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Coupling one-dimensional time-dependent classical and quantum transport models

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A transient model for one-dimensional charge transport in an open quantum system is proposed. In the semiclassical limit, it reduces to the inflow boundary value problem for the classical transport equation. On this basis, the coupling of classical and quantum transport models through an interface is investigated. Suitable interface conditions are derived through asymptotic formulas involving the quantum reflection–transmission coefficients and time delays. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421635]

I. INTRODUCTION

In this work, we propose and analyze a method for coupling classical and quantum transport models in a one-dimensional time-dependent setting. This paper is the followup of a previous work of one of the authors,[1] where the one-dimensional stationary case was investigated. We shall see that the account of the time dependence increases the complexity of the coupling methodology to a large extent.

The problem can be formulated as follows. We consider a particle system (such as certain semiconductor devices, e.g., Resonant Tunnelling Diodes), which consists of a small localized portion (denoted by Q), where the dynamics of the particles is quantum and a large area (denoted by C), where the behavior of the particles can be well approximated by classical mechanics. For computational efficiency, it is desirable to use a classical mechanics model for the particles as long as they are in region C and to shift to a quantum model only when they cross the border between the C and Q regions. Similarly, when a particle leaves the Q region, one should be able to shift back to a classical model.

The problems posed by this procedure are twofold. First, independently of the consideration of the classical region, the quantum region is an open quantum system, which may gain or lose particles. Boundary conditions for open quantum systems are not easily derived. Such boundary conditions were proposed and analyzed in Refs. 2, 3 in the one-dimensional stationary case and in Refs. 4, 5 for the multidimensional stationary case (numerical studies of such boundary conditions can be found in Refs. 6–9, . . .). Approximate boundary conditions for the time-dependent case can be found in Refs. 10–12. In the present paper, we shall present an alternative approach to the search for boundary conditions: the *a priori* construction of density matrices that are exact solutions of the quantum von-Neumann equation, and that are consistent with the statistics of the particles coming into the quantum region.

However, there is not a unique such construction. This is due to the necessary ''delocalization'' of the classical particles when they enter the quantum region. Indeed, the quantum-mechanical picture of a particle is a wave packet. If there is only one classical limit of a given

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quantum wave packet, the reciprocal is obviously untrue. A given classical particle may be the classical limit of many different wave packets. Therefore, when a classical particle crosses the border of the quantum region, one has to choose into which wave packet it will be transformed. Consequently, the construction depends on this arbitrarily chosen wave packet.

In this work, the construction is restricted to the case of a time-independent potential. This is because it makes a large use of the scattering states of the quantum structure, which are well defined only for time-independent potentials. This restriction will be waived in future work.

So far, we have discussed the problem of finding the correct solution of the quantum von-Neumann equation, given the statistics of the incoming particles. Now, we have to examine the reverse question, i.e., how the quantum behavior of the particles in the Q region affects the dynamics in the C region.

For that purpose, we consider the Wigner transform of the density matrix in the Q region and perform a semiclassical limit $\hbar \to 0$. We show that the formal limit of the Wigner distribution function satisfies the usual boundary value problem for the classical transport equation in Q with prescribed incoming data. Furthermore, the outgoing Wigner distribution function at the Q region boundary can be expressed in terms of the incoming data by means of quantum reflection–transmission probabilities and time delays. Since the incoming distribution in the Q region is the outgoing one of the C region and *vice versa*, we can assign similar reflection–transmission conditions to the classical distribution function at the $C-Q$ interface. These conditions only depend on the scattering probabilities and time delays of the quantum structure, but not on the expression of the density matrix in the Q region. Therefore, they lead to a self-contained problem for the classical distribution function, decoupled from that of the quantum region.

In this paper, we first give a general presentation and justification of the above described procedure. Then, we concentrate on the quantum region Q and perform the semiclassical analysis of the Wigner distribution function. Finally, we shall discuss questions regarding current continuity through the interface. We shall only develop formal arguments, and will defer rigorous proofs to a forthcoming paper.[13] A summary of the present approach can be found in Ref. 14.

II. THE COUPLING METHODOLOGY: FORMAL APPROACH

A. Setting of the problem

We consider a one-dimensional system consisting of a large number of independent particles moving along the whole real line. In the sequel, we shall consider electrons, since one of the potential application of the present work is to quantum semiconductor devices. However, the procedure would apply equally well to any other kind of particles. The electrons are subject to a given time-independent potential $V(x)$. We suppose that the gradients of the potential are small apart in a tiny localized region contained in the interval $[a, b]$, where they are large. Therefore, we can consider that the dynamics is classical in the region $C=\mathbb{R}\backslash[a,b]$ and quantum in the region $Q=[a,b]$. What is the precise meaning of small and large in terms of dimensionless parameters and an asymptotic analysis will be the subject of future work. In the present one, we shall take this for granted. Our aim is to find a procedure that couples a classical kinetic description of the particle system in the C region to a quantum statistical model in the Q region.

In $C=\mathbb{R}\backslash[a,b]$, the system is described by the classical particle distribution function $f(x,p,t)$, which is a function of position $x\in\mathbb{R}$, momentum $p\in\mathbb{R}$, and time $t>0$. It is a solution of the one-dimensional collisionless transport (or Vlasov) equation:

$$\partial_t f + v\,\partial_x f + e\frac{\partial V}{\partial x}\partial_p f = 0, \quad x\in\mathbb{R}\backslash[a,b], \quad v=\frac{p}{m}, \tag{1}$$

where m and e are, respectively, the mass and charge, and v, the velocity. At the boundary $\partial C=\{a,b\}$, inflow boundary conditions must be prescribed. At $x=a$ (resp., $x=b$), an inflow velocity for C is such that $v<0$ (resp., $v>0$). We therefore prescribe the boundary conditions

$$f(a,p,t)=f_a(p,t), p<0; \quad f(b,p,t)=f_b(p,t), \quad p>0, \tag{2}$$

where f_a and f_b obviously depend on the dynamics of the Q region.

In $Q=[a,b]$, the system is modeled by the density matrix $\rho(x,x',t)$, which is a solution of the von Neumann equation. However, instead of prescribing boundary conditions for the von Neumann equation at the boundary of the quantum region Q, we take another route. We choose to solve the von Neumann equation on the whole real line, but with a modified potential $\tilde{V}$ that coincides with V in Q and that is constant in C:

$$\tilde{V}(x)=\begin{cases} V_a:=V(a), & x\leqslant a,\\ V(x), & a\leqslant x\leqslant b,\\ V_b:=V(b), & x\geqslant b. \end{cases} \tag{3}$$

Therefore, the von Neumaann equation for ρ reads as

$$i\hbar\rho_t=(\tilde{H}_x-\tilde{H}_{x'})\rho, \quad (x,x',t)\in\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}, \tag{4}$$

where

$$\tilde{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}-e\tilde{V}(x)$$

is the modified particle Hamiltonian in the potential $\tilde{V}$ and $\tilde{H}_x$, $\tilde{H}_{x'}$ are, respectively, the actions of $\tilde{H}$ on the x and x' variables. Now, which solution of the von Neumann equation we must consider, of course, depends of the distribution function in the C region. Therefore, the coupling problem can be summarized as follows: how f_a and f_b are linked with ρ and reciprocally how ρ is linked with f?

We first note that we are not going to consider initial value problems for Eqs. (1) and (4), but solutions for all times $t\in\mathbb{R}$ (so-called eternal solutions). The reason is the following. When entering the Q region, a classical particle must be delocalized into a wave packet. However, a wave packet has a finite extension in space and is in fact very unlikely to be compactly supported. In other words, even very far from the Q region, a classical particle interacts with it because of the tiny but nonzero tail of its wave packet representation. Therefore, the interaction of a classical particle with the Q region is nonlocal in time and actually extends infinitely in the past and in the future.

Now, to understand our coupling methodology, it is illuminating to first consider a classical dynamics in the Q region and derive a classical–classical coupling methodology. Of course, this strange question (why not just use the same classical model everywhere) is investigated just for a clearer exposition of the true classical–quantum coupling.

B. Classical–classical coupling

In this section, we suppose that, in the Q region, the system is described by a classical distribution function g, solution of the Vlasov equation,

$$\partial_t g+v\,\partial_x g+e\frac{\partial V}{\partial x}\partial_p g=0, \quad x\in[a,b], \quad v=\frac{p}{m}. \tag{5}$$

Of course, the boundary ∂Q of Q is $\partial Q=\partial C=\{a,b\}$. However, the incoming velocities for the domain Q at a (resp., b) are now such that $v>0$ (resp., $v<0$). Obviously, the boundary conditions for g at a and b must be

$$g(a,p,t)=g_a(p,t):=f(a,p,t), \quad p>0; \quad g(b,p,t)=g_b(p,t):=f(b,p,t), \quad p<0, \tag{6}$$

where $f(a,p,t)$ (for $p>0$) and $f(b,p,t)$ (for $p<0$) are supposedly known from the resolution of f in the C region. Reciprocally, the boundary conditions (2) for f must obviously be completed by the condition that

$$f_a(p,t) := g(a,p,t), \quad p<0; \quad f_b(p,t) := g(b,p,t), \quad p>0. \tag{7}$$

Now, we introduce the characteristic equations of (5):

$$\frac{dX}{dt} = \frac{P(t)}{m}; \quad \frac{dP}{dt} = e\frac{dV}{dx}(X(t)),$$

which are supposed to be uniquely solvable for a given set of initial conditions. This is certainly true, provided that the potential is smooth, which we shall assume from now on. We consider maximal solutions, which exist until the position X reaches one of the boundaries a or b of the domain. We denote by $(X,P)_{(t;x,p)}$; the solution at time t such that $(X,P)(0)=(x,p)$. Now, it is readily seen that

$$\phi_{(a,p_0,t_0)}(x,p,t) = \delta((x,p)-(X,P)_{(t-t_0;a,p_0)}),$$

is the unique measure solution of (5) that satisfies the boundary condition

$$v\,\phi_{(a,p_0,t_0)}(a,p,t) = \delta(p-p_0)\,\delta(t-t_0).$$

Here and in the remainder of the paper, δ denotes the Dirac delta measure. Writing g_a as a superposition of such elementary distributions:

$$\begin{aligned} g_a(p,t) &= \int_{t_0\in\mathbb{R}} \int_{p_0\in\mathbb{R}^+} g_a(p_0,t_0)\,\delta(p-p_0)\,\delta(t-t_0)dt_0\,dp_0 \\ &= \int_{t_0\in\mathbb{R}} \int_{p_0\in\mathbb{R}^+} (v_0 g_a(p_0,t_0))(v_0^{-1}\delta(p-p_0)\,\delta(t-t_0))dt_0\,dp_0 \end{aligned}$$

(with $v_0=p_0/m$), and similarly for g_b:

$$g_b(p,t) = \int_{t_0\in\mathbb{R}} \int_{p_0\in\mathbb{R}^-} (|v_0|g_b(p_0,t_0))(|v_0|^{-1}\delta(p-p_0)\,\delta(t-t_0))dt_0\,dp_0,$$

we can exactly represent g by the integral formula

$$\begin{aligned} g(x,p,t) = &\int_{t_0\in\mathbb{R}} \int_{p_0\in\mathbb{R}^+} (v_0 g_a(p_0,t_0))\phi_{(a,p_0,t_0)}(x,p,t)dt_0\,dp_0 \\ &+ \int_{t_0\in\mathbb{R}} \int_{p_0\in\mathbb{R}^-} (|v_0|g_b(p_0,t_0))\phi_{(b,p_0,t_0)}(x,p,t)dt_0\,dp_0. \end{aligned} \tag{8}$$

The measures $\phi_{(a,p_0,t_0)}$ (resp., $\phi_{(b,p_0,t_0)}$) are elementary distributions that describe particles entering the Q region at time t_0 through point a with momentum $p_0>0$ (resp., through point b and momentum $p_0<0$).

Now, (8) can be used to compute the outgoing traces of g on ∂Q as functions of its incoming traces g_a and g_b, i.e., [by (6)], of the outgoing traces of f (with respect to C). On the other hand, outgoing traces of g on ∂Q are also incoming traces of f on ∂C by virtue of (7). Therefore, this operation will ultimately give us an expression of the incoming traces of f as functions of its

outgoing traces, which will lead to a self-contained problem for f. Then, knowing f and, in particular, its outgoing traces by the resolution of this problem, we will find g by means of formula (8). We are now going to detail this program.

We start with the computation of the outgoing traces of $\phi_{(a,p_0,t_0)}$ and $\phi_{(b,p_0,t_0)}$. Again, using the smoothness of the potential that rules out any pathology of the trajectories, the characteristic $(X,P)_{(t;a,p_0)}$ with $p_0>0$ exits the domain Q after a certain time $\tau(p_0)$ either by point a with momentum $-p_0$ (in which case, we say that the particle is reflected) or by point b with momentum,

$$p_b(p_0)=\mathrm{sgn}(p_0)\sqrt{p_0^2+2me(V_b-V_a)} \tag{9}$$

(then, the particle is transmitted). The expression (9) obviously follows from the energy conservation, itself a consequence of the time independence of the potential. If the expression inside the square root defining $p_b(p_0)$ is negative, then reflection occurs certainly and the quantity $p_b(p_0)$ needs not be defined. We define reflection and transmission coefficients $R(p_0),T(p_0)$ in such a way that

$$R(p_0)=1-T(p_0)=\begin{cases}1, & \text{in the case of a reflection}\\ 0, & \text{in the case of a transmission.}\end{cases}$$

Then we can write

$$v\,\phi_{(a,p_0,t_0)}(a,p,t)=R(p_0)\,\delta(p+p_0)\,\delta((t-t_0)-\tau(p_0)),\quad p<0, \tag{10}$$

$$v\,\phi_{(a,p_0,t_0)}(b,p,t)=T(p_0)\,\delta(p-p_b(p_0))\,\delta((t-t_0)-\tau(p_0)),\quad p>0. \tag{11}$$

Similar definitions can, of course, be given for characteristics starting from b with momentum $p_0<0$. In particular, we define

$$p_a(p_0)=\mathrm{sgn}(p_0)\sqrt{p_0^2-2me(V_b-V_a)}.$$

This leads to the following expressions:

$$v\,\phi_{(b,p_0,t_0)}(b,p,t)=R(p_0)\,\delta(p+p_0)\,\delta((t-t_0)-\tau(p_0)),\quad p>0, \tag{12}$$

$$v\,\phi_{(b,p_0,t_0)}(a,p,t)=T(p_0)\,\delta(p-p_a(p_0))\,\delta((t-t_0)-\tau(p_0)),\quad p<0. \tag{13}$$

Now, from (10)–(13), we deduce, for $p<0$,

$$\begin{aligned}g(a,p,t)=&\int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^+}g_a(p_0,t_0)R(p_0)\,\delta(p+p_0)\,\delta((t-t_0)-\tau(p_0))dt_0\,dp_0\\&+\int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^-}\frac{|p_0|}{|p_a(p_0)|}g_b(p_0,t_0)T(p_0)\,\delta(p-p_a(p_0))\,\delta((t-t_0)-\tau(p_0))dt_0\,dp_0,\end{aligned}$$

or, after performing the integrations and noting that $p_0'=p_a(p_0)\Leftrightarrow p_0=p_b(p_0')$,

$$g(a,p,t)=R(-p)g_a(-p,t-\tau(-p))+T(p_b(p))g_b(p_b(p),t-\tau(p_b(p))).$$

Similarly, for $p>0$, we have

$$g(b,p,t)=\int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^-} g_b(p_0,t_0)R(p_0)\,\delta(p+p_0)\,\delta((t-t_0)-\tau(p_0))dt_0\,dp_0$$
$$+\int_{t_0\in\mathbb{R}}\int_{p_0\in\mathbb{R}^+}\frac{p_0}{p_b(p_0)}g_a(p_0,t_0)T(p_0)\,\delta(p-p_b(p_0))\,\delta((t-t_0)-\tau(p_0))dt_0\,dp_0,$$

or

$$g(b,p,t)=R(-p)g_b(-p,t-\tau(-p))+T(p_a(p))g_a(p_a(p),t-\tau(p_a(p))).$$

We note that, by time reversibility, $T(p_a(p))=T(-p)$ and $\tau(p_a(p))=\tau(-p)$ [for $p>0$ and when $p_a(p)$ is defined]. Similarly, $T(p_b(p))=T(-p)$ and $\tau(p_b(p))=\tau(-p)$ [for $p<0$ and when $p_b(p)$ is defined]. This finally leads to

$$g(a,p,t)=R(-p)g_a(-p,t-\tau(-p))+T(-p)g_b(p_b(p),t-\tau(-p)),\quad p<0, \tag{14}$$

$$g(b,p,t)=R(-p)g_b(-p,t-\tau(-p))+T(-p)g_a(p_a(p),t-\tau(-p)),\quad p>0. \tag{15}$$

Now, eliminating g by (6) and (7), we use (14) and (15) to set up a self-contained reflection–transmission problem for f:

$$f(a,p,t)=R(-p)f(a,-p,t-\tau(-p))+T(-p)f(b,p_b(p),t-\tau(-p)),\quad p<0, \tag{16}$$

$$f(b,p,t)=R(-p)f(b,-p,t-\tau(-p))+T(-p)f(a,p_a(p),t-\tau(-p)),\quad p>0. \tag{17}$$

These boundary conditions express the incoming traces of f as functions of its outgoing traces. They are very likely to lead to a well-posed problem for f in C (the existence of solutions for similar kinds of boundary conditions can be found in Refs. 15,16). With these boundary conditions, the Vlasov equation (1) can be solved in C without any reference to the distribution function in Q. Of course, via the reflection–transmission coefficients R, T and time delays τ, f depends on the potential in Q. Then, once f is found in C, formula (8) allows us to represent the solution in Q as an integral involving the boundary values of f at a and b.

We are going to duplicate the same methodology for the classical–quantum coupling in the next section.

C. Classical–quantum coupling

The first and nonobvious point is to define the analogs of the elementary distributions $\phi_{(a,p_0,t_0)}$ and $\phi_{(b,p_0,t_0)}$ that characterize particles entering the Q region at time t_0 and point a with momentum $p_0>0$ (resp., at point b and momentum $p_0<0$). We start by recalling the definition of the scattering states of the potential $\tilde{V}$. These are solutions ψ of the stationary Schrödinger equation:

$$\tilde{H}\psi=\mathcal{E}\psi \tag{18}$$

(where $\mathcal{E}$ is the energy) that are bounded on the real line but not square integrable. Elementary analysis[17] shows that for a given energy $\mathcal{E}$, the space of such solutions is of dimension zero, one or two according to the relative position of $\mathcal{E}$ with respect to V_a and V_b. A convenient basis of the solution space is provided by wave functions describing the diffusion of a plane wave coming from infinity by the potential inhomogeneity. These are given by the solutions of the following boundary value problem in the interval $[a,b]$:[2]

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}\psi_p''-eV\psi_p=\left(\frac{p^2}{2m}-eV_a\right)\psi_p,\\
\text{for } p>0,\quad &\hbar\psi_p'(a)+ip\psi_p(a)=2ip,\\
&\hbar\psi_p'(b)=ip_b(p)\psi_p(b);
\end{aligned}
\tag{19}
$$

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}\psi_p''-eV\psi_p=\left(\frac{p^2}{2m}-eV_b\right)\psi_p,\\
\text{for } p<0,\quad &\hbar\psi_p'(a)=-ip_a(p)\psi_p(a),\\
&\hbar\psi_p'(b)+ip\psi_p(b)=2ip.
\end{aligned}
\tag{20}
$$

Let us suppose, to fix the ideas, that $V_b>V_a$. Then $p_b(p)$ is always well defined. On the other hand, $p_a(p)$ is well defined only if $|p|\geqslant\sqrt{2em(V_b-V_a)}$. For $p>0$, the two solutions ψ_p and $\psi_{-p_b(p)}$ form a basis of the solution space of (18) associated with the energy $\mathcal{E}=p^2/2m-eV_a=p_b(p)^2/2m-eV_b$, which is therefore of dimension 2. ψ_p describes the scattering of a plane wave coming from $-\infty$ by the potential inhomogeneity, while $\psi_{-p_b(p)}$ describes the scattering of a plane wave coming from $+\infty$. For $p<0$ and $|p|\leqslant\sqrt{2em(V_b-V_a)}$, then $p_a(p)$ in formula (20) has to be defined as a complex square root: $p_a(p)=\pm i\sqrt{2me(V_b-V_a)-p^2}$. Which sign must be chosen in this definition is unimportant because the solution space is of dimension 1 and the two solutions are then proportional. In this case, the solution (20) represents the pure quantum reflection of a plane wave by a potential barrier.

The boundary conditions appearing in (19),(20) are consequences of the following explicit formula for ψ_p outside $[a,b]$ (this is because the potential $\tilde{V}$ is assumed constant in $\mathbb{R}\backslash[a,b]$):

$$
\text{for } p>0,\quad
\begin{aligned}
&\psi_p(x)=e^{ip[(x-a)/\hbar]}+A(p)e^{-ip[(x-a)/\hbar]},\quad x<a,\\
&\psi_p(x)=B(p)e^{ip_b(p)[(x-b)/\hbar]},\quad x>b;
\end{aligned}
\tag{21}
$$

where

$$
A(p)=\psi_p(a)-1:\quad B(p)=\psi_p(b),\quad p>0;
\tag{22}
$$

and

$$
\text{for } p<0,\quad
\begin{aligned}
&\psi_p(x)=B(p)e^{i[(x-a)/\hbar]p_a(p)},\quad x<a,\\
&\psi_p(x)=e^{i[(x-b)/\hbar]p}+A(p)e^{-ip[(x-b)/\hbar]},\quad x>b;
\end{aligned}
\tag{23}
$$

where

$$
A(p)=\psi_p(b)-1;\quad B(p)=\psi_p(a),\quad p<0.
\tag{24}
$$

In the above formulas, $A(p)$ is the coefficient of the reflected wave (reflection amplitude) whereas $B(p)$ is that of the transmitted wave (transmission amplitude) and the factor in front of the incoming wave ensures that it has amplitude 1. If $p<0$ and $|p|\leqslant\sqrt{2em(V_b-V_a)}$ (again assuming that $V_b>V_a$ to fix the idea), it must be noted that $p_a(p)$ in formula (23) is purely imaginary, so that the wave is evanescent in the region $x<a$.

We recall that the corresponding reflection and transmission coefficients,

$$
R(p)=|A(p)|^2,\quad T(p)=\frac{\Re(p_{a,b}(p))}{p}|B(p)|^2,
\tag{25}
$$

[where $p_{a,b}(p)$ stands for p_a (resp., p_b) when $p<0$ (resp., $p>0$) and $\mathcal{R}$, $\mathcal{T}$ for the real and imaginary parts] satisfy

$$R(p)+T(p)=1, \tag{26}$$

and the reciprocity identity

$$T(p)=T(-p_{a,b}(p)), \quad \text{for all } p\in\mathbb{R} \text{ such that } p_{a,b}(p)\in\mathbb{R}. \tag{27}$$

To any scattering state $\psi_p(x)$ corresponds a time-dependent wave function,

$$\Psi_p(x,t)=\psi_p(x)e^{-i[\mathcal{E}(p)t/\hbar]},$$

where we denote by $\mathcal{E}(p)$ the energy associated with ψ_p:

$$\mathcal{E}(p)=\frac{p^2}{2m}-eV_a, \quad \text{for } p>0 \quad \text{and} \quad \mathcal{E}(p)=\frac{p^2}{2m}-eV_b, \quad \text{for } p<0.$$

However, the probability density $|\Psi_p|^2$ associated with Ψ_p is time independent (which is the definition of a stationary solution of the Schrödinger equation). Therefore, such a wave function is unable to represent a dynamical process such as the motion of an isolated particle.

To do so, one has to call for the concept of a wave packet. Let $\Phi_\hbar(p_0,p_1)$ be a ''localizing function'' that can be viewed as the typical shape of the wave packet. This function is arbitrary, provided it satisfies a certain number of constraints that will be listed below. Let us think of $\Phi_\hbar$ as a non-negative real-valued function, which ''gets peaked'' about $p_0=p_1$ as $\hbar$ tends to zero. We shall make this definition more precise later on. We represent an electron coming into the domain Q at time t_0 with momentum p_0 by the following wave packet:

$$\Psi_{p_0,t_0}(x,t)=\int_{\mathbb{R}}\Phi_\hbar(p_0,p_1)\psi_{p_1}(x)\exp\left(-\frac{i(t-t_0)\mathcal{E}(p_1)}{\hbar}\right)dp_1. \tag{28}$$

An important example of the wave packet profile is the Gaussian wave packet,

$$\Phi_\hbar(p_0,p_1)=\sqrt{C_\hbar}\exp\left(-\frac{(p_0-p_1)^2}{4\sigma_\hbar}\right), \tag{29}$$

where $C_\hbar$ is a normalization constant about which we shall come back below and $\sigma_\hbar$ is the momentum variance of the wave packet. Throughout the paper, $\Phi_\hbar$ will be assumed real-valued.

Although the above formula mixes states corresponding to incoming plane waves from either the left ($p_1>0$) or the right ($p_1<0$), a semiclassical analysis shows that Ψ_{p_0,t_0} corresponds to a particle entering Q at time t_0 through a and moving to the right if $p_0>0$ and entering Q through b and moving to the left if $p_0<0$. More specifically, applying the stationary phase theorem, a formal analysis[17] yields, for $p_0>0$,

$$\Psi_{p_0,t_0}\sim\begin{cases}\Psi^I_{p_0,t_0}+\Psi^R_{p_0,t_0}, & x<a,\\ \Psi^T_{p_0,t_0}, & x>b,\end{cases}$$

where the incident $\Psi^I_{p_0,t_0}$, reflected $\Psi^R_{p_0,t_0}$ and transmitted $\Psi^T_{p_0,t_0}$ wave packets, respectively, represent classical particles moving according to the equations

$$x_I(t)=a+v_0(t-t_0), \quad x<a \quad \text{(incident wave)},$$

$$x_R(t)=a-v_0((t-t_0)-\tau_R(p_0)), \quad x<a \quad \text{(reflected wave)},$$

$$x_T(t)=a+v_0((t-t_0)-\tau_T(p_0)),\quad x>b\quad \text{(trasmitted wave)}.$$

Therefore, up to a limit $\hbar\to 0$, the incident wave packet hits the boundary a at time t_0 coming from the left with momentum p_0. It gives rise to a reflected wave packet that departs from a at time $t_0+\tau_R(p_0)$ where $\tau_R(p_0)$ is a quantum reflection time delay, and to a transmitted wave packet that departs from b at time $t_0+\tau_T(p_0)$ with $\tau_T(p_0)$ is the transmission time delay. These delays are given by the following formula (see also Ref. 17):

$$\tau_R(p)=\frac{1}{v}\frac{dS_R(p)}{dp},\quad \tau_T(p)=\frac{1}{v}\frac{dS_T(p)}{dp},\tag{30}$$

where $S_R(p)$ and $S_T(p)$ are smooth realizations of the complex phases of the scattering amplitudes:

$$A(p)=\sqrt{R(p)}e^{i[S_R(p)/\hbar]},\quad B(p)=\sqrt{\frac{p}{\Re(p_{a,b}(p))}T(p)}\,e^{i[S_T(p)/\hbar]}.$$

In this paper, we shall give a more rigorous meaning to these statements.

The wave packet Ψ_{p_0,t_0} is obviously a solution of the time-dependent Schrödinger equation,

$$i\hbar\frac{\partial\Psi}{\partial t}=\tilde{H}\Psi.\tag{31}$$

From these wave packets, we construct a density matrix that is the quantum analog of the elementary distributions $\phi_{(a,p_0,t_0)}$ or $\phi_{(b,p_0,t_0)}$. It is defined by

$$\begin{aligned}\rho_{q_0,t_0}(x,x',t)&=\Psi_{q_0,t_0}(x,t)\overline{\Psi_{q_0,t_0}(x',t)}\\&=\int_{\mathbb{R}^2}\Phi_\hbar(q_0,p_1)\Phi_\hbar(q_0,q_2)\psi_{p_1}(x)\overline{\psi_{p_2}(x')}\\&\quad\times\exp\left(-\frac{i}{\hbar}(t-t_0)(\mathcal{E}(p_1)-\mathcal{E}(p_2))\right)dp_1\,dp_2,\end{aligned}\tag{32}$$

and represents a particle entering Q at time t_0 through point a if $q_0>0$ (resp., through point b if $q_0<0$). ρ_{q_0,t_0} is a truly time-dependent solution of the von Neumann equation (4).

Of course, for ρ_{q_0,t_0} to represent a physically admissible density matrix, it has to be of trace unity. We recall that the trace of a density matrix $\rho(x,x')$ is given by

$$\mathrm{Tr}\,\rho=\int_{\mathbb{R}}\rho(x,x)dx,$$

while $\rho(x,x)dx$ represents the probability density associated with ρ. In order to compute the trace of (32), it is convenient to highlight its relation with the scattering transform.

First, we recall that the definition of the Fourier transform of a function $g(p)$ is defined by

$$\mathcal{F}g(\eta)=\frac{1}{2\pi}\int e^{i\eta p}g(p)dp,\tag{33}$$

while the inverse Fourier transform of a function $G(x)$ is given by

$$\mathcal{F}^{-1}G(p)=\int e^{-i\eta p}G(\eta)d\eta.\tag{34}$$

The Plancherel identity states that

$$\int \overline{\mathcal{F}g(\eta)}\mathcal{F}f(\eta)d\eta = \frac{1}{2\pi}\int \overline{g}f\,dp. \tag{35}$$

The scattering transform can be viewed as a Fourier transform in which the scattering states $\psi_p(x)$ are used instead of the exponentials e^{ipx}. In particular, it reduces to the Fourier transform (up to a change of variables) in the case of a constant potential. More precisely, we define the scattering transform $\mathcal{G}(g)$ according to

$$\mathcal{G}g(x) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} g(p)\psi_p(x)dp,$$

and the inverse scattering transform:

$$\mathcal{G}^{-1}G(p) = \int_{\mathbb{R}} G(x)\overline{\psi_p(x)}dx.$$

It is immediately seen that, in the case of a constant potential, the scattering and Fourier transforms are related by

$$\mathcal{G}g(x) = \frac{1}{\hbar}\mathcal{F}g\left(\frac{x}{\hbar}\right) = \mathcal{F}[g(\hbar\cdot)](x),$$

$$\mathcal{G}^{-1}G(p) = \mathcal{F}^{-1}G\left(\frac{p}{\hbar}\right) = \hbar\mathcal{F}^{-1}[G(\hbar\cdot)](p).$$

In the general case, $\mathcal{G}^{-1}$ is an isomorphism of Hilbert spaces between L^2_{ac} onto $L^2(\mathbb{R})$, and $\mathcal{G}$ is the inverse isomorphism, where L^2_{ac} denotes the absolutely continuous subspace of $L^2(\mathbb{R})$ associated with the operator $\tilde{H}$. Therefore, we have the analog of Plancherel's formula:

$$\int \overline{\mathcal{G}g(x)}\mathcal{G}f(x)dx = \frac{1}{2\pi\hbar}\int \overline{g}f\,dp. \tag{36}$$

The definition and properties of the scattering transform can be found in Ref. 18.

Now, in view of the scattering transform, Ψ_{p_0,t_0} can be written as

$$\Psi_{p_0,t_0}(x,t) = 2\pi\hbar\mathcal{G}_{p_1}\left[\Phi_\hbar(p_0,p_1)\exp\left(-\frac{i(t-t_0)\mathcal{E}(p_1)}{\hbar}\right)\right](x), \tag{37}$$

where $\mathcal{G}_{p_1}$ indicates that we take the scattering transform with respect to p_1. Then, using (36), we compute

$$\begin{aligned}
\mathrm{Tr}\,\rho_{q_0,t_0}(t) &= \int_{\mathbb{R}} |\Psi_{q_0,t_0}(x,t)|^2\,dx \\
&= (2\pi\hbar)^2\int_{\mathbb{R}}\left|\mathcal{G}_{p_1}\left[\Phi_\hbar(p_0,p_1)\exp\left(-\frac{i(t-t_0)\mathcal{E}(p_1)}{\hbar}\right)\right](x)\right|^2 dx \\
&= 2\pi\hbar\int_{\mathbb{R}}\left|\Phi_\hbar(q_0,p_1)\exp\left(-\frac{i(t-t_0)\mathcal{E}(p_1)}{\hbar}\right)\right|^2 dp_1 = 2\pi\hbar\int_{\mathbb{R}}|\Phi_\hbar(q_0,p_1)|^2\,dp_1.
\end{aligned}$$

Therefore, the density matrix $\rho_{q_0,t_0}(\cdot,\cdot,t)$ is of trace unity if and only if the wave packet function $\Phi_\hbar$ satisfies the normalization condition

$$2\pi\hbar\int_{\mathbb{R}}|\Phi_\hbar(p,q)|^2\,dq=1, \tag{38}$$

which we shall assume satisfied from now on. We note that this normalization condition allows us to define the probability density $P_\hbar(p,q)dq$ according to

$$P_\hbar(p,q)dq=2\pi\hbar|\Phi_\hbar(p,q)|^2\,dq. \tag{39}$$

We also complete the definition of the Gaussian wave packet (29) by giving the expression of the normalizing constant, which, according to (38), must be equal to $C_\hbar=((2\pi)^{3/2}\hbar\sqrt{\sigma_\hbar})^{-1}$.

Now, we recall that Q is an open quantum system where the statistics of incoming particles is described by two distribution functions $g_a(p,t)(p>0)$ and $g_b(p,t)(p<0)$. For simplicity, we define the boundary data $\mathbf{g}$ according to

$$\mathbf{g}(p,t)=g_a(p,t)\quad\text{for } p>0\quad\text{and}\quad\mathbf{g}(p,t)=g_b(p,t)\quad\text{for } p<0. \tag{40}$$

We postulate that the state of the quantum region Q is formed by the superposition of the elementary density matrices ρ_{q_0,t_0}, weighted by the statistics of incoming particles $\mathbf{g}(q_0,t_0)$. We therefore reproduce formula (8) and define the density matrix in Q by the formula

$$\begin{aligned}\rho(x,x',t)&=\int_{\mathbb{R}^2}\frac{|q_0|}{m}\mathbf{g}(q_0,t_0)\rho_{q_0,t_0}(x,x',t)dt_0\,dq_0\\&=\int\frac{|q_0|}{m}\mathbf{g}(q_0,t_0)\Phi_\hbar(q_0,q_1)\Phi_\hbar(q_0,q_2)\psi_{q_1}(x)\overline{\psi_{q_2}}(x')\\&\quad\times\exp\left(-\frac{i}{\hbar}(t-t_0)(\mathcal{E}(q_1)-\mathcal{E}(q_2))\right)dt_0\,dq_0\,dq_1\,dq_2.\end{aligned} \tag{41}$$

This defines how the state of the quantum region Q is computed as a function of the inflow statistics g_a and g_b. Now, we turn to the classical distribution function f in the region C. Of course, it is understood that the inflow statistics for the quantum region Q coincides with the outgoing trace of f, i.e., relation (6) is still valid:

$$g_a(p,t)=f(a,p,t),\quad p>0;\quad g_b(p,t)=f(b,p,t),\quad p<0. \tag{42}$$

The problem is now to find the analog of relation (7). Again, we take our inspiration from the classical case and, more precisely, from the reflection–transmission boundary condition for f, as given by (16) and (17). To use this relation in the quantum–classical coupling case, it is tempting to just replace the classical reflection–transmission coefficients and time delays by the quantum ones. However, this procedure is not current-conservative (see Sec. V). Furthermore, it does not take into account the fact that the quantum delocalization of a particle into a wave packet mixes states of different momenta (or different energies).

In the remainder of this section, we make the following simplifying hypothesis:

$$\Phi_\hbar(p,q)=0,\quad\text{if } p \text{ and } q \text{ have opposite signs.} \tag{43}$$

Under this hypothesis, we specify the following reflection–transmission condition for f at the interface between C and Q:

$$|p|f(a,p,t)=\int_{q>0}P_\hbar(q,-p)R_\hbar(-p)f(a,q,t-\tau_R^\hbar(-p))|q|dq$$
$$+\int_{q<0}P_\hbar(q,p_b(p))T_\hbar(p_b(p))\frac{p}{p_b(p)}f(b,q,t-\tau_T^\hbar(p_b(p)))|q|dq,\quad p<0, \tag{44}$$

$$|p|f(b,p,t)=\int_{q<0}P_\hbar(q,-p)R_\hbar(-p)f(b,q,t-\tau_R^\hbar(-p))|q|dq$$
$$+\int_{q>0}P_\hbar(q,p_a(p))T_\hbar(p_a(p))\frac{p}{p_a(p)}f(a,q,t-\tau_T^\hbar(p_a(p)))|q|dq,\quad p>0. \tag{45}$$

In these formulas, $P_\hbar(q,p)$ is the probability density defined by (39) and $(R_\hbar,T_\hbar)$, $(\tau_R^\hbar,\tau_T^\hbar)$ are the quantum reflection–transmission coefficients and time delays. Note that hypothesis (43) implies that $P_\hbar(q,p)=0$ if p and q have opposite signs. We also remark that the quantum time delays for reflection and transmission are not equal. In the classical formulas (16) and (17), only one of these times is relevant since, for a given value of p, reflection and transmission never occur simultaneously. The probabilistic nature of quantum mechanics, however, makes reflection and transmission occur simultaneously and the associated time delays are different.

We now explain the physics behind these conditions. For instance, let us examine (44), the discussion being obviously identical for (45). It expresses that the particles going out of the quantum zone Q through a (i.e., with momentum $p<0$) originate from particles having entered Q at an earlier time, either through a (i.e., with momentum $-p>0$) or through b [i.e., with momentum $p_b(p)<0$]. However, the entering particles are transformed into wave packets as they cross the border of the Q region, by means of $\Phi_\hbar$. Each entering particle through say a with momentum $q>0$ "excites" a quantum wave of momentum $-p>0$ according to the probability density $P_\hbar(q,-p)$. Therefore the intensity of the wave entering at time t with momentum $-p>0$ per unit time is proportional to

$$\int_{q>0}P_\hbar(q,-p)f(a,q,t)|q|dq.$$

Only the fraction $R(-p)$ will be reflected back to a, the remaining part will be transmitted to b. Furthermore, for the wave to "arrive" at a at time t, it needs to have entered Q at time $t-\tau_R^\hbar(-p)$. Collecting all these remarks leads to the flux of particles exiting Q through a at time t, originating from particles having entered Q through the same point; hence the first integral. The same analysis is valid for the second integral considering waves entering into Q through b and transmitted to a. Simply, the change of p to $p_b(p)$ (if $V_a\neq V_b$) has to be taken into account. The ratio $p/p_b(p)$ takes into account the change of volume in momentum space in the map $p\to p_b(p)$.

Conditions (44), (45) maintain the positivity (i.e., if the outgoing distribution is positive, the incoming one is also positive). Note, however, that the Gaussian wave packet (29) does not satisfy hypothesis (43). It is worth mentioning that quantum time delays may be non positive. Analytical computations for specially unsmooth potentials like delta potentials indicate that time delays may become negative.[19] Nevertheless, for smooth enough potentials, we shall assume that time delays are positive; otherwise the well-posedness of the kinetic problem in C would not be guaranteed.

To summarize our coupling methodology, we first solve the self-contained problem (1) with the reflection–transmission boundary conditions (44) and (45) for f in the classical region C

(provided that the quantum time delays are positive). Then, once f and its boundary values $f(a,p,t)$ (for $p>0$), $f(b,p,t)$ (for $p<0$) are known, we construct the density matrix in the quantum region Q according to (41), where $\mathbf{g}$ is given by (40) and (42).

D. Classical–quantum coupling: Summary of results

We now outline how we can give a rigorous foundation to the above described coupling methodology. The main tool we will use is the Wigner transform.[20] The Wigner transform of the density matrix (41) is defined according to

$$W^{\hbar}(x,p,t)=\frac{1}{2\pi}\int_{\mathbb{R}} e^{i\eta p}\rho\left(x-\frac{\hbar}{2}\eta,x+\frac{\hbar}{2}\eta,t\right)d\eta.$$

Since the wave packets Ψ_{q_0,t_0} are solutions of the Schrödinger equation (31), $W^{\hbar}$ is a solution of the Wigner equation:

$$\partial_t W^{\hbar}+\frac{p}{m}\partial_x W^{\hbar}+\theta_{\hbar}[\tilde{V}]\cdot W^{\hbar}=0,$$

where the pseudodifferential operator $\theta_{\hbar}$ is given by

$$\theta_{\hbar}[\tilde{V}]W^{\hbar}(x,p)=-\frac{ie}{2\pi}\int_{\mathbb{R}} e^{i\eta p}\delta_{\hbar}[\tilde{V}](x,\eta)\mathcal{F}_p^{-1}W^{\hbar}(x,\eta)d\eta,$$

with

$$\delta_{\hbar}[\tilde{V}](x,\eta)=\frac{\tilde{V}\left(x+\frac{\hbar}{2}\eta\right)-\tilde{V}\left(x-\frac{\hbar}{2}\eta\right)}{\hbar},$$

and $\mathcal{F}_p^{-1}$ denotes the inverse Fourier transform (34).

In the remainder of the paper, our goal is to prove that, in the semiclassical limit $\hbar\to 0$, $W^{\hbar}$ converges to a solution $g=g(x,p,t)$ of the Vlasov equation (5) in Q with the inflow boundary conditions (6) at a and b, namely,

$$g(a,p,t)=g_a(p,t),\quad p>0;\quad g(b,p,t)=g_b(p,t),\quad p<0. \tag{46}$$

More precisely, we shall prove the following.

Main Result: Assuming that $\Phi_{\hbar}$ is real, we introduce $\Lambda_{\hbar}$, according to:

$$\Lambda_{\hbar}(p,q,q')=2\pi\hbar\,\Phi_{\hbar}\left(p,q+\frac{\hbar}{2}q'\right)\Phi_{\hbar}\left(p,q-\frac{\hbar}{2}q'\right). \tag{47}$$

We note that

$$\Lambda_{\hbar}(p,q,0)=2\pi\hbar|\Phi_{\hbar}(p,q)|^2=P_{\hbar}(p,q),\quad \int_{\mathbb{R}}\Lambda_{\hbar}(p,q,0)dq=1. \tag{48}$$

We assume additionally that $\Lambda_{\hbar}$ satisfies

$$\lim_{\hbar\to 0}\Lambda_{\hbar}(p,q,q')=\delta(p-q). \tag{49}$$

Then $W^{\hbar}$ formally converges as $\hbar\to 0$ toward g, the solution of

$$\partial_t g + \frac{p}{m}\partial_x g + e\frac{dV}{dx}\partial_p g = 0,$$

$$g(a,p,t) = g_a(p,t), \quad p>0,$$

$$g(b,p,t) = g_b(p,t), \quad p<0.$$

Moreover, we have asymptotically,

$$W^\hbar(a,-p,t) = R_\hbar(p)W^\hbar(a,p,t-\tau_R^\hbar(p)) + T_\hbar(p)W^\hbar(b,p_b(p),t-\tau_T^\hbar(p)), \quad p>0, \tag{50}$$

$$W^\hbar(b,-p,t) = R_\hbar(p)W^\hbar(b,p,t-\tau_R^\hbar(p)) + T_\hbar(p)W^\hbar(a,p_a(p),t-\tau_T^\hbar(p)), \quad p<0, \tag{51}$$

where $R_\hbar(p)$, $T_\hbar(p)$ are the reflection–transmission coefficients (25) and $\tau_R^\hbar(p)$, $\tau_T^\hbar(p)$ are the time delays (30).

Condition (49) guarantees that, in the semiclassical limit, the wave packet gets more and more localized in both position and momentum. For instance, in the case of the Gaussian wave packet (29), we have

$$\Lambda_\hbar(p,q,q') = \frac{1}{2\pi\sigma_\hbar}\exp-\frac{(p-q)^2}{2\sigma_\hbar}\exp-\frac{\hbar^2 q'^2}{8\sigma_\hbar}.$$

Therefore, condition (49) is fulfilled as soon as we simultaneously have

$$\sigma_\hbar \to 0 \quad \text{and} \quad \frac{\hbar^2}{\sigma_\hbar} \to 0, \quad \text{as} \quad \hbar \to 0.$$

For instance, $\sigma_h = O(\hbar)$ as $\hbar \to 0$ is convenient.

This ''formal'' theorem justifies our methodology in that the Wigner transformed density matrix (41) converges in the semiclassical limit toward the solution of the inflow boundary value problem for the Vlasov equation in the region Q. In particular, as $\hbar \to 0$, the trace of the Wigner function at the boundary ∂Q satisfies the dual reflection–transmission problem to that imposed to the classical distribution function f. Indeed, substituting $f(a,p,t)$ to $W^\hbar(a,-p,t)$ and similarly at point b transforms (50), (51) into (16), (17). Therefore, our definition of the density matrix seems established on a solid basis, in spite of the arbitrariness of the wave packet function $\Phi_\hbar$.

The remainder of the paper is organized as follows. In Sec. III we develop the proof of Theorem 2.4 in the case $V_a = V_b$. Then, in Sec. IV, the extension of the result to the case $V_a \neq V_b$ will be outlined. In Sec. V, we prove that the reflection–transmission conditions (44), (45) satisfy the time-integrated current conservation principle. Finally, in Sec. VI, we specialize to the stationary state in order to bridge the gap with earlier work of one of the authors.[1]

III. PROOF OF THE MAIN RESULT IN THE CASE $V_a = V_b$

A. Preliminaries

First, we introduce some notations. We shall need to distinguish between the density matrices $\rho^{(a)}$ and $\rho^{(b)}$ of electrons injected at the boundaries a and b, respectively:

$$\rho^{(a)}(x,x',t) = \int_{\mathbb{R}^+} dq_0 \int_{\mathbb{R}} dt_0 \frac{|q_0|}{m} g_a(q_0,t_0)\Psi_{q_0,t_0}(x,t)\overline{\Psi_{q_0,t_0}(x',t)}, \tag{52}$$

$$\rho^{(b)}(x,x',t) = \int_{\mathbb{R}^-} dq_0 \int_{\mathbb{R}} dt_0 \frac{|q_0|}{m} g_b(q_0,t_0)\Psi_{q_0,t_0}(x,t)\overline{\Psi_{q_0,t_0}(x',t)}, \tag{53}$$

so that $\rho = \rho^{(a)} + \rho^{(b)}$. We also decompose $W^\hbar = W_a^\hbar + W_b^\hbar$ with

$$W^{\hbar}_{a,b}(x,p,t)=\frac{1}{2\pi}\int_{\mathbb{R}} e^{i\eta p}\rho^{(a,b)}\left(x-\frac{\hbar}{2}\eta,x+\frac{\hbar}{2}\eta,t\right)d\eta. \tag{54}$$

The major part of the computation concerns boundary conditions. Indeed, let $\theta(x,p,t)$ be a test function in $\mathcal{D}(\mathbb{R}_x\times\mathbb{R}_p\times\mathbb{R}_t)$. We have the following identity obtained by a simple integration by parts:

$$\int_{(x,p,t)\in[a,b]\times\mathbb{R}^2}\theta\left[\partial_t W^{\hbar}+\frac{p}{m}\partial_x W^{\hbar}+e\frac{dV}{dx}\partial_p W^{\hbar}\right]dx\,dp\,dt=I^{\hbar}_b-I^{\hbar}_a-I^{\hbar}_{ab},$$

where

$$I^{\hbar}_{ab}=\int_{(x,p,t)\in[a,b]\times\mathbb{R}^2}W^{\hbar}\left[\partial_t\theta+\frac{p}{m}\partial_x\theta+e\frac{dV}{dx}\partial_p\theta\right]dx\,dp\,dt,$$

$$I^{\hbar}_b=\int_{\mathbb{R}^2}\frac{p}{m}\theta(b,p,t)W^{\hbar}(b,p,t)dp\,dt,$$

$$I^{\hbar}_a=\int_{\mathbb{R}^2}\frac{p}{m}\theta(a,p,t)W^{\hbar}(a,p,t)dp\,dt.$$

Standard results on semiclassical limits (see, e.g., Refs. 21, 22, 23, 24, 25, etc.) allow us to perform the $\hbar\to 0$ limit in the interior of the interval $[a,b]$, so that

$$\lim_{\hbar\to 0}-I^{\hbar}_{ab}+I^{\hbar}_b-I^{\hbar}_a=0. \tag{55}$$

In particular, we have the following.

Lemma 3.1:

$$\lim_{\hbar\to 0}I^{\hbar}_{ab}=\int_{(x,p,t)\in[a,b]\times\mathbb{R}^2}g\left[\partial_t\theta+\frac{p}{m}\partial_x\theta+e\frac{dV}{dx}\partial_p\theta\right]dx\,dp\,dt. \tag{56}$$

Next, we need to calculate the $\hbar\to 0$ limit of the left boundary term $I^{\hbar}_a$. The right boundary term $I^{\hbar}_b$ can be treated analogously. To this aim, we introduce

$$U(p,t)=\frac{p}{m}\theta(a,p,t), \tag{57}$$

and we remark that $U(0,t)=0$ for all $t\in\mathbb{R}$. We compute

$$I^{\hbar}_a=\int_{\mathbb{R}^2}U(p,t)W^{\hbar}(a,p,t)dp\,dt=\int_{\mathbb{R}^2}U(p,t)W^{\hbar}_a(a,p,t)dp\,dt+\int_{\mathbb{R}^2}U(p,t)W^{\hbar}_b(a,p,t)dp\,dt,$$

where $W^{\hbar}_a$ and $W^{\hbar}_b$ are defined at (54). Let us denote by J^h_a the first integral and K^h_a the second one. We have

$$J_a^\hbar = \int U(p,t) W_a^\hbar(a,p,t)\,dp\,dt$$
$$= \frac{1}{2\pi}\int_{\mathbb{R}^4} dp\,d\eta\,dt_0\,dt \int_{\mathbb{R}^+} dq_0\, e^{i\eta p} U(p,t)\,\frac{|q_0|}{m}\, g_a(q_0,t_0)\,\overline{\Psi_{q_0,t_0}}\left(a+\frac{\hbar}{2}\eta,t\right)$$
$$\times \Psi_{q_0,t_0}\left(a-\frac{\hbar}{2}\eta,t\right). \tag{58}$$

On the other hand, we have

$$\overline{\Psi_{q_0,t_0}}\left(a+\frac{\hbar}{2}\eta,t\right)\Psi_{q_0,t_0}\left(a-\frac{\hbar}{2}\eta,t\right) = \int_{\mathbb{R}^2} \Phi_\hbar(q_0,q_1)\Phi_\hbar(q_0,q_2)\,\overline{\psi_{q_1}}\left(a+\frac{\hbar}{2}\eta\right)\psi_{q_2}\left(a-\frac{\hbar}{2}\eta\right)$$
$$\times \exp\left[i\,\frac{q_1^2-q_2^2}{2m\hbar}(t-t_0)\right] dq_1\,dq_2. \tag{59}$$

Before analyzing (58), we claim that the behavior of the right-hand side of (59) as $\hbar$ tends to zero is left unchanged if we replace the integration set by $\mathbb{R}^2_+$:

$$\overline{\Psi_{q_0,t_0}}\left(a+\frac{\hbar}{2}\eta,t\right)\Psi_{q_0,t_0}\left(a-\frac{\hbar}{2}\eta,t\right) \simeq \int_{\mathbb{R}^2_+} \Phi_\hbar(q_0,q_1)\Phi_\hbar(q_0,q_2)\,\overline{\psi_{q1}}\left(a+\frac{\hbar}{2}\eta\right)\psi_{q_2}\left(a-\frac{\hbar}{2}\eta\right)$$
$$\times \exp\left[i\,\frac{q_1^2-q_2^2}{2m\hbar}(t-t_0)\right] dq_1\,dq_2. \tag{60}$$

This is a consequence of the fact that the wave packet ''is peaked'' around q_0 and q_0 is positive. This claim can be rigorously proven by applying the dominated convergence theorem and will be developed in Ref. 13.

B. First approximation: using the asymptotics of ψ_q in the neighborhood of the boundary

A simple rescaling of the Schrödinger equation (19) leads to

$$\lim_{\hbar\to 0} \psi_q^\hbar\left(a+\frac{\hbar}{2}\eta\right) - e^{i(q/2)\eta} - A(q)e^{-i(q/2)\eta} = 0, \quad \text{for } q>0, \tag{61}$$

uniformly with respect to $\eta \in]-\infty, M]\,(\forall M>0)$. In what follows, we shall forget the subscripts $\hbar$ in the reflection–transmission coefficients and time delays for clarity. Replacing $\psi_q[a+(\hbar/2)\eta]$ by $e^{i(q/2)\eta}+A(q)e^{-iq\eta}$ in (59) leads to the following approximate formula:

$$\overline{\Psi_{q_0,t_0}}\left(a+\frac{\hbar}{2}\eta,t\right)\Psi_{q_0,t_0}\left(a-\frac{\hbar}{2}\eta,t\right) \approx \mathrm{I}_\hbar + \mathrm{II}_\hbar + \mathrm{III}_\hbar + \mathrm{IV}_\hbar, \tag{62}$$

where

$$\mathrm{I}_\hbar = \int_{\mathbb{R}^2} \Phi_\hbar(q_0,q_1)\Phi_\hbar(q_0,q_2) e^{-i([q_1+q_2]/2)\eta} e^{i[(q_1^2-q_2^2)/2m\hbar](t-t_0)} dq_1\,dq_2, \tag{63}$$

$$\mathrm{II}_\hbar = \int_{\mathbb{R}^2} \Phi_\hbar(q_0,q_1)\Phi_\hbar(q_0,q_2)\overline{A(q_1)}A(q_2) e^{i[(q_1+q_2)/2]\eta} e^{i[(q_1^2-q_2^2)/2m\hbar](t-t_0)} dq_1\,dq_2, \tag{64}$$

$$\mathrm{III}_\hbar = \int_{\mathbb{R}^2} \Phi_\hbar(q_0,q_1)\Phi_\hbar(q_0,q_2)\overline{A}(q_1)e^{i[(q_1-q_2)/2]\eta}e^{i[(q_1^2-q_2^2)/2m\hbar](t-t_0)}dq_1\,dq_2, \tag{65}$$

$$\mathrm{IV}_\hbar = \int_{\mathbb{R}^2} \Phi_\hbar(q_0,q_1)\Phi_\hbar(q_0,q_2)A(q_2)e^{i[(q_2-q_1)/2]\eta}e^{i[(q_1^2-q_2^2)/2m\hbar](t-t_0)}dq_1\,dq_2. \tag{66}$$

The first two terms correspond to the contributions of the two plane waves (corresponding to q_1 and q_2) traveling in the same direction, while the last two ones correspond to contributions of opposite traveling waves. We shall see later on that, because of the assumption (49) on the wave packet function $\Phi_\hbar$, the last two integrals have vanishing $\hbar\to 0$ limits.

In order to compute these limits, we perform the change of variables,

$$(z,y)=\left(\frac{q_1+q_2}{2},\frac{q_1-q_2}{\hbar}\right),\quad (q_1,q_2)=\left(z+\frac{\hbar}{2}y,z-\frac{\hbar}{2}y\right),\quad \frac{q_1^2-q_2^2}{2m\hbar}=\frac{yz}{m}, \tag{67}$$

in (63)–(66). Introducing $\Lambda_\hbar$ according to (47), this leads to

$$\mathrm{I}_\hbar=\frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y)e^{-iz\eta}e^{i(yz/m)(t-t_0)}\,dz\,dy, \tag{68}$$

$$\mathrm{II}_\hbar=\frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y)\overline{A}\left(z+\frac{\hbar}{2}y\right)A\left(z-\frac{\hbar}{2}y\right)e^{iz\eta}e^{i(yz/m)(t-t_0)}\,dz\,dy, \tag{69}$$

$$\mathrm{III}_\hbar=\frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y)\overline{A}\left(z+\frac{\hbar}{2}y\right)e^{iy\hbar\eta}e^{i(yz/m)(t-t_0)}\,dz\,dy, \tag{70}$$

$$\mathrm{IV}_\hbar=\frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y)A\left(z-\frac{\hbar}{2}y\right)e^{-iy\hbar\eta}e^{i(yz/m)(t-t_0)}\,dz\,dy. \tag{71}$$

We deduce from (58) that

$$J_a^\hbar\simeq\frac{1}{2\pi}\int e^{i\eta p}U(p,t)\frac{q_0}{m}g_a(q_0,t_0)[(\mathrm{I}_\hbar+\mathrm{II}_\hbar+\mathrm{III}_\hbar+\mathrm{IV}_\hbar)(q_0,t_0,\eta,t)]dp\,d\eta\,dt_0\,dt\,dq_0.$$

We first integrate with respect to p. This gives

$$J_a^\hbar=\int \mathcal{F}_pU(\eta,t)\frac{q_0}{m}g_a(q_0,t_0)[(\mathrm{I}_\hbar+\mathrm{II}_\hbar+\mathrm{II}_\hbar+\mathrm{IV}_\hbar)(q_0,t_0,\eta,t)]dq_0\,dt_0\,d\eta\,dt. \tag{72}$$

C. Second approximation: Using the asymptotics of the reflection amplitude

Let us now work on $\mathrm{II}_\hbar$. We first recall that the reflection coefficient R and the phase S_R of the reflection amplitude are given by

$$A(z)=\sqrt{R(z)}e^{i[s_R(z)/\hbar]}.$$

We suppose that S is a smooth (at least differentiable) determination of the phase and that it converges smoothly when $\hbar\to 0$. We then have

$$\overline{A}\left(z+\frac{\hbar}{2}y\right)A\left(z-\frac{\hbar}{2}y\right)=R(z)e^{-iS_R'(z)y}+O(\hbar),$$

where

$$S_R'(z)=\frac{d}{dz}S_R(z).$$

This finally leads to

$$\mathrm{II}_\hbar \simeq \frac{1}{2\pi}\int \Lambda_\hbar(q_0,z,y)R(z)e^{i\eta z}e^{-iS_R'(z)y}e^{i(yz/m)(t-t_0)}\,dy\,dz.$$

Now, going back to (72), we notice that t appears in $\mathrm{I}_\hbar$, $\mathrm{II}_\hbar$, $\mathrm{III}_\hbar$, $\mathrm{IV}_\hbar$ only through complex exponentials. Therefore, by integrating first with respect to t, we obtain Fourier transforms of U with respect to the time variable. We finally end up with the following formulas:

$$J_a^\hbar = \mathrm{I}_\hbar' + \mathrm{II}_\hbar' + \mathrm{III}_\hbar' + \mathrm{IV}_\hbar',$$

where

$$\mathrm{I}_\hbar' = \int \mathcal{F}_{p,t}U\left(\eta,\frac{yz}{m}\right)\frac{q_0}{m}g_a(q_0,t_0)\Lambda_\hbar(q_0,z,y)e^{-i\eta z}e^{-i(yz/m)t_0}\,dy\,dz\,dt_0\,dq_0\,d\eta,$$

$$\mathrm{II}_\hbar' = \int \mathcal{F}_{p,t}U\left(\eta,\frac{yz}{m}\right)\frac{q_0}{m}g_a(q_0,t_0)\Lambda_\hbar(q_0,z,y)R(z)e^{i\eta z}e^{-iS_R'(z)y}e^{-i(yz/m)t_0}\,dy\,dz\,dt_0\,dq_0\,d\eta,$$

$$\mathrm{III}_\hbar' = \int \mathcal{F}_{p,t}U\left(\eta,\frac{yz}{m}\right)\frac{q_0}{m}g_a(q_0,t_0)\Lambda_\hbar(q_0,z,y)\overline{A}\left(z+\frac{\hbar}{2}\eta\right)e^{iy\hbar\eta}e^{-i(yz/m)t_0}\,dy\,dz\,dt_0\,dq_0\,d\eta,$$

$$\mathrm{IV}_\hbar' = \int \mathcal{F}_{p,t}U\left(\eta,\frac{yz}{m}\right)\frac{q_0}{m}g_a(q_0,t_0)\Lambda_\hbar(q_0,z,y)A\left(z-\frac{\hbar}{2}\eta\right)e^{-iy\hbar\eta}e^{-i(yz/m)t_0}\,dy\,dz\,dt_0\,dq_0\,d\eta,$$

where the integration domain is $\mathbb{R}$ except for the variable q_0, where it is $\mathbb{R}_+$.

D. Third approximation: Using the assumption (49) on the wave packets

Formally, using (49), $\mathrm{I}_\hbar'$ converges in the sense of measures to

$$\mathrm{I}_\hbar' = \frac{2\pi}{m}\int \mathcal{F}_{p,t}U\left(\eta,\frac{yz}{m}\right)z\overline{\mathcal{F}_t g_a\left(z,\frac{yz}{m}\right)}e^{-i\eta z}\mathbf{1}_{z>0}\,dy\,dz\,d\eta,$$

and the other terms are approximated by

$$\mathrm{II}_\hbar' \simeq \frac{2\pi}{m}\int \mathcal{F}_{p,t}U\left(\eta,\frac{yz}{m}\right)z\overline{\mathcal{F}_t g_a\left(z,\frac{yz}{m}\right)}e^{i\eta z}R(z)e^{-iS_R'(z)y}\mathbf{1}_{z>0}\,dy\,dz\,d\eta,$$

$$\mathrm{III}_\hbar' \simeq \frac{2\pi}{m}\int \mathcal{F}_{p,t}U\left(\eta,\frac{yz}{m}\right)z\overline{\mathcal{F}_t g_a\left(z,\frac{yz}{m}\right)}\overline{A}\left(z+\frac{\hbar}{2}y\right)e^{iy\hbar\eta}\mathbf{1}_{z>0}\,dy\,dz\,d\eta,$$

where $\mathbf{1}_{z>0}$ denotes the characteristic function of the set $\{z>0\}$. The estimate for $\mathrm{IV}_\hbar'$ is similar as for $\mathrm{III}_\hbar'$.

Next, letting z fixed and integrating with respect to y leads, in view of the Parseval identity, to

$$\mathrm{I}_\hbar' = \int_{(z,\eta,t)\in\mathbb{R}^+\times\mathbb{R}^2}\mathcal{F}_p U(\eta,t)g_a(z,t)e^{-i\eta z}\,dz\,d\eta\,dt = \int_{(z,t)\in\mathbb{R}^+\times\mathbb{R}}U(z,t)g_a(z,t)dt\,dz.$$

For $\mathrm{II}_\hbar'$, using the same computations, we get

$$\mathrm{II}'_\hbar \simeq \int_{(z,t)\in\mathbb{R}^+\times\mathbb{R}} U(-z,t)g_a(z,t-\tau_R(z))R(z)dt\,dz,$$

where the reflection time delay $\tau_R(z)$ is given by (30).

Next, we claim that $\mathrm{III}'_\hbar$ tends to zero when $\hbar\to 0$. Indeed, integrating first with respect to η in the formula for $\mathrm{III}'_\hbar$; gives

$$\mathrm{III}'_\hbar = \frac{2\pi}{m}\int_{(z,y)\in\mathbb{R}^+\times\mathbb{R}} \mathcal{F}_t U\left(-\hbar y,\frac{yz}{m}\right) z\overline{\mathcal{F}_t g_a\left(z,\frac{yz}{m}\right)A\left(z+\frac{\hbar}{2}y\right)}dy\,dz.$$

We just notice now that $|\overline{A}|\leqslant 1$, and that

$$\mathcal{F}_t U\left(-\hbar y,\frac{yz}{m}\right)\underset{h\to 0}{\to}\mathcal{F}_t U\left(0,\frac{yz}{m}\right)=0,$$

since $U(0,t)=0$. Since $\mathcal{F}_t U$, $\mathcal{F}_t g_a$ are smooth and sufficiently decaying at ∞, the dominated convergence theorem implies $\lim_{\hbar\to 0}\mathrm{III}'_\hbar=0$. Therefore it follows that

$$J_a^\hbar = \int_{\mathbb{R}^2} U(p,t)W_a^\hbar(a,p,t)dp\,dt \simeq \int_{(p,t)\in\mathbb{R}^+\times\mathbb{R}} U(p,t)g_a(p,t)dp\,dt + \int_{(p,t)\in\mathbb{R}^+\times\mathbb{R}} U(-p,t)g_a(p,t-\tau_R(p))R(p)dp\,dt.$$

Proceeding analogously for K_a^h, we find

$$K_a^H = \int_{\mathbb{R}^2} U(p,t)W_b^\hbar(a,p,t)dp\,dt \simeq \int_{(p,t)\in\mathbb{R}^-\times\mathbb{R}} T(p)U(p,t)g_b(p,t-\tau_T(p))dp\,dt,$$

where the transmission time delay $\tau_T(z)$ is given by (30). This leads to the following asymptotic formulas, restoring the dependence with respect to $\hbar$:

$$W_a^\hbar(a,p,t)=g_a(p,t):\quad W_a^\hbar(a,-p,t)=R_\hbar(p)g_a(p,t-\tau_R^\hbar(p)),$$

$$W_b^\hbar(a,p,t)=0:\quad W_b^\hbar(a,-p,t)=T_\hbar(-p)g_a(-p,t-\tau_T^\hbar(-p)),\quad \text{for } p>0. \tag{73}$$

Analogously, we have the following asymptotic formulas:

$$W_b^h(b,p,t)=g_b(p,t);\quad W_b^\hbar(b,-p,t)=R_\hbar(p)g_b(p,t-\tau_R^\hbar(p)),$$

$$W_a^\hbar(b,p,t)=0;\quad W_a^\hbar(b,-p,t)=T_\hbar(-p)g_a(-p,t-\tau_T^\hbar(-p)),\quad \text{for } p<0.$$

Summing the asymptotic formulas for W_a^h and $W_b^\hbar$, we obtain relations (50) and (51), which concludes the proof of Theorem 2.4 in the case $V_a=V_b$.

IV. THE CASE $V_a\neq V_b$

In this section, we briefly describe how the proof should be adapted to the case $V_a\neq V_b$. The asymptotic analysis of $J_a^\hbar$ is unchanged while that of $K_a^\hbar$ needs to be adapted. We recall that

$$K_a^h=\int_{\mathbb{R}^2} U(p,t)W_b^\hbar(a,p,t)dp\,dt,$$

and is given by (58), in which g_a is replaced by g_b and the integration domain of the variable q_0 is $\mathbb{R}_-$. Besides, we can use (60) in which the integration domain is $\mathbb{R}_-^2$ for exactly the same

reasons as those developed in the case $V_a = V_b$. Note that the phase factor $[i(q_1^2 - q_2^2)/2m\hbar](t - t_0)$ is left unchanged since the energy $\mathcal{E}(q_1)$ and $\mathcal{E}(q_2)$ are shifted by the same amount, q_1 and q_2 having the same sign.

Next, we claim that the contribution of terms for which $p_a(q_1)$ [or $p_a(q_2)$] are imaginary is exponentially small as stated in Lemma B.3 of Ref. 1 (again a rigorous proof developed in Ref. 13 relies on the dominated convergence theorem). Now, using the asymptotic expansion

$$\psi_q\left(a + \frac{\hbar}{2}\eta\right) = B(q)e^{+i[pa(q)/2]\eta} + O(\hbar),$$

leads to the asymptotic approximation [an analog of (72)]:

$$K_a^\hbar \simeq \int \mathcal{F}_p U(\eta, f)\frac{|q_0|}{m} g_b(q_0, t_0)\mathrm{I}_\hbar(q_0, t_0, \eta, t)dq_0\, dt_0\, d\eta\, dt,$$

where the integration domain is $\mathbb{R}$ for all variables except for q_0, where it is $\mathbb{R}_-$. The term $\mathrm{I}_\hbar$ is given by

$$\mathrm{I}_\hbar = \frac{1}{2\pi}\int_{\mathbb{R}^2_\hbar} \Lambda_\hbar(q_0, z, y)\overline{B}\left(z + \frac{\hbar}{2}y\right)B\left(z - \frac{\hbar}{2}y\right)e^{-i\,p_a(z+\hbar/2y) + p_a(z-\hbar/2y)/2\eta}e^{i(yz/m)(t-t_0)}\,dz\,dy,$$

where

$$\mathbb{R}^2_\hbar = \left\{(z,y)\in\mathbb{R}^2, \quad s.t.\left(z \pm \frac{\hbar}{2}y\right) < 0, \quad p_a\left(z \pm \frac{\hbar}{2}y\right)\in\mathbb{R}\right\}$$

Using the asymptotics of the transmission amplitude in the same way as in Sec. III C, we find the asymptotic expression for $\mathrm{I}_\hbar$,

$$\mathrm{I}_\hbar \simeq \int_{y\in\mathbb{R}}\int_{z<0, s.t. p_a(z)\in\mathbb{R}} \Lambda_\hbar(q_0, z, y)T(z)\frac{z}{p_a(z)}e^{-ip_a(z)\eta}e^{-i(z/m)\tau_T(z)y}e^{i(yz/m)(t-t_0)}\,dz\,dy.$$

This leads to

$$K_\hbar^a \simeq \int_{z<0, s.t. p_a(z)\in\mathbb{R}}\int_{(t,\eta)\in\mathbb{R}^2} \mathcal{F}_p U(\eta, t)g_b(z, t-\tau_T(z))T(z)\frac{z}{p_a(z)}e^{-i\eta p_a(z)}\,dz\,d\eta\,dt.$$

Letting $z' = p_a(z)$, which yields $z = p_b(z')$ and $z\,dz = z'\,dz'$, we obtain

$$K_\hbar^a \simeq \int_{(z',t,\eta)\in\mathbb{R}_-\times\mathbb{R}^2} \mathcal{F}_p U(\eta, t)g_b(p_b(z'), t-\tau_T(p_b(z')))T(p_b(z'))e^{-i\eta z'}\,dz'\,d\eta\,dt.$$

The integration domain in z' is $\mathbb{R}_-$ because of the following:

(i) if $V_a \leqslant V_b$, the set $\{z<0, p_a(z)\in\mathbb{R}\}$ is nothing but $(-\infty, -\sqrt{2me(V_b - V_a)})$, which leads to $\mathbb{R}_-$ after the change of variable $z' = p_b(z)$;

(ii) if $V_a \geqslant V_b$, then $\{z<0,\ p_a(z)\in\mathbb{R}\} = \mathbb{R}_-$, and the integration interval in z' should be $(-\infty, -\sqrt{2me(V_a - V_b)})$. Integrating on the whole half-line $\mathbb{R}_-$ does not change the result since $T(p_b(z')) = 0$ whenever $z' \in (-\sqrt{2me(V_a - V_b)}, 0)$.

Finally, making use of the reciprocity identities

$$T(p_p(p)) = T(-p), \quad \tau_T(p_b(p)) = \tau_T(-p),$$

as well as the Parseval identity, we obtain

$$K_\hbar^q \simeq \int_{(p,t)\in \mathbb{R}_+\times\mathbb{R}} U(-p,t)T(-p_b(p))g_b(-p_b(p),t-\tau_T(-p_b(p)))dp\,dt,$$

which is the desired asymptotic result.

V. TIME-INTEGRATED CURRENT CONSERVATION

In this section, we go back to the coupling methodology defined by Eqs. (41)–(45). An important criterion for the validity of the coupling methodology is that it is current conservative, i.e., that there is no net creation or destruction of particles. Here, we show that our coupling approach is current conservative, in a time-integrated form. Instantaneous current conservation cannot be obtained because it would violate the time-energy uncertainty principle. Indeed, the quantum wave packet description of a particle implies a certain time delocalization (which is at least equal to $\hbar$ over the energy delocalization). Therefore, it is not possible to *a priori* know how much of a given wave packet has crossed the border between the C and Q region (or vice versa) at a given time. However, we must be certain that, once an infinite time has elapsed, the whole wave packet has crossed the border; hence a current conservation in time-integrated form.

Let us denote by $J_C(a,t)$ and $J_Q(a,t)$ the classical and quantum currents flowing through point a at time t. They are, respectively, defined by

$$J_Q(a,t)=\frac{\hbar}{m}\mathcal{T}\left(\frac{\partial\rho}{\partial x}(a,a,t)\right)=\frac{\hbar}{m}\int_{\mathbb{R}^2}\frac{|q_0|}{m}\mathbf{g}(q_0,t_0)\mathcal{T}[\overline{\Psi_{q_0,t_0}}(a,t)\Psi'_{q_0,t_0}(a,t)]dq_0\,dt_0, \quad (74)$$

$$J_C(a,t)=\int_{\mathbb{R}}\frac{p}{m}f(a,p,t)dp, \quad (75)$$

with **g** defined by (40) and (42). Then we have the following.

Lemma 5.1: Under hypothesis (43), we have

$$\int_{\mathbb{R}}J_Q(a,t)dt=\int_{\mathbb{R}}J_C(a,t)dt, \quad \int_{\mathbb{R}}J_Q(b,t)dt=\int_{\mathbb{R}}J_C(b,t)dt. \quad (76)$$

Proof: We prove the first relation (76). The proof of the second one obviously follows the same method. We start with the computation of $J_Q(a,t)$. Inserting formula (28) in (74) and performing the change of variables $q_1=z+(\hbar/2)y$, $q_2=z-(\hbar/2)y$, we get

$$\begin{aligned}&\int_{\mathbb{R}}J_Q(a,t)dt\\ &=\mathcal{T}\left\{\frac{\hbar}{m^2}\int|q_0|\overline{\mathcal{F}_t\mathbf{g}\left(q_0,\frac{yz}{m}\right)}\Lambda_\hbar(q_0,z,y)\overline{\psi_{z+(\hbar/2)y}(a)}\psi'_{z-(\hbar/2)y}(a)e^{i(yz/m)t}\,dt\,dz\,dy\,dq_0\right\}\\ &=\mathcal{T}\left\{\frac{2\pi\hbar}{m}\int\frac{|q_0|}{|z|}\overline{\mathcal{F}_t\mathbf{g}(q_0,0)}\Lambda_\hbar(q_0,z,0)\overline{\psi_z(a)}\psi'_z(a)dq_0\,dz\right\}.\end{aligned}$$

Since

$$\mathcal{T}(\overline{\psi_z}(a)\psi'_z(a))=\frac{z}{\hbar}(1-R(z))=\frac{z}{\hbar}T(z) \quad (z>0); \quad \mathcal{T}(\overline{\psi_z}(a)\psi'_z(a))=\frac{z}{\hbar}T(z) \quad (z<0),$$

we deduce, with (48),

$$\int_{\mathbb{R}}J_Q(a,t)dt=\int_{\mathbb{R}}\frac{q_0}{m}\tilde{T}_\hbar(q_0)\mathcal{F}_t\mathbf{g}(q_0,0)dq_0=\int_{\mathbb{R}^2}\frac{p}{m}\tilde{T}_\hbar(p)\mathbf{g}(p,t)dp\,dt,$$

where

$$\tilde{T}_\hbar(p)=\int P_\hbar(p,z)T_\hbar(z)dz, \quad \tilde{R}_\hbar(p)=\int P_\hbar(p,z)R_\hbar(z)dz. \tag{77}$$

Now, we turn to the computation of $J_C(a,t)$. Introducing

$$F(x,p)=\int_{\mathbb{R}} f(x,p,t)dt, \tag{78}$$

we have, with (44), (45), and dropping the indices $\hbar$ for simplicity,

$$\begin{aligned}\int_{\mathbb{R}} J_C(a,t)dt &= \int_{p>0} p[F(a,p)-F(a,-p)]dp \\ &= \int_{p>0} pF(a,p)dp - \left\{ \int_{p>0}\int_{q>0} P(q,p)R(p)F(a,q)|q|dq\,dp \right. \\ &\quad \left. + \int_{p>0}\int_{q<0} P(q,-p_b(p))T(-p_b(p))\frac{p}{p_b(p)}F(b,q)|q|dq\,dp \right\}. \end{aligned} \tag{79}$$

By exchanging the p and q variables in the integrals inside the curly brackets, we are led to

$$\begin{aligned}\int_{\mathbb{R}} J_C(a,t)dt &= \int_{p>0}|p|F(a,p)dp - \int_{p>0}F(a,p)|p|\left(\int_{q>0} P(p,q)R(q)dq \right)dp \\ &\quad - \int_{p<0}F(b,p)|p|\left(\int_{q>0} P(p,-p_b(q))T(-p_b(q))\frac{q}{p_b(q)}dq \right)dp. \end{aligned} \tag{80}$$

Now, we have, using the normalization condition (38) together with relation (26),

$$1-\int_{q>0} P(p,q)R(q)dq = \int_{q>0} P(p,q)T(q)dq = \tilde{T}(p), \quad p>0,$$

$$\int_{q>0} P(p,-p_b(q))T(-p_b(q))\frac{q}{p_b(q)}dq = \int_{q>0} P(p,-q)T(-q)dq = \tilde{T}(p), \quad p<0,$$

and therefore, (80) leads to

$$\int_{\mathbb{R}} J_C(a,t)dt = \int_{p>0}|p|\tilde{T}(p)F(a,p)dp - \int_{p<0}|p|\tilde{T}(p)F(b,p)dp.$$

But, with (78) and the fact that the outgoing trace of f coincides with the incoming trace of g [see Eq. (42)], we deduce that

$$\int_{\mathbb{R}} J_C(a,t)dt = \int_{\mathbb{R}^2} \tilde{T}(p)\mathbf{g}(p,t)p\,dp = \int_{\mathbb{R}} J_Q(a,t)dt,$$

which completes the proof.

VI. CLASSICAL–QUANTUM COUPLING IN THE STATIONARY CASE

In the present section, we specialize our method for the stationary case in order to bridge the gap with previous work.[1] We first state the following lemma.

Lemma 6.1: Assume that the function $\mathbf{g}$ *does not depend on time and that hypothesis* (43) *holds true. Then the density matrix* ρ *defined by* (41) *does not depend on time and is given by*

$$\rho(x,x')=\int \tilde{g}(q)\psi_q(x)\overline{\psi_q}(x')dq, \tag{81}$$

with

$$\tilde{g}(p)=2\pi\hbar\int_{\mathbb{R}}\frac{|q|}{|p|}|\Phi_\hbar(q,p)|^2\mathbf{g}(q)dq=\int_{\mathbb{R}}P(q,p)\frac{|q|}{|p|}\mathbf{g}(q)dq. \tag{82}$$

In a previous work, one of the authors[1] proposed a method for the stationary case based on (81) with $\mathbf{g}$ instead of $\tilde{g}$. We have seen that, given the conditions (49) on $\Phi_\hbar(q,p)$, $\tilde{g}$ is close to $\mathbf{g}$ in the limit $\hbar\to 0$. Therefore, these two constructions are consistent.

Proof: Performing the changes of variables $t_1=t_0-t$ and $(q_1,q_2)\to(z,y)$ [defined by (67)] in the expression (41) (in which $\mathbf{g}$ is now independent of t), we obtain

$$\rho(x,x',t)=\frac{1}{2\pi}\int\frac{|q_0|}{m}\boldsymbol{g}(q_0)\Lambda_\hbar(q_0,z,y)\psi_{z+(\hbar/2)y}(x)\overline{\psi_{z-(\hbar/2)y}(x')}\exp\left(it_1\frac{yz}{m}\right)dt_1\,dq_0\,dy\,dz,$$

which ensures that ρ does not depend on time. The integrations with respect to t_1 and y are, respectively, performed and lead to

$$\rho(x,x')=\int\frac{|q_0|}{|z|}\mathbf{g}(q_0)P(q_0,z)\psi_z(x)\overline{\psi_z(x')}dq_0\,dz=\int\tilde{g}(z)\psi_z(x)\overline{\psi_z(x')}dz,$$

which leads to the result.

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Geometric amplitude, adiabatic invariants, quantization, and strong stability of Hamiltonian systems

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Considered is a linear set of ordinary differential equations with a matrix depending on a set of adiabatically varying parameters. Asymptotic solutions have been constructed. As has been shown, an important characteristic determining the qualitative portrait of the system is the real part of Berry's complex geometric phase, which we call the geometric amplitude. For systems with purely imaginary eigenvalues the equivalence has been proven in the adiabatic approximation of system sets without geometric amplitude, Hamiltonian systems, quantizable systems, and strongly stable systems. Classification of the systems without geometric amplitude is given with respect to the kind of matrix of the initial system. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1418718]

I. INTRODUCTION

The interest toward the problem of adiabatic evolution of the dynamic system that seemed to have been solved long ago has increased sharply after the papers by Berry and Hannay.[1–3] They noticed certain unusual properties of some terms in the phase of the well-known adiabatic solutions. These terms can be represented as contour integrals of the nonpotential field in the system parameter space. As a result, they do not depend explicitly on the parameter time dependence, but depend only on the geometry of the contour that the representative point moves along through the parameter space. For this reason, the part of the phase described by these terms has been named geometric. Soon thereafter the geometric phases were measured experimentally and found numerous applications, as an intrinsic part of the adiabatic theory, in diverse areas of modern physics.[4]

In view of the general complex representation of adiabatic solutions to linear systems with slowly varying parameters, it is natural to assume that the geometric phase can be complex as well, i.e., it can change the amplitude of solutions in addition to changing the phase.[5,6] The real part of Berry's complex phase, which is responsible for amplitude variations, will be called the *geometric amplitude*. The complex Berry phases were first considered in Ref. 5. Yet, in that paper, as well as in, for instance, Ref. 6, the geometric amplitude appeared in a system characterized by a nonzero real part of its eigenvalues, i.e., against the background of a far greater real component of the conventional dynamic phase, and hence could not affect the qualitative behavior of the solution. As was shown later, the geometric amplitude can appear in oscillatory systems (i.e., in such systems that have purely imaginary eigenvalues) as well where the real part of the dynamic phase is zero.[7] The example below illustrates the significance of the geometric amplitude in this case. Let the system parameters vary in such a way that the system's representative point moves along a closed contour in the parameter space. In the case of a conventional oscillator the amplitude of the adiabatic solution returns to its initial value together with the parameter values. But if a geometric amplitude is present in the oscillatory system, then the corresponding integral of a nonpotential field along the closed contour in the parameter space assumes a nonzero value, and the system does not return to its initial state. Moreover, if the system's representative point performs a continuous motion along a bounded closed contour (i.e., the variation of the systems parameters is finite), then the system might deviate infinitely far from its initial state.

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Thus, the presence of a geometric amplitude implies instability of the oscillator system. This kind of instability was treated with the use the WKB formalism for such dynamic systems that are described by ordinary differential equations of order n.[7] The unusual properties of geometric instability make it essentially different from the known parametric resonances. First, the geometric instability is independent of the relationship between the phases of parameter variation and phases of the solution. Second, the geometric instability is present with an arbitrary temporal dependence of the system parameters (not necessarily periodic, however, if periodic, then of an arbitrary small frequency) for any nondegenerate contour described by the system in the parameter space. Finally, the geometric instability is physically reversible, in the sense that it would be sufficient to vary the parameters in such a way as to have the representative point move along the same contour in the opposite direction, for the instability to be replaced by damping.

These properties suggest that the geometric amplitude can play an important role in dynamic systems. Meanwhile, in Ref. 7 the author put forward a hypothesis of the absence of geometric amplitude in Hamiltonian and other systems possessing a certain symmetry, and formulated the problem of identifying classes of systems with the geometric amplitude. The same paper indicated the direct connection between the geometric amplitude and the possibility of constructing adiabatic invariants, namely that adiabatic invariants can only be constructed if the geometric amplitude is absent.

In this paper the author has discovered and investigated the close connection relating the geometric amplitude to adiabatic invariants, Hamiltonian formalism, the quantization problem, and strong stability of the system. We create a classification of the systems without geometric amplitudes, in which the central role belongs to Hamiltonian systems. Considered are the dynamic systems with adiabatically varying parameters, that are described by nondegenerate sets of ordinary linear differential equations with different eigenvalues. Instead of the cumbersome WKB formalism for the nth-order equations, we offer a more convenient and natural formalism of the first-order vector equation. While in the conventional Hamiltonian theory a complex structure is introduced as an auxiliary one after the quadratic Hamiltonian has been brought to the normal form, we assume a complex structure to be specified in the initial equation. After that, the problem of determining whether the system is Hamiltonian is formulated. As a result, the general formalism of the problem is simplified.

II. GENERAL FORMALISM

Let us consider the linear system described by an n-dimensional vector equation in $\mathbf{C}^n$:

$$\mathbf{x}' = \mathbf{A}(\bar{\mu})\mathbf{x}, \tag{1}$$

where $\mathbf{x}=(x_1,\ldots,x_n)$ is the vector function to be found (its components will be called coordinates); the prime stands for differentiation with respect to the independent variable t (known further as time); $\mathbf{A}(\bar{\mu})$ is the linear operator specified by a square nondegenerate matrix that is a smooth function without singularities of the set of s adiabatically varying parameters $\bar{\mu}=(\mu_1,\ldots,\mu_s)$, i.e., of the vector in $\mathbf{R}^s$. (Let us note that all the main results of this paper are nearly identically obtainable for the initial system in $\mathbf{R}^{2n}$ as well.) The system parameters are subject to an arbitrary (though nonresonance) adiabatic variation with time:

$$\bar{\mu}=\bar{\mu}(\varepsilon t), \quad \varepsilon \ll 1. \tag{2}$$

Here, ε is the adiabaticity parameter. The matrix $\mathbf{A}(\bar{\mu})$ is assumed to be nondegenerate with all the values of the parameters, and all of its eigenvalues are separated sufficiently far for permitting use of the independent adiabatic solutions of (1).

The adiabatic solutions of the system (1) are obtainable through the standard asymptotic techniques,[8] however we are going to use the following idea (it was proposed by Neistadt and is mentioned in Ref. 9).

Let us bring the matrix $\mathbf{A}(\overline{\mu})$ to a diagonal form by applying a parameter-dependent linear substitution of coordinates. In terms of the new coordinates, the matrix of the transformed system will be only slightly nondiagonal, with the off-diagonal terms being proportional to the first-order time derivatives and having the order of ε. Let us further diagonalize the matrix obtained to first order in ε via another linear substitution of coordinates. In these coordinates the off-diagonal matrix elements will be second order ε^2 values, being proportional to the second-order time derivatives. This procedure can be similarly reiterated. This way, the initial equation can be brought for any finite order of ε approximation to a diagonal form, for which exact solutions can be easily written. In this paper we are interested only in the first approximation diagonalization, which corresponds to either the adiabatic approximation or the averaging method (the applicability of adiabatic solutions is discussed in Appendix A).

Let $\mathbf{D}(\overline{\mu})$ be the transition matrix toward the new coordinates $\mathbf{y}$ where $\mathbf{A}(\overline{\mu})$ is diagonal. Then,

$$\mathbf{x}=\mathbf{D}(\overline{\mu})\mathbf{y}, \quad \mathbf{D}^{-1}(\overline{\mu})\mathbf{A}(\overline{\mu})\mathbf{D}(\overline{\mu})=\mathbf{\Lambda}(\overline{\mu})\equiv\mathrm{diag}(\lambda_1,\ldots,\lambda_n), \tag{3}$$

where $\lambda_j=\lambda_j(\overline{\mu})$ are current eigenvalues of the matrix $\mathbf{A}(\overline{\mu})$. Using the substitution (3), Eq. (1) is reduced to the form

$$\mathbf{y}'=(\mathbf{\Lambda}-\mathbf{D}^{-1}\mathbf{D}')\mathbf{y}. \tag{4}$$

From here on, wherever it is unambiguous, the functional arguments are omitted for brevity. The matrix of Eq. (4) consists of two components, namely the diagonal matrix $\mathbf{\Lambda}$ of order ε^0, and the nondiagonal matrix $\mathbf{D}^{-1}\mathbf{D}'$, whose order is ε^1, as its elements are proportional to the time derivatives of the parameters, viz., $\mathbf{D}'=(d\mathbf{D}/d\overline{\mu})\overline{\mu}'$. In the meantime, the diagonal terms of the matrix $\mathbf{D}^{-1}\mathbf{D}'$ make a linear contribution in ε to the magnitudes of eigenvalues of the matrix of (4). At the same time, the contribution of the off-diagonal elements of $\mathbf{D}^{-1}\mathbf{D}'$ to the eigenvalues is of higher orders, and in the linear approximation they can always be reduced to zero via a minor basis correction, i.e., substitution:

$$\mathbf{y}=(\mathbf{I}+\mathbf{\Delta})\tilde{\mathbf{y}};$$

$$\mathbf{\Delta}_{ij}=\frac{(\mathbf{D}^{-1}\mathbf{D}')_{ij}}{\lambda_j-\lambda_i}, \quad i\neq j; \quad \mathbf{\Delta}_{ii}=0, \tag{5}$$

where $\mathbf{I}$ is the unit matrix, $|\mathbf{\Delta}|\sim\varepsilon$. As a result of the substitution (5), we obtain, instead of Eq. (4):

$$\tilde{\mathbf{y}}'=[\mathbf{\Lambda}-\mathrm{dg}(\mathbf{D}^{-1}\mathbf{D}')+O(\varepsilon^2)]\tilde{\mathbf{y}}. \tag{6}$$

Here and further on, the operator dg denotes making the off-diagonal components of the matrix vanish. The sought-for approximate solutions of Eq. (6) will be as follows:

$$\tilde{\mathbf{y}}(t)\approx\tilde{\mathbf{y}}(0)\exp\left\{\int_0^t\left[\mathbf{\Lambda}(\overline{\mu}(\varepsilon\tau))-\mathrm{dg}\left(\mathbf{D}^{-1}(\overline{\mu}(\varepsilon\tau))\frac{d}{d\tau}\mathbf{D}(\overline{\mu}(\varepsilon\tau))\right)\right]d\tau\right\}, \tag{7}$$

where the symbol $\approx$ stands for asymptotic equivalence at $\varepsilon\to 0$ [in our case, to an accuracy up to $O(\varepsilon^2)$]. Using the substitution $(d/d\tau)\mathbf{D}(\overline{\mu}(\varepsilon\tau))d\tau=(d/d\overline{\mu})\mathbf{D}(\overline{\mu})d\overline{\mu}$, the second term in (7) can be transformed into a contour integral in the space of parameters, with the solutions being

$$\tilde{\mathbf{y}}(t)\approx\tilde{\mathbf{y}}(0)\exp\left\{\int_0^t\mathbf{\Lambda}(\overline{\mu}(\varepsilon\tau))d\tau+\int_l\overline{\mathbf{\Omega}}(\overline{\mu})d\overline{\mu}\right\}, \tag{8}$$

where

$$\overline{\mathbf{\Omega}}(\overline{\mu})=-\mathrm{dg}\left(\mathbf{D}^{-1}(\overline{\mu})\frac{d\mathbf{D}(\overline{\mu})}{d\overline{\mu}}\right) \tag{9}$$

is the s-dimensional field of the diagonal matrices over the $\overline{\mu}$ space; l is the contour in which the representative point moves. From here on, the integration contour is assumed to lie in a certain finite, simply connected region of $\mathbf{R}^s$, being sufficiently far removed from the singularities of field (9) (turning points) that are known to correspond to the eigenvalues merger points λ_j;[10] in our case those are $(s-1)$-dimensional hypersurfaces.

We have reduced the initial set (1) to a nearly diagonal form, and in the adiabatic approximation Eq. (6) and its solutions (8) break down into n independent components (degrees of freedom) over each dimension y_j. To make things simpler, all further derivations will be made for the jth component, the extension to the entire system being trivial. Equation (6) and its solutions (8) take the form

$$\tilde{y}_j'=(\lambda_j-\overline{\omega_j}\overline{\mu}')\tilde{y}_j+O(\varepsilon^2), \tag{10}$$

$$\tilde{y}_j(t)\approx\tilde{y}_j(0)\exp\left\{\int_0^t\lambda_j(\overline{\mu}(\varepsilon\tau))d\tau+\int_l\overline{\omega_j}(\overline{\mu}_j)d\overline{\mu}\right\}, \tag{11}$$

where

$$\overline{\omega_j}(\overline{\mu})=\overline{\mathbf{\Omega}}_{jj}(\overline{\mu})=-\left(\mathbf{D}^{-1}(\overline{\mu})\frac{d\mathbf{D}(\overline{\mu})}{d\overline{\mu}}\right)_{jj} \tag{12}$$

is the jth element of the diagonal field matrix (9), and $O(\varepsilon^2)$ contains terms proportional to different y_k. We have taken into account that $-\mathrm{dg}(\mathbf{D}^{-1}\mathbf{D}')=\overline{\mathbf{\Omega}}\overline{\mu}'$ in (6).

The first term in the exponent (11) is the standard ''fast,'' or dynamic, phase that depends explicitly on time, following the evolution of the initial matrix eigenvalues. The second ''slow'' term is of order ε, as compared to the first one. It does not depend explicitly on time, being dependent only on the representative point trajectory in the space of parameters.

Let us extract the potential component of the field $\overline{\omega_j}(\overline{\mu})$:

$$\overline{\omega_j}(\overline{\mu})=\mathrm{grad}(\varphi_j(\overline{\mu}))+\overline{\omega_j^{(c)}}(\overline{\mu}), \tag{13}$$

where $\varphi_j(\overline{\mu})$ is a scalar function, while $\overline{\omega_j^{(c)}}(\overline{\mu})$ is the nonpotential component of $\overline{\omega_j}(\overline{\mu})$. By substituting (13) in (11), we obtain

$$\tilde{y}_j(t)\approx\tilde{y}_j(0)\exp\left\{\int_0^t\lambda_j(\overline{\mu}(\varepsilon\tau))d\tau+\varphi_j(\overline{\mu}(t))-\varphi_j(\overline{\mu}(0))+\int_l\overline{\omega_j^{(c)}}(\overline{\mu})d\overline{\mu}\right\}. \tag{14}$$

The contribution of the potential field component $\overline{\omega_j}(\overline{\mu})$ to the solutions (14) is determined only by the boundary parametric values, being independent, as it is, of the integration contour in the $\overline{\mu}$ space. Therefore, it is the component that determines the connection of the slow solution amplitude to *current* parameter values, and is responsible for the construction of adiabatic invariants.

The contribution of the nonpotential component, $\overline{\omega_j^{(c)}}(\overline{\mu})$, quite to the contrary, depends considerably on the contour geometry l (i.e., on all *prior* values of the parameters), being nonzero even at cyclic parametric variations that correspond to closed contours in the $\overline{\mu}$ space. The last term in the exponent (14) is Berry's complex geometric phase.

For the convenience of our further argumentation we will separate the real and imaginary parts of Berry's complex phase. Its imaginary part will be called the geometric phase proper:

$$\psi_j(l)=\mathrm{Im}\int_l\overline{\omega_j^{(c)}}(\overline{\mu})d\overline{\mu}, \tag{15}$$

while its real part will become the geometric amplitude:

$$\gamma_j(l)=\mathrm{Re}\int_l \overline{\omega}_j^{(c)}(\overline{\mu})d\overline{\mu}, \tag{16}$$

since it is exactly its increment that entails the solution amplitude variations.

Proposition: *The geometric terms, along with the current eigenvalues* λ_j *determine the qualitative portrait of a linear adiabatic system.*

Really, the behavior of the linear system (1) is determined, at constant parameters, by the eigenvalue set λ_j. Those eigenvalues can also be used to describe the system (1) with parameters that vary adiabatically over small times $t\ll\varepsilon^{-1}$ (the values λ_j change little over this time). To describe the adiabatic behavior of the system (1) over large times $t\gg\varepsilon^{-1}$, let us determine the effective eigenvalues that correspond to the solutions (14) over a given time:

$$\lambda_j^{\mathrm{eff}}(t)=\frac{\ln\tilde{y}_j(t)-\ln\tilde{y}_j(0)}{t}. \tag{17}$$

By substituting the solutions (14) into (17), we shall obtain

$$\lambda_j^{\mathrm{eff}}=\langle\lambda_j\rangle_t+\frac{\gamma_j+i\psi_j}{t}+O(t^{-1}), \tag{18}$$

where $\langle\lambda_j\rangle_t\equiv(1/t)\int_0^t\lambda_j(\overline{\mu}(\varepsilon\tau))d\tau$ are average values of the current eigenvalues. The second term in (18) has the order ε and, generally speaking, does not tend to zero together with t^{-1}, since during continuous circulation of the representative point in the $\overline{\mu}$ space the geometric terms grow without bound. If there is a bound $\tilde{\lambda}_j^{\mathrm{eff}}=\lim_{t\to\infty}\lambda_j^{\mathrm{eff}}(t)$, then the solution behavior over large times [strictly speaking, over times so large that the value of $\lambda_j^{\mathrm{eff}}(t)$ does not leave the small vicinity of its limit] can be ''roughly'' (i.e., neglecting the local deviations) described by the formula $\tilde{y}_j(t)\approx\tilde{y}_j(0)\exp(\tilde{\lambda}_j^{\mathrm{eff}}t)$. For example, at periodic parametric variations with the period $T\sim\varepsilon^{-1}$, the value $\lambda_j^{\mathrm{eff}}(t)$ tends asymptotically to the limit $\tilde{\lambda}_j^{\mathrm{eff}}=\langle\lambda_j\rangle_T+[\gamma_j(l_T)+i\psi_j(l_T)]/T$, where l_T is the closed contour corresponding to one period. The role of the effective eigenvalues can be illustrated by the geometric instability.[7] That paper considered systems with purely imaginary current eigenvalues, $\mathrm{Re}\,\lambda_j=0$ (in the sequel, such systems will be called *oscillatory*). There the solutions demonstrated an exponential growth at the effective rate $\mathrm{Re}\,\tilde{\lambda}_j^{\mathrm{eff}}=\gamma_j(l_T)/T$.

Thus, to qualitatively describe the behavior of a system with adiabatically varying parameters one has to know the effective eigenvalues that are determined by the local eigenvalues $\lambda_j(\overline{\mu})$ and geometric terms [fields $\overline{\omega}_j^{(c)}(\overline{\mu})$]. It is natural that the geometric terms and local eigenvalues are invariant with respect to local coordinate substitutions that depend on the current values of the parameters and their derivatives and can only change the potentials $\varphi_j(\overline{\mu})$ (see Appendix B). All of the above argumentation provide grounds for listing the geometric phases and amplitudes together with such ''basic'' characteristics of a system as eigenvalues λ_j.

III. ADIABATIC INVARIANT CONSTRUCTION, POINCARÉ'S INTEGRAL INVARIANTS, AND THE LIOUVILLE THEOREM

As noted above, the potentials $\varphi_j(\overline{\mu})$ in the solutions (14) depend on the choice of a coordinate system. In particular, we can always transit to such coordinates in which the potentials $\varphi_j(\overline{\mu})$ vanish. Transition to these coordinates in the case of the Hamiltonian systems corresponds to the transition to the canonical action variables. Let us make the substitution

$$z_j=\tilde{y}_j\exp(-\varphi_j(\overline{\mu})).$$

Then, the equations (10) and their solutions (14), considering (13), (15), and (16), will take on the following form:

$$z_j' = (\lambda_j + \overline{\omega}_j^{(c)}\overline{\mu}')z_j + O(\varepsilon^2); \tag{19}$$

$$z_j(t) \approx z_j(0)\exp\left\{\int_0^t \lambda_j(\overline{\mu}(\varepsilon\tau))d\tau + \gamma_j(l) + i\psi_j(l)\right\}. \tag{20}$$

If in the **z** space the solution absolute values should be approximately constant:

$$I_j(t) \equiv |z_j(t)|^2 \approx \text{const}, \tag{21}$$

then they are known as adiabatic invariants of action I_j. In the initial coordinates, they determine, under given initial conditions, the unambiguous connection between the approximate solution amplitude and current parametric values. The following is obvious.

Statement I: *A given degree of freedom possesses an adiabatic invariant of action if and only if*

$$\begin{gathered} \operatorname{Re}\lambda_j = 0, \\ \gamma_j = 0. \end{gathered} \tag{22}$$

Note that the conditions (22) are equivalent to the requirement that the real part of the effective eigenvalue λ_j^{eff}, introduced in the preceding section, be equal to zero. In other words, it should be equivalent to the requirement of conservation of the oscillatory nature of the motion over large times and under adiabatically varying parameters.

The expressions (21) and the conditions (22) correspond to the conservation of the phase flux of the jth degree of freedom in the **z** space. [Since we consider the general case for a complex equation in $\mathbf{C}^n$, each degree of freedom corresponds to one dimension z_j, with the phase flux of one degree of freedom corresponding to the phase flux of the complex plane z_j. It is rather easy to extend all the results given here to the case of real initial system (1) in $\mathbf{R^{2n}}$, where, after diagonalization of the equations, each degree of freedom corresponds to two complex conjugated equations.] Indeed, from (20) and (21) it is easy to see that the time dependence of the area of a z_j-plane element:

$$S_j(t) \equiv \int dz_j \wedge dz_j^* \approx S_j(0)\exp\left\{2\int_0^t \operatorname{Re}\lambda_j\, d\tau + 2\gamma_j\right\},$$

coincides with the values $I_j(t)$ to insignificant factors (the asterisk stands for complex conjugation, while integration of the 2-form is done over the selected area element of the phase z_j plane at a fixed time). When the geometric amplitude $\gamma_j \neq 0$ is present in the oscillatory system the phase flux is not conserved and gets changed by a factor of $\exp(2\gamma_j)$.

We will define Poincaré's kth ($k \leqslant n$) integral invariant through the statement as follows: The area of an arbitrary k-dimensional hypersurface of the kind

$$S^{(k)}(t) = \int \sum_{a_1 < \ldots < a_k} dz_{a_1} \wedge dz_{a_1}^* \wedge \cdots \wedge dz_{a_k} \wedge dz_{a_k}^*,$$

is conserved in the course of time evolution: $S^{(k)}(t) = \text{const}$. (Here, one has to make an important remark. The Poincare's integral invariants are an attribute of Hamiltonian systems. With this in mind, the considered complex invariant structure can be introduced only for the Hamiltonian systems with purely imaginary current eigenvalues. However, Hamiltonian systems may possess eigenvalues of two other kinds as well, namely pairs of opposite real numbers and quadruples with opposite real and imaginary parts.[16] Those two cases of eigenvalue pairs and quadruples are not considered here. Formally speaking, we can leave them out by requiring that the imaginary parts of eigenvalues λ_j be different.) Poincaré's first integral invariant represents a sum of projection areas on the plane z_j:

$$S^{(1)}=\int \sum_{j=1}^{n} dz_j\wedge dz_j^*=\int \sum_{j=1}^{n} dS_j=\text{const.}$$

Statement II: *In the considered adiabatic approximation (when the degrees of freedom z_j are assumed independent) the existence of Poincaré's first integral invariant is equivalent to the presence of n adiabatic invariants $S_j\approx$ const, i.e., for its existence it is necessary and sufficient that the conditions (22) hold for all degrees of freedom.*

Let us consider also changes in the *n*-dimensional phase volume of the system:

$$S^{(n)}\equiv V(t)\equiv\int dz_1\wedge dz_1^*\wedge\cdots\wedge dz_n\wedge dz_n^*\approx V(0)\exp\left\{2\sum_{j=1}^{n}\left(\int_0^t \mathrm{Re}\,\lambda_j\,d\tau+\gamma_j\right)\right\}.$$

Statement III: *The necessary and sufficient conditions for the phase volume of a system to be conserved, $V(t)\approx$ const (Poincaré's nth integral invariant, or Liouville's theorem) are*

$$\sum_{j=1}^{n}\mathrm{Re}\,\lambda_j=0,\qquad \sum_{j=1}^{n}\gamma_j=0. \tag{23}$$

Thus, Liouville's theorem of conservation of the phase volume of a system imposes restrictions on the geometric amplitudes without forbidding their existence. Should one require conservation of the phase areas for each degree of freedom (adiabatic invariants) or conservation of the phase volume for manifolds of dimension less than *n* (Poincaré's integral invariants), that would only be possible if all geometric amplitudes were identical zeros.

IV. HAMILTONIAN FORMALISM

It is known that a system has Poincaré's first integral invariant only when the system is Hamiltonian.[11,12] In this way, it follows from the results of the preceding section [condition (22)] that the absence of geometric amplitudes is necessary and sufficient for an oscillatory system to be Hamiltonian in the approximation considered. We will produce direct proof for this assertion.

In an oscillatory system without geometric amplitudes, the Hamiltonian formalism is naturally introduced when the diagonalized equations are realificated. Indeed, carrying out the realification of (19) and introducing the variables

$$p_j=\mathrm{Re}\,z_j,\quad q_j=\mathrm{Im}\,z_j,$$

we obtain

$$\begin{aligned}p_j'&=\mathrm{Re}(\lambda_j+\overline{\omega}_j^{(c)}\overline{\mu}')p_j-\mathrm{Im}(\lambda_j+\overline{\omega}_j^{(c)}\overline{\mu}')q_j+O(\varepsilon^2)\\ q_j'&=\mathrm{Im}(\lambda_j+\overline{\omega}_j^{(c)}\overline{\mu}')p_j+\mathrm{Re}(\lambda_j+\overline{\omega}_j^{(c)}\overline{\mu}')q_j+O(\varepsilon^2).\end{aligned} \tag{24}$$

Taking into account the conditions (22) and neglecting ε-quadratic components, we find that $2n$ real equations (24) correspond to the canonical equations with a Hamiltonian:

$$H(p,q)=\frac{1}{2}\sum_{j=1}^{n}\mathrm{Im}(\lambda_j+\overline{\omega}_j^{(c)}\overline{\mu}')(p_j^2+q_j^2), \tag{25}$$

where $p\equiv(p_1,\ldots,p_n)$; $q\equiv(q_1,\ldots,q_n)$.

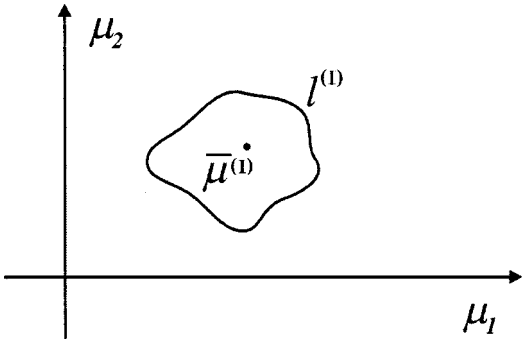

FIG. 1. To the proof of Theorem I. The nonperturbed system realization corresponds to the zero contour at point $\bar{\mu}^{(I)}$, the perturbed one corresponds to the closed contour $l^{(I)}$ around $\bar{\mu}^{(I)}$. Here and in the following figures, for the sake of clearness, we present the case of two-dimensional parameter space: $\bar{\mu}=(\mu_1,\mu_2)$.

Thus, an oscillatory system without geometric amplitudes is a canonical one with a Hamiltonian (25). Let us now prove the opposite: an arbitrary oscillatory Hamiltonian system has no geometric amplitudes.

Let us consider a Hamiltonian system with different imaginary eigenvalues, $\mathrm{Re}\,\lambda_j=0$. We will call a *realization* of a system the system with a certain given time dependence $\bar{\mu}(\varepsilon t)$. As the initial realization we will take the one with arbitrary constant values of the parameters $\bar{\mu}=\bar{\mu}^{(I)}$. It is obvious that the geometric phases and amplitudes of this realization of the system are zero. As the perturbed realization we will consider the realization of the same system where the parameters change in such a way that the representative point is moving along a small closed contour $l^{(I)}$ in the vicinity of the point $\bar{\mu}^{(I)}$ in the parameter space (Fig. 1). The perturbed realization of the system will now possess certain nonzero geometric terms. Their values are independent of a specific parameter-on-time dependence and depend only on the contour $l^{(I)}$ shape. For this reason, without loss of generality, we can assume that in the perturbed realization the parameters depend on time periodically with an arbitrary nonresonance period $T\sim\varepsilon^{-1}$.

Recall that the systems where parameters depend on time periodically are characterized by *multiplicators*, namely the coefficients of eigensolution transformation over one period. Using the explicit form of the solutions (20), we obtain that the system multiplicators in the adiabatic approximation are as follows:

$$\rho_j(l)=\exp\left\{\int_0^T \lambda_j\,dt+\gamma_j(l)+i\psi_j(l)\right\}. \tag{26}$$

In the initial realization $|\rho_j(0)|=1$, i.e., its multiplicators lie on a unit circle. According to the theorem on the strong stability of Hamiltonian systems whose Hamiltonian depends periodically on time,[13] if the perturbation is small enough (i.e., the contour $l^{(I)}$ lies in a sufficiently small vicinity of the point $\bar{\mu}^{(I)}$); then the multiplicators of the perturbed system realization also belong to the unit circle: $|\rho_j(l^{(I)})|=1$. Hence, using (26) for the perturbed realization, we obtain $\gamma_j(l^{(I)})=0$. This proves that the system's geometric amplitudes are equal to zero for an arbitrary small contour in the vicinity of an arbitrary point in the considered region of $\bar{\mu}$ space. Therefore the geometric amplitudes in a Hamiltonian system with $\mathrm{Re}\,\lambda_j=0$ are identical zeros.

This result can be interpreted as the conservation of the oscillatory nature of a Hamiltonian system motion under adiabatic parametric variations. Hence, in particular, it follows [compare (19), (24), (25), taking into account (22)] that a Hamiltonian system with different imaginary eigenvalues and slow varying parameters, similar to a system with constant parameters, is reduced in the adiabatic approximation to the normal form[14] with a Hamiltonian:

$$H(p,q)=\sum_{j=1}^{n} H_j(p_j,q_j)=\frac{1}{2}\sum_{j=1}^{n} w_j(p_j^2+q_j^2), \tag{27}$$

where $iw_j=\lambda_j+\overline{\omega}_j^{(c)}\overline{\mu}'$.

So, we demonstrate that the oscillatory systems have no geometric amplitudes if and only if the system is Hamiltonian. In other words, the following theorem is true.

Theorem I: *Among the system (1) with different imaginary current eigenvalues the sets of Hamiltonian systems and those without geometric amplitudes are, within the adiabatic approximation, coincident. The Hamiltonians of these systems can be reduced to the normal form (27), namely to that of a sum of independent oscillators.*

It should be emphasized that it is exactly in the oscillatory Hamiltonian systems that geometric amplitudes are absent, although they may be present in Hamiltonian systems with a nonzero real part of the current eigenvalues.[5,6] Indeed, the simplest example of such a system may well be the generalized Hannay oscillator[3] with the following Hamiltonian: $H=\frac{1}{2}(\mu_1 p^2+2\mu_2 pq+\mu_3 q^2)$. If one considers the Hannay oscillator in the parametric region $\mu_1\mu_3-\mu_2^2<0$ (corresponding to its eigenvalues being real and its phase portrait being hyperbolic), then the known geometric phase in this system becomes its geometric amplitude. It should be noted that the typical growth rates associated with the geometric amplitude will at all times be much smaller than the typical real part of the system eigenvalues.[7]

V. SYSTEM QUANTIZATION

In this section, we will try to answer the question whether the system (1) can be quantized and what conditions are required for that. As in the preceding section, we will deal with oscillatory systems. We call the spectrum of the jth degree of freedom σ_j the range of $|z_j|^2$ for fixed values of the parameters:

$$\sigma_j(\overline{\mu})=\{|z_j|^2\}|_{\overline{\mu}=\text{const}}.$$

The system quantization will be understood as follows. Let the system (1) with purely imaginary eigenvalues correspond to a certain classical system. It is quite obvious that its spectra are continuous: $\sigma_j=[0,+\infty)$. During quantization we correspond this system to the quantum one so that its dynamic variables z_j satisfy the same differential equations (19), but spectra $\sigma_j(\overline{\mu})$ are discrete and unambiguously determined by the fixed parametric values $\overline{\mu}$.

It is quite clear that the known quantization rules for oscillatory Hamiltonian systems satisfy our requirements (see, for instance, the oscillator quantization in Ref. 15). Indeed, for a Hamiltonian oscillatory system under constant values of parameters σ_j's are, to constant multipliers, spectra of Hamiltonians (27) H_j of independent linear oscillators. We are going to prove that the non-Hamiltonian oscillatory system is unquantizable in principle, and the reason for that can be attributed to the presence of geometric amplitudes.

Consider a realization of a non-Hamiltonian oscillatory system, in which the time dependence of parameters is like shown in Fig. 2. Up to a certain moment of time the parameters preserve certain constant values: $\overline{\mu}=\overline{\mu}^{(II)}$ at $t\in(-\infty,t_1]$; afterward in the finite segment $t\in[t_1,t_2]$ the parameters undergo a single cyclic change, corresponding to the closed contour $l^{(II)}$ with its beginning and end being in the point $\overline{\mu}^{(II)}$; after that the parameter values are equal to the initial ones and remain constant in the sequel: $\overline{\mu}=\overline{\mu}^{(II)}$ at $t\in[t_2,+\infty)$. Let us consider the spectra transformation of this realization in the range $t\in[t_1,t_2]$.

On one hand, in the ranges $t\in(-\infty,t_1]$ and $t\in[t_2,+\infty)$ the considered realization is described by the same differential equations with the same constant parameter values $\overline{\mu}^{(II)}$. That is why its phase portraits in these ranges must coincide:

$$\sigma_j|_{t>t_2}=\sigma_j|_{t<t_1}=\sigma_j(\overline{\mu}^{(II)}).$$

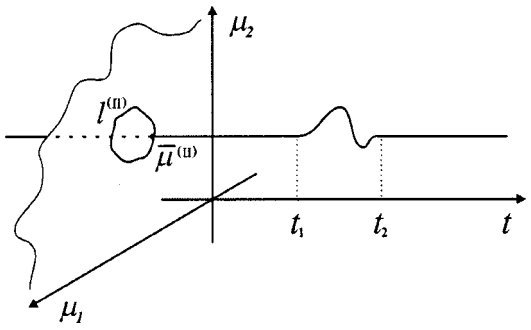

FIG. 2. To the proof of Theorem II. The $\overline{\mu}(t)$ dependence and its projection on the $\overline{\mu}$ space: closed contour $l^{(II)}$ with its beginning and end at point $\overline{\mu}^{(II)}$.

On the other hand, due to the non-Hamiltonian nature of the system, in the range $t\in[t_1,t_2]$ the solution gains geometric amplitudes $\gamma_j^{(II)}=\gamma_j(l^{(II)})$, and, as was shown in Sec. III, the values of $|z_j|^2$ (which are proportional to the phase fluxes of different degrees of freedom) get changed by the factor of $\exp(2\gamma_j^{(II)})$. This means that the spectra of a given system realization undergo the same kind of extension:

$$\sigma_j|_{t>t_2}=\exp(2\gamma_j^{(II)})\sigma_j|_{t<t_1}.$$

Comparing the above assertions, we can avoid a contradiction only if the phase portrait of the system with the constant parameters and its spectra are self-similar with the coefficients $\exp(2\gamma_j^{(II)})$ in each dimension:

$$\sigma_j(\overline{\mu}^{(II)})=\exp(2\gamma_j^{(II)})\sigma_j(\overline{\mu}^{(II)}).$$

Hence an oscillatory system with a nonzero geometric amplitude is unquantizable. Indeed, by choosing different contours $l^{(II)}$ in the considered simply connected region of the $\overline{\mu}$ space, we will obtain that the possible values $\gamma_j^{(II)}=\gamma_j(l^{(II)})$ continuously fill up a certain segment of the real axis. The values of similarity coefficients $\exp(2\gamma_j^{(II)})$ will also continuously fill up the appropriate segment. In particular, by constricting the contour $l^{(II)}$ to the point $\overline{\mu}^{(II)}$ we can make $\gamma_j^{(II)}$ arbitrarily small, with the similarity coefficients being arbitrarily close to one. The classical continuous spectrum $\sigma_j=[0,+\infty)$ is always self-similar with any coefficient. Assume that the quantum discrete spectrum can be self-similar. But in this case the similarity coefficients' values will represent the discrete set, being determined by the interlevel distances. In particular, the quantum spectrum similarity coefficient cannot be made arbitrarily close to one, as this fact would mean that the interlevel distance is arbitrarily small, i.e., the spectrum is continuous. This proves that a non-Hamiltonian system cannot possess a discrete spectrum.

In the Hamiltonian system the phase space is not extended over $t\in[t_1,t_2]$, hence we do not need to require that the spectrum is self-similar. For this reason, the Hamiltonian system spectrum may be discrete.

Thus, the following theorem is true.

Theorem II: *Among the system (1) with different imaginary current eigenvalues the set of quantizable systems coincides, within the adiabatic approximation, with the set of systems without geometric amplitudes (or, according to Theorem I, with the set of Hamiltonian systems).*

The result obtained can be interpreted as yet another confirmation of the so-called Ehrenfest hypothesis.[16,12] According to this hypothesis, during the classical system quantization the quantum numbers correspond to adiabatic invariants. When geometric amplitudes are present, there are no adiabatic invariants in the system, and we cannot correspond a set of certain fixed numbers to each its solution. [Yet, this result does not mean that the system (1) with the geometric amplitudes

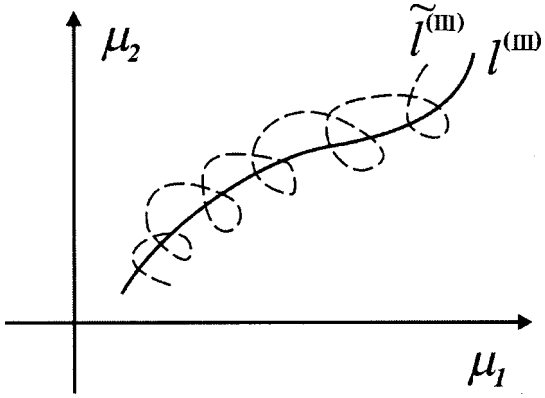

FIG. 3. To the proof of Theorem III. Contour $l^{(III)}$ of the nonperturbed system realization and its corresponding contour $\tilde{l}^{(III)}$ of the perturbed system realization in the space of parameters.

cannot describe a quantum system. Equation (1) can, for example, correspond to the Schrödinger equation of a certain system. We only mean that if the system (1) is classical, then its dependent variables cannot be quantized in the non-Hamiltonian case.]

VI. SYSTEM STRONG STABILITY

In the preceding two sections we established that for oscillatory systems the classes of systems without geometric amplitude, Hamiltonian systems, and quantizable ones are equivalent. In this section, we are going to demonstrate that this class of systems can be regarded as a set of oscillatory systems possessing the property of strong stability.

Let's define the strong stability in the following way.

Definition: *Let a realization of the system (1) with the matrix* $\mathbf{A}=\mathbf{A}_0(\overline{\mu})$ *from a certain class and the dependence* $\overline{\mu}=\overline{\mu}_0(\varepsilon t)$ *be stable, i.e., all of its solutions bounded. If there exists a* $\delta>0$, *such that any perturbed realization of the system (1) with the matrix* $\mathbf{A}=\mathbf{A}_1(\overline{\mu})$ *from the same class and the dependence* $\overline{\mu}=\overline{\mu}_1(\varepsilon t)$, *satisfying the inequality*

$$\|\mathbf{A}_1(\overline{\mu}_1(\varepsilon t))-\mathbf{A}_0(\overline{\mu}_0(\varepsilon t))\|<\delta, \quad \forall t, \tag{28}$$

is also stable, then the initial realization of the system is called strongly stable.

The system is strongly stable if all of its realizations are strongly stable.

Let us demonstrate first that a strongly stable oscillatory system does not have geometric amplitudes, i.e., it is Hamiltonian in the approximation considered. Indeed, let a certain realization of an oscillatory system with nonzero geometric amplitudes be stable. Then, we will select as a perturbed realization, the realization of the same system, in which the representative point would circulate in a certain direction in the $\overline{\mu}$ space around the trajectory of the initial realization (Fig. 3). The trajectories of the representative points for the initial and the perturbed realizations can be done arbitrarily close to each other, such that the condition (28) can be satisfied for arbitrarily small δ. By properly selecting the circulation direction and shape it is always possible to make the geometric amplitude (together with the solution amplitude) grow infinitely, and thus perturbed relization becomes unstable (see the Introduction, Sec. II, Ref. 7). Consequently, a strongly stable oscillatory system must not have geometric amplitude, and it is Hamiltonian in the approximation under consideration.

Now, let us prove the opposite: An oscillatory system of the Hamiltonian class is strongly stable in the approximation considered. This follows directly from the explicit form of the independent solutions (20). Indeed, the oscillatory system eigenvalues are purely imaginary, with the geometric amplitudes in the Hamiltonian systems being identically zero. In this way, the exponent in (20) is purely imaginary for any realization of a Hamiltonian system, and its solutions are

bounded. Since the perturbed system must belong to the same class, in accordance with the above definition, i.e., it must be Hamiltonian, solutions of any of its realization will also be bounded. This concludes the proof of the strong stability of Hamiltonian systems.

The above assertions demonstrate that an oscillatory system with different eigenvalues is strongly stable if and only if the system is Hamiltonian. In other words, the following theorem is true.

Theorem III: *Among the systems (1) with different imaginary eigenvalues, the set of systems with the property of strong stability, in the sense of the above definition, coincides in the adiabatic approximation with the set of Hamiltonian systems (or, in accordance with Theorem I, with the set of systems without geometric amplitudes, or, in accordance with Theorem II, with the set of quantizable systems).*

VII. SYSTEM CLASSIFICATION

As was shown in Sec. II, solutions of a system (1) in the general form possess geometric amplitudes. For this reason, it is natural to perform a classification of such systems that have no geometric amplitudes. This classification will be performed from the standpoint of the matrix type of the initial problem (1). Some of the results to be obtained in this section are well known, and they are given here for the sake of completeness and coherence. Here belong the results concerning the matrix of a Hamiltonian system in the canonical coordinates and in the coordinates connected to the canonical ones via time-independent substitutions.[12,13]

A. Oscillatory systems

In Sec. IV we describe a complete class of oscillatory systems without geometric amplitudes; that turned out to be the set of Hamiltonian systems with different imaginary eigenvalues. In the employed complex canonical $\mathbf{z}$ coordinates the Hamiltonian system has the following form [see (19), taking into account (22)]:

$$\mathbf{z}' = i\tilde{\mathbf{\Lambda}}(\overline{\mu},\overline{\mu}')\mathbf{z} + O(\varepsilon^2), \tag{29}$$

where $\tilde{\mathbf{\Lambda}}(\overline{\mu},\overline{\mu}') = \mathrm{diag}(\lambda_1 + \overline{\omega}_1^{(c)}\overline{\mu}', \ldots, \lambda_n + \overline{\omega}_n^{(c)}\overline{\mu}') \equiv \mathbf{\Lambda}(\overline{\mu}) + \overline{\mathbf{\Omega}}^{(c)}(\overline{\mu})\overline{\mu}'$ is a diagonal real matrix. The initial system (1) is specified, generally speaking, in arbitrary $\mathbf{x}$ coordinates. Let the $\mathbf{x}$ and $\mathbf{z}$ coordinates be connected through a certain transition matrix $\tilde{\mathbf{D}}(\overline{\mu},\overline{\mu}')$ [the dependence on $\overline{\mu}'$ is contained in the substitution (5)]:

$$\mathbf{x} = \tilde{\mathbf{D}}(\overline{\mu},\overline{\mu}')\mathbf{z}. \tag{30}$$

Then the matrix $\mathbf{A}$ of the initial system (1) will be

$$\mathbf{A} = i\tilde{\mathbf{D}}\tilde{\mathbf{\Lambda}}\tilde{\mathbf{D}}^{-1} - \tilde{\mathbf{D}}\tilde{\mathbf{D}}^{-1\prime} + O(\varepsilon^2). \tag{31}$$

Thus, *a set* K *of oscillatory systems (1) without geometric amplitudes is a set of systems (1) with the matrix* $\mathbf{A}(\overline{\mu})$*, representable as (31), where* $\tilde{\mathbf{D}} = \tilde{\mathbf{D}}(\overline{\mu},\overline{\mu}')$ *is an arbitrary complex nondegenerate matrix, while* $\tilde{\mathbf{\Lambda}} = \tilde{\mathbf{\Lambda}}(\overline{\mu},\overline{\mu}')$ *is an arbitrary real diagonal matrix.*

Let us isolate in this set the subsets that may be of special interest. To that end, let us write the system (29) as

$$\mathbf{z}' = \mathbf{J}\mathbf{H}(\overline{\mu},\overline{\mu}')\mathbf{z} + O(\varepsilon^2), \tag{32}$$

where $\mathbf{J} = i\mathbf{I}$ ($\mathbf{I}$ is a unit matrix of order n), while $\mathbf{H}(\overline{\mu},\overline{\mu}') = \tilde{\mathbf{\Lambda}}(\overline{\mu},\overline{\mu}')$ is a Hermitian diagonal matrix. Under realification the matrix $\mathbf{J}$ turns into a unit antisymmetrical matrix of the order $2n$, which defines the symplectic structure, while the matrix $\mathbf{H}(\overline{\mu},\overline{\mu}')$ turns into a real symmetrical matrix Hamiltonian.[12–14]

As is known, canonical substitutions are those that preserve the form of a symplectic structure (while, generally speaking, changing the Hamiltonian) in the new coordinates. In our case, this fact means that the matrix $\mathbf{J}$ turns into itself during canonical substitution of the variables, while Eq. (32) preserves its form with some other Hermitian matrix $\tilde{\mathbf{H}}(\overline{\mu},\overline{\mu}')$ instead of $\mathbf{H}(\overline{\mu},\overline{\mu}')$. It is easy to demonstrate that in the formalism under consideration the set of linear canonical substitutions is represented by the substitutions (30) with the unitary matrix $\tilde{\mathbf{D}}^*(\overline{\mu},\overline{\mu}')=\tilde{\mathbf{D}}^{-1}(\overline{\mu},\overline{\mu}')$ (compare the correspondence of unitary transformations in the quantum mechanics to canonical ones in the classical mechanics).[15,17] After the unitary substitution (30) Eq. (32) turns into

$$\mathbf{x}'=\mathbf{J}\tilde{\mathbf{H}}(\overline{\mu},\overline{\mu}')\mathbf{x}+O(\varepsilon^2),$$

where

$$\tilde{\mathbf{H}}=\tilde{\mathbf{D}}\tilde{\Lambda}\tilde{\mathbf{D}}^{-1}+i\tilde{\mathbf{D}}\tilde{\mathbf{D}}^{-1'}.$$

One can easily see that due to the matrix $\tilde{\mathbf{D}}$ being unitary the matrix $\tilde{\mathbf{H}}$ is Hermitian.

The subset $K_1\subset K$ *of all oscillatory Hamiltonian systems (1), written in the canonical variables, represents the set of systems (1) with the matrix* $\mathbf{A}(\overline{\mu})=\mathbf{J}\tilde{\mathbf{H}}(\overline{\mu})$, *where* $\mathbf{J}=i\mathbf{I}$, *while* $\tilde{\mathbf{H}}(\overline{\mu})$ *is an arbitrary nondegenerate complex Hermitian matrix with different real eigenvalues*.[12,13]

Let us also consider the subset of all systems, associated with the system (32) via substitution of the kind (30), where the matrix is constant $\tilde{\mathbf{D}}(\overline{\mu},\overline{\mu}')=\tilde{\mathbf{D}}=\text{const}$. In this case Eq. (32) turns into the equation

$$\mathbf{x}'=\mathbf{G}\tilde{\tilde{\mathbf{H}}}(\overline{\mu},\overline{\mu}')\mathbf{x}+O(\varepsilon^2),$$

where $\mathbf{G}=i\tilde{\mathbf{D}}\tilde{\mathbf{D}}^*$ is a constant anti-Hermitian matrix, which under the realification defines a new form of the symplectic structure. $\tilde{\tilde{\mathbf{H}}}(\overline{\mu},\overline{\mu}')=\tilde{\mathbf{D}}^{*-1}\tilde{\Lambda}(\overline{\mu},\overline{\mu}')\tilde{\mathbf{D}}^{-1}$ is the Hermitian matrix specifying the matrix Hamiltonian under the realification.

The subset $K_2\subset K$ *of oscillatory Hamiltonian systems (1), represented in arbitrary coordinates and connected with the canonical ones via a constant substitution, is a set of systems (1) with the matrix* $\mathbf{A}(\overline{\mu})=\mathbf{G}\tilde{\tilde{\mathbf{H}}}(\overline{\mu})$. *Here,* $\mathbf{G}$ *is an arbitrary constant nondegenerate complex anti-Hermitian matrix, while* $\tilde{\tilde{\mathbf{H}}}(\overline{\mu})$ *is an arbitrary nondegenerate complex Hermitian matrix, with their product having different purely imaginary eigenvalues*.[12,13]

Evidently, $K_1\subset K_2$.

B. General case

Consider now the general case for nonoscillatory systems when $\operatorname{Re}\mathbf{\Lambda}\neq 0$. Let us make a substitution:

$$\tilde{\mathbf{z}}=\mathbf{z}\exp\left(-\int_0^t \operatorname{Re}\mathbf{\Lambda}(\overline{\mu}(\varepsilon\tau))d\tau\right), \tag{33}$$

which evidently does not affect the geometric terms in the solutions (20) (see Appendix B). Let us assume, as we did before, that the initial $\mathbf{x}$ and $\mathbf{z}$ coordinates are connected through a certain nondegenerate substitution (30). The substitution (33) is equivalent to the transition $\mathbf{\Lambda}\to i\operatorname{Im}\mathbf{\Lambda}$. Therefore, upon the inverse substitution to (30), bringing the equations back to the original $\mathbf{x}$ space we obtain [compare to (1), (3)]:

$$\tilde{\mathbf{x}}'=\tilde{\mathbf{A}}\tilde{\mathbf{x}},\quad \tilde{\mathbf{A}}=i\mathbf{D}\operatorname{Im}\mathbf{\Lambda}\mathbf{D}^{-1}. \tag{34}$$

This equation has purely imaginary current eigenvalues $\tilde{\lambda}_j = i\,\mathrm{Im}\,\lambda_j$ and the same geometric terms in the solutions as the initial equation (1). Thereby the problem has been reduced to the preceding one, and the system has no geometric amplitudes if and only if the system (34) belongs to the above set K of oscillatory Hamiltonian systems. Using (3) and (34), we can write

$$\mathbf{A} = \tilde{\mathbf{A}} + \mathbf{D}\,\mathrm{Re}\,\Lambda\mathbf{D}^{-1}. \tag{35}$$

Thus, *in the general case the complete set* $\mathrm{M} \supset \mathrm{K}$ *of the systems (1) without geometric amplitudes is the set of systems (1) with a matrix representable as (35), where* $\tilde{\mathbf{A}} = \tilde{\mathbf{A}}(\overline{\mu})$ *is an arbitrary matrix from* K; $\mathrm{Re}\,\mathbf{\Lambda}(\overline{\mu})$ *an arbitrary real diagonal matrix and* $\mathbf{D} = \mathbf{D}(\overline{\mu})$ *is the transition matrix bringing* $\tilde{\mathbf{A}}(\overline{\mu})$ *to a diagonal form*.

We will also describe the subsets that may be of special interest.

Lemma: *If the matrix* $\mathbf{A}(\overline{\mu})$ *of the system (1) can be brought to a diagonal form with the unitary matrix* $\mathbf{D}^*(\overline{\mu}) = \mathbf{D}^{-1}(\overline{\mu})$, *then the system has no geometric amplitudes*.

Proof: The geometric terms in the solutions of the system (1) arise from nonpotential components of the matrix field (9) $\overline{\mathbf{\Omega}}(\overline{\mu})$. The condition for the existence of geometric terms is the nonpotentiality of that field:

$$(\mathrm{rot}\,\overline{\mathbf{\Omega}})_{\alpha\beta} \equiv \frac{\partial \mathbf{\Omega}_\alpha}{\partial u_\beta} - \frac{\partial \mathbf{\Omega}_\beta}{\partial \mu_\alpha} \neq 0. \tag{36}$$

Here, the Greek indices relate to the $\overline{\mu}$ space. By substituting (9) into (36), we obtain

$$(\mathrm{rot}\,\overline{\mathbf{\Omega}})_{\alpha\beta} = \mathrm{dg}\left(\frac{\partial \mathbf{D}^{-1}}{\partial \mu_\beta}\frac{\partial \mathbf{D}}{\partial \mu_\alpha} - \frac{\partial \mathbf{D}^{-1}}{\partial \mu_\alpha}\frac{\partial \mathbf{D}}{\partial \mu_\beta} \right) \neq 0.$$

(We recall that the operator dg eliminates off-diagonal matrix components.) Since $\mathbf{D}$ is unitary, it is easy to obtain

$$(\mathrm{rot}\,\overline{\mathbf{\Omega}})_{\alpha\beta} = \mathrm{diag}\left(\frac{\partial \mathbf{D}^*}{\partial \mu_\beta}\frac{\partial \mathbf{D}}{\partial \mu_\alpha} - \frac{\partial \mathbf{D}^*}{\partial \mu_\alpha}\frac{\partial \mathbf{D}}{\partial \mu_\beta} \right) = 2i\,\mathrm{Im}\left(\mathrm{diag}\left(\frac{\partial \mathbf{D}^*}{\partial \mu_\beta}\frac{\partial \mathbf{D}}{\partial \mu_\alpha} \right) \right) \neq 0.$$

Thus, the nonpotential component of the field (9) can only be imaginary, which infers that the solutions can possess a geometric phase, but never an amplitude.

The lemma has been proven.

The set of systems (1) with the matrix $\mathbf{A} = \mathbf{D}\mathbf{\Lambda}\mathbf{D}^{-1}$, *where* $\mathbf{D} = \mathbf{D}(\overline{\mu})$ *is an arbitrary complex unitary matrix, while* $\mathbf{\Lambda} = \mathbf{\Lambda}(\overline{\mu})$ *is an arbitrary complex diagonal matrix, forms the subset* $\mathrm{M}_1 \subset \mathrm{M}$.

The subset M_1 contains, in particular, the subsets of systems (1) with Hermitian, anti-Hermitian, and unitary matrices $\mathbf{A}(\overline{\mu})$. The subset of systems with anti-Hermitian matrices apparently is the subset K_1 described above of oscillatory Hamiltonian systems in the canonical variables.

VIII. CONCLUSIONS

In the paper we considered a linear dynamic system of the general kind, which is described by the complex vector equation with a nondegenerate matrix possessing different eigenvalues. The system matrix is assumed to depend on a set of parameters varying adiabatically. The principal results reported in this paper are as follows.

(1) Adiabatic solutions (8), (11), (14), (20) have been constructed that demonstrate the presence, in the general case of geometric phases and amplitudes.

(2) The geometric terms have been shown to be as important system characteristics as the eigenvalues. Together they determine the qualitative portrait of the system (effective eigenvalues), being invariant with respect to the local coordinate substitutions.

(3) The necessary and sufficient conditions (22) for construction of an adiabatic invariant for one degree of freedom have been formulated. They are the absence of a geometric amplitude and a zero value for the real part of the current eigenvalue of the given degree of freedom.

(4) We analyzed the condition for the existence Poincaré's integral invariants in the system and fulfilment of the Liouville theorem. The Poincaré's first integral invariant is shown to be equivalent, in the adiabatic approximation, to the complete set of n adiabatic invariants. In other words, the conditions for its existence are an oscillatory nature of the system and zero values for all geometric amplitudes. At the same time, the conditions of the Liouville theorem (23), generally speaking, permit the presence of geometric amplitudes in the system (an example of the physical system satisfying the Liouville theorem and containing geometric amplitudes may be the ''beam–plasma system.'' [7]

(5) The main results of this paper can be viewed as the following equivalence relationships. For oscillatory systems in the adiabatic approximation, the equivalence has been shown of classes of systems without geometric amplitudes, Hamiltonian systems, quantizable systems, and strongly stable systems (Theorems I–III):

$$\begin{pmatrix}\text{systems without}\\ \text{geometric amplitudes}\end{pmatrix}\approx\begin{pmatrix}\text{Hamiltonian}\\ \text{systems}\end{pmatrix}\approx\begin{pmatrix}\text{quantizable}\\ \text{systems}\end{pmatrix}\approx\begin{pmatrix}\text{strongly stable}\\ \text{systems}\end{pmatrix}.$$

It might be interesting to compare the equivalence of Hamiltonian and strongly stable systems with the known theorems on strong stability of oscillatory Hamiltonian systems with a time-independent Hamiltonian and with the periodically dependent Hamiltonian.[13,14] The nonlinear counterparts of these theorems are the simplest consequences of the KAM (Kolmogorov–Arnold–Moser) theorem.[12,14] First, the theorems proved in this paper somewhat broaden (in the adiabatic approximation) the class of strongly stable systems to include oscillatory Hamiltonian systems with *an arbitrary* time dependence of parameters. Second, the Hamiltonian nature of systems is not only a sufficient, but also *necessary* condition for the system strong stability in the theorems proved.

(6) Finally, based on the results obtained in this paper, a rather complete classification has been made of the systems without geometric amplitudes from the standpoint of the form of matrix of the initial system. We give a description of the set of all systems without a geometric amplitude, and indicate several subsets that are easily described and may represent special interest.

We have been able to obtain the above results of sufficient generality due to the use of the simplifying assumptions (equation linearity and adiabaticity), as well as to the following important circumstance. Note that the problem of whether a system is Hamiltonian and possesses strong stability was studied many times in the *temporal* statement:

$$\mathbf{x}'=\mathbf{A}(t)\mathbf{x},$$

where the system matrix is an explicit function of time. One can apply to such a problem statement the Birkhoff's remark that in the vicinity of a nonsingular point there should always be coordinate substitution leading the equation up to the trivial Hamiltonian system.[18] We, however, considered the problem of evolution of a nonautonomous system in the *functional* statement: the matrix of the system (1) is time dependent via arbitrary parameter functions $\mathbf{A}=\mathbf{A}(\bar{\mu}(t))$.[19] Note that in the physical problems this statement is more natural. For the system matrix, the difference between the temporal and functional problem statement is not important, since it is simply a composite function of time. However, this circumstance plays an important role when we deal with coordinate substitutions. In the temporal statement all substitutions are simply functions of time, and thus they belong to the same class. Yet, in the functional problem statement the coordinate substitutions are functional of parameters $\bar{\mu}$, which allows us to distinguish between local (the functional is a function of the current value of $\bar{\mu}$) and integral substitutions (the substitution is an integral functional of $\bar{\mu}$ containing the system's prior history) (Appendix B). It is only the local substitutions that leave the eigenvalues and geometric terms invariant. Consequently, if we intend to transform the system without distorting its global qualitative portrait, we must restrict ourselves to

the local variable substitutions. In such a functional problem statement the Birkhoff result does not hold: His proposed substitution may be nonlocal. Therefore the problem of determination of whether a system is Hamiltonian in the vicinity of a nonsingular point becomes nontrivial.

We defined a set of the Hamiltonian systems in the considered approximation, making essential use of the functionality of the problem statement in the proofs of all the theorems.

Our objective in this work is to describe adequately the linear adiabatic systems mainly from the standpoint of mathematical physics. At the same time, we would rather have our attention focused as well on the geometric amplitude in oscillatory systems as a possible physical phenomenon. The linear oscillatory physical systems may be described by equations of a non-Hamiltonian kind and contain geometric amplitudes that promote the development of a geometric instability in the system.[7] In case this phenomenon is discovered in real systems, the geometric amplitude may play an important role due to its unusual properties, which makes it natural to continue the studies in this area. It is hoped that this paper will facilitate the search for systems with geometric amplitude, and if they are discovered, it will help to describe their behavior.

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APPENDIX A: LIMITS OF VALIDITY FOR ADIABATIC SOLUTIONS

By employing the technique of consecutive Neistadt diagonalization, as proposed in Sec. II, we obtain the solutions of Eq. (1) after kth diagonalization in the form of

$$\mathbf{x}(t)=\left(\sum_{j=1}^{k}\mathbf{D}^{(i)}(t)+O_1(\varepsilon^k)\right)\exp\left\{\int_0^t\left(\sum_{j=1}^{k}\mathbf{\Lambda}^{(j)}(\tau)+O_2(\varepsilon^k)\right)d\tau\right\}\mathbf{y}^{(k)}(0), \tag{A1}$$

where $\mathbf{y^{(k)}}(0)$ is the initial conditions vector in the kth basis, the matrices $\mathbf{D}^{(j)}$, and diagonal matrices $\mathbf{\Lambda}^{(j)}$ are proportional to ε^{j-1}, while the correction terms $O(\varepsilon^k)$ are written in a form that provide for inductive transition $k\to k+1$. Here consecutive approximations of the factor before the exponent in (37) correspond to the basis corrections as the solution eigenvectors rotate. The diagonal matrices $\mathbf{\Lambda}^{(j)}$ in the exponent approximate the effective eigenvalues of the solution. The properties of the asymptotic solution (A1), strict conditions of the series convergence and estimation of their residual terms can be found in the standard courses on asymptotic methods,[8] while here we will do simple qualitative estimations.

Comparing the formula (A1) with the substitutions (3), (5) and solutions (8), it is easy to see the correspondence:

$$\mathbf{y^{(1)}}\equiv\mathbf{y},\quad \mathbf{y^{(2)}}\equiv\tilde{\mathbf{y}},\quad \mathbf{D^{(1)}}\equiv\mathbf{D},\quad \mathbf{D^{(2)}}\equiv\mathbf{\Delta},\quad \mathbf{\Lambda^{(1)}}\equiv\mathbf{\Lambda},\quad \mathbf{\Lambda^{(2)}}\equiv\overline{\mathbf{\Omega}}\overline{\mu'},$$

and write the adiabatic solutions used in the article as

$$\mathbf{x}(t)=\left(\sum_{j=1}^{2}\mathbf{D^{(j)}}(t)+O_1(\varepsilon^2)\right)\exp\left\{\int_0^t\left(\sum_{j=1}^{2}\mathbf{\Lambda^{(j)}}(\tau)+O_2(\varepsilon^2)\right)d\tau\right\}\mathbf{y^{(2)}}(0). \tag{A2}$$

At the same time, the transition from the $\tilde{\mathbf{y}}$ coordinates to $\mathbf{z}$ coordinates in Sec. III is associated with ambiguity of the diagonalization matrix choice $\mathbf{D^{(1)}}\equiv\mathbf{D}$. It is simply a choice of the certain most convenient matrix $\mathbf{D^{(1)}}$.

Due to the terms $O_2(\varepsilon^2)$ in the time integral, the solutions (A2) are applicable in the time intervals $t\ll t_{\max}=\varepsilon^{-2}$. At that, the considered in this paper small values $\mathbf{\Lambda}^{(2)}$ are integrated over time and can largely determine the value $\mathbf{x}(t)$ only in the range $t\geqslant t_{\min}=\varepsilon^{-1}$.

Let us now derive the conditions, under which one can neglect the terms $O_1(\varepsilon^2)$. We will consider first the most important for the geometric amplitude effect case of an oscillatory system, i.e., $\mathrm{Re}\,\mathbf{\Lambda^{(1)}}=0$.

In the absence of the geometric amplitude the solutions (A2) are bounded (their Lyapunov indices being zero in the adiabatic approximation) and small corrections to the rotation of solution eigenvectors are insignificant, i.e., the contribution of the values $O_1(\varepsilon^2)$ and even $\mathbf{D^{(2)}}$ to the solutions is small at all times $t \ll t_{\max}$. When the geometric amplitude is present, various solutions (A2) may grow exponentially with time at various growth rates on the order ε. The system is said to have an exponential solution splitting.[20] In this case, even a small error in the projections of solution eigenvectors may result in a large error in the solution. In this case, the condition, under which one can neglect the terms $O_1(\varepsilon^2)$, will be $t \ll t_{\max 1}=\varepsilon^{-1}\ln\varepsilon^{-1}$. Note that $t_{\min} \ll t_{\max 1} \ll t_{\max}$.

If the system has the exponential splitting even in the zero approximation: $\mathrm{Re}\,\mathbf{\Lambda}^{(1)} \neq 0$, then, similarly, the small corrections defining projections of eigenvectors will be essential. The condition, under which one can neglect the terms $O_1(\varepsilon^2)$ is $t \ll t_{\max 2}=\ln\varepsilon^{-1}$. Here $t_{\max 2} \ll t_{\min}$, i.e., within these limits of validity the eigenvalue corrections $\mathbf{\Lambda}^{(2)}$ always provide a small contribution to the solutions. In order to derive the solutions applicable in the time range $t \sim t_{\min}$ and usable for the geometric amplitude research, one has to take into account the eigenvector rotations $\mathbf{D^{(k)}}$ up to $k > \varepsilon^{-1}/\ln\varepsilon^{-1}$. Yet, if one assumes that $\tilde{\mathbf{y}} \equiv \mathbf{y^{(k)}}$ in Eq. (6) and below, then all conclusions of this paper remain true, because the values of the geometric terms in the kth basis are still determined only by the matrix $\mathbf{D^{(1)}}$.

APPENDIX B: NOTE ON THE COORDINATE SUBSTITUTIONS CONSIDERED

Throughout this paper [except for the substitution (33)] we consider *local* linear coordinate substitutions, whose transition matrix depends only on the *current* parameter values and their derivatives. The point is that the set of systems associated with such substitutions can be considered to be qualitatively equivalent.

Contrary to local substitutions, let us consider *integral* ones, which contain information about *prior* parameter values and their derivatives. Substitutions of the kind

$$\tilde{y}_j \to \tilde{y}_j \exp\left(\int_0^t f_j(\overline{\mu}(\varepsilon\tau))d\tau \right), \tag{B1}$$

are equivalent to a change of the current eigenvalues of the system: $\lambda_j \to \lambda_j - f_j$. While substitutions of the kind

$$\tilde{y}_j \to \tilde{y}_j \exp\left(\int_l \overline{g}_j(\overline{\mu})d\overline{\mu} \right), \tag{B2}$$

where $\overline{g}_j(\overline{\mu})$ is the nonpotential field, are equivalent to a change of the geometric terms: $\overline{\omega}_j^{(c)} \to \overline{\omega}_j^{(c)} - \overline{g}_j$ [see solutions (14)]. As shown in Sec. II, with the current eigenvalues and geometric terms determine the qualitative portrait of the system. In particular, using the integral substitutions (B1) and (B2) with $f_j=\lambda_j$, $\overline{g}_j=\overline{\omega}_j^{(c)}$, we can always reduce the system, in the adiabatic approximation, to its trivial form: $\tilde{y}_j'=0$.

Note that local variable substitutions correspond to correction of the current basis, and it is obvious that they cannot change the eigenvalues and geometric phases and amplitudes. For this reason, we can say that the systems connected by local substitutions are equivalent qualitatively.

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Planar Dirac electron in Coulomb and magnetic fields: A Bethe ansatz approach

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The Dirac equation for an electron in two spatial dimensions in the Coulomb and homogeneous magnetic fields is an example of the so-called quasi-exactly solvable models. The solvable parts of its spectrum were previously solved from the recursion relations. In this work we present a purely algebraic solution based on the Bethe ansatz equations. It is realized that, unlike the corresponding problems in the Schrödinger and the Klein–Gordon cases, here the unknown parameters to be solved for in the Bethe ansatz equations include not only the roots of the wave function assumed, but also a parameter from the relevant operator. We also show that the quasi-exactly solvable differential equation does not belong to the classes based on the algebra sl_2. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Recently a new type of spectral problem, the so-called quasi-exactly solvable model (QESM), was discovered by physicists and mathematicians.[1–8] This is a special class of quantum-mechanical problems for which analytical solutions are possible only for parts of the energy spectra and for particular values of the fundamental parameters. The reason for such quasi-exactly solvability is usually the existence of a hidden Lie-algebraic structure.[2–6] More precisely, a quasi-exactly solvable (QES) Hamiltonian can be reduced to a quadratic combination of the generators of a Lie group with finite-dimensional representations.

The first physical example of QESM in atomic physics is the system of two electrons moving in an external oscillator potential discussed in Refs. 9 and 10. The authors of these works apparently were unaware of the mathematical development in QESM. Later, several physical QESMs were discovered, which include the two-dimensional Schrödinger,[11] the Klein–Gordon,[12] and the Dirac equations[13] of an electron moving in an attractive/repulsive Coulomb field and a homogeneous magnetic field. The essential features shared by all these above examples are as follows. The differential equations are solved according to the standard procedure. After separating out the asymptotic behaviors of the system, one obtains an equation for the part which can be expanded as a power series of the basic variable. But instead of the two-step recursion relations for the coefficients of power series so often encountered in exactly solvable problems, one gets three-step recursion relations. The complexity of the recursion relations does not allow one to determine the energy spectrum exactly from the normalizability of the eigenfunctions. However, one can impose a sufficient condition for normalizability by terminating the series at a certain order of power of the variable; i.e., by choosing a polynomial. By doing so one could obtain exact solutions to the original problem, but only for certain energies and for specific values of the parameters of the problem. These parameters, namely, are the frequency of the oscillator potential and the external magnetic fields.

In Ref. 14 a systematic and unified algebraic treatment was given to the above-mentioned systems, with the exception of the Dirac case. This was made possible by realizing that these

systems are governed essentially by the same basic equation, which is quasi-exactly solvable owing to the existence of a hidden sl_2 algebraic structure. This algebraic structure was first realized by Turbiner for the case of two electrons in an oscillator potential.[15] In this algebraic approach, analytic expressions of the solvable parts of the energy spectrum and the allowed parameters were expressible in terms of the roots of a set of Bethe ansatz equations.

In this article we would like to extend the method of Ref. 14 to the planar Dirac equation of an electron in the Coulomb and magnetic fields. It turns out that a set of Bethe ansatz equations can also be set up in this case. However, unlike the systems considered in Ref. 14, here the unknown variables in the Bethe ansatz equations involved not only the roots of the wave functions assumed, but also a parameter from the relevant operator. We also demonstrate that the Bethe ansatz approach yields the same spectrum as that obtained by solving recursion relations. Finally, we show that the quasi-exactly solvability of this system is not related to the sl_2 algebra.

II. THE DIRAC EQUATION

In $2+1$ dimensions the Dirac algebra

$$\{\gamma^\mu,\gamma^\nu\}=2g^{\mu\nu},\quad g^{\mu\nu}=\mathrm{diag}(1,-1,-1) \tag{1}$$

may be represented in terms of the Pauli matrices as $\gamma^0=\sigma_3$, $\gamma^k=i\sigma_k$ or, equivalently, the matrices $(\alpha_1,\alpha_2)=\gamma^0(\gamma^1,\gamma^2)=(-\sigma_2,\sigma_1)$ and $\beta=\gamma^0$. Then the Dirac equation for an electron minimally coupled to an external electromagnetic field has the form (we set $c=\hbar=1$)

$$(i\partial_t-H_D)\Psi(t,\mathbf{r})=0, \tag{2}$$

where

$$H_D=\alpha\mathbf{P}+\beta m-eA^0\equiv\sigma_1P_2-\sigma_2P_1+\sigma_3m-eA^0 \tag{3}$$

is the Dirac Hamiltonian, $P_k=-i\partial_k+eA_k$ is the operator of generalized momentum of the electron, A_μ is the vector potential of the external electromagnetic field, m is the rest mass of the electron, and $-e$ $(e>0)$ is its electric charge. The Dirac wave function $\Psi(t,\mathbf{r})$ is a two-component function. In an external Coulomb field and a constant homogeneous magnetic field $B>0$ along the z direction, the potential A_μ assumes the following forms in the symmetric gauge

$$A^0(r)=Ze/r\ \ (e>0),\quad A_x=-By/2,\quad A_y=Bx/2. \tag{4}$$

We assume the wave functions to have the form

$$\Psi(t,\mathbf{x})=\frac{1}{\sqrt{r}}\exp(-iEt)\,\psi_l(r,\varphi), \tag{5}$$

where E is the energy of the electron, and

$$\psi_l(r,\varphi)=\begin{pmatrix}F(r)e^{il\varphi}\\ G(r)e^{i(l+1)\varphi}\end{pmatrix} \tag{6}$$

with integral number l. The function $\psi_l(r,\varphi)$ is an eigenfunction of the conserved total angular momentum $J_z=L_z+S_z=-i\partial/\partial\varphi+\sigma_3/2$ with eigenvalue $j=l+\frac{1}{2}$. It should be reminded that l is not a good quantum number. Only the eigenvalues j of the conserved total angular momentum J_z are physically meaningful.

By putting Eqs. (5) and (6) into (2), and taking into account the equations

$$P_x\pm iP_y=-ie^{\pm i\varphi}\left(\frac{\partial}{\partial r}\pm\left(\frac{i}{r}\frac{\partial}{\partial\varphi}-\frac{eBr}{2}\right)\right), \tag{7}$$

we obtain

$$\frac{dF}{dr}-\left(l+\frac{1}{2}+\frac{eBr}{2}\right)F+\left(E+m+\frac{Z\alpha}{r}\right)G=0, \tag{8}$$

$$\frac{dG}{dr}+\left(l+\frac{1}{2}+\frac{eBr}{2}\right)G-\left(E-m+\frac{Z\alpha}{r}\right)F=0, \tag{9}$$

where $\alpha\equiv e^2=\frac{1}{137}$ is the fine structure constant. In a strong magnetic field the asymptotic solutions of $F(r)$ and $G(r)$ have the forms $\exp(-eBr^2/4)$ at large r, and r^{γ} with $\gamma=\sqrt{(l+1/2)^2-(Z\alpha)^2}$ for small r. One must have $Z\alpha<\frac{1}{2}$, otherwise the wave function will oscillate as $r\to 0$ when $l=0$ and $l=-1$.

Let us assume

$$F(r)=r^{\gamma}\exp(-eBr^2/4)Q(r),\quad G(r)=r^{\gamma}\exp(-eBr^2/4)P(r). \tag{10}$$

In Ref. 13 we showed that parts of the spectrum could be analytically solved for by imposing the sufficient condition that $Q(r)$ and $P(r)$ be polynomials, thus showing that the system belongs to the QESM. The spectrum was solved in Ref. 13 from the recursion relations for the coefficients in the series expansion in Q and P. In this article, we will show that the same spectrum can also be obtained in a purely algebraic way. This is achieved by the method of factorization which leads to a set of Bethe ansatz equations.[13,14]

Substituting Eq. (10) into Eqs. (8) and (9) and eliminating $P(r)$ from the coupled equations, we have

$$\left\{\frac{d^2}{dr^2}+\left[\frac{2\gamma}{r}-eBr+\frac{Z\alpha/r^2}{E+m+Z\alpha/r}\right]\frac{d}{dr}+E^2-m^2+\frac{2EZ\alpha}{r}+\frac{l+\frac{1}{2}}{r^2}-\frac{\gamma}{r^2}-eB(\Gamma+1)\right.$$
$$\left.+\frac{Z\alpha/r^2}{E+m+Z\alpha/r}\left[\frac{\gamma}{r}-eBr-\frac{l+\frac{1}{2}}{r}\right]\right\}\ Q(r)=0, \tag{11}$$

where $\Gamma=l+\frac{1}{2}+\gamma$. Once $Q(r)$ is solved, the form of $P(r)$ is obtainable from Eqs. (8) and (10). If we let $x=r/l_B$, $l_B=1/\sqrt{eB}$, Eq. (11) becomes

$$\left\{\frac{d^2}{dx^2}+\left[\frac{2\gamma}{x}-x+\frac{Z\alpha}{x((E+m)l_Bx+Z\alpha)}\right]\frac{d}{dx}+(E^2-m^2)l_B^2+\frac{2EZl_B\alpha}{x}+\frac{(l+\frac{1}{2}-\gamma)}{x^2}-(\Gamma+1)\right.$$
$$\left.-\frac{Z\alpha(l+\frac{1}{2}-\gamma)}{x^2[(E+m)l_Bx+Z\alpha]}-\frac{Z\alpha}{(E+m)l_Bx+Z\alpha}\right\}\ Q(x)=0. \tag{12}$$

Equation (12) can be rewritten as

$$\left\{\frac{d^2}{dx^2}+\left[\frac{2\beta}{x}-x-\frac{1}{x+x_0}\right]\frac{d}{dx}+\epsilon+\frac{b}{x}-\frac{c}{x+x_0}\right\}\ Q(x)=0. \tag{13}$$

Here $\beta=\gamma+\frac{1}{2}$, $x_0=Z\alpha/[(E+m)l_B]$, $\epsilon=(E^2-m^2)l_B^2-(\Gamma+1)$, $b=b_0+L/x_0$, $b_0=2EZ\alpha l_B$, $L=(l+\frac{1}{2}-\gamma)$, and $c=x_0+L/x_0$. On expressing l_B in the expression of ϵ in terms of x_0, we get

$$\epsilon=\frac{E-m}{E+m}\left(\frac{Z\alpha}{x_0}\right)^2-(\Gamma+1). \tag{14}$$

It is obvious that the energy E is determined once we know the values of ϵ and x_0. The corresponding value of the magnetic field B is then obtainable from the expression $l_B = Z\alpha/[(E+m)x_0]$. Solution of x_0 is achieved below by means of the Bethe ansatz equations.

III. THE BETHE ANSATZ EQUATIONS FOR $Q(x)$

We observe that the problem of finding the spectrum for Eq. (13) is equivalent to determining the eigenvalues of the operator

$$D = -\frac{d^2}{dx^2} - \left(\frac{2\beta}{x} - x - \frac{1}{x+x_0}\right)\frac{d}{dx} - \frac{b}{x} + \frac{c}{x+x_0}. \tag{15}$$

We want to factorize the operator (15) in the form

$$D = a^+ a + \epsilon. \tag{16}$$

The eigenfunctions of the operator D at $\epsilon = 0$ must satisfy the equation

$$aQ(x) = 0. \tag{17}$$

Suppose polynomial solutions exist for Eq. (13), say Q equals a nonvanishing constant, or $Q = \Pi_{k=1}^{n}(x - x_k)$, where x_k are the zeros of Q, and n is the degree of Q. In the case where Q is a constant (which may be viewed as corresponding to $n = 0$), the operators a and a^+ have the form

$$a = \frac{d}{dx}, \quad a^+ = -\frac{d}{dx} - \left(\frac{2\beta}{x} - x - \frac{1}{x+x_0}\right). \tag{18}$$

If $Q = \Pi_{k=1}^{n}(x - x_k)$, a and a^+ will assume the form

$$a = \frac{d}{dx} - \sum_{k=1}^{n} \frac{1}{x - x_k} \tag{19}$$

and

$$a^+ = -\frac{d}{dx} - \left(\frac{2\beta}{x} - x - \frac{1}{x+x_0}\right) - \sum_{k=1}^{n} \frac{1}{x - x_k}. \tag{20}$$

We now substitute the forms of a and a^+ into Eq. (16) and compare the result with Eq. (15). This leads to conditions that must be satisfied by the various parameters and the roots x_k's. For constant $Q\,(n = 0)$, one has

$$\epsilon = b = c = 0. \tag{21}$$

The fact that $c = 0$ implies

$$x_0^2 = -L. \tag{22}$$

For $n \geqslant 1$, one gets

$$b_0 + \frac{L}{x_0} = 2\beta \sum_{k=1}^{n} \frac{1}{x_k}, \quad \epsilon = n, \tag{23}$$

$$x_0 + \frac{L}{x_0} = \sum_{k=1}^{n} \frac{1}{x_k + x_0}, \tag{24}$$

$$\frac{2\beta}{x_k}-x_k-\frac{1}{x_k+x_0}-2\sum_{j\neq k}^{n}\frac{1}{x_j-x_k}=0,\quad k=1,\ldots,n. \tag{25}$$

Equations (22), (24), and (25) constitute the set of $n+1$ Bethe ansatz equations relevant to this Dirac system, which involve $n+1$ unknown parameters $\{x_0,x_1,\ldots,x_n\}$. It is worthwhile to note that, unlike the corresponding equations in the Schrödinger and the Klein–Gordon cases discussed in Ref. 14, this set of Bethe ansatz equations involved not only the roots x_k, but also a parameter x_0 from D. Summing Eq. (25) over k leads to the expression $b_0=x_0+\Sigma_{k=1}^{n}x_k$, i.e., b_0 is simply the sum of all the roots of the Bethe ansatz equations. From the second equation in Eq. (23) we get

$$E^2-m^2=\frac{1}{l_B^2}(\Gamma+n+1). \tag{26}$$

Since $-\frac{1}{2}\leqslant\Gamma\leqslant 0$ for $Z\alpha<\frac{1}{2}$,[13] we see from Eq. (26) that the solvable parts of the spectrum must satisfy $|E|\geqslant m$.

So we see that the solution of the solvable parts of the spectrum E boils down to solving the Bethe ansatz equations for x_0 in the differential operator, and the roots $x_k(k=1,\ldots,n)$ of $Q(x)$. Once the value of x_0 for each order $n=\epsilon$ is known, the energy E is given by Eq. (14). The corresponding magnetic field B is then determined from the definition of b_0, or from Eq. (26). The Bethe ansatz equations thus provide a systematic solutions of the QES spectrum. Of course, as the order of the degree of Q increases, analytical solutions of the Bethe ansatz equations becomes difficult, and one must resort to numerical methods.

IV. SOLUTIONS FOR $n=0,1$, and 2

In what follows we shall show the consistency of the solutions by the Bethe ansatz approach and that by the recursion relations presented in Ref. 13 for the first three lowest orders ($n=0,1,2$) in Q. Instead of solving for x_0, our strategy is to eliminate it in Eq. (14) by means of Eqs. (22)–(25) so as to obtain an equation obeyed by E for each order of Q. This equation is then compared with the corresponding equation obtained from the recursion relations as presented in Ref. 13.

From Eqs. (21) and (22) we have $x_0^2=-L$ and $\epsilon=0$ when Q is a constant. Substitute these values of x_0 and ϵ into Eq. (14), and using the fact that $\Gamma L=(Z\alpha)^2$, we obtain the corresponding value of E as

$$E=-\frac{m}{2(l+\gamma+1)}. \tag{27}$$

This is the result presented in Ref. 13. The corresponding allowed value of the magnetic field B is then obtained from Eqs. (26) and (27). The fact that x_0 is real leads to $L<0$, which in turn implies that the energy levels given by Eq. (27) are only possible for $l<0$. This is consistent with the conclusion obtained by the method of recursion relations.[13]

For $n=1$, we find from Eqs. (14), (23), (24), and (25) that

$$\Gamma+2=\frac{E-m}{E+m}\frac{(Z\alpha)^2}{x_0^2}, \tag{28}$$

$$b_0+\frac{L}{x_0}=\frac{2\beta}{x_1}, \tag{29}$$

$$\frac{1}{x_1+x_0}=x_0+\frac{L}{x_0}, \tag{30}$$

$$\frac{2\beta}{x_1}-x_1-\frac{1}{x_1+x_0}=0. \tag{31}$$

Equations (29)–(31) imply $x_1=b_0-x_0$. Substituting x_1 into Eq. (30), we obtain

$$x_0^2=L\left[\frac{E+m}{2E(Z\alpha)^2}-1\right]^{-1}. \tag{32}$$

Then from Eqs. (32) and (28), we get

$$\left[4(\Gamma+1)-\frac{\Gamma}{Z^2\alpha^2}\right]E^2+4Em+\frac{\Gamma}{(Z\alpha)^2}m^2=0. \tag{33}$$

The energy E can be solved from Eq. (33) by the standard formula, after which the magnetic field is determined from Eq. (26). Equation (33) does not resemble the one obtained from the recursion relation in Ref. 13. However, on multiplying Eq. (33) by $\Gamma+1$ and making use of the fact that $(Z\alpha)^2=\Gamma(\Gamma-2\gamma)$, we can show, after some algebra, that Eq. (33) is equivalent to the corresponding equation given in Ref. 13.

Finally we consider the case for $n=2$. We have Eq. (14) with $\epsilon=2$, together with Eqs. (23)–(25) in the forms

$$\Gamma+3=\frac{E-m}{E+m}\frac{(Z\alpha)^2}{x_0^2}, \tag{34}$$

$$b_0+\frac{L}{x_0}=\frac{2\beta}{x_1}+\frac{2\beta}{x_2}, \tag{35}$$

$$\frac{1}{x_1+x_0}+\frac{1}{x_2+x_0}=x_0+\frac{L}{x_0}, \tag{36}$$

$$\frac{2\beta}{x_1}-x_1-\frac{1}{x_1+x_0}-\frac{2}{x_2-x_1}=0, \tag{37}$$

$$\frac{2\beta}{x_2}-x_2-\frac{1}{x_2+x_0}-\frac{2}{x_1-x_2}=0. \tag{38}$$

From these equations we find $x_1+x_2=b_0-x_0$ and $x_1x_2=2\beta x_0(b_0-x_0)/(b_0x_0+L)$. Putting these expressions into Eq. (36) and using the fact that $\Gamma=2\beta+L-1$, we arrive at

$$(b_0^2-2\beta)x_0^2+b_0\Gamma x_0+[b_0^2(L-1)-L(2\beta+1)]+\frac{b_0\Gamma L}{x_0}=0. \tag{39}$$

Now multiplying Eq. (39) by Γ, using $\Gamma L=(Z\alpha)^2$, and expressing b_0, l_B, and $1/x_0^2$ in terms of E, we get finally

$$\left\{4(2\Gamma+3)-\frac{1}{(Z\alpha)^2}\left[6\Gamma+2(\gamma+1)+\frac{(2\gamma+1)\Gamma}{\Gamma+3}\right]\right\}\ E^3$$
$$+\left\{12-\frac{1}{(Z\alpha)^2}\left[2(\gamma+1)-\frac{(2\gamma+1)\Gamma}{\Gamma+3}\right]\right\}\ E^2m$$
$$+\frac{1}{(Z\alpha)^2}\left[6\Gamma+2(\gamma+1)+\frac{(2\gamma+1)\Gamma}{\Gamma+3}\right]Em^2+\frac{1}{(Z\alpha)^2}\left[2(\gamma+1)-\frac{(2\gamma+1)\Gamma}{\Gamma+3}\right]m^3=0. \tag{40}$$

Again, this equation does not look the same as that obtained from the recursion relations. But we can show they are in fact equivalent as they differ only by a multiplicative factor $(\Gamma+1)(\Gamma+2)$.

V. THE BETHE ANSATZ EQUATIONS FOR $P(x)$

One may as well solve the QES energy spectrum of the problem from the differential equation of $P(x)$ instead of $Q(x)$. The analysis proceeds in exactly the same way as we did for $Q(x)$. We shall only give the outline below in order to show the similarity and differences between the two sets of Bethe ansatz equations.

The equation for $P(x)$ can be cast into the following form:

$$\left\{\frac{d^2}{dx^2}+\left[\frac{2\beta}{x}-x-\frac{1}{x+x_0'}\right]\frac{d}{dx}+\epsilon'+\frac{b'}{x}-\frac{c'}{x+x_0'}\right\}\ P(x)=0. \tag{41}$$

Here $x_0'=Z\alpha/[(E-m)l_B]$, $\epsilon'=(E^2-m^2)l_B^2-\Gamma$, $b'=b_0+c'$, and $c'=-\Gamma/x_0'$. Other parameters are as defined previously. Instead of Eq. (14) we now have

$$\epsilon'=\frac{E+m}{E-m}\left(\frac{Z\alpha}{x_0'}\right)^2-\Gamma. \tag{42}$$

We note here the sign difference before the mass terms in Eqs. (14) and (42). It is obvious that Eq. (41) is in the same form as Eq. (13), and hence is also quasi-exactly solvable. Suppose $P(x)$ has the factorized form $P(x)=\Pi_{k=1}^{n'}(x-x_k')$. Then the set of Bethe ansatz equations for the parameters $\{x_0',x_1',\ldots,x_{n'}'\}$ is given by

$$-\frac{\Gamma}{x_0'}=\sum_{k=1}^{n'}\frac{1}{x_k'+x_0'}, \tag{43}$$

$$\frac{2\beta}{x_k'}-x_k'-\frac{1}{x_k'+x_0'}-2\sum_{j\neq k}^{n'}\frac{1}{x_j'-x_k'}=0,\quad k=1,\ldots,n'. \tag{44}$$

In place of Eq. (23) we have

$$b_0-\frac{\Gamma}{x_0'}=2\beta\sum_{k=1}^{n'}\frac{1}{x_k'},$$

$$\epsilon'=n',\quad n'=1,2.\ldots \tag{45}$$

Summing Eq. (44) over k gives $b_0=\Sigma_{k=1}^{n'}x_k'$. For any given integral value of $\epsilon'=n'$ the QES part of the energy E is determined from Eq. (42) once the values of x_0' are obtained from the Bethe ansatz equations. The corresponding value of the magnetic field B is then obtainable from the expression $l_B=Z\alpha/[(E-m)x_0']$.

We note here that since the two sets of Bethe ansatz Eqs. (22), (24) and (25), and (43) and (44) give the same spectrum of the QES energy E and the corresponding B, we have, from the values of ϵ, ϵ' and b_0, the following necessary conditions:

$$n'=n+1, \tag{46}$$

$$b_0=x_0+\sum_{k=1}^{n}x_k=\sum_{k=1}^{n+1}x_k'. \tag{47}$$

Conversely, one can easily show that Eqs. (46) and (47) are also the sufficient conditions for the two sets of Bethe ansatz equations to give the same QES energy spectrum and magnetic field. The condition (46) implies that the degree of the polynomial $P(x)$ is of one order higher than that of $Q(x)$, which is in complete agreement with the result obtained in Ref. 13.

VI. NON-sl_2-BASED QUASI-EXACTLY SOLVABILITY

We now demonstrate that the QES Eqs. (13) and (41) cannot be represented as a bilinear combination of the generators of the sl_2 algebra. The question of whether there exists non-sl_2-based one-dimensional QESM was first posed in Ref. 2 in which all sl_2-based QESM are classified. The first example of such a kind was given in Ref. 16, which presents a potential arising in the context of the stability analysis around the kink solution for ϕ^4-type field theory in $1+1$ dimensions.

We shall show that Eq. (13) is not generated by the sl_2 algebra. The same conclusion applies immediately to Eq. (41), since both equations have the same form. Let us rewrite Eq. (13) as

$$\left\{-(x^2+x_0x)\frac{d^2}{dx^2}+[x^3+x_0x^2+(1-2\beta)x-2\beta x_0]\frac{d}{dx}-\epsilon x^2+(c-b-\epsilon x_0)x-bx_0\right\}Q(x)=0. \tag{48}$$

Turbiner[2] has shown that all sl_2-based second order QES differential equations can be cast into the form

$$-P_4(x)\frac{d^2Q}{dx^2}+P_3(x)\frac{dQ}{dx}+(P_2(x)-\lambda)Q=0, \tag{49}$$

where

$$\begin{aligned}P_4(x)&=a_{++}x^4+a_{+0}x^3+(a_{+-}+a_{00})x^2+a_{0-}x+a_{--},\\ P_3(x)&=2(2j-1)a_{++}x^3+[(3j-1)a_{+0}+b_+]x^2+[2j(a_{+-}+a_{00})+a_{00}+b_0]x+ja_{0-}+b_-,\\ P_2(x)&=2j(2j-1)a_{++}x^2+2j(ja_{+0}+b_+)x+a_{00}j^2+b_0j.\end{aligned} \tag{50}$$

Here a_{kl}'s and b_k's $(k,l=+,0,-)$ are constants, and j is a non-negative integer or half-integer. Equation (49) corresponds to the eigenvalue problem

$$HQ=\lambda Q, \quad H=-\sum_{\substack{k,l=+,0,-\\ k\geqslant l}}a_{kl}J^kJ^l+\sum_{k=+,0,-}b_kJ^k, \tag{51}$$

which has a polynomial solution of power $2j$ in x. Here J^k's are the generators of sl_2:

$$J^+ = x^2 \frac{d}{dx} - 2jx, \quad J^0 = x \frac{d}{dx} - j, \quad J^- = \frac{d}{dx}. \tag{52}$$

Comparing Eqs. (48) and (49) we find that the two equations are inconsistent with each other. For instance, the coefficient of x^4 in P_4 requires $a_{++} = 0$, whereas the coefficient of x^3 in P_3 implies $2(2j-1)a_{++} = 1$, which gives a nonvanishing a_{++} for positive integral and half-integral values of j. This shows that Eq. (13) is not sl_2-based.

VII. CONCLUSIONS

In conclusion, we have given an algebraic solution to the planar Dirac equation of an electron in the Coulomb and magnetic fields. The relevant Bethe ansatz equations are presented. Unlike the corresponding equations in the Schrödinger and the Klein-Gordon case discussed in Ref. 14, the unknown variables in this set of Bethe ansatz equations include not only the roots of the polynomial assumed, but also a parameter from the QES differential operator. Equivalence between this approach and that by the recursion relations is demonstrated. Finally, we show that the QES equation for this problem does not belong to any of the classes based on the sl_2 algebra.

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Noncommuting limits in homogenization theory of electromagnetic crystals

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We study the homogeneous properties of metallic 2D photonic crystals. We give a rigorous proof that the limits when the ratio period over wavelength tends to zero and the conductivity tends to infinity do not commute. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1418013]

I. INTRODUCTION

This article concerns the homogenization of 2D dielectric photonic crystals and the fact that the limits $k\to 0$ (k is the Bloch vector) and $\varepsilon\to+\infty$ do not commute for p-polarized waves (it is not the case for s-polarized waves, which is a straightforward case). This result has been claimed by Nicorovici *et al.* in a series of papers[1–3] and it has been claimed to be false by Krokhin *et al.* in a comment.[4] The point of this article is to make the situation clear once and for all, that is, to give a mathematically clean derivation of the result by Nicorovici and to prove that it is right.

II. HOMOGENIZATION RESULT

Rather than letting the Bloch vector tend to zero, we use the following homogenization scheme: We deal with a finite-size photonic crystal, contained in a bounded domain Ω, with period η (the period is a contracted cell ηY, where $Y=[0,1[^2$ and θ is the filling ratio in Y, see Fig. 1 for notations) and a fixed wavenumber k_0 in which case for an incident field u^i the total field u_η satisfies in p-polarization: $\mathrm{div}(\varepsilon_\eta^{-1}\nabla u_\eta)+k_0^2 u_\eta=0$ and $u_\eta-u^i$ satisfies a radiation condition. Function ε_η is defined by

$$\varepsilon_\eta=\begin{cases}\varepsilon\left(\dfrac{x}{\eta}\right) & \text{in } \Omega,\\ 1 & \text{in } \mathbb{R}^2\backslash\Omega,\end{cases}$$

where $y\in Y\to\varepsilon(y)$ represents the relative permittivity inside the basic cell. It is extended to $\mathbb{R}^2$ by periodization. The relative permittivity of one rod is equal to ε_s and the rest of the cell has relative permittivity ε_Ω. We study the limit of u_η when $\eta\to 0$.

It is known that by standard homogenization theory[5,6] u_η tends, in $L^2_{\mathrm{loc}}(\mathbb{R}^2)$, to u_0 satisfying $\mathrm{div}(\varepsilon_{\mathrm{hom}}^{-1}\nabla u_0)+k_0^2 u_0=0$ where

$$\varepsilon_{\mathrm{hom}}^{-1}=\begin{pmatrix}(1-\theta)\varepsilon_\Omega^{-1}+\theta\varepsilon_s^{-1}+\phi_{11}^{\varepsilon_s} & \phi_{12}^{\varepsilon_s}\\ \phi_{21}^{\varepsilon_s} & (1-\theta)\varepsilon_\Omega^{-1}+\theta\varepsilon_s^{-1}+\phi_{22}^{\varepsilon_s}\end{pmatrix}$$

in Ω and $(\varepsilon_{\mathrm{hom}})^{-1}=1$ in $\mathbb{R}^2\backslash\Omega$. The matrix $(\phi_{ij}^{\varepsilon_s})$ is defined in Ref. 5. If we let ε_s formally tend to infinity we get

$$\varepsilon_{\mathrm{hom}}^{-1}\to\begin{pmatrix}(1-\theta)\varepsilon_\Omega^{-1}+\phi_{11}^{\infty} & \phi_{12}^{\infty}\\ \phi_{21}^{\infty} & (1-\theta)\varepsilon_\Omega^{-1}+\phi_{22}^{\infty}\end{pmatrix}, \tag{1}$$

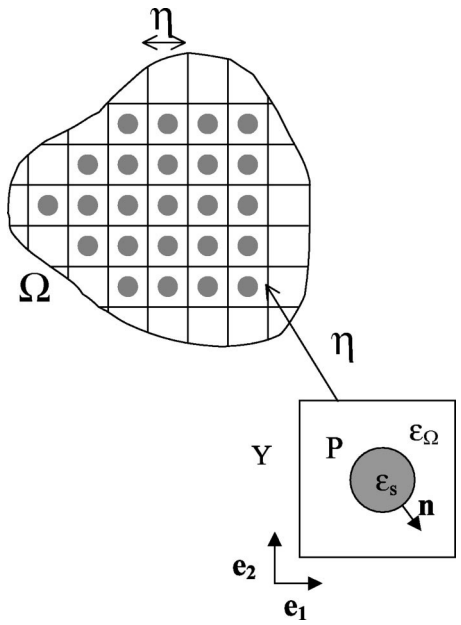

FIG. 1. Sketch of the homogenization problem.

where $\phi_{ij}^{\infty}=\langle \partial w_j/\partial y_i \rangle_Y$, w_j being the unique Y-periodic solution, with null mean, of the following problem

$$\begin{aligned} \Delta w_j &= 0 \quad \text{in } Y\backslash P, \\ \frac{\partial w_j}{\partial n} &= -\mathbf{n}.\mathbf{e_j} \quad \text{on } \partial P, \end{aligned} \tag{2}$$

and $\langle . \rangle_Y$ denotes averaging over Y. For convenience, w_j is extended by 0 on P.

Now let us deal directly with the infinitely conducting crystal; the set of rods is denoted T_η. At step η, the field satisfies $\mathrm{div}(\varepsilon_\eta^{-1}\nabla u_\eta)+k_0^2 u_\eta=0$ in the complementary of the rods with

$$\varepsilon_\eta = \begin{cases} \varepsilon_\Omega \text{ in } \Omega\backslash T_\eta, \\ 1 \text{ in } \mathbb{R}^2\backslash\Omega, \end{cases}$$

and $\partial u_\eta/\partial n=0$ on ∂T_η. Our result is the following.

Theorem: *When* η *tends to* 0, u_η *tends in* L^2_{loc} *to* u_0 *satisfying* $\mathrm{div}(\varepsilon_\infty^{-1}\nabla u_0)+k_0^2 u_0=0$ *in* $\Omega\backslash\partial\Omega$ *where*

$$\begin{aligned} \varepsilon_\infty^{-1} &= \frac{1}{1-\theta}\begin{pmatrix} (1-\theta)\varepsilon_\Omega^{-1}+\phi_{11}^{\infty} & \phi_{12}^{\infty} \\ \phi_{21}^{\infty} & (1-\theta)\varepsilon_\Omega^{-1}+\phi_{22}^{\infty} \end{pmatrix} \quad \text{in } \Omega \\ &= 1 \quad \text{outside } \Omega, \end{aligned}$$

and the following transmission conditions hold on the boundary of $\partial\Omega$:

$$u_0^- = (1-\theta)u_0^+,$$

$$(\varepsilon_\infty^{-1}\nabla u_0^-).\mathbf{n} = \nabla u_0^+.\mathbf{n}.$$

A simple comparison with (1) leads to the following evident conclusion.

Corollary: The limits $\eta\to 0$ *and* $\varepsilon_s\to+\infty$ *do not commute.*

Proof: Step 1: We assume that (u_η) is bounded in $L^2(\Omega)$.

The field u_η is null inside the rods but we can define a function $\tilde{u}_\eta$ such that $u_\eta=\tilde{u}_\eta$ outside T_η and $\tilde{u}_\eta$ belongs to the Sobolev space $H^1_{\mathrm{loc}}(\mathbb{R}^2)$ (see Ref. 6 for a proof), so that $(1-1_{T_\eta})\tilde{u}_\eta=u_\eta$ and $(\tilde{u}_\eta)$ is bounded in $H^1(\Omega)$. Using now a test function ϕ in the Schwartz space $\mathcal{D}(\Omega)$, we find

$$-\int_\Omega 1_{\Omega_\eta}\nabla\tilde{u}_\eta\nabla\phi\, d^2x+k_0^2\varepsilon_\Omega\int_\Omega(1-1_{T_\eta})\tilde{u}_\eta\phi\, d^2x=0.$$

By Rellich–Kondratov theorem, we deduce that up to the extraction of a subsequence we have the following points:

(1) $\tilde{u}_\eta\to\tilde{u}_0$ strongly in $L^2(\Omega)$,
(2) $u_0=(1-1_\Omega\theta)\tilde{u}_0$,
(3) $\chi_\eta=1_{\Omega_\eta}\nabla\tilde{u}_\eta\rightharpoonup\chi_0$ weakly in $L^2(\Omega)$,

so that

$$-\int_\Omega\chi_0\nabla\phi d^2x+k_0^2\int_\Omega u_0\phi\, d^2x=0$$

or equivalently $\mathrm{div}(\chi_0)+k_0^2u_0=0$. We then have to find an expression for χ_0. We set $w_i=w_\eta+x_i$, where $w_\eta=\eta w(x/\eta)$ [note that $w_i\overset{L^2}{\rightharpoonup}x_i$ strongly in $L^2(\Omega)$]. We have

$$\begin{aligned}0&=\int_\Omega[-1_{\Omega_\eta}\nabla\tilde{u}_\eta\nabla(\phi w_i)+k_0^2u_\eta\phi w_i]d^2x\\&=-\int_\Omega\chi_\eta\nabla\phi w_i d^2x+\int_\Omega\nabla\phi\nabla w_i\tilde{u}_\eta d^2x+k_0^2\int_\Omega u_\eta\phi w_i d^2x.\end{aligned}$$

Then letting η tend to 0 in the last expression, we obtain

$$\int_\Omega[-\chi_0x_i+\langle\nabla w_i\rangle_Y.\mathbf{e}_i\tilde{u}_0]\nabla\phi d^2x+k_0^2\int_\Omega u_0\phi x_i d^2x=0.$$

This shows that $\chi_0.\mathbf{e}_i=(\langle\nabla w\rangle_Y+(1-\theta)\mathbf{e}_i).\nabla\tilde{u}_0$ from which we get the following equation, valid in $\mathbb{R}^2$,

$$\mathrm{div}(\varepsilon_\infty^{-1}\nabla\tilde{u}_0)+k_0^2u_0=0.$$

It implies that the following transmission conditions hold on the boundary of Ω:

(1) $u_0^-=(1-\theta)u_0^+$.
(2) $(\varepsilon_{\mathrm{hom}}^{-1}\nabla u_0^-).\mathbf{n}=\nabla u_0^+.\mathbf{n}$.

Step 2: Assuming that the hypothesis of step 1 is false, there is a subsequence, still denoted (u_n), such that $\|u_n\|_\Omega$ diverges to infinity. Let us then deal with the same scattering problem, but with incident field $u^i/\|u_n\|_\Omega$. We can apply the above result to the rescaled field $u_n/\|u_n\|_\Omega$. The uniqueness of the limit problem implies that $\lim_{\eta\to0}u_n/\|u_n\|_\Omega=0$ and a contradiction. The theorem and corollary follow.

A numerical discussion of the theorem and of the unusual transmission conditions is given in Ref. 7.

As a conclusion, we might suggest that a clear mathematical approach should make it possible to avoid any polemical discussion over these issues.

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Covariant geometric quantization of nonrelativistic time-dependent mechanics

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We provide geometric quantization of the vertical cotangent bundle $V^*Q\to Q\to\mathbf{R}$, equipped with the canonical Poisson structure and treated as a momentum phase space of nonrelativistic time-dependent mechanics. We show that this quantization is equivalent to fiberwise quantization of symplectic fibers of $V^*Q\to\mathbf{R}$ and that the quantum algebra of time-dependent mechanics is an instantwise algebra. Quantization of the classical evolution equation defines a connection on this instantwise algebra and describes quantum evolution in time-dependent mechanics as a parallel transport. © *2002 American Institute of Physics.*
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I. INTRODUCTION

We study the covariant (frame-independent) geometric quantization of nonrelativistic mechanics, subject to time-dependent transformations. Its configuration space is a fiber bundle $Q\to\mathbf{R}$ equipped with bundle coordinates (t,q^k), $k=1,\ldots,m$, where t is a fixed Cartesian coordinate on the time axis $\mathbf{R}$. The corresponding momentum phase space is the vertical cotangent bundle V^*Q of $Q\to\mathbf{R}$.[1,2] It is endowed with holonomic bundle coordinates (t,q^k,p_k), subject to time-dependent transition functions

$$q'^k=q'^k(t,q^i),\quad p'_k=\frac{\partial q^j(t,q'^i)}{\partial q'^k}p_j. \tag{1}$$

Of course, all fiber bundles over $\mathbf{R}$ are trivial, but different trivializations,

$$Q\cong\mathbf{R}\times M,\quad V^*Q\cong\mathbf{R}\times T^*M, \tag{2}$$

correspond to different nonrelativistic reference frames. Given such a trivialization, the associated bundle coordinates on V^*Q have time-independent transition functions.

In contrast with the existent quantizations of nonrelativistic mechanics,[3,4] we do not fix a trivialization (2). The key point is that, in this case, the evolution equation is not reduced to the Poisson bracket on V^*Q, but can be expressed into the Poisson bracket on the cotangent bundle T^*Q of Q.[5] Therefore, covariant geometric quantization of time-dependent mechanics on a configuration bundle $Q\to\mathbf{R}$ requires compatible geometric quantization both of the cotangent bundle T^*Q and the vertical cotangent bundle V^*Q of Q.

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The cotangent bundle T^*Q plays the role of the homogeneous momentum phase space of time-dependent mechanics. It is provided with holonomic coordinates $(q^0=t,q^k,p_0=p,p_k)$, where the fiber coordinate p has the affine transformation law

$$p'=p+\frac{\partial q^k(t,q'^i)}{\partial t}p_k. \tag{3}$$

The cotangent bundle T^*Q is equipped with the canonical Liouville form $\Xi=p_\lambda dq^\lambda$, the canonical symplectic form $\Omega=d\Xi$, and the corresponding Poisson bracket

$$\{f,f'\}_T=\partial^\lambda f\partial_\lambda f'-\partial_\lambda f\partial^\lambda f', \quad f,f'\in C^\infty(T^*Q).$$

There is the canonical one-dimensional affine fiber bundle

$$\zeta: T^*Q\to V^*Q, \tag{4}$$

whose kernel is the annihilator of the vertical tangent bundle $VQ\subset TQ$. The fibration (4) provides the vertical cotangent bundle V^*Q with the canonical Poisson structure $\{,\}_V$ such that

$$\zeta^*\{f,f'\}_V=\{\zeta^*f,\zeta^*f'\}_T, \tag{5}$$

$$\{f,f'\}_V=\partial^k f\partial_k f'-\partial_k f\partial^k f', \tag{6}$$

for all $f,f'\in C^\infty(V^*Q)$.[1,6] The corresponding symplectic foliation coincides with the fibration $V^*Q\to\mathbf{R}$.

The relation (5) defines the monomorphism of Poisson algebras

$$\zeta^*:(C^\infty(V^*Q),\{,\}_V)\to(C^\infty(T^*Q),\{,\}_T). \tag{7}$$

Therefore, a compatibility of geometric quantizations of T^*Q and V^*Q implies that this monomorphism is prolonged to a monomorphism of quantum algebras of V^*Q and T^*Q.

Of course, it seems natural to quantize $C^\infty(V^*Q)$ as a subalgebra (7) of the Poisson algebra $C^\infty(T^*Q)$. However, geometric quantization of the Poisson algebra $(C^\infty(T^*Q),\{,\}_T)$ need not imply that of its Poisson subalgebra $\zeta^*C^\infty(V^*Q)$.

Recall that geometric quantization of a symplectic manifold $(Z,\Omega,\{,\})$ provides a representation

$$\pi: f\to i\hat{f}, \quad [\hat{f},\hat{f}']=-i\widehat{\{f,f'\}}, \tag{8}$$

of a certain subalgebra $\mathcal{A}$ of the Poisson algebra $C^\infty(Z)$ by Hermitian operators $\hat{f}$ in a Hilbert space. The geometric quantization procedure falls into three steps: prequantization, polarization and metaplectic correction.[3,4,7] The first one associates to each element f of the Poisson algebra $C^\infty(Z)$ a first order differential operator $\hat{f}$ on sections of a complex line bundle $C\to Z$ such that the Dirac condition (8) holds. Polarization of a symplectic manifold (Z,Ω) is defined as a maximal (regular) involutive distribution $\mathbf{T}\subset TZ$ on Z such that

$$\Omega(u,v)=0, \quad \forall u,v\in\mathbf{T}_z, \quad z\in Z. \tag{9}$$

Given the Lie algebra $\mathbf{T}(Z)$ of $\mathbf{T}$-subordinate vector fields on Z, let $\mathcal{A}\subset C^\infty(Z)$ be the subalgebra of functions f whose Hamiltonian vector fields u_f fulfill the condition

$$[u_f,\mathbf{T}(Z)]\subset\mathbf{T}(Z).$$

Only elements of this algebra are quantized. After metaplectic correction, the quantum algebra $\mathcal{A}$ is represented by operators in a certain subspace of sections of the tensor product $C\otimes\mathcal{D}_{1/2}$ of the prequantization line bundle $C\to Z$ and the fiber bundle $\mathcal{D}_{1/2}\to Z$ of complex half-forms on Z. We will also appeal to geometric quantization of Poisson manifolds.[6,8]

We show that the standard prequantization of the cotangent bundle T^*Q yields the compatible prequantization of the Poisson manifold V^*Q such that the monomorphism ζ^* (7) is prolonged to a monomorphism of prequantum algebras. However, polarization of T^*Q need not induce any polarization of V^*Q, unless it contains the vertical cotangent bundle $V_\zeta T^*Q$ of the fiber bundle ζ (4) spanned by vectors ∂^0 (see Sec. III). A unique canonical real polarization of T^*Q, satisfying the above condition

$$V_\zeta T^*Q\subset\mathbf{T}, \tag{10}$$

is the vertical tangent bundle VT^*Q of $T^*Q\to Q$. The associated quantum algebra $\mathcal{A}_T$ consists of functions on T^*Q which are affine in momenta p_λ. We show that this vertical polarization of T^*Q yields the polarization of the Poisson manifold V^*Q such that the corresponding quantum algebra $\mathcal{A}_V$ consists of functions on V^*Q which are affine in momenta p_k. It follows that $\mathcal{A}_V$ is a subalgebra of $\mathcal{A}_T$ under the monomorphism (7). After metaplectic correction, the compatible Schrödinger representations of $\mathcal{A}_T$ and $\mathcal{A}_V$ by operators on complex half-forms on Q are obtained.

The physical relevance of the Schrödinger quantization of T^*Q, however, is open to question. The scalar product of half-forms on Q implies integration over time, though the time plays the role of a classical evolution parameter in quantum mechanics, based on Schrödinger and Heisenberg equations. At the same time, the Schrödinger quantization of V^*Q provides instantwise quantization of nonrelativistic mechanics. Indeed, a glance at the Poisson bracket (6) shows that the Poisson algebra $C^\infty(V^*Q)$ is a Lie algebra over the ring $C^\infty(\mathbf{R})$ of functions of time alone, where algebraic operations, in fact, are instantwise operations depending on time as a parameter. We show that the Schrödinger quantization of the Poisson manifold V^*Q induces geometric quantization of its symplectic fibers V_t^*Q, $t\in\mathbf{R}$, such that the quantum algebra $\mathcal{A}_t$ of V_t^*Q consists of elements $f\in\mathcal{A}_V$ restricted to V_t^*Q. This agrees with the instantwise quantization of symplectic fibers $\{t\}\times T^*M$ of the direct product (2) in Ref. 3. Moreover, the induced geometric quantization of fibers V_t^*Q, by construction, is determined by their injection to V^*Q, but not projection of V^*Q. Therefore, it is independent of a trivialization (2), and defines frame-independent instantwise quantization of nonrelativistic mechanics.

Turn now to quantization of the evolution equation in time-dependent mechanics. The problem is that the Poisson structure (6) fails to provide any dynamic equation on the momentum phase space V^*Q because all Hamiltonian vector fields

$$u_f=\partial^k f\partial_k-\partial_k f\partial^k,\quad u_f\rfloor df'=\{f,f'\}_V,\quad \forall f'\in C^\infty(V^*Q),$$

for functions f on V^*Q are vertical. Hamiltonian dynamics of time-dependent mechanics is described in a different way as a particular Hamiltonian dynamics on fiber bundles.[9,10]

A Hamiltonian on the momentum phase space $V^*Q\to\mathbf{R}$ of time-dependent mechanics is defined as a global section

$$h:V^*Q\to T^*Q,\quad p\circ h=-\mathcal{H}(t,q^j,p_j), \tag{11}$$

of the affine bundle ζ (4).[1,2] Of course, it is not an element of the Poisson algebra $C^\infty(V^*Q)$. Every Hamiltonian h (11) yields the pull-back Hamiltonian form

$$H=h^*\Xi=p_k dq^k-\mathcal{H}dt \tag{12}$$

on V^*Q. Given a trivialization (2), the form H is the well-known integral invariant of Poincaré–Cartan, where $\mathcal{H}$ is a familiar (frame-dependent) Hamiltonian. For any Hamiltonian form H (12), there exists a unique vector field γ_H on V^*Q such that $\gamma_H\rfloor dt=1$ and

$$\gamma_H \rfloor dH = 0. \tag{13}$$

This vector field defines the Hamilton equations on V^*Q.

Let us consider the Lie derivative

$$\mathbf{L}_{\gamma_H} f = \gamma_H \rfloor df \tag{14}$$

of a function $f \in C^\infty(V^*Q)$ along γ_H. It is the evolution equation in time-dependent Hamiltonian mechanics. If $\mathbf{L}_{\gamma_H} f = 0$, a function f is constant on a solution of the Hamilton equations. Given a trivialization (2), the evolution equation (14) can be written as

$$\mathbf{L}_{\gamma_H} f = \partial_t f + \{\mathcal{H}, f\}_V.$$

However, taken separately, the terms on its right-hand side are ill-behaved under time-dependent transformations. In order to express the evolution equation into a Poisson bracket, let us consider the pull-back $\zeta^* H$ of the Hamiltonian form $H = h^* \Xi$ onto the cotangent bundle T^*Q. It is readily observed that the difference $\Xi - \zeta^* h^* \Xi$ is a horizontal one-form on $T^*Q \to \mathbf{R}$ and that

$$\mathcal{H}^* = \partial_t \rfloor (\Xi - \zeta^* h^* \Xi) = p + \mathcal{H} \tag{15}$$

is a function on T^*Q which we agree to call a covariant (frame-independent) Hamiltonian. Then the evolution equation (14) is brought into the form

$$\zeta^*(\mathbf{L}_{\gamma_H} f) = \{\mathcal{H}^*, \zeta^* f\}_T, \tag{16}$$

adapted for quantization.

The problem is that the covariant Hamiltonian $\mathcal{H}^*$ (15) does not belong to the algebra $\mathcal{A}_T$, unless it is affine in momenta. Let us assume that $\mathcal{H}^*$ is a polynomial of momenta. This is the case of all physical models. Then one can show (see Sec. V) that $\mathcal{H}^*$ can be represented by a finite sum of products of elements of $\mathcal{A}_T$, though this representation by no means is unique. Thereby, it can be quantized as an element of the enveloping algebra $\overline{\mathcal{A}}_T$ of the Lie algebra $\mathcal{A}_T$.

Remark 1: An ambiguity of the operator representation of a classical Hamiltonian is a well-known technical problem of Schrödinger quantization as well as any geometric quantization scheme, where a Hamiltonian does not preserve a polarization (see Ref. 3 for a general, but rather sophisticated, analysis of such Hamiltonians). One can include the covariant Hamiltonian $\mathcal{H}^*$ (15) in a quantum algebra by choosing polarization of T^*Q which contains the Hamiltonian vector field of $\mathcal{H}^*$. This polarization always exists, but does not satisfy the condition (10) and, therefore, does not define any polarization of the Poisson manifold V^*Q (see Sec. VI). Note that, given a trivialization (2), symplectic fibers V_t^*Q, $t \in \mathbf{R}$, of the Poisson bundle $V^*Q \to \mathbf{R}$ can be provided with the instantwise polarization spanned by vectors

$$(\partial_1 \mathcal{H} \partial^1 - \partial^1 \mathcal{H} \partial_1, \ldots, \partial_m \mathcal{H} \partial^m - \partial^m \mathcal{H} \partial_m).$$

However, this polarization need not be regular and, by construction, is frame-dependent. It is a standard polarization in conservative Hamiltonian mechanics of one-dimensional systems, but it requires an exclusive analysis of each physical model.

Given a covariant Hamiltonian $\mathcal{H}^*$ (15) and its representative $\overline{\mathcal{H}}^*$ in $\overline{\mathcal{A}}_T$, the map

$$\nabla : f \to \{\overline{\mathcal{H}}^*, f\}_T$$

is a derivation of the enveloping algebra $\overline{\mathcal{A}}_V \subset \overline{\mathcal{A}}_T$ of the Lie algebra $\mathcal{A}_V$. Moreover, this derivation obeys the Leibniz rule

$$\nabla(rf) = \partial_t r f + r \nabla f, \quad \forall r \in C^\infty(\mathbf{R}),$$

and, consequently, is a connection on the instantwise algebra $\overline{\mathcal{A}}_V$.[11] This property is preserved under quantization. Therefore, the quantized evolution equation describes quantum evolution in nonrelativistic mechanics as a parallel transport along time. The corresponding evolution operator is constructed. It is different for different reference frames.

II. PREQUANTIZATION

We start from the standard prequantization of the cotangent bundle T^*Q.[3,4,7] Since the symplectic form Ω on T^*Q is exact and, consequently, belongs to the zero de Rham cohomology class, a prequantization bundle is the trivial complex line bundle

$$C=T^*Q\times\mathbf{C}\to T^*Q \tag{17}$$

of zero Chern class. Coordinated by (q^λ,p_λ,c), this bundle is provided with the admissible linear connection

$$A=dp_\lambda\otimes\partial^\lambda+dq^\lambda\otimes(\partial_\lambda+ip_\lambda c\partial_c) \tag{18}$$

whose strength form equals $i\Omega$. The A-invariant Hermitian fiber metric on $C\to Q$ is $g(c,c)=c\overline{c}$. The covariant derivative of sections s of the prequantization bundle C (17) relative to the connection A (18) along the vector field u on T^*Q reads

$$\nabla_u s=u^\lambda(\partial_\lambda-ip_\lambda)s+u_\lambda\partial^\lambda s. \tag{19}$$

Given a function $f\in C^\infty(T^*Q)$ and its Hamiltonian vector field

$$u_f=\partial^\lambda f\partial_\lambda-\partial_\lambda f\partial^\lambda,\quad u_f\rfloor\Omega=-df,$$

the covariant derivative (19) along u_f is

$$\nabla_{u_f}s=\partial^\lambda f(\partial_\lambda-ip_\lambda)s-\partial_\lambda f\partial^\lambda s.$$

Then, in order to satisfy the Dirac condition (8), one assigns to each function $f\in C^\infty(T^*Q)$ the first order differential operator

$$\hat{f}(s)=-i(\nabla_{u_f}+if)s=[-i(\partial^\lambda f\partial_\lambda-\partial_\lambda f\partial^\lambda)+(f-p_\lambda\partial^\lambda f)]s \tag{20}$$

on sections s of the prequantization bundle C (17). The prequantum operators (20) for elements f of the Poisson subalgebra $\zeta^*C^\infty(V^*Q)\subset C^\infty(T^*Q)$ read

$$\hat{f}(s)=[-i(\partial^k f\partial_k-\partial_\lambda f\partial^\lambda)+(f-p_k\partial^k f)]s. \tag{21}$$

Turn now to prequantization of the Poisson manifold $(V^*Q,\{,\}_V)$. The Poisson bivector w of the Poisson structure (6) on V^*Q is

$$w=\partial^k\wedge\partial_k=-[w,\vartheta]_{\mathrm{SN}}, \tag{22}$$

where $[,]_{\mathrm{SN}}$ is the Schouten–Nijenhuis bracket and $\vartheta=p_k\partial^k$ is the Liouville vector field on the vertical cotangent bundle $V^*Q\to Q$. The relation (22) shows that the Poisson bivector w is exact and, consequently, has the zero Lichnerowicz–Poisson cohomology class.[1,6] Therefore, let us consider the trivial complex line bundle

$$C_V=V^*Q\times\mathbf{C}\to V^*Q \tag{23}$$

of zero Chern class. Since the line bundles C (17) and C_V (23) are trivial, C can be seen as the pull-back ζ^*C_V of C_V, while C_V is isomorphic to the pull-back h^*C of C with respect to a

section h (11) of the affine bundle (4). Since $C_V=h^*C$ and since the covariant derivative of the connection A (18) along the fibers of ζ (4) is trivial, let us consider the pull-back

$$h^*A=dp_k\otimes\partial^k+dq^k\otimes(\partial_k+ip_kc\partial_c)+dt\otimes(\partial_t-i\mathcal{H}c\partial_c) \tag{24}$$

of the connection A (18) onto $C_V\to V^*Q$.[11] This connection defines the contravariant derivative

$$\nabla_\phi s_V=\nabla_{w^\sharp\phi}s_V \tag{25}$$

of sections s_V of $C_V\to V^*Q$ along one-forms ϕ on V^*Q. This contravariant derivative corresponds to a contravariant connection A_V on the line bundle $C_V\to V^*Q$.[6] Since the vector fields $w^\sharp\phi=\phi^k\partial_k-\phi_k\partial^k$ are vertical on $V^*Q\to\mathbf{R}$, this contravariant connection does not depend on the choice of a section h. By virtue of the relation (25), the curvature bivector of A_V is equal to iw,[12] i.e., A_V is an admissible connection for the Poisson structure on V^*Q. Then the Kostant-Souriau formula

$$\begin{gathered}\hat f(s_V)=(-i\nabla_{u_f}+f)s_V=[-i(\partial^kf\partial_k-\partial_kf\partial^k)+(f-p_k\partial^kf)]s_V,\\ u_f=w^\sharp df=\partial^kf\partial_k-\partial_kf\partial^k,\end{gathered} \tag{26}$$

defines prequantization of the Poisson manifold V^*Q. In particular, the prequantum operators of functions $r\in C^\infty(\mathbf{R})$ of time alone are reduced to multiplication $\hat r s_V=rs_V$. Consequently, the prequantum algebra of V^*Q inherits the structure of a $C^\infty(\mathbf{R})$-algebra.

It is immediately observed that the prequantum operator $\hat f$ (26) coincides with the prequantum operator $\widehat{\zeta^*f}$ (21) restricted to the pull-back sections $s=\zeta^*s_V$. Thus, the above prequantization of the Poisson algebra $C^\infty(V^*Q)$ is equivalent to its prequantization as a subalgebra of the Poisson algebra $C^\infty(T^*Q)$.

Note that, since the complex line bundles C (17) and C_V (23) are trivial, their sections are simply smooth complex functions on T^*Q and V^*Q, respectively. Then the prequantum operators (20) and (26) can be written in the form

$$\hat f=-i\mathbf{L}_{u_f}+(f-\mathbf{L}_\vartheta f), \tag{27}$$

where ϑ denotes the Liouville vector field on $T^*Q\to Q$ or $V^*Q\to Q$, respectively.

III. QUANTIZATION

Given compatible prequantizations of the cotangent bundle T^*Q and the vertical cotangent bundle V^*Q, let us now construct their compatible polarizations and quantizations. We assume that Q is an oriented manifold and that the cohomology group $H^2(Q,\mathbf{Z}_2)$ is trivial.

Recall that polarization of a Poisson manifold $(Z,\{,\})$ is defined as a sheaf $\mathbf{T}^*$ of germs of complex functions on Z whose stalks $\mathbf{T}^*_z$, $z\in Z$, are Abelian algebras with respect to the Poisson bracket $\{,\}$.[12] Let $\mathbf{T}^*(Z)$ be the structure algebra of global sections of the sheaf $\mathbf{T}^*$; it is also called a Poisson polarization.[6,8] A quantum algebra $\mathcal{A}$ associated to the Poisson polarization $\mathbf{T}^*$ is defined as a subalgebra of the Poisson algebra $C^\infty(Z)$ which consists of functions f such that

$$\{f,\mathbf{T}^*(Z)\}\subset\mathbf{T}^*(Z).$$

Polarization of a symplectic manifold yields its Poisson one.

Let $\mathbf{T}^*$ be a polarization of the Poisson manifold $(T^*Q,\{,\}_T)$. Its direct image in V^*Q with respect to the fibration ζ (4) is polarization of the Poisson manifold $(V^*Q,\{,\}_V)$ if the germs of $\mathbf{T}^*$ are constant along the fibers of ζ,[12] i.e., are germs of functions independent of the momentum coordinate p. It follows that the corresponding symplectic polarization $\mathbf{T}$ of T^*Q is vertical with respect to the fibration $T^*Q\to V^*Q$.

The vertical polarization $\mathbf{T}=VT^*Q$ of T^*Q obeys this condition. The associated quantum algebra $\mathcal{A}_T \subset C^\infty(T^*Q)$ consists of functions which are affine in momenta p_λ. The algebra $\mathcal{A}_T$ acts by operators (27) on the space of smooth complex functions s on T^*Q which fulfill the relation $\nabla_u s=0$ for any $\mathbf{T}$-valued (i.e., vertical) vector field $u=u_\lambda \partial^\lambda$ on the cotangent bundle $T^*Q\to Q$. Clearly, these functions are the pull-back of complex functions on Q with respect to the fibration $T^*Q\to Q$. Following the general metaplectic technique, we come to complex half-forms on Q which are sections of the complex line bundle $\mathcal{D}_{1/2}\to Q$ with the transition functions $c'=Sc$ such that $S\overline{S}$ is the Jacobian of coordinate transition functions on Q. Then the formula (27), where $\mathbf{L}_{u_f}$ is the Lie derivative of half-forms, defines the Schrödinger representation of the Lie algebra $\mathcal{A}_T$ by operators

$$\hat{f}\rho=(-i\mathbf{L}_{a^\lambda\partial_\lambda}+b)\rho=\left(-ia^\lambda\partial_\lambda-\frac{i}{2}\partial_\lambda a^\lambda+b\right)\rho, \quad f=a^\lambda(q^\mu)p_\lambda+b(q^\mu)\in\mathcal{A}_T, \tag{28}$$

in the space $\mathcal{D}_{1/2}(Q)$ of complex half-forms ρ on Q. From now on, we assume that a coordinate atlas of Q and a bundle atlas of $\mathcal{D}_{1/2}\to Q$ are defined on the same covering of Q, e.g., by contractible open sets. Let $E\subset\mathcal{D}_{1/2}(Q)$ consist of half-forms of compact support, and let $\overline{E}$ be its completion with respect to the nondegenerate Hermitian form

$$\langle\rho|\rho'\rangle=\left(\frac{1}{2\pi}\right)^m\int_Q\rho\overline{\rho'}. \tag{29}$$

The (unbounded) operators (28) on the domain E in the Hilbert space $\overline{E}$ are Hermitian.

The vertical polarization of T^*Q defines the polarization $\mathbf{T}^*_V$ of the Poisson manifold V^*Q which contains the germs of functions, constant on the fibers of $V^*Q\to Q$. The associated quantum algebra $\mathcal{A}_V$ consists of functions on V^*Q which are affine in momenta. It is a $C^\infty(\mathbf{R})$-algebra. This algebra acts by operators (27) on the space of smooth complex functions s_V on V^*Q which fulfill the relation $\nabla_u s_V=0$ for any vertical vector field $u=u_k\partial^k$ on $V^*Q\to Q$. These functions are also the pull-back of complex functions on Q with respect to the fibration $V^*Q\to Q$. Similarly to the case of $\mathcal{A}_T$, we obtain the Schrödinger representation of the Lie algebra $\mathcal{A}_V$ by the operators

$$\hat{f}\rho=(-i\mathbf{L}_{a^k\partial_k}+b)\rho=\left(-ia^k\partial_k-\frac{i}{2}\partial_k a^k+b\right)\rho, \quad f=a^k(q^\mu)p_k+b(q^\mu)\in\mathcal{A}_V, \tag{30}$$

on half-forms on Q and in the above Hilbert space $\overline{E}$. Moreover, a glance at the expressions (28) and (30) shows that (30) is the representation of $\mathcal{A}_V$ as a subalgebra of the Lie algebra $\mathcal{A}_T$.

It should be emphasized that, written in the coordinate form, the operators (28) and (30) are defined independently of the choice of a coordinate chart, and their coordinate expressions (28) and (30) are maintained under coordinate transformations (1) and (3).

IV. INSTANTWISE QUANTIZATION

As was mentioned earlier, the physical relevance of the space of half-forms on Q with the scalar product (29) is open to question. At the same time, the representation (30) preserves the structure of $\mathcal{A}_V$ as a $C^\infty(\mathbf{R})$-algebra. Therefore, let us show that this representation defines the instantwise quantization of $\mathcal{A}_V$.

First, the prequantization (26) of the Poisson manifold V^*Q yields prequantization of its symplectic leaves V^*_tQ, $t\in\mathbf{R}$, as follows. The symplectic structure on V^*_tQ is

$$\Omega_t=(h\circ i_t)^*\Omega=dp_k\wedge dq^k, \tag{31}$$

where h is an arbitrary section of the fiber bundle ζ (4) and $i_t: V^*_t Q \to V^*Q$ is the natural imbedding. Since $w^\sharp \phi$ is a vertical vector field on $V^*Q \to \mathbf{R}$ for any one-form ϕ on V^*Q, the contravariant derivative (25) defines a connection along each fiber $V^*_t Q$, $t \in \mathbf{R}$, of the Poisson bundle $V^*Q \to \mathbf{R}$. It is the pull-back

$$A_t = i_t^* h^* A = dp_k \otimes \partial^k + dq^k \otimes (\partial_k + i p_k c \partial_c)$$

of the connection h^*A (24) onto the trivial pull-back line bundle

$$i_t^* C_V = V^*_t Q \times \mathbf{C} \to V^*_t Q.$$

It is readily observed that this connection is admissible for the symplectic structure (31) on $V^*_t Q$, and provides prequantization of the symplectic manifold $(V^*_t Q, \Omega_t)$ by the formula

$$\hat{f}_t = -i\mathbf{L}_{u_{f_t}} + (f_t - \mathbf{L}_{\vartheta_t}) = -i(\partial^k f_t \partial_k - \partial_k f_t \partial^k) + (f_t - p_k \partial^k f_t), \tag{32}$$

where $u_{f_t} = \partial^k f_t \partial_k - \partial_k f_t \partial^k$ is the Hamiltonian vector field of a function f_t on $V^*_t Q$ with respect to the symplectic form Ω_t (31). The operators (32) act on smooth complex functions s_t on $V^*_t Q$. In particular, let f_t, s_t and $(\hat{f}s)_t$ be the restriction to $V^*_t Q$ of a real function f and complex functions s and $\hat{f}(s)$ on V^*Q, respectively. We obtain from the formulas (26) and (32) that

$$(\hat{f}s)_t = \hat{f}_t s_t .$$

This equality shows that the prequantization (26) of the Poisson manifold V^*Q is a leafwise prequantization.[12]

Let $\mathbf{T}^*_V$ be the above polarization of the Poisson manifold V^*Q. It yields the pull-back polarization $\mathbf{T}^*_t = i_t^* \mathbf{T}^*_V$ of a fiber $V^*_t Q$ with respect to the Poisson morphism $i_t: V^*_t Q \to V^*Q$. The corresponding distribution $\mathbf{T}_t$ coincides with the vertical tangent bundle of the fiber bundle $V^*_t Q \to Q_t$. The associated quantum algebra $\mathcal{A}_t$ consists of functions on V^*Q_t which are affine in momenta. In particular, the restriction to $V^*_t Q$ of any element of the quantum algebra $\mathcal{A}_V$ of V^*Q obeys this condition and, consequently, belongs $\mathcal{A}_t$. Conversely, any element of $\mathcal{A}_t$ is of this type. For instance, using a trivialization (2) and the corresponding surjection $\pi_t: V^*Q \to V^*_t Q$, one can define the pull-back $\pi_t^* f_t$ of a function $f_t \in \mathcal{A}_t$ which belongs to the quantum algebra $\mathcal{A}_V$ and $f_t = i_t^*(\pi_t^* f_t)$. Thus, $\mathcal{A}_t = i^* \mathcal{A}_V$ and, therefore, the polarization $\mathbf{T}^*_V$ of the Poisson bundle $V^*Q \to \mathbf{R}$ is a fiberwise polarization.

To provide metaplectic correction and to complete geometric quantization of symplectic fibers of the Poisson bundle $V^*Q \to \mathbf{R}$, one can use the following fact.

Any atlas $\{(U; t, q^k)\}$ of bundle coordinates on the fiber bundle $Q \to \mathbf{R}$ induces a coordinate atlas $\{(Q_t \cap U; q^k)\}$ of its fiber Q_t, $t \in \mathbf{R}$. Since

$$\det \begin{pmatrix} 1 & \partial_t q'^k \\ 0 & (\partial_i q'^k) \end{pmatrix} = \det(\partial_i q'^k),$$

the Jacobian J of the transition function between coordinate charts $(U; t, q^k)$ and $(U'; t, q'^k)$ on Q coincides with the Jacobian J_t of the transition function between coordinate charts $(Q_t \cap U; q^k)$ and $(Q_t \cap U'; q'^k)$ on Q_t at points of $Q_t \cap U \cap U'$. It follows that, for any fiber Q_t of Q, the pull-back $i_t^* \mathcal{D} \to Q_t$ of the complex line bundle $\mathcal{D} \to Q$ of complex densities on Q with transition functions $c' = Jc$ is the complex line bundle of complex densities on Q_t with transition functions $J_t = J|_{Q_t}$. Accordingly, any density L on Q yields the pull-back section $L_t = L \circ i_t$ of the line bundle $i^* \mathcal{D} \to Q_t$, i.e., L_t is a density on Q_t. The pull-back $L \to L_t$ takes the coordinate form

$$L = \mathcal{L}(t, q^k) d^m q \wedge dt \to L_t = \mathcal{L}(t, q^k) d^m q|_{t=\text{const}} = \mathcal{L}(t, q^k) \overline{d^m} q,$$

where $\{\overline{dq}^k\}$ are holonomic fiber bases for V^*Q. It is maintained under transformations of bundle coordinates on Q.

Let now $\mathcal{D}_{1/2}\to Q$ be a complex line bundle of complex half-forms on Q with transition functions S such that $S\overline{S}=J$ on $U\cap U'$. Its pull-back $i_t^*\mathcal{D}_{1/2}$ is a complex line bundle over a fiber Q_t, $t\in\mathbf{R}$, with transition functions $S_t=S|_{Q_t}$. These transition functions obey the relation

$$S_t\overline{S}_t=J|_{Q_t}=J_t,$$

i.e., $i_t^*\mathcal{D}_{1/2}\to Q_t$ is the fiber bundle of half-forms on Q_t. Then the formula (32) defines the Schrödinger representation of the quantum algebra $\mathcal{A}_t$ of the symplectic fiber Q_t by (unbounded) Hermitian operators

$$\hat{f}_t\rho_t=(-i\mathbf{L}_{a^k\partial_k}+b)\rho_t=\left(-ia^k\partial_k-\frac{i}{2}\partial_k a^k+b\right)\rho_t,\quad f_t=a^k(q^i)p_k+b(q^i)\in\mathcal{A}_t, \tag{33}$$

in the Hilbert space $\overline{E_t}$ which is the completion of the pre-Hilbert space E_t of half-forms on Q_t of compact support with respect to the scalar product

$$\langle\rho_t|\rho_t'\rangle=\left(\frac{1}{2\pi}\right)^m\int_{Q_t}\rho_t\overline{\rho_t'}.$$

If Q_t is compact, the operators (33) in $\overline{E_t}$ are self-adjoint. Pre-Hilbert spaces E_t constitute a trivial bundle E_R over $\mathbf{R}$.

As in the above case of densities, any half-form ρ on Q yields the section $\rho\circ i_t$ of the pull-back bundle $i_t^*\mathcal{D}_{1/2}\to Q_t$, i.e., a half-form on Q_t. Given an element $f\in\mathcal{A}_V$ and its pull-back $f_t=i_t^*f\in\mathcal{A}_t$, we obtain from the formulas (30) and (33) that

$$\hat{f}\rho\circ i_t=\hat{f}_t(\rho\circ i_t).$$

This equality shows that the Schrödinger quantization of the Poisson manifold V^*Q can be seen as the instantwise quantization. Following this interpretation, let us choose the representation space $E_R(\mathbf{R})$ for $\mathcal{A}_V$ which consists of complex half-forms ρ on Q such that, for any $t\in\mathbf{R}$, the half-form $\rho\circ i_t$ on Q_t is of compact support. It is a pre-Hilbert $C^\infty(\mathbf{R})$-module. The $E_R(\mathbf{R})$ is also the carrier space for the Lie algebra $\mathcal{A}_T$, but its action on $E_R(\mathbf{R})$ is not instantwise.

V. THE QUANTUM EVOLUTION EQUATION

Turn now to quantization of the evolution equation (16). As was mentioned earlier, the problem is that, in the framework of the Schrödinger quantization, the covariant Hamiltonian $\mathcal{H}^*$ (15) does not belong to the quantum algebra $\mathcal{A}_T$, unless it is affine in momenta. Let us restrict our consideration to the physically relevant case of $\mathcal{H}^*$, polynomial in momenta. We aim to show that such $\mathcal{H}^*$ is decomposed in a finite sum of products of elements of the algebra $\mathcal{A}_T$.

Let f be a smooth function on T^*Q which is a polynomial of momenta p_λ. A glance at the transformation laws (1) and (3) shows that it is a sum of homogeneous polynomials of fixed degree in momenta. Therefore, it suffices to justify a desired decomposition of an arbitrary homogeneous polynomial F of degree $k>1$ on T^*Q. We use the fact that the cotangent bundle T^*Q admits a finite bundle atlas.[13] Let $\{U_\xi\}$, $\xi=1,\ldots,r$, be the corresponding open cover of Q and $\{f_\xi\}$ a smooth partition of unity subordinate to this cover. Put

$$l_\xi=f_\xi(f_1^k+\cdots+f_r^k)^{-1/k}.$$

It is readily observed that $\{l_\xi^k\}$ is also a partition of unity subordinate to $\{U_i\}$. Let us consider the local polynomials

$$F_\xi = F|_{U_\xi} = \sum_{(\alpha_1 \dots \alpha_k)} a_\xi^{\alpha_1 \dots \alpha_k}(q) p_{\alpha_1} \cdots p_{\alpha_k}, \quad q \in U_\xi.$$

Then we obtain a desired decomposition

$$F = \sum_\xi l_\xi^k F_\xi = \sum_\xi \sum_{(\alpha_1 \dots \alpha_k)} [l_\xi a_\xi^{\alpha_1 \dots \alpha_k} p_{\alpha_1}][l_\xi p_{\alpha_2}] \cdots [l_\xi p_{\alpha_k}], \tag{34}$$

where all terms $l_\xi a_\xi^{\alpha_1 \dots \alpha_k} p_{\alpha_1}$ and $l_\xi p_\alpha$ are smooth functions on T^*Q. Clearly, the decomposition (34) by no means is unique.

The decomposition (34) shows that one can associate to a polynomial covariant Hamiltonian $\mathcal{H}^*$ an element $\overline{\mathcal{H}}^*$ of the enveloping algebra $\overline{\mathcal{A}_T}$ of the Lie algebra $\mathcal{A}_T$. Recall that $\overline{\mathcal{A}}$ consists of finite sums of tensor products of elements of $\mathcal{A}_T$ modulo the relations

$$f \otimes f' - f' \otimes f - \{f, f'\}_T = 0.$$

To be more precise, a representative $\overline{\mathcal{H}}^*$ belongs to $\mathcal{A}_T + \overline{\mathcal{A}_V}$, where $\overline{\mathcal{A}_V}$ is the enveloping algebra of the Lie algebra $\mathcal{A}_V \subset \mathcal{A}_T$ [see the decomposition (42)]. The enveloping algebra $\overline{\mathcal{A}_V}$ is provided with the anti-automorphism

$$*: f_1 \otimes \cdots \otimes f_k \to (-1)^k f_k \otimes \cdots \otimes f_1,$$

and one can always make a representative $\overline{\mathcal{H}}^*$ Hermitian.

Since the Dirac condition (8) holds, the Schrödinger representation of the Lie algebras $\mathcal{A}_T$ and $\mathcal{A}_V$ is naturally extended to their enveloping algebras $\overline{\mathcal{A}_T}$ and $\overline{\mathcal{A}_V}$, and provides the quantization $\hat{\mathcal{H}}^*$ of a covariant Hamiltonian $\mathcal{H}^*$.

Given an operator $\hat{\mathcal{H}}^*$, the bracket

$$\nabla \hat{f} = i[\hat{\mathcal{H}}^*, \hat{f}] \tag{35}$$

defines a derivation of the quantum algebra $\overline{\mathcal{A}_V}$. Moreover, since $\hat{p} = -i\partial_t$, the derivation (35) obeys the Leibniz rule

$$\nabla(r\hat{f}) = \partial_t r \hat{f} + r \nabla \hat{f}, \quad r \in C^\infty(\mathbf{R}).$$

Therefore, it is a connection on the instantwise algebra $\overline{\mathcal{A}_V}$, which enables one to treat quantum evolution of $\overline{\mathcal{A}_V}$ as a parallel transport along time.[11,14] In particular, $\hat{f}$ is parallel with respect to the connection (35) if

$$[\hat{\mathcal{H}}^*, \hat{f}] = 0. \tag{36}$$

One can think of this equality as being the Heisenberg equation in time-dependent mechanics, while the quantum constraint

$$\hat{\mathcal{H}}^* \rho = 0, \quad \rho \in E_R(\mathbf{R}), \tag{37}$$

plays a role of the Schrödinger equation. It is readily observed that an operator $\hat{f}$ is a solution of the Heisenberg equation (36) iff it preserves the subspaces of solutions of the Schrödinger equation (37).

Given a trivialization (2) and the corresponding decomposition of a covariant Hamiltonian

$$\hat{\mathcal{H}}^* = -i\partial_t + \hat{\mathcal{H}}, \tag{38}$$

one can introduce the evolution operator U for the connection (35). It obeys the equation

$$\hat{\mathcal{H}}^* \circ U = -iU \circ \partial_t, \tag{39}$$

and can be written as the formal time-ordered exponent

$$U = T \exp\left[-i\int_0^t \hat{\mathcal{H}}\, dt'\right]. \tag{40}$$

In particular, if an element $\rho_0 \in E_R(\mathbf{R})$ obeys the relation $\partial_t \rho_0 = 0$, then $U\rho_0$ is a solution of the Schrödinger equation (37).

The evolution operator U can be brought into the frame-covariant form as follows. By definition, any connection

$$\Gamma = (dq^k - \Gamma^k dt) \otimes \partial_k$$

on the configuration bundle $Q \to \mathbf{R}$ yields a section

$$h_\Gamma : V^*Q \ni \sigma \to \Gamma \rfloor \sigma = p_k(dq^k - \Gamma^k dt) \in T^*Q, \quad p \circ h_\Gamma = -\mathcal{H}_\Gamma = -p_k\Gamma^k,$$

of the affine bundle (4). Then any Hamiltonian is split as

$$h = h_\Gamma - \mathcal{H}^0_\Gamma, \quad \mathcal{H} = \mathcal{H}_\Gamma + \mathcal{H}^0_\Gamma, \tag{41}$$

where $\mathcal{H}^0_\Gamma$ is a function on V^*Q. The physical meaning of this splitting becomes clear due to the fact that every trivialization (2) of $Q \to \mathbf{R}$ yields a complete connection Γ on $Q \to \mathbf{R}$ such that $\Gamma^k = 0$ relative to the corresponding coordinates, and *vice versa*. It follows that such a connection is associated to a nonrelativistic reference frame.[1,11]

With the splitting (41), we have the corresponding decomposition of classical and quantum covariant Hamiltonians

$$\mathcal{H}^* = \mathcal{H}^*_\Gamma + \mathcal{H}^0_\Gamma, \quad \hat{\mathcal{H}}^* = \hat{\mathcal{H}}^*_\Gamma + \hat{\mathcal{H}}^0_\Gamma, \tag{42}$$

where function $\mathcal{H}^*_\Gamma$ belongs to the algebra $\mathcal{A}_T$. In particular, let Γ be a complete connection associated to some trivialization of the configuration bundle $Q \to \mathbf{R}$. Under this trivialization, the decomposition (42) takes the coordinate form (38) where $\mathcal{H} = \mathcal{H}^0_\Gamma$. Then the equation (39) for the evolution operator is easily brought into the frame-covariant form

$$\hat{\mathcal{H}}^* \circ U_\Gamma = U_\Gamma \circ \hat{\mathcal{H}}^*_\Gamma.$$

One can think of the operator U_Γ in this equation as describing quantum evolution with respect to the reference frame Γ. It can be written as the time-ordered exponent (40) where $\mathcal{H}$ is replaced with $\mathcal{H}^0_\Gamma$.

In particular, let an element $\rho_\Gamma \in E_R(\mathbf{R})$ obey the equation

$$\hat{\mathcal{H}}^*_\Gamma \rho_\Gamma = 0. \tag{43}$$

Then $U_\Gamma \rho_\Gamma$ is a solution of the Schrödinger equation (37). One can think of ρ_Γ in the equation (43) as being a stationary state relative to the reference frame Γ. Let Γ' be another reference frames. Then the operator

$$U = T \exp\left[-i\int_0^t (\hat{\mathcal{H}}_\Gamma - \hat{\mathcal{H}}_{\Gamma'})dt'\right], \quad \hat{\mathcal{H}}^*_\Gamma \circ U = U \circ \hat{\mathcal{H}}^*_{\Gamma'},$$

defines an isomorphism between the spaces of stationary states relative to the reference frames Γ and Γ'.

APPENDIX: PRESYMPLECTIC QUANTIZATION

In comparison with the previous geometric quantization of the Poisson manifold $(V^*Q,\{,\}_V)$, its presymplectic quantization that follows enables one to include any covariant Hamiltonian $\mathcal{H}^*$ (15) in the quantum algebra.

A glance at the equation (13) shows that one can think of the vector field γ_H as being the Hamiltonian vector field of a zero Hamiltonian with respect to the presymplectic form dH on V^*Q. Therefore, one can examine geometric quantization of the presymplectic manifold (V^*Q,dH). Given a trivialization (2), this quantization has been studied in Ref. 4.

Geometric quantization is not applied directly to a presymplectic manifold (Z,ω), but to its symplectic realization (Z',ω') such that the presymplectic form ω is a pull-back of a symplectic form ω'. The following two possibilities are usually considered: (i) (Z',ω') is a reduction of (Z,ω) along the leaves of the characteristic distribution of the presymplectic form ω of constant rank,[15,16] and (ii) there is a coisotropic imbedding of (Z,ω) to (Z',ω').[17,18]

In application to (V^*Q,dH), the reduction procedure leads to quantization along classical solutions as follows. The kernel of dH is spanned by the vector field γ_H and, consequently, the presymplectic form dH is of constant rank. Its characteristic foliation is made up by integral curves of this vector field, i.e., solutions of Hamilton equations. If the vector field γ_H is complete, this foliation is simple, i.e., is a fibration of V^*Q over a symplectic manifold N of initial values. In this case, we come to the instantwise quantization when functions on V^*Q at a given instant $t\in\mathbf{R}$ are quantized as functions on N.

The second variant of geometric quantization of the presymplectic manifold (V^*Q,dH) is based on the fact that the image $N_h=h(V^*Q)$ of any section h (11) is a one-codimensional imbedded submanifold and, consequently, is coisotropic. It is given by the constraint

$$\mathcal{H}^*=p+\mathcal{H}(t,q^k,p_k)=0.$$

Then the geometric quantization of the presymplectic manifold (V^*Q,dH) consists in geometric quantization of the cotangent bundle T^*Q and setting the quantum constraint condition

$$\hat{\mathcal{H}}^*\psi=0$$

on physically admissible quantum states. This condition implies that $\hat{\mathcal{H}}^*$ belongs to the quantum algebra of T^*Q. It takes place if one uses polarization of T^*Q which contains the Hamiltonian vector field

$$u_{\mathcal{H}^*}=\partial_t+\partial^k\mathcal{H}\partial_k-\partial_k\mathcal{H}\partial^k. \tag{44}$$

Such a polarization of T^*Q always exists. Indeed, any section h (11) of the affine bundle ζ (4) defines the splitting

$$a_\lambda\partial^\lambda=a_k(\partial^k-\partial^k\mathcal{H}\partial^0)+(a_0+a_k\partial^k\mathcal{H})\partial^0$$

of the vertical tangent bundle VT^*Q of $T^*Q\to Q$. Then elements $(\partial^k-\partial^k\mathcal{H}\partial^0)$ together with the Hamiltonian vector field (44) obey the polarization condition (9) and generate a polarization of T^*Q. Clearly, this polarization does not satisfy the condition (10), and does not define any polarization of the Poisson manifold V^*Q.

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Foundations for relativistic quantum theory. I. Feynman's operator calculus and the Dyson conjectures

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In this paper, we provide a representation theory for the Feynman operator calculus. This allows us to solve the general initial-value problem and construct the Dyson series. We show that the series is asymptotic, thus proving Dyson's second conjecture for quantum electrodynamics. In addition, we show that the expansion may be considered exact to any finite order by producing the remainder term. This implies that every nonperturbative solution has a perturbative expansion. Using a physical analysis of information from experiment versus that implied by our models, we reformulate our theory as a sum over paths. This allows us to relate our theory to Feynman's path integral, and to prove Dyson's first conjecture that the divergences are in part due to a violation of Heisenberg's uncertainly relations. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1425080]

I. INTRODUCTION

Following Dirac's quantization of the electromagnetic field in 1927,[1] and his relativistic electron theory in 1928,[2] the equations for quantum electrodynamics (QED) were developed by Heisenberg and Pauli[3,4] in the years 1929–30 (see Miller[5] and Schweber[6]). From the beginning, when researchers attempted to use the straightforward and physically intuitive time-dependent perturbation expansion to compute physical observerables, a number of divergent expressions appeared. Although it was known that the same problems also existed in classical electrodynamics, it was noted by Oppenheimer[7] that there was a fundamental difference in the quantum problem as compared to the classical one. (Dirac[8] had shown that, in the classical case, one could account for the problem of radiation reaction without directly dealing with the self-energy divergence by using both advanced and retarded fields and a particular limiting procedure.)

Early attempts to develop subtraction procedures for the divergent expressions were very discouraging because they depended on both the gauge and the Lorentz frame, making them appear ambiguous. Although the equations of QED were both Lorentz and gauge covariant, it was generally believed that, in a strict sense, they had no solutions expandable in powers of the charge. The thinking of the times was clearly expressed by Oppenheimer[9] in his 1948 report to the Solvay Conference, ''If one wishes to explore these solutions, bearing in mind that certain infinite terms will, in a later theory, no longer be infinite, one needs a covariant way of identifying these terms; and for that, not merely the field equations themselves, but the whole method of approximation and solution must at all stages preserve covariance.''

The solution to the problem posed by Oppenheimer was made (independently) by Tomonaga,[10] Schwinger,[11] and Feynman.[12,13] (These papers may be found in Schwinger.[14]) To-

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monaga introduced what is now known as the interaction representation and showed how the approximation process could be carried out in a covariant manner. Schwinger developed the general theory and applied it to many of the important problems. Feynman took a holistic view of physical reality in his development. He suggested that we view a physical event as occurring on a film which exposes more and more of the outcome as the film unfolds. His idea was to deal directly with the solutions to the equations describing the physical system, rather than the equations themselves. In addition to solving the problem posed by Oppenheimer, Feynman's approach led to a new perturbation series, which provided an easy, intuitive, and computationally simple method to study interacting particles while giving physical meaning to each term in his expansion.

Since Feynman's method and approach was so different, it was not clear how it related to that of Schwinger and Tomonaga. Dyson,[15,16] made a major contribution. Dyson realized that Feynman and Schwinger were both dealing with different versions of Heisenberg's S-matrix. He then formally introduced time-ordering and provided a unified approach by demonstrating the equivalence of the Feynman and Schwinger–Tomonaga theories. This approach also allowed him to show how the Schwinger theory could be greatly simplified and extended to all orders of the perturbation expansion. Dyson's time-ordering idea was actually obtained from discussions with Feynman, who later explored and fully developed it into his time-ordered operator calculus.[17]

A. Background

After the problem proposed by Oppenheimer was resolved, attitudes toward the renormalization program and quantum field theory could be classified into three basic groups. The first group consisted of those who were totally dissatisfied with the renormalization program. The second group considered the renormalization program an interim step and believed that the divergences were an indication of additional physics, which could not be reached by present formulations. The first two groups will not be extensively discussed in this paper. However, we can associate the names of Dirac and Landau with the first group, and Sakata and Schwinger with the second. (See Dirac,[18] Sakata,[19] Schwinger,[20] and also Schweber.[6])

The third group was more positive, and directed its attention toward investigating the mathematical foundations of quantum field theory with the hope of providing a more orderly approach to the renormalization program (assuming that the theory proved consistent). This direction was clearly justified since part of the problem had been consistently blamed on a mathematical issue, the perturbation expansion. Indeed, the whole renormalization program critically depended on the expansion of the S-matrix in powers of the coupling constant. This concern was further supported since attempts to use the expansion when the coupling constant was large led to meaningless results. Additional unease could be attributed to the fact that, at that time, not much was actually known about the physically important cases where one was dealing with unbounded operator-valued functions (distributions).

Researchers working on the mathematical foundations of quantum electrodynamics and quantum field theory adopted the name axiomatic field theory starting in the 1950s. These researchers focused on trying to find out what could be learned about the existence of local relativistic quantum field theories based on certain natural assumptions which included the postulates of quantum mechanics, locality, Poincaré invariance, and a reasonable spectrum. This approach was initiated by the work of Wightman,[21] and Lehmann, Symanzik, and Zimmermann.[22,23] Here, the quantized field is interpreted mathematically as an operator-valued Schwartz distribution. Explicit use of the theory of distributions was a major step, which helped to partially make the theory (mathematically) sound by smoothing out the fields locally. (The recent paper by Wightman[24] provides an inspired introduction to the history of Heisenberg's early observations on the latter concept and its relationship to the divergences.[25])

The axiomatic approach proved very fruitful, providing the first rigorous proofs of a number of important general results, and attracted many able researchers. The favored name today is algebraic quantum field theory. The books by Jost,[26] Streater and Wightman,[27] and Bogolubov and Shirkov[28] are the classics, while more recent work can be found in Haag.[29] (See also the book by Bogolubov, Logunov, and Todorov,[30] and the recent review paper by Buchholz.[31])

For a number of reasons, most notably a lack of nontrivial examples, the axiomatic approach evolved in a number of directions. One major direction is called ''constructive'' quantum field theory. Here, one focuses on attempts to directly construct solutions of various model field theories, which either have exact (nonperturbative) solutions, or have an asymptotic perturbative expansion which can be summed to the exact solution. In this approach, instead of formulating the theory in Minkowski space–time, one passes to imaginary time and formulates it in Euclidean space (an idea which first appeared in Dyson[15]). This leads to a formulation in terms of ''Schwinger functions,'' also known as Euclidean Green's functions. The advantage of this approach is that hyperbolic equations are transformed to elliptic ones, and Gaussian kernels, for which a very rich set of analytic tools has been developed, replace Feynman kernels. The output of this enterprise is truly impressive. Constructive solutions have been obtained for a number of important models. Furthermore, this approach has given us a clearer picture of the problems associated with the rigorous construction of a relativistic quantum field theory and provided new mathematical methods. An early summary of this approach may be found in the lecture notes,[32] while more recent progress is contained in the lecture notes,[33] both edited by Velo and Wightman (see also Refs. 34 and 6). The books by Glimm and Jaffe[35] and Simon[36] give a different flavor and point of departure.

Although a great deal of work has been done in constructive field theory over the last 30 years, many difficult problems still remain. For example, the appearance of difficulties with the constructive approach to polynomial types of field theories is discussed in the paper by Sokal.[37] He conjectured that the $\lambda\varphi^4_{\geqslant 4}$ theory ($\lambda\varphi^4$ in four or more space–time dimensions) is a generalized free field, where λ is the coupling constant. This theory represents a self-interacting boson field. The conjecture was proven by Aizenman and Graham[38] and Fröhlich.[39] Three years later, Gawedzki and Kupiainen[40] proved that, if we change the sign of the coupling constant, the solution exists (as a tempered distribution) and the perturbation expansion is asymptotic to the solution. This state of affairs led Wightman (Ref. 33, p. 1) to lament that, ''We do not know whether the lack of an existence theorem for solutions with the 'right' sign reflects the nonexistence of solutions or merely the lack of a technique to construct them.'' Things are further complicated by the fact that the $\lambda\varphi^4_4$ theory has a perturbative solution! This led Gallavotti[41] to suggest that constructive approaches other than the ferromagnetic lattice approximation, used by Aizenman and Graham, and Fröhlich, may be required.

The most well-known method for quantum field theory calculations is perturbative renormalization theory. This approach is discussed in most standard texts on quantum field theory and has an interesting history that is best told by Wightman.[42] (The first book to include Dyson's reformulation of the Feynman–Schwinger–Tomonaga theory is the classic by Jauch and Rohrlich.[43]) Early work in the perturbative approach focused on the development of different renormalization methods with the hope of identifying those for which rigorous mathematical methods could be used. The methods generally consisted of two parts. First, the Green's functions were regularized in a relativistically and gauge invariant manner[28,34,42,44] to yield well-defined tempered distributions, even on the light cone. Then appropriate counter-terms were introduced so that, in the limit, when the regularization was removed, the various divergences of the S-matrix were also removed. It was found that all renormalization procedures are equivalent up to a finite renormalization (cf. Refs. 42 and 34). Today, theories are classified as ''renormalizable'' or ''unrenormalizable'' according to whether the number of renormalizable constants is finite or infinite, respectively.

Some model theories in less than four space–time dimensions considered in constructive field theory belong to a special subclass of renormalizable theories called ''super renormalizable,'' for which the renormalization process can be carried out without using perturbation theory.[32,33,35,36] For these theories, the renormalized perturbation series can be shown to be Borel summable to the exact nonperturbative solution. A nice summary of these developments was given by Glimm and Jaffe.[35] On the other hand, constructive models of the Gross–Neveu type are renormalizable but not super renormalizable (see Ref. 33).

Feldman *et al.*[45] have studied the mathematical foundations of quantum electrodynamics from the perturbative point of view (see also Rosen in Ref. 33, p. 201). Here, a renormalized formal

power series (renormalized tree expansion) is obtained for a measure on the space of fields within the Euclidean formulation of QED. (The tree expansion method is an outgrowth of Wilson's[46] renormalization group approach as distilled by Gallavotti[41] and co-workers.) It is then shown that QED in four (Euclidean) dimensions is locally Borel summable. Their work is truly remarkable and represents the first (formal) proof that (Euclidean) quantum electrodynamics can be renormalized using gauge invariant counterterms. However, in general, it is a nontrivial problem to return from the Euclidean regime to Minkowski space. The return trip requires application of the Osterwalder–Schrader reconstruction theorem (see Ref. 32). This theorem places conditions on the Euclidean Green's functions which guarantee analytic continuation back to the real-time vacuum expectation values. When these conditions are fulfilled, the Lehmann, Symanzik, and Zimmermann[22,23,32] reduction formulas may then be used to obtain the S-matrix. For technical reasons, they were not able to directly apply the Osterwalder–Schrader theorem. They could still get back to QED in Minkowski space–time by following the methods of Hepp[44] and Lowenstein and Speer.[47] However, nothing could be said about the convergence properties of their series.

B. Purpose

It is clear that Dyson's use of time ordering was the fundamental conceptual tool which allowed him to relate the Feynman and Schwinger–Tomonaga theories. This tool has now become a natural part of almost every branch of physics and is even used in parts of engineering. Its importance to the foundations of quantum field theory led Segal[48] to suggest that the identification of mathematical meaning for Feynman's time-ordered operator calculus is one of the major problems. A number of investigators have attempted to solve this problem. Miranker and Weiss[49] showed how the Feynman ordering process could be done formally using the theory of Banach algebras. Nelson[50] used Banach algebras to developed a theory of ''operants'' as an alternate (formal) approach. Araki,[51] motivated by the work of Fujiwara, used Banach algebras to develop yet another formal approach. (Fujiwara[52] had earlier suggested that the Feynman program could be implemented if one used a sheet of unit operators at every point except at time t, where the true operator should be placed.) Maslov[53] used the idea of a T-product to formally order operators and developed an operational theory. Another important approach to this problem via the idea of an index may be found in the works of Johnson and Lapidus,[54–56] see also Johnson, Lapidus, and DeFacio.[57]

This paper is part of a new investigation into the physical and mathematical foundations of relativistic quantum theory. Our overall goal is to construct a self-consistent relativistic quantum theory of particles and fields. For this paper, we have two specific objectives. Our first (and major) objective is to construct a physically simple and computationally useful representation theory for the Feynman time-ordered operator calculus.

A correct formulation and representation theory for the Feynman time-ordered operator calculus should at least have the following desirable features:

(1) It should provide a transparent generalization of current analytic methods without sacrificing the physically intuitive and computationally useful ideas of Feynman.
(2) It should provide a clear approach to some of the mathematical problems of relativistic quantum theory.
(3) It should explain the connection with path integrals.

In the course of his analysis, unification, and simplification of the Feynman–Schwinger–Tomonaga theory, Dyson made two important suggestions (conjectures). The first conjecture concerned the divergences in QED, while the second was concerned with the convergence of the renormalized perturbation series. In addressing the problem of divergences, Dyson conjectured that they may be due to an idealized conception of measurability resulting from the infinitely precise knowledge of the space–time positions of particles (implied by our Hamiltonian formula-

tion) which leads to a violation of the Heisenberg uncertainty principle. This point of view can be traced directly to the Bohr–Rosenfeld theory of measurability for field operators and, according to Schweber,[6] is an outgrowth of Dyson's discussions with Oppenheimer.

In addressing the renormalized S-matrix,[16] Dyson suggested that it might be more reasonable to expect the expansion to be asymptotic rather than convergent and gave physical arguments to support his claim. The lack of a clear mathematical framework made it impossible to formulate and investigate his suggestions.

Schweber[6] notes that Dyson made two other well-known conjectures. The ''overlapping divergences'' conjecture was proved by Salam,[58] Ward,[59] Mills and Yang,[60] and Hepp.[61] Dyson's conjecture that a certain Feynman integral converges, necessary for showing that the ultraviolet divergences cancel to all orders, was proved by Weinberg.[62]

Our second objective is to provide proofs of the above two conjectures under general conditions that should apply to any formulation of quantum field theory which does not abandon Hamiltonian generators for unitary solution operators. The proof of the first conjecture is, to some extent expected, and is a partial vindication of our belief in the consistency of quantum electrodynamics in the sense that the ultraviolet problem is caused by an effect that is basically ''simple.'' Such a result is partly anticipated since the effect can be made to disappear via appropriate cutoffs. We also identify (special) conditions under which the renormalized perturbation series may actually converge. A proof of the above-mentioned conjectures is implicit in, and is one of the major achievements of, constructive field theory for the models studied. In fact, these theories verify a stronger version of the second conjecture since, as noted earlier, the renormalized perturbation series is summable to the true solution.

The work in this paper is both a generalization and simplification of earlier work[63–65] that is easier and requires the weakest known conditions. We construct a new representation Hilbert space and von Neumann algebra for the Feynman (time-ordered) operator calculus. In order to make the theory applicable to other areas, we develop it using semigroups of contractions and the Riemann integral. A contraction semigroup on a Hilbert space $\mathcal{H}$ can always be extended to a unitary group on a larger space $\mathcal{H}'$. Thus, for quantum theory we may replace the semigroups by unitary groups and assume that our space is $\mathcal{H}'$ without any loss in understanding.

The Riemann integral can be easily replaced by the operator-valued Riemann-complete integral of Henstock[66] and Kurzweil,[67] which generalizes the Bochner and Pettis integrals (see Gill[63]). This integral is easier to understand (and learn) compared to the Lebesgue or Bochner integrals, and provides useful variants of the same theorems that have made those integrals so important. Furthermore, it arises from a simple (transparent) generalization of the Riemann integral that was taught in elementary calculus. Its usefulness in the construction of Feynman path integrals was first shown by Henstock,[68] and has been further explored in the recent book by Muldowney.[69]

In Sec. I D we provide a brief review of the necessary operator theory in order to make the paper self-contained. In Sec. II we construct an infinite tensor product Hilbert space and define what we mean by time ordering. In Sec. III we construct time-ordered integrals and evolution operators and prove that they have the expected properties. In Sec. IV we define what is meant by the phase ''asymptotic in the sense of Poincaré'' for operators, and use it to prove Dyson's second conjecture for contraction semigroups. We then discuss conditions under which the perturbation series may be expected to converge.

In Sec. V we take a photograph of a track left by an elementary particle in a bubble chamber as a prototype to conduct a physical analysis of what is actually known from experiment. This approach is used to rederive our time-ordered evolution operator as the limit of a probabilistic sum over paths. We use it to briefly discuss our theory in relationship to the Feynman path integral, and show that it provides a general and natural definition for the path integral that is independent of measure theory and the space of continuous paths.

The results from Sec. V are applied to the S-matrix expansion in Sec. VI to provide a formulation and proof of Dyson's first conjecture. In particular, we show that, within our formulation, the assumption of precise time information over a particle's trajectory introduces an infinite amount of energy into the system at each point in time. We use Dyson's original notation partly for

reasons of nostalgia, but also to point out what we are not able to explain within our framework. Also, since all renormalization procedures are equivalent, there is no loss.

C. Operator theory

In this section we establish notation and quote some results from operator theory used in the paper. Let $\mathcal{H}$ denote a separable Hilbert space over **C** (complex numbers), $\mathbf{B}(\mathcal{H})$ the set of bounded linear operators, and $\mathbf{C}(\mathcal{H})$ the set of closed densely defined linear operators on $\mathcal{H}$.

Definition 1.0: A family of bounded linear operators $\{U(t,0),\, 0\leqslant t<\infty\}$ defined on $\mathcal{H}$ is a *strongly continuous semigroup (or C_0-semigroup)* if

(1) $U(0,0)=I$, (2) $U(t+s,0)=U(t,0)U(s,0)$, and (3) $\lim_{t\to 0} U(t,0)\varphi=\varphi, \forall\, \varphi\in\mathcal{H}$.

$U(t,0)$ is a contraction semigroup in case $\|U(t,0)\|\leqslant 1$. If we replace (2) by (2′) $U(t,\tau)=U(t,s)U(s,\tau)$, $0\leqslant\tau\leqslant s\leqslant t<\infty$, then we call $U(t,\tau)$ a *strongly continuous evolution family*.

Definition 1.2: A densely defined operator H is said to be *maximal dissipative* if $\mathrm{Re}\langle H\varphi,\varphi\rangle\leqslant 0$, $\forall\,\varphi\in D(H)$, and $\mathrm{Ran}\,(I-H)=\mathcal{H}$ [range of $(I-H)$].

The following results may be found in Goldstein[70] or Pazy.[71]

Theorem 1.2: *Let $U(t,0)$ be a C_0-semigroup of contraction operators on $\mathcal{H}$. Then*

(1) $H\varphi=\lim_{t\to 0}(U(t,0)\varphi-\varphi)/t$ *exists for* φ *in a dense set.*
(2) $R(z,H)=(zI-H)^{-1}$ *exists for* $z>0$ *and* $\|R(z,H)\|\leqslant 1/z$.

Theorem 1.3: *Suppose H is a maximal dissipative operator. Then H generates a unique C_0-semigroup $\{U(t,0)|0\leqslant t<\infty\}$ of contraction operators on $\mathcal{H}$.*

Theorem 1.4: *If H is densely defined with both H and H* dissipative, then H is maximal dissipative.*

II. INFINITE TENSOR PRODUCT VON NEUMANN ALGEBRAS

In this section we define time-ordered operators and construct the representation space which will be used in Sec. III to develop our theory of time-ordered integrals and evolution operators. Much of the material in this section was developed by von Neumann[72] for other purposes, but is perfectly suited for our program. In order to see how natural our approach is, let $\mathcal{H}_\otimes=\hat{\otimes}_s\mathcal{H}(s)$denote the infinite tensor product Hilbert space of von Neumann, where $\mathcal{H}(s)=\mathcal{H}$ for $s\in[a,b]$ and $\hat{\otimes}$ denotes closure. If $\mathbf{B}(\mathcal{H}_\otimes)$ is the set of bounded operators on $\mathcal{H}_\otimes$, define $\mathbf{B}(\mathcal{H}(t))\subset\mathbf{B}(\mathcal{H}_\otimes)$ by

$$\mathbf{B}(\mathcal{H}(t))=\{\mathbf{H}(t)|\mathbf{H}(t)=\hat{\otimes}_{a\geqslant s>t}I_s\otimes H(t)\otimes(\otimes_{t>s\geqslant -a}I_s),\forall H(t)\in\mathbf{B}(\mathcal{H})\},\tag{2.1a}$$

where I_s denotes an identity operator, and let $\mathbf{B}^{\#}(\mathcal{H}_\otimes)$ be the uniform closure of the von Neumann algebra generated by the family $\{\mathbf{B}(\mathcal{H}(t)),|t\in E\}$. If the family $\{H(t)|t\in E\}$ is in $\mathbf{B}(\mathcal{H})$, then the corresponding operators $\{\mathbf{H}(t)|t\in E\}\in\mathbf{B}^{\#}(\mathcal{H}_\otimes)$commute when acting at different times: $t\neq s\Rightarrow$

$$\mathbf{H}(t)\mathbf{H}(s)=\mathbf{H}(s)\mathbf{H}(t).\tag{2.1b}$$

Definition 2.0: The smallest space $\mathcal{FD}_\otimes\subseteq\mathcal{H}_\otimes$ which leaves the family $\{\mathbf{H}(t)|t\in E\}$ invariant is called a Feynman–Dyson space for the family. (This is the film.)

We need the following results about operators on $\mathcal{H}_\otimes$.

Theorem 2.1: [von Neumann (Ref. 72)] *The mapping $\mathbf{T}^t_\theta$: $\mathbf{B}(\mathcal{H})\to\mathbf{B}(\mathcal{H}(t))$ is an isometric isomorphism of algebras.* (*We call $\mathbf{T}^t_\theta$ the time-ordering morphism.*)

Definition 2.2: The vector $\Phi=\otimes_s\phi_s$ is said to be equivalent to $\Psi=\otimes_s\psi_s$ and we write $\Phi\approx\Psi$, if and only if

$$\sum_s |\langle\phi_s,\psi_s\rangle_s-1|<\infty.\tag{2.2}$$

Here, $\langle\cdot,\cdot\rangle_s$ is the inner product on $\mathcal{H}(s)$, and it is understood that the sum is meaningful only if at most a countable number of terms are different from zero.

Let $\mathcal{H}_\Phi=\mathrm{cl}\{\Psi|\Psi=\Sigma_{i=1}^n\Psi_i,\Psi_i\approx\Phi,n\in\mathbf{N}\}$ (closure), $\Phi\in\mathcal{H}_\otimes$, and let $\mathbf{P}_\Phi$ denote the projection from $\mathcal{H}_\otimes$ onto $\mathcal{H}_\Phi$. The space $\mathcal{H}_\Phi$ is known as the *incomplete tensor product generated by* Φ. The details on incomplete tensor product spaces as well as proofs of the next two theorems may be found in von Neumann.[72]

Theorem 2.3: *The above-defined relation is an equivalence relation on* $\mathcal{H}_\otimes$ *and*

(1) *if* Ψ *is not equivalent to* Φ, *then* $\mathcal{H}_\Phi\cap\mathcal{H}_\Psi=\{0\}$ *(i.e.,* $\mathcal{H}_\Phi\perp\mathcal{H}_\Psi$*)*;
(2) *if* $\psi_s\neq\phi_s$ *occurs for at most a finite number of* s, *then* $\Phi=\otimes_s\phi_s\approx\Psi=\otimes_s\psi_s$;
(3) *if* $\mathbf{T}\in\mathbf{B}^\#(\mathcal{H}_\otimes)$, *then* $\mathbf{P}_\Phi\mathbf{T}=\mathbf{T}\mathbf{P}_\Phi$ *so that* $\mathbf{P}_\Phi\mathbf{T}\in\mathbf{B}^\#(\mathcal{H}_\Phi)$.

The second condition in Theorem 2.3 implies that, for each fixed $\Phi=\otimes_s\phi_s$, there is an uncountable number of $\Psi=\otimes_s\psi_s$ equivalent to Φ, while the third condition implies that every bounded linear operator on $\mathcal{H}_\otimes$ restricts to a bounded linear operator on $\mathcal{H}_\Phi$ for each Φ.

We can now construct our film $\mathcal{FD}_\otimes$. Let $\{e^i|\mathbf{i}\in\mathbf{N}\}$ denote an arbitrary ordered complete orthonormal basis (c.o.b) for $\mathcal{H}$. For each $t\in\mathbf{E},\mathbf{i}\in\mathbf{N}$, let $e_t^i=e^i$, $E^i=\otimes_{t\in E}e_t^i$, and define $\mathcal{FD}^i$ to be the incomplete tensor product generated by the vector E^i. Setting $\mathcal{FD}_\otimes=\oplus_{i=1}^\infty\mathcal{FD}^i$, it will be clear in Sec. III that $\mathcal{FD}_\otimes$ is (one of an infinite number of) the natural representation space(s) for Feynman's time-ordered operator theory. It should be noted that $\mathcal{FD}_\otimes$ is a nonseparable Hilbert (space) bundle over $[a,b]$. However, it is not hard to see that each fiber is isomorphic to $\mathcal{H}$.

In order to facilitate the proofs in Sec. III, we need an explicit basis for each $\mathcal{FD}^i$. To construct it, fix i and let f^i denote the set of all functions $\{j(t)|t\in E\}$ mapping $E\to\mathbf{N}\cup\{0\}$ such that $j(t)$ is zero for all but a finite number of t. Let $I(j)=\{j(t)|t\in E\}$ denote the function j and set $E_{I(j)}^i=\otimes_{t\in E}e_{t,j(t)}^i$ with $e_{t,0}^i=e^i$ and $j(t)=k\Rightarrow e_{t,k}^i=e^k$.

Theorem 2.4: *The set* $\{E_{I(j)}^i|I(j)\in f^i\}$ *is a (c.o.b) for each* $\mathcal{FD}^i$.

For each $\Phi^i,\Psi^i\in F^i$, set $a_{I(j)}^i=\langle\Phi^i,E_{I(j)}^i\rangle$, $b_{I(j)}^i=\langle\Psi^i,E_{I(j)}^i\rangle$, so that

$$\Phi^i=\sum_{I(j)\in F^i}a_{I(j)}^iE_{I(j)}^i,\Psi^i=\sum_{I(j)\in F^i}b_{I(j)}^iE_{I(j)}^i\ \text{ and }\ \langle\Phi^i,\Psi^i\rangle=\sum_{I(j)\in F^i}a_{I(j)}^i\overline{b_{I(k)}^i}\langle E_{I(j)}^i,E_{I(k)}^i\rangle.$$

Now,

$$\langle E_{I(j)}^i,E_{I(k)}^i\rangle=\prod_t\langle e_{t,I(j)}^i,e_{t,I(k)}^i\rangle=0,$$

unless $j(t)=k(t)$, $\forall t\in E$, so that

$$\langle\Phi^i,\Psi^i\rangle=\sum_{I(j)\in F^i}a_{I(j)}^i\overline{b_{I(j)}^i}.$$

We need the notion of an exchange operator. (Theorem 2.6 is in Ref. 63.)

Definition 2.5: An exchange operator $\mathbf{E}[t,t']$ *is a linear map defined for pairs* $t,t'\in[a,b]$ *such that*:

(1) $\mathbf{E}[t,t']:\mathbf{B}(\mathcal{H}(t))\to\mathbf{B}(\mathcal{H}(t'))$ *onto,*
(2) $\mathbf{E}[t,s]\mathbf{E}[s,t']=\mathbf{E}[t,t']$,
(3) $\mathbf{E}[t,t']\mathbf{E}[t',t]=1$,
(4) *if* $s\neq t,t'$, *then* $\mathbf{E}[t,t']\mathbf{H}(s)=\mathbf{H}(s),\forall\mathbf{H}(s)\in\mathbf{B}(\mathcal{H}(s))$.

Theorem 2.6:

(1) $\mathbf{E}[\cdot,\cdot]$ exists and is a Banach algebra isomorphism on $\mathbf{B}^\#(\mathcal{H}_\otimes)$.
(2) $\mathbf{E}[s,s']\mathbf{E}[t,t']=\mathbf{E}[t,t']\mathbf{E}[s,s']$ for distinct pairs (s,s') and (t,t') in E.

III. TIME-ORDERED INTEGRALS

In this section we construct time-ordered integrals and evolution operators for a fixed family $\{H(t)|t\in E\}\subset \mathbf{C}(\mathcal{H})$ of generators of contraction semigroups on $\mathcal{H}$. We assume that, for each t, $H(t)$ and $H^*(t)$ are dissipative (so that the family is maximal dissipative for each t). In the following discussion we adopt the notation: (e.o.v.): ''except for at most one s value;'' (e.f.n.v.) ''except for an at most finite number of s values;'' and (a.s.c.): ''almost surely and the exceptional set is at most countable.''

The s value referred to is in our fixed interval E.

For the given family $\{H(t)|t\in E\}\subset \mathbf{C}(\mathcal{H})$, define $\exp\{\tau\mathbf{H}(t)\}$ by

$$\exp\{\tau\mathbf{H}(t)\}=\hat{\otimes}_{s\in[b,t)} I_s\otimes(\exp\{\tau H(t)\})\otimes(\otimes_{s\in(t,a]} I_s), \tag{3.1}$$

and set $\mathbf{H}_z(t)=z\mathbf{H}(t)\mathbf{R}(z,\mathbf{H}(t))$, $z>0$, where $\mathbf{R}(z,\mathbf{H}(t))=(zI_\otimes-\mathbf{H}(t))^{-1}$ is the resolvent of $\mathbf{H}(t)$. It is known that $H_z(t)$ generates a uniformly bounded contraction semigroup and $\lim_{z\to\infty}H_z(t)\phi=H(t)\phi$ for $\phi\in D(H(t))$.

Theorem 3.1: *Suppose for each t, $\{H(t)|t\in E\}\subset \mathbf{C}(\mathcal{H})$ generates a strongly continuous contraction semigroup on $\mathcal{H}$. Then $\mathbf{H}(t)\mathbf{H}_z(t)\Phi=\mathbf{H}_z(t)\mathbf{H}(t)\Phi, \Phi\in D$, (where D denotes the domain of the family $\{\mathbf{H}(t)|t\in E\}$), and*

(1) *The family $\{\mathbf{H}_z(t)|t\in E\}$ generates a uniformly bounded contraction semigroup on $\mathcal{FD}_\otimes$ for each t and $\lim_{z\to\infty}\mathbf{H}_z(t)\Phi=\mathbf{H}(t)\Phi, \Phi\in D$.*
(2) *The family $\{\mathbf{H}(t)|t\in E\}\subset \mathbf{C}(\mathcal{H}_\otimes)$ generates a strongly continuous contraction semigroup on $\mathcal{FD}_\otimes$ (so that $\{\mathbf{H}(t)|t\in E\}\subset \mathbf{C}(\mathcal{FD}_\otimes)$).*

Proof: The proof of (1) is standard. Note that $\mathbf{H}_z(t)=z^2\mathbf{R}(z,\mathbf{H}(t))-zI_\otimes$ and $\|\mathbf{R}(z,\mathbf{H}(t))\|_\otimes \leqslant 1/z$, so $\|\exp\{s\mathbf{H}_z(t)\}\|_\otimes=\|\exp\{-sz\}\exp\{sz^2\mathbf{R}(z,\mathbf{H}(t))\}\|_\otimes\leqslant 1$. Now recall that $\lim_{z\to\infty}\{z\mathbf{R}(z,\mathbf{H}(t))\Phi\}=\Phi, \Phi\in\mathcal{FD}_\otimes$, so that, for $\Phi\in D$, we have that $\lim_{z\to\infty}\mathbf{H}_z(t)\Phi=\lim_{z\to\infty}\{z\mathbf{H}(t)\mathbf{R}(z,\mathbf{H}(t))\Phi\}=\lim_{z\to\infty}\{z\mathbf{R}(z,\mathbf{H}(t))\}\mathbf{H}(t)\Phi=\mathbf{H}(t)\Phi$.

To prove (2), first recall (Gill[73]) that a tensor product norm, $\|\cdot\|_\otimes$, is uniform if, for $\hat{\otimes}_{s\in E}T_s\in\mathbf{B}(\mathcal{H}_\otimes)$,

$$\|\hat{\otimes}_{s\in E} T_s\|_\otimes\leqslant\prod_{s\in E}\|T_s\|. \tag{3.2}$$

Using the uniform property of the (Hilbert space) tensor product norm, it is easy to see that $\exp\{\tau\mathbf{H}(t)\}$ is a contraction semigroup.

To prove strong continuity, we need to identify a dense core for the family $\{\mathbf{H}(t)|t\in E\}\subset\mathbf{C}(\mathcal{FD}_\otimes)$. Let D_1 denote the ordered tensor product of the domains of the family $\{H(t)|t\in E\}\subset\mathbf{C}(\mathcal{H})$, (so that $D_1\subset D$)

$$D_1=\otimes_{s\in E} D(H(s))=\left\{\sum_{i=1}^{n}\otimes_s\varphi_s^i\,|\,\varphi_s^i\in D(H(s)), s\in E\right\}. \tag{3.3}$$

It is clear that D_1 is a dense core in $\mathcal{H}_\otimes$, so $D_0=D_1\cap\mathcal{FD}_\otimes$ is a dense core in $\mathcal{FD}_\otimes$. Using our standard basis, if

$$\Phi,\Psi\in D_0,\quad \Phi=\sum_i\sum_{I(j)}a^i_{I(j)}E^i_{I(j)},\quad \Psi=\sum_i\sum_{I(k)}b^i_{I(k)}E^i_{I(k)};$$

then, since $(\exp\{\tau\mathbf{H}(t)\}-I_\otimes)$ is invariant on $\mathcal{FD}^i$ and $I_\otimes$ is the identity on $\mathcal{FD}_\otimes$, we have

$$\langle(\exp\{\tau\mathbf{H}(t)\}-I_\otimes)\Phi,\Psi\rangle=\sum_i\sum_{I(j)}\sum_{I(k)}a^i_{I(j)}\overline{b^i_{I(k)}}\langle(\exp\{\tau\mathbf{H}(t)\}-I_\otimes)E^i_{I(j)},E^i_{I(k)}\rangle, \tag{3.4a}$$

and

$$\langle(\exp\{\tau\mathbf{H}(t)\}-I_{\otimes})E^i_{I(j)},E^i_{I(k)}\rangle=\prod_{s\neq t}\langle e^i_{s,j(s)},e^i_{s,k(s)}\rangle\langle(\exp\{\tau H(t)\}-I)e^i_{t,j(t)},e^i_{t,k(t)}\rangle$$

$$=\langle(\exp\{\tau H(t)\}-I)e^i_{t,j(t)},e^i_{t,j(t)}\rangle(\text{e.o.v.})$$

$$=\langle(\exp\{\tau H(t)\}-I)e^i,e^i\rangle(\text{e.f.n.v.}), \tag{3.4b}$$

$$\Rightarrow\langle(\exp\{\tau\mathbf{H}(t)\}-I_{\otimes})\Phi,\Psi\rangle$$

$$=\sum_i\sum_{I(j)}a^i_{I(j)}\overline{b^i_{I(j)}}\langle(\exp\{\tau H(t)\}-I)e^i,e^i\rangle(\text{a.s.c.}). \tag{3.4c}$$

Since all sums are finite, we have

$$\lim_{\tau\to 0}\langle(\exp\{\tau\mathbf{H}(t)\}-I_{\otimes})\Phi,\Psi\rangle=\sum_i\sum_{I(j)}a^i_{I(j)}\overline{b^i_{I(j)}}\left\{\lim_{\tau\to 0}\langle(\exp\{\tau H(t)\}-I)e^i,e^i\rangle\right\}=0(\text{a.s.c.}). \tag{3.4d}$$

The if and only if part is now clear. Since $\exp\{\tau\mathbf{H}(t)\}$ is bounded on $\mathcal{H}_{\otimes}$ and the above-mentioned limit exists on D_0 (which is dense in $\mathcal{FD}_{\otimes}$), we see that $\exp\{\tau\mathbf{H}(t)\}$ extends to a contraction semigroup on $\mathcal{FD}_{\otimes}$. Now use the fact that, if a bounded semigroup converges weakly to the identity, it converges strongly (see Pazy,[71] p. 44).

We now assume that the family $\{H(t)|t\in E\}\subset\mathbf{C}(\mathcal{H})$ has a weak Riemann integral $Q=\int_a^b H(t)\mathrm{d}t\in\mathbf{C}(\mathcal{H})$. It follows that the family $\{H_z(t)|t\in E\}\subset\mathbf{B}(\mathcal{H})$ also has a weak Riemann integral $Q_z=\int_a^b H_z(t)\mathrm{d}t\in\mathbf{B}(\mathcal{H})$. Let P_n be a sequence of partitions (of E) so that the mesh $\mu(P_n)\to 0$ as $n\to\infty$. Set

$$Q_{z,n}=\sum_{l=1}^{n}H_z(\overline{t_l})\Delta t_l,\quad Q_{z,m}=\sum_{q=1}^{m}H_z(\overline{s_q})\Delta s_q,\quad \mathbf{Q}_{z,n}=\sum_{l=1}^{n}\mathbf{H}_z(\overline{t_l})\Delta t_l,$$

$$\mathbf{Q}_{z,m}=\sum_{q=1}^{m}\mathbf{H}_z(\overline{s_q})\Delta s_q,\quad \text{and}\ \Delta Q_z=Q_{z,n}-Q_{z,m},\quad \Delta\mathbf{Q}_z=\mathbf{Q}_{z,n}-\mathbf{Q}_{z,m}$$

Let

$$\Phi,\Psi\in D_0;\quad \Phi=\sum_i^J\Phi^i=\sum_i^J\sum_{I(j)}^K a^i_{I(j)}E^i_{I(j)},\quad \Psi=\sum_i^L\Psi^i=\sum_i^L\sum_{I(k)}^M b^i_{I(k)}E^i_{I(k)}.$$

Then we have:

Theorem 3.2 (first fundamental theorem for time-ordered integrals):

$$\langle\Delta\mathbf{Q}_z\Phi,\Psi\rangle=\sum_i^J\sum_{I(j)}^K a^i_{I(j)}\overline{b^i_{I(j)}}\langle\Delta Q_z e^i,e^i\rangle(\text{a.s.c.}). \tag{3.5}$$

Note: The form of (3.5) is quite general since $\Delta\mathbf{Q}_z$ can be replaced by other terms which also give a true relationship. For example, it is easy to show that the family $\{\mathbf{H}_z(t)|t\in E\}$ is weakly measurable, weakly continuous, weakly differentiable, etc., if and only if the same is true for the family $\{H_z(t)|t\in E\}$.

Proof:

$$\langle\Delta\mathbf{Q}_z\Phi,\Psi\rangle=\sum_i\sum_{I(j)}\sum_{I(k)}a^i_{I(j)}\overline{b^i_{I(k)}}\langle\Delta\mathbf{Q}_z E^i_{I(j)},E^i_{I(k)}\rangle$$

(we omit the upper limit). Now

$$\langle \Delta \mathbf{Q}_z E^i_{I(j)}, E^i_{I(k)}\rangle = \sum_{l=1}^{n} \Delta t_l \langle \mathbf{H}_z(\overline{t_l}) E^i_{I(j)}, E^i_{I(k)}\rangle - \sum_{q=1}^{m} \Delta s_q \langle \mathbf{H}_z(\overline{s_q}) E^i_{I(j)}, E^i_{I(k)}\rangle$$

$$= \sum_{l=1}^{n} \Delta t_l \prod_{t\neq \overline{t_l}} \langle e^i_{t,j(t)}, e^i_{t,k(t)}\rangle \langle H_z(\overline{t_l}) e^i_{\overline{t_l}, j(\overline{t_l})}, e^i_{\overline{t_l}, k(\overline{t_l})}\rangle$$

$$- \sum_{q=1}^{m} \Delta s_q \prod_{t\neq \overline{s_q}} \langle e^i_{t,j(t)}, e^i_{t,k(t)}\rangle \langle H_z(\overline{s_q}) e^i_{\overline{s_q}, j(\overline{s_q})}, e^i_{\overline{s_q}, k(\overline{s_q})}\rangle$$

$$= \sum_{l=1}^{n} \Delta t_l \langle H_z(\overline{t_l}) e^i_{\overline{t_l}, j(\overline{t_l})}, e^i_{\overline{t_l}, j(\overline{t_l})}\rangle - \sum_{q=1}^{m} \Delta s_q \langle H_z(\overline{s_q}) e^i_{\overline{s_q}, j(\overline{s_q})}, e^i_{\overline{s_q}, j(\overline{s_q})}\rangle$$

$$= \langle \Delta Q_z e^i, e^i\rangle \text{(e.f.n.v.)}.$$

This result leads to (3.5).

Theorem 3.3 (second fundamental theorem for time-ordered integrals): *If the family* $\{H_z(t)|t\in E\}$ *has a weak Riemann (Riemann-complete) integral, then*

(1) *the family* $\{\mathbf{H}_z(t)|t\in E\}\subset \mathbf{B}^{\#}(\mathcal{FD}_{\otimes})$ *has a weak Riemann (Riemann-complete) integral.*

(2) *If, in addition, we assume that for each* Φ *with* $\|\Phi\|=1$,

$$\sup_{t\in E}\left| \int_a^t (\|\mathbf{H}_z(s)\Phi\|^2 - |\langle \mathbf{H}_z(s)\Phi,\Phi\rangle|^2)\mathrm{d}s\right| < \infty, \tag{3.6}$$

then the family $\{\mathbf{H}_z(t)|t\in E\}$ *has a strong integral* $\mathbf{Q}_z[t,a]=\int_a^t \mathbf{H}_z(s)\mathrm{d}s$ *which generates a uniformly continuous contraction semigroup on* $\mathcal{FD}_{\otimes}$.

Notes:

(1) It is sufficient that $\sup_{t\in E}|\int_a^t(\|\mathbf{H}_z(s)E^i\|^2-|\langle \mathbf{H}_z(s)E^i,E^i\rangle|^2)\mathrm{d}s|<\infty$ for each i.
(2) Condition (3.6) is satisfied if $\|\mathbf{H}_z(s)E^i\|^2$ is Lebesgue integrable for each i. In this case, we replace the Riemann integral by the Riemann-complete integral.
(3) In general, the family $\{\mathbf{H}_z(t)|t\in E\}$ need not be a Bochner or Pettis integral, as it is not required that $\|\mathbf{H}_z(t)\Phi\|, \langle \mathbf{H}_z(t)\Phi,\Phi\rangle$ be (square) Lebesgue integrable. It is possible that $\int_a^b\|\mathbf{H}_z(t)\Phi\|^2\mathrm{d}t=\infty$ and $\int_a^b|\langle \mathbf{H}_z(t)\Phi,\Phi\rangle|^2\mathrm{d}t=\infty$, while (3.6) is zero.

For example, let $f(t)$ be any nonabsolutely (square) integrable function and set $\mathbf{H}_z(t)=f(t)I_{\otimes}$. Then the above-mentioned possibility holds while $\int_a^t(\|\mathbf{H}_z(s)\Phi\|^2-|\langle \mathbf{H}_z(s)\Phi,\Phi\rangle|^2)\mathrm{d}s\equiv 0$ for all t in E.

Proof: The proof of (1) is easy and follows from (3.5). To see that (3.6) makes $\mathbf{Q}_z$ a strong limit, let $\Phi\in D_0$. Then

$$\langle \mathbf{Q}_{z,n}\Phi, \mathbf{Q}_{z,n}\Phi\rangle = \sum_i^J \sum_{I(j),I(h)}^K a^i_{I(j)}\overline{a}^i_{I(h)}\left(\sum_{k,m}^n \Delta t_k \Delta t_m \langle H_z(s_k)E^i_{I(j)}, H_z(s_m)E^i_{I(h)}\rangle\right)$$

$$= \sum_i^J \sum_{I(j)}^K |a^i_{I(j)}|^2\left(\sum_{k\neq m}^n \Delta t_k\Delta t_m \langle H_z(s_k)e^i_{s_k,j(s_k)}, e^i_{s_k,j(s_k)}\rangle \right.$$

$$\left. \times \langle e^i_{s_m,j(s_m)}, H_z(s_m)e^i_{s_m,j(s_k)}\rangle\right)$$

$$+ \sum_i^J \sum_{I(j)}^K |a^i_{I(j)}|^2\left(\sum_k^n (\Delta t_k)^2 \langle H_z(s_k)e^i_{s_k,j(s_k)}, H_z(s_k)e^i_{s_k,j(s_k)}\rangle\right). \tag{3.7}$$

This can be rewritten as

$$\|\mathbf{Q}_{z,n}\Phi\|_{\otimes}^2=\sum_i^J\sum_{I(j)}^K|a^i_{I(j)}|^2\left\{|\langle Q_{z,n}e^i,e^i\rangle|^2+\sum_k^n(\Delta t_k)^2(\|H_z(s_k)e^i\|^2-|\langle H_z(s_k)e^i,e^i\rangle|^2)\right\}(\text{a.s.c.}). \tag{3.8}$$

The last term can be written as

$$\left|\sum_{k,}^n(\Delta t_k)^2(\|H_z(s_k)e^i\|^2-|\langle H_z(s_k)e^i,e^i\rangle|^2)\right|\leqslant\mu_n M\sup_{t\in E}\left|\int_a^t(\|H_z(s)e^i\|^2-|\langle H_z(s)e^i,e^i\rangle|^2)\mathrm{ds}\right|,$$

where M is a constant and μ_n is the mesh of P_n, with $\mu_n\to 0$ as $n\to\infty$. Now note that $\|\mathbf{H}_z(t)E^i\|_{\otimes}=\|H_z(t)e^i\|$ and $\langle\mathbf{H}_z(t)E^i,E^i\rangle=\langle H_z(t)e^i,e^i\rangle$ (e.o.v) so that

$$\sup_{t\in E}\left|\int_a^t(\|H_z(s)e^i\|^2-|\langle H_z(s)e^i,e^i\rangle|^2)\mathrm{ds}\right|$$

$$=\sup_{t\in E}\left|\int_a^t(\|\mathbf{H}_z(s)E^i\|^2-|\langle\mathbf{H}_z(s)E^i,E^i\rangle|^2)\mathrm{ds}\right|(\text{a.s.c.}).$$

We can now use (3.6) to get

$$\|\mathbf{Q}_{z,n}\Phi\|_{\otimes}^2\leqslant\sum_i^J\sum_{I(j)}^K|a^i_{I(j)}|^2\left\{|\langle Q_{z,n}e^i,e^i\rangle|^2+\mu_n M\sup_t\left|\int_a^t(\|\mathbf{H}_z(t)E^i\|^2-|\langle\mathbf{H}_z(t)E^i,E^i\rangle|^2)\mathrm{ds}\right|.\right\}$$

$$(\text{a.s.c.}).$$

Thus, $\mathbf{Q}_{z,n}\Phi$ converges strongly to $\mathbf{Q}_z\Phi$ on D_0 and hence has a strong limit on $\mathcal{FD}_{\otimes}$. To show that $\mathbf{Q}_z[t,a]$ generates a uniformly continuous contraction, it suffices to show that $Q_z[t,a]$ and $Q_z^*[t,a]$ are dissipative. Let Φ be in D_0, then

$$\langle\mathbf{Q}_z[t,a]\Phi,\Phi\rangle=\sum_i^J\sum_{I(j)}^K a^i_{I(j)}\overline{b^i_{I(j)}}\langle Q_ze^i,e^i\rangle(\text{a.s.c.})$$

and, since $Q_{z,n}[t,a]$ is disspative for each n, we have

$$\langle Q_z[t,a]e^i,e^i\rangle=\langle Q_{z,n}[t,a]e^i,e^i\rangle+\langle[Q_z[t,a]-Q_{z,n}[t,a]]e^i,e^i\rangle\leqslant\langle[Q_z[t,a]-Q_{z,n}[t,a]]e^i,e^i\rangle.$$

Letting $n\to\infty$, we get $\langle Q_z[t,a]e^i,e^i\rangle\leqslant 0$, so that $\langle\mathbf{Q}_z[t,a]\Phi,\Phi\rangle\leqslant 0$. The same argument applies to $\mathbf{Q}_z^*[t,a]$. Since $\mathbf{Q}_z[t,a]$ is dissipative and densely defined, it has a (bounded) dissipative closure on $\mathcal{FD}_{\otimes}$.

It should be noted that the theorem is still true if we allow the approximating sums for condition (3.6) to diverge but at an order less than $\mu_n^{-1+\delta}$, $0<\delta<1$, that is,

$$\sup_t\left|\int_a^t(\|\mathbf{H}_z(t)E^i\|^2-|\langle\mathbf{H}_z(t)E^i,E^i\rangle|^2)\mathrm{ds}\right|=\infty,$$

with

$$\left|\sum_{k,}^n(\Delta t_k)^2(\|H_z(s_k)e^i\|^2-|\langle H_z(s_k)e^i,e^i\rangle|^2)\right|\leqslant M\mu_n^{\delta}.$$

We also note that

$$\|\mathbf{Q}_z[t,a]\Phi\|_{\otimes}^2=\sum_i^J\sum_{I(j)}^K|a^i_{I(j)}|^2|\langle Q_ze^i,e^i\rangle|^2(\text{a.s.c.}) \tag{3.9}$$

in either of the above cases. This representation makes it easy to prove the next theorem.

Theorem 3.4:

(1) $\mathbf{Q}_z[t,s]+\mathbf{Q}_z[s,a]=\mathbf{Q}_z[t,a]$(a.s.c.),
(2) $s-\lim_{h\to 0}(\mathbf{Q}_z[t+h,a]-\mathbf{Q}_z[t,a])/h=s-\lim_{h\to 0}(\mathbf{Q}_z[t+h,t])/h=\mathbf{H}_z(t)$(a.s.c.),
(3) $s-\lim_{h\to 0}\mathbf{Q}_z[t+h,t]=0$ (a.s.c.),
(4) $s-\lim_{h\to 0}\exp\{\tau\mathbf{Q}_z[t+h,t]\}=I_\otimes$ (a.s.c.), $\tau\geqslant 0$.

Proof: In each case, it suffices to prove the result for $\Phi\in D_0$. To prove (1), use

$$\|[\mathbf{Q}_z[t,s]+\mathbf{Q}_z[s,a]]\Phi\|_\otimes^2=\sum_i^J\sum_{I(j)}^K|a^i_{I(j)}|^2|\langle[Q_z[t,s]+Q_z[s,a]]e^i,e^i\rangle|^2\text{(a.s.c.)}$$
$$=\sum_i^J\sum_{I(j)}^K|a^i_{I(j)}|^2|\langle Q_z[t,a]e^i,e^i\rangle|^2=\|\mathbf{Q}_z[t,a]\Phi\|_\otimes^2\text{(a.s.c.)}.$$

To prove (2), use (1) to get $\mathbf{Q}_z[t+h,a]-\mathbf{Q}_z[t,a]=\mathbf{Q}_z[t+h,t]$(a.s.c.), so that

$$\lim_{h\to 0}\left\|\frac{\mathbf{Q}_z[t+h,t]}{h}\Phi\right\|_\otimes^2=\sum_i^J\sum_{I(j)}^K|a^i_{I(j)}|^2\lim_{h\to 0}\left|\left\langle\frac{Q_z[t+h,t]}{h}e^i,e^i\right\rangle\right|^2=\|\mathbf{H}_z(t)\Phi\|_\otimes^2\text{(a.s.c.)}.$$

The proof of (3) follows from (2), and the proof of (4) follows from (3).

Theorem 3.5: *Suppose that* $\lim_{z\to\infty}\langle Q_z[t,a]\phi,\psi\rangle=\langle Q[t,a]\phi,\psi\rangle$ *exists for* ϕ *in a dense set* $\forall\psi\in\mathcal{H}$ *(weak convergence). Then*:

(1) $Q[t,a]$ generates a strongly continuous contraction semigroup on $\mathcal{H}$,
(2) $\lim_{z\to\infty}\mathbf{Q}_z[t,a]\Phi=\mathbf{Q}[t,a]\Phi$ for $\Phi\in D_0$ and $\mathbf{Q}[t,a]$ is the generator of a strongly continuous contraction semigroup on $\mathcal{FD}_\otimes$,
(3) $\mathbf{Q}[t,s]+\mathbf{Q}[s,a]=\mathbf{Q}[t,a]$(a.s.c.),
(4) $\lim_{h\to 0}[(\mathbf{Q}[t+h,a]-\mathbf{Q}[t,a])/h]\Phi=\lim_{h\to 0}[(\mathbf{Q}[t+h,t])/h]\Phi=\mathbf{H}(t)\Phi$ (a.s.c.),
(5) $\lim_{h\to 0}\mathbf{Q}[t+h,t]\Phi=0$ (a.s.c.), and
(6) $\lim_{h\to 0}\exp\{\tau\mathbf{Q}[t+h,t]\}\Phi=\Phi$(a.s.c.), $\tau\geqslant 0$.

Proof: The proofs are easy. For (1), first note that $Q[t,a]$ is closable and use $\langle Q[t,a]\phi,\phi\rangle=\langle Q_z[t,a]\phi,\phi\rangle+\langle[Q[t,a]-Q_z[t,a]]\phi,\phi\rangle\leqslant\langle[Q[t,a]-Q_z[t,a]]\phi,\phi\rangle$ and let $z\to\infty$. Then do likewise for $\langle\phi,Q^*[t,a]\phi\rangle$ to get that $Q[t,a]$ is maximal dissipative. To prove (2), use (3.9) in the form

$$\|[\mathbf{Q}_z[t,a]-\mathbf{Q}_{z'}[t,a]]\Phi\|_\otimes^2=\sum_i^J\sum_{I(j))}^K|a^i_{I(j)}|^2|\langle[Q_z[t,a]-Q_{z'}[t,a]]e^i,e^i\rangle|^2\text{(a.s.c.)}.$$

This proves that $\mathbf{Q}_z[t,a]\overset{s}{\to}\mathbf{Q}[t,a]$. Since $\mathbf{Q}[t,a]$ is densely defined, it is closable. The same method as above shows that it is maximal dissipative. Proofs of the other results follow the methods of the previous theorem.

Since $\mathbf{Q}[t,a]$ and $\mathbf{Q}_z[t,a]$ generate contraction semigroups, set $\mathbf{U}[t,a]=\exp\{\mathbf{Q}[t,a]\}$, $\mathbf{U}_z[t,a]=\exp\{\mathbf{Q}_z[t,a]\}$, for $t\in E$. They are evolution operators and the following theorem is a slight modification of a result due to Hille and Phillips,[74] known as the second exponential formula.

Theorem 3.6: *If* $\mathbf{Q}'[t,a]=w\mathbf{Q}[t,a]$ *is the generator of a strongly continuous contraction semigroup, and* $\mathbf{U}^w[t,a]=\exp\{w\mathbf{Q}[t,a]\}$, *then, for each n and* $\Phi\in D[(\mathbf{Q}[t,a])^{n+1}]$, *we have (where w is a parameter)*

$$\mathbf{U}^w[t,a]\Phi=\left\{I_\otimes+\sum_{k=1}^{n}\frac{(w\mathbf{Q}[t,a])^n}{n!}+\frac{1}{n!}\int_0^w(w-\xi)^n\mathbf{Q}[t,a]^{n+1}\mathbf{U}^\xi[t,a]\mathrm{d}\xi\right\}\Phi. \tag{3.10}$$

Proof: The proof is easy. Start with $[\mathbf{U}_z^w[t,a]\Phi-I_\otimes]\Phi=\int_0^w\mathbf{Q}_z[t,a]\mathbf{U}_z^\xi[t,a]\mathrm{d}\xi\Phi$ and use integration by parts to get that

$$[\mathbf{U}_z^w[t,a]\Phi-I_\otimes]\Phi=w\mathbf{Q}_z[t,a]\Phi+\int_0^w(w-\xi)[\mathbf{Q}_z[t,a]]^2\mathbf{U}_z^\xi[t,a]\mathrm{d}\xi\Phi.$$

It is clear how to get the nth term. Finally, let $z\to\infty$ to get (3.10).

Theorem 3.7. *If* $a<t<b$,

(1) $\lim_{z\to\infty}\mathbf{U}_z[t,a]\Phi=\mathbf{U}[t,a]\Phi,\quad\Phi\in\mathcal{FD}_\otimes$,
(2) $\partial/\partial t\,\mathbf{U}_z[t,a]\Phi=\mathbf{H}_z(t)\mathbf{U}_z[t,a]\Phi=\mathbf{U}_z[t,a]\mathbf{H}_z(t)\Phi,\quad\Phi\in\mathcal{FD}_\otimes$, and
(3) $\partial/\partial t\,\mathbf{U}[t,a]\Phi=\mathbf{H}(t)\mathbf{U}[t,a]\Phi=\mathbf{U}[t,a]\mathbf{H}(t)\Phi,\quad\Phi\in D(\mathbf{Q}[b,a])\supset D_0$.

Proof: To prove (1), use the fact that $\mathbf{H}_z(t)$ and $\mathbf{H}(t)$ commute along with

$$\begin{aligned}\mathbf{U}[t,a]\Phi-\mathbf{U}_z[t,a]\Phi&=\int_0^1(\mathrm{d}/\mathrm{ds})(e^{s\mathbf{Q}[t,a]}e^{(1-s)\mathbf{Q}_z[t,a]})\Phi\,\mathrm{ds}\\&=\int_0^1 s(e^{s\mathbf{Q}[t,a]}e^{(1-s)\mathbf{Q}_z[t,a]})(\mathbf{Q}[t,a]-\mathbf{Q}_z[t,a])\Phi\,\mathrm{ds},\end{aligned}$$

so that

$$\|\mathbf{U}[t,a]\Phi-\mathbf{U}_z[t,a]\Phi\|\leqslant\|\mathbf{Q}[t,a]\Phi-\mathbf{Q}_z[t,a]\Phi\|.$$

To prove (2), use

$$\mathbf{U}_z[t+h,a]-\mathbf{U}_z[t,a]=\mathbf{U}_z[t,a](\mathbf{U}_z[t+h,t]-I)=(\mathbf{U}_z[t+h,t]-I)\mathbf{U}_z[t,a],$$

so that,

$$\frac{(\mathbf{U}_z[t+h,a]-\mathbf{U}_z[t,a])}{h}=\mathbf{U}_z[t,a]\frac{(\mathbf{U}_z[t+h,t]-I)}{h}.$$

Now set $\Phi_z^t=\mathbf{U}_z[t,a]\Phi$ and use (3.10) with $n=1$ and $w=1$ to get:

$$\mathbf{U}_z[t+h,t]\Phi_z^t=\left\{I_\otimes+\mathbf{Q}_z[t+h,t]+\int_0^1(1-\xi)\mathbf{U}_z^\xi[t+h,t]\mathbf{Q}_z[t+h,t]^2\mathrm{d}\xi\right\}\Phi_z^t,$$

so that

$$\begin{aligned}\frac{(\mathbf{U}_z[t+h,t]-I)}{h}\Phi_z^t-\mathbf{H}_z(t)\Phi_z^t&=\frac{\mathbf{Q}_z[t+h,t]}{h}\Phi_z^t-\mathbf{H}_z(t)\Phi_z^t\\&\quad+\int_0^1(1-\xi)\mathbf{U}_z^\xi[t+h,t]\frac{\mathbf{Q}_z[t+h,t]^2}{h}\Phi_z^t\,\mathrm{d}\xi.\end{aligned}$$

It follows that

$$\left\|\frac{(\mathbf{U}_z[t+h,t]-I)}{h}\Phi_z^t-\mathbf{H}_z(t)\Phi_z^t\right\|_\otimes\leqslant\left\|\frac{\mathbf{Q}_z[t+h,t]}{h}\Phi_z^t-\mathbf{H}_z(t)\Phi_z^t\right\|_\otimes+\frac{1}{2}\left\|\frac{\mathbf{Q}_z[t+h,t]_2}{h}\Phi_z^t\right\|_\otimes.$$

The result now follows from Theorem (3.4)—(2) and (3).

To prove (3), note that $\mathbf{H}_z(t)\Phi=\mathbf{H}(t)\{z\mathbf{R}(z,\mathbf{H}(t))\}\Phi=\{z\mathbf{R}(z,\mathbf{H}(t))\}\mathbf{H}(t)\Phi$, so that $\{z\mathbf{R}(z,\mathbf{H}(t))\}$ commutes with $\mathbf{U}[t,a]$ and $\mathbf{H}(t)$. Now show that

$$\|\mathbf{H}_z(t)\mathbf{U}_z[t,a]\Phi-\mathbf{H}_{z'}(t)\mathbf{U}_{z'}[t,a]\Phi\|\leqslant\|[\mathbf{U}_z[t,a]\Phi-\mathbf{U}_{z'}[t,a]]\mathbf{H}(t)\Phi\|+\|[z\mathbf{R}(z,\mathbf{H}(t))\Phi - z'\mathbf{R}(z',\mathbf{H}(t))]\mathbf{H}(t)\Phi\|\to 0,\quad z,z'\to\infty,$$

so that, for

$$\Phi\in D(\mathbf{Q}[b,a]),\ \ \mathbf{H}_z(t)\mathbf{U}_z[t,a]\Phi\to\mathbf{H}(t)\mathbf{U}[t,a]\Phi=\frac{\partial}{\partial t}\mathbf{U}[t,a]\Phi.$$

The previous theorems form the core of our approach to the Feynman operator calculus. Our theory applies to both hyperbolic and parabolic equations. In the conventional approach, these two cases require different methods (see Pazy[71]). It is not hard to show that the requirements imposed in these cases are stronger than (our condition of) weak integral. This will be discussed in a later paper devoted to the general problem on Banach spaces.

IV. PERTURBATION THEORY

Definition 4.1: The evolution operator $\mathbf{U}^w[t,a]=\exp\{w\mathbf{Q}[t,a]\}$ is said to be *asymptotic in the sense of Poincaré* if, for each n and each $\Phi_a\in D[(\mathbf{Q}[t,a])^{n+1}]$, we have

$$\lim_{w\to 0} w^{-(n+1)}\left\{\mathbf{U}^w[t,a]-\sum_{k=1}^{n}\frac{(w\mathbf{Q}[t,a])^k}{k!}\right\}\Phi_a=\frac{\mathbf{Q}[t,a]^{n+1}}{(n+1)!}\Phi_a. \tag{4.1}$$

This is the operator version of an asymptotic expansion in the classical sense, but here $\mathbf{Q}[t,a]$ is an unbounded operator.

As noted earlier, Dyson[16] analyzed the (renormalized) perturbation expansion for quantum electrodynamics and suggested that it actually diverges. He concluded that we could, at best, hope that the series is asymptotic. His arguments were based on (not completely convincing) physical considerations, but no precise formulation of the problem was possible at that time. However, the calculations of Hurst,[75] Thirring,[76] Peterman,[77] and Jaffe[78] for specific models all support Dyson's contention that the renormalized perturbation series diverges. In his recent book[79] (pp. 13–16), Dyson's views on the perturbation series and renormalization are reiterated: ''... in spite of all the successes of the new physics, the two questions that defeated me in 1951 remain unsolved.'' Here, he is referring to the question of mathematical consistency for the whole renormalization program, and our ability to (reliably) calculate nuclear processes in quantum chromodynamics. (For other details and references to additional works, see Schweber,[6,80] Wightman,[81] and Zinn-Justin.[82])

The general construction of a physically simple and mathematically satisfactory formulation of quantum electrodynamics is still an open problem. The next theorem establishes Dyson's (second) conjecture under conditions that would apply to any (future) theory that does not require a radical departure from the present foundations of quantum theory (unitary solution operators). It also applies to the renormalized expansions in some areas of condensed matter physics where the solution operators are contraction semigroups.

Theorem 4.2: *Suppose the conditions for Theorem 3.5 are satisfied. Then:*

(1) $\mathbf{U}^w[t,a]=\exp\{w\mathbf{Q}[t,a]\}$ *is asymptotic in the sense of Poincaré.*

(2) *For each n and each* $\Phi_a\in D[(\mathbf{Q}[t,a])^{n+1}]$, *we have*

$$\Phi(t)=\Phi_a+\sum_{k=1}^{n} w^k\int_a^t \mathrm{d}s_1\int_a^{s_1}\mathrm{d}s_2\cdots\int_a^{s_{k-1}}\mathrm{d}s_k\mathbf{H}(s_1)\mathbf{H}(s_2)\cdots\mathbf{H}(s_k)\Phi_a$$
$$+\int_0^w(w-\xi)^n\mathrm{d}\xi\int_a^t\mathrm{d}s_1\int_a^{s_1}\mathrm{d}s_2\cdots\int_a^{s_n}\mathrm{d}s_{n+1}\mathbf{H}(s_1)\mathbf{H}(s_2)\cdots\mathbf{H}(s_{n+1})\mathbf{U}^{\xi}[s_{n+1},a]\Phi_a, \tag{4.2}$$

where $\Phi(t)=\mathbf{U}^w[t,a]\Phi_a$.

Proof: From (3.10), we have

$$\mathbf{U}^w[t,a]\Phi=\left\{\sum_{k=0}^{n}\frac{(w\mathbf{Q}[t,a])^n}{n!}+\frac{1}{n!}\int_0^w(w-\xi)^n\mathbf{Q}[t,a]^{n+1}\mathbf{U}^{\xi}[t,a]\mathrm{d}\xi\right\}\Phi,$$

so that

$$w^{-(n+1)}\left\{\mathbf{U}^w[t,a]\Phi_a-\sum_{k=0}^{n}\frac{(w\mathbf{Q}[t,a])^k}{k!}\Phi_a\right\}$$
$$=+\frac{(n+1)}{(n+1)!}w^{-(n+1)}\int_0^w(w-\xi)^n\mathrm{d}\xi\,\mathbf{U}^{\xi}[t,a]\mathbf{Q}[t,a]^{n+1}\Phi_a.$$

Replace the right-hand side by

$$I=\frac{(n+1)}{(n+1)!}w^{-(n+1)}\int_0^w(w-\xi)^n\mathrm{d}\xi\{\mathbf{U}_z^{\xi}[t,a]+[\mathbf{U}^{\xi}[t,a]-\mathbf{U}_z^{\xi}[t,a]]\}\mathbf{Q}[t,a]^{n+1}\Phi_a.$$

Now, expand the term $\mathbf{U}_z^{\xi}[t,a]$ in a two-term Taylor series about zero to get

$$\mathbf{U}_z^{\xi}[t,a]=I_{\otimes}+\xi\mathbf{Q}_z[t,a]+R_z^{\xi}.$$

Put the above in I, compute the elementary integrals showing that only the $I_{\otimes}$ term gives a nonzero value (of $1/(n+1)$) when $w\to 0$. Then let $z\to\infty$ to get

$$\lim_{w\to 0}(n+1)w^{-(n+1)}\int_0^w\mathrm{d}\xi(w-\xi)^n\mathbf{U}^{\xi}[t,a]\mathbf{Q}[t,a]^{n+1}\Phi_a=\mathbf{Q}[t,a]^{n+1}\Phi_a.$$

This proves that $\mathbf{U}[t,a]=\exp\{\mathbf{Q}[t,a]\}$ is asymptotic in the sense of Poincaré. To prove (4.2), let $\Phi_a\in D[(\mathbf{Q}[t,a])^{n+1}]$ for each $k\leqslant n+1$, and use the fact that (Dollard and Friedman[83])

$$(\mathbf{Q}_z[t,a])^k\Phi_a=\left(\int_a^t\mathbf{H}_z(s)\mathrm{d}s\right)^k\Phi_a=(k!)\int_a^t\mathrm{d}s_1\int_a^{s_1}\mathrm{d}s_2\cdots\int_a^{s_{k-1}}\mathrm{d}s_n\mathbf{H}_z(s_1)\mathbf{H}_z(s_2)\cdots\mathbf{H}_z(s_k)\Phi_a. \tag{4.3}$$

Letting $z\to\infty$ gives the result.

Our conditions are very weak. For example, the recent work of Tang and Li[84] required that $\|H(t)\|$ be Lebesgue integrable.

There are well-known special cases in which the perturbation series may actually converge to the solution. This can happen, for example, if the generator is bounded or if it is analytic in some sector. More generally, when the generator is of the form $\mathbf{H}(t)=\mathbf{H}_0(t)+\mathbf{H}_i(t)$, where $\mathbf{H}_0(t)$ is analytic and $\mathbf{H}_i(t)$ is some reasonable perturbation, which need not be bounded, there are conditions that allow the interaction representation to have a convergent Dyson expansion. These results can be formulated and proven in our formalism. However, the proofs are essentially the same as in the standard case so we will present them in a later paper devoted to the operator calculus on Banach spaces. The recent book by Engel and Nagel[85] provides some new results in this general area.

There are also cases where the (renormalized) series may diverge, but still respond to some summability method. This phenomenon is well-known in classical analysis. In field theory, things can be much more complicated. A good discussion, with references, can be found in the review by Wightman[81] and the book by Glimm and Jaffe.[35]

V. SUM OVER PATHS

In this section we first review and make a distinction between what is actually known and what we think we know about the foundations for our physical view of the micro-world. The objective is to provide the background for a number of physically motivated postulates that will be used to develop a theory of measurement for the micro-world (sufficient for our purposes). This will allow us to relate the theory of Secs. III and IV to Feynman's sum over paths approach and prove Dyson's second conjecture. This section differs from the previous ones in that we shift the orientation and perspective from that of mathematical physics to that of theoretical physics.

In spite of the enormous successes of the physical sciences in the past century, our information and understanding about the micro-world is still rather meager. In the macro-world we are quite comfortable with the view that physical systems evolve continuously in time and our results justify this view. Indeed, the success of continuum physics is the basis for a large part of our technical advances in the twentieth century. On the other hand, the same view is also held at the micro-level and, in this case, our position is not very secure. The ability to measure physical events continuously in time at the micro-level must be considered a belief which, although convenient, has no place in science as an *a priori* constraint.

In order to establish perspective, let us consider this belief within the context of a satisfactory, and well-justified theory, Brownian motion. This theory lies at the interface between the macro- and the micro-worlds. Some presentations of this theory (the careful ones) make a distinction between the mathematical and the physical foundations of Brownian motion and that distinction is important for our discussion.

When Einstein[86] began his investigation of the physical issues associated with this phenomenon, he was forced to assume that physical information about the state of a Brownian particle (position, velocity, etc.) can only be known in time intervals that are large compared with the mean time between molecular collisions. (It is known that, under normal physical conditions, a Brownian particle receives about 10^{21} collisions per second.) Wiener took the mathematical step and assumed that this mean time (between collisions) could be made zero, thus providing a mathematical Brownian particle. This corresponds physically to the assumption that the ratio of the mass of the particle to the friction of the fluid is zero in the limit (see Wiener *et al.*[87]).

From the physical point of view, use of Wiener's idealization of the Einstein model was not satisfactory since it led to problems of unbounded path length and nondifferentiability at all points. The first problem is physically impossible while the second is physically unreasonable. Of course, the idealization has turned out to be quite satisfactory in areas where the information required need not be detailed, such as large parts of electrical engineering, chemistry, and the biological sciences. Ornstein and Uhlenbeck[88] later constructed a model that gives the Einstein view asymptotically but, in small-time regions, is equivalent to the assumption that the particle travels a linear path between collisions. This model provides finite path length and differentiability. (The theory was later idealized by Doob.[89]) What we do know is that the very nature of the liquid state implies collective behavior among the molecules. *This means that we do not know what path the particle travels in between collisions*. However, since the tools and methods of analysis require some form of continuity, some such (in between observation) assumptions must be made. It is clear that the need for these assumptions is imposed by the available mathematical structures within which we must represent physical reality as a model.

Theoretical science concerns itself with the construction of mathematical representations of certain restricted portions of physical reality. Various trends and philosophies that are prevalent at the time temper these constructs. A consistent theme has been the quest for simplicity. This requirement is born out of the natural need to restrict models to the minimum number of variables, relationships, constraints, etc., which give a satisfactory account of known experimental results

and possibly allow the prediction of heretofore unknown consequences. One important outcome of this approach has been to implicitly eliminate all reference to the background within which physical systems evolve. In the micro-world, such an action cannot be justified without prior investigation. We propose to replace the use of mathematical coordinate systems by ''physical coordinate systems'' in order to (partially) remedy this problem.

We denote a physical coordinate system at time t by $\mathbf{R}_p^3(t)$. This coordinate system is attached to an observer (including measuring devices) and is envisioned as $\mathbf{R}^3$ plus any background effects, either local or distant, which affect the observer's ability to obtain precise (ideal) experimental information about physical reality. This in turn affects our observer's ability to construct precise (ideal) representations and make precise predictions about physical reality (in the micro-world).

More specifically, consider the evolution of some micro-system on the interval $E=[a,b]$. Physically this evolution manifests itself as a curve on $\mathbf{X}$, where

$$\prod_{t\in E} \mathbf{R}_p^3(t)=\mathbf{X}.$$

Thus, true physical events occur on $\mathbf{X}$ where actual experimental information is modified by fluctuations in $\mathbf{R}_p^3(t)$, and by the interaction of the micro-system with the measuring equipment. Based on the success of our models, we know that such small changes are in the noise region, and they have no effect on our predictions for macro-systems. However, there is no (physical) reason to believe that the effects will be small on micro-systems.

In terms of our theoretical representations, we are forced to model the evolution of physical systems in terms of wave functions, amplitudes, and/or operator-valued distributions, etc. There are thus two spaces, the physical space of evolution for the micro-system and the observer's space of obtainable information concerning this evolution. The lack of distinction between these two spaces seems to be the cause for some of the confusion and lack of physical clarity. For example, it may be perfectly correct to assume that a particle travels a continuous path on $\mathbf{X}$. However, the assumption that the observer's space of obtainable information includes infinitesimal space–time knowledge of this path is completely unfounded. This leads to our first postulate:

Postulate 1: Physical reality is a continuous process in time.

We thus take this view, fully recognizing that experiment does not provide continuous information about physical reality, and that there is no reason to believe that our mathematical representations contain precise information about the continuous space–time behavior of physical processes at this level.

Since the advent of the special theory of relativity, there has been much discussion about events, which generally means a point in $\mathbf{R}^4$ with the Minkowski metric. In terms of real physics, this is a fiction which is frequently useful for reasons of presentation but so widely used that, to avoid confusion, it is appropriate to define what we mean by a *physical event*.

Definition 5.1: A physical event is a set of physical changes in a given system that can be verified directly by experiment or indirectly via subsequent changes, where conclusions are based on an a priori agreed-upon model of the physical process.

This definition corresponds more closely to what is meant by physical events. It explicitly recognizes the evolution of scientific inference and the need for general agreement about what is being observed (based on specific models).

Before continuing, it will be helpful to have a particular physical picture in mind that makes the above-presented discussion explicit. For this purpose, we take this picture to be a photograph showing the track left by a π-meson in a bubble chamber (and take seriously the amount of information available). In particular, we assume that the following reaction occurs:

$$\pi^+ \rightarrow \mu^+ + \nu.$$

We further assume that the orientation of our photograph is such that the π-meson enters on the left at time $t=0$ and the tracks left by the μ-meson disappear on the right at time $t=T$, where

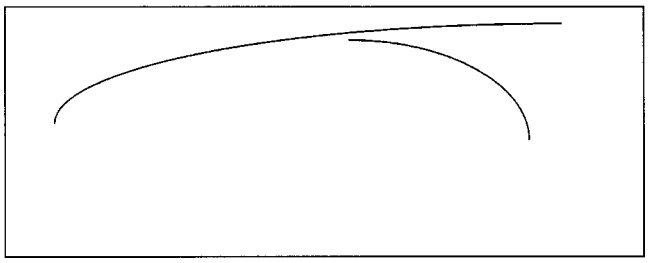

FIG. 1. Ideal picture of the reaction $\pi^+ \to \mu^+ + \nu$.

T is of the order of 10^{-3} s, the time exposure for photographic film. Although the neutrino does not appear in the photograph, we also include a track for it. In Fig. 1 we present a simplified picture of this photograph.

We have drawn the photograph as if we continuously see the particles in the picture. However, experiment only provides us individual bubbles, which do not necessarily overlap, from which we must extract physical information. A more accurate (though still not realistic) depiction is given in Fig. 2.

Let us assume that we have magnified a portion of our photograph to the extent that we may distinguish the individual bubbles created by the π-meson as it passes through the chamber. In Fig. 3, we present a simplified model of adjacent bubbles.

Postulate 2: We assume that the center of each bubble represents the average knowable effect of the particle in a symmetric time interval about the center.

By average knowable effect, we mean the average of the physical observables. In Fig. 3, we consider the existence of a bubble at time τ_j to be caused by the average of the physical observables over the time interval $[t_{j-1}, t_j]$, where $t_{j-1} = (1/2)[\tau_{j-1} + \tau_j]$ and $t_j = (1/2)[\tau_j + \tau_{j+1}]$. This postulate requires some justification. In general, the resolution of film and the relaxation time for distinct bubbles in the chamber vapor are limited. This means that if the π-meson creates two bubbles that are closely spaced in time, the bubbles may coalesce and appear as one. If this does not occur, it is still possible that the film will record the event as one bubble because of its inability to resolve events is such small time intervals.

Let us now recognize that we are dealing with one photograph so that, in order to obtain all available information, we must analyze a large number of photographs of the same reaction obtained under similar conditions (pre-prepared states). It is clear that the number of bubbles and the time placement of the bubbles will vary (independently of each other) from photograph to photograph. Let λ^{-1} denote the average time for the appearance of a bubble in the film.

Postulate 3: We assume that the number of bubbles in any film is a random variable.

Postulate 4: We assume that, given that n bubbles have appeared on a film, the time positions of the centers of the bubbles are uniformly distributed.

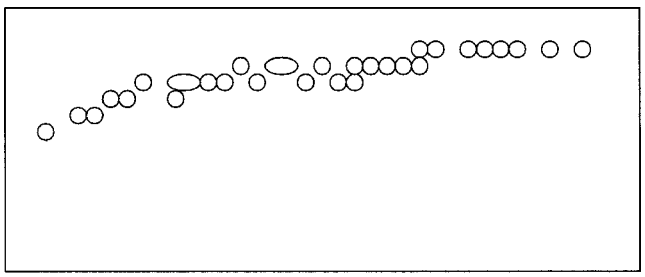

FIG. 2. More accurate picture of the reaction $\pi^+ \to \mu^+ + \nu$.

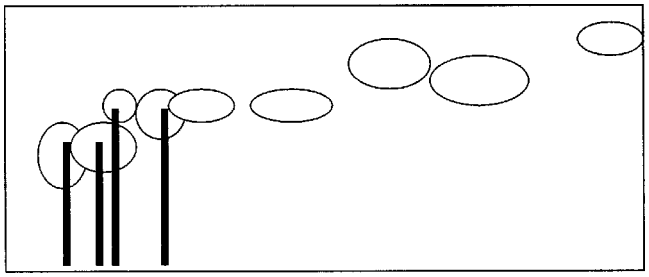

FIG. 3. Highly magnified view showing individual bubbles.

Postulate 5: We assume that $N(t)$, the number of bubbles up to time t in a given film, is a Poisson-distributed random variable with parameter λ.

To motivate Postulate 5, recall that τ_j is the time center of the jth bubble and λ^{-1} is the average (experimentally determined) time between bubbles. The following results can be found in Ross.[90]

Theorem 5.1: *The random variables $\Delta\tau_j=\tau_j-\tau_{j-1}(\tau_0=0)$ are independent identically distributed random variables of exponential type with mean λ^{-1}, for $1\leqslant j\leqslant n$.*

The arrival times $\tau_1,\tau_2,\ldots,\tau_n$ are not independent, but their density function can be computed from

$$\text{Prob}[\tau_1,\tau_2,\ldots,\tau_n]=\text{Prob}[\tau_1]\text{Prob}[\tau_2|\tau_1]\cdots\text{Prob}[\tau_n|\tau_1,\tau_2,\ldots,\tau_{n-1}]. \tag{5.1a}$$

We now use Theorem 5.1 to conclude that, for $k\geqslant 1$,

$$\text{Prob}[\tau_k|\tau_1,\tau_2,\ldots,\tau_{k-1}]=\text{Prob}[\tau_k|\tau_{k-1}]. \tag{5.1b}$$

We do not know this conditional probability. However, the natural assumption is that, given that n bubbles appear, they are equally (uniformly) distributed on the interval. We can now construct what we call the experimental evolution operator. Assume that the conditions for Theorem 3.5 are satisfied and that the family $\{\tau_1,\tau_2,\ldots,\tau_n\}$ represents the time positions of the centers of n bubbles in our film of Fig. 3. Set $a=0$ and define $\mathbf{Q}_E[\tau_1,\tau_2,\ldots,\tau_n]$ by

$$\mathbf{Q}_E[\tau_1,\tau_2,\ldots,\tau_n]=\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}E[\tau_j,s]\mathbf{H}(s)\text{ds}. \tag{5.2a}$$

Here, $t_0=\tau_0=0$, $t_j=(1/2)[\tau_j+\tau_{j+1}]$ (for $1\leqslant j\leqslant n$), and $E[\tau_j,s]$ is the exchange operator defined in Sec. II. The effect of our exchange operator $E[\tau_j,s]$ is to concentrate all information contained in $[t_{j-1},t_j]$ at τ_j. This is how we implement our postulate that the known physical event of the bubble at time τ_j is due to an average of physical effects over $[t_{j-1},t_j]$ with information concentrated at τ_j. We can rewrite $\mathbf{Q}_E[\tau_1,\tau_2,\ldots,\tau_n]$ as

$$\mathbf{Q}_E[\tau_1,\tau_2,\ldots,\tau_n]=\sum_{j=1}^{n}\Delta t_j\left[\frac{1}{\Delta t_j}\int_{t_{j-1}}^{t_j}E[\tau_j,s]\mathbf{H}(s)\text{ds}\right]. \tag{5.2b}$$

Thus, we indeed have an average as required by Postulate 2. The evolution operator is given by

$$U[\tau_1,\tau_2,\ldots,\tau_n]=\exp\left\{\sum_{j=1}^{n}\Delta t_j\left[\frac{1}{\Delta t_j}\int_{t_{j-1}}^{t_j}E[\tau_j,s]\mathbf{H}(s)\text{ds}\right]\right\}. \tag{5.3a}$$

For $\Phi\in\mathcal{FD}_{\otimes}$, we define the function $\mathbf{U}[N(t),0]\Phi$ by

$$\mathbf{U}[N(t),0]\Phi = U[\tau_1,\tau_2,\ldots,\tau_{N(t)}]\Phi. \tag{5.3b}$$

The function $\mathbf{U}[N(t),0]\Phi$ is an $\mathcal{FD}_{\otimes}$-valued random variable, which represents the distribution of the number of bubbles that may appear on our film up to time t. In order to relate $\mathbf{U}[N(t),0]\Phi$ to actual experimental results, we must compute its expected value. Using Postulates 3, 4, and 5, we have

$$\overline{\mathbf{U}}_\lambda[t,0]\Phi = \mathcal{E}[\mathbf{U}[N(t),0]\Phi] = \sum_{n=0}^{\infty} \mathcal{E}\{\mathbf{U}[N(t),0]\Phi | N(t)=n\}\text{Prob}[N(t)=n], \tag{5.4a}$$

$$\mathcal{E}\{\mathbf{U}[N(t),0]\Phi | N(t)=n\} = \int_0^t \frac{d\tau_1}{t}\int_{\tau_1}^t \frac{d\tau_2}{t-\tau_1}\cdots\int_{\tau_{n-1}}^t \frac{d\tau_n}{t-\tau_{n-1}}\mathbf{U}[\tau_n,\ldots,\tau_1]\Phi = \overline{\mathbf{U}}_n[t,0]\Phi, \tag{5.5a}$$

and

$$\text{Prob}[N(t)=n] = \frac{(\lambda t)^n}{n!}\exp\{-\lambda t\}. \tag{5.6}$$

The integral in (5.4a) acts to distribute uniformly the time positions τ_j over the successive intervals $[t,\tau_{j-1}]$, $1\leqslant j\leqslant n$, given that τ_{j-1} has been determined. This is a natural result given our lack of knowledge.

The integral (5.4a) is of theoretical value but is not easy to compute. Since we are only interested in what happens when $\lambda\to\infty$, and as the mean number of bubbles in the film at time t is λt, we can take $\tau_j=(jt/n)$, $1\leqslant j\leqslant n$ ($\Delta t_j = t/n$ for each n). We can now replace $\overline{\mathbf{U}}_n[t,0]\Phi$ by $\mathbf{U}_n[t,0]\Phi$, and with this understanding, we continue to use τ_j, so that

$$\mathbf{U}_n[t,0]\Phi = \exp\left\{\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j} E[\tau_j,s]\mathbf{H}(s)ds\right\}\Phi. \tag{5.5b}$$

We define our experimental evolution operator $\mathbf{U}_\lambda[t,0]\Phi$ by

$$\mathbf{U}_\lambda[t,0]\Phi = \sum_{n=0}^{\infty}\frac{(\lambda t)^n}{n!}\exp\{-\lambda t\}\mathbf{U}_n[t,0]\Phi. \tag{5.4b}$$

We now have the following result, which is a consequence of the fact that Borel summability is regular.

Theorem 5.4: *Assume that the conditions for Theorem 3.5 are satisfied. Then*

$$\lim_{\lambda\to\infty}\overline{\mathbf{U}}_\lambda[t,0]\Phi = \lim_{\lambda\to\infty}\mathbf{U}_\lambda[t,0]\Phi = \mathbf{U}[t,0]\Phi. \tag{5.7}$$

Since $\lambda\to\infty\Rightarrow\lambda^{-1}\to 0$, this means that the average time between bubbles is zero (in the limit) so that we get a continuous path. It should be observed that this continuous path arises from averaging the sum over an infinite number of (discrete) paths. The first term in (5.4b) corresponds to the path of a π-meson that created no bubbles (i.e., the photograph is blank). This event has probability $\exp\{-\lambda t\}$ (which approaches zero as $\lambda\to\infty$). The nth term corresponds to the path of a π-meson that created n bubbles, (with probability $[(\lambda t)^n/n!]\exp\{-\lambda t\}$), etc. Before deriving a physical relationship, let $P[t;s,\lambda]=0$ if $s\leqslant 0$ and, for $0<s<\infty$, define it as

$$P[t;s,\lambda]=e^{-\lambda t}\sum_{k=0}^{\lceil \lambda s\rceil}\frac{(\lambda t)^k}{k!}, \tag{5.8}$$

where $n=\lceil \lambda s\rceil$ is the greatest integer $\leqslant \lambda s$. We can now write $\mathbf{U}[t,0]\Phi$ as

$$\mathbf{U}[t,0]\Phi=\lim_{\lambda\to\infty}\int_0^\infty d_s P[t;s,\lambda]\mathbf{U}_{\lceil \lambda s\rceil}[s,0]\Phi,$$

$$\mathbf{U}_{\lceil \lambda s\rceil}[s,0]\Phi=\exp\left\{\sum_{j=1}^{\lceil \lambda s\rceil}\int_{t_{j-1}}^{t_j}E[\tau_j,u]\mathbf{H}(u)\mathrm{d}u\right\}\Phi. \tag{5.9}$$

Equation (5.9) means that we get both a sum over paths and a probability interpretation for our formalism. This allows us to give a new definition for path integrals.

Suppose the evolution operator $\mathbf{U}[t,0]$ has a kernel, $\mathbf{K}[\mathbf{x}(t),t;\mathbf{x}(0),0]$, such that

(1) $\mathbf{K}[\mathbf{x}(t),t;\mathbf{x}(s),s]=\int_{\mathbf{R}^3}\mathbf{K}[\mathbf{x}(t),t;\mathbf{x}(s),s]\mathbf{K}[\mathbf{x}(s),s;\mathbf{x}(0),0]\mathrm{d}\mathbf{x}(s)$, and
(2) $\mathbf{U}[t,0]\Phi=\int_{\mathbf{R}^3}\mathbf{K}[\mathbf{x}(t),t;\mathbf{x}(0),0]\mathrm{d}\mathbf{x}(0)$.

Then, from Eq. (5.9), we have that

$$\mathbf{U}[t,0]\Phi=\lim_{\lambda\to\infty}\int_0^\infty d_s P[t;s,\lambda]\left\{\prod_{j=1}^{\lceil \lambda s\rceil}\int_{\mathbf{R}^3}\mathbf{K}[\mathbf{x}(t_j),t_j;\mathbf{x}(t_{j-1}),t_{j-1}]_j\prod_{j=1}^{\lceil \lambda s\rceil}\mathrm{d}\mathbf{x}(t_{j-1})\Phi(0)\right\}.$$

Thus, whenever we can associate a kernel with our evolution operator, the time-ordered version always provides a well-defined path-integral as a sum over paths. The definition does not (directly) depend on the space of continuous paths and is independent of a theory of measure on infinite dimensional spaces. Feynman suggested that the operator calculus was more general, in his book with Hibbs[91] (see pp. 355–356).

VI. THE *S*-MATRIX

The objective of this section is to provide a formulation of the S-matrix that will allow us to investigate the sense in which we can believe Dyson's first conjecture. At the end of his second paper on the relationship between the Feynman and Schwinger–Tomonaga theories, he explored the difference between the divergent Hamiltonian formalism that one must begin with and the finite S-matrix that results from renormalization. He takes the view that it is a contrast between a real observer and a fictitious (ideal) observer. The real observer can only determine particle positions with limited accuracy and always gets finite results from his measurements. Dyson then suggests that ''... The ideal observer, however, using non-atomic apparatus whose location in space and time is known with infinite precision, is imagined to be able to disentangle a single field from its interactions with others, and to measure the interaction. In conformity with the Heisenberg uncertainty principle, it can perhaps be considered a physical consequence of the infinitely precise knowledge of (particle) location allowed to the ideal observer, that the value obtained when he measures (the interaction) is infinite.'' He goes on to remark that, if his analysis is correct, the problem of divergences is attributable to an idealized concept of measurability.

In order to explore this idea, we work in the interaction representation with obvious notation. Replace the interval $[t,0]$ by $[T,-T]$, $\mathbf{H}(t)$ by $(-i/\hbar)\mathbf{H}_I(t)$, and our experimental evolution operator $\mathbf{U}_\lambda[T,-T]\Phi$ by the experimental scattering operator $\mathbf{S}_\lambda[T,-T]\Phi$, where

$$\mathbf{S}_\lambda[T,-T]\Phi=\sum_{n=0}^{\infty}\frac{(2\lambda T)^n}{n!}\exp[-2\lambda T]\mathbf{S}_n[T,-T]\Phi, \tag{6.1}$$

$$\mathbf{S}_n[T,-T]\Phi=\exp\left\{(-i/\hbar)\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}E[\tau_j,s]\mathbf{H}_I(s)\mathrm{d}s\right\}\Phi, \tag{6.2}$$

and $\mathbf{H}_I(t)=\int_{\mathbf{R}^3}\mathbf{H}_I(\mathbf{x}(t),t)\mathrm{d}\mathbf{x}(t)$ is the interaction energy. We follow Dyson for consistency (see also the discussion), so that δmc^2 is the mass counter-term designed to cancel the self-energy divergence, and

$$\mathbf{H}_I(\mathbf{x}(t),t)=-ie\mathbf{A}_\mu(\mathbf{x}(t),t)\overline{\psi}(\mathbf{x}(t),t)\gamma_\mu\psi(\mathbf{x}(t),t)-\delta mc^2\overline{\psi}(\mathbf{x}(t),t)\psi(\mathbf{x}(t),t). \tag{6.3}$$

We now give a physical interpretation of our formalism. Rewrite Eq. (6.1) as

$$\mathbf{S}_\lambda[T,-T]\Phi=\sum_{n=0}^{\infty}\frac{(2\lambda T)^n}{n!}\exp\left\{(-i/\hbar)\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}[E[\tau_j,s]\mathbf{H}_I(s)-i\lambda\hbar I_\otimes]\mathrm{d}s\right\}\Phi. \tag{6.4}$$

In this form, it is clear that the term $-i\lambda\hbar I_\otimes$ has a physical interpretation as the absorption of photon energy of amount $\lambda\hbar$ in each subinterval $[t_j,t_{j-1}]$ (cf. Mott and Massey[92]). When we compute the limit, we get the standard S-matrix (on $[T,-T]$). It follows that we must add an infinite amount of photon energy to the mathematical description of the experimental picture (at each point in time) in order to obtain the standard scattering operator. This is the ultraviolet divergence and shows explicitly that the transition from the experimental to the ideal scattering operator requires that we illuminate the particle throughout its entire path. Thus, it appears that we have, indeed, violated the uncertainty relation. This is further supported if we look at the form of the standard S-matrix:

$$\mathbf{S}[T,-T]\Phi=\exp\left\{(-i/\hbar)\int_{-T}^{T}\mathbf{H}_I(s)\mathrm{d}s\right\}\Phi, \tag{6.5}$$

and note that the differential ds in the exponent implies perfect infinitesimal time knowledge at each point, strongly suggesting that the energy should be totally undetermined. If violation of the Heisenberg uncertainty relation is the cause for the ultraviolet divergence then, as it is a variance relation, it will not appear in first order (perturbation) but should show up in all higher-order terms. On the other hand, if we eliminate the divergent terms in second order, we would expect our method to prevent them from appearing in any higher order term of the expansion. The fact that this is precisely the case in quantum electrodynamics is a clear verification of Dyson's conjecture.

If we allow T to become infinite, we once again introduce an infinite amount of energy into the mathematical description of the experimental picture, as this is also equivalent to precise time knowledge (at infinity). Of course, this is the well-known infrared divergence and can be eliminated by keeping T finite (see Dahmen *et al.*[93]) or introducing a small mass for the photon (see Feynman,[12] p. 769). If we hold λ fixed while letting T become infinite, the experimental S-matrix takes the form:

$$\begin{gathered}\mathbf{S}_\lambda[\infty,-\infty]\Phi=\exp\left\{(-i/\hbar)\sum_{j=1}^{\infty}\int_{t_{j-1}}^{t_j}E[\tau_j,s]\mathbf{H}_I(s)\mathrm{d}s\right\}\Phi,\\ \bigcup_{j=1}^{\infty}[t_{j-1},t_j]=(-\infty,\infty),\quad \Delta t_j=\lambda^{-1}.\end{gathered} \tag{6.6}$$

This form is interesting since it shows how a minimal time eliminates the ultraviolet divergence. Of course, this is not unexpected, and has been known at least since Heisenberg[94] introduced his fundamental length as a way around the divergences. This was a prelude to the various lattice approximation methods. The review by Lee[95] is interesting in this regard.

In closing this section, we record our exact expansion for the S-matrix to any finite order. With $\Phi(-\infty)\in D[(\mathbf{Q}[\infty,-\infty])^{n+1}]$, we have

$$\mathbf{S}[\infty,-\infty]\Phi(-\infty)=\sum_{k=0}^{n}\left(\frac{-i}{\hbar}\right)^{k}\int_{-\infty}^{\infty}ds_1\int_{-\infty}^{s_1}ds_2\cdots\int_{-\infty}^{s_{k-1}}ds_k\mathbf{H}_I(s_1)\mathbf{H}_I(s_2)\cdots\mathbf{H}_I(s_k)\Phi(-\infty)$$
$$+\left(\frac{-i}{\hbar}\right)^{n+1}\int_0^1(1-\xi)^n d\xi\int_{-\infty}^{\infty}ds_1\int_{-\infty}^{s_1}ds_2\cdots\int_{-\infty}^{s_n}ds_{n+1}\mathbf{H}_I(s_1)$$
$$\times\mathbf{H}_I(s_2)\cdots\mathbf{H}_I(s_{n+1})\mathbf{S}^{\xi}[s_{n+1},-\infty]\Phi(-\infty). \tag{6.7}$$

It follows that (in a theoretical sense) we can consider the standard S-matrix expansion to be exact, when truncated at any order, by adding the last term of Eq. (6.7) to give the remainder. This result also means that, whenever we can construct an exact nonperturbative solution, it always implies the existence of a perturbative solution valid to any order. However, in general, only in particular cases can we know if the series at some n (without the remainder) approximates the solution.

VII. CONCLUSION

In this paper we have shown how to construct a natural representation Hilbert space for Feynman's time-ordered operator calculus. This space allows us to construct the time-ordered integral and evolution operator (propagator) under the weakest known conditions. Using the theory, we have shown that the perturbation expansion relevant to quantum theory is asymptotic in the sense of Poincaré. This provides a precise formulation and proof of Dyson's second conjecture[16] that, in general, we can only expect the expansion to be asymptotic.

Our investigation into the extent that our continuous models for the micro-world faithfully represent the amount of information available from experiment has led to a derivation of the time-ordered evolution operator in a more physical way. This approach made it possible to prove that the ultraviolet divergence is caused by a violation of the Heisenberg uncertainty relation at each point in time, thus partially confirming Dyson's first conjecture.

We used Dyson's original notation so as to explicitly exhibit the counter-term necessary to eliminate the self-energy divergence that occurs in QED. This divergence is not accounted for and is outside the scope of the current investigation. Thus, within our present framework, we cannot say that all the divergences arise from our disregard of some simple physics, and are not the result of deeper problems. Thus, Dyson's concerns about the mathematical consistency of quantum electrodynamics, and quantum field theory in general, is still an open problem.

Although we are not working in the framework of axiomatic field theory, our approach may make some uneasy since Haag's theorem suggests that the interaction representation does not exist (see Streater and Wightman,[27] p. 161). (Haag's theorem assumes, among other things, that the equal time commutation relations for the canonical variables of a interacting field are equivalent to those of a free field.) In trying to explain this unfortunate result, these authors point out that (see p. 168) ''... What is even more likely in physically interesting quantum field theories is that equal time commutation relations will make no sense at all; the field might not be an operator unless smeared in time as well as space.'' The work in Secs. V and VI of this paper strongly suggests that there is no physical basis to assume that we know anything about canonical variables at one instant in time (see postulate 2 and the following paragraph). Thus, our approach actually confirms the above-mentioned comments of Streater and Wightman.

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Spiked harmonic oscillators

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A complete variational treatment is provided for a family of spiked-harmonic oscillator Hamiltonians $H=-\mathrm{d}^2/\mathrm{d}x^2+Bx^2+\lambda/x^\alpha (B>0,\lambda>0)$, for arbitrary $\alpha>0$. A compact topological proof is presented that the set $S=\{\psi_n\}$ of known exact solutions for $\alpha=2$ constitutes an orthonormal basis of the Hilbert space $L_2(0,\infty)$. Closed-form expressions are derived for the matrix elements of H with respect to S. These analytical results, and the inclusion of a further free parameter, facilitate optimized variational estimation of the eigenvalues of H to high accuracy. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1418247]

I. INTRODUCTION

A family of quantum Hamiltonians known as spiked harmonic oscillators is given by the general Hamiltonian operator

$$H=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+x^2+\frac{\lambda}{x^\alpha}, \tag{1.1}$$

acting in the Hilbert space $L_2(0,\infty)$. Eigenfunctions $\psi\in L_2(0,\infty)$ of H satisfy the Schrödinger equation

$$-\psi''+\left\{x^2+\frac{\lambda}{x^\alpha}\right\}\psi=E\psi \quad \text{with} \quad \psi(0)=0. \tag{1.2}$$

The function ψ is an eigenfunction corresponding to the eigenvalue E and the condition $\psi(0)=0$ is called a *Dirichlet boundary condition*. The name of the operator derives from the graphical shape of the full potential[1] $V(x)=x^2+\lambda/x^\alpha$, which shows a pronounced peak near the origin for $\lambda>0$. Further, the Hamiltonian Eq. (1.1) is characterized by means of two parameters,[1] namely λ playing the role of a coupling constant and $\alpha\geqslant 0$ determining the degree of the singularity of the potential at the origin. Therefore, it has been regarded as a two parameter (α,λ) problem. Recently however, the present authors[2] have studied a more general family of Hamiltonians, known as generalized spiked harmonic oscillators, determined by

$$H=H_0+\frac{\lambda}{x^\alpha}, \quad H_0=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+Bx^2+\frac{A}{x^2} \quad (B>0,\ A\geqslant 0) \tag{1.3}$$

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as an operator in $L_2(0,\infty)$. They argued[2–5] that the basis, constructed from the exact solutions of the singular Gol'dman and Krivchenkov Hamiltonian H_0 in Eq. (1.3), forms a more effective starting point for a perturbative variational treatment of the Hamiltonian (1.1) than the basis of the ordinary harmonic oscillator, as used, for example, in earlier works of Aguilera-Navarro *et al.*[6,7] The objective of the present article is the demonstration of this contention, as well as the establishment of a single variational method suitable for the *complete* set of eigenvalues of the Schrödinger equation (1.2). ''Suitable'' means that, regardless of the values of the parameters λ and α, the presented variational treatment remains valid for all discrete energy eigenvalues E_n, $n=0,1,2,...$ and further, is also valid in the N-dimensional case with an arbitrary angular-momentum quantum number l.

The article is essentially self-contained, providing verification of the most relevant results concerning the generalized spiked harmonic oscillators (1.3). The proof we here give for the completeness of the set $S=\{\psi_n\}$ of eigenfunctions of H_0 is topological in nature and compact. However, the principal advances of the present work over Ref. 2 are twofold. First, we have managed now to derive closed forms for the infinite sums representing the matrix elements of H with respect to S; this, in turn, has allowed us to use these matrices to find accurate energy upper bounds quickly. Second, we have included a free parameter A in the perturbation (1.3) and consequently a final minimization of the matrix eigenvalues over A generates even more accurate eigenvalue approximations, or allows us to determine the eigenvalues to a given accuracy with the use of matrices having smaller dimension D. In Sec. II, we give a brief history of the spiked harmonic oscillator problem and indicate its relevance. Thereafter we present in Sec. III the Gol'dman and Krivchenkov potential[2] as an exactly solvable model of singular type, and prove that the exact solutions of its Schrödinger equation form a complete orthonormal basis of the Hilbert space $L_2(0,\infty)$. This topological fact is accomplished by means of using abscissas of plain convergence, absolute convergence, as well as of holomorphy of the Laplace transform, which abscissas are well discussed in the book of Gustav Doetsch. We further develop in Sec. IV explicit expressions for the matrix elements of the Hamiltonian (1.3) for arbitrary values of α subjected to the restriction $\gamma>\alpha/2$ with special attention given to $\alpha=2$, 4, and 6, for which we have the most complete analytic results. Herein $\gamma=1+\frac{1}{2}\sqrt{1+4A}$ arises out of the energy expressions for the exact solutions of the Gol'dman and Krivchenkov Hamiltonian H_0, whereas $\gamma>\alpha/2$ follows from the necessity of taking inner products of functions of type $f(x)=x^{\gamma-(\alpha+1)/2}\exp(-\beta x^2/2)P(x)$ with one another in the Hilbert space $L_2(0,\infty)$, where $P(x)$ is an arbitrary polynomial. This is followed by our variational treatment in Sec. V, wherein we compare in detail our method with that of the variational approach of Aguliera-Navarro *et al.*[6,7] An extension to the N-dimensional case with arbitrary angular momentum number $l=0,1,2,...$ is provided in Sec. VI. Finally, numerical results with detailed comparisons to previous work, accompanied by concluding remarks, are given in Sec. VII. The difficulty concerning convergence of the eigenvalues approximations calculated from the truncated matrix, in particular the slowness of convergence of the eigenvalues, is looked at in depth for the case of $\alpha=4$. It is proved that there is a critical value $\lambda_c=5/4$ such that convergence is slow when $\lambda<\lambda_c$ and rapid when $\lambda>\lambda_c$.

II. BACKGROUND AND BRIEF HISTORY

There are several reasons for the interest in the spiked harmonic oscillator Hamiltonian.[1–42] First, it represents the simplest model of certain realistic interaction potentials in atomic, molecular, and nuclear physics, and second, its interesting intrinsic properties from the viewpoint of mathematical physics. The potential $V(x)=x^2+\lambda/x^\alpha$ gives rise to a notably long-ago recognized surprise, i.e., no dominance of either of the two interaction potentials x^2 and λ/x^α takes place. Thus, for all values of $\lambda>0$, the term λ/x^α always adds an infinite repulsive barrier near the origin and on the other hand, one can never neglect the x^2 term because its absence demolishes the existence of the ground-state energy.[43,44] Consequently,[7] the potential $x^2+\lambda/x^\alpha$ is like a wide valley extending to ∞. Further, the study for small λ reveals the presence of two different behaviors depending on the value of α. When $\alpha<5/2$, the ground state energy has a power series

expansion[7] in terms of λ. For $\alpha \geqslant 5/2$, the regular perturbation theory fails badly for this kind of (*supersingular*) potential. Another interesting observation is that after the perturbation $\lambda x^{-\alpha}$ is shut off $(\lambda \to 0)$, permanent and irreversible (vestigial) effects of the interaction remain.[5] The latter effect was first noted by Klauder,[8–10] who discussed this remarkable phenomenon in connection with nonrenormalizable covariant quantum field theories. In particular, potentials V, which are sufficiently singular, cannot be smoothly turned off $(\lambda \to 0)$ in the Hamiltonian $H = H_0 + \lambda V$ to restore the free Hamiltonian H_0. This is now know as Klauder's phenomenon.[11–13] Indeed, an obvious approach to obtain information about the spectrum of the Hamiltonian equation (1.1) is to regard the potential $x^{-\alpha}$ as a perturbation of the well-known harmonic oscillator Hamiltonian. By means of the exact solutions u_n of the harmonic oscillator, one attempts to investigate the behavior of the spectrum in terms of the unperturbed eigenfunctions u_n of H_0. Detwiler and Klauder[14] realized that the normal perturbation theory already fails badly for the first correction of the ground-state energy $(n=0)$ for $\alpha \geqslant 3$. Examining the asymptotic behavior of the lowest eigenvalues of H by means of variational arguments, they were able to predict the kind of dependence the ground state energy $E = E(\lambda)$ has on the coupling λ for λ sufficiently small.

Due to the failure of the Rayleigh–Schrödinger series, a modified perturbation theory was required, especially to ascertain the higher-order expressions in the energy expansion in terms of powers of λ. Harrell[1] modified the Rayleigh–Schrödinger series by utilizing the standard (Wentzel–Kramers–Brillouin)-approximation technique for the lowest few orders. This proving to be quite successful, he continued to develop a special perturbation theory, now know as singular perturbation theory, and thereby obtained the first few terms of the perturbed λ-expansion for different values of α. This turned out to be a nonpower series expansion and in fact was of exactly the same order as of Detwiler and Klauder.[14] Its drawback is however, that it is valid only for sufficiently small value of the coupling λ, i.e., for $\lambda \ll 1$.

Since the early work of Detwiler and Klauder and Harrell, spiked harmonic-oscillator Hamiltonian equations (1.1) have become the subject of intensive study lasting over three decades.[2–42] Aguilera-Navarro *et al.*[6] managed to obtain a strong coupling perturbative expansion $(\lambda \gg 2)$ for the ground state energy. Shortly after, Aguilera-Navarro and Guardiola[7] attempted to find a path leading from the weak-coupling regime due to Harrell[1] to the strong coupling regime.[6] Nonetheless, they failed to give a general constructive method to relate the two perturbative regimes for arbitrary values of the exponent α. Special attention was given to certain values of α. Aguilera-Navarro *et al.*[17] analyzed the Hamiltonian (1.1) for $\alpha = 1$ around the three regions $\lambda \to -\infty$, $\lambda \to 0$, and $\lambda \to \infty$ via Rayleigh–Ritz large-order perturbative expansions. Aguilera-Navarro *et al.*[18] studied the particular case of $\alpha = 4$ by using a non-orthonormal set satisfying the correct boundary conditions at $x \to \infty$ and $x \to 0$. Exact and approximate (variational) solutions of the ground state energy of the spiked harmonic oscillator problem have also been reported for particular parameter values in the perturbation potential. Aside from these results, special methods have been developed to compute the eigenvalues numerically with high precision.[30–39]

Most of these results however, concern themselves with different approximation techniques for the ground-state energy for the problem in one spatial dimension. Recently, the N-dimensional case has began to attract the attention of many researchers.[3–5,41,42] In earlier work[2–5] we have pointed out the advantages of basing our variational analysis on an exactly soluble model, which itself has a singular potential term.[2] We examine a family of generalized spiked harmonic-oscillator Hamiltonians (1.1) in terms of a one-dimensional space variable $x\,(0 \leqslant x < \infty)$ with eigenfunctions satisfying Dirichlet boundary condition as stated in Eq. (1.3), that is to say, with wave functions vanishing at the boundaries. The singular orthonormal basis, consisting of the set of exact solutions of H_0, serves as a better starting point for the analysis of the Hamiltonian equation (1.1). In this paper we use these exact solutions of H_0 to provide systematic variational solutions of the spiked harmonic oscillator Hamiltonians (1.1). We first discuss the tools we implement herein, namely the Gol'dman and Krivchenkov orthonormal basis.

III. ORTHONORMALITY OF CONFLUENT HYPERGEOMETRIC SERIES AND SINGULAR POTENTIALS

The purpose of the section is to develop the necessary tools for the variational approach we shall present later. Specifically, we derive in this section the orthonormal basis most suitable for dealing with the Hamiltonian equation (1.3). Although the variational method does not *per se* require the use of a complete orthonormal basis, one can employ in some situations an orthogonal, or even a nonorthogonal,[18] set of sufficiently smooth functions to attain very effective results. In such cases, however, the variational method shall only have meaning for the particular set of chosen functions,[18] and the slightest modification of the original problem shall immediately necessitate a new set of functions or at least some modifications. Since we are interested in a set of basis functions admissible for the entire parameter range of α and λ in Eqs. (1.1) and (1.3) for our variational method, we develop our solution by using the solution of an exactly solvable singular potential whose singularity coincides with that of the spiked harmonic oscillator. Therefore, we use an exactly solvable singular Hamiltonian known as the Gol'dman and Krivchenkov Hamiltonian,[45,46]

$$-\psi''+V_0\left(\frac{a}{x}-\frac{x}{a}\right)^2\psi=E_n\psi, \quad x\in[0,\infty) \quad \text{with} \quad \psi(0)=0, \tag{3.1}$$

namely ψ satisfies the Dirichlet boundary condition. The energy spectrum in terms of the parameters V_0 and a is given by[45]

$$E_n=\frac{4}{a}\sqrt{V_0}\left\{n+\frac{1}{2}+\frac{1}{4}\left(\sqrt{1+4V_0a^2}-2a\sqrt{V_0}\right)\right\}, \tag{3.2}$$

whereas the exact wave functions take the form

$$\psi_n(x)=C_nx^{\nu}\exp\left(-\frac{1}{2}\frac{\sqrt{V_0}}{a}x^2\right){}_1F_1\left(-n,\nu+\frac{1}{2}\frac{\sqrt{V_0}}{a}x^2\right) \tag{3.3}$$

with $\nu=\frac{1}{2}(1+\sqrt{1+4V_0a^2})$. In terms of the Pochhammer symbols,

$$(a)_0=1, \quad (a)_k=a(a+1)(a+2)\ldots(a+k-1)=\frac{\Gamma(a+k)}{\Gamma(a)}, \quad k=1,2,...,$$

expressed in terms of the gamma function Γ, the previous function ${}_1F_1$, known as the confluent hypergeometric function,[47] is defined by

$${}_1F_1(-n;b;z)=\sum_{k=0}^{n}\frac{(-n)_kz^k}{(b)_kk!}. \tag{3.4}$$

To simplify the notation, we introduce parameters $B=V_0a^{-2}$ and $A=V_0a^2$, and thereby obtain an exact solution to the one-dimensional Schrödinger equation with the singular potential

$$V(x)=Bx^2+\frac{A}{x^2}, \quad B>0, A\geqslant 0, \tag{3.5}$$

whose energy spectrum is now given in terms of parameters A and B by

$$E_n=2\beta(2n+\gamma), \quad n=0,1,2,..., \tag{3.6}$$

wherein $\beta=\sqrt{B}$ and $\gamma=1+\frac{1}{2}\sqrt{1+4A}$. The wave functions in this case have the form

$$\psi_n(x)=C_nx^{\gamma-1/2}e^{-(1/2)\beta x^2}\,{}_1F_1(-n;\gamma;\beta x^2) \quad \text{for} \quad n=0,1,2,\ldots. \tag{3.7}$$

The constant C_n in Eq. (3.7) is determined from the normalization condition

$$\int_0^\infty \psi_n^2(x)\mathrm{d}x = 1. \tag{3.8}$$

In order to compute this integral, we need the following lemma, which is a generalization of formula f6 in the appendix of the book *Quantum Mechanics* by Landau and Lifshitz.[46]

Lemma 1: For $\gamma > 0$, and $m,n = 0,1,2,...,$

$$\int_0^\infty x^{2\gamma-1} e^{-\beta x^2}\, {}_1F_1(-n;\gamma;\beta x^2)\, {}_1F_1(-m;\gamma;\beta x^2)\mathrm{d}x = \frac{1}{2}\frac{n!\Gamma(\gamma)}{\beta^\gamma(\gamma)_n}\delta_{mn}, \tag{3.9}$$

where $\delta_{mn} = 0$ for $m \neq n$ and 1 for $m = n$.

Proof: We denote the indefinite integral of the left-hand side of Eq. (3.9) by I_{mn} and have by means of the series representation Eq. (3.4) of the confluent hypergeometric function ${}_1F_1$ that

$$I_{mn} = \sum_{k=0}^{m}\sum_{l=0}^{n}\frac{(-m)_k(-n)_l}{(\gamma)_k(\gamma)_l}\frac{\beta^{k+l}}{k!l!}\int_0^\infty x^{2\gamma+2k+2l-1}e^{-\beta x^2}\mathrm{d}x.$$

Further, after resorting to the integral representation of the gamma function

$$\Gamma(x) = \int_0^\infty e^{-t}t^{x-1}\,\mathrm{d}t, \quad x > 0,$$

and a change of variables, we obtain for $2\gamma + 2k + 2l - 1 > 0$ that

$$I_{mn} = \frac{1}{2\beta^\gamma}\sum_{k=0}^{n}\sum_{l=0}^{m}\frac{(-n)_k(-m)_l}{(\gamma)_k(\gamma)_l}\frac{\Gamma(\gamma+k+l)}{k!l!} = \frac{1}{2\beta^\gamma}\sum_{k=0}^{n}\left[\sum_{l=0}^{m}\frac{(-m)_l(\gamma+k)_l}{(\gamma)_l l!}\right]\frac{(-n)_k\Gamma(\gamma+k)}{(\gamma)_k k!}.$$

The finite sum inside the square brackets is just the series representation of the terminated hypergeometric function ${}_2F_1$, and therefore

$$I_{mn} = \frac{1}{2\beta^\gamma}\sum_{k=0}^{n}{}_2F_1(-m,\gamma+k;\gamma;1)\frac{(-n)_k\Gamma(\gamma+k)}{(\gamma)_k k!}.$$

Applying Chu-Vandermonde's theorem[48] on summing the series ${}_2F_1$ with unit argument, we get

$$I_{mn} = \frac{\Gamma(\gamma)}{2\beta^\gamma(\gamma)_m}\sum_{k=0}^{n}\frac{(-k)_m(-n)_k}{k!}, \tag{3.10}$$

wherein we have invoked the identity

$$(-k)_n = \begin{cases} \dfrac{(-1)^n k!}{(k-n)!} & \text{if } 0 \leqslant n \leqslant k \\ 0 & \text{if } n > k. \end{cases} \tag{3.11}$$

On account of Eq. (3.11), the product $(-k)_m(-n)_k$ in Eq. (3.10) differs from zero only for $n = k = m$, and thus

$$\sum_{k=0}^{n}\frac{(-k)_m(-n)_k}{k!} = n!$$

if $n = m$ or 0 if $n \neq m$, which terminates the proof of our lemma. ■

The reader should realize at this point the connection between the above-mentioned lemma and the orthonormality relation of Laguerre polynomials. In fact, because of the relation[47]

$$ {}_1F_1(-n;\gamma+1;x)=\frac{n!}{(\gamma+1)_n}L_n^{(\gamma)}(x), $$

Eq. (3.9) is just another form of the orthonormality condition for Laguerre ploynomials. Thus the normalization constants C_n of Eq. (3.7) can now be determined via Lemma 1 and the normalization condition Eq. (3.8), and this entails

$$ C_n^{-2}=\frac{1}{2}\frac{n!\Gamma(\gamma)}{\beta^{\gamma}(\gamma)_n}, \tag{3.12} $$

and the normalized wave function equation (3.7) now reads as follows:

$$ \psi_n(x)=(-1)^n\sqrt{\frac{2\beta^{\gamma}(\gamma)_n}{n!\Gamma(\gamma)}}x^{\gamma-1/2}e^{-(1/2)\beta x^2}\,{}_1F_1(-n;\gamma;\beta x^2). \tag{3.13} $$

The alternating coefficients $(-1)^n$ were introduced in the definition of $\psi_n(x)$ to guarantee a smooth transition by means of the identity

$$ {}_1F_1\left(-n,\frac{3}{2},x^2\right)=\frac{(-1)^n}{2x}\frac{n!}{(2n+1)!}H_{2n+1}(x) \tag{3.14} $$

to the odd solutions of the harmonic oscillator problem, namely the case $A=0$ in Eq. (3.7). From the immediately preceeding we arrive at

Theorem 1: For $\psi_n(x)$ defined by Eq. (3.13), the following orthonormality relations

$$ \int_0^{\infty}\psi_n(x)\psi_m(x)\mathrm{d}x=\delta_{mn}, \quad m,n=0,1,2,... $$

hold in $L_2(0,\infty)$.

It may seem that the Hamiltonian H_0 is self-adjoint, whence we could assume the completeness of the normalized eigenfunctions $\{\psi_n(x)\}_{n=0}^{\infty}$ from the general theory of self-adjoint operators. However, we are inhibited from doing this because of the domain of definition of H_0. The Hamiltonian operator H_0 in the Hilbert space $L_2(0,\infty)$ cannot have all of $L_2(0,\infty)$ as its domain of definition on account of the presence of the second derivative in H_0. Consequently, the totality $C_0^{\infty}(0,\infty)$ of infinitely differentiable complex valued functions on $(0,\infty)$ with compact support is initially assumed to be the domain of definition of H_0. $C_0^{\infty}(0,\infty)$ lies dense in $L_2(0,\infty)$ and H_0 is formally adjoint to itself, but not necessarily self-adjoint. To make H_0 self-adjoint, we invoke its Friedrichs extension,[49,50] which is a self-adjoint and exists in principle. If we consider H_0 to stand for its Friedrichs extension, then we need to know its spectrum $\sigma(H_0)=\sigma_d(H_0)\cup\sigma_e(H_0)$, i.e., the disjoint union of its discrete and essential spectrums. $L_2(0,\infty)$ is the direct sum of the eigenspaces of H_0 if and only if the essential spectrum is empty.[51,52] We establish $\sigma_e(H_0)=\varnothing$ by demonstrating completeness for the system $\{\psi_n(x)\}_{n=0}^{\infty}$ in the Hilbert space $L_2(0,\infty)$ of all square integrable functions over the interval $(0,\infty)$ for H_0 in its Friedrichs extension form, by means of the well-known Hahn–Banach theorem.

Theorem 2: The set of $L_2(0,\infty)$-functions $\{\psi_n(x)\}_{n=0}^{\infty}$, defined by Eq. (3.13), is a complete orthonormal basis for the Hilbert space $L_2(0,\infty)$.

Proof: The orthonormality of $\{\psi_n(x)\}_{n=0}^{\infty}$ follows from Theorem 1. To prove completeness, we proceed as follows. On account of the definition (3.13) of $\psi_n(x)$ in terms of the hypergeometric function

$$ {}_1F_1(-n,\gamma,\beta x^2)=\sum_{k=0}^{n}\binom{n}{k}\frac{(-\beta)^{n-k}\Gamma(\beta)}{\Gamma(\gamma+n-k)}x^{2(n-k)} $$

we can express each of the functions ${}_1F_1(-n,\gamma,\beta x^2)(n\geqslant 0)$ uniquely as a finite linear combination of $x^{2n}(n\geqslant 0)$ as well as conversely. This in terms of the span, which we denote by $(L.H.)$, means that $(L.H.)({}_1F_1(-n,\gamma,\beta x^2)(n\geqslant 0))=(L.H.)(x^{2n}(n\geqslant 0))$. We multiply each member of these two sets by $x^{\gamma-1/2}\exp(-\beta x^2/2)$, and thereby obtain a linear subspace of the Hilbert space $L_2(0,\infty)$, whose topological closure satifies

$$ \overline{(L.H.)(\cdot^{\gamma-1/2}\,{}_1F_1(-n,\gamma,\beta\cdot^2)\exp(-\beta\cdot^2/2)(n\geqslant 0))}=\overline{(L.H.)(\cdot^{\gamma-1/2+2n}\exp(-\beta\cdot^2/2)(n\geqslant 0))}, $$

and further, orthogonal complementation yields

$$ \begin{aligned}&[(L.H.)(\cdot^{\gamma-1/2}{}_1F_1(-n,\gamma,\beta^2)\exp(-\beta\cdot^2/2)(n\geqslant 0))]^{\perp}\\ &\quad=[(L.H.)(\cdot^{\gamma-1/2+2n}\exp(-\beta\cdot^2/2)(n\geqslant 0))]^{\perp}.\end{aligned} $$

Now we turn to demonstrating that $[(L.H.)(\cdot^{\gamma-1/2}\,{}_1F_1(-n,\gamma,\beta\cdot^2)\exp(-\beta\cdot^2/2)(n\geqslant 0))]^{\perp}=0$, in other words $\{C_n\cdot^{\gamma-1/2}{}_1F_1(-n,\gamma,\beta\cdot^2)\exp(-\beta\cdot^2/2)\}_{n=0}^{\infty}$ constitutes an orthonormal basis of the Hilbert space $L_2(0,\infty)$ with C_n's given by (3.12). Assuming that $\Phi\in L_2(0,\infty)$ with $\Phi\perp(L.H.)(\cdot^{\gamma-1/2}{}_1F_1(-n,\gamma,\beta\cdot^2)\exp(-\beta\cdot^2/2)(n\geqslant 0))$ leads directly to

$$ \langle\cdot^{\gamma-1/2+2n}\exp(-\beta\cdot^2/2)|\Phi\rangle=\int_0^{\infty}x^{\gamma-1/2+2n}\exp(-\beta x^2/2)\overline{\Phi(x)}\,dx=0\quad(n\geqslant 0). $$

We define

$$ f(s)\equiv\int_0^{\infty}x^{\gamma-1/2}\exp(-sx^2/2)\overline{\Phi(x)}\,dx=\int_0^{\infty}e^{-st}F(t)\,dt, $$

where $F(t)\equiv t^{\gamma/2-3/4}\overline{\Phi(\sqrt{t})}/2$.

Out of the fact that $\Phi\in L_2(0,\infty)$ follows

$$ \begin{aligned}\int_0^{\infty}|e^{-st}F(t)|\,dt&=\int_0^{\infty}1/2t^{\gamma/2-3/4}|\Phi(\sqrt{t})|\exp(-(\Re s)t)\,dt\\ &=\sqrt{2}\int_0^{\infty}t^{\gamma/2-1/2}\exp(-(\Re s)t)|\Phi(\sqrt{t})|\,\frac{1}{\sqrt{2}}t^{-1/4}\,dt\\ &\leqslant\sqrt{2}\sqrt{\int_0^{\infty}|t^{\gamma/2-1/2}\exp(-(\Re s)t)|^2\,dt}\sqrt{\int_0^{\infty}|\Phi(\sqrt{t})|^2\,dt}\\ &=\sqrt{2}\sqrt{\int_0^{\infty}\exp(-2(\Re s)t)t^{\gamma-1}\,dt}\sqrt{\int_0^{\infty}|\Phi(x)|^2\,dx}\\ &=\sqrt{2}\sqrt{\frac{1}{(2\Re s)^{\gamma}}\int_0^{\infty}e^{-t}t^{\gamma-1}\,dt}\|\Phi\|_{L_2(0,\infty)}\\ &=\sqrt{2(\Re s)^{-\gamma}\Gamma(\gamma)}\|\Phi\|_{L_2(0,\infty)}\\ &<\infty.\end{aligned} $$

Herewith the abscissa $\tilde{\alpha}$ of absolute convergence[53] of the Laplace integral $f(s)=\mathcal{L}\{F\}$, namely the smallest real number $\tilde{\alpha}$, such that $\int_0^\infty |e^{-st}F(t)|\mathrm{d}t<\infty$ for all $\Re s>\tilde{\alpha}$, has the property that $\tilde{\alpha}\leqslant 0$. In consequence of our substitution $x=\sqrt{t}$, we have further that

$$\langle \cdot^{\gamma-1/2+2n}\exp(-\beta^2/2)|\Phi\rangle=(-1)^n\int_0^\infty (-t)^n e^{-(\beta/2)t}F(t)\mathrm{d}t=f^{(n)}(\beta/2)=0 \quad (n\geqslant 0). \tag{3.15}$$

Since $f(s)$ is definitely holomorphic in the half-plane $\Re s>0$, because the abscissa of holomorphy $\tilde{\chi}$ satisfies $\tilde{\chi}\leqslant\tilde{\beta}\leqslant\tilde{\alpha}$ ($\tilde{\beta}$ being the abscissa of ordinary convergence of the Laplace Integral[53] $\mathcal{L}\{F\}$), $f(s)$ shall clearly have a Taylor series expansion

$$f(s)=\sum_{n=0}^{\infty}(n!)^{-1}f^{(n)}(\beta/2)(s-\beta/2)^n=0 \quad (|s-\beta/2|<\beta/2) \tag{3.16}$$

in terms of Eq. (3.15) about the point $\beta/2>0$. The radius of convergence of this Taylor series is at least a big as $\beta/2$, since it may happen that the abscissa of holomorphy[53] $\tilde{\chi}$ of the Laplace integral $f(s)=\mathcal{L}\{F\}$ is definitely less than the abscissa $\tilde{\beta}$ of ordinary convergence, not to mention that of absolute convergence $\tilde{\alpha}$. Thus we have that $f(s)\equiv 0$ in the open disk $|s-\beta/2|<\beta/2$ of the s complex plane. By means of the identity theorem of holomorphic functions,[54] we have that the Laplace integral $f(s)=\mathcal{L}\{F\}\equiv 0$ in the half-plane of holomorphy $\Re s>\tilde{\chi}$; and more so in the holomorphy domain of f, which contains its half-plane of holomorphy. The uniqueness of the Laplace-transform implies that $F(t)\equiv 1/2t^{\gamma/2-3/4}\Phi(\sqrt{t})=0$ a.e. in t on the interval $[0,\infty)$. Hence, $\int_0^\infty|\Phi(\sqrt{t})|^2(2\sqrt{t})^{-1}\mathrm{d}t=\int_0^\infty|\Phi(x)|^2\,\mathrm{d}x=0$, namely $\Phi=0$ a.e. on $(0,\infty)$, which is to say that $\{C_n\cdot^{\gamma-1/2}{}_1F_1(-n,\gamma;\beta\cdot^2)\}_{n=0}^\infty$ constitutes a complete orthonormal basis of the Hilbert space $L_2(0,\infty)$. ■

IV. THE MATRIX ELEMENTS FOR SINGULAR POTENTIALS

It is well known that the Schrödinger equation, even in the one-dimensional case, rarely possesses an exact (analytic) solution. Consequently, a multitude of arduous numerical techniques have been implemented to ascertain its energy eigenvalues over several decades; from among these, we mention matrix diagonalization. Our primary aim in this section is to find the matrix elements of the Hamiltonian equation (1.3), whose calculation is achieved by means of

Lemma 2: If $2\gamma-\alpha>0$, then for all pairs of non-negative integers and m and n we have that

$$\int_0^\infty x^{2\gamma-\alpha-1}e^{-\beta x^2}{}_1F_1(-n,\gamma,\beta x^2){}_1F_1(-m,\gamma,\beta x^2)\mathrm{d}x$$

$$=\frac{\beta^{\alpha/2-\gamma}}{2}\frac{\left(\frac{\alpha}{2}\right)_n\Gamma\left(\gamma-\frac{\alpha}{2}\right)}{(\gamma)_n}{}_3F_2\left(-m,\gamma-\frac{\alpha}{2},1-\frac{\alpha}{2};\gamma,1-\frac{\alpha}{2}-n;1\right). \tag{4.1}$$

Proof: Let I_{mn} denote the infinite integral on the left-hand side of Eq. (4.1). Using the series representation equation (3.4) of the confluent hypergeometric function ${}_1F_1$ yields

$$I_{mn}=\sum_{k=0}^{m}\sum_{l=0}^{n}\frac{(-m)_k(-n)_l}{(\gamma)_k(\gamma)_l}\frac{\beta^{k+l}}{k!l!}\int_0^\infty x^{-\alpha+2\gamma+2k+2l-1}e^{-\beta x^2}\,\mathrm{d}x. \tag{4.2}$$

By resorting to the integral representation of gamma function, we obtain under the condition $-\alpha/2+\gamma+k+l>0$ that

$$I_{mn}=\frac{1}{2}\sum_{k=0}^{m}\sum_{l=0}^{n}\frac{(-m)_k(-n)_l}{(\gamma)_k(\gamma)_l}\frac{\beta^{\alpha/2-\gamma}}{k!l!}\Gamma\left(-\frac{\alpha}{2}+\gamma+k-l\right)$$

$$=\frac{1}{2}\beta^{\alpha/2-\gamma}\sum_{k=0}^{m}\left[\sum_{l=0}^{n}\frac{(-n)_l\Gamma\left(-\frac{\alpha}{2}+\gamma+k+l\right)}{(\gamma)_l l!}\right]\frac{(-m)_k}{(\gamma)_k}\frac{1}{k!}. \tag{4.3}$$

This relation we rewrite in terms of the Pochhammer symbols, use $\Gamma(-\alpha/2+\gamma+k+l)=(-\alpha/2+\gamma+k)_l\Gamma(-\alpha/2+\gamma+k)$, invoke Chu–Vandermonde's theorem, and thus write

$$\sum_{l=0}^{n}\frac{(-n)_l\Gamma\left(-\frac{\alpha}{2}+\gamma+k+l\right)}{(\gamma)_l l!}=\sum_{l=0}^{n}\frac{(-n)_l\left(-\frac{\alpha}{2}+\gamma+k\right)_l}{(\gamma)_l l!}\Gamma\left(-\frac{\alpha}{2}+\gamma+k\right)$$

$$=\Gamma\left(-\frac{\alpha}{2}+\gamma+k\right)\,{}_2F_1\left(-n-\frac{\alpha}{2}+\gamma+k;\gamma;1\right)$$

$$=\Gamma\left(-\frac{\alpha}{2}+\gamma+k\right)\frac{\left(\frac{\alpha}{2}-k\right)_n}{(\gamma)_n} \tag{4.4}$$

for the finite sum inside the square brackets of Eq. (4.3). Consequently, we arrive at

$$I_{mm}=\frac{1}{2}\beta^{\alpha/2-\gamma}\sum_{k=0}^{m}\Gamma\left(-\frac{\alpha}{2}+\gamma+k\right)\frac{\left(\frac{\alpha}{2}-k\right)_n}{(\gamma)_n}\frac{(-m)_k}{(\gamma)_k}\frac{1}{k!}$$

$$=\frac{1}{2}\beta^{\alpha/2-\gamma}\frac{\Gamma(\gamma)}{(\gamma)_n}\sum_{k=0}^{m}(-1)^k\binom{m}{k}\frac{\Gamma\left(\frac{\alpha}{2}+n-k\right)\Gamma\left(-\frac{\alpha}{2}+\gamma+k\right)}{\Gamma(\gamma+k)\Gamma\left(\frac{\alpha}{2}-k\right)}, \tag{4.5}$$

wherein we have used the identity $(-m)_k/k!=(-1)^k\binom{m}{k}$. We further simplify expression (4.5) by taking note of

$$(a-k)_n=\frac{(1-a)_k(a)_n}{(1-a-n)_k}$$

in order to justify the relation

$$I_{mn}=\frac{1}{2}\beta^{\alpha/2-\gamma}\frac{\Gamma\left(\gamma-\frac{\alpha}{2}\right)\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n}\sum_{k=0}^{m}\frac{(-m)_k\left(\gamma-\frac{\alpha}{2}\right)_k\left(1-\frac{\alpha}{2}\right)_k}{(\gamma)_k\left(1-\frac{\alpha}{2}-n\right)_k k!}=\frac{1}{2}\beta^{\alpha/2-\gamma}\frac{\Gamma\left(\gamma-\frac{\alpha}{2}\right)\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n}\,{}_3F_2$$

$$\left(-m,\gamma-\frac{\alpha}{2},1-\frac{\alpha}{2};\gamma,1-\frac{\alpha}{2}-n;1\right), \tag{4.6}$$

which is valid for all values of α and γ such that $\gamma-\alpha/2>0$. This completes the proof of the lemma. ■

It should be noted that Eq. (4.1) is a generalization of Eq. (3.9), and under the limit process of $\alpha\to 0^+$ Eq. (4.1) reduced to Eq. (3.9). In order to prove this, we proceed by proving

$$\lim_{\alpha\to 0^+}\left(\frac{\alpha}{2}\right)_n {}_3F_2\left(-m,\gamma-\frac{\alpha}{2},1-\frac{\alpha}{2};\gamma,1-\frac{\alpha}{2}-n;1\right)=n!\,\delta_{mn}. \tag{4.7}$$

This can be demonstrated by bringing in the series representation of the terminated hypergeometric function ${}_3F_2$, which leads to

$$\left(\frac{\alpha}{2}\right)_n {}_3F_2\left(-m,\gamma-\frac{\alpha}{2},1-\frac{\alpha}{2};\gamma,1-\frac{\alpha}{2}-n;1\right)=\sum_{k=0}^{m}\frac{(-m)_k\left(\gamma-\frac{\alpha}{2}\right)_k\left(1-\frac{\alpha}{2}\right)_k(-1)^n\Gamma\left(1-\frac{\alpha}{2}\right)}{k!(\gamma)_k\Gamma\left(1-\frac{\alpha}{2}-n+k\right)}$$

by means of the identities

$$\left(1-\frac{\alpha}{2}-n\right)_k=\frac{\Gamma\left(1-\frac{\alpha}{2}-n+k\right)}{\left(1-\frac{\alpha}{2}\right)_{-n}\Gamma\left(1-\frac{\alpha}{2}\right)}=(-1)^n\frac{\left(\frac{\alpha}{2}\right)_n\Gamma\left(1-\frac{\alpha}{2}-n+k\right)}{\Gamma\left(1-\frac{\alpha}{2}\right)}.$$

Therefore, by taking the limit as $\alpha\to 0^+$, we can easily see that

$$\lim_{a\to 0^+}\left(\frac{\alpha}{2}\right)_n {}_3F_2\left(-m,\gamma-\frac{\alpha}{2},1-\frac{\alpha}{2};\gamma,1-\frac{\alpha}{2}-n;1\right)=\sum_{k=0}^{m}\frac{(-m)_k(-1)^n}{\Gamma(1-n+k)}=\sum_{k=0}^{m}\frac{(-m)_k(-k)_n}{k!},$$

where we have made use of the relation $(1+k)_{-n}=(-1)^n/(-k)_n$. Again, the product $(-m)_k(-k)_n$ leads to the fact that the sum

$$\sum_{k=0}^{m}\frac{(-m)_k(-k)_n}{k!}$$

collapses to $n!$, for the case of $m=k=n$, and 0 otherwise.

The matrix elements of the Hamiltonian (1.3) are now given by means of Lemma 3 in terms of the infinite integral

$$x_{mn}^{-\alpha}=\langle\psi_m|x^{-\alpha}|\psi_n\rangle=C_mC_n\int_0^\infty x^{2\gamma-\alpha-1}e^{-\beta x^2}\,{}_1F_1(-n,\gamma,\beta x^2)\,{}_1F_1(-m,\gamma,\beta x^2)\mathrm{d}x. \tag{4.8}$$

Therefore, as a consequence of Lemma 2 and Eq. (3.12), the matrix elements now assume the explicit forms

$$x_{mn}^{-\alpha}=(-1)^{n+m}\beta^{\alpha/2}\frac{\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n}\frac{\Gamma\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma(\gamma)}\sqrt{\frac{(\gamma)_n(\gamma)_m}{n!m!}}\,{}_3F_2\left(-m,\gamma-\frac{\alpha}{2},1-\frac{\alpha}{2};\gamma,1-n-\frac{\alpha}{2};1\right); \tag{4.9}$$

among which the following is of particular interest

$$x_{0n}^{-\alpha}=(-1)^n\beta^{\alpha/2}\frac{\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n}\frac{\Gamma\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma(\gamma)}\sqrt{\frac{(\gamma)_n}{n!}}. \tag{4.10}$$

In the case of α being a non-negative even number ($\alpha=2,4,6,...$), the hypergeometric function ${}_3F_2$ in Eq. (4.9) may be looked upon as a terminated polynomial of degree $1-\alpha/2$ instead of an m-degree polynomial; thus for $n\geqslant m$ and $\alpha=2,4,6,...$ we have that

$${}_3F_2\left(-\left(\frac{\alpha}{2}-1\right),\gamma-\frac{\alpha}{2},-m;\gamma,1-n-\frac{\alpha}{2};1\right)=\sum_{s=0}^{[\alpha/2-1]}\frac{(-m)_s\left(\gamma-\frac{\alpha}{2}\right)_s\left(1-\frac{\alpha}{2}\right)_s}{s!(\gamma)_s\left(1-\frac{\alpha}{2}-n\right)_s}. \tag{4.11}$$

As a result hereof, the matrix elements (4.9) further simplify into the closed form expressions immediately appearing. These are most suitable for computational purposes as for the case of $\gamma>0$ and $\alpha=0$, we indeed shall have

$$x_{mn}^{0}=\begin{cases}1 & \text{if } n=m\\ 0 & \text{if } n\neq m\end{cases} \tag{4.12}$$

after using Eq. (4.7); as it should have been expected in this specific case. For the case of $\gamma>1$ and $\alpha=2$, we have from Eq. (4.9) that

$$x_{mn}^{-2}=\begin{cases}(-1)^{m+n}\beta\dfrac{\Gamma(\gamma-1)}{\Gamma(\gamma)}\sqrt{\dfrac{n!(\gamma)_m}{m!(\gamma)_n}} & \text{if } n\geqslant m\\ (-1)^{m+n}\beta\dfrac{\Gamma(\gamma-1)}{\Gamma(\gamma)}\sqrt{\dfrac{m!(\gamma)_n}{n!(\gamma)_m}} & \text{if } m\geqslant n.\end{cases} \tag{4.13}$$

On the other hand, if the case is $\gamma>2$ and $\alpha=4$, we then have from Eqs. (4.9) and (4.11) that

$$x_{mn}^{-4}=\begin{cases}(-1)^{m+m}\beta^2\dfrac{\Gamma(\gamma-2)}{\Gamma(\gamma+1)}\sqrt{\dfrac{n!(\gamma)_m}{m!(\gamma)_n}}[\gamma(n-m+1)+2m] & \text{if } n\geqslant m\\ (-1)^{m+n}\beta^2\dfrac{\Gamma(\gamma-2)}{\Gamma(\gamma+1)}\sqrt{\dfrac{m!(\gamma)_n}{n!(\gamma)_m}}[\gamma(m-n+1)+2n] & \text{if } m\geqslant n.\end{cases} \tag{4.14}$$

As a final case that we illustrate, namely $\gamma>3$ and $\alpha=6$, we point to the fact that Eq. (4.9) lets us deduce

$$x_{mn}^{-6}=\begin{cases}(-1)^{m+n}\dfrac{\beta^3}{2}\dfrac{\Gamma(\gamma-3)}{\Gamma(\gamma+2)}\sqrt{\dfrac{n!(\gamma)_m}{m!(\gamma)_n}}[(2+n)(1+n)\gamma(\gamma+1)-2m(1+n)\\ \quad\times(\gamma-3)(\gamma+1)-m(1-m)(\gamma-2)(\gamma-3)] & \text{if } n\geqslant m\\ (-1)^{m+n}\dfrac{\beta^3}{2}\dfrac{\Gamma(\gamma-3)}{\Gamma(\gamma+2)}\sqrt{\dfrac{m!(\gamma)_n}{n!(\gamma)_m}}[(2+m)(1+m)\gamma(\gamma+1)-2n(1+m)\\ \quad\times(\gamma-3)(\gamma+1)-n(1-n)(\gamma-2)(\gamma-3) & \text{if } m\geqslant n.\end{cases} \tag{4.15}$$

Actually, we can derive similar expressions for all even integers beyond 6, i.e., $\alpha=8,10,...$. We point to the cases where $m\geqslant n$, where the derivation is achieved by interchanging the order of the

summation of Eq. (4.2) and applying thereafter Eq. (4.11) in reversed order. The particular case of $A=0$ (or $\gamma=\frac{3}{2}$) and $B=1$, that is, allows us, of course, to recover the result of Aguilera-Navarro *et al.*[6] as a special case.

V. VARIATIONAL APPROACH

In this section we implement the results developed in Sec. IV to calculate the matrix elements of $x^{-\alpha}$ by means of a complete orthonormal basis. Thereby we shall be able to introduce a variational treatment of the spiked harmonic oscillator Hamiltonian given by Eq. (1.1). The principle idea is the representation of the Hamiltonian equation (1.1) as

$$H=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+Bx^2+\frac{\lambda}{x^\alpha}=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+Bx^2+\frac{A}{x^2}+\left(\frac{\lambda}{x^\alpha}-\frac{A}{x^2}\right), \tag{5.1}$$

where, at a later point, $A(\neq 0)$ plays the role of an extra degree of freedom, which shall be determined through a minimization procedure. Although the idea is not complicated, it has many advantages and we mention just a few. First, the range of α is no longer restricted and it can be extended as one pleases, provided the condition $2\gamma>\alpha$ or more explicitly $A>\frac{1}{4}(\alpha-2)^2-\frac{1}{4}$ is satisfied. Second, it substantially reduces the number of basis elements required for the computation of the eigenvalues of the Hamiltonian equation (1.1), even for the intermediate region $\lambda \approx 1$. Third, it be can be adapted effectively and allows easy handling by means of symbolic software such as Mathematica. Fourth, the approach of Aguilera-Navarro *et al.* now becomes a special case, namely set $A=0$ and $B=1$. Fifth, it can be easily extended to the case of N dimensions, where the orbital angular momentum number l is arbitrary, with minor modifications only, as we shall see in Sec. VI.

Let $\psi(x)$ be a *trial function* for Hamiltonian H given by Eq. (5.1), and let us suppose that $\psi(x)$ is expandable as finite linear combinations of the basis functions $\psi_n(x)$ as given by Eq. (3.13), i.e.,

$$\psi(x)=\sum_{n=0}^{D-1} a_n\psi_n(x). \tag{5.2}$$

The problem now is to minimize the eigenenergies of Eq. (5.2) with respect to the variational parameters a_n, $n=0,1,...,D-1$ in the finite dimensional subspace H_D spanned by the D functions ψ_0, $\psi_1,\ldots,\psi_{D-1}$. However, this is equivalent to diagonalizing the Hamiltonian in Eq. (5.2) in the subspace H_D. By separating the Hamiltonian equation (5.1) into two contributions $H_0=-\mathrm{d}^2/\mathrm{d}x^2+Bx^2+Ax^{-2}$ and $H_I=\lambda x^{-\alpha}-Ax^{-2}$, we have

$$H_{mn}=\int_0^\infty \psi_m(x)H\psi_n(x)\mathrm{d}x\equiv\langle\psi_m|H_0|\psi_n\rangle+\langle\psi_m|H_I|\psi_n\rangle,\quad m,n=0,1,2,...,D-1. \tag{5.3}$$

Since the matrix representation of H_0 is diagonal in the basis $\{\psi_n\}_0^\infty$, the first term on the right-hand side of Eq. (5.3) yields the exact solution of Gol'dman and Krivchenkov potential equation (3.6), i.e.,

$$\langle\psi_m|H_0|\psi_n\rangle=2\beta(2n+\gamma)\delta_{mn}\quad(\beta=\sqrt{B},\gamma=1+\tfrac{1}{2}\sqrt{1+4A}),$$

and the second term on the right-hand side of Eq. (5.3) is given by

$$\langle\psi_m|H_I|\psi_n\rangle=\lambda\langle\psi_m|x^{-\alpha}|\psi_n\rangle-A\langle\psi_m|x^{-2}|\psi_n\rangle,$$

where $\langle\psi_m|x^{-\alpha}|\psi_n\rangle$ and $\langle\psi_m|x^{-2}|\psi_n\rangle$ are given by Eqs. (4.9) and (4.13), respectively.

Two important observations follow from these results. First, the matrix elements of the Hamiltonian (5.1) in terms of the Gol'dman and Krivchenkov basis equation (3.13) are given explicitly by $(m,n=0,1,2,...,D-1,n\geqslant m)$

$$H_{mn}=2\beta(2n+\gamma)\delta_{nm}+(-1)^{n+m}\lambda\beta^{\alpha/2}\frac{\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n}\frac{\Gamma\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma(\gamma)}\sqrt{\frac{(\gamma)_n(\gamma)_m}{n!m!}}$$
$$\times {}_3F_2\left(-m,\gamma-\frac{\alpha}{2},1-\frac{\alpha}{2};\gamma,1-n-\frac{\alpha}{2};1\right)-(-1)^{m+n}\frac{A\beta}{\gamma-1}\sqrt{\frac{n!(\gamma)_m}{m!(\gamma)_n}} \tag{5.4}$$

taken over the D-dimensional subspace spanned by basis (3.13). The expressions in Eq. (5.4) are highly suitable for the systematic computer-aided calculations of the energy eigenvalues via diagonalization and subsequent minimization of the matrix

$$\min_A \operatorname{diag}\begin{pmatrix} H_{00} & H_{10} & \cdots & H_{1D-1} \\ H_{10} & H_{11} & \cdots & H_{1D-1} \\ \cdots & \cdots & \cdots & \cdots \\ H_{D-10} & H_{D-11} & \cdots & H_{D-1D-1} \end{pmatrix}. \tag{5.5}$$

Second, by increasing the matrix dimension D, we can always improve these upper energy bounds. In the variational analysis of the ground state energy of the singular potential $V(x)=x^2+\lambda x^{-\alpha}$, Aguilera-Navarro *et al.*[6] utilized an orthonormal basis of harmonic oscillator eigenfunctions on the interval $(0,\infty)$, i.e., the set of Hermite functions generated by the nonsingular harmonic-oscillator potential x^2. This is equivalent to our basis functions for the case $B=1$ and $A=0$, as mentioned earlier. The shortcomings of their approach, however, are as follows. First, validity only holds for $\alpha<3$. Second, a huge set of the basis elements is needed to obtain reasonably accurate eigenvalues, and this even for the intermediate region $(\lambda\approx 1)$.

VI. THE *N*-DIMENSIONAL CASE

In order to extended the scope of our variational analysis to the N-dimensional spiked harmonic oscillator Hamiltonian equation (1.1), we first determine the exact solutions of the N-dimensional Schrödinger equation with a Gol'dman and Krivchenkov potential equation (3.5). To do this, we notice that the A term of the Gol'dman and Krivchenkov potential has the dimensions of kinetic energy, such as the term that appears in higher-dimensional systems. We therefore may replace A in Eq. (3.5) with

$$A\to A+\Lambda(\Lambda+1),\quad \Lambda=l+\tfrac{1}{2}(N-3),\quad N\geqslant 2, \tag{6.1}$$

and thereby obtain an exact solutions of N-dimensional radial Schrödinger equation

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\Lambda(\Lambda+1)}{x^2}+Bx^2+\frac{A}{x^2}\right)\psi_{nl}=E^N_{nl}\psi_{nl}. \tag{6.2}$$

Such exact solutions are generated from the well-known solutions of harmonic oscillator potential by two simple transformations. We first replace the angular momentum l in the harmonic oscillator energy expression $\beta(4n+2l+3)$, $n=0,1,2,...$ by $-\frac{1}{2}+\sqrt{A+(l+\frac{1}{2})^2}$, and subsequently replace l with Λ. Thus, the exact eigenvalues of N-dimensional Schrödinger equation with a Gol'dman and Krivchenkov potential are

$$E^N_{nl}=2\beta(2n+\gamma_N),\quad n,l=0,1,2,..., \tag{6.3}$$

where $\beta=\sqrt{B}$ and $\gamma_N=1+\sqrt{A+(\Lambda+\frac{1}{2})^2}$, while the exact eigenfunctions are given by

$$\psi_{nl}(x)=(-1)^n\sqrt{\frac{2\beta^{\gamma_N}(\gamma_N)_n}{n!\Gamma(\gamma_N)}}x^{\gamma_N-1/2}e^{-(1/2)\beta x^2}\,{}_1F_1(-n;\gamma_N;\beta x^2). \tag{6.4}$$

TABLE I. The rate of convergency for the upper bound of the ground state energy E_0 of the Schrödinger equation $(-\Delta+x^2+\lambda/x^{0.5})\psi=E_0\psi$ for $\lambda=0.1$ and $\lambda=1000$. $E_0^{A=0}$ obtained by diagonalization of the $D\times D$ matrix elements, E_0^A obtained by diagonalization of the $D\times D$ matrix elements then minimizing with respect to the parameter A.

	$\lambda=0.1$		$\lambda=1000$	
$D\times D$	$E_0^{A=0}$	E_0^A	$E_0^{A=0}$	E_0^A
1×1	3.102 277	3.102 185	1025.765 672	415.934 312
2×2	3.102 167	3.102 149	746.081 846	415.932 051
3×3	3.102 151	3.102 143	642.417 430	145.890 659
5×5	3.102 143	3.102 141	549.825 333	415.889 798
10×10	3.102 140	3.102 139 (Exact)	461.349 666	415.889 785 (Exact)

The matrix elements in this case turn out to be

$$\langle\psi_{ml}|x^{-\alpha}|\psi_{nl}\rangle=(-1)^{n+m}\beta^{\alpha/2}\frac{\left(\frac{\alpha}{2}\right)_n}{(\gamma)_n}\frac{\Gamma\left(\gamma_N-\frac{\alpha}{2}\right)}{\Gamma(\gamma_N)}\sqrt{\frac{(\gamma_N)_n(\gamma_N)_m}{n!m!}}$$
$$\times{}_3F_2\left(-m,\gamma_N-\frac{\alpha}{2},1-\frac{\alpha}{2};\gamma_N,1-n-\frac{\alpha}{2};1\right)\quad N\geqslant2. \tag{6.5}$$

Matrix elements for the special cases of $\alpha=2,4,6,...$ are obtained by substituting in Eqs. (4.13)–(4.15) for γ the expression γ_N, where $\gamma_N=1+\sqrt{A+(\Lambda+\frac{1}{2})^2}$. The matrix elements of the Hamiltonian equation (6.2) now turn out to be very similar to those in Eq. (5.4), namely

$$H_{mn}=2\beta(2n+\gamma_N)\delta_{mn}+\lambda\langle\psi_{ml}|x^{-\alpha}|\psi_{nl}\rangle-A\langle\psi_{ml}|x^{-2}|\psi_{nl}\rangle,\quad N\geqslant2. \tag{6.6}$$

Since the purpose of the present work is to consider the variational analysis of the eigenvalues of the Hamiltonian equation (1.1) with Dirichlet boundary condition, we restricted ourselves to the case of $N\geqslant2$ in order to avoid problems stemming from the degeneracy of the spectrum in the case of $N=1$. The one-dimensional case Eq. (5.4) on $L_2(0,\infty)$ is recovered by setting $D=3$ and $l=0$. Further, the recovery of the results of Aguilera-Navarro *et al.* is achieved by substituting $A=0$, $B=1$, $D=3$, and $l=0$ in Eq. (6.6).

VII. NUMERICAL RESULTS

Although the variational method has been used earlier in one form or another, the special form it takes in the present article has a specific purpose. First, the demonstration of the validity of an accurate and uniform approximation not only for the ground state energy of Eq. (1.1), but also for the entire spectrum in arbitrary dimensions with arbitrary angular-momentum number. And second, its applicability to general values of the parameters (α, λ) of the potential, subjected to the restriction $\alpha<2\gamma$. The achievement of these purposes is due to the closed forms we have been able to obtain for the matrix-elements Eq. (4.9). At this point we note that the variational results are upper bounds to the energy levels, in accordance with the variational theorem.

For $\alpha<2$ the variational method gives excellent results for arbitrary value of the coupling λ. The advantage of the minimization process with respect to parameter A is shown in Table I. Herein we compare the numerical values obtained by diagonalization for $\alpha=0.5$ for different dimensions of the matrix equation (5.5) with numerical values obtained by the process of diagonalization and minimization with respect to A. There is an interesting observation, which must be noted here. For given $\alpha<2$, the dimension of the matrix required for obtaining results of a given accuracy depends on the behavior of the coupling λ. For the case where λ is small, however, we can get away with a matrix equation (5.5) of smaller dimension as compared to the case where λ is large. To further

TABLE II. A comparison between the results E^{RP} by means of Ricccati–Padé (Ref. 17) and E^R by means of renomalized series (Ref. 17) and the result of the present work E (correct to seven digits shown) for $\alpha=1$ and various values of the coupling λ.

λ	E^{RP}	E^R	E
0.001	3.001 128	3.001 143	3.001 128
0.01	3.011 276	3.011 417	3.011 276
0.1	3.110 9	3.113 386	3.112 068
1	4.057 906	4.064 649	4.057 888
10	10.577 483	10.577 825	10.577 485

illustrate this point, a one-dimension subspace (1×1 matrix) is adequate for calculating the eigenvalue 3.001 128 (exact to the accuracy quoted) for $\lambda=0.001$ when $\alpha=1$; but for $\lambda=10$, on the other hand, a matrix at least of size 80×80 is necessary to obtain the eigenvalue 10.577 48. In the case of $\alpha=1$, we present in Table II a comparison of our numerical results to some previous work.[17] For $\alpha>2$, the situation is completely reversed.

For $\alpha=2$, the first variational approximation (subspace of dimension one) to the ground state eigenvalues of the spiked harmonic oscillator Hamiltonian is

$$E_0(\alpha=2)=2\beta\gamma+\frac{\lambda\beta}{\gamma-1}-\frac{A\beta}{\gamma-1},\quad \gamma=1+\frac{1}{2}\sqrt{1+4A}. \tag{7.1}$$

The minimization of this expression with respect to the parameter A can be easily performed and leads to $A=\lambda$. On substituting this back into Eq. (7.1) we get $E_0=2\beta(1+\frac{1}{2}\sqrt{1+4A})$, which is the exact result quoted in Eq. (3.6) for $n=0$.

For arbitrary α, the first variational approximation (subspace of dimension 1) of the ground state eigenvalues of the Hamiltonian equation (1.1) is

$$\epsilon_0=\min_A E_0=\min_A\left\{2\beta\gamma+\lambda\beta^{\alpha/2}\frac{\Gamma\left(\gamma-\frac{\alpha}{2}\right)}{\Gamma(\gamma)}-\frac{A\beta}{\gamma-1}\right\},\quad \gamma=1+\frac{1}{2}\sqrt{1+4A}. \tag{7.2}$$

When $D=2$, i.e., subspace of dimension 2, the diagonalization can also be performed analytically via the secular equation, that is to say by means of the expression

$$\epsilon_\pm=\min_A E_\pm=\min_A\{\tfrac{1}{2}[(H_{00}+H_{11})\pm\sqrt{(H_{00}-H_{11})^2+(2H_{01})^2}]\}. \tag{7.3}$$

where $\epsilon_0=\epsilon_-$ and $\epsilon_1=\epsilon_+$. Moreover, one can obtain analytic expressions for upper bound eigenvalues[4] in this case.

Because of the simple formulas for the matrix elements in the cases of $\alpha=4$ and $\alpha=6$ given by (4.14) and (4.15), respectively, the determination of the energy values to any desired accuracy has now been reduced to an easy task. A heuristic scheme for ascertaining the eigenvalues to any required number of digits is as follows. The eigenvalues obtained from successive levels, such as $(1\times1,2\times2,\ldots)$, of the truncated matrix (5.5) are compared, and the calculation ceases when the successive eigenvalues agree with each other up to the prescribed decimal place. It is sufficient, therefore, to use the N-dimensional case for the matrix elements equation (6.5) for calculation purposes. To recover the one-dimensional case, we may set $D=3$ and $l=0$, and to recover the results of Aguilera-Navarro *et al.*, we set $A=0$, $B=1$, $D=3$, and $l=0$. Table III illustrates the use of this procedure for the case of $\alpha=4$ and $\lambda=1000$ in the dimensions $N=2-10$.

Another advantage of the variational approach presented herein is the amount of information that we get about the spectrum of the Hamiltonian equation (1.1) every time we compute the eigenvalues via the diagonalization and minimization. Indeed, we obtain for an arbitrary matrix

TABLE III. Upper bounds E^U for $H=-\Delta+x^2+1000/x^4$ for dimension $N=2-10$, obtained by diagonalization then minimization of the 30×30 matrix elements. The "exact" values E were obtained by direct numerical integration of Schrödinger's equation.

N	E^U	E
2	21.350 246	21.350 246
3	21.369 463	21.369 463
4	21.427 056	21.427 056
5	21.522 859	21.522 859
6	21.656 596	21.656 596
7	21.827 883	21.827 883
8	22.036 232	22.036 232
9	22.281 057	22.281 057
10	22.561 680	22.561 680

(5.5) of size D a set of upper bounds for the eigenvalues $E_0, E_l, \ldots, E_{D-1}$. Each can be improved by either an increase in the dimension of the matrix, or by extracting the desired level through the diagonalization and thereafter minimizing with respect to parameter A, which is illustrated in Table V.

For $\alpha>2$ and small values of λ, the variational method is still applicable, however the eigenvalues converge very slowly, and an immense number of matrix elements are needed in order to obtain accurate results. In principle, the method is still effective as we see from Table V, but at the expense of using a huge number of matrix elements. On the other hand, we obtained accurate eigenvalues with the use of a modest number of matrix elements for λ varying between 1000 and 0.01, as Table VI indicates. An interesting explanation of this lies in the following comment. Let us look at the perturbed Hamiltonian

$$H=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+x^2+\frac{A}{x^2}+\epsilon\left(\frac{\lambda}{x^\alpha}-\frac{A}{x^2}\right) \tag{7.4}$$

instead of the one given by Eq. (5.1), and solve the matrix eigenvalue problem by expanding the determinant in powers of ϵ up to and including ϵ^2. It is well known[6] that we shall end up with the perturbation-like formula (after setting $\epsilon=1$)

$$E=E_0+\lambda\langle\psi_0|x^{-\alpha}|\psi_0\rangle-A\langle\psi_0|x^{-2}|\psi_0\rangle-\sum_{n\neq0}^{D}\frac{|\langle\psi_0|\lambda x^{-\alpha}-Ax^{-2}|\psi_n\rangle|^2}{E_n-E_0}, \tag{7.5}$$

where the summation on the right-hand side is finite and D is the number of the basis functions used. By analyzing this sum, we shall come to understand the slow convergence of the eigenvalues calculated by means of the variational approach. For the sake of simplicity, let us restrict ourselves to the case of $\alpha=4$. With the aid of Eqs. (4.13) and (4.14), the sum in Eq. (7.5) becomes

TABLE IV. For arbitrary size $D\times D$ of the matrix (5.5) for $H=-\Delta+x^2+1000/x^4$, a set of upper bounds for the eigenvalues $E_0, E_1, \ldots, E_{D-1}$ that can improve by increasing the size D.

1×1	2×2	3×3	4×4	5×5	6×6	7×7
21.427 79	21.382 12	21.374 00	21.370 07	21.369 72	21.369 51	21.369 46
	26.298 42	26.189 48	26.166 99	26.155 44	26.154 18	26.153 40
		31.097 17	30.919 24	30.878 34	30.856 56	30.851 94
			35.834 86	35.587 50	35.525 79	35.492 11
				40.520 33	40.205 49	40.121 62
					45.160 79	44.781 42
						49.762 16

TABLE V. Upper bounds E^U for $H=-\mathrm{d}^2/\mathrm{d}x^2+x^2+\lambda/x^\alpha$ ($\alpha=4$ and 6), for small values of λ, obtained by diagonalization of the $D\times D$ matrix elements then minimizing with repect to the parameter A.

	$\lambda=0.0025$		$\lambda=0.005$		$\lambda=0.01$	
E	$\alpha=4$	$\alpha=6$	$\alpha=4$	$\alpha=6$	$\alpha=4$	$\alpha=6$
E^{DKa}	3.106 70	3.353 95	3.148 39	3.423 02	3.205 27	3.505 74
$E^{H\mathrm{b}}$	3.037 61	3.068 22	3.053 19	3.081 13	3.075 22	3.096 48
$E^{K\mathrm{c}}$	3.106 81	3.353 92	3.148 35	3.422 88	3.205 07	3.505 45
$E^{P\mathrm{d}}$	3.103 77	3.343 05	3.146 64	3.413 16	3.204 42	3.496 88
$E^{L\mathrm{e}}$	3.106 81	3.353 92	3.148 35	3.422 88	3.205 07	3.505 45
$E^{U\mathrm{f}}$	3.107 95	3.354 095	3.149 00	3.422 95	3.205 48	3.505 49

[a]From Ref. 14.
[b]From Ref. 1.
[c]From Ref. 32. Richardson extrapolation. Correct to the six digits shown.
[d]From Padé approximant technique (see Ref. 23).
[e]From the Lanczos/grid method (see Ref. 23). Correct to the six digits shown.
[f]From the present work.

$$\sum_{n\neq 0}^{D}\frac{|\langle\psi_0|\lambda x^{-4}-Ax^{-2}|\psi_n\rangle|^2}{E_n-E_0}=\frac{1}{4}\frac{\Gamma^2(\gamma-2)}{\Gamma^2(\gamma)}\left[\lambda^2\sum_{n=1}^{D}\frac{(n+1)!}{(\gamma)_n}+2\lambda(\lambda-A(\gamma-2))\sum_{n=1}^{D}\frac{(n+1)!}{n(\gamma)_n}+(\lambda-A(\lambda-2))^2\sum_{n=1}^{D}\frac{(n+1)!}{n^2(\gamma)_n}\right] \tag{7.6}$$

in this case. For $D\to\infty$, the sums on the right-hand side of Eq. (7.6) have closed-form expressions in terms of hypergeometric functions, particularly

$$\sum_{n\neq 0}^{\infty}\frac{|\langle\psi_0|\lambda x^{-4}-Ax^{-2}|\psi_n\rangle|^2}{E_n-E_0}=\frac{1}{2\gamma}\frac{\Gamma^2(\gamma-2)}{\Gamma^2(\gamma)}[\lambda^2\,{}_2F_1(3,1;\gamma+1;1)+2\lambda(\lambda-A(\gamma-2))\,{}_3F_2(3,1,1;2,\gamma+1;1)+(\lambda-A(\gamma-2))^2\,{}_4F_3(3,1,1,1;2,2,\gamma+1;1)]. \tag{7.7}$$

Herein the conditions of the convergence of hypergeometric functions[48] guarantee that the function ${}_2F_1$ converges for $\gamma>3$, the function ${}_3F_2$ converges for $\gamma>2$, and ${}_4F_3$ converges for $\gamma>1$. Thus, Eq. (7.7) holds for $\gamma>3$ or $A>3.75$ in general, but for $\alpha=4$, the matrix *elements* equation (4.9) holds for $\gamma>2$ or $A>0.75$. This demonstrates the difficulties one encounters with the variational method for small value of λ. To understand this further, we note the relation between λ and the parameter A. Thus for λ that is small, A is small; on the other hand, λ large implies that A is large. This is evident from the first variational approximation, namely Eq. (7.2) yields

TABLE VI. A comparison between the results E^F of Fernández (Ref. 24), and the results E^{HS} of Hall *et al.* (Ref. 29) and the result of the present work E^{HSK} (correct to seven digits shown) for $\alpha=4$ and $\alpha=6$ and various values of the coupling λ.

	$\alpha=4$			$\alpha=6$		
λ	E_0^F	E_0^{HS}	E_0^{HSK}	E_0^F	E_0^{HS}	E_0^{HSK}
1000	21.384 46	21.370 26	21.369 462	12.737 60	12.725 65	12.718 617
100	11.292 41	11.265 86	11.265 080	8.422 60	8.420 96	8.413 358
10	6.649 78	6.609 66	6.606 622	6.016 40	6.014 94	6.003 209
1	4.548 79	4.504 16	4.494 179	4.676 88	4.684 97	4.659 940
0.1	3.626 44	3.600 44	3.575 557	4.019 15	4.042 84	3.915 665
0.01	3.237 75	3.249 80	3.205 486	3.524 93	3.580 70	3.505 492

$$\epsilon_0 = \min_A \left\{ 2\gamma + \frac{\lambda}{(\gamma-1)(\gamma-2)} - \frac{A}{\gamma-1} \right\}, \quad \gamma = 1 + \frac{1}{2}\sqrt{1+4A}. \tag{7.8}$$

After differentiating Eq. (7.8) with respect to A, it can be shown that the relation between A and λ is implicitly given by

$$\lambda = \frac{(\gamma-2)^2(4(\gamma-1)^2-1)}{4(2\gamma-3)}, \tag{7.9}$$

from which it is quite easy to see that λ is an increasing function of γ for all $\gamma > 2$. Thus for Eq. (7.7) to converge, we must have $\gamma > 3$, i.e., $\lambda > 1.25$. This demonstrates that for $\lambda < 1.25$, the accuracy of the eigenvalue calculations by means of the variational method necessitates a matrix of very large order.

VIII. CONCLUSION

In this paper we have carried our study of the spiked harmonic-oscillator problem further by expressing the Hamiltonian H given by Eq. (1.1) as the perturbation of the singular Gol'dman and Krivchenkov Hamiltonian $H_0 = -\mathrm{d}^2/\mathrm{d}x^2 + Bx^2 + A/x^2$, where the expression $\lambda x^{-\alpha} - Ax^{-2}$ is looked upon as the perturbation term. We have provided a compact proof of the fact that the eigenfunctions of order 0 generated by H_0 form a suitable singularity-adapted basis for the appropriate Hilbert space of the full problem. Our principal results are fourfold: (1) the proof of the completeness of the orthogonal set of normalized eigenvalues of H_0 by means of the domains of convergence, absolute convergence, holomorphy of the Laplace transform; (2) the derivation of the compact closed form (1.3) for the matrix elements $x_{mn}^{-\alpha}$ via infinite integrals of products of two confluent hypergeometric functions; (3) a variational method applied to our perturbation of the Hamiltonian H_0, which proves to be very effective for accurate calculation of the eigenvalues of the spiked harmonic oscillator, as the accompanying numerical calculations verify; (4) we show that this variational approach is applicable to the entire discrete spectrum for the spiked harmonic oscillator in N dimensions.

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The noncommutative harmonic oscillator in more than one dimension

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The noncommutative harmonic oscillator, with noncommutativity not only in position space but also in phase space, in arbitrary dimension is examined. It is shown that the $\star$-genvalue problem, which replaces the Schrödinger problem in this case, can be decomposed into separate harmonic oscillator equations for each dimension. The two-dimensional noncommutative harmonic oscillator (four noncommutative phase-space dimensions) is investigated in greater detail. The requirement of the existence of rotationally symmetric solutions leads to a two parameter harmonic oscillator which is completely solved in this case. The angular momentum operator is derived and its $\star$-genvalue problem is shown to be equivalent to the usual eigenvalue problem of the $\star$-genfunction related wave function. The $\star$-genvalues of the angular momentum are found to depend on the energy difference of the oscillations in the two dimensions. Furthermore two examples of a symmetric noncommutative harmonic oscillators are analyzed. The first is the noncommutative two-dimensional Landau problem with harmonic oscillator potential, which shows degeneracy in the energy levels for certain critical values of the noncommutativity parameters, and the second is the three-dimensional harmonic oscillator with noncommuting coordinates and momenta. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1416196]

I. INTRODUCTION

Deformation quantization,[1] through $\star$-product (originally discovered by Groenewold),[2] has recently been receiving increasing attention in field theories on R^d, string theories, and M theory.[3–6]

Recently, in string theory it was realized[7] that the introduction of a constant B field gives rise to noncommutative open string end points, which in turn generate noncommutative D-brane configuration spaces.

The appearance of noncommutative spaces helped to revive the deformation quantization technique of Moyal.[7] This technique was elucidated further in Refs. 8 and 9. In this setup the ordinary product was replaced by the pivotal associative noncommutative $\star$-product, which is essentially unique in flat space.[10] The one-dimensional Schrödinger equation was replaced by the $\star$-genvalue equation, while the wave functions became Wigner functions. The advantage of this approach with respect to the formalism developed in Ref. 11 is that it allows noncommutativity to be introduced in phase space and not just in configuration space.

In the present work we consider the $\star$-genvalue problem for the n-dimensional noncommutative harmonic oscillator ($2n$ phase-space dimensions) with phase-space noncommutativity (the commutative n-dimensional harmonic oscillator with a general quadratic Hamiltonian was studied in Ref. 12). It is again shown that the $\star$-genvalue problem is equivalent to the Schrödinger problem in a suitable representation of the algebra, stemming from the Heisenberg algebra repre-

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sentation of transformed phase-space variables. The energy eigenvalues and eigenfunctions are determined as functions of the noncommutativity parameters.

The case of the two-dimensional harmonic oscillator is examined thoroughly. The angular momentum operator is derived in the rotationally symmetric case. It is shown that the $\star$-genvalues for the function corresponding to this operator contain, apart from the usual angular momentum eigenvalues, a term that depends on the energy difference of the oscillations in the two dimensions.

In the asymmetric two-dimensional case critical values of the noncommutativity parameters arise. For these values the energy spectrum becomes infinitely degenerate at every level. This problem can be identified with the noncommutative Landau problem in harmonic oscillator potential.

The main motivation for studying so extensively the noncommutative harmonic oscillator is its importance in the noncommutative quantization of field theory, as explored in Ref. 13.

The paper is organized as follows.

In Sec. II we summarize known results, namely the definition of the Moyal product of functions in phase space through the Weyl ordering prescription and the equivalence of the stationary $\star$-genvalue problem in one-dimension to the corresponding Schrödinger problem.

Section III is dedicated to the study of the two-dimensional harmonic oscillator $\star$-genvalue equation for a simple case of nontrivial commutation relations. The $\star$-genvalues and functions are determined for the corresponding Hamiltonian by solving the imaginary and real part equations of the $\star$-genvalue equation.

In Sec. IV the $\star$-genvalue problem for the Hamiltonian and the angular momentum, in the two-dimensional problem of Sec. III, is investigated further. The Hamiltonian $\star$-genvalue problem is shown to be equivalent to the Schrödinger eigenvalue problem for an appropriate action of the position and momentum operators on the space of functions (see Ref. 14). The $\star$-genvalue problem for the angular momentum is also shown to be equivalent to the eigenvalue problem of the corresponding operator for the above-mentioned action of position and momentum operators. Finally, the $\star$-genvalues of the angular momentum are shown to depend also on the energy difference of the oscillations in the two dimensions.

In Sec. V the existence of rotationally symmetric $\star$-genfunctions imposes constraints on the possible commutation relations of the n-dimensional harmonic oscillator. In two dimensions these constraints are solved explicitly, leading to commutation relations that depend on two parameters, and the $\star$-genvalue problem for the corresponding noncommutative Hamiltonian is solved. The angular momentum, which is the generator of rotations, is constructed again and its $\star$-genvalues are computed.

Finally Sec. VI copes with the most general phase-space commutation relations. We show that it is possible, through orthogonal transformations, to bring the matrix realizing the commutation relations into a standard symplectic form. In this way we can compute the energy levels, $\star$-genfunctions and the $\star$-commutation relation of creation and annihilation operator-related functions for the n-dimensional harmonic oscillator. As a first application we consider the physically interesting Landau problem of a charged particle in the noncommutative plane in the presence of a constant magnetic field with a harmonic oscillator potential.[15] We find a critical point for the magnetic field at which the energy levels are infinitely degenerate. As a second application the three-dimensional noncommutative harmonic oscillator (in six phase-space dimensions) is considered.

II. OVERVIEW OF THE WIGNER FUNCTIONS AND THE ★-GENVALUE PROBLEM

Let us start with a classical Hamiltonian $H(q,p)=p^2/2m+V(q)$ in one dimension. Upon quantization the canonical variables q,p become operators $\hat{q},\hat{p}$ satisfying the canonical commutation relations $[\hat{q},\hat{p}]=i\hbar$. One way to define the $\star$-product is via the Weyl map, which is a linear map from the classical phase-space functions to quantum operators. Thus we now consider monomials of the form $q^m p^n$ with m,n positive integers. To define the corresponding operator product it is possible to use the Weyl ordering prescription:[16]

$$\hat{W}(q^m p^n)=\frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}\hat{p}^{n-k}\hat{q}^m\hat{p}^k \tag{1}$$

according to which the $\hat{W}(q^m p^n)$ operator is symmetrized in $\hat{q}$ and $\hat{p}$ by use of Heisenberg's commutation relation. This regularization scheme can be extended to act on arbitrary power series functions $f(q,p)$ through linearity. Thus, Weyl ordering is an invertible map from the space of functions on the phase space to the space of quantum operators. We can now use Weyl ordering to define a new product between functions on the phase space:[8,16]

$$\begin{aligned} f(q,p)\star g(q,p)&=\hat{W}^{-1}(\hat{W}(f)\hat{W}(g))\\ &=f(q,p)e^{i(\hbar/2)(\overleftarrow{\partial}_q\overrightarrow{\partial}_p-\overleftarrow{\partial}_p\overrightarrow{\partial}_q)}g(q,p)\\ &=f\left(q+i\frac{\hbar}{2}\overrightarrow{\partial}_p,p-i\frac{\hbar}{2}\overrightarrow{\partial}_q\right)g(q,p). \end{aligned} \tag{2}$$

This is the celebrated $\star$-product which enjoys the properties of noncommutativity, associativity, and uniqueness.

In phase space one can define Wigner quasidistribution functions to calculate matrix elements of observables. The time-independent Wigner function corresponding to a pair of eigenstates $|\psi_n\rangle,|\psi_m\rangle$ of the Schrödinger problem, $\hat{H}|\psi_n\rangle=E_n|\psi_n\rangle$, is represented in two phase-space dimensions by[7]

$$f_{mn}(q,p)=\frac{1}{2\pi}\int \mathrm{d}y\, e^{-iyp}\left\langle q-\frac{\hbar}{2}y\middle|\psi_n\right\rangle\left\langle\psi_m\middle|q+\frac{\hbar}{2}y\right\rangle=f^*_{nm}(q,p), \tag{3}$$

where an asterisk stands for complex conjugation. In this case, one can show by employing the Schrödinger equation and the definition of the star product (2) that Wigner functions obey the $\star$-genvalue equations:[9]

$$H(q,p)\star f_{mn}(q,p)=E_n f_{mn}(q,p),\quad f_{mn}(q,p)\star H(q,p)=E_m f_{mn}(q,p). \tag{4}$$

In (3) for complete sets $|\psi_n\rangle$ one can also derive the completeness relation:

$$\sum_{m,n} f_{mn}(q,p)f^*_{mn}(q',p')=\frac{1}{2\pi\hbar}\,\delta(q-q')\,\delta(p-p'), \tag{5}$$

which enables the construction of arbitrary phase-space functions in terms of $f_{mn}(q,p)$.

For the diagonal case [$m=n$ in (3)] one can prove that the Wigner functions satisfy the diagonal $\star$-genvalue equation:

$$H(q,p)\star f_n(q,p)=f_n(q,p)\star H(q,p)=E_n f_n(q,p) \tag{6}$$

and the orthogonality relation:

$$f_m\star f_n=\frac{1}{2\pi\hbar}\,\delta_{m,n}f_m\,. \tag{7}$$

Furthermore, the real solutions of (6) are required to be of the Wigner type for the wave functions of $\hat{H}|\psi_n\rangle=E_n|\psi_n\rangle$.[8] So, instead of solving the one-dimensional Schrödinger equation one can try to solve the $\star$-genvalue equation to determine directly the diagonal Wigner functions and the corresponding energy spectrum.

III. A TWO-DIMENSIONAL HARMONIC OSCILLATOR

In this case we have four coordinates (q_i,p_j), with $i,j=1,2$, in phase space. The classical Hamiltonian for this model is

$$H(q_i,p_j)=\frac{1}{2}\sum_{i=1}^{2}(q_i^2+p_i^2), \tag{8}$$

where, without loss of generality, parameters have been absorbed in the phase-space variables. Quantum mechanically, the position and momentum operators satisfy the Heisenberg commutation relations. Here we will extend this realization to include nontrivial commutation relations for $\hat{q}_1$, $\hat{q}_2$ and $\hat{p}_1$, $\hat{p}_2$:

$$[\hat{q}_i,\hat{p}_j]=i\hbar\,\delta_{ij},\quad [\hat{q}_1,\hat{q}_2]=i\theta,\quad [\hat{p}_1,\hat{p}_2]=-i\theta, \tag{9}$$

where θ is a real constant. The related star product takes the form:

$$\star=\exp\left[\frac{i}{2}(\overleftarrow{\partial}_{q_1},\overleftarrow{\partial}_{p_1},\overleftarrow{\partial}_{q_2},\overleftarrow{\partial}_{p_2})\begin{pmatrix}0&\hbar&\theta&0\\-\hbar&0&0&-\theta\\-\theta&0&0&\hbar\\0&\theta&-\hbar&0\end{pmatrix}\begin{pmatrix}\vec{\partial}_{q_1}\\\vec{\partial}_{p_1}\\\vec{\partial}_{q_2}\\\vec{\partial}_{p_2}\end{pmatrix}\right]. \tag{10}$$

The resulting $\star$-genvalue equation is

$$\left[\left(q_1+\frac{i\hbar}{2}\partial_{p_1}+\frac{i\theta}{2}\partial_{q_2}\right)^2+\left(p_1-\frac{i\hbar}{2}\partial_{q_1}-\frac{i\theta}{2}\partial_{p_2}\right)^2+\left(q_2+\frac{i\hbar}{2}\partial_{p_2}-\frac{i\theta}{2}\partial_{q_1}\right)^2+\left(p_2-\frac{i\hbar}{2}\partial_{q_2}+\frac{i\theta}{2}\partial_{p_1}\right)^2\right]f(q_1,p_1,q_2,p_2)=2Ef(q_1,p_1,q_2,p_2). \tag{11}$$

Equation (11) splits into an equation for the imaginary part,

$$[\hbar(p_1\partial_{q_1}-q_1\partial_{p_1})+\hbar(p_2\partial_{q_2}-q_2\partial_{p_2})+\theta(q_2\partial_{q_1}-q_1\partial_{q_2})+\theta(p_1\partial_{p_2}-p_2\partial_{p_1})]f=0 \tag{12}$$

and an equation for the real part:

$$\left[(q_1^2+p_1^2+q_2^2+p_2^2)-\frac{(\hbar^2+\theta^2)}{4}(\partial_{q_1}^2+\partial_{p_1}^2+\partial_{q_2}^2+\partial_{p_2}^2)\right]f=2Ef. \tag{13}$$

Equation (12) admits a solution of the form $f(z)$ with $z=2(q_1^2+p_1^2+q_2^2+p_2^2)=4H$. The real part-equation (13) transforms to the ordinary differential equation:

$$\left[z\partial_z^2+2\partial_z+\frac{1}{(\hbar^2+\theta^2)}\left(E-\frac{z}{4}\right)\right]f(z)=0. \tag{14}$$

The problem with this reduction is the inconsistency underlying the number of degrees of freedom. We started with the two-dimensional harmonic oscillator and we ended up with one oscillation equation. So we need to search for a set of transformations that will preserve the number of degrees of freedom. An appropriate set of transformations is

$$\overline{q}_1=q_1,\quad \overline{p}_1=\frac{1}{\sqrt{\hbar^2+\theta^2}}(\hbar_{p_1}+\theta_{q_2}), \tag{15}$$

$$\overline{q_2}=\frac{1}{\sqrt{\hbar^2+\theta^2}}(\hbar q_2-\theta p_1),\quad \overline{p_2}=p_2.$$

The imaginary part equation is then written as

$$[(\overline{p_1}\partial_{\overline{q_1}}-\overline{q_1}\partial_{\overline{p_1}})+(\overline{p_2}\partial_{\overline{q_2}}-\overline{q_2}\partial_{\overline{p_2}})]f=0. \tag{16}$$

This implies that f is a function of $z_1=2(\overline{q_1}^2+\overline{p_1}^2)$ and $z_2=2(\overline{q_2}^2+\overline{p_2}^2)$. The real part equation transforms under the new variables into

$$\left[z_1\partial_{z_1}^2+\partial_{z_1}+z_2\partial_{z_2}^2+\partial_{z_2}+\frac{1}{(\hbar^2+\theta^2)}\left(E-\frac{(z_1+z_2)}{4}\right)\right]f(z_1,z_2)=0. \tag{17}$$

The diagonal $\star$-genfunctions $f_{nm}(z_1,z_2)$ (not to be confused with the nondiagonal Wigner functions in one dimension) associated with this equation are determined through products of Laguerre polynomials:

$$f_{nm}(\tilde{z}_1,\tilde{z}_2)=e^{-(1/2)(\tilde{z}_1+\tilde{z}_2)}L_n(\tilde{z}_1)L_m(\tilde{z}_2), \tag{18}$$

where

$$L_m(\tilde{z}_i)=\frac{1}{m!}e^{\tilde{z}_i}\frac{d^m}{d^m\tilde{z}_i}(e^{-\tilde{z}_i}\tilde{z}_i^m) \tag{19}$$

and $L_0(\tilde{z}_i)=1$, $L_1(\tilde{z}_i)=1-\tilde{z}_i$, $L_2(\tilde{z}_i)=1-2\tilde{z}_i+\tilde{z}_i^2/2$,... with $\tilde{z}_i=z_i/\sqrt{\hbar^2+\theta^2}$. The energies corresponding to these $\star$-genfunctions are

$$E_{nm}=\sqrt{\hbar^2+\theta^2}(n+m+1). \tag{20}$$

The functions corresponding to the annihilation and creation operators are given in terms of the transformed variables as

$$a_i=\frac{1}{\sqrt{2}}(\overline{q_i}+i\overline{p_i}),\quad a_i^\dagger=\frac{1}{\sqrt{2}}(\overline{q_i}-i\overline{p_i}). \tag{21}$$

It is possible to express these functions in terms of the original phase-space variables by reversing our transformations. They satisfy the following modified commutation relations:

$$a_i\star a_j^\dagger-a_j^\dagger\star a_i=\delta_{ij}\sqrt{\hbar^2+\theta^2} \tag{22}$$

and $a_i\star f_{00}(\overline{q_i},\overline{p_i})=0$. They generate the $\star$-Fock space of states as follows:

$$f_{nm}\propto a_1^{\dagger n}a_2^{\dagger m}\star f_{00}\star a_2^m a_1^n. \tag{23}$$

The Hamiltonian takes the following form:

$$H=\sum_{i=1}^{2}\left(a_i^\dagger\star a_i+\frac{\sqrt{\hbar^2+\theta^2}}{2}\right). \tag{24}$$

This completes the solution of the two-dimensional harmonic oscillator $\star$-genvalue problem for the commutation relations we started with.

IV. RELATION TO SCHRÖDINGER EQUATION

In the one-dimensional case the $\star$-genvalue equation is equivalent to the Schrödinger equation, as was shown in Ref. 8. However, in the two-dimensional case one has to search for a suitable representation of the commutation relations before writing down a Schrödinger equation. This problem can be overcome for the harmonic oscillator of Sec. III by using the transformations (15), to transform the commutation relations to two sets of Heisenberg commutation relations with $\hbar$ replaced by $\sqrt{\hbar^2+\theta^2}$, and using the usual representation of the Heisenberg commutation relations in the Hamiltonian. The Schrödinger equation with respect to the new variables becomes

$$\frac{1}{2}\sum_{i=1}^{2}(\hat{\overline{q}}_i^2+\hat{\overline{p}}_i^2)\Psi(\overline{q}_i)=E\Psi(\overline{q}_i) \tag{25}$$

and its eigenfunctions are given by

$$\Psi_{nm}(\overline{q}_i)=\Psi_n(\overline{q}_1)\Psi_m(\overline{q}_2), \tag{26}$$

where Ψ_n are the usual eigenfunctions of the one-dimensional harmonic oscillator. This equation splits into two one-dimensional harmonic oscillator equations. Making use of the one-dimensional equivalence of the Schrödinger problem to the $\star$-genvalue problem we obtain that Eq. (25) (with $\hbar$ replaced by $\sqrt{\hbar^2+\theta^2}$) is equivalent to

$$H(\overline{q}_i,\overline{p}_i)\overline{\star}\overline{f}(\overline{q}_i,\overline{p}_i)=\overline{f}(\overline{q}_i,\overline{p}_i)\overline{\star}H(\overline{q}_i,\overline{p}_i)=E\overline{f}(\overline{q}_i,\overline{p}_i), \tag{27}$$

where

$$\begin{aligned}\overline{f}(\overline{q}_i,\overline{p}_j)&=\overline{f}(\overline{q}_1,\overline{p}_1)\overline{f}\overline{f}(\overline{q}_2,\overline{p}_2)\\&=\frac{1}{(2\pi)^2}\int\int \mathrm{d}y_1\,\mathrm{d}y_2\,e^{-iy_1\overline{p}_1}e^{-iy_2\overline{p}_2}\\&\quad\times\prod_{i=1}^{2}\Psi_i^*\left(\overline{q}_i-\frac{1}{2}\sqrt{\hbar^2+\theta^2}y_i\right)\Psi_i\left(\overline{q}_i+\frac{1}{2}\sqrt{\hbar^2+\theta^2}y_i\right)\\&\equiv\frac{1}{(2\pi)^2}\int\int \mathrm{d}y_1\,\mathrm{d}y_2\,e^{-iy_1\overline{p}_1}e^{-iy_2\overline{p}_2}\prod_{i=1}^{2}\Psi_i^*\Psi_i\,.\end{aligned} \tag{28}$$

The $\overline{\star}$-product, which is the transformed version of the $\star$-product defined in (10), is

$$\overline{\star}=\exp\left[\frac{i}{2}\sqrt{\hbar^2+\theta^2}\sum_{i=1}^{2}(\overleftarrow{\partial}_{\overline{q}_i}\overrightarrow{\partial}_{\overline{p}_i}-\overleftarrow{\partial}_{\overline{\mu}_i}\overrightarrow{\partial}_{\overline{q}_i})\right]. \tag{29}$$

So we have shown that the Schrödinger problem, in the representation of $\hat{q}^i,\hat{p}^j$ defined by the Heisenberg representation of $\hat{\overline{q}}^i,\hat{\overline{p}}^j$, is equivalent to the $\star$-genvalue problem (11).

Next let us investigate what happens with the angular momentum. The phase-space function corresponding to the operator that commutes with the Hamiltonian and generates rotations in the original variables is

$$L=\frac{\hbar}{\hbar^2+\theta^2}\left[\hbar(q_1p_2-q_2p_1)+\frac{\theta}{2}(p_1^2-q_1^2+p_2^2-q_2^2)\right]. \tag{30}$$

Transforming this to the new variables (15) gives

$$\overline{L}(\overline{q}_i,\overline{p}_j)=\frac{\hbar}{\hbar^2+\theta^2}\left[\hbar(\overline{q}_1\overline{p}_2-\overline{q}_2\overline{p}_1)+\frac{\theta}{2}(\overline{q}_2^2+\overline{p}_2^2-\overline{q}_1^2-\overline{p}_1^2)\right]. \tag{31}$$

The angular momentum $\star$-genvalue equation becomes

$$\begin{aligned}
&L(q_i,p_i)\star f(q_i,p_i)\\
&\quad=\overline{L}(\overline{q}_i,\overline{p}_i)\star\overline{f}(\overline{q}_i,\overline{p}_i)\\
&\quad=\frac{1}{(2\pi)^2}\frac{\hbar}{(\hbar^2+\theta^2)}\left[\hbar\left[\overline{q}_1\left(\overline{p}_2-\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_2}\right)-\overline{q}_2\left(\overline{p}_1-\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_1}\right)\right]\right.\\
&\qquad\left.+\frac{\theta}{2}\left[\overline{q}_2^2+\left(\overline{p}_2-\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_2}\right)^2-\overline{q}_1^2-\left(\overline{p}_1-\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_1}\right)^2\right]\right]\\
&\qquad\times\int \mathrm{d}y_1\,\mathrm{d}y_2\exp\left(-iy_1\left(\overline{p}_1+\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_1}\right)\right)\\
&\qquad\times\exp\left(-iy_2\left(\overline{p}_2+\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_2}\right)\right)\prod_{i=1}^{2}\Psi_i^*\Psi_i\\
&\quad=\frac{1}{(2\pi)^2}\frac{\hbar}{(\hbar^2+\theta^2)}\int\int \mathrm{d}y_1\,\mathrm{d}y_2\,e^{-iy_1\overline{p}_1}e^{-iy_2\overline{p}_2}\\
&\qquad\times\left[\hbar\left[\left(\overline{q}_1+\frac{1}{2}\sqrt{\hbar^2+\theta^2}y_1\right)\left(-i\partial_{y_2}-\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_2}\right)\right.\right.\\
&\qquad\left.-\left(\overline{q}_2+\frac{1}{2}\sqrt{\hbar^2+\theta^2}y_2\right)\left(-i\partial_{y_1}-\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_1}\right)\right]\\
&\qquad+\frac{\theta}{2}\left[\left(\overline{q}_2+\frac{1}{2}\sqrt{\hbar^2+\theta^2}y_2\right)^2+\left(-i\partial_{y_2}-\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_2}\right)^2-\left(\overline{q}_1+\frac{1}{2}\sqrt{\hbar^2+\theta^2}y_1\right)^2\right.\\
&\qquad\left.\left.-\left(-i\partial_{y_1}-\frac{i}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_1}\right)^2\right]\right]\prod_{i=1}^{2}\Psi_i^*\Psi_i\\
&\quad=\frac{\hbar}{(\hbar+\theta^2)}[\hbar\sqrt{\hbar^2+\theta^2}m_z+\theta(E_2-E_1)]\overline{f}(\overline{q}_i,\overline{p}_j).
\end{aligned}\tag{32}$$

Here we have used $\overline{p}_ie^{-iy_i\overline{p}_i}=i\partial_{yi}e^{-iy_i\overline{p}_i}$ and partial integration has been performed. Note that

$$\left(\partial_{y_i}+\frac{1}{2}\sqrt{\hbar^2+\theta^2}\vec{\partial}_{\overline{q}_i}\right)\Psi^*\left(\overline{q}_i-\frac{\sqrt{\hbar^2+\theta^2}}{2}y_i\right)=0.$$

The discrete values m_z are the eigenvalues of the angular momentum for the commutative two dimensional harmonic oscillator:

$$\hat{L}\Psi(\overline{q}_i)=(\hat{\overline{q}}_1\hat{\overline{p}}_2-\hat{\overline{q}}_2\hat{\overline{p}}_1)\Psi(\overline{q}_i)=\sqrt{\hbar^2+\theta^2}m_z\Psi(\overline{q}_i). \tag{33}$$

What we have essentially proven is that the solution of the $\star$-genvalue problem for the angular momentum is equivalent to the solution of the eigenvalue problem for the angular momentum operator in the representation we began with. We observe that we pick an extra new term that depends on the energy difference of the two oscillations and is linear in the noncommutativity parameter θ.

V. ROTATIONALLY SYMMETRIC CASE

Up to this point we have considered only the case where $\hat{q}_i$ commute with $\hat{p}_j$, for $i \neq j$, and the $\hat{q}_i, \hat{p}_j$ behave symmetrically, that is $[\hat{q}_1, \hat{q}_2] = -[\hat{p}_1, \hat{p}_2]$. Let us consider the more general situation where the commutation relations are governed by a general antisymmetric matrix M in $2n$ phase-space dimensions. In this case the $\star$-product reads:

$$\star = \exp \frac{i}{2} [\overleftarrow{\partial}_I^T M_{IJ} \vec{\partial}_J], \tag{34}$$

where $\partial_I^T = (\partial_{q_I}, \partial_{p_I})$, and $M_{IJ} = -M_{JI}^T$ are 2×2 matrix blocks. Here the summation convention is assumed. The imaginary part of the $\star$-genvalue equation, generalizing (12) now becomes

$$X_I^T M_{IJ} \partial_J f = 0, \tag{35}$$

where $X_I^T = (q_I, p_I)$. If f is rotationally symmetric, that is $f \equiv f(X_I^T X_I)$, then this equation is satisfied provided that M is antisymmetric. Interestingly enough, if one starts with the $\star$-genvalue problem for this f, ignoring the commutation relations, Eq. (35) would require that the matrix M be antisymmetric.

The real part equation becomes

$$[X_I^T X_I - \tfrac{1}{4} (M_{IK_1} \partial_{K_1})^T (M_{IK_2} \partial_{K_2})] f = 2Ef. \tag{36}$$

Again demanding $f = f(X_I^T X_I)$ to be a solution of (36) we are led to

$$X_I^T X_I f(X_I^T X_I) - \tfrac{1}{2} \mathrm{tr}(M_{IK}^T M_{IK}) f'(X_I^T X_I) - X_{K_1}^T M_{IK_1}^T M_{IK_2} X_{K_2} f''(X_I^T X_I) = 2E f(X_I^T X_I). \tag{37}$$

If this equation is to be satisfied we need

$$M_{IK_1}^T M_{IK_2} = \alpha \delta_{K_1 K_2} I \tag{38}$$

with I the identity matrix. So (38) is the condition for the problem to admit rotational symmetric solutions.

Condition (38) can be solved explicitly in the case of four phase-space dimensions. The most general matrix M that admits rotationally symmetric $\star$-genfunctions is given by

$$M_{11} = \pm M_{22} = \begin{pmatrix} 0 & \hbar \\ -\hbar & 0 \end{pmatrix}, \quad M_{12} = -M_{21} = \begin{pmatrix} \theta & \phi \\ \pm \phi & \mp \theta \end{pmatrix}, \tag{39}$$

where the two signs correspond to the two possible solutions that exist. We are going to more closely examine the first case, since the second can be treated on equal footing. In the present case a transformation that leads to the Heisenberg commutation relations is $\overline{X} = R^T X$, where R is given by

$$R = \begin{pmatrix} \dfrac{\sqrt{\hbar^2 + \phi^2}}{\sqrt{\hbar^2 + \theta^2 + \phi^2}} & 0 & 0 & -\dfrac{\theta}{\sqrt{\hbar^2 + \theta^2 + \phi^2}} \\ -\dfrac{\theta \phi}{\sqrt{\hbar^2 + \theta^2 + \phi^2}\sqrt{\hbar^2 + \phi^2}} & \dfrac{\hbar}{\sqrt{\hbar^2 + \phi^2}} & 0 & -\dfrac{\phi}{\sqrt{\hbar^2 + \theta^2 + \phi^2}} \\ 0 & 0 & 1 & 0 \\ \dfrac{\hbar \theta}{\sqrt{\hbar^2 + \theta^2 + \phi^2}\sqrt{\hbar^2 + \phi^2}} & \dfrac{\phi}{\sqrt{\hbar^2 + \phi^2}} & 0 & \dfrac{\hbar}{\sqrt{\hbar^2 + \theta^2 + \phi^2}} \end{pmatrix}. \tag{40}$$

Certainly this transformation is not unique. It is defined up to symplectic rotations which preserve both the Hamiltonian and the commutation relations in the transformed variables.

The angular momentum, as the generator of rotations, is found to be

$$L=\frac{\hbar}{\hbar^2+\theta^2+\phi^2}\left[\hbar(q_1p_2-q_2p_1)+\frac{\theta}{2}(p_1^2-q_1^2+p_2^2-q_2^2)-\phi(p_1q_1+p_2q_2)\right] \tag{41}$$

and in the transformed variables is reexpressed as

$$\overline{L}=\frac{\hbar}{\hbar^2+\theta^2+\phi^2}\left[\sqrt{\hbar^2+\phi^2}(\overline{q}_1\overline{p}_2-\overline{q}_2\overline{p}_1)+\frac{\theta}{2}(\overline{q}_1^2+\overline{p}_1^2-\overline{q}_2^2-\overline{p}_2^2)\right]. \tag{42}$$

Again the $\star$-genvalue problem for the Hamiltonian is the same as the Schrödinger problem with $\star$-genvalues $E_{n_1,n_2}=\sqrt{\hbar^2+\theta^2+\phi^2}(n_1+n_2+1)$. The same equivalence is valid for the angular momentum $\star$-genvalue problem producing the $\star$-genvalues

$$\frac{\hbar}{(\hbar+\theta^2+\phi^2)}[\sqrt{\hbar^2\phi^2}\sqrt{\hbar^2+\theta^2+\phi^2}m_z+\theta(E_1-E_2)].$$

In the limit $\theta,\phi\to 0$ we can recover from these expressions the usual ones. This solves the general two-dimensional phase-space noncommutative harmonic oscillator that admits rotationally symmetric solutions.

VI. GENERAL CASE

Let us now discard the condition that there exist rotationally symmetric solutions. The matrix M used to define the commutation relations is a general antisymmetric matrix. The following lemma holds:[17]

Lemma 1: Let (V,ω) *be a symplectic vector space and* $g:V\times V\to R$ *be an inner product. Then there exists a basis* $u_1,\ldots,u_n,v_1,\ldots,v_n$ *of* V *which is both g-orthogonal and* ω*-standard. Moreover, this basis can be chosen such that* $g(u_j,u_j)=g(v_j,v_j)$ *for all* j.

This means that it is possible, by rescaling, to find an orthogonal transformation R so that

$$R^TMR=J(M), \tag{43}$$

where

$$J(M)_{IJ}=\alpha_I(M)\,\delta_{IJ}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}. \tag{44}$$

From (34) we see that if we make the transformation $\overline{X}=R^TX$, then the matrix M in the $\star$-product is replaced by $J(M)$ and the Hamiltonian remains invariant because the transformation is orthogonal. So the $\star$-genvalue problem now becomes

$$\overline{H}\overline{\star}\overline{f}=E\overline{f}, \tag{45}$$

where $\overline{\star}$ is

$$\overline{\star}=\exp\left[\frac{i}{2}\overleftarrow{\partial}_I^T J(M)_{IK}\overrightarrow{\partial}_K\right]. \tag{46}$$

The imaginary part equation (35) becomes

$$\sum_i \alpha_i(\overline{q}_i\partial_{\overline{p}_i}-\overline{p}_i\partial_{\overline{q}_i})\overline{f}(\overline{q}_i,\overline{p}_i)=0, \tag{47}$$

where $\alpha_i=\alpha_I(M)$. This equation is satisfied by $\overline{f}\equiv f(z_i)$ where $z_i=2(\overline{q_i^2}+\overline{p_i^2})$. For this $\overline{f}$, the real part equation takes the form:

$$\sum_i \left[z_i\partial_{z_i}^2+\partial_{z_i}-\frac{1}{\alpha_i^2}\left(\frac{z_i}{4}-E_i\right)\right] f(z_i)=0 \tag{48}$$

and the energy is $E=\Sigma_i E_i$. This equation can be separated into a set of equations for each z_i. Solving these equations we get the eigenvalues $E_i=\alpha_i(n_i+1/2)$ and the eigenfunctions:

$$f_{n_i}(z_i)=e^{-(1/2\alpha_i)z_i}L_{n_i}(z_i/\alpha_i). \tag{49}$$

The overall eigenfunctions are products of the $f_{n_i}(z_i)$. The functions corresponding to annihilation and creation operators again take the form (21). They satisfy the following modified commutation relations:

$$\alpha_i\star a_j^\dagger-a_j^\dagger\star a_i=\alpha_i\delta_{ij} \tag{50}$$

and the Hamiltonian becomes

$$H=\sum_i \left(a_i^\dagger\star a_i+\frac{\alpha_i}{2}\right). \tag{51}$$

Again, the $\star$-genvalue problem is equivalent to the Schrödinger problem in the transformed variables. This means that it is also equivalent in the original variables, if one uses the representation for the original variables that result from the usual representation of the transformed ones (the operators corresponding to the transformed variables satisfy the Heisenberg commutation relations).

As an example that does not admit rotationally symmetric solutions we consider the noncommutative Landau problem in harmonic oscillator potential in two dimensions. Assume for convenience that $\hbar=1$. Here the commutation relations are

$$[\hat{q}_i,\hat{p}_j]=i\delta_{ij},\quad [\hat{q}_1,\hat{q}_2]=i\theta,\quad [\hat{p}_1,\hat{p}_2]=iB. \tag{52}$$

The latter commutation relation results from the presence of magnetic field, while the middle one from the noncommutativity of space. The star product is

$$\star=\exp\left[\frac{i}{2}(\overleftarrow{\partial}_{q_1},\overleftarrow{\partial}_{p_1},\overleftarrow{\partial}_{q_2},\overleftarrow{\partial}_{p_2})\begin{pmatrix}0&1&\theta&0\\-1&0&0&B\\-\theta&0&0&1\\0&-B&-1&0\end{pmatrix}\begin{pmatrix}\vec{\partial}_{q_1}\\\vec{\partial}_{p_1}\\\vec{\partial}_{q_2}\\\vec{\partial}_{p_2}\end{pmatrix}\right]. \tag{53}$$

The α_I take the form:

$$\alpha_\pm=\tfrac{1}{2}(\sqrt{(\theta-B)^2+4}\pm(\theta+B). \tag{54}$$

These $\alpha_\pm$ correspond to the frequencies of the Landau harmonic oscillator in the two dimensions. In this case there is no degeneracy in the $\alpha_\pm$ as opposed to the previous cases.

A transformation matrix R that leads to the Heisenberg commutation relations is

$$R=\begin{pmatrix} -\dfrac{\alpha_-(1+B\tilde{\alpha}_-)}{\sqrt{(1-B\theta)^2+\alpha_-^2(1+\beta\tilde{\alpha}_-)^2}} & 0 & -\dfrac{\alpha_+(1-B\tilde{\alpha}_+)}{\sqrt{(1-B\theta)^2+\alpha_+^2(1-B\tilde{\alpha}_+)^2}} & 0 \\ 0 & \dfrac{1}{\sqrt{1+\tilde{\alpha}_-^2}} & 0 & \dfrac{1}{\sqrt{1+\tilde{\alpha}_+^2}} \\ 0 & -\dfrac{\tilde{\alpha}_-}{\sqrt{1+\tilde{\alpha}_-^2}} & 0 & \dfrac{\tilde{\alpha}_+}{\sqrt{1+\tilde{\alpha}_+^2}} \\ -\dfrac{1-B\theta}{\sqrt{(1-B\theta)^2+\alpha_-^2(1+B\tilde{\alpha}_-)^2}} & 0 & \dfrac{1-B\theta}{\sqrt{(1-B\theta)^2+\alpha_+^2(1-B\tilde{\alpha}_+)^2}} & 0 \end{pmatrix}, \tag{55}$$

where we have assumed that $B\theta<1$ and

$$\tilde{\alpha}_\pm=\tfrac{1}{2}(\sqrt{(\theta-B)^2+4}\pm(\theta-B)). \tag{56}$$

Note that if $B\theta=1$ then the fourth row in the transformation matrix becomes zero, so the transformation becomes degenerate, which is not permitted. So there is a critical value for the magnetic field $B_0=1/\theta$. At B_0 the frequency $\alpha_-=0$, so there is an infinite degeneracy at the energy levels, corresponding to the excitations of the α_- oscillator. This problem was solved through a series of transformations in Ref. 15, without resorting to the $\star$-genvalue formalism.

As a further example consider the case of the noncommutative Landau problem with the additional commutation relations $[\hat{q}_1,\hat{p}_2]=i\phi_1$ and $[\hat{p}_1,\hat{q}_2]=i\phi_2$. In this case the frequencies become

$$\alpha_\pm=\tfrac{1}{2}(\sqrt{(B-\theta)^2+4+(\phi_1+\phi_2)^2}\pm\sqrt{(B+\theta)^2+(\phi_1-\phi_2)^2}) \tag{57}$$

and a degeneracy is produced provided that

$$B\theta-\phi_1\phi_2=1. \tag{58}$$

Note that in this case the matrix M in the $\star$-product becomes degenerate again.

As a final example consider the six phase-space dimensional case. The commutation relations we consider are

$$[\hat{q}_i,\hat{p}_j]=i\delta_{ij},\quad [\hat{q}_1,\hat{q}_2]=i\theta_3,\quad [\hat{q}_1,\hat{q}_3]=-i\theta_2,\quad [\hat{q}_2,\hat{q}_3]=i\theta_1. \tag{59}$$

All other commutation relations are trivial. Now the frequencies α_i are

$$\alpha_{1,2}=\sqrt{1+\theta_1^2+\theta_2^2+\theta_3^2},\quad \alpha_3=1. \tag{60}$$

There is twofold degeneracy for the first frequency. The transformation matrix in this case is

$$R=\begin{pmatrix} -\frac{\theta_1\theta_3}{\alpha\beta} & \frac{\theta_2}{\beta} & 0 & \frac{\theta_1\theta_3}{\alpha\beta\gamma} & 0 & -\frac{\theta_1}{\gamma} \\ -\frac{\theta_2}{\alpha\beta} & 0 & -\frac{\theta_1\theta_3}{\beta\gamma} & -\frac{\theta_2\gamma}{\alpha\beta} & \frac{\theta_1}{\gamma} & 0 \\ -\frac{\theta_2\theta_3}{\alpha\beta} & -\frac{\theta_1}{\beta} & 0 & \frac{\theta_2\theta_3}{\alpha\beta\gamma} & 0 & -\frac{\theta_2}{\gamma} \\ \frac{\theta_1}{\alpha\beta} & 0 & -\frac{\theta_2\theta_3}{\beta\gamma} & \frac{\theta_1\gamma}{\alpha\beta} & \frac{\theta_2}{\gamma} & 0 \\ \frac{\beta}{\alpha} & 0 & 0 & -\frac{\beta}{\alpha\gamma} & 0 & -\frac{\theta_3}{\gamma} \\ 0 & 0 & \frac{\beta}{\gamma} & 0 & \frac{\theta_3}{\gamma} & 0 \end{pmatrix}, \tag{61}$$

where

$$\alpha=\sqrt{1+\theta_1^2+\theta_2^2+\theta_3^2},$$

$$\beta=\sqrt{\theta_1^2+\theta_2^2},$$

$$\gamma=\sqrt{\theta_1^2+\theta_2^2+\theta_3^2}.$$

To summarize, we have shown in the present section how to treat in general the $2n$-dimensional phase-space noncommutative harmonic oscillator. We have seen that in the case the matrix M is degenerate there is a zero eigenvalue and also an infinite degeneracy in the energy levels corresponding to excitations of the zero frequency oscillator.

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The supersymmetric technique for random-matrix ensembles with zero eigenvalues

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The supersymmetric technique is applied to computing the average spectral density near zero energy in the large-N limit of the random-matrix ensembles with zero eigenvalues: B, DIII-odd, and the chiral ensembles (classes AIII, BDI, and CII). The supersymmetric calculations reproduce the existing results obtained by other methods. The effect of zero eigenvalues may be interpreted as reducing the symmetry of the zero-energy supersymmetric action by breaking a certain Abelian symmetry. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1423765]

I. INTRODUCTION

There exists a remarkable correspondence between large families of random-matrix ensembles and symmetric superspaces. It has been shown by Zirnbauer that in the large-N limit (N is the matrix dimension) correlation functions in random-matrix ensembles may be represented as integrals over appropriate Riemannian symmetric superspaces (with dimensions independent of N).[1] This relation to symmetric superspaces is based on Efetov's supersymmetric technique introducing auxiliary anticommuting (Grassmann) variables in order to directly average correlation functions over the statistical ensemble.[2]

At the same time, the random-matrix ensembles are known to be in one-to-one correspondence with symmetric spaces (Cartan symmetry classes).[3,4] The classification of Zirnbauer thus establishes a correspondence between large families of symmetric spaces and Riemannian symmetric superspaces.[1] The random-matrix ensembles with zero eigenvalues were not included in the original classification, and later it became apparent that the zero eigenvalues in random-matrix ensembles are related to the reducibility of the corresponding symmetric superspaces.[5–7]

In this paper, I study this relation by explicitly calculating the average density of states in all random-matrix ensembles with zero eigenvalues. There are five such ensembles (Table I): class B [so(N) matrices at odd N], class DIII-odd [so($2N$)/u(N) matrices at odd N], and the three chiral ensembles: unitary AIII, orthogonal BDI, and symplectic CII. In a physical context, the ensembles B and DIII-odd appear in vortices in superconductors with odd pairing,[5,8] the chiral classes—in QCD.[9,10] The zero levels in these ensembles occur as a consequence of the symmetry inverting energy ($E \to -E$) combined with the odd dimension (for classes B and DIII-odd) or with the dimensional imbalance between the two chiral sectors (for the chiral classes). Table I also lists the values of the parameters α and β appearing in the joint probability distribution for energy levels ω_i,

$$dP(\omega_1, \ldots, \omega_n) \propto \prod_{i<j} |\omega_i^2 - \omega_j^2|^\beta \prod_i \omega_i^\alpha d\omega_i \tag{1}$$

(β determines the strength of repulsion between levels, α—the strength of repulsion from zero).

Previously, a supersymmetric calculation of the misroscopic spectral density for the chiral unitary case was done in Ref. 6, and the case of class B was studied in Ref. 5 (in the context of class BD, which is the average of classes B and D). I include these cases for completeness in the corresponding sections.

TABLE I. Random-matrix ensembles with zero eigenvalues.

Cartan class	Symmetric space (compact type)	β	α	Number of zero eigenvalues m
$B-D$	$\mathrm{SO}(N)$	2	$2m$	$m=0$, even N
DIII	$\mathrm{SO}(2N)/\mathrm{U}(N)$	4	$1+4m$	$m=1$, odd N
AIII	$\mathrm{SU}(p+q)/\mathrm{S}(\mathrm{U}(p)\times\mathrm{U}(q))$	2	$1+2m$	$m=\lvert p-q\rvert$
BDI	$\mathrm{SO}(p+q)/\mathrm{SO}(p)\times\mathrm{SO}(q)$	1	m	
CII	$\mathrm{Sp}(p+q)/\mathrm{Sp}(p)\times\mathrm{Sp}(q)$	4	$3+4m$	

From the supersymmetric calculations for the five random-matrix ensembles, we find that zero levels in random-matrix ensembles manifest themselves in reducing the symmetry of the supersymmetric action at zero energy. In the absence of zero levels, this action (a function of the supermatrix Q in Efetov's technique[2]) is invariant with respect to the full supergroup preserving the linear constraints on Q (latter being determined by the symmetries of random matrices). For ensembles with zero levels, the zero-energy action is invariant with respect to only a normal subgroup of this supergroup, but breaks the remaining abelian symmetry. In the large-N limit, the integral over Q is dominated by the saddle-point manifold. This manifold is a Riemannian symmetric superspace,[1] and for ensembles admitting zero levels it is not irreducible: it may be split into orbits of the normal subgroup of the full symmetry (super) group. The quotient by this normal subgroup is an abelian (conventional, not super) group [Z_2 for classes $B-D$ and DIII, and GL(1) for the chiral classes]. If the random-matrix ensemble contains zero levels, the action is not invariant with respect to this residual abelian group, but transforms according to one of its one-dimensional representations.

The paper is organized as follows: In Sec. II, I review the results for the average spectral density in the random-matrix ensembles with zero levels. Next, I describe the details of the supersymmetric calculations for each of the five random-matrix ensembles. The calculation for the ensemble $B-D$ is presented in somewhat more detail, and in the subsequent sections the repeating steps of the derivations are described only briefly. In the last section I discuss common features of these calculations specific for ensembles with zero levels.

II. SPECTRAL DENSITY IN RANDOM-MATRIX ENSEMBLES WITH ZERO LEVELS

In this section I review the results for the average spectral density in the vicinity of the zero eigenvalue. All these results are known and were previously derived by other methods. The reader may use this section as a quick reference.

In what follows we consider zero-curvature random-matrix ensembles and treat them as quantum-mechanical Hamiltonians. Accordingly we use quantum-mechanical terminology such as ''energy levels,'' ''interlevel spacing,'' etc.

In an ensemble of random matrices of size N, with a fixed dispersion of matrix elements, the interlevel spacing in the middle of the spectrum scales as $N^{-1/2}$ for large N. If we measure the energy E in the units of this interlevel spacing Δ, the correlation functions in the vicinity of zero energy (middle of the spectrum) have a finite and universal limit as $N\to\infty$. In this paper I am interested in the average density of states $\rho(x)$ as a function of dimensionless energy $x=E/\Delta$. This function gives the average number of energy levels in any interval $[a;b]$,

$$\langle n\rangle_{[a;b]}=\int_a^b \rho(x)dx. \tag{2}$$

(In the case of $\beta=4$ ensembles DIII and CII, all energy levels are doubly degenerate, and for counting purposes every degenerate pair of states will be counted as a single level.) The function

$\rho(x)$ is symmetric $\rho(x)=\rho(-x)$ and has the normalization $\lim_{x\to\infty}\rho(x)=1$. For an ensemble with m zero levels, $\rho(x)$ has a δ-functional contribution at $x=0$: $\rho(x)=m\,\delta(x)+\tilde{\rho}(x)$, where $\tilde{\rho}(x)$ is continuous at $x=0$.

The results for the average density of states $\rho(x)$ in the ensembles studied in this paper are the following (defining $y=2\pi|x|$, m is the number of zero levels in the chiral ensembles):

Class D:

$$1+\frac{\sin y}{y}, \tag{3}$$

Class B:

$$1-\frac{\sin y}{y}+\delta(x), \tag{4}$$

Class DIII-even:

$$\frac{\pi}{2}y[J_1'(y)J_0(y)+J_1^2(y)]+\frac{\pi}{2}J_1(y), \tag{5}$$

Class DIII-odd:

$$\frac{\pi}{2}y[J_1'(y)J_0(y)+J_1^2(y)]-\frac{\pi}{2}J_1(y)+\delta(x), \tag{6}$$

Class AIII (chiral unitary):

$$\frac{\pi}{4}y\left[J_m^2\left(\frac{y}{2}\right)-J_{m-1}\left(\frac{y}{2}\right)J_{m+1}\left(\frac{y}{2}\right)\right]+m\,\delta(x), \tag{7}$$

Class BDI (chiral orthogonal):

$$\frac{\pi}{2}\left(\frac{y}{2}\left[J_m^2\left(\frac{y}{2}\right)-J_{m-1}\left(\frac{y}{2}\right)J_{m+1}\left(\frac{y}{2}\right)\right]+J_m\left(\frac{y}{2}\right)R_m\left(\frac{y}{2}\right)\right)+m\,\delta(x), \tag{8}$$

Class CII (chiral symplectic):

$$\frac{\pi}{2}(y[J_{2m}^2(y)-J_{2m-1}(y)J_{2m+1}(y)]-J_{2m}(y)\tilde{R}_{2m}(y))+m\,\delta(x), \tag{9}$$

where the functions R_n and $\tilde{R}_n$ are defined as

$$\tilde{R}_n(z)=1-R_n(z)=\int_0^z J_n(z')dz'. \tag{10}$$

These results were previously derived by other methods. The results (3) and (4) are presented in the book of Mehta.[11] They are also straightforward to obtain from mapping of level statistics onto free fermions. A supersymmetric approach to classes B and D was developed in Ref. 5. The result (5) was found by Nagao and Slevin[12] and by Altland and Zirnbauer[13] (contrary to their claim, their result is identical to the result of Nagao and Slevin after some algebraic manipulations with Bessel functions). The result (7) was obtained in the works of Verbaarschot and Zahed,[14] Nagao and Slevin,[15] and Forrester.[16] Also, a supersymmetric calculation of (7) at $m=0$ was reported in Ref. 17, and then at arbitrary m in Ref. 6. To make this paper self-contained, I repeat the derivation of Ref. 6 in the corresponding section. The particular case of formula (8) at m

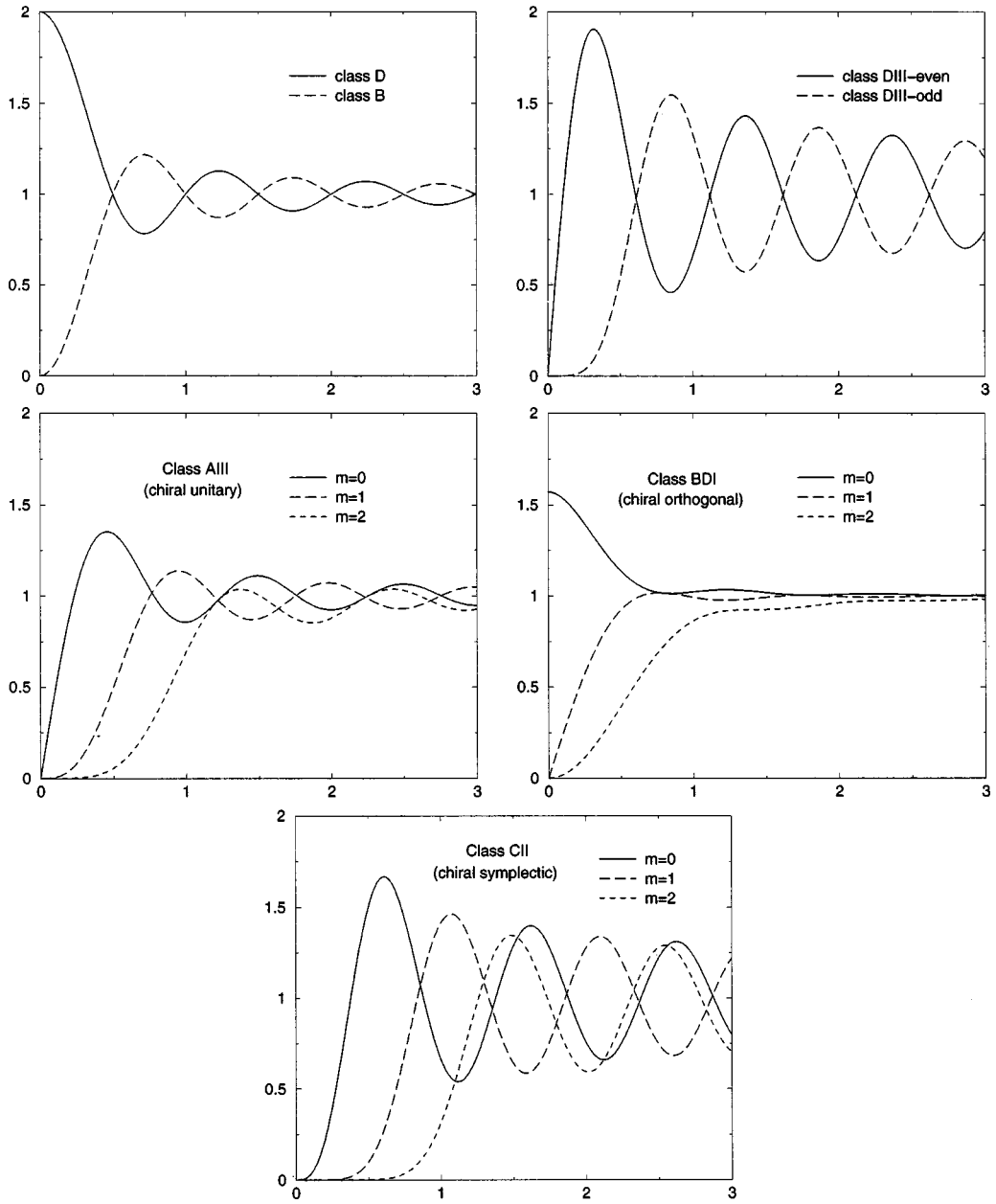

FIG. 1. The average spectral density $\rho(x)$ for ensembles B–D, DIII, AIII, BDI, and CII.

$=1$ can be found in Ref. 12. The case of arbitrary m was treated in Refs. 18 and 19. The latter work also contains the answer for the ensemble CII. The results of Refs. 18 and 19 are presented in the form of complicated integrals. The simple formulas (8) and (9) were later reported in Refs. 20, 21, 22.

The average spectral densities (3)–(9) are plotted in Fig. 1.

III. REMARKS ABOUT NOTATION, SUPERGROUPS, AND SUPERSPACES

In this section I explain some notational conventions used in the subsequent sections. The calculations involve supermatrices acting in a superspace which has the structure $\mathbb{C}^2 \otimes \mathbb{C}^2$ or $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$, depending on the symmetry class. One of the $\mathbb{C}^2$ factors refers to the Fermi–Bose (FB)

sectors and defines the supersymmetric grading. The one or two remaining $\mathbb{C}^2$ factors are either produced by additionally doubling the dimension to take into account the symmetries of the random-matrix ensemble (in classes $B-D$, DIII, and BDI) or are originally present in the matrix structure in the random-matrix ensemble (in class DIII and in the three chiral classes). These $\mathbb{C}^2$ will be labeled to as ''particle–hole'' (PH) or ''1–2'' sectors, without stressing the physical meaning of this terminology. In supermatrices, the FB sectors will be graphically divided by solid lines [see, for example, Eq. (12)], with the BB sector in the upper left corner, and the FF sector in the lower right corner. When the matrices also act in the PH or 1–2 spaces, in order to avoid confusion, these spaces will be explicitly mentioned as a subscript, from the outermost division to the innermost subdivision [see, for example, Eqs. (58)–(60)]. The empty spaces in matrices denote zeros.

The supergroups $\mathrm{GL}(n|m)$ and $\mathrm{OSp}(n|2m)$ appearing in our supersymmetric constructions are defined as follows. The complex supergroup $\mathrm{GL}(n|m)$ consists of all invertible supermatrices of dimension $n+m$. The complex supergroup $\mathrm{OSp}(n|2m)$ is the subgroup of $\mathrm{GL}(n|2m)$ obeying the relation,

$$g^{-1}=\gamma g^{T}\gamma^{-1}, \tag{11}$$

where

$$\gamma=\left(\begin{array}{c|cc} 1_n & & \\ \hline & 0 & 1_m \\ & -1_m & 0 \end{array}\right). \tag{12}$$

Its support is the direct product of $\mathrm{O}(n)$ and $\mathrm{Sp}(m)$. More details about these supergroups may be found in Refs. 23, 1. The reader may also refer to Ref. 2 for conventions regarding manipulations with supermatrices. The Lie superalgebras of $\mathrm{OSp}(n|2m)$ and $\mathrm{GL}(n|m)$ are denoted as $\mathrm{osp}(n|2m)$ and $\mathrm{gl}(n|m)$.

To distinguish between fermionic and bosonic sectors [which is important when performing integration, either compact or noncompact, see below], we shall reserve the notation $\mathrm{OSp}(n|2m)$ for the supergroup with $\mathrm{O}(n)$ in the bosonic and $\mathrm{Sp}(m)$ in the fermionic sector. The same supergroup with $\mathrm{O}(n)$ in the fermionic and $\mathrm{Sp}(m)$ in the bosonic sector we denote as $\mathrm{SpO}(n|2m)$. Also, we use the notation $\mathrm{SpSO}(n|2m)$ for the connected component of $\mathrm{SpO}(n|2m)$ [with the unit superdeterminant].

The notation $\mathrm{Sp}(m)$ in this paper refers to the symplectic group of $2m\times 2m$ matrices. This notation agrees with Refs. 1, 3, 8, but differs from Ref. 23, where the same group is denoted $\mathrm{Sp}(2m)$.

IV. CLASSES *B* AND *D*

In this section we use the supersymmetric technique to compute the density of states for the $\mathrm{so}(N)$ random matrices (class D for even N, class B for odd N). This is the simplest of the five examples considered in this paper, and we describe it in more detail to demonstrate the technique of the calculation. The calculation follows the prescription described in detail by Zirnbauer.[1]

The random-matrix ensembles $B-D$ is unitary (with $\beta=2$). The supermatrix Q used in the calculation of the average density of states has dimension $2+2$ (2 bosonic and 2 fermionic dimensions), is parameterized by $4+4$ independent variables and is an element of $\mathrm{osp}(2|2)$ Lie superalgebra. The saddle-point manifold has dimension $2+2$, and thus the density of states in the large-N limit is computed as an integral over two commuting and two Grassmann variables.

The random-matrix ensemble $B-D$ consists of purely imaginary antisymmetric matrices H,

$$H_{ab}=H_{ba}^{*}=-H_{ba}, \quad a,b=1,\ldots,N. \tag{13}$$

The matrix elements have independent Gaussian distributions,

$$dP(H)\propto\prod_{a>b}\ \exp\left(-\frac{|H_{ab}|^2}{2v^2}\right)dH_{ab}, \tag{14}$$

so that the averages of any number of matrix elements are given by the Wick rule together with the pair average,

$$\langle H_{ab}H_{a'b'}\rangle=v^2(\delta_{ab'}\delta_{ba'}-\delta_{aa'}\delta_{bb'}). \tag{15}$$

From the calculation below we shall see that the energy unit defined as

$$\Delta=\frac{\pi v}{\sqrt{N}} \tag{16}$$

plays the role of the average level spacing near zero energy.

The average density of states can be found by differentiating the generating function,

$$Z(\omega_B,\omega_F)=\int dP(H)\,\frac{\det(H-\omega_F\Delta)}{\det(H-\omega_B\Delta)}, \tag{17}$$

where the integration is performed over the ensemble of random matrices H; ω_B and ω_F are auxiliary variables (complex numbers). We included the energy scale Δ in the definition (17) to make ω_B and ω_F dimensionless.

The ensembles considered in this paper have an $E\to -E$ symmetry, which leads to the symmetry of the generating function,

$$Z(\omega_B,\omega_F)=Z(-\omega_B,-\omega_F)=(-1)^m Z(-\omega_B,\omega_F), \tag{18}$$

where m is the number of zero levels. In the supersymmetric calculation below we neglect the overall sign of $Z(\omega_B,\omega_F)$, but restore it at the end of the calculation from the condition $Z(\omega,\omega)=1$ and from positiveness of the density of states.

The two determinants in (17) may be written as Gaussian integrals over bosonic and fermionic variables (auxiliary fields). Introducing the $(N+N)$-component supervector $\psi_a=(\psi_{Ba},\psi_{Fa})$, $a=1,\ldots,N$, and performing the integration over $dP(H)$, we arrive at the partition function for interacting superfields [the common energy scale v drops out already at this step, thanks to our including Δ in (17)],

$$Z(\omega_B,\omega_F)=\int D(\psi^{\dagger},\psi)\exp\left(-\frac{i\pi\omega_\mu}{\sqrt{N}}\psi_{\mu a}^{\dagger}\psi_{\mu a}-\frac{1}{2}[(\psi_{\mu a}^{\dagger}\psi_{\mu b})(\psi_{\nu b}^{\dagger}\psi_{\nu a})-(\psi_{\mu a}^{\dagger}\psi_{\mu b})(\psi_{\nu a}^{\dagger}\psi_{\nu b})]\right), \tag{19}$$

where μ, ν are fermion-boson indices. In the integral, the Grassmann components in ψ and $\psi^{\dagger}$ are treated as independent variables (total $2N$ Grassmann variables). The integral over bosonic components of ψ and $\psi^{\dagger}$ is taken over the $2N$-dimensional real submanifold $(\psi^{\dagger})_{Ba}=(\psi_{Ba})^{*}$.

To decouple the interaction with the Q-matrix, it is necessary to double the dimension of vector ψ. Combine the old superfields $\psi_{\mu a}$ into the new ones,

$$\Psi_a=\begin{pmatrix}\psi_B\\ \psi_B^\dagger\\ \psi_F\\ \psi_F^\dagger\end{pmatrix}_a, \quad \overline{\Psi}_a=\begin{pmatrix}\psi_B^\dagger\\ -\psi_B\\ \psi_F^\dagger\\ \psi_F\end{pmatrix}_a^T, \tag{20}$$

so that

$$\overline{\Psi}=(\gamma\Psi)^T, \tag{21}$$

where

$$\gamma=\left(\begin{array}{cc|cc}0&1&&\\-1&0&&\\\hline&&0&1\\&&1&0\end{array}\right). \tag{22}$$

In terms of the supervectors Ψ and $\overline{\Psi}$, the partition function may be rewritten as

$$Z(\omega_B,\omega_F)=\int D\Psi\,\exp\left(-\frac{1}{2}\mathrm{STr}\left[\frac{i\pi}{\sqrt{N}}\Psi_a\overline{\Psi}_a\hat{\omega}+\frac{1}{2}(\Psi_a\overline{\Psi}_a)^2\right]\right), \tag{23}$$

where

$$\hat{\omega}=\left(\begin{array}{cc|c}\omega_B&&\\&&\\\hline&&\omega_F\end{array}\right)\otimes\begin{pmatrix}1&0\\0&-1\end{pmatrix}. \tag{24}$$

[With this definition of $\hat{\omega}$ we in fact change the sign of ω_F, which may result in the change of sign of $Z(\omega_B,\omega_F)$, according to (18). We shall not control the overall sign of $Z(\omega_B,\omega_F)$, but restore the correct sign at the end of the calculation.]

The matrix $(\Psi_a\overline{\Psi}_a)$ has the explicit form,

$$\Psi_a\overline{\Psi}_a=\left(\begin{array}{cc|cc}Q_B&-X&\sigma&\rho\\\bar{X}&-Q_B&\bar{\rho}&\bar{\sigma}\\\hline\bar{\sigma}&-\rho&Q_F&0\\\bar{\rho}&-\sigma&0&-Q_F\end{array}\right). \tag{25}$$

This is also the form of the supermatrix Q used to decouple the interaction via Hubbard–Stratonovich transformation,

$$Z(\omega_B,\omega_F)=\int DQ\int D\Psi\exp\left(-\frac{1}{2}\mathrm{STr}\left[\frac{N}{2}Q^2+i\sqrt{N}\left(Q-\frac{\pi}{N}\hat{\omega}\right)\Psi_a\overline{\Psi}_a\right]\right). \tag{26}$$

The integration is performed in the space of matrices Q of the form (25) which is equivalent to the linear constraint,

$$\gamma Q\gamma^{-1}=-Q^T. \tag{27}$$

More precisely, the integral is taken along the real subspace in the complex space (27) where Q_B is real, Q_F is purely imaginary, and $\overline{X}=X^*$ (for convergence of the integral).

After integrating in Ψ, we arrive at

$$Z(\omega_B,\omega_F)=\int DQ\left[\mathrm{SDet}\left(Q-\frac{\pi}{N}\hat{\omega}\right)\right]^{-N/2}\exp\left(-\frac{N}{2}\mathrm{STr}\frac{Q^2}{2}\right). \tag{28}$$

Since we are interested in small energy scales (of the order of several level spacings from zero), we can expand the action to terms linear in ω and obtain

$$Z(\omega_B,\omega_F)=\int DQ\exp\left(-\frac{N}{2}\mathrm{STr}\left[\frac{Q^2}{2}+\ln Q\right]+\mathrm{STr}\frac{\pi}{2}\hat{\omega}Q^{-1}\right). \tag{29}$$

At large N, the integral is determined by the saddle points of the action,

$$S_0(Q)=\mathrm{STr}\left(\frac{Q^2}{2}+\ln Q\right). \tag{30}$$

By varying the action, the equation of the saddle-point manifold is

$$Q^2=-1. \tag{31}$$

By deforming the integration contour onto the saddle-point manifold, the integral reduces to

$$Z(\omega_B,\omega_F)=\int_\Gamma DQ\exp\left(-\frac{N}{2}S_0(Q)-\mathrm{STr}\frac{\pi}{2}\hat{\omega}Q\right) \tag{32}$$

(the transversal directions do not contribute to the integral because of the supersymmetry).

The contour of integration Γ on the saddle-point manifold should be determined from the condition that the original contour of integration can be deformed onto it without making integrals divergent (see also discussion of this procedure in Ref. 1). For the convergence of the integral (19) over the bosonic components of ψ and $\psi^\dagger$, the energy ω_B must have an infinitesimal imaginary part $\mathrm{Im}\,\omega_B<0$. Then, for the convergence of the integral (32), the matrix Q must satisfy $\mathrm{Im}\,Q_B>0$ at infinity on the contour Γ [Q_B is the bosonic diagonal element, as shown in (25)]. Besides, the contour Γ must be compact in the fermionic and noncompact in the bosonic sector (see, e.g., Refs. 1, 2, 24). It is shown in Ref. 1 that Γ is the Riemannian symmetric superspace SpO(2|2)/GL(1|1) (class $CI|DIII$).

The key observation, important for taking into account the parity of N, is that the saddle-point manifold Γ consists of two connected components, which are the images of the two components of the symmetry group SpO(2|2) acting on Γ. This symmetry group acts on Q by conjugation: $Q\mapsto UQU^{-1}$. Explicitly, the two connected pieces of Γ may be obtained by rotating by the connected component of the symmetry group SpSO(2|2) the two representative matrices,

$$Q_1 = \left(\begin{array}{cc|cc} i & & & \\ & -i & & \\ \hline & & -i & \\ & & & i \end{array}\right), \qquad Q_2 = \left(\begin{array}{cc|cc} i & & & \\ & -i & & \\ \hline & & i & \\ & & & -i \end{array}\right). \tag{33}$$

The action (30) is invariant with respect to SpSO(2|2), but acquires an additional shift by $2\pi i$ between the two connected components of the saddle-point manifold.

It is this property of the supersymmetric action that allows to distinguish between odd and even N in the large-N limit: In the even-N case (class D, no zero levels), the contributions from the two pieces of the saddle-point manifold come with equal signs, and in the odd-N case (class B, one zero level)—with opposite signs,

$$Z(\omega_B,\omega_F)=Z_1(\omega_B,\omega_F)+(-1)^N Z_2(\omega_B,\omega_F). \tag{34}$$

The average spectral density $\rho(\omega)$ may be found as

$$\rho(\omega)=-\frac{1}{\pi}\mathrm{Im}\frac{\partial Z(\omega_B,\omega_F)}{\partial \omega_B}\bigg|_{\omega_B=\omega_F=\omega-i0}=\frac{1}{\pi}\mathrm{Im}\frac{\partial Z(\omega_B,\omega_F)}{\partial \omega_F}\bigg|_{\omega_B=\omega_F=\omega-i0}. \tag{35}$$

To take the integral over Γ, we need to parameterize the integration contour: In this section, the parameterization involves the two commuting parameters x,ϕ and the two anticommuting ξ and $\overline{\xi}$ (we never use complex conjugation of anticommuting variables in this paper, and so ξ and $\overline{\xi}$ should be treated as independent variables). The expressions for $\rho(\omega)$ in coordinates takes the form,

$$\rho(\omega)=\mathrm{Im}\int DQ\, Q_F \exp[-\pi\omega(Q_B-Q_F)], \tag{36}$$

where $Q_B(x,\phi,\xi,\overline{\xi})$ and $Q_F(x,\phi,\xi,\overline{\xi})$ are diagonal matrix elements of Q in a particular parameterization, and the measure of integration DQ is

$$DQ=\frac{1}{2\pi}J(x,\phi,\xi,\overline{\xi})dx\,d\phi\,d\xi\,d\overline{\xi}. \tag{37}$$

The Jacobian $J(x,\phi,\xi,\overline{\xi})$ may be found from expressing the invariant metric $\mathrm{STr}(dQ)^2$ in coordinates,

$$\mathrm{STr}(dQ)^2=g^{ij}dx_i dx_j \tag{38}$$

and taking its superdeterminant

$$J(\{x_i\})=(\mathrm{SDet}\, g^{ij})^{1/2}. \tag{39}$$

In parameterizing the saddle-point manifold we use the usual trick of splitting the rotation of the supermatrix Q_i into the two rotations by even and odd generators of the supergroup.[2] Namely, we parameterize

$$Q=U_\xi Q_z U_\xi^{-1}, \tag{40}$$

where Q_z is obtained from Q_1 or Q_2 by even rotations parameterized by x and ϕ (and without mixing between boson–bosonic and fermion–fermionic blocks), and

$$U_\xi = \exp(A), \tag{41}$$

where A is an odd infinitesimal rotation linear in ξ and $\overline{\xi}$.

Supersymmetric calculations of this sort often lead to singularities in superintegrals which need to be resolved by properly taking into account boundary terms (see e.g. Refs. 2, 1). In this paper I avoid such singularities by an appropriate choice of parameterization of the odd rotation U_ξ.

We shall also employ the symmetry relating the two components of the saddle-point manifold. Namely, conjugation by the matrix,

$$T = \left(\begin{array}{cc|cc} 1 & 0 & & \\ 0 & 1 & & \\ \hline & & 0 & 1 \\ & & 1 & 0 \end{array}\right), \tag{42}$$

transforms Q_1 into Q_2 ($Q_2 = T^{-1} Q_1 T$) and the two components of the saddle-point manifold into each other.

Thus we first parameterize the component generated by Q_1, and then the parameterization of the other component may be obtained by applying the operator T.

The even rotations of Q_1 may be parameterized as

$$Q_z = i \cdot \left(\begin{array}{cc|cc} \cosh x & -e^{i\phi}\sinh x & & \\ e^{-i\phi}\sinh x & -\cosh x & & \\ \hline & & -1 & 0 \\ & & 0 & 1 \end{array}\right) \tag{43}$$

(with $x \in [0; +\infty)$, $\phi \in [0; 2\pi]$).

The symmetry (27) of the matrix Q imposes a similar symmetry constraint on the matrix A in (41). The latter constraint admits four independent parameters in the boson-fermion and fermion-boson sectors of A. However, when acting on Q_z, only two of them are independent. At this stage we have a freedom of choosing two of the four infinitesimal rotations for our parameterization. The final result does not depend on our choice [provided the Jacobian (39) is nondegenerate], but a good choice of parameterization may considerably simplify the calculation.

We choose

$$A=\left(\begin{array}{cc|cc} & & \xi & 0 \\ & & 0 & \bar{\xi} \\ \hline \bar{\xi} & 0 & & \\ 0 & -\xi & & \end{array}\right) \tag{44}$$

which leads to

$$U_\xi=\left(\begin{array}{cc|cc} 1-\frac{1}{2}\bar{\xi}\xi & 0 & \xi & 0 \\ 0 & 1-\frac{1}{2}\bar{\xi}\xi & 0 & \bar{\xi} \\ \hline \bar{\xi} & 0 & 1+\frac{1}{2}\bar{\xi}\xi & 0 \\ 0 & -\xi & 0 & 1+\frac{1}{2}\bar{\xi}\xi \end{array}\right). \tag{45}$$

The Jacobian calculation may be simplified using the simple algebraic identity,[2]

$$ds^2=\tfrac{1}{2}\mathrm{STr}(dQ)^2=\tfrac{1}{2}\mathrm{STr}(dQ_z)^2+\tfrac{1}{2}\mathrm{STr}[Q_z,\delta U_\xi]^2+\mathrm{STr}(\delta U_\xi[Q_z,dQ_z]), \tag{46}$$

where $\delta U_\xi=U_\xi^{-1}dU_\xi$.

After some calculation, we find for the parameterization chosen

$$ds^2=dx^2+\sinh^2 x\,d\phi^2-[4(\cosh x+1)+2\sinh^2 x\,\bar{\xi}\xi]d\bar{\xi}\,d\xi+2i\sinh^2 x(\bar{\xi}\,d\xi+\xi\,d\bar{\xi})d\phi \tag{47}$$

and

$$J(x,\phi,\xi,\bar{\xi})=\frac{1}{2}\tanh\frac{x}{2}. \tag{48}$$

Also, by a direct calculation,

$$\begin{aligned} Q_{B1}&=i[\cosh x-(\cosh x+1)\bar{\xi}\xi], \\ Q_{F1}&=i[1+(\cosh x+1)\bar{\xi}\xi]. \end{aligned} \tag{49}$$

Using the operator T to relate the two connected components of the saddle-point manifold, we find for the second component,

$$Q_{B2}=Q_{B1},\quad Q_{F2}=-Q_{F1}, \tag{50}$$

and the Jacobian obviously remains the same (48).

As a consistency check, one may verify that

$$Z_{\pm}(\omega,\omega)=\int \frac{1}{2\pi}\, J(x,\phi,\xi,\bar{\xi})dx\, d\phi\, d\bar{\xi}\, d\xi\, (\exp[-\pi\omega(Q_{B1}-Q_{F1})]\pm\exp[-\pi\omega(Q_{B1}+Q_{F1})])$$
$$=1 \tag{51}$$

(up to a sign).

Now the calculation of the integral (36) is easily done,

$$\rho_1(\omega)=\mathrm{Re}\int_0^\infty dx\int_0^{2\pi} d\phi\int d\bar{\xi}\, d\xi\, \frac{1}{4\pi}\tanh\frac{x}{2}[1+(\cosh x+1)\bar{\xi}\xi]$$
$$\times\exp(-i\pi\omega[(\cosh x-1)-2(\cosh x+1)\bar{\xi}\xi])=\tfrac{1}{2}\,\delta(x)+1, \tag{52}$$

$$\rho_2(\omega)=\mathrm{Re}\int_0^\infty dx\int_0^{2\pi} d\phi\int d\bar{\xi}\, d\xi\, \frac{1}{4\pi}\tanh\frac{x}{2}[1+(\cosh x+1)\bar{\xi}\xi]\exp(-i\pi\omega[\cosh x+1])$$
$$=\frac{1}{2}\,\delta(x)-\frac{\sin(2\pi\omega)}{2\pi\omega} \tag{53}$$

(all the calculations are performed up to an overall sign). The δ-function terms are obtained from imaginary $1/i\omega$ terms by shifting ω to the lower half-plane $\omega\to\omega-i0$.

Combining these results with proper signs, we arrive at the final expressions (3) and (4). The asymptotic value $\rho(\omega\to\infty)=1$ proves that Δ given by (16) is indeed the average level spacing.

Note that $\rho_1(\omega)$ appeared in Ref. 5 as the spectral density in class BD (which is the average of B and D).

V. CLASSES *D*III-EVEN AND *D*III-ODD

For classes DIII-even and DIII-odd, the calculation is similar to that of the previous section. The saddle-point manifold again consists of two connected components, and taking their contributions with different signs distinguishes between odd and even matrix dimension.

The ensembles DIII-even and DIII-odd have $\beta=4$. In the calculation of the average spectral density in these ensembles, the matrix Q has dimension $4+4$ and belongs to a $(8+8)$-dimensional linear space. The saddle-point manifold is $(4+4)$-dimensional.

The ensembles DIII are defined as consisting of $2N\times 2N$ matrices,

$$H=i\begin{pmatrix} H_1 & H_2 \\ H_2 & -H_1 \end{pmatrix}, \tag{54}$$

where H_1 and H_2 are real $N\times N$ antisymmetric matrices ($H_1^T=-H_1$, $H_2^T=-H_2$). Depending on whether N is even or odd, this defines the ensemble DIII-even or DIII-odd, respectively. The matrix elements of H_1 and H_2 are assumed to be distributed independently with a Gaussian distribution, and produce the following pair correlation function for the matrix elements of H:

$$\langle H_{ai,bj}H_{a'i',b'j'}\rangle=v^2(\delta_{ii'}\delta_{jj'}-(-1)^{i+j}\bar{\delta}_{ii'}\bar{\delta}_{jj'})(\delta_{ab'}\delta_{ba'}-\delta_{aa'}\delta_{bb'}), \tag{55}$$

where the indices i, j take values 1 or 2 and distinguish between the two N-dimensional sectors in the $2N$-dimensional linear space, and $\bar{\delta}=\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$ in this "1–2" space.

We express energy in the units

$$\Delta=\frac{\sqrt{2}\,\pi v}{\sqrt{N}} \tag{56}$$

(as the result of the calculation, this is the average level spacing).

The space of Ψ-vectors needs to be doubled. Instead of a single vector Ψ_a we introduce a pair of vectors Ψ_{1a} and Ψ_{2a} (here a takes values $1,\ldots,N$),

$$\Psi_{1a}=\begin{pmatrix}\psi_{1B}\\ \psi_{2B}\\ \psi_{1B}^{\dagger}\\ \psi_{2B}^{\dagger}\\ \psi_{1F}\\ \psi_{2F}\\ \psi_{1F}^{\dagger}\\ \psi_{2F}^{\dagger}\end{pmatrix}_a,\quad \Psi_{2a}=\begin{pmatrix}\psi_{2B}\\ -\psi_{1B}\\ \psi_{2B}^{\dagger}\\ -\psi_{1B}^{\dagger}\\ \psi_{2F}\\ -\psi_{1F}\\ \psi_{2F}^{\dagger}\\ -\psi_{1F}^{\dagger}\end{pmatrix}_a,\quad \bar{\Psi}_{1a}=\begin{pmatrix}\psi_{1B}^{\dagger}\\ -\psi_{2B}^{\dagger}\\ -\psi_{1B}\\ \psi_{2B}\\ \psi_{1F}^{\dagger}\\ -\psi_{2F}^{\dagger}\\ \psi_{1F}\\ -\psi_{2F}\end{pmatrix}_a^T,\quad \bar{\Psi}_{2a}=\begin{pmatrix}\psi_{2B}^{\dagger}\\ \psi_{1B}^{\dagger}\\ -\psi_{2B}\\ -\psi_{1B}\\ \psi_{2F}^{\dagger}\\ \psi_{1F}^{\dagger}\\ \psi_{2F}\\ \psi_{1F}\end{pmatrix}_a^T. \tag{57}$$

The two sets of vectors Ψ, $\bar{\Psi}$ are necessary to reproduce the four terms in the interaction induced by (55).

The corresponding supermatrix Q has the form,

$$Q=\left(\begin{array}{cccc|cccc}
Q_B & X_B & -Y_B & 0 & \bar{\sigma}_1 & -\bar{\sigma}_2 & \rho_1 & -\rho_2\\
X_B & -Q_B & 0 & Y_B & -\bar{\sigma}_2 & -\bar{\sigma}_1 & -\rho_2 & -\rho_1\\
\bar{Y}_B & 0 & -Q_B & X_B & \bar{\rho}_1 & -\bar{\rho}_2 & \sigma_1 & -\sigma_2\\
0 & -\bar{Y}_B & X_B & Q_B & -\bar{\rho}_2 & -\bar{\rho}_1 & -\sigma_2 & -\sigma_1\\
\hline
\sigma_1 & \sigma_2 & -\rho_1 & -\rho_2 & -Q_F & -X_F & 0 & -Y_F\\
\sigma_2 & -\sigma_1 & -\rho_2 & \rho_1 & -X_F & Q_F & -Y_F & 0\\
\bar{\rho}_1 & \bar{\rho}_2 & -\bar{\sigma}_1 & -\bar{\sigma}_2 & 0 & -\bar{Y}_F & Q_F & -X_F\\
\bar{\rho}_2 & -\bar{\rho}_1 & -\bar{\sigma}_2 & \bar{\sigma}_1 & -\bar{Y}_F & 0 & -X_F & -Q_F
\end{array}\right)_{FB,PH,12} \tag{58}$$

Equivalently, Q may be described as obeying the two linear constraints,

$$\gamma_{12}Q\gamma_{12}^{-1}=-Q,\quad \gamma_{12}=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}_{12}, \tag{59}$$

and

$$\gamma_{PH} Q \gamma_{PH}^{-1} = Q^T, \qquad \gamma_{PH} = \gamma = \left(\begin{array}{cc|cc} 0 & 1 & & \\ -1 & 0 & & \\ \hline & & 0 & 1 \\ & & 1 & 0 \end{array}\right)_{FB,PH} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_{12}, \tag{60}$$

where FB and PH indices specifies that the operator acts in the Fermi–Bose and ''particle–hole'' spaces (the doubling of dimension by combining ψ and $\psi^\dagger$ in a single vector Ψ), and ''1–2'' denotes the space corresponding to the two N-dimensional sectors in the original Hamiltonian (54).

Similarly to the previous section, we find for the generating function $Z(\omega_B, \omega_F)$,

$$\begin{aligned} Z(\omega_B,\omega_F) &= \int D\Psi \exp\left(-\frac{1}{4}\mathrm{STr}\left[i\pi \frac{\sqrt{2}}{\sqrt{N}} \Psi_{ia}\overline{\Psi}_{ia}\hat{\omega} + \frac{1}{2}(\Psi_{ia}\overline{\Psi}_{ia})^2 \right] \right) \\ &= \int DQ \int D\Psi \exp\left(-\frac{1}{2}\mathrm{STr}\left[\frac{N}{2}Q^2 + i\sqrt{\frac{N}{2}}\left(Q - \frac{\pi}{N}\hat{\omega} \right)\Psi_{ia}\overline{\Psi}_{ia} \right] \right) \\ &= \int DQ \left[\mathrm{SDet}\left(Q - \frac{\pi}{N}\hat{\omega} \right) \right]^{-N/2} \exp\left(-\frac{N}{2}\mathrm{STr}\,\frac{Q^2}{2} \right), \end{aligned} \tag{61}$$

where

$$\hat{\omega} = \begin{pmatrix} \omega_B & \\ & \omega_F \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_{\mathrm{PH}} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_{12}. \tag{62}$$

At small energies ω_B, ω_F this leads to the formulas (29)–(32), albeit with the new definitions of Q and $\hat{\omega}$.

The saddle-point manifold consists of the two connected pieces represented by

$$Q_1 = \left(\begin{array}{ccccc|ccccc} i & & & & & & & & & \\ & -i & & & & & & & & \\ & & -i & & & & & & & \\ & & & i & & & & & & \\ & & & & i & & & & & \\ \hline & & & & & -i & & & & \\ & & & & & & i & & & \\ & & & & & & & i & & \\ & & & & & & & & -i & \\ & & & & & & & & & -i \end{array}\right), \qquad Q_2 = \left(\begin{array}{ccccc|ccccc} i & & & & & & & & & \\ & -i & & & & & & & & \\ & & -i & & & & & & & \\ & & & i & & & & & & \\ & & & & i & & & & & \\ \hline & & & & & -i & & & & \\ & & & & & & -i & & & \\ & & & & & & & -i & & \\ & & & & & & & & -i & \\ & & & & & & & & & -i \end{array}\right). \tag{63}$$

Similarly to the procedure described in the previous section, first the supermatrices Q_1, Q_2 are rotated by even symmetry-group generators. These rotations do not mix bosonic and fermionic components, i.e., the matrix Q_z contains only boson–boson and fermion–fermion blocks,

$$Q_z = \left(\begin{array}{c|c} Q_z^{(BB)} & \\ \hline & Q_z^{(FF)} \end{array} \right). \tag{64}$$

We shall use the following parameterization of these blocks:

$$Q_z^{(\mathrm{BB})} = \begin{pmatrix} i\cosh\theta_B & n_1\sinh\theta_B & (n_2-in_3)\sinh\theta_B & 0 \\ n_1\sinh\theta_B & -i\cosh\theta_B & 0 & -(n_2-in_3)\sinh\theta_B \\ (n_2+in_3)\sinh\theta_B & 0 & -i\cosh\theta_B & n_1\sinh\theta_B \\ 0 & -(n_2+in_3)\sinh\theta_B & n_1\sinh\theta_B & i\cosh\theta_B \end{pmatrix}_{\mathrm{PH},12}, \tag{65}$$

where (n_1,n_2,n_3) is a vector of a real two-dimensional unit sphere $(n_1^2+n_2^2+n_3^2=1)$. The boson–boson block is the same for the two sectors of the saddle-point manifold.

The fermion–fermion blocks for the two components of the saddle-point manifold are

$$Q_{z1}^{(\mathrm{FF})} = \begin{pmatrix} 0 & 0 & 0 & -ie^{i\theta_F} \\ 0 & 0 & -ie^{i\theta_F} & 0 \\ 0 & -ie^{-i\theta_F} & 0 & 0 \\ -ie^{-i\theta_F} & 0 & 0 & 0 \end{pmatrix}, \tag{66}$$

$$Q_{z2}^{(\mathrm{FF})} = \begin{pmatrix} -i\cos\theta_F & -i\sin\theta_F & 0 & 0 \\ -i\sin\theta_F & i\cos\theta_F & 0 & 0 \\ 0 & 0 & i\cos\theta_F & -i\sin\theta_F \\ 0 & 0 & -i\sin\theta_F & -i\cos\theta_F \end{pmatrix}. \tag{66}$$

The parameter range is $\theta_B\in[0;+\infty)$, $\theta_F\in[0;2\pi]$, and the vector $\mathbf{n}$ runs over the two-dimensional unit sphere S^2.

Like in the previous section, we first do the calculation in the first component of the saddle-point manifold, and then obtain the answers for the second component by using the symmetry operator T mapping one component (generated by Q_1) onto the other (generated by Q_2). One possible choice of such a matrix T is

$$T=\left(\begin{array}{cccc|cccc} 1 & & & & & & & \\ & 1 & & & & & & \\ & & 1 & & & & & \\ & & & 1 & & & & \\ \hline & & & & 1/2 & -i/2 & -i/2 & 1/2 \\ & & & & -i/2 & -1/2 & 1/2 & i/2 \\ & & & & -i/2 & 1/2 & -1/2 & i/2 \\ & & & & 1/2 & i/2 & i/2 & 1/2 \end{array}\right)_{FB,PH,12}. \tag{67}$$

Returning to the parameterization for the first component of the saddle-point manifold, the matrix A involved in the odd rotation (40), (41) is chosen as follows:

$$A=\left(\begin{array}{cccc|cccc} & & & & \xi & \nu & 0 & 0 \\ & & & & -\nu & \xi & 0 & 0 \\ & & & & \bar{\nu} & \bar{\xi} & 0 & 0 \\ & & & & -\bar{\xi} & \bar{\nu} & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & & & & \\ 0 & 0 & 0 & 0 & & & & \\ \bar{\nu} & \bar{\xi} & -\xi & -\nu & & & & \\ -\bar{\xi} & \bar{\nu} & \nu & -\xi & & & & \end{array}\right)_{FB,PH,12}. \tag{68}$$

This matrix satisfies the *flatness* condition $[A,dA]=0$, and this leads to $\delta U_\xi = U_\xi^{-1} dU_\xi = dA$. Using the algebraic identity (46), together with (38), (39), and

$$DQ=\frac{1}{(2\pi)^2} J(\theta_B,\theta_F,\mathbf{n},\xi,\overline{\xi},\nu,\overline{\nu})\, d\theta_B\, d\theta_F\, d^2\mathbf{n}\, d\xi\, d\overline{\xi}\, d\nu\, d\overline{\nu}, \tag{69}$$

one finds after some calculation the explicit form for the invariant measure in the coordinates chosen,

$$DQ=\frac{1}{16\pi^2} e^{-2i\theta_F} \sinh^2\theta_B\, d\theta_B\, d\theta_B\, d\theta_F\, d^2\mathbf{n}\, d\xi\, d\overline{\xi}\, d\nu\, d\overline{\nu} \tag{70}$$

(here $d^2\mathbf{n}$ is the integration over the solid angle on the unit sphere).

The explicit expressions for the diagonal entries of the Q-matrix Q_B and Q_F are found to be

$$Q_{B1}=i[\cosh\theta_B+e^{i\theta_F}(\bar{\xi}\xi-\bar{\nu}\nu)],\quad Q_{F1}=-ie^{i\theta_F}(\bar{\xi}\xi+\bar{\nu}\nu). \tag{71}$$

Using the operator T defined in (67), for the second component of the saddle-point manifold we find

$$\begin{aligned} Q_{B2}&=Q_{B1},\\ Q_{F2}&=i[\cos\theta_F+2\bar{\xi}\xi\bar{\nu}\nu e^{i\theta_F}+\cosh\theta_B(\bar{\nu}\nu-\bar{\xi}\xi)\\ &\quad+in_1\sinh\theta_B(\nu\bar{\xi}-\bar{\nu}\xi)-(n_2+in_3)\bar{\nu}\bar{\xi}\sinh\theta_B+(n_2-in_3)\nu\xi\sinh\theta_B]. \end{aligned} \tag{72}$$

After some calculation, one verifies the normalization:

$$\begin{aligned} Z_1(\omega,\pm\omega)&=\int dQ\,\exp[-2\pi\omega(Q_{B1}\mp Q_{F1})]=0,\\ Z_2(\omega,\pm\omega)&=\int dQ\,\exp[-2\pi\omega(Q_{B2}\mp Q_{F2})]=1. \end{aligned} \tag{73}$$

The density of states is found in terms of Bessel functions,

$$\rho_1(\omega)=\mathrm{Im}\int dQ\,Q_{F1}\exp[-2\pi\omega(Q_{B1}-Q_{F1})]=\frac{1}{2}\delta(\omega)-\frac{\pi}{2}J_1(2\pi\omega) \tag{74}$$

in the first sector, and

$$\rho_2(\omega)=\mathrm{Im}\int dQ\,Q_{B2}\exp[-2\pi\omega(Q_{B2}-Q_{F2})]=\frac{1}{2}\delta(\omega)+\pi^2\omega[J_1'(2\pi\omega)J_0(2\pi\omega)+J_1^2(2\pi\omega)], \tag{75}$$

where in (74) and (75) we assumed $\omega>0$ and are careless about the overall sign of the answers.

Taking these contributions with proper signs, we obtain the answers (5) and (6). Remarkably, in (6), the contributions of $\rho_1(\omega)$ and of $\rho_2(\omega)$ cancel each other to the third order at small ω, producing the correct behavior of the total density of states $\rho(\omega)\propto\omega^5$.

VI. CLASS *A*III (CHIRAL UNITARY)

The supersymmetric calculations for the three chiral random-matrix ensembles differ from those for classes B–D and DIII in that the broken symmetry of the saddle-point manifold is not the discrete Z_2, but the continuous GL(1). The representations of GL(1) are enumerated by the integer winding number whose absolute value equals the number of zero levels in the random-matrix ensemble.

The chiral unitary ensemble considered in this section has $\beta=2$ (unitary bulk statistics). In the calculation of the average density of states, the supermatrix Q has the block form (in the "1–2" space)

$$Q=\begin{pmatrix} 0 & Q_1\\ Q_2 & 0\end{pmatrix}, \tag{76}$$

where Q_1 and Q_2 are $(1+1)$-dimensional supermatrices without linear constraints. Thus the linear space of matrices Q is $4+4$-dimensional, and the saddle-point manifold has dimension $2+2$.

The (Gaussian) chiral unitary ensemble (class AIII in Cartan notation) consists of the matrices of the form,

$$H=\begin{pmatrix} 0 & \tilde{H} \\ \tilde{H}^\dagger & 0 \end{pmatrix}, \tag{77}$$

where $\tilde{H}$ is a rectangular matrix $p\times q$ with complex matrix elements. The matrix elements of $\tilde{H}$ have independent Gaussian distributions,

$$dP(H)\propto\prod_{a,b}\ \exp\left(-\frac{|\tilde{H}_{ab}|^2}{v^2}\right)d\,\mathrm{Re}\,\tilde{H}_{ab}d\,\mathrm{Im}\,\tilde{H}_{ab}\,. \tag{78}$$

The spectrum of such a matrix H consist of $N=\min(p,q)$ pairs of eigenvalues $\pm E_i$ and of $m=|p-q|$ zero eigenvalues. In this paper we are interested in the average density of states near zero in the limit of large matrices $N\to\infty$ while keeping the number of zero levels m fixed. The average level spacing near zero in the large-N limit is

$$\Delta=\frac{\pi v}{2\sqrt{N}}. \tag{79}$$

Following the standard procedure, we introduce p-component superfields Ψ_1 and $\overline{\Psi}_1$, and q-component superfields Ψ_2 and $\overline{\Psi}_2$,

$$\Psi_{1a}=\begin{pmatrix}\psi_{1B}\\ \psi_{1F}\end{pmatrix}_a,\quad \overline{\Psi}_{1a}=\begin{pmatrix}\psi^\dagger_{1B}\\ \psi^\dagger_{1F}\end{pmatrix}^T_a,\quad a=1,\ldots,p, \tag{80}$$

$$\Psi_{2b}=\begin{pmatrix}\psi_{2B}\\ \psi_{2F}\end{pmatrix}_b,\quad \overline{\Psi}_{2b}=\begin{pmatrix}\psi^\dagger_{2B}\\ \psi^\dagger_{2F}\end{pmatrix}^T_b,\quad b=1,\ldots,q. \tag{81}$$

The generating function (17) takes the form,

$$\begin{aligned} Z(\omega_B,\omega_F)&=\int D\Psi\,\exp\left(-\mathrm{STr}\left[\frac{i\pi}{2\sqrt{N}}(\Psi_{1a}\overline{\Psi}_{1a}+\Psi_{2b}\overline{\Psi}_{2b})\hat{\omega}+(\Psi_{1a}\overline{\Psi}_{1a})(\Psi_{2b}\overline{\Psi}_{2b})\right]\right)\\ &=\int D(Q_1,Q_2)\int D\Psi\,\exp\left(-\mathrm{STr}\left[NQ_1Q_2+i\sqrt{N}\left(Q_1-\frac{\pi}{2N}\hat{\omega}\right)\Psi_{2b}\overline{\Psi}_{2b}\right.\right.\\ &\quad\left.\left.+i\sqrt{N}\left(Q_2-\frac{\pi}{2N}\hat{\omega}\right)\Psi_{1a}\overline{\Psi}_{1a}\right]\right)\\ &=\int D(Q_1,Q_2)\left[\mathrm{SDet}\left(Q_1-\frac{\pi}{2N}\hat{\omega}\right)\right]^{-q}\left[\mathrm{SDet}\left(Q_2-\frac{\pi}{2N}\hat{\omega}\right)\right]^{-p}\\ &\quad\times\exp(-N\,\mathrm{STr}\,Q_1Q_2), \end{aligned} \tag{82}$$

where the original integration contour in Q is at $Q_2=Q_1^\dagger$, and

$$\hat{\omega} = \left(\begin{array}{c|c} \omega_B & \\ \hline & \omega_F \end{array}\right). \tag{83}$$

At small energies, expanding the supersymmetric action to terms linear in $\omega_{B,F}$, we find

$$Z(\omega_B,\omega_F) = \int DQ\,[\mathrm{SDet}\,Q_1]^m \exp\left[-NS_0(Q_1,Q_2) + \frac{\pi}{2}\mathrm{STr}\,\hat{\omega}(Q_1^{-1}+Q_2^{-1})\right] \tag{84}$$

with

$$S_0(Q_1,Q_2) = \mathrm{STr}(Q_1Q_2 + \ln Q_1 + \ln Q_2). \tag{85}$$

If Q_1 and Q_2 are combined into a single supermatrix Q according to (76), this action coincides with the standard form (30). The saddle-point manifold Γ is given by the condition,

$$Q_1Q_2 = -1 \tag{86}$$

(which is equivalent to $Q^2=-1$), and the generating function may be written as the integral over the saddle-point manifold,

$$Z_m(\omega_B,\omega_F) = \int_\Gamma DQ\,[\mathrm{SDet}\,Q_1]^m \exp\left[-\frac{\pi}{2}\mathrm{STr}\,\hat{\omega}(Q_1+Q_2)\right]. \tag{87}$$

A parameterization and the calculation of the integral was previously performed in Ref. 6, and I outline their calculation here for completeness. The matrices Q_1 and Q_2 are parameterized as

$$Q_1 = -Q_2^{-1} = \left(\begin{array}{c|c} ie^x & 0 \\ \hline 0 & ie^{i\phi} \end{array}\right) \exp\left(\begin{array}{c|c} 0 & \xi \\ \hline \bar{\xi} & 0 \end{array}\right). \tag{88}$$

The invariant measure deduced from the metric $ds^2=\mathrm{STr}(Q_1Q_2)$ leads to the trivial Jacobian $J=1$ and to the integration measure

$$DQ = \frac{1}{2\pi}dx\,d\phi\,d\xi\,d\bar{\xi}. \tag{89}$$

From the parameterization (88), the diagonal elements of the matrices Q_1 and Q_2 are easily computed. The generating function (87) involves the average of the diagonal elements of Q_1 and Q_2,

$$\begin{aligned} Q_{\mathrm{BB}} &= \tfrac{1}{2}[(Q_1)_{\mathrm{BB}} + (Q_2)_{\mathrm{BB}}] = i\cosh x\,[1-\tfrac{1}{2}\bar{\xi}\xi], \\ Q_{\mathrm{FF}} &= \tfrac{1}{2}[(Q_1)_{\mathrm{FF}} + (Q_2)_{\mathrm{FF}}] = i\cos\phi\,[1+\tfrac{1}{2}\bar{\xi}\xi]. \end{aligned} \tag{90}$$

Also, the m-dependent prefactor in (87) is a plane wave generated by

$$\mathrm{SDet}\,Q_1 = e^{x-i\phi}. \tag{91}$$

The normalization can be verified by computing the integral,

$$Z_m(\omega,\omega)=\int \frac{1}{2\pi}dx\,d\phi\,d\xi\,d\bar{\xi}\,e^{m(x-i\phi)}\exp\left[-i\pi\omega\left(\cosh x\left[1-\frac{1}{2}\bar{\xi}\xi\right]+\cos\phi\left[1+\frac{1}{2}\bar{\xi}\xi\right]\right)\right]$$
$$=\pm 1. \tag{92}$$

The average spectral density is calculated from (35) as the integral (again, up to an overall sign),

$$\rho_m(\omega)=\mathrm{Re}\int \frac{1}{2\pi}dx\,d\phi\,d\xi\,d\bar{\xi}\,e^{m(x-i\phi)}\cosh x\left[1-\frac{1}{2}\bar{\xi}\xi\right]$$
$$\times\exp[-i\pi\omega(\cosh x[1-\tfrac{1}{2}\bar{\xi}\xi]+\cos\phi[1+\tfrac{1}{2}\bar{\xi}\xi])] \tag{93}$$

which after some algebra produces the result (7).

VII. CLASS *BD*I (CHIRAL ORTHOGONAL)

Similarly to the three Wigner–Dyson random-matrix ensembles, the chiral ensembles form the three classes: unitary, orthogonal, and symplectic, depending on the structure of the matrix $\tilde{H}$ in the block form (77). In the chiral orthogonal ensemble (class *BD*I in Cartan notation), the matrix $\tilde{H}$ is real. In this ensemble, the bulk repulsion of the levels corresponds to the orthogonal regime: $\beta=1$. The supermatrix Q involved in the calculation of the average spectral density has the block form (76), but now the matrices Q_1 and Q_2 have dimensions $2+2$ each, with one linear constraint, so the dimension of the linear space of all the matrices Q is $8+8$. The saddle-point equation selects the saddle-point manifold of dimension $4+4$.

The entries of the matrix $\tilde{H}$ in (77) are assumed to be real, with independent Gaussian distributions,

$$dP(H)\propto\prod_{a,b}\ \exp\left(-\frac{|\tilde{H}_{ab}|^2}{2v^2}\right)d\tilde{H}_{ab}\,. \tag{94}$$

As in the chiral unitary ensemble, the spectrum consists of N pairs of opposite energies, and of $m=|p-q|$ zero-energy levels. The average level spacing is given by the same expression (79) [note however a difference between the definitions of v in (78) and in (94), depending on whether $\tilde{H}_{ab}$ are complex or real].

To account for the matrix elements $\tilde{H}_{ab}$ being real, we need to double the dimensions of the superfields Ψ_i and $\bar{\Psi}_i$. The p-component superfields Ψ_1 and $\bar{\Psi}_1$ are defined as

$$\Psi_{1a}=\begin{pmatrix}\psi_{1B}\\ \psi_{1B}^\dagger\\ \psi_{1F}\\ \psi_{1F}^\dagger\end{pmatrix}_a,\quad \bar{\Psi}_{1a}=\begin{pmatrix}\psi_{1B}^\dagger\\ \psi_{1B}\\ \psi_{1F}^\dagger\\ -\psi_{1F}\end{pmatrix}^T_a,\quad a=1,\ldots,p, \tag{95}$$

and similarly, the q-component superfields Ψ_2 and $\bar{\Psi}_2$,

$$\Psi_{2b}=\begin{pmatrix}\psi_{2B}\\ \psi_{2B}^\dagger\\ \psi_{2F}\\ \psi_{2F}^\dagger\end{pmatrix}_b,\quad \bar{\Psi}_{2b}=\begin{pmatrix}\psi_{2B}^\dagger\\ \psi_{2B}\\ \psi_{2F}^\dagger\\ -\psi_{2F}\end{pmatrix}^T_b,\quad b=1,\ldots,q. \tag{96}$$

Repeating the steps of the derivation (82), we arrive at the following expression for the generating function [in place of (84)]:

$$Z_m(\omega_B,\omega_F)=\int DQ\,[\mathrm{SDet}\,Q_1]^{m/2}\exp\left[-\frac{N}{2}S_0(Q_1,Q_2)+\frac{\pi}{4}\mathrm{STr}\,\hat{\omega}(Q_1^{-1}+Q_2^{-1})\right], \tag{97}$$

where $\hat{\omega}$ and $S_0(Q_1,Q_2)$ are given by the old expressions (83) and (85). However, the matrices Q_1 and Q_2 are now two times bigger. Each of them has the explicit form,

$$Q_i=\left(\begin{array}{cc|cc} Q_{Bi} & -X_i & \sigma_i & -\rho_i \\ \bar{X}_i & Q_{Bi} & \bar{\rho}_i & -\bar{\sigma}_i \\ \hline \bar{\sigma}_i & \rho_i & Q_{Fi} & 0 \\ \bar{\rho}_i & \sigma_i & 0 & Q_{Fi} \end{array}\right). \tag{98}$$

Equivalently, this form of the matrices Q_i may be described by the linear constraints,

$$\gamma Q_i \gamma^{-1}=Q_i^T, \tag{99}$$

where

$$\gamma=\left(\begin{array}{cc|cc} 0 & 1 & & \\ 1 & 0 & & \\ \hline & & 0 & 1 \\ & & -1 & 0 \end{array}\right). \tag{100}$$

The saddle-point manifold Γ is determined by the condition (86), and the generating function is expressed as

$$Z_m(\omega_B,\omega_F)=\int_\Gamma DQ\,[\mathrm{SDet}\,Q_1]^{m/2}\exp\left[-\frac{\pi}{4}\mathrm{STr}\,\hat{\omega}(Q_1+Q_2)\right]. \tag{101}$$

In the present section we choose a slightly different form of parameterization than in the previous one. Namely, parameterize

$$Q_1=U_1Q_{z1}U_2^{-1},\quad Q_2=U_2Q_{z2}U_1^{-1}, \tag{102}$$

where the matrices Q_{z1} and Q_{z2} contain only boson–boson and fermion–fermion blocks (contain only even rotations), and the matrices U_1 and U_2 contain only odd rotations. The explicit form of this parameterization is as follows:

$$Q_{z1} = i\left(\begin{array}{cc|cc} e^{x}\cosh\theta & e^{x+iy}\sinh\theta & & \\ e^{x-iy}\sinh\theta & e^{x}\cosh\theta & & \\ \hline & & e^{i\phi} & 0 \\ & & 0 & e^{i\phi} \end{array}\right),$$

$$Q_{z2} = i\left(\begin{array}{cc|cc} e^{-x}\cosh\theta & -e^{-x+iy}\sinh\theta & & \\ -e^{-x-iy}\sinh\theta & e^{-x}\cosh\theta & & \\ \hline & & e^{-i\phi} & 0 \\ & & 0 & e^{-i\phi} \end{array}\right), \tag{103}$$

$$U_1 = \exp(A_1), \qquad U_2 = \exp(A_2), \tag{104}$$

$$A_1 = \left(\begin{array}{cc|cc} & & -\xi & \lambda \\ & & -\bar{\lambda} & \bar{\xi} \\ \hline & & & \\ & & & \end{array}\right), \qquad A_2 = \left(\begin{array}{cc|cc} & & & \\ & & & \\ \hline \bar{\xi} & \lambda & & \\ \bar{\lambda} & \xi & & \end{array}\right). \tag{105}$$

After some calculation, the Jacobian is found to be

$$J = \sinh\theta e^{2(x-i\phi)}, \tag{106}$$

and therefore the measure of integration is

$$DQ = \frac{1}{(2\pi)^2}\sinh\theta\, e^{2(x-i\phi)}\, dx\, dy\, d\theta\, d\phi\, d\bar{\xi}\, d\xi\, d\bar{\lambda}\, d\lambda. \tag{107}$$

Finally, from the explicit calculation of the diagonal elements of Q_1 and Q_2,

$$\begin{aligned} Q_{\mathrm{BB}} &= \tfrac{1}{2}[(Q_1)_{\mathrm{BB}} + (Q_2)_{\mathrm{BB}}] = i[\cosh x\cosh\theta - \tfrac{1}{2}e^{i\phi}(\bar{\xi}\xi - \bar{\lambda}\lambda)], \\ Q_{\mathrm{FF}} &= \tfrac{1}{2}[(Q_1)_{\mathrm{FF}} + (Q_2)_{\mathrm{FF}}] = i[\cos\phi + \tfrac{1}{2}e^{-x}(\cosh\theta[\bar{\xi}\xi - \bar{\lambda}\lambda] - \sinh\theta[e^{iy}\bar{\xi}\bar{\lambda} + e^{-iy}\lambda\xi])]. \end{aligned} \tag{108}$$

Now, after verifying the normalization,

$$Z_m(\omega, \pm\omega) = \int DQ\, e^{m(x-i\phi)}\exp[-\pi\omega(Q_{\mathrm{BB}} \pm Q_{\mathrm{FF}})] = 1, \tag{109}$$

we compute the average density of states as the following integral:

$$\rho_m(\omega)=\mathrm{Re}\int DQ\, e^{m(x-i\phi)}\, Q_{\mathrm{BB}} \exp[-\pi\omega(Q_{\mathrm{BB}}+Q_{\mathrm{FF}})] \tag{110}$$

[where DQ, Q_{BB}, and Q_{FF} are defined in (107) and (108)]. After some algebra and manipulations with Bessel functions, this produces the result (8).

VIII. CLASS *C*II (CHIRAL SYMPLECTIC)

The last symmetry class considered in this paper is *C*II in Cartan notation: the chiral symplectic one. It consists of the matrices H of the block form (77), where the matrix $\tilde{H}$ has an internal 2×2 structure,

$$\tilde{H}=\begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \tag{111}$$

where a and b are rectangular $p\times q$ matrices [the matrix $\tilde{H}$ thus has the dimensions $2p\times 2q$, and the Hamiltonian (77) has the dimension $2(p+q)$]. The spectrum of such a Hamiltonian consists of the $N=\min(p,q)$ pairs of doubly degenerate levels at opposite energies $\pm E_i$, and of $2m=2|p-q|$ zero-energy levels. Since each level has degeneracy two (or a multiple of two), we divide the density of states by two for the purpose of level counting, and count each degenerate level as a single one.

As in the two previous sections, the supermatrix Q is of the form (76). Similarly to the chiral orthogonal case, the matrices Q_1 and Q_2 in this calculation have dimension $2+2$, with one linear constraint. The dimension of the linear space of matrices Q is thus $8+8$, and the dimension of the saddle-point manifold is $4+4$.

The entries of the matrix (111) are assumed to be normalized as

$$dP(A)\propto\prod_{a,b}\ \exp\left(-\frac{|a_{ab}|^2}{v^2}\right) d\,\mathrm{Re}\,a_{ab}\, d\,\mathrm{Im}\,a_{ab}\prod_{a,b}\ \exp\left(-\frac{|b_{ab}|^2}{v^2}\right) d\,\mathrm{Re}\,b_{ab}\, d\,\mathrm{Im}\,b_{ab}\,. \tag{112}$$

With this normalization, the average level spacing is

$$\Delta=\frac{\pi v}{\sqrt{2N}}. \tag{113}$$

Similarly to the *D*III ensemble discussed before, we need to additionally double the set of the superfields to account for the symplectic matrix structure. Namely, in addition to the ''1–2'' sector, distinguishing between the size-p and size-q blocks in (77), we introduce the ''particle–hole'' (PH) sector referring to the two sectors inside the matrix A (111). Thus we arrive to the four pairs of superfields Ψ_{P1}, $\overline{\Psi}_{P1}$, Ψ_{P2}, $\overline{\Psi}_{P2}$, Ψ_{H1}, $\overline{\Psi}_{H1}$, Ψ_{H2}, $\overline{\Psi}_{H2}$,

$$\Psi_{P1a}=\begin{pmatrix} \psi^\dagger_{P1B} \\ \psi_{H1B} \\ \psi^\dagger_{P1F} \\ \psi_{H1F} \end{pmatrix}_a, \quad \overline{\Psi}_{P1a}=\begin{pmatrix} \psi_{P1B} \\ \psi^\dagger_{H1B} \\ -\psi_{P1F} \\ \psi^\dagger_{H1F} \end{pmatrix}^T_a, \quad \Psi_{H1a}=\begin{pmatrix} \psi^\dagger_{H1B} \\ -\psi_{P1B} \\ \psi^\dagger_{H1F} \\ -\psi_{P1F} \end{pmatrix}_a,$$
$$\overline{\Psi}_{H1a}=\begin{pmatrix} \psi_{H1B} \\ -\psi^\dagger_{P1B} \\ -\psi_{H1F} \\ -\psi^\dagger_{P1F} \end{pmatrix}^T_a, \quad a=1,\ldots,p, \tag{114}$$

and similarly for the sector-2 fields Ψ_{P2}, $\overline{\Psi}_{P2}$, Ψ_{H2}, $\overline{\Psi}_{H2}$.

This results in the following form of matrices Q_i:

$$Q_i = \left(\begin{array}{cc|cc} Q_{Bi} & 0 & -\sigma_i & \bar{\rho}_i \\ 0 & Q_{Bi} & \rho_i & \bar{\sigma}_i \\ \hline \bar{\sigma}_i & -\bar{\rho}_i & Q_{Fi} & \bar{X}_i \\ \rho_i & \sigma_i & X_i & Q_{Fi} \end{array}\right)_{FB,PH}, \tag{115}$$

which differs from the chiral orthogonal ensemble by interchanging the bosonic and fermionic sectors (this duality was already described in Ref. 1).

Performing the standard steps of the derivation [similarly to (82)], we arrive at the following answer in the saddle-point approximation:

$$Z_m(\omega_B,\omega_F)=\int_\Gamma DQ\,[\mathrm{SDet}\,Q_1]^m \exp\left[-\frac{\pi}{2}\mathrm{STr}\,\hat{\omega}(Q_1+Q_2)\right] \tag{116}$$

[note the differences from the orthogonal result (101)!].

Finally, the calculation may be performed using the parameterization obtained from that of the previous section by interchanging bosonic and fermionic sectors. Note that under this interchange, the compact variables become noncompact and vice versa. Explicitly, Eqs. (103), (105)–(107) are replaced by

$$Q_{z1} = i\left(\begin{array}{cc|cc} e^{x} & 0 & & \\ 0 & e^{x} & & \\ \hline & & e^{i\phi}\cos\theta & e^{i(\phi+y)}\sin\theta \\ & & -e^{i(\phi-y)}\sin\theta & e^{i\phi}\cos\theta \end{array}\right), \tag{117}$$

$$Q_{z2} = i\left(\begin{array}{cc|cc} e^{-x} & 0 & & \\ 0 & e^{-x} & & \\ \hline & & e^{-i\phi}\cos\theta & -e^{-i(\phi-y)}\sin\theta \\ & & e^{-i(\phi+y)}\sin\theta & e^{-i\phi}\cos\theta \end{array}\right),$$

$$A_1 = \left(\begin{array}{c|cc} & \xi & \lambda \\ \hline & -\bar{\lambda} & -\bar{\xi} \\ & & \end{array}\right), \qquad A_2 = \left(\begin{array}{c|cc} & & \\ \hline & \bar{\xi} & \lambda \\ & \bar{\lambda} & \xi \end{array}\right). \tag{118}$$

$$DQ = \frac{1}{(2\pi)^2} \sin\theta\, e^{2(x-i\phi)}\, dx\, dy\, d\theta\, d\phi\, d\bar{\xi}\, d\xi\, d\bar{\lambda}\, d\lambda. \tag{119}$$

Equation (108) is replaced by

$$\begin{gathered} Q_{\mathrm{BB}} = \tfrac{1}{2}[(Q_1)_{\mathrm{BB}} + (Q_2)_{\mathrm{BB}}] = i[\cosh x + \tfrac{1}{2} e^{i\phi}(\cos\theta[\bar{\xi}\xi + \bar{\lambda}\lambda] + \sin\theta[e^{iy}\bar{\lambda}\xi + e^{-iy}\lambda\bar{\xi}])], \\ Q_{\mathrm{FF}} = \tfrac{1}{2}[(Q_1)_{\mathrm{FF}} + (Q_2)_{\mathrm{FF}}] = i[\cos\phi\cos\theta - \tfrac{1}{2} e^{-x}(\bar{\xi}\xi + \bar{\lambda}\lambda)]. \end{gathered} \tag{120}$$

Taking the integral

$$\rho_m(\omega) = \mathrm{Re} \int DQ\, e^{2m(x-i\phi)}\, Q_{\mathrm{BB}} \exp[-2\pi\omega(Q_{\mathrm{BB}} + Q_{\mathrm{FF}})], \tag{121}$$

we obtain the final result (9). [Note that in (121) we divided the density of states by two to prevent double counting of the doubly degenerate states.]

IX. ZERO LEVELS AND REDUCED SUPERSYMMETRY OF THE ACTION

After presenting the calculations of the average density of states in the five random-matrix ensembles with zero levels, in this section we discuss the specifics of the supersymmetric method due to the zero levels. I do not present here a consistent mathematical analysis of this problem, leaving it for future study. Instead I only summarize the common features of the above calculations specific for the ensembles with zero levels.

The standard supersymmetric procedure to calculate spectral correlation functions in any random-matrix ensemble starts with introducing bosonic and fermionic fields ψ_B and ψ_F.[1,2] Integrating over the Gaussian disorder produces a four-term interaction. This interaction is then decoupled via Hubbard–Stratonovich transformation by a supermatrix Q whose dimension is independent on the matrix size N in the original random-matrix ensemble. Integrating over the superfields (ψ_B, ψ_F), one arrives at an effective action for the supermatrix Q. The supermatrix Q obeys certain linear symmetry relations and thus belongs to a linear superspace L depending on the symmetries of the original random-matrix ensemble. In the superspace L, there acts a supergroup G inherited from the supersymmetry mixing the bosonic and fermionic fields ψ_B and ψ_F. Namely, an element $g \in G$ is a supermatrix acting on Q by conjugation,

$$g: Q \mapsto g Q g^{-1}. \tag{122}$$

The group G then depends on the symmetries of the matrix Q and hence on the symmetry of the random-matrix ensemble.

The effective action $S(Q)$ may, at small energies ω, be expanded to the linear in ω term,

$$S(Q) = S_{\omega=0}(Q) + \omega\, \mathrm{STr}\, \Lambda Q^{-1}, \tag{123}$$

where $\Lambda \in L$ is a particular supermatrix with $\Lambda^2 = 1$.

TABLE II. Supergroups and superspaces involved in the spectral density calculations.

Class	L	G	H	$\Gamma = G/H$	G_0	G/G_0
$B-D$	osp(2|2)	SpO(2|2)	GL(1|1)	SpO(2|2)/GL(1|1)	SpSO(2|2)	Z_2
DIII	osp(4|4)/osp(2|2)$\oplus$osp(2|2)	SpO(2|2)$\times$SpO(2|2)	SpO(2|2)[a]	SpO(2|2)	S[SpO(2|2)$\times$SpO(2|2)][b]	Z_2
AIII	gl(1|1)$\oplus$gl(1|1)	GL(1|1)$\times$GL(1|1)	GL(1|1)[a]	GL(1|1)	S[GL(1|1)$\times$GL(1|1)][b]	GL(1)
BDI	[gl(2|2)/osp(2|2)]$\oplus$[gl(2|2)/osp(2|2)]	GL(2|2)	OSp(2|2)	GL(2|2)/OSp(2|2)	SL(2|2)[c]	GL(1)
CII	[gl(2|2)/osp(2|2)]$\oplus$[gl(2|2)/osp(2|2)]	GL(2|2)	SpO(2|2)	GL(2|2)/SpO(2|2)	$SL_2(2\|2)$[c]	GL(1)

[a] H is diagonal in G: $H=\{(g,g)\}$ in classes DIII and AIII.
[b] S$[H\times H]$ denotes here the subgroup $\{(g_1,g_2)|S\ \mathrm{Det}\ g_1 = S\ \mathrm{Det}\ g_2\}$.
[c] $SL(2|2)=\{g\in GL(2|2)|S\ \mathrm{Det}\ g=1\}$; $SL_2(2|2)=\{g\in GL(2|2)|S\ \mathrm{Det}\ g=\pm 1\}$.

In ensembles without zero eigenvalues, the zero-energy action $S_{\omega=0}(Q)$ is invariant with respect to the supergroup G. The zero-energy action $S_{\omega=0}(N)$ scales linearly with N, and in the large-N limit the integral over Q is determined by the saddle points of $S_{\omega=0}(Q)$. The saddle-point equation, with the appropriate normalization, reads

$$Q^2=-1. \tag{124}$$

This equation is solved by $Q=i\Lambda$, as well as by any matrix obtained from $i\Lambda$ by G-rotations (122). The matrix Λ is invariant under a subgroup $H\subset G$, and the saddle-point manifold Γ is the quotient G/H.

More precisely, Γ is a Riemannian (real) supermanifold in G/H, which makes it a Riemannian symmetric superspace as defined in Ref. 1. This real submanifold should be determined geometrically from deforming the real integration subspace in L while keeping the integral convergent. A good geometric understanding of this contour deformation still needs to be developed, but the rule of thumb for choosing the real integration manifold in Γ is to take the bosonic sector noncompact and the fermionic one compact [this choice also provides a metric of a definite sign on Γ].

For the random-matrix ensembles with zero eigenvalues, the invariance properties of the effective action $S_{\omega=0}(Q)$ are modified. In this case, $S_{\omega=0}(Q)$ is invariant with respect not to the whole supergroup G, but only with respect to its normal subgroup G_0. The subgroup G_0 must contain H, and the factor group G/G_0 is an abelian group (an ordinary group, not a supergroup). The exponent $\exp[S_{\omega=0}(Q)]$ transforms according to one of its (one-dimensional) representations. The degree of this representation equals the number of zero eigenvalues in the random-matrix ensemble.

In the ensembles $B-D$ and DIII, the group G/G_0 is discrete Z_2, and the two representations of Z_2 correspond to the ensembles with and without zero eigenvalues (odd N and even N, respectively). Specifically, the action $S_{\omega=0}(Q)$ has the form,

$$S_{\omega=0}(Q)=NS_0(Q), \tag{125}$$

where $S_0(Q)$ gets incremented by $i\pi$ under the action of the generator of $G/G_0=Z_2$. Hence, $\exp[S_{\omega=0}(Q)]$ transforms according to the even/odd representation of Z_2 for even/odd N.

In the chiral random-matrix ensembles AIII, BDI, and CII, the group G/G_0 is the continuous GL(1), with its representations labeled by the integer ''winding number'' m. The absolute value of m equals the number of zero eigenvalues in the random-matrix ensemble. The action $S_{\omega=0}(Q)$ in the chiral ensembles [which includes the logarithm of the pre-exponent in (87), (101), (116)] is of the form

$$S_{\omega=0}(Q)=NS_0(Q)+mS_1(Q), \tag{126}$$

where $S_0(Q)$ is invariant under G, and $S_1(Q)$ produces phase shifts under $G/G_0=\mathrm{GL}(1)$. The exponent $\exp[S_{\omega=0}(Q)]$ then transforms as the representation of GL(1) of degree m.

The summary of the ''building blocks'' of the supersymmetric calculations in this paper (the calculation of the average spectral density) is presented in Table II. This table is compiled using the results of Ref. 1 and the calculations in the previous sections. The definitions of the supergroups involved in this table may be found in Sec. III. To keep track of the bosonic (noncompact) and fermionic (compact) sectors of the supergroups, we use the notation OSp for the orthosymplectic supergroup with the orthogonal part in the bosonic, and the symplectic part in the fermionic sectors. In the opposite case of orthogonal fermionic and symplectic bosonic sector, we denote the same supergroup SpO. It is important for reducing the action symmetry in ensembles $B-D$ and DIII, that $\mathrm{SpO}(2n|2n)$ has two disconnected components with superdeterminants 1 and -1 [the former of them denoted as $\mathrm{SpSO}(2n|2n)$]. Incidentally, in the ensembles C and CI, dual to $B-D$ and DIII by interchanging fermionic and bosonic sectors, in the supergroup $\mathrm{OSp}(2n|2n)$, with the non-compact orthogonal sector, the second component (with $S\,\mathrm{Det}=-1$) plays no role and should be disregarded as it always corresponds to a divergent integral. The supergroup $\mathrm{GL}(n|n)$ is not

simple either. First, it has a one-dimensional center consisting of scalar matrices. Second, it has a normal subgroup $\mathrm{SL}(n|n)$ consisting of matrices with unit superdeterminant. This latter reduction of the supergroup $\mathrm{GL}(n|n)$ is crucial for the symmetry classification in the case of the chiral ensembles (the last three lines in Table II).

Finally, it is worth mentioning that the conclusion about the reduced supersymmetry of the zero-energy effective action $S_{\omega=0}(Q)$ may be extended to higher-order correlation functions involving averaging several Green's functions (the average spectral density requires averaging only one Green's function). In Ref. 1 a general procedure of calculating correlation functions of arbitrary order (with the number of zero levels $m=0$) was described, and the saddle-point manifold (a Riemannian symmetric superspace) Γ was found to be always reducible for ensembles admitting zero levels. Thus the extension of the calculation of the present paper to higher-order correlations is straightforward (however, explicit parameterization and integral evaluation immediately becomes much more complicated).

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Supersymmetric spin networks

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In this article we study the construction of supersymmetric spin networks, which has a direct interpretation in context of the representation theory of the superalgebra. In particular we analyze a special kind of spin network associated with superalgebra $\mathrm{Osp}(1|2n)$. It turns out that the set of corresponding spin network states forms an orthogonal basis of the Hilbert space $\mathcal{L}^2(\mathcal{A}/\mathcal{G})$, and this argument holds even in the q-deformed case. The $\mathrm{Osp}(n|2)$ spin networks are also discussed briefly. We expect they could provide useful techniques to quantum supergravity and gauge field theories from the point of nonperturbative view. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421423]

I. INTRODUCTION

The notion of spin networks originally was advocated by Roger Penrose in the 1970s when he tried to give a quantum mechanical description of the geometry of space.[1] In his opinion, the final version of quantum geometry should be a combinatorial theory in which we consider the different combinations and permutations of objects such that we could derive the discrete spectra of observables in the quantum mechanical level. After that the idea of spin networks was introduced to many areas, including lattice gauge theory[2] and topological field theory.[3] In the middle of the 1990s, the spin networks were introduced in loop quantum gravity in a quite different way.[4,5] It was exploited to construct the Hilbert space of kinematical quantum states and consequently the discrete spectra of the area and volume of the space were obtained.[6] Later the dynamics of the spin networks were also considered and its evolution gives rise to a casual set of spin networks[7] or spin foams.[8]

It is evident to see the importance of spin networks if we list some basic features they contain. First spin networks are a very general notion in quantum field theory in which gauge fields are involved. In particular, they are gauge invariant objects, in the sense that the corresponding spin network states will be solutions to the Gauss constraint naturally if we take the standard Dirac procedures to quantize the theory. As a result, it would be much easier to find the physically related subspace in Hilbert space. In path integral formulation, we can consider the functional integration on the modular space since a well-defined measure theory can be established in context of spin networks. In loop quantum gravity, they are background independent and nonperturbative objects as well.

Until now we mainly focus on SU(2) spin networks since it has important application to quantum general relativity.[6,8,9] However, in principle we could construct the spin networks associated to other groups or supergroups. More importantly, we have a belief that they could be applied to quantum supergravity and gauge theories as well. Based on this motivation, the supersymmetric spin networks first were introduced in Ref. 10 and then developed in Ref. 11. In Ref. 10 by virtue of supersymmetric spin networks, we carry out a nonperturbative quantization of simple supergravity. In particular, we find the spectrum of area operator taking a discrete form,

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$$\hat{A}|\Gamma^{sg},e_i,v_j\rangle=\sum_i l_p^2\sqrt{j_i\left(j_i+\frac{1}{2}\right)}|\Gamma^{sg},e_i,v_j\rangle, \tag{1}$$

where l_p is the Planck length and $j_i=e_i/2$.

In this article we develop the construction of supersymmetric spin networks. After giving an overview on some general features of spin networks in Sec. II, we study a special kind of super spin network which has superalgebras $\mathrm{Osp}(1|2n)$ in the consequent section, and $\mathrm{Osp}(N|2)$ spin networks are also discussed briefly in Sec. IV. In Sec. V we discuss some possible applications of super spin networks.

II. AN OVERVIEW

A spin network is a graph, $\Gamma(e_i,v_j)$, embedded in a three dimensional manifold M. It is composed of edges (or links) and vertices (either nodes or joints). To each edge, we assign the color, e_i, which is related to the labels of the irreducible representation of groups, and to each vertex we assign an intertwiner operator, v_j, which maps the incoming irreducible representations to the outcoming ones at the vertex. We adopt the convention that the vertex is called a k-valent one if there are k edges meeting at this vertex.

The construction of spin networks has a direct interpretation in representation theory of groups. In spin networks, each edge e labeled by the representation could be understood as a parallel propagator or holonomy of the connection A, $U_e(A)$, along the edge in connection representation. In matrix notation of group theory, it also corresponds to the higher dimensional irreducible representation of the group element. In SU(2) spin networks, we also think of the edge as the combination of many *ropes*, each of which corresponds to the fundamental representation of the group. Therefore, the reason that each edge can be decomposed into many ropes stems from the fact that every higher dimensional irreducible representation of the group can be obtained by employing the symmetrization or antisymmetrization procedures from the fundamental representations. It is this fact that we can decompose the spin network into multi-loop graphs by permuting and connecting all the ropes to form loops, and finally we are able to establish the transformation between spin network states and loop states in the corresponding Hilbert space.

Intertwiner operators associated with every vertex in spin network can be understood as the different ways that we could carry out to connect the ropes when edges meet at the same vertex. Correspondingly, in the language of representation theory of groups, it corresponds to the fact that tensor products of several irreducible representations can be completely decomposed into the direct sum of the irreducible representations. Hence, they are invariant tensors in irreducible representations of groups and given by standard Clebsch–Gordan (CG) theory. In the case of SU(2) spin networks, when the vertex is a tri-valent one, the decomposition of the tensor product is unique. If the edges are more than three, we then can divide the multi-valent vertex into the tri-valent vertices by making use of the intertwiner operator. At the same time, restricted by the expansion of Clebsch–Gordan series, the colors associated with edges which meet at the same vertex must satisfy some conditions consistent with these CG series. We call them admissible conditions. For instance, consider three valences with colors (a,b,c) meet at the same vertex in ordinary SU(2) spin networks. Then they have to satisfy the triangle inequality and the sum of them has to be even numbers; however, in the case of $\mathrm{Osp}(1|2)$, then the sum can be any positive integer.

Associated with each spin network, we can obtain one number by taking the trace of the corresponding matrix product of the propagators along edges in representation space, which is called the evaluation of spin networks. It has very important applications to quantum gravity. In particular, when we consider the action of operators such as area and volume observables on the spin network states, it provides us a practical way to work out the spectra of these observables. In cases of SU(2) and $\mathrm{Osp}(1|2)$, the evaluations of spin networks, in particular the theta graphs, are discussed respectively in Refs. 12 and 10, where $6j$ symbols and recoupling theories play important roles.

Based on the spin network $\Gamma(e_i, v_j)$, we can define a spin network state, $\Phi_{f_\Gamma}(A)$, by means of the cylindrical function with the form

$$\Phi_{f_\Gamma}(A) := f_\Gamma(U_{e_1}(A), \ldots, U_{e_n}(A)), \tag{2}$$

where cylindrical function f_Γ refers to taking the holonomy along each edge and then contracting the holonomy matrix with the intertwiners at each vertex where edges meet. Spin network states have more advantages than loop states since they are linear independent and do form a basis of the Hilbert space, rather than loop states the space of which is over completed and contains some identities. To show the spin network states form a basis in the Hilbert space, we need solve two key problems. One is the definition of inner product of the spin network state, consequently we can show any two different spin network states are orthogonal and linear independent; the other one is the completeness of the spin network states, namely any state in Hilbert space can be expressed in terms of spin network states. In the case of SU(2), these two problems are solved successfully mainly by virtue of the Haar measure and Peter–Weyl theorem in group theory, respectively.[4–6] As a result, SU(2) spin networks play a key role to form a linear independent basis of the Hilbert space in loop quantum gravity.

When we try to extend the notion of spin networks to the supersymmetric case, we need to construct the graphs and find the rules which must be completely consistent with the representation theory of superalgebras. Following constructions of SU(2) and Osp$(1|2)$ spin networks,[4,10] which has been recalled above, let us list some basic procedures that we have to take into account in this article.

(i) The definition of supersymmetric spin networks. At the first sight, it is simple to define the supersymmetric spin networks. We only need to change the representations associated to edges to the corresponding representations of the supergroups and label the vertex by intertwiner operator appropriately. But after that, to make the spin network well defined, we need to consider the following related questions.

(ii) What are the admissible conditions associated with the tri-valent vertex? Or, equivalently, can any tensor product of the irreducible representations be decomposed into the direct sum of the irreducible representations? Due to the features of superalgebras on their own, we will face some troubles at once, because, unlike the Lie algebra, *the tensor products of many kinds of superalgebras are not completely reducible into the irreducible ones*. We could see this trouble elsewhere when we construct the Osp$(2|2)$ spin networks.[11]

(iii) Could we find a way to evaluate the graphs such that we could consider the action of the operators on the corresponding spin network states and then calculate the spectra of the operators? More explicitly, can every edge be decomposed into ropes, as we do in the case of SU(2)? Namely, can any irreducible representation of the supergroups be constructed from the fundamental representation? We will also see only some special sorts of superalgebras have such features. Furthermore, is it possible to carry out a graphic representation of computing the enclosure of edges?

(iv) Does the set of the corresponding spin network states form a basis for the Hilbert space? To show this, first we need to show that any different spin network states are orthogonal and linear independent, and, second, any states in the space can be decomposed into the sum of the spin network states.

To answer these questions, in this article we extend the strategy in SU(2) spin networks to a special kind of supersymmetric spin network which is equipped with superalgebra Osp$(1|2n)$. The analysis of this special one will lead to some general comments on the construction of supersymmetric spin networks with other superalgbras.

But, before we do that, let us recall some basic facts related to superalgebras in the last part of this section. Superalgebras and supergroups were proposed in physics to construct the supersymmetric model in which bosons and fermions are placed in the same supermultiplet and they could change into each other under the supersymmetric transformation. In fact, every superalgebra

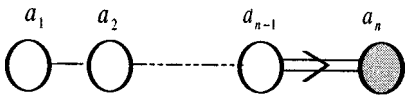

FIG. 1. Dynkin diagram of Osp$(1|2n)$.

or graded algebra contains two kinds of generators. One is even, which is the bosonic part, and the other is odd corresponding to the fermionic part. Contrasting to the ordinary algebras, the even generators of the superalgebra are associated with the *anti*commuting parameters while the odd ones are associated with the *anti*commuting parameters. A special kind of superalgebra is a classical simple Lie superalgebra, whose odd part is completely reducible into one or two irreducible subspaces. Its classification and representation are given in the fundamental paper by Kac.[13] Furthermore, if classical superalgebras admit a nondegenerate metric tensor, they are called basic superalgebras, which is the closest one to simple Lie algebra. All irreducible representations of basic superalgebras are obtainable from a highest weight and the Schur lemma holds under the usual way. However, unlike the ordinary Lie algebras, normally superalgebras have two kinds of representations. One is typical, and the other one is atypical. The typical representations are irreducible and more like the ordinary representations of the Lie algebra, however the atypical ones are in many respects degenerate. In particular, the atypical representations may not be *completely* reducible, for example, if they occur as the semidirect sums of several irreducible atypical representations.

Many kinds of Lie superalgebras do not have properties similar to those of Lie algebras. For example, the complete reducibility is not valid for all the simple Lie superalgebras any more, even for basic ones. Finite reducible but indecomposable representations may appear if we consider the tensor products of irreducible representations. However, the representations of Osp$(1|2n)$ have all the nice properties of those of semisimple Lie algebras. For example, all its reducible representations are fully reducible and therefore a generalized Wigner–Eckhart theorem holds.

The Lie supergroups are obtained by exponentiating Lie superalgebras. Particularly for supergroups SU$(N|M)$ and Osp$(N|2M)$, it is known that all the representations constructable can be obtained from the direct product of fundamental representations.

III. Osp$(1|2n)$ SPIN NETWORKS

A. Definition

First let us concentrate on a special kind of spin network with superalgebra Osp$(1|2n)$ $=B(0,n)$,[14] which is a subset of the orthosympletic Lie superalgebras Osp$(M|2n)$.[15] Its even part is $O(1)\otimes Sp(2n)$ and the Dynkin diagram is shown in Fig.1.

The finite dimensional irreducible representation is characterized by its highest weight Λ $=(a_1,a_2,\ldots,a_n)$, which takes the form

$$\Lambda=a_1\omega_1+a_2\omega_2+\cdots+a_n\omega_n, \tag{3}$$

where $\omega_i(i=1,\ldots,n)$ is the fundamental weight and the coordinate $a_i(i=1,\ldots,n)$ has to be nonnegative integer. The Sp$(2n)$ representation contained in the representation can be read out from the diagram directly by replacing the odd root a_n by $b_n=\frac{1}{2}a_n$. Correspondingly, the edge in Osp$(1|2n)$ spin networks is labeled by e_i, which is defined as a partition of $(a_1,\ldots,a_n)$. In the language of spin networks we also call the weight coordinates colors of the edge. In the simplest case of $n=1$, we see the representation of superalgebra is labeled by only one integer $e_1=2j_1$, and the corresponding spin networks are discussed in detail in Ref. 10.

B. Elements: Edges and vertices

As we mentioned earlier, in general there are two kinds of representations of the superalgebra. One is typical, and the other one is atypical. However, superalgebra Osp$(1|2n)$ has a remarkable

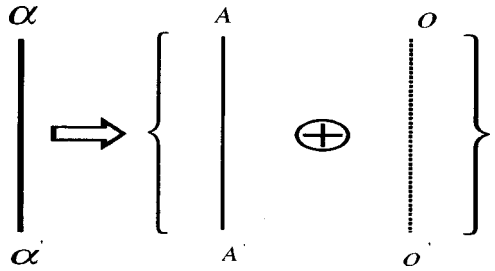

FIG. 2. Composition of unit element with color $(1,0,\ldots,0)$.

feature. It has only typical representation. The fundamental representation is labeled by weight coordinates $(1,0,\ldots,0)$, and the basis vector of the representation is $2n+1$ dimensional and contains one boson and $2n$ fermions,

$$\xi_\alpha = \begin{pmatrix} \psi_A \\ \phi_o \end{pmatrix}, \tag{4}$$

where ψ_A is the fermionic part of the representation and $A=(1,\ldots,2n)$ is the spinor index of $\mathrm{Sp}(2n)$, while ϕ_o is the bosonic part which is only one dimensional. Then the unit element in the fundamental representation can be illustrated as in Fig. 2, in which we denote the $\mathrm{Sp}(2n)$ element by the thin line and the single bosonic part by the dotted line.

The higher finite dimensional representations of the superalgebra can be obtained by symmetrizing and antisymmetrizing the fundamental representations.[16] Note that in the simplest case of $n=1$, we only need to take the symmetrization procedures since the anti-symmetrization of two spinor indices will be identical to the trivial representation. In context of Young tableaus, we have only one row of boxes. However, for $n\geqslant 2$, we need to take both symmetrization and antisymmetrization procedures to obtain all the finite dimensional irreducible representations. For instance, we consider the tensor products of two fundamental representations. We can symmetrize two basis vectors, which is defined as[17]

$$\xi_{(\alpha\beta)} = \xi^1_\alpha \xi^2_\beta + (-)^{g(\alpha)\cdot g(\beta)} \xi^1_\beta \xi^2_\alpha . \tag{5}$$

Also we can antisymmetrize them as

$$\xi_{(\alpha\beta)} = \xi^1_\alpha \xi^2_\beta - (-)^{g(\alpha)\cdot g(\beta)} \xi^1_\beta \xi^2_\alpha , \tag{6}$$

where $g(\alpha)$ is the grade of the index. For fermionic indices, it is one and for bosonic it is zero. If we denote the symmetrization by the square box in the graph, and antisymmetrization by a circle labeled by the number of ropes under consideration, then the unit elements of the supergroup under these representations are illustrated in Fig. 3.

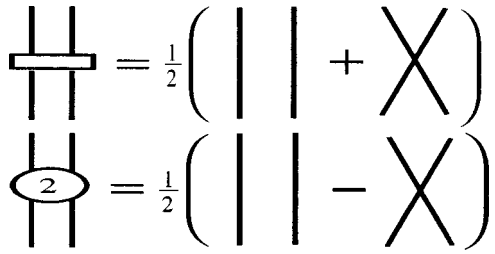

FIG. 3. Symmetrization and antisymmetrization of fundamental representation.

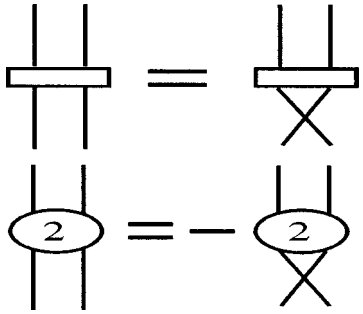

FIG. 4. Property I.

Their weight coordinates are (2,0,...,0) and (0,1,0,...,0), respectively. We also call the unit element symmetrizer in which ropes are symmetrized and antisymmetrizer in which ropes are antisymmetrized. Unlike the symmetrization, we can derive the following properties of the antisymmetrization in graphic representations (see Figs. 4–6).

These properties are easily proved by using the definition of symmetrizers and antisymmetrizers shown in (3). For instance in Fig. 5, when two lines are both symmetrized and antisymmetrized at the same time, then obviously they vanish.

Also, when one graph involves both boxes and circles, we find the order is also important now. For instance, the graphs shown in Fig. 7 are not equivalent.

Continuously taking the antisymmetrization procedures on fundamental representations, we will find it has to be terminated as far as more than $2n$ fundamental representations are involved, since with antisymmetrizing the same index vanishes. To simplify the notation, we only show one line but label the number of ropes which are antisymmetrized in the circle. We draw it as in Fig. 8.

To construct the graphical representation for any highest weight irreducible representation, we need make use of the Young supertableaux. For $\mathrm{Osp}(1|2n)$, the construction of Young supertableaux is simple since it has the same shape as the usual Young tableaus of $\mathrm{Sp}(2n)$ representation $(a_1,a_2,\ldots,a_{n-1},1/2\,a_n)$. The Young tableau associated to $\mathrm{Sp}(2n)$ representation $(a_1,a_2,\ldots,a_{n-1},1/2a_n)$ is defined as a graph with λ_i boxes in the ith row where λ_i is related to the Dynkin labels by

$$\lambda_i=a_i+\lambda_{j+1},\quad \lambda_n=\tfrac{1}{2}a_n, \tag{7}$$

which satisfies $\lambda_1\geqslant\lambda_2\geqslant\cdots\geqslant\lambda_n\geqslant 0$.

Replacing each box in the Young supertableaux by a vertical straight rope and putting them in parallel from left to right, then we define a decomposition of the edge by symmetrizing or antisymmetrizing them corresponding to their positions in Young supertableaux. As a result, if an irreducible representation is obtained by taking both symmetrization and antisymmetrization pro-

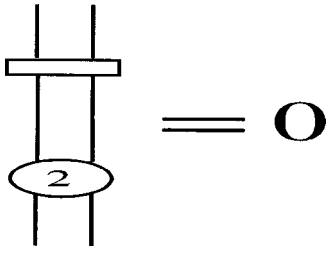

FIG. 5. Property II.

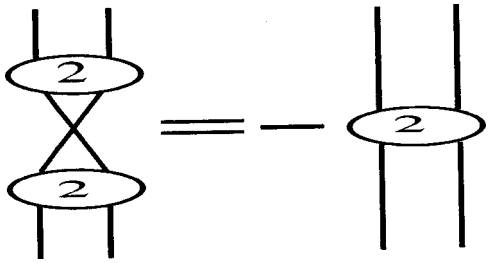

FIG. 6. Property III.

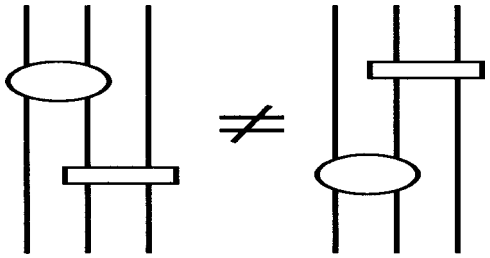

FIG. 7. Two distinguished graphs with different orders of box and circle.

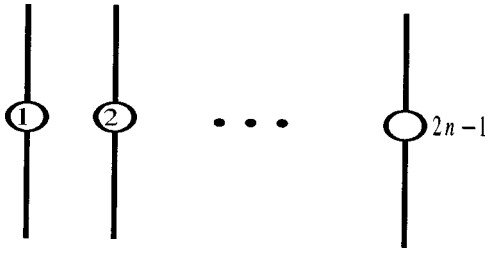

FIG. 8. All the nonvanishing antisymmetrizers in Osp$(1|2n)$ spin networks.

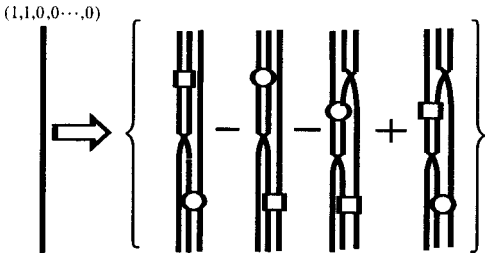

FIG. 9. The graphic representation of $(1,1,0,\ldots,0)$.

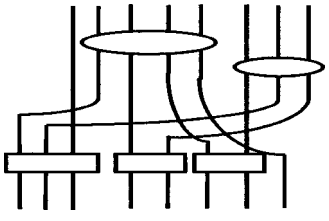

FIG. 10. The rope components of general edges.

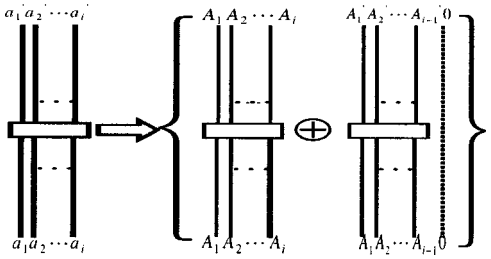

FIG. 11. The rope components of general edges.

cedures, we find there are several inequivalent graphic representations. For example, the representation $(1,1,0,0,\ldots,0)$ could be realized by graphs illustrated in Fig. 9.

In conclusion, we find the edge in spin networks can be decomposed into some components which are the combination of some symmetrized or antisymmetrized ropes. An example of the decomposition is shown in Fig. 10.

Next we consider the vertex and intertwiners in spin networks. In the context of representation theory, it is equivalent to considering the tensor product of irreducible representations. We note that the only Lie superalgebras for which all finite dimensional representations are completely reducible are the direct products of $\mathrm{Osp}(1|2n)$ superalgebras and semi-simple Lie algebras (Djoković–Hochschild theorem[18]). In the context of spin networks, we will have no trouble connecting the edges together at the same vertex. We only need to find out the appropriate admissible conditions and label the vertex by the correct intertwiners, which corresponds to finding the Clebsch–Gordan series for the tensor products of the irreducible representations. To be able to do that, the possible way is to decompose the edge into the direct sum of ones in ordinary $\mathrm{Sp}(2n)$ spin networks since the tensor product of two $\mathrm{Sp}(2n)$ representations is discussed and the CG coefficients are computable.[19] Next, let us go back to consider the decomposition of super edges into the ordinary $\mathrm{Sp}(2n)$ edges. In the case that only symmetrizations are involved, the edge will decomposed into two components, which is illustrated in Fig. 11.

However, if both symmetrization and antisymmetrizations are involved, then we would find the terms will be more than two, and the specific calculation is possible to carry out. Normally we have the following strategy to obtain all the terms in ordinary $\mathrm{Sp}(2n)$ spin networks. The first term in $\mathrm{Sp}(2n)$ spin networks has the same shape as the super one. Then we divide the ropes into symmetrized groups in which each rope is symmetrized with one another. Then we pick out *at most* one rope from each symmetrized group in turn and replace them by the dotted lines such that we will get all the graphs in terms of the ordinary $\mathrm{Sp}(2n)$ spin networks. Finally, we still need to read off any graph which contains at least two dotted but *antisymmetrized* lines since it vanishes. Among all the graphs remaining, we also have to identify some equivalent graphs and maybe it is a little complicated work. However, in context of Young supertableaux, the procedure is simple. We find the supertableaux of $\mathrm{Osp}(1|2n)$ can be decompsed into the direct sum of ordinary tableaux by removing at most one box from each row. So maybe another practical way is to do the

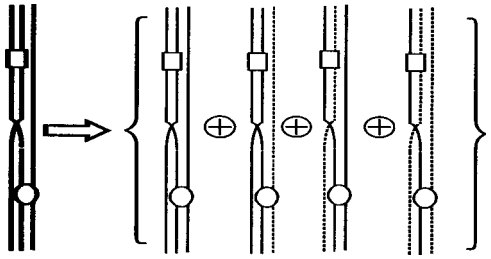

FIG. 12. Decomposition of super spin network into ordinary $\mathrm{Sp}(2n)$ ones.

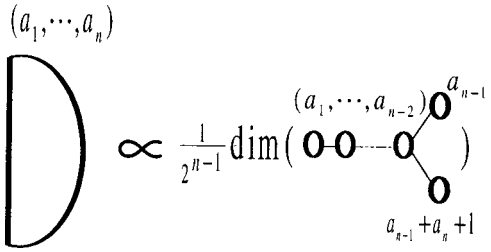

FIG. 13. Closure of the edges.

decomposition in the context of Young tableaux and then transform the Young diagram into edges of the spin networks. For example, the super one $(1,1,0,\ldots,0)$ can be decomposed into four $\mathrm{Sp}(2n)$ terms as shown in Fig. 12.

Then the tensor product of two edges in super spin networks will correspondingly be decomposed to the direct sum of the tensor products of edges in $\mathrm{Sp}(2n)$ spin networks.

C. Evaluation

In this article we have not carried out a specific calculation for the evaluation of $\mathrm{Osp}(1|2n)$ spin networks yet. However, based on the following analysis, we would like to claim that it is definitely possible to do so due to the features of the $\mathrm{Osp}(1|2n)$ superalgebra. Basically we have two ways to evaluate such super spin networks. One way is to decompose the super one into the ordinary $\mathrm{Sp}(2n)$ spin networks, as we argued above; the other way is given as follows. Reference 20 shows that there is a one-to-one correspondence between the graded representation of $\mathrm{Osp}(1|2n)$ and the nonspinorial representations of $\mathrm{O}(2n+1)$. First, if a graded irreducible representation of $\mathrm{Osp}(1|2n)$ and a nonspinorial irreducible representation of $\mathrm{O}(2n+1)$ have the same highest weight, one has

$$\dim(\rho^{\mathrm{osp}(1|2n)}(a_1,\ldots,a_n))=\dim(\rho'^{\mathrm{O}(2n+1)}(a_1,\ldots,a_n)). \tag{8}$$

Moreover, the multiplicity of any weight is the same for both representations. As a direct application of the argument, consider the tensor products of both irreducible representations having the same highest weights. Then we can see the Clebsch–Gordan (CG) series coincide; in particular, since the tensor products are completely reducible, their CG series can be obtained by counting the multiplicities of their weights.

So far, the one-to-one correspondence also gives us an alternative practical way to evaluate the $\mathrm{Osp}(1|2n)$ spin networks by studying the $\mathrm{O}(2n+1)$ spin networks, which should be easy to carry out at first.

In the last part of this section, we conjecture some examples that could be worked out in the future. One is the closure of any edge, namely, the supertrace of the unit element of supergroup $\mathrm{Osp}(1|2n)$ in such finite irreducible representation. Note that the supertrace of supergroups is defined as

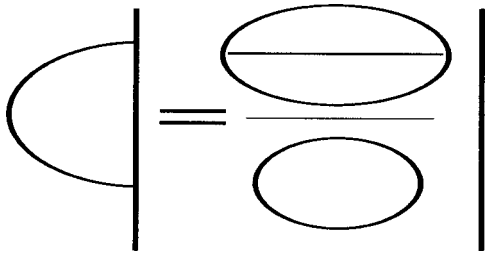

FIG. 14. Identity.

$$\mathrm{Str}(U^{\alpha}_{\beta}) := \mathrm{Tr}(A) - \mathrm{Tr}(D), \tag{9}$$

where we suppose the matrix representation of the supergroup has a structure

$$U = \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \tag{10}$$

This can be done by calculating the dimensions of the Lie algebra $\mathrm{O}(2n+1)$ shown in Fig. 13.

We find the closure of the edge is a nonzero number. Thus we could expect the identity drawn in Fig. 14 to be evident.

They would also be applied to the nonperturbative quantization of eleven dimensional supergravity when we consider the actions of the operators. For instance, we may consider the quadratic Casimir operators and their eigenvalues. In loop quantum gravity, this kind of operator is related to the area observable:

$$C_k(\Lambda) = \frac{1}{4n+2}(\Lambda|\Lambda + 2\rho), \tag{11}$$

where $(|)$ is defined as the inner product of the weights and ρ is defined as

$$\rho = \omega_1 + \omega_2 + \cdots + \omega_n . \tag{12}$$

The supertrace not being zero has more important meaning when we define super spin network states and form the Hilbert space. This good feature will allow us to define generalized ''Ashtekar–Lewandowski'' (AL) measure on the space, moreover, to show the spin network states form a basis of the space.

D. Hilbert space

In this section we begin with the integration theory on the supergroup manifold, and then apply it to spin network states.

Given a manifold M, we define a Lie superalgebra $\mathrm{Osp}(1|2n)$ valued connection one-form A. For instance, in eleven dimensional space–time, we can define the $\mathrm{Osp}(1|32)$ connection as follows,

$$A =: A_{\mu}(x)dx^{\mu} = A^{a}_{\mu}(x)P_a dx^{\mu} + A^{ab}_{\mu}(x)J_{ab}dx^{\mu} + A^{a_1\cdots a_5}_{\mu}(x)Z_{a_1\cdots a_5}dx^{\mu} + \Psi^{\alpha}_{\mu}(x)Q_{\alpha}dx^{\mu}, \tag{13}$$

where $x=(x_0,\ldots,x_{10})$ are local coordinates on M, μ is the space–time index and a,b are internal indices. α is spinor index. $P_a, J_{ab}, Z_{a_1\cdots a_5}$, and Q_{α} are $\mathrm{Osp}(1|2n)$ generators while J_{ab} and $Z_{a_1\cdots a_5}$ are skew symmetric. In (13) we can think of all the components of connection A as the smooth function on the manifold M. Let us denote the space of smooth connections on M as $\mathcal{A}$. Then we define the space of continuous functionals on $\mathcal{A}$ as $\mathrm{Fun}(\mathcal{A})$. Now based on the linear vector space, we want to define a Hilbert space, $\mathcal{L}^2(\mathcal{A})$. Namely, we need introduce some inner product of the quantum states which is the element in $\mathrm{Fun}(\mathcal{A})$, and then consider the completion of $\mathrm{Fun}(\mathcal{A})$. In loop quantum gravity, we carry out all the procedures by introducing a special kind of function of the connection, which is called a cylindrical function. They are defined as the functions of holonomies of the connection. Therefore they are functions of group manifold as well. Then the inner products can be defined by means of taking the integration on the group manifold; as we know, a unique, both left- and right-invariant measure can be defined on it.

Now we extend all the construction mentioned earlier to the supersymmetric case of $\mathrm{Osp}(1|2n)$. First, note the super loop variables can be defined by means of the holonomy of super connections $\mathcal{A}$. For details we refer to Ref. 21:

$$U[\mathcal{A},\gamma](s) := \mathcal{P}\exp\int_{\gamma} ds\,\gamma^{\mu}A_{\mu}(\gamma(s)). \tag{14}$$

Note that U is an element of supergroup $\mathrm{Osp}(1|2n)$. The loop states can be defined as

$$\Psi_{\gamma}(A) := \mathrm{Str}U[A,\gamma], \tag{15}$$

where γ is a loop in the space–time manifold with $\gamma(0)=\gamma(1)$. Though the holonomy is not gauge invariant, their supertrace is gauge invariant indeed.

It is well known that there is a probability measure, the Haar measure, for the compact Lie groups such that we could define a unique normalized both left- and right-invariant integration, namely,

$$\int_G dg = 1, \quad \int dg f(g) = \int dg f(g_0 g g_1) = \int dg f(g^{-1}), \tag{16}$$

where g_0, g_1 are any group elements and $f(g)$ is also an arbitrary function of g. The generalization of the Haar integral for Lie supergroups was discussed in Ref. 22. We refer to that paper for more details on the integration theory on supermanifold. Here we point out that in particular case of $\mathrm{Osp}(1|2n)$, we can also define a generalized Haar measure on the space of functions on the supergroup which are both left- and right-invariant.[23] Therefore it is possible to develop a positive integration theory on the space of connection, $\mathcal{A}$. Here we define the generalized Haar measure on supergroup $\mathrm{Osp}(1|2n)$ as

$$\int_G dg = 1, \quad \int_G g^{(\rho)}_{\alpha\beta} dg = 0, \ \ \rho \neq 0. \tag{17}$$

Next we consider the definition of inner product of spin network states. Associate to every spin network, we can define a corresponding spin network state in the Hilbert space. To show that the set of spin network states does form a basis for the state space in the case of $\mathrm{Osp}(1|2n)$, we carry out the following procedures. In spin networks we know a connection is simply to assign a group element, U_e, to each edge of the graph e by taking the holonomy of the connection A in the irreducible representation ρ_e along the edge. Hence, the space of connections in context of spin networks is

$$\mathcal{A} \cong \bigotimes_{e_i} G^{e_i}, \tag{18}$$

which is the finite product of group G and the measure is defined as

$$\mathcal{D}\mathcal{A} = \bigotimes_{e_i} dU_{e_i}. \tag{19}$$

We call this measure the generalized Ashtekar–Lewandowski measure. Now we could define the inner product of two spin network states by means of cylindrical functions.

Consider a spin network $\Gamma(e_i, v_j)$. We define the cylindrical functions, Φ_{f_Γ}, which only depend on the holonomies of the connection A. Using the generalized Haar measure on $[G]^n$, we then define the scalar product of two cylindrical functions as

$$\langle \Phi_{f_\Gamma} | \Phi_{g_\Gamma} \rangle := \int_{G^n} dU_1 \cdots dU_i \ \overline{f_\Gamma(U_1,\ldots,U_i)} g_\Gamma(U_1,\ldots,U_i). \tag{20}$$

The Hilbert space on which ρ_l is defined can be denoted as $\mathcal{H}_{\rho_l}$. Hence the total Hilbert space associated to the spin networks can be defined as the tensor product of these spaces,

$$\mathcal{H}=\bigotimes_{v_j}\mathcal{H}^{v_j}=\bigotimes_{v_j}\Big(\bigotimes_{e_i}\mathcal{H}_{e_i}\Big)^{v_j}, \tag{21}$$

where e_i are edges meeting at the same vertex v_j. In the case of Osp$(1|2n)$, since any products of finite dimensional irreducible representations are completely reducible, namely,

$$\rho_1\otimes\ldots\otimes\rho_i=\bigoplus_j v^j\rho_j, \tag{22}$$

correspondingly we find the tensor products of the Hilbert spaces can be decomposed into the direct sum of Hilbert spaces on which the irreducible representations of Osp$(1|2n)$ are defined,

$$\mathcal{H}_{e_1}\otimes\ldots\otimes\mathcal{H}_{e_i}=\bigoplus_{\rho_j}K^j\mathcal{H}_{\rho_j}. \tag{23}$$

Furthermore, we can decompose the Hilbert space as the direct sum of the functions on all the irreducible representations and its conjugate:

$$\mathcal{L}^2(\mathcal{A}/\mathcal{G})=\bigoplus_j V_j\otimes V_j^*. \tag{24}$$

Next, to show that the spin network states are orthogonal and linear independent, we exploit the generalized Peter–Weyl theorem:

Theorem: Let ρ be the irreducible representation of Osp$(1|2n)$ with the highest weights ρ^i, and let $U^{\rho}_{\alpha\beta}$, $\alpha,\beta=1,2,\ldots,d_i(d_i=dim\rho^i)$, be the matrix element of ρ^i, Then:

$$\mathrm{Fun}(A)=\bigoplus_i\bigoplus_{\alpha,\beta=1}^{d_i}U^i_{\alpha\beta}, \tag{25}$$

$$\int U^i_{\alpha\beta}\tilde{U}^j_{\gamma\sigma}(-1)^{\beta\gamma+\alpha+\beta}=\delta_{\alpha\gamma}\delta_{ij}\frac{U^i_{\sigma\beta}}{S\dim(i)}, \tag{26}$$

$$\int U^i_{\alpha\beta}\tilde{U}^j_{\gamma\sigma}(-1)^{\beta\gamma}=\delta_{\beta\sigma}\delta_{ij}\frac{U^i_{\alpha\gamma}}{S\dim(i)}. \tag{27}$$

From the formula above, we note that the nonzero supertrace plays an important role. However, for the supergroups whose supertrace vanishes, then we would maybe have some trouble finding the generalized Peter–Weyl theorem.

Now making use of Eqs. (26) and (27) in the generalized Peter–Weyl theorem, and following the procedures in Ref. 4, it is straightforward to show the Osp$(1|2n)$ spin states are orthogonal,

$$\langle\Gamma,e^i,v_j|\Gamma',e^{i'},v_{j'}\rangle=\delta_{\Gamma\Gamma'}\delta_{ii'}\delta_{jj'}. \tag{28}$$

At the same time, using the equation (25) we can show the set of spin network states is completed such that any state in the Hilbert space can be expressed as the sum of the Osp$(1|2n)$ spin network states,

$$|\Phi\rangle=\sum_i C_i|\Gamma_i\rangle. \tag{29}$$

Therefore, the spin network states do form a basis for the Hilbert space $\mathcal{L}^2(\mathcal{A}/\mathcal{G})$.

Finally, we point out that in the case of quantum deformed superalgebra, we could also construct the q-deformed spin networks and the corresponding spin network states, which will have important application when we study the casual evolution of the spin networks and super-

symmetric spin foams. In the q-deformed case, the ordinary sum of two superspins J_1+J_2 cannot give a third superspin any more when q is not equal to one. The notion of coproduct has to be introduced. The generalized Peter–Weyl theorem for $U_q(\mathrm{osp}(1|2n))$ is given in Ref. 24.

In the class of $\mathrm{Osp}(1|2n)$ spin networks, we are particularly interested in the case of $n=16$, namely $\mathrm{Osp}(1|32)$, since this superalgebra is related to the eleven dimensional supergravity[25–27] and M theory.[28] As we know, in eleven dimensional supergravity, the super-Poincare algebras with two- and five-form central charges are obtained by taking an Inonu–Wigner contraction of $\mathrm{Osp}(1|32)$. This superalgebra has many facets in different dimensions, which are studied in Ref. 29. As a result, we expect the $\mathrm{Osp}(1|32)$ spin networks will have its own advantages when we try to carry out a background independent and nonperturbative quantization of the eleven dimensional supergravity and M theory.

IV. Osp($N|2$) SPIN NETWORKS

In previous section we have described $\mathrm{Osp}(1|2n)$ spin networks following the proposal we gave in overview. In this section we will discuss $\mathrm{Osp}(N|2)$ spin networks briefly. We are interested in this kind of spin network because it is related to the chiral supergravities.[30] But in this class the case of $N=2$ is different from the others since the even part of this superalgebra is $\mathrm{SO}(2)\times\mathrm{Sp}(2)$ such that the first number a_1 of Dynkin labels can be any complex number; however, for the others it has to be a non-negative integer. Its construction and application to supergravity are studies in Refs. 11 and 31. Here we consider the general case when N is larger than two.

The basis vectors of the fundamental representation of $\mathrm{Osp}(N|2)$ span a $N+2$ dimensional vector space. Similar to the case of $\mathrm{Osp}(1|2n)$, its higher finite dimensional irreducible representations can be obtained by standard symmetrization and antisymmetrization procedures on fundamental representation. Therefore, in the context of spin networks, we can decompose the edge into ropes.

In fact, any representation of basic Lie superalgebra can be decomposed into the direct sum of irreducible representations of the even subalgebra, which means any edge in super spin networks can be decomposed into the sum of normal edges which are labeled by the irreducible representations of the even subalgebra. In the case of $\mathrm{Osp}(N|2)$, we can decompose the $\mathrm{Osp}(N|2)$ spin networks into the direct sum of the ordinary spin networks with $\mathrm{SO}(N)\otimes\mathrm{Sp}(2)$. In particular, if only the symmetrization procedures are considered, we have simple decompositions. Figure 15 illustrates the basic one which has the color $(2,0,\ldots,0)$.

Since the $\mathrm{SO}(N)$ indices are antisymmetrized, the decomposition of the graphs terminate at the term which contains N dotted lines (see Fig. 16).

However, unlike the case of $\mathrm{Osp}(1|2n)$, some questions arise in the $\mathrm{Osp}(N|2)$ case as we try to construct the Hilbert space based on spin network states. As we mentioned before, both typical and atypical representations are present for other superalgebras except $\mathrm{Osp}(1|2n)$. The key difference of these two types of representations is that all the typical representation is either irreducible or completely reducible; however, the atypical one maybe is not completely reducible (i.e., reducible but not decomposable). In group theory, there is a simple meaning of complete reduc-

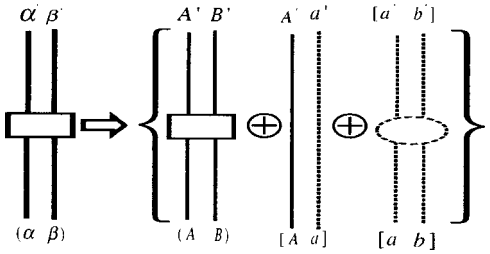

FIG. 15. Symmetrizer with color two.

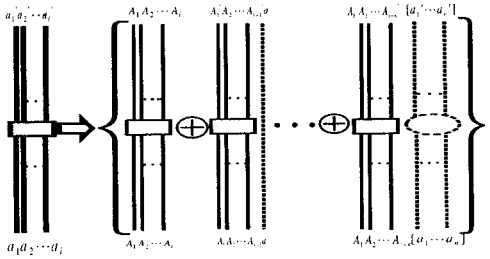

FIG. 16. Symmetrizer with color $(i,0,\ldots,0)$.

ibility, namely the representation space should be a Hilbert space and the representation should be unitary. Correspondingly, in the context of spin networks we will meet some serious problems to show the corresponding spin network states form a basis for the Hilbert space. In this case, we do not know there exists some kind of generalized Peter–Weyl theorem, though the left-invariant Haar integral for such supergroups is also discussed in Ref. 22. But let us note there are some classes, which are called star representations and graded star representations in irreducible representations of the superalgebras.[14,32] Inside each class the complete reducibility is reserved indeed and the CG series can be given also. Thus, spanning spin network states in such subspaces, we still expect they could be well defined to form a basis for such Hilbert spaces. Note that in quantum gravity, only the *physical* Hilbert space is what we want finally. So, it is quite interesting to find some self-consistent subset of spin networks which are well defined and investigate the possible applications to quantum theory.

In the end of this section, let us make a summation by listing the correspondence between the construction of spin networks and the representation theory of the superalgebra.

Spin networks	Representation theory of superalgebra
Edges	Irreducible representation
Vertex	Intertwiner operator
Ropes	Fundamental representations
Admissible conditions	Clebsch–Gordan series
Closure of edges	Supertrace of the unit element
Spin network states	Cylindrical functions
Inner product of spin network states	Generalized Haar measure
Orthogonality and linear independence of states	Generalized Peter–Weyl theorem

V. DISCUSSIONS

In this article we have presented a general introduction to the construction of supersymmetric spin networks. All the strategy in ordinary SU(2) spin networks can be employed in the case of Osp$(1|2n)$ spin networks. In particular, the spin network states form a basis for the Hilbert space $\mathcal{L}^2(\mathcal{A}/\mathcal{G})$. But normally it is becoming more complicated to carry out a practical way to evaluate the spin network graphs, as in general both symmetrization and antisymmetrization procedures are involved in higher finite dimensional irreducible representations. However, it is definitely plausible to give a specific calculation on evaluation of graphs in the future by following strategies given in present article. On the other hand, due to the properties of the superalgebra, it is unclear if we could construct spin network states as the basis of Hilbert space based on any kind of superalgebra. Here we only discussed the Osp$(N|2)$ spin networks briefly and found this problem should be considered seriously.

To apply spin network techniques to quantum supergravities and Yang–Mills theory is very promising and important. At root they are powerful tools to quantize gauge theories along the nonperturbative and background independent approach.

First we expect the corresponding spin network states would be applied to construct the Hilbert space of quantum supergravities. In this framework we could find a practical way to consider the action of the operators, and calculate the spectra of the observables. In Ref. 10, we have made a first step to calculate the spectrum of area operator in $N=1$ Chiral supergravity, and the extension to the case of $N=2$ is also done in Ref. 11.

Second, we propose the holographic hypothesis[33,34] can be tested in the framework of nonperturbative quantum supergravities. This conjecture has been tested in $N=1$ and $N=2$ supergravity, respectively.[31,35] It is the supersymmetric spin networks that make it possible to count the number of degrees of freedom on the boundary such that we find the relations between the area of the boundary and the number of the states do satisfy Bekenstein's conditions.

Until now we only take into account the finite dimensional representation of the superalgebra. It is worth studying what role the spin networks will play if we consider the infinite dimensional representation of the superalgebra.

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condition $G_{\alpha\beta}\xi_{(\alpha\beta)}=0$ (Ref. 16), where $G_{\alpha\beta}$ is the invariant bilinear form taking the form

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & I_n \\ 0 & -I_n & 0 \end{pmatrix}.$$

However, this shift will not affect our construction of the unit element of the supergroups. We just ignore this shift in this article.

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The Fejér average and the mean value of a quantity in a quasiclassical wave packet

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The mean value of a quantity in an equally weighted wave packet was recently found in the classical limit to be the Fejér average of partial sums of Fourier series expansion of the classical quantity, and the number of stationary states in it is equal to that of partial sums. The incompleteness of the Fejér average in representing a classical quantity enables us to define a classical uncertainty relation which turns out to be the counterpart of the quantum one. In this paper, two typical quantum systems, a harmonic oscillator and a particle in an infinite square well, are used to illustrate the above-mentioned points. © *2002 American Institute of Physics.*
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I. INTRODUCTION

During the past few years, the dynamics of wave packets has become a very active field of research—for a review, see Ref. 1. Intensive theoretical and experimental studies show that only the short-term, one or two periods to be precise, behaviors of an initially localized wave packet prove to be similar to those of an appropriate ensemble of classical orbits. Its long-term behaviors such as collapse, (super-)revival, etc., are inevitable and of purely quantum mechanical origin.[1] However, an outstanding problem remains open: In what sense can or cannot the quantum mechanics recover the classical mechanics for a single orbit in the classical limit?

As stated in a standard textbook,[2] in order to obtain a definite classical orbit in the classical limit, we must start from a quasiclassical wave packet of a particular form $|\psi(t)\rangle=\Sigma_m c_m\psi_m$, where the coefficients c_m are noticeably different from zero only in some range δm of values of the quantum number n such that $1\ll\delta m\ll n$; the numbers n are supposed large and the superimposed stationary states ψ_m in the wave packet $|\psi(t)\rangle$ have nearly the same energy E_n.[2] As believed, the mean value of a quantity in such a wave packet must become, in the classical limit, simply the classical value of the quantity; and the mean value was ''proved'' to have a Fourier series form.[2] In fact, the proof given in Ref. 2 is not rigorous in mathematics, as recently pointed out in Ref. 3.

The wave packet we study takes the following simplest form:

$$|\psi(t)\rangle=\frac{1}{\sqrt{2N+1}}\sum_{m=-N}^{N}\psi_{n+m}(x)\exp\left(\frac{-iE_{n+m}t}{\hbar}\right)\quad(N\leqslant n). \tag{1}$$

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It is an equally weighted wave packet (EWWP) which is constructed by superposition of $2N+1$ successive stationary states centered at the nth with an equal weight $1/\sqrt{2N+1}$. Q.H.L. has recently proven in a Letter[3] that in the constraint classical limit;

$$n\to\infty,\hbar\to 0,n\hbar=an\ \ appropriate\ \ classical\ \ action, \tag{2}$$

the quantum mechanical mean value of a quantity in the EWWP goes over to the classical quantity, but the form is Fejér average of partial sums of Fourier series of the classical quantity rather than the Fourier series itself.[3] Let the nth partial sum of Fourier series expansion of a classical quantity f be f_n,

$$f_n=\sum_{k=-n}^{n} c_k \exp\left(\frac{i2k\pi t}{T}\right). \tag{3}$$

The Fejér average $F\langle f\rangle$ of $2N+1$ partial sums is then

$$F\langle f\rangle=\frac{f_0+f_1+f_2+\cdots f_{2N}}{2N+1}. \tag{4}$$

What was proven in Ref. 3 means in the quasiclassical sense that the number $2N+1$ of the stationary states in EWWP (1) is nothing but the number of the partial sums in the Fejér average $F\langle f\rangle$ (4), and

$$\overline{f}=\langle\psi(t)|f|\psi(t)\rangle\approx F\langle f\rangle. \tag{5}$$

We are impressed by the fact that the Fejér average is initially an intellectual creation in pure mathematics to study the convergence of Fourier series. Its existence in physics may reflect the harmony of mind world of mankind and material structure of nature. Since the Fejér average is not familiar to some readers, we give a brief introduction to it in the Appendix.

The Fejér average $F\langle f\rangle$ (4) of a classical quantity can contain an arbitrary number of partial sums for N, which can be an arbitrary integer ranging from 0 to ∞. However, from Eq. (1), quantum mechanics puts an upper bound to N, $N\leqslant n$. In fact, we have $N\ll n$ in the quasiclassical sense as will be shown shortly. Moreover, the minimum of the uncertainty relation $\Delta x\Delta p$ singles out a critical $N=N_c$, for the uncertainty relation cannot be minimized with the number of stationary states being more or less than it. The relation between N_c and n can be reasonably assumed to be given by an exponent equation,

$$N_c\approx n^m,\quad m<1, \tag{6}$$

where m is a constant exponent depending on the form of the potential, and can be called the critical exponent. In this paper, calculations give $m=2/3$ for a harmonic oscillator (HO), and $m=1/2$ for an infinite square well (ISW) potential.

There is no uncertainty associated with a classical quantity; but the representation of Fejér average $F\langle f\rangle$ (4) of the classical quantity is not complete unless $N\to\infty$ (cf. the Appendix). Because of this incompleteness, a classical uncertainty $\Delta_c f$ can be defined by

$$\Delta_c f=\sqrt{F\langle f^2\rangle-(F\langle f\rangle)^2}, \tag{7}$$

which approaches zero as $N\to\infty$. It is the counterpart of the quantum uncertainty Δf for the correspondence relation (5) implies in the semiclassical sense,

$$\Delta_c f\approx\Delta f. \tag{8}$$

Note that in each case in this paper, to compare a classical mechanical result with a quantum mechanical one, the classical quantity takes its semiclassical form.

As a systematic illustration of how the Fejér average relates to the mean value of a quantity in the EWWP, a single HO and a particle in the ISW are studied in Secs. II and III, respectively. Why these two systems are chosen is based on both physical and mathematical considerations. In physics, they are two fundamental models in quantum mechanics and insights into the dynamics exhibited in them speak immediately to a wide range of physical systems.[4] In mathematics, the classical position $x(t)$ and momentum $p(t)$ for a single HO contain only the fundamental frequency terms $\cos(\omega t)$ and $\sin(\omega t)$, respectively; whereas for a particle in the ISW they give the sawtooth and square wave, respectively, which are indispensable in an elementary discussion of Fourier analyses relevant to Fejér average[5–8] that offers the base of our exact treatment. A brief conclusion is given in Sec. IV.

II. FEJÉR AVERAGE AND A SINGLE ONE-DIMENSIONAL HO

A single one-dimensional HO is of great importance in quantum mechanics as well as in classical physics, since it can be used to approximate a single particle moving in an arbitrary continuous potential in the vicinity of a stable equilibrium position. Furthermore, it is analytically calculable throughout. We like to use it to illustrate various aspects of our theory. This section starts with the calculation of mean values of quantities in the EWWP for the HO, from which the Fejér average comes out as a natural result. Next with the minimum of the uncertainty relation $\Delta x \Delta p$, the critical exponent m is obtained. Then the classical uncertainty relation can be defined and found to be in a semiclassical sense comparable to the quantum one. Section II D presents a brief summary.

A. Mean values of quantities in the EWWP for a single HO

For a single one-dimensional HO with mass μ and intrinsic frequency ω, the mean values for the quantities H, H^2, x, x^2, p, p^2 in the EWWP (1) are given by

$$\langle \psi(t)|H|\psi(t)\rangle = (n+\tfrac{1}{2})\hbar\omega, \tag{9}$$

$$\langle \psi(t)|H^2|\psi(t)\rangle = \left[\left(n+\frac{1}{2}\right)\hbar\omega\right]^2 + (n\hbar\omega)^2\frac{N(N+1)}{3n^2}, \tag{10}$$

$$\langle \psi(t)|x|\psi(t)\rangle = \left(\frac{2}{2N+1}\sqrt{\frac{\hbar}{2\mu\omega}}\sum_{m=-N+1}^{N}\sqrt{n+m}\right)\cos\omega t = f(n,N)\left(\frac{2N}{2N+1}\sqrt{\frac{2n\hbar}{\mu\omega}}\right)\cos\omega t, \tag{11}$$

$$\begin{aligned}\langle \psi(t)|x^2|\psi(t)\rangle &= \left(n+\frac{1}{2}\right)\left(\frac{\hbar}{\mu\omega}\right) + \left(\frac{\hbar}{\mu\omega}\right)\frac{1}{2N+1}\sum_{m=-N+2}^{N}\sqrt{(n+m)(n+m-1)}\cos 2\omega t \\ &= \left(n+\frac{1}{2}\right)\left(\frac{\hbar}{\mu\omega}\right) + \left(\frac{n\hbar}{\mu\omega}\right)\frac{2N-1}{2N+1}g(n,N)\cos 2\omega t,\end{aligned} \tag{12}$$

$$\begin{aligned}\langle \psi(t)|p|\psi(t)\rangle &= -\left(\frac{2}{2N+1}\sqrt{\frac{\hbar\mu\omega}{2}}\sum_{m=-N+1}^{N}\sqrt{n+m}\right)\sin\omega t \\ &= -f(n,N)\left(\frac{2N}{2N+1}\sqrt{2\mu n\hbar\omega}\right)\sin\omega t,\end{aligned} \tag{13}$$

$$\begin{aligned}\langle \psi(t)|p^2|\psi(t)\rangle &= \left(n+\frac{1}{2}\right)\mu\hbar\omega - \mu\hbar\omega\frac{1}{2N+1}\sum_{m=-N+2}^{N}\sqrt{(n+m)(n+m-1)}\cos 2\omega t \\ &= \left(n+\frac{1}{2}\right)\mu\hbar\omega - \mu n\hbar\omega\frac{2N-1}{2N+1}g(n,N)\cos 2\omega t,\end{aligned} \tag{14}$$

where $f(n,N)$ and $g(n,N)$ are

$$f(n,N)=\frac{1}{2N}\sum_{m=-N+1}^{N}\sqrt{1+\frac{m}{n}},\ g(n,N)=\frac{1}{2N-1}\sum_{m=-N+2}^{N}\sqrt{\left(1+\frac{m}{n}\right)\left(1+\frac{m-1}{n}\right)}. \quad (15)$$

Since we have $N<n$, $f(n,N)$ and $g(n,N)$ satisfy

$$\sqrt{1+\frac{-N+1}{n}}<f(n,N)<\sqrt{1+\frac{N}{n}}, \quad (16)$$

$$\sqrt{\left(1+\frac{-N+2}{n}\right)\left(1+\frac{-N+1}{n}\right)}<g(n,N)<\sqrt{\left(1+\frac{N}{n}\right)\left(1+\frac{N-1}{n}\right)}. \quad (17)$$

As a consequence, both $f(n,N)$ and $g(n,N)$ approach unity in the following limit;

$$N\to\infty,\quad N/n\to 0. \quad (18)$$

Upon looking more closely, we can find two relations after neglect of terms higher than $O(1/n)$,

$$\frac{2N}{2N+1}f(n,N)=1-\frac{1}{2N}+O\left(\frac{1}{n}\right)\approx\frac{2N}{2N+1}, \quad (19)$$

and

$$\frac{2N-1}{2N+1}g(n,N)=1-\frac{1}{N}+O\left(\frac{1}{n}\right)\approx\frac{2N-1}{2N+1}. \quad (20)$$

Thus, in the classical limit (2) in conjunction with the limit (18), after neglect of the terms higher than $O(1/n)$, results (9)–(14) become the following quantities, respectively:

$$\langle\psi(t)|H|\psi(t)\rangle\approx E, \quad (21)$$

$$\langle\psi(t)|H^2|\psi(t)\rangle\approx E^2, \quad (22)$$

$$\langle\psi(t)|x|\psi(t)\rangle\approx\frac{2N}{2N+1}\sqrt{\frac{2E}{\mu\omega^2}}\cos(\omega t), \quad (23)$$

$$\langle\psi(t)|p|\psi(t)\rangle\approx-\frac{2N}{2N+1}\sqrt{2\mu E}\sin(\omega t), \quad (24)$$

$$\langle\psi(t)|x^2|\psi(t)\rangle\approx\frac{E}{\mu\omega^2}+\frac{2N-1}{2N+1}\frac{E}{\mu\omega^2}\cos(2\omega t)\approx(\langle\psi(t)|x|\psi(t)\rangle)^2, \quad (25)$$

$$\langle\psi(t)|p^2|\psi(t)\rangle\approx\mu E-\frac{2N-1}{2N+1}\mu E\cos(2\omega t)\approx(\langle\psi(t)|p|\psi(t)\rangle)^2. \quad (26)$$

All results on the right-hand side of Eqs. (21)–(26) are the classical quantities in terms of the Fejér average of $(2N+1)$ partial sums of Fourier series. In other words, the mean value of a quantity in the EWWP converges to the Fejér average of the classical quantity in the classical limit. In Sec. II C, the Fejér average of classical quantities will be discussed in more detail.

B. The relation between *N* and *n* determined by minimizing the uncertainty relation

The square of usual uncertainties of x and p as $\langle\psi(t)|x^2|\psi(t)\rangle-(\langle\psi(t)|x|\psi(t)\rangle)^2$ and $\langle\psi(t)|p^2|\psi(t)\rangle-(\langle\psi(t)|p|\psi(t)\rangle)^2$ are time dependent. Because the time average of them over a period suffices to characterize the deviation of quantum mechanics from the classical one, in this subsection we use the following uncertainties:

$$\Delta x=\left(\left(n+\frac{1}{2}\right)-\left(\frac{1}{2N+1}\sum_{m=-N+1}^{N}\sqrt{n+m}\right)^2\right)^{1/2}\left(\frac{\hbar}{\mu\omega}\right)^{1/2}, \tag{27}$$

$$\Delta p=\left(\left(n+\frac{1}{2}\right)-\left(\frac{1}{2N+1}\sum_{m=-N+1}^{N}\sqrt{n+m}\right)^2\right)^{1/2}(\mu\omega\hbar)^{1/2}. \tag{28}$$

The minimum of their product $\Delta x\Delta p$ means to minimize the quantity $(n+1/2)-(\Sigma_{m=-N+1}^{N}\sqrt{n+m}/(2N+1))^2$ at a fixed n. In the quasiclassical case where $N\ll n$ is satisfied, the square root of $\sqrt{n+m}$ can be expanded up to $(m/n)^3$ as (the numerical work will confirm that expansion to this order is accurate enough),

$$\sqrt{n}\left(1+\frac{m}{2n}-\frac{m^2}{8n^2}+\frac{m^3}{16n^3}\right). \tag{29}$$

Then, the summation $\Sigma_{m=-N+1}^{N}\sqrt{n+m}/(2N+1)$ is approximately

$$\begin{aligned}\frac{1}{2N+1}\sum_{m=-N+1}^{N}\sqrt{n+m}&\approx\frac{1}{2N+1}\sum_{m=-N+1}^{N}\sqrt{n}\left(1+\frac{m}{2n}-\frac{m^2}{8n^2}+\frac{m^3}{16n^3}\right)\\&=\frac{N^3-2N(1+2N^2)n/3+8Nn^2+32Nn^3}{16(1+2N)n^{5/2}}.\end{aligned} \tag{30}$$

Treating N as a continuous variable, the zeros of the equation obtained from the derivative of Eq. (30) with respect to N would minimize the uncertainty relation $\Delta x\Delta p$. The only meaningful root is

$$N_c=-\frac{1}{4}+\frac{3\,(-3+4\,n)}{2*2^{2/3}y^{1/3}}+\frac{y^{1/3}}{12*2^{1/3}(-3+4\,n)}, \tag{31}$$

where

$$\begin{aligned}y=&-54\,(-3+4\,n)^3+864\,n\,(-3+4\,n)^2\,(-1+12\,n+48\,n^2)+216\,\sqrt{6}\,\sqrt{n}\,(-3\\&+4\,n)^2\,\sqrt{-1+16\,n-32\,n^2+64\,n^3+3072\,n^4+6144\,n^5}.\end{aligned} \tag{32}$$

When $n\gg 1$, we have approximately, with $[x]$ standing for the integral part of positive number x,

$$N_c\approx[6^{1/3}n^{2/3}]. \tag{33}$$

A comparison of this relation to the numerically exact one, as shown in Fig. 1, shows that this relation is unbelievably accurate in whole range of $n\geqslant 1$. Then the uncertainty relation $\Delta x\Delta p$ is, after simplification,

$$\Delta x\Delta p\approx\frac{\hbar}{2}\frac{3^{2/3}}{2^{1/3}}n^{1/3}=\hbar^{2/3}\left(\frac{3^2}{2^4}\right)^{1/3}(n\hbar)^{1/3}. \tag{34}$$

In the following, we will give its counterpart in classical mechanics.

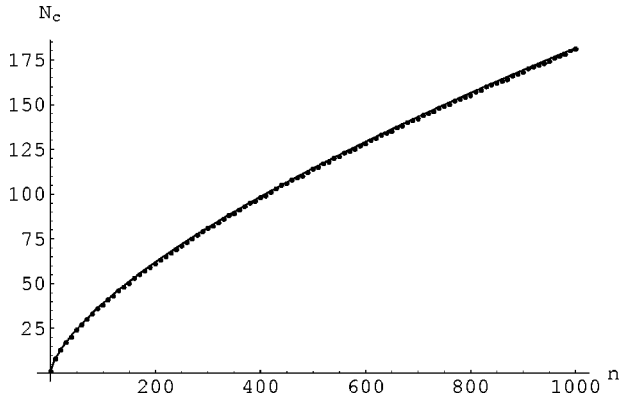

FIG. 1. Comparison of the numerical result of N_c (dotted line) and the approximately analytical one (solid line) $6^{1/3}n^{2/3}$; both are obtained from minimizing of the uncertainty $\Delta x\Delta p$ at each n. These two results coincides with each other in whole range $n\geqslant 1$.

C. Another derivation of the uncertainty relation (34) from the Fejér average approximation of the semiclassical quantities

By definition,[3,5–8] the Fejér averages of the first $(2N+1)$ partial sums of the Fourier series of x, x^2, p, and p^2 are with $N>1$,

$$F\langle x\rangle=\frac{2N}{2N+1}\sqrt{\frac{2E}{\mu\omega^2}}\cos(\omega t), \tag{35}$$

$$F\langle x^2\rangle=\frac{E}{\mu\omega^2}+\frac{2N-1}{2N+1}\frac{E}{\mu\omega^2}\cos(2\omega t), \tag{36}$$

$$F\langle p\rangle=-\frac{2N}{2N+1}\sqrt{2\mu E}\cos(\omega t), \tag{37}$$

$$F\langle p^2\rangle=\mu E-\frac{2N-1}{2N+1}\mu E\cos(2\omega t). \tag{38}$$

The larger the number N, the more accurate are the Fejér average approximations. Analogous to the definition of quantum uncertainties given by Eqs. (27) and (28), the classical uncertainties $\Delta_c x$ and $\Delta_c p$ are defined by

$$\Delta_c x=(\overline{F\langle x^2\rangle-(F\langle x\rangle)^2})^{1/2}=\left(\frac{E}{\mu\omega^2}\left(1-\left(\frac{2N}{2N+1}\right)^2\right)\right)^{1/2}, \tag{39}$$

$$\Delta_c p=(\overline{F\langle p^2\rangle-(F\langle p\rangle)^2})^{1/2}=\left(\mu E\left(1-\left(\frac{2N}{2N+1}\right)^2\right)\right)^{1/2}, \tag{40}$$

where $\overline{f(t)}$ means the time average of the quantity $f(t)$ over a period. The product of $\Delta_c x$ and $\Delta_c p$ is

$$\Delta_c x\Delta_c p=\frac{E}{\omega}\frac{4N+1}{(2N+1)^2}, \tag{41}$$

which reduces to, when $N\gg 1$,

$$\Delta_c x \Delta_c p \approx \frac{E}{N\omega}. \tag{42}$$

We see that the classical uncertainty vanishes only in the limit of N approaching infinity. However, using the relations $N_c \approx [6^{1/3} n^{2/3}]$ and $E \approx n\hbar\omega$, the classical uncertainty relation (42) is in semiclassical form,

$$\Delta_c x \Delta_c p \approx \left\langle \frac{n\hbar}{N_c} \right\rangle \approx 6^{-1/3} \hbar^{2/3} (n\hbar)^{1/3}, \tag{44}$$

which differs from the purely quantum one (34) only in a numerical factor 3/2. Equation (44) can be called a semiclassical uncertainty relation.

D. A brief summary of results obtained by EWWP description of a single HO

(1) For a single one-dimensional HO, analytical calculations give the critical exponent $m=2/3$ and a relation $N_c \approx [6^{1/3} n^{2/3}]$.
(2) The classical uncertainty relation $\Delta_c x \Delta_c p$ is definable, and this uncertainty relation comes from the incompleteness of the Fejér average representation of a classical quantity. After rewriting it into its semiclassical form, we see $\Delta_c x \Delta_c p \approx \Delta x \Delta p$.

III. FEJÉR AVERAGE AND A SINGLE PARTICLE IN AN ISW

A single particle in an ISW is the simplest quantum system whose energy level is not equally spaced, and the wave packet dynamics exhibited in it is essentially the same as that in more complicated system.[4] Since the long-term behaviors of EWWP such as collapse, revival, etc., do not have any analog in classical mechanics, only the first two period behaviors are examined in the following. In Sec. III A, the analytical expressions of mean values x, x^2, p, p^2 in the EWWP for a single particle in an ISW are given. In Sec. III B, the critical exponent $m=1/2$ is numerically determined. In Sec. III C, we show that the inequality of energy level spacing is responsible for the small difference between $\langle f \rangle$ and $F\langle f \rangle$ for $f=x$ and p, respectively. Section IV D presents a brief summary.

A. Mean values of quantities in the EWWP for a single particle in an ISW

For the quantum motion of a particle of mass μ in a one-dimensional ISW with width a, the normalized stationary state function is $\psi_n(x)\exp(-iE_n t/\hbar) = (2/a)^{1/2} \sin(k_n x)\exp(-ip_n^2 t/(2\mu\hbar))$, where $k_n = n\pi/a$, $E_n = p_n^2/(2\mu)$ is the energy and the momenta $p_n = \pm \hbar k_n$ is equally probable. In classical mechanics, the particle moves to and fro within the two impenetrable walls. The classical position x is

$$x = \begin{cases} p_c t/\mu = a\omega t/\pi, & 0 < t < T/2 \\ 2a - a\omega t/\pi \quad T//2 < t < T, \end{cases} \tag{45}$$

where $T = 2a\mu/p_c$ is the time of one period, p_c is the magnitude of momentum, and $\omega = 2\pi/T$ is the frequency. The derivative of position x with respect to time t gives the velocity $p/\mu = \pm p_c/\mu$. The mth partial sum of its Fourier series representing x is given by x_m,

$$x_m = \frac{a}{2} - \frac{4a}{\pi^2} \sum_{r=0}^{m} \frac{\cos[(2r+1)\omega t]}{(2r+1)^2}. \tag{46}$$

Its Fejér average $F\langle x \rangle$ is

$$F\langle x \rangle = \frac{a}{2} - \frac{8a}{\pi^2} \frac{1}{(2N+1)} \sum_{l=0}^{N-1} \sum_{r=0}^{l} \frac{\cos[(2r+1)\omega t]}{(2r+1)^2}. \tag{47}$$

Similarly, we have $F\langle f\rangle$ for $f=x^2,\ p,\ p^2$ [cf. Eqs. (54)–(56)]. Note that there is the famous Gibb's phenomenon when using truncated Fourier series to approximate the classical momentum p, while $F\langle p\rangle$ does not have such a phenomenon.[6–8] The calculation of $\langle f\rangle$ in the EWWP for $f=x,\ x^2,\ p,\ p^2$ is straightforward:

$$\langle x\rangle=\frac{a}{2}+\frac{4a}{\pi^2}\frac{1}{2N+1}\sum_{l=0}^{N-1}\sum_{r=0}^{l}\left\{\left(\frac{1}{(2n+2N-4l+2r-1)^2}-\frac{1}{(2r+1)^2}\right)\right.$$
$$\times\cos\left((2r+1)\left(1+\frac{2N-4l+2r-1}{2n}\right)\omega_n t\right)+\left(\frac{1}{(2n+2N-4l+2r-3)^2}-\frac{1}{(2r+1)^2}\right)$$
$$\left.\times\cos\left((2r+1)\left(1+\frac{2N-4l+2r-3}{2n}\right)\omega_n t\right)\right\}, \tag{48}$$

$$\langle x^2\rangle=\frac{a^2}{3}-\frac{1}{2N+1}\frac{a^2}{2\pi^2}\sum_{m=-N}^{N}\frac{1}{(n+m)^2}+\frac{4a^2}{\pi^2}\frac{1}{2N+1}\sum_{l=1}^{2N}\sum_{r=1}^{l}(-1)^r$$
$$\times\left(\frac{1}{r^2}-\frac{1}{(2n-2N+2l-r)^2}\right)\cos\left(r\left(1-\frac{2N-2l+r}{2n}\right)\omega_n t\right), \tag{49}$$

$$\langle p\rangle=\mu\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle, \tag{50}$$

$$\langle p^2\rangle=\frac{1}{2N+1}\left(\frac{\pi\hbar}{a}\right)^2\sum_{m=-N}^{N}(n+m)^2=\left(\frac{n\pi\hbar}{a}\right)^2\left(1+\frac{N+N^2}{3n^2}\right)=p_n^2\left(1+\frac{N+N^2}{3n^2}\right), \tag{51}$$

where $\omega_n=\pi p_n/(\mu a)=n\hbar\pi^2/(\mu a^2)$. The following set of classical limits;

$$n\to\infty,\quad N\to\infty,\quad N/n\to 0,\quad n\hbar\to p_c a/\pi=\omega\mu(a/\pi)^2\quad(\text{i.e., }|p_n|\to p_c,\ \text{or, }\omega_n\to\omega). \tag{52}$$

constitutes the necessary and sufficient condition to ensure the quantum mechanical averages (48)–(51) to be equal to the following Fejér averages;

$$\langle x\rangle\approx F\langle x\rangle=\frac{a}{2}-\frac{8a}{\pi^2}\frac{1}{2N+1}\sum_{l=1}^{N-1}\sum_{r=1}^{l}\frac{\cos[(2r+1)\omega t]}{(2r+1)^2}, \tag{53}$$

$$\langle x^2\rangle\approx F\langle x^2\rangle=\frac{a^2}{3}+\frac{4a^2}{\pi^2}\frac{1}{2N+1}\sum_{l=1}^{2N}\sum_{r=1}^{l}(-1)^r\frac{\cos(r\omega t)}{r^2}, \tag{54}$$

$$\langle p\rangle\approx F\langle p\rangle=\mu\frac{\mathrm{d}}{\mathrm{d}t}F\langle x\rangle, \tag{55}$$

$$\langle p^2\rangle\approx p_c^2. \tag{56}$$

B. The relation between *N* and *n* determined by minimizing the uncertainty relation

The mean value $\langle p\rangle$ is a continuous function of t; it is zero when the center of EWWP starts to return from either wall of the well. Since the mean value of p^2 is a constant of time, $\Delta p=\sqrt{\langle p^2\rangle}$ when $\langle p\rangle=0$. At this instant, minimizing $\Delta x\Delta p$ amounts to minimizing Δx. The numerical result as given in Fig. 2 shows that $N_c\approx[\sqrt{n}]$, e.g., $N_c=23$ when $n=500$. In all numerical calculations hereafter, the natural units are used in which $a=\mu=\hbar=1$.

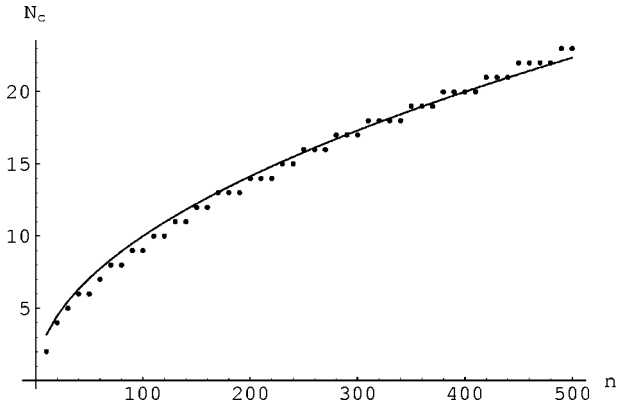

FIG. 2. Corresponding to each n ranging from 10 to 500, there is a unique value of N_c (dotted curve) minimizing the uncertainty $\Delta x \Delta p$. The smooth curve is $\sqrt{n}$. Since $N_c = [\sqrt{n}] \pm 1$ with $[x]$ denoting the integral part of x, $N_c \approx \sqrt{n}$ gives a nice fit.

C. $\langle f \rangle$ and $F\langle f \rangle$ when $n = 500$

When $n = 500$, $N_c = 23$, $p_n = \pm p_c = \pm 500\pi$, and $T = 0.001\,27$, $\langle f \rangle$ and $F\langle f \rangle$ when $f = x$, p are plotted in Fig. 3. The difference between them is small. Is the inequality of the energy level spacing the principal origin of the small difference? In order to examine this problem, we magnify the difference by introducing the reduced uncertainty δf and reduced classical uncertainty $\delta_c f$,

$$\delta f = \sqrt{1 - (\langle f \rangle)^2 / \langle f^2 \rangle}, \quad \delta_c f = \sqrt{1 - (F\langle f \rangle)^2 / F\langle f^2 \rangle}. \tag{57}$$

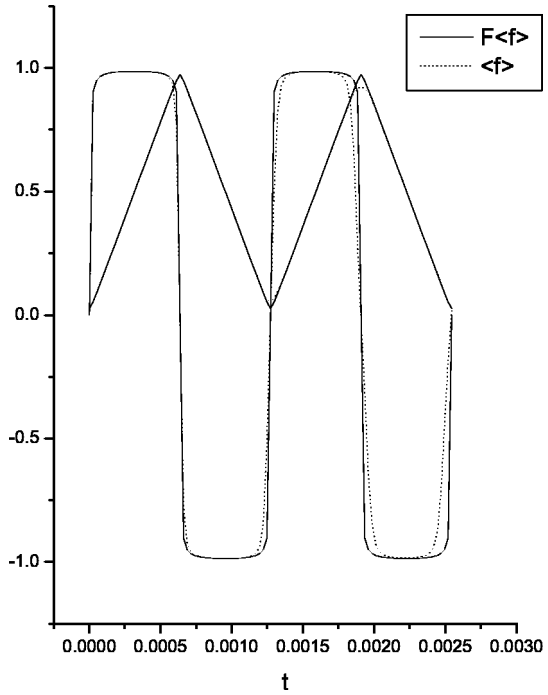

FIG. 3. When $N_c = 23$, $p_n = \pm p_c = \pm 500\pi$, i.e., $n = 500$, and taking 500π as the unit of the momentum, the Fejér averages $F\langle x \rangle$ (solid sawtooth wave), $F\langle p \rangle$ (solid square wave), and the quantum mechanical averages $\langle x \rangle$ (dotted sawtooth curve), and $\langle p \rangle$ (dotted square curve) in the EWWP. In the first period, $\langle x \rangle$ and $F\langle x \rangle$ are almost the same, and so are $\langle p \rangle$ and $F\langle p \rangle$. In some intervals two curves completely coincide, only one curve is possibly visible.

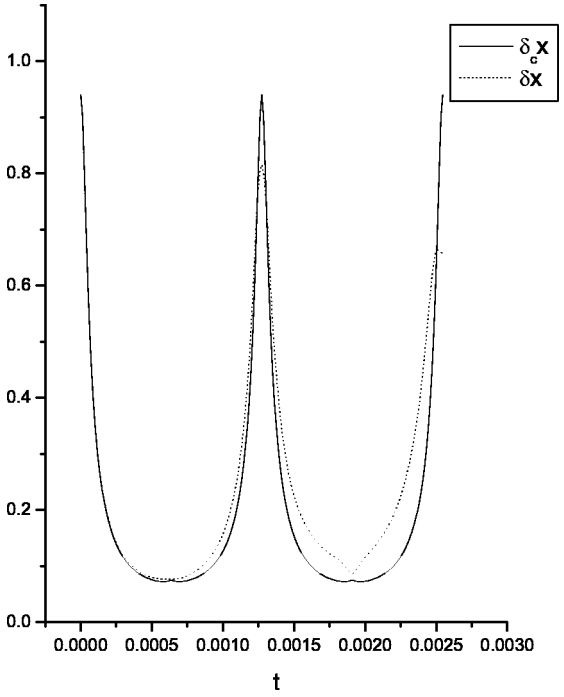

FIG. 4. The difference between $\langle x\rangle$ and $F\langle x\rangle$ viewed from the reduced uncertainty δx (dotted curve) and the classical one $\delta_c x$ (solid curve). The difference between $\langle x\rangle$ and $F\langle x\rangle$ comes from the inequality of energy level spacing. Both curves are entirely different from the classical result $\delta x=0$ $(x\neq 0)$.

In Figs. 4 and 5, we compare the behaviors of δf and $\delta_c f$ for $f=x$, p, respectively. We use solid lines to plot the reduced classical uncertainties $\delta_c f$, and the dotted for either the pure quantum mechanical quantities δf or the semiquantum mechanical ones. By the semiquantum mechanical quantities, we mean those constructed from the pure quantum mechanical ones in which the quantum mechanical matrix elements $f_{n+r,n}=\int_0^a \psi_{n+r}(x) f \psi_n(x)\mathrm{d}x$ are replaced with the rth Fourier amplitudes f_r of the classical quantity f, while the time factors $\exp\{(E_{n+r}-E_n)t/\hbar\}$ remain unchanged. From Eqs. (48) to (50), the pure quantum mechanical quantities and the semi-ones have little difference when n is large and t is small, e.g., $n=500$, $t\leqslant 0.0025$. Therefore when we speak of one of them, both are practically referred to. It is then clear that the difference between solid and dotted lines comes from the inequality of energy level spacing. The longer the time evolves, the more the quantum mechanics deviates from the classical mechanics.

D. A brief summary of results obtained by EWWP description of a single particle in an ISW

(1) For a single particle in an ISW, numerical calculations give a critical exponent $m=1/2$, and relation $N_c\approx\sqrt{n}$.
(2) The small difference between the $\langle f\rangle$ and $F\langle f\rangle$ principally results from the inequality of energy level spacing.

IV. CONCLUSION

Though it is first an intellectual creation in pure mathematics, the Fejér average turns out to be rooted in physics that reflects the objective structure of nature. The quantum mechanical average of a quantity in the EWWP in the quasiclassical sense goes over to the Fejér average of partial sums of Fourier series expansion of the semiclassical quantity, rather than the Fourier series itself as widely accepted.

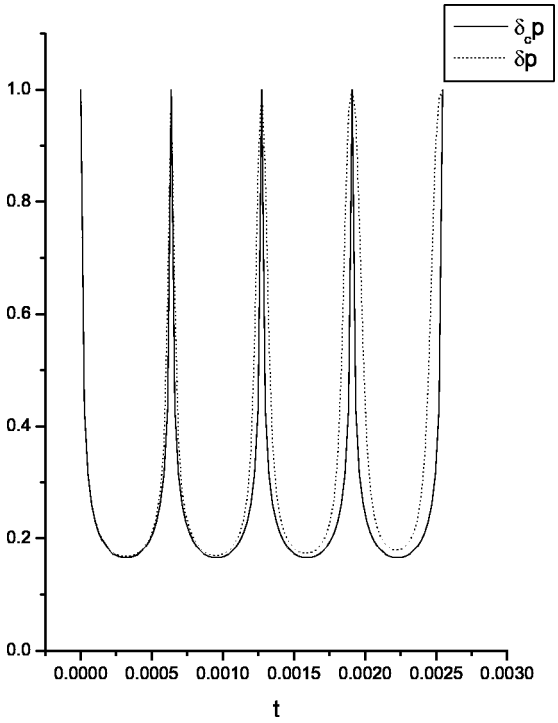

FIG. 5. The difference between $\langle p\rangle$ and $F\langle p\rangle$ viewed from the reduced uncertainty δp (dotted curve) and the reduced classical one $\delta_c p$ (solid curve). Both are entirely different from classical result $\delta p=0$ $(p\neq 0)$.

Two critical exponents $m=1/2,\ 2/3$ are obtained for a single HO and a particle in an ISW, respectively. The critical exponent of the Keplerian motion is of interest and will be studied in the near future.

Because of incompleteness of Fejér average in representing a classical quantity, a classical uncertainty relation $\Delta_c x\Delta_c p$ is definable, which proves to be comparable to the quantum one. This uncertainty is entirely different from the standard deviation associated with an ensemble of classical orbits.[1] In current statistical interpretation of quantum mechanics, the quantum uncertainty is usually interpreted to have a statistical origin.[9]

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APPENDIX: A BRIEF INTRODUCTION TO THE FEJÉR AVERAGE

The Fourier series had not come to mathematicians as a reliable and convenient tool until the discovery of the convergence of the Fejér average of its partial sums in 1900. Fejér's theorem is as follows. The Fejér average of the partial sums of the Fourier series $f_n=\Sigma_{k=-n}^{n} c_k \exp(i2k\pi t/T)$ as $\sigma_n=(f_0+f_1+f_2+\cdots f_{n-1})/n$ approximates the given function $f(t)$ at each point where $f(t+0)$ and $f(t-0)$ exist and $f(t)=\frac{1}{2}[f(t+0)+f(t-0)]$, and uniformly converges to the function $f(t)$ when $f(t)$ is continuous on the circle. Note that the truncated Fourier series f_n of $f(t)$ converges *in the mean* to the function. As a profound consequence, the Gibbs phenomenon of Fourier series does not occur with the Fejér average. On its history, see Ref. 5. On its fundamentals, see, for example, Ref. 6. On its applications, see Ref. 7. On its modern developments, see a recent review.[8]

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Discrete Kaluza–Klein from scalar fluctuations in noncommutative geometry

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We compute the metric associated with noncommutative spaces described by a tensor product of spectral triples. Well-known results of the two-sheets model (distance on a sheet, distance between the sheets) are extended to any product of two spectral triples. The distance between different points on different fibers is investigated. When one of the triples describes a manifold, one finds a Pythagorean theorem as soon as the direct sum of the internal states (viewed as projections) commutes with the internal Dirac operator. Scalar fluctuations yield a discrete Kaluza–Klein model in which the extra component of the metric is given by the internal part of the geometry. In the standard model, this extra component comes from the Higgs field. © *2002 American Institute of Physics*.
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I. INTRODUCTION

In the noncommutative approach to the standard model of elementary particles,[1] space–time appears as the product (in the sense of fiber bundles) of a continuous manifold by a discrete space. In previous papers, we have studied the metric aspect of several classes of discrete spaces,[2] and the metric of the continuum has been approached from a Lie-algebraic approach.[3] Here, within the framework of noncommutative geometry, we investigate how the distance in the continuum evolves when the space–time of Euclidean general relativity is tensorized by an internal space. We find that in many cases the relevant picture is the two-sheets model.[4,5] Indeed, under precise conditions, the metric aspect of ''continuum$\times$discrete'' spaces reduces to the simple picture of two copies of the manifold. It was known[6,7] that the distance on each copy is the geodesic distance while the distance between the copies—the distance on the fiber—is a constant. But this does not give a complete description of the geometry, in particular the distance between different points on different copies. In this paper we show that this distance coincides with the geodesic distance within a $(4+1)$-dimensional manifold whose fifth component comes from the internal part of the geometry. This component is a constant in the simplest cases and becomes a function of the manifold when the metric fluctuates. Restricting ourselves to scalar fluctuations of the metric, which correspond to the Higgs sector in the standard model, it appears that the Higgs field describes the internal part of the metric in terms of a discrete Kaluza–Klein model.

The aim of this paper is to investigate the metric aspect of the standard model geometry. This goal is only partially achieved because we focus on scalar fluctuations and we mention only very briefly mathematical aspects such as the Gromov distance. For a comprehensive approach to these questions, the reader is invited to consult Ref. 8. Other works on distance in noncommutative geometry mainly concern lattices[9–12] and finite spaces. A larger bibliography can be found in Ref.

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2. Naturally, using a Kaluza–Klein picture in noncommutative geometry is not a new idea and one can refer to Refs. 13 and 14 for instance as well as the textbook.[15] In particular, that the distance between the sheets depends on the manifold has been shown in Refs. 16 and 17. Last but not least, for a comprehensive approach to the subject, the most recent and complete reference is Ref. 17.

The paper is written for a four-dimensional manifold but generalization to higher dimension should be straightforward. Sections II and III introduce classical notions of distance in noncommutative geometry and a simple proof that, on a manifold, this distance coincides with the geodesic distance. Section IV extends known results of the two-sheets model—distance on each copy, distance between the copies—to the product of any two spaces (not necessarily a manifold$\times$a discrete space). In Sec. V we show that, under conditions on the internal part of the Dirac operator, a large number of examples actually reduce to a two points fiber space. In the simplest case the internal space is orthogonal to the continuum in the sense of the Pythagorean theorem (in finite spaces, the Pythagorean theorem has already been mentioned by Ref. 18). Section VI studies the scalar fluctuations (terminology is made precise there) of this metric. Section VII presents examples, among them the standard model, and makes precise the link between the Higgs field and the metric.

II. THE DISTANCE FORMULA

Let $\mathcal{A}$ be a unital C^*-algebra represented over a complex Hilbert space $\mathcal{H}$ equipped with a scalar product $\langle .,. \rangle$ defining the norm $\|\psi\|_{\mathcal{H}}^2 \doteq |\langle \psi, \psi \rangle|$ for $\psi \in \mathcal{H}$. The C^*-norm of $\mathcal{A}$ is the operator norm in $\mathcal{H}$,

$$\|a\|_{\mathcal{A}} \doteq \sup_{\psi \in \mathcal{H}} \frac{\|\pi(a)(\psi)\|_{\mathcal{H}}}{\|\psi\|_{\mathcal{H}}},$$

where π is the representation. The so-called Dirac operator D is a self-adjoint operator in $\mathcal{H}$, possibly unbounded. When the spectral dimension is even,[4] the chirality χ is a Hermitean operator which anticommutes with D and commutes with $\pi(\mathcal{A})$. The set $(\mathcal{A},\mathcal{H},D,\pi,\chi)$ is called a spectral triple. The terminology is justified because π is usually infered in the notation $\mathcal{H}$, and once given $(\mathcal{A},\mathcal{H},D)$, χ—if it exists—is uniquely determined by the axioms of noncommutative geometry.[1] Since the algebra appears through its representation, we can, without loss of generality, replace $\mathcal{A}$ by $\mathcal{A}/\ker(\pi)$ and assume that π is faithful. To improve the readability we omit the symbol π unless necessary.

We denote by $\mathcal{P}(\mathcal{A})$ the set of pure states of $\mathcal{A}$. The distance d between two of its elements ω_1, ω_2 is

$$d(\omega_1,\omega_2) \doteq \sup_{a \in \mathcal{A}} \{|\omega_1(a) - \omega_2(a)| / \|[D,a]\| \leqslant 1\},$$

where $\|.\|$ is the operator norm in $\mathcal{H}$ (we do not write $\|[D,a]\|_{\mathcal{A}}$ because $[D,a]$ may not be the representation of an element of $\mathcal{A}$). This supremum is reached[2] by a positive element such that $\|[D,\pi(a)]\| = 1$:

$$d(\omega_1,\omega_2) = \sup_{a \in \mathcal{A}_+} \{|\omega_1(a) - \omega_2(a)| / \|[D,a]\| = 1\}. \tag{1}$$

This formula is invariant under several transformations, including unitary transformation and projection. First, a unitary element u of $\mathcal{A}$ defines both an automorphism of the algebra $\alpha_u(a) \doteq uau^*$ and a *unitary equivalent* triple $(\mathcal{A},\mathcal{H},uDu^*,\pi \circ \alpha_u)$. Obviously distances are not changed under such a transformation because $\|[D,a]\| = \|[uDu^*, \alpha_u(a)]\|$. More interesting is the action of a projection $e \in \mathcal{A}$ $(e^2 = e^* = e)$ given by

$$\alpha_e(a) \doteq eae,$$

which defines the *restricted* spectral triple

$$(\mathcal{A}_e \doteq \alpha_e(\mathcal{A}), \quad \mathcal{H}_e \doteq e\mathcal{H} \doteq \operatorname{ran} e, \quad D_e \doteq eDe|_{\mathcal{H}_e}, \quad \pi_e \doteq \pi|_{\mathcal{H}_e})$$

whose corresponding distance is denoted by d_e. α_e being not injective, for a pure state $\omega \in \mathcal{P}(\mathcal{A})$ the linear form $\omega \circ \alpha_e$ is not necessarily a state of $\mathcal{A}$ (for instance if e is in the kernel of ω). However it is a pure state of the subalgebra $\mathcal{A}_e$. Conversely, any pure state ω_e of $\mathcal{A}_e$ is made a pure state of $\mathcal{A}$ by writing $\omega_e \circ \alpha_e$. In other words, $\mathcal{P}(\mathcal{A}_e) = \mathcal{P}(\mathcal{A}) \circ \alpha_e \subset \mathcal{P}(\mathcal{A})$.

Lemma 1: If a projection e is such that $[D,e]=0$, *the distance between two pure states* ω_1, ω_2 *of* $\mathcal{A}_e$ *is invariant by projection*: $d_e(\omega_1,\omega_2) = d(\omega_1 \circ \alpha_e, \omega_2 \circ \alpha_e)$.

Proof: For $a_e \in \mathcal{A}_e$, $\|[D_e, \pi_e(a_e)]\| = \|[\pi(e)D\pi(e), \pi(a_e)]\| = \|[D, \pi(a_e)]\|$ therefore

$$\begin{aligned} d_e(\omega_1,\omega_2) &= \sup_{a_e \in \mathcal{A}_e} \{|(\omega_1 - \omega_2)(a_e)| / \|[D,\pi(a_e)]\| \leqslant 1\}, \\ &\leqslant \sup_{a \in \mathcal{A}} \{|(\omega_1 \circ \alpha_e - \omega_2 \circ \alpha_e)(a)| / \|[D,\pi(a)]\| \leqslant 1\} \\ &= d(\omega_1 \circ \alpha_e, \omega_2 \circ \alpha_e). \end{aligned}$$

This upper bound is reached by $\alpha_e(a)$ where $a \in \mathcal{A}$ reaches the supremum for the distance d, namely $\|[D,\pi(a)]\| = 1$ and $d(\omega_1 \circ \alpha_e, \omega_2 \circ \alpha_e) = \omega_1 \circ \alpha_e(a) - \omega_2 \circ \alpha_e(a)$. ■

III. DISTANCE IN A MANIFOLD

The spectral triple of a Riemannian spin manifold $\mathcal{M}$ of dimension four with a metric g is

$$\mathcal{A} = C^\infty(\mathcal{M}), \quad \mathcal{H} = L_2(\mathcal{M},S), \quad D = i\gamma^\mu \partial_\mu = i\partial\!\!\!/, \tag{2}$$

where $L_2(\mathcal{M},S)$ is the set of square integrable spinors on $\mathcal{M}$. The Riemannian gamma matrices $\gamma^\mu = \gamma^{\mu *} = e_a^\mu \gamma^a$ are obtained via the vierbein field e_a^μ from the Euclidean gamma matrices γ^a of the associated Clifford algebra. Using $\delta^{ab} e_a^\mu e_b^\nu = g^{\mu\nu}$ and $\gamma^a\gamma^b + \gamma^b\gamma^a = 2\delta^{ab}\mathbb{I}$ one has $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}\mathbb{I}$. The spectral dimension is the dimension of the manifold, so there is a chirality $\gamma^5 = \gamma^0\gamma^1\gamma^2\gamma^3$ made of the Euclidean γ^a's. The scalar product of $\mathcal{H}$ is $\langle \psi, \phi \rangle \doteq \int_{\mathcal{M}} \overline{\psi}(x)\phi(x)\,\mathrm{d}x$ and an element $f \in \mathcal{A}$ is represented over $\mathcal{H}$ by the pointwise multiplication, $\pi(f) \doteq f\mathbb{I}$, so that

$$\|f\|_{\mathcal{A}} = \sup_{\psi \in \mathcal{H}} \left(\frac{\int_{\mathcal{M}} (\overline{f\psi})(x)(f\psi)(x)\mathrm{d}x}{\int_{\mathcal{M}} \overline{\psi}(x)\psi(x)\mathrm{d}x} \right)^{1/2} = \sup_{x \in \mathcal{M}} |f(x)|.$$

By Gelfand transform, $\mathcal{P}(\mathcal{A}) \simeq \mathcal{M}$. The isomorphism $x \in \mathcal{M} \leftrightarrow \omega_x \in \mathcal{P}(\mathcal{A})$ is defined by $\omega_x(f) \doteq f(x)$. The noncommutative distance (1),

$$d(x,y) = \sup_{f \in C^\infty(\mathcal{M})} \{|f(x) - f(y)| / \|[i\partial\!\!\!/, f\mathbb{I}]\| \leqslant 1\},$$

coincides with the geodesic distance $L(x,y)$ between points x,y of $\mathcal{M}$. This is a classical result[4] but the proof introduces ideas and notations important for further presentation so that we shall give it in detail (this version of the proof comes from Ref. 19).

The supremum is reached on $\mathcal{A}_+$, so f is real. For $\psi \in \mathcal{H}$, $[i\partial\!\!\!/, f\mathbb{I}]\psi = i(\partial\!\!\!/ f)\psi$, so

$$\|[i\partial\!\!\!/, f\mathbb{I}]\|^2 = \|(i\partial\!\!\!/ f)^* i\partial\!\!\!/ f\| = \|\gamma^\mu \partial_\mu f \gamma^\nu \partial_\nu f\| = \|g^{\mu\nu}\partial_\mu f \partial_\nu f \mathbb{I}\| = \sup_{q \in \mathcal{M}} \{g^{\mu\nu}(q)\partial_\mu f(q)\partial_\nu f(q)\}.$$

The gradient $\vec{\nabla}$ in the usual sense is the exterior derivative d (not to be confused with the distance) which maps zero-forms (i.e., smooth functions over $\mathcal{M}$) to one-forms:

$$\vec{\nabla} f \doteq (\partial_\mu f)\mathrm{d}x^\mu \in T^*\mathcal{M}.$$

By definition[20] g defines an inner product (thus, a norm) in each cotangent space $T_q^*\mathcal{M}$ in such a manner that

$$\|\vec{\nabla} f(q)\|^2_{T_q^*\mathcal{M}} = g^{\mu\nu}(q)\partial_\mu f(q)\partial_\nu f(q).$$

Omitting the index $T_q^*\mathcal{M}$, one writes

$$\|[i\not{b}, f\mathbb{I}]\| = \sup_{q\in\mathcal{M}} \|\vec{\nabla} f(q)\|.$$

Now, let $c: t\in[0,1]\to\mathcal{M}$ be the minimal geodesic between x and y and let $\cdot$ denote the total derivative with respect to t. For any $f\in C^\infty(\mathcal{M})$,

$$f(x)-f(y) = \int_0^1 \dot{f}(c(t))\mathrm{d}t = \int_0^1 \partial_\mu f(p)\dot{c}^\mu(t)\mathrm{d}t,$$

where $p\doteq c(t)$. The metric defines an isomorphism $T_p\mathcal{M}\simeq T_p^*\mathcal{M}$ such that

$$\partial_\mu f(p)\dot{c}^\mu(t) = g^{\mu\nu}(p)\partial_\mu f(p)\dot{c}_\nu(t) = \langle \vec{\nabla} f(p), \dot{c}_\nu(t)\mathrm{d}x^\nu\rangle,$$

thus, by Cauchy–Schwarz, $|\partial_\mu f(p)\dot{c}^\mu(t)| \leqslant \|\vec{\nabla} f(p)\|\|\dot{c}_\nu(t)\mathrm{d}x^\nu\|$. Assuming that f reaches the supremum, one has $\|\vec{\nabla} f\|\leqslant 1$, so

$$\mathrm{d}(x,y) = |f(x)-f(y)| \leqslant \int_0^1 \|\dot{c}_\nu(t)\mathrm{d}x^\nu\|\mathrm{d}t = L(x,y).$$

This upper bound is reached by the function

$$L: q\mapsto L(q,y). \tag{3}$$

Indeed, $L(x)-L(y)=L(x,y)$ and

$$\sup_{q\in\mathcal{M}} \|\vec{\nabla} L(q)\| \leqslant 1. \tag{4}$$

To prove (4), take $q,q'\in\mathcal{M}$ with coordinates q^μ, q'^μ in a given chart such that q' comes from q by the infinitesimal transformation $\sigma(\epsilon)$, $\epsilon\leqslant 1$, where σ is the flow generated by the vector field $g^{\mu\nu}(\partial_\nu L)\partial_\mu$ with initial condition $\sigma(0)=q$. Then, writing $\mathrm{d}q^\mu \doteq q'^\mu - q^\mu$,

$$q^\mu + \mathrm{d}q^\mu = q'^\mu = \sigma^\mu(\epsilon) = \sigma^\mu(0) + \epsilon\frac{\mathrm{d}\sigma^\mu}{\mathrm{d}t}(0) + \mathcal{O}(\epsilon^2) = q^\mu + \epsilon\, g^{\mu\nu}(q)\partial_\nu L(q) + \mathcal{O}(\epsilon^2),$$

which means that

$$\mathrm{d}q^\mu = \epsilon\, g^{\mu\nu}(q)\partial_\nu L(q) + \mathcal{O}(\epsilon^2). \tag{5}$$

As $L(q',y)$ is the shortest length from q' to y, $L(q',y)\leqslant L(q',q)+L(q,y)$, and one has

$$L(q+\mathrm{d}q) \leqslant L(q',q) + L(q). \tag{6}$$

Using (5),

$$L(q',q) \doteq \sqrt{g_{\lambda\rho}(q)\mathrm{d}q^\lambda dq^\rho} = \sqrt{\epsilon^2 g_{\lambda\rho}(q) g^{\lambda\mu}(q)\partial_\mu L(q)\, g^{\rho\nu}(q)\partial_\nu L(q)} = \epsilon\sqrt{g^{\mu\nu}\partial_\mu L(q)\ \partial_\nu L(q)}.$$

Inserting into the right-hand side of (6) whose left-hand side is developed with respect to ϵ yields

$$L(q)+\partial_\mu L(q)\,\mathrm{d}q^\mu = L(q)+\epsilon\, g^{\mu\nu}(q)\partial_\mu L(q)\partial_\nu L(q)+\mathcal{O}(\epsilon^2)$$
$$\leqslant \epsilon\sqrt{g^{\mu\nu}\partial_\mu L(q)\,\partial_\nu L(q)}+L(q)+\mathcal{O}(\epsilon^2),$$

which is true for all q, hence (4) and finally $\mathrm{d}(x,y)=L(x,y)$.

Note that L is not smooth at y but only continuous. As smooth functions are dense in continuous functions, one may exhibit a sequence of smooth functions converging to L and satisfying the commutator norm condition. One may also define the distance as the supremum over the continuous functions of expression (1), see Ref. 17 for details.

IV. TENSOR PRODUCT OF SPECTRAL TRIPLES

The tensor product of an even spectral triple $T_I=(\mathcal{A}_I,\mathcal{H}_I,D_I,\pi_I)$ with chirality χ_I by the spectral triple $T_E=(\mathcal{A}_E,\mathcal{H}_E,D_E,\pi_E)$ is the spectral triple $T_I\otimes T_E\doteq(\mathcal{A}',\mathcal{H}',D')$ defined by

$$\mathcal{A}'\doteq\mathcal{A}_I\otimes\mathcal{A}_E,\quad \mathcal{H}'\doteq\mathcal{H}_I\otimes\mathcal{H}_E,\quad D'\doteq D_I\otimes\mathbb{I}_E+\chi_I\otimes D_E,$$

where the representation of $\mathcal{A}'$ is $\pi'\doteq\pi_I\otimes\pi_E$. The notation $T_I\otimes T_E$ is a matter of convention for spectral triples do not form a vector space. The product of spectral triples is commutative in the sense that when T_E is even with chirality χ_E, then $T_E\otimes T_I\doteq(\mathcal{A},\mathcal{H},D)$ is well defined by permutation of factors,

$$\mathcal{A}\doteq\mathcal{A}_E\otimes\mathcal{A}_I,\quad \mathcal{H}\doteq\mathcal{H}_E\otimes\mathcal{H}_I,\quad D\doteq D_E\otimes\mathbb{I}_I+\chi_E\otimes D_I, \tag{7}$$

$\pi=\pi_E\otimes\pi_I$, and is equivalent to $T_I\otimes T_E$ up to the unitary operator

$$U\doteq\left(\frac{\mathbb{I}_I+\chi_I}{2}\otimes\mathbb{I}_E+\frac{\mathbb{I}_I-\chi_I}{2}\otimes\chi_E\right).$$

For physics it is interesting to take for this tensor product the product of the continuum by the discrete, namely to study the geometry of the four-dimensional space–time of Euclidean general relativity together with an internal discrete space. In the standard model, the internal space describes the electroweak and strong interactions and is defined by a spectral triple T_I in which the algebra $\mathcal{A}_I$ is chosen such that its unitarities are related to the gauge group of interactions while $\mathcal{H}_I$ is the space of fermions. Both $\mathcal{A}_I$ and $\mathcal{H}_I$ are finite dimensional, so T_I is a finite spectral triple[21] and T_E is the usual spectral triple (2) of a manifold. The spectral dimension of a finite spectral triple is 0 and $\dim(T_E)=\dim(\mathcal{M})=4$: both T_E and T_I are even therefore both $T_E\otimes T_I$ and $T_I\otimes T_E$ are defined.

In this section, we give general results that do not require either T_E to be the spectral triple of a manifold or T_I to be finite. To fix notations we simply assume that T_E is even so that we work with $T_E\otimes T_I$. To study the metric of a noncommutative space, the first goal is to make explicit the set of pure states of the associated algebra. For ω_E and ω_I being pure states of $\mathcal{A}_E$ and $\mathcal{A}_I$, the pair (ω_E,ω_I) is a state of $\mathcal{A}$ which acts as $\omega_E\otimes\omega_I$ (that $\mathbb{I}$ maps to 1 is obvious, the positivity can be seen in Ref. 22 for instance) but this is not necessarily a pure state. Moreover there can be pure states of $\mathcal{A}$ that cannot be written as tensor products. However, as soon as one of the algebras is Abelian, one obtains[23] that $\mathcal{P}(\mathcal{A}_E\otimes\mathcal{A}_I)\simeq\mathcal{P}(\mathcal{A}_E)\times\mathcal{P}(\mathcal{A}_I)$ and any pure state ω of $\mathcal{A}$ writes $\omega=\omega_E\otimes\omega_I$.

In the two-sheets model $\mathcal{A}=C^\infty(\mathcal{M})\otimes\mathbb{C}^2$, therefore any pure state is $\omega_x\otimes\omega_i$ where ω_i, $i=1,2$, is a pure state of $\mathbb{C}^2$ and labels the sheets. It is known[4] that $d(\omega_x\otimes\omega_i,\omega_y\otimes\omega_i)$ is the geodesic distance $L(x,y)$ while $d(\omega_x\otimes\omega_i,\omega_x\otimes\omega_j)$ is a constant. This extends to any product of spectral triples. Once fixed a pure state ω_E, $d(\omega_E\otimes\omega_I,\omega_E\otimes\omega_I')$ depends only on the spectral triple T_I and, similarly, $d(\omega_E\otimes\omega_I,\omega_E'\otimes\omega_I)$ depends only on T_E. This is true even when none of the algebra is commutative: the distance is then defined between states that may be not pure.

Theorem 2: Let d_E, d_I, d be the distance in T_E, T_I, $T_E\otimes T_I$, respectively. For ω_E, ω_E' in $\mathcal{P}(\mathcal{A}_E)$ and ω_I, ω_I' in $\mathcal{P}(\mathcal{A}_I)$,

$$d(\omega_E\otimes\omega_I,\omega_E\otimes\omega_I')=d_I(\omega_I,\omega_I'),$$

$$d(\omega_E\otimes\omega_I,\omega_E'\otimes\omega_I)=d_E(\omega_E,\omega_E').$$

Proof: Let f_j denote the elements of $\mathcal{A}_E$ and m_i those of $\mathcal{A}_I$. A generic element of $\mathcal{A}$ is $a=f^i\otimes m_i$, where the summation index i runs over a finite subset of $\mathbb{N}$. Definition (7) yields

$$[D,a]=[D_E,f^i]\otimes m_i+f^i\chi_E\otimes[D_I,m_i].$$

Multiplying this formula from the left and the right by the unitary operator $\chi_E\otimes\mathbb{I}_I$ allows one to write

$$\|[D_E,f^i]\otimes m_i+f^i\chi_E\otimes[D_I,m_i]\|=\|-[D_E,f^i]\otimes m_i+f^i\chi_E\otimes[D_I,m_i]\|,$$

where we use that $\chi_E=\chi_E^*$ commutes with f^i and anticommutes with D_E. For u,v in a normed space, $2\|u\|\leqslant\|u+v\|+\|u-v\|$, thus

$$\|[D_E,f^i]\otimes m_i\|\leqslant\|[D,a]\|, \tag{8}$$

and $\|f^i\chi_E\otimes[D_I,m_i]\|\leqslant\|[D,a]\|$. One can factorize the left-hand side of Eq. (8) by $\chi_E\otimes\mathbb{I}_I$ in order to have

$$\|f^i\otimes[D_I,m_i]\|\leqslant\|[D,a]\|. \tag{9}$$

For any $\omega_E\in\mathcal{P}(\mathcal{A}_E)$ and $a\in\mathcal{A}_+$, let us define $a_E\in\mathcal{A}_I$ by

$$a_E\doteq\omega_E(f^i)m_i.$$

a_E is self-adjoint. Indeed, positivity of a, i.e., $a=(f^{p^*}\otimes m_p^*)(f^q\otimes m_q)=\frac{1}{2}(f^{pq}\otimes m_{pq}+f^{pq^*}\otimes m_{pq}^*)$ where $f^{pq}\doteq f^{p^*}f^q$ and $m_{pq}=m_p^*m_q$, yields

$$a_E=\tfrac{1}{2}(\omega_E(f^{pq})m_{pq}+\omega_E(f^{pq*})m_{pq}^*)=a_E^*.$$

Thus

$$i[D_I,a_E]=i(\omega_E\otimes\mathbb{I}_I)(f^i\otimes[D_I,m_I])$$

in $\mathcal{B}(\mathcal{H}_I)$ is normal. One knows[23] that for any normal element a of a C^*-algebra, $\|a\|=\sup_{\tau\in\mathcal{S}}|\tau(a)|$, where $\mathcal{S}$ is the set of states. Thus, with $\mathcal{S}_I$ the set of states of $\mathcal{B}(\mathcal{H}_I)$,

$$\begin{aligned}\|[D_I,a_E]\|&=\sup_{\tau_I\in\mathcal{S}_I}|\tau_I([D_I,a_E])|\\&\leqslant\sup_{(\tilde{\omega}_E,\tau_I)\in\mathcal{P}(\mathcal{A}_E)\times\mathcal{S}_I}|(\tilde{\omega}_E\otimes\tau_I)(f^i\otimes[D_I,m_i])|\\&\leqslant\sup_{(\tau_E,\tau_I)\in\mathcal{S}_E\times\mathcal{S}_I}|(\tau_E\otimes\tau_I)(f^i\otimes[D_I,m_i])|\\&=\|f^i\otimes[D_I,m_i]\|,\end{aligned}$$

where we use that $if^i\otimes[D_I,m_i]\in\mathcal{B}(\mathcal{H})$ is also normal. Together with (9),

$$\|[D_I,a_E]\|\leqslant\|[D,a]\|.$$

Since $(\omega_E\otimes\omega_I)(a)-(\omega_E\otimes\omega_I')(a)=\omega_I(a_E)-\omega_I'(a_E)$,

$$d(\omega_E\otimes\omega_I,\omega_E\otimes\omega_I')\leqslant d_I(\omega_I,\omega_I').$$

This upper bound is reached by $\mathbb{I}_E\otimes a_I$ where $a_I\in\mathcal{A}_I$ reaches the supremum for T_I alone, namely $d_I(\omega_I,\omega_I')\doteq|(\omega_I-\omega_I')(a_I)|$ and $1=\|[D_I,\pi_I(a_I)]\|$.

The proof for $d(\omega_E\otimes\omega_I,\omega_E'\otimes\omega_I)$ is similar, using (8) instead of (9). ■

V. METRIC IN THE CONTINUUM×DISCRETE

The key points of Theorem 2 are Eqs. (8) and (9). The first one allows one to forget about the internal part of the commutator and makes sense for states of $\mathcal{A}$ defined by different pure states on $\mathcal{A}_E$ but the same pure state on $\mathcal{A}_I$. When T_E is the spectral triple of a manifold and T_I a finite spectral triple, the noncommutative space described by $T_E\times T_I$ is a fiber bundle over the manifold with a discrete fiber. This can also be seen as the union of several copies of the manifold, indexed by the element of the fiber. Theorem 2 simply says that each of the copies is endowed with the metric of the base. Note that the discussion about the Gromov distance between manifolds with distinct metrics in Ref. 4 may not be transposed here because such manifolds are not described by a tensor product of spectral triples.

In contrast, (9) does not take into account the external part of the commutator and is sufficient to determine the distance between states defined by the same pure state on $\mathcal{A}_I$ (i.e., points on the same fiber within the picture of a continuum×discrete space). Of course the mixed case $d(\omega_E\otimes\omega_I,\omega_E{}'\otimes\omega_I')$—the distance between different points on different copies of the manifold—requires one to take into account both the internal and the external part of the commutator. This makes the computation more difficult. However, for continuum×discrete spaces, some of these distances have a nice interpretation in terms of a discrete Kaluza–Klein model: although the internal space is discrete, the distance appears as the geodesic distance in a ''virtual'' $(4+1)$-dimensional manifold (''virtual'' means that the points between the sheets are not part of the geometry, the embedding into a higher dimensional continuum space is a practical intermediate).

Let us first give a semigeneral result which does not require T_E to be the spectral triple of a manifold (T_E is just supposed to be even to fix notations) but which assumes

$$\mathcal{A}_I\doteq\bigoplus_k\mathcal{A}_k,$$

where k runs over a finite subset of $\mathbb{N}$ and the $\mathcal{A}_k$'s are von Neumann algebras on $\mathbb{C}$. Note that a pure state of a direct sum of algebras is a pure state of one of the algebras, that is

$$\mathcal{P}(A_I)=\bigcup_k\mathcal{P}(\mathcal{A}_k).$$

The reason why we restrict ourselves to von Neumann algebras is that to any normal state[24] ω of $\mathcal{A}_k$ corresponds a projection $\rho\in\mathcal{A}_k$, the so-called support of the state, such that

$$\alpha_\rho(a)\doteq\rho a\rho=\omega(a)\rho. \tag{10}$$

We let $\mathcal{P}(\mathcal{A}_k)_*$ denote the set of normal pure states of $\mathcal{A}_k$. Strictly speaking, the support is defined for normal states of complex algebras. However in the standard model, we shall explicitly exhibit such a projection for the real internal algebra so that, in the following, we deal with an algebra over $\mathbb{K}$ where $\mathbb{K}=\mathbb{C}$ or $\mathbb{R}$. Typically, in physical examples, the $\mathcal{A}_k$ are matrix algebras for which it is known that all states are normal; ρ is nothing but a density matrix. When normal pure states of different components $\mathcal{A}_k$ are involved and D_I commutes with the direct sum of their support, one obtains as an immediate consequence of Lemma 1 that $\mathcal{A}_I$ reduces to $\mathbb{K}^2$.

Proposition 3: Let ρ, ρ' *be the supports of two distinct normal pure states* $\omega_k, \omega_{k'} \in \mathcal{P}(\mathcal{A}_k)_*$, *and let* $p \doteq \rho \oplus \rho'$. *If* $[D_I, p] = 0$ *then, for any* $\omega_E, \omega'_E \in \mathcal{P}(\mathcal{A}_E)$,

$$d(\omega_E \otimes \omega_k, \omega'_E \otimes \omega_{k'}) = d_e(\omega_E \otimes \omega_1, \omega'_E \otimes \omega_2),$$

where ω_1, ω_2 *are the pure states of* $\mathbb{K}^2$ *and* d_e *is the distance associated with* $T_e \doteq T_E \otimes T_r$ *with*

$$\mathcal{A}_r \doteq \mathbb{K}^2, \quad \mathcal{H}_r \doteq p\mathcal{H}_I, \quad D_r \doteq pD_I p|_{\mathcal{H}_r}.$$

Proof: The projection $e \doteq \mathbb{I}_E \otimes p \in \mathcal{A}$ defines the restricted triple $T_e \doteq (\mathcal{A}_e, \mathcal{H}_e, D_e)$ in which

$$\mathcal{A}_e \doteq \alpha_e(\mathcal{A}) = \mathcal{A}_E \otimes \alpha_p(\mathcal{A}_I).$$

Since ρ and ρ' correspond to different components of $\mathcal{A}_I$ they are orthogonal, therefore

$$\alpha_p(\mathcal{A}_I) = \alpha_\rho(\mathcal{A}_k) \oplus \alpha_{\rho'}(\mathcal{A}_{k'}) = \omega_k(\mathcal{A}_k)\rho \oplus \omega_{k'}(\mathcal{A}_{k'})\rho'$$

by (10). $\omega_k, \omega_{k'}$ being surjective on $\mathbb{K}$, $\omega_k(\mathcal{A}_k)\rho$ and $\omega_{k'}(\mathcal{A}_{k'})\rho'$ are isomorphic to $\mathbb{K}$. Hence

$$\mathcal{A}_e = \mathcal{A}_E \otimes \mathbb{K}^2.$$

The state $\omega_i \in \mathcal{P}(\mathbb{K}^2)$ extracts the ith component of a pair of elements of $\mathbb{K}$. In detail, for $a_I \in \mathcal{A}_I$,

$$\alpha_p(a_I) = \omega_k(a_I)\rho \oplus \omega_{k'}(a_I)\rho', \tag{11}$$

so that $\omega_1 \circ \alpha_p(a_I) = \omega_k(a_I)$. Since e acts like the identity on $\mathcal{A}_E$,

$$(\omega_E \otimes \omega_1) \circ \alpha_e = \omega_E \otimes (\omega_1 \circ \alpha_p) = \omega_E \otimes \omega_k,$$

and $(\omega'_E \otimes \omega_2) \circ \alpha_e = \omega'_E \otimes \omega_{k'}$. By hypothesis $[D, e] = \chi_E \otimes [D_I, p] = 0$ so Lemma 1 yields

$$d(\omega_E \otimes \omega_k, \omega'_E \otimes \omega_{k'}) = d_e(\omega_E \otimes \omega_1, \omega'_E \otimes \omega_2).$$

$\mathcal{H}_r$ and D_r are given by Lemma 1. ■

To explicitly compute d_e, we now focus on the case of a continuum$\times$discrete space and we take for T_E the spectral triple of a manifold (2). To simplify the notations, the pure state $\omega_x \otimes \omega_k$ is denoted by x_k. The main result of this section is that the internal space is orthogonal to the manifold, in the sense of the Pythagorean theorem, as soon as the Dirac operator commutes with the sum of the density matrices.

Theorem 4: *Let* $\omega_k, \omega_{k'} \in \mathcal{P}(\mathcal{A}_k)_*, \mathcal{P}(\mathcal{A}_{k'})_*$, $k \neq k'$. *Let* ρ, ρ' *be their supports and* $p \doteq \rho \oplus \rho'$. *If* $[D_I, p] = 0$, *then for any points* x, y *in* $\mathcal{M}$,

$$d(x_k, y_{k'})^2 = d(x_k, y_k)^2 + d(y_k, y_{k'})^2.$$

Proof: The proof consists of three steps. First the problem is reduced to a two-sheets model. Then the distance is shown to be the geodesic distance within a $(4+1)$-dimensional Riemannian manifold which, third, satisfies the Pythagorean theorem.

(1) With notations of Proposition 3,

$$d(x_k, y_{k'}) = d_e(x_1, y_2). \tag{12}$$

Let us be more explicit on $\mathcal{H}_r$, π_r, and D_r,

$$\mathcal{H}_r \doteq p\mathcal{H}_I = \mathcal{H}_k \oplus \mathcal{H}_{k'}, \tag{13}$$

where $\mathcal{H}_k \doteq \rho\mathcal{H}_I$ and $\mathcal{H}_{k'} \doteq \rho'\mathcal{H}_I$. Following (11), one lets $a_r = \omega_k(a_I)\rho \oplus \omega_{k'}(a_I)\rho'$ denote a generic element of $\mathcal{A}_r$. Clearly $\pi_r(\rho) = \mathbb{I}_k$ so

$$\pi_r(a_r) = \omega_k(a_I)\mathbb{I}_k \oplus \omega_{k'}(a_I)\mathbb{I}_{k'}. \tag{14}$$

D_r is the restriction to $\mathcal{H}_r$ of the projection of D_I on $\mathcal{H}_r$, namely

$$D_r \doteq \begin{pmatrix} V & M \\ M^* & W \end{pmatrix}, \tag{15}$$

where M is a linear map from $\mathcal{H}_k$ to $\mathcal{H}_{k'}$, and V, W are endomorphisms of $\mathcal{H}_k$, $\mathcal{H}_{k'}$, respectively. M is supposed to be nonzero for the contrary makes D_r commuting with π_r, that is all states of $\mathcal{A}$ defined by ω_k are at infinite distance from any states defined by $\omega_{k'}$.

Equations (13)–(15) associated with (11) fully determine the triple T_r, and thus T_e. Omitting ρ and ρ' appearing in (11), a generic element of $\mathcal{A}_e$ writes

$$a = f^i \otimes \omega_k(m_i) \oplus f^i \otimes \omega_{k'}(m_i) = f \oplus g,$$

where $m_i \in \mathcal{A}_I$ and $f^i, f \doteq f^i\omega_k(m_i), g \doteq f^i\omega_{k'}(m_i) \in C^\infty(\mathcal{M})$. In accordance with (1), we assume that $f \oplus g$ is positive, i.e., f and g are real functions. x_1 and y_2 act as

$$x_1(a) = f(x), \quad y_2(a) = g(y).$$

a is represented by

$$f\mathbb{I}_E \otimes \mathbb{I}_k \oplus g\mathbb{I}_E \otimes \mathbb{I}_{k'}$$

and the Dirac operator $D_e = i\partial\!\!\!/ \otimes \mathbb{I}_I + \gamma^5 \otimes D_r$ is such that

$$[D_e, a] = \begin{pmatrix} i\partial\!\!\!/ f \otimes \mathbb{I}_k & (g-f)\gamma^5 \otimes M \\ \overline{(f-g)}\gamma^5 \otimes M^* & i\partial\!\!\!/ \otimes \mathbb{I}_{k'} \end{pmatrix}. \tag{16}$$

(2) Let us show that d_e coincides with the geodesic distance on the compact manifold

$$\mathcal{M}' \doteq [0,1] \times \mathcal{M},$$

with coordinates $x'^a = (t, x^\mu)$, equipped with the metric

$$\{g^{ab}(x')\} \doteq \begin{pmatrix} \|M\|^2 & 0 \\ 0 & g^{\mu\nu}(x) \end{pmatrix},$$

and made a spin manifold by adding to the previous γ-matrices

$$\gamma^t = \|M\|\gamma^5.$$

Thanks to Sec. III, it is enough to show that d_e coincides with the distance L' of the triple

$$\mathcal{A}' = C^\infty(\mathcal{M}'), \quad \mathcal{H}' = L_2(\mathcal{M}', S), \quad D' = i\gamma^a\partial_a = i\gamma^t\partial_t + i\partial\!\!\!/.$$

To proceed, let $\mathcal{A}''$ be the subset of $\mathcal{A}'_+$ consisting of all functions

$$\phi(t,x) \doteq (1-t)g(x) + tf(x),$$

where f and g are any real functions on $\mathcal{M}$. Then

$$\|[D',\phi]\|^2=\|\gamma^a\partial_a\phi\|^2=\sup_{(t,x)\in\mathcal{M}'}\{g^{ab}(t,x)\,\partial_a\phi(t,x)\,\partial_b\phi(t,x)\}$$
$$\leqslant\sup_{x\in\mathcal{M}}\{\,|(f-g)(x)|^2\|M\|^2+\sup_{t\in[0,1]}P(t,x)\,\},$$

where

$$P(t,x)\doteq t^2\|\vec{\nabla}(f-g)(x)\|^2+2tg^{\mu\nu}(x)\,\partial_\mu(f-g)(x)\,\partial_\nu g(x)+\|\vec{\nabla}g(x)\|^2$$

is a parabola in t of positive leading coefficient, i.e., which reaches its maximum for $t=0$ or 1. Note that

$$P(0,x)=\|\vec{\nabla}g(x)\|^2,\quad P(1,x)=\|\vec{\nabla}f(x)\|^2$$

and, thanks to (16),

$$\left\|\begin{pmatrix}\mathbb{I}_E\otimes\mathbb{I}_k & 0\\ 0 & 0\end{pmatrix}[D_e,a]\begin{pmatrix}\mathbb{I}_E\otimes\mathbb{I}_k & 0\\ 0 & \gamma^5\otimes\mathbb{I}_{k'}\end{pmatrix}\right\|^2=\left\|\begin{pmatrix}i\not{\partial}f\otimes\mathbb{I}_k & (g-f)\mathbb{I}_E\otimes M\\ 0 & 0\end{pmatrix}\right\|^2$$
$$=\sup_{x\in\mathcal{M}}\{\,\|\vec{\nabla}f(x)\|^2+|f(x)-g(x)|^2\|M\|^2\,\}$$
$$\leqslant\|[D_e,a]\|^2.$$

Similarly, one has $\sup_{x\in\mathcal{M}}\{\|\vec{\nabla}g(x)\|^2+|f(x)-g(x)|^2\|M\|^2\}\leqslant\|[D_e,a]\|^2$, hence

$$\|[D',\phi]\|\leqslant\|[D_e,a]\|.$$

Consequently, since $x_1(a)-y_2(a)=\phi(0,x)-\phi(1,y)$,

$$d_e(x_1,y_2)\leqslant\sup_{\phi\in\mathcal{A}''}\{|\phi(0,x)-\phi(1,y)|/\|[D',\phi]\leqslant1\|\}\leqslant L'((0,x),(1,y)).\tag{17}$$

Proving the converse inequality calls for more precision on the geometry of $\mathcal{M}'$. Because $\{g^{ab}(x')\}$ is block diagonal and does not depend on t, the coefficients of the Levi-Civita connection are

$$\Gamma^t_{t\mu}=\Gamma^t_{\mu t}=\tfrac{1}{2}g^{tt}\partial_\mu g_{tt},\quad \Gamma^\mu_{tt}=-\tfrac{1}{2}g^{\mu\nu}\partial_\nu g_{tt},\quad \Gamma^\mu_{t\nu}=\Gamma^\mu_{\nu t}=\Gamma^t_{tt}=\Gamma^t_{\mu\nu}=0,$$

where $g_{tt}=(g^{tt})^{-1}=\|M\|^{-2}$. The geodesic equations read

$$\frac{\mathrm{d}^2t}{\mathrm{d}\tau^2}+g^{tt}(\partial_\mu g_{tt})\frac{\mathrm{d}t}{\mathrm{d}\tau}\frac{\mathrm{d}x^\mu}{\mathrm{d}\tau}=0,\tag{18}$$

$$\frac{\mathrm{d}^2x^\mu}{\mathrm{d}\tau^2}-\frac{1}{2}g^{\mu\nu}(\partial_\nu g_{tt})\frac{\mathrm{d}t}{\mathrm{d}\tau}\frac{\mathrm{d}t}{\mathrm{d}\tau}+\Gamma^\mu_{\lambda\rho}\frac{\mathrm{d}x^\lambda}{\mathrm{d}\tau}\frac{\mathrm{d}x^\rho}{\mathrm{d}\tau}=0,\tag{19}$$

and, because g_{tt} does not depend on x^μ, reduce to

$$\frac{\mathrm{d}t}{\mathrm{d}\tau}=\text{constant}\doteq g^{tt}K,\quad\text{and}\quad\frac{\mathrm{d}^2x^\mu}{\mathrm{d}\tau^2}+\Gamma^\mu_{\lambda\rho}\frac{\mathrm{d}x^\lambda}{\mathrm{d}\tau}\frac{\mathrm{d}x^\rho}{\mathrm{d}\tau}=0\,,\tag{20}$$

where K is a real constant. In other terms, the projection to $\mathcal{M}$ of a geodesic $\mathcal{G}'$ of $\mathcal{M}'$ is a geodesic $\mathcal{G}$ of $\mathcal{M}$, and the projection of $\mathcal{G}'$ to the submanifold $[0,1]\times\mathcal{G}$ is a straight line (i.e., a geodesic of the submanifold). Let $\{x^a(\tau)\}$ be a geodesic in $\mathcal{M}'$ parametrized by its length element $\mathrm{d}\tau$. Note that, using (20),

$$1=\frac{\mathrm{d}\tau^2}{\mathrm{d}\tau^2}=g_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}\tau}\frac{\mathrm{d}x^\nu}{\mathrm{d}\tau}+g^{tt}K^2. \tag{21}$$

Let $\mathrm{d}s$ be the line element of $\mathcal{M}$. Assuming that $g^{tt}K^2\neq 1$ (this will be discussed later),

$$\mathrm{d}\tau^2=\frac{\mathrm{d}s^2}{1-g^{tt}K^2},\quad \mathrm{d}t=\frac{\mathrm{d}t}{\mathrm{d}\tau}\mathrm{d}\tau=\frac{g^{tt}K\,\mathrm{d}s}{\sqrt{1-g^{tt}K^2}}. \tag{22}$$

For q in $\mathcal{M}$, let $\mathcal{G}'_q$ be the minimum geodesic of $\mathcal{M}'$ between $(0,q)$ and $(1,y)$, and $\mathcal{G}_q$ its projection on $\mathcal{M}$. Let us define the continuous function over $\mathcal{M}$,

$$f_0(q)=\sqrt{1-g^{tt}K^2}L(q)=\sqrt{1-g^{tt}K^2}\int_{\mathcal{G}_q}\mathrm{d}s,$$

where L has been defined in (3). Take $a_0=(f_0,g_0)$, where $g_0=f_0-K$. Then

$$x_1(a_0)-y_2(a_0)=f_0(x)-g_0(y)=f_0(x)+K. \tag{23}$$

But the second equation in (22) gives

$$1=\int_{\mathcal{G}'_x}\mathrm{d}t=\frac{g^{tt}K}{\sqrt{1-g^{tt}K^2}}\int_{\mathcal{G}_x}\mathrm{d}s,$$

inserted in (23) as $K1$,

$$x_1(a_0)-y_2(a_0)=\sqrt{1-g^{tt}K^2}\int_{\mathcal{G}_x}\mathrm{d}s+\frac{g^{tt}K^2}{\sqrt{1-g^{tt}K^2}}\int_{\mathcal{G}_x}\mathrm{d}s=\frac{1}{\sqrt{1-g^{tt}K^2}}\int_{\mathcal{G}_x}\mathrm{d}s.$$

Using the first equation in (22) one obtains

$$x_1(a_0)-y_2(a_0)=\int_{\mathcal{G}'_x}\mathrm{d}\tau=L'((0,x),(1,y)). \tag{24}$$

Moreover, $\not\partial f_0=\not\partial g_0$ and $\partial_\mu f_0=\sqrt{1-g^{tt}K^2}\partial_\mu L$, so (16) yields

$$\|[D_e,a_0]\|^2=\sup_{q\in\mathcal{M}}\{g^{\mu\nu}(q)\partial_\mu f_0(q)\partial_\nu f_0(q)+g^{tt}K^2\}=\sup_{q\in\mathcal{M}}\{(1-g^{tt}K^2)\|\vec{\nabla}L(q)\|^2+g^{tt}K^2\}.$$

Recalling (4), this gives $\|[D_e,a_0]\|\leqslant 1$ so, with (24) (and the same remark as the one at the end of Sec. III, concerning the nonsmoothness of f_0 at y),

$$d_e(x_1,y_2)\geqslant L'((0,x),(1,y)).$$

Together with (17) and (12),

$$d(x_k,y_{k'})=L'((0,x),(1,y)). \tag{25}$$

This result holds as long as $g^{tt}K^2 \neq 1$. If this is not true, then $U \doteq (\mathrm{d}x^\mu/\mathrm{d}\tau)\partial_\mu \in TM$ is zero for (21) indicates that $g(U,U)=0$ and $\mathcal{M}$ is Riemannian. In other words, $x^\mu(\tau)$ is a constant. This cannot be the equation of $\mathcal{G}'_x$ unless $x=y$. As a conclusion, (25) holds as soon as $x \neq y$.

When $x=y$, (12) gives $d(y_k,y_{k'})=d_e(y_1,y_2)$. With d_r denoting the distance associated with the triple T_r alone, Proposition (2) yields $d_e(y_1,y_2)=d_r(\omega_1,\omega_2)$, which is nothing but the distance of the simplest two-points space and equals[4] $1/\|M\|$. Thus

$$d(y_k,y_{k'})=\frac{1}{\|M\|}. \tag{26}$$

The projection $\mathcal{G}_y$ of the geodesic $\mathcal{G}'_x=\mathcal{G}'_y$ is, by (19), a geodesic between y and y, that is to say a point. $\mathcal{G}'_y$ reduces to a straight line in the hyperplane. Thus $\mathrm{d}\tau^2=g_{tt}\,\mathrm{d}t^2$ and

$$L'((0,y),(1,y))=\sqrt{g_{tt}}\int_{\mathcal{G}'_y}\mathrm{d}t=\sqrt{g_{tt}}=\frac{1}{\|M\|}.$$

Consequently $d(y_k,y_{k'})=L'((0,y),(1,y))$ and (25) holds even if $x=y$.

(3) The last step is to show that (25) satisfies the Pythagorean equality. g^{tt} being a constant, Eq. (22) indicates that $\mathrm{d}\tau$ and $\mathrm{d}s$ are equal up to a constant factor. In this way, one may parametrize a geodesic of $\mathcal{M}'$ by $\mathrm{d}s$ rather than $\mathrm{d}\tau$ and obtains, thanks to the geodesic equations,

$$\mathrm{d}t=g^{tt}K'\,\mathrm{d}s,$$

where K' is a real constant. Then

$$\mathrm{d}\tau^2=g_{tt}\,\mathrm{d}t^2+\mathrm{d}s^2=\mathrm{d}s^2(1+g^{tt}K'^2).$$

Thus

$$L'((0,x),(1,y))=\sqrt{1+g^{tt}K'^2}\int_{\mathcal{G}'_x}\mathrm{d}s=\sqrt{1+g^{tt}K'^2}L(x,y)=\sqrt{L(x,y)^2+g^{tt}K'^2L(x,y)^2}. \tag{27}$$

On one side, Theorem 2 gives $L(x,y)=d(x_k,y_k)$. On the other side,

$$g^{tt}K'^2L(x,y)^2=g_{tt}\left(\int_{\mathcal{G}'_x}g^{tt}K'\,\mathrm{d}s\right)^2=g_{tt}\left(\int_{\mathcal{G}'_x}\mathrm{d}t\right)^2=g_{tt}=\frac{1}{\|M\|^2}=d^2(y_k,y_{k'})$$

by (26). Together with (25) and (27),

$$d(x_k,y_{k'})^2=d(x_k,y_k)^2+d^2(y_k,y_{k'}).$$

■

VI. FLUCTUATIONS OF THE METRIC

For a complete presentation of the material of this section and a justification of the terminology, see Refs. 4 and 1. To a triple $(\mathcal{A},\mathcal{H},D)$, the axiom of reality adds an operator J, called the real structure, such that $[JaJ^{-1},b]=0$ for any $a,b\in\mathcal{A}$. This allows one to define a right action of $\mathcal{A}$ over $\mathcal{H}$ which makes sense because of the noncommutativity of the algebra. To define a notion of unitarily equivalent spectral triples preserving the operator J, a unitary element u of $\mathcal{A}$ is implemented by the operator $U\doteq uJuJ^{-1}$ rather than the operator u. Then the action of u defines the *gauge transformed* triple $(\mathcal{A},\mathcal{H},D_A)$ where

$$D_A\doteq UDU^*=D+A+JAJ^{-1} \tag{28}$$

with

$$A \doteq u[D,u^{-1}].$$

The self-adjoint operator A governs the failure of invariance of D under a gauge transformation.[4] Under a gauge transformation, A transforms like a usual vector potential. Since in electrodynamics the vector potential is a one-form, one defines the space Ω^1 of one-form of the noncommutative space $(\mathcal{A},\mathcal{H},D)$ as the set of elements

$$a^i[D,b_i],$$

where $a^i,b_i \in \mathcal{A}$. Note that we use the simplifying notation Ω^1 rather than Ω^1_D, more common in the literature, because we only deal with zero-forms and one-forms (Ω^n_D differs from Ω^n for $n \geqslant 2$). Since A is self-adjoint, the set of vector potentials is simply the subset of self-adjoint elements of Ω^1. For any vector potential A, D_A defined by (28) is called the covariant Dirac operator.

The distance is not invariant under a gauge transformation and the metric is said to fluctuate. To study such fluctuations, one has to replace D by D_A everywhere in the preceding sections. A well-known result makes this replacement less studious than it seems.

Lemma 5: $[a,J\omega J^{-1}]=0, \forall\, \omega \in \Omega^1, a \in \mathcal{A}$.

Proof: $[J^{-1}aJ,[D,b_i]]=0$ (first order axiom) and $[a,Ja^iJ^{-1}]=0$ (axiom of reality) yield

$$\begin{aligned}[a,J\omega J^{-1}] &= [a,Ja^i[D,b_i]J^{-1}] \\ &= aJa^iJ^{-1}J[D,b_i]J^{-1} - Ja^i[D,b_i]J^{-1}a \\ &= Ja^i[D,b_i]J^{-1}a - Ja^i[D,b_i]J^{-1}a = 0.\end{aligned}$$

■

As an immediate consequence,

$$[D_A,a]=[D+A,a]. \tag{29}$$

Let us now work out the one-forms of a tensor product triple $T_E \otimes T_I$. In Refs. 25 and 26 it is shown that

$$\Omega^1 = \Omega^1_E \otimes \Omega^0_I + \chi_E \Omega^0_E \otimes \Omega^1_I,$$

where $\Omega^0_E = \mathcal{A}_E$ is the set of zero-forms of $\mathcal{A}_E$, and similar definitions for the other terms. When T_E is the spectral triple of a manifold,

$$\Omega^1_E \ni f^j[i\not{\partial},g_j\mathbb{I}_E] = if^j(\gamma^\mu \partial_\mu g_j) = i\gamma^\mu f_\mu,$$

where $f^j,g_j,f_\mu \doteq f^j\partial_\mu g_j \in C^\infty(\mathcal{M})$. A one-form of the total spectral triple is

$$\Omega^1 \ni i\gamma^\mu f^i_\mu \otimes a_i + \gamma^5 h^j \otimes m_j,$$

where $a_i \in \mathcal{A}_I$, $h^j \in C^\infty(\mathcal{M})$, $m_j \in \Omega^1_I$. A vector potential is

$$A = i\gamma^\mu \otimes A_\mu + \gamma^5 \otimes H \tag{30}$$

with $A_\mu \doteq f^i{}_\mu a_i$ an $\mathcal{A}_I$-valued skew-adjoint vector field (over $\mathcal{M}$) and $H \doteq h^j m_j$ a Ω^1_I-valued self-adjoint scalar field. For a matrix algebra (or a direct sum of matrix algebras), the skew-adjoint elements form the Lie algebra of the Lie group of unitarities. This Lie group represents the gauge group of the theory, thus A_μ is a gauge potential. In Ref. 1 a formula is given for the fluctuations of the metrics due to A_μ with a zero H. This involves the holonomy of the gauge connexion. Here, we focus on the fluctuations coming from the scalar field H, and for simplicity we assume that $A_\mu = 0$. Then (29) becomes

$$[D_A,a]=[D+\gamma^5\otimes H,a]. \tag{31}$$

From now on, we write $D_A\doteq D+\gamma^5\otimes H$. For simplicity, d still denotes the distance associated with the triple $(\mathcal{A},\mathcal{H},D_A)$. Remembering definition (7), a scalar fluctuation substitutes

$$D_H\doteq D_I+H$$

for D_I. The main difference is that the internal Dirac operator D_H now depends on x so that each point x of the manifold defines an internal triple

$$T_I^x\doteq(\mathcal{A}_I,\mathcal{H}_I,D_H(x)).$$

This interpretation of scalar fluctuations perfectly fits to the adaptation of Theorem 2.

Theorem 2′: *Let L be the geodesic distance in $\mathcal{M}$ and d_x the distance of the spectral triple T_I^x alone. For $x,y\in\mathcal{M}$ and $\omega_k,\omega_{k'}\in\mathcal{P}(\mathcal{A}_I)_*$,*

$$d(x_k,x_{k'})=d_x(\omega_k,\omega_{k'}),$$

$$d(x_k,y_k)=L(x,y).$$

Proof: The adaptation of the proof of Theorem 2 is straightforward. Notations are similar except that ω_E is now ω_x so that a_E is replaced by a_x. With $H=h^j m_j$,

$$\begin{aligned}[D_H(x),a_x]=[D_I+\omega_x(h^j)m_j,\omega_x(f^i)m_i]&=\omega_x(f^i)[D_I,m_i]+\omega_x(h^j)\omega_x(f^i)[m_j,m_i]\\&=(\omega_x\otimes\mathbb{I}_I)(f^i\otimes[D_I,m_i]+h^jf^i\otimes[m_j,m_i])\\&=(\omega_x\otimes\mathbb{I}_I)(f^i\otimes[D_H,m_i]).\end{aligned} \tag{32}$$

Then, $i[D_H(x),a_x]$ being normal,

$$\begin{aligned}\|[D_H(x),a_x]\|=\sup_{\tau_I\in\mathcal{S}_I}|\tau_I([D_H(x),a_x])|&=\sup_{\tau_I\in\mathcal{S}_I}|(\omega_x\otimes\tau_I)(f^i\otimes[D_H,m_i])|\\&\leqslant\sup_{\tilde\omega_E\otimes\tau_I\in\mathcal{P}(\mathcal{A}_E)\otimes\mathcal{S}_I}|(\tilde\omega_E\otimes\omega_I)(f^i\otimes[D_H,m_i])|\\&\leqslant\|f^i\otimes[D_H,m_i]\|.\end{aligned}$$

Equation (9) being replaced by $\|f^i\otimes[D_H,m_i]\|\leqslant\|[D_A,a]\|$, one obtains

$$\|[D_H(x),a_x]\|\leqslant\|[D_A,a]\|.$$

The rest of the proof is then similar as in Theorem 2. ■

Note that in (32) we use that ω_x is a character, i.e., that $\mathcal{A}_E$ is Abelian.

Applied to the two-sheets model, Theorem 2′ simply says that the distance between the sheets is encoded by a scalar field, as has already been shown in Ref. 16 [see also Ref. 7 for a $M_2(\mathbb{C})\oplus\mathbb{C}$ model]. Theorem 4 is modified in a more serious way for the fluctuation introduces an x-dependence for the coefficients of the Kaluza–Klein metric.

Theorem 4′: *Let $\omega_k,\omega_{k'}\in\mathcal{P}(\mathcal{A}_k)_*,\mathcal{P}(\mathcal{A}_{k'})_*$, $k\neq k'$. Let ρ,ρ' be the associated projections and $p\doteq\rho\oplus\rho'$. If $[D_H,p]=0$ for any points of $\mathcal{M}$, then for any points $x,y\in\mathcal{M}$,*

$$d(x_k,y_{k'})=L'((0,x),(1,y)),$$

where L' is the geodesic distance of the spin manifold $\mathcal{M}'\doteq[0,1]\times\mathcal{M}$ equipped with the metric

$$\begin{pmatrix}\|M(x)\|^2 & 0\\ 0 & g^{\mu\nu}(x)\end{pmatrix}$$

in which $g^{\mu\nu}$ is the metric of $\mathcal{M}$ and M is the restriction to the representation of $\mathcal{A}_{k'}$ of the projection of D_H on the representation of $\mathcal{A}_k$.

Proof: Unless otherwise made precise, notations are similar to Theorem 4. The first part of the proof is hardly modified. Let $\psi^r \otimes \xi_r \in \mathcal{H}$. Recalling (31) and the definition (30) of H,

$$[D_A, a]\psi^r \otimes \xi_r = \gamma^5 \psi_r \otimes [D_I, p]\xi_r + \gamma^5 h^j \psi_r \otimes [m_j, p]\xi_r \in \mathcal{H}.$$

Evaluated at $x \in \mathcal{M}$, the above expression yields

$$[D_A, a]\psi^r(x) \otimes \xi_r = \gamma^5 \psi_r(x) \otimes [D_I + H(x), p]\xi_r = 0$$

by hypothesis, which means that $[D_A, a]$ is the zero endomorphism of $\mathcal{H}$ so that Lemma 3 applies and

$$d(x_k, y_{k'}) = d_e(x_1, y_2).$$

The only difference with Theorem 4 is that D_r now depends on x. For instance when $\mathcal{A}_I$ is finite dimensional then M is a matrix whose entries are scalar fields on $\mathcal{M}$.

Now $g^{tt}(x) \doteq \|M(x)\|^2$ depends on x but is still independent with respect to t. The geodesic equations (18) and (19) no longer reduce to (20) but

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}\left(g_{tt}\frac{\mathrm{d}t}{\mathrm{d}\tau}\right) &= \left(\frac{\mathrm{d}}{\mathrm{d}\tau}g_{tt}\right)\frac{\mathrm{d}t}{\mathrm{d}\tau} + g_{tt}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{dt}{d\tau}\right) \\
&= (\partial_\mu g_{tt})\frac{\mathrm{d}t}{\mathrm{d}\tau}\frac{\mathrm{d}x^\mu}{\mathrm{d}\tau} + g_{tt}\frac{\mathrm{d}^2 t}{\mathrm{d}\tau^2} \\
&= g_{tt}\left(g^{tt}(\partial_\mu g_{tt})\frac{\mathrm{d}t}{\mathrm{d}\tau}\frac{\mathrm{d}x^\mu}{\mathrm{d}\tau} + \frac{\mathrm{d}^2 t}{\mathrm{d}\tau^2}\right) \\
&= 0
\end{aligned}$$

by (18). Thus $g_{tt}(\mathrm{d}t/\mathrm{d}\tau) = K$ is a constant. This is almost the first equation in (20), except that

$$\frac{\mathrm{d}t}{\mathrm{d}\tau} = K g^{tt}(x) \tag{33}$$

now depends on x. $a_0 = (f_0, g_0)$ is defined by

$$f_0(q) \doteq \int_{\mathcal{G}_q} \sqrt{1 - K^2 g^{tt}}\,\mathrm{d}s, \quad g_0 \doteq f_0 - K, \tag{34}$$

where $\mathcal{G}'_q$ is the minimal geodesics from $(0,q)$ to the fixed point $(1,y)$ and $\mathcal{G}_q$ its projection to $\mathcal{M}$ (note that $\mathcal{G}_q$ is no longer a geodesic of $\mathcal{M}$). Assuming that

$$K^2 g^{tt}(p) \neq 1 \tag{35}$$

for any $p \in \mathcal{G}_q$ allows one to write

$$\mathrm{d}\tau = \frac{\mathrm{d}s}{\sqrt{1 - K^2 g^{tt}}}$$

and then

$$1=\int_{\mathcal{G}'_q}\mathrm{d}t=\int_{\mathcal{G}'_q}\frac{\mathrm{d}t}{\mathrm{d}\tau}\mathrm{d}\tau=\int_{\mathcal{G}_q}\frac{Kg^{tt}}{\sqrt{1-K^2g^{tt}}}\mathrm{d}s. \tag{36}$$

If (35) does not hold, we call G the set of points p of $\mathcal{G}_q$ for which $1-K^2g^{tt}(p)=0$. G' is the corresponding subset of $\mathcal{G}'_q$. For any $p'\in\mathcal{G}'_q$, (33) yields

$$\frac{\mathrm{d}t}{\mathrm{d}\tau}\mathrm{d}\tau=K^{-1}\,\mathrm{d}\tau,$$

and (36) is replaced by

$$1=\int_{\mathcal{G}_q/G}\frac{Kg^{tt}}{\sqrt{1-K^2g^{tt}}}\mathrm{d}s+\int_{G'}K^{-1}\,\mathrm{d}\tau.$$

Inserted as $K1$ in $x_1(a_0)-y_2(a_0)=f_0(x)+K$, this gives

$$\begin{aligned}x_1(a_0)-y_2(a_0)&=\int_{\mathcal{G}_x}\sqrt{1-K^2g^{tt}}\,\mathrm{d}s+\int_{\mathcal{G}_x/G}\frac{K^2g^{tt}}{\sqrt{1-K^2g^{tt}(x)}}\mathrm{d}s+\int_{G'}\mathrm{d}\tau\\&=\int_{G}\sqrt{1-K^2g^{tt}}\,\mathrm{d}s+\int_{\mathcal{G}_x/G}\frac{\mathrm{d}s}{\sqrt{1-K^2g^{tt}(x)}}+\int_{G'}\mathrm{d}\tau\\&=\int_{\mathcal{G}'_x/G'}\mathrm{d}\tau+\int_{G'}\mathrm{d}\tau\\&=L'((0,x),(1,y)).\end{aligned}$$

The function $f_0(q)$ is in the vicinity of q by definition (34) constant on a codimension 1 hypersurface through q. Choosing an adapted reference frame with $\{x^1,x^2,x^3\}$ being the coordinates in the hypersurface and x^0 the normal coordinate, one has $\mathrm{d}s(q)=\sqrt{g_{00}(q)}\mathrm{d}x^0$ and $\partial_\mu f_0(q)=\delta^0_\mu\partial_0 f_0(q)$, giving

$$\partial_\mu f_0(q)=\delta^0_\mu\sqrt{1-K^2g^{tt}(q)}\sqrt{g_{00}(q)},$$

$$g^{\mu\nu}(q)\partial_\mu f_0(q)\partial_\nu f_0(q)=g^{00}(1-g^{tt}K^2)g_{00}=1-g^{tt}K^2,$$

which leads to $\|[D_e,a_0]\|=1$. Hence the result. ■

A few comments about this theorem. First, since all the coefficients of the metric depend on x, there is no way that the geodesic distance satisfies the Pythagorean theorem. Second, a metric is nondegenerate by definition, and we implicitly assume that $M(x)$ never cancels. This was assumed in Theorem 4 to make the distance finite. Here the point is more subtle for the field M may be zero for some points x. Let $\ker(M)\subset\mathcal{M}$ be the set of such points. For any $q\in\ker(M)$, $d((0,q),(1,q))=+\infty$ by Proposition 2′. Moreover,

$$\begin{aligned}d((0,q),(1,q))&\leqslant d((0,q),(0,x))+d((0,x),(1,y))+d((1,y),(1,q))\\&\leqslant L(p,x)+d((0,x),(1,y))+L(y,q),\end{aligned}$$

so $d((0,x),(1,y))=+\infty$ for any $x,y\in\mathcal{M}$, which contradicts Theorem 4′ if $x=y\notin\ker(M)$. One solution is to assume that any point (t,q) with $q\in\ker(M)$ is at infinite distance from any other point, and define $\mathcal{M}'$ as $[0,1]\times\mathcal{M}/\ker(M)$. If any path between x and y crosses $\ker(M)$, this operation splits $\mathcal{M}'$ into disconnected parts. A better solution is to take into account the nonscalar part A_μ of the fluctuation. [In physical models, $M(x)$ is the representation of the Higgs field in the unbroken phase. Then, at $M=0$ the Higgs potential reaches its local maximum. Neglecting the

gauge potential A_μ, the Faddeev–Popov determinant of the t'Hooft gauge-fixing condition is zero at the maximum of the Higgs potential. This leads to a Gribov problem and questions a quantum treatment of $M(x)$ without gauge field. (observation by Helmuth Hüffel)] This goes beyond the aim of this paper and the reader should consult Ref. 1. ker M is the set of points where fermions have no mass. It could be interesting to link the degeneracy of the metric to singularities when passing from massive to massless fermions.

VII. THE STANDARD MODEL AND OTHER EXAMPLES

We shall investigate the metric of spaces whose internal part is one of those described in Ref. 2. We also give some indications on the distance in the standard model.

A. Commutative spaces

We call commutative space a spectral triple whose internal algebra is $\mathbb{C}^k$, $k\in\mathbb{N}$. Any k-tuple of complex numbers $a=(a^1,\ldots,a^k)$ is represented by a diagonal matrix. For two pure states $\omega_u,\omega_v (u,v\in[1,k])$, $\rho_u\oplus\rho_v$ is the matrix with null coefficients except 1 on the uth and vth elements of the diagonal. Within the graphical framework of Ref. 2, one shows that the internal distance only depends on points that are on some path between u and v. In other terms

$$d_I(u,v)=\tilde{d}_I(u,v),$$

where $\tilde{d}_I$ denotes the distance computed with the Dirac operator $\tilde{D}_I=\rho D_I\rho$ in which

$$\rho\doteq\bigoplus_{i\in P\cup Q}\rho_i,$$

with P the set of points that are not connected to u or v, and Q the set of points that are connected either to u or to v by one and only one path. Note that, for any internal one-form,

$$\rho a_i[D_I,b^i]\rho=a_i[\tilde{D},b^i]$$

so that the tilde operation is coherent with the scalar fluctuation. At any point x of the manifold

$$d_x(\omega_u,\omega_v)=\tilde{d}_x(\omega_u,\omega_v)$$

therefore, to apply Theorem 2, it is enough to check that $[\tilde{D}_H,\rho]=0$. One verifies that whenever a component of the internal Dirac operator is zero, the corresponding component of any internal one-form is also zero, so that $[\tilde{D}_H,\rho_I]=0$ as soon as $[\tilde{D}_I,\rho_I]=0$.

This means that the only path between u and v is the link $u-v$ itself. The simplest case, $k=2$, endows the two-sheets model with a cylindrical metric. The other examples of commutative spaces given in Ref. 2 do not fit the required condition and our next examples will be noncommutative.

B. Two-points space

Let $\mathcal{A}_I=M_n(\mathbb{C})\oplus\mathbb{C}$ be represented over $\mathbb{C}^{n+1}$ by

$$\begin{pmatrix} m & 0\\ 0 & c\end{pmatrix}, \tag{37}$$

where $m\in M_n(\mathbb{C})$ and $c\in\mathbb{C}$. Possible chirality K and Dirac operator Δ are

$$K=\begin{pmatrix}\mathbb{I}_n & 0\\ 0 & -1\end{pmatrix},\quad \Delta=\begin{pmatrix}0 & M\\ M^* & 0\end{pmatrix},$$

where $M \in \mathbb{C}^n$. But there is no operator J to fluctuate the metric. A solution is to make (37) acting over $\mathcal{H}_I = M_{n+1}(\mathbb{C})$ and define

$$D\psi \doteq \Delta\psi + \psi\Delta, \quad \chi_I\psi \doteq K\psi + \psi K, \quad J\psi \doteq \psi^*$$

for any $\psi \in \mathcal{H}_I$. Since $J\Delta J^{-1}\psi = J\Delta\psi^* = (\Delta\psi^*)^* = \psi\Delta$, one has $D\psi = \Delta\psi + J\Delta J^{-1}\psi$. Moreover, for any $a \in \mathcal{A}_I$, $[J\Delta J^{-1}, a]\psi = a\psi\Delta - a\psi\Delta = 0$, so $[D_I, a] = [\Delta, a]$. Note that this result comes directly from Lemma 5 as soon as one knows that Δ is a one-form.[21] Since the operator norm over $\mathbb{C}^n$ is equal to the operator norm over $M_n(\mathbb{C})$,

$$\|[D,a]\| = \|[\Delta,a]\|$$

and the distance is in fact the same as the one computed with the spectral triple $(\mathcal{A}_I, \mathbb{C}^{n+1}, \Delta)$. Note that this point is assumed in Ref. 27.

Let ρ_1 be the density matrix associated with a pure state ω_1 of $M_n(\mathbb{C})$ and ρ_0 the one corresponding to the pure state ω_0 of $\mathbb{C}$. Then

$$\rho_1 \oplus \rho_0 = \begin{pmatrix} \rho_1 & 0 \\ 0 & 1 \end{pmatrix}$$

so that $[D_I, \rho_1 \oplus \rho_0] = 0$ is equivalent to $\rho_1 M = M$. In other terms, M is collinear to the range of ρ_1. A happy coincidence makes that this is precisely the condition under which the internal distance $d_I(\omega_1, \omega_0) = 1/\|M\|$ is finite.[2] Theorem 4 is true for any Dirac operator—$d_I(\omega_0, \omega_1) = +\infty$ makes $d(x_0, y_1) = +\infty$ for any x, y in $\mathcal{M}$—so

$$d(x_0, y_1) = \sqrt{L(x,y)^2 + \frac{1}{\|M\|^2}}$$

when M is in the range of ρ_1, is infinite otherwise.

C. The standard model

The spectral triple of the standard model (see Refs. 4, 1, and 28 and Refs. 29 and 30 for a physical expectation of the Higgs mass) is the tensor product of the usual spectral triple of a manifold T_E by an internal triple in which

$$\mathcal{A}_I = \mathbb{H} \oplus \mathbb{C} \oplus M_3(\mathbb{C})$$

($\mathbb{H}$ is the real algebra of quaternions) is represented over

$$\mathcal{H}_I = \mathbb{C}^{90} = \mathcal{H}^P \oplus \mathcal{H}^A = \mathcal{H}_L^P \oplus \mathcal{H}_R^P \oplus \mathcal{H}_L^A \oplus \mathcal{H}_R^A.$$

The basis of $\mathcal{H}_L^P = \mathbb{C}^{24}$ consists of the left-handed fermions

$$\begin{pmatrix} u \\ d \end{pmatrix}_L, \quad \begin{pmatrix} c \\ s \end{pmatrix}_L, \quad \begin{pmatrix} t \\ b \end{pmatrix}_L, \quad \begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \quad \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}_L, \quad \begin{pmatrix} \mu_\tau \\ \tau \end{pmatrix}_L,$$

and the basis of $\mathcal{H}_R^P = \mathbb{C}^{21}$ is labeled by the right-handed fermions u_R, d_r, c_R, s_R, t_R, b_R and e_R, μ_R, τ_R (the model assumes massless neutrinos). The color index for the quarks has been omitted. $\mathcal{H}_R^A$ and $\mathcal{H}_L^A$ correspond to the antiparticles. ($a \in \mathbb{H}$, $b \in \mathbb{C}$, $c \in M_3(\mathbb{C})$) is represented by

$$\pi_I(a,b,c) \doteq \pi^P(a,b) \oplus \pi^A(b,c) \doteq \pi_L^P(a) \oplus \pi_R^P(b) \oplus \pi_L^A(b,c) \oplus \pi_R^A(b,c)$$

where, writing $B \doteq \left(\begin{smallmatrix} b & 0 \\ 0 & \bar{b} \end{smallmatrix}\right) \in \mathbb{H}$ and $N = 3$ for the number of fermion generations,

$$\pi_L^P(a)\doteq a\otimes\mathbb{I}_N\otimes\mathbb{I}_3\oplus a\otimes\mathbb{I}_N,\quad \pi_R^P(b)\doteq B\otimes\mathbb{I}_N\otimes\mathbb{I}_3\oplus\overline{b}\otimes\mathbb{I}_N,$$

$$\pi_L^A(b,c)\doteq\mathbb{I}_2\otimes\mathbb{I}_N\otimes c\oplus\overline{b}\mathbb{I}_2\otimes\mathbb{I}_N,\quad \pi_R^A(b,c)\doteq\mathbb{I}_2\otimes\mathbb{I}_N\otimes c\oplus\overline{b}\mathbb{I}_n.$$

One defines a real structure

$$J_I=\begin{pmatrix}0 & \mathbb{I}_{15N}\\ \mathbb{I}_{15N} & 0\end{pmatrix}\circ^{-},$$

where $^{-}$ denotes the complex conjugation, and an internal Dirac operator

$$D_I\doteq\begin{pmatrix}D_P & 0\\ 0 & \overline{D_P}\end{pmatrix}=\begin{pmatrix}D_P & 0\\ 0 & 0\end{pmatrix}+J_I\begin{pmatrix}D_P & 0\\ 0 & 0\end{pmatrix}J_I^{-1}$$

whose diagonal blocks are $15N\times 15N$ matrices

$$D_P\doteq\begin{pmatrix}0 & M\\ M^* & 0\end{pmatrix},$$

with M an $8N\times 7N$ matrix

$$M\doteq\begin{pmatrix}(e_{11}\otimes M_u+e_{22}\otimes M_d)\otimes\mathbb{I}_3 & 0\\ 0 & e_2\otimes M_e\end{pmatrix}. \tag{38}$$

Here, $\{e_{ij}\}$ and $\{e_i\}$ denote the canonical basis of $M_2(\mathbb{C})$ and $\mathbb{C}^2$, respectively. M_u, M_d, M_e are the mass matrices

$$M_u=\begin{pmatrix}m_u & 0 & 0\\ 0 & m_c & 0\\ 0 & 0 & m_t\end{pmatrix},\quad M_d=C_{KM}\begin{pmatrix}m_d & 0 & 0\\ 0 & m_s & 0\\ 0 & 0 & m_b\end{pmatrix},\quad M_e=\begin{pmatrix}m_e & 0 & 0\\ 0 & m_\mu & 0\\ 0 & 0 & m_\tau\end{pmatrix}$$

whose coefficients are the masses of the elementary fermions, pondered by the unitary Cabibbo–Kobayashi–Maskawa matrix. The chirality, last element of the spectral triple, is

$$\chi_I=(-\mathbb{I}_{8N})\oplus\mathbb{I}_{7N}\oplus(-\mathbb{I}_{8N})\oplus\mathbb{I}_{7N}.$$

The presence of the conjugate representation $\overline{b}$ in π_I requires one to view $\mathbb{C}$ as a real algebra. Therefore, the pure state ω_0 of $\mathbb{C}$ is no longer the identity but an $\mathbb{R}$-linear function with value in $\mathbb{R}$ which maps 1 to 1. In other words, ω_0 is the real part: $\omega_0(b)=\mathrm{Re}(b)$. As a quaternionic algebra, $\mathbb{H}$ has a single pure state and this remains true for $\mathbb{H}$ seen as a real algebra.

Lemma 6: The single pure state ω_1 of $\mathbb{H}$ is $\omega_1(a)=\frac{1}{2}\mathrm{Tr}(\mathbb{I}_{\mathbb{H}}a)$.

Proof: The representation of $\mathbb{H}$ over the four-dimensional real vector space with basis $\{1,i,j,k\}$ such that $i^2=j^2=k^2=-1$, $ij=-ji=k$, $jk=-kj=i$, and $ki=-ik=j$, is

$$a=\alpha+\beta i+\gamma j+\delta k,$$

where $\alpha,\beta,\gamma,\delta\in\mathbb{R}$. Since $\overline{a}\doteq\alpha-\beta i-\gamma j-\delta k$, $a\overline{a}\in\mathbb{R}^+$ so any $\mathbb{R}$-linear form is positive. Therefore a state is any $\mathbb{R}$-linear form that maps $\mathbb{I}_{\mathbb{H}}=1$ to 1. Let ω be such a state. By linearity,

$$\omega(a)=\alpha+\beta\omega(i)+\gamma\omega(j)+\delta\omega(k),$$

so ω is uniquely determined by its values on i,j,k. Let $\omega_{\omega(i)}$ be the linear form defined by $\omega_{\omega(i)}(i)=\omega(i)$, $\omega_{\omega(i)}(1)=\omega_{\omega(i)}(j)=\omega_{\omega(i)}(k)=0$. Define similarly $\omega_{\omega(1)},\omega_{\omega(j)},\omega_{\omega(k)}$. Then

$$\omega=\omega_{\omega(1)}+\omega_{\omega(i)}+\omega_{\omega(j)}+\omega_{\omega(k)}$$
$$=\lambda(\omega_{\omega(1)}+\omega_{\kappa\omega(i)}+\omega_{\kappa\omega(j)}+\omega_{\kappa\omega(k)})+(1-\lambda)(\omega_{\omega(1)}+\omega_{\kappa'\omega(i)}+\omega_{\kappa'\omega(j)}+\omega_{\kappa'\omega(k)}), \quad (39)$$

where $\lambda,\kappa\in\mathbb{R}/\{1\}$ and $\kappa'\doteq(1-\lambda\kappa)/(1-\lambda)$. Both factors of the right-hand side of (39) map 1 to 1, so they are states and ω is not pure unless $\omega(i)=\omega(j)=\omega(k)=0$. Hence the only pure state of $\mathbb{H}$ is $\omega_1\doteq\omega_{\omega(1)}$.

The quaternion a can also be represented over $\mathbb{C}^2$ by $\left(\begin{smallmatrix}\theta & \rho\\ -\bar{\rho} & \bar{\theta}\end{smallmatrix}\right)$ where $\theta\doteq\alpha+i\beta$. Then $\mathrm{Tr}(a)\doteq 2\,\mathrm{Re}(\theta)=2\alpha=2\omega_1(a)$, that is $\omega_1(a)=\mathrm{Tr}(\frac{1}{2}\mathbb{I}_H a)$. ■

With regard to $\mathcal{P}(M_3(\mathbb{C}))$, we shall only need the following well-known lemma:

Lemma 7: Let $\omega,\omega'\in\mathcal{P}(\mathcal{A}_I)$. Then $\omega=\omega'$ if and only if $\ker(\omega)=\ker(\omega')$.

Proof: Pure states are linear forms, so if they have the same kernel they are proportional. Since they coincide on the identity, they are equal. ■

Noncommutative geometry gives an interpretation of the Higgs field as a one-form of the internal space. By scalar fluctuation, one-forms closely interfere with the metric. Thus the Higgs field has an interpretation in terms of an internal metric. The conclusive result of this paper is a precision of this link between Higgs and metric when the gauge field A_μ is neglected.

Proposition 8: The finite part of the geometry of the standard model with scalar fluctuations of the metric consists of a two-sheets model labeled by the single states of $\mathbb{C}$ and $\mathbb{H}$. Each of the sheets is a copy of the Riemannian four-dimensional space–time endowed with its metric. The fifth component of the metric, corresponding to the discrete dimension, is

$$g^{tt}(x)=(|1+h_1(x)|^2+|h_2(x)|^2)m_t^2$$

where $\left(\begin{smallmatrix}h_1\\ h_2\end{smallmatrix}\right)$ is the Higgs doublet and m_t the mass of the quark top.

Proof: π_I stands for $\pi_I(a,b,c)$ and $\Delta\doteq\left(\begin{smallmatrix}D_P & 0\\ 0 & 0\end{smallmatrix}\right)$ so that $D_I=\Delta+J\Delta J^{-1}$. Since Δ is a one-form,[21] Lemma 5 yields $[J_I\Delta J_I^{-1},\pi_I]=0$, so that we can take $D_H=\Delta+H$. By explicit calculation,[31]

$$H=\begin{pmatrix}0 & \pi_L^P(h)M & 0 & 0\\ M^*\pi_L^P(h^*) & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix},$$

where h is a quaternion-valued scalar field. Thus

$$D_H=\begin{pmatrix}0 & \Phi M & 0 & 0\\ M^*\Phi^* & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}, \quad (40)$$

where

$$\Phi\doteq(h+\mathbb{I}_{\mathbb{H}})\otimes\mathbb{I}_{4N}=\begin{pmatrix}1+h_1 & h_2\\ -\bar{h}_2 & 1+\bar{h}_1\end{pmatrix}\otimes\mathbb{I}_{4N},$$

with h_1 and h_2 being two complex scalar fields.

By (1), the metric of the standard model is identical to the metric associated with the triple $(\mathcal{A}_s,\mathcal{H},D)$, where $\mathcal{A}_s=C^\infty(\mathcal{M})_s\otimes\mathcal{A}_{Is}$ is the subalgebra of self-adjoint elements of $\mathcal{A}$, with

$$\mathcal{A}_{Is}=\mathbb{C}_s\oplus\mathbb{H}_s\oplus M_3(\mathbb{C})_s=\mathbb{R}\oplus\mathbb{R}\oplus M_3(\mathbb{C})_s.$$

The representation π_s associated with this triple coincides with the restriction of π to $\mathcal{A}_s$. Concerning the quaternion, π_s substitutes

$$\begin{pmatrix} \theta & 0 \\ 0 & \theta \end{pmatrix} \quad \text{to} \quad \begin{pmatrix} \theta & \overrightarrow{\rho} \\ -\overrightarrow{\rho} & \overline{\theta} \end{pmatrix}.$$

In other words, to each representation of $\mathbb{H}$ there corresponds the direct sum of twice the fundamental representation of $\mathbb{R}=\mathbb{H}_s$. Now ω_1 seen as a pure state of $\mathbb{H}_s$ is nothing but the identity. The associated projection $\rho_1 \in \mathbb{H}_s$ is nothing but the real number 1 which obviously satisfies (10). The same is true for ω_0 seen as a pure state of $\mathbb{R}=\mathbb{C}_s$. Hence

$$\pi_s(\rho_0 \oplus \rho_1) = \begin{pmatrix} \mathbb{I}_{15N} & & & 0 \\ & 0_{6N} & & \\ & & \mathbb{I}_{2N} & \\ 0 & & & 0_{6N} \\ & & & & \mathbb{I}_N \end{pmatrix}$$

commutes with D_H defined in (40). Proposition 4′ applies to the distance between pure states of $\mathcal{A}$ defined by ω_0 and ω_1. Here

$$\pi_s(\operatorname{ran}\rho_1) = \mathcal{H}_L^P \quad \text{and} \quad \pi_s(\operatorname{ran}\rho_0) = \mathcal{H}_R^P \oplus \mathcal{H}_{\text{lep}}^A,$$

where $\mathcal{H}_{\text{lep}}^A = \mathbb{C}^{3N}$ is the subset of $\mathcal{H}^A$ generated by the antileptons. Thus the extra metric component is

$$g^{tt}(x) = \|\Phi(x)M\|^2.$$

Note that, as desired, ΦM is a $2\alpha^{\mathbb{H}} \times (\alpha^{\mathbb{C}} + \overline{\alpha^{\mathbb{C}}})$ matrix, where $\alpha^{\mathbb{H}} = 4N$ is the degeneracy of the representation of $\mathbb{H}_s$ in π_L^P, and $\alpha^{\mathbb{C}} = 3N$, $\overline{\alpha^{\mathbb{C}}} = 4N$ are defined as well. Using the explicit form (38),

$$\begin{aligned} \|\Phi(x)M\|^2 &= \max\{\|(\Phi(x)\otimes \mathbb{I}_3)(e_{11}\otimes M_u + e_{22}\otimes M_d)\|^2, \|(\Phi(x)\otimes \mathbb{I}_3)(e_2 \otimes M_e)\|^2\} \\ &= (|1+h_1(x)|^2 + |h_2(x)|^2)\max\{m_t^2, m_\tau^2\} = (|1+h_1(x)|^2 + |h_2(x)|^2)m_t^2. \end{aligned}$$

The other distances, involving the pure states of $M_3(\mathbb{C})$, are not finite. Indeed,

$$\|[D_H, \pi_I(a,b,c)]\| = \left\| \left[\begin{pmatrix} 0 & \Phi M \\ M^*\Phi^* & 0 \end{pmatrix}, \pi^P(a,b) \right] \right\|$$

does not put any constraint on c, thus for $\omega_2 \in \mathcal{P}(M_3(\mathbb{C}))$ and $\omega \in \mathcal{P}(\mathcal{A}_I)$,

$$d_I(\omega_2, \omega) \geqslant \sup_{c \in M_3(\mathbb{C})} |\omega_2(c) - \omega(c)|.$$

For $\omega = \omega_0$, $c = \lambda \mathbb{I}_3$ with $\lambda \to \infty$ makes the distance $d_I(\omega_2, \omega_0)$ infinite. Then

$$d_I(\omega_2, \omega_0) = d(x_2, x_0) \leqslant d(x_2, y_0) + d(y_0, x_0) \leqslant d(x_2, y_0) + L(x,y)$$

by Theorem 4′, so that $d(x_2, y_0) = +\infty$. The same is true for $\omega = \omega_1$. The same is also true when $\omega \in \mathcal{P}(M_3(\mathbb{C}))$ because, by Lemma 7, there exists $c' \in ker(\omega_2)$, $c' \notin ker(\omega)$ which makes $d_I(\omega_2, \omega)$ infinite. ■

VIII. CONCLUSION

Noncommutative geometry intrinsically links the Higgs field with the metric structure of space–time. We have not considered the gauge field A_μ so it is not clear whether or not the interpretation of the Higgs as an extra metric component has a direct physical meaning. It is important to study the influence of the gauge fluctuation together with a Higgs field, and see how it probably makes the metric of the strong interaction part finite.

Since $\mathbb{H}$ has only one pure state, the problem of the distance between states defined by distinct pure states of the same component of the internal algebra is not questioned here. One may be tempted to consider states τ of $\mathbb{H}$ that are not pure. But asking $\tau(\overline{q}) = \overline{\tau}(q)$—which is part of the definition of a real state[32] and does not come as a consequence like in the complex case—precisely means that $\tau = \omega_1$. To extend the field of investigation, one can consider states that do not preserve the conjugation—then the supremum is no longer reached by a positive element—but this contradicts the spirit of density matrices in quantum mechanics. More interesting is probably to take into account complexified states, that is real linear functions with value in $\mathbb{C}$.

The reduction of $\mathcal{A}_I$ to $\mathbb{K}^2$ (Proposition 3) is made possible by the orthogonality of the projections. When the two internal pure states are no longer orthogonal, there is no reason why the relevant picture should remain the two-sheets model. The same is true for two orthogonal states whose sum of the projections does not commute with the Dirac operator. In this sense, if these cases do not support a simple ''classical'' picture (such as being the geodesic distance of a discrete Kaluza–Klein manifold), they reflect a purely noncommutative aspect of space–time.

Note that the result—before fluctuation—concerning states defined by the same pure state of one of the algebras (Theorem 2), as well as the reduction from $\mathcal{A}_I$ to $\mathbb{K}^2$, do not assume that $\mathcal{A}_E$ is Abelian. It is only later, to establish the orthogonality between the internal and the external spaces, that T_E is taken as the spectral triple of a manifold. It would be interesting to clarify the importance, or the unimportance, of the commutativity regarding the Pythagorean theorem.

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Pseudo-Hermiticity versus *PT* symmetry: The necessary condition for the reality of the spectrum of a non-Hermitian Hamiltonian

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We introduce the notion of *pseudo-Hermiticity* and show that every Hamiltonian with a real spectrum is pseudo-Hermitian. We point out that all the PT-symmetric non-Hermitian Hamiltonians studied in the literature belong to the class of pseudo-Hermitian Hamiltonians, and argue that the basic structure responsible for the particular spectral properties of these Hamiltonians is their pseudo-Hermiticity. We explore the basic properties of general pseudo-Hermitian Hamiltonians, develop *pseudosupersymmetric quantum mechanics*, and study some concrete examples, namely the Hamiltonian of the two-component Wheeler–DeWitt equation for the FRW-models coupled to a real massive scalar field and a class of pseudo-Hermitian Hamiltonians with a real spectrum. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The past three years have witnessed a growing interest in non-Hermitian Hamiltonians with real spectra.[1–23] Based on the results of various numerical studies, Bender and collaborators[1,4] found certain examples of one-dimensional non-Hermitian Hamiltonians that possessed real spectra. Because these Hamiltonians were invariant under PT transformation, their spectral properties were linked with their PT symmetry. The purpose of this article is to explore the basic structure responsible for the reality of the spectrum of a non-Hermitian Hamiltonian.

By definition, a PT-symmetric Hamiltonian H satisfies

$$PTH(PT)^{-1}=PTHPT=H, \tag{1}$$

where P and T are, respectively, the operators of parity and time-reversal transformations. These are defined according to

$$P\,x\,P=-x, \quad P\,p\,P=T\,p\,T=-p, \quad T\,i1\,T=-i1, \tag{2}$$

where x, p, and 1 are, respectively, the position, momentum, and identity operators acting on the Hilbert space $\mathcal{H}=L^2(\mathbb{R})$ and $i:=\sqrt{-1}$. Note that Eq. (2) applies only for the systems whose classical position x and momentum p are real. In this article we shall only be concerned with these systems.

As we mentioned previously, the only reason for relating the concept of PT-symmetry and non-Hermitian Hamiltonians with a real spectrum is that most of the known examples of the latter satisfy Eq. (1). Certainly there are Hermitian Hamiltonians with a real spectrum that are not PT-symmetric and there are PT-symmetric Hamiltonians that do not have a real spectrum. Therefore, PT-symmetry is neither a necessary nor a sufficient condition for a Hamiltonian to have a real spectrum. This raises the possibility that the PT-symmetry of a Hamiltonian may have

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nothing to do with the reality of its spectrum. The interest in PT-symmetry seems to be mostly because of the lack of an alternative framework replacing the Hermiticity of the Hamiltonian in ordinary (unitary) quantum mechanics. Much of the published work on the subject concerns the study of various examples and the extension of the concepts developed for Hermitian Hamiltonians to the PT-symmetric ones.[1–20] Recently, Znojil,[21] Japaridze,[22] and Kretschmer and Szymanowski[23] have addressed some of the more fundamental issues regarding the mathematical structure and the interpretation of the PT-symmetric quantum mechanics.

Among the common properties of all the PT-symmetric Hamiltonians that have so far been studied are the following.

(1) Either the spectrum of the Hamiltonian is real (PT-symmetry is exact) or there are complex-conjugate pairs of complex eigenvalues (PT-symmetry is broken).[1,4,10,12]

(2) The indefinite inner-product $\langle\langle\,|\,\rangle\rangle$ defined by

$$\langle\langle\psi_1|\psi_2\rangle\rangle := \langle\psi_1|P|\psi_2\rangle, \quad \forall|\psi_1\rangle,|\psi_2\rangle\in\mathcal{H}, \tag{3}$$

is invariant under the time-translation generated by the Hamiltonian.[21,22]

The main motivation for the present investigation is the remarkable fact that there is no evidence that PT-symmetry is the basic structure responsible for these properties. For example, in Ref. 3, the authors construct a class of non-PT-symmetric Hamiltonians with a real spectrum. Another example of a non-Hermitian Hamiltonian with similar properties is the Hamiltonian describing the evolution of the solutions of the two-component Wheeler–DeWitt equation for FRW-models coupled with a real massive scalar field.[24] This Hamiltonian is explicitly ''time dependent,'' ''parity-invariant,'' and non-Hermitian (with respect to the relevant L^2-$norm$ on the space of two-component wave functions), but the corresponding invariant indefinite inner-product does not involve P.

The organization of the article is as follows. In Sec. II, we introduce the concept of a *pseudo-Hermitian* operator and derive the basic spectral properties of pseudo-Hermitian Hamiltonians. These coincide with Properties 1 and 2 (with P replaced with a Hermitian invertible linear operator η). In Sec. III, we consider the class of pseudo-Hermitian Hamiltonians that have a complete biorthonormal eigenbasis and show that the pseudo-Hermiticity is a necessary condition for having a real spectrum. In Sec. IV, we explore the pseudo-Hermitian Hamiltonian of the two-component Wheeler–DeWitt equation for FRW-models coupled with a real massive scalar field. In Sec. V, we develop pseudosupersymmetric quantum mechanics. In Sec. VI, we use pseudosupersymmetry to construct a large class of pseudo-Hermitian Hamiltonians with a real spectrum. In Sec. VII, we present our concluding remarks.

II. PSEUDO-HERMITIAN HAMILTONIANS

We first give a few definitions. Throughout this paper we will assume that all the inner product spaces are complex. The generalization to real inner product spaces is straightforward.

Definition 1: Let $V_\pm$ be two inner product spaces endowed with Hermitian linear automorphisms $\eta_\pm$ (invertible operators mapping $V_\pm$ to itself and satisfying)

$$\forall v_\pm, w_\pm \in V_\pm, \quad (v_\pm, \eta_\pm w_\pm)_\pm = (\eta_\pm v_\pm, w_\pm)_\pm,$$

where $(,)_\pm$ stands for the inner product of $V_\pm$) and $O: V_+ \to V_-$ be a linear operator. Then the $\eta_\pm$-pseudo-Hermitian adjoint $O^\sharp: V_- \to V_+$ of O is defined by $O^\sharp := \eta_+^{-1} O^\dagger \eta_-$. In particular, for $V_\pm = V$ and $\eta_\pm = \eta$, the operator O is said to be η-pseudo-Hermitian if $O^\sharp = O$.

Definition 2: Let V be an inner product space. Then a linear operator $O: V \to V$ is said to be pseudo-Hermitian, if there is a Hermitian linear automorphism η such that O is η-pseudo-Hermitian.

Now, consider a quantum system with a possibly non-Hermitian and time-dependent Hamiltonian $H=H(t)$ and a Hilbert space $\mathcal{H}$ which is endowed with a Hermitian linear automorphism η.

Proposition 1: The Hermitian indefinite inner product $\langle\langle|\rangle\rangle_\eta$ defined by η, i.e.,

$$\langle\langle\psi_1|\psi_2\rangle\rangle_\eta := \langle\psi_1|\eta|\psi_2\rangle, \quad \forall|\psi_1\rangle,|\psi_2\rangle\in\mathcal{H}, \tag{4}$$

is invariant under the time-translation generated by the Hamiltonian H if and only if H is η-pseudo-Hermitian.

Proof: First note that the η-pseudo-Hermiticity of H is equivalent to the condition

$$H^\dagger = \eta\, H\, \eta^{-1}. \tag{5}$$

Now, using the Schrödinger equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{6}$$

its adjoint, and Eq. (4), one has for any two evolving state vectors $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$:

$$i\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle\psi_1(t)|\psi_2(t)\rangle\rangle_\eta = \langle\psi_1(t)|(\eta H - H^\dagger\eta)|\psi_2(t)\rangle.$$

Therefore, $\langle\langle\psi_1(t)|\psi_2(t)\rangle\rangle_\eta$ is a constant if and only if (5) holds. □

Note that choosing $\eta=1$ reduces Eq. (5) to the condition of the Hermiticity of the Hamiltonian. Hence *pseudo-Hermiticity is a generalization of Hermiticity*. Furthermore, observe that a typical PT-symmetric Hamiltonian defined on a real phase space $((x,p)\in\mathbb{R}^2)$ has the form $H=p^2/(2m)+V(x)$ where the potential $V(x)=V_+(x)+iV_-(x)$ has an even real part $V_+(x)$ and an odd imaginary part $V_-(x)$, i.e., $V_\pm(\pm x)=\pm V_\pm(x)$. It is not difficult to see that such a PT-symmetric Hamiltonian satisfies

$$H^\dagger = \frac{p^2}{2m}+V_+(x)-iV_-(x) = \frac{p^2}{2m}+V_+(-x)+iV_-(-x) = P\,H\,P = P\,H\,P^{-1}.$$

Hence it is P-pseudo-Hermitian. In contrast, consider the non-Hermitian Hamiltonians

$$H_1 := p^2+x^2p, \quad H_2 := p^2+i(x^2p+p\,x^2).$$

Clearly, H_1 is PT symmetric, but not P-pseudo-Hermitian, whereas H_2 is P-pseudo-Hermitian and not PT symmetric. Therefore, PT symmetry and P-pseudo-Hermiticity are distinct properties. Note, however, that H_1 may be pseudo-Hermitian with respect to another Hermitian automorphism η. We shall explore the relationship between PT-symmetry and pseudo-Hermiticity in Sec. III.

The defining condition (5) may also be expressed as the intertwining relation

$$\eta\, H = H^\dagger\, \eta. \tag{7}$$

Using this equation together with the eigenvalue equation for the Hamiltonian, namely $H|E_i\rangle = E_i|E_i\rangle$, and its adjoint, we can easily show that any two eigenvectors $|E_i\rangle$ and $|E_j\rangle$ of H satisfy

$$(E_i^*-E_j)\langle\langle E_i|E_j\rangle\rangle_\eta = 0. \tag{8}$$

A direct implication of this equation is the following Proposition.

Proposition 2: An η-pseudo-Hermitian Hamiltonian has the following properties.

(a) The eigenvectors with a nonreal eigenvalue have vanishing η-semi-norm, i.e.,

$$E_i\notin\mathbb{R} \quad \text{implies} \quad \||E_i\rangle\|_\eta^2 := \langle\langle E_i|E_i\rangle\rangle_\eta = 0. \tag{9}$$

(b) Any two eigenvectors are η-orthogonal unless their eigenvalues are complex conjugates, i.e.,

$$E_i \neq E_j^* \quad \text{implies} \quad \langle\langle E_i | E_j \rangle\rangle_\eta = 0. \tag{10}$$

In particular, the eigenvectors with distinct real eigenvalues are η-orthogonal.

In the remainder of this section, we list a number of simple but remarkable consequences of pseudo-Hermiticity.

Proposition 3: Let V be an inner product space endowed with a Hermitian linear automorphism η, $1: V \to V$ denote the identity operator, $O_1, O_2: V \to V$ be linear operators, and $z_1, z_2 \in \mathbb{C}$. Then,

(a) $1^\sharp = 1$;
(b) $(O_1^\sharp)^\sharp = O_1$;
(c) $(z_1 O_1 + z_2 O_2)^\sharp = z_1^* O_1^\sharp + z_2^* O_2^\sharp$,

where z_i^* stands for the complex conjugate of z_i.

Proof: (a) and (b) are trivial consequences of the definition of $\sharp$ and the Hermiticity of η. (c) follows from this definition and the linearity of η and η^{-1}:

$$(z_1 O_1 + z_2 O_2)^\sharp = \eta^{-1}(z_1 O_1 + z_2 O_2)^\dagger \eta = z_1^* \eta^{-1} O_1^\dagger \eta + z_2^* \eta^{-1} O_2^\dagger \eta = z_1^* O_1^\sharp + z_2^* O_2^\sharp.$$

□

Proposition 4: Let V_ℓ, with $\ell \in \{1,2,3\}$, be inner product spaces endowed with Hermitian linear automorphisms η_ℓ and $O_1: V_1 \to V_2$ and $O_2: V_2 \to V_3$ be linear operators. Then $(O_2 O_1)^\sharp = O_1^\sharp O_2^\sharp$.

Proof: This relation follows from the following simple calculation:

$$(O_2 O_1)^\sharp = \eta_1^{-1}(O_2 O_1)^\dagger \eta_3 = \eta_1^{-1} O_1^\dagger \eta_2 \eta_2^{-1} O_2^\dagger \eta_3 = O_1^\sharp O_2^\sharp.$$

□

Corollary: Pseudo-Hermitian conjugation ($O \to O^\sharp$) is a $*$-operation.

Proof: According to Propositions 3 and 4, $\sharp$ has all the properties of a $*$-operation. □

Proposition 5: Let V be an inner product space endowed with a Hermitian linear automorphism η, $U: V \to V$ be a unitary operator, and $O: V \to V$ be a linear operator. Then $\eta_U := U^\dagger \eta U$ is a Hermitian linear automorphism, and O is η-pseudo-Hermitian if and only if $O_U := U^\dagger O U$ is η_U-pseudo-Hermitian. In other words, the notion of pseudo-Hermiticity is unitary-invariant.

Proof: First we recall that because U is unitary, η_U is both Hermitian and invertible. Furthermore, we have

$$\eta_U^{-1} O_U^\dagger \eta_U = U^\dagger \eta^{-1} U U^\dagger O^\dagger U U^\dagger \eta U = U^\dagger (\eta^{-1} O^\dagger \eta) U.$$

□

Proposition 6: Let V be an inner product space, η_1 and η_2 be Hermitian linear automorphisms, and $O: V \to V$ be a linear operator. Then the η_1-pseudo-Hermitian adjoint of O coincides with its η_2-pseudo-Hermitian adjoint if and only if $\eta_2^{-1}\eta_1$ commutes with O.

Proof: This statement holds because $\eta_1^{-1} O^\dagger \eta_1 = \eta_2^{-1} O^\dagger \eta_2$ implies $O^\dagger \eta_1 \eta_2^{-1} = \eta_1 \eta_2^{-1} O^\dagger$. Taking the Hermitian adjoint of this relation yields $[O, \eta_2^{-1}\eta_1] = 0$. □

Corollary: If the Hamiltonian H of a quantum system is pseudo-Hermitian with respect to two different Hermitian linear automorphisms η_1 and η_2 of the Hilbert space, then $\eta_2^{-1}\eta_1$ is a symmetry of the system. Conversely, let η be a Hermitian linear automorphism of the Hilbert space, G be a symmetry group of the system whose elements g are represented by invertible linear operators. Then ηg is a Hermitian linear automorphism and H is ηg-pseudo-Hermitian provided that $g^\dagger \eta g = \eta$.

Proof: This is a direct implication of Proposition 6 and the definition of the symmetry, namely $[g, H] = 0$ or equivalently $g^{-1} H g = H$.[25]

III. PSEUDO-HERMITIAN HAMILTONIANS WITH A COMPLETE BIORTHONORNAL EIGENBASIS

Let H be an η-pseudo-Hermitian Hamiltonian with a complete biorthonormal eigenbasis $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ and a discrete spectrum.[26] Then, by definition,

$$H|\psi_n,a\rangle=E_n|\psi_n,a\rangle,\quad H^\dagger|\phi_n,a\rangle=E_n^*|\phi_n,a\rangle, \tag{11}$$

$$\langle\phi_m,b|\psi_n,a\rangle=\delta_{mn}\delta_{ab}, \tag{12}$$

$$\sum_n\sum_{a=1}^{d_n}|\phi_n,a\rangle\langle\psi_n,a|=\sum_n\sum_{a=1}^{d_n}|\psi_n,a\rangle\langle\phi_n,a|=1, \tag{13}$$

where d_n is the multiplicity (degree of degeneracy) of the eigenvalue E_n, and a and b are degeneracy labels.

Proposition 7: Let H be a pseudo-Hermitian Hamiltonian with these properties. Then the nonreal eigenvalues of H come in complex conjugate pairs with the same multiplicity.

Proof: According to Eqs. (5) and (11),

$$H(\eta^{-1}|\phi_n,a\rangle)=\eta^{-1}H^\dagger|\phi_n,a\rangle=E_n^*(\eta^{-1}|\phi_n,a\rangle). \tag{14}$$

Because η^{-1} is invertible, $\eta^{-1}|\phi_n,a\rangle\neq 0$ is an eigenvector of H with eigenvalue E_n^*. More generally, η^{-1} maps the eigensubspace associated with E_n to that associated with E_n^*. Again, because η^{-1} is invertible, E_n and E_n^* have the same multiplicity. □

Next, we use the subscript "$_0$" to denote real eigenvalues and the corresponding basis eigenvectors and the subscript "$_\pm$" to denote the complex eigenvalues with $\pm$ imaginary part and the corresponding basis eigenvectors. Then in view of Eqs. (11)–(14), we have

$$1=\sum_{n_0}\sum_{a=1}^{d_{n_0}}|\psi_{n_0},a\rangle\langle\phi_{n_0},a|+\sum_{n_+}\sum_{\alpha=1}^{d_{n_+}}(|\psi_{n_+},\alpha\rangle\langle\phi_{n_+},\alpha|+|\psi_{n_-},\alpha\rangle\langle\phi_{n_-},\alpha|), \tag{15}$$

$$H=\sum_{n_0}\sum_{a=1}^{d_{n_0}}E_{n_0}|\psi_{n_0},a\rangle\langle\phi_{n_0},a|+\sum_{n_+}\sum_{\alpha=1}^{d_{n_+}}(E_{n_+}|\psi_{n_+},\alpha\rangle\langle\phi_{n_+},\alpha|+E_{n_+}^*|\psi_{n_-},\alpha\rangle\langle\phi_{n_-},\alpha|). \tag{16}$$

Repeating the calculation leading to Eq. (14), we find

$$\eta^{-1}|\phi_{n_0},a\rangle=\sum_{b=1}^{d_{n_0}}c_{ba}^{(n_0)}|\psi_{n_0},b\rangle,\quad c_{ab}^{(n_0)}:=\langle\phi_{n_0},a|\eta^{-1}|\phi_{n_0},b\rangle, \tag{17}$$

$$\eta^{-1}|\phi_{n_+},\alpha\rangle=\sum_{\beta=1}^{d_{n_+}}c_{\beta\alpha}^{(n_+)}|\psi_{n_-},\beta\rangle,\quad c_{\alpha\beta}^{(n_+)}:=\langle\phi_{n_-},\alpha|\eta^{-1}|\phi_{n_+},\beta\rangle, \tag{18}$$

$$\eta^{-1}|\phi_{n_-},\alpha\rangle=\sum_{\beta=1}^{d_{n_+}}c_{\beta\alpha}^{(n_-)}|\psi_{n_+},\beta\rangle,\quad c_{\alpha\beta}^{(n_-)}:=\langle\phi_{n_+},\alpha|\eta^{-1}|\phi_{n_-},\beta\rangle, \tag{19}$$

where $c_{ab}^{(n_0)}$ and $c_{\alpha\beta}^{(n_\pm)}$ are complex coefficients. The latter may be viewed as entries of complex matrices $c^{(n_0)}$ and $c^{(n_\pm)}$, respectively. Because η and consequently η^{-1} are Hermitian operators, so are the matrices $c^{(n_0)}$ and $c^{(n_\pm)}$. In particular, we can make a unitary transformation of the Hilbert space to map the biorthonormal system of eigenbasis vectors of the Hamiltonian to a new system in which these matrices are diagonal. We can further rescale the basis vectors so that $c^{(n_0)}$

and $c^{(n_\pm)}$ become identity matrices. In the following we shall assume, without loss of generality, that such a transformation has been performed. Then, Eqs. (17)–(19) take the form

$$|\phi_{n_0},a\rangle=\eta|\psi_{n_0},a\rangle,\quad |\phi_{n_\pm},\alpha\rangle=\eta|\psi_{n_\mp},\alpha\rangle. \tag{20}$$

In particular, combining this result with Eq. (12), we have the following η-orthonormalization of the eigenvectors of H

$$\langle\!\langle\psi_{n_0},a|\psi_{m_0},b\rangle\!\rangle_\eta=\delta_{n_0,m_0}\delta_{ab},\quad \langle\!\langle\psi_{n_\pm},\alpha|\psi_{m_\mp},\beta\rangle\!\rangle_\eta=\delta_{n_\pm,m_\mp}\delta_{\alpha\beta}. \tag{21}$$

Next, we solve Eq. (20) for $|\psi_{n_0}\rangle$ and $|\psi_{n_\pm}\rangle$ and substitute the result in Eq. (15). This leads to an explicit expression for η that can be easily inverted to yield η^{-1}. The result is

$$\eta=\sum_{n_0}\sum_{a=1}^{d_{n_0}}|\phi_{n_0},a\rangle\langle\phi_{n_0},a|+\sum_{n_+}\sum_{\alpha=1}^{d_{n_+}}(|\phi_{n_-},\alpha\rangle\langle\phi_{n_+},\alpha|+|\phi_{n_+},\alpha\rangle\langle\phi_{n_-},\alpha|), \tag{22}$$

$$\eta^{-1}=\sum_{n_0}\sum_{a=1}^{d_{n_0}}|\psi_{n_0},a\rangle\langle\psi_{n_0},a|+\sum_{n_+}\sum_{\alpha=1}^{d_{n_+}}(|\psi_{n_-},\alpha\rangle\langle\psi_{n_+},\alpha|+|\psi_{n_+},\alpha\rangle\langle\psi_{n_-},\alpha|). \tag{23}$$

One can easily check that the Hamiltonian H and the operators η and η^{-1} as given by Eqs. (16), (22), and (23) satisfy the η-pseudo-Hermiticity condition (5).

The above-mentioned analysis provides the following necessary and sufficient condition for pseudo-Hermiticity.

Theorem: Let H be a non-Hermitian Hamiltonian with a discrete spectrum and a complete biorthonormal system of eigenbasis vectors $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$. Then H is pseudo-Hermitian if and only if one of the following conditions hold

(1) The spectrum of H is real.
(2) The complex eigenvalues come in complex conjugate pairs and the multiplicity of complex conjugate eigenvalues are the same.

Proof: We have already shown in Proposition 7 that pseudo-Hermiticity of H implies at least one of these conditions. To prove that these conditions are sufficient for the pseudo-Hermiticity of H, we use $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ to express H in the form (16) and construct η according to Eq. (22). Then, by construction, H and η satisfy (5). □

This theorem reveals the relevance of the concept of pseudo-Hermiticity to the spectral properties of the PT-symmetric Hamiltonians considered in the literature. To the best of our knowledge, an analogue of this theorem that would apply to arbitrary PT-symmetric Hamiltonians does not exist. A direct implication of this theorem is the following corollary.

Corollary 1: Every non-Hermitian Hamiltonian with a discrete real spectrum and a complete biorthonormal system of eigenbasis vectors is pseudo-Hermitian.

Note that, in general, a non-Hermitian Hamiltonian may not admit a complete biorthonormal system of eigenvectors. The preceding Theorem and Corollary 1 may not apply for these non-Hermitian Hamiltonians.

Corollary 2: Every PT-symmetric Hamiltonian with a discrete spectrum and a complete biorthonormal system of eigenbasis vectors is pseudo-Hermitian.

Proof: This statement follows from the above-presented Theorem and fact that the eigenvalues of every PT-symmetric Hamiltonian with a complete biorthonormal system of eigenbasis vectors come in complex conjugate pairs. To see this, let $|E\rangle$ be an eigenvector of H with eigenvalue E, i.e., $H|E\rangle=E|E\rangle$, and $|E\rangle'\coloneqq PT|E\rangle$. Then

$$H|E\rangle' = H(PT)|E\rangle = (PT)H|E\rangle = (PT)E|E\rangle = E^*(PT)|E\rangle = E^*|E\rangle',$$

where we have made use of the linearlity of P and the antilinearlity of T. □

IV. PSEUDO-HERMITICITY IN MINISUPERSPACE QUANTUM COSMOLOGY

The Wheeler–DeWitt equation (with a particularly simple factor ordering prescription) for a Freedman–Robertson–Walker (FRW) model coupled to a massive real scalar field has the form

$$\left[-\frac{\partial^2}{\partial\alpha^2}+\frac{\partial^2}{\partial\phi^2}+\kappa\, e^{4\alpha}-m^2e^{6\alpha}\phi^2\right]\psi(\alpha,\phi)=0, \tag{24}$$

where $\alpha=\ln a$, a is the scale factor, ϕ is the scalar field, m is the mass of ϕ, and $\kappa=-1,0$, or 1 depending on whether the universe is open, flat, or closed.[27] In the two-component representation developed in Ref. 24, this equation takes the form of the Schrödinger equation: $i\dot\Psi=H(\alpha)\Psi$ where a dot stands for a derivative with respect to α and

$$\Psi=\frac{1}{\sqrt2}\begin{pmatrix}\psi+i\dot\psi\\ \psi-i\dot\psi\end{pmatrix},\quad H=\frac{1}{2}\begin{pmatrix}1+\mathcal{D} & -1+\mathcal{D}\\ 1-\mathcal{D} & -1-\mathcal{D}\end{pmatrix}, \tag{25}$$

$$\mathcal{D}:=-\frac{\partial^2}{\partial\phi^2}+V(\phi,\alpha),\quad V(\phi,\alpha):=m^2e^{6\alpha}\phi^2-\kappa\, e^{4\alpha}. \tag{26}$$

As seen from these equations $\mathcal{D}/2$, up to an unimportant additive scalar, is the Hamiltonian of a ''time-dependent'' simple harmonic oscillator with unit ''mass'' and ''frequency'' $\omega=m\,e^{3\alpha}$, where α and ϕ play the roles of time t and position x, respectively.

It is not difficult to check that the two-component Hamiltonian H is not Hermitian with respect to the L^2-inner product on the space of two-component state vectors Ψ. However, its eigenvalue problem can be solved exactly.[24] For an open or flat FRW universe ($\kappa=-1,0$) the eigenvalues of H are real. For a closed FRW model, there is a range of values of α for which all the eigenvalues are real. Outside this range they come in complex conjugate imaginary pairs. This suggests that H is a pseudo-Hermitian Hamiltonian. In fact, we can easily check that H is an η-pseudo Hermitian Hamiltonian for

$$\eta=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{27}$$

The indefinite inner product corresponding to (27) is nothing but the Klein–Gordon inner product that is invariant under the ''time-translation'' generated by H.

V. PSEUDOSUPERSYMMETRIC QUANTUM MECHANICS

The application of the ideas of supersymmetric quantum mechanics[28] in constructing non-Hermitian PT-symmetric Hamiltonians has been considered in Refs. 3, 7, 13, 17, and 19 and a formulation of PT-symmetric supersymmetry has been outlined in Refs. 14 and 20. In this section, we develop a straightforward generalization of supersymmetric quantum mechanics that applies for pseudo-Hermitian Hamiltonians.

Definition 3: Consider a $\mathbb{Z}_2$-graded quantum system[29] with the Hilbert space $\mathcal{H}_+\oplus\mathcal{H}_-$ and the involution or grading operator τ satisfying

$$\tau=\tau^\dagger=\tau^{-1}\quad\text{and}\quad\forall|\psi_\pm\rangle\in\mathcal{H}_\pm,\quad\tau|\psi_\pm\rangle=\pm|\psi_\pm\rangle. \tag{28}$$

Let η be an even Hermitian linear automorphism (i.e., $[\eta,\tau]=0$) and suppose that the Hamiltonian H of the system is η-pseudo-Hermitian. Then H (alternatively the system) is said to have a pseudo-supersymmetry generated by an odd linear operator $\mathcal{Q}$ $(i.e.,\{\mathcal{Q},\tau\}=0)$ if H and $\mathcal{Q}$ satisfy the pseudosuperalgebra

$$\mathcal{Q}^2=\mathcal{Q}^{\sharp 2}=0, \quad \{\mathcal{Q},\mathcal{Q}^\sharp\}=2H. \tag{29}$$

A simple realization of pseudosupersymmetry is obtained using the two-component representation of the Hilbert space where the state vectors $|\psi\rangle$ are identified by the column vector $\binom{|\psi_+\rangle}{|\psi_-\rangle}$ of their components $|\psi_\pm\rangle$ belonging to $\mathcal{H}_\pm$. In this representation, one can satisfy the η-pseudo-Hermiticity of the Hamiltonian H, [i.e., Eq. (5)] and the pseudosuperalgebra (29) by setting

$$\tau=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \quad \eta=\begin{pmatrix}\eta_+ & 0\\ 0 & \eta_-\end{pmatrix}, \tag{30}$$

$$\mathcal{Q}=\begin{pmatrix}0 & 0\\ D & 0\end{pmatrix}, \quad H=\begin{pmatrix}H_+ & 0\\ 0 & H_-\end{pmatrix}, \tag{31}$$

where $\eta_\pm$ is a Hermitian linear automorphism of $\mathcal{H}_\pm$, $D:\mathcal{H}_+\to\mathcal{H}_-$ is a linear operator, and

$$H_+ := \tfrac{1}{2}D^\sharp D, \quad H_- := \tfrac{1}{2}D\,D^\sharp. \tag{32}$$

Note that, by definition, $\mathcal{Q}^\sharp=\eta^{-1}\mathcal{Q}^\dagger\eta$,

$$D^\sharp=\eta_+^{-1}D^\dagger\eta_-, \tag{33}$$

and that $H_\pm:\mathcal{H}_\pm\to\mathcal{H}_\pm$ are $\eta_\pm$-pseudo-Hermitian Hamiltonians satisfying the intertwining relations

$$D\,H_+=H_-D, \quad D^\sharp H_-=H_+D^\sharp. \tag{34}$$

As a consequence, H_+ and H_- are isospectral, D maps the eigenvectors of H_+ to those of H_-, and $D^\sharp$ does the converse, except for those eigenvectors that are eliminated by these operators. More specifically, suppose that $H_\pm$ has a complete biorthonormal eigenbasis $\{|\psi_n^\pm,a\rangle,|\phi_n^\pm,a\rangle\}$ satisfying

$$H_\pm|\psi_n^\pm,a\rangle=E_n^\pm|\psi_n^\pm,a\rangle, \quad H_\pm^\dagger|\phi_n^\pm,a\rangle=E_n^{\pm *}|\phi_n^\pm,a\rangle.$$

Then, $D|\psi_n^+,a\rangle$ is either zero in which case $E_n^+=0$, or it is an eigenvector of H_- with eigenvalue E_n^+; $D^\sharp|\psi_n^-,a\rangle$ is either zero in which case $E_n^-=0$, or it is an eigenvector of H_+ with eigenvalue E_n^-. Similarly $D^\dagger$ and $D^{\sharp\dagger}$ relate the eigenvectors $|\phi_n^\pm,a\rangle$ of $H_\pm^\dagger$.

An interesting situation arises when one of the automorphisms $\eta_\pm$ is trivial, e.g., $\eta_+=1$. In this case, H_+ is a Hermitian Hamiltonian with a real spectrum, and pseudosupersymmetry implies that the pseudo-Hermitian Hamiltonian H_-—which is generally non-Hermitian—must have a real spectrum as well. This is not the only way to generate non-Hermitian Hamiltonians with a real spectrum. In the next section we shall use pseudo-supersymmetry to construct a class of non-Hermitian Hamiltonians that have a real spectrum.

VI. A CLASS OF NON-HERMITIAN HAMILTONIANS WITH A REAL SPECTRUM

Consider the class of pseudosupersymmetric systems corresponding to the choices:

$$\mathcal{H}_\pm=\mathcal{H}=L^2(\mathbb{R}), \quad \eta_\pm=\pm P, \tag{35}$$

$$D=p+f(x)+ig(x), \tag{36}$$

where f and g are real-valued functions. We can express these functions in the form

$$f(x)=f_+(x)+f_-(x),\quad g(x)=g_-(x)+g_+(x), \tag{37}$$

where f_+ and g_+ are even functions of x, and f_- and g_- are odd functions. In view of Eqs. (35)–(37), (33), and (32), we have

$$D^\sharp=p-f_+(x)+f_-(x)+i[g_+(x)-g_-(x)], \tag{38}$$

$$H_\pm=\tfrac{1}{2}([p+f_-(x)]^2+g'_-(x)\pm g_-^2-f_+^2-i[2g_-(x)f_+(x)\pm f'_+(x)]+K), \tag{39}$$

$$K:=i\{g_+(x),p\}+g_+(x)[2if_-(x)-g_+(x)], \tag{40}$$

where a prime means a derivative and {,} stands for the anticommutator.

Next, we demand that H_+ is a Hermitian Hamiltonian. The necessary and sufficient condition for the Hermiticity of H_+ and non-Hermiticity of H_- is

$$g_+(x)=0,\quad g_-(x)=-\frac{f'_+(x)}{2f_+(x)}. \tag{41}$$

Introducing the even function $\xi(x):=\ln|f_+(x)/\lambda|$ for some $\lambda\in\mathbb{R}-\{0\}$, and using Eqs. (39)–(41), we have

$$H_+=\tfrac{1}{2}([p+f_-(x)]^2+\tfrac{1}{4}\xi'(x)^2-\tfrac{1}{2}\xi''(x)-\lambda^2e^{2\xi(x)}), \tag{42}$$

$$H_-=\tfrac{1}{2}([p+f_-(x)]^2-\tfrac{1}{4}\xi'(x)^2-\tfrac{1}{2}\xi''(x)-\lambda^2e^{2\xi(x)}+2i\lambda e^{\xi(x)}\xi'(x)). \tag{43}$$

By construction, $H_\pm$ are pseudo-Hermitian pseudo-supersymmetric partners. In particular, they are isospectral. H_+ happens to be a Hermitian operator. This implies that the eigenvalues of both H_+ and H_- are real. Furthermore, for $f_-(x)\neq 0$, H_- is not PT-invariant. This is a concrete example of a non-Hermitian Hamiltonian with a real spectrum that fails to be PT-symmetric.

Equation (43) provides a large class of non-Hermitian Hamiltonians with a real spectrum whose members are determined by the choice of functions f_- and ξ. This class includes Hamiltonians with a discrete spectrum. For example let $\xi(x)=-(x/\ell)^{2n}$, where n is a positive integer and ℓ is a positive real parameter with the dimension of length. Then

$$H_\pm=\tfrac{1}{2}[p+f_-(x)]^2+V_\pm(x),$$

$$V_+=\tfrac{1}{2}(n^2\ell^{-4n}x^{4n-2}+n(2n-1)\ell^{-2n}x^{2n-2}-\lambda^2e^{-2\ell^{-2n}x^{2n}}),$$

$$V_-=\tfrac{1}{2}(-n^2\ell^{-4n}x^{4n-2}+n(2n-1)\ell^{-2n}x^{2n-2}-\lambda^2e^{-2\ell^{-2n}x^{2n}}-4i\lambda n\ell^{-2n}x^{2n-1}e^{-\ell^{-2n}x^{2n}}).$$

It is not difficult to see that H_+ is a Hermitian Hamiltonian with a discrete spectrum. Therefore, H_- has a real discrete spectrum as well.

VII. CONCLUSION

In this article, we have introduced the concept of a pseudo-Hermitian operator and showed that the desirable spectral properties attributed to PT-symmetry are in fact consequences of pseudo-Hermiticity of the corresponding Hamiltonians. We have derived various properties of pseudo-Hermitian conjugation and pseudo-Hermitian operators. In particular, we showed how the defining automorphism η is linked to the eigenvectors of an η-pseudo Hermitian Hamiltonian H with a complete biorthonormal eigenbasis. As the corresponding eigenbasis is subject to gauge transformations, the automorphism with respect to which H is pseudo-Hermitian is not unique. This raises the question of the classification of the equivalence classes of automorphisms that lead

to the same notion of pseudo-Hermiticity for a given Hamiltonian. We have given a brief discussion of this problem and showed its connection with symmetries of the Hamiltonian. We have also developed a generalization of supersymmetry that would apply for general pseudo-Hermitian Hamiltonians, and used it to construct a class of pseudo-Hermitian Hamiltonians with a real spectrum.

A particularly interesting result of our investigations is that all the PT-symmetric Hamiltonians that admit a complete biorthonormal eigenbasis are pseudo-Hermitian. In this sense, pseudo-Hermiticity is a generalization of PT-symmetry.

For a PT-symmetric Hamiltonian, the exactness of PT-symmetry implies the reality of the spectrum. More specifically, if an eigenvector $|E\rangle$ is PT-invariant, $PT|E\rangle=|E\rangle$, then the corresponding eigenvalue E is real. A similar condition for a general pseudo-Hermitian Hamiltonian is not known. Pseudo-Hermiticity is only a necessary condition for the reality of the spectrum, not a sufficient condition. In contrast, PT-symmetry is neither necessary nor sufficient. The exact PT-symmetry is a sufficient condition. But for a given PT-symmetric Hamiltonian it is not easy to determine the exactness of PT-symmetry without actually solving the corresponding eigenvalue problem.

We hope that the concepts developed in this article provide the material for a more rigorous study of the foundation of pseudounitary quantum mechanics.

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Asymptotics of bound states and bands for laterally coupled waveguides and layers

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The asymptotics (in the width of windows) of eigenvalues and bands for two-dimensional waveguides and three-dimensional layers coupled through small windows is obtained. The technique is matching of asymptotic expansions of the solutions of boundary value problems. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1425081]

I. INTRODUCTION

The recent development of nanoelectronics allows physicists to create different mesoscopic structures. It stimulates remarkable progress in semiconductor physics. At the same time this progress has brought interesting mathematical problems with direct relevance to physics. The description of ballistic electron transport in many mesoscopic quantum systems reduces to the description of electron wave propagation in a system of waveguides or layers (see, e.g., Refs. 1–5). The problem of bound states for laterally coupled waveguides recently attracted a new wave of interest. This paper deals with different systems of two-dimensional waveguides and three-dimensional layers coupled through small apertures. First, we consider a system of two waveguides Ω_+, Ω_- of widths d_+, d_- coupled laterally through a small window of width $2a$. It has been proved in Ref. 6 that the Dirichlet Laplacian for this system has an eigenvalue λ_a closed to the threshold and it can be estimated as

$$c_1 a^4 \leqslant \frac{\pi^2}{d_+^2} - \lambda_a \leqslant c_2 a^4 \tag{1}$$

for sufficiently small a (the order of this term was found in Ref. 7 on physical level of rigor). Here c_1, c_2 are some constants, $d_+ > d_-$. The authors used variational technique and obtained only estimates and not asymptotics. Analogous estimates were obtained for the case of n coupling windows.[8] The asymptotics of the eigenvalue in question was obtained in Refs. 9 and 10. Some further results are in Ref. 11 (the asymptotics of resonances close to the Nth threshold) and Ref. 12 (the asymptotics of eigenvalues and resonances for curved coupled waveguides). A method of matching the asymptotic expansions (in a) for the corresponding solutions was used. The scheme of matching was a modification of that suggested in Refs. 13 and 14. One can see that there is some correlation between the result and known weak-coupling asymptotics for Schrödinger operators.[15]

In the beginning of the first part of the present paper we describe briefly the procedure and the results of Ref. 10. The result is in good correlation with estimates in Ref. 8. The case of periodic system of coupling openings is considered. In this situation the matching procedure has some new features. The key idea is that it is necessary to consider each fiber (each value of the quasimomentum) separately and to seek the asymptotic expansion not for the eigenvalue but for some function of the eigenvalue of the operator for fixed fiber. The choice of this function is related to

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the behavior of the Green function for spectral parameter tending to the threshold. The asymptotics of edges of the band which tends to the threshold for $a \to 0$ is obtained.

Then, we consider a coupled two-dimensional quantum waveguide and resonator in the presence of a magnetic field. The quantum mechanical Hamiltonian of a free two-dimensional charged particle in a homogeneous magnetic field that is perpendicular to the plane of confinement of the particle is given in Landau's gauge by the following differential expression:

$$h = -\left(\frac{\partial}{\partial x_1} + Bx_2\right)^2 - \frac{\partial^2}{\partial x_2^2}. \tag{2}$$

More precisely, the aforementioned Hamiltonian H is a self-adjoint operator in $L^2(\mathbf{R}^2)$ which is the closure of the symmetric operator h with domain $C_0^\infty(\mathbf{R}^2)$.[16] In (2) B is the magnetic induction, the system of units is chosen so that the charge of the particle and the physical constants c and $\hbar$ are equal to unity, and the mass of the particle is 1/2. We shall deal with the Hamiltonian in the strip and bounded domain with the Dirichlet boundary condition coupled through a small window. The structure of the spectrum of the Schrödinger operator with magnetic field in a single strip was considered in Ref. 17. A shift of the eigenvalue for the resonator caused by coupling is considered.

In the second part of the paper we deal with a system of two layers Ω_+, Ω_- of widths d_+, d_-,

$$\Omega_\pm = \{(x_1, x_2, x_3) \in \mathbf{R}^2 \times [0, \pm d_\pm]\},$$

coupled laterally through small windows. The problem for the case of one coupling aperture ω_a of the diameter $2a$, $\omega_a = a\omega$, was considered in Ref. 8. It has been proved that the Dirichlet Laplacian for this system has an eigenvalue λ_a close to the threshold and there exist positive constants c_1, c_2, such that

$$e^{-c_1 a^{-3}} \leqslant \frac{\pi^2}{d_+^2} - \lambda_a \leqslant e^{-c_2 a^{-3}} \tag{3}$$

for sufficiently small a, $d_+ > d_-$. The authors used a variational technique.

In the present paper we consider the case of finite and infinite (periodic) systems of coupling windows and obtain the asymptotics of the ground state (for N windows) and the asymptotics of the band (for periodic system of windows). Singly periodic and doubly periodic lattices are considered in the case when there are several window centers in the primitive cell of the lattice. The method of matching of the asymptotic expansions (in a) for the corresponding solutions is used. The scheme of matching described previously is modified. The key idea of the improvement is that one should seek the asymptotic expansion not for the eigenvalue in question but for some function of it. The choice of the function is related to the behavior of the Green function (as a function of spectral parameter) near the threshold. This function changes when we come to the case of periodic system of windows. The case of $d_+ = d_-$ is considered too. It is interesting that in this case the asymptotics is not a limit of that for $d_+ \to d_-$, $d_+ > d_-$ (an additional factor appears). An analogous situation was in the case of waveguides (see previous text). The result (for $N = 1$) is compared with estimates in Ref. 8.

II. COUPLED WAVEGUIDES: SINGLE WINDOW AND FINITE NUMBER OF WINDOWS

Let us describe the procedure of the construction of the asymptotic series for the eigenvalue in the simplest case—two waveguides coupled through a single window. The small parameter a is the halfwidth of the opening. Consider the case when $d_+ > d_-$. Let $\lambda_a = k_a^2$ be the eigenvalue in question. We shall seek the asymptotic series of the following form:

$$\left(\frac{\pi^2}{d_+^2} - k_a^2\right)^{1/2} = \sum_{j=2}^{\infty} \sum_{i=0}^{\infty} k_{ji} a^j (\log a)^i. \tag{4}$$

For the corresponding eigenfunction $\psi_a(x)$ the asymptotic series is the following:

$$\psi_a(x)=\left(\frac{\pi^2}{d_+^2}-k_a^2\right)^{1/2}\sum_{j=0}^{\infty} a^j P_{j+1}(D_y,\log a)G^-(x,y,k)\big|_{y=0}, \quad x\in\Omega^- - S_{a^{1/2}}, \tag{5}$$

$$\psi_a(x)=\sum_{j=1}^{\infty}\sum_{i=0}^{[(j-1)/2]} v_{ji}(x/a)a^j(\log a)^i, \quad x\in S_{2a^{1/2}}, \tag{6}$$

$$\psi_a(x)=-\left(\frac{\pi^2}{d_+^2}-k_a^2\right)^{1/2}\sum_{j=0}^{\infty} a^j P_{j+1}(D_y,\log a)G^+(x,y,k)\big|_{y=0}, \quad x\in\Omega^+ - S_{a^{1/2}}, \tag{7}$$

where S_t is the sphere of radius t with the center at the center of the opening,

$$v_{ji}\in W^1_{2,\mathrm{loc}}(\Omega^+\cup\Omega^-), \quad P_1(D_y,\log a)=a^{(1)}_{10}\frac{\partial}{\partial n_y},$$

$P_m(D_y,\log a)$ are some polynomials in normal and tangential derivatives (in respect to y):

$$P_m(D_y,\log a)=\sum_{q=1}^{m-1}\sum_{i=0}^{[q/2]-1} a^{(m)}_{qi}(\log a)^i D_y^{m-q+1}, \quad m\geqslant 2. \tag{8}$$

$G^{\pm}$ are the Green functions for the waveguides $\Omega^{\pm}$. It is known that its derivatives can be represented in close proximity of the point π^2/d_+^2 in the form

$$\begin{aligned} D_y^j G^+(x,0,k)&=\frac{1}{d_+}\sin\frac{\pi x_2}{d_+}D_x^j\left(\sin\frac{\pi x_2}{d_+}\right)\Bigg|_{x_2=0}\left(\frac{\pi^2}{d_+^2}-k_a^2\right)^{-1/2}+\Phi_j(x,k)\log r+g_j^+(x,k)\\ &\quad+\sum_{i=0}^{[j/2]}\sum_{t=0}^{j-2i-1} b^{(j)}_{it}(k)r^{-j+2(i+t)}\sin(j-2i)\theta,\\ D_y^j G^-(x,0,k)&=\Phi_j(x,k)\log r+g_j^-(x,k)+\sum_{i=0}^{[j/2]}\sum_{t=0}^{j-2i-1} b^{(j)}_{it}(k)r^{-j+2(i+t)}\sin(j-2i)\theta, \end{aligned} \tag{9}$$

where (r,θ) are polar coordinates. Terms $b^{(j)}_{it}(k)$, $\Phi_j(x,k)$, $g_j^-(x,k)$ are analytic in respect to k in some neighborhood of the point π/d_+, $\Phi_j\in C^\infty(\mathbf{R}^2)$ and is antisymmetric with respect to x_2, $g_j^{\pm}\in C^\infty(\Omega^{\pm})$,

$$b^{(j)}_{00}=(-1)^{[(j+1)/2]}(j-1)!/\pi, b^{(3)}_{10}=k^2/(2\pi), \Phi_{1n}(0,k)=-k^2/(2\pi). \tag{10}$$

Boundary problems for the coefficients of the series (6) are obtained by the following way. One substitutes the series (6) and (4) [more precisely, not only (4), but also the corresponding series for k_a] into the Helmholtz equation (for $k=k_a$) with the Dirichlet boundary condition. Then one changes the variables: $\xi=x/a$. The coefficients in the terms with identical powers of a and $\log a$ should be equal. Hence, one obtains the following problems:

$$\begin{aligned} \Delta_\xi v_{ji}&=-\sum_{p=0}^{j-3}\sum_{q=0}^{[p/2]-1}\Lambda_{pq}v_{j-p-2,i-q}, \quad \xi\in\mathbf{R}^2\backslash\Gamma,\\ v_{ji}&=0, \quad \xi\in\Gamma, \end{aligned} \tag{11}$$

where

$$\Gamma=\{\xi:\xi_2=0,\xi_1\in(-\infty,-1]\cup[1,\infty)\},$$

Λ_{pq} are the coefficients of the series

$$k_a^2=\sum_p\sum_q\Lambda_{pq}a^p(\log a)^q.$$

Let $\psi_a^{\pm}(x,k)$ be the series (5), (7), $P_m^{(N)}(D_y,\log a)$ the sums of type (8) where the summation limit $m-1$ is replaced by $\min(m-1,N)$, $\Psi_{a,N}^{\pm}$ the series $\psi_a^{\pm}(x,k)$ in which P_j is replaced by $P_j^{(N)}$, $\hat{\psi}_a^{\pm}(x,k)$, $\hat{k}_N(a)$, $\hat{v}_N(\xi,a)$ the partial sums of the corresponding series. Note that Nth finite sums of the series $\psi_a^{\pm}(x,k)$ and $\Psi_{a,N}^{\pm}(x,k)$ coincide because of the definition of $P_j^{(N)}$. Let us define the operator M_{pq} for the sums $U(x,a)$ of the type (5), (7) (for $k=k_a$) in the following manner: decompose the coefficients of $U(x,a)$ in the asymptotic series for $r\to0$, replace the variables ($\xi=x/a$) and, simultaneously, replace $\log r$ by $\log\rho+\log a$, $\rho=|\xi|$. Mark as $M_{pq}(U)$ the sum of all terms of the type $a^p(\log a)^q\phi(\xi)$. Let

$$M_p=\sum_q M_{pq}. \tag{12}$$

Lemma 1: Let k_a have asymptotics given by (4). Define $L_N(\Psi_{a,N}^{\pm}(x,k_a))$ in the following way:

$$L_1(\Psi_{a,1}^{\pm}(x,k_a))=M_1(\Psi_{a,1}^{\pm}(x,k_a)).$$

$$L_N(\Psi_{a,N}^{\pm}(x,k_a))=L_{N-1}(\Psi_{a,N-1}^{\pm}(x,k_a))+M_N(\Psi_{a,N}^{\pm}(x,k_a)).$$

Then for $N\geqslant1$ the following correlations take place:

$$L_N(\Psi_{a,N}^{\pm}(x,k_a))=\sum_{j=1}^{N}\sum_{i=0}^{[(j-1)/2]}V_{ji}^{\pm}(\xi)a^j(\log a)^i,$$

$$L_N(\Psi_{a,N}^{\pm}(x,k_a))-L_N(\hat{\psi}_{a,N}^{\pm}(x,\hat{k}_N(a)))=O(a\rho^{-N}+a^N(\log a)^N\rho^{-1}),$$

$$(L_N(\Psi_{a,N}^{\pm}(x,k_a))-L_N(\hat{\psi}_{a,N}^{\pm}(x,\hat{k}_N(a))))_{\xi_i}=O(a\rho^{-N-1}+a^N(\log a)^N\rho^{-2}),$$

$$\hat{\psi}_{a,N}^{\pm}(x,\hat{k}_N(a))-L_N(\hat{\psi}_{a,N}^{\pm}(x,\hat{k}_N(a)))=O(r^{N+1}+a^{N+1}(\log a)^N),$$

$$(\hat{\psi}_{a,N}^{\pm}(x,\hat{k}_N(a)))_{x_i}-(L_N(\hat{\psi}_{a,N}^{\pm}(x,\hat{k}_N(a))))_{x_i}=O(r^N+a^{N+1}(\log a)^N/r),$$

for $\rho\to\infty,r\to0$, respectively. Series $V_{ji}^{\pm}(\xi)$ does not depend on N, is the asymptotic solution of (11) for $\rho\to\infty$, and $v_{qm}=V_{qm}^{\pm}(\xi)$ in the right-hand side of (11) has a structure:

$$V_{ji}^{\pm}(\xi)=\sum_{q=-p}^{\infty}\rho^{-q}f_{jiq}^{\pm}(\theta)+\log\rho\sum_{q=1}^{p-2}\rho^qF_{jiq}^{\pm}(\theta), \tag{13}$$

where $p=j-2i$, $F_{jiq}^{\pm}(\theta)$, $f_{jiq}^{\pm}(\theta)$ are linear combinations of $\sin m\theta$, and their sums $V_{ji}^{-}(\xi)+V_{ji}^{+}(\xi)$ are polynomials of $j-2i$ order. Series $V_{Ni}^{\pm}(\xi)$ has a form

$$V_{Ni}^{\pm}(\xi)=\hat{V}_{Ni}^{\pm}(\xi)+k_{N+1,i}k_{20}^{-1}(V_{10}^{\pm}(\xi)\pm\widetilde{V_{10}^{\pm}}(\xi))\pm\frac{k_{20}}{\pi}\sum_{i=0}^{[(N-1)/2]}\sum_{j=2}^{\infty}a_{Nl}^{N-1+p}(-1)^{[(j+1)/2]}$$

$$\times(j-1)!\rho^{-j}\sin j\theta,$$

where $\hat{V}^{\pm}_{Ni}(\xi)$ does not depend on $k_{q+1,p}, a^{(m)}_{qp}$ for $q \geqslant N$,

$$\widetilde{V^{\pm}_{10}}(\xi) = \begin{cases} 0, & \xi_2 > 0, \\ \xi_2, & \xi_2 < 0. \end{cases}$$

The proof consists of direct calculations using asymptotics (9) and (10). Thus, to achieve matching it is necessary to show that there exist values k_{ji}, polynomials P_j, and functions v_{ji} being solutions of (11) such that asymptotics of $v_{ji}, \rho \to \infty$, $\xi_2 > 0 (\xi_2 < 0)$, coincides with the series $V^{+}_{ji}(\xi)(V^{-}_{ji}(\xi))$, correspondingly. We confine our attention in the following to the first term k_{20} only.

Using the described procedure, we obtain the following theorem:

Theorem 1: The leading term of the asymptotics of the eigenvalue λ_a which tends to the lower bound of the continuous spectrum is

$$\lambda_a = \begin{cases} \pi^2/d_+^2 - \left(\dfrac{\pi^3}{4d_+^3}\right)^2 a^4 + o(a^4), & d_+ > d_-, \\ \pi^2/d^2 - \left(\dfrac{\pi^3}{2d^3}\right)^2 a^4 + o(a^4), & d_+ = d_- = d. \end{cases} \tag{14}$$

Remark: The case of coupled curved waveguides is considered in Ref. 12.

The procedure is analogous for the case when there are n coupling windows with the centers at the points $(x_q, 0)$, $q = 1, \ldots, n$, of widths $2a_q = 2a\omega_q$, correspondingly. Let $d_+ > d_-$. Formulas (5)–(7) now have the form:

$$\psi_a(x) = \left(\frac{\pi^2}{d_+^2} - k_a^2\right)^{1/2} \sum_{j=0}^{\infty} \sum_{q=1}^{n} a^j P^q_{j+1}(D_y, \log a) G^{-}(x, y, k)\big|_{y=(x_q,0)}, \quad x \in \Omega^{-} \setminus \cup_q S^q_{a^{1/2}}, \tag{15}$$

$$\psi_a(x) = \sum_{j=1}^{\infty} \sum_{i=0}^{[(j-1)/2]} v^q_{ji}(x/a) a^j (\log a)^i, \quad x \in S^q_{2a^{1/2}}, \tag{16}$$

$$\psi_a(x) = -\left(\frac{\pi^2}{d_+^2} - k_a^2\right)^{1/2} \sum_{j=0}^{\infty} \sum_{q=1}^{n} a^j P^q_{j+1}(D_y, \log a) G^{+}(x, y, k)\big|_{y=(x_q,0)}, \quad x \in \Omega^{+} \setminus \cup_q S^q_{a^{1/2}}, \tag{17}$$

where S^q_t is the corresponding sphere with the center at $(x_q, 0)$. Let us choose

$$P^q_1(D_y, \log a) = \alpha_q \frac{d_+}{\pi} \frac{\partial}{\partial n_y},$$

then, we have

$$a^{-1} M^q_1 (\pi^2/d_+^2 - k_a^2)^{1/2} \sum_{p=1}^{n} P^p_1 G^{+}(x, (x_p, 0), k_a) = -\alpha_q \frac{d_+}{\pi^2} k_{20} \xi_2 \rho_q^{-2} - \sum_{p=1}^{n} \alpha_p \frac{\pi}{d_+^2} \xi_2, \tag{18}$$

$$a^{-1} M^q_1 (\pi^2/d_+^2 - k_a^2)^{1/2} \sum_{p=1}^{n} P^p_1 G^{-}(x, (x_p, 0), k_a) = \alpha_q \frac{d_+}{\pi^2} k_{20} \xi_2 \rho_q^{-2}, \tag{19}$$

where ρ_q is the distance from the center of the qth window, M^q_1 is the expression (12) corresponding to the point $(x_q, 0)$. To construct $v^q_{ji}(x/a)$ we use a harmonic function having the following asymptotics:

$$\hat{Y}_1(\xi)=\begin{cases}\sum_{q=1}^{n}\alpha_q\xi_2+\sum_{j=1}^{\infty}c_{1j}^{q}\rho_q^{-j}\sin j\theta_q, & \xi_2>0,\\ -\sum_{j=1}^{\infty}c_{1j}^{q}\rho_q^{-j}\sin j\theta_q, & \xi_2<0.\end{cases} \tag{20}$$

Here the coefficients

$$c_{11}^{q}=\sum_{p=1}^{n}\alpha_p c_{\omega_q},$$

where c_{ω_q} is the harmonic capacity of the corresponding segment in $\mathbf{R}^2$. It is known (Ref. 18) that it is the following:

$$c_{\omega_q}=(\omega_q/2)^2.$$

Making matching of terms of order $\rho_q^{-1}\sin\theta_q$ in neighborhoods of each opening, we obtain the following system for the determination of α_q:

$$\sum_{q=1}^{n}\alpha_q c_{\omega_{qi}}=\frac{d_+^3}{\pi^3}k_{20}\alpha_i, \quad i=1,2,\ldots,n. \tag{21}$$

The condition of nontrivial solvability of (21) is

$$\det\begin{pmatrix} c_{\omega_1}-\beta & c_{\omega_1} & \ldots & c_{\omega_1}\\ c_{\omega_2} & c_{\omega_2}-\beta & \ldots & c_{\omega_2}\\ . & . & . & .\\ c_{\omega_n} & c_{\omega_n} & \ldots & c_{\omega_n}-\beta\end{pmatrix}=0.$$

Here

$$\beta=\frac{d_+^3}{\pi^3}k_{20}.$$

Simple calculations lead to the value of k_{20}:

$$k_{20}=\frac{\pi^3}{d_+^3}\sum_{i=1}^{n}c_{\omega_i}. \tag{22}$$

Other $n-1$ roots of the equation give us $k_{20}=0$. It means that the terms of such order in the asymptotic series do not give us information about other eigenvalues. The obtained value is the leading term of the asymptotics in a of the ground state only. It was shown in Ref. 8 that for sufficiently small a the discrete spectrum contains only one simple eigenvalue. The case of two identical waveguides can be considered in the analogous way. The result is the following theorem.

Theorem 2: The leading term of the asymptotics of the eigenvalue λ_a which tends to the lower bound of the continuous spectrum for the case of n coupling windows is

$$\lambda_a=\begin{cases} \pi^2/d_+^2-\left(\dfrac{\pi^3}{d_+^3}\displaystyle\sum_{i=1}^{n} c_{\omega_i}\right)^2 a^4+o(a^4), & d_+>d_-, \\ \pi^2/d^2-\left(\dfrac{2\pi^3}{d^3}\displaystyle\sum_{i=1}^{n} c_{\omega_i}\right)^2 a^4+o(a^4), & d_+=d_-=d. \end{cases} \tag{23}$$

Remark: Here we deal with the eigenvalue only. That is why we confine our attention to the lower bound of the continuous spectrum only. There are resonances (quasibound states) near other thresholds (lower bounds of other branches of the continuous spectrum). To obtain its asymptotics it is necessary to construct additional terms of the asymptotic expansions. This problem was analyzed in Ref. 11. In the present work we deal with the Dirichlet boundary condition because it is more natural for quantum waveguide. But the suggested approach can be applied to the case of Neumann or Robin boundary conditions too.

III. COUPLED WAVEGUIDES: PERIODIC SYSTEM OF WINDOWS

Consider waveguides coupled through periodic system of windows ($x^q=qL$). In this case consideration has essentially new features. We shall describe these differences and the result. First, we must replace $(\pi^2 d_+^{-2}-k_a^2)^{1/2}$ in (4), (15), and (17) by another function $f(k_a)$ (see the following). Expressions (15) and (17) should be modified in the following way:

$$\psi_a(x)=\pm f(k_a)\sum_{q=-\infty}^{\infty}\alpha_q\frac{\partial}{\partial n_y}G^{\mp}(x,y,k)\big|_{y=(x^q,0)}+o(a^0), \quad x\in\Omega^{\mp}-\cup_q S_{a^{1/2}}^q, \tag{24}$$

Periodicity leads to the Bloch condition, i.e., $\alpha_q=\exp(i\theta Lq)\alpha_0$, where θ is quasimomentum, $-\pi L^{-1}\leqslant\theta\leqslant\pi L^{-1}$. We shall construct the asymptotics in each fiber, i.e., for fixed value of the quasimomentum (the operator for particular fiber has an eigenvalue). Then by varying θ, we shall obtain band parameters. Matching procedure in a neighborhood of each window is analogous to that for the previous case. The sum on the right-hand side of (18) for $q=0$ is replaced by the series

$$\alpha_0\sum_{q=-\infty}^{\infty}\exp(iqL\theta-\gamma L|\theta|)=(\gamma(\cosh(\gamma L)-\cos(\theta L)))^{-1}\sinh(\gamma L)\alpha_0.$$

Due to this fact we choose the function $f(k_a)$ in the following form:

$$f(k_a)=\gamma(\cosh(\gamma L)-\cos(\theta L))(\sinh(\gamma L))^{-1}.$$

The first terms of the asymptotic expansion (in a) of $f(k_a)$ is sought in the form [compare with (4)]:

$$f(k_a)=L^{-1}(1-\cos(\theta L))+k_{20}a^2+o(a^2). \tag{25}$$

Note that the asymptotics of k_a^2 depends on θ, i.e., we seek asymptotics in each fiber separately.

Matching of terms of order a^{-1} is evident, because one has from (24) and (25) only the following terms of this order:

$$\pm(\pi L)^{-1}(1-\cos(\theta L))\alpha_0\xi_2\rho^{-2}, \quad \xi_2>0(\xi_2<0).$$

As for terms of order a, one gets [instead of (18) and (19)]:

$$a^{-1}M_1^0\left(f(k_a)\sum_{p=-\infty}^{\infty}\alpha_p\frac{\partial G^+}{\partial n_y}(x,(x^p,0),k_a)\right)=-\alpha_0\frac{k_{20}}{\pi}\xi_2\rho_q^{-2}-\alpha_0\frac{\pi^2}{d_+^3}\xi_2,$$

$$a^{-1}M_1^0\left(f(k_a)\sum_{p=-\infty}^{\infty}\alpha_p\frac{\partial G^-}{\partial n_y}(x,(x^p,0),k_a)\right)=\alpha_0\frac{k_{20}}{\pi}\xi_2\rho_q^{-2}.$$

Hence, to match increasing at infinity terms we choose the function v_{10}^0 in the form: $v_{10}^0=-\pi^2 d_+^{-3}\alpha_0 Y_1$. Making equal terms of order $\xi_2\rho_q^{-2}$, one gets $k_{20}=\pi^2 d_+^{-3}/4$. Consequently, the leading term of the asymptotics of the eigenvalue in a fiber is obtained from

$$\gamma(\cosh(\gamma L)-\cos(\theta L))(\sinh(\gamma L))^{-1}=\pi^2 d_+^{-3}a^2/4+o(a^2),\quad \gamma=(\pi^2 d_+^{-2}-k_a^2)^{1/2}.$$

To get a band one should vary the quasimomentum θ, $-\pi L^{-1}\leqslant\theta\leqslant\pi L^{-1}$. To estimate the band edges for small a one can replace the function $\cosh(\gamma L)$ [and $\sinh(\gamma L)$] by the first two terms of its Taylor's series. Changes for the case of two identical waveguides are the same as earlier. The result is the following theorem.

Theorem 3: The asymptotics of the edges of the band which tends to the lower bound of the continuous spectrum for the case of periodic system of coupling windows is as follows:

$$\frac{\pi^2}{d_+^2}-\frac{3\pi^3}{2Ld_+^3}a^2+o(a^2)\leqslant\lambda_a\leqslant\frac{\pi^2}{d_+^2}-\frac{\pi^3}{2Ld_+^3}a^2+o(a^2),\quad d_+>d_-,$$

$$\frac{\pi^2}{d^2}-\frac{3\pi^3}{Ld^3}a^2+o(a^2)\leqslant\lambda_a\leqslant\frac{\pi^2}{d^2}-\frac{\pi^3}{Ld^3}a^2+o(a^2),\quad d_+=d_-=d.$$

Remark: One can see that there is a gap in the spectrum for sufficiently small a.

IV. RESONATOR COUPLED WITH A WAVEGUIDE IN A MAGNETIC FIELD

Consider a system of resonator Ω^{in} coupled through small window ω_a of width $2a$ with a waveguide Ω^{ex}. Let λ_0^{in} be an eigenvalue of the Schrödinger operator with a magnetic field in Ω^{in} (without opening) with the Dirichlet boundary condition and ψ_0 be the corresponding eigenfunction. Let λ_0^{in} be less than the threshold for Ω^{ex}. Then, for sufficiently small a one has a perturbed eigenvalue λ_a^{in} for the system of coupled resonator and waveguide. We seek the asymptotics (the main terms) of k_a^{in}, $k_a^{\text{in}}=\sqrt{\lambda_a^{\text{in}}}$ in the form:

$$k_a^{\text{in}}=k_0+k_{20}a^2+o(a^2),\quad k_0=\sqrt{\lambda_0^{in}}. \tag{26}$$

The asymptotic expansion for the corresponding eigenfunction is as follows:

$$\psi_a(x)=\pm(k^2-k_0^2)\alpha\frac{\partial}{\partial n_y}G^{\text{in,ex}}(x,y,k)\big|_{y=(0,0)}+o(a^0),\quad x\in\Omega^{\text{in,ex}}\setminus S_{a^{1/2}}, \tag{27}$$

$$\psi_a(x)=v_{10}(x/a)a+o(a),\quad x\in S_{2a^{1/2}}, \tag{28}$$

where $G^{\text{in,ex}}$ are the Green functions for $\Omega^{\text{in,ex}}$.

The procedure is analogous to that for coupled waveguides. The difference is that for the Green function of the resonator one has another asymptotics:[20]

$$\frac{\partial G^{\text{in}}}{\partial n_y}(x,(0,0),k)=\frac{\psi_{0n}(0)\psi_0(x)}{k^2-k_0^2}-\pi^{-1}r^{-1}\sin\theta+\Phi_1(x,k)\log r+g_1^{\text{in}}(x,k),$$

$$\frac{\partial G^{\text{ex}}}{\partial n_y}(x,(0,0),k)=-\pi^{-1}r^{-1}\sin\theta+\Phi_1(x,k)\log r+g_1^{ex}(x,k),$$

where ψ_{0n} is the normal derivative of ψ_0.

Boundary problems for the coefficients of the asymptotic series (28) (in our case for one term v_{10}) are obtained in the following way. One substitutes the series (26)–(28) into the following equation (for $k=k_a$) [see (2)] (with the Dirichlet boundary condition):

$$-\Delta u-2iB\left(x_2\frac{\partial u}{\partial x_1}+\frac{\partial(x_2u)}{\partial x_2}\right)+(B^2x_2^2-k^2)u=0.$$

Then, one changes the variables: $\xi=x/a$, and obtains

$$-a^{-1}\Delta v_{10}(\xi)-a2iB\xi_2\frac{\partial v_{10}(\xi)}{\partial\xi_1}+(-E_0^+ +a^2B^2\xi_2^2+\cdots)v_{10}(\xi)+\cdots=0.$$

The coefficients in the terms with identical powers of a (and $\log a$ for the next terms) should be equal. Hence, one obtains the following problem for v_{10} (terms of order a^{-1} in the equation):

$$\Delta_\xi v_{10}=0,\quad \xi\in\mathbf{R}^2\backslash\Gamma,\quad v_{10}=0,\quad \xi\in\Gamma, \tag{29}$$

where $\Gamma=\{\xi:\xi_2=0,\xi_1\in(-\infty,-1]\cup[1,\infty)\}$.

Matching of terms of the asymptotic expansions gives one the value of k_{20}:

$$k_{20}=-\frac{\pi|\psi_{0n}(0)|^2}{8k_0}.$$

The result is as follows.

Theorem 4: The leading term of the asymptotics of the perturbed eigenvalue λ_a^{in} has the following asymptotics

$$\lambda_a^{\text{in}}=\lambda_0^{\text{in}}-\frac{\pi|\psi_{0n}(0)|^2}{4}a^2+o(a^2).$$

Remark: The dependence on B is due to the term ψ_{0n}.

Example: Consider circular resonator Ω^{in}. For this case one can find ψ_{0n} explicitly. Let us deal with physical units in the example: m,e are the mass and charge of an electron, respectively, c is the speed of light, $\hbar$ is Planck's constant, $\mathbf{p}=-i\hbar\nabla$, $\mathbf{A}=2^{-1}\mathbf{B}\times\mathbf{r}$. Then the Schrödinger operator with a magnetic field (the Landau operator) is

$$H=\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)^2.$$

Let Ω^{in} be a disk $\Omega^{\text{in}}=\{(r,\varphi):r\leqslant r_0\}$. Introduce the following notation:

$$\omega=\frac{|e\mathbf{B}|}{cm},\quad \lambda=\left(\frac{\hbar c}{|e\mathbf{B}|}\right)^{1/2},\quad x_0=\frac{r_0}{2\lambda^2}.$$

The spectrum of the operator H with the Dirichlet boundary conditions consists of the eigenvalues E_{st},

$$E_{st}=\hbar\omega(2^{-1}(s+|s|+1)-\epsilon_{st}),\quad s=0,\pm1,\pm2,\ldots,\quad t=1,2,\ldots,$$

ϵ_{st} is a root of the equation $\Phi(\epsilon,|s|+1,x_0)=0$. Here $\Phi(a,c,x)=M(a,c,x)$ is the Kummer function. The corresponding eigenfunction $\psi_{(st)}$ is

$$\psi_{(st)}(r,\varphi)=\left(\frac{m\omega}{2\pi\hbar c_{st}}\right)^{1/2}\frac{r^{|s|}}{(2\lambda^2)^{|s|/2}}\exp\left(is\varphi-\frac{r^2}{4\pi\lambda^2}\right)\Phi\left(\epsilon_{st},|s|+1,\frac{r^2}{2\lambda^2}\right),$$

where c_{st} is normalization constant,

$$c_{st}=\int_0^{x_0}\exp(-x)x^{|s|}(\Phi(\epsilon_{st},|s|+1,x))^2\,dx.$$

The Green function has a form

$$G^{\text{in}}(r,\varphi,r',\varphi';\zeta)=\frac{m\omega}{2\pi\hbar}\exp\left(-\frac{r^2+r'^2}{4\lambda^2}\right)\sum_{s=-\infty}^{\infty}\frac{(rr')^{|s|}}{(2\lambda^2)^{|s|}}\exp is(\varphi-\varphi')$$
$$\times\sum_{t=1}^{\infty}\frac{\Phi\left(\epsilon_{st},|s|+1,\frac{r^2}{2\lambda^2}\right)\Phi\left(\epsilon_{st},|s|+1,\frac{r'^2}{2\lambda^2}\right)}{c_{st}(E_{st}-\zeta)}.$$

One sum can be calculated. Let

$$F_s(q,v,\zeta)=\begin{cases}\Phi(\zeta,|s|+1,q)(\Psi(\zeta,|s|+1,v)-\beta\Phi(\zeta,|s|+1,v)), & q\leqslant v\\ \Phi(\zeta,|s|+1,v)(\Psi(\zeta,|s|+1,q)-\beta\Phi(\zeta,|s|+1,q)), & v\leqslant q.\end{cases}$$

Here

$$\beta=\frac{\Psi(\zeta,|s|+1,x_0)}{\Phi(\zeta,|s|+1,x_0)},\quad \zeta\neq\epsilon_{st},$$

$\Psi(a,c,x)$ is the Trikomi function. Then the Green function takes the form

$$G^{\text{in}}(r,\varphi,r',\varphi';\zeta)=\frac{m\omega}{2\pi\hbar}\exp\left(-\frac{r^2+r'^2}{4\lambda^2}\right)\sum_{s=-\infty}^{\infty}\frac{(rr')^{|s|}}{(2\lambda^2)^{|s|}}\exp is(\varphi-\varphi')$$
$$\times\Gamma\left(\frac{1+s+|s|}{2}-\frac{\zeta}{\hbar\omega}\right)F_s\left(\frac{r^2}{2\lambda^2},\frac{r'^2}{2\lambda^2},\frac{1+s+|s|}{2}-\frac{\zeta}{\hbar\omega}\right).$$

V. COUPLED LAYERS: FINITE NUMBER OF WINDOWS

It is proved in Ref. 8 that for the case of one coupling window there exists an eigenvalue which tends to the threshold when $a\to 0$. Consider the case when there are n coupling windows ω_q^a with centers at the points $x^q,x^q\in\{(x_1,x_2,0),x_i\in\mathbf{R}\}$, $q=1,\ldots,n$, $\omega_q^a=a\omega_q$. We assume that the distances between apertures are of order $|\omega_q|^{1/2}$, i.e., a^0. Let $d_+>d_-$. For n windows there are, generally speaking, n eigenvalues in question. Let us construct the asymptotic series for the ground state (minimal eigenvalue). We shall follow the scheme described previously (for coupled waveguides). The difference is that we start from another form of the asymptotic series. Let $\lambda_a=k_a^2$ be the eigenvalue in question. As for the asymptotic series, it is more convenient to seek the series not for λ_a but for some function of it (the reason will be clear later):

$$(\log(\pi^2-k_a^2d_+^2)^{1/2})^{-1}=\sum_{j=3}^{\infty}k_ja^j. \tag{30}$$

In the paper we shall deal with the first term of the series only (it is sufficient to describe the ground state). For the corresponding eigenfunction $\psi_a(x)$ the asymptotic series is as follows:

$$\psi_a(x)=\pm(\log(\pi^2-k_a^2d_+^2)^{1/2})^{-1}\sum_{j=0}^{\infty}\sum_{q=1}^{n}a^j(P_{j+1}^q(D_y)G^{\pm}(x,y,k_a))\big|_{y=(x_q,0,0)},$$

$$x\in\Omega^{\pm}\setminus\cup_q S_{a^{1/2}}^q, \tag{31}$$

$$\psi_a(x)=\sum_{j=1}^{\infty}v_j^q(x/a)a^j,\quad x\in S_{2a^{1/2}}^q, \tag{32}$$

where S_t^q is the sphere of radius t with the center at x^q,

$$v_j^q\in W_{2,\mathrm{loc}}^1(\Omega^+\cup\Omega^-),\quad P_1^q(D_y)=\alpha_q\frac{\partial}{\partial n_y},$$

$P_m^q(D_y)$ is some polynomial in normal and tangential derivatives (in respect to y):

$$P_m^q(D_y)=\sum_{p=1}^{m-1}a_{pq}^{(m)}D_y^{m-q+1},\quad m\geqslant 2. \tag{33}$$

$G^{\pm}$ are the Green functions for the layers $\Omega^{\pm}$. To find the leading term of the asymptotics of the eigenvalue we need the asymptotics of the derivative of the Green function near the point (0) of the boundary for values of spectral parameter in close proximity of the point π^2/d_+^2:

$$\frac{\partial}{\partial n_y}G^+(x,0,k)=\frac{1}{d_+^2}\sin\frac{\pi x_3}{d_+}\log(\pi^2-k_a^2d_+^2)^{1/2}-\frac{x_3}{2\pi r^3}+g^+(x,k), \tag{34}$$

$$\frac{\partial}{\partial n_y}G^-(x,0,k)=\frac{x_3}{2\pi r^3}+g^-(x,k),\quad r=|x|. \tag{35}$$

Here $g^{\pm}(x,k)$ satisfies the Dirichlet boundary condition and is analytic in k in a neighborhood of $\pi^2d_+^{-2}$. The first term of (34) is obtained from the well-known series for the Dirichlet Green function for the layer

$$G^{\pm}(x,y,k)=\sum_{n=1}^{\infty}\frac{2}{d_{\pm}^2}\sin\frac{\pi nx_3}{d_{\pm}}\sin\frac{\pi ny_3}{d_{\pm}}\frac{i}{4}H_0^{(1)}(i(\pi^2n^2d_{\pm}^{-2}-k^2)^{1/2}((x_1-y_1)^2+(x_2-y_2)^2)^{1/2}).$$

Coefficients v_j^q of the series (32) satisfy boundary problems which are obtained during the process of matching in a neighborhood of the qth window in the following way. One substitutes the series (32), (30) and the corresponding series for k_a into the Helmholtz equation (for $k=k_a$) with the Dirichlet boundary condition. Than one changes the variables (in $S_{2a^{1/2}}^q$): $\xi=x/a$. The coefficients in the terms with identical powers of a should be equal. Hence, one obtains the following problems:

$$\begin{gathered}\Delta_{\xi}v_j^q=-\sum_{p=0}^{j-2}\Lambda_pv_{j-p-2}^q,\quad \xi\in\mathbf{R}^3\setminus\gamma,\\ v_j^q=0,\quad \xi\in\gamma,\end{gathered} \tag{36}$$

where

$$\gamma=\{\xi:\xi_3=0,(\xi_1,\xi_2,0)\in\omega_q\},$$

Λ_p are the coefficients of the series

$$k_a^2=\sum_p \Lambda_p a^p.$$

The definition of $M_p^q(U)$ for a neighborhood of the point x^q is analogous to the definition of $M_p(U)$ for the case of waveguides (see previous text). We need M_1^0 because we deal with the leading terms only.

Thus, to achieve matching it is necessary to show that there exist values k_j, polynomials P_j^q, and functions v_j^q being solutions of (36) such that asymptotics of v_j^q, $\rho\to\infty$, $\xi_2>0(\xi_2<0)$, coincides with the corresponding sums obtained from $\psi_a^{\pm}(x,k)$. We confine our attention in the following to the first term k_3 only.

Taking into account the asymptotics of the Green function (34) in a neighborhood of pth window, one obtains

$$\lim_{k\to\pi/d_+} (\log(\pi^2-k^2d_+^2)^{1/2})^{-1}P_1^qG^+(x,x^q,k)=\frac{\alpha_q}{d_+^2}\sin\pi x_3/d_+,$$

$$\lim_{k\to\pi/d_+} (\log(\pi^2-k^2d_+^2)^{1/2})^{-1}P_1^qG^-(x,x^q,k)=0.$$

Taking into account (30), one has ($M_1=M_1^p$):

$$a^{-1}M_1\left((\log(\pi^2-k_a^2d_+^2)^{1/2})^{-1}\sum_{q=1}^n P_1^qG^+(x,x^q,k_a)\right)=-\frac{1}{2\pi}\alpha_pk_3\xi_3\rho_p^{-3}+\sum_{q=1}^n\frac{\pi}{d_+^3}\alpha_q\xi_3, \tag{37}$$

$$a^{-1}M_1\left((\log(\pi^2-k_a^2d_+^2)^{1/2})^{-1}\sum_{q=1}^n P_1^qG^-(x,x^q,k_a)\right)=\frac{1}{2\pi}\alpha_pk_3\xi_3\rho_p^{-3}, \tag{38}$$

where ρ_p is the distance of a point from the center of the pth window.

Boundary problems for v_1^p,v_2^p have homogeneous right-hand sides. To match the increasing term in (37) it is necessary to choose v_1^p as a harmonic function with the corresponding asymptotics. It is known[21,22] that there exists a harmonic function $Y_1^p(\xi)$, satisfying the boundary condition and having the following asymptotics for $\rho_p\to\infty$:

$$Y_1^p(\xi)=\begin{cases}\xi_3+\frac{3}{2}b_{\omega_p}\xi_3\rho_p^{-3}, & \xi_3>0,\\ -\frac{3}{2}b_{\omega_p}\xi_3\rho_p^{-3}, & \xi_3<0.\end{cases} \tag{39}$$

Here b_{ω_p} is average virtual mass for ω_p. We choose v_1^p in the form:

$$v_1^p(\xi)=\frac{\pi}{d_+^3}\sum_{q=1}^n\alpha_qY_1^p(\xi).$$

Achieving matching of terms of order $\rho_p^{-3}\xi_3$ in neighborhoods of each opening, we obtain the following system for the determination of α_q:

$$\frac{3\pi}{2d_+^3}\sum_{q=1}^n\alpha_qb_{\omega_p}=-\frac{k_3}{2\pi}\alpha_p,\quad p=1,2,\ldots,n. \tag{40}$$

The condition of nontrivial solvability of (40) is

$$\det\begin{pmatrix} b_{\omega_1}+\beta & b_{\omega_1} & \dots & b_{\omega_1} \\ b_{\omega_2} & b_{\omega_2}+\beta & \dots & b_{\omega_2} \\ . & . & . & . \\ b_{\omega_n} & b_{\omega_n} & \dots & b_{\omega_n}+\beta \end{pmatrix}=0. \tag{41}$$

Here

$$\beta=\frac{d_+^3}{3\pi^2}k_3.$$

Summing all the rows, and making simple calculations, we get the value of the determinant (41):

$$(-\beta)^{n-1}\left(\sum_{i=1}^{n} b_{\omega_i}+\beta\right).$$

Hence,

$$-\sum_{i=1}^{n} b_{\omega_i}=\frac{d_+^3}{3\pi^2}k_3,$$

and we get, immediately, the value of k_3:

$$k_3=-\frac{3\pi^2}{d_+^3}\sum_{i=1}^{n} b_{\omega_i}. \tag{42}$$

Other $n-1$ roots ($\beta=0$) of Eq. (42) give us $k_3=0$. It means that the terms of such order in the asymptotic series do not give us information about other eigenvalues. The obtained value is the leading term of the asymptotics in a of the ground state only. The situation is analogous to that for coupled waveguides.

In the case of two identical layers $d_+=d_-=d$ we must make some changes. First, the asymptotics (35) for G^- is now similar to that of G^+ (34). As a result, we obtain

$$a^{-1}M_1^p\left((\log(\pi^2-k_a^2d_+^2)^{1/2})^{-1}\sum_{q=1}^{n} P_1^qG^{\pm}(x,x^q,k_a)\right)=\mp\frac{1}{2\pi}\alpha_pk_3\xi_3\rho_p^{-3}\pm\sum_{q=1}^{n}\frac{\pi}{d_+^3}\alpha_q\xi_3, \tag{43}$$

instead of (37) and (38). Hence, we now need a harmonic function $\tilde{Y}_1^p(\xi)$ with another asymptotics then $Y_1^p(\xi)$ in $\rho_p,\rho_p\to\infty$:

$$\tilde{Y}_1^p(\xi)=\begin{cases}\xi_3+3b_\omega\xi_3\rho_p^{-3}, & \xi_3>0,\\ -\xi_3-3b_\omega\xi_3\rho_p^{-3}, & \xi_3<0.\end{cases} \tag{44}$$

Such function exists. One can see that it is related with Y_1^p in a simple way (in terms of complex variables):

$$\tilde{Y}_1^p(z)=Y_1^p(z)+Y_1^p(-z).$$

Making matching as earlier, we obtain

$$k_3=-\frac{6\pi^2}{d^3}\sum_{i=1}^{n} b_{\omega_i}. \tag{45}$$

Remark: The result is not a formal limit of that for two different layers (as in the case of waveguides). From the point of view of physics the effect is related to the fact that for different layers if energy is slightly greater than the threshold there is only one way to go to infinity, and for identical layers there are simultaneously two ways.

Finally, incorporating (41) and (45), we obtain the result:

Theorem 5: The leading term of the asymptotics of the minimal eigenvalue λ_a which tends to the lower bound of the continuous spectrum for the case of n coupling windows is equal to

$$\lambda_a=\begin{cases}\pi^2/d_+^2-\dfrac{1}{d_+^2}\exp\left(-\dfrac{2d_+^3}{3\pi^2}\left(\displaystyle\sum_{i=1}^{n} b_{\omega_i}\right)^{-1}a^{-3}(1+o(1))\right), & d_+>d_-,\\ \pi^2/d^2-\dfrac{1}{d^2}\exp\left(-\dfrac{d^3}{3\pi^2}\left(\displaystyle\sum_{i=1}^{n} b_{\omega_i}\right)^{-1}a^{-3}(1+o(1))\right), & d_+=d_-=d.\end{cases} \tag{46}$$

For the case of circular window ω of radius R the value of average virtual mass is known:[23]

$$b_\omega=\frac{4}{9\pi}R^3.$$

Hence, one obtains the following corollary:

Corollary 1: The leading term of the asymptotics of the minimal eigenvalue λ_a which tends to the lower bound of the continuous spectrum for the case of n coupling circular windows is equal to

$$\lambda_a=\begin{cases}\pi^2/d_+^2-\dfrac{1}{d_+^2}\exp\left(-\dfrac{3d_+^3}{2\pi^2}\left(\displaystyle\sum_{i=1}^{n} a_i^3\right)^{-1}(1+o(1))\right), & d_+>d_-,\\ \pi^2/d^2-\dfrac{1}{d^2}\exp\left(-\dfrac{3d^3}{4\pi^2}\left(\displaystyle\sum_{i=1}^{n} a_i^3\right)^{-1}(1+o(1))\right), & d_+=d_-=d,\end{cases}$$

where a_i is the radius of the disk ω_i^a.

Corollary 2: The leading term of the asymptotics of the eigenvalue λ_a which tends to the lower bound of the continuous spectrum for the case of one coupling window is equal to

$$\lambda_a=\begin{cases}\pi^2/d_+^2-\dfrac{1}{d_+^2}\exp\left(-\dfrac{2d_+^3}{3\pi^2}a^{-3}b_\omega^{-1}(1+o(1))\right), & d_+>d_-,\\ \pi^2/d^2-\dfrac{1}{d^2}\exp\left(-\dfrac{d^3}{3\pi^2}a^{-3}b_\omega^{-1}(1+o(1))\right), & d_+=d_-=d.\end{cases} \tag{47}$$

Remark: One can compare (47) with estimates in Ref. 8 (3).

VI. LAYERS COUPLED THROUGH PERIODIC SYSTEM OF WINDOWS: SINGLY PERIODIC SYSTEM OF WINDOWS

Consider a case when windows form a singly periodic system. Namely, let Λ_1, $\Lambda_1=\{x,x=(qL,0,0),\ q\in\mathbf{Z}\}$ be the corresponding Bravais lattice, and the primitive cell contains the set Z, $Z=\{z^j,\ j=1,2,\ldots,n\}$, $Z^q=\{z^{j,q}=(z_1^j+qL,z_2,z_3),\ q\in\mathbf{Z},\ j=1,2,\ldots,n\}$, of the windows $(\omega_{q,i}^a)$ centers. The windows are $\omega_{q,i}^a=a\,\omega_{q,i}$, $\omega_{0,i}=\omega_i$. Here we have a band instead of an eigenvalue for a single window. Let us construct the asymptotics of its edges.

Due to periodicity the corresponding solution ψ_a satisfies the Bloch condition:

$$\psi_a(x+L)=e^{i\theta L}\psi_a(x),$$

where θ is a quasimomentum ($-\pi L^{-1}\leqslant\theta\leqslant\pi L^{-1}$). For fixed value of the quasimomentum we have an eigenvalue of the corresponding operator in this fiber. We shall construct the asymptotic expansion of the eigenvalues λ_a^θ in each fiber separately, and then by varying θ, we shall get parameters of the band. Let us seek the asymptotic expansion for the following function f_{Λ_1} of $\lambda_a^\theta=k_{a,\theta}^2$:

$$f_{\Lambda_1}(k_{a,\theta})=L\sqrt{\pi^2-k_{a,\theta}^2d_+^2+\theta^2d_+^2}=k_3^\theta a^3+o(a^3). \tag{48}$$

The asymptotic expansion for the corresponding eigenfunction is as follows:

$$\psi_a(x)=\pm f_{\Lambda_1}(k_{a,\theta})\sum_{p=0}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{z^{j,q}\in Z^q}a^j(P_{p+1}^{q,j}(D_y)G^{\pm}(x,y,k_{a,\theta}))\big|_{y=z^{j,q}},\quad x\in\Omega^{\pm}\setminus\cup_q S_{a^{1/2}}^q, \tag{49}$$

$$\psi_a(x)=\sum_{j=1}^{\infty}v_j^q(x/a)a^j,\quad x\in S_{2a^{1/2}}^q, \tag{50}$$

where $P_1^{q,j}(D_y)=\alpha_q^j(\partial/\partial n_y)$ (the Bloch condition leads to the relation: $\alpha_q^j=e^{i\theta Lq}\alpha_0^j$). Following the above-mentioned procedure of matching (see Sec. V), one obtains for the window $\omega_0^{j'}$ ($\rho=\rho_0^{j'}$):

$$a^{-1}M_1\left(f_{\Lambda_1}(k_{a,\theta})\sum_{q=-\infty}^{\infty}\sum_{z^{j,q}\in Z^q}(P_1^{q,j}(D_y)G^-(x,y,k_{a,\theta}))\bigg|_{y=z^{j,q}}\right)=\frac{1}{2\pi}\alpha_0^jk_3^\theta\xi_3\rho^{-3}, \tag{51}$$

$$\begin{aligned}&a^{-1}M_1\left(f_{\Lambda_1}(k_{a,\theta})\sum_{q=-\infty}^{\infty}\sum_{z^{j,q}\in Z^q}(P_1^{q,j}(D_y)G^+(x,y,k_{a,\theta}))\bigg|_{y=z^{j,q}}\right)\\&\quad=-\frac{1}{2\pi}\alpha_0^jk_3^\theta\xi_3\rho^{-3}+\frac{2\pi^2}{d_+^3}a^{-1}M_1\Bigg(f_{\Lambda_1}(k_{a,\theta})\Bigg(-\frac{1}{2\pi}\alpha_0^{j'}\log\sqrt{\frac{\pi^2}{d_+^2}-k_{a,\theta}^2}\\&\qquad+\sum_{z^{j,0}\in Z^0,j\neq j'}\alpha_0^j\frac{i}{4}H_0^{(1)}\left(i|z^{j,0}|\sqrt{\frac{\pi^2}{d_+^2}-k_{a,\theta}^2}\right)\\&\qquad+\sum_{q=1}^{\infty}\sum_{z^{j,q}\in Z^q}\alpha_0^j\cos(q\theta L)\frac{i}{4}H_0^{(1)}\left(i|z^{j,q}|\sqrt{\frac{\pi^2}{d_+^2}-k_{a,\theta}^2}\right)\Bigg)x_3\Bigg).\end{aligned} \tag{52}$$

Let us take into account the following formula:[24]

$$H_0^{(1)}(mR)=J_0(m\rho)H_0^{(1)}(mr)+2\sum_{n=1}^{\infty}J_n(m\rho)H_n^{(1)}(mr)\cos(n\varphi),\quad \rho<r,\quad m\in\mathbf{C},$$

where φ is the angle between the sides ρ and r in the triangle ρ,r,R. We use this relation with $\rho=|z^0|$, $r=|qL|$, $R=|z^q|$,

$$m=i\sqrt{\frac{\pi^2}{d_+^2}-k_{a,\theta}^2}.$$

Then, we use known formula[24]

$$\sum_{n=1}^{\infty}\cos(nb)K_0(nz)=\frac{\pi}{2\sqrt{z^2+b^2}}+\left(C+\log\frac{z}{4\pi}\right)\Big/\,2+\frac{\pi}{2}\sum_{n=1}^{\infty}\left(\frac{1}{\sqrt{(2n\pi-b)^2+z^2}}-\frac{1}{2n\pi}\right)+\frac{\pi}{2}\sum_{n=1}^{\infty}\left(\frac{1}{\sqrt{(2n\pi+b)^2+z^2}}-\frac{1}{2n\pi}\right).$$

One chooses for our case

$$z=L\sqrt{\frac{\pi^2}{d_+^2}-k_{a,\theta}^2},\quad b=L\theta,$$

and taking into account the correlations

$$K_0(z)=\frac{\pi i}{2}H_0^{(1)}(iz),z>0,\quad I_0(z)=J_0(iz),\quad \sqrt{\frac{\pi^2}{d_+^2}-k_{a,\theta}^2}=i\theta+o(a^0),$$

one transforms (52) to the form:

$$a^{-1}M_1\left(f_{\Lambda_1}(k_{a,\theta})\sum_{q=-\infty}^{\infty}\sum_{z^{j,q}\in Z^q}(P_1^{q,j}(D_y)G^+(x,y,k_{a,\theta}))\Big|_{y=z^{j,q}}\right)$$
$$=-\frac{1}{2\pi}\alpha_0^{j'}k_3^{\theta}\xi_3\rho^{-3}+\frac{\pi^2}{2d_+^2}\sum_{z^{j,0}\in Z^0}\alpha_0^jI_0(i\theta|z^{j,0}|)\xi_3. \tag{53}$$

To match the increasing terms in (51) and (53) we choose $v_1^0(\xi)$ in the following form:

$$v_1^0(\xi)=\frac{\pi^2}{2d_+^2}\sum_{z^{j,0}\in Z^0}\alpha_0^jI_0(i\theta|z^{j,0}|)Y_1(\xi). \tag{54}$$

Matching of terms of order $\xi_3\rho^{-3}$, one gets the following system for α_0^j:

$$\frac{k_3^{\theta}}{2\pi}\alpha_0^{j'}=\frac{\pi^2}{2d_+^2}b_{\omega^{j'}}\sum_{z^{j,0}\in Z^0}\alpha_0^jI_0(i\theta|z^{j,0}|),\quad j'=1,\ldots,n. \tag{55}$$

It is analogous to the system (40). The condition of nontrivial solvability of (55) is

$$\det\begin{pmatrix}\beta_1b_{\omega_1}+\beta & \beta_1b_{\omega_1} & \ldots & \beta_1b_{\omega_1}\\ \beta_1b_{\omega_2} & \beta_1b_{\omega_2}+\beta & \ldots & \beta_1b_{\omega_2}\\ . & . & . & .\\ \beta_1b_{\omega_n} & \beta_1b_{\omega_n} & \ldots & \beta_1b_{\omega_n}+\beta\end{pmatrix}=0. \tag{56}$$

Here

$$\beta=-\frac{d_+^2}{\pi^3}k_3^{\theta},\quad \beta_1=\sum_{z^{j,0}\in Z^0}I_0(i\theta|z^{j,0}|).$$

Summing all the rows, and making simple calculations, we get the value of the determinant (56):

$$(-\beta)^{n-1}\left(\beta_1\sum_{i=1}^{n}b_{\omega_i}+\beta\right).$$

Hence,

$$k_3^{\theta}=\frac{\pi^3}{d_+^2}\sum_{z^{j,0}\in Z^0}\sum_{i=1}^{n} I_0(i\theta|z^{j,0}|)b_{\omega_0^i}.$$

For the eigenvalue in a fiber we have

$$\lambda_a^{\theta}=k_{a,\theta}^2=\frac{\pi^2}{d_+^2}+\theta^2-\frac{\pi^6}{d_+^6L^2}\left(\sum_{z^{j,0}\in Z^0}\sum_{i=1}^{n} I_0(i\theta|z^{j,0}|)b_{\omega_0^i}\right)^2 a^6+o(a^6). \tag{57}$$

It is a dispersion relation. To get a band one must vary θ from $-\pi/L$ to π/L. Due to smallness of a one comes to the conclusion that there is no gap ($b_\omega^2\pi^4 d_+^{-6}a^6<1$). But windows cause a shift of the lower bound of the continuous spectrum:

$$\lambda_{\min,a}=\frac{\pi^2}{d_+^2}-\frac{\pi^6}{d_+^6L^2}\left(\sum_{i=1}^{n} nb_{\omega_0^i}\right)^2 a^6+o(a^6). \tag{58}$$

For the case of two identical layers ($d_-=d_+=d$) it is necessary to change the scheme in the same way as for the case of n coupling windows (see previous text). Formally, it means that in (54) Y_1 should be replaced by $\tilde{Y}_1$ and in (57) and (58) b_ω by $2b_\omega$. The following theorem results.

Theorem 6: The lower bound of the continuous spectrum of Dirichlet Laplacian for layers coupled through singly periodic system of windows is as follows:

$$\lambda_{\min,a}=\begin{cases}\dfrac{\pi^2}{d_+^2}-\dfrac{\pi^6n^2}{d_+^6L^2}\left(\displaystyle\sum_{i=1}^{n} b_{\omega_0^i}\right)^2 a^6+o(a^6), & d_+>d_-,\\[2ex] \dfrac{\pi^2}{d^2}-\dfrac{4\pi^6n^2}{d^6L^2}\left(\displaystyle\sum_{i=1}^{n} b_{\omega_0^i}\right)^2 a^6+o(a^6), & d_+=d_-=d.\end{cases}$$

Corollary 3: The lower bound of the continuous spectrum of the Dirichlet Laplacian for layers coupled through singly periodic system of circular windows $\omega_{q,i}^a$ is as follows:

$$\lambda_{\min,a}=\begin{cases}\dfrac{\pi^2}{d_+^2}-\dfrac{16\pi^4n^2}{81d_+^6L^2}\left(\displaystyle\sum_{i=1}^{n} R_i^3\right)^2 a^6+o(a^6), & d_+>d_-,\\[2ex] \dfrac{\pi^2}{d^2}-\dfrac{64\pi^4n^2}{81d^6L^2}\left(\displaystyle\sum_{i=1}^{n} R_i^3\right)^2 a^6+o(a^6), & d_+=d_-=d.\end{cases}$$

Here R_i is the radius of the circle ω_i.

Note that R_i is dimensionless.

VII. LAYERS COUPLED THROUGH PERIODIC SYSTEM OF WINDOWS: DOUBLY PERIODIC SYSTEM OF WINDOWS

Consider the case of doubly periodic system of windows. Namely, we assume that centers of windows form a two-dimensional lattice. Let Λ_2 be the corresponding Bravais lattice

$$\Lambda_2=\{n_1a_1+n_2a_2\in\mathbf{R}^2|(n_1,n_2)\in\mathbf{Z}^2\},$$

where a_1,a_2 are linearly independent vectors in $\mathbf{R}^2$. The reciprocal lattice Γ_2, the Wigner–Seitz cell $\hat{\Gamma}_2$, and the Brillouin zone $\hat{\Lambda}_2$ are, correspondingly,

$$\Gamma_2=\{n_1b_1+n_2b_2\in\mathbf{R}^2|(n_1,n_2)\in\mathbf{Z}^2\},\quad a_jb_{j'}=2\pi\delta_{jj'},\quad j,j'=1,2,$$

$$\hat{\Gamma}_2=\{s_1a_1+s_2a_2\in\mathbf{R}^2|s_j\in[-1/2,1/2),\quad j=1,2\},$$

$$\hat{\Lambda}_2=\{s_1b_1+s_2b_2\in\mathbf{R}^2|s_j\in[-1/2,1/2),\quad j=1,2\}.$$

The scheme of construction of the main term of the asymptotics of the eigenvalue in a fixed fiber (for fixed quasimomentum) is the same as for one-dimensional lattice Λ_1. That is why we shall not describe here the procedure in detail and shall stress only points that differ from that in Sec. VI.

First, we must replace the function $f_{\Lambda_1}(k_{a,\theta})$ for which the asymptotic expansion is sought (48) by another one $f_{\Lambda_2}(k_{a,\theta})$. Let us describe the choice of this function. The form of $f_{\Lambda_1}(k_{a,\theta})$ is related to the behavior of the sum on the right-hand side of (52) for the values of $k_{a,\theta}$ close to the lower bound of the continuous spectrum of the operator in the fiber $(\pi^2/d_+^2+\theta^2)$. In the case of Λ_1 it is as follows:

$$\frac{d_+}{2L\sqrt{\pi^2-k_{a,\theta}^2d_+^2+\theta^2d_+^2}}.$$

That is why we choose $f_{\Lambda_1}(k_{a,\theta})$ in the form:

$$f_{\Lambda_1}(k_{a,})=L\sqrt{\pi^2-k_{a,\infty}^2d_+^2+\theta^2d_+^2}.$$

For two-dimensional lattice we have double series over Λ_2 on the right-hand side of (52), i.e., (52)is replaced by

$$\begin{aligned}
&a^{-1}M_1\left(f_{\Lambda_2}(k_{a,\theta})\sum_{\lambda\in\Lambda_2}a^j(P_1^\lambda(D_y)G^+(x,y,k_{a,\theta}))\Big|_{y=\lambda}\right)\\
&\quad=-\frac{1}{2\pi}\alpha_0k_3^\theta\xi_3\rho^{-3}+\frac{\pi^2}{d_+^3}a^{-1}M_1\left(f_{\Lambda_2}(k_{a,\theta})\left(-\frac{1}{2\pi}\alpha_0^0\log\sqrt{\frac{\pi^2}{d_+^2}-k_{a,\theta}^2}\right.\right.\\
&\qquad\left.\left.+\sum_{\lambda\in\Lambda_2}\sum_{z^{j,q}\in Z^q}\alpha_0^j\frac{i}{4}H_0^{(1)}\left(i|z^{j,q}+\lambda|\sqrt{\frac{\pi^2}{d_+^2}-k_{a,\theta}^2}\right)\right)\exp(i(\theta,\lambda))x_3\right).
\end{aligned}\tag{59}$$

Here θ, λ are two-dimensional vectors, and (θ,λ) is scalar product. The sum of such type appears in the theory of two-dimensional crystals. It can be transformed by Poisson summation formula to the form:[25]

$$\sum_{\gamma\in\Gamma_2}\frac{|\hat{\Lambda}_2|}{4\pi^2(|\gamma+\theta|^2+\pi^2d_+^{-2}-k_{a,\theta}^2)}\sum_{z^{j,0}\in Z^0}\alpha_0^jI_0\left(\sqrt{\frac{\pi^2}{d_+^2}-k_{a,\theta}^2}|z^{j,0}|\right),$$

where $|\hat{\Lambda}_2|$ is the square of the Brillouin zone $\hat{\Lambda}_2$ for Λ_2, $\theta\in\hat{\Lambda}_2$. Hence, we choose the function $f_{\Lambda_2}(k_{a,\theta})$ in the form

$$\begin{aligned}
f_{\Lambda_2}(k_{a,\theta})&=|\hat{\Lambda}_2|^{-1}4\pi^2(|\gamma_\theta+\theta|^2+\pi^2d_+^{-2}-k_{a,\theta}^2),\\
|\gamma_\theta+\theta|^2&=\min_{\gamma\in\Gamma_2}|\gamma+\theta|^2.
\end{aligned}\tag{60}$$

Correspondingly, we seek asymptotic expansion of $f_{\Lambda_2}(k_{a,\theta})$,

$$f_{\Lambda_2}(k_{a,\theta})=k_{3,\theta}^{\Lambda_2}a^3+o(a^3).\tag{61}$$

In (49) $f_{\Lambda_1}(k_{a,\theta})$ is replaced by $f_{\Lambda_2}(k_{a,\theta})$. Then, following the same procedure as for singly periodic lattice (see previous text), one comes to the following expression for $k^{\Lambda_2}_{3,\theta}$:

$$k^{\Lambda_2}_{3,\theta}=\frac{2\pi^3}{d_+^3}\sum_{z^{j,0}\in Z^0} I_0(i\sqrt{|\hat{\Lambda}_2|^{-1}}2\pi|\gamma_\theta+\theta||z^{j,0}|)\sum_{i=1}^{n} b_{\omega_0^i}.$$

Consequently, in accordance with (60) and (61) one gets

$$k^2_{a,\theta}=|\gamma_\theta+\theta|^2+\pi^2 d_+^{-2}-|\hat{\Lambda}_2|\frac{\pi^3}{2d_+^3}\sum_{z^{j,0}\in Z^0} I_0(i\sqrt{|\hat{\Lambda}_2|^{-1}}2\pi|\gamma_\theta+\theta||z^{j,0}|)\sum_{i=1}^{n} b_{\omega_0^i}a^3+o(a^3). \tag{62}$$

Varying the quasimomentum θ, $\theta\in\hat{\Lambda}_2$, one gets a band. One can see that due to smallness of a there is no gap. As a result, we come to the following theorem (the result for two identical layers is obtained in the same way as earlier).

Theorem 7: The lower bound of the continuous spectrum of the Dirichlet Laplacian for layers coupled through doubly periodic system of windows is as follows:

$$\lambda_{\min,a}=\begin{cases}\dfrac{\pi^2}{d_+^2}-|\hat{\Lambda}_2|\dfrac{\pi n}{2d_+^3}\displaystyle\sum_{i=1}^{n} b_{\omega_0^i}a^3+o(a^3), & d_+>d_-,\\[2ex] \dfrac{\pi^2}{d^2}-|\hat{\Lambda}_2|\dfrac{\pi n}{d^3}\displaystyle\sum_{i=1}^{n} b_{\omega_0^i}a^3+o(a^3), & d_+=d_-=d.\end{cases}$$

Corollary 3: The lower bound of the continuous spectrum of the Dirichlet Laplacian for layers coupled through doubly periodic system of circular windows $\omega^a_{q,i}$ is as follows:

$$\lambda_{\min,a}=\begin{cases}\dfrac{\pi^2}{d_+^2}-|\hat{\Lambda}_2|\dfrac{2n}{9d_+^3}\displaystyle\sum_{i=1}^{n} R_i^3a^3+o(a^3), & d_+>d_-,\\[2ex] \dfrac{\pi^2}{d^2}-|\hat{\Lambda}_2|\dfrac{4n}{9d^3}\displaystyle\sum_{i=1}^{n} R_i^3a^3+o(a^3), & d_+=d_-=d.\end{cases}$$

Here R_i is the radius of the circle ω_i.

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Remarks on the lattice Green's function: The Glasser case

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We have investigated the lattice Green's function for the Glasser cubic lattice. Expressions for its density of states, phase shift, and scattering cross section in terms of complete elliptic integrals of the first kind are derived. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421063]

I. INTRODUCTION

The lattice Green's function is defined as

$$G(E)=\frac{\Omega}{(2\pi)^d}\int_{1\mathrm{BZ}}\frac{F(\vec{K})}{E-E(\vec{K})}\vec{\mathrm{d}}k, \tag{1.1}$$

where $E(\vec{k})$ represents a dispersion relation, $F(\vec{k})$ is an appropriate function, Ω denotes the volume of the crystal in the real space, d is the dimension, and 1BZ indicates that the integration is carried over the first Brillouin zone.

In this paper we report on the lattice Green's function and the article is organized as follows. Section II is devoted to the general definition of the diagonal lattice Green's function and its form, inside and outside the band, for the cubic lattice in terms of the first kind elliptic integrals. This section also contains the formulas for the density of states, the phase shift, and the cross section for a point defect case. In Sec. III we present the results and discussion. Finally, the details of the Green's function derivation inside the band are given in the Appendix.

II. LATTICE GREEN'S FUNCTION

The Green's function for the Glasser cubic lattice is defined as[1–5]

$$G^0(E)=\frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\frac{\mathrm{d}k_x\,\mathrm{d}k_y\,\mathrm{d}k_z}{E-E(k_x,k_y,k_z)}, \tag{2.1}$$

where

$$E(k_x,k_y,k_z)=\cos k_x+\cos k_y+\cos k_z+\cos k_x\cos k_y+\cos k_x\cos k_z+\cos k_y\cos k_z+\cos k_x\cos k_y\cos k_z\,.$$

This case is of practical interest in studying the properties of a Heisenberg ferromagnet with axial anisotropy,[1,6]

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$$G^0(E)=\frac{4}{\pi^2(E+1)}K^2(k), \tag{2.2}$$

where

$$k^2=\frac{1}{2}\left[1-\frac{(E-7)^{1/2}}{(E+1)^{1/2}}\right], \tag{2.3}$$

and $K(k)$ is the complete elliptic integral of the first kind.

The Green's function inside and outside the band can be written as[7] (some mathematical manipulations are given in the appendix)

$$G^0(E)=\begin{cases}\dfrac{4}{\pi^2(E+1)}K^2(k), & |E|>7\\ \dfrac{\sqrt{2}}{\pi^2\sqrt{E+1}}K(k_+)K(k_-)+i\dfrac{1}{\sqrt{2}\pi^2\sqrt{E+1}}[K^2(k_+)-K^2(k_-)], & -1<E<7.\end{cases} \tag{2.4}$$

Therefore, the density of states is

$$\mathrm{DOS}^0(E)=\frac{1}{\sqrt{2}\pi^3\sqrt{E+1}}[K^2(k_+)-K^2(k_-)], \tag{2.5}$$

where

$$k_{\pm}^2=\tfrac{1}{2}(1\pm((7-E)/8)^{1/2}). \tag{2.6}$$

We consider the case where perfect periodicity is destroyed by modifying just one site (the L site). The situation can be thought of physically as arising by substituting the host atom at the L site by a foreign atom,[8] i.e., a localized zero-range potential of strength ε' is introduced. In the tight-binding model, ε' is proportional to the charge difference between the impurity outer electrons and those of the host atom. Thus our Green's function for this single impurity is[7,9,10]

$$G(L,E)=\begin{cases}\dfrac{4K^2(k)}{(E+1)\pi^2-4\varepsilon' K^2(k)}, & |E|>7\\ \dfrac{2\sqrt{2}\pi^2(E+1)^{1/2}K(k_+)K(k_-)-2\varepsilon' K^2(k_+)K^2(k_-)-\varepsilon'[(K^4(k_+)+K^4(k_-))]+i\pi^2((E+1)2)^{1/2}[K^2(k_+)-K^2(k_-)]}{[\sqrt{2}\pi^2(E+1)^{1/2}-2\varepsilon' K(k_+)K(k_-)]^2+\varepsilon'^2[(K^2(k_+)-K^2(k_-))]^2}, & |E|<7\end{cases}. \tag{2.7}$$

The density of states can be written as[7,9,10]

$$\mathrm{DOS}^0(E)=\frac{\sqrt{2}\pi(E+1)^{1/2}[K^2(k_+)-K^2(k_-)]}{[\sqrt{2}\pi^2(E+1)^{1/2}-2\varepsilon' K(k_+)K(k_-)]^2+\varepsilon'^2[K^2(k_+)-K^2(k_-)]^2}. \tag{2.8}$$

The S-wave phase shift, δ_0, is defined as[7,9,10]

$$\tan\delta_0=\frac{\pi\mathrm{DOS}^0(E)}{\dfrac{1}{\varepsilon'}-\mathrm{Re}\,G^0(E)}. \tag{2.9}$$

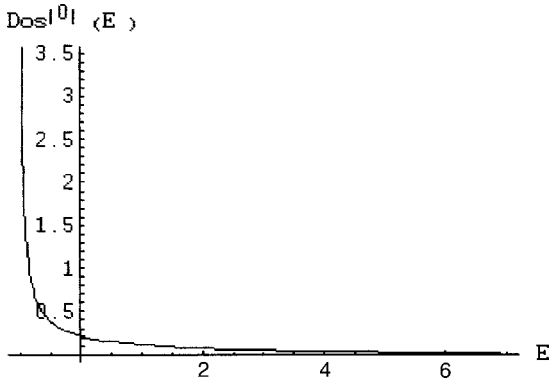

FIG. 1. The density of states (DOS) for the perfect Glasser lattice.

Here, $\mathrm{Re}\,G^0(E)$ refers to the real part of Green's function inside the band. After some mathematical manipulations, we obtain:

$$\tan\delta_0=\frac{K^2(k_+)-K^2(k_-)}{\sqrt{2}(E+1)^{1/2}\pi^2/\varepsilon'-2K(k_+)K(k_-)}. \tag{2.10}$$

The cross section, σ, is defined as[7,9,10]

$$\sigma=\frac{4\pi}{P^2}\frac{\pi^2[\mathrm{DOS}^0(E)]^2}{\left[\mathrm{Re}\,G^0(E)-\dfrac{1}{\varepsilon'}\right]^2+\pi^2[\mathrm{DOS}^0(E)]^2}. \tag{2.11}$$

Here, P refers to the electron momentum.
Therefore, the cross section becomes

$$\sigma=\frac{4\pi}{P^2}\frac{(K^2(k_+)-K^2(k_-))^2}{2\pi^4\left(\dfrac{\sqrt{2}}{\pi^2}K(k_+)K(k_-)-\dfrac{\sqrt{E+1}}{\varepsilon'}\right)^2+(K^2(k_+)-K^2(k_-))^2}. \tag{2.12}$$

III. RESULTS AND DISCUSSION

The results for the Glasser cubic lattice are shown in Figs. 1–8. Figure 1 shows the density of states for the perfect Glasser lattice. It diverges as E goes to minus one and falls off exponentially as expected from Eq. (2.5). The real and imaginary parts of Green's function for the perfect lattice are displayed in Fig. 2, they have the same behavior as noted previously. Figure 3 gives the density

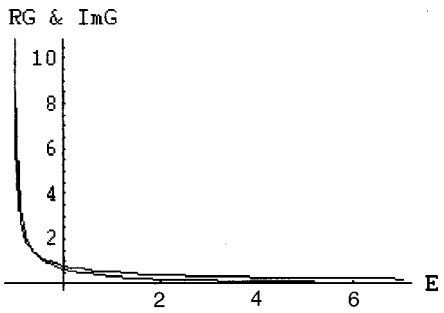

FIG. 2. Real and imaginary parts of Green's function for the perfect Glasser lattice.

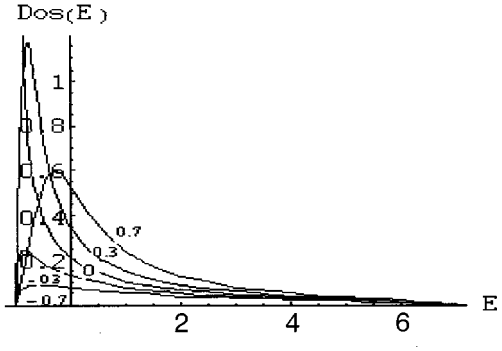

FIG. 3. The DOS for the Glasser lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

of states for the Glasser lattice with a single impurity potential with strength ε' (-0.7, -0.3, 0.0, 0.3, and 0.7). For $\varepsilon'=0.0$ and 0.3 (in arbitrary units), the density of states diverges as E goes to minus one (as previously) and falls off exponentially. The peak value varies with the potential strength and reaches its maximum at $\varepsilon'=0.7$. Figure 4 shows the density of states (DOS) in three dimensions with one axis representing the potential strength ε' varying between -1 and 1 (arbitrary units) whereas the second axis is the energy scale varying between -1 and 7 as indicated in the formalism.

The phase shift, δ_0, is defined as the shift in the phase of the wave function due to the presence of the impurity potential. Figure 5 displays δ_0 for the Glasser lattice with single impurity for different potential strengths ε'. If an attractive potential is turned on, then it gives rise to a positive phase shift and vice versa. That is, a point defect just to the left of the host in the periodic table leads to positive δ_0. The curves are mirror images of each other. The phase shift vanishes as the potential is turned off (perfect lattice); this behavior is clear from the definition of δ_0. In Fig. 6 we have a more general case of the phase shift, δ_0, for the Glasser lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

The cross section, σ, can be defined as the area an impurity atom presents to the incident electron. It is related to some physical quantities such as the conductivity in metals. Figure 7 shows the cross section, σ, for the Glasser lattice with single impurity for different potential strengths ε'. The values are all positive since σ can be viewed as a sort of probability. The cross

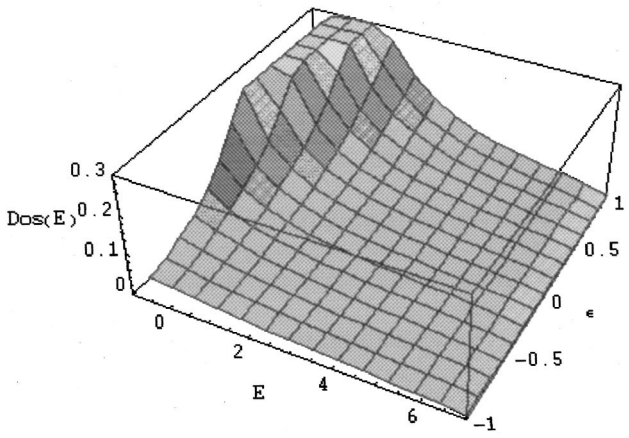

FIG. 4. Three-dimensional DOS for the Glasser lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

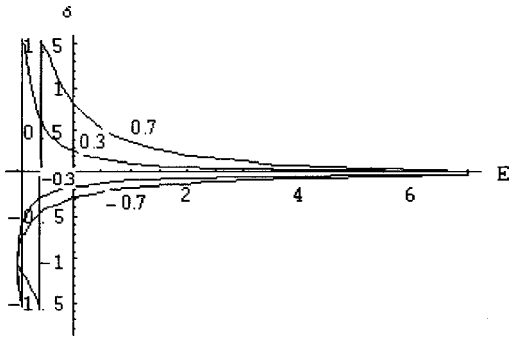

FIG. 5. The phase shift for the Glasser lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

section vanishes for a perfect lattice as expected. Figure 8 displays the cross section, σ, in three dimensions for the Glasser lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

APPENDIX: DERIVATION OF GREEN'S FUNCTION FOR THE GLASSER LATTICE

In this Appendix we derive an expression for Green's function inside the band in terms of complete elliptic integral of the first kind.

Green's function for the Glasser lattice outside the band is given by[3,4,7]

$$G^0(E)=\frac{4K^2(k)}{\pi^2(E+1)}, \tag{A1}$$

where

$$k=\sqrt{\frac{1}{2}[1-\sqrt{1-\beta^{-1}}]}, \quad \beta=\frac{E+1}{8}<1.$$

The complete elliptic integral of the first kind is expressed as

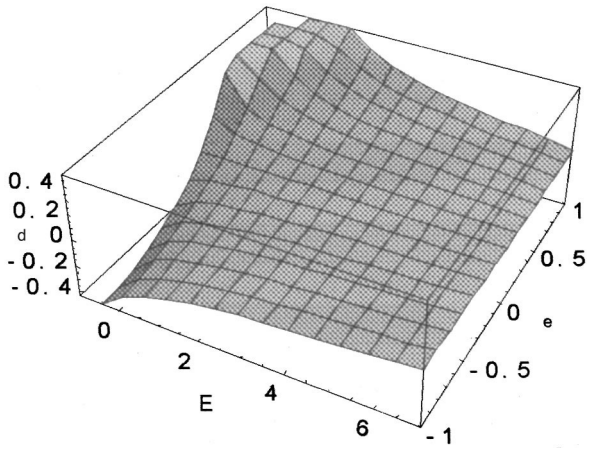

FIG. 6. The phase shift, δ_0, for the Glasser lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

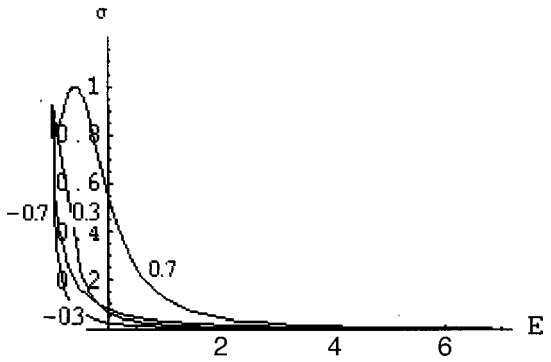

FIG. 7. The cross section, σ, for the Glasser lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

$$K(k)=\frac{\pi}{2}{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;k^2\right), \tag{A2}$$

where
${}_2F_1(\frac{1}{2},\frac{1}{2};1;k^2)$ is the Gauss hypergeometric function.

Kummer's identity is[11]

$${}_2F_1(\tfrac{1}{4},\tfrac{1}{4};1;\beta^{-1})={}_2F_1(\tfrac{1}{2},\tfrac{1}{2};1;\tfrac{1}{2}(1-\sqrt{1-\beta^{-1}})). \tag{A3}$$

Substituting (A3) in (A1) we have

$$G^0(E)=\frac{({}_2F_1(\frac{1}{4},\frac{1}{4};1;\beta^{-1}))^2}{(E+1)}. \tag{A4}$$

Using the following transformations:[12]

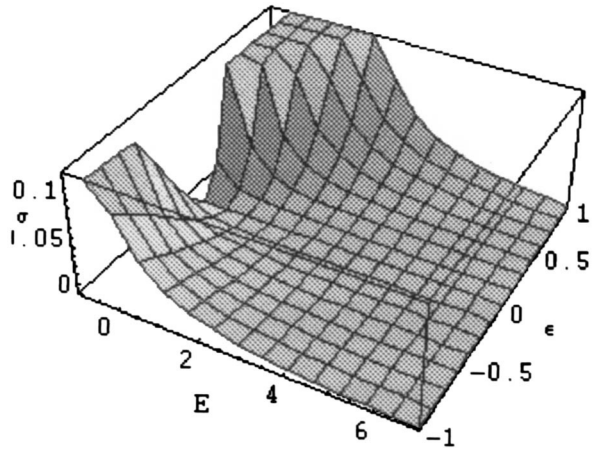

FIG. 8. The cross section, σ, in three dimensions for the Glasser lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

$$ {}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta^{-1}\right)=\beta^{1/4}\left(\frac{(\Gamma(\frac{1}{4}))^2}{2\pi^{3/2}}\,{}_2F_1\left(\frac{1}{4},\frac{1}{4};\frac{1}{2};1-\beta\right)+2\pi^{1/2}\frac{\sqrt{\beta-1}}{(\Gamma(\frac{1}{4}))^2}\,{}_2F_1\left(\frac{3}{4},\frac{3}{4};\frac{3}{2};1-\beta\right)\right), \tag{A5} $$

with

$$ \frac{(\Gamma(\frac{1}{4}))^2}{\pi^{3/2}}\,{}_2F_1\left(\frac{1}{4},\frac{1}{4};\frac{1}{2};1-\beta\right)={}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1+\sqrt{1-\beta})\right)+{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1-\sqrt{1-\beta})\right), \tag{A6} $$

and

$$ \frac{4\pi^{1/2}\sqrt{1-\beta}}{(\Gamma(\frac{1}{4}))^2}\,{}_2F_1\left(\frac{3}{4},\frac{3}{4};\frac{3}{2};1-\beta\right)={}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1-\sqrt{1-\beta})\right) $$
$$ -{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1+\sqrt{1-\beta})\right), \tag{A7} $$

in (A5) we obtain

$$ {}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta^{-1}\right)=\frac{\beta^{1/4}}{2}\left((1+i)\,{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1+\sqrt{1-\beta})\right)\right. $$
$$ \left.+(1-i)\,{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1-\sqrt{1-\beta})\right)\right), \tag{A8} $$

or in terms of complete elliptic integral of the first kind

$$ {}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta^{-1}\right)=\frac{\beta^{1/4}}{\pi}((1+i)K(k_+)+(1-i)K(k_-)), \tag{A9} $$

where

$$ k_{\pm}^2=\frac{1}{2}(1\pm\sqrt{1-\beta}). $$

Substituting (A9), in (A4) then we obtain

$$ G^0(E)=\frac{\beta^{1/2}}{\pi^2(E+1)}((1+i)K(k_+)+(1-i)K(k_-))^2, \tag{A10} $$

then

$$ G^0(E)=\frac{1}{\sqrt{2}\pi^2\sqrt{E+1}}(2K(k_+)K(k_-)+i(K^2(k_+)-K^2(k_-))). \tag{A11} $$

If a single impurity characterized by a localized potential is introduced in the perfect lattice, then according to Dyson's equation Green's function is defined as[8]

$$ G(L,E)=\frac{G^0(E)}{1-\varepsilon' G^0(E)}. \tag{A12} $$

After some mathematical manipulation Eq. (A12) becomes.

$$G(L,E)$$
$$= \frac{2\pi^2\sqrt{2(E+1)}K(k_+)K(k_-) - 2\varepsilon' K^2(k_+)K^2(k_-) + i\pi^2\sqrt{2(E+1)}(K^2(k_+) - K^2(k_-)) - \varepsilon'[K^4(k_+) + K^4(k_-)]}{(\pi^2\sqrt{2(E+1)} - 2\varepsilon' K(k_+)K(k_-))^2 + \varepsilon'^2(K^2(k_+) - K^2(k_-))^2}. \tag{A13}$$

Thus, the *S*-phase shift and scattering cross section can be evaluated in terms of complete elliptic integrals of the first kind as shown in the text.

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Infinite infrared regularization and a state space for the Heisenberg algebra

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We present a method for the construction of a Krein space completion for spaces of test functions, equipped with an indefinite inner product induced by a kernel which is more singular than a distribution of finite order. This generalizes a regularization method for infrared singularities in quantum field theory, introduced by Morchio and Strocchi, to the case of singularities of infinite order. We give conditions for the possibility of this procedure in terms of local differential operators and the Gelfand–Shilov test function spaces, as well as an abstract sufficient condition. As a model case we construct a maximally positive definite state space for the Heisenberg algebra in the presence of an infinite infrared singularity. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1425427]

I. INTRODUCTION

A notable case in which some of the abundant singularities of quantum field theory can be treated rigorously is presented by the method of infrared regularization of Morchio and Strocchi.[1,2] There, the first-order singularity of the two-point function of the massless scalar field in $1+1$-dimensional space–time manifests itself in the nonpositivity of the Wightman inner product on the one-particle space. In momentum space, this two-point function appears as a singular integral kernel which is regularized in the distributional sense as a Cauchy principal value. Since this regularization involves subtraction of values of the test functions at $p=0$, the Wightman inner product induced by the two-point function is clearly no longer positive definite. It turns out that, if the usual positivity axiom of Wightman theory, see Ref. 3, is replaced by a weaker Hilbert space structure condition, the construction of a suitable physical state space is still possible. The one-particle space becomes a Krein space, the natural analogon of a Hilbert space in the case of an indefinite inner product, and it is maximal in the sense that there is no larger Krein space closure of the test function space (we refer to Appendix B, where some basic notions of, and results on, indefinite inner product spaces are gathered). Thus, no physical information gets lost and one can identify a positive definite physical Hilbert subspace. In fact, in the case treated in Refs. 1 and 2 the rank of negativity is one, and thus the Krein space is actually a Pontryagin space. In Ref. 4, we have cast this procedure in abstract form, yielding a method by which every quasipositive space, i.e., a space with finite rank of negativity, can be completed to a Pontryagin space. By this, we generalized the infrared regularization method to singularities of the type of finite order distributions. On the other hand it is by now well known that constructive approaches to interacting quantum fields generically involve much more singular objects, see Refs. 5 and 6, namely ultradistributions and even Fourier hyperfunctions.[7,8] Thus, it is natural to look for a further generalization of the procedure for finding a maximal Krein space closure starting from a space of test functions with an indefinite inner product induced by a singular kernel, to the case of nondistributional infinite order singularities, and therefore to the case of an infinite number of negative degrees of freedom. This is what we will present in the following.

We illustrate the regularization method by a neat (yet unphysical) model in which infinite

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order singularities appear naturally, at least on a heuristic level. (We tend to denote the whole process of defining an indefinite inner product by a generalized function *and* the construction of a maximal Krein space closure as ''regularization.'' The first step, which is the traditional regularization of a singular integral, means going only half way toward a physically conclusive result.) Namely, we will consider the Schrödinger representation of the Heisenberg algebra on a test function space over $\mathbb{R}$ in the presence of a singularity concentrated at $p=0$. This model will be informally described in Sec. II, where also some notions needed subsequently are introduced. Further, we will state the main result, which is that the regularization procedure yields a maximal Krein space and in it a largest possible, positive definite, closed subspace, which can sensibly be considered as the ''physical state space'' for the Heisenberg algebra of ''observables.''

Section III contains the regularization procedure proper. It shows in particular that there is a certain balance that has to be kept between the singularity of the inner product, measured in terms of infinite order (local) differential operators, and the choice of test function space, which we express in terms of the Gelfand–Shilov scheme of spaces, see Ref. 9, Chap. IV. The method itself is, however, general enough to be applied to a much wider class of singularities than infrared ones, and for a lot of other test function spaces.

In Sec. IV, we formulate abstractly a sufficient condition under which the regularization is guaranteed to work. The conditions we give are not the most general and abstract ones possible, since they reflect the limitations of the procedure of Sec. III. Therefore they present no sharp criterion to decide whether an indefinite space admits the construction of a maximal majorant topology by our construction of a Hilbert majorant. Nevertheless, they capture the essential points that enable our construction, and therefore are at least useful to explain the mechanism behind it. Furthermore, our conditions are simple enough to be effective in many concrete cases. We discuss possible further generalizations at the end of Sec. IV.

Appendix A contains a simple, concrete construction of certain neutral elements, i.e., vectors with vanishing inner product, which play an important role in the regularization procedure in Sec. III. Appendix B compiles some basics about indefinite inner product spaces mainly taken from Ref. 10.

II. THE MODEL

Recently, a comprehensive abstract classification of representations of the Heisenberg algebra on an indefinite inner product space has been worked out by Mnatsakanova *et al.* in Ref. 11. There, it was pointed out that this issue is somewhat more difficult to handle than in the positive definite case, which is covered by the Stone–von Neumann uniqueness theorem, see Ref. 12, Chap. IV. Especially, domain questions appear and the notion of irreducibility has to be reconsidered. Here, we take a different approach in considering a very concrete example where the Heisenberg representation is from the beginning assumed to be the quantum mechanical Schrödinger representation

$$\hat{q} \overset{\text{def}}{=} x\cdot, \qquad \hat{p} \overset{\text{def}}{=} -i\frac{d}{dx},$$

on a function space over $\mathbb{R}$.

The following discussion will take place in momentum space, and we will notoriously denote the Fourier transforms of functions with *f, g,* etc., and the variable by *p*. Consider the indefinite inner product

$$\langle f,g\rangle \overset{\text{def}}{=} (f,g)_{L^2} - \sum_{k=0}^{\infty} c_k^2 \overline{f^{(k)}}(0) g^{(k)}(0), \tag{1}$$

with real coefficients c_k (this will turn out to pose no essential restriction in our case, see the following). It can be formally interpreted as being induced by a generalized function (a kernel) on $\mathbb{R}^2$ in the following way:

$$\langle f,g\rangle = (\delta(p-p')-J(\partial_p\partial_{p'})\delta(p)\delta(p'),\overline{f}(p)g(p')). \tag{2}$$

Here, the infinite order differential operator J is given by its symbol

$$J(\xi)\overset{\text{def}}{=}\sum_{k=0}^{\infty} c_k^2\xi^k.$$

The singularity in $\langle .,.\rangle$ can be characterized by the following notion, where we have already adapted the conventional notation a bit, so as to conform with our application in Sec. III:

Definition and Remark 2.1 (Ref. 9, 159 pp.): An entire function $J(\xi)$ in the complex variable ξ is called *infraexponential of order* $1/(2\delta)$ if it fulfills for every $\varepsilon>0$ an estimate

$$|J(\xi)|\leqslant C_\varepsilon e^{\varepsilon|\xi|^{1/(2\delta)}}$$

for some $C_\varepsilon>0$. In this case, the coefficients c_k^2 of the Taylor series of J satisfy the following upper bounds: For every $D>0$ exists a $\theta\in(0,1)$ and a $C>0$ such that

$$|c_k^2|\leqslant C\frac{\theta^k}{D^k e^{2k\delta}k^{2k\delta}}. \tag{3}$$

Now, our first concern is on which test function space the inner product can be defined. To this end, we use the Gelfand–Shilov scheme for the classification of spaces of smooth functions, see Ref. 9, Chap. IV. For $0\leqslant\alpha,\ \beta\leqslant\infty$ the space $\mathscr{S}_\alpha^\beta(\mathbb{R})$ consists of smooth functions f on $\mathbb{R}$ satisfying estimates

$$|p^q f^{(k)}(p)|\leqslant CA^qB^kq^{q\alpha}k^{k\beta}.$$

We need in fact only consider the regularity of the functions in $\mathscr{S}_\alpha^\beta(\mathbb{R})$ at the origin, which is expressed in the following basic estimate: There exists a $B>0$ such that for all $\rho>0$ and a constant C_f depending on f we have

$$|f^{(k)}(0)|\leqslant C_f(B+\rho)^k k^{k\beta}. \tag{4}$$

It is apparent from (3) and (4) that the indefinite inner product is well-defined on $\mathscr{S}_\alpha^\beta$ by (1) as the distribution (2), whenever J is infraexponential of order $\leqslant 1/(2\beta)$. We denoted by $\mathcal{V}=\mathcal{V}_J(\alpha,\beta;\rho)$ a space $\mathscr{S}_\alpha^\beta$ equipped with an indefinite inner product (1) defined by an infraexponential symbol J of order $1/(2\delta)$ for any $\delta\leqslant\beta$.

Further constraints on the choice of test function space now come from the intended Schrödinger representation of the Heisenberg algebra. As the Heisenberg generators act in momentum space by multiplication with p and differentiation id/dp, it is clear that they will not be symmetric operators with respect to the indefinite inner product $\langle .,.\rangle$ on the whole space. A representation on a subspace of $\mathcal{V}$ acts by symmetric operators only if this subspace consists of functions f such that all derivatives of f vanish at $p=0$. This subspace is at the same time also positive definite. In order that it is also maximal in the sense that there is no larger positive definite subspace in $\mathcal{V}$, one has in fact to assume that the coefficients c_k^2 in Eq. (1) are strictly positive, i.e., $c_k\in\mathbb{R}\backslash\{0\}$ for all k, which we do from now on. In turn, this implies that $J(\partial_p\partial_p')$ is a properly infinite differential operator and thus the singularity in (2) must be stronger than a finite order distribution. This excludes as test function space any space $\mathscr{S}_\alpha^\infty$ which allows only distributions of finite order, and thus in particular the Schwartz space $\mathscr{S}=\mathscr{S}_\infty^\infty$. On the other hand, the very strong singularity of

an analytic functional is also excluded: Since for $\beta=1$ the test functions in $\mathcal{V}$ are all analytic in a strip neighborhood of the real axis, the requirement $f^{(k)}(0)=0$ for all k would lead to the trivial subspace.

After these heuristics, we are ready to state our main result, whose proof will follow in the following section. We will characterize the complete, positive definite representation subspace for the Heisenberg algebra by the Fourier transformation. For that, we need another definition.

Definition 2.2: The space of functions $L^2_0(\mathbb{R})$ is defined as

$$L^2_0(\mathbb{R}) \overset{\text{def}}{=} \{f \in L^2(\mathbb{R}) | \mu^k(f)=0, \ \forall k \in \mathbb{N}_0\},$$

where the *k-th moment* $\mu^k(f)$ of a function $f \in L^2(\mathbb{R})$ is given by

$$\mu^k(f) \overset{\text{def}}{=} \int_{\mathbb{R}} x^k f(x) dx,$$

if it exists for a $k \in \mathbb{N}_0$.

Theorem 2.3: *Let* $0 \leqslant \alpha \leqslant \infty$, $1 < \beta < \infty$. *Assume* $\delta > \beta$, *and let J be infraexponential of order* $1/(2\delta)$ *with strictly positive Taylor coefficients. Then, the space* $\mathcal{V}=\mathcal{V}_J(\alpha,\beta;(2\delta)^{-1})$ *admits a maximal completion to a Krein space* $\mathcal{K}$ *with countably infinite rank of negativity. The maximal positive definite subspace of* $\mathcal{K}$, *invariant under the action of the Heisenberg algebra in the Schrödinger representation by self-adjoint operators on it, is the Fourier transform* $\mathcal{F}L^2_0(\mathbb{R})$ *of* $L^2_0(\mathbb{R})$.

The appearance of $\delta > \beta$ results from technicalities of the infrared regularization process, as will become clear in the following. This leaves room for improvement. It should be stressed that the diagonal form $\delta(p-p')$ of (2) outisde the singularity $p=p'=0$ was chosen to allow for a symmetric action of the Heisenberg generators. The regularization procedure itself is nonetheless rather independent of the structure of the kernel outside the singular points. On the other hand, the discussion at the beginning of this section also points to a principal limitation of the regularization method. If the singularity in a certain point p_0 is that of a proper analytic functional, i.e., $\delta \leqslant 1$, and the rank of indefiniteness is infinite, regularization is impossible since the positive subspace would be trivial in that case.

The somewhat exotic representation of the Heisenberg algebra mentioned previously does not fit into the classification of Ref. 11, see also Ref. 13. Rather it corresponds to the ''counterexample'' in the appendix of Ref. 11. As explained there, $L^2_0(\mathbb{R})$ naturally decomposes into two irreducible subspaces of ''left-'' and ''right-movers'' i.e., states with support, respectively, on the negative, and positive half-axis in momentum space, by closure of the two domains $\mathcal{V}_\pm = \{f \in \mathcal{V} | f(p)=0 \text{ for } p \lessgtr 0\}$ in the Krein topology.

III. INFINITE INFRARED REGULARIZATION

In this section we present the proper method for the construction of a Krein space from $\mathcal{V}$. The general strategy is close in spirit to the well-known method for closing a Hilbert space with respect to the action of a given positive bilinear form on it (see Ref. 14, Appendix A.2). The construction of a maximal majorant Hilbert topology for $\mathcal{V}$ leading to a Krein space closure of it, relies mainly on two ingredients: first, the existence of neutral elements within $\mathcal{V}$ which separate the negative degrees of freedom from the rest of the space. Second, there is some ''air'' left between the decay of the coefficients c_k^2 defining $\langle .,. \rangle$ via (1), and the growth of the Taylor coefficients of the functions in $\mathcal{V}$. This is expressed in Eq. (3), the assumption $\delta > \beta$ of Theorem 2.3, and (4). To make use of that margin, we define the ''damping coefficients'' γ_k by

$$\gamma_k \overset{\text{def}}{=} k^{k\delta}. \tag{5}$$

The neutral decomposition elements will be constructed in Appendix A to fulfill the following demands:

Lemma 3.1: Let $0\leqslant\alpha\leqslant\infty$ *and* $1<\beta<\infty$. *Let there be given a sequence of numbers* c_k *satisfying* (3), *and let* γ_k *be as in* (5). *Then there exists a sequence of functions* $\{\chi_k\}_{k\in\mathbb{N}_0}\subset\mathscr{S}^{\beta}_{\alpha}$ *with the following properties*:

(i) $\|\chi_k\|^2_{L^2}=c_k^2\gamma_k^2$,
(ii) $\chi_k^{(i)}(0)=\delta_{ik}\cdot\gamma_k$,
(iii) $(\chi_k,\chi_l)_{L^2}=0$ *for all* $k\neq l$,
(iv) $\langle\chi_k,\chi_l\rangle=0$ *for all k, l.*

We denote by $\mathcal{N}$ *the linear subspace of* $\mathscr{S}^{\beta}_{\alpha}$ *generated by* $\{\chi_k\}_{k\in\mathbb{N}_0}$.

The subspace $\mathcal{N}$ is neutral, $\mathcal{N}\subset\mathcal{V}^0$. We also observe that $\mathcal{V}$ is nondegenerate due to the presence of the L^2-part in the indefinite product (1). This property will prevail in the closure of $\mathcal{V}$ we construct in the following. Now, every $f\in\mathscr{S}^{\beta}_{\alpha}$ has, for every finite $N\geqslant 0$, a unique decomposition

$$f=f^{N+}+\sum_{i=0}^{N}f^i\chi_i\quad\text{with}\quad f^i=\frac{f^{(i)}(0)}{\gamma_i},\tag{6}$$

and $f^{N+}\in\mathscr{S}^{\beta}_{\alpha}$ is such that $\int^{(i)}(0)=0$ for $0\leqslant i\leqslant N$. Furthermore, the sum in the decomposition is clearly in $\mathcal{N}$.

Proposition 3.2: The seminorm p given by the limit

$$p(f)^2\overset{\text{def}}{=}\lim_{N\to\infty}\left[\langle f^{N+},f^{N+}\rangle+\sum_{i=0}^{N}\{|\langle f,\chi_i\rangle|^2+|f^i|^2\}\right]\tag{7}$$

exists and defines a majorant topology τ *on* $\mathcal{V}$.

Proof: Taking Lemma B.3 into account, we have to show that (7), if it is well defined, dominates the inner square. Assuming that the limit in question exists, it is easy to show that $p(f)^2$ majorizes the inner square $|\langle f,f\rangle|$ of f. Namely, using (6) we can express $\langle f,f\rangle$ as

$$\langle f,f\rangle=\langle f^{N+},f^{N+}\rangle+\sum_{i=0}^{N}\{f^i\langle f,\chi_i\rangle+\overline{f^i}\langle\chi_i,f\rangle\}$$

using property (iv) of Lemma 3.1, and the fact that $\langle f^{N+},\chi_i\rangle=\langle f,\chi_i\rangle$ which follows from it. Now, in every term in the sum above we have the elementary estimate for complex numbers $|f^i\langle f,\chi_i\rangle+\overline{f^i}\langle\chi_i,f\rangle|\leqslant|\langle f,\chi_i\rangle|^2+|f^i|^2$. If the first term $\langle f^{N+},f^{N+}\rangle$ in (7) has a limit at all, then it tends to $(f^+,f^+)_{L^2}=\|f^+\|^2_{L^2}\geqslant 0$ for a certain $f^+\in L^2$, showing $p(f)^2\geqslant|\langle f,f\rangle|$ in the limit $N\to\infty$. It remains to show that all the limits involved in (7) exist. In order to show finiteness of the first term it suffices to show that the decomposition (6) of f converges in $L^2(\mathbb{R})$ for $N\to\infty$, since it then tends to $\|f^+\|^2_{L^2}$ and is thus necessarily finite as we have just seen. For the sum defining the decomposition, we have by (i) of Lemma 3.1

$$\left\|\sum_{N=0}^{\infty}f^i\chi_i\right\|^2_{L^2}\leqslant\sum_{N=0}^{\infty}\|f^i\chi_i\|^2_{L^2}=\sum_{N=0}^{\infty}|f^{(i)}(0)c_i|^2<\infty,$$

taking (3) and (4) into account, showing that claim. By definition (1) of the inner product, the ith term in the sum in (7) becomes

$$|\langle f,\chi_i\rangle|^2+|f^i|^2=\left|(f,\chi_i)_{L^2}-\sum_{k=0}^{2} c_k^2\overline{f^{(k)}}(0)\chi_i^{(k)}(0)\right|^2+|f^i|^2$$
$$\leqslant|(f,\chi_i)_{L^2}|^2+c_i^4\gamma_i^2|f^{(i)}(0)|^2+\frac{|f^{(i)}(0)|^2}{\gamma_i^2}.$$

For the first term we find, using the Cauchy–Schwartz estimate, by (3) and (5), and of course the assumption of Theorem 2.3:

$$|(f,\chi_i)_{L^2}|^2\leqslant\|f\|_{L^2}^2|c_i^2\gamma_i^2|\leqslant\|f\|_{L^2}^2\frac{C\theta^i}{D^i e^{2i\delta}}.$$

Further using (4), the second term is bounded by

$$c_i^4\gamma_i^2|f^{(i)}(0)|^2\leqslant\frac{C^2C_f^2}{i^{2i(\delta-\beta)}}\left(\frac{\theta(B+\rho)}{e^{2\delta}D}\right)^{2i}.$$

Finally the third term satisfies

$$\frac{|f^{(i)}(0)|^2}{\gamma_i^2}\leqslant\frac{C_f^2}{i^{2i(\delta-\beta)}}(B+\rho)^{2i}.$$

All three terms decay faster than exponentially in i, making the overall sum in (7) convergent in the limit $N\to\infty$. □

Notice that although we chose to see this independently by considering L^2-convergence, the numerical convergence of the $\langle f^{N+},f^{N+}\rangle$-part of the decomposition could have been inferred in the same way as the convergence of the other terms in (7). In fact, one could have inverted the decomposition (6) to yield $f^{N+}=f-\Sigma_{i=0}^{N}f^i\chi_i$ and then see the convergence of $\langle f^{N+},f^{N+}\rangle$ by majorizing it with the same convergent terms as in the previous proof.

It is apparent from the proof of Proposition 3.2 that the decomposition (6) of f converges in the closure $\overline{\mathcal{V}^\tau}$ of $\mathcal{V}$ with respect to τ. In fact, it is easy to see that the increments $p(f^i\chi_i)^2$ decay fast enough to turn the partial sums in the decomposition into a Cauchy sequence. This allows us to write for every $f\in\mathcal{V}$,

$$f=f^+\sum_{i=0}^{\infty}f^i\chi_i\quad\text{with}\quad f^+\in\overline{\mathcal{V}^\tau}. \tag{8}$$

We further see, using the joint continuity of $\langle .,.\rangle$, see Definition B.2, that the indefinite inner product $\langle .,.\rangle$ has a unique extension to $\overline{\mathcal{V}^\tau}$, which we will also denote by $\langle .,.\rangle$. Thus using (8), Eq. (7) extends to a definition of a quadratic normed topology on the τ-complete space $\overline{\mathcal{V}^\tau}$, i.e., a Hilbert majorant topology on that space:

Corollary 3.3: On the closure $\mathcal{K}\overset{\text{def}}{=}\overline{\mathcal{V}^\tau}=(\mathscr{S}_\alpha^\beta)^{-\tau}$ *we define the Hilbert scalar product*

$$(f,g)\overset{\text{def}}{=}\langle f^+,g^+\rangle+\sum_{i=0}^{\infty}\{\langle f,\chi_i\rangle\langle\chi_i,g\rangle+\overline{f^i}g^i\},\quad\forall f,g\in\mathcal{K}. \tag{9}$$

We denote the Hilbert norm on $\mathcal{K}$ *by* $\|.\|\overset{\text{def}}{=}p(.)=(.,.)^{1/2}$. *In particular, we have the identity* $\langle f^+,f^+\rangle=\|f^+\|_{L^2}^2$.

We set

$$\mathcal{P} \overset{\text{def}}{=} \{f \in \mathcal{V} \,|\, f^{(k)}(0) = 0, \quad \forall k \in \mathbb{N}_0\}.$$

Obviously, $\langle .,. \rangle$ is positive definite on $\mathcal{P}$ and equals the L^2-scalar product on that subspace. The decomposition (8) can now be expressed as follows:

Lemma 3.4: Equation (8) *defines a mapping*

$$P : \mathcal{V} \to \overline{\mathcal{V}}^\tau, \quad f \mapsto f^+,$$

with the following properties:

(i) *P is continuous in the topology* τ.
(ii) *P has a continuous extension to* $\mathcal{K}$.
(iii) *P maps* $\mathcal{K}$ *onto* $\overline{\mathcal{P}}^\tau$.
(iv) *P is an orthogonal projection onto* $\overline{\mathcal{P}}^\tau$ *with respect to* $(.,.)$.
(v) *The decomposition*

$$\mathcal{K} = \overline{\mathcal{P}}^\tau \oplus \overline{\mathcal{N}}^\tau$$

is orthogonal with respect to the scalar product (.,.) (denoted by $\oplus$*).*

Proof: To show (i) we estimate

$$\begin{aligned}
\|f^+\|^2 &= \|f^+\|_{L^2}^2 + \sum_{i=0}^{\infty} |\langle f^+, \chi_i \rangle|^2 \\
&= \|f^+\|_{L^2}^2 + \sum_{i=0}^{\infty} |(f^+, \chi_i)_{L^2}|^2 \\
&\leqslant \|f^+\|_{L^2}^2 \left(1 + \sum_{i=0}^{\infty} \|\chi_i\|_{L^2}^2 \right) \\
&\leqslant \|f^+\|_{L^2}^2 \left(1 + \sum_{i=0}^{\infty} c_i^2 \gamma_i^2 \right) \leqslant C \|f^+\|_{L^2}^2 \leqslant C \|f\|^2.
\end{aligned}$$

In the last step we used that we have $\|f\|^2 \geqslant \langle f^+, f^+ \rangle = \|f^+\|_{L^2}^2$ by Corollary 3.3. Assertion (ii) follows from (i). By (i) and (ii) it suffices to show that $f \in \mathcal{V}$ entails $f^+ \in \overline{\mathcal{P}}^\tau$ to show (iii). For that, by the second to last inequality mentioned previously, it suffices to approximate f^+ in the L^2-norm with elements of $\overline{\mathcal{P}}^\tau$. Such an approximation can be easily constructed, e.g., as $f_\varepsilon^+ = (1 - \rho_\varepsilon) f^+$ for $\varepsilon \to 0$, with the cut-off functions ρ_ε of Lemma A.1. That $P : \mathcal{K} \to \overline{\mathcal{P}}^\tau$ is surjective is now clear, since P is the identity on $\overline{\mathcal{P}}^\tau$. For $f^+ \in \mathcal{P}$ and $\chi \in \mathcal{N}$, the scalar product reduces to

$$(f^+, \chi) = \sum_{i=0}^{\infty} \langle f^+, \chi_i \rangle \langle \chi_i, \chi \rangle = 0,$$

since $\langle \chi_i, \chi \rangle = 0$, and because f^+ and χ have decompositions with vanishing $(f^+)^i$ and χ^+, respectively. Continuity of $\langle .,. \rangle$ then implies statement (iv). Assertion (v) follows from (iv) and the fact that the sum in (8) converges to an element of $\overline{\mathcal{N}}^\tau$. □

To construct the metric operator J that connects the indefinite with the Hilbert scalar product on $\mathcal{K}$, we have to decompose this space somewhat further. To that end, we consider the functionals

$$F_i(f) \overset{\text{def}}{=} \langle \chi_i, f_i \rangle, \quad f \in \mathcal{V}$$

on $\mathcal{V}$. These functionals are nonzero since $\mathcal{V}$ is nondegenerate, they vanish on $\mathcal{N}$, and they are clearly bounded with respect to the norm p. In fact, we have $|F_i(f)|/p(f)\leqslant 1$ for $f\in\mathcal{V}$, by (7). That is, the F_i have unique continuations (also denoted by F_i) to $\mathcal{K}$ by the Hahn–Banach theorem, and by continuity these satisfy the same bound $0<\|F_i\|\leqslant 1$.

Lemma 3.5: The uniquely determined vectors $v_i\in\mathcal{K}$ which represent F_i via $F_i(f)=(v_i,f)$ for all $f\in\mathcal{K}$ are actually contained in $\overline{\mathcal{P}^\tau}$.

Proof: That the vectors v_i exist and are unique in $\mathcal{K}$ follows from Riesz' representation theorem applied to the bounded linear functionals F_i on the Hilbert space $\mathcal{K}$. We have to show that they are in $\overline{\mathcal{P}^\tau}$. Choose a sequence $\{v_{in}\}_{n\in\mathbb{N}}$ in $\mathcal{V}$ that approximates v_i, i.e., $\|v_i-v_{in}\|\to 0$ for $n\to\infty$. Using the decomposition (8) for the v_{in} we calculate (adopting Einstein's summation convention for repeated upper and lower indices)

$$\begin{aligned}\|v_i-v_{in}\|^2&=(v_i-(v_{in})^+-(v_{in})^j\chi_j,v_i-(v_{in})^+-(v_{in})^k\chi_k)\\&=\|v_i-(v_{in})^+\|^2-(v_i-(v_{in})^+-(v_{in})^j\chi_j,(v_{in})^k\chi_k)-((v_{in})^j\chi_j,v_i-(v_{in})^+)\\&=\|v_i-(v_{in})^+\|^2-(v_i-v_{in},(v_{in})^j\chi_j)-((v_{in})^j\chi_j,v_i)+((v_{in})^j\chi_j,(v_{in})^+).\end{aligned}$$

The last term on the right-hand side vanishes for all n due to Lemma 3.4(v). The third term is zero since $(v_i,\chi_j)=F_i(\chi_j)=\langle\chi_i,\chi_j\rangle=0$. We use the Cauchy–Schwartz estimate for the scalar product $(.,.)$ and the fact that $\|\chi_i\|=|(\chi_i)^i|=|\chi_i^{(i)}(0)/\gamma_i|=1$ to estimate the second term as follows:

$$|(v_i-v_{in},(v_{in})^j\chi_j)|\leqslant\|v_i-v_{in}\|\sum_{j=0}^{\infty}|(v_{in})^j|\leqslant C\|v_i-v_{in}\|,$$

with some constant $C>0$ independent of n. In fact, since $(v_{in})^j=v_{in}^{(j)}(0)/\gamma_j$, and using (4) and (5) we see that the sum is finite for all n. Since the sequence v_{in} is convergent in the norm p and by definition (7) of this norm, the sum must actually converge and therefore admits a global bound C as above. In conclusion, since v_{in} is τ-convergent to v_i, i.e., $\|v_i-v_{in}\|\to 0$ for $n\to\infty$, we must have $\|v_i-(v_{in})^+\|\to 0$ by necessity, and thus already Pv_{in} is τ-convergent to v_i. This shows the claim. □

The basic properties of the v_i are collected in the next lemma.

Lemma 3.6: The vectors v_i have the following properties:

(i) $\langle\chi_i,v_i\rangle=(v_i,v_i)=1$,
(ii) $(v_i,v_j)=\langle\chi_i,v_j\rangle=0$ for $i\neq j$,
(iii) $\langle v_i,v_i\rangle=0$,
(iv) $\langle v_i,f\rangle=f^i$ *for all* $f\in\mathcal{V}$.

Proof: Statement (i) is clear from the defining property of v_i, except for the last equality that says $\|v_i\|=1$. This will soon turn out to be true. Let $\{v_{in}\}_{n\in\mathbb{N}}\subset\mathcal{P}$ be a sequence converging to v_i in $\mathcal{K}$, which exists by Lemma 3.5. Then with (9), and since $(v_{in})^j=0$ for all j we have

$$\frac{\|v_{in}\|^2}{|\langle\chi_i,v_{in}\rangle|}=\frac{\langle v_{in},v_{in}\rangle}{|\langle\chi_i,v_{in}\rangle|}+1+\frac{\Sigma_{j\neq i}\langle\chi_j,v_{in}\rangle}{|\langle\chi_i,v_{in}\rangle|}.$$

Now $|\langle\chi_i,v_{in}\rangle|=|(v_i,v_{in})|\to\|v_i\|^2$ by (i), so that the left-hand side tends to 1 for $n\to\infty$ (here we assume that the denominators are nonzero which can be achieved by choosing v_{in} suitably). Since the denominators stay bounded, we must necessarily have $|\langle\chi_j,v_{in}\rangle|\to 0$ for $j\neq i$ showing (ii), and also $\langle v_{in},v_{in}\rangle\to 0$ showing (iii) since v_{in} converges to v_i with respect to $\|.\|=p(.)$ and p majorizes the inner square. Incidentally, this also shows

$$\sup_n\frac{|F_i(v_{in})|}{\|v_{in}\|}=\sup_n\frac{|\langle\chi_i,v_{in}\rangle|}{\|v_{in}\|}=1,$$

and this proves the last equality in (i), since the norm of v_i and that of the linear functional F_i coincide by Riesz' theorem. To show (iv), we consider again the decomposition (8) of a vector $f \in \mathcal{V}$ which yields

$$\langle v_{in}, f\rangle = \langle v_{in}, f^+\rangle + f^i\langle v_{in}, \chi_i\rangle + \sum_{j\neq i} f^j\langle v_{in}, \chi_j\rangle.$$

In this expression we find $\langle v_{in}, f^+\rangle \to 0$, since by (iii) v_{in} converges strongly to 0 in $\overline{\mathcal{P}^\tau}$, and due to Lemma 3.4. By arguments similar to that in the proof of Lemma 3.5, the sum stays bounded independently of n, and since every single term in it converges to 0 by (ii), the sum also tends to 0. This leaves us with the second term which converges to $f^i\langle v_i, \chi_i\rangle = f^i$ by (i). This shows (iv).□

The v_i could be constructed concretely as limits of functions which vanish strongly in the L^2-sense, as in Ref. 1. Lemmas 3.5 and 3.6 allow us to avoid such an explicit construction. The vectors v_i are an orthonormal basis of a closed Hilbert subspace of $\mathcal{K}$. This space is isomorphic to the dual space of $\overline{\mathcal{N}^\tau}$ by definition of the functionals F_i and Lemma 3.5, and we mnemonically denote it by the symbol $\overline{\mathcal{N}^{\tau\langle * \rangle}}$.

Lemma 3.7: Denote by $\mathcal{H}$ the closure $\overline{\mathcal{P}^\tau}_+$ of $\mathcal{P}$ with respect to the topology τ_+ induced by the quadratic Hilbert norm $p_+(.)^2 \overset{\text{def}}{=} \langle .,. \rangle$ on $\mathcal{P}$. The space $\mathcal{K}$ admits the decomposition

$$\mathcal{K} = \mathcal{H} \oplus \overline{\mathcal{N}^{\tau\langle * \rangle}} \oplus \overline{\mathcal{N}^\tau},$$

orthogonal with respect to (.,.).

Proof: First, we must show that the decomposition is indeed possible because $\mathcal{H} \subset \overline{\mathcal{V}^\tau}$. To this end, note that the topology τ_+ is stronger than the restriction of τ to $\mathcal{P}$. In fact, if a sequence in $\mathcal{P}$ converges in the norm p_+ then it converges in the L^2-norm by (1), and by the action of the indefinite product on $\mathcal{P}$ it is easy to see that this suffices to ensure convergence in the norm p. Now, taking Lemma 3.4(v) into account, we have to show that the (.,.)-orthogonal decomposition $\overline{\mathcal{P}^\tau} = \mathcal{H} \oplus \overline{\mathcal{N}^{\tau\langle * \rangle}}$ holds. First, observe that the vectors v_i form a τ-complete orthonormal system in $\overline{\mathcal{N}^{\tau\langle * \rangle}}$. Now, for $f^+, g^+ \in \mathcal{P}$ we have

$$(f^+, g^+) = \langle f^+, g^+\rangle + \sum_{i=0}^{\infty} (f^+, v_i)(v_i, g^+),$$

by the definition of v_i and (9). This shows that a sequence $\{f_n^+\}_{n\in\mathbb{N}}$ in $\mathcal{P}$ converges to a limit $f \in \overline{\mathcal{P}^\tau}$ if and only if $p_+(f_n^+ - f) \to 0$ and independently the (.,.)-orthogonal projection of $f_n^+ - f$ onto the closed subspace $\overline{\mathcal{N}^{\tau\langle * \rangle}}$ of $\overline{\mathcal{P}^\tau}$ tends to zero. Denote by $\overline{\mathcal{N}^{\tau\langle \perp \rangle}}$ the orthogonal complement of $\overline{\mathcal{N}^{\tau\langle * \rangle}}$ in $\mathcal{K}$ with respect to (.,.). By the above-given argument, the subset $\mathcal{P} \cap \overline{\mathcal{N}^{\tau\langle \perp \rangle}}$ of $\overline{\mathcal{P}^\tau}$ is dense in $\mathcal{H}$ with respect to the topology τ_+. This shows that the proposed decomposition is indeed (.,.)-orthogonal. In conclusion, a τ-Cauchy sequence in $\mathcal{P}$ can be identified with a pair $(f, \{\lambda_i\}_{i\in\mathbb{N}_0})$ with an $f \in \mathcal{H}$ and $\lambda_i = (v, v_i)$ for some $v \in \overline{\mathcal{N}^{\tau\langle * \rangle}}$. This shows $\overline{\mathcal{P}^\tau} = \mathcal{H} \oplus \overline{\mathcal{N}^{\tau\langle * \rangle}}$. □

It should be noted that by Lemma 3.6 (iii), the vectors v_i indeed converge to zero in the topology τ_+ of $\mathcal{H}$ but are clearly nonzero in $\overline{\mathcal{P}^\tau} \subset \mathcal{K}$. Furthermore, τ_+ is stronger than the L^2-topology although $p_+(f^+) = \|f^+\|_{L^2}$ for $f^+ \in \mathcal{P}$. We will characterize $\mathcal{H}$ as a function space in the following. We have compiled all information needed to exhibit the Krein space structure of $\mathcal{K}$.

Theorem 3.8: *The space $\mathcal{K}$ is a Krein space with countably infinite rank of indefiniteness. Its Hilbert space structure is maximal and given by the metric operator $J: \mathcal{K} \to \mathcal{K}$, satisfying the identity $\langle .,. \rangle = (., J.)$. It holds*

$$Jv_i = \chi_i, \quad J\chi_i = v_i, \quad \text{and } J|_{\mathcal{H}} = \mathbb{I}_{\mathcal{H}},$$

in the decomposition of Lemma 3.7.

Proof: The strategy of the proof will be as follows: The metric operator exists by Proposition B.5, and we have seen in Lemma 3.7 that we can write down its action in the decomposition $\mathcal{K}=\mathcal{H}\oplus\overline{\mathcal{N}^\pi}^{\langle *\rangle}\oplus\overline{\mathcal{N}^\pi}$. We can then explicitly demonstrate that the operator J on $\mathcal{K}$ acts as stated. This special form of J immediately implies that it is a bounded, completely invertible operator on $\mathcal{K}$. Thus by Proposition B.7, $\mathcal{K}$ is a Krein space and since $J^{-1}=J$ is also bounded, its Hilbert space structure $(\mathcal{K}, J)$ is maximal by Lemma B.8. Now, by definition of the v_i we have $\langle f,\chi_i\rangle=(f,J\chi_i)=(f,v_i)$ for all $f\in\mathcal{K}$, showing $J\chi_i=v_i$. On the other hand, by Lemma 3.6(iv) and (9) we have $\langle f,v_i\rangle=(f,Jv_i)=\overline{f^i}=(f,\chi_i)$, showing $Jv_i=\chi_i$. It remains to consider the restriction of J to $\mathcal{H}$. Take $f^\perp, g^\perp\in\mathcal{P}\cap\overline{\mathcal{N}^\pi}^{\langle\perp\rangle}$ (see the proof of Lemma 3.7) and note that $(f^\perp,g^\perp)=\langle f^\perp,g^\perp\rangle$ for those vectors. Since these vectors are dense in $\mathcal{H}$, it follows that the restriction of J to $\mathcal{H}$ is the identity. This shows the claim. □

To conclude the proof of Theorem 2.3, it finally remains to show that $\mathcal{H}$ is the Fourier transform of the space L_0^2 defined in Definition 2.2. Now $\mathcal{F}$ is a topological isomorphism from $\mathscr{S}_\beta^\alpha$ onto $\mathcal{V}=\mathscr{S}_\alpha^\beta$ and for $f\in\mathscr{S}_\beta^\alpha$ we have

$$i^k\hat{f}^{(k)}(0)=\left(i^k\frac{d^k}{d\xi^k}\int_{\mathbb{R}}e^{-ix\xi}f(x)\mathrm{d}x\right)\Bigg|_{\xi=0}=i^k\int_{\mathbb{R}}(-ix)^kf(x)dx=\mu^k(f).$$

By that, the image of $\mathcal{P}$ under $\mathcal{F}^{-1}$ is the subspace of $\mathscr{S}_\beta^\alpha$ of functions f with $\mu^k(f)=0$ for all k. Since $\mathscr{S}_\beta^\alpha$ is dense in L^2 and the Fourier transformation is an L^2-isometry, we can see $\mathcal{H}=\mathcal{F}L_0^2$. Thus Theorem 2.3 is finally proven.

If we test the vectors v_i with states in the ''physical'' subspace $\mathcal{H}$, i.e., the representation space for the Heisenberg-observables, they appear as completely delocalized states. In fact the action of the momentum operator on them is given by Lemma 3.6(iv):

$$\langle pv_i,f\rangle=\langle v_i,pf\rangle=(pf)^i=0\quad\text{for all}\quad f\in\mathcal{H},\quad i\in\mathbb{N}_0,$$

where we denoted the unique extension of the multiplication operator p from $\mathcal{V}$ to $\mathcal{K}$ also by p. This is different from the case of one single negative degree of freedom in Ref. 1, where the single vector v_0 turns out to be completely delocalized on the whole Krein state space.

IV. A CONDITION SUFFICIENT FOR REGULARIZATION

In this section, we want to give a set of conditions on a general indefinite inner product space $\mathcal{V}$, that will be sufficient for the regularization procedure to work. We did not put this generalization in the beginning, and then deduced the special case $\mathcal{V}=\mathscr{S}_\alpha^\beta$ considered previously from it, for two reasons: First and foremost, we wanted to emphasize the case of indefinite inner products generated by singular kernels acting on a test function space, which we think is particularly interesting in view of possible applications in physics. Second, most of the assertions and proofs in Sec. III are already cast abstract enough to be re-used in the proof of the generalized regularization Theorem 4.1 without any modification. Thus, we can stress the essential points that need modification and thereby highlight the principles which put the regularization procedure to work.

Two elements are essential: First, the existence of neutral decomposition elements χ_i that enable us to isolate the positive part of the indefinite product. Second, a certain balance between the growth, respectively, and decay of (a) the inner products of vectors in the space with the neutral elements, and (b) the coefficients of the linear decomposition of a vector with respect to these. These growth conditions constitute the main difference between the case of finite rank of indefiniteness considered in Ref. 4 and the infinite case, where they serve to render the Hilbert majorant topology well defined in the first place.

Let us now formulate our set of conditions. We assume $\mathcal{V}$ to be a complex linear space with an indefinite inner product $\langle .,.\rangle$, which shall be nondegenerate. Assume the following.

(0) There exists an orthogonal system $\{\tilde{\chi}_i\}_{i\in\mathbb{N}_0}$ of mutually linearly independent, neutral vectors in $\mathcal{V}$.

(1) For all $v \in \mathcal{V}$, the unique decomposition for $N \in \mathbb{N}_0$,

$$v = \tilde{v}^{N+} + \sum_{i=0}^{N} \tilde{v}^i \tilde{\chi}_i, \quad \tilde{v}^i \in \mathbb{C}$$

becomes asymptotically positive in the sense that

$$0 \leqslant \lim_{N\to\infty} \langle \tilde{v}^{N+}, \tilde{v}^{N+} \rangle.$$

(2) There exists a sequence of complex numbers $\{\gamma_i\}_{i\in\mathbb{N}_0}$ such that both sequences $\{\gamma_i \langle \tilde{\chi}_i, v\rangle\}$ and $\{\tilde{v}^i/\gamma_i\}$ are in $l^2(\mathbb{N}_0)$.

These conditions enable us to prove an equivalent of Proposition 3.2. In fact, setting $\chi_i \overset{\text{def}}{=} \gamma_i \tilde{\chi}_i$, we obtain the analog of the finite decomposition (6) for a vector $v \in \mathcal{V}$ with coefficients $v^i = \tilde{v}^i/\gamma_i$. We then have to see that the sum (7) with f replaced by v, defining the majorant norm $p(v)^2$, converges. The convergence of the asymptotically positive part $\lim_{N\to\infty}\langle v^{N+}, v^{N+}\rangle$ then follows, as we have already noted after the proof of Proposition 3.2. Now, the ith summand in the definition of $p(v)^2$ becomes

$$|\langle v, \chi_i\rangle|^2 + |v^i|^2 = |\gamma_i \langle v, \tilde{\chi}_i\rangle|^2 + |\tilde{v}^i/\gamma_i|^2,$$

and the sum converges due to condition (2). Thus, we get a majorant Hilbert topology τ on $\mathcal{V}$. A close inspection of the proofs of the various lemmata in Sec. III shows that the only other point which has to be reconsidered is the proof of statement (i) of Lemma 3.4, that the mapping $P: v \mapsto v^+$ is τ-continuous on $\mathcal{K} \overset{\text{def}}{=} \overline{\mathcal{V}}^{\tau}$. There, we have utilized the L^2-norm, but we will see that this can also be shown independently. In fact, we have

$$\|v^+\|^2 = \left(v - \sum_{i=0}^{\infty} v^i \chi_i, v - \sum_{j=0}^{\infty} v^j \chi_j \right) = \|v\|^2 - 2\,\mathrm{Re} \sum_{i=0}^{\infty} v'(\chi_i, v) + \sum_{i,j=0}^{\infty} v^i \overline{v^j} (\chi_i, \chi_j).$$

We use the two consequences $(\chi_i, \chi_j) = \delta_{ij}$ and $(\chi_i, v) = \overline{v^i}$ of Eq. (9) in the third and second term, respectively, to obtain

$$= \|v\|^2 - \sum_{i=0}^{\infty} |v^i|^2 \leqslant \|v\|^2$$

by definition (7) of $\|v\|^2$. Here again, condition (2) ensures the convergence of the sums appearing. From this point, one can proceed word for word as in Sec. III with the definition of the vectors v_i and the demonstration of their properties. We finally obtain a generalization of Theorem 3.8:

Theorem 4.1: *Let $\mathcal{V}$ satisfy (0)–(2). Then $\mathcal{K}$ is a Krein space with rank of indefiniteness $\#\{\chi_i \neq 0\}$. Its Hilbert space structure is maximal, and the metric operator J acts as in Theorem 3.8.*

Note that (0)–(2) and Theorem 4.1 are formulated as to cover the cases of finite as well as of infinite rank of indefiniteness. Namely, in case the rank of indefiniteness is $N < \infty$, one can find at most N neutral, linearly independent vectors, and one has to use them all to obtain a decomposition that, as demanded by (1), becomes positive (in this case not asymptotically). One then chooses $\tilde{\chi}_i = 0$ for $i > N-1$.

We conclude this paper with some comments on the generalized regularization procedure just described. First, the conditions (0)–(2) certainly do not present the utmost general ones possible. In particular, one can perhaps replace the neutral orthogonal system of (0) by a general system of linear independent vectors which lead to an asymptotically positive decomposition. See Ref. 4 Remark A.13, where we describe how to find a maximal neutral orthogonal system in the case of

finite rank of negativity. Furthermore, whether $\langle v^+, v^+ \rangle$ is positive or negative definite is irrelevant, since one can always go over to $-\langle .,. \rangle$ (the so called *antispace* of $\mathcal{V}$). On the other hand, one cannot easily dispense with either of the l^2-conditions in (2), since they represent rather sharply the convergence conditions that enabled us to construct a majorant. Since we made no presuppositions with respect to $\mathcal{V}$ regarding structure and topology, condition (1) is also indispensible.

In our case of main interest in Sec. III, the essence of conditions (0) and (1) are captured in Lemma 3.1 which is proven in Appendix A. A similar construction of neutral decomposition elements will also have to be carried out in any other concrete case, and is thus at the very center of the regularization procedure, in putting flesh to the bones of the abstract conditions (0) and (1). The construction in Appendix A may serve as a blueprint for that at least in the case of test function spaces over $\mathbb{R}^n$ and inner products generated by kernels whose singularities are ''localized'' enough, e.g., concentrated on a compact set. This may justify that we did not delve into a further abstraction of conditions (0) and (1).

Let us consider an instructive special case. Assume the sequence of coefficients $\{\tilde{v}^i\}$ is bounded for all $v \in \mathcal{V}$. If there holds an estimate

$$|\langle \tilde{\chi}_i, v \rangle| \leqslant C(v) i^{-(1+\delta)},$$

with a constant depending on v and for some $\delta > 0$, we can choose

$$\gamma_i = i^{-(1/2+\varepsilon)}$$

for any $0 < \varepsilon < \delta$. Such polynomial growth and decay conditions are obviously much weaker than the conditions that were present in the case $\mathcal{V} = \mathscr{S}^{\beta}_{\alpha}$, see, e.g., our choice of γ's in (5). Thus the range of cases covered by Theorem 4.1 is considerably widened in comparison to Theorem 3.8 and Theorem 2.3.

The question arises naturally, whether we can find uniform properties on $\mathcal{V}$, as opposed to the pointwise ones (1) and (2), that enable regularization. In essence one would look for a simple quantitative measure that tells us when the construction of the majorant is possible. But this is not straightforward. To simplify the discussion, consider the case where $\{\tilde{v}^i\}$ is bounded in $\mathbb{C}$ for all v (these sets can of course not be uniformly bounded). A simple uniform measure that could replace condition (2) can be formulated in terms of the quantities

$$\overline{\beta}_i \overset{\text{def}}{=} \sup_{v \in \mathcal{V}, \tilde{v}^i = 1} |\langle \tilde{\chi}_i, v \rangle|.$$

Notice that at least $\tilde{\chi}_i$ is in the set over which the supremum is taken, and if this is the only element we have $\tilde{\beta}_i = 0$ due to neutrality of that vector. One can then replace (2) by the condition that there shall exist a sequence $\{\gamma_i^{-1}\}$ in $l^2(\mathbb{N}_0)$ such that also $\{\tilde{\beta}_i \gamma_i\}$ is in $l^2(\mathbb{N}_0)$. This uniform growth condition on $\tilde{\beta}_i$ is however by far too restrictive, since it does not even cover the case considered in Theorem 2.3. The basic reason for this is that in most cases the neutral orthogonal system $\{\tilde{\chi}_i\}$ does not exhaust the space $\mathcal{V}$ in the sense that a complete orthogonal system exhausts a Hilbert space. The inner products with these vectors do not contain enough information about the whole space, and especially its positive part, to decide sharply whether $\mathcal{V}$ is regularizable. The problem of finding a good abstract definition of what we would like to call ''regularizable inner product spaces'' remains therefore open.

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APPENDIX A: CONSTRUCTION OF NEUTRAL DECOMPOSITION ELEMENTS

In this Appendix, we present a simple construction for the neutral decomposing functions of Lemma 3.1. We point out that different and more refined constructions are surely possible, but the one given in the following suffices for our purpose.

We have to show (i)–(iii) since (iv) follows from them. We prove Lemma 3.1 for $\gamma_k=1$, $\forall k$. The general case follows by multiplication of the functions χ_k constructed in the following with the given sequence γ_k. The first thing we need to show is that there are enough functions of compact support in $\mathcal{S}_\alpha^\beta$. For that, we have to consider the spaces $\mathcal{S}_\alpha^{\beta,B}$, which constitute $\mathcal{S}_\alpha^\beta$ as an inductive limit for $B\to\infty$, see Ref. 9, Chap. IV, Sec. 3 for their definition.

Lemma A.1: Let $0\leqslant\alpha\leqslant\infty$ *and* $1<\beta<\infty$. *For* $\varepsilon>0$ *there exists* $B_\varepsilon>0$ *and a function* $\rho_\varepsilon\in\mathcal{S}_\alpha^{\beta,B_\varepsilon}$ *such that*

$$\rho_\varepsilon(x)=\begin{cases}1, & \text{if } |x|<\varepsilon/2\\ 0, & \text{if } |x|>3\varepsilon/2\\ 0\leqslant\rho_\varepsilon(x), & \text{otherwise.}\end{cases}$$

Proof: Under the given conditions, the function ρ_ε can be constructed using the well-known facts about the Gelfand–Shilov spaces, for which we refer to Ref. 9, Chap. IV. The space $\mathcal{S}_\alpha^\beta$ contains the space $\mathcal{S}_0^\beta$ which consists of functions of compact support and is nontrivial for $\beta>1$. Furthermore, for $\phi\in\mathcal{S}_0^\beta$ we have $\phi^2\in\mathcal{S}_0^\beta$. Thus there exists a $B>0$ and a nonzero function ϕ with $\phi(x)\geqslant 0$ in $\mathcal{S}_0^{\beta,B}$, such that supp $\phi\subset[-R,R]$ for some $R>0$. Then

$$\phi_\varepsilon(x)\overset{\text{def}}{=}\frac{\varepsilon}{2R\|\phi\|_{L^1}}\cdot\phi(2Rx/\varepsilon)$$

is an element of $\mathcal{S}_0^{\beta,B_\varepsilon}$ for $B_\varepsilon=2RB/\varepsilon$, see Ref. 9, p. 158. It has L^1-norm 1 and support in $[-\varepsilon/2,\varepsilon/2]$. Since convolution with L^1-functions does not change the regularity, the function $\phi_\varepsilon*\chi_{[-\varepsilon,\varepsilon]}$ is an element of $\mathcal{S}_0^{\beta,B_\varepsilon}$ and therefore *a fortiori* of $\mathcal{S}_\alpha^{\beta,B_\varepsilon}$ with all the desired properties. □

We set

$$\kappa_n(x)\overset{\text{def}}{=}\rho_{1/3}(x-n)/\|\rho_{1/3}\|_{L^2}\ .$$

Since κ_n has support in $[n-1/2,\ n+1/2]$, we have $(\kappa_i,\kappa_j)=0$ for all $i\neq j$. Define a sequence of positive real numbers by

$$\varepsilon_i\overset{\text{def}}{=}\frac{1}{3e}\prod_{k=0}^{i}\min(1,c_k^2). \tag{†}$$

Set

$$\delta_i\overset{\text{def}}{=}\frac{x^i}{i!}\rho_{\varepsilon_i}.$$

Furthermore, for $i\neq j$ define

$$k_{ij}\overset{\text{def}}{=}\text{sign}(i-j)\sqrt{(\delta_j,\delta_i)_{L^2}}.$$

We use the following enumeration for the off-diagonal entries of an infinite matrix (rows and columns counted from 0):

$$\mathbb{N}_0^2\backslash\mathrm{diag}\ni(i,j)\mapsto n(i,j)\overset{\mathrm{def}}{=}\begin{cases}\dfrac{j(j-1)}{2}+i+1 & \text{if } i<j\\ n(j,i), & \text{otherwise.}\end{cases}$$

We use the functions δ_i as building blocks for the desired functions, since they have just the right behavior at 0 to ensure property (ii) of Lemma 3.1. To correct their nonvanishing L^2-overlap with each other we use the corrective

$$K_i\overset{\mathrm{def}}{=}\sum_{j\neq i} k_{ij}\kappa_{n(i,j)}.$$

We must show that this is possible, i.e., that $\|\delta_i+K_i\|_{L^2}^2$ does not exceed c_i^2, in order to satisfy (i). We have

$$\|\delta_i+K_i\|_{L^2}^2=\|\delta_i\|_{L^2}^2+\|K_i\|_{L^2}^2=\sum_{j=0}^{\infty}|(\delta_i,\delta_j)_{L^2}|.$$

The terms in the sum allow for the basic (yet very coarse) estimate

$$|(\delta_i,\delta_j)_{L^2}|\leqslant\frac{2}{i!j!}\left(\frac{3}{2}\min(\varepsilon_i,\varepsilon_j)\right)^{i+j+1}$$

by construction of δ_i. Using (†) we have $\min(\varepsilon_i,\varepsilon_j)\leqslant(i/3\varepsilon)\min(c_i^2,1)$ and therefore we can estimate under the additional assumption $c_i^2\leqslant 1$:

$$\|\delta_i+K_i\|_{L^2}^2\leqslant\sum_{j=0}^{\infty}\frac{2}{i!j!}\left(\frac{c_i^2}{2e}\right)^{i+j+1}\leqslant\frac{2}{i!}\left(\frac{c_i^2}{2e}\right)^{i+1}\sum_{j=0}^{\infty}\frac{c_i^{2j}}{j!}=\frac{2}{i!}\left(\frac{c_i^2}{2e}\right)^{i+1}e^{c_i^2}\leqslant\frac{c_i^2}{i!(2e)^i}\leqslant c_i^2.$$

Now using the function

$$\nu_i=\sqrt{c_i^2-\|\delta_i+K_i\|_{L^2}^2}\,\kappa_{-i}$$

we can set

$$\chi_i\overset{\mathrm{def}}{=}\delta_i+K_i+\nu_i.$$

We are done if we show that χ_i is well defined as a function in $\mathscr{S}_\alpha^\beta$, i.e., that the sum K_i converges in the topology of the namely space. To that end, we have to show convergence in one of the spaces $\mathscr{S}_{\alpha,A}^{\beta,B}$ which constitute the inductive limit $\mathscr{S}_\alpha^\beta=\lim_{\to A,B\to\infty}\mathscr{S}_{\alpha,A}^{\beta,B}$. We show that the increments in the sum K_i, namely $k_{ij}\kappa_{n(i,j)}$, decay fast enough in j to turn the sum into a Cauchy sequence in that topology. In the countably normed space $\mathscr{S}_{\alpha,A}^{\beta,B}$, we therefore have to estimate the increments due to the terms in the sum defining K_i:

$$\|k_{ij}\kappa_{n(i,j)}\|_{\rho,\delta}=\sup_{x_z k.q}\frac{|x^k k_{ij}\kappa_{n(i,j)}|}{(A+\rho)^k(B+\delta)^q k^{k\alpha}q^{q\beta}}\quad\text{with }\rho,\delta>0.$$

We first argue that this quantity can be estimated independently of q. In fact, the functions $\kappa_{n(i,j)}$ are translates of a fixed function in $\mathscr{S}_\alpha^{\beta,B_{1/3}}$, and therefore the supremum over q is smaller than at constant times the supremum over k and x only, if we choose $B=\max(B_{1/3},B_{\varepsilon_i})$:

$$\|k_{ij}\kappa_{n(i,j)}\|_{\rho,\delta} \leqslant C_\kappa \sup_{x,k} \frac{|x^k k_{ij}\kappa_{n(i,j)}|}{(A+\rho)^k k^{k\alpha}}.$$

It suffices to consider this especially for $A \geqslant 1$ and $\alpha = 1$ in which case we have

$$\leqslant C_\kappa \sup_{x,k} \frac{|x^k k_{ij}\kappa_{n(i,j)}|}{k^k}.$$

For j large enough and by definition of $n(i,j)$ we can estimate $|x| \leqslant 2j^2$ on the support of $\kappa_{n(i,j)}$, and with some other constant C'_κ depending only on the function $\kappa_{n(i,j)}$,

$$\leqslant C'_\kappa k_{ij} \sup_k \left(\frac{2j^2}{k}\right)^k.$$

Continuous maximization in k shows

$$\leqslant C'_\kappa k_{ij} e^{cj^2}.$$

Now it is clear from their definition that k_{ij} decay faster than an exponential function of any type in j and thus the claim follows.

APPENDIX B: BASICS OF INDEFINITE INNER PRODUCT SPACES

In this section we recall some facts about indefinite inner product, Krein and Pontryagin spaces needed in the main text. For an extensive discussion of the subject matter we refer the reader to (Refs. 10 and 15). First some notations: Let $\mathcal{V}$ be a vector space equipped with an indefinite inner product $\langle .,. \rangle$ (antilinear in the first, linear in the second argument). The linear span of a subset $\mathcal{A}$ of vectors in $\mathcal{V}$ is denoted by $\langle \mathcal{A} \rangle$. The *linear sum* of subspaces $\mathcal{V}_1,\ldots,\mathcal{V}_n$ of $\mathcal{V}$ is given by $\langle \mathcal{V}_1 \cup \cdots \cup \mathcal{V}_n \rangle$ and denoted by $\mathcal{V}_1 + \cdots + \mathcal{V}_n$. If the spaces $\mathcal{V}_1,\ldots,\mathcal{V}_n$ are linearly independent, their linear sum is termed *direct sum* and denoted by $\mathcal{V}_1 \dot{+} \cdots \dot{+} \mathcal{V}_n$. *Orthogonality* with respect to $\langle .,. \rangle$ is defined, and denoted by the binary relation $\perp$ as usual (but clearly does not have the same strong consequences as in definite inner product spaces). If the $\mathcal{V}_1,\ldots,\mathcal{V}_n$ are mutually orthogonal, their *orthogonal direct sum* is denoted by $\mathcal{V}_1(\dot{+})\cdots(\dot{+})\mathcal{V}_n$, whereas the symbol $\oplus$ is reserved for orthogonal sums with respect to a positive definite inner product, which we will denote with $(.,.)$, following mathematical convention. By *positive definite* we mean as usual $(x,x) \geqslant 0$, $\forall x \neq 0$, and $(x,x) = 0 \Rightarrow x = 0$. A subspace $\mathcal{A}$ of $\mathcal{V}$ is called *positive*, *negative*, or *neutral*, respectively, if one of the possibilities $\langle x,x \rangle > 0$, $\langle x,x \rangle < 0$ or $\langle x,x \rangle = 0$ holds for all $x \in \mathcal{A}$, with $x \neq 0$. One sets

$$\mathcal{V}^{++} \overset{\text{def}}{=} \{x \in \mathcal{V} | \langle x,x \rangle > 0 \text{ or } x = 0\},$$

and calls this subset the *positive part* of $\mathcal{V}$. The *negative* and *neutral* parts $\mathcal{V}^{--}$ and $\mathcal{V}^0$ are defined alike. A subspace $\mathcal{A}$ of $\mathcal{V}$ is called *degenerate*, if its *isotropic part* $\mathcal{A} \cap \mathcal{A}^\perp$ does not only consist of the zero vector. In the main text and the following we will deal merely with *nondegenerate* spaces, i.e., spaces with $\mathcal{V}^\perp = \{0\}$. A nondegenerate inner product space $\mathcal{V}$ is said to be *decomposable* if it admits a *fundamental decomposition*

$$\mathcal{V} = \mathcal{V}^\perp(\dot{+})\mathcal{V}^+(\dot{+})\mathcal{V}^- \quad \text{with } \mathcal{V}^+ \subset \mathcal{V}^{++}, \mathcal{V}^- \subset \mathcal{V}^{--}.$$

For nondegenerate spaces the isotropic part of the decomposition vanishes. The dimension of a maximal negative definite subspace $\mathcal{V}^- \subset \mathcal{V}^{--}$ appearing in a fundamental decomposition of a nondegenerate inner product space is called the *rank of negativity* of $\mathcal{V}$. As proven in Ref. 10,

Corrollaries II.10.4 and IV.7.4, it is a unique positive cardinal denoted by $\varkappa^-(\mathcal{V})$. The *rank of positivity* $\varkappa^+(\mathcal{V})$ is defined in analogy to that. We set $\varkappa \equiv \min(\varkappa^-, \varkappa^+)$ and call this number the *rank of indefiniteness* of $\mathcal{V}$.

Now some less trivial things about the topology of indefinite inner product spaces: A locally convex topology τ on $\mathcal{V}$ defined by a single seminorm p, which is then actually a norm, is called *normed*. If $\mathcal{V}$ is τ-complete, we say that τ is a *Banach topology*. If τ can be defined by a *quadratic norm* $p(x)=(x,x)^{1/2}$, where $(.,.)$ is a positive definite inner product on $\mathcal{V}$, then τ is called a *quadratic normed topology*. Again, if $\mathcal{V}$ is τ-complete, then τ is termed *Hilbert topology*. A normed topology τ_1 is *stronger* than another τ_2, written $\tau_1 \geqslant \tau_2$, if and only if every τ_2-open set is also a τ_1-open set, or equivalently the relation $p_1(x) \geqslant \alpha p_2(x)$ holds for all $x \in \mathcal{V}$, with an $\alpha > 0$. Two norms that define the same topology are called *equivalent*. A locally convex topology τ on $\mathcal{V}$ is called a *partial majorant* of the inner product if $\langle .,. \rangle$ is separately τ-continuous. The *weak topology* on $\mathcal{V}$ is the topology defined by the family of seminorms

$$p_y(x) \overset{\text{def}}{=} |\langle y,x \rangle| \quad \text{for all } x \in \mathcal{V}.$$

Lemma B.1 (Ref. 10, Theorem II.2.1): The weak topology is the weakest partial majorant on $\mathcal{V}$. If a locally convex topology on $\mathcal{V}$ is stronger than the weak topology, then it is a partial majorant.

We will need a stronger concept of topology:

Definition B.2: A locally convex topology τ on $\mathcal{V}$ is called *majorant topology*, if the inner product $\langle .,.. \rangle$ is jointly τ-continuous.

In applications, one can often restrict oneself to majorants defined by a single seminorm which majorizes the inner square, as shown by the following result.

Lemma B.3. (Ref. 10, Lemma IV.1.1. and IV.1.2): It holds:

(i) *To every majorant there exists a weaker majorant defined by a single seminorm.*

(ii) *For a locally convex topology defined by a single seminorm p to be a majorant it is sufficient that p dominates the inner square*:

$$|\langle x,x \rangle| \leqslant \alpha p(x)^2, \quad \alpha > 0, \quad \forall x \in \mathcal{V}.$$

Majorant topologies, and especially majorant Hilbert topologies, have many advantages over partial majorants. Before we describe them, let us see why one would not like to use the weak topology on general indefinite inner product spaces:

Lemma B.4. (Ref. 10, Theorem IV.1.4): The weak topology on the nondegenerate indefinite inner product space $\mathcal{V}$ is a majorant, if and only if $\dim \mathcal{V} < \infty$.

The indefinite inner product on a space equipped with a majorant Hilbert topology admits a simple description by the so-called *metric operator*.

Proposition B.5. (Ref. 10, Theorem IV.5.2): Let $\mathcal{V}$ be an indefinite inner product space with a majorant Hilbert topology τ defined by a norm $\|.\|$. Then there exists a Hermitean linear operator, called metric (or Gram) operator, J on $\mathcal{V}$ such that

$$\langle x,y \rangle = (x,Jy), \quad \forall x,y \in \mathcal{V},$$

where $(.,.)$ is the positive inner product on $\mathcal{V}$ that defines $\|.\|$. Moreover, in this case $\mathcal{V}$ is decomposable and the fundamental decomposition can be chosen so that each of the three components is τ-closed.

The spaces we want to construct in the main text should be complete in a certain sense, which we will now specify.

Definition B.6: If a nondegenerate indefinite inner product space $\mathcal{K}$ admits a decomposition

$$\mathcal{K} = \mathcal{K}^+ (\dot{+}) \mathcal{K}^-, \quad \mathcal{K}^+ \subset \mathcal{K}^{++}, \quad \mathcal{K}^- \subset \mathcal{K}^{--},$$

such that $\mathcal{K}^+,\mathcal{K}^-$ are complete with respect to the restrictions of the weak topology to them (termed *intrinsically complete*), then the space $\mathcal{K}$ is called a *Krein space*.

Krein spaces can easily be characterized:

Proposition B.7. (Ref. 10, Theorem V.1.3): An indefinite inner product space $\mathcal{V}$ is a Krein space if and only if there exists a majorant Hilbert topology τ on $\mathcal{V}$ such that metric operator J is completely invertible.

A Hilbert-space completion $\mathcal{H}$ of an indefinite inner product space $\mathcal{V}$, if it exists together with its metric operator J, is called the *Hilbert space structure* $(\mathcal{H},J)$ associated to $\mathcal{V}$. In applications one would like to find the largest Hilbert space associated to an indefinite inner product space. For that, one considers *minimal* majorant topologies, i.e., topologies τ_* such that no majorant τ is weaker than τ_*. Hilbert space structures given by the completion of $\mathcal{V}$ with respect to a minimal majorant are correspondingly called *maximal*. We find that the Hilbert space structure is maximal, if it leads actually to a Krein space:

Lemma B.8 (Ref. 2, Appendix A.1): A majorant Hilbert topology leads to a maximal Hilbert space structure $(\mathcal{K}, J)$, if and only if J has a bounded inverse. Given a Hilbert space structure one can always construct a maximal one.

The last statement means in effect that every space admitting some majorant Hilbert topology can be completed to a Krein space.

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Lorentz invariant Lagrangians

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The aim of this article is to study certain Lorentz invariant Lagrangians. The first of these Lagrangians could be related to a particle of spin $\frac{1}{2}$ moving in a particular Yang–Mills gauge field. The second Lagrangian is related to the relativistic Newton–Coulomb problem. For each of these Lagrangians, we write the corresponding wave equations and determine the negative energy levels. The article concludes with the construction of a class of Lagrangians associated with pairs of particles, one of which has zero mass. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1420742]

I. INTRODUCTION

The main problem we study in this article is to quantize certain Lorentz invariant Lagrangians; we formally extend the classical two-particle Lagrangians, which have been used in Newtonian gravitation theory and respectively in Pauli's theory of the hydrogen atom.

In the first section, we construct a Lagrangian for a particle moving in a gauge field defined by a Lorentz invariant connection $\mathcal{C}$. The connection $\mathcal{C}$ is defined in a principal bundle $P=\Gamma\to\Sigma$, where Γ is the group of 2×2-complex matrices with positive determinants and Σ is the space of spacelike vectors in Minkowski space. The corresponding Euler–Lagrange equations are similar to Pauli equations, with the differences that they are of order two and refer to a Coulomb field.

We determine the negative energy levels by using representation theory.

The second section is related to the relativistic Kepler–Newton–Coulomb problem, as introduced by L. P. Horwitz (see Ref. 1). We determine the corresponding negative energy levels by using both representation theory as well as the classical theory of second order differential equations of Laplace type.

Representation theory is used in order to determine the eigenvalues of Casimir operators; these values appear in the corresponding radial equations; some of these eigenvalues can also be determined using analysis and imposing specific regularity conditions, as given in Sec. III E.

The final results concerning the energy levels are given in a theorem at the end of Sec. III F.

We had to use many elementary and classical results, which we have written explicitly, in order to dispose of uniform notations for the reader's convenience. Giving proper quotations seems to be a hard task.

We constantly compared the energy spectra obtained in this article to the spectrum obtained by Schrödinger and which is proportional to the sequence $S=(1/n^2)_{n=1,2,3,\ldots}$.

In the two situations we met, certain deviations arose. For instance, in the case of the relativistic Coulomb problem, we obtained a spectrum which is proportional to the sequence $S'=4((2n+1)^{-2})_{n\in\mathbb{N}}=((n+\frac{1}{2})^{-2})_{n\in\mathbb{N}}$.

We assume that we gain the whole of S by introducing the principal series of representations of the group SL(2, $\mathbb{C}$). This can be done by considering some Lorentz invariant Lagrangians associated with two-particle systems, such that one of the two particles lies on the light-cone. These Lagrangians are also linked to two-particle systems, when the particles are separated by a vector of zero length. Though this program is not yet acomplished, the formulas we obtained make our assumption plausible.

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II. THE FIRST LAGRANGIAN

A. A principal SU(1, 1)-bundle

We identify each point $x=(x_0,x_1,x_2,x_3)$ in Minkowski space M with a Hermitian matrix by writing

$$x=\begin{pmatrix} x_0+x_3 & x_1-ix_2 \\ x_1+ix_2 & x_0-x_3 \end{pmatrix},$$

and denote the spatial inversion by a hat; more generally, when $\xi=\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ and ψ are 2×2-matrices, we write

$$\hat{\xi}=\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}, \quad |\xi|^2=-\det(\xi), \quad \langle \xi,\psi\rangle=-\frac{1}{2}\mathrm{Tr}(\psi\hat{\xi}).$$

Let Γ be the group of complex 2×2-matrices with real and positive determinant.

The manifold

$$\Sigma=\{x\in M;\ |x|^2=-\det(x)>0\}$$

is diffeomorphic to $\mathbb{R}^2\times S^2$ and there is a transitive action A of Γ on Σ, which is given by the formula

$$A:\Gamma\times\Sigma\to\Sigma, \quad A(g,x)=gxg^*.$$

Let us consider the Pauli matrix $\sigma_3=\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ and define the map

$$f_3:\Gamma\to\Sigma, \quad f_3(g)=g\sigma_3 g^*.$$

Then

$$f_3^{-1}(\sigma_3)=\mathrm{SU}(1,1), \quad f_3(\Gamma)=\Sigma,$$

and the map f_3 is Γ-equivariant.

The aim of this section is to study the Γ-homogeneous and also principal SU(1, 1)-bundle

$$P=(\Gamma,f_3,\Sigma).$$

For a point $x=(x_0,x_1,x_2,x_3)\in\Sigma$, we denote

$$r=\sqrt{(x_1)^2+(x_2)^2+(x_3)^2}, \quad z=x_1+ix_2,$$

$$R=\sqrt{r^2-(x_0)^2}=\sqrt{-\det(x)}.$$

Each matrix $g=\left(\begin{smallmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{smallmatrix}\right)\in\Gamma$ can be written as a product

$$g=uhv \tag{1}$$

with factors

$$u\in\mathrm{SU}(2), \quad v\in\mathrm{SU}(1,1), \quad h=\mathrm{diag}(h_1,h_2), \quad h_1>0, h_2>0. \tag{2}$$

Let us introduce the notations

$$x=g\sigma_3 g^*, \quad k=h^2\sigma_3=\mathrm{diag}(k_1,k_2).$$

Then $x=uku^*$ and, when we suppose that

$$u=\begin{pmatrix} a & -\overline{b} \\ b & \overline{a} \end{pmatrix},\ \ v=\begin{pmatrix} \alpha & \overline{\beta} \\ \beta & \overline{\alpha} \end{pmatrix},$$

$$|a|^2+|b|^2=1,\ \ |\alpha|^2-|\beta|^2=1,$$

we get

$$2x_0=k_1+k_2,$$

$$2x_3=(k_1-k_2)(|a|^2-|b|^2),$$

$$z=x_1+ix_2=(k_1-k_2)\overline{a}b,$$

$$2r=h_1^2+h_2^2,\ \ R=h_1h_2,$$

$$k_1=x_0+r,\ \ k_2=x_0-r,$$

$$2|a|^2=1+\frac{x_3}{r},\ \ 2|b|^2=1-\frac{x_3}{r},\ \ 2\overline{a}b=\frac{x_1+ix_2}{r}.$$

These relations lead us to the following conclusions:

(1) When the matrix g is given, the matrices h, k are uniquely determined, while the matrices u, v are determined up to a transformation of the form

$$u\mapsto u\ \mathrm{diag}(e^{i\varphi},e^{-i\varphi}),\ \ v\mapsto \mathrm{diag}(e^{-i\varphi},e^{i\varphi})v,\ \ \varphi\in\mathbb{R}.$$

(2) The principal SU(1, 1)-bundle $P=(\Gamma,\ f_3,\Sigma)$ is trivial over each of the sets

$$\Sigma_+=\{x\in\Sigma|x_3>-r\},\ \ \Sigma_-=\{x\in\Sigma|x_3<r\},$$

and we can define the local sections $f_+:\Sigma_+\to\Gamma,\ \ f_-:\Sigma_-\to\Gamma$ by the formulas

$$f_+(x)=u_+(x)h(x),\ \ f_-(x)=u_-(x)h(x), \tag{3}$$

$$u_+(x)=\frac{1}{\sqrt{2r(r+x_3)}}\begin{pmatrix} r+x_3 & -\overline{z} \\ z & r+x_3 \end{pmatrix},$$

$$u_-(x)=\frac{1}{\sqrt{2r(r-x_3)}}\begin{pmatrix} \overline{z} & -r+x_3 \\ r-x_3 & z \end{pmatrix}, \tag{4}$$

$$h(x)=\begin{pmatrix} \sqrt{r+x_0} & 0 \\ 0 & \sqrt{r-x_0} \end{pmatrix}. \tag{5}$$

Then these two local sections are related, over $\Sigma_+\cap\Sigma_-$, by the formula

$$f_+(x)=f_-(x)\ \mathrm{diag}\left(\frac{z}{|z|},\ \frac{\overline{z}}{|z|}\right), \tag{6}$$

showing that the structural group SU(1, 1) of the principal bundle P is reducible to U(1).

B. An invariant Yang–Mills connection

Denote by $V=(E,p,\Sigma)$ the vector bundle with fiber $\mathbb{C}^2$ associated with the principal bundle P. The points of E are equivalence classes

$$[g,\xi]=\{(gv^{-1},v\xi);\ \ v\in \mathrm{SU}(1,1)\},\ \ g\in\Gamma,\ \ \xi\in\mathbb{C}^2. \tag{7}$$

The equation (6) shows that the vector bundle V admits an SU(2)-invariant decomposition into the Whitney sum of two complex line bundles, $V=L_1\oplus L_2$.

By considering the bundle map $f_3:\Gamma\to\Sigma$, we broke the Lorentz symmetry of Minkowski space, since implicitly we distinguish the point $\sigma_3=(0,0,0,1)$; but, considering the bundle P, we gain a richer symmetry, because the group Γ acts transitively on itself by left translations and this action induces a transitive action on Σ.

The Lie algebra sl(2, $\mathbb{C}$) carries an $\mathbb{R}$-bilinear form ω, which is invariant with respect to the linear adjoint representation of SL(2, $\mathbb{C}$) and which is defined by the equation

$$\omega(x,y)=\text{Real part of } \mathrm{Tr}(\hat{x}\ y).$$

When $\omega(x,y)=0$, we say that x is orthogonal to y.

We can use the form ω in order to introduce a Γ-invariant connection $\mathcal{C}$ on the bundle P: the $\mathcal{C}$-horizontal tangent vectors on Γ at a point $g\in\Gamma$ will be the pairs (g,gX) such that $X\in \mathrm{sl}(2,\mathbb{C})\oplus\mathbb{R}\cdot I$ and such that X is orthogonal to all $y\in \mathrm{su}(1,1)$.

The matrices X which are orthogonal to su(1, 1) have the form

$$X=\begin{pmatrix} p+iq & \lambda \\ -\overline{\lambda} & p'+iq \end{pmatrix},\ \ p\in\mathbb{R},\ \ p'\in\mathbb{R},\ \ q\in\mathbb{R},\ \ \lambda\in\mathbb{C}. \tag{8}$$

The equations of the $\mathcal{C}$-horizontal distribution are obtained by writing that the differential matrix $g^{-1}dg$ has the form (8). When we use the decomposition (1), the equations of the $\mathcal{C}$-horizontal distribution take the form

$$d\alpha=-iA\alpha+\overline{B}\beta,\ \ d\beta=B\alpha+iA\beta, \tag{9}$$

where

$$A=-i(\overline{a}da+\overline{b}db),\ \ B=\frac{x_0}{R}(bda-adb). \tag{10}$$

The local sections f_+, f_- defined by formulas (3)–(5) allow us to build the diffeomorphisms

$$\tau_+:\Sigma_+\times \mathrm{SU}(1,1)\to(f_3)^{-1}(\Sigma_+),\ \ \tau_+(x,v)=f_+(x)v, \tag{11}$$

$$\tau_-:\Sigma_-\times \mathrm{SU}(1,1)\to(f_3)^{-1}(\Sigma_-),\ \ \tau_-(x,v)=f_-(x)v. \tag{12}$$

It is convenient to introduce, besides the usual polar coordinates ϑ, φ, a new angle coordinate ψ, so that we have

$$z=r\sin\vartheta\exp(i\varphi),\ \ x_3=r\cos\vartheta,\ \ x_0=r\sin\psi\quad\left(-\frac{\pi}{2}<\psi<\frac{\pi}{2}\right). \tag{13}$$

Then

$$tg\,\psi=\frac{x_0}{R},\ \ tg\,\varphi=\frac{x_2}{x_1},\ \ tg\,\vartheta=\frac{\sqrt{(x_1)^2+(x_2)^2}}{x_3}.$$

The one-forms (10), computed over Σ_+ and Σ_-, become

$$A_+=\frac{x_1dx_2-x_2dx_1}{2r(r+x_3)}=\sin^2\frac{\vartheta}{2}\,d\varphi,$$
$$A_-=-\frac{x_1dx_2-x_2dx_1}{2r(r-x_3)}=-\cos^2\frac{\vartheta}{2}\,d\varphi, \tag{14}$$

$$B_+=-\frac{z^2x_0}{2Rr(r+x_3)}\,d\left(\frac{r+x_3}{z}\right)=-\frac{1}{2}e^{i\varphi}\tan\psi(d\vartheta+i\sin\vartheta d\varphi),$$
$$B_-=-\frac{\overline{z}^2x_0}{2Rr(r-x_3)}\,d\left(\frac{r-x_3}{\overline{z}}\right)=-\frac{1}{2}e^{-i\varphi}\tan\psi(d\vartheta+i\sin\vartheta\,d\varphi). \tag{15}$$

For the reader's convenience, we write down the following formulas, giving the operators of partial derivatives $\partial_\alpha=\partial/\partial_\alpha$:

$$\partial_0=R^{-1}\partial_\psi-tg\psi\,\partial_R,$$

$$\partial_1=R^{-1}\cos\psi\left(-\frac{\sin\varphi}{\sin\vartheta}\partial_\varphi+\cos\varphi\cos\vartheta\,\partial_\vartheta-tg\psi\cos\varphi\sin\vartheta\,\partial_\psi\right)+\frac{\sin\vartheta\cos\varphi}{\cos\psi}\partial_R,$$

$$\partial_2=R^{-1}\cos\psi\left(\frac{\cos\varphi}{\sin\vartheta}\partial_\varphi+\sin\varphi\cos\vartheta\,\partial_\vartheta-tg\psi\sin\varphi\sin\vartheta\,\partial_\psi\right)+\frac{\sin\vartheta\sin\varphi}{\cos\psi}\partial_R,$$

$$\partial_3=-R^{-1}(\cos\psi\sin\vartheta\,\partial_\vartheta+\sin\psi\cos\vartheta\,\partial_\psi)+\frac{\cos\vartheta}{\cos\psi}\partial_R.$$

The connection $\mathcal{C}$ of P induces a connection, also denoted $\mathcal{C}$, on the associated vector bundle V. Since the structural group of V is $SU(1,1)$, V carries an invariant pseudo-Hermitian form H of signature $(1,1)$ and the connection $\mathcal{C}$ is compatible with this structure.

Using the gauge associated with the local section f_+, we can represent a section Φ of V as a pair (Φ^1,Φ^2) of complex valued functions. The covariant derivative D commutes with the action of the group Γ on P and is given by the formula

$$D\Phi=(D\Phi^1,D\Phi^2)=(d\Phi^1+iA\Phi^1-\overline{B}\Phi^2,\,d\Phi^2-B\Phi^1-iA\Phi^2).$$

The group Γ acts on sections $s:\Sigma\to E$ in the bundle V according to the formula $(gs)(x)=g(s(x'))$, where $x'=g^{-1}x(g*)^{-1}$ and

$$g([g_1,\xi])=[gg_1,\xi].$$

This action induces an action α of the Lie algebra of Γ. When we represent the class $[g,\xi]\in E$ through the pair $(g\sigma_3g^*,g\xi)\in\Sigma\times\mathbb{C}^2$, α will associate with the matrices $(i/2)\,\sigma_1,(i/2)\,\sigma_2,(i/2)\,\sigma_3,\frac{1}{2}\sigma_3\in\mathrm{sl}(2,\mathbb{C})$, the following differential operators, acting on maps $\Psi:\Sigma\to\mathbb{C}^2$:

$$d_k=\frac{i}{2}\sigma_k-b_k\sigma_0(k=1,2,3),\quad e_3=\frac{1}{2}\sigma_3+a_3, \tag{16}$$

where

$$b_1=\sin\varphi\,\partial_\vartheta+\cos\varphi\cot\vartheta\,\partial_\varphi,\quad b_2=-\cos\varphi\,\partial_\vartheta+\sin\varphi\cot\vartheta\,\partial_\varphi, \tag{17}$$

$$b_3=-\partial_\varphi,\quad a_3=\cos\vartheta\cos\psi\,\partial_\psi-\sin\vartheta\sin\psi\,\partial_\vartheta. \tag{18}$$

Using the invariant form H of V and the invariant metric of Minkowski space, we get, for any real numbers E_1, C, a Lorentz invariant Lagrangian

$$\mathcal{L}(\Phi)=\int_\Sigma\left(|D\Phi^1|^2-|D\Phi^2|^2+\left(E_1+\frac{C}{R}\right)(|\Phi^1|^2-|\Phi^2|^2)\right)\ dx. \tag{19}$$

C. The Dirac monopole

The bundle P contains an SU(2)-homogeneous principal S^1-subbundle $Q=(\Gamma',q,\Sigma)$ with total space

$$\Gamma'=\{g'=uh|u\in SU(2),\ h=\mathrm{diag}(h_1,h_2),\ h_1>0, h_2>0\},$$

with base-space Σ, projection map $q=f_3|_{\Gamma'}$; the group S^1 acts on Γ' on the right through diagonal matrices diag(exp($i\sigma$),exp($-i\sigma$)).

The connection $\mathcal{C}$ induces a connection $\mathcal{C}'$ on this bundle. The horizontal tangent vectors of Γ' are solutions of the equation

$$d\sigma+iA=0.$$

We easily recognize that the connection $\mathcal{C}'$ represents the vector potential of a Dirac magnetic monopole of magnetic charge 1.

The strength of this magnetic monopole is

$$H=dA=\tfrac{1}{2}\sin\vartheta\ d\vartheta\wedge d\varphi=\frac{1}{2r^3}(x_3\ dx_1\wedge dx_2+x_1\ dx_2\wedge dx_3+x_2\ dx_3\wedge dx_1).$$

As it is well known, reducing the group SL(2,$\mathbb{C}$) to SU(2) is equivalent to fixing the x_0-axis in Minkowski space.

D. The curvature

We now come back to the connection $\mathcal{C}$ and compute the curvature F of $\mathcal{C}$. We have

$$F=d\Lambda-\Lambda\wedge\Lambda,\ \ \Lambda=\begin{pmatrix}-iA & \overline{B}\\ B & iA\end{pmatrix}.$$

More explicitly,

$$F=\begin{pmatrix}-idA+B\wedge\overline{B} & d\overline{B}+2iA\wedge\overline{B}\\ dB-2iA\wedge B & idA-B\wedge\overline{B}\end{pmatrix}.$$

Introducing the differential one-forms

$$f=\frac{\exp(i\varphi)}{\cos\psi}(d\vartheta+i\sin\vartheta\ d\varphi),\ \ j=\frac{d\psi}{\cos\psi},$$

the matrices Λ, F take the forms

$$\Lambda_+=\begin{pmatrix}-i\sin^2\frac{\vartheta}{2}d\varphi & -\frac{1}{2}\sin\psi\ \overline{f}\\ -\frac{1}{2}\sin\psi\ f & i\sin^2\frac{\vartheta}{2}\ d\varphi\end{pmatrix},\quad F_+=\frac{1}{4}\begin{pmatrix}-f\wedge\overline{f} & 2\overline{f}\wedge j\\ 2\,f\wedge j & f\wedge\overline{f}\end{pmatrix}.$$

Using the coordinates R,ϑ,φ,ψ, the metric of Minkowski space, defined as $d\sigma^2=-\det(dx)$ and restricted at Σ, gets the expression

$$d\sigma^2=dR^2+\frac{R^2}{\cos^2\psi}(d\vartheta^2+\sin^2\vartheta\ \ d\varphi^2-d\psi^2). \tag{20}$$

It is now not difficult to compute the Dirac dual $*F$ of the curvature form F and to obtain

$$*F_+=\frac{i}{2}\frac{dR}{R}\wedge\begin{pmatrix} j & -\overline{f} \\ f & -j \end{pmatrix}.$$

It is also not difficult to compute the covariant derivative

$$D(*F_+)=d(*F_+)-[\Lambda,*F_+]=d(*F_+)-\Lambda\wedge *F_+ + *F_+\wedge\Lambda.$$

One verifies the relations

$$df+2i\sin^2\frac{\vartheta}{2}\ \ f\wedge d\varphi+\sin\psi\ \ f\wedge j=0,\ \ dj=0,$$

and obtains the following.

Theorem: The connection $\mathcal{C}$ verifies the Yang–Mills condition

$$D(*F)=0.$$

E. Integrating the Euler–Lagrange equations

In terms of the coordinates R,ϑ,φ,ψ and denoting partial derivatives by indices, the Lagrangian (19) takes the form

$$\begin{aligned}\mathcal{L}(\Phi)=\int_\Sigma\Bigg(&\frac{R^3\sin\vartheta}{\cos^3\psi}(|\Phi^1_R|^2-|\Phi^2_R|^2)-\frac{R\sin\vartheta}{\cos\psi}(|\Phi^1_\psi|^2-|\Phi^2_\psi|^2)+\frac{R\sin\vartheta}{\cos\psi}\Bigg(\left|\Phi^1_\vartheta+\frac{e^{-i\varphi}}{2}\tan\psi\Phi^2\right|^2\\&-\left|\Phi^2_\vartheta+\frac{e^{i\varphi}}{2}\tan\psi\,\Phi^1\right|^2\Bigg)+\frac{R}{\sin\vartheta\cos\psi}\Bigg(\left|\Phi^1_\varphi+i\sin^2\frac{\vartheta}{2}\Phi^1-\frac{i}{2}e^{-i\varphi}\tan\psi\sin\vartheta\,\Phi^2\right|^2\Bigg)\\&-\frac{R}{\sin\vartheta\cos\psi}\Bigg(\left|\Phi^2_\varphi+\frac{i}{2}e^{i\varphi}\tan\psi\sin\vartheta\,\Phi^1-i\sin^2\frac{\vartheta}{2}\Phi^2\right|^2\Bigg)+\left(E_1+\frac{C}{R}\right)\frac{R^3\sin\vartheta}{\cos^3\psi}(|\Phi^1|^2\\&-|\Phi^2|^2)\Bigg)dR\,d\vartheta\,d\varphi\,d\psi.\end{aligned}$$

Looking at the expression to be integrated, we see that there are two corresponding Euler–Lagrange equations for Φ^1 and Φ^2, which can be obtained from one another by interchanging the pairs $(\Phi^1,i),(\Phi^2,-i)$, and there are two other equations, for $\overline{\Phi}^1,\overline{\Phi}^2$, which are obtained from the first ones by complex conjugation.

We can give the Euler–Lagrange equations simple forms by introducing the d'Alembertian

$$\Box=(\partial_0)^2-\sum_{i=1,2,3}(\partial_i)^2. \tag{21}$$

In terms of the coordinates R,ϑ,φ,ψ, one gets

$$\Box=-(\partial_R)^2-\frac{3}{R}\partial_R+\frac{1}{R^2}K, \tag{22}$$

where K is the Casimir operator acting on functions $F:\Sigma\to\mathbb{C}$ and has the expression

$$K=-\cos^2\psi\left((\partial_\vartheta)^2+\cot\vartheta\,\partial_\vartheta+\frac{1}{\sin^2\vartheta}(\partial_\varphi)^2-(\partial_\psi)^2-\tan\psi\,\partial_\psi\right). \tag{23}$$

Note: For the definitions of the Casimir operators used throughout this article, see Secs. II F and III A.

The Euler–Lagrange equations for Φ^1,Φ^2 are written

$$R^2\left(\Box-E_1-\frac{C}{R}\right)\Phi^1=\mathcal{D}_1^+(\Phi^1)+\mathcal{D}_2^+(\Phi^2), \tag{24}$$

$$R^2\left(\Box-E_1-\frac{C}{R}\right)\Phi^2=\mathcal{D}_2^-(\Phi^1)+\mathcal{D}_1^-(\Phi^2), \tag{25}$$

where

$$\mathcal{D}_1^\varepsilon(\Phi)=\varepsilon\frac{i}{2}\frac{\cos^2\psi}{\cos^2(\vartheta/2)}\Phi_\varphi+\frac{1}{4}\left(2-\frac{\cos\vartheta+3}{\cos\vartheta+1}\cos^2\psi\right)\Phi,$$

$$\mathcal{D}_2^\varepsilon(\Phi)=e^{-\varepsilon i\varphi}\sin\psi\cos\psi\left(\Phi_\vartheta-\frac{\varepsilon i}{\sin\vartheta}\Phi_\varphi-\frac{1}{2}tg\frac{\vartheta}{2}\Phi\right).$$

We remark that the two equations (24) and (25) reduce to just one, when we impose the constraint $F^2=\overline{F^1}$.

Suppose we have a particular solution of the form

$$\Phi^1=\rho F^1,\quad \Phi^2=\rho F^2,$$

where ρ is a function of R alone and F^1,F^2 are functions of ϑ,φ and ψ. Then the equations (24), and (25) give

$$\begin{aligned}-\rho^{-1}(R^2\rho_{RR}+3R\rho_R+E_1R^2\rho+CR\rho)&=(F^1)^{-1}((-K+\mathcal{D}_1^+)(F^1)+\mathcal{D}_2^+(F^2))\\&=(F^2)^{-1}(\mathcal{D}_2^-(F^1)+(-K+\mathcal{D}_1^-)(F^2)).\end{aligned}$$

We infer the existence of a constant $\mathbb{K}_0$ such that

$$\rho_{RR}+\frac{3}{R}\rho_R+\left(E_1+\frac{C}{R}-\frac{\mathbb{K}_0}{R^2}\right)\rho=0, \tag{26}$$

$$(-K+\mathcal{D}_1^+)(F^1)+\mathcal{D}_2^+(F^2)=-\mathbb{K}_0F^1, \tag{27}$$

$$\mathcal{D}_2^-(F^1)+(-K+\mathcal{D}_1^-)(F^2)=-\mathbb{K}_0F^2. \tag{28}$$

Considering the map f_+ defined by formula (3), we perform the gauge transformation $F\mapsto G=f_+F$ and ask the new map $G=(G^1,G^2)$ to be **a vector of highest weight**, i.e., we impose the relations

$$d_3G=iMG,\quad (d_1+id_2)G=0,\quad e_3G=NG, \tag{29}$$

where M,N are real numbers and d_1 ,d_2 ,d_3 ,e_3 are the differential matrix operators defined by formulas (16). The equations (29) imply

$$\partial_\varphi G^1=i(M-\tfrac{1}{2})G^1,\quad \partial_\varphi G^2=i(M+\tfrac{1}{2})G^2, \tag{30}$$

$$G^2=-e^{i\varphi}(\partial_\vartheta+i\cot\vartheta\ \ \partial_\varphi)G^1,\ \ (\partial_\vartheta+i\cot\vartheta\ \ \partial_\varphi)G^2=0, \tag{31}$$

$$\cos\vartheta\ \ \cos\psi\ \ G^1_\psi-\sin\vartheta\ \ \sin\psi\ \ G^1_\vartheta=(N-\tfrac{1}{2})G^1, \tag{32}$$

$$\cos\vartheta\ \ \cos\psi\ \ G^2_\psi-\sin\vartheta\ \ \sin\psi\ \ G^2_\vartheta=(N+\tfrac{1}{2})G^2. \tag{33}$$

Denoting $M'=M-\frac{1}{2}$, we find $N=-\frac{1}{2}$ and get the general solution to these equations in the form

$$G^1=C_1\frac{e^{iM'\varphi}(\sin\vartheta)^{M'}(\cos\vartheta-\sin\psi)}{(\cos\psi)^{M'+1}}=C_1\frac{z^{M'}(x_3-x_0)}{R^{M'+1}}, \tag{34}$$

$$G^2=C\frac{e^{i(M'+1)\varphi}(\sin\vartheta)^{(M'+1)}}{(\cos\psi)^{M'+1}}=C\frac{z^{M'+1}}{R^{M'+1}}, \tag{35}$$

where C_1 is a constant. A not very long computation gives

$$\mathbb{K}G=\mathbb{K}_0G, \tag{36}$$

where $\mathbb{K}$ is the Casimir operator (44), defined in the next subsection, and

$$\mathbb{K}_0=M^2+2M+\tfrac{1}{4}=M'^2+3M'+\tfrac{3}{2}. \tag{37}$$

Note that M' must be a positive integer.

Looking at the equations (27), (28), and (36) and having in mind the fact that there exist no Lorentz invariant, non trivial, linear systems of PDEs of the first order, we infer that the equations (27) and (28) transform into the equation (36), when we perform the gauge transformation $G=f_+F$. The gauge map f_+ given by formula (3) can be also written as follows:

$$f_+(x)=R^{1/2}\begin{pmatrix}\cos\dfrac{\vartheta}{2} & -e^{-i\varphi}\sin\dfrac{\vartheta}{2}\\ e^{i\varphi}\sin\dfrac{\vartheta}{2} & \cos\dfrac{\vartheta}{2}\end{pmatrix}\begin{pmatrix}\sqrt{\dfrac{1+\sin\psi}{\cos\psi}} & 0\\ 0 & \sqrt{\dfrac{1-\sin\psi}{\cos\psi}}\end{pmatrix}. \tag{38}$$

Resuming, we can state the following.

Theorem: The equations (34), (35), and (37), joined to $F=(f_+)^{-1}G$, define the solutions to the equations (27) and (28), which are vectors of highest weight with respect to the action of $\mathrm{sl}(2,\mathbb{C})$ on sections in the vector bundle V.

F. Review of classical results

In order to dispose of uniform notations and to be very explicit, we review some classic results. We begin by considering functions

$$F:\mathrm{SL}(2,\mathbb{C})\to\mathbb{C},\ \ g\mapsto F(g,\overline{g}),$$

and introducing the differential operators

$$C_1=-(g^1_jd^j_2+g^2_jd^j_1),\quad C'_1=-(h^1_je^j_2+h^2_je^j_1),$$

$$C_2=-i(g^1_jd^j_2-g^2_jd^j_1),\quad C'_2=i(h^1_je^j_2-h^2_je^j_1),$$

$$C_3=-(g^1_jd^j_1-g^2_jd^j_2),\quad C'_3=-(h^1_je^j_1-h^2_je^j_2),$$

where summation is understood over $j=1,2$ and

$$h_j^i=\overline{g_j^i},\quad d_i^j=\frac{\partial}{\partial g_j^i},\quad e_i^j=\frac{\partial}{\partial \overline{g_j^i}}.$$

Then the following operators are induced by infinitesimal right translations on the group $SL(2,\mathbb{C})$ and generate the Lie algebra $sl(2,\mathbb{C})$:

$$A_k=\frac{1}{2}(C_k+C_k'),\quad B_k=\frac{i}{2}(C_k'-C_k)\quad (k=1,2,3).$$

The Casimir operator K is defined as follows:

$$\begin{aligned}K&=\frac{1}{2}\sum_{k=1}^{3}((C_k)^2+(C_k')^2)\\&=\sum_{k=1}^{3}((A_k)^2-(B_k)^2)\\&=\frac{1}{4}(2g_j^ig_s^kd_k^jd_i^s-g_j^ig_s^rd_i^jd_r^s+2h_j^ih_s^re_r^je_i^s-h_j^ih_s^re_i^je_r^s).\end{aligned}$$

Suppose the function F has the particular form

$$F(g,\overline{g})=\varphi(x),\quad x=g\sigma_3g^*.$$

Then, using the notations

$$\partial_\alpha=\frac{\partial}{\partial x^\alpha},\quad \Box=\partial_0^2-\partial_1^2-\partial_2^2-\partial_3^2,$$

we have

$$K(F)=\left(\sum_{k=1}^{3}(C_k)^2\right)(F)=\left(\sum_{k=1}^{3}(C_k')^2\right)(F),$$

$$((d_1^1d_2^2-d_2^1d_1^2)(F))(g,\overline{g})=\det(\overline{g})\quad(\Box\varphi)(x),\tag{39}$$

$$((e_1^1e_2^2-e_2^1e_1^2)(F))(g,\overline{g})=\det(g)(\Box\varphi)(x),\tag{40}$$

$$K(F)=R^2\Box\varphi+\sum_{\alpha,\beta=0}^{3}x_\alpha x_\beta\ \partial_\alpha\partial_\beta\varphi+3\sum_{\alpha=0}^{3}x_\alpha\ \partial_\alpha\varphi,\tag{41}$$

$$A_i(F)=a_i(\varphi):=(x_0\partial_i+x_i\partial_0)(\varphi),\tag{42}$$

$$B_i(F)=b_i(\varphi):=-(x_j\partial_k-x_k\partial_j)(\varphi),\tag{43}$$

$$(ijk)=(123),(231),(312),$$

$$\left(\sum_{k=1}^{3}A_kB_k\right)(F)=\left(\sum_{k=1}^{3}B_kA_k\right)(F)=0.$$

The Casimir operator of the group $SU(2)$ has the expression

$$K_u=-\sum_{k=1}^{3}(B_k)^2=-r^2\Delta+\sum_{i,j=1}^{3}x_ix_j\partial_i\partial_j+2\sum_{j=1}^{3}x^j\partial_j,$$

where

$$\Delta=(\partial_1)^2+(\partial_2)^2+(\partial_3)^2.$$

When the Casimir operators K,K_u have to act either on maps $\Psi=f_+\Phi:\Sigma\to\mathbb{C}^2$ or on sections of the bundle $P=(\Gamma,f_3,\Sigma)$, their actions are given by the formulas

$$\mathbb{K}=\frac{3}{2}+K+\sum_{k=1}^{3}(a_k+ib_k)\sigma_k, \tag{44}$$

$$\mathbb{K}_u=\frac{3}{4}+K_u+i\sum_{k=1}^{3}b_k\sigma_k. \tag{45}$$

III. THE RELATIVISTIC COULOMB PROBLEM

A. The Lie algebra so(2,3)

There is a spinorial representation of the Lie algebra sl(2,$\mathbb{C}$) on End($\mathbb{C}^2$), which is given by the following endomorphisms:

$$M_{0k}(g)=\frac{1}{2}\sigma_k g\sigma_3,\quad M_{ij}(g)=-\frac{i}{2}\sigma_k g,$$

where $(ijk)=(123),(231),(312)$.

An extension of sl(2,$\mathbb{C}$) is obtained by adding the four endomorphisms:

$$M_{04}(g)=\frac{1}{2}g\sigma_1,\quad M_{k4}(g)=-\frac{i}{2}\sigma_k g\sigma_2.$$

We let $M_{\alpha\beta}=-M_{\beta\alpha}$. Then, omitting to write brackets which vanish, the commutation relations of this extended Lie algebra are

$$[M_{0i}\ ,M_{0j}]=M_{ij},\quad [M_{i4}\ ,M_{j4}]=M_{ij},$$

$$[M_{\alpha i}\ ,M_{i\beta}]=M_{\alpha\beta}.$$

We recognize the structure of the algebra so(2,3). In fact, we produced the fundamental spinorial representation of the algebra so(2,3).

It is not difficult to check that the skew-form $\sigma_0\wedge\sigma_3-i\sigma_1\wedge\sigma_2$ is Lorentz-invariant, showing that so(2,3) is a real form of the simplectic Lie algebra sp(4).

We introduce the notations

$$H_1=M_{03},\quad H_2=M_{12},$$

$$F_+=M_{04}+M_{34},\quad F_-=M_{04}-M_{34},$$

$$G_+=M_{14}+iM_{24},\quad G_-=M_{14}-iM_{24},$$

$$E_{\varepsilon\eta}=[F_\varepsilon\ ,G_\eta]=M_{01}+\varepsilon M_{31}+i\eta(M_{02}-\varepsilon M_{23}),$$

$$\varepsilon,\eta\in\{+,-\}.$$

Suppose we have a linear, finite dimensional, irreducible representation

$$\rho:\mathrm{so}(2,3)\to\mathrm{End}(V).$$

A vector $x_0\in V$, $x_0\neq 0$, is said to be a vector of highest weight if

$$F_+(x_0)=G_+(x_0)=E_{+-}(x_0)=0. \tag{46}$$

Since $E_{++}=[F_+,G_+]$, these conditions also imply

$$E_{++}(x_0)=0,\ (M_{01}+M_{31})(x_0)=0,\ (M_{02}-M_{23})(x_0)=0. \tag{47}$$

The Casimir operator K' of so(2,3) is defined as

$$K'=K+K_1\ , \tag{48}$$

where K is the Casimir operator of sl(2,$\mathbb{C}$), i.e.,

$$K=(M_{01})^2+(M_{02})^2+(M_{03})^2-(M_{12})^2-(M_{23})^2-(M_{31})^2 \tag{49}$$

and where

$$K_1=(M_{14})^2+(M_{24})^2+(M_{34})^2-(M_{04})^2. \tag{50}$$

Direct computations give the following six relations:

$$\begin{aligned}K'&=(H_1)^2-(H_2)^2-\tfrac{1}{2}(F_+F_-+F_-F_+-G_+G_--G_-G_+)\\&\quad-\tfrac{1}{4}(E_{++}E_{--}+E_{--}E_{++}+E_{+-}E_{-+}+E_{-+}E_{+-})\\&=(H_1)^2-(H_2)^2-\tfrac{1}{2}([F_+,F_-]-[G_+,G_-])-F_-F_++G_-G_+\\&\quad-\tfrac{1}{4}([E_{++},E_{--}]+[E_{+-},E_{-+}])-\tfrac{1}{2}(E_{--}E_{++}+E_{-+}E_{+-})\\&=(H_1)^2-(H_2)^2+2H_1+(H_1-iH_2)-\tfrac{1}{2}(E_{--}E_{++}+E_{-+}E_{+-})-(F_-F_+-G_-G_+),\end{aligned}$$

$$[E_{++},E_{--}]=-4(H_1-iH_2),\quad [E_{+-},E_{-+}]=-4(H_1+iH_2),$$

$$[F_+,F_-]=-2H_1,\quad [G_+,G_-]=-2iH_2\ ,$$

which enable us to state the following.

Theorem: (i) Suppose x_0 is a vector of highest weight and that

$$H_1(x_0)=Nx_0,\ H_2(x_0)=iMx_0. \tag{51}$$

Then

$$K'(x_0)=(N^2+M^2+3N+M)x_0. \tag{52}$$

(ii) Due to relations (47), x_0 is a vector of highest weight also with respect to sl(2,$\mathbb{C}$).

(iii) For vectors of highest weight in irreducible representations of sl(2,$\mathbb{C}$), satisfying the relations (46),

$$K(x_0)=(N^2+M^2+2N)x_0\ . \tag{53}$$

(iv) In tensorial representations of so(2,3) or of sl(2,$\mathbb{C}$), M and N are integers, while in spinorial representations, M and N are half integers.

B. The relativistic BLRL vector

We now denote by x^α and $x_\alpha=\eta_{\alpha\beta}x^\beta$ the coordinates of a point x in $\mathbb{R}^4$, where

$$-\eta_{00}=\eta_{11}=\eta_{22}=\eta_{33}=1\ ,\ \ \eta_{\alpha\beta}=0 \qquad \text{for} \quad \alpha\neq\beta.$$

The following differential operators generate the Lie algebra of the Lorentz group:

$$M_{\alpha\beta}=x_\alpha\partial_\beta-x_\beta\partial_\alpha.$$

Following L. P. Horwitz (see Refs. 1–3), we introduce the relativistic BLRL (Bernoulli–Laplace–Runge–Lenz) vector

$$\mathbb{D}=(D_0\ ,D_1\ ,D_2\ ,D_3)$$

with components

$$D_\alpha=2M_{\lambda\alpha}\partial^\lambda+3\partial_\alpha+2kR^{-1}x_\alpha=2\partial^\lambda M_{\lambda\alpha}-3\partial_\alpha+2kR^{-1}x_\alpha=2x_\lambda\partial^\lambda\partial_\alpha-2x_\alpha\partial_\lambda\partial^\lambda+3\partial_\alpha+2kR^{-1}x_\alpha,$$

where k is a real number and

$$R^2=x^\lambda x_\lambda\,,\quad \partial^\lambda=\eta^{\lambda\alpha}\partial_\alpha,\ \ \eta^{\lambda\alpha}=\eta_{\lambda\alpha}.$$

It is not difficult to prove the following.

Proposition: Each component D_α is a Hermitian differential operator which commutes with the Newton–Coulomb Hamiltonian

$$H=-\tfrac{1}{2}\partial^\lambda\partial_\lambda-kR^{-1}.$$

Proposition: The following relations hold:

$$x^\alpha D_\alpha-2kR=-3x^\alpha\ \partial_\alpha+2K,$$

$$D_\alpha\ x^\alpha-2kR=3x^\alpha\ \partial_\alpha+2K+12,$$

$$\{x^\alpha,D_\alpha\}-4kR=4K+12,$$

where $K=-\Sigma_{\alpha<\beta}M^{\alpha\beta}M_{\alpha\beta}$ is the Casimir operator of $\mathrm{sl}(2,\mathbb{C})$.

By direct computations, one derives the relations

$$[M_{\alpha\beta}\ ,M_{\lambda\rho}]=\eta_{\beta\lambda}M_{\alpha\rho}+\eta_{\alpha\rho}M_{\beta\lambda}-\eta_{\beta\rho}M_{\alpha\lambda}-\eta_{\alpha\lambda}M_{\beta\rho},$$

$$[D_\alpha\ ,D_\beta]=-8HM_{\alpha\beta},\quad [M_{\alpha\beta}\ ,D_\lambda]=\eta_{\beta\lambda}D_\alpha-\eta_{\alpha\lambda}D_\beta, \tag{54}$$

$$D^\alpha D_\alpha=2(4K+9)H+4k^2.$$

Let L' be the Lie algebra generated by the operators $M_{\alpha\beta},D_\alpha$ and let us consider a representation space of the Lie algebra L', on which H has a fixed value $E<0$. Then, denoting $D_\alpha=2\sqrt{-2E}\,M_{\alpha4}$, we recognize the commutation relations of the Lie algebra $L'=\mathrm{so}(2,3)$. Taking $\eta_{44}=-1$ and introducing the Casimir operator K' of L',

$$K'=-\sum_{0\leqslant I<J}^{4}M_{IJ}M^{IJ}=K-\frac{D^\alpha D_\alpha}{8E},$$

formula (54), with H replaced by E, gives

$$E=\frac{-2k^2}{4\left(K_0'+\frac{9}{4}\right)}, \tag{55}$$

where K_0' are the eigenvalues of the Casimir operator K', which are given by formula (52).

In order to determine irreducible tensorial representations of L', we try to detect vectors of highest weights, using the equations (47) and (51). More precisely, we look for differentiable functions $f:\Sigma\to\mathbb{C}$ that are solutions of the following system of partial differential equations, characterizing simultaneous (H,M_{12},M_{03}) eigenvectors of highest weights:

$$Hf=Ef,\ \ M_{12}f=iMf,\ \ M_{03}f=Nf, \tag{56}$$

$$(M_{01}+M_{31})f=0,\ \ (M_{02}-M_{23})f=0, \tag{57}$$

$$(D_0+D_3)f=0,\ \ (D_1+iD_2)f=0. \tag{58}$$

The solutions of Eqs. (57) are functions $F(w,R)$ of $w=x^0-x^3$ and R. The equations (56) imply $M=0$ and

$$wF_w=NF,\ \ 2wF_{wR}+RF_{RR}+3F_R+2(k+ER)F=0,$$

and it follows that F has the form $F(w,R)=w^Ng(R)$, where the function g verifies the differential equation

$$Rg''(R)+(2N+3)g'(R)+2(k+ER)g(R)=0.$$

The equations (58) imply $2F_{wR}+3F_R+2kF=0$, and we get $g''=-2Eg$. The general solution of the system (56)–(58) will be, up to a constant factor,

$$f_N(x)=\exp\left(\frac{-2kR}{2N+3}\right)(x^0-x^3)^N$$

with

$$E=\frac{-k^2}{2\left(N+\frac{3}{2}\right)^2}. \tag{59}$$

The relations (52) and (53), giving the eigenvalues of K and K', joined to $M=0$, imply

$$K'(f_N)=N(N+3)f_N,\ \ K(f_N)=N(N+2)f_N.$$

As it is well known, a vector f of highest weight in V is a generator of the representation space V, i.e., $V=L'f$.

The functions $f_{m,N}=(D_1-iD_2)^m(f_N)$ are solutions of the equation $M_{12}f=-imf$. To give an example, we note that

$$f_{1,N}=(D_1-iD_2)(f_N)=-\frac{4nk(x^1-ix^2)}{(2N+3)R}\ f_N.$$

Alternatively, we can treat the eigenvalue problem, in the case of the Hamiltonian $H=-\frac{1}{2}\partial_\lambda\partial^\lambda-kR^{-1}$, by using the reduced symmetry SO(3). Looking for solutions of the system of equations

$$Hf=Ef,\ \ M_{12}f=imf,\quad (M_{23}+iM_{31})f=0,$$

we find

$$f=(x_1+ix_2)^m \;\; r^{-(2m+1)}\psi(R),$$

where ψ is a solution of the following equation:

$$\psi''(R)-\frac{2m-1}{R}\psi'(R)+2\left(E+\frac{k}{R}\right)\psi(R)=0.$$

C. A class of equivalent Lagrangians

The Lagrangian

$$L_1=\frac{m_1}{2}|x'|^2+\frac{m_2}{2}|y'|^2+\frac{C}{R}=\frac{A}{2}|u'|^2+\frac{B}{2}|w'|^2+\frac{C}{R}$$
$$\left(u=x-y,\;\; w=\frac{m_1x+m_2y}{m_1+m_2}\right) \tag{60}$$

is associated with a pair of particles x, y in Minkowski space and is similar to the Lagrangian associated with a two-particle gravitational interaction in Newtonian mechanics. The extremal trajectories obey Kepler's laws (see Ref. 3). The constants A, B are related to the masses m_1, m_2 of the two particles according to the formulas

$$B=(m_1+m_2),\;\; AB=m_1m_2.$$

Consequently, we must have $A>0$, $B>0$, $B\geqslant 4A$.

Let us consider, more generally, Lagrangians of the form

$$L_2=\frac{U}{2}(A|u'|^2+B|w'|^2)+V,$$

where $u=u(s), w=w(s)$ are trajectories in Minkowski space, U,V are functions of $R=|u|$, and A, B are real nonvanishing numbers.

When we introduce the time parameter τ, along each trajectory, such that $ds/d\tau=U$, the Euler–Lagrange equations, for a fixed constant level $L_2-2V=E$, take the form

$$A\frac{d^2u}{d\tau^2}=\left(\frac{d}{dR}(EU+UV)\right)\frac{u}{R},\;\; (Uw')'=0.$$

Besides $E=L_2-2V$, we get two other constants of motion: the vector $P=BUw'$ and the scalar

$$E_{\text{int}}=\frac{A}{2}\left|\frac{du}{d\tau}\right|^2-U(V+E)=U\left(\frac{AU}{2}|u'|^2-V-E\right)=-\frac{|P|^2}{2B}.$$

The extremal trajectories of L_2 obey Kepler's laws, for all energy levels E, when U,V have the form

$$U=\frac{a+bR}{R},\quad V=\frac{c+dR}{a+bR},$$

where a,b,c,d are real numbers and a,bc are not both equal to zero. Under these circumstances, the equations of motion write

$$A\frac{d^2u}{d\tau^2}=-\frac{c+aE}{R^3}u.$$

The constant E_{int} plays the role of internal energy, while $P=BUw'$ is the total momentum vector and $E_{\text{tr}}=-(2B)^{-1}|P|^2$ plays the role of energy of translation. We obtained the equality $E_{\text{int}}=E_{\text{tr}}$.

D. Two-particle relativistic wave equations

The wave equation associated with the Lagrangian L_2 writes

$$\Box_u F-3U^{-1}\frac{dU}{dR}\frac{\partial F}{\partial R}-\frac{2AU(V+E)}{\kappa^2}+\frac{A}{B}\Box_w F=0.$$

In the particular case (60), we get the following wave equation:

$$\Box_u F-\frac{2A}{\kappa^2}\left(E+\frac{C}{R}\right)F+\frac{A}{B}\Box_w F=0.$$

This equation can be given the form

$$\mathcal{H}(F)=E_2F,E_2=E-\frac{\kappa^2}{2B}\Box_w, \tag{61}$$

where $\mathcal{H}$ is the Hamiltonian of the relative motion:

$$\mathcal{H}=\frac{\kappa^2}{2A}\Box_u-\frac{C}{R}. \tag{62}$$

We also introduce the operator of radial derivation

$$X=u^\alpha\partial_\alpha.$$

Making use of formula (41), the wave equation (61) becomes

$$\frac{2AR^2}{\kappa^2}\left(E+\frac{C}{R}-\frac{\kappa^2}{2B}\Box_w\right)F+X^2(F)+2X(F)=KF. \tag{63}$$

Let us suppose that the wave function F is a product of three functions:

$$F(u,w)=f(R)G(u)H(w),$$

where the functions $G(u),H(w)$ satisfy the equations

$$X(G)=0,\quad K(G)=K_0G,\quad \Box_w H=-\frac{\mu^2}{\kappa^2}H, \tag{64}$$

with constant coefficients K_0,μ. Then G is homogeneous of degree 0 and

$$K(fGH)=fK(G)H,\quad R^2\Box G=K_0G.$$

From the wave equation (63) we get the following radial equation:

$$f''(R)+\frac{3}{R}f'(R)+\left(p+\frac{q}{R}-\frac{K_0}{R^2}\right)f(R)=0, \tag{65}$$

where

$$p=\frac{2A}{\kappa^2}\left(E+\frac{\mu^2}{2B}\right),\quad q=\frac{2AC}{\kappa^2}. \tag{66}$$

We assume that E is the energy of the system of two particles, while

$$E_2=E+\frac{\mu^2}{2B}$$

is the energy of the relative motion.

E. The quantization conditions

Using standard methods, we now give some essentially known results concerning the ordinary differential equations of the form

$$f''(x)+\frac{s}{x}f'(x)+\left(p+\frac{q}{x}+\frac{r}{x^2}\right)f(x)=0, \tag{67}$$

where p,q,r,s are real numbers.

We shall solve the equation (67) for $x>0$, under certain regularity conditions and supposing

$$p<0. \tag{68}$$

Problems of this type have been studied since long ago (see Refs. 4 and 5). The regularity conditions generally adopted imply the fact that the solutions f have the form

$$f(x)=\exp(bx)x^a\times\text{polynomial of } x,\quad b<0,$$

and belong to some finite dimensional representation vector spaces of a certain symmetry group.

We shall impose the following regularity conditions:

(i) The function f must be real analytic for all $x>0$.
(ii) f must vanish at infinity.

When we write the solutions of Eq. (67) as follows,

$$f(x)=x^\alpha e^{bx}\vartheta(x),\quad b<0,$$

we get the equation

$$x^2\vartheta''(x)+[2bx^2+(s+2\alpha)x]\vartheta'(x)+[(b^2+p)x^2$$
$$+(q+bs+2\alpha b)x+\alpha(\alpha-1)+r+\alpha s]\vartheta(x)=0.$$

We define h,α,b,l,k such that we have

$$h^2=\frac{(s-1)^2}{4}-r,\quad b^2=-p,\quad \alpha=\frac{1-s}{2}+h,\quad l=2h+1,\quad k=\frac{q}{b}. \tag{69}$$

Then the equation satisfied by ϑ becomes

$$x\vartheta''(x)+(2bx+l)\vartheta'(x)+b(k+l)\vartheta(x)=0. \tag{70}$$

Since we supposed $p<0$, we get two real solutions for b; we choose the negative solution.

Suppose we have a solution f with

$$f(x)=x^{\alpha}e^{bx}\vartheta(x)=x^{\alpha}e^{bx}\sum_{i=-\infty}^{\infty}a_i x^{\beta+i},$$

where $0\leqslant\beta<1$. Then we shall have, for all indices i,

$$(\beta+i+1)(\beta+i+l)a_{i+1}=-2b\left(\beta+i+\frac{k+l}{2}\right)a_i.$$

It follows that the power series $\Sigma_{i=0}^{-\infty}a_i x^i$ is divergent for $x>0$, unless there exists an integer n such that $a_{n-\lambda}=0$ for all $\lambda>0$. Since we look for nontrivial solutions, we shall suppose that $a_n\neq 0$. Then

$$(n+\beta)(n+\beta+l-1)=0.$$

For $i>0$, we introduce the coefficients

$$c_i=\Pi_{j=1}^{i}\left(1+\frac{\beta}{j}\right),\quad a_i'=i!c_i(-2b)^{-i}a_i;$$

since $i!c_i<(i+1)!$, we have $0<c_i<i+1$. We also have

$$f(x)=e^{bx}x^{\alpha+\beta}\vartheta_1(x),\quad \vartheta_1(x)=\sum_{i\geqslant n}(c_i)^{-1}a_i'\frac{(-2bx)^i}{i!},$$

$$(\beta+i+l)a_{i+1}'=\left(\beta+i+\frac{k+l}{2}\right)a_i',$$

$$a_n'\neq 0,$$

and, as long as $\beta+i+l\neq 0$,

$$a_{i+1}'=\left(1+\frac{k-l}{2(\beta+i+l)}\right)a_i'.$$

For i large, all a_i have the same sign and $|a_{i+1}'/a_i'|>2/3$. Then there exist a positive constant C and a natural number N such that, for $i>N$,

$$C|a_i'|>2^i/3^i.$$

Comparing the series $Cx\vartheta(x)$, $\exp(-2bx)$, we get

$$C|a_i'|(-2bx)^i>(-\tfrac{4}{3}bx)^i \text{ for large } i \text{ and } x>0,$$

$$\exp(bx)|x^{1-\beta}\vartheta(x)|>\exp\left(-\frac{bx}{3}\right) \text{ for large positive } x,$$

and we infer that the function f will be bounded at infinity if and only if the number of coefficients $a_i\neq 0$ is finite. Thus there must exist a natural number m such that $a_{m-1}\neq 0$ and $a_i=0$ for $i>m-1$. Then we get

$$\vartheta(x)=x^{\beta}\sum_{i=n}^{m-1}a_i x^i,\quad f(x)=e^{bx}x^{\alpha}\vartheta(x),$$

$$k=2-2m-2\beta-l=1-2(m+\beta+h), \tag{71}$$

$$(\beta+n)(\beta+n+l-1)=0.$$

Note that the number of monomials arising in $\vartheta(x)$ equals $m-n$, so that we must have $m>n$. We also have

$$p=-b^2=-\frac{q^2}{k^2}=-\frac{q^2}{(2\beta+2h+2m-1)^2}. \tag{72}$$

When $q=k=0$, we get

$$h=\frac{1}{2}-m,\quad r=\frac{(1-s)^2}{4}-\left(m-\frac{1}{2}\right)^2.$$

F. The Spectrum

In the radial equation corresponding to the classical Schrödinger equation for the hydrogen atom, one has

$$s=2,\quad r=-l'(l'+1),\quad 2h=-(2l'+1),\quad l'\in\mathbb{N},\quad p=\frac{-q^2}{4(l'+m)^2},$$

where, according to Schrödinger's terminology, $l'+m$ is the principal quantum number, $l'+1$ is the azimuthal quantum number and $m-1$ is the radial quantum number.

The radial equation (26) of the Lagrangian $\mathcal{L}$ in formula (19) has, according to formula (37), $\mathbb{K}_0=M'^2+3M'+\frac{3}{2}$, so that $h^2=(M'+\frac{3}{2})^2+\frac{1}{4}$.

In the case of the equation (65), which is associated with the Lagrangian (60), we get $h^2=K_0+1$, where K_0 is an eigenvalue of the Casimir operator K.

According to formula (53), when F belongs to an irreducible, finite dimensional representation of the group SL(2,$\mathbb{C}$), there exist two positive integers $2M,2N$ such that $K_0+1=M^2+(N+1)^2$.

For a tensorial representation, one has $M=0$, N is an integer and we get $K_0+1=(N+1)^2, h=\pm(N+1), l=\pm 2(N+1)+1$. The relations (71) and $0\leqslant\beta<1$ show that $\beta=0$ and $n(n+l-1)=0$.

Introducing these values in formulas (66), we get the following.

Theorem: Under the regularity conditions (i) and (ii) of Section III E, the negative energy levels E_1,E_2 associated with the Lagrangians (19), respectively with the Hamiltonian (62) with $A>0$, are given by the formulas

$$E_1=\frac{-C^2}{(2\beta_1\pm 2h_1+2m-1)^2},\quad E_2=\frac{-AC^2}{2\kappa^2(m\pm(N+1)-1/2)^2}, \tag{73}$$

where M',m,N are positive integers, $(h_1)^2=(M'^2+\frac{3}{2})^2+\frac{1}{4}$ and β_1 has to be determined by using the equations (69) and (71).

When N is a half integer, E_2 will belong to the Schrödinger spectrum, but the corresponding solution f of the equation (67) will be defined up to sign and will belong to an infinite dimensional representation space of SL(2,$\mathbb{C}$).

Among the unitary, irreducible representations of the group SL(2,$\mathbb{C}$), one distinguishes the principal series of unitary representations (see Ref. 6, Chap. III). For a representation of the principal series, K_0+1 has the form $(N^2-\rho^2)/4$, with $N\in\mathbb{N}$ and $\rho\in\mathbb{R}$. When $\rho=0$, we shall have $h^2=K_0+1=N^2/4$ and, formally, we get

$$E_2=\frac{-AC^2}{2\kappa^2(m\pm N/2-1/2)^2}.$$

This follows:

Proposition: The unitary representations of the principal series with $\rho=0$ give the discrete spectrum obtained by Schrödinger for the atom of hydrogen.

IV. THE NEW LAGRANGIANS

A. Geometric considerations

The representations of the principal series are realized in spaces formed by functions defined on the tangent space of the complex projective line $P^1(\mathbb{C})$.

The complex projective line $P^1(\mathbb{C})$ can be identified, as SL(2,$\mathbb{C}$)-space, with the space Π of straight lines lying on the light-cone

$$\Lambda=\{\xi\in M;|\xi|^2=0\},$$

by identifying each point $[z_1,z_2]\in P^1(\mathbb{C})$ with the vector line generated by the vector

$$\xi=\tfrac{1}{2}(|z_1|^2+|z_2|^2,z_1\overline{z_2}+\overline{z_1}z_2,-i(z_1\overline{z_2}-\overline{z_1}z_2),|z_1|^2-|z_2|^2).$$

The light-cone Λ is the boundary of Σ.

The space Π is a coset space of $\Lambda_0=\Lambda\backslash\{0\}$ and the tangent space $T\Pi$ is a coset space of $T\Lambda_0$. We have

$$T\Lambda_0=\{(\xi,u)\in\Lambda\times M;\xi\neq 0,\langle\xi,u\rangle=0\},$$

$$T\Pi=\{[\xi,u];(\xi,x)\in T\Lambda_0\},$$

where $[\xi,u]=\{(a\xi,au+b\xi);a\in\mathbb{R},a\neq 0,b\in R\}$.

When $(\xi,u)\in T\Lambda_0$ and $|u|^2\neq 0$, we have $|u|^2>0$, i.e., $u\in\Sigma$. Denote

$$T_+\Lambda_0=\{(\xi,u)\in T\Lambda_0;\xi^0>0,|u|^2>0\}$$

and $\pi(\xi,u)=u,\pi_+=\pi|T_+$. When $(\xi,u)\in T_+\Lambda_0$ and $u=\sigma_3=(0,0,0,1)$, we have $\xi^0=\sqrt{(\xi^1)^2+(\xi^2)^2},\xi^3=0$. We then have the following.

Proposition: The triple $(T_+\Lambda_0,\pi_+,\Sigma)$ is a principal $\mathbb{C}^*$-fiber bundle with structure group $\mathbb{C}^*=\{z\in\mathbb{C};z\neq 0\}$.

Suppose that $g\in\Gamma,(\xi,u)=(\sigma_1+\sigma_0,\sigma_3)$ and that $g\xi g^*=\xi,gug^*=u$. Then g has the form $g=\pm\sigma_0+b(\sigma_2+i\sigma_3),b\in\mathbb{R}$ and we can state the following.

Proposition: The space $T_+\Lambda_0$ is isomorphic to Γ/L, where L is the group formed by the matrices $g=\pm\sigma_0+b(\sigma_2+i\sigma_3),b\in\mathbb{R}$.

When $(\xi,u)\in T_+\Lambda_0$ and $\xi^0+\xi^3>0$, the vectors ξ,u can be given, in a unique way, by the expressions

$$\xi=\frac{a}{2}(1+|z|^2,z+\overline{z},-i(z-\overline{z}),1-|z|^2), \tag{74}$$

$$u=\frac{a}{2}(z\overline{Z}+\overline{z}Z,Z+\overline{Z},-i(Z-\overline{Z}),-(z\overline{Z}+\overline{z}Z))+b\xi, \tag{75}$$

where

$$a=\xi^0+\xi^3,\ \ z=\frac{\xi^1+i\xi^2}{\xi^0+\xi^3},\ \ b=\frac{u^0+u^3}{\xi^0+\xi^3},\ \ Z=\frac{u^1+iu^2-(u^0+u^3)z}{\xi^0+\xi^3}.$$

Let $T_0P^1(\mathbb{C})$ be the subspace of nonvanishing tangent vectors of $P^1(\mathbb{C})$. On $T_0P^1(\mathbb{C})$ we can use homogeneous coordinates z_1, z_2, Z_1, Z_2, as well as local coordinates

$$z=\frac{z_2}{z_1},\ \ Z=\dot{z}=\frac{z_1Z_2-z_2Z_1}{(z_1)^2}.$$

Each homographic transformation of $P^1(\mathbb{C})$ prolongs to $T_0P^1(\mathbb{C})$,

$$z\mapsto\frac{az+b}{cz+d},\ \ Z\mapsto\frac{Z}{(cz+d)^2},\ \ ad-bc=1.$$

The group $\mathbb{C}^*$ acts on the fibers of $T_0P^1(\mathbb{C})$ by complex multiplication.

Let $S_{N,\rho}$ be the vector space of smooth functions $F:T_0P^1(\mathbb{C})\to\mathbb{C}$, which satisfy, for all $\lambda\in\mathbb{C},\lambda\neq 0$, the following equation:

$$F(z,\lambda Z)=\left(\frac{\lambda}{|\lambda|}\right)^N|\lambda|^{-1+i\rho}F(z,Z),$$

where N is an integer and ρ is a real number. For F in $S_{N,\rho}$ one has

$$F(z,Z)=f(z)\left(\frac{Z}{|Z|}\right)^{-N}|Z|^{1-i\rho},$$

where

$$f(z)=F\left(\frac{1-z^2}{2},\ \ \frac{1+z^2}{2i},\ \ z\right).$$

Each $S_{N,\rho}$ is a representation space of the group $\mathrm{SL}(2,\mathbb{C})$ and the two-form $|f(z)|^2dz\wedge d\overline{z}$ is an invariant. When we introduce on $S_{N,\rho}$ the norm

$$||F||=\left(\frac{i}{2}\int_{\mathbb{C}}|f(z)|^2dz\wedge d\overline{z}\right)^{1/2},$$

we get by completion the Hilbert space of a unitary representation $R_{N,\rho}$ of the group $\mathrm{SL}(2,\mathbb{C})$.

In Ref. 6 (pp. 130–144) it is proved that each representation $R_{N,\rho}$ is irreducible and that $F\in S_{N,\rho}$ implies $4K(F)=(N^2-\rho^2-4)F$.

B. New invariant Lagrangians

The $\mathrm{SL}(2,\mathbb{C})$-space $T_0P^1(\mathbb{C})$ carries the invariant holomorphic one-form $Z^{-1}dz$.

The space $T_+\Lambda_0$ is defined, as a subset of $M\times M$, by the equations

$$\xi^0=\sqrt{(\xi^1)^2+(\xi^2)^2+(\xi^3)^2},\ \ y^0=\frac{\xi^1y^1+\xi^2y^2+\xi^3y^3}{\xi^0}.$$

Using formulas

$$z=\frac{\xi^1+i\xi^2}{\xi^0+\xi^3},\quad Z=\frac{u^1+iu^2-(u^0+u^3)z}{\xi^0+\xi^3},$$

it is not difficult to prove the following statements:

Proposition: The map $J:(\xi,u)\mapsto(z,Z)$ *defines a principal fibration* $(T_+\Lambda_0,J,T_0P^1(\mathbb{C}))$ *with structure group*

$$L'=\{a\sigma_0+b(\sigma_1-i\sigma_2);\ \ a\neq 0,\ \ b\in\mathbb{R}\}$$

and the map which sends $F\in S_{N,\rho}$ *to* $F^J=F\circ J$ *is an equivariant embedding of* $S_{N,\rho}$ *into the space of functions* $\Phi:T_+\Lambda_0\to\mathbb{C}$.

The space $T_+\Lambda_0$ is a six-dimensional manifold. It is convenient to select six real, independent coordinates on $T_+\Lambda_0$, among or contained in the following variables:

$$R=|u|,\ \ v=u^0+u^3,\ \ \rho=\frac{R}{u^0+u^3},\ \ W=\frac{u^1+iu^2}{u^0+u^3},$$

$$Z=\frac{u^0+u^3}{\xi^0+\xi^3}\ (W-z),\ \ \sigma=|Z|,\ \ H_1=Z^{-1}dz.$$

Note that the following relations hold:

$$u^0=\frac{R}{2\rho}(1-|z|^2+\overline{W}z+W\overline{z}),\ \ u^1=\frac{R}{2\rho}(W+\overline{W}),$$

$$u^2=-\frac{iR}{2\rho}(W-\overline{W}),\ \ u^3=\frac{R}{2\rho}(1+|z|^2-\overline{W}z-W\overline{z}),$$

$$v=ab,\ \ \rho=|z-W|,\ \ \sigma=b\rho,\ \ R=ab\rho,$$

$$H_1=Z^{-1}dz,\ \ \langle d\xi,d\xi\rangle=R^2|H_1|^2=\frac{R^2}{\sigma^2}|dz|^2,$$

$$\langle u,d\xi\rangle=\frac{R^2}{2}(H_1+\overline{H}_1)=\frac{R^2}{2\rho\sigma}[(\overline{W}-\overline{z})dz+(W-z)d\overline{z}],$$

$$\langle du,du\rangle=(dR)^2+\frac{R^2}{\rho^2}[|dW|^2-(d\rho)^2],$$

$$\langle d\xi,du\rangle=\frac{R^2}{2\sigma\rho}\left[((\overline{W}-\overline{z})dz+(W-z)d\overline{z})\ \left(\frac{d\sigma}{\sigma}-\frac{d\rho}{\rho}\right)+dz\ \ d\overline{W}+dW\ \ d\overline{z}\right].$$

We get Lorentz-invariant metrics on $T_+\Lambda_0$ by considering linear combinations of the scalar products

$$A\langle d\xi,d\xi\rangle+B\langle du,du\rangle+C\langle d\xi,du\rangle,\tag{76}$$

with coefficients depending on R.

We look at $\xi\in\Lambda$ as representing a generic electro-magnetic field. A specific electro-magnetic field would be defined by a vector potential $\xi=A(u)$ or, more precisely, by a section $s:\Sigma\to T_+\Lambda_0$, $s(u)=(u,A(u))$.

The manifold $T_+\Lambda_0$ carries the following invariant six-form,

$$du^0 \wedge du^1 \wedge du^2 \wedge du^3 \wedge \frac{dZ \wedge dz}{Z^2} = R^3 dR \wedge dz \wedge d\bar{z} \wedge \frac{d\rho \wedge d\sigma}{2\rho^2\sigma^2} \wedge d\omega.$$

Proposition: The quadratic, differential forms (76) are all degenerate, due to the presence of $\langle d\xi, d\xi \rangle$*; the tangent vectors* $((\xi,u),(\xi',u'))$*, satisfying the equations* $\xi' = C\xi$, $u' = -B\xi$*, are singular.*

The degeneracy of the forms (76) can be removed by introducing a constraint such as $\xi^0 = 1$, which reduces the dimension of the configuration space to five. It is plausible to assume, regarding the formulas above, that Lagrangians of this type produce the whole Schrödinger spectrum.

We finally remark that the Lagrangians which can be built using the invariants indicated above, such as (76), can be linked with two-particle systems $(u, u+\xi)$, for which the difference vector ξ lies on the light-cone.

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Fedosov quantization on symplectic ringed spaces

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We expose the basics of the Fedosov quantization procedure, placed in the general framework of symplectic ringed spaces. This framework also includes some Poisson manifolds with nonregular Poisson structures, presymplectic manifolds, complex analytic symplectic manifolds, etc. © *2002 American Institute of Physics.*
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I. INTRODUCTION

On a symplectic manifold (M,ω) *Fedosov quantization* is an embedding of the algebra $C^\infty(M,\mathbf{C})[[h]]$ of formal power series in h, with complex valued differentiable functions on M as coefficients, into the algebra of the cross sections of the *Weyl algebras bundle* $W(TM)$ by means of parallel translation with respect to a *generalized Abelian connection*. This article is an exposition of the basics of Fedosov quantization. The difference between our exposition and that of the original works (Refs. 1 and 2) consists in the fact that we place Fedosov's construction in the general framework of *symplectic ringed spaces*. The generalization is purely formal, and should be seen as folklore, but, it allows for new applications including a class of Poisson manifolds with possibly nonregular Poisson structure, presymplectic manifolds, holomorphic symplectic manifolds, etc. On the other hand, it is important to notice that in the general case one has an obstruction to the existence of a connection. Therefore, Fedosov quantization can be used only on symplectic ringed spaces where this obstruction vanishes.

II. SYMPLECTIC RINGED SPACES

A *Herz–Reinhart Lie algebra*, or *HRL-algebra* (or *Lie pseudo-algebra*[3,4]), L over a pair (K,C), where K is a commutative ring with unit and C is a commutative K-algebra with unit, is a Lie algebra over K which also is a C-module, and is endowed with a mapping $\iota: L\to\mathcal{D}$, the algebra of derivations of C over K, that is both a K-Lie algebra and a C-module homomorphism, with the compatibility condition

$$[X,fY]=f[X,Y]+(\iota(X)f)Y \quad (f\in C;\ X,Y\in L). \tag{2.1}$$

The fundamental example is $K=\mathbf{R}$, $C=C^\infty(M)$, $L=\Gamma TM$, where M is an arbitrary differentiable manifold, and Γ always denotes spaces of cross sections of vector bundles or sheaves.

Now, we define a *Herz–Reinhart–Lie (HRL)-ringed space*, as a topological space M endowed with a sheaf $\mathcal{C}$ of commutative K-algebras with unit and a *sheaf* $\mathcal{L}$ *of HRL-algebras* over $(K,\mathcal{C})$. This latter notion has the obvious definition, namely, for each open subset U of M the space of sections $\Gamma_U(\mathcal{L})$ is a HRL-algebra over $(K,\Gamma_U(\mathcal{C}))$, and the restrictions are homomorphisms of HRL-algebras. The sheaves of HRL-algebras were studied in Ref. 5 under the name of sheaves of *twisted Lie algebras*. A HRL-ringed space whose sheaf $\mathcal{L}$ is a locally free $\mathcal{C}$-module of rank m will be called an HRL-*ringed space of rank* m.

Example 2.1: An m-dimensional differentiable (respectively, complex analytic) manifold M is a HRL-ringed space of rank m, with $K=\mathbf{R}$ (respectively, $K=\mathbf{C}$), $\mathcal{C}=\mathcal{C}^\infty(M)$ [respectively

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$\mathcal{C}^{\mathrm{hol}}(M)]$, the sheaf of germs of differentiable (respectively, holomorphic) functions on M, and $\mathcal{L}$ the sheaf of germs of differentiable (respectively, holomorphic) vector fields on M.

Example 2.2: Let $p:A\to M$ be a differentiable vector bundle of rank m which is a Lie algebroid of anchor $\iota:A\to TM$.[4] Then, if we take $K=\mathbf{R}$, $\mathcal{C}=\mathcal{C}^\infty(M)$, $\mathcal{L}$ the sheaf A of germs of differentiable cross sections of A, and ι induced by the anchor, we again get a HRL-ringed space of rank m.

Example 2.3: Let M be a differentiable manifold endowed with a foliation $\mathcal{F}$ of codimension m, and let $\nu\mathcal{F}$ be the transversal bundle of $\mathcal{F}$. Take $K=\mathbf{R}$, $\mathcal{C}$ the sheaf of germs of differentiable functions on M which are constant along the leaves of $\mathcal{F}$ (*foliated functions*), $\mathcal{L}$ the sheaf of germs of foliated cross sections of $\nu\mathcal{F}$, and $\iota(X)f=\overline{X}f$, where $f\in\mathcal{C}, X\in\mathcal{L}$, and $\overline{X}$ is a germ of foliated vector field on M which projects onto X. The result is a structure of HRL-ringed space of rank m. (We refer to Ref. 6 for the theory of foliated manifolds.)

Because the structure of HRL-ringed space is similar to that of Lie algebroid, the same formulas as in the latter case[7,4] yield a differential calculus for HRL-ringed spaces.

If we refer to the sheaf

$$\Omega^k(M):=Alt_{\mathcal{C}}(\mathcal{L}^k,\mathcal{C}) \tag{2.2}$$

as the sheaf of germs of differential k-forms ($:=$ denotes a definition), there exists an exterior differential $d:\Omega^k(M)\to\Omega^{k+1}(M)$ defined for $\lambda\in\Omega^k(M)$ by

$$\begin{aligned} d\lambda(X_0,\ldots,X_k)=&\sum_{i=0}^{k}(-1)^i\iota(X_i)(\lambda(X_0,\ldots,\hat{X}_i,\ldots,X_k))\\ &+\sum_{i<j=1}^{k}(-1)^{i+j}\lambda([X_i,X_j],X_0,\ldots,\hat{X}_i,\ldots,\hat{X}_j,\ldots,X_k). \end{aligned} \tag{2.3}$$

In (2.3), and in all the similar formulas of this article, the germs always are at the same point of M. The operator d satisfies $d^2=0$, and leads to a usual definition of de Rham cohomology spaces $H^k(\mathcal{L})$. Notice also the existence of the *wedge product* which makes the graded exterior algebra $\{\Omega^k(M)\}_{k\in\mathbf{N}}$ into a differential graded algebra with respect to the exterior differential d.

Furthermore, if the sheaf $\mathcal{M}$ over M is a $\mathcal{C}$-module, we define the spaces of $\mathcal{M}$-valued differential forms by

$$\Omega^k(M,\mathcal{M}):=Alt_{\mathcal{C}}\mathcal{L}^k,\mathcal{M}), \tag{2.4}$$

and a *connection* on $\mathcal{M}$ is a K-linear homomorphism

$$\nabla:\mathcal{M}\to\Omega^1(M,\mathcal{M}), \tag{2.5}$$

which satisfies the condition

$$\nabla(f\xi)=f\nabla\xi+(df)\xi \quad (f\in\mathcal{C},\ \xi\in\mathcal{M}). \tag{2.6}$$

We will also use the notation $\nabla_Y\xi:=(\nabla\xi)(Y)$.

Using a connection, and in analogy with formula (2.3), for all $\lambda\in\Omega^k(M,\mathcal{M})$ one defines

$$\begin{aligned} \nabla\lambda(X_0,\ldots,X_k)=&\sum_{i=0}^{k}(-1)^i\nabla_{X_i}(\lambda(X_0,\ldots,\hat{X}_i,\ldots,X_k))\\ &+\sum_{i<j=1}^{k}(-1)^{i+j}\lambda([X_i,X_j],X_0,\ldots,\hat{X}_i,\ldots,\hat{X}_j,\ldots,X_k)\in\Omega^{k+1}(M,\mathcal{M}). \end{aligned} \tag{2.7}$$

In particular, (2.7) may be used to define the *curvature of the connection* ∇,

$$\Phi=\nabla^2:\mathcal{M}\to\Omega^2(M,\mathcal{M}), \tag{2.8}$$

where

$$\Phi(\xi)(Y,Z)=\nabla_Y\nabla_Z\xi-\nabla_Z\nabla_Y\xi-\nabla_{[Y,Z]}\xi. \tag{2.9}$$

It is easy to check that Φ is a homomorphism over $\mathcal{C}$, and satisfies the *Bianchi identity*

$$\nabla(\Phi(\xi))(Y,Z,U)=\sum_{\mathrm{Cycl}(Y,Z,U)}\Phi(\nabla_Y\xi)(Z,U). \tag{2.10}$$

In (2.9) and (2.10) $Y,Z,U\in\mathcal{L}$, and $\xi\in\mathcal{M}$.

The operators ∇_Y can be extended to any *tensorial sheaf* produced from $\mathcal{M}$ by the usual formulas of differential geometry. In the whole article, tensor and wedge product sheaves are seen as sheaves of $\mathcal{C}$-multilinear morphisms (e.g., Ref. 8). In particular, the curvature Φ can also be seen as a *two-form with values in* $\mathrm{Hom}_{\mathcal{C}}(\mathcal{M},\mathcal{M})$, and, then, the Bianchi identity takes the simple classical form[3,8]

$$\nabla\Phi=0. \tag{2.11}$$

Our interest will be in connections on $\mathcal{L}$, also called *connections on the HRL-ringed space* M. In this case another important invariant is the *torsion*, defined by

$$T(X,Y)=\nabla_XY-\nabla_YX-[X,Y]\quad(X,Y\in\mathcal{L}). \tag{2.12}$$

From (2.1) and (2.6), it follows that $T\in\Omega^2(M,\mathcal{L})$, and a simple computation yields the *torsion Bianchi identity*

$$(\nabla T)(X,Y,Z)=\sum_{\mathrm{Cycl}(X,Y,Z)}\Phi(X)(Y,Z)\quad(X,Y,Z\in\Gamma\mathcal{L}). \tag{2.13}$$

The torsion of a connection on $\mathcal{L}$ yields the following expression of the exterior differential (2.3):

$$\begin{aligned}d\lambda(X_0,\ldots,X_k)=&\sum_{i=0}^{k}(-1)^i(\nabla_{X_i}\lambda)(X_0,\ldots,\hat{X}_i,\ldots,X_k)\\&+\sum_{i<j=1}^{k}(-1)^{i+j}\lambda(T(X_i,X_j),X_0,\ldots,\hat{X}_i,\ldots,\hat{X}_j,\ldots,X_k).\end{aligned} \tag{2.14}$$

This formula suggests considering the operator

$$\nabla\lambda(X_0,\ldots,X_k)=\sum_{i=0}^{k}(-1)^i(\nabla_{X_i}\lambda)(X_0,\ldots,\hat{X}_i,\ldots,X_k)), \tag{2.15}$$

which coincides with $d\lambda$ if the torsion of ∇ is zero.

From (2.6), we see that the difference $D=\nabla^2-\nabla^1$ of two connections on M is a global section of $\mathrm{Hom}_{\mathcal{C}}(\mathcal{L},\Omega^1(M,\mathcal{L}))=\mathrm{Hom}_{\mathcal{C}}(\mathcal{L}\times\mathcal{L},\mathcal{L})$, i.e., a *tensor field*. Using this remark it follows easily that if ∇ is an arbitrary connection, then

$$\nabla^0_XY:=\tfrac{1}{2}(\nabla_XY+\nabla_YX+[X,Y]) \tag{2.16}$$

is a torsionless connection.

If $\mathcal{M}$ is a locally free $\mathcal{C}$-module of finite rank s over a ringed space $(M,\mathcal{C},\mathcal{L})$ of rank m, we may use local bases $(X_i)_{i=1}^m$ of $\mathcal{L}$, and local bases $(\xi_u)_{u=1}^s$ of $\mathcal{M}$, and get the local equations of the connection ∇,

$$\nabla_{X_i}\xi_u=\sum_{v=1}^{s}\Gamma_{iu}^{v}\xi_v, \tag{2.17}$$

where the *connection coefficients* Γ_{iu}^{v} are local sections of $\mathcal{C}$. The local equations (2.17) may be used in exactly the same way as in classical differential geometry, e.g., Ref. 8. For instance, let us take the case $\mathcal{M}=\mathcal{L}$, and look for the local expression of the torsion. For this purpose, we first notice the existence of *structure equations*:

$$[X_i,X_j]=\sum_{k=1}^{m}s_{ij}^{k}X_k \quad (s_{ij}^{k}=-s_{ji}^{k}\in\mathcal{C}).$$

Then, if we put $T(X_i,X_j)=\Sigma_{k=1}^{m}T_{ij}^{k}X_k$, we get

$$T_{ij}^{k}=\Gamma_{ij}^{k}-\Gamma_{ji}^{k}-s_{ij}^{k}.$$

Clearly, in the case of a differentiable manifold M a connection (2.5) on $\mathcal{M}=\mathcal{L}$ is just a linear connection on M. In the case of a complex analytic manifold a connection is the same thing as a holomorphic connection on the manifold, and it exists iff the *Atiyah class* of the manifold vanishes.[9] In the case of the transversal bundle of a foliation, a connection (2.5) on $\mathcal{L}$ is defined by a *projectable connection* of the foliation, and it exists iff the *Atiyah class of the foliation* vanishes.[6] Therefore, not every ringed space has connections. In the case of a Lie algebroid, a connection (2.5) is a *connection of the algebroid*, and any Lie algebroid has connections.

As a matter of fact, the Atiyah class method,[3,5] yields a general result namely, the following theorem.

Theorem 2.1: *For each HRL-ringed space of finite rank* $(M,K,\mathcal{C},\mathcal{L})$, *there exists a well defined sheaf-cohomology class* $a(M)\in H^1(M,Hom_{\mathcal{C}}(\mathcal{L},Hom_{\mathcal{C}}(\mathcal{L},\mathcal{L})))$ *such that existence of a connection on* $\mathcal{L}$ *is equivalent with* $a(M)=0$.

Proof: For any HRL-ringed space $(M,K,\mathcal{C},\mathcal{L})$ there exists a sheaf $\mathcal{J}$, which plays the role of the jet bundle J^1TM of a differentiable manifold M. Namely, $\mathcal{J}$ is the submodule of $\mathcal{L}\oplus\mathrm{Hom}_K(\mathcal{L},\mathcal{L})$ which consists of the pairs $(X,-\mathrm{ad}_X+\varphi)$, where $X\in\mathcal{L},\varphi\in\mathrm{Hom}_{\mathcal{C}}(\mathcal{L},\mathcal{L})$ and $\mathrm{ad}_X:=[X,]$. The fact that $\mathcal{J}$ is a $\mathcal{C}$-module follows from

$$(fX,-f\mathrm{ad}_X+f\varphi)=(fX,-\mathrm{ad}_{fX}+f\varphi-(df)X). \tag{2.18}$$

Now, we notice the existence of the following exact sequence of $\mathcal{C}$-module sheaves

$$0\to\mathcal{F}:=\mathrm{Hom}_{\mathcal{C}}(\mathcal{L},\mathcal{L})\xrightarrow{\epsilon}\mathcal{J}\xrightarrow{p}\mathcal{L}\to 0, \tag{2.19}$$

where $\epsilon(\varphi)=(0,\varphi)$, and $p(X,-\mathrm{ad}_X+\varphi)=X$.

Then, there exists a connection ∇ on $\mathcal{L}$ iff there exists a splitting of (2.19), i.e., a homomorphism $\psi:\mathcal{J}\to\mathcal{F}$ such that $\psi\circ\epsilon=id$. Indeed, if ψ is given, $\nabla X=\psi(X,-\mathrm{ad}_X)$ is a connection. Conversely, if ∇ is a connection, $\psi(X,-\mathrm{ad}_X+\varphi)=\nabla X+\varphi$ is the required homomorphism.

Furthermore, if $\mathcal{L}$ is locally free and of finite rank, the sequence (2.19) behaves as a sequence of finite dimensional vector spaces, and leads to the exact sequence

$$0\to\mathrm{Hom}(\mathcal{L},\mathcal{F})\xrightarrow{p'}\mathrm{Hom}(\mathcal{J},\mathcal{F})\xrightarrow{\epsilon'}\mathrm{Hom}(\mathcal{F},\mathcal{F})\to 0, \tag{2.20}$$

then to the corresponding exact sequence of sheaf-cohomology

$$0\to H^0(M,\mathcal{A})\overset{p^*}{\to}H^0(M,\mathcal{B})\overset{\epsilon^*}{\to}H^0(M,\mathcal{E})\overset{\delta}{\to}H^1(M,\mathcal{A})\to\cdots. \tag{2.21}$$

In (2.20) and (2.21), the morphisms ϵ', ϵ^*, p', p^* are induced by ϵ and p of (2.19), $\mathcal{A}$, $\mathcal{B}$, $\mathcal{E}$ are the second, third and fourth sheaf of the sequence (2.20), respectively, and δ is the connecting morphism.

It follows that the condition for the existence of a connection is that the identity belongs to the image of ϵ^*, and this is equivalent to $\delta(id)=0$. Hence, if we define the *Atiyah class* by $a(M)=\delta(id)\in H^1(M,\mathrm{Hom}(\mathcal{L},\mathcal{F}))$, we precisely have the required result. Q.E.D.

Now, again, let $(M,\mathcal{C},\mathcal{L})$ be a HRL-ringed space. A two-form $\omega\in\Omega^2(M)$ will be called *nondegenerate* if the sheaf homomorphism $\flat_\omega:\mathcal{L}\to\Omega^1(M)$ defined by

$$\flat_\omega(X)(Y)=\omega(X,Y)\quad (X,Y\in\mathcal{L})$$

is an isomorphism. The inverse of this isomorphism will be denoted by $\#_\omega$. A two-form ω which is nondegenerate and *closed*, i.e., $d\omega=0$ is called a *symplectic form*, and, then, $(M,\mathcal{C},\mathcal{L},\omega)$ is called a *symplectic ringed space*.

Example 2.4: The differentiable and holomorphic symplectic manifolds obviously are examples of symplectic ringed spaces.

Example 2.5: Let (M,ω), where M is a $(2n+h)$-dimensional differentiable manifold and ω is a closed two-form of rank $2n$ over M, be a *presymplectic manifold*. It is well known (e.g., Ref. 10) that ker ω is tangent to an h-dimensional foliation $\mathcal{S}$, called the *characteristic foliation*, and that the form ω is projectable with respect to this foliation. By looking at the earlier Example 2.3, we see that the sheaf $\mathcal{L}$ of germs of projectable cross sections of the transversal bundle $\nu\mathcal{S}$ defines a ringed space structure over $M[\mathcal{C}=\mathcal{C}^\infty(M)]$, which is endowed with the symplectic form induced by ω.

Example 2.6: As in Example 2.2, let $A\to M$ be a Lie algebroid of rank $2m$, with the anchor map $\iota:A\to TM$. Then, any nondegenerate cross section $\omega\in\Gamma\wedge^2A^*$, which is closed with respect to the exterior differential d_A (see Refs. 7 and 4), makes the ringed space $(M,\mathcal{C}^\infty(M),\underline{A})$ into a symplectic ringed space. It is also convenient to say that (A,ω) is a *symplectic Lie algebroid*. Following are some concrete examples of symplectic Lie algebroids.

Example 2.7: If $P\in\Gamma\wedge^2TM$ is a regular Poisson structure of M, and if $\mathcal{S}$ is the symplectic foliation of P (e.g., Ref. 11), then $T\mathcal{S}$ with the leafwise two-form provided by the Poisson bracket of P is a symplectic Lie algebroid.

Example 2.8: Let (M,W) be an arbitrary Poisson manifold. Then T^*M is a Lie algebroid of anchor $\iota=\#_W$. A symplectic structure on this algebroid is a nondegenerate bivector field Q on M which is a cocycle in the Poisson–Lichnerowicz cohomology, i.e., $[W,Q]=0$ (e.g., Ref. 11).

Some of the usual symplectic notions straightforwardly transfer to symplectic ringed spaces. For instance, we may define $\Pi\in Alt_{\mathcal{C}}(\Omega^1(M)\times\Omega^1(M),\mathcal{C})$ by

$$\Pi(\sigma_1,\sigma_2)=\langle\sigma_1,\#_\omega\sigma_2\rangle,\quad \sigma_1,\sigma_2\in\Omega^1(M),$$

and also define $\#_\Pi:=\#_\omega$. Furthermore, we may define the *Hamiltonian gradient* X_f of any $f\in\mathcal{C}$ by $X_f=-\#_\Pi df$, and the *Poisson bracket*

$$\{f,g\}:=\omega(X_f,X_g)=\iota(X_f)g=-\iota(X_g)f=\Pi(df,dg). \tag{2.22}$$

The evaluation

$$0=d\omega(X_f,X_g,X_h)=\sum_{\mathrm{Cycl}(f,g,h)}\iota(X_f)\omega(X_g,X_h)-\sum_{\mathrm{Cycl}(f,g,h)}\omega([X_f,X_g],X_h)$$

$$=\sum_{\mathrm{Cycl}(f,g,h)}\{f,\{g,h\}\}-\sum_{\mathrm{Cycl}(f,g,h)}\langle dh,[X_f,X_g]\rangle$$

$$=\sum_{\mathrm{Cycl}(f,g,h)}\{f,\{g,h\}\}-\sum_{\mathrm{Cycl}(f,g,h)}(\iota[X_f,X_g])h$$

$$=\sum_{\mathrm{Cycl}(f,g,h)}\{f,\{g,h\}\}-\sum_{\mathrm{Cycl}(f,g,h)}(\iota(X_f)\iota(X_g)-\iota(X_g)\iota(X_f))h$$

$$=-\sum_{\mathrm{Cycl}(f,g,h)}\{f,\{g,h\}\}$$

shows that the bracket (2.22) satisfies the Jacobi identity. Since the Leibniz rule also obviously holds, we have a structure of *Poisson algebra sheaves* on $\mathcal{C}$. (See, for instance, Ref. 11 for the definition of a Poisson algebra.)

However, not all the classical symplectic properties hold. For instance, the Jacobi identity for the Poisson bracket (2.22) implies

$$X_{\{f,g\}}-[X_f,X_g]\in\ker\iota, \tag{2.23}$$

hence, the result is zero only at the *injectivity points* of ι. Another negative example is obtained if we consider the operation of a *Schouten–Nijenhuis bracket* on a HRL-ringed space (e.g., Ref. 7). Then, the general algebraic computations of Ref. 12 hold, and we have the formula

$$[\Pi,\Pi](df,dg,dh)=2\sum_{\mathrm{Cycl}(f,g,h)}\{\{f,g\},h\}. \tag{2.24}$$

But, since $\{df/f\in\mathcal{C}\}$ may not span $\Omega^1(M)$, generally, we may have $[\Pi,\Pi]\neq 0$.

Let us come back to the symplectic Lie algebroid (A,ω) of Example 2.6. Then, the symplectic objects $\flat_\omega$, Π, X_f, etc. have interpretations in terms of vector bundles: an isomorphism $\flat_\omega:A\to A^*$, a cross section $\Pi\in\Gamma\wedge^2 A$, cross sections $X_f\in\Gamma A$, etc. The Poisson bracket (2.22) becomes a Poisson algebra structure on $C^\infty(M)$, and there exists a corresponding Poisson bivector field $P\in\Gamma\wedge^2 TM$ such that

$$\{f,g\}=\Pi(d_Af,d_Ag)=P(df,dg),\quad [P,P]=0, \tag{2.25}$$

where the final bracket is the usual Schouten–Nijenhuis bracket on M.

For a better understanding of the relation between P and Π, let us consider the transposed homomorphism $\iota':T^*M\to A^*$ of the anchor $\iota:A\to TM$. Then we have

$$d_Af=\iota'(df),\quad \#_P=-\iota\circ\#_\Pi\circ\iota'. \tag{2.26}$$

Notice that the injectivity points of ι are the same as the surjectivity points of ι'. Accordingly, from (2.23) and (2.24), we see that the relations

$$X_{\{f,g\}}=[X_f,X_g],\quad [\Pi,\Pi]_A=0 \tag{2.27}$$

hold at the injectivity points of ι. If the set of injectivity points of ι is dense in M, the equalities (2.27) hold everywhere on M.

The considerations above suggest the following definition: a Poisson structure P on a differentiable manifold M will be called a *quasi-symplectic Poisson structure* if it is induced by a symplectic Lie algebroid, via formula (2.25).

Example 2.7 tells us that every regular Poisson structure is quasi-symplectic. Other quasi-symplectic Poisson structures are provided by Example 2.8. If (M,W) is a Poisson manifold which has a nonsingular Poisson two-cocycle Q (i.e., $Q\in\Gamma\wedge^2TM$, rank $Q=\dim M$, $[W,Q]=0$), the corresponding object Π of (2.25) is a usual two-form on M, and (2.25) defines a quasi-symplectic Poisson structure given by

$$\{f,g\}=\Pi(X_f^W,X_g^W)\quad[f,g\in C^\infty(M)],\tag{2.28}$$

where the arguments are the W-Hamiltonian vector fields of the functions f,g.

For a more concrete situation of this kind, let (M,Π,ϕ) be a *symplectic-Nijenhuis manifold*, with the symplectic form Π and the Nijenhuis tensor ϕ (see, for instance, Ref. 13). Then, M has a Poisson structure W defined by $\#_W=\phi\circ\#_Q$, where Q is the bivector field given by $\#_Q=\flat_\Pi^{-1}$. W is the first structure of the Poisson hierarchy of the symplectic-Nijenhuis manifold M, and it is compatible with the Poisson structure Q of M, i.e., $[W,Q]=0$.[13] Since Q is nondegenerate, we are in the situation described by the previous paragraph, and we get a quasi-symplectic Poisson structure

$$\begin{aligned}\{f,g\}=\Pi(\#_W df,\#_W dg)&=\langle\flat_\Pi\#_W df,\#_W dg\rangle\\&=-\langle\#_W\flat_\Pi\#_W df,dg\rangle=-\langle\phi\#_W df,dg\rangle=-\langle\phi^2\#_Q df,dg\rangle.\end{aligned}$$

Up to the sign, this is the second structure of the Poisson hierarchy of (M,Π,ϕ).[13] Thus, we have proven the following.

Proposition 2.1: *The second Poisson structure of the Poisson hierarchy of a symplectic-Nijenhuis manifold is a quasi-symplectic Poisson structure.*

Of course, the structures of Proposition 2.1 may have singular points.

One of the main ingredients of Fedosov quantization is a symplectic connection. The well known procedure of constructing symplectic connections on symplectic manifolds, as presented for instance, in Ref. 14, holds without modification on a symplectic ringed space.

Namely, if $(M,\mathcal{C},\mathcal{L})$ is a ringed space which possesses a nondegenerate two-form ω (*almost symplectic ringed space*), a connection ∇ on $\mathcal{L}$ (i.e., on M) is said to *preserve* ω if $\nabla_X\omega=0$, $\forall X\in\mathcal{L}$. If there exists a connection ∇^0 on M, the formula

$$\nabla_XY=\nabla^0_XY+\Theta(X,Y)+A(X,Y),\tag{2.29}$$

where

$$\omega(\Theta(X,Y),Z)=\tfrac{1}{2}(\nabla^0\omega)(Y,Z),\quad\omega(A(X,Y),Z)=B(X,Y,Z),\tag{2.30}$$

$\forall X,Y,Z\in\mathcal{L}$, and $\forall B\in\mathrm{Hom}_{\mathcal{C}}(\mathcal{L}\times\mathcal{L}\times\mathcal{L},\mathcal{C})$ which satisfies the condition $B(X,Y,Z)=B(X,Z,Y)$, yields all the connections of M which preserve ω. Θ and A are well defined by (2.30) because ω is nondegenerate.

Furthermore, formula (2.14) shows that a torsionless, ω-preserving connection may exist only if $d\omega=0$. Conversely, if we are in this latter case, and if we assume that ∇^0 has zero torsion [e.g., this ∇^0 is given by applying (2.16) to the original ∇^0], it turns out that ∇ of (2.29), and with

$$B(X,Y,Z)=\tfrac{1}{6}[(\nabla^0_Y\omega)(X,Z)+(\nabla^0_Z\omega)(X,Y)],\tag{2.31}$$

is an ω-preserving, torsionless connection. Indeed, from (2.29), and since $d\omega=\nabla^0\omega$ [in the sense of (2.15)], we deduce that $\omega(T_\nabla(X,Y),Z)=0$ for the chosen value (2.31) of B.

By definition, a connection which preserves the symplectic form ω and has zero torsion is called a *symplectic connection* on the symplectic ringed space $(M,\mathcal{C},\mathcal{L},\omega)$. Above, we saw that if M has an arbitrary connection, it also has symplectic connections, and we wrote down the expression of one symplectic connection ∇, defined by means of (2.31). It follows that all the symplectic connections are given by

$$\tilde{\nabla}_X Y = \nabla_X Y + C(X,Y),$$

where $Q(X,Y,Z) := \omega(C(X,Y),Z)$ is symmetric in all its arguments.

In analogy with Riemannian geometry, one defines the *covariant curvature tensor* of a symplectic connection, namely,

$$S(X_1,X_2,X_3,X_4) = -\omega(X_1,\Phi(X_2)(X_3,X_4)), \tag{2.32}$$

where Φ is given by (2.8). This tensor has the following symmetry properties:

$$\begin{gathered} S(X_1,X_2,X_3,X_4) = -S(X_1,X_2,X_4,X_3), \\ S(X_1,X_2,X_3,X_4) + S(X_1,X_3,X_4,X_2) + S(X_1,X_4,X_2,X_3) = 0, \\ S(X_1,X_2,X_3,X_4) = S(X_2,X_1,X_3,X_4). \end{gathered} \tag{2.33}$$

The first equality is obvious, the second is the *Bianchi identity* (2.13), and the third follows by expressing the derivations via the connection in the identity

$$(\iota(X_3)\iota(X_4) - \iota(X_4)\iota(X_3) - \iota([X_3,X_4]))(\omega(X_1,X_2)) = 0,$$

where $X_1,X_2,X_3,X_4 \in \mathcal{L}$.

Concerning examples of symplectic connections in cases other than symplectic manifolds, we first quote the case of a presymplectic manifold (M,ω). It is easy to see that a symplectic connection on M seen as a symplectic ringed space, as in Example 2.5, may be identified with a connection on M seen as a differentiable manifold, which preserves ω, has torsion tangent to the characteristic foliation of ω, and defines a transversal projectable connection of the same foliation. Details on the construction of these connections can be found in Ref. 15.

Another interesting case is that of a symplectic structure Q on the tangent Lie algebroid T^*M of a Poisson manifold (M,W) (see Example 2.8). In this case, it is natural to start with a connection D on the differentiable manifold M which satisfies the condition $D_X Q = 0$ $(X \in \Gamma TM)$. D exists since (M,Q^{-1}) is an almost symplectic manifold but, generally, D has a nonzero torsion T_D. The connection D yields a connection ∇ on the Lie algebroid T^*M[11,16] by putting

$$\nabla_\alpha \beta = D_{\#_W \alpha}\beta, \quad \alpha,\beta \in \Gamma T^*M. \tag{2.34}$$

A straightforward computation, which uses the Lie bracket of T^*M,[7,11]

$$\{\alpha,\beta\} = L_{\#_W\alpha}\beta - L_{\#_W\beta}\alpha - d(W(\alpha,\beta)),$$

yields the torsion T_∇ by the formula

$$\langle T_\nabla(\alpha,\beta),X\rangle = \alpha(T_D(\#_W\beta,X)) - \beta(T_D(\#_W\alpha,X)) - (D_X W)(\alpha,\beta). \tag{2.35}$$

Therefore, generally, $T_\nabla \neq 0$, and we must apply the general algorithm to get a torsionless symplectic connection on (T^*M,Q). The passage from ∇ of (2.34) to a torsionless connection is given by (2.16), i.e.,

$$\nabla^0_\alpha \beta = \tfrac{1}{2}(\nabla_\alpha\beta + \nabla_\beta\alpha + \{\alpha,\beta\}). \tag{2.36}$$

Furthermore, from (2.34), (2.36), and $d_{T^*M}Q = 0$ we get

$$(\nabla^0_\alpha Q)(\beta,\gamma) = \tfrac{1}{2}Q(\alpha,T_\nabla(\beta,\gamma)). \tag{2.37}$$

Finally, from (2.30), (2.31), and (2.37), we deduce the expression of a symplectic connection

$$\check{\nabla}_\alpha \beta = \nabla^0_\alpha \beta + E(\alpha,\beta), \tag{2.38}$$

where

$$Q(E(\alpha,\beta),\gamma) = \tfrac{1}{4} Q(\alpha, T_\nabla(\beta,\gamma)) + \tfrac{1}{12}[Q(\beta, T_\nabla(\alpha,\gamma)) + Q(\gamma, T_\nabla(\alpha,\beta))]. \tag{2.39}$$

III. FEDOSOV QUANTIZATION

In this section, we describe the Fedosov quantization procedure, following the original works, Refs. 1 and 2, with minor modifications, and emphasizing the ringed space setting. Other expositions of this procedure can be found in Refs. 17–19, etc.

First we recall the construction of the *Weyl algebra* of a complex symplectic vector space $(E, \omega \in \wedge^2 E)$ of dimension $2m$.

We begin with the associative, commutative algebra of formal Laurent series in the parameter h

$$W(E) := \left\{ w = \sum_{k=-\infty}^{\infty} \sum_{i=0}^{\infty} t_{ki} h^k / t_{ki} \in \odot^i E^*, \quad i + 2k \geqslant 0 \right\}, \tag{3.1}$$

where $\odot$ denotes the symmetric tensor product, and it defines the multiplication in $W(E)$.

This algebra will be graded by asking

$$\deg t_{ki} = i, \quad \deg h = 2, \tag{3.2}$$

and we will write the element $w \in W(E)$ which appears in (3.1) as

$$w = \sum_{p=0}^{\infty} \hat{w}_p, \quad \hat{w}_p = \sum_{2k+i=p} t_{ki} h^k. \tag{3.3}$$

In terms of vector spaces, this means

$$W(E) = \prod_{p=0}^{\infty} V_p(E), \quad V_p(E) = \prod_{k=-\infty}^{[p/2]} \odot^{p-2k} E^*. \tag{3.4}$$

Furthermore, consider the *contraction operators*

$$C^p_\omega : (\odot^i E^*) \otimes (\odot^j E^*) \to \odot^{i+j-2p} E^* \tag{3.5}$$

defined by 0 if $p > \min(i,j)$, and by

$$C^p_\omega(\alpha,\beta)(e_1,\ldots,e_{i+j-2p}) = \sum_{\sigma \in S_{i+j-2p}} \sum_{a_1,\ldots,a_p=1}^{m} \frac{1}{(i+j-2p)!} \cdot \alpha(b_{a_1^*},\ldots,b_{a_p^*}, e_{\sigma(1)},\ldots,e_{\sigma(i-p)}) \times \beta(b_{a_1},\ldots,b_{a_p}, e_{\sigma(i-p+1)},\ldots,e_{\sigma(i+j-2p)}) \tag{3.6}$$

if $p \leqslant \min(i,j)$. In (3.6), S is the symmetric group, $e_l \in E$ $(l = 1,\ldots,i+j-2p)$, and (b_a, b_{a*}) $(a^* := a+m)$ is an arbitrary ω-symplectic basis of E.

The contractions extend to series (3.1), and may be used to define the *Moyal product*

$$w \circ w' := \sum_{q=0}^{\infty} \frac{1}{q!} \left(-\frac{ih}{2} \right)^q C^q_\omega(w,w') \quad [w,w' \in W(E)], \tag{3.7}$$

which makes $W(E)$ into a graded [because of (3.2)], associative algebra, called the *Weyl algebra* of (E,ω).

Computations in the Weyl algebra become easy if we consider an arbitrary basis $(u_i)_{i=1}^{2m}$ of E, and represent an element $t \in \odot^q E^*$ by

$$t = t_{i_1,\dots,i_q} y^{j_1} \cdots y^{j_q} = \sum_{|\alpha|=q} \tau_{\alpha_1 \cdots \alpha_{2m}} (y^1)^{\alpha_1} \cdots (y^{2m})^{\alpha_{2m}} = \sum_{|\alpha|=q} \tau_\alpha y^\alpha. \tag{3.8}$$

In (3.8), (y^i) are the coordinates of a generic vector of E with respect to the basis (u_i), and for their indices we use (here and subsequently) the Einstein summation convention. Furthermore, the coefficients t are symmetric, the second equality is obtained by collecting the various factors y^i into a power of y^i, and the third equality is the formal notation of its left hand side, i.e.,

$$\alpha = (\alpha_1,\dots,\alpha_{2m}) \quad (\alpha_i \geqslant 0), \quad y^\alpha = (y^1)^{\alpha_1} \cdots (y^{2r})^{\alpha_{2m}}, \quad |\alpha| = \alpha_1 + \cdots + \alpha_{2m}.$$

With this representation, an element $w \in W(E)$ becomes

$$w(y,h) = \sum_{k=-\infty}^{k=\infty} \sum_{|\alpha|=0}^{\infty} h^k t_{k,\alpha} y^\alpha, \quad |\alpha| + 2k \geqslant 0, \tag{3.9}$$

the usual product of polynomials corresponds to the symmetric tensor product, and the Moyal product is

$$\begin{aligned} w \circ w' &= \sum_{q=0}^{\infty} \frac{1}{q!} \left(-\frac{ih}{2} \right)^q \omega^{i_1 j_1} \cdots \omega^{i_q j_q} \frac{\partial^q w}{\partial y^{i_1} \cdots \partial y^{i_q}} \frac{\partial^q w'}{\partial y^{j_1} \cdots \partial y^{j_q}} \\ &= \exp\left(-\frac{ih}{2} \omega^{ij} \frac{\partial}{\partial z^i} \frac{\partial}{\partial u^j} \right) (w(z,h) w'(s,h)|_{z=s=y}), \end{aligned} \tag{3.10}$$

where $\omega^{ih} \omega_{hk} = \delta^i_k$ and ω_{hk} are the u-components of ω.

It follows easily that the center $Z(W(E))$ is the algebra of formal power series $\mathbf{C}[[h]]$.[1,2]

The next step consists of *enlarging* the Weyl algebra $W(E)$ to the associative algebra

$$\hat{W}(E) := W(E) \otimes (\oplus_{q=0}^{2m} \wedge^q E^*). \tag{3.11}$$

If (u_i) is the basis used in (3.8), and if (ν^i) is its dual cobasis, $\lambda \in \hat{W}(E)$ may be seen as

$$\lambda = \sum_{k=-\infty}^{\infty} \sum_{p=0}^{\infty} \sum_{q=0}^{2m} h^k \lambda_{kpqi_1 \cdots i_p j_1 \cdots j_q} y^{i_1} \cdots y^{i_p} \nu^{j_1} \wedge \cdots \wedge \nu^{j_q}, \quad p + 2k \geqslant 0, \tag{3.12}$$

where the coefficients are symmetric in the indices i, and skew-symmetric in the indices j. The product of $\hat{W}(E)$ is defined by (3.10) with a wedge product of the partial derivatives which appear in that formula.

In $\hat{W}(E)$, the *commutant* is defined as the natural extension of

$$[\lambda, \mu] = \lambda \circ \mu - (-1)^{\tilde{\lambda}\tilde{\mu}} \mu \circ \lambda, \tag{3.13}$$

where tilde denotes the degree of the wedge product factor of an element of $\hat{W}(E)$.

The center $Z(\hat{W}(E))$ is $\mathbf{C}[[h]] \otimes (\oplus_{q=0}^{2m} \wedge^q E^*)$, and one has the *central projections*[1,2] of λ of (3.12):

$$\lambda_0 := \sum_{k=0}^{\infty} \sum_{q=0}^{2m} h^k \lambda_{k0qj_1\cdots j_q} \nu^{j_1} \wedge \cdots \wedge \nu^{j_q} \in Z(\hat{W}(E)), \tag{3.14}$$

$$\lambda_{00} := \sum_{k=0}^{\infty} h^k \lambda_{k00} \in Z(W(E)). \tag{3.15}$$

The following basis-independent operators are essential in the subsequent computations:[1,2]

$$\delta\lambda := \sum_{j=1}^{2m} \nu^j \wedge \frac{\partial \lambda}{\partial y^j}, \quad \delta^*\lambda = \sum_{j=1}^{2m} y^j (i(u_j)\lambda). \tag{3.16}$$

These operators satisfy the properties

$$\delta^2 = 0, \quad \delta^{*2} = 0, \quad \delta(a \circ b) = (\delta a) \circ b + (-1)^{\tilde{a}} a \circ \delta b. \tag{3.17}$$

Furthermore, $\forall \lambda \in \hat{W}(E)$, one can check the *Hodge decomposition* formula

$$\lambda = \delta\delta^{-1}\lambda + \delta^{-1}\delta\lambda + \lambda_{00}, \tag{3.18}$$

where δ^{-1} is defined on the (p,q)-term of (3.12) by

$$\delta^{-1}\lambda := \frac{1}{p+q}\delta^*\lambda. \tag{3.19}$$

We intend to apply the previous algebraic constructions to symplectic ringed spaces. To be able to do so, in what follows we assume that $\mathcal{C}$ is a subsheaf of the sheaf of germs of continuous, complex valued functions on M and that $(M,\mathcal{C},\mathcal{L},\omega)$ is a symplectic ringed space of finite rank. Then $\mathcal{L}$ must be the sheaf of germs of cross sections of a complex symplectic vector bundle over M.[20] This implies that the rank of the space is even, say $2m$, and that $\mathcal{L}$ has local *symplectic bases*, i.e., local bases $(X_i)_{i=1}^{2m}$ such that

$$\omega(X_a, X_b) = 0, \ \ \omega(X_a, X_{b+m}) = \delta_{ab}, \quad \omega(X_{a+m}, X_{b+m}) = 0, \quad a,b = 1,\ldots,r.$$

Then the previous algebraic constructions may be performed on each stalk of $\mathcal{L}$, and using local symplectic bases of germs (X_i). Accordingly, we get *sheaves of Weyl algebras* $\mathcal{W}(\mathcal{L})$, $\hat{\mathcal{W}}(\mathcal{L})$, and the formulas developed earlier in this section hold, with germs instead of algebraic tensors overall. In particular, there is a *central sheaf* $\mathcal{Z}(\mathcal{W}(\mathcal{L})) = \mathcal{C}[[h]]$, which consists of germs of formal power series in h, and a *central sheaf* $\mathcal{Z}(\hat{\mathcal{W}}(\mathcal{L})) = \mathcal{C}[[h]] \otimes (\oplus_{q=0}^{2m} \wedge^q \mathcal{L})$.

In the ringed setting, Fedosov's quantization will be an embedding of $\mathcal{C}[[h]]$ onto the *parallel germs* of $\mathcal{W}(\mathcal{L})$ with respect to a *generalized symplectic connection*. Accordingly, we shall assume that $(M,\mathcal{C},\mathcal{L},\omega)$ has connections [it has a vanishing Atiyah class $a(M)$, as defined in Sec. II], and take a torsionless, symplectic connection ∇ on this space. Then, ∇ extends to a *covariant exterior differential* $\nabla : \hat{\mathcal{W}}(\mathcal{L}) \to \hat{\mathcal{W}}(\mathcal{L})$ defined by[1,2]

$$\nabla(t \otimes \theta) = \sum_{i=1}^{2m} \nu^i \wedge \nabla_{X_i}(t \otimes \theta) \quad (t \in \odot^q \mathcal{L}^*, \theta \in \wedge^s \mathcal{L}^*), \tag{3.20}$$

where (X_i) is a local basis of $\mathcal{L}$ and (ν^i) is the dual cobasis. The definition is invariant by a change of the local basis, and (3.20) reduces to (2.15) if there is no symmetric factor t. Since the connection has zero torsion, in the case of a differential form θ one has $\nabla\theta = d\theta$. Furthermore, since $\nabla\omega = 0$, (3.10) shows that

$$\nabla(\lambda \circ \mu) = (\nabla\lambda) \circ \mu + (-1)^{\tilde{\lambda}} \lambda \circ \nabla\mu, \quad \lambda, \mu \in \hat{\mathcal{W}}(\mathcal{L}). \tag{3.21}$$

The operator (3.20) is what is actually needed in Fedosov quantization, and, subsequently, we will think of this operator when referring to a connection. Fedosov[1,2] writes the operator ∇ in a convenient way as follows. Consider the local equations (2.17) of the connection ∇, and assume that the basis $(\xi_i = X_i)$ used in these equations is symplectic. Then, the symplectic character of the connection is equivalent to

$$\Gamma_{ijk} = \Gamma_{jik} \quad (\Gamma_{ijk} := \omega_{is}\Gamma^s_{jk}). \tag{3.22}$$

Accordingly, $\forall x \in M$, there exists a germ

$$\Gamma := \tfrac{1}{2}\Gamma_{ijk} y^i y^j \nu^k \in (\hat{\mathcal{W}}(\mathcal{L}))_x, \tag{3.23}$$

and *Fedosov's formula* is

$$\nabla\lambda = d\lambda + \frac{i}{h}[\Gamma, \lambda], \tag{3.24}$$

for λ given by (3.12), and with d applied as if h, y would be constants. Formula (3.24) is easily checked for $\lambda = \lambda_i \nu^i$ and $\lambda = \lambda_i y^i$, and it holds in the general case because d and the commutant $[\Gamma, \ ]$ are derivations of $\hat{\mathcal{W}}(\mathcal{L})$. Notice that the germs (3.23) do not define a global section of $\hat{\mathcal{W}}(\mathcal{L})$.

The same method yields the formulas[1,2]

$$\delta\lambda = -\frac{i}{h}[\varpi, \lambda], \quad \varpi := \delta^* \omega = \omega_{ij} y^i \nu^j, \tag{3.25}$$

$$\nabla\delta + \delta\nabla = 0, \tag{3.26}$$

$$\nabla^2\lambda = \frac{i}{h}[S, \lambda], \quad S := -\frac{1}{4} S_{ijkl} y^i y^j \nu^k \wedge \nu^l, \tag{3.27}$$

S_{ijkl} being the components of the covariant curvature tensor of the symplectic connection ∇, which is known to be symmetric in the first two arguments and skew symmetric in the last two arguments [see (3.33)].

Fedosov's formula (3.24) suggests a definition of *generalized symplectic connections*[1,2] as operators

$$\hat{\nabla}\lambda = \nabla\lambda + \frac{i}{h}[\gamma, \lambda], \tag{3.28}$$

where

$$\gamma = \sum_{k=-\infty}^{\infty} \sum_{p=0}^{\infty} h^k \gamma_{ki_1 \cdots i_p j} y^{i_1} \cdots y^{i_p} \nu^j \quad (p + 2k \geqslant 0) \tag{3.29}$$

are germs which define a global section of $\Gamma(\mathcal{W}(\mathcal{L}) \otimes \mathcal{L}^*)$. Then, a straightforward computation yields the *generalized curvature* Φ defined by means of the formulas

$$\hat{\nabla}^2\lambda = \frac{i}{h}[\Phi, \lambda], \quad \Phi = S + \nabla\gamma + \frac{i}{h}\gamma^2, \tag{3.30}$$

and the *Bianchi identity*

$$\hat{\nabla}\Phi=\nabla\Phi+\frac{i}{h}[\gamma,\Phi]=0. \tag{3.31}$$

By definition, if $\hat{\nabla}^2\lambda=0$ for all $\lambda\in\hat{\mathcal{W}}(\mathcal{L})$, $\hat{\nabla}$ is called an *Abelian connection*.

Now, we come to the result which is at the heart of Fedosov quantization.[1,2,17,19]

Theorem 3.1: *Let $(M,\mathcal{C},\mathcal{L},\omega)$ be a symplectic ringed space of finite rank $2m$, with the sheaf $\mathcal{C}$ being a subsheaf of germs of continuous, complex valued functions, and which has connections. Then, there exist generalized, symplectic, Abelian connections $\hat{\nabla}$ on M. Furthermore, for any Abelian connection $\hat{\nabla}$, for any $a\in\mathcal{C}[[h]]$, there exists a unique $\lambda\in\mathcal{W}(\mathcal{L})$ with central projection $\lambda_{00}=a$, such that $\hat{\nabla}\lambda=0$.*

Proof: Consider a generalized connection (3.28), where $\gamma=\varpi+r$ for ϖ given by (3.25), and for an element

$$r=\sum_{p\geqslant 2}^{\infty}\hat{r}_p\in\mathcal{W}(\mathcal{L})\otimes\mathcal{L}^*, \tag{3.32}$$

which satisfies the condition $\delta^{-1}r=0$. The last condition implies that r has the central projection $r_0=0$; therefore, by the Hodge decomposition (3.18) $r=\delta^{-1}\delta r$.

The curvature form of this connection $\hat{\nabla}$ is given by (3.30) and, in view of (3.10), (3.13), (3.25) and $\nabla\omega=0$, it becomes

$$\Phi=S+\nabla r-\delta r+\frac{i}{h}r^2-\omega. \tag{3.33}$$

Since $\omega\in\mathcal{Z}(\hat{\mathcal{W}}(\mathcal{L}))$, the condition

$$\delta r=S+\nabla r+\frac{i}{h}r^2 \tag{3.34}$$

ensures $\hat{\nabla}^2=0$.

We show that (3.34) has a unique solution r with the required properties. Uniqueness will ensure that the germs r define a global cross section of $\mathcal{W}(\mathcal{L})\otimes\mathcal{L}^*$. Indeed, by applying to (3.34) the operator δ^{-1}, we get

$$\delta^{-1}\delta r=r=\delta^{-1}S+\delta^{-1}\nabla r+\frac{i}{h}\delta^{-1}(r^2), \tag{3.35}$$

which is equivalent to the recurrence formula

$$\hat{r}_p=\widehat{(\delta^{-1}S)}_p+\delta^{-1}\nabla\hat{r}_{p-1}+\frac{i}{h}\delta^{-1}\left(\sum_{i=2}^{p-3}\hat{r}_i\circ\hat{r}_{p-1-i}\right). \tag{3.36}$$

Equations (3.32) and (3.36) imply $\hat{r}_2=0$, and, then,

$$\hat{r}_p=(\delta^{-1}\nabla)^{p-3}\delta^{-1}S+\frac{i}{h}\sum_{s=0}^{p-7}\left[(\delta^{-1}\nabla)^s\delta^{-1}\left(\sum_{j=3}^{p-s-2}\hat{r}_j\circ\hat{r}_{p-s-j-1}\right)\right]\quad(p\geqslant 3). \tag{3.37}$$

Now, it remains to establish that the obtained germ r satisfies Eq. (3.34). From (3.35), using the Hodge decomposition (3.18) and the Bianchi identity (3.33), we get

$$\delta r=\delta\delta^{-1}S+\delta\delta^{-1}\nabla r+\frac{i}{h}\delta\delta^{-1}r^2=S+\nabla r+\frac{i}{h}r^2-\delta^{-1}\delta\left(\nabla r+\frac{i}{h}r^2\right). \tag{3.38}$$

Formulas (3.33) and (3.38) give us the curvature

$$\Phi = \delta^{-1}\delta\left(\nabla r + \frac{i}{h}r^2\right) - \omega,$$

and, since

$$\hat{\nabla}\omega \overset{(2.28)}{=} \nabla\omega + \frac{i}{h}[\varpi + r, \omega] = \nabla\omega = d\omega = 0,$$

the Bianchi identity (3.31) yields

$$\hat{\nabla}\delta^{-1}\delta\left(\nabla r + \frac{i}{h}r^2\right) = 0. \tag{3.39}$$

But, if we look at any λ such that $\delta\lambda = 0$ and $\lambda_{00} = 0$, we have $\lambda = \delta\delta^{-1}\lambda$, and we see that

$$\hat{\nabla}\delta^{-1}\lambda \overset{(2.28)}{=} \nabla\delta^{-1}\lambda - \delta\delta^{-1}\lambda + \frac{i}{h}[r, \delta^{-1}\lambda] = 0$$

implies

$$\lambda = \nabla\delta^{-1}\lambda + \frac{i}{h}[r, \delta^{-1}\lambda]. \tag{3.40}$$

This is equivalent to a recurrence relation

$$\hat{\lambda}_p = \nabla\delta^{-1}\hat{\lambda}_{p-1} + \frac{i}{h} \quad (\text{terms in } \hat{\lambda}_i, \quad i \leqslant p-4), \tag{3.41}$$

which yields $\lambda = 0$. Since

$$\lambda = \delta\left(\nabla r + \frac{i}{h}r^2\right)$$

satisfies the required condition, the last term of (3.38) vanishes, and we are done.

Now, we address the second part of the theorem.

From (3.25) and (3.28), we see that $\hat{\nabla}\lambda = 0$ means

$$\delta\lambda = D\lambda, \quad D\lambda = \nabla\lambda + \frac{i}{h}[r, \lambda]. \tag{3.42}$$

Since $\lambda \in \mathcal{W}(\mathcal{L})$, $\delta^{-1}\lambda = 0$, and (3.18) and (3.42) yield

$$\lambda = \lambda_{00} + \delta^{-1}D\lambda = a + \delta^{-1}D\lambda, \tag{3.43}$$

and, with the decomposition $\lambda = \Sigma_{p=0}^{\infty}\hat{\lambda}_p$, we get the recurrence formula

$$\hat{\lambda}_p = (\hat{a})_p + \delta^{-1}\nabla\hat{\lambda}_{p-1} + \frac{i}{h}\delta^{-1}([r, \lambda]_{p-1}), \tag{3.44}$$

which uniquely defines all the terms $\hat{\lambda}_p$.

Particularly, if

$$a=\sum_{k=0}^{\infty} h^k f_k, \tag{3.45}$$

the first eight terms λ_p are given by

$$\hat{\lambda}_p=\sum_{s=0}^{[p/2]} h^s(\delta^{-1}\nabla)^{p-2s} f_s, \quad 0\leqslant p\leqslant 4, \tag{3.46}$$

$$\hat{\lambda}_p=\sum_{s=0}^{[p/2]} h^s(\delta^{-1}\nabla)^{p-2s} f_s+\frac{i}{h}\sum_{s=0}^{p-5}(\delta^{-1}\nabla)^s\delta^{-1}\sum_{j=3}^{p-s-2}[\hat{r}_j,\hat{\lambda}_{p-s-j-1}], \quad 5\leqslant p\leqslant 8. \tag{3.47}$$

The terms $\hat{\lambda}_p$ for larger values of p include commutants with several factors r. If for any $\mu\in\hat{W}(\mathcal{L})$ we denote

$$\overline{\mu}=\sum_{s=0}^{\infty}(\delta^{-1}\nabla)^s\mu, \tag{3.48}$$

and reorder the terms of λ, as determined by (3.46), (3.47), etc., we obtain

$$\lambda=\overline{a}+\frac{i}{h}\delta^{-1}[r,\overline{a}]+\left(\frac{i}{h}\right)^2\delta^{-1}[r,\delta^{-1}[\overline{r,\overline{a}}]]+\cdots. \tag{3.49}$$

Finally, we must check that (3.43) implies $\hat{\nabla}\lambda=0$. First, we notice that (3.43) implies

$$\delta^{-1}\hat{\nabla}\lambda=\delta^{-1}D\lambda-\delta^{-1}\delta\lambda=\lambda-a-\delta^{-1}\delta\lambda=\delta\delta^{-1}\lambda=0. \tag{3.50}$$

This allows us to use the Hodge decomposition (3.18) for $\hat{\nabla}\lambda$, the Abelian character of $\hat{\nabla}$, and (3.43) to get

$$\hat{\nabla}\lambda=\delta^{-1}\delta\hat{\nabla}\lambda=\delta^{-1}(D\hat{\nabla}\lambda-\hat{\nabla}^2\lambda)=\delta^{-1}D\hat{\nabla}\lambda. \tag{3.51}$$

Since the operator $\delta^{-1}D$ raises the degree, (3.51) yields a recurrence relation for the homogeneous terms of $\hat{\nabla}\lambda$, in the sense of the decomposition (3.3), which shows that $\hat{\nabla}\lambda=0$. Q.E.D.

As a consequence of this main theorem we see that there exists an injection

$$l:\mathcal{C}[[h]]\to\mathcal{W}(\mathcal{L}), \tag{3.52}$$

which sends the formal power series $a\in\mathcal{Z}(\mathcal{L})$ to the $\hat{\nabla}$-parallel section λ of $\mathcal{W}(\mathcal{L})$ which has the central projection $\lambda_{00}=a$.

This injection precisely is Fedosov quantization. The reason to see it as a quantization process with links to quantum physics is that the mapping l leads to a deformation of the commutative product fg into a noncommutative product, also known as a *star product*,[21,22] namely,

$$f*g=l^{-1}(l(f)\circ l(g)), \quad f,g\in\mathcal{C}. \tag{3.53}$$

The definition is correct since (3.21) and (3.28) show that $l(f)\circ l(g)$ belongs to the image of l.

In various concrete cases such as the ones in Examples (2.5)–(2.9), the mapping l is defined by corresponding versions of formulas (3.37), (3.46), (3.47), (3.49), etc. In particular, since a Lie algebroid always has connections, our presentation shows that Fedosov quantization works for the regular Poisson manifolds and, also, for the quasi-symplectic Poisson manifolds, even if the latter are nonregular. In other cases, the vanishing Atiyah class condition is required, and it may be very restrictive. For instance, this happens in the case of holomorphic symplectic manifolds.[9]

Note added in proof. In the paper[23] Nest and Tsygan give the classifications of general star products on symplectic Lie algebroids and holomorphic symplectic manifolds based on Fedosov quantization.

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Planar trajectories in a monopole field

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Motion of a Yang–Mills particle in a monopole field is proposed and planar orbits are observed. The planar orbits are studied further with some numerical analysis of the equations of motion. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In the Yang–Mills quantum field theories, such as electroweak and QCD, particles are assigned with some charges like hypercharge and color. In QED (an Abelian gauge theory) the charge is a conserved quantity that is related to the gauge-invariant property of the Lagrangian and expressed by a unique real number. In the non-Abelian theories the charge can no longer be expressed by a unique real number and might be displayed as a vector in the space of the gauge group (space of symmetry).

Wong extracted the classical equations of motion of a particle with a non-Abelian charge in a classical Yang–Mills field. The force on a (non-Abelian) particle in a (non-Abelian) field is the modification of the Lorentz force in the usual electrodynamics. Now the charge is a vector (in the isospace) and therefore may evolve in time. Wong has given the equation of evolution of the charge isovector, while the length of the charge isovector remains constant.

As an application of the Wong equations of motion we consider the 't Hooft or BPS monopoles and launch a Yang–Mills test particle in the field of the monopole. The speed and the total angular momentum of the particle and the field are constants of motion. We explain the equations of motion and enumerate some results. An interesting consequence of this motion is planar orbits. When a test particle is launched in the field of the monopole, while the direction of its charge isovector is normal to its position and velocity vectors, it will move in the plane normal to the charge isovector forever. We have explained the planar motions and the conditions for bounded orbits and their stability, and performed some numerical analysis of the equations of motion.

II. EQUATIONS OF MOTION OF YANG–MILLS PARTICLES IN YANG–MILLS FIELDS

In analogy with an Abelian system (a classical point charged particle interacting with the electromagnetic field), one can see a rich range of phenomena that occurs in non-Abelian systems. Wong proposed a system of equations to describe the classical dynamics of such systems (consisting of colored particles in non-Abelian fields) by generalizing the Lorentz force and Maxwell equations of electrodynamics. The non-Abelian particle is characterized by an isovector $\vec{I}$ (in analogy with the gauge invariant scalar charge q of an electrically charged point particle) which transforms under the adjoint representation of the internal symmetry group of the field—i.e., the gauge group. The following equations have been formulated by Wong:[1]

$$m\ddot{x}_\mu = eF^a_{\mu\nu} I^a \dot{x}^\nu, \tag{2.1}$$

$$\dot{I}^a + e\epsilon^{abc} A^b_\mu I^c \dot{x}^\mu = 0, \tag{2.2}$$

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where $x(\tau)$ is the world line of the particle in space–time, τ is proper time and ''dot'' denotes differentiation with respect to the proper time. The right-hand side of Eq. (2.1) obviously represents a generalization of the Lorentz force in which A^a_μ is a non-Abelian gauge potential and $F^a_{\mu\nu}$ are the gauge field strengths:

$$F^a_{\mu\nu}=\partial_\mu A^a_\nu-\partial_\nu A^a_\mu+e\,\epsilon^{abc}A^b_\mu A^c_\nu. \tag{2.3}$$

In the above equation e is coupling constant. In the limit we are considering a particle is thus described by an internal isovector $\vec{I}$ as well as its space–time coordinates. An immediate consequence of Eq. (2.2) is

$$\frac{d}{d\tau}I^2=0, \quad \text{where } I^2\equiv I^aI^a, \tag{2.4}$$

which shows the isovector I^a performs a precessional motion in isospace, i.e., the vector I^a sweeps the surface of a sphere in isospace such that the radius of this sphere could be understood as norm (absolute value) of charge isovector. Equivalently one can interpret Eq. (2.4) as a conservation law of scalar charge for a non-Abelian point particle.

III. EQUATIONS OF MOTION OF A YANG–MILLS PARTICLE IN A MONOPOLE FIELD

As an interesting problem, one can consider the interaction between a colored particle and a monopole. After discovery of the first monopole in the Yang–Mills–Higgs theories,[2,3] Schechter[4] and later Fehér[5] investigated the classical motion of a colored test particle in an external field given by the BPS monopole.

The ansatz of 't Hooft–Polyakov monopole for a finite-energy nonsingular classic solution can be of the form[2] (see also Ref. 6)

$$A^{a0}(\vec{r})=J(r)\frac{x^a}{er^2}, \tag{3.1}$$

$$A^{ai}(\vec{r})=\epsilon^{aij}\frac{x^j}{er^2}[1-K(r)], \tag{3.2}$$

$$\Phi^a(\vec{r})=\frac{x^a}{er^2}H(r), \tag{3.3}$$

where $J(r)$, $K(r)$, and $H(r)$ are certain functions of the radius r. In the last equation Φ^a is the Higgs field. For the 't Hooft–Polyakov monopoles, replacing the above ansatz with $J(r)=0$ in Eq. (2.3), a direct calculation shows

$$F^a_{0i}=0, \tag{3.4}$$

$$F^a_{ij}=\frac{1}{er^2}\left\{-2\,\epsilon^{aij}(1-K)+\epsilon^{ijk}\frac{x^ax^k}{r^2}(1-K)^2+(\epsilon^{aik}x^jx^k+\epsilon^{akj}x^ix^k)\frac{1}{r^2}(rK'+2(1-K))\right\}, \tag{3.5}$$

where prime indicates d/dr. Using the identity

$$\epsilon^{ijl}x^lx^k+\epsilon^{ilk}x^lx^j+\epsilon^{ljk}x^lx^i=r^2\,\epsilon^{ijk}, \tag{3.6}$$

Eq. (3.5) is simplified to

$$F^a_{ij}=\epsilon^{ijk}\frac{1}{er^2}\left\{\frac{x^ax^k}{r^2}(K^2-rK'-1)+rK'\,\delta^{ak}\right\}. \tag{3.7}$$

For the BPS monopole K and H are supposed to be[7,8]

$$K=\frac{aer}{\sinh(aer)},\quad H=aer\coth(aer)-1, \tag{3.8}$$

where a is magnitude of Higgs field at vacuum.

At large distances, K and K' vanish exponentially; the field has the form of a pure magnetic monopole. Thus an electrically charged particle coupled to vector potential would move exactly as a charged particle in a pure magnetic field.

In a nonrelativistic frame, $\tau=x_0=t$, using Eqs. (3.7), Eqs. (2.1) and (2.2) can be written in vector notation

$$m\dot{\vec{v}}=\frac{K^2-rK'-1}{r^4}(\vec{v}\times\vec{r})(\vec{r}\cdot\vec{I})+\frac{K'}{r}(\vec{v}\times\vec{I}), \tag{3.9}$$

$$\dot{\vec{I}}=\frac{1-K}{r^2}(\vec{r}\times\vec{v})\times\vec{I}. \tag{3.10}$$

Define at each point along the trajectory of the particle an orthogonal set of vectors,

$$\vec{r},\ \ \vec{w}=\vec{r}\times\vec{v},\ \ \vec{z}=\vec{r}\times\vec{w},\quad \text{where}\ \ \vec{v}=\frac{d\vec{r}}{dt}. \tag{3.11}$$

Then without loss of generality, non-Abelian charge I^a may be written as

$$\vec{I}=\alpha\hat{r}+\beta\hat{w}+\gamma\hat{z}, \tag{3.12}$$

where $\hat{r}$, $\hat{w}$ and $\hat{z}$ are unit vectors along the three directions. The coefficients α, β and γ satisfy

$$\alpha^2+\beta^2+\gamma^2=\text{const}, \tag{3.13}$$

which is a direct consequence of Eq. (2.4). Substituting Eq. (3.12) into Eq. (3.10) gives three equations for α, β and γ:

$$\dot{\alpha}=-\gamma|\vec{w}|K/r^2, \tag{3.14}$$

$$\dot{\beta}=\frac{r\gamma}{|\vec{w}|^2}\dot{\vec{v}}\cdot(\vec{r}\times\vec{v}), \tag{3.15}$$

$$\dot{\gamma}=-\frac{r\beta}{|\vec{w}|^2}\dot{\vec{v}}\cdot(\vec{r}\times\vec{v})+\frac{\alpha|\vec{w}|K}{r^2}. \tag{3.16}$$

Next, using the moving frame (3.11) in Eq. (3.9) we obtain the ordinary equation of motion:

$$m\dot{\vec{v}}=\frac{\beta}{r^2}|\vec{w}|K'\,\hat{r}+\frac{\beta}{r^2}(\vec{r}\cdot\vec{v})K'\,\hat{z}-\frac{1}{r^3}[\,\alpha|\vec{w}|(K^2-1)+\gamma r(\vec{r}\cdot\vec{v})K'\,]\hat{w}. \tag{3.17}$$

In addition to the length of the charge isovector, $|\vec{I}|$, the kinetic energy (or the magnitude of velosity $|\vec{v}|$) and the total angular momentum of the particle and the fields,[9]

$$\vec{J}=m(\vec{r}\times\vec{v})+K\vec{I}+\frac{(1-K)(\vec{r}\cdot\vec{I})}{r^2}\vec{r}, \tag{3.18}$$

are constants of motion.

For small distances near the center of the BPS monopole, $K=aer/\sinh(aer)\sim 1$ and $K'\sim 0$. So from Eqs. (3.9) and (3.10), $m\dot{\vec{v}}=0$ and $\dot{\vec{I}}=0$, which show a free motion around the center of the BPS monopole. Schechter has mentioned some properties of motion at large distances in Ref. 4.

Considering a general solution for equations of motion (3.9) and (3.10) is not easy. So, we explain some specific solutions in some detail.

If the particle is launched in a radial direction, while the charge isovector is also initially radial, the particle will move uniformly in the radial direction. This is the only choice for radial motion. This can be simply seen from the equations of motion (3.9) and (3.10), when $\vec{r}\times\vec{v}$ vanishes as the condition for radial motion. So $m\dot{\vec{v}}=(K'/r)(\vec{v}\times\vec{I})$ and $\dot{\vec{I}}=0$. For a radial motion, the acceleration $\dot{\vec{v}}$ must be in the radial direction, while we see $\vec{v}\times\vec{I}$ is normal to the radial direction (as we know $\vec{v}$ is radial). So the only possible case is a constant charge isovector $\vec{I}$ along the radial axis, and therefore a uniform radial motion occurs because $m\dot{\vec{v}}=0$. If the initial velocity points to the origin, the particle passes through the origin.

If the particle is launched in the field (in any direction) while the charge isovector is normal to the both initial particle's radial direction and velocity vector, then the particle will move on a plane normal to the charge isovector and the charge isovector remains constant. Under these circumstances radial motion is not allowed. We will show bounded orbits are allowed in the planar motion sector, while we have not observed bounded motions in the general three-dimensional theory.

In any case other than the two cases mentioned, the particle will move on a spatial curve. At the end of this section a numerical analysis of the general three-dimensional equations is described. In the next section we explain the planar motion of a particle in field of the BPS monopole.

IV. PLANAR ORBITS

A planar motion is identified by a conserved vector normal to the plane of motion. For nonzero values of position and velocity of a nonuniform motion, the plane of motion is normal to $\vec{r}\times\vec{v}$ at each time. Therefore, if in Eq. (3.17) the component of the force in the direction $\vec{r}\times\vec{v}$ vanishes, a planar motion takes place, provided that the equation of evolution for the charge isovector is valid.

A quick look at Eqs. (3.14)–(3.17) shows if we put $\alpha=\gamma=0$ we get

$$\dot{\alpha}=0, \tag{4.1}$$

$$\dot{\beta}=0, \tag{4.2}$$

$$\dot{\gamma}=-\frac{r\beta}{|\vec{w}|^2}\dot{\vec{v}}\cdot(\vec{r}\times\vec{v}), \tag{4.3}$$

$$m\dot{\vec{v}}=\frac{\beta}{r^2}|\vec{w}|K'\,\hat{r}+\frac{\beta}{r^2}(\vec{r}\cdot\vec{v})K'\,\hat{z}, \tag{4.4}$$

where in the last equation there is no component along $\vec{r}\times\vec{v}$ [i.e., $\dot{\vec{v}}\cdot(\vec{r}\times\vec{v})=0$] on the right-hand side, and therefore the condition for a planar motion is obtained. Using Eq. (4.4) the third equation becomes

$$\dot{\gamma}=0. \tag{4.5}$$

The equations (4.1) and (4.5) are consistent with the assumption $\alpha=\gamma=0$, and Eq. (4.2) becomes

$$\beta=\text{const}\neq 0, \tag{4.6}$$

which is required for the nonvanishing charge isovector. So the equations of motion (3.14)–(3.17) transformed to a new set of consistent equations which has only one equation, Eq. (4.4), to be solved. This equation as we said has no component in the direction normal to the position and velocity vectors, and this was the condition for the planar motion we mentioned at the beginning of this subsection. So $\alpha=\gamma=0$ implies planar motion. We will show also that the planar motion condition necessitates $\alpha=\gamma=0$.

To have no term in the direction normal to the plane of motion (as the condition for planar motion), we need to equate the coefficient of $\hat{w}$ in Eq. (3.17) to zero. So, Eq. (3.17) breaks into two separate equations

$$m\dot{\vec{v}}=\frac{\beta}{r^2}|\vec{w}|K'\,\hat{r}+\frac{\beta}{r^2}(\vec{r}\cdot\vec{v})K'\,\hat{z}, \tag{4.7}$$

$$\alpha|\vec{w}|(K^2-1)+\gamma r(\vec{r}\cdot\vec{v})K'=0, \tag{4.8}$$

where the first equation is the same as Eq. (4.4). With this treatment we are imposing an extra constraint on the original equations of motion, and this is not necessarily consistent with the other equations. To show the consistency, we may solve six equations out of seven (six original equations of motion plus one constraint because of the planar motion condition), and examine the validity of the last one with the resulting solution. From Eq. (4.7), $\dot{\vec{v}}$ has no term in the direction $\vec{r}\times\vec{v}$, so from Eq. (3.15), $\dot{\beta}=0$, which gives $\beta=\beta_0=\text{const}$, and equations for α and γ become

$$\dot{\alpha}=-\frac{\gamma|\vec{w}|K}{r^2}, \tag{4.9}$$

$$\dot{\gamma}=\frac{\alpha|\vec{w}|K}{r^2}. \tag{4.10}$$

So, with a solution for Eq. (4.7) we have to show the consistency of Eqs. (4.8)–(4.10) all together. Replacing α from Eq. (4.8) into Eq. (4.10) we obtain

$$\dot{\gamma}=\gamma\frac{KK'}{1-K^2}\dot{r}, \tag{4.11}$$

where we have used $\vec{r}\cdot\vec{v}=r\,\dot{r}$. Equation (4.11) is solvable and the solution is

$$\gamma=\frac{c_1}{\sqrt{1-K^2}}, \tag{4.12}$$

where c_1 is a constant. Using Eqs. (4.8) and (4.12)

$$\alpha=c_1\frac{r^2K'\,\dot{r}}{|\vec{w}|(1-K^2)^{3/2}}. \tag{4.13}$$

From Eqs. (4.9) and (4.10) [or equivalently from Eq. (3.13) and the fact that β is a constant] one may simply find

$$\alpha^2+\gamma^2=c_2^2, \tag{4.14}$$

where $c_2^2=I^2-\beta_0^2$ is another constant. So, finally we have to show the solutions (4.12) and (4.13) for γ and α satisfy Eq. (4.14). As we see, a solution for $\vec{r}$ and $\vec{v}$ (in fact $\vec{v}$ is enough) is needed to replace for appropriate quantities in (4.13).

The equation (4.7) stands alone and may be solved independently from the other equations. Taking the normal direction to the plane of motion as the z-direction in a cylindrical coordinate, one can write down the equations of motion in the polar plane. We can simply replace $\{\hat{r},\hat{w},\hat{z}\}$ by $\{\hat{r},\hat{k},-\hat{\theta}\}$. In the polar plane

$$\vec{v}=\dot{r}\,\hat{r}+r\dot{\theta}\,\hat{\theta}, \tag{4.15}$$

$$\dot{\vec{v}}=(\ddot{r}-r\dot{\theta}^2)\,\hat{r}+(2\dot{r}\dot{\theta}+r\ddot{\theta})\,\hat{\theta}, \tag{4.16}$$

so Eq. (4.7) in the cylindrical coordinates is

$$m[(\ddot{r}-r\dot{\theta}^2)\,\hat{r}+(2\dot{r}\dot{\theta}+r\ddot{\theta})\,\hat{\theta}\,]=\beta\dot{\theta}K'\,\hat{r}-\beta\frac{\dot{r}}{r}K'\,\hat{\theta}. \tag{4.17}$$

A set of two nonlinear differential equations appears,

$$\begin{aligned} m(\ddot{r}-r\dot{\theta}^2)&=\beta\dot{\theta}K',\\ m(2\dot{r}\dot{\theta}+r\ddot{\theta})&=-\beta\frac{\dot{r}}{r}K', \end{aligned} \tag{4.18}$$

which governs the motion of the particle in the polar plane. From the last equation one finds

$$mr^2\dot{\theta}+\beta K\equiv j=\text{const.} \tag{4.19}$$

Obtaining K' from the former equation of Eq. (4.18) and replacing it in the latter one, we find

$$\dot{r}\ddot{r}+r\dot{r}\dot{\theta}^2+r^2\dot{\theta}\ddot{\theta}=0,$$

which produces another constant of motion

$$\dot{r}^2+r^2\dot{\theta}^2\equiv v^2=\text{const.} \tag{4.20}$$

Both of the constants are in agreement with the overall discussion we had earlier about constants of motion.

Now we can replace $\dot{r}$ and $|\vec{w}|=|r^2\dot{\theta}|$ from Eqs. (4.19) and (4.20),

$$|\vec{w}|=|r^2\dot{\theta}|=\left|\frac{j-\beta K}{m}\right|,\quad \dot{r}^2=v^2-\left(\frac{j-\beta K}{mr}\right)^2, \tag{4.21}$$

into Eq. (4.14),

$$\frac{c_1^2}{1-K^2}\left\{1+\frac{r^4(K')^2[v^2-((j-\beta K)/mr)^2]}{((j-\beta K)/m)^2(1-K^2)^2}\right\}=c_2^2, \tag{4.22}$$

to check validity of this constraint that is imposed from the planar motion condition. In the above equation $K=aer/\sinh(aer)$, and c_1, c_2, m, β, v, j, a and e are constants. This means the right-hand side of Eq. (4.22) must be a constant. This can not happen in general. At least numerically, we may show the above function of r is not a constant for many choices of constants. The only clear possibility is for $r=\text{const}$, i.e., for a circular motion. For $r=\text{const}$, $\dot{r}=0$, so from Eq. (4.13) $\alpha=0$ and from Eq. (4.14) [or Eq. (4.12)] $\gamma=\text{const}$, where from Eq. (4.9) this constant must be zero which ceases $c_1=c_2=0$. For the other cases (i.e., not necessarily circular motions),

Eq. (4.22) necessitates $c_1=c_2=0$ and then $\alpha=\gamma=0$. So a planar orbit is possible if and only if the charge isovector has no component in the plane of motion, which means in the planar motion the charge isovector identifies the plane and remains constant.

V. ANALYTIC DESCRIPTION OF PLANAR ORBITS

A Lagrangian for the two-dimensional motion discussed above is offered as

$$L=T-U=\tfrac{1}{2}m\,(\dot{r}^2+r^2\dot{\theta}^2)+\beta\,\dot{\theta}\,K(r). \tag{5.1}$$

The "potential" $U=-\beta\,\dot{\theta}\,K(r)$ shows the force is not central. For a central force, the angular momentum, $l=mr^2\dot{\theta}$, and the total energy of the system, $T+U$, are constants of motion. But in our problem the total angular momentum of the particle and the fields, which was expressed in Eq. (4.19), and the kinetic part of energy alone [Eq. (4.20)] are constants of motion. Using the Euler–Lagrange equations, the equations of motion (4.18) are simply derived from the Lagrangian (5.1).

Replacing $\dot{\theta}$ from Eq. (4.19) into the first equation of Eqs. (4.18),

$$m\ddot{r}=\beta\left(\frac{j-\beta K}{mr^2}\right)K'+mr\left(\frac{j-\beta K}{mr^2}\right)^2=-\frac{m}{2\dot{r}}\frac{d}{dt}\left(\frac{j-\beta K}{mr}\right)^2, \tag{5.2}$$

gives

$$m\ddot{r}=-\frac{dV(r)}{dr}, \tag{5.3}$$

where

$$V(r)=\frac{m}{2}\left(\frac{j-\beta K}{mr}\right)^2. \tag{5.4}$$

The equation (5.3) is a one-dimensional equation of motion. The first integration of Eq. (5.3) gives

$$E=\tfrac{1}{2}m\dot{r}^2+V(r), \tag{5.5}$$

which is indeed equivalent to Eq. (4.20), i.e., $E=mv^2/2$ and $V(r)=mr^2\dot{\theta}^2/2$.

The "effective potential" $V(r)$ is a function of distance r, and through j depends on the initial conditions of the motion. To see how $V(r)$ is, we may simply analyze its derivative with respect to r:

$$V'(r)=\frac{-1}{2\,m\,r^3}(j-\beta K)(j-\beta K+\beta rK'). \tag{5.6}$$

The derivative $V'(r)$ vanishes if one of its two factors vanishes, i.e., $K(r)=j/\beta$ or $K(r)-rK'(r)=j/\beta$. To find the solutions of these equations we may find the points at which the constant function j/β coincides with the functions $K(r)=r/\sinh(r)$ ($a=e=1$) or $K(r)-rK'(r)=r^2\cosh(r)/\sinh^2(r)$. Looking at Fig. 1, for $0<j<j_c$ (say $\beta=1$) there are two solutions for $V'(r)=0$, therefore $V(r)$ has two extrema at r_1 and r_2. The effective potential $V(r)$ is a non-negative function and $V(r)\to 0$ as $r\to\infty$. So the two extrema must be a minimum and a maximum, respectively, i.e., r_1 is the minimum and r_2 is the maximum. For $0<j\leqslant 1$, $V(r)$ is tangent to the r-axis at the minimum point r_1 [because $V(r)$ is also vanishes for $j=\beta K$], and this is the only point that $V(r)$ touches the r-axis. For $1<j<j_c$, $V(r)$ does not coincide with the r-axis. For $j\neq 1$, $V(r)\to\infty$ as $r\to 0$, but for $j=1$ this limit is finite and $V(r)\to 0$ as $r\to 0$ (so $r_1=0$). For

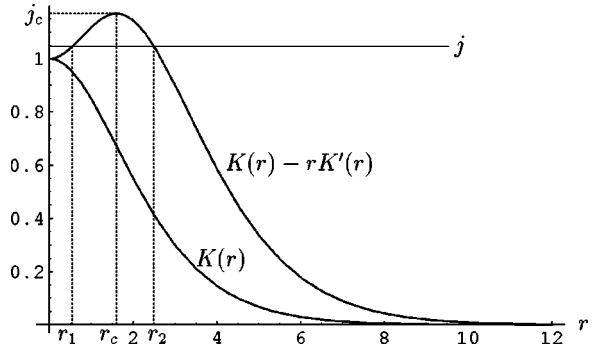

FIG. 1. Solutions of $V'(r)=0$.

$j=j_c$ ($r=r_c$) there is only a saddle point, and for $j\leqslant 0$ and $j>j_c$ there is no extremum and $V(r)$ is monotonically decreasing. Figure 2 shows the possible shapes of $V(r)$.

For a given j we may discuss the orbit of the particle, subject to the initial conditions. The limit value j_c may depend on the other constants of theory such as a, e and β. To see how j_c depends on a and e (instead of setting $a=e=1$ in last steps), we may consider a and e in K as it came in (3.8). Therefore, we have $K=aer/\sinh(aer)$ and $K-rK'=a^2e^2r^2\cosh(aer)/\sinh^2(aer)$. If we plot K and $K-rK'$ in Fig. 1 versus aer, we see r_c is rescaled, but j_c remains unaltered (up to the constant factor β). It is not difficult to find r_c and j_c (with $a=e=\beta=1$):

$$r_c=1.606, \quad j_c=1.169. \tag{5.7}$$

Let see the situation of a motion when j and E (or v) are given. If $0<j<j_c$ but $j\neq 1$, we have the top-left plot in Fig. 2. The altitude and latitude of the extrema from the horizontal and vertical axes are related to the constant j. Figure 3 shows the different possibilities of motion subject to energy E.

If the particle starts its motion with the energy E_4, it will be scattered to infinity and can never come closer to the origin than r_6 (see Fig. 7 in the next subsection). A motion with the energy E_2 will move on a circle of radius r_2 even if it starts its motion from inside or outside of the radius r_2. This motion is unstable, i.e., a small perturbation banishes the particle from the radius r_2. A small perturbation to the left may make a bounded orbit if the perturbed energy is less than E_2, while a small perturbation to the right sends the particle to infinity even if the energy is less than E_2 (see Fig. 8 in the next subsection). A particle with the energy E_3 is bounded and moves between two radii r_3 and r_4 if it starts the motion in between the two radii (see Fig. 7 in the next subsection), but it will be scattered to infinity if starts the motion from $r\geqslant r_5$. A particle with the

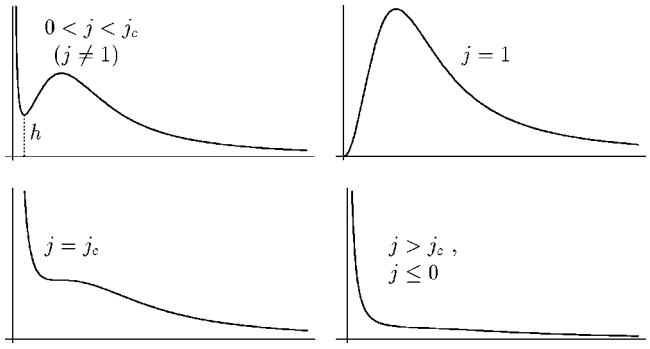

FIG. 2. One dimensional effective potential $V(r)$ (vertical axis) versus radius r (horizontal axis). In the top left plot, the height h is zero for $1<j<j_c$.

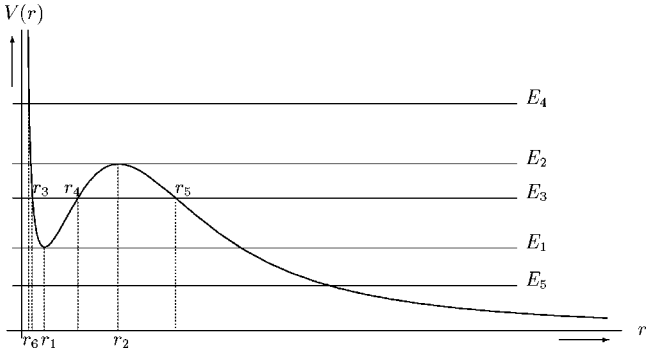

FIG. 3. Different possibilities of motion for $0<j<j_c$ $(j\neq 1)$.

energy E_1 moves on a circle of radius r_1. This is a stable motion (see Fig. 7 in the next subsection). The situation of a particle with the energy E_5 is similar to the particle with the energy E_4. In Fig. 3 r_1 and r_2 are given by r_1 and r_2 in Fig. 1 when j is specified.

For $0<j<1$, $V(r)$ is tangent to the r-axis at r_1, therefore the case with energy E_5 is inappropriate and E_1 lies on the r-axis (so $E_1=0$). A stationary particle (a particle with $E=0$, i.e., $\dot{r}_0=\dot{\theta}_0=0$) settles in this category and remains at r_1 without moving. So a stable circular motion is possible only for $1<j<j_c$.

For $0<j<j_c$, a bounded motion is possible if $E_1\leqslant E\leqslant E_2$. Using Fig. 1, $j=K(r_2)-r_2K'(r_2)=K(r_2)+r_2^2\dot{\theta}_2^2$, which gives $\dot{\theta}_2=-K'(r_2)/r_2$. So $E_2=(\dot{r}_2^2+r_2^2\dot{\theta}_2^2)/2=r_2^2\dot{\theta}_2^2/2=(K'(r_2))^2/2$, where index 2 shows the value of each quantity at r_2. For the minimum value we can do the same. For $1\leqslant j\leqslant j_c$ we have $(K'(r_1))^2/2\leqslant E\leqslant(K'(r_2))^2/2$, and for $0<j\leqslant 1$, $0\leqslant E\leqslant(K'(r_2))^2/2$. For each case radii r_1 and r_2 are determined by j, so with j we can describe the overall properties of the motion. As a problem we may determine the maximum value that E can take for a bounded motion. By equating the derivative of function $(K'(r))^2/2$ to zero, we find $r=1.606$ that is equal to r_c [see Eq. (5.7)] and so the maximum value of $(K'(r))^2/2$ is $E_c=0.0480$. This is not an accident, because in fact the energy E is equal to the potential $V(r)$ at the turning points, so at the turning points $E=V(r)=(j-K)^2/2r^2$. Clearly, the maximum value of E for a bounded motion occurs when $j=j_c$ (see Fig. 1). So if $E>E_c$ we can immediately conclude that the motion is not bounded.

Another point that is worth mentioning isn the following: If the particle is launched into the field from $r>r_m$, (for some r_m) we remain in the category $0<j<1$ for bounded motions. From Fig. 1 one can simply see the maximum distance from the origin for a maximum turning point for the category $1\leqslant j\leqslant j_c$ occurs in $j=1$. Then r_m is the nonzero root of $K(r)-rK'(r)=1$, which gives $r_m=2.676$. Clearly if a particle is launched in the field from $r>r_m$ it will not be bounded if $j\geqslant 1$. So the only possibility for a bounded orbit for this particle is $0<j<1$ (not any motion is necessarily bounded).

Motions with $j\neq 1$ do not pass the origin at all. For the bounded orbits, a particle moves in its path between two circles of radii r_3 and r_4. In the turning points $V(r)=E$, so $\dot{r}=0$. For $0<j<1$, in the radius r_1 [the point which locates between the turning points and minimizes $V(r)$] $V(r)=0$ (see the top-left plot in Fig. 2 with $h=0$), so in this radius $\dot{\theta}=0$ and the orbit must be tangent to a radius at this point (see Fig. 4). In the radius r_1 $(=OP_1=OP_2$ in Fig. 4), $\dot{\theta}=0$, but $\dot{r}\neq 0$ (because $E\neq 0$), so $d\theta/dr=0$. This means at this point the direction of variations of r remains unchanged, while the direction of variations of θ is changed. Therefore, each time that the particle completes a motion between two radii (for example, starting from the upper turning point and returning back to the point after traveling to the lower turning point), it passes two times from the desired point (r_1). So the particle makes an internal loop outside the origin (i.e., the loop does not surround the origin) in each travel. So in a 2π rotation the particle may construct several inner

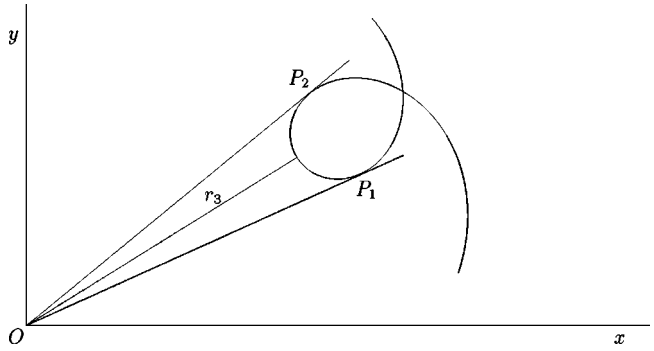

FIG. 4. Internal loops are possible for $0<j<1$.

loops which are lying on the main orbit around the origin. This case does not happen for $1<j<J_c$ because always $V(r)>0$.

This is an important result. For $1<j<J_c$ the particle rotates around the origin once in every 2π rotation (but not necessarily in a closed orbit). This is similar to the Kepler problem in gravitation. This motion definitely can happen only inside the region $r\leqslant r_m$ as we explained earlier. But for $0<j<1$ the situation is different. In a 2π rotation, a particle trajectory may form several loops outside the origin (see Fig. 5). This case may happen anywhere in the plane subject to suitable initial values.

For $j=1$ (the top-right plot in Fig. 2), the situation is the same as $0<j<1$, but here the lower turning point is fixed, $r_3=r_1=0$ (in contrast to the case of $j\neq 1$ where the lower turning point depends on E). In this case, the upper turning point, $r_4\leqslant r_m=2.676$. So in a bounded motion the particle passes the origin periodically. In fact, this case is settled between the two parts of the previously studied case. For $1<j<j_c$ a bounded orbit turns around the origin once in each 2π period, and the particle's orbit comes closer to the origin on a point of its trajectory when j takes a value closer to one (i.e., perihelion becomes shorter). In the limit, for $j=1$ the trajectory crosses the origin, and in each 2π rotation, the particle passes the origin once. When j takes a (positive) value less than 1, the orbit leaves the origin and makes a loop in the opposite side (see Fig. 5).

For $j=1$, $r=0$ is an extremum point of the potential $V(r)$, and $V(r)$ is tangent to the r-axis in $r=0$. So it is important to study any probable ambiguity at the origin. The origin is a turning point, and also the orbit is tangent to a radius at the origin. So it is a question to know about the velocity components at the origin. It is not difficult to show neither $\dot{r}$ nor $\dot{\theta}$ vanishes at $r=0$. One may show

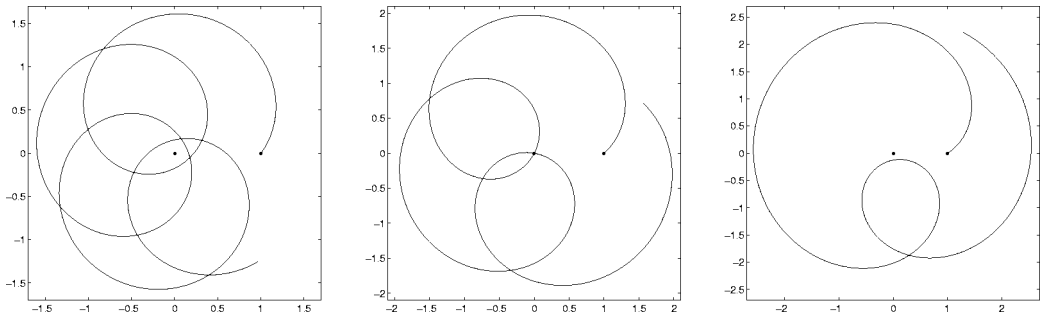

FIG. 5. In the left plot $j>1$, In the middle one $j=1$ and in the right plot $j<1$. In the three cases the particle has started the motion from (0,1) with the same energy, $E=0.025$. The total angular momentum j are 1.03, 1, and 0.97, respectively. The starting point and the origin are marked by black dots.

$$\lim_{r\to 0}\dot{\theta}=\lim_{r\to 0}\left\{\frac{1-K(r)}{r^2}\right\}=\frac{1}{6},$$
$$\lim_{r\to 0}\dot{r}^2=\lim_{r\to 0}\left\{v^2-\left(\frac{1-K(r)}{r}\right)^2\right\}=v^2. \tag{5.8}$$

The above limits may look strange, but still $v^2=\dot{r}^2+r^2\dot{\theta}^2$ is valid.

For $j=j_c$ (bottom-left plot in Fig. 2) a particle with the exact energy E_c has a non-stable circular motion in the saddle point, otherwise the particle is scattered to infinity. For $j\leqslant 0$ and $j>j_c$ the particle is scattered to infinity and there is no chance for bounded orbits.

Finally, if a particle starts its motion from the point (r_0,θ_0) with the velocity $(\dot{r}_0,\dot{\theta}_0)$, we may calculate the two important constants j and E (or equivalently v) and very soon recognize the motion to be bounded or not, and to which of the preceding cases it belongs.

In principle, we have discussed the overall characters and properties of the orbits, but the actual equation of the orbit must be obtained by integrating the differential equations of motion (4.19) and (4.20). Replacing $\dot{\theta}$ from Eq. (4.19) in Eq. (4.20) we get

$$t=\pm\int_{r_0}^{r}\frac{dr}{\sqrt{v^2-((j-\beta K)/mr)^2}}, \tag{5.9}$$

where the motion is supposed to be started from the initial value r_0 at time $t=0$. As it stands Eq. (5.9) gives t as a function of r and the constants of integration E (or v), j and r_0. However, it may be inverted, at least formally, to give r as a function of t and the constants. Once the solution for r is found, the solution for θ follows immediately from Eq. (4.19). At large distances from the center, K and K' vanish and the particle moves in a straight line. Clearly in the areas too close to the center of the monopole, K' vanishes as well (but not K), and a free motion is valid. However, in the other areas K and K' are important and cannot be ignored. Again using $\dot{\theta}$ from Eq. (4.19) and $\dot{r}$ from Eq. (4.20) (after some replacement of $\dot{\theta}$), after some rearrangement of variables an integral equation for the orbit of the particle is found as:

$$\theta-\theta_0=\pm\int_{r_0}^{r}\frac{dr}{r\sqrt{(mvr/(j-\beta K))^2-1}}. \tag{5.10}$$

With the presence of the hyperbolic function in the integral, it seems difficult to solve it by changing the variables. Instead of the above integral equation for the orbit, we may replace dt from Eq. (4.19) into Eq. (5.3) and find a second order differential equation for the orbit. But none of these help us to find analytic solutions for the orbits. So in the next we present some numerical solutions of Eqs. (4.18) and observe the results we found in the previous pages.

VI. NUMERICAL OBSERVATIONS

In this subsection we present some numerical solutions for the set of equations (4.18) for planar motions and Eqs. (3.9) and (3.10) for nonplanar motions. We have used the Runge–Kutta method (of fourth order) for solving first order differential equations. The required programs are written in the ''MATLAB'' programming package. In a planar motion let us suppose a particle of unit mass, $m=1$, and unit charge, $\vec{I}=\beta\hat{k}$, $\beta=+1$, has been launched in the field of a BPS monopole with $a=e=1$, from a point (r_0,θ_0), with an initial velocity $(\dot{r}_0,\dot{\theta}_0)$. The following results are concluded for the different initial values for which we have tested the equations.

The monopole forces the particle to move on a curve in the plane such that if the thumb of the right hand stands in the direction of the charge isovector, then the sense of closing the rest of fingers shows the direction of rotation of particle. In Fig. 6 a particle is launched in four different

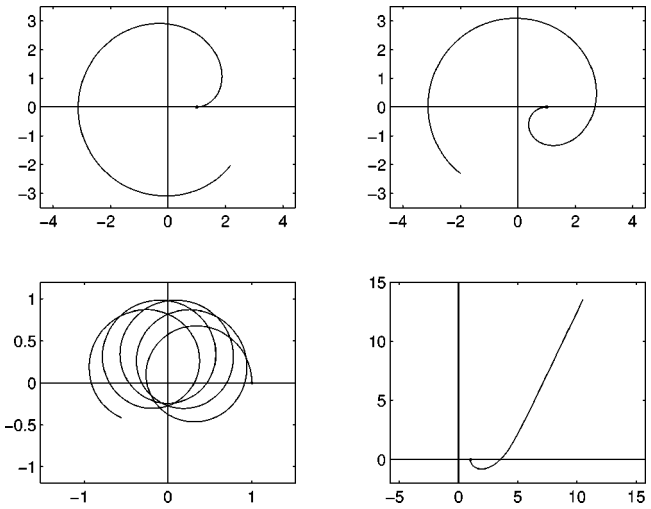

FIG. 6. Particle is launched from point (1,0) (the dark point in the x-axis) with the same speed (0.184) in each case. (The number of significant digits in the velocity is not crucial; it has been chosen for a better illustration of the plots.)

directions (with the same energy), and the particle moves counter-clockwise in each case (the charge isovector is normal to the paper pane and outward). This observation is greatly different from the usual scattering of an electric particle in a Maxwell field. If the behavior of this system was like a usual electrodynamics system, the two bottom plots of Fig. 6 would be the mirror images with respect to the x-axis, while here we see one motion is bounded while the other one is scattered to the infinity. (Note in the last two plots, in spite of the fact that the energy is the same in both cases, j is different so they follow the two different models of $j-E$ graphs we explained in Sec. V.)

This point can be explained analytically when the condition for the planar motion is used in the original equation (3.9). In Eq. (3.9) $\vec{r}\cdot\vec{I}=0$ (for the planar motion), so the equation of motion in a compact form is

$$m\ddot{\vec{r}}=\frac{K'}{r}(\vec{v}\times\vec{I}). \tag{6.1}$$

The term on the right-hand side of Eq. (6.1) is the force that is exerted from the fields onto the particle. The $\vec{I}=\beta\hat{k}$ is a vector normal to the plane of motion and in the upward direction. So the cross-product of $\vec{v}$ and $\vec{I}$ is a vector in the plane of motion and always normal to the velocity vector and in counter-clockwise direction. Therefore, the particle is forced to move counter-clockwise.

Bounded and unbounded orbits are allowed depending on the choice of initial values. Closed bounded orbits may exist for each point in the plane, depending on the initial velocity. There are lots of various orbits: circles, Limaçon-shapes, curves with many loops (loops may surround the center or not), the simple scattered curves and many other complicated curves. A variety of possible orbits are shown in Fig. 7. For closed orbits the initial conditions are specified. For example, in the two top plots of Fig. 7 the initial position of the particle is known [i.e., $(r,\theta)=(1,0)$], the velocities are specified up to some significant digits.

Although the circular motions are closed orbits, in general we can not find a prescription for closed orbits. By numerical methods and trial and error we may find some closed orbits. The top-left plot in Fig. 7 is an example.

Figure 8 shows an unstable motion around the maximum point for $0<j<j_c$. In the top-left plot, the particle is launched from point (1,0) with $(\dot{r}_0,\dot{\theta}_0)=(0.184,0)$, so it will rotate in a radial direction at $r_2=3.163$. This case is calculated only to be compared with the closed top-left plot in

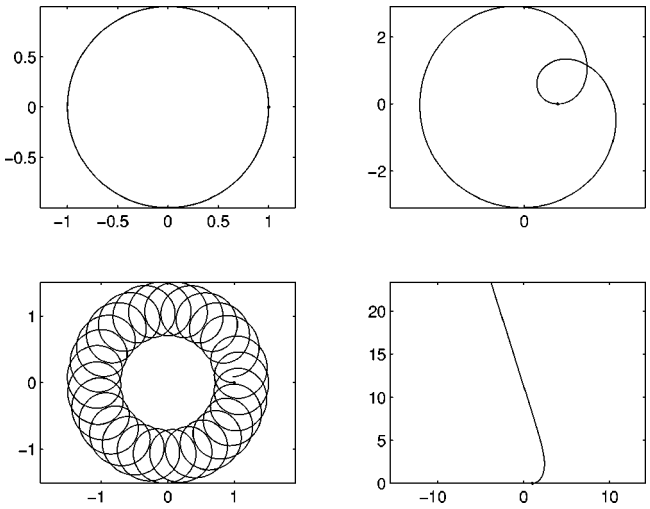

FIG. 7. For each case motion is started from point (1,0) (the dark point), but the initial energy is different for each case. For the circle, initial velocity is 0.266, and for the Limaçon-shape, the initial velocity is $(\dot{r}_0,\dot{\theta}_0)=(0.184,0)$.

Fig. 7. So for any $0<j<j_c$ (i.e., r_0 and $\dot{\theta}_0$ are specified), we can find a value $\dot{r}_0$ and send the particle to rotate on the critical radius r_2. For smaller or bigger energies, the motion will be bounded between two circles, or scattered to infinity, as was explained earlier. The bottom-left and top-right plots show these points. The bottom-right plot is another example of a unstable motion. The particle starts the motion from the same point as the other three, but j and energy are different. We can compare this case with the circular motion in Fig. 7.

VII. NUMERICAL OBSERVATIONS FOR NONPLANAR MOTIONS

Now we explain nonplanar motions which indeed follow the general equations of motion (3.9) and (3.10). Suppose the particle is launched in the field from the point (0,0,10) with an initial velocity $(0,0,-0.1)$ while the charge isovector is initially (0,0,1). As we explained before, the particle moves in the z-direction and passes through the origin in enough time. Now suppose instead of launching the particle in the z-direction, we launch it from the point (0,1,10). So the

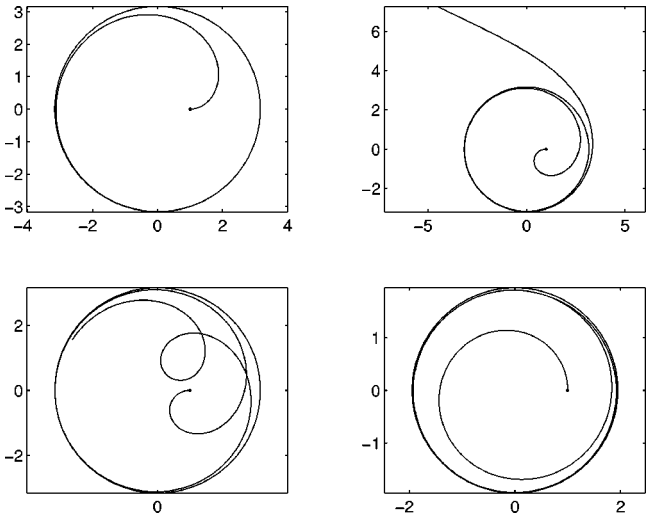

FIG. 8. For each case motion is started from point (1,0) (the dark point). The plots show stability of the orbits around r_2.

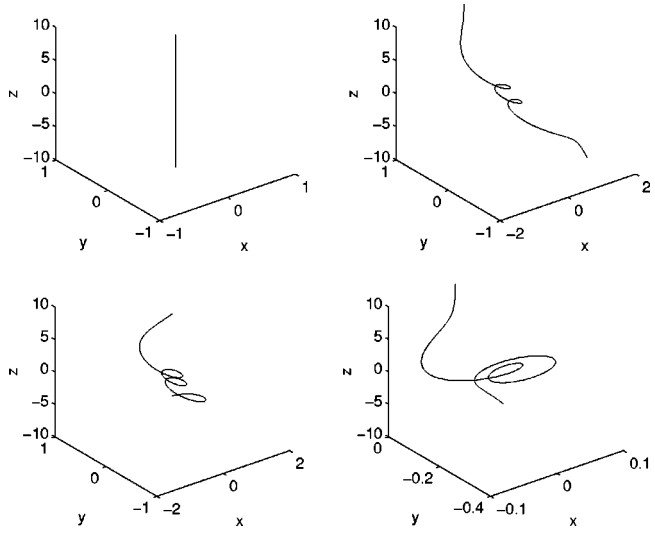

FIG. 9. Spatial orbits.

initial conditions are as before unless an impact parameter is taken into consideration. Of course with these initial conditions the particle moves on a curve which is no longer planar. The top two plots in Fig. 9 show the orbits for the above-mentioned two cases.

Instead of considering an impact parameter in the above case, which leads to a nonplanar motion, any small deviation in the initial velocity in the normal direction to the plane or in the charge isovector in the plane causes nonplanar orbits as well. Examples for these two cases are the bottom plots in Fig. 9. In the right plot the particle is launched from (0,0,10) with the velocity $(0,0.01,-0.1)$ and charge isovector (0,0,1), and in the left plot from (0,0,10) with the velocity $(0,0,-0.1)$ and the charge isovector (0,0.1,1).

By changing the initial values we may collect a wide range of spatial orbits. Organizing these plots to get some useful results is not straightforward, and in addition we need a long time for each computation. As an example, the following observation may lead us to the idea of standard one-dimensional potential we explained on the subject of planar motion. In the continuation of the top two plots in Fig. 9 we can increase the impact parameter. Note that the particle reflects back in the z-direction, when we put (0,2,10) for the location of the particle and the other initial values are unchanged. Now we can decrease the impact parameter and then play with it by adding and subtracting the earlier values to find a plot such that the particle stays around the xy-plane (at least for a while). We may continue this procedure to get a better and better result. In Fig. 10, the left plot is the three-dimensional orbit and the right one shows the time variation of the z component. This plot is resulting from the same initial values as the two top plots in Fig. 9, but with impact parameter 1.953 [i.e., (0,1.953,10) for the initial location]. The particle has a small oscillatory

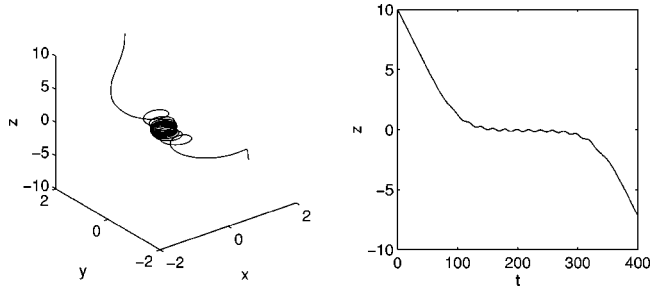

FIG. 10. Nonstable motion.

motion along the z-axis close to the xy-plane for a while. We may increase duration of the delay around the xy-plane for a longer time by changing the value of the impact parameter to a better value.

Based on the observation we explained in the last paragraph, one may compare this situation with the unstable extremum points in the one-dimensional potential model we explained for the planar motions (see Fig. 8), but in a three-dimensional context. So if this is like an unstable extremum, there might exist a stable analog of the one-dimensional potential in the three-dimensional context. If a minimum exists for the general potential model, a stable planar motion would be allowed. This means stability of planar motion might be possible, i.e., if some small normal perturbations disturb the planar motion, the orbit should stay bounded around the plane. In the next topic we analyze this problem in some detail.

It is proper here to say a word about the scattering problem. With the above results from the numerical works, we see the scattering depending on many parameters is not as simple as in the two-dimensional central force problems. We may keep the initial conditions of the problem unchanged but alter the impact parameter. As the impact parameter changes, the plane spanned by the initial and final velocity vectors changes. So it is needed to introduce three scattering angles instead of the one which is used in the usual two-dimensional scattering problems. Even in two-dimensional planar motions the scattering of the particle is not symmetric with respect to the positive and negative values of the impact parameter (see the two bottom plots in Fig. 6). The problem of scattering in three-dimensional motions is a separate problem, so we skip it here.

VIII. STABILITY OF PLANAR MOTIONS

The conditions for planar motion look too strong and therefore the stability of planar motions may be very weak. This means, if a little deviation in the quantities perturbs the planar motion in the normal direction to the plane, the particle will leave the plane and be scattered to infinity. Because the perturbations are generally in three dimensions, we should use the general equations of motion (3.9) and (3.10). So, let us first find the required equations for perturbations in three dimensions.

Suppose small perturbations in $\vec{r}$ and $\vec{I}$ are of the form

$$\vec{r}\to\vec{r}+\vec{\epsilon},\quad \vec{I}\to\vec{I}+\vec{\delta}, \tag{8.1}$$

where $\vec{\epsilon}$ and $\vec{\delta}$ are small quantities. For the other quantities we will have

$$\vec{v}\to\vec{v}+\dot{\vec{\epsilon}},\ \ \dot{\vec{v}}\to\dot{\vec{v}}+\ddot{\vec{\epsilon}},\ \ \dot{\vec{I}}\to\dot{\vec{I}}+\dot{\vec{\delta}},\ \ r\to r+\frac{\vec{\epsilon}\cdot\vec{r}}{r}, \tag{8.2}$$

where in the last one we have kept only the first order approximation. Replacing the unperturbed quantities in equations of motion (3.9) and (3.10) with the perturbed quantities from the right-hand side of the above relations, we find

$$\begin{aligned} m\ddot{\vec{\epsilon}}=&\frac{K^2-rK'-1}{r^4}\{(\vec{v}\times\vec{\epsilon})(\vec{r}\cdot\vec{I})+(\dot{\vec{\epsilon}}\times\vec{r})(\vec{r}\cdot\vec{I})+(\vec{v}\times\vec{r})(\vec{r}\cdot\vec{\delta})+(\vec{v}\times\vec{r})(\vec{\epsilon}\cdot\vec{I})\}\\ &-\frac{4K^2-2rKK'+r^2K''-3rK'-4}{r^3}(\vec{\epsilon}\cdot\vec{r})(\vec{v}\times\vec{r})(\vec{r}\cdot\vec{I})+\frac{K'}{r}\{(\vec{v}\times\vec{\delta})+(\dot{\vec{\epsilon}}\times\vec{I})\}\\ &+\frac{rK''-K'}{r^3}(\vec{\epsilon}\cdot\vec{r})(\vec{v}\times\vec{I}), \end{aligned} \tag{8.3}$$

$$\dot{\vec{\delta}}=\frac{1-K}{r^2}\{(\vec{\epsilon}\times\vec{v})\times\vec{I}+(\vec{r}\times\dot{\vec{\epsilon}})\times\vec{I}+(\vec{r}\times\vec{v})\times\vec{\delta}\}-\frac{2(1-K)+rK'}{r^4}(\vec{\epsilon}\cdot\vec{r})[(\vec{r}\times\vec{v})\times\vec{I}\,], \tag{8.4}$$

where in derivation we have ignored the second order perturbations and used the unperturbed equations (3.9) and (3.10).

Now for the planar motion case, where we have suggested to make a small perturbation in the space, we have

$$m\ddot{\vec{\epsilon}}=\frac{K^2-rK'-1}{r^4}\{(\vec{v}\times\vec{r})(\vec{r}\cdot\vec{\delta})+(\vec{v}\times\vec{r})(\vec{\epsilon}\cdot\vec{I})\}+\frac{K'}{r}\{(\vec{v}\times\vec{\delta})+(\dot{\vec{\epsilon}}\times\vec{I})\}$$
$$+\frac{rK''-K'}{r^3}(\vec{v}\times\vec{I})(\vec{\epsilon}\cdot\vec{r}), \tag{8.5}$$

$$\dot{\vec{\delta}}=\frac{1-K}{r^2}\{(\vec{r}\times\vec{v})\times\vec{\delta}+(\vec{I}\cdot\vec{\epsilon})\,\vec{v}-(\vec{I}\cdot\dot{\vec{\epsilon}})\,\vec{r}\}, \tag{8.6}$$

and we have used $\vec{r}\cdot\vec{I}=\vec{v}\cdot\vec{I}=0$. Only the terms in the second row of Eq. (8.5) can be derived from the planar equation of motion (6.1), and the remaining terms in both equations have appeared by considering the general three-dimensional equations of motion.

Cylindrical coordinates are suitable to write down the equations for each component separately. We may write

$$\vec{\epsilon}=\epsilon_r\hat{r}+\epsilon_\theta\hat{\theta}+\epsilon_z\hat{z},$$
$$\vec{\delta}=\delta_r\hat{r}+\delta_\theta\hat{\theta}+\delta_z\hat{z}. \tag{8.7}$$

So

$$\dot{\vec{\epsilon}}=(\dot{\epsilon}_r-\dot{\theta}\epsilon_\theta)\hat{r}+(\dot{\epsilon}_\theta+\dot{\theta}\epsilon_r)\hat{\theta}+\dot{\epsilon}_z\hat{k},$$
$$\dot{\vec{\delta}}=(\dot{\delta}_r-\dot{\theta}\delta_\theta)\hat{r}+(\dot{\delta}_\theta+\dot{\theta}\delta_r)\hat{\theta}+\dot{\delta}_z\hat{k}, \tag{8.8}$$

and

$$\ddot{\vec{\epsilon}}=(\ddot{\epsilon}_r-\ddot{\theta}\epsilon_\theta-2\dot{\theta}\dot{\epsilon}_\theta-\dot{\theta}^2\epsilon_r)\hat{r}+(\ddot{\epsilon}_\theta+\ddot{\theta}\epsilon_r+2\dot{\theta}\dot{\epsilon}_r-\dot{\theta}^2\epsilon_\theta)\hat{\theta}+\ddot{\epsilon}_z\hat{k}. \tag{8.9}$$

Replacing from Eqs. (8.7)–(8.9) into Eqs. (8.5) and (8.6), and using $\vec{I}=\beta\hat{k}$ ($\beta=$const), $\vec{r}$ and $\vec{v}$ in the polar plane (plane of motion), one may find a complete set of six linear differential equations for six unknown perturbation components:

$$m\ddot{\vec{\epsilon}}=\left\{\beta\frac{K'}{r}\dot{\epsilon}_\theta+\beta K''\dot{\theta}\epsilon_r+K'\dot{\theta}\delta_z\right\}\hat{r}+\left\{-\beta\frac{K'}{r}\dot{\epsilon}_r-\beta\frac{rK''-K'}{r^2}\dot{r}\epsilon_r+\beta\frac{K'}{r}\dot{\theta}\epsilon_\theta-\frac{K'}{r}\dot{r}\delta_z\right\}\hat{\theta}$$
$$+\left\{-\beta\frac{K^2-rK'-1}{r^2}\dot{\theta}\epsilon_z+\frac{1-K^2}{r}\dot{\theta}\delta_r+\frac{K'}{r}\dot{r}\delta_\theta\right\}\hat{k}, \tag{8.10}$$

$$\dot{\vec{\delta}}=\left\{\frac{1-K}{r^2}(-\beta r\dot{\epsilon}_z+\beta\dot{r}\epsilon_z-r^2\dot{\theta}\delta_\theta)\right\}\hat{r}\left\{\frac{1-K}{r}(\beta\dot{\theta}\epsilon_z+r\dot{\theta}\delta_r)\right\}\hat{\theta}, \tag{8.11}$$

where on the left-hand side we may replace $\ddot{\vec{\epsilon}}$ and $\dot{\vec{\delta}}$ from Eqs. (8.9) and (8.8), and write down equations of motion for each component. In the first instance we find $\dot{\delta}_z=0$, so

$$\delta_z=\text{const}. \tag{8.12}$$

Therefore for small perturbations the total component of the charge isovector in the normal direction to the plane of motion, $\beta+\delta_z$, remains constant. For example, if initially the perturbation of the charge isovector takes place in the plane of motion, this perturbation remains in the plane when the perturbation is small.

Let us choose an auxiliary variable $\vec{\sigma}\equiv\dot{\vec{\epsilon}}$

$$\vec{\sigma}=\sigma_r\hat{r}+\sigma_\theta\hat{\theta}+\sigma_z\hat{k},$$
$$\dot{\vec{\sigma}}=(\dot{\sigma}_r-\dot{\theta}\sigma_\theta)\hat{r}+(\dot{\sigma}_\theta+\dot{\theta}\sigma_r)\hat{\theta}+\dot{\sigma}_z\hat{k}. \tag{8.13}$$

Now we can write nine first-order differential equations for the perturbations (let us set $m=1$):

$$\dot{\epsilon}_r=\dot{\theta}\,\epsilon_\theta+\sigma_r,$$

$$\dot{\epsilon}_\theta=-\dot{\theta}\,\epsilon_r+\sigma_\theta,$$

$$\dot{\epsilon}_z=\sigma_z,$$

$$\dot{\sigma}_r=\beta\frac{rK''-k'}{r}\dot{\theta}\,\epsilon_r+\left(\beta\frac{K'}{r}+\dot{\theta}\right)\sigma_\theta+K'\dot{\theta}\,\delta_z,$$

$$\dot{\sigma}_\theta=-\beta\frac{rK''-k'}{r^2}\dot{r}\,\epsilon_r-\left(\beta\frac{K'}{r}+\dot{\theta}\right)\sigma_r+\frac{K'}{r}\dot{r}\,\delta_z, \tag{8.14}$$

$$\dot{\sigma}_z=-\beta\frac{K^2-rK'-1}{r^2}\dot{\theta}\,\epsilon_z+\frac{1-K^2}{r}\dot{\theta}\,\delta_r+\frac{K'}{r}\dot{r}\,\delta_\theta$$

$$\dot{\delta}_r=\beta\frac{1-K}{r^2}\dot{r}\,\epsilon_z-\beta\frac{1-K}{r}\sigma_z+K\dot{\theta}\,\delta_\theta,$$

$$\dot{\delta}_\theta=\beta\frac{1-K}{r}\dot{\theta}\,\epsilon_z-K\dot{\theta}\,\delta_r,$$

$$\dot{\delta}_z=0.$$

Equivalently we may write the above set of equations in matrix form

$$\dot{\vec{S}}=\mathbf{M}\vec{S}, \tag{8.15}$$

where

$$\vec{S}=[\epsilon_r\ \ \epsilon_\theta\ \ \epsilon_z\ \ \sigma_r\ \ \sigma_\theta\ \ \sigma_z\ \ \delta_r\ \ \delta_\theta\ \ \delta_z]^T \tag{8.16}$$

(T stands for the transpose) and

$$\mathbf{M}(\vec{r},\dot{\vec{r}})$$

$$=\begin{bmatrix}
0 & \dot\theta & 0 & 1 & 0 & 0 & 0 & 0 & 0\\
-\dot\theta & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0\\
\dfrac{\beta(rK''-K')\dot\theta}{r} & 0 & 0 & 0 & \dfrac{\beta K'}{r}+\dot\theta & 0 & 0 & 0 & K'\dot\theta\\
-\dfrac{\beta(rK''-K')\dot r}{r^2} & 0 & 0 & -\dfrac{\beta K'}{r}-\dot\theta & 0 & 0 & 0 & 0 & \dfrac{K'\dot r}{r}\\
0 & 0 & \dfrac{\beta(1-K^2+rK')\dot\theta}{r^2} & 0 & 0 & 0 & \dfrac{(1-K^2)\dot\theta}{r} & \dfrac{K'\dot r}{r} & 0\\
0 & 0 & \dfrac{\beta(1-K^2)\dot r}{r^2} & 0 & 0 & -\dfrac{\beta(1-K)}{r} & 0 & K\dot\theta & 0\\
0 & 0 & \dfrac{\beta(1-K)\dot\theta}{r} & 0 & 0 & 0 & -K\dot\theta & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}. \tag{8.17}$$

The matrix **M**, which is a function of the variables $\vec{r}$ and $\dot{\vec{r}}$, is implicitly a function of time t. If **M** was a constant matrix with eigenvalues λ_i and eigenvectors $\vec{R}_i$, the solution of the linear differential equation (8.16) would be $\Sigma_{i=1}^{9} C_i \exp(\lambda_i t)\vec{R}_i$, where C_i are constants. But now the solution cannot be as simple as this, because the eigenvalues of the matrix **M** are functions of time. The only chance for solving the equations in this way is for circular motions when r and $\dot\theta$ are constants and $\dot r$ vanishes. For example, for the circular motion of Fig. (7), $r=1$, $\theta_0=0$, $\dot r=0$, $\dot\theta=0.266$ and $\beta=1$, the eigenvalues of **M** are

$$0.442,\ -0.442,\ 0.509,\ -0.509,\ 0.235i,\ -0.235i,\ 0,\ 0,\ 0.$$

We have used the "MAPLE" programming package to calculate the above values. Using the MAPLE package we can find the eigenvectors as well. Now we need initial values of the perturbation quantities to determine the constants C_i. Suppose in the circular motion, instead of starting the motion at $t=0$ exactly from the point (1,0,0) in the plane of motion, start the motion from (1,0,0.001) and the other initial values of the circular motion do not alter. So we have set a small perturbation only in the z-direction (normal to the plane of motion), i.e., $S(t=0)=[0,0,0.001,0,0,0,0,0,0]^T$. Equating $S(t=0)=\Sigma_{i=1}^{9} C_i\vec{R}_i$, the constants C_i are found. Let us study the result for one of the perturbation's components, e.g., ϵ_z,

$$\epsilon_z = 0.000\,511\, e^{0.509t} + 0.000\,511 e^{-0.509t} - 0.000\,022\,3\, e^{0.235\, i\, t}.$$

Clearly the first exponential term on the right-hand side of the above equation, in spite of its small coefficient, diverges as $t\to\infty$. Therefore, we can judge the circular motion under study is not stable.

An analytic solution of the set of equations (8.14) [or equivalently (8.15)] is not available, so we may examine the equations of perturbation by numerical methods. We can study any solution in the plane, with some small values for perturbation quantities. Suppose a list of data of position and velocity of a planar motion is available. So we may use the data and the set of equations (8.14) and a numerical method such as the Runge–Kutta method (or even simpler methods) for computing the differential equations. It is more convenient to calculate the data of planar motion in a procedure and at the same time compute the perturbation quantities for each set of $(r,\theta,\dot r,\dot\theta)$. We have studied the problem with different choices of the perturbation quantities for different planar solutions, and the results are the same as above. Indeed if the initial perturbation in the charge

isovector is in the z-direction, or the initial perturbation in $\vec{r}$ and $\vec{v}$ is in the plane of motion, the motion will stay planar. The stable and unstable planar motions (for perturbations in the plane) were discussed earlier.

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A planar Runge–Lenz vector

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Following Dahl's method an exact Runge–Lenz vector **M** with two components M_1 and M_2 is obtained as a constant of motion for a two particle system with charges e_1 and e_2 whose electromagnetic interaction is based on Chern–Simons electrodynamics. The Poisson bracket $\{M_1, M_2\} \neq L_z$ but is modified by the appearance of the product $e_1 e_2$ as central charges. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1420399]

A characteristic feature of the nonrelativistic Kepler problem is that there exists apart from the conservation of energy (E) and the angular momentum vector (**L**) another conserved quantity, namely the Runge–Lenz vector (**A**). A textbook[1] derivation of **A** begins with the equation of motion of a mass m under the central force $\mathbf{F} = f(r)(\mathbf{r}/r)$, namely, $d\mathbf{p}/dt = f(r)(\mathbf{r}/r)$, leading to

$$\frac{d}{dt}(\mathbf{p}\times\mathbf{L}) = -mf(r)r^2\frac{d}{dt}\left(\frac{\mathbf{r}}{r}\right) \tag{1}$$

as $d\mathbf{L}/dt = 0$. With $r^2 f(r) =$ a constant (say-k), thereby implying an inverse square law of force, Eq. (1) immediately yields $\mathbf{A} = \mathbf{p}\times\mathbf{L} - mk(\mathbf{r}/r)$; this is the Runge–Lenz vector. With the definition $\mathbf{K} = (-2mE)^{1/2}\mathbf{A}$, one easily obtains the Poisson bracket relations

$$\{\mathbf{K}, E\} = 0, \{\mathbf{L}, E\} = 0, \{L_i, L_j\} = \epsilon_{ijk}L_k, \{L_i, K_j\} = \epsilon_{ijk}K_k, \{K_i, K_j\} = \epsilon_{ijk}L_k. \tag{2}$$

Thus there exists an internal symmetry associated with the nonrelativistic Kepler problem with the invariance group being isomorphic to the four-dimensional rotation group O_4. Until recently, the presence of this internal symmetry had not been tied to a generally accepted invariance principle. In other words, the phenomenological derivation implied in Eq. (1) begs the question of whether the Runge–Lenz vector has a deeper physical origin. Specifically, the question is if there is a space–time transformation, the invariance of the Lagrangian for the Kepler problem under which directly leads to the conservation of **A**.

An affirmative answer to this question was recently obtained by Dahl[2] by regarding the Kepler problem as the zero-order description of a relativistic two-body problem; or, as emphasized by Dahl,[2] it is absolutely necessary to investigate the relativistic two-body problem in order to discover the connection between the dynamical symmetry of the nonrelativistic Kepler problem and special relativity.

Of special relevance to this paper is the fact[3] that for the Kepler problem the angular momentum vector $\mathbf{L} = \mathbf{r}\times\mathbf{p}$ is conserved so that $\mathbf{r}\cdot\mathbf{L} = 0$. Thus **r** always lies in a plane[4] whose normal is parallel to **L**. Since the motion of the particle is planar because of symmetry considerations it is appropriate to ask the following: Suppose the motion of the particle was de facto planar and not due to symmetry considerations as in the case of motion under a central force, could one still obtain a Runge–Lenz vector that is conserved in this $2+1$ dimensional case? Happily, we derive in this paper, following Dahl's method,[2] a bonafide Runge–Lenz vector [see Eq. (23)] associated with the relativistic Lagrangian with Chern–Simons interactions[5–7] for a two-particle system consisting of masses m_1 and m_2 with charges e_1 and e_2, respectively, given by

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$$L=-m_1c^2\left(1-\frac{|\dot{\mathbf{x}}_1^2|}{c^2}\right)^{1/2}-m_2c^2\left(1-\frac{|\dot{\mathbf{x}}_2^2|}{c^2}\right)^{1/2}-\frac{e_1e_2}{\pi c}\frac{\mathbf{k}\cdot\mathbf{r}\times\dot{\mathbf{r}}}{|\mathbf{r}|^2} \tag{3}$$

with $\mathbf{r}=\mathbf{x}_1-\mathbf{x}_2$, $\mathbf{x}_1$ (and $\dot{\mathbf{x}}_1$) and $\mathbf{x}_2$ (and $\dot{\mathbf{x}}_2$) being the position (and velocity) vectors of the masses m_1 and m_2 and $\mathbf{k}$ a fictitious unit vector orthogonal to the plane of $\mathbf{x}_1$ and $\mathbf{x}_2$.

It is easy to obtain (3) starting with the electromagnetic potentials $\mathrm{A}^\mu(\mathbf{x},t)$, $\mu=0,1,2$, for Chern–Simons electrodynamics in the radiation gauge with $\boldsymbol{\nabla}\cdot\mathbf{A}=0$, namely,

$$A^0(\mathbf{x},t)=\frac{e}{2\pi c}\frac{(\mathbf{x}-\mathbf{R}(t))\times\dot{\mathbf{R}}(t).\mathbf{k}}{|\mathbf{x}-\mathbf{R}(t)|^2}, \tag{4a}$$

$$\mathbf{A}(\mathbf{x},t)=\frac{e}{2\pi}\frac{(\mathbf{x}-\mathbf{R}(t))\times\mathbf{k}}{|\mathbf{x}-\mathbf{R}(t)|^2}, \tag{4b}$$

the charge e being located at $\mathbf{R}(t)$. Needless to say Eqs. (4a) and (4b) are the $2+1$ dimensional counterparts of the corresponding $3+1$ dimensional $A^\mu(\mathbf{x},t)$ given by Eqs. (26.19) and (26.20) in Fock[8] for example.

Under an infinitesimal Lorentz transformation given by $\delta\mathbf{x}=-\boldsymbol{\nu}t+(\boldsymbol{\nu}.\mathbf{x}/c^2)\dot{\mathbf{x}}$, it is simple to check the change in the Lagrangian L, defined by

$$\begin{aligned}\delta L&=\frac{\partial L}{\partial\mathbf{x}_1}\cdot\delta\mathbf{x}_1+\frac{\partial L}{\partial\mathbf{x}_2}\cdot\delta\mathbf{x}_2+\frac{\partial L}{\partial\dot{\mathbf{x}}_1}\cdot\delta\dot{\mathbf{x}}_1+\frac{\partial L}{\partial\dot{\mathbf{x}}_2}\cdot\delta\dot{\mathbf{x}}_2\\&=\frac{\mathrm{d}}{\mathrm{d}t}\left(-m_1\mathbf{x}_1.\boldsymbol{\nu}\gamma_1-m_2\mathbf{x}_2.\boldsymbol{\nu}\gamma_2+\frac{e_1e_2}{\pi c}\frac{\mathbf{k}.\delta\mathbf{r}\times\mathbf{r}}{|\mathbf{r}|^2}\right),\end{aligned} \tag{5}$$

without the use of the equations of motion for the two masses m_1 and m_2. Here γ_1 and γ_2 are given by

$$\left(1-\frac{|\dot{\mathbf{x}}_1|^2}{c^2}\right)^{1/2}\quad\text{and}\quad\left(1-\frac{|\dot{\mathbf{x}}_2|^2}{c^2}\right)^{1/2},$$

respectively. Since δL works out to a total differential in (5) without the use of the equations of motion, it is clear that the action $S=\int\mathrm{d}t\,L$ is unaffected by the transformation from $\mathbf{x}\rightarrow\mathbf{x}+\delta\mathbf{x}$, thus making the Lagrangian (3) Lorentz invariant.

The constant of motion is now obtained by using the equations of motion for m_1 and m_2 to rewrite the first equality in (5) as

$$\delta L=\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\mathbf{x}}_1}\cdot\delta\mathbf{x}_1+\frac{\partial L}{\partial\dot{\mathbf{x}}_2}\cdot\delta\mathbf{x}_2\right). \tag{6}$$

From the second equality in (5) and (6) one thus obtains

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\mathbf{x}}_1}\cdot\delta\mathbf{x}_1+\frac{\partial L}{\partial\dot{\mathbf{x}}_2}\cdot\delta\mathbf{x}_2+m_1\mathbf{x}_1.\boldsymbol{\nu}\gamma_1+m_2\mathbf{x}_2.\boldsymbol{\nu}\gamma_2-\frac{e_1e_2}{\pi c}\frac{\mathbf{k}.\delta\mathbf{r}\times\mathbf{r}}{|\mathbf{r}|^2}\right)=0. \tag{7}$$

With the canonical momenta defined by $\mathbf{p_i}=\partial L/\partial\dot{\mathbf{x}}_i$ it is easy to obtain from (3) $\mathbf{p}_1=m_1\dot{\mathbf{x}}_1\gamma_1^{-1}+\mathbf{g}$ and $\mathbf{p}_2=m_2\dot{\mathbf{x}}_2\gamma_2^{-1}-\mathbf{g}$, where $\pi c|\mathbf{r}|^2\mathbf{g}=e_1e_2(\mathbf{r}\times\mathbf{k})$ and thus rework (7) as $(\mathrm{d}/\mathrm{d}t)(\mathbf{K}.\mathbf{v})=0$ with the constant of motion $\mathbf{K}$ given by

$$\mathbf{K}=-t\mathbf{P}+m_1\mathbf{x}_1\gamma_1^{-1}+m_2\mathbf{x}_2\gamma_2^{-1}, \tag{8}$$

the total momentum $\mathbf{P}$ being defined as $\mathbf{P}=\mathbf{p}_1+\mathbf{p}_2$. Equation (8) is the counterpart of Eq. (20) in Ref. 2; also while the latter is derived from the Darwin Lagrangian[8] for the electromagnetic

N-body problem and is correct in the $1/c^2$ approximation, Eq. (8) is exact. Note that $\mathbf{K}$ depends explicitly on time except in the center-of-momentum system which is the Lorentz frame where $\mathbf{P}=\mathbf{0}$.

For the Lagrangian (3) the Hamiltonian H and the angular momentum vector $\mathbf{L}$ are given by

$$H=m_1c^2\gamma_1^{-1}+m_2c^2\gamma_2^{-1}, \quad \mathbf{L}=\mathbf{x}_1\times\mathbf{p}_1+\mathbf{x}_2\mathbf{x}\mathbf{p}_2 \tag{9a}$$

and in the $\mathbf{P}=0$ frame they work out to

$$H=m_1c^2f_1+m_2c^2f_2, \quad \mathbf{L}=\mathbf{r}\times\mathbf{p}=\mathbf{k}(r_1p_2-r_2p_1)=\mathbf{k}L_z \tag{9b}$$

with p_1 and p_2 being the x and y components of the relative momentum vector $\mathbf{p}$ defined by

$$\mathbf{p}=\frac{m_2\mathbf{p}_1-m_1\mathbf{p}_2}{m_1+m_2}.$$

In deriving the Hamiltonian in (9b) we go through the following steps.

(i) Since $m_1\dot{\mathbf{x}}_1\gamma_1^{-1}=\mathbf{p}_1-\mathbf{g}$, therefore $\gamma_1^{-2}=1+(1/m_1^2c^2)|\mathbf{p}_1-\mathbf{g}|^2$. One can now express $\mathbf{p}_1$ and $\mathbf{p}_2$ in terms of $\mathbf{p}$ and $\mathbf{P}$ via the relations

$$\mathbf{p}_1=\frac{m_1}{m_1+m_2}\mathbf{P}+\mathbf{p}, \quad \mathbf{p}_2=\frac{m_2}{m_1+m_2}\mathbf{P}-\mathbf{p} \tag{10}$$

and find that in the center-of-momentum system with $\mathbf{P}=0$,

$$\gamma_1^{-1}=\left(1+\frac{|\mathbf{B}|^2}{m_1^2c^2}\right)^{1/2} \tag{11a}$$

with $\mathbf{B}=\mathbf{p}-\mathbf{g}$.

(ii) The above-given calculation can be repeated with $m_2\dot{\mathbf{x}}_2\gamma_2^{-1}=\mathbf{p}_2+\mathbf{g}$ to obtain the following result in the case when $\mathbf{P}=0$:

$$\gamma_2^{-1}=\left(1+\frac{|\mathbf{B}|^2}{m_2^2c^2}\right)^{1/2}. \tag{11b}$$

We shall relabel γ_1^{-1} and γ_2^{-1} in Eqs. (11a) and (11b) as f_1 and f_2, respectively, in the following. Using these definitions one can now rework $\mathbf{K}$ in Eq. (8) in the center-of-momentum system with $\mathbf{P}=0$ as

$$\mathbf{K}=(m_1f_1+m_2f_2)\mathbf{R}+\mu(f_1-f_2)\mathbf{r} \tag{12}$$

with the reduced mass μ and the center-of-mass (c.m.) position vector $\mathbf{R}$ defined by

$$\mu=\frac{m_1m_2}{m_1+m_2} \quad \text{and} \quad \mathbf{R}=\frac{m_1\mathbf{x}_1+m_2\mathbf{x}_2}{m_1+m_2}.$$

As emphasized by Dahl[2] the c.m. vector $\mathbf{R}$ should now be eliminated from Eq. (12) to make $\mathbf{K}$ a proper dynamical function and as in Ref. 2 we shall do this with the help of the equation of motion for $\mathbf{R}$ in the $\mathbf{P}=0$ limit, namely,

$$\frac{d\mathbf{R}}{dt}=\left(\frac{\partial H}{\partial\mathbf{P}}\right)_{\mathbf{P}=0}=\left(\frac{\mu}{m_2}\frac{\partial H}{\partial\mathbf{p}_1}+\frac{\mu}{m_1}\frac{\partial H}{\partial\mathbf{p}_2}\right)_{p_1=\mathbf{p},\mathbf{p}_2=-\mathbf{p}}. \tag{13}$$

One should now recast the Hamiltonian H in (9a) in terms of the canonical momenta $\mathbf{p}_1$ and $\mathbf{p}_2$ and it is given by

$$H=m_1c^2g_1+m_2c^2g_2,\quad g_1=\left(1+\frac{|\mathbf{S}_1|^2}{m_1^2c^2}\right)^{1/2},\quad g_2=\left(1+\frac{|\mathbf{S}_2|^2}{m_2^2c^2}\right)^{1/2} \tag{14}$$

with $\mathbf{S}_1=\mathbf{p}_1-\mathbf{g}$ and $\mathbf{S}_2=\mathbf{p}_2+\mathbf{g}$. On calculating the partial derivatives required in Eq. (13) it is easy to get

$$(m_1+m_2)\frac{d\mathbf{R}}{dt}=(\gamma_1-\gamma_2)\mathbf{B}. \tag{15}$$

From the Hamiltonian (9b), the equations of motion are

$$\frac{\partial\mathbf{H}}{\partial\mathbf{p}}=T\mathbf{B}=\dot{\mathbf{r}} \tag{16a}$$

with $T=\gamma_1/m_1+\gamma_2/m_2$, γ_1 and γ_2 being defined by Eqs. (11a) and (11b). Since $\mathbf{B}=\mathbf{p}-\mathbf{g}$ it is clear that

$$\mathbf{k}\times\dot{\mathbf{r}}=T(\mathbf{k}\times\mathbf{p}+h\mathbf{r}), \tag{16b}$$

where $\pi c|\mathbf{r}|^2h=-e_1e_2$. With Eq. (16b) the other equation of motion, namely,

$$\frac{\partial H}{\partial\mathbf{r}}=Th\left(\mathbf{k}\times\mathbf{p}-\mathbf{r}\left(h+2\frac{\mathbf{r}.\mathbf{k}\times\mathbf{p}}{|\mathbf{r}|^2}\right)\right)=-\dot{\mathbf{p}}, \tag{16c}$$

yields

$$\dot{\mathbf{p}}=h\left(\mathbf{k}\times\dot{\mathbf{r}}-2\frac{\mathbf{r}}{|\mathbf{r}|^2}\mathbf{k}\times\dot{\mathbf{r}}.\mathbf{r}\right). \tag{17}$$

Equation (17) easily leads to

$$\frac{d}{dt}(\mathbf{p}+h\mathbf{r}\times\mathbf{k})=\frac{d\mathbf{B}}{dt}=0. \tag{18}$$

Thus $\mathbf{B}$ is a constant in time and so are f_1 and f_2 in Eqs. (11a) and (11b). Returning to Eq. (15) we get

$$\frac{d}{dt}\left(\mathbf{R}+\frac{\gamma_2-\gamma_1}{m_1+m_2}\mathbf{B}\right)=\mathbf{0} \tag{19}$$

on using Eq. (18). Thus the c.m. position vector $\mathbf{R}(t)$ is given by

$$(m_1+m_2)\mathbf{R}(t)=\mathbf{B}(\gamma_1-\gamma_2)t+\mathbf{R}_0, \tag{20}$$

where $\mathbf{R}_0$ is a constant. Equation (20) is the counterpart of Eq. (43) in Ref. 2; however we must emphasize here that Eq. (20) in this paper is exact in that it has been derived using the equations of motion given by (16a) and (16c) without recourse to approximation. In contrast, the solution for $\mathbf{R}(t)$ given by Eq. (43) in Dahl's paper[2] has been obtained in the $1/c^2$ approximation to the equation of motion as given by Eq. (39) therein. On using (20) in (12) one obtains the exact form of the vector $\mathbf{K}$ as

$$\mathbf{K}=\left(\frac{m_1-m_2+m_2f_2\gamma_1-m_1f_1\gamma_2}{m_1+m_2}\right)t\mathbf{B}+\mu(f_1-f_2)\mathbf{r}+\mathbf{R}_0\frac{m_1f_1+m_2f_2}{m_1+m_2}. \tag{21}$$

With the Hamiltonian H in (9b), Eq. (21) can be reworked as

$$\mathbf{K}=\frac{H}{(m_1+m_2)c^2}\mathbf{R}_0+\frac{m_1-m_2}{m_1+m_2}\mathbf{M} \tag{22}$$

with

$$\mathbf{M}=Qt\mathbf{B}+m_1m_2\frac{f_1-f_2}{m_1-m_2}\mathbf{r} \tag{23}$$

and $Q=1+(m_2f_2\gamma_1-m_1f_1\gamma_2)/(m_1-m_2)$. For the Chern–Simons Lagrangian given by Eq. (3) of this paper Eq. (22) is the counterpart of Eq. (46) in Ref. 2; Eq. (23) therefore defines the Runge–Lenz vector **M** of the Lagrangian (3) in the center-of-momentum system.

It is easy to see that the above-noted derivation in (22) and (23) needs a second look for the equal mass $m_1=m_2$ case. Indeed a similar discussion is also in order for the Runge–Lenz vector derived from Eq. (45) in Dahl's paper;[2] note however that the remedy there is quite painless, namely: begin with unequal masses $m_1\neq m_2$ and subsequently derive the correct Lenz vector for the equal mass case, $m_1=m_2=m$, the result being a simple replacement of the factor μ in Eq. (46) there by $m/2$. But a corresponding effort here merits a separate discussion and is therefore relegated to the Appendix.

With M_1 denoting the x component of the two-component vector **M** it is clear that $\partial M_1/\partial t=QB_1$; thus one expects the Poisson bracket $\{M_1,H\}=-QB_1$, since **M** is a constant of motion, with H being given by Eq. (9b). It is easy to check this using the following:

$$\{r_1,f_1\}=\frac{\gamma_1B_1}{m_1^2c^2},\{r_1,f_2\}=\frac{\gamma_2B_1}{m_2^2c^2},\{r_i,p_j\}=\delta_{ij},\{f_1,f_2\}=0,\{\mathbf{B},f_1\}=0=\{\mathbf{B},f_2\}. \tag{24}$$

On replacing r_1 by r_2 in the first pair of Poisson brackets in (24) one should also replace B_1 by B_2.

One can also use Eq. (24) to evaluate the Poisson bracket of **M** with L_z, the latter being given in Eq. (9b). Using $\{B_i,L_z\}=-\varepsilon_{ij}B_j$ it is easy to verify that

$$\{M_i,L_z\}=-\varepsilon_{ij}M_j \tag{25}$$

with $\varepsilon_{12}=-\varepsilon_{21}=1$. We shall now evaluate the $\{M_1,M_2\}$ Poisson bracket; by virtue of Eq. (24) and the fact that $\{B_1,B_2\}=0$ it is easy to obtain the result

$$\{M_1,M_2\}=-\frac{\alpha^2}{c^2}(f_1-f_2)\left(\frac{\gamma_1}{m_1^2}-\frac{\gamma_2}{m_2^2}\right)\left(\frac{e_1e_2}{\pi c}+L_z\right) \tag{26}$$

with $(m_1-m_2)\alpha=m_1m_2$. While Eq. (25) is expected, on account of **M** being a vector, (26) does not match with that given by Eq. (2) for the Runge–Lenz vector **K** and is therefore a novel feature of this paper. The fact that the calculation made here is exact and quite unlike the approximate calculation to order $1/c^2$ of the Runge–Lenz vector by Dahl[2] reinforces our confidence in this assertion.

The extra term $e_1e_2/\pi c$ in Eq. (26) is reminiscent of the observation by Witten and Olive[9,10] long ago that in supersymmetric theories with solitons the usual supersymmetry algebra is modified to include topological quantum numbers as central charges. Interestingly, the last factor on the right-hand side of Eq. (26) can be expressed as $e_1e_2/\pi c+L_z=\mu(\mathbf{r}\times\mathbf{l})_z$, where we define $\mathbf{l}=\dot{\mathbf{x}}_1\gamma_1^{-1}-\dot{\mathbf{x}}_2\gamma_2^{-1}$ with

$$\gamma_1=\left(1-\frac{|\dot{\mathbf{x}}_1|^2}{c^2}\right)^{1/2}$$

and

$$\gamma_2=\left(1-\frac{|\dot{\mathbf{x}}_2|^2}{c^2}\right)^{1/2}.$$

Qualitatively, Eqs. (25) and (26) are important to this paper because we have derived them, besides Eq. (24), as Poisson brackets here. This is not the case with the Poisson bracket relations given by Eq. (4) in Ref. 2; indeed Dahl[2] provides only a qualitative understanding [see Eqs. (56)–(58) in Ref. 2] of the said Poisson bracket and is unable to derive Eq. (4) in the $1/c^2$ order description in his paper. Needless to say, Eq. (26) is the $2+1$ dimensional counterpart of the $3+1$ dimensional Poisson bracket given by Eq. (4) in Ref. 2, namely

$$\{M_i,M_j\}=-\frac{2}{\mu}H\sum_{k=1}^{3}\varepsilon_{ijk}L_k. \tag{27}$$

In conclusion, two distinguishing features characterize the derivation of the Runge–Lenz vector (23) associated with the Chern–Simons Lagrangian (3) in this paper: (a) the calculation here is exact and, (b) as an unexpected bonus the Poisson bracket in (26) contains the product e_1e_2 as a central charge.

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APPENDIX

When the masses m_1 and m_2 in the Lagrangian (3) are equal the Runge–Lenz vector $\mathbf{M}$ is worked out initially by assuming that $m_1\neq m_2$; taking the limit of Eq. (22) when $m_2\to m_1$ then yields the desired form of $\mathbf{M}$ as explained in the following. Let us assume here that $m_1=m_2+\varepsilon$ where $\varepsilon>0$. For the second term in Eq. (23) of the text one thus has

$$\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(f_1-f_2)=\lim_{\varepsilon\to 0}\left\{\left(1+\frac{|\mathbf{B}|^2}{c^2(m_2+\varepsilon)^2}\right)^{1/2}-\left(1+\frac{|B|^2}{c^2m_2^2}\right)^{1/2}\right\} \tag{A1}$$

$$=-\frac{|\mathbf{B}|^2}{c^2m_2^3}\gamma_2 \tag{A2}$$

by a Maclaurin expansion of the first term to order ε. Here γ_2 and γ_1 (see the following) are given by Eq. (11) of the text. A similar effort on the first term in Eq. (23) yields

$$\lim_{\varepsilon\to 0}\left(1-\frac{m_1f_1\gamma_2-m_2f_2\gamma_1}{\varepsilon}\right)=2\gamma_2\frac{|\mathbf{B}|^2}{m_2^2c^2}. \tag{A3}$$

Thus when $m_1=m_2=m$, we have instead of Eq. (23) the Runge–Lenz vector

$$\mathbf{M}=\frac{|B|^2\gamma}{mc^2}\left(\frac{2t}{m}\mathbf{B}-\mathbf{r}\right)=\gamma(1-f^2)(m\mathbf{r}-2t\mathbf{B}) \tag{A4}$$

with $f\gamma=1$ and

$$\gamma=\left(1+\frac{|\mathbf{B}|^2}{m^2c^2}\right)^{-1/2}.$$

With the Poisson brackets given by Eq. (24) it is now easy to arrive at the relations $\{M_i,L_z\}=-\epsilon_{ij}M_j$ and

$$\{M_1, M_2\} = -\frac{1}{c^2}\gamma^4(f^4-1)\left(\frac{e_1 e_2}{\pi c}+L_z\right). \tag{A5}$$

Equation (A5) is the equal mass counterpart of Eq. (26) for unequal masses.

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Iper-ideal kinetic constraints in continuum mechanics

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A geometrical approach to Lagrangian formulation of continuum mechanics in the language of jet-bundles theory is proposed. The resulting environment allows one to deal with a particular class of kinetic constraints, through a suitable implementation of Gauss' principle. A variational formulation of systems subject to such constraints is also outlined. Two explicit examples are given. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1420397]

I. INTRODUCTION

During the last ten years, nonholonomic constraints have drawn the renewed interest of many authors; as a result, a satisfactory mathematical description of nonholonomic mechanics has been recently set up using the tools of fiber-bundles and jet-bundles theory.

So far, the main efforts in this field of research have concerned systems with a finite number of degrees of freedom, providing a large number of devoted papers (see, e.g., Refs. 1–13).

Our aim is to extend the analysis to the continuum case, borrowing the ideas from works proposing a modern geometrical approach to classical mechanics of discrete systems.

To this end, we propose a new geometrical framework for continuum mechanics, based on jet-bundles theory and general enough to suit a description of material continua in Lagrangian formulation.

The resulting mathematical environment provides an advance in the geometrical description of continuum mechanics and it is successfully used to deal with a particular class of nonholonomic systems; despite the fact that the class is presently limited, the opinion of the authors is that the implemented geometrical setup may provide the starting point for a deeper analysis of a more general class of constraints.

The plan of the paper is as follows. Section II starts with a brief review of the basic aspects of mechanics of point particles. Continuous systems are subsequently introduced extending previous ideas along the lines developed by Kijowski.[14] In this connection, both kinematics and unconstrained dynamics are examined; in particular one of the main aspects of the construction is a new geometrical description of interactions involving a suitable extension of the concept of dynamical flow. Eventually, we introduce the class of nonholonomic constraints which will form the object of the subsequent developments; as we shall see, such constraints consist in purely kinetic restrictions imposed separately on each point of the continuum.

In Sec. III we discuss the problem of motion for these constrained systems. In general, the implementation of the equations of motion, in the presence of constraints, requires the assignment of a rule, known as *constitutive characterization*, which allows one to determine the constrained dynamics from the free one. Accordingly, we introduce a constitutive characterization called *iper-ideality*, defined through a suitable revisitation of Gauss' principle of minimal constraint; as we shall see, iper-ideality is equivalent to requiring the ideality of the constraints with respect to any infinitesimal part of the continuum. A comparison with d'Alembert principle, completed with the so-called Chetaev conditions, is worked out. Finally the explicit equations of motion are written.

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Section IV is devoted to the deduction of dynamical equations from a variational principle. Once again, the basic idea is borrowed from the discrete case and consists in restricting the class of deformations with respect to which the stationarity condition of the action functional is imposed.

The paper ends with two explicit examples.

II. THE GEOMETRICAL FRAMEWORK

A. Geometric preliminaries

The proposed geometrical formulation of continuum mechanics relies on an extension of the ideas involved in the geometrization of the equations of motion of discrete systems in the language of jet bundles.

For convenience of the reader, we briefly review the basic topics of the matter focusing our attention on the mechanics of a single point particle. The foundations of the theory and further details may be found in Refs. 1, 2, and 15.

(1) The evolution of a material point P is described in a frame-independent scheme, introducing the so-called *space–time* $\mathcal{V}_4$; in classical mechanics, the latter is a four-dimensional differentiable manifold, fibered over the real line $\Re$ with projection t: $\mathcal{V}_4 \to \Re$ given by the absolute time function; $\mathcal{V}_4$ is usually referred to fibered coordinates t, x^1, x^2, x^3, subject to the transformation laws

$$\overline{t} = t + c, \quad \overline{x}^i = \overline{x}^i(t, x^1, x^2, x^3) \quad i, = 1,...,3. \tag{1}$$

(2) Every evolution of P is described by a corresponding section $\gamma: \Re \to \mathcal{V}_4$; this leads to a natural identification of the velocity space of the material point with the first jet bundle $j_1(\mathcal{V}_4)$, associated with the stated fibration; $j_1(\mathcal{V}_4)$ may be canonically embedded into the tangent bundle $T(\mathcal{V}_4)$, according to the identification

$$j_1(\mathcal{V}_4) \simeq \{X \in T(\mathcal{V}_4) \,|\, \langle X, \mathrm{d}t \rangle = 1\}; \tag{2}$$

every fibered coordinate systems t, x^i on $\mathcal{V}_4$ may be lifted to a corresponding jet-coordinate system $t, x^i, \dot{x}^i$ on $j_1(\mathcal{V}_4)$, with transformation laws

$$\overline{t} = t + c, \quad \overline{x}^i = \overline{x}^i(t, x^1, x^2, x^3), \quad \overline{\dot{x}}^i = \frac{\partial \overline{x}^i}{\partial t} + \frac{\partial \overline{x}^i}{\partial x^j} \dot{x}^j. \tag{3}$$

In jet-coordinates, the identification (2) is made explicit by the relation

$$z = \left(\frac{\partial}{\partial t} + \dot{x}^i(z) \frac{\partial}{\partial x^i} \right)_{\pi(z)} \in j_1(\mathcal{V}_4),$$

$\pi: j_1(\mathcal{V}_4) \to \mathcal{V}_4$ being the natural projection. Moreover, denoting by $V(\mathcal{V}_4)$ and $V(j_1(\mathcal{V}_4))$ the vertical bundles associated with the fibrations $\mathcal{V}_4 \to \Re$ and $j_1(\mathcal{V}_4) \to \mathcal{V}_4$, respectively, the affine character of the fibration $j_1(\mathcal{V}_4) \to \mathcal{V}_4$ provides a canonical isomorphism between the vertical spaces $V_{\pi(z)}(\mathcal{V}_4)$ and $V_z(j_1(\mathcal{V}_4))$ for each $z \in j_1(\mathcal{V}_4)$. The latter, known as the *vertical lift* of vectors, is expressed in coordinates as

$$V = V^i \left(\frac{\partial}{\partial x^i} \right)_{\pi(z)} \to \hat{V} = V^i \left(\frac{\partial}{\partial \dot{x}^i} \right)_z. \tag{4}$$

(3) Similarly, the second jet bundle $j_2(\mathcal{V}_4)$ may be regarded as the acceleration space of P; $j_2(\mathcal{V}_4)$, referred to jet-coordinates $t, x^i, \dot{x}^i, \ddot{x}^i$, is an affine bundle over $j_1(\mathcal{V}_4)$, modeled on the vertical bundle $V(j_1(\mathcal{V}_4))$. Once again, we have a canonical identification between points $w \in j_2(\mathcal{V}_4)$ and vectors on $j_1(\mathcal{V}_4)$, expressed by

$$w=\left(\frac{\partial}{\partial t}+\dot{x}^i(w)\frac{\partial}{\partial x^i}+\ddot{x}^i(w)\frac{\partial}{\partial \dot{x}^i}\right)_{\pi(w)}\in j_2(\mathcal{V}_4), \tag{5}$$

π now denoting the projection $j_2(\mathcal{V}_4)\to j_1(\mathcal{V}_4)$.

(4) In the geometrical approach to dynamics, a central role is played by the sections Z: $j_1(\mathcal{V}_4)\to j_2(\mathcal{V}_4)$. Viewing them as vector fields on $j_1(\mathcal{V}_4)$, they are called *dynamical flows*; in local coordinates every such flow has components

$$Z=\frac{\partial}{\partial t}+\dot{x}^i\frac{\partial}{\partial x^i}+Z^i(t,x^j,\dot{x}^j)\frac{\partial}{\partial \dot{x}^i}. \tag{6}$$

From Eq. (6) it is easily seen that the integral curves of a dynamical flow Z are jet-extensions of sections of $\mathcal{V}_4$, and that the difference between two arbitrary dynamical flows is a vertical vector field on $j_1(\mathcal{V}_4)$.

Referring to Refs. 1 and 2 for more detailed accounts, we now recall that the assignment of a frame of reference $\mathcal{I}$ determines the following.

(a) A representation of the space–time manifold $\mathcal{V}_4$ as a Cartesian product $\mathcal{V}_4=\Re\times E_3$; by the absolute time axiom, each fiber $t=\text{const}$ represents an Euclidean three-space E_3, identified with the physical space of $\mathcal{I}$ at time t. In the following, $\mathbf{x}:\mathcal{V}_4\to E_3$ will indicate the relativization process associated with a generic frame of reference $\mathcal{I}$; the restriction of the push-forward $\mathbf{x}_*$ to $V(\mathcal{V}_4)$ gives rise to an identification of vertical vectors on $\mathcal{V}_4$ with vectors on E_3, based on the relation

$$V\in V(\mathcal{V}_4)\to \mathbf{v}:=\mathbf{x}_*(V)\in T(E_3). \tag{7}$$

Choosing as spatial coordinates x^1,x^2,x^3 on $\mathcal{V}_4$ a set of Euclidean coordinates on E_3 (henceforth such a choice will be systematically done), the correspondence (7) is made explicit by the relation

$$V=V^i\frac{\partial}{\partial x^i}\to \mathbf{v}=V^i\mathbf{e}_{(i)} \tag{8a}$$

with $\mathbf{e}_{(i)}:=\mathbf{x}_*(\partial/\partial x^i)$, $i=1,...,3$, forming an orthonormal basis for $V_3:=T(E_3)$. Using the vertical lift (4), we get a similar identification between vertical vectors on $j_1(\mathcal{V}_4)$ and vectors in V_3, namely

$$\hat{V}=V^i\frac{\partial}{\partial \dot{x}^i}\to \mathbf{v}=V^i\mathbf{e}_{(i)}. \tag{8b}$$

(b) A global section $Z_{\mathcal{I}}: j_1(\mathcal{V}_4)\to j_2(\mathcal{V}_4)$, assigning to each $z\in j_1(\mathcal{V}_4)$ the unique element $Z_{\mathcal{I}}(z)\in j_2(\mathcal{V}_4)$ expressing the instantaneous vanishing of the relative acceleration of the given material point P in the kinetic state z. Given an element $w\in j_2(\mathcal{V}_4)$, Eqs. (5) and (6) show that the difference $\rho_{Z_{\mathcal{I}}}(w):=w-Z_{\mathcal{I}}(\pi(w))=(\ddot{x}^i(w)-Z^i_{\mathcal{I}}(\pi(w)))\partial/\partial\dot{x}^i$ is a vertical vector field on $j_1(\mathcal{V}_4)$; this defines a map $\rho_{Z_{\mathcal{I}}}: j_2(\mathcal{V}_4)\to V(j_1(\mathcal{V}_4))$ yielding a (frame-dependent) identification of the acceleration space of P with $V(j_1(\mathcal{V}_4))$. It is easily seen that, in Cartesian coordinates, the components $Z^i_{\mathcal{I}}$ of $Z_{\mathcal{I}}$ are identically zero.

The correspondence between vertical vectors on $\mathcal{V}_4$ [respectively, on $j_1(\mathcal{V}_4)$] and vectors on E_3 allows one to introduce a fiber metric g on $\mathcal{V}_4$ [on $j_1(\mathcal{V}_4)$]. For this purpose, letting $\hat{g}$ denote the Euclidean metric of E_3, we define

$$g(V,W):=\hat{g}(\mathbf{x}_*(V),\mathbf{x}_*(W))\quad \forall V,W\in V(\mathcal{V}_4)\quad [\forall \hat{V},\hat{W}\in V(j_1(\mathcal{V}_4))] \tag{9}$$

whence, in Cartesian coordinates,

$$g_{ij} := g\left(\frac{\partial}{\partial x^i}, \frac{\partial}{\partial x^j}\right) = g\left(\frac{\partial}{\partial \dot{x}^i}, \frac{\partial}{\partial \dot{x}^j}\right) = \hat{g}(\mathbf{e}_{(i)}, \mathbf{e}_{(j)}) = \delta_{ij}. \tag{10}$$

Although the scalar product (9) is defined through the relativization process induced by $\mathcal{I}$, it may be easily verified that it is actually invariant under arbitrary transformations of the frame of reference, thereby representing an intrinsic attribute of the configuration space–time of P.

By means of the fiber metric g, we can invert the correspondences (8) between vectors $\mathbf{v} = v^i \mathbf{e}_{(i)}$ on V_3 and vertical vectors $V = V^i(\partial/\partial x^i)$ on $\mathcal{V}_4$ [or $\hat{V} = V^i(\partial/\partial \dot{x}^i)$ on $j_1(\mathcal{V}_4)$], according to the relation

$$g_{ij} V^j = g\left(V, \frac{\partial}{\partial x^i}\right) = g\left(\hat{V}, \frac{\partial}{\partial \dot{x}^i}\right) := (\mathbf{v}, \mathbf{e}_{(i)}) \tag{11a}$$

equivalent, in Cartesian coordinates, to

$$V^i = v^i. \tag{11b}$$

Collecting all previous results, the geometrical description of the dynamics of a material point P may be formulated as follows.

(i) Through Eq. (11), we first associate with the vector $\mathbf{F}$ on E_3, describing the total force $\mathbf{F} = (F^i/m)\mathbf{e}_{(i)}$ (evaluated in the frame of reference $\mathcal{I}$ and normalized by the inertial mass m of P), the vertical vector field V on $j_1(\mathcal{V}_4)$ given by

$$V := \frac{F^i}{m} \frac{\partial}{\partial \dot{x}^i}. \tag{12}$$

(ii) Then, the dynamical flow

$$Z := Z_{\mathcal{I}} + V \tag{13}$$

provides a frame-independent representation of the dynamics of P, in the sense that the integral curves of Z are the (first jet-extension of) the solutions of the motion of P.

B. Continuous systems: Kinematics

The mathematical description of a continuum is generally based on the introduction of two different spaces: the first one, known as *material space*, takes the physical properties of the continuum into account, while the second one is the space–time $\mathcal{V}_4$, where the evolution of the system is described.

The material space, indicated by $\mathcal{B}$, is regarded as a differentiable manifold of dimension $M \leqslant 3$; we shall denote by $X^1, \ldots, X^M$ a local coordinate system on $\mathcal{B}$, with transformation laws

$$\overline{X}^A = \overline{X}^A(X^1, \ldots, X^M), \quad A = 1, \ldots, M. \tag{14}$$

The physical properties of the continuum will be taken into account by means of a measure of mass μ: $B(\mathcal{B}) \to \Re_+$, which assigns to each Borel set $U \in B(\mathcal{B})$ the total mass $\mu(U)$ contained in it.

From now on, the evolution of the continuum will be described using the so-called "Lagrangian viewpoint," i.e., considering the congruence of world lines of the points of $\mathcal{B}$ in space–time. In this way, we shall be able to extend the ideas outlined in Sec. II A to the continuum case.

The following discussion will be made in a purely mechanical scheme, omitting from our analysis every consideration regarding energetic and thermodynamical aspects. The latter may be taken into account introducing additional spaces for further dependent variables by Cartesian product with $\mathcal{V}_4$, and making use of suitable constitutive relations.

The *configuration* of the continuum at any instant t is described by a map $\varphi_t:\mathcal{B}\rightarrow\Sigma_t\subset\mathcal{V}_4,\Sigma_t$ representing the totality of simultaneous events at time t. Accordingly, the evolution of the system is a map $\varphi:\mathfrak{R}\times\mathcal{B}\rightarrow\mathcal{V}_4$, assigning to each $t\in\mathfrak{R}$ the configuration of the system at that time.

Therefore, we may take as the basic environment for the description of the continuum the Cartesian product $\mathcal{V}_4\times\mathcal{B}$, fibered both on $\mathcal{V}_4$ and $\mathfrak{R}\times\mathcal{B}$, and referred to local fibered coordinates t, x^i,X^A, subject to the transformation laws (1) and (14). In this context, every evolution φ of the continuum may be thought of as a section $\varphi:\mathfrak{R}\times\mathcal{B}\rightarrow\mathcal{V}_4\times\mathcal{B}$, namely

$$\varphi:\begin{cases} t=t \\ X^A=X^A \\ x^i=\varphi^i(t,X^A) \end{cases}. \tag{15}$$

In other words, the Lagrangian formulation of continuum mechanics may be viewed as the study of the sections of the fibered manifold $\mathcal{V}_4\times\mathcal{B}\rightarrow\mathfrak{R}\times\mathcal{B}$.

Special relevance in the following will be held by some geometrical objects induced by the above-mentioned fibration.

To start with, taking Eqs. (1) and (14) into account, it is easily seen that the vertical fiber bundle $V(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$, associated with the fibration $\mathcal{V}_4\times\mathcal{B}\rightarrow\mathfrak{R}\times\mathcal{B}$, is canonically identified with the fiber bundle $V(\mathcal{V}_4)\times\mathcal{B}$. In fact, denoting by $\pi_{\mathcal{V}_4}:\mathcal{V}_4\times\mathcal{B}\rightarrow\mathcal{V}_4$ and $\pi_{\mathcal{B}}:\mathcal{V}_4\times\mathcal{B}\rightarrow\mathcal{B}$ the natural projections, the map $\kappa:V(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})\rightarrow V(\mathcal{V}_4)\times\mathcal{B}$ expressed as

$$\kappa:V^i\frac{\partial}{\partial x^i}_{|z}\in V_z(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})\rightarrow\left(V^i\frac{\partial}{\partial x^i}_{|\pi_{\mathcal{V}_4}(z)},\pi_{\mathcal{B}}(z)\right)\in V_{\pi_{\mathcal{V}_4}(z)}(\mathcal{V}_4)\times\mathcal{B}, \tag{16}$$

$\forall z\in\mathcal{V}_4\times\mathcal{B}$, provides the required identification.

Denoting by $V(j_1(\mathcal{V}_4)\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$ the vertical bundle associated with the fibration $j_1(\mathcal{V}_4)\times\mathcal{B}\rightarrow\mathcal{V}_4\times\mathcal{B}$, the same arguments, together with (an obvious extension of) the vertical lift (4), provide a similar identification between $V(j_1(\mathcal{V}_4)\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$ and $V(j_1(\mathcal{V}_4))\times\mathcal{B}$.

Besides, $\mathcal{V}_4\times\mathcal{B}\rightarrow\mathfrak{R}\times\mathcal{B}$ may be endowed with a fiber metric

$$G:=\pi^*_{\mathcal{V}_4}(\mathbf{x}^*(\hat{g})) \tag{17}$$

giving rise to the scalar product $G(V,W)=V^iW^jG(\partial/\partial x^i,\partial/\partial x^j):=G_{ij}V^iW^j\forall V=V^i(\partial/\partial x^i)$, $W=W^i(\partial/\partial x^i)\in V(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$ [the reader may easily verify that the metric (17) is independent of the choice of the frame of reference $\mathcal{I}$, and thus of the induced relativization process $\mathbf{x}$]; once again, using relation (4) as well as the stated identifications, we may lift G to a fiber metric on $j_1(\mathcal{V}_4)\times\mathcal{B}\rightarrow\mathcal{V}_4\times\mathcal{B}$ (still denoted by G), based on the scalar product $G(\hat{V},\hat{W})=G_{ij}V^iW^j\forall\hat{V}=V^i(\partial/\partial\dot{x}^i)$, $\hat{W}=W^i(\partial/\partial\dot{x}^i)\in V(j_1(\mathcal{V}_4)\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$.

In addition to this, the restriction of the map $\mathbf{x}_*\times id_{\mathcal{B}}$ to $V(\mathcal{V}_4)\times\mathcal{B}$ provides the following correspondence:

$$\mathbf{x}_*\times id_{\mathcal{B}}:(V,p)\in V(\mathcal{V}_4)\times\mathcal{B}\rightarrow(\mathbf{v},p)\in V_3\times\mathcal{B} \tag{18}$$

with V and $\mathbf{v}$ related by Eq. (7).

Conversely, taking the identification (16) into account and following the same arguments stated at the end of Sec. II A, the fiber metric (17) allows one to associate with each pair $(\mathbf{v}=v^i\mathbf{e}_{(i)},p)\in V_3\times\mathcal{B}$ a corresponding element $V=V^i(\partial/\partial x^i)\in V_{\pi^{-1}_{\mathcal{B}}(p)}(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$ by means of the relation

$$G_{ij}V^j=G\left(V,\frac{\partial}{\partial x^i}\right):=\hat{g}(\mathbf{v},\mathbf{e}_{(i)}), \tag{19}$$

equivalent, in Cartesian coordinates, to

$$V^i = v^i. \tag{20}$$

Lifting G to a fiber metric on $j_1(\mathcal{V}_4)\times B \to \mathcal{V}_4\times\mathcal{B}$, the previous arguments may be restated taking $V(j_1(\mathcal{V}_4))$ in place of $V(\mathcal{V}_4)$ and $V(j_1(\mathcal{V}_4)\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$ in place of $V(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$. In particular, the correspondence between elements of $V_3\times\mathcal{B}$ and of $V(j_1(\mathcal{V}_4)\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$ is still expressed by equations of the form (19) and (20).

The first jet bundle of $\mathcal{V}_4\times\mathcal{B}\to\mathfrak{R}\times\mathcal{B}$, henceforth denoted by $j_1(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$, will be referred to local jet-coordinates t, X^A, x^i, x^i_A, x^i_0 (where $x^i_A = \partial\varphi^i/\partial X^A$, and $x^i_0 = \partial\varphi^i/\partial t$), with transformation laws

$$\overline{t} = t + c, \quad \overline{x^i} = \overline{x^i}(t, x^1, x^2, x^3), \quad \overline{X^A} = \overline{X^A}(X^1,\ldots,X^M) \tag{21a}$$

$$\overline{x^i_0} = \frac{\partial\overline{x^i}}{\partial t} + \frac{\partial\overline{x^i}}{\partial x^j}x^j_0, \quad \overline{x^i_A} = \frac{\partial\overline{x^i}}{\partial x^j}\frac{\partial X^B}{\partial\overline{X^A}}X^j_B. \tag{21b}$$

The comparison of Eq. (21b) with Eq. (3) shows that there exists a natural projection $\tau^1_1: j_1(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B}) \to j_1(\mathcal{V}_4)\times\mathcal{B}$, described in local coordinates as

$$\tau^1_1: (t, x^i, X^A, x^i_0, x^i_A) \to (t, x^i, X^A, \dot{x}^i = x^i_0).$$

More generally, the kth jet-extension of $\mathcal{V}_4\times\mathcal{B}\to\mathfrak{R}\times\mathcal{B}$ will be indicated by $j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$ and referred to local jet-coordinates t, $X^A, x^i, x^i_\alpha, \ldots, x^i_{\alpha_1,\ldots,\alpha_k}$ (from now on, Greek letters run in the set $\{0, 1, 2, 3\}$, with the subindex 0 representing the time derivative).

As before, it is an easy matter to verify that the maps $\tau^k_r: j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B}) \to j_r(\mathcal{V}_4)\times B (\forall r < k)$, defined by

$$\tau^k_r: (t, X^A, x^i, x^i_\alpha, \ldots, x^i_{\alpha_1,\ldots,\alpha_k}) \to (t, x^i, X^A, \dot{x}^i = x^i_0, \ddot{x}^i = x^i_{00}, \ldots)$$

are well-defined projections.

The previous mathematical environments allow one to geometrize the mechanical quantities involved in the description of the evolution of a continuum system $\mathcal{B}$.

Every section $\varphi: \mathfrak{R}\times\mathcal{B}\to\mathcal{V}_4\times\mathcal{B}$, describing the evolution of $\mathcal{B}$ in Lagrangian terms, may be lifted to a section $j_1(\varphi): \mathfrak{R}\times\mathcal{B}\to j_1(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$, assigning to each point $(t,p)\in\mathfrak{R}\times\mathcal{B}$ the values of the section and of its tangent plane at (t,p). As a result, the composite map $\tau^1_1\circ j_1(\varphi)$ is a section of the bundle $j_1(\mathcal{V}_4)\times B\to\mathfrak{R}\times\mathcal{B}$, representing the velocity distribution of the points of the continuum. The fibration $j_1(\mathcal{V}_4)\times B\to\mathfrak{R}\times\mathcal{B}$ will therefore be called the *velocity space of the continuum*.

A similar procedure allows one to lift the section $\varphi: \mathfrak{R}\times\mathcal{B}\to\mathcal{V}_4\times\mathcal{B}$ to the second jet bundle $j_2(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$, thus generating a section $j_2(\varphi): \mathfrak{R}\times\mathcal{B}\to j_2(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$, and then project it into $j_2(\mathcal{V}_4)\times\mathcal{B}$ by means of τ^2_2. The resulting section $\tau^2_2\circ j_2(\varphi): \mathfrak{R}\times\mathcal{B}\to j_2(\mathcal{V}_4)\times\mathcal{B}$ represents the distribution of the accelerations of the points of the continuum. Accordingly, the fibered manifold $j_2(\mathcal{V}_4)\times B\to\mathfrak{R}\times\mathcal{B}$ will be called the *acceleration space of the continuum*.

More generally, the section $\varphi: \mathfrak{R}\times\mathcal{B}\to\mathcal{V}_4\times\mathcal{B}$ may be lifted to any jet-extension $j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$, thereby generating a section $j_k(\varphi)$, which, projected into $j_1(\mathcal{V}_4)\times B$ (by means of τ^k_1) or into $j_2(\mathcal{V}_4)\times B$ (by means of τ^k_2), gives rise to corresponding sections

$$\dot{\varphi} := \tau^k_1\circ j_k(\varphi) = \tau^1_1\circ j_1(\varphi): \mathfrak{R}\times\mathcal{B}\to j_1(\mathcal{V}_4)\times\mathcal{B},$$

$$\ddot{\varphi} := \tau^k_2\circ j_k(\sigma) = \tau^2_2\circ j_2(\varphi): \mathfrak{R}\times\mathcal{B}\to j_2(\mathcal{V}_4)\times\mathcal{B}.$$

The situation is summarized into the commutative diagram

$$\begin{array}{ccccc} j_1(\mathcal{V}_4)\times\mathcal{B} & \xleftarrow{\tau_1^k} & j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B}) & \xrightarrow{\tau_2^k} & j_2(\mathcal{V}_4)\times\mathcal{B} \\ \dot{\varphi}\uparrow & & j_k(\varphi)\uparrow & & \ddot{\varphi}\uparrow \\ \mathfrak{R}\times\mathcal{B} & = & \mathfrak{R}\times\mathcal{B} & = & \mathfrak{R}\times\mathcal{B} \end{array} . \tag{22}$$

C. Continuous systems: Dynamics

In this section, it will be shown how interactions may be embodied in the geometrical scheme developed so far.

As is well known, the forces acting on a physical system $\mathcal{B}$ may be classified into:

(i) external forces, due to the interactions of the system with the external world; they are expressed as functions of the motion of the system and possibly of the time variable t;
(ii) internal forces, describing the interactions among the different points of the system and generally represented by more complicated expressions.

The external forces will be modeled introducing the *specific density of external forces* $\mathbf{F}: j_1(\mathcal{V}_4)\times\mathcal{B}\to V_3$, in such a way that, given a section $\varphi:\mathfrak{R}\times\mathcal{B}\to\mathcal{V}_4\times\mathcal{B}$ and a Borel set $U \in B(\mathcal{B})$, the integral

$$\int_U (\mathbf{F}\circ\dot{\varphi})\mu$$

represents the resultant of external forces (evaluated in the frame $\mathcal{I}$) acting on U at time t, in the "kinetic state" $\dot{\varphi}(t,\cdot)$.

Making use of Eqs. (12) and (13), the specific density of external forces $\mathbf{F} = F^i(t,x^i,\dot{x}^i,X^A)\mathbf{e}_{(i)}$ allows one to define a map $Z^{\text{ext}}: j_1(\mathcal{V}_4)\times\mathcal{B}\to j_2(\mathcal{V}_4)\times\mathcal{B}$, fibered on $j_1(\mathcal{V}_4)\times\mathcal{B}$, as expressed by the commutative diagram

$$\begin{array}{ccc} j_1(\mathcal{V}_4)\times\mathcal{B} & \xrightarrow{Z^{\text{ext}}} & j_2(\mathcal{V}_4)\times\mathcal{B} \\ id\downarrow & & \downarrow\pi \\ j_1(\mathcal{V}_4)\times\mathcal{B} & = & j_1(\mathcal{V}_4)\times\mathcal{B} \end{array} , \tag{23}$$

π denoting the natural projection. In local (Cartesian) coordinates, taking Eqs. (12) and (13) into account, Z^{ext} is represented as

$$Z^{\text{ext}}(z,p) = \left(\frac{\partial}{\partial t} + \dot{x}^i(z)\frac{\partial}{\partial x^i} + F^i(z,p)\left.\frac{\partial}{\partial \dot{x}^i}\right|_z, X^A(p) \right). \tag{24}$$

Equation (24) clearly shows that the map Z^{ext} may be thought as a family of dynamical flows, one for each $p\in\mathcal{B}$.

Composing the map (23) with the projection τ_1^k, we may regard external forces as a map (still denoted by) $Z^{\text{ext}}: j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})\to j_2(\mathcal{V}_4)\times\mathcal{B}$, depending at most on first-order time derivatives and not on material ones. We remark that this property is invariant under arbitrary fibered coordinate transformations.

Internal forces are quite different in nature. In fact, the internal forces do not only depend on the kinetic state and (possibly) on time, but also on the *material derivatives* and mixed *time-material* derivatives $x^i_{\alpha_1,\ldots,\alpha_s}$ for s up to an order k, determined by the physical properties of the system; obviously, the time derivative order is limited to the first one, so expressing the condition that forces cannot depend on accelerations. The reader may easily verify that such a condition is actually invariant under arbitrary coordinate transformations in $\mathcal{V}_4\times\mathcal{B}$.

In the present scheme, internal forces may be geometrized introducing the *specific density of internal forces* $\mathbf{f}: j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})\to V_3$; given φ and U as above, the map $\mathbf{f}=f^i(t,X^A,x^i,x^i_\alpha,\ldots,x^i_{\alpha_1,\ldots,\alpha_k})\mathbf{e}_{(i)}$ is such that the integral

$$\int_U (\mathbf{f}\circ j_k(\varphi))\mu$$

yields the resultant of the internal forces acting on U at time t in the configuration $\varphi(t,\cdot)$. In general, $\mathbf{f}$ is deduced as the divergence of a suitable stress tensor associated with the system.

Once again, still taking Eqs. (12) and (13) into account, we may define a map $Z^{\text{int}}: j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})\to j_2(\mathcal{V}_4))\times\mathcal{B}$, fibered over $j_1(\mathcal{V}_4)\times\mathcal{B}$, according to the commutative diagram

$$\begin{array}{ccc} j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B}) & \xrightarrow{\quad Z^{\text{int}}\quad} & j_2(\mathcal{V}_4)\times\mathcal{B} \\ \tau_1^k\downarrow & & \downarrow \\ j_1(\mathcal{V}_4)\times\mathcal{B} & = & j_1(\mathcal{V}_4)\times\mathcal{B} \end{array} \qquad (25)$$

If $z\in j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$, the map Z^{int} is expressed locally as

$$Z^{\text{int}}(z)=\left(\frac{\partial}{\partial t}+x^i_0(z)\frac{\partial}{\partial x^i}+f^i(z)\frac{\partial}{\partial \dot{x}^i}\bigg|_{\tau_1^k(z)},X^A(z)\right). \qquad (26)$$

Collecting all previous results, internal and external forces together give rise to a map $Z: j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})\to j_2(\mathcal{V}_4)\times\mathcal{B}$, fibered over $j_1(\mathcal{V}_4)\times\mathcal{B}$; as mentioned previously, Z only depends on the variables $x^i_{\alpha_1,\ldots,\alpha_s}$ $(s\leqslant k)$ in which the time derivative order is limited to the first one. In local (Cartesian) coordinates we have the representation

$$Z(z)=\left(\frac{\partial}{\partial t}+x^i_0(z)\frac{\partial}{\partial x^i}+(F^i+f^i)(z)\frac{\partial}{\partial \dot{x}^i}\bigg|_{\tau_1^{(k)}(z)},X^A(z)\right). \qquad (27)$$

The map (27) will be called the *dynamical map*.

In continuum mechanics, Newton's second law is written for each subset $U\in B(\mathcal{B})$ as follows:

$$\int_U(\varphi_{00}(t,X^A)-(\mathbf{F}+\mathbf{f})(t,X^A,\varphi^i_\alpha,\ldots,\varphi^i_{\alpha_1,\ldots,\alpha_k}))\mu=0. \qquad (28)$$

The arbitrariness in the choice of $U\subset\mathcal{B}$ allows one to regard Eq. (28) as an equation for the integrand. This is the standard procedure used to convert the integral formulation of the equations of continuum mechanics into the differential one. It will be systematically adopted in all subsequent developments.

In order to investigate the geometric interpretation of Eq. (28) we start with the following

Proposition II.1: Let $Q\to M$ and $Q'\to M'$ be fibered manifolds; suppose that $Q\to M$ is an affine bundle and denote by $V\to M$ the corresponding modeling vector bundle. If $f,g: Q'\to Q$ is a pair of fibered morphisms, then the difference $f-g: Q'\to V$ is a bundle morphism, according to the following commutative diagram:

$$\begin{array}{ccc} Q' & \xrightarrow{\quad f-g\quad} & V \\ \downarrow & & \downarrow \\ M' & \longrightarrow & M \end{array} \qquad (29)$$

The proof is totally straightforward and is omitted.

Applying Proposition II.1 to the maps Z and τ_2^k we have that the difference $(Z-\tau_2^k)$ is a bundle morphism such that diagram

$$\begin{array}{ccc} j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B}) & \xrightarrow{Z-\tau_2^k} & V(j_1(\mathcal{V}_4))\times\mathcal{B} \\ \tau_1^k\downarrow & & \downarrow \\ j_1(\mathcal{V}_4)\times\mathcal{B} & = & j_1(\mathcal{V}_4)\times\mathcal{B} \end{array} \tag{30}$$

is commutative. In local (Cartesian) coordinates, if $z\in j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$, we have

$$(F-\tau_2^k)(z)=\left((F^i+f^i-x^i_{00})(z)\,\frac{\partial}{\partial\dot{x}^i}\bigg|_{\tau_1^k(z)},X^A(z)\right). \tag{31}$$

As a consequence, the geometric counterpart of Eq. (28) is finding the set of all points belonging to $(Z-\tau_2^k)^{-1}(\{0\}\times\mathcal{B})$; the latter singles out a submanifold of $j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$ which, by definition, may be regarded as the partial differential equation

$$(F^i+f^i)(t,X^A,\varphi^i_\alpha,\ldots,\varphi^i_{\alpha_1,\ldots\alpha_k})-\varphi^i_{00}=0 \tag{32}$$

of order k for the unknown $\varphi:\mathfrak{R}\times\mathcal{B}\to\mathcal{V}_4\times\mathcal{B}$.

Finally, Proposition II.1 implies that the difference Z_1-Z_2 between two different dynamical maps is a map $(Z_1-Z_2):j_k(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})\to V(j_1(\mathcal{V}_4))\times B$, fibered over $j_1(\mathcal{V}_4)\times\mathcal{B}$. This fact will be important in the description of constraints on the continuum.

D. Purely kinetic constraints

As is well known, the presence of constraints acting on a given system $\mathcal{B}$ is expressed, in mathematical terms, by corresponding restrictions imposed on the possible evolutions of $\mathcal{B}$, i.e., on the set of sections $\varphi:\mathcal{B}\times\mathfrak{R}\to\mathcal{V}_4\times\mathcal{B}$.

In the subsequent discussion, we shall concentrate on the study of a particular kind of constraint henceforth referred to as *purely kinetic*, expressed as restrictions of the form

$$g^\sigma(t,x^i,x^i_0)=0,\quad \sigma=1,\ldots,r,\quad r\in\{1,2,3\} \tag{33}$$

simultaneously imposed on *all* particles $p\in\mathcal{B}$.

Equation (33) may be viewed alternatively as the Cartesian representation of a submanifold of $j_1(\mathcal{V}_4\times\mathcal{B},\mathfrak{R}\times\mathcal{B})$, or of a submanifold of $j_1(\mathcal{V}_4)$ (identifying x^i_0 with $\dot{x}^i$).

In the latter case, under the regularity assumption $\operatorname{rank}\|\partial g^\sigma/\partial\dot{x}^i\|=r$, Eq. (33) defines an embedding $i:\mathcal{A}\to j_1(\mathcal{V}_4)$, fibered over $\mathcal{V}_4$, summarized into the commutative diagram

$$\begin{array}{ccc} \mathcal{A} & \xrightarrow{i} & j_1(\mathcal{V}_4) \\ \pi\downarrow & & \downarrow\pi, \\ \mathcal{V}_4 & = & \mathcal{V}_4 \end{array} \tag{34}$$

π denoting the natural projection.

The geometry of the *constraints manifold* $\mathcal{A}$ has been thoroughly investigated in the literature (see, e.g., Refs. 1 and 2). For the present purposes, it is sufficient to recall that the push-forward of the embedding i is an injection of the vertical bundle $V(\mathcal{A})$, associated with the fibration $\mathcal{A}\to\mathcal{V}_4$, into the vertical bundle $V(j_1(\mathcal{V}_4))$. For later use, taking the identification (5) into account, we also denote by $\tau(\mathcal{A}):=T(\mathcal{A})\cap j_2(\mathcal{V}_4)$ the intersection between the tangent space on $\mathcal{A}$ and the second-jet space of the fibration $\mathcal{V}_4\to\mathfrak{R}$.

By means of the submanifold $\mathcal{A}$ we may construct—in an obvious way—a second embedding $i:\mathcal{A}\times\mathcal{B}\to j_1(\mathcal{V}_4)\times\mathcal{B}$, fibered over $\mathcal{V}_4\times\mathcal{B}$. Once again, the situation is summarized into the commutative diagram

$$\begin{array}{ccc} \mathcal{A}\times\mathcal{B} & \overset{i}{\to} & j_1(\mathcal{V}_4)\times\mathcal{B} \\ \pi\downarrow & & \downarrow\pi \\ \mathcal{V}_4\times\mathcal{B} & = & \mathcal{V}_4\times\mathcal{B} \end{array} . \tag{35}$$

Let us denote by $V(\mathcal{A}\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$ the vertical bundle associated with the fibration $\mathcal{A}\times\mathcal{B}\to\mathcal{V}_4\times\mathcal{B}$. Then, through (the vertical lift of) Eq. (16), we have the natural identification $V(\mathcal{A}\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})\simeq V(\mathcal{A})\times\mathcal{B}$, systematically used in the following.

Moreover, the push-forward of i is an injection of $V(\mathcal{A})\times\mathcal{B}$ into $V(j_1(\mathcal{V}_4))\times\mathcal{B}$. In view of this, identifying $V(\mathcal{A})\times\mathcal{B}$ with its image $i_*(V(\mathcal{A}))\times\mathcal{B}\subset V(j_1(\mathcal{V}_4))\times\mathcal{B}$, the bundle $V(\mathcal{A})\times\mathcal{B}$ is easily recognized to coincide with the totality of vertical vectors $X^i(\partial/\partial\dot{x}^i)$ satisfying the conditions

$$X^i\frac{\partial g^\sigma}{\partial\dot{x}^i}=0, \quad \forall\sigma=1,...,r. \tag{36}$$

Now, if we identify the submanifold $\mathcal{A}\times\mathcal{B}$ with its image $i(\mathcal{A})\times\mathcal{B}\subset j_1(\mathcal{V}_4)\times\mathcal{B}$, the results stated in Sec. II B allow one to regard $\mathcal{A}\times\mathcal{B}$ itself as the *space of admissible velocities* of $\mathcal{B}$, each point $z\in\mathcal{A}\times\mathcal{B}$ actually representing an admissible kinetic state of a particle of the continuum $\mathcal{B}$. Accordingly, every section $\varphi:\mathcal{B}\times\mathfrak{R}\to\mathcal{V}_4\times\mathcal{B}$ consistent with the constraints (33), i.e., satisfying the requirement

$$g^\sigma(t,\varphi(t,X^A),\dot{\varphi}(t,X^A))=0, \quad \forall(t,X^A)\in\mathfrak{R}\times\mathcal{B},\forall\sigma=1,...,r, \tag{37}$$

will be called *admissible*. Then, the totality of evolutions of $\mathcal{B}$ allowed by the constraints coincides with the class of admissible sections of $\mathcal{V}_4\times\mathcal{B}\to\mathfrak{R}\times\mathcal{B}$. The clear meaning of the requirement (37) is that the image of the first jet-extension of each admissible section under the projection τ_1^k has to be contained in $\mathcal{A}\times\mathcal{B}$.

For later use, we notice that, up to the assignment of initial data $\varphi^i(0,X)$, $\dot{\varphi}^i(0,X)$ s.t. $g^\sigma(0,\varphi(0,X),\dot{\varphi}(0,X))=0\,\forall X\in\mathcal{B}$, Eq. (37) is mathematically equivalent to the "tangency" requirement

$$\frac{\partial g^\sigma}{\partial t}+\frac{\partial g^\sigma}{\partial x^i}\dot{\varphi}^i+\frac{\partial g^\sigma}{\partial\dot{x}^i}\ddot{\varphi}^i=0, \quad \forall(t,X^A)\in\mathfrak{R}\times\mathcal{B};\forall\sigma=1,...,r. \tag{38}$$

III. SOLVING THE DYNAMICS

A. The constitutive characterization of iper-ideality

Within the geometrical framework outlined in Sec. II, the implementation of the equations of motion in the presence of constraints requires the introduction of a rule χ assigning to every free dynamics $\hat{Z}$ a corresponding *effective dynamics* $Z:=\chi(\hat{Z})$ expressing through Eq. (32) the actual evolution of the constrained system.

To start with, let us denote by $j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R})$ the submanifold of $j_k(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R})$ (locally) described by Eq. (33), or, equivalently, the pull-back of $j_k(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R})$ over $\mathcal{A}\times\mathcal{B}$, expressed by the commutative diagram

$$\begin{array}{ccc} j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R}) & \overset{i}{\rightarrow} & j_k(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R}) \\ \downarrow & & \downarrow r_1^k \\ \mathcal{A}\times\mathcal{B} & \overset{i}{\rightarrow} & j_1(\mathcal{V}_4)\times\mathcal{B} \end{array} . \tag{39}$$

From the considerations in Sec. II, taking Eqs. (27), (35), and (38) explicitly into account, it is easily seen that the constrained dynamics Z has to be a differentiable map $Z: j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R}) \rightarrow \tau(\mathcal{A})\times\mathcal{B}$. Within this scheme, it is clear that the required rule χ has to be considered as the *constitutive characterization* of the constraints. Therefore, such a rule χ represents an additional piece of information, related to the physical properties of the devices involved in the implementation of the constraints, which has to be included among the geometrical attributes of the system. In the subsequent discussion we shall characterize a special kind of purely kinetic constraint, defined, as we shall see, by a suitable choice of the rule χ.

First of all, we observe that, due to Proposition II.1, the difference

$$\phi := \chi(\hat{Z}) - \hat{Z} \tag{40}$$

between the effective dynamics and [the restriction to $j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R})$ of] the unconstrained dynamics, defines a differentiable map $\phi: j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R}) \rightarrow V_{\mathcal{A}}(j_1(\mathcal{V}_4))\times\mathcal{B}$, where $V_{\mathcal{A}}(j_1(\mathcal{V}_4))$ denotes the restriction to $\mathcal{A}$ of the vertical bundle $V(j_1(\mathcal{V}_4))$.

In view of the results stated in Sec. II B, the map ϕ has a natural interpretation in terms of *reactive forces*: recalling Eq. (20), the connection between the map ϕ and the distribution $\Phi = \Phi^i e_{(i)}$ of specific density of reactive forces is expressed by

$$\phi^i = \Phi^i. \tag{41}$$

Now, indicating by $\pi_{\tau(\mathcal{A})}$ the projection $\pi_{\tau(\mathcal{A})}: \tau(\mathcal{A})\times\mathcal{B} \rightarrow \mathcal{A}\times\mathcal{B}$, it is easily seen that—independently of the choice of constitutive characterization χ—the reactive force ϕ necessarily satisfies the inequality

$$|\phi_{|z}| = |\chi(\hat{Z})_{|z} - \hat{Z}_{|z}| \geqslant \min\{|Y - \hat{Z}_{|z}|, \quad Y \in \pi_{\tau(\mathcal{A})}^{-1}(\tau_1^k(z))\} \tag{42}$$

for all $z \in j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R})$, the norm $|\cdot|$ being the one induced by the fiber metric G_{ij}. Indeed, by construction, $\chi(\hat{Z})_{|z}$ belongs to $\pi_{\tau(\mathcal{A})}^{-1}(\tau_1^k(z))$.

Borrowing from Ref. 1, we may then state the following

Definition III.1: A set of purely kinetic constraints is said to be iper-ideal if and only if the equality sign identically holds in Eq. (42), i.e., if the corresponding constitutive characterization χ satisfies

$$|\chi(\hat{Z})_{|z} - \hat{Z}_{|z}| = \min\{|Y - \hat{Z}_{|z}|, \quad Y \in \pi_{\tau(\mathcal{A})}^{-1}(\tau_1^k(z))\} \tag{43}$$

for all $z \in j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R})$.

We are now going to see that the constitutive characterization of iper-ideality is essentially equivalent to the requirement that the constraints appear *ideal* with respect to any infinitesimal part of continuum $\mathcal{B}$, ideality being understood in the sense of Gauss' principle of minimal constraint.[1,2]

Indeed, taking the definition of the metric G_{ij} as well as Eq. (41) into account, Eqs. (40) and (43) mean that the motion of any particle of continuum $\mathcal{B}$ is selected among the totality of kinematically admissible evolutions as the one for which the quantity

$$|\phi|^2 = |\Phi|^2 = |\mathbf{a} - \mathbf{F} - \mathbf{f}|^2 \tag{44}$$

attains a minimum at any instant t ($\mathbf{a}$ and $\mathbf{F}+\mathbf{f}$ denote, respectively, the acceleration of the particle and the specific density of active forces). As predicted, this is precisely a restatement of Gauss' principle for any infinitesimal part of $\mathcal{B}$, regarded as the search, within the class of admissible accelerations, for that value $\mathbf{a}$ which minimizes the expression (44) at each instant t.

Once again borrowing from the discrete case[1] and extending the arguments to the present context, Gauss' criterion of minimal constraint may be made equivalent to the principle of virtual work; as we shall see, this is achieved embodying the so-called Chetaev' conditions into the definition of the virtual displacements for any particle of $\mathcal{B}$.

In fact, for each $z \in j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R})$, the image space

$$\rho_z(\hat{Z}) := \{Y-\hat{Z}_{|z} | Y \in \pi^{-1}_{\tau(\mathcal{A})}(\tau_1^k(z))\}$$

is an affine subspace of the vertical space $V_{\tau_1^k(z)}(j_1(\mathcal{V}_4)\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$ $(\simeq V(j_1(\mathcal{V}_4))\times\mathcal{B}_{|\tau_1^k(z)})$, modeled on $V_{\tau_1^k(z)}(\mathcal{A}\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$ $(\simeq V(\mathcal{A})\times\mathcal{B}_{|\tau_1^k(z)})$. For this reason, there exists an element of *minimal norm* in $\rho_z(\hat{Z})$, identified with the unique element $N_z \in \rho_z(\hat{Z})$ *orthogonal* to $V_{\tau_1^k(z)}(\mathcal{A}\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$.

Repeating the reasoning for each $z \in j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R})$, we may define a unique map $\mathcal{P}(\hat{Z}): j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R}) \to \tau(\mathcal{A})\times\mathcal{B}$ such that $\mathcal{P}(\hat{Z})_{|z}-\hat{Z}_{|z}=N_z \forall z$. It is clear that the constitutive characterization (43) is nothing but the ansatz $\chi(\hat{Z}) := \mathcal{P}(\hat{Z})$.

In terms of reactive forces, this implies that the iper-ideality is mathematically equivalent to the orthogonality condition

$$G(\phi_z, X)=0, \quad \forall X \in V_{\tau_1^k(z)}(\mathcal{A}\times\mathcal{B},\mathcal{V}_4\times\mathcal{B}), \forall z \in j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R}). \tag{45}$$

Recalling Eqs. (19), (36), and (41), the scalar product (45) takes the form

$$\Phi_i X^i = 0, \tag{46}$$

Φ_i and X^i denoting, respectively, the (covariant) components of the specific density of reactive force Φ and the components of any vertical vector X satisfying the relations $X^i(\partial g^\sigma/\partial \dot{x}^i)=0$ $\sigma=1,...,r$.

Then, performing the formal substitution $X^i \to \delta\varphi^i$ and defining the virtual displacement $\delta\varphi := (\delta\varphi^1, \delta\varphi^2, \delta\varphi^3)$ for any particle of $\mathcal{B}$, from Eq. (46) we recover the content of the principle of virtual work

$$\Phi \cdot \delta\varphi = 0,$$

for every virtual displacement $\delta\varphi$ obeying the Chetaev conditions $(\partial g^\sigma/\partial \dot{x}^i)\delta\varphi^i=0$ $\sigma=1,...,r$.[1,2,16–18]

B. The equations of motion

In this section we shall examine the construction of the equations of motion for a continuum $\mathcal{B}$ subject to iper-ideal purely kinetic constraints.

First of all, it is worth observing that the identical vanishing of the scalar product $G(\phi,X) = G_{ij}\phi^i X^j = \phi_i X^i = 0$ for all vertical vectors $X = X^i(\partial/\partial\dot{x}^i) \in V(\mathcal{A}\times\mathcal{B},\mathcal{V}_4\times\mathcal{B})$ implies the relations $\phi_i = \lambda_\sigma(\partial g^\sigma/\partial\dot{x}^i)$ or, equivalently, $\phi^i = \lambda_\sigma(\partial g^\sigma/\partial\dot{x}^j)G^{ij}$ for some functions $\lambda_\sigma \in \mathcal{F}(j_k^{\mathcal{A}}(\mathcal{V}_4\times\mathcal{B},\mathcal{B}\times\mathfrak{R}))$, because of the tangency condition $X^i(\partial g^\sigma/\partial\dot{x}^i)=0$ $\sigma=1,...,r$.

This fact, together with Eq. (40), allows one to represent the constrained dynamical map $Z := \chi(\hat{Z})$ in the form

$$Z = \hat{Z} + \lambda_\sigma \frac{\partial g^\sigma}{\partial \dot{x}^i} G^{ij} \frac{\partial}{\partial \dot{x}^j}. \tag{47}$$

In comparison with Eq. (30), Eq. (47) yields the corresponding constrained equations of motion for $\mathcal{B}$, expressed as

$$\ddot{\varphi}^i = F^i + f^i + \lambda_\sigma \frac{\partial g^\sigma}{\partial \dot{x}^j} G^{ij}. \tag{48}$$

The final step is the determination of the multipliers λ_σ. This is easily achieved imposing the "tangency" condition (38), resulting in

$$\frac{\partial g^\gamma}{\partial t} + \frac{\partial g^\gamma}{\partial x^i}\dot{\varphi}^j + (F^i + f^i)\frac{\partial g^\gamma}{\partial \dot{x}^i} + \lambda_\sigma \frac{\partial g^\sigma}{\partial \dot{x}^j} G^{ij} \frac{\partial g^\gamma}{\partial \dot{x}^i} = 0, \quad \gamma = 1,...,r. \tag{49}$$

In view of the regularity assumption $\|\partial g^\sigma/\partial \dot{x}^i\| = r$, ensuring the nonsingularity of the matrix $\Gamma^{\sigma\gamma} := (\partial g^\sigma/\partial \dot{x}^j) G^{ij} (\partial g^\gamma/\partial \dot{x}^i)$, Eq. (49) may be solved uniquely for the λ_σ's, yielding the explicit expressions

$$\lambda_\sigma = \Gamma_{\sigma\gamma}\left[-\left(\frac{\partial g^\gamma}{\partial t} + \frac{\partial g^\gamma}{\partial x^i}\dot{\varphi}^i \right) - (F^i + f^i)\frac{\partial g^\gamma}{\partial \dot{x}^i} \right], \tag{50}$$

$\Gamma_{\sigma\gamma}$ denoting the inverse of the matrix $\Gamma^{\sigma\gamma}$.

Finally, we get the required equations of motion for the system, simply inserting the result (50) into Eq. (48).

IV. VARIATIONAL FORMULATION

The aim of this section is to derive the constrained equations of motion (48), (38) from a suitable variational problem, basing our discussion on the usual variational formulation for general field theories. For simplicity, we focus our attention on first-order variational calculus only. Extensions to higher order cases are essentially straightforward and are left to the reader.

First of all, we consider the totality of local sections $\varphi: \Re \times \mathcal{B} \to \mathcal{V}_4 \times \mathcal{B}$ and denote it by Γ. As is well known, Γ may be endowed with a smooth infinite dimensional manifold structure. Given a section $\varphi \in \Gamma$, we shall call *deformation* of φ a differentiable map $\psi: \Re \times \mathcal{B} \times (-\sigma, \sigma) \to \mathcal{V}_4 \times \mathcal{B} (\sigma \in \Re)$ satisfying the conditions

$$\psi(\cdot, 0) = \varphi(\cdot), \quad \psi_\xi(\cdot) := \psi(\cdot, \xi) \in \Gamma, \quad \forall \xi \in (-\sigma, \sigma). \tag{51}$$

In view of Eq. (51), a deformation of φ defines a curve in Γ, passing through φ for $\xi = 0$. Then, the tangent vector to ψ at φ identifies an element $V \in T_\varphi \Gamma$, defined by the relation

$$V(\cdot) := \frac{d\psi}{d\xi}(\cdot, \xi)_{|\xi = 0}. \tag{52}$$

From Eq. (52) it is easily seen that V has the nature of a vertical vector field along the section φ, namely of a map $V: \Re \times \mathcal{B} \to V_{\varphi(\Re \times \mathcal{B})}(\mathcal{V}_4 \times \mathcal{B}, \Re \times \mathcal{B})$ such that the following diagram

$$\begin{array}{ccc} \Re \times \mathcal{B} & \overset{V}{\rightarrow} & V(\mathcal{V}_4 \times \mathcal{B}, \Re \times \mathcal{B}) \\ \downarrow id & & \downarrow \pi \\ \Re \times \mathcal{B} & \overset{\varphi}{\rightarrow} & \mathcal{V}_4 \times \mathcal{B} \end{array} \tag{53}$$

is commutative, π denoting the canonical projection.

Any map V as in diagram (53) will be called an *infinitesimal deformation* of φ.

Now, let $\mathcal{L}$ be a differentiable $(M+1)$-form on $j_1(\mathcal{V}_4\times\mathcal{B},\Re\times\mathcal{B})$, semibasic with respect to the fibration $j_1(\mathcal{V}_4\times\mathcal{B},\Re\times\mathcal{B})\to\Re\times\mathcal{B}$. In local coordinates, $\mathcal{L}=L(t,X^A,x^i,x^i_\alpha)\times \mathrm{d}t\wedge\mathrm{d}X^1\wedge\cdots\wedge\mathrm{d}X^M$.

For any compact domain $D\subset\Re\times\mathcal{B}$, let us denote by Γ_D the totality of sections $\varphi\in\Gamma$ defined in some open neighborhood $U\subset\Re\times\mathcal{B}$ of D. By means of $\mathcal{L}$, we may then define a real-valued functional I_D on Γ_D, according to the relation

$$I_D(\varphi):=\int_D j_1(\varphi)^*(\mathcal{L}),\quad \forall\varphi\in\Gamma_D. \tag{54}$$

Given a section $\varphi\in\Gamma_D$ and an infinitesimal deformation $V\in T_\varphi\Gamma$, we shall call *first variation* of I_D at φ with respect to V (Gateaux derivative at φ in the direction V) the expression

$$\frac{\delta I_D}{\delta V}(\varphi):=\frac{\mathrm{d}}{\mathrm{d}\xi}\int_D j_1(\psi_\xi)^*(\mathcal{L})_{|_{\xi=0}}, \tag{55}$$

ψ_ξ being any deformation of φ "tangent to V" [i.e., satisfying Eq. (52)].

Following the usual terminology, we shall call the *critical point* of I_D any section $\varphi\in\Gamma_D$ making the functional I_D stationary, i.e., satisfying the condition

$$\frac{\delta I_D}{\delta V}(\varphi)=0$$

for all infinitesimal deformations $V\in T_\varphi\Gamma$.

By definition, the standard variational problem associated with the $(M+1)$-form $\mathcal{L}$—usually called the *Lagrangian*—consists in the search for sections $\varphi\in\Gamma$ which are critical points of all functionals I_D (54) for all compact domains D, with respect to all infinitesimal variations vanishing at the boundary of D, namely such that

$$\frac{\delta I_D}{\delta V}(\varphi)=0,\quad \forall\ \text{compact domain}\ D\subset\Re\times\mathcal{B},\forall V\in T_\varphi\Gamma\ \text{ s.t. }\ V_{|\partial D}=0. \tag{56}$$

For convenience, we introduce the notation $X^0:=t$ and refer the manifolds $\Re\times\mathcal{B}$ and $j_1(\mathcal{V}_4\times\mathcal{B},\Re\times\mathcal{B})$ to local coordinates X^α and X^α, x^i, x^i_α, $\alpha=0,...,M$, respectively. We also denote by $\mathrm{d}S:=\mathrm{d}X^0\wedge\cdots\wedge\mathrm{d}X^M$ the local volume element in $\Re\times\mathcal{B}$.

Taking the condition at the boundary $V_{|\partial D}=0$ explicitly into account, it is a straightforward matter to get the well-known expression[14,19]

$$\frac{\delta I_D}{\delta V}(\varphi)=\int_D\left[\frac{\partial L}{\partial x^i}-\mathrm{d}_\alpha\left(\frac{\partial L}{\partial x^i_\alpha}\right)\right]V^i\circ j_2(\varphi)\mathrm{d}S\ , \tag{57}$$

where the d_α's indicate the formal derivatives $\mathrm{d}_\alpha:\mathcal{F}(j_1(\mathcal{V}_4\times\mathcal{B},\Re\times\mathcal{B}))\to\mathcal{F}(j_2(\mathcal{V}_4\times\mathcal{B},\Re\times\mathcal{B}))$ with respect to any X^α, i.e., $\mathrm{d}_\alpha f=\partial f/\partial X^\alpha+(\partial f/\partial x^i)x^i_\alpha+(\partial f/\partial x^i_\beta)x^i_{\beta\alpha}\forall f=f(X^\alpha,x^i,x^i_\alpha)$.

Because of the arbitrariness in the choice of the compact domains D as well as of the infinitesimal deformations V, it follows from Eq. (57) that a section φ is a solution of the variational problem (56) if and only if it satisfies the well known Euler–Lagrange equations

$$\left[\frac{\partial L}{\partial x^i}-\mathrm{d}_\alpha\left(\frac{\partial L}{\partial x^i_\alpha}\right)\right]\circ j_2(\varphi)=0,\quad i=1,...,3. \tag{58}$$

As mentioned previously, our aim is now to set up a variational formulation for the equations of motion (48), (38) of a continuum system $\mathcal{B}$ subject to purely kinetic constraints.

To this end, let us suppose the existence of a Lagrangian $\mathcal{L}$ which describes the dynamical behavior of the system in the absence of kinetic constraints, by means of the corresponding Euler–Lagrange equations (58).

Borrowing from the arguments developed for the discrete case,[20,21] the idea is not to study the stationarity of functionals (54) with respect to all infinitesimal deformations V vanishing at the boundary, but only with respect to the ones satisfying the Chetaev conditions

$$\frac{\partial g^{\sigma}}{\partial \dot{x}^{i}} V^{i} = 0, \quad \sigma = 1,...,r. \tag{59}$$

We shall call the latter a *constrained* variational problem.

The solutions of (57) and (59) may be obtained by means of the usual Lagrange multipliers' method (see, e.g., Ref. 22), from which we derive the existence of some functions λ_{σ} such that a section φ is a solution of the constrained variational problem if and only if it satisfies the equations

$$\left[\frac{\partial L}{\partial x^{i}} - \mathrm{d}_{\alpha}\left(\frac{\partial L}{\partial x^{i}_{\alpha}}\right)\right] \circ j_2(\varphi) = \lambda_{\sigma} \frac{\partial g^{\sigma}}{\partial \dot{x}^{i}} \circ j_2(\varphi), \quad i = 1,...,3, \tag{60}$$

clearly identical to Eq. (48). The argument is straightforward. The details are left to the reader.

In general, Eq. (60) alone is not sufficient to single out any solution φ. In fact, in addition to (the significant components of) the section φ, we need to determine the multipliers λ_{σ}, too. To restore determinacy, some additional conditions are required.

In this specific case, the significant ansatz is to impose that the solutions φ satisfy the ''tangency'' requirement (38). As already pointed out, this, together with the assignment of consistent initial data, is mathematically equivalent to requiring consistency with the equations of constraints (33), and it is actually sufficient to determine the unknowns λ_{σ}. We underline that these supplementary conditions concern exclusively the solutions, and not their deformations.

We have thus shown that the admissible evolutions of the system $\mathcal{B}$ can be characterized as the solutions $\varphi: \mathfrak{R} \times \mathcal{B} \to \mathcal{V}_4 \times \mathcal{B}$ of a suitable constrained variational problem. An explicit example will be given in Sec. V.

Remark: We notice that the complementary case, consisting in the study of constraints depending on material derivatives only, has been considered in Ref. 23. Although the authors use a geometrical framework quite similar to the one proposed here, they deduce the equations of motion through a variational principle which, in the case of finite dimensional systems subject to nonholonomic constraints, reduces to vakonomic mechanics and thus yields incorrect equations of motion.

For this reason, the approach proposed in Ref. 23 does not seem appropriate to deal with purely kinetic constraints, contrary to the one proposed here based on Gauss' and D'Alembert's principles. Therefore, as mentioned by Marsden and co-workers,[23] it appears that a distinction between time and material partial derivatives is needed.

However, a unified approach would be desirable and, in our opinion, it may be implemented in the framework of infinite-dimensional manifolds. A first step in this direction has been made in Ref. 24.

V. EXAMPLES

A. Rotating continuum

Let us denote by $\{\underline{k}_1, \underline{k}_2, \underline{k}_3\}$ an orthonormal basis in the physical space of a given frame of reference $\mathcal{I}$. We consider a continuum $\mathcal{B}$ subject to a kinetic constraint which keeps it rotating around $\underline{k}_3$ with a constant angular velocity $\underline{\omega} = \omega \underline{k}_3$, so that the tangential velocity $\underline{v}_T(p)$ of each point $p \in \mathcal{B}$ is proportional to the distance from the axis of rotation. The tangential velocity is meant as the component of the velocity of each p which is tangent to the circle centered on $\underline{k}_3$, lying on the plane orthogonal to $\underline{k}_3$ and passing through p at each instant t.

If $\varphi:\Re\times\mathcal{B}\to\mathcal{V}_4$ describes the evolution of the continuum in the frame of reference $\mathcal{I}$, we define:
(1) $\underline{R}=\underline{R}(t,X^A)$ the radius vector, which connects the point $p\in\mathcal{B}$ having coordinates $\{X^1,\ldots,X^M\}$ and the axis of rotation, and lies in the plane orthogonal to $\underline{k}_3$ containing p;
(2) $\hat{R}=(1/\rho)\underline{R}$ where $\rho=\sqrt{\varphi_1^2+\varphi_2^2}$;
(3) $\hat{l}=\underline{k}_3\wedge\hat{R}$.

If $\varphi=\Sigma_{i=1}^3\varphi_i\underline{k}_i$ we have

$$\underline{R}=\varphi_1\underline{k}_1+\varphi_2\underline{k}_2,\quad \hat{l}=\frac{1}{\rho}(-\varphi_2\underline{k}_1+\varphi_1\underline{k}_2).$$

We can describe the constraint by means of

$$\omega|\underline{R}|=|\dot{\varphi}\cdot\hat{l}|. \tag{61}$$

This means that, given a circle centered on $\underline{k}_3$, lying on a plane orthogonal to $\underline{\omega}$, the tangential component of the velocity of each of its points is proportional to the product of the radius of the circle by the magnitude ω of the angular velocity.

Equation (61) may be rephrased as

$$\omega(\varphi_1^2+\varphi_2^2)=|\varphi_1\dot{\varphi}_2-\varphi_2\dot{\varphi}_1|.$$

We thus define the constraints in implicit form by means of the relation

$$g:=|\varphi_1\dot{\varphi}_2-\varphi_2\dot{\varphi}_1|-\omega(\varphi_1^2+\varphi_2^2)=0. \tag{62}$$

Denoting by (F_1,F_2,F_3) the components of the specific density of internal and external forces together and recalling Eqs. (48)–(50) we have

$$\lambda=\frac{1}{\rho^2}[2\omega(\varphi_1\dot{\varphi}_1+\varphi_2\dot{\varphi}_2)-\nu(F_1\varphi_2-F_2\varphi_1)], \tag{63}$$

where

$$\nu=\frac{|\varphi_1\dot{\varphi}_2-\varphi_2\dot{\varphi}_1|}{\varphi_1\dot{\varphi}_2-\varphi_2\dot{\varphi}_1}.$$

The sign of ν is uniquely determined by the choice of initial data. The reader may easily verify that the first term on the right-hand side of (63) is the part of reactive force which annihilates Coriolis force, while the second balances the tangential component of real (internal and external) physical forces.

From all the above-mentioned considerations, we obtain that the equations of motion for the constrained continuum are

$$\begin{cases}\ddot{\varphi}_1=F_1-\dfrac{\varphi_2}{\rho^2}[2\omega\nu(\varphi_1\dot{\varphi}_1+\varphi_2\dot{\varphi}_2)-(F_1\varphi_2-F_2\varphi_1)],\\ \ddot{\varphi}_2=F_2+\dfrac{\varphi_1}{\rho^2}[2\omega\nu(\varphi_1\dot{\varphi}_1+\varphi_2\dot{\varphi}_2)-(F_1\varphi_2-F_2\varphi_1)],\\ \ddot{\varphi}_3=F_3.\end{cases} \tag{64}$$

We finally observe that Eq. (64) represents every continuum subject to the constraint described by Eq. (62); different continua correspond to different choices of the functions F_i.

B. Vibrating string

In a Cartesian frame of reference, let us consider a homogeneous elastic string with fixed ends, moving without friction on a horizontal plane. In addition to this, we require that the string makes transversal vibrations only.

Although both restrictions are positional in nature, we shall deal with them as (integrable) kinetic constraints; actually, the aim is to provide an example in which the iper-ideality condition turns out to be a common physical requirement. Moreover, we shall discuss the problem using the variational formulation.

To this end, denoting by ℓ_0 the rest length of the string, we identify the material space $\mathcal{B}$ of the system with the closed interval $[0,\ell_0]\subset\mathfrak{R}$ and refer it to a coordinate ξ. Moreover, we denote by μ_0 the (constant) density of the string. Finally we indicate by x^1, x^2, x^3 the Cartesian coordinates in the physical space of the given frame chosen in such a way that the horizontal plane coincides with $x^3=0$ and the ends of the string belong to the x^1 axis. Accordingly, the jet-coordinates will be indicated by $t,\xi,x^i,x^i_t,x^i_\xi,x^i_{tt},x^i_{t\xi},x^i_{\xi\xi},\dots$.

In this way, the imposed constraints are, respectively, expressed by

$$g^1 := x^3_t = 0, \quad g^2 := x^1_t = 0. \tag{65}$$

As far as the constraint $g^1=0$ is concerned, the iper-ideality condition is easily recognized to reproduce the requirement of absence of friction.

The implementation of a variational formulation requires the construction of a suitable Lagrangian for the system $\mathcal{B}$. To this purpose, we consider the string as a sequence of material points all connected to the neighbors by springs; in other words, given any pair of points P_1 and P_2 belonging to the string and having distance $\delta\xi$ in the rest configuration, we endow them with a potential energy equal to the one of a spring of rest length $\delta\xi$ and elastic constant $\chi/\delta\xi$, namely

$$\delta U = -\frac{\chi}{2\delta\xi}(\delta s-\delta\xi)^2 = -\frac{\chi}{2}\left(\frac{\delta s}{\delta\xi}-1\right)^2\delta\xi,$$

where δs is the actual length of the piece of string between P_1 and P_2. The constant χ depends on the structural properties of the string; in fact $\chi=ES$, where E is the Young's modulus and S is the (constant) section of the string. Therefore, by an obvious limit process $\delta\xi\to 0$, the total internal potential energy of the system is given by the integral

$$U = -\frac{\chi}{2}\int_0^{\ell_0}\left(\frac{\mathrm{d}s}{\mathrm{d}\xi}-1\right)^2\mathrm{d}\xi.$$

On the other hand, the kinetic energy of the spring is expressed as

$$T = \frac{1}{2}\int_0^{\ell_0}\mu_0\sum_{i=1}^{3}(x^i_t(t,\xi))^2\mathrm{d}\xi.$$

Collecting all the results and taking the weight potential into account, we may define the Lagrangian

$$\mathcal{L} = \left(\frac{\mu_0}{2}\sum_{i=1}^{3}(x^i_t)^2-\frac{\chi}{2}\left(\sqrt{\sum_{i=1}^{3}(x^i_\xi)^2}-1\right)^2-\mu_0 g x^3\right)\mathrm{d}t\wedge\mathrm{d}\xi \tag{66}$$

viewed as a two-form on $j_1(\mathcal{V}_4\times[0,\ell_0],\mathfrak{R}\times[0,\ell_0])$, semibasic with respect to the fibration $j_1(\mathcal{V}_4\times[0,\ell_0],\mathfrak{R}\times[0,\ell_0])\to\mathfrak{R}\times[0,\ell_0]$.

The Euler–Lagrange–Chetaev equations (60) associated with the Lagrangian (66) assume the form

$$\begin{cases} \mu_0\varphi^1_{tt}=\dfrac{\partial}{\partial\xi}\left[\chi\left(\sqrt{\sum_{i=1}^{3}(\varphi^i_\xi)^2}-1\right)\dfrac{\varphi^1_\xi}{\sqrt{\Sigma^3_{i=1}(\varphi^i_\xi)^2}}\right]+\lambda_1, \\ \mu_0\varphi^2_{tt}=\dfrac{\partial}{\partial\xi}\left[\chi\left(\sqrt{\sum_{i=1}^{3}(\varphi^i_3)^2}-1\right)\dfrac{\varphi^2_3}{\sqrt{\Sigma^3_{i=1}(\varphi^i_\xi)^2}}\right], \\ \mu_0\varphi^3_{tt}=\dfrac{\partial}{\partial\xi}\left[\chi\left(\sqrt{\sum_{i=1}^{3}(\varphi^i_\xi)^2}-1\right)\dfrac{\varphi^3_\xi}{\sqrt{\Sigma^3_{i=1}(\varphi^i_\xi)^2}}\right]-\mu_0 g+\lambda_2. \end{cases} \tag{67}$$

Imposing the tangency conditions (38), which in the present case are

$$\varphi^1_{tt}=0, \quad \varphi^3_{tt}=0 \tag{68}$$

directly from Eq. (67) we get the following expressions:

$$\begin{cases} \lambda_1=-\dfrac{\partial}{\partial\xi}\left[\chi\left(\sqrt{\sum_{i=1}^{3}(\varphi^i_\xi)^2}-1\right)\dfrac{\varphi^1_\xi}{\sqrt{\Sigma^3_{i=1}(\varphi^i_\xi)^2}}\right], \\ \lambda_2=\mu_0 g-\dfrac{\partial}{\partial\xi}\left[\chi\left(\sqrt{\sum_{i=1}^{3}(\varphi^i_\xi)^2}-1\right)\dfrac{\varphi^3_\xi}{\sqrt{\Sigma^3_{i=1}(\varphi^i_\xi)^2}}\right] \end{cases}$$

for the multipliers λ. Recalling Eq. (48), the latter provide the explicit description of (the density of) the reactive forces.

Choosing the initial data and the boundary conditions consistent with the constraints, namely

$$\varphi^1(0,\xi)=\frac{\ell}{\ell_0}\xi, \quad \varphi^2(0,\xi)=\psi(\xi), \quad \varphi^3(0,\xi)=0,$$

$$\varphi^1_t(0,\xi)=0, \quad \varphi^2_t(0,\xi)=\dot\psi(\xi), \quad \varphi^3_t(0,\xi)=0,$$

$$\varphi^1(t,0)=0, \quad \varphi^2(t,0)=0, \quad \varphi^3(t,0)=0,$$

$$\varphi^1(t,\ell_0)=\ell, \quad \varphi^2(t,\ell_0)=0, \quad \varphi^3(t,\ell_0)=0,$$

Eq. (68) is solved by

$$\varphi^1(t,\xi)=\frac{\ell}{\ell_0}\xi, \quad \varphi^3(t,\xi)=0. \tag{69}$$

If we replace Eq. (69) in the second equation of (67), we get the partial differential equation

$$\mu_0\varphi^2_{tt}=\frac{\partial}{\partial\xi}\left[\chi\left(\sqrt{\left(\frac{\ell}{\ell_0}\right)^2+(\varphi^2_\xi)^2}-1\right)\frac{\varphi^2_\xi}{\sqrt{\left(\frac{\ell}{\ell_0}\right)^2+(\varphi^2_\xi)^2}}\right], \tag{70}$$

which rules the evolution of φ^2. Under the approximation of small deformations, we may neglect all the quadratic terms in φ^2_ξ in Eq. (70), thus obtaining the well-known D'Alembert equations

$$\varphi^2_{tt}=\frac{\chi}{\mu_0}\left(1-\frac{\ell_0}{\ell}\right)\varphi^2_{\xi\xi}$$

for the linear elastic string.

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On a general link between anomalous diffusion and nonextensivity

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Stochastic processes of systems with composable entropy measures are studied. The processes are described by Fokker–Planck equations which are nonlinear with respect to their probability densities and whose diffusion coefficients are derived from the entropy measures in questions. In nonextensive (extensive) systems anomalous (normal) diffusion is found. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421062]

I. INTRODUCTION

Anomalous diffusion is a phenomenon which can be found in various fields of physics[1–3] ranging from surface diffusion[4] and diffusion through porous media[5] to plasma physics.[6] Anomalous diffusion can be described by non-Fickian linear diffusion equations,[7,8] continuous time random walks,[9–12] fractional Fokker–Planck equations,[13–17] and nonlinear diffusion equations.[5,18–24] The focus of the present article is on nonlinear diffusion equations which have recently been discussed in the context of nonextensive thermostatistics. The interest in such a link between anomalous diffusion and nonextensivity[25] has been fueled by a work of Plastino and Plastino.[26] They derived a nonlinear Fokker–Planck equation (NLFPE) whose stationary solution agrees with the equilibrium distribution obtained by maximizing the nonextensive entropy proposed by Tsallis[27–32] under the constraints of canonical ensembles. Note that in this article nonlinear (or generalized) Fokker–Planck equations are evolution equations for probability densities which are nonlinear with respect to their probability densities as opposed to conventional Fokker–Planck equations which are linear with respect to their probability densities.[33–44] The NLFPE proposed by Plastino and Plastino and modifications of it have been extensively studied in the literature.[45–59] In particular, for the entropy functional

$$S[\mathcal{P}] := B\left[\int_{-\infty}^{\infty} \tilde{S}(\mathcal{P}(x))\mathrm{d}x\right] \tag{1}$$

acting on the probability density $\mathcal{P}(x)$ and involving the outer function $B(z) \in C^{\infty}(\mathbb{R})$ and the entropy kernel $\tilde{S} \in C^{\infty}(0,\infty)$, the NLFPE

$$\frac{\partial}{\partial t}\mathcal{P}(x,t) = -\frac{\partial}{\partial x}\left[M\{\mathcal{P}(x,t)\}\left(h(x)\mathcal{P}(x,t) - \frac{\rho[\mathcal{P}]}{\alpha}\frac{\partial}{\partial x}\hat{L}[\tilde{S}\{\mathcal{P}(x,t)\}]\right)\right] \tag{2}$$

was derived.[51] Here, $\mathcal{P}(x,t)$ describes the time-dependent process probability density, $h(x)$ is the drift, $M\{\cdot\}$ is a function or functional of $\mathcal{P}(x,t)$, the factor $1/\alpha$ with $\alpha > 0$ corresponds to the overall fluctuation strength, the functional $\rho[\cdot]$ is defined by

$$\rho[y] := \left.\frac{\mathrm{d}B(z)}{\mathrm{d}z}\right|_{\int_{-\infty}^{\infty}\tilde{S}(y(x))\mathrm{d}x}, \tag{3}$$

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and the differential operator $\hat{L}$ is given by

$$\hat{L}[\chi(y)] := \chi(y) - y\frac{\mathrm{d}\chi(y)}{\mathrm{d}y}. \tag{4}$$

It can be shown that the stationary solution of the NLFPE (2) agrees with the equilibrium distribution derived by maximizing the entropy (1) under the constraints of canonical ensembles.[51] The nonlinear diffusion equation corresponding to the NLFPE (2) can be obtained by putting $M \equiv 1$ and $h(x) \equiv 0$. In this case, we get

$$\frac{\partial}{\partial t}\mathcal{P}(x,t) = \frac{\rho[\mathcal{P}(x,t)]}{\alpha}\frac{\partial^2}{\partial x^2}\hat{L}[\tilde{S}\{\mathcal{P}(x,t)\}]. \tag{5}$$

Note that in contrast to conventional nonlinear diffusion equations[5,18–24] but in line with the Fokker–Planck equation approach, the density function $\mathcal{P}(x,t)$ is normalized to unity [i.e., $\int \mathcal{P}(x,t)\mathrm{d}x = 1$]. In the following, we consider continuous solutions $\mathcal{P}(x,t)$ which are infinitely differentiable on their domains of nonvanishing function values. That is, we assume that (i) $\mathcal{P}(x,t) \geqslant 0$, (ii) $\mathcal{P}(x,\cdot) \in C^0(\mathbb{R})$, and (iii) $\mathcal{P}(x,\cdot) \in C^\infty(\mathrm{supp}\{\mathcal{P}(x,\cdot)\})$ with $\mathrm{supp}\{\mathcal{P}(x,\cdot)\} := \{x : \mathcal{P}(x,\cdot) > 0\}$. Recently, several special cases of Eq. (5) have been examined and explicit solutions have been derived. For the nonextensive entropy proposed by Tsallis anomalous diffusion was found.[46,48,49,53,59] For the extensive Renyi entropy normal diffusion and for the nonextensive Sharma–Mittal entropy anomalous diffusion was found except for the limiting case in which the Sharma-Mittal entropy reduces to the Renyi entropy.[53] For other generalized entropy measures,[30,51,60–65] such a discussion has not been carried out so far. Similarly, until now, a general link between nonextensivity (extensivity) of entropy functionals and anomalous (normal) diffusion which can be applied to all kinds of entropy measures has not been established. In the following, we will derive such a link for composable entropy functionals (Ref. 32, Sec. II.1), that is, for functionals satisfying

$$S[\mathcal{W}] = S[\mathcal{R}_1] + S[\mathcal{R}_2] + N(S[\mathcal{R}_1], S[\mathcal{R}_2]), \tag{6}$$

where the probability densities $\mathcal{R}_1(x)$ and $\mathcal{R}_2(x)$ describe two statistically independent subsystems yielding the joint probability density $\mathcal{W}(x,y) := \mathcal{R}_1(x)\mathcal{R}_2(y)$. Here, $N(u,v) \in C^2(\mathbb{R} \times \mathbb{R})$ denotes an arbitrary function of the entropies $S[\mathcal{R}_1]$ and $S[\mathcal{R}_2]$ of the subsystems. Note that the commutativity of the multiplication [i.e., $\mathcal{R}_1(x)\mathcal{R}_2(y) = \mathcal{R}_1(y)\mathcal{R}_2(x)$] implies the symmetry of N [i.e., $N(u,v) = N(v,u)$]. If N depends on $S[\mathcal{P}]$, we will call the functional S a nonextensive functional. More precisely, S is nonextensive if $\partial N/\partial u|_{u=S[\mathcal{P}(x,t)]} \not\equiv 0$ for $\mathcal{P}(x,t)$ given by Eq. (5). In contrast, if N does not depend on $S[\mathcal{P}]$, we will refer to S as an extensive functional. In particular, for $N = \mathrm{const}$, we can introduced the shifted functional $S' = S + N$, which satisfies the well-known relation of extensive entropies $S'[\mathcal{R}_1\mathcal{R}_2] = S'[\mathcal{R}_1] + S'[\mathcal{R}_2]$ (cf., e.g., Refs. 66–68).

II. NONEXTENSIVITY AND ANOMALOUS DIFFUSION

From Eq. (5) we can derive the evolution equation of the mean $\langle x \rangle$ (which is $\mathrm{d}\langle x \rangle/\mathrm{d}t = 0$) and the second moment $\langle x^2 \rangle$ (which is $\mathrm{d}\langle x^2 \rangle/\mathrm{d}t = 2\,\alpha^{-1}\rho\int \hat{L}\,\mathrm{d}x$). Using Eq. (4), for the variance $\sigma^2 := \langle x^2 \rangle - \langle x \rangle^2$ we then obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma^2(t) = \underbrace{\frac{2}{\alpha}\rho[\mathcal{P}]\int_{-\infty}^{\infty}\left[\tilde{S}(\mathcal{P}(x,t)) - \mathcal{P}(x,t)\left.\frac{\mathrm{d}\tilde{S}(z)}{\mathrm{d}z}\right|_{z=\mathcal{P}(x,t)}\right]\mathrm{d}x}_{\mathcal{Y}[\mathcal{P}]}. \tag{7}$$

Consequently, if the functional $\mathcal{Y}[\mathcal{P}]$ is constant with respect to time we have normal diffusion [i.e., $\sigma^2(t) \propto t$]. Otherwise, we find anomalous diffusion [i.e., $\sigma^2(t) \not\propto t$]. We now derive $\mathcal{Y}$ from

the assumed nonextensivity/extensivity property (6). To this end, let $\mathcal{R}_1(x)$ be defined on the real line and $\mathcal{R}_2(y)$ be defined on the interval $[0,a]$ with $a>0$. Furthermore, let $\mathcal{R}_2(y)$ denote the uniform distribution on $[0,a]$, that is, $\mathcal{R}_2(y)\equiv 1/a$. Then, from Eqs. (1) and (6) it follows

$$B\left[a\int_{-\infty}^{\infty}\tilde{S}\left(\frac{\mathcal{R}_1(x)}{a}\right)\mathrm{d}x\right]=S[\mathcal{R}_1]+B\left[a\tilde{S}\left(\frac{1}{a}\right)\right]+N\left(S[\mathcal{R}_1],B\left[a\tilde{S}\left(\frac{1}{a}\right)\right]\right). \tag{8}$$

Next, we differentiate Eq. (8) with respect to a and put $a=1$. Thus, we obtain

$$\mathcal{Y}[R_1]=C+\left.\frac{\partial N(S[\mathcal{R}_1],v)}{\partial v}\right|_{v=C} \tag{9}$$

with

$$C:=\left(\tilde{S}(1)-\left.\frac{\mathrm{d}\tilde{S}(z)}{\mathrm{d}z}\right|_{z=1}\right)\left.\frac{\mathrm{d}B(z)}{\mathrm{d}z}\right|_{z=\tilde{S}(1)}. \tag{10}$$

Consequently, the variance $\sigma^2(t)$ satisfies the evolution equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma^2(t)=\frac{2C}{\alpha}+\frac{2}{\alpha}\frac{\partial N(S[\mathcal{P}],v)}{\partial v}_{v=C} \tag{11}$$

with $\mathcal{P}(x,t)$ determined by the diffusion equation (5). Since C does not depend on the time variable t, we deal with normal diffusion if the second term on the right hand side of Eq. (11) does not depend on time. Otherwise, we find anomalous diffusion. Therefore, at issue is how $S[\mathcal{P}]$ and $\partial N(S[\mathcal{P}],v)/\partial v|_{v=C}$ evolve as functions of time. From Eq. (5) it follows that $S[\mathcal{P}]$ satisfies the relation

$$\frac{\mathrm{d}}{\mathrm{d}t}S[\mathcal{P}]=\frac{1}{\alpha}(\rho[\mathcal{P}])^2\int_{-\infty}^{\infty}\mathcal{P}(x,t)\left(\frac{\partial}{\partial x}\left.\frac{\mathrm{d}\tilde{S}(z)}{\mathrm{d}z}\right|_{z=\mathcal{P}(x,t)}\right)^2\mathrm{d}x\geqslant 0 \tag{12}$$

[see Ref. 52, Eq. (6) for $M\equiv 1$]. We require now that the entropy functional S is sensitive to unlikely events. More precisely, we require the existence of an interval $(0,l]$ of finite length l (i.e., $l>0$) such that the derivative $\mathrm{d}\tilde{S}(z)/\mathrm{d}z$ maps all elements of $(0,l]$ to nonvanishing function values (i.e., $\exists l:\forall z\in(0,l]:\mathrm{d}\tilde{S}(z)/\mathrm{d}z\neq 0$). We find that for entropies of this kind the expression

$$\frac{\partial}{\partial x}\left.\frac{\mathrm{d}\tilde{S}(z)}{\mathrm{d}z}\right|_{z=\mathcal{P}(x,t)} \tag{13}$$

can have at most a finite number of zeros for $x\in I_k$, where the intervals I_k are defined by $I_k=[x_l^k,x_r^k]$ with $x_l^k<x_r^k$, I_k mutually disjoint, and $0<\mathcal{P}(z,t)\leqslant l$ for all $z\in I_k$. That is, $\partial\mathrm{d}\tilde{S}/\partial x\mathrm{d}z\not\equiv 0$ for $z=\mathcal{P}(x,t)$ and $x\in I_k$. Since we restrict our considerations to continuous probability densities which decay to zero in a smooth fashion (cf. Sec. I), the existence of such intervals is guaranteed. From Eq. (12) we can then read off that

$$\frac{\mathrm{d}}{\mathrm{d}t}S[\mathcal{P}]\geqslant\frac{1}{\alpha}(\rho[\mathcal{P}])^2\sum_k\int_{I_k}\mathcal{P}(x,t)\left(\frac{\partial}{\partial x}\left.\frac{\mathrm{d}\tilde{S}(z)}{\mathrm{d}z}\right|_{z=\mathcal{P}(x,t)}\right)^2\mathrm{d}x>0. \tag{14}$$

In sum, entropies which are sensitive to unlikely events are strictly monotonically increasing functions for the diffusion processes defined by Eq. (5). We are now in the position to examine the evolution of $\partial N(S[\mathcal{P}],v)/\partial v|_{v=C}$. Differentiating this expression with respect to the time variable t yields

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial N(S[\mathcal{P}],v)}{\partial v}\right|_{v=C}=\left.\frac{\partial^2 N(u,v)}{\partial u\,\partial v}\right|_{v=C,u=S[\mathcal{P}]}\frac{\mathrm{d}S[\mathcal{P}]}{\mathrm{d}t}. \tag{15}$$

Using this result and differentiating Eq. (11) with respect to t, we obtain

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\sigma^2(t)=\frac{2}{\alpha}\underbrace{\frac{\mathrm{d}S[\mathcal{P}]}{\mathrm{d}t}}_{>0}\left.\frac{\partial^2 N(u,v)}{\partial u\,\partial v}\right|_{v=C,u=S[\mathcal{P}]}. \tag{16}$$

Therefore, we have normal diffusion [i.e., $\mathrm{d}^2\sigma^2(t)/\mathrm{d}t^2=0$] if and only if

$$\left.\frac{\partial^2 N(u,v)}{\partial u\,\partial v}\right|_{v=C,u=S[\mathcal{P}]}=0. \tag{17}$$

Since we found in Sec. I that extensivity and nonextensivity, respectively, can be defined by means of the derivative $\partial N(u,v)/\partial u|_{u=S[\mathcal{P}]}$, we can now draw our final conclusions (which are only valid within the NLPFE framework and for composable entropies, of course).

(i) Nonextensive systems with $\partial N(u,v)/\partial v|_{v=C}=0$ and extensive systems show normal diffusion. Normal diffusion only occurs in nonextensive systems with $\partial N(u,v)/\partial v|_{v=C}=0$ and extensive systems.

(ii) Nonextensive systems with $\partial N(u,v)/\partial v|_{v=C}\neq 0$ show anomalous diffusion. Anomalous diffusion only occurs in nonextensive systems satisfying $\partial N(u,v)/\partial v|_{v=C}\neq 0$.

Roughly speaking, nonextensivity implies anomalous diffusion and extensivity implies normal diffusion. But there is an exception to this rule: in nonextensive systems for which the first order partial derivative of $N(u,v)$ with respect to u vanishes for $u=C$ normal diffusion can also occur.

III. CONCLUDING REMARKS

Let us conclude with a few remarks. First, the theory developed here applies to the Renyi entropy,[69,70] the Sharma–Mittal entropy,[71] and the entropy proposed by Tsallis.[27] For the Renyi entropy we find $N\equiv 0$, which implies that the corresponding nonlinear diffusion equation (5) describes normal diffusion. The two other entropies are composable and nonextensive and satisfy

$$S[\mathcal{W}]=S[\mathcal{R}_1]+S[\mathcal{R}_2]+\underbrace{(1-q)S[\mathcal{R}_1]S[\mathcal{R}_2]}_{N(S[\mathcal{R}_1],S[\mathcal{R}_2])}, \tag{18}$$

where $q\neq 1$ measures the degree of nonextensivity.[27,53] Substituting $N(u,v)=(1-q)uv$ into Eq. (16), we obtain

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\sigma^2(t)=\frac{2(1-q)}{\alpha}\frac{\mathrm{d}S[\mathcal{P}]}{\mathrm{d}t}\neq 0 \quad \text{for } q\neq 1, \tag{19}$$

which illustrates that for these entropies the nonlinear diffusion equation (5) describes anomalous diffusion. Consequently, we reobtain the results previously derived in Refs. 46, 48, 49, 53, and 59. Note that in these studies explicit solutions or scaling arguments have been used, whereas we have exploited the very definition of nonextensive entropies.

Second, for semi-nonextensive systems (i.e., systems for which the energy is an extensive variable whereas the entropy is a nonextensive one) Abe derived explicit expressions for the nonlinearity N [cf. Eq. (6)] of composable entropies.[72] Such systems can exhibit an equilibrium state only for entropy measures satisfying

$$\frac{\partial S[\mathcal{W}=\mathcal{R}_1\mathcal{R}_2]}{\partial S[\mathcal{R}_1]}=\rho[\mathcal{W}]\tilde{g}(S[\mathcal{R}_1])\tilde{h}(S[\mathcal{R}_2])$$

$$\Rightarrow \frac{\partial S[\mathcal{W}=\mathcal{R}_2\mathcal{R}_1]}{\partial S[\mathcal{R}_2]}$$

$$=\rho[\mathcal{W}]\tilde{g}(S[\mathcal{R}_2])\tilde{h}(S[\mathcal{R}_1])$$

$$=\frac{\partial S[\mathcal{W}=\mathcal{R}_1\mathcal{R}_2]}{\partial S[\mathcal{R}_2]}, \tag{20}$$

where $\rho[\cdot]$ is defined by Eq. (3) (and coincides with the function k in Ref. 72) and $\tilde{g}(z)$ and $\tilde{h}(z)$ denote differentiable functions. It can be shown that in the absence of an outer function [i.e., for $\rho\equiv 1$, $B(z)=z$] this decomposition implies

$$S[\mathcal{W}]=S[\mathcal{R}_1]+S[\mathcal{R}_2]+\lambda S[\mathcal{R}_1]S[\mathcal{R}_2], \tag{21}$$

where λ is a separation constant.[72] Obviously, Eq. (21) is a generalization of Eq. (18) (which has been derived for two particular generalized entropies only) and the evolution of the variance can be read off from Eq. (19) by replacing $1-q$ with λ. Consequently, the nonlinear Fokker–Planck approach to stochastic processes employed in the present study predicts the occurrence of anomalous diffusion in semi-nonextensive systems with composable entropies that can be cast into the form (1) with $B(z)=z$. Moreover, Abe suggested to describe the entropy of black holes by a composable measure with $\rho\not\equiv 1$ and $N(u,v)=2\sqrt{uv}$. In this case, Eq. (16) reads

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\sigma^2(t)=\frac{2}{\alpha\sqrt{C}}\frac{\mathrm{d}}{\mathrm{d}t}\sqrt{S[\mathcal{P}]}, \tag{22}$$

which describes anomalous diffusion provided that S is sensitive to unlikely events (i.e., $\mathrm{d}S>0$, cf. Sec. II). We can easily verify that a simple example of a composable entropy with $N(u,v)=2\sqrt{uv}$ is given by $S:=[S_{\mathrm{BGS}}]^2$, where S_{BGS} denotes the Boltzmann–Gibbs–Shannon entropy $S_{\mathrm{BGS}}[\mathcal{P}]:=-\int\mathcal{P}\ln\mathcal{P}\mathrm{d}x$.[66–68] Then, we obtain $B(z)=z^2$ and (on account of the sensitivity of S_{BGS} to unlikely events) $\mathrm{d}S>0$.

In the absence of an outer function B [i.e., for $B(z)\equiv z$] we usually find $\tilde{S}(1)=0$. The reason for this is that many entropy functionals S are derived from entropies $S_d:=\Sigma_{i=1}^{M}\tilde{S}(p_i)=\Sigma_{i=1}^{M}p_i\tilde{s}(p_i)$ for discrete sets of probabilities p_i. In these cases, by convention, one defines $\tilde{s}(z)$ (information of an event with probability z) in such a way that it vanishes in the case of the certain event with probability one, that is, $\tilde{s}(1)=0\Rightarrow\tilde{S}(1)=1\tilde{s}(1)=0$. For $B(z)\equiv z$ and $\tilde{S}(1)=0$ the constant C reads $C=-\mathrm{d}\tilde{S}(z)/\mathrm{d}z|_{z=1}$. In this special case, the evolution equation of the variance reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma^2(t)=-\frac{2}{\alpha}\frac{\mathrm{d}\tilde{S}(z)}{\mathrm{d}z}\bigg|_{z=1}+\frac{2}{\alpha}\frac{\partial N(S[\mathcal{P}],v)}{\partial v}\bigg|_{v=-\mathrm{d}\tilde{S}(z)/\mathrm{d}z|_{z=1}}. \tag{23}$$

In particular, for the Boltzmann–Gibbs–Shannon entropy $S=S_{\mathrm{BGS}}=-\int\mathcal{P}\ln\mathcal{P}\mathrm{d}x$ we obtain $\mathrm{d}\tilde{S}(z)/\mathrm{d}z=-1-\ln z$ and the well-known relation $\mathrm{d}\sigma^2(t)/\mathrm{d}t=2\alpha^{-1}\Rightarrow\sigma^2(t)=2t/\alpha$.

Finally, the derivation presented in the preceding section does not hold for diffusion processes with infinite variances such as Lévy distributions, cf., e.g., Refs. 3 and 10. In this context, limitations of the approach to anomalous diffusion by means of nonlinear Fokker–Planck equations in combination with the calculation of process variances were illustrated in detail in Refs. 53

and 55. In order to circumvent such problems, one may follow Tsallis and Bukman who introduced the notion of pseudo anomalous diffusion for Lévy distributions and examined the evolution of normalization constants instead of process variances.[59]

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Fluctuation operators and spontaneous symmetry breaking

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We develop an alternative approach to this field, which was to a large extent developed by Verbeure *et al*. It is meant to complement their approach, which is largely based on a noncommutative central limit theorem and coordinate space estimates. In contrast to that we deal directly with the limits of l-point truncated correlation functions and show that they typically vanish for $l \geqslant 3$ provided that the respective scaling exponents of the fluctuation observables are appropriately chosen. This direct approach is greatly simplified by the introduction of a smooth version of spatial averaging, which has a much nicer scaling behavior and the systematic development of Fourier space and energy-momentum spectral methods. We both analyze the regime of normal fluctuations, the various regimes of poor clustering and the case of spontaneous symmetry breaking or Goldstone phenomenon. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1424474]

I. INTRODUCTION

In the past decade in a series of papers Verbeure and co-workers developed a beautiful and ingeneous framework to study so-called macroscopic fluctuation phenomena in systems and various regimes of quantum statistical mechanics (see the cited literature). The approach is to a large extent based on a quantum variant of the *central limit theorem* and is mainly performed in real (i.e., configuration) space. Among other things, the general goal is to study the limit behavior of correlation functions of so-called *fluctuation observables*, i.e., appropriately renormalized averages of microscopic observables, averaged over volumes, V, which approach the whole space, $\mathbb{R}^n$, say. Typically, one arrives, depending on the type of clustering of the microscopic l-point functions, at certain simple limit algebras as, e.g., CCR.

We approach the field from a slightly different angle. In a first step we choose another averaging procedure, which avoids sharp volume cut-offs and, *a fortiori*, has a very nice and transparent scaling behavior. This is then exploited in the following analysis which systematically develops so-called Fourier-space and energy-momentum spectral methods of observables and correlation functions. We consider it to be an advantage that the calculations turn out to be relatively transparent and lead in a direct way to the desired results.

We first treat the case of *normal fluctuations* and L^1-clustering. We show that all the truncated l-point functions vanish for $l \geqslant 3$ while they approach a finite, nontrivial limit for $l = 2$. The analysis is done both for the $(k = 0)$-and the $(k \neq 0)$-modes. We emphasize that the calculations for net-momentum different from zero also remain very simple. A variant of the method is then applied to the case of L^2-clustering.

In the second part of the article we embark on the analysis of fluctuations in the presence of *spontaneous symmetry breaking (ssb)*. In a first step we prove some general results in the context of ssb and the *Goldstone phenomenon*. We then address the problem of macroscopic fluctuations within this context. Among other things, we give a general and rigorous proof that the limit fluctuations are always classical for temperature states (a phenomenon already observed by Verbeure *et al.* in various simple models). The article ends with a treatment of extremely poor

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clustering, which can be controlled by a new method we develop in the last section. To sum up, we think that in our view the two different frameworks seem to neatly complement each other and should lead to further interesting results if combined.

II. THE SCENARIO OF NORMAL FLUCTUATIONS

The following analysis works for statistical equilibrium states and/or for vacuum states in quantum field theory. To avoid constant mentioning of the respective scenario we are actually working in, we usually treat equilibrium (i.e., KMS) states, to fix the framework. Now, let Ω be the vacuum or equilibrium state (rather its GNS representation; usually we work within a concrete Hilbert space, $\mathcal{H}$). As an abstract state we denote it by ω. Expectations of observables are written as

$$\langle A\rangle = \omega(A) = (\Omega, A\Omega) \tag{1}$$

with A taken from the *local algebra*, $\mathcal{A}_0 \subset \mathcal{A}$, the latter one being the *quasi-local* norm closure of $\mathcal{A}_0$. We assume Ω to be *cyclic* with respect to $\mathcal{A}_0$ or $\mathcal{A}$. That is, we assume

$$\overline{\mathcal{A}_0 \cdot \Omega} = \mathcal{H}. \tag{2}$$

There are certain differences as to the (assumed) locality properties of the dynamics between (non-)relativistic statistical mechanics and relativistic quantum field theory (RQFT). Denoting the time evolution (acting on the algebra of observables) by α_t, we are confronted with the following phenomenon.

Observation 2.1: In RQFT part of the usual framework is the assumption

$$\alpha_t : \mathcal{A}_0 \to \mathcal{A}_0, \tag{3}$$

while in statistical mechanics (due to weaker locality behavior) we have in the generic case only

$$\alpha_t : \mathcal{A} \to \mathcal{A} \tag{4}$$

with $\mathcal{A}_0$ usually not left invariant as the observables will typically develop infinitely extended tails.

Furthermore, we assume once and for all that our system is in a *pure, translation invariant phase*, that is, Ω is extremal translation invariant under the space translations (which can, as in the case of lattice systems, also be a discrete subgroup). There can, of course, exist several coexisting pure phases at the same external parameters as in the regime below a phase transition threshold. These assumptions imply that we can expect certain *cluster properties*, i.e., decay of *correlations* (see e.g., Ref. 1).

A. Definition of ordinary fluctuation operators

We begin by defining the *fluctuation operators* in the *normal* situation as it was done in Ref. 2.

We assume, for the time being, L^1-clustering for the two-point-function, that is,

$$\int |\langle A(x)B\rangle^T| d^n x < \infty \quad A, B \in \mathcal{A} \tag{5}$$

with $A(x)$ the translate of A and

$$\langle AB\rangle^T = \langle AB\rangle - \langle A\rangle \cdot \langle B\rangle. \tag{6}$$

Once and for all we assume, to simplify notation, in our particular context that the occurring observables are normalized to $\langle A\rangle = 0$ unless otherwise stated.

Definition 2.2: We define the normal (finite volume) fluctuation operators as

$$A_V^F := 1/V^{1/2} \cdot \int_V A(x) d^n x =: 1/V^{1/2} \cdot A_V . \tag{7}$$

In a next step one wants to give sense to these objects in the limit $V \to \infty$. From the L^1-condition we, however, infer

$$|(A_V^F \Omega, B\Omega)| \leqslant 1/V^{1/2} \int_{\mathbb{R}^n} |(A(x)\Omega, B\Omega)| d^n x \to 0. \tag{8}$$

Hence, $A_V^F \Omega \to 0$ on a dense set. Furthermore, we have

$$(A_V^F \Omega, A_V^F \Omega) = 1/V \int_V \int_V (A(x)\Omega, A(y)\Omega) dx dy = 1/V \int_V dx \left(\int_{V-x} \langle A^* A(y-x) \rangle d(y-x) \right). \tag{9}$$

This is less than or equal to

$$(1/V) \cdot V \cdot \sup_x \left(\int_{V-x} |(\ldots)| \right) \leqslant \int_{\mathbb{R}^n} |F(y-x)| d^n (y-x) < \infty \tag{10}$$

[for convenience we sometimes denote a general two-point function by $F(x-y)$]. This suffices to prove weak convergence to zero for $A_V^F \Omega$ on the total Hilbert space $\mathcal{H}$.

Remark 2.3: We note that this proves also the well-known normal-fluctuation result $\langle A_V \cdot A_V \rangle \leqslant V$ *in the* L^1*-case. Under certain well-specified conditions the fluctuations can even be weaker than normal. If, e.g.,* Q_V *is the local integral over a conserved quantity, we proved a divergence significantly weaker than* $\sim V$ *(cf. Ref. 3). But, in general, the local fluctuations will diverge in the limit* $V \to \infty$ *in contrast perhaps to ordinary intuition, even if the quantity is globally conserved due to quantum fluctuations (see also the section about spontaneous symmetry breaking).*

A weaker than normal divergence can occur in the following situation. An asymptotic behavior $\sim V$ does only prevail if $\int_V F(u) du \neq 0$ in the limit $V \to \infty$. On the other side such correlation functions tend to oscillate about zero (for physical reasons; there are, e.g., usually preferred relative positions in, say, a quantum liquid). In other words, while

$$\int F(u) du = 0 \tag{11}$$

may seem to be rather ungeneric at first glance, it can nevertheless happen in a specific context. The general situation is analyzed in the above reference; certain examples of better than normal fluctuations were also found by Verbeure *et al.* in, e.g., Ref. 4 (see also Ref. 5).

For the fluctuation operators themselves we have, due to locality, for $A, B \in \mathcal{A}_0$,

$$[A_V, B] \quad \text{independent of} \quad V \quad \text{for} \quad V \supset V_0 \supset V_B \tag{12}$$

for some V_0 which contains the localization region V_B for $B \in \mathcal{A}_0$. We then have

$$\lim_V (A_V^F \cdot C\Omega, B\Omega) = \lim_V ([A_V^F, C]\Omega, B\Omega) + \lim_V (A_V^F \Omega, C^* B\Omega). \tag{13}$$

We have already shown that the second term goes to zero. In the first term the commutator becomes

$$[A_V^F, C] = V^{-1/2} \cdot [A_{V_0}, C], \tag{14}$$

and hence the first term goes also to zero. In case we assume only $A \in \mathcal{A}$, a further L^1-condition for the three-point function is needed to arrive at the same result. As $\mathcal{A}_0\Omega$ is assumed to be dense in $\mathcal{H}$ and $\|A_V^F\| < \infty$ uniformly in V, we have the following.

Proposition 2.4: L^1-clustering implies that

$$A_V^F \to 0 \quad \textit{weakly on } \mathcal{H}, \quad \|A_V^F\Omega\| < \infty \quad \textit{uniformly in } V, \tag{15}$$

but $\|A_V^F\Omega\|$ bounded away from zero in general. That is, A_V^F does not converge strongly to zero and, a fortiori, there is no convergence in norm.

This clearly shows that, in order to have nontrivial limit operators, one has to leave the original Hilbert space of microscopic observables and has to define or construct an entirely new representation living on a different state.

B. A smoothed version of fluctuation operators

Since we employ in the following so-called *Fourier methods* and related calculational tools, it is advantageous to change to a smoother version of fluctuation operators. As everybody knows, sharp volume cut-offs are both a little bit artificial and technically nasty, since they may sometimes lead to nongeneric or spurious effects. In other branches of rigorous statistical mechanics or axiomatic quantum field theory volume integrations have therefore frequently been emulated or implemented in a slightly different way (see, e.g., Ref. 6).

Two choices have basically been in use with the second version having much nicer properties in several respects as we will explain below. Instead of integrating over a sharp volume, V, centered, e.g., around the coordinate origin, one integrates the shifted observable, $A(x)$, over a smooth test function localized basically in V but having smooth tails.

Remark: As V we choose in the following a ball centered at the origin with radius R and let R go to infinity.

Definition 2.5: Two admisssible families of test functions are the following ones: $f_R(x) \geqslant 0$ *smooth with*

$$f_R(x) := \begin{cases} 1 & \text{for } |x| \leqslant R, \\ 0 & \text{for } |x| \geqslant R+h, \end{cases} \tag{16}$$

or

$$f_R(x) := f(|x|/R) \quad \text{with} \quad f(s) = \begin{cases} 1 & \text{for } |x| \leqslant 1, \\ 0 & \text{for } |x| \geqslant 2. \end{cases} \tag{17}$$

Note that the latter choice has much nicer behavior under Fourier transform while working with the Fourier transforms of the former version or, e.g., the indicator function of the volume V is quite cumbersome). On the other hand, the latter version has tails which are also scaled.

Lemma 2.6:

$$\hat{f}_R(k) = \text{const} \cdot R^n \cdot \hat{f}(R \cdot k), \tag{18}$$

where here and in the following ''const'' denotes an (in this context) irrelevant numerical factor which, *a fortiori*, may change in the course of a calculation. With the help of this smearing functions we now define the following.

Definition 2.7 (smooth volume integration): We redefine the fluctuation operators in the following way:

$$A_R^F := R^{-n/2} \cdot \int A(x) \cdot f_R(x) d^n x \tag{19}$$

with f_R, unless otherwise stated, the family given in the second example above (remember $\langle A \rangle := 0$).

III. THE LIMITING CASE FOR NORMAL FLUCTUATIONS

In order to arrive at a rigorous definition of fluctuation operators in a certain limit state we will follow a line of arguments which may complement the treatment of Verbeure *et al.* in several respects. We will study directly the macroscopic limit of the n-point functions with the help of certain *momentum space methods*. As they are perhaps not so common in statistical physics we will give the technical details next.

A. Some generalities

Any n-point (correlation) function of the kind $\langle A_1(x_1)\cdots A_n(x_n)\rangle$ with the $A_i(x_i)$ the translates of the observables A_i (which may also contain an implicit time variable t_i which is, however, kept fixed in the following) is written as $W(x_1,\ldots,x_n)$. With the state Ω being translation invariant we have

$$W(x_1,\ldots,x_n)=W(x_1-x_2,\ldots,x_{n-1}-x_n). \tag{20}$$

To express cluster properties in a clear way, we introduce the so-called *truncated correlation functions* via the following recursion relation:

$$W(x_1,\ldots,x_n)=\sum_{\text{part}}\prod_{P_i} W^T(x_{i_1},\ldots,x_{i_k}), \tag{21}$$

where the sum extends over all partitions of the set $\{1,\ldots,n\}$ into subsets P_i with the elements in each subset ordered as $i_1<i_2\cdots<i_k$. The first elements of the recursion are

$$W(x)=W^T(x)=0 \quad \text{in our case,} \tag{22}$$

$$W^T(x_1,x_2)=W(x_1,x_2)-W(x_1)W(x_2). \tag{23}$$

Observation 3.1: In the truncated correlation functions the vacuum state, ground state or equilibrium state, Ω, has been eliminated in a symmetric way, so that we have, in a sense to be specified,

$$W^T(x_1,\ldots,x_n)\to 0 \quad for \quad \sup|x_i-x_j|\to\infty. \tag{24}$$

In this section we assume the following *cluster property*:

$$W^T(x_1,\ldots,x_n)\in L^1 \ \text{ in the variables } \ \{x_1-x_2,\ldots,x_{n-1}-x_n\}. \tag{25}$$

From the above we see that the original hierarchy of n-point functions can be reconstructed from the new hierarchy of truncated n-point functions, which have more transparent cluster properties. The L^1-condition allows us to Fourier transform the $W^T(x_1,\ldots,x_l)$ and we get from translation invariance:

$$\begin{aligned}
\text{const}\cdot\int \tilde{W}^T(p_1,\ldots,p_l)\cdot e^{-i\Sigma p_i x_i}\prod\, dp_i &= W^T(x_1,\ldots,x_l)\\
&= W^T(x_1-x_2,\ldots,x_{l-1}-x_l)\\
&= \text{const}\int \hat{W}^T(p_1,p_1+p_2,\ldots,p_1+\cdots+p_{l-1})\\
&\quad\cdot\delta(p_1+\cdots+p_l)e^{-i\Sigma p_i x_i}\prod\, dp_i\\
&= \text{const}\int \hat{W}^T(q_1,\ldots,q_{l-1})e^{-i\Sigma_{i=1}^{l-1} q_i y_i}\prod_{i=1}^{l-1} dq_i
\end{aligned} \tag{26}$$

with

$$y_i := x_i - x_{i+1}, \quad q_i = \sum_{j=1}^{i} p_j, \quad i \leqslant (l-1). \tag{27}$$

The functional determinant $\det(\partial q/\partial p)$ is one and we can regard $\hat{W}^T$ either as a function of the q_i's or the p_i's. We hence have the following lemma.

Lemma 3.2: As a Fourier transform of a L^1-function, $\hat{W}^T(p_1,\ldots,p_{l-1}) = \hat{W}^T(q_1,\ldots,q_{l-1})$ is a continuous and bounded function which decreases at infinity in the q-variables.

B. The ($k=0$)-modes

We now study the limit of truncated l-point functions with the entries being fluctuation operators A_R^F, more precisely their Fourier transforms, i.e.,

$$\begin{aligned}\langle A_R^F(1)\cdots A_R^F(l)\rangle^T &= \text{const}\cdot R^{ln/2}\cdot \int \hat{f}(Rp_1)\cdots\hat{f}(-R[p_1+\cdots+p_{l-1}])\cdot \hat{W}^T(p_1,\ldots,p_{l-1})\prod dp_i \\ &= \text{const}\cdot R^{ln/2}\cdot R^{-(l-1)n}\cdot \int \hat{f}(p_1')\cdots\hat{f}(-[p_1'+\cdots+p_{l-1}']) \\ &\quad \cdot \hat{W}^T(p_1'/R,\ldots,p_{l-1}'/R)\prod dp_i' \,. \end{aligned} \tag{28}$$

Here $\hat{W}$ is continuous and bounded and the $\hat{f}$'s are of rapid decrease. Hence we can perform the limit $R\to\infty$ under the integral and get the following theorem.

Theorem 3.3: *The expression $\langle A_R^F(1)\cdots A_R^F(l)\rangle^T$ scales as $\sim R^{(2-l)n/2}$. This implies that for $l>2$ the above limit is zero; for $l=2$ the limit is a finite number bounded away from zero in general. In other words, we have*

$$\lim_{R\to\infty} \langle A_R^F(1)\cdots A_R^F(l)\rangle^T = 0 \quad \text{for } l>2 \tag{29}$$

and

$$\lim_{R\to\infty} \langle A_R^F(1)\cdots A_R^F(l)\rangle = \lim_{R\to\infty} \sum_{\text{part}} \prod_{\{ij\}} \langle A_R^F(i) A_R^F(j)\rangle. \tag{30}$$

The relation between the original microscopic system $(\mathcal{A},\omega)$ and the coarse-grained system of fluctuation operators is a little bit subtle. Note that ω_F, the limit state to be constructed, can no longer be considered as a state or something like that on the original algebra nor can the fluctuation operators be considered as a representation of, say, $\mathcal{A}$. One aspect of the impending problems can perhaps best be seen by realizing that, e.g.,

$$(A\cdot B)_V^F \neq A_V^F \cdot B_V^F, \tag{31}$$

which pertains also in the limit. That is, in a sense to be defined, we have

$$(A\cdot B)^F \neq A^F \cdot B^F, \tag{32}$$

the same holding in general for all the higher products. This is one source of nonuniqueness as there is no invariant discrimination between an observable regarded as a single object to be scaled and as a product of other observables, where now each factor has to be scaled separately. The appropriate point of view has to be a different one [as has also been emphasized by Verbeure *et al.*, cf. e.g., Ref. 2(b), p. 540f and private communication].

The picture remains relatively clear for the intermediate scales, $V<\infty$. We have a start system $(\mathcal{A},\omega)$, labeled by, say, $V=0$. On every scale V we have a new algebra, $\mathcal{A}_V^F$ (actually a subalgebra of $\mathcal{A}$), generated by the observables A_V^F, $A\in\mathcal{A}$ [including arbitrary finite products $(A_1\cdots A_n)_V^F$]. If we prefer to consider this algebra on scale V as a new abstract algebra (i.e., forgetting about the underlying finer algebra $\mathcal{A}$), we get also a new, coarse-grained state via the identification

$$\omega_V^F(\Pi A_V^{F,i}) := \omega(\Pi A_V^{F,i}). \tag{33}$$

(A related philosophy was expounded by Buchholz and Verch in, e.g., Ref. 7 within the context of the algebraic analysis of ultra-violet behavior in quantum field theory.)

The map

$$R_V:\mathcal{A}\to\mathcal{A}_V^F \tag{34}$$

can be viewed as kind of a *renormalization map*, which however, does *not* preserve the algebraic structure (i.e., the algebras are in general not *isomorphic*). Furthermore, one gets a "*new*" dynamics on this algebra by defining

$$\alpha_t^V(A_V^F) := (\alpha_t(A))_V^F. \tag{35}$$

Remark 3.4: In our context α_t is assumed to commute with the space translations or with a corresponding lattice version, that is, we have $\alpha_t(A_V^F)=(\alpha_t A)_V^F$. (Furthermore, it may turn out to be reasonable to scale the time variable on the lhs also.)

On the other hand, in order to construct the limit theory itself, one can proceed in a slightly different direction. The above limits of n-point functions define a consistent hierarchy of new n-point functions which then allow us to define a *new* limit system via the so-called *reconstruction theorem* (for a pendant in quantum field theory, see, e.g., Ref. 8). Put differently, we define limit objects, $\{A_i^F\}$, the so-called fluctuation operators, which live in a new Hilbert space built upon the new state, ω_F, defined by the limits:

$$\omega_F(A_1^F\cdots A_n^F) := \lim_{R\to\infty}\langle A_{1,R}^F\cdots A_{n,R}^F\rangle = \sum_{\text{part}}\prod_{\{ij\}}\omega_F(A_i^F\cdot A_j^F). \tag{36}$$

Note, however, that the so-called *Gelfand-ideal*, I_F, is large, that is, there are many elements of $\mathcal{A}$ which are mapped to zero by this limit with

$$I_F := \{A;\omega_F((A^F)^*\cdot A^F)=0\}. \tag{37}$$

This is, of course, typical for such kinds of *mean-values*, as, e.g., all space-translates of A yield the same limit element. Shifting one of the observables in the above l-point functions by, say, a_i yields an extra factor $e^{ip_ia_i}$ in the Fourier transform which, after the above coordinate tranformation goes over into $e^{ip_i'/R\cdot a_i}$ which goes to one. Summing up, we have the following.

Conclusion 3.5: With the help of Eq. (36) we construct a new limit system, consisting of the algebra of fluctuation operators, $\mathcal{A}_F$, and the limit state ω_F. The well-known GNS construction (see e.g., Ref. 9) allows us to construct the corresponding Hilbert-space representation with

$$\omega_F(A_1^F\cdots A_n^F)=(\Omega_F,A_1^F\cdots A_n^F\Omega_F) \tag{38}$$

(where, by abuse of notation, we do not discriminate between operators and their equivalence classes on the rhs).

As all the n-point functions decay into a product of two-point functions, all the commutators are c-numbers:

$$[A^F,B^F]=\omega_F([A^F,B^F]). \tag{39}$$

The system of fluctuation operators is a quasi-free system (cf. Ref. 10).

Taking now self-adjoint elements one can, as in Ref. 2, represent the new system as a representation of the *CCR* over the real vector space of s.a. operators. Our scalar product, induced by the hierarchy of n-point functions, can be split in the following way:

$$(A^F\Omega_F, B^F\Omega_F) = \mathrm{Re}(\cdots) + i\,\mathrm{Im}(\cdots) =: s_F(A^F,B^F) + (i/2)\sigma_F(A^F,B^F), \tag{40}$$

$$\omega_F([A^F,B^F]) = \sigma_F(A^F,B^F), \tag{41}$$

where σ_F defines a *symplectic form*. The *Weyl-operators*, e^{iA^F} with A^F s.a., fulfill the *CCR* relations

$$\omega_F(e^{iA^F}) = e^{-1/2 s_F(A^F,A^F)}, \tag{42}$$

$$e^{iA^F}\cdot e^{iB^F} = e^{i(A^F+B^F)}\cdot e^{-i/2\sigma_F(A^F,B^F)}. \tag{43}$$

In our context the first equation can, e.g., be verified as follows: Only the $2n$-point functions are different from zero. On the lhs we hence have

$$\omega_F(e^{iA^F}) = \sum\ (-1)^n/(2n)!\cdot\omega_F([A^F]^{2n}). \tag{44}$$

It remains to count the number of partitions of a $2n$-set into two-sets. This number is $(2n)!/2^n\cdot n!$. In (44) we now get for A^F s.a. on the rhs

$$\sum_n\ 1/n!\left(-\frac{1}{2}\cdot\omega_F(A^FA^F)\right)^n = e^{-1/2 s_F(A^FA^F)}. \tag{45}$$

□

The above general cluster result of the limit n-point functions makes the study of the limit time evolution relatively straightforward. In a first step it suffices to study the two-point functions. We define the time evolution in the limit theory by

$$\omega_F(A^F(t')\cdot B^F(t)) := \lim\omega(A_V^F(t')\cdot B_V^F(t)) = \lim\omega(A(t')_V^F\cdot B(t)_V^F). \tag{46}$$

On the limiting GNS–Hilbert space constructed above we now get a bounded *sesquilinear form* $(x,y(t))$ which, by standard results, yields a bounded operator $U^F(t)$ implementing the time evolution. Here we use that the limit n-point functions are products of two-point functions. Furthermore, we infer with the help of the above limit process that

$$(U_t^Fx, U_t^Fy) = \omega_F(\cdots) = \lim\omega(\cdots) = (x,y). \tag{47}$$

In other words, we arrive at the following conclusion.

Theorem 3.6: *The preceding construction yields a strongly continuous unitary time evolution on the limiting GNS–Hilbert space.*

Another point worth mentioning (since it might perhaps be overlooked) is the question of the nontriviality of the commutators

$$[A^F,B^F] = \omega_F([A^F,B^F]). \tag{48}$$

In principle it could happen that all the expectation values on the rhs vanish. In that case the limit algebra would be *Abelian* and the fluctuations *classical*. In a more general context (cf., e.g., Ref. 7) this problem is more complicated. In our situation this question can, however, be answered in a rather straightforward way. We have

$$\lim_V \omega([A_V^F, B_V^F]) = \lim_V \omega([A_V, V^{-1} \cdot B_V]). \tag{49}$$

For $A, B \in \mathcal{A}_0$, i.e., local, the rhs equals

$$\lim_V \omega([A_V, B]). \tag{50}$$

We know candidates which lead to a vanishing of the limit for all $B \in \mathcal{A}_0$. For A chosen s.a. these are the generators of *conserved symmetries*, written

$$Q := \int A(x) d^n x. \tag{51}$$

Usually they are assumed to commute with the time evolution, expressed as $Q(t) = Q$, hence the above limit would also be zero on the full quasi-local algebra. This situation, more specifically the case of *spontaneous symmetry breaking (ssb)* and *Goldstone phenomenon*, will be dealt with in more detail in Sec. V. In any case, as conserved symmetries are usually not so numerous, we may presume that, in the generic case, not all of these commutators will be zero.

For A, B not necessarily strictly local our above more general formalism is useful. With

$$\omega(A(x)B) = F_{AB}(x), \quad \omega(BA(x)) = G_{AB}(x), \tag{52}$$

the vanishing of the commutator would imply

$$\begin{aligned} 0 = [A^F, B^F] &= \lim_R R^n \cdot \int |\hat{f}(Rp)|^2 (\hat{F}_{AB}(p) - \hat{G}_{AB}(p)) d^n p \\ &= \lim_R \int |\hat{f}(p)|^2 (\hat{F}_{AB}(p/R) - \hat{G}_{AB}(p/R)) d^n p \\ &= (\hat{F}_{AB}(0) - \hat{G}_{AB}(0)) \cdot \int |\hat{f}(p)|^2 d^n p. \end{aligned} \tag{53}$$

by the theorem of dominated convergence (note that we are in the L^1-situation). Hence we have the following result.

Proposition 3.7:

$$[A^F, B^F] = 0 \Leftrightarrow \hat{F}_{AB}(0) = \hat{G}_{AB}(0), \tag{54}$$

that is,

$$\int F_{AB}(x) d^n x = \int G_{AB}(x) d^n x \tag{55}$$

or

$$\int (\Omega, [A(x), B]\Omega) d^n x = 0, \tag{56}$$

which is the same result as in the strictly local case.

C. The $(k \neq 0)$-modes

Up to now only the $(k = 0)$-modes of fluctuation operators, i.e., $\lim_V V^{-n/2} \cdot \int_V A(x) d^n x$, have been studied. For various reasons it is useful to have corresponding formulas at hand for fluctua-

tion observables containing a certain net-momentum. This problem was studied by Verbeure *et al.* in, e.g., Ref. 11 and the results were applied in, e.g., Ref. 12 in the analysis of *Goldstone modes*. In the original (real-space) approach the necessary calculations turned out to be quite involved and far from being simple. This is another case in point to demonstrate the merits of our Fourier space scaling methods.

Instead of the original scaling operators, A_V^F or A_R^F, we now study their $k\neq 0$-variants, $A_R^F(k)$. We begin with a technical lemma.

Lemma 3.8:

$$\hat{A}(k) := (2\pi)^{-n/2}\int e^{ikx}A(x)d^nx \tag{57}$$

is an operator-valued distribution. [We use the convention $\hat{f}(k)=(2\pi)^{-n/2}\int e^{-ikx}f(x)d^nx$.]

Remark: For a systematic use and proofs of such energy-momentum techniques in quantum statistical mechanics we refer to, e.g., Ref. 13, where also some more mathematical background is provided.

Integrating now over $e^{iqx}\cdot f_R(x)$, we get the q-mode fluctuation operators:

$$\begin{aligned} A_R^F(q) &:= R^{-n/2}\int A(x)e^{iqx}f_R(x)d^nx \\ &= R^{n/2}\int \hat{A}(k+q)\hat{f}(Rk)d^nk \\ &= R^{n/2}\int \hat{A}(k)\hat{f}(R(k-q))d^nk. \end{aligned} \tag{58}$$

We can now proceed in exactly the same way as above in the case of the zero-mode analysis and calculate the truncated l-point functions $\langle A_R^F(1,q_1)\cdots A_R^F(l,q_l)\rangle^T$ (where the indices 1 to l label different observables). The only thing that changes are the test functions, i.e., $f_R(x)\to e^{iq_kx}\cdot f_R(x)$. We arrive at the conclusion:

Theorem 3.9 (q-mode fluctuation operators): *In the case of L^1-clustering all truncated correlation functions vanish for $l\geqslant 3$ and the l-point functions are again sums of products of two-point functions. The concrete form of the limit-two-point functions is given in formula (62).*

If we calculate the limit-two-point functions explicitly, we get

$$\begin{aligned} \langle A_R^F(q_1)\cdot B_R^F(q_2)\rangle^T &= R^n\int \langle\hat{A}(k_1+q_1)\hat{B}(k_2+q_2)\rangle^T\cdot\delta(k_1+q_1+k_2+q_2)\cdot\hat{f}(Rk_1)\hat{f}(Rk_2)dk_1dk_2 \\ &= R^n\int \langle\hat{A}(k_1+q_1)\hat{B}(-(k_1+q_1))\rangle^T\cdot\hat{f}(Rk_1)\hat{f}(-R(k_1+q_1+q_2))dk_1 \\ &= R^n\int \langle\hat{A}(k)\hat{B}(-k)\rangle^T\cdot\hat{f}(R(k-q_1))\hat{f}(-R(k+q_2))dk. \end{aligned} \tag{59}$$

With $k' := R(k-q_1)$ we arrive at

$$\int \hat{W}^T(k'/R+q_1)\cdot\hat{f}(k')\hat{f}(-k'-R(q_1+q_2))dk'. \tag{60}$$

By assumption $\hat{W}^T$ is in L^1 and $\hat{f}$ is of rapid decrease, so the limit can again be carried out under the integral and we have the following observation.

Observation 3.10: For $q_1+q_2\neq 0$ it holds

$$\lim_R \langle A_R^F(q_1)\cdot B_R^F(q_2)\rangle^T = 0. \tag{61}$$

For $q=q_1=-q_2$ we get on the other side,

$$\lim_R \langle A_R^F(q)\cdot B_R^F(-q)\rangle^T = \hat{W}^T(q)\cdot \int \hat{f}(k)\hat{f}(-k)dk. \tag{62}$$

In other words, the limit tests the spectral momentum of the two-point function.

IV. THE CASE OF L^2-CLUSTERING

Before we embark on an investigation of the situation in the regime where phase transitions, vacuum degeneracy and/or spontaneous symmetry breaking (ssb) prevail, we briefly address the case where the clustering is weaker than L^1 but still L^2, say. Our above Fourier space approach can also easily handle this more singular situation. We hence assume now that the truncated l-point functions cluster only in the L^2-sense in the difference variables.

Now we cannot conclude that the Fourier transform is bounded and continuous, but we know it is again an L^2-function. We repeat the first steps of the above calculation with, however, another *scaling exponent*, α, which we leave open for the moment.

Definition 4.1: In the general case we define fluctuation operators by

$$A_R^F := R^{-\alpha}\cdot \int A(x) f_R(x) d^n x. \tag{63}$$

We get

$$\langle A_R^F(1)\cdots A_R^F(l)\rangle^T = \text{const}\cdot R^{l(n-\alpha)}\cdot \int \hat{f}(Rp_1)\cdots\hat{f}(-Rq_{l-1})\cdot \hat{W}^T(q_1,\ldots,q_{l-1})\prod dq_i, \tag{64}$$

where the $\{p_i\}$ are linear functions of the $\{q_i\}$ as described earlier. We now apply the Cauchy–Schwartz inequality:

$$|lhs| \leqslant \text{const}\cdot R^{l(n-\alpha)}\left[\int (\hat{f}(Rp_1)\cdots\hat{f}(-Rq_{l-1}))^2\prod dq_i\right]^{1/2} \cdot\left[\int (\hat{W}^T(q_1,\ldots,q_{l-1}))^2\prod dq_i\right]^{1/2}. \tag{65}$$

In the first integral on the rhs we make again a variable transformation from q_i to $q_i' := Rq_i$, yielding an overall scaling factor

$$R^{l(n-\alpha)}\cdot R^{-(l-1)n/2}. \tag{66}$$

We again want the limits of the two-point functions to be both finite and nontrivial, i.e., different from zero in general.

Proposition 4.2: To make the rhs of (65) finite in the limit for $l=2$ the maximal α to choose is

$$3n-4\alpha=0, \quad i.e., \quad \alpha=(\tfrac{3}{4})n. \tag{67}$$

For a general l this leads to the scaling exponent $(n-(\frac{1}{2})l\cdot n)/2$, which is negative for $l\geqslant 3$. Hence, all higher truncated l-point functions vanish in the limit.

However, to guarantee that the result is really nontrivial, we have to analyze the situation in more detail as the above estimate is only an inequality. In the case of L^1-clustering $\alpha=n/2$ was appropriate. The largest value which can occur in the L^2-case is the above maximal $\alpha=(\frac{3}{4})n$. If we want to avoid that the two-point functions vanish in the limit we have to choose in the L^2-case

$$(\tfrac{1}{2})n<\alpha\leqslant(\tfrac{3}{4})n \tag{68}$$

depending on the concrete decay of the two-point functions in configuration space. We see that, evidently, the situation is now less canonical as compared to the L^1-case.

Remark: A related situation (on a lattice) was analyzed by Verbeure *et al.* in Ref. 14, where a clustering weaker than L^1 was considered with, however, the additional input that the local algebras, sitting at the points of the lattice, form a finite dimensional *Lie algebra*. In that case, suitable scaling exponents are chosen to render the autocorrelation functions finite and nonvanishing, while, on the other side, the finiteness of the limit three-point functions has to be imposed as an extra assumption. Under this proviso one gets the existence of a limit Lie algebra, but nevertheless results are only partial while perhaps, on the other side, being also more interesting.

We do not want to dwell too much on this point at the moment, as progress seems to be, to a certain extent, model dependent. Furthermore, we develop a different approach in the last section which is able to cope with any kind of poor cluster behavior.

If we want to guarantee the *a priori* existence or vanishing of the truncated three-point functions with the help of our L^2-estimate (65), we have to restrict the chosen α in the following way.

Corollary 4.3: If the appropriate α fulfills $\alpha>(\frac{2}{3})n$, we get a negative scaling exponent for $l\geqslant 3$ as

$$n-(\tfrac{1}{3})ln\leqslant 0 \quad \text{for} \quad l\geqslant 3. \tag{69}$$

For $\alpha=\frac{2}{3}$ the three-point functions are finite.

Remark 4.4: One would get corresponding relations for smaller α but higher correlation functions, beginning from a certain order, $l_0(\alpha)$ say. On the other hand, one cannot guarantee the a priori existence of the l-point functions for $2<l<l_0(\alpha)$ as the general scaling relation reads for $l\geqslant l_0(\alpha)$

$$l(2\alpha-n)>n \quad and \quad \alpha>(1/2)n, \tag{70}$$

α being so chosen that the two-point functions are nontrivial.

V. SPONTANEOUS SYMMETRY BREAKING (SSB) AND THE GOLDSTONE PHENOMENON

A. General remarks

Before we study fluctuation operators in the regime of vacuum-, ground-, equilibrium-state degeneracy, we want to briefly comment, in order to set the stage, on the (rigorous) implementation of *ssb* in the various areas with particular emphasis on (quantum) statistical mechanics, i.e., condensed matter physics. As this topic has, however, been much discussed in the past from various points of view, we do not intend to give an exaustive commentary. We only mention some earlier work being of relevance for our argumentation and sketch the general framework.

We assume that our state, ω or Ω, is (non-)invariant under some automorphism group of $\mathcal{A}_0$ or $\mathcal{A}$. Furthermore, and this is important (while frequently not clearly stated), we assume the time evolution, α_t, to commute with the automorphism group, α_g.

Definition 5.1: α_g is called a symmetry group if

$$\alpha_g\cdot\alpha_t=\alpha_t\cdot\alpha_g. \tag{71}$$

Definition 5.2: If

$$(\Omega,\alpha_g(A)\Omega)=(\Omega,A\Omega) \tag{72}$$

for all $A\in\mathcal{A}$, the symmetry is called conserved and can be implemented by a unitary group of operators in the representation space

$$\alpha_g(A)\to U(g)AU(g^{-1}). \tag{73}$$

On the other side, if

$$(\Omega,\alpha_g(A)\Omega)\neq(\Omega,A\Omega) \tag{74}$$

for some A, A the symmetry-breaking observable, *the symmetry is called* spontaneously broken *since it still commutes with the time evolution (i.e., formally: with the Hamiltonian, modulo* boundary terms *due to* long-range correlations).

In most cases the (continuous) symmetry group derives from a clearly identifiable *generator* (we restrict ourselves, for convenience, to one-parameter groups) which is built from a local operator density, i.e.,

$$U(s)=e^{isQ},\quad Q(t)=\int q(x,t)d^nx,\quad Q(t)=Q(0)\coloneqq Q. \tag{75}$$

Note that there are many technical subtleties lurking behind these operator identities, all of which we cannot mention in the following. [For more details and references see, e.g., Ref. 15. A nice review is Ref. 16, where many of the widely scattered results have been compiled.]

Remark 5.3: In many situations the generator density is the zero-component of a conserved current. Formally, the conservation law encodes the time independence of the global charge, Q. Furthermore, for convenience, we assume the symmetry to commute with the space translations, i.e., $U(x)QU(-x)=Q$. This is, in fact, frequently the case and simplifies certain calculations.

The most crucial consequence is that in case the symmetry is spontaneously broken, some of the above relations do only hold in a formal or algebraic sense. More specifically, we have the following theorem.

Theorem 5.4: *If α_g is spontaneously broken, the global generator Q does only exist in a formal sense as a limit*

$$Q=\lim_V Q_V,\quad Q_V\coloneqq\int_V q(x)d^nx. \tag{76}$$

We have

$$ssb\Leftrightarrow\lim_V(\Omega,[Q_V,A]\Omega)\neq 0 \tag{77}$$

for some $A\in\mathcal{A}$ and Q is in that case only definable as a nasty operator (see below).

In the following we will take (77) as the defining relation of *ssb* (the technical details of the various statements can be found in the literature, mentioned above).

The notion of *ssb* is closely connected with another phenomenon, the so-called *Goldstone-phenomenon*. While there exists a clear picture in, say, *relativistic quantum field theory*, the corresponding picture is a little bit blurred in the nonrelativistic regime. In the relativistic context we have sharp *zero-mass Goldstone modes*, i.e., true particles due to relativistic covariance. On the other hand, in, e.g., condensed matter physics or statistical mechanics, the situation is less generic. In general we no longer have sharp excitation modes; we have rather to expect excitation modes having a *finite lifetime* for momentum different from zero but becoming infinitely sharply peaked for momentum $k\to 0$. The proper view is to analyze these excitation branches in the *full* Fourier space of *energy-momentum* as has, e.g., been done in Ref. 15(d) and earlier in the author's doctoral thesis, the principal object being the spectral-resolution of the two-point correlation functions [in a neighborhood of $(E,k)=(0,0)$]. The *ssb* or Goldstone phenomenon manifests itself in this quantity by a singular contribution in the spectral measure. One should mention at this place the

work of Bros and Buchholz (see, e.g., Ref. 17) about quantum field theory in temperature (i.e., KMS-) states. In this particlar context the residual causality and locality properties of the underlying relativistic theory lead to a, in some respects, more generic behavior as compared to the ordinary nonrelativistic condensed matter regime.

In the nonrelativistic regime it turns out that the concrete structure of the Goldstone mode depends usually on the details of the microscopic interactions (that means both the so-called energy-momentum dispersion law which can be, to give an example, quadratic or linear near $k=0$ in the case of magnons or phonons, say, and the k-dependent width of the branch). This led to the desire to characterize the presence of a Goldstone phenomenon by a simple (if qualitative) property. Sometimes one finds in the literature the saying that the Goldstone phenomenon consists of the vanishing of a *mass-gap* above the ground state. But this statement is in some sense frequently empty. From Ref. 18 we know, e.g., that a *short-ranged Galilei-covariant* theory, with a nonvanishing particle density, cannot have a mass-gap due to *phonon-excitations* which signal the trivial breaking of the Galilei-boosts. Furthermore, in most cases KMS–Hamiltonians have as spectrum the whole real line.

Remark 5.5: Models like the famous BCS-model (having a gap) are no case in point as they are implicitly breaking Galilei-invariance as do all such mean-field-models. This becomes apparent when analyzing the interaction part of the corresponding Hamiltonian. The complete fermion- or boson-liquid is, on the other side, again Galilei-invariant, hence has no mass-gap, but may, of course, still display, e.g., superfluidity.

In the next subsection we will provide a, as we think, more satisfying and completely general characterization of the Goldstone phenomenon which is independent of the details of the model under discussion.

B. Some rigorous results for the symmetry generator in the presence of *ssb*

After the above introductory remarks we want to prove a couple of rigorous results which characterize to some extent the presence of *ssb* in the (non-)relativistic regime. The main observation is that the symmetry generator is no longer defined as a nice operator in the representation (Hilbert or *GNS*-) space when *ssb* is present and that this, at first glance, mathematical result encodes some interesting physics.

Let us work, for simplicity, in the context of *temperature states*. This has the advantage that Ω is separating, i.e.,

$$A\Omega = B\Omega \Rightarrow A = B. \tag{78}$$

The first task is to give $Q := \lim_V Q_V$ a rigorous meaning. The standard procedure (see the above mentioned literature) is to define Q via

$$QA\Omega := \lim_V [Q_V, A]\Omega, \quad Q\Omega := 0, \tag{79}$$

for, e.g., $A \in \mathcal{A}_0$. For V sufficiently large, the commutator on the rhs becomes independent of V, hence there is a chance to get a well-defined Q (at least on a dense set of vectors), as on the lhs we have by *separability*

$$A\Omega = B\Omega \Rightarrow A = B \Rightarrow [Q_V, A-B] = 0. \tag{80}$$

For $A \in \mathcal{A}$ one has to employ cluster properties.

Observation 5.6: We have already seen above that, while such a Q may exist, the corresponding $\|Q_V\Omega\|$ *will nevertheless diverge for* $V \to \mathbb{R}^n$*! This shows that the connection between the global generator and its local approximations is not that simple. The best one can usually expect, even in the case of symmetry conservation, is a weak convergence on a dense set*

$$(B\Omega, QA\Omega) = \lim_V (B\Omega, Q_V\Omega), \tag{81}$$

but, due to the above divergence of $\|Q_V\Omega\|$*, we cannot even have weak convergence on the full Hilbert space. (For more details, see the above cited literature, in particular Ref. 15(c), where the various possibilities in the respective fields have been compared.)*

We see from the above that Q can be defined as a densely defined operator but usually we want to have more. A conserved continuous symmetry is given by a s.a. generator. Let us see under what conditions the above Q is at least *symmetric* provided that the Q_V are symmetric. We assume the symmetry to be conserved, i.e.,

$$\lim_V (\Omega, [Q_V, A]\Omega) = 0 \quad \text{for all} \quad A \in \mathcal{A}. \tag{82}$$

We then have

$$(B\Omega, QA\Omega) = \lim_V (B\Omega, [Q_V, A]\Omega) = \lim_V (([Q_V, B]\Omega, A\Omega) + (Q_v\Omega, B^*A\Omega) - (A^*B\Omega, Q_V\Omega)). \tag{83}$$

Conclusion 5.7: Q *is symmetric if* $\lim_V (A\Omega, Q_V\Omega) = 0$ *for all* $A \in \mathcal{A}_0$*. Under the same proviso it follows*

$$(B\Omega, QA\Omega) = \lim_V (B\Omega, Q_V\Omega). \tag{84}$$

What is the situation if the symmetry is spontaneously broken? For convenience we replace again the sharp volume-integration by our smooth one, i.e.,

$$Q_V \to Q_R := \int q(x) f_R(x) d^n x. \tag{85}$$

We know that there exists a symmetry-breaking observable A s.t.

$$\lim_R (\Omega, [Q_R, A]\Omega) \neq 0 \Rightarrow QA\Omega = \lim_R [Q_R, A]\Omega \neq 0. \tag{86}$$

Due to the assumed translation invariance, i.e.,

$$U(a)QU(-a) = Q \quad \text{or, what is the same,} \quad U(a)q(x)U(-a) = q(x+a), \tag{87}$$

we have

$$(\Omega, QA\Omega) = (\Omega, Q \cdot V^{-1} A_V \Omega) \tag{88}$$

and

$$Q \cdot V^{-1} A_V \Omega = V^{-1} \int_V U(x) d^n x \cdot QA\Omega, \tag{89}$$

where $U(x)$ is the unitary representation of the translations.

Remark: As a result of a discussion with Detlev Buchholz, following a seminar talk about the article, we will give a technically more detailed proof of the above statement in the Appendix at the end of the article. This seems to be advisable since, as we are showing below, the global operator, Q, turns out to be nonclosable, which will make certain limit manipulations more cumbersome.

Lemma 5.8:

$$s-\lim_V V^{-1}\int_V U(x)d^nx=P_\Omega, \tag{90}$$

P_Ω the projector on the (in our case) unique vacuum-,ground-, equilibrium-state.

Proof: The result is well-known (see, e.g., Ref. 1). We give however a very short and slightly different proof using our smooth volume integration. With $V_R:=\int f_R(x)d^nx$, a *spectral resolution* yields

$$V_R^{-1}\cdot\int U(x)f_R(x)d^nx=\text{const}\cdot\left(\int f(x)d^nx\right)^{-1}\cdot\int\hat{f}(Rp)dE_p\,. \tag{91}$$

Applied to a vector ψ we can now employ Lebesgue's theorem of dominated convergence and get

$$\lim_V V^{-1}\int U(x)d^nx\cdot\psi=(\hat{f}(0))^{-1}\cdot\hat{f}(0)P_\Omega\psi=P_\Omega\psi. \tag{92}$$

□

This yields

$$0\neq P_\Omega QA\Omega=\lim_V Q\cdot V^{-1}A_V\Omega. \tag{93}$$

On the other hand,

$$\lim_V\|V^{-1}A_V\Omega\|=\|P_\Omega A\Omega\|=0 \tag{94}$$

by an analogous reasoning [note that we assumed $(\Omega,A\Omega)=0$].

We have now a sequence of vectors, $V^{-1}A_V\Omega$, converging to zero in norm while $Q\cdot V^{-1}A_V\Omega$ converges to $P_\Omega QA\Omega\neq 0$. Summing up what we have shown we arrive at the following conclusion:

Conclusion 5.9 (Goldstone theorem): If we have ssb and a separating vector, Ω (representing the ground or temperature state), Q can still be defined as an operator which is, however, not closable, hence, a fortiori, not symmetric (note that symmetric operators are closable). This abstract result has as a practical consequence the physical property exhibited in the preceding formulas. They express the content of the Goldstone phenomenon in the most general and model-independent way. We infer that Q induces transitions from a singular part of the continuous spectrum, passing through $(E,p)=(0,0)$, to the extremal invariant state Ω. On the other side, a conserved symmetry implies

$$Q\Omega=0,\quad P_\Omega[Q,A]\Omega=0\Rightarrow P_\Omega QA\Omega=0. \tag{95}$$

We show now that the above result really contains the original Goldstone phenomenon. Let us, e.g., assume that we have the above result and, on the other side, a gap in the energy spectrum above the state Ω. We emphasized above that an important ingredient of the notion of *ssb* is the time independence of, say, the above expression. We employ again the spectral resolution of operators with respect to energy-momentum. We hence have

$$0\neq c=P_\Omega Q\int\hat{A}(k,E)e^{-itE}dkdE\Omega \tag{96}$$

with c being independent of t. We choose a real testfunction $g(t)$ with $\int g(t)dt=1$. This yields

$$0\neq c=P_\Omega Q\int A(t)\cdot g(t)dt\Omega=P_\Omega Q\int\hat{A}(E)\hat{g}(E)dE\Omega. \tag{97}$$

If there is a gap above zero, we may choose the support of $\hat{g}$ so that

$$\mathrm{supp}(\hat{g}) \cap \mathrm{supp}(\mathrm{spec}(H)) = 0. \tag{98}$$

Since, by assumption, P_Ω has been extracted in the energy support of A, we get the result $c = 0$, that is, no symmetry breaking. But we can infer more about the nature of the energy-momentum spectrum near (0,0). We see that $P_\Omega QA(g(t))\Omega$ depends only on the value of $\hat{g}(E)$ in $E = 0$, which is one in our case, but not on the shape of g. Inspecting Eq. (93) we can infer the following: The Fourier transform of the rhs contracts around $k = 0$ in the limit $V \to \infty$. On the other side we learned that in the limit both sides have their energy support concentrated in $E = 0$. The lhs shows that the limit vector is parallel to Ω. Whereas we do not want to go into the partly intricate details of the limiting processes of *nonclosable operators* (note that it is, e.g., dangerous to use the adjoint, Q^*, in the reasoning as it is not densely defined), the latter part of the above theorem should now be obvious.

This sharp excitation around $(E,k) = (0,0)$ extends into the full energy-momentum plane in form of a (usually) smeared excitation branch (having a finite k-dependent life-time). For the regime of temperature states the situation was analyzed in some detail in Ref. 15(d) and already in the authors doctoral thesis. We see from the above that a similar situation prevails in the more general case of a separable Ω and, analogously, for ground-state models where Q can be defined in the above way. Even if the above Q is not definable as a nonclosable limit operator we arrive at a similar result by exploiting the limit-expectation values instead of the strong vector- or operator limits, but we do not want to dwell more into the corresponding details in this article which deals with a different topic.

VI. THE CANONICAL (GOLDSTONE) PAIR IN THE PRESENCE OF *ssb*

As far as we can see, the notion of a *canonical Goldstone pair* was introduced by Verbeure *et al.* in Ref. 12. In the following section we want to prove only a few general (model-independent) results, whereas much more could be shown by combining the framework, developed above, with the techniques mentioned in the preceding section.

We remarked above that *ssb* is characterized by the nonvanishing (but time-independence) of the following commutator limit:

$$0 \neq c = \lim_V (\Omega, [Q_V, A(t)]\Omega). \tag{99}$$

To fix the notation: usually a pure phase is characterized by the nonvanishing of a so-called *order parameter* in the presence of *ssb*. This is an observable, B say, with

$$(\Omega, B\Omega) = \begin{cases} c \neq 0 & \text{in the broken phase,} \\ 0 & \text{in the conserved phase (above } T_c\text{, say).} \end{cases} \tag{100}$$

From (99) we see that as order parameter we have to choose

$$B := \lim_V [Q_V, A], \tag{101}$$

while A is the symmetry breaking observable.

Example 6.1: In the Heisenberg ferromagnet with spontaneous magnetization in, say, the z-direction, the order parameter is S_z or $\langle S_z \rangle$. As generator of the broken symmetry one may take ΣS_x and as symmetry breaking observable, e.g., S_y.

We have seen that we can write

$$0 \neq c = \lim_V (\Omega, [Q_V, A]\Omega) = \lim_V (\Omega, [Q_V, V^{-1}A_V]\Omega) = \lim_R (\Omega, [Q_R, V_R^{-1}A_R]\Omega), \tag{102}$$

where

$$Q_R := \int q(x) f_R(x) d^n x, \quad A_R := \int_{S_R} A(x) d^n x \tag{103}$$

with V_R the volume of the sphere, S_R, with radius R.

We can now split the scaling exponent among the two observables (the volume of the unit sphere being absorbed in the constant):

$$0 \neq \text{const} = \lim_R (\Omega, [R^{-\alpha} Q_R, R^{-(n-\alpha)} A_R] \Omega). \tag{104}$$

This form of scaling may yield something reasonable if the scaling exponents can be so adjusted that also

$$(\Omega, R^{-\alpha} Q_R R^{-\alpha} Q \Omega) \text{ and } (\Omega, R^{-(n-\alpha)} A R^{-(n-\alpha)} A \Omega) \tag{105}$$

remain finite in this limit.

In general it does not seem to be easy to get both rigorous and general estimates on the scaling behavior of these quantities. Fortunately, in the case of temperature (KMS) states, such estimates are available. In Refs. 19–21 the following special (*real-space-*) version of the *Bogoliubov inequality* has been proved and employed for the observables Q_R and $V_R^{-1} A_R$:

$$|\langle [Q_R, V_R^{-1} A_R] \rangle|^2 \leqslant \langle V_R^{-1} A_R V_R^{-1} A_R \rangle \cdot \langle [Q_R, [Q_R, H]] \rangle. \tag{106}$$

The delicate term is the double commutator on the rhs. If Q is spontaneously broken, boundary terms will survive in the commutator of Q_R and the Hamiltonian, H, when taking the limit $R \to \infty$, while in a formal sense they commute. The double commutator saves us two powers of R, so to say. That is we arrive after some cumbersome manipulations at

$$\langle [Q_R, [Q_R, H]] \rangle \sim R^{(n-2)} \text{ for } R \to \infty, \tag{107}$$

hence

$$\langle V_R^{-1} A_R V_R^{-1} A_R \rangle \gtrsim R^{(2-n)} \text{ for } R \to \infty \tag{108}$$

as the limit on the lhs is a constant different from zero in the case of ssb.

Theorem 6.2: *For temperature states we have for the symmetry-breaking observable*

$$\langle A_R A_R \rangle \gtrsim R^{(n+2)}. \tag{109}$$

That is, compared with the ordinary, normal scaling behavior ($\sim R^n$), *the divergence is worse. From this one infers the following decay of the two-point correlation function itself:*

$$|\langle A(x) A \rangle| \gtrsim R^{(n-2)}. \tag{110}$$

Putting all the pieces together we now have to make the following identification:

$$n - \alpha \geqslant (n+2)/2 \Rightarrow \alpha \leqslant (n-2)/2 \tag{111}$$

in order that the limit commutator is nontrivial, i.e., nonclassical. On the other hand, the divergence behavior of $\langle Q_R Q_R \rangle$ can frequently be inferred either from covariance properties [as in relativistic quantum field theory; see, e.g., Ref. 6(c)] or from an analysis of the spectral behavior in concrete (nonrelativistic) models. Summing up we have the following.

Conclusion 6.3 (canonical pair): For a covariant four-current in relativistic quantum field theory the two-point function in Fourier space contains a prefactor $\sim p^2$ *which yields (after some*

calculations) an $\alpha=\frac{1}{2}$ (for space dimension, $n=3$). On the other side, if we do not have such nice covariance properties, the divergence of $\langle Q_R Q_R\rangle$ is generically much worse than $\sim R$ (in three dimensions). This holds, in particular, for the above temperature states. It follows that for temperature states we cannot find a critical exponent α so that both the autocorrelations remain finite in the limit and the commutator nontrivial. That is, for temperature states the limit fluctuations are classical (an observation already made by Verbeure et al. for special models, see, e.g., Ref. 12).

The situation seems to be less generic for ground state models, i.e., the temperature-zero case. For one, we do not automatically have an *a priori* estimate as in the above conclusion, from which we can infer that it is the autocorrelation of A_R which is ill-behaved. For another, in temperature states, as was shown in, e.g., Ref. 15(d) by the author, the spectral weight has to become infinite along the Goldstone excitation branch in a specific way (which is governed by the dispersion law of the Goldstone mode) for energy-momentum approaching zero. This sort of singularity is mainly responsible for the poor decay of the respective autocorrelation function. This phenomenon may be absent in the case of ground states as has also been shown for certain Bose-gas models in Ref. 12, where some of these questions have been dealt with in greater detail. Note in particular that a variety of aspects may depend on the precise shape of the Goldstone mode near energy-momentum equal to (0,0) as was shown in the above mentioned paper of the author or in the unpublished doctoral thesis.

On the other side, there has been some interesting work of Pitaevskii and Stringari (see, e.g., Ref. 22), who showed that variants of the *uncertainty principle* may lead to nontrivial results in certain cases for ground state systems if one can exploit and control certain additional *sum rules*.

Remark 6.4: Note that the ordinary uncertainty principle (for, e.g., Hermitian operators and ignoring possible domain questions) reads

$$\tfrac{1}{4}\cdot|\langle[A,B]\rangle|^2\leqslant\langle AA\rangle\cdot\langle BB\rangle. \tag{112}$$

One sees that instead of the double commutator of the local symmetry generator and the Hamiltonian now a term like $\langle Q_R Q_R\rangle$ occurs. While we have an *a priori* estimate of the large-R behavior of the double commutator, the behavior of $\langle Q_R Q_R\rangle$ is probably less generic (in particular in the ground state situation) and we need some extra information of the kind mentioned above.

VII. THE CASE OF ssb OR VERY POOR DECAY OF CORRELATIONS

In the preceding sections we studied the case of L^1- or L^2-clustering. In this last section we want to briefly show how we can proceed in the case of extremely poor clustering. We want, however, for the sake of brevity and in order to better illustrate the method, to concentrate on the simpler case of a uniformly poor decay of all the correlation functions we are discussing. This is of course not always the case but the scheme can be easily generalized (we discuss this topic in more detail in Ref. 23, where we treat this question in the context of the renormalization group analysis).

We hence assume that the truncated l-point functions cluster weaker than L^2 or L^1, say, in the difference variables, $y_i:=x_{i+1}-x_i$ (see Sec. III A). The following reasoning works both in the case of non-L^1 or non-L^2 clustering. In the latter case one would again use the *Cauchy–Schwarz inequality* (as in Sec. III B). To illustrate the method we choose the non-L^1 procedure.

So let us assume

$$W^T(y_1,\ldots,y_{l-1})\notin L^1. \tag{113}$$

For each l we assume the existence of a weight factor with a suitable exponent, $\alpha_l\in\mathbb{R}$:

$$P_l(y):=\left(1+\sum y_i^2\right)^{\alpha_l/2}, \tag{114}$$

so that

$$F(y) := P_l(y)^{-1} \cdot W^T(y) \in L^1 \quad \text{for} \quad \alpha_l > \alpha_l^{\inf}. \tag{115}$$

On the other side, we define the fluctuation operators with the exponent γ, which will be adjusted later:

$$A_R^F := R^{-\gamma} \cdot A_R \,. \tag{116}$$

It follows

$$W^T(y) = P_l(y) \cdot F(y) \tag{117}$$

with $F(y)$ an (in general, l-dependent) L^1-function.

For the limit correlation functions we then get

$$\langle A_R^F(1) \cdots A_R^F(l) \rangle^T = R^{ln} \cdot R^{-l\gamma} \cdot \int \hat{F}(q) \cdot \hat{P}_l(q) [\hat{f}(Rp_1) \cdots \hat{f}(-Rq_{l-1})] \prod \, dq_i \tag{118}$$

(cf. Sec. III A).

Remark 7.1: We write the Fourier transform of $P_l(y)$ formally as

$$\hat{P}_l(q) = \left(1 + \sum \, D_{q_i}^2 \right)^{\alpha_l/2} \tag{119}$$

(with D_{q_i} the partial derivatives). For noninteger $\alpha_l/2$ this is a pseudo-differential operator. At the moment, for the sake of brevity, we do not want to say more about the corresponding mathematical framework (see Ref. 23 for a complete discussion). What we in fact only need are the scaling properties of the expression. If one wants to be careful, one may equally well take the explicit expression for the Fourier transform of the above polynomial in the y-coordinates applied to the product of the f_R's and exploit its scaling properties.

In any case, we get (with this proviso) and the usual variable transformation $p_i' := Rp_i$:

$$\langle A_R^F(1) \cdots A_R^F(l) \rangle^T = R^{ln - l\gamma - (l-1)n + \alpha_l} \cdot \int \hat{F}(q'/R) \cdot \left(R^{-2} + \sum \, D_{q_i'}^2 \right)^{\alpha_l/2}$$

$$\times [\hat{f}(p_1') \cdots \hat{f}(-q_{l-1}')] \prod \, dq_i' \,. \tag{120}$$

Again only the explicit scaling prefactor matters in the limit $R \to \infty$. [Note that for nonminimal α_l we may have $\hat{F}(0) = 0$. Technical intricacies like this one will be discussed at length in Ref. 23.] To get a finite result for *all* correlation functions we have to adjust the scaling parameter, γ, so that the exponents vanish or are negative. We choose α_2 for $l = 2$ so that the limit two-point function is finite and nonvanishing, that is,

$$n - 2\gamma + \alpha_2 = 0 \to \gamma = (n + \alpha_2)/2. \tag{121}$$

Inserting this γ in the general expression for $l \geqslant 3$, we conclude that the scaling prefactor is finite in the limit provided that

$$\alpha_l \leqslant l\gamma - n = ((l-1)n + l\alpha_2)/2 \tag{122}$$

with γ fixed by the two-point function. For $\alpha_l < l\gamma - n$ we can even conclude that all(!) higher limit correlation functions vanish and that the resulting theory is (quasi-)free. The latter would, for example, be the case if

$$\alpha_l \leqslant (l-1) \cdot \alpha_2 \tag{123}$$

holds, since we then have (with $\alpha_2<n$)

$$\alpha_l \leqslant (l-1)\cdot\alpha_2 < (l-\tfrac{1}{2})\alpha_2 = (2l-1)\cdot\alpha_2/2 < ((l-1)n+l\alpha_2)/2, \tag{124}$$

but nothing can be concluded in general for, say, $\alpha_l = l\cdot\alpha_2$.

We see that it is of tantamount importance to better understand the assymptotic behavior of truncated l-point functions and, in particular, the rate of decay as a function of l. We address this topic in more detail in Ref. 23.

APPENDIX: NONCLOSABLE SYMMETRY GENERATORS

The rigorous implementation of the formula

$$U(a)q(x)U(-a) = q(x+a) \tag{A1}$$

is

$$\begin{aligned} U(a)Q_R U(-a) &= U(a)\int q(x) f_R(x) d^n x U(-a) \\ &= \int q(x+a) f_R(x) d^n x \\ &= \int q(y) f_R(y-a) d^n y =: Q_R(a). \end{aligned} \tag{A2}$$

The first question is: how does the global Q behave under translations? To answer this question we have to take recourse to the definition of the global Q as a limit of local operations. We have

$$U(a)QA\Omega = U(a)\lim_R [Q_R, A]\Omega = \lim_R [Q_R(a), A(a)]\Omega \tag{A3}$$

since it holds

$$\lim_n U(a)\psi_n = U(a)\lim_n \psi_n \tag{A4}$$

as $U(a)$ is bounded. If A is local, we have for sufficiently large R (and hence, in the limit)

$$\lim_R [(Q_R(a) - Q_R(0)), A(a)] = 0. \tag{A5}$$

We hence arive at

$$U(a)QA\Omega = \lim_R [Q_R, A(a)]\Omega = QA(a)\Omega = QU(a)A\Omega. \tag{A6}$$

Lemma 7.2: On the dense set $\mathcal{A}_0\Omega$, Q commutes with the translations.

In a next step we have to analyze the action of Q on integrals or averages like $\int_V U(x)AU(-x)d^n x\Omega$. More specifically, we want to show that Q commutes, so to speak, with the operation of *integration*. We have

$$Q\cdot\int_V A(x)d^n x\Omega := \lim_R \left[Q_R, \int_V A(x) d^n x \right]\Omega. \tag{A7}$$

We approximate the integral by a sum, that is

$$\int_V A(x)d^n x\psi := \lim_i \sum_i d^n x_i \cdot A(x_i)\psi, \tag{A8}$$

and get (as the Q_R are assumed to be nice, that is, closed operators)

$$\left[Q_R, \int_V A(x)d^n x\right]\Omega = \lim_i \left[Q_R, \sum_i d^n x_i \cdot A(x_i)\right]\Omega = \lim_i \sum_i d^n x_i \cdot U(x_i)[Q_R(-x_i), A]\Omega. \tag{A9}$$

We again choose R so large that

$$[Q_R(-x), A] = [Q_R, A] \quad \text{for all } x \in V, \tag{A10}$$

which leads to

$$\left[Q_R, \int_V A(x)d^n x\right]\Omega = \lim_i \sum_i d^n x_i \cdot U(x_i)[Q_R, A]\Omega = \int_V U(x)d^n x \cdot [Q_R, A]\Omega. \tag{A11}$$

Taking now the limit $R \to \infty$, we get obtain the following lemma.

Lemma 7.3:

$$Q\int_V A(x)d^n x\Omega = \int_V U(x)d^n x \cdot QA\Omega. \tag{A12}$$

This shows, that our manipulations can be justified.

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Dynamical body frames, orientation-shape variables and canonical spin bases for the nonrelativistic *N*-body problem

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After the separation of the center-of-mass motion, a new privileged class of canonical Darboux bases is proposed for the nonrelativistic N-body problem by exploiting a geometrical and group theoretical approach to the definition of *body frame* for deformable bodies. This basis is adapted to the rotation group SO(3), whose canonical realization is associated with a symmetry Hamiltonian *left action*. The analysis of the SO(3) coadjoint orbits contained in the N-body phase space implies the existence of a *spin frame* for the N-body system. Then, the existence of appropriate nonsymmetry Hamiltonian *right actions* for nonrigid systems leads to the construction of an N-dependent discrete number of *dynamical body frames* for the N-body system, hence to the associated notions of *dynamical* and *measurable* orientation and shape variables, angular velocity, rotational and vibrational configurations. For $N=3$ the dynamical body frame turns out to be unique and our approach reproduces the *xxzz gauge* of the gauge theory associated with the *orientation-shape* SO(3) principal bundle approach of Littlejohn and Reinsch. For $N\geqslant 4$ our description is different, since the dynamical body frames turn out to be *momentum dependent*. The resulting Darboux bases for $N\geqslant 4$ are connected to the coupling of the *spins* of particle clusters rather than the coupling of the *centers of mass* (based on Jacobi relative normal coordinates). One of the advantages of the spin coupling is that, unlike the center-of-mass coupling, it admits a relativistic generalization. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In this paper we deal with the construction of a specialized system of coordinates for the nonrelativistic N-body problem which could be instrumental to nuclear, atomic and molecular physics, as well as to celestial mechanics. In particular, we shall exploit the technique of the canonical realizations of Lie symmetry groups[1–5] within the framework of the nonrelativistic version of the *rest-frame Wigner covariant instant form* of dynamics[6,7] to the effect of obtaining coordinates adapted (locally in general) to the SO(3) group. In most of the paper we consider only free particles, since the mutual interactions are irrelevant to the definition of the kinematics.

Isolated systems of N particles possess $3N$ degrees of freedom in configuration space and $6N$

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in phase space. The Abelian nature of the overall translational invariance, with its associated three commuting Noether constants of motion, allows for the decoupling and, therefore, for the elimination of either three configurational variables or three pairs of canonical variables, respectively (separation of the center-of-mass motion). In this way one is left with either $3N$-3 relative coordinates $\vec{\rho}_a$ or $6N$-6 relative phase space variables $\vec{\rho}_a$, $\vec{\pi}_a$, $a=1,...,N-1$ and the center-of-mass angular momentum or spin is $\vec{S}=\Sigma_{a=1}^{N-1}\vec{\rho}_a\times\vec{\pi}_a$. In the nonrelativistic theory most of the calculations employ the sets of $3N-3$ *Jacobi normal relative coordinates* $\vec{s}_a$ which diagonalize the quadratic form associated with the relative kinetic energy (the spin becomes $\vec{S}=\Sigma_{a=1}^{N-1}\vec{s}_a\times\vec{\pi}_{sa}$, with $\vec{\pi}_{sa}$ momenta conjugated to the $\vec{s}_a$'s). Each set of relative Jacobi normal coordinates $\vec{s}_a$, $a=1,...,N-1$, is associated with a *different clustering* of the N particles, corresponding to the centers of mass of the various subclusters. In special relativity Jacobi normal coordinates do not exist, as it will be shown in Ref. 8, and a different strategy must be used.

On the other hand, the non-Abelian nature of the overall rotational invariance entails the impossibility of an analogous intrinsic separation of *rotational* (or *orientational*) configurational variables from others which could be called *shape* or *vibrational*. As a matter of fact, this is one of the main concerns of molecular physics and of advanced mechanics of deformable bodies. Recently, a new approach inspired by the geometrical techniques of fiber bundles has been proposed in these fields of research: a self-contained and comprehensive exposition of this viewpoint and a rich bibliography can be found in Ref. 9.

In the theory of deformable bodies one loses any intrinsic notion of *body frame*, which is a fundamental tool for the description of rigid bodies and their associated Euler equations. *A priori*, for a given configuration of a nonrelativistic continuous body, and in particular for an N-body system, any barycentric orthogonal frame could be named *body frame* of the system with its associated notion of *vibrations*.

This state of affairs suggested[9] replacing the kinematically accessible region of the nonsingular configurations[10] in the $(3N\text{-}3)$-dimensional relative configuration space by a SO(3) principal fiber bundle over a $(3N\text{-}6)$-dimensional base manifold, called *shape* space. The SO(3) fiber on each shape configuration carries the *orientational* variables (e.g., the usual Euler angles) referred to the chosen *body frame*. A local cross section of the principal fiber bundle selects just one orientation of a generic N-body configuration in each fiber [SO(3) orbit] and this is equivalent to a *gauge convention*, namely to a possible definition of a *body frame* (*reference orientation*), to be adopted after a preliminary choice of the *shape* variables. It turns out that this principal bundle is trivial only for $N=3$, so that in this case global cross sections exist, and in particular the identity cross section may be identified with the *space frame*. Any global cross section is a copy of the 3-body shape space and its coordinatization gives a description of the *internal vibrational* motions associated with the chosen gauge convention for the reference orientation. For $N\geqslant 4$, however, global cross sections do not exist[11] and the definition of the reference orientation (*body frame*) can be given only locally. This means that the shape space cannot be identified with a $(3N\text{-}6)$-dimensional submanifold of the $(3N\text{-}3)$-dimensional relative configuration space. The *gauge convention* about the reference orientation and the consequent individuation of the internal *vibrational degrees of freedom* requires the choice of a connection Γ on the SO(3) principal bundle (i.e., a concept of *horizontality*) and this leads in turn to the introduction of a SO(3) gauge potential on the base manifold. In this way a natural gauge invariant concept of *purely rotational* N-body configurations exists (*vertical* velocity vector field, i.e., null shape velocities). Of course a gauge fixing is needed in order to select a particular Γ-horizontal cross section and the correlated gauge potential on the shape space. Obviously, physical quantities like the rotational or vibrational kinetic energies and, in general, any observable feature of the system must be gauge invariant. Note instead that both the space frame and the body frame components of the angular velocity are gauge quantities in the *orientation-shape bundle* approach and their definition depends upon the gauge convention. See Ref. 9 for a review of the gauge fixings used in molecular physics literature and, in particular, for the virtues of a special connection C corresponding to the shape configurations with vanishing center-of-mass angular momentum $\vec{S}$. The C-horizontal cross sections are

orthogonal to the fibers with respect to the Riemannian metric dictated by the kinetic energy.

This *orientation-shape* approach replaces the usual Euler kinematics of rigid bodies and entails in general a coupling between the internal *shape* variables and some of the *orientational* degrees of freedom. In Ref. 9 it is interestingly shown that the nontriviality of the SO(3) principal bundle, when extended to continuous deformable bodies, is at the heart of the explanation of problems like the *falling cat* and the *diver*. A characteristic role of SO(3) gauge potentials in this case is to *generate rotations by changing the shape*.

In Ref. 9 the Hamiltonian formulation of this framework is also given, but no explicit procedure for the construction of a canonical Darboux basis for the orientational and shape variables is worked out. See Refs. 9, 12 for the existing sets of shape variables for $N=3,4$ and for the determination of their physical domain.

Independent of this SO(3) principal bundle framework and having in mind the relativistic N-body problem where only Hamiltonian methods are available, we have been induced to search for a *constructive procedure* for building canonical Darboux bases in the $(6N\text{-}6)$-dimensional relative phase space, suited to the non-Abelian canonical reduction of the overall rotational symmetry. Our procedure surfaced from the following independent pieces of information.

(A) In recent years a systematic study of relativistic kinematics of the N-body problem, in the framework of the *rest-frame Wigner covariant instant form of dynamics* has been developed in Ref. 13 and then applied to the isolated system composed by N scalar charged particles plus the electromagnetic field.[14,15]

These papers contain the construction of a special class of canonical transformations, of the Shanmugadhasan type.[16,6] Such transformations are simultaneously adapted to the following: (i) the Dirac first class constraints appearing in the Hamiltonian formulation of relativistic models; (ii) the timelike Poincaré orbits associated with most of their configurations. In the Darboux bases one of the final canonical variables is the square root of the Poincaré invariant P^2 (P_μ is the conserved time-like four-momentum of the isolated system). Subsequently, by using the constructive theory of the canonical realizations of Lie groups[1–5] a new family of canonical transformations was introduced in Ref. 17. This latter leads to the definition of the so-called *canonical spin bases*, in which also the Pauli–Lubanski Poincaré invariant $W^2=-P^2\vec{S}_T^2$ for time-like Poincaré orbits[18] becomes one of the final canonical variables. The construction of the spin bases exploits the clustering of spins rather than the Jacobi clustering of centers of mass.

In spite of its genesis in a relativistic context, the technique used in the determination of the spin bases, related to a *typical form*[1] of the canonical realizations of the $E(3)$ group, can be easily adapted to the nonrelativistic case, where W^2 is replaced by the invariant $\vec{S}^2$ of the extended Galilei group.

(B) These results provide the starting point for the construction of a canonical Darboux basis adapted to the non-Abelian SO(3) symmetry. The three non-Abelian Noether constants of motion $\vec{S}$ are arranged in these canonical Darboux bases as an array containing the canonical pair S^3, $\beta=\tan^{-1}(S^2/S^1)$ and the unpaired variable $S=|\vec{S}|$[19] [*scheme A* of the canonical realization of SO(3)[2]]. The angle canonically conjugated to S, say α, is an *orientational* variable, which, being coupled to the internal *shape* degrees of freedom, cannot be a constant of motion. Being conjugate to a constant of the motion, it is an *ignorable* variable in the Hamiltonian formalism, so that its equation of motion can be solved by quadratures after the solution of the other equations. In conclusion, in this non-Abelian case one has only two (instead of three as in the Abelian case) commuting constants of motion, namely S and S^3 (like in quantum mechanics).

This is also the outcome of the momentum map canonical reduction[20–22] by means of adapted coordinates. Let us stress that α, S^3, β are a local coordinatization of any coadjoint orbit of SO(3) contained in the N-body phase space. Each coadjoint orbit is a 3-dimensional embedded submanifold and is endowed with a Poisson structure whose neutral element is α. This latter is also the essential coordinate for the definition of the *flag* of spinors (see Refs. 23 and 2, Sec. V). On the other hand, the spinor flag is nothing else than a unit vector $\hat{R}$ orthogonal to $\vec{S}$,[24] which is going to be a fundamental tool in what follows.

By fixing nonzero values of the variables S^3, $\beta=\tan^{-1}(S^2/S^1)$ through second class constraints, one can define a $(6N\text{-}8)$-dimensional reduced phase space. However, the canonical reduction cannot be furthered by eliminating S, since α is not a constant of motion.

(C) The group-theoretical treatment of rigid bodies[21] (see Chap. IV, Sec. 10 of Ref. 21) is based on the existence of the realization of the (free and transitive) *left* and *right* Hamiltonian actions of the SO(3) rotation group on either the tangent or cotangent bundle over their configuration space. Given a *laboratory or space frame* $\hat{f}_r$, the generators of the *left* Hamiltonian action[25] are the non-Abelian constants of motion S^1, S^2, S^3, $[\{S^r,S^s\}=\epsilon^{rsu}S^u]$, viz., the spin components in the *space frame*. In the approach of Ref. 9 the SO(3) principal bundle is built starting from the *relative configuration space* and, upon the choice of a body-frame convention, a gauge-dependent SO(3) *right* action is introduced.

Correspondingly, taking into account the *relative phase space* of any isolated system, one may investigate whether one or more SO(3) *right* Hamiltonian actions could be implemented besides the global canonical realization of the SO(3) *left* Hamiltonian action, which is a symmetry action. In other words, one may look for solutions $\check{S}^r$, $r=1,2,3$ [with $\Sigma_r(\check{S}^r)^2=\Sigma_r(S^r)^2=S^2$], of the partial differential equations $\{S^r,\check{S}^s\}=0$, $\{\check{S}^r,\check{S}^s\}=-\epsilon^{rsu}\check{S}^u$ and then build corresponding *left* invariant Hamiltonian vector fields. Alternatively, one may look for the existence of a pair $\check{S}^3$, $\gamma=\tan^{-1}(\check{S}^2/\check{S}^1)$, of canonical variables satisfying $\{\gamma,\check{S}^3\}=-1$, $\{\gamma,S^r\}=\{\check{S}^3,S^r\}=0$ and also $\{\gamma,\alpha\}=\{\check{S}^3,\alpha\}=0$. Local theorems given in Refs. 1, 2 guarantee that this is always possible provided $N\geqslant 3$. See Chap. IV of Ref. 21 for what is known in general about the actions of Lie groups on symplectic manifolds. Clearly, the functions $\check{S}^r$ do not generate symmetry actions, because they are not constants of the motion.

The inputs coming from (A), (B), (C) together with the technique of the spin bases introduced in Ref. 17 suggest the following strategy for the geometrical and group-theoretical identification of a privileged class of canonical Darboux bases for the N-body problem.

(1) Every such basis must be a *scheme B* (i.e., a canonical completion of *scheme A*)[1,2] for the canonical realization of the rotation group SO(3), viz., it must contain its invariant S and the canonical pair S^3, $\beta=\tan^{-1}(S^2/S^1)$. Therefore, all the remaining variables in the canonical basis except α are SO(3) scalars.

(2) As said above, the existence of the angle α satisfying $\{\alpha,S\}=1$ and $\{\alpha,S^3\}=\{\alpha,\beta\}=0$ leads to the geometrical identification of a unit vector $\hat{R}$ orthogonal to $\vec{S}$ and, therefore, of a orthonormal frame $\hat{S}$, $\hat{R}$, $\hat{S}\times\hat{R}$ (the notation $\hat{}$ means unit vector), which will be called *spin frame*.

(3) The study of the equations $\hat{R}^2=1$ and $\{\vec{S}\cdot\hat{R},\hat{R}^i\}=0$ entails the symplectic result $\{\hat{R}^i,\hat{R}^j\}=0$. As a byproduct we get a canonical realization of an $E(3)$ group with generators $\vec{S}$, $\hat{R}$ $[\{\hat{R}^i,\hat{R}^j\}=0, \{\hat{R}^i,S^j\}=\epsilon^{ijk}\hat{R}^k]$ and fixed values of its invariants $\hat{R}^2=1$, $\vec{S}\cdot\hat{R}=0$ (nonirreducible type 3 realization according to Ref. 17).

(4) In order to implement a SO(3) *Hamiltonian right action* in analogy with the rigid body theory,[21] we must construct an orthonormal triad or *body frame* $\hat{N}$, $\hat{\chi}$, $\hat{N}\times\hat{\chi}$. The decomposition,

$$\vec{S}=\check{S}^1\hat{\chi}+\check{S}^2\hat{N}\times\hat{\chi}+\check{S}^3\hat{N}\overset{\text{def}}{=}\check{S}^r\hat{e}_r, \tag{1.1}$$

identifies the SO(3) scalar generators $\check{S}^r$ of the right action provided they satisfy $\{\check{S}^r,\check{S}^s\}=-\epsilon^{rsu}\check{S}^u$. This latter condition together with the obvious requirement that $\hat{N}$, $\hat{\chi}$, $\hat{N}\times\hat{\chi}$ be SO(3) vectors $[\{\hat{N}^r,S^s\}=\epsilon^{rsu}\hat{N}^u$, $\{\hat{\chi}^r,S^s\}=\epsilon^{rsu}\hat{\chi}^u$, $\{\hat{N}\times\hat{\chi}^r,S^s\}=\epsilon^{rsu}\hat{N}\times\hat{\chi}^u]$ entails the equations[26]

$$\{\hat{N}^r,\hat{N}^s\}=\{\hat{N}^r,\hat{\chi}^s\}=\{\hat{\chi}^r,\hat{\chi}^s\}=0. \tag{1.2}$$

To each solution of these equations is associated a couple of canonical realizations of the $E(3)$ group (type 2, nonirreducible): one with generators $\vec{S}$, $\vec{N}$ and nonfixed invariants $\check{S}^3=\vec{S}\cdot\hat{N}$ and $|\vec{N}|$; another with generators $\vec{S}$, $\vec{\chi}$ and nonfixed invariants $\check{S}^1=\vec{S}\cdot\hat{\chi}$ and $|\vec{\chi}|$. These latter contain the relevant information for constructing the angle α and the new canonical pair $\check{S}^3$, $\gamma=\tan^{-1}(\check{S}^2/\check{S}^1)$ of SO(3) scalars. Since $\{\alpha,\check{S}^3\}=\{\alpha,\gamma\}=0$ must hold, it follows that the vector $\vec{N}$ necessarily belongs to the $\vec{S}-\hat{R}$ plane. The three canonical pairs S, α, S^3, β, $\check{S}^3$, γ will describe the *orientational* variables of our Darboux basis, while $|\vec{N}|$ and $|\vec{\chi}|$ will belong to the *shape* variables. Alternatively, an anholonomic basis can be constructed by replacing the above six variables by $\check{S}^r$ (or S^r) and three uniquely determined Euler angles $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$.

Let us consider the case $N=3$ as a first example. It turns out that a solution of Eqs. (1.2) corresponding to a *body frame* (determined only by the 3-body system configuration, as in the *rigid body* case) is completely individuated once two orthonormal vectors $\vec{N}$ and $\vec{\chi}$, functions of the relative coordinates and independent of the momenta, are found such that $\vec{N}$ lies in the $\vec{S}-\hat{R}$ plane.[27] We do not know whether in the case $N=3$ other solutions of Eqs. (1.2) exist leading to momentum-dependent body frames. Anyway, our constructive method necessarily leads to momentum-dependent solutions of Eqs. (1.2) for $N\geqslant 4$ and therefore to momentum-dependent or *dynamical body frames*.

We can conclude that in the N-body problem there are *hidden structures allowing the identification of special dynamical body frames which, being independent of gauge conditions, are endowed with a physical meaning*.

The following particular results can be proven.

(i) For $N=2$, a single $E(3)$ group can be defined: it allows the construction of an orthonormal *spin frame* $\hat{S}$, $\hat{R}$, $\hat{R}\times\hat{S}$ in terms of the measurable relative coordinates and momenta of the particles.

(ii) For $N=3$, $\vec{S}=\vec{S}_1+\vec{S}_2$, a pair of $E(3)$ groups emerge associated with $\vec{S}_1$ and $\vec{S}_2$, respectively. In this case, besides the orthonormal *spin frame*, an orthonormal *dynamical body frame* $\hat{N}$, $\hat{\chi}$, $\hat{N}\times\hat{\chi}$ can be defined such that $\check{S}^1=\vec{S}\cdot\hat{\chi}$, $\check{S}^2=\vec{S}\cdot\hat{N}\times\hat{\chi}$, $\check{S}^3=\vec{S}\cdot\hat{N}$ are the canonical generators of a SO(3) Hamiltonian *right* action. The nonconservation of $\check{S}^r$ entails that *the dynamical body frame evolves in a way dictated by the equations of motion*, just as it happens in the rigid body case.

It can be shown that for $N=3$ this definition of a *dynamical body frame* can be reinterpreted as a special global cross section (*xxzz gauge*, where *x* stays for $\hat{\chi}$ and *z* for $\hat{N}$; this outcome is independent from the particular choice made for $\vec{N}$ and $\vec{\chi}$) of the trivial SO(3) principal bundle of Ref. 9, namely a privileged choice of body frame. Actually, the three canonical pairs of orientational variables S^3, $\beta=\tan^{-1}(S^2/S^1)$; S, α; $\check{S}^3$, $\gamma=\tan^{-1}(\check{S}^2/\check{S}^1)$, can be replaced by the anholonomic basis of three Euler angles $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ and by $\check{S}^1$, $\check{S}^2$, $\check{S}^3$ as it is done in Ref. 9. In our construction, however, the Euler angles $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ are determined as the *unique set* of *dynamical orientation variables*. Then, the remaining canonical pairs q^μ, p_μ, $\mu=1,2,3$, of this spin-adapted Darboux basis describe the *dynamical shape* phase space.

While the above *dynamical body frame* can be identified with the global cross section corresponding to the *xxzz gauge*, all other global cross sections cannot be interpreted as *dynamical body frames* (or *dynamical right* actions), because the SO(3) principal bundle of Ref. 9 is built starting from the relative configuration space and, therefore, it is a *static*, velocity-independent, construction. As a matter of fact, after the choice of the shape configuration variables q^μ and of a space frame in which the relative variables have components ρ^r_a, the approach of Ref. 9 begins with the definition of the body-frame components $\check{\rho}^r_a(q^\mu)$ of the relative coordinates, in the form $\rho^r_a=R^{rs}(\theta^\alpha)\check{\rho}^s_a(q^\mu)$,[28] and then extends it in a *velocity-independent* way to the relative velocities $\dot{\rho}^r_a \overset{\text{def}}{=} R^{rs}(\theta^\alpha)\check{v}^s_a$. In

our construction we get instead $\rho_a^r = R^{rs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{\rho}_a^s(q^\mu)$ in the *xxzz gauge*, so that in the present case ($N=3$) all *dynamical* variables of our construction coincide with the *static* variables in the *xxzz gauge*. On the other hand, in the relative phase space, the construction of the *evolving dynamical body frame* is based on nonpoint canonical transformations.

(iii) For $N=4$, where $\vec{S}=\vec{S}_1+\vec{S}_2+\vec{S}_3$, it is possible to construct *three* sets of *spin frames* and *dynamical body frames* corresponding to the hierarchy of clusterings $((ab)c)$ [i.e., ((12)3), ((23)1), ((31)2)] of the relative spins $\vec{S}_a$.[29] The associated three canonical Darboux bases share the three variables S^3, β, S (viz., $\vec{S}$), while both the remaining three orientational variables and the shape variables depend on the spin clustering. This entails the existence of three different SO(3) *right* actions with nonconserved canonical generators $\check{S}^r_{(A)}$, $A=1,2,3$. Therefore, one can define three anholonomic bases $\tilde{\alpha}_{(A)}$, $\tilde{\beta}_{(A)}$, $\tilde{\gamma}_{(A)}$, $\check{S}^r_{(A)}$ and associated shape variables $q^\mu_{(A)}$, $p_{(A)\mu}$, $\mu=1,...,6$, connected by canonical transformations leaving S^r fixed. These anholonomic bases and the associated *evolving dynamical body frames*, however, have no relations with the $N=4$ *static* nontrivial SO(3) principal bundle of Ref. 9, which admits only local cross sections. As a matter of fact, one gets $\rho_a^r = R^{rs}(\tilde{\alpha}_{(A)},\tilde{\beta}_{(A)},\tilde{\gamma}_{(A)})\check{\rho}_{(A)a}(q^\mu_{(A)},p_{(A)\mu},\check{S}^r_{(A)})$ instead of $\rho_a^r = R^{rs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{\rho}_a^s(q^\mu)$.

These results imply that, for $N=4$, the 18-dimensional relative phase space admits three operationally well defined *dynamical body frames*, and associated *right* actions, and its coordinates are naturally split in three different ways into 6 dynamical rotational variables and 12 generalized dynamical shape variables. As a consequence, we get three possible definitions of *dynamical vibrations*. Each set of 12 generalized dynamical canonical shape variables is obviously defined modulo canonical transformations so that it should even be possible to find local canonical bases corresponding to the local cross sections of the $N=4$ *static* nontrivial SO(3) principal bundle of Ref. 9.

Our results can be extended to arbitrary N, with $\vec{S}=\Sigma_{a=1}^{N-1}\vec{S}_a$. There are as many independent ways (say K) of spin clustering as in quantum mechanics. For instance for $N=5$, $K=15$: 12 spin clusterings correspond to the pattern $(((ab)c)d)$ and 3 to the pattern $((ab)(cd))$ $[a,b,c,d=1,...,4]$. For $N=6$, $K=105$: 60 spin clusterings correspond to the pattern $((((ab)c)d)e)$, 15 to the pattern $((ab)(cd)e)$ and 30 to the pattern $(((ab)c)(de))$ $[a,b,c,d,e=1,...,5]$. Each spin clustering is associated to (a) a related *spin frame*; (b) a related *dynamical body frame*; (c) a related Darboux spin canonical basis with orientational variables S^3, β, S, $\alpha_{(A)}$, $\check{S}^3_{(A)}$, $\gamma_{(A)}=\tan^{-1}(\check{S}^2_{(A)}/\check{S}^1_{(A)})$, $A=1,...,K$ [their anholonomic counterparts are $\tilde{\alpha}_{(A)}$, $\tilde{\beta}_{(A)}$, $\tilde{\gamma}_{(A)}$, $\check{S}^r_{(A)}$ with uniquely determined orientation angles] and shape variables $q^\mu_{(A)}$, $p_{\mu(A)}$, $\mu=1,...,3N-6$. Furthermore, for $N\geq 4$ we find the following relation between spin and angular velocity: $\check{S}^r = \mathcal{I}^{rs}(q^\mu_{(A)})\check{\omega}^s_{(A)} + f^\mu(q^\nu_{(A)})p_{(A)\mu}$.

Let us conclude this Introduction with some remarks.

The $\vec{S}=0$, *C-horizontal*, cross section of the *static* SO(3) principal bundle corresponds to N-body configurations that cannot be included in the previous Hamiltonian construction based on the canonical realizations of SO(3): these configurations (which include the singular ones) have to be analyzed independently since they are related to the exceptional orbit of SO(3), whose little group is the whole group.

While physical observables have to be obviously independent of the gauge-dependent *static body frames*, they do depend on the *dynamical body frame*, whose axes are operationally defined in terms of the relative coordinates and momenta of the particles. In particular, a *dynamical* definition of *vibration*, which replaces the $\vec{S}=0$ *C-horizontal* cross section of the *static* approach,[30] is based on the requirement that the components of the *angular velocity* vanish. Actually, the angular velocities with respect to the dynamical body frames become now *measurable quantities*, in agreement with the phenomenology of extended deformable bodies.

In this connection, let us recall that the main efforts done in developing canonical transformations for the N-body problem took place in the context of celestial mechanics. As a conse-

quence, these transformations are necessarily adapted to the Newtonian gravitational potential. This latter, together with the harmonic potential, corresponds to the only interactions having extra dynamical symmetries besides the rotational one. The particularity of the final canonical transformations which have been worked out in that mechanical context is that of containing the Hamiltonian as one among the final momenta. This is in particular true for the $N=2$ body problem (Delauny variables) and for the $N=3$ body problem (Jacobi's methos of *the elimination of the nodes*). On the other hand, it is well-known that, for generic nonintegrable interactions, putting the Hamiltonian in the canonical bases is quite useless, since it does not bring to *isolating integrals* of the motion having the capability of reducing the dimensions of phase space. We stress again here that our construction rests only on the left and right actions of the SO(3) group and is therefore completely independent of the interactions (e.g., the treatment of spinning stars in astrophysics).

It is an open problem whether the use of more general body frames for $N=3$ and $N\geqslant 4$ obtained by using the freedom of making arbitrary configurations dependent rotations[27] may be used to simplify the free Hamiltonian and/or some type of interaction.

It is hoped that our results may be instrumental for nuclear, atomic and molecular physics, since a description based on spin clustering rather than on the standard Jacobi center-of-mass clusterings was lacking until now.

Let us observe that the extension of the *dynamical body frames* to continuous deformable bodies (see Ref. 31 for an initial study of the relativistic configurations of a Klein–Gordon field from this point of view) is a lacking piece of kinematical information and will be studied elsewhere.

The fact that we use nonpoint canonical transformations will make the quantization more difficult than in the orientation-shape bundle approach, where a separation of rotations from vibrations in the Schrödinger equation is reviewed in Ref. 9. The quantizations of the original canonical relative variables and of the canonical spin bases will give equivalent quantum theories only if the nonpoint canonical transformations are unitarily implementable. These problems are completely unexplored.

In a future paper[8] we shall study the relativistic N-body problem, where the definition and separation of the center-of-mass motion are known to be a complicated issue. Moreover the schematization with rigid bodies does not exist in special relativity: the only relativistic concept of rigidity are Born's rigid motions.[32] This problem has found a solution within the Wigner-covariant rest-frame instant form of dynamics.[13] It will be shown that concepts like reduced masses, Jacobi normal relative coordinates and tensor of inertia do not exist at the relativistic level. Yet, in the framework of the rest-frame instant form, both the orientation-shape SO(3) principal bundle approach and the canonical spin bases can be defined just as in the nonrelativistic case.

In Sec. II the rest-frame description of N free particles is introduced.

In Sec. III the *canonical spin bases*, the *spin frame* and the *dynamical body frames* are introduced and the cases $N=2$, $N=3$ and $N\geqslant 4$ are analyzed separately.

In Appendix A detailed calculations are given for the case $N=3$.

In Appendix B some notions on Euler angles are reviewed.

In Appendix C the construction of the *canonical spin bases* is given for the $N=4$ case.

See the preliminary version[33] of this paper for a more complete review of the SO(3) principal bundle approach (see also Refs. 34–37), many more technical details on the new canonical transformations and some examples of interaction potentials.

II. THE NONRELATIVISTIC REST-FRAME DESCRIPTION

In this section we give a summary of the description of N nonrelativistic free particles in the rest frame.

Given the coordinates $\vec{\eta}_i(t)$, $i=1,...,N$, of N particles of mass m_i, the standard Lagrangian is $L=\Sigma_{i=1}^{N}(m_i/2)\dot{\vec{\eta}}_i^2$. By introducing the center-of-mass coordinates $\vec{q}_{\rm nr}$ and a set of relative variables, the Lagrangian can be rewritten as $L=(m/2)\dot{\vec{q}}_{\rm nr}+$ (quadratic form in the relative veloci-

ties), $m=\Sigma_{i=1}^{N} m_i$. The canonical momenta are $\vec{p}_i = m_i \dot{\vec{\eta}}_i$, while the total momentum conjugated to $\vec{q}_{\rm nr}$ is $\vec{P}=\Sigma_{i=1}^{N}\vec{p}_i$. The Hamiltonian is $H=\Sigma_{i=1}^{N}(\vec{p}_i^{\,2}/2m_i)=\vec{P}^2/2m+$ (quadratic form in the relative momenta).

The rest-frame description (equivalent to the decoupling of the center of mass) is obtained by imposing the vanishing of the conserved total momentum $\vec{P}=\Sigma_{i=1}^{N}\vec{p}_i=0$. It can be obtained as the nonrelativistic $c\to\infty$ limit of the relativistic rest-frame instant form of Ref. 8. Equivalently we can start from the Lagrangian

$$L_D(t)=\sum_{i=1}^{N}\frac{m_i}{2}[\dot{\vec{\eta}}_i(t)+\vec{\lambda}(t)]^2, \quad S_D=\int dt\, L_D(t) \tag{2.1}$$

in which the Lagrange multipliers $\vec{\lambda}(t)$ are considered as configurational variables.

The canonical momenta are

$$\vec{\kappa}_i(t)=\frac{\partial L_D(t)}{\partial \dot{\vec{\eta}}_i(t)}=m_i[\dot{\vec{\eta}}_i(t)+\vec{\lambda}(t)],$$
$$\vec{\pi}_\lambda(t)=\frac{\partial L_D(t)}{\partial \dot{\vec{\lambda}}(t)}=0. \tag{2.2}$$

Therefore, $\vec{\pi}_\lambda(t)\approx 0$ is a primary constraint. The canonical and Dirac Hamiltonians are [the variables $\vec{\mu}(t)$ being the Dirac multipliers in front of the primary constraints $\vec{\pi}_\lambda(t)\approx 0$]

$$H_c=\vec{\pi}_\lambda\cdot\dot{\vec{\lambda}}+\sum_{i=1}^{N}\vec{\kappa}_i\cdot\dot{\vec{\eta}}_i-L_D=\sum_{i=1}^{N}\frac{\vec{\kappa}_i^{\,2}}{2m_i}-\vec{\lambda}\cdot\vec{\kappa}_+, \quad \vec{\kappa}_+=\sum_{i=1}^{N}\vec{\kappa}_i,$$
$$H_D=\sum_{i=1}^{N}\frac{\vec{\kappa}_i^{\,2}}{2m_i}-\vec{\lambda}\cdot\vec{\kappa}_+ +\vec{\mu}\cdot\vec{\pi}_\lambda. \tag{2.3}$$

The time constancy of the primary constraints implies the following secondary constraint:

$$\dot{\vec{\pi}}_\lambda(t)\stackrel{\circ}{=}\{\vec{\pi}_\lambda(t),H_D\}=\vec{\kappa}_+\approx 0, \tag{2.4}$$

which is the nonrelativistic rest-frame condition.

There are two first class constraints $\vec{\pi}_\lambda\approx 0$, $\vec{\kappa}_+\approx 0$: $\vec{\lambda}(t)$ and a center-of-mass variable are gauge variables. The Hamilton and Euler–Lagrange equations are ($\stackrel{\circ}{=}$ means evaluated on the trajectories which minimize the action principle)

$$\dot{\vec{\eta}}_i(t)\stackrel{\circ}{=}\{\vec{\eta}_i(t),H_D\}=\frac{\vec{\kappa}_i(t)}{m_i}-\vec{\lambda}(t), \quad \dot{\vec{\lambda}}(t)\stackrel{\circ}{=}\vec{\mu}(t),$$
$$\dot{\vec{\kappa}}_i(t)\stackrel{\circ}{=}0, \quad \dot{\vec{\pi}}_\lambda(t)\stackrel{\circ}{=}\vec{\kappa}_+\approx 0, \tag{2.5}$$
$$m_i(\ddot{\vec{\eta}}_i+\dot{\vec{\lambda}})(t)\stackrel{\circ}{=}0.$$

This is the nonrelativistic limit of the relativistic rest-frame instant form of dynamics: Minkowski spacetime is replaced by Galilei spacetime and the Wigner hyperplanes are replaced by the inertial observers seeing the isolated system as instantaneously at rest in the $t=\text{const}$ hyperplanes. Defining the nonrelativistic center of mass,

$$\vec{q}_{\rm nr}=\sum_{i=1}^{N}\frac{m_i}{m}\,\vec{\eta}_i\,, \tag{2.6}$$

with $m=\Sigma_{i=1}^{N}m_i$, the gauge fixing $\vec{q}_{\rm nr}\approx 0$ implies $\vec{\lambda}(\tau)\approx 0$ and the decoupling of the center of mass, see Eq. (2.9).

In analogy with the relativistic case of Ref. 13, let us introduce the following family of nonrelativistic point canonical transformations:

$$\begin{array}{|c|}\hline \vec{\eta}_i \\ \hline \vec{\kappa}_i \\ \hline \end{array} \qquad \longrightarrow \qquad \begin{array}{|c|c|}\hline \vec{q}_{nr} & \vec{\rho}_a \\ \hline \vec{\kappa}_+ & \vec{\pi}_a \\ \hline \end{array} \tag{2.7}$$

defined by

$$\vec{\eta}_i=\vec{q}_{\rm nr}+\frac{1}{\sqrt{N}}\sum_{a=1}^{N-1}\Gamma_{ai}\vec{\rho}_a\,,$$

$$\vec{\kappa}_i=\frac{m_i}{m}\,\vec{\kappa}_+ +\sqrt{N}\sum_{a=1}^{N-1}\gamma_{ai}\vec{\pi}_a\,,$$

$$\vec{q}_{\rm nr}=\sum_{i=1}^{N}\frac{m_i}{m}\,\vec{\eta}_i\,,$$

$$\vec{\kappa}_+=\sum_{i=1}^{N}\vec{\kappa}_i\,,$$

$$\vec{\rho}_a=\sqrt{N}\sum_{i=1}^{N}\gamma_{ai}\vec{\eta}_i\,,$$

$$\vec{\pi}_a=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\Gamma_{ai}\vec{\kappa}_i\,, \tag{2.8}$$

$$\vec{S}=\sum_{a=1}^{N-1}\vec{\rho}_a\times\vec{\pi}_a\,,$$

$$\Gamma_{ai}=\gamma_{ai}-\sum_{k=1}^{N}\frac{m_k}{m}\gamma_{ak}\,,\quad \gamma_{ai}=\Gamma_{ai}-\frac{1}{N}\sum_{k=1}^{N}\Gamma_{ak}\,,$$

$$\sum_{i=1}^{N}\gamma_{ai}=0,\quad \sum_{i=1}^{N}\frac{m_i}{m}\Gamma_{ai}=0,$$

$$\sum_{i=1}^{N}\gamma_{ai}\gamma_{bi}=\delta_{ab}\,,\quad \sum_{i=1}^{N}\gamma_{ai}\Gamma_{bi}=\delta_{ab}\,,$$

$$\sum_{a=1}^{N-1} \gamma_{ai}\gamma_{aj} = \delta_{ij} - \frac{1}{N}, \quad \sum_{a=1}^{N-1} \gamma_{ai}\Gamma_{aj} = \delta_{ij} - \frac{m_i}{m}.$$

Here, the γ_{ai}'s (and the Γ_{ai}'s) are numerical parameters depending on $\frac{1}{2}(N-1)(N-2)$ free parameters.[13,38]

Then, by using the equations of motion $m[\dot{\vec{q}}_{\rm nr}(t) + \vec{\lambda}(t)] \stackrel{\circ}{=} 0$, we get the Lagrangian $L_{\rm rel}$ and the Hamiltonian $H_{\rm rel}$ describing the relative motions after the separation of the center-of-mass motion,

$$L_D(t) = \sum_{i=1}^{N} \frac{m_i}{2}\left[\dot{\vec{q}}_{\rm nr}(t) + \vec{\lambda}(t) + \frac{1}{\sqrt{N}}\sum_{a=1}^{N-1} \Gamma_{ai}\dot{\vec{\rho}}_a(t)\right]^2$$

$$\stackrel{\circ}{=} L_{\rm rel}(t) = \frac{1}{2}\sum_{a,b}^{1\cdot N-1} k_{ab}[m_i, \Gamma_{ai}]\dot{\vec{\rho}}_a(t)\cdot\dot{\vec{\rho}}_b(t),$$

$$k_{ab}[m_i, \Gamma_{ci}] = k_{ba}[m_i, \Gamma_{ci}] = \frac{1}{N}\sum_{i=1}^{N} m_i\Gamma_{ai}\Gamma_{bi},$$

$$k^{-1}_{ab}[m_i, \Gamma_{ci}] = N\sum_{i=1}^{N} \frac{\gamma_{ai}\gamma_{bi}}{m_i},$$

$$\Downarrow$$

$$\vec{\pi}_a(t) = \sum_{b=1}^{N-1} k_{ab}[m_i, \Gamma_{ci}]\dot{\vec{\rho}}_b(t),$$

$$\Rightarrow H_{\rm rel} = \frac{1}{2}\sum_{ab}^{1\ldots N-1} k^{-1}_{ab}[m_i, \Gamma_{ai}]\vec{\pi}_a(t)\cdot\vec{\pi}_b(t). \tag{2.9}$$

The same result can be obtained by adding the gauge fixings $\vec{q}_{\rm nr} \approx 0$ which imply $\vec{\lambda}(t) = 0$, and by going to Dirac brackets with respect to the second class constraints $\vec{\kappa}_+ \approx 0$, $\vec{q}_{\rm nr} \approx 0$. The $(6N\text{-}6)$-dimensional reduced phase space is now spanned by $\vec{\rho}_a$, $\vec{\pi}_a$ and from Eq. (2.8) we have $\vec{S} \equiv \Sigma_{a=1}^{N-1}\vec{\rho}_a \times \vec{\pi}_a$.

At the nonrelativistic level[9,39] the next problem for each N is to diagonalize the matrix $k_{ab}[m_i, \Gamma_{ai}]$. The off-diagonal terms of the matrix $k_{ab}[m_i, \Gamma_{ai}]$ are called *mass polarization terms*, while its eigenvalues are the *reduced masses* (see for instance Ref. 40).

III. CANONICAL SPIN BASES

Following the preliminary work of Ref. 17, we look for a set of nonpoint canonical transformations from the relative canonical variables $\vec{\rho}_a = \sqrt{N}\Sigma_{i=1}^{N}\gamma_{ai}\vec{\eta}_i$, $\vec{\pi}_a = (1/\sqrt{N})\,\Sigma_{i=1}^{N}\Gamma_{ai}\vec{\kappa}_i$ of Eq. (2.8) to a canonical basis adapted to the SO(3) subgroup[1,2] of the extended Galilei group and containing one of its invariants, namely the modulus of the spin. Jacobi coordinates will not be used.

A. 2-body systems

The relative variables are $\vec{\rho} = \vec{\rho}$, $\vec{\pi}$ and the Hamiltonian is $H_{\rm rel} = \vec{\pi}^2/2\mu$, where $\mu = m_1 m_2/(m_1 + m_2)$ is the reduced mass. The spin is $\vec{S} = \vec{\rho} \times \vec{\pi}$ $[S = \sqrt{\vec{S}^2}]$.

Let us define the following decomposition:

$$\vec{\rho}=\rho\hat{R},\quad \rho=\sqrt{\vec{\rho}^2},\quad \hat{R}=\frac{\vec{\rho}}{\rho}=\hat{\rho},\quad \hat{R}^2=1,$$

$$\vec{\pi}=\tilde{\pi}\hat{R}-\frac{S}{\rho}\hat{R}\times\hat{S}=\tilde{\pi}\hat{\rho}-\frac{S}{\rho}\hat{\rho}\times\hat{S}, \tag{3.1}$$

$$\tilde{\pi}=\vec{\pi}\cdot\hat{R}=\vec{\pi}\cdot\hat{\rho},\quad \hat{S}=\frac{\vec{S}}{S},\quad \hat{S}\cdot\hat{R}=0.$$

Therefore, besides the standard *space or laboratory frame* with unit vectors $\hat{f}_r$, we can build a *spin frame*, whose basis unit vectors $\hat{S}$, $\hat{R}$, $\hat{S}\times\hat{R}$ are identified by the 2-body system itself. Since $\{S^i,S^j\}=\epsilon^{ijk}S^k$, $\{\hat{R}^i,\hat{R}^j\}=0$, $\{\hat{R}^i,S^j\}=\epsilon^{ijk}\hat{R}^k$, $\vec{S}$ and $\hat{R}$ are the generators of an $E(3)$ group containing SO(3) as a subgroup. The $E(3)$ invariants turn out to have the fixed values $\hat{R}^2=1$ and $\vec{S}\cdot\hat{R}=0$.

As shown in Ref. 17, it is instrumental to consider the following nonpoint canonical transformation adapted to the SO(3) group valid when $\vec{S}\neq 0$ (the invariant $S=|\vec{S}|$ becomes one of the new canonical variables),

$$\begin{array}{|c|}\hline \vec{\rho}\\ \hline \vec{\pi}\\ \hline\end{array}\quad\longrightarrow\quad \begin{array}{|cc|c|}\hline \alpha & \beta & \rho\\ \hline S & S^3 & \tilde{\pi}\\ \hline\end{array}\ , \tag{3.2}$$

where

$$\alpha=\tan^{-1}\frac{1}{S}\left(\vec{\rho}\cdot\vec{\pi}-\frac{(\rho)^2}{\rho^3}\pi^3\right),$$

$$\beta=\tan^{-1}\frac{S^2}{S^1},\quad \sin\beta=\frac{S^2}{\sqrt{(S)^2-(S^3)^2}},\quad \cos\beta=\frac{S^1}{\sqrt{(S)^2-(S^3)^2}}. \tag{3.3}$$

The two pairs of canonical variables α, S, β, S^3 form the irreducible kernel of the *scheme A* of a (nonirreducible, type 3; see Ref. 17) canonical realization of the group $E(3)$ generated by $\vec{S}$, $\hat{R}$, with fixed values of the invariants $\hat{R}^2=1$, $\hat{R}\cdot\vec{S}=0$, just as the variables S^3, β and S form the *scheme A* of the SO(3) group with invariant S.

Geometrically we have the following:

(i) The angle α is the angle between the plane determined by $\vec{S}$ and $\hat{f}_3$ and the plane determined by $\vec{S}$ and $\hat{R}$.

(ii) The angle β is the angle between the plane $\vec{S}-\hat{f}_3$ and the plane $\hat{f}_3-\hat{f}_1$.

We have

$$\begin{aligned} S^1&=\sqrt{(S)^2-(S^3)^2}\cos\beta,\\ S^2&=\sqrt{(S)^2-(S^3)^2}\sin\beta,\end{aligned} \tag{3.4}$$

$$\hat{R}^1=\hat{\rho}^1=\sin\beta\sin\alpha-\frac{S^3}{S}\cos\beta\cos\alpha,$$

$$\hat{R}^2=\hat{\rho}^2=-\cos\beta\sin\alpha-\frac{S^3}{S}\sin\beta\cos\alpha,$$

$$\hat{R}^3=\hat{\rho}^3=\frac{1}{S}\sqrt{(S)^2-(S^3)^2}\cos\alpha,$$

$$(\hat{S}\times\hat{R})^1=\hat{S}^2\hat{R}^3-\hat{S}^3\hat{R}^2=\sin\beta\cos\alpha+\frac{S^3}{S}\cos\beta\sin\alpha,$$

$$(\hat{S}\times\hat{R})^2=\hat{S}^3\hat{R}^1-\hat{S}^1\hat{R}^3=-\cos\beta\cos\alpha+\frac{S^3}{S}\sin\beta\sin\alpha,$$

$$(\hat{S}\times\hat{R})^3=-\hat{S}^1\hat{R}^2-\hat{S}^2\hat{R}^1=\frac{1}{S}\sqrt{(S)^2-(S^3)^2}\sin\alpha,$$

$$\hat{S}\times\hat{R}(\alpha)=\frac{\partial\hat{R}(\alpha)}{\partial\alpha}=\hat{R}\left(\alpha+\frac{\pi}{2}\right),$$

$$\Rightarrow\alpha=-\tan^{-1}\frac{(\hat{S}\times\hat{R})^3}{[\hat{S}\times(\hat{S}\times\hat{R})]^3}. \tag{3.5}$$

From the last line of this equation we see that the angle α can be expressed in terms of $\hat{S}$ and $\hat{R}$. Given the Hamiltonian description of any isolated system (a deformable body) in its rest frame with conserved spin $\vec{S}(q,p)$ (q,p denote a canonical basis for the system), a solution $\alpha(q,p)$ of the equations $\{\alpha(q,p),S(q,p)\}=1$, $\{\alpha(q,p),\beta(q,p)\}=\{\alpha(q,p),S^3(q,p)\}=0$, allows us to construct the unit vector $\hat{R}$ associated with the isolated system and then to build the spin frame and the $E(3)$ group.

Let us remark that *the Delaunay Hamilton–Jacobi transformation for the 2-body problem with the Newton potential*, used in celestial mechanics (see for instance Sec. 2.5 of Ref. 41), is *different* from Eq. (3.2). In fact, even if it contains S^3, β, S, it has (i) an angle α' differing from α for the choice of the origin; (ii) the Hamiltonian and a conjugate variable replacing ρ, $\tilde{\pi}$.

The following inverse canonical transformation holds true:

$$\vec{\rho}=\rho\hat{R}(\alpha,\beta,S,S^3),$$

$$\vec{\pi}=\tilde{\pi}\hat{R}(\alpha,\beta,S,S^3)+\frac{S}{\rho}\hat{S}(\beta,S,S^3)\times\hat{R}(\alpha,\beta,S,S^3),$$

$$\Rightarrow\vec{\pi}^2=\tilde{\pi}^2+\frac{S^2}{\rho^2}. \tag{3.6}$$

In this degenerate case, the *dynamical* shape variables ρ, $\tilde{\pi}$ coincide with the *static* ones and describe the vibration of the dipole.

The rest-frame Hamiltonian for the relative motion becomes ($\check{I}$ is the barycentric tensor of inertia of the dipole)

$$H_{\rm rel}=\frac{1}{2}\left[\check{I}^{-1}S^2+\frac{\tilde{\pi}^2}{\mu}\right],\quad \check{I}=\mu\rho^2,\quad \mu=\frac{m_1m_2}{m_1+m_2}, \tag{3.7}$$

while the body frame angular velocity is

$$\check{\omega}=\frac{\partial H_{\rm rel}}{\partial\check{S}}=\frac{\check{S}}{\check{I}}. \tag{3.8}$$

When $\vec{S}\neq 0$, Eq. (3.2) explicitly shows that a non-Abelian symmetry group like SO(3) does not allow a canonical reduction like in the Abelian case of translations. In this latter case we can eliminate the three Abelian constants of motion $\vec{\kappa}_+\approx 0$ and gauge fix the three conjugate variables $\vec{q}_{\rm nr}\approx 0$. In the non-Abelian case we could surely fix S^3, β by imposing second class constraints $S^3-a\approx 0$, $\beta-b\approx 0$, and eliminate this pair of canonical variables by going to Dirac brackets. However, since α is not a constant of motion [see later on Eq. (3.7); we get instead $(d/dt)(S-s)\overset{\circ}{=}0$], we can only add by hand the first class constraint $S-s\approx 0$ $(s\neq 0)$. It is only after the solution of the equations of motion, that we could also complete the reduction by adding $\alpha-\alpha_{\rm solution}\approx 0$ as a gauge-fixing. Let us remark that, since S is a constant of the motion, the angle α is an *ignorable* variable, which does not occur in the Hamiltonian.

In the absence of interactions the solution for α can be easily worked out (in any case it can be obtained by quadratures after the solution of the other equations of motion). The Hamilton equations, equivalent to $\ddot{\vec{\rho}}\overset{\circ}{=}0$, are $\dot{\rho}\overset{\circ}{=}\tilde{\pi}/\mu$, $\dot{\tilde{\pi}}\overset{\circ}{=}(S)^2/\mu\rho^3$, $\dot{S}\overset{\circ}{=}0$, $\dot{\alpha}\overset{\circ}{=}S/\mu\rho^2$. The solution $\vec{\rho}\overset{\circ}{=}\vec{b}t+\vec{a}$ ($\vec{a}$, $\vec{b}$ constant vectors) implies $\rho\overset{\circ}{=}|\vec{b}t+\vec{a}|$, $\hat{R}\overset{\circ}{=}(\vec{b}t+\vec{a})/|\vec{b}t+\vec{a}|$, $\tilde{\pi}\overset{\circ}{=}2\mu\vec{b}\cdot(\vec{b}t+\vec{a})/|\vec{b}t+\vec{a}|$, $S\overset{\circ}{=}\mu\sqrt{2}|\vec{a}\times\vec{b}|$, $\alpha\overset{\circ}{=}\arccos(\hat{R}^3S/\sqrt{(S)^2-(S^3)^2})$.

In the 2-body case the condition $\vec{S}\approx 0$, imposed as three first class constraints, is equivalent to $\vec{\rho}-k\vec{\pi}\approx 0$ and selects only the solution $\vec{\rho}(t)\overset{\circ}{=}\vec{A}e^{Bt}$ (k, $\vec{A}$ and B are constants).

B. 3-body systems

In the case $N=3$ the range of the indices is $i=1,2,3$, $a=1,2$. The spin is $\vec{S}=\Sigma_{a=1}^2\vec{\rho}_a\times\vec{\pi}_a=\Sigma_{a=1}^2\vec{S}_a$ after the canonical transformation (2.7) and the relative motions are governed by the Hamiltonian (2.9) for $N=3$.

Again, we shall assume $\vec{S}\neq 0$, because the exceptional SO(3) orbit $S=0$ has to be studied separately. This is done by adding $S\approx 0$ as a first class constraint and studying the following two disjoint strata with a different number of first class constraints separately: (a) $\vec{S}\approx 0$, but $\vec{S}_1=-\vec{S}_2\neq 0$; (b) $\vec{S}_a\approx 0$, $a=1,2$ (in this case we have $\vec{\rho}_a-k_a\vec{\pi}_a\approx 0$).[42]

For each value of $a=1,2$, we consider the nonpoint canonical transformation (3.2),

$$\begin{array}{|c|}\hline \vec{\rho}_a \\ \hline \vec{\pi}_a \\ \hline \end{array} \quad \longrightarrow \quad \begin{array}{|cc|c|}\hline \alpha_a & \beta_a & \rho_a \\ \hline S_a & S_a^3 & \tilde{\pi}_a \\ \hline \end{array} \tag{3.9}$$

where

$$\alpha_a=\tan^{-1}\frac{1}{S_a}\left(\vec{\rho}_a\cdot\vec{\pi}_a-\frac{(\rho_a)^2}{\rho_a^3}\pi_a^3\right),$$

$$\beta_a=\tan^{-1}\frac{S_a^2}{S_a^1},\quad \sin\beta_a=\frac{S_a^2}{\sqrt{(S_a)^2-(S_a^3)^2}},\quad \cos\beta_a=\frac{S_a^1}{\sqrt{(S_a)^2-(S_a^3)^2}}. \tag{3.10}$$

$$\vec{\rho}_a=\rho_a\hat{R}_a,\quad \rho_a=\sqrt{\vec{\rho}_a^2},\quad \hat{R}_a=\frac{\vec{\rho}_a}{\rho_a}=\hat{\rho}_a,\quad \hat{R}_a^2=1, \tag{3.11}$$

$$\vec{\pi}_a=\tilde{\pi}_a\hat{R}_a+\frac{S_a}{\rho_a}\hat{S}_a\times\hat{R}_a,\quad \tilde{\pi}_a=\vec{\pi}_a\cdot\hat{R}_a.$$

$$\vec{\rho}_a=\rho_a\hat{\rho}_a(\alpha_a,\beta_a,S_a,S_a^3)=\rho_a\hat{R}_a(\alpha_a,\beta_a,S_a,S_a^3),$$

$$\vec{\pi}_a=\tilde{\pi}_a\hat{\rho}_a(\alpha_a,\beta_a,S_a,S_a^3)+\frac{S_a}{\rho_a}\hat{S}_a(\beta_a,S_a,S_a^3)\times\hat{\rho}_a(\alpha_a,\beta_a,S_a,S_a^3)$$

$$=\tilde{\pi}_a\hat{R}_a(\alpha_a,\beta_a,S_a,S_a^3)+\frac{S_a}{\rho_a}\hat{S}_a(\beta_a,S_a,S_a^3)\times\hat{R}_a(\alpha_a,\beta_a,S_a,S_a^3). \tag{3.12}$$

We have now *two* unit vectors $\hat{R}_a$ and *two* $E(3)$ realizations generated by $\vec{S}_a$, $\hat{R}_a$, respectively, and fixed invariants $\hat{R}_a^2=1$, $\vec{S}_a\cdot\hat{R}_a=0$ (nonirreducible, type 2; see Ref. 17).

Then, the *simplest choice*, within the existing arbitrariness,[27] for the orthonormal vectors $\vec{N}$ and $\vec{\chi}$ functions only of the relative coordinates is (it is the canonical transformation of Ref. 17 with the interchange $\vec{\rho}_a\leftrightarrow\vec{\pi}_a$)

$$\vec{N}=\frac{1}{2}(\hat{R}_1+\hat{R}_2)=\frac{1}{2}(\hat{\rho}_1+\hat{\rho}_2),\quad \hat{N}=\frac{\vec{N}}{|\vec{N}|},\quad |\vec{N}|=\sqrt{\frac{1+\hat{\rho}_1\cdot\hat{\rho}_2}{2}},$$

$$\vec{\chi}=\frac{1}{2}(\hat{R}_1-\hat{R}_2)=\frac{1}{2}(\hat{\rho}_1-\hat{\rho}_2),\quad \hat{\chi}=\frac{\vec{\chi}}{|\vec{\chi}|},\quad |\vec{\chi}|=\sqrt{\frac{1-\hat{\rho}_1\cdot\hat{\rho}_2}{2}}=\sqrt{1-\vec{N}^2},$$

$$\vec{N}\times\vec{\chi}=-\frac{1}{2}\hat{\rho}_1\times\hat{\rho}_2,\quad |\vec{N}\times\vec{\chi}|=|\vec{N}||\vec{\chi}|=\frac{1}{2}\sqrt{1-(\hat{\rho}_1\cdot\hat{\rho}_2)^2}, \tag{3.13}$$

$$\vec{N}\cdot\vec{\chi}=0,\quad \{N^r,N^s\}=\{\chi^r,\chi^s\}=\{N^r,\chi^s\}=0,$$

$$\hat{R}_1=\hat{\rho}_1=\vec{N}+\vec{\chi},\quad \hat{R}_2=\hat{\rho}_2=\vec{N}-\vec{\chi},\quad \hat{R}_1\cdot\hat{R}_2=\hat{\rho}_1\cdot\hat{\rho}_2=\vec{N}^2-\vec{\chi}^2.$$

Likewise, we have for the spins

$$\vec{S}=\vec{S}_1+\vec{S}_2,$$

$$\vec{W}=\vec{S}_1-\vec{S}_2,$$

$$\vec{S}_1=\tfrac{1}{2}(\vec{S}+\vec{W}),\quad \vec{S}_2=\tfrac{1}{2}(\vec{S}-\vec{W}), \tag{3.14}$$

$$\{W^r,W^s\}=\epsilon^{rsu}S^u.$$

We therefore succeeded in constructing an orthonormal triad (the *dynamical body frame*) and two $E(3)$ realizations (nonirreducible, type 3; see Ref. 17): one with generators $\vec{S}$, $\vec{N}$ and nonfixed invariants $|\vec{N}|$ and $\vec{S}\cdot\hat{N}$, the other with generators $\vec{S}$ and $\vec{\chi}$ and nonfixed invariants $|\vec{\chi}|$ and $\vec{S}\cdot\hat{\chi}$. As said in the Introduction, Eq. (1.1), this is equivalent to the determination of the nonconserved generators $\check{S}^r$ of a Hamiltonian *right action* of SO(3): $\check{S}^1=\vec{S}\cdot\hat{\chi}=\vec{S}\cdot\hat{e}_1$, $\check{S}^2=\vec{S}\cdot\hat{N}\times\hat{\chi}=\vec{S}\cdot\hat{e}_2$, $\check{S}^3=\vec{S}\cdot\hat{N}=\vec{S}\cdot\hat{e}_3$.

The realization of the $E(3)$ group with generators $\vec{S}$, $\vec{N}$ and nonfixed invariants $\vec{N}^2$, $\vec{S}\cdot\vec{N}$ leads to the final canonical transformation introduced in Ref. 17

$$\begin{array}{|c|}\hline \vec{\rho}_a \\ \hline \vec{\pi}_a \\ \hline \end{array}\quad\longrightarrow\quad \begin{array}{|cc|cc|c|}\hline \alpha_1 & \beta_1 & \alpha_2 & \beta_2 & \rho_a \\ \hline S_1 & S_1^3 & S_2 & S_2^3 & \tilde{\pi}_a \\ \hline \end{array}\quad\longrightarrow\quad \begin{array}{|ccc|c|c|}\hline \alpha & \beta & \gamma & |\vec{N}| & \rho_a \\ \hline S=\check{S} & S^3 & \check{S}^3=\vec{S}\cdot\hat{N} & \xi & \tilde{\pi}_a \\ \hline \end{array} \tag{3.15}$$

where

$$|\vec{N}|=\sqrt{\frac{1+\hat{\rho}_1\cdot\hat{\rho}_2}{2}},$$

$$\check{S}^3=\vec{S}\cdot\hat{N}=\frac{1}{\sqrt{2}}\sum_{a=1}^{2}\vec{\rho}_a\times\vec{\pi}_a\cdot\frac{\hat{\rho}_1+\hat{\rho}_2}{\sqrt{1+\hat{\rho}_1\cdot\hat{\rho}_2}}\equiv S\cos\psi,$$

$$\cos\psi=\hat{S}\cdot\hat{N}=\frac{\check{S}^3}{S},\quad \sin\psi=\frac{1}{S}\sqrt{(S)^2-(\check{S}^3)^2},$$

$$S=\check{S}=\left|\sum_{a=1}^{2}\vec{\rho}_a\times\vec{\pi}_a\right|,$$

$$S^3=\sum_{a=1}^{2}(\vec{\rho}_a\times\vec{\pi}_a)^3,$$

$$\alpha=-\tan^{-1}\frac{(\hat{S}\times\hat{N})^3}{[\hat{S}\times(\hat{S}\times\hat{N})]^3}=-\tan^{-1}\frac{[\hat{S}\times(\hat{\rho}_1+\hat{\rho}_2)]^3}{[\hat{S}\times(\hat{S}\times[\hat{\rho}_1+\hat{\rho}_2])]^3},\tag{3.16}$$

$$\beta=\tan^{-1}\frac{S^2}{S^1},$$

$$\gamma=\tan^{-1}\frac{\vec{S}\cdot(\hat{N}\times\hat{\chi})}{\vec{S}\cdot\hat{\chi}}=\tan^{-1}\frac{\check{S}^2}{\check{S}^1},$$

$$\Rightarrow\sin\gamma=\frac{\check{S}^2}{\sqrt{(\check{S})^2-(\check{S}^3)^2}},\quad \cos\gamma=\frac{\check{S}^1}{\sqrt{(\check{S})^2-(\check{S}^3)^2}},$$

$$\xi=\frac{\vec{W}\cdot(\hat{N}\times\hat{\chi})}{|\vec{\chi}|}=\frac{\vec{W}\cdot(\hat{N}\times\hat{\chi})}{\sqrt{1-\vec{N}^2}}=\frac{\sqrt{2}\Sigma_{a=1}^{2}(-)^{a+1}\vec{\rho}_a\times\vec{\pi}_a\cdot(\hat{\rho}_2\times\hat{\rho}_1)}{[1-\hat{\rho}_1\cdot\hat{\rho}_2]\sqrt{1+\hat{\rho}_1\cdot\hat{\rho}_2}}.$$

For $N=3$ the *dynamical shape variables*, functions of the relative coordinates $\vec{\rho}_a$ only, are $|\vec{N}|$ and ρ_a, while the conjugate shape momenta are ξ, $\tilde{\pi}_a$.

Let us remark that *this transformation is different from the canonical transformation* of Ref. 43 introduced for the method of *elimination of the nodes*. Since S is a constant of motion, the conjugate variable α is *ignorable* and does not occur in the Hamiltonian. We recover the result that the effective order of the 3-body equations of motion is 8, before using the conservation of the energy.

The final array (3.15) is nothing other than a *scheme* B^1 of a realization of the $E(3)$ group with generators $\vec{S}$, $\vec{N}$ (nonirreducible type 3). In particular, the two canonical pairs S^3, β, S, α, constitute the irreducible kernel of the $E(3)$ *scheme A*, whose invariants are $\check{S}^3$, $|\vec{N}|$; γ and ξ are the so-called *supplementary variables* conjugated to the invariants; finally, the two pairs ρ_a, $\tilde{\pi}_a$

are so-called *inessential variables*. Let us remark that S^3, β, S, α, γ, ξ, are a local coordinatization of every $E(3)$ coadjoint orbit with $\check{S}^3=\text{const}$, $|\vec{N}|=\text{const}$ and fixed values of the inessential variables, present in the 3-body phase space.

We can now reconstruct $\vec{S}$ and define a *new* unit vector $\hat{R}$ orthogonal to $\vec{S}$ by adopting the prescription of Eq. (3.5).

The vectors $\hat{S}$, $\hat{R}$, $\hat{S}\times\hat{R}$ build up the *spin frame* for $N=3$. The angle α conjugate to S is explicitly given by

$$\alpha=-\tan^{-1}\frac{(\hat{S}\times\hat{N})^3}{[\hat{S}\times(\hat{S}\times\hat{N})]^3}=-\tan^{-1}\frac{(\hat{S}\times\hat{R})^3}{[\hat{S}\times(\hat{S}\times\hat{R})]^3}. \tag{3.17}$$

The two expressions of α given here are consistent with the fact that $\hat{S}$, $\hat{R}$ and $\hat{N}$ are coplanar, so that $\hat{R}$ and $\hat{N}$ differ only by a term in $\hat{S}$.

As a consequence of this definition of $\hat{R}$, we get the following expressions for the *dynamical body frame* $\hat{N}$, $\hat{\chi}$, $\hat{N}\times\hat{\chi}$ in terms of the final canonical variables,

$$\hat{N}=\cos\psi\hat{S}+\sin\psi\hat{R}=\frac{\check{S}^3}{S}\hat{S}+\frac{1}{S}\sqrt{(S)^2-(\check{S}^3)^2}\hat{R}=\hat{N}[S,\alpha;S^3,\beta;\check{S}^3,\gamma],$$

$$\hat{\chi}=\sin\psi\cos\gamma\hat{S}-\cos\psi\cos\gamma\hat{R}+\sin\gamma\hat{S}\times\hat{R}=\frac{\check{S}^1}{S}\hat{S}-\frac{\check{S}^3}{S}\frac{\check{S}^1\hat{R}+\check{S}^2\hat{S}\times\hat{R}}{\sqrt{(S)^2-(\check{S}^3)^2}}=\hat{\chi}[S,\alpha;S^3,\beta;\check{S}^3,\gamma],$$

$$\begin{aligned}\hat{N}\times\hat{\chi}&=\sin\psi\sin\gamma\hat{S}-\cos\psi\sin\gamma\hat{R}-\cos\gamma\hat{S}\times\hat{R}\\&=\frac{\check{S}^2}{S}\hat{S}-\frac{\check{S}^3}{S}\frac{\check{S}^1\hat{R}-\check{S}^2\hat{S}\times\hat{R}}{\sqrt{(S)^2-(\check{S}^3)^2}}=(\hat{N}\times\hat{\chi})[S,\alpha;S^3,\beta;\check{S}^3,\gamma],\end{aligned}$$

$$\Downarrow \tag{3.18}$$

$$\hat{S}=\sin\psi\cos\gamma\hat{\chi}+\sin\psi\sin\gamma\hat{N}\times\hat{\chi}+\cos\psi\hat{N}\overset{\text{def}}{=}\frac{1}{S}[\check{S}^1\hat{\chi}+\check{S}^2\hat{N}\times\hat{\chi}+\check{S}^3\hat{N}],$$

$$\hat{R}=-\cos\psi\cos\gamma\hat{\chi}-\cos\psi\sin\gamma\hat{N}\times\hat{\chi}+\sin\psi\hat{N},$$

$$\hat{R}\times\hat{S}=-\sin\gamma\hat{\chi}+\cos\gamma\hat{N}\times\hat{\chi}.$$

While ψ is the angle between $\hat{S}$ and $\hat{N}$, γ is the angle between the plane $\hat{N}-\hat{\chi}$ and the plane $\hat{S}-\hat{N}$. As in the case $N=2$, α is the angle between the plane $\hat{S}-\hat{f}_3$ and the plane $\hat{S}-\hat{R}$, while β is the angle between the plane $\hat{S}-\hat{f}_3$ and the plane $\hat{f}_3-\hat{f}_1$. See Fig. 1.

Owing to the results of Appendix A, which allow us to re-express $S_a=|\vec{S}_a|$, S^3_a, $\beta_a=\tan^{-1}(S^2_a/S^1_a)$ in terms of the final variables and owing to Eqs. (3.13), (3.17) which allow us to get $\alpha_a=-\tan^{-1}[(\hat{S}_a\times\hat{R}_a)^3/(\hat{S}_a\times(\hat{S}_a\times\hat{R}_a))^3]$, we can reconstruct the inverse canonical transformation.

The existence of the *spin frame* and of the *dynamical body frame* allows to define two decompositions of the relative variables, which make explicit the inverse canonical transformation. For the relative coordinates we get from Eqs. (3.13) and (A3),

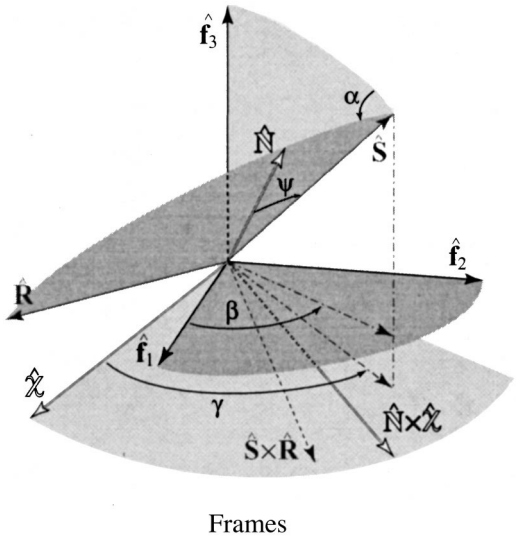

FIG. 1. *Space* frame ($\hat{f}_r$), *spin* frame ($\hat{S}$, $\hat{R}$, $\hat{S}\times\hat{R}$) and *dynamical body* frame ($\hat{N}$, $\hat{\chi}$, $\hat{N}\times\hat{\chi}$) for $N\geqslant 3$ particles. ψ—angle between $\hat{N}$ and $\hat{S}$; α—angle between the planes $\hat{S}-\hat{f}_3$ and $\hat{S}-\hat{R}$; β—angle between $\hat{f}_1$ and the projection of $\hat{S}$ onto the plane $\hat{f}_1-\hat{f}_2$; γ—angle between $\hat{\chi}$ and the projection of $\hat{S}$ onto the plane $\hat{\chi}-\hat{N}\times\hat{\chi}$.

$$
\begin{aligned}
\vec{\rho}_a &= \rho_a \hat{R}_a \\
&= \rho_a[\vec{N}+(-)^{a+1}\vec{\chi}] \\
&= \rho_a[|\vec{N}|\hat{N}+(-)^{a+1}\sqrt{1-\vec{N}^2}\hat{\chi}] \\
&= [\vec{\rho}_a\cdot\hat{S}]\hat{S}+[\vec{\rho}_a\cdot\hat{R}]\hat{R}+[\vec{\rho}_a\cdot\hat{S}\times\hat{R}]\hat{S}\times\hat{R} \\
&= \vec{\rho}_a[S,\alpha;S^3,\beta;\check{S}^3,\gamma;\rho_a,|\vec{N}|]. \qquad (3.19)
\end{aligned}
$$

The analogous formulas for the relative momenta are [see Eq. (A3) for the expression of the body frame components of $\vec{\pi}_a$]

$$
\begin{aligned}
\vec{\pi}_a &= \tilde{\pi}_a\hat{R}_a+\frac{S_a}{\rho_a}\hat{S}_a\times\hat{R}_a \\
&= \tilde{\pi}_a\hat{\rho}_a+\frac{S_a}{\rho_a}\hat{S}_a\times\hat{\rho}_a \\
&= [\vec{\pi}_a\cdot\hat{N}]\hat{N}+[\vec{\pi}_a\cdot\hat{\chi}]\hat{\chi}+[\vec{\pi}_a\cdot\hat{N}\times\hat{\chi}]\hat{N}\times\hat{\chi} \\
&= [\vec{\pi}_a\cdot\hat{S}]\hat{S}+[\vec{\pi}_a\cdot\hat{R}]\hat{R}+[\vec{\pi}_a\cdot\hat{S}\times\hat{R}]\hat{S}\times\hat{R} \\
&= \vec{\pi}_a[S,\alpha;S^3,\beta;\check{S}^3,\gamma;|\vec{N}|,\xi;\rho_a,\tilde{\pi}_a]. \qquad (3.20)
\end{aligned}
$$

Finally, the results of Appendix B allow us to perform a sequence of a canonical transformation to Euler angles $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ with their conjugate momenta, followed by a transition to the anholonomic basis used in the orientation-shape bundle approach,[9]

$$
\begin{array}{|c c c|} \hline \alpha & \beta & \gamma \\ S=\check{S} & S^3 & \check{S}^3 \\ \hline \end{array}
\quad\longrightarrow\quad
\begin{array}{|c c c|} \hline \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} \\ p_{\tilde{\alpha}} & p_{\tilde{\beta}} & p_{\tilde{\gamma}} \\ \hline \end{array}
\quad\xrightarrow{non\ can.}\quad
\begin{array}{|c c c|} \hline \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} \\ \check{S}^1 & \check{S}^2 & \check{S}^3 \\ \hline \end{array}
$$

$$S=\check{S}=\sqrt{(\check{S}^1)^2+(\check{S}^2)^2+(\check{S}^3)^2},$$

$$S^3=-\sin\tilde{\beta}\cos\tilde{\gamma}\check{S}^1+\sin\tilde{\beta}\sin\tilde{\gamma}\check{S}^2+\cos\tilde{\beta}\check{S}^3,$$

$$\alpha=\arctan\frac{p_{\tilde{\beta}}\tan\tilde{\beta}}{\check{S}-\dfrac{p_{\tilde{\alpha}}p_{\tilde{\gamma}}}{\check{S}\cos\tilde{\beta}}},\tag{3.21}$$

$$\gamma=\frac{\pi}{2}-\tilde{\gamma}-\arctan\frac{\cot\tilde{\beta}p_{\tilde{\gamma}}-\dfrac{p_{\tilde{\alpha}}}{\sin\tilde{\beta}}}{p_{\tilde{\beta}}},$$

$$\beta=\tilde{\alpha}+\arctan\frac{\cot\tilde{\beta}p_{\tilde{\alpha}}-\dfrac{p_{\tilde{\gamma}}}{\sin\tilde{\beta}}}{p_{\tilde{\beta}}}-\frac{\pi}{2}.$$

Here $p_{\tilde{\alpha}}$, $p_{\tilde{\beta}}$, $p_{\tilde{\gamma}}$ are the functions of $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$, $\check{S}^r$ given in Eqs. (B3). The equations (B3), (3.21), (3.13) and $\check{S}^2=\vec{S}\cdot\hat{N}\times\hat{\chi}$ lead to the determination of the *dynamical orientation variables* $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ in terms of $\vec{\rho}_a$, $\vec{\pi}_a$. Let us stress that, while in the orientation-shape bundle approach the orientation variables θ^α are gauge variables, the Euler angles $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ are *uniquely determined* in terms of the original configurations and momenta.

In conclusion, the complete transition to the anholonomic basis used in the *static* theory of the orientation-shape bundle is (another possible anholonomic basis is $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$, S^r)

α	β	γ	$\lvert\vec{N}\rvert$	ρ_a
$S=\check{S}$	S^3	$\check{S}^3$	ξ	$\tilde{\pi}_a$

$\xrightarrow{non\ can.}$

$\tilde{\alpha}$	$\tilde{\beta}$	$\tilde{\gamma}$	$\lvert\vec{N}\rvert$	ρ_a
$\check{S}^1$	$\check{S}^2$	$\check{S}^3$	ξ	$\tilde{\pi}_a$

(3.22)

In order to further the comparison with the orientation-shape bundle approach, let us note the following relation between the space and body components of the relative coordinates. Eqs. (3.20), (3.22), (3.18) and (B2) imply

$$\rho^r_a=\mathcal{R}^r{}_s(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{\rho}^s_a(q),$$

with

$$\check{\rho}^1_a(q)=(-)^{a+1}\rho_a\sqrt{1-\vec{N}^2},\quad \check{\rho}^2_a(q)=0,\quad \check{\rho}^3_a(q)=\rho_a|\vec{N}|,$$

and

$$S^r=\mathcal{R}^r{}_s(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{S}^s,\tag{3.23}$$

so that the final visualization of our sequence of transformations is

$\vec{\rho}_a$
$\vec{\pi}_a$

$\xrightarrow{non\ can.}$

$\tilde{\alpha}$	$\tilde{\beta}$	$\tilde{\gamma}$	$q^\mu(\vec{\rho}_a)$
$\check{S}^1$	$\check{S}^2$	$\check{S}^3$	$p_\mu(\vec{\rho}_a,\vec{\pi}_a)$

(3.24)

Note furthermore that we get $\check{\rho}_a^2=\vec{\rho}_a\cdot\hat{N}\times\hat{\chi}=0$ by construction and this entails that using our *dynamical body frame* is equivalent to a convention (*xxzz gauge*) about the body frame of the type of *xxz* and similar gauges quoted in Ref. 9.

Finally, we can give the expression of the Hamiltonian for relative motions in terms of the anholonomic Darboux basis of Eqs. (3.21). By using Eq. (A3) we get

$$
\begin{aligned}
H_{\rm rel}=&\frac{1}{2\vec{N}^2}\left[\frac{1}{2}\left(\frac{k^{-1}{}_{11}}{\rho_1^2}+\frac{k^{-1}{}_{22}}{\rho_2^2}\right)+\frac{k^{-1}{}_{12}}{\rho_1\rho_2}\right](\check{S}^1)^2+\frac{1}{2}\left[\frac{1}{2}\left(\frac{k^{-1}{}_{11}}{\rho_1^2}+\frac{k^{-1}{}_{22}}{\rho_2^2}\right)+\frac{k^{-1}{}_{12}(2\vec{N}^2-1)}{\rho_1\rho_2}\right](\check{S}^2)^2\\
&+\frac{1}{2(1-\vec{N}^2)}\left[\frac{1}{2}\left(\frac{k^{-1}{}_{11}}{\rho_1^2}+\frac{k^{-1}{}_{22}}{\rho_2^2}\right)-\frac{k^{-1}{}_{12}}{\rho_1\rho_2}\right](\check{S}^3)^2+\sqrt{1-\vec{N}^2}\left[\frac{\xi}{2}\left(\frac{k^{-1}{}_{11}}{\rho_1^2}-\frac{k^{-1}{}_{22}}{\rho_2^2}\right)\right.\\
&\left.+2k^{-1}{}_{12}|\vec{N}|\sqrt{1-\vec{N}^2}\left(\frac{\tilde{\pi}_1}{\rho_2}-\frac{\tilde{\pi}_2}{\rho_1}\right)\right]\check{S}^2-\frac{1}{2|\vec{N}|\sqrt{1-\vec{N}^2}}\left(\frac{k^{-1}{}_{11}}{\rho_1^2}-\frac{k^{-1}{}_{22}}{\rho_2^2}\right)\check{S}^1\check{S}^3+k^{-1}{}_{11}\\
&\times\left[\tilde{\pi}_1^2+\frac{\xi^2(1-\vec{N}^2)}{4\rho_1^2}\right]+k^{-1}{}_{22}\left[\tilde{\pi}_2^2+\frac{\xi^2(1-\vec{N}^2)}{4\rho_2^2}\right]+2k^{-1}{}_{12}\left[(2\vec{N}^2-1)\tilde{\pi}_1\tilde{\pi}_2-|\vec{N}|(1-\vec{N}^2)\right.\\
&\left.\times\xi\left(\frac{\tilde{\pi}_1}{\rho_2}+\frac{\tilde{\pi}_2}{\rho_1}\right)+\frac{\xi^2(1-\vec{N}^2)(2\vec{N}^2-1)}{4\rho_1\rho_2}\right]\overset{\rm def}{=}\frac{1}{2}[\check{S}^r(\check{\mathcal{I}}^{-1})^{rs}\check{S}^s+\tilde{g}^{\mu\nu}(p_\mu-\vec{S}\cdot\vec{\mathcal{A}}_\mu)(p_\nu-\check{\vec{S}}\cdot\check{\vec{\mathcal{A}}}_\nu)],
\end{aligned}
\tag{3.25}
$$

where $q^\mu=(\rho_1,\rho_2,|\vec{N}|)$, $p_\mu=(\tilde{\pi}_1,\tilde{\pi}_2,\xi)$ are the dynamical shape variables. By reason of comparison, in the last line we have presented the Hamiltonian in the form of the static SO(3) principal bundle approach. In Appendix E of Ref. 33 there is the determination of the quantities $\check{\mathcal{A}}_\mu^r(q)$ [the SO(3) gauge potential], $\tilde{g}^{\mu\nu}(q)$ (the inverse metric), $\check{\mathcal{I}}^{-1rs}(q)$ (the tensor of inertia) appearing in the *xxzz gauge*. Recall that the special *xxzz gauge* potentials $\check{\mathcal{A}}_\mu^r(q)$ are measurable quantities in our approach. The same holds for the angular velocity in the evolving dynamical body frame.

By evaluating $p_\mu|_{\dot{q}=0}$, we can recover the rotational kinetic energy (the centrifugal potential) $H_{\rm rel}^{\rm (rot)}=\frac{1}{2}\check{S}^r(\check{\mathcal{I}}^{-1})^{rs}\check{S}^s$ of the *xxzz gauge*. In our approach the measurable *vibrational* kinetic energy $H_{\rm rel}^{\rm (vib)}$ for $\vec{S}\neq 0$ nonsingular $N=3$ configurations can be obtained by restricting $\check{S}^r$ in $H_{\rm rel}$ to the value $\check{S}^r|_{\check{\omega}^s=0}$ [see Eq. (3.32) and Appendix E of Ref. 33], upon the requirement that the dynamical angular velocity vanishes in the *xxzz gauge*. Let us remark that we get $H_{\rm rel}\neq H_{\rm rel}^{\rm (rot)}+H_{\rm rel}^{\rm (vib)}$, differently from the static orientation-shape bundle result associated with the C-connection. In order to get the theory with the Jacobi normal coordinates one has to perform our sequence of canonical transformations after having diagonalized k_{ab}.

The Hamiltonian in the basis (3.15) can be obtained with the following replacements $\check{S}^1=\sqrt{(S)^2-(\check{S}^3)^2}\cos\gamma$ and $\check{S}^2=\sqrt{(S)^2-(\check{S}^3)^2}\sin\gamma$.

C. *N*-body systems

Let us now consider the general case with $N\geqslant 4$ without introducing Jacobi normal coordinates. Instead of coupling the centers of mass of particle clusters as it is done with Jacobi coordinates (*center-of-mass clusters*), the *canonical spin bases* will be obtained by coupling the spins of the 2-body subsystems (*relative particles*) $\vec{\rho}_a$, $\vec{\pi}_a$, $a=1,...,N-1$, defined in Eqs. (2.7), in all possible ways (*spin clusters* from the addition of angular momenta). Let us stress that we can build a *spin basis* with a pattern of *spin clusters* completely unrelated to a possible pre-existing *center-of-mass clustering*.

Let us consider the case $N=4$ as a prototype of the general construction. We have now three relative variables $\vec{\rho}_1$, $\vec{\rho}_2$, $\vec{\rho}_3$ and related momenta $\vec{\pi}_1$, $\vec{\pi}_2$, $\vec{\pi}_3$. In the following formulas we use the convention that the subscripts a, b, c mean any permutation of 1,2,3.

By using the explicit construction given in Appendix C, we define the following sequence of canonical transformations (we assume $S\neq 0$; $S_A\neq 0$, $A=a,b,c$) corresponding to the *spin clustering* pattern $abc\mapsto(ab)c\mapsto((ab)c)$ [build first the spin cluster (ab), then the spin cluster $((ab)c)$]:

$$
\begin{array}{|cccc|}\hline \vec{\rho}_a & \vec{\rho}_b & \vec{\rho}_c & \\ \vec{\pi}_a & \vec{\pi}_b & \vec{\pi}_c & \\ \hline \end{array} \longrightarrow
$$

$$
\longrightarrow \begin{array}{|cc|cc|cc|ccc|}\hline \alpha_a & \beta_a & \alpha_b & \beta_b & \alpha_c & \beta_c & \rho_a & \rho_b & \rho_c \\ S_a & S_a^3 & S_b & S_b^3 & S_c & S_c^3 & \tilde{\pi}_a & \tilde{\pi}_b & \tilde{\pi}_c \\ \hline \end{array} \longrightarrow
$$

$$
\xrightarrow{(ab)c} \begin{array}{|cc|c|cc|ccc|}\hline \alpha_{(ab)} & \beta_{(ab)} & \gamma_{(ab)} & \alpha_c & \beta_c & |\vec{N}_{(ab)}| & \rho_a & \rho_b & \rho_c \\ S_{(ab)} & S^3_{(ab)} & \check{S}^3_{(ab)}=\vec{S}_{(ab)}\cdot\hat{N}_{(ab)} & S_c & S_c^3 & \xi_{(ab)} & \tilde{\pi}_a & \tilde{\pi}_b & \tilde{\pi}_c \\ \hline \end{array} \longrightarrow
$$

$$
\longrightarrow \begin{array}{|cc|c|c|cc|ccc|}\hline \alpha_{((ab)c)} & \beta_{((ab)c)} & \gamma_{((ab)c)} & |\vec{N}_{((ab)c)}| & \gamma_{(ab)} & |\vec{N}_{(ab)}| & \rho_a & \rho_b & \rho_c \\ S=\check{S} & S^3 & \check{S}^3=\vec{S}\cdot\hat{N}_{((ab)c)} & \xi_{((ab)c)} & \vec{S}_{(ab)}\cdot\hat{N}_{(ab)} & \xi_{(ab)} & \tilde{\pi}_a & \tilde{\pi}_b & \tilde{\pi}_c \\ \hline \end{array} \longrightarrow
$$

$$
\xrightarrow{non\ can.} \begin{array}{|ccc|c|c|cc|ccc|}\hline \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} & |\vec{N}_{((ab)c)}| & \gamma_{(ab)} & |\vec{N}_{(ab)}| & \rho_a & \rho_b & \rho_c \\ \check{S}^1 & \check{S}^2 & \check{S}^3 & \xi_{((ab)c)} & \Omega_{(ab)}=\vec{S}_{(ab)}\cdot\hat{N}_{(ab)} & \xi_{(ab)} & \tilde{\pi}_a & \tilde{\pi}_b & \tilde{\pi}_c \\ \hline \end{array} \tag{3.26}
$$

The first nonpoint canonical transformation is based on the existence of the three unit vectors $\hat{R}_A$, $A=a,b,c$, and of three $E(3)$ realizations with generators $\vec{S}_A$, $\hat{R}_A$ and fixed values ($\hat{R}_A^2=1$, $\vec{S}_A\cdot\hat{R}_A=0$) of the invariants. Use Eqs. (3.10), (3.11) and (3.12).

In the next canonical transformation the spins of the *relative particles a* and *b* are coupled to form the spin cluster (ab), leaving the *relative particle c* as a spectator. We use Eq. (3.13) to define $\vec{N}_{(ab)}=\frac{1}{2}(\hat{R}_a+\hat{R}_b)$, $\vec{\chi}_{(ab)}=\frac{1}{2}(\hat{R}_a-\hat{R}_b)$, $\vec{S}_{(ab)}=\vec{S}_a+\vec{S}_b$, $\vec{W}_{(ab)}=\vec{S}_a-\vec{S}_b$. We get $\vec{N}_{(ab)}\cdot\vec{\chi}_{(ab)}=0$, $\{N^r_{(ab)},N^s_{(ab)}\}=\{N^r_{(ab)},\chi^s_{(ab)}\}=\{\chi^r_{(ab)},\chi^s_{(ab)}\}=0$ and a new $E(3)$ realization generated by $\vec{S}_{(ab)}$ and $\vec{N}_{(ab)}$, with nonfixed invariants $|\vec{N}_{(ab)}|$, $\vec{S}_{(ab)}\cdot\hat{N}_{(ab)}\overset{\text{def}}{=}\Omega_{(ab)}$. From Eqs. (3.20) it follows that

$$
\begin{aligned}
\vec{\rho}_a&=\rho_a[|\vec{N}_{(ab)}|\hat{N}_{(ab)}+\sqrt{1-\vec{N}^2_{(ab)}}\hat{\chi}_{(ab)}],\\
\vec{\rho}_b&=\rho_b[|\vec{N}_{(ab)}|\hat{N}_{(ab)}-\sqrt{1-\vec{N}^2_{(ab)}}\hat{\chi}_{(ab)}],\\
\vec{\rho}_c&=\rho_c\hat{R}_c\,.
\end{aligned}
\tag{3.27}
$$

Equation (3.16) defines $\alpha_{(ab)}$ and $\beta_{(ab)}$, so that Eq. (3.5) defines a unit vector $\hat{R}_{(ab)}$ with $\vec{S}_{(ab)}\cdot\hat{R}_{(ab)}=0$, $\{\hat{R}^r_{(ab)},\hat{R}^s_{(ab)}\}=0$. This unit vector identifies the *spin cluster* (ab) in the same way as the unit vectors $\hat{R}_A=\hat{\vec{\rho}}_A$ identify the *relative particles A*.

The next step is the coupling of the *spin cluster* (ab) with unit vector $\hat{R}_{(ab)}$ [described by the canonical variables $\alpha_{(ab)}$, $S_{(ab)}$, $\beta_{(ab)}$ $S^3_{(ab)}$] with the *relative particle c* with unit vector $\hat{R}_c$ and described by α_c, S_c, β_c, S_c^3: this builds the *spin cluster* $((ab)c)$.

Again, Eq. (3.13) allows us to define $\vec{N}_{((ab)c)}=\frac{1}{2}(\hat{R}_{(ab)}+\hat{R}_c)$, $\vec{\chi}_{((ab)c)}=\frac{1}{2}(\hat{R}_{(ab)}-\hat{R}_c)$, $\vec{S}=\vec{S}_{((ab)c)}=\vec{S}_{(ab)}+\vec{S}_c$, $\vec{W}_{((ab)c)}=\vec{S}_{(ab)}-\vec{S}_c$. Since we have $\vec{N}_{((ab)c)}\cdot\vec{\chi}_{((ab)c)}=0$ and $\{N^r_{((ab)c)},N^s_{((ab)c)}\}=\{N^r_{((ab)c)},\chi^s_{((ab)c)}\}=\{\chi^r_{((ab)c)},\chi^s_{((ab)c)}\}=0$ due to $\{\hat{R}^r_{(ab)},\hat{R}^s_c\}=0$, a new $E(3)$ realization generated by $\vec{S}$ and $\vec{N}_{((ab)c)}$ with nonfixed invariants $|\vec{N}_{((ab)c)}|$, $\vec{S}\cdot\hat{N}_{((ab)c)}=\check{S}^3$ emerges. Equation (3.16) defines $\alpha_{((ab)c)}$ and $\beta_{((ab)c)}$, so that Eq. (3.5) allows us to identify a final unit vector $\hat{R}_{((ab)c)}$ with $\vec{S}\cdot\hat{R}_{((ab)c)}=0$ and $\{\hat{R}^r_{((ab)c)},\hat{R}^s_{((ab)c)}\}=0$.

In conclusion, when $S\neq 0$, we find both a *spin frame* $\hat{S}$, $\hat{R}_{((ab)c)}$, $\hat{R}_{((ab)c)}\times\hat{S}$ and a *dynamical body frame* $\hat{\chi}_{((ab)c)}$, $\hat{N}_{((ab)c)}\times\hat{\chi}_{((ab)c)}$, $\hat{N}_{((ab)c)}$, like in the 3-body case. There is an *important difference*, however: the orthonormal vectors $\vec{N}_{((ab)c)}$ and $\vec{\chi}_{((ab)c)}$ depend on the momenta of the

relative particles a and b through $\hat{R}_{(ab)}$, so that our results do not share any relation with the $N=4$ nontrivial SO(3) principal bundle of the orientation-shape bundle approach.

The final 6 *dynamical shape variables* are $q^{\mu}=\{|\vec{N}_{((ab)c)}|,\gamma_{(ab)},|\vec{N}_{(ab)}|,\rho_a,\rho_b,\rho_c\}$. While the last four depend only on the original relative coordinates $\vec{\rho}_A$, $A=a,b,c$, the first two depend also on the original momenta $\vec{\pi}_A$: therefore they are *generalized shape variables*. By using Appendix B, we obtain

$$\rho_A^r=\mathcal{R}^{rs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{\rho}_A^s(q^{\mu},p_{\mu},\check{S}^r),\quad A=a,b,c. \tag{3.28}$$

This means that for $N=4$ the dynamical body frame components $\check{\rho}_A^r$ depend also on the dynamical shape momenta and on the dynamical body frame components of the spin. It is clear that this result stands completely outside the orientation-shape bundle approach.

As shown in Appendix F of Ref. 33, starting from the Hamiltonian $H_{\mathrm{rel}((ab)c)}$ expressed in the final variables, we can define a rotational Hamiltonian $H^{(\mathrm{rot})}_{\mathrm{rel}((ab)c)}$ and a vibrational Hamiltonian $H^{(\mathrm{vib})}_{\mathrm{rel}((ab)c)}$ (vanishing of the physical dynamical angular velocity $\check{\omega}^r_{((ab)c)}=0$), but $H_{\mathrm{rel}((ab)c)}$ fails to be the sum of these two Hamiltonians showing once again the nonseparability of rotations and vibrations. Let us stress that in the rotational Hamiltonian we find an *inertia-like tensor* depending only on the dynamical shape variables. A similar result, however, does not hold for the spin-angular velocity relation.

The price to be paid for the existence of 3 global *dynamical body frames* for $N=4$ is a more complicated form of the Hamiltonian kinetic energy. On the other hand, *dynamical vibrations* and *dynamical angular velocity* are measurable quantities in each dynamical body frame.

For $N=5$ we can repeat the previous construction either with the sequence of spin clusterings $abcd\mapsto(ab)cd\mapsto((ab)c)d)\mapsto(((ab)c)d)$ or with the sequence $abcd\mapsto(ab)(cd)\mapsto((ab)\times(cd))$ (a, b, c, d any permutation of 1,2,3,4) as stated in the Introduction. Each *spin cluster* $(\cdots)$ will be identified by the unit vector $\hat{R}_{(\cdots)}$, the axis of the *spin frame* of the cluster. All the final *dynamical body frames* built with this construction will have their axes depending on both the original configurations and momenta.

This construction is trivially generalized to any N: we have only to classify all the possible *spin clustering patterns*.

Therefore, for $N\geq 4$ our sequence of canonical and noncanonical transformations leads to the following result, to be compared with Eq. (3.22) of the 3-body case,

$$\begin{array}{|c|}\hline \vec{\rho}_A \\ \hline \vec{\pi}_A \\ \hline \end{array} \quad \overset{non\ can.}{\longrightarrow} \quad \begin{array}{|ccc|c|}\hline \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} & q^{\mu}(\vec{\rho}_A,\vec{\pi}_A) \\ \hline \check{S}^1 & \check{S}^2 & \check{S}^3 & p_{\mu}(\vec{\rho}_A,\vec{\pi}_A) \\ \hline \end{array} \tag{3.29}$$

This state of affairs suggests that for $N\geq 4$ and with $S\neq 0$, $S_A\neq 0$, $A=a,b,c$, namely when the standard $(3N\text{-}3)$-dimensional orientation-shape bundle is not trivial, the original $(6N\text{-}6)$-dimensional relative phase space admits the definition of as many *dynamical body frames* as spin canonical bases, which are globally defined (apart isolated coordinate singularities) for the nonsingular N-body configurations with $\vec{S}\neq 0$ (and with nonzero spin for each spin subcluster).

These *dynamical body frames* do not correspond to local cross sections of the static nontrivial orientation-shape SO(3) principal bundle and the spin canonical bases do not coincide with the canonical bases associated with the static theory.

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APPENDIX A: SOME FORMULAS FOR THE CASE $N=3$

In this appendix we justify Eq. (3.19). To find the expression of $\vec{\pi}_a\cdot\hat{N}$, $\vec{\pi}_a\cdot\hat{\chi}$, $\vec{\pi}_a\cdot\hat{N}\times\hat{\chi}$ let us consider the following quantities:

$$\vec{S}_1=\vec{\rho}_1\times\vec{\pi}_1=\rho_1[\vec{N}\times\vec{\pi}_1+\vec{\chi}\times\vec{\pi}_1],$$

$$\vec{S}_2=\vec{\rho}_2\times\vec{\pi}_2=\rho_2[\vec{N}\times\vec{\pi}_2-\vec{\chi}\times\vec{\pi}_2],$$

$$\vec{S}=\vec{S}_1+\vec{S}_2=\vec{N}\times[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2]+\vec{\chi}\times[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2],$$

$$\vec{W}=\vec{S}_1-\vec{S}_2=\vec{N}\times[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2]+\vec{\chi}\times[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2],$$

$$\vec{S}\cdot\vec{N}=|\vec{N}|\check{S}^3=|\vec{N}||\vec{\chi}|[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2]\cdot\hat{N}\times\hat{\chi}=|\vec{N}||\vec{\chi}|b_3,$$

$$\vec{S}\cdot\vec{\chi}=|\vec{\chi}|\check{S}^1=-|\vec{N}||\vec{\chi}|[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2]\cdot\hat{N}\times\hat{\chi}=-|\vec{N}||\vec{\chi}|a_3,$$

$$\vec{S}\cdot\vec{N}\times\vec{\chi}=|\vec{N}\times\vec{\chi}|\check{S}^2=\vec{N}^2|\vec{\chi}|[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2]\cdot\hat{\chi}-\vec{\chi}^2|\vec{N}|[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2]\cdot\hat{N}=\vec{N}^2|\vec{\chi}|a_2-\vec{\chi}^2|\vec{N}|b_1,$$

$$\vec{W}\cdot\vec{N}=-\vec{S}\cdot\vec{\chi},\tag{A1}$$

$$\vec{W}\cdot\vec{\chi}=-\vec{S}\cdot\vec{N},$$

$$\vec{W}\cdot\vec{N}\times\vec{\chi}=\vec{N}^2|\vec{\chi}|[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2]\cdot\hat{\chi}-\vec{\chi}^2|\vec{N}|[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2]\cdot\hat{N}=\vec{N}^2|\vec{\chi}|b_2-\vec{\chi}^2|\vec{N}|a_1,$$

$$\rho_1\tilde{\pi}_1=\vec{\rho}_1\cdot\vec{\pi}_1=\rho_1[\vec{\pi}_1\cdot\vec{N}+\vec{\pi}_1\cdot\vec{\chi}],$$

$$\rho_2\tilde{\pi}_2=\vec{\rho}_2\cdot\vec{\pi}_2=\rho_2[\vec{\pi}_2\cdot\vec{N}-\vec{\pi}_2\cdot\vec{\chi}],$$

$$\rho_1\tilde{\pi}_1+\rho_2\tilde{\pi}_2=\vec{\rho}_1\cdot\vec{\pi}_1+\vec{\rho}_2\cdot\vec{\pi}_2=[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2]\cdot\vec{N}+[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2]\cdot\vec{\chi}=|\vec{N}|a_1+|\vec{\chi}|b_2,$$

$$\rho_1\tilde{\pi}_1-\rho_2\tilde{\pi}_2=\vec{\rho}_1\cdot\vec{\pi}_1-\vec{\rho}_2\cdot\vec{\pi}_2=[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2]\cdot\vec{N}+[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2]\cdot\vec{\chi}=|\vec{N}|b_1+|\vec{\chi}|a_2,$$

where

$$a_1=[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2]\cdot\hat{N},$$

$$a_2=[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2]\cdot\hat{\chi},$$

$$a_3=[\rho_1\vec{\pi}_1+\rho_2\vec{\pi}_2]\cdot\hat{N}\times\hat{\chi},$$

$$b_1=[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2]\cdot\hat{N},\tag{A2}$$

$$b_2=[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2]\cdot\hat{\chi},$$

$$b_3=[\rho_1\vec{\pi}_1-\rho_2\vec{\pi}_2]\cdot\hat{N}\times\hat{\chi}.$$

Since $\vec{S}\cdot\hat{N}=\check{S}^3$, $\vec{S}\cdot\hat{\chi}=\sin\psi\cos\gamma=\check{S}^1$, $\vec{S}\cdot\hat{N}\times\hat{\chi}=\sin\psi\sin\gamma=\check{S}^2$, $\vec{W}\cdot\hat{N}\times\hat{\chi}=\xi\sqrt{1-\vec{N}^2}$, from Eq. (A1) we get $\vec{\pi}_a$ in terms of the final canonical variables:

$$\vec{\pi}_1\cdot\hat{N}=\frac{a_1+b_1}{2\rho_1}=\tilde{\pi}_1|\vec{N}|-\frac{\sqrt{1-\vec{N}^2}}{2\rho_1}[\check{S}^2+\xi\sqrt{1-\vec{N}^2}],$$

$$\vec{\pi}_2\cdot\hat{N}=\frac{a_1-b_1}{2\rho_2}=\tilde{\pi}_2|\vec{N}|+\frac{\sqrt{1-\vec{N}^2}}{2\rho_2}[\check{S}^2-\xi\sqrt{1-\vec{N}^2}],$$

$$\vec{\pi}_1\cdot\hat{\chi}=\frac{a_2+b_2}{2\rho_1}=\tilde{\pi}_1\sqrt{1-\vec{N}^2}+\frac{|\vec{N}|}{2\rho_1}[\check{S}^2+\xi\sqrt{1-\vec{N}^2}],$$

$$\vec{\pi}_2\cdot\hat{\chi}=\frac{a_2-b_2}{2\rho_2}=-\tilde{\pi}_2\sqrt{1-\vec{N}^2}+\frac{|\vec{N}|}{2\rho_2}[\check{S}^2-\xi\sqrt{1-\vec{N}^2}], \tag{A3}$$

$$\vec{\pi}_1\cdot\hat{N}\times\hat{\chi}=\frac{a_3+b_3}{2\rho_1}=\frac{1}{2\rho_1}\left[-\frac{\check{S}^1}{|\vec{N}|}+\frac{\check{S}^3}{\sqrt{1-\vec{N}}^2}\right],$$

$$\vec{\pi}_2\cdot\hat{N}\times\hat{\chi}=\frac{a_3-b_3}{2\rho_2}=-\frac{1}{2\rho_2}\left[\frac{\check{S}^1}{|\vec{N}|}+\frac{\check{S}^3}{\sqrt{1-\vec{N}^2}}\right].$$

With these results we can obtain the expression of the spin quantities $\vec{W}$, $\vec{S}_a$ in terms of the final variables [see Eq. (C6) of Ref. 33].

APPENDIX B: EULER ANGLES

Let us denote by $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ the Euler angles chosen as orientation variables θ^α.

Let $\hat{f}_1=\hat{\imath}$, $\hat{f}_2=\hat{\jmath}$, $\hat{f}_3=\hat{k}$ be the unit 3-vectors along the axes of the space frame and $\hat{e}_1=\hat{\chi}$, $\hat{e}_2=\hat{N}\times\hat{\chi}$, $\hat{e}_3=\hat{N}$, the unit 3-vectors along the axes of a *body frame*. Then we have

$$\vec{S}=S^r\hat{f}_r=R^{rs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{S}^s\hat{f}_r=\check{S}^s\hat{e}_s,$$
$$\hat{e}_s=(R^T)^{sr}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\hat{f}_r=\mathcal{R}_s{}^r(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\hat{f}_r. \tag{B1}$$

There are two main conventions for the definition of the Euler angles $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$.

(A) The *y-convention* [see Refs. 44 (Appendix B) and 45]:

(i) perform a first rotation of an angle $\tilde{\alpha}$ around $\hat{f}_3$ [$\hat{f}_1\mapsto\hat{e}'_1=\cos\tilde{\alpha}\hat{f}_1+\sin\tilde{\alpha}\hat{f}_2$, $\hat{f}_2\mapsto\hat{e}'_2=-\sin\tilde{\alpha}\hat{f}_1+\cos\tilde{\alpha}\hat{f}_2$, $\hat{f}_3\mapsto\hat{e}'_3=\hat{f}_3$];

(ii) perform a second rotation of an angle $\tilde{\beta}$ around $\hat{e}'_2$ [$\hat{e}'_1\mapsto\hat{e}''_1=\cos\tilde{\beta}\hat{e}'_1-\sin\tilde{\beta}\hat{e}'_3$, $\hat{e}'_2\mapsto\hat{e}''_2=\hat{e}'_2$, $\hat{e}'_3\mapsto\hat{e}''_3=\sin\tilde{\beta}\hat{e}'_1+\cos\tilde{\beta}\hat{e}'_3$];

(iii) perform a third rotation of an angle $\tilde{\gamma}$ around $\hat{e}''_3$ [$\hat{e}''_1\mapsto\hat{e}_1=\cos\tilde{\gamma}\hat{e}''_1+\sin\tilde{\gamma}\hat{e}''_2$, $\hat{e}''_2\mapsto\hat{e}_2=-\sin\tilde{\gamma}\hat{e}''_1+\cos\tilde{\gamma}\hat{e}''_2$]. In this way we get

$$\begin{pmatrix}\hat{\chi}\\ \hat{N}\times\hat{\chi}\\ \hat{N}\end{pmatrix}\equiv\begin{pmatrix}\hat{e}_1\\ \hat{e}_2\\ \hat{e}_3\end{pmatrix}=\mathcal{R}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\begin{pmatrix}\hat{f}_1\\ \hat{f}_2\\ \hat{f}_3\end{pmatrix},$$

$$\mathcal{R}_r{}^s(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})$$
$$= R^{Trs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})$$
$$= \begin{pmatrix} \cos\tilde{\gamma}\cos\tilde{\beta}\cos\tilde{\alpha}-\sin\tilde{\gamma}\sin\tilde{\alpha} & \cos\tilde{\gamma}\cos\tilde{\beta}\sin\tilde{\alpha}+\sin\tilde{\gamma}\cos\tilde{\alpha} & -\cos\tilde{\gamma}\sin\tilde{\beta} \\ -(\sin\tilde{\gamma}\cos\tilde{\beta}\cos\tilde{\alpha}+\cos\tilde{\gamma}\sin\tilde{\alpha} & -\sin\tilde{\gamma}\cos\tilde{\beta}\sin\tilde{\alpha}+\cos\tilde{\gamma}\cos\tilde{\alpha} & \sin\tilde{\gamma}\sin\tilde{\beta} \\ \sin\tilde{\beta}\cos\tilde{\alpha} & \sin\tilde{\beta}\sin\tilde{\alpha} & \cos\tilde{\beta} \end{pmatrix},$$

with

$$\tan\tilde{\alpha}=\frac{\hat{N}^2}{\hat{N}^1},\quad \cos\tilde{\beta}=\hat{N}^3,\quad \tan\tilde{\gamma}=-\frac{\hat{\chi}^3}{(\hat{N}\times\hat{\chi})^3}. \tag{B2}$$

Since $\hat{N}$ and $\hat{\chi}$ are functions of $\vec{\rho}_a$ only, see Eq. (3.13), we get $\{\tilde{\alpha},\tilde{\beta}\}=\{\tilde{\beta},\tilde{\gamma}\}=\{\tilde{\gamma},\tilde{\alpha}\}=0$.

(B) The *x-convention* (see Refs. 46, 44 (in the text) and 2): the Euler angles θ, φ and ψ are: (i) $\theta=\tilde{\beta}$; (ii) $\cos\varphi=-\sin\tilde{\alpha}$, $\sin\varphi=\cos\tilde{\alpha}$; (iii) $\cos\psi=\sin\tilde{\gamma}$, $\sin\psi=-\cos\tilde{\gamma}$.

We use the *y-convention*. Following Ref. 2, let us introduce the canonical momenta $p_{\tilde{\alpha}}$, $p_{\tilde{\beta}}$, $p_{\tilde{\gamma}}$ conjugated to $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$: $\{\tilde{\alpha},p_{\tilde{\alpha}}\}=\{\tilde{\beta},p_{\tilde{\beta}}\}=\{\tilde{\gamma},p_{\tilde{\gamma}}\}=1$ (note that this Darboux chart does not exist globally). Then, the results of Ref. 2 imply

$$\begin{aligned}
S^1&=-\sin\tilde{\alpha}p_{\tilde{\beta}}+\frac{\cos\tilde{\alpha}}{\sin\tilde{\beta}}p_{\tilde{\gamma}}-\cos\tilde{\alpha}\cot\tilde{\beta}p_{\tilde{\alpha}},\\
S^2&=\cos\tilde{\alpha}p_{\tilde{\beta}}+\frac{\sin\tilde{\alpha}}{\sin\tilde{\beta}}p_{\tilde{\gamma}}-\sin\tilde{\alpha}\cot\tilde{\beta}p_{\tilde{\alpha}},\\
S^3&=p_{\tilde{\alpha}},\\
\check{S}^1&=\sin\tilde{\gamma}p_{\tilde{\beta}}-\frac{\cos\tilde{\gamma}}{\sin\tilde{\beta}}p_{\tilde{\alpha}}+\cos\tilde{\gamma}\cot\tilde{\beta}p_{\tilde{\gamma}},\\
\check{S}^2&=\cos\tilde{\gamma}p_{\tilde{\beta}}+\frac{\sin\tilde{\gamma}}{\sin\tilde{\beta}}p_{\tilde{\alpha}}-\sin\tilde{\gamma}\cot\tilde{\beta}p_{\tilde{\gamma}},\\
\check{S}^3&=p_{\tilde{\gamma}},\\
&\Downarrow\\
p_{\tilde{\alpha}}&=S^3=-\sin\tilde{\beta}\cos\tilde{\gamma}\check{S}^1+\sin\tilde{\beta}\sin\tilde{\gamma}\check{S}^2+\cos\tilde{\beta}\check{S}^3,\\
p_{\tilde{\beta}}&=-\sin\tilde{\alpha}S^1+\cos\tilde{\alpha}S^2=\sin\tilde{\gamma}\check{S}^1-\cos\tilde{\gamma}\check{S}^2,\\
p_{\tilde{\gamma}}&=\check{S}^3=\cos\tilde{\alpha}\sin\tilde{\beta}S^1+\sin\tilde{\alpha}\sin\tilde{\beta}S^2+\cos\tilde{\beta}S^3.
\end{aligned} \tag{B3}$$

APPENDIX C: 4-BODY CASE

Let us give the main steps of the construction of the spin basis in the case $N=4$. From Eqs. (3.27) we have

$$\vec{\rho}_a=\rho_a[|\vec{N}_{(ab)}|\hat{N}_{(ab)}+\sqrt{1-\vec{N}^2_{(ab)}}\hat{\chi}_{(ab)}],$$

$$\vec{\rho}_b=\rho_b[|\vec{N}_{(ab)}|\hat{N}_{(ab)}-\sqrt{1-\vec{N}^2_{(ab)}}\hat{\chi}_{(ab)}], \tag{C1}$$

$$\vec{\rho}_c=\rho_c\hat{R}_c\,.$$

The definitions given after Eqs. (3.27) and Appendix B imply

$$\vec{N}\overset{\text{def}}{=}\vec{N}_{((ab)c)}=\frac{1}{2}(\hat{R}_{(ab)}+\hat{R}_c),$$

$$\vec{\chi}\overset{\text{def}}{=}\vec{\chi}_{((ab)c)}=\frac{1}{2}(\hat{R}_{(ab)}-\hat{R}_c),$$

$$\vec{N}\times\vec{\chi}=-\frac{1}{2}\hat{R}_{(ab)}\times\hat{R}_c\,, \tag{C2}$$

$$\Downarrow$$

$$\vec{\rho}_c=\rho_c[|\vec{N}|\hat{N}-\sqrt{1-\vec{N}^2}\hat{\chi}],$$

$$\Rightarrow\rho^r_c=\mathcal{R}^{rs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{\rho}^s_c(|\vec{N}|,\rho_c).$$

Let us remember that the dynamical shape variables of Eq. (3.26) are $q^\mu=\{|\vec{N}|,\gamma_{(ab)},|\vec{N}_{(ab)}|,\ \rho_a,\ \rho_b,\ \rho_c\}$. Then, from Eqs. (3.16) and (3.18), for the subsystem (ab) we get

$$\hat{R}_{(ab)}=\vec{N}+\vec{\chi},\quad \vec{S}_{(ab)}\cdot\hat{R}_{(ab)}=0,$$

$$\vec{S}_{(ab)}\overset{\text{def}}{=}\vec{S}_a+\vec{S}_b=S_{(ab)}(\sin\psi_{(ab)}[\cos\gamma_{(ab)}\,\hat{\chi}_{(ab)}+\sin\gamma_{(ab)}\hat{N}_{(ab)}\times\hat{\chi}_{(ab)}]=\cos\psi_{(ab)}\hat{N}_{(ab)}),$$

$$\hat{\chi}_{(ab)}=\tfrac{1}{2}(\hat{R}_a-\hat{R}_b)=\cos\gamma_{(ab)}(\sin\psi_{(ab)}\hat{S}_{(ab)}-\cos\psi_{(ab)}\hat{R}_{(ab)})-\sin\gamma_{(ab)}\hat{R}_{(ab)}\times\hat{S}_{(ab)}\,,$$

$$\hat{N}_{(ab)}=\cos\psi_{(ab)}\hat{S}_{(ab)}+\sin\psi_{(ab)}\hat{R}_{(ab)}\,, \tag{C3}$$

$$\hat{N}_{(ab)}\times\hat{\chi}_{(ab)}=\sin\gamma_{(ab)}(\sin\psi_{(ab)}\hat{S}_{(ab)}-\cos\psi_{(ab)}\hat{R}_{(ab)})+\cos\gamma_{(ab)}\hat{R}_{(ab)}\times\hat{S}_{(ab)}\,,$$

$$\cos\psi_{(ab)}=\frac{\Omega_{(ab)}}{S_{(ab)}},\quad \sin\psi_{(ab)}=\sqrt{1-\left(\frac{\Omega_{(ab)}}{S_{(ab)}}\right)^2},\quad \Omega_{(ab)}=\vec{S}_{(ab)}\cdot\hat{N}_{(ab)}\,.$$

We have, moreover,

$$\vec{S}_c=\tfrac{1}{2}(\vec{S}-\vec{W}_{((ab)c)}),$$

$$\vec{W}_{((ab)c)}\cdot\vec{N}=-\vec{S}\cdot\vec{\chi},\quad \vec{W}_{((ab)c)}\cdot\vec{\chi}=-\vec{S}\cdot\vec{N},$$

$$\check{W}^1=-\frac{|\vec{N}|\check{S}^3}{\sqrt{1-\vec{N}^2}},\quad \check{W}^2=\xi\sqrt{1-\vec{N}^2},$$

$$\check{W}^3 = -\frac{\sqrt{1-\vec{N}^2}}{|\vec{N}|}\cos\gamma\sqrt{(S)^2-(\check{S}^3)^2},$$

$$\gamma_{((ab)c)} = \tan^{-1}\frac{\vec{S}\cdot(\hat{N}\times\hat{\chi})}{\vec{S}\cdot\hat{\chi}} = \tan^{-1}\frac{\check{S}^2}{\check{S}^1},$$

$$\xi_{((ab)c)} = \frac{\vec{W}_{((ab)c)}\cdot(\hat{N}\times\hat{\chi})}{\sqrt{1-\vec{N}^2}},$$

$$\begin{aligned}\vec{S}_{(ab)} &= \tfrac{1}{2}(\vec{S}+\vec{W})_{((ab)c)}\\ &= \check{S}^1_{(ab)}\hat{\chi}+\check{S}^2_{(ab)}\hat{N}\times\hat{\chi}+\check{S}^3_{(ab)}\hat{N}\\ &= \tfrac{1}{2}(\check{S}^1+\check{W}^1_{((ab)c)})\hat{\chi}+\tfrac{1}{2}(\check{S}^2+\check{W}^2_{((ab)c)})\hat{N}\times\hat{\chi}+\tfrac{1}{2}(\check{S}^3+\check{W}^3_{((ab)c)})\hat{N},\end{aligned}$$

$$\begin{aligned}&\vec{S}=\vec{S}_a+\vec{S}_b+\vec{S}_c=\vec{S}_{(ab)}+\vec{S}_c\overset{\text{def}}{=}\vec{S}_{((ab)c)}=\check{S}^1\hat{\chi}+\check{S}^3\hat{N}+\check{S}^2\hat{N}\times\hat{\chi},\\ &\check{S}^1_{(ab)}=\frac{1}{2}\left(\check{S}^1-\frac{|\vec{N}|}{\sqrt{1-\vec{N}^2}}\check{S}^3\right),\\ &\check{S}^2_{(ab)}=\tfrac{1}{2}(\check{S}^2+\xi_{((ab)c)}\sqrt{1-\vec{N}^2}),\\ &\check{S}^3_{(ab)}=\frac{1}{2}\left(\check{S}^3-\frac{\sqrt{1-\vec{N}^2}}{|\vec{N}|}\check{S}^1\right),\end{aligned}\tag{C4}$$

$$\check{S}^1=\cos\gamma_{((ab)c)}\sqrt{(S)^2-(\check{S}^3)^2},\quad \check{S}^2=\sin\gamma_{((ab)c)}\sqrt{(S)^2-(\check{S}^3)^2},$$

$$S_{(ab)}=\sqrt{(\check{S}^1_{(ab)})^2+(\check{S}^2_{(ab)})^2+(\check{S}^3_{(ab)})^2}=\frac{1}{2}\sqrt{(\check{S}^2+\xi_{((ab)c)}\sqrt{1-\vec{N}^2})^2+\left(\frac{\check{S}^1}{|\vec{N}|}-\frac{\check{S}^3}{\sqrt{1-\vec{N}^2}}\right)^2},$$

$$\hat{S}_{(ab)}=\frac{1}{2S_{(ab)}}\left[(\check{S}^2+\xi_{((ab)c)}\sqrt{1-\vec{N}^2})\hat{N}\times\hat{\chi}+\left(\check{S}^1-\frac{|\vec{N}|}{\sqrt{1-\vec{N}^2}}\check{S}^3\right)\hat{\chi}+\left(\check{S}^3-\frac{\sqrt{1-\vec{N}^2}}{|\vec{N}|}\check{S}^1\right)\hat{N}\right],$$

$$\hat{R}_{(ab)}=|\vec{N}|\hat{N}+\sqrt{1-\vec{N}^2}\hat{\chi},$$

$$\begin{aligned}\hat{R}_{(ab)}\times\hat{S}_{(ab)}=\frac{1}{2S_{(ab)}}\Bigg[&(\check{S}^2+\xi_{((ab)c)}\sqrt{1-\vec{N}^2})(\sqrt{1-\vec{N}^2}\hat{N}-|\vec{N}|\hat{\chi})\\ &+\left(|\vec{N}|\left(\check{S}^1-\frac{|\vec{N}|}{\sqrt{1-\vec{N}^2}}\check{S}^3\right)-\sqrt{1-\vec{N}^2}\left(\check{S}^3-\frac{\sqrt{1-\vec{N}^2}}{|\vec{N}|}\check{S}^1\right)\right)\hat{N}\times\hat{\chi}\Bigg].\end{aligned}$$

The final result is $[\check{S}^1=1/S\sqrt{(S)^2-(S^3)^2}\cos\beta_{((ab)c)},\ \check{S}^2=1/S\sqrt{(S)^2-(S^3)^2}\sin\beta_{((ab)c)}]$

$$\hat{N}_{(ab)}=\cos\psi_{(ab)}\hat{S}_{(ab)}+\sin\psi_{(ab)}\hat{R}_{(ab)}$$
$$=\left[\frac{\Omega_{(ab)}\left(\check{S}^3-\frac{\sqrt{1-\vec{N}^2}}{|\vec{N}|}\check{S}^1\right)}{2(S_{(ab)})^2}+|\vec{N}|\sqrt{1-\left(\frac{\Omega_{(ab)}}{S_{(ab)}}\right)^2}\right]\hat{N}+\left[\frac{\Omega_{(ab)}\left(\check{S}^1-\frac{|\vec{N}|}{\sqrt{1-\vec{N}^2}}\check{S}^3\right)}{2(S_{(ab)})^2}\right.$$
$$\left.+\sqrt{1-\vec{N}^2}\sqrt{1-\left(\frac{\Omega_{(ab)}}{S_{(ab)}}\right)^2}\right]\hat{\chi}+\frac{\Omega_{(ab)}(\check{S}^2+\xi_{((ab)c)}\sqrt{1-\vec{N}^2}}{2(S_{(ab)})^2}\hat{N}\times\hat{\chi},$$

$$\hat{\chi}_{(ab)}=\cos\gamma_{(ab)}(\sin\psi_{(ab)}\hat{S}_{(ab)}-\cos\psi_{(ab)}\hat{R}_{(ab)})-\sin\gamma_{(ab)}\hat{R}_{(ab)}\times\hat{S}_{(ab)}$$
$$=\left(\cos\gamma_{(ab)}\left[\sqrt{1-\left(\frac{\Omega_{(ab)}}{S_{(ab)}}\right)^2}\frac{\left(\check{S}^3-\frac{\sqrt{1-\vec{N}^2}}{|\vec{N}|}\check{S}^1\right)}{2S_{(ab)}}-|\vec{N}|\frac{\Omega_{(ab)}}{S_{(ab)}}\right]\right.$$
$$\left.-\frac{\sqrt{1-\vec{N}^2}\sin\gamma_{(ab)}}{2S_{(ab)}}(\check{S}^2+\xi_{((ab)c)}\sqrt{1-\vec{N}^2})\right)\hat{N}$$
$$+\left(\cos\gamma_{(ab)}\left[\sqrt{1-\left(\frac{\Omega_{(ab)}}{S_{(ab)}}\right)^2}\frac{\left(\check{S}^1-\frac{|\vec{N}|}{\sqrt{1-\vec{N}^2}}\check{S}^3\right)}{2S_{(ab)}}-\sqrt{1-\vec{N}^2}\frac{\Omega_{(ab)}}{S_{(ab)}}\right]\right.$$
$$\left.+\frac{|\vec{N}|\sin\gamma_{(ab)}}{2S_{(ab)}}(\check{S}^2+\xi_{((ab)c)}\sqrt{1-\vec{N}^2})\right)\hat{\chi}+(\cos\gamma_{(ab)}\sqrt{1-\left(\frac{\Omega_{(ab)}}{S_{(ab)}}\right)^2}$$
$$\times\left(\frac{\check{S}^2+\xi_{((ab)c)}\sqrt{1-\vec{N}^2}}{2S_{(ab)}}\right)-\frac{\sin\gamma_{(ab)}}{2S_{(ab)}}\left[|\vec{N}|\left(\check{S}^1-\frac{|\vec{N}|}{\sqrt{1-\vec{N}^2}}\check{S}^3\right)\right.$$
$$\left.-\sqrt{1-\vec{N}^2}\left(\check{S}^3-\frac{\sqrt{1-\vec{N}^2}}{|\vec{N}|}\check{S}^1\right)\right]\hat{N}\times\hat{\chi}. \tag{C5}$$

Then, Eqs. (C1) and (C2) imply

$$\rho_a^r=\mathcal{R}^{rs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{\rho}_a^s[|\vec{N}|,\gamma_{(ab)},|\vec{N}_{(ab)}|,\rho_a;\xi,\Omega_{(ab)};\check{S}^r],$$
$$\rho_b^r=\mathcal{R}^{rs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{\rho}_b^s[|\vec{N}|,\gamma_{(ab)},|\vec{N}_{(ab)}|,\rho_a;\xi,\Omega_{(ab)};\check{S}^r], \tag{C6}$$
$$\rho_c^r=\mathcal{R}^{rs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{\rho}_c^s[|\vec{N}|,\rho_c].$$

This means that $\check{\rho}^r_{a\text{ or }b}$ depend not only on the dynamical shape variables $q^\mu=\{|\vec{N}|=|\vec{N}_{((ab)c)}|,\gamma_{(ab)},|\vec{N}_{(ab)}|,\rho_a,\rho_b,\rho_c\}$ but also on some of the conjugate shape momenta $p_\mu=\{\xi_{((ab)c)},\Omega_{(ab)}=\vec{S}_{(ab)}\cdot\hat{N}_{(ab)},\xi_{(ab)},\tilde{\pi}_a,\tilde{\pi}_b,\tilde{\pi}_c\}$ and the dynamical body frame components $\check{S}^r$ of the spin.

By using Eq. (A3), for the canonical momenta we get [$|\vec{N}|=|\vec{N}_{((ab)c)}|$, $S_{(ab)}$ given by Eq. (C4)]

$$\vec{\pi}_a = \left[\tilde{\pi}_a |\vec{N}_{(ab)}| - \frac{\sqrt{1-\vec{N}^2_{(ab)}}}{2\rho_a} \left(\sqrt{(S_{(ab)})^2 - (\Omega_{(ab)})^2} \sin\gamma_{(ab)} + \xi_{(ab)} \sqrt{1-\vec{N}^2_{(ab)}} \right) \right] \hat{N}_{(ab)}$$
$$+ \left[\tilde{\pi}_a \sqrt{1-\vec{N}^2_{(ab)}} + \frac{|\vec{N}_{(ab)}|}{2\rho_a} \left(\sqrt{(S_{(ab)})^2 - (\Omega_{(ab)})^2} \sin\gamma_{(ab)} + \xi_{(ab)} \sqrt{1-\vec{N}^2_{(ab)}} \right) \right] \hat{\chi}_{(ab)}$$
$$- \frac{1}{2\rho_a} \left((\sqrt{S_{(ab)}})^2 - (\Omega_{(ab)})^2 \right) \frac{\cos\gamma_{(ab)}}{|\vec{N}_{(ab)}|} - \frac{\Omega_{(ab)}}{\sqrt{1-\vec{N}^2_{(ab)}}} \hat{N}_{(ab)} \times \hat{\chi}_{(ab)},$$

$$\vec{\pi}_b = \left[\tilde{\pi}_b |\vec{N}_{(ab)}| + \frac{\sqrt{1-\vec{N}^2_{(ab)}}}{2\rho_b} \left(\sqrt{(S_{(ab)})^2 - (\Omega_{(ab)})^2} \sin\gamma_{(ab)} - \xi_{(ab)} \sqrt{1-\vec{N}^2_{(ab)}} \right) \right] \hat{N}_{(ab)}$$
$$- \left[\tilde{\pi}_b \sqrt{1-\vec{N}^2_{(ab)}} - \frac{|\vec{N}_{(ab)}|}{2\rho_b} \left(\sqrt{(S_{(ab)})^2 - (\Omega_{(ab)})^2} \sin\gamma_{(ab)} - \xi_{(ab)} \sqrt{1-\vec{N}^2_{(ab)}} \right) \right] \hat{\chi}_{(ab)}$$
$$- \frac{1}{2\rho_b} \left(\sqrt{(S_{(ab)})^2 - (\Omega_{(ab)})^2} \frac{\cos\gamma_{(ab)}}{|\vec{N}_{(ab)}|} + \frac{\Omega_{(ab)}}{\sqrt{1-\vec{N}^2_{(ab)}}} \right) \hat{N}_{(ab)} \times \hat{\chi}_{(ab)},$$

$$\vec{\pi}_c = \left[\tilde{\pi}_c |\vec{N}| + \frac{\sqrt{1-\vec{N}^2}}{2\rho_c} \left(\check{S}^2 - \xi_{((ab)c)} \sqrt{1-\vec{N}^2} \right) \right] \hat{N} - \left[\tilde{\pi}_c \sqrt{1-\vec{N}^2} - \frac{|\vec{N}|}{2\rho_c} \left(\check{S}^2 - \xi_{((ab)c)} \sqrt{1-\vec{N}^2} \right) \right] \hat{\chi}$$
$$- \frac{1}{2\rho_c} \left(\frac{\check{S}^1}{|\vec{N}|} + \frac{\check{S}^3}{\sqrt{1-\vec{N}}^2} \right) \hat{N} \times \hat{\chi}, \tag{C7}$$

$$\vec{\pi}^2_a = \tilde{\pi}^2_a + \frac{1}{4\rho^2_a} \left[\xi^2_{(ab)} (1-\vec{N}^2_{(ab)}) + \left(\sin^2\gamma_{(ab)} + \frac{\cos^2\gamma_{(ab)}}{\vec{N}^2_{(ab)}} \right) \left((S_{(ab)})^2 - (\Omega_{(ab)})^2 \right) + \frac{(\Omega_{(ab)})^2}{1-\vec{N}^2_{(ab)}} \right.$$
$$\left. + 2\sqrt{(S_{(ab)})^2 - (\Omega_{(ab)})^2} \left(\xi_{(ab)} \sqrt{1-\vec{N}^2_{(ab)}} \sin\gamma_{(ab)} - \frac{\Omega_{(ab)} \cos\gamma_{(ab)}}{|\vec{N}_{(ab)}| \sqrt{1-\vec{N}^2_{(ab)}}} \right) \right],$$

$$\vec{\pi}^2_b = \tilde{\pi}^2_b + \frac{1}{4\rho^2_b} \left[\xi^2_{(ab)} (1-\vec{N}^2_{(ab)}) + \left(\sin^2\gamma_{(ab)} + \frac{\cos^2\gamma_{(ab)}}{\vec{N}^2_{(ab)}} \right) \left((S_{(ab)})^2 - (\Omega_{(ab)})^2 \right) + \frac{(\Omega_{(ab)})^2}{1-\vec{N}^2_{(ab)}} \right.$$
$$\left. - 2\sqrt{(S_{(ab)})^2 - (\Omega_{(ab)})^2} \left(\xi_{(ab)} \sqrt{1-\vec{N}^2_{(ab)}} \sin\gamma_{(ab)} - \frac{\Omega_{(ab)} \cos\gamma_{(ab)}}{|\vec{N}_{(ab)}| \sqrt{1-\vec{N}^2_{(ab)}}} \right) \right],$$

$$\vec{\pi}^2_c = \tilde{\pi}^2_c + \frac{1}{4\rho^2_c} \left[\xi^2_{((ab)c)} (1-\vec{N}^2) + (\check{S}^2)^2 + \frac{(\check{S}^1)^2}{\vec{N}^2} + \frac{(\check{S}^3)^2}{1-\vec{N}^2} \right.$$
$$\left. - 2 \left(\xi_{((ab)c)} \sqrt{1-\vec{N}^2} \check{S}^2 - \frac{\check{S}^1 \check{S}^3}{|\vec{N}| \sqrt{1-\vec{N}^2}} \right) \right].$$

To evaluate $\vec{\pi}_c$ one defines an auxiliary variable $\vec{\pi}_{(ab)}$ such that $\vec{S}_{(ab)}=\hat{R}_{(ab)}\times\vec{\pi}_{(ab)}$ (its component along $\hat{R}_{(ab)}$ is arbitrary; remember that $\hat{R}_{(ab)}\cdot\vec{S}_{(ab)}=0$). Then we use the equations $\vec{S}=\vec{S}_{(ab)}+\vec{S}_c$ and $\vec{W}=\vec{S}_{(ab)}-\vec{S}_c$ (with $\vec{S}_c=\vec{\rho}_c\times\vec{\pi}_c$) to extract the form of $\vec{\pi}_c$ like in the 3-body case [Eq. (A3)].

The resulting Hamiltonian is not a polynomial of second order in the dynamical body frame components of the spin, unlike that of the static orientation-shape bundle approach. Yet, the rotational part of the Hamiltonian, determined by putting the dynamical shape velocities equal to zero ($\dot{q}^\mu=0$), can be shown to have the standard form of the rigid body case (see Appendix F of Ref. 33), with a nonstandard *dynamical inertia-like tensor* depending only on the shape variables.

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[25] We follow the convention of Ref. 9; note that this action is usually denoted as a *right* action in mathematical texts. The S^r's are the Hamiltonians, associated with the momentum map from the symplectic manifold to $so(3)^*$ [the dual of the Lie algebra $so(3)$], which allow the implementation of the symplectic action through Hamiltonian vector fields.
[26] With $\check{S}^r=\vec{S}\cdot\hat{e}_r$, the conditions $\{\check{S}^r,\check{S}^s\}=-\epsilon^{rsu}\check{S}^u$ imply the equations $\vec{S}\cdot\hat{e}_r\times\hat{e}_s+S^iS^j\{\hat{e}^i_r,\hat{e}^j_s\}=\epsilon_{rsu}S^k\hat{e}^u_k$, hence the quoted result.
[27] Let us remark that any pair of orthonormal vectors $\vec{N}$, $\vec{\chi}$ function only of the relative coordinates can be used to build a body frame. This freedom is connected to the possibility of redefining a body frame by using a configuration-dependent arbitrary rotation, which leaves $\vec{N}$ in the $\vec{S}$–$\hat{R}$ plane.
[28] R is a rotation matrix, θ^α are arbitrary gauge orientational parameters and $\check{\rho}^r_a(q^\mu)$ is assumed to depend on the shape variables only and not on their conjugate momenta.

[29] In a way analoguous to the angular momentum composition in quantum mechanics, note that this spin clustering is independent of the center-of-mass clustering associated with the Jacobi coordinates: the existence of these two unrelated clusterings might prove to be a useful and flexible tool in molecular physics.
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Structures in BC_N Ruijsenaars–Schneider models

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We construct the classical r-matrix structure for the Lax formulation of BC_N Ruijsenaars–Schneider systems proposed in Commun. Math. Phys., **115**, 127 (1988). The r-matrix structure takes a quadratic form similar to the A_N Ruijsenaars–Schneider Poisson bracket behavior, although the dynamical dependence is more complicated. Commuting Hamiltonians stemming from the BC_N Ruijsenaars–Schneider Lax matrix are shown to be linear combinations of particular Koornwinder–van Diejen ''external fields'' Ruijsenaars–Schneider models, for specific values of the exponential one-body couplings. Uniqueness of such commuting Hamiltonians is established once the first of them and the general analytic structure are given. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The integrable relativistic extensions of Calogero–Moser N-body integrable systems were originally introduced by Ruijsenaars and Schneider[1] (classical case) and Ruijsenaars[2] (quantum case) for an underlying Lie algebra structure A_N. They have been the subject of numerous investigations in these last years. Their exact connection to field-theoretical integrable systems, initially described in Ref. 1, was clarified in Ref. 3; their dynamical classical r-matrix structure, first tackled in Refs. 4, 5 was finally established in Ref. 6 and characterized as a quadratic structure, à la Sklyanin,[7,8] stemming from the dynamical linear r-matrix structure of Calogero-Moser systems.[9] This in turn is connected to the realization of such systems[10] as ''Hamiltonian reduction,'' in a more general sense, see Ref. 11, of dynamical systems living on a Heisenberg double,[11–13] where the quadratic r-matrix structure is natural.[11] More complete descriptions may be found in Ref. 14.

Using a $\mathbb{Z}_2$-folding of the original A_{2N} or A_{2N+1} algebra lead[15] to a consistent construction of classical integrable Hamiltonians and Lax formulation for resp. BC_N and C_N Ruijsenaars trigonometric systems. Classical elliptic-interaction BC_N and C_N models were subsequently introduced in Ref. 16. More recently the Lax matrices, obtained by the aforementioned folding procedure for Lie algebra structures BC_N, C_N, and D_N, were explicited in a series of papers.[17,18] Their classical r-matrix structure remained unknown.

Several one-body extensions of the Ruijsenaars–Schneider systems were also considered. First of all, quantum integrable trigonometric one-body-potential (or ''external field extensions''), and rational limits thereof, were constructed in Ref. 19. The quantum integrability proof, and construction of the quantum Hamiltonians themselves, rested upon polynomial-algebraic arguments pioneered by Koornwinder[20] and interestingly indicating a connection to BC_N-type algebras. In this case, both classical Lax formulation and classical r-matrix construction are lacking. Conjectural quantum elliptic Hamiltonians were introduced in Ref. 16. The BC_N and C_N elliptic classical potentials obtained by the folding procedure, were identified with classical limits of a specific realization (albeit with a smaller number of free parameters) of this conjecture. Explicit construction of quantum elliptic van Diejen-type Hamiltonians was then achieved in Ref. 21 using

corner-transfer-matrix methods. It pointed again to a BC_N structure underlying at least some particular Koornwinder–van Diejen potentials. The corner-transfer-matrix method used in Ref. 21 however does not relate clearly to the previous procedures, using as it does two types of Lax operators.

This series of results begs several questions and we wish to address here two points which remained unclarified.

First of all we construct the classical r-matrix for the folded Lax matrices of trigonometric BC_N systems. (We expect that the C_N and D_N case, and the elliptic potentials, may be treated by similar techniques although the elliptic case may endow more complicated algebraic manipulations.) This problem may seem academic, since in any case commutation of the Hamiltonians follows from the construction itself.[15] However it actually sheds light on the delicate question of interplay between the folding procedure $A_{2N} \to BC_N$ and the initial ''quadratization'' of Poisson structure entailed by the change of base symplectic manifold for the ''Hamiltonian'' reduction from T^*g (cotangent bundle Lie group) to $D\,g_H$ (Heisenberg double of Lie group). Similar difficulties occur when considering the quantum deformation of BC- or D-type algebras, compared with deformation of A_N algebras (this fact was pointed out to us by Arnaudon). Indeed it will eventually turn out that the classical r-matrix for hyperbolic Ruijsenaars–Schneider BC_N models may be recast under a quadratic form, similar to the A_N case, but contrary to what occurred in the Calogero–Moser models[22] the structure (after folding) exhibits now a dependence in both sets of conjugated dynamical variables, and the quadratic r-matrix is thus not directly related to the linear dynamical r-matrix structure for BC_N Calogero–Moser models.

The second problem which we consider here deals with the connection between the initial trigonometric classical Koornwinder–van Diejen Hamiltonians and the ''canonical'' Poisson commuting Hamiltonians generated by the traces of powers of the Lax matrix for BC_N systems. The previous results hint at some nice dovetailing between the two approaches (folding and algebraic-polynomial arguments) at least in some particular cases. Indeed the two sets of Hamiltonians exhibit a striking similarity of structure. It will be shown that the Koornwinder–van Diejen Hamiltonians, with a certain choice of one-body potential are in fact combinations of the ''canonical ones.'' More importantly this property of ''uniqueness up to linear transformations'' is shown to be true for any set of Poisson-commuting Hamiltonians once the functional structure (to be explicited hereafter) is given.

II. THE CLASSICAL r-MATRIX STRUCTURE

A. The BC_N Ruijsenaars–Schneider models and notations

The canonical variables are a set of rapidities $\{\theta_i, i=1,\cdots,N\}$ and conjugate positions q_i such that $\{\theta_i, q_j\}=\delta_{ij}$. The Hamiltonian reads

$$H=\sum_{\substack{j=1\\ \varepsilon=\pm 1}}^{N} e^{-\varepsilon\,\beta\,\theta_j} f_j + \mathcal{U}, \tag{1}$$

where

$$f_j=\left[f(q_j)\, f(2\,q_j) \prod_{\substack{k=1,\\ k\neq=j}}^{N} f(q_j-q_k)\, f(q_j+q_k) \right]^{1/2} \quad \text{and} \quad \mathcal{U}=\prod_{k=1}^{N} f(q_k).$$

Function f may take different forms, namely,

$$f(q)=1-\frac{g^2}{q^2}\,(\text{rational}),$$

$$f(q)=1-\frac{\sinh^2\gamma}{\sinh^2\dfrac{\nu q}{2}}\,(\text{hyperbolic}),$$

$$f(q)=1-\frac{\sin^2\gamma}{\sin^2\dfrac{\nu q}{2}}\,(\text{trigonometric}).$$

The most general elliptic case where

$$f(q)=(\lambda+\nu\mathcal{P}(q)),\quad \mathcal{P}=\text{Weierstrass function}$$

will not yet be considered here.

The trigonometric and hyperbolic cases define the same model at least locally up to a redefinition of the parameters (the global structure of trigonometric versus hyperbolic models is however quite different, owing to topological properties, as can be seen for instance in Ref. 23). The rational case is obtained by an easy limit procedure from one of these models. We shall therefore consider in the following only the hyperbolic version.

Let us note that one can also write $f(q)=v(q)\,v(-q)$, with

$$v(q)=\frac{\sinh\left(\dfrac{\nu q}{2}+\gamma\right)}{\sinh\dfrac{\nu q}{2}}$$

or even as a rational function of an exponential variable,

$$v(q)=\lambda^{-1/2}\frac{z-\lambda}{z-1}\quad\text{with}\quad z=e^{\nu q}\quad\text{and}\quad \lambda=e^{-2\gamma}.$$

This rational formulation will be useful to establish some functional identities à la Liouville.[11]

B. The BC_N Lax operator

The Lax formulation of BC_N Ruijsenaars–Schneider system may be obtained as a folding of the A_{2N} case.[15] The reduction works as follows: labeling the $2N+1$ rapidities $\{\theta_i, i=-N\cdots N\}$ and conjugate positions $\{q_i, i=-N\cdots N\}$, one sets $\theta_i=\varepsilon_i\theta_{|i|}$ and $q_i=\varepsilon_i q_{|i|}$ with

$$\varepsilon_i=\begin{cases}+1 & \text{for } 1\leqslant i\leqslant N\\ 0 & \text{for } i=0\\ -1 & \text{for } -1\geqslant i\geqslant -N\end{cases}.$$

The Lax matrix for the A_{2N} cases is

$$\mathcal{L}=\sum_{i,j=-N}^{N}\mathcal{L}_{ij}\,e_{ij}$$

$$\mathcal{L}_{ij}(q_1,\ldots,q_N,q_0,q_{-1},\ldots,q_{-N},\theta_j)=c(q_i-q_j)\,e^{-\beta\theta_j}\prod_{\substack{k=-N,\\ k\neq j}}^{N}f^{1/2}(q_j-q_k),\qquad(2)$$

where $\{e_{ij}\}$ is the standard basis for $(2N+1)\times(2N+1)$ matrices; f was given in the previous subsection and

$$c(q)=\frac{\sinh\gamma}{\sinh\left(\dfrac{\nu q}{2}+\gamma\right)}=(1-\lambda)\,\frac{z^{1/2}}{z-\lambda}.$$

The Lax matrix for the BC_N Ruijsenaars–Schneider systems then reads[17]

$$L=\sum_{i,j=-N}^{N} L_{ij}\,e_{ij} \quad \text{with} \quad L_{ij}=\mathcal{L}_{ij}(q_1,\ldots,q_N,0,-q_1,\ldots,-q_N,\varepsilon_j\,\theta_{|j|}). \tag{3}$$

It can be rewritten, $L_{ij}=c(q_i-q_j)\,e^{-\beta\,\varepsilon_j\,\theta_{|j|}}\,f_j$, extending the definition of f_j given in (1) to $j\in\{-N\cdots N\}$. Note that with this extension of f_j one has $f_0=\mathcal{U}$ and $f_j=f_{-j}$.

It has been shown that the Lax operator (2) satisfies the quadratic fundamental Poisson bracket,[6]

$$\{\overset{\otimes}{\mathcal{L}},\mathcal{L}\}=\mathcal{L}\otimes\mathcal{L}a_1-a_2\mathcal{L}\otimes\mathcal{L}+\mathcal{L}_2\,s_1\,\mathcal{L}_1-\mathcal{L}_1\,s_2\,\mathcal{L}_2, \tag{4}$$

where $\mathcal{L}_1=\mathcal{L}\otimes 1$, $\mathcal{L}_2=1\otimes\mathcal{L}$ and the quadratic structure coefficients read

$$a_1=a+w, \quad s_1=s-w,$$

$$a_2=a+s-s^{\pi}-w, \quad s_2=s^{\pi}+w.$$

For any matrix M, the matrix M^{π} is defined by

$$\text{if } M\equiv\sum_{ijkl=-N}^{N} M_{ijkl}\,e_{ij}\otimes e_{kl}, \text{ then } M^{\pi}=\sum_{ijkl=-N}^{N} M_{ijkl}\,e_{kl}\otimes e_{ij}.$$

Matrices a,s,w take the form,

$$a=\alpha\sum_{\substack{j,k=-N\\k\neq j}}^{N}\coth\frac{\nu}{2}(q_k-q_j)\,e_{jk}\otimes e_{kj}, \tag{5}$$

$$s=-\alpha\sum_{\substack{j,k=-N\\k\neq j}}^{N}\frac{1}{\sinh\dfrac{\nu}{2}(q_k-q_j)}\,e_{jk}\otimes e_{kk},$$

$$w=\alpha\sum_{\substack{j,k=-N\\k\neq j}}^{N}\coth\frac{\nu}{2}(q_k-q_j)\,e_{kk}\otimes e_{jj},$$

where $\alpha\equiv\beta\,(\nu/2)$.

It must be recalled here that the most general structure of Poisson bracket for a Lax operator of a Liouville-integrable system is a linear one,[24]

$$\{\overset{\otimes}{L},L\}=[r,L_1]-[r^{\pi},L_2]. \tag{6}$$

The quadratic form (4) corresponds to the case where the r-matrix itself assumes a linear dependency in L of type,

$$r=b\,L_2+L_2\,c, \tag{7}$$

with b and c arbitrary matrices determining the quadratic coefficients a_1,a_2,s_1,s_2,

$$a_1=c^{\pi}-c,\ \ a_2=b^{\pi}-b,\ \ s_1=c+b^{\pi},\ \text{ and }\ s_2=s_1^{\pi}.$$

In the next subsection, we will show that the BC_N Ruijsenaars–Schneider Lax operator (3) also satisfies a quadratic fundamental Poisson bracket (4) albeit with a fundamental difference with respect to (5) regarding the dependence on the dynamical variables. We will give explicitly the generalizations of the matrices $a_1, a_2, s_1,$ and $s_2,$ hereafter denoted "quadratic r-matrices" for obvious semantic reasons.

C. Computation of the classical *r*-matrix

Let us calculate the Poisson brackets of the Lax matrix (3),

$$\{L_{ij},L_{kl}\}=\beta\, L_{ij}L_{kl}\left(\varepsilon_l\frac{\partial \ln L_{ij}}{\partial q_{|l|}}-\varepsilon_j\frac{\partial \ln L_{kl}}{\partial q_{|j|}}\right)$$

and express it in terms of the Lax matrix (2),

$$\varepsilon_l\frac{\partial \ln L_{ij}}{\partial q_{|l|}}=\left(\frac{\partial \ln \mathcal{L}_{ij}}{\partial q_l}-\frac{\partial \ln \mathcal{L}_{ij}}{\partial q_{-l}}\right).$$

We thus get

$$\{L_{ij},L_{kl}\}=\{\mathcal{L}_{ij},\mathcal{L}_{kl}\}+\beta\, L_{ij}L_{kl}\left(\frac{\partial \ln \mathcal{L}_{kl}}{\partial q_{-j}}-\frac{\partial \ln \mathcal{L}_{ij}}{\partial q_{-l}}\right).$$

The Poisson bracket of the first term on the right-hand side keeps the same form (4) where one should fold the dynamical variables ($\theta_i=\varepsilon_i\,\theta_{|i|}$ and $q_i=\varepsilon_i\,q_{|i|}$). We thus only need to concentrate on the remaining term, introducing the four-index object,

$$U_{ijkl}\equiv\frac{2}{\nu}\left(\frac{\partial \ln \mathcal{L}_{kl}}{\partial q_{-j}}-\frac{\partial \ln \mathcal{L}_{ij}}{\partial q_{-l}}\right).$$

Straightforward calculations yield

$$U_{ijkl}=\delta_{j,-l}\,u_j+(\delta_{i,-l}-\delta_{j,-l})\,t_{ij}-(\delta_{j,-k}-\delta_{j,-l})\,t_{kl},$$

where

$$t_{ij}=-\frac{2}{\nu}(\ln c)'(q_i-q_j)=\coth\left(\frac{\nu}{2}(q_i-q_j)+\gamma\right)=\frac{z_i+\lambda\, z_j}{z_i-\lambda\, z_j},$$

$$u_j=\frac{2}{\nu}\sum_{\substack{k=-N,\\ k\neq j}}^{N}(\ln f)'(q_k-q_j)$$

$$=\sum_{\substack{k=-N,\\ k\neq j}}^{N}2\coth\frac{\nu}{2}(q_j-q_k)+\coth\left(\frac{\nu}{2}(q_k-q_j)+\gamma\right)$$

$$-\coth\left(\frac{\nu}{2}(q_j-q_k)+\gamma\right)$$

$$= \sum_{\substack{k=-N,\\ k\neq j}}^{N} 2\,\frac{z_j+z_k}{z_j-z_k} + \frac{z_k+\lambda\, z_j}{z_k-\lambda\, z_j} - \frac{z_j+\lambda\, z_k}{z_j-\lambda\, z_k}$$

$$= \sum_{\substack{k=-N,\\ k\neq j}}^{N} 2\, a_{jk} + t_{kj} - t_{jk},$$

with

$$a_{jk} = \coth\frac{\nu}{2}(q_j-q_k) = \frac{z_j+z_k}{z_j-z_k} \quad \text{for } j\neq k.$$

Note the following properties of these objects on the folded space:

$$t_{-j-i} = t_{ij}, \quad a_{-j-i} = a_{ij}, \quad \text{and} \quad u_{-i} = -u_i.$$

In the expression of U_{ijkl}, the terms in $\delta_{j,-l}$ are not on the same footing as the others since they are separately antisymmetric under the exchange of the two spaces (operation π) whereas the remaining terms verify this property only altogether.

We thus first take care of the $\delta_{j,-l}$ terms, introducing the matrix ρ,

$$\rho = \alpha \sum_{k,l=-N}^{N} L_{kl}\left(\frac{1}{2}u_l - t_{kl}\right) e_{-l-l}\otimes e_{kl},$$

realizing them as a linear r-matrix form (6),

$$([\rho, L_1] - [\rho^{\pi}, L_2])_{ijkl} = \alpha\, L_{ij}L_{kl}\,(\delta_{j,-l}(u_j - t_{ij} + t_{kl}) + \delta_{i,-l}(\tfrac{1}{2}u_l - t_{kl}) - \delta_{j,-k}(\tfrac{1}{2}u_j - t_{ij}))$$

$$= \alpha\, L_{ij}L_{kl}\,(U_{ijkl} - \tilde{U}_{ijkl}),$$

$$\text{with } \tilde{U}_{ijkl} = \delta_{i,-l}(t_{ij} + t_{kl} - \tfrac{1}{2}u_l) - \delta_{j,-k}(t_{ij} + t_{kl} - \tfrac{1}{2}u_j).$$

We may furthermore bring it back to our sought general quadratic form by setting $\rho = \tau L_2$ [i.e., taking $b=\tau$ and $c=0$ in (7)], since the matrix L is invertible,

$$\tau = \rho\, L_2^{-1} = \alpha \sum_{i,k,l=-N}^{N} L_{k-i}\, L_{-il}^{-1}\left(\frac{1}{2}u_{-i} - t_{k-i}\right) e_{ii}\otimes e_{kl}. \tag{8}$$

One should immediately note, from the explicit form of L (3), that this matrix τ actually does not depend on the rapidities θ_i's. We are therefore still in the ''canonical'' quadratic structure (à la Suris) of type (4) with dynamical quadratic r-matrices depending only on one set of canonical variables (the q_i's).

We will now show that there exists a matrix σ, such that $\sigma^{\pi} = \sigma$ and

$$\alpha\, L_{ij}L_{kl}\,\tilde{U}_{ijkl} = [L_2\,\sigma\, L_1 - L_1\,\sigma^{\pi}\, L_2]_{ijkl}.$$

This corresponds to setting $c=\sigma$ and $b=0$ in (7) and thus actually formally completes the quadratic r-matrix structure (4).

In order to ensure self-consistency of the dependence in the indices, we assume the following tensorial structure:

$$\sigma = \sum_{m,n=-N}^{N} \sigma_{mn}\, e_{mn}\otimes e_{-n-m}, \quad \text{satisfying} \quad \sigma^{\pi} = \sigma, \ \text{i.e.,} \ \sigma_{-n-m} = \sigma_{mn},$$

yielding

$$[L_2\,\sigma\,L_1-L_1\,\sigma^{\pi}\,L_2]_{ijkl}=\delta_{i,-l}\sum_{n=-N}^{N}\sigma_{in}\,L_{k-n}\,L_{nj}-\delta_{j,-k}\sum_{n=-N}^{N}\sigma_{kn}\,L_{i-n}\,L_{nl}\,.$$

The set of equations to be solved then reads

$$\delta_{i,-l}\left(\sum_{n=-N}^{N}\sigma_{in}\frac{L_{k-n}\,L_{nj}}{L_{ij}L_{kl}}-\alpha\left(t_{ij}+t_{kl}-\frac{1}{2}u_l\right)\right)$$
$$=\delta_{j,-k}\left(\sum_{n=-N}^{N}\sigma_{kn}\frac{L_{i-n}\,L_{nl}}{L_{ij}L_{kl}}-\alpha\left(t_{ij}+t_{kl}-\frac{1}{2}u_j\right)\right),$$

or, equivalently,

$$\sum_{n=-N}^{N}\sigma_{in}\frac{L_{k-n}\,L_{nj}}{L_{ij}L_{k-i}}-\alpha\left(t_{ij}+t_{k-i}+\frac{1}{2}u_i\right)=\delta_{j,-k}\,s_{ik},\quad\text{with}\quad s_{ik}=s_{ki}\,.$$

Direct calculations yield

$$\frac{L_{k-n}\,L_{nj}}{L_{ij}L_{k-i}}=\frac{e^{\beta\,\theta_n}f_n}{e^{\beta\,\theta_i}f_i}\left((1-\delta_{j,-k})\frac{t_{nj}-t_{n-k}}{t_{ij}-t_{i-k}}+\delta_{j,-k}\frac{t_{nj}^2-1}{t_{ij}^2-1}\right),$$

and equations become

$$\sum_{n=-N}^{N}\tilde{\sigma}_{in}\,(t_{nj}-t_{n-k})=\alpha\left(t_{ij}^2-t_{i-k}^2+\frac{1}{2}u_i\,t_{ij}-\frac{1}{2}u_i\,t_{i-k}\right)\sum_{n=-N}^{N}\tilde{\sigma}_{in}\frac{t_{nj}^2-1}{t_{ij}^2-1}-\alpha\left(2\,t_{ij}+\frac{1}{2}u_i\right)$$
$$=s_{i-j},\quad\text{with}\quad\tilde{\sigma}_{in}=\frac{e^{\beta\,\theta_n}f_n}{e^{\beta\,\theta_i}f_i}\sigma_{in}\,.$$

Let us recall here that the only additional contraints on matrices $\tilde{\sigma}$ and s read

$$\begin{cases}\tilde{\sigma}_{-j-i}=\dfrac{f_i^2}{f_j^2}\tilde{\sigma}_{ij}\\ s_{ij}=s_{ji}\,.\end{cases}\tag{9}$$

According to the previous equations, the matrix s is determinated given the matrix $\tilde{\sigma}$, and $\tilde{\sigma}$ is obtained, up to a one-dimensional degree of freedom v_i, by

$$\sum_{n=-N}^{N}\tilde{\sigma}_{in}\,t_{nj}=\alpha\,(t_{ij}^2+\tfrac{1}{2}u_i\,t_{ij}+v_i),\tag{10}$$

since t is invertible.

Remains to verify that one can find v_i's, such that the compatibility relations (9) be satisfied, namely,

$$\sum_{m=-N}^{N}t_{im}\,f_m^2\,t_{mj}(t_{mj}-t_{im}+u_m)=\sum_{m=-N}^{N}f_m^2\,(v_{-m}\,t_{mj}-v_m\,t_{im}),\tag{11}$$

$$(v_i+1)\sum_{n,m=-N}^{N}(t_{-jm}^2-1)\,(t^{-1})_{mn}=(v_{-j}+1)\sum_{n,m=-N}^{N}(t_{im}^2-1)\,(t^{-1})_{mn}\,.\tag{12}$$

Equation (12) directly yields $v_i=-1+\eta\,\Sigma_{n,m=-N}^{N}(t_{im}^2-1)\,(t^{-1})_{mn}$, with η an arbitrary constant.

In order to solve (11) we shall first compute its left-hand side.

We do so by twofold evaluation of the following contour integral in the complex plane around infinity,

$$I_{ij}=\frac{1}{2\pi i}\oint_{C_\infty}\frac{dz}{z}\,\frac{z_i+\lambda z}{z_i-\lambda z}\,\frac{z+\lambda z_j}{z-\lambda z_j}\prod_{k=-N}^{N}\frac{z-\lambda z_k}{z-z_k}\,\frac{z_k-\lambda z}{\lambda(z_k-z)}.$$

Contour C_∞ is oriented counterclockwise and loops around infinity. Residue at infinity gives $I_{ij}=-1$.

Whereas I_{ij} also equals the sum of residues at poles of the meromorph integrand in the whole complex plane, that is, a single pole at $z=0$ with residue -1 and a set of double poles at $z=z_m$. We thus obtain

$$\sum_{m=-N}^{N}\left[\frac{z_i+\lambda z}{z_i-\lambda z}\,\frac{z+\lambda z_j}{z-\lambda z_j}\,\frac{(z-\lambda z_m)\,(z_m-\lambda z)}{-\lambda z}\prod_{\substack{k=-N,\\ k\neq m}}^{N}\frac{z-\lambda z_k}{z-z_k}\,\frac{z_k-\lambda z}{\lambda(z_k-z)}\right]'(z=z_m)=0.$$

Noticing that

$$\begin{aligned}u_m&=\frac{2}{\nu}\sum_{\substack{k=-N,\\ k\neq m}}^{N}(\ln f)'(q_k-q_m)\\&=-\frac{2}{\nu}\frac{\partial}{\partial q_m}\ln\prod_{\substack{k=-N,\\ k\neq m}}^{N}f(q_k-q_m)\\&=-2\,z_m\frac{\partial}{\partial z_m}\ln\prod_{\substack{k=-N,\\ k\neq m}}^{N}\frac{z_m-\lambda z_k}{z_m-z_k}\,\frac{z_k-\lambda z_m}{\lambda(z_k-z_m)}\\&=-2\,z_m\left[\ln\prod_{\substack{k=-N,\\ k\neq m}}^{N}\frac{z-\lambda z_k}{z-z_k}\,\frac{z_k-\lambda z}{\lambda(z_k-z)}\right]'(z=z_m)\end{aligned}$$

and also

$$z_m\left[\ln\left(\frac{z_i+\lambda z}{z_i-\lambda z}\,\frac{z+\lambda z_j}{z-\lambda z_j}\right)\right]'(z=z_m)=\frac{1}{2}\left((t_{im}-t_{mj})-\left(\frac{1}{t_{im}}-\frac{1}{t_{mj}}\right)\right),$$

we obtain

$$\sum_{m=-N}^{N}t_{im}\,f_m^2\,t_{mj}\left[t_{mj}-t_{im}+u_m+\left(\frac{1}{t_{im}}-\frac{1}{t_{mj}}\right)\right]=0,$$

or equivalently,

$$\sum_{m=-N}^{N}t_{im}\,f_m^2\,t_{mj}(t_{mj}-t_{im}+u_m)=\sum_{m=-N}^{N}f_m^2\,(t_{im}-t_{mj}).$$

This derivation of Liouville-type functional identities stems from similar derivations to be found in Ref. 10.

Equation (11) now reads

$$\sum_{m=-N}^{N}t_{im}\,f_m^2\,(v_m+1)=\sum_{m=-N}^{N}(v_{-m}+1)\,f_m^2\,t_{mj}=\sum_{m=-N}^{N}t_{-jm}\,f_m^2\,(v_m+1),$$

and can be solved straightforwardly, $v_i=-1+\xi\,(1/f_i^2)\,\Sigma_{m=-N}^{N}(t^{-1})_{im}$, with ξ any constant.

We thereby prove the consistency of (9) and (10), since $v_i=-1$ is an obvious solution (with $\eta=\xi=0$).

In addition, performing calculations of the same type of contour integrals, one gets

$$\sum_{n,m=-N}^{N}(t_{im}^2-1)\,(t^{-1})_{mn}=-\frac{4\lambda}{(\lambda-1)^2}\frac{1}{f_i^2}\sum_{m=-N}^{N}(t^{-1})_{im}\propto\frac{1}{D_i^+},$$

with

$$D_i^+=\prod_{\substack{k=-N,\\ k\neq i}}^{N}\frac{z_i-\lambda\,z_k}{z_i-z_k}.$$

The two forms which the v_i's should satisfy, are actually identical, $v_i=-1+(\zeta/D_i^+)$, ζ being an arbitrary constant.

We fix this remaining gauge, setting $\zeta=(1-\lambda^{2N+1})/(1-\lambda)$, in order to obtain the simplest form for $\tilde{\sigma}$ from relation (10),

$$\tilde{\sigma}_{ij}=\alpha\frac{D_j^+}{D_i^+}(\delta_{i,j}\,s_i-(1-\delta_{i,j})\,a_{ij}),\quad\text{where}\quad s_i=\frac{1+\lambda}{1-\lambda}+\sum_{m=-N}^{N}\frac{1}{2}(t_{mi}+t_{im}).$$

We finally give the expression of the matrix σ,

$$\sigma=\alpha\sum_{i,j=-N}^{N}\frac{\mathcal{A}_j}{\mathcal{A}_i}(\delta_{i,j}\,s_i-(1-\delta_{i,j})\,a_{ij})\,e_{ij}\otimes e_{-j-i},\quad\text{with}\quad\mathcal{A}_i=\sqrt{\frac{D_i^+}{D_{-i}^+}}e^{-\beta\,\theta_i}.\tag{13}$$

The r-matrix structure is now completely defined by a quadratic Poisson bracket of type (4) where the quadratic r-matrices a_1, a_2, s_1, and s_2 are changed into

$$\begin{aligned}
a_1&\to\tilde{a}_1=a_1,\\
s_1&\to\tilde{s}_1=s_1+\sigma+\tau^{\pi},\\
s_2&\to\tilde{s}_2=\tilde{s}_1^{\pi}=s_2+\sigma^{\pi}+\tau=s_2+\sigma+\tau,\\
a_2&\to\tilde{a}_2=\tilde{a}_1+\tilde{s}_1-\tilde{s}_2=a_2+\tau^{\pi}-\tau,
\end{aligned}\tag{14}$$

and matrices σ and τ are, respectively, defined by Eqs. (13) and (8).

D. Comments

One should notice that this quadratic r-matrix structure is now fully dynamical, depending both on the positions q_i's and rapidities θ_i's. Moreover, its conjugating factor $\mathcal{A}_i$, which bears this double dependance, is deeply connected to the structure of the matrix L under folding,

$$L_{ij}^{-1}=\frac{\mathcal{A}_j}{\mathcal{A}_i}L_{-i-j}.$$

We have here an interesting first example of a ''doubly dynamical'' r-matrix dependence, stemming from the interplay between the folding procedure leading from A_{2N} to BC_N, and the quadratic structure of Ruijsenaars–Schneider-type models. This seems to open new perspectives, first of all on the classification of such doubly dynamical r-matrices. The only other example known to us at this time is the classical linear r-matrix structure for the Lax formulation of the A_N elliptic Calogero–Moser model in the absence of the spectral parameter.[25] Proof of its double dynamical

dependence is given in Ref. 26 although the explicit form is yet conjectural.[27] Curiously however, it occurs in relation with an A_N model with no folding and may therefore be of a different nature.

Interpretation of doubly dynamical objects in the frame of quantum group theory is yet lacking. ''Simply'' dynamical r-matrices are known to be connected to the theory of Drinfel'd-twisted quantum groups, specifically of the type of Felder's Dynamical Quantum Groups[28] (see, for instance, Refs. 29, 30). Whether doubly dynamical objects have such connections is a new problem and we have no further comments to make on this point. A very recent result[31] may however give indications on how to twist quantum groups by non-Abelian twisted cocycles (here the twist would occur ''along'' a Heisenberg algebra).

III. THE CANONICAL HAMILTONIANS

A. Preliminaries

We first describe the Poisson-commuting Hamiltonians[15] generated by traces of powers of the BC_N Lax matrix (3). Subsequent comparison with Koornwinder–van Diejen Hamiltonians is made easier by using as an algebraic basis the coefficients of the characteristic polynomial of the Lax operator. They read for any integer $l \in \{1 \cdots N\}$,

$$\mathcal{H}_l = \sum_{\substack{\mathcal{J} \subset \{-N \cdots N\} \\ |\mathcal{J}| = l}} m_{\mathcal{J}}(L),$$

with $m_{\mathcal{J}}(L)$ the principal minor of L with lines and columns indexed by $\mathcal{J}$.

Taking into account the form of L and properties of Cauchy matrices,

$$m_{\mathcal{J}}(L) = e^{-\beta\theta_{\mathcal{J}}} \prod_{\substack{j \in \mathcal{J} \\ k \notin \mathcal{J}}} f^{1/2}(q_j - q_k), \quad \text{where} \quad \theta_{\mathcal{J}} = \sum_{j \in \mathcal{J}} \theta_j .$$

Because of the folding, we now rearrange these terms so as to sort them with respect to linearly independent exponentials of rapidities. We thus decompose $\mathcal{J} = \varepsilon J \cup S$, separating indices of $\mathcal{J}$ such that their opposite does not belong to $\mathcal{J}$ (set $\varepsilon J = \{\varepsilon_j |j| / j \in \mathcal{J} \wedge -j \notin \mathcal{J}\}$ and $J = \{|j| / j \in \varepsilon J\} \subset \{1 \cdots N\}$) and the complementary parts, symmetric under folding S,

$$\mathcal{H}_l = \sum_{\substack{J \subset \{1 \cdots N\},\ |J| \leqslant l \\ \varepsilon_j = \pm 1,\ j \in J}} \mathcal{U}_{J^c, l-|J|}\, e^{-\beta\theta_{\varepsilon J}} \prod_{\substack{j \in \varepsilon J \\ k \notin \varepsilon J}} f^{1/2}(q_j - q_k), \tag{15}$$

with

$$\mathcal{U}_{K,p} = \sum_{\substack{S \subset \mathcal{A}_K = K \cup -K \cup \{0\} \\ S = -S,\ |S| = p}} \prod_{\substack{s \in S \\ k \in \mathcal{A}_K \setminus S}} f^{1/2}(q_s - q_k) = \sum_{\substack{S \subset \mathcal{A}_K \\ S = -S,\ |S| = p}} \prod_{\substack{s \in S \\ k \in \mathcal{A}_K \setminus S}} v(q_s - q_k). \tag{16}$$

We now recall the Koornwinder–van Diejen Hamiltonians[16] in the classical case,

$$H_l = \sum_{\substack{J \subset \{1 \cdots N\},\ |J| \leqslant l \\ \varepsilon_j = \pm 1,\ j \in J}} U_{J^c, l-|J|}\, e^{-\beta\theta_{\varepsilon J}}\, V^{1/2}_{\varepsilon J; J^c}\, V^{1/2}_{-\varepsilon J; J^c}, \tag{17}$$

where, after some rearrangements,

$$V_{\varepsilon J; K} = \prod_{j \in \varepsilon J} \frac{w(q_j)}{v(2\, q_j)\, v(q_j)} \prod_{\substack{j \in \varepsilon J \\ k \in \mathcal{A}_K \cup -\varepsilon J}} v(q_j - q_k)$$

and

$$U_{K,p}=(-1)^p \sum_{\substack{\varepsilon I\subset \mathcal{A}_K \\ |I|=p}} \prod_{i\in \varepsilon I} \frac{w(q_i)}{v(2q_i)\,v(q_i)} \prod_{\substack{i,i'\in \varepsilon I \\ i<i'}} \frac{v(-q_i-q_{i'})}{v(q_i+q_{i'})} \prod_{\substack{i\in \varepsilon I \\ k\in \mathcal{A}_K\setminus \varepsilon I}} v(q_i-q_k).$$

The potentials w are particular functions and may be interpreted as an interaction with some external field.

Direct computation yields

$$V_{\varepsilon J;J^c}V_{-\varepsilon J;J^c}=\prod_{j\in \varepsilon J} \frac{w(q_j)}{v(2q_j)\,v(q_j)} \frac{w(-q_j)}{v(-2q_j)\,v(-q_j)} \prod_{\substack{j\in \varepsilon J \\ k\notin \varepsilon J}} f(q_j-q_k).$$

Setting $w(q_j)=v(2q_j)\,v(q_j)$, which is an admissible choice according to Ref. 16, H_l (17) takes actually the same form as $\mathcal{H}_l$ (15), up to the crucial change of $\mathcal{U}_{K,p}$ into $U_{K,p}$. $U_{K,p}$ takes a simpler form, for this choice of one-body potential w,

$$U_{K,p}=(-1)^p \sum_{\substack{\varepsilon I\subset \mathcal{A}_K \\ |I|=p}} \prod_{\substack{i,i'\in \varepsilon I \\ i<i'}} \frac{v(-q_i-q_{i'})}{v(q_i+q_{i'})} \prod_{\substack{i\in \varepsilon I \\ k\in \mathcal{A}_K\setminus \varepsilon I}} v(q_i-q_k), \tag{18}$$

nevertheless *it is generally not equal to* $\mathcal{U}_{K,p}$ (the notation used in Ref. 17 is in this respect misleading).

They are actually only equal for $p=0$, where trivially, $U_{K,0}=1=\mathcal{U}_{K,0}$. For instance when $p=1$, one gets

$$U_{K,1}=-\sum_{i\in \mathcal{A}_K\setminus\{0\}} \prod_{\substack{k\in \mathcal{A}_K \\ k\neq i}} v(q_i-q_k) \quad \text{and} \quad \mathcal{U}_{K,1}=\prod_{\substack{k\in \mathcal{A}_K \\ k\neq 0}} v(q_k).$$

We compute a suitable contour integral on the same lines as in the previous section to obtain the Liouville-type functional identity,

$$\sum_{i\in \mathcal{A}_K} \prod_{\substack{k\in \mathcal{A}_K \\ k\neq i}} v(q_i-q_k)=\frac{\sinh \gamma(2|K|+1)}{\sinh \gamma},$$

and thus show that

$$U_{K,1}=\mathcal{U}_{K,1}-\frac{\sinh \gamma(2|K|+1)}{\sinh \gamma}.$$

It will now be shown that these two relations, for $p=0$ and $p=1$, between the $U_{K,p}$'s and $\mathcal{U}_{K,1}$'s are actually sufficient to establish that the two sets of Hamiltonians define the same family of commuting dynamical flows, namely one set of Hamiltonians is a triangular linear combination of the other set.

A more general result will in fact be proved in the following subsection.

B. Uniqueness theorem

Theorem 1: *Let q_i and θ_i, $i\in\mathbb{N}$, be a set of conjugated variables such that $\{\theta_i,q_j\}=\delta_{ij}$. Let I and K be arbitrary finite sets of indices included in $\mathbb{N}$. Assume the existence of a set of complex functions $u_{K,p}$ depending upon the set of indices K and a natural integer p, and of another set of complex functions $v_{\varepsilon J,I}$ depending upon the sets of indices J and I $(J\subset I)$ and a $|J|$-uple of signs $\varepsilon=(\varepsilon_j, j\in J)$, such that:*

(a) $u_{K,p}$ and $v_{\varepsilon J,I}$ be independent of the rapidities θ_is;

(b) $u_{K,0}=1$, $v_{\varnothing,I}=1$, *and* $v_{\varepsilon\{j\},I}\neq 0$;
(c) $S^I=\{h_l^I=\sum_{\substack{J\subset I,\,|J|\leqslant l\\ \varepsilon_j=\pm 1,\,j\in J}} u_{J^c,l-|J|}\, e^{-\beta\theta_{\varepsilon J}}\, v_{\varepsilon J,I},\ l\in\{1\cdots|I|\}\}$ *be a family of Poisson-commuting functions* $(\theta_{\varepsilon J}=\sum_{j\in J}\varepsilon_j\theta_j)$.

If there exists a second set of complex functions $\tilde{u}_{K,p}$ *obeying the first two conditions; such that* $\tilde{S}^I=\{\tilde{h}_l^I=\sum_{\substack{J\subset I,\,|J|\leqslant l\\ \varepsilon_j=\pm 1,\,j\in J}} \tilde{u}_{J^c,l-|J|}\, e^{-\beta\theta_{\varepsilon J}}\, v_{\varepsilon J,I},\ l\in\{1\cdots|I|\}\}$ *be a new family of Poisson-commuting functions; and* $\tilde{u}_{K,1}=u_{K,1}+c_1(|K|)$, *then there exist coefficients* $c_r(m)$, $(r,m)\in\mathbb{N}^2$, *independent of all dynamical variables, connecting the two families of Hamiltonians as*

$$\tilde{h}_l^I=\sum_{s=0}^{l} c_{l-s}(|I|-s)\, h_s^I, \quad \text{with} \quad \forall m\in\mathbb{N}, c_0(m)=1.$$

Proof: The strategy of the proof relies upon a recursive procedure on p, showing that

$$\tilde{u}_{K,p}=\sum_{r=0}^{p} c_{p-r}(|K|-r)\, u_{K,r}, \quad \forall K\subset\mathbb{N} \text{ finite and such that } |K|\geqslant p. \tag{19}$$

Let l_0 be a strictly positive integer; the recursion hypothesis hereafter denoted r.h., states that (19) is valid for any $p\leqslant l_0$.

The assumptions in the theorem immediately imply the validity of r.h. for $l_0=1$, which can be directly rewritten as

$$\tilde{h}_1^I=h_1^I+c_1(|I|). \tag{20}$$

Let us assume r.h. up to l_0 and establish it for l_0+1. We have

$$\tilde{h}_{l_0+1}^I=\tilde{u}_{I,l_0+1}+\sum_{\substack{J\subset I,1\leqslant|J|\leqslant l_0+1\\ \varepsilon_j=\pm 1,j\in J}} \tilde{u}_{J^c,l_0+1-|J|}\, e^{-\beta\theta_{\varepsilon J}}\, v_{\varepsilon J,I}.$$

Since $l_0+1-|J|\leqslant l_0$ in the previous summation, we apply r.h. to get

$$\tilde{h}_{l_0+1}^I=\tilde{u}_{I,l_0+1}+\sum_{s=1}^{l_0+1} c_{l_0+1-s}(|I|-s)\sum_{\substack{J\subset I,1\leqslant|J|\leqslant s\\ \varepsilon_j=\pm 1,j\in J}} u_{J^c,s-|J|}\, e^{-\beta\theta_{\varepsilon J}}\, v_{\varepsilon J,I}$$

$$=\tilde{u}_{I,l_0+1}-\sum_{s=1}^{l_0+1} c_{l_0+1-s}(|I|-s)\, u_{I,s}+\sum_{s=1}^{l_0+1} c_{l_0+1-s}(|I|-s)\, h_s^I. \tag{21}$$

We now use the Poisson-commutation property of $\tilde{S}^I$ as

$$\{\tilde{h}_{l_0+1}^I,\tilde{h}_1^I\}=0.$$

Combining (20), (21) and the Poisson-commutation property of S^I yields

$$0=\left\{\tilde{u}_{I,l_0+1}-\sum_{s=1}^{l_0+1} c_{l_0+1-s}(|I|-s)\,u_{I,s},h_1^I\right\}$$

$$=\sum_{j\in I,\varepsilon=\pm 1}\beta\,\varepsilon\,e^{-\beta\,\varepsilon\,\theta_j}v_{\varepsilon\{j\},I}\frac{\partial}{\partial q_j}$$

$$\times\left(\tilde{u}_{I,l_0+1}-\sum_{s=1}^{l_0+1} c_{l_0+1-s}(|I|-s)\,u_{I,s}\right).$$

By functional independence of $\Sigma_{\varepsilon=\pm 1}\varepsilon\,e^{-\beta\,\varepsilon\,\theta_j}v_{\varepsilon\{j\},I}$, it follows that the function obtained as $\tilde{u}_{I,l_0+1}-\Sigma_{s=1}^{l_0+1}c_{l_0+1-s}(|I|-s)\,u_{I,s}$ *does not depend on any dynamical variable*. Hence it defines the coefficient $c_{l_0+1}(|I|)$, thereby proving the r.h. to order l_0+1. Finally, relation (19) immediately implies the result of the theorem. □

C. Comments

An immediate consequence of this theorem is the existence of linear triangular relations between the BC_N Ruijsenaars–Schneider Hamiltonians and the classical Koornwinder–van Diejen Hamiltonians when $w(q_j)=v(2\,q_j)\,v(q_j)$. Such relations were indicated in Ref. 32 for the lowest and highest-order Hamiltonians.

The explicit coefficient have to be computed order by order since at this time no general recursion formula is available. As an example we have worked out the first two functions,

$$U_{K,1}=\mathcal{U}_{K,1}+c_1(|K|)\quad\text{and}\quad U_{K,2}=\mathcal{U}_{K,2}+c_1(|K|-1)\,\mathcal{U}_{K,1}+c_2(|K|)$$

with

$$c_1(|K|)=-\frac{\sinh\gamma(2\,|K|+1)}{\sinh\gamma},$$

$$c_2(|K|)=\frac{1}{2}\left(\frac{\sinh\gamma(2\,|K|-1)}{\sinh\gamma}\,\frac{\sinh\gamma(2\,|K|+1)}{\sinh\gamma}-\frac{\sinh 4\,\gamma\,|K|}{\sinh 2\,\gamma}-2\right).$$

No obvious pattern appears yet. As a consequence, an algebraic interpretation of the Koornwinder–van Diejen Hamiltonians in connection with the canonical Hamiltonians is still lacking.

More generally, the theorem implies that a hierarchy of Poisson-commuting Hamiltonians with the generic form given is uniquely determinated by the giving of the family of v-functions and the first Hamiltonian, or equivalently the first ''potential term'' $u_{K,1}$. In the Koornwinder–van Diejen case, this first Hamiltonian is given in Ref. 20.

We wish to end this section with a conjecture on the classical Koornwinder–van Diejen Hamiltonians with a general one-body potential chosen as in Ref. 19 [this time dropping the restriction to $w(q_j)=v(2\,q_j)\,v(q_j)$]. They have not yet been constructed by a Lax formalism. We expect that the suitable Lax matrix for this hierarchy may be obtained by multiplying the BC_N Lax matrix (3) by a $2\,N+1$ diagonal matrix: $L_W=LD_W$, with $D_{W_{ii}}=\mathcal{W}(q_i)\,\mathcal{W}(-q_i)$. This one-body potential function $\mathcal{W}$ has to be determinated by integrability conditions. In addition, we conjecture that, after some canonical transformation on the dynamical variables, the Hamiltonians $\mathcal{H}_W^l$ generated by $\mathrm{tr}(L_W^l)$ will take the same form as the Koornwinder–van Diejen Hamiltonians (17) up to the change of $U_{K,p}$ into some $\mathcal{U}_{W_{K,p}}$. The theorem will then apply, thereby yielding the full connection between BC_N-type Ruijsenaars–Schneider potentials and the classical Koornwinder–van Diejen Hamiltonians.

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The global finite structure of generic envelope loci for Hamilton–Jacobi equations

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We discuss in some detail the existence of global generating functions describing Lagrangian submanifolds connected with evolution problems for Hamilton–Jacobi (H–J) equations. First, we produce a physical application of a result by Viterbo: for generic (in a suitable sense) Hamiltonian functions and initial data, the envelopes, i.e., the wave front sets, related to Hamilton–Jacobi problems are globally finitely generated. Furthermore, we show how to compute global space–time generating functions with finite parameters for geometric solutions of a H–J equation of the evolution kind. © *2002 American Institute of Physics.*
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I. INTRODUCTION: THE HAMILTON–JACOBI PROBLEM

Dynamical mechanical systems, even infinite-dimensional evolution systems, like the wave propagation problems of Continuum Mechanics or Optics, are often governed by a Hamilton–Jacobi equation, for some Hamiltonian function $H:\mathbb{R}\times T^*Q\to\mathbb{R}$. Here, we take as standard scenario T^*Q, the symplectic manifold of dynamics, and in what follows $Q=\mathbb{R}^n$ is the ''space,'' while $\mathcal{Q}=\mathbb{R}^{n+1}$ is the ''space–time.''

We are interested in a Cauchy Problem, which, in the so-called *classical* formulation, reads as

$$\frac{\partial S}{\partial t}(q,t)+H\left(t,q,\frac{\partial S}{\partial q}(q,t)\right)=0,$$

(Classical Cauchy Problem)

$$S(q,t)\big|_{t=0}=\sigma(q).$$

It is well known that it is not possible to find classical *global* solutions for the above (CCP): this is mainly due to the nonlinearity of the problem. From the physical point of view, the main objects of interest related to the solutions are often precisely these obstructions, sometimes called *caustics*.

In order to overcome the difficulties connected to the obstructions to existence of global solutions, we can begin from a simple observation in the classical case, that is when a global classical solution exists. Let

$$S:\mathbb{R}^n\times\mathbb{R}\to\mathbb{R},\quad (q,t)\mapsto S(q,t),$$

be a classical solution of the above problem, and, transforming it to the so-called ''homogeneous version,'' set

$$\mathcal{Q}:=\mathbb{R}^n\times\mathbb{R},\quad x:=(q,t),\quad (x,\xi):=(q,t;p,\tau),$$

$$\mathcal{H}:T^*\mathcal{Q}\to\mathbb{R},\quad \mathcal{H}(x,\xi):=\tau+H(t,q,p).$$

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Then the differential of $S:\mathcal{Q}\to\mathbb{R}$ is a 1-form $dS:\mathcal{Q}\to T^*\mathcal{Q}$, and setting

$$\mathrm{im}(dS):=\left\{(x,\xi):\xi=\frac{\partial S}{\partial x}(x),x\in\mathcal{Q}\right\}\subset T^*\mathcal{Q},$$

the H–J equation reads as

$$\mathrm{im}(dS)\subset\mathcal{H}^{-1}(0).$$

As is usual, we introduce the Liouville 1-form $\theta_{\mathcal{Q}}=\xi\,dx$ on $T^*\mathcal{Q}$, so that $d\theta_{\mathcal{Q}}$ is the standard symplectic 2-form on $T^*\mathcal{Q}$.

We note that

$$(1)\quad \dim\ \mathrm{im}(dS)=\dim\mathcal{Q},$$

$$(2)\quad d\theta_{\mathcal{Q}}\big|_{\mathrm{im}(dS)}=(d\xi\wedge dx)\big|_{\mathrm{im}(dS)}=\frac{\partial^2 S}{\partial x\,\partial x}dx\wedge dx\equiv 0,$$

It is a well known fact in symplectic geometry—see, e.g., Arnold and Novikov (1990)—that the two properties (1) and (2) characterize the *Lagrangian submanifolds* of $T^*\mathcal{Q}$. Furthermore, $\Lambda=\mathrm{im}(dS)$ is *transverse* to the fibers of $\mathcal{Q}$ (since it has a graph structure).

We recognize here a way to overcome the difficulty in finding a global solution: instead of a function $S(x)$, we are now searching for a *Lagrangian submanifold* Λ (i.e., such that $\dim\Lambda=\dim\mathcal{Q}$, and $d\theta_{\mathcal{Q}}\big|_{\Lambda}=0$) satisfying what can be considered the ''new'' geometric version of the H–J equation:

$$\Lambda\subset\mathcal{H}^{-1}(0).$$

A crucial theorem in symplectic geometry, due mainly to Maslov (1965) and Hörmander (1971), characterizes the Lagrangian submanifolds locally: let Λ be a Lagrangian submanifold of $T^*\mathcal{Q}$; then for each point $\lambda\in\Lambda$ there exists a description of Λ by means of a local *generating function*, $U(\subset\mathcal{Q})\times\mathbb{R}^k\ni(x,u)\mapsto S(x,u)\in\mathbb{R}$, such that (locally)

$$\Lambda=\left\{(x,y):\xi=\frac{\partial S}{\partial x}(x,u),\quad 0=\frac{\partial S}{\partial u}(x,u),\quad \text{for some } u\in\mathbb{R}^k\right\},$$

where S can be assumed to satisfy the rank condition:

$$\mathrm{rk}\left(\frac{\partial^2 S}{\partial x\,\partial u}\ \frac{\partial^2 S}{\partial u\,\partial u}\right)\Bigg|_{\partial S/\partial u=0}=\max=k.$$

Whenever, locally at λ, we can describe Λ without introducing auxiliary parameters u—in other words, if Λ is the image of dS, so that $k=0$—then λ is a point of transverse intersection of Λ with the fiber $T^*\mathcal{Q}\to\mathcal{Q}$. The following questions arise naturally:

(1) How to obtain Λ satisfying the H-J equation $\Lambda\subset\mathcal{H}^{-1}(0)$?
(2) Given a Lagrangian submanifold Λ, is it possible to find a *global* generating function $S(x,u)$ for it?

The answer to question (1) is formally easy: by a standard procedure of the gluing of characteristics of the Hamiltonian field X_H (which we suppose to be complete) we obtain the geometric object Λ:

$$\Lambda=\bigcup_{t\in I\subset\mathbb{R}}\Phi^t_{X_H}(\mathrm{im}(d\sigma))\quad \Phi^t_{X_H}:\text{flow of } X_H.$$

Hence, by Maslov–Hörmander, we can construct the local generating functions; see also Benenti and Tulczyjew (1979).

Question (2) is crucial, especially whenever we want to generate *true* solutions (in the sense of ''functions,'' not submanifolds) to H–J equations.

In fact, if we know a *global* generating function of the Lagrangian submanifold solution of some H–J problem, then we have the following.

(a) We can try to generate the *viscosity* solution (Crandall–Evans–Lions) by some suitable inf/sup procedure on the auxiliary parameters u. These techniques were first introduced by Hopf (1965); also, an existence and uniqueness theorem exists in this context; see Bardi and Capuzzo-Dolcetta (1997) and Cardin (1993);
(b) sometimes, with due care, we can generate the Chaperon–Sikorav–Viterbo solution by a Morse (Lusternik–Schnirelman) procedure; see, e.g., Dubrovin, Fomenko and Novikov (1990). Rather surprisingly, this last solution sometimes differs from the viscosity solution for the same problem; see Viterbo (1990), Viterbo (1996), Capitanio (1999).

Very important developments on the links between viscosity and geometric solutions of the H–J equation, mainly on the classification and stability of the singularities, have been performed by Izumiya and Kossioris; among many interesting papers, see, e.g., Izumiya and Kossioris (1997).

Here, one might naturally suspect that global generating functions $S(x,u)$ of geometric solutions for a H–J equation exist *only* for Hamiltonian functions that are *integrable* on the fiber zero ($\mathcal{H}=0$). This idea arises from the following fact: if there exists a *complete integral*, $W(x^i,a^A)$, $i=1,...,n+1$, $A=1,...,n$, then the H–J general problem with initial data σ on a submanifold Σ of co-dimension one into $\mathcal{Q}$,

$$\mathcal{H}\left(x,\frac{\partial S}{\partial x}(x)\right)=0, \quad \text{or} \quad \Lambda\subset\mathcal{H}^{-1}(0);$$

$$S|_{\Sigma}=\sigma, \quad \text{or} \quad S(\tilde{x}^i(\chi^A))=\sigma(\chi^A),$$

admits—see Cardin (1989)—the following *global* generating function describing the Lagrangian submanifold solution Λ:

$$S(x^i;\chi^A,a^B):=W(x^i,a^B)-W(\tilde{x}^i(\chi^A),a^B)+\varphi(\chi^A).$$

For example, if $\mathcal{H}(x,\xi)=\tau+H(p)$, then a complete integral is $W(x,a)=W(t,q,a)=-tH(a)+q\cdot a$, and the above formula works. It is remarkable that just by means of this formula Bardi and Evans (1984) found that the inf-sup procedure generates precisely the viscosity solution. Nevertheless, in the sequel, we will see that the above belief is false, more precisely, it is too pessimistic.

In order to exploit this point, we start from a very remarkable fact, more or less well known: *every* Lagrangian submanifold $\Lambda\subset\mathcal{H}^{-1}(0)\subset T^*\mathcal{Q}$, where $\mathcal{H}(x,\xi)=\tau+H(q,p,t)$ (i.e., of the evolution kind), admits a *formal* global generating function. This function is precisely the Action Functional of the related Calculus of Variations, and the auxiliary parameters belong to an *infinite*-dimensional space, the space of curves. We remind the reader that, if locally the q-components of the characteristics related to H do not cross each other, then, locally, a suitable interpretation of $A=\int_{t_0}^{t_1}L\,dt$ gives us Hamilton's Principal Function, which is a well known local complete integral. As we will soon see, in order to obtain a global generating function from the Action Functional we will *relax* the above restriction on the intersection of the q-characteristics.

Some remarks follow.

- Surely, the first powerful use of this idea was done by Feynman; see, e.g., Feynman and Hibbs (1965), where, roughly speaking, he generalized the *phase* functions—generating functions with a finite number of auxiliary parameters—of stationary phase theory for high frequency integrals, using the aforementioned Action Functionals.
- It is notable that Berry and Upstill, in a well known survey on global Optics—see p. 265 of Berry and Upstill (1980)—gave some pioneering ideas about the possibility of reducing to a finite number of auxiliary parameters.
- The search for global generating functions has a long story. A first theorem by Lees (1979) defined the obstructions in a cohomological and *k*-theoretical framework, but Giroux (1988) found a gap in that proof. Besides Giroux, Chaperon (1984), Laudenbach (1987) and Sikorav (1987) proved similar theorems, but only for *compact* parallelizable manifolds $\mathcal{Q}$.
- Here, we will consider some ideas of Viterbo (1990), more precisely we will give the details of his reduction procedure in the *noncompact* case: $Q=\mathbb{R}^n$, see also Aebischer *et al.* (1994). Some of the mathematical techniques were introduced by Amann, Conley, and Zehnder, see Amann and Zehnder (1980), Conley and Zehnder (1984), in connection with the search for periodic solutions of Hamiltonian systems.

First, we recall that a *Hamiltonian isotopy* is a canonical transformation, obtained via the flow of a Hamiltonian vector field X_H, generated by a Hamiltonian function H, possibly depending on the real evolution parameter $s\in[0,T]$.

Theorem 1: *Let $\Lambda\subset T^*\mathbb{R}^n$ be a Lagrangian submanifold connected by a Hamiltonian isotopy, generated by H, to the zero-section of $T^*\mathbb{R}^n$. If the second derivatives of H are globally uniformly bounded, then Λ admits a global generating function with a finite number of auxiliary parameters.*

Remark: The generating function coming from Theorem 1 generally does not satisfy the above rank condition of the Maslov–Hörmander theorem; really, that condition assures that the locus,

$$\left\{(q,p):p=\frac{\partial S}{\partial q}(q,u),\quad 0=\frac{\partial S}{\partial u}(q,u)\right\},$$

is a *smooth* Lagrangian manifold: we do not impose this fact, since it is a hypothesis of Theorem 1.

A constructive and physically meaningful consequence of Theorem 1 concerning envelopes—wave front sets—will be presented in Sec. III. Furthermore, in Sec. IV we built the global space–time generating functions with finite parameters of the Lagrangian submanifolds solving Cauchy problems for generic H–J equations of the evolution type.

II. A PROOF OF THEOREM 1

Let us consider the set of curves

$$\Gamma:=\{\gamma(\cdot)=(q(\cdot),p(\cdot))\in H^{1,2}([0,T],\mathbb{R}^{2n}):p(0)=0\}.$$

By the Rellich–Kondrachov theorem (or by the Sobolev imbedding theorem),

$$H^{1,2}((0,T),\mathbb{R}^{2n})\hookrightarrow\mathcal{C}^0([0,T],\mathbb{R}^{2n}),$$

compactly, so in the above definition it is understood that the elements of Γ are the natural continuous extension of the curves of $H^{1,2}((0,T),\mathbb{R}^{2n})$: more explicitly the continuous curves in $T^*\mathbb{R}^n$, $t\mapsto\gamma(t)$, arriving to the zero-section, such that $\dot\gamma=d\gamma/dt\in L^2:=L^2((0,T),\mathbb{R}^{2n})$. The following is self-evident.

Lemma 1 (linear structure of Γ): The set Γ has a natural structure of linear space, and then $T_\gamma\Gamma=\Gamma$, for all $\gamma\in\Gamma$.

An equivalent way to describe the curves of Γ is to assign the q-projection of the end point, $q(T)\in\mathbb{R}^n$, and the velocity $\dot{\gamma}$, for each $s\in[0,T]$, of the curve γ by means of a function $\phi\in L^2$.

Lemma 2 (the bijection g): For all $\phi\in L^2$ *set* $\phi=(\phi_q,\phi_p)$. The map g,

$$g:\mathbb{R}^n\times L^2\to\Gamma,\quad (q(T),\phi)\mapsto g(q(T),\phi)(s):=\left(q(T)-\int_s^T\phi_q(r)dr,\int_0^s\phi_p(r)dr\right),$$

is a bijection.

Proof: Let $\gamma(\cdot)=(q(\cdot),p(\cdot))\in\Gamma$, since $(\dot{q}(s),\dot{p}(s))\in L^2$, then $\gamma(s)=g(q(T),(\dot{q}(s),\dot{p}(s)))$. This proves that g is surjective.

Now, let $q(T)$, $\overline{q}(T)\in\mathbb{R}^n$ ϕ, $\overline{\phi}\in L^2$, such that $g(q(T),\phi)=g(\overline{q}(T),\overline{\phi})$; in other words,

$$\left(q(T)-\int_s^T\phi_q(r)dr,\int_0^s\phi_p(r)dr\right)=\left(\overline{q}(T)-\int_s^T\overline{\phi}_q(r)dr,\int_0^s\overline{\phi}_p(r)dr\right).$$

Thus, for all $s\in[0,T]$ one has

$$\overline{q}(T)-q(T)-\int_s^T(\overline{\phi}_q(r)-\phi_q(r))dr=0,\quad \int_0^s(\overline{\phi}_p(r)-\phi_p(r))dr=0^*,$$

hence

$$\overline{q}(T)=q(T),\quad \overline{\phi}_q=\phi_q,\quad \overline{\phi}_p=\phi_p.$$

This shows that g is injective.

Let $\{\Phi^s\}_{s\in[0,T]}$ be a Hamiltonian isotopy of $T^*\mathbb{R}^n$, where $H=H(s,q,p)$, $s\in[0,T]$, is the Hamiltonian generating it:

$$\Phi^s=\Phi_{X_H}^{s,0},\quad \Phi_{X_H}^{0,0}=\mathrm{id}_{\mathbb{R}^{2n}}.$$

We remind that the flow Φ^s transforms Lagrangian manifolds into Lagrangian manifolds: $\Lambda_s=\Phi^s(\Lambda_0)$. Our hypothesis is

$$\Lambda=\Lambda_T=\Phi^T(\Lambda_0),$$

where $\Lambda_0=\{(q,p)\in T^*\mathbb{R}^n:q\in\mathbb{R}^n,p=0\}$ is the *zero-section* of $T^*\mathbb{R}^n=\mathbb{R}^{2n}$. Set

$$\mathbb{E}=\begin{pmatrix}\mathbb{O}&-\mathbb{I}\\ \mathbb{I}&\mathbb{O}\end{pmatrix},\quad \gamma=\begin{pmatrix}p\\ q\end{pmatrix},\quad \dot{\gamma}=\begin{pmatrix}\dot{p}\\ \dot{q}\end{pmatrix},\quad \nabla H=\begin{pmatrix}\dfrac{\partial H}{\partial p}\\ \dfrac{\partial H}{\partial q}\end{pmatrix},$$

the Hamilton's equations related to $X_H=\mathbb{E}\nabla H$,

$$\dot{p}=-\frac{\partial H}{\partial q},\quad \dot{q}=\frac{\partial H}{\partial q},$$

can be written in the form $\dot{\gamma}-\mathbb{E}\nabla H=0$, or, equivalently,

$$\mathbb{E}\dot{\gamma}+\nabla H=0.$$

The map,

$$A:\Gamma\to\mathbb{R},\quad \gamma\mapsto A|\gamma|:=\int_0^T[p(s)\cdot\dot q(s)-H(s,q(s),p(s))]ds,$$

is the Action Functional of the Hamilton–Helmholtz variational principle related to the Hamiltonian H.

Lemma 3 (Hamilton–Helmholtz): A curve $\gamma\in\Gamma$ solves the Hamilton's equations if and only if

$$(\delta\text{:Gâteaux derivative})\quad \delta A[\gamma]\delta\gamma=0,\quad \forall\,\delta\gamma\in\Gamma\ \ \textit{such that}\ \ \delta q(T)=0.$$

Proof: By a direct computation: $\forall\,\delta\gamma\in T_\gamma\Gamma=\Gamma$,

$$\begin{aligned}
\delta A|\gamma|\delta\gamma&=\frac{dA}{d\lambda}(\gamma+\lambda\,\delta\gamma)|_{\lambda=0}\\
&=\frac{DA}{D\gamma}\delta\gamma\\
&=\int_0^T\left(\delta p\cdot\dot q+p\cdot\delta\dot q-\frac{\partial H}{\partial q}\cdot\delta q-\frac{\partial H}{\partial p}\cdot\delta p\right)ds\\
&=\int_0^T\left(\dot q-\frac{\partial H}{\partial p}\right)\cdot\delta p\ \ ds-\int_0^T\frac{\partial H}{\partial q}\cdot\delta q\ \ ds+\int_0^T p\cdot\delta\dot q\ \ ds\\
&=\int_0^T\left(\dot q-\frac{\partial H}{\partial p}\right)\cdot\delta p\ \ ds-\int_0^T\frac{\partial H}{\partial q}\cdot\delta q\ \ ds+p\cdot\delta q\Big|_0^T-\int_0^T\dot p\cdot\delta q\ \ ds\\
&=\int_0^T\left(\dot q-\frac{\partial H}{\partial p}\right)\cdot\delta p\ \ ds-\int_0^T\left(\dot p+\frac{\partial H}{\partial q}\right)\cdot\delta q\ \ ds+p(T)\cdot\delta q(T)\\
&=-\int_0^T(\mathbb{E}\dot\gamma+\nabla H)\cdot\delta\gamma\ \ ds+p(T)\cdot\delta q(T).
\end{aligned}$$

□

Lemma 4 below allows us to regard the Action functional A as a generating function of Λ_T with infinite parameters (in L^2).

Lemma 4 (∞-parameters generating function): The map,

$$W:=A\circ g:\mathbb{R}^n\times L^2\to\mathbb{R},\quad (q(T),\phi)\mapsto W(q(T),\phi):=A\circ g(q(T),\phi)=A[g(q(T),\phi)],$$

generates Λ_T, that is,

$$\Lambda_T=\left\{(q(T),p(T)):\ \ q(T)\in\mathbb{R}^n,\quad p(T)=\frac{\partial W}{\partial q(T)}(q(T),\phi),\quad \frac{DW}{D\phi}(q(T),\phi)=0\right\}.$$

Proof: Let us write explicitly W:

$$W(q(T),\phi)=\int_0^T\left[\phi_q(s)\int_0^s\phi_p(r)dr-H\left(s,q(T)-\int_s^T\phi_q(r)dr,\int_0^s\phi_p(r)dr\right)\right]ds;$$

then, by writing $DW/D\phi$ the Gateaux derivative on infinite-dimensional spaces,

$$\frac{DW}{D\phi}\delta\phi=\int_0^T\Bigg[\delta\phi_q(s)\int_0^s\phi_p(r)dr+\phi_q(s)\int_0^s\delta\phi_q(r)dr-\frac{\partial H}{\partial q}\Bigg(-\int_s^T\delta\phi_q(r)dr\Bigg)$$
$$-\frac{\partial H}{\partial p}\int_0^s\delta\phi_p(r)dr\Bigg]ds.$$

Let us rewrite the first term. Preliminarily, one has

$$\frac{d}{ds}\Bigg(\int_0^s\phi_p(r)dr\int_T^s\delta\phi_q(r)dr\Bigg)=\phi_p(s)\int_T^s\delta\phi_q(r)dr+\delta\phi_q(s)\int_0^s\phi_p(r)dr;$$

by integrating from $s=0$ to $s=T$ one obtains

$$0=\Bigg(\int_0^s\phi_p(r)dr\int_T^s\delta\phi_q(r)dr\Bigg)\Bigg|_0^T=\int_0^T\Bigg(\delta\phi_q(s)\int_0^s\phi_p(r)dr-\phi_p(s)\int_s^T\delta\phi_q(r)dr\Bigg)ds,$$

and hence

$$\int_0^T\delta\phi_q(s)\int_0^s\phi_p(r)dr\ \ ds=\int_0^T\phi_p(s)\int_s^T\delta\phi_q(r)dr\ \ ds.$$

Using this result to rewrite the expression of $DW/D\phi$ we obtain

$$\frac{DW}{D\phi}\delta\phi=\int_0^T\Bigg[\phi_p(s)\int_s^T\delta\phi_q(r)dr+\phi_q(s)\int_0^s\delta\phi_p(r)dr-\frac{\partial H}{\partial q}\Bigg(-\int_s^T\delta\phi_q(r)dr\Bigg)$$
$$-\frac{\partial H}{\partial p}\int_0^s\delta\phi_p(r)dr\Bigg]ds$$
$$=\int_0^T\Bigg[-\Bigg(\phi_p(s)+\frac{\partial H}{\partial q}\Bigg)\Bigg(-\int_s^T\delta\phi_q(r)dr\Bigg)-\Bigg(-\phi_q(s)+\frac{\partial H}{\partial p}\Bigg)\int_0^s\delta\phi_p(r)dr\Bigg]ds$$
$$=-\int_0^T(\mathbb{E}\dot\gamma+\nabla H)\delta\gamma\ \ ds,$$

where $\delta\gamma=(-\int_s^T\delta\phi_q(r)dr,\int_0^s\delta\phi_p(r)dr)\in\Gamma$. Hence, one obtains that

$$\frac{\partial W}{\partial q(T)}\Bigg|_{DW/D\phi=0}=\int_0^T\Bigg(-\frac{\partial H}{\partial q}\Bigg)ds=\int_0^T\dot p(s)ds=p(T).$$

Fourier Expansions and Fixed Point: For every $\phi\in L^2$ let us consider the Fourier expansion,

$$\phi(s)=\sum_{k\in\mathbb{Z}}\phi_k e^{i(2\pi k/T)s}.$$

For each fixed $N\in\mathbb{N}$ let us consider the projection maps on the basis $\{e^{i(2\pi k/T)s}\}_{k\in\mathbb{Z}}$ of L^2,

$$\mathbb{P}_N\phi(s):=\sum_{|k|\leqslant N}\phi_k e^{i(2\pi k/T)s},\quad \mathbb{Q}_N\phi(s):=\sum_{|k|>N}\phi_k e^{i(2\pi k/T)s}.$$

Clearly,

$$\mathbb{P}_N L^2\oplus\mathbb{Q}_N L^2=L^2,$$

and for $\phi \in L^2$ we will write $u := \mathbb{P}_N \phi$ and $v := \mathbb{Q}_N \phi$.

Remark: The idea to prove the existence of a generating function with finitely many parameters is to show that the "infinite" tail $\mathbb{Q}_N \dot{\gamma}$ of $\dot{\gamma}$, for γ a curve in Γ solving Hamilton's equations, can be dropped out from the expression of the Action functional; in other words, γ is completely determined by a suitable choice of its "finite" part $\mathbb{P}_N \dot{\gamma}$, for suitable (large) $N \in \mathbb{N}$.

Lemma 5 (Lipschitz): For fixed $q(T) \in \mathbb{R}^n$ and $u \in \mathbb{P}_N L^2$, the map,

$$\mathbb{Q}_N L^2 \to (\Gamma, \|\cdot\|_{L^2}), \quad v \mapsto g(q(T), u+v),$$

is Lipschitz with

$$\mathrm{Lip}(g) \leqslant \frac{T}{2\pi N}(1+\sqrt{2N}).$$

Proof: In some more details, the above map is

$$v \mapsto \left(q(T) - \int_s^T (u_q + v_q)(r)dr, \int_0^s (u_p + v_p)(r)dr \right).$$

For each v_1, $v_2 \in \mathbb{Q}_N L^2$, let us consider the Fourier expansion:

$$v := v_2 - v_1 = \sum_{|k|>N} v_k e^{i(2\pi k/T)s}, \quad v_k = (q_k, p_k).$$

We compute $g(q(T), u+v_2) - g(q(T), u+v_1)$:

$$\begin{aligned}
g(v_2) - g(v_1) &= \left(-\int_s^T (v_{q2} - v_{q1})(r)dr, \int_0^s (v_{p2} - v_{p1})(r)dr \right) \\
&= \left(-\int_s^T \sum_{|k|>N} q_k e^{i(2\pi k/T)r} dr, \int_0^s \sum_{|k|>N} p_k e^{i(2\pi k/T)r} dr \right) \\
&= T\left(\sum_{|k|>N} \frac{q_k e^{i(2\pi k/T)r}}{i2\pi k}\bigg|_T^s, \quad \sum_{|k|>N} \frac{p_k e^{(2\pi k/T)r}}{i2\pi k}\bigg|_0^s \right) \\
&= T\left(\sum_{|k|>N} \frac{(q_k, p_k)}{i2\pi k} e^{i(2\pi k/T)s} - \sum_{|k|>N} \frac{(q_k, q_k)}{i2\pi k} \right) \\
&= T\left(\sum_{|k|>N} \frac{v_k}{i2\pi k} e^{i(2\pi k/T)s} - \sum_{|k|>N} \frac{v_k}{i2\pi k} \right).
\end{aligned}$$

Hence the estimate of $\|g(q(T), u+v_2) - g(q(T), u+v_1)\|_{L^2}$ follows:

$$\begin{aligned}
\|g(v_2) - g(v_1)\|_{L^2} &\leqslant T\left(\left\| \sum_{|k|>N} \frac{v_k}{i2\pi k} e^{i(2\pi k/T)t} \right\|_{L^2} + \left\| \sum_{|k|>N} \frac{v_k}{i2\pi k} \right\|_{L^2} \right) \\
&\leqslant T\left(\frac{1}{2\pi N}\|v\|_{L^2} + \|\langle v, \mathbb{Q}_N \,\mathrm{iD}_{[0,T]} \rangle_{L^2}\|_{L^2} \right) \\
&\leqslant T\left(\frac{1}{2\pi N}\|v\|_{L^2} + \|v\|_{L^2} \|\mathbb{Q}_N \,\mathrm{id}_{[0,T]}\|_{L^2} \right) \\
&\leqslant T\left(\frac{1}{2\pi N}\|v\|_{L^2} + \frac{1}{2\pi}\sqrt{\frac{2}{N}}\|v\|_{L^2} \right)
\end{aligned}$$

$$\leqslant \frac{T}{2\pi N}(1+\sqrt{2N})\|v\|_{L^2}.$$

Lemma 6 (contraction map): Suppose that

$$\sup_{y\in\mathbb{R}^{2n}s\in[0,T]}|\nabla^2_{yy}H| = C < +\infty \quad (y := (q,p)).$$

For N large enough: $TC/2\pi N(1+\sqrt{2N})<1$, for every fixed $q(T)\in\mathbb{R}^n$ and $u\in\mathbb{P}_N L^2([0,T|;\mathbb{R}^{2n})$ the map:

$$\mathbb{Q}_N L^2([0,T];\mathbb{R}^{2n})\to\mathbb{Q}_N L^2([0,T];\mathbb{R}^{2n}),$$

$$v\to\mathbb{Q}_N\mathbb{E}\nabla H(g(q(T),u+v)),$$

is a contraction map.

Proof:

$$\begin{aligned}&\|\mathbb{Q}_N\mathbb{E}\nabla H(g(q(T),u+v_2))-\mathbb{Q}_N\mathbb{E}\nabla H(g(q(T),u+v_1))\|_{L^2}\\ &\leqslant \sup_{y\in\mathbb{R}^{2n}s\in[0,T]}|\nabla^2_{yy}H|\|g(q(T),u+v_2)-g(q(T),u+v_1)\|_{L^2}\\ &\leqslant \frac{TC}{2\pi N}(1+\sqrt{2N})\|v_2-v_1\|_{L^2}.\end{aligned}$$

□

By the Banach–Caccioppoli theorem there exists one and only one fixed point $f(q(T),u)$ for the above contraction map. By standard arguments one can easily see that this fixed point depends smoothly on $q(T)$ and u. In the formula, $f(q(T),u)$ is such that

$$f(q(T),u)=\mathbb{Q}_N\mathbb{E}\nabla H(g(q(T),u+f(q(T),u))).$$

It is crucial to observe that, if we solve the *finite* (say, algebraic) equation for u,

$$u=\mathbb{P}_N\mathbb{E}\nabla H(g(q(T),u+f(q(T),u))),$$

and we sum the last two formulas, then the resulting equation,

$$\dot\gamma=\mathbb{E}\nabla H(\gamma),$$

implies that the curve $\gamma=g(q(T),u+f(q(T),u))$ *solves* the Hamilton canonical differential equations, and it is starting from the zero section (so that $\gamma\in\Gamma$). Furthermore, we point out that $\dim(\mathbb{P}_N L^2([0,T];\mathbb{R}^{2n}))=2n(2N+1):=k(n,N)$.

To conclude the proof of Theorem 1 we need to show the following.

Lemma 7 (the finite-parameters generating function): The following function:

$$S:\mathbb{R}^n\times\mathbb{R}^{k(n,N)}\to\mathbb{R},$$

$$(q(T),u)\to S(q(T),u):=A\circ g(q(T),u+f(q(T),u))=W(q(T),u+f(q(T),u)),$$

is a global generating function for $\Lambda=\Phi^T(\Lambda_0)$.

Proof: We write

$$\frac{\partial S}{\partial u}(q(T),u)=\frac{DW}{D\phi}\left(\frac{D\phi}{Du}+\frac{D\phi}{Dv}\frac{Df}{Du}\right)$$

(note that $D\phi/Du$ and $D\phi/Dv$ are the projectors $\mathbb{P}_N$ and $\mathbb{Q}_N$, respectively),

$$\frac{\partial S}{\partial u}(q(T),u) = -\int_0^T [\mathbb{P}_N(\mathbb{E}\dot\gamma + \nabla H(\gamma))]\big|_{\gamma = g(q(T),u+f(q(T),u))} ds$$
$$-\int_0^T [\mathbb{Q}_N(\mathbb{E}\dot\gamma + \nabla H(\gamma))]\big|_{\gamma = g(q(T),u+f(q(T),u))} \frac{Df}{Du} ds.$$

By the very construction of $f(q(T),u)$ the second integral vanishes, so

$$\frac{\partial S}{\partial u}(q(T),u) = -\int_0^T [\mathbb{P}_N(\mathbb{E}\dot\gamma + \nabla H(\gamma))]\big|_{\gamma = g(q(T),u+f(q(T),u))} ds,$$

so that

$$\frac{\partial S}{\partial u}(q(T),u) = 0 \quad \text{is equivalent to} \quad [\mathbb{P}_N(\mathbb{E}\dot\gamma + \nabla H(\gamma))]\big|_{\gamma = g(q(T),u+f(q(T),u))} = 0.$$

On the other hand,

$$\frac{\partial S}{\partial q(T)} = \frac{\partial W}{\partial q(T)} + \frac{DW}{D\phi}\frac{D\phi}{Dv}\frac{Df}{Dq(T)},$$

$$\frac{\partial S}{\partial q(T)} = \frac{\partial W}{\partial q(T)} - \int_0^T [\mathbb{Q}_N(\mathbb{E}\dot\gamma + \nabla H(\gamma))]\big|_{\gamma = g(q(T),u+f(u(T),u))} \frac{Df}{Dq(T)} ds;$$

hence

$$\frac{\partial S}{\partial q(T)}(q(T),u) = \frac{\partial W}{\partial q(T)}(q(T),\phi)\big|_{\phi = u+f(q(T),u)}.$$

Now it is easy to conclude that the pair $(q(T),\phi) \in \mathbb{R}^n \times L^2$ satisfies

$$p(T) = \frac{\partial W}{\partial q(T)}(q(T),\phi),$$

$$0 = \frac{DW}{D\phi}(q(T),\phi),$$

if and only if the pair $(q(T),u) \in \mathbb{R}^n \times \mathbb{R}^{k(n,N)}$, where

$$\phi = u + f(q(T),u), \quad \text{so that } u = \mathbb{P}_N\phi,$$

satisfies

$$p(T) = \frac{\partial S}{\partial q(T)}(q(T),u),$$

$$0 = \frac{\partial S}{\partial u}(q(T),u).$$

III. THE GLOBAL FINITE ENVELOPE STRUCTURE OF THE PHASE FRONT SETS

Let us recall the general evolution problem, $q \in \mathbb{R}^n$,

$$\frac{\partial S}{\partial t}(t,q)+H\left(t,q,\frac{\partial S}{\partial q}(t,q)\right)=0,$$

$$S(t,q)|_{t=0}=\sigma(q),$$

where, e.g., we may suppose the initial data $\sigma(q)$ to be a suitable regularization of a Heaviside function defined around a one-co-dimensional surface $\Sigma \subset \mathbb{R}^n$ (a smooth Riemann problem), as could be a model to propagation phenomena starting from (some neighborhood of) Σ. The canonical transformation $(q,p) \to (\tilde{q},\tilde{p})$ generated by the function

$$F(q,\tilde{q})=\tilde{p}\cdot q+\sigma(q),$$

is given by

$$p=\frac{\partial F}{\partial q}(q,\tilde{p}):\ \ p=\tilde{p}+\frac{\partial \sigma}{\partial q}(q),$$

$$\tilde{q}=\frac{\partial F}{\partial \tilde{p}}(q,\tilde{p}):\ \ \tilde{q}=q.$$

The transformed Hamiltonian function of $H(q,p,t)$ is

$$K(\tilde{q},\tilde{p},t)=H\left(\tilde{q},\tilde{p}+\frac{\partial \sigma}{\partial q}(\tilde{q}),t\right),$$

so that the characteristics of X_K starting at $t=0$ from the zero-section $\{(\tilde{q},0)\}$ of T^*Q correspond to the characteristics of X_H starting from the initial Lagrangian submanifold $\Lambda_0 = \{(q,\partial\sigma/\partial q(q))\}$. Let us now consider the Action Functional of the Hamilton–Helmholtz variational principle related to the Hamiltonian function K,

$$A[\gamma] := \int_0^T [\tilde{p}(s)\cdot \dot{\tilde{q}}(s)-K(\tilde{q}(s),\tilde{p}(s),s)]ds,$$

defined for $\gamma \in \Gamma = \{(\tilde{q}(\cdot),\tilde{p}(\cdot)) \in H^{1,2}([0,T],\mathbb{R}^{2n}):\tilde{p}(0)=0\}$. We have seen above that A is a global generating function for $\hat{\Lambda}_T = \{(\tilde{q}(T),\tilde{p}(T))\}$ with infinite parameters. If the condition

$$\sup_{y\in\mathbb{R}^{2n},t\in[0,T]}|\nabla^2_{yy}K(y,t)|<+\infty \quad (y=(\tilde{q},\tilde{p})\in\mathbb{R}^{2n})$$

holds, then Theorem 1 allows us to describe the generalized Envelope at the time $t=T$, i.e. Λ_T, by a global generating function $\tilde{S}(\tilde{q},u_1,\ldots,u_N)$ with *finite* parameters $N<+\infty$. Finally, by turning from $(\tilde{q},\tilde{p})$ to the original setting (q,p), the Lagrangian submanifold is now generated by (check the structure of the canonical transformation above)

$$S(q,u)=\sigma(q)+\tilde{S}(q,u).$$

Note that the above condition on $\nabla^2_{yy}K$ involves both H and σ.

IV. THE GLOBAL GENERATING FUNCTION FOR THE SPACE–TIME SOLUTION

Now we consider the set of curves (as above),

$$\Gamma := \{\gamma(\cdot)=(q(\cdot),p(\cdot)) \in H^{1,2}([0,T],\mathbb{R}^{2n}):p(0)=0\},$$

the *new* functional,

$$\hat{A}:[0,T]\times\Gamma\to\mathbb{R},\quad (t,\gamma(\cdot))\mapsto\hat{A}[t,\gamma(\cdot)]:=\int_0^t[p(r)\cdot\dot{q}(r)-H(r,q(r),p(r))]dr,$$

and the *new* bijection:

$$\hat{g}:[0,T]\times\mathbb{R}^n\times L^2([0,T],\mathbb{R}^{2n})\to[0,T]\times\Gamma,$$

$$(t,q,\phi)\mapsto\hat{g}(t,q,\phi)=(t,\gamma(\cdot)),\quad \gamma(s)=(q(s),p(s)):=\left(q-\int_s^t\phi_q(r)dr,\int_0^S\phi_p(r)dr\right).$$

The second value of the map $\hat{g}(t,q,\phi)$ is the curve $\gamma(\cdot)=(q(\cdot),p(\cdot))$ which is (*i*) starting from $p(0)=0$, such that (*ii*) $\dot{\gamma}(\cdot)=\phi(\cdot)$, and (*iii*) $q(t)=q$.

Consider the infinite-parameters function:

$$\hat{W}:=\hat{A}\circ\hat{g}:[0,T]\times\mathbb{R}^n\times L^2\to\mathbb{R},$$

$$(t,q,\phi)\mapsto\hat{W}(t,q,\phi):=\hat{A}\circ\hat{g}(t,q,\phi).$$

We will prove that $\hat{W}$ generates $\hat{\Lambda}:=\cup_{t\in[0,T]}\Lambda_t$, the Lagrangian submanifold of $T^*([0,T]\times\mathbb{R}^n)$; i.e., that

$$\hat{\Lambda}=\left\{(t,q;\tau,p):t\in[0,T],\ q\in\mathbb{R}^n,\ \tau=\frac{\partial\hat{W}}{\partial t}(t,q,\phi),\ p=\frac{\partial\hat{W}}{\partial q}(t,q,\phi),\quad \frac{D\hat{W}}{D\phi}(t,q,\phi)=0\right\},$$

is the geometric solution of the Hamilton–Jacobi problem,

$$\frac{\partial S}{\partial t}+H\left(t,q,\frac{\partial S}{\partial q}\right)=0,\quad S(0,q)=0.$$

In order to prove this, we write explicitly $\hat{W}$:

$$\hat{W}(t,q,\phi)=\int_0^t\left[\int_0^s\phi_p(r)dr\cdot\phi_q(s)-H\left(s,q-\int_s^t\phi_q(r)dr,\int_0^s\phi_p(r)dr\right)\right]ds;$$

then, for $D\hat{W}/D\phi=0$, we compute $\partial\hat{W}/\partial q$:

$$\frac{\partial\hat{W}}{\partial q}=-\int_0^t\frac{\partial H}{\partial q}ds=\int_0^t\dot{p}(s)ds=p(t).$$

Finally, we compute, $\partial\hat{W}/\partial t$:

$$\frac{\partial \hat{W}}{\partial t}(t,q,\phi)=p(t)\cdot\dot{q}(t)-H\left(t,q,\frac{\partial \hat{W}}{\partial q}\right)+\int_0^t \frac{\partial H}{\partial q}\left(s,q-\int_s^t \phi_q(r)dr,\int_0^s \phi_p(r)dr\right)\phi_q(t)ds$$

$$=p(t)\cdot\dot{q}(t)-H\left(t,q,\frac{\partial \hat{W}}{\partial q}\right)+\int_0^t \frac{\partial H}{\partial q}ds\dot{q}(t)$$

$$=\frac{\partial \hat{W}}{\partial q}\dot{q}-H-\frac{\partial}{\partial q}\left(\int_0^t [p\cdot\dot{q}-H]d\tau\right)\dot{q}(t)$$

$$=-H\left(t,q,\frac{\partial \hat{W}}{\partial q}\right).$$

Therefore, $\hat{W}(t,q,\phi)$ is a global generating function, with infinite parameters ϕ, for the geometric solution $\hat{\Lambda}$ within $T^*([0,T]\times\mathbb{R}^n)$.

Now, with minor changes, the reduction machinery used in the preceding sections still works for $\hat{W}$, and, by means of the trick of Sec. III, we obtain global generating functions for general initial problems (for nontrivial σ). In some more detail, for fixed $N\in\mathbb{N}$, $(t,q)\in[0,T]\times\mathbb{R}^n$, and $u(\cdot)\in\mathbb{P}_N L^2([0,T];\mathbb{R}^{2n})$, the map,

$$\mathbb{Q}_N L^2\to(\Gamma,\|\cdot\|_{L^2}),$$

$$v(\cdot)\mapsto\hat{g}(t,q,u(\cdot)+v(\cdot)),$$

is Lipschitz with constant

$$\frac{T}{2\pi N}(1+\sqrt{2N}),$$

and the theory goes in the same way above, so, lastly, we can determine a global generating function with finite parameters $S(t,q,u)$ for $\hat{\Lambda}$, which is solving, for all $(t,q)\in[0,T]\times\mathbb{R}^n$ and for some $u\in\mathbb{R}^k$,

$$\frac{\partial S}{\partial t}(t,q,u)+H\left(t,q,\frac{\partial S}{\partial q}(t,q,u)\right)=0,\quad S(0,q,u)=0,\quad \frac{\partial S}{\partial u}(t,q,u)=0.$$

Now, for more general initial data $\sigma\neq 0$, we may argue in a strictly similar way as done in Sec. III.

More precisely, consider coordinates $\hat{t},\hat{q},\hat{p}$ and let now $S(\hat{t},\hat{q},u)$ be a generating $\hat{\Lambda}$, geometrical solution of H–J starting, at $\hat{t}=0$, from the zero-section $(\hat{p}\equiv 0)$ for the Hamiltonian $K(\hat{t},\hat{q},\hat{p}):=H(\hat{t},\hat{q},\hat{p}+(\partial\sigma/\partial q)(\hat{q}))$ where $\nabla^2 K$ are bounded; moreover, let us consider the canonical transformation $\Psi:(t,q;\tau,p)\mapsto(\hat{t},\hat{q};\hat{\tau},\hat{p})$ generated by the function

$$G(t,q,\hat{\tau},\hat{p})=\hat{\tau}t+\hat{p}\cdot q+\sigma(q),$$

$$\tau=\frac{\partial G}{\partial t}:\quad \tau=\hat{\tau},$$

$$p=\frac{\partial G}{\partial q}:\quad p=\hat{p}+\frac{\partial\sigma}{\partial q}(q),$$

$$\hat{t}=\frac{\partial G}{\partial\hat{\tau}}:\quad \hat{t}=t,$$

$$\hat{q}=\frac{\partial G}{\partial \hat{p}}: \quad \hat{q}=q.$$

If we let $\hat{S}(\hat{t},\hat{q},u)$ be the finite global generating function of $\hat{\Lambda}$, it is an easy matter to see that the Lagrangian submanifold,

$$\Lambda=\Psi^{-1}(\hat{\Lambda}),$$

is the geometrical solution of the $H-J$ equation $\tau+H=0$, starting, at $t=0$, from $\mathrm{im}(d\sigma)$, and we note that a global generating function for it is given by

$$S(t,q,u)=\hat{S}(t,q,u)+\sigma(q).$$

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On harmonic oscillators on the two-dimensional sphere S^2 and the hyperbolic plane H^2

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Two Harmonic Oscillators (isotropic and nonisotropic 2:1) are studied on the two-dimensional sphere S^2 and the hyperbolic plane H^2. Both systems are integrable and super-integrable with constants of motion quadratic in the momenta. These properties are shown to derive from a complex factorization for the constants of motion, which holds for arbitrary values of the curvature κ, and the dynamics of the Euclidean harmonic 1:1 and 2:1 oscillators is directly recovered for $\kappa=0$. The harmonic oscillators on either the standard unit sphere (radius $R=1$) or the unit Lobachewski plane (''radius'' $R=1$) appear as the particular values of the κ-dependent potentials for the values $\kappa=1$ and $\kappa=-1$. Finally a particular potential is proposed for representing the general spherical (hyperbolic) $n:1$ anisotropic harmonic oscillator on a two-dimensional manifold of constant curvature. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1423402]

I. INTRODUCTION

Dynamics on a nonflat configuration space Q remains as a very partially studied subject, even in the simplest two-dimensional constant curvature cases where Q is either the sphere S^2 or the hyperbolic (Lobachewski) plane H^2 (see Refs. 1, 2, 3 for the case of spherical central potentials). In fact, there exist some noncentral but rather simple problems, e.g., the nonisotropic harmonic oscillators, still awaiting to be studied in manifolds of nonzero curvature.

It is well known that integrable systems, in the classical sense of Arnold–Liouville, must have as many independent constants of motion in involution as degrees of freedom. On the other hand, a system is called super-integrable if it is integrable and, in addition, possesses more independent first integrals than degrees of freedom. It is known that these additional first integrals give rise to a higher degree of regularity in the phase space (e.g., the existence of periodic orbits) since the trajectories are restricted to submanifolds with less than n dimensions. In particular, if a system with n degrees of freedom possesses $2n-1$ independent first integrals, then it is called maximally super-integrable. The Kepler problem, the harmonic oscillator and the Calogero–Moser system are some cases of this very particular class of systems (for other super-integrable systems see Refs. 4–15 and references therein).

In a recent paper[16] the existence of super-integrable systems on the two-dimensional sphere S^2 and on the hyperbolic plane H^2 was analyzed. The study was focused on the quadratic super-integrability, that is, on the existence of systems that, besides the energy, admit two further independent constants of motion quadratic in the velocities (quadratic super-integrability is related with super-separability in the sense of Ref. 14). Some of the spherical (hyperbolic) potentials obtained by this approach were already known, but some others were apparently new. Particularly

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interesting was the existence of a potential that seems to represent the spherical (hyperbolic) version of the Euclidean nonisotropic 2:1 oscillator $4x^2+y^2$ or x^2+4y^2 (for other Euclidean nonisotropic oscillators the additional constant of motion is not quadratic, but higher order in momenta). We recall that the spherical version of the central oscillator was studied by Higgs in Ref. 2 and is known as the Higgs oscillator.

The main objective of this article is to develop a deeper analysis of these two spherical (hyperbolic) oscillators: the central Higgs oscillator and noncentral 2:1 oscillator. We will show, as a basic point, that these two systems are endowed with the same fundamental properties as the standard Euclidean one. This means that those properties to be considered as fundamental (e.g., the existence of constants of motion, super-integrability, complex factorization) are preserved under non-Euclidean deformations. Conversely, the Euclidean Oscillator can be considered as a very particular case (the flat limit) of the general ''curved'' Harmonic Oscillator. We will carry out this approach by considering the curvature as a parameter.

The article is organized as follows: In Sec. II we discuss the fundamental properties of the Euclidean Harmonic Oscillator related with the existence of super-integrability. We are interested in obtaining non-Euclidean deformations of these Euclidean properties. Section III is devoted to the geometry of the Riemannian two-dimensional (2-D) manifolds of constant curvature. We first discuss some properties of the curvilinear systems of coordinates and then we introduce a formalism with the curvature κ as a parameter (this formalism was already used in Ref. 16). This is made so that the Euclidean geometry is directly recovered for $\kappa=0$.

In Secs. IV and V we study the integrability and the super-integrability of both oscillators (isotropic central oscillator and non-isotroipc 2:1 oscillator) in the the sphere S^2 and in the hyperbolic plane H^2 with curvature κ (these two sections have been written in such a way that can be read independently). First, in Sec. IV, the study is presented in ''geodesic polar'' coordinates, and then, in Sec. V, we will obtain the results by using ''geodesic parallel'' coordinates. The dynamics in the Euclidean plane (studied in Sec. II) appears as a very particular case. The harmonic oscillators on either the standard unit sphere (radius $R=1$) or the unit Lobachewski plane (''radius'' $R=1$) correspond to the values $\kappa=1$ and $\kappa=-1$. Finally, in Sec. VI we provide a discussion and an outlook to the results obtained.

II. SUPER-INTEGRABILITY OF THE EUCLIDEAN HARMONIC OSCILLATOR

The two-dimensional harmonic oscillator,

$$L_{\mathrm{HO}}=(\tfrac{1}{2})(v_x^2+v_y^2)-(\tfrac{1}{2})(\omega_1^2x^2+\omega_2^2y^2),$$

is a trivially integrable system, since it is a direct sum of one-degree of freedom systems and, therefore, it has the two one-degree of freedom energies, $I_1=E_x$ and $I_2=E_y$, as involutive integrals. If the oscillator is isotropic then it has the angular momentum as an additional integral of motion. If the oscillator is nonisotroipc then the angular momentum is not preserved but in the very particular case in which the quotient of the two frequencies is rational the system has a third additional nonlinear integral.

In geometric terms the phase space is foliated by tori and every integral curve is a curve with constant slope on a torus. The slope of the curve is determined by the ratio ω_2/ω_1. Thus, if this ratio is irrational the corresponding curve will be dense on the torus.[17,18] If this ratio is rational then the orbit becomes closed and the motion will be periodic.

The super-integrability of the rational case, $\omega_1=n_1\omega_0$, $\omega_2=n_2\omega_0$, with integers n_1,n_2, can be approached by using a complex formalism.[18,19] The following proposition states the existence of the additional constant of motion and give a method for obtaining it explicitly.

Proposition 1: Let J_1, J_2, be the following two functions:

$$J_1=v_x+\mathrm{i}n_1\omega_0x, \quad J_2=v_y+\mathrm{i}n_2\omega_0y.$$

Then the complex function J_{12} defined as

$$J_{12}=J_1^{n_2}(J_2^*)^{n_1}$$

is a constant of motion.

Proof: The time-evolution of the functions J_1, J_2, is given by

$$\frac{d}{dt}J_1=-\mathrm{i}\,n_1\omega_0 J_1 \quad \frac{d}{dt}J_2=-\mathrm{i}\,n_2\omega_0 J_2.$$

Hence we have

$$\frac{d}{dt}J_{12}=n_2J_1^{(n_2-1)}(J_2^*)^{n_1}\dot{J}_1+n_1J_1^{n_2}(J_2^*)^{(n_1-1)}\dot{J}_2^*=J_1^{n_2}(J_2^*)^{n_1}(\mathrm{i}\,\omega_0)(n_2n_1-n_1n_2)=0. \quad (1)$$

Therefore J_{12} is a constant of motion. Notice that J_{12}, which can be considered as coupling the two degrees of freedom, depends on the relation between ω_2 and ω_1. As stated above, J_{12} is well defined as a constant of motion only if the quotient ω_2/ω_1 is rational.

Since J_{12} is a complex function it determines two different real first integrals,

$$I_3=\mathrm{Im}(J_{12}), \quad I_4=\mathrm{Re}(J_{12}),$$

which are polynomials in the velocities (momenta) of degree n_1+n_2-1 and n_1+n_2, respectively. Only one of these two functions must be considered as fundamental, because I_1,I_2,I_3,I_4 are functionally dependent (I_3 is independent of I_1 and I_2, but I_4 is a dependent function of I_1, I_2 and I_3).

Next we give the expressions of I_3 and I_4 for the first two rational cases.

(i) Isotropic case $\omega_1=\omega_2=\omega_0$:

$$I_4=\mathrm{Re}(J_{12})=v_xv_y+\omega_0^2xy, \quad I_3=\mathrm{Im}(J_{12})=\omega_0(xv_y-yv_x); \quad (2)$$

$\mathrm{Im}(J_{12})$ is just the angular momentum, and $\mathrm{Re}(J_{12})$ is the nondiagonal component of the Fradkin tensor.[20]

(ii) The nonisotroipc case with $\omega_1=2\omega_0$, $\omega_2=\omega_0$:

$$\begin{aligned} I_4&=\mathrm{Re}(J_{12})=v_xv_y^2+\omega_0^2(4xv_y-yv_x)y,\\ I_3&=\mathrm{Im}(J_{12})=(xv_y-yv_x)v_y-\omega_0^2xy^2. \end{aligned} \quad (3)$$

Summarizing: Proposition 1 states two properties: (i) super-integrability of the rational case, and (ii) complex factorization of the additional constant of motion, that can be considered as the two fundamental features characterizing the two-dimensional harmonic oscillator. In fact, they can even be considered as defining properties. That is, any dynamical system defined in a non-Euclidean space must satisfy the appropriate non-Euclidean versions of points (i) and (ii) to be in fact considered as an (non-Euclidean) Harmonic Oscillator.

III. GEOMETRY AND DYNAMICS ON THE SPHERE S^2 AND THE HYPERBOLIC PLANE H^2

A two-dimensional manifold M can be described by using different coordinate systems. If we consider it as an imbedded submanifold of $\mathbb{R}^3$, then the points of M can be characterized by the

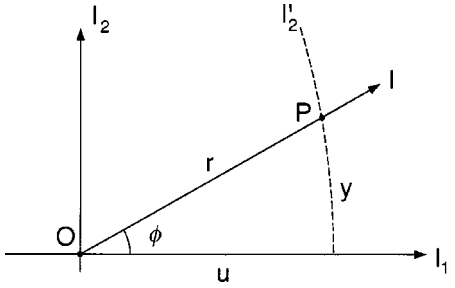

FIG. 1. Polar (r,ϕ) and parallel (u,y) coordinates based on the oriented geodesic l_1 and reference point O. All these coordinates are lengths or angles measured in the intrinsic metric of the space of constant curvature. The figure follows the pattern of a stereographic projection of the sphere from the South Pole, with O at the North Pole, but the geometrical meaning of these coordinates holds for any value of the curvature.

three external coordinates (x,y,z) plus an additional constraint. Nevertheless, in differential geometric terms, a more appropriate approach is to develop the study by using two-dimensional systems of coordinates adapted to M.

On any general two-dimensional Riemannian space (not neccesarily of constant curvature) there are two distinguished types of local coordinate systems: ''geodesic parallel'' and ''geodesic polar'' coordinates. They reduce to the familiar Cartesian and polar coordinates on the Euclidean plane (see Refs. 16 and 21) and both are based on an origin point O and an oriented geodesic l_1 through O (Fig. 1).

For any point P in some suitable neigboorhood of O, there is a unique geodesic l joining O and P. The (geodesic) polar coordinates (r,ϕ) of P, relative to the origin O and the positive geodesic ray of l_1, are the (positive) distance r between O and P measured along l, and the angle ϕ between l and the positive ray l_1, measured around O. These coordinates are defined in a neigborhood of O not extending beyond the cut locus of O; polar coordinates are singular at O, and ϕ is discontinuous on the positive ray of l_1.

Now, consider the geodesic l_2' through P and orthogonal to l_1 and let P_1 be the intersection point of l_2' and l_1 nearest to P. The (geodesic) parallel coordinates (u,y) of P, relative to the origin O and base geodesic l_1, are defined as the distance u between O and P_1, measured along l_1, and the distance y, between P_1 and P, measured along l_2'. Again these coordinates will be regular and without singularities in some suitable strip centered in l_1. If instead of l_1 another line is taken as the base, we obtain another system of geodesic parallel coordinates. Figure 2 also display the particular case with base l_2, orthogonal to l_1 through O; these second sets of parallel coordinates will be denoted (v,x).

These systems are suitable for most general purposes, because the coordinates (r,ϕ), (u,y) and (v,x) have a *direct* geometric significance, as distances and angles measured in the intrinsic metric of the surface. Closed expressions are usually only possible for spaces of *constant curva-*

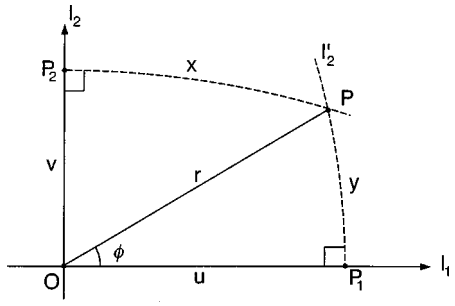

FIG. 2. The three coordinate systems (r,ϕ), (u,y) and (v,x) of a point P. Relationships among these coordinates are discussed in the text for any curvature value κ.

ture. In the constant *positive* curvature case, i.e., the sphere, the geodesics are great circles, and relations among distances and angles are the subject of spherical geometry. Polar coordinates on the sphere are singular at the origin (pole) O and also at its antipodal point (the cut locus of O). Parallel coordinates are singular in the two poles of the base geodesic. While in the Euclidean plane a line orthogonal to both l_1 and l_2 do not exist (nor does it exist in the hyperbolic plane), there is such a line l_3 for the sphere (the polar of the point O); so we have here a third set of parallel coordinates. These three sets are based on three geodesics mutually orthogonal by pairs and the third system with base l_3 is essentially equivalent to the polar coordinates whose center is the pole of l_3.

The notation has been chosen to emphasize the similarities with the Euclidean case. For a point P, r is the distance measured in either S^2 or H^2 (with curvature κ) from P to the origin point O, and ϕ determines the orientation of the line OP through O. On the other side, x, y are the geodesic distances from P to the two "coordinate axes" l_1, l_2; there are other two quantities, u, v which are distances, measured along l_1, l_2, between O and the orthogonal projections of P on l_1, l_2. In the Euclidean case, we have the identities $x=u, y=v$, but once we deal with nonzero curvature these equalities are no longer true; recall that y is the distance from P to the "x" coordinate axis, but *u is not* the distance from P to the "y" coordinate axis. Both polar (r,ϕ) and the two systems of parallel coordinates (u,y) and (v,x) are always *orthogonal*; however, the coordinate system (x,y) made up of the distances to the two coordinate axes is orthogonal in the Euclidean plane, but *not* in S^2 nor in H^2.

For a sphere of radius R the "geographic" coordinates (θ,ϕ) (where θ is the latitude and ϕ the longitude) are closely related to both polar and parallel type coordinate systems: $(R(\pi/2-\theta),\phi)$ are *polar* coordinates with an origin in the North pole, while $(R\phi, R\theta)$ are *parallel* coordinates with the equator as the base line. This equivalence does not exist in the Euclidean and hyperbolic case, where polar and parallel coordinates are very different, so there are reasons to keep their consideration separate, even for the sphere, in the context in which we are working. The fundamental properties of the harmonic oscillator on manifolds of constant curvature will be more clearly seen this way.

The metric of the sphere of curvature $\kappa = 1/R^2$ is given in parallel and polar coordinates by

$$ds^2 = \cos^2(y/R)\,du^2 + dy^2, \quad ds^2 = dr^2 + R^2 \sin^2(r/R)\,d\phi^2,$$

reducing to du^2+dy^2 and $dr^2+r^2\,d\phi^2$ when $R\to\infty$. It is possible to write these expressions in a form which holds simultaneously for the sphere, the Euclidean plane and the hyperbolic plane, by introducing the following "tagged" trigonometric functions:[22]

$$\mathrm{C}_\kappa(x) = \begin{cases} \cos\sqrt{\kappa}\,x, & \text{if } \kappa>0, \\ 1, & \text{if } \kappa=0, \\ \cosh\sqrt{-\kappa}\,x, & \text{if } \kappa<0, \end{cases} \qquad \mathrm{S}_\kappa(x) = \begin{cases} \dfrac{1}{\sqrt{\kappa}}\sin\sqrt{\kappa}\,x, & \text{if } \kappa>0, \\ x, & \text{if } \kappa=0, \\ \dfrac{1}{\sqrt{-\kappa}}\sinh\sqrt{-\kappa}\,x, & \text{if } \kappa<0, \end{cases}$$

and

$$\mathrm{T}_\kappa(x) = \frac{\mathrm{S}_\kappa(x)}{\mathrm{C}_\kappa(x)}.$$

When $\kappa=1$ the three "tagged" functions are the ordinary trigonometrical functions, i.e., $\mathrm{S}_1(x)=\sin x$, $\mathrm{C}_1(x)=\cos x$, $\mathrm{T}_1(x)=\tan x$. For $\kappa=0$ one gets the "parabolic" sine $\mathrm{S}_0(x)=x$, cosine $\mathrm{C}_0(x)=1$, and tangent $\mathrm{T}_0(x)=x$. For $\kappa=-1$, these functions are the hyperbolic cosine, sine, and tangent. Therefore, in the flat case $\kappa=0$ all $\mathrm{C}_\kappa(x)$ are replaced by 1, while all $\mathrm{S}_\kappa(x)$, $\mathrm{T}_\kappa(x)$ are

replaced by its variable x; this suggests that in the curved case, $C_\kappa(x)$ should be looked at as a kind of ''curved'' deformation of the function 1, while both $S_\kappa(x)$ and $T_\kappa(x)$ are two kinds of deformations of the linear function x.

The idea is to obtain relations between the different coordinates (u,y), (v,x), (r,ϕ), in a way that holds regardless of the value of κ. In the cases $\kappa>0$ or $\kappa<0$ they reduce to formulas of spherical or hyperbolic trigonometry, while for $\kappa=0$ they are well-known Euclidean relations.

In any rectangular triangle, as P_1PO in Fig. 1, the three sides r,u,y, and the angle ϕ at O are related by the following equations:

$$S_\kappa(y)=S_\kappa(r)\sin\phi, \quad C_\kappa(r)=C_\kappa(u)C_\kappa(y),$$

$$T_\kappa(u)=T_\kappa(r)\cos\phi, \quad T_\kappa(y)=S_\kappa(u)\tan\phi,$$

and similar equations for the triangle P_2PO (sides r,v,x, angle $\pi/2-\phi$ at O):

$$S_\kappa(x)=S_\kappa(r)\cos\phi, \quad C_\kappa(r)=C_\kappa(v)C_\kappa(x),$$

$$T_\kappa(v)=T_\kappa(r)\sin\phi, \quad T_\kappa(x)\tan\phi=S_\kappa(v).$$

Starting from these equations we get many relations with a rather symmetrical appearance in the pairs x,y and u,v. The change from *polar* to *parallel* coordinates, in any constant curvature plane, can be read from these equations.

The harmonic oscillator potential will be closely related with the particular function $T_\kappa^2(r)$ that can be presented, in terms of (y,u) or (x,v), in several alternative ways:

$$T_\kappa^2(r)=T_\kappa^2(u)+\frac{T_\kappa^2(y)}{C_\kappa^2(u)}=\frac{T_\kappa^2(u)}{C_\kappa^2(y)}+T_\kappa^2(y)=T_\kappa^2(v)+\frac{T_\kappa^2(x)}{C_\kappa^2(v)}=\frac{T_\kappa^2(v)}{C_\kappa^2(x)}+T_\kappa^2(x). \tag{4}$$

These expressions can be considered as different κ-deformed versions of the Pythagorean theorem. In fact for the $\kappa=0$ Euclidean plane we have $u=x$, $v=y$, and they reduce to $r^2=x^2+y^2$.

IV. THE 1:1 AND 2:1 HARMONIC OSCILLATORS ON A 2-D SPACE OF CONSTANT CURVATURE I: POLAR COORDINATES

In the Euclidean plane, central potentials are better discussed in polar coordinates. This is also true for $\kappa\neq0$. Nevertheless we know that nonisotroipc Euclidean oscillators are better presented in Cartesian coordinates. As we deal with both types when the configuration space is assumed to be a space of constant curvature κ, our idea is to develop both approaches. In this section the study is presented in geodesic polar coordinates, and in the next section we will make use of parallel coordinates (we begin with polar coordinated because it is the usual way of presenting the Higgs oscillator). In any case the properties we are looking for are intrinsic properties of the harmonic oscillator considered as a dynamical system, that is, as a vector field defined on the tangent bundle of a particular manifold (sphere S^2 or hyperbolic plane H^2). So all the issues we are interested in, such as integrability, super-integrability, or complex factorization, will prove to be reached by both approaches. Nevertheless we will find some differences between both approaches; this will be important with a view to facilitate further generalizations to other $n:1$ oscillators.

The differential element of distance on a manifold Q of constant curvature (S^2 if $\kappa>0$, the Euclidean plane if $\kappa=0$, or H^2 if $\kappa<0$) becomes, when written in ''geodesic polar'' coordinates:

$$ds^2=dr^2+S_\kappa^2(r)\,d\phi^2.$$

Thus a general standard Lagrangian has the following form:

$$L(\kappa)=(\tfrac{1}{2})(v_r^2+S_\kappa^2(r)v_\phi^2)-U(r,\phi,\kappa),$$

in such a way that for $\kappa=0$ we recover the standard Euclidean system,

$$\lim_{\kappa\to 0} L(\kappa)=(\tfrac{1}{2})(v_r^2+r^2v_\phi^2)-V(r,\phi),\quad V(r,\phi)=U(r,\phi,0).$$

The systems we are concerned with are systems endowed with quadratic integrals of motion depending on the curvature κ as a parameter, but we will first recall, as a previous step, the properties of the linear constants, which arise from exact Noether symmetries. An exact Noether symmetry is a complete vector field Y defined on the configuration space Q such that its natural lift Y^t to phase space TQ is an exact symmetry of the Lagrangian, that is, $Y^t(L)=0$. Then, if we denote by θ_L the Cartan one-form,

$$\theta_{\mathrm{L}}=\left(\frac{\partial L}{\partial v_r}\right)dr+\left(\frac{\partial L}{\partial v_\phi}\right)d\phi,$$

the function I defined as $I=i(Y^t)\theta_L$ is a constant of motion. The important point is that if L is a natural Lagrangians of mechanical type (Riemannian metric minus a potential) then the constant I is linear function in the velocities, and the vector field Y must necessarily be symmetry of the kinetic term (isometry of the metric) and symmetry of the potential.

In this particular spherical (hyperbolic) case the kinetic term is endowed with the following three symmetries:

$$Y_{P_1}(\kappa)=(\cos\phi)\frac{\partial}{\partial r}-\left(\frac{\mathrm{C}_\kappa(r)}{\mathrm{S}_\kappa(r)}\sin\phi\right)\frac{\partial}{\partial\phi},$$

$$Y_{P_2}(\kappa)=(\sin\phi)\frac{\partial}{\partial r}+\left(\frac{\mathrm{C}_\kappa(r)}{\mathrm{S}_\kappa(r)}\cos\phi\right)\frac{\partial}{\partial\phi},$$

$$Y_J(\kappa)=\frac{\partial}{\partial\phi}.$$

These three vector fields generate a Lie algebra,

$$[Y_{P_1},Y_{P_2}]=-\kappa Y_J,\quad [Y_{P_1},Y_J]=-Y_{P_2},\quad [Y_{P_2},Y_J]=Y_{P_1},$$

isomorphic to the Lie algebra of isometries of the spherical (Euclidean, hyperbolic) space; only if $\kappa=0$ (Euclidean plane) Y_{P_1} and Y_{P_2} conmute.

Constants of motion linear in the velocities only appear for some specific potentials. In particular, we have three cases.

(i) If the potential U is of the form $U=U(z(r,\phi))$, $z(r,\phi)=\mathrm{S}_\kappa(r)\sin\phi$, then

$$P_1(\kappa)=i(Y^t_{P_1}(\kappa))\theta_L=(\cos\phi)v_r-(\mathrm{C}_\kappa(r)\mathrm{S}_\kappa(r)\sin\phi)v_\phi$$

is a constant of motion.

(ii) If the potential U is of the form $U=U(z'(r,\phi))$, $z'(r,\phi)=\mathrm{S}_\kappa(r)\cos\phi$, then

$$P_2(\kappa)=i(Y^t_{P_2}(\kappa))\theta_L=(\sin\phi)v_r+(\mathrm{C}_\kappa(r)\mathrm{S}_\kappa(r)\cos\phi)v_\phi$$

is a constant of motion.

(iii) If the potential U depends only on r, i.e., $U=U(r)$; then

$$J(\kappa)=i(Y^t_J(\kappa))\theta_L=\mathrm{S}^2_\kappa(r)v_\phi$$

is a constant of motion.

Notice that, in geometric terms, the two functions z and z' are in fact the "tagged" sines $z=S_k(y)$ and $z'=S_k(x)$. Concerning (iii) it represents the Kepler area law which in this form holds for any κ.

The most general linear constant of motion turns out to be a linear combination of $P_1(\kappa)$, $P_2(\kappa)$, $J(\kappa)$, with constant coefficients:

$$I_{11}=a_1P_1(\kappa)+a_2P_2(\kappa)+cJ(\kappa).$$

Suppose now that L has a constant of the motion $I=I(r,\phi,v_r,v_\phi)$ which is quadratic in the velocities

$$I=I_{22}+I_{20}(r,\phi,\kappa),\quad I_{22}=av_r^2+2bv_rv_\phi+cv_\phi^2,$$

where a, b, and c, are functions of r and ϕ (κ-dependent). Then the three functions a, b, and c must take the form

$$a=a_0\cos^2\phi+c_0\sin^2\phi+b_0\sin\phi\cos\phi,$$

$$b=(\tfrac{1}{2})\mathrm{S}_\kappa(r)\mathrm{C}_\kappa(r)[(c_0-a_0)\sin 2\phi+b_0\cos 2\phi]+(\tfrac{1}{2})\mathrm{S}_\kappa^2(r)(-a_1\cos\phi+c_1\sin\phi),$$

$$c=\mathrm{S}_\kappa^2(r)\mathrm{C}_\kappa^2(r)(a_0\sin^2\phi+c_0\cos^2\phi-b_0\sin\phi\cos\phi)+\mathrm{S}_\kappa^3(r)\mathrm{C}_\kappa(r)(c_1\cos\phi+a_1\sin\phi)+a_2\mathrm{S}_\kappa^4(r)\ ,$$

where a_0, b_0, c_0; a_1, c_1; a_2 are real parameters. The most general form for I_{22} turns out to be a linear combination of binary products of linear constants:

$$I_{22}(\kappa)=a_0P_1^2(\kappa)+b_0P_1(\kappa)P_2(\kappa)+c_0P_2^2(\kappa)+a_1P_2(\kappa)J(\kappa)+c_1P_1(\kappa)J(\kappa)+a_2J^2(\kappa)\ .$$

In the flat $\kappa=0$ limit, we have $\mathrm{S}_\kappa(r)\to r$ and $\mathrm{C}_\kappa(r)\to 1$, so all these equations coincide with the ones obtained for $Q=E^2$. In the more general κ-dependent approach, the case where the configuration space is Euclidean can be considered, not as a limit case, but simply as the particular case $\kappa=0$. Generically r appears through $\mathrm{S}_\kappa(r)$, and there are also some factors which in the curved case appear through a tagged cosine of r, $\mathrm{C}_\kappa(r)$, which in the Euclidean case degenerates to $\mathrm{C}_0(r)\equiv 1$ and which therefore becomes invisible; of course these terms turn visible once we deal with the case of nonzero curvature κ. We also notice that the dependence on the curvature κ is only present in the radial part of the functions. The angular functions (e.g., $\cos\phi$,$\sin\phi$) are κ-independent.

A. Isotropic oscillator

Let us consider the following spherical (Euclidean, hyperbolic) Lagrangian with curvature κ,

$$L=(\tfrac{1}{2})(v_r^2+\mathrm{S}_\kappa^2(r)v_\phi^2)-(\tfrac{1}{2})\omega_0^2\,U_{11}(r,\phi,\kappa),\quad U_{11}=\mathrm{T}_\kappa^2(r),$$

so that the standard oscillator potential on the unit sphere (Higgs oscillator), on the Euclidean plane, or on the unit Lobachewski plane, arise as the following three particular cases:

$$U_{11}(1)=\tan^2 r,\quad V_{11}=U_{11}(0)=r^2,\quad U_{11}(-1)=\tanh^2 r.$$

The Euclidean oscillator V_{11} (parabolic potential without singularities) appears in this formalism as making a separation between two different situations (see Fig. 3). The spherical potential is

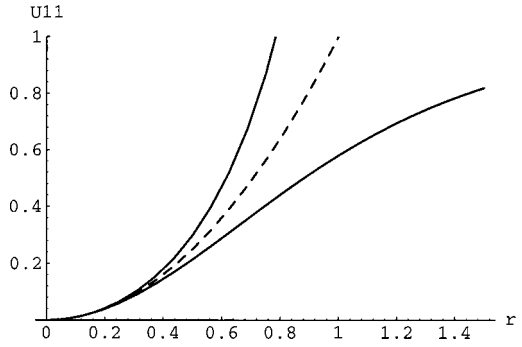

FIG. 3. Plot of U_{11} as a function of r, for $\kappa=-1$ (lower curve), $\kappa=0$ (dashed line) and $\kappa=1$ (upper curve).

represented by a well with singularities on the border (impenetrable walls at the equatorial circle $r=\pi/2\sqrt{\kappa}$ if the potential center is at the poles), and the hyperbolic potential by a well with finite depth since $U_{11}\to 1/|\kappa|$ when $r\to\infty$.

The dynamics is given by the following κ-dependent vector field:

$$X_{11}=v_r\frac{\partial}{\partial r}+v_\phi\frac{\partial}{\partial\phi}+f_r\frac{\partial}{\partial v_r}+f_\phi\frac{\partial}{\partial v_\phi},$$

$$f_r=(\mathrm{S}_\kappa(r)\mathrm{C}_\kappa(r))v_\phi^2-\omega_0^2\left(\frac{\mathrm{S}_\kappa(r)}{\mathrm{C}_\kappa^3(r)}\right),$$

$$f_\phi=-2\left(\frac{\mathrm{C}_\kappa(r)}{\mathrm{S}_\kappa(r)}\right)v_r v_\phi.$$

This is an integrable system endowed with two fundamental quadratic integrals of motion:

$$I_1(\kappa)=P_1^2(\kappa)+\omega_0^2(\mathrm{T}_\kappa(r)\cos\phi)^2,\quad I_2(\kappa)=P_2^2(\kappa)+\omega_0^2(\mathrm{T}_\kappa(r)\sin\phi)^2.$$

These constants are sum of two squares (as in the Euclidean plane) so they can be interpreted as the modulus of appropriate complex functions. Notice also that they can be considered as the κ-deformed versions of the two Euclidean one-degree of freedom energies; nevertheless, for $\kappa\neq 0$, the sum $I_1(\kappa)+I_2(\kappa)$ does not represent the total energy.

We begin our analysis by considering the time-derivative of the the two κ-dependent functions $P_1(\kappa)$ and $P_2(\kappa)$. They are given by

$$\frac{d}{dt}P_1(\kappa)=-\omega_0^2\left(\frac{\mathrm{S}_\kappa(r)}{\mathrm{C}_\kappa^3(r)}\right)\cos\phi,\quad \frac{d}{dt}P_2(\kappa)=-\omega_0^2\left(\frac{\mathrm{S}_\kappa(r)}{\mathrm{C}_\kappa^3(r)}\right)\sin\phi\ .$$

In a similar way, the time-derivative of the two velocity-independent functions $\mathrm{T}_\kappa(r)\cos\phi$, $\mathrm{T}_\kappa(r)\sin\phi$, is given by

$$\frac{d}{dt}(\mathrm{T}_\kappa(r)\cos\phi)=\frac{P_1(\kappa)}{\mathrm{C}_\kappa^2(r)},\quad \frac{d}{dt}(\mathrm{T}_\kappa(r)\sin\phi)=\frac{P_2(\kappa)}{\mathrm{C}_\kappa^2(r)}.$$

The following proposition states the super-integrability of the system and proves the existence of a complex factorization.

Proposition 2: Let K_1, K_2, *be the following two functions*:

$$K_1 = P_1(\kappa) + \mathrm{i}\omega_0(\mathrm{T}_\kappa(r)\cos\phi), \quad K_2 = P_2(\kappa) + \mathrm{i}\omega_0(\mathrm{T}_\kappa(r)\sin\phi).$$

Then (i) The modulus of K_1 *and* K_2 *are constants of motion and coincide with* $I_1(\kappa), I_2(\kappa)$:

$$|K_1|^2 = I_1(\kappa), \quad |K_2|^2 = I_2(\kappa).$$

(ii) The complex function K_{12} *defined as*

$$K_{12} = K_1 K_2^*$$

is also a constant of motion.

Proof: (i) follows directly from the definition of K_1 and K_2. For proving (ii) we analyze the time-evolution of K_1 and K_2. We have

$$\frac{d}{dt}K_1 = \frac{d}{dt}P_1(\kappa) + \mathrm{i}\,\omega_0\frac{d}{dt}(\mathrm{T}_\kappa(r)\cos\phi) = -\omega_0^2\left(\frac{\mathrm{S}_\kappa(r)}{\mathrm{C}_\kappa^3(r)}\right)\cos\phi + \mathrm{i}\,\omega_0\frac{P_1(\kappa)}{\mathrm{C}_\kappa^2(r)} = \left(\frac{\mathrm{i}\omega_0}{\mathrm{C}_\kappa^2(r)}\right)K_1,$$

and a similar calculus leads to

$$\frac{d}{dt}K_2 = \left(\frac{\mathrm{i}\omega_0}{\mathrm{C}_\kappa^2(r)}\right)K_2.$$

Thus we obtain

$$\frac{d}{dt}(K_1 K_2^*) = 0,$$

which states the function K_{12} as an additional constant of motion. It can be decomposed into real and imaginary parts as follows:

$$K_{12} = I_4(\kappa) + \mathrm{i}I_3(\kappa),$$

where $I_4(\kappa)$, $I_3(\kappa)$ are real constants of motion, respectively, quadratic and linear in the velocities, and given by

$$I_4(\kappa) = P_1(\kappa)P_2(\kappa) + \omega_0^2(\mathrm{T}_\kappa^2(r)\cos\phi\sin\phi), \quad I_3(\kappa) = \omega_0 J(\kappa).$$

These are the general κ-dependent versions of the flat space constants denoted I_4, I_3. A direct calculation shows that

$$I_1(\kappa) + I_2(\kappa) + \kappa(J(\kappa))^2 = (\tfrac{1}{2})[v_r^2 + \mathrm{S}_\kappa^2(r)v_\phi^2 + \omega_0^2 U_{11}(r,\phi,\kappa)],$$

which means that in any space of nonzero constant curvature κ the total energy can be written as a sum of *three* summands, one of which carries the spherical (Euclidean, hyperbolic) angular momentum with the curvature κ as a coefficient and vanishes into the limit $\kappa \to 0$.

Summarizing: the isotropic harmonic oscillator is super-integrable for any value of the curvature κ (positive, zero or negative) and an additional constant of motion K_{12} can be obtained by complex factorization. The fundamental integral of motion $I_3(\kappa)$ represents the spherical or hyperbolic version of the angular momentum (because the potential U_{11} is central independently of

the value of the curvature). Concerning $I_4(\kappa)$, it represents the κ-dependent spherical or hyperbolic versions of the so–called Fradkin constant.[20]. Next, we give the expressions of these two constants for three particular cases.

(i) Higgs oscillator in the unit sphere (radius $R=1$). In this case we have

$$P_1=(\cos\phi)v_r-(\cos r\ \sin r\sin\phi)\,v_\phi,$$
$$P_2=(\sin\phi)v_r+(\cos r\ \sin r\cos\phi)v_\phi,$$
$$J=\sin^2 r\,v_\phi,$$

and then I_4, I_3, are given by

$$I_4=P_1P_2+\omega_0^2(\tan^2 r\cos\phi\sin\phi),\quad I_3=\omega_0 J.$$

(ii) Isotropic oscillator in the unit Lobachewski plane (''radius'' $R=1$). In this case we have

$$P_1=(\cos\phi)v_r-(\cosh r\sinh r\sin\phi)v_\phi,$$
$$P_1=(\sin\phi)v_r+(\cosh r\sinh r\cos\phi)v_\phi,$$
$$J=\sinh^2 rv_\phi,$$

and then I_4, I_3, are given by

$$I_4=P_1P_2+\omega_0^2(\tanh^2 r\cos\phi\sin\phi),\quad I_3=\omega_0 J.$$

(iii) The expressions for $\kappa=0$ become the usual formulas for the standard isotropic oscillator.

B. Nonisotropic 2:1 oscillator

As mentioned in the Introduction, systems on the two-dimensional sphere (Euclidean, hyperbolic plane) with the first integrals quadratic in the velocities were studied in Ref. 16. Several different potentials were obtained as solutions of a system of two coupled differential equations depending on the parameter κ. One of the potentials obtained in this approach was

$$U_{21}(r,\phi,\kappa)=\frac{1}{1-\kappa(\mathrm{S}_\kappa(r)\sin\phi)^2}\left[4\left(\frac{\mathrm{T}_\kappa(r)\cos\phi}{1-\kappa(\mathrm{T}_\kappa(r)\cos\phi)^2}\right)^2+(\mathrm{S}_\kappa(r)\sin\phi)^2\right],$$

which satisfies

$$\lim_{\kappa\to 0}U_{21}=4r^2\cos^2\phi+r^2\sin^2\phi$$

and was interpreted as representing the potential of the spherical (hyperbolic) version of the 2:1 harmonic oscillator.

So, let us now study the following spherical (hyperbolic) Lagrangian with curvature κ:

$$L=(\tfrac{1}{2})(v_r^2+\mathrm{S}_\kappa^2(r)v_\phi^2)-(\tfrac{1}{2})\omega_0^2U_{21}(r,\phi,\kappa).$$

The dynamics is given by the following vector field:

$$X_{21}=v_r\frac{\partial}{\partial r}+v_\phi\frac{\partial}{\partial\phi}+f_r\frac{\partial}{\partial v_r}+f_\phi\frac{\partial}{\partial v_\phi},$$

where the κ-dependent forces f_r and f_ϕ are given by

$$f_r = \mathrm{S}_\kappa(r)\mathrm{C}_\kappa(r)v_\phi^2 - (\omega_0^2 \mathrm{S}_\kappa(r)\mathrm{C}_\kappa(r))\left[\frac{\mathrm{C}_\kappa^2(r)(4\cos^2\phi+\sin^2\phi)+\kappa \mathrm{S}_\kappa(r)(3+\cos^2\phi)\cos^2\phi}{(\mathrm{C}_\kappa^2(r)-\kappa \mathrm{S}_\kappa^2(r)\cos^2\phi)^3}\right],$$

$$f_\phi = -2\left(\frac{\mathrm{C}_\kappa(r)}{\mathrm{S}_\kappa(r)}\right)v_r v_\phi + (\omega_0^2 \sin\phi\cos\phi)\left[\frac{3\mathrm{C}_\kappa^2(r)+\kappa \mathrm{S}_\kappa^2(r)\cos^2\phi}{(\mathrm{C}_\kappa^2(r)-\kappa \mathrm{S}_\kappa^2(r)\cos^2\phi)^3}\right].$$

It was proved in Ref. 16 that this system possesses the following two quadratic integrals of motion:

$$\begin{aligned} I_1(\kappa) &= P_1^2(\kappa) + 4\omega_0^2\left(\frac{\mathrm{T}_\kappa(r)\cos\phi}{1-\kappa(\mathrm{T}_\kappa(r)\cos\phi)^2}\right)^2, \\ I_2(\kappa) &= P_2^2(\kappa) + \kappa J^2(\kappa) + \omega_0^2[1+\kappa(\mathrm{T}_\kappa(r)\cos\phi)^2]\left(\frac{\mathrm{T}_\kappa(r)\sin\phi}{1-\kappa(\mathrm{T}_\kappa(r)\cos\phi)^2}\right)^2. \end{aligned} \tag{5}$$

For further convenience, it will be useful to write the constant I_2 as

$$I_2(\kappa) = P_2^2(\kappa) + \kappa J^2(\kappa) + \omega_0^2 F(r,\phi,\kappa)(\mathrm{T}_\kappa(r)\sin\phi)^2,$$

where we have denoted by $F(r,\phi,\kappa)$ the following function:

$$F(r,\phi,\kappa) = \frac{1+\kappa(\mathrm{T}_\kappa(r)\cos\phi)^2}{(1-\kappa \mathrm{T}_\kappa^2(r)\cos^2\phi)^2}.$$

Notice that if we denote by $I_0(\kappa)$ the trivial constant of motion (energy),

$$I_0(\kappa) = (\tfrac{1}{2})(v_r^2 + \mathrm{S}_\kappa^2(r)v_\phi^2) + (\tfrac{1}{2})\omega_0^2 U_{21}(r,\phi,\kappa);$$

then

$$2I_0(\kappa) = I_1(\kappa) + I_2(\kappa).$$

Let us now denote by K_1 the following complex function:

$$K_1 = P_1(\kappa) + (2\mathrm{i}\omega_0)\left(\frac{\mathrm{T}_\kappa(r)\cos\phi}{1-\kappa(\mathrm{T}_\kappa(r)\cos\phi)^2}\right).$$

By using

$$\frac{d}{dt}P_1(\kappa) = -\left(\frac{4\omega_0^2}{\mathrm{C}_\kappa^2(r)}\right)F(r,\phi,\kappa)\left[\frac{\mathrm{T}_\kappa(r)\cos\phi}{1-\kappa\,\mathrm{T}_\kappa^2(r)\sin^2\phi}\right],$$

$$\frac{d}{dt}\left(\frac{\mathrm{T}_\kappa(r)\cos\phi}{1-\kappa \mathrm{T}_\kappa^2(r)\sin^2\phi}\right) = \left(\frac{1}{\mathrm{C}_\kappa^2(r)}\right)F(r,\phi,\kappa)\,P_1(\kappa),$$

we get the time-evolution of the function K_1 given by

$$\frac{d}{dt}K_1 = \left(\frac{2\mathrm{i}\omega_0}{\mathrm{C}_\kappa^2(r)}\right)F(r,\phi,\kappa)\,K_1.$$

It seems that the following step must be the analysis of the time evolution of $P_2(\kappa)$ (as we have done for the case of the central Higgs oscillator). Nevertheless instead of considering $P_2(\kappa)$ by

itself, we will consider two other related functions obtained by addition (subtraction) of a new term related with the spherical (hyperbolic) version of the angular momentum:

$$\frac{d}{dt}[P_2(\kappa)+\sqrt{\kappa}\,J(\kappa)]=-\left(\frac{\omega_0}{\mathrm{C}_\kappa(r)}\right)^2\left(\frac{1}{1+\sqrt{\kappa}\,\mathrm{T}_\kappa(r)\cos\phi}\right)^2\left[\frac{\mathrm{T}_\kappa(r)\sin\phi}{1+\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi}\right],$$

$$\frac{d}{dt}[P_2(\kappa)-\sqrt{\kappa}J(\kappa)]=-\left(\frac{\omega_0}{\mathrm{C}_\kappa(r)}\right)^2\left(\frac{1}{1-\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi}\right)^2\left[\frac{\mathrm{T}_\kappa(r)\sin\phi}{1-\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi}\right].$$

On the other hand, the time-derivative of the two velocity-independent functions,

$$\left[\frac{\mathrm{T}_\kappa(r)\sin\phi}{1+\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi}\right],\quad\left[\frac{\mathrm{T}_\kappa(r)\sin\phi}{1-\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi}\right],$$

is given by

$$\frac{d}{dt}\left[\frac{\mathrm{T}_\kappa(r)\sin\phi}{1+\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi}\right]=\left(\frac{1}{\mathrm{C}_\kappa^2(r)}\right)\left(\frac{1}{1+\sqrt{\kappa}\,\mathrm{T}_\kappa(r)\cos\phi}\right)^2[P_2(\kappa)+\sqrt{\kappa}\,J(\kappa)],$$

$$\frac{d}{dt}\left[\frac{\mathrm{T}_\kappa(r)\sin\phi}{1-\sqrt{\kappa}\,\mathrm{T}_\kappa(r)\cos\phi}\right]=\left(\frac{1}{\mathrm{C}_\kappa^2(r)}\right)\left(\frac{1}{1-\sqrt{\kappa}\,\mathrm{T}_\kappa(r)\cos\phi}\right)^2[P_2(\kappa)-\sqrt{\kappa}\,J(\kappa)].$$

These relations to us suggests to define not one, but two functions, similar to K_2:

$$K_2^+=P_2(\kappa)+\sqrt{\kappa}J(\kappa)+\mathrm{i}\omega_0\left(\frac{\mathrm{T}_\kappa(r)\sin\phi}{1+\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi}\right),$$

$$K_2^-=P_2(\kappa)-\sqrt{\kappa}J(\kappa)+\mathrm{i}\,\omega_0\left(\frac{\mathrm{T}_\kappa(r)\sin\phi}{1-\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi}\right),$$

whose time derivatives are given by

$$\frac{d}{dt}K_2^+=\left(\frac{\mathrm{i}\omega_0}{\mathrm{C}_\kappa^2(r)}\right)\left[\frac{1}{(1+\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi)^2}\right]K_2^+,$$

$$\frac{d}{dt}K_2^-=\left(\frac{\mathrm{i}\omega_0}{\mathrm{C}_\kappa^2(r)}\right)\left[\frac{1}{(1-\sqrt{\kappa}\mathrm{T}_\kappa(r)\cos\phi)^2}\right]K_2^-.$$

Then we have the following proposition.

Proposition 3: Let the complex functions K_1, K_2^+, K_2^- be defined as above. Then the complex function K_{122} defined as

$$K_{122}=K_1\,K_2^{+*}\,K_2^{-*}$$

is a constant of motion.

Proof: We have already obtained the time derivatives of everyone of the three functions K_1, K_2^+, K_2^-. Because of this, the time evolution of K_{122} is given by

$$\frac{d}{dt}K_{122}=\dot{K}_x K_2^+ * K_2^- * + K_1 \dot{K}_y^+ * K_2^- * + K_1 K_2^+ * \dot{K}_2^- *$$

$$=\left(\frac{\mathrm{i}\,\omega_0}{\mathrm{C}_\kappa^2(r)}\right)\left[2F(r,\phi,\kappa)-\frac{1}{(1+\sqrt{\kappa}\,\mathrm{T}_\kappa(r)\cos\phi)^2}-\frac{1}{(1-\sqrt{\kappa}\,\mathrm{T}_\kappa(r)\cos\phi)^2}\right]K_{122}\,.$$

But the function F is such that the term in square brackets vanishes identically, and we arrive at

$$\frac{d}{dt}K_{122}=0.$$

Thus we have shown that complex function $K_{122}=I_4(\kappa)+\mathrm{i}\,I_3(\kappa)$ as well as the two associated real functions, $I_4(\kappa)$ and $I_3(\kappa)$, are all of them constants of motion. After some computations (we omit the details) we have obtained

$$I_4(\kappa)=[P_2^2(\kappa)-\kappa J^2(\kappa)]\,P_1(\kappa)+\omega_0^2 I_{41}(\kappa),$$

$$I_3(\kappa)=P_2(\kappa)\,J(\kappa)-\omega_0^2 I_{30}(\kappa),$$

with

$$I_{41}(\kappa)=\left(\frac{\mathrm{T}_\kappa(r)\sin\phi)}{(1-\kappa\,\mathrm{T}_\kappa^2(r)\cos^2\phi)^2}\right)[I_{41}^a(\kappa)+\kappa\,I_{41}^b(\kappa)],$$

$$I_{41}^a(\kappa)=4P_2(\kappa)\mathrm{T}_\kappa(r)\cos\phi-P_1(\kappa)\mathrm{T}_\kappa(r)\sin\phi,$$

$$I_{41}^b(\kappa)=(\mathrm{T}_\kappa^2(r)\cos^2\phi)(4J(\kappa)+P_1(\kappa)\mathrm{T}_\kappa(r)\sin\phi),$$

$$I_{30}(\kappa)=\frac{\mathrm{T}_\kappa^3(r)\cos\phi\sin^2\phi}{(1-\kappa\,\mathrm{T}_\kappa^2(r)\cos^2\phi)^2}.$$

We close this section observing that, although these κ-dependent polar coordinates (r,ϕ) prove to be convenient for the central U_{11} case, the results of this noncentral subsection [actually, even the function $U_{21}(r,\phi)$ itself] suggest the convenience of a new study in a new and more appropriate system of coordinates.

V. THE 1:1 AND 2:1 HARMONIC OSCILLATORS ON A 2-D SPACE OF CONSTANT CURVATURE II: PARALLEL COORDINATES

The dynamics of a system defined in a two-dimensional space with constant curvaure κ can also be studied by using the ''geodesic parallel'' system of coordinates introduced in Sec. II. In this case the differential element of distance is

$$ds^2=\mathrm{C}_\kappa^2(y)du^2+dy^2,$$

so a standard Lagrangian (kinetic term minus potential function) has the following form:

$$L(\kappa)=(\tfrac{1}{2})(\mathrm{C}_\kappa^2(y)v_u^2+v_y^2)-U(u,y,\kappa),$$

in such a way that the Euclidean system is just given by the particular value of $L(\kappa)$ in $\kappa=0$,

$$\lim_{\kappa\to 0} L(\kappa)=(\tfrac{1}{2})\,(v_x^2+v_y^2)-V(x,y),\quad V(x,y)=U(x,y,0)\,.$$

The kinetic term remains invariant under the action of the three κ-dependent vector fields Y_{P_1}, Y_{P_2}, $Y_J(\kappa)$, whose expressions in parallel coordinates are

$$Y_{P_1}(\kappa)=\frac{\partial}{\partial u},\quad Y_{P_2}(\kappa)=\kappa\,\mathrm{S}_\kappa(u)\mathrm{T}_\kappa(y)\,\frac{\partial}{\partial u}+\mathrm{C}_\kappa(u)\,\frac{\partial}{\partial y},$$

$$Y_J(\kappa)=\mathrm{C}_\kappa(u)\mathrm{T}_\kappa(y)\,\frac{\partial}{\partial u}-\mathrm{S}_\kappa(u)\,\frac{\partial}{\partial y}.$$

Moreover, the potentials U_1, U_2, U_J, now characterized by the following dependence:

$$U_1=U(y),\quad U_2=U(\mathrm{S}_\kappa(u)\mathrm{C}_k(y)),\quad \text{and}\quad U_J=U\left(\frac{\mathrm{T}^2_\kappa(u)}{\mathrm{C}^2_\kappa(y)}+\mathrm{T}^2_\kappa(y)\right)$$

(remark that these expressions embody the same dependence as derived in the previous section) are endowed with $Y_{P_1}(\kappa)$, $Y_{P_2}(\kappa)$, $Y_J(\kappa)$, as exact Noether symmetries. The associated linear constants of motion are given by

$$\begin{gathered}P_1(\kappa)=\mathrm{C}^2_\kappa(y)\,v_u,\quad P_2(\kappa)=\kappa\,\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(y)\mathrm{S}_\kappa(y)\,v_u+\mathrm{C}_\kappa(u)\,v_y,\\ J(\kappa)=\mathrm{C}_\kappa(u)\mathrm{C}_\kappa(y)\mathrm{S}_\kappa(y)\,v_u-\mathrm{S}_\kappa(u)\,v_y,\end{gathered}\tag{6}$$

and hence the more general form for a linear constant of motion I_{11}, is as a linear combination of these three functions, $I_{11}=a_1P_1(\kappa)+a_2P_2(\kappa)+cJ(\kappa)$.

The constants of motion which are quadratic in the velocities arise from generalized Noether symmetries (hidden symmetries) of $L(\kappa)$, and they have the following expression:

$$I=I_{22}+I_{20}(u,y,\kappa),$$

with the term I_{22} again given by a linear combination of quadratic pairings,

$$I_{22}(\kappa)=a_0P_1^2(\kappa)+b_0P_1(\kappa)P_2(\kappa)+c_0P_2^2(\kappa)+a_1P_2(\kappa)J(\kappa)+c_1P_1(\kappa)J(\kappa)+a_2J^2(\kappa).$$

In contrast to the formalism in polar coordinates (r,ϕ), the κ-dependence is now present in both coordinates, u and y, because both are lengths.

A. Isotropic oscillator

The Lagrangian of isotropic spherical (Euclidean, hyperbolic) oscillator with curvature κ is

$$L=\left(\frac{1}{2}\right)(\mathrm{C}^2_\kappa(y)v_u^2+v_y^2)-\left(\frac{1}{2}\right)\omega_0^2\,U_{11}(u,y,\kappa),\quad U_{11}=\frac{\mathrm{T}^2_\kappa(u)}{\mathrm{C}^2_\kappa(y)}+\mathrm{T}^2_\kappa(y).$$

This potential is indeed the same discussed with polar coordinates as $\mathrm{T}^2_\kappa(r)$ [see (4)]. In Sec. III we pointed out that the fuction $\mathrm{T}^2_\kappa(r)$ admits several alternative expressions in terms of the coordinates (u,y) which can be considered as curvature versions of the Pythagorean theorem. Because of this, the potential $U_{11}=U_{11}(u,y,\kappa)$ can also be written as

$$U_{11}=\mathrm{T}_\kappa^2(u)+\frac{\mathrm{T}_\kappa^2(y)}{\mathrm{C}_\kappa^2(u)}.$$

The dynamics is given by the following κ-dependent vector field:

$$X_{11}=v_u\frac{\partial}{\partial u}+v_y\frac{\partial}{\partial y}+f_u\frac{\partial}{\partial v_u}+f_y\frac{\partial}{\partial v_y},$$

$$f_u=2\,\kappa\,\mathrm{T}_\kappa(y)\,v_u v_y-\omega_0^2\left(\frac{\mathrm{S}_\kappa(u)}{\mathrm{C}_\kappa^3(u)\,\mathrm{C}_\kappa^4(y)}\right),$$

$$f_y=-\,\kappa\,\mathrm{C}_\kappa(y)\,\mathrm{S}_\kappa(y)\,v_u^2-\omega_0^2\left(\frac{\mathrm{S}_\kappa(y)}{\mathrm{C}_\kappa^2(u)\,\mathrm{C}_\kappa^3(y)}\right).$$

The following two κ-dependent functions remain constant along the trajectories of X_{11}:

$$I_1(\kappa)=P_1^2(\kappa)+\omega_0^2\,\mathrm{T}_\kappa^2(u),\quad I_2(\kappa)=P_2^2(\kappa)+\omega_0^2\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(u)}\right)^2. \tag{7}$$

They are integrals of motion quadratic in the velocities (momenta in the Hamiltonian formalism) which correspond to the κ-deformed versions of the two Euclidean one-degree of freedom energies.

The following proposition states the super-integrability of the system and proves the existence of a complex factorization.

Proposition 4: Let K_1, K_2, be the following two functions:

$$K_1=P_1(\kappa)+\mathrm{i}\,\omega_0\,\mathrm{T}_\kappa(u),\quad K_2=P_2(\kappa)+\mathrm{i}\,\omega_0\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(u)}\right).$$

Then the complex function K_{12} defined as

$$K_{12}=K_1K_2^*$$

is a constant of motion.

Proof: The time-evolution of the functions K_1, K_2 is given by

$$\frac{d}{dt}K_1\equiv X_{11}(K_1)=X_{11}[\mathrm{C}_\kappa^2(y)\,v_u]+\mathrm{i}\,\omega_0\,X_{11}[\mathrm{T}_\kappa(u)]=\left(\frac{\mathrm{i}\,\omega_0}{\mathrm{C}_\kappa^2(u)\mathrm{C}_\kappa^2(y)}\right)K_1,$$

$$\frac{d}{dt}K_2\equiv X_{11}(K_2)=X_{11}[P_2(\kappa)]+\mathrm{i}\,\omega_0\,X_{11}\left[\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(u)}\right]=\left(\frac{\mathrm{i}\,\omega_0}{\mathrm{C}_\kappa^2(u)\mathrm{C}_\kappa^2(y)}\right)K_2.$$

Hence we have

$$\frac{d}{dt}K_{12}=X_{11}(K_1)K_2^*+K_1\,X_{11}(K_2^*)=0,$$

which states the function K_{12} as an additional constant of motion. The associated real integrals of motion I_4, I_3 are

$$I_4=\mathrm{Re}(K_1 K_2^*)=P_1(\kappa)P_2(\kappa)+\omega_0^2\,\mathrm{T}_\kappa(u)\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(u)}\right),$$

$$I_3=\mathrm{Im}(K_1 K_2^*)=\omega_0\,P_2(\kappa)\mathrm{T}_\kappa(u)-\omega_0\,P_1(\kappa)\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(u)}\right)=\omega_0\,J(\kappa).$$

We close with two properties. First, the relation between the modulus of the functions K_1, K_2, and the two fundamental constants of motion is the same that of the Euclidean plane,

$$|K_1|^2=I_1(\kappa),\quad |K_2|^2=I_2(\kappa).$$

Second, the three constants of motion $I_1(\kappa),I_2(\kappa),I_3(\kappa)$ are functionally independent, and the total energy is related to them as

$$(\tfrac{1}{2})(\mathrm{C}_\kappa^2(y)v_u^2+v_y^2)+(\tfrac{1}{2})\omega_0^2\,U_{11}(u,y,\kappa)=(\tfrac{1}{2})(I_1(\kappa)+I_2(\kappa)+\kappa\,J^2(\kappa)),$$

because of

$$P_1^2(\kappa)+P_2^2(\kappa)+\kappa\,J^2(\kappa)=\mathrm{C}_\kappa^2(y)v_u^2+v_y^2.$$

B. Nonisotropic 2:1 oscillator

In parallel coordinates the Lagrangian of the spherical (hyperbolic) 2:1 harmonic oscillator with curvature κ is

$$L=(\tfrac{1}{2})(\mathrm{C}_\kappa^2(y)v_u^2+v_y^2)-(\tfrac{1}{2})\omega_0^2\,U_{21}(u,y,\kappa),$$

$$U_{21}=\frac{\mathrm{T}_\kappa^2(2\,u)}{\mathrm{C}_\kappa^2(y)}+\mathrm{T}_\kappa^2(y)=\mathrm{T}_\kappa^2(2\,u)+\frac{\mathrm{T}_\kappa^2(y)}{\mathrm{C}_\kappa^2(2\,u)}.$$

Therefore, the dynamics is represented by the following κ-dependent vector field:

$$X_{21}=v_u\frac{\partial}{\partial u}+v_y\frac{\partial}{\partial y}+f_u\frac{\partial}{\partial v_u}+f_y\frac{\partial}{\partial v_y},$$

$$f_u=2\,\kappa\,\mathrm{T}_\kappa(y)v_u v_y-2\,\omega_0^2\left(\frac{\mathrm{S}_\kappa(2\,u)}{\mathrm{C}_\kappa^3(2\,u)\mathrm{C}_\kappa^4(y)}\right),$$

$$f_y=-\kappa\,\mathrm{C}_\kappa(y)\mathrm{S}_\kappa(y)\,v_u^2-\omega_0^2\left(\frac{\mathrm{S}_\kappa(y)}{\mathrm{C}_\kappa^2(2\,u)\mathrm{C}_\kappa^3(y)}\right).$$

This system possesses two integrals of motion quadratic in the velocities:

$$I_1(\kappa)=P_1(\kappa)^2+4\,\omega_0^2\left(\frac{\mathrm{T}_\kappa(u)}{1-\kappa\,\mathrm{T}_\kappa^2(u)}\right)^2,$$

$$I_2(\kappa)=P_2^2(\kappa)+\kappa\,J^2(\kappa)+\omega_0^2\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2\,u)}\right)^2=[v_y^2+\kappa\,\mathrm{C}_\kappa^2(y)\mathrm{S}_\kappa^2(y)v_u^2]+\omega_0^2\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2\,u)}\right)^2.$$

In the two-dimensional sphere S^2 (hyperbolic plane) with curvature κ, the expression for the tangent of the double-angle is $\mathrm{T}_\kappa(2\,\alpha)=2\,\mathrm{T}_\kappa(\alpha)/(1-\kappa\,\mathrm{T}_\kappa^2(\alpha))$; thus the function $I_1(\kappa)$ can also be rewritten as follows:

$$I_1(\kappa)=P_1(\kappa)^2+\omega_0^2\,\mathrm{T}_\kappa^2(2\,u).$$

The dynamics is κ-dependent and so are the two integrals of motion. Hence the following two equations:

$$X_{21}(I_1(\kappa))=0,\quad X_{21}(I_2(\kappa))=0,$$

remain true for any value (positive, negative or null) of the curvature κ. Moreover, if we denote by $I_0(\kappa)$ the trivial constant of motion:

$$I_0(\kappa)=(\tfrac{1}{2})(\mathrm{C}_\kappa^2(y)v_u^2+v_y^2)+(\tfrac{1}{2})\omega_0^2\,U_{21}(u,y,\kappa),$$

then we have

$$2I_0(\kappa)=I_1(\kappa)+I_2(\kappa).$$

So the total energy $I_0(\kappa)$ splits as a sum of two terms, $I_1(\kappa)$ and $I_2(\kappa)$, as was the case in the Euclidean plane. Nevertheless, for $\kappa\neq 0$ the second integral contains an additional term proportional to the angular momentum. For the zero curvature limit, this additional term vanishes, and we obtain the correct Euclidean expressions,

$$\lim_{\kappa\to 0} I_1(\kappa)=v_x^2+4\omega_0^2x^2,\qquad \lim_{\kappa\to 0} I_2(\kappa)=v_y^2+\omega_0^2y^2.$$

Let us denote by K_1, K_2^+, K_2^-, the following three complex functions:

$$K_1=P_1(\kappa)+\mathrm{i}\,\omega_0\,\mathrm{T}_\kappa(2\,u),$$

$$K_2^+=[P_2(\kappa)+\sqrt{\kappa}\,J(\kappa)]+\mathrm{i}\,\omega_0(\mathrm{C}_\kappa(u)+\sqrt{\kappa}\,\mathrm{S}_\kappa(u))\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2\,u)}\right),$$

$$K_2^-=[P_2(\kappa)-\sqrt{\kappa}\,J(\kappa)]+\mathrm{i}\,\omega_0(\mathrm{C}_\kappa(u)-\sqrt{\kappa}\,\mathrm{S}_\kappa(u))\left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2\,u)}\right).$$

The first function can be considered as a ''curved'' version of the Euclidean function J_1 (see the notation of Sec. II), and K_2^+, K_2^-, two different κ-dependent deformations of the Euclidean function J_2.

Proposition 5: Let the complex functions K_1, K_2^+, K_2^-, be defined as above. Then

(i) *The modulus of K_1 is a constant of motion and coincides with $I_1(\kappa)$; the sums of the modulus of K_2^+ and K_2^- is a constant of motion and coincides with $I_2(\kappa)$.*

(ii) *The complex function K_{122}, defined as*

$$K_{122}=K_1\,K_2^{+*}\,K_2^{-*},$$

is a constant of motion.

Proof: (i) The modulus of the first function K_1 is the constant value of the first integral of motion,

$$|K_1|^2 = P_1^2(\kappa) + \omega_0^2[\mathrm{T}_\kappa(2u)]^2 = I_1(\kappa),$$

and the sum of the modulus of K_2^+ and K_2^- coincides with $2I_2(\kappa)$:

$$|K_2^+|^2 + |K_2^-|^2 = 2\left(P_2^2(\kappa) + \kappa J^2(\kappa) + \omega_0^2 \left[\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2u)} \right]^2 \right) = 2I_2(\kappa).$$

(ii) The time evolution of the first function K_1 is given by

$$\frac{d}{dt} K_1 \equiv X_{21}(K_1) = \frac{d}{dt}(\mathrm{C}_\kappa^2(y) v_u) + (\mathrm{i}\omega_0) \frac{d}{dt} \mathrm{T}_\kappa(2u) = \left[\frac{2\mathrm{i}\omega_0}{\mathrm{C}_\kappa^2(2u)\mathrm{C}_\kappa^2(y)} \right] K_1,$$

and a similar calculus leads to

$$\frac{d}{dt} K_2^+ \equiv X_{21}(K_2^+) = \mathrm{i}\omega_0 \left[\frac{\mathrm{C}_\kappa(u) + \sqrt{\kappa}\,\mathrm{S}_\kappa(u)}{\mathrm{C}_\kappa(2u)\mathrm{C}_\kappa(y)} \right]^2 K_2^+,$$

$$\frac{d}{dt} K_2^- \equiv X_{21}(K_2^-) = \mathrm{i}\omega_0 \left[\frac{\mathrm{C}_\kappa(u) - \sqrt{\kappa}\,\mathrm{S}_\kappa(u)}{\mathrm{C}_\kappa(2u)\mathrm{C}_\kappa(y)} \right]^2 K_2^-.$$

The important point is that we get the following expression for the time evolution of the function product $K_{22} = K_2^+ K_2^-$:

$$\begin{aligned} \frac{d}{dt}(K_2^+ K_2^-) &= X_{21}(K_2^+) K_2^- + K_2^+ X_{21}(K_2^-) \\ &= \left[\frac{\mathrm{i}\omega_0}{\mathrm{C}_\kappa^2(2u)\mathrm{C}_\kappa^2(y)} \right] [(\mathrm{C}_\kappa(u) + \sqrt{\kappa}\,\mathrm{S}_\kappa(u))^2 + (\mathrm{C}_\kappa(u) - \sqrt{\kappa}\,\mathrm{S}_\kappa(u))^2](K_2^+ K_2^-) \\ &= \left[\frac{2\mathrm{i}\omega_0}{\mathrm{C}_\kappa^2(2u)\mathrm{C}_\kappa^2(y)} \right] (K_2^+ K_2^-). \end{aligned}$$

Thus we arrive at the property

$$\frac{d}{dt} K_{122} = X_{21}(K_1)(K_2^{+*} K_2^{-*}) + K_1 X_{21}(K_2^{+*} K_2^{-*}) = 0$$

and the function K_{122} is an integral of motion. As it is complex, we obtain two real κ-dependent constants, $I_3(\kappa)$ and $I_4(\kappa)$, defined in the usual form

$$K_{122} = I_4(\kappa) + \mathrm{i} I_3(\kappa).$$

After some simplification the expressions for these two constants become

$$I_3(\kappa) = J(\kappa) P_2(\kappa) + \omega_0^2 \left(\frac{\mathrm{S}_\kappa(u)\mathrm{C}_\kappa(u)}{\mathrm{C}_\kappa^2(2u)} \right) \mathrm{T}_\kappa^2(y),$$

$$I_4(\kappa) = [P_2^2(\kappa) - \kappa J^2(\kappa)] P_1(\kappa) + \omega_0^2 [2\,\mathrm{T}_\kappa(2u)\, v_y - \mathrm{C}_\kappa(y)\mathrm{S}_\kappa(y)\, v_u] \left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(2u)} \right).$$

We close this section with the following observations.

(i) Although K_2^+ and K_2^- are two different κ-dependent functions, $K_2^+ \neq K_2^-$, they have the same function J_2 as the Euclidean limit. We have

$$\lim_{\kappa\to 0} K_1 = v_x + \mathrm{i}\,\omega_0\,(2x), \quad \lim_{\kappa\to 0} K_2^+ = \lim_{\kappa\to 0} K_2^- = v_y + \mathrm{i}\,\omega_0\, y.$$

The coefficient $n_1=2$ in the Euclidean function J_1 (see the notation of Sec. II) is now present, not as a global multiplicative factor on the imaginary part of K_1, but as a coefficient inside the argument of the tangent function.

(ii) The Euclidean function J_2 is κ-deformed in two different ways, K_2^+ and K_2^-, in such a way that the Euclidean square factor J_2^2 becomes the product $K_2^+ K_2^-$.

(iii) The transition of U_{11} to U_{21} is very simple: just the change $\mathrm{T}_\kappa(u)$ by $\mathrm{T}_\kappa(2\,u)$ in the potential expressed in parallel coordinates.

VI. FINAL COMMENTS AND OUTLOOK

We have started with a discussion of the curvilinear systems of coordinates on 2-D spaces of constant curvature and then we have studied the two oscillators with quadratic super-integrability. We have proved that they can be considered as κ-deformations of the Euclidean oscillator or, alternatively, that the classic and well-known Euclidean oscillator appears just as a very particular case of a much more general ''curved'' system. Concerning our approach, two important points are, first, that the results have been obtained for a general value of the curvature κ, in such a way that they cover simultaneously the case of a Euclidean plane ($\kappa=0$), the 2-sphere ($\kappa>0$) and the hyperbolic plane ($\kappa<0$); and, second, that all the computations have been carried out in both ''geodesic polar'' and ''geodesic parallel'' coordinates. The ''geodesic parallel'' coordinates may seem rather unusual, but they have proved to be the more appropriate ones for the study of the nonisotropic case.

The results obtained in Sec. V suggest that the appropriate potential $U_{n1}(u,y,\kappa)$ for representing the general nonisotropic $n{:}1$ oscillator, with an n integer, on a 2-D manifold of constant curvature κ, is given by

$$U_{n1} = \frac{\mathrm{T}_\kappa^2(n\,u)}{\mathrm{C}_\kappa^2(y)} + \mathrm{T}_\kappa^2(y) = \mathrm{T}_\kappa^2(n\,u) + \frac{\mathrm{T}_\kappa^2(y)}{\mathrm{C}_\kappa^2(n\,u)}.$$

This potential satisfies the appropriate Euclidean limit,

$$\lim_{\kappa\to 0} U_{n1}(\kappa) = (nx)^2 + y^2,$$

and is integrable for arbitrary values of the integer n. The two fundamental integrals of motion are both quadratic in the velocities

$$I_1(\kappa) = P_1^2(\kappa) + \omega_0^2\,[\mathrm{T}_\kappa(n\,u)]^2,$$

$$I_2(\kappa) = [P_2^2(\kappa) + \kappa\, J^2(\kappa)] + \omega_0^2 \left(\frac{\mathrm{T}_\kappa(y)}{\mathrm{C}_\kappa(n\,u)}\right)^2,$$

and can be considered as κ-deformations of the two quadratic Euclidean energies:

$$\lim_{\kappa\to 0} I_1(\kappa) = v_x^2 + \omega_0^2\,(nx)^2, \quad \lim_{\kappa\to 0} I_2(\kappa) = v_y^2 + \omega_0^2\, y^2.$$

It seems natural to conjecture that U_{n1} (for any integer value of n) is super-integrable as well, and that the corresponding additional (nonquadratic) integral can also be obtained through a complex constant similar to the one obtained for the $2{:}1$ case in Sec. V. A more difficult problem seems to be the obtaining of the spherical (hyperbolic) version of the rational $n_1{:}n_2$ oscillator, since a direct

generalization will lead to problems with the domain and range of the potential (in this general case, the spherical system looks more complicated than the hyperbolic one). We think that these are open questions that must be investigated.

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Attractors for second-order lattice dynamical systems with damping

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We consider the existence and the approximation of the global attractor for second-order damped lattice dynamical systems. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Recently, various properties of the solutions for lattice dynamical systems have been studied by many authors; see Refs. 1–5 and the references therein. Lattice systems arise in many applications, for example, in chemical reaction theory, image processing and pattern recognition, material science, and biology. They possess their own form, but in some cases they arise as spatial discretizations of partial differential equations.

In this paper, by introducing a new weight norm that is equivalent to the usual norm in the phase space, we shall consider the existence and approximation of the global attractor for the second-order damped lattice dynamical system:

$$\ddot{u}_i-\gamma(\dot{u}_{i-1}-2\dot{u}_i+\dot{u}_{i+1})+h(\dot{u}_i)-(u_{i-1}-2u_i+u_{i+1})+\lambda u_i+f(u_i)=g_i,\quad i\in Z, \tag{1}$$

where $\gamma\geqslant 0$ and $\lambda>0$ are constants, g_i is given, and f, $h\in C^1(R,R)$ satisfy some monotonic conditions. Equation (1) can be regarded as a model of damped coupled nonlinear oscillators (see Ref. 1, pp. 442–451) and a model of a discrete analog of the following continuous strongly damped semilinear wave equation in R:

$$u_{tt}-\gamma u_{xxt}+h(u_t)-u_{xx}+\lambda u+f(u)=g, \tag{2}$$

which arises in wave phenomena of various areas with a strong damping in mathematical physics. The global attractor and its dimension to Eq. (2) in bounded domain have been widely studied; see Refs. 6–9 and the references therein. It is important to have some rigorous study on the dynamics of system (1). Here we shall study the asymptotic behavior for system (1) when the initial date belongs to the space l^2.

This paper is organized as follows. In the second section, we show the existence and uniqueness of solutions for system (1). In Sec. III, we prove the existence of an absorbing set of (1) (that is, the uniform boundedness of solutions). In Sec. IV, we prove the asymptotic compactness for the semigroup associated with (1) and the existence of the global attractor. In Sec. V, we consider the finite-dimensional approximations to the global attractor.

II. EXISTENCE AND UNIQUENESS OF SOLUTIONS

In this section, we present the existence and uniqueness of solutions for system (1). We consider the system

$$\ddot{u}_i-\gamma(\dot{u}_{i-1}-2\dot{u}_i+\dot{u}_{i+1})+h(\dot{u}_i)-(u_{i-1}-2u_i+u_{i+1})+\lambda u_i+f(u_i)=g_i,\quad i\in Z, \tag{3}$$

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with the initial conditions

$$u_i(0)=u_{i,0}, \quad \dot{u}_i(0)=u_{1i,0}, \quad i\in Z, \tag{4}$$

where $\gamma\geqslant 0$, $\lambda>0$, $g=(g_i)_{i\in Z}$, and f, $h\in C^1(R,R)$.

We make the following assumptions on f, h:

$$f(s)s\geqslant \nu G(s)\geqslant 0, \quad \forall s\in R, \tag{5}$$

$$h(0)=0, \quad 0<\alpha\leqslant h'(s)\leqslant \beta<+\infty, \quad \forall s\in R; \tag{6}$$

here ν, α, β are positive constants and $G(s)=\int_0^s f(t)dt$, $s\in R$. Obviously, $f(s)=\Sigma_{j=0}^m a_j s^{2j+1}$, with $a_j>0$, $j=0,1,...,m$, satisfies (5).

We also assume that α, β, γ, λ satisfy

$$0\leqslant \gamma\leqslant \frac{\beta^2+4\lambda}{\alpha\lambda}. \tag{7}$$

For our purpose, we introduce some spaces and operators. Let $l^2=\{u=(u_i)_{i\in Z}|\Sigma_{i\in Z}|u_i|^2<\infty\}$. Define the linear operators B, $\overline{B}$, A from l^2 to l^2 as follows. For any $u=(u_i)_{i\in Z}\in l^2$,

$$(Bu)_i=u_{i+1}-u_i, \quad (\overline{B}u)_i=u_{i-1}-u_i, \quad (Au)_i=-(u_{i-1}-2u_i+u_{i+1}), \quad \forall i\in Z.$$

Then we have

$$A=\overline{B}B=B\overline{B}.$$

For any two elements of l^2, $u=(u_i)_{i\in Z}$, $v=(v_i)_{i\in Z}\in l^2$, define bilinear forms as

$$(u,v)=\sum_{i\in Z} u_i v_i, \quad \|u\|^2=(u,u)=\sum_{i\in Z}|u_i|^2;$$

$$(u,v)_\lambda=\rho(Bu,Bv)+\lambda(u,v), \tag{8}$$

$$\|u\|_\lambda^2=(u,u)_\lambda=\rho\|Bu\|^2+\lambda\|u\|^2=\sum_{i\in Z}(\rho|u_{i+1}-u_i|^2+\lambda|u_i|^2),$$

where ρ is chosen as

$$\rho=1-\frac{\alpha\lambda}{\beta^2+4\lambda}\gamma\geqslant 0.$$

It is easy to check that above two bilinear forms $(\cdot,\cdot)$ and $(\cdot,\cdot)_\lambda$ in (8) are both the inner products; moreover, the norms $\|\cdot\|$ and $\|\cdot\|_\lambda$ are equivalent to each other because

$$\lambda\|u\|^2\leqslant\|u\|_\lambda^2=\sum_{i\in Z}(\rho|u_{i+1}-u_i|^2+\lambda|u_i|^2)\leqslant(4\rho+\lambda)\|u\|^2.$$

Denote by l^2, l_λ^2 the spaces with the inner products and norms in (8), respectively,

$$l^2=(l^2,(\cdot,\cdot),\|\cdot\|), \quad l_\lambda^2=(l^2,(\cdot,\cdot)_\lambda,\|\cdot\|_\lambda);$$

then l^2 and l_λ^2 are Hilbert spaces.

Let $E=l_\lambda^2\times l^2$, endowed with the inner product and norm as, for $\varphi_j=(u^{(j)},v^{(j)})=((u_i^{(j)}),(v_i^{(j)}))_{i\in Z}\in E$, $j=1,2$,

$$(\varphi_1,\varphi_2)_E=(u^{(1)},u^{(2)})_\lambda+(v^{(1)},v^{(2)})=\sum_i\ [\rho(Bu^{(1)})_i(Bu^{(2)})_i+\lambda u_i^{(1)}u_i^{(2)}+v_i^{(1)}v_i^{(2)}],$$

$$\|\varphi\|_E^2=(\varphi,\varphi)_E,\quad \forall\varphi\in l_\lambda^2\times l^2. \tag{9}$$

Now we consider the existence and uniqueness of solutions of system (3)–(4). With the above notations, Eq. (3) can be written as

$$\ddot{u}+\gamma A\dot{u}+h(\dot{u})+Au+\lambda u+f(u)=g,\quad t>0, \tag{10}$$

and the initial data (4) are

$$u(0)=(u_{i,0})_{i\in Z}=u_0,\quad \dot{u}(0)=(u_{1i,0})_{i\in Z}=u_{10}, \tag{11}$$

where

$$u=(u_i)_{i\in Z},\quad h(\dot{u})=(h(\dot{u}_i))_{i\in Z},\quad f(u)=(f(u_i))_{i\in Z},\quad g=(g_i)_{i\in Z}.$$

It is convenient to reduce (10) to an evolution equation of the first order in time. Let $v=\dot{u}+\varepsilon u$, where ε is chosen as

$$\varepsilon=\frac{\alpha\lambda}{\beta^2+4\lambda}>0; \tag{12}$$

then system (10)–(11) is equivalent to the following initial value problem in Hilbert space E:

$$\dot{\varphi}+C(\varphi)=F(\varphi),\quad \varphi(0)=(u_0,v_0)^T=(u_0,u_{10}+\varepsilon u_0)^T, \tag{13}$$

where

$$\varphi=(u,v)^T,\quad v=\dot{u}+\varepsilon u,\quad F(\varphi)=(0,-f(u)+g)^T,$$

$$C(\varphi)=\begin{pmatrix}\varepsilon u-v\\ Au+\lambda u-\gamma\varepsilon Au+\varepsilon^2u+\gamma Av-\varepsilon v\end{pmatrix}+\begin{pmatrix}0\\ h(v-\varepsilon u)\end{pmatrix}. \tag{14}$$

Let us show that the function $F(\varphi)-C(\varphi)$ is locally Lipschitz continuous from E to E. By condition (5), $f(0)=0$, and for any $u=(u_i)_{i\in z}\in l^2$,

$$\|f(u)\|^2=\sum_{i\in Z}|f(u_i)|^2=\sum_{i\in Z}|f'(\theta_iu_i)|^2|u_i|^2,$$

where $\theta_i\in(0,1)$. By $|\theta_iu_i|\leqslant|u_i|\leqslant\|u\|$,

$$\|f(u)\|\leqslant\|u\|\max_{s\in[0,\|u\|]}|f'(s)|; \tag{15}$$

thus, from $f\in C^1$, it follows that $f(u)\in l^2$, i.e., f maps l^2 into l^2, hence, F maps E into itself.

By (6),

$$\|h(v-\varepsilon u)\|^2=\sum_{i\in Z}|h'(\tilde{\theta}_i(v_i-\varepsilon u_i))|^2|v_i-\varepsilon u_i|^2\leqslant 2\beta^2(\|v\|^2+\varepsilon^2\|u\|^2); \tag{16}$$

thus, if $\varphi=(u,v)\in E$, then $h(v-\varepsilon u)\in l^2$, i.e., $H(\varphi)=(0,h(v-\varepsilon u))^T$ maps E into E.

Let B be a bounded set in E, $\varphi_j=(u^{(j)},v^{(j)})=((u_i^{(j)}),(v_i^{(j)}))_{i\in Z}\in B$, $j=1,2$, similar to (15), there exists $L(B)$ depending on B such that

$$\|F(\varphi_1)-F(\varphi_2)\|_E^2=\|f(u^{(1)})-f(u^{(2)})\|^2$$

$$=\sum_{i\in z}|f'(u_i^{(1)}+\theta_i(u_i^{(2)}-u_i^{(1)})|^2|u_i^{(1)}-u_i^{(2)}|^2)$$

$$\leqslant\left(\max_{s\in[0,\|u^{(1)}\|+\|u^{(2)}\|]}|f'(s)|\right)\cdot\|u^{(1)}-u^{(2)}\|^2\leqslant L(B)\|\varphi_1-\varphi_2\|_E^2,$$

and similar to (16),

$$\|H(\varphi_1)-H(\varphi_2)\|_E^2=\|h(v^{(1)}-\varepsilon u^{(1)})-h(v^{(2)}-\varepsilon u^{(2)})\|^2$$

$$=\sum_{i\in z}|h'(\xi_i)|^2|(v_i^{(1)}-v_i^{(1)})-\varepsilon(u_i^{(1)}-u_i^{(2)})|^2$$

$$\leqslant 2\beta^2(\|v^{(1)}-v^{(1)}\|^2+\varepsilon^2\|u^{(1)}-u^{(2)}\|^2)$$

$$\leqslant 2\beta^2(1+\varepsilon^2/\lambda)\|\varphi_1-\varphi_2\|_E^2,$$

which imply that $F(\varphi)-C(\varphi)$ is locally Lipschitz from E to E. By the standard theory of ordinary differential equations, we obtain the existence and uniqueness of local solution φ for problem (13).

Lemma 2.1: If $g=(g_i)_{i\in Z}\in l^2$ and f, h satisfy (5), (6), then for any initial data $\varphi(0)=(u_0,v_0)^T\in E$, there exists a unique local solution $\varphi(t)=(u(t),v(t))^T$ of (13) such that $\varphi\in C^1((0,T_0),E)$ for some $T_0>0$. If $T_0<+\infty$, then $\lim_{t\to T_0}\|\varphi(t)\|_E=+\infty$.

In fact, it is shown from Lemma 3.2 below that the local solution $\varphi(t)$ of (13) exists globally, that is, $\varphi\in C^1(R_+,E)$, which implies that maps

$$S(t):\varphi(0)=(u_0,v_0)\in E\to\varphi(t)=S(t)\varphi(0)=(u(t),v(t))\in E,\quad t\geqslant 0, \tag{17}$$

generates a continuous semigroup $\{S(t)\}_{t\geqslant 0}$ on E, where $v(t)=\dot{u}(t)+\varepsilon u(t)$.

Remark: It is easy to see that the solutions of problem (13) are backward unique in time t, i.e., the solution $\varphi(t)\in C^1(R,E)$.

III. ABSORBING SET

In this section, we consider the uniform boundedness of solutions of system (13). First, we present a positivity of the nonlinear operator C.

Lemma 3.1: For any $\varphi=(u,v)^T\in E$,

$$(C(\varphi),\varphi)_E\geqslant\sigma\|\varphi\|_E^2+\frac{\alpha}{2}\|v\|^2, \tag{18}$$

where

$$\sigma=\frac{\alpha\lambda}{\sqrt{\beta^2+4\lambda}(\beta+\sqrt{\beta^2+4\lambda})}. \tag{19}$$

Proof: It is easy to check that

$$(Bu,v)=(u,\overline{B}v)\quad\text{and}\quad(Au,v)=(Bu,Bv),\quad\forall u,v\in l^2. \tag{20}$$

By the definition of $(\cdot,\cdot)_E$ in (9), (14), and (20),

$$(C(\varphi),\varphi)_E=\varepsilon[\rho\|Bu\|^2+\lambda\|u\|^2]+\varepsilon^2(u,v)+\gamma(Av,v)+(h(v-\varepsilon u),v)-\varepsilon(v,v),$$

and by (6),

$$\varepsilon^2(u,v)+(h(v-\varepsilon u),v)=\varepsilon^2\sum_{i\in Z}u_iv_i+\sum_{i\in Z}h'(\tau_i(v_i-\varepsilon u_i))(v_i-\varepsilon u_i)v_i$$
$$\geqslant\alpha\|v\|^2-\varepsilon(\beta-\varepsilon)\|u\|\cdot\|v\|;$$

then

$$(C(\varphi),\varphi)_E-\sigma\|\varphi\|_E^2-\frac{\alpha}{2}\|v\|^2\geqslant(\varepsilon-\sigma)[\rho\|Bu\|^2+\lambda\|u\|^2]+\gamma\|Bv\|^2$$
$$+\left(\frac{\alpha}{2}-\varepsilon-\sigma\right)\|v\|^2-\beta\varepsilon\|u\|\cdot\|v\|$$
$$\geqslant(\varepsilon-\sigma)[\rho\|Bu\|^2+\lambda\|u\|^2]+\left(\frac{\alpha}{2}-\varepsilon-\sigma\right)\|v\|^2-\frac{\beta\varepsilon}{\sqrt{\lambda}}[\rho\|Bu\|^2$$
$$+\lambda\|u\|^2]^{1/2}\|v\|,$$

and a simple computation from (12), (19) shows

$$4(\varepsilon-\sigma)\left(\frac{\alpha}{2}-\varepsilon-\sigma\right)=\frac{\beta^2\varepsilon^2}{\lambda}.$$

Thus, the proof is completed.

Now we consider the boundedness of solutions $\varphi(t)$ of (13).

Lemma 3.2: If (5)–(7) hold and $g\in l^2$, then there exists a bounded ball $O=O_E(0,r_0)$, centered at 0 with radius r_0, such that for every bounded set B of E, there exists $T(B)\geqslant 0$ such that

$$S(t)B\subset O,\quad \forall t\geqslant T(B), \tag{21}$$

where $r_0^2=(2/\alpha\mu)\|g\|^2$. Therefore, there exists a constant $T_0\geqslant 0$ depending on O such that

$$S(t)O\subset O,\quad \forall t\geqslant T_0. \tag{22}$$

Proof: Assume that (5)–(7) hold and $g\in l^2$. Let $\varphi(t)=(u(t),v(t))^T\in E$ be a solution of (13), where $v(t)=\dot{u}(t)+\varepsilon u(t)$. Taking the inner product $(\cdot,\cdot)_E$ of (13) with $\varphi(t)$, we have

$$\frac{1}{2}\frac{d}{dt}\|\varphi\|_E^2+(C(\varphi),\varphi)_E+(f(u),\dot{u})+\varepsilon(f(u),u)=(g,v). \tag{23}$$

By (18),

$$(C(\varphi),\varphi)_E\geqslant\sigma\|\varphi\|_E^2+\frac{\alpha}{2}\|v\|^2. \tag{24}$$

By (5),

$$(f(u),\dot{u})=\sum_{i\in Z}f(u_i)\dot{u}_i=\frac{d}{dt}\left(\sum_{i\in Z}G(u_i)\right), \tag{25}$$

$$(f(u),u)=\sum_{i\in Z}f(u_i)u_i\geqslant\nu\sum_{i\in Z}G(u_i), \tag{26}$$

and

$$(g,v)\leqslant\frac{1}{2\alpha}\|g\|^2+\frac{\alpha}{2}\|v\|^2. \tag{27}$$

By putting (24)–(27) into (23), we find

$$\frac{d}{dt}\left[\|\varphi\|_E^2+2\sum_{i\in Z}G(u_i)\right]+\mu\left[\|\varphi\|_E^2+2\sum_{i\in Z}G(u_i)\right]\leqslant\frac{1}{\alpha}\|g\|^2, \tag{28}$$

where $\mu=\min\{2\sigma,\nu\varepsilon\}$. Since

$$G(u_i)\geqslant 0,\quad \|\varphi\|_E^2+2\sum_{i\in Z}G(u_i)\geqslant 0,$$

by Gronwall's inequality,

$$\|\varphi\|_E^2+2\sum_{i\in Z}G(u_i)\leqslant\left[\|\varphi(0)\|_E^2+2\sum_{i\in Z}G(u_{i0})\right]e^{-\mu t}+\frac{1}{\alpha\mu}\|g\|^2(1-e^{-\mu t}). \tag{29}$$

By (5),

$$\sum_{i\in Z}G(u_{i0})\leqslant\frac{1}{\nu}\sum_{i\in Z}f(u_{i0})_{ui0}\leqslant\frac{1}{\nu}\max_{s\in[0,\|u(0)\|]}|f'(s)|\cdot\|u(0)\|^2. \tag{30}$$

By (29) and (28),

$$\|\varphi\|_E^2\leqslant\left[\|\varphi(0)\|_E^2+\frac{2}{\nu}\max_{s\in[0,\|u(0)\|]}|f'(s)|\cdot\|u(0)\|^2\right]e^{-\mu t}+\frac{1}{\alpha\mu}\|g\|^2(1-e^{-\mu t}) \tag{31}$$

and

$$\limsup_{t\to\infty}\|\varphi\|_E^2\leqslant\frac{1}{\alpha\mu}\|g\|^2. \tag{32}$$

Inequality (31) [or (32)] implies that the semigroup $\{S(t)\}_{t\geqslant 0}$ possesses a bounded absorbing set in E. The proof is completed.

From (31), for any initial data $\varphi(0)=(u_0,v_0)^T\in E$, then the solution $\varphi(t)=(u(t),v(t))^T$ is bounded for all $t\in[0,+\infty)$, that is, the solution $\varphi(t)$ exists globally on $[0,+\infty)$, maps $\{S(t)_{t\geqslant 0}\}$ defined by (17) form a semigroup on E.

IV. GLOBAL ATTRACTOR

In this section, we prove the existence of a global attractor for the semigroup $\{S(t)_{t\geqslant 0}\}$ associated with (13) on E. For this purpose, we need to prove the asymptotic compactness of $\{S(t)_{t\geqslant 0}\}$.

Lemma 4.1: If (5)–(7) hold, $g\in l^2$ and $\varphi(0)=(u_0,v_0)\in O$, then $\forall\,\eta>0$, there exist $T(\eta)$ and $K(\eta)$ such that the solution $\varphi(t)=(\varphi_i)_{i\in Z}=((u_i(t)),(v_i(t)))_{i\in Z}\in E$ of problem (13), $v(t)=\dot{u}(t)+\varepsilon u(t)$, satisfies

$$\sum_{|i|\geqslant K(\eta)}\|\varphi_i(t)\|_E^2=\sum_{|i|\geqslant K(\eta)}[\rho|(Bu(t))_i|^2+\lambda|u_i(t)|^2+|v_i(t)|^2]\leqslant\eta,\quad\forall t\geqslant T(\eta), \tag{33}$$

where $(Bu(t))_i=u_{i+1}(t)-u_i(t)$.

Proof: Choosing a smooth function $\theta\in C^1(R^+,R)$ satisfies

$$\theta(s)=0,\quad 0\leqslant s\leqslant 1,$$

$$0\leqslant\theta(s)\leqslant 1,\quad 1\leqslant s\leqslant 2, \tag{34}$$

$$\theta(s)=1, \quad s\geqslant 2;$$

then there exists a constant C_0 such that $|\theta'(s)|\leqslant C_0$ for $s\in R^+$.

Let $\varphi(t)=(u(t),v(t))=(\varphi_i)_{i\in Z}=((u_i(t)),(v_i(t)))_{i\in Z}$ be a solution of (13), where $v(t)=\dot{u}(t)+\varepsilon u(t)$, $\varphi_i=(u_i,v_i)$, ε is as in (12).

Let k be a fixed integer. Set $w_i=\theta(|i|/k)u_i$, $z_i=\theta(|i|/k)v_i$, $y=(w,z)=((w_i),(z_i))_{i\in Z}$. Taking the inner product $(\cdot,\cdot)_E$ of (13) with y, we have

$$(\dot{\varphi},y)_E+(C(\varphi),y)_E=(F(\varphi),y)_E. \tag{35}$$

It is possible to check that

$$(\dot{\varphi},y)_E=\frac{1}{2}\frac{d}{dt}\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)\|\varphi_i\|_E^2, \tag{36}$$

where

$$\|\varphi_i\|_E^2=\rho|(Bu)_i|^2+\lambda|u_i|^2+|v_i|^2=\rho|u_{i+1}-u_i|^2+\lambda|u_i|^2+|v_i|^2, \tag{37}$$

and

$$\begin{aligned}(C(\varphi),y)_E=&\varepsilon\rho(Bu,Bw)-\rho(Bv,Bw)+\lambda\varepsilon(u,w)-\lambda(v,w)+(Bu,Bz)+\lambda(u,z)+\varepsilon^2(u,z)\\&-\varepsilon\gamma(Bu,Bz)-\varepsilon(v,z)+(h(v-\varepsilon u),z),\end{aligned} \tag{38}$$

$$\begin{aligned}(Bu,Bw)(t)&=\sum_{i\in Z}\left\{\left[\theta\left(\frac{|i+1|}{k}\right)-\theta\left(\frac{|i|}{k}\right)\right](u_{i+1}-u_i)u_{i+1}+\theta\left(\frac{|i|}{k}\right)(u_{i+1}-u_i)^2\right\}\\&\geqslant-\frac{4C_0r_0^2}{k}+\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)(u_{i+1}-u_i)^2, \quad \forall t\geqslant T_0,\end{aligned}$$

$$(Bv,Bw)=\sum_{i\in Z}\left[\theta\left(\frac{|i+1|}{k}\right)(v_{i+1}-v_i)u_{i+1}-\theta\left(\frac{|i|}{k}\right)(v_{i+1}-v_i)u_i\right],$$

$$(Bu,Bz)=\sum_{i\in Z}\left[\theta\left(\frac{|i+1|}{k}\right)(u_{i+1}-u_i)v_{i+1}-\theta\left(\frac{|i|}{k}\right)(u_{i+1}-u_i)v_i\right],$$

$$\begin{aligned}(1-\varepsilon\gamma)(Bu,Bz)-\rho(Bv,Bw)&=\rho\sum_{i\in Z}\left(\theta\left(\frac{i+1}{k}\right)-\theta\left(\frac{|i|}{k}\right)\right)(u_{i+1}v_i-u_iv_{i+1})\\&\geqslant-\rho\sum_{i\in Z}\frac{|\theta'(\tau_i)|}{k}|u_{i+1}v_i-u_iv_{i+1}|\\&\geqslant-\frac{4\rho C_0r_0^2}{k}, \quad \forall t\geqslant T_0,\end{aligned}$$

$$(u,w)=\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)u_i^2, \quad (v,w)=\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)u_iv_i=(u,z), \quad (v,z)=\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)v_i^2,$$

$$\varepsilon^2(u,z)+(h(v-\varepsilon u),z)\geqslant\alpha\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)u_i^2-\varepsilon(\beta-\varepsilon)\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)u_iv_i.$$

By (38) and the proof of (18),

$$(C(\varphi),y)\geqslant -\frac{8\rho C_0 r_0^2}{k}+\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)\left[\sigma\|\varphi_i\|_E^2+\frac{\alpha}{2}|v_i|^2\right],\quad \forall t\geqslant T_0. \tag{39}$$

And

$$(F(\varphi),y)_E=-(f(u),z)+(g,z),$$

$$\begin{aligned}(f(u),z)&=\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)f(u_i)\dot{u}_i+\varepsilon\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)f(u_i)u_i\\&\geqslant\frac{d}{dt}\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)G(u_i)+\varepsilon\nu\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)G(u_i),\end{aligned} \tag{40}$$

$$\begin{aligned}(g,z)=\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)g_iv_i&=\sum_{|i|\geqslant k}\theta\left(\frac{|i|}{k}\right)g_iv_i\leqslant\frac{\alpha}{2}\sum_{|i|\geqslant k}\theta^2\left(\frac{|i|}{k}\right)v_i^2+\frac{1}{2\alpha}\sum_{|i|\geqslant k}g_i^2\\&\leqslant\frac{\alpha}{2}\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)v_i^2+\frac{1}{2\alpha}\sum_{|i|\geqslant k}g_i^2.\end{aligned} \tag{41}$$

Putting inequalities (36), (39)–(41) into (35), we obtain

$$\frac{d}{dt}\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)[\|\varphi_i\|_E^2+2G(u_i)]+\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)[2\sigma\|\varphi_i\|_E^2+2\varepsilon\nu G(u_i)]\leqslant\frac{8\rho C_0r_0^2}{k}+\frac{1}{\alpha}\sum_{|i|\geqslant k}g_i^2.$$

Since $g\in l^2$, then $\forall\,\eta>0$, there exists $K(\eta)$ such that

$$\frac{8\rho C_0r_0^2}{k}+\frac{1}{\alpha}\sum_{|i|\geqslant k}g_i^2\leqslant\eta,\quad \forall k\geqslant K(\eta),$$

i.e., for $t\geqslant T_0, k\geqslant K(\eta)$,

$$\frac{d}{dt}\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)[\|\varphi_i\|_E^2+2G(u_i)]+\mu\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)[\|\varphi_i\|_E^2+2G(u_i)]\leqslant\eta,$$

where $\mu=\min\{2\sigma,\varepsilon\nu\}$. So, by Gronwall's inequality,

$$\begin{aligned}\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)[\|\varphi_i\|_E^2+2G(u_i)]&\leqslant e^{-\mu(t-T_0)}\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)[\|\varphi_i(T_0)\|_E^2+2G(u_i(T_0))]+\frac{\eta}{\mu}\\&\leqslant e^{-\mu(t-T_0)}r_0^2\left(1+\frac{2}{\nu}M_0\right)+\frac{\eta}{\mu},\quad \forall t\geqslant T_0,\end{aligned}$$

where $M_0=\max_{s\in[0,r_0/\nu]}|f'(s)|$. Taking

$$T(\eta)=\max\left\{T_0,T_0+\frac{1}{\mu}\ln\frac{\mu}{\eta}\left(1+\frac{2}{\nu}M_0\right)r_0^2\right\},$$

then for $t\geqslant T(\eta)$ and $k\geqslant K(\eta)$, we have

$$\sum_{|i|\geqslant 2k}\|\varphi_i\|_E^2\leqslant\sum_{i\in Z}\theta\left(\frac{|i|}{k}\right)\|\varphi_i\|_E^2\leqslant\frac{2\eta}{\mu}, \tag{42}$$

which implies Lemma 4.1. The proof is completed.

Lemma 4.2: If (5)–(7) hold and $g \in l^2$, then the semigroup $\{S(t)\}_{t\geqslant 0}$ is asymptotically compact in E, that is, if $\{\varphi_n\}$ is bounded in E and $t_n \to +\infty$, then $\{S(t_n)\varphi_n\}$ is precompact in E.

Proof: Since $\{\varphi_n\} \subset E = l^2_\lambda \times l^2$ is bounded, assume that $\|\varphi_n\|_E \leqslant r$ for some positive constant r, $n = 1,2,\ldots$. By Lemma 3.2, there exists T_r such that

$$S(t)\{\varphi_n\} \subset O, \quad \forall t \geqslant T_r, \tag{43}$$

where O is the absorbing set in Lemma 2.3. By $t_n \to +\infty$, there exists $N_1(r)$ such that $t_n \geqslant T_r$ if $n \geqslant N_1(r)$, thus,

$$S(t_n)\{\varphi_n\} \subset O, \quad \forall n \geqslant N_1(r). \tag{44}$$

Since E is a Hilbert space and by (44), there exists $\varphi_0 \in E$ and a subsequence of $\{S(t_n)\varphi_n\}$ (denoted still by $\{S(t_n)\varphi_n\}$), such that

$$S(t_n)\varphi_n \to \varphi_0, \quad \text{weakly in } E. \tag{45}$$

In fact, the convergence here is a strong one, i.e., $\forall \eta > 0$, there exists $N(\eta)$ such that

$$\|S(t_n)\varphi_n - \varphi_0\|_E \leqslant \eta, \quad \forall n \geqslant N(\eta).$$

For $\eta > 0$, by Lemma 4.1 and (43), there exist $K_1(\eta), T(\eta)$ such that

$$\sum_{|i|\geqslant K_1(\eta)} \|(S(t)(S(T_r))\varphi_n)_i\|^2_E \leqslant \frac{\eta^2}{8}, \quad t \geqslant T(\eta).$$

By $t_n \to +\infty$, there exists $N_2(r,\eta)$ such that $t_n \geqslant T_r + T(\eta)$ if $n \geqslant N_2(r,\eta)$; hence,

$$\sum_{|i|\geqslant K_1(\eta)} \|(S(t_n)\varphi_n)_i\|^2_E = \sum_{|i|\geqslant K_1(\eta)} \|(S(t_n - T_r)S(T_r)\varphi_n)_i\|^2_E \leqslant \frac{\eta^2}{8}. \tag{46}$$

Again, since $\varphi_0 \in E$, there exists $K_2(\eta)$ such that

$$\sum_{|i|\geqslant K_2(\eta)} \|(\varphi_0)_i\|^2_E \leqslant \frac{\eta^2}{8}. \tag{47}$$

Let $K(\eta) = \max\{K_1(\eta), K_2(\eta)\}$, by (45),

$$((S(t_n)\varphi_n)_i)_{|i|\leqslant K(\eta)} \to ((\varphi_0)_i)_{|i|\leqslant K(\eta)}, \quad \text{strongly in} \quad R^{2K(\eta)+1}_\lambda \times R^{2K(\eta)+1}, \quad \text{as} \quad n \to +\infty,$$

that is, there exists $N_3(\eta)$ such that

$$\sum_{|i|\leqslant K(\eta)} \|(S(t_n)\varphi_n)_i - (\varphi_0)_i\|^2_E \leqslant \frac{\eta^2}{2}, \forall n \geqslant N_3(\eta). \tag{48}$$

Setting $N(\eta) = \max\{N_1(r), N_2(r,\eta), N_3(\eta)\}$, from (46)–(48), then for $n \geqslant N(\eta)$,

$$\begin{aligned}\|S(t_n)\varphi_n - \varphi_0\|^2_E &= \sum_{|i|\leqslant K(\eta)} \|(S(t_n)\varphi_n)_i - (\varphi_0)_i\|^2_E + \sum_{|i|> K(\eta)} \|(S(t_n)\varphi_n)_i - (\varphi_0)_i\|^2_E \\ &\leqslant \frac{\eta^2}{2} + 2\sum_{|i|> K(\eta)} (\|(S(t_n)\varphi_n)_i\|^2_E - \|(\varphi_0)_i\|^2_E) \leqslant \eta^2.\end{aligned}$$

The proof is completed.

As a direct consequence of Lemma 3.2, Lemma 4.2 and Theorem I.1.1 in Ref. 10, we obtain the existence of a global attractor for semigroup $\{S(t)\}_{t\geqslant 0}$.

Theorem 4.1: If (5)–(7) hold and $g \in l^2$, then the semigroup $\{S(t)\}_{t\geqslant 0}$ associated with (13) possesses a global attractor ß in E.

Remark: Since the solutions of problem (13) are backward unique in time, the invariance of the global attractor ß means

$$S(t)ß = ß, \quad \text{for } t \in R. \tag{49}$$

V. APPROXIMATION OF ATTRACTOR

In this section, we present the approximation to the global attractor ß by the global attractors of finite-dimensional ordinary differential systems.

Let $n \in Z_+$ be a positive integer, we consider the $(2n+1)$-dimensional ordinary differential equations:

$$\begin{gathered}\ddot{w}_i - \gamma(\dot{w}_{i-1} - 2\dot{w}_i + \dot{w}_{i+1}) + h(\dot{w}_i) = (w_{i-1} - 2w_i + w_{i+1}) - \lambda w_i - f(w_i) + g_i, \\ i = -n, \quad -n+1, \quad \ldots, \quad n-1, \quad n, \quad w_{-n} = w_{n+1}, \quad w_n = w_{-n+1},\end{gathered} \tag{50}$$

with the initial values

$$w_i(0) = w_{i0}, \quad \dot{w}_i(0) = z_{i0} \in R, \quad i = -n, -n+1, \ldots, n-1, n. \tag{51}$$

Then equations (50)–(51) can be written as

$$\begin{gathered}\ddot{w} + \gamma\tilde{A}\dot{w} + h(\dot{w}) = -\tilde{A}w - \lambda w - \tilde{f}(w) + \tilde{g}, \\ w(0) = (w_{i0})_{|i|\leqslant n}, \quad \dot{w}(0) = (z_{i0})_{|i|\leqslant n} \in R^{2n+1},\end{gathered} \tag{52}$$

where $w = (w_i)_{|i|\leqslant n}$, $h(\dot{w}) = (h(\dot{w}_i))_{|i|\leqslant n}$, $\tilde{f}(w) = (f(w_i))_{|i|\leqslant n}$, $\tilde{g} = (g_i)_{|i|\leqslant n}$,

$$\tilde{A} = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \ddots & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ -1 & 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix}_{(2n+1)\times(2n+1)}.$$

Let us introduce some Hilbert spaces and operators similar to Sec. II.
Let

$$B = \begin{pmatrix} -1 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \ddots & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdots & -1 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & -1 \end{pmatrix}_{(2n+1)\times(2n+1)};$$

then

$$\tilde{A} = \tilde{B}\tilde{B}^T = \tilde{B}^T\tilde{B}.$$

For any $w = (w_i)_{|i|\leqslant n}$, $z = (z_i)_{|i|\leqslant n} \in R^{2n+1}$, define

$$(w,z)=\sum_{|i|\leqslant n} w_i z_i, \|w\|^2=\sum_{|i|\leqslant n} |w_i|^2,$$

$$(w,z)_\lambda=\rho(\tilde{B}w,\tilde{B}z)+\lambda(w,z),$$

$$\|w\|_\lambda^2=\rho\|\tilde{B}w\|^2+\lambda\|w\|^2=\sum_{|i|\leqslant n}(\rho|w_{i+1}-w_i|^2+\lambda|w_i|^2),$$

where ρ is as in Sec. II. Let $R_\lambda^{2n+1}=(R^{2n+1},\|\cdot\|_\lambda)$, $\tilde{E}=R_\lambda^{2n+1}\times R^{2n+1}$, endowed with the inner product and norm as follows: for $W_j=(w^{(j)},z^{(j)})=((w_i^{(j)}),(z_i^{(j)}))_{|i|\leqslant n}\in\tilde{E}$, $j=1,2$,

$$(W_1,W_2)_{\tilde{E}}=(w^{(1)},w^{(2)})_\lambda+(z^{(1)},z^{(2)})=\sum_i [\rho(\tilde{B}w^{(1)})_i(\tilde{B}w^{(2)})_i+\lambda w_i^{(1)}w_i^{(2)}+z_i^{(1)}z_i^{(2)}],$$

$$\|W_1\|_E^2=(W_1,W_1)_{\tilde{E}};$$

then $\tilde{E}$ is a Hilbert space.

Let $z=\dot{w}+\varepsilon w$, where ε is as in (12); then problem (52) is equivalent to the following first-order system in Hilbert space $\tilde{E}$:

$$\dot{Y}+\tilde{C}(Y)=\tilde{F}(Y),\quad Y(0)=(w(0),z(0)+\varepsilon w(0))^T\in\tilde{E}, \tag{53}$$

where $Y=(w,z)$,

$$\tilde{F}(Y)=\begin{pmatrix}0\\ -\tilde{f}(w)+\tilde{g}\end{pmatrix},$$

$$\tilde{C}(Y)=\begin{pmatrix}\varepsilon w-z\\ \tilde{A}w+\lambda w+\varepsilon^2 w-\varepsilon\gamma\tilde{A}w+\gamma\tilde{A}z-\varepsilon z+h(z-\varepsilon w)\end{pmatrix}.$$

Obviously, the problem (53) is well posed in $\tilde{E}$, that is, for any $Y(0)\in\tilde{E}$, there exists a unique solution $Y\in C([0,+\infty),\tilde{E})\cap C^1((0,+\infty),\tilde{E})$, and maps of solutions $S_n(t):Y(0)\to Y(t)=S_n(t)Y(0)\in\tilde{E}$ generate a continuous semigroup $\{S_n(t)\}_{t\geqslant 0}$ on $\tilde{E}$.

Similar to Lemma 3.2 and Theorem 4.1, we have the following lemma.

Lemma 5.1: If (5)–(7) hold and $g\in l^2$, then there exists a bounded ball $\tilde{O}=\tilde{O}_{\tilde{E}}(0,r_0)$, centered at 0 with radius r_0, such that $\tilde{O}$ is an absorbing set of $\{S_n(t)\}_{t\geqslant 0}$, where r_0 is the same constant in Lemma 3.2, which is independent of n. The semigroup $\{S_n(t)\}_{t\geqslant 0}$ possesses a global attractor $ß_n\subset\tilde{O}\subset\tilde{E}$.

It is easy to see that

$$S_n(t)ß_n=ß_n,\quad \text{for}\quad \text{all}\ \ t\in R.$$

To prove $ß_n$ being an approximation to ß, in the following, we extend the element $w=(w_i)_{|i|\leqslant n}\in R^{2n+1}$ to an element of l^2 such that $w_i=0$ for $|i|>n$ (we still denote it by w).

Lemma 5.2: If (5)–(7) hold, $g\in l^2$, and $\varphi_n(0)\in ß_n$, then there exists a subsequence $\{\varphi_{n_k}(0)\}$ of $\{\varphi_n(0)\}$ and $\varphi_0\in ß$ such that $\varphi_{n_k}(0)$ converges to φ_0 in E.

Proof: Let $\varphi_n(t)=S_n(t)\varphi_n(0)=(u_n(t),v_n(t))\in\tilde{E}=R_\lambda^{2n+1}\times R^{2n+1}$ be a solution of problem (53). Since $\varphi_n(0)\in ß_n$, $\varphi_n(t)\in ß_n\subset\tilde{O}$ for all $t\in R$, thus, for any $t\in R$, $n=1,2,...$,

$$\|\varphi_n(t)\|_{\tilde{E}}=\|\varphi_n(t)\|_E=(\rho\|Bu_n\|^2+\lambda\|u_n\|^2+\|v_n\|^2)^{1/2}\leqslant r_0. \tag{54}$$

By (53),

$$\|\dot{\varphi}_n(t)\|_E \leqslant \|\tilde{C}(\varphi_n(t))\|_E + \|\tilde{F}(\varphi(t))\|_E . \tag{55}$$

Here

$$\|\tilde{C}\varphi_n(t)\|_E^2 \leqslant 8\{\varepsilon^2\rho\|Bu_n\|^2 + \rho\|Bv_n\|^2 + (\lambda\varepsilon^2 + \lambda^2 + \varepsilon^4 + 2\beta^2\varepsilon^2)\|u_n\|^2$$
$$+ (\lambda + \varepsilon^2 + 2\beta^2)\|v_n\|^2 + (1-\varepsilon\gamma)^2\|\tilde{A}u_n\|^2 + \gamma^2\|\tilde{A}v_n\|^2\},$$

and

$$\|Bv_n\|^2 \leqslant 4\|v_n\|^2, \quad \|\tilde{A}u_n\|^2 \leqslant 16\|u_n\|^2, \quad \|\tilde{A}v_n\|^2 \leqslant 16\|v_n\|^2;$$

thus, by (54), there exists $C_1(r_0)$ and $C_2(r_0,\|g\|)$ such that

$$\|\tilde{C}\varphi_n(t)\|_E^2 \leqslant C_1(r_0), \quad \|\tilde{F}(\varphi(t))\|_E \leqslant C_2(r_0,\|g\|), \quad \forall t \in R, \quad n = 1,2,\ldots . \tag{56}$$

So, by (55) and (56),

$$\|\dot{\varphi}_n(t)\|_E \leqslant C_3(r_0,\|g\|), \quad \forall t \in R, \quad n = 1,2,\ldots . \tag{57}$$

Let J_k ($k=1, 2,\ldots$) be a sequence of compact intervals of R such that $J_k \subset J_{k+1}$ and $\cup_k J_k = R$. Taking $s, t \in J_k$, we have

$$\|\varphi_n(t) - \varphi_n(s)\|_E < 2C_3(r_0,\|g\|)|t-s|,$$

which implies the equicontinuity of $\{\varphi_n(t)\}_{n=1}^{\infty}$ in $C(J_k,E)$. By (54), $\{\varphi_n(t)\}_{n=1}^{\infty}$ is uniformly bounded in E for fixed t, hence there exists a subsequence of $\{\varphi_n(t)\}_{n=1}^{\infty}$ (still denoted by $\{\varphi_n(t)\}_{n=1}^{\infty}$) and $\tilde{\varphi}_t \in E$, such that

$$\varphi_n(t) \to \tilde{\varphi}_t, \quad \text{weakly in } E, \quad \text{as } n \to +\infty. \tag{58}$$

Similar to the proof of Lemma 4.2, we show that the weak convergence in (58) is a strong one, that is, $\forall t \in J_k$, $\{\varphi_n(t)\}_{n=1}^{\infty}$ is precompact in E. By Ascoli's theorem, there exists a subsequence $\{\varphi_{n_1}(t)\}$ of $\{\varphi_n(t)\}$ and $\varphi_t \in C(J_1,E)$ such that $\varphi_{n_1}(t)$ converges to φ_t in $C(J_1,E)$. Again, by Ascoli's theorem and induction, there exists a subsequence of $\{\varphi_{n_{k+1}}(t)\}$ of $\{\varphi_{n_k}(t)\}$ such that $\varphi_{n_{k+1}}(t)$ converges to φ_t in $C(J_{k+1},E)$. Taking a diagonal subsequence in the usual way, there exists a subsequence $\{\varphi_{n_k}(t)\}$ of $\{\varphi_n(t)\}$ and $\varphi(t) \in C(R,E)$ such that

$$\varphi_n(t) \to \varphi(t), \quad \text{in } C(J,E), \quad \text{as } n \to +\infty, \quad \text{for any compact set } J \subset R. \tag{59}$$

By (54), for $\varphi(t) = (u(t),v(t)) = (u_i(t),v_i(t))_{i\in Z} \in E$, $v(t) = \dot{u}(t) + \varepsilon u(t)$,

$$\|\varphi(t)\|_E = (\rho\|Bu\|^2 + \lambda\|u\|^2 + \|v\|^2)^{1/2} \leqslant C_4(r_0), \quad \forall t \in R. \tag{60}$$

Now we will prove $\varphi(t) \in$ ß, the global attractor for semigroup $\{S(t)_{t\geqslant 0}\}$ associated with problem (13). We denote $\{\varphi_{n_k}(t)\}$ by $\{\varphi_n(t)\}$, from (57),

$$\dot{\varphi}_n(t) \to \dot{\varphi}(t), \quad \text{weak star in } L^{\infty}(R,E), \quad \text{as } n \to +\infty. \tag{61}$$

Let $i \in Z$ and $n \geqslant |i|$. Since $\varphi_n(t) = (u_{n,i}(t),v_{n,i}(t))_{|i|\leqslant n} \in \tilde{E}$ is the solution of problem (53), for every $t \in R$,

$$\ddot{u}_{n,i} - \gamma(\dot{u}_{n,i-1} - 2\dot{u}_{n,i} + \dot{u}_{n,i+1}) + h(\dot{u}_{n,i}) = (u_{n,i-1} - 2u_{n,i} + u_{n,i+1}) - \lambda u_{n,i} - f(u_{n,i}) + g_i ; \tag{62}$$

then $\forall \delta \in C_0^\infty(J)$; we have

$$\int_J [\ddot{u}_{n,i} - \gamma(\dot{u}_{n,i-1} - 2\dot{u}_{n,i} + \dot{u}_{n,i+1})]\delta(t)dt + \int_J h(\dot{u}_{n,i})\delta(t)dt$$
$$= \int_J [(u_{n,i-1} - 2u_{n,i} + u_{n,i+1}) - \lambda u_{n,i+1} + g_i]\delta(t)dt + \int_J f(u_{n,i})\delta(t)dt,$$

where

$$\left| \int_J f(u_{n,i})\delta(t)dt - \int_J f(u_i)\delta(t)dt \right|$$
$$\leqslant \int_J |f(u_{n,i}) - f(u_i)\| \delta(t)|dt|$$
$$\leqslant \sup_{t\in J}|f'(u_{n,i} + \vartheta_i(u_i - u_{n,i}))| \sup_{t\in J}|u_i - u_{n,i}| \int_J |\delta(t)|dt \to 0 \quad (n\to\infty),$$

and

$$\left| \int_J h(\dot{u}_{n,i})\delta(t)dt \right| - \int_J h(\dot{u}_i)\delta(t)dt$$
$$\leqslant \int_J |h(\dot{u}_{n,i}) - h(\dot{u}_i)\| \delta(t)|dt|$$
$$\leqslant \sup_{t\in J}|h'(\dot{u}_{n,i} + \tilde{\vartheta}_i(\dot{u}_i - \dot{u}_{n,i}))| \sup_{t\in J}|\dot{u}_i(t) - \dot{u}_{n,i}(t)| \int_J |\delta(t)|dt$$
$$\leqslant \beta \sup_{t\in J}|\dot{u}_i(t) - \dot{u}_{n,i}(t)| \int_J |\delta(t)|dt \to 0 \quad (n\to\infty),$$

because by (59), $\sup_{t\in J}|u_i - u_{n,i}| \to 0$, $\sup_{t\in J}|\dot{u}_i(t) - \dot{u}_{n,i}(t)| \to 0$ as $n\to\infty$ and by (54), (60),

$$|u_{n,i} + \vartheta(u_i - u_{n,i})| \leqslant \|u(t)\| + \|u_n(t)\| \leqslant C_5(r_0, \|g\|), \quad \forall t \in R.$$

Therefore, we have

$$\ddot{u}_i - \gamma(\dot{u}_{i-1} - 2\dot{u}_i + \dot{u}_{i+1}) + h(\dot{u}_i) = (u_{i-1} - 2u_i + u_{i+1}) - \lambda u_i - f(u_i) + g_i, \quad t \in J. \tag{63}$$

Since J is arbitrary, (63) holds for all $t \in R$, which means $\varphi(t) = (u(t), v(t))$ is a solution of (13). By (60), $\varphi(t)$ is bounded for $t \in R$, so, $\varphi(t) \in ß$, hence, $\varphi_n(0) \to \varphi(0) \in ß$. The proof is completed.

As a direct consequence of Lemma 5.2, we obtain the upper semicontinuity of ß.

Theorem 4.1: If (5)–(7) hold and $g \in l^2$, then $\lim_{n\to+\infty} d_E(ß_n, ß) = 0$, where $d_E(ß_n, ß) = \sup_{a\in ß_n} \inf_{b\in ß} \|a - b\|_E$.

Remark: For the mapping $S_0(t): (u_0, u_{10})^T \to (u(t), \dot{u}(t))^T \in l^2 \times l^2$ associated with problem (3)–(4) in the space $l^2 \times l^2$ with the usual inner product and norm, since $S_0(t) = R_{-\varepsilon} S(t) R_\varepsilon$, $R_\varepsilon = \left(\begin{smallmatrix} 1 & 0 \\ \varepsilon & 1 \end{smallmatrix}\right)$ is an isomorphism on $l^2 \times l^2$ and $\{S(t)\}_{t\geqslant 0}$ possesses a global attractor ß in E, the global attractor of $\{S_0(t)\}_{t\geqslant 0}$ in E is $R_{-\varepsilon} ß$, which implies that $\{S_0(t)\}_{t\geqslant 0}$ possesses a global attractor in $l^2 \times l^2$ because $l^2 \times l^2$ and E have the same elements and their norms are equivalent.

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A direct method for integrable couplings of TD hierarchy

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A direct method for establishing integrable couplings is proposed in this paper. As an example illustration, integrable couplings of TD hierarchy are obtained by constructing a suitable transformation of Lax pairs and a new Lie algebra. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1398061]

I. INTRODUCTION

Integrable couplings are a quite new interesting aspect in the field of soliton theory. It originates from an investigation on soliton equations. Mathematically, the problem of integrable couplings may be defined in the following way.

For a given integrable system of evolution equations

$$u_t = K(u), \tag{1}$$

the following system:

$$\begin{cases} u_t = K(u) \\ v_t = S(u,v) \end{cases}, \tag{2}$$

is called integrable coupling of (1), if (2) is also integrable and $S(u,v)$ includes u or its x-derivatives explicitly.

Two methods for discovering integrable couplings were proposed in Refs. 1–3:

(1) the original system and its linearized system

$$\begin{cases} u_t = K(u) \\ u_t = K'(u)[v] \end{cases}, \tag{3}$$

(2) the perturbation approach.

The above two methods have the common characteristics: Starting from the original equation (1) yields the integrable coupling of only one equation. In this paper, we proceed first to consider an isospectral problem, then a suitable loop algebra $\tilde{G}$ is constructed. The results obtained are integrable couplings of a family of evolution equations. As an example illustration, we try to establish the integrable couplings of TD hierarchy. However, it is not easy to obtain directly the integrable coupling. Thus a transformation of Lax pairs is made first. The second section is the TD hierarchy obtained by the Lax transformation. In the third section, integrable couplings of TD hierarchy are presented. Finally some remarks are made in Sec. IV.

Consider the isospectral problem

$$\varphi_x = U_1(u,\lambda)\varphi, \lambda_t = 0, u = (q,r)^T, \varphi = (\varphi_1, \varphi_2)^T, \tag{4}$$

where $U_1 = U_1(u,\lambda)$ is a matrix of order 2, T means transposition of the matrix.

Solving the adjoint representation of Eq. (4)

$$V_x = [U_1, V] \equiv U_1 V - V U_1, V = \begin{pmatrix} a & b \\ c & -a \end{pmatrix}, \tag{5}$$

yields recursion relations on a_i, b_i, c_i, $i \geqslant 1$, where

$$a=\sum_{i\geqslant 0} a_i\lambda^{-i}, b=\sum_{i\geqslant 0} b_i\lambda^{-i}, c=\sum_{i\geqslant 0} c_i\lambda^{-i}.$$

The Lax pair is obtained by using Tu-model[4]

$$\varphi_x=U_1\varphi, \varphi_{t_n}=V_1^{(n)}\varphi. \tag{6}$$

The compatibility of (6) leads to the zero-curvature equation

$$U_{1t}-V_{1x}^{(n)}+[U_1, V_1^{(n)}]=0. \tag{7}$$

By the use of the trace identity,[4] the generalized Hamiltonian hierarchy in the Liouville sense is obtained

$$u_{t_n}=\begin{pmatrix} q \\ r \end{pmatrix}_{t_n}=J\frac{\delta H_n}{\delta u}=JL\frac{\delta H_{n-1}}{\delta u}, \tag{8}$$

where J, L are a Hamiltonian operator and a recursion operator, respectively, $\delta/\delta u$ denotes variational derivative.

Consider the isospectral problem

$$\varphi_x=U(u,\lambda)\varphi, U=U_1(u,\lambda)+e(u,\lambda), \tag{9}$$

the matrix U is homogeneous rank, the second-order matrix $e(u,\lambda)$ meets that

$$[e,V]=0, [e,V_1^{(n)}]=0. \tag{10}$$

Let $f_n=f_n(u,\lambda)$ have the same order with U and meet the following:

$$[U_1,f_n]=0, [e,f_n]=0, e_{t_n}=f_{nx}. \tag{11}$$

Put $V^{(n)}=V_1^{(n)}+f_n$, we have

$$U_{t_n}-V_x^{(n)}+[U,V^{(n)}]=U_{1t_n}-V_{1x}^{(n)}+[U_1,V_1^{(n)}]=0, \tag{12}$$

that is, the compatibility of the new Lax pairs

$$\varphi_x=U\varphi, \varphi_{t_n}=V^{(n)}\varphi, \tag{13}$$

leads to (8) as well. In fact, $e=e(u,\lambda)$ and $f_n=f_n(u,\lambda)$ are chosen easily which satisfy (10) and (11). For example, we may take the forms $e=g(u,\lambda)E_2$, $f_n=h_n(u,\lambda)E_2$, where E_2 denotes second-order unit matrix. When reducing the zero-curvature equation derived from (9) to the Hamiltonian hierarchy, we have that[4]

$$\left\langle V,\frac{\partial U}{\partial\lambda}\right\rangle=\left\langle V,\frac{\partial U_1}{\partial\lambda}\right\rangle, \left\langle V,\frac{\partial U}{\partial u}\right\rangle=\left\langle V,\frac{\partial U_1}{\partial u}\right\rangle. \tag{14}$$

Thus the same trace identities are obtained

$$\frac{\delta}{\delta u}\left\langle V,\frac{\partial U}{\partial\lambda}\right\rangle=\left(\lambda^{-\gamma}\frac{\partial}{\partial\lambda}\lambda^{\gamma}\right)\left\langle V,\frac{\partial U}{\partial u}\right\rangle, \frac{\delta}{\delta u}\left\langle V,\frac{\partial U_1}{\partial\lambda}\right\rangle=\left(\lambda^{-\gamma}\frac{\partial}{\partial\lambda}\lambda^{\gamma}\right)\left\langle V,\frac{\partial U_1}{\partial u}\right\rangle. \tag{15}$$

Therefore, (4) and (9) lead to the same Hamiltonian system. But the Lax pair (6) is different from (13).

II. TD HIERARCHY

Taking the loop algebra $\tilde{A}_1$ with the basis $h_1=\left(\begin{smallmatrix}1&0\\0&0\end{smallmatrix}\right)$, $h_2=\left(\begin{smallmatrix}0&0\\0&1\end{smallmatrix}\right)$, $e=\left(\begin{smallmatrix}0&1\\0&0\end{smallmatrix}\right)$, $f=\left(\begin{smallmatrix}0&0\\1&0\end{smallmatrix}\right)$ for which we have that

$$[h_1,e]=-[h_2,e]=e,[h_1,f]=-[h_2,f]=-f,[e,f]=h_1-h_2\equiv h,h_i(n)=\lambda^n h_i,$$

$$e(n)=\lambda^n e,f(n)=\lambda^n f,\deg h_i(n)=\deg e(n)=\deg f(n)=n,i=1,2.$$

Consider the spectral problem of TD equation[5]

$$\begin{gathered}\varphi_x=U_1\varphi,U_1=U_1(u,\lambda)=\begin{pmatrix}-\lambda+r & q\\ q & \lambda\end{pmatrix}=-h(1)+rh_1(0)+q(e(0)+f(0)),\\ \varphi=(\varphi_1,\varphi_2)^T,u=(q,r)^T.\end{gathered}\tag{16}$$

Solving the adjoint equation

$$V_x=[U_1,V],\tag{17}$$

yields that

$$\begin{cases}a_{nx}=q(c_n-b_n),b_{n+1}=\frac{1}{2}(rb_n-2qa_n-b_{nx})\\ c_{nx}=2c_{n+1}+2qa_n-rc_n,a_0=-1,b_0=c_0=0,a_1=0,b_1=c_1=q\,.\\ a_2=\frac{1}{2}q^2,b_2=\frac{1}{2}(qr-q_x),c_2=\frac{1}{2}(qr+q_x)\end{cases}\tag{18}$$

Let

$$\varphi_x=U_1\varphi,\varphi_{t_n}=V_1^{(n)}\varphi,V_1^{(n)}=\begin{pmatrix}\sum_{i=0}^{n}a_i\lambda^{n-i}+q^{-1}(b_{n+1}+c_{n+1}) & \sum_{i=0}^{n}b_i\lambda^{n-i}\\ \sum_{i=0}^{n}c_i\lambda^{n-i} & -\sum_{i=0}^{n}a_i\lambda^{n-i}\end{pmatrix}.\tag{19}$$

Then the compatibility of the Lax pairs (19) leads to the well-known TD hierarchy as follows:

$$u_{t_n}=\begin{pmatrix}q\\ r\end{pmatrix}_{t_n}=J\frac{\delta H_n}{\delta u}=J\begin{pmatrix}b_{n+1}+c_{n+1}\\ a_{n+1}\end{pmatrix}=JL^{n-1}\begin{pmatrix}b_2+c_2\\ a_2\end{pmatrix},\tag{20}$$

where $J=\left(\begin{smallmatrix}0&\partial q^{-1}\\ q^{-1}\partial&0\end{smallmatrix}\right)$ is a Hamiltonian operator, $L=\frac{1}{2}\left(\begin{smallmatrix}r&\partial q^{-1}\partial-4q\\ \partial^{-1}q\partial&\partial^{-1}r\partial\end{smallmatrix}\right)$, $\partial\equiv\partial/\partial x$, $\partial^{-1}\partial=\partial\partial^{-1}=1$. Put $e=-r/2\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$, $f_n=-1/2q\,(b_{n+1}+c_{n+1})\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$, it is easy to verify that e and f_n meet (10) and (11).

Taking loop algebra $\overline{A_1}$ with the basis

$$h(n)=\begin{pmatrix}\lambda^n&0\\0&-\lambda^n\end{pmatrix},\quad e(n)=\begin{pmatrix}0&\lambda^n\\0&0\end{pmatrix},\quad f(n)=\begin{pmatrix}0&0\\\lambda^n&0\end{pmatrix},$$

$$[h(m),f(n)]=-2\,f(m+n),[h(m),e(n)]=2e(m+n),[e(m),f(n)]=h(m+n),$$

then the compatibility of the following Lax pair

$$\varphi_x = U\varphi = (U_1 + e)\varphi = \begin{pmatrix} -\lambda + \frac{r}{2} & q \\ q & \lambda - \frac{r}{2} \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} = \left(-h(1) + \frac{r}{2}h(0) + q(e(0) + f(0)) \right) \varphi,$$

$$\varphi_{t_n} = V^{(n)}\varphi = (V_1^{(n)} + f_n)\varphi,$$

$$V^{(n)} = \begin{pmatrix} \sum_{i=0}^{n} a_i \lambda^{n-i} + \frac{1}{2q}(b_{n+1} + c_{n+1}) & \sum_{i=0}^{n} b_i \lambda^{n-i} \\ \sum_{i=0}^{n} c_i \lambda^{n-i} & -\sum_{i=0}^{n} a_i \lambda^{n-i} - \frac{1}{2q}(b_{n+1} + c_{n+1}) \end{pmatrix}, \tag{21}$$

also gives rise to the TD hierarchy (20) and eq. $V_x = [U, V]$ is equivalent to (18).

III. INTEGRABLE COUPLINGS OF TD HIERARCHY

To obtain integrable couplings of TD hierarchy, we will establish a suitable loop algebra $\tilde{G}$. Let G be a linear space with basis $\{e_1, e_2, e_3, e_4, e_5\}$, we define the commutative relations as follows:

$$\begin{cases} [e_1, e_2] = 2e_2, [e_1, e_3] = -2e_3, [e_1, e_4] = e_4 \\ [e_1, e_5] = -e_5, [e_2, e_3] = e_1, [e_2, e_4] = 0 \\ [e_2, e_5] = e_4, [e_3, e_4] = e_5, [e_3, e_5] = 0 \\ [e_4, e_5] = 0 \end{cases}. \tag{22}$$

Set $a = \Sigma_{i=0}^{5} a_i e_i$, $b = \Sigma_{i=0}^{5} b_i e_i$, $c = \Sigma_{i=0}^{5} c_i e_i$, where a_i, b_i, c_i are all arbitrary constants or functions, then we have

$$[a, [b, c]] + [b, [c, a]] + [c, [a, b]] = 0, \tag{23}$$

that is, Jacobi identity holds. Thus G is a Lie algebra. If we let

$$\begin{cases} e_i(n) = e_i \lambda^n, i = 1,2,3,4,5 \\ [e_i(m), e_j(n)] = [e_i, e_j]\lambda^{m+n}, 1 \leqslant i, j \leqslant 5, \\ \deg e_i(n) = n, i = 1,2,3,4,5 \end{cases} \tag{24}$$

then the loop algebra $\tilde{G}$ is constructed. Set the subalgebras $\tilde{G}_1$, $\tilde{G}_2$ to have bases $\{e_1(n), e_2(n), e_3(n)\}, \{e_4(n), e_5(n)\}$, respectively. Of course, $\tilde{G}_1$ and $\tilde{G}_2$ meet the relations as follows:

$$\tilde{G}_1 \text{ is isomorphic to } \overline{A_1}, [\tilde{G}_1, \tilde{G}_2] \subset \tilde{G}_2. \tag{25}$$

Taking the form of linear spectral problem

$$\begin{cases} \Psi_x = [U, \Psi], \lambda_t = 0 \\ \Psi_t = [V, \Psi] \end{cases}, \tag{26}$$

where $\Psi = \Sigma_{i=1}^{5} \Psi_i e_i, \Psi_i$ is an arbitrary function, $U = U(u, \lambda) \in \tilde{G}, V = V(u, \lambda) \in \tilde{G}$, and $u = (u_1, u_2, \ldots, u_p)^T$ is a function vector. λ is a spectral parameter. The compatibility of (26) leads to that

$$\Psi_{xt}=[U_t,\Psi]+[U,\Psi_t]=[U_t,\Psi]+[U,[V,\Psi]]=\Psi_{tx}=[V_x,\Psi]+[V,\Psi_x]$$

$$=[V_x,\Psi]+[V,[U,\Psi]],$$

$$[U_t,\Psi]+[U,[V,\Psi]]-[V_x,\Psi]-[V,[U,\Psi]]=0. \tag{27}$$

By using Jacobi identity (23) and (27) may reduce to that

$$[U_t,\Psi]-[V_x,\Psi]+[[U,V],\Psi]=0. \tag{28}$$

Since Ψ is arbitrary, (28) reduces to the zero-curvature equation

$$U_t-V_x+[U,V]=0. \tag{29}$$

In particular, we take the isospectral problem

$$\Psi_x=[U,\Psi],\lambda_t=0,$$

$$U=-e_1(1)+u_1(e_2(0)+e_3(0))+\frac{u_2}{2}e_1(0)+u_3e_4(0)+u_4e_5(0), \tag{30}$$

$$V=\sum_{m=0}^{\infty}(a_me_1(-m)+b_me_2(-m)+c_me_3(-m)+d_me_4(-m)+f_me_5(-m)).$$

Solving the adjoint representation equation

$$V_x=[U,V], \tag{31}$$

yields that

$$\begin{gathered}a_{mx}=u_1(c_m-b_m),b_{mx}=-2b_{m+1}-2u_1a_m+u_2b_m,c_{mx}=2c_{m+1}+2u_1a_m-u_2c_m,\\ d_{m+1}=u_1f_m+\frac{u_2}{2}d_m-u_3a_m-u_4b_m-d_{mx},\\ f_{mx}=f_{m+1}+u_1d_m-\frac{u_2}{2}f_m-u_3c_m+u_4a_m,\\ a_0=-1,b_0=c_0=d_0=f_0=0,a_1=0,b_1=c_1=u_1,d_1=u_3,f_1=-u_4.\end{gathered} \tag{32}$$

Set

$$\begin{cases}V_{1+}^{(n)}=\\ \displaystyle\sum_{m=0}^{n}(a_me_1(n-m)+b_me_2(n-m)+c_me_3(n-m)+d_me_4(n-m)+f_me_5(n-m)).\\ V_{1-}^{(n)}=\lambda^nV-V_{1+}^{(n)}\end{cases}$$

Then we have

$$-V_{1+x}^{(n)}+[U,V_{1+}^{(n)}]=V_{1-x}^{(n)}-[U,V_{1-}^{(n)}]. \tag{33}$$

Note that the terms in the left-hand side of (33) are of degree $\geqslant 0$, while the terms of the right-hand side are of degree $\leqslant 0$. Thus by using Tu-model, we have

$$-V_{1+x}^{(n)}+[U,V_{1+}^{(n)}]=2b_{n+1}e_2(0)-2c_{n+1}e_3(0)+d_{n+1}e_4(0)-f_{n+1}e_5(0).$$

In terms of (21), taking $V^{(n)}=V_{1+}^{(n)}+1/2u_1(b_{n+1}+c_{n+1})e_1(0)$, we have

$$-V_x^{(n)}+[u,V^{(n)}]=(b_{n+1}-c_{n+1})(e_2(0)+e_3(0))-\left(\frac{1}{2u_1}(b_{n+1}+c_{n+1})\right)_x e_1(0)$$
$$+\left(d_{n+1}-\frac{u_3}{2u_1}(b_{n+1}+c_{n+1})\right)e_4(0)+\left(\frac{u_4}{2u_1}(b_{n+1}+c_{n+1})-f_{n+1}\right)e_5(0).$$

The zero-curvature equation (29) determines the system

$$u_t=\begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix}_t=\begin{pmatrix}c_{n+1}-b_{n+1}\\\left(\frac{1}{u_1}(b_{n+1}+c_{n+1})\right)_x\\-d_{n+1}+\frac{u_3}{2u_1}(b_{n+1}+c_{n+1})\\f_{n+1}-\frac{u_4}{2u_1}(b_{n+1}+c_{n+1})\end{pmatrix}=\begin{pmatrix}\frac{1}{u_1}a_{n+1,x}\\\left(\frac{1}{u_1}(b_{n+1}+c_{n+1})\right)_x\\-d_{n+1}+\frac{u_3}{2u_1}(b_{n+1}+c_{n+1})\\f_{n+1}-\frac{u_4}{2u_1}(b_{n+1}+c_{n+1})\end{pmatrix}$$
$$=\begin{pmatrix}0&u_1^{-1}\partial&0&0\\\partial u_1^{-1}&0&0&0\\\frac{u_3}{2u_1}&0&-1&0\\-\frac{u_4}{2u_1}&0&0&-1\end{pmatrix}\begin{pmatrix}b_{n+1}+c_{n+1}\\a_{n+1}\\d_{n+1}\\f_{n+1}\end{pmatrix}=J\begin{pmatrix}b_{n+1}+c_{n+1}\\a_{n+1}\\d_{n+1}\\f_{n+1}\end{pmatrix}. \tag{34}$$

From (32), we have

$$\begin{pmatrix}b_{n+1}+c_{n+1}\\a_{n+1}\\d_{n+1}\\f_{n+1}\end{pmatrix}=\frac{1}{2}\begin{pmatrix}u_2&\partial u_1^{-1}\partial-4u_1&0&0\\\partial^{-1}u_1\partial&\partial^{-1}u_2\partial&0&0\\-u_4&u_4u_1^{-1}\partial-2u_3&u_2-2\partial&2u_1\\u_3&u_3u_1^{-1}\partial-2u_4&-2u_1&u_2+2\partial\end{pmatrix}\begin{pmatrix}b_n+c_n\\a_n\\d_n\\f_n\end{pmatrix}$$
$$=L\begin{pmatrix}b_n+c_n\\a_n\\d_n\\f_n\end{pmatrix}. \tag{35}$$

In terms of (35), the hierarchy (34) reduces to the following:

$$u_t=\begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix}_t=JL^n\begin{pmatrix}b_1+c_1\\a_1\\d_1\\f_1\end{pmatrix}. \tag{36}$$

The hierarchy (36) is derived from the zero-curvature equation (29), therefore, it is integrable. Comparison J and L in (36) with those in (20), we see that (36) is integrable coupling of the TD hierarchy (20).

IV. CONCLUDING REMARKS

This paper proposed a new method—called a direct method to find integrable couplings of evolution equations, which developed the existed method for seeking for integrable couplings in Refs. 1–3. However, one open problem remains. The integrable couplings obtained by the direct method are integrable in the Lax sense. Can we generalize the well-known trace identity into the loop algebra $\tilde{A}_2$ so that the integrable couplings which are obtained by our method are integrable in the Liouville sense? Can we use the similar method to discover the integrable couplings of BPT hierarchy? These are problems to tackle in future.

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Propagator, tree-level unitarity and effective nonrelativistic potential for higher-derivative gravity theories in *D* dimensions

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A prescription for computing the propagator for D-dimensional higher-derivative gravity theories, based on the Barnes–Rivers operators, is presented. A systematic study of the tree-level unitarity of these theories is developed and the agreement of their linearized versions with Newton's law is investigated by computing the corresponding effective nonrelativistic potential. Three-dimensional quadratic gravity with a gravitational Chern–Simons term is also analyzed. A discussion on the issue of light bending within the framework of both D-dimensional quadratic gravity and three-dimensional quadratic gravity with a Chern–Simons term is provided as well. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1415743]

I. INTRODUCTION

Undoubtedly, Einstein's field theory accounts very well for all known macroscopic gravitational phenomena. However, as a quantum theory it is less satisfactory: it has an S matrix which, despite being finite at the one-loop level,[1] diverges at the two-loop order.[2] This is not surprising, since one of the most difficult field theories when it comes to quantization is certainly the theory of the space–time structure itself. It is not known what the correct quantum theory of gravitation is.

Now, as is well known, the four-dimensional space–time is the most problematic place for a quantum field theory to live. Indeed, quantum field theories are notorious for being ill defined in four-dimensional space–time but can often be handled in space–times of a different dimensionality. Dimensional regularization is a common example of such a procedure: results that are divergent in four dimensions are convergent for $D>4$. The divergences of the four-dimensional theory are removed by considering our space–time as a limit $D\to 4$ of higher-dimensional space–times.[3] On the other side of the dimensionality spectrum, there are field theories in space–times with $2\leqslant D<4$. In some cases, such quantum models are exactly soluble and provide a valuable insight into the clockwork of quantum field theory.

In this vein, here we study—at the tree level—various higher-derivative gravity theories. First, we shall consider gravitational theories which will be called, for short, D-dimensional higher-derivative gravity theories. These theories share some basic points with general relativity:

(i) General covariance and
(ii) the action is extremized under variation of the metric.

On the other hand, they differ from general relativity in the following respects:

(i) The field equations for the metric are of fourth order.

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(ii) Space–time is allowed to have any number of dimensions, which is a condition absolutely necessary in the context of string theory.

Quadratic gravity in four dimensions is the most typical example of such a theory.[4–6] At this point it is reasonable to pose the question: What is the use of probing into these theories? Before answering this question, let us comment, in passing, on some results recently obtained concerning quadratic gravity in four dimensions. In a series of papers on the photon propagation around a massive body in quadratic theories of gravitation it was shown that, unlike Einstein's gravity, quadratic gravity produces dispersive photon propagation.[7–9] To be more specific, quadratic gravity produces energy-dependent photon scattering. An interesting consequence of this fact is that gravity's rainbows and higher-derivative gravity can coexist without conflict.[9] In this sense quadratic gravity is closer to quantum electrodynamics than any currently known gravitational theory. In fact, dispersive photon propagation is a trivial phenomenon in the context of QED. Based on the fact that the rainbow effect which is present in quadratic gravity is undetectable, nowadays it is possible to find a new constraint on the value of the contribution of the quadratic part. This is a very important result given the scarcity of observational constraints on gravitational theories. In addition, it was also found that the gravitational deflection predicted by quadratic gravity is always smaller than that predicted by Einstein's theory.[7–9] It is worth mentioning that the R^2 sector of the theory of gravitation with higher derivatives does not contribute anything to the gravitational deflection.[10,11] After this little digression we return to the question raised previously. Our motivation for studying D-dimensional higher-derivative gravity theories is to try to answer, among other things, the following questions:

(i) Which is the lowest dimension in which these theories make sense?
(ii) Are these D-dimensional theories unitary at the tree level?
(iii) Is the massless excitation a dynamical degree of freedom in any dimension?
(iv) Does D-dimensional linearized quadratic gravity agree with Newton's theory in the limiting case of motion at low velocity in a weak gravitational field?
(v) Is the gravitational deflection within the context of the theories mentioned above greater or smaller than that related to the corresponding Einstein's theory?

Second, we shall analyze three-dimensional quadratic gravity with a gravitational Chern–Simons term. Now the action is extremized *à la* Palatini (independently varied connection). In other words, the propagation of the metric and affine structures of space–time are independent. Our goal here is, first of all, to find out how the nature of the field excitations is affected by the addition of a gravitational Chern–Simons term to the Lagrangian concerning three-dimensional quadratic gravity. Second, we shall study the tree-level unitarity of the above theory, the nonrelativistic limit of its linearized version and light bending within the framework of the same.

The plan of this work is as follows. In Sec. II we find the appropriate Lagrangian for computing the propagator concerning D-dimensional quadratic gravity. In Sec. III we present an algorithm for computing the propagator for D-dimensional higher-derivative gravity theories based on the Barnes–Rivers operators.[12–16] Using this prescription we get the propagator for D-dimensional quadratic gravity in an unconventional gauge. From this result we obtain in a straightforward way the propagator in a series of interesting gauges which for $D=4$ reduce to well known results which are broadly used in the literature.[17] In Sec. IV we study in a systematic way the tree-level unitarity of D-dimensional higher-derivative gravity theories. It is shown that for $D>2$ quadratic gravity is nonunitary at the tree level. On the other hand, we get that D-dimensional $R+R^2$ gravity is unitary at the tree level for $D>2$. Section V is devoted to the study of the effective nonrelativistic potential for D-dimensional quadratic gravity. An expression for computing this potential is obtained for $D>2$ and from that we get, in particular, the potential for three-dimensional linearized quadratic gravity. Unlike the Newtonian potential, this potential is well behaved: it is finite at the origin and zero at infinity. In Sec. VI we analyze the gravitational deflection in the framework of D-dimensional quadratic gravity. Section VII deals with three-

dimensional quadratic gravity with a gravitational Chern–Simons term. Finally, a summary of the main results is presented in Sec. VIII.

In our notation the signature is $(+-\cdots-)$. The curvature tensor is defined by $R^{\alpha}_{\beta\gamma\delta}=-\partial_{\delta}\Gamma^{\alpha}_{\beta\gamma}+\cdots$, the Ricci tensor by $R_{\mu\nu}=R^{\alpha}_{\mu\nu\alpha}$, and the curvature scalar by $R=g^{\mu\nu}R_{\mu\nu}$, where $g_{\mu\nu}$ is the metric tensor. Natural units are used throughout.

II. FINDING THE APPROPRIATE LAGRANGIAN FOR COMPUTING THE PROPAGATOR CONCERNING *D*-DIMENSIONAL QUADRATIC GRAVITY

The action for quadratic gravity in $D>1$ dimensions is given by

$$I=\int d^{D}x\sqrt{(-1)^{D-1}g}\left[\frac{2R}{\kappa^{2}}+\frac{\alpha}{2}R^{2}+\frac{\beta}{2}R^{2}_{\mu\nu}+\frac{\gamma}{2}R^{2}_{\mu\nu\rho\sigma}+\frac{\delta}{2}\Box R\right], \tag{1}$$

where κ^{2} is a suitable constant with dimension L^{D-2} which in four dimensions is equal to $32\pi G$, with G being Newton's constant, and α, β, γ and δ are constants with dimension L^{4-D}. The $\Box R$ term in this action is manifestly a total covariant divergence and can be ignored. For $D=1$ the space is flat and all the tensors $R_{\mu\nu\alpha\beta}$, $R_{\mu\nu}$, R identically vanish. Of course, there can be no dynamics in a space which does not possess both a spacelike and a timelike dimension. The lowest dimension in which the quadratic theory makes sense is thus $D=2$.

Proposition 1: We can drop out the $R^{2}_{\mu\nu\rho\sigma}$ term of the linearized Lagrangian related to gravity with higher derivatives in dimensions higher than second.

Proof: Let $\mathcal{L}^{1}(\mathcal{L}^{2})$ be the Lagrangian corresponding to the gravity theory without (with) the $R^{2}_{\mu\nu\rho\sigma}$ term, namely,

$$\mathcal{L}^{1}\equiv\sqrt{(-1)^{D-1}g}\left[\frac{2R}{\kappa^{2}}+\frac{\alpha}{2}R^{2}+\frac{\beta}{2}R^{2}_{\mu\nu}\right], \tag{2}$$

$$\mathcal{L}^{2}\equiv\sqrt{(-1)^{D-1}g}\left[\frac{2R}{\kappa^{2}}+\frac{\alpha}{2}R^{2}+\frac{\beta}{2}R^{2}_{\mu\nu}+\frac{\gamma}{2}R^{2}_{\mu\nu\rho\sigma}\right]. \tag{3}$$

Decomposing the metric, $g_{\mu\nu}$, as

$$g_{\mu\nu}=\eta_{\mu\nu}+\kappa h_{\mu\nu}, \tag{4}$$

where $\eta_{\mu\nu}$ is the Minkowski metric, and inserting (4) into (2) and (3) yields

$$\mathcal{L}^{1}_{lin.}=\frac{b}{4}[\Box h_{\mu\nu}\Box h^{\mu\nu}-(A^{\mu}_{,\mu})^{2}-F^{2}_{\mu\nu}+(1+4c)(A^{,\alpha}_{\alpha}-\Box\phi)^{2}]-\frac{1}{2}[h^{\mu\nu}\Box h_{\mu\nu}+A^{2}_{\nu}+(A_{\nu}-\phi_{,\nu})^{2}], \tag{5}$$

$$\mathcal{L}^{2}_{lin.}=\left(\frac{b}{4}+d\right)\left[\Box h_{\mu\nu}\Box h^{\mu\nu}-(A^{\mu}_{,\mu})^{2}-F^{2}_{\mu\nu}+\frac{(b/4)\,(1+4c)}{b/4+d}(A^{,\alpha}_{\alpha}-\Box\phi)^{2}\right]-\frac{1}{2}[h^{\mu\nu}\Box h_{\mu\nu}+A^{2}_{\nu}+(A_{\nu}-\phi_{,\nu})^{2}],$$

where $A^{\mu}\equiv h^{\mu\nu}_{,\nu}$, $\phi\equiv h$, $F_{\mu\nu}=A_{\mu,\nu}-A_{\nu,\mu}$, $b\equiv\beta\kappa^{2}/2$, $c\equiv\alpha/\beta$, and $d\equiv\gamma\kappa^{2}/2$. Indices are lowered (raised) using $\eta_{\mu\nu}(\eta^{\mu\nu})$. □

It is worth mentioning that we could have arrived at the conclusion that the $R^{2}_{\mu\nu\rho\sigma}$ term need never be considered in calculating the propagator by simply noting that the linearized Gauss–Bonet invariant is a total derivative in any space–time dimension, the restriction to $D=4$ coming in only when we take the full nonlinear structure into account.

Thus, we come to the conclusion that the appropriate Lagrangian for computing the propagator concerning quadratic gravity in $D>2$ dimensions is

$$\overline{\mathcal{L}}=\sqrt{(-1)^{D-1}g}\left[\frac{2R}{\kappa^2}+\frac{\alpha}{2}R^2+\frac{\beta}{2}R_{\mu\nu}^2\right]. \tag{6}$$

Proposition 2: In two dimensions

$$\frac{\alpha}{2}R^2+\frac{\beta}{2}R_{\mu\nu}^2+\frac{\gamma}{2}R_{\mu\nu\rho\sigma}^2=\left(\frac{\alpha}{2}+\frac{\beta}{4}+\frac{\gamma}{2}\right)R^2.$$

Proof: In two dimensions both the Riemann tensor and the Ricci tensor can be expressed in terms of the curvature scalar. Indeed,[18]

$$R_{\mu\nu\rho\sigma}=\tfrac{1}{2}R(g_{\mu\sigma}g_{\nu\rho}-g_{\mu\rho}g_{\nu\sigma}),$$

and

$$R_{\mu\nu}=\tfrac{1}{2}Rg_{\mu\nu}.$$

Therefore,

$$\frac{\alpha}{2}R^2+\frac{\beta}{2}R_{\mu\nu}^2+\frac{\gamma}{2}R_{\mu\nu\rho\sigma}^2=\frac{\alpha}{2}R^2+\frac{\beta}{2}\frac{R^2}{2}+\frac{\gamma}{2}R^2=\left(\frac{\alpha}{2}+\frac{\beta}{4}+\frac{\gamma}{2}\right)R^2.$$

□

Obviously, for $D=2$ the suitable Lagrangian for calculating the propagator related to quadratic gravity is $\overline{\mathcal{L}}=\sqrt{-g}[2R/\kappa^2+(\alpha/2)R^2]$. Nonetheless, we will not discuss this theory here. From now on we shall assume that $D>2$.

III. FINDING THE PROPAGATOR FOR *D*-DIMENSIONAL HIGHER-DERIVATIVE GRAVITY THEORIES

We begin by describing a prescription for computing the propagator for gravity theories with higher derivatives in $D>2$ dimensions. The algorithm is used afterward to get the propagator for D-dimensional quadratic gravity in an unconventional gauge. From this result we obtain the propagator in a series of gauges which in the $D=4$ case reduce to well known gauges that are widely used in the literature.[17]

A. The prescription

Let $\overline{\mathcal{L}}$ be the Lagrangian for any metric theory of gravity with higher derivatives. To compute the graviton propagator we need the bilinear part of this Lagrangian. The latter is obtained by decomposing the metric, $g_{\mu\nu}$, as in (4), and inserting (4) into $\overline{\mathcal{L}}$. Let $\mathcal{L}_g$ be the resulting Lagrangian. In the specific case of gauge-invariant theories, we add to $\mathcal{L}_g$ a gauge-fixing Lagrangian $\mathcal{L}_{gf}$. Accordingly, $\mathcal{L}=\mathcal{L}_g+\mathcal{L}_{gf}$ can be written as

$$\mathcal{L}=\tfrac{1}{2}h^{\mu\nu}\mathcal{O}_{\mu\nu,\rho\sigma}h^{\rho\sigma}. \tag{7}$$

In performing these calculations it is extremely convenient to work in terms of the Barnes–Rivers operators[12–16] in the space of symmetric rank-two tensors. The complete set of D-dimensional operators is given by

$$P^1_{\mu\nu,\rho\sigma}=\tfrac{1}{2}(\theta_{\mu\rho}\omega_{\nu\sigma}+\theta_{\mu\sigma}\omega_{\nu\rho}+\theta_{\nu\rho}\omega_{\mu\sigma}+\theta_{\nu\sigma}\omega_{\mu\rho}),$$

$$P^2_{\mu\nu,\rho\sigma}=\frac{1}{2}(\theta_{\mu\rho}\theta_{\nu\sigma}+\theta_{\mu\sigma}\theta_{\nu\rho})-\frac{1}{D-1}\theta_{\mu\nu}\theta_{\rho\sigma},$$

$$P^0_{\mu\nu,\rho\sigma}=\frac{1}{D-1}\,\theta_{\mu\nu}\theta_{\rho\sigma},$$

$$\overline{P}^0_{\mu\nu,\rho\sigma}=\omega_{\mu\nu}\omega_{\rho\sigma},$$

$$\bar{\bar{P}}^0_{\mu\nu,\rho\sigma}=\theta_{\mu\nu}\omega_{\rho\sigma}+\omega_{\mu\nu}\theta_{\rho\sigma},$$

where $\theta_{\mu\nu}$ and $\omega_{\mu\nu}$ are the usual transverse and longitudinal vector projection operators

$$\theta_{\mu\nu}=\eta_{\mu\nu}-\frac{k_\mu k_\nu}{k^2},\quad \omega_{\mu\nu}=\frac{k_\mu k_\nu}{k^2},$$

which satisfy the relations

$$\theta_{\mu\rho}\theta^\rho_\nu=\theta_{\mu\nu},\quad \omega_{\mu\rho}\omega^\rho_\nu=\omega_{\mu\nu},\quad \theta_{\mu\rho}\omega^\rho_\nu=0.$$

Here k_μ is the momentum of the graviton exchanged and $k^2\equiv k_\mu k^\mu$.

The set of operators $\{P^1,P^2,P^0,\overline{P}^0\}$ is a complete set of projection operators for symmetric rank-two tensors, i.e., they are idempotent, mutually orthogonal and satisfy the completness relation

$$[P^1+P^2+P^0+\overline{P}^0]_{\mu\nu,\rho\sigma}=\tfrac{1}{2}(\eta_{\mu\rho}\eta_{\nu\sigma}+\eta_{\mu\sigma}\eta_{\nu\rho})\equiv I_{\mu\nu,\rho\sigma}.$$

In the rest frame of a massive tensor field, the family of operators $\{P^1,P^2,P^0,\overline{P}^0\}$ project out the spin-1, spin-2, and two spin-0 parts of the field. The operator $\bar{\bar{P}}^0$, in turn, is nothing but the sum of two spin-0 transfer operators, namely,

$$\bar{\bar{P}}^0_{\mu\nu,\rho\sigma}\equiv[P^{\theta\omega}+P^{\omega\theta}]_{\mu\nu,\rho\sigma},$$

where $P^{\theta\omega}_{\mu\nu,\rho\sigma}\equiv\theta_{\mu\nu}\omega_{\rho\sigma}$ and $P^{\omega\theta}_{\mu\nu,\rho\sigma}\equiv\omega_{\mu\nu}\theta_{\rho\sigma}$. Its multiplicative table is given by

$$\bar{\bar{P}}^0P^1=P^1\bar{\bar{P}}^0=\bar{\bar{P}}^0P^2=P^2\bar{\bar{P}}^0=O,$$

$$(\bar{\bar{P}}^0)^2=(D-1)(P^0+\overline{P}^0),$$

$$P^0\bar{\bar{P}}^0=\bar{\bar{P}}^0\overline{P}^0=P^{\theta\omega},$$

$$\overline{P}^0\bar{\bar{P}}^0=\bar{\bar{P}}^0P^0=P^{\omega\theta},$$

where O is the null operator.

The expansion of the operator $\mathcal{O}$ in the basis $\{P^1,P^2,P^0,\overline{P}^0,\bar{\bar{P}}^0\}$ is trivially obtained using the following tensorial identities:

$$\tfrac{1}{2}(\eta_{\mu\rho}\eta_{\nu\sigma}+\eta_{\mu\sigma}\eta_{\nu\rho})=[P^1+P^2+P^0+\overline{P}^0]_{\mu\nu,\rho\sigma},$$

$$\eta_{\mu\nu}\eta_{\rho\sigma}=[(D-1)P^0+\overline{P}^0+\bar{\bar{P}}^0]_{\mu\nu,\rho\sigma},$$

$$\frac{1}{k^2}(\eta_{\mu\rho}k_\nu k_\sigma+\eta_{\mu\sigma}k_\nu k_\rho+\eta_{\nu\rho}k_\mu k_\sigma+\eta_{\nu\sigma}k_\mu k_\rho)=[2P^1+4\overline{P}^0]_{\mu\nu,\rho\sigma},\tag{8}$$

$$\frac{1}{k^2}(\eta_{\mu\nu}k_\rho k_\sigma+\eta_{\rho\sigma}k_\mu k_\nu)=[\bar{\bar{P}}^0+2\overline{P}^0]_{\mu\nu,\rho\sigma},$$

$$\frac{1}{k^4}(k_\mu k_\nu k_\rho k_\sigma)=\overline{P}^0_{\mu\nu,\rho\sigma}.$$

The identities,

$$P^2_{\mu\nu,\rho\sigma}=\frac{1}{2}(\eta_{\mu\rho}\eta_{\nu\sigma}+\eta_{\mu\sigma}\eta_{\nu\rho})-\frac{1}{D-1}\eta_{\mu\nu}\eta_{\rho\sigma}-\left[P^1+\frac{D-2}{D-1}\overline{P}^0-\frac{1}{D-1}\bar{\bar{P}}^0\right]_{\mu\nu,\rho\sigma},$$
$$P^0_{\mu\nu,\rho\sigma}=\frac{1}{D-1}\eta_{\mu\nu}\eta_{\rho\sigma}-\frac{1}{D-1}[\overline{P}^0+\bar{\bar{P}}^0]_{\mu\nu,\rho\sigma}, \tag{9}$$

in turn, greatly facilitate the task of casting the propagator in a form wherein the terms proportional to the graviton momentum are omitted, which in practice widely simplifies computations involving conserved currents.

We will not display the demonstrations of (8) and (9) since they follow straightforwardly from the very definition of the operators $P^1,\ldots,\bar{\bar{P}}^0$.

We are now ready to find the propagator, $\mathcal{O}^{-1}$. To accomplish this we have to invert the operator $\mathcal{O}$. Expanding the latter in the basis $\{P^1,P^2,P^0,\overline{P}^0,\bar{\bar{P}}^0\}$ with the help of the identities (8), we get

$$\mathcal{O}=x_1P^1+x_2P^2+x_0P^0+\overline{x}_0\overline{P}^0+\bar{\bar{x}}_0\bar{\bar{P}}^0.$$

Assume then that $\mathcal{O}^{-1}=y_1P^1+y_2P^2+y_0P^0+\overline{y}_0\overline{P}^0+\bar{\bar{y}}_0\bar{\bar{P}}^0$, where $y_1,y_2,\ldots,\bar{\bar{y}}_0$ are parameters to be determined. Since $\mathcal{O}\mathcal{O}^{-1}=I$, we promptly obtain the following set of simultaneous equations:

$$\begin{aligned}
x_1y_1&=1,\\
x_2y_2&=1,\\
x_0y_0+(D-1)\bar{\bar{x}}_0\bar{\bar{y}}_0&=1,\\
\overline{x}_0\overline{y}_0+(D-1)\bar{\bar{x}}_0\bar{\bar{y}}_0&=1,\\
\bar{\bar{x}}_0y_0+\overline{x}_0\bar{\bar{y}}_0&=0,\\
\bar{\bar{x}}_0\overline{y}_0+x_0\bar{\bar{y}}_0&=0.
\end{aligned} \tag{10}$$

Before going on we need a lemma.

Lemma: If $x_1\neq0$, $x_2\neq0$, *and* $[x_0\overline{x}_0-(D-1)\bar{\bar{x}}_0]\neq0$, *then (10) has one and only one solution.*

Proof: Row reducing the argumented matrix of the system (10) to echelon form yields

$$\begin{bmatrix}
x_1 & 0 & 0 & 0 & 0 & 1\\
0 & x_2 & 0 & 0 & 0 & 1\\
0 & 0 & x_0 & 0 & (D-1)\bar{\bar{x}}_0 & 1\\
0 & 0 & \bar{\bar{x}}_0 & 0 & \overline{x}_0 & 0\\
0 & 0 & 0 & \overline{x}_0 & (D-1)\bar{\bar{x}}_0 & 1\\
0 & 0 & 0 & \bar{\bar{x}}_0 & x_0 & 0
\end{bmatrix}\sim\begin{bmatrix}
x_1 & 0 & 0 & 0 & 0 & 1\\
0 & x_2 & 0 & 0 & 0 & 1\\
0 & 0 & x_0 & 0 & (D-1)\bar{\bar{x}}_0 & 1\\
0 & 0 & 0 & \overline{x}_0 & (D-1)\bar{\bar{x}}_0 & 1\\
0 & 0 & 0 & 0 & [x_0\overline{x}_0-(D-1)\bar{\bar{x}}_0^2] & -\bar{\bar{x}}_0\\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.$$

□

Therefore, the propagator is given by

$$\mathcal{O}^{-1}=\frac{1}{x_1}P^1+\frac{1}{x_2}P^2+\frac{1}{x_0\overline{x}_0-(D-1)\bar{\bar{x}}_0^2}[\overline{x}_0P^0+x_0\overline{P}^0-\bar{\bar{x}}_0\bar{\bar{P}}^0]. \tag{11}$$

In summary, the prescription for computing the propagator consists of the following procedures.

(1) Linearize the original Lagrangian using (4).
(2) Add to the previous result a suitable gauge-fixing Lagrangian. Obviously, we only do this in the case of gauge-invariant theories.
(3) Cast the resulting Lagrangian into the bilinear form $\mathcal{L}=\frac{1}{2}h^{\mu\nu}\mathcal{O}_{\mu\nu,\rho\sigma}h^{\rho\sigma}$.
(4) Find the coefficients $x_1,x_2,\ldots,\bar{\bar{x}}_0$ by expanding the operator $\mathcal{O}$ in the basis $\{P^1,P^2,P^0,\overline{P}^0,\bar{\bar{P}}^0\}$ with the help of the identities (8).
(5) Insert these coefficients in (11).

B. Propagator for *D*-dimensional quadratic gravity in an unconventional gauge

Let us then find the propagator by means of the prescription developed in Sec. III A. Of course, the linearization of (6) leads to (5). So, $\mathcal{L}_g\equiv\mathcal{L}^{1}_{lin.}$. Lagrangian (5) is invariant under the infinitesimal coordinate transformation $x^\mu\rightarrow x^\mu+\kappa\xi^\mu(x)$, where $\xi^\mu(x)$ is an infinitesimal vector field. It must be infinitesimal to avoid inconsistency with (4). Under this transformation we have from (4)

$$h_{\mu\nu}(x)\rightarrow h_{\mu\nu}(x)-\xi_{\mu,\nu}-\xi_{\nu,\mu}. \tag{12}$$

The presence of the local gauge symmetry (12) requires the addition of a gauge-fixing term, $\mathcal{L}_{gf}$, to Lagrangian (5). It is common practice to choose a linear combination of A_μ and $\phi_{,\mu}$ as gauge functions. However, looking at (5) we clearly see the presence not only of this linear combination but also of its curl ($F_{\mu\nu}$) and its divergence ($A^\mu_{,\mu}-\Box\phi$). Hence, we choose the following unconventional gauge-fixing Lagrangian,

$$\mathcal{L}_{gf}=\lambda_1(A_\nu-\lambda\phi_{,\nu})^2+\frac{b}{4}[\lambda_2(A^\mu_{,\mu}-\lambda\Box\phi)^2+\lambda_3F^2_{\mu\nu}],$$

where λ, λ_1, λ_2, and λ_3 are suitable gauge parameters. Casting the Lagrangian, $\mathcal{L}=\mathcal{L}_g+\mathcal{L}_{gf}$, into the bilinear form $\mathcal{L}=\frac{1}{2}h^{\mu\nu}\mathcal{O}_{\mu\nu,\rho\sigma}h^{\rho\sigma}$, and expanding the operator $\mathcal{O}$ in the basis $\{P^1,P^2,\ldots,\bar{\bar{P}}^0\}$ with the help of (8), we obtain

$$\mathcal{O}=x_1P^1+x_2P^2+x_0P^0+\overline{x}_0\overline{P}^0+\bar{\bar{x}}_0\bar{\bar{P}}^0,$$

whereupon

$$x_1\equiv\frac{b}{2}\left(\lambda_3k^4+\frac{2\lambda_1k^2}{b}\right),$$

$$x_2\equiv\frac{b}{2}\left(k^4+\frac{2k^2}{b}\right),$$

$$x_0\equiv\frac{b}{2}\left[Dk^4-\frac{2(D-2)k^2}{b}+4(D-1)k^4c+(D-1)k^4\lambda_2\lambda^2+\frac{4(D-1)k^2\lambda_1\lambda^2}{b}\right],$$

$$\overline{x}_0\equiv\frac{b}{2}\left(k^4\lambda_2-2k^4\lambda\lambda_2+\frac{4k^2\lambda_1}{b}-\frac{8k^2\lambda\lambda_1}{b}+k^4\lambda_2\lambda^2+\frac{4k^2\lambda_1\lambda^2}{b}\right),$$

$$\bar{\bar{x}}_0\equiv\frac{b}{2}\left(\frac{4k^2\lambda_1\lambda^2}{b}+k^4\lambda_2\lambda^2-k^4\lambda\lambda_2-\frac{4k^2\lambda\lambda_1}{b}\right).$$

The propagator in momentum space is given by (11). From this result we can find the propagator in a series of interesting gauges, by judiciously choosing the parameters λ, λ_1, λ_2, and λ_3. We list below the most important covariant gauges that result from such choices.

(1) *Julve–Tonin gauge* ($\lambda=0$)*:*[19]

$$\mathcal{L}_{gf}=\lambda_1 A_\nu^2+\frac{b}{4}[\lambda_2(A^\mu_{,\mu})^2+\lambda_3 F^2_{\mu\nu}].$$

Propagator:

$$\mathcal{O}^{-1}=\frac{m_1^2}{k^2(m_1^2\lambda_1-\lambda_3k^2)}P^1+\frac{m_1^2}{k^2(m_1^2-k^2)}P^2+\frac{m_0^2}{2k^2[k^2-[(D-2)/2]\,m_0^2]}P^0 + \frac{m_1^2}{(2m_1^2\lambda_1-\lambda_2k^2)k^2}\overline{P}^0, \tag{13}$$

where

$$m_0^2\equiv\frac{2}{D\beta\kappa^2/4+(D-1)\kappa^2\alpha},\quad m_1^2\equiv-\frac{4}{\beta\kappa^2}.$$

Absence of tachyons requires $\beta<0$ and $(D-1)\alpha+\beta D/4>0$. Note that the choice $\lambda=0$ gives a propagator that only contains the spin-projection operators, i.e., P^1, P^2, P^0, $\overline{P}^0$, and it gives also a propagator all parts of which behave like k^{-4}.

(2) *de Donder gauge* ($\lambda_2=\lambda_3=0,\lambda=\frac{1}{2}$)*:*

$$\mathcal{L}_{gf}=\lambda_1(A_\nu-\tfrac{1}{2}\partial_\nu\phi)^2.$$

Propagator:

$$\mathcal{O}^{-1}=\frac{1}{\lambda_1k^2}P^1+\frac{m_1^2}{k^2(m_1^2-k^2)}P^2+\frac{m_0^2}{2k^2[k^2-[(D-2)/2]\,m_0^2]}P^0 +\left[\frac{2}{\lambda_1k^2}+\frac{(D-1)m_0^2}{2k^2[k^2-[(D-2)/2]\,m_0^2]}\right]\overline{P}^0+\frac{m_0^2}{2k^2[k^2-[(D-2)/2]\,m_0^2]}\bar{\bar{P}}^0.$$

(3) *Feynman gauge* ($\lambda_2=\lambda_3=0,\lambda_1=1,\lambda=\frac{1}{2}$):

$$\mathcal{L}_{gf}=(A_\nu-\tfrac{1}{2}\partial_\nu\phi)^2.$$

Propagator:

$$\mathcal{O}^{-1}=\frac{1}{k^2}P^1+\frac{m_1^2}{k^2(m_1^2-k^2)}P^2+\frac{m_0^2}{2k^2[k^2-[(D-2)/2]\,m_0^2]}P^0 +\left[\frac{2}{k^2}+\frac{(D-1)m_0^2}{2k^2[k^2-[(D-2)/2]\,m_0^2]}\right]\overline{P}^0+\frac{m_0^2}{2k^2[k^2-[(D-2)/2]\,m_0^2]}\bar{\bar{P}}^0.$$

IV. A SYSTEMATIC STUDY OF TREE-LEVEL UNITARITY

Now we present a method for analyzing the unitarity at the tree level of D-dimensional higher-derivative gravity theories.

In order to verify whether ghosts and tachyons are absent in a given theory of gravity with higher derivatives we require that the corresponding propagator has only first poles at k^2-M^2

$=0$ with real masses M (no tachyons) and with positive residues (no ghosts).[20–22] Therefore, to probe the tree-level unitarity of D-dimensional higher-derivative gravity theories we couple the propagator to external conserved currents, $T^{\mu\nu}$, compatible with the symmetries of the theory, and afterward we examine the current-current amplitude at the poles. The transition amplitude in momentum space, in turn, can be cast in the form

$$\mathcal{A}=\mathsf{g}^2 T^{\mu\nu}\mathcal{O}^{-1}_{\mu\nu,\rho\sigma}T^{\rho\sigma}, \tag{14}$$

where g is the effective coupling constant of the theory. Note that only the spin-projectors P^2 and P^0 will give a non-null contribution to the current-current amplitude since $k_\mu T^{\mu\nu}=0$.

Let us then expand the sources in a suitable basis. The set of independent vectors in momentum space,

$$k^\mu\equiv(k^0,\mathbf{k}),\quad \tilde{k}^\mu\equiv(k^0,-\mathbf{k}),\quad \varepsilon_i^\mu\equiv(0,\vec{\epsilon}_i),\quad i=1,\ldots,D-2,$$

where $\vec{\epsilon}_1,\ldots,\vec{\epsilon}_{D-2}$ are mutually orthogonal unit vectors which are also orthogonal to $\mathbf{k}$, serves our purpose. Accordingly, the symmetric current tensor $T^{\mu\nu}(k)$ can be written as

$$T^{\mu\nu}=ak^\mu k^\nu+b\tilde{k}^\mu\tilde{k}^\nu+c^{ij}\varepsilon_i^{(\mu}\varepsilon_j^{\nu)}+dk^{(\mu}\tilde{k}^{\nu)}+e^i k^{(\mu}\varepsilon_i^{\nu)}+f^i\tilde{k}^{(\mu}\varepsilon_i^{\nu)}. \tag{15}$$

The current conservation, $k_\mu T^{\mu\nu}=0$, gives the following constraints for the coefficients a, b, d, e^i and f^i

$$ak^2+(k_0^2+\mathbf{k}^2)\frac{d}{2}=0, \tag{16}$$

$$b(k_0^2+\mathbf{k}^2)+d\frac{k^2}{2}=0, \tag{17}$$

$$e^i k^2+f^i(k_0^2+\mathbf{k}^2)=0. \tag{18}$$

If we saturate the indices of $T^{\mu\nu}$ with momenta k_μ, we obtain the equation $k_\mu k_\nu T^{\mu\nu}=0$, which yields a consistency relation for the coefficients a, b, and d:

$$ak^4+b(k_0^2+\mathbf{k}^2)^2+dk^2(k_0^2+\mathbf{k}^2)=0. \tag{19}$$

Now, all we have to do is to compute the residue of $\mathcal{A}$ at each first pole of the propagator and verify whether its sign is positive.

Proposition 3: Higher-derivative gravity is nonunitary at the tree level in $D>2$ dimensions. If $m_0^2>0$ $[D\beta/4+(D-1)\alpha>0]$ and $m_1^2>0(-\beta>0)$, the theory is nontachyonic and has one normal massless spin-2 particle, one massive spin-2 ghost and one normal massive spin-0 particle. The massless excitation is not a dynamical degree of freedom in $D=3$.

Proof: From (14) and (13) we promptly obtain

$$\begin{aligned}\mathcal{A}&=\mathsf{g}^2 T^{\mu\nu}\left\{\frac{m_1^2}{k^2(m_1^2-k^2)}P^2+\frac{m_0^2}{2k^2[k^2-(D-2)m_0^2/2]}P^0\right\}T^{\rho\sigma}\\&=\mathsf{g}^2\left\{\frac{T_{\mu\nu}T^{\mu\nu}-T^2/(D-2)}{k^2}-\frac{T_{\mu\nu}T^{\mu\nu}-T^2/(D-1)}{k^2-m_1^2}\right.\\&\quad\left.+\frac{T^2}{(D-1)(D-2)[k^2-(D-2)m_0^2/2]}\right\},\end{aligned} \tag{20}$$

where $T=\eta_{\mu\nu}T^{\mu\nu}$. Thus, we have two poles for the spin-2 sector, i.e., $k^2=0$, $k^2=m_1^2$, and one pole for the spin-0 sector, namely, $k^2=(D-2)m_0^2/2$. Let us then find the sign of the residue at these poles. We assume that D-dimensional quadratic gravity has no tachyons, which implies $m_0^2>0$ and $m_1^2>0$.

• *Pole* $k^2=0$. From (16)–(18) and (20), we get that the residue of $\mathcal{A}$ at the pole $k^2=0$ is

$$\text{Res}\,\mathcal{A}|_{k^2=0}=\mathrm{g}^2\left[(c^{ij})^2-\frac{(c^{ii})^2}{D-2}\right]_{k^2=0}.$$

Therefore, the massless excitation is not a dynamical degree of freedom in three dimensions. For $D>3$ the result above tells us that $\text{Res}\,\mathcal{A}|_{k^2=0}>0$.

• *Pole* $k^2=(D-2)m_0^2/2$. In this case

$$\text{Res}\,\mathcal{A}|_{k^2=(D-2)m_0^2/2}=\left[\frac{\mathrm{g}^2T^2}{(D-1)(D-2)}\right]_{k^2=(D-2)m_0^2/2},$$

which implies that the residue of the current-current amplitude at the pole $k^2=(D-2)m_0^2/2$ is always positive for $D>2$. Thence, the scalar massive particle is a physical one.

• *Pole* $k^2=m_1^2$. The residue of the transition amplitude at the pole $k^2=m_1^2$ is given by

$$\begin{aligned}\text{Res}\,\mathcal{A}|_{k^2=m_1^2}&=-\mathrm{g}^2\Bigg\{ab(k_0^2+\mathbf{k}^2)^2+b^2k^4+bdk^2(k_0^2+\mathbf{k}^2)+(c^{ij})^2-\frac{1}{2}(k_0^2+\mathbf{k}^2)e^if^i-\frac{k^2}{2}(f^i)^2\\&\quad-\frac{1}{D-1}[ak^2+bk^2-c^{ii}+d(k_0^2+\mathbf{k}^2)]^2\Bigg\}_{k^2=m_1^2},\\&=-\mathrm{g}^2\Bigg\{[(a-b)k^2]^2+(c^{ij})^2+\frac{k^2}{2}[(e^i)^2-(f^i)^2]-\frac{1}{D-1}[(b-a)k^2-c^{ii}]^2\Bigg\}_{k^2=m_1^2},\end{aligned}$$

where use has been made of (16)–(19). This expression can also be written as

$$\begin{aligned}\text{Res}\,\mathcal{A}|_{k^2=m_1^2}=-\mathrm{g}^2\Bigg\{&\frac{D-2}{D-1}[(a-b)k^2]^2+\left[(c^{ij})^2-\frac{(c^{ii})^2}{D-1}\right]+\frac{k^2}{2}[(e^i)^2-(f^i)^2]\\&-\frac{2}{D-1}(a-b)k^2c^{ii}\Bigg\}_{k^2=m_1^2}.\end{aligned}$$

Now, assuming as usual that $T\geqslant 0$, we get that $c^{ii}\leqslant 0$, which implies that $\text{Res}\,\mathcal{A}|_{k^2=m_1^2}<0$ for $D>2$. So, we have a nontachyonic massive spin-2 ghost in the propagator of higher-derivative gravity. In conclusion we way say that D-dimensional higher-derivative gravity is nonunitary at the tree level. □

Corollary 1: D-dimensional $R+R^2$ gravity is unitary at the tree level for $D>2$. In three dimensions the massless excitation is not a dynamical degree of freedom.

Proof: Clear. □

V. EFFECTIVE NONRELATIVISTIC POTENTIAL

In principle any relativistic theory of gravitation ought to agree with Newton's theory in the limiting case of motion at low velocity in a weak gravitational field. Accordingly it is worthwhile to probe whether D-dimensional linearized quadratic gravity leads to the right nonrelativistic law for gravitational interactions. To do this we compute the effective nonrelativistic potential for the interaction of two identical massive bosons of zero spin via a graviton exchange. The expression for the potential is

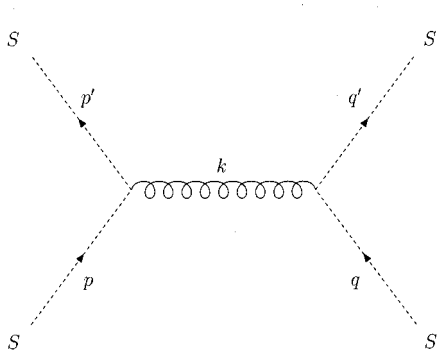

FIG. 1. One-graviton-exchange contribution to the scattering of two identical spinless massive bosons. S denotes a scalar particle with mass m.

$$U(r)=\frac{1}{4m^2}\,\frac{1}{(2\pi)^{D-1}}\int d^{D-1}\mathbf{k}\mathcal{M}_{N.R.}e^{-i\mathbf{k}\cdot\mathbf{r}}, \tag{21}$$

whereupon $\mathcal{M}_{N.R.}$ is the nonrelativistic limit of the Feynman amplitude for the process $S+S\rightarrow S+S$, where S stands for a spinless boson of mass m. The corresponding Feynman diagram is shown in Fig. 1.

The Lagrangian for the interaction of gravity with a free, massive scalar field $\tilde{\phi}$ is

$$\mathcal{L}_{int}=-\frac{\kappa h^{\mu\nu}}{2}\left[\partial_\mu\tilde{\phi}\partial_\nu\tilde{\phi}-\frac{1}{2}\,\eta_{\mu\nu}(\partial_\alpha\tilde{\phi}\partial^\alpha\tilde{\phi}-m^2\tilde{\phi}^2)\right].$$

From the previous expression the Feynman rule for the elementary vertex may readily be deduced. It is shown in Fig. 2. The invariant amplitude for the process shown in Fig. 1 is

$$\begin{aligned}\mathcal{M}=&\frac{m_1^2}{k^2(m_1^2-k^2)}\,\frac{\kappa^2}{2}\Bigg\{(p.q)(p'.q')+(p.q')(p'.q)+(p.p')(m^2-q.q')+(q.q')(m^2-p.p')\\&+\frac{D}{2}(m^2-p.p')(m^2-q.q')-\frac{1}{2(D-1)}[Dm^2-(D-2)p.p'][Dm^2-(D-2)q.q']\Bigg\}\\&+\frac{m_0^2}{k^2(k^2-[(D-2)/2]\,m_0^2)}\,\frac{\kappa^2}{8(D-1)}[Dm^2-(D-2)p.p'][Dm^2-(D-2)q.q'].\end{aligned}$$

In the nonrelativistic limit this expression reduces to

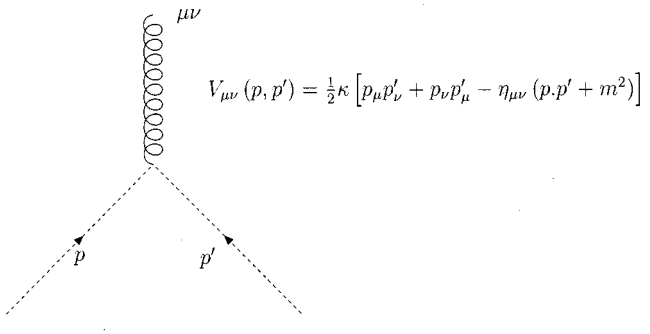

FIG. 2. The relevant Feynman rule for boson-boson interaction.

$$\mathcal{M}_{N.R.}=-\frac{D-2}{D-1}\frac{\kappa^2 m^4 m_1^2}{\mathbf{k}^2(\mathbf{k}^2+m_1^2)}+\frac{\kappa^2 m^4 m_0^2}{2(D-1)\mathbf{k}^2(\mathbf{k}^2+[(D-2)/2]\,m_0^2)}. \tag{22}$$

Substituting (22) into (21) we obtain[23]

$$U(r)=I_1+I_2,$$

where

$$I_1\equiv-\frac{\kappa^2 m^2 m_1^2}{4(2\pi)^{D-1}}\frac{D-2}{D-1}\int_0^\infty\int_0^\pi\cdots\int_0^\pi\int_0^\pi\int_0^{2\pi}\left[\frac{e^{-i\mathbf{k}.\mathbf{r}}}{\mathbf{k}^2(\mathbf{k}^2+m_1^2)}|\mathbf{k}|^{D-2}d|\mathbf{k}|\sin^{D-3}\right.$$
$$\left.\times\,\theta_{D-2}d\theta_{D-2}\cdots\sin^2\theta_3 d\theta_3\sin\theta_2\,d\theta_2 d\theta_1\right], \tag{23}$$

$$I_2\equiv\frac{\kappa^2 m^2 m_0^2}{8(2\pi)^{D-1}}\frac{1}{D-1}\int_0^\infty\int_0^\pi\cdots\int_0^\pi\int_0^\pi\int_0^{2\pi}\left[\frac{e^{-i\mathbf{k}.\mathbf{r}}}{\mathbf{k}^2(\mathbf{k}^2+[(D-2)/2]\,m_0^2)}|\mathbf{k}|^{D-2}d|\mathbf{k}|\sin^{D-3}\right.$$
$$\left.\times\,\theta_{D-2}d\theta_{D-2}\cdots\sin^2\theta_3 d\theta_3\sin\theta_2 d\theta_2 d\theta_1\right]. \tag{24}$$

Hence, the problem of computing the effective nonrelativistic potential was reduced to quadratures. We give in the following two examples to illustrate the efficacy of the method: linearized quadratic gravity in three and four dimensions, respectively.

• *Three-dimensional linearized quadratic gravity*. For $D=3$ the expressions (23) and (24) tell us that

$$U(r)=\frac{\kappa^2 m^2}{8(2\pi)^2}\int_0^\infty\left(\int_0^{2\pi}e^{-i|\mathbf{k}|r\cos\theta}d\theta\right)\left(\frac{1}{\mathbf{k}^2+m_1^2}-\frac{1}{\mathbf{k}^2+m_0^2/2}\right)|\mathbf{k}|d|\mathbf{k}|$$
$$=\frac{\kappa^2 m^2}{16\pi}\int_0^\infty\left(\frac{1}{\mathbf{k}^2+m_1^2}-\frac{1}{\mathbf{k}^2+m_0^2/2}\right)J_0(|\mathbf{k}|r)|\mathbf{k}|d|\mathbf{k}|,$$

where J_0 is the Bessel function of the first kind of order zero. Now, from a mathematical point of view, $\int_0^\infty[xJ_0(ax)/(x^2+b^2)]\,dx$ only makes sense if[24] $a>0$, $\mathrm{Re}\,b>0$. Accordingly, we assume that $m_0^2>0(\frac{3}{4}\beta+2\alpha>0)$ and $m_1^2>0(-\beta>0)$, which is nothing but the condition for absence of tachyons (both positive and negative energy) in the dynamical field. Performing the integration yields

$$U(r)=2\overline{G}m^2[K_0(m_1 r)-K_0(m_0 r/\sqrt{2})],$$

where K_0 is the modified Bessel function of the order of zero and $\overline{G}\equiv\kappa^2/32\pi$.

Therefore, the potential is given by

$$V(r)=2\overline{G}m[K_0(m_1 r)-K_0(m_0 r/\sqrt{2})].$$

Note that $V(r)$ behaves as $2\overline{G}m\ln(m_0/m_1\sqrt{2})$ at the origin and as $2\overline{G}m[\sqrt{\pi/2m_1 r}e^{-m_1 r}-\sqrt{\pi/m_0 r\sqrt{2}}e^{-m_0 r/\sqrt{2}}]$ asymptotically.[25]

Three comments are in order here:

(i) Unlike the Newtonian potential, $V_N=2Gm\ln r_0/r$, which has a logarithmic singularity at the origin and is unbounded at infinity, the potential concerning three-dimensional linearized quadratic gravity is extremely well behaved: it is finite at the origin and zero at the infinity.

(ii) $V(r)\to 0$ as m_0 and $m_1\to\infty$, confirming in this way the well known fact that the standard correspondence of three-dimensional linearized Einstein's theory with Newton's theory breaks down.[26]

(iii) Recently it was shown that the solution of the linearized field equations concerning three-dimensional linearized quadratic gravity, having as source a static point like mass m, is given by[27]

$$h_{00}=\frac{\kappa m}{8\pi}[K_0(m_1 r)-K_0(m_0 r/\sqrt{2})],$$

$$h_{11}=h_{22}=\frac{\kappa m}{8\pi}[2\ln r+K_0(m_1 r)+K_0(m_0 r/\sqrt{2})].$$

Since $V=\kappa h_{00}/2$, we see that this independent computation of the potential leads to the same result as that obtained via the effective nonrelativistic potential. The former is, in a sense, a major test of our semiclassical computation.

• *Four-dimensional linearized quadratic gravity*. The effective nonrelativistic potential is computed in this case as follows:

$$U(r)=\frac{\kappa^2 m^2}{6(2\pi)^2}\int_0^\infty\left(\int_0^\pi e^{-i|\mathbf{k}|r\cos\theta}\sin\theta d\theta\right)\left[-\frac{3}{4}\frac{1}{\mathbf{k}^2}+\frac{1}{\mathbf{k}^2+m_1^2}-\frac{1}{4(\mathbf{k}^2+m_0^2)}\right]\mathbf{k}^2 d|\mathbf{k}|$$

$$=\frac{\kappa^2 m^2}{6(2\pi)^2}\frac{1}{r}\mathrm{Im}\left[\int_{-\infty}^{+\infty}e^{ix}\left(-\frac{3}{4x}+\frac{x}{x^2+m_1^2r^2}-\frac{1}{4}\frac{x}{x^2+m_0^2r^2}\right)dx\right]. \tag{25}$$

Now, the condition for the existence of integrals like $\int_{-\infty}^{+\infty}[(x\sin x)/(x^2+a^2)]dx$ $(a\neq 0)$ is that $a>0$. In this case they can be easily evaluated by the method of contour integration. Therefore, assuming that $3\alpha+\beta>0$ and $-\beta>0$, which corresponds to the absence of tachyons in the dynamical field, we promptly obtain from (25)

$$U(r)=Gm^2\left[-\frac{1}{r}+\frac{4}{3}e^{-m_1 r}-\frac{1}{3}e^{-m_0 r}\right].$$

So, the potential for linearized higher-derivative gravity is given by the expression[4,7]

$$V(r)=Gm\left[-\frac{1}{r}+\frac{4}{3}\frac{e^{-m_1 r}}{r}-\frac{1}{3}\frac{e^{-m_0 r}}{r}\right],$$

which agrees asymptotically with Newton's law. At the origin it tends to the finite value $Gm((m_0-4m_1)/3)$.

From the computation of $V(r)$ for linearized quadratic gravity in three and four dimensions we learned that the existence of the potential is related to the absence of tachyons in the dynamical field. Consequently, we may conjecture that this is so in any dimension $D>2$. This issue will be treated elsewhere.

VI. GRAVITATIONAL DEFLECTION

Using the mathematical apparatus developed in the last sections we consider now the issue of light bending within the framework of D-dimensional quadratic gravity. Accordingly, let us con-

sider the interaction between a fixed source and a light ray. The associated energy-momentum tensors will be designated respectively as $T^{\mu\nu}$ and $F^{\mu\nu}$. The current-current amplitude for this process is given by

$$\mathcal{A}=\mathsf{g}^2 T_{\mu\nu}\mathcal{O}^{-1}_{\mu\nu,\rho\sigma}F^{\rho\sigma}.$$

But, on mass shell, $k_\mu T^{\mu\nu}=0$ and $k_\mu F^{\mu\nu}=0$, implying that only P^2 and P^0 will give a non-null contribution to the current-current amplitude. Therefore,

$$\mathcal{A}=\mathsf{g}^2 T^{\mu\nu}F^{\rho\sigma}\left[\frac{m_1^2}{k^2(m_1^2-k^2)}P^2+\frac{m_0^2}{2k^2[k^2-[(D-2)/2]m_0^2]}P^0\right]_{\mu\nu,\rho\sigma}.$$

Now, taking (9) into account and recalling that the energy-momentum tensor for light (electromagnetic radiation) is traceless, while $T^{\mu\nu}=\eta^{\mu 0}\eta^{\nu 0}T^{00}$ for a static source, we promptly obtain

$$\mathcal{A}=\mathsf{g}^2 T^{00}F^{00}\left[\frac{1}{k^2}-\frac{1}{k^2-m_1^2}\right].$$

Since $\mathsf{g}^2T^{00}F^{00}/k^2$ is precisely the current-current amplitude for the interaction between a fixed source and a light ray in the context of D-dimensional linearized general relativity, we come to the conclusion that the gravitational deflection predicted by D-dimensional linearized quadratic gravity is always smaller than that predicted by D-dimensional linearized Einstein's theory.

Let us then discuss in more detail the result above in the particular case $D=3$. Proposition 3 tell us that the massless excitation is not a dynamical degree of freedom in three dimensions. Consequently, only $-\mathsf{g}^2T^{00}F^{00}/(k^2-m_1^2)$ will contribute to light deflection. Thus, we come to the surprising result that in the framework of three-dimensional linearized quadratic gravity a light ray is deflected upward instead of downward as its four-dimensional counterpart. This is, perhaps, a property peculiar to quadratic gravity in $D=3$. It is worth mentioning that a classical computation of the gravitational deflection[27] assures us of the correctness of our result which is based on a semiclassical approach.

VII. THREE-DIMENSIONAL QUADRATIC GRAVITY WITH A GRAVITATIONAL CHERN–SIMONS TERM

To conclude we consider quadratic gravity with a gravitational Chern–Simons term. The topological Chern–Simons Lagrangian is given by

$$\mathcal{L}_{C.S.}=\frac{1}{2\mu}\varepsilon^{\mu\nu\lambda}\left(R^{\alpha}_{\beta\mu\nu}\Gamma^{\beta}_{\alpha\lambda}-\frac{2}{3}\Gamma^{\alpha}_{\beta\mu}\Gamma^{\beta}_{\gamma\nu}\Gamma^{\gamma}_{\alpha\lambda}\right)=\frac{\varepsilon^{\lambda\mu\nu}}{\mu}\Gamma^{\rho}_{\sigma\lambda}\left(\partial_\mu\Gamma^{\sigma}_{\rho\nu}+\frac{2}{3}\Gamma^{\sigma}_{\omega\mu}\Gamma^{\omega}_{\nu\rho}\right), \tag{26}$$

where μ is a dimensionless parameter. Linearizing (26), we obtain

$$\mathcal{L}_{C.S.lin.}=\frac{1}{2}\frac{1}{M}h^{\mu\nu}\mathcal{P}_{\mu\nu,\rho\sigma}h^{\rho\sigma}, \tag{27}$$

where[28]

$$\mathcal{P}_{\mu\nu,\rho\sigma}\equiv\frac{\Box\partial^\lambda}{4}[\varepsilon_{\mu\lambda\rho}\theta_{\nu\sigma}+\varepsilon_{\mu\lambda\sigma}\theta_{\nu\rho}+\varepsilon_{\nu\lambda\rho}\theta_{\mu\sigma}+\varepsilon_{\nu\lambda\sigma}\theta_{\mu\rho}], \tag{28}$$

and $M\equiv\mu/\kappa^2$. In order to have a complete basis for the operator space of the field equations concerning higher-derivative gravity theories in three dimensions with a Chern–Simons term, we

TABLE I. Multiplication table for the three-dimensional operators P^1, P^2, P^0, $\overline{P}^0$, $\bar{\bar{P}}^0$, and P.

	P^1	P^2	P^0	$\overline{P}^0$	$\bar{\bar{P}}^0$	P
P^1	P^1	O	O	O	O	O
P^2	O	P^2	O	O	O	P
P^0	O	O	P^0	O	$P^{\theta\omega}$	O
$\overline{P}^0$	O	O	O	$\overline{P}^0$	$P^{\omega\theta}$	O
$\bar{\bar{P}}^0$	O	O	$P^{\omega\theta}$	$P^{\theta\omega}$	$2(P^0+\overline{P}^0)$	O
P	O	P	O	O	O	$-k^6P^2$

include in the collection of three-dimensional operators $\{P^1,P^2,P^0,\overline{P}^0,\bar{\bar{P}}^0\}$ (see Sec. III A) the operator P (28). The multiplication table for these operators is displayed in Table I.

We are now ready to compute the propagator. Expanding both operators $\mathcal{O}$ and $\mathcal{O}^{-1}$ in the basis $\{P^1,P^2,P^0,\overline{P}^0,\bar{\bar{P}}^0\}$, we obtain

$$\mathcal{O}=x_1P^1+x_2P^2+x_0P^0+\overline{x}_0\overline{P}^0+\bar{\bar{x}}_0\bar{\bar{P}}^0+pP,$$

$$\mathcal{O}^{-1}=y_1P^1+y_2P^2+y_0P^0+\overline{y}_0\overline{P}^0+\bar{\bar{y}}_0\bar{\bar{P}}^0+qP.$$

With the help of Table I and taking into account that $\mathcal{O}\mathcal{O}^{-1}=I$, we find that $y_1=1/x_1$, $y_2=x_2/(x_2^2-p^2k^6)$, $y_0=\overline{x}_0/(x_0\overline{x}_0-2\bar{\bar{x}}_0^2)$, $\overline{y}_0=x_0/(x_0\overline{x}_0-2\bar{\bar{x}}_0^2)$, $\bar{\bar{y}}_0=-\bar{\bar{x}}_0(x_0\overline{x}_0-2\bar{\bar{x}}_0^2)$, and $q=-p/(x_2^2-p^2k^6)$, while the propagator is given by

$$\mathcal{O}^{-1}=\frac{1}{x_1}P^1+\frac{x_2}{x_2^2-p^2k^6}P^2+\frac{\overline{x}_0}{x_0\overline{x}_0-2\bar{\bar{x}}_0^2}P^0+\frac{x_0}{x_0\overline{x}_0-2\bar{\bar{x}}_0^2}\overline{P}^0-\frac{\bar{\bar{x}}_0}{x_0\overline{x}_0-2\bar{\bar{x}}_0^2}\bar{\bar{P}}^0-\frac{p}{x_2^2-p^2k^6}P. \tag{29}$$

Accordingly, let us then find the propagator for quadratic gravity with a Chern–Simons term. This theory is defined by the Lagrangian

$$\overline{\mathcal{L}}=-\frac{2R\sqrt{g}}{\kappa^2}+\frac{\varepsilon^{\mu\nu\lambda}}{\mu}\Gamma^{\rho}_{\sigma\lambda}\left(\partial_\mu\Gamma^{\sigma}_{\rho\nu}+\frac{2}{3}\Gamma^{\sigma}_{\omega\mu}\Gamma^{\omega}_{\nu\rho}\right)+\left(\frac{\alpha}{2}R^2+\frac{\beta}{2}R^2_{\mu\nu}\right)\sqrt{g}.$$

In the Julve–Tonin gauge the operator $\mathcal{O}$ has the form

$$\mathcal{O}=-k^2\left(\lambda_1+\lambda_3\frac{b}{2}k^2\right)P^1+k^2\left(k^2\frac{b}{2}-1\right)P^2+\left[k^2+bk^4\left(\frac{3}{2}+4c\right)\right]P^0$$
$$-k^2\left(\frac{b}{2}\lambda_2k^2+2\lambda_1\right)\overline{P}^0+\frac{P}{M},$$

and the propagator is given by

$$\mathcal{O}^{-1}=\frac{-2}{k^2[2\lambda_1+b\lambda_3k^2]}P^1+\left[-\frac{1}{k^2}+\frac{1}{1+(bM_2^2/2)}\frac{1}{k^2-M_2^2}+\frac{1}{1+(bM_1^2/2)}\frac{1}{k^2-M_1^2}\right]P^2$$
$$+\left[\frac{1}{k^2}-\frac{1}{k^2-m^2}\right]P^0-\frac{1}{k^2[2\lambda_1+\lambda_2(b/2)k^2]}\overline{P}^0$$
$$-\left[\frac{4}{b^2M(M_1^2-M_2^2)}\left(\frac{1}{k^2-M_1^2}-\frac{1}{k^2-M_2^2}\right)\frac{1}{k^4}\right]P, \tag{30}$$

where

$$M_1^2 \equiv \left(\frac{2}{b^2M^2}\right)[1+bM^2+\sqrt{1+2bM^2}],$$

$$M_2^2 \equiv \left(\frac{2}{b^2M^2}\right)[1+bM^2-\sqrt{1+2bM^2}],$$

$$m^2 \equiv \frac{-1}{b\left(\frac{3}{2}+4c\right)}.$$

If we do not want tachyons in the dynamical field, we may choose, for instance, $b>0$ and $(\frac{3}{2}+4c)<0$. In this case the theory is causal at the tree level. In this vein we assume from now on m^2, M_1^2, M_2^2, and $M^2>0$.

We discuss in the following tree-level unitarity, nonrelativistic limit and gravitational deflection for quadratic-Chern-Simons gravity in $D=3$.

A. Tree-level unitarity

From (14) and (30) we obtain at once

$$\mathcal{A}=\mathrm{g}^2\left[\frac{2}{b^2}\frac{bM_2^2-2}{(M_2^2-M_1^2)M_2^2}\frac{T_{\mu\nu}T^{\mu\nu}-\frac{1}{2}T^2}{k^2-M_2^2}+\frac{2}{b^2}\frac{2-bM_1^2}{(M_2^2-M_1^2)M_1^2}\frac{T_{\mu\nu}T^{\mu\nu}-\frac{1}{2}T^2}{k^2-M_1^2}-\frac{\frac{1}{2}T^2}{k^2-m^2}\right.$$
$$\left.+\frac{4}{b^2M_1^2M_2^2}\frac{T^2-T_{\mu\nu}T^{\mu\nu}}{k^2}\right]. \tag{31}$$

Therefore, if $b>0$ and $(\frac{3}{2}+4c)<0$, (20) tells us that $\mathrm{Res}\,\mathcal{A}|_{k^2=M_1^2}>0$, $\mathrm{Res}\,\mathcal{A}|_{k^2=M_2^2}>0$, $\mathrm{Res}\,\mathcal{A}|_{k^2=m^2}<0$, and $\mathrm{Res}\,\mathcal{A}|_{k^2=0}=0$.

Proposition 4: Quadratic gravity with a gravitational Chern–Simons term is nonunitary at the tree level. If $b>0$ and $(\frac{3}{2}+4c)<0$, the theory in nontachyonic and has one normal massless spin-2 particle, one normal spin-2 particle of mass M_2, one normal spin-2 particle of mass M_1 and one spin-0 ghost of mass m. The massless excitation is not a dynamical degree of freedom.

Corollary 2: $R+R^2$ gravity with a Chern–Simons term is nonunitary at the tree level. If $\alpha<0$, the theory is nontachyonic and has one physical massless spin-2 particle, one physical particle of spin-2 and mass M and one spin-0 ghost of mass $m\equiv\sqrt{-1/2\alpha\kappa^2}$. The massless excitation is not a dynamical degree of freedom.

Proof: Clear. □

Therefore, we come to the conclusion that neither quadratic gravity with a Chern–Simons term nor $R+R^2$ gravity with a Chern–Simons term is unitary at the tree level.

A detailed comparison between three-dimensional quadratic gravity with quadratic gravity with a Chern–Simons term clearly shows that the harmless massive scalar mode of the former becomes a troublesome massive spin-0 ghost within the context of the latter, while the massive spin-2 ghost related to three-dimensional quadratic gravity is now replaced by two massive physical particles both of spin-2. On the other hand, if we make a comparison between three-dimensional $R+R^2$ gravity with $R+R^2$ gravity with a Chern–Simons term, we come to the conclusion that the gravitational Chern–Simons term is responsible for breaking down the unitarity of the former.

B. Nonrelativistic limit

In this case the invariant amplitude for the process $S+S\rightarrow S+S$, where S denotes a spinless boson of mass $\tilde{m}$, as well as for its nonrelativistic limit, are given respectively by

$$\mathcal{M}=\kappa^2\Bigg[-\frac{1}{2k^2}+\frac{1}{bM_2^2+2}\,\frac{1}{k^2-M_2^2}+\frac{1}{b^2M_1^2+2}\,\frac{1}{k^2-M_1^2}\Bigg]\times\Bigg[(p\cdot q)(p'\cdot q')+(p\cdot q')(p'\cdot q)$$
$$+p\cdot p'(\tilde{m}^2-q\cdot q')+(\tilde{m}^2-p\cdot p')q\cdot q'+\frac{3}{2}(\tilde{m}^2-q\cdot q')(\tilde{m}^2-p\cdot p')-\frac{1}{4}(3\tilde{m}^2-p\cdot p')$$
$$\times(3\tilde{m}^2-q\cdot q')\Bigg]+\frac{\kappa^2}{8}\Bigg\{(3\tilde{m}^2-p\cdot p')(3\tilde{m}^2-q\cdot q')\Bigg[\frac{1}{k^2}-\frac{1}{k^2-m^2}\Bigg]\Bigg\}$$

and

$$\mathcal{M}_{N.R.}=\kappa^2\tilde{m}^4\Bigg[\frac{1}{2}\,\frac{1}{\mathbf{k}^2+m^2}-\frac{1}{2+bM_2^2}\,\frac{1}{\mathbf{k}^2+M_2^2}-\frac{1}{2+bM_1^2}\,\frac{1}{\mathbf{k}^2+M_1^2}\Bigg]. \tag{32}$$

Inserting (32) into (21) and performing the integration yields

$$U(r)=2\tilde{m}^2\overline{G}\Bigg[K_0(rm)-\frac{1}{1+(bM_1^2/2)}K_0(rM_1)-\frac{1}{1+(bM_2^2/2)}K_0(rM_2)\Bigg].$$

As a result, the potential is given by the expression

$$V(r)=2\tilde{m}\overline{G}\Bigg[K_0(rm)-\frac{1}{1+(bM_1^2/2)}K_0(rM_1)-\frac{1}{1+(bM_2^2/2)}K_0(rM_2)\Bigg].$$

Note that $V(r)$ behaves as $2\tilde{m}\overline{G}\,\ln M_1^{1+(bM_1^2/2)}M_2^{1+(bM_2^2/2)}/m$ at the origin and as

$$2\tilde{m}\overline{G}\Bigg[\sqrt{\frac{\pi}{2mr}}e^{-rm}-\frac{1}{1+(bM_1^2/2)}\sqrt{\frac{\pi}{2M_1r}}e^{-M_1r}-\frac{1}{1+(bM_2^2/2)}\sqrt{\frac{\pi}{2M_2r}}e^{-M_2r}\Bigg]$$

asymptotically. Two comments are in order here:

(i) Unlike the Newtonian potential $V_N=2\overline{G}\tilde{m}\ln r_0/r_1$ which has a logarithmic singularity at the origin and is unbounded at infinity, the potential concerning linearized quadratic Chern–Simons gravity in $(2+1)D$ is extremely well behaved: it is finite at the origin and zero at infinity.

(ii) $V(r)\rightarrow 0$ as α and $\beta\rightarrow 0$, confirming in this way the fact that the standard correspondence of three-dimensional linearized Einstein–Chern–Simons gravity with Newton's theory breaks down.[29,30]

C. Light deflection

The current-current amplitude for the interaction of a light ray with a fixed source is given by

$$\mathcal{A}=\mathsf{g}^2T^{\mu\nu}F^{\rho\sigma}\Bigg[\Bigg(-\frac{1}{k^2}+\frac{1}{1+(bM_2^2/2)}\,\frac{1}{k^2-M_2^2}+\frac{1}{1+(bM_1^2/2)}\,\frac{1}{k^2-M_1^2}\Bigg)P^2$$
$$+\Bigg(\frac{1}{k^2}-\frac{1}{k^2-m^2}\Bigg)P^0\Bigg]_{\mu\nu,\rho\sigma}.$$

Taking (9) into account we can rewrite the expression above as

$$\mathcal{A}=\mathcal{A}_0+\mathcal{A}_1,$$

where

$$\mathcal{A}_0\equiv-\frac{\mathrm{g}^2T_{00}F_{00}}{k^2},$$

$$\mathcal{A}_1\equiv\mathrm{g}^2T_{00}F_{00}\left(\frac{1}{1+(bM_2^2/2)}\,\frac{1}{k^2-M_2^2}+\frac{1}{1+(bM_1^2/2)}\,\frac{1}{k^2-M_1^2}\right).$$

Of course, only $\mathcal{A}_1$ will contribute to light deflection since the massless excitation is not a degree of freedom. Hence, the light ray will be deflected downward as usual.

VIII. SUMMARY AND DISCUSSION

We proposed a prescription for finding the propagator concerning higher-derivative gravity theory in D dimensions based on the Barnes–Rivers operators. Using this algorithm, we computed the propagator for the latter in an unconventional gauge and, by a suitable choice of the gauge parameters, we reobtained the propagator in a series of gauges which are used in day-to-day physics.

A systematic study of the tree-level unitarity of D-dimensional higher-derivative gravity theory was presented afterward. It was shown that it is nonunitary at the tree level: the term quadratic in the Ricci tensor is the Achille's heel of the theory. This term is responsible for the presence of a massive spin-2 particle of negative residue, i.e., a ghost, in the bare propagator. Nevertheless, this may be a hasty conclusion. Indeed, as pointed out by Antoniadis and Tomboulis,[15] this excitation is unstable in four dimensions. Perhaps it would be unstable as well in any dimension. Therefore, D-dimensional quadratic gravity cannot yet be rejected as a viable possibility.

On the other hand, D-dimensional $R+R^2$ gravity is unitary at the tree level. We call attention to the fact that our discussion was confined to a particular style of variational principle. Perhaps there are richer unitary combinations in higher dimensions with the connection varied independently. If this is the case, that would be worth knowing. This matter will be the object of a future investigation.

The problem of computing the effective nonrelativistic potential for D-dimensional quadratic gravity was then reduced to quadratures. It seems that the existence of this potential in any dimension is related to the absence of tachyons (both positive and negative energy) in the dynamical field. It was also shown that, unlike three-dimensional linearized gravity which has no Newtonian limit, three-dimensional linearized quadratic gravity has a potential that, despite being rather different from the corresponding Newtonian one, is extremely well behaved.

It was shown afterward that the gravitational deflection is always smaller than that predicted by the corresponding Einstein's theory. This conclusion is totally independent of the value of D. For $D=3$ we arrive at the astonishing result that a light ray would be deflected upward instead of downward as its four-dimensional counterpart. It can be shown, in addition, that in $D=3$ a gravitational force is exerted on a slowly moving test particle.[31] This force greatly resembles that of a straight $U(1)$-gauge cosmic string in the framework of linearized quadratic gravity in four dimensions[32] and it is absent in three-dimensional general relativity.

Finally, we discussed three-dimensional quadratic gravity augmented by a Chern–Simons term. It was shown that neither the latter nor three-dimensional $R+R^2$ gravity with a Chern–Simons term are unitary at the tree level. On the other hand, as it was shown previously, light deflection has the ''wrong sign'' within the context of three-dimensional quadratic gravity. The addition of a topological massive term to the latter ''repairs'' the aforementioned sign. Is worth mentioning that ''antigravity'' is possible in the context of three-dimensional quadratic Chern–Simons gravity.[33]

To conclude we raise two interesting questions:

(i) Is it possible that gravity's rainbows and quadratic gravity theories can coexist without conflict in any dimension?

(ii) Is the photon propagation dispersive in the framework of three-dimensional quadratic gravity with a Chern–Simons term such as in four-dimensional quadratic gravity? These issues will be discussed elsewhere.

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On the problem of algebraic completeness for the invariants of the Riemann tensor. II

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We study the set of invariants CZ [E. Zakhary and J. Carminati, J. Math. Phys. **42**, 1474 (2001)] for the class of space–times whose Ricci tensors do not possess a null eigenvector. We show that all cases are completely backsolvable in terms of sets of invariants from CZ. We provide algebraically complete sets for each canonically different space–time. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In a previous paper[1] we introduced a new set of polynomial Riemann invariants CZ, satisfying the minimum degree property, which was claimed to be ''determining.'' (The various new definitions which are used here were introduced in the previous article.[1] In particular, we shall use the term ''complete'' to mean ''algebraically complete'' when referring to sets of invariants.) The main purpose of this article and a sequel will be to rigorously establish this fact. This will be achieved with the use of a ''backsolving'' technique. Moreover, we will explicitly give algebraically complete sets of invariants for each canonically different space–time. Essential to our approach is the notion of ''maximally backsolvable,'' which is the ability to backsolve, with a given set of invariants, for all of the theoretically possible, ''independent,'' Riemann curvature information, i.e., we call a set of invariants ''maximal'' if it contains all of the theoretically possible (not necessarily all) curvature information from the Riemann tensor, once all of the possible remaining tetrad freedom, which can act on the curvature components, is completely used up. It follows that such a maximal set must be determining and vice versa. Also, we need to further distinguish when a maximal set contains *all* of the information in the Riemann tensor and when it does not. We call a set of invariants ''curvature complete'' if it contains *all* of the independent information that is in the Riemann tensor and complete backsolving is then achievable. Clearly, curvature complete implies maximal but not vice versa.

Regarding explicitly giving algebraically complete sets of invariants for each canonically different space–time, we will show that this is always possible by choosing certain subsets of CZ. We will, in general, not give explicit solutions of the independent curvature components in terms of our invariants as in many cases this is not possible since the resulting polynomial expressions are very large and of high degree. As was shown previously,[1] for some Segre and Weyl types not all of the information that is in the Riemann tensor is in its second order polynomial invariants. Hence, complete backsolving is not always possible for these cases but maximal backsolving should always, at least in principle, be achievable with an algebraically complete set of invariants. Note, obviously, that ''completely backsolvable'' implies ''maximally backsolvable'' but not vice versa.

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Our backsolving procedure is carried out, in almost all cases, in the Ricci canonical frames corresponding to the different Segre types (and general Petrov type). We note that the backsolving for the Ricci (or Weyl) components only in terms of the pure Ricci (or pure Weyl) invariants, in their respective canonical frames, has been previously done by Carminati and McLenaghan[2] and Zakhary.[3]

Regarding our method of proof, after having established that a set of invariants is maximal or determining by backsolving and if necessary using the index theorem, we then check that we have retained the minimum possible number of invariants [i.e., that it cannot be further reduced (in number[4] of invariants) and still achieve the same "measure" [5] of backsolving]. It follows that once this is done, we have established that the set is algebraically complete. In cases where complete backsolving has been achieved (i.e., we have curvature complete sets), which is for all of class A (see below), the "minimal number" property is established by simply observing that the number[4] of invariants is the same as the number[4] of unknown functions in the curvature components (after all of the possible remaining tetrad freedom, which can act on the curvature components, is completely used up).

Since the backsolving method yields, in general, nonunique solutions, this could lead to significantly different space–times and/or Petrov types. A full investigation of this issue is planned for the future. However, our main concern in this article and a future paper (as was in Ref. 1) is centered on how much algebraically independent information that is in the Riemann tensor is present in its polynomial invariants and the backsolving technique introduced is achieving this.

Any Segre type falls into one of two classes: class A, in which the Ricci tensor does not possess a null eigenvector, and class B, in which the Ricci tensor possesses a null eigenvector. As we shall show in this article and a future paper, all space–times in class A are always completely backsolvable (CB), while space–times in class B are completely backsolvable except for special cases (excluding the trivial Segre type [(1,111)]). These exceptional cases will be designated as "not (generally) completely backsolvable" (NCB).[6] We will also show, in a future paper, that there is a geometric link between the NCB space–times in class B and the alignment of the eigenvectors of the Ricci tensor with the repeated principal null directions (PNDs) of the Weyl tensor. In this article, we will consider only those Segre types in class A.

Recall, the CZ set consists of the following invariants:[1]

$$
\begin{aligned}
R &:= g^{ab}g^{cd}R_{acdb},\\
w_1 &:= \tfrac{1}{6}\Psi_{ABCD}\Psi^{ABCD},\\
w_2 &:= \tfrac{1}{6}\Psi_{ABCD}\Psi^{CD}{}_{EF}\Psi^{EFAB},\\
r_1 &:= \tfrac{1}{3}\Phi_{AB\dot{A}\dot{B}}\Phi^{AB\dot{A}\dot{B}},\\
r_2 &:= \tfrac{1}{6}\Phi_{AB\dot{A}\dot{B}}E^{AB\dot{A}\dot{B}},\\
r_3 &:= \tfrac{1}{12}E_{AB\dot{A}\dot{B}}E^{AB\dot{A}\dot{B}},\\
m_1 &:= \Psi_{ABCD}\Phi^{CD}{}_{\dot{C}\dot{D}}\Phi^{AB\dot{C}\dot{D}},\\
m_2 &:= \Psi_{(AB}{}^{EF}\Psi_{CD)EF}\Phi^{AB}{}_{\dot{C}\dot{D}}\Phi^{CD\dot{C}\dot{D}},\\
m_3 &:= \Psi_{ABCD}\Phi^{AE\dot{A}\dot{B}}\Phi^{B}{}_{E\dot{A}\dot{C}}\Phi^{CF\dot{C}\dot{D}}\Phi^{D}{}_{F\dot{D}\dot{B}},\\
m_4 &:= \Psi^{AB}{}_{CD}\Phi^{CD}{}_{\dot{A}\dot{B}}\overline{\Psi}^{\dot{A}\dot{B}}{}_{\dot{C}\dot{D}}\Phi_{AB}{}^{\dot{C}\dot{D}},\\
m_5 &:= \Psi_{(AB}{}^{CD}\Psi_{EF)CD}\overline{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}\Phi^{AB\dot{C}\dot{D}}\Phi^{EF\dot{A}\dot{B}},\\
m_6 &:= \Psi^{AB}{}_{CD}\Psi^{CD}{}_{EF}\Phi^{EF}{}_{\dot{A}\dot{B}}\overline{\Psi}^{\dot{A}\dot{B}}{}_{\dot{C}\dot{D}}\overline{\Psi}^{\dot{C}\dot{D}}{}_{\dot{E}\dot{F}}\Phi_{AB}{}^{\dot{E}\dot{F}},
\end{aligned}
\tag{1}
$$

TABLE I. Relations between sets.

CZ set	Equivalent invariants in ZC set (Ref. 8)	Equivalent invariants in CM set (Ref. 9)
R	R	R
w_1	I	$\frac{1}{6}w_1$
w_2	J	$\frac{1}{6}w_2$
r_1	I_6	$\frac{1}{3}r_1$
r_2	I_7	$\frac{1}{3}r_2$
r_3	I_8	$\frac{1}{3}r_3-\frac{1}{12}r_1^2$
m_1	K	m_1
m_2	L	$m_2-\frac{1}{3}w_1r_1$
m_3	$-M$	$\cdots$
m_4	M_1	m_3
m_5	M_2	$m_5-\frac{1}{3}w_1\overline{m}_1$
m_6	$\cdots$	$\cdots$

where

$$E^{AB}{}_{\dot{C}\dot{D}} := 2\Phi^{A}{}_{E\dot{F}(\dot{C}}\Phi^{BE\dot{F}}{}_{\dot{D})}. \tag{2}$$

For future reference, we give, in Table I the relations between the various sets. Further, we give other tables (Tables II and III)[7–9] which summarize the syzygies for the different Petrov and Segre types of the Weyl and Ricci tensors, respectively.

II. RICCI CANONICAL FRAMES

In this section we will set up the canonical frames for the different Segre types using Hall's approach.[10] Our analysis is somewhat more detailed than Hall's in that we give more explicit descriptions of the canonical forms together with the remaining tetrad freedom for each case. Briefly, a local real null tetrad $\{l^a,n^a,x^a,y^a\}$, with l^a and n^a being null vectors and x^a and y^a being spacelike vectors, is introduced on the space–time manifold M. The only nonvanishing inner products are $l^a n_a=1$ and $x^a x_a=y^a y_a=-1$. In this case the completeness relation takes the form

$$g_{ab}=l_a n_b+n_a l_b-x_a x_b-y_a y_b. \tag{3}$$

We note that the Newman–Penrose (NP) complex null tetrad $\{l^a,n^a,m^a,\overline{m}^a\}$ is related to the above tetrad via the relation $m^a=(1/\sqrt{2})(x^a+iy^a)$.

The covariant Ricci tensor with components R_{ab} can be written as

$$\begin{aligned} R_{ab}=&2R^1 l_{(a}n_{b)}+R^2 l_a l_b+R^3 n_a n_b+2R^4 l_{(a}x_{b)}+2R^5 l_{(a}y_{b)}+2R^6 n_{(a}x_{b)}\\ &+2R^7 n_{(a}y_{b)}+2R^8 x_{(a}y_{b)}+R^9 x_a x_b+R^{10} y_a y_b. \end{aligned} \tag{4}$$

TABLE II. The Weyl syzygies.

Petrov types	Syzygies
I	$\cdots$
II, D	$w_1^3=w_2^2$
III, N, O	$w_1=w_2=0$

TABLE III. The Ricci syzygies.

Ricci degeneracy	Segre types	Syzygies
{1111}	[1,111], [Z$\overline{\text{Z}}$,11]	⋯
{112}	[1,1(11)], [(1,1)11], [Z$\overline{\text{Z}}$,(11)], [2,11]	$r_2^2(4r_1^3-6r_1r_3+r_2^2)=r_3^2(3r_1^2-4r_3)$
{22}	[(1,1)(11)], [2,(11)]	$r_2=r_3=0$
{13}	[1,(111)], [(1,11)1], [(2,1)1], [3,1]	$r_2^2=r_1^3, r_3=r_1^2$
{4}	[(3,1)], [(2,11)], [(1,111)]	$r_1=r_2=r_3=0$

The mixed Ricci tensor with components $R^a{}_b$ can be represented as a linear transformation $\mathbf{R}: T_p(M)\to T_p(M)$ with matrix $R^a{}_b$.

The classification of the Ricci tensor **R** depends on the following general results due to Churchill:[11]

(i) There always exists a two-dimensional subspace of $T_p(M)$ which is an invariant two-space of **R**.
(ii) If **V** is an invariant two-space of **R**, then so is the two-space orthogonal to **V**.
(iii) **R** has two distinct spacelike eigenvectors.
(iv) **R** has a null invariant two-space ⇔**R** has a null eigenvector.

It follows that the canonical forms of the Ricci tensor naturally split into two different classes (as previously stated): class A, the Ricci tensor has no null eigenvectors, and class B, the Ricci tensor has a null eigenvector. Below, we summarize the results of our investigation for class A.

For later use, we present the transformations of the null tetrad, Weyl and Ricci components, in the following compact form:

$$X'=\Pi X\overline{\Pi}^T,\quad \Psi'=\Xi\Psi\Xi^T,\quad \Phi'=\Xi\Phi\overline{\Xi}^T,$$

where

$$X=\begin{bmatrix}\mathbf{l} & \mathbf{m}\\ \overline{\mathbf{m}} & \mathbf{n}\end{bmatrix},\quad \Pi=\begin{bmatrix}A & B\\ C & D\end{bmatrix},\quad \Psi=\begin{bmatrix}\Psi_0 & \Psi_1 & \Psi_2\\ \Psi_1 & \Psi_2 & \Psi_3\\ \Psi_2 & \Psi_3 & \Psi_4\end{bmatrix},$$

$$\Phi=\begin{bmatrix}\Phi_{00} & \Phi_{01} & \Phi_{02}\\ \Phi_{10} & \Phi_{11} & \Phi_{12}\\ \Phi_{20} & \Phi_{21} & \Phi_{22}\end{bmatrix},\quad \Xi=\begin{bmatrix}A^2 & 2AB & B^2\\ AC & AD+BC & BD\\ C^2 & 2CD & D^2\end{bmatrix},$$

and $AD-BC=1$.

A. Class A: The Ricci tensor has no null eigenvectors

1. PP type I, Segre type [1,111]:

Canonical form of R_{ab}*:*

$$R_{ab}=2\rho_1 l_{(a}n_{b)}+\rho_2(l_al_b+n_an_b)-\rho_3x_ax_b-\rho_4y_ay_b,$$

with

$$\rho_2 \neq 0,\ \rho_2 \neq \rho_4,\ \rho_1 \pm \rho_2 \neq \rho_3,\ \rho_1 \pm \rho_2 \neq \rho_4.$$

Inner products:

$$R_{ab}l^b = \rho_1 l_a + \rho_2 n_a,\ R_{ab}n^b = \rho_2 l_a + \rho_1 n_a,\ R_{ab}x^b = \rho_3 x_a,\ R_{ab}y^b = \rho_4 y_a.$$

Eigenvectors: $l^a + n^a,\ l^a - n^a,\ x^a,\ y^a$.
Eigenvalues: $\rho_1 + \rho_2,\ \rho_1 - \rho_2,\ \rho_3,\ \rho_4$.
Canonical form of Ricci components Φ_{ab}*:*

$$\Phi_{00} = \Phi_{22} = -\tfrac{1}{2}\rho_2 \neq 0,$$

$$\Phi_{11} = \tfrac{1}{8}(\rho_3 + \rho_4 - 2\rho_1),$$

$$\Phi_{02} = \Phi_{20} = \tfrac{1}{4}(\rho_3 - \rho_4) \neq 0,$$

$$\Phi_{01} = \Phi_{12} = 0,$$

with

$$4\Phi_{11}^2 \neq (\Phi_{00} \pm \Phi_{02})^2.$$

Remaining tetrad freedom: None.

2. PP type I, Segre type [$Z\bar{Z}$,11]:

Canonical form of R_{ab}*:*

$$R_{ab} = 2\rho_1 l_{(a}n_{b)} + \rho_2(l_a l_b - n_a n_b) - \rho_3 x_a x_b - \rho_4 y_a y_b,$$

with

$$\rho_2 \neq 0,\ \rho_3 \neq \rho_4.$$

Inner Products:

$$R_{ab}l^b = \rho_1 l_a - \rho_2 n_a,\ R_{ab}n^b = \rho_2 l_a + \rho_1 n_a,\ R_{ab}x^b = \rho_3 x_a,\ R_{ab}y^b = \rho_4 y_a.$$

Eigenvectors: $l^a + in^a,\ l^a - in^a,\ x^a,\ y^a$.
Eigenvalues: $\rho_1 + i\rho_2,\ \rho_1 - i\rho_2,\ \rho_3,\ \rho_4$.

Canonical form of Ricci components Φ_{ab}*:*

$$\Phi_{00} = -\Phi_{22} = \tfrac{1}{2}\rho_2 \neq 0,$$

$$\Phi_{11} = \tfrac{1}{8}(\rho_3 + \rho_4 - 2\rho_1),$$

$$\Phi_{02} = \Phi_{20} = \tfrac{1}{4}(\rho_3 - \rho_4) \neq 0,$$

$$\Phi_{01} = \Phi_{12} = 0.$$

Remaining tetrad freedom: None.

3. PP type D, Segre type [1,1(11)]:

Canonical form of R_{ab}*:*

$$R_{ab} = 2\rho_1 l_{(a}n_{b)} + \rho_2(l_a l_b + n_a n_b) - \rho_3 x_a x_b - \rho_3 y_a y_b,$$

with

$$\rho_2 \neq 0,\ \rho_1 \pm \rho_2 \neq \rho_3 .$$

Inner products:

$$R_{ab}l^b = \rho_1 l_a + \rho_2 n_a ,\ R_{ab}n^b = \rho_2 l_a + \rho_1 n_a ,\ R_{ab}x^b = \rho_3 x_a ,\ R_{ab}y^b = \rho_3 y_a .$$

Eigenvectors: $l^a + n^a,\ l^a - n^a,\ x^a,\ y^a$.
Eigenvalues: $\rho_1 + \rho_2,\ \rho_1 - \rho_2,\ \rho_3,\ \rho_3$.

Canonical form of Ricci components Φ_{ab}*:*

$$\Phi_{00} = \Phi_{22} = -\tfrac{1}{2}\rho_2 \neq 0, \quad \Phi_{11} = \tfrac{1}{4}(\rho_3 - \rho_1), \quad \Phi_{01} = \Phi_{02} = \Phi_{12} = 0,$$

with

$$4\Phi_{11}^2 \neq \Phi_{00}^2 .$$

Remaining tetrad freedom: Spatial rotations: $D = \overline{A},\ A\overline{A} = 1,\ B = C = 0$.

4. PP type D, Segre type [$Z\overline{Z}$,(11)]

Canonical form of R_{ab}*:*

$$R_{ab} = 2\rho_1 l_{(a}n_{b)} + \rho_2(l_a l_b - n_a n_b) - \rho_3 x_a x_b - \rho_3 y_a y_b ,$$

with

$$\rho_2 \neq 0.$$

Inner Products:

$$R_{ab}l^b = \rho_1 l_a - \rho_2 n_a ,\ R_{ab}n^b = \rho_2 l_a + \rho_1 n_a ,\ R_{ab}x^b = \rho_3 x_a ,\ R_{ab}y^b = \rho_3 y_a .$$

Eigenvectors: $l^a + in^a,\ l^a - in^a,\ x^a,\ y^a$.
Eigenvalues: $\rho_1 + i\rho_2,\ \rho_1 - i\rho_2,\ \rho_3,\ \rho_3$.

Canonical form of Ricci components Φ_{ab}*:*

$$\Phi_{00} = -\Phi_{22} = \tfrac{1}{2}\rho_2 \neq 0, \quad \Phi_{11} = \tfrac{1}{4}(\rho_3 - \rho_1), \quad \Phi_{01} = \Phi_{02} = \Phi_{12} = 0.$$

Remaining tetrad freedom: Spatial rotations: $D = \overline{A},\ A\overline{A} = 1,\ B = C = 0$.

5. PP Type O, Segre Type [1,(111)]:

Canonical form of R_{ab}*:*

$$R_{ab} = 2\rho_1 l_{(a}n_{b)} + \rho_2(l_a l_b + n_a n_b) - (\rho_1 - \rho_2)(x_a x_b + y_a y_b),$$

with

$$\rho_2 \neq 0.$$

Inner products:

$$R_{ab}l^b = \rho_1 l_a + \rho_2 n_a ,\ R_{ab}n^b = \rho_2 l_a + \rho_1 n_a ,\ R_{ab}x^b = (\rho_1 - \rho_2)x_a ,$$

$$R_{ab}y^b = (\rho_1 - \rho_2)y_a .$$

Eigenvectors: $l^a+n^a,\ l^a-n^a,\ x^a,\ y^a$.
Eigenvalues: $\rho_1+\rho_2,\ \rho_1-\rho_2,\ \rho_1-\rho_2,\ \rho_1-\rho_2$.

Canonical form of Ricci components Φ_{ab}*:*

$$\Phi_{00}=2\Phi_{11}=\Phi_{22}=-\tfrac{1}{2}\rho_2\neq 0,$$

$$\Phi_{01}=\Phi_{02}=\Phi_{12}=0.$$

Remaining tetrad freedom: 3-d spatial rotations SO(3): $D=\overline{A},\ C=-\overline{B},\ A\overline{A}+B\overline{B}=1$.

At this point, we would like to compare our canonical forms with those as given by MacIntosh *et al.*[12] and Joly and MacCallum.[7] Specifically, apart from changes due to $\mathbf{l}\leftrightarrow\mathbf{n}$ interchange, our work differs from theirs in that Φ_{11} could be zero for Segre types [1,111], [$Z\overline{Z}$,11], [1,1(11)] and [$Z\overline{Z}$,(11)] (and also [2,11] and [(1,1)11]), whereas they report that Φ_{11} is necessarily nonzero for these types.

III. COMPLETE BACKSOLVING

In this section, we will prove that the CZ set is determined for class A by explicitly showing that complete backsolving is always possible for each Segre type, for certain selected subsets chosen from CZ. These subsets are all algebraically complete since they are all curvature complete and a simple count[4] shows that they are, in each case, the smallest possible sets. Most of the computations were done with the algebraic computing system Maple.

A. Segre type [1,111]

In this case, the algebraically complete set of invariants is $\{R,w_1,w_2,r_1,r_2,r_3,m_1,m_2,m_3\}$ and we will now show that complete backsolving is always possible, at least in principle. We begin with the backsolving for the Ricci components Φ_{ab}. In our canonical frame, the Ricci invariants are

$$r_1=\tfrac{2}{3}(\Phi_{00}^2+\Phi_{02}^2+2\Phi_{11}^2),$$

$$r_2=2\Phi_{11}(\Phi_{00}^2-\Phi_{02}^2),$$

$$r_3=\tfrac{1}{3}(\Phi_{00}^4-2\Phi_{00}^2\Phi_{02}^2+8\Phi_{00}^2\Phi_{11}^2+8\Phi_{02}^2\Phi_{11}^2+\Phi_{02}^4).$$

Since the Jacobian which is given by $\frac{64}{9}J$, where

$$J=\Phi_{00}\Phi_{02}(\Phi_{00}+\Phi_{02}+2\Phi_{11})(\Phi_{00}+\Phi_{02}-2\Phi_{11})(\Phi_{00}-\Phi_{02}+2\Phi_{11})(\Phi_{00}-\Phi_{02}-2\Phi_{11})$$

is always nonzero, it follows that the Ricci invariants $r_1,\ r_2,\ r_3$ are always backsolvable for Φ_{ab}.

To facilitate the backsolving of the Weyl components Ψ_a, we make the following substitutions:

$$\Psi_0=x+y,\ \ \Psi_1=u+v,\ \ \Psi_3=u-v,\ \ \Psi_4=x-y.$$

The Weyl and mixed invariants then take the form

$$w_1=\tfrac{1}{3}(x^2-y^2-4u^2+4v^2+3\Psi_2^2),$$

$$w_2=2\Psi_2u^2-2\Psi_2v^2-\Psi_2^3-2u^2x+4yuv-2v^2x+\Psi_2x^2-\Psi_2y^2,$$

$$m_1=2(\Phi_{00}^2-4\Phi_{11}^2+\Phi_{02}^2)\Psi_2+4\Phi_{00}\Phi_{02}x,$$

$$m_2 = -2\Psi_2^2\Phi_{02}^2 + 8\Psi_2^2\Phi_{11}^2 - 2\Psi_2^2\Phi_{00}^2 + \tfrac{16}{3}\Phi_{11}^2 v^2 - \tfrac{4}{3}\Phi_{02}^2 v^2 - \tfrac{4}{3}\Phi_{00}^2 v^2 - \tfrac{16}{3}\Phi_{11}^2 u^2 + \tfrac{4}{3}\Phi_{02}^2 u^2 + \tfrac{4}{3}\Phi_{00}^2 u^2 - 8\Phi_{00} v^2 \Phi_{02} - 8\Phi_{00} u^2 \Phi_{02} - \tfrac{8}{3}\Phi_{11}^2 x^2 + \tfrac{8}{3}\Phi_{11}^2 y^2 + \tfrac{2}{3}\Phi_{02}^2 x^2 - \tfrac{2}{3}\Phi_{02}^2 y^2 + \tfrac{2}{3}\Phi_{00}^2 x^2 - \tfrac{2}{3}\Phi_{00}^2 y^2 + 8\Psi_2 \Phi_{00}\Phi_{02} x,$$

$$m_3 = 2(4\Phi_{00}^2\Phi_{11}^2 + 2\Phi_{00}^2\Phi_{02}^2 + 4\Phi_{02}^2\Phi_{11}^2 - \Phi_{00}^4 - \Phi_{02}^4)\Psi_2 - 16\Phi_{00}\Phi_{02}\Phi_{11}^2 x.$$

We begin by noting that the system $\{m_1, m_3\}$ which contains only the Weyl variables x and Ψ_2 has Jacobian equal to $-8J$ which is nonzero. Hence, we may regard x and Ψ_2 as (locally) implicit functions of m_1 and m_3 and Φ_{ab} (which in turn are determined by the Ricci invariants). Next, we solve w_1 for u^2 and use this equation to eliminate u from m_2. We can always solve this resulting equation for v^2, since its coefficient is nonzero. Finally, after solving w_2 for $4yuv$ and squaring, we substitute the solutions for u^2 and v^2 into this expression to obtain a polynomial equation of degree 6 in y with the coefficients being polynomials in x, Ψ_2, Φ_{ab}, and invariants. This polynomial can always be solved for y, since the coefficient of y^6 is $J/(\Phi_{00}\Phi_{02}) \neq 0$.

B. Segre type [$Z\bar{Z}$,11]

For this Segre type, the complete set of invariants is the same as that for [1,111], and the backsolving follows virtually the same procedure, providing the following substitutions: $\Psi_0 = x + y$, $\Psi_1 = u + v$, $\Psi_3 = i(v - u)$, $\Psi_4 = y - x$ are used instead of the previous ones.

C. Segre type [1,1(11)]

For this Segre type, the Ricci canonical frame is determined up to a spatial rotation. At the appropriate stage, we will use this remaining tetrad freedom to simplify the Weyl components. We will show that in all subcases complete backsolving can be achieved.

We begin with the backsolving for the Ricci components Φ_{ab}. In our canonical frame, the independent Ricci invariants are

$$r_1 = \tfrac{2}{3}(\Phi_{00}^2 + 2\Phi_{11}^2),$$

$$r_2 = 2\Phi_{00}^2\Phi_{11}.$$

Since the Jacobian $J = \frac{8}{3}\Phi_{00}(\Phi_{00} - 2\Phi_{11})(\Phi_{00} + 2\Phi_{11}) \neq 0$, it follows that the Ricci invariants r_1, r_2 are always backsolvable for Φ_{ab}.

Case 1: $\Psi_0 \neq 0$: In this case, we may use the tetrad freedom to make Ψ_0 real. Further, we shall need to treat the cases where $\Psi_3 = 0$ separately.

Case 1A: $\Psi_3 \neq 0$: We now show that the complete set is $\{R, w_1, w_2, r_1, r_2, m_1, m_2, m_4\}$. We begin by expressing the invariants in this frame.

$$w_1 = \tfrac{1}{3}(\Psi_0\Psi_4 - 4\Psi_1\Psi_3 + 3\Psi_2^2),$$

$$w_2 = 2\Psi_1\Psi_2\Psi_3 - \Psi_2^3 - \Psi_0\Psi_3^2 - \Psi_1^2\Psi_4 + \Psi_0\Psi_2\Psi_4,$$

$$m_1 = 2\Psi_2(\Phi_{00}^2 - 4\Phi_{11}^2),$$

$$m_2 = \tfrac{2}{3}(\Phi_{00}^2\Psi_0\Psi_4 + 2\Phi_{00}^2\Psi_1\Psi_3 + 12\Phi_{11}^2\Psi_2^2 - 4\Phi_{11}^2\Psi_0\Psi_4 - 3\Phi_{00}^2\Psi_2^2 - 8\Phi_{11}^2\Psi_1\Psi_3),$$

$$m_4 = \Phi_{00}^2\Psi_4\bar{\Psi}_4 + 16\Phi_{11}^2\Psi_2\bar{\Psi}_2 + \Phi_{00}^2\Psi_0^2 + 8\Phi_{00}\Phi_{11}\Psi_3\bar{\Psi}_3 + 2\Phi_{00}^2\Psi_2\bar{\Psi}_2 + 8\Phi_{00}\Phi_{11}\Psi_1\bar{\Psi}_1.$$

m_1 can always be solved for Ψ_2 since $\Phi_{00}^2 - 4\Phi_{11}^2 \neq 0$. We can always solve w_1 and m_2 to get $\Psi_1 = C_1/\Psi_3$ and $\Psi_4 = C_4/\Psi_0$, where C_1, C_4 are given by Φ_{ab}, Ψ_2 and invariants. Substituting these expressions into w_2 we get the quadratic polynomial equation

$$\psi^2+(w_2-2C_1\Psi_2-C_4\Psi_2+\Psi_2^3)\psi+C_1^2C_4=0$$

where $\psi=\Psi_0\Psi_3^2$. This can always be solved for ψ in terms of Φ_{ab}, Ψ_2 and invariants. Substituting $\Psi_3=(\psi/\Psi_0)^{1/2}$ into m_4, we get a quartic polynomial equation in Ψ_0, which can always be solved for Ψ_0 since the coefficient of Ψ_0^4 is $\Phi_{00}^2(\psi\bar{\psi})^{1/2}\neq 0$.

Case 1B(i): $\Psi_3=0$ & $\Psi_4\neq 0$: In this case, the complete set is $\{R,w_1,w_2,r_1,r_2,m_1,m_4\}$. This is established as follows. The non-Ricci invariants, when expressed in this frame, take the form

$$w_1=\tfrac{1}{3}(\Psi_0\Psi_4+3\Psi_2^2),$$

$$w_2=\Psi_0\Psi_2\Psi_4-\Psi_2^3-\Psi_1^2\Psi_4,$$

$$m_1=2\Psi_2(\Phi_{00}^2-4\Phi_{11}^2),$$

$$m_4=\Phi_{00}^2\Psi_4\bar{\Psi}_4+16\Phi_{11}^2\Psi_2\bar{\Psi}_2+\Phi_{00}^2\Psi_0^2+2\Phi_{00}^2\Psi_2\bar{\Psi}_2+8\Phi_{00}\Phi_{11}\Psi_1\bar{\Psi}_1.$$

Again, m_1 can always be solved for Ψ_2 since $\Phi_{00}^2-4\Phi_{11}^2\neq 0$. We can always solve w_1 and w_2 to get

$$\Psi_1^2=\Psi_0(3\Psi_2w_1-4\Psi_2^3-w_2)/[3(w_1-\Psi_2^2)] \quad \text{and} \quad \Psi_4=3(w_1-\Psi_2^2)/\Psi_0\neq 0.$$

After solving the invariant m_4 for $\Psi_1\bar{\Psi}_1$ and squaring, we substitute the expressions for Ψ_1^2, $\bar{\Psi}_1$ and Ψ_4 to get a polynomial equation of degree 8 in Ψ_0 with coefficients being polynomials in Φ_{ab}, Ψ_2 and invariants. The leading term of this polynomial is $3\Phi_{00}^4(\Psi_2^2-w_1)\Psi_0^8$. Since $\Psi_4\neq 0$, the coefficient of Ψ_0^8 is nonzero and consequently the polynomial algebraically determines Ψ_0 for suitably restricted values of the invariants.

Case 1B(ii): $\Psi_3=\Psi_4=0$: In this case, the complete set is $\{R,w_1,r_1,r_2,m_4,m_5\}$. To prove this, we consider the non-Ricci invariants, which in this frame become

$$w_1=\Psi_2^2,$$

$$m_4=16\Phi_{11}^2\Psi_2\bar{\Psi}_2+\Phi_{00}^2\Psi_0^2+2\Phi_{00}^2\Psi_2\bar{\Psi}_2+8\Phi_{00}\Phi_{11}\Psi_1\bar{\Psi}_1,$$

$$m_5=2\Phi_{00}^2\Psi_0^2\Psi_2-2\Phi_{00}^2\Psi_2^2\bar{\Psi}_2-8\Phi_{00}\Phi_{11}\Psi_1\bar{\Psi}_1\Psi_2-2\Phi_{00}^2\Psi_0\Psi_1^2-16\Phi_{11}^2\Psi_2^2\bar{\Psi}_2.$$

w_1 can always be solved for Ψ_2. We eliminate Ψ_1 and $\bar{\Psi}_1$ from m_4 and m_5 to obtain a polynomial in Ψ_0 in the following manner. First, we eliminate the product $\Psi_1\bar{\Psi}_1$ from m_4 and m_5 and solve for Ψ_1^2. Then, we solve m_4 for $\Psi_1\bar{\Psi}_1$, square this result and substitute in the previous expression for Ψ_1^2. The resulting condition is a polynomial (bi-cubic) of degree 6 in Ψ_0.

$$\begin{aligned}\Psi_0^6\Phi_{00}^6+2\Phi_{00}^4(2\Psi_2\Phi_{00}^2\bar{\Psi}_2-m_4-56\Psi_2\Phi_{11}^2\bar{\Psi}_2)\Psi_0^4+\Phi_{00}^2(4\bar{\Psi}_2^2\Psi_2^2\Phi_{00}^4\\ -4\Phi_{00}^2\bar{\Psi}_2\Psi_2m_4+64\Phi_{00}^2\bar{\Psi}_2^2\Psi_2^2\Phi_{11}^2+256\Psi_2^2\Phi_{11}^4\bar{\Psi}_2^2+m_4^2+48\Phi_{11}^2\Psi_2\bar{m}_5\\ +64\Psi_2\Phi_{11}^2\bar{\Psi}_2m_4+48\Phi_{11}^2m_5\bar{\Psi}_2)\Psi_0^2-16\Phi_{11}^2(\Psi_2m_4+m_5)(m_4\bar{\Psi}_2+\bar{m}_5)=0.\end{aligned}$$

Since the last term in the polynomial condition is negative definite, it has a positive solution for Ψ_0^2. Thus Ψ_0 is (implicitly) determined in terms of the invariants and, therefore, we conclude that all of the Ricci and Weyl components are now determined (implicitly and nonuniquely) in terms of the invariants.

Case 2: $\Psi_0=0$ *and* $\Psi_1\neq 0$: In this case, we may use the tetrad freedom to make Ψ_1 real.

Case 2A: $\Phi_{11}\neq 0$ *or* $\Psi_4\neq 0$: In this case, the complete set is $\{R,w_1,w_2,r_1,r_2,m_1,m_4\}$. To show this, we begin by expressing the invariants in this frame:

$$w_1=\tfrac{1}{3}(3\Psi_2^2-4\Psi_1\Psi_3),$$

$$w_2=2\Psi_1\Psi_2\Psi_3-\Psi_2^3-\Psi_1^2\Psi_4,$$

$$m_1=2\Psi_2(\Phi_{00}^2-4\Phi_{11}^2),$$

$$m_4=\Phi_{00}^2\Psi_4\overline{\Psi}_4+16\Phi_{11}^2\Psi_2\overline{\Psi}_2+8\Phi_{00}\Phi_{11}\Psi_3\overline{\Psi}_3+2\Phi_{00}^2\Psi_2\overline{\Psi}_2+8\Phi_{00}\Phi_{11}\Psi_1^2.$$

m_1 can always be solved for Ψ_2 since $\Phi_{00}^2-4\Phi_{11}^2\neq 0$. Using the invariants w_1, w_2 and m_1 we obtain

$$\Psi_2=m_1/[2(\Phi_{00}^2-4\Phi_{11}^2)],\quad \Psi_3=A_3/\Psi_1,\quad \Psi_4=A_4/\Psi_1^2$$

where $A_3=3(\Psi_2^2-w_1)/4$ and $A_4=(\Psi_2^3-3\Psi_2w_1-2w_2)/2$.

Substituting these expressions into m_4 we get the bi-cubic polynomial equation

$$8\Phi_{00}\Phi_{11}\Psi_1^6-[m_4-2(\Phi_{00}^2-8\Phi_{11}^2)\Psi_2\overline{\Psi}_2]\Psi_1^4+8\Phi_{00}\Phi_{11}A_3\overline{A}_3\Psi_1^2+\Phi_{00}^2A_4\overline{A}_4=0.$$

For suitably restricted values of the invariants, this polynomial equation can be solved for Ψ_1.

Case 2B: $\Phi_{11}=\Psi_4=0$: The complete set is $\{R,w_1,w_2,r_1,m_6\}$. As before, we show this by first expressing the invariants in this frame:

$$w_1=\tfrac{1}{3}(3\Psi_2^2-4\Psi_1\Psi_3),$$

$$w_2=2\Psi_1\Psi_2\Psi_3-\Psi_2^3,$$

$$m_6=2\Phi_{00}^2(4\Psi_1^2\Psi_3\overline{\Psi}_3-2\Psi_1\Psi_3\overline{\Psi}_2^2+2\Psi_1^4-2\Psi_1\Psi_2^2\overline{\Psi}_3+\Psi_2^2\overline{\Psi}_2^2+2\Psi_3^2\overline{\Psi}_3^2).$$

Eliminating the product $\Psi_1\Psi_3$ between w_1 and w_2 yields the equation $\Psi_2^3-3w_1\Psi_2-2w_2=0$, which always determines Ψ_2 in terms of w_1 and w_2. Next, we solve w_1 for Ψ_3 to obtain $\Psi_3=3(\Psi_2^2-w_1)/(4\Psi_1)$. Substituting these results into the expression for m_6 yields the following polynomial condition which is quadratic in Ψ_1^4:

$$256\Psi_1^8\Phi_{00}^2-32(2m_6-9\overline{w}_1w_1\Phi_{00}^2-\Psi_2^2\Phi_{00}^2\overline{\Psi}_2^2+3\overline{w}_1\Psi_2^2\Phi_{00}^2+3\overline{\Psi}_2^2w_1\Phi_{00}^2)\Psi_1^4$$
$$+81\Phi_{00}^2(w_1-\Psi_2^2)^2(\overline{w}_1-\overline{\Psi}_2^2)^2=0.$$

For suitably restricted values of the invariants, this polynomial equation can be solved for Ψ_1.

Case 3: $\Psi_0=\Psi_1=0$, *and* $\Psi_3\neq 0$: In this case, we may use the tetrad freedom to make Ψ_3 real.

Case 3A: $\Phi_{11}\neq 0$ *or* $\Psi_4\neq 0$: We will now show that the complete set is $\{R,w_1,r_1,r_2,m_4,m_5\}$. We begin by expressing the invariants in this frame:

$$w_1=\Psi_2^2,$$

$$m_4=16\Phi_{11}^2\Psi_2\overline{\Psi}_2+\Phi_{00}^2\Psi_4\overline{\Psi}_4+2\Phi_{00}^2\Psi_2\overline{\Psi}_2+8\Phi_{00}\Phi_{11}\Psi_3^2,$$

$$m_5=2\Phi_{00}^2\Psi_4\overline{\Psi}_4\Psi_2-2\Phi_{00}^2\Psi_2^2\overline{\Psi}_2-8\Phi_{00}\Phi_{11}\Psi_2\Psi_3^2-2\Phi_{00}^2\overline{\Psi}_4\Psi_3^2-16\Phi_{11}^2\Psi_2^2\overline{\Psi}_2.$$

w_1 determines Ψ_2. Combining m_4 and m_5 we obtain the following rational expression for $\overline{\Psi}_4$:

$$\overline{\Psi}_4=(2\Psi_2 m_4-24\Psi_3^2\Psi_2\Phi_{00}\Phi_{11}-m_5-6\Psi_2^2\overline{\Psi}_2\Phi_{00}^2-48\Psi_2^2\overline{\Psi}_2\Phi_{11}^2)/(2\Phi_{00}^2\Psi_3^2).$$

Substituting this equation and its complex conjugate into the expression for m_4 we obtain the bi-cubic

$$\begin{aligned}&32\Psi_3^6\Phi_{11}\Phi_{00}^3+4\Phi_{00}^2(2\Psi_2\Phi_{00}^2\overline{\Psi}_2-m_4+160\Psi_2\Phi_{11}^2\overline{\Psi}_2)\Psi_3^4+24\Phi_{00}\Phi_{11}(12\Psi_2^2\Phi_{00}^2\overline{\Psi}_2^2\\&+96\Psi_2^2\Phi_{11}^2\overline{\Psi}_2^2-4\overline{\Psi}_2\Psi_2 m_4+\overline{m}_5\Psi_2+\overline{\Psi}_2 m_5)\Psi_3^2+(48\overline{\Psi}_2^2\Psi_2\Phi_{11}^2-2\overline{\Psi}_2 m_4\\&+6\overline{\Psi}_2^2\Psi_2\Phi_{00}^2+\overline{m}_5)(6\Psi_2^2\overline{\Psi}_2\Phi_{00}^2-2\Psi_2 m_4+m_5+48\Psi_2^2\overline{\Psi}_2\Phi_{11}^2)=0,\end{aligned}$$

which determines Ψ_3.

Case 3B: $\Phi_{11}=\Psi_4=0$: The complete set is $\{R,w_1,r_1,m_6\}$ since the invariants in this frame are

$$w_1=\Psi_2^2,$$

$$m_6=2\Phi_{00}^2(\Psi_2^2\overline{\Psi}_2^2+2\Psi_3^4),$$

which always determine Ψ_2 and Ψ_3.

Case 4: $\Psi_0=\Psi_1=\Psi_3=0$: In this case, if $\Psi_4\neq 0$, we may use the tetrad freedom to make Ψ_4 real. The invariants in this frame are

$$w_1=\Psi_2^2,$$

$$m_4=16\Phi_{11}^2\Psi_2\overline{\Psi}_2+\Phi_{00}^2\Psi_4^2+2\Phi_{00}^2\Psi_2\overline{\Psi}_2,$$

which always determine Ψ_2 and Ψ_4. Hence the complete set is $\{R,w_1,r_1,r_2,m_4\}$. Note that if $\Psi_4=0$, then w_1 determines Ψ_2 (and m_4 is dependent).

D. Segre type [$z\bar{z}$,(11)]

The backsolving analysis for this Segre type is virtually identical to that for Segre type [1,1(11)] except for minor sign differences.

E. Segre type [1,(111)]

For this Segre type, it is easier to use the Weyl canonical frame. The Ricci components for this Segre type, in general, are[3] $\Phi_{00}=\pm 2\alpha^2$, $\Phi_{01}=\pm 2\alpha\beta$, $\Phi_{02}=\pm 2\beta^2$, $\Phi_{11}=\pm(\alpha\gamma+\beta\overline{\beta})$, $\Phi_{12}=\pm 2\beta\gamma$, and $\Phi_{22}=\pm 2\gamma^2$ (with same sign all through) where α and γ are real, β is complex and $0\leqslant\beta\overline{\beta}<\alpha\gamma$. The only independent Ricci invariant is $r_1=4(\alpha\gamma-\beta\overline{\beta})^2$, therefore, $\gamma=(2\beta\overline{\beta}+\sqrt{r_1})/(2\alpha)$. Note that, in this case, α cannot equal zero.

1. Segre type [1,(111)], Petrov type I:

For this Petrov type $w_2^2\neq w_1^3$. In our Weyl canonical frame, the only nonzero Weyl components are Ψ_2 and $\Psi_0=\Psi_4$ where $\Psi_0^2\neq 9\Psi_2^2$. The Weyl invariants in this frame are $w_1=\frac{1}{3}(\Psi_0^2+3\Psi_2^2)$ and $w_2=\Psi_2(\Psi_0^2-\Psi_2^2)$. The Jacobian of this system of equations is $\frac{2}{3}\Psi_0(\Psi_0^2-9\Psi_2^2)\neq 0$ and, hence, it is backsolvable for Ψ_0 and Ψ_2.

We will now show that the complete set is $\{R,w_1,w_2,r_1,m_4,m_5\}$. The mixed invariants in this frame are

$$\begin{aligned}m_4=4(&\Psi_0\overline{\beta}^4\overline{\Psi}_0+6\Psi_0\alpha^2\beta^2\overline{\Psi}_2+6\Psi_2\alpha^2\overline{\beta}^2\overline{\Psi}_0+\Psi_0\beta^4\overline{\Psi}_0+6\Psi_2\overline{\Psi}_2\alpha^2\gamma^2+\Psi_0\overline{\Psi}_0\gamma^4\\&+6\Psi_2\beta^2\overline{\Psi}_2\overline{\beta}^2+6\Psi_2\beta^2\overline{\Psi}_0\gamma^2+24\Psi_2\alpha\beta\overline{\Psi}_2\overline{\beta}\gamma+6\Psi_0\overline{\beta}^2\overline{\Psi}_2\gamma^2+\Psi_0\alpha^4\overline{\Psi}_0),\end{aligned}$$

$$m_5 = 8(4\overline{\Psi}_2\alpha\gamma\beta\overline{\beta} + \overline{\Psi}_2\overline{\beta}^2\beta^2 + \overline{\Psi}_2\alpha^2\gamma^2 + \overline{\Psi}_0\beta^2\gamma^2 + \overline{\Psi}_0\alpha^2\overline{\beta}^2)\Psi_0^2 + 8\Psi_2(6\alpha^2\beta^2\overline{\Psi}_2 + \overline{\Psi}_0\gamma^4 + \overline{\Psi}_0\beta^4 + \overline{\Psi}_0\overline{\beta}^4 + 6\overline{\beta}^2\overline{\Psi}_2\gamma^2 + \overline{\Psi}_0\alpha^4)\Psi_0 - 24\Psi_2^2(4\overline{\Psi}_2\alpha\gamma\beta\overline{\beta} + \overline{\Psi}_2\overline{\beta}^2\beta^2 + \overline{\Psi}_2\alpha^2\gamma^2 + \overline{\Psi}_0\beta^2\gamma^2 + \overline{\Psi}_0\alpha^2\overline{\beta}^2).$$

After eliminating γ using the Ricci invariant r_1, and some simple recombining, these equations reduce to

$$16(\overline{q}^4\Psi_0 + \Psi_0 + 6\overline{q}^2\Psi_2)(6q^2\overline{\Psi}_2 + q^4\overline{\Psi}_0 + \overline{\Psi}_0)\alpha^8 + 32\overline{q}\sqrt{\overline{r_1}}q(3\Psi_2 + \overline{q}^2\Psi_0)(\overline{\Psi}_0q^2 + 3\overline{\Psi}_2)\alpha^6 + (24r_1\overline{q}^2q^2\overline{\Psi}_0\Psi_0 + 24r_1\Psi_0\overline{q}^2\overline{\Psi}_2 - 4u_4 + 24r_1\Psi_2q^2\overline{\Psi}_0)\alpha^4 + 8\Psi_0\overline{\Psi}_0r_1^{3/2}q\alpha^2\overline{q} + \Psi_0\overline{\Psi}_0r_1^2 = 0, \tag{5}$$

$$8\overline{q}^2(6q^2\overline{\Psi}_2 + \overline{\Psi}_0q^4 + \overline{\Psi}_0)\alpha^4 + 8\overline{q}\sqrt{\overline{r_1}}q(\overline{\Psi}_0q^2 + 3\overline{\Psi}_2)\alpha^2 + 2r_1\overline{\Psi}_0q^2 + u_5 = 0, \tag{6}$$

where the nonzero term $(3\Psi_2 - \Psi_0)(3\Psi_2 + \Psi_0)$ has been cancelled from Eq. (6) and where $q = \beta/\alpha$ and u_4 and u_5 are defined by

$$u_4 = m_4 - 6r_1\overline{\Psi}_2\Psi_2,$$

$$m_5 = u_5(3\Psi_2 - \Psi_0)(3\Psi_2 + \Psi_0) + 2\Psi_2m_4 - 18r_1\overline{\Psi}_2\Psi_2^2 + 2r_1\overline{\Psi}_2\Psi_0^2.$$

Solving Eq. (6) for q^4 and substituting it into Eq. (5) yields

$$16\overline{q}\sqrt{\overline{r_1}}\Psi_0q(\overline{q}-1)(\overline{q}+1)(\overline{q}^2+1)(\overline{\Psi}_0q^2 + 3\overline{\Psi}_2)\alpha^6 + (24\overline{\Psi}_2\overline{q}^4\Psi_0r_1 + 20\overline{q}^4\Psi_0r_1\overline{\Psi}_0q^2 - 12\Psi_2\overline{q}^2u_5 - 4\Psi_0r_1\overline{\Psi}_0q^2 - 2\overline{q}^4\Psi_0u_5 - 4u_4\overline{q}^2 - 2\Psi_0u_5)\alpha^4 - 8\Psi_0\overline{\Psi}_0r_1^{3/2}q\alpha^2\overline{q}^3 + \Psi_0\overline{\Psi}_0r_1^2\overline{q}^2 = 0. \tag{7}$$

Finally, making one more variables change $\{f = q^2, h = q\overline{q}\alpha^2\}$ Eqs. (6) and (7) become

$$(48f\overline{\Psi}_2 + 8\overline{\Psi}_0f^2 + 8\overline{\Psi}_0)h^2 + 8\sqrt{r_1}f(\overline{\Psi}_0f + 3\overline{\Psi}_2)h + f(2\overline{\Psi}_0r_1f + u_5) = 0 \tag{8}$$

and

$$16\sqrt{r_1}\Psi_0(\overline{f}-1)(\overline{f}+1)(\overline{\Psi}_0f + 3\overline{\Psi}_2)h^3 + (-4u_4\overline{f} - 2\Psi_0u_5 + 24r_1\Psi_0\overline{f}^2\overline{\Psi}_2 + 20\Psi_0r_1\overline{\Psi}_0f\overline{f}^2 - 12\Psi_2\overline{f}u_5 - 4\Psi_0r_1\overline{\Psi}_0f - 2\Psi_0u_5\overline{f}^2)h^2 + 8\Psi_0\overline{\Psi}_0r_1^{3/2}h\overline{f}^2f + \Psi_0\overline{\Psi}_0r_1^2\overline{f}^2f = 0. \tag{9}$$

Next we compute the resultant of Eqs. (8) and (9) with respect to f to obtain the consistency condition

$$-1024r_1\Psi_0^2(\overline{f}-1)^2(\overline{f}+1)^2(3\overline{\Psi}_2 - \overline{\Psi}_0)(3\overline{\Psi}_2 + \overline{\Psi}_0)h^6 - 512\Psi_0^2r_1^{3/2}(\overline{f}-1)(\overline{f}+1)(5\overline{f}^2-1) \times (3\overline{\Psi}_2 - \overline{\Psi}_0)(3\overline{\Psi}_2 + \overline{\Psi}_0)h^5 + (384r_1\Psi_0\overline{f}^3\overline{\Psi}_2u_4 + 64u_4{}^2\overline{f}^2 + 16128\overline{\Psi}_2^2\Psi_0^2r_1{}^2\overline{f}^2 + 32\Psi_0^2u_5{}^2\overline{f}^2 + 16\Psi_0^2u_5{}^2 + 384\overline{\Psi}_2\Psi_0r_1u_4\overline{f} - 192\overline{\Psi}_2\Psi_0^2r_1u_5 + 384\Psi_2\overline{f}^2u_5u_4 + 64\overline{\Psi}_0^2\Psi_0^2r_1{}^2 + 64\Psi_0u_5\overline{f}^3u_4 + 16\Psi_0^2u_5{}^2\overline{f}^4 + 192\Psi_2\overline{f}^3u_5{}^2\Psi_0 + 192\Psi_2\overline{f}u_5{}^2\Psi_0 + 1152r_1\Psi_0\overline{f}^3\overline{\Psi}_2\Psi_2u_5 - 23040r_1{}^2\Psi_0^2\overline{f}^4\overline{\Psi}_2^2 + 1152r_1\Psi_0^2\overline{f}^2\overline{\Psi}_2u_5 - 192r_1\Psi_0^2\overline{f}^4\overline{\Psi}_2u_5 + 1152\overline{\Psi}_2\Psi_0r_1\Psi_2\overline{f}u_5$$

$$+576\Psi_2^2\overline{f}^2u_5{}^2+2624\overline{\Psi}_0^2\Psi_0^2r_1{}^2\overline{f}^4-1664\overline{\Psi}_0^2\Psi_0^2r_1{}^2\overline{f}^2+64u_4\overline{f}\Psi_0u_5)h^4$$

$$-32\overline{f}\sqrt{r_1}(-18r_1\Psi_2u_5\Psi_0\overline{\Psi}2-6r_1u_4\Psi_0\overline{\Psi}_2-u_4\Psi_0u_5-44r_1{}^2\overline{f}^3\overline{\Psi}_0^2\Psi_0^2-\overline{f}^3\Psi_0^2u_5{}^2$$

$$+12r_1\overline{f}^3\overline{\Psi}_2\Psi_0^2u_5-54r_1\overline{f}^2\overline{\Psi}_2\Psi_0\Psi_2u_5-2\overline{f}u_4{}^2-\overline{f}\Psi_0^2u_5{}^2-18\overline{f}\Psi_2^2u_5{}^2-3\overline{f}^2\Psi_0u_5u_4$$

$$-144r_1^2\overline{f}\overline{\Psi}_2^2\Psi_0^2-12\overline{f}\Psi_2u_5u_4-18r_1\overline{f}^2\overline{\Psi}_2\Psi_0u_4-9\overline{f}^2\Psi_2u_5{}^2\Psi_0+360r_1{}^2\overline{f}^3\overline{\Psi}_2^2\Psi_0^2$$

$$-3\Psi_2u_5{}^2\Psi_0+12r_1{}^2\overline{f}\overline{\Psi}_0^2\Psi_0^2-36r_1\overline{f}\overline{\Psi}_2\Psi_0^2u_5)h^3-8\overline{f}r_1(36r_1\overline{f}^3\overline{\Psi}_2\Psi_0^2u_5-3\Psi_2u_5{}^2\Psi_0$$

$$+360r_1{}^2\overline{f}^3\overline{\Psi}_2^2\Psi_0^2-3\overline{f}^3\Psi_0^2u_5{}^2-u_4\Psi_0u_5-52r_1{}^2\overline{f}^3\overline{\Psi}_0^2\Psi_0^2-21\overline{f}^2\Psi_2u_5{}^2\Psi_0-2\overline{f}u_4{}^2$$

$$-12\overline{f}\Psi2u_5u_4-3\overline{f}\Psi_0^2u_5{}^2-7\overline{f}^2\Psi_0u_5u_4-18\overline{f}\Psi_2^2u_5{}^2+4r_1{}^2\overline{f}\overline{\Psi}_0^2\Psi_0^2-36r_1\overline{f}^2\overline{\Psi}_2\Psi_0u_4$$

$$-108r_1\overline{f}^2\overline{\Psi}_2\Psi_0\Psi_2u_5-48r_1\overline{f}\overline{\Psi}_2\Psi_0^2u_5-72r_1^2\overline{f}\overline{\Psi}_2^2\Psi_0^2)h^2-8\overline{f}^2\Psi_0r_1{}^{3/2}(36r_1^2\Psi_0\overline{f}^2\overline{\Psi}_2^2$$

$$-8r_1{}^2\Psi_0\overline{f}^2\overline{\Psi}_0{}^2+12r_1\Psi_0\overline{\Psi}_2\overline{f}^2u_5-18r_1\overline{f}\overline{\Psi}_2\Psi_2u_5-6r_1\overline{f}\overline{\Psi}_2u_4-6r_1\overline{\Psi}_2\Psi_0u_5-6\overline{f}u_5{}^2\Psi_2$$

$$-\Psi_0u_5{}^2\overline{f}^2-u_5{}^2\Psi_0-2\overline{f}u_5u_4)h-\overline{f}^2r_1{}^2\Psi_0(-4r_1{}^2\Psi_0\overline{f}^2\overline{\Psi}_0^2+12r_1\Psi_0\overline{\Psi}_2\overline{f}^2u_5-\Psi_0u_5{}^2\overline{f}^2$$

$$-6\overline{f}u_5{}^2\Psi_2-2\overline{f}u_5u_4-u_5{}^2\Psi_0)=0. \tag{10}$$

Finally, we take the resultant with respect to $\overline{f}$ of Eq. (10) with the complex conjugate of Eq. (8) to obtain, after some nonzero common factors have been cancelled,

$$4\,294\,967\,296r_1^2(\Psi_0-3\Psi_2)^2(\Psi_0+3\Psi_2)^2(3\overline{\Psi}_2-\overline{\Psi}_0)^2(3\overline{\Psi}_2+\overline{\Psi}_0)^2h^{16}$$

$$+193\,273\,528\,320r_1{}^{5/2}(\Psi_0^2\overline{\Psi}_2^2-9\Psi_2^2\overline{\Psi}_2^2+\Psi_2^2\overline{\Psi}_0^2)(-2\Psi_0^2\overline{\Psi}_0^2+9\Psi_0^2\overline{\Psi}_2^2$$

$$-81\Psi_2^2\overline{\Psi}_2^2+9\Psi_2^2\overline{\Psi}_0^2)h^{15}-134\,217\,728r_1(\Psi_0-3\Psi_2)(\Psi_0+3\Psi_2)(3\overline{\Psi}_2-\overline{\Psi}_0)(3\overline{\Psi}_2+\overline{\Psi}_0)$$

$$\times(-3276\overline{\Psi}_2^2r_1^2\Psi4^2+29\,160\overline{\Psi}_2^2r_1^2\Psi_2^2+216\overline{\Psi}_2^2\Psi_2\overline{u}_5r_1-24\overline{\Psi}_2\Psi_0^2r_1u_5+216\overline{\Psi}_2r_1u_5\Psi_2^2$$

$$+36\overline{\Psi}_2r_1\Psi_2u_4+364\overline{\Psi}_0^2\Psi_0^2r_1^2-3276r_1^2\Psi_2^2\overline{\Psi}_0^2-24\Psi_2\overline{\Psi}_0^2\overline{u}_5r_1-u_4^2)h^{14}+\cdots=0.$$

This is a polynomial of degree 16 in h. The leading term is

$$4\,294\,967\,296r_1^2(\Psi_0-3\Psi_2)^2(\Psi_0+3\Psi_2)^2(3\overline{\Psi}_2-\overline{\Psi}_0)^2(3\overline{\Psi}_2+\overline{\Psi}_0)^2h^{16},$$

which is always nonzero. Hence, with suitable restrictions on the values of the invariants, this polynomial can, in principle, determine h. Once h is determined, the remaining variables α,β and γ are determined and complete backsolving has been achieved.

2. Segre type [1,(111)], Petrov type II:

For this Petrov type $w_2^2=w_1^3$ and $\Psi_2^2=w_1$. In our Weyl canonical frame, the only nonzero Weyl components are Ψ_2 and $\Psi_4=1$. In this case, the complete set is $\{R,w_1,r_1,m_4,m_5\}$. To show this we consider the mixed invariants, which in this frame become

$$m_4=2(2\alpha^4+12\Psi_2\alpha^2\overline{\beta}^2+12\overline{\Psi}_2\alpha^2\beta^2+72\beta^2\overline{\beta}^2\Psi_2\overline{\Psi}_2+36\sqrt{r_1}\beta\overline{\beta}\Psi_2\overline{\Psi}_2+3r_1\Psi_2\overline{\Psi}_2),$$

$$m_5=2(4\Psi_2\alpha^4-12\Psi_2^2\alpha^2\overline{\beta}^2+24\Psi_2\overline{\Psi}_2\alpha^2\beta^2-72\beta^2\overline{\beta}^2\Psi_2^2\overline{\Psi}_2-36\sqrt{r_1}\beta\overline{\beta}\Psi_2^2\overline{\Psi}_2-3r_1\Psi_2^2\overline{\Psi}_2).$$

Eliminating $\overline{\beta}$ from m_4 and m_5 yields

$$\alpha^2+6\Psi_2\beta^2=0$$

or

$$12\Psi_2\alpha^4+\Psi_2\overline{\Psi}_2\alpha^2\beta^2-\Psi_2 m_4-m_5=0$$

or both.

Eliminating $\overline{\beta}$ from m_4 and $\overline{m}_5$ and substituting the resulting expression for β into these two equations yields, respectively,

$$144r_1\Psi_2\overline{\Psi}_2\alpha^4=m_4^2+12r_1\Psi_2\overline{m}_5+36r_1\Psi_2^2\overline{\Psi}_2^2$$

or

$$186\,624r_1\Psi_2\overline{\Psi}_2\alpha^{12}+\cdots=0,$$

which is a polynomial of degree 12 in α. Separately, each of these polynomials can determine α and hence β; then r_1 determines γ.

3. Segre type [1,(111)], Petrov type III:

For this Petrov type $w_1=w_2=0$. In our Weyl canonical frame, the only nonzero Weyl component is $\Psi_3=1$.

The complete set is $\{R,r_1,m_4,m_5\}$. The mixed invariants in this frame take the form

$$m_4=64\alpha^2\beta\overline{\beta}+8\sqrt{r_1}\alpha^2,$$

$$m_5=32\alpha^3\beta.$$

Eliminating β and $\overline{\beta}$ from m_4, m_5 and $\overline{m}_5$ we get

$$128\sqrt{r_1}\alpha^6-16m_4\alpha^4+m_5\overline{m}_5=0,$$

which can be solved for α. Then β and γ are determined by m_5 and r_1, respectively, and complete backsolving has been achieved.

4. Segre type [1,(111)], Petrov type D:

For this Petrov type $w_1=\Psi_2^2$ which determines Ψ_2. In our Weyl canonical frame, the only nonzero Weyl component is Ψ_2. We will use the remaining tetrad freedom to simplify the Ricci components.

Case 1: $\beta\neq0$: In this case, we can make $\beta=1/\alpha$ (real). We will show that the complete set is $\{R,w_1,r_1,m_4\}$. Note that $m_5^2=w_1m_4^2$. Substituting $\gamma=(2\beta\overline{\beta}+\sqrt{r_1})/(2\alpha)$ and $\beta=1/\alpha$ into the mixed invariant m_4 we get $m_4=6\Psi_2\overline{\Psi}_2(\alpha^4r_1+12\alpha^2\sqrt{r_1}+24)/\alpha^4$. This determines α and hence, β and then γ.

Case 2: $\gamma\neq0$ *and* $\beta=0$: In this case, we can make $\alpha=1$, and hence, $\gamma=\frac{1}{2}\sqrt{r_1}$. The complete set is $\{R,w_1,r_1\}$. Note that $m_5^2=w_1m_4^2=36w_1^2\overline{w}_1r_1^2$.

5. Segre type [1,(111)], Petrov type N:

For this Petrov type $w_1=w_2=0$. In our Weyl canonical frame, the only nonzero Weyl component is $\Psi_4=1$. We can use the remaining tetrad freedom to make $\beta=0$ (since $\alpha\neq0$).

In this case, $m_4=4\alpha^4$, $m_5=0$ and $\gamma=\sqrt{r_1}/(2\alpha)$. Hence, the complete set is $\{R,r_1,m_4\}$ and complete backsolving is always possible.

TABLE IV. The complete sets for the different Segre types with no null eigenvector.

PP type	Segre type	Conditions (in Ricci canonical frame)	Complete sets (and subsets thereof)
I	[1,111] [$Z\bar{Z}$,11]		$\{R,w_1,w_2,r_1,r_2,r_3,m_1,m_2,m_3\}$
D	[1,1(11)] [$Z\bar{Z}$,(11)]	$\Psi_0=\Psi_4=\Phi_{11}=0$ $\{\Psi_0=\Psi_1=0$ and $(\Psi_4\neq 0$ or $\Phi_{11}\neq 0)\}$ or $\{\Psi_3=\Psi_4=0$ and $(\Psi_0\neq 0$ or $\Phi_{11}\neq 0)\}$ Otherwise	$\{R,w_1,w_2,r_1,m_6\}$ $\{R,w_1,r_1,r_2,m_4,m_5\}$ $\{R,w_1,w_2,r_1,r_2,m_1,m_2,m_4\}$
O	[1,(111)]		$\{R,w_1,w_2,r_1,m_4,m_5\}$

6. Segre type [1,(111)], Petrov type O

For this Petrov type $w_1=w_2=0$ and $\Psi_i=0$. We can use the tetrad freedom to make $\alpha=\gamma$ and $\beta=0$, i.e., the Ricci canonical frame as well. In this case, $m_4=m_5=0$ and $\alpha^2=\frac{1}{4}r_1$. Hence, the complete set is $\{R,r_1\}$.

IV. SUMMARY OF RESULTS

In Table IV, we give the complete sets of invariants for the different Segre types (with ''essential'' special cases) whose Ricci tensors do not have a null eigenvector. The ''essential'' special cases in this table, although expressed in the Ricci canonical frame, are linked to invariant geometric properties. If $\Psi_0=\Psi_4=0$, then it follows that the two PNDs of the Weyl tensor lie in the two-plane spanned (real or complex) by the two eigenvectors, which lie in the timelike blade $\{l^a,n^a\}$, of the Ricci tensor. If $\Psi_0=\Psi_1=0$, then the Weyl tensor is algebraically special and the repeated PND lies in the two-plane spanned (real or complex) by the two eigenvectors, which lie in the timelike blade $\{l^a,n^a\}$, of the Ricci tensor. Similarly for $\Psi_3=\Psi_4=0$. Finally, if $\Phi_{11}=0$, then the sum of the eigenvalues of the eigenvectors in the timelike blade $\{l^a,n^a\}$ equals twice the eigenvalue of either eigenvector in the spacelike blade $\{x^a,y^a\}$.

V. CONCLUSION

In this second article on the problem of algebraic completeness for the invariants of the Riemann tensor, we have exhaustively analyzed all canonically different space–times in which the Ricci tensor does not have a null eigenvector. In each case, we have given algebraically complete sets. It follows from this work, at least for these cases (class A), that the set CZ is determining, as previously claimed.[1] In a sequel paper, we will present a complete analysis of all Segre types which correspond to the cases when the Ricci tensor has a null eigenvector (class B). Interestingly, we will then show that complete backsolving is, in general,[13] not always possible when there is an alignment between an eigenvector of the Ricci tensor with the repeated principal null directions of the Weyl tensor (excluding [(1,111)]). As previously mentioned, we suspect that some space–times within such classes will, in general, prove to be more difficult to distinguish as inequivalent. As a final point, there still remains to fully clarify the geometric meaning of the invariants, principally the mixed ones. This will be the main focus of future work in this area.

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[4] Equivalent real.
[5] Number (equivalent real) of curvature unknowns solved for in terms of the invariants and remaining, if any, curvature components.

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[13] Special cases do exist which allow complete backsolving. Thus an alignment between an eigenvector of the Ricci tensor with a repeated principal null vector of the Weyl tensor is a necessary but not sufficient condition to prevent complete backsolving. More details on this aspect will be provided in a sequel paper.

On solitons with nonminimally coupled scalar fields

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A nonsingular static and spherically symmetric space–time endowed with nonminimally coupled scalar field described by the action $S=\int d^4x\,(\sqrt{-g}/2)(R-g^{\alpha\beta}\phi_{,\alpha}\phi_{,\beta}-\xi R\,\phi^2)$ is presented for the case in which the coupling parameter $\xi>1/6$. This solitonlike space–time is obtained using the technique of conformal transformation that associates solutions produced by ordinary scalar fields in general relativity with those with nonminimally coupled scalar fields. The dynamical stability of the solution is examined through the Galerkin method. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421060]

I. INTRODUCTION

Nonminimally coupled scalar fields are characterized by the following action integral,

$$S=\int d^4x\,\frac{\sqrt{-g}}{2}(R-g^{\alpha\beta}\,\phi_{,\alpha}\,\phi_{,\beta}-\xi R\,\phi^2), \tag{1.1}$$

where we are adopting $8\pi G=c=1$ and ξ is the coupling constant between the scalar field and the gravitational field. This constant is a free parameter, since particle theory and quantum field calculations are not able to provide a definitive value. Nonminimally coupled scalar fields have been taken into consideration in the inflationary cosmological scenario,[1] with black holes and the No-Hair theorem,[2] and recently connected with gravitational collapse.[3] Some authors in the realm of inflationary scenario have investigating possible constraints on ξ based in the recent observational results from the cosmic microwave background.[4] There are two exceptional cases given by $\xi=0$ and that corresponds to minimal coupling and $\xi=\frac{1}{6}$ for the conformal coupling.

We report here an interesting result concerning the existence of a soliton solution with nonminimally coupled scalar field. In classical field theories a soliton configuration is characterized by a finite distribution of matter confined to a finite region of space for all time, without singularity, and, in general is associated to the existence of conserved Noether currents in the theories. However, there are soliton solutions without an explicit conserved Noether current.[5] The interest on such solitonic configurations relies on the problem of dark matter in cosmology, because the visible and baryonic matter can account for only a small fraction of the total mass of the Universe. Then, a possible solution of this problem is to consider that the dark matter is nonbaryonic in the form of soliton configuration such as scalar soliton stars, oscillating soliton stars, boson stars, Q-balls[6] and nontopological solitons that can arise in a second-order phase transition in the early universe.[7]

The plan of this work is as follows. In Sec. II we present the solution obtained by the technique of conformal transformation together with the discussion of its basic properties. Section

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III deals with the problem of stability of the soliton under small radial perturbations, in which the we have used the Galerkin method. Finally, Sec. IV is devoted to our conclusions.

II. THE CONFORMAL TRANSFORMATION AND THE SOLITONLIKE SOLUTION

The starting point is to consider static and spherically symmetric space–times endowed with a nonminimally coupled scalar field. For the sake of simplicity, we make use of the conformal transformation technique that allows us to transform the action (1.1) in the Einstein frame. This is done if the metric on the Einstein frame, $\tilde{g}_{\mu\nu}$, is related to the metric of the physical frame $g_{\mu\nu}$ by

$$\tilde{g}_{\mu\nu}=\Omega^2 g_{\mu\nu}, \tag{2.1}$$

where $\Omega^2=1-\xi\phi^2$. Also, we introduce the scalar field Φ such that

$$\Phi=\int \frac{\sqrt{1-\xi(1-6\xi)\phi^2}}{1-\xi\phi^2}d\phi. \tag{2.2}$$

Introducing (2.1) and (2.2) into the action (1.1), we obtain

$$S=\int d^4x\frac{\sqrt{-\tilde{g}}}{2}(\tilde{R}-\tilde{g}^{\alpha\beta}\Phi_{,\alpha}\Phi_{,\beta}), \tag{2.3}$$

where Φ is the minimally coupled scalar field in the Einstein frame. Therefore, once a given solution is known in the Einstein frame, it is possible to determine the solution in the physical frame from relations (2.1) and (2.2). Also, it is worthwhile mentioning that the conformal transformation does not modify the symmetries present in the space–time. There is a vast literature about applications of conformal transformations that is not restricted to nonminimally coupled scalar fields, but it can be also used for general scalar-tensor theories and for nonlinear theories of gravity.[8]

To generate static and spherically symmetric space–times with nonminimally coupled scalar fields, we consider the most general asymptotically flat solution for static and spherically symmetric space–time found by Janis *et al.*[9] and also by Wyman:[10]

$$d\tilde{s}^2=-w^{2\alpha}dt^2+w^{-2\alpha}dr^2+r^2w^{2(1-\alpha)}(d\vartheta^2+\sin^2\vartheta\,d\varphi^2), \tag{2.4}$$

$$\Phi=\pm\sqrt{2(1-\alpha^2)}\ln w, \tag{2.5}$$

where $w=\sqrt{1-2M/r}$, M is a positive quantity, and the parameter α is restricted to $0\leqslant\alpha<1$, since the mass measured by an observer at infinity (the Bondi mass), αM, must be positive. The case $\alpha=1$ corresponds to the Schwarzshild space–time. The above solution has a naked singularity at $r=2M$ if $2M<r<\infty$, or at $r=0$ if $-\infty<r<0$, which is in accordance with the No-Hair theorem concerning the absence of a black hole with scalar charge. Bekenstein[11] was the first to present the method of conformal transformation applied to the case $\xi=\frac{1}{6}$, and generate all classes of static and spherically symmetric solutions for conformally coupled scalar fields. The main result was a solution representing a black hole with a nontrivial scalar field, which in principle threatened the No-Hair theorem. However, later it was shown[12] that the Bekenstein solution is actually unstable under small radial perturbations. In order to complete the analysis connected with this issue, Bekenstein and Saa[2] have proved that there is no black hole configurations with general nonminimally coupled scalar fields. Then, the question is: why would we be interested in searching for any new solution for static and spherically symmetric space–times with nonminimally scalar fields, if, except for the Bekenstein black hole, all remaining solutions have naked singularities? If this information is true, then our analysis would not make sense, but we are going to show that there exist a class of solitonlike configurations generated by nonminimally coupled scalar fields.

Let us consider the case $\xi>\frac{1}{6}$. Integrating Eq. (2.2), the resulting relation between Φ and ϕ is

$$\Phi = -\sqrt{\frac{6\,\xi-1}{\xi}}\sinh^{-1}\sqrt{\xi\,(6\,\xi-1)}\,\phi + \sqrt{\frac{3}{2}}\ln\left|\frac{\sqrt{6}\,\xi\,\phi+\sqrt{1-\xi\,(1-6\,\xi)\,\phi^2}}{\sqrt{6}\,\xi\,\phi-\sqrt{1-\xi\,(1-6\,\xi)\,\phi^2}}\right|. \tag{2.6}$$

From above, it is not possible to derive an expression $\phi=\phi(r)$ after substituting Eq. (2.5) into Eq. (2.6), except for the conformally coupled case $\xi=\frac{1}{6}$. This difficulty is overcome if we consider ϕ as the new ''radial'' coordinate, so that $r=r(\phi)$, and consequently $w=w(\phi)$. Therefore, the line element in the physical frame can be written as

$$d\,s^2 = -\frac{w^{2\,\alpha}}{(1-\xi\,\phi^2)}\,d\,t^2 + \frac{w^{-2\,\alpha}}{(1-\xi\,\phi^2)}\left(\frac{d\,r}{d\,\phi}\right)^2 d\,\phi^2 + \Sigma(\phi)^2\,(d\,\vartheta^2+\sin^2\vartheta\,d\,\varphi^2), \tag{2.7}$$

where $\Sigma(\phi)$ is the proper radius of the two-spheres given by

$$\Sigma(\phi)^2 = \frac{r^2\,(\phi)\,w^{2\,(1-\alpha)}}{1-\xi\,\phi^2}, \tag{2.8}$$

with $r(\phi)=2\,M/[1-w^2\,(\phi)]$. The function for $w(\phi)$ is determined after substituting Eq. (2.5) into Eq. (2.6). For sake of completeness, we have

$$w(\phi) = \left(\pm\frac{\sqrt{6}\,\xi\,\phi+\sqrt{1+\xi\,(6\,\xi-1)\,\phi^2}}{-\sqrt{6}\,\xi\,\phi+\sqrt{1+\xi\,(6\,\xi-1)\,\phi^2}}\right)^{\gamma}\exp\left(-2\,\gamma\,\sqrt{\frac{6\,\xi-1}{6\,\xi}}\sinh^{-1}(\sqrt{\xi\,(6\,\xi-1)}\,\phi)\right), \tag{2.9}$$

where $\gamma=\pm\sqrt{3}/2\,\sqrt{1-\alpha^2}$. The solutions can be divided into types $A(B)$ according the sign $+(-)$ taken on the rhs of the above equation. Indeed, both types of solution A and B are equivalent due the symmetry of the Eqs. (2.7)–(2.9) under the change $\phi\to-\phi$ and $\gamma\to-\gamma$. For our proposal, we shall consider type A solutions only. Another very important quantity is the local mass function m defined by

$$1-\frac{2\,m}{\Sigma} = g^{\mu\nu}\Sigma_{,\mu}\Sigma_{,\nu} = \Omega^2\,w^{2\,\alpha}\left(\frac{d\,r}{d\,\phi}\right)^{-2}\left(\frac{d\,\Sigma}{d\,\phi}\right)^2, \tag{2.10}$$

with m being interpreted as the effective gravitational mass inside the sphere of radius Σ.

At this point a complete analysis is obtained after accomplishing the following items: (a) behavior of the proper area Σ^2 taking into account that $|\gamma|\geqslant\sqrt{3}/2$ (this corresponds to $0\leqslant\alpha<1$); (b) behavior of the mass function; (c) determination of singularities and regular event horizons; and (d) behavior of radial null rays. As already mentioned, it was shown in previous works that regular event horizons are present only for $\xi=\frac{1}{6}$ and $\gamma=1$ (or $\alpha=\frac{1}{2}$) corresponding to the Bekenstein black hole.

In order to study the behavior of the proper area $\Sigma(\phi)^2$, the scalar field is restricted to assume values inside the interval $|\phi|<1/\sqrt{\xi}$, necessary for the positiveness of the conformal factor $\Omega^2=1-\xi\,\phi^2$. Thus, for all $|\gamma|\geqslant\sqrt{3}/2$, except $|\gamma|=1$, the proper area varies from $\Sigma^2\,(|\phi|=1/\sqrt{\xi})=0$ to $\Sigma^2\,(|\phi|=0)=\infty$ for $|\gamma|>1$, or is infinity in both extremes, namely, $\Sigma^2\,(|\phi|=1/\sqrt{\xi})=\infty$ and $\Sigma^2\,(|\phi|=0)=\infty$, if $\sqrt{3}/2\leqslant|\gamma|\leqslant1$. In both cases, the space–time is asymptotically flat and has a naked singularity at $|\phi|=1/\sqrt{\xi}$, since invariants like R, $R_{\mu\nu}R^{\mu\nu}$ diverge in this region. Considering now the case $\gamma=1$ (type A solution), the scalar field varies in the following intervals: $\phi_*\leqslant\phi\leqslant0$ and $0\leqslant\phi\leqslant1/\sqrt{\xi}$, where $\phi_*<-1/\sqrt{\xi}$ is a solution of $w(\phi_*)^2=1$ (Ref. 13) distinct from $\phi=0$. Both domains of ϕ correspond to different solutions, and we are interested in the solution of the first interval ($\phi_*\leqslant\phi\leqslant0$). The proper area Σ^2 becomes unbounded at $\phi=0$ or $\phi=\phi_*$, having a minimum value distinct from zero for $\phi\in[\phi_*,0]$ as shown in Fig. 1. If one inspects the behavior of the conformal factor $\Omega^2=1-\xi\,\phi^2$, it is immediate to conclude that for $\phi=-1/\sqrt{\xi}$, Ω^2 vanishes, and inside the interval $\phi_*\leqslant\phi\leqslant-1/\sqrt{\xi}$, Ω^2 becomes negative, but the metric remains finite and keeps its signature.[14] This fact can be confirmed analytically after substituting

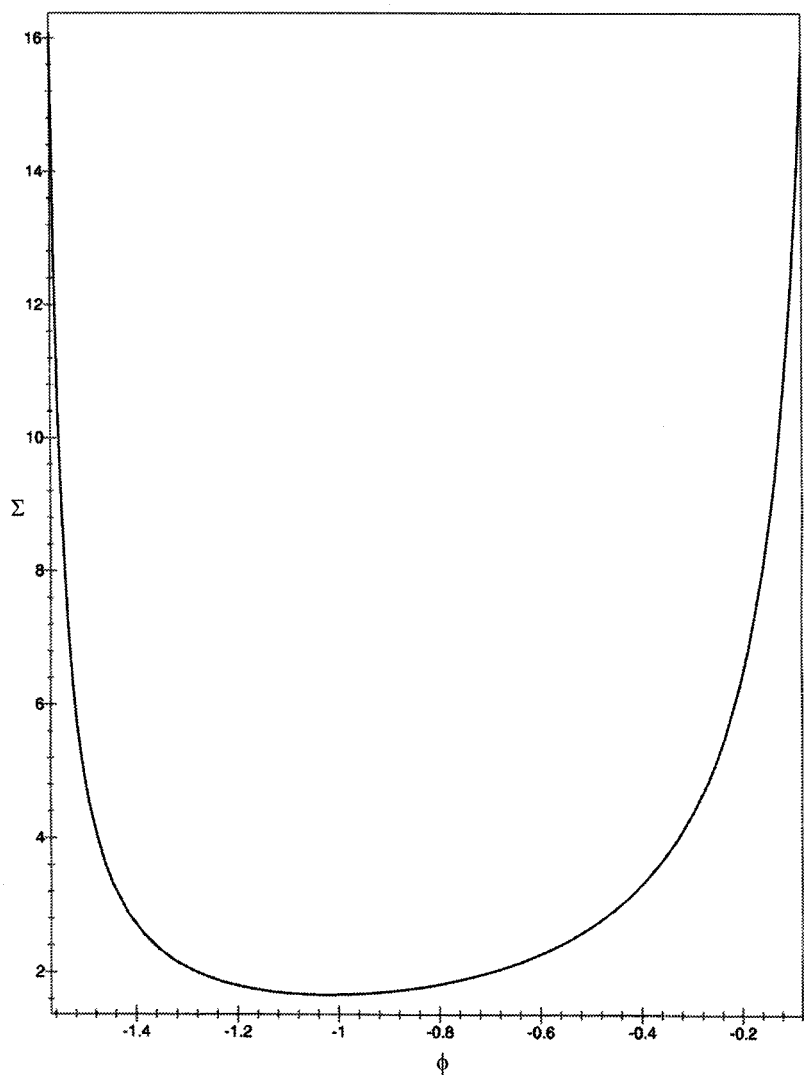

FIG. 1. Plot of the proper radius Σ given by Eq. (2.8), where we have assumed $\xi=1.0$ and $M=1.0$. In this case $\phi_* \approx -1.596\,441\,702\,3$ that characterizes the asymptotically flat region together with $\phi=0$. Here the minimum of the proper radius occurs for $\phi\approx -1.020\,491$.

$\alpha=\frac{1}{2}$ (or $\gamma=1$) into Eq. (2.8), for instance, where for $\phi=-1/\sqrt{\xi}$ both $w(\phi)$ and the conformal factor $\Omega^2=1-\xi\,\phi^2$ vanish, but the quantity $w(\phi)/(1-\xi\,\phi^2)$ remains finite and positive; also for $\phi_*<\phi<-1/\sqrt{\xi}$, both terms of are negative, rendering, again, a positive quantity. The same result is valid for all metric coefficients. We have studied the behavior of the invariants like R, $R_{\mu\nu}R^{\mu\nu}$, $R_{\mu\nu\tau\beta}R^{\mu\nu\tau\beta}$ and $W_{\mu\nu\tau\beta}W^{\mu\nu\tau\beta}$, where $W_{\mu\nu\tau\beta}$ is the Weyl tensor, and the result is depicted in Fig. 2. As we can see, such invariants reach to a finite maximum value at the minimum of the proper area Σ^2 and tend to zero as the proper area approaches to infinity, either for $\phi\to 0$ and $\phi\to\phi_*$. A better understanding of the structure of the space–time is obtained analyzing the behavior of radial light rays, which is done properly using the coordinates (t,Σ). After a straightforward calculation, it follows

$$\frac{d\,\Sigma}{d\,t}=\pm\,\frac{1}{2\,\sqrt{w\,(1-\xi\,\phi^2)}}\left(\frac{1+3\,w^2}{2}-\frac{3\,\xi\,(1-w^2)\,|\phi|}{\sqrt{6}\,\sqrt{1-\xi\,(1-6\,\xi)\,\phi^2}}\right), \tag{2.11}$$

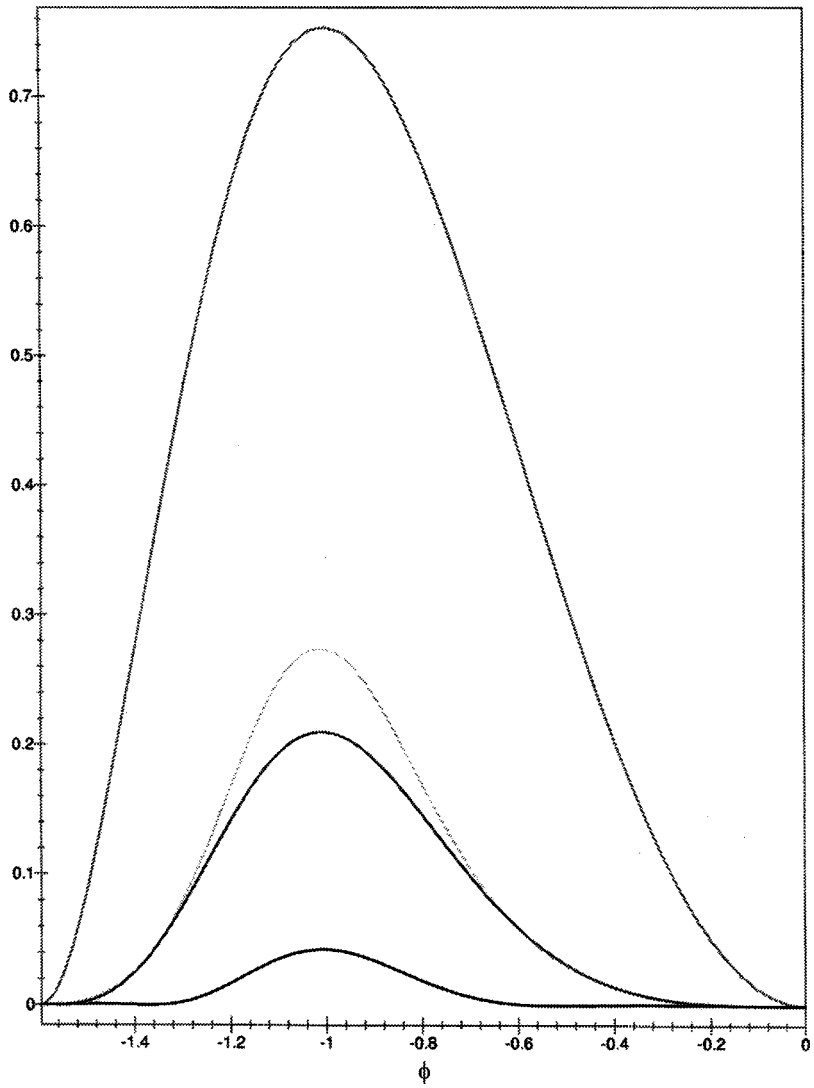

FIG. 2. Invariants R, $R_{\mu\nu}R^{\mu\nu}$, $R_{\mu\nu\tau\beta}R^{\mu\nu\tau\beta}$ and $W_{\mu\nu\tau\beta}W^{\mu\nu\tau\beta}$ versus the scalar field ϕ are plotted for $\xi=1.0$ and $M=1.0$. The maximum value of them occurs at the minimum of the proper radius and tends to zero for either $\phi\to\phi_*$ and $\phi\to 0$.

where the signal $+(-)$ denotes outgoing (ingoing) radial light rays. In Fig. 3, the plot of the above equation is shown, making clear that an initially, say, ingoing ray ($d\Sigma/dt<0$) becomes an outgoing ray ($d\Sigma/dt>0$) after bouncing at the minimum of the proper area where $d\Sigma/dt=0$. An interesting effect appears when the above expression is evaluated in both asymptotic limits, that is, for $\phi=0$ we have $|d\Sigma/dt|=1$, and for $\phi=\phi_*$, it follows $|d\Sigma/dt|=1/\sqrt{\xi\phi_*^2-1}$, such that this ratio is always less than 1 (indeed, we have shown numerically that this is true for all $\xi>\frac{1}{6}$). Therefore, in the asymptotic region characterized by $\phi=\phi_*$, the radial null ray behaves as if it propagates in a medium with an effective "index of refraction" $n=\sqrt{\xi\phi_*^2-1}$. In the limit $\xi\gg\frac{1}{6}$ the velocity of light approaches to 1 (here with the units adopted $c=1$), whereas for ξ tending to $\frac{1}{6}$ the velocity decreases, and in the exact limit $\xi=\frac{1}{6}$ corresponding to the Bekenstein black hole, the velocity vanishes. This means that the light rays are frozen in the event horizon of the black hole in which the proper radius has a finite value and $\phi_*=-\infty$. The last quantity to be

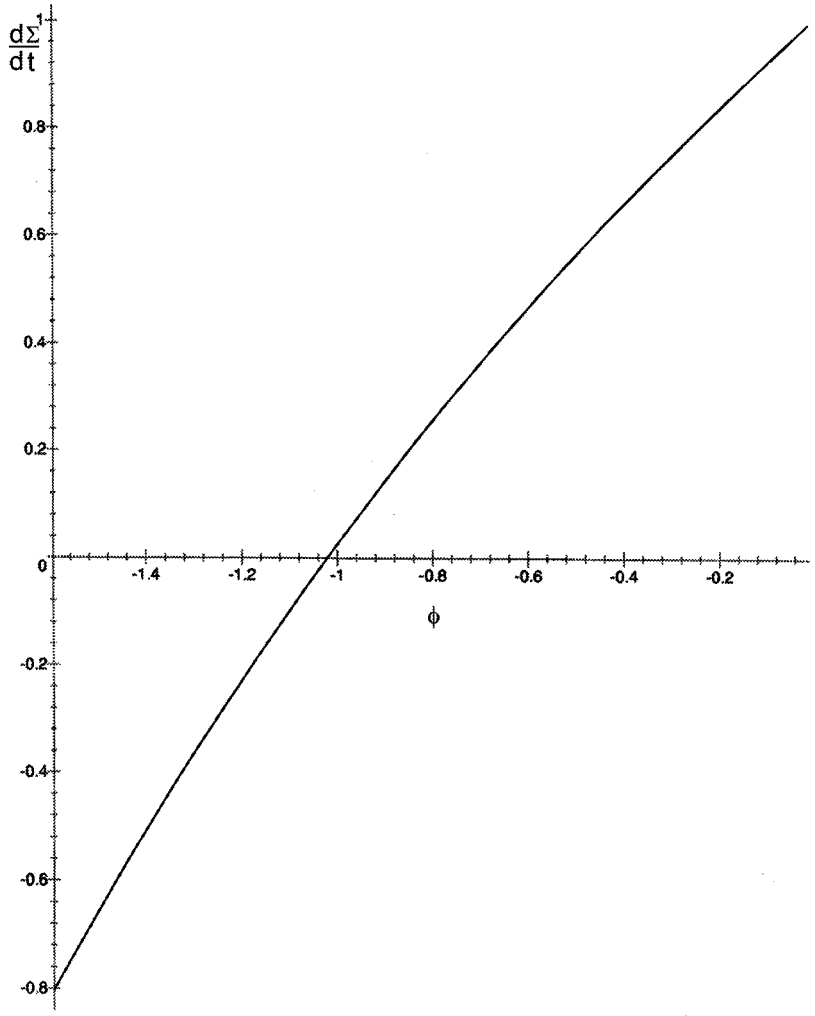

FIG. 3. Behavior of $d\,\Sigma/d\,t$ for radial light rays. The bounce take place at $\Sigma_{\min}$, where $d\,\Sigma/d\,t=0$ for $\phi \approx -1.020\,491$, with the choice $\xi=1.0$. In the asymptotic limit $\phi\to\phi_{*}\approx -1.596\,441\,702\,3$, $d\,\Sigma/d\,t\to 0.814\,53$.

studied is the local mass function defined in Eq. (2.10), whose behavior is sketched in Fig. 4 for $\gamma=1$ and $\xi>\frac{1}{6}$. According to it, the mass function is positive everywhere and has maximum finite value at the minimum of the proper area.

III. STABILITY ANALYSIS AND THE GALERKIN METHOD

We will proceed with the discussion of the stability of the soliton under radial perturbations. For this we first consider the following general spherically symmetric line element

$$ds^2=-e^{\nu(t,\rho)}dt^2+e^{\lambda(t,\rho)}d\rho^2+e^{\beta(t,\rho)}(d\theta^2+\sin^2\theta\,d\varphi^2), \tag{3.1}$$

where ρ is a suitable radial coordinate whose relations with the coordinate r and the scalar field of the background solution, ϕ_0, will be given later. From now on the subscript ''0'' denotes the quantities related to the static background solution described in the last section. The metric functions and the scalar field are perturbations around the background configuration written as

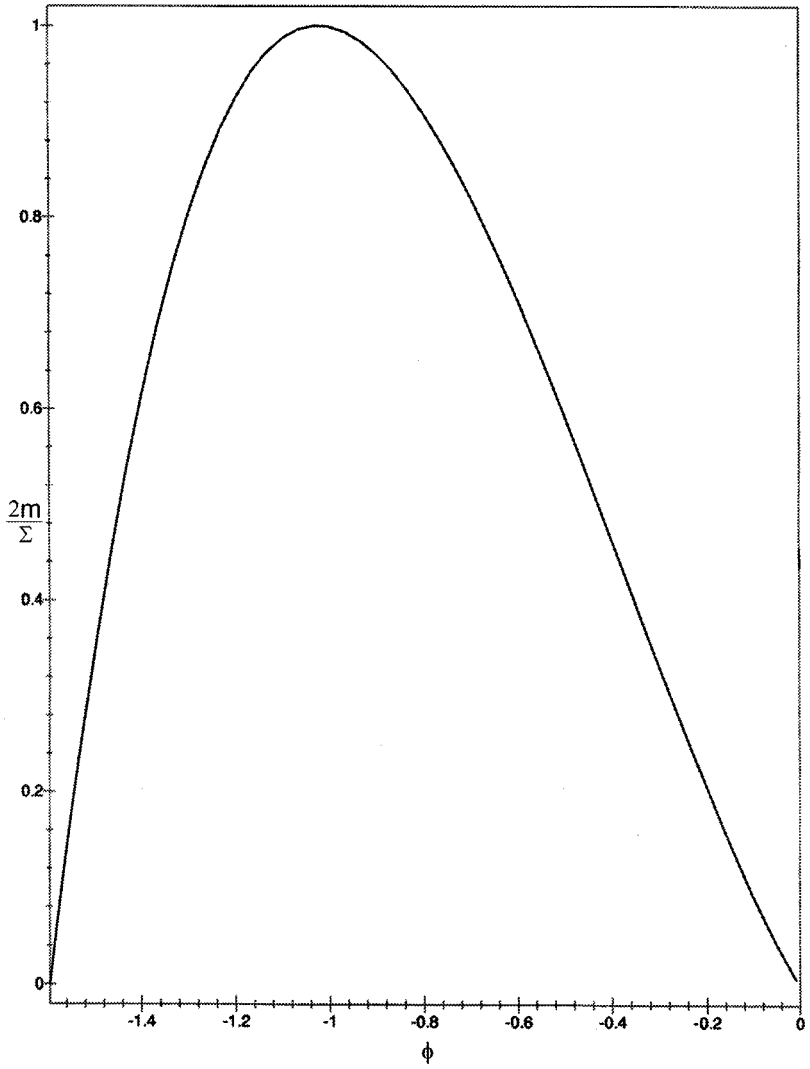

FIG. 4. Behavior of the mass function for $\xi=1.0$ and $M=1.0$, showing that it is positive everywhere.

$$\nu=\nu_0(\rho)+\delta\nu(t,\rho),\quad \lambda=\lambda_0(\rho)+\delta\nu(t,\rho),$$
$$\beta=\beta_0(\rho)+\delta\beta(t,\rho),\quad \phi=\phi_0(\rho)+\delta\phi(\rho,t). \tag{3.2}$$

The set of equations for $\delta\nu$, $\delta\lambda$, $\delta\beta$ and $\delta\phi$ is obtained after substituting the previous ansatz into the field equations and collecting only linear terms in the perturbations. It is possible to decouple the equation for $\delta\phi$ from the other perturbed functions, and afterwards to express $\delta\nu$, $\delta\lambda$ and $\delta\beta$ in terms of $\delta\phi$. Then, the stability/instability is actually determined by the behavior of $\delta\phi$. In order to perform the mentioned decoupling, we impose the following coordinate condition,[12]

$$\delta\nu+2\,\delta\beta=\delta\lambda, \tag{3.3}$$

together with $\nu_0+2\beta_0=\lambda_0$, that is, the same condition is valid for the background metric.

We begin with the equation of motion of the scalar field generated by the action (1.1)

$$g^{\alpha\mu}\phi_{,\alpha;\mu}+h(\phi)g^{\alpha\beta}\phi_\alpha\phi_\mu=0, \tag{3.4}$$

where

$$h(\phi)=\frac{1}{\Delta}\frac{d\Delta}{d\phi}=-\frac{\xi(1-6\xi)\phi}{1-\xi(1-6\xi)\phi^2},$$

with $\Delta=\sqrt{1-\xi(1-6\xi)\phi^2}$, were introduced as a matter of convenience. Note that if $\xi=0$ or $\xi=\frac{1}{6}$, $\Delta=1$ and $h(\phi)=0$. Considering in the above equation the background scalar field together with the coordinate condition $\nu_0+2\beta_0=\lambda_0$, it can be shown that $d\phi_0/d\rho=\text{const}/\Delta_0$. Then, in the special cases $\xi=0,\frac{1}{6}$ the radial coordinate ρ is proportional do the scalar field ϕ_0. Taking the line element (3.1), the ansatz (3.2) and the condition (3.3), the following linearized equation for $\delta\phi$ is derived:

$$e^{\lambda_0-\nu_0}(\ddot{\delta\phi})-(\delta\phi)''-2h(\phi_0)\phi_0'(\delta\phi)'-\left(\frac{dh}{d\phi}\right)_0\phi_0^2\delta\phi=0, \tag{3.5}$$

where prime and dot denote derivative with respect to ρ and t, respectively. The next step is to introduce the function $\psi(\rho,t)$ by

$$\delta\phi=\frac{\psi e^{-\beta_0/2}}{\Delta_0}, \tag{3.6}$$

such that Eq. (3.5) becomes

$$\frac{\partial^2\psi}{\partial x^2}+V(x)\psi=\frac{\partial^2\psi}{\partial t^2}, \tag{3.7}$$

where $V(x)=\frac{1}{2}e^{-2\beta_0}(\frac{1}{2}\beta_0'^2-\beta_0'')$ and x is a new variable related to ρ by $dx/d\rho=e^{\beta_0}$. Also, $dx/d\phi_0=e^{\beta_0}\Delta_0$, which provides a useful relation between ϕ_0 and x, since the background solution is given in function of ϕ_0. In Fig. 5 the potential is plotted as a function of ϕ_0. As expected $V(x(\phi_0))$ is a well behaved function, its maximum value occurs for the minimum of $\Sigma(\phi_0)$, and it vanishes at $\phi_0=\phi_*,0$ which characterizes the asymptotic flat regions. It can be shown that the these asymptotic regions correspond to $x=+\infty,-\infty$, respectively. To Eq. (3.7) suitable boundary conditions must be specified in order to determine the dynamical stability of the soliton. We choose

$$\psi\to 0 \quad \text{for} \quad \phi_0\to 0,\phi_*. \tag{3.8}$$

In the sequence we use the Galerkin method[15] to study the dynamical stability of the background solution. This method is known in applications involving the derivation of finite-dimensional dynamical systems from approximations of infinite-dimensional systems, where one of the most celebrated systems of this form is the one obtained by Lorenz.[16] To begin with we express ψ as a finite sum of time-dependent modal coefficients multiplied by elements of a suitable basis as

$$\psi=\sum_{j=1}^{N}a_j(t)b_j(\phi_0), \tag{3.9}$$

where $b_j(\phi_0)=\sqrt{2/L}\sin j\pi(\phi_0-\phi_*)/L$, $L=|\phi_*|$ are the basis functions that satisfies the boundary conditions (3.8) and are orthonormal, or $(b_j,b_k)=\int_{\phi_*}^{0}b_j(\phi_0)b_k(\phi_0)d\phi_0=\delta_{jk}$. Substituting Eq. (3.9) into Eq. (3.7) and taking the inner product with each basis function, say, $b_k(\phi_0)$, $k=1,2,...,N$, the ϕ_0 dependence will be removed by the spatial integration and we will be left with a set of N coupled ordinary differential equations for the coefficients $a_j(t)$. Then, after direct calculation,

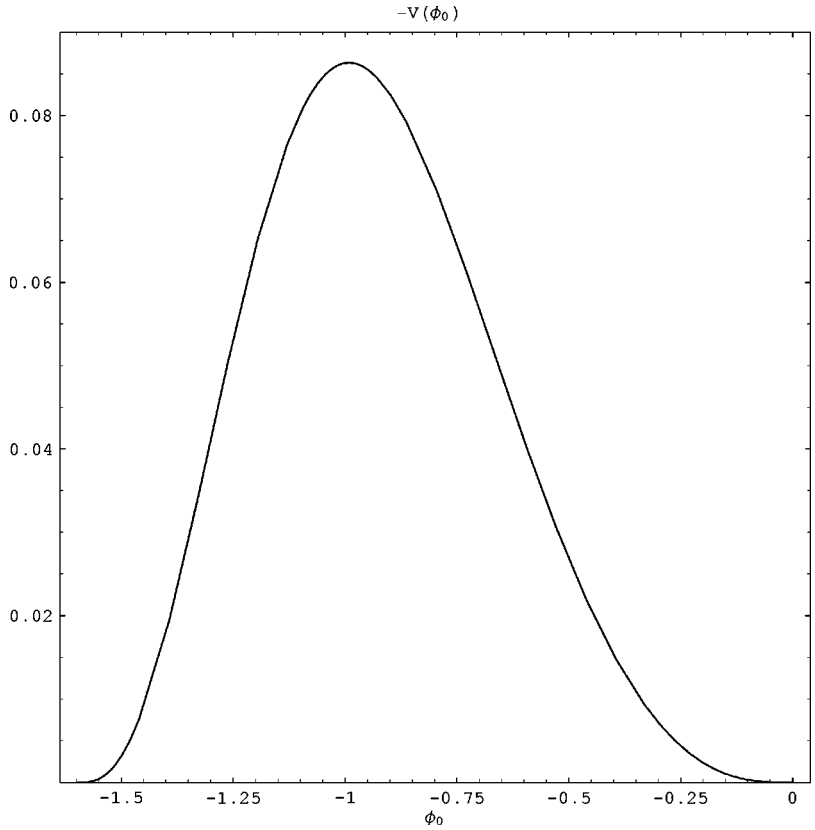

FIG. 5. Potential $V(\phi_0)$ for $\xi=1.0$ and $M=1.0$.

$$\sum_{j=1}^{N} a_j(t)\left[\frac{1}{2}\int_{\phi_*}^{0}\left(\frac{d\phi_0}{dx}\right)^2\left(\frac{d^2b_j}{d\phi_0^2}b_k-\frac{db_j}{d\phi_0}\frac{db_k}{d\phi_0}\right)d\phi_0+(Vb_j,b_k)\right]=\ddot{a}_k(t). \tag{3.10}$$

The first term on the lhs was obtained by integration by parts after taking into account the relation between x and ϕ_0, whereas the rhs is a consequence of the orthogonality condition. Note that the potential is expressed as a function of ϕ_0, or $V(\phi_0)=\frac{1}{2}e^{-2\beta_0}(\frac{1}{2}\beta'^2-\beta'')$ with $e^{\beta_0(\phi_0)}=\Sigma^2(\phi_0)$ given by Eq. (2.8).

The evaluation of the integrals on the lhs of Eq. (3.10) is performed using the background solution of Fig. 1 in which $\xi=1.0$, $M=1.0$ and $\phi_*\approx-1.596\,441\,702\,3$. Choosing the truncation of order five ($N=5$), the set of coupled ordinary differential equations is

$$\begin{aligned}\ddot{a}_1(t)=&-0.091\,674\,171\,681\,681\,25a_1(t)-0.036\,715\,247\,928\,300\,85a_2(t)\\&+0.152\,808\,191\,765\,106\,3a_3(t)+0.073\,750\,165\,035\,988\,63a_4(t)\\&-0.028\,833\,005\,465\,299\,63a_5(t),\end{aligned}$$

$$\begin{aligned}\ddot{a}_2(t)=&-0.021\,125\,139\,415\,259\,99a_1(t)-0.182\,175\,598\,496\,4850a_2(t)\\&-0.040\,747\,263\,640\,001\,60a_3(t)+0.277\,739\,497\,569\,803\,4a_4(t)\\&+0.113\,557\,063\,854\,599\,9a_5(t),\end{aligned}$$

$$\ddot{a}_3(t) = 0.057\,469\,035\,104\,788\,86 a_1(t) - 0.031\,992\,557\,900\,804\,12 a_2(t) - 0.360\,250\,782\,811\,640\,0 a_3(t) - 0.071\,039\,065\,011\,462\,57 a_4(t) + 0.446\,499\,972\,214\,607\,3 a_5(t), \tag{3.11}$$

$$\ddot{a}_4(t) = 0.022\,063\,739\,688\,377\,25 a_1(t) + 0.145\,486\,338\,858\,8478 a_2(t) - 0.056\,014\,320\,562\,388\,30 a_3(t) - 0.611\,788\,072\,949\,546\,4 a_4(t) - 0.109\,873\,233\,512\,505\,2 a_5(t),$$

$$\ddot{a}_5(t) = -0.007\,321\,852\,906\,258\,496 a_1(t) + 0.049\,500\,537\,610\,535\,84 a_2(t) + 0.274\,359\,783\,320\,026\,4 a_3(t) - 0.089\,803\,091\,260\,416\,16 a_4(t) - 0.935\,094\,586\,190\,751\,3 a_5(t),$$

where we have retained only those terms in the sum containing modal coefficients with indices 1 to 5. It is not difficult to show that the solution for each mode has the form of $e^{\kappa t}$, where κ is found to be

$$\pm 1.060\,072\,109\,542\,642 i, \quad \pm 0.835\,466\,769\,461\,132\,2 i, \quad \pm 0.466\,451\,337\,306\,448\,5 i, \quad \pm 0.182\,644\,756\,929\,545\,0 i, \quad \pm 0.329\,073\,934\,727\,850\,6 i. \tag{3.12}$$

For higher-order truncations, the number of equations for the modal coefficients increases, and we have verified that κ is always pure imaginary numbers. This result indicates that all modes oscillate about the background solution, implying the stability of the solution under small radial perturbations.

IV. CONCLUSIONS

We have discussed a static solitonlike solution generated by nonminimally coupled scalar field. The solution was obtained using the technique of conformal transformation that relates the actions integrals (1) and (4). In addition, we have examined the problem of dynamical stability under small radial perturbations, in which the Galerkin method was applied successfully. This method allowed us to reduce Eq. (3.7) to a set of five coupled linear differential equations for the temporal evolution of the perturbations provided that we have restricted ourselves to a truncation of order five in the decomposition (3.9). The system has shown to be identical to a set of coupled harmonic oscillators whose characteristics frequencies are given by (3.12), therefore indicating the stability of the soliton under radial perturbations. As a matter of fact, the effect of higher-order truncations is to increase the number of equations, but not change the nature of the system as a set of coupled harmonic oscillators. As a final remark, we point out the possibility of using the Galerkin method to study semi-analytically the behavior of nonlinear perturbations of either the soliton presented here or any other static configuration, as for instance, a boson star. In this case the resulting finite set of ordinary differential equations is no longer linear and a wealthy behavior is expected.

ACKNOWLEDGMENTS

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[14] It is worthing mentioning that this behavior is also found for the Bekenstein solution characterized by $\xi=\frac{1}{6}$ and $|\gamma|=1$, where the scalar field varies inside the interval $|\phi|<\infty$. Since the conformal factor is $\Omega^2=1-1/6\phi^2$, it is evident that Ω^2 vanishes at $\phi=\sqrt{6}$ and assumes negative values for $|\phi|>\sqrt{6}$.
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On the structure of degenerate solutions of the Einstein conformally invariant scalar system

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We address the question of the existence and construction of nontrivial, regular solutions of the Einstein–conformally invariant massless scalar field equations, i.e., solutions (g,Φ) satisfying $(1-\alpha\Phi^2)R_{\mu\nu}=\alpha(4\nabla_\mu\Phi\nabla_\nu\Phi-2\Phi\nabla_\mu\nabla_\nu\Phi-g_{\mu\nu}\nabla^\sigma\Phi\nabla_\sigma\Phi)$, $\nabla^\mu\nabla_\mu\Phi=0$, and additionally geometry and the scalar field are regular across the degeneracy region defined as the zeros of $(1-\alpha\Phi^2)$. Under the assumptions (1) the solution (g,Φ) is minimally of class C^3 and admits a hypersurface orthogonal, timelike Killing vector field ξ, and (2) relative to the three spacelike hypersurfaces perpendicular to the Killing field, the degeneracy region constitute regular two-surfaces, and the induced positive definite three metric possesses a degenerate Ricci, we show that the conformal system admits nontrivial, regular across the degeneracy region solutions and we demonstrate that any such solution necessarily admits an additional local $G(3)$ group of isometries possessing two-dimensional orbits of constant Gaussian curvature coinciding with the $\Phi=$cons-equipotential two surfaces. Those solutions exhibit similar properties as the Levi–Civita–Ehlers–Kundt class of static solutions of Einstein's vacuum equations. We investigate this coincidence and in particular we probe the origin of the additional local $G(3)$ group of isometries exhibited by both classes of solutions. From the partial differential equations point of view, both systems, i.e., conformal system as well as the vacuum system, degenerate or become singular, the conformal system along solutions subject to $\alpha\Phi^2=1$ within the static region, the vacuum along solutions subject to $V=(-\xi\cdot\xi)^{1/2}\to 0^+$. We demonstrate that as a consequence of the singular nature of the dynamical equations, among all solutions possessing degenerate Ricci in the open vicinity of $\alpha\Phi^2=1$, respectively, $V\to 0^+$, the only regular across degeneracy region solutions are those characterized by a vanishing York–Cotton tensor and, furthermore, such solutions necessarily admit an additional local $G(3)$ group of isometries possessing two-dimensional orbits of constant Gaussian curvature.
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I. INTRODUCTION

It is well known that the n-dimensional conformally invariant generalization of the flat Laplace or massless Klein–Gordon equation is provided by[1]

$$g^{AB}\nabla_A\nabla_B\Phi-\frac{(n-2)}{4(n-1)}R\Phi=0. \tag{1a}$$

If Φ is a solution of this equation and Ω is any smooth positive function, then $\bar{\Phi}=\Omega^{1-n/2}\Phi$ also

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satisfies (1a) provided all geometrical quantities are formed using the conformal metric $\bar{g}_{AB} = \Omega^2 g_{AB}$. Augmenting the conformally invariant action functional $S[g,\Phi]$ by the Einstein–Hilbert term and specializing to $n=4$ space–time dimensions, a theory involving a massless scalar field Φ conformally coupled to the background scalar curvature R is generated. The combined action functional is given by

$$S[g,\Phi] = \int \left(\frac{1}{16\pi G} R - \frac{1}{12}\Phi^2 R + \frac{1}{2}\nabla^\mu \Phi \nabla_\mu \Phi \right) \sqrt{-g}\, d^4x. \tag{1b}$$

and yields, after some rearrangement, the following coupled system:

$$(1-\alpha\Phi^2) R_{\mu\nu} = \alpha(4\nabla_\mu \Phi \nabla_\nu \Phi - 2\Phi \nabla_\mu \nabla_\nu \Phi - g_{\mu\nu} \nabla^\sigma \Phi \nabla_\sigma \Phi), \tag{1c}$$

$$\nabla^\mu \nabla_\mu \Phi = 0, \tag{1d}$$

where in the above $\alpha = k/6 = 8\pi G/6$ stands for an ''effective'' coupling constant and all indices involved are four-dimensional. Thus the concept of the conformally invariant scalar wave equation (1a) leads to a system which is no longer conformally invariant and, moreover, (1c) and (1d) exhibit features that are absent whenever Φ is minimally coupled to gravity. The presence of the second derivatives on the right-hand side of (1c), as well as the presence of the $(1-\alpha\Phi^2)$ factor on its left-hand side, are two notable features.

Bekenstein,[2,3] by cleverly exploiting conformal techniques, was able to generate solutions of the conformal equations starting from solutions of the minimally coupled equations. Additional solutions and properties of solutions can be found in Refs. 4–9. The black hole sector of the theory has been explored in Refs. 10–12, and in summary the theory admits no other classes of static black holes besides the familiar Schwartzschild class, Refs. 10 and 12 The stationary black hole sector has not been exploited in all details, but the circular sector contains only the Kerr family.[11] Solutions of cosmological interest have been presented in Refs. 2 and 13. Noakes, in Ref. 14, has shown that (1c) and (1d) admit a well-posed initial value formulation, a property that is an asset for the theory. Despite all this activity, still the peculiar structure of Eqs. (1c) and (1d) raises a number of questions begging for an answer. If (g,Φ) is a solution (1c) and (1d), then its Ricci tensor fails in general to be semi positive definite i.e., if l is an arbitrary smooth timelike or null vector field, then $R_{\mu\nu} l^\mu l^\nu$ can have any sign. As consequence one cannot easily infer geodesic incompleteness, formation of trapped surface, or, for a black hole space–time, a well-behaved domain of outer communication.[1,15] In short, the analysis of the global structure of space–times (M, g, Φ) with (g,Φ) a solution of (1c) and (1d) is not a trivial issue. The present article primarily is focused on exploring consequences of the intriguing $(1-\alpha\Phi^2)$ factor multiplying the left-hand side of (1c). If (g,Φ) is a solution of (1c) and (1d) so that $(1-\alpha\Phi^2)$ is vanishing but only locally, then (1c) shows that regularity of the simplest scalar invariant $R^{\mu\nu}R_{\mu\nu}$ across zeros of $(1-\alpha\Phi^2)$ requires a special relationship between Φ its first and second derivatives. But what is the precise nature of such interrelationship guaranteeing regularity of (g,Φ) across zeros of $(1-\alpha\Phi^2)$?

If such solutions (g,Φ) exist (and in fact exist), then from the partial differential equation's point of view the system (1c) and (1d) degenerates or becomes singular, in the sense that its highest-order derivatives are nullified on the set of points where $1-\alpha\Phi^2=0$. This latter set will be referred to hereafter as the degeneracy region associated with the particular solution (g,Φ). Accordingly, an answer to the above-posed questions calls for an understanding of the regularity properties of solutions of (1c) and (1d) in the local vicinity of the degeneracy region. Such inquiry is also relevant in another respect that partially motivated the present work. As is well known, Müller zum Hagen,[16] some time ago, has shown that all static, minimally C^3 solutions of Einstein's vacuum equations are real analytic tensor fields within the static region. This analyticity property follows from the fact that sufficiently regular vacuum metrics, whenever expressed relative to a local harmonic chart, satisfy a second-order manifestly elliptic system of equations. Standard result of the so-called elliptic regularity theory then implies real analyticity for the

space–time metric. As it is shown in Ref. 17, Müller zum Hagen theorem extends to suitably smooth static solutions of the nonvacuum Einstein's equations provided the latter equations do not degenerate anywhere within the static region. In that regard static solutions of the Einstein–Klein–Gordon, electrovacuum, or Dilaton gravity of class C^3, or more generally of class $C^{2+\mu}$, $0<\mu<1$, exhibit the same analyticity property as their vacuum counterparts:[17] both geometry and matter fields are analytic within the static region of the space–time manifold. However, an extension of this analyticity property to solutions along which the dynamical equations degenerate runs into obstacles and, in fact, establishing their analyticity (if it holds) is by no means a trivial problem. The conformal system (1c) and (1d) is perhaps the simplest set of equations exhibiting such behavior. It degenerates on static solutions (g,Φ) subject to the vanishing of $(1-\alpha\Phi^2)$ within the static domain. Thus an understanding of the behavior of solutions of (1c) and (1d) across degeneracies would be helpful in formulating a suitable extension of Müller zum Hagen theorem encompassing also solutions along which the relevant equations degenerate.

For orientation purposes, it is worth mentioning here that degenerate set of equations are encountered in other context as well. For instance, the ''conformal vacuum Einstein equations'' written in the ''unphysical manifold,'' degenerate on any solution which is asymptotically flat at future $\mathcal{J}^+$, past $\mathcal{J}^-$ or spacelike infinity i^0.[18] Also the conformally rescaled vacuum Einstein equations degenerate on static, asymptotically Euclidean solutions in the vicinity of the point at infinity.[19–21] Moreover, degeneracies in the Einstein equations may also occur away from the asymptotic regions. On numerous occasions the field equations written relative to a local coordinate chart exhibit such degeneracies.[22] Analysis of the above-mentioned systems reveals that solutions along which a given set of equations degenerates may be smooth across degeneracies. Friedrich, in Ref. 18, has shown that the ''conformal vacuum Einstein equations'' admit analytic solutions across degeneracies while the work of Beig and Simon, and also of Kundu,[21] shows that sufficiently smooth asymptotically flat, static, or stationary solutions of Einstein vacuum equation with nonzero ADM mass are analytic in a vicinity of the point at infinity. The results of Refs. 18 and 21 have been established via a ''desingularization'' procedure, i.e., via a process by which solutions along which the original equations become singular are shown to satisfy an effective set of regular equations. An analysis, then, of the latter system establishes the existence of smooth solutions across the degeneracy region. In brief, therefore, an analysis of solutions of a degenerate system of equations possesses the challenge of constructing an effective set of regular equations where one regains the full strength of the highest-order derivatives. However, and depending upon the structure of the original set, the effective equivalent set is not obvious and often requires considerable labor in constructing it.

The present article is focused on an analysis and properties of solutions (g,Φ) along which the conformal equations (1c) and (1d) degenerate. As far as we are aware, the only knowledge regarding the behavior of solutions of (1c) and (1d) near degeneracies is provided by the work of Ref. 6. In this work static, spherically symmetric, and asymptotically flat solutions of the conformal system have been analyzed and those results are very illuminating within the present context. The conformal system admits the following classes of static, asymptotically flat, and spherically symmetric solutions:[6]

$$ds^2=-\left(1-\frac{r_0}{r}\right)^2dt^2+\left(1-\frac{r_0}{r}\right)^{-2}dr^2+r^2(d\theta^2+\sin^2\theta\,d\varphi^2), \tag{2a}$$

$$\Phi=-\alpha^{-1/2}\frac{r_0}{r-r_0},\quad r_0>0, \tag{2b}$$

$$ds^2=-K^2(r)dt^2+Q^2(r)[dr^2+r^2(d\theta^2+\sin^2\theta d\varphi^2)], \tag{2c}$$

$$K(r)=\frac{1}{2}(R^{(\eta-1)(\eta+3)/4\eta}+R^{(\eta+1)(\eta-3)/4\eta}),\quad Q(r)=\frac{(r-r_0)^2}{2r^2}(R^{(3-\eta)/2\eta}+R^{(3+\eta)/2\eta}),$$

$$\Phi(r)=\alpha^{-1/2}\frac{1-R}{1+R},\quad R(r)=\left(\frac{r+r_0}{r-r_0}\right)^{4\eta/(\eta^2+3)},\quad \eta>0. \tag{2d}$$

However, the curvature of the above metrics exhibits diverse behavior. The curvature of (2a) and (2b) is perfectly smooth across the zeros of the $1-\alpha\Phi^2$, occurring at $r=2r_0$ clearly within the static region. In fact, (2a) and (2b) are the only regular, asymptotically flat, spherical and analytic metric within the static region.[6] On the other hand, the curvature of (2c) and (2d), away from the value $\eta=1$, exhibits different behavior. Even though the factor $1-\alpha\Phi^2$ admits roots (again at $r=2r_0$), the curvature diverges as those roots are approached. The paradigm of (2a)–(2d) suggests that (1c) and (1d) admit solutions where the geometry and the field Φ are perfectly regular over zeros of $(1-\alpha\Phi^2)$, but also solutions where the zeros of $(1-\alpha\Phi^2)$ are accompanied by a singular geometry. Moreover, the ''majority'' of static, spherically symmetric, and asymptotically flat solutions of (1c) and (1d) are singular ''across degeneracies,'' one parameter family of singular solutions versus isolated regular ones. Notice, however, that a third class, involving all those static, with or without spherical symmetry, solutions where the factor $(1-\alpha\Phi^2)$ is nowhere vanishing within the static region is not *a priori* excluded. This class can be handled rather ''straightforwardly'' and according two theorems established by Bekenstein[23] can be put, via a conformal transformation, into a correspondence with solutions of the Einstein–Klein–Gordon massless minimally coupled to gravity equations or even static vacuum solutions of Einstein equations.

The discussion so far and, in particular, the existence of the regular class (2a) and (2b) shows that (1c) and (1d) admit at least one class of regular solution across degeneracies. Naturally then we ask: Do (1c) and (1d) admit other classes of solutions exhibiting the same regularity properties as the class (2a) and (2b)? If so, how one can construct them explicitly? In principle, the construction question can be addressed by taking advantage of the fact that the initial value formulation of the theory is well posed[14] or casting (1c) and (1d) into a system of elliptic equations, once considerations are restricted to static solutions. Unfortunately, however, there are a number of technical difficulties that have to be surpassed first. Solutions of the initial value constraints or choice of boundary data for the elliptic system have to be first addressed and those steps are by no means trivial tasks.

In the present article we shall adopt a method that bypasses the above-mentioned difficulties and it is tailored towards to the construction of degenerate solutions of (1c) and (1d). We shall, however, restrict our considerations to the question of the existence and regularity properties of degenerate solutions (g,Φ) of (1c) and (1d) admitting a hypersurface orthogonal timelike Killing vector field. Since, moreover, very little is known about the connection between the regularity properties of degenerate solutions and the structure of zeros of the $(1-\alpha\Phi^2)$ factor, we shall also invoke some assumptions regarding the structure of the latter ''zero set.'' The hypersurface orthogonal property of the Killing field allows us to project (1c) and (1d) along the local spacelike hypersurfaces perpendicular to the Killing field, thus casting (1c) and (1d) into an equivalent system involving a positive definite metric, the redshift factor, and the scalar field as the field variables. Since the projected equations involve a positive definite metric, the eigenstructure of the associated Ricci tensor is rather simple. We exploit this property and, in fact, the present article is focused exclusively on the investigation of the structure of static solutions of (1c) and (1d) admitting a degenerate three Ricci tensor.[24] Degeneracy on Ricci implies that any static solutions of (1c) and (1d) satisfy a set of nontrivial integrability conditions. Those integrability conditions have been analyzed in detail for the particular case that the redshift factor and the scalar field are functionally related. This functional relation reduces considerably the complexity of the field equations and associated integrability conditions. The latter enable us to write an effective set of regular equations satisfied by any solution of (1c) and (1d) along which the conformal equations degenerate. The study of this effective system allowed us to infer the local existence of solutions

of (1c) and (1d) regular across degenerate regions. Moreover, we have been able to integrate the effective equations and thus provide explicit solutions of (1c) and (1d) regular across the degeneracy regions. Their construction is discussed in detail in Sec. III. Since, as it will become clear further below, all static solutions of (1c) and (1d) admitting a degenerate Ricci and regular across the degeneracy region necessarily admit a local $G(3)$ group of isometries with two-dimensional orbits of constant Gaussian curvature, we devote some effort to understanding the origin of those additional local isometries. As a part of this effort in Sec. IV we turn our attention to Einstein vacuo equations. This vacuum set, written relative to a specific coordinate gauge, also degenerates on any static solution approaching the regions where the magnitude of the Killing field vanishes. We then compare the properties of degenerate classes of solutions of the two systems, and the results of this section make contact with the Levi–Civita–Ehlers–Kundt class of static solutions of the vacuum Einstein equations.[25,26] This contact furnishes further insights into the structure of solutions of the conformal system and those insights are discussed in Sec. IV as well as in the concluding part of the article. As a byproduct, using the integration techniques developed in the present work an *ab initio* construction of the Levi–Civita–Ehlers–Kundt class of vacuum degenerate solutions is also presented.

II. ON STATIC, REGULAR SOLUTIONS OF THE CONFORMAL EQUATIONS

We start by considering a space–time manifold (M,g,Φ) with M a C^k, for some integer k, $k\geqslant 4$, connected, orientable, and paracompact manifold and (g,Φ) a solution of (1c) and (1d) admitting a timelike, hypersurface orthogonal, Killing vector field ξ. We restrict considerations to "classical solutions," i.e., solutions of class C^m, $m\geqslant 3$, so that the field equations and Bianchi identities are pointwise well defined and, in this section, we disregard any (g,Φ) subject to an everywhere constant scalar field Φ. Exploiting the timelike and hypersurface orthogonal property of ξ, a standard construction[1] yields a set of local coordinates, referred to hereafter as Killing coordinates, so that the space–time metric takes the form

$$ds^2=g_{\mu\nu}dx^\mu dx^\nu=-V^2dt^2+\gamma_{ab}dx^a dx^b. \tag{3a}$$

Relative to such coordinates a solution (g,Φ) of (1c) and (1d) satisfies

$$(1-\Phi^2)(R_{ab}-V^{-1}D_aD_bV)=(4D_a\Phi D_b\Phi-2\Phi D_aD_b\Phi-\gamma_{ab}D^c\Phi D_c\Phi), \tag{3b}$$

$$(1-\Phi^2)D^aD_aV=VD^a\Phi D_a\Phi+2\Phi D^a\Phi D_aV, \tag{3c}$$

$$VD^aD_a\Phi=-D^a\Phi D_aV, \tag{3d}$$

where above and hereafter the effective coupling constant α has been absorbed in the field Φ. For part of this article, it is convenient to work with (U,Λ_{ab}) where $V=e^U$, $\gamma_{ab}=V^{-2}\Lambda_{ab}$ instead of (V,γ_{ab}). Performing the local conformal transformation $\gamma_{ab}=V^{-2}\Lambda_{ab}$, the above equations lead into the following equivalent system:

$$(1-\Phi^2)(\overline{R}_{ab}-2\overline{D}_aU\overline{D}_bU)=4\overline{D}_a\Phi\overline{D}_b\Phi-2\Phi\overline{D}_a\overline{D}_b\Phi-2\Phi\overline{D}_a\Phi\overline{D}_bU-2\Phi\overline{D}_aU\overline{D}_b\Phi$$
$$-2\Lambda_{ab}\overline{D}^c\Phi\overline{D}_c\Phi, \tag{4a}$$

$$(1-\Phi)^2\overline{D}^a\overline{D}_aU=\overline{D}^a\Phi\overline{D}_a\Phi+2\Phi\overline{D}^a\Phi\overline{D}_aU, \tag{4b}$$

$$\overline{D}^a\overline{D}_a\Phi=0, \tag{4c}$$

where $(\overline{R}_{ab},\overline{D})$ stand for the Ricci tensor and covariant derivative computed using the positive definite metric Λ.

We are interested in analyzing solutions (Λ,U,Φ) subject to the vanishing of the $1-\Phi^2$ factor within the static region. However, at this point, we know nothing about the structure of the

''zero set,'' i.e., the set defined by $\{x \in M | 1-\Phi^2=0\}$, except that it is a closed subset of M.[27] Its precise nature requires the advance knowledge of the solution itself and the existence of solutions characterized by a topologically complicated zero set cannot be *a priori* excluded. We break this circular state by first imposing conditions on $\{x \in M | 1-\Phi^2=0\}$ and subsequently investigate whether (4a)–(4c) admits solutions compatible with such conditions. As we have also indicated in the Introduction, we shall also functionally relate U and the scalar field Φ and more precisely we shall inquire whether the set (4a)–(4c) admits solutions satisfying

(a) the equipotential ''surfaces'' of U and Φ coincide and
(b) with reference to the local (x^1,x^2,x^3) coordinates covering the $t=$const spacelike hypersurfaces, the (local) level surface $\{(x^1,x^2,x^3)|1-\Phi^2(x^1,x^2,x^3)=0\}$ is not a critical one, i.e., $\overline{D}_a\Phi|_{\Phi^2=1} \neq 0$.

Condition (a) implies that $U=U(\Phi)$ and this relation eliminates the field U from (4a)–(4c), yielding a slightly simpler system to work with. Even though the condition $U=U(\Phi)$ is restrictive, nevertheless it sheds considerable light on the nature of degenerate solutions of (4a)–(4c). In the conclusion section, a few comments regarding the existence of solutions of (4a)–(4c) away from this assumption will be made. Condition (b) ensures that each connected component of the local level surface $\{(x^1,x^2,x^3)|1-\Phi^2(x^1,x^2,x^3)=0\}$ is a regular two-surface. The fact that $\overline{D}_a\Phi|_{\Phi^2=1} \neq 0$ coupled with the differentiability assumptions on Φ implies that an open vicinity of any $\Phi^2=1$ equipotential surface is characterized by the absence of critical points and this property will be used heavily in the upcoming sections. In the alternative possibility, i.e., if (b) is not imposed, then the local level surface $\{(x^1,x^2,x^3)|1-\Phi^2(x^1,x^2,x^3)=0\}$ may admit critical points.[28] The analysis and properties of solutions of (4a)–(4c) near critical points is a rather delicate and difficult issue. Ultimately a complete understanding of the behavior of degenerate solutions of (4a)–(4c) [or of (1c) and (1d)] has to address that possibility. In the present article we gloss it over on the grounds that an understanding of solutions of (4a)–(4c) near critical points would require altogether different techniques than those employed in the present work. We do, however, hope to present such an analysis in the near future. For this section and unless otherwise explicitly stated, all solutions of (3b)–(3d), or equivalently of (4a)–(4c), will be assumed to obey conditions (a) and (b) defined above.

We begin by first utilizing the relation $U=U(\Phi)$ combined with (4b) and (4c). After some algebra, Eqs. (4b) and (4c) imply

$$U(\Phi)=-\frac{1}{2}\left[\ln(1-\Phi^2)+C_1\ln\left(\frac{1-\Phi}{1+\Phi}\right)\right]+C_2, \tag{5a}$$

where (C_1,C_2) are arbitrary integration constants. Substituting this expression into (4a) and tracing, we arrive at

$$(1-\Phi^2)^2\overline{R}=2(C_1^2-1)\overline{D}^a\Phi\overline{D}_a\Phi, \tag{5b}$$

which, combined with condition (b), implies that scalar curvature $\overline{R}$ is regular on any $\Phi^2=1$ equipotential surface provided $C_1^2=1$. Accordingly, regularity of the geometry on $\Phi^2=1$ implies via (5b) that $\overline{R}$ must be vanishing in an open vicinity of any $\Phi^2=1$ equipotential surface. Choosing for the moment $C_1=1$, relation (5a) leads to

$$U(\Phi)=-\ln(1-\Phi)+C_2, \tag{6a}$$

which is manifestly regular on and near any equipotential surface labeled by $\Phi=-1$, but it fails to be so on equipotential surfaces labeled by $\Phi=1$. The choice $C_1=-1$ leads to

$$U(\Phi)=-\ln(1+\Phi)+C_2, \tag{6b}$$

which now exhibits the ''reverse'' behavior, namely it is regular in the vicinity of $\Phi=1$ but singular on the $\Phi=-1$ ones. Since, however, a singular $U(\Phi)$ implies singular space–time geometry, it follows that all solutions of (1c) and (1d) are singular, if they satisfy conditions (a) and (b) and at the same time both types of equipotential surfaces labeled by $\Phi=1$ and $\Phi=-1$ coexist within the static region covered by the local Killing coordinates. Notice that since $\xi\cdot\xi=-e^{2U}$, the above-mentioned singularities are timelike in character. Thus we restrict considerations hereafter to the construction of solutions admitting only one type of equipotential surface taken without loss of generality to be described by $\Phi=1$. Substituting (6b) in (4a)–(4c) combined with $\overline{R}=0$ leads to

$$(1-\Phi^2)\overline{R}_{ab}=6\overline{D}_a\Phi\overline{D}_b\Phi-2\Phi\overline{D}_a\overline{D}_b\Phi-2\Lambda_{ab}\overline{D}^c\Phi\overline{D}_c\Phi, \tag{7a}$$

$$\overline{D}^a\overline{D}_a\Phi=0. \tag{7b}$$

Solutions (Λ,Φ) of this system are characterized by $R=0$ and, if Φ takes the value $\Phi=1$ somewhere within the local $t=$const spacelike hypersurface, then necessarily (7a) and (7b) degenerate on such solutions. Furthermore, every regular solution (g,Φ) satisfies an important property: its York–Cotton tensor R_{abc} (Ref. 29) satisfies

$$\Phi(1-\Phi^2)\overline{R}_{abc}=4\overline{D}_b\Phi\overline{R}_{ca}-4\overline{D}_c\Phi\overline{R}_{ab}-2\overline{D}^d\Phi\overline{R}_{dc}\Lambda_{ba}+2\overline{D}^d\Phi\overline{R}_{db}\Lambda_{ca}, \tag{8a}$$

where we recall that $\overline{R}_{abc}$ is defined by $\overline{R}_{abc}=\overline{D}_b\overline{R}_{ca}-\overline{D}_c\overline{R}_{ba}+\frac{1}{4}(\Lambda_{ab}\overline{D}_c\overline{R}-\Lambda_{ac}\overline{D}_b\overline{R})$. The derivation of (8a) proceeds via differentiation of (7a), antisymmetrization, use of the Ricci identity $\overline{D}_a\overline{D}_b\overline{D}_c\Phi-\overline{D}_b\overline{D}_a\overline{D}_c\Phi=\overline{R}_{abcd}\overline{D}^d\Phi$, and the fact that at three dimensions the Riemann tensor is determined entirely by the Ricci curvature, i.e.,

$$\overline{R}_{abcd}=\Lambda_{ac}\overline{R}_{db}-\Lambda_{bc}\overline{R}_{da}+\Lambda_{bd}\overline{R}_{ca}-\Lambda_{ad}\overline{R}_{cb}+\tfrac{1}{2}(\Lambda_{ad}\Lambda_{cb}-\Lambda_{ac}\Lambda_{db})\overline{R}. \tag{8b}$$

Relation (8a) is satisfied by all regular solutions of (7a) and (7b), and this property is of fundamental importance. As it has been derived here, it holds for every regular solution (Λ,Φ) of (7a) and (7b), but in the sequel we shall use it as a consistency-integrability condition in the following sense: Let $(\overline{\Lambda},\overline{\Phi})$ be a smooth configuration consisting of a three Riemannian metric $\overline{\Lambda}$ and a scalar function $\overline{\Phi}$. In order that this configuration satisfies (7a) and (7b), it is necessary that the Ricci tensor of $\overline{\Lambda}$ and the gradient of $\overline{\Phi}$ satisfy (8a). However, (8a) constrains the Ricci curvature of $\overline{\Lambda}$ and this constraint sheds considerable light onto the nature of potential solutions of (7a) and (7b). Moreover, (8a) must hold true across the $\Phi=1$ equipotential surfaces, provided regular across $\Phi=1$ solution exists. Validity of (8a) across degeneracies demands a fine balance between the Ricci and the gradient of $\overline{\Phi}$. In particular, whenever (8a) is applied to metrics possessing a degenerate Ricci, it imposes strong constraints on the behavior of the Ricci eigenvalues and, in turn, those constraints will help us to identify the classes of regular metrics across the $\Phi=1$ equipotential surface from those that are singular.

With those comments in mind, we first inquire whether in a local vicinity of the $\Phi=1$ equipotential surface, the system (7a) and (7b) admits solutions (Λ,Φ) characterized by a degenerate Ricci tensor. More precisely, we look for solutions (Λ,Φ) so that in an open vicinity of $\Phi=1$ their Ricci is given by

$$\overline{R}_{ab}=\overline{\lambda}(3\hat{\Phi}_a\hat{\Phi}_b-\Lambda_{ab}), \tag{9a}$$

where $\hat{\Phi}=\hat{\Phi}^a\partial/\partial x^a=[\overline{D}^a\Phi/(\overline{D}^a\Phi\overline{D}_a\Phi)^{1/2}]\partial/\partial x^a$ and $\overline{\lambda}$ is a scalar field, a measure of the Ricci eigenvalues. It is implicitly assumed in (9a) that $\overline{\lambda}$ is not identically vanishing and is at least of

class C^1. The special case of an identically vanishing $\overline{\lambda}$ will be discussed at the end of this section while the most general case of a degenerate Ricci will be addressed in Sec. VI. Combining (9a) with Eq. (7a) one finds

$$\overline{D}_a\overline{D}_b\Phi \equiv \lambda_\Phi(3\hat{\Phi}_a\hat{\Phi}_b - \Lambda_{ab}), \tag{9b}$$

where hereafter λ_Φ is defined by

$$\lambda_\Phi := \frac{2\Phi^a\Phi_a - (1-\Phi^2)\overline{\lambda}}{2\Phi}. \tag{9c}$$

Thus $\overline{D}_a\overline{D}_b\Phi$ viewed as a real symmetric matrix admits $D_a\Phi$ also as its distinct eigendirection with corresponding eigenvalue determined by $\overline{\lambda}$ and the gradient of Φ. Notice that had we assumed that a solution (Λ, Φ) existed so that in the open vicinity of $\Phi=1$ the real symmetric matrix $\overline{D}_a\overline{D}_b\Phi$ is given by (9b), then (7a) and (7b) would imply Ricci degeneracy over the same region and thus there is no loss in generality by assuming degeneracy in the Ricci.

With regard to the system (9a)–(9c) one notices the following: If $(\Lambda,\Phi,\overline{\lambda})$ is any regular solution of (9a)–(9c) so that $\Phi=1$ is a regular two-surface, then this (Λ,Φ) necessarily satisfies (7a) and (7b) and, moreover, (7a) and (7b) degenerates on such solutions. Indeed, substituting the right-hand sides of (9a) and (9b) into the left- and right-hand sides of (7a) and (7b), respectively, yields an equality, provided (9c) holds. But if (9c) holds, then multiplying (9a) by $(1-\Phi^2)$ and using (9c) we obtain

$$\begin{aligned}(1-\Phi)\overline{R}_{ab} &= (1-\Phi^2)\overline{\lambda}(3\hat{\Phi}_a\hat{\Phi}_b - \Lambda_{ab}) \\ &= (1-\Phi^2)\frac{2(\Phi^c\Phi_c - \Phi\lambda_\Phi)}{1-\Phi^2}(3\hat{\Phi}_a\hat{\Phi}_b - \Lambda_{ab}) \\ &= 6\overline{D}_a\Phi\overline{D}_b\Phi - 2\Phi\overline{D}_a\overline{D}_b\Phi - 2\Lambda_{ab}\overline{D}^c\Phi\overline{D}_c\Phi.\end{aligned} \tag{9d}$$

where the above string of equalities holds away from $\Phi=1$, but by continuity arguments they are also valid across $\Phi=1$. Thus particular solutions of the manifestly regular system (9a) and (9b), subject to $\Phi=1$ locally, also satisfy the system (7a) and (7b) and, moreover, the latter system degenerates on such solutions. Accordingly the system (9a)–(9c) offers the means of constructing degenerate solutions of (7a) and (7b) and, in fact, one could construct all degenerate solutions of (7a) and (7b) subject of course to the satisfaction of (9a). Indeed, if (7a) and (7b) admits a regular solution (Λ, Φ) so that its Ricci tensor is given by (9a), then (Λ,Φ) satisfy (9a) and (9b) for a λ_Φ determined by (9c). Regularity of the geometry on and around $\Phi=1$ implies $\overline{R}^{ab}\overline{R}_{ab}=6\overline{\lambda}^2$ and that $\overline{\lambda}$ is necessarily bounded. But for such $\overline{\lambda}$ Eq. (7a) implies that $\overline{D}_a\overline{D}_b\Phi$ is also degenerate with a corresponding eigenvalue λ_Φ related to $\overline{\lambda}$ via (9c) from which it follows that (Λ,Φ) satisfy (9a)–(9c).

In view of those remarks, we now turn our attention to the local properties of solutions (Λ,Φ) satisfying (9a)–(9c). At first, if $(\Lambda,\Phi,\overline{\lambda})$ is any such solution, then the Ricci identity applied to $\overline{D}_a\Phi$ in view of (9b) and (8b) implies

$$\begin{aligned}&(3\hat{\Phi}_b\hat{\Phi}_c - \Lambda_{bc})\overline{D}_a\lambda_\Phi - (3\hat{\Phi}_a\hat{\Phi}_c - \Lambda_{ac})\overline{D}_b\lambda_\Phi + 3\lambda_\Phi(\hat{\Phi}_b\overline{D}_a\hat{\Phi}_c - \hat{\Phi}_a\overline{D}_b\hat{\Phi}_c) \\ &\quad = \overline{\lambda}(\Phi^d\Phi_d)^{1/2}(\hat{\Phi}_b\Lambda_{ac} - \hat{\Phi}_a\Lambda_{bc}),\end{aligned} \tag{10a}$$

where, in arriving at the above results, use of the following easily verifiable relation obtained from (9b) has been made:

$$\overline{D}_a\hat{\Phi}_b=\lambda_\Phi\frac{\hat{\Phi}_a\hat{\Phi}_b-\Lambda_{ab}}{(\Phi^c\Phi_c)^{1/2}}. \tag{10b}$$

Substituting (9a) in (8a) it follows that the right-hand side of the latter is identically zero and thus necessarily Λ is locally conformally flat. Consistency would require $\overline{D}_a\overline{R}_{cb}-\overline{D}_c\overline{R}_{ab}=0$ and this relation demands that the ''eigenvalue'' $\overline{\lambda}$, Φ_a, and Λ_{ab} ought to satisfy

$$\overline{R}_{abc}\equiv(3\hat{\Phi}_c\hat{\Phi}_a-\Lambda_{ca})\overline{D}_b\overline{\lambda}-(3\hat{\Phi}_b\hat{\Phi}_a-\Lambda_{ba})\overline{D}_c\overline{\lambda}+3\overline{\lambda}(\hat{\Phi}_c\overline{D}_b\hat{\Phi}_a-\hat{\Phi}_b\overline{D}_c\hat{\Phi}_a)=0. \tag{10c}$$

Relations (10a) and (10c) constitute a set of tensorial consistency relations required to be satisfied by λ_Φ, $\overline{\lambda}$, $\overline{D}_a\Phi$ as well as Λ_{ab}. Indeed, starting from (10c) and after contracting it with $\hat{\Phi}^b$ we find

$$\overline{R}_{abc}\hat{\Phi}^a\equiv 2(\hat{\Phi}_c\overline{D}_b\overline{\lambda}-\hat{\Phi}_b\overline{D}_c\overline{\lambda})=0. \tag{11a}$$

Utilizing this relation back in R_{abc} we obtain

$$\overline{R}_{abc}\equiv\Lambda_{ba}\overline{D}_c\overline{\lambda}-\Lambda_{ca}\overline{D}_b\overline{\lambda}+3\overline{\lambda}(\hat{\Phi}_c\overline{D}_b\hat{\Phi}_a-\hat{\Phi}_b\overline{D}_c\hat{\Phi}_a)=0. \tag{11b}$$

Forming now $\overline{R}_{abc}\Lambda^{ab}$ it yields

$$\overline{R}_{abc}\Lambda^{ab}\equiv 2\overline{D}_c\overline{\lambda}+3\overline{\lambda}\hat{\Phi}_c\overline{D}^b\hat{\Phi}_b=0, \tag{11c}$$

while, on the other hand, contracting (11b) with $\hat{\Phi}^c$ we get

$$\overline{R}_{abc}\hat{\Phi}^c\equiv\Lambda_{ba}\hat{\Phi}^c\overline{D}_c\overline{\lambda}-\hat{\Phi}_a\overline{D}_b\overline{\lambda}+3\overline{\lambda}\overline{D}_b\hat{\Phi}_a=0, \tag{11d}$$

where in arriving at the above equation use of the fact that $\hat{\Phi}^a$ is a unit geodesic field has been made a conclusion that follows directly from (10b). Although in this and the next section we shall not make use of (11b), nevertheless it is an important relation and its significance will become clear in Sec. VI. Contacting (11c) with any arbitrary smooth vector field Y perpendicular to $\hat{\Phi}^c$ yields

$$\overline{R}_{abc}\Lambda^{ab}Y^c\equiv 2Y^c\overline{D}_c\overline{\lambda}=0, \tag{12a}$$

a relation implying that the gradient of $\overline{\lambda}$ is parallel to Φ^a. On the other hand, forming $\overline{R}_{abc}\Lambda^{ab}\Phi^c$ and rearrangement yields

$$\frac{4\Phi^c\overline{D}_c\overline{\lambda}}{3\overline{\lambda}}-\frac{\Phi^a\overline{D}_a(\Phi^c\Phi_c)}{\Phi^c\Phi_c}=0, \tag{12b}$$

from which we infer

$$\Phi^c\overline{D}_c\left[\log\left(\frac{\overline{\lambda}}{(\Phi^c\Phi_c)^{3/4}}\right)\right]=0. \tag{12c}$$

However, this relation yields

$$\overline{\lambda}=A^2(\Phi^c\Phi_c)^{3/4}, \tag{12d}$$

and A^2 a nonvanishing function constant along the integral curves of $\Phi^c\partial/\partial x^c$. Substituting (12d) back into (9a) and applying the contracted Bianchi identity on $\overline{R}_{ab}$ we eventually conclude with the help of (12a) that A is constant. Thus the satisfaction of the integrability conditions (10c) leads to the ''specification'' of $\overline{\lambda}$ [and thus also of λ_Φ via (9c)]. Let us now turn our attention to condition (10a). As it stands, it involves $\overline{\lambda}$ and λ_Φ, but eliminating λ_Φ using (9c) and straightfor-

ward but long algebra shows that (10a) reduces to (9a). Accordingly, satisfaction of (10a) and (9c) implies satisfaction of (9a). Notice, however, if condition (9c) is not *a priori* imposed, then (10a) yields the following differential constraint relating $\overline{\lambda}$ and λ_Φ:

$$2\Phi^a \overline{D}_a \lambda_\Phi - 6\lambda_\Phi^2 = 2\overline{\lambda}(\Phi^c \Phi_c). \tag{13}$$

This constraint implies that not every solution of (9a) and (9b) is necessarily a solution of (7a) and (7b), but rather, and as we have discussed above, only those solutions of (9a) and (9b) subject additionally to satisfaction of (9c) are solutions of (7a) and (7b). Of course (9c) satisfies (13) as it can easily verified.

Thus the analysis of the integrability conditions (10a) and (10c) leads us to the following problem: Construct all (Λ,Φ) satisfying in the vicinity of the $\Phi=1$ equipotential surface the following equations:

$$\overline{R}_{ab} = A^2(\Phi^c \Phi_c)^{3/4}(3\hat{\Phi}_a \hat{\Phi}_b - \Lambda_{ab}), \tag{14a}$$

$$\overline{D}_a \overline{D}_b \Phi = \frac{1}{2\Phi}(\Phi^c \Phi_c - (1-\Phi^2)A^2(\Phi^c \Phi_c)^{3/4})(3\hat{\Phi}_a \hat{\Phi}_b - \Lambda_{ab}). \tag{14b}$$

Accordingly, the problem of the existence and properties of degenerate solutions of (7a) and (7b) is now shifted in constructing solutions of the above regular effective system of equations characterized by the property that the level surface (or surfaces) defined by $\Phi=1$ are regular two-surfaces. Here the relatively ''simple'' structure of the effective system (14a) and (14b) is mainly due to the special choice of Ricci shown in (9a). In latter sections we shall move away from metrics obeying (9a) but still characterized by a degenerate Ricci. Again we shall construct an effective system of equations but the latter system would be much more complex in comparison to (14a) and (14b). For the moment we turn our attention to the integration of the system (14a) and (14b).

III. THE LOCAL BEHAVIOR OF GEOMETRY AND FIELD NEAR $\Phi=1$

The construction of all Riemannian metrics and fields satisfying (14a) and (14b) is not a trivial task since this system is a set of partial differential equations and at this point no spatial symmetries have been imposed (and, in fact, will not be imposed). Nevertheless, we shall be able to integrate it thanks to the insights furnished by the integrability conditions exploited in the previous section. At first (14b), or equivalently (10b) coupled with the regular nature of the $\Phi=1$ surface, implies that the components of the extrinsic curvature of the family of two-surfaces $\Phi=c$, $c \in (1-\epsilon,1+\epsilon)$, are proportional to their intrinsic two-metric $\gamma^{(2)}$ and that is an important insight. In order to take advantage of it, we shall cast Eqs. (14a) and (14b) into an equivalent first-order system describing the ''evolution'' of the intrinsic metric $\gamma^{(2)}$ and components of the extrinsic curvature K across the equipotential surfaces. Such a procedure is best performed by employing Israel's coordinates[30] adapted to the present situation. Such coordinates are well defined once considerations are constricted to solutions obeying condition (b) of Sec. II. Under that assumption, the equipotential surface $\Phi=1$ is a regular two-space and this coupled with the minimally C^3 assumption on Φ, it follows that $\overline{D}_a\Phi$ is nonvanishing in a local vicinity of $\Phi=1$ equipotential surface. Accordingly, the vector field $n=n^a\partial/\partial x^a=\hat{\Phi}^a\partial/\partial x^a$ ''normal'' to $\Phi=c$, $c\in(1-\epsilon,1+\epsilon)$ is nonsingular for some $\epsilon>0$. Let now (θ^1,θ^2) be arbitrary local coordinates on the $\Phi=1$ surface. Israel's coordinates are constructed by first extending (θ^1,θ^2) of the $\Phi=1$ surface by Lie dragging, them along the integral curves of the ''normal'' field, i.e., $n^a\partial\theta^i/\partial x^a=0$, $i=1,2$. We augment (θ^1,θ^2) by taking as a third coordinate the value of the scalar field Φ viewed as parametrizing the family of the equipotential surfaces. The set (Φ,θ^1,θ^2) provides a local coordinazation of an open vicinity of the $\Phi=1$ surface and, relative to such coordinates, the metric can be written in the form

$$ds^2=\frac{d\Phi^2}{\Phi^a\Phi_a}+\gamma^{(2)}_{ij}d\theta^i d\theta^j=\frac{d\Phi^2}{S^2(\Phi,\theta^1,\theta^2)}+\gamma_{ij}(\Phi,\theta^1,\theta^2)d\theta^i d\theta^j, \tag{15a}$$

where hereafter γ_{ij} stands for the intrinsic metric of the $\Phi=\text{const}$ two-surfaces. Relative to those coordinates, the components of the extrinsic curvature or second fundamental form K_{ij} are given by[1]

$$K_{ij}=\frac{1}{2}L_n\gamma_{ij}=\frac{1}{2}(\Phi^a\Phi_a)^{1/2}\frac{\partial\gamma_{ij}}{\partial\Phi}=\frac{1}{2}S\frac{\partial\gamma_{ij}}{\partial\Phi}. \tag{15b}$$

Projecting Eq. (14a) along the normal and perpendicular directions to the $\Phi=\text{const}$ two-surfaces, we lead into

$$-R^{(2)}-K^{ij}K_{ij}+K^2=4A^2S^{3/2}, \tag{16a}$$

$$D_iK-D_jK^j{}_i=0, \tag{16b}$$

$$-S\frac{\partial K_{ij}}{\partial\Phi}+2K_{il}K^l{}_j-KK_{ij}+\frac{1}{2}R^{(2)}\gamma_{ij}+\frac{1}{S}D_iD_jS-\frac{2}{S^2}D_iSD_jS=-A^2S^{3/2}\gamma_{ij}, \tag{16c}$$

$$\frac{1}{2}S\frac{\partial\gamma_{ij}}{\partial\Phi}=K_{ij}, \tag{16d}$$

$$\frac{\partial S}{\partial\Phi}+K=0, \tag{16e}$$

where in the above $R^{(2)}$ is the scalar curvature of the $\Phi=c$, $c\in(1-\epsilon,1+\epsilon)$ two-surfaces. Equations (16a)–(16e) constitute a complete set of equations describing the ''evolution'' of (γ_{ij},K_{ij}) along the family of $\Phi=c$, $c\in(1-\epsilon,1+\epsilon)$ surfaces. Equations (16a) and (16b) are the ''Hamiltonian'' and ''momentum'' constraint, respectively, while Eqs. (16d) and (16c) are the ''evolution'' equation for (γ_{ij},K_{ij}). Equation (16e) stands for the $(2+1)$ content of $\overline{D}^a\overline{D}_a\Phi=0$.

Our task is now shifted to the integration of the system (16a)–(16e). We shall first satisfy the ''Hamiltonian'' and ''momentum'' constraints and then move into the evolution equations. To start with we recall that Eq. (10b) or equivalently (14b) implies that $\overline{D}_a\hat{\Phi}_b=-\lambda_\Phi\gamma_{ab}/S$ and, in view of the fact that $\hat{\Phi}=[1/(\Phi^a\Phi_a)^{1/2}]d\Phi=n_\Phi d\Phi$ is the field of the unit normals of the $\Phi=c$, $c\in(1-\epsilon,1+\epsilon)$, it follows that relative to the (Φ,θ^1,θ^2) coordinates, the components of K_{ij} are also given by

$$K_{ij}=\overline{D}_i\hat{\Phi}_j=-\frac{\lambda_\Phi\gamma_{ij}}{S}=-\frac{1}{2}\frac{\partial S}{\partial\Phi}\gamma_{ij}, \tag{17a}$$

where in passing to the second equality use of (10b) has been made which, via the relation $(\partial/\partial\Phi)\equiv(\Phi^a/\Phi^b\Phi_b)(\partial/\partial x^a)$, leads to the following string of useful equalities:

$$\lambda_\Phi=\frac{1}{2}\hat{\Phi}^a\hat{\Phi}^b\overline{D}_a\overline{D}_b\Phi=\frac{\Phi^a\Phi^b}{2S^2}\overline{D}_a\overline{D}_b\Phi=\frac{1}{4}\Phi^aD_a(\log S^2)=\frac{1}{4}\frac{\partial S^2}{\partial\Phi}=\frac{1}{2}S\frac{\partial S}{\partial\Phi}. \tag{17b}$$

Substituting the right-hand side of (17a) in the ''momentum constraint'' (16b) it follows that $S(\Phi,\theta^1,\theta^2)$ satisfies

$$\frac{\partial^2S}{\partial\theta^i\partial\Phi}=0. \tag{18a}$$

This equation can be satisfied by any S of the form $S(\Phi,\theta^1,\theta^2)=f(\Phi)+g(\theta^1)+h(\theta^2)$. However, using the fact that $S=(\Phi^a\Phi_a)^{1/2}=(\overline{\lambda}/A^2)^{2/3}$ and appealing to the content of (12a) by identifying Y with $(\partial/\partial\theta^1),(\partial/\partial\theta^2)$, respectively, it follows immediately that

$$\frac{\partial S}{\partial\theta^1}=\frac{\partial S}{\partial\theta^2}=0, \tag{18b}$$

and thus $S=S(\Phi)$ alone, a conclusion of extreme importance. Taking now the trace part of the evolution equation (16c) combined with the ''Hamiltonian constraint'' we lead into

$$-S\frac{d^2S}{d\Phi^2}+\frac{1}{2}\left(\frac{dS}{d\Phi}\right)^2+2A^2S^{3/2}=0, \tag{18c}$$

$$R^{(2)}=K^2+S\frac{\partial K}{\partial\Phi}-2A^2S^{3/2}, \tag{18d}$$

but now (18d) coupled with the fact that A^2 is a constant implies that $R^{(2)}$ is a function only of Φ and thus the Gaussian curvature $G=\frac{1}{2}R^{(2)}$ of any $\Phi=\text{const}$ surface is constant in the sense $R^{(2)}=R^{(2)}(\Phi)$ and this is a second important conclusion. On the other hand, the integration of (18c) yields

$$S(\Phi)=\left(\frac{A^2}{2}\Phi^2+C_1\Phi+C_2\right)^2, \tag{18e}$$

where C_1 and C_2 are arbitrary integration constants. The components of the intrinsic metric γ_{ij} are computed by taking into account that, on the one hand, $K_{ij}=-\frac{1}{2}(\partial S/\partial\Phi)\gamma_{ij}$ while on the other hand from (15b), $K_{ij}=1/2S\partial\gamma_{ij}/\partial\Phi$. It follows from those two equations that $\partial(\gamma_{ij}S)/\partial\Phi=0$, implying further the following expression for the components of the two-metric:

$$\gamma_{ij}=\frac{B}{S(\Phi)}\hat{\gamma}_{ij}, \tag{18f}$$

where B is an arbitrary nonvanishing integration constant and we have taken $\hat{\gamma}_{ij}$ to be a two-Riemannian metric of constant Gaussian curvature $G=(\pm1,0)$. Since two-dimensional spaces of constant Gaussian curvature are locally isometric to a two-Euclidean plane, two-sphere, and the Lobachevsky plane, respectively,[31] there exist local canonical coordinates $(\hat{x}^1,\hat{x}^1)$ such that $\hat{\gamma}_{ij}$ on any $\Phi=\text{const}$ surface can be written in the standard form:

$$ds^2_{(2)}=(d\hat{x}^1)^2+\Sigma^2(\hat{x}^1)(d\hat{x}^2)^2, \tag{18g}$$

with $(\Sigma^2(\hat{x})=\sin^2(\hat{x}),\sinh^2(\hat{x}),1)$ for the case that G equals to $(1,-1,0)$ respectively. With the help of (18f) and the form of $S(\Phi)$ shown in (18e), it follows that the trace-free part of the evolution equations (16c) is identically satisfied. On the other hand, (16e) by virtue of the first and last equalities in (17a) is identically satisfied while requiring equality between the last two expressions requires that (18e) has to satisfy

$$\frac{1}{2}\frac{\partial S}{\partial\Phi}=\frac{\lambda_\Phi}{S}=\frac{2S-(1-\Phi^2)A^2S^{1/2}}{2\Phi}, \tag{18h}$$

and this yields an identity provided $C_2=A^2/2$. Thus eventually $S(\Phi)$ reduces to

$$S(\Phi)=\left(\frac{A^2}{2}\Phi^2+C\Phi+\frac{A^2}{2}\right)^2. \tag{18i}$$

From (18f) it follows that the scalar curvature $R^{(2)}$ of any $\Phi=\text{const}$ surface is given by $R^{(2)}=\pm 2S(\Phi)/B$ and zero, respectively, while use of (18i) in Eq. (18d) gives $R^{(2)}=2S(\Phi)\times(C^2;A^4)$. Consistency of those two expressions fixes a relation between the free parameters $C^2;A^4$ and B. The relation $B=(C^2-A^4)^{-1}>0$ leads to a three-metric relative to which the family of $\Phi=c,\ c\in(1-\epsilon,1+\epsilon)$, equipotential surfaces possess positive Gaussian curvature, while the relations $B=(A^4-C^2)^{-1}>0$, $C^2=A^4$, furnishes metrics where the $\Phi=c,\ c\in(1-\epsilon,1+\epsilon)$, surfaces posses negative and zero curvature, respectively. In summary, therefore, all three metrics Λ satisfying (14a) are given by

$$ds^2=\frac{d\Phi^2}{S(\Phi)^2}+\frac{B}{S(\Phi)}[(dx^1)^2+\Sigma^2(x^1)(dx^2)^2],\quad \Phi\in(1-c,1+c),\ \ c>0, \tag{19a}$$

with $S(\Phi)$ given by (18i) and the constant B is paired to the specific form of $\Sigma(x)$ according to

$$(B=(C^2-A^4)^{-1}>0,\quad \Sigma(x)=\sin x);$$

$$(B=(A^4-C^2)^{-1}>0,\quad \Sigma(x)=\sinh x);\quad (B=1,\ C^2=A^4,\Sigma(x)=1). \tag{19b}$$

As an overall check, the scalar curvature of (19a) for all choices implied by (19b) is identically zero, while a computation of Ricci and $\overline{D}_a\overline{D}_b\Phi$ returns us back (14a) and (14b) as it should be. Notice hereafter we shall disregard the metrics with plane orbits obtained by taking $C=-A^2$ in (19b). Such solutions satisfy $\lim_{\Phi\to 1}\overline{D}^a\Phi\overline{D}_a\Phi=0$, and although they are interesting, their analysis will get us away from the main focus of this article.

The metrics defined by (18g) admit a three-parameters group of isometries acting on any $\Phi=\text{const}$ two-surfaces and if, $\xi_{(i)}$, $i=1,2,3$, stand for the corresponding Killing vectors, they satisfy the following algebra:

$$[\xi_i,\xi_j]=\varepsilon_{ijk}\xi_k,\quad G=1,$$

$$[\xi_1,\xi_2]=\xi_3,\quad [\xi_2,\xi_3]=\xi_1,\quad [\xi_3,\xi_1]=\xi_2,\quad G=-1,$$

$$[\xi_1,\xi_2]=\xi_3,\quad [\xi_2,\xi_3]=\xi_1,\quad [\xi_3,\xi_1]=0,\quad G=0.$$

Because of (18f) and (18i), it is clear that the above Killing vectors generate a local three-parameter Lie group of isometries $G(3)$ for the full three-metric (19a). Thus we arrive at the conclusion that all solutions of (14a) and (14b) necessarily admit a local $G(3)$ group of isometries possessing two-dimensional orbits of constant Gaussian curvature identified with the equipotential $\Phi=c,\ c\in(1-\epsilon,1+\epsilon)$, two-surfaces.[32]

The corresponding space–time metrics can be easily constructed. In fact, it is convenient to express them relative to the same spatial coordinate chart (Φ,θ^1,θ^2) augmented with the Killing parameter taken as the timelike coordinate.[32] Relative to such coordinates they take the following form:

$$ds^2=-\frac{dt^2}{(1+\Phi)^2}+\frac{(1+\Phi)^2}{S(\Phi)}\left(\frac{d\Phi^2}{S(\Phi)}+Bds^2_{(2)}\right),\quad \Phi\in(1-c,1+c),\ \ c>0, \tag{20}$$

where $S(\Phi)$ and $ds^2_{(2)}$ are given by (18i) and (18g), respectively. It can be verified that Φ is a harmonic coordinate relative to the above space–time metric, i.e., $\nabla^a\nabla_a\Phi=0$ and the above metrics combined with (6b) satisfy (4a)–(4c).

Before we analyze their properties, let us for the moment consider the special case where the scalar $\overline{\lambda}$ defined in (9a) is assumed to be identically vanishing in the open vicinity of $\Phi=1$. In that event Eq. (9c) fixes λ_Φ to

$$\lambda_\Phi = \frac{\Phi^a \Phi_a}{\Phi},$$

and thus the conformal system leads (7a) and (7b) to the following effective set of equations:

$$R_{ab} = 0, \tag{21a}$$

$$\overline{D}_a \overline{D}_b \Phi = \frac{\Phi^c \Phi_c}{\Phi}(3\hat{\Phi}_a \hat{\Phi}_b - \Lambda_{ab}). \tag{21b}$$

This system can be integrated by applying the same technique used for (14a) and (14b). Because of (21a) the constraint (10c) is trivially satisfied while a substitution of the value of λ_Φ in (10a) yields also an identity. The $2+1$ splitting of (21a) yields a set of equations obtained directly from (16a)–(16e) by setting $A=0$, while from (21b) one obtains

$$\overline{D}_a \hat{\Phi}_b = \frac{\Phi^c \Phi_c}{\Phi} \frac{(\hat{\Phi}_a \hat{\Phi}_b - \Lambda_{ab})}{(\Phi_c \Phi^c)^{1/2}} = \frac{(\Phi^c \Phi_c)^{1/2}}{\Phi}(\hat{\Phi}_a \hat{\Phi}_b - \Lambda_{ab}).$$

Following identical steps as that carried out in the integration of (14a) and (14b), one now gets in the place of (18c) and (18d)

$$-S\frac{d^2 S}{d\Phi^2} + \frac{1}{2}\left(\frac{dS}{d\Phi}\right)^2 = 0, \tag{22a}$$

$$R^{(2)} = K^2 + S\frac{\partial K}{\partial \Phi}. \tag{22b}$$

Equation (22a) implies

$$S(\Phi) = (C^2 \Phi + C_1)^2, \tag{23a}$$

and the analog of (18h) for the present system requires the above $S(\Phi)$ ought to satisfy

$$\frac{1}{2}\frac{\partial S}{\partial \Phi} = \frac{\lambda_\Phi}{S} = \frac{\Phi^a \Phi_a}{S\Phi} = \frac{S}{\Phi}, \tag{23b}$$

which is the case, provided $C_1 = 0$. However, now $S(\Phi)$ reduces to $S(\Phi) = C^4 \Phi^2$, where we have to rename the integration constant, and in turn (22b) implies

$$R^{(2)} = 2C^4 S(\Phi).$$

Thus for every solution of (21a) and (21b) the $\Phi = c$, $c \in (1-c, 1+c)$, two-spaces are spaces of positive Gaussian curvature. Notice that $C=0$ implies $\overline{D}_a \Phi = 0$, a case excluded by choice. For $S(\Phi) = C^4 \Phi^2$, Eq. (15a) implies that the solution may be written in the form

$$ds^2 = \frac{d\Phi^2}{C^8 \Phi^4} + \frac{1}{C^8 \Phi^2}(d\theta^2 + \sin^2\theta d\phi^2), \tag{24a}$$

yielding the following space–time metric:

$$ds^2 = -\frac{dt}{(1+\Phi)^2} + \frac{(1+\Phi)^2}{C^8 \Phi^4} d\Phi^2 + \frac{(1+\Phi)^2}{C^8 \Phi^2}(d\theta^2 + \sin^2\theta d\phi^2). \tag{24b}$$

Introducing a new coordinate r via $r^2 = (1/C^8)[(1+\Phi)^2/\Phi^2]$, then (24b) can be written in the form

$$ds^2=-\left(1-\frac{r_0}{r}\right)^2 dt^2+\left(1-\frac{r_o}{r}\right)^{-2} dr^2+r^2(d\theta^2+\sin^2\theta d\phi^2),$$

$$\Phi=\frac{r_o}{r-r_o}, \quad r_0=\pm\frac{1}{C^4}, \tag{24c}$$

but this is the solution (2a) and (2b) discussed earlier on, originally discovered by Bekenstein[2,3] and also by Bocharova *et al.* (Ref. 4), rederived in Ref. 6 and analyzed further in Ref. 12. We may add parenthetically that the metrics (2c) and (2d) discussed earlier on, cannot be reached via the techniques of this section. Such metrics satisfy $\bar{R}\neq 0$ (in fact $\bar{R}$ diverges as $\Phi=1$) and thus via Eqs. (5) and (6) are automatically excluded from the present considerations.

Finally, for completeness, let us also examine an intermediate case, i.e., the case where the scalar $\bar{\lambda}$ in (9a) is a nonzero constant. In that event the contracting Bianchi identity applied to (9a) implies $\bar{D}^a\bar{R}_{ab}=6\bar{\lambda}\lambda_\Phi(\bar{D}^a\Phi\bar{D}_a\Phi)^{-1/2}\hat{\Phi}_b$ and thus necessarily $\bar{\lambda}\lambda_\Phi=0$. The case $\bar{\lambda}=0$ has been examined above, while the case $\lambda_\Phi=0$ and $\bar{\lambda}\neq 0$ implies via (9b) that $\bar{D}_a\bar{D}_b\Phi=0$. The contracted Ricci identity applied to $\bar{D}_a\Phi$ yields $\bar{D}^a\bar{D}_a\bar{D}_b\Phi=\bar{R}_{ab}\bar{D}^a\Phi+\bar{D}_b(\bar{D}^a\bar{D}_a\Phi)$, from which we obtain $\bar{R}_{ab}\bar{D}^b\Phi=0$, requiring in turn $\bar{\lambda}=0$. Notice that imposing simultaneously $\bar{\lambda}=0$ and $\lambda_\Phi=0$, then (9c) requires $\bar{D}^a\Phi\bar{D}_a\Phi=0$, i.e., $\bar{D}_a\Phi$ vanishes in the local vicinity of $\Phi=1$ and thus $\Phi=$const. This case, however, has been excluded by choice and one expects all solutions to be vacuum solutions.

In summary we have constructed four classes of nontrivial solutions of the conformal system obeying conditions (a) and (b) and satisfying $1-\Phi^2=0$ within the region covered by the Killing chart. In Sec. V we shall establish their regular nature in the vicinity of the degeneracy, i.e., along and across the $\Phi^2=1$ two-surface. Those solutions are highly symmetric, admitting a local $G(3)$ group of isometries possessing two-dimensional orbits of constant Gaussian curvature, and this striking property needs further elaboration. What is the origin of those local isometries? Is there something special in the structure of (7a) and (7b) that dictates this high degree of symmetry on its solutions, or they are artifacts of the special form of the Ricci employed in (9a)? Do solutions of other degenerate system of equations exhibit such property? In the upcoming sections we shall attempt to provide some insights in the above interrelated questions. We shall do so by comparing properties of solutions of (7a) and (7b) to solutions of a distinct degenerate system of equations. This latter degenerate system of equations is provided by the Einstein' vacuum equations. The two systems exhibit structural similarities and, due to the fact that static solutions of Einstein vacuum equation have been studied for a longer period of time, this comparison offers complementary insights.

IV. STATIC, VACUUM, DEGENERATE SOLUTIONS

In accordance with the above plan, in this section, we shall briefly recall a few aspects of Einstein vacuum equations that will be useful in the sequel. We consider a space–time manifold (M,g), with M a C^k, for some integer k, $k\geqslant 4$, connected, orientable, and paracompact manifold and g a minimally C^3 solution of Einsteins vacuum equations admitting a timelike, hypersurface orthogonal, Killing vector field ξ. Utilizing the timelike and hypersurface orthogonal property of ξ, local Killing coordinates can be employed so that the metric can be written in the form (3a). Relative to such coordinates, Eqs. (3b)–(3d) with $\Phi=0$ yield the effective Einstein vacuum equations

$$VR_{ab}=D_aD_bV, \tag{25a}$$

$$D^aD_aV=0, \tag{25b}$$

where $V^2=-\xi^\mu\xi_\mu$, and γ stands for a positive definite metric, on each $t=$const local coordinate slice. For our purpose, we shall view the above equations as defined on a smooth, orientable,

connected, and paracompact three-dimensional manifold Σ. A triplet then (Σ,γ,V), with (γ,V) satisfying (25a) and (25b), V a positive function on Σ and γ a Riemannian metric, gives rise to four-dimensional Ricci flat solutions of Einstein's vacuum equations. As is well known, (25a) and (25b) does not admit nonflat solutions on any closed manifold Σ. Moreover, a classical theorem due to Lichnerowicz[33] asserts that if (Σ,γ) is complete and $V\to 1$ at infinity, then necessarily $V=1$ everywhere and Σ is the standard R^3 with the flat metric or quotients of R^3 by discrete isometry groups (for a recent derivation of Lichnerowicz theorem under weaker conditions, see the work in Ref. 34). Thus nontrivial solutions (γ,V) of (25a) and (25b) require Σ to be on open manifold possessing nontrivial metric boundary $\dot{\Sigma}$ defined by $\dot{\Sigma}=\bar{\Sigma}-\Sigma$ where $\bar{\Sigma}$ is the Cauchy completion of Σ. Solution (Σ,γ,V), which cannot be extended into a larger domain Σ' consistent with $V>0$, possesses a metric boundary $\dot{\Sigma}$ that may contain nonempty components where $V=0$. Following the terminology in Ref. 34 we designate hereafter this part of $\dot{\Sigma}$ by S and refer to it as the "horizon" associated with the particular solution (Σ,γ,V). If nonempty, it may contain several disconnected components and some of them may even be noncompact. For our purpose we shall be interested in examining solutions (Σ,γ,V) that possess a nonempty S and moreover, (γ,V) extends smoothly up to and including S. In particular, we shall look for solutions subject to the condition that all geometrical scalars are bounded as the "horizon" S is approached and hereafter such solutions, if they exist, will be referred to as a regular in the "open vicinity" of $V=0$. Such solutions will obey $D_aV\neq 0$ on S (Ref. 35) and thus a local vicinity of S can be "foliated" by a sequence of $V=c$, $c\in(0,c)$, $c>0$ equipotential surfaces much the same way as the $\Phi=c$, $c\in(1-\epsilon,1+\epsilon)$, $\epsilon>0$ equipotential surfaces foliate the local vicinity of $\Phi=1$. Moreover, if such solutions exist then by considering any sequence of points in Σ with a limit point on S, the system (25a) and (25b) degenerates on any (γ,V) as the "horizon" S is approached. However, such behavior is also exhibited by the conformal Eqs. (7a) and (7b) as well. If (Λ,Φ) is any solution of (7a) and (7b) satisfying $\Phi>1$, then by considering any sequence of points in the vicinity of $\Phi=c$, $c\in(1,1+\epsilon)$, $\epsilon>0$, and having a limit point on $\Phi=1$, then (7a) and (7b) degenerates along such sequence [although such solutions can be extended as solutions of (7a) and (7b) to a larger domain]. From this viewpoint, the (regular) "horizon" S plays an identical role as the (regular) $\Phi=1$ equipotential surface played in the analysis of regular solutions of the conformal system. Besides this degeneracy aspect, both (25a) and (25b), respectively, (7a) and (7b) contain the second derivatives of the V, respectively, Φ, and as we shall shortly see that is of crucial importance. A minor difference between the two is due to the fact that the right-hand side of (7a) contains additionally the gradient of Φ. Below we shall access the significance of that gradient, but it ought to be stressed that as far as the structure of the equations is concerned, this gradient is insignificant. The crucial structural similarities between the two systems lies in the factors V, respectively $(1-\Phi^2)$ multiplying the highest-order derivatives in the field equations as well as the presence of the second derivatives of V, respectively, Φ, on their right-hand sides. Those two properties are responsible for many common properties shared by corresponding solutions of the two systems.

In the previous section we have seen that solutions of the conformal system possessing a degenerate Ricci and regular in the open vicinity of $\Phi=1$ equipotential surface necessarily possesses an additional local $G(3)$ group of isometries. Due to the similarities between the conformal and vacuo system discussed above it is natural to inquire first whether the vacuo system (25a) and (25b) admits degenerate solutions (γ,V) smooth up to and including the horizon and second, whether such solutions, if they exist, exhibit similar properties to those of the conformal system. Thus we shall look for solutions (γ,V) of (25a) and (25b) subject to the condition that the Ricci tensor of γ is given by [compare to (9a)]

$$R_{ab}=\lambda(3\hat{V}_a\hat{V}_b-\gamma_{ab}), \tag{26a}$$

where $\hat{V}^a\equiv V^a/(V^bV_b)^{1/2}$ and λ is minimally a C^1 function of the local coordinates. Such a Ricci implies via (25a)

$$D_aD_bV=V\lambda(3\hat{V}_a\hat{V}_b-\gamma_{ab})=\lambda_V(3\hat{V}_a\hat{V}_b-\gamma_{ab}). \tag{26b}$$

Moreover, it is rather easy to show that any solution (γ,V) of (25a) and (25b) possesses a York–Cotton tensor R_{abc} satisfying

$$VR_{abc}=2R_{ba}V_c-2R_{ca}V_b+\gamma_{ba}R_{cd}V^d-\gamma_{ca}R_{bd}V^d, \tag{27}$$

a relation which is the analog of Eq. (8a) for the conformal system. Substituting the right-hand side of (26a) in (27) it follows immediately that $R_{abc}=0$. By arguments similar to the conformal case it follows that the analogs to Eqs. (10a) and (10c) are for the present case given by

$$\begin{aligned}&(3\hat{V}_b\hat{V}_c-\gamma_{bc})D_a\lambda_V-(3\hat{V}_a\hat{V}_c-\gamma_{ac})D_b\lambda_V+3\lambda_V(\hat{V}_bD_a\hat{V}_c-\hat{V}_aD_b\hat{V}_c)\\&\quad=\lambda(V_aV^a)^{1/2}[\gamma_{ac}\hat{V}_b-\gamma_{bc}\hat{V}_a],\end{aligned} \tag{28a}$$

$$R_{abc}\equiv(3\hat{V}_c\hat{V}_a-\gamma_{ca})D_b\lambda-(3\hat{V}_b\hat{V}_a-\gamma_{ba})D_c\lambda+3\lambda(\hat{V}_cD_b\hat{V}_a-\hat{V}_bD_c\hat{V}_a)=0. \tag{28b}$$

As long as $\lambda_V=\lambda V$ it follows that satisfaction of (28b) implies satisfaction of (28a) and similar arguments as those used in the previous section leads us into a set of equations analogous to (11a)–(11d) with the sole exception that $\hat{\Phi}_a$ is replaced by $\hat{V}_a$. Thus contracting (28b) with $\gamma^{ac}V^b$ it follows again that

$$V^aD_a[\log(\lambda(V^bV_b)^{-3/4})]=0, \tag{29a}$$

implying $\lambda=A^2(V^bV_b)^{3/4}$. Imposing further the contracted Bianchi identity to (26a), it implies eventually that A^2 is a constant. Thus we lead into the following set of effective equations describing in the open vicinity of $V=0$, vacuo solutions possessing a degenerate Ricci:

$$R_{ab}=A^2(V^bV_b)^{3/4}(3\hat{V}_a\hat{V}_b-\gamma_{ab}), \tag{30a}$$

$$D_aD_bV=A^2V(V^bV_b)^{3/4}(3\hat{V}_a\hat{V}_b-\gamma_{ab}),\quad V\in(0,\epsilon),\quad \epsilon>0. \tag{30b}$$

Obviously this system is identical in structure to that of (14a) and (14b). As a consequence the integration of (30a) and (30b) proceeds in parallel to the method employed for (14a) and (14b) and thus we shall be rather sketchy. The fact that a vicinity of $V=0$ is characterized by the absence of critical points of V allows us to introduce again Israel coordinates.[30] In fact Israel in the original 1967 paper introduced those coordinates precisely to analyze solutions of (25a) and (25b) without, of course, imposing conditions (26a). Thus we shall write locally the metric in the form (15a) with the sole exception that $\Phi^a\Phi_a$ is replaced by V^aV_a. Projecting (30a) and (30b) along the $V=$const two-surface we lead into the system analogous to (16a) where (V,D_aV) replaces $(\Phi,\overline{D}_a\Phi)$ and in (15a) it is now understood that $S(V,\theta^1,\theta^2)$. Applying the same steps that lead us into (18c) and (18d), one now gets

$$S(V)=\left(\frac{A^2}{2}V^2+C_1V+C_2\right)^2.$$

However, since the components of the extrinsic curvature of the $V=$const surfaces are different than the $\Phi=$const surfaces, indeed are given by $K_{ij}=-A^2VS^{1/2}\gamma_{ij}$ [compare to (17a)], it follows now that (18h) rewritten for the present case requires that $C_1=0$, implying that

$$S(V)=\left(\frac{A^2}{2}V^2+C\right)^2. \tag{30c}$$

Completing the integration procedure of (30a) and (30b) we are led to the following three classes of vacuum metric, the analogs of (19a) and (19b) for the conformal case:

$$ds^2=\frac{dV^2}{S(V)^2}+\frac{1}{BS(V)}[(dx^1)^2+\Sigma^2(x^1)(dx^2)^2], \tag{31a}$$

$$B=-2A^2C, \quad C<0, \quad \Sigma(x)=\sin x;$$

$$B=2A^2C, \quad C>0, \quad \Sigma(x)=\sinh x; \quad B=1, \quad C=0, \quad \Sigma(x)=1. \tag{31b}$$

However, it is clear that those solutions exhibit identical symmetry properties as those of the conformal system (7a) and (7b). Indeed, they admit a local $G(3)$ group of isometries possessing two-dimensional orbits of constant Gaussian curvature coinciding with the $V=c$, $c\in(0,\epsilon)$ equipotential surfaces. The corresponding algebra of the infinitesimal generators is identical to the corresponding algebra obeyed by the conformal solutions. Before we continue it is worthwhile to consider the associated space–time metrics. Using (31a), it follows that corresponding space–time metrics are given by

$$ds^2=-V^2dt^2+\frac{dV^2}{S(V)^2}+\frac{1}{BS(V)}[dx^{1^2}+\Sigma^2(x^1)dx^{2^2}], \quad V\in(0,c), \quad c>0, \tag{31c}$$

which are the analogs of (20). Due to the relatively simple form of $S(V)$ the above metrics can be reexpressed in a different coordinate gauge. In fact, setting $S(V)=1/Br^2$ where r is an arbitrary coordinate we lead into

$$ds^2=-\left(1-\frac{2M}{r}\right)dt^2+\left(1-\frac{2M}{r}\right)^{-1}dr^2+r^2(dx^2+\sin^2 x dy^2),$$

$$2M<r<\infty, \quad \text{if } M>0 \quad \text{and} \quad 0<r<\infty, \quad \text{if } M<0, \tag{32a}$$

$$ds^2=-\left(\frac{2M}{r}-1\right)dt^2+\left(\frac{2M}{r}-1\right)^{-1}dr^2+r^2(dx^2+\sinh^2 x dy^2), \quad 0<r<2M, \tag{32b}$$

$$ds^2=-\frac{1}{r}dt^2+rdr^2+r^2(dx^2+dy^2), \quad 0<r<\infty, \tag{32c}$$

where we have defined $M=1/(2C)^{3/2}A$. For the case of (32c) the ranges of each of the (x,y) coordinates is the entire real line, while for the classes (32a) and (32b) the corresponding (x,y) ranges are the familiar ones associated with metrics of constant nonzero Gaussian curvature. The metrics (32a)–(32c) have been derived long ago by Levi–Civita[25] and much later by Ehlers and Kundt[26] with an entirely different motive and point of view than the one pursued here. Here they have been derived as the static solutions of (25a) and (25b) possessing a degenerate Ricci given by (26a) and, as we shall verify in the next sections, possessing regular ''horizon'' S. In the classification scheme of Ref. 26 they belong to the class A and we have chosen to present brief derivation here since, and as far as we are aware, their construction has not been discussed in the current literature.[36] The structure and properties of the above solutions will be compared with the class of solutions of the conformal system constructed in the previous section and this is the subject of the next section.

V. REGULARITY PROPERTIES OF THE DEGENERATE SOLUTIONS

We now briefly turn our attention to the regularity properties of the metrics constructed in the last two sections. At first, for all classes of solutions, the geometry is regular as the degenerate points of the corresponding equations are approached. Indeed from (19a) and (19b) or (32a) and (32b) one gets

$$\overline{R}^{ab}\overline{R}_{ab}=6\overline{\lambda}^2,$$

where $\overline{\lambda}$ equals $A^2S^{3/2}(\Phi)$, respectively, $A^2S^{3/2}(V)$, for the conformal respectively vacuum case, and thus their regular nature as $\Phi=1$, respectively, $V\to 0^+$, is manifest. Examining the Kretchman scalar $K=R^{\mu\nu\sigma\tau}R_{\mu\nu\sigma\tau}$ and $\hat{G}=C^{\mu\nu\sigma\tau}C_{\mu\nu\sigma\tau}$ for the corresponding four metrics (20) one obtains the following expressions:[37]

$$K=\frac{F(\Phi)}{(1+\Phi)^8},\quad \hat{G}=\frac{3(C-A^2)^2(A^2\Phi^2+2C\Phi+A^2)^6}{4(1+\Phi)^8},\quad G=1, \tag{33a}$$

$$K=\frac{F(\Phi)}{(1+\Phi)^8},\quad \hat{G}=\frac{3(C-A^2)^2(A^2\Phi^2+2C\Phi+A^2)^6}{4(1+\Phi)^8},\quad G=-1, \tag{33b}$$

$$K=\frac{3A^{16}(1+\Phi)^8}{32},\quad \hat{G}=0,\quad G=0, \tag{33c}$$

where the function $F(\Phi)$ is defined by

$$F(\Phi)=\tfrac{1}{32}[3A^4\Phi^4+4A^2(4A^2-C)\Phi^3+2(15A^4-8A^2C+2C^2)\Phi^2+4A^2(4A^2-C)\Phi$$
$$+3(9A^4-16A^2C+8C^2)](A^2\Phi^2+2C\Phi+A^2)^6 \tag{33d}$$

and satisfies $F(-1)=56(A^2-C)^8$ and $F(1)=8(23A^4-18A^2C+7C^2)(A^2+C)^6$. The corresponding invariants for the vacuum metrics (31b) and (31c) are given by

$$K=\hat{G}=\tfrac{3}{4}A^4(A^2V^2+2C)^6,\quad G=1, \tag{33e}$$

$$K=\hat{G}=\tfrac{3}{4}A^4(A^2V^2-2C)^6,\quad G=-1, \tag{33f}$$

$$K=\hat{G}=\tfrac{3}{4}A^{16}V^{12},\quad G=0. \tag{33g}$$

Expressions (33a)–(33c) imply that the space–time metrics (20) are regular across the $\Phi=1$ timelike hypersurface, while (33e)–(33g) imply regularity of the geometry as the $V=0$ null hypersurface is approached [disregarding here the case of $M<0$ in (32a)].

As it is clear from their derivations, the metrics (19a) and (19b) and thus also the space–time metrics (20) are local solutions valid within the space–time region covered by the local Killing chart. However, we may extend them maximally and consistently with the existence of the timelike Killing field, by enlarging the Φ-coordinate range, i.e., assuming $\Phi\in(-1,\infty)$ and similarly $V\in(0,\infty)$ [or possibly $V\in(0,1)$]. Let us first consider extension of (20). Disregarding the innocuous coordinate singularities associated with the local (x^1,x^2), coordinates, then for all $t\in(-\epsilon,\epsilon)$ and $\Phi\in(-1,\infty)$ the extended metrics (20) satisfy the conformal equations (1c) and (1d). The three spaces $\Phi=c$, $c\in(-1,\infty)$, are timelike hypersurfaces and, for the special case where the equipotential surfaces $\Phi=\text{const}$, $t=\text{const}$ are assumed to be complete, simply connected Riemannian two-spaces, and thus identified as either the two-sphere, hyperbolic two-space, or the Euclidean plane, respectively, then any $\Phi=c$, $c\in(-1,\infty)$, timelike hypersurface is topologically $(-\epsilon,\epsilon)\times K$ with K either a two-sphere, the hyperbolic two-space or the Euclidean two-space, respectively.[38] However, the so-extended solutions exhibit curvature singularities. In-

deed an examination of (33a) and (33b) shows that the space–time curvature grows unbounded as $\Phi \to -1$ and thus no further extension of the space–time is possible across the $\Phi=-1$ ''timelike hypersurface.'' Exception to that rule constitutes the metrics with plane orbits. For such metrics K, $\hat{G}$ are given by (33c), and thus both of them have smooth limit as $\Phi \to -1^{+}$. This two-''plane'' is at infinite proper distance away from any point on any $t=$const spacelike hypersurface and, moreover, an analysis of the ''outgoing'' timelike, resp. null geodesics, shows that it is located at the ''space–time boundary.'' An infinite amount of proper time, resp. affine parameter, along outgoing causal geodesics is required in order to be reached. In addition to the above-discussed timelike singularities, the extended metrics (20) also exhibit unbounded growth as $\Phi \to \infty$. However, the structure of this singularity is not immediately obvious. In order to get some insights into its structure, let us first introduce advanced Eddington–Finkelstein coordinates[1,15] associated with the line element (20). In such (u,Φ,x^1,x^2) coordinate systems, with $du=dt+[(1+\Phi)^2/S(\Phi)]d\Phi$, (20) takes the form

$$ds^2=-\frac{du^2}{(1+\Phi)^2}+2\frac{2}{S(\Phi)}du d\Phi+\frac{B(1+\Phi)^2}{S(\Phi)}ds^2_{(2)}.$$

An analysis of the geometry using this coordinates is rather tedious. However, since we are only interested in analyzing the structure of the geometry as $\Phi \to \infty$, it is sufficient to examine the behavior of the geometry for large values of Φ. In such limits the leading behavior of the above line element takes the following form:

$$ds^2=-\frac{du^2}{\Phi^2}+2\frac{du d\Phi}{\Phi^4}+\frac{1}{\Phi^2}ds^2_{(2)},$$

where hereafter and for notational simplicity we have set all constants to unit values. Defining further a new coordinate x via $x=-1/\Phi$, $x\in(-\epsilon,0)$, $\epsilon>0$, it follows that the above line element takes the form

$$ds^2=-x^2du^2+2x^2dudx+x^2ds^2_{(2)}=-y^{2/3}du^2+2dudy+y^{2/3}ds^2_{(2)}, \tag{33h}$$

where in passing to the second equality we have defined the coordinate y via $dy=x^2dx$. However, in the above form, the limit $\Phi \to \infty$ corresponds to $y \to 0^{-}$. An analysis of the curvature for $y \in (-\epsilon',0)$ shows that $K=R^{\mu\nu\sigma\tau}R_{\mu\nu\sigma\tau}\equiv 4/27[(27y^{4/3}-6y^{2/3}+2)/y^{8/3}]$ and thus all null geodesic generators of each $u=$const null hypersurface terminate after a finite amount of affine parameter in a curvature singularity. Moreover, the set $y \to 0^{-}$ corresponds to a ''null hypersurface'' and thus the structure of $\Phi \to \infty$ singularity for all extended metrics (20) corresponds to a ''null singularity.''

Let us now briefly discuss the regularity properties of the vacuum metrics (32a)–(32c). At first (33e)–(33g) shows no pathologies in the geometry takes place as the ''$V=0$'' null hypersurface is approached, and the ''bad behavior'' of the metric across ''$V=0$'' is simply a coordinate singularity. The metric (32a) (for $M>0$) as well as (32b) can be analytically extended across the corresponding Killing horizons and their analytical extensions are discussed in the work of Ehlers and Kundt.[26] No analytical extension is required for the case of the metric (32c) since the $V \to 0^{+}$ null hypersurface occurs at the boundary of the space–time, a situation similar to that encountered in the analysis of the metrics (20) possessing plane orbits at the limit $\Phi \to -1$. On the other hand, if the magnitude of the timelike Killing vector is left unrenormalized, then (33) shows that all classes of vacuum metrics becomes singular as the $V \to \infty$ timelike hypersurface is approached and this property is in accord with the behavior of the metrics (20) at the limit of $\Phi \to \infty$ with the exception that the later singularities are null whereas the former are timelike. Imposing asymptotic flatness on (32a)–(32c), one gets the well-known results.

A high degree of subtlety is, however, exhibited by the metric (24c). At first and by construction, (24) is a solution of (1c) and (1d) within the static region, i.e., for all $r>r_0$. An examination

of the scalar invariants K and C shows that both of them are regular for all $r>r_0$. Moreover, the metric can be extended so that it is manifestly regular at $r=r_0$. Indeed, for an analysis along the same lines as those that lead us into (33h) one gets

$$ds^2=-x^2du^2+2dudx+(1-x)^2ds^2_{(2)},\quad x\in(-\epsilon,0),$$

as the $\Phi\to\infty$ limit of the line element (20). However, now $K=R^{\mu\nu\sigma\tau}R_{\mu\nu\sigma\tau}=8(3x^2+1)/(1-x)^2$ from which now it follows that the $x=0$ null hypersurface is regular one, an expectable fact since (20) is isometric to the metric of the extreme Reisner–Nordstrom manifold. Thus the geometry can be extended through the Killing horizon and details of this extension are for instance, discussed in Ref. 15. However, due to the fact that the scalar field Φ diverges as the Killing horizon is approached, the solution (24c) cannot be extended across the Killing horizon as a solution of the conformal equations (7a) and (7b). The reason for this failure as well as its implications are discussed in detail in Ref. 12.

VI. DEGENERATE SINGULAR SOLUTIONS

In the last three sections we have analyzed solutions of the conformal system (7a) and (7b) as well as of the vacuum system (25a) and (25b) possessing a degenerate Ricci tensor given by (9a), resp. (26a). However, as we indicated in Sec. II, the Ricci of (9a), resp. (26a), is rather special in the sense that its unique principal direction is normal to $\Phi=\text{const}$, resp. $V=\text{const}$, equipotential surfaces. Thus it is of considerable interest to investigate whether (7a) and (7b), resp. (25a) and (25b), admit other regular solutions across degeneracies subject to the condition that the unique principal direction of the Ricci is no longer normal to the above-mentioned two spaces. Accordingly, in this section we shall examine whether (7a) and (7b), resp. (25a) and (25b), admit solutions possessing a degenerate Ricci such that in the vicinity of $\Phi=1$, respectively, $V\to0^+$, the distinct Ricci eigenvector X is no longer parallel to $\overline{D}_a\Phi$, resp. D_aV. More precisely, we assume a Ricci given by

$$\overline{R}_{ab}=\overline{\lambda}(3X_aX_b-\Lambda_{ab}),\tag{34a}$$

and shall focus our attention primarily on the conformal system (7a) and (7b). As we shall see, the treatment of the vacuum system follows identical steps.

Combining (34a) with Eqs. (7a) and (7b), it follows that the scalar field Φ satisfies

$$2\Phi\overline{D}_a\overline{D}_b\Phi=2(3\Phi_a\Phi_b-\Lambda_{ab}\Phi^c\Phi_c)-\overline{\lambda}(1-\Phi^2)(3X_aX_b-\Lambda_{ab}),\tag{34b}$$

and thus the real symmetric matrix $\overline{D}_a\overline{D}_b\Phi$ longer exhibits identical eigenstructure as the corresponding Ricci. Substituting further (34a) in (8a) and straightforward algebra yield

$$\begin{aligned}\Phi(1-\Phi^2)[&(3X_cX_a-\Lambda_{ca})\overline{D}_b\overline{\lambda}-(3X_bX_a-\Lambda_{ba})\overline{D}_c\overline{\lambda}\\&+3\overline{\lambda}(X_c\overline{D}_bX_a+X_a\overline{D}_bX_c-X_b\overline{D}_cX_a-X_a\overline{D}_cX_b)]\\&=6\overline{\lambda}[2X_a(X_c\Phi_b-\Phi_cX_b)-\Lambda_{ca}(\Phi_b-X^d\Phi_dX_b)+\Lambda_{ab}(\Phi_c-X^d\Phi_dX_c)].\end{aligned}\tag{34c}$$

We write this equation hereafter in the form $\Phi(1-\Phi^2)\overline{R}_{abc}=\overline{S}_{abc}$, where $\overline{S}_{abc}$ stands for the right-hand side of (34c). It is clear that $\Phi(1-\Phi^2)\overline{R}_{abc}=\overline{S}_{abc}$ is the generalization of the constraint $\overline{R}_{abc}=0$ encountered in the previous sections. However, the structure of the new constraint shows that if (7a) and (7b) admit a solution (Λ,Φ) subject to (34a), then Λ is no longer locally conformally flat and thus we are dealing with a more ''complex geometry.'' Moreover, since (34c) is ''singular'' as the $\Phi=1$ two-surface is approached, it is expected that if (7a) and (7b) admit solutions characterized by a Ricci given by (34a), then their properties would be different than the

properties of their counterparts constructed in the previous sections. On the other hand, differentiating once more (34b) and appealing to the Ricci commutation relation, we obtain the following condition, which is the analog of (10a):

$$
\begin{aligned}
&2\Phi(\overline{D}_c\overline{D}_a\overline{D}_b\Phi-\overline{D}_a\overline{D}_c\overline{D}_b\Phi)+2\Phi_c\overline{D}_a\overline{D}_b\Phi-2\Phi_a\overline{D}_c\overline{D}_b\Phi\\
&\quad=6(\Phi_a\overline{D}_c\overline{D}_b\Phi-\Phi_c\overline{D}_a\overline{D}_b\Phi)-2\Phi^d(\Lambda_{ab}\overline{D}_c\overline{D}_d\Phi-\Lambda_{cb}\overline{D}_a\overline{D}_d\Phi)-3\overline{\lambda}(1-\Phi^2)\\
&\qquad\times(X_a\overline{D}_cX_b-X_c\overline{D}_aX_b+X_b\overline{D}_cX_a-X_b\overline{D}_aX_c)+(3X_bX_c-\Lambda_{bc})[(1-\Phi^2)\overline{D}_a\overline{\lambda}-2\Phi\overline{\lambda}\Phi_a]\\
&\qquad-(3X_bX_a-\Lambda_{ba})[(1-\Phi^2)\overline{D}_c\overline{\lambda}-2\Phi\overline{\lambda}\Phi_c].
\end{aligned}
$$

Substituting (34b) in the above and after lengthy algebra it yields Eqs. (34c). Thus it is sufficient to examine the content of the integrability condition (34c). Forming $\Phi(1-\Phi^2)\overline{R}_{abc}X^a=\overline{S}_{abc}X^a$ it yields

$$
\Phi(1-\Phi^2)[2X_c\overline{D}_b\overline{\lambda}-2X_b\overline{D}_c\overline{\lambda}+3\overline{\lambda D}_bX_c-3\overline{\lambda D}_cX_b]=6\overline{\lambda}[X_c\Phi_b-\Phi_cX_b], \tag{35a}
$$

while the combination $\Phi(1-\Phi^2)\overline{R}_{abc}X^aX^c=\overline{S}_{abc}X^aX^c$ yields

$$
\Phi(1-\Phi^2)[2\overline{D}_b\overline{\lambda}-2X_bX^c\overline{D}_c\overline{\lambda}-3\overline{\lambda}X^c\overline{D}_cX_b]=6\overline{\lambda}[\Phi_b-X^c\Phi_cX_b]. \tag{35b}
$$

Combining the contents of $\Phi(1-\Phi^2)\overline{R}_{abc}X^aX^c=\overline{S}_{abc}X^aX^c$, and $\Phi(1-\Phi^2)\overline{R}_{abc}X^a=\overline{S}_{abc}X^a$ with $\Phi(1-\Phi^2)\overline{R}_{abc}=\overline{S}_{abc}$, it yields $\Phi(1-\Phi^2)\hat{R}_{abc}=0$ where hereafter $\hat{R}_{abc}$ is defined by

$$
\begin{aligned}
\hat{R}_{abc}\equiv&(X_cX_a-\Lambda_{ca})\overline{D}_b\overline{\lambda}-(X_bX_a-\Lambda_{ba})\overline{D}_c\overline{\lambda}+3\overline{\lambda}(X_a\overline{D}_bX_c-X_a\overline{D}_cX_b-X_c\overline{D}_bX_a+X_b\overline{D}_cX_a)\\
&+2X^d\overline{D}_d\overline{\lambda}\Lambda_{ca}X_b-2X^d\overline{D}_d\overline{\lambda}\Lambda_{ab}X_c+3\overline{\lambda}\Lambda_{ca}X^d\overline{D}_dX_b-3\overline{\lambda}\Lambda_{ba}X^d\overline{D}_dX_c=0.
\end{aligned} \tag{35c}
$$

However, $\Phi(1-\Phi^2)\hat{R}_{abc}=0$ and continuity arguments show that $\hat{R}_{abc}=0$ in the open vicinity of $\Phi=1$. Forming $\hat{R}_{abc}X^c$ it follows that

$$
\hat{R}_{abc}X^c\equiv(\Lambda_{ba}-X_bX_a)X^c\overline{D}_c\overline{\lambda}-3\overline{\lambda}X_bX^c\overline{D}_cX_a+3\overline{\lambda D}_bX_a=0, \tag{35d}
$$

while a contraction of above with Λ_{ab} implies

$$
\hat{R}_{abc}X^c\Lambda^{ab}\equiv2X^a\overline{D}_a\overline{\lambda}+3\overline{\lambda D}_aX^a=0. \tag{35e}
$$

Considering now $\hat{R}_{abc}\Lambda^{ab}=0$ and taking into account the above equation results in

$$
\hat{R}_{abc}\Lambda^{ab}\equiv\overline{D}_c\overline{\lambda}-3\overline{\lambda}X^d\overline{D}_dX_c-X_cX^d\overline{D}_d\overline{\lambda}=0. \tag{35f}
$$

The content of this equation combined with $\hat{R}_{abc}X^c=0$ yields

$$
\hat{R}_{abc}X^c\equiv\Lambda_{ba}X^c\overline{D}_c\overline{\lambda}-X_b\overline{D}_a\overline{\lambda}+3\overline{\lambda D}_bX_a=0. \tag{36a}
$$

This is an important equation and we shall make use of it later on. For the moment we shall combine $\Phi(1-\Phi^2)\overline{R}_{abc}=\overline{S}_{abc}$ with the content of $\hat{R}_{abc}=0$. Indeed $\Phi(1-\Phi^2)\overline{R}_{abc}X^aX^b=\overline{S}_{abc}X^aX^b$ combined with the content of $\hat{R}_{abc}\Lambda^{ab}=0$ yields

$$
\Phi(1-\Phi^2)[\overline{D}_a\overline{\lambda}-X_aX^b\overline{D}_b\overline{\lambda}]=6\overline{\lambda}[\Phi_a-X^b\Phi_bX_a]. \tag{36b}
$$

Contracting the above equation with any arbitrary smooth vector field Y^a perpendicular to X^a yields

$$
\Phi(1-\Phi^2)Y^a\overline{D}_a\overline{\lambda}=6\overline{\lambda}Y^a\overline{D}_a\Phi,
$$

which in turn implies

$$Y^a\overline{D}_a\left[\log\left(\frac{\overline{\lambda}^{1/3}(1-\Phi^2)}{\Phi^2}\right)\right]=0,$$

and thus eventually we conclude

$$\overline{\lambda}^{1/3}=\frac{G^2(x)\Phi^2}{(1-\Phi^2)}, \tag{36c}$$

where in the above $G^2(x)$ stands for a nonvanishing function constant along the integral curves of the vector field X and in the above x stands for a set of comoving ''coordinates'' enumerating the integral curves of X. However, now (36c) implies that $\overline{R}_{ab}\overline{R}^{ab}$ is given by

$$\overline{R}^{ab}\overline{R}_{ab}=6\overline{\lambda}^2=\frac{6G^{12}(x)\Phi^{12}}{(1-\Phi^2)^6},$$

which shows that if a solution (Λ,Φ) of (7a) and (7b) exist so that the Ricci tensor of Λ is given by (34a), then the geometry is necessarily singular as $\Phi^2\to 1$. The only way that such a singularity can be avoided is to assume that $G(x)\equiv 0$, but this possibility implies that $\overline{R}_{ab}=0$ in the vicinity of $\Phi=1$ and such a Ricci returns as to the system (21a) and (21b) analyzed in Sec. III. Thus (7a) and (7b) does not admit regular solutions across $\Phi=1$ possessing a Ricci given by (34a). Interestingly and in concordance to the results of Secs. II and IV, an identical conclusion holds true for the vacuo system (25a) and (25b) as well. In fact, starting from (25a) and (25b) and looking for solutions (γ,V) subject to (34a), then the analog of (34c) takes the form $VR_{abc}=S_{abc}$, where, in this particular case, S_{abc} is given by

$$S_{abc}=3\lambda[2X_a(X_bV_c-X_cV_b)+\gamma_{ba}(X^dV_dX_c-V_c)-\gamma_{ca}(X^dV_dX_b-V_b)]. \tag{37a}$$

Repetition of the steps that leads into (35c) shows that $\hat{R}_{abc}=0$, where the three tensor $\hat{R}_{abc}$ has precisely the same form as that shown in Eq. (35c). It follows then that the corresponding eigenvalue λ satisfies

$$\lambda^{1/3}=\frac{G^2(x)}{V}, \tag{37b}$$

which is the analog of (36c). Accordingly vacuum solutions (γ,V) subject to (34a) become singular as $V\to 0^+$.

The above conclusions regarding the behavior of solutions of (7a) and (7b) characterized by a Ricci given by (34a) were reached via an analysis of the integrability conditions alone and thus it is not clear whether such solutions really exist. If they exist, and are defined in an open neighborhood of $\Phi=1$, respectively in $V\in(0,c)$, then they must become singular across $\Phi=1$, resp. $V\to 0^+$. It would therefore be of an independent interest to devote some effort to analyze the existence question. Moreover, if we will be able to construct them explicitly, them we shall be able to study the local isometry groups (if any), and thus compare their symmetry properties to those exhibited by solutions of (14a) and (14b), resp. (26a) and (26b). We shall show below that such solutions indeed exist and shall present their explicit construction. Since, however, the integration procedure is rather lengthy, we shall report below our findings and the reader is referred to the Appendix for details of the intermediate computations leading to their constructions.

Our effective system of equations consists of (34a) and (34b) augmented by the integrability condition (34c). By arguments along the lines that lead us to the equivalence of (7a) and (7b) to that of (14a) and (14b) via (9a)–(9c), here as well it is easily inferred that any solution (Λ,Φ) of (7a) and (7b) subject to (34a) necessarily satisfies (34b) and (34c) and conversely solutions of

(34a) and (34b) satisfying additionally (34c) are also solutions of (7a) and (7b). Of course here our considerations are restricted to the local vicinity of $\Phi=c,\ c\in(1,1+\epsilon)$ [or $\Phi=c,\ c\in(1-\epsilon,1)$]. One of the most important insights furnished by the integrability condition (34c) is the content of (36a). It implies the existence of a local coordinate system (x,y,z) covering the open vicinity of $\Phi=c,\ c\in(1,1+\epsilon)$, and such that the metric Λ can be written in the following form:

$$ds^2=\bar{\lambda}^{-2/3}\left(\frac{dx^2}{a^2(x)}+\frac{dy^2}{b^2(y)}+b^2(y)dz^2\right). \tag{38}$$

Relative to such coordinates the eigenvector X is parallel to $\partial/\partial x$, while (y,z) are local coordinates on the family of the two-surfaces perpendicular to $\partial/\partial x$ (see the Appendix). With the help of the above insight the integration of the field equations (34a) and (34b) remarkably can be accomplished and, after a long and tedious intermediate algebra, leads us to the solutions described by

$$\bar{\lambda}^{2/3}=(x+y)^2,$$

$$a^2(x)=2x^3+\frac{2k^3+mk-n}{k^2}x^2+mx+n>0, \tag{39a}$$

$$b^2(y)=2y^3-\frac{2k^3+mk-n}{k^2}y^2+my-n>0, \tag{39b}$$

$$\Phi(x,y)=\left(\frac{2k(x+y)(x+k)}{2k(x+k)y-2k^2x-km+2n}\right)^{1/2}, \tag{39c}$$

where in the above (k,m,n) are integration constants chosen so that for a given range of the (x,y) coordinates, the metric coefficients ought to be consistent with the positive definite character of the metric. Furthermore, for such choices of (k,m,n), an analysis of $\Phi(x,y)$ given by (39c) or more conveniently using (A30), shows that the intersection of any $x=c,\ c<\infty$, local two-coordinate surface with $\Phi=1$ appears as $\lim y\to\infty$. Moreover, (38), (39a), and (39b) show that the proper distance of any point $y=y_0$ lying on any $x=c,\ c<\infty$, is at finite proper distance away from the limiting value $\lim y\to\infty$ and at $\lim y\to\infty$ the scalar invariant $R^{ab}R_{ab}$ diverges. Thus and in accord with (36c), indeed the geometry is singular as points subject to $\Phi(x,y)=1$ are approached. Away from such singular regions, (38) and (39a)–(39c) show that the metric admits a local group of isometrics generated by $\partial/\partial z$, a situation that is in sharp contrast to the previously constructed solutions. Even though still symmetric, one parameter local group of isometrics, not as symmetric as the corresponding solutions of (7a) and (7b) possessing a Ricci given by (9a). We shall return to that point below, after the construction of the corresponding vacuum solutions. For the vacuo case the corresponding equations are

$$R_{ab}=\lambda(3X_aX_b-\Lambda_{ab}), \tag{40a}$$

$$D_aD_bV=V\lambda(3X_aX_b-\Lambda_{ab}). \tag{40b}$$

We are again looking for solution valid in the local vicinity of the ''horizon,'' and relative to the same coordinate gauge shown in (38) the above system admits the following solutions (see also the Appendix for details):

$$\lambda^{2/3}=(x+y)^2,$$
$$a^2(x)=2x^3+mx+n>0,\quad b^2(y)=2y^3+my-n>0, \tag{41a}$$

$$V(x,y)=\frac{c_1a(x)}{x+y}, \tag{41b}$$

where again in the above (m,n,c_1) are integration constants subject to $c_1>0$. The set of points lying on the horizon correspond to the limit of $y\to\infty$ for all x finite. Like the corresponding solution of the conformal system, (41a) and (41b) also admit a local group of isometrics generated by $\partial/\partial z$.

The space–time metric associated with (39a)–(39c), (41a), and (41b) can be easily inferred. Indeed for the conformal system it is given by

$$ds^2=-\frac{dt^2}{(1+\Phi)^2}+\frac{(1+\Phi)^2}{(x+y)^2}\left(\frac{dx^2}{a^2(x)}+\frac{dy^2}{b^2(y)}+b^2(y)dz^2\right), \tag{42a}$$

$$\Phi(x,y)=\left(\frac{2k(x+y)(x+k)}{2k(x+k)y-2k^2x-km+2n}\right)^{1/2}, \tag{42b}$$

while for the vacuum case it is given by

$$ds^2=\frac{1}{(x+y)^2}\left(-a^2(x)dt^2+\frac{dx^2}{a^2(x)}+\frac{dy^2}{b^2(y)}+b^2(y)dz^2\right). \tag{43}$$

It can be verified directly that (42a) and (42b), resp. (43), satisfy the covariant equations (1c) and (1d), resp. $G_{\mu\nu}=0$, while their counterparts (39a)–(39c), resp. (41a) and (41b), satisfy (7a) and (7b), resp. (25a) and (25b), of course away from the degeneracies. The vacuum solution (43) belongs to the C-class of metrics in the classification scheme proposed by Ehlers and Kundt.[26] Judging from the corresponding comments in Ref. 26, it appears that originally this solution was derived by Levi–Civita.[25] Maintaining the same nomenclature as that adopted in Ref. 26 we shall refer to (42a) and (42b) as the corresponding C-class of solutions for the conformal system. To the best of our knowledge, the solutions (42a) and (42b) are new and, due to their complexity, we shall refrain from discussing here their global structure and particularly the structure of the singularity occurring as $\Phi\to 1$. This analysis will be presented elsewhere. With the above explicit form of the C-class of solutions, it appears that the metrics possessing a degenerate Ricci and satisfying (7a) and (7b) is now complete and those solutions, except (24c), are in correlation with the corresponding degenerate solutions of the vacuo system (25a) and (25b).

It is worthwhile at this point to return to the important issue of the origin of the additional local isometrics present in all constructed degenerate solutions of (7a) and (7b), resp. (25a) and (25b). Actually there are two intertwined issues involved here; first, the issue of the origin of the local isometrics and, second the regularity of the solutions across degeneracies. The analysis of the previous sections shows that a degenerate Ricci is not by itself solely responsible for the origin of the local isometrics, but, rather, it is Ricci degeneracy combined with the fundamental constraints (8a), resp. (27). Whenever a particular solution possesses a (degenerate) Ricci so that the right-hand-sides of (8a), resp. (27), are identically zero, and this occurs only when $\overline{D}_a\Phi$ resp. D_aV, are parallel to the Ricci principal distinct eigendirection, as it can be easily inferred from the right-hand sides of (8a), resp. (27), then the corresponding Ricci eigenvalue has a gradient parallel to its distinct eigendirections [see Eq. (12a)]. This fact combined with the Hamiltonian constraint shows that the two surfaces perpendicular to the Ricci eigendirection lack any distinct direction and thus are maximally symmetric [see Eqs. (18b) and (18d)]. The existence then of the local $G(3)$ admitting orbits of constant Gaussian curvature follows naturally. However away from this case, whenever a solution is characterized by a three-metric, which even though it possesses a degenerate Ricci it is not by itself conformally flat, then the Ricci eigenvalue exhibits a gradient that possesses a nonvanishing component tangential to the family of the two-surfaces perpendicular to the distinct Ricci eigendirection [see Eq. (36b)]. As a consequence this family of two-surfaces, their existence guaranteed by relations like (36a), is no longer a space of constant Gaussian curvature [see Eqs. (A26)]. As a consequence the solution cannot have a $G(3)$ possessing orbits of constant Gaussian curvature. However, as it is clear from (42) and (43), Ricci degeneracy guarantees only the existence of an additional local $G(1)$.

As far as the regularity of the geometry across the degeneracy region is concerned, it should be stressed that this issue involves the full system i.e., (7a) and (7b), resp. (25a) and (25b). In the previous sections we have worked with an effective regular set of equations, augmented by a set of singular integrability conditions i.e., Eqs. (8a) and (27). Whenever a particular solution possesses as a degenerate Ricci so that the right-hand sides of (8a) and (27) are vanishing then this solution satisfies a system of effective equations, namely (10c), (14a), and (14b), resp. (26a), and (26b), and (28b), which has no traces of the singular nature of the original singular equations i.e., (7a), (7b), (25a), and (25b). Accordingly, any regular solution of the effective equations is necessarily regular over the degeneracy regions as well, since the latter region is not registered as anything peculiar in the structure of the effective equations [in that regard, recall the arguments before and above Eq. (9d)]. The fact that all regular solutions of the effective equations (10c), (14a), and (14b), resp. (26a), (26b), and (28b) exhibit high symmetry is to be interpreted as due to the special nonsingular structure of the effective system. Once, however, a particular solution possesses a degenerate Ricci so that the right-hand sides of (8a) and (27) are no longer vanishing, the situation is different. In such events the corresponding effective system is no longer regular since it also contains the integrability conditions (8a), resp. (27), which themselves are singular along solutions subject to $\Phi=1$, resp. $V\rightarrow 0^{+}$. Equations (36c) and (37b) then describe the consequences.

This summary makes clear the importance of the York–Cotton tensor. Its special role in controlling the symmetries and regularity properties of any solution of (7a), and (7b), resp. (25a), and (25b) is due to the special singular structure of (7a) and (7b), resp. (25a) and (25b) since as we have shown earlier, all solutions of those equations necessarily satisfy (8a), resp. (27). We may recall that such a property of the York–Cotton tensor is encountered in other situations as well. In Robinson's derivations of the uniqueness of the Schwartzschild black hole,[39] the vanishing of R_{abc} on the asymptotically Euclidean three-manifold Σ possessing a regular S was one of the key elements in the proof. The existence of the SO(3) symmetry then followed as the consequence of the vanishing of the York–Cotton tensor combined with the asymptotically Euclidean character of the geometry of Σ.

VII. DISCUSSION

In this work we have analyzed some consequences of the $(1-\Phi^2)$ factor multiplying the left-hand side of Eq. (1c) and, as it is clear, its presence adds a special flavor to the dynamics of the conformal system. In accord with the results of Refs. 18 and 21, the mere fact that the conformal system degenerates on specific classes of solutions, it does not follow that such solutions are singular over degeneracies. The regular solutions constructed in the previous sections offer another concrete example. It also clear from the analysis presented here that an understanding of the properties of solutions across degeneracies is a subtle and involved issue. The solutions constructed in this work although on the one hand offer insights to the dynamics of the conformal system, on the other hand call for more work. Although we have been able to construct and analyze classes of regular solutions across degeneracies, they were derived under the assumption that such solutions possess a degenerate Ricci and, moreover, the zeros of the $1-\Phi^2$ factor possess a ''nice'' structure. Naturally they lead us to ask: Do there exist other regular across degeneracies solution characterized by a nondegenerate Ricci? If yes, are they always accompanied by additional local isometries? And what is the role of the York–Cotton tensor if any? We do not have an answer to those questions, but we may add that the fundamental constraint (8a), holding for every solution of (7a) and (7b), imposes constraints on the two distinct Ricci eigenvalues. A preliminary analysis of the constraints indicates that it is conceivable that the conformal system may admit regular solutions across the degeneracy region possessing a non degenerate Ricci. Unfortunately, however, progress towards settling that issue is obstructed by the complicated nature of the integrability conditions that is a set of coupled tensorial differential constraints. As far as the presence of additional local isometries as a requirement of regularity across degeneracies, we may note that a contraction of (8a) by itself yields

$$\overline{R}^{abc}\overline{R}_{abc}=\frac{A^{abc}A_{abc}}{1-\Phi^2},$$

where A_{abc} is an expression involving gradients of the Ricci eigenvalues and corresponding eigenvectors. Thus any solution (Λ,Φ) would be singular as $\Phi^2\to 1$, unless some special arrangement is operating at the level of the York–Cotton tensor and the Ricci curvature. On the other hand, the comparison of the singular conformal equations to vacuum Einstein equations describing static solutions offers support to the contention that regularity of the solution across the singularities of the equations may be accompanied by additional isometries. Some time ago Israel[40] and much later Geroch and Hartle[41] analyzed the so-called distorted class of black hole solutions of Einstein vacuum equations. Such solutions possess a regular event horizon, distorted by the presence of some axisymmetric distribution of matter. It can be easily seen that the distorted class of black holes can be put into a correspondence with local solutions of (25a) and (25b) possessing a regular ''horizon'' *S*. Xanthopoulos *et al.*[42,43] showed that the distorted classes of black holes are necessary for type *D* on the event horizon. Moreover, those solutions, within the present formalism, do not possess a degenerate Ricci, but of course are axisymmetric and thus provided examples of regular solutions as the degenerate region is approached possessing a local $G(1)$ and whose Ricci is not degenerate in the local vicinity of the ''horizon'' *S*. The question of whether there exist local static black hole solutions possessing a regular horizon and without any additional symmetry is for the moment an open question. Some progress towards resolving that question is discussed in Ref. 44.

On an entirely different aspect, the results of the present work can be extended into different directions. An obvious natural extension concerns the question of the existence of static, regular across degeneracies solutions of (1c) and (1d) without imposing the functional relationship $U(\Phi)$ nor the condition (b) introduced in Sec. II. As far as the first question is concerned, some progress has been made in Ref. 45. It was shown there that (1c) and (1d) indeed admit regular across degeneracies solutions and those solutions as well as their properties and construction will be discussed elsewhere. Moreover, the method discussed in the present article can be applied to analyze the structure of solutions of other singular systems of equations, particularly equations associated with theories involving scalar fields arbitrarily coupled to the background curvature. One such system is provided by the theory involving Einstein gravity and a scalar field Φ nonconformally coupled to the background curvature. For such theories the factor $(1-\alpha\Phi^2)$ is replaced by $(1-k\xi\Phi^2)$ and the dynamical equations have similar structure as those of the conformal system. It would be therefore illuminating to extend the present analysis to such theories and compare the behavior of their solutions to the corresponding solutions presented here.

Finally, in closing we may add that scalar fields and relativistic gravity mix rather well. Primarily due to their simplicity, scalar fields often are employed to get insights into the complex dynamics of Einstein field equations. Soliton-like solutions[46] as well as models of strongly gravitating sources involving matter and scalar fields arbitrarily coupled to gravity with or without Higgs-type potentials have been studied in detail in the current literature.[47] Even though still direct observational evidence supporting the existence of long range scalar fields is lacking, current cosmological observations are interpreted as favoring an accelerating universe, and the possibility that scalars fields may provide a natural explanation is currently under active investigation.[48] Therefore, theories involving scalar fields besides their pure mathematical importance may turn out to be of physical importance as well. Observations will tell.

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APPENDIX: C-CLASS METRICS FOR THE CONFORMAL SYSTEM

In this appendix we shall present some intermediate computations leading to the construction of the singular metrics discussed in Sec. VI. Our problem is the integration of the system (34a) and (34b) and as we have indicated earlier on, an extremely important insight is offered by the following relation, natural consequence of the integrability condition (8a) [see in particular, Eqs. (11d) and (36a)]:

$$\Lambda_{ab}X^c\overline{D}_c\overline{\lambda}-X_a\overline{D}_b\overline{\lambda}+3\overline{\lambda}\overline{D}_aX_b=0. \tag{A1}$$

The significance of this relation has been pointed out in the influential report of Ehlers and Kundt in Ref. 26 and that remark helped us enormously. An initial attempt, centered on adopting the integration technique of Sec. III to the system (34a) and (34b), lead us into a complex set of unyielding coupled differential equations. It was only after we became aware of Ref. 26 that we were able to integrate (34a) and (34b).

In order to see the implications of (A1), let us first consider a conformal transformation generated by an arbitrary conformal factor Ω^2, i.e., define $g_{ab}=\Omega^2\Lambda_{ab}$. Standard formula using the behavior of the connection under conformal transformation[1] shows that the following identity holds true:

$$D_a(\Omega X_b)=\Omega\overline{D}_aX_b-X_a\overline{D}_b\Omega+\Lambda_{ab}X^c\overline{D}_c\Omega, \tag{A2}$$

where in the above the covariant derivative operator D_a is formed using the g metric. However, a comparison of (A2) with (A1) implies that by choosing $\Omega=\overline{\lambda}^{1/3}$ as the conformal factor, then

$$D_a(\overline{\lambda}^{1/3}X_b)=0, \tag{A3}$$

implying that $g_{ab}=\overline{\lambda}^{1/3}\Lambda_{ab}$ admits $\overline{\lambda}^{1/3}X_a$, a parallel vector field. However, the existence of such a field imposes strong constraints on g_{ab} (and thus also on Λ_{ab} and $\overline{\lambda}$). A theorem in Ref. 29 (see also Ref. 26) assures that in the region admitting parallel fields exist local coordinates (x,y,z) so that x is parallel to $\partial/\partial x$ and g admits the following representation:

$$ds^2=g_{ab}dx^adx^b=dx^2+ds^2_{(2)},$$

from which we also conclude that

$$ds^2=\Lambda_{ab}dx^adx^b=\overline{\lambda}^{-2/3}g_{ab}dx^adx^b=\overline{\lambda}^{-2/3}(dx^2+ds^2_{(2)}), \tag{A4}$$

where $ds^2_{(2)}=\hat{\gamma}_{ij}(y,z)dx^idx^j$. Thus, relative to the coordinate (x,y,z) predicted by the existence of the parallel field $\overline{\lambda}^{1/3}X_a$, the coordinate dependence of the metric Λ has been constrained considerably. We write (A4) in the following form,

$$ds^2=\frac{dx^2}{S^2(x,y,z)}+\frac{1}{S^2(x,y,z)}\hat{\gamma}_{ij}(y,z)dx^idx^j=\frac{dx^2}{S^2}+\gamma_{ij}dx^idx^j, \tag{A5}$$

and project first Eq. (34a) along and perpendicular to $x=$const local coordinate surfaces, thus getting

$$-R^{(2)}-K^{ij}K_{ij}+K^2=4S^3, \tag{A6}$$

$$D_iK-D_jK^j{}_i=0, \tag{A7}$$

$$-S\frac{\partial K_{ij}}{\partial x}+2K_{il}K^l{}_j-KK_{ij}+\frac{1}{2}R^{(2)}\gamma_{ij}+\frac{1}{S}D_iD_jS-\frac{2}{S^2}D_iSD_jS=-S^3\gamma_{ij}, \tag{A8}$$

$$\frac{1}{2}S\frac{\partial\gamma_{ij}}{\partial x}=K_{ij}, \tag{A9}$$

where the extrinsic curvature of the $x=\text{const}$ two-surfaces is given by

$$K_{ij}=\frac{1}{2}L_n\gamma_{ij}=\frac{1}{2}S\frac{\partial}{\partial x}\frac{\hat{\gamma}_{ij}}{S^2}=-\frac{\hat{\gamma}_{ij}}{S^2}\frac{\partial S}{\partial x}=-\frac{\partial S}{\partial x}\gamma_{ij}. \tag{A10}$$

Substituting this K_{ij} into the Hamiltonian, momentum constraint and evolution equations, we get

$$R^{(2)}+4S^3-2\left(\frac{\partial S}{\partial x}\right)^2=0, \tag{A11}$$

$$\frac{\partial^2 S}{\partial x\partial x^i}=0, \tag{A12}$$

$$\left[S\frac{\partial^2 S}{\partial x^2}-\left(\frac{\partial S}{\partial x}\right)^2-S^3\right]\gamma_{ij}+\frac{1}{S}D_iD_jS-\frac{2}{S^2}D_iSD_jS=0. \tag{A13}$$

But Eq. (A12) implies that one may write

$$S(x,y,z)=f(x)+g(y)+h(z), \tag{A14}$$

where $(f(x),g(y),h(z))$ are arbitrary functions that ought to be specified. Taking the trace of (A13) leads into

$$2\left[S\frac{\partial^2 S}{\partial x^2}-\left(\frac{\partial S}{\partial x}\right)^2-S^3\right]+\frac{1}{S}D^iD_iS-\frac{2}{S^2}D^iSD_iS=0. \tag{A15}$$

It is convenient from this point onward to work with the metric $\hat{\gamma}_{ij}(y,z)$, and relative to this metric the Hamiltonian and the trace of the evolution equation read

$$S^2\hat{R}^{(2)}+2S\hat{D}^i\hat{D}_iS-2\hat{D}^iS\hat{D}_iS+4S^3-2\left(\frac{\partial S}{\partial x}\right)^2=0, \tag{A16}$$

$$2\left[S\frac{\partial^2 S}{\partial x^2}-\left(\frac{\partial S}{\partial x}\right)^2-S^3\right]+S\hat{D}^i\hat{D}_iS-2\hat{D}^iS\hat{D}_iS=0, \tag{A17}$$

where in the above $\hat{R}^{(2)}$ and all geometrical tensors are formed using $\hat{\gamma}_{ij}=\hat{\gamma}_{ij}(y,z)$. Due to the fact that local coordinates (x,y,z) involve a considerable amount of gauge freedom, we exploit this freedom and define a new set $(\overline{x},\overline{y},\overline{z})$ by

$$\overline{x}=f(x),\qquad \overline{y}=g(y),\qquad \overline{z}=h(z).$$

Relative to such coordinates, the scalar function S takes the form $S=\overline{x}+\overline{y}+\overline{z}$ and the metric (A5) transforms into

$$ds^2=\frac{1}{S^2}\left(\frac{d\overline{x}^2}{a^2(\overline{x})}+\hat{\gamma}_{ij}(\overline{y},\overline{z})d\overline{x}^i d\overline{x}^j\right). \tag{A18}$$

Expressing the derivatives of S in terms of $(\overline{x},\overline{y},\overline{z})$ via

$$\frac{\partial S}{\partial x}=\frac{\partial S}{\partial\overline{x}}\frac{\partial\overline{x}}{\partial x}=\frac{\partial\overline{x}}{\partial x}\equiv a(\overline{x}),\quad \frac{\partial^2 S}{\partial x^2}=a\frac{da}{d\overline{x}}=\frac{1}{2}\frac{da^2}{d\overline{x}},$$

then Eqs. (A16) and (A17) take the form

$$S^2\hat{R}^{(2)}+2S\hat{D}^i\hat{D}_iS-2\hat{D}^iS\hat{D}_iS+4S^3-2a^2=0, \tag{A19}$$

$$S\hat{D}^i\hat{D}_iS-2\hat{D}^iS\hat{D}_iS+S\frac{da^2}{d\bar{x}}-2a^2-2S^3=0. \tag{A20}$$

Differentiating now (A20) with respect to $\bar{x}$ we obtain

$$\hat{D}^i\hat{D}_iS+S\frac{d^2a^2}{d\bar{x}^2}-\frac{da^2}{d\bar{x}}-6S^2=0, \tag{A21}$$

and an additional differentiation of (A21) yields

$$S\left[\frac{d^3a^2}{d\bar{x}^3}-12\right]=0, \tag{A22}$$

from which we get

$$a^2(\bar{x})=2\bar{x}^3+\frac{l}{2}\bar{x}^2+m\bar{x}+n, \tag{A23}$$

where l, m, n are arbitrary integration constants. Substituting this equation back in (A21) we obtain

$$\hat{D}^i\hat{D}_iS=6(\bar{y}+\bar{z})^2-l(\bar{y}+\bar{z})+m, \tag{A24}$$

while substituting (A23) and (A24) back into (A20) we get

$$\hat{D}^iS\hat{D}_iS=2(\bar{y}+\bar{z})^3-\frac{l}{2}(\bar{y}+\bar{z})^2+m(\bar{y}+\bar{z})-n, \tag{A25}$$

and upon substituting (A23)–(A25) back into (A19) we get

$$\hat{R}=-12(\bar{y}+\bar{z})+l. \tag{A26}$$

Since Eqs. (A24)–(A26) involves only the coordinates $\bar{y}$ and $\bar{z}$ via the combination $\bar{y}+\bar{z}$, we take advantage of it and define new coordinates (y,z) via

$$y=\bar{y}+\bar{z}, \qquad z=z(\bar{y},\bar{z})$$

with $z=z(\bar{y},\bar{z})$ arbitrary for the moment function of its arguments. Using the arbitrariness in the choice of z, we demand

$$\hat{\gamma}^{yz}=(\hat{\gamma}^{\bar{y}\bar{y}}+\hat{\gamma}^{\bar{y}\bar{z}})\frac{\partial z}{\partial\bar{y}}+(\hat{\gamma}^{\bar{y}\bar{z}}+\hat{\gamma}^{\bar{z}\bar{z}})\frac{\partial z}{\partial\bar{z}}=0.$$

The above equation is a first-order linear partial differential equation and locally always admits solutions. In terms of the new coordinates (y,z), S takes the simpler form: $S=x+y$ and, for such S, (A25) fixes $\hat{\gamma}^{yy}$ to the form

$$\hat{\gamma}^{yy}=y^3-\frac{l}{2}y^2+my-n \tag{A27}$$

with the help of which Eq. (A24) implies

$$\frac{\partial\sqrt{\hat{\gamma}}}{\partial y}=0.$$

Since the two-metric is diagonal, we also get $\hat{\gamma}_{yy}=c^2\hat{\gamma}_{zz}^{-1}$ where c^2 is an arbitrary constant that is absorbed here after the z coordinate. Thus eventually we lead

$$ds^2=\frac{1}{S^2}\left(\frac{dx^2}{a^2(x)}+\frac{dy^2}{b^2(y)}+b^2(y)dz^2\right) \tag{A28}$$

with

$$a^2(x)=2x^3+\frac{l}{2}x^2+mx+n,\quad b^2(y)=2y^3-\frac{l}{2}y^2+my-n. \tag{A29}$$

Computing the scalar curvature $\hat{R}^{(2)}$ of the $x=$const using the metric $\hat{\gamma}_{ij}$, we find that $\hat{R}=-12y+l$, showing that (A26) is identically satisfied. Moreover, returning back to the trace-free part of the evolution equations (A13), using (A28) and (A29) and the form of S, we find that it is identically satisfied.

Up to this point we have constructed all metrics satisfying $\overline{R}_{ab}=\overline{\lambda}(3X_aX_b-\Lambda_{ab})$ subject to $(\overline{\lambda},X)$ satisfying (A1). In order, however, to complete the solution of (34a) and (34b) we must also specify Φ for the conformal case (or V for the vacuum case). Let us first consider the conformal case. Starting from the equation $\overline{D}^a\overline{D}_a\Phi=0$ and utilizing Eq. (36c) it follows via $\overline{\lambda}^{-1/3}=S=x+y$ that

$$\Phi(x,y)=\left(\frac{x+y}{x+y+G^2(x)}\right)^{1/2},\quad G^2(x)>0. \tag{A30}$$

Demanding that this Φ satisfy $\overline{D}_a\overline{D}^a\Phi=0$ and, after algebra, using (A28) and (A29) we obtain the following consistency relations for $G(x)$:

$$\begin{aligned}&H_1(x)y^3+[(3x+G^2)H_1(x)+\tfrac{1}{2}H_2(x)]y^2+x[(3x+2G^2)H_1(x)+H_2(x)]y\\&\quad+x^2[(x+G^2)H_1(x)+\tfrac{1}{2}H_2(x)]=0,\end{aligned} \tag{A31}$$

where $H_1(x)$ and $H_2(x)$ are defined by

$$H_1(x)=(4x^2+lx^2+2mx+2n)\frac{d^2G^2}{dx^2}+(6x^2+lx+m)\frac{dG^2}{dx}-(6G^2+12x+l)G^2, \tag{A32}$$

$$H_2(x)=2\left(2x^2+\frac{l}{2}x^2+mx+n\right)\left(2+\frac{dG^2}{dx}\right)\frac{dG^2}{dx}-[4G^4+(12x+l)G^2+2(6x^2+lx+m)]G^2. \tag{A33}$$

Since, however, (A31) must be satisfied identically, it follows that necessarily $H_1(x)=H_2(x)=0$. Due the fact that $H_1(x)=0$ can be viewed as a differential equation for $G^2(x)$, and $H_1(x)=0$ possesses analytic coefficients, we look for polynomial solutions $G(x)$. It takes a rather long and tedious algebra to show that the following function $G^2(x)$ satisfies (A32) and (A33),

$$G^2(x)=-\frac{2k(x+k)^2-2k^3+mk-2n}{2k(x+k)}, \tag{A34}$$

provided the integration constants appearing in (A29) are adjusted so that $a^2(x)$ and $b^2(y)$ have the form

$$a^2(x)=2x^3+\frac{2k^3+mk-n}{k^2}x^2+mx+n>0, \tag{A35}$$

$$b^2(y)=2y^3-\frac{2k^3+mk-n}{k^2}y^2+my-n>0. \tag{A36}$$

Using (A34), then the corresponding expression for the scalar field Φ takes the form

$$\Phi(x,y)=\left(\frac{2k(x+y)(x+k)}{2k(x+k)y-2k^2x-km+2n}\right)^{1/2}. \tag{A37}$$

Up to this point we have satisfied only the trace-free part of Eq. (34b). In order to complete the solution we must also satisfy the other components of Eq. (34b). Setting

$$K_{ab}=2\Phi\overline{D}_a\overline{D}_b\Phi-2(3\Phi_a\Phi_b-\Lambda_{ab}\Phi^d\Phi_d)+\overline{\lambda}(1-\Phi^2)(3X_aX_b-\Lambda_{ab}) \tag{A38}$$

and substituting in (A34)–(A37), then after a long and tedious algebra we find that K_{ab} is diagonal and, in fact, as long as $H_1(x)=H_2(x)=0$, then necessarily $K_{ab}=0$. Thus the set of functions (A35)–(A37) describes the general solution of (7a) and (7b) subject to Ricci given by (34a) and of course satisfaction of the integrability conditions (34c).

Let us now briefly discuss the integration of the vacuum system (40a) and (40b). As it is clear from the above integration procedure, we only need to verify Eq. (40b) for the metric (A28) and (A29). From Eq. (37b) we have $V=G^2(x)/(x+y)$ and, demanding $D^aD_aV=0$, we obtain the following ordinary equations for $G^2(x)$:

$$G_1(x)y^2+G_2(x)y+x(G_2(x)+xG_1(x)-2lx)=0, \tag{A39}$$

where $G_1(x)$ and $G_2(x)$ are defined by

$$G_1(x)=a^2\frac{d^2G^2}{dx^2}+\frac{1}{2}\frac{da^2}{dx}\frac{dG^2}{dx}-\left(6x+\frac{5}{2}l\right)G^2, \tag{A40}$$

$$G_2(x)=2xa^2\frac{d^2G^2}{dx^2}+\left(x\frac{da^2}{dx}-3a^2\right)\frac{dG^2}{dx}-\left(\frac{1}{2}\frac{da^2}{dx}-lx-2m\right)G^2. \tag{A41}$$

Again (A39) must be satisfy identically, and thus necessarily $G_1(x)=0$, $G_2(x)=0$, and additionally $l=0$. Forming a linear combination of $G_1(x)=G_2(x)=0$, namely, $G_2(x)-2xG_1(x)=0$, we obtain

$$a^2\frac{dG^2}{dx}+\frac{1}{2}\frac{da^2}{dx}G^2-2(6x^2+m)G^2=0.$$

Since, on the other hand, $a^2(x)=2x^3+mx+n$, it follows that the above equation can be written in the form

$$\frac{1}{G^2}\frac{dG^2}{dx}-\frac{1}{2a^2}\frac{da^2}{dx}=0,$$

which in turn implies

$$\frac{d}{dx}\left[\log\left(\frac{G^2}{a}\right)\right]=0$$

from which we infer that $G^2(x)=c_1^2 a(x)$. Substituting the above equation in (A40) and (A41) we find that they are identically satisfied. Finally, the vacuum metric is given by (A28) combined with $a^2(x)$ and $b^2(y)$ given by (A29) with $l=0$ while $V(x,y)$ given by

$$V(x,y)=\frac{c_1^2 a(x)}{x+y}.$$

That set of functions constitutes the general solution of (40a) and (40b).

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[19] The behavior of static or stationary vacuum asymptotically Euclidean solutions of Einstein equations has been the subject of many investigations. Within Geroch's (Ref. 20) coordinates-free description of asymptotic flatness at spatial infinity, a conformally rescaled positive metric $\tilde{g}=\Omega^2 g$ defined on an unphysical three manifold $(\tilde{M},\tilde{g})$ satisfies a formally degenerate system of equations in the neighborhood of the so-called point at infinity Λ attached to M so that $\tilde{M}=M\cup\{\Lambda\}$ is diffeomorphic to an open ball of R^3. The analysis of $\tilde{g}$ near Λ has been performed in Ref. 21 where the analyticity of $\tilde{g}$ is also established.
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static solution of the conformal equations (4a)–(4c). Again regularity of Ω requires $1-\Phi^2\neq 0$ and thus similar comments apply to the content of the this theorem as well.

[24] Unfortunately the term ''degenerate'' will appear in various places in the text with different meanings. It has been used in the title, and there and elsewhere in the text degenerate solutions refers to solutions which in the first place are defined in the vicinity of degeneracy and, moreover, in the same region satisfy the relevant equations. The term degenerate equations has been explained in the text while the term degenerate Ricci refers to a Ricci where at least two of its eigenvalues coincide at a point or in an open vicinity of a given point.

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[28] In such an event the level surface of Φ is in general many-sheeted and a proof of this property can be found, for instance, in the appendix of Israel-1967 paper (Ref. 30). Additional discussion can also be found in P. Kellogg, *Potential Theory* (Dover, New York, 1931).

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[32] It should be noted though that during this integration procedure the range of the Φ-coordinate nonwhere enters in a crucial manner, except that one implicitly assumes that the level surface of $\Phi=c$ admits no critical points. It is that property that allows us to consider the solutions as valid in a Φ-range given by $(1-\epsilon,1+\epsilon)$, $\epsilon>0$. In fact, since by construction $S(\Phi)|_{\Phi=1}\neq 0$, one may introduce a new coordinate r defined via $d\Phi/dr=c/S(\Phi)$, and obeying $\Phi(r=1)=1$. This ordinary equation admits a local solution and thus it is clear that $\Phi(r)$ satisfies $1-\Phi(r)=0$. We have avoided introducing this parametrization since the resulting $\Phi(r)$ is a rather complex expression involving in general transcendental functions.

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A rigidity theorem for nonvacuum initial data

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In this note we prove a theorem on nonvacuum initial data for general relativity. The result presents a ''rigidity phenomenon'' for the extrinsic curvature, caused by the nonpositive scalar curvature. More precisely, we claim that in the case of an asymptotically flat nonvacuum initial data if the spatial metric has everywhere nonpositive scalar curvature, then the extrinsic curvature cannot be compactly supported. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421422]

I. INTRODUCTION

According to our experiences there are many different gravitational configurations in our physical world. Therefore, if general relativity is a correct theory of gravitational phenomena (at least at low energies), then it is important to know whether or not these various patterns can be modeled in general relativity, i.e., Einstein equations provide enough solutions for describing many different gravitational fields. Unfortunately or fortunately, Einstein equations form an extraordinarily difficult system of nonlinear partial differential equations for the four dimensional Lorentzian metric mainly because of the rich self-interactions of the gravitational field; hence in general it is a hard job to write down explicit solutions in this theory. Therefore, all methods which prove at least the existence of solutions are very important. From this viewpoint, the Cauchy problem or initial value formulation of general relativity is maybe the most powerful method to generate plenty of solutions.

As it is well known, the initial value formulation gives rise to a correspondence between globally hyperbolic space–times and gravitational initial data. Maybe we can say without an exaggeration that the class of globally hyperbolic space–times is the most important class of space–times from the physical point of view. Consequently, the initial data formulation provides not only many but also physically relevant solutions. The constraint equations between initial data are in the focal point of the initial data formulation. The question is whether or not these constraint equations are easier to solve than the original Einstein equation itself, making the method effective. Of course, the answer is typically yes.

This motivates the serious efforts made in order to understand the structure and provide solutions of constraint equations. Far from being complete we just mention the early works of Lichnerowicz (1944), Bruhat (1962), Choquet-Bruhat and Geroch (1969), Choquet-Bruhat and York (1980), Fisher and Marsden (1979), and Christodoulou and Klainerman (1993). These papers mainly deal with the analytical properties of the solutions. Witt proved the existence of solutions on a general three-manifold (Witt, 1986). More recently, in a sequence of papers Isenberg, Moncrief, Choquet-Bruhat, and York proved the existence of solutions under milder and milder assumptions (cf., e.g., Isenberg, 1995; Choquet-Bruhat *et al.*, 1992; Isenberg and Moncrief, 1996, moreover Choquet-Bruhat *et al.*, 2000).

The constraint equations involve the scalar curvature of the metric on the underlying Cauchy surface which is a three dimensional smooth manifold. Various properties of the solutions depend crucially on the scalar curvature, especially on its sign. But we know that in the problem of describing the sign of the scalar curvature, especially on a compact manifold, one encounters the topology of the space. Parallel to the investigations of solutions of the constraint equations by

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physicists and mathematicians, mathematicians proved remarkable results on the properties of the scalar curvature of Riemannian manifolds. By an early general result of Kazdan and Warner (1975) we know that for compact manifolds of dimension greater than two there is no constraint on the scalar curvature *if there is at least one point where it is negative*. This shows that it is easy to construct manifolds with negative scalar curvature. If we wish to construct manifolds with non-negative scalar curvature, however, we have to face various obstacles coming from the topology of the manifold. We just mention two basic examples. By results of Lichnerowicz and Hitchin, on spin manifolds it is often impossible to construct metrics of positive scalar curvature because of a subtle topological invariant, the so-called $\hat{A}$-genus (Hitchin, 1974; Lichnerowicz, 1963). Moreover, in three dimensions, the size of the fundamental group provides another obstruction for positive scalar curvature by results of Gromow and Lawson (1983) and Schoen–Yau (1984). An excellent survey on this branch of differential geometry is Besse (1987).

These observations make it not surprising that the topology of the Cauchy surface has a strong influence on the properties of initial data on it. The goal of this article is to understand this link a bit better. Our motivation is a paper by Witt (1986) who studied the problem of existence of initial data on general three-manifolds and examined certain characteristics of these initial data. In Sec. III we prove a theorem which states that on open Riemannian manifolds with everywhere nonpositive scalar curvature the extrinsic curvature field of nonvacuum initial data cannot be compactly supported, i.e., it has a ''tail'' at infinity although this tail may have sufficiently fast fall-off to make such an initial data still asymptotically flat. The proof of this theorem is elementary and is based on the following idea.

By using the initial data set (M,g,k) and the assumption that $\operatorname{supp} k$ is compact, we construct another ''universal'' initial data set $(M,g,\varphi g)$ where $\varphi: M \to \mathbb{R}$ is a compactly supported at least once continuously differentiable (or C^1-) function on M (with a little more effort this function could be smoothened but we do not need this). However, this leads us to a contradiction if the scalar curvature of g is nonpositive everywhere. In other words, we deform the original initial data set into a standard one whose properties are easier to understand.

II. BACKGROUND MATERIAL

First let us introduce some notations. Let W be a smooth manifold. We will call a tensor field T of type (m,n) over W if it is a smooth section of the bundle

$$T^{(m,n)}W := \underbrace{TW \otimes \ldots \otimes TW}_{m} \otimes \underbrace{T^*W \otimes \ldots \otimes T^*W}_{n}.$$

Remember that an *initial data set for general relativity* is a triple (M,g,k), where M is a (not necessarily compact) connected, oriented, smooth three-manifold, $g=(g_{ij})$ is a smooth, complete Riemannian metric on M, i.e., a nondegenerate smooth symmetric tensor field of type (0,2) on M while $k=(k_{ij})$ is a smooth, symmetric tensor field on M also of (0,2)-type. These fields must satisfy the following constraint equations (Hawking and Ellis, 1973; Wald, 1984):

$$\begin{aligned} s_g - |k|_g^2 + \mathrm{tr}^2 k &= 16\pi\rho, \\ \operatorname{div}(k - (\mathrm{tr}k)g) &= 8\pi J, \\ \rho \geqslant |J|_g &\geqslant 0. \end{aligned} \tag{1}$$

Here s_g is the scalar curvature of the metric g and $|\cdot|_g$ denotes various norms given by the induced scalar product on $T^{(m,n)}M$, e.g., $|k|_g^2 = \langle k,k\rangle = k_{ij}k^{ij}$. The operator $\mathrm{tr}: T^{(m,n)}M \to T^{(m-1,n-1)}M$ is the trace with respect to the metric, e.g., $\mathrm{tr}k = k^i_i$. For the sake of simplicity in the second equation we also denote by g and k the (1,1)-tensors with respect to the metric g [i.e., $g=(g^i_j)$, $k=(k^i_j)$ in the second equation]. The linear differential operator $\operatorname{div}: C^\infty(T^{(m,n)}M) \to C^\infty(T^{(m-1,n)}M)$ is the covariant divergence, defined by

$$\mathrm{div}T:=\mathrm{tr}(\nabla T),$$

where T is a tensor field of (m,n)-type and ∇ is the Levi–Civitá covariant derivative of the metric g. The smooth function $\rho:M\to\mathbb{R}$ is the energy-density, and the smooth covector field $J\in C^\infty(T^*M)$ with $|J|_g^2=\langle J,J\rangle=J_iJ^i$ is interpreted as the momentum-density of matter.

Supposing the energy- and momentum-densities correspond to classical nondissipative matter sources or vacuum ($J=0$, $\rho=0$), the coupled Einstein equations can be used to evolve the initial data set (M,g,k) into a (globally hyperbolic) smooth space–time (N,h) where $N\cong M\times\mathbb{R}$ and M is a Cauchy surface in N. Furthermore, $h|_M=g$ and k is the second fundamental form or extrinsic curvature of M in (N,h) (Hawking and Ellis, 1973; Wald, 1984)

Also remember that the open oriented three-manifold M has an *end* $E\subset M$ if there is a compact set $C\subset M$ such that $M\backslash C=E$ and $E\cong S_g\times(\mathbb{R}^+\backslash\{0\})$ where S_g is a compact, oriented surface of genus g and $\mathbb{R}^+=[0,\infty)$. An initial value data set (M,g,k) is called *asymptotically flat along E if M has an end* $E\cong S^2\times(\mathbb{R}^+\backslash\{0\})$ and the following asymptotical fall-off conditions hold for the complete metric g and the field k (r parametrizes $\mathbb{R}^+$ in E):

$$(g|_E)_{ij}=\delta_{ij}+O(1/r),\quad (k|_E)_{ij}=O(1/r^2),$$

$$\partial_l(g|_E)_{ij}=O(1/r^2),\quad \partial_l(k|_E)_{ij}=O(1/r^3),$$

$$\partial_l\partial_k(g|_E)_{ij}=O(1/r^3).$$

Notice that the definition of a manifold with an end does not exclude the possibility that M still has a boundary, different from the end E (strictly speaking, E is not a boundary). But the boundary points are added to M because $C=M\backslash E$ is compact according to our assumption. Consequently geodesic completeness of g requires that this extra boundary must be empty, in other words M is diffeomorphic to the punctured manifold $\tilde{M}\backslash\{y\}$ where $\tilde{M}$ is a connected, compact, oriented three-manifold without boundary.

Finally, the *support* of a tensor field $T\in C^\infty(T^{(m,n)}W)$ is the closed set

$$\mathrm{supp}T:=\overline{\{x\in W|T(x)\neq 0\}}.$$

After this background material, we are in a position to prove our theorem. The motivation is the following.

III. THE THEOREM

It was proved by Witt (1986) that every three-manifold with an end admits a nonvacuum, asymptotically flat initial data set. For a typical three-manifold, the resulting Cauchy developed space–time does not admit maximal slices, however; i.e., there are no maximal spacelike submanifolds whose extrinsic curvature is identically zero. One may raise the question: to what extent are these slices not maximal? In other words, what are the conditions on a Riemannian manifold (M,g) for its extrinsic curvature in the Cauchy development to be compactly supported at least? We will answer this question in our theorem.

Theorem (rigidity for nonvacuum initial data): *Let (M,g) be a connected, oriented, complete Riemannian three-manifold with an end $E\cong S^2\times(\mathbb{R}^+\backslash\{0\})$. Suppose the scalar curvature s_g of g is nonpositive everywhere and there is a nonvacuum initial data set (M,g,k) on it which is asymptotically flat along the end E. Then* $\mathrm{supp}\,k$ *is noncompact.*

Proof: Since the scalar curvature is nonpositive, the set $\mathrm{supp}\,s_g$ consists of the closure of those points where s_g is negative. Then the first and third (in)equalities of (1) show that $\mathrm{supp}\,s_g\subseteq\mathrm{supp}\,k$; therefore, if the scalar curvature is negative everywhere, the statement is trivially true, consequently we may assume that $\mathrm{supp}\,s_g\subset M$. In the same fashion, since (M,g,k) is a nonvacuum data set, there is a point $x_0\in M$ such that $\rho(x_0)\neq 0$. This yields $\mathrm{supp}\,\rho\neq\emptyset$. Being the scalar curvature nonpositive, via the first and third (in)equalities of (1) again we have $k(x_0)\neq 0$,

i.e., $\operatorname{supp}\rho\subseteq\operatorname{supp}k$. Therefore, if the energy density is supported everywhere, the theorem is again trivially valid, consequently we may assume $\operatorname{supp}\rho\subset M$. Consider a subset $C\subset M$ such that $\operatorname{supp}s_g\subset C$ and $\operatorname{supp}\rho\subset C$ and suppose the decomposition $M=C\cup E$ is valid where E denotes the end of M. Consequently, by the structure of M we may assume that C is compact. This shows that there is a constant

$$0<a:=\sup_{x\in C}(-|k(x)|_g^2+\operatorname{tr}^2k(x))<\infty.$$

Consider a triple $(M,g,\varphi g)$ where $\varphi:M\to\mathbb{R}$ is a C^1-function. This triple is a weak initial data set if it obeys the constraint equations (here by "weak" we mean that the initial data set in question is not smooth, only C^k for some $k\in\mathbb{N}$):

$$s_g+6\varphi^2=16\pi\rho,$$

$$-2\operatorname{div}(\varphi g)=-2\operatorname{tr}(\nabla(\varphi g))=-2\operatorname{tr}(\mathrm{d}\varphi\otimes g)=8\pi J,$$

$$\rho\geqslant|J|_g\geqslant 0.$$

In the second equation we have used the fact that $\nabla g=0$. These (in)equalities can be combined into a first order partial differential inequality for the unknown function φ:

$$\tfrac{1}{4}(s_g+6\varphi^2)\geqslant|\mathrm{d}\varphi|_g, \tag{2}$$

taking into account that $|\operatorname{tr}(\mathrm{d}\varphi\otimes g)|_g=|\mathrm{d}\varphi|_g$. *Assume $\varnothing\neq\operatorname{supp}k\subset M$ is compact, i.e., the theorem is not true.* In this case we construct a compactly supported function φ out of the original data (M,g,k) such that $(M,g,\varphi g)$ is a weak initial data set. We achieve this in three steps.

(*i*) *Construction of φ in the compact interior of M.* Let us identify the end $E\subset M$ with $S^2\times(\mathbb{R}^+\setminus\{0\})$. By assumption $\operatorname{supp}k$ is compact in M, consequently there is an $R_1\in\mathbb{R}^+$ satisfying $S^2\times(R_1,\infty)\not\subset\operatorname{supp}k$. Note that this is possible only if $s_g|_{S^2\times(R_1,\infty)}=0$. We can take the choice $C:=M\setminus(S^2\times(R_1,\infty))$ for the compact set used in the definition of the constant a. We construct the function φ in C as follows:

$$\varphi(x):=-\sqrt{a},\quad x\in C.$$

In other words φ is a constant negative function on M except the infinite tube $S^2\times(R_1,\infty)$. Note that with this function (2) is trivially satisfied in C because (M,g,k) is an initial data set on C.

(*ii*) *Construction of φ along an annulus in E.* Consider an inner point $x_0\in C\subset M$ where $\rho(x_0)>0$ and $k(x_0)\neq 0$. There is an open (geodesic) ball $B_\varepsilon(x_0)\subset M$ of radius $\varepsilon>0$ such that $\rho|_{B_\varepsilon(x_0)}>0$ and $k|_{B_\varepsilon(x_0)}\neq 0$. Consider the annulus $U_\varepsilon:=\overline{B_\varepsilon(x_0)\setminus B_{\varepsilon/2}(x_0)}\cong S^2\times[\varepsilon/2,\varepsilon]$. Take another constant $R_1<R_2<\infty$ and the diffeomorphism

$$\beta:U_\varepsilon\to S^2\times[R_1,R_2],\quad x_t=(p,t)\mapsto\left(p,R_1+\frac{2t-\varepsilon}{\varepsilon}(R_2-R_1)\right)=(p,r),$$

where $p\in S^2$ and the point $x_t\in U_\varepsilon$ is identified with $(p,t)\in S^2\times[\varepsilon/2,\varepsilon]$. Here $S^2\times[R_1,R_2]$ is also an annulus in the tube E. By assumption g is asymptotically flat, i.e., the function $\sqrt{g^{11}}\geqslant 0$ is bounded, consequently there is a constant

$$0<b:=\sup_{x\in M}\sqrt{g^{11}(x)}<\infty$$

(here $x^1=r$). Choose a smooth function $\psi:[R_1,R_2]\to\mathbb{R}^-$. Viewing it as a function on $S^2\times[R_1,R_2]$ (i.e., a function depending only on r), one obtains the estimate

$$b|\psi'| \geqslant |\sqrt{g^{11}}\psi'| = |\mathrm{d}\psi|_g , \tag{3}$$

where prime denotes differentiation with respect to r. Now we define ψ as follows:

$$\psi(\beta(x_t)) := \begin{cases} -\sqrt{a}, & \text{if } t = \dfrac{\varepsilon}{2} \\ \text{arbitrary but the derivative of } \psi \text{ is small}, & \text{if } t \in \left(\dfrac{\varepsilon}{2}, \varepsilon\right), \\ 0, & \text{if } t = \varepsilon . \end{cases}$$

In this definition the smallness of ψ' means the following. Consider a differentiable curve $\gamma : [\varepsilon/2, \varepsilon] \to U_\varepsilon$ given by

$$t \mapsto x_t := (\Theta_{\varepsilon/2} + A \sin(R_2 - R_1)t,\ \phi_{\varepsilon/2} + A \sin(R_2 - R_1)t, t).$$

This is a high-speed curve because it oscillates rapidly inside $B_\varepsilon(x_0)$. More precisely, for its speed $|\dot{\gamma}(t)|_g \sim R_2 - R_1$ is valid (dot denotes differentiation with respect to t). We can take a choice for the point x_0 and the amplitude A, and initial phases $\Theta_{\varepsilon/2}$ and $\phi_{\varepsilon/2}$ of the curve γ such that

$$\mathrm{d}\left(\sqrt{-|k(x_t)|_g^2 + \mathrm{tr}^2 k(x_t)}\right)(\dot{\gamma}(t)) \sim -(R_2 - R_1) < 0$$

holds for each $t \in [\varepsilon/2, \varepsilon]$. Then we suppose

$$0 \leqslant \psi'(\beta(x_t)) \leqslant \min\left(-\frac{\varepsilon}{4(R_2 - R_1)} \mathrm{d}\left(\sqrt{-|k(x_t)|_g^2 + \mathrm{tr}^2 k(x_t)}\right)(\dot{\gamma}(t)), \frac{16\pi}{b}\rho(x_t) \right). \tag{4}$$

It is also clear that such a function exists if R_2 is suitably large: let ψ be an arbitrarily smooth, negative-valued function $\psi : S^2 \times [R_1, R_2] \to \mathbb{R}^-$ with initial value $\psi(p, R_1) = \psi(\beta(x_{\varepsilon/2})) = -\sqrt{a}$. Suppose there is an interval $[R, R+T] \subset [R_1, R_2]$ such that ψ' obeys (4), but there is a constant $c > 0$ with $\psi'(p,r) \geqslant c$ if $r \in [R, R+T]$. This constant can be chosen to be independent of $R_2 - R_1$. In this case we can estimate for large R_1 and R_2 as follows:

$$\psi(p, R_2) \geqslant -\sqrt{a} + \frac{1}{2}\int_{R_1}^{R_2} \psi'(p,r)\mathrm{d}r \geqslant -\sqrt{a} + \frac{1}{2}\int_{R}^{R+T} \psi'(p,r)\mathrm{d}r \geqslant -\sqrt{a} + \frac{c}{2}T.$$

In other words, if T, that is, $R_2 - R_1$, is sufficiently large, we can achieve that $\psi(p, R_2) = 0$. We choose φ on $S^2 \times [R_1, R_2]$ to be the ψ just constructed.

It is not difficult to check that φ obeys (2) in $S^2 \times [R_1, R_2]$. Indeed, by the definition of the constant a we have

$$\varphi(p, R_1) = \varphi(\beta(x_{\varepsilon/2})) = -\sqrt{a} \leqslant -\sqrt{-|k(x_{\varepsilon/2})|_g^2 + \mathrm{tr}^2 k(x_{\varepsilon/2})}.$$

Taking suitable large R_1 and R_2, exploiting the decay of the metric g and using (4) this implies that for each $t \in [\varepsilon/2, \varepsilon]$ we have

$$\begin{aligned} \varphi(\beta(x_t)) = \varphi(p,r) &= -\sqrt{a} + \int_{R_1}^{r} \mathrm{d}\varphi(p,\varrho)(\beta'(x_\tau))\mathrm{d}\varrho \\ &= -\sqrt{a} + \int_{R_1}^{r} \varphi'(p,\varrho)\Big(g_{11}(p,\varrho) + A\frac{\varepsilon}{2}(g_{12}(p,\varrho) + g_{13})(p,\varrho) \\ &\quad \times \cos\frac{\varepsilon}{2}(\varrho + R_2)\Big)\mathrm{d}\varrho \end{aligned}$$

$$\leqslant -\sqrt{a}+2\int_{R_1}^{r}\varphi'(p,\varrho)\,\mathrm{d}\varrho$$

$$=-\sqrt{a}+\frac{4(R_2-R_1)}{\varepsilon}\int_{\varepsilon/2}^{t}\varphi'(\beta(x_\tau))\,\mathrm{d}\tau$$

$$\leqslant -\sqrt{-|k(x_{\varepsilon/2})|_g^2+\mathrm{tr}^2k(x_{\varepsilon/2})}-\int_{\varepsilon/2}^{t}\mathrm{d}\big(\sqrt{-|k(x_\tau)|_g^2+\mathrm{tr}^2k(x_\tau)}\big)(\dot\gamma(\tau))\,\mathrm{d}\tau$$

$$=-\sqrt{-|k(x_t)|_g^2+\mathrm{tr}^2k(x_t)}.$$

Consequently,

$$\varphi^2(\beta(x_t))\geqslant -|k(x_t)|_g^2+\mathrm{tr}^2k(x_t).$$

Therefore, since $s_g(\beta(x_t))=0$ and $0\geqslant s_g(x_t)$, we can write

$$\tfrac{1}{4}(s_g(\beta(x_t))+6\varphi^2(\beta(x_t)))=\tfrac{3}{2}\varphi^2(\beta(x_t))\geqslant s_g(x_t)-|k(x_t)|_g^2+\mathrm{tr}^2k(x_t)=16\pi\rho(x_t).$$

Moreover, also by (4), we have for the same $x_t\in U_\varepsilon$ that $16\pi\rho(x_t)\geqslant b\varphi'(\beta(x_t))$. This gives rise to our key inequality

$$\tfrac{3}{2}\varphi^2(\beta(x_t))\geqslant b\varphi'(\beta(x_t)),\tag{5}$$

showing via (3) that (2) is again satisfied in the annulus $S^2\times[R_1,R_2]$.

(iii) Construction of φ along the remaining part of the infinitely long tube in M. Finally, define

$$\varphi(x):=0\quad\text{if } x\in S^2\times[R_2,\infty).$$

Again, (2) is trivially valid.

Consider the function $\varphi:M\to\mathbb{R}^-$ defined through (i)–(iii). This is a continuous negative function on M and is compactly supported: it is equal to zero for all $r\geqslant R_2$ and equal to the constant $-\sqrt{a}$ if $r\leqslant R_1$. Its derivative is also compactly supported in $S^2\times[R_1,R_2]$ and is positive. Moreover, φ can be adjusted to be C^1 on M (note that φ is smooth except at the junction points): it is clearly C^1 at $r=R_2$ by (5). However, by exploiting the freedom in the construction of φ in the inner points of the annulus, we can deform it to be C^1 at $r=R_1$ as well [i.e., we may assume that $\varphi'(p,r)\to 0$ as $r\to R_1$]. In this way we have constructed a weak C^1 initial data set $(M,g,\varphi g)$ (with a little effort we could smooth this data but we do not need this).

The compactly supported φ depends nontrivially only on r with $(p,r)=\beta(x_t)\in S^2\times[R_1,R_2]$ and satisfies the ordinary differential inequality (5). Now we demonstrate that it is impossible. Dividing by φ'^2 and taking reciprocies in (5) we get

$$\left(\frac{\varphi'}{\varphi}\right)^2\leqslant\frac{3\varphi'}{2b},$$

which is nothing but

$$-\sqrt{\frac{3\varphi'}{2b}}\leqslant\frac{\varphi'}{\varphi}\leqslant\sqrt{\frac{3\varphi'}{2b}}.$$

By integrating the left inequality from R_1 to $r<R_2$ we arrive at the following estimate:

$$\log\sqrt{a}-\sqrt{\frac{3}{2b}}\int_{R_1}^{R_2}\sqrt{\varphi'(p,\varrho)}\,\mathrm{d}\varrho\leqslant\log(-\varphi(p,r)).$$

At this point we have used the inequality

$$0<\int_{R_1}^{r}\sqrt{\varphi'(p,\varrho)}\,\mathrm{d}\varrho\leqslant\int_{R_1}^{R_2}\sqrt{\varphi'(p,\varrho)}\,\mathrm{d}\varrho<\infty$$

for the non-negative function φ'. This shows that the logarithm of φ is bounded from below. However, being φ compactly supported, $\log(-\varphi(p,r))$ is unbounded, as r approaches R_2. Consequently the last but one inequality shows a contradiction yielding our original assumption, that $\operatorname{supp} k$ is compact, was wrong. We finished the proof. ◇

Remarks. (1) We would like to summarize here how the original initial data (M,g,k) was used in the construction because apparently its behavior has been taken into account only in a particular small ball $B_\varepsilon(x_0)$. But, in fact, the construction is sensitive for the global characteristics of the original initial data. In step (i) we considered (M,g,k) in the whole interior C by exploiting the existence of the constant a which is in some sense the maximum of k in the whole compact C. This enabled us to ''pump up'' the original initial data in C into a standard one which corresponds to the extremal point(s) of the original extrinsic curvature in some sense. Concerning part (iii), we have seen in the beginning of the proof that the only interesting possibility for our would-be initial data with compactly supported extrinsic curvature was the case where both the scalar curvature and energy-density were compactly supported. Consequently all fields in the initial data vanish along the tube for very large r yielding the hypothetical initial data did not carry ''information'' along an infinitely long part of the end E. This is in accordance with the fact that our adjusted universal initial data $(M,g,\varphi g)$ was also trivial on this portion. Finally, part (ii), which is the descending regime, is nothing but a magnification of the behavior of (M,g,k) in a small ball where matter is present via the diffeomorphism β. Indeed this small ball is responsible for the details of the fall-off of φ (we could have used equally well any other ball), however, the fact that this function can vanish within a finite distance is again guaranteed by the global properties of the original would-be initial data set: namely the only interesting case was when all fields were compactly supported.

(2) Note that even if $\operatorname{supp} k$ is noncompact the nonvacuum data (M,g,k) may be asymptotically flat, as it is shown by Witt (1986) who constructs nonvacuum, asymptotically flat initial data for every three-manifold with an end. But the above theorem is sharp in the following sense. If we allow for a Riemannian manifold (M,g) to have positive scalar curvature in a suitable region in M, it is possible to construct nonvacuum asymptotically flat initial data with compactly supported second fundamental form. An example is the Tolman–Bondi solution. This is because in this case the key inequality (5) can be written in the form

$$\tfrac{1}{4}(s_g+6\varphi^2)\geqslant b\varphi'$$

with $s_g>0$ in the positive scalar curvature regime and it may have compactly supported solutions. But if s_g is still negative somewhere, then k is nonzero in that point; consequently, the initial surface is not a maximal slice in this case.

(3) Notice that the above considerations do not remain valid for *vacuum initial data*. For example, the Schwarzschild space–time has initial data with nonpositive scalar curvature (namely it is identically zero) but the extrinsic curvature of the initial surface is compactly supported (namely identically zero, i.e., the initial surface is a maximal slice). We conjecture that the analog of the above theorem for vacuum initial data is the following: if (M,g) is an asymptotically flat three-manifold with *some*where negative scalar curvature, then any vacuum initial data set (M,g,k) cannot be asymptotically flat (i.e., the extrinsic curvature cannot decay at the required rate). But in this moment we are unable to prove this.

IV. CONCLUDING REMARKS

In the previous section we have studied gravitational initial data from a general point of view. We have found that in the case of nonpositive scalar curvature, the behavior of the extrinsic curvature becomes very ''rigid:'' for open manifolds, the fall-off of the extrinsic curvature cannot be arbitrary.

The negativity of the scalar curvature becomes important by an early general result of Kazdan and Warner (1975):

Theorem (Kazdan–Warner): *Let W be a compact manifold with* $\dim W \geqslant 3$, *and $f: W \to \mathbb{R}$ be a smooth function on it such that there is a point $x \in W$ obeying $f(x) < 0$. Then there is a smooth Riemannian metric h on W such that $s_h = f$,* i.e., *whose scalar curvature is the prescribed function f.* ◇

The theorem demonstrates that a compact manifold of sufficiently large dimension always can be endowed with a metric with somewhere negative scalar curvature. This shows, taking into account the constraint equations, that it is relatively easy to construct initial data with somewhere non-zero extrinsic curvature.

The classical results of Gromow and Lawson (1983) and Schoen and Yau (Schoen, 1984), however, show that closed three-manifolds whose prime decomposition contains a $K(\pi,1)$ factor (this implies such manifolds have infinite fundamental groups) do not carry any metric with positive scalar curvature. Consequently, initial data with positive scalar curvature must be rare at least in the compact case.

If the compact $\tilde{M}$ does not have positive scalar curvature, the punctured, open manifold $M = \tilde{M} \backslash \{y\}$ of this type, which is nothing but a manifold with an end, does not have a metric with non-negative scalar curvature, too. Consequently, these punctured manifolds do not admit nonvacuum, asymptotically flat initial data with identically zero extrinsic curvature. Furthermore, if the scalar curvature is everywhere nonpositive, then this extrinsic curvature has noncompact support, as we have seen.

These results are quite surprising because all the fields in question are defined in the class of smooth functions, so one would expect that initial data can be altered *locally* in a nontrivial way. In other words, we have reduced the local degrees of freedom of the gravitational field in some sense.

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The Fermat principle in general relativity and applications

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In this paper we use a general version of Fermat's principle for light rays in general relativity and a curve shortening method to write the Morse relations for light rays joining an event with a smooth timelike curve in a Lorentzian manifold with boundary. The Morse relations are obtained under the most general assumptions and one can apply them to have a mathematical description of the *gravitational lens effect* in a very general context. Moreover, Morse relations can be used to check if existing models are corrected. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Fermat's principle in classical optics states that the trajectory of a light ray from a source A to a target B is such that it is a minimizer, or better, a stationary curve for the travel time among all the paths joining points A and B.

This variational principle can be extended in the context of general relativity where the trajectory of a light ray under the action of the gravitational field in vacuum is given by a null geodesic in the Lorentzian manifold modeling the space–time generated by a gravitational mass distribution.

A formulation of Fermat's principle is given once the following data are determined:

(1) a set of *trial curves* joining the light source and the observer;
(2) a *functional* that associates to each trial curve a real number, which has to be related to a measurement of the *time* passed from the instant at which the photon departed from the light source to the instant at which the photon arrives to the observer.

A mathematical proof of Fermat's principle consists in proving that the trajectory of a light ray is *characterized* as a stationary point of the time functional in the set of trial curves.

The geodesics in a semi-Riemannian manifold are characterized as solutions of differential equations, and the *local* theory of the light rays can be developed in terms of systems of differential equations in $\mathbb{R}^n$. However, the variational approach has the advantage of providing techniques for proving *global* existence results, and also for producing several kinds of estimates on the number of solutions, given in terms of the topology of the space of trial curves. To this aim in this paper we prove the *Morse relations* for light rays, which will be presented in detail in Sec. II. We now proceed to a general discussion of the mathematical problem, its physical applications, and a presentation of the results that will be proven in this paper.

We fix a Lorentzian manifold $(\mathcal{M},g)$ that is the mathematical model of our relativistic space–time, and we assume that $\mathcal{M}$ is endowed with a time orientation given by the choice of a continuous timelike vector field W on $\mathcal{M}$. Such assumption is indeed very mild; namely, given

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any Lorentzian manifold, there always exists a twofold covering $\tilde{\mathcal{M}}$ of $\mathcal{M}$ that admits a time orientation (cf. Ref. 1), and clearly there is a two-to-one correspondence between the geodesics in $\tilde{\mathcal{M}}$ and those on $\mathcal{M}$. If we want to study the light rays emitted by some source at a given time in the past, represented by an event p of $\mathcal{M}$, and reaching an observer sometimes during its life, whose worldline is given by a timelike curve γ in $\mathcal{M}$, then we need to determine all the lightlike future pointing geodesics joining p and γ in $\mathcal{M}$. We are assuming here that both the source and the receivers are *pointlike*, i.e., they have dimensions which are neglectible with respect to their distance; a variational principle for light rays between a spatially extended source and a spatially extended receiver may be found in Ref. 2.

In analogy with the principle in classical optics, the set of trial curves is chosen to be the set of all possible future pointing trajectories joining the source with the observer, and that are run at the speed of light. This amounts to saying that a trial curve is a curve whose tangent vector is everywhere in the light cone, and it belongs to the same half light cone as the vector field W.

The choice of the *regularity* to impose on the trial curves and, most of all, the choice of the functional to be extremized are rather delicate questions, which have deep consequences for the mathematical theory to be developed.

The first relativistic formulation of the principle, valid in the case of a *static* space–time, is due to Weyl (see Ref. 3); the validity of the general relativistic Fermat's principle was successively extended to the case of *stationary* space–times by Levi-Civita (see Ref. 4). For *conformally stationary* space–times an alternative formulation of the principle is given in Ref. 5.

The first attempt to extend Fermat's principle beyond the (conformally) stationary case is due to Uhlenbeck (see Ref. 6), who considered a Lorentzian manifold diffeomorphic to a space–time splitting $\mathcal{M}_0\times\mathbb{R}$ and a time-dependent metric which is diagonal with respect to this product. The variational principle proven in Ref. 6 employs the time functional given by the projection onto the second factor calculated at the final point of each trial curve. Such functional does not depend on the parametrization of the trial curve as, for instance, the *length* functional for curves in a Riemannian manifold, and this lack of *rigidity* makes it a difficult task to obtain results of the existence and multiplicity of critical points. For this reason, in order to prove the classical Morse relations the author employs an action functional whose Lagrangian function depends quadratically on the velocities. This kind of functional has a strict relationship with the *energy* functional for Riemannian geodesics, obtained by *removing the square root* inside the integral that defines the length. The same variational principle was used in Ref. 7 to obtain Morse relations for light rays on orthogonal splitting Lorentzian manifolds, using an infinite dimensional setting and covering some gaps that occur in Ref. 6. Such a variational principle was extended in Ref. 8 to *stably causal* Lorentzian manifolds having a smooth time function and applied in Refs. 9 and 10 to obtain multiplicity results and Morse relations for light rays joining an event p with a timelike curve γ in the presence of a smooth convex boundary.

A very general version of the principle, valid in all space–times, was given recently by Kovner (see Ref. 11), who introduced the so called *arrival time* functional with respect to the observer γ, defined on the space of *piecewise smooth* lightlike curves joining p and γ. Such functional is given by fixing any (future pointing) parametrization of γ, and assigning to each trial curve the value of the parameter of γ at the arrival point. Any two future pointing parametrizations of γ differ by an order preserving diffeomorphism between two intervals of the real line; it is an easy observation that the stationary points of the arrival time functional do not indeed depend on the choice of the parametrization of γ.

A rigorous mathematical proof of the Kovner's claim was given in Ref. 12. However, the proof in Ref. 12 needs the assumption that the critical points have nonzero derivative everywhere.

An alternative variational principle on the space of lightlike curves z with a suitable prescribed parametrization and satisfying $\dot{z}(s)\neq 0$ for all s, can be found in Ref. 13. However, using this approach it is not possible to obtain Morse relations, as will be clear from the discussion presented in Appendix B.

In Ref. 10 the reader will find a more detailed presentation of the different versions of the

relativistic Fermat principle and some examples and applications to the multiple image effect (the so called "gravitational lens effect").

In Ref. 14 published in 1979, Walsh, Carlswell, and Weymann discussed the possibility that the double quasar $0957+561$ would be a good candidate for a gravitational lens effect. Such a name refers to the phenomena occurring when a multiple image of some stellar object is observed. The multiple image effects are due to the deflection of the light in the presence of a gravitational field. We refer, e.g., to Refs. 15 and 16 for a detailed physical description of the gravitational lens effect and many physical examples. In Refs. 17 and 18 it is shown how one can use the Morse relations to check if a model is corrected or not. The version of the relativistic Fermat principle introduced by Kovner also allows one to treat nonstationary situations such as a gravitational wave sweeping over a gravitational lensing situation. More details can be found in Ref. 19.

Some natural questions arise in the study of the gravitational lensing effect; for instance, an attempt is made to understand under which circumstances a multiple imaging of a distant source can occur, and, in this case, how many images of the source can be seen. In mathematical terms, these questions can be answered by giving conditions on the topology and the metric of the space–time that guarantee a multiplicity of lightlike geodesics between p and γ lying inside an open set Λ, which represent the region of the universe in which to localize the description for any gravitational lens. As already mentioned, a technique for investigating these issues is provided by the Morse theory, which is a well-established mathematical theory that relates the critical points of a smooth functional with the topology of the underlying space.

The main purpose of this paper is to develop an infinite dimensional Morse theory under *minimal* assumptions on the global structure of the space–time and on the timelike curve γ. This, in particular, allows us to extend the results in Refs. 5, 6, 7, and 10 concerning Morse relations. Most of all, we want to push the results beyond the compactness assumption of *global hyperbolicity* made in Refs. 6 and 7; we also generalize the results of Ref. 10 in the following directions:

(1) we do not assume the *stable causality* of the Lorentzian manifold $(\mathcal{M},g)$, which will only be assumed to be time orientable;
(2) we do not assume any regularity for the boundary $\partial\Lambda$ of the region Λ;
(3) we do not assume that γ is embedded as a *closed* subset of $\Lambda\subseteq\mathcal{M}$.

Observe in particular that the second generalization above allows one to also extend the results to light rays moving on a region of the universe exterior to a static blackhole (see Ref. 20). For the functional framework, we will employ Kovner's arrival time functional, denoted by τ; observe that the definition of τ does not require the existence of a *global time function* on Λ, which was a crucial assumption in Refs. 7 and 10.

For a correct physical interpretation of our results, all the relevant information about the light rays joining p and γ must be encoded in the open subset Λ. For this reason, if $\Lambda\neq\mathcal{M}$, we assume the following *convexity* property of Λ:

$$\begin{aligned}&\textit{every lightlike geodesic starting from any event in } \Lambda\\ &\textit{and moving outside } \overline{\Lambda} \textit{ does not come back in } \Lambda.\end{aligned}\tag{$*$}$$

Note that assumption $(*)$ is not strictly necessary to develop our theory. As a matter of fact, we will use a more general assumption: the light convexity of the boundary of Λ (cf. (3) in Sec. III). Observe also that in the Minkowski space–time a set $\Lambda_0\times\mathbb{R}$ satisfies condition $(*)$ precisely when Λ_0 is convex. Other simple examples of space–times satisfying $(*)$ are the regions outside the event horizon of the Schwarzschild and Reissner–Nordström space–times (see Ref. 21).

Our Morse relations are given for future pointing lightlike geodesics; we remark here that there is also a time-reversed version of Fermat's principle. Namely, p can be interpreted as a pointlike receiver at a particular instant of time and γ as the worldline of a pointlike light source, in which case one is interested in determining the past pointing light rays from p to γ. Clearly, the results proven in the paper are still valid in the past pointing case. From a mathematical point of

view, the case of past pointing light rays is completely analogous, and will not be treated explicitly in this paper.

In Sec. II we will give a formal statement of our results, and we will present arguments to show that our assumptions cannot be weakened to obtain a Morse theory.

The reader is referred to classical books such as those noted in Refs. 1, 20, and 22 for the main notions and properties in Lorentzian geometry.

Finally, we remark that alternative approaches to the study of the Morse theory for light rays are available in Refs. 23–25; the author applies the Morse theory in a time independent *quasi-Newtonian* setting.

II. STATEMENT OF THE RESULTS AND SOME DISCUSSION ABOUT THE ASSUMPTIONS

Let $(\mathcal{M},g)$ be a smooth Lorentz manifold, Λ an open connected subset of $\mathcal{M}$, $p\in\Lambda$, $\gamma:]\alpha,\beta[\to\Lambda$ a smooth timelike curve such that $p\notin\gamma(]\alpha,\beta[)$. Here and in the rest of the paper we will often set $\langle\cdot,\cdot\rangle\equiv g(z)[\cdot,\cdot]$.

We assume that $(\mathcal{M},g)$ is time orientable. This means that there exists a smooth vector field W on $\mathcal{M}$ such that $\langle W(z),W(z)\rangle<0$ for any $z\in\mathcal{M}$. With respect to the orientation W we assume that

(1) *γ is future pointing,*

namely

$$\langle\dot\gamma(s),W(\gamma(s))\rangle<0\,\forall s\in]\alpha,\beta[.$$

Since we want to study future pointing light rays joining p and γ in Λ, we shall only consider past and future relative to Λ. More precisely given two points q_1 and q_2 in Λ, we say that q_2 is in the future of q_1 [in symbols $q_2\in J^+(q_1,\Lambda)$] if there exists a piecewise smooth curve $y:[0,1]\to\Lambda$ such that $\langle\dot y,\dot y\rangle\leqslant 0$ (i.e., y is a causal curve), $\langle\dot y,W(y)\rangle<0$ (i.e., y is future pointing), $y(0)=q_1, y(1)=q_2$. In general if $A\subset\Lambda$ the future of A (in Λ) is the set

$$J^+(A,\Lambda)=\bigcup_{a\in A}J^+(a,\Lambda),$$

while the past of A (in Λ) is the set

$$J^-(A,\Lambda)=\{q\in\Lambda: A\cap J^+(q,\Lambda)=\varnothing\}.$$

To have future pointing lightlike curves joining p and γ in Λ, clearly we need the following assumptions:

(2) *there exists $q_+\in\gamma(]\alpha,\beta[)\cap J^+(p,\Lambda)$.*

Moreover a light-convexity assumption on the closure $\overline{\Lambda}$ of the open subset Λ is needed:

(3) *$\overline{\Lambda}$ is light convex, i.e., all the lightlike geodesics in $\Lambda\cup\partial\Lambda$ with endpoints in Λ are enterely contained in Λ.*

Here $\partial\Lambda$ is the topological boundary of Λ. Finally, to be able to define the arrival time functional we need

(4) $\gamma:]\alpha,\beta[\mapsto\Lambda$ *is injective.*

By (4), on the space of the curves joining p and γ on the interval $[0,1]$, the arrival time functional is well defined

$$\tau(z)=\gamma^{-1}(z(1)). \tag{2.1}$$

The following assumptions says that τ is bounded from below on the set of the future pointing lightlike curves joining p and γ.

(5) *There exists $q_-\in\gamma(]\alpha,\beta[)\setminus J^+(p,\Lambda)$.*

Since we do not require that $\partial\Lambda$ is smooth we are not able to use the same penalizing argument as in Refs. 9 and 10 to overcome the difficulties due to the presence of the boundary. To

develop a Morse theory for the arrival time functional we should need a flow which is strictly decreasing far from the critical points. Since the boundary is not smooth a convenient approach is a shortening method.

Assumption (3) is necessary because we need a flow that it is invariant with respect to the lightlike curves with image in Λ. Note that to develop a Morse theory the presence of the boundary is a difficulty to bypass because we want to treat with ''free'' critical points lying in $\overline{\Lambda}$. Note also that, even if the boundary would be smooth, a shortening method seems technically more simple that the penalized techniques used in Refs. 7, 9, and 10. Moreover, since τ is invariant by reparametrizations, as well as the space of future pointing lightlike curves joining p and γ, a shortening approach also seems to be a good help to overcome this kind of difficulty.

To use the shortening method we need an assumption assuring the existence of minimizers in Λ between events and timelike curves. For this reason we also need the following assumption (6) *there exists a smooth timelike vector field W in $\mathcal{M}$ having the following properties:* (a) *γ is an integral curve of W* (*namely $\dot{\gamma}=W(\gamma)$ for any $s\in]\alpha,\beta[$*), (b) *for any $q\in J^+(p,\Lambda)\cup J^-(\gamma(]\alpha,\beta[),\Lambda)$ if γ_q is the maximal integral curve of W such that $\gamma_q(0)=q$, there is $\overline{q}\in[\mathrm{Im}\,\gamma_q\cap\Lambda]\backslash J^+(p,\Lambda)$.*

Here Im γ_q denotes the image of the curve γ_q. Note that assumption (6) is certainly satisfied if Λ is invariant with respect to the flow of W.

Morse theory gives an algebraic relation (in terms of formal series) between the critical points of a suitable functional (in our case the arrival time functional) and the topology of the space where the functional is defined. At this point there are two options: to introduce a Sobolev space of lightlike curves or to use broken lightlike geodesics as space of trial curves.

To state Morse relations we prefer here to use the second choice since it does not require the use of any auxiliary (Riemann) structure. Nevertheless in Sec. III we shall give an infinite dimensional formulation of the Fermat principle using Sobolev spaces. Indeed, even if we use a shortening procedure it is more convenient than an infinite dimensional approach to study the arrival time functional close to its critical points. This is due to the fact that here it is hard to try to reduce (as, e.g., in Refs. 6 and 7) the study of the functional τ on a space of curves joining two fixed points.

For this reason we are not able to adapt to our case the Milnor finite dimensional approximation scheme (cf. Ref. 26) close to critical points.

Now set

$$\begin{aligned}\mathcal{B}^+_{p,\gamma}(\Lambda)&\\ &=\{z:[0,1]\to\Lambda : z \textit{ is a } C^2 \textit{ piecewice curve such that } z(0)\\ &=p, z(1)\in\gamma(]\alpha,\beta[) \textit{ and, on any interval } [a,b]\subset]\alpha,\beta[\\ &\textit{where } z \textit{ is of class } C^2,\ z \textit{ is a constant or a future pointing light-like geodesic}\}.\end{aligned} \tag{2.2}$$

We point out that a curve $z\in\mathcal{B}^+_{p,\gamma}(\Lambda)$ may be constant on some interval $[a,b]\subset[0,1]$ (and therefore $z_{|[a,b]}$ is not a lightlike geodesic). Nevertheless the topological structure of the problem is carried on by the space $\mathcal{B}^+_{p,\gamma}(\Lambda)$, instead of the space $\hat{\mathcal{B}}^+_{p,\gamma}(\Lambda)$ of the broken lightlike geodesics (without subintervals where z is constant). A simple example in Appendix B shows that Morse relations cannot be written using $\hat{\mathcal{B}}^+_{p,\gamma}(\Lambda)$.

In Sec. V we shall prove the homotopy equivalence between $\mathcal{B}^+_{p,\gamma}(\Lambda)$ (endowed with the uniform topology) and the Sobolev spaces of future pointing, lightlike, $H^{1,r}$-curves joining p and γ ($r\in[1,+\infty]$).

Using the space $\mathcal{B}^+_{p,\gamma}(\Lambda)$ we can state our last assumptions. In Sec. III we shall prove that it is equivalent to the one formulated in Refs. 9 and 10.

For any $c\in]\alpha,\beta[$ [cf. (4)] we denote by τ^c the c-sublevel of the functional τ in $\mathcal{B}^+_{p,\gamma}(\Lambda)$:

$$\tau^c=\{z\in\mathcal{B}^+_{p,\gamma}(\Lambda):\tau(z)\leqslant c\}. \tag{2.3}$$

Definition 2.1: Fix $c>\alpha$. We say that $\mathcal{B}^+_{p,\gamma}(\Lambda)$ is c-precompact if any sequence $\{z_n:n\in\mathbb{N}\}\subset\tau^c$ has a subsequence uniformly convergent in $\overline{\Lambda}$, up to reparametrizations. We say that τ is pseudocoercive in $\mathcal{B}^+_{p,\gamma}(\Lambda)$, if $\mathcal{B}^+_{p,\gamma}(\Lambda)$ is c-precompact for any $c\in]\alpha,\beta[$.

Note that by assumption (5) there exists $\hat{s}>\alpha$ such that τ^c is the empty set for any $c\in]\alpha,\hat{s}]$.)

Whenever $\Lambda=\mathcal{M}$ pseudocoercivity coincides with the global hyperbolicity of the set of the events in the future of p, (cf. Ref. 9).

Before stating our main result, we recall some definitions.

Definition 2.2: Let $(\mathcal{M},\langle\cdot,\cdot\rangle)$ be a Lorentzian manifold, and $z:[0,1]\to\mathcal{M}$ be a geodesic. A smooth vector field ζ along z is called a Jacobi field if it satisfies

$$D_s^2\zeta+R(\zeta,\dot{z})\dot{z}=0, \tag{2.4}$$

where R is the curvature tensor of the metric $\langle\cdot,\cdot\rangle$ (cf. Ref. 22). *A point $z(s)$, $s\in]0,1]$ is said to be conjugate to $z(0)$ along z if there exists a nonvanishing Jacobi field ζ along $z_{|[0,s]}$ such that*

$$\zeta(0)=\zeta(s)=0. \tag{2.5}$$

The multiplicity of the conjugate point $z(s)$ is the maximal number of linearly independent Jacobi fields satisfying (2.5).

By (2.4) the set of the Jacobi fields is a vector space of dimension $2\dim\mathcal{M}$. Hence the multiplicity of a conjugate point is finite and, by (2.5), is at most $\dim\mathcal{M}$ [actually it is at most $\dim\mathcal{M}-1$ because $\zeta(s)=s\dot{z}(s)$ is a Jacobi field which is zero only at $s=0$].

Definition 2.3: The index $\mu(z)$ is the number of conjugate points $z(s)$, $s\in]0,1[$ to $z(0)$, counted with their multiplicity.

It is well known that the index of a lightlike geodesic is finite (see Ref. 22).

Definition 2.4: Let p be a point and γ a timelike curve on a Lorentzian manifold $(\mathcal{M},g)$. Then p and γ are said to be nonconjugate by lightlike geodesics if for any lightlike geodesic $z:[0,1]\to\mathcal{M}$ joining p and γ, $z(1)$ is nonconjugate to p along z.

It is well known that such a condition is true except for a residual set of pairs (p,γ). For some results whenever p and γ are conjugate see Ref. 27.

Let X be a topological space and $\mathbb{K}$ a field. For any $l\in\mathbb{N}$ let $H_l(X;\mathbb{K})$ be the lth homology group of X with coefficients in $\mathbb{K}$. Since $\mathbb{K}$ is a field, then $H_l(X;\mathbb{K})$ is a vector space whose dimension $\beta_l(X;\mathbb{K})$ (eventually $+\infty$) is called the lth *Betti number of X* (with coefficients in $\mathbb{K}$). The *Poincaré polynomial* $\mathcal{P}(X;\mathbb{K})$ is defined as the following formal series:

$$\mathcal{P}(X;\mathbb{K})(\kappa)=\sum_{l\in\mathbb{N}}\beta_l(X;\mathbb{K})\kappa^l.$$

Let $\mathcal{G}^+_{p,\gamma}(\Lambda)$ be the set of the future pointing lightlike geodesics joining p and γ and having image contained in Λ. The main result of this paper is the following theorem.

Theorem 2.5: *Let Λ, p, γ satisfy* (1)–(6). *Assume that the following assumptions hold true:*

(L_1) *p and γ are nonconjugate*;

(L_2) *τ is pseudocoercive on $\mathcal{B}^+_{p,\gamma}(\Lambda)$*;

then for any field $\mathbb{K}$ there exists a formal series $S(\kappa)$ with coefficients in $\mathbb{N}\cup\{+\infty\}$, such that

$$\sum_{z\in\mathcal{G}^+_{p,\gamma}(\Lambda)}\kappa^{\mu(z)}=\mathcal{P}(\mathcal{B}^+_{p,\gamma}(\Lambda);\mathbb{K})(\kappa)+(1+\kappa)S(\kappa). \tag{2.6}$$

The same result holds for the lightlike geodesics joining p and γ in the past of p, under an obvious modification of the assumptions.

Remark 2.6: Observe that the Betti numbers $\beta_l(X;\mathbb{K})$ [and the coefficient of the formal series $S(\kappa)$ in (2.6)] depend in a substantial way on the choice of the field $\mathbb{K}$. On the other hand, the left-hand side of the equality (2.6) does not depend on $\mathbb{K}$, hence one can obtain more information on $\mathcal{G}^+_{p,\gamma}(\Lambda)$ by letting the coefficient field $\mathbb{K}$ be arbitrary in (2.6). For example, a result of Serre, where the choice of $\mathbb{K}$ is essential (cf. Ref. 28), is used to prove part (b) of Theorem 2.11.

Remark 2.7: Note that assumption (L_2) cannot be removed. Indeed, let $(\mathcal{M}_0,\langle\cdot,\cdot\rangle_0)$ be a Riemannian manifold such that there exist two points p_1, $p_2\in\mathcal{M}_0$ which are not joined by any geodesic for the metric $\langle\cdot,\cdot\rangle_0$. Consider the (static) Lorentzian manifold $(\mathcal{M},\langle\cdot,\cdot\rangle)$, where $\mathcal{M}=\mathcal{M}_0\times\mathbb{R}$ and $\langle\cdot,\cdot\rangle$ is given by

$$\langle\zeta,\zeta\rangle=\langle\xi,\xi\rangle_0-\theta^2,$$

for any $z=(x,t)\in\mathcal{M}_0\times\mathbb{R}$ and $\zeta=(\xi,\theta)\in T_z\mathcal{M}$. Let $\Lambda=\mathcal{M}$. Consider the point $p=(p_1,0)$ and the timelike curve $\gamma(s)=(p_2,s)$. Clearly assumptions (1)–(6) are satisfied, but not (L_2). Theorem 2.5 does not hold for p and γ, since there are no lightlike geodesics joining p and γ, while $\mathcal{P}(\mathcal{B}^+_{p,\gamma}(\Lambda),\mathbb{K})(\kappa)\neq=0$ for any field $\mathbb{K}$.

Remark 2.8: Let c_l be the number of the future pointing lightlike geodesics joining p and γ having index q. Then (2.6) can be written in the following way:

$$\sum_{l=0}^{\infty} c_l\kappa^l=\sum_{l=0}^{\infty}\beta_l(\mathcal{B})^+_{p,\gamma}(\Lambda;\mathbb{K})\kappa^l+(1+\kappa)S(\kappa). \tag{2.7}$$

From (2.7) we deduce that a certain number of future pointing light rays joining p and γ are obtained according to the topology of $\mathcal{B}^+_{p,\gamma}(\Lambda)$. In particular, setting $\kappa=1$ in (2.7), we have the following estimate on the number $\mathrm{card}(\mathcal{G}^+_{p,\gamma}(\Lambda))$ of the light rays joining p and γ:

$$\mathrm{card}(\mathcal{G}^+_{p,\gamma}(\Lambda))=\sum_{l=0}^{\infty}\beta_l(\mathcal{B}^+_{p,\gamma}(\Lambda);\mathbb{K})+2S(1). \tag{2.8}$$

Since $S(1)$ is non-negative we also get the classical Morse inequalities

$$c_l\geqslant\beta_l(\mathcal{B}^+_{p,\gamma}(\Lambda);\mathbb{K}),\quad \forall l\in\mathbf{N}. \tag{2.9}$$

An example of the influence of the topology of $\mathcal{B}^+_{p,\gamma}(\Lambda)$ on the number of future pointing, lightlike geodesics between p and γ is given by the next theorem.

Theorem 2.9: *Under the assumptions of* Theorem 1.5 *we have the following.*

(a) *If* $\mathcal{B}^+_{p,\gamma}(\Lambda)$ *is contractible the number* $\mathrm{card}\,\mathcal{G}^+_{p,\gamma}(\Lambda)$ *is infinite or odd.*
(b) *If* $\mathcal{B}^+_{p,\gamma}(\Lambda)$ *is not contractible, there exist at least two future pointing light rays joining p and* γ. (We recall that a topological space is said to be *contractible* if it is homotopically equivalent to a point.)

Actually, the topology of $\mathcal{B}^+_{p,\gamma}(\Lambda)$ is in general not known for arbitrary Lorentzian manifold. More information can be obtained if its topology can be related to the topology of the manifold Λ. Let $\Omega(\Lambda)$ be the *based loop space* of all the continuous curves $z:[0,1]\to\Lambda$ such that $z(0)=z(1)=\overline{z}$. Since Λ is connected, $\Omega(\Lambda)$ does not depend on $\overline{z}$. We equip $\Omega(\Lambda)$ with the *uniform topology*. Since the Poincaré polynomial is a homotopical invariant, we have the following result as an immediate consequence of Theorem 2.5.

Theorem 2.10: *Besides the assumptions of Theorem 2.5, assume also:*
(L_3) $\mathcal{B}^+_{p,\gamma}(\Lambda)$ *has the same homotopy type of the based loop space* $\Omega(\Lambda)$.
Then for any field $\mathcal{K}$ *there exists a formal series* $S(\kappa)$ *with coefficients in* $\mathbb{N}\cup\{+\infty\}$, *such that*

$$\sum_{z\in\mathcal{G}^+_{p,\gamma}(\Lambda)} r^{\mu(z)}=\mathcal{P}(\Omega(\Lambda),\mathbb{K})(\kappa)+(1+\kappa)S(\kappa). \tag{2.10}$$

In Appendix A we give a general condition assuring that (L_3) is satisfied. Thanks to the results proved in Sec. 5 and Appendix A we see that assumption (L_3) is certainly satisfied if $(\Lambda,\langle\cdot,\cdot\rangle)$ is conformally stationary and this is the case, with a good approximation, of the accepted cases of multiple quasars (see, e.g., Ref. 16).

Theorem 2.11: *Under the assumptions of Theorem 2.10 we have:*

(a) If Λ is contractible, then the number of the future pointing lightlike geodesics joining p with γ and with image in Λ is infinite or odd.
(b) If Λ is noncontractible, then the number of the future pointing lightlike geodesics joining p with γ and with image in Λ is infinite.

Conditions assuring the finiteness of the images can be found in Ref. 29. To write Morse relations for light rays using the arrival time functional τ it does not seem that the pseudocoercivity assumption can be weakened. Indeed it is necessary to have that the sublevels τ^c of the arrival time functional are complete with respect to a suitable metric and the Palais–Smale sequences are precompact (with respect to such a metric). Note that the sequences in Definition 2.1 are allowed to reach $\partial\Lambda$. The light convexity of $\overline{\Lambda}$ will guarantee the existence of minimizers with image entirely included in Λ.

Morse relations are proved regarding lightlike geodesics as critical points of the functional τ. They are written using the geometric index μ instead of the Morse index thanks to Theorem 5.13. Its proof is based on a different approach to the index theorem for lightlike geodesics, with respect to the one of Ref. 22, where the index theorem is proved on a quotient space of the admissible variations. For the proof of Theorem 5.13 we have to choose a suitable manifold where the critical points of τ are lightlike geodesics.

III. MINIMIZERS FOR THE ARRIVAL TIME ON SOBOLEV CURVE SPACES

We begin the section by introducing the Sobolev spaces $H^{1,r}([0,1],\Lambda)$ with $r\in[1,+\infty]$. This can be rapidly done in the following way.

Let W be the smooth timelike vector field on $\mathcal{M}$ whose existence is assumed in (1). The manifold $\mathcal{M}$ can be equipped by a natural Riemannian structure setting

$$\langle\zeta,\zeta\rangle_R=\langle\zeta,\zeta\rangle-\frac{2\langle W(z),\zeta\rangle^2}{\langle W(z),W(z)\rangle.} \tag{3.1}$$

The Riemannian metric (3.1) can be used to introduce a Riemann distance on Λ that we shall denote by d_R. Such a distance allows us to introduce the space of the absolutely continuous curves between $[0,1]$ and Λ (denoted by $AC([0,1],\Lambda)$). Finally for any $r\in[1,+\infty[$ we set

$$H^{1,r}([0,1],\Lambda)=\left\{z\in AC([0,1],\Lambda):\int_0^1(\langle\dot z,\dot z\rangle_R)^{r/2}\,\mathrm{ds}<+\infty\right\}$$

while

$$H^{1,\infty}([0,1],\Lambda)=\{z\in AC([0,1],\Lambda):\sup\{\langle\dot z(s),\dot z(s)\rangle_R:s\in[0,1]\}<+\infty\}.$$

Using local coordinates and the Palais definition of the Sobolev manifold (cf. Ref. 30) we see that the above defined spaces do not depend on the choice of W. Moreover we set

$$\Omega^{1,r}_{p,\gamma}(\Lambda)=\{z\in H^{1,r}([0,1],\Lambda):z(0)=p,z(1)\in\gamma(]\alpha,\beta[)\}. \tag{3.2}$$

For any absolutely continuous curve z we can extend the classical definition of causal curve saying that z is a causal curve if $\langle\dot z(s),\dot z(s)\rangle\leqslant 0$ almost everywhere (a.e.). Moreover we say that a causal curve is future pointing if

$$\langle \dot{z}(s), W(z(s))\rangle < 0 \quad \textit{for almost every } s \textit{ such that } \dot{z}(s) \neq 0.$$

It is possible to prove that the above-presented notions are equivalent to the ones given in Ref. 20 for continuous curves, whenever we deal with absolutely continuous curves. This can be done using Proposition 3.2.

To develop a Morse theory for light rays the following spaces will be also used:

$$\mathcal{L}^{+,r}_{p,\gamma}(\Lambda) = \{z \in \Omega^{1,r}_{p,\gamma}([0,1],\Lambda) : \langle \dot{z}, \dot{z}\rangle = 0 \text{ a.e. and } z \text{ is future pointing}\}. \tag{3.3}$$

More in general for any event p_* and any future pointing, injective, timelike curve $\gamma_* :]\alpha_*, \beta_*[\to \Lambda$ we shall use the following notation:

$$\mathcal{L}^{+,r}_{p_*,\gamma_*}([a,b],\Lambda) = \{z \in H^{1,r}([a,b],\Lambda):$$

$$\langle \dot{z}, \dot{z}\rangle = 0 \text{ a.e., } z \textit{ is future pointing, } z(a) = p_* \text{ and } z(b) \in \gamma_*(]\alpha_*, \beta_*[\}.$$

We shall denote by the same symbol τ the functional defined by $\gamma_*^{-1}(z(b))$ on the space $\mathcal{L}^{+,r}_{p_*,\gamma_*}([a,b],\Lambda)$.

Remark 3.1: Note that the above-mentioned spaces are not smooth manifold: a tangent space is not well defined on the curves z such that $\dot{z}(s) = 0$ on a subset of $[0,1]$ having positive Lebesgue measure.

For this reason if we want to deal with smooth manifolds we need to use an approximation of $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ by suitable smooth manifolds and to study *a priori* estimates for the limit process (cf. Refs. 9 and 10). In this paper we shall work directly on $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ showing first that assumptions (1)–(6) and pseudocoercivity allow one to find smooth minimizers in Λ which are lightlike geodesics.

This is a further motivation to choose a shortening procedure for the arrival time functional, since it permits one to bypass the nonsmoothness of the spaces defined by (3.3). It will be possible to write Morse relations using the Poincaré polynomial of $\mathcal{B}^{+}_{p,\gamma}(\Lambda)$ because we shall prove in Sec. IV that it is homotopically equivalent to $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$.

The next result is a local version of the relativistic Fermat principle and it is the first step for the shortening procedure.

Proposition 3.2: Let $q \in \mathcal{M}$. Then there exists $\rho(q) > 0$ having the following property. For any γ_* timelike injective curve and integral curve of Y such that:

(1) $0 < \mathrm{d}_R(q, \mathrm{Im}\ \gamma_*) \leqslant \rho(q)$,
(2) $\mathrm{Im}\ \gamma_* \cap J^+(q,\mathcal{M}) \neq \varnothing$,
(3) $\mathrm{Im}\ \gamma_* \setminus J^+(q,\mathcal{M}) \neq \varnothing$,

there exists a unique future pointing lightlike geodesic joining q and γ_* and minimizing the arrival time on $\mathcal{L}^{+,r}_{q,\gamma_*}(\mathcal{M})$.

The proof can be, e.g., obtained as a limit process of timelike problems using the results of Ref. 31. Anyway here we shall give a variational proof working directly in the lightlike case. The proof is quite different from the classical geometrical one (cf. Ref. 20). The following remarks will be used for the proof of Proposition 3.2 and other results in the present paper.

Remark 3.3: For any $z \in \Lambda$ there exists a neighborhood $\mathcal{U}_z$ of z and a coordinate system $\varphi = (x_1, \ldots, x_{N-1}, t)$ $(N = \dim \Lambda)$ on $\mathcal{U}_z$ such that $W = \partial/\partial t$ and $\mathcal{U}_z = \Sigma \times]a,b[$ where Σ is a spacelike hypersurface parametrized by $x_1, \ldots, x_{N-1}$.

Moreover, in the coordinates $x = (x_1, \ldots, x_{N-1})$ and $t \in]a,b[$ the metric g is given by

$$g(x,t)[(\xi,\theta),(\xi,\theta)] = \langle \alpha(x,t)\xi, \xi\rangle_0 + 2\langle \delta(x,t)), \xi\rangle_0 \theta - \beta(x,t)\theta^2,$$

where $(\xi,\theta)\in T_{(x,(a+b)/2)}\Sigma\times\mathbb{R}$, $\langle\cdot,\cdot\rangle_0$ is the restriction of g to Σ, α is a smooth, symmetric positive definite operator, δ is a smooth vector field on Σ, and β is a smooth positive real function. Note that $\langle\cdot,\cdot\rangle_0$ is a Riemannian metric on Σ.

Indeed it is sufficient to choose $\Sigma=\{(x,t):t=(a+b)/2\}$, $\alpha(x,t)$, $\delta(x,t)$, and $\beta(x,t)$ such that

$$\langle\alpha(x,t)\xi_1,\xi_2\rangle_0=g(x,t)[\xi_1,\xi_2]\quad\text{for any}\quad\xi_1,\xi_2\in T_{(x,(a+b)/2)}\Sigma,$$

$$\delta(x,t)=[G_0(x,t)]^{-1}(\overline{\delta}(x,t)),\quad\overline{\delta}(x,t)=\sum_{i=1}^{N-1}g_{iN}(x,t)\frac{\partial}{\partial x_i},$$

$$G_0(x,t)=(g_{i,j})_{i,j=1,\ldots,N-1},$$

and $\beta(x,t)=-g(x,t)[W,W]$.

Remark 2.4: We will assume henceforth that W is *renormalized* in such a way that

$$\langle W(z),W(z)\rangle=-1\quad\text{for any}\quad z\in\mathcal{M}.$$

In particular, $\langle\dot\gamma,\dot\gamma\rangle\equiv-1$, and so the parameter of γ can be interpreted as proper time.

Therefore, in the coordinate systems $(x_1,\ldots,x_{N-1},t)$ with $\partial/\partial t=W$ (cf. Remark 3.3), $z=(x,t)\in\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ if and only if

$$\dot t=\langle\delta,\dot x\rangle_0+\sqrt{\langle\delta,\dot x\rangle_0^2+\langle\alpha\dot x,\dot x\rangle_0}\tag{3.4}$$

because

$$\beta(x,t)=-\langle W(z),W(z)\rangle\equiv1.$$

Moreover, in such a coordinate system, any integral curve of W can be written as

$$s\mapsto(\overline{x},s),$$

for some $\overline{x}\in\Sigma$.

In order to prove Proposition 2.2, the following preliminary results are needed.

Lemma 2.5: Under the assumptions of Proposition 3.2, if $\rho(q)$ is sufficiently small, there exists a minimizer of τ on $\mathcal{L}^{+,1}_{q,\gamma_*}(\mathcal{M})$ having $H^{1,\infty}$ regularity.

Proof: By Remarks 3.3–3.4 and the assumptions of Proposition 3.2, if $\rho(q)$ is sufficiently small, we can consider a sufficiently small neighborhood $\mathcal{U}$ of q such that $\mathcal{U}=V\times I$, where V is an open neighborhood contained in Σ, $I=]-\lambda_0,\lambda_0[$, $q=(q_0,0)\in V\times I$, the curve $\gamma_*(t)=(q_*,t)$ is defined in $]-\lambda_0,\lambda_0[$ and $\mathrm{d_R}(q_0,q_*)\to0$ whenever $\mathrm{d_R}(q,\mathrm{Im}\,\gamma_*)\to0$. If $z\in\mathcal{L}^+_{p,\gamma}$ and takes its values in $\mathcal{U}$, then $z(s)=(x(s),t(s))$, $x(0)=q_0$, $x(1)=q_*$, and $t(s)$ satisfies the Cauchy problem

$$\begin{cases}\dot t=\langle\delta(x,t),\dot x\rangle_0+\sqrt{\langle\alpha(x,t)\dot x,\dot x\rangle_0+\langle\delta(x,t),\dot x\rangle_0^2},\\ t(0)=0.\end{cases}\tag{3.5}$$

Moreover

$$\tau(z)=t_x(1)=\int_0^1\langle\delta(x,t_x),\dot x\rangle_0\,\mathrm{d}s+\int_0^1\sqrt{\langle\alpha(x,t_x)\dot x,\dot x\rangle_0+\langle\delta(x,t_x),\dot x\rangle_0^2}\,\mathrm{d}s,$$

where t_x is the solution of the above-mentioned Cauchy problem above. Using a minimal Riemannian geodesic between q_0 and q_* in V shows that

$$\inf_{\mathcal{L}^{+}_{q,\gamma_*}} \tau \to 0 \quad \text{as} \quad \mathrm{d}_R(q,\gamma_*) \to 0.$$

We show now the existence of a minimizer for τ.

Consider a minimizing sequence (z_m) for τ and set $z_m=(x_m,t_m)$. The coercivity of α shows that the Riemann length of x_m is bounded. Then by (3.5) we deduce that $\dot{t}_m$ is bounded in L^1. Then we can reparametrize z_m proportionally to arclength obtaining a curve $y_m \in \mathcal{L}^{+,1}_{q,\gamma_*}(\Lambda)$ such that $y_m(\theta)=z_m(\sigma)$ where

$$\theta=\frac{\int_a^\sigma \langle -\dot{z}_m, W(z_m)\rangle \mathrm{d}s}{\int_a^b \langle -\dot{z}_m, W(z_m)\rangle \mathrm{d}s}.$$

Since

$$\int_a^b |\dot{z}_m| \mathrm{d}s$$

is uniformly bounded, there exists a positive constant M independent of $m \in \mathbb{N}$ such that

$$\left| \int_a^b \langle \dot{z}_m, W(z_m)\rangle \mathrm{d}s \right| \leq M.$$

Then it is not difficult to see that $\dot{y}_m$ is uniformly bounded.

So we have a sequence of curves $z_m=(x_m,t_m)$ such that, up to a reparametrization (and replacing y_m with z_m),

$$(x_m,t_m) \text{ uniformly converges to a curve } z=(x,t);$$

$$\text{the sequence } (\dot{x}_m) \text{ is bounded in } L^\infty;$$

$$\text{the sequence } (\dot{x}_m) \text{ weakly converges to } \dot{x} \text{ in } L^2.$$

In particular the sequence $(\dot{x}_m)$ weakly converges to $\dot{x}$ in L^1 and then by well-known properties of the weak convergence (see, e.g., Ref. 32),

$$\int_0^1 \sqrt{\langle \alpha(x,t)\dot{x},\dot{x}\rangle_0 + \langle \delta(x,t)\dot{x},\dot{x}\rangle_0^2}\, \mathrm{d}s \leq \liminf_{m\to\infty} \int_0^1 \sqrt{\langle \alpha(x,t)\dot{x}_m,\dot{x}_m\rangle_0 + \langle \delta(x,t)\dot{x}_m,\dot{x}_m\rangle_0^2}\, \mathrm{d}s.$$

Moreover, we clearly have

$$\left| \int_a^b \left(\sqrt{\langle \alpha(x,t)\dot{x}_m,\dot{x}_m\rangle_0 + \langle \delta(x,t),\dot{x}_m\rangle_0^2} - \sqrt{\langle \alpha(x_m,t_m)\dot{x}_m,\dot{x}_m\rangle_0 + \langle \delta(x_m,t_m),\dot{x}_m\rangle_0^2} \right) \mathrm{d}s \right|$$

$$\leq \int_a^b \left(\left| \langle (\alpha(x_m,t_m)-\alpha(x,t))\dot{x}_m,\dot{x}_m\rangle_0 \right| + \left| \langle \delta(x_m,t_m)+\delta(x,t),\dot{x}_m\rangle_0 \langle \delta(x_m,t_m) - \delta(x,t),\dot{x}_m\rangle_0 \right| \right)^{1/2} \mathrm{d}s \mapsto 0 \quad \text{as} \quad m \to +\infty.$$

Finally, by the uniform convergence of (x_m,t_m) to (x,t),

$$\int_a^b \langle \delta(x_m,t_m),\dot{x}_m\rangle_0 \to \int_a^b \langle \delta(x,t),\dot{x}\rangle_0.$$

It follows that for any $s_1<s_2$,

$$\liminf_{m\to\infty}(t_m(s_2)-t_m(s_1))=\liminf_{m\to\infty}\Bigg(\int_{s_1}^{s_2}\langle\delta(x_m,t_m),\dot{x}_m\rangle_0\,\mathrm{d}s + \int_{s_1}^{s_2}\sqrt{\langle\alpha(x_m,t_m)\dot{x}_m,\dot{x}_m\rangle_0+\langle\delta(x_m,t_m),\dot{x}_m\rangle_0^2}\,\mathrm{d}s\Bigg)$$
$$\geqslant\Bigg(\int_{s_1}^{s_2}\langle\delta(x,t),\dot{x}\rangle_0\,\mathrm{d}s+\int_{s_1}^{s_2}\sqrt{\langle\alpha(x,t)\dot{x},\dot{x}\rangle_0+\langle\delta(x,t),\dot{x}\rangle_0^2}\,\mathrm{d}s\Bigg).$$

So we have obtained:

$$\begin{cases}\dot{t}\geqslant\langle\delta(x,t),\dot{x}\rangle_0+\sqrt{\langle\alpha(x,t)\dot{x},\dot{x}\rangle_0+\langle\delta(x,t),\dot{x}\rangle_0^2},\\ t(0)=0.\end{cases}$$

Let t_x be the solution of the above-assigned Cauchy problem relative to the curve x. Comparison theorems for ordinary differential equations show that $t_x\leqslant t$. Hence, (x,t_x) is a minimizer for τ.

Finally, our (reparametrized) minimizing sequence z_m satisfies:

$$\begin{cases}\langle\dot{z}_m,W(z_m)\rangle \text{ is bounded and}\\ \dot{z}_m \text{ is weakly convergent to } \dot{z} \text{ in } L^2.\end{cases}$$

Therefore $\langle\dot{z},W(z)\rangle$ is bounded and the minimizer z is therefore in $H^{1,\infty}$. □

Lemma 3.6: Assume $q\notin\gamma_*([\alpha,\beta[)$. Let z be a minimizer of τ on $\mathcal{L}^{+,1}_{q,\gamma_*}(\mathcal{M})$ such that $z\in H^{1,\infty}([0,1],\mathcal{M})$. Then there exists a curve $y\in\mathcal{L}^{+,\infty}_{q,\gamma_*}$ such that y minimizes τ and

$$\inf\{\|\dot{y}(s)\|_{\mathrm{R}}:s\in[0,1]\backslash N\}>0, \tag{3.6}$$

where N is a subset of $[0,1]$ having zero Lebesgue measure.

Moreover,

$$y([0,1])=z([0,1]).$$

Proof: Choose $y(\theta)=z(\sigma)$ where

$$\theta=\frac{\int_0^\sigma\langle-\dot{z},W(z)\rangle\mathrm{d}s}{\int_0^1\langle-\dot{z},W(z)\rangle\mathrm{d}s}.$$

It is easy to see that $y\in\mathcal{L}^{+,\infty}_{q,\gamma_*}(\Lambda)$, $y([0,1])=z([0,1])$ and

$$\langle\dot{y}(\theta),W(\theta)\rangle=\int_0^1\langle-\dot{z},W(z)\rangle\mathrm{d}s \text{ a.e.} \tag{3.7}$$

Since $\int_0^1\langle-\dot{z},W(z)\rangle\mathrm{d}s\neq0$ we deduce immediately (3.6). □

Lemma 3.7: Let z be a curve in $\mathcal{L}^{+,\infty}_{p,\gamma}$ satisfying (3.6). Then there exists a neighborhood $\mathcal{V}$ of z in $H^{1,\infty}([0,1],\Lambda)$ such that $\mathcal{V}\cap\mathcal{L}^{+,\infty}_{p,\gamma}$ is a C^1-manifold and for any $z\in\mathcal{V}$ its tangent space is given by

$$T_z(\mathcal{L}^{+,\infty}_{p,\gamma})=\{\zeta\in H^{1,\infty}([0,1],T\Lambda):\zeta(s)\in T_{z(s)}\Lambda \text{ for any } s,$$
$$\zeta(0)=0,\zeta(1)\|\dot{\gamma}(\tau(z)),\langle D_s\zeta,\dot{z}\rangle=0 \text{ a.e.}\}.$$

Here $T\Lambda$ denotes the tangent bundle of Λ and D_s the covariant derivative along z.

Proof: Consider the map $\psi:\Omega^{1,\infty}_{p,\gamma}(\Lambda)\to L^\infty([0,1],\mathbb{R})$ such that

$$\psi(z)=\sqrt{2}\langle \dot{z},W(z)\rangle+\sqrt{\langle \dot{z},\dot{z}\rangle+2\langle \dot{z},W(z)\rangle^2}=\sqrt{2}\langle \dot{z},W(z)\rangle+\sqrt{\langle \dot{z},\dot{z}\rangle_R}.$$

Note that $\psi^{-1}(0)=\mathcal{L}^{+,\infty}_{p,\gamma}$. The set $\Omega^{1,\infty}_{p,\gamma}(\Lambda)$ is a manifold and, for any $z\in\Omega^{1,\infty}_{p,\gamma}$, its tangent space is

$$T_z\Omega^{1,\infty}_{p,\gamma}=\{\zeta\in H^{1,\infty}([0,1],T\Lambda):\zeta(s)\in T_{z(s)}\Lambda \text{ for any } s\in[0,1],$$

$$\zeta(0)=0,\quad \zeta(1)\|\dot{\gamma}(\tau(z))\}.$$

By the above-mentioned formula we immediately deduce that ψ is of class C^1 in a neighborhood of z. We claim that, $\forall z\in\mathcal{V}\cap\mathcal{L}^{+,\infty}_{p,\gamma}$, the differential $d\psi(z)[\,\cdot\,]$ is surjective.

Indeed let U_z be the parallel transport of $\dot{\gamma}(\tau(z))$ along z, i.e., the solution of the Cauchy problem

$$\begin{cases} D_{\dot{z}}U_z=0,\\ U_z(1)=\dot{\gamma}(\tau(z)).\end{cases}$$

Then for any $\varphi\in L^\infty([0,1],\mathbb{R})$ it is easy to show the existence of $\lambda\in H^{1,\infty}([0,1],\mathbb{R})$ such that $\lambda(0)=0$,

$$d\psi(z)[\lambda U_z]=\varphi,$$

and the kernel of $d\psi(z)$ splits. Then $V\cap\psi^{-1}(0)$ is a manifold whose tangent space at z is the kernel of $d\psi(z)$ in $T_z\Omega^{1,\infty}_{p,\gamma}$. □

Remark 3.8: The functional τ is differentiable on $\Omega^{1,\infty}_{p,\gamma}$. Since τ is defined by setting $\gamma(\tau(z))=z(1)$, its differential satisfies

$$\dot{\gamma}(\tau(z))d\tau(z)[\zeta]=\zeta(1)$$

and therefore

$$d\tau(z)[\zeta]=0,$$

if and only if

$$\zeta(1)=0 \text{ for any } \zeta\in T_z(\mathcal{L}^{+,\infty}_{p,\gamma}).$$

Now let V be a smooth vector field along z such that $V(0)=V(1)=0$ and U_z the parallel transport of $\gamma(\tau(z))$ along z. If z satisfies (3.6) put

$$\lambda(s)=\int_0^s\left\langle D_rV,\frac{\dot{z}}{\langle U_z,\dot{z}\rangle}\right\rangle dr.$$

Then $V-\lambda U_z\in T_z(\mathcal{L}^{+,\infty}_{p,\gamma})$ and if z is a critical point of τ on $\mathcal{L}^{+,\infty}_{p,\gamma}$ it is

$$\tau(z)[V-\lambda U_z]=0 \text{ for any } V$$

and therefore

$$0=\lambda(1)=\int_0^1\left\langle D_sV,\frac{\dot{z}}{\langle U_z,\dot{z}\rangle}\right\rangle ds \text{ for any } V.$$

Conversely if z satisfies the above-mentioned condition, $\zeta(1)=0$ for any V, hence z is a critical point of τ.

The following theorem is the relativistic Fermat principle proved in $H^{1,\infty}$ (see also Ref. 12).

Theorem 3.9 (Fermat principle): *Let $z \in \mathcal{L}^{+,\infty}_{p,\gamma}$ such that (3.6) is satisfied. Then, z is a critical point of τ if and only if it is a reparametrization of a C^2-geodesic in $\mathcal{L}^{+,\infty}_{p,\gamma}$.*

Proof: If z is a critical point of τ [satisfying (3.6)] it is

$$\int_0^1 \left\langle D_r V, \frac{\dot{z}}{\langle U_z, \dot{z}\rangle} \right\rangle \mathrm{d}r = 0$$

for any V along z such that $V(0)=V(1)=0$. If y is a reparametrization of z such that $\langle U_w, \dot{w}\rangle$ is constant we deduce $\int_0^1 \langle D_r V, \dot{y}\rangle = 0$ for any V and therefore y is a smooth geodesic.

Conversely if z is a reparametrization of a C^2-geodesic, it is $D_s(\mu' \dot{z}) = 0$ for some $\mu \in H^{1,\infty}([0,1],\mathbb{R})$. Then $\langle U_z, \mu' \dot{z}\rangle$ is constant, so

$$\int_0^1 \left\langle D_r V, \frac{\dot{z}}{\langle U_z, \dot{z}\rangle} \right\rangle \mathrm{d}r = 0$$

for any V such that $V(0)=V(1)=0$. Then, by Remark 3.8 we deduce that z is a critical point of τ. □

We are finally ready to prove Proposition 3.2.

Proof of Proposition 2.2: By Lemmas 3.5 and 3.6 and Theorem 3.9 there exists a future pointing lightlike geodesic w joining q and γ_*, minimizing τ on $\mathcal{L}^{+,r}_{q,*}$. The uniqueness of w is a consequence of the local invertibility of the exponential map (cf. Ref. 1).

Remark 3.10: Fix $z \in \mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ and $[a_1,a_2] \subset [0,1]$. Let γ_2 be the integral curve of W such that $\gamma_2(0) = z(a_2)$. Since it is future pointing, a simple contradiction argument shows that, whenever $\mathrm{d}_R(z(a_1), z(a_2)) \to 0$, the infimum of τ on $\mathcal{L}^{+,r}_{z(a_1),\gamma_2}([a_1,a_2],\Lambda)$ tends to 0, and if $z(a_1) = z(a_2)$ the infimum is 0.

Remark 3.11: Since τ and $\mathcal{L}^{+,r}_{q,\gamma_*}(\Lambda)$ are invariant by reparametrizations, it is clear that there are nonsmooth minimizers. Note that, among the minimizers there are also curves having null derivatives in subsets of $[0,1]$ with positive Lebesgue measure.

Now we shall prove the equivalence between Definition 2.1 and the corresponding definition given in Refs. 9 and 10 [where the pseudocoercivity of τ is given in $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$].

Lemma 3.12: Let $z \in \mathcal{L}^{+,1}_{p,\gamma}(\Lambda)$. Then there exists z_n in $\mathcal{B}^{+}_{p,\gamma}(\Lambda)$ such that $z_n \to z$ uniformly.

Proof: We can apply Proposition 3.2 to obtain the existence of a minimizer in the space $\mathcal{L}^{+,1}_{z(a_1),\gamma_2}([a_1,a_2],\Lambda)$ where γ_2 is the integral curve of w such that $\gamma_2(0) = z_2$. Since z is fixed, if $a_2 - a_1$ is sufficiently small, $\int_{a_1}^{a_2} \sqrt{\langle \dot{z}, \dot{z}\rangle_R}\, \mathrm{d}s$ is small and also the length [with respect to the Riemann structure (3.1)] of the geodesic minimizing τ is small. Then, choosing a suitable partition of the interval $[0,1]$ allows one to construct a broken geodesic $\hat{z}$ such that the distance between z and $\hat{z}$ with respect to the $H^{1,1}$-norm is arbitrarily small. Therefore, the uniform distance can be made as small as we want and we are done. □

By Lemma 3.12 it follows immediately

Proposition 3.13: For any $r \in [1,+\infty]$, τ is pseudocoercive on $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ if and only if it is pseudocoercive on $\mathcal{B}^{+}_{p,\gamma}(\Lambda)$.

For any $z \in H^{1,1}([0,1],\Lambda)$ denote by $\ell(z)$ its length induced by the Riemann structure (3.1).

Lemma 3.14: Assume τ is pseudocoercive on $\mathcal{B}^{+}_{p,\gamma}(\Lambda)$. Then, for any $c \in]\alpha,\beta[$ there exists $D(c) > 0$ such that

$$\tau(z) \leqslant c \Rightarrow \ell(z) \leqslant D(c) \quad \text{for any} \quad z \in \mathcal{L}^{+,r}_{p,\gamma}(\Lambda).$$

Proof: Assume by contradiction the existence of a sequence z_n in $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ such that $\tau(z_n) \leqslant c \in]\alpha,\beta[$ and $\ell(z_n) \to +\infty$. Since τ and ℓ are invariant by reparametrizations, by the pseudocoercivity of τ (and Proposition 3.13) we can assume that z_n has a subsequence (that we

shall continue to denote by z_n) uniformly convergent to a continuous curve $z:[0,1]\to\overline{\Lambda}$. Since $z([0,1])$ is compact, it can be covered by a finite number of open neighborhoods U_i in $\mathcal{M}$ such that, on any U_i, the metric g has the form

$$ds^2=\langle\alpha(x,t)\xi,\xi\rangle_0+2\langle\delta(x,t),\xi\rangle_0\theta-\theta^2$$

(cf. Remarks 3.3 and 3.4). If $]a_n^i,b_n^i[$ is an interval such that $z_n(s)\in U_i$ for any $s\in]a_n^i,b_n^i[$ and $z_n=(x_n,t_n)$ we have

$$t_n(b_n^i)-t_n(a_n^i)=\int_{a_n^i}^{b_n^i}\dot{t}_n\,ds=\int_{a_n^i}^{b_n^i}(\langle\delta,\dot{x}_n\rangle_0+\sqrt{\langle\delta,\dot{x}_n\rangle_0^2+\langle\alpha\dot{x}_n,\dot{x}_n\rangle_0})ds.$$

Since any $\overline{U_i}$ is compact and the number of U_i is finite we deduce that $\int_{a_n^i}^{b_n^i}\sqrt{\langle\dot{x}_n,\dot{x}_n\rangle_0}\,ds$ (and consequently $\int_{a_n^i}^{b_n^i}|\dot{t}_n|ds$) is bounded independently by n and i. Finally, since any z_n is included in

$$\bigcup_i U_i$$

and $\dot{z}_n=(\dot{x}_n,\dot{t}_n)$ on any U_i, we deduce that $\int_{a_n^i}^{b_n^i}\|\dot{z}_n\|_R\,ds$ is bounded independently by n and i. Then $\ell(z_n)$ is bounded getting a contradiction. □

Lemma 3.14 will be used, together with the following proposition, to construct the shortening flow for τ.

Proposition 3.15: Let W, Λ, and $\gamma:]\alpha,\beta[\to\Lambda$ satisfy (1)–(6) of Sec. II. Assume that τ is pseudocoercive on $\mathcal{B}^+_{p,\gamma}(\Lambda)$ and fix $c\in]\alpha,\beta[$.

Then there exists $\rho_*(c)>0$ satisfying the following property. Let $z\in\tau^c\cap\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$, $[a,b]\subset[0,1]$, $z_1,z_2\in z([0,1])$ with $z_1=z(a),z_2=z(b)$, and $d_R(z_1,z_2)\leqslant\rho_*(c)$. Let $\gamma_i:]\alpha_i^-,\beta_i^+[\to\Lambda(i=1,2)$ be the maximal integral curve (in Λ) of

$$\begin{cases}\dot{\eta}=W(\eta),\\ \eta(0)=z_i,\quad i=1,2.\end{cases}\tag{3.8}$$

Moreover, for any $\hat{z}_1\in\gamma(]\alpha_1^-,0])$ with $d_R(\hat{z}_1,z_1)\leqslant\rho_*(c)$ there exists a unique future pointing lightlike geodesic Γ such that $\Gamma(a)=\hat{z}_1$, $\Gamma(b)$ is in the image of γ_2, $\Gamma(s)\in\Lambda$ for any $s\in[a,b]$, and

$$\tau(\Gamma)=\inf\{\tau(y):y\in\mathcal{L}^{+,r}_{\hat{z}_1,\gamma_2}([a,b],\Lambda)\}.\tag{3.9}$$

Proof: By pseudocoercivity it is immediate to check the existence of K, compact subset of $\overline{\Lambda}$, such that

$$z\in\tau^c\Rightarrow z([0,1])\subset K.\tag{3.10}$$

Now take a finite family $U_1,\ldots,U_m$ of open subsets of $\mathcal{M}$ covering K and such that any U_i is compact and U_i satisfies the properties of Remarks 3.3 and 3.4. By Proposition 3.2 and Remark 3.10 if $\rho_*(c)$ is sufficiently small there exists a minimizer w in $\mathcal{L}^{+,r}_{\hat{z}_1,\gamma_2}([a,b],U_i)$ for some $i=1,\ldots,m$. [Note that, by assumption (6), $w(b)\in\Lambda$]. Since

$$\bigcup_{i=1}^m\overline{U_i}$$

is compact, by the local invertibility of the exponential map [and the minimality of $\tau(w)$] we see that, if $\rho_*(c)$ is sufficiently small, the minimizing geodesic is unique. Then we have just to prove that the minimizer is included in Λ. If $z_1=z_2$ this is obvious. Then suppose that $z_1\neq z_2$. If $\rho_*(c)$ is sufficiently small and $\mathrm{d}_R(z_1,z_2)\leqslant\rho_*(c)$, $z_1,z_2\in U_i\cap\Lambda$ (for some i). Then, using Proposition 3.2 and choosing $\rho_*(c)$ sufficiently small, we can construct two continuous maps $\theta_1,\theta_2:[0,1]\to U_i\cap\Lambda$ having the following properties:

(1) for any $\lambda\in[0,1]$, $\theta_2(\lambda)$ is in the future of $\theta_1(\lambda)$,
(2) $\theta_1(0)=\hat{z}_1\theta_2(0)=z_2$,
(3) $\theta_1(\lambda)\neq\theta_2(\lambda)$ for any $\lambda\neq 1$,
(4) $\theta_1(1)=\theta_2(1)$,
(5) for any $\lambda\in[0,1]$ there exists a unique minimizer of τ on $\mathcal{L}_{\theta_1(\lambda),\gamma_2(\lambda)}([a,b],U_i)$ where $\gamma_2(\lambda)$ is the maximal integral curve of W such that $\gamma_2(\lambda)(0)=\theta_2(\lambda)$.

Now set

$$A=\{\lambda\in[0,1]:\ \textit{the lightlike or constant geodesic minimizing } \tau \textit{ on } \mathcal{L}_{\theta_1(\lambda),\gamma_2(\lambda)}([a,b],U_i) \textit{ does not intersect } \partial\Lambda\}.$$

Since $\theta_1(1)=\theta_2(1)\in\Lambda,1\in A$. Take

$$\lambda_0\equiv\inf A\geqslant 0.$$

By the definition of λ_0, there exists $\lambda_n\to\lambda_0^+$ and a sequence w_n of lightlike geodesic minimizing τ on $\mathcal{L}^{+,r}_{\theta_1(\lambda_n),\gamma_2(\lambda_n)}([a,b],U_i)$ such that $w_n([0,1])\subset\Lambda$. Unless to consider a subsequence, by (3.4) we obtain the existence of a lightlike geodesic w such that

$$w_n\to w \text{ with respect to the } C^2-\text{norm},$$

$$w(a)=\theta_1(\lambda_0),\quad w(b)\in\gamma_2^{-1}(\lambda_0)\quad(\gamma_2\subset\Lambda),$$

$$w([a,b])\subset\overline{\Lambda}.$$

If $w([a,b])\subset\Lambda$, then $\lambda_0=0$ and we are done. If $w([a,b])\cap\partial\Lambda\neq\varnothing$, since $\theta_1(\lambda_0)\neq\theta_2(\lambda_0)$ are in Λ we get a contradiction with the light-convexity of $\overline{\Lambda}$. □

IV. HOMOTOPICAL EQUIVALENCE BETWEEN $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ AND $\mathcal{B}^{+}_{p,\gamma}(\Lambda)$

In this section [under assumptions (1)–(6)] we shall introduce a shortening flow and we shall use it to prove that $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ and $\mathcal{B}^{+}_{p,\gamma}(\Lambda)$ are homotopically equivalent for any $r\in[1,+\infty]$. This flow will also be used to get the deformation of the sublevels of τ for the Morse theory, whenever we are far from lightlike geodesics.

Indeed far from lightlike geodesics, τ will be strictly decreasing with a speed uniformly far from zero. In other words τ will verify the Palais–Smale compactness condition along the flow.

To construct the shortening flow we shall use the same ideas as in Ref. 26 adapting them to our case. Note that here we cannot use the finite dimensional approach near critical curves (used in Ref. 26 for Riemannian geodesics) because we are not working with fixed end points. So the shortening approach will be used only far from geodesics.

The shortening procedure can be introduced in the following way. Fix $c>\inf\{\tau(z),z\in\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)\}$. Consider $D(c)$ as in Lemma 3.14, $\rho_*(c)$ as in Proposition 3.15, and take $N=N(c)$ such that

$$\frac{D(c)}{N}<\rho_*(c).$$

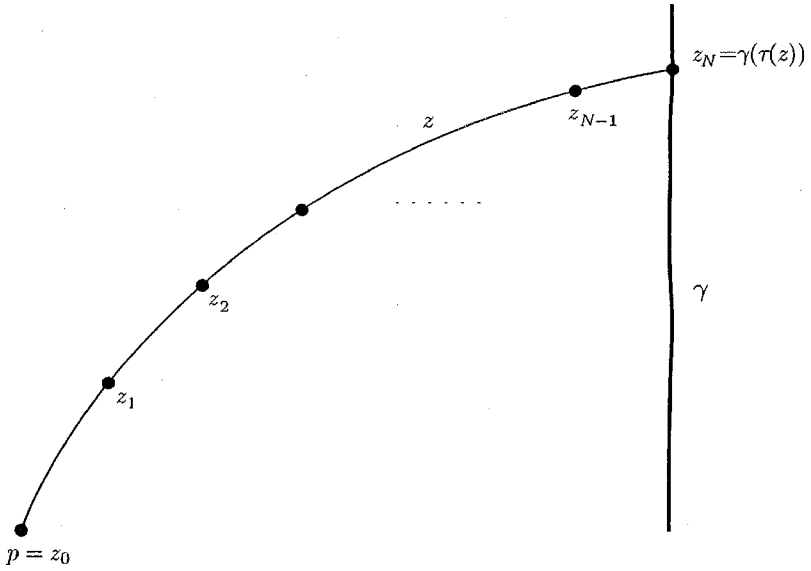

FIG. 1.

Choose a partition $\{0=s_0<s_1,\ldots,s_{N-1}<s_N=1\}$ of $[0,1]$ such that for any $i\in\{1,\ldots,N\}$,

$$s_i-s_{i-1}=\frac{1}{N}.$$

For any $z\in\tau^c\cap\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$, choose $N+1$ points $z_0,z_1,\ldots,z_N$ on $z([0,1])$ such that $z(0)=p$, $z_N=z(1)$, and $\mathrm{d}_R(z_i,z_{i-1})=l(z)/N$, for any $i\in\{1,\ldots,N\}$, where $l(z)$ denotes the length of z with respect to the Riemannian structure (3.1) (see Fig. 1).

Denote by γ_i $(i=1,\ldots,N)$ the maximal integral curve of W such that $\gamma_i(0)=z_i$ (see Fig. 2). Observe that $\gamma_N(s)=\gamma(s+\tau(z))$ for all s.

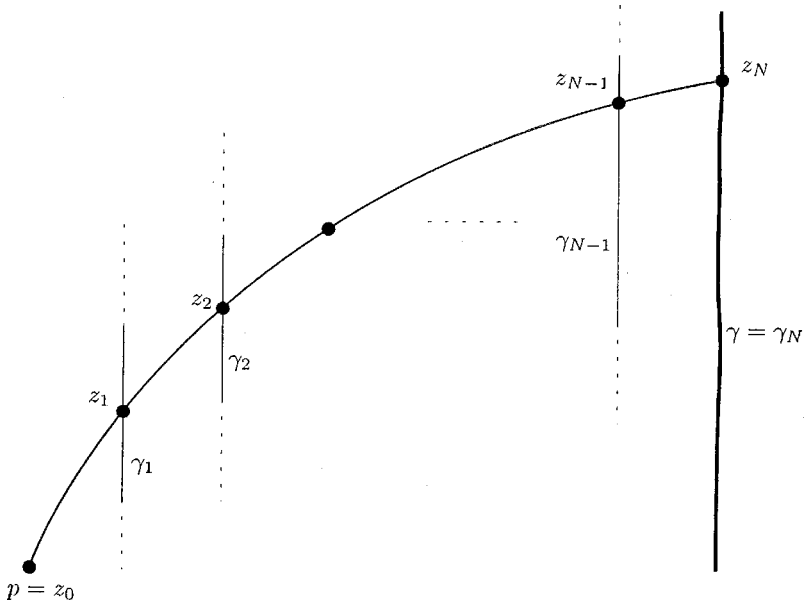

FIG. 2.

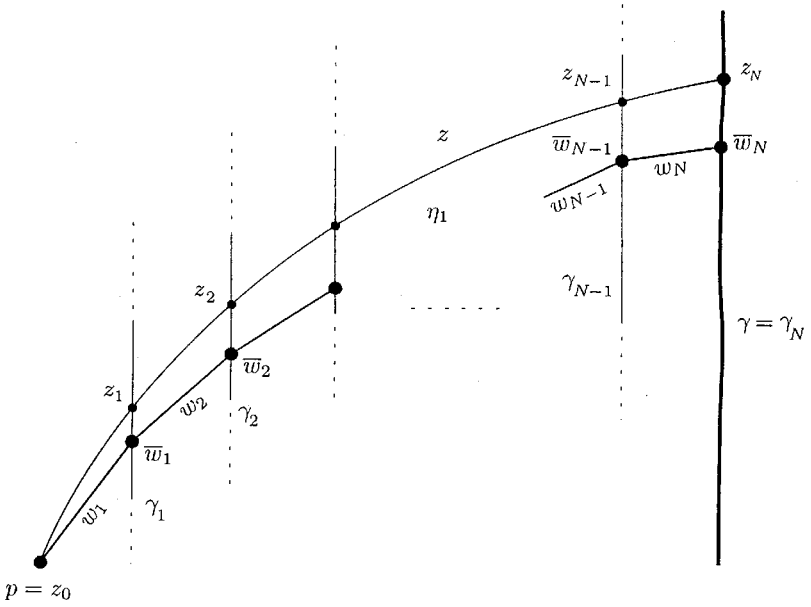

FIG. 3.

Let w_1 be the lightlike geodesic minimizing τ on $\mathcal{L}^{+,r}_{p,\gamma_1}([s_0,s_1],\Lambda)$ (recall that $z_0=p$ and $s_0=0$), w_2 the lightlike geodesic minimizing τ on $\mathcal{L}^{+,r}_{w_1(s_1),\gamma_2}([s_1,s_2],\Lambda)$, and so on (see Fig. 3). In Figs. 3–5, the points $w_i(s_i)$ are denoted by $\overline{w_i}$.

Note that the number N can be chosen big enough in order that $\mathrm{d}_R(w_i(s_i),z_{i+1})\leqslant\rho_*(c)$, for any $i=1,\ldots,N-1$ and for any $z\in\tau^c$.

Remark 4.1: Let $K=K(c)$ be a compact subset of $\overline{\Lambda}$ as in (3.10). By compactness, $K(c)$ can be covered by a finite family (U_j) satisfying Remark 3.3. Moreover, N can be chosen so large that $z([s_{i-1},s_i])$ and the minimizer of τ on $\mathcal{L}^{+,r}_{w_{i-1}(s_{i-1}),\gamma_i}([s_{i-1},s_i],\Lambda)$ are contained in some U_j.

The Lorentzian metric on U_j is described as

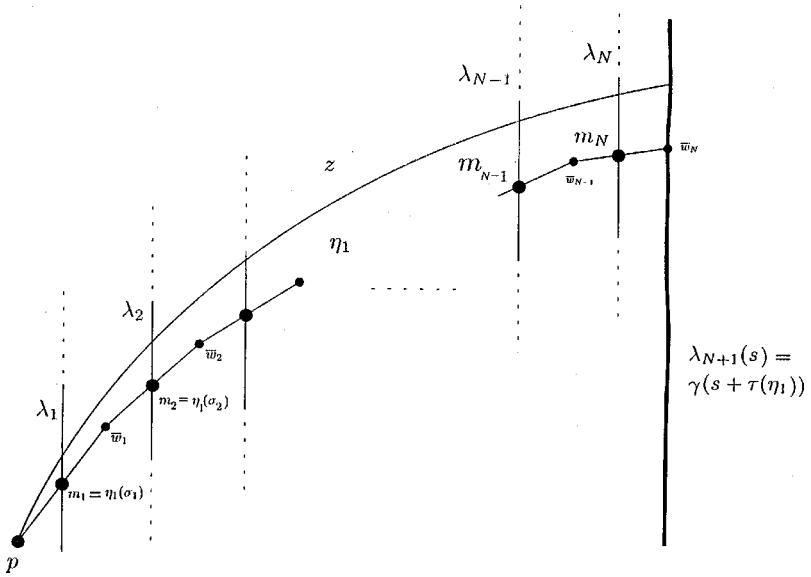

FIG. 4.

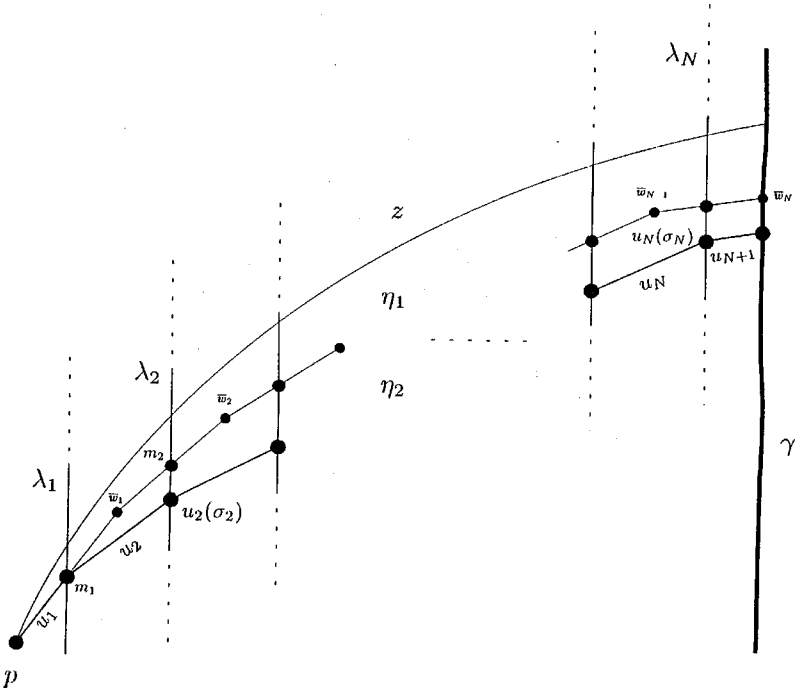

FIG. 5.

$$\langle \zeta, \zeta \rangle = \langle \alpha_j(x,t)\xi, \xi \rangle_0 + 2\langle \delta_j(x,t), \xi \rangle_0 \theta - \theta^2 \tag{4.1}$$

(cf. Remark 3.3), where $\alpha_j(x,t)$ is a positive linear operator, $\delta_j(x,t)$ is smooth vector field, $z = (x,t) \in U_j$, and $\zeta = (\xi, \theta) \in T_z\mathcal{M}$.

With the above notation, for any future pointing curve z with image contained in some U_j, the condition $\langle \dot{z}, \dot{z} \rangle = 0$ holds if and only if

$$\dot{t} = \langle \delta_j(x,t), \dot{x} \rangle_0 + \sqrt{\langle \alpha_j(x,t), \dot{x}, \dot{x} \rangle_0 + \langle \delta_j(x,t), \dot{x} \rangle_0^2}. \tag{4.2}$$

Moreover, any γ_i is an integral curve of W, so, in U_j, it has the form $s \mapsto (x_j, t_j + s)$, if $z_j = (x_j, t_j)$.

Note that $\mathcal{L}^{+,r}_{p,\gamma_1}([s_0, s_1], \Lambda)$ is nonempty, since it contains the restriction $z_{|[s_0,s_1]}$. Now, using elementary comparison theorems for ordinary differential equations and the metric (4.1) on U_j allow one to deduce also that any space $\mathcal{L}^{+,r}_{w_{i-1}(s_{i-1}),\gamma_i,\epsilon}([s_{i-1}, s_i], \Lambda)$ is nonempty for any $i \in \{2, \ldots, N\}$.

Note also that, if η_1 is the curve defined by setting $\eta_1([s_{i-1}, s_i]) = w_i$, then $\tau(\eta_1) \leqslant \tau(z) \leqslant c$ (always by comparison theorems in O.D.E.). In particular $\eta_1([0,1])$ is contained in $K(c)$.

Remark 4.2: A second curve η_2 will be constructed in the following way starting from η_1. On any minimizer w_i $(i = 1, \ldots, N)$ consider the point m_i such that $\mathrm{d}(w_i(s_{i-1}), m_i) = \mathrm{d}(m_i, w(s_i))$.

For $i = 1, \ldots, N$, we denote by λ_i the maximal integral curve of W such that $\lambda_i(0) = m_i$; moreover, we set $\lambda_{N+1}(s) = \gamma(s + \tau(\eta_1))$ (see Fig. 4).

Consider now the following subdivision of the interval $[0,1]$. Let $\sigma_0 = 0$, $\sigma_1 = 1/2N$, $\sigma_j = (2j-1)/2N$ for $j = 2, \ldots, N$, and $\sigma_{N+1} = 1$.

Denote by u_1 the minimizer of τ on $\mathcal{L}^{+,r}_{p,\lambda_1}([\sigma_0, \sigma_1], \Lambda)$, by u_2 the minimizer of τ on $\mathcal{L}^{+,r}_{u_1(\sigma_1),\lambda_2}([\sigma_1, \sigma_2], \Lambda)$ and so, inductively, we denote by u_j the minimizer of τ in $\mathcal{L}_{u_{j-1}(\sigma_{j-1}),\lambda_j,\epsilon}([\sigma_{j-1}, \sigma_j], \Lambda)$, $j = 2, \ldots, N+1$.

Finally, (see Fig. 5) we denote by η_2 the curve such that

$$\eta_2|_{[\sigma_{j-1},\sigma_j]} = u_j .$$

Using again comparison theorems in ordinary differential equations one proves that $\tau(\eta_2) \leqslant \tau(\eta_1)$.

The continuous flow $\eta(\sigma,z)$ can be constructed as follows. Fix $\sigma \in [0,1]$ and consider for instance the interval $[s_0,s_1]$. We choose $\eta(\sigma,z)_{|[s_0,s_1]}$ as follows. Set $p=(x_0,0)$ and $\gamma_1(s) = (x_1,t_1+s)$ (in some neighborhood U_j as in Remark 4.1). Since $z(s)=(x(s),t(s))$, the curve $x(s)$ joins x_0 with x_1.

Let $y(\sigma)$ be the minimizer of the functional

$$y \mapsto \int_{s_0}^{\sigma s_1} \langle \delta_i(y,t_y),\dot{y}\rangle_0 \, \mathrm{ds} + \int_{s_0}^{\sigma s_1} \sqrt{\langle \alpha_i(y,t_y),\dot{y},\dot{y}\rangle_0 + \langle \delta_i(y,t_y),\dot{y}\rangle_0^2} \, \mathrm{ds}$$

with boundary conditions $y(0)=x_0$ and $y(\sigma s_1)=x(\sigma s_1)$, where t_y is the solution of (4.2) with $t_y(0)=0$ in the interval $[0,\sigma s_1]$.

Denote by $\hat{y}(\sigma)$ the extension of $y(\sigma)$ to $[s_0,s_1]$ taking $\hat{y}(s)=x(s)$ for $s \in [\sigma s_1,s_1]$. Finally, denote by $\hat{t}_y$ the corresponding solution of (4.2) in the interval $[s_0,s_1]$. The curve $(\hat{y}(\sigma),\hat{t}_y(\sigma))$ will be $\eta(\sigma,z)$ in the interval $[s_0,s_1]$. In the same way we can construct $\eta(\sigma,z)$ on the other intervals $[s_{i-1},s_i]$. Note that, by construction, $\eta(1,z)=\eta_1$. Similarly, we can extend the flow η to a map defined on $[0,2]\times\tau^c$ in such a way that $\eta(2,z)=\eta_2$.

Now, we iterate the above-mentioned shortening argument, replacing the original curve z with the curve η_2. Successively we apply the above-mentioned construction, starting from η_2. By induction we obtain a flow $\eta(\sigma,z)$, defined on $\mathbb{R}^+\times\tau^c$.

Since $\tau(\eta(\sigma,z)) \leqslant \tau(z)$ for any σ and for any z, using η we immediately deduce

Lemma 4.3: Fix $r \in [1,+\infty]$. For any $c \in]\alpha,\beta[$, $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)\cap\tau^c$ is homotopically equivalent to $\mathcal{B}^+_{p,\gamma}\cap\tau^c$.

Moreover choosing a suitable continuous map $\rho_*(c)$ $(c \in]\alpha,\beta[)$ and arguing as in Sec. 9 of Ref. 7 we can also obtain the following result.

Proposition 4.4: $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ is homotopically equivalent to $\mathcal{B}^+_{p,\gamma}(\Lambda)$.

Suppose that $\tau(\eta_1)=\tau(\eta_2)$ and consider the situation is a single interval $[\sigma_j,\sigma_{j+1}]$. Since $\tau(\eta_1)=\tau(\eta_2)$ simple comparison theorems in O.D.E. show that η_1 is a minimizer on the interval $[\sigma_j,\sigma_{j+1}]$. Suppose that it consists of two (nonconstant) lightlike geodesics. If it is not a lightlike geodesic, by the above-given construction it has a discontinuity at $s_{j+1}=(\sigma_{j+1}+\sigma_j)/2$. Denote by U_{η_1} the parallel transport of $\dot{\gamma}(\tau(\eta_1))$ along the curve η_1. Since η_1 is a minimizer satisfying (3.6), by Lemma 3.7 and Remark 3.8 it is

$$\int_{\sigma_j}^{\sigma_{j+1}} \frac{\langle D_s V,\, \dot{\eta}_1\rangle}{\langle U_{\eta_1},\dot{\eta}_1\rangle} \mathrm{ds} = 0$$

for any C^∞-vector field along η_1 such that $V(0)=0, V(1)=0$. In particular $\dot{\eta}_1/\langle U_{\eta_1},\dot{\eta}_1\rangle$ is a C^1 curve. Therefore $\dot{\eta}_1(s^-_{j+1})=\dot{\eta}_1(s^+_{j+1})$, so η_1 is the image of a future pointing lightlike geodesic in the interval $[\sigma_j,\sigma_{j+1}]$.

Then, whenever we are far from lightlike geodesics and there are not intervals where η_1 is a constant, $\tau(\eta_2)<\tau(\eta_1)$. If η_1 possesses some interval where it is a constant it is possible to construct a ''localized'' flow where τ is strictly decreasing ignoring such intervals and using the above-given construction of the flow in a small neighborhood of η_1.

Finally compactness arguments similar to the ones used for the shortening method for Riemannian geodesics (cf. Ref. 26) allow one to obtain the analogous of the classical deformation results (see, e.g. Refs. 33 and 34) for the functional τ on $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$.

Since, to obtain Morse relations, we shall work with respect to the $H^{1,2}$ structure, we give the statements of the deformation results only for $r=2$.

Proposition 4.5: Let c be a regular value for τ on $\mathcal{L}^{+,2}_{p,\gamma}$ [namely $\tau^{-1}(\{c\})$ *does not contain geodesics*].

Then, there exists a positive number $\delta=\delta(c)$ and a continuous map $H\in C^0([0,1]\times\tau^{c+\delta},\tau^{c+\delta})$, such that:

(a) $H(0,z)=z$, *for every* $z\in\tau^{c+\delta}$,
(b) $H(1,\tau^{c+\delta})\subseteq\tau^{c-\delta}$,
(c) $H(\sigma,z)\in\tau^{c-\delta}$
for any $\sigma\in[0,1]$ *and* $z\in\tau^{c-\delta}$;

Proposition 4.6: Let K_c be the set of lightlike geodesics on $\tau^{-1}(\{c\})\cap\mathcal{L}^{+,2}_{p,\gamma}$. Then for any open neighborhood U of K_c, there exists a positive number $\delta=\delta(U,c)$ and a homotopy $H\in C^0([0,1]\times\tau^{c+\delta},\tau^{c+\delta})$, such that

(a) $H(0,z)=z$, *for any* $z\in\tau^{c+\delta}$,
(b) $H(1,\tau^{c+\delta}\backslash U)\subset\tau^{c-\delta}$,
(c) $H(\sigma,z)\in\tau^{c-\delta}$, *for every* $\sigma\in[0,1]$ *and* $z\in\tau^{c-\delta}$.

Remark 4.7: There are two main differences between the shortening method described previously and the classical shortening method for Riemannian geodesics. In our case, we locally minimize a functional which is is not given in an integral form. Second, we minimize the functional in the space of curves joining a point with a curve, and not two fixed points.

Remark 4.8: The flows used in Propositions 4.5 and 4.6 are just what we need for a Ljusternik–Schnirelmann theory. Then, without using the nondegeneracy assumption of Theorem 2.5 we can obtain the existence of at last $\mathrm{cat}(\mathcal{B}^+_{p,\gamma}(\Lambda))$ future pointing lightlike geodesic in $\mathcal{B}^+_{p,\gamma}(\Lambda)$. (Here cat X denotes the minimal number of contractible subsets of X covering it). Moreover if $\mathrm{cat}(\mathcal{B}^+_{p,\gamma}(\Lambda))=+\infty$ there is a sequence z_n of future pointing lightlike geodesics in $\mathcal{B}^+_{p,\gamma}(\Lambda)$ such that $\tau(z_n)\to\beta$.

V. ON THE BEHAVIOR OF τ NEAR LIGHTLIKE GEODESICS

To develop a Morse theory we shall use the space $\mathcal{L}^{+,2}_{p,\gamma}(\Lambda)$ [that contains $\mathcal{B}^{+,2}_{p_1\gamma}(\Lambda)$], because $H^{1,2}([0,1],\Lambda)$ is an Hilbert manifold (endowed with its natural metric). Since $\mathcal{L}^{+,2}_{p,\gamma}(\Lambda)$ is invariant by reparametrization as well as τ, it will be useful to consider equivalence classes of curves or, better, to single out one parametrization. This will be done on an open neighborhood $\mathcal{N}_w$ of $w([0,1])$ for any lightlike geodesic w.

Toward this goal consider the parallel vector field U_w along w of $\dot\gamma(\tau(w))$ (which is a timelike vector). Since γ is an integral curve of W, by Remark 4.4 it is $\langle U_w,U_w\rangle\equiv-1$. Now, by the pseudocoercivity of τ it follows that w does not have self-intersection, so its image is a submanifold and U_w can be extended to a smooth vector field Y on Λ such that

$$\langle Y(z),Y(z)\rangle=-1 \quad \text{for any } z\in\Lambda, \tag{5.1}$$

$$D_{\dot w(s)}Y(w(s))=0 \quad \text{for any } s\in[0,1] \tag{5.2}$$

(cf. Ref. 35). Using the vector field Y we define the following space:

$$\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)=\left\{z\in\mathcal{L}^{+,2}_{p,\gamma}(\Lambda):\langle Y(z),\dot z\rangle=\int_0^1\langle Y(z),\dot z\rangle\mathrm{d}s \ \text{ a.e.}\right\}. \tag{5.3}$$

Note that by (5.2), the geodesic w is in $\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ and

$$\int_0^1\langle Y(w),\dot w\rangle\mathrm{d}s<0..$$

The space $\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ will be used to study Morse theory near the critical point w for the functional τ. The first step in this direction is to prove that $\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ is a C^1-manifold.

Remark 5.1: It is well known that the space $\Omega^{+,2}_{p,\gamma}(\Lambda)$ defined by (3.2) is a C^∞-manifold and its tangent space at any z is given by

$$T_z\Omega^{+,2}_{p,\gamma}(\Lambda)=\{\zeta\in H^{1,2}([0,1],\mathcal{T}\Lambda):$$

$$\zeta(s)\in T_{z(s)}\Lambda \text{ for any } s,\zeta(0)=0,\zeta(1)) \text{ is parallel to } \dot\gamma(\tau(z))\}$$

where $\mathcal{T}\Lambda$ denotes the tangent bundle of Λ.

Remark 5.2: Consider the map

$$\phi:\Omega^{+,2}_{p,\gamma}(\Lambda)\to\left\{h\in L^2([0,1],\mathbb{R}):\int_0^1 h\,\mathrm{d}s=0\right\}$$

defined as

$$\phi(z)=\langle Y(z),\dot z\rangle-\int_0^1\langle Y(z),\dot z\rangle\mathrm{d}s. \tag{5.4}$$

It is a standard computation to prove that ϕ is of class C^∞ and its differential satisfies:

$$\mathrm{d}\phi(z)[\zeta]=\langle Y,D_s\zeta\rangle+\langle D_\zeta Y,\dot z\rangle-\int_0^1(\langle Y,D_s\zeta\rangle+\langle D_\zeta Y,\dot z\rangle)\mathrm{d}s, \tag{5.5}$$

where D is the Levi-Civita connection relative to the Lorentzian structure g.

Proposition 5.3: The space

$$\mathcal{P}^{+,2}_{p,\gamma}(\Lambda)=\left\{z\in\Omega^{+,2}_{p,\gamma}(\Lambda):\langle Y(z),\dot z\rangle=\int_0^1\langle Y(z),\dot z\rangle\mathrm{d}s<0\right\} \tag{5.6}$$

is a manifold whose tangent space is given by

$$T_z\mathcal{P}^{+,2}_{p,\gamma}(\Lambda)=\left\{\zeta\in T_z\Omega^{+,2}_{p,\gamma}(\Lambda):\langle Y,D_s\zeta\rangle+\langle D_\zeta Y,\dot z\rangle=\int_0^1(\langle Y,D_s\zeta\rangle+\langle D_\zeta Y,\dot z\rangle)\mathrm{d}s\right\}. \tag{5.7}$$

Proof: Consider the map ϕ defined by (5.4). By (5.5) and the implicit function theorem it is sufficient to prove that for any $h\in L^2([0,1],\mathbb{R})$ such that $\int_0^1 h\,\mathrm{d}s=0$ there exists $\zeta\in T_z\Omega^{+,2}_{p,\gamma}(\Lambda)$ such that

$$\langle Y,D_s\zeta\rangle+\langle D_\zeta Y,\dot z\rangle=h. \tag{5.8}$$

Choose $\zeta=\mu Y$ with $\mu(0)=0$. Then ζ satisfies (5.8) if and only if μ satisfies the Cauchy problem

$$\begin{cases}-\dot\mu+\mu\langle D_Y Y,\dot z\rangle=h,\\ \mu(0)=0,\end{cases}$$

because, by (5.1), $\langle Y,Y\rangle\equiv-1$. Such a problem has a (unique) solution in $H^{1,2}([0,1],\mathbb{R})$ and we are done. □

Remark 5.4: For any $z\in\mathcal{P}^{+,2}_{p,\gamma}(\Lambda)$, $\|\dot z\|_R$ is uniformly far from 0. [Here $\|\cdot\|_R$ is the norm induced by the Riemann structure (3.1)]. Indeed if $z\in\mathcal{P}^{+,2}_{p,\gamma}(\Lambda)$ it is

$$0<-\int_0^1\langle Y(z),\dot z\rangle\mathrm{d}s=-\langle Y(z),\dot z\rangle\leqslant|\langle Y(z),\dot z\rangle_R|\leqslant\|Y(z)\|_R\|\dot z\|_R.$$

Lemma 5.5: Let $\psi:\mathcal{P}^{+,2}_{p,\gamma}(\Lambda)\to L^2([0,1],\mathbb{R})$ *defined as*

$$\psi(z)=\sqrt{2}\langle \dot z, W(z)\rangle+\sqrt{\langle \dot z,\dot z\rangle_R}. \tag{5.9}$$

Then ψ *is of class* C^1 *and, for any* $\zeta\in\mathcal{P}^{+,2}_{p,\gamma}(\Lambda)$,

$$\begin{aligned}\mathrm{d}\psi(z)[\zeta]=&\sqrt{2}(\langle D_s\zeta, W(z)\rangle+\langle D_\zeta W,\dot z\rangle)\\&+\frac{1}{\sqrt{\langle \dot z,\dot z\rangle_R}}(\langle D_s\zeta,\dot z\rangle+2\langle \dot z, W(z)\rangle(\langle D_s\zeta, W(z)\rangle+\langle D_\zeta W,\dot z\rangle)).\end{aligned} \tag{5.10}$$

Note that, by Remark 5.4, since $\zeta\in H^{1,2}$ it is $\mathrm{d}\psi(z)[\zeta]\in L^2$.

Proof: Standard computations show that the differential of the map

$$\psi_1(z)=\sqrt{2}\langle \dot z, W(z)\rangle$$

along the direction ζ is given by

$$\mathrm{d}\psi_1(z)[\zeta]=\sqrt{2}(\langle D_s\zeta, W(z)\rangle+\langle D_\zeta W,\dot z\rangle).$$

To evaluate the differential of the map

$$\psi_2(z)=\sqrt{\langle \dot z,\dot z\rangle_R}$$

(at an instant s_0) we can assume that [in a neighborhood of $z(s_0)$] we are in $\mathbb{R}^n$ and

$$\langle \zeta,\zeta\rangle_R=\langle L(z)[\zeta],\zeta\rangle_E,$$

where $\langle\cdot,\cdot\rangle_E$ is the Euclidean scalar product of $\mathbb{R}^n$ and $L(z)$ is a smooth positive definite linear operator. Using such a position the vector fields in the tangent space at any curve z (on a suitable interval $[s_0-\delta,s_0+\delta]$) will be $H^{1,2}$-vector fields (defined on $[s_0-\delta,s_0+\delta]$) with values in $\mathbb{R}^n$.

Suppose that ζ is of class C^1. Then, by Remark 5.4, $\dot z+\lambda\dot\zeta$ is uniformly far from 0 for any λ sufficiently small, and

$$\mathrm{d}\psi_2(z)[\zeta]=\lim_{\lambda\to0}\frac{1}{\lambda}(\sqrt{\langle L(z+\lambda\zeta)[\dot z+\lambda\dot\zeta],\dot z+\lambda\dot\zeta\rangle_E}-\sqrt{\langle L(z)[\dot z],\dot z\rangle_E}).$$

Therefore there exists $\theta=\theta(\lambda,s)\in[0,1]$ such that

$$\mathrm{d}\psi_2(z)[\zeta]=\lim_{\lambda\to0}\frac{\langle \mathrm{d}L(z+\lambda\theta\zeta)[\zeta][\dot z+\lambda\dot\zeta],\dot z+\lambda\dot\zeta\rangle_E+2\langle L(z+\lambda\theta\zeta)[\dot\zeta],\dot z+\lambda\theta\dot\zeta\rangle_E}{2\sqrt{\langle L(z+\lambda\theta\zeta)[\dot z+\lambda\theta\dot\zeta],\dot z+\lambda\theta\dot\zeta\rangle_E}},$$

where the limit is done with respect to the L^2-norm.

Then, by the Lebesgue convergence theorem we obtain

$$\mathrm{d}\psi_2(z)[\zeta]=\frac{\langle \mathrm{d}L(z)[\zeta][\dot z],\dot z\rangle_E+2\langle L(z)[\dot\zeta],\dot z\rangle_E}{2\sqrt{\langle L(z)[\dot z],\dot z\rangle_E}},$$

which is a map in $L^2([s_0-\delta,s_0+\delta])$ by Remark 5.4.

Since

$$\langle L(z)[\dot z],\dot z]\rangle_E=\langle \dot z,\dot z\rangle_R=\langle \dot z,\dot z\rangle+2\langle W(z),\dot z\rangle^2$$

and

$$\langle \mathrm{d}L(z)[\zeta][\dot{z}],\dot{z}\rangle_E + 2\langle L(z)[\dot{\zeta}],\dot{z}\rangle_E = \mathrm{d}(\langle L(z)[\dot{z}],\dot{z}\rangle_E)[\zeta],$$

we obtain

$$\mathrm{d}\psi_2(z)[\zeta] = \frac{1}{\sqrt{\langle \dot{z},\dot{z}\rangle_R}}(\langle D_s\zeta,\dot{z}\rangle + 2\langle \dot{z},W(z)\rangle(\langle D_s\zeta,W(z)\rangle + \langle D_\zeta W,\dot{z}\rangle)). \tag{5.11}$$

Now consider $\zeta \in H^{1,2}([s_0-\delta,s_0+\delta],\mathbb{R}^n)$ and ζ_1 of class C^1. Then (in local coordinates) for any λ sufficiently small with respect to $\|\dot{\zeta}_1\|_{L^\infty}$, there exist $C_1, C_2 > 0$ such that

$$\begin{aligned}
&\left|\frac{\psi_2(z+\lambda\zeta_1)-\psi_2(z+\lambda\zeta)}{\lambda}\right| \\
&= \frac{1}{\lambda}\left|\frac{\langle L(z+\lambda\zeta_1)[\dot{z}+\lambda\dot{\zeta}_1],\dot{z}+\lambda\dot{\zeta}_1\rangle_E - \langle L(z+\lambda\zeta)[\dot{z}+\lambda\dot{\zeta}],\dot{z}+\lambda\dot{\zeta}\rangle_E}{\sqrt{\langle L(z+\lambda\zeta_1)[\dot{z}+\lambda\dot{\zeta}_1],\dot{z}+\lambda\dot{\zeta}_1\rangle_E} + \sqrt{\langle L(z+\lambda\zeta)[\dot{z}+\lambda\dot{\zeta}],\dot{z}+\lambda\dot{\zeta}\rangle_E}}\right| \\
&\leqslant \frac{C_1\|\zeta-\zeta_1\|_{L^\infty}\langle \dot{z}+\lambda\dot{\zeta}_1,\dot{z}+\lambda\dot{\zeta}_1\rangle_E}{\sqrt{\langle L(z+\lambda\zeta_1)[\dot{z}+\lambda\dot{\zeta}_1],\dot{z}+\lambda\dot{\zeta}_1\rangle_E}} \\
&\quad + \frac{C_2|\dot{z}+\lambda\dot{\zeta}_1+\dot{z}+\lambda\dot{\zeta}|_E|\zeta_1-\zeta|_E}{\sqrt{\langle L(z+\lambda\zeta_1)[\dot{z}+\lambda\dot{\zeta}_1],\dot{z}+\lambda\dot{\zeta}_1\rangle_E} + \sqrt{\langle L(z+\lambda\zeta)[\dot{z}+\lambda\dot{\zeta}],\dot{z}+\lambda\dot{\zeta}\rangle_E}},
\end{aligned}$$

where $|\cdot|_E$ is the Euclidean norm in $\mathbb{R}^n$. Then there exists $C>0$ such that

$$\left|\frac{\psi_2(z+\lambda\zeta_1)-\psi_2(z+\lambda\zeta)}{\lambda}\right| \leqslant C(\|\zeta_1-\zeta\|_{L^\infty}|\dot{z}+\lambda\dot{\zeta}_1|_E + |\dot{\zeta}_1-\dot{\zeta}|_E).$$

Therefore, since $\dot{z}$ is in L^2, $\|\dot{\zeta}_1\|_{L^2}$ is bounded (according to the L^2-norm of ζ) and $\zeta(0)=\zeta_1(0)$ we deduce the existence of a constant C_0 such that for any $\lambda \leqslant 1$,

$$\frac{1}{\lambda}\|\psi_2(z+\lambda\zeta_1)-\psi_2(z+\lambda\zeta)\|_{L^2} \leqslant C_0\|\zeta_1-\zeta\|_{H^{1,2}}. \tag{5.12}$$

Now, by the Lebesgue convergence theorem and Remark 5.4 it is not difficult to see that the linear operator $\mathrm{d}\psi_2(z)$ is continuous as linear map from $T_z\mathcal{P}^{+,2}_{p,\gamma}(\Lambda)$ to $L^2([0,1],\mathbb{R})$. Then for any $\epsilon > 0$ there exists $\vartheta \in]0,\epsilon[$ such that

$$\|\zeta_1-\zeta\|_{H^{1,2}} \leqslant \vartheta \Rightarrow \|\mathrm{d}\psi_2(z)[\zeta]-\mathrm{d}\psi_2(z)[\zeta_1]\|_{L^2} < \epsilon. \tag{5.13}$$

Moreover always fixing ζ_1 such that $\|\zeta_1-\zeta\|_{H^{1,2}} \leqslant \vartheta$, for any $\lambda \leqslant 1$ we have

$$\frac{1}{\lambda}\|\psi_2(z+\lambda\zeta_1)-\psi_2(z+\lambda\zeta)\|_{L^2} \leqslant C_0\vartheta \leqslant C_0\epsilon. \tag{5.14}$$

Finally

$$\begin{aligned}
\frac{\psi_2(z+\lambda\zeta)-\psi_2(z)}{\lambda} - \mathrm{d}\psi_2(z)[\zeta] &= \frac{\psi_2(z+\lambda\zeta_1)-\psi_2(z)}{\lambda} - \mathrm{d}\psi_2(z)[\zeta_1] + \frac{\psi_2(z+\lambda\zeta)-\psi_2(z+\lambda\zeta_1)}{\lambda} \\
&\quad + \mathrm{d}\psi_2(z)[\zeta_1] - \mathrm{d}\psi_2(z)[\zeta].
\end{aligned}$$

Since ψ_2 is differentiable at z along the direction ζ_1, for any λ sufficiently small it is

$$\left\| \frac{\psi_2(z+\lambda\zeta_1)-\psi_2(z)}{\lambda} - d\psi_2(z)[\zeta_1] \right\|_{L^2} \leqslant \epsilon,$$

so, combining (5.13) and (5.14) gives the existence of $\hat{\lambda}$ such that $|\lambda| \leqslant \hat{\lambda}$ implies

$$\left\| \frac{\psi_2(z+\lambda\zeta)-\psi_2(z)}{\lambda} - d\psi_2(z)[\zeta] \right\|_{L^2} \leqslant \epsilon + C_0\epsilon + \epsilon,$$

proving that (5.11) is satisfied for any $\zeta \in H^{1,2}$.

The continuity of $d\psi_2(\cdot)$ (which is a consequence of Remark 5.4 and the Lebesgue Theorem) says that ψ_2 is of class C^1 in $\mathcal{P}^{+,2}_{p,\gamma}(\Lambda)$ and its differential is given by (5.11). □

Remark 5.6: If $z \in \mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ then $\dot{z} \neq 0$ almost everywhere and it is lightlike. Since $\langle Y(z), \dot{z} \rangle$ is negative and Y is timelike, there exists a positive constant ν_z such that

$$-\langle Y(z), \dot{z} \rangle \geqslant \nu_z \|Y(z)\|_R \|\dot{z}\|_R .$$

Moreover $\langle Y(z), \dot{z} \rangle$ is constant, therefore $\|\dot{z}\|_R$ is uniformly bounded.

Now we can finally prove that $\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ is a manifold in a neighborhood of w.

Proposition 5.7: There exists an open neighborhood $\mathcal{O}_w$ of the geodesic w in $\Omega^{+,2}_{p,\gamma}(\Lambda)$ such that $\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda) \cap \mathcal{O}_w$ is a manifold of class C^1 and, for any $z \in \mathcal{Q}^{+,2}_{p,\gamma}(\Lambda) \cap \mathcal{O}_w$,

$$T_z(\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda) \cap \mathcal{O}_w) = \Big\{ \zeta \in \Omega^{+,2}_{p,\gamma}(\Lambda) : \langle D_s\zeta, \dot{z} \rangle = 0 \ \text{ a.e., and}$$

$$\langle Y, D_s\zeta \rangle + \langle D_\zeta Y, \dot{z} \rangle = \int_0^1 (\langle Y, D_s\zeta \rangle + \langle D_\zeta Y, \dot{z} \rangle) ds \ \text{a.e.,} \Big\}. \tag{5.15}$$

Proof: Let $\psi : \mathcal{P}^{+,2}_{p,\gamma}(\Lambda) \to L^2([0,1]\mathbb{R})$ be the C^1-map given by (5.9). By (5.10) its differential at any point $z \in \mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ is

$$d\psi(z)[\zeta] = \frac{\langle D_s\zeta, \dot{z} \rangle}{\sqrt{\langle \dot{z}, \dot{z} \rangle_R}}.$$

Since our result is of local nature (in a neighborhood of the geodesic w), by (5.7) it suffices to show that, for any $h \in L^2([0,1]\mathbb{R})$, there exists $\zeta \in T_z\Omega^{+,2}_{p,\gamma}(\Lambda)$ such that

$$\begin{cases} \langle Y(w), D_s\zeta \rangle + \langle D_\zeta Y(w), \dot{w} \rangle = \displaystyle\int_0^1 (\langle Y, D_s\zeta \rangle + \langle D_\zeta Y(w), \dot{w} \rangle) ds, \\ \dfrac{\langle D_s\zeta, \dot{w} \rangle}{\sqrt{\langle \dot{w}, \dot{w} \rangle_R}} = h . \end{cases}$$

Choose $\zeta(s) = \mu(s) Y(w(s)) + \lambda(s)\dot{w}(s)$. Since $\langle Y, Y \rangle \equiv -1$, denoting by c_w the real constant $\langle Y, \dot{w} \rangle$, it will be sufficient to verify the existence of two real functions μ and λ such that $\mu(0) = 0$, $\lambda(0) = \lambda(1) = 0$ and

$$\begin{cases} \mu' + \mu\langle D_Y Y, \dot{w} \rangle + \lambda' c_w \quad \text{is constant,} \\ \mu' c_w = h\sqrt{\langle \dot{w}, \dot{w} \rangle_R}, \end{cases}$$

and this can be done choosing

$$\mu(s)=\frac{1}{c_w}\int_0^s h\sqrt{\langle \dot w,\dot w\rangle_R}\,\mathrm{d}r,$$

and

$$c_w\lambda'=c+\frac{1}{c_w}h\sqrt{\langle \dot w,\dot w\rangle_R}-\frac{\langle D_YY,\dot w\rangle}{c_w}\int_0^s h\sqrt{\langle \dot w,\dot w\rangle_R}\,\mathrm{d}r,$$

where (integrating both terms of the above mentioned equality) the constant c can be chosen so that $\lambda(1)=\lambda(0)=0$. □

Remark 5.8: To describe the tangent space $T_z(\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)\cap\mathcal{O}_w)$ we can operate in the following way. Take $\zeta\in T_z\mathcal{P}^{+,2}_{p,\gamma}(\Lambda)$ and choose $\mu\in H^{1,2}([0,1],\mathbb{R})$ such that $\mu(0)=0$ and

$$\langle D_{\dot z}[\zeta-\mu Y],\dot z\rangle=0,$$

namely, μ has to satisfy

$$\begin{cases}\langle D_{\dot z}\zeta,\dot z\rangle-\mu' c_z-\mu\langle D_{\dot z}Y,\dot z\rangle=0,\\ \mu(0)=0,\end{cases}$$

where $c_z\equiv\langle Y,\dot z\rangle$ is a negative constant. Then μ is given by

$$\mu(s)=\int_0^s\frac{\langle D_{\dot z}\zeta,\dot z\rangle}{c_z}\exp\left(-\int_r^s\frac{\langle D_{\dot z}Y,\dot z\rangle}{c_z}\mathrm{d}\sigma\right)\mathrm{d}r, \tag{5.16}$$

and by (5.16):

$$\mathrm{d}\tau(z)[\zeta-\mu Y]=-\langle\dot\gamma(\tau(z),\zeta(1)\rangle+\langle\dot\gamma(\tau(z)),Y(z(1)\rangle\mu(1)$$

where

$$\mu(1)=\int_0^1\frac{\langle D_{\dot z}\zeta,\dot z\rangle}{c_z}\exp\left(-\int_r^1\frac{\langle D_{\dot z}Y,\dot z\rangle}{c_z}\mathrm{d}\sigma\right)\mathrm{d}r.$$

Then, using Remark 5.4 and the same technique of the proof of Lemma 5.5 allows one to deduce that τ is of class C^2 on $\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)\cap\mathcal{O}_w$.

In Sec. III we proved the existence (for any timelike curve sufficiently closed to a fixed event) of minimizing lightlike geodesics for the functional τ. Now we need a sort of converse of the above-mentioned principle.

Proposition 5.9: Any future pointing lightlike geodesic w is a critical point of τ on $\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)\cap\mathcal{O}_w$.

Proof: Take $V\in T_w\Omega^{+,2}_{p,\gamma}(\Lambda)$ such that $V(0)=V(1)=0$ and $\mu\in H^{1,2}([0,1],\mathbb{R})$ such that $\mu(0)=0$ and

$$\langle D_{\dot w}[V-\mu Y],\dot w\rangle=0. \tag{5.17}$$

By (5.16), Proposition 5.7, and Remark 5.8 it will be sufficient to prove that

$$0=\mathrm{d}\tau(w)[V-\mu Y]=\mu(1)\langle Y(w(1)),\dot\gamma(\tau(w))\rangle. \tag{5.18}$$

Now by (5.17)

$$\mu(1)=\int_0^1\frac{\langle D_{\dot w}V,\dot w\rangle}{\langle Y,\dot w\rangle}\mathrm{d}s$$

because $D_{\dot w}\dot w=0$. Then $\mu(1)=0$ for any V because $\langle Y,\dot w\rangle$ is constant ($\neq 0$) and w is a geodesic. □

Remark 5.10: The above-mentioned proof also shows that, for any $\zeta\in T_w(\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)\cap\mathcal{O}_w)$, since w is a geodesic it is $\zeta(1)=0$.

Remark 5.11: Let w be a future pointing lightlike geodesic. The same computations as in Ref. 13 allow one to prove that, for any $\zeta\in T_w\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$, the Hessian of τ along the direction ζ is given by

$$H^\tau(w)[\zeta,\zeta]=\frac{-1}{\langle\dot\gamma(\tau(w)),\dot w(1)\rangle}\int_0^1(\langle D_s\zeta,D_s\zeta\rangle-\langle R(\zeta,\dot w)\dot w,\zeta\rangle)\mathrm{d}s. \tag{5.19}$$

Now we equip $T_w\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ with the Hilbert structure

$$\langle\zeta_1,\zeta_2\rangle=\int_0^1\langle D^Y_s\zeta_1,D^Y_s\zeta_2\rangle_Y\,\mathrm{d}s, \tag{5.20}$$

where $\langle\zeta,\zeta\rangle_Y=\langle\zeta,\zeta\rangle-2\langle Y(w),\zeta\rangle^2$ [which is equivalent to (3.1)] and D^Y_s is the covariant derivative with respect to $\langle\zeta,\zeta\rangle_Y$.

Proposition 5.12: The linear map associated with the quadratic form (5.19) on $T_w\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ is a compact perturbation of the identity with respect to the Hilbert structure (5.20).

Proof: It is

$$\langle D_s\zeta,D_s\zeta\rangle=\langle D_s\zeta,D_s\zeta\rangle+2\langle D_s\zeta,Y(w)\rangle^2-2\langle D_s\zeta,Y(w)\rangle^2=\langle D_s\zeta,D_s\zeta\rangle_Y-2\langle D_s\zeta,Y(w)\rangle^2. \tag{5.21}$$

Now there exists a bilinear map Γ defined on the vector fields on Λ such that

$$D_s\zeta=D^Y_s\zeta+\Gamma(w)[\zeta,\zeta].$$

Moreover, by (5.15)

$$\langle D_s\zeta,Y(w)\rangle=-\langle D_\zeta Y,\dot w\rangle+\int_0^1(\langle D_s\zeta,Y(w)\rangle+\langle D_\zeta Y,\dot w\rangle)\mathrm{d}s \tag{5.22}$$

while, by Remark 5.10,

$$\int_0^1\langle D_s\zeta,Y(w)\rangle=-\int_0^1\langle\zeta,D_sY\rangle. \tag{5.23}$$

Since $H^{1,2}$ is compactly embedded in L^∞, combining (5.21), (5.22) and (5.23) gives the proof. □

Now denote by $m(w,\tau)$ the maximal dimension of a subspace of $T_w(\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)\cap\mathcal{O}_w)$ where the restriction of $H^\tau(w)[\cdot,\cdot]$ is negative definite. It is called the Morse index of the quadratic form $H^\tau(w)[\cdot,\cdot]$. The following index theorem holds:

Theorem 5.13: *Let w be a geodesic in $\mathcal{Q}^{+,2}_{\nu,\gamma}(\Lambda)$. Then*

$$m(w,\tau)=\mu(w).$$

To prove Theorem 5.13 some preliminary results are needed.

Lemma 5.14: Let ζ be a Jacobi field along w such that $\zeta(0)=0,\zeta(1)=0$. Then $\zeta\in T_w\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$.

Proof: Let ζ be a Jacobi field along w with $\zeta(0)=0$ and $\zeta(1)=0$. It is immediately checked that $\langle\dot w,D_s\zeta\rangle\equiv 0$. Therefore we just have to prove that the function

$$\varphi(s)=\langle D_s\zeta,Y(w)\rangle+\langle\zeta,D_\zeta Y\rangle$$

is constant. Since $D_sY\equiv 0$ and w is a geodesic

$$\varphi'(s)=\langle D_s^2\zeta,Y(w)\rangle+\langle\zeta,D_sD_\zeta Y\rangle.$$

Now, since ζ is a Jacobi field and

$$D_sD_\zeta Y=D_\zeta D_sY+R(\dot w,\zeta)Y$$

(cf. Ref. 22), it is

$$\begin{aligned}\varphi'(s)&=-\langle R(\zeta,\dot w)\dot w,Y(w)\rangle+\langle D_\zeta D_sY+R(\dot w,\zeta)Y,\dot w\rangle\\&=-\langle R(\zeta,\dot w)\dot w,Y(w)\rangle+\langle R(\dot w,\zeta)Y,\dot w\rangle=0\end{aligned}$$

because of the symmetry properties of the curvature tensor R (cf. Ref. 22). □

An integration by parts shows immediately that the following Lemma holds.

Lemma 5.15: If ζ is a Jacobi field along w such that $\zeta(0)=0$ and $\zeta(1)=0$, then

$$H^\tau(w)[\zeta,\zeta_1]=0\quad\text{for any}\quad\zeta_1\in T_w\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda).\tag{5.24}$$

Lemma 5.16: Let $\zeta\in T_w\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ such that (5.24) *is satisfied. Then ζ is a C^2-Jacobi field along w such that $\zeta(0)=0$ and $\zeta(1)=0$.*

Proof: If $\zeta\in T_w\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$, $\zeta(0)=0$ and by Remark 5.10, $\zeta(1)=0$ because w is a geodesic. Then, assuming that (5.24) holds, we have to verify that ζ is of class C^2 and it satisfies (2.4).

Let V be a C^∞-vector field along w such that $V(0)=0$, $V(1)=0$. Set $c_w=\langle Y(w),\dot w\rangle$ (which is a nonzero constant) and choose

$$\mu(s)=\int_0^s\frac{1}{c_w}\langle D_sV,\dot w\rangle.$$

Now let λ be the unique real map such that

$$\langle D_sV,Y(w)\rangle+\langle\dot w,D_VY\rangle-\mu'\langle Y(w),Y(w)\rangle-\mu\langle\dot w,D_YY\rangle-\lambda' c_w=\text{const},$$

$$\lambda(0)=\lambda(1)=0.$$

A straightforward computation shows that $\zeta_1=V-\mu Y(w)-\lambda\dot w\in T_w\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$. Therefore by (5.24) we have

$$\int_0^1(\langle D_s\zeta,D_sV-\mu'Y(w)-\lambda'\dot w\rangle-\langle R(\zeta,\dot w)\dot w,V-\mu Y(w)-\lambda\dot w\rangle)\,\mathrm{d}s=0$$

for any C_0^∞-vector field V along w. Now $\langle D_s\zeta,\dot w\rangle\equiv0$ and $\langle R(\zeta,\dot w)\dot w,\dot w\rangle\equiv0$. This allows us to deduce immediately that ζ is of class C^2. So, to obtain (2.4), it suffices to prove that, for any V,

$$\int_0^1(-\mu'\langle D_s\zeta,Y(w)\rangle+\mu\langle R(\zeta,\dot w)\dot w,Y(w)\rangle)\,\mathrm{d}s=0,\tag{5.25}$$

which is equivalent to

$$\int_0^1(-\langle D_sV,\dot w\rangle\langle D_s\zeta,Y(w)\rangle+\langle V,\dot w\rangle\langle R(\zeta,\dot w)\dot w,Y(w)\rangle)\,\mathrm{d}s=0.$$

Then an integration by parts shows that (5.25) is equivalent to

$$\frac{\mathrm{d}}{\mathrm{d}s}(\langle D_s\zeta,Y(w)\rangle\dot w)+\langle R(\zeta,\dot w)\dot w,Y(w)\rangle)=0.$$

Now, w is a geodesic while, by (5.15),

$$\langle D_s\zeta, Y(w)\rangle = \int_0^1 (\langle D_s\zeta, Y(w)\rangle + \langle D_\zeta Y, \dot w\rangle)\mathrm{d}s - \langle D_\zeta Y, \dot w\rangle,$$

therefore (5.25) is equivalent to

$$-\frac{\mathrm{d}}{\mathrm{d}s}(\langle D_\zeta Y, \dot w\rangle) + \langle R(\zeta, \dot w)\dot w, Y(w)\rangle = 0.$$

But

$$D_s D_\zeta Y = D_\zeta D_s Y + R(\dot w, \zeta)Y,$$

w is a geodesic and $D_s Y \equiv 0$, therefore (5.25) follows by the symmetry properties of R. □

Proof of Theorem 5.13: We prove a generalization of the Morse index theorem for Riemannian geodesics (see, e.g., Refs. 21 and 26) to lightlike geodesics. For any $\sigma \in]0,1]$ set

$$T_\sigma = \{\zeta \in H^{1,2}([0,\sigma]), \mathcal{T}\Lambda) : \zeta(s) \in T_{w(s)} \text{ for any } s \in]0,\sigma],$$

$$\zeta(0) = 0, \quad \zeta(\sigma) = 0,$$

$$\langle Y, D_s\zeta\rangle + \langle D_\zeta Y, \dot w\rangle \equiv c_\zeta \text{ a.e. in } [0,\sigma],$$

$$\langle D_s\zeta, \dot w\rangle = 0 \text{ a.e. in } [0,\sigma]\}.$$

Note that $T_1 = T_w\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$. Set, for any $\zeta \in T_\sigma$,

$$H_\sigma[\zeta,\zeta] = \int_0^\sigma (\langle D_s\zeta, D_s\zeta\rangle - \langle R(\zeta, \dot w)\dot w, \zeta\rangle)\mathrm{d}s.$$

Note that

$$H^\tau(w)[\cdot,\cdot] = \frac{-1}{\langle \dot\gamma(\tau(w)), \dot w(1)\rangle} H_1([\cdot,\cdot],$$

while $-\langle \dot\gamma(\tau(w)), \dot w(1)\rangle > 0$ because

$$\dot\gamma(\tau(w)) = Y(\gamma(\tau(w))) = Y(w(1))$$

and $\langle Y(w(s)), \dot w(s)\rangle$ is constant.

Therefore, denoting by $i(H_1)$ the Morse index of the quadratic form H_1 we have to prove that

$$i(H_1) = \mu(w). \tag{5.26}$$

On T_σ we define the Hilbert structure

$$\langle \zeta, \zeta\rangle_\sigma = \int_0^\sigma \langle D^Y_r\zeta, D^Y_r\zeta\rangle_Y \mathrm{d}r. \tag{5.27}$$

Denote by L_σ the linear operator in T_σ such that

$$\langle L_\sigma\zeta_1, \zeta_2\rangle_\sigma = H_\sigma([\zeta_1, \zeta_2]). \tag{5.28}$$

By Proposition 5.12 we see that

$$L_\sigma = I_\sigma - K_\sigma,$$

where I_σ is the identity on T_σ and $K_\sigma : T_\sigma \to T_\sigma$ is a compact operator. We shall denote by w_σ the geodesic $w_{|[0,\sigma]}$. It is well known that T_σ has the following orthogonal decomposition consisting of eigenspaces of L_σ,

$$T_\sigma = H_\sigma^+ \oplus H_\sigma^0 \oplus H_\sigma^-,$$

where (5.28) is positive definite on H_σ^+, definite negative on H_σ^-, and $H_\sigma^0 = \mathrm{Ker}\, L_\sigma$.

For any $\sigma \in]0,1]$ let $\lambda_1(\sigma) \geqslant \cdots \geqslant \lambda_k(\sigma)$ be the eigenvalues of the compact operator K_σ. Any eigenvalues are here repeated according to its (finite) multiplicity. By Lemmas 5.15–5.16 $w(\sigma)$ is conjugate to $w(0)$ with multiplicity equal to m if and only if there exists $k \in \mathbb{N}$ such that

$$\lambda_k(\sigma) < 1, \quad \lambda_{k+1}(\sigma), \ldots, \lambda_{k+m}(\sigma) = 1, \quad \text{and} \quad \lambda_{k+m+1}(\sigma) > 1.$$

Since K_σ is compact the eigenvalues of K_σ are characterized by the well-known Poincaré formula:

$$\lambda_k(\sigma) = \max_{\dim V = k} \Big[\min_{\zeta \in V, |\zeta|_\sigma = 1} (\langle K_\sigma \zeta, \zeta \rangle_\sigma) \Big], \tag{5.29}$$

which holds whenever the eigenvalues are positive. (Here $|\cdot|_\sigma = \langle \cdot, \cdot \rangle_\sigma^{1/2}$). Since we are interested in studying the behavior of $\lambda_k(\sigma)$ when its value is close to 1, we shall assume that all the $\lambda_k(\sigma)$'s are positive. The general case can be treated by small changes.

Using (5.29) it is not difficult to prove that any λ_k is a continuous function of σ. Moreover using (5.21)–(5.23) it is easy to show that there exists $\sigma_0 > 0$ such that, for any $\sigma \in]0,\sigma_0]$, H_σ is positive definite on T_σ. Then it will be sufficient to show that

$$\text{any } \lambda_k \text{ is strictly increasing.} \tag{5.30}$$

Fix $k \in \mathbb{N}$ and $0 \leqslant \sigma_1 < \sigma_2 \leqslant 1$. By (5.29) there exists a subspace V of T_{σ_1} having dimension k such that

$$\lambda_k(\sigma_1) = \min_{\zeta \in V, |\zeta|_{\sigma_1} = 1} (\langle K_{\sigma_1} \zeta, \zeta \rangle_{\sigma_1}). \tag{5.31}$$

For any $\zeta \in V$ set $c_\zeta \equiv \langle D_s \zeta, Y(w) \rangle + \langle \dot{w}, D_\zeta Y \rangle$ and $c_w \equiv \langle \dot{w}, Y(w) \rangle$. Take the vector field

$$A_\zeta = \zeta + \lambda \dot{w}$$

where $\lambda' = -c_\zeta / c_w$ and $\lambda(\sigma_1) = 0$. Since $\zeta \in T_{\sigma_1}$, w is a lightlike geodesic and $D_s Y \equiv 0$ it is

$$\langle D_s A_\zeta, \dot{w} \rangle \equiv 0, \tag{5.32}$$

$$\langle D_s A_\zeta, Y(w) \rangle + \langle \dot{w}, D_{A_\zeta} Y \rangle \equiv 0, \tag{5.33}$$

and

$$A_\zeta(\sigma_1) = 0, A_\zeta(0) = \lambda(0) \dot{w}(0). \tag{5.34}$$

Now denote by $\hat{A}_\zeta$ the extension to $[0,\sigma_2]$ of A_σ obtained by setting $\hat{A}_\zeta = 0$ on $[\sigma_1, \sigma_2]$. Note that, for any $\zeta \in V$,

$$\langle K_{\sigma_2} \hat{A}_\zeta, \hat{A}_\zeta \rangle_{\sigma_2} = \langle K_{\sigma_1} \zeta, \zeta \rangle_{\sigma_1}.$$

Now set

$$B_\zeta = \hat{A}_\zeta + \mu \dot{w},$$

where μ satisfies

$$\mu' = \text{const}, \quad \mu(0) = -\lambda(0), \quad \mu(\sigma_2) = 0. \tag{5.35}$$

Since $\hat{A}_\zeta$ satisfies (5.32)–(5.34) (with A_ζ replaced by $\hat{A}_\zeta$), thanks to (5.35) we deduce that $B_\zeta \in T_{\sigma_2}$. Note that the map

$$B_\cdot : V \to T_{\sigma_2}$$

is a linear and injective. Then the space

$$V_* = \{B_\zeta : \zeta \in V\}$$

is a subspace of T_{σ_2} having dimension k. Moreover, by our construction,

$$\langle K_{\sigma_2} B_\zeta, B_\zeta \rangle_{\sigma_2} = \langle K_{\sigma_1} \zeta, \zeta \rangle_{\sigma_1} \text{for any} \zeta \in V.$$

Then, by (5.29) and (5.31)

$$\lambda_k(\sigma_1) = \min_{\zeta \in V, |\zeta|_{\sigma_1} = 1} ((\langle K_{\sigma_1} \zeta, \zeta \rangle_{\sigma_1}) = \min_{\zeta \in V_*, |\zeta|_{\sigma_2} = 1} (\langle K_{\sigma_2} \zeta, \zeta \rangle_{\sigma_2}) \leqslant \lambda_k(\sigma_2). \tag{5.36}$$

To conclude the proof assume by contradiction that

$$\lambda \equiv \lambda_k(\sigma_1) = \lambda_k(\sigma_2). \tag{5.37}$$

By the spectral properties of K_{σ_2}, T_{σ_2} admits the orthogonal decomposition

$$T_{\sigma_2} = H^- \oplus H^0 \oplus H^+,$$

such that $\lambda I_{\sigma_2} - K_{\sigma_2}$ is negative definite on H^-, positive definite on H^+, and $H^0 = \text{Ker}(\lambda I_{\sigma_2} - K_{\sigma_2})$.

We claim that

$$V_* \cap (H^0 \oplus H^+) = \{0\}. \tag{5.38}$$

Indeed if $\zeta = \zeta_0 + \zeta_+ \in V_* \cap (H^0 \oplus H^+)$, where $\zeta_0 \in H^0$ and $\zeta_+ \in H^+$, if $\zeta_+ \neq = 0$ and $|\zeta|_{\sigma_2} = 1$ it is

$$\langle K_{\sigma_2} \zeta_0, \zeta_0 \rangle_{\sigma_2} + \langle K_{\sigma_2} \zeta_+, \zeta_+ \rangle_{\sigma_2} = \lambda \langle \zeta_0, \zeta_0 \rangle_{\sigma_2} + \langle K_{\sigma_2} \zeta_+, \zeta_+ \rangle_{\sigma_2} < \lambda \langle \zeta_0, \zeta_0 \rangle_{\sigma_2} + \lambda \langle \zeta_+, \zeta_+ \rangle_{\sigma_2} = \lambda$$

in contradiction with (5.36) and (5.37) because $\zeta \in V_*$. Then $\zeta_+ = 0$ and

$$\zeta = \zeta_0 \in \text{Ker}(\lambda I_{\sigma_2} - K_{\sigma_2}).$$

Then the same proof of Lemma 5.16 allows one to deduce that ζ is of class C^2. Since $\mu \dot{w}$ is of class C^2 then $\hat{A}_\zeta$ is of class C^2, and by the construction of $\hat{A}_\zeta$ we deduce that

$$D_s(A_\zeta)(\sigma_1) = 0.$$

Since ζ is a Jacobi field in $[0, \sigma_1]$, w is a geodesic and λ' is constant, $A_\zeta = \zeta + \lambda \dot{w}$ satisfies (2.4) with initial condition $A_\zeta(\sigma_1) = 0$ and $D_s(A_\zeta)(\sigma_1) = 0$. Then by the uniqueness of the Cauchy

problem it is $A_\zeta \equiv 0$. Since $\zeta(0)=0$, then $\lambda(0)=0$ and therefore $\lambda \equiv 0$. This implies that $\mu \equiv 0$ and $B_\sigma \equiv 0$ proving (5.38). Then the orthogonal projection of V_* on H^- has dimension n and

$$\lambda_k(\sigma_1)=\lambda < \min_{\zeta \in V_*, |\zeta|_{\sigma_2}=1} \langle K_{\sigma_2}\zeta,\zeta\rangle_{\sigma_2} \leqslant \lambda_k(\sigma_2)$$

proving (5.30) and concluding the proof of Theorem 5.13. □

VI. PROOF OF THEOREMS 2.5, 2.9, AND 2.11

Now we are finally ready to prove Theorem 2.5.

Proof of Theorem 2.5: Whenever we are far from the geodesics in $\mathcal{L}^{+,2}_{p,\gamma}(\Lambda)$, we can use the shortening flow at Sec IV to obtain a flow where τ is strictly decreasing.

Near any geodesic we can construct an homotopy equivalence between $\mathcal{L}^{+,2}_{p,\gamma}(\Lambda)$ and $\mathcal{Q}^{+,2}_{p,\gamma}(\Lambda)$ simply by a convex combination between the identity in $H^{1,2}([0,1],\mathbb{R})$ and the parametrization described by the condition

$$\langle \dot z, Y(z)\rangle = \int_0^1 \langle \dot z, Y(z)\rangle ds \quad \text{a.e.}$$

Then we can use the shortening flow for τ far from geodesics and, thanks to Proposition 5.7, Remark 5.8, and Proposition 5.9, we can use the classical Morse theory (see, e.g., Refs. 33 and 34) to describe the topology nearby a geodesic. In this way we obtain

$$\sum_{w \in \mathcal{G}_{p,\gamma}(\Lambda)} \lambda^{m(w,\tau)} = \mathcal{P}(\mathcal{L}^{+,2}_{p,\gamma}(\Lambda))(\kappa) + (1+\kappa)S(\kappa),$$

where S is a formal series with coefficients in $\mathbb{N}\cup\{+\infty\}$.

Since $\mathcal{B}^+_{p,\gamma}(\Lambda)$ is homotopically equivalent to $\mathcal{L}^{+,2}_{p,\gamma}(\Lambda)$ (cf. Proposition 4.4), applying Theorem 5.13 gives the proof of (2.6). □

Proof of Theorem 2.9: Assume that $\mathcal{B}^+_{p,\gamma}(\Lambda)$ is contractible. Then the Poincaré polynomial of $\mathcal{B}^+_{p,\gamma}(\Lambda)$ with respect to any field $\mathbb{K}$ is given by

$$\mathcal{P}(\mathcal{B}^+_{p,\gamma}(\Lambda),\mathbb{K})(\kappa)=1.$$

Let $\mathcal{G}^+_{p,\gamma}(\Lambda)$ be the set of future pointing lightlike geodesics joining p with γ. Formula (2.6) gives

$$\operatorname{card}\mathcal{G}^+_{p,\gamma}(\Lambda)=1+2S(1).$$

Then $\operatorname{card}\mathcal{G}^+_{p,\gamma}(\Lambda)$ is odd or infinite, according to whether $S(1)$ is finite or infinite. If $\mathcal{B}^+_{p,\gamma}(\Lambda)$ is not contractible, $\operatorname{cat}\mathcal{B}^+_{p,\gamma}(\Lambda)\geqslant 2$ so the conclusion follows by Remark 4.8. □

Proof of Theorem 2.11: If Λ is contractible, then $\Omega(\Lambda)$ is contractible. Then by assumption (L_3), $\mathcal{B}^+_{p,\gamma}(\Lambda)$ is contractible and the proof follows from the first part of Theorem 2.9. If Λ is not contractible by (L_3) and a result of Serre,[28] for a suitable field $\mathbb{K}$ the Poincaré polynomial $\mathcal{P}(\mathcal{B}^+_{p,\gamma}(\Lambda),\mathbb{K})$ has infinitely many coefficients different from zero and the conclusion follows from formula (2.6). □

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APPENDIX A: ON THE TOPOLOGY OF $\mathcal{B}^+_{p,\gamma}(\Lambda)$

Under light-convexity and pseudocoercivity of τ we have seen in Sec. IV that $\mathcal{B}^+_{p,\gamma}(\Lambda)$ is homotopically equivalent to $\mathcal{L}^{+,r}_{p,\gamma}(\Lambda)$ (for any $r\in[1,+\infty]$).

In this Appendix we shall give a general condition assuring that $\mathcal{L}^{+,1}_{p,\gamma}(\Lambda)$ is homeomorphic to $\Omega^{1,1}_{p,\gamma}(\Lambda)$. Then, using a standard technique one sees that $\Omega^{1,1}_{p,\gamma}(\Lambda)$ is homotopically equivalent to the based loop space of Λ.

Proposition A1: Suppose that there exists a smooth hypersurface Λ_0 in Λ and a smooth timelike vector field Y in Λ such that

(1) *Y is complete in Λ.*
(2) *$\Lambda=\{\eta(\sigma,y): y\in\Lambda_0, \sigma\in\mathbb{R}, \dot\eta=Y(\eta), \eta(0)=y\}$.*
(3) *For any integral curve η of Y there exists a unique $s\in\mathbb{R}$ such that $\eta(s)\in\Lambda_0$.*
(4) *$\gamma:\mathbb{R}\to\Lambda$ is an integral curve of Y with $\gamma(0)\in\Lambda_0$.*
(5) *$p\in\Lambda_0$ and $p\neq\gamma(0)$.*
(6) *The Cauchy problem*

$$\begin{cases} \sigma' = \dfrac{-1}{\langle Y,Y\rangle}\left(\langle Y,\eta_y[\dot y]\rangle + \dfrac{1}{2}\sqrt{\langle Y,\eta_y[\dot y]\rangle^2 - \langle Y,Y\rangle\langle \eta_y[\dot y],\eta_y[\dot y]\rangle}\right), \\ \sigma(0)=0 \end{cases} \tag{A1}$$

can be solved in the interval $[0,1]$ for any $y\in H^{1,1}([0,1],\Lambda)$ such that $y(0)=p$ and $y(1)=\gamma(0)$.

Then $\mathcal{L}^{+,1}_{p,\gamma}(\Lambda)$ *is homeomorphic to* $\Omega^{1,1}_{p,\gamma}(\Lambda)$.

[Here $Y=Y(\eta(\sigma,y))$ and η_y denotes the derivative of η with respect to the second variable].

Proof: Take $z(s)=\eta(\sigma(s),y(s))$. Suppose $y\in H^{1,1}([0,1],\Lambda)$, $y(0)=p$ and $y(1)=\gamma(0)$. If σ satisfies (6) a straightforward computation shows that the curve $z(s)$ is in $\mathcal{L}^{+,1}_{p,\gamma}(\Lambda)$. Conversely $z\in\mathcal{L}^{+,1}_{p,\gamma}(\Lambda)$ can be projected on Λ_0 using the integral curve of Y [cf. assumption (3)]. Since (A.1) has a unique solution we are done. □

APPENDIX B: MORSE RELATIONS ON THE SPACE OF THE PIECEWISE LIGHTLIKE GEODESICS

In this Appendix we show by a simple example that we cannot write Morse relations using the topology of the piecewise (non-null) lightlike geodesics (endowed with the topology of the uniform convergence). This space, as in Sec. II, will be denoted by $\hat{\mathcal{B}}^{+}_{p,\gamma}(\Lambda)$.

On the space $\mathbb{R}^2\times\mathbb{R}$ we consider the flat Minkowski metric

$$ds^2 = dx_1^2 + dx_2^2 - dt^2.$$

Take $p=(y_0,0)$ and $\gamma(s)=(y_1,s)$. It is immediate to verify that $\hat{\mathcal{B}}^{+}_{p,\gamma}(\Lambda)$ is homeomorphic to the space $\mathcal{C}_{y_0,y_1}$ of the piecewise nonzero geodesics in $\mathbb{R}^2$ (with respect to the Euclidean metric) joining y_0 with y_1 endowed with the uniform topology. Considering the positions on the unit circle assumed by the unit speed of any broken geodesic it is not difficult to show that $\mathcal{C}_{y_0,y_1}$ has infinitely many connect components. Then, if Morse relations hold, one should obtain the existence of infinitely many geodesics joining p and γ and this is clearly false.

Analogously one sees that in the $(2+1)$-dimensional Minkowski space–time the infinite dimensional space where the relativistic Fermat principle is proved has infinitely many connect components. Then also in this case it is not possible to write the Morse relations.

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Scaling behavior in the Einstein–Yang–Mills monopoles and dyons

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Scaling behavior in the moduli space of monopole and dyon solutions in the Einstein–Yang–Mills theory in the asymptotically anti-de Sitter space is derived. The mass of monopoles and dyons scales with respect to their magnetic and electric charges, independent of the values of the cosmological constant and gauge coupling constant. The stable monopole and dyon solutions are approximated by solutions in the fixed anti-de Sitter spacetime. Unstable solutions can be viewed as the Bartnik–McKinnon solutions dressed with monopole and dyon solutions in the fixed anti-de Sitter space. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421637]

I. INTRODUCTION

It has been shown that there exist a continuum of stable and unstable monopole and dyon solutions in the Einstein–Yang–Mills theory in the asymptotically anti-de Sitter (AdS) space.[1,2] They generalize a discrete family of unstable particlelike solutions in the asymptotically Minkowski or de Sitter space.[3] Similarly, black hole solutions exist with discrete values of magnetic charges in the asymptotically flat or de Sitter space,[4,5] and with continuous values of non-Abelian electric and magnetic charges in the asymptotically AdS space.[6,2,7,8]

Monopole and dyon solutions are characterized by their mass and non-Abelian magnetic/electric charges. The spectrum defines the moduli space of the solutions, which varies with the cosmological constant (Λ) and the gauge and gravitational coupling constants (e and G). The spectrum consists of infinitely many discrete points for $\Lambda \geqslant 0$, whereas it has a finite number of continuous branches for $\Lambda < 0$. When the parameter $\Lambda < 0$ approaches zero, an already-existing branch of monopole and dyon solutions collapses to a single point in the moduli space. At the same time new branches of solutions emerge. A fractal structure in the moduli space has been observed.[2,9]

In this paper we derive a scaling law for the mass spectrum of the solutions with respect to their magnetic and electric charges (Q_M and Q_E), the cosmological constant $\Lambda(<0)$, and the ratio of the gravitational constant to the gauge coupling constant $v \equiv 4\pi G/e^2$. Some of the results in Ref. 2 indicate that the mass of monopoles and dyons is expressed in terms of a universal function $f(Q_M, Q_E)$. We shall show that this follows from the factorization property of the solutions and that $f(Q_M, Q_E)$ is determined by the monopole and dyon solutions in the fixed AdS background metric.

AdS spacetime has many special properties. In some models it accommodates the holographic principle; the information on the boundary of the space determines physics in the bulk.[10] We shall see a trace of this property in the classical Einstein–Yang–Mills theory. The existence of stable monopole and dyon solutions in the asymptotically AdS space seems tightly connected to boundary data on non-Abelian charges, though a more thorough investigation is necessary.

II. MONOPOLES AND DYONS

There exist static, spherically symmetric monopole and dyon solutions in the Einstein–Yang–Mills theory. The action of the system is

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$$S=\int d^4x\sqrt{-g}\left[\frac{1}{16\pi G}(R-2\Lambda)-\frac{1}{4}F^{a\mu\nu}F^{a}{}_{\mu\nu}\right]. \tag{1}$$

The Einstein and Yang–Mills equations are given by

$$\begin{aligned} &R^{\mu\nu}-\tfrac{1}{2}g^{\mu\nu}(R-2\Lambda)=8\pi GT^{\mu\nu},\\ &F^{\mu\nu}{}_{;\mu}+e[A_\mu,F^{\mu\nu}]=0. \end{aligned} \tag{2}$$

The metric of spacetime is given by

$$\begin{aligned} &ds^2=-\frac{H}{p^2}dt^2+\frac{dr^2}{H}+r^2(d\theta^2+\sin^2\theta\, d\phi^2),\\ &H=1-\frac{2m}{r}-\frac{\Lambda}{3}r^2, \end{aligned} \tag{3}$$

where H, p, and m depend on r only. $m(r)/G$ represents a total mass contained inside r in the $c=1$ unit. (Numerical values below are given in the $c=\hbar=G=1$ unit.) The $SU(2)$ Yang–Mills fields take

$$A^{(0)}=\frac{\tau^j}{2e}\left\{u(r)\frac{x_j}{r}dt-\epsilon_{jkl}\frac{1-w(r)}{r^2}x_k\,dx_l\right\}, \tag{4}$$

in the Cartesian coordinates ($x_1^2+x_2^2+x_3^2=r^2$). The gauge coupling constant is denoted as e. With these ansatz (3) and (4) the Einstein and Yang–Mills equations (2) reduce to

$$\left(\frac{H}{p}w'\right)'=-\frac{p}{H}u^2w-\frac{w}{p}\frac{(1-w^2)}{r^2}, \tag{5}$$

$$(r^2pu')'=\frac{2p}{H}w^2u, \tag{6}$$

$$m'=v\left[H(w')^2+\frac{(1-w^2)^2}{2r^2}+\frac{1}{2}r^2p^2(u')^2+\frac{u^2w^2p^2}{H}\right], \tag{7}$$

$$p'=-\frac{2v}{r}p\left[(w')^2+\frac{u^2w^2p^2}{H^2}\right], \tag{8}$$

with the boundary conditions $u=m=0$ and $w=p=1$ at the origin. The set of the equations contains two parameters: the cosmological constant Λ and the ratio of the gravitational constant to the gauge coupling constant $v=4\pi G/e^2$.

There are soliton-type solutions with finite masses. There are infinitely many conserved, gauge-covariant charges. In the spherically symmetric case the nonvanishing charges of importance are[1,2]

$$\begin{pmatrix}Q_E\\ Q_M\end{pmatrix}=\frac{e}{4\pi}\int dS_k\sqrt{-g}\,\mathrm{Tr}\begin{pmatrix}F^{k0}\\ \tilde{F}^{k0}\end{pmatrix}\frac{x^j\tau^j}{r}=\begin{pmatrix}-u_1p_\infty\\ 1-w_\infty^2\end{pmatrix}, \tag{9}$$

where u_1, p_∞, and w_∞ are defined by the asymptotic expansion $u\sim u_\infty+(u_1/r)+\ldots$, etc. Each solution is specified by its mass (multiplied by G), $M=m(\infty)$, non-Abelian electric and magnetic charges, Q_E and Q_M, and the number, n, of the nodes of $w(r)$. For $\Lambda\geqslant 0$ the spectrum of the solutions is discrete, $u(r)=0$ ($Q_E=0$), $n=1,2,3,\ldots$, and all solutions are unstable. For $\Lambda<0$ the

spectrum is completely different. It is continuous. For each $n(=0,1,2,...)$ there are a family of solutions with continuous values of Q_E and Q_M.[1,2] In particular, the nodeless solutions ($n=0$) are stable. In the moduli space of the solutions, M of a particular point (solution) is a function of Λ, v, n, Q_E, and Q_M. M, Λ, and v have dimensions of (length), (length)$^{-2}$, and (length)^2, respectively, whereas n, Q_E, and Q_M are dimensionless. We show that M is expressed in terms of a universal function of Q_E and Q_M up to an overall factor.

III. SOLUTIONS IN THE FIXED AdS BACKGROUND METRIC

To understand why stable solutions exist only in the asymptotically AdS space ($\Lambda<0$), we consider soliton solutions in the fixed AdS background metric, setting $p=1$ and $H=1-\Lambda r^2/3$ in Eqs. (5) and (6) and on the rhs of Eq. (7). Introduce $x=(|\Lambda|/3)^{1/2}r$ and $\hat{u}=(3/|\Lambda|)^{1/2}u$. Then Eqs. (5), (6), and (7) become

$$\frac{d}{dx}\left\{(1+x^2)\frac{dw}{dx}\right\}=-\frac{w(1-w^2)}{x^2}-\frac{\hat{u}^2 w}{1+x^2},$$
$$\frac{d}{dx}\left\{x^2\frac{d\hat{u}}{dx}\right\}=\frac{2w^2\hat{u}}{1+x^2}, \tag{10}$$

and

$$\frac{dm}{dx}=v\sqrt{\frac{|\Lambda|}{3}}\left\{(1+x^2)\left(\frac{dw}{dx}\right)^2+\frac{(1-w^2)^2}{2x^2}+\frac{x^2}{2}\left(\frac{d\hat{u}}{dx}\right)^2+\frac{\hat{u}^2w^2}{1+x^2}\right\}. \tag{11}$$

The equations for $\hat{u}(x)$ and $w(x)$ do not involve either v or Λ. The charges of the solutions are

$$Q_M=1-w_\infty^2, \quad Q_E=x^2\left.\frac{d\hat{u}}{dx}\right|_{x=\infty}. \tag{12}$$

Hence a family of the solutions in the fixed AdS background metric satisfy

$$w(r;\Lambda,w_\infty,Q_E)^{\mathrm{AdS}}=\tilde{w}^{\mathrm{AdS}}(x;w_\infty,Q_E),$$
$$u(r;\Lambda,w_\infty;Q_E)^{\mathrm{AdS}}=\sqrt{\frac{|\Lambda|}{3}}\tilde{u}^{\mathrm{AdS}}(x;w_\infty,Q_E). \tag{13}$$

Here $\{\tilde{w}^{\mathrm{AdS}}(r),\tilde{u}^{\mathrm{AdS}}(r)\}$ represents a solution for $\Lambda=-3$. Further dm/dx is expressed in terms of $\hat{u}$ and w with an overall factor $v(|\Lambda|/3)^{1/2}$, which implies that

$$m(r;\Lambda,v,w_\infty,Q_E)^{\mathrm{AdS}}=v\sqrt{\frac{|\Lambda|}{3}}\tilde{m}^{\mathrm{AdS}}(x;w_\infty,Q_E),$$
$$M^{\mathrm{AdS}}=m^{\mathrm{AdS}}|_{r=\infty}=v\sqrt{|\Lambda|}f(Q_M,Q_E), \tag{14}$$

where $\tilde{m}^{\mathrm{AdS}}(r)$ is the mass function for $v=1$ and $\Lambda=-3$. $f(Q_M,Q_E)$ defines a universal scaling function, as we shall see below. Note that f is a double-valued function of Q_M as $Q_M=1-w_\infty^2$.

The size of the solutions also scales. One definition of the size, l, of a solution is given in terms of $m(r)$ by $m(l)=0.5\cdot m(\infty)$, where we have arbitrarily taken a size factor 0.5. It immediately follows that

$$l^{\mathrm{AdS}}=\frac{1}{\sqrt{|\Lambda|}}h(Q_M,Q_E). \tag{15}$$

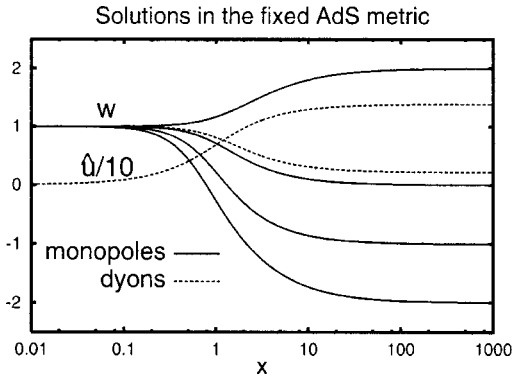

FIG. 1. $w(x)$ and $\hat{u}(x)$ of typical monopole and dyon solutions in the fixed AdS metric. The particular dyon solution displayed in the figure has $(Q_M, Q_E) = (0.954, 0.527)$.

Typical solutions are depicted in Fig. 1. Both $w(x)$ and $\hat{u}(x)$ monotonically decrease or increase. The solutions have, at most, one node in $w(r)$. Most of the energy of each solution is localized in $x < 10$.

There is a special solution,[11]

$$\hat{u} = 0, \quad w = \frac{1}{\sqrt{1+x^2}}, \tag{16}$$

for which $Q_E = 0$, $Q_M = 1$, and $M = (\sqrt{3}\pi/8)v|\Lambda|^{1/2}$. $Q_M = 1$ corresponds to the same quantized magnetic charge as for the 't Hooft and Polyakov monopole.

Further, $w^{\mathrm{AdS}} \sim 1$ and $m^{\mathrm{AdS}} \sim 0$ for $x < 0.1$. It is also numerically confirmed that

$$\mathrm{Max}_r \frac{2m^{\mathrm{AdS}}}{r} \cdot \frac{1}{1-(\Lambda r^2/3)} \sim \begin{cases} 0.03(v|\Lambda|)^{1/2} M^{1/2} |\Lambda|^{1/4}, & \text{for } w_\infty > 1, \\ 0.1 M |\Lambda|^{1/2}, & \text{for } w_\infty < 1, \end{cases} \tag{17}$$

for monopole solutions. As far as $v|\Lambda|$ and $M|\Lambda|^{1/2}$ are small enough, corrections to the metric may be ignored, and the solution in the fixed AdS background metric gives a good approximation to a solution in the EYM theory. [$p(r) \sim 1$ for those solutions.]

IV. FACTORIZATION

Let us turn to the EYM solutions in the $\Lambda = 0$ case. Set $u = 0$. Expressed in terms of $y = r/\sqrt{v}$, $H = 1 - (2\overline{m}/y)$, and $\overline{m} = m/\sqrt{v}$, Eqs. (5), (7), and (8) contain no parameter;

$$\begin{aligned} \frac{d}{dy}\left(\frac{H}{p}\frac{dw}{dy}\right) &= -\frac{w}{p}\frac{(1-w^2)}{y^2}, \\ \frac{d\overline{m}}{dy} &= \frac{(1-w^2)^2}{2y^2} + H\left(\frac{dw}{dy}\right)^2, \\ \frac{dp}{dy} &= -\frac{2p}{y}\left(\frac{dw}{dy}\right)^2. \end{aligned} \tag{18}$$

Solutions $\{w, p, \overline{m}\}$ are functions of y only. In each solution $w(r)$ crosses the axis n times ($n = 1,2,...$), and approaches $(-1)^n$ asymptotically. A physical mass is given by M/G, or $\overline{m}(\infty)\sqrt{v}/G = \overline{m}(\infty) M_{\mathrm{Pl}}/\sqrt{\alpha}$ where $\alpha = e^2/4\pi$ and $G = M_{\mathrm{Pl}}^{-2}$. The mass of the nth Bartnik–McKinnon solution is

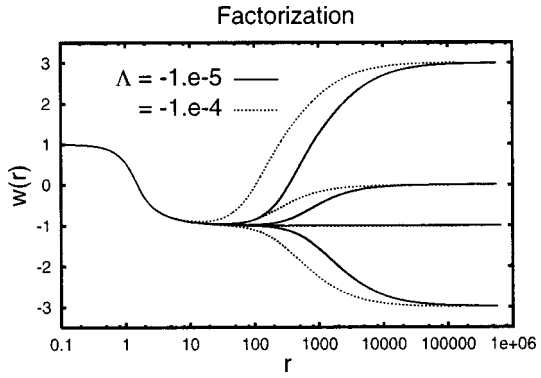

FIG. 2. Factorization property of the EYM monopole solutions. $\Lambda=-10^{-4}$ and -10^{-5} with $v=1$.

$$(\text{mass})_n^{\Lambda=0}(v)=\frac{M_{\text{Pl}}}{\sqrt{\alpha}}e_n \quad (n=1,2,...). \tag{19}$$

$e_n=M_n^{\Lambda=0}|_{v=1}$ is numerically given by $(e_1,e_2,\ldots)=(0.8286,0.9713,...)$. For $n\gg 1$, $e_n\sim 1-1.081e^{-\pi n/\sqrt{3}}$.[12] $w_n^{\Lambda=0}(r)$, $p_n^{\Lambda=0}(r)$, and $m_n^{\Lambda=0}(r)$ of the nth solution reach their asymptotic values at $r\sim a_n\sqrt{v}$, where $a_n\sim 10^n$.[5] The size of the Bartnik–McKinnon solutions is characterized by $l_n^{\Lambda=0}\sim a_n\sqrt{v}$.

Monopole and dyon solutions in $\Lambda<0$ are labeled by $(n,v,\Lambda,w_\infty,Q_E)$. The index n runs over 0, 1, 2,.... We would like to show that for $l_n^{\Lambda=0}\sqrt{|\Lambda|}\ll 1$, the Einstein–Yang–Mills monopole solutions are well approximated by

$$\begin{aligned} w_n&=w_n^{\Lambda=0}(r;v)w^{\text{AdS}}(r;\Lambda,(-1)^n w_\infty,Q_E),\\ u_n&=u^{\text{AdS}}(r;\Lambda,(-1)^n w_\infty,Q_E)/p_n^{A=0}(\infty;v),\\ p_n&=p_n^{\Lambda=0}(r;v),\\ m_n&=m_n^{\Lambda=0}(r;v)+m^{\text{AdS}}(r;\Lambda(-1)^n w_\infty;Q_E,v), \end{aligned} \tag{20}$$

where it has been understood that $w_0^{\Lambda=0}(r;v)=p_0^{\Lambda=0}(r;v)=1$ and $m_0^{\Lambda=0}(r;v)=0$. First, the solution in the fixed AdS metric approximately solves the EYM equations for $n=0$, as remarked above.

Secondly, for $n\geqslant 1$ we consider two regions; [I] $r<0.1(3/|\Lambda|)^{1/2}$ and [II] $r>a_n\sqrt{v}$. The two regions overlap with each other if $|\Lambda|v<0.03a_n^{-2}$. In the region I, $w^{\text{AdS}}\sim 1$, $m^{\text{AdS}}\sim 0$, and $-\Lambda r^2/3\ll 1$ so that the solution is well approximated by that in the $\Lambda=0$ case, provided u^2 is sufficiently small. In the region II, $w_n^{\Lambda=0}\sim(-1)^n$, $p_n^{\Lambda=0}\sim p_n^{\Lambda=0}|_{r=\infty}$, and $m_n^{\Lambda=0}\sim\sqrt{v}e_n$. In Eqs. (5)–(8) the value of constant p is irrelevant with pu substituted by u. H is approximated by $H=1-\Lambda r^2/3$ as $m_n^{\Lambda=0}/r<1/a_n\ll 1$. Hence the solutions are given by those in the fixed AdS background metric with w at $r=\infty$ given by $(-1)^n w_\infty$. The solutions in the asymptotically AdS space are obtained by dressing solutions in the fixed-AdS background metric to the Bartnik–McKinnon solutions in the asymptotically flat space, as expressed in (20).

The factorization property of the solutions, (20), is confirmed by numerical evaluation of the solutions. In Fig. 2, $w(r)$ of the monopole solutions at $\Lambda=-10^{-4}$, -10^{-5}, and $v=1$ with various $w_\infty=3$, 0, -1, -3 are depicted. For $r<10$ these solutions are well approximated by the first Bartnik–McKinnon solution at $\Lambda=0$. For larger r the solutions are essentially given by $-w^{\text{AdS}}(x;\Lambda=-1,-w_\infty)$.

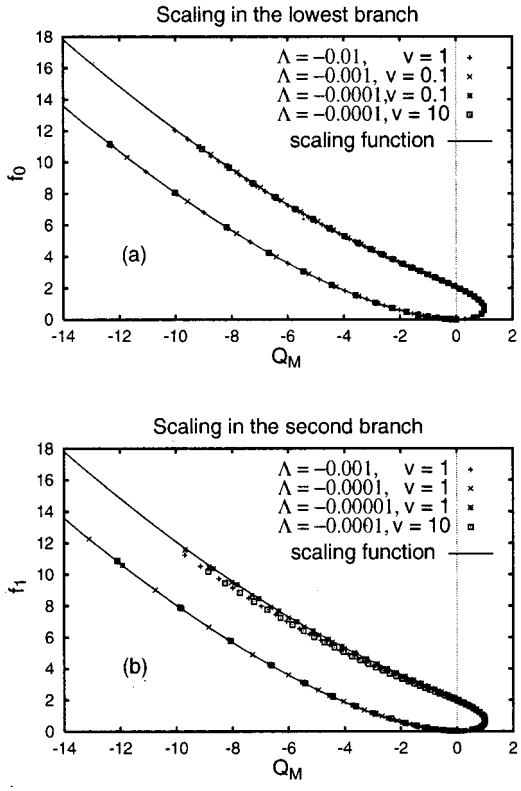

FIG. 3. Scaling (a) for $f_0 \equiv M_0(v,\Lambda,w_\infty,0)/(v|\Lambda|^{1/2})$, and (b) for $f_1 \equiv (M_1(v,\Lambda,w_\infty,0) - v^{1/2}e_1)/(v|\Lambda|^{1/2})$. The scaling function $f(Q_M,0)$ is also depicted.

V. SCALING

A scaling law follows from the factorization property. From (14) and (20),

$$\frac{M_n(v,\Lambda,w_\infty,Q_E) - \sqrt{v}\,e_n}{v\sqrt{|\Lambda|}} = f(Q_M,Q_E), \tag{21}$$

the rhs of which is independent of Λ and v, and also of n. The scaling law is valid for $|\Lambda|v < 0.03a_n^{-2}$ and small $|Q_E|$.

In Fig. 3 numerical data of monopole solutions for the lowest $(n=0)$ and second $(n=1)$ branches is depicted. It is seen that all data for $v|\Lambda| < 0.01$ falls on the universal function $f(Q_M,0)$ for $n=0$, and for $v|\Lambda| < 0.0001$ for $n=1$. It follows from (21) that the mass is given by

$$(\text{mass})_n(v,\Lambda,w_\infty,Q_E) = \frac{e_n}{\sqrt{a}} M_{\text{Pl}} + \frac{\sqrt{|\Lambda|}}{\alpha} f(Q_M,Q_E). \tag{22}$$

In the lowest branch the magnitude of the mass is determined by $\sqrt{|\Lambda|}/\alpha$, whereas in the higher branches it is given by $M_{\text{Pl}}/\sqrt{\alpha}$.

The size of a monopole or dyon is essentially the same as that of the solution in the fixed AdS background metric, as the dressed fields cover the inside Bartnik–McKinnon core. $h(Q_M,0)$ in (15) is depicted in Fig. 4.

As $\Lambda(<0)$ approaches 0, the branch in the $Q_M - M$ plane collapses to a flat line $M = \sqrt{v}\,e_n$. The size of the solution grows as $|\Lambda|^{-1/2}$ so that Bartnik–McKinnon solutions with higher n can be accommodated inside the AdS solutions, allowing more solutions in higher branches. This explains the phenomenon observed in Ref. 2. In the $\Lambda = 0$ limit only solutions with $Q_M = 0$ survive.

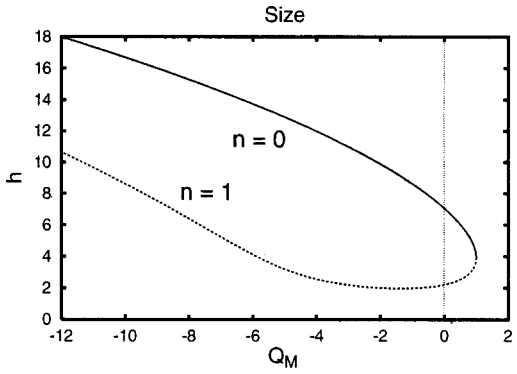

FIG. 4. Scaling function, $h(Q_M,0)$, for the size in (9). The portion with $n=0$ or $n=1$ corresponds to solutions with no node or one node in $w^{\mathrm{AdS}}(x)$, respectively.

VI. SUMMARY

In this paper we have examined monopole-dyon solutions in the Einstein–Yang–Mills theory in the asymptotically AdS space. The monopole and dyon solutions in the lowest branch $(n=0)$ are essentially the solutions in the fixed AdS background metric. The solutions in the higher branches $(n>0)$ are obtained by dressing monopole and dyon solutions in the fixed AdS background metric around the Bartnik–McKinnon solutions in the asymptotically flat space. As all Bartnik–McKinnon solutions are unstable, the monopole and dyon solutions in the higher branches are unstable, whereas the nodeless solutions are stable against small perturbations.

Because of the factorization property of the solutions there arises a scaling law in the mass of the solutions when regarded as a function of e, G, Λ, Q_M, and Q_E. Up to an overall factor it scales to a universal function $f(Q_M,Q_E)$ determined by the solutions in the fixed AdS metric. The factorization/dressing mechanism is expected to apply for black hole solutions as well.

In quantum theory Q_M and Q_E are expected to be quantized. Solutions with minimal $|Q_M|$ or $|Q_E|$ must be absolutely stable. The stable solutions discussed in the present paper are, in nature, nontopological solitons. They exist only with gravitational force. In this sense they may be called gravitational solitons.[13]

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Character expansions for the orthogonal and symplectic groups

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Formulas for the expansion of arbitrary invariant group functions in terms of the characters for the Sp($2N$), SO($2N+1$), and SO($2N$) groups are derived using a combinatorial method. The method is similar to one used by Balantekin to expand group functions over the characters of the U(N) group. All three expansions have been checked for all N by using them to calculate the known expansions of the generating function of the homogeneous symmetric functions. An expansion of the exponential of the traces of group elements, appearing in the finite-volume gauge field partition functions, is worked out for the orthogonal and symplectic groups. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1418014]

I. INTRODUCTION

The expansion of invariant functions of a group into its characters (traces of the representation matrices)[1] is very useful in a number of physical situations. In U(N) lattice gauge theories and in the lattice expansion of the nonlinear U(N)×U(N) sigma model calculation of certain U(N) group integrals are needed.[2–6] If the integrands can be expanded in terms of the U(N) characters, then such integrals can easily be calculated.[3,7,8] Similar U(N) integrals also arise in the statistical theory of nuclear reactions.[9] In 1980 Itzykson and Zuber calculated a particular unitary group integral[10] which turned out to be a special case of a more general formula by Harish-Chandra.[11] The Itzykson–Zuber integral and its generalizations[12–15] are also easily dealt with using character expansions.[1]

The character expansion of an invariant function of group elements is given by

$$f(\det U, TrU, \ldots) = \sum_r a_r \chi_r(U), \tag{1.1}$$

where $\chi_r(U)$ is the character of the representation r. Since group characters form an orthogonal set[16] the coefficients can be obtained by explicitly integrating the product of this function with the characters over the group manifold:

$$a_r = \int dU \chi_r^*(U) f(\det U, TrU, \ldots). \tag{1.2}$$

(Note that a_0 is the integral of the function itself over the group manifold). It is rather difficult to obtain complicated character expansions by explicit integration. In 1984 Balantekin[8] developed a combinatorial method that enabled one to solve for the coefficients in some expansions over the

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U(N) group characters that was quite simple in comparison to performing group integrals. Needing a more general version, the result was recently extended in its range of applicability.[1]

In a parallel development it was shown that the spectral density of the Dirac operator for a gauge theory near its zero eigenvalues should only depend on the symmetries in question.[17–19] Although the original work[17–19] used a Gaussian random matrix model, the results from the random matrix theory can be proven to be universal.[20–24] This implies that the spectral density of the Dirac operator near the origin can be extracted from random matrix theories which provide a description of common aspects of various quantum phenomena (for a review see Ref. 25). Hence to study the low-energy limit of, for example, quantum chromodynamics (QCD), one needs to choose a random matrix theory with the global symmetries of the QCD partition function. The partition functions calculated from the effective field theory and random matrix theory agree.[17,26,27] These random matrix theories are characterized by the Dyson index β which is the number of independent variables per matrix element.[19,28] For fermions in the fundamental representation $\beta=1$ for $N_c=2$ and $\beta=2$ for $N_c\geqslant 2$ where N_c is the number of colors. For fermions in the adjoint representation and $N_c\geqslant 2$ we have $\beta=4$. For $\beta=2$ the low-energy (finite-volume) QCD partition function is the same as the one-link integral of two-dimensional lattice QCD[5,29] and is calculated using the U(N) character expansion[1] and other methods.[30,14,31] For $\beta=4$ the zero momentum Goldstone modes belong to the coset space $\mathrm{SU}(N_f)/\mathrm{SO}(N_f)$[30,15] where N_f is the number of fermion flavors. Hence the finite-volume partition function is a group integral where the argument is the exponential of an SO(N_f) group element. Similarly in the $\beta=1$ case the coset space of the Goldstone modes is $\mathrm{SU}(2N_f)/\mathrm{Sp}(2N_f)$.[30,15] Massive partition functions of random matrix ensembles with $\beta=1$ and 4 were considered in Refs. 24 and 32. To calculate these partition functions it is very useful to have expressions for character expansions over the orthogonal and symplectic groups. Explicit expressions for these partition functions, for example, may help in finding solutions of Virasoro constraints which were found so far only for the $\beta=2$ case. (For the application of Virasoro constraints on the effective finite volume partition function, see, for example, Refs. 33–35).

The present work is an extension of Balantekin's method of finding the expansion coefficients for expansions over the characters for the symplectic group Sp($2N$), the odd dimensional special orthogonal group SO($2N+1$), and the even dimensional special orthogonal group SO($2N$). Some background material will be treated in Sec. II, including general information about the characters of the groups in question. The procedures for developing the expansions for the different groups are similar, so Sec. III will treat the general idea. The specific expressions will be derived in Sec. IV for Sp($2N$), in Sec. V for SO($2N+1$), and in Sec. VI for SO($2N$). Finally, some examples of expansions will be given for each of the groups in Sec. VII.

For quick reference, the expansions and the most general expressions for their coefficients for Sp($2N$), SO($2N+1$), and SO($2N$) are found in Eqs. (4.10) and (4.11), (5.8) and (5.9), and (6.10) and (6.12), respectively.

II. BACKGROUND AND FORMULAS FOR CHARACTERS

In order to calculate expressions for the character expansions, we will need expressions for the characters. These characters have been furnished by Weyl.[36] For reference, the Weyl formulas for the U(N), Sp($2N$), SO($2N+1,\mathfrak{R}$), and SO($2N,\mathfrak{R}$) group characters are reprinted below. [We have included the formula for the U(N) group characters for completeness even though we will not need them in the present work.]

In the following, $\det[\mathcal{A}_{ij}]$ refers to the determinant of the $N\times N$ matrix $\mathcal{A}$ whose entry in the ith row and jth column is $\mathcal{A}_{ij}$. Furthermore, we will denote a matrix in the unitary group as U, the symplectic group as P, and the orthogonal group as R, and the eigenvalues of any of these matrices are labeled by t_i. For the U(N) case, there are N eigenvalues that are all phases. For the Sp($2N$) and SO($2N$) cases, there are $2N$ eigenvalues, but they come in pairs of a phase and its reciprocal. Thus, a complete list of eigenvalues would be $t_1,t_2,\ldots,t_N,t_1^{-1},t_2^{-1},\ldots,t_N^{-1}$. For the SO($2N+1$) case, it is the same as the even dimensional cases with an additional eigenvalue of

$t=1$. The determinants given below, then, are determinants of $N\times N$ matrices which contain functions of only the individual eigenvalues, not their reciprocals. Finally, the character is a function of the representation, which is labeled by a partition $(n_1,n_2,\ldots,n_N)$ where the nonnegative integers n_i satisfy $n_1\geqslant n_2\geqslant\cdots\geqslant n_N$. Each representation corresponds to a permissible Young tableau.

The expressions for the simple characters of the U(N), Sp($2N$), and SO($2N+1$) groups are

$$\chi_{(n_1,n_2,\ldots,n_N)}(U)=\frac{\det[t_i^{n_j+N-j}]}{\det[t_i^{N-j}]}, \tag{2.1}$$

$$\chi_{(n_1,n_2,\ldots,n_N)}(P)=\frac{\det[t_i^{n_j+N-j+1}-t_i^{-(n_j+N-j+1)}]}{\det[t_i^{N+1-j}-t_i^{-(N+1-j)}]}, \tag{2.2}$$

and

$$\chi_{(n_1,n_2,\ldots,n_N)}(R)=\frac{\det[t_i^{n_j+N-j+1/2}-t_i^{-(n_j+N-j+1/2)}]}{\det[t_i^{N+1/2-j}-t_i^{-(N+1/2-j)}]}, \tag{2.3}$$

respectively.

The SO($2N$) case requires more attention. We define

$$\mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R)=\frac{\det[t_i^{n_j+N-j}+t_i^{-(n_j+N-j)}-\delta_{jN}\delta_{n_N0}]}{\det[t_i^{N-j}+t_i^{-(N-j)}-\delta_{jN}]} \tag{2.4}$$

and

$$\mathcal{S}_{(n_1,n_2,\ldots,n_N)}(R)=\frac{\det[t_i^{n_j+N-j}-t_i^{-(n_j+N-j)}]}{\det[t_i^{N-j}+t_i^{-(N-j)}-\delta_{jN}]}. \tag{2.5}$$

(The notation in the previous two equations is nonstandard, but they give the proper elements as stated in Ref. 16 in a more modern and manipulable form.) $\mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R)$ alone is the simple character of SO($2N$) if and only if $n_N=0$. If $n_N\neq 0$, then $\mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R)$ is a double character. For this case, the simple characters are given by $\frac{1}{2}(\mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R)\pm\mathcal{S}_{(n_1,n_2,\ldots,n_N)}(R))$. In the present work, only the expression for $\mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R)$ given in Eq. (2.4) will be needed. This statement will be justified in Sec. VI where SO($2N$) is treated.

One last property of these expressions that will be useful for checking the reliability of the expansions derived in this article is the value of the characters for representations corresponding to Young tableaux of one row ($n_1=n$, all others are 0) and one column ($n_n=1$ for all n up to some value, all others are 0). The characters for representations with one row, labeled (n), and one column, labeled (1^n), are

$$\chi_{(n)}(U)=h_n(t_i),\quad \chi_{(1^n)}(U)=a_n(t_i), \tag{2.6}$$

$$\chi_{(n)}(P)=h_n(t_i,t_i^{-1}),\quad \chi_{(1^n)}(P)=a_n(t_i,t_i^{-1})-a_{n-2}(t_i,t_i^{-1}), \tag{2.7}$$

$$\chi_{(n)}(R)=h_n(t_i,t_i^{-1},1)-h_{n-2}(t_i,t_i^{-1},1),\quad \chi_{(1^n)}(R)=a_n(t_i,t_i^{-1},1), \tag{2.8}$$

$$\mathcal{C}_{(n)}(R)=h_n(t_i,t_i^{-1})-h_{n-2}(t_i,t_i^{-1}),\quad \mathcal{C}_{(1^n)}(R)=a_n(t_i,t_i^{-1}), \tag{2.9}$$

for the U(N), Sp($2N$), SO($2N+1$), and SO($2N$) groups, respectively. The functions $h_n(t_i)$ are the homogeneous symmetric functions of order n, and the functions $a_n(t_i)$ are the elementary symmetric functions of order n. Further discussion is given in Ref. 1.

III. GENERAL PROPERTIES OF THE DERIVATION

We are now ready to derive the form for the expansions of group functions over the characters of the various groups mentioned in the previous section. As with any expansion, the crux of this issue is being able to determine and calculate the coefficients in the expansion. The goal of the next four sections will be to find these coefficients.

The derivation is very similar to the one used by Balantekin[1] in finding the coefficients of the expansion over the unitary group characters. As the expressions for the group characters for $\mathrm{Sp}(2N)$, $\mathrm{SO}(2N+1)$, and $\mathrm{SO}(2N)$ are all similar, the derivations for all three will proceed in much the same manner. To make the general method more transparent, the common aspects of the derivation will be presented in this section without mention of the specific groups. The following three sections will be devoted to using the result of this section to derive expressions for the coefficients in the expansions over the characters in each group.

We begin by noting that each of the expressions for the characters given by Eqs. (2.2)–(2.4) are all ratios of determinants, so that we can write

$$\chi_{(n_1,n_2,\ldots,n_N)}(M)=\frac{\mathcal{N}}{\mathcal{D}}, \tag{3.1}$$

where M is a matrix element of the group in question and $\mathcal{N}$ and $\mathcal{D}$ refer to numerator and denominator. For any of these groups, the denominator $\mathcal{D}$ can be expressed generally as

$$\mathcal{D}=\det[t_i^{N-j+q}\pm t_i^{-(N-j+q)}-\delta_{q0}\delta_{jN}], \tag{3.2}$$

where q can take on the value 1 for the $\mathrm{Sp}(2N)$ group, $\frac{1}{2}$ for the $\mathrm{SO}(2N+1)$ group, and 0 for the $\mathrm{SO}(2N)$ group. In this form, we choose the appropriate value of q and the proper sign of the $\pm$ sign to specify which group we are discussing. Namely, we see that the minus sign will be used for $\mathrm{Sp}(2N)$ and $\mathrm{SO}(2N+1)$ whereas the plus sign will be used for $\mathrm{SO}(2N)$.

In following the derivation of the $\mathrm{U}(N)$ expansion given in Ref. 1, we define a ''generating function,'' $G(x,t)$, to be some function of a variable t and any necessary parameters x. Later, we will take t to be an eigenvalue of a group matrix. For now, we expand the generating function in a power series in the variable t around $t=0$. Thus,

$$G(x,t)=\sum_{n=-\infty}^{\infty}A_n(x)t^n. \tag{3.3}$$

We assume that the series expansion converges for $|t|=1$. However, there are no other restrictions on the coefficients, so that some of the $A_n(x)$ can be zero. For instance, if the expansion is a Taylor series, then $A_n\equiv 0$ for all $n<0$.

Now, we define a function $\mathcal{F}$ by

$$\mathcal{F}=\mathcal{D}\prod_{i=1}^{N}G(x,t_i)G(x,t_i^{-1}), \tag{3.4}$$

where $\mathcal{D}$ is given in Eq. (3.2). By using the definition of $G(x,t)$ from Eq. (3.3), $\mathcal{F}$ can be written as (suppressing the x dependence of A_n)

$$\mathcal{F}=\mathcal{D}\left[\sum_{n=-\infty}^{\infty}A_nt_1^n\right]\left[\sum_{n=-\infty}^{\infty}A_nt_1^{-n}\right]\left[\sum_{n=-\infty}^{\infty}A_nt_2^n\right]\left[\sum_{n=-\infty}^{\infty}A_nt_2^{-n}\right]\cdots\left[\sum_{n=-\infty}^{\infty}A_nt_N^n\right]\left[\sum_{n=-\infty}^{\infty}A_nt_N^{-n}\right], \tag{3.5}$$

or, by combining the product of sums over the same variable, it can be written as

$$\mathcal{F}=\mathcal{D}\left[\sum_{n=-\infty}^{\infty}\sum_{p=-\infty}^{\infty}A_nA_pt_1^{n-p}\right]\left[\sum_{n=-\infty}^{\infty}\sum_{p=-\infty}^{\infty}A_nA_pt_2^{n-p}\right]\cdots\left[\sum_{n=-\infty}^{\infty}\sum_{p=-\infty}^{\infty}A_nA_pt_N^{n-p}\right]. \quad (3.6)$$

To proceed, we use the expression for $\mathcal{D}$ in Eq. (3.2). This determinant can be laboriously expanded as an alternating sum of products of the elements [see Eq. (A3)]. Upon doing so, we can combine the factors of the variable t_i in the determinant with the factor in Eq. (3.6) of the same variable. However, before naively doing so, we notice that there is a symmetry in the exponents in the determinant. We also notice that the double summations of the t_i's are unaffected by interchange of the dummy indices n and p. So the symmetry of the exponents will be preserved if we use $n-p$ in the product of the first term, $p-n$ in the product of the second term, and split the delta term in half using $n-p$ in the first one and $p-n$ in the second one. Upon doing so, we find that the new expression is again a determinant. Rewriting this as a determinant, we obtain

$$\mathcal{F}=\det\left[\sum_{n=-\infty}^{\infty}\sum_{p=-\infty}^{\infty}A_nA_p\left(t_i^{N-j+q+n-p}\pm t_i^{-(N-j+q+n-p)}-\frac{1}{2}\delta_{q0}\delta_{jN}(t_i^{n-p}+t_i^{p-n})\right)\right]. \quad (3.7)$$

Now, we change variables, defining a new integer $r=N-j+n-p$. This gives

$$\mathcal{F}=\det\left[\sum_{p=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}A_{r-N+j+p}A_p\left(t_i^{r+q}\pm t_i^{-(r+q)}-\frac{1}{2}\delta_{q0}\delta_{jN}(t_i^{r-N+j}+t_i^{N-j-r})\right)\right]. \quad (3.8)$$

The order of the summation for r and p is interchangeable. Also, the delta term chooses only $N=j$. Thus,

$$\mathcal{F}=\det\left[\sum_{r=-\infty}^{\infty}\sum_{p=-\infty}^{\infty}A_{r-N+j+p}A_p\left(t_i^{r+q}\pm t_i^{-(r+q)}-\frac{1}{2}\delta_{q0}\delta_{jN}(t_i^{r}+t_i^{-r})\right)\right]. \quad (3.9)$$

We notice that all of the dependence on the dummy variable p can be isolated by defining

$$c_{r,j}=\sum_{p=-\infty}^{\infty}A_{r-N+j+p}A_p\,. \quad (3.10)$$

Also, by combining the delta term with the other term [again remembering that it is only present for the SO($2N$) case in which $q=0$ and we use the $+$ sign], we can write our expression for $\mathcal{F}$ as

$$\mathcal{F}=\det\left[\sum_{r=-\infty}^{\infty}c_{r,j}(t_i^{r+q}\pm t_i^{-(r+q)})\left(1-\frac{1}{2}\delta_{q0}\delta_{jN}\right)\right]. \quad (3.11)$$

We have come to the point in the derivation where it will be necessary to specialize Eq. (3.11) for the three different types of groups by making appropriate choices for q and the $\pm$ sign. This will be taken up in the next three sections.

IV. THE EXPANSION OVER SP(2*N*) CHARACTERS

We begin with the Sp($2N$) case, as it is the simplest one. The starting point will be Eq. (3.11). For the Sp($2N$) case, $q=1$ and we choose the minus sign. Thus, we have

$$\mathcal{F}=\det\left[\sum_{r=-\infty}^{\infty}c_{r,j}(t_i^{r+1}-t_i^{-(r+1)})\right], \quad (4.1)$$

where $c_{r,j}$ is defined in Eq. (3.10). Before proceeding, it is beneficial to change dummy indices again by letting $r+1\rightarrow r$. This gives us

$$\mathcal{F}=\det\left[\sum_{r=-\infty}^{\infty} c'_{r,j}(t_i^r-t_i^{-r})\right], \tag{4.2}$$

where

$$c'_{r,j}=\sum_{p=-\infty}^{\infty} A_{r-N+j-1+p}A_p\,. \tag{4.3}$$

This sum over r from $-\infty$ to ∞ can be broken up into positive r, negative r, and $r=0$. The $r=0$ term vanishes because $t_i^0-t_i^0=0$. Then, changing the negative values to positive by replacing r with $-r$ and collecting terms, we get

$$\mathcal{F}=\det\left[\sum_{r=0}^{\infty} d_{r,j}(t_i^r-t_i^{-r})\right], \tag{4.4}$$

where

$$d_{r,j}=c'_{r,j}-c'_{-r,j}\,. \tag{4.5}$$

Equation (4.4) is very similar to an expression that is treated in Theorem 1.2.1 from Ref. 37. We will need a slightly more general form of this theorem, which we present in the Appendix. Using the result, Eq. (A8), we get

$$\mathcal{F}=\sum_{r_1>r_2>\cdots>r_N\geqslant 0}^{\infty} \det[d_{r_j,i}]\det[t_i^{r_j}-t_i^{-r_j}]. \tag{4.6}$$

Now, if, in the summation, $r_N=0$, then both determinants vanish, so we can restrict $r_N\geqslant 1$. Let us define

$$r_j=n_j+N-j+1. \tag{4.7}$$

Then, $r_j>r_{j+1}$ implies that $n_j\geqslant n_{j+1}$. Furthermore, since $r_N\geqslant 1$, then $n_N\geqslant 0$. Thus, we can write the summation as

$$\mathcal{F}=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty} \det[d_{n_j+N-j+1,i}]\det[t_i^{n_j+N-j+1}-t_i^{-(n_j+N-j+1)}]. \tag{4.8}$$

In the above expression, the second determinant is seen to be exactly the numerator in the Weyl formula for the characters of the symplectic group given in Eq. (2.2). We even have the appropriate restrictions on the values of the n_i that are necessary to make the equation valid. Thus, we can write the above expression as

$$\mathcal{F}=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty} \det[d_{n_j+N-j+1,i}]\mathcal{N}. \tag{4.9}$$

Now we recall our definition of $\mathcal{F}$ from Eq. (3.4). If we divide both sides by the denominator $\mathcal{D}$ and recall that our expression for the character of the Sp($2N$) group is $\chi_{(n_1,n_2,\ldots,n_N)}(P)=\mathcal{N}/\mathcal{D}$, then we obtain

$$\prod_{i=1}^{N} G(x,t_i)G(x,t_i^{-1})=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty} \det[d_{n_j+N-j+1,i}]\chi_{(n_1,n_2,\ldots,n_N)}(P). \tag{4.10}$$

This is our desired character expansion over the Sp($2N$) group! It is a sum over all irreducible representations of the symplectic group. Expressions for the coefficients are obtained using Eqs. (4.5) and (4.3). The result is

$$d_{n_j+N-j+1,i}=\sum_{p=-\infty}^{\infty} A_p(A_{n_j+i-j+p}-A_{-n_j-2N-2+i+j+p}). \tag{4.11}$$

In the special case in which the expansion of the generating function $G(x,t)$ is a Taylor series expansion with $A_p\equiv 0$ for all $p<0$, this simplifies slightly to

$$d_{n_j+N-j+1,i}=\sum_{p=0}^{\infty} A_p(A_{p+|n_j+i-j|}-A_{p+n_j+2N+2-i-j}). \tag{4.12}$$

We defer examples of the usage of this expansion until Sec. VII.

V. THE EXPANSION OVER SO($2N+1$) CHARACTERS

Once again, we start from Eq. (3.11). For SO($2N+1$), we have $q=\frac{1}{2}$ and we choose the minus sign. Then, we have

$$\mathcal{F}=\det\left[\sum_{r=-\infty}^{\infty} c_{r,j}(t_i^{r+1/2}-t_i^{-(r+1/2)})\right] \tag{5.1}$$

and $c_{r,j}$ is defined in Eq. (3.10).

This sum over r from $-\infty$ to ∞ can be broken up into ranges of $r\geqslant 0$ and $r<0$, which gives

$$\mathcal{F}=\det\left[\sum_{r=0}^{\infty} c_{r,j}(t_i^{r+1/2}-t_i^{-(r+1/2)})+\sum_{r=-\infty}^{-1} c_{r,j}(t_i^{r+1/2}-t_i^{-(r+1/2)})\right]. \tag{5.2}$$

Changing variables in the second summation using $r\to -(r+1)$ and collecting terms, we get

$$\mathcal{F}=\det\left[\sum_{r=0}^{\infty} d_{r,j}(t_i^{r+1/2}-t_i^{-(r+1/2)})\right], \tag{5.3}$$

where

$$d_{r,j}=c_{r,j}-c_{-r-1,j}\,. \tag{5.4}$$

Once again, we refer to Eq. (A8) in the Appendix to simplify Eq. (5.3) and we write

$$\mathcal{F}=\sum_{r_1>r_2>\cdots>r_N\geqslant 0}^{\infty} \det[d_{r_j,i}]\det[t_i^{r_j+1/2}-t_i^{-(r_j+1/2)}]. \tag{5.5}$$

If we define

$$r_j=n_j+N-j, \tag{5.6}$$

then the summation becomes

$$\mathcal{F}=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty} \det[d_{n_j+N-j,i}]\det[t_i^{n_j+N-j+1/2}-t_i^{-(n_j+N-j+1/2)}]. \tag{5.7}$$

The second determinant is simply the numerator of the Weyl formula for SO($2N+1$) as given in Eqs. (2.3), so using the definition of $\mathcal{F}$ from Eq. (3.4) and dividing by $\mathcal{D}$ gives

$$\prod_{i=1}^{N} G(x,t_i)G(x,t_i^{-1}) = \sum_{n_1 \geqslant n_2 \geqslant \cdots \geqslant n_N \geqslant 0}^{\infty} \det[d_{n_j+N-j,i}]\chi_{(n_1,n_2,\ldots,n_N)}(R). \tag{5.8}$$

This is the expansion for the SO($2N+1$) group, again a sum over all irreducible representations. Note, however, that this expression does not include the spinor representations of SO($2N+1$). The expression for the coefficient is found using Eqs. (5.4) and (3.10) with the result given by

$$d_{n_j+N-j,i} = \sum_{p=-\infty}^{\infty} A_p(A_{n_j+i-j+p} - A_{-n_j-2N-1+i+j+p}). \tag{5.9}$$

In the special case of a Taylor series with $A_p \equiv 0$ for all $p<0$, this simplifies to

$$d_{n_j+N-j,i} = \sum_{p=0}^{\infty} A_p(A_{p+|n_j+i-j|} - A_{p+n_j+2N+1-i-j}). \tag{5.10}$$

We conclude this section with a reminder that care must be taken in the usage of the above formulas for SO($2N+1$). One must remember that the number 1 is always an additional eigenvalue of the matrix R. Thus, in forming group functions, one must manually include a factor of $G(x,1)$ on both sides of the equation in order to have a function on the left hand side that treats all eigenvalues equally. This tricky point will be illustrated by example in Sec. VII, after we treat the SO($2N$) case in the next section.

VI. THE EXPANSION OVER SO(2*N*) CHARACTERS

One more time, we start from Eq. (3.11). Recall that for SO($2N$), we have $q=0$ and we use the + sign. Thus, we have

$$\mathcal{F} = \det\left[\sum_{r=-\infty}^{\infty} c_{r,j}(t_i^r + t_i^{-r})\left(1 - \frac{1}{2}\delta_{jN}\right)\right], \tag{6.1}$$

where $c_{r,j}$ is defined in Eq. (3.10). The delta function term serves to divide each entry in the last column by a factor of 2. When taking the determinant, a factor of 2 comes out and divides the equation. Thus,

$$\mathcal{F} = \frac{1}{2}\det\left[\sum_{r=-\infty}^{\infty} c_{r,j}(t_i^r + t_i^{-r})\right]. \tag{6.2}$$

This sum over r from $-\infty$ to ∞ can be broken up into positive r, negative r, and $r=0$. Then changing the negative values to positive by replacing r with $-r$ and collecting terms, we get

$$\mathcal{F} = \frac{1}{2}\det\left[\sum_{r=0}^{\infty} d_{r,j}\left(1 - \frac{1}{2}\delta_{r0}\right)(t_i^r + t_i^{-r})\right], \tag{6.3}$$

where

$$d_{r,j} = c_{r,j} + c_{-r,j} \tag{6.4}$$

and the δ_{r0} is inserted to ensure the correct coefficient for $r=0$. Once again, we can use Eq. (A8) from the Appendix to simplify Eq. (6.3) which gives

$$\mathcal{F} = \frac{1}{2}\sum_{r_1 > r_2 > \cdots > r_N \geqslant 0}^{\infty} \det[d_{r_j,i}]\det\left[(t_i^{r_j} + t_i^{-r_j})\left(1 - \frac{1}{2}\delta_{r_j 0}\right)\right]. \tag{6.5}$$

Let us define

$$r_j = n_j + N - j. \tag{6.6}$$

Then the summation becomes

$$\mathcal{F} = \frac{1}{2} \sum_{n_1 \geqslant n_2 \geqslant \cdots \geqslant n_N \geqslant 0}^{\infty} \det[d_{n_j+N-j,i}] \det\left[(t_i^{n_j+N-j} + t_i^{-(n_j+N-j)}) \left(1 - \frac{1}{2} \delta_{n_j+N-j,0} \right) \right]. \tag{6.7}$$

Focusing on the second determinant on the right hand side, we can multiply the two binomials to give

$$\det\left[t_i^{n_j+N-j} + t_i^{-(n_j+N-j)} - \frac{1}{2} \delta_{n_j+N-j,0} (t_i^{n_j+N-j} + t_i^{-(n_j+N-j)}) \right]. \tag{6.8}$$

Now, the delta function is only nonzero when $n_j + N - j = 0$, which can only occur for $j = N$ and $n_N = 0$ because n_j is non-negative. In this event, the exponents vanish and the sum in parentheses becomes 2, which cancels the $\frac{1}{2}$. Thus, we can write Eq. (6.7) as

$$\mathcal{F} = \frac{1}{2} \sum_{n_1 \geqslant n_2 \geqslant \cdots \geqslant n_N \geqslant 0}^{\infty} \det[d_{n_j+N-j,i}] \det[t_i^{n_j+N-j} + t_i^{-(n_j+N-j)} - \delta_{jN} \delta_{n_N 0}]. \tag{6.9}$$

We see that the second determinant is precisely the appropriate numerator in the Weyl formula for the quantity $\mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R)$ given in Eq. (2.4). By recalling the definition of $\mathcal{F}$ from Eq. (3.4) and dividing by $\mathcal{D}$, we get

$$\prod_{i=1}^{N} G(x,t_i) G(x,t_i^{-1}) = \sum_{n_1 \geqslant n_2 \geqslant \cdots \geqslant n_N \geqslant 0}^{\infty} \frac{1}{2} \det[d_{n_j+N-j,i}] \mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R), \tag{6.10}$$

This is the character expansion for SO($2N$). As with the SO($2N+1$) case, the expansion does not include the spinor representations. Note that the above expansion is not an expansion over the simple characters of the SO($2N$) group because the $\mathcal{C}$'s are double characters if $n_N > 0$ as discussed in Sec. II. If one desires an expansion over the simple characters, one can write

$$\mathcal{C} = \tfrac{1}{2}(\mathcal{C} + \mathcal{S}) + \tfrac{1}{2}(\mathcal{C} - \mathcal{S}), \tag{6.11}$$

which puts the two simple characters on the right hand side, as explained earlier. At the present time, we find it simpler to apply the formula in the state that it is in. The expression for the coefficient is found using Eqs. (6.4) and (3.10) and is found to be

$$d_{n_j+N-j,i} = \sum_{p=-\infty}^{\infty} A_p (A_{n_j+i-j+p} + A_{-n_j-2N+i+j+p}). \tag{6.12}$$

In the special case of a Taylor series with $A_p = 0$ for all $p < 0$, this simplifies to

$$d_{n_j+N-j,i} = \sum_{p=0}^{\infty} A_p (A_{p+|n_j+i-j|} + A_{p+n_j+2N-i-j}). \tag{6.13}$$

The derivations of the expansions are complete. We now turn to some examples.

VII. EXAMPLES OF CHARACTER EXPANSIONS

In this section, we give some examples of expansions of group functions over the characters of the Sp($2N$), SO($2N+1$), and SO($2N$) groups. In Sec. VII A, we will present the expansion of

the generating function of the homogeneous symmetric functions. This can be used as a check of the formulas derived in the present article, as the expansions are known. In Sec. VII B, we present the expansion for the function $\exp(xTrM)$, where M is some matrix element of one of the three groups we treat.

A. Homogeneous symmetric functions

Consider the generating function of the homogeneous symmetric functions, namely

$$G(x,t)=\frac{1}{1-xt}=\sum_{n=0}^{\infty} x^n t^n. \tag{7.1}$$

Thus, we have $A_n(x)=x^n$ for $n\geqslant 0$ and $A_n(x)=0$ otherwise. Consider the $\mathrm{Sp}(2N)$ expansion. Note that

$$\prod_{i=1}^{N} G(x,t_i)G(x,t_i^{-1})=\frac{1}{\det[I-xP]}, \tag{7.2}$$

where I is the $2N\times 2N$ identity matrix. The expansion is given by Eq. (4.10). Since the series expansion of the generating function in Eq. (7.1) does not contain negative powers of t, the coefficients are given by Eq. (4.12). Thus, the coefficients are given by

$$\det[d_{n_j+N-j+1,i}]=\det\left[\sum_{p=0}^{\infty} x^p(x^{p+|n_j+i-j|}-x^{p+n_j+2N+2-i-j})\right], \tag{7.3}$$

which after simplifying becomes

$$\det[d_{n_j+N-j+1,i}]=\det\left[\frac{x^{|n_j+i-j|}-x^{n_j+2N+2-i-j}}{1-x^2}\right]. \tag{7.4}$$

We simplify by noticing that if $n_2\geqslant 1$, then the first column of the determinant is a multiple of the second column, thereby making the determinant vanish. Thus, n_2 must be zero in order to have a nonvanishing coefficient. Now, since $n_2\geqslant n_3$ and so on, we see that the only surviving terms in the expansion are those for which $n_2=n_3=\cdots=n_N=0$. This corresponds to one row Young tableaux, labeled (n) earlier. The above determinant then becomes

$$\det[d_{n_j+N-j+1,i}]=\det\left[\frac{x^{|n_1\delta_{1j}+i-j|}-x^{n_1\delta_{1j}+2N+2-i-j}}{1-x^2}\right]. \tag{7.5}$$

This, in turn, can be written as

$$\det[d_{n_j+N-j+1,i}]=\frac{x^{n_1}}{(1-x^2)^N}\det[x^{|i-j|}-x^{2N+2-i-j}]. \tag{7.6}$$

By an induction argument on the dimension of the determinant on the right hand side, one can prove that

$$\det[x^{|i-j|}-x^{2N+2-i-j}]=(1-x^2)^N \tag{7.7}$$

and thus

$$\det[d_{n_j+N-j+1,i}]=x^{n_1}, \tag{7.8}$$

where we recall that all n's other than n_1 are 0. Then, the character expansion is Eq. (4.10) with the coefficients found above is

$$\frac{1}{\det[I-xP]}=\prod_{i=1}^{N}\left(\frac{1}{1-xt_i}\right)\left(\frac{1}{1-xt_i^{-1}}\right)=\sum_{n_1=0}^{\infty}x^{n_1}\chi_{(n_1)}(P). \tag{7.9}$$

If we use Eq. (2.7), which relates the character of one row Young tableaux to the homogeneous symmetric functions, we have

$$\frac{1}{\det[I-xP]}=\prod_{i=1}^{N}\left(\frac{1}{1-xt_i}\right)\left(\frac{1}{1-xt_i^{-1}}\right)=\sum_{n=0}^{\infty}x^{n}h_n(t_i,t_i^{-1}). \tag{7.10}$$

However, this is exactly the defining equation for the homogeneous symmetric functions. Thus, we see that the expansion derived for Sp($2N$) agrees with the known expansion.

To perform the same expansion over the SO($2N+1$) group, one must use caution. As alluded to earlier, we must manually include the eigenvalue 1. Mathematically, we have

$$\frac{1}{\det[I-xR]}=G(x,1)\prod_{i=1}^{N}G(x,t_i)G(x,t_i^{-1}), \tag{7.11}$$

where $G(x,t)$ is still given by Eq. (7.1) and I is the $(2N+1)\times(2N+1)$ identity matrix. Then, we have the expansion from Eq. (5.8) and we scale both sides by $G(x,1)=(1-x)^{-1}$ to get

$$G(x,1)\prod_{i=1}^{N}G(x,t_i)G(x,t_i^{-1})=\frac{1}{1-x}\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty}\det[d_{n_j+N-j,i}]\chi_{(n_1,n_2,\ldots,n_N)}(R). \tag{7.12}$$

The coefficient is given by Eq. (5.10)

$$\det[d_{n_j+N-j,i}]=\det\left[\sum_{p=0}^{\infty}x^{p}(x^{p+|n_j+i-j|}-x^{p+n_j+2N+1-i-j})\right], \tag{7.13}$$

or, after simplifying,

$$\det[d_{n_j+N-j,i}]=\det\left[\frac{x^{|n_j+i-j|}-x^{n_j+2N+1-i-j}}{1-x^2}\right]. \tag{7.14}$$

Once again it can be shown that if $n_2\geqslant 1$, the first two columns are multiples and the coefficient vanishes. It can also be shown using the result of the similar expression for the Sp($2N$) expansion that if $n_1=n$ and all other $n_i=0$, then

$$\det[d_{n_j+N-j,i}]=\frac{x^n}{1+x} \tag{7.15}$$

so that

$$\frac{1}{\det[I-xR]}=\frac{1}{(1-x)}\prod_{i=1}^{N}\frac{1}{(1-xt_i)}\frac{1}{(1-xt_i^{-1})}=\sum_{n=0}^{\infty}\frac{x^n}{1-x^2}\chi_{(n)}(R). \tag{7.16}$$

Finally, using the value of the single row characters for the SO($2N+1$) group from Eq. (2.8), one can show that

$$\frac{1}{\det[I-xR]}=\frac{1}{(1-x)}\prod_{i=1}^{N}\frac{1}{(1-xt_i)}\frac{1}{(1-xt_i^{-1})}=\sum_{n=0}^{\infty}x^{n}h_n(t_i,t_i^{-1},1), \tag{7.17}$$

which again agrees with the definition of the homogeneous symmetric functions.

We continue on with the same expansion for the SO($2N$) group. Using the same generating function and using the character expansion from Eq. (6.10), we have

$$\frac{1}{\det[I-xR]}=\prod_{i=1}^{N}\frac{1}{(1-xt_i)}\frac{1}{(1-xt_i^{-1})}=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty}\frac{1}{2}\det[d_{n_j+N-j,i}]\mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R). \tag{7.18}$$

Note the appearance of the factor of $\frac{1}{2}$ in this expression. The coefficient is given by Eq. (6.13) to be

$$\det[d_{n_j+N-j,i}]=\det\left[\sum_{p=0}^{\infty}x^p(x^{p+|n_j+i-j|}+x^{p+n_j+2N-i-j})\right], \tag{7.19}$$

or, after simplification,

$$\det[d_{n_j+N-j,i}]=\det\left[\frac{x^{|n_j+i-j|}+x^{n_j+2N-i-j}}{1-x^2}\right]. \tag{7.20}$$

Once again, the first two columns are multiples if $n_2\geqslant 1$, so the only surviving coefficients are the ones corresponding to $n_1=n$, all others are zero. Again, the determinant can be evaluated with the help of the result from the Sp($2N$) case, and the result is

$$\det[d_{n_j+N-j,i}]=\frac{2x^n}{1-x^2}. \tag{7.21}$$

We note that the 2 cancels with the $\frac{1}{2}$ built into the SO($2N$) expansion and the remaining expression is exactly the same as the SO($2N+1$) expression. Thus, we see that the expansions derived in the present work indeed give the correct expansion. In all three of these examples, we have tacitly assumed that N is at least 2, but one can check that the expansions are correct for the $N=1$ cases as well.

We could also consider the generating function for the alternating symmetric functions, $G(x,t)=1-xt$, and calculate the expansions as another check for reliability. One can check that the expansions derived from the present work in fact give the known expansions. This task will not be undertaken in the present work.

B. Expansion of exp(*x Tr* M)

Now that we have confidence in the character expansions derived here, we can start considering more interesting examples. Of course, any generating function can be chosen as long as it can be expanded in a power series. For our example, we will choose the exponential function because it is expected that this technique will prove useful in performing group integrals that arise in low-energy effective QCD partition functions and the integrals are of exponential functions.

We begin by defining the generating function

$$G(x,t)=e^{xt}=\sum_{n=0}^{\infty}\frac{x^n}{n!}t^n \tag{7.22}$$

so that $A_n(x)=x^n/n!$ for $n\geqslant 0$ and zero otherwise. Let us first consider Sp($2N$). We have

$$\prod_{i=1}^{N}G(x,t_i)G(x,t_i^{-1})=e^{x(t_1+t_2+\cdots+t_N+t_1^{-1}+t_2^{-1}+\cdots+t_N^{-1})}=\exp(xTrP). \tag{7.23}$$

Our character expansion is given by Eq. (4.10) as

$$\exp(xTrP)=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty}\det[d_{n_j+N-j+1,i}]\chi_{(n_1,n_2,\ldots,n_N)}(P), \tag{7.24}$$

where the coefficients are given directly by Eq. (4.12) as

$$\det[d_{n_j+N-j+1,i}]=\det\left[\sum_{p=0}^{\infty}\frac{x^p}{p!}\left(\frac{x^{p+|n_j+i-j|}}{(p+|n_j+i+j|)!}-\frac{x^{p+n_j+2N+2-i-j}}{(p+n_j+2N+2-i-j)!}\right)\right]. \tag{7.25}$$

This can be recognized as a modified Bessel function, which has the expansion

$$I_\lambda(x)=\sum_{p=0}^{\infty}\frac{1}{p!(p+\lambda)!}\left(\frac{x}{2}\right)^{2p+\lambda}. \tag{7.26}$$

Note also that $I_\lambda(x)=I_{-\lambda}(x)$ for any x. Thus, we can rewrite the coefficient as (dropping the absolute value sign)

$$\det[d_{n_j+N-j+1,i}]=\det[I_{n_j+i-j}(2x)-I_{n_j+2N+2-i-j}(2x)] \tag{7.27}$$

so that, finally,

$$\exp(xTrP)=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty}\det[I_{n_j+i-j}(2x)-I_{n_j+2N+2-i-j}(2x)]\chi_{(n_1,n_2,\ldots,n_N)}(P). \tag{7.28}$$

We proceed with the same expansion for the SO($2N+1$) group. Using the same generating function, Eq. (5.8) gives us the expansion as

$$\prod_{i=1}^{N}\exp(xt_i)\exp(xt_i^{-1})=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty}\det[d_{n_j+N-j,i}]\chi_{(n_1,n_2,\ldots,n_N)}(R), \tag{7.29}$$

where Eq. (5.10) gives

$$\det[d_{n_j+N-j,i}]=\det\left[\sum_{p=0}^{\infty}\frac{x^p}{p!}\left(\frac{x^{p+|n_j+i-j|}}{(p+|n_j+i-j|)!}-\frac{x^{p+n_j+2N+1-i-j}}{(p+n_j+2N+1-i-j)!}\right)\right], \tag{7.30}$$

or, using the definition of the modified Bessel function,

$$\det[d_{n_j+N-j,i}]=\det[I_{n_j+i-j}(2x)-I_{n_j+2N+1-i-j}(2x)]. \tag{7.31}$$

Thus, our expression is

$$\prod_{i=1}^{N}\exp(xt_i)\exp(xt_i^{-1})=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty}\det[I_{n_j+i-j}(2x)-I_{n_j+2N+1-i-j}(2x)]\chi_{(n_1,n_2,\ldots,n_N)}(R). \tag{7.32}$$

Now, the left hand side is not yet $\exp(xTrR)$. We need to include the eigenvalue 1. Thus we multiply both sides by e^x and we get

$$\exp(xTrR)=\exp(x)\prod_{i=1}^{N}\exp(xt_i)\exp(xt_i^{-1})$$

$$=e^{x}\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty}\det[I_{n_j+i-j}(2x)-I_{n_j+2N+1-i-j}(2x)]\chi_{(n_1,n_2,\ldots,n_N)}(R), \tag{7.33}$$

which is the desired expansion. We emphasize the appearance of the e^x on the right hand side of the expression. This extra term is unique to the SO($2N+1$) group.

As our final example, we develop the same expansion for the SO($2N$) group. As before, we write the expansion from Eq. (6.10) as

$$\exp(xTrR)=\prod_{i=1}^{N}\exp(xt_i)\exp(xt_i^{-1})=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N>0}^{\infty}\frac{1}{2}\det[d_{n_j+N-j,i}]\mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R). \tag{7.34}$$

The coefficients are given by Eq. (6.13) as

$$\det[d_{n_j+N-j,i}]=\det\left[\sum_{p=0}^{\infty}\frac{x^p}{p!}\left(\frac{x^{p+|n_j+i-j|}}{(p+|n_j+i-j|)!}+\frac{x^{p+n_j+2N-i-j}}{(p+n_j+2N-i-j)!}\right)\right]. \tag{7.35}$$

Again using the modified Bessel equation expansion, we get

$$\det[d_{n_j+N-j,i}]=\det[I_{n_j+i-j}(2x)+I_{n_j+2N-i-j}(2x)]. \tag{7.36}$$

Thus, the desired expansion is

$$\exp(xTrR)=\sum_{n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0}^{\infty}\frac{1}{2}\det[I_{n_j+i-j}(2x)+I_{n_j+2N-i-j}(2x)]\mathcal{C}_{(n_1,n_2,\ldots,n_N)}(R). \tag{7.37}$$

Once again, we emphasize the factor of $\frac{1}{2}$ in this expression. This is unique to the SO($2N$) expansion.

VIII. CONCLUSIONS

The present article, along with Refs. 1 and 8 completes the program of finding character expansions for all classical Lie groups. We expect these formulas to be useful in a wide range of applications. We already described some of these applications in the Introduction.

One should emphasize that the success in understanding the relationship between the random matrix theories and the low-lying eigenvalues of the QCD Dirac operator suggests investigating other aspects of QCD in a statistical framework (for a recent review see Ref. 38). More recently a similarity between disordered systems in condensed matter physics and QCD, namely the existence of a universal energy scale known as Thouless energy, was suggested.[39–41] This problem can be treated using the supersymmetry approach.[42,25,43] In the supersymmetry approach to this problem one needs to calculate integrals over supergroups.[44,45] One should note that integration over unitary supergroups was already considered in Refs. 13 and 45–47. Invariant integration over an Osp($N/2M$) manifold was also previously discussed in Refs. 48 and 49. An approach based on Gelfand–Tzetlin coordinates was developed and a recursion formula for both ordinary and supergroup integrals was found.[50–53] Character expansions for supergroups may be useful to understand the nature and extent of this approach. The characters of supergroups are given by formulas similar to the Weyl formulas except that complete symmetric functions are replaced by the graded homogeneous symmetric functions or alternately traces by supertraces.[54–57] Since our character

expansion formulas are basically combinatorial in nature they are applicable to the supergroups as well by the appropriate substitution of traces with supertraces. Thus one can obtain character expansions of the orthosymplectic supergroup Osp($N/2M$) from our formulas for SO(N)[54] and of the supergroup P(N) from our formulas for Sp($2N$).[55]

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APPENDIX: A THEOREM ON DETERMINANTS

Here we take up the issue of slightly generalizing a theorem on determinants that can be found in Hua's book.[37] His Theorem 1.2.1 states that

$$\det\left[\sum_{r=0}^{\infty} d_{r,j}t_i^r\right]=\sum_{r_1>r_2>\ldots>r_N\geqslant 0}^{\infty} \det[d_{r_j,i}]\det[t_i^{r_j}]. \tag{A1}$$

We would like to prove the following more general statement, which we state as a theorem.

Theorem 1: *Let $f_r(t)$ be an arbitrary function of the variable t with dependence on the index r. Then the following equality holds*:

$$\det\left[\sum_{r=0}^{\infty} d_{r,j}f_r(t_i)\right]=\sum_{r_1>r_2>\ldots>r_N\geqslant 0}^{\infty} \det[d_{r_j,i}]\det[f_{r_j}(t_i)]. \tag{A2}$$

To prove the theorem, we recall the expansion of determinants of $N\times N$ matrices, namely,

$$\det[\mathcal{A}_{i,j}]=\sum_{m_1=1}^{N}\sum_{m_2=1}^{N}\cdots\sum_{m_N=1}^{N}\epsilon_{m_1m_2\cdots m_N}\mathcal{A}_{1,m_1}\mathcal{A}_{2,m_2}\cdots\mathcal{A}_{N,m_N}, \tag{A3}$$

where the tensor $\epsilon_{m_1m_2\cdots m_N}$ is completely antisymmetric. Then, the left hand side of Eq. (A2) becomes

$$\begin{aligned}\det\left[\sum_{r=0}^{\infty} d_{r,j}f_r(t_i)\right]=&\sum_{m_1=1}^{N}\sum_{m_2=1}^{N}\cdots\sum_{m_N=1}^{N}\epsilon_{m_1m_2\cdots m_N}\left[\sum_{r_1=0}^{\infty} d_{r_1,m_1}f_{r_1}(t_1)\right]\\&\times\left[\sum_{r_2=0}^{\infty} d_{r_2,m_2}f_{r_2}(t_2)\right]\cdots\left[\sum_{r_N=0}^{\infty} d_{r_N,m_N}f_{r_N}(t_N)\right].\end{aligned} \tag{A4}$$

Isolating the dependence on the m_i's, we get

$$\begin{aligned}\det\left[\sum_{r=0}^{\infty} d_{r,j}f_r(t_i)\right]=&\sum_{r_1=0}^{\infty}\sum_{r_2=0}^{\infty}\cdots\sum_{r_N=0}^{\infty} f_{r_1}(t_1)f_{r_2}(t_2)\cdots f_{r_N}(t_N)\\&\times\left[\sum_{m_1=1}^{N}\sum_{m_2=1}^{N}\cdots\sum_{m_N=1}^{N}\epsilon_{m_1m_2\cdots m_N}d_{r_1,m_1}d_{r_2,m_2}\cdots d_{r_N,m_N}\right].\end{aligned} \tag{A5}$$

We recognize the term on the right hand side in the large brackets as a determinant, so

$$\det\left[\sum_{r=0}^{\infty} d_{r,j} f_r(t_i)\right] = \sum_{r_1=0}^{\infty}\sum_{r_2=0}^{\infty}\cdots\sum_{r_N=0}^{\infty} f_{r_1}(t_1) f_{r_2}(t_2)\cdots f_{r_N}(t_N)\det[d_{r_i,j}]. \tag{A6}$$

Now, if any of the r_i are equal, then the determinant on the right hand side will vanish because two rows would be identical. Thus, the sum can be restricted to distinct values of the r_i's. Next, since the r_i's are all different, we would like to order them in descending order so that $r_i > r_{i+1}$. In doing so, we would like to not change the form of the determinant on the right hand side. So, for any switch of labels, we permute the rows to leave the form unchanged. This brings in a factor of $+1$ or -1, depending on how many permutations are needed. We can express this simply by using the Nth rank alternating tensor as

$$\det\left[\sum_{r=0}^{\infty} d_{r,j} f_r(t_i)\right] = \sum_{r_1>r_2>\cdots>r_N\geqslant 0}^{\infty} \det[d_{r_i,j}] \sum_{m_1=1}^{N}\sum_{m_2=1}^{N}\cdots\sum_{m_N=1}^{N} \epsilon_{m_1 m_2\cdots m_N} f_{r_{m_1}}(t_1) f_{r_{m_2}}(t_2)\cdots f_{r_{m_N}}(t_N). \tag{A7}$$

Here we note that the term involving m_i sums is a determinant. Thus, taking the transpose of the determinant of the d's, we conclude

$$\det\left[\sum_{r=0}^{\infty} d_{r,j} f_r(t_i)\right] = \sum_{r_1>r_2>\cdots>r_N\geqslant 0}^{\infty} \det[d_{r_j,i}]\det[f_{r_j}(t_i)], \tag{A8}$$

which proves the theorem.

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Algebro-geometric solution of the 2+1 dimensional Burgers equation with a discrete variable

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The quasiperiodic solution of the 2+1 dimensional Burgers equation with a discrete variable is obtained through three steps: (a) decomposition into a symplectic map plus two finite-dimensional Hamiltonian systems; (b) straightening out of both the discrete and the continuous flows in the Jacobian variety; (c) inversion into the original variables. Inner relation with the modified Kadomtsev–Petviashvili equation is presented. The explicit theta function solutions for these two 2+1 integrable models are given. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The most attractive point in the celebrated Liouville–Arnold theory is the straightening out of various flows on the invariant torus, which reveals the basic structure of the Liouville integrability.[1] There were a series of brilliant examples in the development of classical mechanics, such as the two-body problem of Newton, the geodesic flow on the ellipsoid of Jacobi, the harmonic oscillator constrained on the sphere of C. Neumann, and the integrable tops of Euler, Lagrange, and Kovalevski. They have a common feature: the motions are all quasiperiodic. The ingenious mathematical skill in solving these problems is essentially reduced in finding the angular variables and proving the uniform way of their evolution. Hence, in the window of angular coordinates, the motion is linear locally, and quasiperiodic globally.

The discovery of the N-soliton solution to the Korteweg–de Vries equation (KdV) in 1967 is a prominent event in mathematical physics. As for the quasiperiodic solutions, after a series of independent works by Novikov,[2] Matveev,[3] Lax,[4,5] and Marchenko,[6] the final expression,

$$u(x,t) = -2\partial_x^2 \ln \theta(\Omega_1 x + \Omega_2 t + K) + C, \tag{1.1}$$

was found by Its and Matveev in 1975.[7,8] This is tremendous progress along the direction initiated by the pioneer studies in classic mechanics. Since the solution is closely related to the finite-band spectrum of the associated differential operator, it is also called the finite-band solution. The angular argument $\phi = \Omega_1 x + \Omega_2 t + K$ suggests the straightening out of x- and t-flows:

$$\frac{\mathrm{d}\phi}{\mathrm{d}x} = \Omega_1, \quad \frac{\mathrm{d}\phi}{\mathrm{d}t} = \Omega_2. \tag{1.2}$$

Further exciting results appeared later, including the finite-band solution of the 1+1 dimensional discrete Toda equation,[9–14] that of the Kadomtsev–Petviashvili (KP) equation and others, which could be found in the wonderful work of Belokolos, *et al.*[15] The straightening out of the discrete flow

$$\phi(n+1) - \phi(n) = \Omega_S, \quad (\mathrm{mod}\, T) \tag{1.3}$$

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was first proved by Toda through the spectral analysis of the discrete Toda eigenvalue problem.[11–13] As for the KP equation, we have the beautiful formula in Ref. 15:

$$w(x,y,t)=2\partial_x^2 \ln \theta(\Omega_1 x+\Omega_2 y+\Omega_3 t+D)+w_0, \tag{1.4}$$

which suggests the straightening out of the x-, y-, and t-flows in the framework of the angular variable $\phi=\Omega_1 x+\Omega_2 y+\Omega_3 t+D$:

$$\frac{d\phi}{dx}=\Omega_1, \quad \frac{d\phi}{dy}=\Omega_2, \quad \frac{d\phi}{dt}=\Omega_3. \tag{1.5}$$

However, the number of positive results remain very limited for the $(2+1)$-dimensional case since it is very hard to find the angular variable. Based on the observation and analysis of the Lax representation of soliton models, we have developed an approach to get finite-band solutions of spatially multidimensional integrable models. The well-known formula (1.4) for the KP equation is again derived through different means.[16] We also succeeded in getting an algebro-geometric solution of the special $(2+1)$-dimensional Toda lattice model.[17]

Our method is divided into three steps:

(a) decomposition;
(b) straightening out;
(c) inversion.

First the well-known Lax representation is used to decompose the higher dimensional integrable system into lower dimensional ones. A clear formalism of the decomposition is obtained through the so-called nonlinearization technique.[16–28] Second, the resulting finite-dimensional integrable system (the nonlinearized eigenvalue problem) serves as a base to construct the associated algebraic curve and the Abel–Jacobi coordinates, through which the flows are straightened out and the linear superposition yields the solution of the $(2+1)$-dimensional integrable models, expressed in the Abel–Jacobi coordinates. Third, an inverse procedure is indispensable in transforming the explicit solution in the original coordinates, which manifests abundant diversity in different examples. The main tool in our theory is the algebraic curve associated with the Lax matrix.

In the present paper we are going to investigate the $2+1$ dimensional Burgers equation with a discrete variable

$$B_y=2BB_x+\tfrac{1}{2}B_{xx}+\Delta^{-1}B_{xx}, \tag{1.6}$$

where Δ is the onward difference operator with regard to the discrete variable: $\Delta f(n)=f(n+1)-f(n)$, which is closely related to the first two members of the Kac–van Moerbeke (KvM) lattice hierarchy:

$$\frac{da(n)}{dx}=X_0=a(n)[a^2(n+1)-a^2(n-1)], \tag{1.7}$$

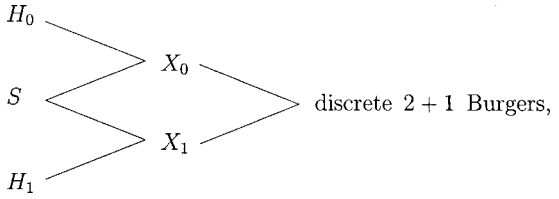
$$\begin{aligned}\frac{da(n)}{dy}=X_1=a(n)[&a^2(n+2)a^2(n+1)+a^4(n+1)+a^2(n+1)a^2(n)-a^2(n)a^2(n-1)\\&-a^4(n-1)-a^2(n-1)a^2(n-2)].\end{aligned} \tag{1.8}$$

The Kac–van Moerbeke equation (1.7) and its variants are sometimes called the Langmuir lattice, the Volterra system or the discrete Korteweg–de Vries equation, which have attracted wide attention.[9,14,29–38] A thorough investigation is made by Bulla *et al.*, for the algebro-geometric solutions of the KvM hierarchy.[39]

Let $a(n,x,y)$ be a compatible solution of Eqs. (1.7) and (1.8). Then $B(n,x,y)=a^2(n,x,y)$ solves Eq. (1.1), which is verified by direct calculations. The KvM hierarchy is the isospectral class of the discrete eigenvalue problem

$$E\chi=U\chi, \quad U=\frac{1}{a}\begin{pmatrix} 0 & a^2 \\ -1 & \lambda \end{pmatrix}, \tag{1.9}$$

where E is the shift operator: $Ef(n)=f(n+1)$. The nonlinearization of N copies of Eq. (1.9) with $\lambda=\alpha_1,\alpha_2,\ldots,\alpha_N$ yields an integrable symplectic map $\mathcal{S}$ in the symplectic space $(\mathbb{R}^{2N},\mathrm{d}p\wedge\mathrm{d}q)$ with N functionally independent integrals $H_0,H_1,\ldots,H_{N-1}$, involutive with each other (see Sec. II). Let $(p(n,\tau_k),q(n,\tau_k))$ be the compatible solution of the H_k-flow and the discrete flow generated by $\mathcal{S}$. Then the nonlinearized map $f_{\mathcal{S}}$ maps (p,q) exactly into a solution of the KvM flow X_k (see Sec. III). Thus we have the decomposition diagram:



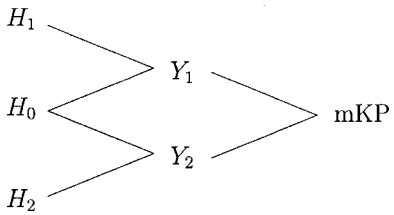
(1.10)

which is the basis of computing the algebro-geometric solution of Eq. (1.6).

The discrete 2+1 Burgers model (1.6) has an inner relation with the modified Kadomtsev–Petviashvili (mKP) equation:

$$v_t=\tfrac{1}{16}(v_{xx}-2v^3)_x+\tfrac{3}{4}\partial_x^{-1}v_{yy}-\tfrac{3}{4}v_x\partial_x^{-1}v_y, \tag{1.11}$$

which is a continuous 2+1 dimensional integrable model, and whose decomposition leads to the same Hamiltonian functions $\{H_k\}$ as noted previously (see Sec. IV):



(1.12)

In other words, the algebro-geometric solution of the discrete 2+1 model (1.6) is built up with the "bricks" H_0,H_1, and $\mathcal{S}$, while that of the continuous 2+1 model (1.11) is made up of the bricks H_0,H_1, and H_2.

The meaning of straightening out of the flows is that the velocities of the Abel–Jacobi coordinates along the H_k flow and the discrete $\mathcal{S}$ flow are constants:

$$\frac{\mathrm{d}\phi}{\mathrm{d}\tau_k}=\Omega_k, \quad \frac{\mathrm{d}\psi}{\mathrm{d}\tau_k}=-\Omega_k, \quad k=0,1,2,\ldots, \tag{1.13}$$

$$\begin{aligned} \phi(2m+1)-\phi(2m-1)=\psi(2m+1)-\psi(2m-1)\equiv\Omega_{\mathcal{S}} \pmod T, \\ \phi(2m+2)-\phi(2m)=\psi(2m+2)-\psi(2m)\equiv\Omega_{\mathcal{S}} \pmod T. \end{aligned} \tag{1.14}$$

Let $\omega=(\omega_1,\ldots,\omega_g)$ be the standard holomorphic differential of the associated elliptic curve Γ. It is interested to see that the continuous speed Ω_k is the kth coefficient in the asymptotic expansion of ω, while the discrete speed $\Omega_{\mathcal{S}}$ is the integral of ω from ∞_1 and ∞_2 (see Secs. IV and V).

The discrete evolution (1.14) is a little more complicated than (1.3) in the Toda case. We have given another proof of Eq. (1.3) through the nonlinearization approach,[17] which makes it possible to treat other types of examples, including the present one.

Thus through the ''window'' of the Abel–Jacobi coordinate we have a clear evolution picture of various flows; the special algebro-geometric solutions of higher dimensional integrable models could be essentially reduced as a linear superposition. The same pictures are observed in the KP and the 2+1 Toda cases. The final explicit solutions, expressed resorting to the theta function, are obtained through the Abel–Riemann–Jacobi inversion.[16,17,40,41]

II. THE KAC–van MOERBEKE HIERARCHY

The Kac–van Moerbeke hierarchy is the isospectral class of the discrete eigenvalue problem

$$E\begin{pmatrix} p_j \\ q_j \end{pmatrix} = U(a,\alpha_j)\begin{pmatrix} p_j \\ q_j \end{pmatrix}, \tag{2.1}$$

$$U(a,\lambda) = \frac{1}{a}\begin{pmatrix} 0 & a^2 \\ -1 & \lambda \end{pmatrix}, \tag{2.2}$$

where E is the shift operator: $Ef(n)=f(n+1)$. Denote $E^-f(n)=f(n-1)$, $\Delta=E-1$, and

$$\sigma_1=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_2=\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma_3=\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Proposition 2.1. (Fundamental identity): Let $\sigma(a,\lambda)$ be a linear map defined by

$$V=\sigma(a,\lambda)[G]=\{(a^2E-E^-a^2-\lambda^2)G\}\sigma_1+(2\lambda E^-a^2G)\sigma_2+(-2\lambda G)\sigma_3. \tag{2.3}$$

Then the discrete commutative relation

$$(EV)U-UV=U_*\{(K-\lambda^2J)G\} \tag{2.4}$$

holds for any function G, where

$$K=a(E+1)(a^2E-E^-a^2), \quad J=a\Delta, \tag{2.5}$$

$$U_*(a)\delta a=\left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} U(a+\epsilon\delta a)=\frac{1}{a^2}\begin{pmatrix} 0 & a^2 \\ 1 & -\lambda \end{pmatrix}\delta a. \tag{2.6}$$

Corollary 2.2: $(K-\lambda^2J)G=0$ implies $\det\sigma[G]=$constant, independent of n.
Proof: By (2.4), $V=\sigma[G]$ satisfies $V_{n+1}=UV_nU^{-1}$. Thus $\det V_{n+1}=\det V_n$.
The Lenard gradients $\{g_k\}$ are universal polynomials of a:

$$\begin{gathered} g_{-1}(n)=1, \quad g_0(n)=a^2(n)+a^2(n-1), \\ g_1(n)=a^2(n+1)a^2(n)+[a^2(n)+a^2(n-1)]^2+a^2(n-1)a^2(n-2), \text{ etc.}, \end{gathered} \tag{2.7}$$

satisfying the recursive formula:

$$Jg_{-1}=0, \quad Kg_{j-1}=Jg_j, \tag{2.8}$$

which means $(K-\lambda^2J)g_\lambda=0$ for the generating function:

$$g_\lambda=\sum_{j=0}^{\infty} g_{j-1}\lambda^{-2j}. \tag{2.9}$$

By Corollary 2.2, $\det \sigma[g_\lambda]=$constant. Since the Lenard gradients are universal polynomials of a, this constant can be determined by considering the class of a with rapidly decaying condition as $n\to\infty$. This yields

$$\det \sigma[g_\lambda]=-\lambda^4. \tag{2.10}$$

The discrete Kac–van Moerbeke equations are defined as ($m=0,1,2,\ldots$):

$$\frac{da}{d\tau_m}=X_m=Jg_m. \tag{2.11}$$

The first two are Eqs. (1.7) and (1.8) with $x=\tau_0$ and $y=\tau_1$.

III. THE INTEGRABLE SYMPLECTIC MAP

Consider N copies of Eq. (2.1) with distinct eigenvalues $\alpha_1,\ldots,\alpha_N$, and write them in the vector form:

$$\begin{aligned} p(n+1)&=a(n)q(n),\\ a(n)q(n+1)&=Aq(n)-p(n), \end{aligned} \tag{3.1}$$

where $p=(p_1,\ldots,p_N)^T$, $q=(q_1,\ldots,q_N)^T$, and $A=\mathrm{diag}(\alpha_1,\ldots,\alpha_N)$. Denote the usual inner product of two N-dimensional vectors ξ, η by $\langle\xi,\eta\rangle$. According to the principle of nonlinearization,[18] consider the Bargmann condition

$$g_0=\sum_{j=1}^{N}\alpha_j q_j^2, \tag{3.2}$$

i.e.,

$$a^2(n)+a^2(n-1)=\langle Aq(n),q(n)\rangle. \tag{3.3}$$

Lemma 3.1: The sufficient condition for Eq. (3.2) is

$$a=\sqrt{\langle Aq,q\rangle-\langle p,q\rangle}\equiv f_{\mathcal{S}}(p,q). \tag{3.4}$$

Proof: By (3.1) we have

$$\begin{aligned} a^2(n)&=\langle Aq(n),q(n)\rangle-\langle p(n),q(n)\rangle=\langle a(n)q(n+1),q(n)\rangle=\langle p(n+1),q(n+1)\rangle,\\ a^2(n-1)&=\langle p(n),q(n)\rangle. \end{aligned} \tag{3.5}$$

Hence we obtain Eq. (3.3).

We take Eq. (3.4) as the starting point and call it the Bargmann constraint, which implies the Bargmann condition (3.2). Equations (3.4) and (3.2) are not equivalent as in the case of the Toda lattice.[17] Nevertheless, it is enough for our purpose. Substituting Eq. (3.4) into Eq. (3.1), we obtain a symplectic map:

$$\begin{aligned} E\begin{pmatrix}p\\q\end{pmatrix}&=\begin{pmatrix}aq\\ a^{-1}(Aq-p)\end{pmatrix}\equiv\mathcal{S}\begin{pmatrix}p\\q\end{pmatrix},\\ a&=\sqrt{\langle Aq,q\rangle-\langle p,q\rangle}, \end{aligned} \tag{3.6}$$

with

$$\mathrm{d}p(n+1)\wedge\mathrm{d}q(n+1)=\mathrm{d}p(n)\wedge\mathrm{d}q(n).$$

Lemma 3.2: For the solution $(p_j,q_j),\alpha_j$ of the spectral problem (2.1), we have

$$(K-\alpha_j^2 J)q_j^2=0, \tag{3.7}$$

$$\sigma(a,\lambda)q_j^2=[-(\lambda^2-\alpha_j^2)q_j^2-2\alpha_j p_j q_j]\sigma_1+(2\lambda p_j^2)\sigma_2+(-2\lambda q_j^2)\sigma_3. \tag{3.8}$$

Proof: By direct calculations.

Lemma 3.3: Under the Bargmann constraint (3.4), the equation $(K-\lambda^2 J)G_\lambda=0$ has a solution

$$G_\lambda=g_{-1}+\sum_{j=1}^{N}\frac{\alpha_j q_j^2}{\lambda^2-\alpha_j^2}=1+Q_\zeta(Aq,q), \tag{3.9}$$

where $\zeta=\lambda^2$ and

$$Q_\zeta(\xi,\eta)=\sum_{j=1}^{N}\frac{\xi_j\eta_j}{\lambda^2-\alpha_j^2}.$$

Proof: Using Eqs. (3.7) and (3.2), we calculate

$$(K-\lambda^2 J)G_\lambda=Jg_0+\sum_{j=1}^{N}\frac{\alpha_j(\alpha_j^2-\lambda^2)q_j^2}{\lambda^2-\alpha_j^2}=J\left(g_0-\sum_{j=1}^{N}\alpha_j q_j^2\right)=0.$$

We define the Lax matrix of the Kac–van Moerbeke hierarchy as

$$V_\lambda=\sigma(f_{\mathcal{S}}(p,q),\lambda)[G_\lambda], \tag{3.10}$$

which satisfies the stationary zero-curvature equation (discrete version):

$$(EV_\lambda)U-UV_\lambda=0. \tag{3.11}$$

By corollary 2.2, its determinant gives rise to the generating function of the conserved integrals of the symplectic map $\mathcal{S}$:

$$F_\lambda=\det V_\lambda. \tag{3.12}$$

The expression of V_λ and F_λ is obtained from Eq. (3.8):

$$\frac{1}{\lambda}V_\lambda=\begin{pmatrix}-\lambda & 2\langle p,q\rangle\\ -2 & \lambda\end{pmatrix}-2\begin{pmatrix}\lambda Q_\zeta(p,q) & -Q_\zeta(Ap,p)\\ Q_\zeta(Aq,q) & -\lambda Q_\zeta(p,q)\end{pmatrix}, \tag{3.13}$$

$$\frac{1}{\lambda^2}F_\lambda=-\lambda^2-4Q_\zeta(A^2p,q)+4Q_\zeta(Ap,p)+4\langle p,q\rangle Q_\zeta(Aq,q)+4\{Q_\zeta(Ap,p)Q_\zeta(Aq,q)$$

$$-\lambda^2Q_\zeta^2(p,q)\}=-\lambda^2+\sum_{m=0}^{\infty}\lambda^{-2m-2}F_m. \tag{3.14}$$

Hence we have the integrals of the map $\mathcal{S}$ $(m=1,2,\ldots)$:

$$\begin{aligned}\tfrac{1}{4}F_0&=-\langle A^2p,q\rangle+\langle Ap,p\rangle+\langle p,q\rangle\langle Aq,q\rangle-\langle p,q\rangle^2,\\ \frac{1}{4}F_m&=-\langle A^{2m+2}p,q\rangle+\langle A^{2m+1}p,p\rangle+\langle p,q\rangle\langle A^{2m+1}q,q\rangle\\ &\quad+\sum_{k+j=m-1}\langle A^{2j+1}p,p\rangle\langle A^{2k+1}q,q\rangle-\sum_{k+j=m}\langle A^{2j}p,q\rangle\langle A^{2k}p,q\rangle.\end{aligned}\tag{3.15}$$

The proof of the involutivity of $\{F_m\}$ is based on the generating function method. Consider F_λ as a Hamiltonian function in the symplectic space $(\mathbb{R}^{2N},\mathrm{d}p\wedge\mathrm{d}q)$ and denote the flow variable by t_λ. Then the canonical equation is expressed as

$$\frac{\mathrm{d}}{\mathrm{d}t_\lambda}\begin{pmatrix}p_k\\ q_k\end{pmatrix}=\begin{pmatrix}-\partial F_\lambda/\partial q_k\\ \partial F_\lambda/\partial p_k\end{pmatrix}=W(\lambda,\alpha_k)\begin{pmatrix}p_k\\ q_k\end{pmatrix},\tag{3.16}$$

$$W(\lambda,\mu)=-\frac{4\lambda\mu}{\lambda^2-\mu^2}V_\lambda+2\lambda\left(-\frac{2}{\lambda+\mu}V_\lambda^{11}+V_\lambda^{21}\right)\sigma_1.\tag{3.17}$$

Proposition 3.4:

$$\frac{\mathrm{d}}{\mathrm{d}t_\lambda}V_\mu=[W(\lambda,\mu),V_\mu],\quad\forall\lambda,\mu\in\mathbb{C},\tag{3.18}$$

$$(F_\mu,F_\lambda)=0,\quad\forall\lambda,\mu\in\mathbb{C},\tag{3.19}$$

$$(F_j,F_k)=0,\quad\forall j,k=0,1,2,\ldots.\tag{3.20}$$

Proof: A direct calculation yields (3.18), which implies the invariance of $F_\mu=\det V_\mu$ along the t_λ-flow. By definition, the Poisson bracket is essentially a derivative along the phase flow, thus we have:

$$0=\frac{\mathrm{d}F_\mu}{\mathrm{d}t_\lambda}=(F_\mu,F_\lambda).$$

The expansion of (3.19) according to the negative powers of λ,μ gives rise to (3.20).

IV. DECOMPOSITION OF THE INTEGRABLE MODELS

In order to decompose the KvM equations and further the 2+1 discrete Burgers equation, one should establish the inner relation between the Hamiltonian vector field $I\nabla F_m$ and the KvM vector field X_m. It turns out that the derivative map $\mathrm{d}f_{\mathcal{S}}$ does map $I\nabla F_m$ into X_m, but with an annoying remainder. F_m should be adjusted into some H_m so that $\mathrm{d}f_{\mathcal{S}}$ maps $I\nabla H_m$ exactly into X_m. Fortunately, just as in the case of KP and Toda, the square root of F_λ yields the desired generating function H_λ of $\{H_m\}$ [see Eq. (4.8)]. Later (in Sec. VI) we shall see that H_λ is essentially the eigenvalue of the Lax matrix V_λ, acting on the invariant solution space of the linear equation $E\chi=U\chi$ under the commutative condition (3.11).

We start from the Bargmann condition (3.2), which becomes ($k=0,1,2,\ldots$)

$$\sum_{j=1}^{N}\alpha_j^{2k+1}q_j^2(n)=g_k+c_2g_{k-2}+\cdots+c_kg_0+c_{k+1}g_{-1},\tag{4.1}$$

after being exerted k times by the operator $J^{-1}K$. An extra term cg_{-1} appears each time, since the linear space $\ker J$ is one dimensional with the generator g_{-1}. The coefficient c_m is a constant of

motion. It is surprising that c_{m+2} is the desired H_m up to a factor 2 [see Eq. (4.10)]. Two kinds of linear combinations of Eq. (4.1) give the following two important relations.

Proposition 4.1: The solution $(p(n),q(n))^T=\mathcal{S}^n(p_0,q_0)$ of the discrete flow generated by the symplectic map $\mathcal{S}$ is mapped by f_S into a solution of the stationary KvM equation:

$$X_N+c_{N1}X_{N-1}+\cdots+c_{NN}X_0=0. \tag{4.2}$$

Proof: Define a polynomial

$$\alpha(\lambda^2)=\prod_{j=1}^{N}(\lambda^2-\alpha_j^2)=\lambda^{2N}+\alpha_{N1}\lambda^{2N-2}+\cdots+\alpha_{NN}. \tag{4.3}$$

Let $\lambda=\alpha_j$. A linear combination of Eq. (4.1) with the coefficients $\alpha_{NN},\cdots,\alpha_{N1},1$ yields

$$0=\sum_{j=1}^{N}\alpha(\alpha_j^2)\alpha_j q_j^2=g_N+c_{N1}g_{N-1}+\cdots+c_{NN}g_0+c_{N,N+1}g_{-1},$$

which becomes Eq. (4.2) after being acted with J.

Proposition 4.2: Under the Bargmann constraint (3.4), G_λ and g_λ have a direct relation:

$$G_\lambda=c_\lambda g_\lambda, \tag{4.4}$$

where c_λ is the generating function of the coefficients $\{c_k\}$ in Eq. (4.1),

$$c_\lambda=1+\sum_{k=2}^{\infty}c_k\lambda^{-2k}. \tag{4.5}$$

Proof: Multiplied by λ^{-k-1} and summed with respect to k from 0 to ∞, the linear combination of Eq. (4.1) becomes Eq. (4.4).

As a corollary we have the following expressions for the Lax matrix V_λ and the generation function F_λ of the conserved integrals:

$$V_\lambda=c_\lambda\sigma_\lambda[g_\lambda], \tag{4.6}$$

$$F_\lambda=-c_\lambda^2\lambda^4, \tag{4.7}$$

where Eq. (2.10) is used. Introduce H_λ by $c_\lambda=1+2H_\lambda$. Then

$$(1+2H_\lambda)^2=-\frac{1}{\lambda^4}F_\lambda, \tag{4.8}$$

from which the coefficients $\{H_m\}$ of the expansion

$$H_\lambda=\sum_{m=0}^{\infty}\frac{H_m}{\lambda^{2m+4}} \tag{4.9}$$

are determined uniquely ($c_{k+2}=2H_k$),

$$\begin{aligned}&H_0=-\tfrac{1}{4}F_0,\quad H_1=-\tfrac{1}{4}F_1,\\ &H_m=-\tfrac{1}{4}F_m-\sum_{\substack{i+j=m-2\\ i,\,j\geqslant 0}}H_iH_j,\quad m=2,3,4,\ldots.\end{aligned} \tag{4.10}$$

Specifically,

$$H_0=\langle A^2p,q\rangle-\langle Ap,p\rangle-\langle p,q\rangle\langle Aq,q\rangle+\langle p,q\rangle^2. \tag{4.11}$$

We shall see later (in Sec. VIII) that the integral H_0 is the starting point to link up the discrete 2+1 model (1.6) and the continuous 2+1 model (1.11).

Denote the variables of the H_λ- and H_m-flows by τ_λ and τ_m, respectively. Resorting to Eqs. (3.1) and (3.16), we have the evolution equation of $a=f_{\mathcal{S}}(p,q)$ alone these flows:

$$\frac{\mathrm{d}a}{\mathrm{d}t_\lambda}=-4\lambda^4JG_\lambda, \tag{4.12}$$

$$\frac{\mathrm{d}a}{\mathrm{d}\tau_\lambda}=\frac{1}{\lambda^2}Jg_\lambda, \tag{4.13}$$

in virtue of

$$\frac{\mathrm{d}}{\mathrm{d}\tau_\lambda}=\frac{-1}{4\lambda^4c_\lambda}\frac{\mathrm{d}}{\mathrm{d}t_\lambda}, \tag{4.14}$$

which is a corollary of Eq. (4.8). Comparing the coefficients in the asymptotic expansions of both sides of Eq. (4.13), we get

$$\frac{\mathrm{d}a}{\mathrm{d}\tau_m}=Jg_m=X_m. \tag{4.15}$$

Theorem 4.3: Let $(p(n,\tau_m),q(n,\tau_m)^T$ be a compatible solution of the discrete flow (3.6) ($\mathcal{S}$-flow for short) and the H_m-flow:

$$\frac{\mathrm{d}}{\mathrm{d}\tau_m}\begin{pmatrix}p\\q\end{pmatrix}=I\nabla H_m=\begin{pmatrix}-\partial H_m/\partial p\\ \partial H_m/\partial q\end{pmatrix}. \tag{4.16}$$

Then $a(n,\tau_m)=f_{\mathcal{S}}(p(n,\tau_m),q(n,\tau_m))$ solves the mth KvM equation (4.15).

Theorem 4.4: Let $(p(n,x,y),q(n,x,y)^T$ be a compatible solution of the $\mathcal{S}$-flow, H_0-flow, and H_1-flow with $x=\tau_0,y=\tau_1$. Then

$$B(n,x,y)=\langle Aq(n,x,y),q(n,x,y)\rangle-\langle p(n,x,y),q(n,x,y)\rangle \tag{4.17}$$

is a solution of the discrete 2+1 dimensional Burgers equation (1.6).

Proposition 4.5:

$$\mathrm{d}f_{\mathcal{S}}(p,q):\quad I\nabla H_m\to X_m. \tag{4.18}$$

Proof:

$$X_m=\frac{\mathrm{d}a}{\mathrm{d}\tau_m}=\mathrm{d}f_{\mathcal{S}}(p,q)\left[\frac{\mathrm{d}}{\mathrm{d}\tau_m}\begin{pmatrix}p\\q\end{pmatrix}\right]=\mathrm{d}f_{\mathcal{S}}[I\nabla H_m].$$

Decomposition diagram: discrete $\mathcal{S}$ flow / continuous H_m flow → KvM flow X_m. (4.19)

V. STRAIGHTENING OUT OF THE CONTINUOUS H_k-FLOW

In later analysis, especially in the construction of the algebraic curve Γ, it is indispensable to consider the analytic dependence upon $\zeta=\lambda^2$, rather than λ. Note that $F_\lambda,\lambda^{-1}V_\lambda^{12},\lambda^{-1}V_\lambda^{21}$ are rational functions of $\zeta=\lambda^2$ with simple poles at $\zeta=\alpha_j^2$, which are factorized as:

$$F_\lambda = -V_\lambda^{12}V_\lambda^{21} - (V_\lambda^{11})^2 = \frac{-\zeta\beta(\zeta)}{\alpha(\zeta)} = \frac{-R(\zeta)}{\alpha^2(\zeta)}, \tag{5.1}$$

$$V_\lambda^{12} = 2\lambda[\langle p,q\rangle + Q_\zeta(Ap,p)] = 2\lambda\langle p,q\rangle\frac{m(\zeta)}{\alpha(\zeta)}, \tag{5.2}$$

$$V_\lambda^{21} = -2\lambda[1 + Q_\zeta(Aq,q)] = -2\lambda\frac{n(\zeta)}{\alpha(\zeta)}, \tag{5.3}$$

where

$$\alpha(\zeta) = \prod_{j=1}^{N}(\zeta - \alpha_j^2), \quad \beta(\zeta) = \prod_{j=1}^{N+1}(\zeta - \beta_j^2),$$

$$R(\zeta) = \zeta\alpha(\zeta)\beta(\zeta) = \zeta\prod_{j=1}^{2N+1}(\zeta - \zeta_j), \tag{5.4}$$

$$m(\zeta) = \prod_{j=1}^{N}(\zeta - \gamma_j), \quad n(\zeta) = \prod_{j=1}^{N}(\zeta - \varepsilon_j).$$

with $\zeta_j = \alpha_j^2, j = 1,\ldots,N; \zeta_{N+j} = \beta_j^2, j = 1,\ldots,N+1$. $\{\gamma_j\}$ and $\{\varepsilon_j\}$ are called elliptic coordinates.

Note: $m(\zeta)$ and $n(\zeta)$ are polynomials of ζ, while m and n are indices. The shortage of letters causes the abuse of symbols. There will be no confusion since $m(\zeta)$ and $n(\zeta)$ are used temporarily and do not appear in the final results of this section.

Proposition 5.1:

$$\frac{\langle Ap,p\rangle}{\langle p,q\rangle} = \sum_{j=1}^{N}(\alpha_j^2 - \gamma_j), \quad \langle Aq,q\rangle = \sum_{j=1}^{N}(\alpha_j^2 - \epsilon_j), \tag{5.5}$$

$$\partial_x \ln a(n-1) = \sum_{j=1}^{N}(\gamma_j(n) - \epsilon_j(n)). \tag{5.6}$$

Proof: The first asymptotic terms of Eqs. (5.2) and (5.3) give rise to Eq. (5.5). By Eq. (4.11), the canonical system of the H_0-flow is

$$\begin{aligned} p_x &= (-A^2 + \langle Aq,q\rangle - 2\langle p,q\rangle)p + 2\langle p,q\rangle Aq, \\ q_x &= (A^2 - \langle Aq,q\rangle + 2\langle p,q\rangle)q - 2Ap. \end{aligned} \tag{5.7}$$

Thus

$$\langle p,q\rangle_x = 2\langle p,q\rangle\langle Aq,q\rangle - 2\langle Ap,p\rangle,$$

$$\partial_x \ln a^2(n-1) = \partial_x \ln\langle p,q\rangle = 2\langle Aq,q\rangle - 2\frac{\langle Ap,p\rangle}{\langle p,q\rangle} = 2\sum_{j=1}^{N}(\gamma_j - \epsilon_j).$$

The calculation of the evolution of the elliptic coordinates along the F_λ-flow is based on the components of the Lax equation (3.18):

$$\frac{\mathrm{d}}{\mathrm{d}t_\lambda} V_\mu^{12} = -2W_{\lambda\mu}^{12}V_\mu^{11} + 2W_{\lambda\mu}^{11}V_\mu^{12},$$

$$\frac{\mathrm{d}}{\mathrm{d}t_\lambda} V_\mu^{21} = 2W_{\lambda\mu}^{21}V_\mu^{11} - 2W_{\lambda\mu}^{11}V_\mu^{21},$$

and (5.1) with $\zeta=\gamma_k$ and ε_k, respectively:

$$V_\lambda^{11}|_{\zeta=\gamma_k} = \frac{[R(\gamma_k)]^{1/2}}{\alpha(\gamma_k)}, \quad V_\lambda^{11}|_{\zeta=\epsilon_k} = \frac{[R(\epsilon_k)]^{1/2}}{\alpha(\epsilon_k)}.$$

Differentiate Eqs. (5.2) and (5.3) with respect to t_λ, and let $\zeta=\gamma_k$ and ϵ_k, respectively. Then we have

$$\begin{aligned}\frac{1}{2\sqrt{R(\gamma_k)}}\frac{\mathrm{d}\gamma_k}{\mathrm{d}t_\lambda} &= -\frac{4\zeta m(\zeta)}{\alpha(\zeta)(\zeta-\gamma_k)m'(\gamma_k)},\\ \frac{1}{2\sqrt{R(\epsilon_k)}}\frac{d\epsilon_k}{\mathrm{d}t_\lambda} &= \frac{4\zeta n(\zeta)}{\alpha(\zeta)(\zeta-\epsilon_k)n'(\epsilon_k)}.\end{aligned} \tag{5.8}$$

Resorting to the interpolation formula, we have ($j=1,2,\ldots,N$)

$$\begin{aligned}\sum_{k=1}^{N}\frac{\gamma_k^{N-j}}{2\sqrt{R(\gamma_k)}}\frac{\mathrm{d}\gamma_k}{\mathrm{d}t_\lambda} &= -\frac{4\zeta^{N-j+1}}{\alpha(\zeta)},\\ \sum_{k=1}^{N}\frac{\epsilon_k^{N-j}}{2\sqrt{R(\varepsilon_k)}}\frac{\mathrm{d}\epsilon_k}{\mathrm{d}t_\lambda} &= \frac{4\zeta^{N-j+1}}{\alpha(\zeta)}.\end{aligned} \tag{5.9}$$

These formulas lead naturally to the consideration of the elliptic curve Γ given by the affine equation, $\xi^2 - R(\zeta) = 0$. The genus is $g=N$ since $\deg R = 2N+2$. Denote $P(\zeta) = (\zeta, \xi = \sqrt{R(\zeta)})$. The usual holomorphic differentials on Γ:

$$\tilde{\omega}_j = \frac{\zeta^{g-j}\,\mathrm{d}\zeta}{2\sqrt{R(\zeta)}}, \quad j=1,\ldots,g \tag{5.10}$$

imply the introduction of the quasi-Abel–Jacobi coordinates:

$$\tilde{\phi}_j = \sum_{P\in D_1}\int_{P_0}^{P}\tilde{\omega}_j, \quad \tilde{\psi}_j = \sum_{P\in D_2}\int_{P_0}^{P}\tilde{\omega}_j, \tag{5.11}$$

with fixed point $P_0\in\Gamma$ and the divisors: $D_1 = \Sigma_1^g P(\gamma_k)$, $D_2 = \Sigma_1^g P(\epsilon_k)$, which make Eq. (5.9) very simple:

$$\frac{\mathrm{d}\tilde{\phi}_j}{\mathrm{d}t_\lambda}=-\frac{4\zeta^{g-j+1}}{\alpha(\zeta)},\quad \frac{\mathrm{d}\tilde{\psi}_j}{\mathrm{d}t_\lambda}=\frac{4\zeta^{g-j+1}}{\alpha(\zeta)}. \tag{5.12}$$

Hence

$$\frac{\mathrm{d}\tilde{\phi}_j}{\mathrm{d}\tau_\lambda}=\frac{\zeta^{g-j}}{\sqrt{R(\zeta)}},\quad \frac{\mathrm{d}\tilde{\psi}_j}{\mathrm{d}\tau_\lambda}=-\frac{\zeta^{g-j}}{\sqrt{R(\zeta)}} \tag{5.13}$$

by (4.14), (4.8), and (5.1).

The Abel–Jacobi coordinates are obtained through some normalization. Let $a_1,b_1,\ldots,a_g,b_g$ be the canonical basis of the homology group of cycles on Γ, and $C=(A_{jk})_{g\times g}^{-1}$, where A_{jk} is equal to the integral of $\tilde{\omega}_j$ along the path a_k. Then we have the normalized holomorphic differential $\omega=C\tilde{\omega}$ with the following properties:

$$\int_{a_k}\omega_j=\delta_{jk},\quad \int_{b_k}\omega_j=B_{jk}, \tag{5.14}$$

where the matrix $B=(B_{jk})$ is symmetric and has positively definite imaginary part and is used to construct the Riemann theta function of Γ.[16,17,40,41] The Abel map is defined as

$$\mathcal{A}(P)=\int_{P_0}^{P}\omega$$

and is extended linearly to the whole divisor group of Γ, $\mathcal{A}$: $\mathrm{Div}(\Gamma)\to\mathcal{J}(\Gamma)=\mathbb{C}^g/\mathcal{T}$, where the lattice $\mathcal{T}$ is spanned by the periodic vectors $\{\delta_k,B_k\}$ with components given by Eq. (5.14). The Abel–Jacobi coordinates are defined as

$$\phi=\mathcal{A}(D_1)=C\tilde{\phi},\quad \psi=\mathcal{A}(D_2)=C\tilde{\psi}. \tag{5.15}$$

Theorem 5.2 (Straightening out of the continuous flow): The H_k-flow is straightened out by the Abel–Jacobi coordinates:

$$\frac{\mathrm{d}\phi}{\mathrm{d}\tau_k}=\Omega_k,\quad \frac{\mathrm{d}\psi}{\mathrm{d}\tau_k}=-\Omega_k, \tag{5.16}$$

where the angular speed Ω_k is determined as the coefficient in the asymptotic expansion of the normalized holomorphic differential ω at infinities $\infty_s(s=1,2)$ with $z=\zeta^{-1}$:

$$\omega=\frac{1}{2}(-1)^{s-1}\sum_{k=0}^{\infty}\Omega_k z^k\,\mathrm{d}z. \tag{5.17}$$

The proof is completed with the help of the following lemmas, which also give the algorithm to calculate Ω_k.

Lemma 5.3: Let $S_k=\zeta_1^k+\cdots+\zeta_{2g+1}^k$. Then the coefficients in

$$\frac{\zeta^{g+1}}{\sqrt{R(\zeta)}}=\sum_{k=0}^{\infty}\Lambda_k\zeta^{-k} \tag{5.18}$$

are determined by the recursive formula

$$\Lambda_0=1,\quad \Lambda_1=\tfrac{1}{2}S_1,$$
$$\Lambda_k=\frac{1}{2k}\left(S_k+\sum_{\substack{i+j=k\\ i,j\geqslant 1}} S_i\Lambda_j\right). \tag{5.19}$$

Lemma 5.4: Let $C_1,\ldots,C_g$ be the column vectors of C. Then the coefficients in

$$\frac{\zeta^{g+1}}{\sqrt{R(\zeta)}}(C_1\zeta^{-1}+\cdots+C_g\zeta^{-g})=\sum_{k=0}^{\infty}\Omega_k\zeta^{-k-1} \tag{5.20}$$

are written as

$$\Omega_k=\Lambda_kC_1+\Lambda_{k-1}C_2+\cdots+\Lambda_1C_k \tag{5.21}$$

with supplementary defined $\Lambda_{-s}=0$, $s=1,2,\ldots$. Specifically:

$$\Omega_0=C_1,\quad \Omega_1=\Lambda_1C_1+C_2,\quad \Omega_2=\Lambda_2C_1+\Lambda_1C_2+C_3. \tag{5.22}$$

Proof of theorem 5.2:

$$\frac{\mathrm{d}\phi}{\mathrm{d}\tau_\lambda}=C\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}\tau_\lambda}=\left(C_1\frac{\mathrm{d}\tilde{\phi}_1}{\mathrm{d}\tau_\lambda}+\cdots+C_g\frac{\mathrm{d}\tilde{\phi}_g}{\mathrm{d}\tau_\lambda}\right)=(C_1\zeta^{-1}+\cdots+C_g\zeta^{-g})\frac{\zeta^g}{\sqrt{R(\zeta)}}=\sum_{k=0}^{\infty}\Omega_k\zeta^{-k-2},$$

$$\frac{\mathrm{d}\phi}{\mathrm{d}\tau_\lambda}=(\phi,H_\lambda)=\sum_{k=0}^{\infty}(\phi,H_k)\zeta^{-k-2}.$$

Hence $(\phi,H_k)=\Omega_k$. The second equation of (5.16) is obtained similarly. Note that for the same ζ there are two corresponding points $P(\zeta)=(\zeta,\sqrt{R(\zeta)})$ and $P^-(\zeta)=(\zeta,-\sqrt{R(\zeta)})$ on the upper and lower sheets of Γ, respectively. Thus in the local coordinate $z=\zeta^{-1}$ near the infinities $\infty_s(s=1,2)$, we have

$$\omega=C\tilde{\omega}=C_1\tilde{\omega}_1+\cdots+C_g\tilde{\omega}_g=(C_1\zeta^{-1}+\cdots+C_g\zeta^{-g})\frac{\zeta^g\,\mathrm{d}\zeta}{2[R(\zeta)]^{1/2}}$$

$$=\frac{1}{2}(-1)^s\sum_{k=0}^{\infty}\Omega_k\zeta^{-k-2}\,\mathrm{d}\zeta=\frac{1}{2}(-1)^{s-1}\sum_{k=0}^{\infty}\Omega_kz^k\,\mathrm{d}z.$$

Note: It is in this section (and only in this section) that a_k and B_k are used to designate the cycle and periodic vector, respectively. In other sections, they have different meaning. There is some abuse of letters, but no confusion.

VI. STRAIGHTENING OUT OF THE DISCRETE FLOW $\mathcal{S}^n$

In the present section p and q are designated as scalars, not N dimensional vectors. It would not cause any confusion since no p,q are contained in the final results of this section. Consider the discrete eigenvalue problem

$$\chi(n+1)=U_n\chi(n),\quad U_n=\frac{1}{a(n)}\begin{pmatrix}0 & a^2(n)\\ -1 & \lambda\end{pmatrix}. \tag{6.1}$$

with $\chi(n)=(p(n),q(n))^T$. The fundamental solution matrix

$$M(n)=(\chi^{(1)}(n),\chi^{(2)}(n))=\begin{pmatrix} p^{(1)}(n) & p^{(2)}(n) \\ q^{(1)}(n) & q^{(2)}(n) \end{pmatrix}, \quad M(0)=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

has an explicit expression:

$$M(n+1)=U_nU_{n-1}\cdots U_0. \tag{6.2}$$

Denote $a_k=a(k)$ for short. By mathematical induction, we have

$$M(1)=\frac{1}{a_0}\begin{pmatrix} 0 & a_0^2 \\ -1 & \lambda \end{pmatrix}, \quad M(2)=\frac{1}{a_0a_1}\begin{pmatrix} -a_1^2 & a_1^2\lambda \\ -\lambda & \lambda^2-a_0^2 \end{pmatrix},$$

$$M(3)=\frac{1}{a_0a_1a_2}\begin{pmatrix} -a_2^2\lambda & a_2^2\lambda^2-a_0^2a_2^2 \\ -\lambda^2+a_1^2 & \lambda^3-(a_0^2+a_1^2)\lambda \end{pmatrix},$$

$$M(4)=\frac{1}{a_0a_1a_2a_3}\begin{pmatrix} -a_3^2\lambda^2+a_1^2a_3^2 & a_3^2\lambda^3-(a_0^2+a_1^2)a_3^2\lambda \\ -\lambda^3+(a_1^2+a_2^2)\lambda & \lambda^4-(a_0^2+a_1^2+a_2^2)\lambda^2+a_0^2a_2^2 \end{pmatrix},$$

$$p^{(1)}(n)=\frac{-a(n-1)}{a(0)\cdots a(n-2)}\left\{\lambda^{n-2}-\left[\sum_{j=1}^{n-3}a^2(j)\right]\lambda^{n-4}+\cdots\right\}, \tag{6.3}$$

$$p^{(2)}(n)=\frac{a(n-1)}{a(0)\cdots a(n-2)}\left\{\lambda^{n-1}-\left[\sum_{j=0}^{n-3}a^2(j)\right]\lambda^{n-3}+\cdots\right\},$$

$$q^{(1)}(n)=\frac{-1}{a(0)\cdots a(n-1)}\left\{\lambda^{n-1}-\left[\sum_{j=1}^{n-2}a^2(j)\right]\lambda^{n-3}+\cdots\right\},$$

$$q^{(2)}(n)=\frac{1}{a(0)\cdots a(n-1)}\left\{\lambda^{n}-\left[\sum_{j=0}^{n-2}a^2(j)\right]\lambda^{n-2}+\cdots\right\}.$$

Lemma 6.1: The following functions are polynomials of $\zeta=\lambda^2$ with degrees as tabled:

$\lambda^{-1}p^{(1)}(2k-1)$	$k-2$	$p^{(1)}(2k)$	$k-1$
$p^{(2)}(2k-1)$	$k-1$	$\lambda^{-1}p^{(2)}(2k)$	$k-1$
$q^{(1)}(2k-1)$	$k-1$	$\lambda^{-1}q^{(1)}(2k)$	$k-1$
$\lambda^{-1}q^{(2)}(2k-1)$	$k-1$	$q^{(2)}(2k)$	k

The discrete commutative equation (3.11) satisfied by the Lax matrix V_λ is the key to straightening out the discrete flow generated by the symplectic map $\mathcal{S}$. It implies that the solution space of the linear equation (6.1): $E\chi=U\chi$ is invariant under the action of V_λ. Let ρ and χ be the eigenvalue and eigenfunction, respectively, of the linear operator V_λ in the solution space. Then they satisfy:

$$E\chi=U\chi, \quad V_\lambda\chi=\rho\chi. \tag{6.4}$$

Evidently $\det|\rho-V_\lambda|=\rho^2+F_\lambda=0$, which yields the algebraic curve Γ used in Sec. V. There are two eigenvalues $\rho^\pm=\pm\rho$, whereby Eqs. (5.1), (4.7), and (4.8):

$$\rho=\lambda^2(1+2H_\lambda)=\frac{[R(\zeta)]^{1/2}}{\alpha(\zeta)}. \tag{6.5}$$

Proposition 6.2: The eigenvalue ρ of the Lax matrix V_λ is the generating function of the conserved integrals $\{H_m\}$ of the symplectic map $\mathcal{S}$.

The eigenfunction of the Lax matrix V_λ is called the Baker function after some kind of normalization. It could be taken as

$$\chi^{\pm}(n)=c^{\pm}\chi^{(1)}(n)+\chi^{(2)}(n), \tag{6.6}$$

where

$$c^{\pm}=\frac{V_\lambda^{11}(0)\pm\rho}{V_\lambda^{21}(0)}=\frac{-V_\lambda^{12}(0)}{V_\lambda^{11}(0)\mp\rho}. \tag{6.7}$$

The proof is based on the equation

$$0=(V_\lambda(n)\mp\rho)\chi^{\pm}(n)=(V_\lambda(n)\mp\rho)M(n)\begin{pmatrix} c^{\pm} \\ 1 \end{pmatrix},$$

which yields Eq. (6.7) after letting $n=0$. There is a wonderful relation between the elliptic coordinates and the Baker function.

Proposition 6.3 (formula of Dubrovin–Novikov type): Let $q^{\pm}(n,\lambda)$ be the second component of the Baker function $\chi^{\pm}(n,\lambda)$. Then

$$q^{+}(n,\lambda)q^{-}(n,\lambda)=\frac{V_\lambda^{21}(n)}{V_\lambda^{21}(0)}=\prod_{j=1}^{N}\frac{\lambda^2-\epsilon_j(n)}{\lambda^2-\epsilon_j(0)}. \tag{6.8}$$

Proof: Resorting to Eqs. (3.11) and (6.2), we have

$$V_\lambda(n)M(n)=M(n)V_\lambda(0), \tag{6.9}$$

which serves as the main tool in the direct calculation to derive Eq. (6.8).

Proposition 6.4: For $\lambda\to\infty$,

$$q^{+}(n,\lambda)=\frac{\lambda^n}{a(0)\cdots a(n-1)}[1+O(\lambda^{-2})], \tag{6.10}$$

$$q^{-}(n,\lambda)=a(0)\cdots a(n-1)\lambda^{-n}[1+O(\lambda^{-2})]. \tag{6.11}$$

Proof: By Eqs. (3.13), (6.5), and (5.3), we have

$$V_\lambda^{11}=-\lambda^2-2\lambda^2Q_\zeta(p,q)=-\lambda^2-2\langle p,q\rangle+O(\lambda^{-2}), \tag{6.12}$$

$$\rho=\lambda^2+2\lambda^2H_\lambda=\lambda^2+O(\lambda^{-2}),\quad V_\lambda^{21}(0)=-2\lambda+O(\lambda^{-1}). \tag{6.13}$$

Substituting into Eq. (6.7), we get

$$c^{+}=\langle p,q\rangle\lambda^{-1}+O(\lambda^{-3}),\quad c^{-}=\lambda+O(\lambda^{-1}). \tag{6.14}$$

Put this and Eq. (6.3) into $q^{+}=c^{+}q^{(1)}+q^{(2)}$, and we have Eq. (6.10). The estimation Eq. (6.11) for q^{-} is obtained from Eq. (6.10) and $q^{+}q^{-}=1+O(\lambda^{-2})$, which is a corollary of the Dubrovin–Novikov formula (6.8).

According to Eqs. (5.2), (5.3), (6.12), and (6.3), λc^{+} and λc^{-} are analytic functions of ζ, which can be regarded as the values of the single-valued function $[\lambda c](P)$ on the upper and lower sheets of Γ. Furthermore, resorting to Lemma 6.1 and the following expressions:

$$q^{\pm}(2k,\lambda)=(\lambda c^{\pm})\left\{\frac{1}{\lambda}q^{(1)}(2k,\lambda)\right\}+q^{(2)}(2k,\lambda),$$

$$\lambda q^{\pm}(2k-1,\lambda)=(\lambda c^{\pm})q^{(1)}(2k-1,\lambda)+\zeta\left\{\frac{1}{\lambda}q^{(2)}(2k-1,\lambda)\right\},$$

we have two meromorphic functions on Γ: $q(2k,P)$ and $[\lambda q](2k-1,P)$.

In the local coordinates $z=\zeta^{-1},\hat{\xi}=\zeta^{-N-1}\xi$, the equation of Γ near infinity is written as

$$\hat{\xi}^2-R_*(z)=0,\quad R_*=\prod_{j=1}^{2N+1}(1-\zeta_j z). \tag{6.15}$$

There are two infinities $\infty_s=(z=0,\hat{\xi}=(-1)^s)$, $s=1,2$, located on the upper ($s=2$) and lower ($s=1$) sheets, respectively. By Proposition 6.4, the principal asymptotic terms of $q(2k,P)$ near ∞_2 and ∞_1 are

$$\frac{z^{-k}}{a(0)\cdots a(2k-1)},\quad a(0)\cdots a(2k-1)z^k,$$

respectively, while those of $[\lambda q](2k-1,P)$ are

$$\frac{z^{-k}}{a(0)\cdots a(2k-2)},\quad a(0)\cdots a(2k-2)z^{k-1},$$

respectively. Based on the Dubrovin-Novikov formula (6.8) and through an elementary analysis, we have

Proposition 6.5: The Baker function $q(2k,P)$ has

(i) g simple poles at $\epsilon_1(0),\ldots,\epsilon_g(0)$ and a pole of kth order at ∞_2;

(ii) g simple zeros at $\epsilon_1(2k),\ldots,\epsilon_g(2k)$ and a zero of the kth order at ∞_1. The Baker function $[\lambda q](2k-1,P)$ has

(i) g simple poles at $\epsilon_1(0),\ldots,\epsilon_g(0)$ and a pole of kth order at ∞_2;

(ii) $g+1$ simple zeros at $0,\epsilon_1(2k-1),\ldots,\epsilon_g(2k-1)$ and a zero of the $(k-1)$th order at ∞_1.

Note: In the above-given expressions, we use ϵ_j, instead of $(\epsilon_j,\sqrt{R(\epsilon_j)})$, for short.

Theorem 6.6 (Straightening out of the discrete flow):

$$\psi(2k)-\psi(0)\equiv k\Omega_{\mathcal{S}}\pmod{\mathcal{T}}, \tag{6.16}$$

$$\psi(2k-1)-\psi(0)\equiv k\Omega_{\mathcal{S}}-\eta_1\pmod{\mathcal{T}}, \tag{6.17}$$

or

$$\psi(n)-\psi(0)\equiv\frac{n}{2}\Omega_{\mathcal{S}}+\frac{(-1)^n-1}{4}(\eta_1+\eta_2),\pmod{\mathcal{T}}, \tag{6.18}$$

where $\mathcal{T}$ is the lattice spanned by the periodic vectors and

$$\Omega_{\mathcal{S}}=\int_{\infty_1}^{\infty_2}\omega,\quad \eta_s=\int_{\infty_s}^{P_0}\omega,\quad (s=1,2), \tag{6.19}$$

with $P_0=(0,\sqrt{R(0)})$.

Proof: For $n=2k$, consider the meromorphic differential on Γ:

$$\omega_{\mathcal{S}}(2k)=\left\{\frac{\mathrm{d}}{\mathrm{d}\zeta}\ln q(2k,P)\right\}\mathrm{d}\zeta \tag{6.20}$$

with the residue $-1,1$ at $\epsilon_j(0),\epsilon_j(2k)$, respectively, and the residue $-k,k$ at ∞_2,∞_1, respectively. Expand Eq. (6.20) as a linear combination[13,40]

$$\omega_{\mathcal{S}}(2k)=\Omega+k\omega[\infty_1,\infty_2]+\sum_{j=1}^{g}\omega[\epsilon_j(2k),\epsilon_j(0)]+\sum_{j=1}^{g}e_j\omega_j, \tag{6.21}$$

where ω_j is the normalized Abel differential of the first kind given by Eq. (5.14), Ω is the Abel differential of the second kind, and $\omega(P,Q)$ is the Abel differential of the third kind with the residue $1,-1$ at P,Q, respectively, and the properties

$$\int_{a_j}\omega(P,Q)=0,\quad \int_{b_j}\omega(P,Q)=2\pi\sqrt{-1}\int_{Q}^{P}\omega_j.$$

Integrating (6.21) along a_i and b_i, we have

$$\sum_{j=1}^{g}\int_{\epsilon_j(0)}^{\epsilon_j(2k)}\omega=k\int_{\infty_1}^{\infty_2}\omega+\sum_{j=1}^{g}(n_jB_j+m_j\delta_j),$$

for some integers n_j,m_j. This completes the proof of Eq. (6.16).

For $n=2k-1$, consider the meromorphic differential

$$\begin{aligned}\omega_{\mathcal{S}}(2k-1)&=\left\{\frac{\mathrm{d}}{\mathrm{d}\zeta}\ln[\lambda q](2k-1,P)\right\}\mathrm{d}\zeta=\Omega+(k-1)\omega[\infty_1,\infty_2]+\omega[0,\infty_2]\\&\quad+\sum_{j=1}^{g}\omega[\epsilon_j(2k-1),\epsilon_j(0)]+\sum_{j=1}^{g}e_j\omega_j.\end{aligned} \tag{6.22}$$

Similar treatments lead to the proof of Eq. (6.17).

In order to investigate the evolution of anther Abel–Jacobi coordinate ϕ along the discrete flow generated by the symplectic map $\mathcal{S}$, consider the Baker function with the following normalization:

$$\begin{aligned}p^{\pm}(n,\lambda)&=p^{(1)}(n,\lambda)+d^{\pm}p^{(2)}(n,\lambda),\\d^{\pm}&=(c^{\pm})^{-1}=-\frac{V_\lambda^{11}(0)\mp\rho}{V_\lambda^{12}(0)}.\end{aligned} \tag{6.23}$$

In a similar way, we have:

Proposition 6.7:

$$p^{+}(n,\lambda)p^{-}(n,\lambda)=\frac{V_\lambda^{12}(n)}{V_\lambda^{12}(0)}=\prod_{j=1}^{g}\frac{\zeta-\gamma_j(n)}{\zeta-\gamma_j(0)}, \tag{6.24}$$

$$\begin{aligned}p^{+}(n,\lambda)&=\frac{a(n-1)\lambda^n}{\langle p,q\rangle a(0)\cdots a(n-2)}[1+O(\lambda^{-2})],\\p^{-}(n,\lambda)&=\frac{\langle p,q\rangle a(0)\cdots a(n-2)\lambda^{-n}}{a(n-1)}[1+O(\lambda^{-2})].\end{aligned} \tag{6.25}$$

The functions $p(2k,P)$ and $[\lambda p](2k-1,P)$ are defined similarly, by which we construct the meromorphic differentials

$$\omega_{\mathcal{S}}(2k)=\left\{\frac{\mathrm{d}}{\mathrm{d}\zeta}\ln p(2k,P)\right\}\mathrm{d}\zeta, \tag{6.26}$$

$$\omega_{\mathcal{S}}(2k-1)=\left\{\frac{\mathrm{d}}{\mathrm{d}\zeta}\ln[\lambda p](2k-1,P)\right\}\mathrm{d}\zeta. \tag{6.27}$$

$\omega_{\mathcal{S}}(2k)$ has the residue $k,-k,1,-1$, at $\infty_1,\infty_2,\gamma_j(2k),\gamma_j(0)$, respectively, while $\omega_{\mathcal{S}}(2k-1)$ has the residue $k-1,-k,1,1,-1$, at $\infty_1,\infty_2,0,\gamma_j(2k-1),\gamma_j(0)$, respectively. Having these preparations, finally we obtain:

Theorem 6.8 (Straightening out of the discrete flow):

$$\phi(2k)-\phi(0)\equiv k\Omega_{\mathcal{S}},\quad (\mathrm{mod}\,\mathcal{T}), \tag{6.28}$$

$$\phi(2k-1)-\phi(0)\equiv k\Omega_{\mathcal{S}}-\eta_1,\quad (\mathrm{mod}\,\mathcal{T}), \tag{6.29}$$

or

$$\phi(n)-\phi(0)\equiv\frac{n}{2}\Omega_{\mathcal{S}}+\frac{(-1)^n-1}{4}(\eta_1+\eta_2),\quad (\mathrm{mod}\,\mathcal{T}). \tag{6.30}$$

Now we have a clear evolution picture of the continuous H_m-flows and discrete $\mathcal{S}$-flow in the ''window'' of the Abel–Jacobi coordinates: (i) they are straightened out and have uniform velocities; (ii) they commute each other. Therefore, the compatible solution of various flow is obtained simply through a linear superposition. Specifically, for the KvM equation (2.11) with the label m we have

$$\begin{aligned}\phi(n,\tau_m)&=\frac{n}{2}\Omega_{\mathcal{S}}+\tau_m\Omega_m+\frac{(-1)^n-1}{4}(\eta_1+\eta_2)+\phi_0,\\ \psi(n,\tau_m)&=\frac{n}{2}\Omega_{\mathcal{S}}-\tau_m\Omega_m+\frac{(-1)^n-1}{4}(\eta_1+\eta_2)+\psi_0,\end{aligned} \tag{6.31}$$

based on the decomposition diagram (4.19). Moreover, for the 2+1 Burgers equation (1.6) with a discrete variable, we have

$$\begin{aligned}\phi(n,x,y)&=\frac{n}{2}\Omega_{\mathcal{S}}+x\Omega_0+y\Omega_1+\frac{(-1)^n-1}{4}(\eta_1+\eta_2)+\phi_0,\\ \psi(n,x,y)&=\frac{n}{2}\Omega_{\mathcal{S}}-x\Omega_m-y\Omega_1+\frac{(-1)^n-1}{4}(\eta_1+\eta_2)+\psi_0,\end{aligned} \tag{6.32}$$

based on the decomposition diagram (1.10).

VII. INVERSION. ALGEBRO-GEOMETRIC SOLUTION

Equation (6.32) gives the explicit solution of the 2+1 Burgers equation (1.6) with a discrete variable in the Abel–Jacobi coordinates (ϕ,ψ). In order to get the solution in the original coordinate B, the following steps should be completed:

$$(\phi,\psi)\to(\gamma_j,\epsilon_j)\to a\to B. \tag{7.1}$$

We have $B=a^2$ and

$$\partial_x \ln a(n)=\sum_{j=1}^{g}\left[\gamma_j(n+1)-\epsilon_j(n+1)\right] \tag{7.2}$$

by Eq. (5.6). To express $\Sigma\gamma_j$ and $\Sigma\epsilon_j$ by means of (ϕ,ψ), we use the Riemann theorem,[40,41] which asserts that there exist constant vectors K_1 and K_2 (the Riemann constants) such that $\theta(\mathcal{A}(P(\zeta))-\phi-K_1)$ has exactly g zeros: $\gamma_1,\ldots,\gamma_g$; and $\theta(\mathcal{A}(P(\zeta))-\psi-K_2)$ has exactly g zeros: $\epsilon_1,\ldots,\epsilon_g$ as well. Resorting to the asymptotic expansion (5.17) and through a standard treatment,[16,17] we obtain:

$$\sum_{j=1}^{g}\gamma_j=I_1(\Gamma)-\sum_{s=1}^{2}\operatorname*{Res}_{\infty_s}\zeta d\ln\theta(\mathcal{A}(P(\zeta))-\phi-K_1)=I_1(\Gamma)+\frac{1}{2}\sum_{j=1}^{g}\Omega_0^j\partial_j\ln\frac{\theta(\phi+K_1+\eta_1)}{\theta(\phi+K_1+\eta_2)}, \tag{7.3}$$

$$\sum_{j=1}^{g}\epsilon_j=I_1(\Gamma)-\sum_{s=1}^{2}\operatorname*{Res}_{\infty_s}\zeta d\ln\theta(\mathcal{A}(P(\zeta))-\psi-K_2)=I_1(\Gamma)-\frac{1}{2}\sum_{j=1}^{g}\Omega_0^j\partial_j\ln\frac{\theta(-\psi-K_2-\eta_1)}{\theta(-\psi-K_2-\eta_2)}, \tag{7.4}$$

where ∂_j denotes the differentiation with regard to the jth argument of the theta function and

$$I_k(\Gamma)=\sum_{j=1}^{g}\int_{a_j}\zeta^k\omega_j. \tag{7.5}$$

After these preparations, we transform the solution (6.32) into the original coordinate B through direct calculations.

Theorem 7.1: The $2+1$ dimensional Burgers equation with a discrete argument (1.6) has the quasiperiodic solution:

$$\begin{aligned}
&B(2k-1,x,y)\\
&=\frac{\theta[x\Omega_0+y\Omega_1+(k+1)\Omega_S+\phi_0+K_1+\eta_2]\theta[x\Omega_0+y\Omega_1-(k+1)\Omega_S-\psi_0-K_2-\eta_2]}{\theta[x\Omega_0+y\Omega_1+k\Omega_S+\phi_0+K_1+\eta_2]\theta[x\Omega_0+y\Omega_1-k\Omega_S-\psi_0-K_2-\eta_2]}\\
&\quad\cdot\frac{\theta[y\Omega_1+k\Omega_S+\phi_0+K_1+\eta_2]\theta[y\Omega_1-k\Omega_S-\psi_0-K_2-\eta_2]}{\theta[y\Omega_1+(k+1)\Omega_S+\phi_0+K_1+\eta_2]\theta[y\Omega_1-(k+1)\Omega_S-\psi_0-K_2-\eta_2]}B(2k-1,0,y),
\end{aligned} \tag{7.6}$$

$$\begin{aligned}
B(2k,x,y)&=\frac{\theta[x\Omega_0+y\Omega_1+(k+1)\Omega_S+\phi_0+K_1]\theta[x\Omega_0+y\Omega_1-(k+1)\Omega_S-\psi_0-K_2]}{\theta[x\Omega_0+y\Omega_1+k\Omega_S+\phi_0+K_1]\theta[x\Omega_0+y\Omega_1-k\Omega_S-\psi_0-K_2]}\\
&\quad\cdot\frac{\theta[y\Omega_1+k\Omega_S+\phi_0+K_1]\theta[y\Omega_1-k\Omega_S-\psi_0-K_2]}{\theta[y\Omega_1+(k+1)\Omega_S+\phi_0+K_1]\theta[y\Omega_1-(k+1)\Omega_S-\psi_0-K_2]}B(2k,0,y),
\end{aligned}$$

VIII. THE MODIFIED KADOMTSEV–PETVIASHVILI EQUATION

The canonical equations (5.7) of the Hamiltonian H_0 defined by Eq. (4.11) is put in the linear form

$$\begin{pmatrix}p_j\\q_j\end{pmatrix}_x=\hat{U}(u,v,\alpha_j)\begin{pmatrix}p_j\\q_j\end{pmatrix},\quad \hat{U}(u,v,\lambda)=\begin{pmatrix}-\lambda^2+u & -\lambda v\\ -2\lambda & \lambda^2-u\end{pmatrix} \tag{8.1}$$

with the nonlinearization condition (the Bargmann constraint):

$$\begin{pmatrix}u\\v\end{pmatrix}=\begin{pmatrix}\langle Aq,q\rangle-2\langle p,q\rangle\\ -2\langle p,q\rangle\end{pmatrix}\equiv f_C(p,q). \tag{8.2}$$

In a standard way, Eq. (8.1) leads to the 2+1 dimensional mKP equation (1.11) and its algebro-geometric solution, just as in the above-presented example of the 2+1 Burgers equation and in the previous examples of the KP equation[16,17] and the special 2+1 Toda equation.[17] The general structure and steps are basically the same, though with different features in various continuous and discrete models. We list the main steps and results without proof as follows.

Proposition 8.1 (The fundamental identity): Let $G=(G_1,G_2)^T$ be an arbitrary smooth function of x ($\partial=\partial/\partial_x$), and $\hat{\sigma}$ be a linear operator defined as

$$\hat{V}=\hat{\sigma}(u,v,\lambda)[G]=\{(\tfrac{1}{2}\partial+u-\lambda^2)G_2\}\sigma_1+\{\lambda(\tfrac{1}{2}\partial G_1-vG_2)\}\sigma_2+(-2\lambda G_2)\sigma_3. \tag{8.3}$$

Then

$$\hat{V}_x-[\hat{U},\hat{V}]=\hat{U}_*\{(\hat{K}-\lambda^2\hat{J})G\}, \tag{8.4}$$

where

$$\hat{K}=\begin{pmatrix} 0 & \frac{1}{2}\partial^2+\partial u \\ -\frac{1}{2}\partial^2+u\partial & v\partial+\partial v \end{pmatrix}, \quad \hat{J}=\begin{pmatrix} \partial & \partial \\ \partial & 0 \end{pmatrix}, \tag{8.5}$$

$$\hat{U}_*\begin{pmatrix} \delta u \\ \delta v \end{pmatrix}=\begin{pmatrix} \delta u & -\lambda\delta v \\ 0 & -\delta u \end{pmatrix}. \tag{8.6}$$

The Lenard gradients are defined recursively by $\hat{J}\hat{g}_m=\hat{K}\hat{g}_{m-1}$, with

$$\hat{g}_{-2}=\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \hat{g}_{-1}=\begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \hat{g}_0=\begin{pmatrix} v \\ u-v \end{pmatrix},$$

$$\hat{g}_1=\begin{pmatrix} -\frac{1}{2}v_x+2uv-\frac{3}{2}v^2 \\ \frac{1}{2}u_x+u^2-3uv+\frac{3}{2}v^2 \end{pmatrix}, \tag{8.7}$$

$$\hat{g}_2=\begin{pmatrix} \frac{1}{4}v_{xx}+\frac{3}{2}vv_x-\frac{3}{2}uv_x+3u^2v-6uv^2+\frac{5}{2}v^3 \\ \frac{1}{4}u_{xx}-\frac{1}{4}v_{xx}+\frac{3}{2}uu_x-\frac{3}{2}u_xv+u^3-6u^2v+\frac{15}{2}uv^2-\frac{5}{2}v^3 \end{pmatrix}, \quad \text{etc.}$$

with

$$\det\hat{\sigma}_\lambda[\hat{g}_\lambda]=-\lambda^4, \quad \hat{g}_\lambda=\hat{g}_{-1}+\sum_{k=0}^{\infty}\hat{g}_k\lambda^{-k-1}. \tag{8.8}$$

The associated soliton vector field is defined as $Y_j=J\hat{g}_j$ with

$$Y_0=\begin{pmatrix} u_x \\ v_x \end{pmatrix}, \quad Y_1=\begin{pmatrix} \partial(\frac{1}{2}u_x-\frac{1}{2}v_x+u^2-uv) \\ \partial(-\frac{1}{2}v_x+2uv-\frac{3}{2}v^2) \end{pmatrix},$$

$$Y_2=\begin{pmatrix} \partial(\frac{1}{4}u_{xx}+\frac{3}{2}(uu_x-u_xv-uv_x+vv_x)+u^3-3u^2v+\frac{3}{2}uv^2) \\ \partial(\frac{1}{4}v_{xx}+\frac{3}{2}(vv_x-uv_x)+3u^2v-6uv^2+\frac{5}{2}v^3) \end{pmatrix}. \tag{8.9}$$

Proposition 8.2: Let $(u(x,y,t),v(x,y,t))$ be the compatible solution of

$$\begin{pmatrix} u \\ v \end{pmatrix}_y = Y_1, \quad \begin{pmatrix} u \\ v \end{pmatrix}_t = Y_2. \tag{8.10}$$

Then $v(x,y,t)$ satisfies the $2+1$ dimensional mKP equation (1.11).

Let $(p_j, q_j)^T$ be the solution of Eq. (8.1). Then

$$\hat{\nabla}\alpha_j = \begin{pmatrix} \delta\alpha_j/\delta u \\ \delta\alpha_j/\delta v \end{pmatrix} = \begin{pmatrix} -2p_jq_j \\ \alpha_j q_j^2 \end{pmatrix}. \tag{8.11}$$

It is easy to see that Eq. (8.2) is equivalent with

$$\hat{g}_0 = \sum_{j=1}^{N} \hat{\nabla}\alpha_j. \tag{8.12}$$

The Lenard eigenvalue problem $(K-\alpha_j^2 J)G=0$ has the solution $\hat{\nabla}\alpha_j$, which is used to construct the solution of $(K-\lambda^2 J)G=0$ with general eigenparameter $\lambda^2=\zeta$;

$$\hat{G}_\lambda = \hat{g}_{-1} + \sum_{j=1}^{N} \frac{\hat{\nabla}\alpha_j}{\lambda^2-\alpha_j^2} = \begin{pmatrix} -2Q_\zeta(p,q) \\ 1+Q_\zeta(Aq,q) \end{pmatrix}, \tag{8.13}$$

under the Bargmann condition (8.2) or (8.12). By the fundamental identity (8.4), the commutator equation $\partial\hat{V}-[\hat{U},\hat{V}]=0$ has a solution

$$\hat{V}_\lambda = \hat{\sigma}[\hat{G}_\lambda] = \begin{pmatrix} -\lambda^2[1+2Q_\zeta(p,q)] & 2\lambda[\langle p,q\rangle + Q_\zeta(Ap,p)] \\ -2\lambda[1+2Q_\zeta(Aq,q)] & \lambda^2[1+2Q_\zeta(p,q)] \end{pmatrix}, \tag{8.14}$$

which coincides with the Lax matrix (3.13) of the KvM hierarchy: $\hat{V}_\lambda = V_\lambda$. Hence in the context of the soliton hierarchy $\{Y_m\}$, we again obtain the integrals $\{F_m\}$, generated as the coefficients of the asymptotic expansion of $F_\lambda = \det V_\lambda$. Again we have the integrals $\{H_m\}$ by Eqs. (4.7), (4.8), and (4.10). The present formalism enables us to establish the direct relation between $\{H_m\}$ and $\{Y_m\}$.

Proposition 8.3: (i) f_C defined by the Bargmann condition (8.2) maps the solution $(p(x),q(x))^T$ of the H_0-flow (5.7), or equivalently (8.1)+(8.2), into a solution of the stationary soliton equation

$$Y_N + \hat{c}_{N1}Y_{N-1} + \cdots + \hat{c}_{NN}Y_0 = 0. \tag{8.15}$$

(ii) Let $(p(x,\tau_m),q(x,\tau_m))^T$ be the compatible solution of the H_0- and the H_m-flows. Then $(u(x,\tau_m),v(x,\tau_m))^T = f_C(p,q)$ satisfies both Eq. (8.15) and

$$\frac{\mathrm{d}}{\mathrm{d}\tau_m}\begin{pmatrix} u \\ v \end{pmatrix} = Y_m. \tag{8.16}$$

Besides,

$$\mathrm{d}f_C(I\nabla H_m) = Y_m. \tag{8.17}$$

(iii) Let $(p(x,y,t),q(x,y,t))^T$ be the compatible solution of the H_0-, H_1-, and H_2-flow with the flow variables $x=\tau_0, y=\tau_1$, and $t=\tau_2$, respectively. Then

$$v(x,y,t) = -2\langle p(x,y,t), q(x,y,t)\rangle \tag{8.18}$$

is a solution of the mKP equation (1.11).

Graphically, for the decomposition of the mKP equation, we have diagram (1.12), and for the Y_m-flow, we have the diagram:

$$\begin{matrix} H_0 \\ H_m \end{matrix} \searrow \quad Y_m \tag{8.19}$$

Since there is no more discrete flow $\mathcal{S}$, which is a little more complicated since it splits into two series according to n even or odd, we have a rather simple evolution picture:

$$\begin{gathered} \left.\begin{matrix} \text{Bargmann} & \text{flow} \\ \text{stationary} & \text{flow} \end{matrix}\right\} \phi=\phi_0+x\Omega_0, \quad \psi=\psi_0-x\Omega_0, \\ H_m\text{-flow:} \quad \phi=\phi_0+\tau_m\Omega_m, \quad \psi=\psi_0-\tau_m\Omega_m, \\ Y_m\text{-flow:} \quad \phi=\phi_0+x\Omega_0+\tau_m\Omega_m, \quad \psi=\psi_0-x\Omega_0-\tau_m\Omega_m, \\ \text{mKP-flow:} \quad \phi=\phi_0+x\Omega_0+y\Omega_1+t\Omega_2, \quad \psi=\psi_0-x\Omega_0-y\Omega_1-t\Omega_2. \end{gathered} \tag{8.20}$$

The feature of linear superposition is clear. By Eqs. (5.5), (5.7), (8.3), and (8.4) we have

$$\partial_x \ln v=\frac{v_x}{v}=\frac{\langle p,q\rangle_x}{\langle p,q\rangle}=2\sum_{j=1}^{g}(\gamma_j-\epsilon_j)=\partial_x \ln\frac{\theta(\phi+K_1+\eta_1)\theta(-\psi-K_2-\eta_1)}{\theta(\phi+K_1+\eta_2)\theta(-\psi-K_2-\eta_2)}, \tag{8.21}$$

so long as ϕ and ψ contain the terms $x\Omega_0$ and $-x\Omega_0$, respectively. Thus we get:

Theorem 8.4: The modified Kadomtsev–Petviashvili equation (1.11) has the algebro-geometric solution:

$$\begin{aligned} v(x,y,t)=&\frac{\theta(x\Omega_0+y\Omega_1+t\Omega_2+\phi_0+K_1+\eta_1)\theta(x\Omega_0+y\Omega_1+t\Omega_2-\psi_0-K_2-\eta_1)}{\theta(x\Omega_0+y\Omega_1+t\Omega_2+\phi_0+K_1+\eta_2)\theta(x\Omega_0+y\Omega_1+t\Omega_2-\psi_0-K_2-\eta_2)} \\ &\cdot\frac{\theta(y\Omega_1+t\Omega_2+\phi_0+K_1+\eta_2)\theta(y\Omega_1+t\Omega_2-\psi_0-K_2-\eta_2)}{\theta(y\Omega_1+t\Omega_2+\phi_0+K_1+\eta_1)\theta(y\Omega_1+t\Omega_2-\psi_0-K_2-\eta_1)}v(0,y,t). \end{aligned} \tag{8.22}$$

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On the symplectic structures for geometrical theories

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We present a new approach for constructing covariant symplectic structures for geometrical theories, based on the concept of adjoint operators. Such geometric structures emerge by direct exterior derivation of underlying symplectic potentials. Differences and similarities with other approaches and future applications are discussed. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421636]

I. INTRODUCTION

Usually quantum field theories are studied by means of Feynman path integrals or by means of canonical quantization. Path integral quantization has the virtue to preserve all relevant symmetries, including Poincaré invariance; however, the resultant theory has not (unlike the canonical formalism) necessarily the standard interpretation in terms of quantum mechanical states and operators. On the other hand, the canonical formalism is considered to be the antithesis of a manifestly covariant treatment.

However, more recently, the essence of the canonical formulation has been developed independently by Witten *et al.*[1,2] and Suckerman[3] in such a way that manifestly preserves Poincaré invariance as well as other relevant symmetries. Such a formulation is based on a covariant description of Poisson brackets in terms of a symplectic structure defined on the manifold representing the phase space of classical solutions; thus, quantization is carried out as the replacement of Poisson brackets with commutators, and the resultant quantum theory will be of the conventional type. Specifically, the Witten *et al.* approach requires the construction, *a priori*, of a bilinear product on variations of classical solutions. Subsequently, one needs to verify that such a bilinear form corresponds to a nondegenerate closed two-form on the phase space. Moreover, the bilinear form must be a covariantly conserved current in its spacetime dependence, as required for obtaining a symplectic structure manifestly covariant. More specifically, in such a description, the classical phase space is defined as *the space of solutions of the classical equations of motion*: such a definition is manifestly covariant. The construction of a covariantly conserved two-form J^μ on such phase space yields a symplectic structure ω, defined as $\omega \equiv \int_\Sigma J^\mu \, d\Sigma_\mu$ (Σ being an initial value hypersurface), independent of the choice of Σ and, in particular, Poincaré invariant. Additionally, in terms of the symplectic structure ω, the fact that Poisson brackets satisfy the Jacoby identity, is equivalent that ω to be a closed two-form on the phase space, which holds if J^μ itself is closed. With these properties, J^μ is known as *the symplectic current*. Such a quantization scheme has been applied, for example, for the analysis of two-dimensional gravity (Ref. 4 and references therein), and for the investigation of the Wess–Zumino–Witten model on a circle.[5]

Although in the present article we shall obtain essentially the same geometric structures described above, the main novelty is that such structures emerge in a direct and natural way using the concept of adjoint operators. Particularly, the concept of self-adjoint operators shows that, in the cases considered here, there exist, in general, covariantly conserved currents, which correspond on the phase space, to zero-, one-, and, two-forms. Such differential forms are not independent, but that the two-form turns out to be the exterior derivative of the corresponding one-

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form, and correspond, thus, to an *exact* two-form (and automatically to a closed two-form, as required for the symplectic structure). In this manner, the present approach allows us to find, unlike the Witten–Zuckerman procedure, fundamental one-forms playing the role of *symplectic potentials* for the theory.

In the next section, we shall discuss the key concept of adjoint operators, and its consequences on the existence of covariantly conserved currents. The interpretation of the terms involved in such a definition as wedge products on the phase space is also discussed. In Sec. III only the non-Abelian gauge theories and pure general relativity are considered with the purpose of clarifying our basic ideas and to have a direct comparison with previously known results, particularly with those given in Ref. 2. In Sec. IV, we shall finish with some concluding remarks on our results and possible extensions of the present approach.

Concepts and definitions on differential forms, wedge products, exterior derivative, etc., come entirely from Ref. 2.

II. ADJOINT OPERATORS AND CONSERVED CURRENTS

The general relationship between adjoint operators and covariantly conserved currents has been already given in previous works (Ref. 6 and references cited therein), however, we shall discuss it in this section for completeness.

If $\mathcal{P}$ is a linear partial differential operator that takes matrix-valued tensor fields into themselves, then, the adjoint operator of $\mathcal{P}$, is that operator $\mathcal{P}^\dagger$, such that

$$\mathrm{Tr}\{f^{\rho\sigma\cdots}[\mathcal{P}(g_{\mu\nu\cdots})]_{\rho\sigma\cdots}-[\mathcal{P}^\dagger(f^{\rho\sigma\cdots})]^{\mu\nu\cdots}g_{\mu\nu\cdots}\}=\nabla_\mu J^\mu, \tag{1}$$

where Tr denotes the trace and J^μ is some vector field. From this definition, if $\mathcal{Q}$ and $\mathcal{R}$ are any two linear operators, one easily finds the following properties:

$$(\mathcal{QR})^\dagger=\mathcal{R}^\dagger\mathcal{Q}^\dagger, \quad (\mathcal{Q}+\mathcal{R})^\dagger=\mathcal{Q}^\dagger+\mathcal{R}^\dagger,$$

and in the case of a function F,

$$F^\dagger=F,$$

which will be used implicitly below.

From Eq. (1) we can see that this definition automatically guarantees that, if the field f is a solution of the linear system $\mathcal{P}(f)=0$, and g a solution of the adjoint system $\mathcal{P}^\dagger(g)=0$, then we obtain the continuity law $\nabla_\mu J^\mu=0$, which establishes that J^μ is a covariantly conserved current depending on the fields f and g. This fact means that for any homogeneous equation system, one can always construct a conserved current, taking into account the adjoint system. This general result contains the self-adjoint case ($\mathcal{P}^\dagger=\mathcal{P}$) as a particular one, for which f and g correspond to two independent solutions (in fact, the cases treated in the present article are self-adjoint). Although this result has been established assuming only tensor fields and the presence of a single equation, such a result can be extended in a direct way to equations involving spinor fields, matrix fields, and the presence of more than one field.[6,7]

Our main task in this work is to apply this very general result for the analysis of the symplectic forms on the phase space of the theories under consideration. Hence, it is important to clarify, in the first instance, what the fields f, g, J^μ and the differential operators $\mathcal{P}$, $\mathcal{P}^\dagger$, and ∇_μ will mean on the phase space at the level of Eq. (1). First, such operators will depend only on the background fields, and will correspond thus to zero-forms. Second, although in our previous works we have identified the fields f and g with solutions of the equations governing the first-order variations $[\mathcal{P}(f)=0=\mathcal{P}(g)]$, in the present work we shall see that it is possible to find simultaneously that $\mathcal{P}(G)=0$, where G is some background field. Thus, since the background fields and the first-order variations correspond, on the phase space, to zero-forms and one-forms, respectively,[2] the left-hand side of Eq. (1) must be understood as a wedge product, $\mathrm{Tr}\{f\wedge\mathcal{P}(g)$

$-\mathcal{P}^{\dagger}(f)\wedge g\}=\nabla_{\mu}J^{\mu}$, on such phase space, and something similar for the field J^{μ} in its dependence on the fields f and g. This subject will be clarified in the examples below.

III. GEOMETRICAL THEORIES AND THEIR SYMPLECTIC STRUCTURES

In this section we shall see that the problem of finding the symplectic structures (and in some cases the symplectic potentials), is reduced to identify some fields satisfying some homogeneous linear equations.

A. Yang–Mills theory

Let us consider first the Yang–Mills equations:

$$\partial\!\!\!/^{\mu}F_{\mu\nu}=0, \tag{2}$$

where $F_{\mu\nu}=\partial\!\!\!/_{\mu}A_{\nu}-\partial\!\!\!/_{\nu}A_{\mu}$ is the Yang–Mills curvature, A_{μ} the background gauge connection, and $\partial\!\!\!/_{\mu}\equiv\partial_{\mu}+[A_{\mu},\ \ ]$, the gauge covariant derivative.

From Eq. (2), the variations of the background fields are governed by the equations

$$\partial\!\!\!/^{\mu}\delta F_{\mu\nu}+[\delta A^{\mu},F_{\mu\nu}]=[\delta^{\alpha}_{\nu}\partial\!\!\!/^{\mu}\partial\!\!\!/_{\mu}-\partial\!\!\!/^{\alpha}\partial\!\!\!/_{\nu}]\delta A_{\alpha}+[\delta A_{\alpha},F^{\alpha}{}_{\nu}]\equiv[\mathcal{P}(\delta A_{\alpha})]_{\nu}=0, \tag{3}$$

where $\delta F_{\mu\nu}=\partial\!\!\!/_{\mu}\delta A_{\nu}-\partial\!\!\!/_{\nu}\delta A_{\mu}$, is the variation of the curvature, δA_{μ} the variation of the gauge connection, and the operator $\mathcal{P}$ is a homogeneous linear operator depending only on the background fields. Up to here, the usual equations for the Yang–Mills fields and their variations.

Now the idea is to apply our present approach for obtaining all on the symplectic structure for the theory, directly from the basic equations (2) and (3). For this purpose, let B_{μ} and C_{μ} be any two matrix-valued fields (which will be identified below as a pair of gauge connection variations in one case, and as the background gauge connection and its variation in the particular case of Abelian fields), and using the explicit form of the operator $\mathcal{P}$ in Eq. (3), we have that

$$\begin{aligned}B^{\nu}\wedge[\mathcal{P}(C_{\alpha})]_{\nu}-[\mathcal{P}(B^{\nu})]^{\alpha}\wedge C_{\alpha}=\partial\!\!\!/_{\mu}[B^{\nu}\wedge(\partial\!\!\!/^{\mu}C_{\nu}-\partial\!\!\!/_{\nu}C^{\mu})+(\partial\!\!\!/^{\nu}B^{\mu}-\partial\!\!\!/^{\mu}B^{\nu})\wedge C_{\nu}]\\ +[F_{\mu\nu},B^{\mu}\wedge C^{\nu}],\end{aligned} \tag{4}$$

where

$$B^{\nu}\wedge[C_{\alpha},F^{\alpha}{}_{\nu}]-[B_{\alpha},F^{\alpha}{}_{\nu}]\wedge C^{\nu}=[F_{\mu\nu},B^{\mu}\wedge C^{\nu}], \tag{5}$$

and identities of the form $B^{\nu}\wedge\partial\!\!\!/^{\alpha}\partial\!\!\!/_{\nu}C_{\alpha}\equiv\partial\!\!\!/_{\mu}(B^{\nu}\partial\!\!\!/_{\nu}C^{\mu}-\partial\!\!\!/^{\nu}B^{\mu}\wedge C_{\nu})+\partial\!\!\!/_{\nu}\partial\!\!\!/^{\alpha}B^{\nu}\wedge C_{\alpha}$ have been used. Taking the trace of Eq. (4), we obtain

$$\mathrm{Tr}[B^{\nu}\wedge[\mathcal{P}(C_{\alpha})]_{\nu}-[\mathcal{P}(B^{\nu})]^{\alpha}\wedge C_{\alpha}]=\partial_{\mu}\,\mathrm{Tr}[B_{\nu}\wedge\partial\!\!\!/^{[\mu}C^{\nu]}-\partial\!\!\!/^{[\mu}B^{\nu]}\wedge C_{\nu}], \tag{6}$$

which has the form of Eq. (1) with $\mathcal{P}=\mathcal{P}^{\dagger}$. Thus, we can obtain the continuity equation:

$$\partial_{\mu}J^{\mu}=0,\quad J^{\mu}\equiv\mathrm{Tr}[B_{\nu}\wedge\partial\!\!\!/^{[\mu}C^{\nu]}-\partial\!\!\!/^{[\mu}B^{\nu]}\wedge C_{\nu}], \tag{7}$$

provided that

$$[\mathcal{P}(C_{\alpha})]_{\nu}=0\quad\text{and}\quad[\mathcal{P}(B^{\nu})]^{\alpha}=0. \tag{8}$$

As we shall see, the whole physical information about the covariant symplectic structure of the Yang–Mills theory is contained in Eq. (7), it remains only to identify the fields B_{μ} and C_{μ} satisfying Eqs. (8). In according to Eq. (3), the obvious case is to choose such fields as a pair of variations, say $B_{\mu}=\delta A^{1}_{\mu}$, and $C_{\mu}=\delta A^{2}_{\mu}$ (they have not to correspond necessarily to the same variation). In this manner, J^{μ} in Eq. (7) corresponds, in this case, to the following (nondegenerate) two-form on the phase space:

$$J_\mu = \mathrm{Tr}[\,\delta A_1^\nu \wedge \delta F^2_{\mu\nu} - \delta F^1_{\mu\nu} \wedge \delta A_2^\nu] = \tfrac{1}{2}\delta\,\mathrm{Tr}[A_1^\nu\,\delta F^2_{\mu\nu} - F^2_{\mu\nu}\,\delta A_1^\nu - F^1_{\mu\nu}\,\delta A_2^\nu + A_2^\nu\,\delta F^1_{\mu\nu}] \equiv \delta\theta_\mu, \tag{9}$$

where $F^i_{\mu\nu} = \partial_\mu A^i_\nu - \partial_\nu A^i_\mu$, $\delta F^i_{\mu\nu} = \partial_\mu \delta A^i_\nu - \partial_\nu \delta A^i_\mu$ $(i=1,2)$, and we have used the Leibniz rule for the exterior derivative δ, and the fact that $\delta^2 = 0$. In particular, if $\delta A^1_\mu = \delta A_\mu = \delta A^2_\mu$, from Eq. (9) $J_\mu = 2\,\mathrm{Tr}(\delta A^\nu \wedge \delta F_{\mu\nu})$, which is essentially the Crncović–Witten current.[2] Furthermore, we have defined the one-form θ_μ as

$$\theta_\mu \equiv \tfrac{1}{2}\mathrm{Tr}[A_1^\nu\,\delta F^2_{\mu\nu} - F^2_{\mu\nu}\,\delta A_1^\nu - F^1_{\mu\nu}\,\delta A_2^\nu + A_2^\nu\,\delta F^1_{\mu\nu}], \tag{10}$$

in this manner, θ_μ is the *symplectic potential* for the theory. Note that, according to Eq. (9), the symplectic potential is defined up to the exterior derivative of any matrix-valued field λ_μ: $J_\mu = \delta(\theta_\mu + \delta\lambda_\mu)$.

In the particular case of Abelian fields, from Eqs. (2) and (3) we have that $[\mathcal{P}(A_\alpha)]_\nu = 0$, where A_α is the background gauge connection. In this manner, we can identify $B_\nu = \delta A^1_\nu$ and $C_\nu = A^2_\nu$ (a variation and a background gauge connection, respectively), and then the symplectic potential θ_μ given in Eq. (10) is [like the corresponding symplectic current in Eq. (9)] covariantly conserved. Moreover, we can identify for Abelian fields $B_\nu = A^1_\nu$, and $C_\nu = A^2_\nu$ (a pair of background fields) in Eq. (8); thus, from Eq. (7) $J_\mu = A_1^\nu F^2_{\mu\nu} - A_2^\nu F^1_{\mu\nu}$, which is a covariantly conserved zero-form on the phase space (a conserved current for the exact theory).

Since J_μ in Eq. (9) is an *exact* two-form (it comes from the variations of the symplectic potential θ_μ), corresponds automatically to a closed two-form ($\delta J^\mu = \delta^2\theta^\mu = 0$), as required for the symplectic structure. Unlike the Crncović–Witten approach, we do not need to verify the covariant conservation of our symplectic current, such a property is guaranteed for Eqs. (7) and (8). Therefore, $\omega = \int_\Sigma J^\mu\, d\Sigma_\mu$ is the symplectic structure with the wanted properties for the Yang–Mills theory.[2] Moreover, since the present symplectic structure is essentially the Crncović–Witten result, it has the same invariance properties under gauge transformations.[2] Specifically, as shown in Ref. 2, under gauge transformations of the gauge connection $A_\mu \to A_\mu + \partial_\mu\varepsilon + [A_\mu, \varepsilon]$, δA^i_μ and $\delta F^i_{\mu\nu}$ transform homogeneously, and then J^μ and ω are gauge invariant. Furthermore, following Ref. 2, one can verify easily that ω has vanishing components in the gauge directions in field space [see Eq. (30) in such a reference], which allows us to construct the symplectic structure on the corresponding gauge-invariant space (reduced phase space).

The above results are obtained displaying explicitly the variation of the gauge connection δA_α in Eq. (3). However, it is not the only way for obtaining such results. One can consider Eq. (3) in its original form $\partial^\mu \delta F_{\mu\nu} + [\delta A^\mu, F_{\mu\nu}] = 0$, and the relation $\delta F_{\mu\nu} = \partial_\mu \delta A_\nu - \partial_\nu \delta A_\mu$, as a system of equations governing the field variations $\delta F_{\mu\nu}$, and δA_μ, considering them as independent field variables:

$$\begin{bmatrix} \partial^\mu & -[F^\alpha{}_\nu, \quad] \\ 1 & (\delta^\alpha_\mu \partial_\nu - \delta^\alpha_\nu \partial_\mu) \end{bmatrix} \begin{bmatrix} \delta F_{\mu\nu} \\ \delta A_\alpha \end{bmatrix} = 0,$$

and using again the definition (1) with $\mathcal{P}$ now being the matrix operator in the preceding equation, one obtains essentially the same results.

B. General relativity

The variations of the vacuum Einstein equations $R_{\mu\nu} = 0$ are

$$\nabla_\alpha \delta\Gamma^\alpha_{\mu\nu} - \nabla_\mu \delta\Gamma^\alpha_{\nu\alpha} = 0, \tag{11}$$

where ∇_α is the covariant derivative compatible with the background metric $g_{\mu\nu}$, and $\delta\Gamma^\alpha_{\mu\nu} = \frac{1}{2}g^{\alpha\beta}(\nabla_\mu \delta g_{\nu\beta} + \nabla_\nu \delta g_{\mu\beta} - \nabla_\beta \delta g_{\mu\nu})$, the variation of the metric connection.[2] Displaying explicitly the metric variations $\delta g_{\mu\nu}$, Eqs. (11) take the form

$$[g^{\alpha}_{\nu}\nabla^{\beta}\nabla_{\mu}+g^{\alpha}_{\mu}\nabla^{\beta}\nabla_{\nu}-g^{\alpha}_{\mu}g^{\beta}_{\nu}\nabla^{\rho}\nabla_{\rho}-g^{\alpha\beta}\nabla_{\mu}\nabla_{\nu}+g_{\mu\nu}(g^{\alpha\beta}\nabla^{\rho}\nabla_{\rho}-\nabla^{\beta}\nabla^{\alpha})]\delta g_{\alpha\beta}=0, \quad (12)$$

which can be written in a compact form as

$$[\mathcal{E}(\delta g_{\alpha\beta})]_{\mu\nu}=0, \quad (13)$$

where $\mathcal{E}$ is the linear operator (depending only on the background fields) appearing in Eq. (12). With the same idea of the above case, let $A_{\mu\nu}$, and $B_{\mu\nu}$ be any two 2-index (symmetric) tensor fields (in the first case these fields will be identified as a pair of metric variations for constructing the symplectic current, and as the background metric and a metric variation in the second case for obtaining the corresponding symplectic potential), and using the explicit form of the operator $\mathcal{E}$, we have that

$$B^{\mu\nu}\wedge[\mathcal{E}(A_{\alpha\beta})]_{\mu\nu}-[\mathcal{E}(B^{\mu\nu})]_{\alpha\beta}\wedge A^{\alpha\beta}=\nabla_{\mu}S^{\mu\alpha\beta\lambda\rho\gamma}(B_{\alpha\beta}\wedge\nabla_{\lambda}A_{\rho\gamma}-\nabla_{\lambda}B_{\rho\gamma}\wedge A_{\alpha\beta}), \quad (14)$$

where

$$S^{\mu\alpha\beta\lambda\rho\gamma}=g^{\mu(\rho}g^{\gamma)(\alpha}g^{\beta)\lambda}-\tfrac{1}{2}g^{\mu\lambda}g^{\alpha(\rho}g^{\gamma)\beta}-\tfrac{1}{2}g^{\mu(\alpha}g^{\beta)\lambda}g^{\rho\gamma}-\tfrac{1}{2}g^{\alpha\beta}g^{\mu(\rho}g^{\lambda)\lambda}+\tfrac{1}{2}g^{\alpha\beta}g^{\mu\lambda}g^{\rho\gamma}. \quad (15)$$

Like the Yang–Mills case, Eq. (14) has the form of Eq. (1) with $\mathcal{E}=\mathcal{E}^{\dagger}$. Then, we obtain the local continuity equation:

$$\nabla_{\mu}J^{\mu}=0, \quad J^{\mu}\equiv S^{\mu\alpha\beta\lambda\rho\gamma}(B_{\alpha\beta}\wedge\nabla_{\lambda}A_{\rho\gamma}-\nabla_{\lambda}B_{\rho\gamma}\wedge A_{\alpha\beta}), \quad (16)$$

provided that

$$[\mathcal{E}(A_{\alpha\beta})]_{\mu\nu}=0 \quad \text{and} \quad [\mathcal{E}(B^{\mu\nu})]_{\alpha\beta}=0. \quad (17)$$

In according to Eq. (13), an obvious identification for the fields $A_{\mu\nu}$, and $B_{\mu\nu}$ satisfying Eqs. (17) is

$$A_{\alpha\beta}=\delta g^{1}_{\alpha\beta} \quad \text{and} \quad B_{\mu\nu}=\delta g^{2}_{\mu\nu}, \quad (18)$$

we mean, a pair of variations. In this manner, from Eq. (16),

$$J^{\mu}=S^{\mu\alpha\beta\lambda\rho\gamma}(\delta g^{2}_{\alpha\beta}\wedge\nabla_{\lambda}\delta g^{1}_{\rho\gamma}-\nabla_{\lambda}\delta g^{2}_{\rho\gamma}\wedge\delta g^{1}_{\alpha\beta}), \quad (19)$$

corresponds to a covariantly conserved two-form on the phase space. The last expression can be rewritten, using Eq. (15), in terms of the variations of the metric connection:

$$J^{\mu}=(\delta\Gamma^{\mu}_{\alpha\beta})_1\wedge[\delta g_2^{\alpha\beta}+\tfrac{1}{2}g^{\alpha\beta}(\delta\ln g)_2]-(\delta\Gamma^{\nu}_{\alpha\nu})_1\wedge[\delta g_2^{\mu\alpha}+\tfrac{1}{2}g^{\mu\alpha}(\delta\ln g)_2]-(1\leftrightarrow 2), \quad (20)$$

where $(\delta\Gamma^{\mu}_{\alpha\beta})_1=\frac{1}{2}g^{\mu\rho}[\nabla_{\alpha}\delta g^{1}_{\beta\rho}+\nabla_{\beta}\delta g^{1}_{\alpha\rho}-\nabla_{\rho}\delta g^{1}_{\alpha\beta}]$, $(\delta\ln g)_2=g^{\mu\nu}\delta g^{2}_{\mu\nu}=-g_{\mu\nu}\delta g_2^{\mu\nu}$, and $(1\leftrightarrow 2)$ means a term similar to the first one, just interchanging the subscripts 1 and 2, such as Eq. (19). If we set $\delta g^{1}_{\mu\nu}=\delta g^{2}_{\mu\nu}=\delta g_{\mu\nu}$, J^{μ} in Eq. (20) reduces exactly to the Crncović–Witten current [see Eq. (34) of Ref. 2].

However, the choice (18) for the fields $A_{\alpha\beta}$, and $B_{\mu\nu}$, is not the unique one for satisfying Eqs. (17). We can keep $A_{\alpha\beta}=\delta g^{1}_{\alpha\beta}$, but to identify $B_{\mu\nu}$ as the background metric $g_{\mu\nu}$, since $\nabla_{\lambda}g_{\mu\nu}=0$, and the explicit form of $\mathcal{E}$ in Eq. (12), we have that

$$[\mathcal{E}(g_{\mu\nu})]_{\alpha\beta}=0. \quad (21)$$

Therefore, from Eq. (16), we have that the one-form

$$\theta^{\mu} \equiv S^{\mu\alpha\beta\lambda\rho\gamma} g_{\alpha\beta} \nabla_{\lambda} \delta g^{1}_{\rho\gamma}, \tag{22}$$

is also a covariantly conserved current on the phase space. θ^{μ} can also be rewritten in terms of the variations of the metric connection:

$$\theta^{\mu} = g^{\mu\alpha} (\delta\Gamma^{\nu}_{\alpha\nu})_1 - g^{\alpha\beta} (\delta\Gamma^{\mu}_{\alpha\beta})_1 . \tag{23}$$

Moreover, the conserved currents J^{μ} and θ^{μ} given in Eqs. (19)–(20) and (22)–(23), respectively, are not independent. Considering that $\delta\sqrt{g} = \frac{1}{2}\sqrt{g}\,\delta \ln g$, from Eq. (23), we have that

$$\begin{aligned} \delta(\sqrt{g}\,\theta^{\mu}) = {} & \sqrt{g}[\,\delta g^{\mu\alpha}_{2} \wedge (\delta\Gamma^{\nu}_{\alpha\nu})_1 - \delta g^{\alpha\beta}_{2} \wedge (\delta\Gamma^{\mu}_{\alpha\beta})_1] \\ & - \tfrac{1}{2}\sqrt{g}[g^{\mu\alpha} (\delta\Gamma^{\nu}_{\alpha\nu})_1 - g^{\alpha\beta} (\delta\Gamma^{\mu}_{\alpha\beta})_1] \wedge (\delta \ln g)_2 , \end{aligned} \tag{24}$$

where we have considered also that $\delta^2 = 0$, the Leibniz rule for the exterior derivative, and a variation of the background metric appearing in Eq. (23), in general, different from $\delta g^{1}_{\mu\nu}$, and denoted conveniently by $\delta g^{2}_{\mu\nu}$. Making a direct comparison, the right-hand side of Eq. (24) corresponds, by a factor of $\sqrt{g}$, to the first term on the right-hand side of Eq. (20). With an interchange of the superscripts 1 and 2 in Eq. (24) (which corresponds to identify $A_{\alpha\beta}$ with the background metric and $B_{\mu\nu}$ with the metric variation), we obtain essentially the second term on the right-hand side of Eq. (20). In this manner, we can rewrite

$$\theta^{\mu} = S^{\mu\alpha\beta\lambda\rho\gamma} (g^{2}_{\alpha\beta} \nabla_{\lambda} \delta g^{1}_{\rho\gamma} + g^{1}_{\alpha\beta} \nabla_{\lambda} \delta g^{2}_{\rho\gamma}), \tag{25}$$

and then

$$\delta(\sqrt{g}\,\theta^{\mu}) = \sqrt{g} J^{\mu}, \tag{26}$$

which means that $\sqrt{g} J^{\mu}$ is an *exact* two-form, and $\sqrt{g}\,\theta^{\mu}$ is then the *symplectic potential* for the theory (which is defined up to the exterior derivative of any vector field). Since $\nabla_{\lambda} g_{\mu\nu} = 0$ and $g = g(g_{\mu\nu})$, $\sqrt{g}\,\theta^{\mu}$ and $\sqrt{g} J^{\mu}$ are, like θ^{μ} and J^{μ}, also covariantly conserved.

In the Crncović–Witten approach, one needs to show that $\nabla_{\mu} J^{\mu} = 0$; in the present approach J^{μ} comes directly from the continuity equation (16). Moreover, from Eq. (26), $\sqrt{g} J^{\mu}$ is an exact two-form, and automatically a closed two-form, as required for the symplectic structure $\omega = \int_{\Sigma} \sqrt{g} J^{\mu} d\Sigma_{\mu}$, which has the wanted properties. Since ω is essentially that given in Ref. 2, it has the same invariance properties under gauge transformations described in such a reference.

If we choose $A_{\mu\nu} = g^{1}_{\mu\nu}$, and $B_{\alpha\beta} = g^{2}_{\alpha\beta}$ (a pair of background solutions), both satisfying Eq. (21), then from the local equation (16), we have that $J^{\mu} = 0$, which means that there no exist a (local) conserved current for the exact theory different to the trivial one.

Finally, if we consider Eq. (11) and the relation between $\delta\Gamma$ and $\delta g_{\mu\nu}$ as a system for these field variations (considering them as independent), one obtains essentially the same results.

IV. CONCLUDING REMARKS

As we have seen, the present approach based on the concept of (self-)adjoint operators leads, in a rigorous way, to local continuity laws for the theory under study. Such continuity equations disclose the existence of different conserved currents, in particular those associated with a covariant description of the corresponding symplectic structure.

The symplectic structures described in Refs. 1–3, are always related to a pair of solutions of the equations governing the variations of classical solutions. In the present scheme, the self-adjoint case corresponds, as we have seen in the examples, to that case. Nevertheless, as discussed in Sec. II, there exists a more general case, which establishes the possibility of constructing a (nondegenerate) two-form related to a solution of the equations governing the variations, and a solution of the corresponding adjoint system. No such possibility was previously known in the literature. However, such a two-form is not necessarily closed, remaining to study under what conditions this

two-form represents a symplectic structure. In fact, there are several cases in physics involving operators that are not self-adjoint, where the present approach will be useful: usual free massless fields equations of spin greater that one on a curved spacetime, equations for first-order variations coming from string-inspired actions, etc. Works along these lines are in progress and will be the subject of forthcoming communications.

On the other hand, the Zuckerman formalism, unlike the present one, requires an explicit extension for covering fermionic fields.[3] Even though in the present article we have limited our discussion to bosonic field theories, the adjoint operator formalism allows us to treat bosonic and fermionic fields (and the simultaneous presence of both) on the same footing, since the fundamental definition (1), which is our starting point, extends for spinor fields.[7] In this case, we are particularly interested in superstring theory, and works along these lines are also in progress.

Finally, the connection between adjoint operators and conserved currents used in the present article, has been also used in Ref. 6, although for a different purpose: for obtaining conserved quantities from non-Hermitian systems. In this manner, a scheme based on adjoint operators has different ramifications of wide interest in physics, whose applications also will be the aim of future investigations.

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APPENDIX: NO "PUZZLE" FOR THE SYMPLECTIC CURRENT

In the Crncović–Witten approach,[2] unlike the present scheme, there is not a procedure for obtaining the explicit form for the symplectic structure (or for the symplectic potential). In fact, it may be very difficult to guess such an explicit form for more general and complicated cases. However, without invoking the concept of adjoint operators used in the present scheme, one may be able to obtain the explicit form of the potential symplectic, starting directly from the basic equations for the variations. For example, in the general relativity case, the equation (11) for the variations can be rewritten in the form

$$\nabla_\alpha(\delta\Gamma^\alpha_{\mu\nu}-\delta^\alpha_\mu\delta\Gamma^\lambda_{\nu\lambda})=0, \tag{A1}$$

which implies that the tensor field $T^\alpha_{\mu\nu}\equiv\delta\Gamma^\alpha_{\mu\nu}-\delta^\alpha_\mu\delta\Gamma^\lambda_{\nu\lambda}$ is a covariantly conserved one-form on the phase space. Since $\nabla_\lambda g_{\mu\nu}=0$, and $g=g(g_{\mu\nu})$, the one-form $T^\alpha\equiv\sqrt{g}g^{\mu\nu}T^\alpha_{\mu\nu}$ is also covariantly conserved: $\nabla_\alpha T^\alpha=0$. Using Eq. (23), it is very easy to find that $g^{\mu\nu}T^\alpha_{\mu\nu}=\theta^\alpha$, thus $T^\alpha=\sqrt{g}\,\theta^\alpha$. In this manner, T^α coming from Eq. (A1), is the symplectic potential, whose variations generate automatically a closed two-form. However, regardless of adjoint operators, one must verify the covariant conservation of such a two-form in order to obtain a covariant description.

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Hyper-complex four-manifolds from the Tzitzéica equation

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It is shown how solutions to the Tzitzéica equation can be used to construct a family of (pseudo) hyper-complex metrics in four dimensions. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1426687]

I. INTRODUCTION

A striking *universal* feature of integrable systems is that the same integrable equations often arise from many unrelated sources. The Tzitzéica equation[1]

$$\omega_{xy}=e^{\omega}-e^{-2\omega} \tag{1}$$

is a good example. It first arose in a study of surfaces in $\mathbb{R}^3$ for which the ratio of the negative Gaussian curvature to the fourth power of a distance from a tangent plane to some fixed point is a constant. Tzitzéica has shown that if x and y are coordinates on such a surface in which the second fundamental form is off-diagonal, then there exists a real function $\omega(x,y)$ such that the Peterson–Codazzi equations reduce to (1). Moreover, he has demonstrated[2] that (1) is a consistency condition for an otherwise overdetermined system of partial differential equations (PDEs) for $\psi_i(x,y)$, $i=1,2,3$:

$$\begin{aligned}\partial_x\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix}&=\begin{pmatrix}-\omega_x & 0 & \lambda\\ 1 & \omega_x & 0\\ 0 & 1 & 0\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix},\\ \partial_y\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix}&=\begin{pmatrix}0 & e^{-2\omega} & 0\\ 0 & 0 & e^{\omega}\\ \lambda^{-1}e^{\omega} & 0 & 0\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix}.\end{aligned} \tag{2}$$

[Strictly speaking the linear system given by Tzitzéica consisted of three second order PDEs for one function. These three equations can be recovered from (2) if one eliminates ψ_1 and ψ_2 by cross-differentiating.] The above linear system is in modern terminology known as a ''Lax pair with a spectral parameter.'' It underlines the complete integrability of the Tzitzéica equation.[3]

Equation (1) reappeared in the context of soliton solutions,[4] gas dynamics[5] as well as geometry of affine spheres.[6] In this article I shall reveal yet another occurrence of (1), and show how its solutions can be used to generate explicit pseudo-hyper-complex structures in four dimensions. This will be done by regarding (2) as a reduced Lax pair for SL(3,$\mathbb{R}$) anti-self-dual Yang–Mills (ASDYM) equations, embedding SL(3,$\mathbb{R}$) in Diff($\mathbb{RP}^2$), and reinterpreting the Lax pair in terms of vector fields on $\mathcal{M}=\mathbb{R}^2\times\mathbb{RP}^2$. Four independent vector fields in this Lax pair will provide a null frame for a pseudo-hyper-complex conformal structure on $\mathcal{M}$.

In the next section the Lax formulation of the pseudo-hyper-complex condition in four dimensions will be given following Refs. 7 and 8. In Sec. III the connection with the ASDYM will be established, and the explicit embedding of **sl**(3,$\mathbb{R}$) in **diff**($\mathbb{RP}^2$) will be given. The resulting

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pseudo-hyper-complex structure will be constructed in Sec. IV. All considerations in this section will be local. Finally, Sec. V contains the twistor interpretation of the construction.

II. PSEUDO HYPER-COMPLEX STRUCTURES

A smooth real $4n$-dimensional manifold $\mathcal{M}$ equipped with three real endomorphisms $I,S,T:T\mathcal{M}\to T\mathcal{M}$ of the tangent bundle satisfying the algebra of pseudo-quaternions

$$-I^2=S^2=T^2=1, \quad IST=1,$$

is called pseudo-hyper-complex iff the almost complex structure

$$\mathcal{J}_\lambda=aI+bS+cT \tag{3}$$

is integrable for any point of the hyperboloid $a^2-b^2-c^2=1$. [We identify two sheets of this hyperboloid with two unit discs D_- and D_+, and use λ as a projective coordinate on a Riemann sphere $\mathbb{CP}^1=D_-+D_++S^1$. The coordinate λ plays a role of a complex spectral parameter in the Lax pair (4).] This integrability is equivalent to a vanishing of its Nijenhuis tensor

$$N(X_1,X_2):=(\mathcal{J}_\lambda)^2[X_1,X_2]-\mathcal{J}_\lambda[\mathcal{J}_\lambda X_1,X_2]-\mathcal{J}_\lambda[X_1,\mathcal{J}_\lambda X_2]+[\mathcal{J}_\lambda X_1,\mathcal{J}_\lambda X_2]$$

for arbitrary vectors X_1 and X_2. A convenient matrix representation of the canonical pseudo-hyper-complex structure on $\mathbb{R}^4$ is given by

$$I=\begin{pmatrix} 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ -1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\end{pmatrix}, \quad S=\begin{pmatrix} 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\end{pmatrix}, \quad T=\begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}.$$

In the general case the components of I,S,T depend smoothly on coordinates on $\mathcal{M}$. The endomorphism I endows $\mathcal{M}$ with the structure of a two-dimensional complex manifold, and S and T determine a pair of transverse null foliations. Let g be a metric of signature $(2n,2n)$ on $\mathcal{M}$. If $(\mathcal{M},\mathcal{J}_\lambda)$ is pseudo-hyper-complex and

$$g(TX_1,TX_2)=g(SX_1,SX_2)=-g(IX_1,IX_2)=-g(X_1,X_2)$$

for all vectors X_1,X_2, then the triple $(\mathcal{M},\mathcal{J}_\lambda,g)$ is called a pseudo-hyper-Hermitian structure.

From now on we shall restrict ourselves to oriented four manifolds, where the notions of pseudo-hyper-complex and pseudo-hyper-Hermitian structures coincide. To see it choose any vector $X\in T\mathcal{M}$, and define a conformal structure $[g]$ of signature $(++--)$, by choosing a conformal frame of vector fields (X,IX,SX,TX). Any $g\in[g]$ is then pseudo-hyper-Hermitian. We shall use the following characterization of the pseudo-hyper-Hermiticity condition:

Proposition 1:[7] *Let (X,Y,U,V) be four independent real vector fields on a four-dimensional real manifold $\mathcal{M}$, and let*

$$L_0=X-\lambda V, \quad L_1=U-\lambda Y, \quad \textit{where } \lambda\in\mathbb{CP}^1. \tag{4}$$

If

$$[L_0,L_1]=0 \tag{5}$$

for every λ, then (X,Y,U,V) is a null tetrad for a pseudo-hyper-Hermitian contravariant metric

$$g=X\otimes Y+Y\otimes X-U\otimes V-V\otimes U$$

on $\mathcal{M}$. Every pseudo-hyper-Hermitian metric arises in this way.

For a future reference we write Eq. (4) in full:

$$[X,U]=0, \quad [Y,V]=0, \quad [X,Y]-[U,V]=0. \tag{6}$$

Given the null tetrad (X,Y,U,V) we define the pseudo hyper-complex structure by

$$\begin{gathered} I(X)=-V, \quad I(U)=-Y, \quad I(Y)=U, \quad I(V)=X, \\ S(X)=V, \quad S(U)=Y, \quad S(Y)=U, \quad S(V)=X, \\ T(X)=X, \quad T(U)=U, \quad T(Y)=-Y, \quad T(V)=-V. \end{gathered} \tag{7}$$

Proposition 1 asserts that integrability of I, S, T is guaranteed by (6). Let $\nu\in\Lambda^4(T^*\mathcal{M})$ be the volume form on $\mathcal{M}$. The covariant metric is conveniently expressed in a dual frame

$$\begin{gathered} e_X=\nu(\ldots,Y,U,V), \quad e_Y=\nu(X,\ldots,U,V), \\ e_U=\nu(X,Y,\ldots,V), \quad e_V=\nu(X,Y,U,\ldots), \end{gathered}$$

and is given by

$$g=e_X\otimes e_Y+e_Y\otimes e_X-e_U\otimes e_V-e_V\otimes e_U.$$

The result of Boyer[9] originally formulated for hyper-complex manifolds still applies (with some sign alterations) in the $(++--)$ signature: a four-manifold is pseudo-hyper-complex iff there exists a basis $(\Omega_1,\Omega_2,\Omega_3)$ of the space of self-dual two forms Λ^2_+, and a one-form $\mathcal{A}$ (called a Lee form) such that

$$\mathrm{d}\Omega_i=\mathcal{A}\wedge\Omega_i. \tag{8}$$

If we change a representative of a pseudo-conformal structure according to $g\to e^f g$, then

$$\Omega_i\to e^f\Omega_i, \quad \mathcal{A}\to\mathcal{A}+\mathrm{d}f.$$

Therefore, if $\mathcal{A}$ is exact, then g is conformally pseudo-hyper-Kähler (Ricci-flat).

III. FROM THE TZITZÉICA EQUATION TO ASDYM

The idea of looking at integrable systems as reductions of the anti-self-dual Yang-Mills (ASDYM) equations goes back to Ward.[10] In this section the list of possible reductions will be enlarged by showing that (1) arises from the SL(3,$\mathbb{R}$) ASDYM with two commuting translational symmetries. In Sec. III A the connection matrices will be reinterpreted as vector fields on the projective plane.

Consider the flat metric of signature (2,2) on $\mathbb{R}^4$, which in double null coordinates $x^a=(x,y,u,v)$ takes a form

$$\mathrm{d}x\mathrm{d}y-\mathrm{d}u\mathrm{d}v,$$

and choose the volume element $\mathrm{d}x\wedge\mathrm{d}y\wedge\mathrm{d}u\wedge\mathrm{d}v$. Let $A\in T^*\mathbb{R}^4\otimes\mathbf{sl}(3,\mathbb{R})$ be a connection one-form on a real rank-three vector bundle, and let F be its curvature two-form. In a local trivalization $A=A_a\mathrm{d}x^a$ and $F=F_{ab}\mathrm{d}x^a\wedge\mathrm{d}x^b$, where $F_{ab}=[D_a,D_b]$ takes its values in $\mathbf{sl}(3,\mathbb{R})$. Here $D_a=\partial_a-A_a$ is the covariant derivative. The connection is defined up to gauge transformations $A\to h^{-1}Ah-h^{-1}\mathrm{d}h$, where $h\in\mathrm{Map}(\mathbb{R}^4,\mathrm{SL}(3,\mathbb{R}))$. The ASDYM equations on A_a are $F=-*F$, or

$$F_{xu}=0, \quad F_{xy}-F_{uv}=0, \quad F_{yv}=0.$$

These equations are equivalent to the commutativity of the Lax pair

$$L_0 = D_x - \lambda D_v, \quad L_1 = D_u - \lambda D_y \tag{9}$$

for every value of the parameter λ.

We shall require that the connection possess two commuting translational symmetries X_1, X_2, which in our coordinates are in $X_1 = \partial_u$ and $X_2 = \partial_v$ directions. The direct calculation shows that the ASDYM equations are solved by the following ansatze for Higgs fields A_u and A_v, and gauge fields A_x and A_y

$$\begin{aligned} A_u &= -\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ e^{\omega} & 0 & 0 \end{pmatrix}, \quad A_v = -\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ A_x &= -\begin{pmatrix} -\omega_x & 0 & 0 \\ 1 & \omega_x & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad A_y = -\begin{pmatrix} 0 & e^{-2\omega} & 0 \\ 0 & 0 & e^{\omega} \\ 0 & 0 & 0 \end{pmatrix}, \end{aligned} \tag{10}$$

iff $\omega(x,y)$ satisfies the Tzitzéica equation (1). We note that the reduced Lax pair (9) could be obtained directly from (2) multiplying the second equation by λ.

We connect the ASDYM equations and those on a pseudo-hyper-complex four-dimensional metric (5) by considering gauge potentials that take values in a Lie algebra of vector fields on some manifold. Proposition 1 reveals one such connection: We make the identification: $X = D_x$, $Y = D_y$, $U = D_u$, $V = D_v$. By comparing (9) with (4), we see that the pseudo-hyper-complex equation is a reduction of the ASDYM with the infinite-dimensional gauge group Diff($\mathcal{M}$) by translations along the four coordinate vectors ∂_x, ∂_y, ∂_u, ∂_v.

To reveal the connection with the Tzitzéica equation we shall proceed in a slightly different way: Consider the ASDYM equations with the gauge group G, being a sup-group of Diff(Σ), where Σ is some two-dimensional real manifold. We can represent the components of the connection form of A by vector fields on Σ depending also on the coordinates on $\mathbb{R}^4$. Now we suppose that A is invariant under two translations. The reduced Lax pair will then descend to $\mathcal{M} = \mathbb{R}^2 \times \Sigma$ and give rise to a pseudo-hyper-complex metric. A similar idea has been used in Refs. 11 and 12 to construct new classes of hyper-Kähler four-manifolds out of solutions to some integrable ODEs and PDEs.

Because we are interested in the case $G = \mathrm{SL}(3,\mathbb{R})$, we take Σ to be a real projective plane $\mathbb{RP}^2$ with a natural $\mathrm{PSL}(3,\mathbb{R})$ group action. The relevant vector fields will be constructed in the next subsection.

A. sl(3,$\mathbb{R}$) as a subalgebra of diff($\mathbb{RP}^2$)

To construct a null tetrad for a pseudo-hyper-complex metric we will need an explicit embedding $\mathbf{sl}(3,\mathbb{R}) \to \mathbf{diff}(\mathbb{RP}^2)$. Let

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \in \mathrm{SL}(3,\mathbb{R}).$$

Consider the projective transformations of a plane with local coordinates (p,q):

$$p \to \frac{A_{11}p + A_{12}q + A_{13}}{A_{31}p + A_{32}q + A_{33}}, \quad q \to \frac{A_{21}p + A_{22}q + A_{23}}{A_{31}p + A_{32}q + A_{33}}.$$

This gives rise to a representation of the Lie algebra $\mathbf{sl}(3,\mathbb{R})$ of $\mathrm{SL}(3,\mathbb{R})$ by vector fields on $\mathbb{RP}^2$. The easiest way to obtain this representation is to consider the infinitesimal linear left action of $\mathrm{SL}(3,\mathbb{R})$ on $\mathbb{R}^3$. The generators of this action pushed down to the projective plane are

$$\partial_p, \quad \partial_q, \quad p\partial_q, \quad q\partial_p, \quad -p^2\partial_p - pq\partial_q, \quad -pq\partial_p - q^2\partial_q,$$
$$p\partial_p - q\partial_q, \quad p\partial_p + 2q\partial_q.$$

More precisely, a vector field corresponding to an element

$$M = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & -a_{11}-a_{33} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \in \mathbf{sl}(3,\mathbb{R})$$

is

$$\begin{aligned} X_M = {} & [a_{13} + (a_{11} - a_{33})p + a_{12}q - a_{31}p^2 - a_{32}pq]\partial_p \\ & + [a_{23} + a_{21}p - (a_{11} + 2a_{33})q - a_{31}pq - a_{32}q^2]\partial_q. \end{aligned} \tag{11}$$

IV. CURVED METRICS FROM THE TZITZÉICA EQUATION

Consider the reduced ASDYM Lax pair (9),

$$L_0 = \partial_x - A_x - \lambda A_v, \quad L_1 = -A_u - \lambda(\partial_y - A_y),$$

such that $[L_0, L_1] = 0$ yields (1) and use (11) to replace the matrices (10) by vector fields. Now compare the resulting Lax pair with (4), and read off the null tetrad for a hyper-complex metric (some care needs to be taken with signs because $[X_M, X_N] = -X_{[M,N]}$). This yields

$$\begin{gathered} X = \partial_x + (-\omega_x p + pq)\partial_p + (\omega_x q - p + q^2)\partial_q, \quad U = -e^{\omega}p^2\partial_p - e^{\omega}pq\partial_q, \\ Y = \partial_y - e^{-2\omega}q\partial_p - e^{\omega}\partial_q, \quad V = \partial_p. \end{gathered} \tag{12}$$

The first two equations in (6) are satisfied trivially, and the third one yields

$$[X,Y] - [U,V] = (\omega_{xy} + e^{-2\omega} - e^{\omega})(p\partial_p - q\partial_q),$$

which is 0 if $\omega(x,y)$ satisfies Eq. (1). Let $p = \exp(P), q = \exp(Q)$. The frame of dual one-forms is

$$\begin{aligned} & e_X = \mathrm{d}x, \quad e_U = (\omega_x e^{-\omega-P} + e^{-\omega-P+Q} - e^{-\omega-Q})\mathrm{d}x - e^{-P-Q}\mathrm{d}y - e^{-\omega-P}\mathrm{d}Q, \\ & e_Y = \mathrm{d}y, \quad e_V = (2\omega_x e^{P} - e^{2P-Q})\mathrm{d}x + (e^{Q-2\omega} - e^{\omega+P-Q})\mathrm{d}y - e^{P}\mathrm{d}Q + e^{P}\mathrm{d}P. \end{aligned} \tag{13}$$

Finally, the metric is given by

$$g = 2(e_X e_Y - e_U e_V). \tag{14}$$

It is instructive to verify our calculation by considering the dual formulation of Boyer. Using the identification between the two-forms, and endomorphisms given by g, define a basis $(\Omega_I, \Omega_S, \Omega_T)$ of Λ^2_+ by

$$\Omega_I(X_1,X_2) = -g(IX_1,X_2), \quad \Omega_S(X_1,X_2) = -g(SX_1,X_2), \quad \Omega_T(X_1,X_2) = -g(TX_1,X_2),$$

so that

$$\Omega_S = e_X \wedge e_U - e_Y \wedge e_V, \quad \Omega_T = e_X \wedge e_Y - e_U \wedge e_V, \quad \Omega_I = e_X \wedge e_U + e_Y \wedge e_V.$$

The Lee form $\mathcal{A}$ can be found, such that Eqs. (8) reduce down to (1). Indeed, taking

$$\mathcal{A} = (3e^{P-Q} - 4\omega_x)\mathrm{d}x + (3e^{\omega-Q} - \omega_y)\mathrm{d}y - \mathrm{d}P + 2\mathrm{d}Q$$

yields

$$d\Omega_I - \mathcal{A}\wedge\Omega_I = 0, \quad d\Omega_S - \mathcal{A}\wedge\Omega_S = 0,$$

$$d\Omega_T - \mathcal{A}\wedge\Omega_T = e^{\omega}[\omega_{xy} + e^{-2\omega} - e^{\omega}]dx\wedge dy\wedge d(P+Q) = 0.$$

The metric (14) is therefore never conformal to pseudo-hyper-Kähler because $d\mathcal{A}\neq 0$. Even the simplest solution $\omega = 0$ yields a nontrivial hyper-complex structure

$$g = (e^{P} - e^{2P-2Q})dx^2 + (3 - 2e^{P-2Q} - e^{2Q-P})dxdy + (e^{-P} - e^{2Q})dy^2 - 2dQ^2 + 2dQdP$$
$$+ (e^{P-Q} - e^{Q})dxdP + e^{-Q}dydP + (e^{Q} - 2e^{P-Q})dxdQ + (e^{Q-P} - 2e^{Q})dydQ.$$

[It is worth remarking that a Tzitzéica surface corresponding to $\omega = 0$ (so called Jonas Hexenhut) is also nontrivial.] The Backlund transformations for the Tzitzéica equation[2,13,14] may now be used to generate more complicated metrics.

V. THE TWISTOR CORRESPONDENCE

From the point of view of the Yang–Mills equations, the solutions (14) that we have obtained are metrics on the total space of $\mathcal{E}$, the $\mathbb{RP}^2$-bundle associated to the Yang–Mills bundle. In this section we explain how our construction ties in with the twistor correspondences.

Consider the manifold $\mathcal{Z} = \mathbb{R}^{2,2}\times\mathbb{CP}^1$ [$\mathbb{R}^{2,2}$ denotes $\mathbb{R}^4$ with a flat metric of signature (2,2)]. It decomposes into two open sets

$$\mathcal{Z}_+ = \{(x^a,\lambda)\in\mathcal{Z};\ \mathrm{Im}(\lambda) > 0\} = \mathbb{R}^{2,2}\times D_+,$$

$$\mathcal{Z}_- = \{(x^a,\lambda)\in\mathcal{Z};\ \mathrm{Im}(\lambda) < 0\} = \mathbb{R}^{2,2}\times D_-,$$

where $D_\pm$ are two copies of a Poincare disc. These submanifolds are separated by

$$\mathcal{F}_0 = \{(x^a,\lambda)\in\mathcal{Z};\ \mathrm{Im}(\lambda) = 0\} = \mathbb{R}^{2,2}\times\mathbb{RP}^1.$$

The complex structures on $\mathcal{Z}_\pm$ are specified by a distribution $\mathcal{D}$ of anti-holomorphic vector fields

$$\mathcal{D} = \{\partial_x - \lambda\partial_v,\ \partial_u - \lambda\partial_y,\ \partial_{\bar\lambda}\}.$$

The above distribution with $\lambda\in\mathbb{RP}^1$ defines a foliation of $\mathcal{F}_0$ with a quotient $\mathcal{Z}_0$ which leads to a double fibration:

$$\mathcal{M} \overset{r}{\leftarrow} \mathcal{F}_0 \overset{s}{\rightarrow} \mathcal{Z}_0. \tag{15}$$

The *twistor space* $\mathcal{Z}$ is a three complex dimensional union of two open subsets $\mathcal{Z}_\pm$ separated by a three-dimensional real boundary (*real twistor space*) $\mathcal{Z}_0 := s(\mathcal{F}_0)$.

Each point $\mathbf{x}\in\mathbb{R}^{2,2}$ determines a holomorphic curve $L_{\mathbf{x}}$ made up of two sheets $D_\pm$ of complex structures (3) compactified by adding S^1:

$$\mathbf{x} = (x,y,u,v) \rightarrow L_{\mathbf{x}} = \{(\omega^0,\omega^1,\lambda):\omega^0(\lambda) = v + \lambda x,\ \omega^1(\lambda) = u + \lambda y,\ \lambda\in\mathbb{CP}^1\}.$$

The normal bundle $N = T\mathcal{Z}|_{L_x}/TL_x$ of L_x in $\mathcal{Z}$ is a direct sum of two line bundles with a Chern class equal to one $\mathcal{O}(1)\oplus\mathcal{O}(1)$. If $\mathbf{x}$ and $\mathbf{x}'$ both lie on a self-dual null plane in $\mathbb{R}^{2,2}$ then $L_{\mathbf{x}}$ and $L_{\mathbf{x}}{}'$ intersect in $\mathcal{Z}$ at one point for which $\lambda\in\mathbb{RP}^1$.

Now we turn to the SL(3,$\mathbb{R}$) ASDYM equations on $\mathbb{R}^{2,2}$ with two commuting symmetries X_1, X_2. Let $\mathcal{E} = \mathbb{R}^{2,2}\times\mathbb{RP}^2$ be the bundle associated to the Yang–Mills bundle by the representation of SL(3,$\mathbb{R}$) as projective transformations of $\mathbb{RP}^2$. The SL(3,$\mathbb{R}$) ASDYM connection defines, by a $(++--)$ version of a Ward construction,[15] two holomorphic vector bundles $E_{W_\pm}\rightarrow\mathcal{Z}_\pm$.

The following construction describes also the general case of $G=\mathrm{Diff}(\mathbb{RP}^2)$. For this it is convenient to use the bundles $\mathcal{E}_{W_\pm}$ associated to $E_{W_\pm}$ by the G action on $\mathbb{RP}^2$ (the Ward bundles have infinite-dimensional fibers).

On the other hand, any pseudo-hyper-complex four-metric corresponds to a deformed twistor space $\mathcal{Z}_\mathcal{M}$.[7,9]

Proposition 2: Let $\mathcal{Z}_\mathcal{M}$ be a three-dimensional complex manifold with

(i) *a four parameter family of rational curves with normal bundle $\mathcal{O}(1)\oplus\mathcal{O}(1)$,*
(ii) *a holomorphic projection $\mu:\mathcal{Z}_\mathcal{M}\to\mathbb{CP}^1$, and*
(iii) *an anti-holomorphic involution $\rho:\mathcal{Z}_\mathcal{M}\to\mathcal{Z}_\mathcal{M}$ fixing a real equator of each rational curve.*

Then the real moduli space $\mathcal{M}$ of the ρ-invariant curves is equipped with conformal class $[g]$ of pseudo-hyper-Hermitian metrics. Conversely, given a real analytic pseudo-hyper-Hermitian metrics, there exists a corresponding twistor space with the above structures.

The existence of the holomorphic projection μ reflects the fact that the Lax pair (4) for the pseudo-hyper-complex equations does not contain vector fields ∂_λ.

In this article we have explained how the quotient q of $\mathcal{E}$ by lifts of X_1,X_2 is, by Proposition 4, equipped with a pseudo-hyper-complex metric. To give a more complete picture we can construct the deformed twistor space directly from $\mathcal{E}_{W_\pm}$ and show that this is the twistor space of $\mathcal{M}$.

Given an analytic solution to (1) one can obtain the corresponding twistor space by equipping $\mathcal{M}\times\mathbb{CP}^1$ with a structure of a complex manifold $\mathcal{Z}$: The basis of [0,1] vectors is given by the distribution $\mathcal{D}_\mathcal{M}$ consisting of the Lax pair for the Tzitzéica equation together with the standard complex structure on the $\mathbb{CP}^1$. The point is that this distribution can be obtained directly from $\mathcal{D}$. To see it consider the following chain of correspondences:

$$\begin{array}{ccccc}
\mathcal{Z}_\mathcal{M}=\mathcal{Z}_{\mathcal{M}_-}\cup\mathcal{Z}_{\mathcal{M}_0}\cup\mathcal{Z}_{\mathcal{M}_+} & \overset{\tilde\kappa}{\leftarrow} & \mathcal{E}_W=\mathbb{R}^{2,2}\times\mathbb{RP}^2\times\mathbb{CP}^1 & \overset{\pi}{\to} & \{\mathcal{Z},\mathcal{D}\}\\
\downarrow & & \uparrow & & \downarrow\\
\mathcal{M} & \overset{\kappa}{\leftarrow} & \mathcal{E}=\mathbb{R}^{2,2}\times\mathbb{RP}^2 & \to & \mathbb{R}^{2,2}.
\end{array}$$

Here $\mathcal{Z}$ and $\mathcal{Z}_\mathcal{M}$ are the twistor spaces of $\mathbb{R}^{2,2}$ and $\mathcal{M}$, respectively. The twistor space $\mathcal{Z}_\mathcal{M}$ is defined as the quotient $\tilde\kappa$ of $\mathcal{E}_W$ by lifts of symmetries X_1,X_2. The complex structures on $\mathcal{Z}_{\mathcal{M}_\pm}$ are given a subbundle

$$\mathcal{D}_M=\tilde\kappa(\pi^*\mathcal{D})=\{L_0,L_1,\partial_\lambda^-\}\subset T\mathcal{Z}_\mathcal{M},$$

where

$$L_0=\partial_x+(-\omega_x p+pq)\partial_p+(\omega_x q-p+q^2)\partial_q-\lambda\partial_p,$$

$$L_1=-e^\omega p^2\partial_p-e^\omega pq\partial_q-\lambda(\partial_y-e^{-2\omega}q\partial_p-e^\omega\partial_q).$$

Here π is a holomorphic fibration of the associated Ward bundle. The real three-dimensional surface $\mathcal{Z}_{\mathcal{M}_0}\subset\mathcal{Z}_\mathcal{M}$ is a quotient of $\mathbb{R}^{2,2}\times\mathbb{RP}^2\times\mathbb{RP}^1$ by the four-dimensional real distribution $\{L_0,L_1,X_1,X_2\}$. Moreover, $\mathcal{Z}_\mathcal{M}$ is holomorphically fibered over $\mathbb{CP}^1$ and it has a $\mathcal{O}(1)\oplus\mathcal{O}(1)$ rational curve embedded in it. Both structures are pulled back from $\mathcal{Z}$ and projected by $\tilde\kappa$. The compatibility of these projections is a consequence of the commutativity of the the above diagram, which follows from the integrability the the distribution spanned by (lifts of)

$$X_1,\ X_2,\ L_0,\ L_1,\ \partial_\lambda^-$$

and from the fact that (X_1,X_2) commute with (L_0,L_1).

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Dimensionally dependent tensor identities by double antisymmetrization

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Some years ago, Lovelock showed that a number of apparently unrelated familiar tensor identities had a common structure, and could all be considered consequences in n-dimensional space of a pair of fundamental identities involving trace-free (p,p)-forms where $2p \geqslant n$. We generalize Lovelock's results, and by using the fact that associated with *any* tensor in n-dimensional space there is associated a fundamental tensor identity obtained by antisymmetrizing over $n+1$ indices, we establish a very general ''master'' identity for *all* trace-free (k,l)-forms. We then show how various other special identities are direct and simple consequences of this master identity; in particular we give direct application to Maxwell, Lanczos, Ricci, Bel, and Bel-Robinson tensors, and also demonstrate how relationships between scalar invariants of the Riemann tensor can be investigated in a systematic manner. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1425428]

I. INTRODUCTION

In an n-dimensional space any tensor expression $T_{a_1 a_2 \ldots a_k}$ with $k > n$ indices satisfies a tensor identity

$$T_{[a_1 a_2 \ldots a_k]} = 0. \tag{1}$$

Such mathematically obvious identities can be very useful in practical calculations. However, the antisymmetrization process may not be so explicit since it need not be applied only on free indices; it could also involve dummy indices, some of which could be absorbed into traces, as we shall demonstrate in the following example. (Here, and in the rest of this paper, we use the abstract index notation.[1] However, any index notation would probably work well as long as the above-mentioned property holds.)

Example I.1: Dianyan Xu[2] constructed the following two scalar identities for the Riemann tensor in *four dimensional* spaces,

$$R^a{}_b R^{bcde} R_{acde} = \tfrac{1}{4} R R^{abcd} R_{abcd} + 2 R^{ac} R^{bd} R_{abcd} + 2 R^a{}_b R^b{}_c R^c{}_a - 2 R R^a{}_b R^b{}_a + \tfrac{1}{4} R^3 \tag{2}$$

and

$$R^a{}_c{}^b{}_d R^c{}_e{}^d{}_f R^e{}_a{}^f{}_b = \tfrac{1}{2} R^{ab}{}_{cd} R^{cd}{}_{ef} R^{ef}{}_{ab} - \tfrac{3}{8} R R^{ab}{}_{cd} R^{cd}{}_{ab} - 3 R^{ac} R^{bd} R_{abcd} - 4 R^a{}_b R^b{}_c R^c{}_a + \tfrac{9}{2} R R^a{}_b R^b{}_a - \tfrac{5}{8} R^3. \tag{3}$$

These were obtained after a lengthy calculation by decomposing the Riemann tensor R_{abcd} into its Weyl and Ricci components, and then *using spinor methods*; in fact Dianyan Xu claimed that it was not possible to obtain these identities from the algebraic properties of the Riemann tensor alone.

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However, it was pointed out by Harvey[3] that the first identity could be obtained directly by expanding

$$R^{ab}{}_{[ab}R^{cd}{}_{cd}R^{e}{}_{e]}=0 \tag{4}$$

and the second identity by expanding

$$R^{ab}{}_{[ab}R^{cd}{}_{cd}R^{ef}{}_{ef]}=0 \tag{5}$$

and combining the result with the first identity.

So it is now clear that identities of the type of (2) and (3) exist not only for Riemann tensors, nor even just for Riemann candidates (any four-tensors with the index symmetries of a Riemann tensor); they are in fact valid for any tensors which permit the antisymmetrization constructions (4) and (5). However it should be noted that to get the precise forms of (2) and (3) some of the symmetries of the Riemann tensor must be used.

Harvey's approach also confirmed that both identities were valid in four and lower dimensions—irrespective of the signature of the space (a fact that was missing from Dianyan Xu's spinor derivation). So this insight into the structure of the two identities not only led to a better appreciation of the relevance of these identities in the original context (concerning counterterms in Lagrangians[3–5]), but also highlights the importance of identities built from the antisymmetrization property (1) in the study of Riemann scalar invariants.

Of course the pattern and discussion above suggest how to obtain many more analogous identities for other tensors, for higher dimensions, and for higher order. In fact the identities (2) and (3) can be obtained more directly and compactly by instead using the Weyl tensor C_{abcd} (the trace-free part of the Riemann tensor), e.g., (3) can be obtained from the identity $C^{ab}{}_{[ab}C^{cd}{}_{cd}C^{ef}{}_{ef]}=0$.[3,5–7]

It is also interesting to note that it is not just scalar identities which can be constructed in this manner; for example, similar tensor identities can be considered to underlie the familiar Cayley–Hamilton theorem:

Example I.2: Antisymmetrizing over $n+1$ indices for matrices $M^{a}{}_{b}$ in n dimensions gives the Cayley–Hamilton theorem

$$M^{c_1}{}_{[c_1}M^{c_2}{}_{c_2}\ldots M^{c_n}{}_{c_n}\delta^{b}_{a]}=0. \tag{6}$$

Considering the Cayley–Hamilton theorem from this viewpoint suggests generalizations involving more than one matrix,

$$M^{c_1}{}_{[c_1}N^{c_2}{}_{c_2}\ldots P^{c_n}{}_{c_n}\delta^{b}_{a]}=0. \tag{7}$$

This generalized Cayley–Hamilton theorem has been used to find relations, (syzygies), between scalar invariants of matrices involving more than one matrix.[7–9]

An important question is whether this technique of antisymmetrizing is just a useful ''trick'' in very special circumstances, or whether there is deeper structure to be better understood and more fully exploited.

Some time ago Lovelock[10] noted the significance of certain types of identities—which he called *dimensionally dependent identities*—and demonstrated their existence and importance in quite a wide context (Lovelock[10] has defined a dimensionally dependent identity as an identity which is a direct consequence of the dimension of the space taking on a particular value, and which therefore is not valid for arbitrary dimension n in general). By showing precisely how and where dimensionality plays its role in familiar identities, Lovelock revealed a technique which could be generalized to arbitrary dimension. In fact Lovelock's technique simply involved the antisymmetrizing process being applied in n dimensions, to tensors with *two* sets of indices (upper and lower, in practice) and specialized in two theorems to trace-free tensors with an equal number p of upper and lower indices where $2p\geqslant n$.

Lovelock's investigations were motivated mostly by familiar four-dimensional identities satisfied by Weyl tensors (and Weyl candidates, i.e., tensors with the algebraic symmetries of the Weyl tensor); however, there are other identities which appear to be of a similar nature, but which cannot be confirmed by Lovelock's two theorems. It is the purpose of this paper to investigate dimensionally dependent identities in a systematic manner and obtain a more complete picture; in doing so we develop results more general than Lovelock's, and demonstrate that these new results can be used to confirm identities which cannot be obtained from Lovelock's results, and also to confirm other identities which can only be confirmed indirectly from Lovelock's results.

In Sec. II we make some general observations and present some examples as further motivation for the subsequent sections. We summarize and illustrate Lovelock's results[10] in Sec. III. Lovelock's theorems applied only to trace-free (p,p)-forms in n dimensions where $2p \geqslant n$. However, in Sec. IV, we shall develop more general results in the form of a "master" identity which will be applicable to any tensor in any dimension, and in particular to trace-free (k,l)-forms in any dimension. In Sec. V we will then show that a number of important identities are consequences of this master identity. In particular, we show that the simplification of the gravity–matter coupling terms in the Weyl wave equation and in the Bel tensor, and the complete symmetry of the super-energy tensor for the Lanczos potential of the Weyl tensor are all trivial consequences when the master identity is specialized to four dimensions; in a similar manner we confirm the complete symmetry of the Bel–Robinson tensor in four and five dimensions. In addition, we demonstrate how the results permit a systematic study of relationships between scalar invariants of the Riemann tensor. We also illustrate how the importance of dimensionally dependent identities have been overlooked by reducing the algebraic Rainich condition, and point out the potential usefulness of these results in more general situations.

II. IDENTITIES BY DOUBLE ANTISYMMETRIZATION

We consider the tensor $T^{\mathcal{A}}{}_{a_1}$ where we have adopted the convention that $\mathcal{A}$ denotes an arbitrary number of additional lower and/or upper indices.[1]

Associated with this tensor $T^{\mathcal{A}}{}_{a_1}$, in n-dimensional space, there will always be an identity

$$T^{\mathcal{A}}{}_{[a_1}\delta^{b_2}_{a_2}\delta^{b_3}_{a_3}\ldots\delta^{b_{n+1}}_{a_{n+1}]}=0. \tag{8}$$

For future reference we should note that such identities cannot be made "simpler," in the sense that taking the trace of (8) (on explicit indices, i.e., indices which are not implicit in $\mathcal{A}$) simply gives zero on the left-hand side also.

An alternative approach would be to assume the presence of a volume element $\eta_{a_1a_2\ldots a_n}$, and formulate analogous results in the η notation making use of duals; but we shall concentrate on developing results using the δ notation.

There will of course be one such identity associated with each separate index on T. We could obtain other identities, with less deltas, by taking more than one index of T explicitly into the antisymmetrization operation, but these new identities would involve only the antisymmetrized part of T with respect to the explicit indices.

However, when the tensor T is in fact antisymmetric in a group of k indices, then we can get an identity involving less deltas than the original identity

$$T^{\mathcal{A}}{}_{[a_1\ldots a_k}\delta^{b_{k+1}}_{a_{k+1}}\delta^{b_{k+2}}_{a_{k+2}}\ldots\delta^{b_{n+1}}_{a_{n+1}]}=0, \tag{9}$$

but without losing any part of T. Again, it is important to note that taking the trace of (9), on explicit indices, simply gives zero on the left-hand side also.

We next consider a tensor with both upper and lower indices, each of which contain groups of antisymmetric indices, i.e., $T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{b_1\ldots b_l}=T^{\mathcal{A}}{}_{[a_1\ldots a_k]}{}^{[b_1\ldots b_l]}$ is a (k,l)-*form* with respect to its explicit indices; then we have the associated identity

$$T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{[b_1\ldots b_l}\delta^{b_{k+1}}_{a_{k+1}}\ldots\delta^{b_{n+1}]}_{a_{n+1}}=0 \tag{10}$$

when $l\geqslant k$. (The analogous case obtained by antisymmetrizing on the lower indices for $k\leqslant l$ is obvious.)

Such classes of tensors include many familiar tensors (Riemann, Weyl, Ricci, Maxwell, Lanczos, torsion) and they shall be the main focus of our investigation in this paper.

It is important to note that, although some traces of (10) yield the trivial identity, *there are some traces of* (10) *which yield a nontrivial identity involving the trace of* T. It is these nontrivial traces which yield Lovelock's identities, and our generalizations of them. We illustrate this with the following example.

Example II.1: We consider the (2,2)-form $R_{ab}{}^{cd}$.

In three dimensions: $R_{ef}{}^{[gh}\delta^c_a\delta^{d]}_b=0$.

Contracting once over e and g gives

$$R_{f[a}{}^{[hc}\delta^{d]}_{b]}-R_{ef}{}^{e[h}\delta^c_a\delta^{d]}_b=0, \tag{11}$$

and then over h and f gives,

$$R_{ab}{}^{cd}-4R_{e[a}{}^{e[c}\delta^{d]}_{b]}+R_{ef}{}^{ef}\delta^{[c}_a\delta^{d]}_b=0. \tag{12}$$

From this last result follows the well-known fact that the trace-free part of a Riemann tensor is identically zero in three dimensions.

In four dimensions: $R_{gh}{}^{[ij}\delta^d_a\delta^e_b\delta^{f]}_c=0$.

Contracting once over g and i gives

$$3R_{h[a}{}^{[jd}\delta^e_b\delta^{f]}_{c]}-2R_{gh}{}^{g[j}\delta^d_a\delta^e_b\delta^{f]}_c=0, \tag{13}$$

and then over h and j gives

$$3R_{[ab}{}^{[de}\delta^{f]}_{c]}-6R_{g[a}{}^{g[d}\delta^e_b\delta^{f]}_{c]}+R_{gh}{}^{gh}\delta^{[d}_a\delta^e_b\delta^{f]}_c=0. \tag{14}$$

A third contraction gives zero on the left-hand side also.

All of the above-mentioned identities can be expressed in a more concise form if R_{abcd} is decomposed into trace-free and trace parts.

We note that certain of these contractions yield identities which, if we were to encounter them not knowing their source, would seem (to our surprise) to come from antisymmetrizing over n or $n-1$ explicit indices in n dimensions; on the other hand, when one takes into account *all* the terms in each identity and also notes that these contractions involve antisymmetrizing over upper and lower indices, of course, we would realize that our first judgment was superficial, and we have a disguised antisymmetrization over $n+1$ indices. However, we have noted previously that the identities exist in their most concise form when presented in terms of the trace free part of R_{abcd}; so such identities can be even more deceptive especially when constructed explicitly in terms of a trace-free tensor.

So we now specialize to the important special situation where the (k,l)-form $T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{b_1\ldots b_l}=T^{\mathcal{A}}{}_{[a_1\ldots a_k]}{}^{[b_1\ldots b_l]}$ is *trace-free*, i.e., $T^{\mathcal{A}}{}_{a_1a_2\ldots a_k}{}^{a_1b_2\ldots b_l}=0$, and the underlying structure of the resulting identities become less transparent. To illustrate this we will give three simple examples involving, respectively, a trace-free (2,2)-form $W_{ab}{}^{cd}$ [of which the Weyl conformal curvature tensor $C_{ab}{}^{cd}$ is a special example being a symmetric trace-free (2,2)-form since $C_{abcd}=C_{cdab}$, with the additional property $C_{[abc]d}=0$], a trace-free (2,1)-form $L_{ab}{}^c$ [of which the torsion and Lanczos potential with the additional property $L_{[abc]}=0$ (Ref. 11) are special examples], and a trace-free (1,1)-form $S^a{}_b$ (of which the trace-free symmetric Ricci tensor $\tilde{R}^a{}_b$, the trace-free symmetric energy tensor $\tilde{T}^a{}_b$ and the antisymmetric Maxwell tensor $F^a{}_b$, are special examples).

Example II.2: We now apply the above-presented arguments to the trace-free (2,2)-form $W_{ab}{}^{cd}$.

In three dimensions: $W_{ef}{}^{[gh}\delta_a^c\delta_b^{d]}=0$.

Contracting over f and h gives

$$W_{e[a}{}^{[gc}\delta_{b]}^{d]}=0, \tag{15}$$

and then over e and g gives

$$W_{ab}{}^{cd}=0. \tag{16}$$

In four dimensions: $W_{gh}{}^{[ij}\delta_a^d\delta_b^e\delta_c^{f]}=0$.

Contracting over h and j gives

$$W_{g[a}{}^{[id}\delta_b^e\delta_{c]}^{f]}=0, \tag{17}$$

and then over g and i gives

$$W_{[ab}{}^{[de}\delta_{c]}^{f]}=0. \tag{18}$$

A third contraction gives zero on the left-hand side also.

In five dimensions: $W_{ij}{}^{[kl}\delta_a^e\delta_b^f\delta_c^g\delta_d^{h]}=0$.

Contracting over j and l gives

$$W_{i[a}{}^{[ke}\delta_b^f\delta_c^g\delta_{d]}^{h]}=0, \tag{19}$$

and then over i and k gives

$$W_{[ab}{}^{[ef}\delta_c^g\delta_{d]}^{h]}=0. \tag{20}$$

A third contraction gives zero on the left-hand side also.

So, in each of the three cases, the first identity is obvious in the sense that it is an explicit antisymmetrization over $n+1$ indices in n dimensions. What is particularly interesting, and at first sight perhaps surprising in these situations, is the existence of simple identities in n dimensions which involve explicit antisymmetrization over only $n-1$ indices. But of course, in addition, there is antisymmetrization on both lower and upper indices and the comparatively simple versions are due to the vanishing of the trace of W.

Example II.3: Consider the trace-free (2,1)-form $L_{ab}{}^{c}$.

When we apply the above-mentioned arguments we obtain,

In three dimensions: $L_{[fa}{}^{g}\delta_b^d\delta_{c]}^{e}=0$.

Contracting once on the upper index on L gives

$$L_{[ab}{}^{[d}\delta_{c]}^{e]}=0, \tag{21}$$

and contracting once more gives zero on the left-hand side also.

In four dimensions: $L_{[ha}{}^{i}\delta_b^e\delta_c^f\delta_{d]}^{g}=0$.

Contracting once on the upper index on L gives

$$L_{[ab}{}^{[e}\delta_c^f\delta_{d]}^{g]}=0, \tag{22}$$

and once more gives zero on the left-hand side also.

So, once again, we obtain identities in n dimensions involving explicit antisymmetrization over less than $n+1$ indices; although in this case it involves n indices.

Example II.4: Consider the trace-free (1,1)-form $S_a{}^{b}$.

When we apply the above-mentioned arguments we obtain,

In three dimensions: $S_{[g}{}^{h}\delta_a^d\delta_b^e\delta_{c]}^{f}=0$.

Contracting once on the upper index on S gives

$$S_{[a}{}^{[d}\delta^{e}_{b}\delta^{f]}_{c]}=0, \tag{23}$$

and contracting once more gives zero on the left-hand side also.

In four dimensions: $S_{[i}{}^{j}\delta^{e}_{a}\delta^{f}_{b}\delta^{g}_{c}\delta^{h}_{d]}=0$.

Contracting once on the upper index on S gives

$$S_{[a}{}^{[e}\delta^{f}_{b}\delta^{g}_{c}\delta^{h]}_{d]}=0, \tag{24}$$

and once more gives zero on the left-hand side also.

So, once again, we obtain identities in n dimensions involving explicit antisymmetrization over only n indices.

In the above-given examples we have obtained obvious identities by antisymmetrization over $n+1$ indices in n dimensions; but in addition, as a result of taking traces, we have obtained less obvious identities containing *less* deltas and explicit antisymmetrization over *less than* $n+1$ indices. The existence of these additional identities, which contain less deltas than the obvious ones, are very important for building up more complicated identities. For example, consideration of the obvious four-dimensional identity for the Weyl tensor $C_{[ab}{}^{fg}\delta^{h}_{c}\delta^{i}_{d}\delta^{j}_{e]}=0$ (with 10 free indices), would not suggest the possibility of any third-order *scalar* identities for C; on the other hand, the less obvious one formed from the double trace, $C_{[ab}{}^{[fg}\delta^{h]}_{c]}=0$ (with 6 free indices), certainly permits the constructions of third-order Weyl scalar identities by multiplication with a pair of C tensors.

For each case considered we have gone as far as we could, in the sense that taking an additional trace simply reduces the left-hand side to zero. Nevertheless, this does not in itself mean that there could not exist additional identities with even less deltas than those given previously; however, for each of the cases it can be shown directly that removing further deltas gives a restriction rather than an identity, e.g., *in four dimensions*, when the trace is calculated for $L_{[ab}{}^{[c}\delta^{g]}_{f]}=0$ we find that $L_{ab}{}^{c}=0$.

In Sec. III we shall give results due to Lovelock[10] and show that the results for three and four dimensions of Example II.2 follow directly as a special case; it will also be shown that the result for five dimensions can be deduced, more subtly, from Lovelock's results. In Sec. IV we will derive even more general results of which Lovelock's and the above-mentioned three examples will be seen to be special cases.

III. LOVELOCK'S DIMENSIONALLY DEPENDENT IDENTITIES

Some years ago, Lovelock[10] noted that familiar tensors, (such as the Weyl and Maxwell tensors), with antisymmetry and trace-free properties, obeyed assorted—apparently unrelated—identities. However, although there was no common structural link in the original derivations of these assorted identities, Lovelock[10] showed that they could all be considered to be consequences of two underlying basic tensor identities. These underlying identities had a very simple structure and were a mathematically trivial consequence of dimension alone. We will now quote Lovelock's two theorems, each of which he proved in two different ways; our proofs are essentially more concise presentations of one of his versions.

Theorem III.1: *In an n-dimensional space let* $T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{b_1\ldots b_k}=T^{\mathcal{A}}{}_{[a_1\ldots a_k]}{}^{[b_1\ldots b_k]}$ *be trace-free on its explicit indices. If* $2k>n$ *then*

$$T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{b_1\ldots b_k}=0. \tag{25}$$

Proof: Since $2k>n$, antisymmetrizing over $2k$ indices gives an identity

$$0=T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{i_1\ldots i_k}\delta^{b_1}_{i_1}\ldots\delta^{b_k}_{i_k]}. \tag{26}$$

Since the tensor T is trace-free, we get

$$0 = T^{\mathcal{A}}{}_{a_1 \ldots a_k}{}^{i_1 \ldots i_k} \delta^{b_1}_{i_1} \ldots \delta^{b_k}_{i_k}. \tag{27}$$

Absorbing the deltas gives the theorem. □

Theorem III.2: *In an n-dimensional space let* $T^{\mathcal{A}}{}_{a_1 \ldots a_k}{}^{b_1 \ldots b_k} = T^{\mathcal{A}}{}_{[a_1 \ldots a_k]}{}^{[b_1 \ldots b_k]}$ *be trace-free on its explicit indices. If* $2k = n$ *then*

$$T^{\mathcal{A}}{}_{[a_1 \ldots a_k}{}^{[b_1 \ldots b_k} \delta^{b_{k+1}]}_{a_{k+1}]} = 0. \tag{28}$$

Proof: The proof is analogous to the proof of Theorem II.1 but this time the antisymmetrization is over $2k+1$ indices. Starting with

$$0 = T^{\mathcal{A}}{}_{[a_1 \ldots a_k}{}^{i_1 \ldots i_k} \delta^{b_{k+1}}_{a_{k+1}} \delta^{b_1}_{i_1} \ldots \delta^{b_k}_{i_k]} = T^{\mathcal{A}}{}_{[a_1 \ldots a_k}{}^{i_1 \ldots i_k} \delta^{[b_{k+1}}_{a_{k+1}} \delta^{b_1}_{i_1} \ldots \delta^{b_k]}_{i_k}, \tag{29}$$

since the tensor is trace-free, we get

$$0 = T^{\mathcal{A}}{}_{[a_1 \ldots a_k}{}^{i_1 \ldots i_k} \delta^{[b_{k+1}}_{a_{k+1}]} \delta^{b_1}_{i_1} \ldots \delta^{b_k]}_{i_k}. \tag{30}$$

Absorbing the deltas gives the theorem. □

(This proof shows that this second theorem is actually true for the weaker condition, $2k \geqslant n$; but the validity of the second theorem when $2k > n$ also follows from the first theorem, which has the more fundamental condition.)

The theorems immediately yield the familiar results in Example II.2:

Example III.3: Theorem III.1 with $k=2$ applied to the trace-free (2,2)-form W_{abcd} gives $W_{abcd}=0$ when $n \leqslant 3$.

From Theorem III.2 we find directly $W^{[cd}{}_{[ef} \delta^{a]}_{b]} = 0$ when $n \leqslant 4$.

An additional well-known result is found by multiplying this with $W^{ef}{}_{cd}$ to get

$$W^{ac}{}_{de} W^{de}{}_{bc} = \tfrac{1}{4} \delta^a_b W^{cd}{}_{ef} W^{ef}{}_{cd}. \tag{31}$$

Multiplying with $W^{ef}{}_{ga} W^{bg}{}_{cd}$ instead yields the scalar identity cubic in $W^{ab}{}_{cd}$,

$$W^{ab}{}_{ce} W^{cd}{}_{af} W^{ef}{}_{bd} = \tfrac{1}{4} W^{ab}{}_{cd} W^{cd}{}_{ef} W^{ef}{}_{ab}. \tag{32}$$

The third result in Example II.2 may also be obtained—but in a more indirect manner; we consider the tensor $T^{abef}{}_{cdkl} = W^{[ab}{}_{[cd} \delta^e_k \delta^{f]}_{l]}$ and *by a direct calculation* we can confirm its trace to be zero in five dimensions. Hence, from Theorem III.1, it follows immediately that $T^{abef}{}_{cdkl}$ is identically zero in five dimensions.

The results in Example II.4 can also be obtained in the same way.

As well as showing how familiar identities were direct consequences of his theorems, Lovelock[10] also deduced some new interesting identities. More recently, additional important, and sometimes unexpected, identities have been shown to follow from Lovelock's theorems.[12–15]

However, we emphasize again that the results in Examples II.3 and II.4 cannot be deduced *directly* from Lovelock's theorems.

IV. GENERAL THEOREMS ON DIMENSIONALLY DEPENDENT IDENTITIES

The natural generalization of Lovelock's theorems is the following theorem.

Theorem IV.1: *In an n-dimensional space let* $T^{\mathcal{A}}{}_{a_1 \ldots a_k}{}^{b_1 \ldots b_l} = T^{\mathcal{A}}{}_{[a_1 \ldots a_k]}{}^{[b_1 \ldots b_l]}$ *be trace-free on its explicit indices. Then*

$$T^{\mathcal{A}}{}_{[a_1 \ldots a_k}{}^{[b_1 \ldots b_l} \delta^{b_{l+1}}_{a_{k+1}} \ldots \delta^{b_{l+d}]}_{a_{k+d}]} = 0, \tag{33}$$

where $n+1\leqslant d+k+l$ *and* $d\geqslant 0$.

Proof: The proof is analogous to the proof of Theorem III.2. This time we antisymmetrize over $k+l+d\geqslant n+1$ indices to get the identity.

$$0=T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{i_1\ldots i_l}\delta^{b_{l+1}}_{a_{k+1}}\ldots\delta^{b_{l+d}}_{a_{k+d}}\delta^{b_1}_{i_1}\ldots\delta^{b_l}_{i_l]}=T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{i_1\ldots i_l}\delta^{[b_{l+1}}_{a_{k+1}}\ldots\delta^{b_{l+d}}_{a_{k+d}}\delta^{b_1}_{i_1}\ldots\delta^{b_l]}_{i_l}. \tag{34}$$

Since the tensor T is trace-free, we get

$$0=T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{i_1\ldots i_l}\delta^{[b_{l+1}}_{a_{k+1}}\ldots\delta^{b_{l+d}}_{a_{k+d}]}\delta^{b_1}_{i_1}\ldots\delta^{b_l]}_{i_l}. \tag{35}$$

Absorbing the deltas gives the result. □

Remarks:

(1) For completeness, we add that if we adopt the convention that tensors with only lower or only upper indices are considered ''trace-free,'' then the above-mentioned results also hold for the two classes of tensors where $k=0$ or $l=0$. In addition, for the case $k=0$ and $l=0$, i.e., T a scalar, we simply get the trivial result of the vanishing of the Kronecker delta symbol with $n+1$ index pairs in n-dimensional space.

(2) The theorem generalizes Lovelock's results by associating, in n-dimensional space, an identity with *any* tensor, since—no matter what its index configuration—part of it can be considered as a (k,l)-form, with the above-mentioned conventions when $k=0$ or $l=0$. But it is for trace-free double forms with $k\neq 0\neq l$ that it will be most useful. So when $l=0$ or $k=0$ and $d=0$ we have identity (9); when $k=l\neq 0$ and $d=0$ this is Theorem III.1 and when $k=l\neq 0$ and $d=1$ this is Theorem III.2. Had we wished only to generalize to the case $k=l$ for any d, we could have used Theorem III.1 directly in our proof, as in Example II.2.

(3) No stronger result on T can be obtained by taking the trace of (33), since then the left-hand side just collapses to zero. In addition, the discussion at the end of Sec. II would strongly suggest that the conditions on d cannot be relaxed for nonzero T; we shall confirm later in Theorem IV.5 that this is indeed so.

(4) Of course this theorem does not mean that we cannot construct results beginning with double forms which are not trace-free. Rather, what will happen is that if we begin with such a tensor we will get an apparently more complicated identity with explicit trace terms; if the double form is then decomposed into trace-free and trace parts, the resulting simplification will leave us with the identity which would be obtained by beginning with the trace-free part of the double form.

We shall now illustrate the relevance of the new results in Theorem IV.1 to familiar tensors as follows,

Example IV.2: Applying Theorem IV.1 to the trace-free (2,1)-form $L_{ab}{}^{c}$ $(l=1,k=2)$ in dimensions $n=3$ with $d=1$ gives the identity

$$L_{[ab}{}^{[d}\delta^{e]}_{c]}=0 \tag{36}$$

and in dimensions $n=4$, with $d=2$,

$$L_{[ab}{}^{[e}\delta^{f}_{c}\delta^{g]}_{d]}=0. \tag{37}$$

For trace-free (2,2)-forms $(l=k=2)$ in dimensions $n=5$ with $d=2$ gives the identity

$$W_{[ab}{}^{[ef}\delta^{g}_{c}\delta^{h]}_{d]}=0. \tag{38}$$

For trace-free (1,1)-forms $S^{a}{}_{b}$ $(l=k=1)$, in dimensions $n=4$ with $d=3$ gives the identity

$$S_{[a}{}^{[e}\delta^{f}_{b}\delta^{g}_{c}\delta^{h]}_{d]}=0. \tag{39}$$

Analogous basic identities can be found in other dimensions, and all such identities can then be exploited to build up other useful important identities, as we shall demonstrate in Sec. V.

We now consider whether we can generalize these results in another manner, by asking whether any kind of converses exist. First, by way of example, we consider the identity (38) obtained from Theorem IV.1 for the trace-free (2,2)-forms when $n\leqslant 5$. As mentioned in the third remark above, we would like to confirm explicitly that the stronger condition $W_{[ab}{}^{[de}\delta_{c]}^{f]}=0$, which holds in four dimensions, does not hold in dimensions $n=5$. A related task would be to confirm explicitly that the same identity (38) as holds in $n\leqslant 5$ dimensions does not hold in higher dimensions. We shall see from Theorem IV.5 that we can confirm explicitly an even stronger version of these results.

Second, with respect to the same example, a natural question to ask is whether the trace-free condition is also a necessary condition, i.e., whether any forms with *nonzero trace* can satisfy this identity $W_{[ab}{}^{[ef}\delta_{c}^{g}\delta_{d]}^{h]}=0$ in dimensions $n\leqslant 5$. Whether an alternative (2,2)-form—lacking the trace-free properties but perhaps with different symmetry properties—can satisfy the basic identity is not obviously ruled out. As an example, we could ask whether a (2,2)-form like the Riemann tensor $R_{ab}{}^{cd}$—lacking the trace-free properties of $W_{ab}{}^{cd}$, but having the additional properties $R_{a[bcd]}=0$ and $R_{abcd}=R_{cdab}$—can satisfy the identities. However, we shall see from Theorem IV.6 that *only trace-free* (2,2)-forms satisfy the identity (38) in dimensions $n\leqslant 5$.

We first present a lemma which is then used in the proof of the two theorems. We emphasize that this lemma is also useful in its own right, and we shall demonstrate how it can be viewed as a generalization of a familiar result for the Kronecker delta.

Lemma IV.3: In n-dimensional space let $T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{b_1\ldots b_l}=T^{\mathcal{A}}{}_{[a_1\ldots a_k]}{}^{[b_1\ldots b_l]}$, k, l *and* $d\geqslant 0$ *and* $(k+d)(l+d)>0$. *Then*

$$T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{[b_1\ldots b_l}\delta_{a_{k+1}}^{b_{l+1}}\ldots\delta_{a_{k+d}}^{b_{l+d}]}\delta_{b_{l+d}}^{a_{k+d}}=\frac{d(n-(d+k+l-1))}{(k+d)(l+d)}T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{[b_1\ldots b_l}\delta_{a_{k+1}}^{b_{l+1}}\ldots\delta_{a_{k+d-1}}^{b_{l+d-1}]}+\frac{(-1)^{k+l}kl}{(k+d)(l+d)}T^{\mathcal{A}}{}_{c[a_1\ldots a_{k-1}}{}^{c[b_1\ldots b_{l-1}}\delta_{a_k}^{b_l}\ldots\delta_{a_{k+d-1}}^{b_{l+d-1}]}. \tag{40}$$

Proof: If k, l, or d is zero the lemma is trivial. Assume they are nonzero.

On the left-hand side the last two deltas combine to give

$$T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{[b_1\ldots b_l}\delta_{a_{k+1}}^{b_{l+1}}\ldots\delta_{a_{k+d-1}}^{b_{l+d-1}}\delta_{c]}^{c]}. \tag{41}$$

By summing over all possible positions of the dummy indices c we get

$$\frac{(k+d-1)!(l+d-1)!}{(k+d)!(l+d)!}\sum_{i,j}c_{ij}T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{[b_1\ldots b_l}\delta_{a_{k+1}}^{b_{l+1}}\ldots\delta_{|c|}^{b_{k_i}}\ldots\delta_{a_{l_j}}^{|c|}\ldots\delta_{a_{k+d-1}}^{b_{l+d-1}]}, \tag{42}$$

where $c_{ij}=\pm 1$ depending on whether the index configuration is an even or an odd permutation.

It is now clear that we get only the two types of terms that are on the right-hand side of the theorem; the last type when both dummy indices are on T and the other type when at least one of them is on a δ. What remains is to confirm the coefficients, which essentially means counting how many of each kind occurs and what sign they have.

When both dummy indices are on T they can be moved to the first position. That means that they have moved a total of $(k+d-1)+(l+d-1)$ positions and changed sign equally many times. That gives a factor $(-1)^{k+l}$. There are a total of kl such terms.

When both dummy indices are on the same δ they have moved equally many positions; thus such terms are added. There are d such terms and we also get a factor n since $\delta_i^i=n$.

When both dummy indices are on different δ one of them can be absorbed thereby distorting the order of the other indices. Once that order is restored we have overall an odd permutation; thus such terms are subtracted. There is a total of $d(d-1)$ such terms.

The same situation occurs when one of the dummy indices is on a δ and the other one is on T. There are ld such terms with the upper index on T and kd with the lower index on T.

Taking all this together gives the identity in the lemma. □

When we consider $k=0$ and $l=0$, with T a nonzero constant, in Lemma IV.3 we get a familiar identity for the Kronecker delta,

Corollary IV.4: In n-dimensional space

$$\delta^{[b_1}_{[a_1}\cdots\delta^{b_d]}_{a_d]}\delta^{a_d}_{b_d}=\frac{(n-d+1)}{d}\,\delta^{[b_1}_{[a_1}\cdots\delta^{b_{d-1}]}_{a_{d-1}]}. \tag{43}$$

We now use Lemma IV.3 to establish the two theorems.

Theorem IV.5: *In an n-dimensional space let* $T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{b_1\ldots b_l}=T^{\mathcal{A}}{}_{[a_1\ldots a_k]}{}^{[b_1\ldots b_l]}$. *If*

$$T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{[b_1\ldots b_l}\delta^{b_{l+1}}_{a_{k+1}}\cdots\delta^{b_{l+d}]}_{a_{k+d}]}=0 \tag{44}$$

then

$$n+1>d+k+l\Rightarrow T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{b_1\ldots b_l}=0. \tag{45}$$

Proof: The basic idea is to repeatedly take traces of Eq. (44) getting a sequence of equations; in the last of these no δ remains. The result follows from substituting equations at the end of this sequence into earlier ones. However, care must be taken so that no unwanted canceling of terms occur which forces this process to stop prematurely.

To make the proof easier to overview we define the following notation. Let $(d,k,l)=T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{[b_1\ldots b_l}\delta^{b_{l+1}}_{a_{k+1}}\cdots\delta^{b_{l+d}]}_{a_{k+d}]}$ and if k and l are less than the actual number of indices on T then we contract over the remaining ones. Thus Lemma IV.3 can be written as

$$\text{trace }(d,k,l)=\frac{d(n-(d+k+l-1))}{(k+d)(l+d)}(d-1,k,l)+\frac{(-1)^{k+l}kl}{(k+d)(l+d)}(d,k-1,l-1)$$

and T itself as $(0,k,l)$ and the trace of T as $(0,k-1,l-1)$.

We observe that the coefficients in Lemma IV.3 are nonzero if d is nonzero and k and l are nonzero, respectively.

First assume that $k+l$ is even, then the coefficients in Lemma IV.3 are non-negative. Start with Eq. (44) and multiply with $\delta^{a_{k+d}}_{b_{l+d}}$ and use Lemma IV.3. Then we get $0=(d-1,k,l)+(d,k-1,l-1)$ where we have omitted the coefficients.

Doing that once more gives us $0=(d-2,k,l)+(d-1,k-1,l-1)+(d,k-2,l-2)$. Repeating this process gives a sequence of equations as illustrated in Fig. 1 where each row corresponds to one equation.

The last equation is $0=(0,k-l,0)$ (assuming $k\geqslant l$). Putting this into the second to last equation gives $0=(0,k-l+1,1)$ by using that $0=(j,k,l)\Rightarrow 0=(j+1,k,l)$. Feeding the new information into earlier equations gives the desired conclusion $0=(0,k,l)$.

If $k+l$ is odd then there is a minus sign in Lemma IV.3, which means that there is a risk of cancellation in the above-mentioned process. However, checking how the signs propagate gives us Fig. 2 where the sign at a node is the sign of the term and the sign at the edge is the sign of the coefficient in the identity in Lemma IV.3.

It is now clear that there will be no cancellations since each term originates as the difference between two terms with different sign. □

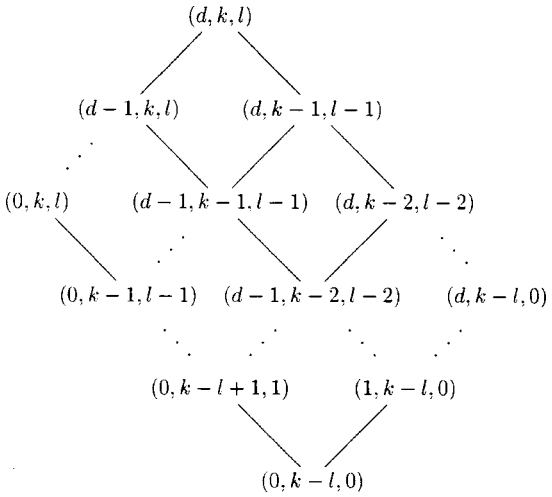

FIG. 1. Sequence of equations.

Theorem IV.6: *In an n-dimensional space let* $T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{b_1\ldots b_l}=T^{\mathcal{A}}{}_{[a_1\ldots a_k]}{}^{[b_1\ldots b_l]}$ *where* $n+1\geqslant k+l$ *and let* $d=n-k-l+1$. *Then*

$$T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{[b_1\ldots b_l}\delta^{b_{l+1}}_{a_{k+1}}\ldots\delta^{b_{l+d}]}_{a_{k+d}]}=0\Leftrightarrow T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{b_1\ldots b_l}\ \textit{is trace-free on its explicit indices.} \tag{46}$$

Proof: $\Leftarrow$: Follows directly from Theorem IV.1

$\Rightarrow$: The case $d=0$ is trivial. Assume $d>0$. Contracting

$$0=T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{[b_1\ldots b_l}\delta^{b_{l+1}}_{a_{k+1}}\ldots\delta^{b_{l+d}]}_{a_{k+d}]} \tag{47}$$

once and using Lemma IV.3 gives

$$0=T^{\mathcal{A}}{}_{i[a_1\ldots a_{k-1}}{}^{i[b_1\ldots b_{l-1}}\delta^{b_l}_{a_k}\ldots\delta^{b_{l+d-1}]}_{a_{k+d-1}]}. \tag{48}$$

The theorem now follows from Theorem IV.5 applied to the tensor

$$\tilde{T}^{\mathcal{A}}{}_{a_1\ldots a_{k-1}}{}^{b_1\ldots b_{l-1}}=T^{\mathcal{A}}{}_{ia_1\ldots a_{k-1}}{}^{ib_1\ldots b_{l-1}}. \tag{49}$$

□

Example IV.7: We know that for the Weyl curvature tensor C_{abcd} [a trace-free symmetric (2,2)-form], $C_{[ab}{}^{[ef}\delta^g_c\delta^{h]}_{d]}=0$ in dimensions $n\leqslant 5$. From Theorem IV.5 we can conclude that this

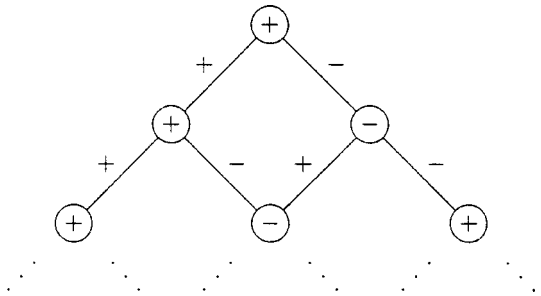

FIG. 2. Signs.

tensor [or indeed *any* nonzero (2,2)-form] cannot satisfy the stronger condition $C_{[ab}{}^{[de}\delta_{c]}^{f]}=0$ in dimensions $n\geqslant 5$; in addition we can conclude that there are absolutely no nonzero (2,2)-forms $T_{ab}{}^{cd}$ satisfying $T_{[ab}{}^{[ef}\delta_{c}^{g}\delta_{d]}^{h]}=0$ *in dimensions greater than five*.

From Theorem IV.6 we can conclude that there are no (2,2)-forms $R_{ab}{}^{cd}$ *with nonzero trace* (e.g., a Riemann tensor) satisfying the identity $R_{[ab}{}^{[ef}\delta_{c}^{g}\delta_{d]}^{h]}=0$ in dimensions $n=5$.

The trace in Lemma IV.3 is not the only trace that is possible for expressions of the type we are investigating. For completeness we here present the other possibility.

Lemma IV.8: Let $T^{\mathcal{A}}{}_{a_1\ldots a_k}{}^{cb_1\ldots b_l}=T^{\mathcal{A}}{}_{[a_1\ldots a_k]}{}^{c[b_1\ldots b_l]}$, k *and* $d\geqslant 0$ *and* $k+d>0$. *Then*

$$T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{c[b_1\ldots b_l}\delta_{a_{k+1}}^{b_{l+1}}\ldots\delta_{a_{k+d}}^{b_{l+d}]}\delta_{c}^{a_{k+d}}=\frac{d(-1)^{l+d-1}}{k+d}T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{[b_1\ldots b_l b_{l+1}}\delta_{a_{k+1}}^{b_{l+2}}\ldots\delta_{a_{k+d-1}}^{b_{l+d}]}+\frac{k(-1)^{k+d-1}}{k+d}T^{\mathcal{A}}{}_{c[a_1\ldots a_{k-1}}{}^{c[b_1\ldots b_l}\delta_{a_k}^{b_{l+1}}\ldots\delta_{a_{k+d-1}}^{b_{l+d}]}. \tag{50}$$

Proof: If k or d is zero the lemma is trivial. Assume they are nonzero.

Absorbing the last delta on the left-hand side gives

$$T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{c[b_1\ldots b_l}\delta_{a_{k+1}}^{b_{l+1}}\ldots\delta_{c]}^{b_{l+d}]}. \tag{51}$$

By summing over all possible positions of the lower dummy index c we get

$$\frac{(k+d-1)!}{(k+d)!}\sum_i c_i T^{\mathcal{A}}{}_{[a_1\ldots a_k}{}^{c[b_1\ldots b_l}\delta_{a_{k+1}}^{b_{l+1}}\ldots\delta_{|c|}^{b_i}\ldots\delta_{a_{k+d-1}}^{b_{l+d}]}, \tag{52}$$

where $c_i=\pm 1$ depending on whether the index configuration is an even or an odd permutaion.

When the c is on a delta it can be absorbed giving terms of the same type as the first term on the right-hand side of (50) There are d such terms and on each of them the indices have been moved a total of $l+d-1$ steps.

When the c is on T it can be moved to the first position of the lower indices giving terms of the same type as the second term on the right-hand side of (50). There are k such terms and on each of them the index has been moved a total of $k+d-1$ steps. □

V. APPLICATIONS

In the previous sections we have noted that, associated with each tensor are a number of fundamental identities; and it is from such identities that more involved and more subtle identities can be constructed, which in turn yield familiar identities. So, we shall now exploit our results in two particular types of applications.

A. Identities involving scalar invariants of Riemann tensors

Relationships between scalar invariants of tensors [such as (2), (3), and (32)] play a very important role in classical invariant theory, as well as in many practical applications. For instance, the study of the scalar invariants of the Riemann tensor in four dimensions has posed many interesting problems, which have not all been resolved.[3,5–9,16,17] The theorems given in this paper provide important tools for a systematic study of invariants of the Weyl, trace-free Ricci, and Lanczos tensors. However, now we shall just apply our results to some representative examples.

Example V.1: Although we can form different scalars from two (2,2)-forms $W_{ab}{}^{cd}$, in *four dimensions*, the simplest basic identity is $W^{[cd}{}_{[ef}\delta_{b]}^{a]}=0$ (with 6 free indices), and so we can immediately see that it cannot yield relationships between scalar invariants involving only two (2,2)-forms.

However, we already know that multiplying this identity by $W^{ef}{}_{ga}W^{bg}{}_{cd}$ gives us the scalar identity (32), which yields a relationship between some cubic scalar invariants; while multiplying by other quadratic terms will give different relationships between different cubic scalar invariants. Clearly we can also choose various suitable expressions involving three (2,2)-forms, which will yield scalar identities of fourth order when multiplied with $W^{[cd}{}_{[ef}\delta^{a]}_{b]}=0$. Hence, it is possible to investigate, for each order, all such possible relationships between all scalar invariants of that order.

When we consider higher dimensions we have analogous basic identities. In *five dimensions* the simplest basic identity is $W_{[ab}{}^{[ef}\delta^{g}_{c}\delta^{h]}_{d]}=0$ (with eight free indices), and hence the lowest order where we can get relationships between scalar invariants from this identity is also at third order; while in *six dimensions* with the simplest basic identity having 10 free indices there can exist no relationships between scalar invariants at third order coming from this identity. These results can be applied to the Weyl tensor, where they may simplify a little because of its extra symmetries.

It is interesting to note that Dianyan Xu's work[2] was motivated by a concern that nontrivial relationships might exist between counterterms in the Lagrangian (essentially invariant scalars constructed from products of the Riemann tensor) of a renormalizable quantum field theory; in particular, if his identities (2), (3), or any other cubic scalar identities, are true in six dimensions then work by Jack and Parker[4] would need to be reevaluated. However, Jack and Parker[5] have subsequently shown explicitly that no such third-order identities can exist in six dimensions; our result in the above-mentioned example agrees with this. Jack and Parker[5] have conjectured that in $2n$ dimensions there do not exist any identities between Riemann scalars of order n; we shall show how our results relate to this conjecture in a subsequent paper.

Example V.2: In order to confirm that the second identity found in Ref. 2 was a four-dimensional one, Harvey first established the intermediate third-order identity (5) by antisymmetrizing over *six* indices and this intermediate identity is therefore valid in five as well as in four dimensions; in our previous example we noted that five dimensions was the lowest dimension where such third-order identities could be constructed for the Weyl tensor. However, one would suspect that the second four-dimensional identity (3) could be obtained directly; this is confirmed by using the four-dimensional identity $C^{[cd}{}_{[ef}\delta^{a]}_{b]}=0$ and expanding $C^{ef}{}_{ai}C^{ib}{}_{cd}C^{[cd}{}_{[ef}\delta^{a]}_{b]}=0$. It can also be obtained, in the manner of Harvey, by antisymmetrizing over 5 indices and expanding

$$R^{ab}{}_{[ab}R^{ef}{}_{cd}R^{cd}{}_{e]f}=0. \tag{53}$$

Example V.3: An important application of the identity in Example IV.2 is to find relationships between scalar invariants of the Lanczos potential[11] in four dimensions. Since the identity $L_{[ab}{}^{[e}\delta^{f}_{c}\delta^{g]}_{d]}=0$ has seven free indices, the lowest order relationship between scalar invariants that we can obtain from it is of order four. For example, by expanding

$$0=L_{[ab}{}^{[e}\delta^{f}_{c}\delta^{g]}_{d]}L^{ab}{}_{e}L_{fg}{}^{h}L^{cd}{}_{h}, \tag{54}$$

we obtain the relationship

$$\begin{aligned}0=&L_{abc}L^{abc}L_{def}L^{def}+L_{abc}L^{abf}L_{def}L^{dec}-4L_{afc}L^{aec}L_{deh}L^{dfh}-2L_{abc}L^{abd}L_{def}L^{cef}\\&-4L_{abc}L^{ad}{}_{f}L^{bfh}L^{c}{}_{dh}.\end{aligned} \tag{55}$$

This of course will not be the only relationship; we could instead multiply the original identity by $L^{ab}{}_{e}L_{fh}{}^{c}L_{g}{}^{hd}$. Therefore, we can investigate all possible contractions of the original identity with three Lanczos tensors and find the corresponding relationship between all possible quartic Lanczos scalars in a systematic manner.

There is an important caveat in the above-given examples. By a systematic study we are able to obtain all relationships between scalar invariants of a particular order *which arise from our dimensionally dependent identities*. Of course, we would like to be able to conclude that we have obtained *all* such possible relationships. Recent work on invariant theory by Gover[18] links rela-

tionships involving scalar invariants of tensors in n dimensions to antisymmetrizing over $n+1$ indices. Although this does not, at this stage, enable us to conclude that all relationships between scalar invariants originate from our dimensionally dependent identities, it would lead us to believe that the results in this paper will be useful in such difficult tasks as determining complete and independent sets of scalar invariants, and their syzygies.

B. Simplifying complicated expressions in four dimensions

There have recently been situations[12–15] where rather complicated tensor expressions in n dimensions have been shown, unexpectedly, to be identically zero when specialized to four dimensions via Lovelock's theorems. So we would anticipate that the more general results obtained in this paper should also be useful in simplifying such expressions, and we now give some examples.

Example V.4: In Ref. 13 Lovelock's identities were used to show that, when the wave equation for the Weyl tensor is constructed from the Bianchi identities, the sum of terms which involve products of Weyl and trace-free Ricci tensors disappeared in *four, and only four, dimensions*, because from the four-dimensional identity $C_{[ab}{}^{[de}\delta_{c]}^{f]}=0$ we can obtain $C_{[ab}{}^{[de}\delta_{c]}^{f]}\tilde{R}_f{}^c=0$ whose left-hand side, when expanded, is precisely this sum of terms.

We shall now show that the analogous component of the Bel tensor[19] disappears in four dimensions by virtue of the same identity. The Bel tensor is given in n dimensions by

$$B_{abcd}=R_{aecf}R_b{}^e{}_d{}^f+R_{aedf}R_b{}^e{}_c{}^f-\tfrac{1}{2}g_{ab}R_{efcg}R^{ef}{}_d{}^g-\tfrac{1}{2}g_{cd}R_{aefg}R_b{}^{efg}+\tfrac{1}{8}g_{ab}g_{cd}R_{efgh}R^{efgh}. \tag{56}$$

When the standard decomposition is substituted we obtain[20]

$$B_{abcd}=\mathcal{T}_{abcd}+\mathcal{Q}_{abcd}+\mathcal{M}_{abcd}, \tag{57}$$

where $\mathcal{T}_{abcd}$ is the Bel–Robinson tensor consisting of quadratic terms in the Weyl tensor, $\mathcal{M}_{abcd}$ consists of quadratic terms in the Ricci tensor R_{ab}, and $\mathcal{Q}_{abcd}$ consists of products of Weyl and Ricci components (gravity-matter coupling term),[21]

$$\begin{aligned}\mathcal{Q}_{abcd}=\frac{1}{n-2}(&-4C^i{}_{(cd)(a}\tilde{R}_{b)i}-4C^i{}_{(ab)(c}\tilde{R}_{d)i}\\&+2\tilde{R}_{ij}(C_a{}^i{}_{(c}{}^j g_{d)b}-C_c{}^i{}_d{}^j g_{ab}+C_b{}^i{}_{(c}{}^j g_{d)a}-C_a{}^i{}_b{}^j g_{cd}))+\frac{2}{n(n-1)}R(C_{acbd}+C_{adbc}).\end{aligned} \tag{58}$$

The structure of $\mathcal{Q}$ (maximum of one delta, or equivalently as presented here with some indices lowered, maximum of one g) suggests that we investigate the *four-dimensional* identity $C_{[ac}{}^{[bd}\delta_{e]}^{f]}=0$; when we multiply this identity by $\tilde{R}^f{}_e$ we obtain the identity

$$C_{dij[a}g_{c]b}\tilde{R}^{ij}-C_{bij[a}g_{c]d}\tilde{R}^{ij}+C_{aci[b}\tilde{R}_{b]}{}^i+C_{bdi[a}\tilde{R}_{c]}{}^i=0. \tag{59}$$

By symmetrizing over the index pair (cd) we get precisely the identity

$$4C^i{}_{(cd)(a}\tilde{R}_{b)i}+4C^i{}_{(ab)(c}\tilde{R}_{d)i}-2\tilde{R}_{ij}(C_a{}^i{}_{(c}{}^j g_{d)b}-C_c{}^i{}_d{}^j g_{ab}+C_b{}^i{}_{(c}{}^j g_{d)a}-C_a{}^i{}_b{}^j g_{cd})=0 \tag{60}$$

and so the gravity–matter coupling term (58) simplifies, *in four dimensions*, to

$$\mathcal{Q}_{abcd}=R(C_{acbd}+C_{adbc})/6. \tag{61}$$

Bonilla and Senovilla[20] have obtained this result, but since they were working with duals, they did not encounter the four-dimensional identity explicitly; Zund[22] has also found the remarkably simple gravity–matter coupling term, using spinors.

The possibility of the *five-dimensional* identity $C_{[ab}{}^{[cd}\delta_e^f\delta_{h]}^{g]}=0$ supplying significant simplification is obviously ruled out since, after multiplication with one trace-free Ricci tensor, there will still be at least one term with two deltas.

Example V.5: The four-dimensional identity for the Lanczos potential $L_{ab}{}^c$,

$$2L^{def}g_{[a|c|}C_{b]def}-2L_{[a}{}^{de}C_{b]edc}-\tfrac{1}{2}L^{de}{}_cC_{deab}=0 \tag{62}$$

plays an important role in the derivation of the wave equation of the Lanczos potential.[23] Its existence was first noted because the spinor equivalence of the left-hand side collapsed; subsequently, it was proven by Edgar[12] by using four-dimensional duals, and also by using Lovelock's four-dimensional identity $C_{[ab}{}^{[cd}\delta_{e]}^{f]}=0$. We can also deduce it by using the four-dimensional identity in Example IV.2, and then expanding

$$L_{[ab}{}^{[c}\delta_d^f\delta_{e]}^{g]}C^{de}{}_{fg}=0. \tag{63}$$

The remaining examples involve identitities which cannot be deduced *directly* from Lovelock's identities.

Example V.6: In Ref. 16, Bonanos demonstrated that a complicated tensor

$$\begin{aligned}\chi'_{abcd}=&\tilde{R}_{ac}\tilde{R}_b{}^m\tilde{R}_{md}+\tilde{R}_{bd}\tilde{R}_a{}^m\tilde{R}_{mc}-\tilde{R}_{ad}\tilde{R}_b{}^m\tilde{R}_{mc}-\tilde{R}_{bc}\tilde{R}_a{}^m\tilde{R}_{md}+\tilde{R}_a{}^m\tilde{R}_m{}^n\tilde{R}_{nc}g_{bd}+\tilde{R}_b{}^m\tilde{R}_m{}^n\tilde{R}_{nd}g_{ac}\\&-\tilde{R}_a{}^m\tilde{R}_m{}^n\tilde{R}_{nd}g_{bc}-\tilde{R}_b{}^m\tilde{R}_m{}^n\tilde{R}_{nc}g_{ad}-\tfrac{1}{2}(\tilde{R}_{mn}\tilde{R}^{mn})(\tilde{R}_{ac}g_{bd}+\tilde{R}_{bd}g_{ac}-\tilde{R}_{ad}g_{bc}-\tilde{R}_{bc}g_{ad})\\&-\tfrac{1}{3}(\tilde{R}_{mn}\tilde{R}^{mr}\tilde{R}^n{}_r)(g_{ac}g_{bd}-g_{ad}g_{bc})\end{aligned} \tag{64}$$

of third order in the trace-free Ricci tensor $\tilde{R}_{ab}$, which had been used in the study of Riemann invariants in four dimensions,[17] was in fact, surprisingly, identically zero.

In Ref. 14 it was demonstrated how this result could be seen as an *indirect* consequence of Lovelock's results.[10] By applying Theorem III.2 to the trace-free Plebanski tensor $P_{ab}{}^{cd}$ which is the ''square'' of the Ricci tensor given by

$$P_{ab}{}^{cd}=2\tilde{R}_{[a}{}^{[c}\tilde{R}_{b]}{}^{d]}+2\tilde{R}_{[a}{}^i\tilde{R}_{|i|}{}^{[c}\delta_{b]}^{d]}-\tfrac{1}{3}\tilde{R}_j{}^i\tilde{R}_i{}^j\delta_{[a}^c\delta_{b]}^d, \tag{65}$$

the following identity of second order in the trace-free Ricci tensor was obtained:

$$2\tilde{R}_{[a}{}^{[c}\tilde{R}_b{}^d\delta_{e]}^{f]}+2\tilde{R}_{[a}{}^i\tilde{R}_{|i|}{}^{[c}\delta_b^d\delta_{e]}^{f]}-\tfrac{1}{3}\tilde{R}_j{}^i\tilde{R}_i{}^j\delta_{[a}^c\delta_b^d\delta_{e]}^f=0. \tag{66}$$

It was then shown in Ref. 14 that the identically zero tensor χ'_{abcd} found by Bonanos was just a direct consequence of multiplying the identity (66) by $\tilde{R}_f{}^e$.

But we now have the complete picture. The basic identity in four dimensions for the trace-free Ricci tensor is the first-order identity (39),

$$\tilde{R}_{[a}{}^{[c}\delta_b^d\delta_e^f\delta_{g]}^{h]}=0. \tag{67}$$

By successive multiplications by the trace-free Ricci tensor we obtain, first of all, the identity (66) which is second order in the trace-free Ricci tensor; subsequently by multiplying the left-hand side of (67) by $\tilde{R}_f{}^e\tilde{R}_h{}^g$ we obtain the third-order identity which is χ'_{abcd} identically zero, and finally the fourth-order identity, which is the Cayley–Hamilton theorem for the matrix representation of $\tilde{R}_a{}^b$ in four dimensions, as shown in Ref. 14.

Example V.7: The Bel–Robinson tensor[24] is given in n dimensions by

$$\mathcal{T}_{abcd}=C_{aecf}C_b{}^e{}_d{}^f+C_{aedf}C_b{}^e{}_c{}^f-\tfrac{1}{2}g_{ab}C_{efcg}C^{ef}{}_d{}^g-\tfrac{1}{2}g_{cd}C_{aefg}C_b{}^{efg}+\tfrac{1}{8}g_{ab}g_{cd}C_{efgh}C^{efgh}. \tag{68}$$

It is obviously symmetric over the first and last pair of indices, but in order to investigate its symmetry over *all* indices we need to examine,

$$\mathcal{T}_{a[bc]d}=\tfrac{1}{4}C_{adef}C_{bc}{}^{ef}-C_{eaf[b}C_{c]}{}^e{}_d{}^f-C_{fge[a}g_{d][b}C_{c]}{}^{efg}+\tfrac{1}{8}g_{a[b}g_{c]d}C_{efgh}C^{efgh}. \tag{69}$$

Its structure (maximum of two deltas) suggests that we investigate the five-dimensional identity $C_{[bc}{}^{[ad}\delta_e^g\delta_{f]}^{h]}=0$; by multiplying with $C_{gh}{}^{ef}$ we obtain precisely the right-hand side of (69). So the Bel–Robinson tensor is completely symmetric in both four and five dimensions, but of course this calculation does not give us any information about higher dimension. [Although we know that $C_{[ab}{}^{[cd}\delta_g^e\delta_{h]}^{f]}=0$ is *not* an identity in higher dimensions, we are considering the more complicated expression (69).] However, by taking the nontrivial double trace on (69) we obtain

$$\mathcal{T}^a{}_{[ab]}{}^b=\frac{(n-4)(n-5)}{16}C_{abcd}C^{abcd}, \tag{70}$$

which shows that the dimensions four and five are both necessary and sufficient conditions for the Bel–Robinson tensor to be completely symmetric.

The fact that $\mathcal{T}_{abcd}$ is completely symmetric, in, and only in, dimensions four and five was originally given by Senovilla[21] from its definition in terms of duals, but in a less direct manner, where each dimension was considered separately.

Example V.8: The Bel–Robinson tensor (constructed from the Weyl tensor), discussed in the last example, has the wrong dimension for energy, so Roberts[25] has proposed instead using an analogous construction with the Lanczos potential of the Weyl tensor which has the correct dimensions for energy. He has suggested looking at the most general expression quadratic in the Lanczos potential, but if instead we use Senovilla's definition of **super-energy tensor**[21] we find the super-energy tensor associated with the Lanczos potential $L_{ab}{}^c$ [a trace-free (2,1)-form] is given in n dimensions by

$$\mathcal{T}^L_{abcd}=L_{aec}L_b{}^e{}_d+L_{aed}L_b{}^e{}_c-\tfrac{1}{2}g_{ab}L_{efc}L^{ef}{}_d-g_{cd}L_{aef}L_b{}^{ef}+\tfrac{1}{4}g_{ab}g_{cd}L_{efg}L^{efg}. \tag{71}$$

It is obviously symmetric over the first and last pair of indices, respectively. It is not symmetric over all indices which can be shown by choosing a local orthonormalized basis and $L_{131}=-L_{311}=-L_{232}=L_{322}=1$, all others zero in n dimensions. Then $\mathcal{T}^L_{1[12]2}=\pm\frac{1}{2}$ (the sign depends on the signature).

The Bel–Robinson tensor in the previous example had the pairwise symmetry $\mathcal{T}_{abcd}=\mathcal{T}_{cdab}$. That symmetry can be imposed on the super-energy tensor for the Lanczos potential by examining

$$T^L{}_{abcd}=\tfrac{1}{2}\mathcal{T}^L_{abcd}+\tfrac{1}{2}\mathcal{T}^L_{cdab} \tag{72}$$

instead. In order to investigate whether this makes it symmetric over *all* indices we examine

$$T^{La}{}_{[bc]}{}^d=T^{L[a}{}_{[bc]}{}^{d]}=\tfrac{1}{4}L_{bce}L^{ade}-L^{[a}{}_{e[b}L_{c]}{}^{|e|d]}-\tfrac{1}{2}\delta^{[a}_{[b}L_{|ef|c]}L^{|ef|d]}-\delta^{[a}_{[b}L_{c]ef}L^{d]ef}$$
$$+\tfrac{1}{4}\delta^a_{[b}\delta^d_{c]}L_{efg}L^{efg}. \tag{73}$$

Its structure (maximum of two deltas) suggests that we investigate the four-dimensional identity $L_{[ef}{}^{[g}\delta_b^a\delta_{c]}^{d]}=0$. By multiplying with $L^{ef}{}_g$ we obtain the right-hand side of (73), so $T^L{}_{abcd}$ is completely symmetric in four dimensions and lower. It is, however, necessary to use the additional symmetry of the Lanczos potential $L_{[abc]}=0$ so this result does not hold for any (2,1)-form.

By taking the nontrivial double trace of (73) we obtain (by using $L_{[abc]}=0$ again)

$$T^{La}{}_{[ab]}{}^{b}=\frac{(n-4)(n-3)}{8}L_{abc}L^{abc}, \tag{74}$$

which shows that the dimension being four or less is both a necessary and sufficient condition for the symmetrized super-energy tensor $T^{L}{}_{abcd}$ for the Lanczos potential to be completely symmetric.

Although we can follow Senovilla's construction for the super-energy tensor from any (2,1)-form $L_{ab}{}^{c}$ in n dimensions, we should point out that the Lanczos potential for the Weyl tensor is unlikely to exist generally in dimensions above four.[15]

Example V.9: The four-dimensional algebraic Rainich identity associated with the energy momentum tensor $T^{a}{}_{b}=F^{a}{}_{c}F^{c}{}_{b}-\frac{1}{4}\delta^{a}_{b}F^{c}{}_{d}F^{d}{}_{c}$ of an electromagnetic field F_{ab} is given by

$$T^{a}{}_{c}T^{c}{}_{b}=\tfrac{1}{4}\,\delta^{a}_{b}T^{c}{}_{d}T^{d}{}_{c}\,. \tag{75}$$

When written out in full this identity is

$$F^{a}{}_{c}F^{c}{}_{d}F^{d}{}_{e}F^{e}{}_{b}-\tfrac{1}{2}F^{a}{}_{c}F^{c}{}_{b}F^{d}{}_{e}F^{e}{}_{d}-\tfrac{1}{4}\delta^{a}_{b}F^{c}{}_{d}F^{d}{}_{e}F^{e}{}_{f}F^{f}{}_{c}+\tfrac{1}{8}\delta^{a}_{b}F^{c}{}_{d}F^{d}{}_{c}F^{e}{}_{f}F^{f}{}_{e}=0. \tag{76}$$

But this is simply the Cayley–Hamilton theorem for $F^{a}{}_{b}$ as given in Example I.2,

$$F^{c}{}_{[c}F^{d}{}_{d}F^{e}{}_{e}F^{f}{}_{f}\delta^{a}_{b]}=0 \tag{77}$$

when specialized to antisymmetric F_{ab}. Equivalently the structure immmediately suggests specializing the four-dimensional identity for trace-free (1,1)-forms $F^{[f}{}_{[c}\delta^{g}_{d}\delta^{h}_{e}\delta^{a]}_{b]}=0$ given in (39) to antisymmetric forms, from which we obtain the identity

$$F^{[f}{}_{[c}\delta^{g}_{d}\delta^{h}_{e}\delta^{a]}_{b]}F^{c}{}_{f}F^{d}{}_{g}F^{e}{}_{h}=0 \tag{78}$$

which, when expanded and specialized to antisymmetric F_{ab}, is identical to (76)

A more direct way to obtain (76) is to expand

$$F^{cd}F^{ef}F_{[cd}F_{ef}\delta^{a}_{b]}=0. \tag{79}$$

VI. SUMMARY AND DISCUSSION

Of course, Lovelock's identities and our generalizations found in this paper are not really ''new'' since they are just simple and direct specializations of those fundamental identities found by antisymmetrizing over $n+1$ indices in n dimensions. Rather, the significance of these identities is that they highlight the fact that there exist heavily disguised versions of these fundamental identities when trace-free and antisymmetry properties are also introduced; and since we often are dealing with tensors with these explicit properties it is often the specializations of the fundamental identities which are relevant in practical applications.

The use of dimensionally dependent identities is a powerful method which has been largely overlooked, perhaps because of its simplicity. A very striking example of this is to be seen in the algebraic Rainich condition for the electromagnetic energy tensor in four dimensions. Over the past 75 years this condition has been obtained by a variety of very different methods: Rainich[26] used invariant planes, while others have used duality rotations,[27] complex duals,[28,29] and complicated matrix manipulation based on the Cayley–Hamilton theorem;[30] in spinors, a simple direct calculation has been given.[1] In fact Rainich's result was one of the motivations for Lovelock's work[10] and although he rederived the result using an explicit four-dimensional identity,[10,31] it is still a somewhat roundabout and contrived calculation. We have shown in example V.9 that the result can be viewed as simply the four-dimensional Cayley–Hamilton theorem when considered as a dimensionally dependent identity, or equivalently a trivial application of our basic result.

In this particular example, as in the others in Sec. V, we have been able to focus directly on the fundamental dimensionally dependent identity underlying the result. By identifying this un-

derlying identity in our various applications to four dimensions in this paper, we are in a position to explore directly the possibility of generalizations to other dimensions and to other forms. We shall present such generalizations in a subsequent paper.

Of course, it is possible to establish results peculiar to four dimensions without having to deal explicitly with dimensionally dependent identities; this is most easily done by using spinors, where the dimension is built into the formalism. Indeed, it was the apparent discrepency between results in spinors and tensors which originally gave the clue to the existence of a number of these four-dimensional identities. If we were only dealing with four-dimensional spaces with Lorentz signature, then spinors would be the more efficient formalism to use; on the other hand, the advantage of the tensor formalism is that once we have identified the underlying four-dimensional tensor identity, generalizations to other dimensions can be sought.

In a similar way, when explicit four-dimensional duals are used, then the dimension can also be built in by some of the identities satisfied by duals. For instance, the key identities associated with duals in work on super-energy tensors by Senovilla [Eqs. (2) and (3) in Ref. 21] have dimension n built in explicitly; so these are dimensionally dependent identities constructed from identities of the form

$$T^{A}_{[a_1}\eta_{a_2a_3\ldots a_{n+1}]}=0. \tag{80}$$

In this context, it is significant that the four-dimensional identity (31) is obtained in Ref. 21 essentially by taking double duals.

As emphasized in Sec. V, important applications of these results will be to Riemann tensors. Of course the Riemann tensor has additional symmetries to those of a (2,2)-form; these additional symmetries have not been explicitly considered in this paper, but would need to be considered explicitly in an exhaustive treatment of invariants of the Riemann tensor.

In conclusion, we emphasize that when examining what actually was required in the proofs of the theorems in Sec. IV one discovers that very little structure was needed. First, the results hold pointwise so the manifold structure is not needed. Second, there was no raising or lowering of indices so no assumption on what to use for that is needed; indeed not even the existence of such operations is needed. Third, no metric was used. This means that those theorems can be applied to objects other than tensors, e.g., spinors when $n=2$; matrices when the number of indices on the objects are appropriate; or other indexed objects such as Christoffel symbols or tensors in coordinate index notation or tetrad index notation.

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Singularity formation in 2+1 wave maps

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We present numerical evidence that singularities form in finite time during the evolution of $2+1$ wave maps from spherically equivariant initial data of sufficient energy. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1418717]

I. INTRODUCTION

While it has been shown that wave maps on a $1+1$-dimensional Minkowski spacetime base evolved from smooth initial data exist for all time,[1,2] and that those on an $m+1$ $(m\geqslant 3)$ Minkowski spacetime base can blow up in finite time,[3] the global existence for the $2+1$ case remains as yet unresolved. Scaling considerations identify $2+1$ as the critical dimension for wave maps, and so there is considerable interest in determining if indeed $2+1$ wave maps developed from smooth initial data can become singular in finite time or not. Here, we describe numerical work that strongly supports the contention that, at least for some sets of smooth initial data, they can.

There are special classes of $2+1$ wave maps for which global existence has been shown to hold: (a) spherically equivariant wave maps with convex,[4] or slightly more general targets,[5] (b) spherically symmetric wave maps with compact targets (plus a further technical condition on the target),[6] (c) general wave maps (general target) with sufficiently small energy.

Not included in any of these three classes are spherically equivariant wave maps from $2+1$ Minkowski spacetime into the round two-sphere with initial data of arbitrary energy. Shatah and Struwe[7] have conjectured that singular behavior should be found in this class. Our numerical results reported here strongly support the validity of this conjecture.

We examine one-parameter families of data, with small values of the parameter corresponding to small energy data and therefore global existence, and with large values of the parameter corresponding to data possibly leading to singularity formation. One might hope to find especially interesting wave map development for data at or near the transition between small and large values. While this sort of ''critical'' behavior has been seen and studied in $3+1$ wave maps,[8,9] we have not found nearly as clear an indication of universal critical behavior for the present $2+1$ case. This criticality issue needs further study, and is not treated in this paper. Here, our focus is on numerical evidence for singular wave map evolution from regular initial data.

We note that our studies of singularity formation in $2+1$ wave maps have been carried out independently of the work of Bizoń, Chmaj, and Tabor[10] using numerical algorithms that differ from theirs. However, their results and ours agree substantially.

II. THE EQUATIONS

Generally a wave map is defined to be a map ϕ^A from a spacetime (the ''base'') into a Riemannian geometry (the ''target''), with ϕ^A a critical point for the action

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$$S[\phi]=\int_{M^{m+1}}\eta^{\mu\nu}g_{AB}(\phi)(\partial_\mu\phi^A\,\partial_\nu\phi^B), \tag{1}$$

where g_{AB} is the Riemannian metric on the target manifold N^n, and $\eta^{\mu\nu}$ is the (inverse) Lorentz-signature metric on the spacetime M^{m+1}. The Euler–Lagrange equations for this action take the form

$$\partial^\mu\partial_\mu\phi^A+\Gamma^A_{BC}\,\partial_\mu\phi^B\,\partial^\mu\phi^C=0, \tag{2}$$

where Γ^A_{BC} represents the Christoffel symbols corresponding to the target metric g_{AB}. This is a semilinear hyperbolic PDE system for ϕ^A. We note that for certain targets, wave maps are known to physicists as ''nonlinear sigma models.''

As noted above, the case of primary interest here is $2+1$ Minkowski spacetime for the base and the round two sphere for the target. In this case, the wave map PDE system (2) may be rewritten in the following form:

$$\Box\phi^a+(\partial_\mu\phi^b\,\partial^\mu\phi^c)\,\delta_{bc}\phi^a=0, \tag{3}$$

where the indices a,b,c take the values $\{1,2,3\}$ (indexing the ambient Euclidean 3-space for the target two sphere), and δ_{bc} is the metric for this ambient space. If we now impose the condition that the maps ϕ^a be spherically equivariant with angular wrapping number k, and write $\phi^a(r,\theta,t)$ in the ''hedgehog'' form

$$\phi^a=\begin{pmatrix}\sin\chi(r,t)\sin k\theta\\ \sin\chi(r,t)\cos k\theta\\ \cos\chi(r,t)\end{pmatrix}, \tag{4}$$

where r is the radial distance from the origin and θ is the azimuthal angle; then the wave map PDE system (2) reduces to the single equation,

$$\ddot{\chi}=\frac{1}{r}(r\chi')'-\frac{k^2\sin 2\chi}{2r^2} \tag{5}$$

where a prime and an overdot denote partial derivatives with respect to r and t, respectively. Thus, the study of the Cauchy problem for $2+1$ spherically equivariant (k-wrapped) wave maps into the round two sphere focuses on finding solutions $\chi(r,t)$ to Eq. (5) with regular initial data $\chi(r,0),\dot{\chi}(r,0)$. Note that regularity at $r=0$ requires that we set $\chi(0,t)=0$ for all t.

While it may be interesting to examine if there is any variation of the behavior of solutions for wrapping numbers k greater than one, we restrict our attention here to the single angular wrapping case $k=1$.

As for any field theory on Minkowski space, there is a divergence-free stress–energy tensor $T_{\mu\nu}$ associated with wave maps. From $T_{\mu\nu}$, we obtain the energy density function for spherically equivariant wave maps,

$$\rho(r,t)=\frac{1}{2}[\dot{\chi}^2+(\chi')^2]+\frac{\sin^2\chi}{2r^2}, \tag{6}$$

whose integral

$$E(t)=\int_r\rho(r,t)r\,dr \tag{7}$$

is conserved [i.e., $E(t)=E(0)$ for all t]. The energy is a useful monitor of numerical accuracy, as discussed below.

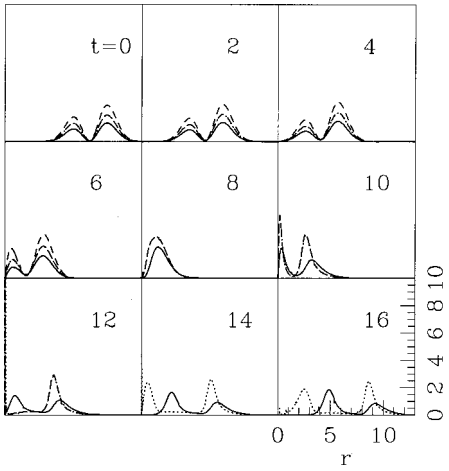

FIG. 1. Snapshots of the energy densities (times r) for a single family of initial data with varying amplitude. At $t=0$ the initial energy densities corresponding to ingoing Gaussian initial data ($R_0=8,\delta=2.3$) are shown. Supercritical ($A=1.4$) is shown as long-dashed line that exists only until $t=6$. Subcritical ($A=1.0$) is shown as a solid line. Two near-critical evolutions are also shown: slightly subcritical ($A=1.19$) is shown as a dotted line and slightly supercritical ($A=1.195$) is shown as a short-dashed line. The two near-critical evolutions coincide at the scale of this graph until $t=12$ after which we cannot compute the apparently singular supercritical solution. The energy densities reached by the supercritical solutions extend significantly off the scale of this graph.

III. NUMERICAL STUDIES OF SINGULARITY FORMATION

Our numerical experiments consist of specifying parametrized families of initial data $\{\chi_\lambda(r,0),\dot{\chi}_\lambda(r,0)\}$ and numerically evolving a number of sets of such data in each family. A typical family—one of the simplest—is the approximately ingoing Gaussian pulse,

$$\chi(r,0)=Ae^{-(r-R_0)^2/\delta^2}, \quad \dot{\chi}(r,0)=\chi'(r,0). \tag{8}$$

This family has three parameters A, R_0, and δ, with the most important one for our discussion being the scale parameter A. Note that the ingoing character of these solutions, which results from the choice of $\dot{\chi}(r,0)$, minimizes outer boundary effects. Note also that while, analytically, $\chi(0,0)$ is not zero, for the choices of R_0 and δ that we make, we can force $\chi(0,0)$ to be zero and retain smoothness to within numerical accuracy.

We evolve using a second-order finite difference approximation to Eq. (5). We use an iterative Crank–Nicholson scheme implemented with RNPL,[11] and also make use of the adaptive mesh framework developed by Choptuik.[12] We have verified that the code generates solutions that converge quadratically in the grid spacing and conserve energy. In arguing that we are indeed generating singularities, we will discuss the convergence and energy conservation tests in more detail below.

For a general set of ingoing Gaussian pulse data, regardless of amplitude, the wave map evolution has the pulse maximum and energy density maximum initially moving inward (decreasing r). For small (subcritical) values of A, this inward motion of the maximum proceeds for a finite time, after which the maximum ''bounces'' away from the origin and begins to move outward (see Fig. 1). There is a general dispersal of the energy density; and for large t, there is very little energy density remaining near the origin.

For large (supercritical) values of A, the behavior of the evolving wave map is qualitatively the same initially. However, rather than bouncing away from the origin, the maxima for supercritical data continue to approach the origin (Fig. 1), with the concentration of energy around the origin appearing to grow without bound. As the energy density and the gradient of the function χ grow very large at the origin, the numerical evolution inevitably becomes unable to resolve the gradient, and the solution becomes sufficiently nonsmooth to cause the numerical evolution to

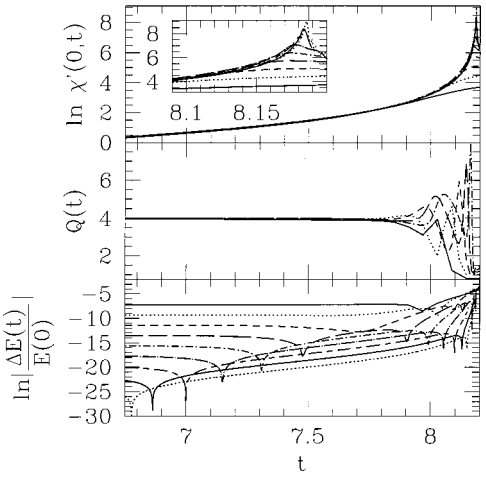

FIG. 2. Results of a supercritical evolution for an initially ingoing Gaussian pulse ($A=2, R_0=10, \delta=2.3, R_{\max}=30$). The results are shown for increasing resolutions $n=2^8$ (solid), $n=2^9$ (dot), $n=2^{10}$ (short dash), $n=2^{11}$ (long dash), $n=2^{12}$ (dot–short dash), $n=2^{13}$ (dot–long dash), $n=2^{14}$ (short dash–long dash), $n=2^{15}$ (solid), and $n=2^{16}$ (dot), where $h=R_{\max}/n$. The top frame shows the rapid growth of $\chi'(0,t)$ near the time of the blowup ($t\approx 8$). The middle frame shows the convergence factor [defined in Eq. (9)]. Factors greater than one indicate convergence. The bottom frame shows the change in energy with respect to the initial energy. As the resolution increases, so does the level of energy conservation.

stop. If this accumulation is indeed a singularity forming, there is no hope for the numerical evolution to resolve it, being itself of finite resolution. The task then is to examine the behavior of the numerical solution up to this point.

Before doing so, we first discuss a couple of standard tests of a numerical solution. We let $\chi(r,t)$ be some solution to the (continuum) partial differential equation (5) and let $\tilde{\chi}_h(r,t)$ be the solution to a discrete form of that equation, for corresponding initial data, on a grid spacing $h \equiv \Delta r$. The hope is that, as the grid spacing Δr gets smaller, the solutions to the discrete equation generated by the evolution code converge to the solutions of the PDE, $\tilde{\chi}(r,t)\to\chi(r,t)$. Because in general the explicit solutions to the PDE are unknown, we instead consider a series of numerical solutions on grids of increasing resolution, say $\tilde{\chi}_{4h}, \tilde{\chi}_{2h}, \tilde{\chi}_h$. If these are to converge to the PDE solution, then they must converge themselves. To examine this convergence, we define a convergence factor (Q) as follows:

$$Q \equiv \frac{|\tilde{\chi}_{4h}-\tilde{\chi}_{2h}|_2}{|\tilde{\chi}_{2h}-\tilde{\chi}_h|_2}, \tag{9}$$

where the norms are the l_2 norm. For these solutions to converge, the difference between solutions for increasing resolution must decrease and hence Q must be greater than one. For second-order schemes, Q is expected to be 4.

Another common test of numerical accuracy focuses on the degree to which energy is conserved by the numerical evolution. The evolution governed by the PDE (5) does conserve energy; the question is whether this remains true for the numerical evolution. Letting $E_{\rm num}(t)$ denote the energy calculated from the numerical solution at time t (on the finite grid), and setting $\Delta(t) \equiv \ln|(E_{\rm num}(t)-E_{\rm num}(0))/E_{\rm num}(0)|$, we monitor $\Delta(t)$ for different choices of grid spacing. The expectation is that $\Delta(t)$ should decrease with increasing resolution; if we observe this, our confidence in the accuracy of our numerical solution is enhanced.

In Fig. 2, we show the evolution in time of three quantities—$\ln\chi'(0,t)$, $Q(t)$, and $\Delta(t)$—for numerical runs of supercritical ingoing Gaussian pulse data, done with nine different grid spacings. In the top frame, we show the behavior of the derivative of χ at the origin as a function of time. The figure shows that as the pulse travels inward, the derivative increases. Until just before $t=8$, all the resolutions show the same behavior as would be expected for a convergent evolution.

However, near the blow-up time, the solutions diverge with higher resolutions providing a larger derivative. The convergence factor $Q(t)$ is shown in the middle frame; it likewise shows second-order convergence up to times close to the blow-up time. In the bottom frame, the change in energy $\Delta(t)$ is shown. We see that as the resolution is increased, energy conservation improves.

What does this tell us about singularity formulation in wave maps evolved from (supercritical) ingoing Gaussian pulse data? We first argue that these results are consistent with what would be expected for such a formation. As the singularity forms, higher- and higher-frequency components become important, and they are represented numerically only if one uses higher and higher grid resolutions. Hence, the behavior of the derivative of χ as the resolution improves would be expected to show larger and larger gradients, as seen in Fig. 2(a). Next, we note that the formation of a singularity should not hinder convergence except quite near the formation time, as is seen in Fig. 2(b). Finally, energy conservation should be fine until the high-frequency components play their role, as we see in Fig. 2(c). Hence, the results observed appear to be consistent with a singularity forming near $t=8$.

This does not guarantee that a singularity forms in these wave maps. There are other effects that might produce the apparently unbounded growth of the derivative of χ and of the energy density near the origin in these numerical simulations. For example, perhaps some unphysical, unstable mode grows because of the particulars of our chosen evolution scheme. We believe that this is not the case, for a number of reasons. First, the presence of such a mode would likely cause much larger growth in $\Delta(t)$ than we see. Second, such modes would have to be excited only after some time (roughly independent of resolution) and only for families of sufficiently large energy. This is not consistent with our observations. Third, the excitation of this sort of instability would almost certainly depend critically on the precise finite difference scheme. Because Bizoń and his collaborators[10] observe similar behavior, using a different numerical evolution scheme, this does not appear to be the case. Thus, we believe it very unlikely that the effects we are seeing are the result of a numerically unstable nonsingular mode.

Another situation in which one might numerically observe the formation of singularities that do not, in fact, evolve analytically from the corresponding data is if the continuum PDE solution is regularized by high-frequency components which cannot be seen by the finite grid resolutions we use. The rather strong convergence behavior we see in our numerical solutions leads us to believe that this is not happening. We note in particular that such unresolved components would have to be separated in frequency space from the nontrivial low-frequency components by a substantial margin, with a large range of dynamically irrelevant frequencies separating the two regimes. This seems to be very unlikely.

IV. CONCLUSION

The numerical studies we present here very strongly support the contention, previously conjectured by Shatah and Struwe,[7] that smooth initial data for wave maps from $2+1$ Minkowski spacetime into the round two sphere can develop singularities (with unbounded derivatives) in finite time. As we note, there are many ways in which the numerical exploration of possible singularity formation might produce misleading indications. However, we believe that as a consequence of the numerical tests we have carried out, together with those done independently by Bizoń and his collaborators,[10] the formation of singularities is the most likely conclusion.

There is much more one would like to know about these spatially equivariant wave maps, as well as about those without such symmetry. One would like to know, for example, if the solutions assume any universal form as one approaches the singularity. Our work (see Fig. 3) supports the results of Bizoń *et al.*,[10] which indicate that indeed the family of static spherically equivariant wave maps,

$$\chi(r)=\pm 2\arctan(\lambda r), \tag{10}$$

does serve as a sort of universal model for singularity formation. This needs to be studied further. One would also very much like to understand the behavior of the wave maps that evolve from

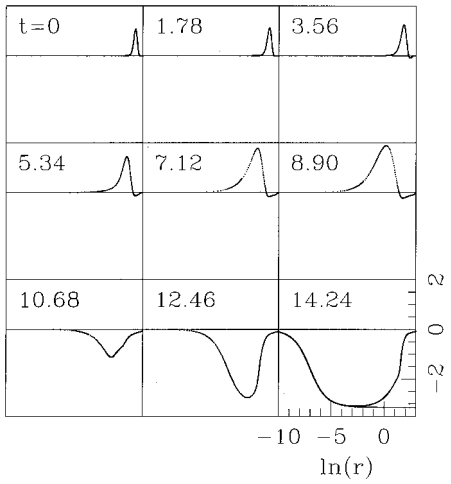

FIG. 3. Near-critical evolutions approach the static solution, Eq. (10). Nine frames equally spaced in time are shown for both *sub*- and *super*critical evolutions. The solutions are indistinguishable in the graph at these times and are shown with dots. After $t=14.24$, the two solutions have quite different fates, but both approach the form of the static solution. In the final frame, the static solution $\chi(r)=-2\arctan(1116r)$ is shown.

initial data near the transition from subcritical to supercritical data. The recent numerical work of Bizoń *et al.*[10] suggests that the static solutions (10) play a central role in the evolution of the transitional wave maps as well in that of supercritical ones; however, this issue needs further investigation. (Note the absence of any self-similar solutions to the $2+1$ wave map equations; for $3+1$ wave maps, such solutions play a key role in the behavior of solutions evolving from critical or near critical data).

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Uniqueness of a convex sum of products of projectors

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Relative to a given factoring of the Hilbert space, the decomposition of an operator into a convex sum of correlated products of pairs of distinct 1-projectors, one set of projectors linearly independent, is unique. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Utilizing the Tridecompositional Uniqueness Theorem of Elby and Bub,[1] I establish the uniqueness, relative to a given factoring of the Hilbert space, of a decomposition of a state operator into a convex sum of correlated products of pairs of distinct 1-projectors,

$$\boldsymbol{\rho}=\sum_j w_j|a_j\rangle\langle a_j|\otimes|b_j\rangle\langle b_j|, \tag{1}$$

one set of projectors linearly independent.

In the Appendix, I present a slightly strengthened version and simplified proof of the Tridecompositional Uniqueness Theorem.

For the remainder of this paper I use the notation $|a_jb_k\rangle$ for the direct product $|a_j\rangle\otimes|b_k\rangle$.

II. PRELIMINARIES

All vectors are normalized.

Definition 1: $|a\rangle$ and $|b\rangle$ are collinear iff $|a\rangle=e^{i\alpha}|b\rangle$, $\alpha\in\mathcal{R}$; we denote this $|a\rangle\|b\rangle$.

Definition 2: The set $\{|a_j\rangle\}$ is noncollinear iff no pair of the set is collinear.

Definition 3: $\boldsymbol{\rho}$ is an operator on $\mathcal{H}_1\otimes\mathcal{H}_2$. The null space of $\boldsymbol{\rho}$ on $\mathcal{H}_\alpha$ is $\mathcal{N}_\alpha\doteq\{|\phi\rangle\in\mathcal{H}_\alpha|\rho|\phi\rangle=0\}$ $(\alpha\in\{1,2\})$.

Lemma 1: *With sets* $\{|a_j\rangle\in\mathcal{H}_1\}$, $\{|b_j\rangle\in\mathcal{H}_2\}$, *and* $\{w_j>0\}$, $j\in\{1\cdots N\}$, *and the operator* $\boldsymbol{\rho}=\Sigma w_j|a_jb_j\rangle\langle a_jb_j|$, *the set* $\{|a_j\rangle\}$ *spans* $\mathcal{G}_1\doteq(\mathcal{N}_1)^\perp$ *and the set* $\{|b_j\rangle\}$ *spans* $\mathcal{G}_2\doteq(\mathcal{N}_2)^\perp$.

Proof: For $|\phi\rangle\in\mathcal{N}_1$ and any $|\beta\rangle\in\mathcal{H}_2$, $\langle\phi\beta|\boldsymbol{\rho}|\phi\beta\rangle=0=\Sigma w_j|\langle a_j|\phi\rangle|^2|\langle b_j|\beta\rangle|^2$; thus $\langle a_j|\phi\rangle=0\forall|\phi\rangle\in\mathcal{N}_1$, so $|a_j\rangle\in(\mathcal{N}_1)^\perp=\mathcal{G}_1$. If $\{|a_j\rangle\}$ does not span $\mathcal{G}_1$, there is a vector in $\mathcal{G}_1$ orthogonal to $\{|a_j\rangle\}$; but any such vector is annihilated by ρ and is thus in $\mathcal{N}_1$, a contradiction.□

The following result appears in Ref. 2, in the midst of the proof of another theorem:

Lemma 2: $|\Psi\rangle$ *and* $|\Phi\rangle$ *are vectors in* $\mathcal{H}_1\otimes\mathcal{H}_2$. *If* $\mathrm{Tr}_2\{|\Psi\rangle\langle\Psi|\}=\mathrm{Tr}_2\{|\Phi\rangle\langle\Phi|\}$, *then there exists a unitary transformation* $\mathbf{U}$ *on* $\mathcal{H}_2$ *such that* $|\Psi\rangle=(1\otimes\mathbf{U})|\Phi\rangle$.

III. THE UNIQUENESS THEOREM

Theorem 1: *With noncollinear sets* $\{|a_j\rangle\in\mathcal{H}_1\}$ *and* $\{|b_j\rangle\in\mathcal{H}_2\}$, $j\in\{1\cdots n\}$, *one set linearly independent, and with noncollinear sets* $\{|A_k\rangle\in\mathcal{H}_1\}$ *and* $\{|B_k\rangle\in\mathcal{H}_2\}$, $k\in\{1\cdots N\}$, *one set linearly independent, and with sets* $\{w_j>0\}$ *and* $\{W_k>0\}$, *if*

$$\sum_{j=1}^{n} w_j|a_jb_j\rangle\langle a_jb_j|=\sum_{k=1}^{N} W_k|A_kB_k\rangle\langle A_kB_k|,$$

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then $N=n$, *and, for all* $j\in\{1\cdots n\}$,

$$|A_j\rangle\|\,|a_{\pi(j)}\rangle,\quad |B_j\rangle\|\,|b_{\pi(j)}\rangle,\quad \textit{and}\quad W_j=w_{\pi(j)},$$

with $\pi(\cdot)$ *a permutation function on* $\{1\cdots n\}$.

Proof: Call the operator $\boldsymbol{\rho}$. Apply Lemma 1, with $d_1\doteq\dim\mathcal{G}_1$ and $d_2\doteq\dim\mathcal{G}_2$, and recall: A set of m vectors spans a space of dimension $d\leqslant m$; $d=m$ iff the vectors are linearly independent. Without loss of generality we take the set $\{|a_j\rangle\}$, which spans $\mathcal{G}_1$, to be linearly independent; thus $n=d_1$. Either $\{|A_k\rangle\}$ or $\{|B_k\rangle\}$ must be linearly independent; in either case, $N=n$: If $\{|A_k\rangle\}$ is linearly independent, then $N=d_1=n$. On the other hand, if $\{|B_k\rangle\}$ is linearly independent, then $N=d_2$; the n vectors $\{|b_j\rangle\}$ must span $\mathcal{G}_2$, hence $n\geqslant d_2=N$. Similarly, the N vectors $\{|A_k\rangle\}$ must span $\mathcal{G}_1$, hence $N\geqslant d_1=n$, thus $N=n$.

Introduce a third Hilbert space $\mathcal{H}_3$, with $\dim\mathcal{H}_3\geqslant n$; $\{|c_j\rangle\}$ and $\{|C_j\rangle\}$ are orthonormal bases of $\mathcal{H}_3$. Construct the two vectors,

$$|\psi\rangle=\sum_{j=1}^{n}\sqrt{w_j}|a_jb_jc_j\rangle\ \text{ and }\ |\Psi\rangle=\sum_{j=1}^{n}\sqrt{W_j}|A_jB_jC_j\rangle;$$

clearly, $\boldsymbol{\rho}=\mathrm{Tr}_3\{|\psi\rangle\langle\psi|\}=\mathrm{Tr}_3\{|\Psi\rangle\langle\Psi|\}$. By Lemma 2, there exists a unitary transformation $\mathbf{U}$ on $\mathcal{H}_3$ such that $|\psi\rangle=(1\otimes1\otimes\mathbf{U})|\Psi\rangle$; defining $|D_j\rangle\doteq\mathbf{U}|C_j\rangle$, we have

$$\sum_{j=1}^{n}\sqrt{w_j}|a_jb_jc_j\rangle=\sum_{j=1}^{n}\sqrt{W_j}|A_jB_jD_j\rangle,$$

to which we apply Theorem A. □

IV. DISCUSSION

"Uniqueness" is relative to the identification of system and apparatus. Elby and Bub claim that Eq. (1) "suffers from a version of the basis degeneracy problem." For example, with $\langle a_1|a_2\rangle=\langle b_1|b_2\rangle=0$, the sum-of-products expression

$$\boldsymbol{\rho}=\tfrac{1}{2}|a_1b_1\rangle\langle a_1b_1|+\tfrac{1}{2}|a_2b_2\rangle\langle a_2b_2| \tag{2}$$

(which, according to Theorem 1, is unique) is the diagonalization of a degenerate Hermitian operator (with eigenvalues 1/2 twice, and 0 twice). The eigenvectors may be taken to be $|a_1b_1\rangle$, $|a_2b_2\rangle$, $|a_1b_2\rangle$ and $|a_2b_1\rangle$—products of vectors taken pairwise from $\mathcal{H}_1$ and $\mathcal{H}_2$. Because of this degeneracy, we can rotate the eigenvectors into $|q_{1,2}\rangle=2^{-1/2}(|a_1b_1\rangle\pm|a_2b_2\rangle)$, $|q_3\rangle=|a_1b_2\rangle$, and $|q_4\rangle=|a_2b_1\rangle$. Then Eq. (2) may be written

$$\boldsymbol{\rho}=\tfrac{1}{2}|q_1\rangle\langle q_1|+\tfrac{1}{2}|q_2\rangle\langle q_2|; \tag{3}$$

"the pointer reading loses its 'special' status."

This argument is flawed—after all, the same claim may be made against the tridecompositional uniqueness theorem itself:

$$|\Psi\rangle=\frac{1}{\sqrt{2}}(|a_1b_1c_1\rangle+|a_2b_2c_2\rangle)=\frac{1}{\sqrt{2}}(|q_1d_1\rangle+|q_2d_2\rangle), \tag{4}$$

with $|d_{1,2}\rangle=2^{-1/2}(|c_1\rangle\pm|c_2\rangle)$. Equation (4) is no more a counterexample to the tridecompositional uniqueness theorem than Eq. (3) is a counterexample to Theorem 1, and for the same reason: the "special" nature of a pointer basis is based on the uniqueness of the form of the

decomposition in Eq. (1), which in turn is based on a particular identification of system and apparatus. One cannot speak of the ''pointer basis'' without having settled on the ''pointer''—the apparatus—thus having already specified the factor spaces.

Only having chosen a fixed identification of the subsystems (and the associated factoring of the space) may either of these uniqueness theorems then be applied.

APPENDIX: THE TRIDECOMPOSITIONAL UNIQUENESS THEOREM

This version of the Tridecompositional Uniqueness Theorem[1] avoids two assumptions of the original: that the linearly dependent set is in the same space in each expansion, and that the expansions each have the same number of terms. The proof here is similar to that of Ref. 1, but is considerably shorter and, perhaps, clearer.

Definition A: $|\Psi\rangle$ is factorable in $\mathcal{H}_1\otimes\mathcal{H}_2$ iff there exist $|\alpha\rangle\in\mathcal{H}_1$ and $|\beta\rangle\in\mathcal{H}_2$ such that $|\Psi\rangle=|\alpha\beta\rangle$.

Lemma A (Similar to Lemma 1 of Ref. 1): *With the set* $\{|a_j\rangle\in\mathcal{H}_1\}$ *linearly independent and the set* $\{|b_j\rangle\in\mathcal{H}_2\}$ *noncollinear,* $|\Psi\rangle=\Sigma_j s_j|a_j b_j\rangle$ *is factorable in* $\mathcal{H}_1\otimes\mathcal{H}_2$ *iff the set* $\{s_j\in\mathcal{C}\}$ *contains exactly one nonzero element.*

Proof: Let $|\Psi\rangle=|\alpha\beta\rangle$, with $|\alpha\rangle\in\mathcal{H}_1$ and $|\beta\rangle\in\mathcal{H}_2$. Expand $|\alpha\rangle=\Sigma_j a_j|a_j\rangle$, so $|\Psi\rangle=\Sigma_j a_j|a_j\beta\rangle$; the set $\{|a_j\rangle\}$ is linear independent, so, for each j, $a_j|\beta\rangle=s_j|b_j\rangle$. For every $s_j\neq 0$, $|b_j\rangle\|\,|\beta\rangle$. If more than one $s_j\neq 0$, $\{|b_j\rangle\}$ is not noncollinear, contrary to hypothesis, contradicting the assumption of factorability. The converse is obvious. □

Theorem A (Tridecompositional uniqueness): *With noncollinear sets* $\{|a_j\rangle\in\mathcal{H}_1\}$, $\{|b_j\rangle\in\mathcal{H}_2\}$, *and* $\{|c_j\rangle\in\mathcal{H}_3\}$, $j\in\{1\cdots n\}$, *two sets linearly independent, and noncollinear sets* $\{|A_k\rangle\in\mathcal{H}_1\}$, $\{|B_k\rangle\in\mathcal{H}_2\}$, *and* $\{|C_k\rangle\in\mathcal{H}_3\}$, $k\in\{1\cdots N\}$, *two sets linearly independent, and sets* $\{\phi_j\in\mathcal{C}|\,\phi_j\neq 0\}$ *and* $\{\varphi_k\in\mathcal{C}|\varphi_k\neq 0\}$, *if*

$$\sum_{j=1}^{n}\phi_j|a_j b_j c_j\rangle=\sum_{k=1}^{N}\varphi_k|A_k B_k C_k\rangle,$$

then $N=n$, *and, for all* $j\in\{1\cdots n\}$,

$$|A_j\rangle\|\,|a_{\pi(j)}\rangle,|B_j\rangle\|\,|b_{\pi(j)}\rangle,\quad |C_j\rangle\|\,|c_{\pi(j)}\rangle,\ \text{and}\ |\varphi_j|=|\phi_{\pi(j)}|,$$

with $\pi(\cdot)$ *a permutation function on* $\{1\cdots n\}$.

Proof: Take $\{|C_k\rangle\}$ and $\{|c_j\rangle\}$ to be linearly independent (with no loss of generality: in each expansion, two of the three sets are linearly independent, requiring coincidence in at least one space). These sets must span the same subspace of $\mathcal{H}_3$; thus $N=n$. Expand $|c_j\rangle=\Sigma_k\gamma_{jk}|C_k\rangle$; then $\varphi_k|A_k B_k\rangle=\Sigma_j\phi_j\gamma_{jk}|a_j b_j\rangle$. For each k, Lemma A requires $\gamma_{jk}=0$ for all but one j; define the function π: $\{1\cdots n\}\to\{1\cdots n\}$ by the relation $\gamma_{\pi(k)k}\neq 0$. We have $|c_{\pi(k)}\rangle=\gamma_{\pi(k)k}|C_k\rangle$, so $|c_{\pi(k)}\rangle\|\,|C_k\rangle$ (and normalization requires $|\gamma_{\pi(k)k}|=1$). Because the set $\{|C_k\rangle\}$ is noncollinear, $\pi(\cdot)$ must be 1:1, i.e., a permutation function on $\{1\cdots n\}$. We also have $\varphi_k|A_k B_k\rangle=\phi_{\pi(k)}\gamma_{\pi(k)k}|a_{\pi(k)}b_{\pi(k)}\rangle$, so $|a_{\pi(k)}\rangle\|\,|A_k\rangle$ and $|b_{\pi(k)}\rangle\|\,|B_k\rangle$; normalization requires $|\varphi_k|=|\phi_{\pi(k)}|$. □

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New cohomology ring for supermanifolds

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In this paper the concept of pesudodifferential forms on supermanifolds is extended and a new complex is introduced. At last it is shown that the corresponding cohomology ring is sensitive to ''super'' structure. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1416888]

I. INTRODUCTION

Supermanifolds, in local view, are spaces with commuting and anticommuting variables. Supermanifolds provide a framework for quantum field theory. In this regard, one can consider fermion fields as anticommuting fields.

In order to understand the geometry and topology of supermanifolds, different concepts of differential geometry have been extended to supermanifolds. However, some concepts have not found any satisfactory generalization. Characteristic classes is an example. In conventional differential geometry, there is a duality between characteristic classes and Schubert cells.[1] Although the superanalog of Schubert cells defined,[2] it is not clear in what homology theory these supercells are closed.[3] It seems that homology classes corresponding to supercells are in cyclic cohomology of a proper algebra. Since there is a correspondence between cyclic cohomology classes and cycles $(\Omega,d,\int)$ where (Ω,d) is a differential graded algebra and $\int$ is a closed trace on Ω,[4] thus proper generalization of differential forms, exterior differential operator and integration lead to find cyclic cohomology classes, different from the ones associated with underlying manifold. One cycle is defined by Monge in Refs. 5, 6. In Ref. 5 a $\mathbf{Z}^2$-graded de Rham like cohomology developed which is not determined by cohomology of its underlying manifold and has a functorial definition within the category of supermanifolds. An integration theory is extended for these $\mathbf{Z}_2$-forms in Ref. 6. Establishing Stokes theorem shows that the integral is a closed trace. But projection which is used in the definition of an integral causes the fast elimination of odd variables. So its cycle does not seem to define a new invariant for supermanifolds.

In this paper we extend $\mathcal{P}$, the algebra of pseudodifferential forms, to an algebra of matrices over $\mathcal{P}$, in rough statement. This idea comes from the point which Connes made in Ref. 4. There, he proves the Gauss–Bonnet theorem for Σ, smooth closed surface in $\mathbf{R}^3$, by considering the algebra of 2×2 matrices with entries in $C^\infty(\Sigma)$.

At last we show that the corresponding cohomology ring is sensitive to a ''super'' structure. This provides a counterexample for the conjecture of Voronov.[5]

Integration theory is introduced in the coming paper.

II. PRELIMINARIES

Let M be a topological space and $\mathcal{A}$ be a sheaf of $\mathbf{Z}_2$-graded commutative real algebras on M. By a real supermanifold with dimension (m,n) we mean a pair $(M,\mathcal{A})$ with the following conditions.

(i) M is a second countable Hausdorff space.

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(ii) For every point $m \in M$ there exists a neighborhood U in which $\mathcal{A}|_U$ is isomorphic to $C^\infty(U)\otimes\wedge\mathbf{R}^n$ as the sheaves of $\mathbf{Z}_2$-graded commutative algebras. U is called a splitting neighborhood. Let $z^1,\ldots,z^m$ be a coordinate function on U and $e^1,\ldots,e^n$ be a basis for $\mathbf{R}^n$. Then z^i's are called even coordinates and e^j's are called odd coordinates.

Let $T_{\mathcal{A}}$ be the sheaf of derivations of $\mathcal{A}$. A $\mathbf{R}$-linear map $X:\mathcal{A}\to\mathcal{A}$ is called a derivation if $X(ab)=X(a)b+(-1)^{\tilde{a}\tilde{X}}aX(b)$ where $\tilde{a}$ and $\tilde{X}$ are degrees (or parities) of a and X according to $\mathbf{Z}_2$-graded structures of $\mathcal{A}$ and $\mathrm{Hom}(\mathcal{A},\mathcal{A})$, respectively.[7]

This sheaf is locally free and is generated by $\{\partial/\partial z^j, \partial/\partial e^i\}$. These derivations have the same parity as the coordinates $\{z^i,e^j\}$. The cotangent sheaf Ω^1_M can be defined as $\mathrm{Hom}_{\mathcal{A}}(T_{\mathcal{A}},\Pi\mathcal{A})$. Here Π can be considered as a formal factor of degree 1 and $\Pi\mathcal{A}$ is an $\mathcal{A}$-module such that

$$\Pi a+\Pi b=\Pi(a+b),$$

$$a(\Pi b)=(-1)^{\tilde{a}}\Pi(ab).$$

Locally, Ω^1_M is generated by $\{dz^i,de^j\}$. Obviously these differentials are of a parity opposite to the parity of coordinates $\{z^i,e^j\}$. Thus the elements $\partial/\partial z^j, de^i$ are commutative and $\partial/\partial e^j, dz^i$ are anticommutative. It is natural to consider functions $\omega(z^i,e^j,\partial/\partial z^i,de^j,dz^i,\partial/\partial e^j)$ which depend on commuting differentials as infinitely differentiable functions.[8] Berezine calls them pseudodifferential forms.

The sheaf of such forms, denoted by $\mathcal{P}$, is Grassmann algebra with generators $\partial/\partial e^j, dz^i$, and a coefficient in $\mathcal{P}_0$, the sheaf of smooth functions of $z^i,e^j,\partial/\partial z^i,de^j$.

III. EXTENDED BEREZIN PESUDODIFFERENTIAL FORMS

On pseudodifferential forms, Berezine introduced the differential

$$d=\sum_i dz^i\frac{\partial}{\partial z^i}+\sum_j de^j\frac{\partial}{\partial e^j}+\sum_i dw^i\frac{\partial}{\partial w^i}+\sum_j dt^j\frac{\partial}{\partial t^j},$$

where $w^i=\partial/\partial z^i$ and $t^j=de^j$.

Obviously the action of d does not produce integral forms. Thus in order to make a complete analogy with a de Rham complex we extend d. For this, it is necessary to have a proper extension of $\mathcal{A}$.

The sheaf of $T_{\mathcal{A}}$ is a locally free sheaf of $\mathcal{A}$-modules. It is locally generated by $\{\partial/\partial z^i, \partial/\partial e^j\}$. The parities of $\partial/\partial z^i$ and $\partial/\partial z^j$ are 0 and 1, respectively. Denote by τ_M the sheaf of algebras which is generated by $T_{\mathcal{A}}$ over $\mathcal{A}$. Obviously τ_M has a structure of a real supermanifold with dimension $(2m,2n)$ and is called a supermanifold that corresponds to $T_{\mathcal{A}}$. For this consider the homomorphism of algebras induced by transition maps due to the splitting representation of $T_{\mathcal{A}}$.

Denote by δ_M the supermanifold corresponding to ΠT_{τ_M}.

Now consider the sheaf $\mathcal{E}_M$ of all endomorphism φ on ΠT_{τ_M}.

Definition 3.1: By the extended pesudodfferential forms we mean the elements of $\mathcal{P}\otimes\mathcal{E}_M$.

There is a structure of algebra on $\mathcal{P}\otimes\mathcal{E}_M$ which is defined by

$$(a\otimes\varphi)\cdot(b\otimes\psi)=ab\otimes\varphi\psi;$$

let $\Omega^{p,q}(U)$ be a $\mathcal{A}(U)$-module with generators

$$\left\{dz^{i_1}\ldots dz^{i_k}\frac{\partial}{\partial e^{j_1}}\ldots\frac{\partial}{\partial e^{j_l}},\frac{\partial}{\partial z^{t_1}}\ldots\frac{\partial}{\partial z^{t_s}}de^{r_1}\ldots de^{r_u},k+l=p\ s+u=q\right\};$$

any element of algebra on $\Omega^{p,q}(U)\otimes\mathcal{E}_M$ is called a (p,q) form. There is also a differential on the algebra of all extended pesudodifferential forms defined as follows:

$$\tilde{d}(a\otimes\varphi)=\sum_{z^i} dz^i\left(\frac{\partial}{\partial z^i}a\right)\otimes\varphi+\sum_{z^i} de^i\left(\frac{\partial}{\partial e^i}a\right)\otimes\varphi+(-1)^{\tilde{a}}\sum_{e^j} a\otimes\frac{\partial}{\partial e^j}L_{\Pi\,\partial/\partial\,(\partial/\partial e^j)}\varphi$$
$$+(-1)^{\tilde{a}}\sum_{z^i} a\otimes\frac{\partial}{\partial z^i}L_{\Pi\,\partial/\partial\,(\partial/\partial z^i)}\varphi. \tag{1}$$

By $L_{\Pi[\partial/\partial(\partial/\partial e^j)]}\varphi$ we mean the Lie derivation along $\Pi[\partial/\partial(\partial/\partial e^j)]$. For this, consider φ as a 1.1 tensor on τ_M. Then the Lie derivative of the covariant component, say ω, is just $(d\bigcirc i(\Pi[\partial/\partial(\partial/\partial e^j)])+i(\Pi[\partial/\partial(\partial/\partial e^j)])\bigcirc d)(\omega)$ and the Lie derivative of contravariant component, say X, is $[X,\Pi[\partial/\partial(\partial/\partial e^j)]]$. A straightforward computation shows the following.

Proposition 3.2: $\tilde{d}$ does note depend upon the choice of coordinates.

Proof: The first two summations on the left-hand side of the equality in (1) obviously make an invariant statement under the change of coordinates. Now consider the last two summations. Let $y^k=y(z^i,e^j), f^l=f(z^i,e^j)$ be a new coordinate; we have

$$\frac{\partial}{\partial e^j}=\frac{\partial y^k}{\partial e^j}\frac{\partial}{\partial y^k}+\frac{\partial f^l}{\partial e^j}\frac{\partial}{\partial f^l},$$

$$\frac{\partial}{\partial z^i}=\frac{\partial y^k}{\partial z^i}\frac{\partial}{\partial y^k}+\frac{\partial f^l}{\partial z^i}\frac{\partial}{\partial f^l},$$

$$\frac{\partial}{\partial\dfrac{\partial}{\partial e^j}}=\frac{\partial e^j}{\partial y^k}\frac{\partial}{\partial\dfrac{\partial}{\partial y^k}}+\frac{\partial e^j}{\partial f^l}\frac{\partial}{\partial\dfrac{\partial}{\partial f^l}},$$

$$\frac{\partial}{\partial\dfrac{\partial}{\partial z^i}}=\frac{\partial z^i}{\partial y^k}\frac{\partial}{\partial\dfrac{\partial}{\partial y^k}}+\frac{\partial z^i}{\partial f^l}\frac{\partial}{\partial\dfrac{\partial}{\partial f^l}}.$$

By substitution we get

$$\sum a\otimes\left(\frac{\partial y^k}{\partial e^j}\frac{\partial}{\partial y^k}+\frac{\partial f^l}{\partial e^j}\frac{\partial}{\partial f^l}\right)L_{\Pi((\partial e^j/\partial y^t)[\partial/\partial(\partial/\partial y^t)]\,+\,(\partial e^j/\partial f^r)[\partial/\partial(\partial/\partial f^r)])}\varphi$$
$$+\sum a\otimes\left(\frac{\partial y^k}{\partial z^i}\frac{\partial}{\partial y^k}+\frac{\partial f^l}{\partial z^i}\frac{\partial}{\partial f^l}\right)L_{\Pi(\partial z^i/\partial y^t)[\partial/\partial(\partial/\partial y^t)]\,+\,(\partial z^i/\partial f^r)[\partial/\partial(\partial/\partial f^r)])}\varphi$$
$$=\sum a\otimes\left(\frac{\partial}{\partial y^k}L_{\Pi[\partial/\partial(\partial/\partial y^k)]}\varphi+\frac{\partial}{\partial f^l}L_{\Pi[\partial/\partial(\partial/\partial f^l)]}\varphi\right).$$

Thus the last two summations are also invariant under a change of coordinates.

Theorem 3.3: $(\mathcal{P}\otimes\mathcal{E}_M,\tilde{d})$ is a complex of differential graded algebra.

Proof: It is sufficient to prove $\tilde{d}^2=0$. It can be checked by direct computation. Let us use L_i, L_j instead of $L_{\Pi[\partial/\partial(\partial/\partial z^i)]}$ and $L_{\Pi[\partial/\partial(\partial/\partial e^j)]}$ respectively, then

$$\tilde{d}(a\otimes\varphi)=dz^i\left(\frac{\partial}{\partial z^i}a\right)\otimes\varphi+de^j\left(\frac{\partial}{\partial e^j}a\right)\otimes\varphi+(-1)^{\tilde{a}}a\otimes\frac{\partial}{\partial e^j}L_j\varphi+(-1)^{\tilde{a}}a\otimes\frac{\partial}{\partial z^i}L_i\varphi,$$

$$\begin{aligned}\tilde{d}(\tilde{d}(a\otimes\varphi)) &= dz^k\,dz^i\left(\frac{\partial}{\partial z^k}\frac{\partial}{\partial z^i}\right)a\otimes\varphi - de^l\,dz^j\left(\frac{\partial}{\partial e^l}\frac{\partial}{\partial z^j}a\right)\otimes\varphi + (-1)^{\tilde{a}}\,dz^i\left(\frac{\partial}{\partial z^i}a\right)\otimes\frac{\partial}{\partial e^l}L_l\varphi \\ &+ (-1)^{\tilde{a}+1}\,dz^i\left(\frac{\partial}{\partial z^i}a\right)\otimes\frac{\partial}{\partial z^k}L_k\varphi + dz^k\,de^j\left(\frac{\partial}{\partial z^k}\frac{\partial}{\partial e^j}a\right)\otimes\varphi + de^l\,de^j\left(\frac{\partial}{\partial e^l}\frac{\partial}{\partial e^j}a\right) \\ &\otimes\varphi + (-1)^{\tilde{a}-1}\,de^j\left(\frac{\partial}{\partial e^j}a\right)\otimes\frac{\partial}{\partial e^l}L_l\varphi + (-1)^{\tilde{a}-1}\,de^j\left(\frac{\partial}{\partial e^j}a\right)\otimes\frac{\partial}{\partial z^k}L_k\varphi \\ &+ (-1)^{\tilde{a}}\Big[dz^k\frac{\partial}{\partial z^k}a\otimes\frac{\partial}{\partial e^j}L_j\varphi + de^l\frac{\partial}{\partial e^l}a\otimes\frac{\partial}{\partial e^j}L_j\varphi + (-1)^{\tilde{a}+1}a\otimes\frac{\partial}{\partial e^l}\frac{\partial}{\partial e^j}\underline{L_l}\,\underline{L_j}\varphi \\ &+ (-1)^{\tilde{a}+1}a\otimes\frac{\partial}{\partial z^k}\frac{\partial}{\partial e^j}L_kL_j\varphi\Big] + (-1)^{\tilde{a}}\Big[dz^k\frac{\partial}{\partial z^k}a\otimes\frac{\partial}{\partial z^i}L_i\varphi + de^l\frac{\partial}{\partial e^l}a\otimes\frac{\partial}{\partial z^i}L_i\varphi \\ &+ (-1)^{\tilde{a}}a\otimes\frac{\partial}{\partial e^l}\frac{\partial}{\partial z^i}L_lL_i\varphi + (-1)^{\tilde{a}}a\otimes\frac{\partial}{\partial z^k}\frac{\partial}{\partial z^i}\underline{L_k}\,\underline{L_i}\varphi\Big].\end{aligned}$$

Since $\partial/\partial e^l$'s are odd and $L_lL_j - L_jL_l = 0$ thus the first underlined term is zero. Equality $L_kL_i = -L_iL_k$ implies that the second underlined term is zero too. Other terms are cancelled by their inverses.

To establish a correspondence with cyclic cohomology classes, we need $\varphi = \tilde{d}f_1\wedge\cdots\wedge\tilde{d}f_{m+n}$ to be an integral form for every $f_i\in\mathcal{A}$ (Ref. 4, p. 186). So φ must contain a section of Berezinian of M (Ref. 7, p. 213). Obviously, $\tilde{d}$ satisfies this condition. As far as we know, it is not true for other presented complexes on supermanifolds.

IV. COHOMOLOGY

A $\mathbf{Z}^2$-graded cohomology groups corresponding to complex of extended pesudodifferential forms can be defined as follows:

$$H_{\tilde{d}}^{(p,q)}(\mathcal{M},\mathcal{A}) = \frac{\operatorname{Ker}\tilde{d}|_{\Omega^{p,q}\otimes\mathcal{E}_M}}{\operatorname{Im} g\tilde{d}|_{(\Omega^{p-1,q}\oplus\Omega^{p,q-1})\otimes\mathcal{E}_M}}.$$

Now we show that these groups are sensitive to the ''super'' structure. For this, it is sufficient to compute them for a purely odd supermanifold $\mathbf{R}^{(0,1)}$.

Proposition 4.1:

$$H_{\tilde{d}}^{(1,1)}(\mathbf{R}^{(0,1)}) = \mathbf{R}^2.$$

Proof: On $\mathcal{E}_{\mathbf{R}^{(0,1)}}$ there are two endomorphism with nonvanishing differentials. Call them $E_1 = ed(\partial/\partial e)\otimes\partial/\partial e$, $E_2 = ed(\partial/\partial e)\otimes\partial/\partial(\partial/\partial e)$. We have $\tilde{d}(1\otimes E_1) = 2de\otimes\partial/\partial e$ and $\tilde{d}(1\otimes E_2) = 2de\otimes\partial/\partial(\partial/\partial e)$. Thus $H_{\tilde{d}}^{(1,1)}(\mathbf{R}^{(0,1)})$ as an $\mathbf{R}$-vector space is generated by the classes of two 1–1 forms $de\otimes(\partial/\partial e)E_1$ and $de\otimes(\partial/\partial e)E_2$.

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Covariant localizations in the torus and the phase observables

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We describe all the localization observables of a quantum particle in a one-dimensional box in terms of sequences of unit vectors in a Hilbert space. An alternative representation in terms of positive semidefinite complex matrices is furnished and the commutative localizations are singled out. As a consequence, we also get a vector sequence characterization of the covariant phase observables. [DOI: 10.1063/1.1425958]

I. INTRODUCTION

We investigate the problem of the localization of a free quantum particle moving in a one-dimensional box with periodic boundary conditions, adopting the point of view that observables are represented as appropriate normalized positive operator measures. (For that approach, see, e.g., Refs. 1–4.) Therefore, if one chooses the one-dimensional torus $\mathbb{T}$ as the configuration space of the system, then a localization observable E is a map that defines for any (Borel) subset $X \subset \mathbb{T}$ a bounded operator $E(X)$ such that, if ψ is the (vector) state of the system, the number $\langle \psi | E(X)\psi \rangle$ is the probability that a localization measurement of the particle in that state leads to a result in X. For example, the group of motions of the system is the torus itself that acts on the vector states by means of the *geometric* representation. The basic requirement for E to represent a localization observable is, therefore, that E is covariant with respect to this action. Hence a localization observable is a normalized positive operator measure covariant under the geometric action of the torus $\mathbb{T}$.

In the following we call such observables $\mathbb{T}$-covariant localization observables and we show that they are characterized in terms of sequences of unit vectors in an infinite dimensional Hilbert space. In this framework we select the measures that are projection valued or commutative, and we discuss the problem of the equivalence of such operator measures. As a by-product, we also get a representation of the phase observables, that is, the normalized positive operator measures which are covariant under the shifts generated by the number observable. Our proof is based on a direct application of a theorem due to Cattaneo,[5] which generalizes Mackey's imprimitivity theorem for positive operator measures. Instead, one could use the results of Holevo,[6,7] based also on group theoretical arguments, to obtain a classification in terms of measurable fields of sesquilinear forms, which in the present context can be described as infinite-dimensional positive semidefinite complex matrices with diagonal elements equal to one. For the sake of comparison, we also derive the

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matrix characterization by direct methods, using only basic analysis and measure theory. This approach has been used in Ref. 8 to work out all the phase observables in terms of *phase matrices*.

II. $\mathbb{T}$-COVARIANT LOCALIZATION OBSERVABLES

Let $\mathbb{T}=\{z\in\mathbb{C}:|z|=1\}$ denote the one-dimensional torus, regarded as a compact (second countable) Abelian group. Let $\mathcal{B}(\mathbb{T})$ be the Borel σ-algebra of $\mathbb{T}$, μ the Haar measure on $\mathbb{T}$, $L_2(\mathbb{T},\mu)$ the Hilbert space of square integrable Borel functions $f:\mathbb{T}\to\mathbb{C}$, and $\mathcal{L}(L_2(\mathbb{T},\mu))$ the set of bounded operators on $L_2(\mathbb{T},\mu)$.

The group $\mathbb{T}$ acts on $L_2(\mathbb{T},\mu)$ via the geometric action

$$[U(a)f](z)=f(az),\quad a\in\mathbb{T},\ \ f\in L_2(\mathbb{T},\mu),\ \ z\in\mathbb{T},$$

which is unitary and continuous with respect to the strong operator topology.

A $\mathbb{T}$-covariant localization observable is a positive normalized operator measure on $\mathbb{T}$, $E:\mathcal{B}(\mathbb{T})\to\mathcal{L}(L_2(\mathbb{T},\mu))$, such that, for all $X\in\mathcal{B}(\mathbb{T})$, $a\in\mathbb{T}$,

$$U(a)E(X)U(a)^*=E(aX). \tag{1}$$

Since the action of $\mathbb{T}$ on itself is transitive, Eq. (1) means that (U,E) is a transitive system of $\mathbb{T}$-covariance based on $\mathbb{T}$ and, hence, (U,E) is described by Ref. 5, Proposition 2.

In order to apply the cited result, let us notice the following facts. The stability subgroup of any point of $\mathbb{T}$ is the trivial subgroup $\{1\}$. The trivial representation σ of $\{1\}$ acting on $L_2(\mathbb{T},\mu)$ contains all the (trivial) representations of $\{1\}$ and the corresponding imprimitivity system (R,P) for $\mathbb{T}$ based on $\mathbb{T}$ induced by σ acts on $L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)\simeq L^2(\mathbb{T},\mu,L_2(\mathbb{T},\mu))$ as

$$(R(a)\varphi)(z_1,z_2)=\varphi(az_1,z_2),$$

$$(P(X)\varphi)(z_1,z_2)=\chi_X(z_1)\varphi(z_1,z_2),$$

where $\varphi\in L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$, $a\in\mathbb{T}$, $X\in\mathcal{B}(\mathbb{T})$, and z_1, $z_2\in\mathbb{T}$.

Proposition 2 of Ref. 5 shows that, given a $\mathbb{T}$-covariant localization observable E, there exists an isometry

$$V:L_2(\mathbb{T},\mu)\to L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu),$$

which intertwines the action U with R and such that

$$E(X)=V^*P(X)V,\quad X\in\mathcal{B}(\mathbb{T}). \tag{2}$$

Conversely, given an intertwining isometry V from $L_2(\mathbb{T},\mu)$ to $L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$, Eq. (2) defines a positive normalized operator measure E satisfying Eq. (1).

Hence, to classify all the $\mathbb{T}$-covariant localization observables, one has to determine all the isometric mappings V such that

$$VU(a)=R(a)V,\quad a\in\mathbb{T}. \tag{3}$$

To perform this task, observe that the monomials e_n, $n\in\mathbb{Z}$, $e_n(z)=z^n$, $z\in\mathbb{T}$, form an orthonormal basis of $L_2(\mathbb{T},\mu)$ and the action of U on them is diagonal, that is,

$$U(a)e_n=a^ne_n.$$

Moreover, the vectors

$$(e_ne_j)(z_1,z_2)=e_n(z_1)e_j(z_2)=z_1^nz_2^j,$$

where n, $j \in \mathbb{Z}$, form an orthonormal basis of $L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$, and the action of R on them is simply

$$R(a)e_n e_j = a^n e_n e_j .$$

It follows that, for any $n \in \mathbb{Z}$, the subspace of $L_2(\mathbb{T},\mu)$ generated by e_n and the subspace of $L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$ generated by $\{e_n e_j\}_{j\in\mathbb{Z}}$ carry the representation of $\mathbb{T}$, $z \mapsto z^n$.

Hence, if $V: L_2(\mathbb{T},\mu) \to L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$ is an isometry intertwining U and R, for any $n \in \mathbb{Z}$, Ve_n must be in the vector space $\mathrm{span}\{(e_n e_j)\}_{j\in\mathbb{Z}} \simeq L_2(\mathbb{T},\mu)$, that is, $Ve_n = e_n h_n$ for some unit vector h_n in $L_2(\mathbb{T},\mu)$.

Conversely, if $(h_n)_{n\in\mathbb{Z}}$ is a sequence of unit vectors in $L_2(\mathbb{T},\mu)$, then the mapping $e_n \mapsto e_n h_n$ extends to a unique linear isometry $V: L_2(\mathbb{T},\mu) \to L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu)$ which intertwines the actions U and R and, by means of Eq. (2), the corresponding operator measure E is explicitly given by

$$\begin{aligned}\langle e_n | E(X) e_m\rangle &= \langle e_n | V^* P(X) V e_m\rangle \\ &= \langle Ve_n | P(X) V e_m\rangle \\ &= \langle e_n h_n | P(X) e_m h_m\rangle = \langle h_n | h_m\rangle \int_X z^{m-n} \mathrm{d}\mu(z),\end{aligned}$$

where n, $m \in \mathbb{Z}$. Then, if $|e_n\rangle\langle e_m|$ denotes the rank one operator $L_2(\mathbb{T},\mu) \ni f \mapsto \langle e_m | f\rangle e_n \in L_2(\mathbb{T},\mu)$, we may thus write, for all $X \in \mathcal{B}(\mathbb{T})$,

$$E(X) = \sum_{n,m\in\mathbb{Z}} \langle h_n | h_m\rangle \int_X z^{m-n}\, \mathrm{d}\mu(z) |e_n\rangle\langle e_m|, \tag{4}$$

where the double series converges in the weak operator topology. We observe that two sequences of unit vectors $(h_n)_{n\in\mathbb{Z}}$ and $(k_n)_{n\in\mathbb{Z}}$ define the same $\mathbb{T}$-covariant localization observable if and only if $\langle h_n | h_m\rangle = \langle k_n | k_m\rangle$ for all n, $m \in \mathbb{Z}$.

For the sake of completeness we also compute the adjoint map $V^*: L_2(\mathbb{T}\times\mathbb{T},\mu\times\mu) \to L_2(\mathbb{T},\mu)$. We get

$$\begin{aligned}\langle V^* e_n e_j | e_p\rangle &= \langle e_n e_j | V e_p\rangle \\ &= \langle e_n e_j | e_p h_p\rangle = \begin{cases} 0, & \text{when } n \neq p, \\ \langle e_j | h_n\rangle, & \text{when } n = p, \end{cases}\end{aligned} \tag{5}$$

showing that for any n, $j \in \mathbb{Z}$,

$$V^* e_n e_j = \langle h_n | e_j\rangle e_n . \tag{6}$$

We now discuss the problem of the equivalence. Two $\mathbb{T}$-covariant localization observables E and E' are equivalent if there is a unitary operator $W: L_2(\mathbb{T},\mu) \to L_2(\mathbb{T},\mu)$ such that, for all $a \in \mathbb{T}$, $X \in \mathcal{B}(\mathbb{T})$,

$$WU(a) = U(a)W, \quad WE(X) = E'(X)W.$$

Clearly, this definition is the requirement that (U,E) and (U,E') are equivalent as $\mathbb{T}$-covariant systems.

The first condition implies now that for each $n \in \mathbb{Z}$, $We_n = z_n e_n$, for some $z_n \in \mathbb{T}$. Therefore, the equivalence of (U,E) and (U,E') equals the fact that for each n, $m \in \mathbb{Z}$ and $X \in \mathcal{B}(\mathbb{T})$,

$$\langle e_n | E'(X) e_m\rangle = z_n \overline{z_m} \langle e_n | E(X) e_m\rangle,$$

for some z_n, $z_m \in \mathbb{T}$. Then, taking into account Eq. (4), two sequences of unit vectors $(h'_n)_{n\in\mathbb{Z}}$ and $(h_n)_{n\in\mathbb{Z}}$ define equivalent $\mathbb{T}$-covariant localization observables if and only if for each n, $m \in \mathbb{Z}$,

$$\langle h'_n | h'_m \rangle = \langle z_n h_n | z_m h_m \rangle.$$

Finally, we consider the problem of projection-valued measures. Let $\mathcal{K}$ be the closed subspace of $L_2(\mathbb{T}\times\mathbb{T}, \mu\times\mu)$ generated by $\{P(X)e_n h_n : X \in \mathcal{B}(\mathbb{T}), n \in \mathbb{Z}\}$. The space $\mathcal{K}$ is stable under the action of the imprimitivity system (R,P). Since the projection measure P acts only on the vector e_n and $\{\chi_X e_n : X \in \mathcal{B}(\mathbb{T})\}$ generates $L_2(\mathbb{T}, \mu)$, one has

$$\mathcal{K} \simeq L_2(\mathbb{T}, \mu) \otimes L,$$

where L is the closed subspace generated by the vectors h_n, $n \in \mathbb{Z}$. According to Ref. 5, Proposition 1, E is projection valued if and only if $V(L_2(\mathbb{T}, \mu)) = \mathcal{K}$, that is, L is one-dimensional.

We summarize the above construction in the form of a theorem.

Theorem 1: *Any $\mathbb{T}$-covariant localization observable $E: \mathcal{B}(\mathbb{T}) \to L_2(\mathbb{T}, \mu)$ is of the form*

$$E(X) = \sum_{n,m\in\mathbb{Z}} \langle h_n | h_m \rangle \int_X z^{m-n} \, d\mu(z) |e_n\rangle\langle e_m|, \quad X \in \mathcal{B}(\mathbb{T}),$$

for some sequence of unit vectors $(h_n)_{n\in\mathbb{Z}}$ in $L_2(\mathbb{T}, \mu)$. Two sequences of unit vectors $(h_n)_{n\in\mathbb{Z}}$ and $(k_n)_{n\in\mathbb{Z}}$ in $L_2(\mathbb{T}, \mu)$ determine the same $\mathbb{T}$-covariant localization observable if and only if $\langle h_n | h_m \rangle = \langle k_n | k_m \rangle$ for all n, $m \in \mathbb{Z}$.

Two such operator measures E and E' are equivalent if and only if

$$\langle h'_n | h'_m \rangle = \langle z_n h_n | z_m h_m \rangle,$$

for some sequence $(z_n)_{n\in\mathbb{Z}}$ in $\mathbb{T}$.

The operator measure E is projection valued exactly when the vectors h_n, $n \in \mathbb{Z}$, are of the form $h_n = z_n h$ for some unit vector h and phase factors $z_n \in \mathbb{T}$.

A. Commutative localizations

By means of the above theorem, we are now in position to characterize the commutative $\mathbb{T}$-covariant localization observables. We recall that such an observable E is commutative if $E(X)E(Y) = E(Y)E(X)$, for all X, $Y \in \mathcal{B}(\mathbb{T})$, that is, if E is a commutative operator measure.

Let $(h_n)_{n\in\mathbb{Z}}$ be a sequence of unit vectors in $L_2(\mathbb{T}, \mu)$, E the corresponding operator measure given by Theorem 1, and define, for all n, $m \in \mathbb{Z}$, $c_{n,m} = \langle h_n | h_m \rangle$.

Proposition 1: The $\mathbb{T}$-covariant localization observable E is commutative if and only if

$$c_{n,n+k} c_{n+k,m} = c_{n,m-k} c_{m-k,m} \tag{7}$$

for all, n, m, $k \in \mathbb{Z}$.

Proof: Define $\mu_{n,m,Y}(X) := \langle n | [E(X)E(Y) - E(Y)E(X)] | m \rangle$ for all n, $m \in \mathbb{Z}$ and X, $Y \in \mathcal{B}(\mathbb{T})$. Let $k \in \mathbb{Z}$, and calculate

$$\int_{\mathbb{T}} z^k \, d\mu_{n,m,Y}(z) = [c_{n,n+k} c_{n+k,m} - c_{n,m-k} c_{m-k,m}] \int_Y z^{n+k-m} \, d\mu(z).$$

If $E(X)E(Y) = E(Y)E(X)$ for all X, $Y \in \mathcal{B}(\mathbb{T})$, then $\mu_{n,m,Y}(X) = 0$ and, thus, $c_{n,n+k} c_{n+k,m} = c_{n,m-k} c_{m-k,m}$ for all n, m, $k \in \mathbb{Z}$.

Conversely, if $c_{n,n+k} c_{n+k,m} = c_{n,m-k} c_{m-k,m}$, n, m, $k \in \mathbb{Z}$, holds, then

$$\mu_{n,m,Y}(X) = \sum_{k=-\infty}^{\infty} (c_{n,n+k} c_{n+k,m} - c_{n,m-k} c_{m-k,m}) \int_X z^{-k} \, d\mu(z) \int_Y z^{k+n-m} \, d\mu(z) = 0$$

for all $n, m \in \mathbb{Z}$ and $X, Y \in \mathcal{B}(\mathbb{T})$. Therefore, $E(X)E(Y)=E(Y)E(X)$ for all $X, Y \in \mathcal{B}(\mathbb{T})$. □

An example of a commutative $\mathbb{T}$-covariant localization observable is the following one. Let $\xi \in [-1,1]$ and $\phi, \psi \in L_2(\mathbb{T},\mu)$ be two-unit vectors such that

$$\langle \psi | \phi \rangle = \xi.$$

Consider the sequence of unit vectors $(h_n)_{n\in\mathbb{Z}}$, with

$$h_n = \psi, \quad \text{for even } n \text{ (including 0)},$$

$$h_n = \phi, \quad \text{for odd } n.$$

The coefficients $c_{n,m}=\langle h_n|h_m\rangle$, $n, m \in \mathbb{Z}$, satisfy condition (7) so that the corresponding $\mathbb{T}$-covariant localization observable E^ξ is commutative. Notice that E^ξ is projection valued if and only if $\xi = \pm 1$.

B. Matrix characterization

To end this section, we discuss an alternative characterization of the $\mathbb{T}$-covariant localization observables. If follows from Theorem 1 that the operator measure E is uniquely defined in terms of the complex matrix elements $c_{n,m}=\langle h_n|h_m\rangle$, $n, m \in \mathbb{Z}$. It is clear that they satisfy the following two conditions:

(a) $c_{n,n}=1$, for all $n \in \mathbb{Z}$,
(b) $\Sigma_{n,m=-k}^{k} c_{n,m}|e_n\rangle\langle e_m| \geqslant O$, for all $k \in \mathbb{N}$.

Conversely, it is known, (see, for example, Ref. 9, Chap. 3), that given a family of complex numbers $\{c_{n,m} \in \mathbb{C} | n,m \in \mathbb{Z}\}$ which has the properties (a) and (b), there exists a sequence of unit vectors $(h_n)_{n\in\mathbb{Z}}$ such that $c_{n,m}=\langle h_n|h_m\rangle$ and, hence, a $\mathbb{T}$-covariant localization observable E defined by

$$E(X) = \sum_{n,m\in\mathbb{Z}} c_{n,m} \int_X z^{m-n}\, \mathrm{d}\mu(z) |e_n\rangle\langle e_m|,$$

for all $X \in \mathcal{B}(\mathbb{T})$.

For completeness, we give a simple construction of a sequence of unit vectors which generates the matrix. The construction is slightly more general than actually needed here.

Let $J \subseteq \mathbb{Z}$ (especially $J=\mathbb{Z}$ or $J=\mathbb{N}$). A matrix $(b_{n,m})_{n,m\in J}$ is *positive semidefinite* if for all sequences $(d_n)_{n\in J} \subset \mathbb{C}$, for which $d_n \neq 0$ for only finitely many $n \in J$,

$$\sum_{n,m\in J} \overline{d_n} b_{n,m} d_m \geqslant 0.$$

For $J=\mathbb{Z}$ this is equivalent to the above condition (b). [Condition (a) is equivalent to the fact that $\|h_n\|=1$ for all $n \in \mathbb{Z}$.]

Proposition 2: Fix $J \subseteq \mathbb{Z}$. Let $l_2(J)$ be a sequence space with the basis $(\chi_{\{n\}})_{n\in J}$. A matrix $(b_{n,m})_{n,m\in J}$ is positive semidefinite if and only if there is a sequence $(h_n)_{n\in J}$ of vectors of $l_2(J)$ such that $b_{n,m}=\langle h_n|h_m\rangle$ for all $n, m \in J$.

Proof: Consider a sequence $(h_n)_{n\in J}$ of vectors of $l_2(J)$ and put $b_{n,m}=\langle h_n|h_m\rangle$. If $(d_n)_{n\in J} \subset \mathbb{C}$ is a sequence for which $d_n \neq 0$ for only finitely many $n \in J$, then

$$\sum_{n,m\in J} \overline{d_n} b_{n,m} d_m = \left\langle \left(\sum_{n\in J} d_n h_n \right) \middle| \left(\sum_{m\in J} d_m h_m \right) \right\rangle \geqslant O,$$

the sums being finite.

Suppose then that $(b_{n,m})_{n,m\in J}$ is positive semidefinite. It follows that $b_{n,n}\geqslant 0$, $b_{n,m}=\overline{b_{m,n}}$, and

$$\begin{vmatrix} b_{n,n} & b_{n,m} \\ b_{m,n} & b_{m,m} \end{vmatrix} = b_{n,n}b_{m,m} - |b_{n,m}|^2 \geqslant 0 \tag{8}$$

for all $n<m$. Especially, if $b_{n,n}b_{m,m}=0$, then $b_{n,m}=0$. Then the doubles series

$$\sum_{\substack{n,m\in J \\ b_{n,n}\neq 0\neq b_{m,m}}} \frac{b_{n,m}}{\sqrt{b_{n,n}b_{m,m}}(|n|+1)(|m|+1)} |\chi_{\{n\}}\rangle\langle\chi_{\{m\}}|$$

converges in the weak operator topology to a bounded and positive operator S. Let A be its square root and, for all $n\in J$,

$$h_n := \sqrt{b_{n,n}}(|n|+1)A\chi_{\{n\}}.$$

Then, taking into account that $S=A^2$, one gets, for all n, $m\in J$ such that $b_{n,n}b_{m,m}\neq 0$,

$$\langle h_n|h_m\rangle = \sqrt{b_{n,n}}(|n|+1)\sqrt{b_{m,m}}(|m|+1)\langle\chi_{\{n\}}|A^2\chi_{\{m\}}\rangle = b_{n,m}.$$

If $b_{n,n}b_{m,m}=0$, for example, $b_{n,n}=0$, then $h_n=0$ and, for all $m\in J$, $b_{n,m}=0=\langle h_n|h_m\rangle$. □

The above proposition, when applied together with the natural isomorphism $l_2(\mathbb{Z}) \ni \chi_{\{n\}}\mapsto e_n\in L_2(\mathbb{T},\mu)$, gives then a vector sequence representation of the matrix $(c_{n,m})_{n,m\in\mathbb{Z}}$ of a $\mathbb{T}$-covariant localization observable E. In Sec. IV we prove by direct methods a characterization of $\mathbb{T}$-covariant localization observables in terms of the matrix $(c_{n,m})_{n,m\in\mathbb{Z}}$. The same result can also be obtained from a theorem of Holevo (Ref. 7, Theorem 1), whose proof is also based on group theoretical arguments.

III. COVARIANT PHASE OBSERVABLES

Theorem 1 leads also to a characterization of the covariant phase observables. To describe them, let $\mathcal{H}$ be a complex separable Hilbert space, and let $(|n\rangle)_{n\in\mathbb{N}}$ be an orthonormal basis of $\mathcal{H}$. We call it the number basis. We define the number operator

$$N := \sum_{n\in\mathbb{N}} n|n\rangle\langle n|$$

with the domain $\mathcal{D}(N) := \{\psi\in\mathcal{H}: \Sigma_{n\in\mathbb{N}} n^2|\langle n|\psi\rangle|^2<\infty\}$, and the unitary "phase shifter" as

$$U^N(a) := \sum_{n\in\mathbb{N}} a^n|n\rangle\langle n|,$$

for all $a\in\mathbb{T}$. We say that a positive normalized operator measure $\tilde{E}:\mathcal{B}(\mathbb{T})\to\mathcal{L}(\mathcal{H})$ is a *phase observable* if it is covariant under the phase shifts, that is, if for any $X\in\mathcal{B}(\mathbb{T})$, $a\in\mathbb{T}$,

$$U^N(a)\tilde{E}(X)U^N(a)^* = \tilde{E}(aX). \tag{9}$$

To determine all the phase observables, let $T:\mathcal{H}\to L_2(\mathbb{T},\mu)$ be the linear isometry with the property

$$T|n\rangle = e_n, \quad \text{for all } n\in\mathbb{N}.$$

Clearly, T intertwines the unitary actions U^N and U, $TU^N=UT$, and $X\mapsto T\tilde{E}(X)T^*$ is a $\mathbb{T}$-covariant localization observable acting in $L_2(\mathbb{T},\mu)$. Using Theorem 1, and the fact that $T^*T=I$, one has the following result.

Corollary 1: A normalized positive operator measure $\tilde{E}:\mathcal{B}(\mathbb{T})\to\mathcal{L}(\mathcal{H})$ is a phase observable if and only if it is of the form

$$\tilde{E}(X)=T^*E(X)T,\quad X\in\mathcal{B}(\mathbb{T}),$$

for some $\mathbb{T}$-covariant localization observable E.

Equivalently, $\tilde{E}:\mathcal{B}(\mathbb{T})\to\mathcal{L}(\mathcal{H})$ is a phase observable if and only if

$$\tilde{E}(X)=\sum_{n,m\in\mathbb{N}}\langle\xi_n|\xi_m\rangle\int_X z^{m-n}\,\mathrm{d}\mu(z)|n\rangle\langle m|,\quad X\in\mathcal{B}(\mathbb{T}),$$

for some sequence of unit vectors $(\xi_n)_{n\in\mathbb{N}}$ of $\mathcal{H}$. Two sequences of unit vectors $(\xi_n)_{n\in\mathbb{N}}$ and $(\eta_n)_{n\in\mathbb{N}}$ define the same phase observable exactly when $\langle\xi_n|\xi_m\rangle=\langle\eta_n|\eta_m\rangle$ for all n, $m\in\mathbb{N}$.

Two phase observables $\tilde{E}$ and $\tilde{E}'$ are equivalent (in the sense of covariance systems) if and only if any of their generating vector sequences (ξ_n) and (ξ_n') are such that, for each n, $m\in\mathbb{N}$, $\langle\xi_n'|\xi_m'\rangle=\langle z_n\xi_n|z_m\xi_m\rangle$ for some z_n, $z_m\in\mathbb{T}$.

Since $T:\mathcal{H}\to L_2(\mathbb{T},\mu)$ is not surjective, there is no projection-valued phase observable.

We note, in addition, that Proposition 1, when applied to phase observables, gives Eq. (7) for all n, m, $k\in\mathbb{N}$ with $m\geqslant k$. For $n=m$ this gives $|c_{n,n+k}|=|c_{n-k,n}|$ for all $n\geqslant k$, which implies that $c_{n,m}=0$ for all $n\neq m$ (for details, see Ref. 11). This means that the only commutative phase observable is the trivial one

$$\mathcal{B}(\mathbb{T})\ni X\mapsto\mu(X)I\in\mathcal{L}(\mathcal{H}).$$

Following Ref. 8 we say that a positive semidefinite complex matrix $(c_{n,m})_{n,m\in\mathbb{N}}$ is a *phase matrix* if $c_{n,n}=1$ for all $n\in\mathbb{N}$. According to Ref. 8, Phase Theorem 2.2, any phase observable $\tilde{E}:\mathcal{B}(\mathbb{T})\to\mathcal{L}(\mathcal{H})$ is of the form

$$\tilde{E}(X)=\sum_{n,m\in\mathbb{N}}c_{n,m}\int_X z^{m-n}\,\mathrm{d}\mu(z)|n\rangle\langle m|$$

for a unique phase matrix $(c_{n,m})$, and any phase matrix determines a phase observable in this way. The equivalence of the two characterizations of the phase observables is again a consequence of Proposition 2.

IV. COVARIANT LOCALIZATIONS IN A BOX: A DIRECT METHOD

We determine next the covariant localizations by direct methods, using only basic analysis and measure theory. Actually, we determine all the normalized (not necessarily positive nor self-adjoint) operator measures which are translation covariant on the interval $[0,2\pi)$. In the rest of this article, we use the interval $[0,2\pi)$ instead of $\mathbb{T}$ when it simplifies the calculations. Note that the Haar measure μ is the normalized Lebesgue measure on $\mathcal{B}([0,2\pi))$, the Borel σ-algebra of $[0,2\pi)$ transferred by the map $\theta\mapsto e^{i\theta}$.

Let, again, $\mathcal{H}$ be a complex separable Hilbert space, but choose now an orthonormal basis $(|n\rangle)_{n\in\mathbb{Z}}\subset\mathcal{H}$ labeled by the integers. Define the "extended number operator" as follows: $\hat{N}:=\Sigma_{n\in\mathbb{Z}}n|n\rangle\langle n|$ with its domain $\mathcal{D}(\hat{N}):=\{\psi\in\mathcal{H}:\Sigma_{n\in\mathbb{Z}}n^2|\langle n|\psi\rangle|^2<\infty\}$, and define the corresponding unitary shift operators as

$$R(\theta):=e^{i\theta\hat{N}}=\sum_{n\in\mathbb{Z}}e^{in\theta}|n\rangle\langle n|$$

for all $\theta\in\mathbb{R}$.

We say that $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$ is an operator measure if it is σ-additive with respect to the weak operator topology. If $E(X)^*=E(X)$, or $E(X)\geqslant O$, for all $X\in\mathcal{B}([0,2\pi))$, we say that E is self-adjoint, or positive. If $E([0,2\pi))=I$, we say that the operator measure E is normalized. Finally, E is covariant if $R(\theta)E(X)R(\theta)^*=E(X\oplus\theta)$ for all $X\in\mathcal{B}([0,2\pi))$ and $\theta\in\mathbb{R}$, where the symbol $\oplus$ means addition modulo 2π.

Before characterizing covariant normalized operator measures we prove the following lemma:

Lemma 1: Fix $q\in\mathbb{Z}$, and let $\nu_q:\mathcal{B}([0,2\pi))\to\mathbb{C}$ be a σ-additive set function such that $\nu_q(X\oplus\theta)=e^{iq\theta}\nu_q(X)$ for all $X\in\mathcal{B}([0,2\pi))$ and $\theta\in[0,2\pi)$, and for which $\nu_q([0,2\pi))=\delta_{0,q}$. Then $\nu_q(X)=c_q(2\pi)^{-1}\int_X e^{iq\theta}\,\mathrm{d}\theta$ for all $X\in\mathcal{B}([0,2\pi))$, where $c_q\in\mathbb{C}$ and $c_0=1$.

Proof: Fix $q\in\mathbb{Z}$, and let $k\in\mathbb{Z}^+$. Now

$$\begin{aligned}\delta_{0,q}=\nu_q([0,2\pi))&=\nu_q\left(\bigcup_{l=0}^{k-1}[l2\pi k^{-1},(l+1)2\pi k^{-1})\right)\\&=\sum_{l=0}^{k-1}\nu_q([0,2\pi k^{-1})+l2\pi k^{-1})\\&=\left[\sum_{l=0}^{k-1}e^{i2\pi qk^{-1}l}\right]\nu_q[0,2\pi k^{-1})=\begin{cases}k\nu_q[0,2\pi k^{-1}), & \text{when } qk^{-1}\in\mathbb{Z},\\0, & \text{when } qk^{-1}\notin\mathbb{Z}.\end{cases}\end{aligned}\tag{10}$$

Suppose that $q\in\mathbb{Z}$ and $k\in\mathbb{Z}^+$ are such that $qk^{-1}\notin\mathbb{Z}$. Then $\int_0^{2\pi k^{-1}}e^{iq\theta}\,\mathrm{d}\theta\neq0$, and we can define

$$c_q(k):=\frac{\nu_q([0,2\pi k^{-1}))}{(2\pi)^{-1}\int_0^{2\pi k^{-1}}e^{iq\theta}\,\mathrm{d}\theta},$$

so that

$$\nu_q([0,2\pi k^{-1}))=c_q(k)\frac{1}{2\pi}\int_0^{2\pi k^{-1}}e^{iq\theta}\,\mathrm{d}\theta=c_q(k)\frac{e^{iq2\pi k^{-1}}-1}{iq2\pi}.$$

On the other hand, for all $r\in\mathbb{Z}^+$, $q(rk)^{-1}\notin\mathbb{Z}$, and

$$\nu_q([0,2\pi k^{-1}))=\nu_q\left(\bigcup_{l=0}^{r-1}[l2\pi(rk)^{-1},(l+1)2\pi(rk)^{-1})\right)=\left[\sum_{l=0}^{r-1}e^{i2\pi q(rk)^{-1}l}\right]\nu_q([0,2\pi(rk)^{-1}))$$

$$=c_q(rk)\frac{e^{iq2\pi k^{-1}}-1}{iq2\pi}.$$

This shows that $c_q(k)=c_q(rk)$, $r\in\mathbb{Z}^+$. Since $q(|q|+1)^{-1}\notin\mathbb{Z}$, one has $c_q(k)=c_q((|q|+1)k)=c_q(|q|+1)$. Thus, for all $k\in\mathbb{Z}^+$, for which $qk^{-1}\notin\mathbb{Z}$, the number $c_q(k)$ is the same, and we may define $c_q:=c_q(|q|+1)$ for all $q\in\mathbb{Z}$ and $q\neq0$.

If $qk^{-1}\in\mathbb{Z}$, $q\in\mathbb{Z}$, $k\in\mathbb{Z}^+$, Eq. (10) gives

$$\nu_q([0,2\pi k^{-1}))=\frac{\delta_{0,q}}{k}=\frac{1}{2\pi}\int_0^{2\pi k^{-1}}e^{iq\theta}\,\mathrm{d}\theta.\tag{11}$$

Thus, if we define $c_0:=1$ we get

$$\nu_q([0,2\pi k^{-1}))=c_q\frac{1}{2\pi}\int_0^{2\pi k^{-1}}e^{iq\theta}\,\mathrm{d}\theta, \tag{12}$$

for all $k\in\mathbb{Z}^+$ and $q\in\mathbb{Z}$.

Let $q\in\mathbb{Z}$. Now one gets

$$\nu_q\left(\bigcup_{p=1}^{\infty}\{p^{-1}\}\right)=\nu_q(\{0\})\sum_{p=1}^{\infty}e^{iqp^{-1}},$$

which implies that $\nu_q(\{0\})=0$. Thus the measure ν_q is nonatomic, that is, $\nu_q(\{x\})=e^{ixq}\nu_q(\{0\})=0$, $x\in[0,2\pi)$, which implies that its distribution function $x\mapsto\nu_q([0,x))$ is continuous. From Eq. (12) it follows that for all $k\in\mathbb{Z}^+$, $p\in\{1,2,...,k\}$,

$$\nu_q([0,2\pi pk^{-1}))=\nu_q\left(\bigcup_{l=0}^{p-1}[l2\pi k^{-1},(l+1)2\pi k^{-1})\right)=c_q\,\frac{1}{2\pi}\int_0^{2\pi pk^{-1}}e^{iq\theta}\,\mathrm{d}\theta. \tag{13}$$

Since $x\mapsto\nu_q([0,x))$ is continuous, and the set $\{2\pi pk^{-1}\in[0,2\pi)|k\in\mathbb{Z}^+,p\in\{1,2,...,k\}\}$, is dense in $[0,2\pi)$, it follows that for all $x\in(0,2\pi]$

$$\nu_q([0,x))=c_q\,\frac{1}{2\pi}\int_0^{x}e^{iq\theta}\,\mathrm{d}\theta.$$

By the Hahn extension theorem

$$\nu_q(X)=c_q\,\frac{1}{2\pi}\int_X e^{iq\theta}\,\mathrm{d}\theta \tag{14}$$

for all $X\in\mathcal{B}([0,2\pi))$ and $q\in\mathbb{Z}$. □

Theorem 2: *Let $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$ be a covariant normalized operator measure. For any $X\in\mathcal{B}([0,2\pi))$,*

$$E(X)=\sum_{n,m\in\mathbb{Z}}c_{n,m}\,\frac{1}{2\pi}\int_X e^{i(n-m)\theta}\,\mathrm{d}\theta|n\rangle\langle m|, \tag{15}$$

where $c_{n,m}\in\mathbb{C}$ and $c_{n,n}=1$ for all $n,m\in\mathbb{Z}$. If E is self-adjoint, then $\overline{c_{n,m}}=c_{m,n}$ for all $n,m\in\mathbb{Z}$, and if E is positive, then

$$\sum_{n,m=-k}^{k}c_{n,m}|n\rangle\langle m|\geqslant O, \tag{16}$$

for all $k\in\mathbb{N}$.

Proof: Denoting, in Lemma 1, $q=n-m$ and $\nu_q(X)=\langle n|E(X)|m\rangle$, Eq. (15) follows. If E is self-adjoint, then from (15) one gets

$$\overline{c_{n,m}}=2\pi\lim_{\epsilon\to0+}\frac{\overline{\langle n|E([0,\epsilon))|m\rangle}}{\epsilon}=c_{m,n}$$

for all n, $m\in\mathbb{Z}$.

Suppose that E is positive and, thus, self-adjoint. Hence, if (16) does not hold, one may choose a $\varphi\in\mathcal{H}$ and an $l\in\mathbb{N}$ such that $\Sigma_{n,m=-l}^{l}c_{n,m}\langle\varphi|n\rangle\langle m|\varphi\rangle<0$, and define a function

$$g:[0,2\pi)\to\mathbb{R},\quad \theta\mapsto g(\theta):=\sum_{n,m=-l}^{l} c_{n,m}e^{i(n-m)\theta}\langle\varphi|n\rangle\langle m|\varphi\rangle.$$

Due to the continuity of g one can choose an $\epsilon\in(0,2\pi)$ such that $\int_0^\epsilon g(\theta)\mathrm{d}\theta<0$. Thus, denoting $I_l:=\Sigma_{n=-l}^{l}|n\rangle\langle n|$,

$$\langle I_l\varphi|E([0,\epsilon))I_l\varphi\rangle=\frac{1}{2\pi}\int_0^\epsilon g(\theta)\,\mathrm{d}\theta<0,$$

which contradicts the positivity of E. □

For later use we note that the positive semi-definiteness condition (16) of the matrix $(c_{n,m})_{n,m\in\mathbb{Z}}$ can be written equivalently as the following determinant condition (see, e.g., Ref. 9, Chap. 3.1)

$$\begin{vmatrix} c_{k_1,k_1} & c_{k_1,k_2} & \cdots & c_{k_1,k_s} \\ c_{k_2,k_1} & c_{k_2,k_2} & \cdots & c_{k_2,k_s} \\ \vdots & \vdots & \ddots & \vdots \\ c_{k_s,k_1} & c_{k_s,k_2} & \cdots & c_{k_s,k_s} \end{vmatrix}\geqslant 0 \tag{17}$$

for all $s\in\mathbb{Z}^+$, $\{k_1,k_2,\ldots,k_s\}\subset\mathbb{Z}$, and $k_1<k_2<\cdots<k_s$. Note that in this case $c_{n,m}=\overline{c_{m,n}}$ and $|c_{n,m}|\leqslant 1$ for all n, $m\in\mathbb{Z}$.

Remark 1: One may ask if the converse statement of Theorem 2 is also true. Let $(c_{n,m})_{n,m\in\mathbb{Z}}$ be an infinite-dimensional complex matrix, and suppose that $c_{n,n}=1$ for all $n\in\mathbb{Z}$. Let $\mathcal{M}:=\mathrm{lin}\{|n\rangle|n\in\mathbb{Z}\}$, and define the following function for all φ, $\psi\in\mathcal{M}$:

$$\mathbb{R}\ni\theta\mapsto C_{\varphi,\psi}(\theta):=\sum_{n,m=-\infty}^{\infty} c_{n,m}e^{i(n-m)\theta}\langle\varphi|n\rangle\langle m|\psi\rangle\in\mathbb{C}.$$

For φ, $\psi\in\mathcal{M}$, define

$$E_{\varphi,\psi}([0,2\pi)):=\frac{1}{2\pi}\int_0^{2\pi} C_{\varphi,\psi}(\theta)\,\mathrm{d}\theta=\langle\varphi|\psi\rangle.$$

Clearly, $E_{\varphi,\psi}([0,2\pi))=\langle\varphi|\psi\rangle$, and $(\varphi,\psi)\mapsto E_{\varphi,\psi}([0,2\pi))$ is a bounded sesquilinear form defined on the dense subspace $\mathcal{M}$ of $\mathcal{H}$. Hence the mapping $(\varphi,\psi)\mapsto E_{\varphi,\psi}([0,2\pi))$ has a unique bounded extension to $\mathcal{H}$ which is $(\varphi,\psi)\mapsto\langle\varphi|\psi\rangle$. We let $E([0,2\pi))$ denote the unique bounded operator, which, actually, is the identity operator I.

Consider the following sesquilinear form defined for all $X\in\mathcal{B}([0,2\pi))$:

$$\mathcal{M}\times\mathcal{M}\ni(\varphi,\psi)\mapsto E_{\varphi,\psi}(X):=\frac{1}{2\pi}\int_X C_{\varphi,\psi}(\theta)\,\mathrm{d}\theta\in\mathbb{C}.$$

This form need not be bounded, so that it does not necessarily define a bounded operator on $\mathcal{H}$. Thus, the formal notation

$$E(X)=\sum_{n,m\in\mathbb{Z}} c_{n,m}\frac{1}{2\pi}\int_X e^{i(n-m)\theta}\,\mathrm{d}\theta|n\rangle\langle m|,\quad X\in\mathcal{B}([0,2\pi)), \tag{18}$$

must be understood as the sesquilinear form $(\varphi,\psi)\mapsto E_{\varphi,\psi}(X)$ defined on $\mathcal{M}$.

Since $R(\theta)\mathcal{M}=\mathcal{M}$, it follows that $X\to E(X)$ is covariant in the sense that

$$E_{R(\theta)*\varphi,R(\theta)*\psi}(X)=E_{\varphi,\psi}(X\oplus\theta)$$

for all $\varphi,\ \psi\in\mathcal{M},\ \theta\in[0,2\pi)$, and $X\in\mathcal{B}([0,2\pi))$.

Finally, if $E_{\varphi,\psi}(X)\geqslant 0$ for all $X\in\mathcal{B}([0,2\pi))$ and $\varphi\in\mathcal{M}$, we say that E is positive. If E is positive, then the matrix $(c_{n,m})_{n,m\in\mathbb{Z}}$ is positive semidefinite (see the proof of Theorem 2). Hence, $0\leqslant E_{\varphi,\varphi}(X)\leqslant E_{\varphi,\varphi}([0,2\pi))=\|\varphi\|^2$, $\varphi\in\mathcal{M}$, $X\in\mathcal{B}([0,2\pi))$, and $(\varphi,\psi)\mapsto E_{\varphi,\psi}(X)$ is bounded on $\mathcal{M}$. In this case, the sesquilinear form $E(X)$, for all $X\in\mathcal{B}([0,2\pi))$, can be regarded as a bounded operator with the unique matrix elements $E_{|n\rangle,|m\rangle}(X)=c_{n,m}(2\pi)^{-1}\int_X e^{i(n-m)\theta}\,\mathrm{d}\theta$, $n,\ m\in\mathbb{Z}$. The mapping $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$ is σ-additive (see the proof of Phase Theorem 2.2 of Ref. 8). Thus, Eq. (18) defines weakly a covariant normalized positive operator measure $X\mapsto E(X)$.

A. Projection-valued covariant normalized positive operator measures

The application of Ref. 5, Proposition 1, in Sec. II gave, in Theorem 1, also a characterization of the $\mathbb{T}$-covariant projection measures. In the present approach one has to determine separately which of the solutions of Theorem 2 are projection valued. We shall do that next.

Proposition 3: Let $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$ be a covariant normalized positive operator measure with the associated structure matrix $(c_{n,m})_{n,m\in\mathbb{Z}}$. E is projection valued, that is, $E(X)^2=E(X)$ for all $X\in\mathcal{B}([0,2\pi))$, if and only if $|c_{n,m}|=1$ for all $n,m\in\mathbb{Z}$.

Proof: Let $x\in(0,1)$ and $n\in\mathbb{Z}$. Using the equations $\Sigma_{k=1}^{\infty}k^{-2}=\pi^2/6$ and $y^2=\pi^2/3+4\Sigma_{k=1}^{\infty}k^{-2}\cos(k(y+\pi))$, $y\in(-\pi,\pi)$, one gets

$$\begin{aligned}\langle n|E([0,2\pi x))^2|n\rangle&=\sum_{s=-\infty}^{\infty}|c_{n,s}|^2\left|\frac{1}{2\pi}\int_0^{2\pi x}e^{i(s-n)\theta}\,\mathrm{d}\theta\right|^2\ (\text{put}\ \ k:=s-n)\\&\leqslant x^2+\frac{1}{2\pi^2}\sum_{k=1}^{\infty}\frac{|e^{2\pi ikx}-1|^2}{k^2}\\&=x^2+\frac{1}{\pi^2}\sum_{k=1}^{\infty}\frac{1}{k^2}-\frac{1}{\pi^2}\sum_{k=1}^{\infty}\frac{\cos(2\pi xk)}{k^2}=x=\langle n|E([0,2\pi x))|n\rangle,\end{aligned}$$

where the equality sign holds only when $|c_{n,m}|=1$ for all $n,m\in\mathbb{Z}$.

On the other hand, if $|c_{n,m}|=1$, then $c_{n,m}=e^{i(v_n-v_m)}$, $v_n\in[0,2\pi)$, for all $n,\ m\in\mathbb{Z}$, since $(c_{n,m})_{n,m\in\mathbb{Z}}$ is the structure matrix of E.[10] Define the following unitary transformations: $W:\mathcal{H}\to\mathcal{H}$, $|n\rangle\mapsto e^{-iv_n}|n\rangle$ and $T:\mathcal{H}\to L^2[0,2\pi)$, $|n\rangle\mapsto f_n$, where $f_n(x)=1/\sqrt{2\pi}e^{-inx}$, $x\in[0,2\pi)$. Now E is unitarily equivalent to the canonical spectral measure E^Q, $E^Q(X)f=\chi_X f$, $X\in\mathcal{B}([0,2\pi))$, $f\in L^2[0,2\pi)$, that is, $E(X)=W^*T^*E^Q(X)TW$, and, thus, E is projection valued.□

Remark 2: The $\mathbb{T}$-covariant localization observables $E:\mathcal{B}(\mathbb{T})\to\mathcal{L}(\mathcal{H})$ are compactly supported, supp $E=\mathbb{T}$. Therefore, all their moment operators

$$V^{(k)}=\int_{\mathbb{T}}z^k\,\mathrm{d}E(z),\quad E^{(k)}=\int_{\mathbb{T}}\arg(z)^k\,\mathrm{d}E(z),$$

with $k\in\mathbb{Z}$, are bounded operators. The cyclic moments $V^{(k)}$ are contractions whereas the phase moments $E^{(k)}$ are self-adjoint. The operator measure E is uniquely determined by both of its moment operator sequences $(V^{(k)})_{k\in\mathbb{Z}}$ and $(E^{(k)})_{k\in\mathbb{Z}}$.

The operator measure E is projection valued if and only if all its cyclic moment operators $V^{(k)}$, $k\in\mathbb{Z}$, are unitary. If E is not projection valued, then, at least, some of the moment operators $V^{(k)}$ are nonunitary. However, if the first cyclic moment operator $V^{(1)}$ of E is unitary, then E is projection measure. Indeed,

$$V^{(1)}=\sum_{n\in\mathbb{Z}}c_{n,n+1}|n\rangle\langle n+1|,$$

so that $V^{(1)}(V^{(1)})^*=I$ implies that $|c_{n,n+1}|=1$ for all $n\in\mathbb{Z}$. By induction, using (17), one then quickly computes that $|c_{n,n+k}|=1$ for all $n\in\mathbb{Z}$ and $k\in\mathbb{Z}^+$, which confirms that E is a projection measure (and hence all $V^{(k)}$ are unitary).

We recall further that $E^{(2)}=(E^{(1)})^2$ exactly when E is projection valued (Ref. 12, Appendix, Sec. 3). In view of that, it is interesting to observe that, due to the covariance condition, the operator measure E (projection valued or not) is uniquely determined already by its first phase moment operator

$$E^{(1)}=\int_{\mathrm{T}}\arg(z)\,\mathrm{d}E(z)=\int_0^{2\pi}\theta\,\mathrm{d}E(\theta)=\pi I+\sum_{n\neq m=-\infty}^{\infty}\frac{c_{n,m}}{i(n-m)}|n\rangle\langle m|$$

since $c_{n,m}=i(n-m)\langle n|E^{(1)}|m\rangle$ for all $n\neq m$. Clearly, the spectral measure $E^{E^{(1)}}$ of the bounded self-adjoint operator $E^{(1)}$ is shift covariant if and only if it is unitarily equivalent to E^Q.

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Global time asymmetry as a consequence of a wave packets theorem

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When $t \to \infty$ any wave packet in the Liouvillian representation of the density matrices becomes a Hardy class function from below. This fact, in the global frame of the Reichenbach diagram, is used to explain the observed global time asymmetry of the universe. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421061]

I. INTRODUCTION

Many authors consider time asymmetry as having a *global* origin.[1] In the last few years, we have shared this position following Davies's reinterpretation of a remarkable idea conceived by Reichenbach.[2] Reichenbach's original idea concerning the arrow of time was that it appears in quasi-isolated systems with nonmaximum entropy at a certain time $t=0$, and he used a ''branched diagram'' originating out of an unstable state to explain this *local* phenomenon. Even if this unstable state can be—at least, theoretically—produced by a fluctuation, in practice it is actually due to the noncomplete isolation of the system before $t=0$. In fact, the truth is that it was interacting with a wider system containing it, in such a way that the energy flowing from this environment results in the production of the unstable initial state of the smaller or *branched* system. This idea was afterwards put in a cosmological scenario by Davies: ''In daily life the arrow of time manifiests itself in the way of quasi-isolated branch systems separated off from the main environment in uncorrelated, less-than-maximum entropy state. Such an explanation suppose, of course, that the wider environment is a less-than-maximum entropy state itself. So long as we confine our attention to subsystems, the question of why their initial state are able to possess less-than-maximum entropy can always be explained by appealing to the wider environment. An examination of realistic branch systems usually shows that they emerge as a result a chain, or hierarchy of branching which, if traced back, expand out into wider and wider regions of the universe. Thus, most of the important time-asymmetric phenomena on Earth are driven by the thermodynamics disequilibrium that exists in the vicinity of the sun, while the sun's own disequilibrium can be traced back to its nuclear constitution, which in turns takes back to the big bang. Eventually, the origin of the arrow of time always refers back to the initial cosmological condition. There exists an arrow of time only because the universe originated in a less-than-maximum entropy state'' (see also the coincident opinion of Feynman in Ref. 1).

We have developed this idea in great detail in several papers.[1] Its obvious simplest graphical representation is the Reichenbach diagram (Fig. 1), where each box represents a physical process, and the lines in the interior of some boxes represent unstable states. The arrow incoming from the left of each box represents the energy that produces the unstable state originating the process of the branch system, while the outgoing arrows emerging from the right of the box represent the energy produced by the process. The big box at the far left-hand side is the initial instability that originates all the branch systems of the diagram: the big-bang (the existence of the unstable initial state was explained in previous papers[3]). Originally, this figure can be considered as a macro-

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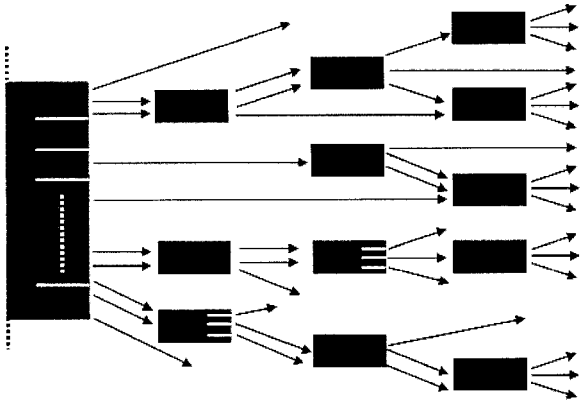

FIG. 1.

scopic process diagram, but as the deep essence of the phenomena is just nonequilibrium, it can be also considered as a microscopic-quantum one, using the quantum mechanics of an unstable system.[4] Then, the Reichenbach diagram is the combination of all the scattering processes within the evolution of the universe, beginning at the initial global instability or big-bang, which is considered as the source of all energy that subsequently flows through all the lines of the diagram. In each scattering process, the incoming energy is used to produce unstable forming states that decay, thus originating the outgoing ones. So, the set of outgoing lines of the diagram can be considered as evolutions from an unstable state toward equilibrium. Essentially, the whole diagram can be considered as only having outgoing lines. In fact, the incoming lines in each scattering "*S*" are just outgoing lines of a previous process. Moreover, the incoming lines (with their associated forming states), cannot be considered as *spontaneous evolutions*, since they just show the pumping of energy from a precedent process, which is really coupled with the scattering system "*S*," making these incoming lines representatives of *nonspontaneous* or forced evolutions. On the contrary, spontaneity clearly characterizes outgoing lines. Considered as a whole, the Reichenbach diagram symbolizes the asymmetrical flow of all the energy within the universe from its initial instability toward a final equilibrium state, resolving this flow as a sum of scattering processes.

Then, time asymmetry (which cannot be explained as a consequence of the local time-symmetric physical *laws*), can be easily explained as a consequence of the time asymmetry of the *universe* (as Fig. 1 shows), which must be considered—in cosmology, at least—as a really existent *physical object* and, as such, endowed with symmetries and asymmetries. Furthermore, the states corresponding to outgoing spontaneous states belong to some space Ψ_- while the incoming nonspontaneous ones belong to another space Ψ_+. These spaces are related by: $\Psi_+ = K\Psi_- \neq \Psi_-$, where K is Wigner time-reversal operator,[5] and time asymmetry—as well as other interesting phenomena—can be considered as a consequence of the existence of such a time-asymmetric space of physical admissible states.[6] *The aim of this paper is to mathematically characterize these spaces.*

For causality reasons, the space Ψ_- was associated with the space of Hardy class functions from below,[7] but this is not completely satisfactory, because it means to postulate causality *before* defining past and future. If all the lines in the Reichenbach diagram would be electromagnetic waves, this choice would be natural, since the outgoing waves of electromagnetic scattering *can* be represented as states belonging to the just mentioned Hardy space.[8] This conclusion can be extended to all hyperbolic scatterings, but not to the parabolic equation of nonrelativistic quantum mechanics. Nevertheless, we are going to show that *far from the scatterer, the outgoing lines belong to a Hardy space if the physical admissible states are wave packets of density matrices.* Thus, eventually all the spontaneously evolving states of the universe would belong to such a type of space, that we will call Ψ_-. On the other hand, the unphysical nonspontaneous time-inverted states would belong to a space Ψ_+. (In the usual popularization language, Ψ_- would be the space

of the spontaneous evolutions: the sugar lump dissolving in the coffee, or the elephant breaking the crystal shop. While Ψ_+ will be the space of impossible—or better, nonspontaneous—evolutions: the sugar lump concentrating in the coffee, or the elephant reconstructing the crystal shop.) The arrow of time would be the consequence of this asymmetry.

II. THE BAKER'S TRANSFORMATION

As a didactical introduction to the subject we will show how spaces Ψ_- and Ψ_+ appear in the famous Baker transformation.

Let us consider the unit square $S=[0,1]\times[0,1]$ with its restricted Lebesgue measure μ and the Baker's transformation:

$$B(x,y)=\begin{cases}(2x,\frac{1}{2}y) & \text{if } 0\leqslant x\leqslant\frac{1}{2}\\ (2x-1,\frac{1}{2}y+\frac{1}{2}) & \text{if } \frac{1}{2}\leqslant x\leqslant 1\end{cases}. \tag{1}$$

Let us consider the *independent and generating partition* of B,[9] i.e., the partition of the unit square into its left and right halves or ''vertical'' rectangles, $P=\{\Delta_1,\Delta_2\}$. ''Independence'' of the partition P with respect to B means that

$$\mu\left(\bigcap_{n=-m_1}^{m_2} B^n(\Delta_{i_n})\right)=\prod_{n=-m_1}^{m_2}\mu(\Delta_{i_n}), \tag{2}$$

where $\Delta_{i_n}\in P$. The ''generating'' character of the partition P with respect to B means that any Borel measurable set of the unit square can be obtained by forming *countable* unions and intersections of sets of the form

$$\bigcap_{n=-m_1}^{m_2} B^n(\Delta_{i_n}) \quad \text{with} \quad \Delta_{i_n}\in P.$$

Let $U:L^2(S,\mu)\to L^2(S,\mu)$ be the unitary map

$$(U^n\rho)(w)=\rho(B^{-n}(w)), \tag{3}$$

where $\rho\in L^2(S,\mu)$, $w\in S$. As is well known, U has a countable uniform Lebesgue spectrum, and therefore[10] there is a *system of imprimitivity* in $L^2(S,\mu)$ based on $\mathbb{Z}$ for the group $\{U^n:n\in\mathbb{Z}\}$. In other words, there is a spectral measure E defined on $\mathbb{Z}$ and taking its values in the set of the orthogonal projection operators of $L^2(S,\mu)$, such that

$$\forall n,m\in\mathbb{Z}:\ U^{-n}E_mU=E_{m+n}, \tag{4}$$

where $E_m=E(\{m\})$ and $E_{m+n}=E(\{m+n\})$. Then, we can define the *age operator*[9] by

$$A=\int_{\mathbb{Z}} n\,\mathrm{d}E=\sum_{n=-\infty}^{+\infty} nE_n. \tag{5}$$

As a consequence of Eqs. (4) and (5), and taking into account the properties of E, we have

$$\forall n\in\mathbb{Z}:\ U^{-n}AU=A+nI. \tag{6}$$

The age operator A has $\mathbb{Z}$ as uniform spectrum with countable multiplicity. In fact, the functions

$$\alpha_0(w)=\begin{cases}+1 & \text{if } w\in\Delta_1\\ -1 & \text{if } w\in\Delta_2\end{cases},$$

together with its transformed by U^n: $\alpha_n=U^n(\alpha_0)$, and all their finite products

$$\alpha_F=\alpha_{n_1}\cdots\alpha_{n_r}$$

$[F=\{n_1,\ldots,n_r\}\ n_j\in\mathbb{Z}]$ constitute an orthonormal eigenbasis $\{\alpha_F:F\subset\mathbb{Z}\}$ of A, each α_F being a "state" of age $n=\max\{n_1,\ldots,n_r\}$, in the sense that

$$A\alpha_F=n\alpha_F. \tag{7}$$

(Clearly, there are countably many states corresponding to each eigenvalue or age n, showing its multiplicity.) Because of Eq. (4), U acts as a *right bilateral shift*[10] on this basis:

$$U\alpha_F=\alpha_{F+1} \tag{8}$$

(where $F+1:=\{n_1+1,\ldots,n_r+1\}$). Equations (6) and (8) show how the age brought about by the dynamical evolution and growing with it matches with the progress of external (or observer's) time labeling the dynamical group.

Now, we can decompose $L^2(S,\mu)$ as a direct sum of two Hardy functions spaces[10] H^2_+ and H^2_- such that

$$H^2_+=\left\{\rho:\rho\in L^2(S,\mu)\wedge\rho=\sum_{F\subset\mathbb{Z}^+}a_F\alpha_F\right\} \tag{9}$$

having only non-null Fourier coefficients $a_F\in\mathbb{C}$ for positive indices, and

$$H^2_-=\left\{\rho:\rho\in L^2(S,\mu)\wedge\rho=\sum_{F\subset\mathbb{Z}^-_0}a_F\alpha_F\right\} \tag{10}$$

having only nonvanishing Fourier coefficients for negative (or zero) indices.

Then, it is obvious that

$$UH^2_+\subset H^2_+,UH^2_-\subset H^2_+\oplus H^2_-=L^2(S,\mu)\neq H^2_- \tag{11}$$

and that

$$\lim_{n\to+\infty}U^n(H^2_+\oplus H^2_-)=H^2_+. \tag{12}$$

We will describe this fact by saying that the states belonging to H^2_+ are "stable toward the future" under the induced evolution U, while those belonging to H^2_- are "unstable." In this way, when acted on by U^n, any function belonging to $L^2(S,\mu)$ will end in space H^2_+ in the "far future" (precisely when $n\to+\infty$). Of course, with respect to the inverse evolution U^{-1} "toward the past"—a *left bilateral shift*—we must reverse these terms, and also change Eq. (12) into

$$\lim_{n\to+\infty}U^{-n}(H^2_+\oplus H^2_-)=H^2_-. \tag{13}$$

In Sec. III we will consider the "quantum version" of what we have said previously.

III. PURE STATES AND THE HAMILTONIAN

Let us begin considering just pure states $|\psi\rangle$, belonging to a Hilbert space $\mathcal{H}$, of a quantum system with Hamiltonian H, such that

$$H|\omega,n\rangle=\omega|\omega,n\rangle, \tag{14}$$

where $0\leqslant\omega<\infty$ or $\omega\in\mathbb{R}^+$ and n belongs to a set of indices N, which is the same for any ω (for didactical reasons we will assume that this set is numerable, and therefore the index n will be discrete). Thus, H can be considered as a typical scattering Hamiltonian just endowed with an absolutely continuous and uniform energy spectrum. Precisely, there is a nuclear space Φ and a rigging of it with $\mathcal{H}$,

$$\Phi\subset\mathcal{H}\subset\Phi^{\times},$$

such that

$$\{|\omega,n\rangle:\omega\in\mathbb{R}^+\wedge n\in N\}\subset\Phi^{\times}$$

(we wil denote by $\Phi^{\times}$ the antidual space of Φ, composed of all continuous antilinear functionals on Φ, and by Φ' its dual) is a generalized eigenbasis of H[11,12] in the sense that

$$\forall\varphi,\psi\in\Phi:\langle\varphi|\psi\rangle=\sum_n\int_0^{\infty}\mathrm{d}\omega\langle\varphi|\omega,n\rangle\langle\omega,n|\psi\rangle, \tag{15}$$

where the left-hand side means the scalar product in $\mathcal{H}$ (antilinear in its left factor), while on the right-hand side $\langle\varphi|\omega,n\rangle$ means the evaluation of the antilinear functional $|\omega,n\rangle$ on φ, and $\langle\omega,n|\psi\rangle$ is the evaluation of the linear functional $\langle\omega,n|$ on ψ. This justifies Dirac's notation:

$$|\psi\rangle=\sum_n\int_0^{\infty}\mathrm{d}\omega|\omega,n\rangle\langle\omega,n|\psi\rangle. \tag{16}$$

Moreover, let us consider that real physical states are wave packets, mathematically modeled by Schwarz functions of $\omega\in\mathbb{R}^+$, for each value of n, so,

$$f(\omega)=\langle\omega,n|\psi\rangle\in\mathcal{S}^+=\mathcal{S}(\mathbb{R}^+). \tag{17}$$

($\mathcal{S}^+$ is the space of all infinite differentiable complex-valued functions defined on $[0,+\infty)$, such that converge to zero for $\omega\to+\infty$ faster than the inverse of any polynomial.)

Taking into account all the values of n we can say that

$$f(\omega)=\langle\omega,n|\psi\rangle\in\bigoplus_n\mathcal{S}_n^+. \tag{18}$$

This mathematical model is adopted for the following reasons:

(1) It is clear that we do not find infinite energies in nature, and so $\langle\omega,n|\psi\rangle$ must somehow go to zero when $\omega\to+\infty$.
(2) In order to use derivatives in our calculations it is not enough to postulate that the states belong to a Hilbert space. They must be representable by differentiable functions. We postulate that they are infinitely differentiable. After all, we cannot find an experimental contradiction to this assumption.
(3) But since these functions must also be square integrable, we can take for granted that they go to zero when $\omega\to+\infty$. We postulate that they go to zero faster than the inverse of any polynomial.

Of course, we are free to choose other spaces instead of $\mathcal{S}^+$, but it is evident that $\mathcal{S}^+$ is the simplest model endowed with all the usual properties of wave packets (that is why the same choice is made in Ref. 13).

IV. MIXED STATES AND THE LIOUVILLIAN

We will use the notation of Ref. 14. Then, the Liouville operator reads

$$L=[H,.]=H\times I-I\times H. \tag{19}$$

Let us consider the space of "density matrices" $\mathcal{L}=\mathcal{H}\otimes\mathcal{H}$, the rigged Hilbert space

$$\Phi\otimes\Phi\subset\mathcal{H}\otimes\mathcal{H}\subset\Phi^{\times}\otimes\Phi',$$

and the generalized basis

$$\{|\omega,n\rangle\langle\omega',n'|:\omega,\omega'\in\mathbb{R}^{+}\wedge n,n'\in N\} \tag{20}$$

(where $|\omega,n\rangle\langle\omega',n'|=|\omega,n\rangle\otimes\langle\omega',n'|\in\Phi^{\times}\otimes\Phi'$).

Let us define the Riezs indices:[14]

$$\begin{gathered}\nu=\omega-\omega', \quad -\infty<\nu<\infty,\\ \sigma=\frac{1}{2}(\omega+\omega'), \quad \frac{|\nu|}{2}\leqslant\sigma<\infty.\end{gathered} \tag{21}$$

It will be convenient to label the basis (20) as

$$|\omega,n\rangle\langle\omega',n'|=|\nu,\sigma,n,n'). \tag{22}$$

Then:

$$L|\nu,\sigma,n,n')=\nu|\nu,\sigma,n,n'). \tag{23}$$

So

$$\left\{|\nu,\sigma,n,n'):\nu\in\mathbb{R}\wedge\frac{|\nu|}{2}\leqslant\sigma<\infty\wedge n,n'\in N\right\} \tag{24}$$

is a generalized eigenbasis of the Liouvillian, ν being the corresponding generalized eigenvalue and σ, n, n', the "degeneration indices." From (21) we see that $\nu\in\mathbb{R}$, while n and $n'\in\mathbb{N}$, and $\sigma\in\mathbb{R}^{+}$, and these spaces have the same cardinality for any ν. So L has uniform Lebesgue spectrum $\mathbb{R}$.

In the basis (24) "the ν-wave function" reads

$$\rho(\nu)=(\rho|\nu,\sigma,n,n'). \tag{25}$$

Following the ideas of Sec. III (and taking into account that we are considering mixed states as "density matrices," identified with *tensor products* of pure states), it is physically justified to suppose that these functions are sums of products of functions $f(\omega)\in\mathcal{S}(\mathbb{R}^{+})$, namely:

$$f(\omega)g(\omega')=f\left(\sigma+\frac{\nu}{2}\right)g\left(\sigma-\frac{\nu}{2}\right). \tag{26}$$

They will have infinite derivatives with respect to ν, since f and g are infinitely differentiable. Moreover, $\rho(\nu)$ goes to zero when $\nu\to\pm\infty$ faster than the inverse of any polynomial since this is a property of f and g. Thus, for any σ, n, n':

$$\rho(\nu)=(\rho|\nu,\sigma,n,n')\in\mathcal{S}(\mathbb{R}). \tag{27}$$

V. THE AGE OPERATOR

Since L has uniform Lebesgue spectrum $\mathbb{R}$, there is a system of imprimitivity in $\mathcal{L}$ based on $\mathbb{R}$ for the group $\{U_t : t \in \mathbb{R}\}$. In other words, there is a spectral measure E defined on $\mathbb{R}$ and taking its values in the set of the orthogonal projection operators of $\mathcal{L}$,[10] such that

$$\forall t,s \in \mathbb{R}: U_t^{-1} E_s U_t = E_{t+s}, \tag{28}$$

where $E_s = E((-\infty, s])$, and $E_{t+s} = E((-\infty, t+s])$. Then we can define the *age operator*[15] by

$$A = \int_{\mathbb{R}} t \, \mathrm{d}E. \tag{29}$$

As a consequence of Eqs. (28) and (29), and taking into account the properties of E, we have

$$\forall t \in \mathbb{R}: U_t^{-1} A U_t = A + tI. \tag{30}$$

The age operator A has $\mathbb{R}$ as a uniform Lebesgue spectrum. In fact, for the physical states we have

$$A\rho(\nu,\sigma,n,n') \doteq i \frac{\partial}{\partial \nu} \rho(\nu,\sigma,n,n')|_{\sigma,n,n'=\text{const}}, \tag{31}$$

that is equivalent to the commutation relation

$$[A,L] = i. \tag{32}$$

(A and L have essentially the same commutation relation as position and momentum operators q and p.) Then $\hat{\rho}(a,\sigma,n,n')$, the Fourier transform in variables $\nu \leftrightarrow a$ of $\rho(\nu,\sigma,n,n')$, is an eigenvector of A, precisely:

$$A\hat{\rho}(a,\sigma,n,n') = a\hat{\rho}(a,\sigma,n,n'). \tag{33}$$

Moreover $\hat{\rho}(a,\sigma,n,n') \in \mathcal{S}(\mathbb{R})$ in the variable a since it is the Fourier transform of $\rho(\nu,\sigma,n,n')$. Then, the time evolution of $\hat{\rho}(a,\sigma,n,n')$ reads:

$$\begin{aligned}(\widehat{e^{-iLt}\rho})(a,\sigma,n,n') &= (\widehat{e^{-i\nu t}\rho})(a,\sigma,n,n') \\ &= \int_{-\infty}^{+\infty} e^{-i\nu t} \rho(\nu,\sigma,n,n') e^{-iat} \mathrm{d}\nu \\ &= \int_{-\infty}^{+\infty} e^{-i(a+t)\nu} \rho(\nu,\sigma,n,n') \mathrm{d}\nu = \hat{\rho}(a+t,\sigma,n,n').\end{aligned} \tag{34}$$

Thus, L is the generator of the time translations, and $\hat{\rho}(a,\sigma,n,n')$ increase its age as $a \to a + t$ becoming $\hat{\rho}(a+t,\sigma,n,n')$. This fact justifies the name given to A. But Eq. (34) tells us that during its time evolution, the wave packet $\hat{\rho}(a,\sigma,n,n') \in \mathcal{S}(\mathbb{R})$ does not change its shape, being merely shifted to the left. So, in the basis (24) all physical states are wave packets at any time, and we have

$$\lim_{t \to +\infty} \hat{\rho}(a+t,\sigma,n,n') = 0 \tag{35}$$

(in the pointwise convergence sense) because functions in Schwarz space go to zero when its variable goes toward the infinite.

VI. THE THEOREM

The quantum version of the Baker's transformation example would be as follows. Let us consider a quantum system whose states ρ are ''density matrices'' belonging to a Hilbert–Liouville space $\mathcal{L}$. Let L be the Liouville superoperator in $\mathcal{L}$, assumed as having $\mathbb{R}$ as uniform Lebesgue spectrum. This amounts to saying that the evolution superoperator $\exp[-iLt]$ is a bilateral shift, closely related with Hardy classes.[16,10]

We can decompose the space of physical states $\Psi=\Phi\otimes\Phi$ as $\Psi_+\oplus\Psi_-$, where

$$\Psi_+=\{\rho\in\Psi:[\forall a<0:\hat{\rho}(a,\sigma,n,n')=0]\}=\{\rho\in\Psi:\hat{\rho}(a,\sigma,n,n')\in L^2(\mathbb{R}^+)\}, \tag{36}$$

$$\Psi_-=\{\rho\in\Psi:[\forall a>0:\hat{\rho}(a,\sigma,n,n')=0]\}=\{\rho\in\Psi:\hat{\rho}(a,\sigma,n,n')\in L^2(\mathbb{R}^-)\} \tag{37}$$

are spaces of wave packets that are also Hardy class functions in the ν variable from above (Ψ_+), or below (Ψ_-), because of a Paley–Wiener Theorem (Ref. 12, Theorem II, p. 47). Then our theorem states that:

Theorem: *The limit of any physical state, when $t\to+\infty$, belongs to Ψ_-.*

Proof: Because of the fact that $L^2(\mathbb{R})=L^2(\mathbb{R}^-)\oplus L^2(\mathbb{R}^+)$, we can decompose any $\hat{\rho}(a)$ [abbreviation for $\hat{\rho}(a,\sigma,n,n')$] as

$$\hat{\rho}(a)=\hat{\rho}_-(a)+\hat{\rho}_+(a), \tag{38}$$

where

$$\begin{aligned}&\hat{\rho}_-(a)=\hat{\rho}(a)\quad\text{for}\quad a<0,\quad \hat{\rho}_-(a)=0\quad\text{for}\quad a>0,\\ &\hat{\rho}_+(a)=\hat{\rho}(a)\quad\text{for}\quad a>0,\quad \hat{\rho}_+(a)=0\quad\text{for}\quad a<0.\end{aligned} \tag{39}$$

In particular

$$\hat{\rho}(a+t)=\hat{\rho}_-(a+t)+\hat{\rho}_+(a+t) \tag{40}$$

(first the shift to the left, and then the decomposition into the negative and positive parts with respect to $a=0$, not with respect to $a+t=0$).

From Eqs. (40) and (35) we see that $\hat{\rho}_+(a+t)\to0$ in $L^2(\mathbb{R}^+)$, when $t\to+\infty$, and therefore $\hat{\rho}(a+t)-\hat{\rho}_-(a+t)\to0$ in $L^2(\mathbb{R}^+)$. So, when $t\to+\infty$ the function $\hat{\rho}(a+t)$ belongs to $L^2(\mathbb{R}^-)$, and thus its inverse Fourier transform, namely $(e^{-iLt}\rho)(\nu)$, belongs to Ψ_-. □

So, we have proved

$$\lim_{t\to+\infty} e^{-iLt}\Psi=\Psi_- \tag{41}$$

the wave packets analog of Eq. (13) for the left shift, as announced.

VII. CONCLUSION

As the typical distance among the scatterers is much bigger than the characteristic dimension of the scatterers itself, most of the states can be considered far from these scatterers. Therefore, most of the physical states *do* belong to space Ψ_-, thus explaining time-asymmetry (see Sec. I). Moreover, using the space of physical admissible states Ψ_-, most of the irreversible phenomena of nature can be foreseen, obtaining the same results as those of other formalisms (such as ''coarse-graining,'' Lindblad, etc.[17]).

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Generalized coherent and intelligent states for exact solvable quantum systems

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The so-called Gazeau–Klauder and Perelomov coherent states are introduced for an arbitrary quantum system. We give also the general framework to construct the generalized intelligent states which minimize the Robertson–Schrödinger uncertainty relation. As illustration, the Pöschl–Teller potentials of trigonometric type will be chosen. We show the advantage of the analytical representations of Gazeau–Klauder and Perelomov coherent states in obtaining the generalized intelligent states in analytical way. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Coherent states, known as the closest states to classical ones, play an important role in many different contexts of theoretical and experimental physics, especially quantum optics.[1–3] Schrödinger first discovered the coherent states for the harmonic oscillator potential in 1926[4] and much work has been done since then on their properties and applications.[5,6] The coherent states have also been found in systems with the Lie group symmetry.[7,8] Recently, coherent states have been found in special Hamiltonians.[9] These coherent states are called minimum uncertainty coherent states. In coherent states the standard deviation of X (coordinate) and P (momentum) are equal and their product is minimum over states. There are also quantum states where, though we have minimum uncertainty for the standard deviation of coordinate and momentum, they are not equal any more; those states are called squeezed states. These states are as important as coherent ones. Their generation plays an important role in many different branches of physics.

There exist three definitions of coherent states. The first one defines the usual coherent states as eigenstates of the annihilation operator a^- for each individual oscillator mode of the electromagnetic field

$$a^-|z\rangle = z|z\rangle. \tag{1}$$

Here $[a^-,a^+]=1$ $((a^-)^\dagger = a^+)$ and z is a complex constant with conjugate $\overline{z}$. The resulting unit normalized states $|z\rangle$ are given by

$$|z\rangle = e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle, \tag{2}$$

where $|n\rangle$ is an element of the Fock space $\mathcal{H}\equiv\{|n\rangle, n\geqslant 0\}$. A second definition of coherent states for oscillators assumes the existence of a unitary "displacement" operator $D(z)$ defined as

$$D(z) = \exp(za^+ - \overline{z}a^-). \tag{3}$$

The coherent states parametrized by z are given by the action of $D(z)$ on the ground state $|0\rangle$. The unitarity of $D(z)$ ensures the correct normalization of $|z\rangle$. The Baker–Campbell–Hausdorff relation (BCH)

$$e^A e^B = e^{A+B+(1/2)[A,B]}, \tag{4}$$

valid only for any two operators A and B that both commute with the commutator $[A,B]$, implies the equivalence of this definition with the one above.

A third definition is based on the uncertainty relation, with the position X and momentum P given, as usual, by

$$X = \frac{1}{\sqrt{2}}(a^- + a^+), \quad P = \frac{i}{\sqrt{2}}(a^+ - a^-). \tag{5}$$

The coherent states defined above have the minimum-uncertainty value $2\Delta X \Delta P = 1$ and maintain this relation in time (temporal stability of coherent states). Coherent states have two important properties. First, they are not orthogonal to each other. Second, they provide a resolution of the identity, i.e., they form an over-complete set states.

A central goal of this article is to extend the above three definitions for an arbitrary quantum system (exactly solvable) and compare the equivalence between them. Note that an attempt in this sense was considered by Nieto *et al.*[9] concluding that the three definition are generally inequivalents. Our analysis is different from the Nieto *et al.* ones for several reasons which will be clear in the sequel of this article.

The method we adopt is an extension of the group-theoretical approach to coherent states which generalizes the displacement operator definition. We call the obtained coherent states: coherent states of Perelomov type. The latter will be compared with Gazeau–Klauder coherent states constructed using the approach adopted by Barut–Girardello[10,11] (see also Refs. 12–14) for an arbitrary quantum system. To extend to third definition, we solve the eigenvalue equation of states minimizing the Robertson–Schrödinger uncertainty relation which extends the Heisenberg one. These states are called generalized intelligent states (GIS).[15,16] We show that the set of GIS includes the Gazeau–Klauder coherent states in a particular situation.

This article is organized as follows: Creation and annihilation operators for an arbitrary quantum system (exactly solvable) are introduced in Sec. II. These operators are used to define Gazeau–Klauder coherent states in Sec. III. Section IV is devoted to giving a general algorithm leading to the Perelomov coherent states. States minimizing the Robertson–Schrödinger uncertainty relation are constructed in Sec. V. The results of Secs. III–V are applied to a quantum system evolving in Pöschl–Teller potentials. In particular, using the analytical representations of Gazeau–Klauder coherent states and Perelomov ones, we give the generalized intelligent states under analytical forms (Sec. VI). The last section concerns a summary of the main results of this work.

II. CREATION AND ANNIHILATION OPERATORS FOR AN ARBITRARY QUANTUM SYSTEM

We start with general consideration on the creation and annihilation operators from the factorization of a given Hamiltonian admitting a nondegenerate discrete infinite energy spectrum. Let us assume that the Hamiltonian H of a quantum system admits infinite spectrum of energy $\{E_n, n=0,1,2,\dots\}$ such that the fundamental energy $E_0=0$ and the others are in increasing order, i.e.,

$$E_0 = 0 < E_1 < E_2 < \cdots < E_{n-1} < E_n < \cdots. \tag{6}$$

For such a system, we know that the fundamental state $\psi_0(x)$ and the potential $V(x)$ are closely related so that the factorization is possible. Indeed, the time independent Schrödinger equation for $\psi_0(x)$ reads

$$H\psi_0(x)=\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right)\psi_0(x)=0, \tag{7}$$

and we have

$$V(x)=\frac{1}{2}\frac{\psi_0''(x)}{\psi_0(x)}, \tag{8}$$

where the prime means the derivation with respect to x.

The usual factorization of H is then given by

$$H=A^+A^- \tag{9}$$

with

$$A^+=\frac{1}{\sqrt{2}}\left(-\frac{d}{dx}+W(x)\right), \quad A^-=\frac{1}{\sqrt{2}}\left(\frac{d}{dx}+W(x)\right), \tag{10}$$

where the superpotential $W(x)$ satisfies the Riccati equation

$$V(x)=\tfrac{1}{2}(W^2(x)-W'(x)). \tag{11}$$

It is clear, from Eqs. (8) and (11), that $W(x)$ takes the form

$$W(x)=-\frac{\psi_0'(x)}{\psi_0(x)}. \tag{12}$$

From Eq. (10), we have

$$[A^-,A^+]=W'(x), \tag{13}$$

which generalizes the usual one for the harmonic oscillator ($W(x)=x$). The operators A^+ and A^- are not the creation and annihilation operators of H. Then, we are interested now in identifying the operators creating and annihilating the quantum states of the system under consideration. The key ingredients in constructing them is to define the operator $H_+=A^-A^+$ obtained from $H=H_-=A^+A^-$ by reversing the order of A^- and A^+. The operator H_+ is in fact a Hamiltonian corresponding to a new potential $V_+(x)$:

$$H_+=-\frac{1}{2}\frac{d^2}{dx^2}+V_+(x), \quad V_+(x)=\frac{1}{2}(W^2(x)+W'(x)). \tag{14}$$

The potentials $V_-(x)=V(x)$ and $V_+(x)$ are known as supersymmetric partner potentials and $H_-\equiv H$ and H_+ are isospectrals (H_+ is also exactly solvable). Indeed, the Schrödinger equation for H_-,

$$H_-|\psi_n\rangle=E_n|\psi_n\rangle, \tag{15}$$

implies

$$H_+(A^-|\psi_n\rangle)=E_n(A^-|\psi_n\rangle). \tag{16}$$

Similarly, the Schrödinger equation for H_+,

$$H_+|\theta_n\rangle = e_n|\theta_n\rangle, \tag{17}$$

implies

$$H_-(A^+|\theta_n\rangle) = e_n(A^+|\theta_n\rangle), \tag{18}$$

where e_n are the eigenvalues and $|\theta_n\rangle$ are eigenstates of H_+. From the latter equations and the fact that $E_0=0$, it is clear that the energies and eigenstates of H_- and H_+ are related by

$$e_n = E_{n+1},$$

$$A^-|\psi_{n+1}\rangle = \sqrt{E_{n+1}}e^{i(E_{n+1}-E_n)\alpha}|\theta_n\rangle, \tag{19}$$

$$A^+|\theta_n\rangle = \sqrt{e_n}e^{-i(E_{n+1}-E_n)\alpha}|\psi_{n+1}\rangle, \tag{20}$$

where $\alpha \in \mathbf{R}$. Notice that if the eigenstates $|\psi_{n+1}\rangle$ ($|\theta_n\rangle$) of H_- (H_+) are normalized, then the wavefunctions $|\theta_n\rangle$ ($|\psi_{n+1}\rangle$) in Eqs. (19) and (20) are also normalized. Further, the operator A^- (A^+) converts an eigenfunction of H_- (H_+) into an eigenfunction of H_+ (H_-) with the same energy. Thus, the operators A^- and A^+ connect the states $|\psi_n\rangle$ and $|\theta_n\rangle$ and cannot be considered as creation and annihilation operators for $H \equiv H_-$. To define the ladder operators for the quantum system described by H, we consider the unitary transformation U connecting the basis $\{|\psi_n\rangle\}$ and $\{|\theta_n\rangle\}$ as follows:

$$|\theta_n\rangle = U|\psi_n\rangle \tag{21}$$

with

$$UU^+ = U^+U = I. \tag{22}$$

The explicit structure of the unitary operator U is given by

$$U = \sum_{n,m} U_{nm}|\psi_n\rangle\langle\psi_m|, \tag{23}$$

where the elements U_{nm} are evaluated by

$$U_{nm} = \langle\psi_n|\theta_m\rangle = \int \psi_n^*(x)\,\theta_m(x)\,dx. \tag{24}$$

Note that in the harmonic oscillator case $U=I$.

At this stage, we can introduce the creation and annihilation operators of H by

$$a^+ = A^+U, \quad a^- = U^+A^-. \tag{25}$$

The actions of the operators a^+ and a^- on the states $\{|\psi_n\rangle\}$ are given by

$$a^+|\psi_n\rangle = \sqrt{E_{n+1}}e^{-i(E_{n+1}-E_n)\alpha}|\psi_{n+1}\rangle, \tag{26}$$

$$a^-|\psi_n\rangle = \sqrt{E_n}e^{i(E_n-E_{n-1})\alpha}|\psi_{n-1}\rangle. \tag{27}$$

Note that $a^+a^- = A^+A^- = H$. It is easy to show that

$$|\psi_n\rangle = \frac{(a^+)^n}{\sqrt{E(n)}}e^{iE_n\alpha}|\psi_0\rangle, \quad n>0, \tag{28}$$

where we have defined

$$E(n)=E_1E_2\cdots E_n \tag{29}$$

and, for $n=0$, $E(0)=1$.

The exponential factor appearing in all these expressions produces only a phase factor and will be significant for the temporal stability of the coherent states we will construct in the following. From Eqs. (26) and (27), we have also

$$[a^-,a^+]|\psi_n\rangle=(E_{n+1}-E_n)|\psi_n\rangle. \tag{30}$$

Let us now introduce the operator N such that

$$N|\psi_n\rangle=n|\psi_n\rangle, \tag{31}$$

which is, in general (for an arbitrary quantum system), different from the product a^+a^- $(=H)$. We can see that it satisfies the following properties:

$$a^-N=(N+1)a^-, \quad a^+(N+1)=Na^+. \tag{32}$$

We are then able to define an operator G such that

$$[a^-,a^+]=G(N), \tag{33}$$

which acts in the states $|\psi_n\rangle$ as

$$G(N)|\psi_n\rangle=(E_{n+1}-E_n)|\psi_n\rangle. \tag{34}$$

The operator G is Hermitian.

III. GAZEAU–KLAUDER COHERENT STATES

A. Eigenstates of annihilation operator

The Gazeau–Klauder coherent states are eigenstates of the annihilation operator of the system under consideration. For the system governed by the Hamiltonian H $(=A^+A^-=a^+a^-)$, such states are labeled by $|z,\alpha\rangle$, $z\in\mathbf{C}$ and $\alpha\in\mathbf{R}$ (α is the parameter entering in Eqs. (26) and (27)), and they are assumed to be the solution of the eigenvalue equation

$$a^-|z,\alpha\rangle=z|z,\alpha\rangle. \tag{35}$$

To have their explicit form we decompose it in the basis $\{|\psi_n\rangle\}$ such that

$$|z,\alpha\rangle=\sum_{n=0}^{+\infty} a_n|\psi_n\rangle \tag{36}$$

and insert this equation in (35). Using Eq. (27), we find

$$a_n=\frac{z^n}{\sqrt{E(n)}}e^{-iE_n\alpha}a_0, \quad n>0, \tag{37}$$

with $E(n)$ is given by (29). For $n=0$, the state $|\psi_0\rangle$ is an eigenstate of a^- with eigenvalue 0. Finally, the coherent states $|z,\alpha\rangle$ take the form

$$|z,\alpha\rangle=a_0\sum_{n=0}^{+\infty}\frac{z^n}{\sqrt{E(n)}}e^{-iE_n\alpha}|\psi_n\rangle. \tag{38}$$

The constant a_0 will be fixed by imposing the normalization to unity. We get

$$|a_0|^{-2}=\sum_{n=0}^{+\infty}\frac{|z|^{2n}}{E(n)}. \tag{39}$$

The coherent states (38) are continuous in $z\in\mathbf{C}$ and $\alpha\in\mathbf{R}$. Moreover, the presence of the phase factor in the definition equations (26) and (27) of the a^- and a^+ actions leads to temporal stability of the coherent states. Indeed, we have

$$e^{iHt}|z,\alpha\rangle=|z,\alpha+t\rangle. \tag{40}$$

The analysis of completeness (in fact, the overcompleteness) requires us to compute the identity resolution, that is,

$$\int |z,\alpha\rangle\langle z,\alpha|d\mu(z)=I_{\mathcal{H}}. \tag{41}$$

Note that the integral is over the disk $\{z\in\mathbf{C},|z|<\mathcal{R}\}$, where the radius of convergence $\mathcal{R}$ is

$$\mathcal{R}=\lim_{n\to+\infty}\sqrt[n]{E(n)} \tag{42}$$

and the measure $d\mu(z)$ has to be determined. To determine it, we suppose that $d\mu(z)$ depends only on $|z|$ (isotropy condition). We take

$$d\mu(z)=[a_0]^{-2}h(r^2)rdrd\varphi;\quad z=re^{i\varphi}. \tag{43}$$

Hence, the identity resolution can be written in the following form:

$$I_{\mathcal{H}}=\sum_{n=0}^{+\infty}|\psi_n\rangle\langle\psi_n|\left[\frac{\pi}{E(n)}\int_0^{\mathcal{R}^2}h(u)u^n du\right]. \tag{44}$$

The last equation is satisfied when we have

$$\int_0^{\mathcal{R}^2}h(u)u^n du=\frac{E(n)}{\pi}. \tag{45}$$

It is clear that the identity resolution is then equivalent to the determination of the function $h(u)$ satisfying Eq. (45). For $\mathcal{R}\to\infty$, the function $h(u)$ is the inverse Mellin transform of $\pi^{-1}E(s-1)$,

$$h(u)=\frac{1}{2\pi^2 i}\int_{c-i\infty}^{c+i\infty}E(s-1)u^{-s}ds;\quad c\in\mathbf{R}. \tag{46}$$

Note that explicit computation of the function $h(u)$ requires the knowledge of the spectrum of the quantum mechanical system under consideration.

Using Eq. (35), one can obtain the mean value of the Hamiltonian H in the states $|z,\alpha\rangle$:

$$\langle z,\alpha|H|z,\alpha\rangle=|z|^2. \tag{47}$$

This relation in known as the action identity.

Finally, we remark that the coherent states $|z,\alpha\rangle$ can be written as an operator $U(z)$ acting in the ground state $|\psi_0\rangle$

$$U(z)=a_0\exp\left(z\frac{N}{g(N)}a^+\right) \tag{48}$$

such that we have

$$|z,\alpha\rangle=U(z)|\psi_0\rangle. \tag{49}$$

In (48), $g(N)\equiv H=a^+a^-$. The operator $U(z)$ is not unitary and cannot be interpreted as the displacement operator in the Perelomov's sense.

A final comment can be made in connection with the work of Gazeau and Klauder.[11] In fact, the coherent states (38) satisfy all the requirements (continuity, temporal stability, identity resolution, action identity) given in their approach but they are more general since we are working with $z\in\mathbf{C}$ and $\alpha\in\mathbf{R}$. They are eigenstates of the annihilation operator a^-. Additional properties of this set of states will be considered in Sec. V.

B. Fock–Bargmann representation

It is well known that the Fock–Bargmann representation enables one to find simple solutions to a number of problems, exploiting the theory of analytical entire functions. In this subsection, generalizing the pioneering work of Bargmann[17] for the usual harmonic oscillator, we give the Bargmann representation of an arbitrary quantum mechanical system. We recall that in the Fock–Bargmann representation for the standard harmonic oscillator, the creation operator a^+ is the multiplication by z while the annihilation operator a^- is the differentiation with respect to z.

For an arbitrary quantum system, we define the Fock–Bargmann space as a space of functions which are holomorphic on a ring D of the complex plane. The scalar product is written with an integral of the form

$$\langle f|g\rangle=\int\overline{f(z)}g(z)d\mu(z), \tag{50}$$

where $d\mu(z)$ is the measure defined above (see Eq. (43)). Let $|f\rangle$ be an arbitrary quantum state of the system under study,

$$|f\rangle=\sum_{n=0}^{+\infty}f_n|\psi_n\rangle,\quad\text{with}\quad\sum_{n=0}^{+\infty}|f_n|^2<\infty. \tag{51}$$

Any state $|f\rangle$ is represented, in the Fock–Bargmann representation, as a function of the complex variable z (using the so-called coherent states associated with the quantum system under consideration):

$$f(z)\equiv\langle\overline{z},\alpha|f\rangle=\sum_{n=0}^{+\infty}\frac{z^n}{\sqrt{E(n)}}e^{iE_n\alpha}f_n. \tag{52}$$

In particular, to the vectors $|\psi_n\rangle$ there correspond the monomials

$$\langle\overline{z},\alpha|\psi_n\rangle=\frac{z^n}{\sqrt{E(n)}}e^{iE_n\alpha}. \tag{53}$$

Using Eqs. (52) and (53), we can prove the following result: In the Fock–Bargmann representation, we realize the annihilation operator a^- by

$$a^-=z^{-1}g\left(z\frac{d}{dz}\right), \tag{54}$$

the creation operator a^+ by

$$a^+ = z, \tag{55}$$

and the operator number by

$$N = z\frac{d}{dz}. \tag{56}$$

The Fock–Bargmann representation exists if we have a measure such that

$$\int |z,\alpha\rangle\langle z,\alpha| d\mu(z) = I_{\mathcal{H}}. \tag{57}$$

The existence of the measure, discussed previously for the so-called Gazeau–Klauder coherent states, ensures that the scalar product takes the form (50). We note that in the case where

$$g\left(z\frac{d}{dz}\right) = z\frac{d}{dz}, \quad \text{i.e.,} \quad g(N) = N, \tag{58}$$

we recover the well-known Fock–Bargmann representation of the harmonic oscillator. The Fock–Bargmann realization discussed here will be the main tool to construct the generalized intelligent states (see Sec. VI).

IV. COHERENT STATES OF PERELOMOV'S TYPE

In view of the second definition of coherent states for the standard harmonic oscillator (group-theoretical approach), we define, for an arbitrary quantum system, the states

$$|z,\alpha\rangle = \exp(za^+ - \bar{z}a^-)|\psi_0\rangle, \quad \text{for} \quad z \in \mathbf{C}, \tag{59}$$

which we call of Perelomov's type. We have to compute the action of the displacement operator

$$D(z) = \exp(za^+ - \bar{z}a^-) \tag{60}$$

on the ground state $|\psi_0\rangle$ of the quantum system under study. We will give the result of this action in a closed form. An illustration is treated for the Pöschl–Teller and square-well potentials (in Sec. VI).

Using the actions of the annihilation and creation operators on the Hilbert space $\{|\psi_n\rangle, n = 0,1,2,\ldots\}$ (Eqs. (26) and (27)), one can, after more or less complicated computations, show that the states $|z,\alpha\rangle$ can be written as follows:

$$|z,\alpha\rangle = \sum_{n=0}^{+\infty} \frac{z^n}{\sqrt{F_n(|z|)}} e^{-iE_n\alpha}|\psi_n\rangle. \tag{61}$$

The quantities $F_n(|z|)$ satisfy

$$F_n(|z|)E(n)(c_n(|z|))^2 = 1, \tag{62}$$

where the coefficients $c_n(|z|)$ are given by

$$c_n(|z|) = \sum_{j=0}^{+\infty} \frac{(-|z|^2)^j}{(n+2j)!}\left(\sum_{i_1=1}^{n+1} E_{i_1}\sum_{i_2=1}^{i_1+1} E_{i_2}\cdots\sum_{i_j=1}^{i_{j-1}+1} E_{i_j}\right). \tag{63}$$

Setting

$$\pi(n+1,j)=\sum_{i_1=1}^{n+1} E_{i_1}\sum_{i_2=1}^{i_1+1} E_{i_2}\cdots\sum_{i_j=1}^{i_{j-1}+1} E_{i_j} \quad \text{and} \quad \pi(n+1,0)=1, \tag{64}$$

one can verify that the π's satisfy the following relation:

$$\frac{\pi(n+1,j)-\pi(n,j)}{E_{n+1}}=\pi(n+2,j-1). \tag{65}$$

Using this recurrence formula, one can show that the coefficients $c_n(|z|=r)$ satisfy the following differential equation:

$$\frac{dc_n(r)}{dr}=\frac{1}{r}c_{n-1}(r)-\frac{n}{r}c_n(r)-E_{n+1}c_{n+1}(r)r. \tag{66}$$

Hence, solving this equation, we can obtain explicitly the coherent states $|z,\alpha\rangle$ of Perelomov's type. Of course, to solve this equation for an arbitrary quantum system is, in general, not an easy task. However, solutions in some particular (and interesting physical system) will be given in Sec. VI. Here, as a first illustration of the approach leading to coherent states of Perelomov's type, we give the standard harmonic oscillator coherent states using the above considerations. In this case we show that (61) coincides with (2). For the harmonic oscillator $E_n=n$ and $E(n)=n!$.

To solve Eq. (66), we set

$$c_n(r)=\frac{1}{n!}\sum_{m=0}^{+\infty} a_m r^m. \tag{67}$$

Substituting this expression in (66), we get the coefficients a_m,

$$a_{2p}=\frac{(-1)^p}{2^p p!}a_0 \quad \text{and} \quad a_{2p+1}=0, \tag{68}$$

where $a_0=1$ because $c_0(r=0)=1$. Finally, we have

$$F_n(|z|)=n!\exp(|z|^2) \tag{69}$$

and

$$|z,\alpha\rangle=\exp\left(-\frac{|z|^2}{2}\right)\sum_{n=0}^{+\infty}\frac{z^n}{\sqrt{n!}}e^{-i\alpha n}|n\rangle. \tag{70}$$

We recover a well-known result.

V. GENERALIZED INTELLIGENT STATES

These states minimize the Robertson–Schrödinger uncertainty relation,[18,19] and generalize the Gazeau–Klauder coherent states.

Using the creation a^+ and annihilation a^- operators, we introduce the Hermitian operators

$$X=\frac{1}{\sqrt{2}}(a^+ + a^-), \quad P=\frac{i}{\sqrt{2}}(a^+ - a^-), \tag{71}$$

which satisfy the commutation relation

$$[X,P]=iG(N)\equiv iG. \tag{72}$$

The operator $G(N)$, defined by (34) is not necessarily a multiple of the unit operator (for an arbitrary quantum system). It is well known that for two Hermitian operators X and P satisfying the noncanonical commutation relation (72), the variances $(\Delta X)^2$ and $(\Delta P)^2$ satisfy the Robertson–Schrödinger uncertainty relation

$$(\Delta X)^2(\Delta P)^2 \geqslant \tfrac{1}{4}(\langle G\rangle^2+\langle F\rangle^2), \tag{73}$$

where the operator F is defined by

$$F=\{X-\langle X\rangle, P-\langle P\rangle\} \tag{74}$$

or by

$$F=i[(2a^- -\langle a^-\rangle)\langle a^-\rangle+(-2a^+ +\langle a^+\rangle)\langle a^+\rangle - a^{-2}+a^{+2}] \tag{75}$$

in terms of the operators a^- and a^+. The symbol $\{,\}$ in (74) stands for the anticommutator. When there is a correlation between X and P, i.e., $\langle F\rangle \neq 0$, the relation (73) is a generalization of the usual one (the Heisenberg uncertainty condition),

$$(\Delta X)^2(\Delta P)^2 \geqslant \tfrac{1}{4}\langle G\rangle^2. \tag{76}$$

The special form (76) is identical to the general form (73) if X and P are uncorrelated, i.e., $\langle F\rangle = 0$. The general uncertainty relation (73) is better suited to determine the lower bound on the product of variances in the measurement of observables corresponding to the noncanonical operators. The so-called generalized intelligent states are obtained when the equality in the Robertson–Schrödinger uncertainty relation is realized.[20] The inequality in (73) becomes equality for the states satisfying the equation (see also Refs. 20–23)

$$(X+i\lambda P)|\psi\rangle = z\sqrt{2}|\psi\rangle, \quad \lambda, z\in \mathbf{C}. \tag{77}$$

As a consequence, we have the following relations

$$(\Delta X)^2=|\lambda|\Delta, \quad (\Delta P)^2=\frac{1}{|\lambda|}\Delta, \tag{78}$$

with

$$\Delta=\tfrac{1}{2}\sqrt{\langle G\rangle^2+\langle F\rangle^2}. \tag{79}$$

The average values $\langle G\rangle$ and $\langle F\rangle$, in the states satisfying the eigenvalue equation (77) can be expressed in terms of the variances as follows:

$$\langle G\rangle = 2\,\mathrm{Re}(\lambda)\langle\Delta P\rangle^2, \quad \langle F\rangle = 2\,\mathrm{Im}(\lambda)\langle\Delta P\rangle^2. \tag{80}$$

It is clear, from (78) that if $|\lambda|=1$, we have

$$(\Delta X)^2=(\Delta P)^2. \tag{81}$$

We call the states satisfying (81) with $|\lambda|=1$ the generalized coherent states. For $|\lambda|\neq 1$, the states are called generalized squeezed states.

Using Eq. (77) one can obtain some general relations for the average values and dispersions of X and P in the states which minimize the Robertson–Schrödinger uncertainty relation (73). We have

$$(\Delta X)^2=\tfrac{1}{2}(\mathrm{Re}(\lambda)\langle G\rangle+\mathrm{Im}(\lambda)\langle F\rangle), \tag{82}$$

$$(\Delta P)^2=\frac{1}{2|\lambda|^2}(\mathrm{Re}(\lambda)\langle G\rangle+\mathrm{Im}(\lambda)\langle F\rangle), \tag{83}$$

$$\mathrm{Im}(\lambda)\langle G\rangle=\mathrm{Re}(\lambda)\langle F\rangle. \tag{84}$$

In order to give a complete classification of the so-called generalized intelligent states for an arbitrary quantum system, we have to solve the eigenvalue equation (77). Such computation was considered previously by the authors in Refs. 15 and 16. The states minimizing the Robertson–Schrödinger uncertainty relation are given by

$$|\psi\rangle\equiv|z,\lambda,\alpha\rangle=\sum_{n=0}^{+\infty} d_n|\psi_n\rangle, \quad d_n\equiv d_n(z,\alpha,\lambda). \tag{85}$$

For the case where $\lambda\neq -1$, the coefficients d_n are given by the following expression:

$$d_n=d_0\frac{(2z)^n}{(1+\lambda)^n\sqrt{E(n)}}\left[\sum_{h=0(1)[n/2]}(-1)^h\frac{(1-\lambda^2)^h}{(2z)^{2h}}\Delta(n,h)\right]e^{-i\alpha E_n}, \tag{86}$$

where the symbol $[n/2]$ stands for the integer part of $n/2$ and the function $\Delta(n,h)$ is defined by

$$\Delta(n,h)=\sum_{j_1=1}^{n-(2h-1)} E_{j_1}\left[\sum_{j_2=j_1+2}^{n-(2h-3)} E_{j_2}\cdots\left[\cdots\left[\sum_{j_h=j_{h-1}+2}^{n-1} E_{j_h}\right]\right]\cdots\right]. \tag{87}$$

We note that the case $\lambda=-1$, leading to the unnormalized solution, is not of interest.

The states $|z,\lambda,\alpha\rangle$ can be also given as the action of some operator on the ground state $|\psi_0\rangle$ of H. A more or less complicated manipulation gives the following result:

$$|z,\lambda,\alpha\rangle=U(\lambda,z)|\psi_0\rangle, \tag{88}$$

where

$$U(\lambda,z)=d_0\sum_{n=0}^{\infty}\left(\left(\frac{2z}{\lambda+1}\right)\frac{a^+}{g(N)}+\left(\frac{\lambda-1}{\lambda+1}\right)\frac{1}{g(N)}(a^+)^2\right)^n. \tag{89}$$

Note that the states $|z,\lambda,\alpha\rangle$ are stable temporally. As a first illustration of this construction, we can obtain the generalized intelligent states for the standard harmonic oscillator ($g(N)=N$). We have (up to normalization constant)

$$|z,\lambda,\alpha\rangle=\exp\left[\left(\frac{\lambda-1}{\lambda+1}\right)\frac{(a^+)^2}{2}\right]\exp\left[\left(\frac{2z}{\lambda+1}\right)a^+\right]|0\rangle, \tag{90}$$

where $|0\rangle$ is the ground states for the harmonic oscillator.

The Gazeau–Klauder coherent states correspond to the situation $\lambda=1$. In this case, the coefficients d_n are given by

$$d_n=d_0\frac{z^n}{\sqrt{E(n)}}e^{-i\alpha E_n}, \tag{91}$$

and the coherent states $|z,\lambda=1,\alpha\rangle$ coincide with Gazeau–Klauder ones $|z,\alpha\rangle$ given by Eq. (38). The normalization factor d_0 is given by Eq. (39). The states $|z,\lambda=1,\alpha\rangle\equiv|z,\alpha\rangle$ minimize the Heisenberg uncertainty relation (76) and are eigenvectors of the annihilation operator a^-. We have

$$(\Delta X)^2=(\Delta P)^2=\tfrac{1}{2}\langle G\rangle, \tag{92}$$

where

$$\langle G\rangle=d_0^2\sum_{n=0}^{+\infty}\frac{|z|^{2n}}{E(n)}E_{n+1}-|z|^2 \quad \text{and} \quad \langle F\rangle=0. \tag{93}$$

The latter equation traduces the fact that there is no correlation between X and P. For the harmonic oscillator, it is easy to see that $\langle G\rangle=1$ and 2 $(\Delta X)^2=2(\Delta P)^2=1$.

As we mentioned above, the coherent states minimizing Robertson–Schrödinger uncertainty relation correspond to the case $|\lambda|=1$. The case $\lambda=1$ corresponds to the Gazeau–Klauder coherent states and $\lambda=-1$ is not allowed by our construction. Setting $\lambda=e^{i\theta}$ ($\theta\neq k\pi;k\in\mathbf{N}$), the states $|z,\lambda,\alpha\rangle$ are coherent and dispersions are given by

$$(\Delta X)^2=(\Delta P)^2=\frac{1}{2|\cos\theta|}\langle G\rangle. \tag{94}$$

The main value of the operator F is nonvanishing (vanishes only in the Gazeau–Klauder coherent states, i.e., $\lambda=1$) and it is given by

$$\langle F\rangle=\mathrm{tg}\theta\langle G\rangle. \tag{95}$$

From the latter equation, we conclude that the presence of the correlation ($\langle F\rangle\neq 0$) does not forbid the system to be prepared in coherent states. This result is true for any quantum system. The properties of the states $|z,\lambda,\alpha\rangle$ turned out to be sensitive about the spectral properties of the commutator $[a^-,a^+]=G(N)$.

To close this section, we note that the minimization of the Robertson–Schrödinger uncertainty relation leads to more general expressions of coherent states associated to an arbitrary quantum system. The Gazeau–Klauder coherent states ($\lambda=1$) (eigenvectors of the annihilation operator) constitute a particular case of such coherent state classess ($|\lambda|=1$).

VI. APPLICATION: PÖSCHL–TELLER POTENTIALS

We start by recalling the eigenvalues and eigenstates of infinite square well and Pöschl–Teller potentials[24] (see also Ref. 25 and references therein). We consider the Hamiltonian

$$H=-\frac{d^2}{dx^2}+V_{\kappa,\kappa'}(x) \tag{96}$$

describing a particle on the line, and submitted to the potential

$$V_{\kappa,\kappa'}(x)=\begin{cases}\dfrac{1}{4a^2}\left[\dfrac{\kappa(\kappa-1)}{\sin^2(x/2a)}+\dfrac{\kappa'(\kappa'-1)}{\cos^2(x/2a)}\right]-\dfrac{(\kappa+\kappa')^2}{4a^2}, & 0<x<\pi a\\ \infty \quad x\leqslant 0, \quad x\geqslant \pi a,\end{cases} \tag{97}$$

for $\kappa>1$ and $\kappa'>1$. It is well known that the Pöschl–Teller potentials interpolate between the harmonic oscillator and infinite square well. The infinite square well takes place in the limit $\kappa=\kappa'=1$.

The Hamiltonian H can be written in the factorized form

$$H=A^+_{\kappa,\kappa'}A^-_{\kappa,\kappa'}, \tag{98}$$

where the operators $A^-_{\kappa,\kappa'}$ and $A^+_{\kappa,\kappa'}$ are given by

$$A^{\pm}_{\kappa,\kappa'} = \mp \frac{d}{dx} + W_{\kappa,\kappa'}(x) \tag{99}$$

in terms of the superpotentials $W_{\kappa,\kappa'}(x)$,

$$W_{\kappa,\kappa'}(x) = \frac{1}{2a}\left[\kappa \mathrm{cotg}\left(\frac{x}{2a}\right) - \kappa' \tan\left(\frac{x}{2a}\right)\right]. \tag{100}$$

The eigenvectors are given by

$$\psi_n(x) = [c_n(\kappa,\kappa')]^{-1/2}\left(\cos\frac{x}{2a}\right)^{\kappa'}\left(\sin\frac{x}{2a}\right)^{\kappa} P_n^{(\kappa-1/2,\kappa'-1/2)}\left(\cos\left(\frac{x}{a}\right)\right) \tag{101}$$

with $c_n(\kappa,\kappa')$ the normalization constant which takes the form

$$c_n(\kappa,\kappa') = a\frac{\Gamma(n+\kappa+1/2)\Gamma(n+\kappa'+1/2)}{\Gamma(n+1)\Gamma(n+\kappa+\kappa')\Gamma(2n+\kappa+\kappa')} \tag{102}$$

and $P_n^{(\alpha,\beta)}$'s stands for the Jacobi polynomials.

The eigenvalues of H are given by

$$H|\psi_n\rangle = n(n+\kappa+\kappa')|\psi_n\rangle. \tag{103}$$

To find the annihilation and creation operators for the Pöschl–Teller system, we follow the strategy given in Sec. II. So, we denote H by H_- and $V_{\kappa,\kappa'}(x)$ by $V^-_{\kappa,\kappa'}(x)$. The Hamiltonian $H_+ = A^-_{\kappa,\kappa'}A^+_{\kappa,\kappa'}$ (supersymmetric partner of $H \equiv H_-$),

$$H_+ = -\frac{1}{2}\frac{d^2}{dx^2} + V^+_{\kappa,\kappa'}(x), \tag{104}$$

describes a quantum system trapped in the potentials

$$V_{\kappa,\kappa'}(x) = \begin{cases} \dfrac{1}{8a^2}\left[\dfrac{\kappa(\kappa-1)}{\sin^2(x/2a)} + \dfrac{\kappa'(\kappa'-1)}{\cos^2(x/2a)}\right] - \dfrac{(\kappa+\kappa')^2}{8a^2}, & 0 < x < \pi a, \\ 0, \quad x \leqslant 0, \quad x \geqslant \pi a. \end{cases} \tag{105}$$

The eigenstates of H_+ are given by

$$\theta_n(x) = [c_n(\kappa+1,\kappa'+1)]^{-1/2}\left(\cos\frac{x}{2a}\right)^{\kappa'+1}\left(\sin\frac{x}{2a}\right)^{\kappa+1} P_n^{(\kappa+1/2,\kappa'+1/2)}\left(\cos\left(\frac{x}{a}\right)\right), \tag{106}$$

where the $c_n(\kappa,\kappa')$ are defined by (102).

The eigenvalues are $e_n = (n+1)(n+\kappa+\kappa'+1)$. Using the operators $A^-_{\kappa,\kappa'}$ and $A^+_{\kappa,\kappa'}$ and the unitary transformation U connecting $\psi_n(x)$ and $\theta_n(x)$ (see Sec. II), we define the creation and annihilation operators by

$$a^+_{\kappa,\kappa'} = A^+_{\kappa,\kappa'}U \quad \text{and} \quad a^-_{\kappa,\kappa'} = U^+A^-_{\kappa,\kappa'}. \tag{107}$$

The creation and annihilation operators $a^+_{\kappa,\kappa'}$ and $a^-_{\kappa,\kappa'}$ act on $|\psi_n\rangle$ as follows,

$$\begin{aligned} a^+_{\kappa,\kappa'}|\psi_n\rangle &= \sqrt{(n+1)(n+1+\kappa+\kappa')}e^{-i\alpha(2n+1+\kappa+\kappa')}|\psi_{n+1}\rangle, \\ a^-_{\kappa,\kappa'}|\psi_n\rangle &= \sqrt{n(n+\kappa+\kappa')}e^{i\alpha(2n-1+\kappa+\kappa')}|\psi_{n-1}\rangle, \end{aligned} \tag{108}$$

and satisfy the following commutation relation,

$$[a^{-}_{\kappa,\kappa'}, a^{+}_{\kappa,\kappa'}] = G_{\kappa,\kappa'}(N), \tag{109}$$

where

$$G_{\kappa,\kappa'}(N) \equiv G(N) = 2N + (1 + \kappa + \kappa'). \tag{110}$$

We note that $N \neq a^{+}_{\kappa,\kappa'} a^{-}_{\kappa,\kappa'} = H$.

A. Gazeau–Klauder coherent states

Using the result of Sec. III, the so-called Gazeau–Klauder coherent states (eigenstates of the annihilation operator $a^{-}_{\kappa,\kappa'}$) read as

$$|z,\alpha\rangle = \mathcal{N}(|z|) \sum_{n=0}^{+\infty} \frac{z^n e^{-i\alpha n(n+\kappa+\kappa')}}{\sqrt{\Gamma(n+1)\Gamma(n+\kappa+\kappa'+1)}} |\psi_n\rangle, \tag{111}$$

with $\mathcal{N}(|z|)$ the normalization constant which takes the form

$$[\mathcal{N}(|z|)]^2 = \frac{|z|^{\kappa+\kappa'}}{I_{\kappa+\kappa'}(2|z|)}, \tag{112}$$

where $I_{\kappa+\kappa'}(2|z|)$ is the modified Bessel function of the first kind.

The identity resolution is given explicitly by

$$\int |z,\alpha\rangle\langle z,\alpha| d\mu(z) = I_{\mathcal{H}}, \tag{113}$$

where the measure can be computed by the inverse Mellin transform[26]

$$d\mu(z) = \frac{2}{\pi} I_{\kappa+\kappa'}(2r) K_{(\kappa+\kappa)'/2}(2r) r dr d\phi, \quad z = r^{i\phi}. \tag{114}$$

The Gazeau–Klauder coherent states of the infinite square well are obtained from the Pöschl–Teller ones simply by putting $\kappa + \kappa' = 2$.

The Gazeau–Klauder coherent states form an overcomplete family of states (resolving the unity by integration with respect to the measure given by (114)), and provide a representation of any state $|f\rangle$ by an entire function

$$f(z,\alpha) = \sqrt{\frac{I_{\kappa+\kappa'}(2|z|)}{|z|^{\kappa+\kappa'}}} \langle \overline{z},\alpha | f\rangle = \sum_{n=0}^{+\infty} \langle \psi_n | f\rangle \frac{z^n e^{i\alpha n(n+\kappa+\kappa')}}{\sqrt{\Gamma(n+1)\Gamma(n+\kappa+\kappa'+1)}}. \tag{115}$$

In particular, the analytic functions corresponding to the vectors $|\psi_n\rangle$ are

$$\mathcal{F}_n(z,\alpha) = \frac{z^n e^{i\alpha n(n+\kappa+\kappa')}}{\sqrt{\Gamma(n+1)\Gamma(n+\kappa+\kappa'+1)}}. \tag{116}$$

Using the Fock–Bargmann representation discussed in Sec. III B, the creation and annihilation operators, for a quantum system evolving in Pöschl–Teller (or in the infinite square well) potentials, are realized by

$$a^{+}_{\kappa,\kappa'} = z, \quad a^{-}_{\kappa,\kappa'} = z \frac{d^2}{dz^2} + (\kappa + \kappa' + 1) \frac{d}{dz}, \tag{117}$$

and the operator $G_{\kappa,\kappa'}(N)$, in this representation, acts as

$$G=2z\frac{d}{dz}+(\kappa+\kappa'+1). \tag{118}$$

In fact, one can verify that

$$a^{+}_{\kappa,\kappa'}\mathcal{F}_n(z,\alpha)=\sqrt{(n+1)(n+1+\kappa+\kappa')}e^{-i\alpha(2n+1+\kappa+\kappa')}\mathcal{F}_{n+1}(z,\alpha), \tag{119}$$

$$a^{-}_{\kappa,\kappa'}\mathcal{F}_n(z,\alpha)=\sqrt{n(n+\kappa+\kappa')}e^{i\alpha(2n-1+\kappa+\kappa')}\mathcal{F}_{n-1}(z,\alpha), \tag{120}$$

$$G_{\kappa,\kappa'}(N)\mathcal{F}_n(z,\alpha)=(2n+1+\kappa+\kappa')\mathcal{F}_n(z,\alpha). \tag{121}$$

This realization will be useful, as we will see, to construct the Pöschl–Teller generalized intelligent states which minimize the Robertson–Schrödinger uncertainty relation.

B. Pöschl–Teller coherent states of Perelomov's type

In Sec. IV, we defined coherent states of Perelomov's type for an arbitrary quantum system. The expressions of these states are given by infinite series (more or less complicated). As a first illustration, we discussed the harmonic oscillator system. Here, we construct the Pöschl–Teller coherent states à la Perelomov. In this order, we have to solve the differential equation (66) for the Pöschl–Teller potentials ($E_n=n(n+\kappa+\kappa')$). In this case, the solutions are

$$c_n(r)=\frac{1}{n!r^n}ß^{-(1/2)(\kappa+\kappa'+1)}_{m,n+(1/2)(\kappa+\kappa'+1)}(\cosh(2r)), \tag{122}$$

because the Jacobi functions ß satisfy the following differential equation.[27]

$$\frac{d}{dr}ß^{l}_{m,n-l}(\cosh(2r))=nß^{l}_{m,n-1-l}(\cosh(2r))-(n-2l)ß^{l}_{m,n+1-l}(\cosh(2r)), \tag{123}$$

where $l=-\frac{1}{2}(\kappa+\kappa'+1)$ and m is a free integer parameter which will be fixed after. These functions play an important role in the representation theory of the $QU(2)$ group of unimodular quasi-unitary matrices.

The differential equation (123) admits several solutions. However, an admissible solution is obtained by noting that $D(z=0)=\mathbf{1}$. Using the definition of the Jacobi functions,[27] the unique solution, compatible with the condition $D(z=0)=\mathbf{1}$, is given by

$$c_n(r)=\frac{1}{n!r^n}ß^{-(1/2)(\kappa+\kappa'+1)}_{(1/2)(\kappa+\kappa'+1),n+(1/2)(\kappa+\kappa'+1)}(\cosh(2r)), \tag{124}$$

which can be written also as

$$c_n(r)=\frac{1}{n!}(\cosh(r))^{-(\kappa+\kappa'+1)}\left(\frac{\tanh r}{r}\right)^n. \tag{125}$$

The coherent states of Perelomov's type take the form

$$|z,\alpha\rangle=(1-\tanh^2|z|)^{(1/2)(\kappa+\kappa'+1)}\sum_{n=0}^{+\infty}\left(\frac{z\tanh|z|}{|z|}\right)^n \times\left[\frac{\Gamma(n+\kappa+\kappa'+1)}{\Gamma(n+1)\Gamma(\kappa+\kappa'+1)}\right]^{1/2}e^{-i\alpha n(n+\kappa+\kappa')}|\psi_n\rangle. \tag{126}$$

Finally, setting $\zeta = z\tanh|z|/|z|$, we obtain

$$|\zeta,\alpha\rangle \equiv (1-|\zeta|^2)^{(1/2)(\kappa+\kappa'+1)} \sum_{n=0}^{+\infty} \zeta^n \left[\frac{\Gamma(n+\kappa+\kappa'+1)}{\Gamma(n+1)\Gamma(\kappa+\kappa'+1)}\right]^{1/2} e^{-i\alpha n(n+\kappa+\kappa')}|\psi_n\rangle. \quad (127)$$

We note that the parameter ζ belongs to the unit disk $D=\{\zeta\in\mathbf{C}, |\zeta|<1\}$.

The states are stable temporally. Indeed,

$$e^{-iHt}|\zeta,\alpha\rangle = |\zeta,\alpha+t\rangle. \quad (128)$$

The identity resolution is given by

$$\int |\zeta,\alpha\rangle\langle\zeta,\alpha| d\mu(\zeta) = I_{\mathcal{H}}, \quad (129)$$

where the measure is

$$d\mu(\zeta) = \frac{\kappa+\kappa'}{\pi}\frac{d^2\zeta}{(1-|\zeta|^2)^2}. \quad (130)$$

There are two main consequences arising from the former result. First, we can express any coherent state $|\zeta',\alpha'\rangle$ in terms of the others:

$$|\zeta',\alpha'\rangle = \int |\zeta,\alpha\rangle\langle\zeta,\alpha|\zeta',\alpha'\rangle d\mu(\zeta). \quad (131)$$

The kernel $\langle\zeta,\alpha|\zeta',\alpha'\rangle$ is easy to evaluate from (127):

$$\langle\zeta,\alpha|\zeta',\alpha'\rangle = \sqrt{(1-|\zeta|^2)^{(\kappa+\kappa'+1)}(1-|\zeta'|^2)^{(\kappa+\kappa'+1)}} \times \sum_{n=0}^{+\infty} \overline{\zeta}^n \zeta'^n \frac{\Gamma(n+\kappa+\kappa'+1)}{\Gamma(n+1)\Gamma(\kappa+\kappa'++1)} e^{-i(\alpha'-\alpha)n(n+\kappa+\kappa')}. \quad (132)$$

The coherent states are normalized ($\langle\zeta,\alpha|\zeta,\alpha\rangle=1$), but they are not orthogonal to each other.

Second, an arbitrary element state of the Hilbert space $\mathcal{H}$, let us call it $|f\rangle$, can be written in terms of the coherent states,

$$|f\rangle = \int (1-|\zeta|^2)^{(1/2)(\kappa+\kappa'+1)} f(\overline{\zeta},\alpha)|\zeta,\alpha\rangle d\mu(\zeta), \quad (133)$$

where the analytic function

$$f(\overline{\zeta},\alpha) = (1-|\zeta|^2)^{-(1/2)(\kappa+\kappa'+1)}\langle\overline{\zeta},\alpha|f\rangle \sum_{n=0}^{+\infty} \zeta^n \left[\frac{\Gamma(n+\kappa+\kappa'+1)}{\Gamma(n+1)\Gamma(\kappa+\kappa'+1)}\right]^{1/2} e^{i\alpha n(n+\kappa+\kappa')}\langle\psi_n|f\rangle \quad (134)$$

determines in a complete way the state $|f\rangle\in\mathcal{H}$. The state $|\psi_n\rangle$ is represented by the function

$$\mathcal{F}'_n(\zeta,\alpha) = \zeta^n \left[\frac{\Gamma(n+\kappa+\kappa'+1)}{\Gamma(n+1)\Gamma(\kappa+\kappa'+1)}\right]^{1/2} e^{i\alpha n(n+\kappa+\kappa')}. \quad (135)$$

The creation $a^+_{\kappa,\kappa'}$, annihilation $a^-_{\kappa,\kappa'}$, and $G_{\kappa,\kappa'}(N)$ operators act in the Hilbert space of analytic functions $f(\zeta,\alpha)$ as first-order differential operators:

$$a^{+}_{\kappa,\kappa'}=\zeta^2\frac{d}{d\zeta}+(\kappa+\kappa'+1)\zeta,\quad a^{-}_{\kappa,\kappa'}=\frac{d}{d\zeta},$$
$$G_{\kappa,\kappa'}(N)\equiv G=2\zeta\frac{d}{d\zeta}+(\kappa+\kappa'+1). \tag{136}$$

One can verify that

$$a^{+}_{\kappa,\kappa'}\mathcal{F}'_n(\zeta,\alpha)=\sqrt{(n+1)(n+1+\kappa+\kappa')}e^{-i\alpha(2n+1+\kappa+\kappa')}\mathcal{F}'_{n+1}(\zeta,\alpha), \tag{137}$$

$$a^{-}_{\kappa,\kappa'}\mathcal{F}'_n(\zeta,\alpha)=\sqrt{n(n+\kappa+\kappa')}e^{i\alpha(2n-1+\kappa+\kappa')}\mathcal{F}'_{n-1}(\zeta,\alpha), \tag{138}$$

$$G_{\kappa,\kappa'}(N)\mathcal{F}'_n(\zeta,\alpha)=(2n+1+\kappa+\kappa')\mathcal{F}'_n(\zeta,\alpha). \tag{139}$$

The analytic representation of the Gazeau–Klauder coherent states and the analytical realization of the Perelomov ones in the unit disk are related through a Laplace transform. Indeed, one can verify easily that

$$\mathcal{F}'_n(\zeta,\alpha)=\frac{\zeta^{-(\kappa+\kappa'+1)}}{\sqrt{\Gamma(\kappa+\kappa'+1)}}\int_0^{+\infty}z^{\kappa+\kappa'}\mathcal{F}_n(z,\alpha)e^{-z/\zeta}dz, \tag{140}$$

which means that the function $\mathcal{F}'_n(1/\zeta,\alpha)$ is the Laplace transform of $z^{\kappa+\kappa'}\mathcal{F}_n(z,\alpha)$. A similar result was obtained in Ref. 28 showing that the representation in the unit disk and Barut–Girardello one, based on the su(1,1) coherent states, are related through a Laplace transform.

C. Pöschl–Teller generalized intelligent states

The generalized intelligent states can be determined by using two analytic representation, one based on the so-called Gazeau–Klauder coherent states (Sec. III) and the other one on the Perelomov's coherent states (Sec. IV).

1. The Gazeau–Klauder analytic representation

We introduce the analytic function

$$\Phi_{(z',\lambda,\alpha)}(z)=\sqrt{\frac{I_{\kappa+\kappa'}(2|z|)}{|z|^{\kappa+\kappa'}}}\langle\overline{z},\alpha|z',\lambda,\alpha\rangle \tag{141}$$

by means of which one converts the eigenvalues equation

$$[(1+\lambda)a^{-}_{\kappa,\kappa'}+(1-\lambda)a^{+}_{\kappa,\kappa'}]|z',\lambda,\alpha\rangle=2z'|z',\lambda,\alpha\rangle \tag{142}$$

into the second-order linear homogeneous differential equation

$$\left[(1+\lambda)\left(z\frac{d^2}{dz^2}+(\kappa+\kappa'+1)\frac{d}{dz}\right)+(1-\lambda)z-2z'\right]\Phi_{(z',\lambda)}(z)=0. \tag{143}$$

We first consider the general case $\lambda\neq\pm1$. Setting

$$\Phi_{(z',\lambda)}(z)=\exp\left(\pm\sqrt{\frac{\lambda-1}{\lambda+1}}z\right)F_{(z',\lambda)}(z), \tag{144}$$

the equation can be transformed in the Kummer equation

$$\left[Z\frac{d^2}{dZ^2}+(\kappa+\kappa'+1-Z)\frac{d}{dZ}-\left(\frac{\kappa+\kappa'+1}{2}\mp\frac{z'}{\sqrt{\lambda^2-1}}\right)\right]F_{(z',\lambda)}(z)=0, \tag{145}$$

where $Z=\mp 2\sqrt{(\lambda-1)/(\lambda+1)}z$.

Then the solutions of Eq. (143) are given by

$$\Phi_{(z',\lambda)}(z)=\exp\left(\pm\sqrt{\frac{\lambda-1}{\lambda+1}}z\right)\,{}_1F_1\left(\frac{\kappa+\kappa'+1}{2}\mp\frac{z'}{\sqrt{\lambda^2-1}},\kappa+\kappa'+1;\mp 2\sqrt{\frac{\lambda-1}{\lambda+1}}z\right) \tag{146}$$

or

$$\Phi_{(z',\lambda)}(z)=\exp\left(\pm\sqrt{\frac{\lambda-1}{\lambda+1}}z\right)z^{-(\kappa+\kappa')}{}_1F_1\left(\frac{1-(\kappa+\kappa')}{2}\mp\frac{z'}{\sqrt{\lambda^2-1}},1-(\kappa+\kappa');\mp 2\sqrt{\frac{\lambda-1}{\lambda+1}}z\right). \tag{147}$$

The first solution (146) is always analytic, but the solution (147) is not. (Remember that $\kappa>1$ and $\kappa'>1$.) The upper and lower signs in Eq. (146) are equivalent, because the confluent hypergeometric function ${}_1F_1(\alpha,\gamma;z)$ can be written in two equivalents forms which are related by Kummer's transformation:

$${}_1F_1(\alpha,\gamma;z)=e^z{}_1F_1(\gamma-\alpha,\gamma,-z). \tag{148}$$

Using the properties of this hypergeometric functions, we conclude that the squeezing parameter λ obeys the condition

$$\sqrt{\left|\frac{\lambda-1}{\lambda+1}\right|}<1\Leftrightarrow \mathrm{Re}(\lambda)>0, \tag{149}$$

which is exactly the restriction on λ imposed by the positivity of the commutator $[a^-_{\kappa,\kappa'},a^+_{\kappa,\kappa'}]=G_{\kappa,\kappa'}(N)$ [see Eqs. (109) and (110)].

We consider now the degenerate cases $\lambda=-1$ and $\lambda=1$. For the $\lambda=-1$ Eq. (143) does not have any normalized analytic solution (the operator $a^+_{\kappa,\kappa'}$ does not have any eigenstate). For $\lambda=1$, using the power series of ${}_1F_1(a,b;z)$, we get

$$\Phi_{(z',\lambda=1)}(z)={}_0F_1(\kappa+\kappa'+1;zz'). \tag{150}$$

The result (150) coincides with the solution (111) (up to normalization constant) for $\lambda=1$, and we recover the Pöschl–Teller coherent states defined as the $a^-_{\kappa,\kappa'}$ eigenstates.

2. The Perelomov coherent state basis and analytic representation in the unit disk

To solve the eigenvalues equation (142), using the analytic representation of Perelomov coherent states in the unit disk, we introduce the analytic function

$$\Phi_{(\zeta',\lambda)}(\zeta)=(1-|\zeta|^2)^{-(1/2)(\kappa+\kappa'+1)}\langle\overline{\zeta},\alpha|\zeta',\lambda,\alpha\rangle. \tag{151}$$

Equation (142) is then converted to the following differential equation:

$$\left[[(1-\lambda)\zeta^2+(1+\lambda)]\frac{d}{d\zeta}+(1-\lambda)(\kappa'+\kappa+1)\zeta-2\zeta'\right]\Phi_{(\zeta',\lambda)}(\zeta)=0. \tag{152}$$

Admissible values of λ and ζ' are determined by the requirements that the functions $\Phi_{(\zeta',\lambda)}(\zeta)$ must be analytic in the unit disk. We consider the general case. The solution of Eq. (152) is

$$\Phi_{(\zeta',\lambda)}(\zeta)=\mathcal{N}^{-1/2}\prod_{l=\pm 1}\left(1+l\left(\frac{\lambda-1}{\lambda+1}\right)^{1/2}\zeta\right)^{-(1/2)(\kappa+\kappa'+1)+l\,\zeta'/\sqrt{\lambda^2-1}}, \tag{153}$$

where $\mathcal{N}$ is a normalization constant. The condition of analyticity requires

$$\left|\frac{\lambda-1}{\lambda+1}\right|<1\Leftrightarrow \mathrm{Re}\,\lambda>0. \tag{154}$$

If $\mathrm{Re}\,\lambda<0$, the function $\Phi_{(\zeta',\lambda)}(\zeta)$ cannot be analytic in the unit disk.

The decomposition of the generalized intelligent states $|\zeta',\lambda,\alpha\rangle$ over the Hilbert orthonormal basis $\{|\psi_n\rangle\}$ can be obtained by expanding the function $\Phi_{(\zeta',\alpha)}(\zeta)$ into a power series in ζ. This can be done using the following relations:

$$\left(1+\left(\frac{\lambda-1}{\lambda+1}\right)^{1/2}\zeta\right)^{\alpha_+}\left(1-\left(\frac{\lambda-1}{\lambda+1}\right)^{1/2}\zeta\right)^{\alpha_-}=\sum_{n=0}^{+\infty}\zeta^n\left(2\sqrt{\frac{\lambda-1}{\lambda+1}}\right)^n P_n^{(\alpha_+-n,\alpha_--n)}(0), \tag{155}$$

where

$$\alpha_\pm=-\frac{1}{2}(\kappa+\kappa'+1)\pm\frac{\zeta'}{\sqrt{\lambda^2-1}}. \tag{156}$$

Then, the function $\Phi_{(\zeta',\alpha)}(\zeta)$ can be expanded in terms of the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$. Using the relation between the hypergeometric function and Jacobi polynomials,[27] one can show

$$|\zeta',\lambda,\alpha\rangle=\mathcal{N}^{-1/2}\sum_{n=0}^{+\infty}\left[\frac{\Gamma(\kappa+\kappa'+1)}{n!\Gamma(\kappa+\kappa'+1+n)}\right]^{1/2}\left[\frac{\Gamma(\alpha_++1)}{\Gamma(\alpha_+-n+1)}\right]\left(2\sqrt{\frac{\lambda-1}{\lambda+1}}\right)^n$$
$$\times{}_2F_1(-n,-n-(\kappa+\kappa'),\alpha_+-n+1;\tfrac{1}{2})e^{-i\alpha E_n}|\psi_n\rangle \tag{157}$$

or

$$|\zeta',\lambda,\alpha\rangle=\mathcal{N}^{-1/2}\sum_{n=0}^{+\infty}\left[\frac{n!\Gamma(\kappa+\kappa'+1)}{\Gamma(\kappa+\kappa'+1+n)}\right]^{1/2}\left(2\sqrt{\frac{\lambda-1}{\lambda+1}}\right)^n P_n^{(\alpha_+-n,\alpha_--n)}(0)e^{-i\alpha E_n}|\psi_n\rangle. \tag{158}$$

The generalized intelligent states $\Phi_{(\zeta',\lambda)}(\zeta)$ and $\Phi_{(z',\lambda)}(z)$ are related through a Laplace transform. In fact, Eq. (152) can be written as

$$\left[[(1+\lambda)\zeta^2+(1-\lambda)]\frac{d}{d\zeta}-\frac{(1-\lambda)(\kappa'+\kappa+1)}{\zeta}+2\zeta'\right]\Phi_{(\zeta',\lambda)}\left(\frac{1}{\zeta}\right)=0. \tag{159}$$

Using

$$\Phi_{(\zeta',\lambda)}\left(\frac{1}{\zeta}\right)=\frac{\zeta^{-(\kappa+\kappa'+1)}}{\sqrt{\Gamma(\kappa+\kappa'+1)}}\int_0^{+\infty}z^{\kappa+\kappa'}\Phi_{(\zeta',\lambda)}(z)e^{-z/\zeta}dz. \tag{160}$$

It is easy to see that the eigenvalue equation (159) becomes

$$\left[(1+\lambda)\left(z\frac{d^2}{dz^2}+(\kappa+\kappa'+1)\frac{d}{dz}\right)+(1-\lambda)z-2\zeta'\right]\Phi_{(\zeta',\lambda)}(z)=0, \tag{161}$$

which coincides with those in (143) ($\zeta'=z'$) that gives the generalized intelligent states (146).

VII. SUMMARY

In this work, we have explicitly constructed the Gazeau–Klauder and Perelomov coherent states for an arbitrary quantum system. As an application of this construction, we considered the system trapped in the Pöschl–Teller potential type. We showed that the analytical representations of Gazeau–Klauder and Perelomov coherent states (which are related through a Laplace transform) enable us to compute the generalized intelligent states for the Pöschl–Teller potentials. Finally, it should be interesting to investigate further applications of the results obtained on this work. Indeed, it is interesting, in our opinion, to construct the coherent states and generalized intelligent states for the shape invariant potentials.[29] This matter will be considered in a forthcoming work.

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Semiclassical properties and chaos degree for the quantum Baker's map

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We study the chaotic behavior and the quantum-classical correspondence for the Baker's map. Correspondence between quantum and classical expectation values is investigated and it is numerically shown that it is lost at the logarithmic timescale. The quantum chaos degree is computed and it is demonstrated that it describes the chaotic features of the model. The correspondence between classical and quantum chaos degrees is considered. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The study of chaotic behavior in classical dynamical systems dates back to Lobachevsky and Hadamard, who have studied the exponential instability property of geodesics on manifolds of negative curvature, and to Poincare, who initiated the inquiry into the stability of the solar system. One believes now that the main features of chaotic behavior in the classical dynamical systems are rather well understood (see, for example, Refs. 1 and 2). However, the status of ''quantum chaos'' is much less clear although significant progress has been made on this front.

Sometimes one says that an approach to quantum chaos, which attempts to generalize the classical notion of sensitivity to initial conditions, fails for two reasons: first, there is no quantum analog of the classical phase space trajectories and, second, the unitarity of linear Schrödinger equations precludes sensitivity to initial conditions in the quantum dynamics of state vector. Let us remind, however, that in fact there exists a quantum analog of the classical phase space trajectories. It is quantum evolution of expectation values of appropriate observables in suitable states. Also, let us remind that the dynamics of a classical system can be described either by the Hamilton equations or by the linear Liouville equations. In quantum theory the linear Schrödinger equation is the counterpart of the Liouville equation while the quantum counterpart of the classical Hamilton equation is the Heisenberg equation. Therefore, the study of quantum expectation values should reveal the chaotic behavior of quantum systems. In this article we demonstrate this fact for the quantum Baker's map.

If one has the classical Hamilton equations

$$dq/dt=p, \quad dp/dt=-V'(q),$$

then the corresponding quantum Heisenberg equations have the same form

$$dq_h/dt=p_h, \quad dp_h/dt=-V'(q_h),$$

where q_h and p_h are quantum canonical operators of position and momentum. For the expectation values one gets the Ehrenfest equations

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$$d\langle q_h\rangle/dt=\langle p_h\rangle, \quad d\langle p_h\rangle/dt=-\langle V'(q_h)\rangle.$$

Note that the Ehrenfest equations are classical equations but for nonlinear $V'(q_h)$ they are neither Hamilton equations nor even differential equations because one can not write $\langle V'(q_h)\rangle$ as a function of $\langle q_h\rangle$ and $\langle p_h\rangle$. However, these equations are very convenient for the consideration of the semiclassical properties of quantum system. The expectation values $\langle q_h\rangle$ and $\langle p_h\rangle$ are functions of time and initial data. They also depend on the quantum states. One of important problems is to study the dependence of expectation values from the initial data. In this article we will study this problem for the quantum Baker's map.

The main objective of ''quantum chaos'' is to study the correspondence between classical chaotic systems and their quantum counterparts in the semiclassical limit.[3,4] The quantum-classical correspondence for dynamical systems has been studied for many years (see for example Refs. 5–10 and reference therein). A significant progress in understanding this correspondence has been achieved in the Wentzel–Kromers–Brillouin (WKB) approach when one considers the Planck constant h as a small variable parameter. Then it is well known that in the limit $h\to 0$ quantum theory is reduced to the classical one.[11] However, in physics the Planck constant is a fixed constant although it is very small. Therefore, it is important to study the relation between classical and quantum evolutions when the Planck constant is fixed. There is a conjecture[12–14,8] that a characteristic timescale τ appears in the quantal evolution of chaotic dynamical systems. For time less than τ there is a correspondence between quantum and classical expectation values, while for times greater that τ the predictions of the classical and quantum dynamics no longer coincide. The important problem is to estimate the dependence τ on the Planck constant h. Probably a universal formula expressing τ in terms of h does not exist and every model should be studied case by case. It is expected that certain quantum and classical expectation values diverge on a timescale inversely proportional to some power of h.[15] Other authors suggest that a breakdown may be anticipated on a much smaller logarithmic timescale.[16–23] The characteristic time τ associated with the hyperbolic fixed points of the classical motion is expected to be of the logarithmic form $\tau=(1/\lambda)\ln(C/h)$, where λ is the Lyapunov exponent and C is a constant which can be taken to be the classical action. Such a logarithmic timescale has been found in the numerical simulations of some dynamical models.[7] It was shown also that the discrepancy between quantum and classical evolutions is decreased by even a small coupling with the environment, which in the quantum case leads to decoherence.[7]

The chaotic behavior of the classical dynamical systems is often investigated by computing the Lyapunov exponents. An alternative quantity measuring chaos in dynamical systems, which is called the chaos degree, has been suggested in Ref. 24 in the general framework of information dynamics.[25] The chaos degree was applied to various models in Ref. 26. An advantage of the chaos degree is that it can be applied not only to classical systems but also to quantum systems as well.

In this work we study the chaotic behavior and the quantum-classical correspondence for the Baker's map.[15,27] The quantum Baker's map is a simple model invented for the theoretical study of quantum chaos. Its mathematical properties have been studied in numerical works. In particular its semiclassical properties have been considered,[16–23] quantum computing and optical realizations have been proposed,[28–30] various quantization procedures have been discussed,[18,31–33] and a symbolic dynamics representation has been given.[33]

It is well known that for the consideration of the semiclassical limit in quantum mechanics it is very useful to use coherent states. We define an analog of the coherent states for the quantum Baker's map. We study the quantum Baker's map by using the correlation functions of the special form which corresponds to the expectation values, translated in time by the unitary evolution operator and taken in the coherent states.

To explain our formalism we first discuss the classical limit for correlation functions in ordinary quantum mechanics. Correspondence between quantum and classical expectation values for the Baker's map is investigated and it is numerically shown that it is lost at the logarithmic timescale. The chaos degree for the quantum Baker's map is computed and it is demonstrated that

it describes the chaotic features of the model. The dependence of the chaos degree on the Planck constant is studied and the correspondence between classical and quantum chaos degrees is established.

II. QUANTUM VERSUS CLASSICAL DYNAMICS

In this section we discuss an approach to the semiclassical limit in quantum mechanics by using the coherent states (see Ref. 6). Then in the next section an extension of this approach to the quantum Baker's map will be given. Consider the canonical system with the Hamilton function

$$H=\frac{p^2}{2}+V(x) \tag{1}$$

in the plane $(p,x)\in\mathbf{R}^2$. We assume that the canonical equations

$$\dot{x}(t)=p(t), \quad \dot{p}(t)=-V'(x(t)) \tag{2}$$

have a unique solution $(x(t),p(t))$ for times $|t|<T$ with the initial data

$$x(0)=x_0, \quad p(0)=v_0. \tag{3}$$

This is equivalent to the solution of the Newton equation

$$\ddot{x}(t)=-V'(x(t)), \tag{4}$$

with the initial data

$$x(0)=x_0, \quad \dot{x}(0)=v_0. \tag{5}$$

We denote

$$\alpha=\frac{1}{\sqrt{2}}(x_0+iv_0). \tag{6}$$

The quantum Hamilton operator has the form

$$H_h=\frac{p_h^2}{2}+V(q_h),$$

where p_h and q_h satisfy the commutation relations

$$[p_h,q_h]=-ih.$$

The Heisenberg evolution of the canonical variables is defined as

$$p_h(t)=U(t)p_hU(t)^*, \quad q_h(t)=U(t)q_hU(t)^*,$$

where

$$U(t)=\exp(-itH_h/h).$$

For the consideration of the classical limit we take the following representation,

$$p_h=-ih^{1/2}\partial/\partial x, \quad q_h=h^{1/2}x,$$

acting to functions of the variable $x\in\mathbf{R}$. We also set

$$a=\frac{1}{\sqrt{2}h^{1/2}}(q_h+ip_h)=\frac{1}{\sqrt{2}}\left(x+\frac{\partial}{\partial x}\right),\quad a^*=\frac{1}{\sqrt{2}h^{1/2}}(q_h-ip_h)=\frac{1}{\sqrt{2}}\left(x-\frac{\partial}{\partial x}\right).$$

Then,

$$[a,a^*]=1.$$

The coherent state $|\alpha\rangle$ is defined as

$$|\alpha\rangle=W(\alpha)|0\rangle, \tag{7}$$

where α is a complex number, $W(\alpha)=\exp(\alpha a^*-a\alpha^*)$ and $|0\rangle$ is the vacuum vector, $a|0\rangle=0$. The vacuum vector is the solution of the equation

$$(q_h+ip_h)|0\rangle=0. \tag{8}$$

In the x-representation one has

$$|0\rangle=\exp(-x^2/2)/\sqrt{2\pi}. \tag{9}$$

The operator $W(\alpha)$ one can write also in the form

$$W(\alpha)=Ce^{iq_hv_0/h^{1/2}}e^{-ip_hx_0/h^{1/2}}, \tag{10}$$

where $C=\exp(-v_0x_0/2h)$.

The mean value of the position operator with respect to the coherent vectors is the real valued function

$$q(t,\alpha,h)=\langle h^{-1/2}\alpha|q_h(t)|h^{-1/2}\alpha\rangle. \tag{11}$$

Now one can present the following basic formula describing the semiclassical limit

$$\lim_{h\to 0}q(t,\alpha,h)=x(t,\alpha). \tag{12}$$

Here $x(t,\alpha)$ is the solution of (4) with the initial data (5) and α is given by (6).

Let us notice that for time $t=0$ the quantum expectation value $q(t,\alpha,h)$ is equal to the classical one:

$$q(0,\alpha,h)=x(0,\alpha)=x_0 \tag{13}$$

for any h. We are going to compare the time dependence of two real functions $q(t,\alpha,h)$ and $x(t,\alpha)$; these functions are approximately equal. The important problem is to estimate for which t the large difference between them will appear. It is expected that certain quantum and classical expectation values diverge on a timescale inversely proportional to some power of h.[15] Other authors suggest that a breakdown may be anticipated on a much smaller logarithmic timescale.[16–23] One of very interesting examples[5] of classical systems with chaotic behavior is described by the Hamilton function

$$H=\frac{p_1^2}{2}+\frac{p_2^2}{2}+\lambda x_1^2x_2^2.$$

The consideration of this classical and quantum model within the described framework will be presented in another publication.

III. COHERENT STATES FOR THE QUANTUM BAKER'S MAP

The classical Baker's transformation maps the unit square $0 \leqslant q,\ p \leqslant 1$ onto itself according to

$$(q,p) \to \begin{cases} (2q, p/2), & \text{if} \quad 0 \leqslant q \leqslant \frac{1}{2}, \\ (2q-1, (p+1)/2), & \text{if} \quad \frac{1}{2} < q \leqslant 1. \end{cases}$$

This corresponds to compressing the unit square in the p direction and stretching it in the q direction, while preserving the area, then cutting it vertically and stacking the right part on top of the left part.

The classical Baker's map has a simple description in terms of its symbolic dynamics.[34] Each point (q,p) is represented by a symbolic string

$$\xi = \cdots \xi_{-2} \xi_{-1} \xi_0 . \xi_1 \xi_2 \cdots, \tag{14}$$

where $\xi_k \in \{0,1\}$, and

$$q = \sum_{k=1}^{\infty} \xi_k 2^{-k}, \quad p = \sum_{k=0}^{\infty} \xi_{-k} 2^{-k-1}.$$

The action of the Baker's map on a symbolic string ξ is given by the shift map (Bernoulli shift) U defined by $U\xi = \xi'$, where $\xi'_k = \xi_{k+1}$. This means that, at each time step, the dot is shifted one place to the right while the entire string remains fixed. After n steps the q coordinate becomes

$$q_n = \sum_{k=1}^{\infty} \xi_{n+k} 2^{-k}. \tag{15}$$

This relation defines the classical trajectory with the initial data

$$q = q_0 = \sum_{k=1}^{\infty} \xi_k 2^{-k}. \tag{16}$$

Quantum Baker's maps are defined on the D-dimensional Hilbert space of the quantized unit square. To quantize the unit square one defines the Weyl unitary displacement operators $\hat{U}$ and $\hat{V}$ in D—dimensional Hilbert space, which produces displacements in the momentum and position directions, respectively, and the following commutation relation is obeyed,

$$\hat{U}\hat{V} = \epsilon \hat{V}\hat{U},$$

where $\epsilon = \exp(2\pi i/D)$. We choose $D = 2^N$, so that our Hilbert space will be the N qubit space $\mathbb{C}^{\otimes N}$. The constant $h = 1/D = 2^{-N}$ can be regarded as the Plank constant. The space $\mathbb{C}^2$ has a basis

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The basis in $\mathbb{C}^{\otimes N}$ is

$$|\xi_1\rangle \otimes |\xi_2\rangle \otimes \cdots \otimes |\xi_N\rangle, \quad \xi_k = 0,1.$$

We write

$$\xi = \sum_{k=1}^{N} \xi_k 2^{N-k}.$$

Then $\xi=0,1,\ldots,2^N-1$ and we denote

$$|\xi\rangle=|\xi_1\xi_2\cdots\xi_N\rangle=|\xi_1\rangle\otimes|\xi_2\rangle\otimes\cdots\otimes|\xi_N\rangle.$$

We will also use for this basis notations $\{|\eta\rangle=|\eta_1\eta_2\cdots\eta_N\rangle,\quad \eta_k=0,1\}$ and $\{|j\rangle=|j_1j_2\cdots j_N\rangle, j_k=0,1\}$.

The operators $\hat{U}$ and $\hat{V}$ can be written as

$$\hat{U}=e^{2\pi i\hat{q}},\quad \hat{V}=e^{2\pi i\hat{p}},$$

where the position and momentum operators $\hat{q}$ and $\hat{p}$ are operators in $\mathbb{C}^{\otimes N}$ which are defined as follows. The position operator is

$$\hat{q}=\sum_{j=0}^{2^N-1} q_j|j\rangle\langle j|=\sum_{j_1,\ldots,j_N} q_j|j_N\ldots j_1\rangle\langle j_1\ldots j_N|,$$

where

$$|j\rangle=|j_1j_2\cdots j_N\rangle,\quad j_k=0,1,$$

is the basis in $\mathbb{C}^{\otimes N}$,

$$j=\sum_{k=1}^{N} j_k2^{N-k},$$

and

$$q_j=\frac{j+\frac{1}{2}}{2^N},\quad j=0,1,\ldots,2^N-1.$$

The momentum operator is defined as

$$\hat{p}=F_N\hat{q}F_N^*,$$

where F_N is the quantum Fourier transform acting to the basis vectors as

$$F_N|j\rangle=\frac{1}{\sqrt{D}}\sum_{\xi=0}^{D-1} e^{2\pi i\xi j/D}|\xi\rangle,$$

where $D=2^N$.

The symbolic representation of quantum Baker's map T was introduced by Schack and Caves[33] and studied in Refs. 35 and 36. Let us explain the symbolic representation of the quantum Baker's map as a special case:[33] By applying a partial quantum Fourier transform

$$G_m=\overbrace{I\otimes\cdots\otimes I}^{m}\otimes F_{N-m}$$

to the position eigenstates, one obtains the following quantum Baker's map T:

$$T|.\xi_1\cdots\xi_N\rangle\equiv|\xi_1.\xi_2\cdots\xi_N\rangle,$$

where

$$T=G_{N-1}\circ G_N^{-1}$$

and

$$|\xi_1\cdots\xi_{N-m}.\xi_{N-m+1}\cdots\xi_N\rangle \equiv G_m|\xi_{N-m+1}\cdots\xi_N\xi_{N-m}\cdots\xi_1\rangle$$
$$= |\xi_{N-m+1}\rangle\otimes\cdots\otimes|\xi_N\rangle\otimes F_{N-m}|\xi_{N-m}\rangle\otimes\cdots\otimes|\xi_1\rangle.$$

The quantum Baker's map T is the unitary operator in $\mathbb{C}^{\otimes N}$ with the following matrix elements,

$$\langle\xi|T|\eta\rangle = \frac{1-i}{2}\exp\left(\frac{\pi}{2}i|\xi_1-\eta_N|\right)\prod_{k=2}^{N}\delta(\xi_k-\eta_{k-1}), \tag{17}$$

where $|\xi\rangle=|\xi_1\xi_2\cdots\xi_N\rangle$, $|\eta\rangle=|\eta_1\eta_2\cdots\eta_N\rangle$ and $\delta(x)$ is the Kronecker symbol, $\delta(0)=1$; $\delta(x)=0$, $x\neq 0$.

We define the coherent states by

$$|\alpha\rangle = Ce^{2\pi i\hat{q}v}e^{-2\pi i\hat{p}x}|\psi_0\rangle. \tag{18}$$

Here $\alpha=x+iv$, x and v are integers, C is the normalization constant and $|\psi_0\rangle$ is the vacuum vector. This definition should be compared with (10). The vacuum vector can be defined as the solution of the equation

$$(q_h+ip_h)|\psi_0\rangle=0$$

[compare with (8)]. We will use the simpler definition which in the position representation is

$$\langle q_j|\psi_0\rangle = C\exp(-q_j^2/2)$$

[compare with (9)]. Here C is a normalization constant.

IV. CHAOS DEGREE

Let us review the entropic chaos degree defined in Ref. 24. This entropic chaos degree is given by a probability distribution φ and a dynamics (channel) Λ^* sending a state to a state; $\varphi=\Sigma_k p_k\delta_k$, where δ_k is the delta measure such as

$$\delta_k(j)\equiv\begin{cases}1 & (k=j),\\ 0 & (k\neq j).\end{cases}$$

Then the entropic chaos degree is defined as

$$D(\varphi;\Lambda^*)=\sum_k p_k S(\Lambda^*\delta_k) \tag{19}$$

with the von Neumann entropy S, equivalent to the Shannon entropy because the probability distribution φ is a classical object.

A dynamics $\mathcal{F}$ of the orbit produces the above channel Λ^*, so let $\{x_n\}$ be the orbit and $\mathcal{F}$ be a map from x_n to x_{n+1}.

Take a finite partition $\{B_k\}$ of $I=[a,b]^l$ $(a,b\in\mathbf{R})\subset\mathbf{R}^l$ such as

$$I=\bigcup_k B_k \quad (B_i\bigcap B_j=\varnothing, i\neq j)$$

for a map $\mathcal{F}$ on I with $x_{n+1}=\mathcal{F}(x_n)$ (a difference equation). The state $\varphi^{(n)}$ of the orbit determined by the difference equation is defined by the probability distribution $(p_i^{(n)})$, that is, $\varphi^{(n)}=p^{(n)}=\Sigma_i p_i^{(n)}\delta_i$, where for an initial value $x\in I$ and the characteristic function 1_A

$$p_i^{(n)} \equiv \frac{1}{m+1} \sum_{k=n}^{m+n} 1_{B_i}(\mathcal{F}^k x).$$

When the initial value x is distributed due to a measure ν on I, the above $p_i^{(n)}$ is given as

$$p_i^{(n)} \equiv \frac{1}{m+1} \int_I \sum_{k=n}^{m+n} 1_{B_i}(\mathcal{F}^k x) d\nu.$$

In the case that $\mathcal{F}$ is a classical Baker's transformation, if the orbit is not stable and periodic, then it is shown that the $m \to \infty$ limit of $p_i^{(n)}$ exists and equals a natural invariant measure for a fixed $n \in \mathbf{N}$.[37]

The joint distribution $(p_{ij}^{(n,n+1)})$ between the time n and $n+1$ is defined by

$$p_{ij}^{(n,n+1)} \equiv \frac{1}{m+1} \sum_{k=n}^{m+n} 1_{B_i}(\mathcal{F}^k x) 1_{B_j}(\mathcal{F}^{k+1} x)$$

or

$$p_{ij}^{(n,n+1)} \equiv \frac{1}{m+1} \int_I \sum_{k=n}^{m+n} 1_{B_i}(\mathcal{F}^k x) 1_{B_j}(\mathcal{F}^{k+1} x) d\nu.$$

Then the channel Λ_n^* at n is determined by

$$\Lambda_n^* \equiv \left(\frac{p_{ij}^{(n,n+1)}}{p_i^{(n)}} \right) \Rightarrow p^{(n+1)} = \Lambda_n^* p^{(n)},$$

and the chaos degree is given by

$$D_c(p^{(n)}; \Lambda_n^*) = sup_{\{B_k\}} \left\{ \sum_i p_i^{(n)} S(\Lambda_n^* \delta_i) = \sum_{i,j} p_{ij}^{(n,n+1)} \log \frac{p_i^{(n)}}{p_{ij}^{(n,n+1)}}; \{B_k\} \right\}. \tag{20}$$

We can judge whether the dynamics causes a chaos or not by the value of D as

$$D > 0 \Leftrightarrow \text{chaotic}, \quad D = 0 \Leftrightarrow \text{stable}.$$

Therefore, it is enough to find a partition $\{B_k\}$ such that D is positive when the dynamics produces chaos.

This classical chaos degree was applied to several dynamical maps, such as a logistic map, a Baker's transformation and a Tinkerbel map, and it could explain their chaotic characters.[24,26] Our chaos degree has several merits compared with usual measures such as the Lyapunov exponent.

V. EXPECTATION VALUES AND CHAOS DEGREE

In this section, we show a general representation of the mean value of the position operator $\hat{q}$ for the time evolution, which is constructed by the quantum Baker's map. Then we give the algorithm to compute the chaos degree for the quantum Baker's map.

To study the time evolution and the classical limit $h \to 0$ which corresponds to $N \to \infty$ of the quantum Baker's map T, we introduce the following the mean value of the position operator $\hat{q}$ for time $n \in \mathbf{N}$ with respect to a single basis $|\xi\rangle$:

$$r_n^{(N)} = \langle \xi | T^n \hat{q} T^{-n} | \xi \rangle, \tag{21}$$

where $|\xi\rangle = |\xi_1 \xi_2 \cdots \xi_N\rangle$.

From (17), the following formula of the matrix elements of T^n for any $n \in \mathbf{N}$ is easily obtained:

$$\langle \xi | T^n | \zeta \rangle = \begin{cases} \left(\frac{1-i}{2}\right)^n \left(\prod_{k=1}^{N-n} \delta(\xi_{n+k} - \zeta_k)\right) \left(\prod_{l=1}^{n} A_{\xi_l \zeta_{N-n+l}}\right) & \text{if } n < N, \\ \left(\frac{1-i}{2}\right)^n \left(\prod_{k=1}^{n} A_{\xi_k \zeta_k}\right) & \text{if } n = N, \\ \left(\frac{1-i}{2}\right)^n \left(\prod_{k=1}^{p} (A^{m+1})_{\xi_k \zeta_{N-p+k}}\right) \left(\prod_{l=1}^{N-p} (A^m)_{\xi_{p+l} \zeta_l}\right) & \text{if } n = mN + p, \\ \left(\frac{1-i}{2}\right)^n \prod_{k=1}^{N} (A^m)_{\xi_k \zeta_k} & \text{if } n = mN, \end{cases} \tag{22}$$

where A is the 2×2 matrix with the element $A_{x_1 x_2} = \exp((\pi/2)\, i |x_1 - x_2|)$ for $x_1, x_2 = 0,\ 1,\ p = 1, \ldots, N-1$ and $m \in \mathbf{N}$.

Using these formulas, the following theorems are obtained and their proofs are given in the Appendix.

Theorem 5.1:

$$r_n^{(N)} = \begin{cases} \sum_{k=1}^{N-n} \xi_{n+k} 2^{-k} + \frac{2^n}{2^{N+1}} & \text{if } n < N, \\ \frac{1}{2} & \text{if } n = N, \\ \frac{1}{2^n} \sum_{j=0}^{2^N - 1} \frac{j + \frac{1}{2}}{2^N} \prod_{k=1}^{p} |(A^{m+1})_{\xi_k j_{N-p+k}}|^2 \prod_{l=1}^{N-p} |(A^m)_{\xi_{p+l} j_l}|^2 & \text{if } n = mN + p, \\ \frac{1}{2^n} \sum_{j=0}^{2^N - 1} \frac{j + \frac{1}{2}}{2^N} \prod_{k=1}^{N} |(A^m)_{\xi_k j_k}|^2 & \text{if } n = mN, \end{cases} \tag{23}$$

where A is the 2×2 matrix with the element $A_{x_1 x_2} = \exp((\pi/2)\, i |x_1 - x_2|)$ for $x_1, x_2 = 0,\ 1,\ p = 1, \ldots, N-1$ and $m \in \mathbf{N}$.

By diagonalizing the matrix A, we obtain the following formula of the absolute square of the matrix elements of A^n for any $n \in \mathbf{N}$.

Lemma 5.2: For any $n \in \mathbf{N}$, we have

$$|(A^n)_{kj}|^2 = \begin{cases} 2^n \cos^2\left(\frac{n\pi}{4}\right) & \text{if } k = j \\ 2^n \sin^2\left(\frac{n\pi}{4}\right) & \text{if } k \neq j \end{cases}.$$

Combining Theorem 5.1 and Lemma 5.2, we obtain the following two theorems with respect to the mean value $r_n^{(N)}$ of the position operator.

Theorem 5.3: *For the case $n = mN + p$, $p = 1, 2, \ldots, N-1$ and $m \in \mathbf{N}$, we have*

$$r_n^{(N)}=\begin{cases}\sum_{k=1}^{N-p}\xi_{p+k}2^{-k}+\dfrac{2^p}{2^{N+1}} & \text{if } m=0(\mathrm{mod}\,4),\\ \sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{-k}+\dfrac{2^N-2^p+1}{2^{N+1}} & \text{if } m=1(\mathrm{mod}\,4),\\ \sum_{k=1}^{N-p}\eta_{p+k}2^{-k}+\dfrac{2^p}{2^{N+1}} & \text{if } m=2(\mathrm{mod}\,4),\\ \sum_{k=N-p+1}^{N}\xi_{k-(N-p)}2^{-k}+\dfrac{2^N-2^p+1}{2^{N+1}} & \text{if } m=3(\mathrm{mod}\,4),\end{cases} \tag{24}$$

where $\eta_k=\xi_k+1(\mathrm{mod}2)$, $k=1,\ldots,N$.

Theorem 5.4: *For the case* $n=mN$, $m\in\mathbf{N}$, *we have*

$$r_N^{(n)}=\begin{cases}\sum_{k=1}^{N}\xi_k2^{-k}+\dfrac{1}{2^{N+1}} & \text{if } m=0(\mathrm{mod}\ 4),\\ \dfrac{1}{2} & \text{if } m=1,3(\mathrm{mod}\ 4),\\ \sum_{k=1}^{N}\eta_k2^{-k}+\dfrac{1}{2^{N+1}} & \text{if } m=2(\mathrm{mod}\ 4).\end{cases} \tag{25}$$

Using formulas (23)–(25), the probability distribution $(p_i^{(n)})$ of the orbit of mean value $r_n^{(N)}$ of the position operator $\hat{q}$ for the time evolution, which is constructed by the quantum Baker's map, is given by

$$p_i^{(n)}\equiv\frac{1}{m+1}\sum_{k=n}^{m+n}1_{B_i}(r_n^{(N)})$$

for an initial value $r_0^{(N)}\in[0,1]$ and the characteristic function 1_A. The joint distribution $(p_{ij}^{(n,n+1)})$ between the time n and $n+1$ is given by

$$p_{ij}^{(n,n+1)}\equiv\frac{1}{m+1}\sum_{k=n}^{m+n}1_{B_i}(r_k^{(N)})1_{B_j}(r_{k+1}^{(N)}).$$

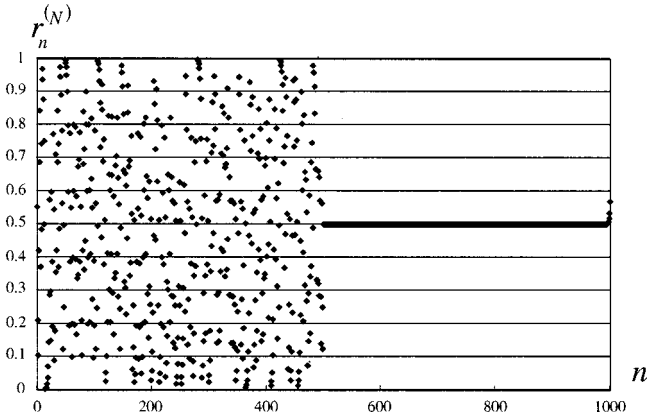

FIG. 1. The distribution of $r_N^{(n)}$ for the case $N=500$.

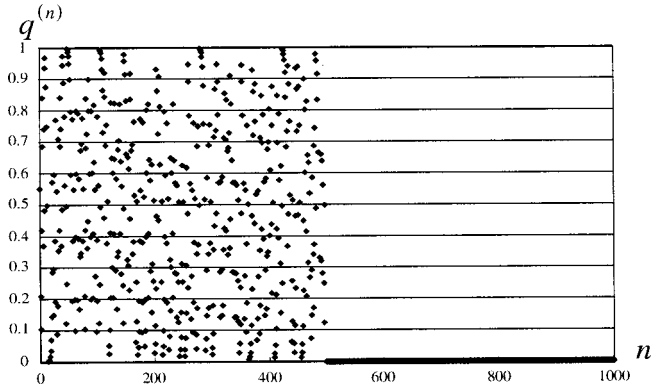

FIG. 2. The distribution of the classical value $q^{(n)}$ for the case $N=500$.

Thus the chaos degree for the quantum Baker's map is calculated by

$$D_q(p^{(n)};\Lambda_n^*)=\sum_{i,j} p_{ij}^{(n,n+1)}\log\frac{p_i^{(n)}}{p_{ij}^{(n,n+1)}}, \tag{26}$$

whose numerical value is shown in the next section.

VI. NUMERICAL SIMULATION OF THE CHAOS DEGREE AND CLASSICAL-QUANTUM CORRESPONDENCE

We compare the dynamics of the mean value $r_n^{(N)}$ of position operator $\hat{q}$ with that of the classical value q_n in the q direction. We take an initial value of the mean value as

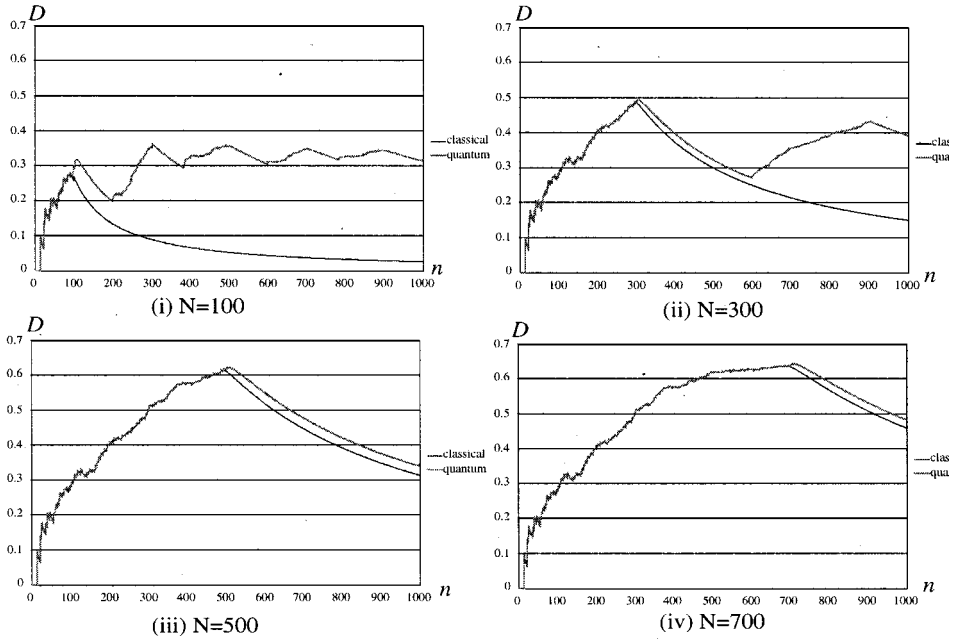

FIG. 3. The change of the chaos degree for several N's up to time $n=1000$.

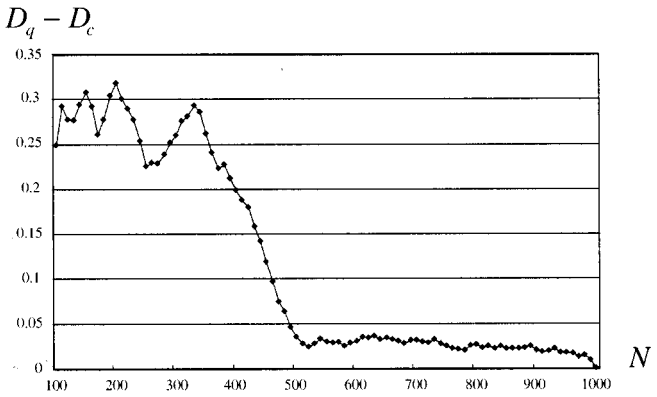

FIG. 4. The difference of the chaos degree between quantum and classical for the case $n=1000$.

$$r_0^{(N)}=\sum_{l=1}^{N}\xi_l 2^{-l}+\frac{1}{2^{N+1}}=0\cdot\xi_1\xi_2\cdots\xi_N 1,$$

where ξ_i is a pseudo-random number valued with 0 or 1. At the time zero we assume that the classical value q_0 in the q direction takes the same value as the mean value $r_0^{(N)}$ of position operator $\hat{q}$. The distribution of $r_n^{(N)}$ for the case $N=500$ is shown in Fig. 1 up to the time $n=1000$. The distribution of the classical value q_n for the case $N=500$ in the q direction is shown in Fig. 2 up to the time $n=1000$.

Figure 3 represents the change of the chaos degree for the case $N=100,300,500,700$ up to the time $n=1000$.

The correspondence between the chaos degree D_q for the quantum Baker's map and the chaos degree D_c for the classical Baker's map for some fixed N's (100,300,500,700 here) is shown for the time less than $T=\log_2(1/h)=\log_2 2^N=N$, and it is lost at the logarithtic time scale T. Here we took a finite partition $\{B_k\}$ of $I=[0,1]$ such as $B_k=[k/100,(k+1)/100))(k=0,1,\ldots,98)$ and $B_{99}=[99/100,1]$ to compute the chaos degree numerically.

The difference of the chaos degrees between the chaos degree D_q for the quantum Baker's map and the chaos degree D_c for the classical Baker's map for a fixed time n (1000, here) is displayed w.r.t. N in Fig. 4.

Thus we conclude that the dynamics of the mean value $r_n{}^{(N)}$ reduces the classical dynamics q_n in the q direction in the classical limit $N\to\infty(h\to 0)$.

The appearance of the logarithmic timescale have been proved rigorously in our recent paper.[38]

ACKNOWLEDGMENTS

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APPENDIX A:

Proof of Theorem 5.1: By a direct calculation, we obtain

$$
\begin{aligned}
r_n^{(N)} &= \langle \xi | T^n \hat{q} T^{-n} | \xi \rangle \\
&= \langle \xi | T^n \left(\sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} |j\rangle\langle j| \right) T^{-n} | \xi \rangle \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} \langle \xi | T^n | j \rangle \langle j | T^{-n} | \xi \rangle \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} \langle \xi | T^n | j \rangle \langle j | T^{*n} | \xi \rangle \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} \langle \xi | T^n | j \rangle \overline{\langle \xi | T^n | j \rangle} \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} |\langle \xi | T^n | j \rangle|^2 .
\end{aligned}
$$

Using (22), the mean value $r_n^{(N)}$ in the case $n<N$ can be expressed as

$$
\begin{aligned}
r_n^{(N)} &= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} |\langle \xi | T^n | j \rangle|^2 \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} \left| \left(\frac{1-i}{2} \right)^n \left(\prod_{k=1}^{N-n} \delta(\xi_{n+k} - j_k) \right) \left(\prod_{l=1}^{n} A_{\xi_l j_{N-n+l}} \right) \right|^2 \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} \left(\frac{1-i}{2} \right)^n \left(\prod_{k=1}^{N-n} \delta(\xi_{n+k} - j_k) \right) \left(\prod_{l=1}^{n} A_{\xi_l j_{N-n+l}} \right) \\
&\quad \times \overline{\left(\frac{1-i}{2} \right)^n \left(\prod_{k=1}^{N-n} \delta(\xi_{n+k} - j_k) \right) \left(\prod_{l-1}^{n} A_{\xi_l j_{N-n+l}} \right)} \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} \left(\frac{1-i}{2} \right)^n \left(\frac{1+i}{2} \right)^n \left(\prod_{k=1}^{N-n} \delta(\xi_{n+k} - j_k) \right) \left(\prod_{l=1}^{n} |A_{\xi_l j_{N-n+l}}|^2 \right) \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} \left(\frac{1-i}{2} \right)^n \left(\frac{1+i}{2} \right)^n \left(\prod_{k=1}^{N-n} \delta(\xi_{n+k} - j_k) \right) \\
&= \frac{1}{2^{N+n}} \sum_{j_1, \cdots j_N} \left\{ \left(\sum_{k=1}^{N} j_k 2^{N-k} \right) + \frac{1}{2} \right\} \left(\prod_{k=1}^{N-n} \delta(\xi_{n+k} - j_k) \right) \\
&= \frac{1}{2^{N+n}} \sum_{j_1, \cdots j_N} \left(\sum_{k=1}^{N} j_k 2^{N-k} \right) \left(\prod_{k=1}^{N-n} \delta(\xi_{n+k} - j_k) \right) + \frac{1}{2^{N+n+1}} \sum_{j_1, \cdots j_N} \left(\prod_{k=1}^{N-n} \delta(\xi_{n+k} - j_k) \right) \\
&= \frac{1}{2^{N+n}} \sum_{j_{N-n+1}, \cdots j_N} \left(\sum_{l=1}^{N-n} \xi_{n+l} 2^{N-l} + \sum_{l=N-n+1}^{N} j_l 2^{N-l} \right) + \frac{1}{2^{N+n+1}} \left(\sum_{j_{N-n+1}, \cdots j_N} 1 \right)
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{2^{N+n}}\left(\sum_{l=1}^{N-n} \xi_{n+l}2^{N-l}\right)\left(\sum_{j_{N-n+1},\cdots j_N} 1\right) + \frac{1}{2^{N+n}}\sum_{j_{N-n+1},\cdots j_N}\left(\sum_{l=N-n+1}^{N} j_l 2^{N-l}\right) \\
&\quad + \frac{1}{2^{N+n+1}}\left(\sum_{j_{N-n+1},\cdots j_N} 1\right) \\
&= \frac{2^n}{2^{N+n}}\left(\sum_{l=1}^{N-n} \xi_{n+l}2^{N-l}\right) + \frac{1}{2^{N+n}}\sum_{j_{N-n+1},\cdots j_N}\left(\sum_{l=N-n+1}^{N} j_l 2^{N-l}\right) + \frac{2^n}{2^{N+n+1}} \\
&= \frac{1}{2^N}\left(\sum_{l=1}^{N-n} \xi_{n+l}2^{N-l}\right) + \frac{1}{2^{N+n}}\sum_{j_{N-n+1},\cdots j_N}\left(\sum_{l=1}^{n} j_{N-n+l}2^{n-l}\right) + \frac{1}{2^{N+1}} \\
&= \frac{1}{2^N}\left(\sum_{l=1}^{N-n} \xi_{n+l}2^{N-l}\right) + \frac{1}{2^{N+n}}\frac{1}{2}(2^n-1)2^n + \frac{1}{2^{N+1}} \\
&= \frac{1}{2^N}\left(\sum_{l=1}^{N-n} \xi_{n+l}2^{N-l}\right) + \frac{2^n}{2^{N+1}}.
\end{aligned}
$$

For the case $n=N$, we similarly obtain

$$
\begin{aligned}
r_n^{(N)} &= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N}|\langle\xi|T^n|j\rangle|^2 \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N}\left|\left(\frac{1-i}{2}\right)^N\left(\prod_{k=1}^{N} A_{\xi_k j_k}\right)\right|^2 \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N}\left|\left(\frac{1-i}{2}\right)^N\right|^2\prod_{k=1}^{N}|A_{\xi_k j_k}|^2 \\
&= \frac{1}{2^{2N}}\sum_{j=0}^{2^N-1}\left(j+\frac{1}{2}\right) \\
&= \frac{1}{2^{2N}}\frac{1}{2}(2^N-1)2^N + \frac{1}{2^{N+1}} = \frac{1}{2}.
\end{aligned}
$$

For $n=mN+p,\ p=1,2,\ldots,N-1,\ m\in\mathbf{N}$,

$$
\begin{aligned}
r_n^{(N)} &= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N}|\langle\xi|T^n|j\rangle|^2 \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{/2}}{2^N}\left|\left(\frac{1-i}{2}\right)^n\left(\prod_{k=1}^{p}(A^{m+1})_{\xi_k j_{N-p+k}}\right)\left(\prod_{l=1}^{N-p}(A^m)_{\xi_{p+l}j_l}\right)\right|^2 \\
&= \frac{1}{2^n}\sum_{j=0}^{2^N-1}\frac{j+\frac{1}{2}}{2^N}\prod_{k=1}^{p}|(A^{m+1})_{\xi_k j_{N-p+k}}|^2\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2,
\end{aligned}
$$

and for $n=mN,\ m\in\mathbf{N}$,

$$
\begin{aligned}
r_N^{(n)} &= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} |\langle \xi | T^n | j \rangle|^2 \\
&= \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} \left| \left(\frac{1-i}{2} \right)^n \prod_{k=1}^{N} (A^m)_{\xi_k j_k} \right|^2 \\
&= \frac{1}{2^n} \sum_{j=0}^{2^N-1} \frac{j+\frac{1}{2}}{2^N} \prod_{k=1}^{N} |(A^m)_{\xi_k j_k}|^2 .
\end{aligned}
$$

■

Proof of Lemma 5.2: By a direct calculation, the matrix A is diagonalized as follows:

$$A = FDF^*, \tag{A1}$$

where

$$F = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad D = \begin{pmatrix} 1+i & 0 \\ 0 & 1-i \end{pmatrix}.$$

From (A1), we have

$$
\begin{aligned}
A^n &= FD^nF^* \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} (1+i)^n & 0 \\ 0 & (1-i)^n \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} (1+i)^n + (1-i)^n & (1+i)^n - (1-i)^n \\ (1+i)^n - (1-i)^n & (1+i)^n + (1-i)^n \end{pmatrix}.
\end{aligned} \tag{A2}
$$

Using (A2), it follows that for any $k=j$, $k=1,2$,

$$
\begin{aligned}
|(A^n)_{kj}|^2 &= \tfrac{1}{2}\{(1+i)^n + (1-i)^n\} \overline{\tfrac{1}{2}\{(1+i)^n + (1-i)^n\}} \\
&= \tfrac{1}{4}\{(1+i)^n + (1-i)^n\}\{(1-i)^n + (1+i)^n\} \\
&= \tfrac{1}{4}\{(1+i)^n + (1-i)^n\}^2 \\
&= \frac{1}{4}\left\{ \left(\sqrt{2}\frac{1+i}{\sqrt{2}} \right)^n + \left(\sqrt{2}\frac{1-i}{\sqrt{2}} \right)^n \right\}^2 \\
&= \frac{1}{4}\left\{ (\sqrt{2})^n \left(\frac{1+i}{\sqrt{2}} \right)^n + (\sqrt{2})^n \left(\frac{1-i}{\sqrt{2}} \right)^n \right\}^2 \\
&= \frac{2^n}{4}\left\{ \left(\exp\left(\frac{\pi}{4} i \right) \right)^n + \left(\exp\left(-\frac{\pi}{4} i \right) \right)^n \right\}^2 \\
&= \frac{2^n}{4}\left\{ \exp\left(\frac{n\pi}{4} i \right) + \exp\left(-\frac{n\pi}{4} i \right) \right\}^2 \\
&= \frac{2^n}{4}\left[\left\{ \cos\left(\frac{n\pi}{4} \right) + i \sin\left(\frac{n\pi}{4} \right) \right\} + \left\{ \cos\left(\frac{n\pi}{4} \right) - i \sin\left(\frac{n\pi}{4} \right) \right\} \right]^2 \\
&= \frac{2^n}{4}\left\{ 2 \cos\left(\frac{n\pi}{4} \right) \right\}^2 = 2^n \cos^2\left(\frac{n\pi}{4} \right)
\end{aligned}
$$

and for any $k \neq j$, $k=1,2$,

$$
\begin{aligned}
|(A^n)_{kj}|^2 &= \tfrac{1}{2}\{(1+i)^n-(1-i)^n\}\overline{\tfrac{1}{2}\{(1+i)^n-(1-i)^n\}} \\
&= \tfrac{1}{4}\{(1+i)^n-(1-i)^n\}\{(1-i)^n-(1+i)^n\} \\
&= -\tfrac{1}{4}\{(1+i)^n-(1-i)^n\}^2 \\
&= -\frac{1}{4}\left\{\left(\sqrt{2}\frac{1+i}{\sqrt{2}}\right)^n-\left(\sqrt{2}\frac{1-i}{\sqrt{2}}\right)^n\right\}^2 \\
&= -\frac{1}{4}\left\{(\sqrt{2})^n\left(\frac{1+i}{\sqrt{2}}\right)^n-(\sqrt{2})^n\left(\frac{1-i}{\sqrt{2}}\right)^n\right\}^2 \\
&= -\frac{2^n}{4}\left\{\left(\exp\left(\frac{\pi}{4}i\right)\right)^n-\left(\exp\left(-\frac{\pi}{4}i\right)\right)^n\right\}^2 \\
&= -\frac{2^n}{4}\left[\left\{\cos\left(\frac{n\pi}{4}\right)+i\sin\left(\frac{n\pi}{4}\right)\right\}-\left\{\cos\left(\frac{n\pi}{4}\right)-i\sin\left(\frac{n\pi}{4}\right)\right\}\right]^2 \\
&= -\frac{2^n}{4}\left\{2i\sin\left(\frac{n\pi}{4}\right)\right\}^2 \\
&= 2^n\sin^2\left(\frac{n\pi}{4}\right).
\end{aligned}
$$

■

Proof of Theorem 5.3: For the case $n=mN+p$, $p=1,\ldots,N-1$ and $m\in\mathbf{N}$,

$$
r_n^{(N)}=\frac{1}{2^n}\sum_{j=0}^{2^N-1}\frac{j+\frac{1}{2}}{2^N}\prod_{k=1}^{p}|(A^{m+1})_{\xi_k j_{N-p+k}}|^2\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2.
$$

By a direct calculation, we obtain

$$
\begin{aligned}
r_n^{(N)} &= \frac{1}{2^n}\sum_{j=0}^{2^N-1}\frac{j+\frac{1}{2}}{2^N}\prod_{k=1}^{p}|(A^{m+1})_{\xi_k j_{N-p+k}}|^2\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2 \\
&= \frac{1}{2^n}\sum_{j=0}^{2^N-1}\frac{j+\frac{1}{2}}{2^N}\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=1}^{p}|(A^{m+1})_{\xi_k j_{N-p+k}}|^2 \\
&= \frac{1}{2^{n+N}}\sum_{j=0}^{2^N-1}\left(j+\frac{1}{2}\right)\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=1}^{p}|(A^{m+1})_{\xi_k j_{N-p+k}}|^2 \\
&= \frac{1}{2^{n+N}}\sum_{j_1,\cdots,j_N}\left\{\left(\sum_{k=1}^{N}j_k2^{N-k}\right)+\frac{1}{2}\right\}\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=1}^{p}|(A^{m+1})_{\xi_k j_{N-p+k}}|^2 \\
&= \frac{1}{2^{n+N}}\sum_{j_1,\cdots,j_N}\left\{\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}j_k2^{N-k}\right)+\frac{1}{2}\right\} \\
&\quad\times\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=1}^{p}|(A^{m+1})_{\xi_k j_{N-p+k}}|^2 \\
&= \frac{1}{2^{(m+1)N+p}}\sum_{j_1,\cdots,j_N}\left\{\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}j_k2^{N-k}\right)+\frac{1}{2}\right\} \\
&\quad\times\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=N-p+1}^{N}|(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2. \qquad \text{(A3)}
\end{aligned}
$$

(i) $m=0(\mathrm{mod}\,4)$

From the above lemma, we have

$$|(A^m)_{\xi_{p+l}j_l}|^2=\begin{cases}2^m & \text{if } j_l=\xi_{p+l},\\ 0 & \text{if } j_l\neq\xi_{p+l},\end{cases}\qquad |(A^{m+1})_{\xi_{k-(N-p)j_k}}|^2=2^m$$

for any $l=1,\cdots,N-p$ and $k=N-p+1,\cdots,N$. Using this formula the product of absolute squares can be expressed as

$$\begin{aligned}&\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=N-p+1}^{N}|(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2\\ &\quad=\begin{cases}(2^m)^{N-p}(2^m)^p & \text{if } j_l=\xi_{p+l} \text{ for all } l=1,\cdots,N-p,\\ 0 & \text{otherwise,}\end{cases}\\ &\quad=\begin{cases}2^{mN} & \text{if } j_l=\xi_{p+l} \text{ for all } l=1,\cdots,N-p,\\ 0 & \text{otherwise.}\end{cases}\end{aligned}$$

Equation (A3) can be rewritten as

$$\begin{aligned}r_n^{(N)}&=\frac{1}{2^{(m+1)N+p}}\sum_{j_1,\cdots,j_N}\left\{\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}j_k2^{N-k}\right)+\frac{1}{2}\right\}\\ &\quad\times\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=N-p+1}^{N}|(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2\\ &=\frac{2^{mN}}{2^{(m+1)N+p}}\sum_{j_{N-p+1},\cdots,j_N}\left\{\left(\sum_{k=1}^{N-p}\xi_{p+k}2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}j_k2^{N-k}\right)+\frac{1}{2}\right\} \qquad \text{(A4)}\\ &=\frac{1}{2^{N+p}}\left(\sum_{k=1}^{N-p}\xi_{p+k}2^{N-k}\right)\left(\sum_{j_{N-p+1},\cdots,j_N}1\right)\\ &\quad+\frac{1}{2^{N+p}}\sum_{j_{N-p+1},\cdots,j_N}\left(\sum_{k=N-p+1}^{N}j_k2^{N-k}\right)+\frac{1}{2^{N+p}}\frac{1}{2}\left(\sum_{j_{N-p+1},\cdots,j_N}1\right)\\ &=\frac{1}{2^N}\sum_{k=1}^{N-p}\xi_{p+k}2^{N-k}+\frac{1}{2^{N+p}}\sum_{j_{N-p+1},\cdots,j_N}\left(\sum_{k=N-p+1}^{N}j_k2^{N-k}\right)+\frac{1}{2^{N+1}}\\ &=\frac{1}{2^N}\sum_{k=1}^{N-p}\xi_{p+k}2^{N-k}+\frac{1}{2^{N+p}}\sum_{j_{N-p+1},\cdots,j_N}\left(\sum_{k=1}^{p}j_{N-p+k}2^{p-k}\right)+\frac{1}{2^{N+1}}\\ &=\frac{1}{2^N}\sum_{k=1}^{N-p}\xi_{p+k}2^{N-k}+\frac{1}{2^{N+p}}\sum_{k=0}^{2^p-1}k+\frac{1}{2^{N+1}}\\ &=\frac{1}{2^N}\sum_{k=1}^{N-p}\xi_{p+k}2^{N-k}+\frac{1}{2^{N+p}}\frac{1}{2}(2^p-1)2^p+\frac{1}{2^{N+1}}\\ &=\sum_{k=1}^{N-p}\xi_{p+k}2^{-k}+\frac{2^p}{2^{N+1}}.\end{aligned}$$

(ii) $m=1(\mathrm{mod}\,4)$

From the above lemma, we have

$$|(A^m)_{\xi_{p+l}j_l}|^2=2^{m-1},\quad |(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2=\begin{cases}2^{m+1} & \text{if } j_k\neq\xi_{k-(N-p)},\\ 0 & \text{if } j_k=\xi_{k-(N-p)},\end{cases}$$

for any $l=1,\cdots,N-p$ and $k=N-p+1,\cdots,N$. Using this formula the product of absolute squares can be expressed as

$$\begin{aligned}&\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=N-p+1}^{N}|(A^{m+1})_{\xi_{k-(N-p)}j_k}|\\ &\quad=\begin{cases}(2^{m-1})^{N-p}(2^{m+1})^p & \text{if } j_k\neq\xi_{k-(N-p)} \text{ for all } k=N-p+1,\cdots,N,\\ 0 & \text{otherwise}\end{cases}\\ &\quad=\begin{cases}2^{(m-1)N+2p} & \text{if } j_k\neq\xi_{k-(N-p)} \text{ for all } k=N-p+1,\cdots,N,\\ 0 & \text{otherwise.}\end{cases}\end{aligned}$$

Let $\eta_{k-(N-p)}=\xi_{k-(N-p)}+1(\mathrm{mod}2), k=N-p+1,\ldots,N$. It follows that

$$\begin{aligned}r_n^{(N)}&=\frac{1}{2^{(m+1)N+p}}\sum_{j_1,\cdots,j_N}\left\{\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}j_k2^{N-k}\right)+\frac{1}{2}\right\}\\ &\quad\times\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=N-p+1}^{N}|(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2\\ &=\frac{2^{(m-1)N+2p}}{2^{(m+1)N+p}}\sum_{j_1,\cdots,j_{N-p}}\left\{\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{N-k}\right)+\frac{1}{2}\right\} \qquad \text{(A5)}\\ &=\frac{1}{2^{2N-p}}\sum_{j_1,\cdots,j_{N-p}}\left\{\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{N-k}\right)+\frac{1}{2}\right\}\\ &=\frac{1}{2^{2N-p}}\sum_{j_1,\cdots,j_{N-p}}\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\frac{1}{2^{2N-p}}\left(\sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{N-k}\right)\left(\sum_{j_1,\cdots,j_{N-p}}1\right)\\ &\quad+\frac{1}{2^{2N-p}}\frac{1}{2}\left(\sum_{j_1,\cdots,j_{N-p}}1\right)\\ &=\frac{1}{2^{2N-p}}\sum_{j_1,\cdots,j_{N-p}}\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\frac{2^{N-p}}{2^{2N-p}}\left(\sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{N-k}\right)+\frac{2^{N-p}}{2^{2N-p}}\frac{1}{2}\\ &=\frac{1}{2^{2N-p}}\sum_{j_1,\cdots,j_{N-p}}\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{-k}+\frac{1}{2^{N+1}}\\ &=\frac{2^p}{2^{2N-p}}\sum_{j_1,\cdots,j_{N-p}}\left(\sum_{k=1}^{N-p}j_k2^{N-p-k}\right)+\sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{-k}+\frac{1}{2^{N+1}}\\ &=\frac{2^p}{2^{2N-p}}\sum_{k=0}^{2^{N-p}-1}k+\sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{-k}+\frac{1}{2^{N+1}}\\ &=\frac{2^p}{2^{2N-p}}\frac{1}{2}(2^{N-p}-1)2^{N-p}+\sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{-k}+\frac{1}{2^{N+1}}\\ &=\sum_{k=N-p+1}^{N}\eta_{k-(N-p)}2^{-k}+\frac{2^N-2^p+1}{2^{N+1}}.\end{aligned}$$

(iii) $m=2(\mathrm{mod}\,4)$

From the above lemma, we have

$$|(A^m)_{\xi_{p+l}j_l}|^2=\begin{cases}2^m & \text{if } j_l\neq\xi_{p+l}\\ 0 & \text{if } j_l=j_{p+l}\end{cases},\quad |(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2=2^m$$

for any $l=1,\cdots,N-p$ and $k=N-p+1,\cdots,N$. Using this formula the product of absolute squares can be expressed as

$$\begin{aligned}&\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=N-p+1}^{N}|(A^{m+1})_{\xi_{k-(N-p)}j_k}|\\&=\begin{cases}(2^m)^{N-p}(2^m)^p & \text{if } j_l\neq\xi_{p+l} \text{ for all } l=1,\ldots,N-p,\\ 0 & \text{otherwise,}\end{cases}\\&=\begin{cases}2^{mN} & \text{if } j_l\neq\xi_{p+l} \text{ for all } l=1,\ldots,N-p,\\ 0 & \text{otherwise.}\end{cases}\end{aligned}$$

Let $\eta_{p+l}=\xi_{p+l}+1(\mathrm{mod}\,2)$, $l=1,\ldots,N-p$. It follows that

$$\begin{aligned}r_n^{(N)}&=\frac{1}{2^{(m+1)N+p}}\sum_{j_1,\cdots,j_N}\left\{\left(\sum_{k=1}^{N-p}j_k2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}j_k2^{N-k}\right)+\frac{1}{2}\right\}\\&\quad\times\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=N-p+1}^{N}|(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2\\&=\frac{2^{mN}}{2^{(m+1)N+p}}\sum_{j_{N-p+1},\cdots,j_N}\left\{\left(\sum_{k=1}^{N-p}\eta_{p+k}2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}j_k2^{N-k}\right)+\frac{1}{2}\right\}.\end{aligned}$$

Substituting η_{p+k} for ξ_{p+k} in (A4), we get

$$r_n^{(N)}=\sum_{k=1}^{N-p}\eta_{p+k}2^{-k}+\frac{2^p}{2^{N+1}}.$$

(iv) $m=3(\mathrm{mod}\,4)$

From the above lemma, we have

$$|(A^m)_{\xi_{p+l}j_l}|^2=2^{m-1},|(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2=\begin{cases}2^{m+1} & \text{if } j_k=\xi_{k-(N-p)},\\ 0 & \text{if } j_k\neq\xi_{k-(N-p)},\end{cases}$$

for any $l=1,\ldots,N-p$ and $k=N-p+1,\ldots,N$. Using this formula the product of absolute squares can be expressed as

$$\begin{aligned}&\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=N-p+1}^{N}|(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2\\&=\begin{cases}(2^{m-1})^{N-p}(2^{m+1})^p & \text{if } j_k=\xi_{k-(N-p)} \text{ for all } k=N-p+1,\ldots,N,\\ 0 & \text{otherwise,}\end{cases}\\&=\begin{cases}2^{(m-1)N+2p} & \text{if } j_k=\xi_{k-(N-p)} \text{ for all } k=N-p+1,\cdots,N,\\ 0 & \text{otherwise.}\end{cases}\end{aligned}$$

Equation (A3) can be rewritten as

$$r_n^{(N)}=\frac{1}{2^{(m+1)N+p}}\sum_{j_1,\cdots,j_N}\left\{\left(\sum_{k=1}^{N-p} j_k 2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N} j_k 2^{N-k}\right)+\frac{1}{2}\right\}$$
$$\times\prod_{l=1}^{N-p}|(A^m)_{\xi_{p+l}j_l}|^2\prod_{k=N-p+1}^{N}|(A^{m+1})_{\xi_{k-(N-p)}j_k}|^2$$
$$=\frac{2^{(m-1)N+2p}}{2^{(m+1)N+p}}\sum_{j_1,\cdots,j_{N-p}}\left\{\left(\sum_{k=1}^{N-p} j_k 2^{N-k}\right)+\left(\sum_{k=N-p+1}^{N}\xi_{k-(N-p)}2^{N-k}\right)+\frac{1}{2}\right\}.$$

Substituting $\xi_{k-(N-p)}$ for $\eta_{k-(N-p)}$ in (A5), we get

$$r_n^{(N)}=\sum_{k=N-p-1}^{N-p}\xi_{k-(N-p)}2^{-k}+\frac{2^N-2^p+1}{2^{N+1}}.$$

■

Proof of Theorem 5.4: For any $n=mN$, $m\in\mathbf{N}$,

$$r_n^{(N)}=\frac{1}{2^n}\sum_{j=0}^{2^N-1}\frac{j+\frac{1}{2}}{2^N}\prod_{k=1}^{N}|(A^m)_{\xi_k j_k}|^2.$$

By a direct calculation, we obtain

$$r_n^{(N)}=\frac{1}{2^n}\sum_{j=0}^{2^N-1}\frac{j+\frac{1}{2}}{2^N}\prod_{k=1}^{N}|(A^m)_{\xi_k j_k}|^2$$
$$=\frac{1}{2^{n+N}}\sum_{j=0}^{2^N-1}(j+\tfrac{1}{2})\prod_{k=1}^{N}|(A^m)_{\xi_k j_k}|^2$$
$$=\frac{1}{2^{(m+1)N}}\sum_{j_1,\cdots,j_N}\left\{\left(\sum_{k=1}^{N} j_k 2^{N-k}\right)+\frac{1}{2}\right\}\prod_{k=1}^{N}|(A^m)_{\xi_k j_k}|^2.$$

(i) $m=0(\mathrm{mod}\,4)$

From the above lemma, we have

$$|(A^m)_{\xi_k j_k}|^2=\begin{cases}2^m & \text{if } j_k=\xi_k,\\ 0 & \text{if } j_k\neq\xi_k,\end{cases}$$

for any $k=1,\ldots,N$. Using this formula the product of absolute squares can be expressed as

$$\prod_{l=1}^{N}|(A^m)_{\xi_k j_k}|^2=\begin{cases}2^{mN} & \text{if } j_k=\xi_k \quad \text{for all } k=1,\ldots,N,\\ 0 & \text{otherwise.}\end{cases}$$

Using this formula the mean value $r_n^{(N)}$ of the position operator can be expressed as

$$r_n^{(N)}=\frac{1}{2^{(m+1)N}}\sum_{j_1,\cdots,j_N}\left\{\left(\sum_{k=1}^{N} j_k 2^{N-k}\right)+\frac{1}{2}\right\}\prod_{k=1}^{N}|(A^m)_{\xi_k j_k}|^2$$
$$=\frac{2^{mN}}{2^{(m+1)N}}\left\{\left(\sum_{k=1}^{N}\xi_k 2^{N-k}\right)+\frac{1}{2}\right\}=\sum_{k=1}^{N}\xi_k 2^{-k}+\frac{1}{2^{N+1}}.$$

(ii) $m=1,3(\mathrm{mod}\,4)$

From the above lemma, we have

$$|(A^m)_{\xi_k j_k}|^2 = 2^{m-1}$$

for any $k=1,\ldots,N$. Note that

$$\prod_{l=1}^{N} |(A^m)_{\xi_k j_k}|^2 = 2^{(m-1)N}.$$

Using this formula the mean value $r_n^{(N)}$ of the position operator can be expressed as

$$\begin{aligned} r_n^{(N)} &= \frac{1}{2^{(m+1)N}} \sum_{j_1,\cdots,j_N} \left\{ \left(\sum_{k=1}^{N} j_k 2^{N-k} \right) + \frac{1}{2} \right\} \prod_{k=1}^{N} |(A^m)_{\xi_k j_k}|^2 \\ &= \frac{2^{(m-1)N}}{2^{(m+1)N}} \sum_{j_1,\cdots,j_N} \left\{ \left(\sum_{k=1}^{N} j_k 2^{N-k} \right) + \frac{1}{2} \right\} \\ &= \frac{1}{2^{2N}} \cdot \left\{ \sum_{j_1,\cdots,j_N} \left(\sum_{k=1}^{N} j_k 2^{N-k} \right) + \frac{1}{2} \left(\sum_{j_1,\cdots,j_N} 1 \right) \right\} \\ &= \frac{1}{2^{2N}} \sum_{k=0}^{2^N-1} k + \frac{1}{2^{N+1}} = \frac{1}{2^{2N}} 2^{N-1}(2^N-1) + \frac{1}{2^{N+1}} = \frac{1}{2}. \end{aligned}$$

(iii) $m=2 \pmod 4$

From the above lemma, we have

$$|(A^m)_{\xi_k j_k}|^2 = \begin{cases} 2^m & \text{if } j_k \neq \xi_k, \\ 0 & \text{if } j_k = \xi_k, \end{cases}$$

for any $k=1,\ldots,N$. Using this formula the product of absolute squares can be expressed as

$$\prod_{l=1}^{N} |(A^m)_{\xi_k j_k}|^2 = \begin{cases} 2^{mN} & \text{if } j_k \neq \xi_k \text{ for all } k=1,\ldots,N \\ 0 & \text{otherwise.} \end{cases}$$

Let $\eta_k = \xi_k + 1 \pmod 2$, $k=1,\ldots,N$. It follows that

$$\begin{aligned} r_n^{(N)} &= \frac{1}{2^{(m+1)N}} \sum_{j_1,\cdots,j_N} \left\{ \left(\sum_{k=1}^{N} j_k 2^{N-k} \right) + \frac{1}{2} \right\} \prod_{k=1}^{N} |(A^m)_{\xi_k j_k}|^2 \\ &= \frac{2^{mN}}{2^{(m+1)N}} \left\{ \left(\sum_{k=1}^{N} \eta_k 2^{N-k} \right) + \frac{1}{2} \right\} = \sum_{k=1}^{N} \eta_k 2^{-k} + \frac{1}{2^{N+1}}. \end{aligned}$$

■

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Symplectic areas, quantization, and dynamics in electromagnetic fields

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A gauge invariant quantization in a closed integral form is developed over a linear phase space endowed with an inhomogeneous Faraday electromagnetic tensor. An analog of the Groenewold product formula (corresponding to Weyl ordering) is obtained via a membrane magnetic area, and extended to the product of N symbols. The problem of ordering in quantization is related to different configurations of membranes: A choice of configuration determines a phase factor that fixes the ordering and controls a symplectic groupoid structure on the secondary phase space. A gauge invariant solution of the quantum evolution problem for a charged particle in an electromagnetic field is represented in an exact continual form and in the semiclassical approximation via the area of dynamical membranes. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1426688]

I. INTRODUCTION AND OVERVIEW

The works by Berezin,[1] Berry,[2] as well as by Marinov[3] have introduced and focused attention on several geometrical formulas representing the phases of three primary quantum objects (the noncommutative product, semiclassical Wigner eigenfunctions, and the evolution Wigner functions) in terms of symplectic area of simple two-dimensional membranes whose boundary consists of line segments and pieces of Hamiltonian trajectories in phase space. The area of these membranes is determined with respect to the canonical 2-form

$$\omega_0=\tfrac{1}{2}J_{jk}dx^k\wedge dx^j,\quad x=(q,p)\in\mathbb{R}^{2n},\quad J=\begin{bmatrix}0 & I\\ -I & 0\end{bmatrix}.$$

Attempts to generalize some of these formulas to phase spaces with a generic symplectic form have been undertaken. For spaces with flat symplectic connection, a product of membrane type was constructed in Ref. 4. For curved symmetric spaces (see Ref. 5) the opportunity to represent the quantum product via the area of triangle membranes was mentioned by Berezin, and it was actually proved by Weinstein,[6] that the semiclassical phase of the product-generating kernel is given by such an area in this case. Over Kählerian manifolds formulas for the noncommutative product and for the solutions of stationary or evolution problems via the area of membranes in the complexification of phase space were obtained in Refs. 7–9 (see also Ref. 10). However, formulas which use only the usual symplectic area are still unavailable for the general case.

In the present paper we analyze three problems related to this topic.

A first and trivial remark, which one can make regarding generalization of the original approach of the works,[1,2,3] is that the specific matrix J in the definition of the symplectic form ω_0

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can be replaced by an arbitrary skew-symmetric matrix without any changes in the geometrical picture. In particular, one can take J to be the matrix $\left[\begin{smallmatrix} F & I \\ -I & 0 \end{smallmatrix}\right]$, where the constant block F represents a homogenous electromagnetic field. But the next and more interesting generalization to consider is that of inhomogeneous (not constant) tensors F.

The second natural question is about ordering. All treatments of the geometrical picture of works[1,2,3] were made for one specific ordering choice: For the Weyl symmetrization of the noncommutative coordinates (operators). What happens with other possible orderings?

The third question which our paper addresses is the application of such Weyl and non–Weyl symbolic calculus, in the presence of an inhomogeneous field, to solving the Cauchy problem and developing a semiclassical representation.

We begin with the first question and consider the linear phase space $\mathbb{R}^{2n}$ with the following inhomogeneous symplectic form

$$\omega_F=\omega_0+F, \quad F=\tfrac{1}{2}F_{jk}(q)\,dq^k\wedge dq^j. \tag{1.1}$$

In cases $n=3$, $n=4$ the form (1.1) describes the structure of the phase space for charged particles in an electromagnetic field;[11,12] the additional summand F is the Faraday 2-form multiplied by the charge coupling constant e/c. For simplicity of notation we include this constant in F_{jk}; also note that the order of indices j,k in (1.1) is opposite to that used in some textbooks.[13]

In detail one has the following. In the three-dimensional case with $q=(q^1,q^2,q^3)$ then

$$F_{jk}=\frac{e}{c}\epsilon_{kjl}B^l \quad (j,k=1,2,3),$$
$$F=\frac{e}{c}(B^1(q)dq^2\wedge dq^3+B^2(q)dq^3\wedge dq^1+B^3(q)dq^1\wedge dq^2). \tag{1.2a}$$

Here B is the magnetic field, and $dF=0$ is equivalent to $\operatorname{div}B=0$. In the four-dimensional case with $q=(q^0,q^1,q^2,q^3)$, $q^0\equiv ct$ one has

$$F_{jk}=\frac{e}{c}\epsilon_{kjl}B^l, \quad (j,k=1,2,3), \quad F_{0j}=\frac{e}{c}E_j \quad (j=1,2,3),$$
$$F=\frac{e}{c}(B^1(t,q)\,dq^2\wedge dq^3+B^2(t,q)\,dq^3\wedge dq^1+B^3(t,q)\,dq^1\wedge dq^2)+eE_j(t,q)dq^j\wedge dt. \tag{1.2b}$$

The electric field is denoted by E, and $dF=0$ is equivalent to the pair of Maxwell equations $c^{-1}\partial B/\partial t+\operatorname{curl}E=0$, $\operatorname{div}B=0$; see Refs. 13 and 14.

The form ω_F is called the *magnetic symplectic form*. We show how this form generates the Weyl–symmetrized associative product $\star_F$ of functions over the phase space.

The general mathematical framework for such products was established by Bayen, Flato, Fronsdal, Lichnerowicz, and Sternheimer,[15] by Berezin,[1] Rieffel,[16] Fedosov[17] and intensively developed in many other works. The specific ''magnetic'' product $\star_F$ we construct and investigate is just a particular example of these quantization schemes. The method which we use to determine $\star_F$ follows Ref. 18 and is based on the creation of the left (right) regular representation for the magnetic commutation relations between the quantum position and the kinetic momentum.

The q^j,p_k are coordinates corresponding to the position of the charged particle and its gauge invariant kinetic momentum. The commutation relations between the corresponding quantum operators $\hat{q}^j,\hat{p}_k$ are the following:

$$[\hat{q}^j,\hat{q}^k]=0, \quad [\hat{q}^j,\hat{p}_k]=i\hbar\,\delta^j_k, \quad [\hat{p}_j,\hat{p}_k]=i\hbar F_{kj}(\hat{q}). \tag{1.3}$$

The usual realization of these operators in the Hilbert space $L^2(\mathbb{R}^n_q)$ is $\hat{q}=q$, $\hat{p}=-i\hbar\partial/\partial q - (e/c)\Phi(q)$, where $(e/c)d(\Phi dq)=F$, and Φ is the gauge potential. Specifically, for $n=3$:

$$\Phi=(\mathcal{A}_1,\mathcal{A}_2,\mathcal{A}_3), \quad \mathrm{curl}\mathcal{A}=B, \quad \hat{p}_j=-i\hbar\frac{\partial}{\partial q_j}-\frac{e}{c}\mathcal{A}_j(q) \quad (j=1,2,3), \tag{1.4a}$$

for $n=4$

$$\Phi=(-a,\mathcal{A}_1,\mathcal{A}_2,\mathcal{A}_3), \quad \mathrm{curl}\mathcal{A}=B, \quad -\left(\frac{1}{c}\frac{\partial\mathcal{A}}{\partial t}+\frac{\partial a}{\partial q}\right)=E,$$

$$\hat{p}_0=-\frac{i\hbar}{c}\frac{\partial}{\partial t}+\frac{e}{c}a(t,q), \quad \hat{p}_j=-i\hbar\frac{\partial}{\partial q_j}-\frac{e}{c}\mathcal{A}_j(t,q) \quad (j=1,2,3). \tag{1.4b}$$

All the formulas obtained in the paper depend on the symplectic form (1.1) only, but not on the choice of potentials, and so, all results are gauge independent.

The noncommutative product $\star_F$ which we construct necessarily reproduces the commutation relations (1.3) on coordinate functions

$$q^j\underset{F}{\star}q^k-q^k\underset{F}{\star}q^j=0, \quad q^j\underset{F}{\star}p_k-p_k\underset{F}{\star}q^j=i\hbar\delta^j_k, \quad p_j\underset{F}{\star}p_k-p_k\underset{F}{\star}p_j=i\hbar F_{kj}(q).$$

The operators of left multiplication $q\star_F$ and $p\star_F$, as well as right multiplication, are derived without difficulty from these relations, using the noncommutative calculus;[18,19] the result incorporates Valatin's[20] primitive of the closed 2-form F (see Sec. II). We note that the problem of a finding a gauge invariant symbol product in a convenient closed form was first addressed by Stratonovich.[21]

In Sec. III we derive explicit formulas for $\star_F$ in two equivalent forms, both valid when $F=0$ and when $F\neq 0$. The first is analogous to the exponential Janus derivative representation[22–24] due to Groenewold. The second is a modification of the $(F=0)$ Berezin's integral for the noncommutative product. In both versions there appears an additional electromagnetic action, or flux, over triangles in phase space. Moreover, the Groenewold-type product formula admits generalization for N multipliers via the magnetic area of polygon membranes.

Our exact formulas for the $\star_F$ product can be easily expanded to obtain formal $\hbar\to 0$ power series. Higher-order terms beyond the Poisson bracket contribution are functions of derivatives of F_{jk}. This series coincides structurally with that obtained by Müller.[25]

Our integral formula for $\star_F$ is similar to that found in Ref. 26 and is also related to constructions[27–29] of the Wigner function in the presence of electromagnetic fields, but the method and the geometric interpretation is our case are completely different. In Sec. IV we show that the $\star_F$ product can be produced by a convolution over $T\mathbb{R}^n$. This convolution is generated by a version of the Connes' tangential groupoid[30–32] but with an additional rapidly oscillating factor represented by the electromagnetic flux.

In Sec. V we analyze, following the general approach of Ref. 33, the structure of the symplectic groupoid corresponding to $\star_F$. This structure is given on the secondary cotangent bundle $T^*(T^*\mathbb{R}^n)=T^*\mathbb{R}^n\oplus\mathbb{R}^{2n}$. The first cotangent bundle, $T^*\mathbb{R}^n=\mathbb{R}^n_q\otimes\mathbb{R}^n_p$, is the primary phase space, over which we construct the product $\star_F$. We show how the symplectic groupoid structure on $T^*(T^*\mathbb{R}^n)$ senses the magnetic correction F in the symplectic form, and how the space $\mathbb{R}^{2n}$, dual to $T^*\mathbb{R}^n$, is equipped with a pseudogroup structure controlled by a hidden magnetic momentum of membranes.

From this point of view, we claim that in the formula for $\star_F$ it would be more natural to consider not the usual geodesic triangle, but the triangle with three additional ''wings'' directed vertically (i.e., parallel to the p-direction) in the phase space. The shape of wings is determined by the symplectic groupoid structure.

Then in Sec. VI we investigate what happens if the Weyl ordering of noncommuting coordinates is changed to some other ordering. The wide (matrix) family of orderings introduced in Ref. 34 we relate to phases in the exponential representation of the $*$-product. These phases can be again presented as symplectic areas of membranes. The membranes are combinations of the basic triangle with additional wings that are now not necessarily vertical. The shape and direction of the wings exactly control the choice of the ordering in quantization, and again it is related to the symplectic groupoid structure over the secondary phase space $T^*(T^*\mathbb{R}^n)$.

The symplectic area of the wings give three additional contributions to the phase. The transform from the original Berezin phase (the Weyl case) to the new one, generated by the wings, can be considered as a type of gauge transformation of the ''symplectic potential.'' On the level of $*$-products this is the transformation from the distinguished Weyl choice to other ordering choices. In a sense this is the ''gauge'' of quantization.

The special features of the Weyl quantization which have made it the preferred choice[2,23,24,35,36] for physical applications are: (1) It treats $\hat{q}$ and $\hat{p}$ symmetrically; (2) self-adjoint operators have real symbols; and, (3) the Groenewold–Moyal bracket is an even function of $\hbar$, in particular its leading semiclassical correction is $O(\hbar^2)$, not $O(\hbar)$. From the symplectic point of view, the Weyl ordering seems distinguished since the corresponding membranes are of the simplest shape (having no wings).

The Wick normal and anti-normal orderings $\hat{z}^{*}_{2},\hat{z}_{1}$ and $\hat{z}^{*}_{1},\hat{z}_{2}$ (where $z=q+ip$) correspond to pure imaginary wings of membranes in the product formulas.

Other convenient orderings—the standard $\hat{q}_{2},\hat{p}_{1}$ and anti-standard $\hat{q}_{1},\hat{p}_{2}$—correspond to the case when the wings are parallel to the basic triangle and the total membrane becomes a plane rectangle. These standard and anti-standard cases correspond to the push- and pull-groupoid structure on $T\mathbb{R}^n$ (see Sec. IV). From the symplectic point of view these cases are singular because of the totally caustic character of the graph of symplectic groupoid multiplication corresponding to these cases.

In Secs. VII and VIII we apply these ideas to the quantum dynamical problem: A charged particle in an electromagnetic field. The basic results for this system were found by Dirac, Fock, Peierls, and Schwinger. Gauge invariant versions of the WKB approximation were developed[37–42] mostly in terms of integral kernels (Green functions). In the context of the present paper we can use the $\star_F$ symbol calculus to obtain a phase space gauge invariant treatment of this problem.

We first study, in Sec. VII, the pure magnetic situation without electric field. We represent the gauge invariant version of the quantum evolution equation over phase space and show how the Berry and Marinov geometrical representation for the solution of the Hamilton–Jacobi equation, as well the geometrical phase summation rule are generalized in the presence of the magnetic field.

At the end of Sec. VII, using the membrane generalization of the Groenewold formula, we represent the symbol of the evolution operator exactly in a continual form. This continual membrane formula is dual to the Feynman path integral representation.

Then, in Sec. VIII, we consider a time-dependent electromagnetic field and represent the gauge invariant quantum equations over phase space in both the nonrelativistic and relativistic cases. Here we use dynamical quantum products which are time-dependent. The evolution of commutation relations in time is controlled by the electric field.

We describe the semiclassical solution of the Cauchy problem using membranes in seven-dimensional contact space $\mathbb{R}_t\times\mathbb{R}^3_q\times\mathbb{R}^3_p$. The boundary of these dynamic membranes are given by

the solution of two classical systems: one for the given particle and an additional one for a "virtual" particle of infinite mass.

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II. MAGNETIC PRODUCT FOR WEYL ORDERING

We begin with the definition of magnetic product on a function space over $\mathbb{R}^{2n}$. The logic is the following: We transform relations (1.3) to the standard Heisenberg relations, apply the standard operators of regular representation, and then transform back to the magnetic variables. As the result, we obtain a formula for magnetic product in terms of left and right regular representation of the algebra (1.3).

First we recall the properties of closed forms on $\mathbb{R}^n$.

Lemma 1: Let $F=\frac{1}{2}F_{jk}(q)dq^k\wedge dq^j$ be a closed two-form on $\mathbb{R}^n$. Consider the vector-valued 1-form Fdq with components $(F(q)\,dq)_j=F_{jk}(q)\,dq^k$ and define the two point vector potential

$$A(q,q')=\frac{1}{|q-q'|}\int_{q'}^{q}|\tilde{q}-q'|F(\tilde{q})d\tilde{q}, \tag{2.1}$$

where the integral is taken along the straight line path from q' to q, and $|\cdot|$ denotes the Euclidean norm on $\mathbb{R}^n$. Then for an arbitrary fixed $q'\in\mathbb{R}^n$ the 1-form $A(q,q')dq$ is a primitive of F

$$d(A\,dq)=F.$$

The choice of a primitive (2.1) *(gauge choice) is uniquely characterized by the orthogonality condition*

$$A(q,q')\cdot(q-q')=0. \tag{2.2}$$

Note that construction (2.1) is different from that usually used in proofs of the known Poincaré lemma in the theory of differential forms. On the other hand, (2.1) is just a simple particular case of the solution of Lie system related to a general Poisson bracket; (see Ref. 18, p. 81, and references therein). Formula (2.1) was obtained by Valatin[20] for electromagnetic tensors. The characteristic condition (2.2) was stressed by Dirac (see Ref. 20, p. 101).

We need several other properties of Valatin's primitive.

Lemma 2: The following formulas hold:

$$d_{q'}(A(q,q')\,dq)=d_q(A(q',q)\,dq'),$$

$$A(q,q')-A(q',q)=\int_{q'}^{q}F(\tilde{q})\,d\tilde{q},$$

$$A(q,q')+A(q',q)=\frac{1}{|q-q'|}\int_{q_m}^{q}|\tilde{q}-\tilde{q}^*|(F(\tilde{q})-F(\tilde{q}^*))\,d\tilde{q},$$

where the integrals are taken along the straight line paths, and $\tilde{q}^*=2q_m-\tilde{q}$ is the point symmetric to $\tilde{q}$ with respect to the middle point $q_m=\frac{1}{2}(q+q')$.

Let Δ be the triangle in $\mathbb{R}^n$ with vertices q, q', q''. Consider the integral (flux) of the form F:

$$\mathrm{Flux}_{q''}(q,q')\equiv\int_{\Delta}F. \tag{2.3}$$

Note that here and everywhere in the sequel the orientation of a membrane corresponds to the sequence of its vertices (or sides) read from right to left; so the orientation of Δ corresponds to the sequence $q\leftarrow q'\leftarrow q''$.

Lemma 3: The following formulas hold:

$$\mathrm{Flux}_{q''}(q,q')=\int_{q'}^{q}A(\tilde{q},q'')d\tilde{q},$$
$$\frac{\partial}{\partial q}\mathrm{Flux}_{q''}(q,q')=A(q,q'')-A(q,q'), \tag{2.4}$$

where the integral in (2.4) *is taken along the straight line path.*

Now let us fix the second argument of $A(q,q')$ at some point, say, $q'=0$ and introduce the operators

$$\hat{p}'=\hat{p}+A(\hat{q},0).$$

Since $\hat{q}$, $\hat{p}$ satisfy relations (1.3), the new set of operators $\hat{q}$, $\hat{p}'$ satisfy the standard Heisenberg commutation relations

$$[\hat{q}^j,\hat{p}'_k]=i\hbar\delta^j_k, \quad [\hat{q}^j,\hat{q}^k]=[\hat{p}'_j,\hat{p}'_k]=0. \tag{2.5}$$

Any Weyl-symmetrized function of operators $\hat{q},\hat{p}$ can be transformed to a function of operators $\hat{q}$, $\hat{p}'$ by the formula

$$f(\hat{q},\hat{p})=f\left(\frac{\overset{3}{\hat{q}}+\overset{1}{\hat{q}}}{2},\overset{2}{\hat{p}'}-\overset{3}{\tilde{A}}(\overset{1}{\hat{q}},\hat{q})\right), \tag{2.6}$$

where

$$\tilde{A}(q,q')\equiv\int_0^1 A(q\mu+q'(1-\mu),0)d\mu.$$

We have used here formulas of noncommutative analysis[19] and Ref. 18, pp. 277–295; the superscripts on top of operators denote the order of application.

Throughout the paper we will not give a characterization of the spaces the symbols must belong to in order that (2.6) and the subsequent product formulas are well defined. This is a separate technical (and often not simple) question which has been extensively investigated in the pseudodifferential operator literature.[18,34,43,44] The reader can consider all formulas as formally algebraic or, depending on the formula, assume an appropriate simple symbol class such as polynomials, smooth rapidly decreasing functions, etc.

For the Heisenberg algebra (2.5) the operators of left and right regular representation are well known. Namely, consider arbitrary Weyl-symmetrized function g' with operator arguments $\hat{q},\hat{p}'$:

$$\hat{g}'\equiv g'(\hat{q},\hat{p}')=g'\left(\frac{\overset{3}{\hat{q}}+\overset{1}{\hat{q}}}{2},\overset{2}{\hat{p}'}\right). \tag{2.7}$$

Then the following left and right multiplication formulas hold:[18,34,43,45]

$$\begin{aligned}
&\hat{q}\hat{g}'=\widehat{L'_q g'}, \quad L'_q=q+\tfrac{1}{2}i\hbar\partial_{p'};\\
&\hat{p}'\hat{g}'=\widehat{L'_p g'}, \quad L'_p=p'-\tfrac{1}{2}i\hbar\partial_q;\\
&\hat{g}'\hat{q}=\widehat{R'_q g'}, \quad R'_q=q-\tfrac{1}{2}i\hbar\partial_{p'};\\
&\hat{g}'\hat{p}'=\widehat{R'_p g'}, \quad R'_p=p'+\tfrac{1}{2}i\hbar\partial_q.
\end{aligned} \tag{2.8}$$

Here we denote $\partial_q \equiv \partial/\partial q$ and $\partial_{p'} = \partial/\partial p'$. Operators L', R' satisfying multiplication formulas (2.8) are called the left and right regular representation of the given algebra, in our case, the algebra (2.5).

On the right-hand side of the formula (2.6) operators $\overset{1}{\hat{q}}$ and $\overset{3}{\hat{q}}$ in arguments of $\tilde{A}$ can be considered as multiplication by $\hat{q}$ from the left and from the right, and so they can be replaced by L'_q and R'_q acting on arguments of f. Thus we obtain from (2.6)

$$f(\hat{q},\hat{p}) = f'\left(\frac{\overset{3}{\hat{q}}+\overset{1}{\hat{q}}}{2}, \overset{2}{\hat{p}'}\right) = f'(\hat{q},\hat{p}'),$$

where

$$f'(q,p') = f(q,p' - \tilde{A}(\overleftarrow{L'_q},\overleftarrow{R'_q})) = \exp\{-\tilde{A}(L'_q,R'_q)\partial_{p'}\}f(q,p'),$$

and the left arrows mean that operators act on arguments standing to their left. After substitution of explicit formulas for L'_q, R'_q from (2.8) we conclude

$$f'(q,p') = \exp\{-\tilde{A}(q+\tfrac{1}{2}i\hbar\partial_{p'}, q-\tfrac{1}{2}i\hbar\partial_{p'})\partial_{p'}\}f(q,p').$$

Note that by Lemma 2

$$\tilde{A}(q+u/2,q-u/2)u = \int_{q-u/2}^{q+u/2} A(\tilde{q},0)\,d\tilde{q} = \mathrm{Flux}_0(q+u/2,q-u/2).$$

So we obtain the transformation formula

Proposition 1: Any Weyl-symmetrized function f in operators $\hat{q}$, $\hat{p}$, satisfying commutation relations (1.3), *can be transformed to the Weyl-symmetrized function f' in operators $\hat{q}$, $\hat{p}'$ satisfying Heisenberg relations* (2.5). *This transform is given by formula*

$$f' = U_F f, \quad U_F = \exp\left\{\frac{i}{\hbar}\mathrm{Flux}_0\left(q+\frac{1}{2}i\hbar\partial_p, q-\frac{1}{2}i\hbar\partial_p\right)\right\}, \tag{2.9}$$

where the Flux_0 *was defined in* (2.3).

Using this transform one easily obtains all objects which are needed for the algebra (1.3). For instance, the operators of left and right regular representation for (1.3) are the following

$$L_q = U_F^{-1}\cdot L'_q\cdot U_F, \quad R_q = U_F^{-1}\cdot R'_q\cdot U_F,$$

$$L_p = U_F^{-1}\cdot L'_p\cdot U_F - A(L_q,0), \quad R_p = U_F^{-1}\cdot R'_p\cdot U_F - A(R_q,0).$$

Applying explicit formulas (2.8) for L', R', (2.9) for U_F and using Lemma 3 we get

$$\begin{aligned} L_q &= q+\tfrac{1}{2}i\hbar\partial_p, \quad R_q = q-\tfrac{1}{2}i\hbar\partial_p, \\ L_p &= p-\tfrac{1}{2}i\hbar\partial_q - A(L_q,R_q), \quad R_p = p+\tfrac{1}{2}i\hbar\partial_q - A(R_q,L_q). \end{aligned} \tag{2.10}$$

Lemma 4: Operators L_q, L_p satisfy commutation relations (1.3), *and operators R_q, R_p satisfy the conjugate relations (with opposite signs). Operators L commute with R.*

If we know the regular representation of commutation relations, we know the product of symbols (see Ref. 18 Appendix 2).

Theorem 1: *The product of Weyl-symmetrized functions in operators satisfying relations* (1.3) *is given by*

$$f(\hat{q},\hat{p})\cdot g(\hat{q},\hat{p})=(f\underset{F}{\star}g)(\hat{q},\hat{p}), \tag{2.11}$$

where $\star_F$ *is the associative product of functions over* $\mathbb{R}^{2n}$ *defined by*

$$f\underset{F}{\star}g=f(L_q,L_p)g=g(R_q,R_p)f.$$

We call $\star_F$ the *magnetic product* of Weyl-symmetrized type. In particular, we have $L_q=q\star_F$, $L_p=p\star_F$, and $R_q=\star_F q$, $R_p=\star_F p$. These multiplication operators satisfy relations (1.3) and their conjugate companions; left and right multiplications commute with each other.

Note that the magnetic product, $\star_F$, since it one-to-one corresponds, by (2.11), to the operator product in the Hilbert space $L^2(\mathbb{R}^n)$, is an example of Rieffel's ''strict deformation quantization.'' [16] Moreover, the operator realization $f\to f(\hat{q},\hat{p})$ possesses the usual trace property

$$trf(\hat{q},\hat{p})=\frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}}f(x)dx.$$

In particular, this means that the space of symbols $L^2(\mathbb{R}^{2n})$ is invariant with respect to the $\star_F$ product (and isomorphic to the algebra of Hilbert–Schmidt operators on $L^2(\mathbb{R}^n)$). Also note the following useful identity:

$$\int_{\mathbb{R}^{2n}}(f\underset{F}{\star}g)(x)\,dx=\int_{\mathbb{R}^{2n}}f(x)g(x)\,dx,$$

which implies that the product $\star_F$ is ''closed'' in the sense of Connes, Flato, and Sternheimer.[46]

III. EXPONENTIAL FORMULA FOR MAGNETIC PRODUCT

The next useful stage in evaluation of the $\star_F$-product is to bring it into an exponential form. First, we apply Proposition 1 and the usual Groenewold formula[22,43] known for Weyl-symmetrized product of symbols over the Heisenberg algebra, namely

$$f'\star g'=f'\exp\left\{-\frac{i\hbar}{2}\overleftarrow{\partial}J^{-1}\overrightarrow{\partial}\right\}g'=f'(q+\vec{u}/2,p)\,g'(q-\tilde{u}/2,p), \tag{3.1}$$

where

$$\tilde{u}=i\hbar\overleftarrow{\partial}_p,\quad \vec{u}=i\hbar\overrightarrow{\partial}_p,\quad \partial=(\partial_q,\partial_p).$$

From (2.9) we calculate

$$U_Ff\star U_Fg=f\exp\left\{\frac{i}{\hbar}\mathrm{Flux}_0(q+(\tilde{u}+\vec{u})/2,q+(\vec{u}-\tilde{u})/2)\right.$$
$$\left.+\frac{i}{\hbar}\mathrm{Flux}_0(q+(\vec{u}-\tilde{u})/2,q-(\tilde{u}+\vec{u})/2)-\frac{i\hbar}{2}\overleftarrow{\partial}J^{-1}\overrightarrow{\partial}\right\}g.$$

Applying the inverse transformation U_F^{-1} we obtain

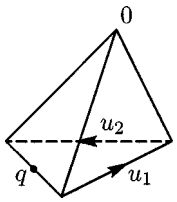

FIG. 1. Membrane $\Delta_q(u_2,u_1)$ is the base plane.

$$U_F^{-1}(U_F f\star U_F g)=f\exp\Big\{-\frac{i}{\hbar}\mathrm{Flux}_0(q+(\tilde{u}+\vec{u})/2,q-(\tilde{u}+\vec{u})/2)+\frac{i}{\hbar}\mathrm{Flux}_0(q+(\tilde{u}+\vec{u})/2,$$
$$q+(\vec{u}-\tilde{u})/2)+\frac{i}{\hbar}\mathrm{Flux}_0(q+(\vec{u}-\tilde{u})/2,q-(\tilde{u}+\vec{u})/2)-\frac{i\hbar}{2}\overleftarrow{\partial}J^{-1}\vec{\partial}\Big\}g.$$

The sum of three fluxes which appeared at last exponent can be simplified if we look at the geometrical picture. Indeed, the three fluxes represent integrals of the form F over three triangles with common vertex 0. They are sides of the tetrahedron. By the Stokes theorem these three fluxes together are equal to the flux over the bottom triangle; see Fig. 1, in which the vectors u_1 and u_2 represent the operators $\vec{u}$ and $\tilde{u}$, respectively.

The relation

$$f\underset{F}{\star}g=U_F^{-1}(U_F f\star U_F g),$$

and the representation of its right-hand side which we have derived above generate the following statement.

Proposition 2: The magnetic product $\star_F$, *corresponding to commutation relations* (1.3), *can be calculated by the formula*

$$(f\underset{F}{\star}g)(q,p)=f(q,p)\exp\Big\{\frac{i}{\hbar}\phi(q,i\hbar\overleftarrow{\partial}_p,i\hbar\vec{\partial}_p)+\frac{i\hbar}{2}(\overleftarrow{\partial}_q\vec{\partial}_p-\overleftarrow{\partial}_p\vec{\partial}_q)\Big\}g(q,p). \tag{3.2}$$

Here

$$\phi(q,u_2,u_1)=\int_{\Delta_q(u_2,u_1)}F, \tag{3.3}$$

and $\Delta_q(u_2,u_1)$ *is a membrane in* $\mathbb{R}^n$ *whose boundary is the triangle constructed by the middle point* q *of one side and by the two other sides* u_2, u_1. *The magnetic flux* (3.3) *can also be represented in the form*

$$\phi=\int_0^1 d\mu\int_0^\mu d\nu\, u_2 F(q+(\mu-\tfrac{1}{2})u_1+(\nu-\tfrac{1}{2})u_2)u_1.$$

Note the differential operators in the exponent (3.2) act only on the arguments of target functions f and g, but not on the argument q in the flux ϕ.

Also note that operators $i\hbar\partial_p$, which we substitute into the flux ϕ in the exponent (3.2), are of order $O(\hbar)$ over the space of non-oscillating functions as $\hbar\to 0$. So the flux ϕ actually is of order $O(\hbar^2)$, and the right-hand side of (3.2) can be easily expanded as a power series in $\hbar$. Thus for nonoscillating (as $\hbar\to 0$) functions f,g

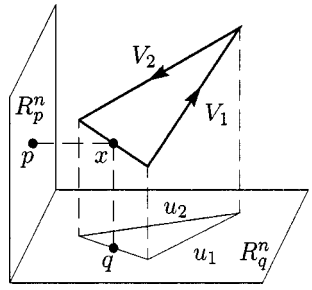

FIG. 2. Membrane $\Sigma_x(V_2,V_1)$.

$$f\underset{F}{\star}g\simeq\sum_{|\gamma|,|\varepsilon|=0}^{\infty}\frac{(-1)^{|\varepsilon|}}{\gamma!\varepsilon!}\left(-\frac{i\hbar}{2}\right)^{|\gamma|+|\varepsilon|}\partial_q^{\varepsilon}\partial_p^{\gamma}f\exp\left\{-\frac{i\hbar}{2}\sum_{|\alpha|,|\beta|=0}^{\infty}\frac{c_{|\alpha|,|\beta|}}{\alpha!\beta!}\right.$$
$$\left.\times\left(-\frac{i\hbar}{2}\right)^{|\alpha|+|\beta|}(\vec{\partial}_p)^{\alpha}\langle\vec{\partial}_p,\partial^{\alpha+\beta}F(q)\vec{\partial}_p\rangle(\vec{\partial}_p)^{\beta}\right\}\partial_q^{\gamma}\partial_p^{\varepsilon}g,$$

where

$$c_{s,m}=\frac{e[m+1]}{(s+1)(m+1)}-\frac{e[s+m]}{(s+1)(s+m+2)},$$

and $e[l]=0$ if l is even, and $e[l]=1$ if l is odd. Here $\langle\cdot,\cdot\rangle$ is the Euclidean scalar product in $\mathbb{R}^n$ and the Greek letters are multi-indices. Of course, the first two terms of this expansion are

$$f\underset{F}{\star}g=fg-\frac{i\hbar}{2}\{f,g\}_F+O(\hbar^2),$$

where $\{,\}_F$ is the Poisson bracket on $\mathbb{R}^{2n}$ corresponding to the symplectic form ω_F, i.e.,

$$\{f,g\}_F=\partial_p f\partial_q g-\partial_q f\partial_p g+\langle\partial_p f,F(q)\partial_p g\rangle. \tag{3.4}$$

In the case where F is restricted to be the pure magnetic form (1.2a), then the $\hbar$ series above is equivalent to the one derived in Ref. 25.

Now we return to the formula (3.2) and observe that it is still not presented in a completely symplectic manner. We have there the flux ϕ, which is the integral of the form F over the triangle in q-space. The other part of the exponent in (3.2) can also be related to the area of a triangle, but in the (q,p)-space; see Fig. 2.

This triangle $\Sigma_x(V_2,V_1)$ is constructed by the middle point x of one side, and by the two opposite sides V_2, V_1. Its projection onto $\mathbb{R}_q^n$ coincides with the triangle $\Delta_q(u_2,u_1)$.

Theorem 2: *The magnetic product can be represented in the form*

$$(f\underset{F}{\star}g)(x)=\exp\left\{\frac{i}{\hbar}\int_{\Sigma_x(\hat{V}_2,\hat{V}_1)}\omega_F\right\}f(x_2)g(x_1)\Big|_{x_1=x_2=x}, \tag{3.5}$$

where ω_F is the magnetic symplectic form (1.1), $\hat{V}=(i\hbar\partial_p,i\hbar\partial_q)$, *and* $x=(q,p)\in\mathbb{R}^{2n}$.

In (3.5) one has to evaluate first the symplectic ω_F-area of the membrane $\Sigma_x(V_2,V_1)$, and then substitute the operators $\hat{V}_1,\hat{V}_2$ for the vectors V_1,V_2; the operator $\hat{V}_1$ is applied to the argument x_1 and $\hat{V}_2$ to the argument x_2.

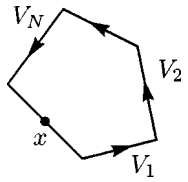

FIG. 3. Membrane $\Sigma_x(V_N,\dots,V_1)$.

Actually, formula (3.5) may be immediately generalized to the case of several multipliers. Consider a membrane in $\mathbb{R}^{2n}$ whose boundary is formed by N vectors $V_1,V_2,\dots,V_N$ as sides of a polygon, and by additional point x as a middle point of the $(N+1)$th side. Denote this membrane by $\Sigma_x(V_N,\dots,V_1)$; see Fig. 3.

Corollary 1: The following formula holds:

$$(f_N \underset{F}{\star} \cdots \underset{F}{\star} f_1)(x) = \exp\left\{\frac{i}{\hbar}\int_{\Sigma_x(\hat{V}_N,\dots,\hat{V}_1)} \omega_F\right\} f_N(x_N)\cdots f_1(x_1)\Big|_{x_1=\cdots=x_N=x}. \tag{3.6}$$

An immediate consequence of (3.5) is an integral formula for $f\star_F g$. Indeed, in (3.5) we have a pseudodifferential operator acting on f and g. By the usual formulas via Fourier and inverse Fourier transform we easily calculate this action and obtain an integral representation for $f\star_F g$. The triangle $\Sigma_x(V_2,V_1)$ in this new formula will be described not by the sides V_2,V_1, but by the middle points x_2,x_1 of those sides. Such a triangle in $\mathbb{R}^{2n}$, constructed by three middle points x,x_2,x_1, we denote by $\Sigma(x,x_2,x_1)$.

Proposition 3: The magnetic product is given by the integral formula

$$(f\underset{F}{\star}g)(x) = \frac{1}{(\pi\hbar)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}} \exp\left\{\frac{i}{\hbar}\int_{\Sigma(x,x_2,x_1)}\omega_F\right\} f(x_2)g(x_1)\,dx_2\,dx_1. \tag{3.7}$$

Actually, the magnetic part F of the form ω_F is integrated in (3.5) and (3.7) over the projection of $\Sigma(x,x_2,x_1)$ onto q-space.

In the case $F=0$, (3.7) becomes the Berezin formula for the Weyl-symmetrized product, and (3.6) becomes equivalent to the N-factor products obtained in Refs. 23 and 24.

IV. TANGENTIAL GROUPOID AND MAGNETIC COCYCLE

Formula (3.7) for magnetic noncommutative product over $\mathbb{R}^{2n}=T^*\mathbb{R}^n$ can also be derived from the Connes type tangential groupoid structure on $T\mathbb{R}^n$,[30–32] equipped with an additional magnetic phase factor (cocycle).

The space $T\mathbb{R}^n$ consists of pairs (q,u), where $q\in\mathbb{R}^n$ and $u\in T_q\mathbb{R}^n$. Vector u is interpreted as a "displacement" at point q. The first and simplest groupoid structure on $T\mathbb{R}^n$ is given by formula $(q_2,u_2)\circ(q_1,u_1)=(q_1,u_2+u_1)$ iff $q_1=q_2$. This groupoid is commutative; it is called the *Galileo groupoid*. This structure is shown in Fig. 4. The set of units of this groupoid consists of all pairs $(q,0)$; so, the set of units is the configuration space $\mathbb{R}^n_q$ considered as the zero-section in $T\mathbb{R}^n$.

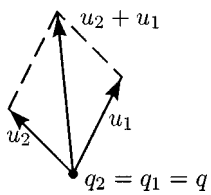

FIG. 4. Galileo groupoid.

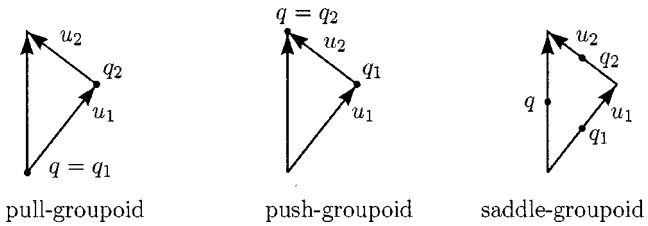

FIG. 5. Pull-groupoid; push-groupoid; saddle-groupoid.

Other geometric combinations of the vectors u_1, u_2 and the points q_1, q_2 may be assembled to give noncommutative groupoids. Three simple possibilities are shown in Fig. 5. The multiplication rule, for instance, in the *pull-groupoid* is $(q_2,u_2)\circ(q_1,u_1)=(q_1,u_2+u_1)$ iff $q_1+u_1=q_2$. For the *saddle-groupoid* one has

$$(q_2,u_2)\circ(q_1,u_1)=(q,u_2+u_1) \quad \text{iff} \quad q_1+u_1/2=q_2-u_2/2.$$

In this case, q is the middle point of the third side of the triangle: $q=q_1+u_2/2=q_2-u_1/2$.

All these groupoids are specific cases of a general *τ-groupoid*, where $0\leqslant\tau\leqslant 1$. Pull-, push-, and saddle-cases correspond to $\tau=1$, $\tau=0$, and $\tau=1/2$, respectively. In Fig. 6 one can see the generic case corresponding to some $\tau \quad (1/2<\tau<1)$; in this case $q_2=q_1+\tau u_1+(1-\tau)u_2$ and $q=q_1+(1-\tau)u_2$. The set of units for all of these groupoids is $\mathbb{R}^n_q\subset T\mathbb{R}^n$.

On any (measurable) groupoid there is a convolution of distributions[30,47]

$$(\phi_2\odot\phi_1)(a)=\int_{a=b\circ c}\phi_2(b)\phi_1(c)\,d\mu_b(c), \tag{4.1}$$

where $d\mu_b$ is the Haar measure on fibres of the left groupoid mapping $c\to c\circ c^{-1}$. For example, in the case of saddle-groupoid we have

$$(\phi_2\odot\phi_1)(q,u)=\int_{\mathbb{R}^n}\phi_2(q+u_1/2,u-u_1)\phi_1(q-(u-u_1)/2,u_1)du_1. \tag{4.2}$$

Each convolution over $T\mathbb{R}^n$ generates a noncommutative product over $T^*\mathbb{R}^n$ just by Fourier transform between u and p coordinates

$$f^{\sim}(q,u)\equiv\frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n}e^{iup/\hbar}f(q,p)\,dp=\frac{1}{(2\pi)^n}\int_{\mathbb{R}^n}e^{iuk}f(q,\hbar k)\,dk. \tag{4.3}$$

For example, if one takes the saddle-groupoid convolution $\odot$ (4.2) then the corresponding product over $T^*\mathbb{R}^n$ is the usual Groenewold–Moyal product $\star$ (3.1), i.e.,

$$(f\star g)^{\sim}=f^{\sim}\odot g^{\sim}. \tag{4.4}$$

Remark 1: In this approach the quantum convolution $\odot$ is not an $\hbar$-deformation of a commutative one. The deformation parameter $\hbar$ appears only in the Fourier transform (4.3); this is

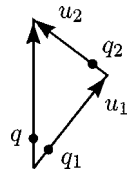

FIG. 6. τ-groupoid.

what makes it possible to include into the quantization scheme functions over $T^*\mathbb{R}^n$ that oscillate rapidly as $\hbar \to 0$. For nonoscillating functions $f(q,p)$ the transform (4.3) admits the classical limit $\hbar = 0$. With this limit one obtains the correspondence $f(q,p) \rightsquigarrow f(q,0)\,\delta(u)$ between the classical commutative algebra of functions over the phase space $T^*\mathbb{R}^n$ and the commutative subalgebra of distributions over $T\mathbb{R}^n$ of the type $\varphi(q)\,\delta(u)$ concentrated at the zero "displacement" $u=0$. Displacement by a nonzero vector u_0, represented over $T\mathbb{R}^n$ as the distribution $\delta(u-u_0)$, after the transform inverse to (4.3) generates the phase space observable $f(q,p)=\exp\{-iu_0 p/\hbar\}$. The corresponding operator $\hat{f}$ (if the magnetic tensor $F=0$) is just the Heisenberg translation operator $\hat{f}\psi(q)=\psi(q-u_0)$. This is the simplest example of rapidly oscillating functions f which one has to include into algebra of observables over $T^*\mathbb{R}^n$, but which lie outside the formal deformation quantization approach;[15,17] see also Refs. 31 and 48.

Now let us return to the relation (4.4) between star-product and convolution. The question arises: how to get the magnetic product $\star_F$ (3.7) via the groupoid structure on $T\mathbb{R}^n$? Let us slightly generalize (4.1) by introducing an exponential phase factor

$$(\phi_2 \odot \phi_1)(a) = \int_{a=b\circ c} e^{i\Phi(b,c)}\phi_2(b)\,\phi_1(c)\,d\mu_b(c). \tag{4.5}$$

Here Φ is a groupoid cocycle, i.e.,

$$\Phi(d,b\circ c)-\Phi(d\circ b,c)+\Phi(b,c)-\Phi(d,b)=0, \quad \Phi(b,c)=-\Phi(c^{-1},b^{-1}),$$

for any multiplicable $b,c,d \in T\mathbb{R}^n$. The cocycle Φ is called the coboundary iff

$$\Phi(b,c)=\psi(b)+\psi(c)-\psi(b\circ c), \quad \psi(b^{-1})=-\psi(b).$$

If Φ in (4.5) is a coboundary, then convolutions (4.5) and (4.1) are actually equivalent.

In the case of saddle-groupoid we can take the following magnetic cocycle (coboundary):

$$\Phi=\frac{1}{\hbar}\int_{\Delta(q,q_2,q_1)} F, \tag{4.6}$$

where F is the Faraday 2-form over $\mathbb{R}^n$, and $\Delta(q,q_2,q_1)$ is the triangle with middle points q, q_2, q_1. In this case the coboundary function ψ at the point $b=(q,u)$ is given by the integral $\psi(b) = 1/\hbar \int A(\tilde{q},0)\,d\tilde{q}$ along the chord $[q-\frac{1}{2}u, q+\frac{1}{2}u]$. Note that ψ controls the additional phase factor in the gauge invariant version of the Wigner function.[21,28,29]

Proposition 4: Let $\odot_F$ be the saddle-groupoid convolution, equipped with the magnetic cocycle (4.6). *Then the Fourier transform* (4.3) *relates this convolution to the magnetic product $\star_F$ via*

$$\underset{F}{(f\star g)}\tilde{} = \underset{F}{\tilde{f}\odot \tilde{g}}.$$

Note that other types of groupoids (like pull-, push-) will also generate some magnetic products over $\mathbb{R}^{2n}=T^*\mathbb{R}^n$. In Sec. VI we will consider a variety of such products. On the other hand, we will show that not all of products over $T^*\mathbb{R}^n$ are generated from the convolution over $T\mathbb{R}^n$ in this fashion.

In Sec. V we analyze the magnetic product (3.7) from the view point of symplectic groupoid structure of the secondary phase space (on the secondary cotangent) $T^*(T^*\mathbb{R}^n)$. Regarding this we mention the following.

Proposition 5: Each groupoid structure on $T\mathbb{R}^n$ whose set of units is $\mathbb{R}^n_q$, uniquely determines a symplectic groupoid structure on $T^*(T^*\mathbb{R}^n)$. Here $T^*\mathbb{R}^n$ is equipped with the symplectic form

$\omega_0 = dp \wedge dq$. If, in addition, on $T\mathbb{R}^n$ a cocycle of type (4.6) *is given, then on $T^*(T^*\mathbb{R}^n)$ we have a symplectic groupoid structure corresponding to the magnetic form ω_F.*

V. SYMPLECTIC GROUPOID AND MEMBRANES WITH WINGS

Formula (3.7) represents the exact magnetic product. On the other hand, it is known,[18] in a very general context, how to construct quantum products of functions over an arbitrary Poisson manifold $\mathcal{N}$ in the semiclassical approximation, to all orders in $\hbar \to 0$. This approximate product takes the form

$$(f*g)(x) \simeq \int \int K_\hbar(x,x_2,x_1) f(x_2) g(x_1)\, dx_1\, dx_2. \tag{5.1}$$

Here $x, x_2, x_1 \in \mathcal{N}$, and $K_\hbar$ is a "wave function" corresponding to some Lagrangian submanifold Λ_* in the "phase space" $\mathcal{E} \times \mathcal{E} \times \mathcal{E}$, where $\mathcal{E}$ is the symplectic groupoid over $\mathcal{N}$. In our case $\mathcal{N} = \mathbb{R}^{2n} = T^*\mathbb{R}^n$ with Poisson bracket (3.4). The Lagrangian submanifold Λ_* is the graph of groupoid multiplication in $\mathcal{E}$. If this graph is one-to-one projected onto the "configuration" space $\mathcal{N} \times \mathcal{N} \times \mathcal{N}$ along the polarization then the function $K_\hbar$ is just a Wentzel–Kramers–Brillouin (WKB) function

$$K_\hbar = \exp\{iS/\hbar\}\varphi + O(\hbar), \tag{5.2}$$

whose phase S is the Poincaré–Cartan action on Λ_* and φ is the solution of the corresponding transport equation.

In specific cases, for instance, in our case $\mathcal{N} = \mathbb{R}^{2n}$ with bracket (3.4), the asymptotic formula (5.1) becomes exact and the remainder $O(\hbar)$ in (5.2) is absent. Indeed, let us compare (5.1), (5.2) with formula (3.7) for the magnetic product $\star_F$. First, one can describe the symplectic groupoid $\mathcal{E}$ in our specific case. Let us set $\mathcal{E} = T^*\mathbb{R}^{2n} = \mathbb{R}^{2n}_x \oplus \mathbb{R}^{2n}_y$, and denote by (x,y) points in $\mathcal{E}$. The space $\mathbb{R}^{2n}_x$ is imbedded into $\mathcal{E}$ as a zero section $\{y=0\}$. The symplectic form on $\mathcal{E}$ is $dy \wedge dx$. The operators L, R (2.10) of left and right regular representation of algebra (1.3) generate two mappings

$$l: \mathcal{E} \to \mathbb{R}^{2n}, \quad r: \mathcal{E} \to \mathbb{R}^{2n}. \tag{5.3}$$

Here $l = (l_q, l_p)$ and $r = (r_q, r_p)$ are just symbols of $L = (L_q, L_p)$ and $R = (R_q, R_p)$, i.e.,

$$L = l(x, -i\hbar\partial_x), \quad R = r(x, -i\hbar\partial_x).$$

In our case formula (2.10) reads

$$\begin{aligned} l_q(x,y) &= x_q - y_p/2, \quad l_p(x,y) = x_p + y_q/2 - A(l_q, r_q), \\ r_q(x,y) &= x_q + y_p/2, \quad r_p(x,y) = x_p - y_q/2 - A(r_q, l_q). \end{aligned} \tag{5.4}$$

Mappings (5.3) are Poisson and anti-Poisson, i.e., l preserves brackets, r changes the sign of brackets [recall that on $\mathbb{R}^{2n}$ we have the bracket (3.4), and the bracket on $\mathcal{E}$ corresponds to the symplectic form $dy \wedge dx$].

The groupoid structure on $\mathcal{E}$ is defined as follows: points $m_2, m_1 \in \mathcal{E}$ are called *multiplicable* iff $r(m_2) = l(m_1)$; the product $m = m_2 \circ m_1$, by definition, is a point in $\mathcal{E}$ such that $l(m) = l(m_2)$, $r(m) = r(m_1)$. The subspace $\mathbb{R}^{2n}_x \subset \mathcal{E}$ is the set of units of this groupoid, and mappings (5.3) are left and right reduction mappings:

$$l(m) = m \circ m^{-1}, \quad r(m) = m^{-1} \circ m.$$

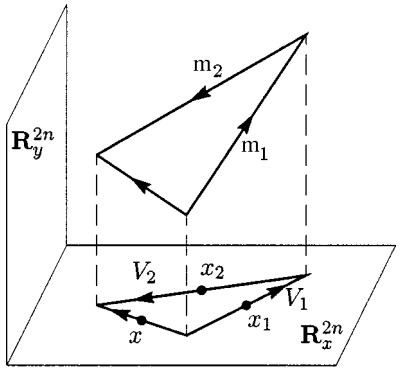

FIG. 7. Groupoid structure on $T^*\mathbb{R}^{2n}$.

The graph $\Lambda_* \subset \mathcal{E}\times\mathcal{E}\times\mathcal{E}$ of this groupoid multiplication consists of all multiplicable points and their products

$$\Lambda_* = \{(m, m_2, m_1) \mid m = m_2 \circ m_1\}. \tag{5.5}$$

If on $\mathcal{E}\times\mathcal{E}\times\mathcal{E}$ we introduce the symplectic form $dy\wedge dx - dy_2\wedge dx_2 - dy_1\wedge dx_1$, then the submanifold Λ_* is Lagrangian (see details in Refs. 33 and 49).

In the case $F=0$ (i.e., A=0) formulas (5.4) are interpreted as "middle point of chord" relations: $x=\frac{1}{2}(l+r)$, $y=JV$, where $V=l-r\in T\mathbb{R}^{2n}$. So, the groupoid structure on $\mathbb{R}^{4n} = T^*\mathbb{R}^{2n}$ is given by the triangle rule (see Fig. 7)

$$\begin{gathered} m = m_2 \circ m_1, \quad m=(x,y), \quad m_1=(x_1,y_1), \quad m_2=(x_2,y_2), \\ y = y_1 + y_2, \quad x = x_1 + \tfrac{1}{2}J^{-1}y_2 = x_2 - \tfrac{1}{2}J^{-1}y_1. \end{gathered} \tag{5.6}$$

For arbitrary given triple of points $x, x_2, x_1 \in \mathbb{R}^{2n}$ we uniquely construct the triangle for which these points are the middle points of its sides, and so reconstruct elements $m, m_2, m_1 \in \mathcal{E}$ such that $m = m_2 \circ m_1$. This means that the graph Λ_* is one-to-one projected onto $\mathbb{R}^{2n}\times\mathbb{R}^{2n}\times\mathbb{R}^{2n}$ along the "vertical" y-polarization. Hence, the kernel $K_\hbar$ has the WKB form (5.2), and its phase is

$$S(x, x_2, x_1) = \int_{(0,0,0)}^{(x,x_2,x_1)} (y\,dx - y_2\,dx_2 - y_1\,dx_1). \tag{5.7}$$

Here y, y_2, y_1 are determined via x, x_2, x_1 following the triangle multiplication rule; the initial point (0,0,0) corresponds to triple of elements $m_0 = m_0 \circ m_0$, where $m_0 = (0,0) \in \mathcal{E}$.

The integral (5.7) is taken over an arbitrary path on Λ_* connecting the triple (0,0,0) (i.e., the degenerate triangle) with the triple (x, x_2, x_1) (i.e., the given triangle). This path is actually a family of triangles in $\mathbb{R}^{2n}$; see Fig. 8. The phase (5.7) in the case $F=0$ (for more general "symmetric" cases see in Ref. 6) is just equal to the area of the final triangle

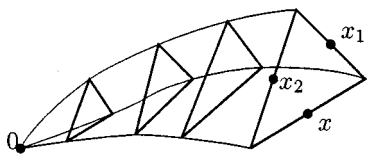

FIG. 8. Path on graph Λ_*.

$$S(x,x_2,x_1)=\int_{\Delta(x,x_2,x_1)}\omega_0.$$

Now let us see what happens in the general magnetic case $F\neq 0$. From (5.4) it follows that the groupoid structure now is given by formulas:

$$x=\tfrac{1}{2}(l+r)+V_F,\quad y=JV+Y_F,\quad \text{where}\quad V=l-r. \tag{5.8}$$

Here we have introduced notations

$$\begin{gathered}V_F=(0;A^s)\in\mathbb{R}^n_q\oplus\mathbb{R}^n_p,\quad Y_F=(A^a;0)\in\mathbb{R}^n_{y_q}\oplus\mathbb{R}^n_{y_p},\\ A^s=\tfrac{1}{2}(A(l_q,r_q)+A(r_q,l_q)),\quad A^a=A(l_q,r_q)-A(r_q,l_q).\end{gathered} \tag{5.9}$$

Comparing with the multiplication rule (5.6) in the case $F=0$ we see that points x, x_2, x_1 are no longer the middle points of sides of the basic triangle and do not even belong to those sides. They are shifted in the p-direction by the vectors V_F.

Another difference from the case $F=0$ is that the usual multiplication rule $y=y_1+y_2$ [see (5.6)] fails to hold for inhomogeneous magnetic case. New magnetic rule is

$$y=y_1+y_2+\left(\int_\Delta \nabla F;0\right), \tag{5.10}$$

where the vector-valued closed two-form ∇F is defined by $\nabla F=\frac{1}{2}\nabla F_{jk}dq^k\wedge dq^j$, and $\Delta=\Delta(q,q_2,q_1)$ is the triangle in q-space with middle points (q,q_2,q_1), which are projections of $x,x_2,x_1\in\mathbb{R}^{2n}$ onto $\mathbb{R}^n_q$. We have obtained the interesting physical quantity:

$$-\int_\Delta \nabla F=\oint_{\partial\Delta}F dq\sim\text{hidden momentum.}$$

The vector 2-form ∇F is a measure of *magnetic inhomogeneity*. So, this form controls the modification of the usual $(F=0)$ multiplication rule. The space $\mathbb{R}^{2n}_y$ (dual to $\mathbb{R}^{2n}_x$) now is not even a group, it is a pseudogroup over the Poisson manifold $\mathbb{R}^{2n}_x$ [see details in general case in Ref. 18, the word ''pseudo''—reflects the fact that the product (5.10) in the y-space depends on x-coordinates as additional parameters, and the condition of ''associativity'' of the product (5.10) senses this dependence]. The nontrivial part of the pseudogroup structure (5.10) is determined by the hidden momentum of the membrane Δ in the magnetic field.

Formula (5.7) in the case $F\neq 0$ still represents the phase in the product (3.7) if we put there the corrected values $y=JV+Y_F$. But now the triangle no longer represents the groupoid multiplication rule, and from this point of view, it seems unnatural to keep this triangle in the formula for the phase.

Actually, we have another configuration (see Fig. 9) related to the triple (x,x_2,x_1). This

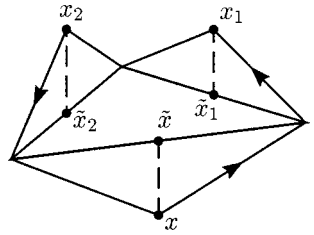

FIG. 9. Membrane $\Sigma_F(x,x_2,x_1)$.

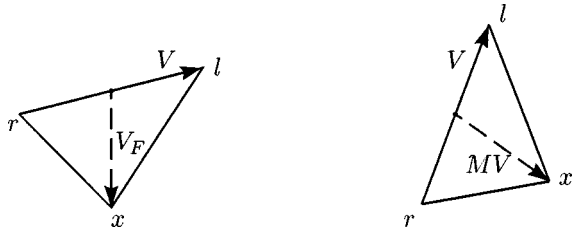

FIG. 10. Magnetic wing and *M*-wing.

configuration consists of triangle $\Sigma(\tilde{x},\tilde{x}_2,\tilde{x}_1)$, where $\tilde{x}=x-V_F$, and also of three additional triangles directed "vertically" (parallel to p) with "top" vertices x, x_2, x_1. We call them *magnetic wings*.

A magnetic wing is characterized by a sequence of its vertices $[l,x,r]$ related to each other by (5.8) (see Fig. 10, left picture). The configuration of membrane with wings, as we see, exactly corresponds to the new groupoid multiplication rule for $F\neq 0$.

Lemma 5:

$$\int_{\Sigma(\tilde{x},\tilde{x}_2,\tilde{x}_1)}\omega_F=\int_{\Sigma(x,x_2,x_1)}\omega_F,\quad \int_{\text{vertical wing}}\omega_F=0.$$

Both statements of the Lemma follow from the orthogonality condition (2.2).

Denote by $\Sigma_F(x,x_2,x_1)$ the triangle $\Sigma(\tilde{x},\tilde{x}_2,\tilde{x}_1)$ together with three magnetic wings described above; see Fig. 9. The boundary of this figure consists of six straight line segments. The figure itself looks like inflected hexagon. More generally, Σ_F could be any membrane in the phase space $\mathbb{R}^{2n}$ with that six segment boundary. In view of Lemma 5 we have

$$\int_{\Sigma(x,x_2,x_1)}\omega_F=\int_{\Sigma_F(x,x_2,x_1)}\omega_F.$$

Theorem 3: *The magnetic product over $T^*\mathbb{R}^n$ is given by*

$$(f\underset{F}{\star}g)(x)=\frac{1}{(\pi\hbar)^{2n}}\int\int\exp\left\{\frac{i}{\hbar}\int_{\Sigma_F(x,x_2,x_1)}\omega_F\right\}f(x_2)g(x_1)dx_2dx_1, \tag{5.11}$$

where Σ_F is the wing membrane corresponding to the magnetic groupoid structure (5.8) *on* $T^*(T^*\mathbb{R}^n)$.

VI. ORDERING IN QUANTIZATION

Now we demonstrate that membrane wings introduced in previous section are actually very natural objects in the quantization framework. We show how different configurations of wings relate to different choices in the ordering problem. In particular, we'll see why the Weyl ordering choice (Weyl symmetrization) looks like an optimal choice.

Let us take a constant real $2n\times 2n$ matrix M (actually, a linear operator in the space tangent to $T^*\mathbb{R}^n$) which obeys the condition

$$M^TJ+JM=0, \tag{6.1}$$

where M^T is the transposed matrix. One can represent M by its $n\times n$ blocks as follows:

$$M=\begin{pmatrix}N & K\\ S & -N^T\end{pmatrix}.$$

Now let us take an arbitrary function $f=f(q,p)$ (say, a polynomial) and determine the following general ordering of operators $\hat{q},\hat{p}'$ (generators of the Heisenberg algebra):

$$\hat{f}^M \equiv f(\tfrac{1}{2}N(\overset{4}{\hat{q}}-\overset{2}{\hat{q}})+\tfrac{1}{2}(\overset{2}{\hat{q}}+\overset{4}{\hat{q}})-\tfrac{1}{2}K(\overset{5}{\hat{p}'}-\overset{1}{\hat{p}'}),\quad \overset{3}{\hat{p}'}-\tfrac{1}{2}S(\overset{4}{\hat{q}}-\overset{2}{\hat{q}})-\tfrac{1}{2}N^T(\overset{5}{\hat{p}'}-\overset{1}{\hat{p}'})). \tag{6.2}$$

We would like to obtain the product formula

$$\hat{f}^M\cdot\hat{g}^M=\hat{k}^M,\quad k=\overset{M}{f*g}. \tag{6.3}$$

To derive the product $*^M$ we first note that the M-ordering (6.2) is related to the Weyl ordering via

$$\hat{f}^M=(U^M f)(\hat{q},\hat{p}'), \tag{6.4}$$

where

$$U^M=\exp\left\{\frac{i}{\hbar}S^M(\hat{V})\right\},\quad \hat{V}=(i\hbar\partial_p,i\hbar\partial_q),$$

and the function S^M is defined by the matrix M as follows

$$S^M(V)=\tfrac{1}{2}\langle JMV,V\rangle=\int_{\Delta^M(V)}\omega_0.$$

Here $\Delta^M(V)$ is the triangle, called the *M-wing*, generated by vector V and by vector MV applied at the middle point of V (see Fig. 10), right picture.

Using U^M we can calculate the product (6.3) by the formula

$$\overset{M}{f*g}\equiv U^{-M}(U^M f\star U^M g),$$

where $\star$ is the Weyl-symmetrized product (without magnetic correction, at first). Looking at exponential representation of the Weyl product, one concludes that

$$\overset{M}{f*g}=\exp\left\{\frac{i}{\hbar}\Phi^M(\hat{V}_2,\hat{V}_1)\right\}f(x_2)g(x_1)|_{x_1=x_2=x},$$

where $\hat{V}=(i\hbar\partial_p,i\hbar\partial_q)$. In this formula we use the notation

$$\Phi^M(V_2,V_1)=\int_{\Sigma(V_2,V_1)}\omega_0+S^M(V_1)+S^M(V_2)-S^M(V_1+V_2),$$

where $\Sigma(V_2,V_1)$ is the triangle generated by vectors V_1, V_2.

The phase function Φ^M can be written as the symplectic area of the *wing membrane* $\Sigma_x^M(V_2,V_1)$ generated by four triangles:

$$\Sigma_x^M(V_2,V_1)=\Delta(V_2,V_1)\cup\Delta^M(V_1)\cup\Delta^M(V_2)\cup\Delta^M(V_1+V_2).$$

Its boundary consists of six line segments. For reasons of uniformity in notation the point x is shown; actually, the ω_0-area of $\Sigma_x^M(V_2,V_1)$ is independent of x.

The picture for Σ_x^M is the same as in Fig. 9, but wings now are M-wings as in Fig. 10 (right picture).

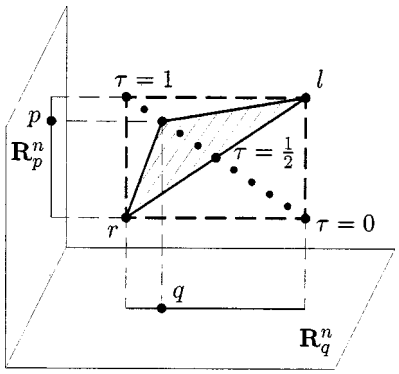

FIG. 11. τ—wings.

Theorem 4: *For an arbitrary real* $2n\times 2n$ *matrix* M*, satisfying* (6.1)*, there is a star-product over* $\mathbb{R}^{2n}$ *given by the wing membranes:*

$$(f\overset{M}{*}g)(x)=\exp\left\{\frac{i}{\hbar}\int_{\Sigma_x^M(\hat{V}_2,\hat{V}_1)}\omega_0\right\}f(x_2)g(x_1)|_{x_1=x_2=x}. \tag{6.5}$$

This product corresponds to the M-ordering rule (6.2) *of noncommutative operators* $\hat{q}$, $\hat{p}'$ (*generators of the Heisenberg algebra*)*, so that formula* (6.3) *holds.*

The family of orderings (6.2) was introduced and studied in detail in Ref. 34, where the following pseudodifferential formulas for M-product were obtained:

$$(f\overset{M}{\star}g)(x)=\overset{2}{f}(x-i\hbar(\tfrac{1}{2}-M)J^{-1}\overset{1}{\partial}_x)g(x)=\overset{2}{g}(x+i\hbar(\tfrac{1}{2}+M)J^{-1}\overset{1}{\partial}_x)f(x).$$

In the particular case

$$M=(\tfrac{1}{2}-\tau)\begin{pmatrix} I & 0\\ 0 & -I\end{pmatrix}, \tag{6.6}$$

the ordering (6.2) simplifies to

$$\hat{f}^\tau=f(\tau\overset{1}{\hat{q}}+(1-\tau)\overset{3}{\hat{q}},\overset{2}{\hat{p}'}). \tag{6.7}$$

The family of τ-wings corresponding to this family of orderings is represented in Fig. 11. The whole membrane Σ_x^M for the specific case $\tau=0$ is shown in Fig. 12.

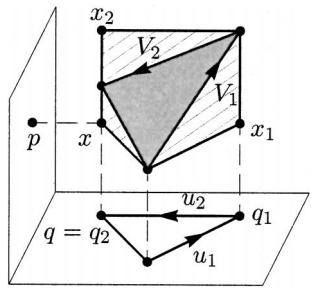

FIG. 12. Membrane Σ_x^M for $\tau=0$.

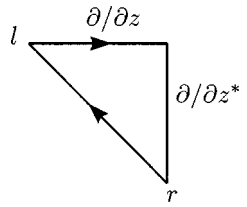

FIG. 13. Pure imaginary wing.

The cases $\tau=0$ and $\tau=1$ are called the standard and anti-standard ordering choices (they correspond to push- and pull- groupoid structures on $T\mathbb{R}^n$, see Sec. IV), and the case $\tau=1/2$ is the Weyl ordering (corresponding to the saddle-groupoid structure on $T\mathbb{R}^n$). In the later case $M=0$ and wings in membranes Σ^M are absent.

Matrix M is assumed to be real, but if we formally take $M=iJ/2$ (i.e., $N=0$, $S=-i/2$, $K=i/2$), then the transform $U^M=\exp\{-\hbar(\partial_q^2+\partial_p^2)/4\}$ relates Weyl ordering to the Wick normal ordering choice. In this case wings are pure imaginary (see Fig. 13), and the membrane Σ^M coincides with hexagon membrane introduced in Refs. 7 and 8.

Remark 2: In the general case, block N of the matrix M controls the position of the point $q\in\mathbb{R}^n$ with respect to the middle point of the vector u in the $T\mathbb{R}^n$-groupoid interpretation. The block S controls an additional $T\mathbb{R}^n$-groupoid cocycle (in u-coordinates) which appears in the convolution formula (see Sec. IV). In contrast to that, the block K in the matrix M generates the transformation of distributions over $T\mathbb{R}^n_q$ of the following type: $\exp\{-i\hbar K\partial_q\cdot\partial_q/2\}$. This is not a point transformation. Thus the product $*^M$ corresponding to matrix M with $K\neq 0$ can not be obtained from the groupoid convolution over $T\mathbb{R}^n$ by construction of Sec. 4. In particular, the Wick product is of such type.

Now let us consider the symplectic groupoid structure on the secondary phase space $T^*(T^*\mathbb{R}^n)$ corresponding to the $*^M$ product (6.3). In the same way as in Sec. II we calculate for the Heisenberg algebra (2.5) operators of left and right representations corresponding to the ordering choice (6.2). We know the transformation from (6.2) to the Weyl ordering; it is given by operator (6.4). Thus the left operators $L^M_q=q*^M$, $L^M_{p'}=p'*^M$ and right operators $R^M_q=*^Mq$, $\mathbb{R}^M_{p'}=*^Mp'$ are given by

$$L^M=U^{-M}\cdot L'\cdot U^M,\quad R^M=U^{-M}\cdot R'\cdot U^M, \tag{6.8}$$

where L', R' are determined in (2.8). We represent L^M,R^M via their symbols l,r:

$$L^M=l(x,-i\hbar\partial_x),\quad R^M=r(x,-i\hbar\partial_x),$$

and easily calculate l, r by (6.8) and by the definition of U^M. The result is

$$l(x,y)=x+(\tfrac{1}{2}-M)J^{-1}y,\quad r(x,y)=x-(\tfrac{1}{2}+M)J^{-1}y.$$

The inverse mapping $(l,r)\to(x,y)$ is given by

$$x=\tfrac{1}{2}(l+r)+MV,\quad V\equiv l-r=J^{-1}y. \tag{6.9}$$

For example, for the ordering cases (6.7), formulas (6.9) are represented in Fig. 11.

The corresponding symplectic groupoid structure on $T^*(T^*\mathbb{R}^n)=\mathbb{R}^{2n}_x\oplus\mathbb{R}^{2n}_y$ is given by the rule represented in Fig. 14. We observe that this structure is exactly given by the membrane with wings Σ^M which we described at the beginning of this section. What is new now is that we have identified the positions of points x,x_2,x_1 exactly as vertices of wings of the membrane Σ^M.

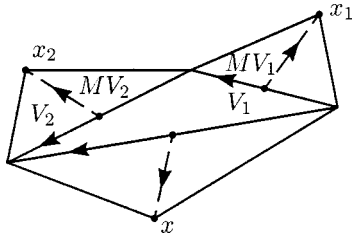

FIG. 14. M-groupoid.

Corollary 2: Let $\det(\frac{1}{2}-M)\neq 0$, *then the integral version of the product formula* (6.5) *reads*

$$(f\overset{M}{*}g)(x)=\frac{1}{(2\pi\hbar)^{2n}|\det(\frac{1}{2}-M)|}\int\int \exp\left\{\frac{i}{\hbar}\int_{\Sigma^M(x,x_2,x_1)}\omega_0\right\}f(x_2)g(x_1)dx_2dx_1, \quad (6.10)$$

where $\Sigma^M(x,x_2,x_1)$ *is the membrane with three* M*-wings having vertices* x, x_2, x_1.

Note that for the τ-ordering case (6.6) the denominator in formula (6.10) $\det(\frac{1}{2}-M)=\tau^n(1-\tau)^n$ is zero if $\tau=0$ or $\tau=1$. We see that the cases $\tau=0$ (standard ordering) and $\tau=1$ (anti-standard ordering) are special. In these cases the graph Λ_* of the groupoid multiplication (see Sec. V) is not one-to-one projected onto the "configuration space" $\mathbb{R}^{2n}_x\times\mathbb{R}^{2n}_{x_2}\times\mathbb{R}^{2n}_{x_1}$, i.e., the graph is totally caustic and the integral kernel $K_\hbar(x,x_2,x_1)$ (5.1) is not of WKB-type (5.2). This is one of essential differences between representations (6.5) and (6.10) for the $*$-product.

Corollary 3: For several multipliers there is the following product formula

$$(f_N\overset{M}{*}\cdots\overset{M}{*}f_1)(x)=\exp\left\{\frac{i}{\hbar}\int_{\Sigma^M_x(\hat{V}_N,\ldots,\hat{V}_1)}\omega_0\right\}f_N(x_N)\cdots f_1(x_1)\Big|_{x_1=\cdots=x_N=x}, \quad (6.11)$$

where $\Sigma^M_x(V_N,\ldots,V_1)$ *is the membrane with* $N+1$ *wings.*

These formulas are naturally generalized for products of differently quantized multipliers, i.e., for the case when each multiplier has its own ordering choice

$$\begin{gathered}\hat{f}_N^{M_N}\cdot\cdots\ \hat{f}_1^{M_1}=\hat{k}^{M_{N+1}},\\ k(x)=\exp\left\{\frac{i}{\hbar}\int_{\Sigma_x^{M_{N+1},\ldots,M_1}(\hat{V}_N,\ldots,\hat{V}_1)}\omega_0\right\}f_N(x_N)\cdots f_1(x_1)\Big|_{x_1=\cdots=x_N=x}.\end{gathered} \quad (6.12)$$

Here the membrane $\Sigma_x^{M_{N+1},\ldots,M_1}$ is constructed by $N+1$ wings each of different configuration determined by different matrices $M_{N+1},\ldots,M_1$.

In conclusion of this section we consider the magnetic case $F\neq 0$. For simplicity, we concentrate on the τ-ordering choice

$$\hat{f}^\tau=f(\overset{1}{\tau}\hat{q}+\overset{3}{(1-\tau)}\hat{q},\overset{2}{\hat{p}}), \quad (6.13)$$

where $\hat{q}$, $\hat{p}$ satisfy the magnetic commutation relations (1.3).

We first transform the magnetic τ-ordering to the magnetic Weyl ordering:

$$\hat{f}^\tau=(U^\tau f)(\hat{q},\hat{p}),\quad U^\tau=\exp\{(\tfrac{1}{2}-\tau)\hat{u}\partial_q\}, \quad (6.14)$$

where $\hat{u}=i\hbar\partial_p$. Then for product of two τ-ordered observables we have from (2.11)

$$\hat{f}^{\tau}\cdot\hat{g}^{\tau}=(U^{\tau}f)(\hat{q},\hat{p})\cdot(U^{\tau}g)(\hat{q},\hat{p})=(U^{\tau}f\underset{F}{\star}U^{\tau}g)(\hat{q},\hat{p}),$$

where $\star_F$ is the magnetic product (3.2), (3.5), corresponding to the Weyl ordering. Transforming back the Weyl symbol to τ-symbol by the transform $(U^{\tau})^{-1}$, we obtain the product formula

$$\hat{f}^{\tau}\cdot\hat{g}^{\tau}=\hat{k}^{\tau},$$

where

$$k\equiv f\overset{\tau}{\underset{F}{\star}}g=(U^{\tau})^{-1}(U^{\tau}f\underset{F}{\star}U^{\tau}g).$$

By formula (3.2) we calculate the new τ-magnetic product as follows

$$\begin{aligned}(f\overset{\tau}{\underset{F}{\star}}g)(q,p)=&\exp\left\{\left(\tau-\frac{1}{2}\right)\hat{u}\partial_q\right\}\left(\exp\left\{\frac{i}{\hbar}\phi(q,\hat{u}_2,\hat{u}_1)+\frac{1}{2}(\hat{u}_1\partial_{q_2}-\hat{u}_2\partial_{q_1})\right\}\right.\\&\left.\times\exp\left\{\left(\frac{1}{2}-\tau\right)(\hat{u}_1\partial_{q_1}+\hat{u}_2\partial_{q_2})\right\}f(q_2,p_2)g(q_1,p_1)\right)\Big|_{q_1=q_2=q,\ p_1=p_2=p}\\=&\exp\left\{\frac{i}{\hbar}\phi\left(q+\left(\tau-\frac{1}{2}\right)(\hat{u}_1+\hat{u}_2),\hat{u}_2,\hat{u}_1\right)+\frac{1}{2}(\hat{u}_1\partial_{q_2}-\hat{u}_2\partial_{q_1})+\left(\tau-\frac{1}{2}\right)\right.\\&\left.\times((\hat{u}_1+\hat{u}_2)(\partial_{q_1}+\partial_{q_2})-\hat{u}_1\partial_{q_1}-\hat{u}_2\partial_{q_2})\right\}f(q_2,p_2)g(q_1,p_1)\Big|_{q_1=q_2=q,\ p_1=p_2=p}.\end{aligned}\tag{6.15}$$

Note that the flux $\phi(q,u_2,u_1)$ was defined by (3.3) via the triangle $\Delta_q(u_2,u_1)$ in $\mathbb{R}^n$ with the middle point q of one of sides. Now we see that the position of the middle point $\tilde{q}$ differs from q by an additional vector $(\tau-\frac{1}{2})(u_1+u_2)$. So,

$$q=\tilde{q}+(\tfrac{1}{2}-\tau)(u_1+u_2)=\tilde{q}+(MV)_q,$$

where M is matrix (6.6) corresponding to τ-ordering, and $V=V_1+V_2$ is a vector in $\mathbb{R}^{2n}$ whose q-component is $u=u_1+u_2$.

The total phase in (6.14) is equal to the magnetic area of the membrane in $\mathbb{R}^{2n}$ constructed by the triangle with sides V_1,V_2,V_1+V_2 and by three additional wings generated by matrix M of special type (6.6). The configuration of the wings in this special case is shown in Fig. 11.

The position of the vertex of the wing is $x^{\tau}=\tilde{x}+MV$, where $\tilde{x}=(l+r)/2$. But actually this position should be changed to match the symplectic groupoid multiplication rule. To find this rule we have to calculate the operators of left and right regular representation in our τ-case. In view of (6.14) these operators are given by formulas

$$L^{\tau}=(U^{\tau})^{-1}\cdot L\cdot U^{\tau},\quad R^{\tau}=(U^{\tau})^{-1}\cdot R\cdot U^{\tau},$$

where L, R are operators (2.10), corresponding to the magnetic Weyl ordering. From (6.14) and (2.10) we obtain

$$L_q^{\tau}=q+\tau i\hbar\partial_p,\quad R_q^{\tau}=q-(1-\tau)i\hbar\partial_p,$$

$$L_p^{\tau}=p-(1-\tau)i\hbar\partial_q-A(L_q^{\tau},R_q^{\tau}),\quad R_p^{\tau}=p+\tau i\hbar\partial_q-A(R_q^{\tau},L_q^{\tau}).$$

So, if we represent these operators by symbols $L^{\tau}=l(x,-i\hbar\partial_x)$, $R^{\tau}=r(x,-i\hbar\partial_x)$, then two groupoid mappings appear

$$l:T^*\mathbb{R}^{2n}\to\mathbb{R}^{2n},\quad r:T^*\mathbb{R}^{2n}\to\mathbb{R}^{2n},$$

where

$$\begin{aligned} l(x,y)&=x+(\tfrac{1}{2}-M)J^{-1}y-(0;A(l_q,r_q)),\\ r(x,y)&=x-(\tfrac{1}{2}+M)J^{-1}y-(0;A(r_q,l_q)). \end{aligned} \tag{6.16}$$

From (6.16) we reconstruct x and y via l,r

$$x=\tfrac{1}{2}(l+r)+V_F+MV,\quad y=JV+Y_F, \tag{6.17}$$

where $V=l-r$, and vectors V_F,Y_F are given by the same formulas as in (5.9) (i.e., the same as in the case $\tau=1/2$ or $M=0$).

Relations (6.17) determine the final configuration of the *magnetic τ-wing*. Position of the vertex x of this magnetic wing is shifted by vector V_F with respect to position x^τ.

Lemma 6: The magnetic area of the magnetic τ-wing with the vertex x is equal to the magnetic area of the wing with vertex x^τ.

In view of this lemma the phase (6.15) can be represented by the area of a membrane $\Sigma_x^\tau(V_2,V_1)$ constructed by the triangle of vectors V_1,V_2,V_1+V_2, and by three magnetic τ-wings over each of these vectors. The point x is the vertex of the magnetic τ-wing over V_1+V_2.

Theorem 5: *The magnetic product corresponding to τ-ordering* (6.13) *of noncommutative coordinates $\hat q,\hat p$ is given by formula*

$$(f\underset{F}{\overset{\tau}{\star}}g)(x)=\exp\left\{\frac{i}{\hbar}\int_{\Sigma_x^\tau(\hat V_2,\hat V_1)}\omega_F\right\}f(x_2)g(x_1)\Big|_{x_1=x_2=x},$$

where Σ_x^τ is a membrane with magnetic τ-wings.

The immediate corollaries from this statement are formulas for several multipliers and also the integral formula for $\star_F^\tau$ via the magnetic area of membranes $\Sigma^\tau(x,x_2,x_1)$ supplied with magnetic τ-wings. These corollaries are formulated by the same way as (6.10)–(6.12), but with magnetic form ω_F in the exponent.

VII. DYNAMICS VIA MEMBRANE AREA

Quantum dynamics of a charged (spinless) particle in electromagnetic field can be described:

(i) in the nonrelativistic case by the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=\left[\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial q}-\frac{e}{c}\mathcal{A}\right)^2+ea\right]\psi, \tag{7.1}$$

(ii) in the relativistic case by the Klein–Gordon equation

$$\left(i\hbar\frac{\partial}{\partial t}-ea\right)^2\psi=c^2\left[\left(-i\hbar\frac{\partial}{\partial q}-\frac{e}{c}\mathcal{A}\right)^2+m^2c^2\right]\psi, \tag{7.2}$$

where $\mathcal{A}$ and a are magnetic and electric potentials of the field, and metric is assumed to be Euclidean.

First, we consider the pure magnetic time-independent situation $a=0$, $\mathcal{A}=\mathcal{A}(q)$. Let us introduce operators $\hat p=-i\hbar\partial/\partial q-(e/c)\mathcal{A}(q)$. Then the dynamical equations can be reduced to studying the evolution operator $\exp\{-itH(\hat p)/\hbar\}$, where $H(p)=p^2/2m$ in the nonrelativistic case, and $H(p)=\pm c\sqrt{p^2+m^2c^2}$ in the relativistic case.

More generally, in a presence of an additional non-Euclidean metric (gravitational field) the Hamiltonian will depend on the q-coordinate as well: $H=H(q,p)$. Say, $H\simeq g^{jk}(q)p_jp_k/2m$ in the nonrelativistic case.

So, the general problem is to study the operator

$$U^t=\exp\left\{-\frac{it}{\hbar}\hat{H}\right\},\quad \hat{H}=H(\hat{q},\hat{p}). \tag{7.3}$$

In particular, we are interested in its asymptotic behavior as $\hbar\to 0$.

Note that the symbol H and the permutation relations between quantum coordinates $\hat{q}$, $\hat{p}$ (1.3) are independent of the gauge choice of the magnetic potential $\mathcal{A}$. Thus the semiclassical approximation for U^t as $\hbar\to 0$, written in terms of the phase space symbol $H(q,p)$ and the phase space noncommutative structure (1.3), is automatically gauge invariant.

Let us represent the operator U^t in the Weyl-symmetrized form

$$U^t=\mathcal{U}^t(\hat{q},\hat{p}),$$

then for symbol $\mathcal{U}^t$ one obtains the following equations

$$i\hbar\frac{\partial\mathcal{U}^t}{\partial t}=H\underset{F}{\star}\mathcal{U}^t,\quad \mathcal{U}^0=1. \tag{7.4}$$

Using Theorem 1 we transform (7.4) to a pseudodifferential form

$$i\hbar\frac{\partial\mathcal{U}^t(x)}{\partial t}=\mathcal{H}_\hbar(x,-i\hbar\partial_x)\,\mathcal{U}^t(x),\quad \mathcal{U}^0=1. \tag{7.5}$$

Here $\mathcal{H}_\hbar(x,y)$ is the Weyl symbol of the operator $H(L_q,L_p)$, and L_q, L_p are given by (2.10). Obviously,

$$\mathcal{H}_\hbar=\mathcal{H}_0+O(\hbar^2),\quad \mathcal{H}_0\equiv H(l), \tag{7.6}$$

where l is the Weyl symbol of L, i.e., $L=l(x,-i\hbar\partial_x)$. The explicit formulas for $l=(l_q,l_p)$ are found in (5.4).

In view of (7.6) the principal term of the semiclassical solution of the Cauchy problem (7.5) is determined by the Hamilton function $\mathcal{H}_0$. For small enough time interval $t\in[0,T]$ the approximate solution has the simplest WKB-form

$$\mathcal{U}^t(x)=\exp\left\{\frac{i}{\hbar}S(t,x)\right\}u^t(x)+O(\hbar), \tag{7.7}$$

where the phase S is the solution of the Hamilton–Jacobi equation

$$\frac{\partial S}{\partial t}+\mathcal{H}_0\left(x,\frac{\partial S}{\partial x}\right)=0,\quad S|_{t=0}=0, \tag{7.8}$$

and the nonoscillatory amplitude u^t is the solution of the ''transport'' equation

$$\frac{\partial u^t}{\partial t}+\frac{\partial}{\partial x}\left(\frac{\partial\mathcal{H}_0}{\partial y}\left(x,\frac{\partial S}{\partial x}\right)u^t\right)=0,\quad u^0=1. \tag{7.9}$$

In order to solve (7.8) and (7.9) one has to consider the Hamiltonian system

$$\dot{X}=\frac{\partial\mathcal{H}_0}{\partial Y},\quad \dot{Y}=-\frac{\partial\mathcal{H}_0}{\partial X},\quad X|_{t=0}=x^0,\quad Y|_{t=0}=0, \tag{7.10}$$

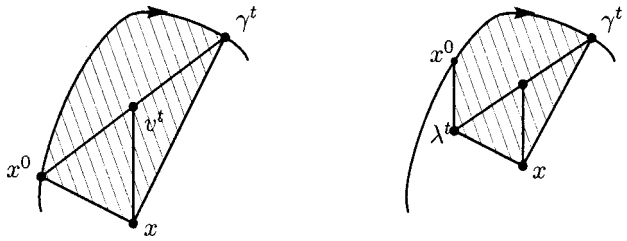

FIG. 15. Membrane Σ_x^t and trajectory of virtual particle.

and determine

$$S=\int_0^t (Y\dot{X}-\mathcal{H}_0)\,d\tilde{t},\quad u^t=\det\left(\frac{\partial X}{\partial x^0}\right)^{-1/2}, \tag{7.11}$$

where $x^0=(q^0,p^0)$ is taken from the equation

$$X(x^0,t)=x.$$

The time interval $t\in[0,T]$ over which the Jacobian $\mathcal{D}X/\mathcal{D}x^0\geqslant\delta>0$ (for any $x^0\in\mathbb{R}^{2n}$) is exactly the interval where the solution $\mathcal{U}^t$ can be represented in the WKB form (7.7).

Lemma 7: Trajectories of (7.10) *are given by formulas*

$$\begin{aligned} X(x^0,t)&=\tfrac{1}{2}(\gamma^t(x^0)+x^0)+v^t(x^0),\\ Y(x^0,t)&=J(\gamma^t(x^0)-x^0)+y^t(x^0), \end{aligned} \tag{7.12}$$

where

$$v^t=(0;\tfrac{1}{2}(A(\gamma_q^t,q^0)+A(q^0,\gamma_q^t))),\quad y^t=(A(\gamma_q^t,q^0)-A(q^0,\gamma_q^t);0),$$

and $\gamma^t=(\gamma_q^t,\gamma_p^t)$ *is the trajectory of the Hamiltonian system corresponding to the function* H *and the magnetic Poisson bracket* (3.4)

$$\begin{aligned} &\dot{\gamma}_q=\frac{\partial H}{\partial p}(\gamma_q,\gamma_p),\quad \dot{\gamma}_p=-\frac{\partial H}{\partial q}(\gamma_q,\gamma_p)-F(\gamma_q)\frac{\partial H}{\partial p}(\gamma_q,\gamma_p),\\ &\gamma|_{t=0}=x^0=(q^0,p^0). \end{aligned} \tag{7.13}$$

The proof of this lemma follows from (5.8) and from the fact that $\mathcal{H}_0=H(l)$, and so components of the mapping $r:\mathbb{R}_x^{2n}\oplus\mathbb{R}_y^{2n}\to\mathbb{R}^{2n}$ (5.4) are integrals of motion for system (7.10), i.e., $r(X,Y)=r(x^0,0)=x^0$ is constant in time.

After substitution of (7.12) into (7.11) one obtains the following result.

Theorem 6: *Let* $\hat{q}$, $\hat{p}$ *satisfy commutation relations* (1.3) *with magnetic tensor* F_{kj}, *and* $\hat{H}=H(\hat{q},\hat{p})$. *Then for small enough time* t *the semiclassical approximation for the magnetic Weyl symbol of the evolution operator* $\exp\{-(it/\hbar)\hat{H}\}=\mathcal{U}^t(\hat{q},\hat{p})$ *is given by the formula*

$$\mathcal{U}^t=\mathcal{J}^{-1/2}\exp\left\{\frac{i}{\hbar}\int_\Sigma\omega_F-\frac{it}{\hbar}H\right\}+O(\hbar). \tag{7.14}$$

Here the membrane $\Sigma=\Sigma_x^t$ (*see Fig.* 15, *left picture*) *is constructed from the piece of the Hamilton trajectory* (7.13), *which connects points* x^0 *and* $\gamma^t(x^0)$, *and from the magnetic wing with vertices* $[\gamma^t(x^0),x,x^0]$, *where*

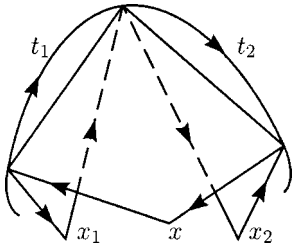

FIG. 16. Group property for membranes with wings.

$$x=\tfrac{1}{2}(\gamma^t(x^0)+x^0)+v^t(x^0). \tag{7.15}$$

Here

$$v^t(x^0)=(0;\tfrac{1}{2}(A(\gamma^t(x^0)_q,q^0)+A(q^0,\gamma^t(x^0)_q))),\quad x^0\equiv(q^0,p^0),$$

and A is the Valatin primitive (2.1). *The Jacobian* $\mathcal{J}$ *in* (7.14) *is given by*

$$\mathcal{J}(x^0,t)=\det[\tfrac{1}{2}(I+d\gamma^t(x^0))+dv^t(x^0)],\quad \mathcal{J}\geqslant\delta>0\quad for\quad t\in[0,T],$$

the Hamilton function H in (7.14) *is evaluated on the trajectory, i.e.,* $H=H(x^0)$, *and* x^0 *is assumed to be expressed in terms of* x,t *via Eq.* (7.15).

Remark 3: The group property of the family of symbols $\mathcal{U}^t$ over $\mathbb{R}^{2n}$ reads

$$\mathcal{U}^{t_2}\underset{F}{\star}\mathcal{U}^{t_1}=\mathcal{U}^{t_2+t_1}. \tag{7.16}$$

In terms of WKB-phase functions (7.14), the identity (7.16) requires that

$$\int_{\Sigma^{t_2}_{x_2}}\omega_F+\int_{\Sigma^{t_1}_{x_1}}\omega_F+\int_{\Sigma_F(x,x_2,x_1)}\omega_F=\int_{\Sigma^{t_2+t_1}_{x}}\omega_F, \tag{7.17}$$

(see Fig. 16), where $\Sigma_F(x,x_2,x_1)$ is the hexagon membrane with magnetic wings, defined at the end of Sec. V. Note that in the case $F=0$ formula (7.17) coincides with the phase addition rule obtained by Marinov.[3] In that particular case the magnetic "anomaly" v^t in (7.15) is absent and the magnetic wings of the membranes disappear.

Also note that the Hamilton function H could be time-dependent. In this case the first membrane phase factor in formula (7.14) is the same, but the second phase factor becomes $\exp\{-(i/\hbar)\int_0^t H(\tilde{\gamma}^{\tilde{t}}(x^0),\tilde{t})d\tilde{t}\}$; the trajectory γ^t is now the solution of system (7.13) with time-dependent Hamiltonian H.

Remark 4: One can use not only Weyl but any other ordering choice to represent the evolution operator as a function in coordinates $\hat{q},\hat{p}$. Then formula (7.14) still holds with membrane Σ constructed by wings corresponding to the given ordering choice (see Sec. VI); Eq. (7.15) and the Jacobian $\mathcal{J}$ are changed following (6.17). Moreover, in Ref. 34 it was proved that using and combining different orderings it is possible to avoid the difficulty with time limitations $t\in[0,T]$ where the WKB-approximation works.

For the Wick ordering choice the wings are pure imaginary (see Fig. 13) and the membrane representation (7.14) coincides with those obtained in Ref. 9. In this case the Jacobian $\mathcal{J}$ is never zero and representation (7.14) is global in t.

In conclusion of this section we apply formula (3.6) to derive the symbol $\mathcal{U}^t$ not asymptotically but in an exact continual form. Namely, one can use the approximation $\mathcal{U}^{t/N}=\exp\{-(it/\hbar N)H\}+O(N^{-2})$ and obtain the Trotter type formula

$$\mathcal{U}^t = \lim_{N\to\infty} \exp\left\{ -\frac{it}{\hbar N} H \right\} \underset{F}{\star} \cdots \underset{F}{\star} \exp\left\{ -\frac{it}{\hbar N} H \right\},$$

(N multipliers). Applying (3.6), one derives

$$\mathcal{U}^t(x) = \lim_{N\to\infty} \exp\left\{ \frac{i}{\hbar} \int_{\Sigma_x(\hat{V}_N,\ldots,\hat{V}_1)} \omega_F \right\} \exp\left\{ -\frac{it}{\hbar N} \sum_{j=1}^{N} H(x_j) \right\} \Bigg|_{x_1=\cdots=x_N=x}. \tag{7.18}$$

Now the question is how to represent this formula in a continual form.

Note that each vector field v on $\mathbb{R}^{2n}$ and any point $x\in\mathbb{R}^{2n}$, $t\in\mathbb{R}$ determines a membrane $\Sigma_x^t(v)\subset\mathbb{R}^{2n}$ whose boundary is constructed from a piece $\{\Gamma^\mu | 0\leqslant\mu\leqslant t\}$ of the trajectory of the field v in $\mathbb{R}^{2n}$ and from the magnetic wing with vertices $[\Gamma^t, x, \Gamma^0]$ (or, the magnetic τ-wing if one wants to use the general τ-ordering). The integral over the membrane in (7.18) is an approximation of the integral over $\Sigma_x^t(v)$ with a convenient choice of v.

Theorem 7: *The following continual formula for the symbol of the evolution operator* (7.3) *holds:*

$$\mathcal{U}^t(x) = \exp\left\{ \frac{i}{\hbar} \int_{\Sigma_x^t(\hat{v})} \omega_F \right\} \exp\left\{ -\frac{i}{\hbar} \int_0^t H(x(\mu))\, d\mu \right\} \Bigg|_{x(\mu)\equiv x}. \tag{7.19}$$

Here $\{x(\mu)=(q(\mu),p(\mu)) | 0\leqslant\mu\leqslant t\}$ *are continuous paths in* $\mathbb{R}^{2n}$ *and* $\hat{v}=(i\hbar\,\delta/\delta p(\mu), i\hbar\,\delta/\delta q(\mu))$ *is the variational derivative operator acting on the path functional.*

Formula (7.19) is dual to the Feynman path-integral formula.[24,50–53] The difference between (7.19) and the path integral is the same as between (3.5) and (3.7). The known Wick and Hori derivations[54,55] for the symbol of the evolution operator (see also generalizations in Ref. 56) are structurally close to (7.19), but use a different first exponential factor. The membrane exponential factor in (7.19) clearly demonstrates the influence of the magnetic form ω_F to the quantum dynamics.

VIII. ELECTROMAGNETIC FIELDS AND SPACE–TIME MEMBRANES

Let us now consider general time-dependent case, i.e., $\mathcal{A}=\mathcal{A}(t,q)$, $a=a(t,q)$ in (7.1), (7.2). We again study the Cauchy problem for the Schrödinger or Klein–Gordon equations.

As a first step one can remove the electric potential a from equations by introducing the new wave function $\psi\exp\{(ie/\hbar)\int_0^t a\,dt\}$. After such a transform the magnetic potential $\mathcal{A}$ is replaced by $\mathcal{A}+c\int_0^t(\partial a/\partial q)\,dt$, but the electromagnetic tensor F_{jk} (1.2b) remains unchanged. So, without loss of generality one can assume that

$$a\equiv 0, \quad E=-c^{-1}\partial\mathcal{A}/\partial t, \quad B=\operatorname{curl}\mathcal{A}.$$

The quantum dynamical equations have the following form:

(i) in the nonrelativistic case

$$i\hbar\frac{\partial\psi}{\partial t} = H(\hat{q},\hat{p}(t))\psi, \quad \text{where} \quad H \simeq \frac{1}{2m} g^{jk}(q) p_j p_k, \tag{8.1a}$$

(ii) in the relativistic case

$$\hbar^2\frac{\partial^2\psi}{\partial t^2} + H^2(\hat{q},\hat{p}(t))\psi = 0, \quad \text{where} \quad H^2 \simeq c^2(g^{jk}(q)p_j p_k + m^2c^2). \tag{8.1b}$$

In the latter case the metric g^{jk} is assumed to be non-negative definite; the symbols $\simeq$ in (8.1a) and (8.1b) mean that some terms of order $\hbar$, $\hbar^2$ could be added to the Hamilton function.[23,29,38,57,58]

In Eqs. (8.1) for each fixed time t the operators $\hat{p}(t)=-i\hbar\partial/\partial q-(e/c)\mathcal{A}(t,q)$ and $\hat{q}=q$ satisfy relations (1.3) with time-dependent tensor

$$F_{jk}(t,q)=\frac{e}{c}\epsilon_{kjl}B^l(t,q),\quad q\in\mathbb{R}^3,\quad j,k=1,2,3.$$

The time derivative of the operators $\hat{p}(t)$ in (8.1) is the following:

$$\frac{d}{dt}\hat{p}_j(t)=eE_j(t,q),\quad j=1,2,3. \tag{8.2}$$

So we see that the electric field is responsible for ''dynamical evolution'' of the quantum magnetic algebra (1.3).

Let us introduce two-point electric potential

$$\beta(t,q,q')\equiv\int_q^{q'}E(t,\tilde{q})d\tilde{q} \tag{8.3}$$

(the integral is taken along the straight line segment), and also the two-point magnetic potential

$$\alpha(t,q,q')\equiv\frac{1}{|q-q'|}\int_{q'}^{q}|\tilde{q}-q'|B(t,\tilde{q})\times d\tilde{q}. \tag{8.4}$$

We stress that these potentials are different from those used by Valatin[20] in the time dependent case, since in our present definitions there is no integration over the time variable. Time and space are separated because we study the Cauchy problem in time.

Lemma 8: The relation holds:

$$-\frac{\partial\beta}{\partial q}-\frac{1}{c}\frac{\partial\alpha}{\partial t}=E(t,q).$$

Now from (8.2) and from composition formulas (2.11) we obtain the following statement.

Proposition 6:

(i) *The time derivative of any Weyl-symmetrized function in quantum coordinates $\hat{q}$, $\hat{p}(t)$ is given by*

$$-i\hbar\frac{d}{dt}f(\hat{q},\hat{p}(t))=f^e(\hat{q},\hat{p}(t),t),$$

where

$$f^e(q,p,t)=e\beta(t,L_q,R_q)f(q,p),$$

and $L_q=q+\frac{1}{2}i\hbar\partial_p$, $R_q=q-\frac{1}{2}i\hbar\partial_p$ are operators of the regular representation (2.10);

(ii) *the composition of two Weyl-symmetrized functions is given by*

$$[f_2(\hat{q},\hat{p}(t))]\cdot[f_1(\hat{q},\hat{p}(t))]=k(\hat{q},\hat{p}(t)),\quad k=f_2(L_q,L_p(t))f_1,$$

where $L_p(t)=p-\frac{1}{2}i\hbar\partial_q-(e/c)\,\alpha(t,L_q,R_q)$.

The solution of the evolution problem (8.1a) has the general form

$$\psi(t,q)=\mathcal{U}^t(\hat{q},\hat{p}(t))(\psi|_{t=0}). \tag{8.5}$$

In view of Proposition 6 equations for symbol $\mathcal{U}^t$ are the following:

$$\left[-i\hbar\frac{\partial}{\partial t}+e\beta(t,L_q,R_q)+H(L_q,L_p(t))\right]\mathcal{U}^t(x)=0,\quad \mathcal{U}^0=1. \tag{8.6}$$

The operator acting on $\mathcal{U}^t$ can be represented [as in (7.5)] via a symbol $\mathcal{H}_\hbar$ over $\mathbb{R}_t\times\mathbb{R}^6_x\times\mathbb{R}^6_y$. In the same way as in (7.6) we have

$$\mathcal{H}_\hbar=\mathcal{H}_0+O(\hbar^2),\quad \mathcal{H}_0(t,x,y)=e\beta(t,l_q(x,y),r_q(x,y))+H(l_q(x,y),l_p(t,x,y)), \tag{8.7}$$

where $x=(q,p)$, $y=(y_q,y_p)$, and

$$l_q=q-\frac{1}{2}y_p,\quad r_q=q+\frac{1}{2}y_p,\quad l_p=p+\frac{1}{2}y_q-\frac{e}{c}\alpha(t,l_q,r_q).$$

[Of course, here we just re-state identities (5.4) in a new notation.] As in Sec. VII, the WKB-solution of (8.6) has the form (7.7), (7.11), where (X,Y) is now the trajectory of the Hamiltonian system

$$\dot X=\frac{\partial\mathcal{H}_0}{\partial y}(t,X,Y),\quad \dot Y=-\frac{\partial\mathcal{H}_0}{\partial x}(t,X,Y),\quad X|_{t=0}=x^0,\quad Y|_{t=0}=0. \tag{8.8}$$

The solution of problem (8.1b) with additional Cauchy data $\partial\psi/\partial t|_{t=0}=0$ can also be constructed in the form (8.5), where $\mathcal{U}^t$ satisfies the equations

$$\left[i\hbar\frac{\partial}{\partial t}-e\beta(t,L_q,R_q)\right]^2\mathcal{U}^t=H^2(L_q,L_p(t))\mathcal{U}^t,\quad \mathcal{U}^0=1,\quad \frac{\partial}{\partial t}\mathcal{U}^t|_{t=0}=0.$$

The WKB-approximation has the form

$$\mathcal{U}^t=\frac{1}{2}\sum_{\pm}\ \exp\left\{\frac{i}{\hbar}S_\pm\right\}u^t_\pm+O(\hbar), \tag{8.9}$$

where the phases $S_\pm$ and amplitudes $u^t_\pm$ correspond [by formulas (7.11)] to the Hamilton function $\mathcal{H}_0$ of type (8.7) with $\pm$ signs in the definition of H. The Hamiltonian system (8.8) again plays the basic role.

The difference in Hamiltonian system (8.8) from the earlier (7.10) is that function $\mathcal{H}_0$ in (8.8) now depends on l_q, l_p and on r_q as well. So, r_p is not an integral of motion for (8.8). Thus instead of dynamical system (7.13) we get now two systems: one for $\gamma=l(t,X,Y)$ and another for $\lambda=r(t,X,Y)$. They are the following:

$$\dot\gamma_q=\frac{\partial H}{\partial p}(\gamma_q,\gamma_p),\quad \dot\gamma_p=-\frac{\partial H}{\partial q}(\gamma_q,\gamma_p)-\frac{e}{c}B(t,\gamma_q)\times\dot\gamma_q+eE(t,\gamma_q) \tag{8.10}$$

and

$$\dot\lambda_q=0,\quad \dot\lambda_p=eE(t,\lambda_q), \tag{8.11}$$

with one and the same initial condition $\gamma|_{t=0}=\lambda|_{t=0}=x^0$.

The function $H(q,p)$ has the following form: $H(q,p)=g^{jk}(q)p_jp_k/2m$ in the nonrelativistic case and $H(q,p)=\pm c\sqrt{g^{jk}(q)p_jp_k+m^2c^2}$ in the relativistic case.

Note that (8.10) is the standard dynamical system for charged massive particle in the electromagnetic field. The additional system (8.11) can be interpreted as the dynamical system for a particle of charge e and mass $m=\infty$. The appearance of this additional ''virtual particle'' is due to the presence of the electric field E.

The phase S of the WKB-solution is given by (7.11); hence

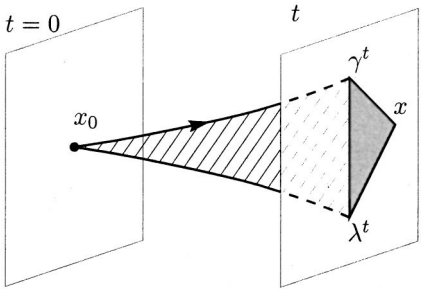

FIG. 17. Dynamical membrane $\Sigma_{t,x}$.

$$S(t,x)=\int_0^t Y\dot{X}\,d\tilde{t}-e\int_0^t \beta(\tilde{t},\gamma_q^{\tilde{t}},\lambda_q^{\tilde{t}})\,d\tilde{t}-\int_0^t H(\gamma^{\tilde{t}})\,d\tilde{t}. \tag{8.12}$$

Lemma 9: The following identity holds:

$$\int_0^t Y\dot{X}\,d\tilde{t}=\int_{\Sigma_x^t}\omega_F=\int_{\Sigma_x^t}\omega_0+\frac{e}{c}\int_{\tilde{\Sigma}_q^t}B(t,\tilde{q})\,d\tilde{q}\wedge d\tilde{q}, \tag{8.13}$$

where the membrane $\Sigma_x^t\subset\mathbb{R}^6=T^*\mathbb{R}^3$ *is constructed from the two trajectories* $\gamma=\gamma^t$ (8.10) *and* $\lambda=\lambda^t$ (8.11) *and from the magnetic wing with vertices* $[\gamma^t,x,\lambda^t]$, *where* $x=(q,p)$ (*see Fig.* 15, *right picture*). *The projection of* Σ_x^t *onto* $\mathbb{R}^3$ *is the membrane* $\tilde{\Sigma}_q^t$ *constructed by a piece of the trajectory* $\{\gamma_q^{\tilde{t}}\,|\,0\leqslant\tilde{t}\leqslant t\}$ *and by the chord* $[q^0,\gamma_q^t]$ *with middle point* q.

This is the membrane area interpretation of the first term in (8.12). The second term in view of definition (8.3) can also be written as two-dimensional area, but in extended space-time:

$$-e\int_0^t\beta\,d\tilde{t}=e\int_0^t d\tilde{t}\int_{q^0}^{\gamma_q^{\tilde{t}}}E(\tilde{t},\tilde{q})\,d\tilde{q}=e\int_{\tilde{\Sigma}_{t,q^0}}E\,dq\wedge dt. \tag{8.14}$$

Here $\tilde{\Sigma}_{t,q^0}$ is a membrane in $\mathbb{R}_t\times\mathbb{R}_q^3$ whose boundary consists of the trajectory (the world line) $\{(\tilde{t},\gamma^{\tilde{t}})\,|\,0\leqslant\tilde{t}\leqslant t\}+$ the chord $[\gamma^t,q^0]+$ the straight time-segment $\{(\tilde{t},q^0)\,|\,0\leqslant\tilde{t}\leqslant t\}$.

Now one can combine (8.13) and (8.14) and apply the Stokes theorem to transform the integration area to be of the most elegant geometry. Let us denote by $\Sigma_{t,x}$ the membrane in $\mathbb{R}_t\times\mathbb{R}_x^6$ whose boundary is constructed by the world line of the given particle $\{(\tilde{t},\gamma^{\tilde{t}})\,|\,0\leqslant\tilde{t}\leqslant t\}$, the world line of the virtual infinitely heavy particle $\{(\tilde{t},\lambda^{\tilde{t}})|0\leqslant\tilde{t}\leqslant t\}$, and also by the magnetic wing with vertices $[\lambda^t,x,\gamma^t]$ (see Fig. 17). We refer to $\Sigma_{t,x}$ as a *dynamical membrane*.

Proposition 7: The WKB-phase of symbol $\mathcal{U}^t$ *in* (8.5) *can be represented as*

$$S(t,x)=\int_{\Sigma_{t,x}}(\omega_0+F)-\int_0^t H(\gamma^{\tilde{t}})\,d\tilde{t}, \tag{8.15}$$

where $\omega_0=\frac{1}{2}Jdx\wedge dx$, *the two-form* F *is given by* (1.2b), $\Sigma_{t,x}$ *is the dynamical membrane in* $\mathbb{R}^7=\mathbb{R}_t\times\mathbb{R}_x^6$, *and* γ^t *is the solution of classical dynamical system* (8.10).

Remark 5: The closed two-form $\tilde{\omega}_F=\omega_0+F$, which appeared in (8.15), generates a contact structure on $\mathbb{R}^7=\mathbb{R}_t\times\mathbb{R}_x^6$.[59,60] The "virtual" system (8.11) is the characteristic system for $\tilde{\omega}_F$. More precisely, the vector field on $\mathbb{R}^7$ corresponding to (8.11) is

$$v_0=\frac{\partial}{\partial t}+eE(t,q)\frac{\partial}{\partial p},\quad x=(q,p).$$

This is the null-field for $\tilde{\omega}_F$

$$v_0 \rfloor \tilde{\omega}_F = 0,$$

and the flow of v_0 preserves $\tilde{\omega}_F$

$$\mathcal{L}_{v_0} \tilde{\omega}_F = 0.$$

Here we denote by $\mathcal{L}$ the Lie derivative and use the sign $\rfloor$ for the contraction of a vector field and a form: $v \rfloor \omega(u) \equiv \omega(u,v)$ for all u. If one denotes by v_H the vector field on $\mathbb{R}^7$ corresponding to (8.10)

$$v_H = \frac{\partial}{\partial t} + \frac{\partial H}{\partial p}(q,p)\frac{\partial}{\partial q} + \left(eE(t,q) - \frac{e}{c} B(t,q) \times \frac{\partial H}{\partial p}(q,p) - \frac{\partial H}{\partial q}(q,p) \right) \frac{\partial}{\partial p},$$

then

$$v_H \rfloor \tilde{\omega}_F = dH - v_0(H)\, dt, \quad \mathcal{L}_{v_H} \tilde{\omega}_F = d(v_0(H)) \wedge dt.$$

Here $v_0(H) = eE\, \partial H / \partial p$; so we see how the electric field E determines the "nonconservation" properties of the charged particle dynamics in the contact space $\mathbb{R}^7 = \mathbb{R}_t \times \mathbb{R}^6_x$.

Now let us return to the WKB-representation (7.7), (7.11) of symbol $\mathcal{U}^t$ and calculate the Jacobian $\mathcal{J} = \mathcal{D}X / \mathcal{D}x^0$. The trajectory X of system (8.9) is given now by a modification of (7.12): $X(x^0,t) = \frac{1}{2}(\gamma^t(x^0) + \lambda^t(x^0)) + v^t(x^0)$, where v^t is the same as in (7.12). Since the solution $\lambda = \lambda^t$ of (8.11) is easily calculated: $\lambda^t_q = q^0$, $\lambda^t_p = p^0 + e\int_0^t E(\tilde{t}, q^0)\, d\tilde{t}$, we derive

$$\mathcal{J} = \det\left[\frac{1}{2}(I + d\gamma^t) + \begin{pmatrix} 0 & 0 \\ C^t & D^t \end{pmatrix} \right]. \tag{8.16}$$

Here

$$C^t \equiv \frac{e}{c} \frac{\partial}{\partial q^0}(\alpha^s(t, \gamma^t_q(x^0), q^0)) + e\int_0^t \frac{\partial E(\tilde{t}, q^0)}{\partial q^0} d\tilde{t}, \quad D^t \equiv \frac{e}{c} \frac{\partial}{\partial p^0}(\alpha^s(t, \gamma^t_q(x^0), q^0)).$$

The function α^s is determined by $\alpha^s(t,q,q') \equiv \frac{1}{2}(\alpha(t,q,q') + \alpha(t,q',q))$, where the two-point magnetic potential α is given by (8.4). The point x^0 everywhere in these formulas has to be expressed via t,x by means of the equation

$$x = \tfrac{1}{2}(\gamma^t(x^0) + \lambda^t(x^0)) + v^t(x^0). \tag{8.17}$$

This equation is uniquely solvable while the Jacobian is positive

$$\mathcal{J} \geqslant \delta > 0, \quad t \in [0,T]. \tag{8.18}$$

So, we conclude with the following result.

Theorem 8: *The symbol $\mathcal{U}^t$ of the evolution operator* (8.5) *solving the equation of motion* (8.1a) *or* (8.1b) *can be represented* [*for sufficiently small time* (8.18)] *in the WKB-form* (7.7) *or* (8.9) *over the contact space $\mathbb{R}^7 = \mathbb{R}_t \times \mathbb{R}^6_x$. The phases S are given by membrane formula* (8.15) *and amplitudes $u^t = \mathcal{J}^{-1/2}$ by* (8.16).

Remark 6: Of course, the contact space $\mathbb{R}^7$ can be symplectified (see Refs. 59 and 60) up to $\mathbb{R}^8 = (\mathbb{R}_{p_0} \oplus \mathbb{R}_t) \times \mathbb{R}^6_x$ with symplectic form $\omega'_F = dp_0 \wedge dt + \tilde{\omega}_F$. The dynamical membrane $\Sigma_{t,x}$ in (8.15) can be blown up to a membrane $\Sigma'_{t,x}$ in such a way that the path γ^t is put on the level $p_0 = -H$, and the path λ^t is put on the level $p_0 = 0$; so, the summand $\int_0^t H\, d\tilde{t}$ in (8.15) is included into the membrane area, and altogether one obtains

$$S(t,x)=\int_{\Sigma'_{t,x}}\omega'_F\,.$$

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Ensemble fluctuations and the origin of quantum probabilistic rule

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We demonstrate that the origin of the so-called quantum probabilistic rule (which differs from the classical Bayes' formula by the presence of cos θ-factor) might be explained in the framework of ensemble fluctuations which are induced by preparation procedures. In particular, quantum rule for probabilities (with nontrivial cos θ-factor) could be simulated for macroscopic physical systems via preparation procedures producing ensemble fluctuations of a special form. We discuss preparation and measurement procedures which may produce probabilistic rules which are neither classical nor quantum; in particular, hyperbolic ''quantum theory.''
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I. INTRODUCTION

It is well known that the classical probabilistic rule based on the Bayes' formula for conditional probabilities cannot be applied to quantum formalism, see, e.g., Refs. 1–3 for extended discussions. In fact, all special features of quantum systems are just consequences of violations of the classical probability rule, Bayes' theorem.[1] In this paper we restrict our investigations to the two-dimensional case. Here Bayes' formula (the formula of total probability) has the form ($i=1,2$):

$$\mathbf{p}(A=a_i)=\mathbf{p}(C=c_1)\mathbf{p}(A=a_i/C=c_1)+\mathbf{p}(C=c_2)\mathbf{p}(A=a_i/C=c_2), \tag{1}$$

where A and C are physical variables which take, respectively, values a_1, a_2 and c_1, c_2. Symbols $\mathbf{p}(A=a_i/C=c_j)$ denote conditional probabilities. There is a large diversity of opinions on the origin of violations of (1) in quantum mechanics. The common opinion is that violations of (1) are induced by special (quite mysterious) features of quantum systems.

Let ϕ be a quantum state. Let $\{\phi_i\}_{i=1}^2$ be an orthogonal basis consisting of eigenvectors of the operator $\hat{C}$ corresponding to the physical observable C.

The quantum theoretical rule (derived in the Hilbert space formalism) has the form ($i=1,2$):

$$q_i=\mathbf{p}_1\mathbf{p}_{1i}+\mathbf{p}_2\mathbf{p}_{2i}\pm 2\sqrt{\mathbf{p}_1\mathbf{p}_{1i}\mathbf{p}_2\mathbf{p}_{2i}}\cos\theta, \tag{2}$$

where $q_i=\mathbf{p}_\phi(A=a_i)$, $\mathbf{p}_j=\mathbf{p}_\phi(C=c_j)$, $\mathbf{p}_{ij}=\mathbf{p}_{\phi_i}(A=a_j)$, $i,j=1,2$. Here probabilities have indexes corresponding to quantum states. The common opinion is that this quantum probabilistic rule must be considered as a peculiarity of nature. However, there exists an opposition to this general opinion, namely the probabilistic opposition. The main domain of activity of this probabilistic opposition is Bell's inequality and the EPR paradox,[4] see, e.g., Refs. 1, 5–11. The general idea supported by the probabilistic opposition is that special quantum behavior can be understood on the basis of local realism, if we are careful with the probabilistic description of physical phenomena. It seems that the origin of all ''quantum troubles'' is probabilistic rule (2). It seems that the violation of Bell's inequality is just a new representation of the old contradiction between

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rules (1) and (2) (the papers of Accardi[1] and De Muynck, De Baere, and Martens[7] contain extended discussions on this problem). Therefore, the main problem of the probabilistic justification of quantum mechanics is to find the clear probabilistic explanation of the origin of quantum probabilistic rule (2) and the violation of classical probabilistic rule (1) and explain why (2) is sometimes reduced to (1).

Accardi[5] introduced a notion of the *statistical invariant* to investigate the relation between classical Kolmogorovean and quantum probabilistic models, see also Gudder and Zanghi in Ref. 6. He was also the first who mentioned that Bayes' postulate is a ''hidden axiom of the Kolmogorovean model... which limits its applicability to the statistical description of the natural phenomena.'' [5] In fact, this investigation plays a crucial role in our analysis of classical and quantum probabilistic rules.

An interesting investigation on this problem is contained in the paper of Shummhammer.[11] He supports the idea that quantum probabilistic rule (2) is not a peculiarity of nature, but just a consequence of one special method of the probabilistic description of nature, the so-called method of *maximum predictive power*. We do not directly support the idea of Shummhammer. It seems that the origin of (2) is not only a consequence of the use of one special method for the description of nature, but merely a consequence of our manipulations with nature, ensembles of physical systems, in quantum preparation/measurement procedures.

In this paper we provide probabilistic analysis of quantum rule (2). In our analysis ''probability'' has the meaning of the *frequency probability*, namely the limit of frequencies in a long sequence of trials (or for a large statistical ensemble). Hence, in fact, we follow von Mises' approach to probability.[12] It seems that it would be impossible to find the roots of quantum rule (2) in the conventional probability framework, A. N. Kolmorogov, 1933.[13] In the conventional measure-theoretical framework probabilities are defined as sets of real numbers having some special mathematical properties. Classical rule (1) is merely a consequence of the definition of conditional probabilities. In the Kolmogorov framework to analyze the transition from (1) to (2) is to analyze the transition from one definition to another. In the frequency framework we can analyze behavior of trails which induce one or another property of probability. Our analysis shows that quantum probabilistic rule (2) can be explained on the basis of ensemble fluctuations (one of the possible sources of ensemble fluctuations is the so-called ensemble nonreproducibility, see De Baere;[7] see also Ref. 10 for the statistical variant of nonreproducibility). Such fluctuations can generate (under special conditions) the $\cos\theta$-factor in (2). Thus trigonometric fluctuations of quantum probabilities can be explained without using the wave arguments.

An unexpected consequence of our analysis is that quantum probability rule (2) is just one of the possible perturbations (by ensemble fluctuations) of classical probability rule (1). In principle, there might exist experiments which would produce perturbations of classical probabilistic rule (1) which differ from quantum probabilistic rule (2).

II. QUANTUM FORMALISM AND ENSEMBLE FLUCTUATIONS

A. Frequency probability theory

The frequency definition of probability is more or less standard in quantum theory; especially in the approach based on preparation and measurement procedures.[14,3]

Let us consider a sequence of physical systems $\pi=(\pi_1,\pi_2,\dots,\pi_N,\dots)$. Suppose that elements of π have some property, e.g., position, and this property can be described by natural numbers: $L=\{1,2,\dots,m\}$, the set of labels. Thus, for each $\pi_j\in\pi$, we have a number $x_j\in L$. So π induces a sequence

$$x=(x_1,x_2,\dots,x_N,\dots),\quad x_j\in L. \tag{3}$$

For each fixed $\alpha\in L$, we have the relative frequency $\nu_N(\alpha)=n_N(\alpha)/N$ of the appearance of α in $(x_1,x_2,\dots,x_N)$. Here $n_N(\alpha)$ is the number of elements in $(x_1,x_2,\dots,x_N)$ with $x_j=\alpha$. von Mises[12] said that x satisfies the principle of the *statistical stabilization* of relative frequencies, if, for each fixed $\alpha\in L$, there exists the limit

$$\mathbf{p}(\alpha)=\lim_{N\to\infty}\nu_N(\alpha). \tag{4}$$

This limit is said to be a probability of α.

We shall not consider the so-called principle of *randomness*, see Ref. 12 for details. This principle, despite its importance for the foundations of probability theory, is not related to our frequency analysis. We shall be interested only in the statistical stabilization of relative frequencies.

Remark 2.1 (randomness): The second von Mises' principle, randomness, was introduced to exclude from consideration deterministic sequences that satisfy the principle of statistical stabilization. For example, $x=(010101\ldots0101\ldots)$ satisfies the principle of the statistical stabilization, but, of course, it could not be considered as a random sequence. By the principle of randomness limits in (4) must be invariant with respect to selections of subsequences in (3) by using some class of so-called place selections. The notion of place selection induces numerous difficulties in von Mises theory, see, e.g., Ref. 10. In fact, the problem—to define randomness by using place selections—was not solved. Mathematicians escape this problem by using other approaches, e.g., Kolmogorov complexity or Marti–Löf tests for randomness, see, e.g., Ref. 10.

B. Preparation and measurement procedures and quantum formalism

We consider a statistical ensemble S of quantum particles described by a quantum state ϕ. This ensemble is produced by some preparation procedure $\mathcal{E}$, see, e.g., Refs. 14 and 3 for details. There are two discrete physical observables $C=c_1,c_2$ and $A=a_1,a_2$.

The total number of particles in S is equal to N. Suppose that n_i^c, $i=1,2$, particles in S would give the result $C=c_i$ and n_i^a, $i=1,2$, particles in S would give the result $A=a_i$. Suppose that, among those particles which would produce $C=c_i$, there are n_{ij}, $i,j=1,2$, particles which would give the result $A=a_j$. So

$$n_i^c=n_{i1}+n_{i2},\quad n_j^a=n_{1j}+n_{2j},\quad i,j=1,2.$$

We use the objective realist model in that both C and A are *objective properties* of a quantum particle, see Refs. 2, 3, and 10 for details. Such a viewpoint to quantum observables could be called Einstein's viewpoint. In such a model we can consider in the ensemble S subensembles $S_j(C)$ and $S_j(A),j=1,2$, of particles having properties $C=c_j$ and $A=a_j$, respectively. Set

$$S_{ij}(A,C)=S_i(C)\cap S_j(A).$$

Then n_{ij} is the number of elements in the ensemble $S_{ij}(A,C)$ (subensemble of S). We remark that the "existence" of the objective property ($C=c_i$ and $A=a_j$) need not imply the possibility to measure this property. For example, such a measurement is impossible in the case of incompatible observables. So in general ($C=c_i$ and $A=a_j$) is a kind of hidden property.

The quantum experience says that the following frequency probabilities are well defined for all observables C, A:

$$\mathbf{p}_i=\mathbf{p}_\phi(C=c_i)=\lim_{N\to\infty}\mathbf{p}_i^{(N)},\quad \mathbf{p}_i^{(N)}=\frac{n_i^c}{N}; \tag{5}$$

$$q_i=\mathbf{p}_\phi(A=a_i)=\lim_{N\to\infty}q_i^{(N)},\quad q_i^{(N)}=\frac{n_i^a}{N}. \tag{6}$$

Can we say something about the behavior of frequencies $\tilde{\mathbf{p}}_{ij}^{(N)}=n_{ij}/N$, $N\to\infty$?

In fact, not so much. Suppose that they stabilize, when $N\to\infty$. This implies that probabilities $\tilde{\mathbf{p}}_{ij}=\mathbf{p}_\phi(C=c_i,A=a_j)=\lim_{N\to\infty}\tilde{\mathbf{p}}_{ij}^{(N)}$ would be well defined. The quantum experience says that

(in general) this probability distribution could not be measured. Thus it may be the frequencies $\tilde{\mathbf{p}}_{ij}^{(N)}$ fluctuate, when $N\to\infty$. Such fluctuations can, nevertheless, produce the statistical stabilization (5), (6), see Ref. 10 for details.

Remark 2.2: The common interpretation of experimental violations of Bell's inequality is that realism cannot be used in quantum theory (at least in the local framework). However, Bell's considerations only imply that we cannot use realist models under the assumption that $\tilde{\mathbf{p}}_{ij}^{(N)}$ stabilize. The realist models with fluctuating frequencies $\tilde{\mathbf{p}}_{ij}^{(N)}$ can coexist with violations of Bell's inequality, see Ref. 10.

Let us now consider statistical ensembles T_i, $i=1,2$, of quantum particles described by the quantum states ϕ_i which are eigenstates of the operator $\hat{C}$: $\hat{C}\phi_i=c_i\phi_i$. These ensembles are produced by some preparation procedures $\mathcal{E}_i$. For instance, we can suppose that particles produced by a preparation procedure $\mathcal{E}$ for the quantum state ϕ pass through additional filters F_i, $i=1,2$. In quantum formalism we have

$$\phi=\sqrt{\mathbf{p}_1}\phi_1+\sqrt{\mathbf{p}_2}e^{i\theta}\phi_2. \tag{7}$$

In the objective realist model this representation may induce the illusion that ensembles T_i, $i=1,2$, for states ϕ_i must be identified with subensembles $S_i(C)$ of the ensemble S for the state ϕ. However, there are no physical reasons for such an identification. There are two main sources of troubles with this identification.

(a) The additional filter F_1 (and F_2) changes the properties of quantum particles. The probability distribution of the property A for the ensemble $S_1(C)=\{\pi\in S: C(\pi)=c_1\}$ [and $S_2(C)$] may differ from the corresponding probability distribution for the ensemble T_1 (and T_2) obtained by filtration. So different preparation procedures produce different distributions of properties.

(b) As we have already mentioned, frequencies $\tilde{\mathbf{p}}_{ij}^{(N)}=n_{ij}/N$ may fluctuate. Even if additional filters do not change properties of quantum particles, nonreproducibility implies that the distribution of the property A may be essentially different for statistical ensembles $S_1(C)$ and $S_2(C)$ (subensembles of S) and T_1 and T_2. Moreover, distributions may be different even for subensembles $S_1(C)$ and $S_1'(C)$ [or $S_2(C)$ and $S_2'(C)$, of two different ensembles S and S' of quantum particles prepared in the same quantum state ϕ, see Ref. 10].

Fluctuations of physical properties which could be induced by (a) or (b) will be called *ensemble fluctuations*.

Of course, principle (a) looks more attractive from the experimentalist (instrumentalists) point of view. This is the original viewpoint of Heisenberg, who paid much attention to the role of perturbations in quantum measurements. Similar ideas were presented by Bohr, who paid much attention to the role of experimental arrangement. Principle (a) implies that the transition from one context (complex of physical conditions) given by the preparation procedure $\mathcal{E}$ to other contexts given by the preparation procedures $\mathcal{E}_j$, $j=1,2$, produces statistical perturbations of properties of physical systems. Principle (a) has some relation to von Mises' principle of randomness. Filters F_j can be considered as place selections in the original ensemble S. Principle (a) is the hypothesis that we could not perform such place selection without changing properties of the physical systems.

Principle (b) looks more exotic, since we always observe the statistical stabilization of frequencies in our experiments. However, we shall also keep in mind this possibility.

Suppose that m_{ij} is the number of particles in the ensemble T_i having the objective property $A=a_j$.

The quantum experience says that the following frequency probabilities are well defined:

$$\mathbf{p}_{ij}=\mathbf{p}_{\phi_i}(A=a_j)=\lim_{N\to\infty}\mathbf{p}_{ij}^{(N)},\quad \mathbf{p}_{ij}^{(N)}=m_{ij}/n_i^c.$$

Here it is assumed that an ensemble T_i consists of n_i^c particles, $i=1,2$. It is also assumed that $n_i^c = n_i^c(N) \to \infty$, $N \to \infty$. In fact, the latter assumption holds true if both probabilities $\mathbf{p}_i$, $i=1,2$, are nonzero.

We remark that probabilities $\mathbf{p}_{ij} = \mathbf{p}_{\phi_i}(A=a_j)$ cannot be (in general) identified with conditional probabilities $\mathbf{p}_{\phi}(A=a_j/C=c_i) = \tilde{\mathbf{p}}_{ij}/\mathbf{p}_i$. As we have remarked, these probabilities are related to statistical ensembles prepared by different preparation procedures, namely by $\mathcal{E}_i$, $i=1,2$, and $\mathcal{E}$. The latter probabilities may be not exist at all, see principle (b).

Let $\{\psi_j\}_{j=1}^2$ be an orthonormal basis consisting of eigenvectors of the operator A. We can restrict our consideration to the case:

$$\phi_1 = \sqrt{\mathbf{p}_{11}}\psi_1 + e^{i\gamma_1}\sqrt{\mathbf{p}_{12}}\psi_2, \quad \phi_2 = \sqrt{\mathbf{p}_{21}}\psi_1 + e^{i\gamma_2}\sqrt{\mathbf{p}_{22}}\psi_2. \tag{8}$$

As $(\phi_1, \phi_2) = 0$, we obtain

$$\sqrt{\mathbf{p}_{11}\mathbf{p}_{21}} + e^{i(\gamma_1 - \gamma_2)}\sqrt{\mathbf{p}_{12}\mathbf{p}_{22}} = 0.$$

Hence, $\sin(\gamma_1 - \gamma_2) = 0$ (we suppose that all probabilities $\mathbf{p}_{ij} > 0$) and $\gamma_2 = \gamma_1 + \pi k$. We also have

$$\sqrt{\mathbf{p}_{11}\mathbf{p}_{21}} + \cos(\gamma_1 - \gamma_2)\sqrt{\mathbf{p}_{12}\mathbf{p}_{22}} = 0.$$

This implies that $k = 2l+1$ and $\sqrt{\mathbf{p}_{11}\mathbf{p}_{21}} = \sqrt{\mathbf{p}_{12}\mathbf{p}_{22}}$. As $\mathbf{p}_{12} = 1 - \mathbf{p}_{11}$ and $\mathbf{p}_{21} = 1 - \mathbf{p}_{22}$, we obtain that

$$\mathbf{p}_{11} = \mathbf{p}_{22}, \quad \mathbf{p}_{12} = \mathbf{p}_{21}. \tag{9}$$

These equalities are equivalent to the condition: $\mathbf{p}_{11} + \mathbf{p}_{21} = 1, \mathbf{p}_{12} + \mathbf{p}_{22} = 1$. So the matrix of probabilities $(\mathbf{p}_{ij})_{i,j=1}^2$ is the so-called *double stochastic matrix*, see, e.g., Ref. 3 for general considerations.

Thus, in fact,

$$\phi_1 = \sqrt{\mathbf{p}_{11}}\psi_1 + e^{i\gamma_1}\sqrt{\mathbf{p}_{12}}\psi_2, \quad \phi_2 = \sqrt{\mathbf{p}_{21}}\psi_1 - e^{i\gamma_1}\sqrt{\mathbf{p}_{22}}\psi_2. \tag{10}$$

So $\varphi = d_1\psi_1 + d_2\psi_2$, where

$$d_1 = \sqrt{\mathbf{p}_1\mathbf{p}_{11}} + e^{i\theta}\sqrt{\mathbf{p}_2\mathbf{p}_{21}}, \quad d_2 = e^{i\gamma_1}\sqrt{\mathbf{p}_1\mathbf{p}_{12}} - e^{i(\gamma_1+\theta)}\sqrt{\mathbf{p}_2\mathbf{p}_{22}}.$$

Thus

$$q_1 = \mathbf{p}_{\phi}(A=a_1) = |d_1|^2 = \mathbf{p}_1\mathbf{p}_{11} + \mathbf{p}_2\mathbf{p}_{21} + 2\sqrt{\mathbf{p}_1\mathbf{p}_{11}\mathbf{p}_2\mathbf{p}_{21}}\cos\theta; \tag{11}$$

$$q_2 = \mathbf{p}_{\phi}(A=a_2) = |d_2|^2 = \mathbf{p}_1\mathbf{p}_{12} + \mathbf{p}_2\mathbf{p}_{22} - 2\sqrt{\mathbf{p}_1\mathbf{p}_{12}\mathbf{p}_2\mathbf{p}_{22}}\cos\theta. \tag{12}$$

C. Probability relations connecting preparation procedures

Let us forget at the moment about the quantum theory. We consider an arbitrary preparation procedure $\mathcal{E}$ for microsystems or macrosystems. Suppose that $\mathcal{E}$ produced an ensemble S of physical systems. Let $C(=c_1, c_2)$ and $A(=a_1, a_2)$ be physical quantities which can be measured for elements $\pi \in S$. Let $\mathcal{E}_1$ and $\mathcal{E}_2$ be preparation procedures which are based on filters F_1 and F_2 corresponding, respectively, to values c_1 and c_2 of C. Denote statistical ensembles produced by these preparation procedures by symbols T_1 and T_2, respectively. Symbols N, n_i^c, n_i^a, n_{ij}, m_{ij} have the same meaning as in the previous considerations. Probabilities $\mathbf{p}_i$, $\mathbf{p}_{ij}$, q_i are defined in the same way as in the previous considerations. The only difference is that, instead of indexes corresponding to quantum states, we use indexes corresponding to statistical ensembles: $\mathbf{p}_i = \mathbf{P}_S(C=c_i)$, $q_i = \mathbf{P}_S(A=a_i)$, $\mathbf{p}_{ij} = \mathbf{P}_{T_i}(A=a_i)$.

In the classical frequency framework we obtain:

$$q_1^{(N)}=\frac{n_1^a}{N}=\frac{n_{11}}{N}+\frac{n_{21}}{N}=\frac{m_{11}}{N}+\frac{m_{21}}{N}+\frac{(n_{11}-m_{11})}{N}+\frac{(n_{21}-m_{21})}{N}.$$

But, for $i=1,2,$ we have

$$\frac{m_{1i}}{N}=\frac{m_{1i}}{n_1^c}\cdot\frac{n_1^c}{N}=\mathbf{p}_{1i}^{(N)}\mathbf{p}_1^{(N)},\quad \frac{m_{2i}}{N}=\frac{m_{2i}}{n_2^c}\cdot\frac{n_2^c}{N}=\mathbf{p}_{2i}^{(N)}\mathbf{p}_2^{(N)}.$$

Hence

$$q_i^{(N)}=\mathbf{p}_1^{(N)}\mathbf{p}_{1i}^{(N)}+\mathbf{p}_2^{(N)}\mathbf{p}_{2i}^{(N)}+\delta_i^{(N)}, \tag{13}$$

where

$$\delta_i^{(N)}=\frac{1}{N}[(n_{1i}-m_{1i})+(n_{2i}-m_{2i})],\quad i=1,2.$$

In fact, this rest term depends on the statistical ensembles $S,\ T_1,\ T_2,\ \delta_i^{(N)}=\delta_i^{(N)}(S,T_1,T_2)$.

D. Behavior of fluctuations

First we remark that $\lim_{N\to\infty}\delta_i^{(N)}$ exists for all physical measurements. This is a consequence of the property of statistical stabilization of relative frequencies for physical observables (in classical as well as in quantum physics). It may be that this property is a peculiarity of nature. It may be that this is just a property of our measurement and preparation procedures, see Ref. 10 for an extended discussion. In any case we always observe that

$$q_i^{(N)}\to q_i,\quad \mathbf{p}_i^{(N)}\to\mathbf{p}_i,\quad \mathbf{p}_{ij}^{(N)}\to\mathbf{p}_{ij},\quad N\to\infty.$$

Thus there exist limits

$$\delta_i=\lim_{N\to\infty}\delta_i^{(N)}=q_i-\mathbf{p}_1\mathbf{p}_{1i}-\mathbf{p}_2\mathbf{p}_{2i}.$$

Suppose that ensemble fluctuations produce negligibly small (with respect to N) changes in properties of particles. Then

$$\delta_i^{(N)}\to 0,\quad N\to\infty. \tag{14}$$

This asymptotic implies classical probabilistic rule (1). In particular, this rule appears in all experiments of classical physics. Hence, preparation and measurement procedures of classical physics produce ensemble fluctuations with asymptotic (14). We also have such a behavior in the case of compatible observables in quantum physics. Moreover, we can obtain the same classical probabilistic rule for incompatible observables C and A if the phase factor $\theta=\pi/2+\pi k$. Therefore classical probabilistic rule (1) is not directly related to commutativity of corresponding operators in quantum theory. It is a consequence of asymptotic (14) for ensemble fluctuations.

Suppose now that filters $F_i,\ i=1,2,$ produce relatively large (with respect to N) changes in properties of particles. Then

$$\lim_{N\to\infty}\delta_i^{(N)}=\delta_i\neq 0. \tag{15}$$

Here we obtain probabilistic rules which differ from the classical one—(1). In particular, this implies that behavior of ensemble fluctuations (15) cannot be produced in experiments of classical

physics. A rather special class of ensemble fluctuations (15) is produced in experiments of quantum physics. However, ensemble fluctuations of form (15) are not reduced to quantum fluctuations (see further considerations).

To carefully study behavior of fluctuations $\delta_i^{(N)}$, we represent them as

$$\delta_i^{(N)}=2\sqrt{\mathbf{p}_1^{(N)}\mathbf{p}_{1i}^{(N)}\mathbf{p}_2^{(N)}\mathbf{p}_{2i}^{(N)}}\lambda_i^{(N)},$$

where

$$\lambda_i^{(N)}=\frac{1}{2\sqrt{m_{1i}m_{2i}}}[(n_{1i}-m_{1i})+(n_{2i}-m_{2i})].$$

We have used the fact:

$$\mathbf{p}_1^{(N)}\mathbf{p}_{1i}^{(N)}\mathbf{p}_2^{(N)}\mathbf{p}_{2i}^{(N)}=\frac{n_1^c}{N}\cdot\frac{m_{1i}}{n_1^c}\cdot\frac{n_2^c}{N}\cdot\frac{m_{2i}}{n_2^c}=\frac{m_{1i}m_{2i}}{N^2}.$$

We have: $\delta_i=2\sqrt{\mathbf{p}_1\mathbf{p}_{1i}\mathbf{p}_2\mathbf{p}_{2i}}\lambda_i$, where the coefficients $\lambda_i=\lim_{N\to\infty}\lambda_i^{(N)}$, $i=1,2$.

In classical physics the coefficients $\lambda_i=0$. We have the same situation in quantum physics for all compatible observables as well as for some incompatible observables. In the general case in quantum physics we can only say that

$$|\lambda_i|\leqslant 1. \tag{16}$$

Hence, for quantum fluctuations, we always have

$$\left|\frac{(n_{1i}-m_{1i})+(n_{2i}-m_{2i})}{2\sqrt{m_{1i}m_{2i}}}\right|\leqslant 1,\quad N\to\infty.$$

Thus quantum ensemble fluctuations induce a relatively small (but in general nonzero!) variations of properties.

E. Fluctuations which induce the quantum probabilistic rule

Let us consider preparation procedures $\mathcal{E}$, $\mathcal{E}_j$, $j=1,2$, which have the deviations, when $N\to\infty$, of the following form ($i=1,2$):

$$\epsilon_{1i}^{(N)}=n_{1i}-m_{1i}=2\xi_{1i}^{(N)}\sqrt{m_{1i}m_{2i}}, \tag{17}$$

$$\epsilon_{2i}^{(N)}=n_{2i}-m_{2j}=2\xi_{2i}^{(N)}\sqrt{m_{1i}m_{2i}}, \tag{18}$$

where the coefficients ξ_{ij} satisfy the inequality

$$|\xi_{1i}^{(N)}+\xi_{2i}^{(N)}|\leqslant 1,\quad N\to\infty. \tag{19}$$

Suppose that $\lambda_i^{(N)}=\xi_{1i}^{(N)}+\xi_{2i}^{(N)}\to\lambda_i$, $N\to\infty$, where $|\lambda_i|\leqslant 1$. We can represent $\lambda_i^{(N)}=\cos\theta_i^{(N)}$. Then $\theta_i^{(N)}\to\theta_i, \mathrm{mod}\, 2\pi$, when $N\to\infty$. Thus $\lambda_i=\cos\theta_i$.

We obtained that

$$\delta_i=2\sqrt{\mathbf{p}_1\mathbf{p}_{1i}\mathbf{p}_2\mathbf{p}_{2i}}\cos\theta_i,\quad i=1,2. \tag{20}$$

Thus fluctuations of the form (17), (18) produce the probability rule ($i=1,2$):

$$q_i=\mathbf{p}_1\mathbf{p}_{1i}+\mathbf{p}_2\mathbf{p}_{2i}+2\sqrt{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_{1i}\mathbf{p}_{2i}}\cos\theta_i. \tag{21}$$

The usual probabilistic calculations give us

$$1=q_1+q_2=\mathbf{p}_1\mathbf{p}_{11}+\mathbf{p}_2\mathbf{p}_{21}+ +\mathbf{p}_1\mathbf{p}_{12}+\mathbf{p}_2\mathbf{p}_{22}+2\sqrt{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_{11}\mathbf{p}_{21}}\cos\theta_1+2\sqrt{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_{12}\mathbf{p}_{22}}\cos\theta_2$$
$$=1+2\sqrt{\mathbf{p}_1\mathbf{p}_2}[\sqrt{\mathbf{p}_{11}\mathbf{p}_{21}}\cos\theta_1+\sqrt{\mathbf{p}_{12}\mathbf{p}_{22}}\cos\theta_2].$$

Thus we obtain the relation

$$\sqrt{\mathbf{p}_{11}\mathbf{p}_{21}}\cos\theta_1+\sqrt{\mathbf{p}_{12}\mathbf{p}_{22}}\cos\theta_2=0. \tag{22}$$

Suppose that ensemble fluctuations (17) and (18) satisfy the additional condition

$$\lim_{N\to\infty}\mathbf{p}_{11}^{(N)}=\lim_{N\to\infty}\mathbf{p}_{22}^{(N)}. \tag{23}$$

This condition implies that the matrix of probabilities is a double stochastic matrix. Hence, we get

$$\cos\theta_1=-\cos\theta_2. \tag{24}$$

So we demonstrated that ensemble fluctuations (17) and (18) in combination with the double stochastic condition (23) produce quantum probabilistic relations (11) and (12).

It must be noticed that the existence of the limits $\lambda_i=\lim_{N\to\infty}\lambda_i^{(N)}$ does not imply the existence of limits $\xi_{1i}=\lim_{N\to\infty}\xi_{1i}^{(N)}$ and $\xi_{2i}=\lim_{N\to\infty}\xi_{2i}^{(N)}$. For example, let $\xi_{1i}^{(N)}=\lambda_i\cos^2\alpha_i^{(N)}$ and $\xi_{2i}^{(N)}=\lambda_i\sin^2\alpha_i^{(N)}$, where "phases" $\alpha_i^{(N)}$ fluctuate $\mathrm{mod}\,2\pi$. Then numbers ξ_{1i} and ξ_{2i} are not defined, but $\lim_{N\to\infty}[\xi_{1i}^{(N)}+\xi_{2i}^{(N)}]=\lambda_i$, $i=1,2$, exist.

If $\xi_{ij}^{(N)}$ stabilize, then probabilities for the simultaneous measurement of incompatible observables would be well defined:

$$\mathbf{p}(A=a_1,C=c_1)=\lim_{N\to\infty}\frac{n_{11}}{N}=\mathbf{p}_1\mathbf{p}_{11}+2\sqrt{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_{11}\mathbf{p}_{21}}\xi_{11},\ldots.$$

The quantum formalism implies that in general such probabilities do not exist.

Remark 2.3: The magnitude of fluctuations can be found experimentally. Let C and A be two physical observables. We prepare free statistical ensembles S, T_1, T_2 corresponding to states ϕ, ϕ_1, ϕ_2. By measurements of C and A for $\pi\in S$ we obtain frequencies $\mathbf{p}_1^{(N)}$, $\mathbf{p}_2^{(N)}$, $q_1^{(N)}$, $q_2^{(N)}$, by measurements of A for $\pi\in T_1$ and for $\pi\in T_2$ we obtain frequencies $\mathbf{p}_{1i}^{(N)}$. We have

$$f_i(N)=\lambda_i^{(N)}=\frac{q_i^{(N)}-\mathbf{p}_1^{(N)}\mathbf{p}_{1i}^{(N)}-\mathbf{p}_2^{(N)}\mathbf{p}_{2i}^{(N)}}{2\sqrt{\mathbf{p}_1^{(N)}\mathbf{p}_{1i}^{(N)}\mathbf{p}_2^{(N)}\mathbf{p}_{2i}^{(N)}}}.$$

It would be interesting to obtain graphs of functions $f_i(N)$ for different pairs of physical observables. Of course, we know that $\lim_{N\to\infty}f_i(N)=\pm\cos\theta$. However, it may be that such graphs can present a finer structure of quantum states.

III. ON THE MAGNITUDE OF FLUCTUATIONS WHICH PRODUCE THE CLASSICAL PROBABILISTIC RULE

We remark that the classical probabilistic rule (which is induced by ensemble fluctuations with $\xi_i^{(N)}\to 0$) can be observed for fluctuations having relatively large absolute magnitudes. For instance, let

$$\epsilon_{1i}^{(N)}=2\xi_{1i}^{(N)}\sqrt{m_{1i}},\quad \epsilon_{2i}^{(N)}=2\xi_{2i}^{(N)}\sqrt{m_{2i}},\quad i=1,2, \tag{25}$$

where sequences of coefficients $\{\xi_{1i}^{(N)}\}$ and $\{\xi_{2i}^{(N)}\}$ are bounded ($N\to\infty$). Here

$$\lambda_i^{(N)}=\frac{\xi_{1i}^{(N)}}{\sqrt{m_{2i}}}+\frac{\xi_{2i}^{(N)}}{m_{1i}}\to 0, \quad N\to\infty$$

(as usual, we assume that $\mathbf{p}_{ij}>0$).

Example 3.1: Let $N\approx 10^6$, $n_1^c\approx n_2^c\approx 5\times 10^5$, $m_{11}\approx m_{12}\approx m_{21}\approx m_{22}\approx 25\times 10^4$. So $\mathbf{p}_1=\mathbf{p}_2=1/2$; $\mathbf{p}_{11}=\mathbf{p}_{12}=\mathbf{p}_{21}=\mathbf{p}_{22}=1/2$ (symmetric state). Suppose we have fluctuations (25) with $\xi_{1i}^{(N)}\approx\xi_{2i}^{(N)}\approx 1/2$. Then $\epsilon_{1i}^{(N)}\approx\epsilon_{2i}^{(N)}\approx 500$. So $n_{ij}=24\times 10^4\pm 500$. Hence, the relative deviation $\epsilon_{ji}^{(N)}/m_{ji}=500/25\times 10^4\approx 0.002$.

Thus fluctuations of the relative magnitude $\approx 0{,}002$ produce the classical probabilistic rule.

It is evident that fluctuations of essentially larger magnitude

$$\epsilon_{1i}^{(N)}=2\xi_{1i}^{(N)}(m_{1i})^{1/2}(m_{21})^{1/\alpha}, \quad \epsilon_{2i}^{(N)}=2\xi_{2i}^{(N)}(m_{2i})^{1/2}(m_{1i})^{1/\beta}, \quad \alpha,\beta>2, \tag{26}$$

where $\{\xi_{1i}^{(N)}\}$ and $\{\xi_{2i}^{(N)}\}$ are bounded sequences ($N\to\infty$), also produce (for $\mathbf{p}_{ij}\neq 0$) the classical probability rule.

Example 3.2: Let all numbers $N,\ldots,m_{ij}$ be the same as in Example 3.1 and let deviations have behavior (26) with $\alpha=\beta=4$. Here the relative deviation $\xi_{ij}^{(N)}/mij\approx 0.045$.

IV. CLASSICAL, QUANTUM, AND "SUPERQUANTUM" PHYSICS

In this section we find relations between different classes of physical experiments. First we consider the so-called classical and quantum experiments. Classical experiments produce the classical probabilistic rule (Bayes' formula). Therefore the corresponding ensemble fluctuations have the asymptotic $\delta_i^{(N)}\to 0$, $N\to\infty$.

Nevertheless, we cannot say that classical measurements give just a subclass of quantum measurements. In the classical domain we have no symmetric relations $\mathbf{p}_{11}=\mathbf{p}_{22}$ and $\mathbf{p}_{12}=\mathbf{p}_{21}$. This is the special condition which connects the preparation procedures $\mathcal{E}_1$ and $\mathcal{E}_2$. This relation is a peculiarity of quantum preparation/measurement procedures.

Experiments with nonclassical probabilistic rules are characterized by the condition $\delta_i^{(N)}\to 0$, $N\to\infty$. Quantum experiments give only a particular class of nonclassical experiments. Quantum experiments produce ensemble fluctuations of form (17) and (18), where coefficients $\xi_{1i}^{(N)}$ and $\xi_{20}^{(N)}$ satisfy (19) and the orthogonality relation

$$\lim_{N\to\infty}(\xi_{11}^{(N)}+\xi_{21}^{(N)})+\lim_{N\to\infty}(\xi_{12}^{(N)}+\xi_{22}^{(N)})=0. \tag{27}$$

In particular, nonclassical domain contains (nonquantum) experiments which satisfy condition of boundedness (19), but do not satisfy orthogonality relation (27). Here we have only the relation of quasiorthogonality (22). In this case the matrix of probabilities is not double stochastic. The corresponding probabilistic rule has the form:

$$q_i=\mathbf{p}_1\mathbf{p}_{1i}+\mathbf{p}_2\mathbf{p}_{2i}+2\sqrt{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_{1i}\mathbf{p}_{2i}}\cos\theta_i. \tag{28}$$

Here in general $\mathbf{p}_{11}+\mathbf{p}_{21}\neq 1$, $\mathbf{p}_{12}+\mathbf{p}_{22}\neq 1$.

We remark that, in fact, (28) and (22) imply that

$$q_1=\mathbf{p}_1\mathbf{p}_{11}+\mathbf{p}_2\mathbf{p}_{21}+2\sqrt{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_{11}\mathbf{p}_{21}}\cos\theta_1;$$

$$q_2=\mathbf{p}_1\mathbf{p}_{12}+\mathbf{p}_2\mathbf{p}_{22}-2\sqrt{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_{11}\mathbf{p}_{21}}\cos\theta_1.$$

V. HYPERBOLIC "QUANTUM" FORMALISM

Let us consider ensembles S, T_1, T_2 such that ensemble fluctuations have magnitudes (17) and (18) where

$$|\xi_{1i}^{(N)}+\xi_{2i}^{(N)}|\geqslant 1+c, c>0, \quad N\to\infty. \tag{29}$$

Here the coefficients $\lambda_i=\lim_{N\to\infty}(\xi_{1i}^{(N)}+\xi_{2i}^{(N)})$ can be represented in the form $\lambda_i=\mathrm{ch}\,\theta_i$, $i=1,2$. The corresponding probability rule is the following:

$$q_i=\mathbf{p}_1\mathbf{p}_{1i}+\mathbf{p}_2\mathbf{p}_{2i}+2\sqrt{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_{1i}\mathbf{p}_{2i}}\,\mathrm{ch}\,\theta_i, \quad i=1,2.$$

The normalization $q_1+q_2=1$ gives the orthogonality relation:

$$\sqrt{\mathbf{p}_{11}\mathbf{p}_{21}}\,\mathrm{ch}\,\theta_1+\sqrt{\mathbf{p}_{12}\mathbf{p}_{22}}\,\mathrm{ch}\,\theta_2=0. \tag{30}$$

Thus

$$\mathrm{ch}\,\theta_2=-\,\mathrm{ch}\,\theta_1\sqrt{\frac{\mathbf{p}_{11}\mathbf{p}_{21}}{\mathbf{p}_{12}\mathbf{p}_{22}}}$$

and, hence,

$$q_2=\mathbf{p}_1\mathbf{p}_{12}+\mathbf{p}_2\mathbf{p}_{22}-2\sqrt{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_{11}\mathbf{p}_{21}}\,\mathrm{ch}\,\theta_1.$$

Such a formalism can be called a *hyperbolic quantum formalism*. It describes a part of nonclassical reality which is not described by ''trigonometric quantum formalism.'' Experiments (and preparation procedures $\mathcal{E}$, $\mathcal{E}_1$, $\mathcal{E}_2$) which produce hyperbolic quantum behavior could be simulated on computer. On the other hand, at the moment we have no ''natural'' physical phenomena which are described by the hyperbolic quantum formalism. ''Trigonometric quantum behavior'' corresponds to essentially better control of properties in the process of preparation than ''hyperbolic quantum behavior.'' Of course, the aim of any experimenter is to approach ''trigonometric behavior.'' However, in principle there might exist such natural phenomena that ''trigonometric quantum behavior'' could not be achieved. In any case even the possibility of computer simulation demonstrates that quantum mechanics (trigonometric) is not complete (in the sense that not all physical reality is described by the standard quantum formalism). (We can compare the hyperbolic quantum formalism with the hyperbolic geometry.)

Example 6.1: Let $\mathbf{p}_1=\alpha$, $\mathbf{p}_2=1-\alpha$, $\mathbf{p}_{11}=\cdots=\mathbf{p}_{22}=1/2$. Then

$$q_1=\tfrac{1}{2}+\sqrt{\alpha(1-\alpha)}\lambda_1, \quad q_2=\tfrac{1}{2}-\sqrt{\alpha(1-\alpha)}\lambda_1.$$

If α is sufficiently small, then λ_1 can be, in principle, larger than 1: $\lambda_1=\mathrm{ch}\,\theta$.

A kind of Hilbert space representation of the hyperbolic transformations of probabilities was proposed in Ref. 15.

VI. QUANTUM BEHAVIOR FOR MACROSCOPIC SYSTEMS

Our analysis shows that ''quantum statistical behavior'' can be demonstrated by ensembles consisting of macroscopic systems, e.g., balls having colors $C=c_1$, red, or c_2, blue, and weights $A=a_1=1$ or $a_2=2$. Suppose that additional filters F_i, $i=1,2$, produce fluctuations (17), (18), and (27). Then, instead of classical Bayes' formula (1), we obtain quantum probability rule (2).

In the context of the statistical simulation of quantum statistical behavior via fluctuations (17) and (18) [with (27)] it would be useful to note that, in fact, we can choose constant coefficients $\xi_{ij}^{(N)}=\xi_{ij}$. Moreover, we have $\xi_{11}=-\xi_{12}$ and $\xi_{21}=-\xi_{22}$. The latter is a consequence of the general relations:

$$\frac{\xi_{11}^{(N)}}{\xi_{12}^{(N)}}\to-1, \quad \frac{\xi_{22}^{(N)}}{\xi_{21}^{(N)}}\to-1, \quad N\to\infty. \tag{31}$$

Asymptotic (31) can be obtained from (17) and (18):

Proof: By (17) we have

$$(n_{11}-m_{11})+(n_{12}-m_{12})=2\xi_{11}\sqrt{m_{11}m_{21}}+2\xi_{12}\sqrt{m_{12}m_{22}}. \tag{32}$$

The left-hand side is equal to zero: $(n_{11}+n_{12})-(m_{11}+m_{12})=n_1^c-n_1^c=0$ (as the ensemble T_1 has n_1^c elements). Hence, by (23) we get

$$\xi_{11}=-\xi_{12}\sqrt{\frac{m_{12}}{m_{21}}\frac{m_{22}}{m_{11}}}\to-\xi_{12},\quad N\to\infty$$

(as $\mathbf{p}_{11}=\mathbf{p}_{22}$ and $\mathbf{p}_{12}=\mathbf{p}_{21}$). In the same way we obtain that

$$\xi_{21}=-\xi_{22}\sqrt{\frac{m_{12}}{m_{21}}\frac{m_{22}}{m_{11}}}\to-\xi_{22},\quad N\to\infty.$$

VII. CORRELATIONS BETWEEN PREPARATION PROCEDURES

In this section we study the frequency meaning of the fact that in the quantum formalism the matrix of probabilities is double stochastic. We remark that this is a consequence of orthogonality of quantum states ϕ_1 and ϕ_2 corresponding to distinct values of a physical observable C. We have

$$\frac{\mathbf{p}_{11}}{\mathbf{p}_{12}}=\frac{\mathbf{p}_{22}}{\mathbf{p}_{21}}. \tag{33}$$

Suppose that (a), see Sec. II, is the origin of quantum behavior. Hence, all quantum features are induced by the impossibility to create new ensembles T_1 and T_2 without changing properties of quantum particles. Suppose that, for example, the preparation procedure $\mathcal{E}_1$ practically destroys the property $A=a_1$ (transforms this property into the property $A=a_2$). So $\mathbf{p}_{11}=0$. As a consequence, the $\mathcal{E}_1$ makes the property $A=a_2$ dominating. So $\mathbf{p}_{12}\approx 1$. Then the preparation procedure $\mathcal{E}_2$ *must* practically destroy the property $A=a_2$ (transforms this property into the property $A=a_1$). So $\mathbf{p}_{22}\approx 0$. As a consequence, the $\mathcal{E}_2$ makes the property $A=a_1$ dominating. So $\mathbf{p}_{21}\approx 1$.

Frequency relation (23) can be represented in the following form:

$$\frac{m_{11}}{n_1^c}-\frac{m_{22}}{n_2^c}\approx 0,\quad N\to\infty. \tag{34}$$

We recall that the number of elements in the ensemble T_i is equal to n_i^c.

Thus

$$\left(\frac{n_{11}-m_{11}}{n_1^c}\right)-\left(\frac{n_{22}-m_{22}}{n_2^c}\right)\approx\frac{n_{11}}{n_1^c}-\frac{n_{22}}{n_2^c}. \tag{35}$$

This is nothing than the relation between fluctuations of property A under the transition from the ensemble S to ensembles T_1, T_2 and distribution of this property in the ensemble S.

VIII. PHYSICAL CONSEQUENCES

By using frequency probabilistic analysis of transitions from one context (complex of physical conditions, preparation procedure) to other contexts we derived general transformation of probabilities induced by such transitions. In particular, quantum interference rule (2) was obtained as a particular case of our general transformation of probabilities.

The following consequences of our investigation might be interesting for physicists.

A. Contextualism

The crucial role of context (complex of physical conditions, experimental arrangement) in experiments with elementary particles was many times (at many occasions) underlined by ''fathers'' of quantum theory (especially, Heisenberg, Bohr, Dirac, see, e.g., Refs. 16 and 17); see also later investigations of Accardi, Ballentine, De Baere, De Muynck, Gudder, Khrennikov, Pitowsky.[1,5–10,15] In particular, Heisenberg mentioned that perturbations of quantum systems induced by context transitions are responsible for the violation of the classical rule of addition of probabilities (the formula of total probability) and the appearance of the quantum rule (interference), see Ref. 16. In fact, Bohr's complementarity principle is nothing other than the philosophy of contextualism. In this paper we present quantative probabilistic measure of statistical perturbations induced by context transitions. This gives the possibility to formulate contextual ideas in the mathematical framework.

B. Wave–particle dualism

It is well known, see, e.g., the historical introduction in Dirac's book[17] or see Feynman in Ref. 18, that the wave–particle dualism was proposed to solve the contradiction between the ''classical'' and ''quantum'' rules for the addition of probabilistic alternatives. The violation of the classical rule was observed in the well-known two slit experiment (by comparing results of measurements for three different complexes of physical conditions: both slits are open, only one of the slits is open). By using the frequency probabilistic framework we obtained ''quantum interference'' without applying wave arguments. Of course, as we have mentioned in this article, we can introduce complex amplitudes of probabilities, see Ref. 15. However, this wave description is just a mathematical description, complex linearization of nonlinear transformation of probabilities. So, in principle, we could use purely corpuscular phemenology.

C. Quantumlike behavior for macrosystems

Our derivation of ''quantum interference'' was purely mathematical. The only physical constraint is that context transitions induce statistical perturbations of relatively small magnitude. In principle, such perturbations could be produced in experiments with macroscopic systems. Thus we predict the possibility to observe quantumlike interference for macroscopic objects. In particular, recent experiments of the group of Zeilinger[19] and the Boulder-group[20] can be interpreted as successful steps in this direction.

By using contextual probabilistic calculus developed in this paper we can associate complex ''wave-amplitudes'' with macroscopic objects. This approach eliminates the gap between micro- and macroworlds. In particular, well-known experiments with Bose–Einstein condensate can be interpreted as the successful step in this direction.

D. Macroscopic quantum computers

The above arguments give the possibility to create experimental situations in that macrosystems would exhibit wave behavior. This implies the possibility to create computing devices based on quantumlike calculus of probabilities and composed of macrosystems.

E. Macroscopic quantum cryptography

The same arguments imply that, in principle, there could be created quantumlike cryptographic schemes based on macrosystems.

F. Hyperbolic interference

One of the unexpected consequences of our frequency probabilistic analysis of experimental statistical data is the possibility to produce not only usual trigonometric, but also hyperbolic interference. This is the concrete experimental prediction. We hope that in the future there will be performed experiments to observe hyperbolic interference.

G. Superquantum scale

We obtained hyperbolic interference for complexes of physical conditions that produce statistical perturbations of relatively large magnitude. Here physical systems are ''supersensitive'' to perturbations produced by measurement devices. Such a behavior would be natural for physical systems having essentially higher sensitivity (to perturbations induced by our macroscopic devices) than ordinary quantum systems (elementary particles). We can talk about ''superquantum'' scale of sizes and energies. In particular, on this scale there must exist a new *hyperbolic Planck constant*. Formally such a parameter appears in the hyperbolic analogue of Schrödinger equation in hyperbolic quantum mechanics, see Ref. 15. Of course, in accordance with our general ideology, hyperbolic interference also could be produced in some experiments with macrosystems.

H. Hyperbolic quantum computing and cryptography

Hyperbolic interference could be used (in a similar way as trigonometric) to realize hyperbolic quantumlike computing and cryptographic schemes. On one hand, hyperbolic quantumlike computing and cryptographic schemes might be realized for super quantum scales. On the other hand, they might be realized for macrosystems.

I. Cognitive quantumlike models

Our probabilistic derivation of interference rules was performed in the general framework. In principle, we can use quantumlike probabilistic calculus to investigate statistical data obtained in cognitive experiments, see Ref. 21.

IX. CONCLUSION

We demonstrated that the so-called quantum probabilistic rule has a natural explanation in the framework of ensemble fluctuations induced by preparation procedures. In particular, the quantum rule for probabilities (with nontrivial $\cos\theta$-factor) could be simulated for macroscopic physical systems via preparation procedures producing the special ensemble fluctuations.

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Global minimizer for the Ginzburg-Landau functional of an inhomogeneous superconductor

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In this paper, we prove that the global minimizer of the Ginzburg-Landau functional of an inhomogeneous superconductor in an external magnetic field below the first critical field H_{c_1} is the vortexless solution. Here, H_{c_1} is defined as the value of h_{ex}, the applied field, for which the minimal energy among vortexless configurations is equal to the minimal energy among single-vortex configurations. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1428808]

I. INTRODUCTION

We are interested in describing the global minimizers of the Ginzburg-Landau functional

$$J(u,A)=\frac{1}{2}\int_{\Omega}|\nabla_A u|^2+|h-h_{ex}|^2-h_{ex}^2+\frac{\kappa^2}{2}(a(x)-|u|^2)^2 \tag{1.1}$$

that corresponds to the free energy of a superconductor in a prescribed, constant magnetic field h_{ex}. Here $\Omega\subset\mathbb{R}^2$ is the smooth, bounded, simply connected section of the superconductor and $a(x):\Omega\to\mathbb{R}$ is a given function satisfying $0<\min_{\bar{\Omega}}a(x)\leqslant a(x)\leqslant 1$ in Ω. The unknowns in Eq. (1.1) are the complex-valued order parameter $u\in H^1(\Omega,\mathbb{C})$ and the $U(1)$ connection $A\in H^1(\Omega,\mathbb{R}^2)$. Here $h=\operatorname{curl}A$ is the induced magnetic field and $\nabla_A u=\nabla u-iAu$. The order parameter u indicates the local state of the material: $|u|$ is the density of superconducting electron pairs, so that, when $|u|\simeq 1$, the material is in its superconducting state, whereas when $|u|\simeq 0$, it is in its normal state. $\kappa=1/\varepsilon>0$ is the Ginzburg-Landau parameter depending on the material.

Minimizers of $J(u,A)$ in $H^1(\Omega,\mathbb{C})\times H^1(\Omega,\mathbb{R}^2)$ solve the Euler equations

$$(G.L.)\begin{cases}-\nabla_A^2 u=\kappa^2 u(a(x)-|u|^2) & \text{in } \Omega\\ -\nabla^{\perp}h=(iu,\nabla_A u) & \text{in } \Omega\end{cases},$$

with the boundary conditions

$$\begin{aligned}h&=h_{ex} \quad \text{on } \partial\Omega\\ (\nabla u-iAu)\cdot n&=0 \quad \text{on } \partial\Omega.\end{aligned} \tag{1.2}$$

Here $\nabla^{\perp}$ denotes $(-\partial_{x_2},\partial_{x_1})$, n is the unit outer normal vector to $\partial\Omega$ and $(z,w)=Re(z\bar{w})$, where z and w are in $\mathbb{C}$.

The mathematical and physical importance of solutions is to determine the zeros of the solutions for a certain range of value of h_{ex}. The points where the the zeros of u appear, with their

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topological degrees, are called the vortices of the map u. Understanding the vortex structures in the solutions and describing the vortices as h_{ex} varies are of significance both in mathematics and in physics.

There have been many works toward dealing with such problems. The first work is due to F. Bethuel, H. Brezis, and F. Helein.[1] They discuss the functional

$$F(u)=\frac{1}{2}\int_{\Omega}|\nabla u|^2+\frac{1}{2\epsilon^2}(1-|u|^2)^2 \tag{1.3}$$

with Dirichlet boundary condition $u=g:\partial\Omega\to S^1$. They proved that minimizes of $F(u)$ in $H^1_g(\Omega,\mathbb{R}^2)$ have $|\deg(g,\partial\Omega)|$ isolated vortices of degree one and they located them by minimizing a renomalized energy. The extensions to the functional

$$F_a(u,\Omega)=\frac{1}{2}\int_{\Omega}|\nabla u|^2+\frac{1}{2\epsilon^2}(a(x)-|u|^2)^2 \tag{1.4}$$

with Dirichlet boundary conditions were made by Ding and Liu.[2] They showed that the vortices of the minimizers are located at the points where $a(x)$ takes its minimum value. Bethuel, Brezis, and Helein[3] studied the functional (1.1) with $h_{ex}=0$, $a(x)\equiv 1$ and replaced by a gauge invariant variant of the Dirichlet condition. Results similar to those in Ref. 1 are obtained. However, all the above discussions are assumed that there is a nonzero topological degree in the Dirichlet boundary conditions which implies the existence of vortices in the minimizers.

Recently numbers of works on the minimizers of $J(u,A)$ with applied fields (without imposing boundary conditions) were done by Aftalion, Sandier, and Serfaty.[4–9] As we may see, there is no *a priori* bound on the numbers of the vortices for the minimizers in $H^1\times H^1$ at this time. To overcome this difficulty, i.e., to have *a priori* control on the numbers of the vortices, Serfaty studied in Refs. 5 and 6 the local minimizers in some open subdomain of functional space of the functional

$$G(u,A)=\frac{1}{2}\int_{\Omega}|\nabla_A u|^2+|h-h_{ex}|^2-h_{ex}^2+\frac{1}{2\varepsilon^2}(1-|u|^2)^2.$$

By constructing the local minimizer, Serfaty obtained the first critical magnetic field H_{c_1} and the location of vortices. In Ref. 8, Sandier and Serfaty concluded that if $h_{ex}\leqslant H_{c_1}$, then global minimizer of $G(u,A)$ in $H^1\times H^1$ is the vortexless solution. For other discussions, refer to Refs. 7 and 9 and references therein.

We studied the local minimizers of $J(u,A)$ in D^a_M where D^a_M is defined with some suitable $M>0$ as

$$D^a_M=\{(u,A):F_a(u,\Omega)<M|\ln\varepsilon|\} \tag{1.5}$$

and the following Theorem was obtained.[10]

Theorem A: *There exist* $k_1=1/2\max_{\bar{\Omega}}|\xi_0(x)/a(x)|$, $k_2^\varepsilon=O_\varepsilon(1)$, $k_3^\varepsilon=o_\varepsilon(1)$ *and* $\varepsilon_0=\varepsilon_0(M)>0$ *such that*

$$H_{c_1}=k_1|\ln\varepsilon|+k_2^\varepsilon \tag{1.6}$$

and for $\epsilon<\epsilon_0$, *the following holds:*

(*i*) *If* $h_{ex}\leqslant H_{c_1}$, *a solution of* (*G.L.*), *that is minimizing* $J(u,A)$ *in* D^a_M *exists, and satisfies* $\frac{1}{2}\min_\Omega a(x)\leqslant|u|\leqslant 1$.

(*ii*) *If* $H_{c_1}+k_3^\varepsilon\leqslant h_{ex}\leqslant H_{c_1}+O(1)$, *a solution of* (*G.L.*) *that is minimizing* $J(u,A)$ *in* D^a_M *exists. It has a bounded positive number of vortices* a_i^ε *of degree one such that* $\mathrm{dist}(a_i^\varepsilon,\Lambda)\to 0$ *as*

$\varepsilon \to 0$, *where* $\Lambda = \{x \in \Omega : |\xi_0(x)/a(x)| = \max_\Omega |\xi_0/a|\}$, $-\mathrm{div}(1/a\,\nabla\xi_0) + \xi_0 = -1$ *in* Ω, $\xi_0 = 0$ *on* $\partial\Omega$ *and there exists a constant* $C > 0$ *such that* $\mathrm{dist}(a_i^\varepsilon, a_j^\varepsilon) \geqslant C$ *for* $i \neq j$.

In this paper, we will study the global minimizers of $J(u,A)$ in $H^1 \times H^1$ and our main result is the following theorem.

Theorem 1.1: *Let* Ω *be a smooth, bounded, simply connected domain in* $\mathbb{R}^2$. *Assume that* $a(x) \in C^2(\overline{\Omega})$ *and* $0 < b_0 = \min_{\overline{\Omega}} a(x) \leqslant a(x) \leqslant 1$ *in* Ω. *Then there exists a value* $H'_{c_1} = H_{c_1} - O(|\ln|\ln\varepsilon||)$ *such that, for any sufficiently small* ε, *if* $h_{ex} \leqslant H'_{c_1}$, *a globally minimizing solution of the functional* $J(u,A)$ *in* $H^1 \times H^1$ *satisfies* $|u| \geqslant \frac{3}{4} b_0$ on $\overline{\Omega}$ *and coincides with the solution found in (i) of Theorem A*.

The energy J that we are going to study in this paper is slightly different from the classical Ginzburg-Landau energy in the sense that there is a term penalizing the variation of the order parameter u. We denote this function by $a(x)$. The minima of $a(x)$ corresponds to the impurities in the material. In the original study by Ginzburg and Landau, $a(x) \equiv 1$. The modified functional (1.1) was first written down by Likharev.[11] Then this model has been used and developed in Refs. 4 and 12.

This paper is organized as follows. In the next section, we shall give some basic estimates. In Sec. III, we shall split the energy J. In Sec. IV, we shall prove Theorem 1.1. In Sec. V, we shall prove Lemma 2.2 which is given in Sec. II.

II. PRELIMINARY RESULTS

Consider (u,A) such that

$$J(u,A) = \min_{(v,B) \in H^1(\Omega,\mathbb{C}) \times H^1(\Omega,\mathbb{R}^2)} J(v,B),$$

then (u,A) satisfies $(G.L.)$. Recall that $J(u,A)$ is invariant under $\mathbb{U}(1)$-gauge transformations, i.e., of the type

$$v = e^{i\phi}u, \quad B = A + \nabla\phi \quad \text{for any} \quad \phi \in H^2(\Omega,\mathbb{R})$$

which make the problem non-compact. Therefore, we shall impose the gauge condition

$$\mathrm{div}(aA) = 0 \ \text{ in } \ \Omega, \quad A \cdot n = 0 \ \text{ on } \ \partial\Omega. \tag{2.1}$$

Since we assumed that Ω is simply connected, there is a function $\xi \in H^2(\Omega,\mathbb{R})$ such that

$$aA = \nabla^\perp \xi = (-\xi_{x_2}, \xi_{x_1}) \ \text{ in } \ \Omega, \quad \xi = 0 \ \text{ on } \ \partial\Omega. \tag{2.2}$$

Hence

$$h = \mathrm{curl} A = \mathrm{div}\left(\frac{1}{a}\nabla\xi\right) \quad \text{in } \ \Omega, \tag{2.3}$$

$$h = h_{ex} \quad \text{on } \ \partial\Omega, \tag{2.4}$$

$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \ \partial\Omega. \tag{2.5}$$

Now, let ξ_0 be the unique solution of the following equation:

$$-\mathrm{div}\left(\frac{1}{a}\nabla\left(\mathrm{div}\left(\frac{1}{a}\nabla\xi_0\right)\right)\right) + \mathrm{div}\left(\frac{1}{a}\nabla\xi_0\right) = 0 \quad \text{in } \ \Omega, \tag{2.6}$$

$$\operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)=0 \quad \text{on } \partial\Omega, \tag{2.7}$$

$$\xi_0=0 \quad \text{on } \partial\Omega. \tag{2.8}$$

Then, by Lemma 4.4 in Ref. 10, ξ_0 satisfies

$$-\operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)+\xi_0=-1 \quad \text{in } \Omega, \tag{2.9}$$

$$\xi_0=0 \quad \text{on } \partial\Omega. \tag{2.10}$$

Denote

$$J_0=-\frac{1}{2}h_{ex}^2\int_\Omega\left|\operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)\right|^2+\frac{1}{a}|\nabla\xi_0|^2, \tag{2.11}$$

and decompose ξ as in Ref. 10 such that

$$\xi=h_{ex}\xi_0+\zeta. \tag{2.12}$$

Then $\zeta=0$ and $\operatorname{div}((1/a)\nabla\zeta)=0$ on $\partial\Omega$. From now on, we shall assume that

$$h_{ex}\leqslant C|\ln\varepsilon|. \tag{2.13}$$

Lemma 2.1: Let (u,A) *be a solution of* $(G.L.)$ *with gauge condition* (2.1). *Then the following holds:*

$$\|\nabla u\|_{L^\infty(\Omega)}\leqslant\frac{C}{\varepsilon}, \quad \|u\|_{L^\infty(\Omega)}\leqslant 1, \tag{2.14}$$

$$\|\nabla\xi\|_{L^\infty(\Omega)}\leqslant Ch_{ex}. \tag{2.15}$$

Moreover, if (u,A) *is a minimizer of the energy* J, *then*

$$J(u,A)\leqslant J_0+\frac{1}{2}\int_\Omega|\nabla\sqrt{a}|^2\leqslant Ch_{ex}^2, \tag{2.16}$$

$$\|\nabla u\|_{L^2(\Omega)}\leqslant Ch_{ex}. \tag{2.17}$$

Proof: Equations (2.14)–(2.16) have been proven in Ref. 10. Now, we shall show Eq. (2.17). By using Eq. (2.16), we have

$$\int_\Omega|\nabla_A u|^2\leqslant Ch_{ex}^2.$$

Noting

$$\int_\Omega|\nabla_A u|^2=\int_\Omega|\nabla u|^2-\frac{1}{a}(iu,\xi_{x_2}u_{x_1}-\xi_{x_1}u_{x_2})+|u|^2|A|^2\leqslant Ch_{ex}^2,$$

we see that

$$\int_\Omega |\nabla u|^2 \leqslant Ch_{ex}^2 + C\|\nabla \xi\|_{L^\infty(\Omega)} \cdot \|\nabla u\|_{L^2(\Omega)} \leqslant Ch_{ex}^2 + C\|\nabla \xi\|_{L^\infty(\Omega)}^2 + \frac{1}{2}\int_\Omega |\nabla u|^2. \quad (2.18)$$

Then, by using Eq. (2.15) in Eq. (2.18), we get

$$\int_\Omega |\nabla u|^2 \leqslant Ch_{ex}^2, \quad (2.19)$$

which is the relation (2.17). □

Lemma 2.2: Let $u \in H^1(\Omega,\mathbb{C})$ be such that $\|\nabla u\|_{L^\infty(\Omega)} \leqslant C/\varepsilon$, and $F_a(u,\Omega) \leqslant Ch_{ex}^2$. Then, for any $\alpha > 2$, there is an $\varepsilon_0 > 0$ such that $\forall\, \varepsilon < \varepsilon_0$ there exists a finite family of disjoint balls $\{B_i\}_{i\in I} = \{B(a_i, r_i)\}_{i\in I}$ such that

$$\{x : |u(x)| < \tfrac{3}{4} b_0\} \subset \cup_{i\in I} B_i, \quad (2.20)$$

$$F_a(u, B_i) \geqslant \pi a(a_i)|d_i|(|\ln \varepsilon| - O(|\ln|\ln \varepsilon||)), \quad (2.21)$$

where $d_i = deg(u, \partial B_i)$ if $\overline{B_i} \subset \Omega$, and $d_i = 0$ otherwise. Moreover

$$r_i \leqslant C|\ln \varepsilon|^{-\alpha}, \quad (2.22)$$

$$\text{Card } I \leqslant Ch_{ex}^2. \quad (2.23)$$

Proof: The proof of this Lemma is postponed to Sec. V. □

III. SPLITTING OF THE ENERGY $J(u,A)$

Denote $\tilde{\Omega} = \Omega \backslash \cup_{i\in I} B_i$, where $\{B_i\}_{i\in I}$ is the family of balls defined in Lemma 2.2 with $\alpha > 5$, then we have the following Lemmas.

Lemma 3.1: We have

$$\frac{1}{2}\int_\Omega |\nabla_A u|^2 = \frac{1}{2}\int_\Omega \left|\nabla u - \frac{i}{a}\nabla^\perp \zeta\ u\right|^2 + \frac{1}{2}h_{ex}^2 \int_\Omega \frac{1}{a}|\nabla \xi_0|^2 + h_{ex}\int_\Omega \frac{1}{a}\nabla \xi_0 \nabla \zeta + 2\pi h_{ex}\sum_{i\in I} d_i \xi_0(a_i) + o(1). \quad (3.1)$$

Proof: We divide the proof into three steps.

Step 1: In this step, we show that

$$\begin{aligned} |\nabla u - iAu|^2 &= \left|\nabla u - \frac{i}{a}h_{ex}\nabla^\perp \xi_0 u - \frac{i}{a}\nabla^\perp \zeta\ u\right|^2 \\ &= \left|\nabla u - \frac{i}{a}\nabla^\perp \zeta\ u\right|^2 + \frac{1}{a^2}h_{ex}^2|u|^2|\nabla \xi_0|^2 + 2\left(\nabla u - \frac{i}{a}\nabla^\perp \zeta u, -\frac{i}{a}h_{ex}\nabla^\perp \xi_0 u\right) \\ &= \left|\nabla u - \frac{i}{a}\nabla^\perp \zeta u\right|^2 + \frac{1}{a^2}h_{ex}^2|u|^2|\nabla \xi_0|^2 + 2h_{ex}\left(\nabla u,\ -\frac{i}{a}\nabla^\perp \xi_0 u\right) \\ &\quad + \frac{2}{a^2}h_{ex}|u|^2 \nabla \xi_0 \nabla \zeta. \end{aligned} \quad (3.2)$$

Step 2: If $\alpha > 5$, we claim that

$$\int_\Omega \left(\nabla u, -\frac{i}{a} h_{ex} \nabla^\perp \xi_0 u \right) = 2\pi h_{ex} \sum_{i \in I} d_i \xi_0(a_i) + o(1). \tag{3.3}$$

In order to prove Eq. (3.3), by using Eqs. (2.13), (2.17), (2.22), and (2.23), we first have

$$\left| \int_{\cup B_i} \left(\nabla u, -\frac{i}{a} h_{ex} \nabla^\perp \xi_0 u \right) \right| \leqslant C(\mathrm{Card} I) h_{ex} \|\nabla u\|_{L^2(\Omega)} \max_{i \in I} r_i \leqslant C |\ln \varepsilon|^{4-\alpha}. \tag{3.4}$$

On the other hand,

$$\int_{\tilde{\Omega}} \left(\nabla u, -\frac{i}{a} h_{ex} \nabla^\perp \xi_0 u \right) = h_{ex} \int_{\tilde{\Omega}} \frac{1}{a} (iu, (\xi_0)_{x_2} u_{x_1} - (\xi_0)_{x_1} u_{x_2}). \tag{3.5}$$

By the change of variables $v = u/|u|$, $\eta = |u|$ and integrating by parts of the integral term on the right-hand side of Eq. (3.5), we obtain

$$\begin{aligned} \int_{\tilde{\Omega}} \frac{1}{a} (iu, (\xi_0)_{x_2} u_{x_1} - (\xi_0)_{x_1} u_{x_2}) &= \int_{\tilde{\Omega}} \frac{1}{a} \eta^2 (iv, dv \wedge d\xi_0) + \int_{\tilde{\Omega}} \frac{1}{a} \eta ((\xi_0)_{x_2} \eta_{x_1} - (\xi_0)_{x_1} \eta_{x_2}) (iv, v) \\ &= \int_{\tilde{\Omega}} (iv, (\xi_0)_{x_2} v_{x_1} - (\xi_0)_{x_1} v_{x_2}) + \int_{\tilde{\Omega}} \frac{1}{a} (\eta^2 - a)(iv, (\xi_0)_{x_2} v_{x_1} \\ &\quad - (\xi_0)_{x_1} v_{x_2}) = C + D. \end{aligned} \tag{3.6}$$

But since

$$C = \int_{\tilde{\Omega}} (iv, (\xi_0)_{x_2} v_{x_1} - (\xi_0)_{x_1} v_{x_2}) = \int_{\tilde{\Omega}} (iv, dv \wedge d\xi_0) = \sum_{i \in I} \int_{\partial B_i} \xi_0 \left(iv, \frac{\partial v}{\partial \tau} \right), \tag{3.7}$$

$$D \leqslant C \left(\int_\Omega (a - \eta^2)^2 \right)^{1/2} \|\nabla v\|_{L^2(\tilde{\Omega})} \|\nabla \xi_0\|_{L^\infty} = o(|\ln \varepsilon|^{-1}), \tag{3.8}$$

we can rewrite Eq. (3.6) as

$$\int_{\tilde{\Omega}} \frac{1}{a} (iu, (\xi_0)_{x_2} u_{x_1} - (\xi_0)_{x_1} u_{x_2}) = \sum_{i \in I} \int_{\partial B_i} \xi_0 \left(iv, \frac{\partial v}{\partial \tau} \right) + o(|\ln \varepsilon|^{-1}). \tag{3.9}$$

Now, denote $\mathcal{J} = \{i \in I : \overline{B_i} \subset \Omega\}$ and let $U_i = \{x \in B_i : |u| \leqslant \frac{1}{2} b_0\}$ $\forall\, i \in \mathcal{J}$. Then, by noting U_i does not intersect ∂B_i and by using Stokes' theorem, we get

$$\begin{aligned} &\left| \int_{\partial B_i} (\xi_0 - \xi_0(a_i)) \left(iv, \frac{\partial v}{\partial \tau} \right) - \int_{\partial U_i} (\xi_0 - \xi_0(a_i)) \left(iv, \frac{\partial v}{\partial \tau} \right) \right| \\ &\quad = \left| \int_{B_i \setminus U_i} d\xi_0 \wedge (iv, dv) \right| \leqslant C \|\nabla \xi_0\|_{L^\infty} r_i \left(\int_{B_i \setminus U_i} |\nabla v|^2 \right)^{1/2} \leqslant C |\ln \varepsilon|^{-\alpha}. \end{aligned} \tag{3.10}$$

Hence,

$$h_{ex} \int_{\partial B_i} (\xi_0 - \xi_0(a_i))(iv, dv) = h_{ex} \int_{\partial U_i} (\xi_0 - \xi_0(a_i))(iv, dv) + o(|\ln \varepsilon|^{-2}). \tag{3.11}$$

On the other hand, in the case that $\alpha \geqslant 5$, we have

$$h_{ex}\left|\int_{\partial U_i}(\xi_0-\xi_0(a_i))(iv,dv)\right|=h_{ex}\left|\int_{\partial U_i}(\xi_0-\xi_0(a_i))\frac{(iu,du)}{|u|^2}\right|$$
$$=\frac{4}{b_0^2}\left|\int_{\partial U_i}(\xi_0-\xi_0(a_i))(iu,du)\right|$$
$$=\frac{4}{b_0^2}\left|\int_{U_i}d\xi_0\wedge(iu,du)+(\xi_0-\xi_0(a_i))(idu,du)\right|$$
$$\leqslant Ch_{ex}r_i\|\nabla u\|_{L^2}+Ch_{ex}r_i\|\nabla\xi_0\|_{L^\infty}\int_\Omega|\nabla u|^2$$
$$\leqslant C|\ln\varepsilon|^{3-\alpha}\leqslant o(|\ln\varepsilon|^{-2}). \tag{3.12}$$

Thus, from Eqs. (3.10)–(3.12), we get

$$h_{ex}\int_{\partial B_i}\xi_0\left(iv,\frac{\partial v}{\partial\tau}\right)=2\pi h_{ex}d_i\xi_0(a_i)+o(|\ln\varepsilon|^{-2}). \tag{3.13}$$

Now, $\forall\, i\in I\backslash\mathcal{J}$, letting $U_i=B_i\cap\{|u|\leqslant\frac{1}{2}b_0\}$ and noting that $\xi_0=0$ on $\partial\Omega$, we have

$$h_{ex}\int_{\partial B_i\cap\Omega}\xi_0(iv,dv)=h_{ex}\int_{\partial U_i\cap\Omega}\xi_0(iv,dv)+o(|\ln\varepsilon|^{-2})$$
$$=\frac{4}{b_0^2}\left|\int_{U_i\cap\Omega}d\xi_0\wedge(iu,du)+\xi_0(idu,du)\right|+o(|\ln\varepsilon|^{-2})=o(|\ln\varepsilon|^{-2}). \tag{3.14}$$

Therefore, combining Eqs. (3.4), (3.5), (3.9), (3.13), and (3.14) and noting Card $I\leqslant Ch_{ex}^2$, the claim (3.3) is proved.

Step 3: From Eqs. (3.2) and (3.3), we obtain

$$\frac{1}{2}\int_\Omega|\nabla_A u|^2=\frac{1}{2}\int_\Omega\left|\nabla u-\frac{i}{a}\nabla^\perp\zeta\ \ u\right|^2+\frac{1}{2}h_{ex}^2\int_\Omega\frac{1}{a^2}|u|^2|\nabla\xi_0|^2+h_{ex}\int_\Omega\frac{1}{a^2}|u|^2\nabla\xi_0\nabla\zeta$$
$$+2\pi h_{ex}\sum_{i\in I}d_i\xi_0(a_i)+o(1). \tag{3.15}$$

But we know that

$$\frac{1}{\varepsilon^2}\int_\Omega(a(x)-|u|^2)^2\leqslant Ch_{ex}^2,$$

and thus we get

$$h_{ex}^2\int_\Omega\frac{1}{a^2}|a-|u|^2||\nabla\xi_0|^2\leqslant Ch_{ex}^2\left(\int_\Omega(a-|u|^2)^2\right)^{1/2}\leqslant C\varepsilon h_{ex}^3\leqslant o(1). \tag{3.16}$$

With the same manipulations, we also have

$$h_{ex}\left|\int_\Omega(a-|u|^2)\nabla\xi_0\nabla\zeta\right|\leqslant C\varepsilon h_{ex}^3\leqslant o(1). \tag{3.17}$$

Hence, combining Eqs. (3.15) with (3.16) and (3.17), we obtain Eqs. (3.1) and thus the proof of Lemma 3.1 is completed. □

Lemma 3.2: We have

$$\frac{1}{2}\int_\Omega (|h-h_{ex}|^2-h_{ex}^2)+\frac{1}{2}h_{ex}^2\int_\Omega \frac{1}{a}|\nabla\xi_0|^2+h_{ex}\int_\Omega \frac{1}{a}\nabla\xi_0\nabla\zeta = J_0+\int_\Omega \left|\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)\right|^2. \tag{3.18}$$

Proof: First, consider

$$\begin{aligned}\int_\Omega |h-h_{ex}|^2-h_{ex}^2 &= \int_\Omega h^2-2hh_{ex}\\ &= \int_\Omega \left|h_{ex}\operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)+\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)\right|^2-2h_{ex}\left(h_{ex}\operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)+\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)\right)\\ &= h_{ex}^2\int_\Omega \left|\operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)\right|^2+\int_\Omega \left|\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)\right|^2-2h_{ex}^2\int_\Omega \operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)\\ &\quad +2h_{ex}\int_\Omega \operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)-2h_{ex}\int_\Omega \operatorname{div}\left(\frac{1}{a}\nabla\zeta\right).\end{aligned} \tag{3.19}$$

But we know that

$$\int_\Omega \frac{1}{a}|\nabla\xi_0|^2+\left|\operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)\right|^2=\int_\Omega \operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)$$

and

$$\int_\Omega \frac{1}{a}\nabla\zeta\nabla\xi_0+\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)\operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)=\int_\Omega \left(\operatorname{div}\frac{1}{a}\nabla\zeta\right).$$

Therefore

$$\begin{aligned}&\frac{1}{2}\int_\Omega (|h-h_{ex}|^2-h_{ex}^2)+\frac{1}{2}h_{ex}^2\int_\Omega \frac{1}{a}|\nabla\xi_0|^2+h_{ex}\int_\Omega \frac{1}{a}\nabla\xi_0\nabla\zeta\\ &\quad =-\frac{1}{2}h_{ex}^2\int_\Omega \frac{1}{a}|\nabla\xi_0|^2+\left|\operatorname{div}\left(\frac{1}{a}\nabla\xi_0\right)\right|^2+\left|\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)\right|^2\\ &\quad =J_0+\int_\Omega \left|\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)\right|^2.\end{aligned}$$

Thus the proof of Lemma 3.2 is completed. □

Lemma 3.3: We have

$$\frac{1}{2}\int_\Omega \left|\nabla u-\frac{i}{a}u\nabla^\perp\zeta\right|^2+\frac{1}{2\varepsilon^2}(a-|u|^2)^2\geqslant\sum_{i\in I} F_a(u,B_i)+o(1). \tag{3.20}$$

Proof: We know the fact that

$$\frac{1}{2}\int_\Omega \left|\nabla u-\frac{i}{a}u\nabla^\perp\zeta\right|^2\geqslant\int_{\cup_{i\in I}B_i}\left|\nabla u-\frac{i}{a}u\nabla^\perp\zeta\right|^2=\int_{\cup_{i\in I}B_i}|\nabla u|^2+\frac{1}{a^2}|u\nabla^\perp\zeta|^2-\frac{2}{a}(\nabla u,\ iu\nabla^\perp\zeta).$$

But when $\alpha>5$,

$$\left|\int_{\cup_{i\in I}B_i}\left(\nabla u,\ \frac{i}{a}u\nabla^{\perp}\zeta\right)\right|\leqslant C(\mathrm{Card}I)\|\nabla\zeta\|_{L^{\infty}}\|\nabla u\|_{L^2}\max_{i\in I}r_i\leqslant C|\ln\varepsilon|^{4-\alpha}=o(1).$$

Hence,

$$\frac{1}{2}\int_{\Omega}\left|\nabla u-\frac{i}{a}u\nabla^{\perp}\zeta\right|^2\geqslant\frac{1}{2}\sum_{i\in I}\int_{B_i}|\nabla u|^2+o(1).$$

Now, if we add the term $1/\varepsilon^2(a-|u|^2)^2$ to both sides of the above inequality, we have

$$\frac{1}{2}\int_{\Omega}\left|\nabla u-\frac{i}{a}u\nabla^{\perp}\zeta\right|^2+\frac{1}{\varepsilon^2}(a-|u|^2)^2\geqslant\sum_{i\in I}F_a(u,B_i).$$

This completes the proof of Lemma 3.3. □

IV. PROOF OF THEOREM 1.1

Let $(u_\varepsilon,A_\varepsilon)$ be the minimizing solution, then it follows from Lemmas 3.1 and 3.2 that

$$J(u_\varepsilon,A_\varepsilon)=\frac{1}{2}\int_{\Omega}\left|\nabla u_\varepsilon-\frac{i}{a}u_\varepsilon\nabla^{\perp}\zeta\right|^2+\frac{1}{2\varepsilon^2}(a-|u_\varepsilon|^2)^2+\int_{\Omega}\left|\mathrm{div}\left(\frac{1}{a}\nabla\zeta\right)\right|^2+J_0$$

$$+2\pi h_{ex}\sum_{i\in I}d_i\xi_0(a_i)+o(1) \tag{4.1}$$

Then, by using Lemma 3.3 and Eq. (2.21), we get from Eq. (4.1)

$$J(u_\varepsilon,A_\varepsilon)\geqslant J_0+2\pi h_{ex}\sum_{i\in I}d_i\xi_0(a_i)+\pi\sum_{i\in I}a(a_i)|d_i|(|\ln\varepsilon|-O(|\ln|\ln\varepsilon\|)). \tag{4.2}$$

On the other hand, we have by minimality

$$J(u_\varepsilon,A_\varepsilon)\leqslant J\left(\sqrt{a},\frac{1}{a}\nabla^{\perp}\xi_0\right)=J_0+\frac{1}{2}\int_{\Omega}|\nabla\sqrt{a}|^2. \tag{4.3}$$

Thus, combining Eqs. (4.2) and (4.3) and noting $\xi_0<0$, we obtain

$$\begin{aligned}\pi\sum_{i\in I}a(a_i)|d_i|(|\ln\varepsilon|-O(|\ln|\ln\varepsilon||))&\leqslant 2\pi h_{ex}\sum_{i\in I}|d_i||\xi_0(a_i)|\\&\leqslant 2\pi h_{ex}\sum_{i\in I}|d_i|a(a_i)\left|\frac{\xi_0(a_i)}{a(a_i)}\right|\\&\leqslant 2\pi h_{ex}\left(\sum_{i\in I}|d_i|a(a_i)\right)\max\left|\frac{\xi_0(a_i)}{a(a_i)}\right|.\end{aligned}$$

Now, if $\Sigma_{i\in I}|d_i|\neq 0$, then $\Sigma_{i\in I}|d_i|a(a_i)\neq 0$ and thus

$$h_{ex}\geqslant\frac{1}{2\max|\xi_0/a|}(|\ln\varepsilon|-O(|\ln|\ln\varepsilon\|))=H'_{c_1}.$$

But since $H_{c_1}=1/2\max|\xi_0/a|\,|\ln\varepsilon|+O(1)$, we see that

$$H'_{c_1}=H_{c_1}-O(|\ln|\ln\varepsilon||). \tag{4.4}$$

Moreover, we deduce that $d_i=0$, $\forall\, i\in I$ if $h_{ex}<H'_{c_1}$ and hence we can reduce Eq. (4.1) to

$$J(u_\varepsilon,A_\varepsilon)=\frac{1}{2}\int_\Omega\left|\nabla u_\varepsilon-\frac{i}{a}u_\varepsilon\nabla^\perp\zeta\right|^2+\frac{1}{2\varepsilon^2}(a-|u_\varepsilon|^2)^2+\int_\Omega\left|\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)\right|^2+J_0+o(1). \tag{4.5}$$

Here, noting that

$$\int_\Omega\left|\nabla u_\varepsilon-\frac{i}{a}u_\varepsilon\nabla^\perp\zeta\right|^2=\int_\Omega|\nabla u_\varepsilon|^2+\frac{1}{a^2}|u_\varepsilon|^2|\nabla^\perp\zeta|^2+\frac{1}{a}(iu_\varepsilon,\zeta_{x_2}(u_\varepsilon)_{x_1}-\zeta_{x_1}(u_\varepsilon)_{x_2}), \tag{4.6}$$

and with the same manipulations as in Step 2 of the Lemma 3.1, the third term on the right-hand side of Eq. (4.6) becomes

$$\int_\Omega\frac{1}{a}(iu_\varepsilon,\zeta_{x_2}(u_\varepsilon)_{x_1}-\zeta_{x_1}(u_\varepsilon)_{x_2})=2\pi\sum_{i\in I}d_i\zeta(a_i)+o(1)=o(1), \tag{4.7}$$

we obtain from Eq. (4.5)

$$\begin{aligned}J(u_\varepsilon,A_\varepsilon)&=\frac{1}{2}\int_\Omega|\nabla u_\varepsilon|^2+\frac{1}{2\varepsilon^2}(a-|u_\varepsilon|^2)^2+\frac{1}{a}|u_\varepsilon|^2|\nabla^\perp\zeta|^2+\int_\Omega\left|\operatorname{div}\left(\frac{1}{a}\nabla\zeta\right)\right|^2+J_0+o(1)\\&\geqslant F_a(u_\varepsilon,\Omega)+J_0+o(1).\end{aligned} \tag{4.8}$$

On the other hand, we also have by minimality that

$$J(u_\varepsilon,A_\varepsilon)\leqslant J_0+\frac{1}{2}\int_\Omega|\nabla\sqrt{a}|^2,$$

and thus

$$F_a(u_\varepsilon,\Omega)\leqslant\frac{1}{2}\int_\Omega|\nabla\sqrt{a}|^2+o(1). \tag{4.9}$$

Now, we claim that

$$\frac{1}{2}\int_\Omega|\nabla u_\varepsilon|^2\to\frac{1}{2}\int_\Omega|\nabla\sqrt{a}|^2\quad\text{as}\quad\varepsilon\to0. \tag{4.10}$$

In fact, for any given sequence $\varepsilon_n\to0$ as $n\to\infty$, we see by Eq. (4.9) that there exists a subsequence (still denote $\{\varepsilon_n\}_{n=1}^\infty$) $\varepsilon_n\to0$ as $n\to\infty$, and $u_0\in H^1(\Omega,\mathbb{C})$ such that $u_{\varepsilon_n}\to u_0$ weakly in $H^1(\Omega,\mathbb{C})$. Thus, we have from Eq. (4.9) that

$$\int_\Omega(a-|u_{\varepsilon_n}|^2)^2\leqslant C\varepsilon_n,$$

and hence $|u_0|=\sqrt{a}$ a.e. in Ω. On the one hand, we have

$$\int_\Omega|\nabla u_0|^2\leqslant\liminf_{n\to\infty}\int_\Omega|\nabla u_{\varepsilon_n}|^2\leqslant\int_\Omega|\nabla\sqrt{a}|^2,$$

and on the other hand, we get by direct calculation,

$$\int_\Omega |\nabla u_0|^2 \geqslant \int_\Omega |\nabla |u_0||^2 = \int_\Omega |\nabla \sqrt{a}|^2,$$

so that the following equality holds:

$$\int_\Omega |\nabla u_0|^2 = \int_\Omega |\nabla \sqrt{a}|^2. \tag{4.11}$$

Combining Eqs. (4.9) and (4.11), we have

$$\int_\Omega |\nabla u_{\varepsilon_n}|^2 \leqslant \int_\Omega |\nabla u_0|^2 + o(1).$$

Hence, as $n \to \infty$,

$$\begin{aligned}\int_\Omega |\nabla u_{\varepsilon_n} - \nabla u_0|^2 &= \int_\Omega |\nabla u_{\varepsilon_n}|^2 + |\nabla u_0|^2 - \nabla \overline{u}_{\varepsilon_n} \nabla u_0 - \nabla u_{\varepsilon_n} \nabla \overline{u_0} \\ &\leqslant 2 \int_\Omega |\nabla u_0|^2 - \nabla \overline{u}_{\varepsilon_n} \nabla u_0 - \nabla u_{\varepsilon_n} \nabla \overline{u}_0 + o(1) = o(1). \end{aligned} \tag{4.12}$$

Therefore, $u_{\varepsilon_n} \to u_0$ strongly in $H^1(\Omega, \mathbb{C})$ and thus

$$\int_\Omega |\nabla u_{\varepsilon_n}|^2 \to \int_\Omega |\nabla \sqrt{a}|^2, \tag{4.13}$$

which is the proof of our claim (4.10). Combining now Eqs. (4.9) with (4.10), we also have

$$\frac{1}{2\varepsilon^2} \int_\Omega (a - |u_\varepsilon|^2)^2 \to 0 \quad \text{as} \quad \varepsilon \to 0, \tag{4.14}$$

from which we conclude that $|u_\varepsilon(x)| \geqslant \frac{3}{4} b_0$ in Ω. In fact, as $|\nabla u_\varepsilon| \leqslant C/\varepsilon$, if $|u_\varepsilon(x_0)| < \frac{3}{4} b_0$, then there exist constants λ, $\mu > 0$ such that $\forall\, \varepsilon > 0$,

$$\frac{1}{\varepsilon^2} \int_{B(x_0, \lambda\varepsilon)} (a - |u_\varepsilon|^2)^2 \geqslant \mu > 0, \tag{4.15}$$

which contradicts Eq. (4.14). Hence, u is the vortexless solution. Since u is the vortexless solution, we may re-use the computation of Ref. 10 to find that

$$J(u, A) = J_0 + F_a(u, \Omega) + \tilde{V}(\zeta) + o(1),$$

where $\tilde{V}(\zeta) \geqslant 0$. Hence $F_a(u, \Omega) \leqslant \frac{1}{2} \int_\Omega |\nabla \sqrt{a}|^2 + o(1)$, and by the definition of D_M^a, we have $(u, A) \in D_M^a$. This proves that for $h_{ex} < H'_{c_1}$, a globally minimizing solution $(u_\varepsilon, A_\varepsilon)$ for the functional $J(u, A)$ coincides with the solution found in (i) of Theorem A. Hence, the Theorem 1.1 is proved.

V. PROOF OF LEMMA 2.2

In this section, the methods in Refs. 13 and 5 are used to prove Lemma 2.2. We also need the Lemmas 5.3, 5.4, and 5.5. In order to prove those Lemmas, we need the following two lemmas.[8]

Lemma 5.1: Let $u : S_t \to \mathbb{C}$, *where* S_t *is a circle of radius* t *in* $\mathbb{R}^2$ *such that* $t > \varepsilon$. *Let* $m = \min\{\min_{S_t} |u|, 1\}$. *If* $m \neq 0$, $d = \deg(u, S_t)$. *If* $m = 0$, *let* $d = 0$. *Then*

$$\int_{S_t}\frac{1}{2}|\nabla u|^2+\frac{a(x)}{4\varepsilon^2}(1-|u|^2)^2\geqslant m^2\frac{\pi d^2}{t}+\frac{C_1(1-m)^{C_1}}{\varepsilon}, \tag{5.1}$$

where C_1 is an absolute constant.

Lemma 5.2: If $u:\Omega\to\mathbb{C}$, there exist $\rho(\Omega)$ and $C(\Omega)>0$ such that $\forall\, x\in\Omega$, $\forall\varepsilon<r<\rho$, letting $m=\min_{S_r\cap\Omega}|u|$,

$$\int_{S_r}\frac{1}{2}|\nabla u|^2+\frac{1}{4\varepsilon^2}(1-|u|^2)^2\geqslant\frac{(1-m)^C}{C\varepsilon}. \tag{5.2}$$

Lemma 5.3: Let $u:\Omega\to\mathbb{C}$ be such that $|\nabla u|<C/\varepsilon$. Then there exist disjoint balls $B_1,\cdots,B_k$ with radii r_i such that $\forall\, 1\leqslant i\leqslant k$,

$$(i)\quad r_i>\varepsilon,$$

$$(ii)\quad \left\{|u|<\frac{3b_0}{4}\right\}\subset\cup_i B_i \ \text{ and } B_i\cap\left\{|u|<\frac{3b_0}{4}\right\}\neq\varnothing,$$

$$(iii)\quad F_a(u,B_i\cap\Omega)\geqslant\frac{C_2 r_i}{\varepsilon}, \tag{5.3}$$

where C_2 is a constant.

Proof: We divide this proof into four steps.

Step 1: Let $S_1,\cdots,S_k$ be the connected components of $\{|u|<4b_0/5\}$ that intersect $\{|u|<3b_0/4\}$ and $x_1\in S_1,\cdots,x_k\in S_k$ be points such that $|u(x_i)|<3b_0/4$. For every i, define $r_i=\sup\{r>0:\partial B(x_i,r)\cap\{|u|<4b_0/5\}\neq\varnothing\}$, then

$$F_a(u,B(x_i,r_i)\cap\Omega)\geqslant\frac{C_2 r_i}{\varepsilon}. \tag{5.4}$$

Indeed, if $r_i\leqslant 2\varepsilon$, since $|\nabla u|\leqslant C/\varepsilon$, we have

$$F_a(u,B(x_i,r_i)\cap\Omega)\geqslant\frac{1}{\varepsilon^2}\int_{B(x_i,r_i)\cap\Omega}(a(x)-|u|^2)^2\geqslant C\geqslant\frac{C}{2}\,\frac{r_i}{\varepsilon},$$

and the conclusion (5.4) is true. If $r_i>2\varepsilon$, by the definition of r_i, we have that $\forall\, t\in[\varepsilon,t_i]$, $\min_{\partial B(x_i,t)}|u|<4b_0/5$. Now, let $v=\sqrt{u}/\sqrt{a}$, then by Lemma 5.2, $\forall\, t\in[\varepsilon,r_i]$, we have

$$\int_{\partial B(x_i,t)\cap\Omega}\frac{1}{2}|\nabla v|^2+\frac{1}{4\varepsilon^2}(1-|v|^2)^2\geqslant\frac{C}{\varepsilon}.$$

Thus, if $\varepsilon\leqslant\varepsilon_0$ as long as ε_0 is small enough, we get from the above equation that

$$\begin{aligned}F_a(u,\partial B(x_i,t)\cap\Omega)&=\int_{\Omega\cap\partial B(x_i,t)}\frac{1}{2}|\sqrt{a}\nabla v+v\nabla\sqrt{a}|^2+\frac{a^2}{4\varepsilon^2}(1-|v|^2)^2\\&\geqslant\frac{1}{2}\int_{\Omega\cap\partial B(x_i,t)}a\left[|\nabla v|^2+\frac{a}{2\varepsilon^2}(1-|v|^2)^2\right]-C|v||\nabla v|\\&\geqslant\frac{1}{2}b_0\int_{\Omega\cap\partial B(x_i,t)}|\nabla v|^2+\frac{b_0}{2\varepsilon^2}(1-|v|^2)^2-C-\frac{b_0}{4}\int_{\Omega\cap\partial B(x_i,t)}|\nabla v|^2\end{aligned}$$

$$\geqslant \frac{1}{4} b_0 \int_{\Omega \cap \partial B(x_i,t)} |\nabla v|^2 + \frac{b_0}{2\varepsilon^2}(1-|v|^2)^2 - C \geqslant \frac{C}{\varepsilon} - C \geqslant \frac{C}{\varepsilon}$$

Hence

$$F_a(u,\Omega \cap B(x_i,r_i)) \geqslant \int_{\varepsilon}^{r_i} F_a(u,\partial B(x_i,t)\cap\Omega)\,\mathrm{d}t \geqslant \frac{C}{\varepsilon}(r_i-\varepsilon) \geqslant \frac{Cr_i}{\varepsilon}.$$

The conclusion (5.4) is true in this case.

Step 2: We write B_i for $B(x_i,r_i)$ for the simplicity of our notation. Then, we claim that $\forall\, i \neq j$, either $B_j \subset B_i$ (in this case, we drop B_j) or $x_j \notin B_i$. In fact, assume that $x_j \in B_i$. By the definition of balls B_i, $\partial B_i \cap \cup_l S_l = \varnothing$, thus

$$S_j = (S_j \cap \overline{B_i^C}) \cup (S_l \cap B_i).$$

Since $x_j \in B_i$, $S_j \cap B_i \neq \varnothing$, using the connectedness of S_j, $S_j \subset B_i$, and we can drop B_j. The claim is proved.

Step 3: Dropping the unnecessary balls, we reduce to balls B_i such that $\cup_i S_i \subset \cup_k B_k$ and $\forall\, i \neq j$, $x_j \notin B_i$. It follows from the Besicovitch covering Lemma, any $x \in \cup B_i$ belongs to at most N of the balls, where N is an absolute constant.

Step 4: The rest of the proof of Lemma 5.3 is the same argument as the Lemma III.4 in Ref. 8. The proof of Lemma 5.3 is completed. □

Lemma 5.4: $\forall\, \alpha > 2$, $|\ln\varepsilon|^{-\alpha} > r > s > \varepsilon$, *if* $B_r(b)$ *and* $B_s(b)$ *are two concentric balls with respective radii* r *and* s, *and if* $u: B_r \backslash \overline{B}_s \to \mathbb{C}$ *is such that* $F_a(u, B_r \backslash \overline{B}_s) \leqslant C|\ln\varepsilon|^2$, $|u| > \frac{3}{4} b_0$, $d = \deg(u, \partial B_r)$, *then*

$$F_a(u, B_r \backslash \overline{B}_s) \geqslant a(b)|d| \left(\Lambda_\varepsilon\left(\frac{r}{|d|}\right) - \Lambda_\varepsilon\left(\frac{s}{|d|}\right)\right) + o(1), \tag{5.5}$$

where Λ_ε *is a function that satisfies the following properties:*

(*i*) $\Lambda_\varepsilon(s)/s$ *is decreasing on* $\mathbb{R}^+$,

(*ii*) $\sup_{s\in\mathbb{R}^+} \Lambda_\varepsilon(s)/s \leqslant C_2/\varepsilon$,

(*iii*) *there exist* $\varepsilon_0, t_0 > 0$ *such that if* $\varepsilon < \varepsilon_0$ *and* $\varepsilon < t < t_0$ *then* $|\Lambda_\varepsilon(t) - \pi \ln t/\varepsilon| \leqslant C$.

Proof: Let $v: S_t \to \mathbb{C}$ and $m = \min\{\min_{s_t}|u|, 1\}$ then by Lemma 5.1, we have

$$\begin{aligned}
\int_{S_t} \frac{1}{2}|\nabla v|^2 + \frac{a(x)}{4\varepsilon^2}(1-|v|^2)^2 &\geqslant m^2 \frac{\pi d^2}{t} + \frac{C_1(1-m)^{C_1}}{\varepsilon} \\
&\geqslant (m^{C'}) \frac{\pi|d|}{t} + \frac{C_1(1-m)^{C'}}{\varepsilon} \\
&\geqslant \min_{m\in[0,1]} \left\{ (m^{C'}) \frac{\pi|d|}{t} + \frac{C_1(1-m)^{C'}}{\varepsilon} \right\} = \frac{\tilde{a}\tilde{b}}{(\tilde{a}^q + \tilde{b}^q)^{1/q}},
\end{aligned}$$

where $C' = \max(2, C_1) \geqslant 2$, $\tilde{a} = \pi|d|/t$ and $\tilde{b} = C_1/\varepsilon$. Denote $f_\varepsilon(s) = \tilde{a}\tilde{b}/(\tilde{a}^q + \tilde{b}^q)^{1/q}$, $\tilde{a}(s) = \pi/s$, $\tilde{b}(s) = C_1/\varepsilon$, $\lambda_\varepsilon(s) = \min\{f_\varepsilon(s), C_1/\varepsilon\}$ and $\Lambda_\varepsilon(t) = \int_0^t \lambda_\varepsilon(s)\mathrm{d}s$, respectively. Here C_1 is defined in Lemma 5.1. Then Λ_ε satisfies properties (i), (ii) and (iii) of this lemma.

Now we prove (5.5). Let $\alpha > 2$, $|\ln\varepsilon|^{-\alpha} > r > s > \varepsilon$ and $u = \sqrt{a}v$, then

$$F_a(u,B_r)-F_a(u,B_s)\geqslant\int_r^s F_a(u,S_t)\mathrm{d}t=\frac{1}{2}\int_r^s\int_{S_t}\left[|\nabla u|^2+\frac{1}{2\varepsilon^2}(a-|u|^2)^2\right]\mathrm{d}\omega_t\ \mathrm{d}t$$
$$\geqslant\frac{1}{2}\int_r^s\int_{S_t}a\left[|\nabla v|^2+\frac{1}{2\varepsilon^2}(1-|v|^2)^2\right]-C|\nabla v|.$$

Noting that

$$\int_r^s\int_{S_t}|\nabla v|\leqslant|B_r\setminus B_s|\left(\int_{B_r\setminus B_s}|\nabla v|^2\right)^{1/2}\leqslant C|\ln\varepsilon|^{-2\alpha}|\ln\varepsilon|=o(1),$$

we have

$$F_a(u,B_r)-F_a(u,B_s)\geqslant\frac{1}{2}a(b)\int_r^s\int_{S_t}|\nabla v|^2+\frac{a}{2\varepsilon^2}(1-|v|^2)^2-C\int_r^s\int_{S_t}t\left[|\nabla v|^2+\frac{a}{2\varepsilon^2}(1-|v|^2)^2\right]$$
$$+o(1)\geqslant\frac{1}{2}a(b)\int_r^s\int_{S_t}|\nabla v|^2+\frac{a}{2\varepsilon^2}(1-|v|^2)^2-C|\ln\varepsilon|^{-\alpha+2}+o(1)$$
$$\geqslant\frac{1}{2}a(b)\int_r^s\int_{S_t}|\nabla v|^2+\frac{a}{2\varepsilon^2}(1-|v|^2)^2+o(1).$$

Hence,

$$F_a(u,B_r)-F_a(u,B_s)\geqslant\frac{1}{2}a(b)\int_r^s\int_{S_t}|\nabla v|^2+\frac{a}{2\varepsilon^2}(1-|v|^2)^2+o(1)$$
$$\geqslant a(b)\int_r^s\lambda_\varepsilon\left(\frac{t}{|d|}\right)\mathrm{d}t\geqslant a(b)\ \ |d|\left(\Lambda_\varepsilon\left(\frac{r}{|d|}\right)-\Lambda_\varepsilon\left(\frac{s}{|d|}\right)\right)+o(1),$$

and the proof of Lemma 5.4 is completed. □

Lemma 5.5: Let $u:\Omega\to\mathbb{C}$ *be such that* $|\nabla u|\leqslant C/\varepsilon$; *and* $\{B_i\}_i$ *be a family of balls of radii* r_i *satisfying the results of Lemma 5.3. Define*

$$d_i=\begin{cases}\deg(u,\partial B_i) & \text{if } \overline{B_i}\subset\Omega\\ 0 \quad \text{otherwise}\end{cases}. \tag{5.6}$$

Denote $s_0=\min_{\{i:d_i\neq0\}}r_i/|d_i|$. *Then, for every* $|\ln\varepsilon|^3\geqslant s\geqslant s_0$, *there exists a family* $B(s)$ *of disjoint balls* $B_1(s),\cdots,B_{k(s)}(s)$ *of radii* $r_i(s)$ *such that*

(*i*) *the family of balls is monotone, i.e., if* $s<t$ *then* $\cup_iB_i(s)\subset\cup_iB_i(t)$,

(*ii*) *for every* i, $F_a(u,B_i(s))\geqslant a(a_i)r_i(s)\,(\Lambda_\varepsilon(s)/s)$, *where* Λ_ε *is defined in Lemma 5.4,* $B_i(s)=B_i(a_i,r_i(s))$,

(*iii*) *if* $\overline{B_i}(s)\subset\Omega$ *and* $d_i(s)=\deg(u,\partial B_i(s))$, *then* $r_i(s)\geqslant s|d_i(s)|$.

Proof: This proof is exactly the same as Proposition III.1 in Ref. 8. □

Proof of Lemma 2.2: In order to apply Lemma 5.5 we first need to check s_0. From the assertion (iii) of Lemma 5.3, we have $C_1r_i<\varepsilon F_a(u,B_i\cap\Omega)\leqslant C\varepsilon|\ln\varepsilon|^2$, note that $s_0=\min_{\{i:d_i\neq0\}}r_i/|d_i|$. So, $s_0\leqslant C\varepsilon|\ln\varepsilon|^2$. We can apply Lemma 5.5 for all $s\geqslant C\varepsilon|\ln\varepsilon|^2$. We choose

$$s_1=\frac{1}{|\ln\varepsilon|^{\alpha+1}}. \tag{5.7}$$

It follows from Lemma 5.5 that final family of balls $B(s_1)$ such that if $\overline{B_i}(s_1)\subset\Omega$ for every i,

$$F_a(u,B_i(s_1)) \geqslant a(a_i)\frac{\Lambda_\varepsilon(s_1)}{s_1} r_i(s_i) \tag{5.8}$$

with $r_i(s_1) \geqslant s_1|d_i(s_1)|$. Therefore $F_a(u,B_i(s_1)) \geqslant a(a_i)\Lambda_\varepsilon(s_1)|d_i(s_1)|$, where $B_i(s_1) = B_i(a_i, r_i(s_1))$, and by Lemma 5.4

$$F_a(u,B_i(s_1)) \geqslant a(a_i)|d_i(s_1)|\left(\pi \ln\frac{s_1}{\varepsilon} - C\right) \geqslant \pi a(a_i)|d_i(s_1)|(|\ln\varepsilon| - O(|\ln|\ln\varepsilon||),$$

thus Eq. (2.21) is proved. By Eq. (5.8), we have

$$r_i(s_1)\frac{\Lambda_\varepsilon(s_1)}{s_1} \leqslant C|\ln\varepsilon|^2.$$

From Lemma 5.4, we know that $\Lambda_\varepsilon(s) \simeq \pi \ln s/\varepsilon$, note that Eq. (5.5),

$$\Lambda_\varepsilon(s_1) \geqslant \pi|\ln\varepsilon| - O(|\ln|\ln\varepsilon||).$$

Hence

$$r_i(s_1) \leqslant C\frac{s_1}{\Lambda_\varepsilon(s_1)}|\ln\varepsilon|^2 \leqslant \frac{C}{|\ln\varepsilon|^{\alpha+1}} \cdot \frac{|\ln\varepsilon|^2}{|\ln\varepsilon|} \leqslant \frac{C}{|\ln\varepsilon|^{\alpha}}$$

which is conclusion (2.22). From Lemma 5.3, $F_a(u,B_i \cap \Omega) \geqslant C_2 r_i/\varepsilon$ with $r_i > \varepsilon$, so, $F_a(u,B_i \cap \Omega) \geqslant C_2$. Since $F_a(u,\Omega) \leqslant C|\ln\varepsilon|^2$, we see that the number of balls there has to be bounded by $C|\ln\varepsilon|^2$. Thus, we have shown (2.23) and the proof of Lemma 2.2 is completed. □

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A spectral quadruple for de Sitter space

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A set of data supposed to give possible axioms for spacetimes with a sufficient number of isometries in spectral geometry is given. These data are shown to be sufficient to obtain $1+1$ dimensional de Sitter spacetime. The data rely at the moment somewhat on the guidance given by a required symmetry, in part to allow explicit calculations in a specific model. The framework applies also to the noncommutative case. Finite spectral triples are discussed as an example. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1420744]

I. INTRODUCTION

Spacetime is the fairy tale of a classical manifold. It is irreconcilable with quantum effects in gravity and most likely, in a strict sense, it does not exist. But to dismiss a mythical being that has inspired generations just because it does not really exist is foolish. Rather it should be understood together with the story tellers through whom and in whom the being exists.

The story tellers of spacetime are the physical fields. It is the interaction with fields that lets one believe that there was a spacetime in which particles of a field have propagated.

Here, the fairy tale of classical spacetime will be uncritically retold again: no quantum effects will be considered and the result will be an ordinary manifold of Lorentzian signature. And yet it is not at all the same old story: the story tellers, the fields are put into the place they deserve—at the center of the matter.

The right framework to allow the fields to play their distinguished role is noncommutative geometry, in particular the notion of a spectral triple.[1–3] A spectral triple $(A,\mathcal{H},D,J,\gamma)$ consists of a pre-C^*-algebra A represented (faithfully) on a Hilbert space $\mathcal{H}$, an unbounded self-adjoint operator D on $\mathcal{H}$, an antiunitary operator J and of a grading operator γ on $\mathcal{H}$. These structures satisfy a set of seven conditions given in Ref. 3.

(1) **Classical dimension.** The inverse D^{-1} of D is an infinitesimal of order $1/n$. Here, n is the dimension of the space.
(2) **First order condition.** For any a in the algebra A and b in the opposite algebra (represented with the help of J),
$$[[D,a],b^{\mathrm{op}}]=0. \tag{1}$$
(3) **Regularity.** The elements a of the algebra A as well as their commutators $[D,a]$ with D are smooth vectors of the derivation $[|D|,\bullet]$.
(4) **Orientability.** There exists the image γ of a Hochschild cycle in degree n such that for n even
$$\gamma=\gamma^*, \quad \gamma^2=\mathbf{1}, \quad \gamma D=-D\gamma, \tag{2}$$
and for n odd
$$\gamma=\mathbf{1}. \tag{3}$$
(5) **Finiteness.** The subspace of smooth Hilbert space vectors $\mathcal{H}_\infty$ is a finite projective module over A with a local Hermitean structure.
(6) **Poincaré duality.** The intersection form $K_\bullet\times K_\bullet\to\mathbb{Z}$ on the K-theory $K_\bullet$ is invertible.

(7) **Reality.** J satisfies

$$J^2=(-1)^{[(n-1)n(n+1)(n+2)]/8}, \quad JD=(-1)^{[n(n+1)(n+2)]/12}DJ, \tag{4}$$

and for n even

$$J\gamma=(-1)^{n/2}\gamma J. \tag{5}$$

If the algebra A is commutative then in a rather deep sense the spectral triple is more or less the same as a spin manifold M with positive definite metric[3] that can be recovered (for a proof see Refs. 4 and 5) in the following way: the algebra A is the algebra of functions on the spin manifold, $\mathcal{H}$ is the Hilbert space of square-integrable sections of the spinor bundle over M, D is the Dirac operator, C is the charge conjugation, and γ is the volume element. All spin manifolds with positive definite metric can be obtained in this way. A generalization covering the orientable Riemannian case without a spin structure was recently given by Lord.[6]

The possibility of choosing a noncommutative algebra A even allows to go beyond ordinary manifolds.

However, this description is not directly applicable to spin manifolds with Lorentzian signature. One problem seems to be that in this case the canonical inner product on spinor fields is not positive definite.

A way to deal with this is to foliate spacetime with spacelike leaves and to describe the Euclidean geometry of the leaves as above. Under the assumption that the spinor fields satisfy the Dirac equation, spinor fields on different leaves belonging to the same solution can be identified.[7] Then the algebras $A(t)$ for different leaves are represented on the same Hilbert space and their causal relationships may be tested by examination of their commutators. This can be exploited to obtain considerable information on the geometry and render further structures typical for Hamiltonian approaches, e.g., the lapse and the shift superfluous.[8]

The Hilbert space $\mathcal{H}$ has in this picture a clear physical interpretation as the phase space of a spinor field. An interpretation of the algebras $A(t)$ was suggested in Ref. 9 and will be scrutinized in future work.

However, previous results did not show how to obtain meaningful spectral information nor what axioms to start with in order to get interesting spacetime geometries. As a first step in this direction, the definition of a spectral quadruple, a set of data that aspires to take the place of such axioms is given. The spectral quadruple is called so because, compared to the spectral triple, a key structure (the time vector) is added. The spectral quadruple is to be understood as a working hypothesis rather than as a fixed concept. Nevertheless, in specific examples, the data of the spectral quadruple are strongly suggested and turn out to be sufficient to reconstruct spacetime. In particular, $1+1$-dimensional de Sitter space is worked out in great detail, based on the realization that postulated symmetries allow to completely carry out explicit calculations. Such an undertaking is not easy even in the Riemannian case[10] where a set of conditions as reviewed above is available. The example of de Sitter space provides at the same time a model against which any set of axioms may be tested.

This paper is structured as follows: Practical calculations to extract the spacetime geometry of a globally hyperbolic spin manifold out of commutators[11] and the generators of evolution (Hamiltonians) are reviewed in Sec. II. These motivate the definition of a spectral quadruple in Sec. III. This definition is to provide definiteness rather than definitiveness and is to be understood as a working hypothesis. In Sec. IV, the representation theory of the relevant symmetry group, $\mathrm{SL}_2(\mathbb{R})$ is reviewed. The spacetime of the postulated spectral quadruple is calculated in Sec. V. A discrete spectral quadruple is discussed as a further example in Sec. VI. The Conclusion contains a discussion of the obtained results and of possibilities for further investigations. A collection of calculations and formulas for $1+1$ de Sitter spacetime, that might be useful for other purposes also, is contained in the Appendix.

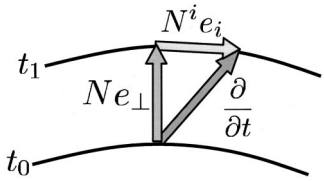

FIG. 1. The $n+1$ splitting of spacetime in the ADM formalism. The time vector $\partial/\partial t$ giving the evolution from a Cauchy hypersurface at time t_0 to the infinitesimally later Cauchy hypersurface at time t_1 can be decomposed into its part $N^i e_i$ parallel to the hypersurfaces and into its orthogonal part $Ne_\perp$. Here e_i, $e_\perp$ are unit vectors adapted to the hypersurfaces and N^i, N are the shift and the lapse.

II. THE RECONSTRUCTION OF SPACETIME FROM COMMUTATORS

In this section, a globally hyperbolic n-dimensional spacetime M with a given foliation Σ_t, $t \in \mathbb{R}$ by spacelike Cauchy hypersurfaces is preassumed. This is sufficient to define a family A_t of commutative algebras, the algebras of smooth functions on the hypersurfaces Σ_t,

$$A_t = C^\infty(\Sigma_t), \tag{6}$$

and to consider their action on the classical phase space (the space of solutions) $\mathcal{H}$ of a Dirac spinor field satisfying the Dirac equation

$$(\not{D} - m)\psi = 0, \quad \text{for } \psi \in \mathcal{H}. \tag{7}$$

This action is just the pointwise multiplication of the initial data of the spinor field by functions on the corresponding Cauchy space slice,

$$(a_t \psi)(x) = a_t(x)\psi(x) \quad \text{for } a_t \in A_t,\ \psi \in \mathcal{H}, \text{ and } x \in \Sigma_t. \tag{8}$$

It is well defined, since a solution is uniquely given by its initial values on any Cauchy hypersurface.

While the algebras A_t are themselves commutative, they do not commute with each other. We proceed now, following Ref. 11, to express this noncommutativity in terms of commutators and then show that the knowledge of the calculated commutators is sufficient to recover the preassumed spacetime manifold including its metric structure and spin structure.

The commutators of interest will be those of functions taken at different times and of functions with the (generically time-dependent) Hamiltonian H of the family A_t of algebras. In the calculations, we will assume to be given the standard data of the Hamiltonian description of gravity, the ADM (Arnowitt–Deser–Misner) formalism.[12] A time flow identifying the Cauchy surfaces in the family and the metric tensor g_{ij} on the hypersurfaces describe the leaves. Also needed is a lapse function N describing the infinitesimal distance between hypersurfaces and the shift function N^i expressing, how much the identification of neighboring hypersurfaces (the time vector field $\partial/\partial t$) is shifted from the normal direction $e_\perp$ along the spatial directions e_i (see Fig. 1),

$$\frac{\partial}{\partial t} = Ne_\perp + N^i e_i. \tag{9}$$

In addition, the Dirac generators $\not{e}_\perp$, $\not{e}_i$ corresponding to the vectors $e_\perp$, e_i and the canonical spin connection ω will appear in the calculations. (Here, the common slash notation is used. The natural insertion γ^μ of covectors a_μ into the Clifford algebra generated by covectors is just indicated by a slash, $\not{a} := \gamma^\mu a_\mu$.)

With this, the Hamiltonian of the spinor field can be written as

$$iH = -N(\omega_\perp^S + \not{e}_\perp \not{e}_i g^{ij} D_j - m\not{e}_\perp) + N^i \partial_i . \tag{10}$$

It is obtained by $n+1$ splitting of the Dirac equation (7)

$$\left(-\gamma_\perp \left(\frac{1}{N} D_t - \frac{N^i}{N} D_i \right) + \gamma_i g^{ij} D_j - m \right) \psi = 0, \tag{11}$$

multiplying from the right by $\not{e}_\perp$ and then extracting the time derivative term. The form (10) is then obtained using the splitting of the spin connection form in the time direction,

$$\omega_t^S = N\omega_\perp^S + N^i \omega_i^S . \tag{12}$$

The commutator of the Hamiltonian with a function $f = f(t_0)$ belonging to a particular algebra A_{t_0} is easily computed,

$$[f, iH] = N \not{e}_\perp \not{e}_i g^{ij} (\partial_j f) - N^i \partial_i f. \tag{13}$$

The commutator of two functions $g \in \Sigma_{t_0}$, $f \in \Sigma_{t_1}$ is a more subtle issue. A not so short calculation, taking into account the possible time dependence of the Hamiltonian, gives the following expansion in time $t_1 - t_0$:

$$[f(t_1), g(t_0)] = (t_1 - t_0)^0 0 \tag{14}$$

$$+ (t_1 - t_0)^1 0 \tag{15}$$

$$- (t_1 - t_0)^2 (N^2 g^{ij} g^{kl} (\partial_i f)[\not{e}_j, \not{e}_k] \partial_l g) \tag{16}$$

$$+ (t_1 - t_0)^3 4 \not{e}_\perp m N^3 g^{ij} (\partial_i f)(\partial_j g) + \begin{pmatrix} \text{terms vanishing} \\ \text{in } 1+1 \text{ dimensions} \end{pmatrix} \tag{17}$$

$$+ O((t_1 - t_0)^4). \tag{18}$$

Note 1. All functions on the right-hand side are taken at the time t_0. It is understood that $f(t_0) \in A_{t_0}$ is the element corresponding to $f(t_1) \in A_{t_1}$ under the identification of A_{t_0}, A_{t_1} induced from the identification of Σ_{t_0}, Σ_{t_1}.

The formulas (10)–(17) contain a wealth of information. They are interpreted in the following remarks.

Remark 1. Commutativity. The vanishing of the zeroth order (14) just expresses the commutativity of the algebra of functions. This is a particularity typical of classical geometry and is, of course, not to be expected to hold in generalizations to noncommutative geometry.

Remark 2. First order condition. The vanishing of the first order (15) can be traced back to the fact that the spinor field obeys a first order differential equation. It can be restated in the following formula valid for any Hamiltonian originating from an arbitrary choice of slicing and time:

$$[[f(t_0), iH], g(t_0)] = 0. \tag{19}$$

Remark 3. Conformal structure. The second order (16) provides the generators $[\not{e}_i, \not{e}_k]$ of spatial orthonormal rotations, also called Coriolis fields. Thus, while it does not provide a length scale, it allows to compare ratios of lengths in different spatial directions. This means that the second order fixes the conformal structure. This term is absent in $1+1$ dimensions as there is no conformal information to talk about.

Remark 4. Time vector and scale. In $1+1$ dimensions, the third order provides the time vector $\not{e}_\perp$. This is uniquely extractable by requiring that it be normalized,

$$\not{e}_\perp^2 = -1. \tag{20}$$

Moreover, the term sets a scale for the metric, the inverse mass $1/m$ of the Dirac field. This scale could not be extracted, e.g., from the spectrum of the Hamiltonian, since an arbitrary rescaling of time by a constant factor will give a rescaling of the Hamiltonian. In this sense the Hamiltonian alone is not sufficient to set a scale.

However, in the general case of $n+1$ dimensions, it is more useful to abandon the expansion to orders higher than one in time (for high energy and low energy expansions, see Ref. 13) and rather *postulate* the existence of a suitable time vector $\not{e}_\perp$ with the correct properties. This allows to avoid a complicated extraction procedure for $\not{e}_\perp$ and m. The ADM data for spacetime can then be extracted from

$$[[iH,\not{e}_\perp],f] \to N g^{ij} \not{e}_j, \tag{21}$$

$$tr(iH\not{e}_\perp) \to Nm, \tag{22}$$

$$tr([iH,f]) \to N^i. \tag{23}$$

This is the approach taken in the next section.

Remark 5. Gauge and spatial Clifford generators. The use of the commutator (13) is the following: Given the time vector, it is easy to recognize the commutator's two terms in an operational way and to extract thus the shift N^i, the spatial Clifford generators $\not{e}_\perp$ together with their correspondence with spatial codirections. The lapse N is obtained by checking the prefactor of the first term against (17). Thus the commutator (13) expresses the arbitrary choices (gauge freedom) of the ADM formalism, including the choice of a spinor basis and is in this sense a somewhat supplementary structure.

The following corollary and remark show that in $1+1$ dimensions the idea of reconstructing spacetime from commutators of the algebras A_t meets complete fulfillment (massive case) as well as complete failure (massless case). Both are due to special properties of the dimension.

Corollary 1. In $1+1$ *dimensions and under the assumption that* $m \neq 0$, *the geometric structure of spacetime can be recovered from the knowledge of the commutators* (*13*) *and* (*15*)–(*17*).

Remark 6. If $m=0$ in $1+1$ dimensions then the commutator $[f(t_1),g(t_0)]$ vanishes at all times. Any (generalized) eigenspaces of an algebra A_{t_0} can be split into a right-moving eigenvector and a left-moving eigenvector. These form a common eigenbasis for all algebras $A_\cdot$.

III. THE SPECTRAL QUADRUPLE

In this section, the structures and properties that were found useful in Sec. II to recover a spacetime manifold from spectral data are pronounced to be first principles, whose collection is called a spectral quadruple. At the same time, they are fused with an imposed symmetry, though it is hoped that the general suggestions are still visible. The imposition of symmetry is done for two reasons: First, it provides a computationally manageable example and in direct generalization the possibility of a large set of important analogous examples. Second, the imposed symmetries provide automatic smoothness which allows to leave this further difficulty for this work on the side lines. (For a physically motivated principle of smoothness see Ref. 9.)

Given a category (a collection of objects and morphisms between objects that can be composed, satisfying a certain set of axioms), a subset of morphisms such that each of its elements has an inverse morphism forms a groupoid.

The following Definition 1 is to be understood as a conceptual step and does not attempt to be free of any redundance. Note that, in the notation of the definition, the dependence of the operators $\not{e}_\perp = \not{e}_\perp(\bullet)$, $\gamma = \gamma(\bullet)$ on the symbolically written index $\bullet$ is present but mostly suppressed.

Definition 1. *The* **spectral quadruple** $(A_\bullet,\mathcal{H},G,C,\gamma(\bullet),\not{e}_\perp(\bullet))$ *consists of a collection of algebras* $A_\bullet$ *represented on the Hilbert space* $\mathcal{H}$*, of a groupoid* G *and of an antilinear operator* C*. In addition, for each of the algebras* $A_\bullet$ *two operators* $\not{e}_\perp$, γ *are given. These structures satisfy the following conditions.*

(1) **Evolution.** *Any two algebras* A_0, A_1 *of the collection* $A_\bullet$ *are required to be mutually unitarily equivalent through a (not necessarily unique) unitary* $U(A_0,A_1)$ *and not mutually commutative,* $[A_{t_1},A_{t_2\neq t_1}]\neq 0$*. The groupoid* G *consists of a subset of all possible unitary equivalences between the algebras in the collection* $A_\bullet$*. It is assumed that for each algebra* A_0 *in the collection there exists an evolution, a (not necessarily unique) differentiable path* $\alpha_t: t\in\mathbb{R}\rightarrow\mathbb{U}_t(\mathbb{A}_0,\mathbb{A}_t)$ *with* $\alpha_0=1$ *such that the generator (derivative) at* $t=0$*, denoted by* iH *is compatible with the further requirements.*

(2) **Charge conjugation.** *The antilinear operator* C *commutes with* G *and satisfies*

$$C^2=(-1)^{s(n)} \tag{24}$$

for the spacetime dimension n *and with*

$$s(n):=\tfrac{1}{8}(n-1)(n-2)(n-3)(n-4). \tag{25}$$

(3) **First order condition (dynamics)**

$$[[f,iH],g^{\mathrm{op}}]=0 \quad \text{for any } f,g\in A_0 \text{ and any generator } iH, \tag{26}$$

with $g^{\mathrm{op}}=Cg^*C$.

(4) **The time vector.** *For each algebra* A_0 *in the collection* $A_\bullet$ *there exists an operator* $\not{e}_\perp$ *called the time vector satisfying*

$$\not{e}_\perp^2=-1, \tag{27}$$

$$\not{e}_\perp^*=-\not{e}_\perp, \tag{28}$$

and the compatibility conditions in (5) and (6) of this definition.

(5) **The volume element.** *For any* A_t *there exists an operator* γ *such that*

$$\gamma^2=\pm 1, \tag{29}$$

$$\{\not{e}_\perp,\gamma\}=0 \quad \text{for even spacetime dimension,} \tag{30}$$

$$[\not{e}_\perp,\gamma]=0 \quad \text{for odd spacetime dimension,} \tag{31}$$

and

$$\gamma=\not{e}_\perp\sum_{f_\bullet\in A_t} f_{i_0}[D,f_{i_1}]\cdots[D,f_{i_n}] \quad \text{for even spacetime dimension } n+1, \tag{32}$$

$$\gamma=\sum_{f_\bullet\in A_t} f_{i_0}[D,f_{i_1}]\cdots[D,f_{i_n}] \quad \text{for odd spacetime dimension } n+1, \tag{33}$$

and for suitable functions $f_\bullet$ *where* D *is given by*

$$D=\begin{cases}\gamma[iH,\gamma] & \text{for even spacetime dimension,}\\ iH & \text{for odd spacetime dimension.}\end{cases} \tag{34}$$

(6) **Geometry of space.** *For any algebra* A_t *of the collection* $(A_t,\mathcal{H},\not{e}_\perp[H,\not{e}_\perp],\gamma,C)$ *is*

(i) *a* spectral triple for odd spacetime dimension,
(ii) *a spectral triple for even spacetime dimension, if restricted to each of the two eigenspaces of* $\not{\epsilon}_\perp$.

Remark 7. The right-hand sides of Eqs. (32) and (33) are to be understood as (images of) Hochschild cycles. The principal part of the operator D [compare with (10)] is the same as the principal part of the spatial Dirac operator but multiplied from the left by $\not{\epsilon}_\perp$. Since $\not{\epsilon}_\perp^2 = -1$, this has no effect on the form of (33) but requires the appearance of $\not{\epsilon}_\perp$ in (33), to cancel one superfluous $\not{\epsilon}_\perp$ coming from the commutators. Note that, together with the requirements in parts 5, 6 of the definition, it follows that

$$D\gamma = (-1)^{n+1}\gamma D. \tag{35}$$

Remark 8. A minimal version of G would be $G=\mathbb{R}$.

An interesting model in this respect would be the classical evolution induced from the modular automorphism group determined by a quasifree state on the Dirac-quantized phase space H. This would make contact with the work of Connes and Rovelli.[14]

However, G may be much larger and it is in this context that the concept of many-fingered time of general relativity comes to its full expression.

For a large G, the definition does not exclude the possibility that, along with generators iH satisfying the definition, there may be some that may not satisfy the definition. These are to be thought of as in some sense singular and are to be avoided (see Remark 11).

Remark 9. The last requirement in the definition of a spectral quadruple puts things on the safe side in order to be sure that reasonable spacetime geometries deserving to be called manifolds will be obtained. It is to be noted though that $\not{\epsilon}_\perp[H,\not{\epsilon}_\perp]$ is in general not the spatial Dirac operator, though it can be used as such for making sure the corresponding spatial section is a manifold, since only the principal symbol of the Dirac operator matters and is in this way obtained correctly.

Remark 10. **Spacetime points.** Compared with the situation in the preceding section, the definition of the spectral quadruple provides for more general situations, in particular for a many-fingered time. This leads to an additional difficulty: Assume, that the algebras in the collection are commutative. Then it is fine to take the characters of an algebra as being points of spacetimes. However, some characters of different algebras in the collection describe the same point. In order to compare characters, one has to extend them as functionals on a larger algebra encompassing all of the collection $A_\bullet$. But since the characters are distributions, they cannot be extended to all bounded operators on $\mathcal{H}$. It is natural to expect that this algebra should be determined by a smoothness principle common to the whole collection $A_\bullet$.

Two types of spectral quadruples are of particular interest.

Definition 2. *A* general spectral quadruple *is a spectral quadruple where G is given by all smooth unitary equivalences* $U(A_\bullet, A_\bullet)$.

A symmetric spectral quadruple *is a spectral quadruple distinguished by the following conditions*:

(1) G is *a finite dimensional Lie group (and iH is then in the Lie algebra of G).*
(2) *For any algebra* A_{t_0}, *the subgroup K preserving the algebra coincides with a maximal compact subgroup of* G.
(3) *The operators* $\not{\epsilon}_\perp$, γ *commute with the group* K,

$$[k, \not{\epsilon}_\perp] = 0, \tag{36}$$

$$[k, \gamma] = 0, \tag{37}$$

for any $k \in K$.

Remark 11. Specializing Remark 8 to a symmetric spectral quadruple, the generator iH for an algebra A_0 is not to be chosen as a compact generator in the Lie algebra of G preserving A_0 as it may not fulfill the geometry-of-space requirement in Definition 1 of a spectral quadruple.

Following these general consideration, we will choose a particular class of symmetric spectral quadruples which we will call de Sitter spectral quadruples.

The group G is chosen to be $\mathrm{SL}_2(\mathbb{R})$.

The set of algebras is generated from one algebra by the action of G. This algebra in turn is generated from one unitary generator u,

$$u^* = u^{-1}. \tag{38}$$

The mutual position of G and u on the representation space $\mathcal{H}$ is partially determined by the commutation relation of u, $\not{e}_\perp$, and γ with a compact generator T_{21} of the Lie algebra of G,

$$[T_{21}, u] = iu, \tag{39}$$

$$[T_{21}, \not{e}_\perp] = 0, \tag{40}$$

$$[T_{21}, \gamma] = 0. \tag{41}$$

The above set of structures is irreducibly represented. This requirement is to avoid dealing with multiple copies.

Note 2. The compact generators of a Lie group generate the maximal compact subgroup of a Lie group.[15] In the case of $\mathrm{SL}_2(\mathbb{R})$ a compact subalgebra of the Lie algebra is just one-dimensional and thus spanned by one element T_{21}. This indicates how to proceed in higher dimensional cases.

As is clear from the definitions, the Hilbert space $\mathcal{H}$ of a de Sitter spectral quadruple is in particular the representation space of a unitary representation of $G = \mathrm{SL}_2(\mathbb{R})$. Therefore, in the next section, the representation theory of $G = \mathrm{SL}_2(\mathbb{R})$ will be reviewed.

IV. $\mathrm{SL}_2(\mathbb{R})$ AND ITS REPRESENTATION THEORY

The group $\mathrm{SL}_2(\mathbb{R})$ is treated in a number of sources. The present review is based on Refs. 15–19.

Definition 3. *The group $SL_2(\mathbb{R})$ is the Lie group of 2×2-matrices of real numbers with unit determinant. $sl_2(\mathbb{R})$ is the Lie algebra of traceless 2×2-matrices of real numbers.*

Remark 12 (see Ref. 15). The Lie group $\mathrm{SL}_2(\mathbb{R})$ and the Lie algebra $\mathrm{sl}_2(\mathbb{R})$ have the following decomposition (Iwasawa decomposition):

$$\mathrm{SL}_2(\mathbb{R}) = K\times A\times N = \underbrace{\begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}}_{\text{maximal compact}} \underbrace{\begin{pmatrix} a & 0 \\ 0 & a^{-1} \end{pmatrix}\begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix}}_{\text{solvable}},$$

$$\mathrm{sl}_2(\mathbb{R}) = k\times a\times n = \underbrace{\begin{pmatrix} 0 & c \\ -c & 0 \end{pmatrix}}_{\text{antisymmetric}} \underbrace{\begin{pmatrix} d & 0 \\ 0 & -d \end{pmatrix}\begin{pmatrix} 0 & n \\ 0 & 0 \end{pmatrix}}_{\text{solvable}},$$

for $\phi, a, b, c, d, n \in \mathbb{R}$.

$\mathrm{SL}_2(\mathbb{R})$ is a simple Lie group and has thus a nondegenerate Killing metric on its Lie algebra with signature $(-,+,+)$.

$\mathrm{SL}_2(\mathbb{R})$ is a double cover for SO(1,2).

The Lie algebra $\mathrm{sl}_2(\mathbb{R})$ can be given by three generators T_{01}, T_{02}, and T_{21} satisfying the following commutation relations:

$$[T_{01}, T_{21}] = -T_{02}, \quad [T_{02}, T_{21}] = +T_{01}, \quad [T_{01}, T_{02}] = -T_{21}. \tag{42}$$

In a complex representation, raising and lowering operators may be defined

$$T_{\pm} = T_{01} \mp i T_{02}. \tag{43}$$

Together with T_{21}, these operators generate the complexification of $\mathrm{sl}_2(\mathbb{R})$. Their commutation relations are

$$[T_{21}, T_{\pm}] = \pm i T_{\pm}, \tag{44}$$

$$[T_{+}, T_{-}] = -2i T_{21}. \tag{45}$$

In addition, the following holds in unitary representations:

$$T_{21}^{*} = -T_{21}, \tag{46}$$

$$T_{01}^{*} = -T_{01}, \tag{47}$$

$$T_{02}^{*} = -T_{02}, \tag{48}$$

$$T_{\pm}^{*} = -T_{\mp}. \tag{49}$$

Representations. The group $\mathrm{SL}_2(\mathbb{R})$ is a noncompact group. Its unitary representations are thus bound to be infinite dimensional while there are nonunitary finite dimensional representations, e.g., the defining representation.

Any representation can be decomposed into irreducible representations of the maximal compact subgroup K which is just the circle group U_1. The irreducible representations of U_1 are one dimensional and given by $\pi_n : \phi \to e^{in\phi}$ with $n \in \mathbb{Z}$. The maximal compact subgroup can be taken to be generated by T_{21}. That the eigenvalues of T_{21} are to be integers or half-integers is a global requirement of the group representation and can in this case not be seen on the level of the generator T_{21} alone but comes from the requirement that the representation of $K = U_1$ should be single valued.

We will consider only admissible unitary representations[16] in which all eigenspaces of T_{21} are only finite dimensional.

The eigenvectors of T_{21} will be labeled by $|n\rangle$:

$$T_{21}|n\rangle = in|n\rangle \quad \text{for } n \text{ integer or half-integer} \tag{50}$$

and will be assumed to be normalized

$$\langle n|n\rangle = 1. \tag{51}$$

For any eigenvector in such an irreducible representation, the vectors $T_{-}T_{+}|n\rangle$, $T_{-}T_{+}|n\rangle$ are proportional to $|n\rangle$.

Define

$$T_{+}|n\rangle = c_n |n+1\rangle. \tag{52}$$

It follows from unitarity (49),

$$T_{-}|n+1\rangle = -\overline{c_n}|n\rangle. \tag{53}$$

From (49) and (45), it follows that

$$\langle n|[T_{+}, T_{-}]n\rangle = -2i\langle n|T_{21}n\rangle, \tag{54}$$

$$-\langle T_{-}n|T_{-}n\rangle + \langle T_{+}n|T_{+}n\rangle = 2n, \tag{55}$$

$$|c_n|^2-|c_{n-1}|^2=2n, \tag{56}$$

and solving the recursion relation gives

$$|c_n|^2=(n+\tfrac{1}{2})^2+R^2m^2, \tag{57}$$

with R^2m^2 being a real number (possibly negative; writing for this number the expression R^2m^2 is convenient for latter interpretation and has no importance here). Since $|c_n|^2$ is positive, R^2m^2 has to satisfy the following condition:

$$(n+\tfrac{1}{2})^2+R^2m^2\geqslant 0 \tag{58}$$

for all half-integers n appearing in the representation. This condition allows us to get insight into the classification of the unitary irreducible representations of $\mathrm{SL}_2(\mathbb{R})$:

(i) As long as $R^2m^2>0$, the condition (58) is always satisfied and c_n never vanishes. Given one eigenvector $|n\rangle$ of the Hermitean operator $-iT_{21}$ and for some half-integer n, one obtains eigenvectors $|n+k\rangle$, for all $k\in\mathbb{R}$. These then span the representation space of the irreducible representation. These representations, labeled by the number R^2m^2 and by whether the eigenvalues are integers or true half integers (i.e., integers$+\frac{1}{2}$), are referred to as the *principal series.*

(ii) If $0\geqslant R^2m^2>\frac{1}{4}$ then the condition (58) is always satisfied and c_n never vanishes under the assumption that the eigenvalues are integers. These representations are called the *complementary series.*

(iii) If the condition (58) cannot be satisfied for eigenvalues shifted by an arbitrary amount, then some c_n have to vanish in order not to run into contradictions with (58) while applying raising and lowering operators. This bounds the eigenvalues of $-iT_{21}$ in the unitary irreducible representation from above or from below. The number R^2m^2 has then to satisfy

$$R^2m^2=-(n_0+\tfrac{1}{2})^2 \tag{59}$$

for some half integer n_0. These unitary irreducible representations are thus discretely indexed by n_0 and by whether the eigenvalues of $-iT_{21}$ are bound from above or from below. This set of unitary irreducible representations is the *discrete series.*

V. THE SYMMETRIC SPECTRAL QUADRUPLES OF DE SITTER SPACE

The Hilbert space of the spectral quadruple is required to carry a representation of the group $\mathrm{SL}_2(\mathbb{R})$ and has in addition to accommodate the operators u, $\not{e}_\perp$, and γ. Since $\not{e}_\perp$ and γ commute with T_{21}, they can be considered separately on each eigenspace of T_{21}. Mutually, $\not{e}_\perp$ and γ anticommute and do not vanish, as follows from the definition of the spectral quadruple. Thus they force the eigenspaces $\mathcal{H}_n$ of T_{21} to be at least two dimensional. In addition, u is an invertible raising operator and its inverse u^* an invertible lowering operator, as follows from Eq. (39). Thus all the eigenspaces $\mathcal{H}_n$ of T_{21} are bound to have the same dimension. From the requirement of irreducibility and from the invertibility of the operator u we obtain that this dimension has to be 2 and that the discrete series can therefore not be a candidate.

We will further assume that the eigenvalues are true half-integers, as we are interested in interpreting the representation space as the phase space of a spinor field. This excludes the complementary series of representations as well as the part of the principal series with integer eigenvalues of $-iT_{21}$.

A common orthonormal eigenbasis $|n,\pm\rangle$ for the mutually commuting anti-Hermitean operators T_{21}, $\not{e}_0$ can be given as

$$T_{21}|n,\pm\rangle=in|n,\pm\rangle, \tag{60}$$

$$\not{e}_0|n,\pm\rangle = \pm i|n,\pm\rangle, \tag{61}$$

$$\langle n',\mathrm{sign}'|n,\mathrm{sign}\rangle = \delta_{n'n}\delta_{\mathrm{sign}'\mathrm{sign}}. \tag{62}$$

The eigenvectors are then unique, up to phases. The relative phases are fixed by requiring further

$$u|n,\pm\rangle = |n+1,\pm\rangle. \tag{63}$$

This leaves only two phases free, one of them an overall phase.

The order-one condition. The only unspecified operators of the spectral quadruple are now T_+ and T_-, the raising and lowering operators.

They are given by their restrictions

$$T_\pm(n):\mathcal{H}_n \to \mathcal{H}_{n\pm1}. \tag{64}$$

The eigenspaces $\mathcal{H}_n$ can be identified using the unitary bijections given by restrictions of u. Then the operators $T_\pm(n)$ can all be understood to operate on a common, two-dimensional Hilbert space.

The order-one condition for the raising and lowering operators can then be written as

$$T_\pm(n+1) - 2T_\pm(n) + T_\pm(n-1) = 0. \tag{65}$$

Note that

$$T_+(n)^* = -T_-(n+1), \tag{66}$$

$$T_-(n)^* = -T_+(n-1), \tag{67}$$

so that both equations (65) can be solved recursively, if two restrictions $T_\pm(\bullet)$ are known.

In order to keep the symmetric way in which the raising and lowering operators appear in the calculations, we choose the two required restrictions to be $T_+(+\frac{1}{2})$, $T_-(-\frac{1}{2})$.

From the preceding section, it is clear that the $T_\pm(n)$ have to be unitaries times the factor $\sqrt{(n+\frac{1}{2})^2+R^2m^2}$.

We set

$$T_+(+\tfrac{1}{2}) = \sqrt{1+R^2m^2}\,u_+, \quad u_+^* u_+ = u_+ u_+^* = \mathbf{1}, \tag{68}$$

$$T_-(-\tfrac{1}{2}) = \sqrt{1+R^2m^2}\,u_-, \quad u_-^* u_- = u_- u_-^* = \mathbf{1}. \tag{69}$$

Solving the order-one recursion condition, one obtains

$$T_+(n) = \sqrt{1+R^2m^2}\left(\left(+\frac{n}{2}-\frac{1}{4}\right)(u_+ + u_-^*) + u_+\right), \tag{70}$$

$$T_-(n) = \sqrt{1+R^2m^2}\left(\left(-\frac{n}{2}-\frac{1}{4}\right)(u_- + u_+^*) + u_-\right). \tag{71}$$

Charge conjugation. It remains to determine the 2×2-matrices u_+, u_-.

For that purpose we use a general parametrization of unitary 2×2 matrices,

$$u_+ = e^{i\rho_+}\frac{1}{\sqrt{1+x_+^2+y_+^2}}\begin{pmatrix} -ix_+ + \tanh\theta_+ & \dfrac{1}{\cosh\theta_+} + iy_+ \\ -\dfrac{1}{\cosh\theta_+} + iy_+ & ix_+ + \tanh\theta_+ \end{pmatrix}, \tag{72}$$

$$u_- = e^{i\rho_-}\frac{1}{\sqrt{1+x_-^2+y_-^2}}\begin{pmatrix} -ix_- + \tanh\theta_- & \dfrac{1}{\cosh\theta_-} + iy_- \\ -\dfrac{1}{\cosh\theta_-} + iy_- & ix_- + \tanh\theta_- \end{pmatrix}. \tag{73}$$

As a consequence of the commutation of the charge conjugation C with G in the definition of a spectral quadruple, one obtains

$$e^{i\rho} := e^{i\rho_+} = -e^{i\rho_-}, \tag{74}$$

$$x := x_+ = -x_-, \tag{75}$$

$$\theta := \theta_+ = \theta_-, \tag{76}$$

$$y := y_+ = y_-. \tag{77}$$

Out of the remaining four parameters, two of them, ρ and y can be set to zero, since they exactly correspond to the two remaining phases in the above choice of basis. ρ is the overall phase and y is connected with a phase freedom in the spinor basis as will become apparent once the geometric interpretation of the de Sitter quadruple is reached.

Thus the de Sitter spectral quadruples form a two-parametric family. Comparing with the representation theory of $\mathrm{SL}_2(\mathbb{R})$, one finds that x can be identified with the parameter Rm while there are no further restrictions on θ. Thus the two matrices u_+ and u_- can be written as

$$u_+ = \begin{pmatrix} -iRm + \tanh\theta & \dfrac{1}{\cosh\theta} \\ -\dfrac{1}{\cosh\theta} & iRm + \tanh\theta \end{pmatrix}, \tag{78}$$

$$u_- = \begin{pmatrix} -iRm + \tanh\theta & -\dfrac{1}{\cosh\theta} \\ \dfrac{1}{\cosh\theta} & iRm + \tanh\theta \end{pmatrix}. \tag{79}$$

Following Remark 4 and Remark 10 (or Corollary 1 and Remark 10, since this is the special, $1+1$-dimensional case), the corresponding spacetime geometry can be directly calculated.

The result is $1+1$ dimensional de Sitter space of radius R containing a Dirac spinor field of mass m. The mass m and the radius R may be reinterpreted at will, as long as Rm is kept constant. In that sense, the mass of the Dirac field becomes the meter stick. The parameter does not change the geometry: The algebra generated by u, from which all other algebras are obtained by symmetry group actions describes a spacelike circle invariant under the action of T_{21}. There is a one parameter set of such circles. θ can be chosen as that parameter.

Instead of carrying out the detailed calculations, one can get these results by checking that the de Sitter spectral quadruples obtained here are identical with the spectral data of $1+1$ de Sitter space calculated in the Appendix, see (A122)–(A127).

Remark 13. The fact that different symmetric spectral quadruples describe the same geometry is not surprizing. It is a consequence of G having been chosen too small to provide for all unitary equivalences that take any smooth spacelike circle into any other smooth spacelike circle on de Sitter. A one-to-one correspondence between spacetimes and spectral quadruples should be searched for with a sufficiently large choice of G only.

Remark 14. Going through a direct calculation, one cannot avoid the problem of extending characters of one algebra in the collection to generalized vectors, on which other algebras may act.

This requires to see the characters as distributions (functionals) on a dense subspace of the Hilbert space.[20] But suitable subspaces of test vectors are in this case obtained for free from the action of the group G: They can be chosen to consist of vectors with rapidly decaying coordinates in the eigenbasis of T_{21}. In this point, the employed Lie symmetry provides substantial help with matters of smoothness.

VI. FINITE SPECTRAL QUADRUPLES

A finite spectral quadruple is based on a collection of finite dimensional algebras with the necessary additional structures.

Here, we will build a spectral quadruple out of a spectral triple $(A_0,\mathcal{H},D,\gamma,J)$. This allows us to take advantage of the fact that the relevant spectral triples have already been fully characterized:[21,22] Finite spectral triples are classified by their algebra A which is a finite direct sum of matrix algebras, $A=\oplus_{i=1}^{k} M_{n_i}(\mathbb{C})$ and a symmetric and invertible $k\times k$ matrix with integer entries, the intersection form $q_{ij}:K_\bullet(A)\times K_\bullet(A)\to\mathbb{Z}$, from which the remaining data of the spectral quadruple can be read off. In particular, the Hilbert space $\mathcal{H}$ is given by

$$\mathcal{H}=\bigoplus_{i,j}^{k}\mathcal{H}_{ij}:=\bigoplus_{i,j}^{k}(\mathbb{C}^{n_i}\otimes\mathbb{C}^{|q_{ij}|}\otimes\mathbb{C}^{n_j}), \tag{80}$$

on which the algebra A acts by left multiplication as $a\otimes\mathbf{1}\otimes\mathbf{1}$ for $a\in A$ while the opposite algebra JA^*J, with $J:H_{ij}\to H_{ji}$, $J(v_i\otimes v_{ij}\otimes v_j)=\overline{v_j}\otimes\overline{v_{ij}}\otimes\overline{v_i}$ antilinear, acts by right matrix multiplication as $\mathbf{1}\otimes\mathbf{1}\otimes\mathbf{a}^{\mathbf{T}}$ for $a\in A$. Furthermore,

$$\gamma\mathcal{H}_{ij}=\mathcal{H}_{ij},\quad \gamma|_{\mathcal{H}_{ij}}=\mathrm{sign}(q_{ij})\mathbf{1}_{\mathcal{H}_{ij}}, \tag{81}$$

and the Dirac operator $D:\mathcal{H}_{kl}\to\mathcal{H}_{ij}$ satisfies the equations

$$D_{ij\,kl}=D^{+}_{ij\,kl},\quad D_{ij\,kl}=\overline{D_{ji\,lk}}, \tag{82}$$

following from the requirements

$$D=D^*, \tag{83}$$

$$JD=DJ. \tag{84}$$

The Dirac operator is further restricted by the order-one condition of a spectral triple.

Example 1. *Let a finite spectral triple be given by the algebra*

$$A=\mathbb{C}\oplus\mathbb{C} \tag{85}$$

and by the intersection form

$$q=\begin{pmatrix}1 & -1\\ -1 & 0\end{pmatrix}. \tag{86}$$

Then

$$\mathcal{H}=\mathbb{C}^3, \tag{87}$$

$$\gamma=\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix}, \tag{88}$$

$$J = \text{complex conjugation} \times \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{89}$$

The representations π, π^{op} of the algebra A and of the opposite algebra A^{op} are given by

$$\pi(z_1 \oplus z_2) = \begin{pmatrix} z_1 & 0 & 0 \\ 0 & z_1 & 0 \\ 0 & 0 & z_2 \end{pmatrix}, \tag{90}$$

$$\pi^{\mathrm{op}}(z_1 \oplus z_2) = \begin{pmatrix} z_1 & 0 & 0 \\ 0 & z_2 & 0 \\ 0 & 0 & z_2 \end{pmatrix}, \tag{91}$$

and

$$D = \begin{pmatrix} 0 & m & \overline{m} \\ \overline{m} & 0 & 0 \\ m & 0 & 0 \end{pmatrix} \quad \text{for} \quad m \in \mathbb{C}. \tag{92}$$

In order to construct a spectral quadruple, it is now sufficient to find in addition to the spectral triple data an operator $\not{\epsilon}_\perp$:

$$\not{\epsilon}_\perp^2 = -\mathbf{1}, \tag{93}$$

$$\not{\epsilon}_\perp^* = -\not{\epsilon}_\perp, \tag{94}$$

$$[\not{\epsilon}_\perp, \gamma] = 0, \tag{95}$$

as required by the definition of a $1+0$-dimensional spectral quadruple, and to supply a Hamiltonian H as a function of time.

The operator $\not{\epsilon}_\perp$ and the Hamiltonian H can be chosen as

$$\not{\epsilon}_\perp := i\gamma(t), \tag{96}$$

$$H(t) := \not{\epsilon}_\perp(t) D(t). \tag{97}$$

Denoting the evolution operator by $U(t)$, one can write the time dependent operator $D(t)$ as $U^{-1}(t) D_0(t) U(t)$ with respect to a comoving basis in which the representation of the algebra remains diagonal. Here $D_0(t)$ has the same form for all times t as the Dirac operator D just with its entries replaced by smooth functions.

In particular, $D_0(t)$ has the form (92), if the spectral triple of Example 1 is taken. The equal time distance of the two points x_t, y_t of this discrete spectral geometry can be calculated via Connes' distance formula:[1]

$$d(x_t, y_t) = \sup_{a_t \in A_t, \|[D(t), a_t]\| \leq 1} \{|x_t(a_t) - y_t(a_t)|\} \tag{98}$$

$$= \sup_{a_0 \in A_0, \|[D_0(t), a_0]\| \leq 1} \{|x_0(a_0) - y_0(a_0)|\} \tag{99}$$

$$= \frac{1}{|m(t)|}. \tag{100}$$

Thus this spectral quadruple describes two points with varying spatial distance $1/|m(t)|$.

To determine the distance between the points, rather than to prescribe it, one would have to provide the corresponding theory of gravity given by an action functional. For example, one could use a spectral action for the Wick rotated system, thus avoiding problems of nondefiniteness of a Lorentzian action. Alternatively, one could try to write down an action directly, in terms of H and its time derivative $\dot{H}$. However, H is noninvertible and it becomes difficult to write a term invariant under time parametrization. For instance, typical terms like $\dot{H}^2/H^3$, $\sqrt[4]{\dot{H}}$ are pested with singularities while $\dot{H}/H$ leads to the solution $H=0$. But this is beyond the scope of the present work.

Remark 15. The here presented type of a discrete spectral quadruple is built in a rather naive way on the basis of a discrete spectral triple, just by adding time. Its value is in showing how the Lorentzian signature is taken up in the discrete case [see especially (96)] rather than in examining all possibilities of the discrete case.

VII. CONCLUSION

In this work, we have arrived at a spectral characterization of spin manifolds with Lorentzian metric through a spectral quadruple. While the spectral geometry of Riemannian spin manifolds as given by the spectral triple has motivated and was incorporated into the spectral quadruple, the spectral quadruple is not just a stack of spectral triples with time vectors $\not{e}_\perp$ and some sign changes added on. The results are derived from the Hamiltonian rather than from the Dirac operator, allowing thus for the many-fingered time typical of general relativity. The requirements of the order-one condition and of charge conjugation are significantly generalized with the first of the two containing the main information on dynamics: These requirements are not to hold for one algebra but instantly for all algebras in the collection $A\!\!\!\bullet$ at once.

Note also that the axioms do not presuppose global hyperbolicity. The lack of global hyperbolicity and the eventual occurrence of closed timelike curves leaves one still with a meaningful structure. For example, closed timelike curves will not allow an arbitrary choice of initial data on spatial sections and will thus severely restrict the size of the phase space but still a fuzzy description of spacetime is eventually left. This should not be seen as a failure. It simply means that certain details of geometry, though possibly existent in mathematical imagination, are automatically dropped, if there is no field to resolve them. This is not unrelated to the features of the Euclidean spectral quadruple presented in Joke 1 at the end of this section.

On the practical side, the notion of a spectral quadruple is backed up by the nontrivial example of de Sitter spectral quadruples which successfully describe $1+1$-dimensional de Sitter space. This is an achievement in itself as it is not so easy, despite the generality of spectral geometry, to produce examples. (This does not mean that there are no examples available in the Riemannian case, as the collection has been built up for some time. But still this is an area in need of substantial further work.) While the requirements of the spectral quadruple are in a preliminary form and confrontation with further examples is definitely needed, a number of important examples is under firm control: It is clear, how to deal with generalizations to higher dimensional de Sitter spaces and other cosmologies of high symmetries. Situations of such high symmetries are not just toy examples but have claim to be directly interpreted: the Friedmann–Robertson–Walker class of models is the one used as the background of realistic cosmology.

With this in hand it is now only natural to have a second look at the standard model of elementary particle physics along the lines of Ref. 23. Judging from the results of Sec. VI, in particular Eq. (97), no fermion doubling is to be expected.

Joke 1. It is amusing to note that the machinery of the spectral quadruple which was designed to deal with Lorentzian manifolds can be turned onto Euclidean situations. To give an example, we define a class of symmetric spectral quadruples which we will call ''spherical spectral almost quadruples.'' The word *almost* refers to one necessary adaptation of the definition of a spectral quadruple to the Euclidean signature: instead of $\not{e}_\perp^2=-\mathbf{1}$ we require $\not{e}_\perp^2=+\mathbf{1}$.

The group G is chosen to be SU_2.

The set of algebras is generated from one algebra by the action of G. This algebra in turn is generated from one unitary generator u:

$$u^* = u^{-1}. \tag{101}$$

The mutual position of G and u on the representation space $\mathcal{H}$ is partially determined by the commutation relation of u, $\not{e}_\perp$, and γ with a compact generator T_{21} of the Lie algebra of G:

$$[T_{21}, u] = iu, \tag{102}$$

$$[T_{21}, \not{e}_\perp] = 0, \tag{103}$$

$$[T_{21}, \gamma] = 0. \tag{104}$$

The above set of structures is irreducibly represented. This requirement is to avoid dealing with multiple copies.

The resulting space should be thought of as being a sphere S^2 with an axis of rotational symmetry determined by the chosen generator T_{21}. The algebra generated by u describes a circle preserved under the rotational symmetry generated by T_{21}. This circle may or may not be chosen at the equator of the sphere and is moved over the sphere by the action of the group SU_2. In this way any point of the sphere is reached by some circles. However, points of the sphere can be resolved only in a limit for the following reason: In analogy with the de Sitter example, the algebras are represented on the space of solutions of the counterpart of the Dirac equation

$$\not{D}\psi = (l + \tfrac{1}{2})\psi \tag{105}$$

for a fixed angular momentum l of the spherical harmonics. Since SU_2 is a compact group, the Hilbert space of any unitary irreducible representation is finite dimensional and so is the Hilbert space of the spectral quadruple. As seen from the point of view of a true sphere only maximally localized vectors in the Hilbert space rather than points of the sphere may be found and the representation of the algebras generates the matrix algebra on the Hilbert space. Thus the spherical spectral almost quadruples describe the fuzzy spheres.

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APPENDIX: SPINORS ON de SITTER SPACE

In this appendix, a self-contained exposition of de Sitter space and of spinor fields on de Sitter space is given. The main purpose is to collect formulas and facts on this model for use as a testing case for Lorentzian spectral geometry. We will concentrate on two-dimensional de Sitter space. However, at instances where this restriction does not bring any simplification, the general n-dimensional case is dealt with directly.

In the course of this, an important particularity is obtained: There is a set of spectral data that can be compared with the spectral quadruples of Sec. V to provide for one of the main results of this paper: The de Sitter spectral quadruples describe de Sitter space.

The first three subsections deal with the differential geometry, with the symmetries and with the spin geometry of de Sitter space from both the point of view of an imbedding into Minkowski space as well as from the intrinsic point of view. In the following two sections, the Dirac operator

of de Sitter space is discussed and employed to construct the action of the symmetries on the space of solutions of the Dirac equation. There, the spectral data in a form comparable to the de Sitter spectral quadruples are obtained.

The geometry of de Sitter space

Definition 4. *The n-dimensional de Sitter geometry is a submanifold of $n+1$ dimensional Minkowski space given in a fixed Lorentz frame by the equation*

$$-(x^0)^2+(x^1)^2+\cdots+(x^n)^2=R^2 \tag{A1}$$

with the metric induced from the metric of the Minkowski imbedding space,

$$ds^2=-(dx^0)^2+(dx^1)^2+\cdots+(dx^n)^2. \tag{A2}$$

The induced metric has signature

$$(-,\underbrace{+,+,\ldots,+,+}_{n-1}).$$

Remark 16. The intrinsic de Sitter geometry may be defined without any reference to an imbedding space. This is not done here as the imbedding space proves to be a very useful technical tool for doing calculations. But for the sake of clarity, some calculations are done or redone in an entirely intrinsic way.

Following Definition 4, the two-dimensional de Sitter geometry can be embedded into the three-dimensional Minkowski space as the hyperboloid

$$-(x^0)^2+(x^1)^2+(x^2)^2=R^2, \tag{A3}$$

and can be parametrized by generalized spherical coordinates

$$x^0=R\sinh\theta, \qquad \theta\in(-\infty,\infty), \tag{A4}$$

$$x^1=R\cosh\theta\cos\phi, \qquad \phi\in[0,2\pi), \tag{A5}$$

$$x^2=R\cosh\theta\sin\phi, \tag{A6}$$

The coordinate vectors of the spherical coordinates $(\partial/\partial\theta)$ $(\partial/\partial\phi)$ are expressed in terms of the Cartesian basis $(\partial/\partial x^0)$, $(\partial/\partial x^1)$, $(\partial/\partial x^2)$ of Minkowski space by

$$\frac{\partial}{\partial\theta}=\frac{\partial x^i}{\partial\theta}\frac{\partial}{\partial x^1}=R\cosh\theta\frac{\partial}{\partial x^0}+R\sinh\theta\cos\phi\frac{\partial}{\partial x^1}+R\sinh\theta\sin\phi\frac{\partial}{\partial x^2}, \tag{A7}$$

$$\frac{\partial}{\partial\phi}=\frac{\partial x^i}{\partial\phi}\frac{\partial}{\partial x^1}=R\cosh\theta\left(-\sin\phi\frac{\partial}{\partial x^1}+\cos\phi\frac{\partial}{\partial x^2}\right). \tag{A8}$$

The induced metric is then

$$g_{\theta\theta}=-R^2, \quad g_{\theta\phi}=g_{\phi\theta}=0, \quad g_{\phi\phi}=R^2\cosh^2\theta, \tag{A9}$$

$$g_{\cdot\cdot}=\begin{matrix}\\ \theta\\ \phi\end{matrix}\overset{\begin{matrix}\theta & \phi\end{matrix}}{\begin{pmatrix}-R^2 & 0\\ 0 & R^2\cosh^2\phi\end{pmatrix}}, \quad g^{\cdot\cdot}=\begin{matrix}\\ \theta\\ \phi\end{matrix}\overset{\begin{matrix}\theta & \phi\end{matrix}}{\begin{pmatrix}-\frac{1}{R^2} & 0\\ 0 & \frac{1}{R^2\cosh^2 0}\end{pmatrix}}. \tag{A10}$$

The symbol • is used to indicate various types of indices without giving them names.

The Christoffel symbols of the unique torsion-free metric connection $\nabla_\bullet$ can be calculated as

$$\Gamma^A{}_{BC} = \tfrac{1}{2} g^{AD}(g_{BD,C} + g_{DC,B} - g_{BC,D}) \tag{A11}$$

with the nonzero components

$$\Gamma^\theta{}_{\phi\phi} = \cosh\theta \sinh\theta, \tag{A12}$$

$$\Gamma^\phi{}_{\theta\phi} = \Gamma^\phi{}_{\phi\theta} = \frac{\sinh\theta}{\cosh\theta}. \tag{A13}$$

The wave operator (Laplace–Beltrami) is then

$$\Box f = g^{AB}\nabla_A\nabla_B f = g^{AB}\left(\frac{\partial}{\partial\xi^A}\frac{\partial}{\partial\xi^B} - \Gamma^C{}_{AB}\frac{\partial}{\partial\xi^C}\right) f \tag{A14}$$

$$= -\frac{1}{R^2}\left(\frac{1}{\cosh\theta}\frac{\partial}{\partial\theta}\theta\frac{\partial}{\partial\theta} - \frac{1}{\cosh^2\theta}\frac{\partial^2}{\partial\phi^2}\right) f, \tag{A15}$$

Apart from the above intrinsic structures, the extrinsic curvature $K_A{}^B$ of the imbedding of de Sitter space into Minkowski space may be calculated, see Lemma 3.

Symmetries

The de Sitter spacetime is a homogeneous space with respect to the Lorentz group of the embedding space. The Lorentz group is generated by boosts and rotations. The generators can be given explicitly, decorated for convenience by a double index: rotation with axis x^0,

$$L_{21} = x^1\frac{\partial}{\partial x^2} - x^2\frac{\partial}{\partial x^1} = \frac{\partial}{\partial\phi}; \tag{A16}$$

boost with axis x^1,

$$L_{02} = x^0\frac{\partial}{\partial x^2} + x^2\frac{\partial}{\partial x^0} = \sin\phi\frac{\partial}{\partial\theta} + \cos\phi\tanh\theta\frac{\partial}{\partial\phi}; \tag{A17}$$

boost with axis x^2,

$$L_{01} = x^0\frac{\partial}{\partial x^1} + x^1\frac{\partial}{\partial x^0} = \cos\phi\frac{\partial}{\partial\theta} - \sin\phi\tanh\theta\frac{\partial}{\partial\phi}. \tag{A18}$$

The generators satisfy the commutation relations

$$[L_{01}, L_{21}] = L_{02}, \tag{A19}$$

$$[L_{02}, L_{21}] = -L_{01}, \tag{A20}$$

$$[L_{01}, L_{02}] = L_{21}. \tag{A21}$$

The Casimir operator is

$$L^\bullet L_\bullet = -R^2\nabla^A\nabla_A. \tag{A22}$$

The action of (the double cover of) these symmetries on spinors and spinor fields is given in the next section, after a description of spinors.

Spinors on de Sitter space

It is possible to construct spinors either intrinsically or as seen from the Minkowski space into which the de Sitter geometry is embedded.

In both cases it is useful to fix a frame (triad).

For the extrinsic description we chose

$$b_i = \frac{\partial}{\partial x^i}. \tag{A23}$$

For the intrinsic description, only two vector fields e_0, e_2 are needed but for further calculations it is useful to add a third vector field e_1, normal to the manifold in embedding space. The resulting triad is then

$$e_0 = \frac{1}{R}\frac{\partial}{\partial \theta} = \frac{1}{R}\frac{\partial x^i}{\partial \theta}\frac{\partial}{\partial x^i}, \tag{A24}$$

$$e_1 = \frac{\partial}{\partial R} = \frac{1}{R}x^i\frac{\partial}{\partial x^i}, \tag{A25}$$

$$e_2 = \frac{1}{R\cosh\theta}\frac{\partial}{\partial \phi} = \frac{1}{R\cosh\theta}\frac{\partial x^i}{\partial \phi}\frac{\partial}{\partial x^i}, \tag{A26}$$

$$e_0 = \cosh\theta\frac{\partial}{\partial x^0} + \sinh\theta\cos\phi\frac{\partial}{\partial x^1} + \sinh\theta\sin\phi\frac{\partial}{\partial x^2}, \tag{A27}$$

$$e_1 = \sinh\theta\frac{\partial}{\partial x^0} + \cosh\theta\cos\phi\frac{\partial}{\partial x^1} + \cosh\theta\sin\phi\frac{\partial}{\partial x^2}, \tag{A28}$$

$$e_2 = -\sin\phi\frac{\partial}{\partial x^1} + \cos\phi\frac{\partial}{\partial x^2}. \tag{A29}$$

The two frames coincide for

$$\theta = 0, \quad \phi = 0. \tag{A30}$$

The triad can then be chosen to generate the corresponding Clifford algebra for the Clifford generators $\not{e}_\bullet$ by the anticommutation relations

$$\not{e}_i\not{e}_j + \not{e}_j\not{e}_i = g_{ij}\mathbf{1}. \tag{A31}$$

The same anticommutation relations are satisfied by the Clifford generators corresponding to $b_\bullet$ but usually denoted by $\gamma_\bullet$ rather than by $\not{b}_\bullet$. One is free to choose a basis in the spinor space and this freedom will be used here to get the following representation of the Clifford generators $\gamma_\bullet$ (and similarly for $\not{e}_\bullet$):

$$\gamma_0 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad \gamma_1 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{A32}$$

The choice was made in such a way as to make γ_0 diagonal which seems to be useful in later computations.

Intrinsic description

The vectors e_0, e_2 are inside the de Sitter space and e_1 is orthogonal to it. e_1 can of course not be part of an intrinsic description but is useful for matters of comparison with extrinsic calculations.

The intrinsic spin connection D_A can be calculated from the connection form

$$\omega^b_{Ac} = e^b_B \nabla_A e^B_c = e^b_B \partial_A e^B_c + e^b_C \Gamma^{CB}{}_A e^B_c . \tag{A33}$$

The forms

$$e^0 = R\, d\theta, \tag{A34}$$

$$e^2 = R \cosh\theta\, d\phi \tag{A35}$$

are a basis dual to e_0, e_2,

$$\omega^0_{A2} = e^0_B \nabla_A e^B_2 = \underbrace{e^0_B \partial_A e^B_2}_{0} + e^0_C \Gamma^C{}_{AB} e^B_2 = \frac{1}{\cosh\theta} \Gamma^\theta{}_{A\phi} = \frac{1}{\cosh\theta} d\phi\, \Gamma^\theta{}_{\phi\phi} = \sinh\theta\, d\phi, \tag{A36}$$

$$\nabla_0 e_0 = 0, \quad \nabla_0 e_2 = 0, \tag{A37}$$

$$\nabla_2 e_0 = \frac{1}{R} \tanh\theta e_2, \quad \nabla_2 e_2 = \frac{1}{R} \tanh\theta e_0 . \tag{A38}$$

From the (tangent space) connection form ω_A, the spin connection form ω^S_A can be obtained as

$$\omega^S_A = \frac{1}{4} \omega^b_{Ac} \not{e}_b \not{e}^c = \frac{1}{2} \not{e}_0 \not{e}^2 \sinh\theta d\phi = \frac{1}{2} \not{e}_0 \not{e}^2 \sinh\theta \frac{e^2}{R\cosh\theta}. \tag{A39}$$

The intrinsic Dirac operator is then

$$\not{D} = \not{e}^a D_a = \not{e}^0 \frac{1}{R} \frac{\partial}{\partial\theta} + \not{e}^2 \frac{1}{R\cosh\theta} \frac{\partial}{\partial\phi} + \frac{1}{2R} \not{e}^0 \tanh\theta. \tag{A40}$$

Extrinsic description

Definition 5. *Let M be given as a submanifold in $\mathbb{R}^{n+1}$ of codimension 1, equipped with the metric induced from a global (translation invariant) metric on $\mathbb{R}^{n+1}$. The* **Levi-Civita covariant spin derivative** *(in an extrinsic basis) along a line parametrized by λ is given by*

$$\nabla_{d/d\lambda} \psi = \frac{d\psi}{d\lambda} + \frac{1}{2} \not{n} \frac{d\not{n}}{d\lambda}. \tag{A41}$$

This may be used to define an extrinsic Dirac operator, as discussed in the next section.

Comparison of extrinsic and intrinsic calculations

The intrinsic calculations proceed from the extrinsic point of view in a moving frame $e_\bullet$, related to the global frame $b_\bullet$ by orthogonal transformations. It is thus useful to know the spin matrices implementing those orthonormal transformations on spinor space.

The generators of rotations and boosts in spinor space can be constructed out of the Clifford generators γ_i by

$$\omega_{ij} = \tfrac{1}{4}[\gamma_i, \gamma_j]. \tag{A42}$$

The Clifford generators γ_i satisfy

$$[\gamma_0,\gamma_1]=2\gamma_2, \tag{A43}$$

$$[\gamma_0,\gamma_2]=-2\gamma_1, \tag{A44}$$

$$[\gamma_1,\gamma_2]=-2\gamma_0. \tag{A45}$$

It follows for the generators of rotations and boosts on the spinor space

$$[\omega_{01},\omega_{21}]=-\omega_{02}, \tag{A46}$$

$$[\omega_{02},\omega_{21}]=\omega_{01}, \tag{A47}$$

$$[\omega_{01},\omega_{02}]=-\omega_{21}. \tag{A48}$$

These are the commutation relations of the Lie algebra $\mathrm{sl}_2(\mathbb{R})$ [see Sec. IV for additional facts on $\mathrm{sl}_2(\mathbb{R})$ and on the corresponding Lie group $\mathrm{Sl}_2(\mathbb{R})$], the generators of (the double cover of) the group of Lorentz transformations.

The boost and rotation spin matrices are

$$S_{01-\mathrm{boost}}=\begin{pmatrix} e^{\theta/2} & 0 \\ 0 & e^{-\theta/2}\end{pmatrix},\quad S^{-1}_{01-\mathrm{boost}}=\begin{pmatrix} e^{-\theta/2} & 0 \\ 0 & e^{\theta/2}\end{pmatrix}, \tag{A49}$$

$$S_{02-\mathrm{boost}}=\begin{pmatrix} \cosh\left(\frac{\theta}{2}\right) & \sinh\left(\frac{\theta}{2}\right) \\ \sinh\left(\frac{\theta}{2}\right) & \cosh\left(\frac{\theta}{2}\right)\end{pmatrix},\quad S^{-1}_{02-\mathrm{boost}}=\begin{pmatrix} \cosh\left(\frac{\theta}{2}\right) & -\sinh\left(\frac{\theta}{2}\right) \\ -\sinh\left(\frac{\theta}{2}\right) & \cosh\left(\frac{\theta}{2}\right)\end{pmatrix}, \tag{A50}$$

$$S_{12-\mathrm{rotation}}=\begin{pmatrix} \cos\left(\frac{\phi}{2}\right) & \sin\left(\frac{\phi}{2}\right) \\ -\sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right)\end{pmatrix},\quad S^{-1}_{12-\mathrm{rotation}}=\begin{pmatrix} \cos\left(\frac{\phi}{2}\right) & -\sin\left(\frac{\phi}{2}\right) \\ \sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right)\end{pmatrix}. \tag{A51}$$

As the fact that the frames $b_\bullet$, $e_\bullet$ agree in a point [see (A30)] and from the knowledge of the spin matrices, the the transformation from $b_\bullet$ the global frame of Minkowski space to a local frame $e_\bullet$ can be calculated as $S_{\theta,\phi}=S_{12-\mathrm{rotation}}S_{01-\mathrm{boost}}$,

$$S_{\theta,\phi}=\begin{pmatrix} e^{\theta/2}\cos\left(\frac{\phi}{2}\right) & \frac{\sin(\phi/2)}{e^{\theta/2}} \\ -\left(e^{\theta/2}\sin\left(\frac{\phi}{2}\right)\right) & \frac{\cos(\phi/2)}{e^{\theta/2}}\end{pmatrix},\quad S^{-1}_{\theta,\phi}=\begin{pmatrix} \frac{\cos(\phi/2)}{e^{\theta/2}} & -\left(\frac{\sin(\phi/2)}{e^{\theta/2}}\right) \\ e^{\theta/2}\sin\left(\frac{\phi}{2}\right) & e^{\theta/2}\cos\left(\frac{\phi}{2}\right)\end{pmatrix}. \tag{A52}$$

This is the spin matrix that allows an explicit comparison of extrinsic and intrinsic calculations.

At times, it is also useful to know the spin matrix implementing the reflection exchanging b_1 and b_2:

$$S_{1\leftrightarrow 2}=S^{-1}_{1\leftrightarrow 2}=\begin{pmatrix} -1 & 1 \\ 1 & 1\end{pmatrix}. \tag{A53}$$

The full action of the symmetry group $\mathrm{Sl}_2(\mathbb{R})$ on spinor fields is given by the simultaneous action on the spinor space and on the spacetime manifold. The full symmetry generators are

$$T_{ij} = -L_{ij} + \omega_{ij} \tag{A54}$$

and satisfy the commutation relations

$$[T_{01}, T_{21}] = -T_{02}, \tag{A55}$$

$$[T_{02}, T_{21}] = T_{01}, \tag{A56}$$

$$[T_{01}, T_{02}] = -T_{21} \tag{A57}$$

analogous to (A19)–(A21) and (A46)–(A48). From the point of view of representation theory, it is useful to work with the rising and lowering operators

$$T_{\pm} = T_{01} \mp i T_{02}, \tag{A58}$$

satisfying

$$[T_{\pm}, T_{21}] = -T_{02} \mp i T_{01} = \mp T_{\pm}, \tag{A59}$$

$$[T_{+}, T_{-}] = -2i T_{21}. \tag{A60}$$

The Dirac operator on de Sitter space

In the following, it is shown that the Dirac operator on Minkowski space commutes with the generators of the Lorentz group action on Minkowski space spinors. Then the Dirac operator on a surface of codimension 1 in flat space is defined and re-expressed in terms of the intrinsic curvature of the surface and calculated for spacelike hyperboloids in Minkowski space. It is further shown that the Dirac operators on the hyperboloids also commute with the generators of the Lorentz group.

Lemma 2. *The Dirac operator* $\not{D}_M = \gamma^i \partial_i$ *commutes with the symmetry generators* $T_{ij} = -L_{ij} + \omega_{ij}$.

Proof. By definition

$$L_{ij} = x^k g_{k[i} \partial_{j]} \quad \text{with } g_{k[i} \partial_{j]} = g_{ki} \partial_j - g_{kj} \partial_i, \tag{A61}$$

$$\omega_{ij} = \tfrac{1}{4}[\gamma_i, \gamma_j]. \tag{A62}$$

A direct calculation gives then

$$[\not{D}_M, T_{ij}] = -\gamma^l (\partial_l L^k_{ij}) \partial_k - [\omega_{ij}, \gamma^k] \partial_k = \underbrace{(\gamma_i \delta^k_j - \gamma_j \delta^k_i - \tfrac{1}{4}[[\gamma_i, \gamma_j], \gamma^k])}_{\text{vanishes}} \partial_k. \tag{A63}$$

The coordinates of the commutator vanish for the following reasons.

If $i = j$ then it vanishes due to antisymmetry in i, j.

If i, j, k are all different then the Kronecker δs vanish and $[\gamma_i, \gamma_j]$ commutes with γ_k, thus everything vanishes.

If $k = i \neq j$ then δ^k_j vanishes and

$$[[\gamma_i, \gamma_j], \gamma^k] = 2[\gamma_i \gamma_j, \gamma^k] = -2\{\gamma_i, \gamma^k\} \gamma_j = -4 \delta^k_i \gamma_j,$$

and the resulting term cancels with $-\gamma_j \delta^k_i$.

If $k = j \neq i$ then use antisymmetry in i, j to transform it into the previous case.

Definition 6. (*The Dirac operator on a surface of codimension 1.*) *Let e_A be a Vielbein on the $n-1$-dimensional surface in n-dimensional flat space and let $\gamma^\bullet$ be global generators of the global Clifford algebra. Then the Dirac operator on the surface is given by*

$$\not{D} = \gamma^A e_A^B \nabla_B , \tag{A64}$$

where $\nabla_\bullet$ is the extrinsic connection of Definition 5.

A direct calculation, using the definition $K_A{}^B := e_A^C \partial_C n^B$ of the extrinsic curvature $K_A{}^B$ gives

$$\not{D}\psi = \gamma^A e_A^B \partial_B \psi + \tfrac{1}{2}\gamma^A e_A^B \not{n} \partial_B \not{n} \psi \tag{A65}$$

$$= \not{e}^B \partial_B \psi + \tfrac{1}{2} \underbrace{\not{e}^B \not{n}}_{\text{anticommute}} \partial_B \not{n} \psi \tag{A66}$$

$$= \not{e}^B \partial_B \psi - \tfrac{1}{2} \not{n} \underbrace{\not{e}^B \partial_B \not{n}}_{\not{e}^A K_{AB} \not{e}^B} \tag{A67}$$

$$= \not{e}^B \partial_B \psi - \tfrac{1}{2} K_A{}^A \not{n} . \tag{A68}$$

In the following lemma, the needed extrinsic curvature is calculated.

Lemma 3. *The extrinsic curvature tensor $K_A{}^B$ and its trace $K_A{}^A$ of the hyperboloid $-(x^0)^2 + \Sigma_i (x^i)^2 = R^2$ in n-dimensional Minkowski space are given by*

$$K_A{}^B = \frac{1}{R} \delta_A^B , \tag{A69}$$

$$K_A{}^A = \frac{n-1}{R} . \tag{A70}$$

Proof. Due to the transitive action of the symmetries on the hyperboloid, it is sufficient to calculate the formulas in one point only which may conveniently be chosen to be

$$x^\alpha = (0, R, 0, 0, \ldots, 0)$$

with normalized coordinates around this point,

$$x^A = \frac{1}{R}(x^0, x^2, x^3, \ldots, x^{n-1}),$$

and with the normal vector

$$n^\alpha = \frac{1}{R}(x^0, x^1 x^2, x^3, \ldots, x^{n-1}).$$

Then a simple calculation gives

$$K_A{}^B = \frac{dn^B}{dx^A} = \frac{1}{R} \delta_A^B . \tag{A71}$$

Corollary 4. On the hyperboloid $-(x^0)^2 + \Sigma_i (x^i)^2 = R^2$ in n-dimensional Minkowski space, the Dirac operator $\not{D}$ is given by

$$\not{D} = \not{e}^B \partial_B - \frac{n-1}{2R} \not{n}. \tag{A72}$$

Corollary 5. On the hyperboloid $-(x^0)^2+(x^i)^2=R^2$ *in n-dimensional Minkowski space, the Dirac operator* $\not{D}$ *can be induced from the Dirac operator* $\not{D}_M$ *on Minkowski space by extending the spinors outside the hyperboloid by (value on hyperboloid)*$\times e^{-n-1/2R(r-R)}$ *along the rays* λx^α, *with r being the spacetime interval as measured form the origin.*

Corollary 6. The Dirac operator $\not{D}$ *on the hyperboloid commutes with the symmetry generators* T_{ij}.

Proof. Note first that the symmetry generators T_{ij} preserve the hyperboloid $-(x^0)^2+(x^i)^2=R^2$ in n-dimensional Minkowski space. The Minkowski space Dirac operator $\not{D}_M$ commutes with the symmetry generators T_{ij}. From the previous corollary, $\not{D}$ can be understood to be a restriction of $\not{D}_M$ to a subset of functions behaving radially as $e^{-(n-1)/2R(r-R)}$.

The implementation of symmetries on the spinor field on de Sitter

The de Sitter hyperboloid embedded in Minkowski space is left invariant under the action of the Lorentz group and thus an an action of the Lorentz group can be given on spinor fields on this hyperboloid.

A representation of the Lorentz group can be given by restricting to the spinor fields ψ which are solutions of the Dirac equation:

$$(\not{D} - m)\psi = 0. \tag{A73}$$

This is reasonable, since the Dirac operator commutes with the generators of the Lorentz group and since the space of solutions of the Dirac equation is equipped with an invariant sesquilinear positive definite inner product:

$$(\psi_1, \psi_2) = \int_\Sigma \overline{\psi_1 \gamma^A} \psi_2 \, d_A\Sigma, \tag{A74}$$

with Σ being an arbitrary spacelike Cauchy surface on the hyperboloid.

The Hilbert space of the representation is then the classical phase space of spinor fields, the space of initial values of the spinor field on a Cauchy surface satisfying the Dirac equation. In order to give the action of the Lorentz group on the initial values, the Dirac equation has to be used.

The Cauchy hypersurface will be taken a sphere S^{n-2} on the hyperboloid at $x^0=$constant. It has a normal vector $\vec{n}=1/R\,(x^0,x^1,\ldots,x^{n-1})$ and an (unnormalized) spatial normal vector $\vec{r}=(0,x^1,\ldots,x^{n-1})$. The time evolution vector will be taken as

$$\frac{\partial}{\partial t} := e_0 = \frac{1}{R}\frac{\partial}{\partial \theta} = \cosh\theta \frac{\partial}{\partial x^0} + \sinh\theta \frac{\vec{r}}{|\vec{r}|} \tag{A75}$$

$$= \frac{1}{\cosh\theta}\left(\frac{\partial}{\partial x^0} + \sinh\theta \vec{n}\right). \tag{A76}$$

The Dirac operator can then be written as

$$\not{D} = \not{e}^0 \partial_t + \not{e}^I \partial_I - \frac{n-1}{2R}\not{n}, \tag{A77}$$

and using the Dirac equation

$$(\not{D} - m)\psi = 0, \tag{A78}$$

the infinitesimal time evolution can be given as

$$\partial_t = [\not{e}_J, \not{e}_0] g^{JI} \partial_I + \frac{n-1}{2R} \not{e}_0 \not{n} + m \not{e}_0 \tag{A79}$$

$$= \underbrace{\frac{\not{n}}{R \cosh\theta} L_{21} + \frac{1}{R} \not{e}_0 \not{n} + m \not{e}_0}_{\text{for 2-dim. de Sitter space}}. \tag{A80}$$

The generators T_{ij} of the Lorentz transformations in three-dimensional Minkowski space acting on spinor fields on the de Sitter space of radius R can now be expressed in terms of ∂_t, ∂_ϕ which in turn can be expressed in terms of the Cartan subalgebra generator T_{21}, eliminating all derivatives in the following formulas:

$$\frac{\partial}{\partial t} = \frac{\not{n}}{R \cosh\theta} (L_{21} - \not{e}_0 \cosh\theta) + m \not{e}_0 \tag{A81}$$

$$= \frac{\not{n}}{R \cosh\theta} \left(- T_{21} + \frac{1}{2} \gamma_0 - \not{e}_0 \cosh\theta \right) + m \not{e}_0, \tag{A82}$$

$$\frac{\partial}{\partial \phi} = - T_{21} + \frac{1}{2} \gamma_0, \tag{A83}$$

$$\omega_{21} = \tfrac{1}{2} \gamma_0, \tag{A84}$$

$$\omega_{02} = - \tfrac{1}{2} \gamma_1, \tag{A85}$$

$$\omega_{01} = \tfrac{1}{2} \gamma_2, \tag{A86}$$

$$L_{21} = \frac{\partial}{\partial \phi}, \tag{A87}$$

$$L_{02} = R \sin\phi \frac{\partial}{\partial t} + \cos\phi \tanh\theta \frac{\partial}{\partial \phi}, \tag{A88}$$

$$L_{01} = \cos\phi \frac{\partial}{\partial \theta} - \sin\phi \tanh\theta \frac{\partial}{\partial \phi}, \tag{A89}$$

$$T_{21} = - \frac{\partial}{\partial \phi} + \frac{1}{2} \gamma_0, \tag{A90}$$

$$T_{02} = - R \sin\phi \frac{\partial}{\partial t} - \cos\phi \tanh\theta \frac{\partial}{\partial \phi} - \frac{1}{2} \gamma_1, \tag{A91}$$

$$T_{01} = - R \cos\phi \frac{\partial}{\partial t} + \sin\phi \tanh\theta \frac{\partial}{\partial \phi} + \frac{1}{2} \gamma_2. \tag{A92}$$

There are now two natural bases in the space of spinors on $S^{n-2}(x^0) = S^1(x^0)$, namely the eigenbasis $|L{:}n, \pm\rangle$ of L_{21} and the eigenbasis $|T{:}n, \pm\rangle$ of T_{21}. The first choice looks to be simpler, if written in the local basis of eigenvectors of γ_0:

$$|L{:}n,+\rangle=\begin{pmatrix} e^{in\phi} \\ 0 \end{pmatrix}, \tag{A93}$$

$$|L{:}n,-\rangle=\begin{pmatrix} 0 \\ e^{-in\phi} \end{pmatrix}. \tag{A94}$$

with n being integers $\dots,-2,-1,0,+1,+2,\dots$ and is maybe somewhat easier to visualize. Compare it with the second basis

$$|T{:}n,+\rangle=\begin{pmatrix} e^{-i(n-1/2)\phi} \\ 0 \end{pmatrix}, \quad |T{:}n,-\rangle=\begin{pmatrix} 0 \\ e^{-i(n+1/2)\phi} \end{pmatrix}, \tag{A95}$$

with n being half-integers $\dots,-\frac{5}{2},-\frac{3}{2},-\frac{1}{2},+\frac{1}{2},+\frac{3}{2},+\frac{5}{2},\dots$.

However it is more appropriate to use the second one since it is the full symmetry generators T_{ij} that are to play the key role in the representation theory of the symmetry group; the generators L_{ij} may not exist on the spinor bundle of a higher dimensional example, due to its nontriviality and is thus not the right concept to be used. To give a meaning to L_{ij} one would have to enlarge the spinor bundle, e.g., by adding to it an inverse bundle.

Note 3. For the reasons given above, the calculations of the action of the symmetry generators $T_{\bullet}$ will be continued in the basis $|T{:}n,\pm\rangle$. But for completeness, analogous results in the basis $|L{:}n,\pm\rangle$ are stated here, in advance,

$$T_{21}|L{:}n,+\rangle=\frac{i}{2}(1-2n)|L{:}n,+\rangle,$$

$$T_{21}|L{:}n,-\rangle=\frac{i}{2}(-1-2n)|L{:}n,-\rangle,$$

$$T_{01}|L{:}n,+\rangle=\tfrac{1}{2}[n|L{:}n,-\rangle+(n-1)|L{:}n-2,-\rangle-is|L{:}n+1,+\rangle-is|L{:}n-1,+\rangle],$$

$$T_{01}|L{:}n,-\rangle=\tfrac{1}{2}[-n|L{:}n,+\rangle-(n+1)|L{:}n+2,+\rangle+is|L{:}n+1,-\rangle+is|L{:}n-1,-\rangle],$$

$$T_{02}|L{:}n,+\rangle=\frac{i}{2}[-n|L{:}n,-\rangle+(n-1)|L{:}n-2,-\rangle+is|L{:}n+1,+\rangle-is|L{:}n-1,+\rangle],$$

$$T_{02}|L{:}n,-\rangle=\frac{i}{2}[-n|L{:}n,+\rangle+(n+1)|L{:}n+2,+\rangle-is|L{:}n+1,-\rangle+is|L{:}n-1,-\rangle],$$

$$T_{+}|L{:}n,+\rangle=(n-1)|L{:}n-2,-\rangle-is|L{:}n-1,+\rangle, \tag{A96}$$

$$T_{+}|L{:}n,-\rangle=-n|L{:}n,+\rangle+is|L{:}n-1,-\rangle, \tag{A97}$$

$$T_{-}|L{:}n,+\rangle=n|L{:}n,-\rangle-is|L{:}n+1,+\rangle, \tag{A98}$$

$$T_{-}|L{:}n,-\rangle=-(n+1)|L{:}n+2,+\rangle+is|L{:}n+1,-\rangle. \tag{A99}$$

We now proceed with the calculation of the action of the $\mathrm{sl}_2(\mathbb{R})$-symmetries (Lorentz symmetries) on the space of solutions of the Dirac equation in the basis $|T{:}n,\bullet\rangle$.

By definition,

$$T_{21}|T{:}n,\pm\rangle=in|T{:}n,\pm\rangle, \tag{A100}$$

$$\not{e}_0 = \cosh\theta \underbrace{\not{b}^0}_{=\gamma^0} + \sinh\theta \frac{\vec{\not{r}}}{R}, \tag{A101}$$

$$\not{n} = \sinh\theta \not{b}^0 + \cosh\theta \frac{\vec{\not{r}}}{R}, \tag{A102}$$

$$\frac{\vec{\not{r}}}{R} := \frac{x^1}{R}\gamma_1 + \frac{x^2}{R}\gamma_2 = e^{i\phi}(\gamma_1 - i\gamma_2) + e^{-i\phi}(\gamma_1 + i\gamma_2) \tag{A103}$$

$$= -ie^{i\phi}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + ie^{-i\phi}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{A104}$$

The actions on the basis are

$$\frac{\vec{\not{r}}}{R}|T{:}n,\pm\rangle := \pm i|T{:}n,\mp\rangle, \tag{A105}$$

$$\not{e}_0|T{:}n,\pm\rangle := \pm i\cosh\theta|T{:}n,\pm\rangle \pm i\sinh\theta|T{:}n,\mp\rangle, \tag{A106}$$

$$\not{n}|T{:}n,\pm\rangle := \pm i\sinh\theta|T{:}n,\pm\rangle \pm i\cosh\theta|n,\mp\rangle. \tag{A107}$$

A direct calculation of $\partial/\partial\theta = R\,(\partial/\partial t)$ from (A82) using (A104)–(A106) gives

$$\frac{\partial}{\partial\theta}|T{:}n,\pm\rangle = \left(\left(\pm n - \frac{1}{2}\right)\tanh\theta \pm iRm\cosh\theta\right)|T{:}n,\pm\rangle \tag{A108}$$

$$+\left(\left(\pm n + \frac{1}{2}\right) \pm iRm\sinh\theta\right)|T{:}n,\mp\rangle, \tag{A109}$$

$$T_+|T{:}n,\pm\rangle = [(n+\tfrac{1}{2})\tanh\theta(1\mp 1) \mp iRm\cosh\theta]|T{:}n+1,\pm\rangle \tag{A110}$$

$$\mp[n+\tfrac{1}{2}+iRm\sinh\theta]|T{:}n+1,\mp\rangle, \tag{A111}$$

$$T_-|T{:}n,\pm\rangle = [-(n-\tfrac{1}{2})\tanh\theta(1\pm 1) \mp iRm\cosh\theta]|T{:}n-1,\pm\rangle \tag{A112}$$

$$\mp[n-\tfrac{1}{2}+iRm\sinh\theta]|T{:}n-1,\mp\rangle. \tag{A113}$$

In matrix notation, on the subspace $|T{:}n,\bullet\rangle$, one gets

$$T_+(n) = \begin{pmatrix} -iRm\cosh\theta & n+\frac{1}{2}+iRm\sinh\theta \\ -(n+\frac{1}{2}+iRm\sinh\theta) & 2(n+\frac{1}{2})\tanh\theta + iRm\cosh\theta \end{pmatrix} u, \tag{A114}$$

$$T_-(n) = \begin{pmatrix} -2(n-\frac{1}{2})\tanh\theta - iRm\cosh\theta & n-\frac{1}{2}+iRm\sinh\theta \\ -(n-\frac{1}{2}+iRm\sinh\theta) & iRm\cosh\theta \end{pmatrix} u^*, \tag{A115}$$

and the time vector $\not{e}_0$ is given by

$$\not{e}_0 = i\begin{pmatrix} \cosh\theta & -\sinh\theta \\ \sinh\theta & -\cosh\theta \end{pmatrix}. \tag{A116}$$

These matrices are understood to be given with respect to the basis $|T{:}n,\pm\rangle$. This basis is however not orthonormal. In order to find an orthogonal basis which would be suitable for comparison with representation–theoretic calculations, the structure of the inner product on the space of spinor fields has to be clarified.

Spacetime spinor fields are equipped with a Hermitean inner product, the Dirac product $B(\bullet,\bullet)$ which is given as the intertwiner B

$$\gamma_\mu^+ B = -B\gamma_\mu, \tag{A117}$$

$$B = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}, \tag{A118}$$

so that the inner product can be calculated as

$$B(\psi,\varphi) = (\overline{\psi}_1 \quad \overline{\psi}_2)\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \tag{A119}$$

Note 4. There is a second possibility to choose a Hermitean inner product A by taking the opposite sign in the intertwining relation:

$$\gamma_\mu^+ A = +A\gamma_\mu. \tag{A120}$$

But this is irreconcilable with other choices already made or to be required, in particular, the Dirac operator was defined to be $\not{D} = \gamma^\mu \partial_\mu$ rather than $i\gamma^\mu\partial_\mu$; the Dirac equation was chosen to be $(\not{D} - m)\psi = 0$; the Dirac operator is required to be formally self-adjoint,

$$B(\psi, \not{D}\varphi) - B(\not{D}\psi, \varphi) = \partial_\mu B(\psi, \gamma^\mu \varphi);$$

The physical time directions given by the metric are negative definite (rather than positive definite), i.e., $p_\mu p^\mu = -m^2$ for an approximate plane wave (rather than $p_\mu p^\mu = +m^2$)

It follows from the global hyperbolicity of the spacetime and the formal self-adjointness of the Dirac operator that the following is a well-defined Hermitean inner product on the space of solutions of the Dirac equation, independent of the spacelike Cauchy surface Σ, see (A74):

$$(\psi,\varphi) = \int_{S^1(\theta = \text{constant})} B(\psi(\phi), e^0 \varphi(\phi))\, d\phi. \tag{A121}$$

With respect to this inner product, the normalized eigenvectors $e_{\pm i}$ of $\not{e}_0$ for the eigenvalues $\pm i$ are

$$e_{\pm i} = \frac{1}{\sqrt{2\cosh\theta \pm 2}}\begin{pmatrix} \cosh\theta \pm 1 \\ \sinh\theta \end{pmatrix}, \tag{A122}$$

and in this orthogonal eigenbasis of $\not{e}_0$ we have

$$\not{e}_0 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \tag{A123}$$

$$\not{e}_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{A124}$$

$$T_+(n)=\begin{pmatrix} -iRm+(n+\frac{1}{2})\tanh\theta & \frac{1}{\cosh\theta}(n+\frac{1}{2}) \\ -\frac{1}{\cosh\theta}(n+\frac{1}{2}) & iRm+(n+\frac{1}{2})\tanh\theta \end{pmatrix}, \tag{A125}$$

$$T_-(n)=\begin{pmatrix} -iRm-(n-\frac{1}{2})\tanh\theta & \frac{1}{\cosh\theta}(n-\frac{1}{2}) \\ -\frac{1}{\cosh\theta}(n-\frac{1}{2}) & iRm-(n-\frac{1}{2})\tanh\theta \end{pmatrix}, \tag{A126}$$

and in particular

$$u_+=T_+(+\tfrac{1}{2})=\begin{pmatrix} -iRm+\tanh\theta & \frac{1}{\cosh\theta} \\ -\frac{1}{\cosh\theta} & iRm+\tanh\theta \end{pmatrix}, \tag{A127}$$

$$u_-=T_-(-\tfrac{1}{2})=\begin{pmatrix} -iRm+\tanh\theta & -\frac{1}{\cosh\theta} \\ \frac{1}{\cosh\theta} & iRm+\tanh\theta \end{pmatrix}. \tag{A128}$$

These data may be compared with the data of the de Sitter spectral quadruples obtained in Sec. V.

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Baxter T-Q equation for shape invariant potentials. The finite-gap potentials case

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The Darboux transformation applied recurrently on a Schrödinger operator generates what is called a *dressing chain*, or from a different point of view, a set of supersymmetric shape invariant potentials. The finite-gap potential theory is a special case of the chain. For the finite-gap case, the equations of the chain can be expressed as a time evolution of a Hamiltonian system. We apply Sklyanin's method of separation of variables to the chain. We show that the classical equation of the separation of variables is the Baxter T-Q relation after quantization. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1426689]

I. INTRODUCTION

What is the most universal method of solving completely integrable models? From Sklyanin's point of view[1] it is the separation of variables in its most general form. Therefore, it is desirable to understand old methods of integration in the light of the modern approach to the separation of variables. One of the most important ''old'' techniques applied with success to many physical and mathematical problems is the Darboux transformation. In short, the two main themes of this paper can be best described by two keywords: The Darboux transformation and the Sklyanin method of separation of variables. The Darboux transformation is a fundamental tool in the supersymmetric approach to quantum mechanics and in the theory of dressing chains.[2,3] Though our example is different from the DST model studied in Ref. 4, this paper and Ref. 4 are closely related. The Sklyanin method aims to connect the separation of variables as we know it from the Hamiltonian mechanics with the new techniques of exactly solving mathematical physics problem, namely the Inverse Scattering Method and its quantum version.[5] The worked example in this paper is the dressing chain representation of the finite-gap potential theory. We review the main ideas from the Darboux transformations with an emphasis on the Hamiltonian view-point on the finite-gap theory, following Veselov and Shabat.[2] We then work the Sklyanin method[1,6,7] on the finite-gap theory. We find the canonical separated variables for the dressing chain representation of the finite-gap potential theory. From the Quantum Inverse Scattering Theory point of view, the equation for the separated variables is the classical version of the Baxter T-Q equation. Then the quantum version of the finite-gap theory is presented, together with the corresponding R-matrix and the Baxter Q-operator. The conclusions and outlook will close the paper.

II. THE DARBOUX TRANSFORMATION AND THE HAMILTONIAN APPROACH FOR THE FINITE-GAP THEORY

Consider the Schrödinger operator for a potential $u(x)$, $\mathcal{H}=-D^2+u(x)$ where $D\equiv d/dx$. Factorize it as a product of two first order operators

$$\mathcal{H}=A^*A, \tag{2.1}$$

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where $A=D-f(x)$ and $A^*=-D-f(x)$. The Darboux transformation sends $\mathcal{H}_1=A^*A$ into $\mathcal{H}_2=AA^*+\alpha\mathbf{1}$ where $\mathbf{1}$ is the identity operator and α is a constant. The functions f_1 and f_2 obtained from the factorization

$$\mathcal{H}_i=-(D+f_i)(D-f_i), \tag{2.2}$$

are related by the equation

$$(f_1+f_2)'=f_1^2-f_2^2+\alpha, \tag{2.3}$$

where the prime means differentiation with respect to x. From the supersymmetric quantum-mechanics point of view, Eq. (2.3) is exactly the shape invariance condition,[3] written in terms of the superpotentials $W_i=-f_i$.

We can continue this process of factorization and Darboux transformation and obtain a chain of equations

$$(f_i+f_{i+1})'=f_i^2-f_{i+1}^2+\alpha_i \quad i=1,2,\ldots. \tag{2.4}$$

This chain is called a *dressing chain*. In what follows we will consider only periodic chains

$$f_i=f_{i+N}, \quad \alpha_i=\alpha_{i+N}, \tag{2.5}$$

where the period N is a positive integer. Supersymmetrically speaking, periodic chains correspond to the cyclic shape invariant potentials.[8] The properties of the dressing chain depend drastically on the period N and the sum $\alpha=\alpha_1+\cdots+\alpha_N$. There are four cases to be considered depending if N is even or odd and α is equal to zero or not. The finite-gap theory, to be studied in this paper, corresponds to the case N odd and $\alpha=0$. In this case the chain is a completely integrable Hamiltonian system. We will use for the case $\alpha=0$ instead of the constant α_i, the constants β_i related with α by $\beta_i-\beta_{i+1}=\alpha_i$. If we regard the variable x in $f_i(x)$ as a *time* variable, then the dressing chain expresses the time evolution of the variables $f_i(x)$, $i=1,\ldots,N$. Their evolution is generated by the Hamiltonian

$$H=\sum_{i=1}^{N}\left(\tfrac{1}{3}f_i^3+\beta_i f_i\right), \tag{2.6}$$

with the Poisson bracket

$$\{f_i,f_j\}=(-1)^{(j-i)\mathrm{mod}N}, \tag{2.7}$$

$$\{f_i,f_i\}=0. \tag{2.8}$$

This Poisson bracket is not canonical. To obtain canonical variables, first let us denote by g_i a set of variables defined by

$$g_i=f_i+f_{i+1}, \tag{2.9}$$

with the Poisson structure

$$\{g_i,g_{i-1}\}=1, \tag{2.10}$$

all other brackets being zero. Though the variables g_i seem to be redundant at this point, later on they will prove to be useful. Now, the canonical variables (X_i,x_i)

$$\{X_i,X_j\}=\{x_i,x_j\}=0, \quad \{X_i,x_j\}=\delta_{ij}, \tag{2.11}$$

will generate the Poisson structure for the variables g_i if

$$g_i = X_i + x_{i+1}. \tag{2.12}$$

As we mentioned before, the finite-gap case ($N=2n+1=$odd) is completely integrable. Therefore, the Hamiltonian responsible for the time evolution belongs to a set of n-independent involutive Hamiltonians. To show this, we use the method of inverse scattering theory. The Lax matrix build on canonical variables (X_i, x_i) is

$$L_i^{(x)}(u) = \begin{pmatrix} x_i & 1 \\ x_i X_i + \beta_i + u & X_i \end{pmatrix}, \tag{2.13}$$

where $(x) \equiv (X_i, x_i)$ and u is a complex parameter. Then we construct the monodromy matrix

$$L^{(x)}(u) = \prod_{i=N}^{1} L_i^{(x)}(u) = L_N^{(x)}(u) L_{N-1}^{(x)}(u) \cdots L_1^{(x)}(u) \tag{2.14}$$

and take its trace

$$\tau_N(u) = TrL(u). \tag{2.15}$$

The trace $\tau_N(u)$ generates the set of involutive Hamiltonians

$$\tau_N(u) = H_1 u^n + H_3 u^{n-1} + \cdots + H_{2N+1}. \tag{2.16}$$

The Hamiltonian H_3 is just the Hamiltonian for the chain. The fact that the set of the Hamiltonians is involutive, is a consequence of the classical r-matrix identity. Denoting by id_2 the unit 2×2 matrix and introducing the notations for the tensor products $l^{(1)} = l \otimes id_2$, $l^{(2)} = id_2 \otimes l$, the r-matrix identity for the Lax matrices $l_i(u) = L_i^{(x)}(u)$

$$\{l_i^{(1)}(u_1), l_j^{(2)}(u_2)\} = [r_{12}(u_1 - u_2), l_i^{(1)}(u_1) l_i^{(2)}(u_2)]\delta_{ij}, \tag{2.17}$$

where

$$r_{12}(u) = -\frac{1}{u}\mathcal{P}_{12}, \tag{2.18}$$

and $\mathcal{P}_{12}$ is the permutation operator in $\mathbf{C}^2 \otimes \mathbf{C}^2$. It is important to notice that although the Lax matrix is written in terms of the variable (X,x), the Hamiltonians H_i (2.16) depend only on the variables g_i, $i=1,2,\ldots,N$. Moreover, it is possible to generate the Hamiltonians H_i as a trace of a monodromy matrix written directly in terms of the chain variables f_i

$$F(u) = \prod_{i=1}^{N} \begin{pmatrix} f_i & 1 \\ f_i^2 + \beta_i + u & f_i \end{pmatrix}, \tag{2.19}$$

$$\tau_N(u) = TrF(u). \tag{2.20}$$

The connection of the dressing chain with the finite-gap theory for the Schrödinger operators is described in Ref. 2. For the finite-gap theory see also[9,10] and the references therein. Here we will emphasize only those notions which will be important later on. To each solution $f_i(x)$ of the dressing chain, or in other words, to each solution of the time evolution of the Hamiltonian system, corresponds a sequence of N finite-gap Schrödinger operators

$$\mathcal{H}_i = -D^2 + u_i(x), \tag{2.21}$$

where the potentials $u_i(x)$ are given by

$$u_i = f_i' + f_i^2. \tag{2.22}$$

The spectral curve of these operators is the spectral curve of the monodromy matrix $F(u)$

$$\det(F(\lambda)-\mu\,\mathbf{1})=0, \tag{2.23}$$

where **1** is the unit matrix, and it can be written as

$$\mu^2-\tau_N(\lambda)\,\mu-\prod_{i=1}^{N}(\lambda+\beta_i)=0. \tag{2.24}$$

From the Darboux transformation we can obtain a recurrence relation between the logarithmic derivatives of the Bloch eigenfunctions. The Bloch eigenfunctions ψ_i of the operator $\mathcal{H}_i$ are given by

$$\mathcal{H}_i\psi_i=(\lambda+\beta_i)\psi_i\,. \tag{2.25}$$

Due to the Darboux transformation, two successive Bloch eigenfunctions are connected through

$$\psi_{i+1}=(D-f_i)\psi_i\,. \tag{2.26}$$

This implies that for the logarithmic derivatives $\chi_i=D\ln\psi_i$ we have the recurrence

$$\chi_i=f_i+\frac{\beta_i+\lambda}{f_i+\chi_{i+1}}. \tag{2.27}$$

III. SKLYANIN METHOD OF SEPARATION OF VARIABLES

To understand the Sklyanin method,[1,5–7] let us start with an old example. For a Hamiltonian of the form

$$H=\tfrac{1}{2}(p_1^2+\cdots+p_n^2)+\tfrac{1}{2}(\omega_1q_1^2+\cdots+\omega_nq_n^2), \tag{3.1}$$

we notice that the variables are not only *canonical*, $\{p_i,q_j\}=\delta_{ij}$ but also *separated*, i.e., each pair $(p_i(t),q_i(t))$ lies on the curve

$$p_i^2+\omega_iq_i^2=\text{const.} \tag{3.2}$$

In general, let us consider a Hamiltonian system having d degrees of freedom and integrable in Liouville's sense. This means that it is given a $2d$-dimensional symplectic manifold and d independent Hamiltonians H_i in involution

$$\{H_i,H_j\}=0,\quad i,j=1\cdots d. \tag{3.3}$$

A system of canonical variables $\lambda\equiv\{\lambda_i\}_{i=1}^d$ and $\mu\equiv\{\mu_i\}_{i=1}^d$ satisfying

$$\{\lambda_i,\lambda_j\}=\{\mu_i,\mu_j\}=0,\quad \{\lambda_i,\mu_j\}=\delta_{ij}\,, \tag{3.4}$$

will be called *separated* if there exists d relations of the form

$$W_j(\lambda_j,\mu_j,H_1,\ldots,H_d)=0. \tag{3.5}$$

For the dressing chain the variables (X,x) are canonical but not separated. We can raise then the question of how to find *canonical separated* variables for the dressing chain. If the integrable system is solvable via the Inverse Scattering Method then we can use a method proposed by Sklyanin to find the transformation from the canonical variables (X,x) to the canonical separated variables (λ,μ). The desired transformation will be obtained as a composition of Bäcklund transformations. The next section is devoted to the Bäcklund transformation for the dressing chain.

IV. BÄCKLUND TRANSFORMATIONS

Following Sklyanin, we need to find a canonical transformation (we will use also the name Bäcklund transformation) from the variables (X,x) to (Y,y). The important property is that the canonical transformation will depend on the spectral parameter λ. This parameter λ will allow us to find at the end the canonical separated variables. Being a canonical transformation, the Poisson structure and the set of Hamiltonians H_i must remain unchanged when expressed in the variable (Y,y). Since Lax matrix $L(u)$ is a monodromy matrix

$$L^{(x)}(u)=L_N^{(x)}(u)\cdots L_2^{(x)}(u)L_1^{(x)}(u), \tag{4.1}$$

we can transform the Lax matrices at each site $L_i^{(x)}(u)$

$$M_i(u-\lambda)L_i^{(x)}(u)=L_i^{(y)}(u)M_{i-1}(u-\lambda), \tag{4.2}$$

because the trace $\tau_N(u)$ is invariant due to $M_N(u-\lambda)L^{(x)}(u)=L^{(y)}(u)M_N(u-\lambda)$. To keep the same Poisson structure we ask that the matrices $M_i(u)$ should obey the same Poisson bracket (2.17) as $L_i(u)$ obeys. Practically, we first have to choose one out of many matrices which obeys the r-matrix Poisson bracket (2.17) and then be lucky enough to find that (4.2) has a solution $Y(X,x)$, $y(X,x)$ for every spectral parameter u. The solution will depend on the parameter λ which is exactly what we want. The technical way to solve (4.2) is quite interesting. The idea is to use, besides the phase spaces (X,x) and (Y,y), two more spaces: (S,s) and (T,t). The phase spaces (S,s) and (T,t) are auxiliary spaces, the Bäcklund transformation being between (X,x) and (Y,y). With the help of these auxiliary spaces, we can write a version of (4.2) as

$$M_i^{(s)}(u-\lambda)L_i^{(x)}(u)=L_i^{(y)}(u)M_i^{(t)}(u-\lambda). \tag{4.3}$$

To go back to (4.2) we simply need to impose the constraints

$$t_i=s_{i-1}, \quad T_i=S_{i-1}. \tag{4.4}$$

We apply now the above method to the dressing chain. The Lax matrix is

$$L_i^{(x)}(u)=\begin{pmatrix} x_i & 1 \\ x_iX_i+\beta_i+\lambda & X_i \end{pmatrix}. \tag{4.5}$$

Here (x) stands for the pair of variables (X,x) and u is the spectral parameter. We choose the matrix M to be identical with L. Because in (4.3) the index i is the same on both sides, we can drop it and write the matrix equation as

$$\begin{pmatrix} s & 1 \\ u-\lambda+sS & S \end{pmatrix}\begin{pmatrix} x & 1 \\ u+\beta+xX & X \end{pmatrix}=\begin{pmatrix} y & 1 \\ u+\beta+yY & Y \end{pmatrix}\begin{pmatrix} t & 1 \\ u-\lambda+tT & T \end{pmatrix}. \tag{4.6}$$

The solution to the system is

$$S=-x+\xi, \tag{4.7}$$

$$X=-s+\frac{\lambda+\beta}{t-x}, \tag{4.8}$$

$$T=-y+\frac{\lambda+\beta}{t-x}, \tag{4.9}$$

$$Y=-t+\xi. \tag{4.10}$$

We remark that ξ is a free variable. This is a consequence of the fact that the conserved Hamiltonians depend only on the combination X_i+x_{i+1}. The generating function $F_\lambda(y,t|x,s)$ is

$$F_\lambda(y,t|x,s)=y(t-\xi)-(x-\xi)s-(\lambda+\beta)\ln(t-x), \tag{4.11}$$

from which we get

$$X=\frac{\partial F_\lambda}{\partial x}, \quad S=\frac{\partial F_\lambda}{\partial s}, \tag{4.12}$$

$$Y=-\frac{\partial F_\lambda}{\partial y}, \quad T=-\frac{\partial F_\lambda}{\partial t}. \tag{4.13}$$

To simplify the formulas we choose the $\xi=x$. The generating function becomes

$$F_\lambda=y(t-x)-(\lambda+\beta)\ln(t-x). \tag{4.14}$$

The constrains $t_i=s_{i-1}$, $T_i=S_{i-1}$ give

$$X_i=-s_i+\frac{\lambda+\beta_i}{s_{i-1}-x_i}, \tag{4.15}$$

which can be solved, in principle, for s_i. Then

$$Y_i+y_{i+1}=X_{i+1}+x_i+s_{i+1}-s_{i-1}. \tag{4.16}$$

In terms of the old variables $g_i=X_i+x_{i+1}$ the transformation reads

$$g_i=z_i-\frac{\lambda+\beta_i}{z_{i-1}}, \tag{4.17}$$

$$\tilde{g}_i=g_{i+1}+z_{i-1}-z_{i+1}, \tag{4.18}$$

where $\tilde{g}_i$ are the transformed variables and

$$z_i=x_{i+1}-s_i. \tag{4.19}$$

Note that (4.17) and (4.18) are just the canonical transformations we were looking for. To obtain the concrete form of these transformations we need to solve (4.17) for z_i, and then to use these values to find $\tilde{g}_i$. Because for an arbitrary λ equation (4.17) cannot be explicitly solved, we leave the canonical transformation in an implicit form. However, for special values of λ, the canonical transformation can be explicitly solved, as we are going to exemplify in Sec. X, Eqs. (10.2)–(10.4).

The first equation in (4.17) is the discrete Riccati equation. It can be linearized with the help of the following change of variables:

$$z_i=\frac{\psi_{i+1}}{\psi_i}. \tag{4.20}$$

We obtain

$$\psi_{i+1}=\psi_i g_i+(\lambda+\beta_i)\psi_{i-1}, \quad i=0,\ldots,N. \tag{4.21}$$

The periodic boundary condition $z_0=z_N$ implies

$$\psi_1\psi_{N-1}=\psi_0\psi_N. \tag{4.22}$$

From (4.14), the generating function for the canonical transformation is

$$X_i=\frac{\partial\Phi_\lambda}{\partial x_i}, \tag{4.23}$$

$$Y_i=-\frac{\partial\Phi_\lambda}{\partial y_i}, \tag{4.24}$$

$$\Phi_\lambda(\boldsymbol{y},\boldsymbol{x})=\sum_{i=1}^{N} F_\lambda(y_i s_{i-1}|x_i s_i)=\sum_{i=1}^{N} y_i(s_{i-1}-x_i)-(\lambda+\beta_i)\ln(s_{i-1}-x_i). \tag{4.25}$$

Here we denote by $\boldsymbol{x}=(x_1,\ldots,x_N)$. Finally in terms of z_i the generating function can be written as

$$\Phi_\lambda(\boldsymbol{y},\boldsymbol{x})=\sum_{i=1}^{N} y_i(-z_{i-1})-(\lambda+\beta_i)\ln(-z_{i-1}). \tag{4.26}$$

V. CANONICAL TRANSFORMATIONS AND DARBOUX FACTORIZATION

To decipher the meaning of the variables z_i present in the canonical transformation (4.17) we will use the knowledge obtained from the Darboux method of factorization. First, from (4.17), find z_{i-1}

$$-z_{i-1}=\frac{\lambda+\beta_i}{g_i-z_i}. \tag{5.1}$$

Then, compare this result with formula (2.27) that gives the recurrence relation between two logarithmic derivatives of the Bloch eigenfunctions

$$\chi_i=f_i+\frac{\lambda+\beta_i}{f_i+\chi_{i+1}}. \tag{5.2}$$

We obtain thus

$$z_{i-1}=f_i-\chi_i, \tag{5.3}$$

which in terms of the superpotentials $W_i=-f_i$ reads as

$$-z_i=W_i+\chi_i.$$

Therefore the variable z_i taken with a minus sign, is the sum between the superpotential W_i and the logarithmic derivative of the Bloch eigenfunction. It is interesting to obtain the time evolution of the variables z_i. From

$$-\psi_i''+u_i\psi_i=(\lambda+\beta_i)\psi_i, \tag{5.4}$$

$$u_i=f_i'+f_i^2, \tag{5.5}$$

$$z_{i-1}'=f_i'-(\psi_i'/\psi_i)', \tag{5.6}$$

we get

$$z_{i-1}'=\chi_i^2-f_i^2+\lambda+\beta_i. \tag{5.7}$$

VI. SEPARATED CANONICAL VARIABLES

At this point we have the canonical Bäcklund transformations (4.17). Let us use the symbol B_λ for this transformation. Our goal is to find separated canonical variables. Following Sklyanin, we consider the composition $B_{\lambda_1\cdots\lambda_N}=B_{\lambda_1}\circ\cdots\circ B_{\lambda_N}$ of Bäcklund transformations and the corresponding generating function $F_{\lambda_1\cdots\lambda_N}(y,x)$. If we treat λ's as dynamical variables and y's as parameters then $F_{\lambda_1\cdots\lambda_N}(y,x)$ becomes the generating function of the N-parametric canonical transformation from (X,x) to (μ,λ) given by

$$X_i=\frac{\partial F_{\lambda_1\cdots\lambda_N}}{\partial x_i},\quad \mu_i=-\frac{\partial F_{\lambda_1\cdots\lambda_N}}{\partial \lambda_i}. \tag{6.1}$$

This transformation is not only canonical but also separates the variables. See Ref. 5 for details.

Each pair (λ_i,μ_i) lie on a curve given implicitly by

$$W(\lambda_i,\mu_i)=0. \tag{6.2}$$

To find the curve W we use the parameter μ which is the variable conjugated to λ

$$\mu=-\frac{\partial F_\lambda}{\partial\lambda}, \tag{6.3}$$

and search for a function $f(\mu)$ such that

$$\det(f(\mu)-L(\lambda))=0. \tag{6.4}$$

Then the spectral curve W is

$$W(\lambda_i,f(\mu_i);H_i)\equiv\det(f(\mu_i)-L(\lambda_i))=0. \tag{6.5}$$

For the dressing chain

$$f(\mu)=-e^\mu. \tag{6.6}$$

To prove this, we will show that $-e^\mu$ is an *eigenvalue* for $L(\lambda)$ so the property $\det(f(\mu)-L(\lambda))=0$ is immediate.

From the definition of μ (6.3) and from the generating function (4.26) we get

$$z_1\cdots z_N=-e^\mu. \tag{6.7}$$

Now, by a simple computation

$$L_i^{(x)}(\lambda)\begin{pmatrix}1\\-s_{i-1}\end{pmatrix}=z_{i-1}\begin{pmatrix}1\\-s_i\end{pmatrix}. \tag{6.8}$$

This proves that for $L=L_N\cdots L_1$ the eigenvalue is $z_1\cdots z_N$.

The spectral curve $W(\lambda,\mu)$ can be expressed in terms of the trace τ_N and β_i

$$\det(v-L(\lambda))=v^2-\tau_N(\lambda)\,v+\prod_{i=1}^{N}(\lambda+\beta_i), \tag{6.9}$$

so

$$e^{2\mu}+\tau_N(\lambda)\,e^\mu-\prod_{i=1}^{N}(\lambda+\beta_i)=0. \tag{6.10}$$

Here

$$\tau_N(\lambda)=H_1\lambda^n+H_3\lambda^{n-1}+\cdots+H_{2N+1}, \tag{6.11}$$

where $N=2n+1$ and $H_1,H_3,\ldots,H_{2N+1}$ are integrals of the chain.

VII. QUANTUM CASE

To get the quantum version of the theory described so far we will use the R-matrix approach. This will ensure the commutativity of the Hamiltonians H_i after quantization. From classical variables (x,X) we move to the quantum variables (x,∂_x). The local quantum Lax matrix

$$L(u|x,\partial_x)=\begin{pmatrix} x & 1 \\ u+x\partial_x & \partial_x \end{pmatrix}, \tag{7.1}$$

verifies the quantum commutation relation

$$R_{12}(u_1-u_2)L^{(1)}(u_1)L^{(2)}(u_2)=L^{(2)}(u_2)L^{(1)}(u_1)R_{12}(u_1-u_2), \tag{7.2}$$

where

$$R_{12}(u)=u+\mathcal{P}_{12}, \tag{7.3}$$

is the $SL(2)$-invariant solution to the quantum Yang–Baxter equation.[11] The monodromy operator and its trace are defined like in the classical case. The commutativity of the Hamiltonians H_i

$$[H_i,H_j]=0, \tag{7.4}$$

is a consequence of (7.2). The whole machinery of the Quantum Inverse Scattering Method can be put to work at this stage. We will limit to study only the Baxter Q-operator and the Baxter T-Q relation. The Q-operator will depend upon the spectral parameter λ. Let us denote it by $Q(\lambda)$. The interesting aspect is that the classical Bäcklund transformation B_λ is the classical limit of the similarity transformation

$$\mathcal{O}\rightarrow Q(\lambda)\mathcal{O}Q^{-1}(\lambda). \tag{7.5}$$

For details see Ref. 5. In the next section we will explicitly construct $Q(\lambda)$ as an integral operator.

VIII. *Q*-OPERATOR

For the Baxter Q-operator we require the three usual properties. First, it has to commute with the trace of the monodromy matrix $\tau_N(u)=\Pi_{i=N}^{1}L(u|x_i,\partial_{x_i})$

$$[\tau_N(u),Q(\lambda)]=0, \tag{8.1}$$

second, it has to commute with itself

$$[Q(\lambda_1),Q(\lambda_2)]=0, \tag{8.2}$$

and the last important property imposed is the Baxter T-Q equation, i.e., the Q-operator should satisfy a finite difference equation

$$\tau_N(\lambda)Q(\lambda)=A(\lambda)Q(\lambda-1)+B(\lambda)Q(\lambda+1), \tag{8.3}$$

where $A(\lambda)$ and $B(\lambda)$ are two functions (not operators) of the spectral parameter λ.

We will follow Ref. 4 and construct $Q(\lambda)$ as an integral operator

$$(Q(\lambda)\psi)(\boldsymbol{x})=\int d\boldsymbol{t}\int d\boldsymbol{y}\prod_{i=1}^{N}R_{\lambda+\beta_i-1}(t_i,x_i|t_{i-1}y_i)\psi(\boldsymbol{y}). \tag{8.4}$$

Here $d\boldsymbol{t}=dt_N\cdots dt_1$ and similar for alike symbols. If we introduce the $\mathcal{R}$-operator as

$$(\mathcal{R}_\lambda\psi)(s,x)=\int dy\int dtR_\lambda(s,x|t,y)\psi(y), \tag{8.5}$$

the formula (8.4) can be understand in the general sense of the trace of a monodromy matrix

$$Q(\lambda)=Tr_{t_N}\mathcal{R}^1_{\lambda+\beta_N-1}\cdots\ \mathcal{R}^N_{\lambda+\beta_1-1}. \tag{8.6}$$

In the notation $R_\lambda(t,y|s,x)$ we recognize the *auxiliary* indexes *s*, *t*, and the *quantum* indexes *x*, *y*. The *Q*-operator can be expressed as an integral operator

$$(Q(\lambda)\psi)(\boldsymbol{x})=\int dy_1\cdots\ \int dy_N\mathcal{Q}_\lambda(\boldsymbol{x}|\boldsymbol{y})\psi(\boldsymbol{y}), \tag{8.7}$$

with the kernel

$$\mathcal{Q}_\lambda(\boldsymbol{x}|\boldsymbol{y})=\int dt_N\cdots\ \int dt_1\prod_{i=N}^{1}R_{\lambda+\beta_i-1}(t_{i-1},x_i|t_i,y_i). \tag{8.8}$$

After this general introduction, we move forward to find the concrete form of the operator $\mathcal{R}_\lambda$. The first property of the Baxter Q-operator, namely the commutation $[\tau_N(u),Q(\lambda)]=0$ is fulfilled if $\mathcal{R}_\lambda$ is a solution of an equation similar to (7.2)

$$M(u-\lambda|s,\partial_s)L(u|x,\partial_x)\mathcal{R}_\lambda=\mathcal{R}_\lambda L(u|y,\partial_y)M(u-\lambda|t,\partial_t), \tag{8.9}$$

where $L(u|x,\partial_x)$ is the local quantum Lax matrix (7.1) and $M(u-\lambda)$ is another matrix which obeys the quantum commutation (7.2.) The main difficulty is how to choose the matrix $M(u-\lambda)$ so that, Eq. (8.9) for $\mathcal{R}(\lambda)$ has a solution for every complex parameter u and by the other hand the Q-operator thus obtained has the required properties. The second property of the Q-operator comes from the Yang–Baxter equation which can be obtained from (8.9) by a standard technique, see Ref. 11. Returning to Eq. (8.9) we take M to be of the same form as the Lax matrix (7.1). We obtain

$$\begin{pmatrix} s & 1\\ u-\lambda+s\partial_s & \partial_s\end{pmatrix}\begin{pmatrix} x & 1\\ u+x\partial_x & \partial_x\end{pmatrix}R_\lambda(t,y|s,x)=R_\lambda(t,y|s,x)\begin{pmatrix} y & 1\\ u+y\partial_y & \partial_y\end{pmatrix}\begin{pmatrix} t & 1\\ u-\lambda+t\partial_t & \partial_t\end{pmatrix}. \tag{8.10}$$

On the right-hand side of the above equation, move $R_\lambda(ty,sy)$ from the left side of the matrices product, to the right side. We have to change $\partial_x\to-\partial_x$ and $x\partial_x\to-1-x\partial_x$. Then the equation becomes

$$\begin{aligned}&\begin{pmatrix} s & 1\\ u-\lambda+s\partial_s & \partial_s\end{pmatrix}\begin{pmatrix} x & 1\\ u+x\partial_x & \partial_x\end{pmatrix}R_\lambda(t,y|s,x)\\ &\quad=\begin{pmatrix} y & 1\\ u-1-y\partial_y & -\partial_y\end{pmatrix}\begin{pmatrix} t & 1\\ u-\lambda-1-t\partial_t & -\partial_t\end{pmatrix}R_\lambda(t,y|s,x).\end{aligned} \tag{8.11}$$

The solution is:

$$R_\lambda(t,y|s,x)=\rho_\lambda\delta(s-y)e^{y(t-x)}(t-x)^{-\lambda-1}. \tag{8.12}$$

We notice that $R\sim\exp(F_\lambda)$ for $\beta=1$. Due to the Dirac function, the solution is gauge independent, i.e., the solution does not depend on the free variable ξ from (4.11). The $\mathcal{R}$-operator (8.5) becomes, after integration over y and changing the variable $t-x=\xi$

$$(\mathcal{R}\psi)(s,x)=\rho_\lambda\int d\xi e^{s\xi}\,\xi^{-\lambda-1}\psi(x+\xi,s), \tag{8.13}$$

or

$$(\mathcal{R}\psi)(s,x)=\rho_\lambda s^\lambda\int d\xi e^{\xi}\,\xi^{-\lambda-1}\psi(x+s^{-1}\xi,s). \tag{8.14}$$

The branch for the many valued function s^λ from (8.14) is fixed by making a cut along $(-\infty,0)$ and taking $\arg(s)\in[-\pi,\pi]$. We have to specify the factor ρ_λ and the integration contour (in the complex ξ pane) in (8.14). The integration contour is the Hankel contour for the Gamma function[12]

$$\int_{-\infty}^{(0+)} e^{\xi}\xi^{-z}d\xi=\frac{2\pi i}{\Gamma(z)}. \tag{8.15}$$

The previous formula inspired us to choose

$$\rho_\lambda=\frac{1}{2\pi i}\Gamma(\lambda+1). \tag{8.16}$$

Then

$$(\mathcal{R}_\lambda(\psi))(s,x)=\frac{1}{2\pi i}\Gamma(\lambda+1)s^\lambda\int d\xi e^{\xi}\xi^{-\lambda-1}\psi(x+s^{-1}\xi,s). \tag{8.17}$$

We are ready now to write the kernel of the Q-operator (8.8). From (8.12) and (8.6) we obtain

$$\mathcal{Q}_\lambda(\boldsymbol{x}|\boldsymbol{y})=\prod_{i=1}^{N} w_i(\lambda;y_{i-1},y_i,x_i), \tag{8.18}$$

where

$$w_i(\lambda;y_{i-1},y_i,x_i)=\frac{1}{2\pi i}\Gamma(\lambda+\beta_i)e^{y_i(y_{i-1}-x_i)}(y_{i-1}-x_i)^{-\lambda-\beta_i}. \tag{8.19}$$

Therefore we have found an explicit form for the Baxter Q-operator (8.18). Next we are going to investigate the third property of the Q-operator, namely the Baxter T-Q equation.

IX. BAXTER T-Q EQUATION

This last paragraph aims to show that the Baxter T-Q equation is the quantum version of the classical separation of variables (6.1). The computation parallels the one in Ref. 4. Start from the left side of the Baxter T-Q equation (8.3)

$$[\tau(\lambda)Q(\lambda)\psi](\boldsymbol{x})=Tr\left[\int d\boldsymbol{t}d\boldsymbol{y}\left(\prod_{i=N}^{1} L(\lambda|x_i,\partial_{x_i})R_{\lambda+\beta_i-1}(t_i,x_i|t_{i-1},y_i)\right)\psi(\boldsymbol{y})\right]. \tag{9.1}$$

We can integrate over t_i and get

$$[\tau(\lambda)Q(\lambda)\psi](\boldsymbol{x})=Tr\left[\int d\boldsymbol{y}\left(\prod_{i=N}^{1}L(\lambda|x_i,\partial_{x_i})w_i\right)\psi(\boldsymbol{y})\right], \tag{9.2}$$

where w_i are given by (8.19).

Move all w_i to the left using

$$L(\lambda|x_i,\partial_{x_i})w_i=w_i\widetilde{L}(\lambda|x_i,\partial_{x_i}), \tag{9.3}$$

with

$$\widetilde{L}(\lambda|x_i,\partial_{x_i})=\begin{pmatrix} x_i & 1 \\ \lambda+\beta_i+x_i\partial_{x_i}\ln w_i & \partial_{x_i}\ln w_i\end{pmatrix}, \tag{9.4}$$

or

$$\widetilde{L}(\lambda|x_i,\partial_{x_i})=\begin{pmatrix} x_i & 1 \\ -x_iy_i+\dfrac{(\lambda+\beta_i)y_{i-1}}{y_{i-1}-x_i} & -y_i+\dfrac{(\lambda+\beta_i)}{y_{i-1}-x_i}\end{pmatrix}. \tag{9.5}$$

At this point we can write

$$[\tau(\lambda)Q(\lambda)\psi](\boldsymbol{x})=\int d\boldsymbol{y}\prod_{i=N}^{1}w_iTr(\widetilde{L}(\lambda|x_N,\partial_{x_N})\cdots\widetilde{L}(\lambda|x_1,\partial_{x_1}))\psi(\boldsymbol{y}). \tag{9.6}$$

The last step is to perform a gauge transformation which leaves the trace invariant and make the matrices $\widetilde{L}(\lambda|x_i,\partial_{x_i})$ triangular, so the trace will be easy to compute

$$\widetilde{L}(\lambda|x_i,\partial_{x_i})\to N_i^{-1}\widetilde{L}(\lambda|x_i,\partial_{x_i})N_{i-1}. \tag{9.7}$$

With the help of the following gauge matrix:

$$N_i=\begin{pmatrix}1 & 0\\ y_i & 1\end{pmatrix}, \tag{9.8}$$

the triangular form for $\widetilde{L}(\lambda|x_i,\partial_{x_i})$ is

$$N_i^{-1}\widetilde{L}(\lambda|x_i,\partial_{x_i})N_{i-1}=\begin{pmatrix}-(y_{i-1}-x_i) & 1\\ 0 & \dfrac{\lambda+\beta_i}{y_{i-1}-x_i}\end{pmatrix}. \tag{9.9}$$

The entries of the previous matrix can be expressed in terms of the w_i (8.19)

$$-(y_{i-1}-x_i)=-(\lambda+\beta_i)\frac{w_i(\lambda-1)}{w_i(\lambda)}, \tag{9.10}$$

$$\frac{\lambda+\beta_i}{y_{i-1}-x_i}=\frac{w_i(\lambda+1)}{w_i(\lambda)}, \tag{9.11}$$

so we get for the trace

$$Tr(\tilde{L}(\lambda|x_N,\partial_{x_N})\cdots\tilde{L}(\lambda|x_1,\partial_{x_1}))=\prod_{i=1}^{N}-(\lambda+\beta_i)\frac{w_i(\lambda-1)}{w_i(\lambda)}+\prod_{i=1}^{N}\frac{w_i(\lambda+1)}{w_i(\lambda)}. \tag{9.12}$$

The last result implies the Baxter T-Q equation

$$\tau(\lambda)Q(\lambda)=-\prod_{i=1}^{N}(\lambda+\beta_i)Q(\lambda-1)+Q(\lambda+1). \tag{9.13}$$

Compare (9.13) with the classical result (6.10) written in the form

$$e^{\mu}+\tau_N-\prod_{i=1}^{N}(\lambda+b_i)e^{-\mu}=0. \tag{9.14}$$

The connection is obvious if we quantify the canonical pair (μ,λ) as

$$\mu\to\frac{d}{d\lambda},\quad \lambda\to\lambda. \tag{9.15}$$

Then (9.14) becomes an operator acting on the Q-operator

$$\left(e^{\mu}+\tau_N-\prod_{i=1}^{N}(\lambda+\beta_i)e^{-\mu}\right)Q(\lambda)=0, \tag{9.16}$$

which is the T-Q equation up to a minus sign. To obtain a T-Q equation which exactly matches the classical formula, we have to choose for ρ_λ the one in (8.16) multiplied with $(-1)^\lambda$.

X. THE CASE $N=3$

It is instructive to study the case $N=3$ which corresponds to the one-gap potentials. The trace (2.15) of the monodromy matrix (2.14) for $N=3$ is

$$\tau_3(u)=(g_1+g_2+g_3)u+g_1g_2g_3+g_1\beta_3+g_2\beta_1+g_3\beta_2. \tag{10.1}$$

The variables g_i, $i=1,2,3$ are (2.12): $g_1=X_1+x_2$, $g_2=X_2+x_3$, and $g_3=X_3+x_1$. The transformation $B(\lambda)$ [(4.17), (4.18)] can be explicitly found for $\lambda=-\beta_i$, $i=1,2,3$. For example, for $\lambda=-\beta_2$ we get

$$\tilde{g}_1=g_3+\frac{\beta_3-\beta_2}{g_2}, \tag{10.2}$$

$$\tilde{g}_2=g_1-\frac{\beta_3-\beta_2}{g_2}+\frac{\beta_1-\beta_2}{g_3+\dfrac{\beta_3-\beta_2}{g_2}}, \tag{10.3}$$

$$\tilde{g}_3=g_2-\frac{\beta_1-\beta_2}{g_3+\dfrac{\beta_3-\beta_2}{g_2}}. \tag{10.4}$$

This transformation can be recovered from the Bäcklund transformations T_k, $k=1,2,3$ from.[2,13] Recall that T_k is given by

$$T_k(g_{k\pm1})=g_{k\pm1}\pm\frac{\beta_{k+1}-\beta_k}{g_k}, \tag{10.5}$$

$$T_k(\beta_k)=\beta_{k+1}, \tag{10.6}$$

$$T_k(\beta_{k+1})=\beta_k, \tag{10.7}$$

the remaining β_j and g_j being not changed. We also need to introduce the shift S acting as

$$S(\beta_i)=\beta_{i-1}, \tag{10.8}$$

$$S(g_i)=g_{i-1}. \tag{10.9}$$

In terms of these last transformations, we can write

$$B(-\beta_2)=T_2ST_1. \tag{10.10}$$

We cannot recover T_k from $B(\lambda)$ because of the difference in nature between these transformations. T_k transforms the parameters β_j so it changes solutions of one system of equations (2.4) to solutions of another system of the same type (2.4). The transformations $B(\lambda)$ change the solutions of the same system (2.4) among themselves. In this respect $B(\lambda)$ is an auto-Bäcklund transformation.

We can try to solve the discrete Riccati equation (4.20) for ψ_i. In this case, we will get $\psi_1,\ldots,\psi_3$ in terms of ψ_0 and ψ_4

$$\psi_1=\frac{1}{Z}[\psi_4-\psi_0(g_2g_3+\lambda+\beta_3)(\lambda+\beta_1)], \tag{10.11}$$

$$\psi_2=\frac{1}{Z}[\psi_4g_1+\psi_0g_3(\lambda+\beta_2)(\lambda+\beta_1)], \tag{10.12}$$

$$\psi_3=\frac{1}{Z}[\psi_4(g_1g_2+\lambda+\beta_2)-\psi_0(\lambda+\beta_1)(\lambda+\beta_2)(\lambda+\beta_3)], \tag{10.13}$$

with $Z=g_1g_2g_3+g_1(\lambda+\beta_3)+g_3(\lambda+\beta_2)$. It obvious that $z_i=\psi_{i+1}/\psi_i$ will depend on ψ_4 and ψ_0 only through their ratio ψ_4/ψ_0. This ratio is not a free parameter because the periodic boundary condition $z_0=z_3$ imposes a restriction on it.

Though the τ-functions are not one of the major players of this paper, it is worthwhile to mention the connection it has with canonical transformations.

The τ-functions for the dressing chain were reported in Ref. 14 for $N=3$. For $N=3$ case, the dressing chain (2.4) written in variables g_i, (2.9), is

$$\begin{aligned} g_0'&=-g_0(g_1-g_2)+\beta_0-\beta_1,\\ g_1'&=-g_1(g_2-g_0)+\beta_1-\beta_2,\\ g_2'&=-g_2(g_0-g_1)+\beta_2-\beta_0. \end{aligned} \tag{10.14}$$

With the change of variables

$$g_0=F_1'-F_2'+c,\quad g_1=F_2'-F_0'+c,\quad g_2=F_0'-F_1'+c, \tag{10.15}$$

where the constant c is given by $3c=g_0+g_1+g_2$, the system of equations (10.14) transforms into

$$\begin{aligned} &F_0''+F_1''+(F_0'-F_1')^2-c\,(F_0'-F_1')+\beta_1=0,\\ &F_1''+F_2''+(F_1'-F_2')^2-c\,(F_1'-F_2')+\beta_2=0, \end{aligned} \tag{10.16}$$

$$F_2''+F_0''+(F_2'-F_0')^2-c\,(F_2'-F_0')+\beta_0=0.$$

The τ-functions $\tau_0,\ \tau_1,\ \tau_2$ are now given by

$$F_0=\log\tau_0,\quad F_1=\log\tau_1,\quad F_2=\log\tau_2. \tag{10.17}$$

In terms of the τ-functions, the dressing chain becomes a Hirota type system of equations

$$(D_x^2-cD_x+\beta_1)\,\tau_0\cdot\tau_1=0,\quad (D_x^2-cD_x+\beta_2)\,\tau_1\cdot\tau_2=0,\quad (D_x^2-cD_x+\beta_0)\,\tau_2\cdot\tau_0=0, \tag{10.18}$$

where for a polynomial P, the operator $P(D_x)$ is defined as

$$P(D_x)\,F(x)\cdot G(x)=P(\partial_y)\,F(x+y)G(x-y)\big|_{y=0}. \tag{10.19}$$

At this point the goal is to work the canonical transformation (4.17) and (4.18) in terms of the τ-functions. The canonical transformation (4.17), (4.18) namely

$$g_i=z_i-\frac{\lambda+\beta_i}{z_{i-1}} \tag{10.20}$$

and

$$\tilde{g}_i=g_{i+1}+z_{i-1}-z_{i+1}, \tag{10.21}$$

cannot be written explicitly as a formula which comprise only $\tilde{g}_i$ and g_i. Therefore, we use the following strategy: Given g_i, we have to solve for z_i in (10.20), and then obtain the transformed variables $\tilde{g}_i$ with the aid of (10.21). As a result, the canonical transformation for the τ-functions will be written in terms of the variables z_i.

First, by simple manipulations of (10.14) and (10.15) we get

$$F_0''=g_1g_2-c^2-\frac{\beta_0+\beta_1-\beta_2}{2}, \tag{10.22}$$

and similarly for F_1'' and F_2''. Using (10.17) we get

$$(\log e^{-\gamma_0x^2}\tau_0)''=g_1g_2, \tag{10.23}$$

and similarly for τ_1 and τ_2. Here $\gamma_0=-\frac{1}{2}(c^2+(\beta_0+\beta_1-\beta_2)/3)$.

After we apply the canonical transformation we obtain the function $\tilde{\tau}_0$ given by

$$(\log e^{-\gamma_0x^2}\tilde{\tau}_0)''=\tilde{g}_1\tilde{g}_2. \tag{10.24}$$

Now it is easy to write the canonical transformation for $\tau_0,\ \tau_1,\ \tau_2$ in terms of the variable z_i. Use (10.20) and (10.21) in (10.23) and (10.24) and get

$$\begin{aligned}
(\log e^{-\gamma_0x^2}\tau_0)''&=\left(z_1-\frac{\lambda+\beta_1}{z_0}\right)\left(z_2-\frac{\lambda+\beta_2}{z_1}\right),\\
(\log e^{-\gamma_1x^2}\tau_1)''&=\left(z_2-\frac{\lambda+\beta_2}{z_1}\right)\left(z_0-\frac{\lambda+\beta_0}{z_2}\right),\\
(\log e^{-\gamma_2x^2}\tau_2)''&=\left(z_0-\frac{\lambda+\beta_0}{z_2}\right)\left(z_1-\frac{\lambda+\beta_1}{z_0}\right)
\end{aligned} \tag{10.25}$$

and

$$(\log e^{-\gamma_0 x^2}\tilde{\tau}_0)''=\left(z_0-\frac{\lambda+\beta_2}{z_1}\right)\left(z_1-\frac{\lambda+\beta_0}{z_2}\right),$$

$$(\log e^{-\gamma_1 x^2}\tilde{\tau}_1)''=\left(z_1-\frac{\lambda+\beta_0}{z_2}\right)\left(z_0-\frac{\lambda+\beta_1}{z_0}\right), \tag{10.26}$$

$$(\log e^{-\gamma_2 x^2}\tilde{\tau}_2)''=\left(z_2-\frac{\lambda+\beta_1}{z_0}\right)\left(z_0-\frac{\lambda+\beta_2}{z_1}\right),$$

with

$$\gamma_0=-\frac{1}{2}\left(c^2+\frac{\beta_0+\beta_1-\beta_2}{3}\right),\quad \gamma_1=-\frac{1}{2}\left(c^2+\frac{\beta_1+\beta_2-\beta_0}{3}\right),\quad \gamma_2=-\frac{1}{2}\left(c^2+\frac{\beta_2+\beta_0-\beta_1}{3}\right).$$

The meaning of the transformations as presented in (10.25) and (10.26) is that first we must factorize like in (10.25) and then use the factorization variables z_i to obtain the transformed τ-functions, like in (10.26).

For the case $N=3$, the canonical transformation must be carried on three times, each time with another λ in order to obtain separated canonical variables, see (6.1). In variables g_i, these transformations read as

$$\tilde{g}_i=g_{i+1}+z_{i-1}-z_{i+1},\quad g_i=z_i-\frac{\lambda_1+\beta_i}{z_{i-1}},$$

$$\tilde{\tilde{g}}_i=\tilde{g}_{i+1}+\tilde{z}_{i-1}-\tilde{z}_{i+1},\quad \tilde{g}_i=\tilde{z}_i-\frac{\lambda_2+\beta_i}{\tilde{z}_{i-1}}, \tag{10.27}$$

$$\tilde{\tilde{\tilde{g}}}_i=\tilde{\tilde{g}}_{i+1}+\tilde{\tilde{z}}_{i-1}-\tilde{\tilde{z}}_{i+1},\quad \tilde{\tilde{g}}_i=\tilde{\tilde{z}}_i-\frac{\lambda_3+\beta_i}{\tilde{\tilde{z}}_{i-1}}.$$

If we add μ_1, μ_2, μ_3 given by (6.7)

$$e^{\mu_1}=-z_1z_2z_3,\quad e^{\mu_1}=-\tilde{z}_1\tilde{z}_2\tilde{z}_3,\quad e^{\mu_1}=-\tilde{\tilde{z}}_1\tilde{\tilde{z}}_2\tilde{\tilde{z}}_3, \tag{10.28}$$

the variables $(\lambda_1,\lambda_2,\lambda_3,\mu_1,\mu_2,\mu_3)$ are separated canonical variables. The time evolution of these variables, inherited from the dressing chain (10.14) is such that, (6.10),

$$e^{2\mu_1}+e^{\mu_1}-(\lambda_1+\beta_1)(\lambda_1+\beta_2)(\lambda_1+\beta_3)=0, \tag{10.29}$$

and similarly for the pairs (λ_2,μ_2) and (λ_3,μ_3). Here $\tau_N(\lambda_1)$ is given by (10.1) with λ_1 instead of u.

If we use the notation $\tau^{(1)}=\tau$, $\tau^{(2)}=\tilde{\tau}$, $\tau^{(3)}=\tilde{\tilde{\tau}}$ and similarly for z_i, the transformations (10.27) for the τ-functions, can be compactly expressed as follows:

factorization:

$$(\log e^{-\gamma_i x^2}\tau_i^{(k)})''=\left(z_{i+1}^{(k)}-\frac{\lambda_k+\beta_{i+1}}{z_i^{(k)}}\right)\left(z_{i+2}^{(k)}-\frac{\lambda_k+\beta_{i+2}}{z_{i+1}^{(k)}}\right),$$

transformation

$$(\log e^{-\gamma_i x^2}\tau_i^{(k+1)})''=\left(z_i^{(k)}-\frac{\lambda_k+\beta_{i+2}}{z_{i+1}^{(k)}}\right)\left(z_{i+1}^{(k)}-\frac{\lambda_k+\beta_i}{z_{i+2}^{(k)}}\right).$$

Here $i=0,1,2$, modulo 3, and $k=1,2,3$. The variables μ are given by (10.28) as before.

XI. HAMILTONIAN FLOW FOR THE CASE $N=3$

Here we discuss the time dependence of the canonical variables (X_i,x_i). We regard the variable x (i.e., the *space* variable) in the system of Eqs. (2.4) as being a time t for the Hamiltonian flow. The Hamiltonian that governs the motion in time is in variables f_i (2.9) given by

$$H=\tfrac{1}{3}(f_1^3+f_2^3+f_3^3+\beta_1 f_1+\beta_2 f_2+\beta_3 f_3). \tag{11.1}$$

It is useful to list all the variables which appeared so far

$$g_1=f_1+f_2, \quad f_1=\tfrac{1}{2}(g_1-g_2+g_3), \quad g_1=X_1+x_2, \tag{11.2}$$

$$g_2=f_2+f_3, \quad f_2=\tfrac{1}{2}(g_2-g_3+g_1), \quad g_2=X_2+x_3, \tag{11.3}$$

$$g_3=f_3+f_1, \quad f_3=\tfrac{1}{2}(g_3-g_1+g_2), \quad g_3=X_3+x_1. \tag{11.4}$$

The evolution of the variable x_1 in time is given by

$$\frac{dx_1}{dt}=\{x_1,H\}. \tag{11.5}$$

The Poisson bracket can be computed for two arbitrary functions f and g from

$$\{f,g\}=\sum_{\alpha,\beta}\frac{\partial f}{\partial y_\alpha}\frac{\partial g}{\partial y_\beta}\{y_\alpha,y_\beta\}, \tag{11.6}$$

where $(y_1,\ldots,y_{2N})=(X_1,\ldots,X_N,x_1,\ldots,x_N)$. In this way we arrive at

$$2\frac{dx_1}{dt}=(f_1^2+f_2^2-f_3^2+\beta_1+\beta_2-\beta_3)\{x_1,X_1\}, \tag{11.7}$$

which gives the evolution for x_1 knowing that the variables (X_1,x_1) are canonical, i.e.,

$$\{x_1,X_1\}=1. \tag{11.8}$$

From the paper of Veselov and Shabat[2] we even know the solutions for the dressing chain in terms of the elliptic Weierstrass $\mathcal{P}$-functions

$$f_i(t)=\frac{1}{2}\frac{\mathcal{P}'(t+a_i)-\mathcal{P}'(b_i)}{\mathcal{P}(t+a_i)-\mathcal{P}(b_i)}. \tag{11.9}$$

We can integrate (11.7) to

$$\begin{aligned}2x_1(t)=&\xi(t+a_3+b_3)+\xi(t+a_3)+\xi(b_3)-\xi(t+a_1+b_1)-\xi(t+a_1)-\xi(b_1)\\&-\xi(t+a_2+b_2)-\xi(t+a_2)-\xi(b_2)+\beta_1+\beta_2-\beta_3.\end{aligned} \tag{11.10}$$

Here $\xi'=-\mathcal{P}, b_i=\mathcal{P}(\beta_i)$ and $a_{i+1}-a_i=b_i$.

In the quantum case the Hamiltonians are generated from the Lax matrix (7.1). The trace of the monodromy matrix is

$$\tau_3(u)=H_1u+H_3, \tag{11.11}$$

where

$$H_1 = x_1 + x_2 + x_3 + \partial_{x_1} + \partial_{x_2} + \partial_{x_3}, \tag{11.12}$$

$$H_3 = \partial_{x_1}\partial_{x_2}\partial_{x_3} + x_1\,\partial_{x_1}\partial_{x_3} + x_2\,\partial_{x_2}\partial_{x_1} + x_3\,\partial_{x_3}\partial_{x_2} + x_2x_1\,\partial_{x_1} + x_3x_2\,\partial_{x_2} + x_1x_3\,\partial_{x_3} + x_1x_2x_3. \tag{11.13}$$

An interesting feature of the quantum case is the absence of evolution of the variables $g_i = \partial_{x_i} + x_{i+1}$ due to

$$[g_i, H_3] = 0. \tag{11.14}$$

This means that there is no quantum analog of the dressing chain in terms of the variables g_i. The only surviving variables are $X_i = \partial_{x_i}$ and x_i which each separately evolve in time under the Hamiltonian H_3.

XII. CONCLUSIONS

For the finite-gap potentials we have shown that the Darboux transformations can be viewed as canonical transformations if we apply the method of separation of variables proposed by Sklyanin. Not only the finite-gap case ($N=$ odd, $\alpha=0$) is interesting but also the other cases. For example, the spectrum of the potentials which are solution of the chain in the case $\alpha\neq 0$ and arbitrary N is described as following. The ground state is at zero energy; the next $(p-1)$ eigenvalues are $E_l = \Sigma_{k=0}^{l}\alpha_k$, $l=0,1,\ldots,(p-2)$, and all other eigenvalues are obtained by adding arbitrary multiples of the quantity $\alpha \equiv \alpha_0 + \alpha_1 + \cdots + \alpha_{p-1}$. The general formula for the excited energy levels is[8]

$$n\alpha + \sum_{k=0}^{l} \alpha_k;\ \{n=0,1,2,\ldots,\infty;\ l=0,1,\ldots,(p-1)\}. \tag{12.1}$$

The above potentials (also called *cyclic shape invariant potentials*) are a direct generalization of the harmonic oscillator. For $N=3$ the potentials are Painlevé transcendents.[2]

In this work we have also shown that there exists a quantum version of the dressing chain, namely the time evolution of the variables (X,x) under the Hamiltonian H_1. From here there are many ways to proceed. One way is along Bethe–Ansatz procedure. It will be interesting to find the spectrum of the quantum Hamiltonians. Also, each Hamiltonian H_i has its own time t_i for evolution, so there must be a τ-function which depends on all time variables $\tau(t_1,t_2,\ldots,t_N)$. The τ-function for the dressing chain was reported in Ref. 14 for $N=3$ in connection with the Painlevé equations. See also Refs. 15, 18, and 19.

We have analyzed the role of τ-functions in connection with the factorization method and canonical transformation. The τ-functions are an important tool in understanding integrable systems and we believe that the connections between the τ-functions and the Darboux transformations is worth to be studied further.

Finally, a word about KdV. The finite-gap potential theory provides solutions of the periodic boundary problems for KdV equation. The KdV equation

$$u_{xt} = u_{xxx} - 6uu_{xx}, \tag{12.2}$$

is a partial differential equation in two variables. One variable x we interpreted as a time variable associated with the Hamiltonian H_1. To what Hamiltonian is the second variable, i.e., t, associated? For $\beta_i=0$ the Hamiltonian is $H_5^2 - H_1H_3$. This result is buried in the paper.[16] What is the meaning of the Sklyanin separation of variables for KdV equation, both classical and quantum? From the conformal field point of view, the quantum KdV and the T-Q relation was already studied in the paper of Ref. 17.

In conclusion, the Darboux transformation together with the new approach of the separation of variables is a promising research direction.

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Regularizing divergences in the von Neumann entropy

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We study the decoherence process of a harmonic oscillator in a dissipative environment by considering the von Neumann entropy. Derivatives of the von Neumann entropy around the initial time exhibit divergences when the system is initially in a pure state. A regularization procedure based on the zeta function technique is considered in order to extract information about decoherence. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1428809]

Quantum-mechanical coherence is of central importance in quantum mechanics. Fundamental implications were pointed out in the early days of the quantum theory.[1,2] Presently, a problem which has received considerable attention is the irreversible loss of quantum coherence, namely quantum decoherence.[3,4] The unavoidable presence of the environment makes a quantum system experience a dissipative dynamics,[5–8] which is mainly responsible for destroying quantum coherence.[4]

Great effort has been devoted to the generation of pure quantum states in a variety of quantum optical devices.[9–13] Recently, great importance has been given to the study of those quantum-mechanical systems which are capable of preserving quantum-mechanical coherence,[14,15] One important issue closely related to this problem is the characterization of the time scales of the decoherence process.[16–19] Presently, the understanding of these ideas is very important because of their potential applications in quantum computing, the challenge to provide us with faster computing machines.

A pure state is defined as $\rho(t)=|\psi(t)\rangle\langle\psi(t)|$, in such a way that $\rho^2(t)=\rho(t)$ and Tr $\rho^2(t)=1$. A mixed state instead is defined by the class of states which satisfies the inequality Tr $\rho^2 \leqslant 1$; this simple relation leads to the definition of the linear entropy of a quantum state $S_l(t)=1-\mathrm{Tr}\ \rho^2(t)$, a quantity which is positive $S_l(t)\geqslant 0$ and bounded $S_l(t)\leqslant 1$.

In a recent paper,[19] fundamental questions such as which are the states that remain pure under the time evolution of an open system were addressed. To that end, the dissipative process described by a Lindblad form[20]

$$\partial_t\rho=\frac{\gamma}{2}(2\,f\rho f^\dagger-f^\dagger f\rho-\rho f^\dagger f\,), \tag{1}$$

was considered and time derivatives of $S_l(t)$ were used both to find whether the eigenstates of f are the only states that remain pure under Eq. (1) and the time scale for the onset of instabilities. In particular, it was found that the instabilities of $S_l(t)$ are at least of third order in time if the initial state is an eigenstate of f. That is, when considering an initial pure state which is an eigenstate of the operator f, i.e., $f|\psi_0\rangle\langle\psi_0|=\beta|\psi_0\rangle\langle\psi_0|$, it is found that

$$S_{l1}(0)=S_{l2}(0)=0,\quad S_{l3}(0)=\gamma^3|\beta|^2(\langle A^2\rangle-\langle A\rangle^2), \tag{2}$$

where $A=[f,f^\dagger]$ and

$$S_{ln}(0)=\left.\frac{d^nS_l(t)}{dt^n}\right|_{t=0}. \tag{3}$$

If A is a constant, then fluctuations of A are zero in an eigenstate of f. However, this can occur only for either $f=a$ or $f=\mu a+\nu a^{\dagger}$, that is, the initial state being either a coherent state or a squeezed state; they remain pure for all times. This result establishes that the linear entropy is unstable at third order in time for any other kind of states associated to other classes of restricted Lindblad dynamics given by Eq. (1). This result does not contradict that found in Refs. 21 and 22 because, as is known, the condition for the Lindblad theory is that the time scale considered for the open system should be very long compared to the relaxation time of the reservoir.

Since in general any nonlinear invariant of the density matrix is a good measure of quantum coherence, it is natural to ask how those results look if one uses an alternative and widely known functional of ρ: the von Neumann entropy $S(t)=-\mathrm{Tr}\,\rho(t)\ln\rho(t)$, which is an ideal parameter with which to characterize the decoherence, and is in fact the key to understanding the connection between decoherence and fluctuations.

In this work we address this problem, our main result being related to the appearance of divergences of the derivatives of the von Neumann entropy around an initial pure state of the system. We show here how to solve the problem of their presence by using the zeta function technique, well known in both spectral and quantum field theory.

We know that the von Neumann entropy can be written in terms of the eigenvalues of ρ as

$$S=-\sum_{i}\lambda_i\ln\lambda_i\,. \tag{4}$$

For a pure state there exists only the eigenvalues 0 and 1 of ρ; and then, S can be conveniently expressed as

$$S=-\lim_{\lambda_i\to 1}\lambda_i\ln\lambda_i+\sum_{i'\neq i}\lim_{\epsilon_{i'}\to 0}\epsilon_{i'}\ln\epsilon_{i'}\,. \tag{5}$$

It is clear that $S\to 0$, when we consider the limit $\epsilon_{i'}\ln\epsilon_{i'}\to 0$ when $\epsilon_{i'}\to 0$. A different situation arises when we calculate the derivatives of the von Neumann entropy around the initial time for the system initially in a pure state. In this case we have

$$S_1(0)=-\lim_{\lambda_i(0)\to 1}\dot{\lambda}_i(0)\ln\lambda_i(0)-\lim_{\lambda_i(0)\to 1}\dot{\lambda}_i(0)-\sum_{i'}\lim_{\epsilon_{i'}(0)\to 0}\dot{\epsilon}_{i'}(0)\ln\epsilon_{i'}(0)-\sum_{i'}\lim_{\epsilon_{i'}(0)\to 0}\dot{\epsilon}_{i'}(0). \tag{6}$$

We observe that in the decoherence process $\dot{\lambda}_i(0)<0$, $\dot{\epsilon}_{i'}(0)>0$ for some $\epsilon_{i'}$, such that $S_1(0)$ is divergent because of the presence of the $\ln\epsilon_{i'}(0)$. This simple calculation raises the question of whether one can consider the derivatives of the von Neumann entropy as giving physical information about the decoherence process. In this work we consider this question and show, by comparing with previous results using the linear entropy, that the von Neumann entropy contains the correct information, and in order to extract it unambiguously from the calculation we must consider a procedure to regularize the von Neumann entropy and separate from its derivatives, in a consistent way, the finite and infinite parts.

A first step to analyze the problem is to characterize which kinds of divergence appear when we consider the derivatives of the entropy evaluated in a pure state. In order to do this we expand the logarithm as

$$\ln(1+(\rho-1))=\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}(\rho-1)^n. \tag{7}$$

In a pure state we have $(\rho-1)^n=(-1)^n(1-\rho)$, so that $\ln(1+(\rho-1))=-(1-\rho)\zeta(1)$, where $\zeta(1)$ is the Riemann zeta function $\zeta(s)=\Sigma_{n=1}^{\infty}n^{-s}$ evaluated at $s=1$. From here, it follows that the entropy is $S=\mathrm{Tr}\rho(1-\rho)\zeta(1)$, a result that in principle is not well defined because $\rho(1-\rho)=0$

and $\zeta(1)$ diverges logarithmically. However, if we consider the series term by term, it is evident that the entropy vanishes in agreement with Eq. (5). Moreover, when calculating derivatives of $S(t)$, derivatives of the $\ln\rho$ appear and we can use the formal expansion (7). In this case, $S_1(t)$ is given by

$$S_1 = -\frac{d}{dt}\mathrm{Tr}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\rho(\rho-1)^n = -\mathrm{Tr}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\left[\rho_1(\rho-1)^n+\rho\frac{d}{dt}(\rho-1)^n\right]$$

$$= \mathrm{Tr}\,\rho_1(1-\rho)\zeta(1)+\mathrm{Tr}\sum_{n=1}^{\infty}\frac{1}{n}\rho(1-\rho)^{n-1}\rho_1, \qquad (8)$$

where $\rho_n = d^n\rho(t)/dt^n$. By taking into account that $\rho(1-\rho)^{n-1}=0$ for $n>1$, we have

$$S_1 = -[1+\zeta(1)]\mathrm{Tr}\,\rho\rho_1. \qquad (9)$$

A similar calculation shows that

$$S_2 = -[1+\zeta(1)]\mathrm{Tr}(2\rho\rho_1^2+\rho\rho_2)+2\zeta(0)\mathrm{Tr}(2\rho\rho_1^2-\rho_1^2), \qquad (10)$$

where $\zeta(0)=-1/2$.

It must be stressed that expressions in Eqs. (9) and (10) are completely general because they are calculated assuming only that the initial state is pure for any dissipative dynamics and therefore are applicable to the exact dynamics. These results contain the divergence $\zeta(1)$, the presence of which cannot be an accident as could be implied from the previous calculation for S. For example, in Eq. (9) the precise value of $\mathrm{Tr}\,\rho\rho_1$ depends on the particular dynamics and the initial conditions. In the particular case outlined in Eq. (2), for an eigenstate of f evolving according to Eq. (1), we obtain that $\mathrm{Tr}\,\rho\rho_1=0$, but S_1 is not well defined because of $\zeta(1)$. In addition, in the case of the second derivative of S, it is not difficult to prove that for the particular case of an eigenstate of f evolving according to Eq. (1), $\mathrm{Tr}\,2\rho\rho_1^2=\mathrm{Tr}\,\rho_1^2$, and

$$S_2 = -[1+\zeta(1)]\mathrm{Tr}(\rho_1^2+\rho\rho_2). \qquad (11)$$

The finite factor in S_2 is similar to that found in the case of the linear entropy[19]

$$S_{l2}(t) = -2\,\mathrm{Tr}(\rho_1^2+\rho_0\rho_2), \qquad (12)$$

which vanishes according to Eq. (2) for an eigenstate of f, so that the second derivative of the von Neumann entropy is still $S_2=0\cdot\infty$, which is not well defined.

From this analysis we realize that divergences in the derivatives of the von Neumann entropy around a pure state are independent of the particular kind of dissipative dynamics. A way out of the problem is simply to discard any divergent term appearing in the calculations, but this will only give a correct result after one manage to define, without ambiguity, the finite part of the von Neumann entropy and its derivatives. This is the essence of a regularization procedure. It is important to keep in mind that the divergences in the derivatives of the von Neumann entropy are related to the existence of zero eigenvalues of the density matrix.

In order to solve the problem, we can benefit from well-established regularization techniques widely used in field theory. It is well known that the calculation of functional determinants of some Hermitian operators involves the evaluation of the logarithm of the operator which contains zero modes (zero eigenvalues). The technique used in this case to regularize the expressions (remove divergent parts arising from zero modes) is the zeta function regularization.[23–26] We show in what follows that the von Neumann entropy can be defined in terms of the zeta function in a similar way.

The zeta function associated with a Hermitian operator, the density matrix $\rho(t)$ in our case, is defined as

$$\zeta_\rho(s,t)=\mathrm{Tr}\,\rho(t)^{-s}=\sum_n \lambda_n^{-s}(t), \tag{13}$$

where $\lambda_n(t)$ are the eigenvalues of $\rho(t)$. We included here a time dependence of the zeta function which comes from the temporal dependence of the density matrix. It is easy to see from this definition that the von Neumann entropy reads

$$S(t)=\frac{d}{ds}\zeta_\rho(s,t)\big|_{s=-1}=-\mathrm{Tr}\,\rho(t)\ln\rho(t). \tag{14}$$

The usefulness of this definition resides in the fact that one can represent the zeta function as an integral

$$\zeta_\rho(s,t)=\frac{1}{\Gamma(s)}\int_0^\infty d\tau\,\tau^{s-1}\,\mathrm{Tr}\,e^{-\tau\rho(t)}, \tag{15}$$

where $\mathrm{Tr}\,e^{-\tau\rho(t)}=\Sigma_i e^{-\tau\lambda_i(t)}$. When the operator involved has zero modes, the integral above leads to a divergent part associated with each zero modes. The procedure to remove the divergences is to redefine the integrand in the equation above, such that

$$\zeta_\rho(s,t)=\frac{1}{\Gamma(s)}\int_0^\infty d\tau\,\tau^{s-1}\mathrm{Tr}[e^{-\tau\rho(t)}-P_0(\rho(t))], \tag{16}$$

where $P_0(\rho(t))$ is the projector onto the zero modes of $\rho(t)$.[24,25] In this way the remnant part in the integral is associated only with the nonzero modes, which is the convergent part. We should stress that in this way the expression

$$S(t)=\lim_{s\to-1}\frac{d}{ds}\zeta_\rho(s,t) \tag{17}$$

is an analytic function of time.

Now, let us apply this technique to the problem at hand. It is clear that if we take as the initial condition that the system is in a pure state, we have

$$e^{-\tau\rho}=1-\rho+\rho e^{-\tau}, \tag{18}$$

such that at $t=0$ we have

$$\zeta_\rho(s,0)=\frac{1}{\Gamma(s)}\int_0^\infty d\tau\,\tau^{s-1}\,\mathrm{Tr}[1-\rho+\rho e^{-\tau}-P_0(\rho)]=1+\frac{1}{\Gamma(s)}\int_0^\infty d\tau\,\tau^{s-1}\,\mathrm{Tr}[1-\rho-P_0(\rho)]. \tag{19}$$

This expression clearly shows the existence of a divergence of the zeta function when evaluating in a pure state. In this way, in a pure state the projector onto zero modes is $P_0=1-\rho$, so that $\zeta_\rho(s,0)=1$, and hence the entropy in a pure state vanishes, as it should. This procedure is actually giving us a way to recognize, without ambiguity, the finite part of the $\zeta_\rho(s,0)$, which can be identified with the term in the integrand containing the exponential factor $e^{-\tau}$. Clearly, any other term inside gives rise to a divergence with no physical interpretation. This is precisely the idea we want to extend to solve the problem with the derivatives of the von Neumann entropy.

We are interested in evaluating temporal derivatives of the entropy using Eq. (14). To that end, we must know the temporal derivatives of $\zeta_\rho(s,t)$. In general, we have that

$$\frac{d}{dt}\mathrm{Tr}[e^{-\tau\rho(t)}]=-\tau\sum_{n=2}\frac{(-\tau)^{n-1}}{(n-1)!}\mathrm{Tr}\,\rho^{n-1}\rho_1=-\tau\sum_{n=1}\frac{(-\tau)^n}{n!}\mathrm{Tr}\,\rho^n\rho_1. \tag{20}$$

Assuming an initial pure state, we have

$$\frac{d}{dt}\mathrm{Tr}[e^{-\tau\rho(t)}]\big|_{t=0} = -\tau\sum_{n=1}\frac{(-\tau)^n}{n!}\mathrm{Tr}\,\rho\rho_1 = \tau\,\mathrm{Tr}\,\rho\rho_1 - \tau\sum_{n=0}\frac{(-\tau)^n}{n!}\mathrm{Tr}\,\rho\rho_1$$
$$= \tau\,\mathrm{Tr}\,\rho\rho_1 - \tau e^{-\tau}\mathrm{Tr}\,\rho\rho_1; \tag{21}$$

then, the derivative of $\zeta_\rho(s,t)$ is

$$\frac{d}{dt}\zeta_\rho(s,t)\bigg|_{t=0} = \frac{1}{\Gamma(s)}\int_0^\infty d\tau\,\tau^{s-1}\,\mathrm{Tr}\left\{\tau(1-e^{-\tau})\rho\rho_1 - \frac{d}{dt}P_0\bigg|_{t=0}\right\}. \tag{22}$$

According to the argument given above, we recognize in this expression the existence of a (logarithmic) divergence; this may be assumed to be removed by a counterterm given by the derivative of P_0.

$$\mathrm{Tr}\frac{d}{dt}P_0\bigg|_{t=0} = \tau\,\mathrm{Tr}\,\rho\rho_1. \tag{23}$$

Then, the convergent part is given by

$$\frac{d}{dt}\zeta_\rho(s,t)\bigg|_{t=0} = -\frac{\Gamma(s+1)}{\Gamma(s)}\mathrm{Tr}\,\rho\rho_1, \tag{24}$$

and therefore the first derivative of the entropy at $t=0$ for an initial pure state is obtained by deriving with respect to s according to Eq. (17)

$$S_1(0) = \frac{d}{ds}\frac{d}{dt}\zeta_\rho(s,0)\big|_{s=-1} = -\mathrm{Tr}\,\rho\rho_1. \tag{25}$$

Notice that this result coincides with that of Eq. (9) once the divergent $\zeta(1)$ is discarded.

The second derivative of the von Neumann entropy can be calculated in a similar way. In this case, in order to subtract the divergence we assume this is removed with

$$\mathrm{Tr}\frac{d^2}{dt^2}P_0 = \tau\,\mathrm{Tr}(\rho_1^2 - 2\rho\rho_1^2) + \tau\,\mathrm{Tr}(2\rho\rho_1^2 + \rho\rho_2) + (-3\tau^2 + 2\tau^3 + 2\tau)\mathrm{Tr}\,\rho\rho_1\rho\rho_1, \tag{26}$$

and then the finite part of the $\zeta_\rho(s,t)$ at $t=0$ is

$$\frac{d}{dt}\zeta_\rho(s,t)\big|_{t=0} = -s\,\mathrm{Tr}\,(2\rho\rho_1^2 + \rho\rho_2) + (s^2 - s)\,\mathrm{Tr}\,\rho\rho_1\rho\rho_1; \tag{27}$$

therefore, the second time derivative of S is

$$S_2(0) = \frac{d}{ds}\frac{d^2}{dt^2}\zeta_\rho(s,0)\big|_{s=-1} = -\mathrm{Tr}(2\rho\rho_1^2 + \rho\rho_2) - 3\,\mathrm{Tr}\rho\rho_1\rho\rho_1. \tag{28}$$

This expression is similar to that found in Eq. (11) once the divergent $\zeta(1)$ is discarded. The particular case of an eigenstate of f, $S_2(0)$, gives a similar result to Eq. (12), because in that case $\mathrm{Tr}\,2\rho\rho_1^2 = \mathrm{Tr}\,\rho_1^2$ and because the term $\mathrm{Tr}\,\rho\rho_1\rho\rho_1 = 0$.

Of course, in some cases it is not necessary to calculate higher-order derivatives because the first-order derivative is nonzero, and this derivative gives enough information about the decoher-

ence process.[19] However, for the case in Eq. (1) we have to calculate higher-order derivatives. In this case, applying the same procedure and discarding the divergent part, we find that the finite part of the third derivative of the von Neumann entropy is

$$S_3(0)=\frac{d}{ds}\frac{d^3}{dt^3}\zeta_\rho(s,0)\big|_{s=-1}=-\mathrm{Tr}(\rho\rho_3+3\rho_1\rho_2).$$

This can be compared with the corresponding derivative of the linear entropy

$$S_{l3}(t)=-2\,\mathrm{Tr}(3\rho_1\rho_2+\rho_0\rho_3), \tag{29}$$

showing that upon a factor we get essentially the same information.

These calculations show that the regularized expression for the von Neumann entropy in Eq. (17) allows us to distinguish, without ambiguity, the divergent part of its derivatives. The information that these derivatives give about the decoherence process is similar to that found by the linear entropy upon a factor. In addition, we have found a new application of the zeta function technique, unknown in the literature, to the best of our knowledge.

Since the completion of this work, we have been informed of a recent reference,[27] where some remote connection of the zeta function techniques to information theory has been discussed. This is a subject that warrants further investigation.

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Noncommutative cohomological field theory and GMS soliton

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We show that it is possible to construct a quantum field theory that is invariant under the translation of the noncommutative parameter $\theta_{\mu\nu}$. This is realized in a noncommutative cohomological field theory. As an example, a noncommutative cohomological scalar field theory is constructed, and its partition function is calculated. The partition function is the Euler number of Gopakumar, Minwalla, and Strominger (GMS) soliton space. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Recently noncommutative geometry and noncommutative field theory revived in the string theory.[1] There are some correspondences between commutative and noncommutative geometry.[26] For example, in the gauge theory, it was shown that the commutative theory with some background field is equivalent to the noncommutative theory.[2] After that, a few kinds of nontrivial solitons in the noncommutative space are discovered. In the gauge theory, U(1) instanton solution was discovered by Nekrasov and Schwartz,[3] and in the scalar theory a nontrivial solution was discovered by Gopakumar, Minwalla, and Strominger,[4] which is called the GMS soliton. There is no corresponding solution in the commutative space, i.e., the GMS soliton is a specific solution in the noncommutative space.

In the noncommutative space, it is difficult to define the length or metric. There are few examples, like a noncommutative torus case, derived the differential geometry, e.g., connection and curvature.[5] But in general noncommutative space, to define the Riemannian geometry is difficult. What we can do is to classify the geometry to the extent of the algebric K-theory. However, it is not enough to classify the noncommutative space from a point of view of differential topology. If there are some characteristic classes that do not vary under the shift from commutative to noncommutative space, then they are useful for the classification of spaces. For instance, in the noncommutative torus the Euler number is independent of the noncommutative parameter θ.[6] We expect that some other topological invariants would be extended to noncommutative space and independent of θ.

The aim of this article is to construct a quantum field theory that is invariant under the transformation of the noncommutative parameter $\theta^{\mu\nu}$. This parameter characterizes the noncommutativity of spaces as

$$[x^{\mu},x^{\nu}]=\frac{\theta^{\mu\nu}}{2\pi i}, \tag{1.1}$$

where x^{μ} are the coordinates of the noncommutative space. Noncommutative parameter independence of the theory means that the partition function of the theory is independent of $\theta^{\mu\nu}$. Cohomological field theory is nominated as such a theory. We construct a cohomological field theory

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on the noncommutative space, and we show that it is actually a usual cohomological field theory in the $\theta^{\mu\nu}=0$ limit. This fact means that noncommutative space succeed to some geometric or topological information of commutative space.

Another purpose of this article is to construct a concrete example of the invariants under the transformation of noncommutative parameter $\theta^{\mu\nu}$. The discovery of the GMS solution is one of the most important developments in recent work on noncommutative field theory. Therefore, we calculate the Euler number of the GMS soliton space as the example of $\theta^{\mu\nu}$ independent partition function. We will see the relation between the GMS soliton and commutative cohomological field theory.

Our example of the noncommutative cohomological field theory is a balanced scalar model that has two multiplets, the scalar and the vector. We consider the case that the potential is a general degree polynomial of the scalar field. In the commutative space, the degree of the potential determines the structure of the vacuum. We will show that in the noncommutative space there is similar picture of vacuum structure. As a result of investigation, the correspondence between the commutative limit $\theta\to 0$ and the noncommutative limit $\theta\to\infty$ is obtained. Especially in the large θ limit, the potential term plays a dominant role, and there are the specific GMS solutions. A point of this article is how we deal with the GMS solitons in quantum field theory.

This article is organized as follows. In Sec. II, we will construct the $\theta^{\mu\nu}$ invariant quantum field theory in general. In Sec. III, we construct a scalar model as a simple example. Balanced topological theory will be used there. It is necessary to introduce potential in topological scalar field theory. The partition function is calculated in both limits, commutative and noncommutative. In Sec. IV, we introduce the Morse theory on the noncommutative field theory, and show that the Euler number of the GMS soliton space is well-defined. In the last section, we summarize and discuss our result.

II. GENERAL FORMALISM

The aim of this section is to make a theory that is invariant under the shift of the noncommutative parameter $\theta_{\mu\nu}$. We discuss how we construct the cohomological field theory on the noncommutative space.

A. Cohomological field theory on noncommutative space

The noncommutative parameter is defined in the commutation relation Eq. (1.1). We introduce the infinitesimal rescaling operator δ_s as follows:

$$(1-\delta_s)[x^\mu,x^\nu]\equiv[x'^\mu,x'^\nu]=\frac{\theta^{\mu\nu}-\delta\theta^{\mu\nu}}{2\pi i}. \tag{2.1}$$

This commutation relation is given by defining δ_s as

$$x'^\mu=x^\mu-\delta_s x^\mu, \tag{2.2}$$

$$\delta_s x^\mu=(\tfrac{1}{2}\delta\theta^{\mu\nu}(\theta^{-1})_{\nu\rho})x^\rho. \tag{2.3}$$

This transformation corresponds to $x'^\mu=\sqrt{\theta}x^\mu$ in Ref. 4. We denote the inverse matrix of the transformation (2.2) by

$$J^\mu_\rho\equiv\delta^\mu{}_\rho+\tfrac{1}{2}\delta\theta^{\mu\nu}(\theta^{-1})_{\nu\rho}. \tag{2.4}$$

Then, the integration measure and the differential operator are transformed into

$$dx^D=\det\mathbf{J}dx'^D,\quad \frac{\partial}{\partial x^\mu}=(J^{-1})_{\mu\nu}\frac{\partial}{\partial x'^\nu}, \tag{2.5}$$

where det$\mathbf{J}$ is the Jacobian. By (2.5) the Moyal product(see, e.g., Ref. 7) is shifted as

$$(1-\delta_s)(*_\theta)=\delta_s(\exp(2\pi i\overleftarrow{\partial}_\mu(\theta-\delta\theta)^{\mu\nu}\vec{\partial}_\nu))=*_{\theta-\delta\theta}, \tag{2.6}$$

because $\delta_s(\overleftarrow{\partial}_\mu\theta^{\mu\nu}\vec{\partial}_\nu)=\overleftarrow{\partial}_\mu\delta\theta^{\mu\nu}\vec{\partial}_\nu$. Note that this transformation is just a rescaling of the coordinate, so that any action and its partition function are not changed under this transformation,

$$S_\theta=\int dx^D\mathcal{L}(*_\theta,\partial_\mu)=\int \det\mathbf{J}dx'^D\mathcal{L}\left(*_{\theta-\delta\theta},(J^{-1})^{\mu\nu}\frac{\partial}{\partial x'^\nu}\right), \tag{2.7}$$

where $\mathcal{L}(*_\theta,\partial_\mu)$ is an explicit description to emphasize that the products of fields are the Moyal product and it contains derivative terms in the Lagrangian. For convenience, we will often omit $*_\theta$ when we do not misunderstand. In the next step, we shift the noncommutative parameter:

$$\theta\rightarrow\theta'=\theta+\delta\theta. \tag{2.8}$$

This shift changes the action and the partition function in general, as follows:

$$S_{\theta'}=\int \det\mathbf{J}dx'^D\mathcal{L}\left(*_\theta,(J^{-1})^{\mu\nu}\frac{\partial}{\partial x'^\nu}\right). \tag{2.9}$$

Compared with (2.7), the shift is regarded as a rescaling without the Moyal product.

On the contrary, our purpose is to construct a field theory invariant under this shift. Immediately we expect the cohomological field theory would be an example since it is scale invariant theory.[8–10] Cohomological field theory is understood through several ways. Twisted SUSY is one of them, but noncommutative SUSY is not adverted here.[11–13] Meanwhile, a geometrical point of view is closely studied in Sec. IV. The Lagrangian of cohomological field theory is BRST-exact. We denote the BRST operator by $\hat{\delta}$, and generic bosonic fields by ϕ_i, which are sections of some vector bundle $s_a(*_\theta\phi_i)$. The BRST operator is defined as

$$\begin{aligned}&\hat{\delta}\phi_i=\psi_i, \quad \hat{\delta}\psi_i=0,\\ &\hat{\delta}\chi^a=H^a, \quad \hat{\delta}H^a=0,\end{aligned} \tag{2.10}$$

where ϕ_i and H^a are bosonic and ψ_i and χ^a are fermionic fields. Following the Mathai–Quillen formalism, the action of the cohomological field theory is written as

$$V=\chi^a(is_a+H_a), \tag{2.11}$$

$$S_\theta=\int dx^D\mathcal{L}(*_\theta,\partial_\mu)=\int dx^D\hat{\delta}V. \tag{2.12}$$

The partition function is defined by

$$Z_\theta=\int \mathcal{D}\phi\mathcal{D}\psi\mathcal{D}\chi\mathcal{D}H\exp(-S_\theta). \tag{2.13}$$

In the commutative space, the Mathai–Quillen formalism tells us that the partition function gives a representation of the Euler number of the space $\mathcal{M}=\{s_a^{-1}(0)\}$.

This partition function is invariant under an infinitesimal transformation which commutes with the BRST transformation (2.10).

$$\hat{\delta}\delta'=\pm\delta'\hat{\delta}, \tag{2.14}$$

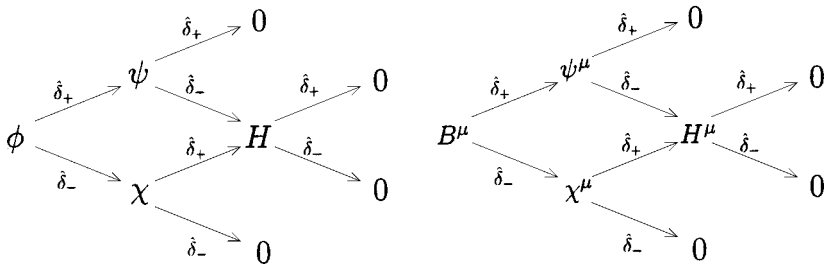

FIG. 1. BRST multiplets in the balanced scalar model. $\delta_+(\delta_-)$ carries ghost number $+1(-1)$.

$$\delta' Z_\theta = \int \mathcal{D}\phi\mathcal{D}\psi\mathcal{D}\chi\mathcal{D}H\,\delta'\left(-\int dx^D \hat{\delta}V\right)\exp(-S_\theta)$$
$$= \int \mathcal{D}\phi\mathcal{D}\psi\mathcal{D}\chi\mathcal{D}H\,\hat{\delta}\left(-\int \delta' V\right)\exp(-S_\theta) = 0.$$

The vacuum expectation value (VEV) of any BRST-exact observable is zero. Note that the path integral measure is invariant under δ' transformation since every field has only one supersymmetric partner and the Jacobian is totally canceled.

We introduce the θ-shift operator as

$$\delta_s x_\mu = -\delta_s x_\mu, \delta_\theta \theta_{\mu\nu} = \theta_{\mu\nu} + \delta\theta_{\mu\nu}. \tag{2.15}$$

Generally, it is possible to define δ_θ to commute with the BRST operator. Following (2.14), the partition function is invariant under this θ-shift and it means that the Euler number of the space $\mathcal{M}$ is independent of the noncommutative parameter θ.

In the end of this section, we list some general nature of this partition function. First, the Gaussian integral is formally defined and an exact result can be given by one-loop calculation. Second, naively the commutative limit ($\theta\to 0$) is given by removing potential terms without constant field, and the $\theta\to\infty$ limit is given by omitting kinetic terms in the action, because the limit $\theta\to 0$ ($\theta\to\infty$) means $\mathbf{J}\to 0$ ($\mathbf{J}\to\infty$) in Eq. (2.9).

In the next section, as an example of noncommutative cohomological field theory, we investigate the balanced scalar model.

III. BALANCED SCALAR MODEL

In this section, we study a concrete example of noncommutative cohomological field theory as θ-shift invariant field theory. For simplicity, we use a real scalar model to construct a cohomological field theory. However, there is no nontrivial example under usual construction of cohomological field theory. Therefore, we introduce the balanced topological field theory.[14,15] This theory is used in the investigation of the Vafa–Witten theory whose partition function is the sum of Euler number of the zero section space $\mathcal{M}$ without a sign, in general.[16–18] When we calculate the Vafa–Witten theory, zero mode integration is not essential because there is no ghost number anomaly. On the contrary, in this article, we carefully calculate the zero mode integration to compare the commutative limit with the large θ limit.

A. The action

We construct the balanced scalar model. The theory is composed of bosonic scalar fields ϕ and H, fermionic scalar fields ψ and χ, bosonic vector fields B_μ and H_μ, fermionic vector fields ψ_μ and χ_μ, and every field is Hermitian field. We give the BRST transformations (Fig. 1) as

$$\hat{\delta}_+\phi = \psi, \quad \hat{\delta}_-\phi = \chi,$$

$$
\begin{aligned}
-\hat{\delta}_-\psi &= \hat{\delta}_+\chi = H,\\
\hat{\delta}_+\psi &= \hat{\delta}_-\chi = \hat{\delta}_+H = \hat{\delta}_-H = 0,\\
\hat{\delta}_+B^\mu &= \psi^\mu,\ \hat{\delta}_-B^\mu = \chi^\mu,\\
-\hat{\delta}_-\psi^\mu &= \hat{\delta}_+\chi^\mu = H^\mu,\\
\hat{\delta}_+\psi^\mu &= \hat{\delta}_-\chi^\mu = \hat{\delta}_+H^\mu = \hat{\delta}_-H^\mu = 0,
\end{aligned}
\tag{3.1}
$$

where $\hat{\delta}_+$ and $\hat{\delta}_-$ satisfy the following relations,

$$
\hat{\delta}_+^2 = \hat{\delta}_-^2 = 0, \quad \hat{\delta}_+\hat{\delta}_- + \hat{\delta}_-\hat{\delta}_+ = 0. \tag{3.2}
$$

The action of the balanced scalar model is

$$
S = \int dx^D \sqrt{g}\mathcal{L}, \tag{3.3}
$$

where the Lagrangian $\mathcal{L}$ is given by an exact form with a ghost-number zero functional $\mathcal{F}$ as

$$
\mathcal{L} = i\hat{\delta}_+\hat{\delta}_-\mathcal{F}. \tag{3.4}
$$

In our case, the functional $\mathcal{F}$ is chosen as

$$
\mathcal{F} = B^\mu\partial_\mu\phi - i\chi^\mu\psi_\mu - i\chi\psi + V(\phi,B^\rho), \tag{3.5}
$$

where $V(\phi,B^\rho)$ is a potential. Therefore the Lagrangian $\mathcal{L}$ becomes

$$
\begin{aligned}
\mathcal{L} &= i\hat{\delta}_+\hat{\delta}_-\mathcal{F} = i\hat{\delta}_+\left\{\chi^\mu\partial_\mu\phi + B^\mu\partial_\mu\chi - i\chi^\mu H_\mu - i\chi H + \left(\chi\frac{\delta}{\delta\phi}\right)V(\phi,B^\rho) + \left(\chi^\mu\frac{\delta}{\delta B^\mu}\right)V(\phi,B^\rho)\right\}\\
&= i\hat{\delta}_+\left[\chi\left\{-\partial_\mu B^\mu + \frac{\delta}{\delta\phi}V(\phi,B^\rho) - iH\right\} + \chi^\mu\left\{\partial_\mu\phi + \frac{\delta}{\delta B^\mu}V(\phi,B^\rho) - iH_\mu\right\}\right] = \mathcal{L}_B + \mathcal{L}_F,
\end{aligned}
\tag{3.6}
$$

where $\mathcal{L}_B(\mathcal{L}_F)$ is the bosonic (fermionic) part of the Lagrangian,

$$
\mathcal{L}_B = iH\left\{-\partial_\mu B^\mu + \frac{\delta}{\delta\phi}V(\phi,B^\rho) - iH\right\} + iH^\mu\left\{\partial_\mu\phi + \frac{\delta}{\delta B^\mu}V(\phi,B^\rho) - iH_\mu\right\}, \tag{3.7}
$$

$$
\begin{aligned}
\mathcal{L}_F &= i\chi\left\{\partial_\mu\psi^\mu - \left(\psi\frac{\delta}{\delta\phi}\right)\frac{\delta}{\delta\phi}V(\phi,B^\rho) - \left(\psi^\mu\frac{\delta}{\delta B^\mu}\right)\frac{\delta}{\delta\phi}V(\phi,B^\rho)\right\}\\
&\quad - i\chi^\mu\left\{\partial_\mu\psi + \left(\psi\frac{\delta}{\delta\phi}\right)\frac{\delta}{\delta B^\mu}V(\phi,B^\rho) + \left(\psi^\nu\frac{\delta}{\delta B^\nu}\right)\frac{\delta}{\delta B^\mu}V(\phi,B^\rho)\right\}.
\end{aligned}
\tag{3.8}
$$

Here we consider the only case that the potential has separated form as

$$
V(\phi,B^\rho) = V(\phi) + \tfrac{1}{2}B_\mu B^\mu. \tag{3.9}
$$

As a result of taking this potential, B^μ has only zero solution in the large θ limit, and this is a necessary condition to investigate the GMS soliton space. If there is a nontrivial B^μ solution, then the moduli space is changed from GMS soliton moduli space and we are not interested in such a case. $\mathcal{L}_B$ and $\mathcal{L}_F$, therefore, become

$$\mathcal{L}_B = iH\left\{ -\partial_\mu B^\mu + \frac{\delta V(\phi)}{\delta\phi} - iH \right\} + iH^\mu(\partial_\mu\phi + B_\mu - iH_\mu), \tag{3.10}$$

$$\mathcal{L}_F = i\chi\left\{ \partial_\mu\psi^\mu - \psi\frac{\delta^2 V(\phi)}{\delta\phi^2} \right\} - i\chi^\mu(\partial_\mu\psi + \psi_\mu). \tag{3.11}$$

Note that every product of fields should be defined by replacing the normal product by the Moyal product when we consider the noncommutative field theory.

B. Commutative limit $\theta\to 0$

We consider the balanced scalar model in two-dimensional flat noncommutative space. One can get the theory on noncommutative space by changing the ordinary product into the star (Moyal) product $*_\theta$. Although noncommutativity is represented by the noncommutative parameter θ in the star product, this parameter is absorbed by the rescaling,

$$x^\mu \to \sqrt{\theta}x^\mu,$$

$$*_\theta \to *_{\theta=1}. \tag{3.12}$$

However, the action is changed as follows:

$$S_B = \int d^2x\,\theta\left[iH*\left\{ -\frac{\partial_\mu B^\mu}{\sqrt{\theta}} + \frac{\delta V(*\phi)}{\delta\phi} - iH \right\} + iH^\mu *\left(\frac{\partial_\mu\phi}{\sqrt{\theta}} + B_\mu - iH_\mu \right) \right], \tag{3.13}$$

$$S_F = \int d^2x\,\theta\left[i\chi*\left\{ \frac{\partial_\mu\psi^\mu}{\sqrt{\theta}} - \psi\frac{\delta^2 V(*\phi)}{\delta\phi^2} \right\} - i\chi^\mu *\left(\frac{\partial_\mu\psi}{\sqrt{\theta}} + \psi_\mu \right) \right], \tag{3.14}$$

where $S_B(S_F)$ is the bosonic (fermionic) part of the action and $*$ means $*_{\theta=1}$ implicitly.

Let us consider the $\theta\to 0$ limit and calculate its partition function, which is compared with the $\theta\to\infty$ limit in the next subsection. The partition function is calculated as

$$\mathcal{Z} = \int \mathcal{D}\phi\mathcal{D}\chi\mathcal{D}\psi\mathcal{D}\chi^\mu\mathcal{D}\psi^\mu\mathcal{D}B^\mu\mathcal{D}H\mathcal{D}H^\mu \exp(-S_B - S_F). \tag{3.15}$$

The part of the action which contributes to the nonzero modes of ϕ and H is

$$\int d^2x\sqrt{\theta}i(H^\mu * \partial_\mu\phi - H*\partial_\mu B^\mu). \tag{3.16}$$

We perform the integration of the nonzero modes of H^μ and B^μ, and it yields delta functionals,

$$\delta(\sqrt{2\pi\theta}\partial_\mu\phi)\,\delta(\sqrt{2\pi\theta}\partial_\mu H). \tag{3.17}$$

Therefore, for ϕ and H, only zero mode integrals remains. Next, the part of the action which contributes to the nonzero modes of χ and ψ is

$$\int d^2x\sqrt{\theta}i(\chi*\partial_\mu\psi^\mu - \chi^\mu*\partial_\mu\psi). \tag{3.18}$$

Integration of nonzero modes of χ,ψ and χ^μ,ψ^μ yields the factor

$$[\det(i\sqrt{\theta}\partial_\mu)]_{\chi_\varnothing\psi^\mu}[\det(i\sqrt{\theta}\partial_\mu)]_{\chi^\mu\psi_\varnothing}, \tag{3.19}$$

where the fields with the subscript $_\varnothing$ denote nonzero modes. Therefore, for χ and ψ, only zero modes remain and the partition function $\mathcal{Z}$ becomes

$$\mathcal{Z}=\frac{[\det(i\sqrt{\theta}\partial_\mu)]_{\chi^\mu\psi_\varnothing}}{[\det(\sqrt{2\pi\theta}\partial_\mu)]_{H^\mu\phi_\varnothing}}\frac{[\det(i\sqrt{\theta}\partial_\mu)]_{\chi_\varnothing\psi^\mu}}{[\det(\sqrt{2\pi\theta}\partial_\mu)]_{H_\varnothing B^\mu}}\int dy\,d\chi_0 d\psi_0\mathcal{D}\chi^\mu\mathcal{D}\psi^\mu\mathcal{D}B^\mu dH_0\mathcal{D}H^\mu \times\exp(-S_B'-S_F'), \tag{3.20}$$

where the fields with the subscript $_0$ denote zero modes and the variable y denotes the zero mode of ϕ (this is just a real constant number) and

$$S_B'=\int d^2x\,\theta\left[H_0\left\{H_0+i\frac{\delta V(y)}{\delta y}\right\}+H^\mu*(H_\mu+iB_\mu)\right], \tag{3.21}$$

$$S_F'=\int d^2x\,\theta i\left[-\chi_0\psi_0\frac{\delta^2V(y)}{\delta y^2}-\chi^\mu*\psi_\mu\right]. \tag{3.22}$$

The factors in front of the integral in Eq. (3.20) cancel each other and only $[\det(2\pi)]^{-1}_{H^\mu\phi_\varnothing}$ remains. H^μ, B^μ and the zero mode of H can be integrated out, and it yields the factor

$$\frac{1}{[v\,\theta/\pi]^{1/2}_{H_0}}\frac{1}{[\det(\theta/\pi)]^{1/2}_{H^\mu\phi_0}}\frac{1}{[\det(\theta/4\pi)]^{1/2}_{H_0B^\mu}}, \tag{3.23}$$

where v is the volume of space–time. This volume is infinity but this will be canceled out by ϕ, χ and ψ zero mode integration, later. Integration of χ^μ,ψ^μ yields the factor $[\det(i\theta)]_{\chi^\mu\psi^\mu}$, and the partition function $\mathcal{Z}$ becomes

$$\mathcal{Z}=\sqrt{\frac{\pi}{v\,\theta}}\det(-1)\int dy\,d\chi_0 d\psi_0\exp(-S_B''-S_F''), \tag{3.24}$$

where

$$S_B''=\int d^2x\frac{\theta}{4}\left\{\frac{\delta V(y)}{\delta y}\right\}^2, \tag{3.25}$$

$$S_F''=-\int d^2x\,\theta i\chi_0\psi_0\frac{\delta^2V(y)}{\delta y^2}. \tag{3.26}$$

Before integrating y, we expand $\delta V(y)/\delta y$ as

$$\frac{\delta V(y)}{\delta y}=y\frac{\delta^2V(y)}{\delta y^2}\bigg|_{y=y_c}+\mathcal{O}(y^2), \tag{3.27}$$

where y_c is a point of the extrema of the potential,

$$\frac{\delta V(y)}{\delta y}\bigg|_{y=y_c}=0, \tag{3.28}$$

and we should sum up all y_c in the calculation of $\mathcal{Z}$:

$$\mathcal{Z}=\sqrt{\frac{\pi}{v\,\theta}}\det(-1)\sum_{y_c}\int dy\,d\chi_0 d\psi_0\exp(-S'), \tag{3.29}$$

where

$$S' = v\,\theta\left[\frac{1}{4}\left\{ y\,\frac{\delta^2 V(y)}{\delta y^2}\bigg|_{y=y_c}\right\}^2 - i\chi\psi\frac{\delta^2 V(y)}{\delta y^2}\bigg|_{y=y_c}\right]. \tag{3.30}$$

Note that these zero modes do not depend on x^μ; then the volume v is factorized out. By integrating the zero modes of ϕ,χ and ψ, we get the partition function,

$$\mathcal{Z} = \sqrt{\frac{\pi}{v\,\theta}}\det(-1)\sum_{y_c}\frac{iv\,\theta\,\delta^2 V(y)/\delta y^2\,|_{y=y_c}}{\{(v\,\theta/4\pi)\;\delta^2 V(y)/\delta y^2\,|^2_{y=y_c}\}^{1/2}}$$

$$= 2\pi i\,\det(-1)\sum_{y_c}\;\mathrm{sgn}\left[\frac{\delta^2 V(y)}{\delta y^2}\bigg|_{y=y_c}\right]. \tag{3.31}$$

The factor in front of Σ_{y_c} is removable as a normalizing factor.

Generally, the potential $V(\phi)$ is a polynomial of the scalar field ϕ:

$$V(\phi) = b_0 + b_1\phi + \frac{b_2}{2!}\phi^2 + \cdots + \frac{b_m}{m!}\phi^m (m \geqslant 2), \tag{3.32}$$

and so the result Eq. (3.31) becomes

$$\mathcal{Z} = \begin{cases} \mathrm{sgn}[b_m]: & m \text{ is even number,} \\ 0: & m \text{ is odd number.} \end{cases} \tag{3.33}$$

In the limit $\theta \to 0$, it seems that the kinetic term plays a dominant role, but the effect of the potential term survives. By this effect, the degree of the polynomial completely determines the partition function as a cyclic form of Eq. (3.33).

C. Noncommutative limit $\theta \to \infty$

In the strong noncommutative limit $\theta \to \infty$, the terms that have derivatives are effectively ignored, and the remaining terms which are potential and mass terms in the balanced scalar model determine the field configuration. In the noncommutative space, there is a specific field configuration, that is, a GMS soliton.[4] This soliton is the solution of the field equation, and there are infinite solutions. Hence, the partition function is the sum of contributions from infinite vacuum states.

In the large θ limit, the balanced scalar model, Eqs. (3.10) and (3.11), is written as

$$S = S_B + S_F, \tag{3.34}$$

where

$$S_B = \int d^2x\,\theta\left[H * \left\{\frac{\delta V(*\phi)}{\delta\phi} - H\right\} + H^\mu * (B_\mu - H_\mu)\right], \tag{3.35}$$

$$S_F = \int d^2x\,\theta\left[-i\chi * \left(\psi\frac{\delta}{\delta\phi}\right)\frac{\delta V(*\phi)}{\delta\phi} + i\chi^\mu * \psi_\mu\right]. \tag{3.36}$$

After integrating over the fields H, H^μ, the action is

$$S = \int d^2x\,\theta\left[\frac{1}{4}\,\frac{\delta V(*\phi)}{\delta\phi}\,\frac{\delta V(*\phi)}{\delta\phi} - i\chi * \left(\psi\frac{\delta}{\delta\phi}\right)\frac{\delta V(*\phi)}{\delta\phi} + \frac{1}{4}B^\mu * B_\mu + i\chi^\mu * \psi_\mu\right]. \tag{3.37}$$

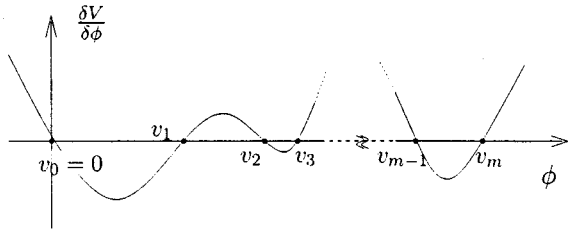

FIG. 2. $\delta V/\delta\phi$, $b_m>0$ and m is odd.

Integration of the fields B^μ, χ^μ and ψ_μ is simply performed, and the partition function is written as

$$\mathcal{Z}=\int \mathcal{D}\phi\mathcal{D}\chi\mathcal{D}\psi e^{-S}, \tag{3.38}$$

where the action is

$$S=\int d^2x\theta\left[\frac{1}{4}\frac{\delta V(*\phi)}{\delta\phi}\frac{\delta V(*\phi)}{\delta\phi}-i\chi*\left(\psi\frac{\delta}{\delta\phi}\right)\frac{\delta V(*\phi)}{\delta\phi}\right]. \tag{3.39}$$

In the large θ limit, the derivative terms are irrelevant, and the potential terms dominate. (Actually the kinetic term integral is survived for next order integral but it yields nothing because of the BRST symmetry.) The field configuration is determined by the form of the potential. In particular the stationary field configuration is obtained by solving the field equation:

$$\frac{\delta V(*\phi)}{\delta\phi}=0. \tag{3.40}$$

In the calculation of the partition function, we should treat these GMS solitons as the stationary points, and the quantum fluctuation is a perturbation from the GMS soliton. In the following section, we discuss the treatment of the GMS soliton in the partition function, and understand the GMS soliton from a topological view point.

We consider the ϕ^{m+2} potential,

$$V(\phi)=\{\phi\text{-polynomial of}(m+2)\text{degree}\}, \tag{3.41}$$

and the field equation takes the following factorized form

$$\frac{\delta V}{\delta\phi}=b_m\phi*(\phi-v_1)*(\phi-v_2)*\cdots*(\phi-v_m), \tag{3.42}$$

where we assume the v_i are real constant numbers with $v_1<v_2<\cdots<v_{m-1}<v_m$ (see Fig. 2). The GMS soliton is given by

$$\phi_{\mathrm{GMS}}=\lambda_i\mathbf{P}_i, \tag{3.43}$$

where $\mathbf{P}_i$ is a projection, and satisfies the idempotent relation $\mathbf{P}_i*\mathbf{P}_j=\delta_{ij}\mathbf{P}_i$. The coefficient λ_i is determined by Eq. (3.42). In the Moyal plane, this projection is given by the Laguerre polynomial $2(-1)^i e^{-x^2}\mathrm{L}_i(2x^2)$.[4] It is possible to choose concrete representation of a corresponding Weyl mapped projection operator, for example,

$$\hat{\mathbf{P}}_i=|i\rangle\langle i|, \tag{3.44}$$

where $|i\rangle$ is the number representation base.[19,20] The Weyl mapped GMS soliton is written as

$$\hat{\phi}_{GMS}=\lambda_i\hat{\mathbf{P}}_i. \tag{3.45}$$

We substitute the GMS solution to ϕ of Eq. (3.42):

$$\left.\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\right|_{GMS}=b_m\lambda_i(\lambda_i-v_1)(\lambda_i-v_2)\cdots(\lambda_i-v_m)\mathbf{P}_i=0. \tag{3.46}$$

The solutions of Eq. (3.46) are given by

$$\lambda_i=0,v_1,v_2,\ldots,v_m. \tag{3.47}$$

These solutions are coefficients of the GMS soliton. The general GMS solution is a linear combination of the projections,

$$\hat{\phi}_{\mathrm{GMS}}=\sum_i\lambda_i\hat{\mathbf{P}}_i=v_1\sum_{i\in\mathbf{S}_1}\hat{\mathbf{P}}_i+v_2\sum_{i\in\mathbf{S}_2}\hat{\mathbf{P}}_i+\cdots+v_m\sum_{i\in\mathbf{S}_m}\hat{\mathbf{P}}_i=v_1\hat{\mathbf{P}}_{\mathbf{S}_1}+v_2\hat{\mathbf{P}}_{\mathbf{S}_2}+\cdots+v_m\hat{\mathbf{P}}_{\mathbf{S}_m}, \tag{3.48}$$

where $\mathbf{S}_A(A\in\{1,2,\ldots,m\})$ is a set of the indices of the projections, and it is defined that if the coefficient of a projection $\hat{\mathbf{P}}_i$ is v_A in (3.48), then the index "i" belongs to $\mathbf{S}_A$. For example, if a GMS soliton takes the form $\hat{\phi}_{\mathrm{GMS}}=v_1(\hat{\mathbf{P}}_1+\hat{\mathbf{P}}_2)+v_2(\hat{\mathbf{P}}_0)$, then $\mathbf{S}_1=\{1,2\}$ and $\mathbf{S}_2=\{0\}$. We define $\hat{\mathbf{P}}_{\mathbf{S}_A}\equiv\Sigma_{i\in\hat{\mathbf{S}}_A}\mathbf{P}_i$. For $A\neq B(A,B\in\{1,2,\ldots,m\})$ the sets $\mathbf{S}_A$ and $\mathbf{S}_B$ are disjoint to each other $\mathbf{S}_A\cap\mathbf{S}_B=\varnothing$, and the projections are orthogonal, $\hat{\mathbf{P}}_{\mathbf{S}_A}\cdot\hat{\mathbf{P}}_{\mathbf{S}_B}=0$. In the commutative space, the field equation (3.42) has only constant solutions. On the contrary, in the noncommutative space, there exist GMS solitons that are operators for the Hilbert space of quantized coordinate, and this fact make new solutions with linear combinations of projections. The indices of the projection are not bound above; then the number of the element of $\mathbf{S}_A$ (rank $\mathbf{S}_A$) is allowed to be infinite. In the following, we introduce a cut-off N of total number of the rank $\mathbf{S}_A$, and then there are N projections $\{\hat{\mathbf{P}}_0,\hat{\mathbf{P}}_1,\hat{\mathbf{P}}_2,\ldots,\hat{\mathbf{P}}_{N-1}\}$. After the calculation we take the limit $N\to\infty$.

Next step, we perform a Gaussian integral around each vacuum. Note that, in the commutative space, the number of the solution is $(m+1)$, On the contrary, in the noncommutative space there are $(m+1)^N$ solutions. In the commutative space, we can take the quantum fluctuation from the vacua of the finite number of simply constant solutions of Eq. (3.42). On the contrary, there are infinite GMS solitons in noncommutative space. Let us take the quantum fluctuation around each of the GMS solitons as $\phi=\phi|_{\mathrm{GMS}}+\phi_q$. We expand the Lagrangian around the specific GMS soliton,

$$\mathcal{L}_{\mathbf{S}}=\frac{1}{4}\left(\phi_q\frac{\delta}{\delta\phi}\right)\frac{\delta V(*\phi)}{\delta\phi}\bigg|_{\mathrm{GMS}}*\left(\phi_q\frac{\delta}{\delta\phi}\right)\frac{\delta V(*\phi)}{\delta\phi}\bigg|_{\mathrm{GMS}}-i\chi*\left(\psi\frac{\delta}{\delta\phi}\right)\frac{\delta V(*\phi)}{\delta\phi}\bigg|_{\mathrm{GMS}}. \tag{3.49}$$

The subscript $\mathbf{S}$ of $\mathcal{L}$ means that the Lagrangian is expanded around the GMS soliton specified by $\mathbf{S}$ that is the family of $\{\mathbf{S}_1,\mathbf{S}_2,\ldots,\mathbf{S}_m\}$. (The rank k single GMS soliton space is an infinite dimensional moduli space of solution and it is concretely described as the coset space $U(N)/U(k)U(N-k)$.[21] In our case, the GMS solution space contains not only a single soliton but also multi-solitons that have any rank solutions. The moduli space specified by $\mathbf{S}$ is $U(N)/U(n_0)U(n_1)\cdots U(N-1)$, where n_i is the rank of $\mathbf{S}_i$.) On the Moyal plane, the field operators $\hat{\phi}_q$, $\hat{\chi}$ and $\hat{\psi}$ are expanded as

$$\hat{\phi}_q=\sum_{i,j=0}^{\infty}\phi_{ij}|i\rangle\langle j|,$$

$$\hat{\chi}=\sum_{i,j=0}^{\infty}\chi_{ij}|i\rangle\langle j|, \tag{3.50}$$

$$\hat{\psi}=\sum_{i,j=0}^{\infty}\psi_{ij}|i\rangle\langle j|.$$

The field operators $\hat{\phi}_q$, $\hat{\chi}$ and $\hat{\psi}$ are Hermitian operators,

$$\phi_q^{\dagger}=\phi_q, \quad \chi^{\dagger}=\chi, \quad \psi^{\dagger}=\psi. \tag{3.51}$$

We rewrite the field such as $\phi_{ij}=\phi_{ij}^R+i\phi_{ij}^I$ ($\phi_{ij}^R,\phi_{ij}^I\in\mathbf{R}$). Then the Hermitian conditions need that real (imaginary) parts are symmetric (anti-symmetric):

$$\begin{aligned}&\phi_{ij}^R=\phi_{ji}^R,\phi_{ij}^I=-\phi_{ji}^I,\\ &\chi_{ij}^R=\chi_{ji}^R, \quad \chi_{ij}^I=-\chi_{ji}^I,\\ &\psi_{ij}^R=\psi_{ji}^R, \quad \psi_{ij}^I=-\psi_{ji}^I.\end{aligned} \tag{3.52}$$

In the operator picture, the integration in the action is replaced by the trace over the field operators. The Lagrangian is always described as the Weyl mapped Lagrangian

$$S_{\mathbf{S}}=\mathrm{Tr}\hat{\mathcal{L}}_{\mathbf{S}}=S_B^{\mathbf{S}}+S_F^{\mathbf{S}}, \tag{3.53}$$

where $S_B^{\mathbf{S}}$ and $S_F^{\mathbf{S}}$ are given by

$$S_B^{\mathbf{S}}=\frac{1}{4}\theta\mathrm{Tr}\left(\hat{\phi}_q\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}\left(\hat{\phi}_q\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}, \tag{3.54}$$

$$S_F^{\mathbf{S}}=-i\theta\mathrm{Tr}\hat{\chi}\left(\hat{\psi}\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}. \tag{3.55}$$

First, we consider the bosonic part of the action. The second derivative of the potential is

$$\begin{aligned}\left(\hat{\phi}_q\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}&=\left(\hat{\phi}_q\frac{\delta}{\delta\hat{\phi}}\right)\{b_m\hat{\phi}(\hat{\phi}-v_1)(\hat{\phi}-v_2)\cdots(\hat{\phi}-v_m)\}\bigg|_{\mathrm{GMS}}\\ &=b_m[\hat{\phi}_q(\hat{\phi}-v_1)(\hat{\phi}-v_2)\cdots(\hat{\phi}-v_m)\\ &\quad+\hat{\phi}\hat{\phi}_q(\hat{\phi}-v_2)\cdots(\hat{\phi}-v_m)+\hat{\phi}(\hat{\phi}-v_1)\phi_q\cdots(\hat{\phi}-v_m)\\ &\quad\vdots\\ &\quad+\hat{\phi}(\hat{\phi}-v_1)(\hat{\phi}-v_2)\cdots\hat{\phi}_q]_{\hat{\phi}=\hat{\phi}_{\mathrm{GMS}}}.\end{aligned} \tag{3.56}$$

We put the GMS soliton into Eq. (3.56), and we get

$$\left(\hat{\phi}_q\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}$$

$$= b_m \sum_{A=0}^{m} \sum_{B=A}^{m} \prod_{i=0}^{A-1} (v_B - v_i) \sum_{C=0}^{A} \prod_{j=A+1}^{m} (v_C - v_j) \hat{\mathbf{P}}_{\mathbf{S}_B} \hat{\phi} \hat{\mathbf{P}}_{\mathbf{S}_C}$$

$$= b_m \sum_{A=0}^{m} \prod_{i=0}^{A-1} (v_A - v_i) \prod_{j=A+1}^{m} (v_A - v_j) \hat{\mathbf{P}}_{\mathbf{S}_A} \hat{\phi}_q \hat{\mathbf{P}}_{\mathbf{S}_A}$$

$$+ b_m \sum_{\substack{A>B \\ A,B \in \{0,\cdots,r\}}} \sum_{k=B}^{A} \prod_{i=0}^{k-1} (v_A - v_i) \prod_{j=k+1}^{m} (v_B - v_j) \hat{\mathbf{P}}_{\mathbf{S}_A} \hat{\phi}_q \hat{\mathbf{P}}_{\mathbf{S}_B}, \tag{3.57}$$

where we define the zeroth solution and the zeroth projection by

$$v_0 \equiv 0, \hat{\mathbf{P}}_{\mathbf{S}_0} \equiv \hat{\mathbf{1}} - \hat{\mathbf{P}}_{\mathbf{S}_1} - \hat{\mathbf{P}}_{\mathbf{S}_2} - \cdots - \hat{\mathbf{P}}_{\mathbf{S}_r}, \tag{3.58}$$

and we introduce the following symbols for convenience:

$$\prod_{i=0}^{-1} (v_0 - v_i) \equiv 1, \quad \prod_{j=m+1}^{m} (v_m - v_j) \equiv 1. \tag{3.59}$$

The coefficient of the cross term $\hat{\mathbf{P}}_{\mathbf{S}_A} \hat{\phi}_q \mathbf{P}_{\mathbf{S}_B} (A > B)$ in Eq. (3.57) is

$$\sum_{k=B}^{A} \prod_{i=0}^{k-1} (v_A - v_i) \prod_{j=k+1}^{m} (v_B - v_j). \tag{3.60}$$

Equation (3.60) is written as

$$\sum_{k=B}^{A} \prod_{i=0}^{k-1} (v_A - v_i) \prod_{j=k+1}^{m} (v_B - v_j) = (v_A - v_0)(v_A - v_1) \cdots (v_A - v_{B-1})(v_{A+1} - v_B) \times (v_{A+2} - v_B) \cdots (v_{m-1} - v_B)(v_m - v_B) \$_{A-B}, \tag{3.61}$$

where $\$_{A-B}$ is defined as

$$\begin{aligned} \$_{A-B} \equiv & (v_B - v_{B+1})(v_B - v_{B+2}) \cdots (v_B - v_A) \\ & + (v_A - v_B)(v_B - v_{B+2}) \cdots (v_B - v_A) \\ & \vdots \\ & + (v_A - v_B)(v_{B+1} - v_A) \cdots (v_{A-1} - v_A). \end{aligned} \tag{3.62}$$

We can see $\$_{A-B}$ always vanishes for any set of v_i (see Appendix D). Then the cross term does not appear. Finally, the remaining terms are closed in each set $\mathbf{S}_A$ such as

$$\left(\hat{\phi}_q \frac{\delta}{\delta \hat{\phi}} \right) \frac{\delta V(\hat{\phi})}{\delta \hat{\phi}} \bigg|_{\mathrm{GMS}} = b_m \sum_{A=0}^{m} \prod_{i=0}^{A-1} (v_A - v_i) \prod_{j=A+1}^{m} (v_A - v_j) \hat{\mathbf{P}}_{\mathbf{S}_A} \hat{\phi}_q \hat{\mathbf{P}}_{\mathbf{S}_A}. \tag{3.63}$$

Then the bosonic part of the action is written as

$$S_B^{\mathbf{S}} = \frac{1}{4} \theta \sum_{A=0}^{m} \left(b_m \prod_{i=0}^{A-1} (v_A - v_i) \prod_{j=A+1}^{m} (v_A - v_j) \right)^2 \mathrm{Tr}[\hat{\mathbf{P}}_{\mathbf{S}_A} \hat{\phi}_q \hat{\mathbf{P}}_{\mathbf{S}_A} \hat{\phi}_q]. \tag{3.64}$$

For the fermionic part, the calculation is the same as the bosonic part. Here $(\hat{\psi}(\delta/\delta\hat{\phi}) \times(\delta V(\hat{\phi})/\delta\hat{\phi})$ is given as

$$\left(\hat{\psi}\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}} = b_m \sum_{A=0}^{m}\prod_{i=0}^{A-1}(v_A - v_i)\prod_{j=A+1}^{m}(v_A - v_j)\hat{\mathbf{P}}_{\mathbf{S}_A}\hat{\psi}\hat{\mathbf{P}}_{\mathbf{S}_A}. \tag{3.65}$$

Then the fermionic part of the action is written as

$$S_F^{\mathbf{S}} = -i\theta b_m \sum_{A=0}^{m}\prod_{i=0}^{A-1}(v_A - v_i)\prod_{j=A+1}^{m}(v_A - v_j)\mathrm{Tr}[\hat{\chi}\hat{\mathbf{P}}_{\mathbf{S}_A}\hat{\psi}\hat{\mathbf{P}}_{\mathbf{S}_A}]. \tag{3.66}$$

We substitute $\mathbf{P}_{\mathbf{S}_A} = \Sigma_{i\in\mathbf{S}_A}\mathbf{P}_i$ into Eqs. (3.64) and (3.66), and use Eq. (3.50), Then we get the action,

$$S_{\mathbf{S}} = S_B^{\mathbf{S}} + S_F^{\mathbf{S}} = \sum_{A=0}^{m}\left\{\frac{1}{4}\theta\sum_{i,j\in\mathbf{S}_A}(b_m\zeta_A)^2\phi_{ij}\phi_{ji} - i\theta\sum_{i,j\in\mathbf{S}_A}b_m\zeta_A\chi_{ij}\psi_{ji}\right\}, \tag{3.67}$$

where we define

$$\zeta_A \equiv \prod_{k=0}^{A-1}(v_A - v_k)\prod_{l=A+1}^{m}(v_A - v_l), A\in\{0,1,2,\ldots,m\}. \tag{3.68}$$

Note that the ϕ_{ij}, χ_{ij} and ψ_{ij} are the c-numbers. Using the result in Appendix C, we can estimate both the partition function in the operator representation and in the commutative field representation with the Moyal product, but the results have no difference. Here, we perform the integral in the operator representation. Then the pathintegral becomes simply an integral of real number (real Grassmann number):

$$\begin{aligned}\mathcal{Z}_{\mathbf{S}} &= \int \mathcal{D}\chi\mathcal{D}\psi\mathcal{D}\phi e^{-S_{\mathbf{S}}} \\ &= \int \prod_{A=0}^{m}\prod_{\substack{m>n \\ i,j\in\mathbf{S}_A}}\left(\frac{d\phi_{ij}}{\sqrt{4\pi\theta}}\right)d\chi_{ij}d\psi_{ij}\exp\{-S_B^{\mathbf{S}} - S_F^{\mathbf{S}}\} \\ &= \prod_{A=0}^{m}[\sqrt{b_m\zeta_A}]^{-n_A^2}[b_m\zeta_A]^{n_A^2},\end{aligned} \tag{3.69}$$

and we get

$$\mathcal{Z}_{\mathbf{S}} = \prod_{A=0}^{m}[\mathrm{sgn}(b_m\zeta_A)]^{n_A}. \tag{3.70}$$

Here n_A is the number of the elements belonging to the set $\mathbf{S}_A$, and we call this number the ''rank'' of $\mathbf{S}_A$; $n_A = \mathrm{rank}\,\mathbf{S}_A$. The noncommutative parameter θ contained under integral measure $d\phi$ in the second line of (3.69) comes from the integral of H. The path integral of the fields ϕ_{ij}, χ_{ij} and ψ_{ij} with indices $(i\in\mathbf{S}_A, j\in\mathbf{S}_B, A\neq B)$ is done with the weight of the kinetic terms, which contributes ''1'' in the partition function. The number of the GMS solitons specified by $\mathbf{S} = \{\mathbf{S_1}, \mathbf{S_2}, \ldots, \mathbf{S_m}\}$ is $N!/n_0!n_1!\cdots n_m!$, where $n_i = \mathrm{rank}\,\mathbf{S_i}$. Therefore, the total partition function that includes all the GMS solitons is given by

$$\mathcal{Z}_{\text{Total}} = \lim_{N\to\infty} \sum_{\mathbf{S}} \mathcal{Z}_{\mathbf{S}}$$

$$= \lim_{N\to\infty} \sum_{\substack{n_0,\cdots,n_m=0 \\ n_0+\cdots+n_m=N}}^{N} \frac{N!}{n_0!n_1!\cdots n_m!} \prod_{A=0}^{m} [\text{sgn}(b_m\zeta_A)]^{n_A} \tag{3.71}$$

$$= \lim_{N\to\infty} (\text{sgn}[b_m])^N (\text{sgn}\,\zeta_0 + \text{sgn}\,\zeta_1 + \cdots + \text{sgn}\,\zeta_m)^N. \tag{3.72}$$

Under the same condition of $v_0 < v_1 < \cdots < v_m$ as in the previous section (see Fig. 2, too), the sign of ζ_A is a simple form,

$$\text{sgn}(\zeta_A) = (-1)^{m-A}, A \in \{0,1,2,\ldots,m\}. \tag{3.73}$$

Then the partition function is

$$\mathcal{Z}_{\text{Total}} = \lim_{N\to\infty} (\text{sgn}[b_m])^N (-1)^m (\underbrace{1-1+1-1+\cdots}_{m+1})^N$$

$$= \begin{cases} \lim_{N\to\infty} (\text{sgn}[b_m])^N & : m \text{ is even number,} \\ 0 & : m \text{ is odd number.} \end{cases} \tag{3.74}$$

Note that through a simple calculation, the partition function Eq. (3.71) is rewritten as

$$\mathcal{Z}_{\text{Total}} = \lim_{N\to\infty} [\text{sgn}(b_m)]^N (-1)^m \sum_{n_p=0}^{N} (-1)^{n_p} \frac{N!}{(N-n_p)!n_p!} [(m+1)/2]^{n_p} ([m/2]+1)^{N-n_p}, \tag{3.75}$$

where the bracket $[\cdots]$ is the Gauss notation. The integer n_p is the number of negative solutions, and it is the sum of n_{2i+1}. This number n_p is related to the Morse theory. This is discussed in the next section.

IV. EULER NUMBER OF GMS SOLITON SPACE

In this section we discuss the properties of the partition function from the point of view of quantum geometry.

A. Noncommutative Mathai–Quillen formalism

In the beginning, we study the partition function with Mathai–Quillen formalism.

As in the usual cohomological field theory, ψ is a tangent vector to the zero section, i.e., the tangent vector to the solution space, $\{\phi, B_\mu | s^a(\phi, B_\mu, \theta) = 0\} = \mathcal{M}$. Note that the vanishing theorem asserts that the zero section space is identified with the GMS solution space. In our theory, since $B^\mu B_\mu = 0$ has only a trivial solution, the zero section space is identified with $\{\phi |\ \delta V/\delta\phi = 0\}$. A condition like the vanishing theorem appears in general in the balanced topological field theory.

In the commutative limit ($\theta \to 0$), the relevant terms of the bosonic action are

$$|\partial_\mu \phi|^2 + \left|\frac{\delta V}{\delta \phi}\right|^2. \tag{4.1}$$

So the lowest energy solutions (true vacua) are constant that satisfy $\delta V/\delta\phi=0$. The number of solutions is $m+1$, that is, the exponent of $\delta V/\delta\phi$ in the commutative limit. Hence, there is no problem in defining the Euler number of the space $\mathcal{M}$ which consists of $m+1$ isolated points as $\pm\Sigma_{k=0}^{m}(-1)^k$. On the contrary, in the large θ limit, the number of GMS soliton solutions is infinite, that is, rank of K_0. Generally, it is a difficult case to define the Euler number of $\mathcal{M}$. However, as we saw in the previous sections, the partition function is invariant under the shift of θ. Finally, the Euler number of the moduli space is invariant under the noncommutative deformation of $\delta V/\delta\phi=0$.

The Gaussian integral in the noncommutative field theories is not familiar in general. But in this case, it is well-defined by the supersymmetry. As we see at first, the result of the path integral in the strong noncommutative limit does not contradict the commutative limit. This is evidence of the validity of the Gaussian integral of the noncommutative field theory. Note that the large θ limit is not the strong coupling limit. We have to consider two parameters, the noncommutative parameter θ and the coupling constant g multiplying overall. In order to get exact results by perturbative calculations, it is necessary for g to approach zero.

In the cohomological field theory, the partition function does not depend on an overall parameter like this g.

We summarize the previous sections by taking account of the fact that the partition function of cohomological field theory can be regarded as the Euler number of $\mathcal{M}$ by Mathai–Quillen formalism.[22]

Theorem IV.1 (θ-shift invariants): *The partition functions Z_θ of the noncommutative cohomological field theories are invariant under the shift of the noncommutative parameter θ:*

$$\frac{\delta}{\delta\theta}Z_\theta=0. \tag{4.2}$$

■

Theorem IV.2 (Euler number of GMS solution space): *On the Moyal plane, when the GMS solution space for real scalar field ϕ is*

$$\mathcal{M}_m=\{\,\phi\,|\,b_m(\cdots\underbrace{(\phi*_\theta(\phi-v_1))*_\theta(\phi-v_2))\cdots*_\theta(\phi-v_m)}_{m+1})=0,\ b_m>0\,\}, \tag{4.3}$$

and any two of v_i are different ($v_i\neq v_j$ for $i\neq j$), then the Euler number of the space $\mathcal{M}_m$ is given by

$$\chi_m=\begin{cases}1 & :\text{m is even number,}\\ 0 & :\text{m is odd number.}\end{cases} \tag{4.4}$$

■

B. Noncommutative Morse theory

In this subsection, we see that the noncommutative cohomological field theory can be regarded as the noncommutative Morse theory.[23,27]

In the commutative limit, the partition function of our theory is given by the Hessian of $\delta^2V/\delta\phi^2$ as we saw in Sec. III. Especially, the zero mode of $\partial_\mu\phi=0$ is just a real constant number. Then the determinant of the Hessian at the critical point p is determined by the sign of the second derivative of the real function at p, where the critical point p is the solution of $dV(x)/dx\,|_p=0 (x\in\mathbf{R})$. We denote the number of negative eigenvalues of the Hessian as n_p. In the commutative limit n_p is either 0 or 1, so the partition function is written by

$$Z=\sum_p \frac{\det \delta^2 V(p)/\delta p^2}{|\det \delta^2 V(p)/\delta p^2|}=\sum_p (-1)^{n_p}=\begin{cases}1: & m \text{ is even number},\\ 0: & m \text{ is odd number}.\end{cases} \tag{4.5}$$

By the fundamental theorem of Morse theory, this is the Euler number of the isolated points $\{p\}$ and this result is consistent with the result of applying Mathai–Quillen formalism to cohomological field theory.

On the other hand, the partition function is determined by the determinant of the operator valued Hessian $\delta^2 V(\phi)/\delta\phi^2$ in the large θ limit. The critical points are operators, too, i.e. GMS solitons are critical points and they exist infinitely at each p. But for each critical point, we can estimate $\det(\delta^2 V(\phi)/\delta\phi^2)$. Now we introduce the Morse index M_{n_p}. M_{n_p} is defined as the number of GMS solitons satisfying the condition that the Hessian consisting of the GMS solitons has n_p negative eigenvalues. As we saw in Sec. III and the Appendix, the n_p is the number of projection operators $\mathbf{P}_i$ whose coefficients belong to p_- in the GMS solution. Here we define p_- and p_+ as the set of critical points that satisfy

$$\begin{aligned}\left.\frac{\delta^2 V(p)}{\delta p^2}\right|_{p_-} &< 0,\\ \left.\frac{\delta^2 V(p)}{\delta p^2}\right|_{p_+} &> 0.\end{aligned} \tag{4.6}$$

In the case of positive b_m, the critical points are $p_-=\{v_0,v_2,\ldots,v_m\}$, and $p_+=\{v_1,v_3,\ldots,v_{m-1}\}$ (see Fig. 2). The number of p_- elements is $[(m+1)/2]$, and the number of p_+ is $[m/2]+1$. Then the number of combinations that n_p projections is combined with $[(m+1)/2]$ points of p_- in the soliton is $[(m+1)/2]^{n_p}$. When the total number of projections is fixed by N, then the remaining $(N-n_p)$ projections are combined with p_+ and its number of combinations is $([m/2]+1)^{(N-n_p)}$. Then the Morse index is given by

$$M_{n_p}(m,N)=[(m+1)/2]^{n_p}([m/2]+1)^{(N-n_p)}\cdot\frac{N!}{(N-n_p)!n_p!}. \tag{4.7}$$

M_{n_p} is divergent in the limit of $N\to\infty$. But we can define the Euler number of the isolated GMS soliton solutions as the fundamental theorem of Morse theory,

$$\chi_m=\sum_{\mathrm{GMS}}(-1)^{n_p}=\sum_{n_p}(-1)^{n_p}M_{n_p} \tag{4.8}$$

$$=(-[(m+1)/2]+[m/2]+1)^N=\begin{cases}1: & m \text{ is even number},\\ 0: & m \text{ is odd number}.\end{cases} \tag{4.9}$$

This is a result consistent with Sec. III and the Mathai–Quillen formalism. Therefore we can conclude that the noncommutative cohomological field theory makes it possible to generalize the Morse theory for the noncommutative field theory.

V. CONCLUSION AND DISCUSSION

We have studied the noncommutative cohomological field theory. Especially, the balanced scalar model is investigated carefully. A couple of theorems are provided. First, the partition function is invariant under the shift of the noncommutative parameter. Second, the Euler number of the GMS soliton space on the Moyal plane is calculated and it is ''1'' for the scalar potential with even degree and ''0'' for odd degree. (Note that the potential in the original GMS paper corresponds to $\delta V(\phi)/\delta\phi$ in our theory. So, the degree of potential is shifted from m to $m+1$.) In

general, Mathai–Quillen formalism tells us that the partition function of cohomological field theory is the Euler number of solution space $\mathcal{M}$ when the space is commutative. We expect that the noncommutative case is the same as the commutative case. Indeed, as we saw in the previous section, it is possible to identify the partition function of the noncommutative cohomological field theory with the Euler number as a result of the fundamental theorem of Morse theory, that is extended to the noncommutative field theory. In this article, we saw this relation in a scalar model, but it is expected that there is no obstacle to applying general cases.

It is possible to use our method for more complex models. For example, we can estimate the Euler number of the moduli space of instantons on noncommutative $\mathbf{R}^4$. In that case, the partition function is the Euler number of the instanton moduli space, and there is some new moduli space of the new instanton like Nekrasov–Schwarz.[3,24] For another example, we can change the base manifold to noncommutative torus. In that case, we will have to use the Powers–Rieffel projection for calculation in the strong noncommutative limit.[20,25] From another point of view, we should study other types of noncommutativity. For example, the noncommutative parameter is a locally defined type, a fuzzy sphere type and so on. To study such various cases it is important to construct the local geometry of noncommutative spaces. They are left as future works.

Most of the geometric nature of the noncommutative space is still unknown. But, as we saw, it is likely that some kinds of commutative space are succeeded by noncommutative space. We will have to study a huge number of them to throw light on the noncommutative geometry.

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APPENDIX A: LARGE θ LIMIT: ϕ^3 POTENTIAL

In this appendix, we show calculations in the large θ limit for simple examples of the balanced scalar model. One example is the ϕ^3 potential, and another is the ϕ^4 potential that is discussed in Appendix B.

We consider the cubic potential,

$$V(\phi)=b_0+b_1\hat{\phi}+\frac{1}{2}b_2\phi*\phi+\frac{1}{3!}b_3\phi*\phi*\phi. \tag{A1}$$

The field equation is written as

$$\frac{\delta V}{\delta\phi}=b_1+b_2\phi+\frac{1}{2}b_3\phi*\phi=\frac{1}{2}b_3(\phi-\alpha)*(\phi-\beta), \tag{A2}$$

where we put

$$\alpha,\beta=-(b_2/b_3)\pm\sqrt{(b_2/b_3)^2-2(b_1/b_3)}. \tag{A3}$$

We consider the case where both α and β are real numbers. By the redefinition of the field ϕ by a translation,

$$\phi'\equiv\phi-\alpha, \tag{A4}$$

the field equation is written as

$$\frac{\delta V}{\delta\phi}=\frac{1}{2}b_3\phi'*(\phi'-(\beta-\alpha))=0. \tag{A5}$$

The GMS solution is given by

$$\hat{\phi}'_{\mathrm{GMS}}=\lambda_i\hat{\mathbf{P}}_i\,, \tag{A6}$$

where the projection operator is $\hat{P}_i=|i\rangle\langle i|$. We put the GMS solution to the field equation,

$$\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}=\frac{1}{2}b_3\lambda_i(\lambda_i-(\beta-\alpha))\hat{\mathbf{P}}_i=0. \tag{A7}$$

The solution is

$$\lambda_i=0,\quad \lambda_i=\beta-\alpha\equiv v\,. \tag{A8}$$

The general GMS solution is a linear combination of projections with coefficients λ_i,

$$\hat{\phi}_{\mathrm{GMS}}=v\sum_{i\in\mathbf{S}}\hat{\mathbf{P}}_i=v\hat{\mathbf{P}}_S\,. \tag{A9}$$

The bosonic part of the action is

$$S_B^{\mathbf{S}}=-\frac{1}{4}\theta\,\mathrm{Tr}\left(\hat{\phi}_q\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}\left(\hat{\phi}_q\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}. \tag{A10}$$

The linear terms of expansion of $V(\hat{\phi})$ around the GMS soliton are

$$\begin{aligned}\left(\hat{\phi}_q\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}&=\left(\hat{\phi}_q\frac{\delta}{\delta\hat{\phi}}\right)\left[\frac{b_3}{2}\hat{\phi}(\hat{\phi}-v)\right]_{\phi=\phi_{\mathrm{GMS}}}\\&=\frac{b_3}{2}\{\hat{\phi}_q(\hat{\phi}_{\mathrm{GMS}}-v)+\hat{\phi}_{\mathrm{GMS}}\hat{\phi}_q\}\\&=\frac{b_3v}{2}\{-\hat{\phi}_q(\hat{\mathbf{1}}-\hat{\mathbf{P}}_S)+\hat{\mathbf{P}}_S\hat{\phi}_q\}.\end{aligned} \tag{A11}$$

Hence, we get

$$S_B^{\mathbf{S}}=-\frac{1}{4}\theta\left(\frac{b_3v}{2}\right)^2\mathrm{Tr}[\,\hat{\phi}_q(\hat{\mathbf{1}}-\hat{\mathbf{P}}_S)\hat{\phi}_q(\hat{\mathbf{1}}-\hat{\mathbf{P}}_S)+\hat{\mathbf{P}}_S\hat{\phi}_q\hat{\mathbf{P}}_S\hat{\phi}_q]. \tag{A12}$$

The fermionic part of the action is

$$S_F^{\mathbf{S}}=-i\theta\mathrm{Tr}\hat{\chi}\left(\hat{\psi}\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}. \tag{A13}$$

As is the same as the bosonic part, the leading terms of quantum field are given by

$$\left(\hat{\psi}\frac{\delta}{\delta\hat{\phi}}\right)\frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}=\frac{b_3v}{2}\{-\hat{\psi}(\hat{\mathbf{1}}-\hat{\mathbf{P}}_{\mathbf{S}})+\hat{\mathbf{P}}_{\mathbf{S}}\hat{\psi}\}. \tag{A14}$$

Then the fermionic part of the action is written as

$$S_F^{\mathbf{S}}=-\frac{\theta b_3v}{2}\mathrm{Tr}[-\hat{\chi}(\hat{\mathbf{1}}-\hat{\mathbf{P}}_S)\hat{\psi}(\hat{\mathbf{1}}-\hat{\mathbf{P}}_S)+\hat{\chi}\hat{\mathbf{P}}_S\hat{\psi}\hat{\mathbf{P}}_S]. \tag{A15}$$

The partition function is given by

$$\begin{aligned}\mathcal{Z}_{\mathrm{S}} &= \int \mathcal{D}\chi\mathcal{D}\psi\mathcal{D}\phi e^{-S} \\ &= \int \prod_{\substack{i>j \\ i,j\neq\in S}} \frac{d\phi_{ij}}{\sqrt{4\pi\theta}} d\chi_{ij} d\psi_{ij} \prod_{\substack{i>j \\ i,j\in S}} \frac{d\phi_{ij}}{\sqrt{4\pi\theta}} d\chi_{ij} d\psi_{ij} e^{-S_B^{\mathrm{S}} - S_F^{\mathrm{S}}} \\ &= \left[\sqrt{\left(\frac{b_3 v}{2}\right)^2}\right]^{-(N-n)^2} \left[\sqrt{\left(\frac{b_3 v}{2}\right)^2}\right]^{-n^2} \left[-\frac{b_3 v}{2}\right]^{(N-n)^2} \left[\frac{b_3 v}{2}\right]^{n^2}, \end{aligned} \tag{A16}$$

and we get

$$\mathcal{Z}_{\mathrm{S}} = [-\mathrm{sgn}(b_3)]^{(N-n)^2} [\mathrm{sgn}(b_3)]^{n^2} = [-\mathrm{sgn}(b_3)]^{N-n} [\mathrm{sgn}(b_3)]^n, \tag{A17}$$

where $n = \mathrm{rank}\, S$. There are $N!/(N-n)!n!$ sets of the GMS solution which has the rank n. Then the total partition function is the sum over $\mathcal{Z}_{\mathrm{S}}$ with the weight $N!/(N-n)!n!$,

$$\begin{aligned}\mathcal{Z}_{\mathrm{Total}} &= \sum_{\mathrm{S}} \mathcal{Z}_{\mathrm{S}} \\ &= \lim_{N\to\infty} \sum_{n=0}^{N} {}_N C_n [-\mathrm{sgn}(b_3)]^{N-n} [\mathrm{sgn}(b_3)]^n. \end{aligned} \tag{A18}$$

From the binomial theorem, we find that

$$\mathcal{Z}_{\mathrm{Total}} = 0. \tag{A19}$$

In the ϕ^3 potential, the partition function is zero.

APPENDIX B: LARGE θ LIMIT: ϕ^4 POTENTIAL

Here we consider another simple example which has ϕ^4 potential,

$$V(\phi) = b_0 + b_1\phi + \frac{1}{2} b_2 \phi * \phi + \frac{1}{3!} b_3 \phi * \phi * \phi + \frac{1}{4!} b_4 \phi * \phi * \phi * \phi. \tag{B1}$$

The field equation is always written as a factorization form

$$\frac{\delta V}{\delta \phi} = \frac{1}{3!} b_4 (\phi - \alpha) * (\phi - \beta) * (\phi - \gamma). \tag{B2}$$

As is the same as the ϕ^3, we translate the scalar field

$$\phi' \equiv \phi - \alpha. \tag{B3}$$

Then the field equation is rewritten as

$$\frac{\delta V}{\delta \phi} = \frac{1}{3!} b_4 \phi' * (\phi' - (\beta - \alpha)) * (\phi' - (\gamma - \alpha)) = \frac{1}{3!} b_4 \phi' * (\phi' - v_1) * (\phi' - v_2), \tag{B4}$$

where we define

$$v_1 \equiv (\beta - \alpha), v_2 \equiv (\gamma - \alpha). \tag{B5}$$

For simplicity we take α, β and γ are real numbers. We put the GMS solution $\phi'_{\mathrm{GMS}} = \lambda_i \mathbf{P}_i$ into the field equation; then

$$\frac{\delta V}{\delta \phi} = \frac{1}{3!} b_4 \lambda_i (\lambda_i - v_1)(\lambda_i - v_2)\mathbf{P}_i = 0. \tag{B6}$$

The solution is

$$\lambda_i = 0, v_1, v_2. \tag{B7}$$

The general GMS solution is a linear combination of projections with coefficients λ_i,

$$\phi_{\mathrm{GMS}} = v_1 \sum_{i \in \mathbf{S_1}} \mathbf{P}_i + v_2 \sum_{i \in \mathbf{S_2}} \mathbf{P}_i \tag{B8}$$

$$= v_1 \mathbf{P}_{\mathbf{S_1}} + v_2 \mathbf{P}_{\mathbf{S_2}}. \tag{B9}$$

The bosonic part of the action is given by

$$S_B^{\mathbf{S}} = -\frac{1}{4} \mathrm{Tr} \left[\left(\hat{\phi}_q \frac{\delta}{\delta \hat{\phi}} \right) \frac{\delta V(\hat{\phi})}{\delta \hat{\phi}} \bigg|_{\mathrm{GMS}} \left(\hat{\phi}_q \frac{\delta}{\delta \hat{\phi}} \right) \frac{\delta V(\hat{\phi})}{\delta \hat{\phi}} \bigg|_{\mathrm{GMS}} \right]. \tag{B10}$$

The linear terms of expansion of $V(\hat{\phi})$ around the GMS soliton are

$$\begin{aligned}
\left(\hat{\phi}_q \frac{\delta}{\delta \hat{\phi}} \right) \frac{\delta V(\hat{\phi})}{\delta \hat{\phi}} \bigg|_{\mathrm{GMS}} &= \left(\phi_q \frac{\delta}{\delta \hat{\phi}} \right) \left[\frac{b_4}{3!} \hat{\phi}(\hat{\phi} - v_1)(\hat{\phi} - v_2) \right]_{\hat{\phi} = \hat{\phi}_{\mathrm{GMS}}} \\
&= \frac{b_4}{3!} \{ \hat{\phi}_q (\hat{\phi}_{\mathrm{GMS}} - v_1)(\hat{\phi}_{\mathrm{GMS}} - v_2) + \hat{\phi}_{\mathrm{GMS}} \hat{\phi}_q (\hat{\phi}_{\mathrm{GMS}} - v_2) \\
&\quad + \hat{\phi}_{\mathrm{GMS}} (\hat{\phi}_{\mathrm{GMS}} - v_2) \hat{\phi}_q \} \\
&= \frac{b_4}{3!} \{ (v_1 v_2) \hat{\phi}_q (\hat{\mathbf{1}} - \hat{\mathbf{P}}_{\mathbf{S_1}} - \hat{\mathbf{P}}_{\mathbf{S_2}}) + (v_1 \hat{\mathbf{P}}_{\mathbf{S_1}} v_2 \hat{\mathbf{P}}_{\mathbf{S_2}}) \hat{\phi}_q [- v_2 (\hat{\mathbf{1}} - \hat{\mathbf{P}}_{\mathbf{S_1}} - \hat{\mathbf{P}}_{\mathbf{S_2}}) \\
&\quad + (v_1 - v_2) \hat{\mathbf{P}}_{\mathbf{S_1}}] + v_2 (v_2 - v_1) \hat{\mathbf{P}}_{\mathbf{S_2}} \hat{\phi}_q \}.
\end{aligned} \tag{B11}$$

The bosonic part of the action is

$$\begin{aligned}
S_B^{\mathbf{S}} = -\frac{1}{4} \theta \mathrm{Tr} [& (b_4 \zeta_0)^2 \hat{\phi}_q (\hat{\mathbf{1}} - \hat{\mathbf{P}}_{\mathbf{S_1}} - \hat{\mathbf{P}}_{\mathbf{S_2}}) \hat{\phi}_q (\hat{\mathbf{1}} - \hat{\mathbf{P}}_{\mathbf{S_1}} - \hat{\mathbf{P}}_{\mathbf{S_2}}) \\
& + (b_4 \zeta_1)^2 \hat{\mathbf{P}}_{\mathbf{S_1}} \hat{\phi}_q \hat{\mathbf{P}}_{\mathbf{S_1}} \hat{\phi}_q + (b_4 \zeta_2) \hat{\mathbf{P}}_{\mathbf{S_2}} \hat{\phi}_q \hat{\mathbf{P}}_{\mathbf{S_2}} \hat{\phi}_q],
\end{aligned} \tag{B12}$$

where we define

$$\zeta_0 \equiv \frac{1}{3!} v_1 v_2, \quad \zeta_1 \equiv \frac{1}{3!} v_1 (v_1 - v_2), \quad \zeta_2 \equiv \frac{1}{3!} v_2 (v_2 - v_1). \tag{B13}$$

The fermionic part of the Lagrangian is written as

$$S_F^{\mathbf{S}} = -i\theta \mathrm{Tr}\hat{\chi}\left(\hat{\psi}\frac{\delta}{\delta\hat{\phi}} \right) \frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}}. \tag{B14}$$

The BRST operation is given by

$$\left(\hat{\psi}\frac{\delta}{\delta\hat{\phi}} \right) \frac{\delta V(\hat{\phi})}{\delta\hat{\phi}}\bigg|_{\mathrm{GMS}} = \frac{b_4}{3!}\{(v_1v_2)\hat{\psi}(\hat{\mathbf{1}}-\hat{\mathbf{P}}_{\mathbf{S}_1}-\hat{\mathbf{P}}_{\mathbf{S}_2}) + (v_1\hat{\mathbf{P}}_{\mathbf{S}_1}+v_2\hat{\mathbf{P}}_{\mathbf{S}_2})\hat{\psi}$$
$$\times[-v_2(\hat{\mathbf{1}}-\hat{\mathbf{P}}_{\mathbf{S}_1}-\hat{\mathbf{P}}_{\mathbf{S}_2}) + (v_1-v_2)\hat{\mathbf{P}}_{\mathbf{S}_1}] + v_2(v_2-v_1)\hat{\mathbf{P}}_{\mathbf{S}_2}\hat{\psi}\}. \tag{B15}$$

Then the fermionic part is

$$S_F^{\mathbf{S}} = -i\theta \mathrm{Tr}[b_4\zeta_0\hat{\chi}(\hat{\mathbf{1}}-\hat{\mathbf{P}}_{\mathbf{S}_1}-\hat{\mathbf{P}}_{\mathbf{S}_2})\hat{\psi}(\hat{\mathbf{1}}-\hat{\mathbf{P}}_{\mathbf{S}_1}-\hat{\mathbf{P}}_{\mathbf{S}_2}) + b_4\zeta_1\hat{\chi}\hat{\mathbf{P}}_{\mathbf{S}_1}\hat{\psi}\hat{\mathbf{P}}_{\mathbf{S}_1} + b_4\zeta_2\hat{\chi}\hat{\mathbf{P}}_{\mathbf{S}_2}\hat{\psi}\hat{\mathbf{P}}_{\mathbf{S}_2}]. \tag{B16}$$

The partition function is given by

$$\mathcal{Z}_{\mathbf{S}} = \int \mathcal{D}\chi\mathcal{D}\psi\mathcal{D}\phi e^{-S} \tag{B17}$$

$$= \int \prod_{\mathbf{S}=\mathbf{S}_0}^{S_2} \left[\prod_{\substack{m>n \\ i,j\in\mathbf{S}}} \frac{d\phi_{ij}}{\sqrt{4\pi\theta}} d\chi_{ij} d\psi_{ij} e^{-S_B^{\mathbf{S}}-S_F^{\mathbf{S}}} \right.$$
$$= [\sqrt{(b_4\zeta_0)^2}]^{-(N-n_1-n_2)^2}[\sqrt{(b_4\zeta_1)^2}]^{-n_1^2}[\sqrt{(b_4\zeta_2)^2}]^{-n_2^2}$$
$$\times [b_4\zeta_0]^{(N-n_1-n_2)^2}[b_4\zeta_1]^{n_1^2}[b_4\zeta_2]^{n_2^2}. \tag{B18}$$

Hence, we get

$$\mathcal{Z}_{\mathbf{S}} = [\mathrm{sgn}(b_4\zeta_0)]^{(N-n_1-n_2)^2}[\mathrm{sgn}(b_4\zeta_1)]^{n_1^2}[\mathrm{sgn}(b_4\zeta_2)]^{n_2^2}, \tag{B19}$$

where $n_1 = \mathrm{rank}\, S_1$, and $n_2 = \mathrm{rank}\, S_2$. From the definition of ζ_i's, one of $\mathrm{sgn}(\zeta_i)$ is always negative, and the others are positive. Then the partition function is always written as

$$\mathcal{Z}_{\mathbf{S}} = [\mathrm{sgn}(b_4)]^{(N-n_1-n_2)^2}[-\mathrm{sgn}(b_4)]^{n_1^2}[\mathrm{sgn}(b_4)]^{n_2^2} \tag{B20}$$

$$= [\mathrm{sgn}(b_4)]^{N-n_1-n_2}[-\mathrm{sgn}(b_4)]^{n_1}[\mathrm{sgn}(b_4)]^{n_2}. \tag{B21}$$

There are $N!/(N-n_1-n_2)!n_1!n_2!$ sets of the GMS solution when the ranks of $\mathbf{S}_1$ and $\mathbf{S}_2$ are n_1 and n_2. Then the total partition function is the sum over $\mathcal{Z}_{\mathbf{S}}$ with the weight $N!/(N-n_1-n_2)!n_1!n_2!$:

$$\mathcal{Z}_{\mathrm{Total}} = \sum_{\mathbf{S}} \mathcal{Z}_{\mathbf{S}}$$
$$= \lim_{N\to\infty} \sum_{n_1,n_2=0}^{N} \frac{N!}{(N-n_1-n)!n_1!n_2!}[\mathrm{sgn}(b_4)]^{N-n_1-n_2}[-\mathrm{sgn}(b_4)]^{n_1}[\mathrm{sgn}(b_4)]^{n_2}$$
$$= \lim_{N\to\infty} (\mathrm{sgn}(b_4) - \mathrm{sgn}(b_4) + \mathrm{sgn}(b_4))^N = \lim_{N\to\infty} (\mathrm{sgn}(b_4))^N. \tag{B22}$$

In the ϕ^4 potential, the partition function takes a nonvanishing value $\lim_{N\to\infty}(\mathrm{sgn}(b_4))^N$.

APPENDIX C: GAUSSIAN INTEGRAL IN THE NONCOMMUTATIVE SPACE

In our calculations, the Gaussian functional integral appears, whose form is

$$\int \mathcal{D}\phi \exp\left\{ -\int d^2x \phi(x) * V(\phi(x))\Big|_{\mathrm{GMS}} * \phi(x) \right\}, \tag{C1}$$

and we convert it into the number representation. Generally, the difference of the operator ordering may yield some difference of the result. Therefore we must show that our prescription is correct.

Generally operators can be represented in the number representation as

$$\hat{O} = \sum_{m,n} O_{mn} |m\rangle\langle n|, \tag{C2}$$

where $\hat{O}$ is any operator and $|m\rangle\langle n|$ is the basis of the number representation. Any operator can be represented as the Weyl ordered operator, so the basis $|m\rangle\langle n|$ can be written as

and its Weyl ordered symbol corresponding to the basis $|m\rangle\langle n|$ is

$$|m\rangle\langle n| = \underbrace{\int \frac{d^2k}{(2\pi)^2} \tilde{f}_{mn}(k) e^{i(k_1\hat{x}^1 + k_2\hat{x}^2)}}_{\text{Weyl ordered operator}}, \tag{C3}$$

$$f_{mn}(x) = \int \frac{d^2k}{(2\pi)^2} \tilde{f}_{mn}(k) e^{i(k_1x^1 + k_2x^2)}. \tag{C4}$$

Here, we consider the following integral,

$$\begin{aligned} \int d\hat{x}_1 d\hat{x}_2 |m\rangle\langle n|p\rangle\langle q| &= \int d\hat{x}_1 d\hat{x}_2 \int \frac{d^2k}{(2\pi)^2} \frac{d^2k'}{(2\pi)^2} \tilde{f}_{mn}(k) \tilde{f}_{pq}(k') e^{i(k_1\hat{x}^1 + k_2\hat{x}^2)} e^{i(k_1'\hat{x}^1 + k_2'\hat{x}^2)} \\ &= \int \frac{d^2k}{(2\pi)^2} \tilde{f}_{mn}(k) \tilde{f}_{pq}(-k), \end{aligned} \tag{C5}$$

where we set $[x^1, x^2] = 1$ for simplicity and use the Baker–Campbell–Hausdorff formula. On the other hand, since $|m\rangle\langle n|p\rangle\langle q| = |m\rangle \delta_{np} \langle q|$,

$$\int d\hat{x}_1 d\hat{x}_2 |m\rangle \delta_{np} \langle q| = \int d\hat{x}_1 d\hat{x}_2 \int \frac{d^2k}{(2\pi)^2} \tilde{f}_{mq}(k) \delta_{np} e^{i(k_1\hat{x}^1 + k_2\hat{x}^2)} = \int d^2k \tilde{f}_{mq}(k) \delta^2(k) \delta_{np}. \tag{C6}$$

Therefore, we can derive a relation:

$$\int \frac{d^2k}{(2\pi)^2} \tilde{f}_{mn}(k) \tilde{f}_{pq}(-k) = \int d^2k \tilde{f}_{mq}(k) \delta^2(k) \delta_{np}. \tag{C7}$$

Using Eq. (C7), we get the following relation:

$$\int d^2x f_{mn}(x) * f_{pq}(x) = \int d^2x f_{mq}(x) \delta_{np}. \tag{C8}$$

A similar calculation gives

$$\int d^2x f_{p_1q_1}(x)*f_{p_2q_2}(x)*\cdots*f_{p_nq_n}(x)=\int d^2x f_{p_1q_n}(x)\delta_{q_1p_2}\delta_{q_2p_3}\cdots\delta_{q_{n-1}p_n}. \tag{C9}$$

It is possible to expand any function in terms of $f_{mn}(x)$, so $\phi(x)$ and $V(\phi)|_{\mathrm{GMS}}$ in Eq. (C1) are expanded as

$$\phi(x)=\sum_{mn}\phi_{mn}f_{mn}(x), \tag{C10}$$

$$V(\phi)|_{\mathrm{GMS}}=\sum_{l}V_l f_{ll}(x). \tag{C11}$$

Therefore we perform the functional integral (C1) using Eqs. (C8) and (C9) as follows:

$$\int \mathcal{D}\phi\exp\left\{-\int d^2x\phi_{mn}V_l\phi_{pq}(f_{mn}(x)*f_{ll}(x)*f_{pq})\right\}=[\det|V_l|^{1/2}]^{-1}. \tag{C12}$$

On the other hand, a calculation in the number representation gives

$$\int \mathcal{D}\hat{\phi}\exp\{-\mathrm{Tr}\phi_{mn}V_l\phi_{pq}(|m\rangle\langle n|l\rangle\langle l|p\rangle\langle q|)\}=\int \mathcal{D}\phi\exp(-\phi_{ml}V_l\phi_{lm})=[\det|V_l|^{1/2}]^{-1}, \tag{C13}$$

which is the same result as Eq. (C12) without normalizing constant which is canceled out. Therefore, we can perform integration in both representations, and the number operator is used in our calculations.

APPENDIX D: $\$_n=0$

We prove a theorem here.

The theorem which we will prove here is

$$\sum_{i=B}^{A}\prod_{\alpha=0}^{i-1}(v_A-v_\alpha)\prod_{\beta=i+1}^{r}(v_B-v_\beta)=0, \tag{D1}$$

where integers A,B satisfy $0\leqslant B<A\leqslant r$, and v_i is any real number. We defined the following notation formally for convenience:

$$\prod_{\alpha=0}^{-1}(v_A-v_\alpha)=\prod_{\alpha=r+1}^{r}(v_A-v_\alpha)=1. \tag{D2}$$

Its proof is as follows.

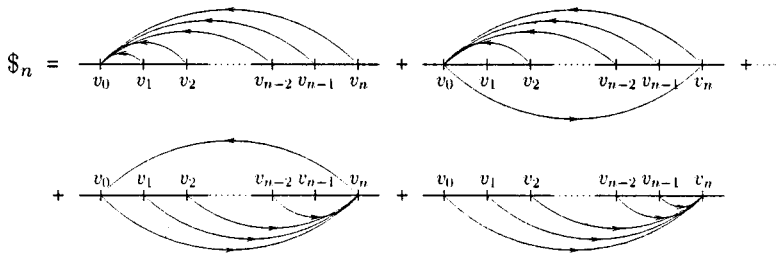

FIG. 3. Graphical representation of $\$_n$. The arrow $v_i \leftarrow v_j$ means $(v_j - v_i)$, and all arrows in one figure should be multiplied.

Proof:

$$\sum_{i=B}^{A}\prod_{\alpha=0}^{i-1}(v_A-v_\alpha)\prod_{\beta=i+1}^{r}(v_B-v_\beta)$$

$$=\sum_{i=B}^{A}(v_A-v_0)(v_A-v_1)\cdots(v_A-v_{i-1})^{\vee}(v_B-v_{i+1})(v_B-v_{i+2})(v_B-v_m)$$

$$=\underbrace{(v_A-v_0)(v_A-v_1)\cdots(v_A-v_{B-1})}_{B}\ \underbrace{(v_B-v_{B+1})(v_B-v_{B+2})\cdots(v_B-v_m)}_{r-B}$$

$$+\underbrace{(v_A-v_0)(v_A-v_1)\cdots(v_A-v_B)}_{B+1}\ \underbrace{(v_B-v_{B+2})(v_B-v_{B+3})\cdots(v_B-v_m)}_{r-B-1}$$

$$+\cdots$$

$$+\underbrace{(v_A-v_0)(v_A-v_1)\cdots(v_A-v_{A-1})}_{A}\ \underbrace{(v_B-v_{A+1})(v_B-v_{A+2})\cdots(v_B-v_m)}_{r-A}$$

$$=(v_A-v_0)(v_A-v_1)\cdots(v_A-v_{B-1})\cdot(v_B-v_{A+1})(v_B-v_{A+2})\cdots(v_B-v_m)$$
$$\times\{1\cdot(v_B-v_{B+1})(v_B-v_{B+2})\cdots(v_B-v_A)+(v_A-v_B)\cdot(v_B-v_{B+2})$$
$$\times(v_B-v_{B+3})\cdots(v_B-v_A)+\cdots$$
$$+(v_A-v_B)(v_A-v_{B+1})\cdots(v_A-v_{A-1})\cdot 1\}. \tag{D3}$$

To show that $\{\cdots\}$ in Eq. (D3) equals zero, we define $\$_n$ as (Fig. 3)

$$\$_n=(v_0-v_1)(v_0-v_2)(v_0-v_3)\cdots(v_0-v_n)+(v_n-v_0)\cdot(v_0-v_2)(v_0-v_3)\cdots(v_0-v_n)$$
$$+(v_n-v_0)(v_n-v_1)\cdot(v_0-v_3)\cdots(v_0-v_n)+\cdots+(v_n-v_0)\cdots(v_n-v_{n-3})\cdot(v_0-v_{n-1})$$
$$\times(v_0-v_n)+(v_n-v_0)\cdots(v_n-v_{n-3})(v_n-v_{n-2})\cdot(v_0-v_n)+(v_n-v_0)\cdots(v_n-v_{n-3})$$
$$\times(v_n-v_{n-2})(v_n-v_{n-1}). \tag{D4}$$

We prove $\$_n=0$ using mathematical induction as follows. First, for $n=1$,

$$\$_1=(v_0-v_1)+(v_1-v_0)=0. \tag{D5}$$

Next, we suppose $\$_n=0$.

And we consider $\$_{n+1}$ as (Fig. 4)

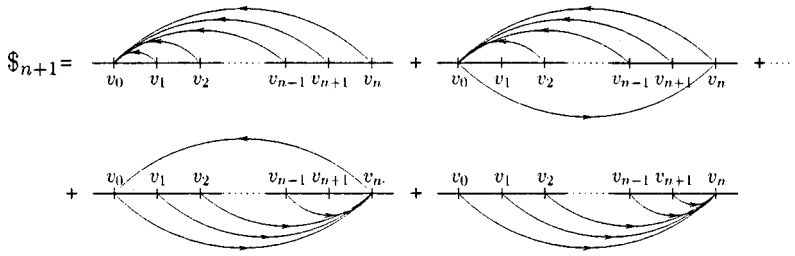

FIG. 4. Graphical representation of $\$_{n+1}$. We put v_{n+1} between v_{n-1} and v_n in the proof.

$$
\begin{aligned}
\$_{n+1} &= (v_0-v_1)(v_0-v_2)(v_0-v_3)\cdots(v_0-v_{n-1})(v_0-v_{n+1})(v_0-v_n)+(v_n-v_0)\cdot(v_0-v_2)\\
&\quad\times(v_0-v_3)\cdots(v_0-v_{n-1})(v_0-v_{n+1})(v_0-v_n)+(v_n-v_0)(v_n-v_1)\cdot(v_0-v_3)\cdots(v_0\\
&\quad-v_{n-1})(v_0-v_{n+1})(v_0-v_n)+\cdots+(v_n-v_0)\cdots(v_n-v_{n-2})\cdot(v_0-v_{n+1})(v_0-v_n)\\
&\quad+(v_n-v_0)\cdots(v_n-v_{n-2})(v_n-v_{n-1})\cdot(v_0-v_n)+(v_n-v_0)\cdots(v_n-v_{n-2})(v_n-v_{n-1})\\
&\quad\times(v_n-v_{n+1})\\
&=\{\$_n-(v_n-v_0)(v_n-v_1)\cdots(v_n-v_{n-1})\}(v_0-v_{n+1})+(v_n-v_0)(v_n-v_1)\cdots(v_n-v_{n-1})\\
&\quad\times\{(v_0-v_n)+(v_n-v_{n+1})\}\\
&=(v_n-v_0)(v_n-v_1)\cdots(v_n-v_{n-1})\{-(v_0-v_{n+1})+(v_0-v_n)+(v_n-v_{n+1})\}=0. \qquad \text{(D6)}
\end{aligned}
$$

Therefore $\$_n=0$ is valid for any n. Using it, $\{\cdots\}$ in Eq. (D3) equals zero, so the proof is completed.

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Closure of orbits and dynamical symmetry of screened Coulomb potential and isotropic harmonic oscillator

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It is shown that for any central potential $V(r)$ there exist a series of conserved aphelion and perihelion vectors $\tilde{\mathbf{R}}=\mathbf{p}\times\mathbf{L}-g(r)\mathbf{r}$, $g(r)=rV'(r)$. However, if and only if $V(r)$ is a pure or screened Coulomb potential, $\tilde{\mathbf{R}}$ and $\mathbf{L}$ constitute an SO_4 algebra in the subspace spanned by the degenerate states with a given energy eigenvalue $E<0$ at the aphelia and perihelia ($\dot{r}=0$). For a pure Coulomb potential, $\tilde{\mathbf{R}}$ is reduced to the Pauli–Runge–Lenz (PRL) vector $\mathbf{R}$ and for a screened Coulomb potential $\tilde{\mathbf{R}}$ is reduced to the extended PRL vector $\mathbf{R}'$. While $d\mathbf{R}/dt=0$ always holds, $d\mathbf{R}'/dt=0$ holds only at the aphelia and perihelia. Moreover, the space spanning the SO_4 algebra for a screened Coulomb potential is smaller than that for a pure Coulomb potential. The relation of closed orbits for a screened Coulomb potential with that for a pure Coulomb potential is clarified. The ratio of the radial frequency ω_r and angular frequency ω_ϕ, $\omega_r/\omega_\phi=\kappa=1$ for a pure Coulomb potential irrespective of the angular momentum L and energy $E(<0)$. For a screened Coulomb potential κ is determined by the angular momentum L, and when κ is any rational number ($\kappa<1$), the orbit is closed. The situation for a pure or screened isotropic harmonic oscillator is similar. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1430900]

I. INTRODUCTION

The orbits of a classical particle in an arbitrary central potential, due to the angular momentum conservation, always lie in a plane perpendicular to the angular momentum. However, the orbits are in general not closed. In classical mechanics, there is a celebrated Bertrand's theorem,[1,2] which says that the only central forces that result in closed orbits for all bound particles are the inverse square law and Hooke's law. The closure of orbits is guaranteed by an additional conserved quantity (apart from the energy and angular momentum)—the Runge–Lenz vector for Kepler's problem[3,4] and a quadrupole tensor for the isotropic harmonic oscillator,[5,6] which implies a higher dynamical symmetry than the geometric symmetry (space isotropy).[7–9]

In a previous paper, Bertrand's theorem was extended. It was shown[10,11] that for a screened Coulomb potential (in natural units)

$$V(r)=-1/r-\lambda/r^2 \quad (0<\lambda\ll 1) \tag{1}$$

there may exist an infinite number of closed orbits (rather than ellipses) characterized by a series of conserved aphelion and perihelion vectors, i.e., extended Runge–Lenz vector ($m=1$)

$$\mathbf{R}'=\mathbf{p}\times\mathbf{L}-(1+2\lambda/r)\mathbf{r}/r, \tag{2}$$

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$d\mathbf{R}'/dt=0$ at the aphelia and perihelia ($\dot{r}=0$), and each closed orbit corresponds to a discrete angular momentum

$$L=\sqrt{2\lambda/(1-\kappa^2)} \tag{3}$$

(κ being a rational number). It was also shown[12] that $\mathbf{L}$ and $\mathbf{R}'$ constitute an SO_4 algebra in the subspace spanned by the degenerate states belonging to a given bound energy eigenvalue $E<0$ at the aphelia and perihelia ($\dot{r}=0$). However, in this case only the energy (but not angular momentum) raising and lowering operators can be constructed from the factorization of radial Schrödinger equation.[10,12] A similar situation exists for the isotropic harmonic oscillator.

In this paper we will show that for an arbitrary central potential $V(r)$, there always exist a series of conserved aphelion and perihelion vectors,

$$\tilde{\mathbf{R}}=\mathbf{p}\times\mathbf{L}-g(r)\mathbf{r}, \tag{4}$$

where $g(r)=rV'(r)$, and $d\tilde{\mathbf{R}}/dt=0$ at $\dot{r}=0$. However, it is found that in general $\mathbf{L}$ and $\tilde{\mathbf{R}}$ do not constitute an SO_4 algebra at the aphelia and perihelia ($\dot{r}=0$). Therefore, the existence of $\tilde{\mathbf{R}}$ does not imply the closure of an orbit. In Sec. II we will show a theorem concerning the restriction on the form of $V(r)$ that $\mathbf{L}$ and $\tilde{\mathbf{R}}$ constitute an SO_4 algebra. A similar theorem concerning the extended quadrupole tensor for the screened isotropic harmonic oscillator will be presented in Sec. III. However, whether these restrictions imply the closure of orbits needs further investigation. Finally, the closure of orbits for a bound particle in the screened Coulomb potential and isotropic harmonic oscillator will be discussed in Sec. IV from another perspective.

II. DYNAMICAL SYMMETRY OF A SCREENED COULOMB POTENTIAL

Using the angular momentum conservation, it is easy to show that for an arbitrary central potential $V(r)$, there always exist a series of conserved aphelion and perihelion vectors $\tilde{\mathbf{R}}=\mathbf{p}\times\mathbf{L}-g(r)\mathbf{r}$, $g(r)=rV'(r)$. However, not all $\tilde{\mathbf{R}}$ can constitute an SO_4 algebra with $\mathbf{L}$ in a subspace spanned by the degenerate states belonging to a given bound energy eigenvalue $E<0$ at the aphelia and perihelia ($\dot{r}=0$). In fact, we have the following theorem.

Theorem 1: If and only if $V(r)$ is a pure or screened Coulomb potential, $\mathbf{L}$ and $\tilde{\mathbf{R}}$ constitute a closed SO_4 algebra in a subspace spanned by the degenerate states belonging to a given bound energy eigenvalue $E<0$ at the aphelia and perihelia ($\dot{r}=0$).

Proof: The quantum counterpart of $\tilde{\mathbf{R}}$ [see Eq. (4)] is

$$\tilde{\mathbf{R}}=\tfrac{1}{2}(\mathbf{p}\times\mathbf{L}-\mathbf{L}\times\mathbf{p})-g(r)\mathbf{r}. \tag{5}$$

In addition to the well-known commutation relations

$$[L_\alpha,L_\beta]=i\epsilon_{\alpha\beta\gamma}L_\gamma, \tag{6}$$

$$[L_\alpha,\tilde{R}_\beta]=i\epsilon_{\alpha\beta\gamma}\tilde{R}_\gamma, \tag{7}$$

it can be shown for the operator $\tilde{\mathbf{R}}$ (5),

$$\tilde{\mathbf{R}}\times\tilde{\mathbf{R}}=-2i\left[\frac{p^2}{2}-\frac{3g(r)+rg'(r)}{2}\right]\mathbf{L}. \tag{8}$$

Therefore, only when

$$\frac{p^2}{2}-\frac{3g(r)+rg'(r)}{2}=H, \tag{9}$$

where H is the Hamiltonian, do $\mathbf{L}$ and $\tilde{\mathbf{R}}$ constitute an SO_4 algebra in a subspace spanned by the degenerate states belonging to a given bound energy eigenvalue $E<0$ at the aphelia and perihelia ($\dot{r}=0$), i.e., $-[3g(r)+rg'(r)]/2=V(r)$. Thus, $V(r)$ must satisfy the following differential equation of Euler type;

$$r^2\frac{d^2V}{dr^2}+4r\frac{dV}{dr}+2V=0. \tag{10}$$

Solving the equation, we get

$$V(r)=\frac{C_1}{r}+\frac{C_2}{r^2}, \tag{11}$$

where C_1 and C_2 are two integral constants. To ensure the existence of bound states, $C_1<0$. Thus, we have two cases:

(1) $C_2=0$.

$V(r)$ is a pure Coulomb potential and $\tilde{\mathbf{R}}$ is reduced to the well-known Pauli–Runge–Lenz vector $\mathbf{R}=\frac{1}{2}(\mathbf{p}\times\mathbf{L}-\mathbf{L}\times\mathbf{p})-\mathbf{r}/r$.

(2) $C_2\neq=0$.

$V(r)$ is just the screened Coulomb potential (in natural units) $V(r)=-1/r-\lambda/r^2(0<\lambda\ll 1)$ and $\tilde{\mathbf{R}}$ is reduced to $\mathbf{R}'=\frac{1}{2}(\mathbf{p}\times\mathbf{L}-\mathbf{L}\times\mathbf{p})-(1+2\lambda/r)\mathbf{r}/r$, i.e., the extended Pauli–Runge–Lenz vector introduced in Refs. 11 and 12.

It is noted that for the pure Coulomb potential, $rg(r)-1=0$, and for the screened Coulomb potential, $rg(r)-1=2\lambda/r$. $rg(r)-1$ may be considered as a deviation from a pure Coulomb potential. From the above-given discussions, only when the deviation from the Coulomb potential $rg(r)-1\propto 1/r$, $\tilde{\mathbf{R}}$ and $\mathbf{L}$ constitute an SO_4 algebra in a subspace spanned by the states belonging to a given bound energy eigenvalue $E<0$ at the aphelia and perihelia ($\dot{r}=0$). However, even in this case there exist two distinct features between the two algebras. (a) While $d\mathbf{R}/dt=0$ always holds for a pure Coulomb potential, $d\mathbf{R}'/dt=0$ holds only at the aphelia and perihelia. (b) For the screened Coulomb potential, the L degeneracy of the energy eigenstates is removed. Therefore, the dimension of the subspace spanning the SO_4 algebra for the screened Coulomb potential is smaller than that for the pure Coulomb potential.

The two-dimensional (2D) case is similar. For any 2D central potential $V(\rho)$, one also can construct a conserved aphelion and perihelion vector,

$$\tilde{\mathbf{R}}=\mathbf{p}\times\mathbf{L}-g(\rho)\rho, \tag{12}$$

where $g(\rho)=\rho V'(\rho)$, $d\tilde{\mathbf{R}}/\mathbf{dt}=\mathbf{0}$ at $\dot{\rho}=0$. The quantum counterpart of $\tilde{\mathbf{R}}$ is

$$\tilde{\mathbf{R}}=\tfrac{1}{2}(\mathbf{p}\times\mathbf{L}-\mathbf{L}\times\mathbf{p})-g(\rho)\rho. \tag{13}$$

Also, it can be shown that, if and only if $V(\rho)$ is a pure or screened Coulomb potential,

$$[L_z,\tilde{R}_x]=i\tilde{R}_y, \tag{14}$$

$$[L_z,\tilde{R}_y]=-i\tilde{R}_x, \tag{15}$$

$$[\tilde{R}_x,\tilde{R}_y]=-2iHL_z, \tag{16}$$

i.e. $(L_z=xp_y-yp_x,\tilde{R}_x,\tilde{R}_y)$ constitute an SO_3 algebra in the subspace spanned by the states belonging to a given bound energy eigenvalue $E<0$ at the aphelia and perihelia ($\dot{\rho}=0$).

III. DYNAMICAL SYMMETRY OF A SCREENED ISOTROPIC HARMONIC OSCILLATOR

Now we address the isotropic harmonic oscillator. First we consider the 2D case. It can be shown that for an arbitrary 2D central field $V(\rho)$, there always exist two conserved aphelion and perihelion quantities,

$$\tilde{Q}_{xy}=h(\rho)xy+p_xp_y, \tag{17}$$

$$\tilde{Q}_1=\tfrac{1}{2}[h(\rho)(x^2-y^2)+(p_x^2-p_y^2)], \tag{18}$$

where $h(\rho)=V'(\rho)/\rho$, and $\mathrm{d}\tilde{Q}_{xy}/\mathrm{d}t=0$ and $\mathrm{d}\tilde{Q}_1/\mathrm{d}t=0$ at the aphelia and perihelia ($\dot{\rho}=0$). Similar to theorem 1, we have

Theorem 2: If and only if $V(\rho)$ is a pure or screened isotropic harmonic oscillator, do the operators $(L_z,\tilde{Q}_{xy},\tilde{Q}_1)$ constitute an SU_2 algebra.

Proof: For any $h(\rho)$, we have the following commutation relations:

$$[L_z,\tilde{Q}_{xy}]=-2i\tilde{Q}_1, \tag{19}$$

$$[L_z,\tilde{Q}_1]=2i\tilde{Q}_{xy}, \tag{20}$$

$$[\tilde{Q}_{xy},\tilde{Q}_1]=-2i[h(\rho)+\tfrac{1}{4}\rho h'(\rho)]L_z. \tag{21}$$

Therefore, only when

$$h(\rho)+\tfrac{1}{4}\rho h'(\rho)=C, \quad C>0 \tag{22}$$

do $(L_z,\tilde{Q}_{xy},\tilde{Q}_1)$ constitute an SU_2 algebra, i.e.,

$$\rho V''(\rho)+3V'(\rho)-4C\rho=0. \tag{23}$$

Solving the equation, we obtain

$$V(\rho)=C_1+C_2/\rho^2+\frac{C}{2}\rho^2, \tag{24}$$

where C_1 and C_2 are two integral constants. Neglecting a trivial additional constant of $V(\rho)$, i.e., letting $C_1=0$, we have two cases:

(1) $C_2=0$.

$V(\rho)$ is a pure isotropic harmonic oscillator and $\tilde{Q}_{xy}$ and $\tilde{Q}_1$ (in natural units $C=1$) are reduced to the well-known conserved quantities[8,9]

$$Q_{xy}=xy+p_xp_y, \tag{25}$$

$$Q_1=\tfrac{1}{2}[(x^2-y^2)+(p_x^2-p_y^2)]. \tag{26}$$

(2) $C_2\neq 0$.

$V(\rho)$ is just the screened isotropic harmonic oscillator (in natural units)

$$V(\rho)=\tfrac{1}{2}\rho^2-\lambda/\rho^2 \quad (0<\lambda\ll 1), \tag{27}$$

and

$$Q'_{xy}=(1+2\lambda/\rho^4)xy+p_xp_y, \tag{28}$$

$$Q_1' = \tfrac{1}{2}[(1+2\lambda/\rho^4)(x^2-y^2)+(p_x^2-p_y^2)], \tag{29}$$

which was introduced in Ref. 12.

It is noted that for a pure isotropic harmonic oscillator, $h(\rho)-1=0$, and for a screened isotropic harmonic oscillator, $h(\rho)-1=2\lambda/\rho$. $h(\rho)-1$ may be considered as a deviation from a pure isotropic harmonic oscillator. From the above discussions, only when the deviation from the isotropic harmonic oscillator $h(\rho)-1\propto 1/\rho$ do $(L_z,\tilde{Q}_{xy},\tilde{Q}_1)$ constitute an SU_2 algebra. However, while $\mathrm{d}Q_{xy}/\mathrm{d}t=0$ and $\mathrm{d}Q_1/\mathrm{d}t=0$ always hold for a pure isotropic harmonic oscillator, for a screened isotropic harmonic oscillator $\mathrm{d}Q_{xy}'/\mathrm{d}t=0$ and $\mathrm{d}Q_1'/\mathrm{d}t=0$ hold only at the aphelia and perihelia.

Now we turn to the three-dimensional case. Similarly, we can construct a conserved aphelion and perihelion quadrupole tensor for any central field $V(r)$,

$$\tilde{Q}_{xy}=h(r)xy+p_xp_y, \tag{30}$$

$$\tilde{Q}_{yz}=h(r)yz+p_yp_z, \tag{31}$$

$$\tilde{Q}_{zx}=h(r)zx+p_zp_x, \tag{32}$$

$$\tilde{Q}_1=\tfrac{1}{2}[h(r)(x^2-y^2)+(p_x^2-p_y^2)]=\tfrac{1}{2}(\tilde{Q}_{xx}-\tilde{Q}_{yy}), \tag{33}$$

$$\tilde{Q}_0=\frac{1}{2\sqrt{3}}[h(r)(x^2+y^2-2z^2)+(p_x^2+p_y^2-2p_z^2)]=\frac{1}{2\sqrt{3}}(\tilde{Q}_{xx}+\tilde{Q}_{yy}-2\tilde{Q}_{zz}), \tag{34}$$

where $h(r)=V'(r)/r$. It can be shown that at the points $\dot{r}=0$, $\mathrm{d}\tilde{Q}_{xy}/\mathrm{d}t=\mathrm{d}\tilde{Q}_{yz}/\mathrm{d}t=\mathrm{d}\tilde{Q}_{zx}/\mathrm{d}t=\mathrm{d}\tilde{Q}_1/\mathrm{d}t=\mathrm{d}\tilde{Q}_0/\mathrm{d}t=0$.

In a similar way as in the 2D case, it can be shown that if and only if $V(r)$ is a pure or screened isotropic harmonic oscillator in the eigen-coordinates[8,12] do $(L_\xi,\tilde{Q}_{\xi\eta},\tilde{Q}_1)$ constitute an SU_2 algebra.

IV. CLOSURE OF ORBITS

From the above-mentioned text, it has been shown that on the one hand the screened Coulomb potential and isotropic harmonic oscillator have higher dynamical symmetry than the geometric symmetry (space isotropy), and on the other hand there may exist profound relations between a pure Coulomb potential (isotropic harmonic oscillator) and a screened Coulomb potential (isotropic harmonic oscillator). To display this point of view, let us investigate further the condition of closure of classical orbits ($L=\sqrt{2\lambda/(1-\kappa^2)}$, $\kappa<1$ being any rational number) for a particle in a screened Coulomb potential or screened isotropic harmonic oscillator.

Consider the bound states. Let Φ be the angle between the rays leading from the center to the successive aphelion and perihelion, then Φ is given by the integral[13]

$$\Phi=\int_{r_p}^{r_a}\frac{L/r^2}{\sqrt{2(E-V(r)-L'^2/2r^2)}}\mathrm{d}r, \tag{35}$$

where $r_p(r_a)$ is the distance between the center and the perihelion (aphelion). It was shown[13] that the orbit is closed only when Φ is commensurable with 2π. It is easy to verify that for a Coulomb potential, $\Phi\equiv\pi$, and for an isotropic harmonic oscillator, $\Phi\equiv\pi/2$, which result in closed orbits for *all* bound particles. This may be considered as an alternative argument for the Bertrand's theorem.

Now we discuss the screened Coulomb potential. For a particle in this field, the equations of motion are

$$\dot{r}=\sqrt{2(E+1/r-L^2/2r^2)}, \tag{36}$$

$$\dot{\phi}=L/r^2, \tag{37}$$

and

$$\Phi_{\mathrm{sc}}=\int_{r_p}^{r_a}\frac{L/r^2}{\sqrt{2(E+1/r-L'^2/2r^2)}}\mathrm{d}r, \tag{38}$$

where

$$L'=\sqrt{L^2-2\lambda}. \tag{39}$$

By contrast, let us consider another particle in a pure Coulomb potential with energy E and angular momentum L'; the equations of motion are

$$\dot{r}=\sqrt{2(E+1/r-L'^2/2r^2)}, \tag{40}$$

$$\dot{\phi}=L'/r^2, \tag{41}$$

and

$$\Phi_c=\int_{r_p'}^{r_a'}\frac{L'/r^2}{\sqrt{2(E+1/r-L'^2/2r^2)}}\mathrm{d}r. \tag{42}$$

Comparing (36) and (40), it is seen that the radial motions of the two particles are the same. Therefore, we get $r_p'=r_p$, $r_a'=r_a$. Let

$$L'/L=\kappa, \tag{43}$$

$\kappa\leqslant 1$ for $\lambda\geqslant 0$. From (38) and (42), we have

$$\Phi_{\mathrm{sc}}=\Phi_c/\kappa=\pi/\kappa. \tag{44}$$

Obviously, if and only if κ is a rational number, the orbit of a particle in the screened Coulomb potential is closed. In this case, the radial frequency ω_r and angular frequency ω_ϕ are commensurable, and $\omega_r/\omega_\phi=\kappa$. For a pure Coulomb potential, $\kappa=1$, and for a screened Coulomb potential when κ is a rational number ($\kappa<1$), the orbit is closed. Equations (43) and (39) imply that κ is determined by the angular momentum, or inversely,

$$L=\sqrt{2\lambda/(1-\kappa^2)}\quad(\kappa<1,\ \text{rational}), \tag{45}$$

which is just Eq. (3). The above-presented discussion intuitively clarifies the relation of the closure of orbits for a pure and a screened Coulomb potential, and why there exist an infinite number of closed orbits for a particle in the screened Coulomb potential with suitable discrete angular momenta and any negative energy ($E<0$).

In quantum mechanics, it is well known that for a pure Coulomb potential, $\omega_r/\omega_\phi=(\partial E/\partial n_r)/(\partial E/\partial l)=1$. Similarly, it can be shown that in the large quantum number limit, for a screened Coulomb potential $\omega_r/\omega_\phi=(\partial E/\partial n_r)/(\partial E/\partial l)=\kappa$.

A similar situation exists for the isotropic harmonic oscillator, but $\omega_r/\omega_\phi=2\kappa$. For a pure isotropic harmonic oscillator, $\kappa=1$, and for a screened isotropic harmonic oscillator when κ is a rational number ($\kappa<1$), the orbit is closed.

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On the Kolmogorov-like generalization of Tsallis entropy, correlation entropies and multifractal analysis

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The generalization à la Kolmogorov of Tsallis entropy, introduced by the authors in a previous work [J. Math. Phys. **37**, 4480 (1996)], is revisited. Invariance properties are pointed out under weaker conditions than before. This result leads us to wonder if Tsallis entropy at the Kolmogorov abstraction level brings new information with respect to the generalization that Kolmogorov did of Shannon entropy. The negative answer motivates us to look for other generalizations of Tsallis entropy in order to avoid the lack of new information. Correlation entropies seem to be good candidates for this purpose. The relationship of this kind of entropy with the multifractal analysis is studied with the help of the thermodynamic formalism. We also outline its usefulness to generalize properties of Tsallis entropy. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1429323]

I. INTRODUCTION

The concept of entropy, first introduced in classical thermodynamics, was reinterpreted by Shannon in his Mathematical Theory of Communications[1] as a measure of uncertainty. Shannon did his formulation at a level which involves just probabilistic vectors. He defines entropy as the positive number

$$H_1 = -\sum_{i=0}^{k-1} p_i \log p_i , \tag{1}$$

where $(p_0, p_1, \ldots, p_{k-1})$ is a probability vector, i.e., $\Sigma p_i = 1$.

After Gibbs gave his formulation of the statistical mechanics, it was posed the fundamental problem of relating temporal and ensembles averages (ergodic problem of the classical statistical mechanics). It was evident that the simple structure considered in Shannon theory was not enough to treat a problem of this nature, therefore a more elaborated one was necessary. In particular, dynamical aspects should be considered. It is the context in which Kolmogorov[2] generalizes Shannon entropy. He did it by using structures including measure preserving transformations that allow one to codify in a discrete way the temporal evolution of the systems. For a given partition of phase space, the quantity of information is calculated by replacing in Eq. (1) probabilities by the measure of the partition members. Then, Kolmogorov–Shannon entropy involves the average of the quantity of information of successive partitions.

One parameter families of entropies that contain Shannon entropy as a particular member have been introduced. Among these, we mention Renyi[3] and Tsallis[4] entropies. This last one appeared motivated by problems that require a nonextensive formalism.[5] It has been applied to study, e.g., gravitational systems[6,7] and phenomena like anomalous diffusion[8] and turbulence.[9]

For a probability vector $(p_0, p_1, \ldots, p_{k-1})$ Tsallis entropy reads

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$$H_q = \frac{1 - \sum_{i=0}^{k-1} p_i^q}{q-1}, \tag{2}$$

where q is any real number. Notice that for $q \to 1$, Shannon entropy is recovered.

In a previous work,[10] hereafter denoted I, we have generalized Tsallis entropy in the same sense that Kolmogorov did for Shannon's. There we have shown that, for any q, the Kolmogorov–Tsallis family of entropies is invariant under isomorphisms and that invariance is complete for Bernoulli schemes. This last result says to us that two Bernoulli schemes with the same entropy are ''finitarilly'' isomorphic.

The main goal of this article is to point out the true role played by the members of the Kolmogorov–Tsallis family of entropies about their ability to bring new information with respect to that contained in Kolmogorov–Shannon entropy. The invariance of the Kolmogorov-Tsallis entropies and a theorem by Ya Sinai[11] lead us to conclude that, under certain conditions, mainly the ergodicity, there is no substantial contribution of new information. Nevertheless, we do not believe that this claim invalidates the many results in several fields, especially in physics, deduced from Tsallis entropy [Eq. (2)] because in these cases what is actually considered is a particular quantity of information. In fact, in I it was shown that, for Bernoulli schemes, Tsallis entropy is obtained from one step in the definition of the Kolmogorov–Tsallis entropy if the quantity of information is calculated for a particular partition (the canonical generator).

The cause of the lack of new information may be due to the use of partitions. This is implicit in the statement of Sinai's theorem.[11] A way to introduce a family of entropies without using partitions is to consider correlation entropies.[12] These entropies are associated to a structure that involves, besides a measure, a metric. They are not only invariants under isomorphisms, in a measure theoretic sense, but also under other conditions which are not taken into account in Sinai's theorem. These additional conditions are related to the metric and are imposed on the function that determines the isomorphism. The family of correlation entropies that we shall introduce directly conducts to Tsallis entropy in the particular case of Bernoulli schemes (endowed with a metric). Also it contains, as a particular member, Kolmogorov–Shannon entropy, as it can be shown from the Brin–Katok theorem.[13] The correlation approach allows us to extend, in a relatively direct way, some properties of the Tsallis entropy to the level of abstract dynamical systems.

The article is organized as follows. In the next section, the main definitions and results of I are briefly reviewed and one of the isomorphism theorems thereof is reformulated under weaker conditions. In Sec. III we analyze the possibility that Kolmogorov–Tsallis entropy gives new information with respect to Kolmogorov–Shannon's. Section IV is devoted to introducing the correlation entropies in the above mentioned sense and also to establish invariant conditions for them. Then, a multifractal analysis is discussed for correlation entropies.

II. KOLMOGOROV–TSALLIS ENTROPY

The mathematical idea of measure preserving transformations generalizes, in some sense, the physical concept of dynamical system. Let recall that, physically, a dynamical system is understood as a collection of particles or states which obey a law that determines their temporal evolution and in such a way that the Liouville theorem is satisfied besides. Recall that the equilibrium condition are mathematically interpreted as the existence of an invariant measure which is the probability that a state belongs to a certain subspace of the phase space in a given instant.

From a mathematical point of view a dynamical system or, more precisely, a measure preserving dynamical system is a quadruple $\mathcal{S}=(X,\mathcal{B},\mu,T)$, where X is a set (phase space), $\mathcal{B}$ is a σ-algebra, μ is a probability measure on $\mathcal{B}$ and T is an invertible map $T:X\to X$ which is measurable and preserves μ, i.e., *for any* $B\in\mathcal{B}$, $T^{-1}B\in\mathcal{B}$ *and* $\mu(T^{-1}B)=\mu(B)$.

A particular structure that we shall frequently mention is the so called *Bernoulli schemes*. In this case the phase space is

$$BS(p)=\{x=(x_i)_{i\in\mathbf{Z}}:x_i\in\Omega,\forall i\in\mathbf{Z}\}\equiv\prod_{-\infty}^{\infty}\{0,1,2,\ldots,k-1\},\tag{3}$$

where p is a probability vector and $\Omega=\{0,1,\ldots,k-1\}$.

The σ-algebra $\mathcal{B}$ is that generated by the semi-algebra of the cylinders $C^{-m,\ldots,m}_{\alpha_{-m},\ldots,\alpha_m}=\{x\in\Sigma_A:x_i=\alpha_i:i=-m,\ldots,m\}$. The measure is defined in the following way: to each point $\{x_i\}$ is assigned a probability $P(\{x_i\})=p_{x_i}$ and the measure of the cylinder $C^{-m,\ldots,m}_{\alpha_{-m},\ldots,\alpha_m}$ is the product measure

$$\mu(C)=P(\{\alpha_{-m}\})\cdots P(\{\alpha_m\})=p_{\alpha_{-m}}\cdots p_{\alpha_m}.\tag{4}$$

These measures can be extended to the whole σ-algebra $\mathcal{B}$ by the extension Kolmogorov theorem.[14,15]

The measure preserving transformation is, finally, the Bernoulli shift $\sigma:BS(p)\to BS(p)$ given by $\sigma x=x'$, where $x'_i=x_{i+1}$.

The generalization à la Kolmogorov of Shannon entropy (1) is defined, first, by measuring the available quantity of information H_1 which is associated to a partition of the phase space X. If $\mathcal{A}=\{A_0,A_1,\ldots,A_{k-1}\}$ is such that $\cup_{i=0}^{k-1}A_i=X$; $A_i\cap A_j=\phi\ \forall i\neq j$, then

$$H_1(\mathcal{A})=-\sum_{i=0}^{k-1}\mu(A_i)\log\mu(A_i).\tag{5}$$

Here $\mu(A_i)$ is interpreted as the probability that a random point lies in A_i. Further, the average of this information quantity, when the experiment repeats infinitely, is calculated. Finally, all the available information is involved by taking the supreme over all the partitions by measurable sets.

Next we review the generalization presented in I. In order to generalize Tsallis entropy Eq. (2) according to the previous procedure, we begin by replacing "probabilities p_i by measures $\mu(A_i)$:"

$$H_q(\mathcal{A})=(q-1)^{-1}\left(1-\sum_{i=0}^{k-1}[\mu(A_i)]^q\right),\tag{6}$$

where q is any real number. The case $q=1$ will be imposed by continuity, and so Eq. (6) yields expression (5).

Given $x\in X$, we consider the following points of its orbit: x, Tx, $T^2x,\ldots,T^{n-1}x$. Since $\mathcal{A}$ is a partition, for each one of these points there is only one member of $\mathcal{A}$ to which it belongs. Then we can associate to each point x a string $\ell=(\ell_0,\ell_1,\ldots,\ell_{n-1})$, which will be called the name of x *of length* n. The assignation is done according to $T^ix\in A_{\ell_i}$, $i=0,1,\ldots,n-1$. Consequently, a new partition can be obtained from $\mathcal{A}$:

$$\mathcal{A}^n=\{A^n(\ell):A^n(\ell)\text{ is the set of points with same name }\ell\text{ of length }n\}.\tag{7}$$

Definition 2.1: The *mean generalized entropy*, associated to a transformation T that preserves a measure μ, is

$$h_q(T)=(q-1)^{-1}[1-\exp(\tilde{h}_q(T))]\tag{8}$$

with

$$\tilde{h}_q(T)=\sup_{\mathcal{A}}\tilde{h}_q(\mathcal{A},T)\tag{9}$$

and

$$\tilde{h}_q(\mathcal{A},T)=\overline{\lim_{n\to\infty}}\frac{1}{n}\{\log[1+(1-q)H_q(\mathcal{A}^n)]\},\tag{10}$$

where, for $H_q(\mathcal{A}^n)$, the sum in Eq. (6) must be taken over all the names of length n.

Remark: For the particular case of Bernoulli schemes $BS(p_0,p_1,\ldots,p_{k-1})$, as partition is considered the "canonical generator" $\mathcal{G}=\{G_i\}$, with $G_i=\{x=(x_l)_{l\in\mathbf{Z}}: x_0=i\}=C_i^0$ for $0\leqslant i\leqslant k-1$. Then $\mu(\mathcal{G}^n)=p_{\alpha_{-m}}\cdots p_{\alpha_m}$ and

$$[\tilde{h}_q(\mathcal{G},\sigma)]_{BS(p_0,p_1,\ldots,p_{k-1})}=\log\sum_{i=0}^{k-1}p_i^q,\tag{11}$$

which leads to Tsallis entropy for arbitrary q [Eq. (2)]:

$$[h_q(\mathcal{G},\sigma)]_{BS(p)}\equiv H_q(p)=(q-1)^{-1}\left[1-\sum_{i=0}^{k-1}p_i^q\right],\tag{12}$$

and the Shannon expression [Eq. (1)] is recovered for $q\to 1$.

Remark: We have (by the Kolmogorov–Sinai theorem) $H_1(p)\equiv h_1(\mathcal{G},\sigma)=h_1(\sigma)$. However, for arbitrary q, $H_q(p)$ does not necessarily agree with $h_q(\sigma)$.

A. Isomorphism theorems and other properties

In I we have proved the following isomorphism theorem:

Theorem I.1: Let $\mathcal{S}=(X,\mathcal{B},\mu,T)$ and $\mathcal{S}'=(X',\mathcal{B}',\mu',T')$ be a two isomorphic dynamical system. Then $h_q(T)=h_q(T')$.

Actually, it can be reformulated under a weaker hypothesis. Before doing this we recall the definition of *factor*.

Definition: A dynamical system $\mathcal{S}'=(X',\mathcal{B}',\mu',T')$ is a factor of the dynamical system $\mathcal{S}=(X,\mathcal{B},\mu,T)$ if there exists a measurable subjective map $f:X\to X'$, such that

(i) For every $B'\in\mathcal{B}$, $\mu(f^{-1}B')=\mu'(B')$.
(ii) For every x, $f(Tx)=T'(fx)$.

Two systems $\mathcal{S}$ and $\mathcal{S}'$ are *weakly isomorphic* if $\mathcal{S}$ is a factor of $\mathcal{S}'$ and $\mathcal{S}'$ is a factor of $\mathcal{S}$. When f is bijective the systems are *isomorphic*.

Theorem 2.2: Let $\mathcal{S}'=(X',\mathcal{B}',\mu',T')$ be a factor of the dynamical system $\mathcal{S}=(X,\mathcal{B},\mu,T)$. Then $h_q(T)\leqslant h_q(T')$ for $q>1$ and $h_q(T)\geqslant h_q(T')$ for $q<1$.

The proof is similar to that given for Theorem I.1, so we omit the details.

The equality holds when the systems are weakly isomorphic. In this case the generalized entropy becomes an invariant under weak isomorphisms.

The generalization in the spirit of Kolmogorov for the Renyi entropy was done in Ref. 12. There the analogous invariant result was proved.

Proposition 2.3: For any integer $m\geqslant 2$ it holds

$h_q(T^m)=(q-1)^{-1}[1-\exp(m\tilde{h}_q(T))]$ for every q.

Proof: We write $\tilde{H}_q(\mathcal{A})=1+(1-q)H_q(\mathcal{A})$. We recall that a partition $\mathcal{A}$ is a refinement of a partition $\mathcal{C}$, if any element of $\mathcal{C}$ can be expressed as union of elements of $\mathcal{A}$. If $q<1$, then $\tilde{H}_q(\mathcal{A})\geqslant\tilde{H}_q(\mathcal{C})$, whereas for $q>1$ is $\tilde{H}_q(\mathcal{A})\leqslant\tilde{H}_q(\mathcal{C})$.

Let $q<1$. We consider a partition $\mathcal{A}$, and let $\mathcal{A}^m$ be the partition by names of length m obtained from $\mathcal{A}$ and T. We have $\tilde{H}_q((\mathcal{A}^m)^n)=1+(1-q)H_q((\mathcal{A}^m)^n)$ where now $(\mathcal{A}^m)^n$ is the partition with names of length n obtained from $\mathcal{A}^m$ and T^m. Then

$$\tilde{h}_q(\mathcal{A}^m,T^m)=\overline{\lim_{n\to\infty}}\frac{1}{n}\{\log[\tilde{H}_q((\mathcal{A}^m)^n)]\}=\overline{\lim_{n\to\infty}}\frac{m}{mn}\{\log[\tilde{H}_q(\mathcal{A}^{mn})]\}$$

$$\geqslant m\overline{\lim_{s\to\infty}}\frac{1}{s}\tilde{H}_q(\mathcal{A}^s)=m\tilde{h}_q(\mathcal{A},T), \tag{13}$$

where $\mathcal{A}^{mn}$ is the partition with names of length mn built from the partition first given and T.

Thus, by taking the supreme over the finite partitions, we have

$$\tilde{h}_q(T^m)\geqslant m\tilde{h}_q(T). \tag{14}$$

For the other inequality, we have the following.

If $l\in\mathbf{N}$, then a partition by names of length l, with respect to $(\mathcal{A},T)$, involves the orbits $x,Tx,\ldots,T^{l-1}x$, for any point x. A partition by names of length n, with respect to $(\mathcal{A}^m,T^m)$ involves the orbits $x,T^mx,\ldots,(T^m)^{n-1}x$. Further, if $l=mn,mn+1,\ldots,mn+m$, then $\mathcal{A}^l$ is a refinement of $(\mathcal{A}^m)^n$. Then

$$\frac{1}{n}\{\log[\tilde{H}_q((\mathcal{A}^m)^n)]\}\leqslant\frac{1}{n}\{\log[\tilde{H}_q(\mathcal{A}^l)]\}=\frac{l}{n}\frac{1}{l}\{\log[\tilde{H}_q(\mathcal{A}^l)]\}\leqslant\frac{mn+m}{n}\frac{1}{l}\{\log[\tilde{H}_q(\mathcal{A}^l)]\}.$$

Consequently,

$$\frac{1}{n}\{\log[\tilde{H}_q(\mathcal{A}^{mn})]\}\leqslant m\left(1+\frac{1}{n}\right)\frac{1}{l}\{\log[\tilde{H}_q(\mathcal{A}^l)]\},$$

and thus

$$\sup_{j\geqslant n}\frac{1}{j}\{\log[\tilde{H}_q(\mathcal{A}^{mj})]\}\leqslant m\sup_{j\geqslant n}\left(1+\frac{1}{j}\right)\sup_{l=mj,mj+1,\ldots,mj+n}\frac{1}{l}\{\log[\tilde{H}_q(\mathcal{A}^l)]\}.$$

Therefore,

$$\tilde{h}_q(T^m)=\overline{\lim_{n\to\infty}}\frac{1}{n}\{\log[\tilde{H}_q((\mathcal{A}^m)^n)]\}=\lim_{j\to\infty}\sup_{j\geqslant n}\frac{1}{j}\{\log[\tilde{H}_q(\mathcal{A}^m)^j]\}\leqslant m\overline{\lim_{n\to\infty}}\frac{1}{l}\{\log[\tilde{H}_q(\mathcal{A}^l)]\}.$$

Finally,

$$\tilde{h}_q(\mathcal{A},T^m)\leqslant m\tilde{h}_q(\mathcal{A},T), \tag{15}$$

for every finite partition $\mathcal{A}$.

For $q>1$ the demonstration is similar, taking into account the inversion of the above inequalities. ■

Proposition 2.4: $h_q(T_1\times T_2)=(q-1)^{-1}[1-\exp(\tilde{h}_q(T_1))\exp(\tilde{h}_q(T_2))]$, where the product of transformation is defined in the usual form.

Proof: We consider two dynamical systems, $S_1=(X_1,\mathcal{B}_1,\mu_1,T_1)$ and $S_2=(X_2,\mathcal{B}_2,\mu_2,T_2)$, and define their ''product:''

$$S_1\times S_2=(X_1\times X_2,\mathcal{B},\mu,T_1\times T_2),$$

where $\mathcal{B}$ is the σ-algebra generated by rectangles $A_{1i}\times A_{2j}$ with $A_{\alpha k}\in\mathcal{B}_\alpha(\alpha=1,2)$ and μ is the product measure $\mu(A_{1i}\times A_{2j})=\mu_1(A_{1i})\cdot\mu_2(A_{2j})$. Let $\mathcal{A}'$ and $\mathcal{A}''$ be partitions of X_1 and X_2, respectively, and let $\mathcal{A}$ be a product partition of $\mathcal{A}'$ and $\mathcal{A}''$.

Since the σ-algebra considered is generated by the rectangles, we have

$$\tilde{h}_q(T_1\times T_2)=\sup\{\tilde{h}_q(\mathcal{A}'\times\mathcal{A}'',T_1\times T_2):\mathcal{A}' \text{ partition of } X_1\ \mathcal{A}'' \text{ partition of } X_2\}.$$

$$\tilde{h}_q(\mathcal{A}'\times\mathcal{A}'',T_1\times T_2)=\overline{\lim_{n\to\infty}}\frac{1}{n}\tilde{H}_q((\mathcal{A}'\times\mathcal{A}'')^n)=\overline{\lim_{n\to\infty}}\frac{1}{n}\log\left(\sum_{\mathscr{C}}[\mu_1((\mathcal{A}')^n)]^q\right)$$
$$+\overline{\lim_{m\to\infty}}\frac{1}{n}\log\left(\sum_{\mathscr{C}}[\mu_2((\mathcal{A}'')^n)]^q\right),$$

where both sums are extended over the names $\mathscr{C}$, of length n for T_1 and T_2. Then,

$$\tilde{h}_q(\mathcal{A}'\times\mathcal{A}'',T_1\times T_2)=\tilde{h}_q(\mathcal{A}',T_1)+\tilde{h}_q(\mathcal{A}'',T_2).$$

Because this is valid for any partition by rectangles, it results in

$$\tilde{h}_q(T_1\times T_2)=\tilde{h}_q(T_1)+\tilde{h}_q(T_2),$$

and so

$$h_q(T_1\times T_2)=(q-1)^{-1}[1-\exp(\tilde{h}_q(T_1))\exp(\tilde{h}_q(T_2))]. \tag{16}$$

■

III. LACK OF NEW INFORMATION IN THE ERGODIC CASE

In view of the previous results, it is natural to ask if the statement of Theorem I.1 (or its stronger version Theorem 2.2) could actually be due to the lack of new information, with respect to that involved in $h_1(T,\mu)$, of the members of the entropy family. We have an answer in the case that the systems are ergodic. For definition of ergodicity and related topics, see, for example, Refs. 16 and 14.

Herein we consider as an additional hypothesis that the space (X,μ) be "countable," i.e., $L^2(X,\mu)$ have a dense countable subset. We recall the following basic result.

Theorem (Ya Sinai):[11] Let $\mathcal{S}=(X,\mathcal{B},\mu,T)$ be an ergodic Lebesgue space and a $BS(p)$ Bernoulli scheme such that $h_1(T)\geqslant[h_1]_{BS(p)}$, then $BS(p)$ is a factor of T.

This theorem, together with Theorem I.1 (or Theorem 2.2) and Proposition 2.6 will serve as a basis to answer the question about the lack of new information.

Proposition 2.6: Let $\mathcal{S}=(X,\mathcal{A},\mu,T)$ be an ergodic Lebesgue space such that $h_1(T)\geqslant\log K$, for some integer $K>1$. Then, for $q>1$,

$$h_q(T)\leqslant\frac{1-K^{1-q}}{q-1}. \tag{17}$$

Proof: Let T be ergodic with $h_1(T)\geqslant\log K$, for some integer $K>1$. The right hand side of the inequality is the classical entropy of the Bernoulli scheme $BS(p)$, with $p=(1/K,\ldots,1/K)$.

By Sinai theorem $BS(1/K,\ldots,1/K)$ is a factor of T. Then by Theorem I.1 (or Theorem 2.2),

$$\tilde{h}_q(T)\geqslant[\tilde{h}_q]_{BS(p)}\geqslant[\tilde{h}_q,\mathcal{G}]_{BS(p)}=\log K^{1-q}, \tag{18}$$

where the last equality follows by taking in Eq. (12) $p_i=1/K$. Thus

$$h_q(T)\leqslant\frac{1-K^{1-q}}{q-1}, \quad \text{for} \quad q>1. \tag{19}$$

■

Definition: A dynamical system is a *Bernoulli automorphism* if it is isomorphic to a Bernoulli scheme.

We are now in conditions of demonstrating that the family h_q does not contain new information with respect to h_1.

Theorem 2.7: Let $\mathcal{S}=(X,\mathcal{A},\mu,T)$ be a Lebesgue space with T ergodic and $h_1(T)>0$. Then

$$h_q(T)=\begin{cases}\Psi_q(h_1) & \text{if } q>1,\\ \infty & \text{if } q<1,\end{cases} \tag{20}$$

where Ψ_q is a certain function.

Proof: (I) Case $q<1$. We will use the following result.[12]

Lemma (Takens and Verbistki): Let h be a real number such that $0\leqslant -t\log t<h<\infty$, with $t\in[0,1]$. Then there exists a natural number m and a vector $p=(p_0,\ldots,p_{m-1})$ such that

(i) $\Sigma_{i=0}^{m-1}p_i=t$, (ii) $-\Sigma_{i=0}^{m-1}p_i\log p_i=h$.

Then let us consider $0<q<1$, $n\in\mathbf{N}$ and define $p_i=n^{-(1+q)/2q}$, $i=0,1,2,\ldots,n-1$. We have

$$\sum_{i=0}^{n-1}p_i=n\times n^{-(1+q)/2q}=n^{(q-1)/2q}\to 0,\quad \text{with } n\to\infty \tag{21}$$

and

$$-\sum_{i=0}^{n-1}p_i\log p_i=\frac{1+q}{2q}n^{(q-1)/2q}\log n\to 0,\quad \text{with } n\to\infty. \tag{22}$$

Let $t=1-\Sigma_{i=0}^{n-1}p_i=1-n^{(q-1)/2q}$,

$\overline{h}=h_1(T)+\Sigma_{i=0}^{n-1}p_i\log p_i=h_1(T)-\dfrac{1+q}{2q}n^{(q-1)/2q}$.

Now by the above lemma (notice that $\overline{h}>-t\log t$, for n large enough), there is a natural number m and a vector $(w_{0,\ldots,}w_{m-1})$ with $\Sigma w_i=t$ and $-\Sigma w_i\log w_i=\overline{h}$. Let us define

$p=(p_0,\ldots,p_{n-1},p_n,\ldots,p_{n+m-1})$, where $p_i=n^{-(1+q)/2q}$, $i=0,1,2,\ldots,n-1$, $p_n=w_0,\ldots,p_{n+m-1}=w_{m-1}$.

Then

$$\sum_{i=0}^{n+m-1}p_i=1 \quad\text{and}\quad -\sum_{i=0}^{n+m-1}p_i\log p_i=h_1(T).$$

We have determined a Bernoulli scheme $BS(p)$ with classical entropy equal to $h_1(T)$. Therefore by the Sinai theorem $BS(p)$ is a factor of T and so by Theorem I.1 (or Theorem 2.2) we have $h_q(T)\geqslant[h_q]_{BS(p)}$. On the other hand, since $\Sigma_{i=0}^{m-1}p_i^q\geqslant\Sigma_{i=0}^{n-1}p_i^q=n^{(q-1)/2q}$, and with $\mathcal{G}$ the canonical generator we get

$$[\tilde{h}_q(\mathcal{G})]_{BS(p_0,\ldots,p_{n-1})}=\log\left(\sum p_i^q\right)=\log(n^{(q-1)/2q}). \tag{23}$$

Therefore,

$$h_q(T)\geqslant[h_q]_{BS(p)}\geqslant\frac{1-\Sigma_{i=0}^{n-1}p_i^q}{q-1}=\frac{1-n^{(q-1)/2q}}{q-1}. \tag{24}$$

Because n can be taken arbitrarily large, we have $h_q(T)=\infty$, for $q<1$.

For q negative, we have $q<q_0$ with $0<q_0<1$, and, since $h_q>h_{q_0}$, the theorem also holds in this case.

(II) Case $q>1$. We shall consider first the particular situation in which T^m is ergodic, for any $m\geqslant 2$ and $h_1(T^m)>0$. For each $x>0$, we choose a negative number $M_q = M_q(x)$ with the following property: for any $y>0$, $x\geqslant y$ if and only if $M_q x\geqslant(1-q)y$.

If, in particular, $x=h_1(T)>0$, and K is an integer such that $K>1$, it holds that $h_1(T)\geqslant\log K$ if and only if $M_q h_1(T)\geqslant(1-q)\log K$. Besides $h_1(T)\geqslant\log K$ implies $BS(1/K,\ldots,1/K)$ is a factor of T (by Sinai theorem), and consequently $\tilde{h}_q(T)\geqslant(1-q)\log K$ (cf. Proposition 2.6).

Also we have $h_1(T)\geqslant \tilde{h}_q(T)/(1-q)$; if $q>1$, this deduces directly from the corresponding definitions. Therefore $M_q h_1(T)\geqslant\tilde{h}_q(T)$, and so

$$\frac{M_q h_1(T)}{1-q}\leqslant\frac{\tilde{h}_q(T)}{1-q}. \tag{25}$$

If it were

$$\frac{M_q h_1(T)}{1-q}<\frac{\tilde{h}_q(T)}{1-q}, \tag{26}$$

then, by applying Proposition 2.6 in particular to T^m, we have

$$\frac{\tilde{h}_q(T^m)}{1-q}-\frac{M_q h_1(T^m)}{1-q}=m\left(\frac{\tilde{h}_q(T)}{1-q}-\frac{M_q h_1(T)}{1-q}\right)\to+\infty,\quad \text{with } m\to+\infty. \tag{27}$$

Then for an m large enough there will an integer $K>1$ such that

$$\frac{M_q h_1(T^m)}{1-q}<\log K<\frac{\tilde{h}_q(T)}{1-q}. \tag{28}$$

Now we have a contradiction with Proposition 2.6 applied to T^m. Let recall that we are assuming that all the positive iterations of T are ergodic.

Therefore, if T is ergodic and T^m is ergodic, $m\geqslant 2$, it holds $M_q h_1(T)=\tilde{h}_q(T)$.

Next we consider the general situation in which it is required that just T be ergodic. For a given ergodic transformation T with $h_1(T)>0$, there exists a Bernoulli scheme with classical entropy equal to $h_1(T)$.[16,17] This also will be valid for dynamical systems isomorphic to Bernoulli schemes, which are called *Bernoulli automorphisms*. Thus if T is ergodic with $h_1(T)>0$, there exists Bernoulli automorphism S with $h_1(T)= h_1(S)$. Then by the Sinai theorem S is a factor of T, so that $\tilde{h}_q(T)\geqslant\tilde{h}_q(S)$. For any transformation T there is associated an operator $\mathcal{L}_T: L^2(X,\mu)\to L^2(X,\mu)$, defined by $\mathcal{L}_T[f](x)=f(Tx)$. It says that this operator has discrete spectrum if there is an orthonormal basis of eigenfunctions. By a theorem of Rohlin, if $T:X\to X$ is a Bernoulli automorphism with X countable, the associated operator $\mathcal{L}_T$ has discrete spectrum (see e.g., Ref. 16, p. 109). It can be proved (Ref. 16, p. 66) that if $\mathcal{L}_T$ has discrete spectrum, then T is strong-mixing. What is actually proved is

$$\lim_{n\to\infty}(\mathcal{L}_T^n f,g)=(f,1)(1,g),$$

where $(.,.)$ denotes the usual product in the Hilbert space $L^2(X,\mu)$.

Thus the Bernoulli automorphism S is mixing and so S^m is ergodic for any $m\geqslant 1$.[18]

Recall that $h_1(T)\geqslant\tilde{h}_q(T)/(1-q)$, if $q>1$. Consequently,

$$M_q h_1(T)\geqslant\tilde{h}_q(T)\geqslant\tilde{h}_q(S)=M_q h_1(S)=M_q h_1(T). \tag{29}$$

Now $\Psi_q(h_1)=(q-1)^{-1}[1-\exp(M_q h_1)]$, and the theorem is proved. ■

Remarks: A similar theorem for Renyi entropy was proved in Ref. 12.

According to Theorem 2.7, the ergodicity implies a functional relationship between $h_1(T)$ and $h_q(T)$ (for $q>1$). If this relationship does not occur, then the dynamical system (X,T,μ) cannot be ergodic. In this way the generalization of the Tsallis entropy may be useful to detect ergodicity.

It would be interesting to relax the condition of ergodicity in Theorem 2.7. It is a matter for future investigation. So far we could anticipate that for $q>1$ the dependence is not directly with $h_1(T)$, but with a quantity which involves it. For $q<1$ the result would be the same, i.e., $h_q(T)=\infty$. If $T^n x=x$, for some n, the last assertion could not be true. This is clear from Proposition 2.3 and the fact of $h_q(id)=0$. Therefore, it must be required that the set $\{x:T^n x=x,$ for some $n\}$ have zero measure. The hypothesis $h_1(T)>0$ might be also relaxed.

IV. CORRELATION ENTROPIES

Let (X,d) be a compact metric space in which are also given a probability measure μ and a continuous map $T:X\to X$. Let consider the metric $d_n(x,y)=\max\{d(T^i(x)),T^i(y)):i=0,1,\ldots,n-1\}$ and let denote with $B_{\varepsilon,n}(x)$ the ball of radius ε in the metric d_n.

Definition 3.1: The *generalized correlation entropy is*

$$h_q^{\mathrm{corr}}(T)=\frac{1-e^{\tilde{h}_q^{\mathrm{corr}}(T)}}{q-1}, \tag{30}$$

where

$$\tilde{h}_q^{\mathrm{corr}}(T)=\lim_{\varepsilon\to 0}\tilde{h}_{q,\varepsilon}^{\mathrm{corr}}(T) \tag{31}$$

and the average of the information quantity is given by

$$\tilde{h}_{q,\varepsilon}^{\mathrm{corr}}(T)=\overline{\lim_{n\to\infty}}\frac{1}{n}\log\left[\int_X \mu(B_{\varepsilon,n}(x))^{q-1}d\mu\right]. \tag{32}$$

It can see that this entropy generalizes $h_1(T)$. For this the following result is used.

Theorem (Brin-Katok[13]): Let $T:X\to X$ be a continuous map in a compact metric space (X,d) and let μ be a T-invariant Borel measure in X. The following functions are defined in X:

$$\overline{h_1}(x,T)=\lim_{\varepsilon\to 0}\overline{\lim_{n\to\infty}}-\frac{1}{n}\log\mu(B_{\varepsilon,n}(x)) \tag{33}$$

$$\underline{h_1}(x,T)=\lim_{\varepsilon\to 0}\underline{\lim_{n\to\infty}}-\frac{1}{n}\log\mu(B_{\varepsilon,n}(x)) \tag{34}$$

($\overline{h_1}(x,T)$, $\underline{h_1}(x,T)$ are called the *upper and lower local entropies*, respectively). Then

(i) the local entropy does exist, i.e., $\overline{h_1}(x,T)=\underline{h_1}(x,T)=h_1(x,T)$, for every $x\in X$, and
(ii) $h_1(x)$ is a T-invariant function and $\int h_1(x)d\overline{\mu}=h_1(T)$.

Corollary 3.2: $\lim_{q\to 1}\tilde{h}_q^{\mathrm{corr}}(T)=h_1(T)$.

Proof: This corollary follows immediately by using standard results in measure theory (Fatou lemma, Monotone convergence theorem) and the Brin–Katok theorem. ■

The invariance is established in the following terms:

Proposition 3.3: Let (X_1,d_1) and (X_2,d_2) be compact metrizable spaces, and let us consider maps $T_1: X_1\to X_1$, $T_2: X_2\to X_2$ and T_i invariant measures μ_1, μ_2. Let $f:X_1\to X_2$ be a measurable bijection such that $f\circ T_1=T_2\circ f$ and $\mu_1(f^{-1}(A)) = \mu_2(A)$, for every measurable set A. If the condition

$$\frac{1}{K}d_1(x,y)\leqslant d_2(f(x),f(y))\leqslant Kd_1(x,y), \quad \text{for some } K>1, \tag{35}$$

holds for $x,y\in X_1$, then $h_q^{\mathrm{corr}}(T_1) = h_q^{\mathrm{corr}}(T_2)$.

A map f which verifies the above condition is called of *bounded distortion*.

Proof: Let $x,y\in X_1$. We have

$$\frac{1}{K}d_1(T_1^i x,T_1^i y)\leqslant d_2(f(T_1^i x),f(T_1^i y))\leqslant Kd_1(T_1^i x,T_1^i y); \quad i=0,1,\ldots,n-1. \tag{36}$$

Let us call

$$B^1_{\varepsilon,n}(x)=\{y:\max\{d_1(T_1^i x,T_1^i y):i=0,1,\ldots,n-1\}<\varepsilon\},$$

$$B^2_{\varepsilon,n}(x')=\{y':\max\{d_2(T_2^i x',T_2^i y'),i=0,1,\ldots,n-1\}<\varepsilon\}.$$

The condition of bounded distortion is equivalent to

$$\frac{1}{K}d_1(T_1^i x,T_1^i y)\leqslant d_2(T_2^i(f(x)),T_2^i(f(y)))\leqslant Kd_1(T_1^i x,T_1^i y), \quad i=0,1,\ldots,n-1. \tag{37}$$

Then we have $B^1_{\varepsilon,n}(x)\subset f^{-1}(B^2_{K\varepsilon,n}(f(x)))$, or

$$\mu_1(B^1_{\varepsilon,n}(x))\leqslant \mu_1(f^{-1}(B^2_{K\varepsilon,n}(f(x))))=\mu_2(B^2_{K\varepsilon,n}(f(x))). \tag{38}$$

Analogously

$$\mu_2(B^2_{\varepsilon,n}(f(x)))\leqslant \mu_1(B^1_{K\varepsilon,n}(x)). \tag{39}$$

Thus, for $q>1$,

$$\overline{\lim_{n\to\infty}}\frac{1}{n}\log\left[\int_{X_1}\mu_1(B^1_{\varepsilon,n}(x))^{q-1}d\mu_1\right]\leqslant\overline{\lim_{n\to\infty}}\frac{1}{n}\log\left[\int_{X_2}\mu_2(B^2_{K\varepsilon,n}(z))^{q-1}d\mu_2\right],$$

and

$$\overline{\lim_{n\to\infty}}\frac{1}{n}\log\left[\int_{X_2}\mu_2(B^2_{\varepsilon,n}(z))^{q-1}d\mu_2\right]\leqslant\overline{\lim_{n\to\infty}}\frac{1}{n}\log\left[\int_{X_1}\mu_1(B^1_{K\varepsilon,n}(x))^{q-1}d\mu_1\right].$$

For $q<1$, we proceed in a similar way but invert the inequalities.

Therefore, with $\varepsilon\to 0$ we have $\tilde{h}_q^{\mathrm{corr}}(T_1)=\tilde{h}_q^{\mathrm{corr}}(T_2)$ and, finally, $h_q^{\mathrm{corr}}(T_1) = h_q^{\mathrm{corr}}(T_2)$. ■

The invariance conditions related with the metric impose a restriction not taken into account in Sinai theorem. So, to have new information it should work in spaces with "more structure."

A. Bernoulli schemes

We shall see that the correlation entropies generalize Tsallis entropy, i.e., for Bernoulli schemes $BS(p_0,p_1,\ldots,p_{k-1})$, we have $h_q^{\mathrm{corr}}=H_q=(1-\Sigma_{i=0}^{k-1}p_i^q/(q-1)$. The metric considered is

$$d^{BS}(x,y)=2^{-|n|},$$

where $n=\min\{|i|:x_i=y_i\}$.

For each m, the ball $B_{2^{-m},n}(x)$, in the metric d_n^{BS}, with respect to the shift σ, is the cylinder

$$\{y:x_i=y_i:i=-n,\ldots,m-n+1\}.$$

Thus $\mu(B_{2^{-m},n}(x))=\Pi_{i=-m}^{n-m+1}p_{x_i}$, so that

$$[\tilde{h}_q^{\mathrm{corr}}]_{BS}=\overline{\lim_{n,m\to\infty}}\frac{1}{n}\log\left[\int_X\mu(B_{2^{-m},n}(x))^{q-1}d\mu\right]=\log\left(\sum p_i^q\right), \tag{40}$$

where the last equality is obtained by direct calculus. Then

$$[h_q^{\mathrm{corr}}]_{BS}=\frac{1-\Sigma p_i^q}{q-1}=H_q(p_0,p_1,\ldots,p_{k-1}). \tag{41}$$

V. RELATIONSHIP WITH MULTIFRACTAL ANALYSIS

The concept of ''multifractal analysis'' was suggested in relation to the scaling behavior of physical measures on strange attractors.[19] In the study of chaotic behaviors one is frequently faced with invariant sets with a complex mathematical structure and the multifractal analysis treats the so-called *fractal decomposition* of these sets. The aim of this procedure is to encode information about very complex structures by means of a sufficiently well behaved real function.

Here we will relate (Proposition 4.1) the correlation entropies introduced earlier to the function

$$\tau(q):=P(q\varphi)-qP(\varphi), \tag{42}$$

where $P(\varphi)$ is the *topological pressure* associated to a given potential φ.

More precisely, let $T:X\to X$ be a homeomorphism with X a compact metric space. A map $\varphi:X\to\mathbf{R}$ will be called a ''potential'' and the topological pressure associated to it is the number[17,16]

$$P(\varphi)=\sup_{\mu}\left\{h_1(T,\mu)+\int\varphi d\mu\right\}, \tag{43}$$

where the supreme is taken over all the Borel measures μ, T-invariant on X.

The function $\tau(q)$ has been used to describe completely the multifractal spectrum for local entropies and its properties, e.g., the convexity, have been studied.[20,21]

Now we give some definitions and declare the main hypothesis under which the relationship between the correlation entropy and the function $\tau(q)$ holds. These conditions are much weaker than those used in the multifractal analysis done by other authors.[20]

An *equilibrium state* for the potential φ is a measure μ_φ which satisfies

$$P(\varphi)=h_1(T,\mu_\varphi)+\int\varphi\,d\mu_\varphi. \tag{44}$$

Under certain conditions imposed on the map T and the potential φ an equilibrium state can be constructed.[17] The *specification property* for a map $T:X\to X$, introduced by R. Bowen in Ref. 22, reads as follows.

A homeomorphism $T:X\to X$ has the *specification property* if, given a finite disjoint collection of integer intervals $I_1,\ldots,I_k$, then, for $\varepsilon>0$, there is an integer $M(\varepsilon)$ and a function $\Phi:I=\cup I_i\to X$ such that

(i) $\mathrm{dist}(I_i, I_j) > M(\varepsilon)$ (Euclidean distance),
(ii) $T^{n_1-n_2}(\Phi(n_1)) = \Phi(n_2)$, and
(iii) $d(T^n(x), \Phi(n)) < \varepsilon$, for some $x: T^m(x) = x$, with $m \geqslant M(\varepsilon) + \mathrm{length}(I)$ and for every $n \in I$.

A homeomorphism $T: X \to X$ is called *expansive* if there is a constant $\delta > 0$, such that $d(T^n(x), T^n(y)) < \delta$, for any integer n, implies $x = y$.

For a potential φ we put

$$S_n(\varphi)(x) = \sum_{i=0}^{n-1} \varphi(T^i(x)). \tag{45}$$

Following Ref. 17, we say that a potential φ belongs to the class $\nu_T(X)$ if the following condition is fulfilled:

There are constants $\varepsilon, K > 0$ in a such way that

$$d_n(x,y) < \varepsilon \Rightarrow |S_n(\varphi)(x) - S_n(\varphi)(y)| < K. \tag{46}$$

A measure μ on X is called a *Gibbs state* if, for sufficiently small $\varepsilon > 0$, there are constants A_ε, $B_\varepsilon > 0$, such that, for any $x \in X$ and for any positive integer n, there is

$$A_\varepsilon \{\exp[S_n(\varphi)(x)] - nP(\varphi)\} \leqslant \mu(B_{n,\varepsilon}(x)) \leqslant B_\varepsilon \{\exp[S_n(\varphi)(x)] - nP(\varphi)\}. \tag{47}$$

Theorem:[17–23] Let T be an expansive homeomorphism which has the specification property and φ be a potential belonging to the class $\nu_T(X)$, Then μ_φ is an equilibrium state associated to φ, which is a Gibbs state. Besides, it is ergodic.

Proposition 4.1: Under the same hypothesis of the previous theorem it holds that

$$h_q^{\mathrm{corr}}(T) = \frac{1 - \exp[\tau(q)]}{q-1}. \tag{48}$$

Proof: Let μ be the equilibrium state μ_φ associated to the potential φ, which exists. It is a Gibbs state by the theorem above. For $E \subset X$, an (n,ε)-separate set[16,17] we have

$$\int_X \mu(B_{n,\varepsilon}(x))^{q-1} d\mu \geqslant \sum_{x_i \in B_{n,\varepsilon/2}} \int_{B_{n,\varepsilon/2}} \mu(B_{n,\varepsilon}(x))^{q-1} d\mu \geqslant \sum_{x_i \in E} \mu(B_{n,\varepsilon}(x_i))^q. \tag{49}$$

This is because $x \in B_{n,\varepsilon}(x_i) \Rightarrow B_{n,\varepsilon}(x_i) \subset B_{n,\varepsilon}(x)$. Denote

$$Z_n(\varphi, E) = \sum_{x \in E} \exp[S_n(\varphi)(x)].$$

We shall need the following estimations.[17]

(i) Let $E \subset X$ be a finite set. If E_n are (n,ε)-separate, then the topological pressure can be calculated by

$$P(\varphi) = \lim_{n \to \infty} \frac{1}{n} \log Z_n(\varphi, E_n). \tag{50}$$

(ii) If δ is the constant of the expansiveness and $\varepsilon < \delta/2$, then there exists a constant $C = C(\varphi, \varepsilon)$ such that

$$|\log Z_n(\varphi, E_n) - nP(\varphi)| < C \quad \text{for all } n \text{ and all maximal } (n,\varepsilon)\text{-separated sets.} \tag{51}$$

We consider first $q>1$. By using that E is (n,ε)-separated and that μ is a Gibbs state, we obtain

$$\int_X \mu(B_{n,\varepsilon}(x))^{q-1}d\mu \geqslant \sup_E\left\{\sum_{x_i\in E} A_{\varepsilon/2}^q \exp\left[-qnP(\varphi)+\sum_{j=0}^{n-1} q\varphi(T^j(x_i))\right]\right\}. \tag{52}$$

Therefore, using estimations and taking corresponding limits, we have

$$\tilde{h}_q^{\mathrm{corr}}(T)=\lim_{\varepsilon\to 0}\overline{\lim_{n\to\infty}}\frac{1}{n}\log\left[\int_X \mu(B_{\varepsilon,n}(x))^{q-1}d\mu\right]\geqslant P(q\varphi)-qP(\varphi)=\tau(q). \tag{53}$$

For the other inequality, let E be $(n,\varepsilon/2)$-separated,

$$\int_X \mu(B_{n,\varepsilon/2}(x))^{q-1}d\mu \leqslant \sum_{x_i\in E}\int_{B_{n,\varepsilon/2}(x_i)} \mu(B_{n,\varepsilon/2}(x))^{q-1}d\mu \leqslant \sum_{x_i\in E}\mu(B_{n,\varepsilon}(x_i))^{q-1}d\mu, \tag{54}$$

since $x\in B_{n,\varepsilon/2}(x_i)\Rightarrow B_{n,\varepsilon/2}(x)\subset B_{n,\varepsilon}(x_i)$. Thus by using again the estimations and that μ is a Gibbs state,

$$\int_X \mu(B_{n,\varepsilon/2}(x))^{q-1}d\mu \leqslant \sup_E\left\{\sum_{x_i\in E} B_\varepsilon^q \exp\left[-qnP(\varphi)+\sum_{j=0}^{n-1} q\varphi(T^j(x_i))\right]\right\}, \tag{55}$$

so that

$$\tilde{h}_q^{\mathrm{corr}}(T)\leqslant P(q\varphi)-qP(\varphi)=\tau(q). \tag{56}$$

The case $q<1$ is proved similarly by inverting inequalities. Finally,

$$h_q^{\mathrm{corr}}(T)=\frac{1-\exp[\tau(q)]}{q-1}. \tag{57}$$

■

The facts that $\tau(q)$ is strictly convex and its derivative is

$$\frac{d\tau}{dq}=\int_X \varphi d\mu_q - P(\varphi), \tag{58}$$

where μ_q is the equilibrium state for the potential $\varphi_q=q\varphi-qP(\varphi)$, were demonstrated first in Ref. 20 and, under the weaker hypothesis considered in the above results, in Ref. 21.

We finish by outlining the usefulness of this correlation approach to extend properties of the Tsallis entropies to general dynamical systems. We show as a sample two of them, say the properties (i) and (ii) of Lemma 1 in Ref. 24.

$$(i)\quad \tilde{h}_q^{\mathrm{corr}}(\lambda T_1+(1-\lambda)T_2)\overset{\leqslant}{\geqslant}\lambda^{q-1}\int_X(\mu_1(B_{n,\varepsilon}(x)))^{q-1}+(1-\lambda)^{q-1}\int_X \mu_2(B_{n,\varepsilon}(x))^{q-1}. \tag{59}$$

We have $\int_X(\mu_1(B_{n,\varepsilon}(x))+\mu_2(B_{n,\varepsilon}(x)))^{q-1}d\mu \overset{\leqslant}{\geqslant}\int_X(\mu_1(B_{n,\varepsilon}(x)))^{q-1}+\int_X\mu_2(B_{n,\varepsilon}(x))^{q-1}$, $\leqslant$ or $\geqslant$ accordingly to $q<1$ or $q>1$. The result follows immediately.

For the special case of Bernoulli schemes, (i) of Lemma 1 in Ref. 24 is obtained.

$$(ii)\quad h_q^{\mathrm{corr}}(T)\leqslant\frac{1-\exp[(1-q)h_{\mathrm{top}}]}{q-1},\quad \text{for } 0<q<1, \tag{60}$$

where h_{top} is the topological entropy of T. To prove it we use that, for $0<q<1$, it holds that

$$\frac{\tilde{h}_q^{\text{corr}}(T)}{1-q} \leqslant \tilde{h}_0^{\text{corr}}(T) = \tau(0) = P(0), \tag{61}$$

and, since $P(0)=h_{\text{top}}$,[16,17] we get

$$\tilde{h}_q^{\text{corr}}(T) \leqslant (1-q)h_{\text{top}}, \tag{62}$$

given Eq. (60) which generalizes property (ii) of Lemma 1 in Ref. 24.

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Short distance asymptotics of Ising correlations

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We prove that the short distance asymptotics for the even Ising model scaling functions from below T_c is given by the Luther–Peschel formula. Generalizations to the odd scaling functions and holonomic fields are given. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1425960]

I. INTRODUCTION

In this paper we will use the Sato–Miwa–Jimbo (SMJ) characterization of the scaling functions for the two-dimensional Ising model to show that the short distance asymptotics of the even scaling functions below the critical point are given by the Luther–Peschel formula[1] (see Theorem 1). We will then present results for the odd correlations below T_c and also for holonomic quantum fields which are a consequence of the same technique used to prove Theorem 1.

This paper is a sequel to Ref. 2 and the reader is referred to that paper for a more detailed explanation of the Ising model scaling limits than we will give here. Continuum limits for the two-dimensional Ising correlations on a lattice were first considered in Ref. 3, where, in addition, a connection with Painlevé transcendents was discovered. In a series of papers Sato, Miwa, and Jimbo showed that the continuum correlations (the scaling functions) were associated with monodromy preserving deformations of the Euclidean Dirac equation and that this connection sufficed to account for the appearance of the Painlevé transcendents.[4–8] Here we exploit the fact that the SMJ formula for the log derivative of the scaling function (a τ function in their terminology) can be expressed in terms of the Fourier coefficients of a solution to the *linear* Dirac equation. We analyze the linear problem in order to control the short distance asymptotics. This analysis was suggested by the success of Riemann–Hilbert techniques in obtaining asymptotics for nonlinear integrable systems,[9] where a similar connection with a linear problem is a central feature.

We would like to point out that the two point function both for the Ising model and for holonomic fields in general has been analyzed in more detail than the result we obtain here, see Refs. 10–12. In particular, the constant term in the short distance asymptotics is obtained—our result for the log derivative has nothing to say about this.

We will begin by recalling some of the results of Ref. 2, where a sketch of the the proof was presented. The SMJ characterization involves certain solutions to the Dirac equation in two dimensions so we will start with a description of the situation of interest to us. The Euclidean Dirac operator in $\mathbf{R}^2$ (with a mass perturbation) is given by

$$mI-\not{\partial}=\begin{bmatrix} m & -2\partial \\ -2\bar{\partial} & m \end{bmatrix},$$

where

$$\partial := \frac{1}{2}\left(\frac{\partial}{\partial x_1}-i\frac{\partial}{\partial x_2}\right),$$

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$$\overline{\partial} := \frac{1}{2}\left(\frac{\partial}{\partial x_1} + i\frac{\partial}{\partial x_2}\right).$$

Although we will *not* be working exclusively with holomorphic functions, the presence of ∂ and $\overline{\partial}$ in the Dirac operator makes it very convenient to introduce the complex variable $z = x_1 + ix_2$ with $\overline{z} = x_1 - ix_2$; we thus identify $\mathbf{R}^2$ with $\mathbf{C}$ in the usual fashion. For brevity we will write $f(z)$ for a function of two real variables even though it is customary to use a notation like $f(z,\overline{z})$ to avoid the temptation to regard $f(z)$ as a holomorphic function of z.

Let $\mathbf{a} = \{a_1, a_2, \ldots, a_N\}$ denote a collection of N distinct points in $\mathbf{C}$. The solutions of the Dirac equation that we are interested in are smooth sections of a rank 2 vector bundle over the punctured plane $\mathbf{C}\backslash\mathbf{a}$.

For the purpose of allowing some later remarks we will begin by defining a slightly more general family of *line* bundles, $\mathcal{E}_\lambda$, than is relevant for the Ising model. For $j = 1,2,\ldots,N$ suppose *real* numbers λ_j are given with $|\lambda_j| \leqslant \frac{1}{2}$. Define

$$\Lambda_j = e^{2\pi i \lambda_j}$$

and write

$$\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N).$$

Roughly speaking the smooth sections of the bundle $\mathcal{E}_\lambda \to \mathbf{C}\backslash\mathbf{a}$ will be multivalued functions on $\mathbf{C}\backslash\mathbf{a}$ with values in $\mathbf{C}$ which have multiplier Λ_j when continued about a loop that circles a_j counterclockwise. This can be made precise in an elegant fashion by working on the simply connected covering space of $\mathbf{C}\backslash\mathbf{a}$ and then restricting attention to smooth sections that transform appropriately under the action of $\pi_1(\mathbf{C}\backslash\mathbf{a})$ by deck transformations. However, some later developments will be clearer for us if we can use functions with specific branching behavior as multipliers taking sections of $\mathcal{E}_\lambda$ to sections of the trivial bundle over $\mathbf{C}\backslash\mathbf{a}$. It will be easiest to be precise about this multiplier action if we define the bundles $\mathcal{E}_\lambda$ by giving transition functions, in spite of the fact that this is a little clumsy.

To begin, note that there are only a finite number of lines each of which consists of all multiples of $a_i - a_j$ for i and j distinct. Thus it is possible to choose a vector $\mathbf{r} \neq 0$ which is not contained in any of these lines. Then the rays, $\mathbf{r}_j$, defined by

$$\mathbf{r}_j = \{z : z = a_j + t\mathbf{r}, t > 0\},$$

do not intersect. Choose an argument $\theta_{\mathbf{r}}$ for $\mathbf{r}$ so that $\mathbf{r} = |\mathbf{r}| e^{i\theta_{\mathbf{r}}}$ with $|\theta_{\mathbf{r}}| \leqslant \pi$ and let $\theta(z)$ denote the polar angle with

$$\theta_{\mathbf{r}} - \pi < \theta(z) < \theta_{\mathbf{r}} + \pi, \quad z = |z| e^{i\theta(z)}.$$

This angle is branched along the ray $-\mathbf{r}$. For $\epsilon > 0$ define a tubular neighborhood, $\mathbf{t}_j(\epsilon)$, of $\mathbf{r}_j$ by

$$\mathbf{t}_j(\epsilon) = \{z : \mathrm{dist}(z, \mathbf{r}_j) < \epsilon\} \cap \left\{z : |\theta(z_j) - \theta_{\mathbf{r}}| < \frac{\pi}{4}\right\}.$$

Now choose $\epsilon > 0$ small enough so that the tubular neighborhoods $\mathbf{t}_j(\epsilon)$ are mutually disjoint *and* so that the disks,

$$D_j(2\epsilon) := \{z : |z - a_j| < 2\epsilon\},$$

are also mutually disjoint (this will be useful later on).

We now introduce a covering of $\mathbf{C}\backslash\mathbf{a}$ over each element of which the bundle $\mathcal{E}_\lambda$ is trivial. Let

$$\mathcal{U}_0 := \{z \in \mathbf{C}\backslash\mathbf{a} : z \notin r_j \text{ for } j = 1,2,\ldots,N\}.$$

Let

$$\mathcal{U}_j := \mathbf{t}_j(\epsilon) \quad \text{for } j=1,2,...,N.$$

Now we glue together the trivial bundles,

$$\mathcal{U}_k \times \mathbf{C} \to \mathcal{U}_k \quad \text{for } k=0,1,...,N,$$

by giving the transition functions s_j that define the bundle $\mathcal{E}_\lambda$. For $j=1,...,N$ define

$$s_j(z)=\begin{cases}\Lambda_j & \text{for } \theta(z_j)<0\\ 1 & \text{for } \theta(z_j)>0.\end{cases}$$

Then the bundle $\mathcal{E}_\lambda$ is defined by the following transition maps between vectors $(z,v)_0 \in \mathcal{U}_0 \times \mathbf{C}$ in the trivial bundle over $\mathcal{U}_0$ and vectors $(z,v)_j \in \mathcal{U}_j \times \mathbf{C}$ in the trivial bundle over $\mathcal{U}_j$ (for $k=1,2,...,N$),

$$(z,v)_0=(z,s_j(z)v)_j \quad \text{for } z \in \mathcal{U}_0 \cap \mathcal{U}_j.$$

The function $s_j(z)$ is smooth since it is constant on each of the two components of $\mathcal{U}_0 \cap \mathcal{U}_j$. The bundle that is relevant for the Ising model is the one with the choice $\Lambda_j=-1$ for all $j=1,2,...,N$. For simplicity we will denote this bundle by $\mathcal{E}$ with no subscript.

The rank 2 *vector* bundles that are more directly of interest to us are $\mathcal{E}_\lambda \otimes \mathbf{C}^2$ and $\mathcal{E} \otimes \mathbf{C}^2$, the direct sum of two copies of $\mathcal{E}_\lambda$ and $\mathcal{E}$, respectively. For simplicity we will use the same notation, $\mathcal{E}_\lambda$ and $\mathcal{E}$, to denote these vector bundles and when necessary make distinctions by referring to the *line bundles* $\mathcal{E}_\lambda$ and $\mathcal{E}$.

The differential operator $mI-\not\partial$ acts on $C^\infty(\mathcal{E}_\lambda)$, the space of smooth sections of the vector bundle $\mathcal{E}_\lambda$, since it commutes with multiplication by constants. We will now define a family of *local* smooth sections of $C^\infty(\mathcal{E}_\lambda)$ which are simultaneously solutions of the Dirac equation, $(mI-\not\partial)w=0$ and eigenfunctions for the infinitesimal rotation about a_j,

$$R_j=z_j\partial_j-\overline{z_j}\overline{\partial_j}+\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

which commutes with $mI-\not\partial$. We write $z_j=z-a_j$ and $\partial_j=\partial_{z_j}$. Note that this infinitesimal rotation has eigenvalues which are translated by $\pm\frac{1}{2}$ compared to the infinitesimal monodromy. Following SMJ we will parametrize our local wave functions by the R_j eigenvalue rather than the infinitesimal monodromy.

Let $\Theta(z)$ denote the angular coordinate at 0 defined so that for $z \notin \{t\mathbf{r}: t>0\}$ we have,

$$z=|z|e^{i\Theta(z)} \quad \text{with } \theta_{\mathbf{r}}<\Theta(z)<\theta_{\mathbf{r}}+2\pi.$$

For l a real number we define a function $w_l(z)$ for $z \in \mathbf{C}\backslash\mathbf{r}$ by

$$w_l^0(z)=\begin{pmatrix}e^{i(l-1/2)\Theta(z)} & I_{l-1/2}(m|z|)\\ e^{i(l+1/2)\Theta(z)} & I_{l+1/2}(m|z|)\end{pmatrix},$$

where I_k is the modified Bessel function of order k. For $z \in \mathbf{C}\backslash(-\mathbf{r})$ we define

$$w_l^\pi(z)=\begin{pmatrix}e^{i(l-1/2)\theta(z)} & I_{l-1/2}(m|z|)\\ e^{i(l+1/2)\theta(z)} & I_{l+1/2}(m|z|)\end{pmatrix}.$$

The only difference being, of course, the choice of angle. Where defined these are solutions to the Dirac equation $(mI-\not\partial)w=0$ and are eigenfunctions of the infinitesimal rotation $Rw_l=lw_l$ about 0.[6] Now let l denote a real number and define (for $|z_j|<2\epsilon$ say)

$$w_l(z_j) = w_l^0(z_j) \text{ in the } \mathcal{U}_0 \text{ trivialization,}$$

$$w_l(z_j) = w_l^{\pi}(z_j) \text{ in the } \mathcal{U}_j \text{ trivialization.}$$

Then it is easy to check that $w_l(z_j)$ is a *local* section of $C^\infty(\mathcal{E}_\lambda)$ provided $l \equiv \frac{1}{2} + \lambda_j \bmod \mathbf{Z}$. Now define a conjugation on $\mathbf{C}^2$ by

$$\begin{pmatrix} a \\ b \end{pmatrix}^* = \begin{pmatrix} \overline{b} \\ \overline{a} \end{pmatrix}.$$

This conjugation commutes with the Dirac operator $\not{\partial}$ and we define

$$w_l^*(z) = \begin{pmatrix} \overline{w}_{l,2}(z) \\ \overline{w}_{l,1}(z) \end{pmatrix}.$$

One can check that $w_l^*(z_j)$ is a local smooth section of $C^\infty(\mathcal{E}_\lambda)$ if and only if $l \equiv \frac{1}{2} - \lambda_j \bmod \mathbf{Z}$. It is a result of SMJ that every solution to $(mI - \not{\partial})w = 0$ in $C^\infty(\mathcal{E}_\lambda)$ has local expansions,

$$w(z) = \sum_{k \in \mathbf{Z}+1/2} a_k^j(w) w_{k+\lambda_j}(z_j) + b_k^j(w) u^*_{k-\lambda_j}(z_j), \tag{1}$$

valid for $0 < |z_j| < 2\epsilon$.[6,13] As the reader may check the coefficients $a_k^j(w)$ and $b_k^j(w)$ are simply related to Fourier coefficients in the expansion of the restriction of w to say the circle $|z_j| = \epsilon$. We will refer to these coefficients as local expansion coefficients.

For the Ising case $\lambda_j = \pm \frac{1}{2}$ and it is better not to use this form of the expansion (which would require a somewhat arbitrary choice of $\pm \frac{1}{2}$ at each a_j); instead we will just write

$$w(z) = \sum_{n \in \mathbf{Z}} \epsilon_n^j(w) w_n(z_j) + c_n^{j*}(w) w_n^*(z_j). \tag{2}$$

Note that we have changed the names of the local expansion coefficients in (2) to $c_n^j(w)$ and $c_n^{j*}(w)$ so that it coincides with the terminology in Ref. 6. Our way of writing (1) is different than the corresponding local expansions in Ref. 6 and so we have given different names to the local expansion coefficients.

Before we move on we will make one further observation about local expansions in a neighborhood of ∞. Suppose that $R > 0$ is big enough so that all the points a_j for $j = 1,2,...,N$ are inside the circle of radius R. Then $\{z : |z| > R\} \setminus \cup_j \mathbf{r}_j$ splits into N distinct components and the $\mathcal{U}_0$ trivialization is not very convenient for the description of sections of $\mathcal{E}$ over this set. In particular suppose that N is even. Then we can alternately flip the signs of sections supported in adjacent components of the $\mathcal{U}_0$ trivialization to produce a trivialization $\mathcal{U}_\infty$ for $\mathcal{E}$ over $\{z : |z| > R\}$. Actually the $\mathcal{U}_0$ trivialization is not defined over the rays $\mathbf{r}_j$ but because of the sign flips on adjacent components it is easy to see that $\mathcal{U}_\infty$ extends to a trivialization of $\mathcal{E}$ over the exterior of the disk of radius R. It is also clear that $\mathcal{U}_\infty$ is only determined itself up to an overall sign which we fix by declaring the $\mathcal{U}_\infty$ trivialization of the $\mathcal{U}_0$ section $\Pi_j (z - a_j)^{\epsilon_j}$ for $|\epsilon| = 0$ to be

$$\prod_j \left(1 - \frac{a_j}{z}\right)^{\epsilon_j} \quad \text{for } |z| > R,$$

where the fractional powers in this last product are the holomorphic functions of z normalized to be 1 at $z = \infty$.

It can be shown (Refs. 6 and 13) that sections $w \in L^2(\mathcal{E})$ which are solutions to the Dirac equation in the exterior of the disk of radius R have convergent expansions (in the $\mathcal{U}_\infty$ trivialization),

$$w(z)=\sum_{n\in\mathbf{Z}} c_n^{\infty}(w)\hat{w}_n(z), \tag{3}$$

where,

$$\hat{w}_u(z):=\begin{bmatrix} -e^{in\theta}K_n(m|z|) \\ e^{-i(n-1)\theta}K_{n-1}(m|z|)\end{bmatrix}.$$

The functions K_n are the modified Bessel functions that tend to zero at ∞. The reader should note that there is more than one definition of these functions (differing by a factor $e^{in\pi}$). We are using the version defined in Ref. 14. Also note that because n is an integer the choice of angle θ is irrelevant.

Now write $x\cdot y=x_1y_1+x_2y_2$ for the standard bilinear form on $\mathbf{C}^2$, so that $\overline{x}\cdot y$ is the standard Hermitian form. For $w, v\in C_0^{\infty}(\mathcal{E}_\lambda)$ define an inner product,

$$(w,v)=\frac{i}{2}\int_C \overline{w}\cdot v\ \mathrm{d}z\ \mathrm{d}\overline{z},$$

which is well defined since $\overline{w}(z)\cdot v(z)$ descends to a compactly supported function on $\mathbf{C}\backslash\mathbf{a}$. We will write $L^2(\mathcal{E}_\lambda)$ for the Hilbert space completion of $C_0^{\infty}(\mathcal{E}_\lambda)$ with respect to the norm induced by this inner product.

For the rest of this introduction we will specialize our considerations to the situation relevant to the Ising model. For n an integer we write,

$$w_n^R=\tfrac{1}{2}(w_n+w_n^*),\quad w_n^I=\frac{1}{2i}(w_n-w_n^*),$$

for the real and imaginary parts of w_n with respect to the conjugation $*$. Since $\Lambda_j=-1$ is real for all j it follows that $w_n^R(z_j)$ and $w_n^I(z_j)$ are local sections of $C^{\infty}(\mathcal{E})$. In Ref. 2 it is shown that for $j=1,2,...,N$ there exists a real solution $\mathcal{W}_j(\mathcal{W}_j^*=\mathcal{W}_j)$ to the Dirac equation,

$$(mI-\not{\partial})\mathcal{W}_j=0,$$

which is in $L^2(\mathcal{E})$ and which has leading order local expansions given by

$$\mathcal{W}_j(z)=\delta_{ij}w_0^I(z_i)+T_{ij}w_0^R(z_i)+\cdots \quad \text{for } i=1,2,...,N. \tag{4}$$

Note that the coefficients $w_n(z)$ are less and less locally singular at $z=0$ as n increases. The $+\cdots$ in (4) refer to terms with w_n and w_n^* for $n>0$. Also note that in (4) it is not necessary to specify what the coefficients T_{ij} are—they are already uniquely determined by the other conditions on $\mathcal{W}_j$.[2]

We are now ready to present the SMJ characterization of the Ising model scaling function from below T_c, $\tau_-(ma)=\tau_-(ma_1,ma_2,\ldots,ma_N)$. It is,

$$\mathrm{d}_a\log\tau_-(ma)=\frac{m}{2i}\sum_j c_1^j(\mathcal{W}_j)\mathrm{d}a_j-\overline{c_1^j(\mathcal{W}_i)}\mathrm{d}\overline{a_j}. \tag{5}$$

The reader might want to consult Ref. 15 or 2 for an explanation of what exactly τ_- is and how it is related to two-dimensional Ising correlations. Most of the rest of this paper will be devoted to understanding the solution $\mathcal{W}_j$ well enough in the limit $m\to 0$ so that we can compute the limiting values of the coefficients $mc_1^j(\mathcal{W}_j)$ which appear in (5). Our principal result is

Theorem 1 (Luther–Peschel Asymptotics): *Suppose that N is even. Then*

$$\lim_{m\to 0} \mathrm{d}_a \log \tau_-(ma) = \frac{1}{2}\mathrm{d}_a \log \sum_{|\epsilon|=0} \prod_{i<j} |a_i - a_j|^{2\epsilon_i\epsilon_j} \tag{6}$$

where the sum is over all choices of $\epsilon_k = \pm\frac{1}{2}$ *with*

$$|\epsilon| := \epsilon_1 + \epsilon_2 + \cdots + \epsilon_N = 0.$$

After the proof of this result we will indicate the changes that are needed to adapt the proof to the case where N is odd. We find for N odd,

$$\lim_{m\to 0} \mathrm{d}_a \log \tau_-(ma) = \frac{1}{2}\mathrm{d}_a \log \sum_{|\epsilon|=\pm 1/2} \prod_{i<j} |a_i - a_j|^{2\epsilon_i\epsilon_j}.$$

We will also indicate how to derive the short distance behavior of the correlations for holonomic fields.

Very briefly the rest of the paper is organized as follows. In Sec. II we characterize $\mathcal{W}_j$ as the solution to a boundary value problem on a finite domain. In Sec. III we introduce the Green function for the $m\to 0$ limit of this boundary value problem. In Sec. IV we introduce the associated boundary value projection. In Sec. V we discuss the inversion of a suitable restriction of this projection. In Sec. VI we discuss how to put these results together to give the perturbation scheme which we use to approximate $\mathcal{W}_j$ in the limit $m\to 0$. In Sec. VII we examine the application of the same technique to other problems.

II. AN EQUIVALENT BOUNDARY VALUE PROBLEM

The tool we will use in dealing with the $m\to 0$ limit of $\mathcal{W}_j$ is a characterization of $\mathcal{W}_j$ as the solution to an inhomogeneous boundary value problem. We will now describe this characterization. It is a result of SMJ[6] that the space of solutions $w \in C^\infty(\mathcal{E})$ to the Dirac equation,

$$(mI - \not{\partial})w = 0,$$

which are also in $L^2(\mathcal{E})$ is N dimensional. We write $\mathbf{N}$ for this space of solutions. For $w \in \mathbf{N}$ define

$$c_0(w) = (c_0^1(w), c_0^2(w), \ldots, c_0^N(w)) \in \mathbf{C}^N,$$

with a similar definition for $c_0^*(w)$. Now let $\mathcal{N}$ denote the image of $\mathbf{N}$ in $\mathbf{C}^N \oplus \mathbf{C}^N$ under the map,

$$\mathbf{N} \ni w \to (c_0(w), c_0^*(w)).$$

Suppose now that $\mathcal{I}$ is any subspace of $\mathbf{C}^N \oplus \mathbf{C}^N$ which is *transverse* to $\mathcal{N}$. If $f \in C_0^\infty(\mathcal{E})$ then in Ref. 2 it was proved that there exists a unique solution $w \in L^2(\mathcal{E})$ to

$$(mI - \not{\partial})w = f,$$

which satisfies the boundary condition $(c_0(w), c_0^*(w)) \in \mathcal{I}$. It was also shown there that the subspace $\mathcal{I}$ given by the set of vectors (v, v) for $v \in \mathbf{C}^N$ (the diagonal subspace) is transverse to $\mathcal{N}$. Henceforth we will work with the subspace $\mathcal{I}$ which corresponds to the boundary condition,

$$c_0(w) = c_0^*(w). \tag{7}$$

Now we will make a subtraction from $\mathcal{W}_j$ which will put the result in the subspace of sections of $\mathcal{E}$ satisfying (7). Let $\varphi(z)$ denote a non-negative function in $C_0^\infty(\mathbf{R}^2)$ which is identically 1 for $|z| < 1$ and identically 0 outside the ball of radius 2. Define,

$$\varphi_{j,\epsilon}(z)=\varphi\left(\frac{z-a_j}{\epsilon}\right).$$

Then since ϵ has been chosen small enough we know that $\varphi_{j,\epsilon}$ is one in a neighborhood of a_j and vanishes near a_i for all $i\neq j$. Now define

$$\delta\mathcal{W}_j(z)=m^{1/2}(\mathcal{W}_j(z)-\varphi_{j,\epsilon}(z)w_0^I(z-a_j)). \tag{8}$$

Then consulting (4) we see that if we look at the local expansion for $\delta\mathcal{W}_j$ in an ϵ neighborhood of a_j then the local expansion coefficients satisfy condition (7). The scale factor $m^{1/2}$ has been introduced so that the following limit exists:

$$\lim_{m\to 0} m^{1/2}w_0^I(z_j)=\frac{1}{\sqrt{2\pi i}}\begin{bmatrix} z_j^{-1/2} \\ -\overline{z_j}^{-1/2}\end{bmatrix}.$$

Here we used $\Gamma(\frac{1}{2})=\sqrt{\pi}$, the fractional powers of z_j and $\overline{z_j}$ that occur are branched along $z=\mathbf{r}_j$ and we employ the convention that the section w_0^I can be identified with its $\mathcal{U}_0$ trivialization (which appears on the right-hand side). Using the fact that both $\mathcal{W}_j$ and $w_0^I(z_j)$ satisfy the massive Dirac equation we find that

$$(m-\not{\partial})\,\delta\mathcal{W}_j=\begin{bmatrix} 0 & -2\partial\varphi_j \\ -2\overline{\partial}\varphi_j & 0\end{bmatrix}m^{1/2}w_0^I(z_j):=f_j. \tag{9}$$

We are now prepared to give an alternative characterization of $\delta\mathcal{W}_j$. Choose $R>0$ big enough so that $D_i(2\epsilon)$ is contained inside $|z|=R$ for $i=1,2,...,N$. Let $D_\infty=\{z:|z|\geqslant R\}$ and define the bounded domain, Ω, by

$$\Omega=\mathbf{C}\backslash\{\cup_{i=1}^n D_i(\epsilon)\cup D_\infty\}.$$

We write $H^k(\mathcal{E}_\Omega)$ for the Sobolev space of sections of $\mathcal{E}$ over Ω which are in $L^2(\Omega)$ together with all their weak derivatives up to and including those of order k.

Lemma 1: The smooth section $\delta\mathcal{W}_j$ of $\mathcal{E}_\Omega$ (the restriction of $\mathcal{E}$ to Ω) is uniquely characterized by the following three properties:

(1) *$\delta W_j\in H^1(\mathcal{E}_\Omega)$ satisfies the inhomogeneous Dirac equation (9) in Ω.*
(2) *For $i=1,2,...,N$ the local Fourier expansions (2) for $\delta\mathcal{W}_j$ restricted to $C_\epsilon(a_i)$ have coefficients $c_k^i(\delta\mathcal{W}_j)$ and $c_k^{i*}(\delta\mathcal{W}_j)$ that vanish for $k<0$ and are equal for $k=0$.*
(3) *The section $\delta\mathcal{W}_j$ has a Fourier expansion $\delta\mathcal{W}_j=\Sigma_{n\in\mathbf{Z}}c_n^\infty(\delta\mathcal{W}_j)\hat{w}_n(z)$, on the circle of radius R.*

Remark: Henceforth we interpret the local expansions (2) as the Fourier expansions of the restrictions of the $\mathcal{U}_0$ trivialization of $\delta\mathcal{W}_j$ to $|z_i|=\epsilon$ in powers $e^{i(n+1/2)\Theta_i}$ for $n\in\mathbf{Z}$. In a similar fashion we interpret (3) as the Fourier expansions of the $\mathcal{U}_\infty$ trivialization of $\delta\mathcal{W}_j$ restricted to the circle of radius R.

Proof of Lemma 1: Because the solution, $\delta\mathcal{W}_j$, of condition (1) of the Lemma is assumed to be in $H^1(\mathcal{E}_\Omega)$ it follows from local elliptic regularity that the solution is actually in $C^\infty(\mathcal{E}_\Omega)$. The support properties of the inhomogeneous term f_j makes it possible to enlarge each circle $C_\epsilon(a_i)$ to an annular region in which $\delta\mathcal{W}_j$ satisfies the homogeneous Dirac equation. In this region it will have a convergent local expansion of type (2). Since the Fourier coefficients $c_k^i(\delta\mathcal{W}_j)$ and $c_k^{i*}(\delta\mathcal{W}_j)$ [for the restriction of $\delta\mathcal{W}_j$ to $C_\epsilon(a_i)$] vanish for $k<0$ and are equal for $k=0$ it follows (by the uniqueness of Fourier expansions) that the same is true for the local expansion coefficients in the annulus. Since the Bessel functions $I_l(r)$ are monotone increasing functions of r for $l\geqslant 0$ this restriction on the local expansions implies that they converge in a domain $0<|z_i|<\epsilon'$, where

ϵ' is slightly bigger than ϵ (only a finite number of Fourier coefficients will get larger for smaller values of $|z_j|$). This shows that a solution, $\delta\mathcal{W}_j$, to (1) and (2) of the Lemma extends to a solution of the Dirac equation which is in L^2 near a_i and has appropriate restrictions on its local expansion coefficients. The same sort of argument shows that restriction (3) allows one to extend $\delta\mathcal{W}_j$ to an L^2 solution to the Dirac equation in a neighborhood of ∞. Q.E.D.

Without much difficulty the reader should be able to verify the following formula for the local expansion coefficients $mc_1^j(\mathcal{W}_j)$ that appear in the SMJ formula for the log derivative of the τ function:

$$mc_1^j(\mathcal{W}_j)=\frac{\sqrt{m}}{2\pi I_{1/2}(m\epsilon)}\int_{\theta_{\mathbf{r}}}^{\theta_{\mathbf{r}}+2\pi}(\delta\mathcal{W}_j)_1(\epsilon e^{i\Theta_j})\exp\left(-i\frac{\Theta_j}{2}\right)\mathrm{d}\Theta_j. \tag{10}$$

In this formula $(\delta\mathcal{W}_j)_1$ is the first component of $\delta\mathcal{W}_j$ in the $\mathcal{U}_0$ trivialization. The formula follows easily from the standard formula for Fourier coefficients and the fact that the subtraction of $\varphi_j w_0(z_j)$ does not alter the local expansion coefficients at level 1, so that $c_1^j(\delta\mathcal{W}_j)=\sqrt{m}c_1^j(\mathcal{W}_j)$.

Our strategy in controlling the $m\to 0$ limit of the coefficients $mc_1^j(\mathcal{W}_j)$ will be to use the characterization of Lemma 1 in conjunction with formula (10). Since

$$\lim_{m\to 0}\frac{\sqrt{m}}{I_{1/2}(m\epsilon)}=\sqrt{\frac{2}{\epsilon}}\Gamma\left(\frac{3}{2}\right)=\sqrt{\frac{\pi}{2\epsilon}},$$

it will suffice for our purposes to control the $m\to 0$ convergence of $\delta\mathcal{W}_j$ in $L^p(C_\epsilon(a_i))$ for any $p\geqslant 1$ and all i. Here $C_\epsilon(a_i)$ is the circle of radius ϵ about a_i.

Next we introduce convenient orthornormal bases for the subspaces that are of interest to us. Define

$$e_n^{(m)}(r,\Theta)=\begin{bmatrix}e^{i(n-1/2)\Theta}\alpha_n^{(m)}(mr)\\ e^{i(n+1/2)\Theta}\beta_n^{(m)}(mr)\end{bmatrix},$$

where

$$\alpha_n^{(m)}(mr)=\frac{I_{n-1/2}(mr)}{\sqrt{I_{n-1/2}^2(mr)+I_{n+1/2}^2(mr)}},\quad \beta_n^{(m)}(mr)=\frac{I_{n+1/2}(mr)}{\sqrt{I_{n-1/2}^2(mr)+I_{n+1/2}^2(mr)}}.$$

Also define $e_n^{(m)*}(r,\Theta)=\left[\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right]\overline{e_n^{(m)}}(r,\Theta)$. The collection

$$\{e_n^{(m)}(\epsilon,\Theta_j),e_n^{(m)*}(\epsilon,\Theta_j)\},$$

as n ranges over the integers is an orthonormal basis for $L^2(C_\epsilon(a_j))$ (with values in $\mathbf{C}^2$). Here we write

$$\Theta_j(z):=\Theta(z-a_j).$$

Definition 1: Let $W_j^{(m)}$ denote the subspace of $L^2(C_\epsilon(a_j))$ which is the L^2 closure of the span of $e_n^{(m)}(\epsilon,\Theta_j)$, and $e_n^{(m)*}(\epsilon,\Theta_j)$ for $n>0$ and the vector $e_0^{(m)}(\epsilon,\Theta_j)+e_0^{(m)*}(\epsilon,\Theta_j)$.

Define

$$\hat{e}_n^{(m)}(r,\theta)=\begin{bmatrix}e^{-in\theta}\alpha_n^{\infty}(mr)\\ e^{-i(n-1)\theta}\beta_n^{\infty}(mr)\end{bmatrix}$$

with

$$\alpha_n^{\infty}(mr)=\frac{-K_n(mr)}{\sqrt{K_{n-1}^2(mr)+K_n^2(mr)}},\quad \beta_n^{\infty}(mr)=\frac{K_{n-1}(mr)}{\sqrt{K_{n-1}^2(mr)+K_n^2(mr)}}.$$

Then $\{\hat{e}_n^{(m)}(R,\theta)\}$, where n ranges over the integers, is an orthonormal set in $L^2(C_R)$.

Definition 2: Let $W_{\infty}^{(m)}$ be the L^2 closure of the span of the $\hat{e}_n^{(m)}(R,\theta)$ for $n\in\mathbf{Z}$.

The boundary conditions (2) and (3) in Lemma 1 become

$$\delta\mathcal{W}_j|_{C_{\epsilon}(a_i)}\in W_i^{(m)},\quad \delta\mathcal{W}_j|_{C_R}\in W_{\infty}^{(m)}.$$

As a first step toward controlling the $m\to 0$ limit of the solution of the boundary value problem described in Lemma 1 we will now record some elementary estimates for the convergence of $e_n^{(m)}(r,\Theta)$ and $\hat{e}_n^{(m)}(r,\theta)$ to their limits as $m\to 0$. For $l>0$ the Bessel function $I_l(r)$ behaves like a constant times r^l as $r\to 0$. It immediately follows that (for $n\geqslant 1$),

$$\lim_{m\to 0}\alpha_n^{(m)}(mr)=1,\quad \lim_{m\to 0}\beta_n^{(m)}(mr)=0,$$

and hence that

$$\lim_{m\to 0}e_n^{(m)}(r,\Theta)=e_n(\Theta):=\begin{bmatrix}e^{i(n-1/2)\Theta}\\0\end{bmatrix}\quad \text{for } n\geqslant 1.$$

For similar reasons we find that

$$\lim_{m\to 0}\hat{e}_n^{(m)}(r,\theta)=\hat{e}_n(\theta):=\begin{bmatrix}-e^{-in\theta}\\0\end{bmatrix}\quad \text{for } n\geqslant 1,$$

and recalling that $K_n(r)=K_{-n}(r)$ we find

$$\lim_{m\to 0}\hat{e}_n^{(m)}(r,\theta)=\hat{e}_n(\theta):=\begin{bmatrix}0\\e^{-i(n-1)\theta}\end{bmatrix}\quad \text{for } n\geqslant 0.$$

For $l>0$, $I_l(r)$ is an increasing function of r and since $I_l'(r)=-(l/r)I_l(r)+I_{l-1}(r)$ the right-hand side is non-negative and hence

$$\frac{I_l(r)}{I_{l-1}}\leqslant\frac{r}{l}\quad \text{for } l>0. \tag{11}$$

For $n>0$, $K_n(r)$ is a decreasing function of r and since $K_n'(r)=(n/r)K_n(r)-K_{n+1}(r)$ the right-hand side is nonpositive and hence

$$\frac{K_n(r)}{K_{n+1}(r)}\leqslant\frac{r}{n}\quad \text{for } n>0. \tag{12}$$

Now suppose that $0<a<b$, then we have,

$$\frac{a}{\sqrt{a^2+b^2}}\leqslant\frac{a}{b}, \tag{13}$$

and

$$1\geqslant\frac{b}{\sqrt{b^2+a^2}}=\frac{1}{\sqrt{1+(a/b)^2}}\geqslant 1-\frac{1}{2}\left(\frac{a}{b}\right)^2. \tag{14}$$

Using Eqs. (11), (12), (13), and (14), we obtain the following estimates:

$$|\alpha_n^{(m)}(mr)-1| \leqslant \frac{1}{2}\left(\frac{I_{n+1/2}(mr)}{I_{n-1/2}(mr)}\right)^2 \leqslant \frac{1}{2}\left(\frac{mr}{n+1/2}\right)^2 \quad \text{for } n \geqslant 1, \tag{15}$$

$$|\beta_n^{(m)}(mr)| \leqslant \frac{I_{n+1/2}(mr)}{I_{n-1/2}(mr)} \leqslant \frac{mr}{n+1/2} \quad \text{for } n \geqslant 1, \tag{16}$$

and

$$|\alpha_n^{\infty}(mr)+1| \leqslant \frac{1}{2}\left(\frac{K_{n-1}(mr)}{K_n(mr)}\right)^2 \leqslant \frac{1}{2}\left(\frac{mr}{n-1}\right)^2 \quad \text{for } n \geqslant 2, \tag{17}$$

$$|\beta_n^{\infty}(mr)| \leqslant \frac{K_{n-1}(mr)}{K_n(mr)} \leqslant \frac{mr}{n-1} \quad \text{for } n \geqslant 2. \tag{18}$$

For $n \leqslant -1$ we also have

$$|\alpha_n^{\infty}(mr)| \leqslant \frac{K_{|n|}(mr)}{K_{|n|+1}(mr)} \leqslant \frac{mr}{|n|}, \tag{19}$$

and

$$|\beta_n^{\infty}(mr)-1| \leqslant \frac{1}{2}\left(\frac{K_{|n|}(mr)}{K_{|n|+1}(mr)}\right)^2 \leqslant \frac{1}{2}\left(\frac{mr}{|n|}\right)^2. \tag{20}$$

We will use these bounds in Sec. V to estimate the norm of a graph operator for the inversion of a certain projection. The n dependence in these bounds will be of use to us there. Note that estimates (17) and (18) obviously fail for $n=1$. However, the first part of those estimates still holds for $n=1$ and since

$$\frac{K_0(mr)}{K_1(mr)} \xrightarrow{m\to 0} 0,$$

it follows that $|\alpha_1^{\infty}(mr)+1|$ and $|\beta_1^{\infty}(mr)|$ both tend to 0 as $m\to 0$. For the same reason even though (19) and (20) are not valid for $n=0$ we still find that $|\alpha_0^{\infty}(mr)|$ and $|\beta_0^{\infty}(mr)-1|$ both tend to 0 as $m\to 0$.

We write

$$W^{(m)} := W_{\infty}^{(m)} \oplus W_1^{(m)} \oplus \cdots \oplus W_N^{(m)},$$

and $W^{(0)}$ for the $m\to 0$ limit of $W^{(m)}$. The estimates we have just given allow us to calculate the limiting behavior of the basis elements of $W^{(m)}$. This makes it natural to define

$$W_j^{(0)} = \mathrm{span}_{n\geqslant 1}\left\{\begin{bmatrix} e^{i(n-1/2)\Theta_j} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ e^{-i(n-1/2)\Theta_j} \end{bmatrix}\right\} \oplus C\begin{bmatrix} e^{-i\Theta_j/2} \\ e^{i\Theta_j/2} \end{bmatrix}, \tag{21}$$

for $j=1,\ldots,N$ and

$$W_{\infty}^{(0)} = \mathrm{span}_{n\geqslant 1}\left\{\begin{bmatrix} e^{-in\theta} \\ 0 \end{bmatrix}\right\} \oplus \mathrm{span}_{n\geqslant 1}\left\{\begin{bmatrix} 0 \\ e^{in\theta} \end{bmatrix}\right\}, \tag{22}$$

with

$$W^{(0)} := W_\infty^{(0)} \oplus W_1^{(0)} \oplus W_2^{(0)} \cdots \oplus W_N^{(0)}.$$

To be a little more precise we will write $W^{(0)}$ for the L^2 closure of the span of the basis vectors given previously [recall that $W^{(m)}$ was also a closed subspace of L^2].

We will always regard

$$W_j^{(0)} \subset L^2(\mathcal{E}_{C_\epsilon(a_j)}), \quad W_\infty^{(0)} \subset L^2(\mathcal{E}_{C_R}),$$

so that $W^{(0)} \subset L^2(\mathcal{E}_{\partial\Omega})$. Notice that the basis elements of the subspaces $W_j^{(0)}$ can be regarded as *smooth* sections of $\mathcal{E}_{C_\epsilon(a_j)}$ in the $\mathcal{U}_0$ trivialization. Similarly the basis elements of $W_\infty^{(0)}$ can be regarded as *smooth* sections of $\mathcal{E}_{C_R}$ in the $\mathcal{U}_\infty$ trivialization. We will do this henceforth and it will make a difference for us when we look at the subspaces of $W^{(0)}$ obtained by taking the closure of the span of the same basis elements in the Sobolev spaces $W^{1/2,p}(\mathcal{E}_{\partial\Omega})$.

III. THE $m=0$ GREEN FUNCTION

The Green function we want to understand has the following matrix kernel:

$$G_0(z,z') = -\frac{1}{4\pi i}\begin{bmatrix} \Sigma_j u_j(z)\overline{v_j(z')} & g(z,z') \\ \overline{g(z,z')} & \Sigma_j \overline{u_j(z)} v_j(z') \end{bmatrix}, \tag{23}$$

where

$$u_j(z) := (z-a_j)^{-1/2} \prod_{k\neq j} \frac{(z-a_k)^{1/2}}{(a_j-a_k)^{1/2}}, \tag{24}$$

$$g(z,z') := \sum_{|\epsilon|=0} c(\epsilon) \frac{\Pi_j (z-a_j)^{\epsilon_j} (z'-a_j)^{-\epsilon_j}}{z'-z}, \tag{25}$$

with $\epsilon = (\epsilon_1, \ldots, \epsilon_n)$ and each $\epsilon_j = \pm \frac{1}{2}$. Also

$$|\epsilon| := \sum_{j=1}^{N} \epsilon_j, \quad c(\epsilon) := \frac{\Pi_{j<k} |a_j - a_k|^{2\epsilon_j \epsilon_k}}{\Sigma_{|\epsilon|=0} \Pi_{j<k} |a_j - a_k|^{2\epsilon_j \epsilon_k}}, \tag{26}$$

and

$$v_j(z) = (z-a_j)^{-1/2} \sum_{|\epsilon|=0, \epsilon_j = 1/2} c(\epsilon) \prod_{k\neq j} \frac{(z-a_k)^{\epsilon_k}}{(a_j-a_k)^{\epsilon_k}}. \tag{27}$$

The multivalued functions $(z-a_j)^{\epsilon_j}$ are all defined using the argument Θ_j and are consequently branched along $z \in \mathbf{r}_j$. We regard $G_0(z,z')$ as defining an operator, G_0, acting on sections of $\mathcal{E}_\Omega$ in the following manner:

$$G_0 f(z) := \int_\Omega G_0(z,z') f(z') \mathrm{d}z' \, \mathrm{d}\overline{z'}, \tag{28}$$

where the section $f(z')$ is identified with its $\mathcal{U}_0$ trivialization. We also regard $G_0 f$ as a section of $\mathcal{E}_\Omega$ given in the $\mathcal{U}_0$ trivialization.

When working with $G_0 f(z)$ for $|z| > R$ it is useful to rewrite $v_j(z)$ and $g(z,z')$ in terms appropriate for the $\mathcal{U}_\infty$ trivialization. The conversion from the $\mathcal{U}_0$ to the $\mathcal{U}_\infty$ trivialization is given as follows:

$$\prod_k (z-a_k)^{\epsilon_k} \to \prod_k \left(1-\frac{a_k}{z}\right)^{\epsilon_k} \quad \text{for } |\epsilon|=0 \text{ and } |z|>R,$$

where the fractional powers on the right are holomorphic functions of z normalized to be 1 at $z=\infty$. In a similar fashion,

$$v_j(z) \to z^{-1}\left(1-\frac{a_j}{z}\right)^{-1/2} \sum_{|\epsilon|=0,\epsilon_j=1/2} c(\epsilon) \prod_{k\neq j} \frac{\left(1-\frac{a_k}{z}\right)^{\epsilon_k}}{(a_j-a_k)^{\epsilon_k}} \quad \text{for } |z|>R. \tag{29}$$

Our goal in this section is to show that G_0 inverts $-\not{\partial}$ with $W^{(0)}$ boundary conditions. It is precisely this property that determines our interest in G_0. We will at the same time establish some elementary but useful estimates.

It is helpful to recall some well-known results for the kernel $1/(z'-z)$. Let $f \in C^1(\overline{\Omega})$ (the continuously differentiable functions on Ω which are continuous together with their derivative on the closure of Ω) and define

$$Tf(z) := \frac{1}{2\pi i} \int_\Omega \frac{f(z')}{z'-z} \mathrm{d}z' \, \mathrm{d}\overline{z'}. \tag{30}$$

Then

Theorem 2: *The distribution derivative of Tf is*

$$\mathrm{d}T\, f = T(\partial_z f)\mathrm{d}z + f\, \mathrm{d}\overline{z}. \tag{31}$$

For $p>2$ one has the estimate,

$$\|Tf\|_{W^{1,p}(\Omega)} \leqslant C_p \|f\|_{W^{1,p}(\Omega)}, \tag{32}$$

for a constant C_p that depends only on p and Ω, and $W^{k,p}(\Omega)$ is the subspace of $L^p(\Omega)$ which consists of functions whose first k weak derivatives are in $L^p(\Omega)$.

Proof: Suppose $f \in C^1(\overline{\Omega})$ and $\phi \in C_0^\infty(\Omega)$. To compute the distribution derivative $\partial_z Tf(z)$ we wish to ''integrate by parts'' in

$$-\int_\Omega Tf(z)\partial_z \phi(z) \mathrm{d}z \, \mathrm{d}\overline{z}.$$

To stay away from the singularity in the kernel we introduce

$$T_\epsilon f(z) := \frac{1}{2\pi i} \int_{\Omega \setminus D_\epsilon(z)} \frac{f(z')}{z'-z} \mathrm{d}z' \, \mathrm{d}\overline{z'},$$

where $D_\epsilon(z)=\{z' : |z'-z|<\epsilon\}$. Also suppose for simplicity that ϵ is chosen small enough so that the distance from the support of ϕ to the boundary of Ω is greater than ϵ. For ϵ this small it follows that for all z in the support of ϕ the set of z' with $|z-z'|=\epsilon$ is completely contained in Ω.

In order to do the ''integration by parts'' efficiently we calculate the exterior derivative of a particular three form on the domain $\Omega \times \Omega \setminus \{z=z'\}$,

$$\mathrm{d}\left(\frac{f(z')\phi(z)-f(z)\phi(z')}{z'-z}\right)\mathrm{d}\overline{z}\,\mathrm{d}z'\,\mathrm{d}\overline{z'}$$
$$=\left(\frac{f(z')\partial\phi(z)-\partial f(z)\phi(z')}{z'-z}+\frac{f(z')\phi(z)-f(z)\phi(z')}{(z'-z)^2}\right)\mathrm{d}z\,\mathrm{d}\overline{z}\,\mathrm{d}z'\,\mathrm{d}\overline{z'}.$$

Now integrate this last identity over

$$(\Omega\times\Omega)_\epsilon:=\Omega\times\Omega\backslash\{(z,z'):|z'-z|<\epsilon\},$$

and use Stokes' theorem. Then make use of

$$\int_{(\Omega\times\Omega)_\epsilon}\frac{f(z')\phi(z)-f(z)\phi(z')}{(z'-z)^2}\mathrm{d}z\,\mathrm{d}\overline{z}\,\mathrm{d}z'\,\mathrm{d}\overline{z'}=0,$$

which follows from the fact that the integrand is odd under the transformation $(z,z')\to(z',z)$ and the domain $(\Omega\times\Omega)_\epsilon$ is invariant under this map. After multiplication by $1/2\pi i$ the resulting identity simplifies directly to,

$$-\int_\Omega T_\epsilon f(z)\partial_z\phi(z)\mathrm{d}z\,\mathrm{d}\overline{z}=\int_\Omega T_\epsilon(\partial f)(z)\phi(z)\mathrm{d}z\,\mathrm{d}\overline{z}$$
$$+\frac{1}{2\pi i}\int_\Omega \mathrm{d}z'\,\mathrm{d}\overline{z'}\int_{|z-z'|=\epsilon}\frac{f(z')\phi(z)-f(z)\phi(z')}{z'-z}\mathrm{d}\overline{z}.$$

Since both f and ϕ are $C^1(\Omega)$ it is easy to see that the second term on the right-hand side of this last equation tends to 0 in the limit $\epsilon\to0$. Because $1/(z'-z)$ is in $L^1_{\mathrm{loc}}(\mathbf{C}^2)$ it follows that $T_\epsilon f\to Tf$ in the sense of distributions as $\epsilon\to0$. Hence,

$$\partial Tf=T\partial f,$$

which is the first part of (31). To obtain the second part consider the exterior derivative,

$$\mathrm{d}\left(\frac{f(z')\phi(z)}{z'-z}\right)\mathrm{d}z\,\mathrm{d}z'\,\mathrm{d}\overline{z'}=-\overline{\partial}_z\left(\frac{f(z')\phi(z)}{z'-z}\right)\mathrm{d}z\,\mathrm{d}\overline{z}\,\mathrm{d}z'\,\mathrm{d}\overline{z'}=-\left(\frac{f(z')\overline{\partial}\phi(z)}{z'-z}\right)\mathrm{d}z\,\mathrm{d}\overline{z}\,\mathrm{d}z'\mathrm{d}\overline{z'}.$$

Integrate this over $(\Omega\times\Omega)_\epsilon$ and multiply the result by $1/2\pi i$. Using Stokes' theorem again, one finds that

$$-\int_\Omega T_\epsilon f(z)\overline{\partial}\phi(z)\mathrm{d}z\,\mathrm{d}\overline{z}=-\frac{1}{2\pi i}\int_\Omega \mathrm{d}z'\,\mathrm{d}\overline{z'}\int_{|z-z'|=\epsilon}\frac{f(z')\phi(z)}{z'-z}\mathrm{d}z.$$

As $\epsilon\to0$ the right-hand side tends to

$$\int_\Omega \mathrm{d}z'\,\mathrm{d}\overline{z'}\,f(z')\phi(z').$$

Hence,

$$\overline{\partial}Tf=f,$$

which is the second part of (31).

To prove the second part of the theorem we first observe that since Ω is a bounded domain it is straightforward to show that T defines a bounded operator on $L^p(\Omega)$ for $p>2$. Hölder's inequality implies that

$$\left| \int_\Omega \frac{f(z')}{z'-z} i\, dz'\, d\overline{z'} \right| \leqslant \|f\|_{L^p(\Omega)} \left(\int_\Omega |z'-z|^{-q} i\, dz'\, d\overline{z'} \right)^{1/q},$$

where $1/p+1/q=1$. However since $p>2$ it follows that $1<q<2$ and hence that

$$z \to \int_\Omega |z'-z|^{-q} i dz'\, d\overline{z'}$$

is a bounded function on Ω. It follows at once that T is bounded on $L^p(\Omega)$ since Ω is a finite domain and bounded functions are in $L^p(\Omega)$ [note: the analogue of T on $\Omega=\mathbf{C}$ is also bounded on $L^p(\mathbf{C})$ for $p>2$ (see Ref. 16)].

To see that it defines a bounded operator on $W^{1,p}(\Omega)$ for $p>2$ it is enough to use (31), which implies that for $f \in C^1(\overline{\Omega})$,

$$\|dT\, f\|_{D^p(\Omega)} \leqslant \|T\partial f\|_{L^p(\Omega)} + \|f\|_{L^p(\Omega)} \leqslant C\|f\|_{W^{1,p}(\Omega)} \quad \text{for } p>2,$$

where we used the fact that T is bounded on L^p $(p>2)$. Since the boundary of Ω is smooth, $C^1(\overline{\Omega})$ is dense in $W^{1,p}(\Omega)$, and the second part of the theorem is proved. QED

We will now use theorem 2 to establish that G_0 is a Green function for $-\not\partial$ on $W^{1,p}(\mathcal{E}_\Omega)$ for $p>2$. Incidentally, we work in the space $W^{1,p}(\mathcal{E}_\Omega)$ only in order to simplify some boundary estimates by using the Sobolev trace theorems; we could work in $L^p(\mathcal{E}_\Omega)$ at the cost of using more complicated global ellipticity estimates (see Ref. 17).

Theorem 3: *Suppose $p>2$ and suppose that $f \in W^{1,p}(\mathcal{E}_\Omega)$ and that f is compactly supported in Ω. Then $G_0 f \in W^{1,p}(\mathcal{E}_\Omega)$ and*

(1) $\|G_0 f\|_{W^{1,p}} \leqslant C_p \|f\|_{W^{1,p}}$,
(2) $-\not\partial G_0 f = f$,
(3) $G_0 f|_{\partial\Omega} \in W^{(0)}$.

Proof: Let $z_j^\epsilon = (z-a_j)^\epsilon$ be defined using the argument Θ_j so that these functions are branched along $\mathbf{r}_j$. For any choice $\boldsymbol{\epsilon}_j = \pm 1/2$ the function,

$$\mathbf{z}^{\boldsymbol{\epsilon}} := \prod_{j=1}^{N} z_j^{\boldsymbol{\epsilon}_j},$$

defines a map,

$$C^\infty(\mathcal{E}_\Omega) \ni f(z) \to \mathbf{z}^{\boldsymbol{\epsilon}} f(z) \in C^\infty(\Omega),$$

which has an inverse,

$$C^\infty(\Omega) \ni f(z) \to \mathbf{z}^{-\boldsymbol{\epsilon}} f(z) \in C^\infty(\mathcal{E}_\Omega),$$

where in each case sections of $C^\infty(\mathcal{E}_\Omega)$ are identified with their $\mathcal{U}_0$ trivializations. Since the derivatives of $\mathbf{z}^{\pm\boldsymbol{\epsilon}}$ are bounded on Ω it follows that these maps induce bounded maps,

$$W^{1,p}(\mathcal{E}_\Omega) \ni f(z) \to \mathbf{z}^{\boldsymbol{\epsilon}} f(z) \in W^{1,p}(\Omega)$$

and

$$W_{1,p}(\Omega) \ni f(z) \to \mathbf{z}^{-\boldsymbol{\epsilon}} f(z) \in W^{1,p}(\mathcal{E}_\Omega).$$

The upper right matrix element of the kernel $G_0(z',z)$ is a linear combination of terms,

$$\frac{\mathbf{z}^{\epsilon}(\mathbf{z}')^{-\epsilon}}{z'-z},$$

each of which is the kernel of an operator we can interpret as a composition,

$$W^{1,p}(\mathcal{E}_\Omega) \xrightarrow{\mathbf{z}^{-\epsilon}} W^{1,p}(\Omega)^{1/(z'-z)} W^{1,p}(\Omega) \xrightarrow{\mathbf{z}^{\epsilon}} W^{1,p}(\mathcal{E}_\Omega),$$

which is bounded for $p>2$ as a consequence of Theorem 2. To be more precise we note that it is the *line bundle* $\mathcal{E}_\Omega$ which appears in this composition. The same argument for $\overline{\mathbf{z}}^{\pm c}$ and $1/(\overline{z'}-\overline{z})$ coupled with the complex conjugate version of Theorem 2 shows that the lower left kernel in $G_0(z,z')$ determines a bounded linear transformation on $W^{1,p}(\mathcal{E}_\Omega)$. The diagonal elements of $G_0(z,z')$ are finite rank L^2 kernels with a range that consists of smooth sections of $\mathcal{E}_\Omega$. Consequently, they determine bounded operators on $W^{1,p}(\mathcal{E}_\Omega)$ as well and this finishes the proof of part (1) of the theorem.

The proof of part (2) of the theorem is a straightforward computation using (1) of Theorem 2 (and its complex conjugate), the fact that $\overline{\partial}_z \mathbf{z}^{\epsilon}=0$, $\partial \overline{\mathbf{z}}^{\epsilon}=0$, $\overline{\partial}_z u_j(z)=0$, $\partial_z \overline{u}_j(z)=0$, and finally,

$$\sum_{|\epsilon|=0} c(\epsilon)=1.$$

Note that both $\overline{\partial}$ and ∂ act on $C^\infty(\mathcal{E}_\Omega)$ since the transition functions that define the bundle are piecewise constant.

To establish part (3) of the theorem it is useful to observe that the subspace $W_j^{(0)}$ consists of L^2 boundary values on $C_\epsilon(a_j)$, of functions,

$$\begin{bmatrix} z_j^{1/2} h_1(z) \\ z_j^{1/2} \overline{h_2}(z) \end{bmatrix} + c_0 \begin{bmatrix} z_j^{-1/2} \\ \overline{z_j}^{1/2} \end{bmatrix},$$

where h_1 and h_2 are holomorphic functions on the disk $D_\epsilon(a_j)$ and c_0 is a complex constant (technically, h_1 and h_2 should be in the appropriate Hardy space). We wish to show that

$$\int_\Omega G_0(z,z') f(z') \mathrm{d}z' \, \mathrm{d}\overline{z'},$$

restricted to $z \in C_\epsilon(a_j)$, lies in $W_j^{(0)}$. Because we have assumed that the support of f is contained inside Ω it follows that for z' in the support of f we have $|z'-a_j|>|z-a_j|$ and so

$$\frac{1}{z'-z} = \frac{1}{z_j'-z_j} = \sum_{n=0}^{\infty} \frac{1}{z_j'} \left(\frac{z_j}{z_j'} \right)^n$$

will converge uniformly for $z \in D_\epsilon(a_j)$ and z' in the support of f. Substituting this expansion in the formula for $G_0 f(z)$ (and the analogue obtained by taking complex conjugates) one sees easily that the boundary value of $G_0 f(z)$ has the form,

$$\begin{bmatrix} z_j^{-1/2} h_1(z) \\ \overline{z_j}^{-1/2} \overline{h_2}(z) \end{bmatrix},$$

where h_1 and h_2 are holomorphic in $D_\epsilon(a_j)$. The only issue is whether the coefficient of $z_j^{-1/2}$ in the first component is the same as the coefficient of $\overline{z_j}^{-1/2}$ in the second component. A computation shows that the coefficient of $z_j^{-1/2}$ in the Fourier expansion on $C_\epsilon(a_j)$ of the first component of $G_0 f$ is

$$-\frac{1}{4\pi i}\int_\Omega dz'\,d\overline{z}'\left\{\overline{v_j}(z')f_1(z')+\sum_{|\epsilon|=0,\epsilon_j=1/2}c(\epsilon)z_j'^{-1/2}\prod_{k\neq j}\frac{(z'-a_k)^{\epsilon_k}}{(a_j-a_k)^{\epsilon_k}}f_2(z')\right\},$$

where we used the fact that

$$\sum_{|\epsilon|=0,\epsilon_j=-1/2}S(\epsilon)=\sum_{|\epsilon|=0,\epsilon_j=1/2}S(-\epsilon).$$

Computing the coefficient of $\overline{z}_j^{-1/2}$ in the Fourier expansion of the second component of G_0f we find

$$-\frac{1}{4\pi i}\int_\Omega dz'\,d\overline{z}'\left\{v_j(z')f_2(z')+\sum_{|\epsilon|=0,\epsilon_j=1/2}c(\epsilon)\overline{z}_j'^{-1/2}\prod_{k\neq j}\frac{\overline{(z'-a_k)^{\epsilon_k}}}{\overline{(a_j-a_k)^{\epsilon_k}}}f_1(z')\right\}.$$

Comparing these two coefficients using the definition of $v_j(z)$ we see that they are the same. Thus $G_0f|_{C_\epsilon(a_j)}\in W_j^{(0)}$.

To finish the proof we need to show that

$$G_0f|_{C_R}\in W_\infty^{(0)}.$$

Recalling the definition of $W_\infty^{(0)}$ we see that it consists of boundary values on C_R of functions,

$$\begin{bmatrix}h_1(z)\\ \overline{h_2}(z)\end{bmatrix},$$

where $h_1(z)$ and $h_2(z)$ are holomorphic functions on D_∞ which vanish at $z=\infty$. The condition $|\epsilon|=0$ in the sum that defines $g(z,z')$ makes it easy to see that

$$\int_\Omega g(z,z')f_2(z')dz'\,d\overline{z}'$$

is holomorphic for $z\in D_\infty$ and tends to 0 at ∞. For precisely the same reason,

$$\int_\Omega \overline{g(z,z')}f_1(z')dz'\,d\overline{z}'$$

is antiholomorphic in D_∞ and vanishes at ∞. The diagonal contributions,

$$-\frac{1}{4\pi i}\int_\Omega\sum_j u_j(z)\overline{v_j}(z')f_1(z')dz'\,d\overline{z}',$$

and

$$-\frac{1}{4\pi i}\int_\Omega\sum_j \overline{u_j}(z)v_j(z')f_2(z')dz'\,d\overline{z}',$$

do not at first appear to vanish at infinity since $u_j(z)$ does not tend to 0 at ∞. However in the lemma which follows this theorem we will prove the homogeneous function identity,

$$\sum_j u_j(z)\overline{v_j}(z')=\sum_j v_j(z)\overline{u_j}(z'). \tag{33}$$

Since $v_j(z)$ is holomorphic for $|z|>R$ and does tend to 0 at ∞ [see (29)] this identity finishes the proof of the theorem. Q.E.D.

We turn to the proof of the identity (33).

Lemma 2: The following identity is true for the functions u_j and v_j defined in (24) *and* (27),

$$\sum_j u_j(z)\overline{v_j}(z')=\sum_j v_j(z)\overline{u_j}(z').$$

Proof: Suppose that $v(z)$ is a holomorphic function branched along the rays $\mathbf{r}_j$ such that

$$V(z)=v(z)\prod_k z_k^{-1/2}$$

is holomorphic in the punctured plane, $\mathbf{C}\backslash\mathbf{a}$, with simple poles at each a_j and which tends to 0 as $z\to\infty$ (this will be the case for each of the functions v_j). Then $V(z)$ has the partial fraction decomposition,

$$V(z)=\sum_k \frac{V_k}{z-a_k},$$

where $V_k=\mathrm{Res}_{z=a_k}V(z)$. Rewriting this in terms of $v(z)$ one finds

$$v(z)=\sum_k V_k z_k^{-1/2}\prod_{l\neq k} z_l^{1/2}=\sum_k V_k\prod_{l\neq k}(a_k-a_l)^{1/2}u_k(z).$$

Thus we have,

$$v_j(z)=\sum_k v_{kj}u_k(z),$$

where the coefficients v_{kj} are found by residue calculation to be

$$v_{jj}=\sum_{|\epsilon|=0,\epsilon_j=1/2} c(\epsilon),$$

and for $k\neq j$,

$$v_{kj}=\frac{(a_k-a_j)^{1/2}}{(a_j-a_k)^{1/2}}\sum_{\substack{|\epsilon|=0\\ \epsilon_j=1/2,\epsilon_k=-1/2}} c(\epsilon)\prod_{l\neq j,k}\frac{(a_k-a_l)^{\epsilon_l}}{(a_j-a_l)^{\epsilon_l}}. \tag{34}$$

We will now show that $v_{kj}=\overline{v_{jk}}$, which will have (33) as a simple consequence. Since v_{jj} is real it is clear that $v_{jj}=\overline{v_{jj}}$. Now suppose that $k\neq j$ and note that

$$\frac{(a_k-a_j)^{1/2}}{(a_j-a_k)^{1/2}}=\frac{\overline{(a_j-a_k)^{1/2}}}{\overline{(a_k-a_j)^{1/2}}},$$

since cross multiplication produces the identity

$$|a_k-a_j|=|a_j-a_k|.$$

Thus the first factor in (34) is Hermitian symmetric and it remains only to check that the second factor is also. First we rewrite $c(\epsilon)$ for $\epsilon_j=\frac{1}{2}$ and $\epsilon_k=-\frac{1}{2}$ in the following manner:

$$c(\epsilon)_{\epsilon_k=-1/2}^{\epsilon_j=1/2}=\frac{|a_j-a_k|^{-1/2}}{\mathbf{c}}\prod_{\substack{\alpha<\beta\\ \alpha,\beta\notin\{j,k\}}}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta}\prod_{l\neq j,k}\frac{|a_j-a_l|^{\epsilon_l}}{|a_k-a_l|^{\epsilon_l}},$$

where $\mathbf{c}:=\sum_{\alpha<\beta}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta}$. Now define,

$$s_{kj}(\epsilon)=\frac{|a_j-a_k|^{-1/2}}{\mathbf{c}}\prod_{\substack{\alpha<\beta\\ \alpha,\beta\notin\{j,k\}}}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta}.$$

The second factor in (34) becomes

$$\sum_{\substack{|\epsilon|=0\\ \epsilon_j=1/2,\epsilon_k=-1/2}} s_{kj}(\epsilon)\prod_{l\neq j,k}\frac{|a_j-a_l|^{\epsilon_l}(a_k-a_l)^{\epsilon_l}}{|a_k-a_l|^{\epsilon_l}(a_j-a_l)^{\epsilon_l}}.$$

Since $s_{kj}(\epsilon)$ is real and obviously equal to $s_{jk}(\epsilon)$ this last expression will be Hermitian symmetric provided that

$$\prod_{l\neq j,k}\frac{|a_j-a_l|^{\epsilon_l}}{|a_k-a_l|^{\epsilon_l}}\frac{(a_k-a_l)^{\epsilon_l}}{(a_j-a_l)^{\epsilon_l}}=\prod_{l\neq j,k}\frac{|a_k-a_l|^{\epsilon_l}}{|a_j-a_l|^{\epsilon_l}}\frac{\overline{(a_j-a_l)^{\epsilon_l}}}{\overline{(a_k-a_l)^{\epsilon_l}}}.$$

But this follows directly from cross multiplication as before. We have shown that $v_{kj}=\overline{v}_{jk}$ and the following simple calculation now proves the identity (33):

$$\sum_j u_j(z)\overline{v}_j(z')=\sum_{j,k}u_j(z)\overline{v}_{kj}\overline{u}_k(z')=\sum_{j,k}v_{jk}u_j(z)\overline{u}_k(z')=\sum_k v_k(z)\overline{u}_k(z').$$

Q.E.D.

IV. THE PROJECTION ON $W^{(0)}$

In this section we will introduce the projection P_0 from $L^2(\mathcal{E}_{\partial\Omega})$ onto $W^{(0)}$ which is naturally associated with the Green function G_0. Another goal is a description of the complementary subspace for P_0 acting on $H^{1/2}(\mathcal{E}_{\partial\Omega})$. We will show that the complementary projection $I-P_0$ projects $H^{1/2}(\mathcal{E}_{\partial\Omega})$ onto the boundary values of sections $\Psi\in H^1(\mathcal{E}_\Omega)$ which are solutions to the Dirac equation, $\not{\partial}\Psi=0$ in Ω.

It is useful to start with a calculation. Write

$$G_0(z,z')=\begin{bmatrix}G_{11}(z,z') & G_{12}(z,z')\\ G_{21}(z,z') & G_{22}(z,z')\end{bmatrix},$$

for the matrix elements of G_0.

Now suppose that $f\in C^1(\mathcal{E}_{\overline{\Omega}})$ and choose $z\in\mathbf{C}\backslash\overline{\Omega}$. Then,

$$\begin{aligned}-G_0(\not{\partial}f)(z)&=-2\int_\Omega\begin{bmatrix}G_{11}(z,z')\partial_{z'}f_2(z')+G_{12}(z,z')\overline{\partial}_{z'}f_1(z')\\ G_{21}(z,z')\partial_{z'}f_2(z')+G_{22}(z,z')\overline{\partial}_{z'}f_1(z')\end{bmatrix}\mathrm{d}z'\,\mathrm{d}\overline{z}'\\ &=-2\int_\Omega d_{z'}\begin{bmatrix}G_{11}(z,z')f_2(z')\mathrm{d}\overline{z}'-G_{12}(z,z')f_1(z')\mathrm{d}z'\\ G_{21}(z,z')f_2(z')\mathrm{d}\overline{z}'-G_{22}(z,z')f_1(z')\mathrm{d}z'\end{bmatrix},\end{aligned}$$

which Stokes' theorem transforms into

$$-G_0(\not{\partial}f)(z)=-2\int_{\partial\Omega}\begin{bmatrix}G_{11}(z,z')f_2(z')\mathrm{d}\overline{z}'-G_{12}(z,z')f_1(z')\mathrm{d}z'\\ G_{21}(z,z')f_2(z')\mathrm{d}\overline{z}'-G_{22}(z,z')f_1(z')\mathrm{d}z'\end{bmatrix}.$$

The first equality follows from the fact that $G_{k2}(z,z')$ is holomorphic for $z' \in \Omega$ and $G_{k1}(z,z')$ is antiholomorphic in $z' \in \Omega$ (remember z is outside of Ω). Of course, this is not precisely accurate since these functions are branched along the rays $\mathbf{r}_j$. However, it is not hard to argue that the application of Stokes' theorem is still correct using the fact that $G_{k2}(z,z')f_1(z')$ and $G_{k1}(z,z')f_2(z')$ are continuous for z' on the rays $\mathbf{r}_j$. Also note that the orientation of $\partial\Omega$ appropriate for this Stokes' calculation is that C_R has the usual counterclockwise orientation and the circles $C_\epsilon(a_j)$ are all *clockwise oriented*. With this as our motivation, we define, for $f \in L^2(\mathcal{E}_{\partial\Omega})$,

$$P_0 f(z) := -2\int_{\partial\Omega}\begin{bmatrix} G_{11}(z,z')f_2(z')d\overline{z}' - G_{12}(z,z')f_1(z')dz' \\ G_{21}(z,z')f_2(z')d\overline{z}' - G_{22}(z,z')f_1(z')dz' \end{bmatrix}, \tag{35}$$

where we understand this as a section of $\mathcal{E}_{\partial\Omega}$ by letting $z \to \partial\Omega$ from outside of Ω. As usual sections of $\mathcal{E}$ are identified with their $\mathcal{U}_0$ or $\mathcal{U}_\infty$ trivializations. If $-\partial f$ is compactly supported in Ω we saw in the last section that the restriction of $-G_0\partial f$ to $\partial\Omega$ is in $W^{(0)}$. Thus (35) suggests that if $f|_{\partial\Omega} \in W^{(0)}$, we should have $P_0 f = f$. Our first result in this section is,

Theorem 4: *The map P_0 defined by* (35) *is a projection from $L^2(\mathcal{E}_{\partial\Omega})$ onto $W^{(0)}$. P_0 restricts to a continuous map,*

$$P_0 : H^{1/2}(\mathcal{E}_{\partial\Omega}) \to H^{1/2}(\mathcal{E}_{\partial\Omega}).$$

Proof: We will show that P_0 maps $L^2(\mathcal{E}_{\partial\Omega})$ into $W^{(0)}$. Observe first that the functions, f, in $L^2(\mathcal{E}_{C_\epsilon(a_j)})$, which are restrictions to $z \in C_\epsilon(a_j)$ of the type

$$f(z) = \sum_{n=-L}^{L}\begin{bmatrix} f_{1n} z_j^{n+1/2} \\ f_{2n}\overline{z}_j^{n+1/2} \end{bmatrix}, \tag{36}$$

for L finite, are dense in $L^2(\mathcal{E}_{C_\epsilon(a_j)})$, and have extensions to $\mathbf{C}\backslash\mathbf{r}_j$ which are solutions to $\partial f = 0$. If φ is a C_0^∞ function which is 1 for $|z| \leqslant 1.5\epsilon$ and 0 for $|z| > 2\epsilon$ and f is a function of type (36) then it is easy to see that $\varphi_j f(z) := \varphi(z_j) f(z)$ is a section of $\mathcal{E}_\Omega$ and $\partial(\varphi_j f)$ is compactly supported inside Ω. For such a function the calculation that we began this section with shows that

$$-G_0\partial(\varphi_j f)|_{\partial\Omega} = P_0 f,$$

and it follows from Theorem 3 that $P_0 f \in W^{(0)}$. The first part of the theorem now follows from the fact that $W^{(0)}$ is closed in $L^2(\mathcal{E}_{\partial\Omega})$ and P_0 is continuous on L^2. We won't bother to give the proof that P_0 is continuous on L^2 since the argument we now present to show that P_0 is continuous on $H^{1/2}(\mathcal{E}_{\partial\Omega})$ adapts directly to show L^2 continuity.

Observe first that the finite rank part of P_0 associated with the kernels G_{11} and G_{22} has a range which is a subset of $C^\infty(\mathcal{E}_{\partial\Omega}) \subset H^{1/2}(\mathcal{E}_{\partial\Omega})$ and is clearly continuous in L^2 and hence also in $H^{1/2}$. Next consider the part of P_0 associated with G_{12}. The component of this operator which maps $H^{1/2}(\mathcal{E}_{C_\epsilon(a_j)})$ into $H^{1/2}(\mathcal{E}_{C_\epsilon(a_k)})$ can be written as a sum of operators each of which has a factorization of the following sort:

$$H^{1/2}(\mathcal{E}_{C_\epsilon(a_j)}) \xrightarrow{z_j^{1/2}} H^{1/2}(C_\epsilon(a_j)) \xrightarrow{\phi(z)} H^{1/2}(C_\epsilon(a_j))$$

$$\xrightarrow{1/(z'-z)} H^{1/2}(C_\epsilon(a_k)) \xrightarrow{\psi(z)} H^{1/2}(C_\epsilon(a_k)) \xrightarrow{z_k^{1/2}} H^{1/2}(\mathcal{E}_{C_\epsilon(a_k)})),$$

where the first, second, fourth, and fifth maps are multiplication operators and the third map is

$$f(z)\to\frac{1}{2\pi i}\int_{C_\epsilon(a_j)}\frac{f(z')}{z'-z}\,dz', \tag{37}$$

which must be interpreted as a suitable boundary value when $j=k$. In this factorization $\phi(z)$ and $\psi(z)$ are smooth functions and hence determine bounded maps on $H^{1/2}$. The Cauchy projection (37) is easily seen to be continuous from $H^{1/2}(C_\epsilon(a_j))$ to $H^{1/2}(C_\epsilon(a_k))$ even when $j=k$. Nothing changes if C_R is one or both of the two components of $\partial\Omega$ that are involved and it follows that the part of P_0 associated with G_{12} is bounded on $H^{1/2}(\mathcal{E}_{\partial\Omega})$. The kernel G_{21} is just the complex conjugate of G_{12} and so it too defines a bounded operator on $H^{1/2}(\mathcal{E}_{\partial\Omega})$. This completes the proof that P_0 is continuous on $H^{1/2}(\mathcal{E}_{\partial\Omega})$.

To finish the proof of the theorem we need to show that if $f\in W^{(0)}$ then $P_0 f=f$. Clearly it is enough to show this for the basis elements (21) and (22). For the calculation on $W_j^{(0)}$ it is preferable to use the alternate forms for G_{11} and G_{22} found in Lemma 2. Thus (35) becomes

$$P_0 f(z)=\frac{1}{2\pi i}\int_{\partial\Omega}\left[\begin{array}{c}\Sigma_k\, v_k(z)\overline{u_k}(z')f_2(z')d\overline{z'}-g(z,z')f_1(z')dz' \\ g(z,z')f_2(z')d\overline{z'}-\Sigma_k\overline{v_k}(z)u_k(z')f_1(z')dz'\end{array}\right]. \tag{38}$$

The following residue calculations suffice to evaluate P_0 on the basis elements of $W_j^{(0)}$ [note that in these results $C_\epsilon(a_j)$ is counterclockwise oriented, as usual],

$$\frac{1}{2\pi i}\int_{C_\epsilon(a_j)}u_k(z)z_j^{n-1/2}dz=\delta_{jk}\delta_{n0}\quad\text{for } n=0,1,2,\ldots.$$

And for $n=0,1,2,\ldots$,

$$\frac{1}{2\pi i}\int_{C_\epsilon(a_j)}\sum_{|\epsilon|=0}c(\epsilon)\frac{\Pi_k z_k^{\epsilon_k}(z_k')^{-\epsilon_k}}{z'-z}(z')^{n-1/2}dz'=\begin{cases}z_j^{n-1/2}-\delta_{n0}v_j(z) & \text{for } z\in C_\epsilon(a_j)\\ -\delta_{n0}v_j(z) & \text{for } z\in\partial\Omega\backslash C_\epsilon(a_j).\end{cases}$$

One finds [being careful to recall the orientation of the $C_\epsilon(a_j)$ component of $\partial\Omega$ is clockwise] that P_0 fixes the elements of the basis for $W_j^{(0)}$. The reader might find the cancellation of the $v_j(z)$ terms that appear in the calculation of the action of P_0 on $\left[\begin{smallmatrix}z_j^{-1/2}\\ z_j^{-1/2}\end{smallmatrix}\right]$ instructive.

To compute the action of P_0 on the basis elements for $W_\infty^{(0)}$ the original form for the kernel of the Green function G_0 is preferable and one can do the needed calculation with the following residues:

$$\frac{1}{2\pi i}\int_{C_R}v_k(z)z^{-n}\,dz=0\quad\text{for } n=1,2,3,\ldots,$$

which follows from the fact that $v_k(z)$ is holomorphic in the exterior of C_R and vanishes at ∞ in the $\mathcal{U}_\infty$ trivialization. And for $n=1,2,3,\ldots$,

$$\frac{1}{2\pi i}\int_{C_R}\sum_{|\epsilon|=0}c(\epsilon)\frac{\Pi_k z_k^{\epsilon_k}(z_k')^{-\epsilon_k}}{z'-z}(z')^{-n}\,dz'=\begin{cases}z^{-n} & \text{for } z\in C_R\\ 0 & \text{for } z\in\partial\Omega\backslash C_R.\end{cases}$$

Again one finds that P_0 fixes the basis (22) and this finishes the proof of the theorem. Q.E.D.

Next we turn to a characterization of the complementary projection $I-P_0$.

Theorem 5: *The projection $I-P_0$ maps $H^{1/2}(\mathcal{E}_{\partial\Omega})$ into the subspace of $H^{1/2}(\mathcal{E}_{\partial\Omega})$ which consists of boundary values of functions $\Psi\in H^1(\mathcal{E}_\Omega)$ which satisfy the Dirac equation*

$$\not{\partial}\Psi=0$$

in Ω. *Furthermore, there exists a constant C so that for all* $f \in H^{1/2}(\mathcal{E}_{\partial\Omega})$ *we have*

$$\|(I-P_0)f\|_{H^1(\mathcal{E}_\Omega)} \leqslant C\|f\|_{H^{1/2}(\mathcal{E}_{\partial\Omega})}. \tag{39}$$

Proof: Using (38) and the well-known identity,

$$(z'-z_{\text{int}})^{-1}-(z'-z_{\text{ext}})^{-1}=2\pi i\,\delta(z'-z),$$

for the difference of the interior and exterior boundary values of the Cauchy kernel on a circle we find the following formula for $P_0^c := I-P_0$,

$$P_0^c f(z) = -\frac{1}{2\pi i}\int_{\partial\Omega}\left[\frac{\Sigma_k v_k(z)\tilde{u}_k(z')f_2(z')\mathrm{d}\overline{z'}-g(z,z')f_1(z')\mathrm{d}z'}{g(z,z')f_2(z')\mathrm{d}\overline{z'}-\Sigma_k\ \overline{v_k}(z)u_k(z')f_1(z')\mathrm{d}z'}\right], \tag{40}$$

with the difference compared to (38) being that in this formula z tends to $\partial\Omega$ from the interior of Ω. It is clear from this formula that $(I-P_0)f(z)$ extends to a section of $\mathcal{E}_\Omega$ which is in the null space of $\not{\partial}$. We need only establish the estimate (39) to finish the proof. The finite rank operator,

$$f \to \frac{1}{2\pi i}\int_{\partial\Omega}\sum_k\ v_k(z)\overline{u_k}(zx')f(z')\mathrm{d}\overline{z'},$$

is obviously continuous on $H^{1/2}(\mathcal{E}_{\partial\Omega})$ since each u_k is in L^2 and the functions $v_k \in C^\infty(\mathcal{E}_\Omega)\subset H^1(\mathcal{E}_\Omega)$. The other finite rank operator that occurs in (40) is continuous from $H^{1/2}(\mathcal{E}_{\partial\Omega})$ into $H^1(\mathcal{E}_\Omega)$ for the same reason. Next we turn to the operator,

$$f \to \frac{1}{2\pi i}\int_{\partial\Omega} g(z,z')f(z')\mathrm{d}z'.$$

This operator is a linear combination of operators each of which we wish to interpret as a composition,

$$H^{1/2}(\mathcal{E}_{\partial\Omega}) \xrightarrow{\mathbf{z}^{-\epsilon}} H^{1/2}(\partial\Omega) \xrightarrow{1/(z'-z)} H^1(\Omega) \xrightarrow{\mathbf{z}^{\epsilon}} H^1(\mathcal{E}_\Omega).$$

The first and third maps are multiplication operators which are obviously continuous. The middle map is shorthand for the operator,

$$f \to \frac{1}{2\pi i}\int_{\partial\Omega}\frac{f(z')}{z'-z}\mathrm{d}z',$$

which is well known to be continuous from $H^{1/2}(\partial\Omega)$ to $H^1(\Omega)$. For the reader's convenience we recall a simple argument for this continuity.

Write $z_j = z-a_j$ and consider a function, f, defined on $\partial\Omega$ by

$$f(z)=\begin{cases}\Sigma_{n=-L}^{L} f_n z_j^n & \text{for } z\in C_c(a_j)\\ 0 & \text{for } z\in\partial\Omega\backslash C_\epsilon(a_j)\end{cases}. \tag{41}$$

Define $P_{\text{int}}f(z)$ for z in Ω by

$$P_{\text{int}}f(z)=\frac{1}{2\pi i}\int_\Omega\frac{f(z')}{z'-z}\mathrm{d}z'.$$

Then

$$P_{\text{int}}f(z)=\sum_{n=-L}^{-1} f_n z_j^n .$$

Since Ω is bounded the Poincaré inequality[18] implies that the $H^1(\Omega)$ norm of $P_{\text{int}}f$ is bounded by the $L^2(\Omega)$ norm of

$$\partial P_{\text{int}}f(z)=\sum_{n=-L}^{-1} n f_n z_j^{n-1}.$$

The $L^2(\Omega)$ norm of $\partial P_{\text{int}}f$ is in turn dominated by the L^2 norm of $\partial P_{\text{int}}f$ on $|z_j|\geqslant\epsilon$. To compute this norm it suffices to observe that (for n, $m=-1,-2,...$),

$$\int_{|z_j|\geqslant\epsilon} z_j^{n-1}\overline{z_j}^{m-1} i\,dz\,d\overline{z}=\int_{|z_j|\geqslant\epsilon} d\left(\frac{z_j^n\overline{z_j}^{m-1}}{n} i\,d\overline{z}\right)=-\frac{1}{n}\int_{C_\epsilon(a_j)} z_j^n\overline{z_j}^{m-1} i\,d\overline{z}=\frac{2\pi}{|n|}\epsilon^{2n}\delta_{nm}.$$

We then see that

$$\|P_{\text{int}}f\|^2_{H^1(\Omega)}\leqslant C\sum_{n=-L}^{-1}\epsilon^{2n}|n|f_n\overline{f_n}\leqslant C\|f\|^2_{H^{-1/2}(C_\epsilon(a_j))}.$$

Now suppose that

$$f(z)=\begin{cases}\displaystyle\sum_{n=-L}^{L} f_n z^n & \text{for } z\in C_R\\ 0 & \text{for } z\in\partial\Omega\backslash C_R .\end{cases} \tag{42}$$

Then the argument we just gave is easily modified to show that

$$\|P_{\text{int}}f\|_{H^1(\Omega)}\leqslant C\|f\|_{H^{1/2}(C_R)}.$$

Sums of functions of type (41) for $j=1,2,...,N$ and type (42) are dense in $H^{1/2}(\partial\Omega)$ and it follows that P_{int} extends to a continuous map from $H^{1/2}(\partial\Omega)$ to $H^1(\Omega)$.[19]

Taking complex conjugates the result we just proved also shows that the map,

$$f\to-\frac{1}{2\pi i}\int_{\partial\Omega}\overline{g(z,z')}f(z')d\overline{z}',$$

is bounded from $H^{1/2}(\mathcal{E}_{\partial\Omega})$ to $H^1(\mathcal{E}_\Omega)$. This finishes the proof of the theorem. QED

V. INVERTING THE PROJECTION $P_0: W^{(m)}\to W^{(0)}$

Remark: In this section we will write $W^{(m)}$ for $W^{(m)}\cap H^{1/2}(\mathcal{E}_{\partial\Omega})$ and $W^{(0)}$ for $W^{(0)}\cap H^{1/2}(\mathcal{E}_{\partial\Omega})$. We will prove the following theorem.

Theorem 6: *For all sufficiently small values of m the projection*

$$P_0: W^{(m)}\to W^{(0)}$$

is an isomorphism. Furthermore, there is a linear map δ from $W^{(0)}$ into $(I-P_0)H^{1/2}(\mathcal{E}_{\partial\Omega})$ and a constant C which is independent of f and m so that for all $f\in W^{(0)}$,

(1) $f+\delta f\in W^{(m)}$,

(2) $\|\delta f\|_{H^{1/2}(\mathcal{E}_{\partial\Omega})} \leqslant Cm\|f\|_{H^{1/2}_{(\mathcal{E}_{\partial\Omega})}}$.

Remark: The map δ gives $W^{(m)}$ as a graph over $W^{(0)}$.

Proof: Suppose first that $f \in W^{(m)}$ and let f_j denote the restriction of f to $C_\epsilon(a_j)$ and let f_∞ denote the restriction of f to C_R. Write $e^{(m)}_{n,j}$ for $e^{(m)}_n(\epsilon,\Theta_j)$ and $\hat{e}^{(m)}_{n,\infty}$ for $\hat{e}^{(m)}_n(R,\theta)$. Then the Fourier expansions of f on $C_\epsilon(a_j)$ and C_R can be written,

$$f_j = a_{0,j}(e^{(m)}_{0,j} + e^{(m)}_{0,j}*) + \sum_{n=1}^{\infty} \{a_{n,j}e^{(m)}_{n,j} + b_{n,j}e^{(m)}_{n,j}*\} \tag{43}$$

and

$$f_\infty = \sum_{n=-\infty}^{\infty} a_{n,\infty}\hat{e}^{(m)}_{n,\infty}. \tag{44}$$

Now let $p_0 f$ denote the element of $W^{(0)}$ which has the same "Fourier coefficients" in the $m \to 0$ limiting basis. That is,

$$p_0 f_j = a_{0,j}(e_{0,j} + e^*_{0,j}) + \sum_{n=1}^{\infty} \{a_{n,j}e_{n,j} + b_{n,j}e^*_{n,j}\} \tag{45}$$

and

$$p_0 f_\infty = \sum_{n=-\infty}^{\infty} a_{n,\infty}\hat{e}_{n,\infty}, \tag{46}$$

where $e_{n,j}$ denotes the basis vector $e_n(\Theta_j)$ and $\hat{e}_{n,\infty}$ denotes the vector $\hat{e}_n(\theta)$. It is easy to check that

$$\langle e^{(m)}_{k,j} - e_{k,j}, e^{(m)}_{l,j} - e_{l,j}\rangle_{H^{1/2}(\mathcal{E}_{\partial\Omega})} = \delta_{kl}\|e^{(m)}_{k,j} - e_{k,j}\|^2_{H^{1/2}(\mathcal{E}_{\partial\Omega})},$$

and from (15) and (16) it follows that

$$\|e^{(m)}_{k,j} - e_{k,j}\|_{H^{1/2}(\mathcal{E}_{\partial\Omega})} \leqslant Cm.$$

Analogous results for $e^{(m)}_{k,j}*$ and for $\hat{e}^{(m)}_k$ [which follow from (17) and (18)] imply the inequality

$$\|p_0 f - f\|_{H^{1/2}(\mathcal{E}_{\partial\Omega})} \leqslant Cm\|f\|_{H^{1/2}(\mathcal{E}_{\partial\Omega})}, \tag{47}$$

for some constant C and all $f \in W^{(m)}$. Now write $\Delta p_0 = p_0 - I$. Then for $f \in W^{(m)}$ we have

$$f + \Delta p_0 f \in W^{(0)}.$$

It follows from this that

$$(I - P_0)(f + \Delta p_0 f) = 0,$$

or

$$(I - P_0)f = -(1 - P_0)\Delta p_0 f.$$

From this, (47), and the fact that P_0 is bounded on $H^{1/2}(\mathcal{E}_{\partial\Omega})$ it follows that

$$\|f - P_0 f\|_{H^{1/2}(\mathcal{E}_{\partial\Omega})} \leqslant Cm\|f\|_{H^{1/2}(\mathcal{E}_{\partial\Omega})},$$

for some constant C and all $f \in W^{(m)}$. When m is small enough so that $Cm<1$ this last inequality implies that $P_0: W^{(m)} \to W^{(0)}$ is injective since $P_0 f = 0$ gives $\|f\| \leqslant Cm\|f\|$ with $Cm<1$, which in turn forces $\|f\|=0$.

Now start with $f_0 \in W^{(0)}$ with Fourier expansion given by (45) and (46) and define $p_m f_0 \in W^{(m)}$ to be the element of $W^{(m)}$ with the Fourier expansion (43) and (44). Then the same estimates we gave previously imply that for $f_0 \in W^{(0)}$ we have

$$\|\Delta p_m f_0\|_{H^{1/2}(\mathcal{E}_{\partial\Omega})} \leqslant Cm\|f_0\|_{H^{1/2}(\mathcal{E}_{\partial\Omega})},$$

for $\Delta p_m := p_m - I$ and some constant C. Now choose m small enough so that the map,

$$P_0 + P_0 \Delta p_m : W^{(0)} \to W^{(0)},$$

is invertible. Define

$$g_0 := (P_0 + P_0 \Delta p_m)^{-1} f_0.$$

Then one can easily check that

$$g_0 + \Delta p_m g_0 \in W^{(m)}$$

and

$$P_0(g_0 + \Delta p_m g_0) = f_0.$$

This shows that $P_0: W^{(m)} \to W^{(0)}$ is subjective. Furthermore if we define

$$\delta = (I - P_0)\Delta p_m (P_0 + P_0 \Delta p_m)^{-1}$$

as a map from $W^{(0)}$ to $(I-P_0)H^{1/2}(\mathcal{E}_{\partial\Omega})$, then it is easy to check that $f_0 + \delta f_0 \in W^{(m)}$ and δ satisfies the estimate (2) of the theorem. Q.E.D.

VI. CONVERGENCE RESULTS

In this section we provide the details for the approximation scheme for $\delta \mathcal{W}_j$ that was outlined in Ref. 2. Let f_j denote the section of $\mathcal{E}_\Omega$ defined in (9). As a first approximation to $\delta \mathcal{W}_j$ we define

$$\delta_1 \mathcal{W}_j = G_0(1 + mG_0)^{-1} f_j. \tag{48}$$

We will show that for all sufficiently small m, $\delta_1 \mathcal{W}_j$ is well defined and

$$(m - \not{\partial})\, \delta_1 \mathcal{W}_j = f_j, \tag{49}$$

with $\delta_1 \mathcal{W}_{j|_{\partial\Omega}} \in W^{(0)}$. Thus $\delta_1 \mathcal{W}_j$ satisfies the same differential equation as $\delta \mathcal{W}_j$ but has boundary values in $W^{(0)}$ instead of $W^{(m)}$. Next we define

$$\delta_2 \mathcal{W}_j = \delta(\delta_1 \mathcal{W}_1). \tag{50}$$

Then the boundary values of $\delta_1 \mathcal{W}_j + \delta_2 \mathcal{W}_j$ are in $W^{(m)}$ but since $\not{\partial}\delta_2 \mathcal{W}_j = 0$ on Ω we find that

$$(m - \not{\partial})(\delta_1 \mathcal{W}_j + \delta_2 \mathcal{W}_j) = f_j + m\delta_2 \mathcal{W}_j.$$

Now let $\delta_3 \mathcal{W}_j$ denote the solution of

$$(m - \not{\partial})\, \delta_3 \mathcal{W}_j = -m\delta_2 \mathcal{W}_j, \tag{51}$$

such that $\delta_3 \mathcal{W}_{j|_{\partial\Omega}} \in W^{(m)}$. The solution we are interested in is then

$$\delta\mathcal{W}_j=\delta_1\mathcal{W}_j+\delta_2\mathcal{W}_j+\delta_3\mathcal{W}_j\,.$$

The following theorem gives convergence results that will allow us to calculate (10) in the limit $m\to 0$. We write f_{0j} for the $m\to 0$ limit of f_j,

$$f_{0j}(z)=i\sqrt{\frac{2}{\pi}}\begin{bmatrix}-\overline{z_j}^{1/2}\partial\varphi_j(z)\\ z_j^{-1/2}\overline{\partial}\varphi_j(z)\end{bmatrix}. \tag{52}$$

Theorem 7: *For $\delta_k\mathcal{W}_j$ defined previously $(k=1,2,3)$ we have,*
(1) *As $m\to 0$, $\delta_1\mathcal{W}_j$ converges to G_0f_{0j} in $W^{1,p}(\mathcal{E}_\Omega)$ for all $p>2$.*
(2) *$\|\delta_2\mathcal{W}_j\|_{H^1(\mathcal{E}_\Omega)}\leqslant Cm$ for some constant C independent of m.*
(3) *The Fourier coefficient,*

$$\int_{\theta_{\mathbf{r}}}^{\theta_{\mathbf{r}}+2\pi}(\delta_3\mathcal{W}_j)_1(\epsilon e^{i\Theta_j})\exp\left(-i\frac{\Theta_j}{2}\right)\mathrm{d}\Theta_j\,, \tag{53}$$

tends to 0 *as* $m\to 0$.

Remark: As we shall see in the following, the upshot of these estimates is that we can compute the $m\to 0$ limit of $mc_1^j(\mathcal{W}_j)$ by calculating the appropriate Fourier coefficient of G_0f_{0j}. Also in the course of proving (1)–(3) of theorem 7 we will confirm the properties asserted for $\delta_k\mathcal{W}_j$, $k=1,2,3$, when they were introduced above.

Proof: Estimate 1 of theorem 3 shows that for $p>2$, G_0 is bounded on $W^{1,p}(\mathcal{E}_\Omega)$. Thus for small enough m, the map $I+mG_0$ is invertible on $W^{1,p}(\mathcal{E}_\Omega)$. Since it is clear that $f_j\in C_0^\infty(\mathcal{E}_\Omega)\subset W^{1,p}(\mathcal{E}_\Omega)$ it follows that $\delta_1\mathcal{W}_j\in W^{1,p}(\mathcal{E}_\Omega)$ for $p>2$. Since $\delta_1\mathcal{W}_j$ is in the image of G_0, part (3) of theorem 3 implies that the boundary value of $\delta_1\mathcal{W}_j$ on $\partial\Omega$ is in $W^{(0)}$. We use part (2) of theorem 3 to do the following calculation:

$$\begin{aligned}(m-\not{\partial})G_0(I+mG_0)^{-1}f_j&=mG_0(I+mG_0)^{-1}f_j+(I+mG_0)^{-1}f_j\\&=(mG_0+I)(I+mG_0)^{-1}f_j=f_j\,,\end{aligned}$$

which confirms (49). Since G_0 is bounded on $W^{1,p}(\mathcal{E}_\Omega)$ the operator $(I+mG_0)^{-1}$ converges uniformly to I on $W^{1,p}(\mathcal{E}_\Omega)$ as $m\to 0$. Thus to finish the proof of 1 we need only show that for all $p>2$ the section f_j converges in $W^{1,p}(\mathcal{E}_\Omega)$ to f_{0j}. Using (9) one finds

$$f_j=i\sqrt{m}\begin{bmatrix}\exp\left(i\frac{\Theta_j}{2}\right)(I_{1/2}(mr)-I_{-1/2}(mr))\partial\varphi_j(z)\\ \exp\left(-i\frac{\theta_j}{2}\right)(I_{-1/2}(mr)-I_{1/2}(mr))\overline{\partial}\varphi_j(z)\end{bmatrix}. \tag{54}$$

The simple estimate,

$$I_{\pm 1/2}(mr)=\left(\frac{mr}{2}\right)^{\pm 1/2}\sum_{n=0}^{\infty}\frac{(mr)^{2n}}{2^{2n}n!\Gamma(n\mp 1/2)}\leqslant\left(\frac{mr}{2}\right)^{\pm 1/2}\frac{\exp\left(\frac{2m\epsilon}{2}\right)^2}{\Gamma(3/2)},$$

which is valid for $r<2\epsilon$ (which contains the support of $\partial\varphi_j$ and $\overline{\partial}\varphi_j$) shows that dominated convergence applies to

$$\lim_{m\to 0}\int_\Omega|f_j-f_{0j}|^p i\,\mathrm{d}z\,\mathrm{d}\overline{z}=0,$$

for all $p \geqslant 1$. The same estimate shows that dominated convergence applies to the $m \to 0$ limit of the integral,

$$\int_\Omega |\mathrm{d}f_j - \mathrm{d}f_{0j}|^p i \, \mathrm{dz} \, \mathrm{d}\bar{z}$$

and this proves that f_j converges to f_{0j} in $W^{1,p}(\mathcal{E}_\Omega)$. Now fix $p > 2$. Since f_j converges in $W^{1,p}(\mathcal{E}_\Omega)$ as $m \to 0$ it follows that its norm in this space is uniformly bounded. Hence the $W^{1,p}$ norm of $\delta_1 \mathcal{W}_j$ is also uniformly bounded. However since the domain Ω is bounded the $W^{1,p}(\mathcal{E}_\Omega)$ norm for $p > 2$ dominates (a constant times) the $H^1(\mathcal{E}_\Omega)$ norm. This shows that $\delta_1 \mathcal{W}_j$ is uniformly bounded in $H^1(\mathcal{E}_\Omega)$ as $m \to 0$. The Sobolev trace theorem[18] implies that the boundary value of $\delta_1 \mathcal{W}_j$ is uniformly bounded in $H^{1/2}(\mathcal{E}_{\partial\Omega})$ and estimate 2 of theorem 6 then shows that $\delta_2 \mathcal{W}_j = \delta(\delta_1 \mathcal{W}_j)$ has norm in $H^{1/2}(\mathcal{E}_\Omega)$ bounded by Cm. Finally estimate (39) shows that the extension of $\delta_2 \mathcal{W}_j$ to Ω has $H^1(\mathcal{E}_\Omega)$ norm dominated by Cm, which is estimate (2) of theorem 7.

Before we turn to the proof of part (3) of theorem 7 it will be useful to establish the following estimates for solutions to the massive Dirac equation.

Theorem 8: *Suppose that $\Psi \in L^2(\mathcal{E}_\Omega)$ is a weak solution to the Dirac equation,*

$$(m - \not{\partial})\Psi = f,$$

in Ω, where $f \in C_0^\infty(\mathcal{E}_\Omega)$. Suppose that $\Psi|_{\partial\Omega} \in W^{(m)}$ so that for $z \in C_\epsilon(a_j)$ the section Ψ has the local expansion

$$\Psi(z) = \sum_{n \geqslant 0} c_n^j(\Psi) w_n(z_j) + c_n^j(\Psi) w_n^*(z_j),$$

with $c_0^j(\Psi) = c_0^{j*}(\Psi)$, and for $z \in C_R$ the section Ψ has the local expansion

$$\Psi(z) = \sum_{n \in \mathbf{Z}} c_n^\infty(\Psi) \hat{w}_n(z).$$

Then,

$$\|\Psi\|_{L^2(\mathcal{E}_\Omega)} \leqslant \frac{1}{m} \|f\|_{L^2(\mathcal{E}_\Omega)}, \tag{55}$$

$$\sum_j |c_0^j(\Psi)|^2 \leqslant \frac{1}{8} \|f\|^2_{L^2(\mathcal{E}_\Omega)}, \tag{56}$$

$$4\pi \sum_{n \geqslant 0} \{|c_n^j(\Psi)|^2 + |c_n^{j*}(\Psi)|^2\} I_{n+1/2}(m\epsilon) I_{n-1/2}(m\epsilon) \epsilon \leqslant \frac{1}{m} \|f\|^2_{L^2(\mathcal{E}_\Omega)}, \tag{57}$$

$$4\pi \sum_{n \in \mathbf{Z}} |c_n^\infty(\Psi)|^2 K_n(mR) K_{n-1}(mR) R \leqslant \frac{1}{m} \|f\|^2_{L^2(\mathcal{E}_\Omega)}. \tag{58}$$

Proof: Since $f \in C_0^\infty(\mathcal{E}_\Omega)$, the existence theorem in Ref. 2 then gives us a weak solution $\Psi \in L^2(\mathcal{E}_\Omega)$ of

$$(m - \not{\partial})\Psi = f,$$

which is smooth as a consequence of local elliptic regularity. Next we calculate the exterior derivative of $2i\bar{\Psi}_1 \Psi_2 \mathrm{d}\bar{z}$ using the fact that Ψ satisfies the Dirac equation,

$$d(2i\overline{\Psi}_1\Psi_2\,d\overline{z}) = m|\Psi|^2 i\,dz\,d\overline{z} - (\overline{\Psi}_1 f_1 + \Psi_2 \overline{f}_2) i\,dz\,d\overline{z}.$$

Integrating this equality over Ω and using Stokes' theorem we find

$$m\|\Psi\|^2_{L^2(\mathcal{E}_\Omega)} - 2i\int_{\partial\Omega}\overline{\Psi}_1\Psi_2\,d\overline{z} = \int_\Omega (\overline{\Psi}_1 f_1 + \Psi_2\overline{f}_2) i\,dz\,d\overline{z}. \tag{59}$$

From this we deduce the inequality

$$m\|\Psi\|^2_{L^2(\mathcal{E}_\Omega)} - 2i\int_{\partial\Omega}\overline{\Psi}_1\Psi_2\,d\overline{z} \leqslant \|\Psi\|_{L^2(\mathcal{E}_\Omega)}\|f\|_{L^2(\mathcal{E}_\Omega)}. \tag{60}$$

Next we compute the boundary term in (60) using the local expansions for Ψ. We find

$$-2i\int_{C_R}\overline{\Psi}_1\Psi_2\,d\overline{z} = 4\pi\sum_n |c_n^\infty(\Psi)|^2 K_n(mR)K_{n-1}(mR)R, \tag{61}$$

and recalling the appropriate orientation of $\partial\Omega$,

$$2i\int_{C_\epsilon(a_j)}\overline{\Psi}_1\Psi_2\,d\overline{z} = 4\pi\sum_{n\geqslant 0}(|c_n^j(\Psi)|^2 + |c_n^{j*}(\Psi)|^2) I_{n+1/2}(m\epsilon)I_{n-1/2}(m\epsilon)\epsilon$$
$$+ 4\pi\overline{c}_0^j(\Psi)c_0^{j*}(\Psi)I^2_{-1/2}(m\epsilon)\epsilon + 4\pi\overline{c}_0^{j*}(\Psi)c_0^j(\Psi)I^2_{1/2}(m\epsilon)\epsilon.$$

The boundary condition $c_0^j(\Psi) = c_0^{j*}(\Psi)$ implies that the right-hand side of this last equation is positive definite. Thus the boundary term on the left-hand side of (60) is positive and we immediately deduce

$$m\|\Psi\|^2_{L^2(\mathcal{E}_\Omega)} \leqslant \|\Psi\|_{L^2(\mathcal{E}_\Omega)}\|f\|_{L^2(\mathcal{E}_\Omega)},$$

which is (55). Now (61) and (60) coupled with the positivity of all the boundary contributions and (55) together imply (57) and (58). For the same reasons we can pick out just one term from each of the $C_\epsilon(a_j)$ boundary terms to find the inequality

$$4\pi\sum_j |c_0^j(\Psi)|^2 I^2_{-1/2}(m\epsilon)\epsilon \leqslant \frac{1}{m}\|f\|^2_{L^2(\mathcal{E}_\Omega)}.$$

This must be true for all ϵ and since

$$\lim_{\epsilon\to 0} I^2_{-1/2}(m\epsilon)\epsilon = \frac{2}{m\pi},$$

we have proved (56). (Theorem 8.) QED

Now suppose as in the preceeding theorem that Ψ is an $L^2(\mathcal{E}_\Omega)$ solution to,

$$(m - \not{\partial})\Psi = f,$$

where $f \in C_0^\infty(\mathcal{E}_\Omega)$. To finish the proof of (3) of Theorem 7 we want to estimate $c_1^j(\Psi)$ in terms of f. To do this we first introduce the function

$$V_j(z) = (z - a_j)^{-3/2}\prod_{k\neq j}(a_j - a_k)^{1/2}(z - a_k)^{-1/2},$$

which we take to be branched along the rays $\mathbf{r}_j$. Next observe that if Ψ is identified with its $\mathcal{U}_0$ trivialization then $V_j\Psi$ is differentiable on Ω and

$$\mathrm{d}(2V_j\Psi_1\,\mathrm{d}z) = -\overline{\partial}(2V_j\Psi_1)\mathrm{d}z\,\mathrm{d}\overline{z} = -2V_j\overline{\partial}\Psi_1\,\mathrm{d}z\,\mathrm{d}\overline{z} = mV_j\Psi_2\,\mathrm{d}z\,\mathrm{d}\overline{z} - V_j f_2\,\mathrm{d}z\,\mathrm{d}\overline{z}.$$

Stokes' theorem implies

$$\int_{\partial\Omega} 2V_j\Psi_1\,\mathrm{d}z = \int_\Omega mV_j\Psi_2\,\mathrm{d}z\,\mathrm{d}\overline{z} - \int_\Omega V_j f_2\,\mathrm{d}z\,\mathrm{d}\overline{z},$$

from which, together with (55), we deduce the inequality

$$\left|\int_{\partial\Omega} V_j\Psi_1\,\mathrm{d}z\right| \leqslant \|V_j\|_{L^2(\Omega)}\|f\|_{L^2(\mathcal{E}_\Omega)}. \tag{62}$$

Next we wish to estimate the boundary integrals over $C_\epsilon(a_k)$. First observe that in a neighborhood of a_k the function V_j has a "Laurent" expansion in powers of $z_k = z - a_k$,

$$V_j(z) = \sum_{n\geqslant -1} c_n^k(V_j) z_k^{n-1/2},$$

and z is restricted to an annulus about $|z_k| = \epsilon$. One finds

$$\frac{1}{2\pi\epsilon i}\int_{C_\epsilon(a_k)} V_j\Psi_1\,\mathrm{d}z = c_1^k(\Psi)c_{-1}^k(V_j)I_{1/2}(m\epsilon)\epsilon^{-3/2} + c_0^k(\Psi)c_0^k(V_j)I_{-1/2}(m\epsilon)\epsilon^{-1/2}$$

$$+ \sum_{n\geqslant 0} c_n^{k*}(\Psi)c_n^k(V_j)I_{n+1/2}(m\epsilon)\epsilon^{n-1/2}.$$

Observe that the term with $c_1^k(\Psi)$ is present only for $k = j$ since one can easily check that

$$c_{-1}^k(V_j) = \delta_{jk}.$$

Next we use the fact that the Taylor expansion of V_j for $|z| \geqslant R$ has the form

$$V_j(z) = \sum_{n<-1} c_n^\infty(V_j) z^n$$

to calculate

$$\frac{1}{2\pi R i}\int_{C_R} V_j\Psi_1(z)\mathrm{d}z = -\sum_{n<-1} c_n^\infty(V_j)R^n c_{n+1}^\infty(\Psi)K_{n+1}(mR).$$

Note: The coefficients $c_n^\infty(V_j)$ are zero for $n > -(N/2) - 1$, where N is the number of branch points, but we will not need this.

Next we use (57) and Cauchy's inequality for the l^2 norm with weight,

$$I_{n+1/2}(m\epsilon)I_{n-1/2}(m\epsilon)\epsilon,$$

to estimate

$$\sum_{n\geqslant 0} |c_n^{k*}(\Psi)\|c_n^k(V_j)|I_{n+1/2}(m\epsilon)\epsilon\epsilon^{n-1/2} \leqslant A_k B_k, \tag{63}$$

where

$$A_k^2 = \sum_{n \geqslant 0} |c_k^{k*}(\Psi)|^2 I_{n+1/2}(m\epsilon) I_{n-1/2}(m\epsilon)\epsilon$$

and

$$B_k^2 = \sum_{n \geqslant 0} \left| \frac{c_k^k(V_j)\epsilon^{n-1/2}}{I_{n-1/2}(m\epsilon)} \right|^2 I_{n+1/2}(m\epsilon) I_{n-1/2}(m\epsilon)\epsilon.$$

Combining this with (11) we see that

$$B_k^2 \leqslant \sum_{n \geqslant 0} |c_n^k(V_j)\epsilon^{n-1/2}|^2 \frac{m\epsilon^2}{n+1/2} \leqslant \epsilon m \|V_j\|^2_{L^2(C_\epsilon a_k))},$$

since $c_n^k(V_j)\epsilon^{n-1/2}$ are Fourier coefficients for V_j on the circle $C_\epsilon(a_k)$. The norm of V_j that appears here is actually the $H^{-1/2}$ norm, but this won't matter for us. This last estimate for B_k combined with (57) for A_k give us

$$A_k B_k \leqslant \sqrt{\frac{\epsilon}{4\pi}} \|V_j\|_{L^2(C_\epsilon(a_k))} \|f\|_{L^2(\mathcal{E}_\Omega)}. \tag{64}$$

In a similar fashion we estimate

$$\sum_{n<-1} |c_n^\infty(V_j) R^n\|_{n+1}^\infty(\Psi)| K_{n+1}(mR) R \leqslant A_\infty B_\infty, \tag{65}$$

where

$$A_\infty^2 = \sum_{n<-1} |c_{n+1}^\infty(\Psi)|^2 K_{n+1}(mR) K_n(mR) R \leqslant \frac{1}{4\pi m} \|f\|^2_{L^2(\mathcal{E}_\Omega)},$$

and

$$B_\infty^2 = \sum_{n<-1} |c_n^\infty(V_j) R^n|^2 \frac{K_{n+1}(mR)}{K_n(mR)} R.$$

In this equation it is important for us that $n<-1$. For $n<-1$ we have

$$\frac{K_{n+1}(mR)}{K_n(mR)} = \frac{K_{|n|-1}(mR)}{K_{|n|}(mR)} \leqslant \frac{mR}{|n|-1},$$

so that

$$B_\infty^2 \leqslant mR \|V_j\|^2_{L^2(C_R)},$$

and

$$A_\infty B_\infty \leqslant \sqrt{\frac{R}{4\pi}} \|V_j\|_{L^2(C_R)} \|f\|_{L^2(\mathcal{E}_\Omega)}. \tag{66}$$

Combining the expressions for the boundary integrals with the estimates that follow from (63) to (66) we find the following lower bound;

$$\frac{1}{2\pi}\left|\int_{\partial\Omega} V_j \Psi_1 \, dz\right| \geq |c_1^j(\Psi)| I_{1/2}(m\epsilon)\epsilon^{-1/2} - \sum_k |c_0^k(V_j)||c_0^k(\Psi) I_{-1/2}(m\epsilon)\epsilon^{1/2}$$
$$- C\|V_j\|_{L^2(\partial\Omega)}\|f\|_{L^2(\mathcal{E}_\Omega)},$$

for a constant C which is independent of m. Now we put together this lower bound with (62) to find

$$I_{1/2}(m\epsilon)|c_1^j(\Psi)| \leq C(I_{-1/2}(m\epsilon)\sum_k |c_0^k(\Psi)| + \|f\|_{L^2(\mathcal{E}_\Omega)}, \tag{67}$$

where the constant C is independent of m but incorporates all the dependence on V_j. The form of this estimate that we will use is now obtained by combining (56) with (67). We find

$$I_{1/2}(m\epsilon)|c_1^j(\Psi)| \leq C(I_{-1/2}(m\epsilon)+1)\|f\|_{L^2(\mathcal{E}_\Omega)} \tag{68}$$

for a different constant C.

We are now prepared to finish the proof of part (3) of Theorem 7. Recall that $\delta_3\mathcal{W}_j$ is defined as the solution to

$$(m-\not\partial)\,\delta_3\mathcal{W}_j = -m\,\delta_2\mathcal{W}_j, \tag{69}$$

with boundary values in $W^{(m)}$. We could make this description technically precise and prove the existence of such a solution using H^1 estimates along the lines of the L^2 estimate (55). The relevant estimates can be obtained via a Stokes' theorem calculation involving the exterior derivative,

$$2id((\overline{\Psi}_1\overline{\partial}\Psi_1 + \overline{\Psi}_2\overline{\partial}\Psi_2)d\overline{z} - (\overline{\Psi}_1\partial\Psi_1 + \overline{\Psi}_2\partial\Psi_2)dz)$$

for a solution Ψ to

$$(M-\not\partial)\Psi = f.$$

However it will be simpler to proceed differently. The solution of (69) which is relevant to us is the one constructed via functional analysis in Ref. 2. This solution is a weak L^2 solution to (69) inside Ω which extends to a solution of the homogeneous equation $(m-\not\partial)\,\delta_3\mathcal{W}_j = 0$ outside Ω and is globally in $L^2(\mathcal{E})$. We can obtain such a solution by approximating the right-hand side $\delta_2\mathcal{W}_j$ in $L^2(\mathcal{E}_\Omega)$ by a sequence of functions $f_n \in C_0^\infty(\mathcal{E}_\Omega)$. Theorem 8 shows that the resulting sequence of solutions to the approximate equations tends strongly in $L^2(\mathcal{E}_\Omega)$ to a weak solution to (69). The norms on the left-hand sides of (57) and (58) are equivalent to the L^2 norms of limiting solution in the components of the exterior of Ω and so the resulting solution is globally in $L^2(\mathcal{E})$ (this is a consequence of the same Stokes' theorem calculation that went into the proof of Theorem 8 but done in the components of the exterior of Ω). We may thus identify the limiting solution with $\delta_3\mathcal{W}_j$ and by obtaining the solution $\delta_3\mathcal{W}_j$ in this fashion we see that estimate (68) remains valid, so that

$$I_{1/2}(m\epsilon)|c_1^j(\delta_3\mathcal{W}_j)| \leq C(I_{-1/2}(m\epsilon)+1)m\|\delta_2\mathcal{W}_j\|_{L^2(\Omega)}.$$

The left-hand side of this last inequality is the Fourier coefficient (53) and the right-hand side tends to 0 using estimate (2) of Theorem 7. This finishes the proof of Theorem 7. Q.E.D.

Remark: The norms on the left-hand side of (57) and (58) which are the appropriate norms for boundary values of L^2 solutions also appear to be equivalent to the $H^{-1/2}$ norms on the corresponding circles. The loss of one half derivative for boundary values of solutions to $(m=0)$ Dirac equations is a general property.[17] In our case, this would follow from the following Bessel function estimate:

$$\frac{K_n(r)}{K_{n-1}(r)} \leqslant 2(n-1)\left(1+\frac{1}{r}\right)$$

for $r>0$ and $n \geqslant 2$ which seems to be true.

We now substitute $\delta\mathcal{W}_j = \delta_1\mathcal{W}_j + \delta_2\mathcal{W}_j + \delta_3\mathcal{W}_j$ into (10) and use Theorem 7 to determine the limit as $m \to 0$. According to part (1) of Theorem 7, $\delta_1\mathcal{W}_j$ converges to $G_0 f_{0j}$ in $W^{1,p}(\mathcal{E}_\Omega)$ for $p>2$. The Sobolev trace theorem implies that it converges in $W^{1/2,p}(\mathcal{E}_{\partial\Omega})$ and this is enough to show that the Fourier coefficient of $\delta_1\mathcal{W}_j$ which appears in (10) converges to

$$\sqrt{\frac{\pi}{2\epsilon}}\frac{1}{2\pi}\int_{\theta_{\mathbf{r}}}^{\theta_{\mathbf{r}}+2\pi}(G_0 f_{0,j})_1(\epsilon e^{i\Theta_j})\exp\left(-i\frac{\Theta_j}{2}\right)\mathrm{d}\Theta_j. \tag{70}$$

Estimate (2) of Theorem 7 implies that the $H^1(\mathcal{E}_\Omega)$ norm of $\delta_2\mathcal{W}_j$ tends to 0 as $m \to 0$ and again the Sobolev trace theorem implies that the boundary value tends to 0 in $H^{1/2}(\mathcal{E}_{\partial\Omega})$, which is enough to show that the contribution made by $\delta_2\mathcal{W}_j$ to (10) is 0 in this limit. Finally part (3) of Theorem 7 shows that $\delta_3\mathcal{W}_j$ makes no contribution to the $m \to 0$ limit of (10). Thus to finish the proof of Theorem 1 we need only calculate (70).

We turn now to the calculation of (70). Using the definition of $f_{0,j}$ found in (52) we see that

$$(G_0 f_{0,j})_1(z) = i\sqrt{\frac{2}{\pi}}\int_\Omega(-G_{11}(z,z')\overline{z}_j'^{-1/2}\partial\varphi(z') + G_{12}(z,z')z_j'^{-1/2}\overline{\partial}\varphi)\mathrm{d}z'\,\mathrm{d}\overline{z}'.$$

Using the fact that $G_{11}(z,z')$ is antiholomorphic in z' and $G_{12}(z,z')$ is holomorphic in z we can rewrite this last integral as the integral of an exact form,

$$i\sqrt{\frac{2}{\pi}}\int_\Omega \mathrm{d}(-G_{11}(z,z')\overline{z}_j'^{-1/2}\varphi(z')\mathrm{d}\overline{z}' - G_{12}(z,z')z_j'^{-1/2}\varphi(z')\mathrm{d}z').$$

Since $\varphi(z)=1$ on $C_\epsilon(a_j)$ and vanishes on the rest of $\partial\Omega$, Stokes' theorem implies that the last integral is

$$i\sqrt{\frac{2}{\pi}}\int_{C_\epsilon(a_j)} G_{11}(z,z')\overline{z}_j'^{-1/2}\,\mathrm{d}\overline{z}' + G_{12}(z,z')z_j'^{-1/2}\,\mathrm{d}z'.$$

Now substitute

$$G_{11}(z,z') - \frac{1}{4\pi i}\sum_k v_k(z)\overline{u}_k(z)$$

and (25) for $G_{12}(z,z')$ in this last integral and use the residue calculations that are found in the results that follow (38) to find

$$(G_0 f_{0,j})_1(z) = -i\frac{z_j^{-1/2}}{\sqrt{2\pi}} + i\sqrt{\frac{2}{\pi}}v_j(z).$$

Using this result it is now a simple matter to convert the Fourier integral (70) into the following residue calculation:

$$\frac{1}{2\pi}\int_{C_\epsilon(a_j)} z_j^{-2}\sum_{|\epsilon|=0,\epsilon_j=1/2} c(\epsilon)\prod_{\neq j}\frac{(z-a_k)^{\epsilon_k}}{(a_j-a_k)^{\epsilon_k}}\mathrm{d}z,$$

which in turn gives

$$i\frac{\partial}{\partial z}\sum_{|\epsilon|=0,\epsilon=1/2} c(\epsilon)\prod_{k\neq j}\frac{(z-a_k)^{\epsilon_k}}{(a_j-a_k)^{\epsilon_k}}\bigg|_{z=a_j} = i\sum_{|\epsilon|=0,\epsilon_j=1/2} c(\epsilon)\sum_{k\neq j}\frac{\epsilon_k}{a_j-a_k}.$$

Dividing by $2i$ to get the limiting value of the coefficient that appears in the $m\to 0$ of the log derivative of the tau function we find

$$\lim_{m\to 0}\frac{mc_1^j(\mathcal{W}_j)}{2i} = \frac{1}{2}\sum_{|\epsilon|=0,\epsilon_j=1/2} c(\epsilon)\sum_{k\neq j}\frac{\epsilon_k}{a_j-a_k}. \tag{71}$$

To finish the proof of Theorem 1 we compare this result with

$$\frac{\partial}{\partial a_j}\sum_{|\epsilon|=0}\prod_{\alpha<\beta}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta} = \sum_{|\epsilon|=0}\sum_{k\neq j}\frac{\epsilon_j\epsilon_k}{a_j-a_k}\prod_{\alpha<\beta}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta}, \tag{72}$$

which we obtained using

$$\frac{\partial}{\partial a_j}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta} = \frac{\epsilon_\alpha\epsilon_\beta}{a_\alpha-a_\beta}(\delta_{\alpha j}-\delta_{\beta j})|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta}.$$

In (71) observe that the $|\epsilon|=0$ sum has two different possible values for ϵ_j, either $\epsilon_j=\frac{1}{2}$ or $\epsilon_j=-\frac{1}{2}$. However since the summand on the right-hand side of (71) is clearly invariant under the complete sign reversal $\epsilon_\alpha\to-\epsilon_\alpha$ it follows that the whole sum is just twice the result for $\epsilon_j=\frac{1}{2}$. That is,

$$\frac{\partial}{\partial a_j}\sum_{|\epsilon|=0}\prod_{\alpha<\beta}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta} = \sum_{|\epsilon|=0,\epsilon_j=1/2}\sum_{k\neq j}\frac{\epsilon_k}{a_j-a_k}\prod_{\alpha<\beta}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta}.$$

Comparing this with (71) and recalling the definition of $c(\epsilon)$ we have finished the proof of Theorem 1.

VII. ODD CORRELATIONS AND HOLONOMIC FIELDS

In this section we make some observations about the application of the technique used to prove Theorem 1 to work out the asymptotics of the odd Ising scaling functions from below T_c and also the short distance behavior of the correlations for holonomic quantum fields.

First we treat the case where N is odd. The one difference in the analogue of Lemma 1 for N odd is that the subspace $W_\infty^{(m)}$ is now the L^2 closure of the span of

$$\hat{w}_n(z) = \begin{bmatrix} -e^{-i(n+1/2)\theta} & K_{n+1/2}(m|z|) \\ -e^{-i(n-1/2)\theta} & K_{n-1/2}(m|z|)\end{bmatrix},$$

for $n\in\mathbf{Z}$. For definiteness we make the choice $0<\theta<2\pi$ and choose the $\mathcal{U}_\infty$ trivialization (in the complement of $\theta=0$) so that finite linear combinations of the $\hat{w}_n(z)$ are smooth sections of $\mathcal{E}$ in the $\mathcal{U}_\infty$ trivialization. Without difficulty one can compute the $m\to 0$ limit of the normalized versions of these vectors and as a consequence we define $W_\infty^{(0)}$ as the L^2 closure of the span of

$$\left\{\begin{bmatrix} e^{-i(n+1/2)\theta}\\ 0\end{bmatrix}\right\}_{n\geq 1}, \begin{bmatrix} -e^{-i(\theta/2)}\\ e^{i(\theta/2)}\end{bmatrix}, \left\{\begin{bmatrix} 0\\ e^{i(n+1/2)\theta}\end{bmatrix}\right\}_{n\geq 1}.$$

Next we introduce a Green function $-\not{\partial}$ with $W^{(0)}$ boundary conditions in the following manner:

$$G_0(z,z')=-\frac{1}{4\pi i}\begin{bmatrix}\sum_j u_j(z)\overline{v_j(z')} & g(z,z')\\ g(z,z') & \sum_j \overline{u_j(z)}v_j(z')\end{bmatrix}, \tag{73}$$

where

$$u_j(z):=(z-a_j)^{-1/2}\prod_{k\neq j}\frac{(z-a_k)^{1/2}}{(a_j-a_k)^{1/2}}, \tag{74}$$

$$g(z,z'):=\sum_{|\epsilon|=\pm 1/2} c(\epsilon)\frac{\Pi_j(z-a_j)^{\epsilon_j}(z'-a_j)^{-\epsilon_j}}{z'-z}, \tag{75}$$

with $\epsilon=(\epsilon_1,\ldots,\epsilon_N)$ and each $\epsilon_j=\pm\frac{1}{2}$. Also

$$|\epsilon|:=\sum_{j=1}^{N}\epsilon_j,\quad c(\epsilon):=\frac{\Pi_{j<k}|a_j-a_k|^{2\epsilon_j\epsilon_k}}{\sum_{|\epsilon|=\pm 1/2}\Pi_{j<k}|a_j-a_k|^{2\epsilon_j\epsilon_k}}, \tag{76}$$

and

$$v_j(z)=(z-a_j)^{-1/2}\sum_{|\epsilon|=\pm 1/2,\epsilon_j=1/2} c(\epsilon)\prod_{k\neq j}\frac{(z-a_k)^{\epsilon_k}}{(a_j-a_k)^{\epsilon_k}}. \tag{77}$$

The multivalued functions $(z-a_j)^{\epsilon_j}$ are all defined using the argument Θ_j and are consequently branched along $z\in\mathbf{r}_j$. We regard $G_0(z,z')$ as defining an operator, G_0, acting on sections of $\mathcal{E}_\Omega$ in the following manner:

$$G_0 f(z):=\int_\Omega G_0(z,z')f(z')\mathrm{d}z'\,\mathrm{d}\overline{z'}, \tag{78}$$

where the section $f(z')$ is identified with its $\mathcal{U}_0$ trivialization. We also regard $G_0 f$ as a section of $\mathcal{E}_\Omega$ given in the $\mathcal{U}_0$ trivialization.

The homogeneous function identity,

$$\sum_k \overline{u_k}(z)v_k(z')=\sum_k \overline{v_k}(z)u_k(z'),$$

can be proved along the lines of Lemma 2 and this makes it possible to establish the desired results concerning the Green function and the projection P_0. One matter that requires a little further analysis is the proof that $G_0 f$ has boundary values on C_R which are in $W_\infty^{(0)}$. For this purpose it is useful to introduce a $\mathcal{U}_\infty$ trivialization for $\mathcal{E}$ over $\{z:|z|>R\}\backslash\{t\in\mathbf{R}:t>0\}$ by introducing square root $z^{1/2}=|z|^{1/2}e^{i\theta/2}$ for $0<\theta<2\pi$, which is branched along the positive real axis. Smooth sections of $\mathcal{E}$ over $\{z:|z|>R\}\backslash\{t\in\mathbf{R}:t>0\}$ can then be represented in the $\mathcal{U}_\infty$ trivialization as products $z^{1/2}\phi(z)$ for a smooth map ϕ from $D_\infty:=\{z:|z|>R\}$ into $\mathbf{C}^2$. For the purpose of analyzing the behavior of the Green function $G_0(z,z')$ for $|z|>R$ it is useful to note that $v_j(z)$ has a representation in this domain given by

$$v_j(z)=z^{-1/2}\left(1-\frac{a_j}{z}\right)^{-1/2}\sum_{|\epsilon|=1/2,\epsilon_j=1/2}c(\epsilon)\prod_{k\neq j}\frac{\left(1-\frac{a_k}{z}\right)^{\epsilon_k}}{(a_j-a_k)^{\epsilon_k}}$$

$$+z^{-3/2}\left(1-\frac{a_j}{z}\right)^{-1/2}\sum_{|\epsilon|=-1/2,\epsilon_j=1/2}c(\epsilon)\prod_{k\neq j}\frac{\left(1-\frac{a_k}{z}\right)^{\epsilon_k}}{(a_j-a_k)^{\epsilon_k}}.$$

Using this one can check that for $\varphi\in C_0^\infty(\mathcal{E}_\Omega)$ we have $G_0\varphi|_{C_R}\in W_\infty^{(0)}$ provided the following reality conditions are satisfied:

$$\sum_{|\epsilon|=1/2,\epsilon_j=1/2}c(\epsilon)\prod_{k\neq j}(a_j-a_k)^{-\epsilon_k}=\sum_{|\epsilon|=1/2,\epsilon_j=1/2}\overline{c(\epsilon)}\prod_{k\neq j}\overline{(a_j-a_k)}^{\epsilon_k}.$$

This will be true for our choice of $c(\epsilon)$ provided that

$$\sum_{|\epsilon|=1/2,\epsilon_j=1/2}\prod_{\substack{\alpha<\beta\\ \alpha,\beta\neq j}}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta}\prod_{k\neq j}|a_j-a_k|^{\epsilon_k}(a_j-a_k)^{-\epsilon_k},$$

is real. However, under the transformation $\epsilon_k\to-\epsilon_k$ for $k\neq j$ the product

$$\prod_{k\neq j}|a_j-a_k|^{\epsilon_k}(a_j-a_k)^{-\epsilon_k},$$

maps into its complex conjugate while in the preceeding sum the coefficient of this product is real and invariant. This implies reality for the sum.

The rest of the analysis closely follows that in the even case and so we will only quote the final result. For N odd we have

$$\lim_{m\to0}\mathrm{d}_a\log\tau_-(ma)=\frac{1}{2}\mathrm{d}_a\log\sum_{|\epsilon|=\pm1/2}\prod_{\alpha<\beta}|a_\alpha-a_\beta|^{2\epsilon_\alpha\epsilon_\beta}.$$

Finally we describe the situation for the tau functions for holonomic fields in the formalism of Ref. 13. Suppose that for $j=1,...,N$ we have

$$-\tfrac{1}{2}<\lambda_j<\tfrac{1}{2},$$

and for simplicity we also suppose that

$$\sum_j\lambda_j=0.$$

The restricted local expansion that determines the subspace $W_j^{(m)}$ is

$$w(z)=\sum_{\substack{k\in\mathbf{z}+1/2\\ k>0}}a_k^j(w)w_{k-\lambda_j}(z_j)+b_k^j(w)w^*_{k+\lambda_j}(z_j).$$

At infinity the restricted expansion that determines $W_\infty^{(m)}$ is

$$w(z)=\sum_{k\in\mathbf{z}+1/2}c_k(w)\hat{w}_k(z).$$

Without difficulty one can check that the limiting subspaces, $W_j^{(0)}$, are spanned by

$$\begin{bmatrix} z_j^{k-\lambda_j} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \overline{z}_j^{k+\lambda_j} \end{bmatrix} \quad \text{for} \quad k=\frac{1}{2},\frac{3}{2},\ldots$$

and $W_\infty^{(0)}$ is spanned by

$$\begin{bmatrix} z^{-n} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \overline{z}^{-n} \end{bmatrix} \quad \text{for} \quad n=1,2,3,\ldots .$$

The mass 0 Green function for the Dirac operator of interest is clearly (see Proposition 1.1 in Ref. 13),

$$G_0(z,z')=-\frac{1}{4\pi}\begin{bmatrix} 0 & g(z,z') \\ \overline{g(z,z')} & 0 \end{bmatrix},$$

where

$$g(z,z')=\frac{\Pi_j z_j^{-\lambda_j}(z_j')^{\lambda_j}}{z'-z}.$$

There are no ''chiral symmetry breaking'' terms. In the notation of (4.3) of Ref. 13 we have

$$\mathrm{d}_a \log \tau(ma,\lambda)=\frac{m}{2}\sum_j \{a^j_{1/2,j}(-\lambda)\mathrm{d}a_j+\overrightarrow{a}^j_{1/2,j}(\lambda)\mathrm{d}\overline{a}_j\},$$

and we find for the $m\to 0$ limit,

$$\lim_{m\to 0}\mathrm{d}_a \log \tau(ma,\lambda)=\sum_{j=1}^{N}\left\{\sum_{k\neq j}\frac{\lambda_j\lambda_k}{a_j-a_k}\mathrm{d}a_j+\sum_{k\neq j}\frac{\lambda_j\lambda_k}{\overline{a}_j-\overline{a}_k}\mathrm{d}\overline{a}_j\right\},$$

which is also just

$$\mathrm{d}_a \log \prod_{j<k}|a_j-a_k|^{\lambda_j\lambda_k}.$$

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Classical Hamiltonian systems with $sl(2)$ coalgebra symmetry and their integrable deformations

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Several families of classical integrable systems with two degrees of freedom are derived from phase-space realizations of $sl(2)$ Poisson coalgebras. As a remarkable fact, the existence of the N-dimensional integrable generalization of all these systems is always ensured (by construction) due to their underlying dynamical coalgebra symmetry. By following the same approach, different integrable deformations for such systems are obtained from the q-deformed analogues of $sl(2)$. The well-known Jordan-Schwinger realization is also proven to be related to a (non-coassociative) coalgebra structure on $sl(2)$ and the $2N$ dimensional integrable Hamiltonian generated by such Jordan-Schwinger representation is obtained. Finally, the relation between complete integrability and the properties of the initial phase-space realization is elucidated through two more examples based on the Heisenberg-Weyl and $so(3,2)$ Poisson coalgebras. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1428810]

I. INTRODUCTION

A Poisson coalgebra (A,Δ) is a Poisson algebra A endowed with a Poisson map Δ between A and $A\otimes A$ that defines a way to construct tensor product representations of A. In the case where A is the dynamical algebra for a one-particle problem, the coproduct Δ provides a two-particle realization of the same dynamical symmetry. In fact, under certain conditions the coproduct Δ can be generalized to a Poisson map between A and $A\otimes A\otimes \ldots {}^{N)}\otimes A$, and the N-particle realization of the symmetry arises. By following this approach, a systematic construction of completely integrable (classical and quantum) Hamiltonians from coalgebras has been introduced in Ref. 1 and several applications of this formalism have been proposed (see, for instance, Refs. 2–4).

It is worth stressing that, in order to obtain the complete integrability from the coalgebra structure, the phase-space realization of the symmetry coalgebra has to fulfill some ''non-degeneracy'' conditions. Actually, classical complete integrability is guaranteed provided that the coalgebra comes from a simple Lie algebra of rank r endowed with a symplectic realization on a $2r$-dimensional phase space and the coproducts $\Delta(C_i)$ of the r Casimirs are non-trivial and functionally independent (note that this was the case for all the examples presented within the previous references). Under these conditions the very role of the coproduct map is to provide the explicit form of all the integrals of motion. By construction, such integrals are organized in a hierarchical way: the k-th integral is defined on the k-th order tensor product of the initial representation. From this perspective, the coproduct can be also seen as the vehicle that ''propagates'' the integrability from the initial (trivial) Hamiltonian system to a new non-trivial family of systems with an arbitrary number of degrees of freedom. Moreover, since quantum deformations (see, for instance, Refs. 5–8) can be understood in a classical mechanical context as deformations of Poisson algebras preserving a coalgebra structure, such construction can be applied for them and leads to a systematic derivation of integrable deformations of Hamiltonian systems.

The aim of the present paper is two-fold. On one hand, we use the $sl(2)$ Poisson coalgebra and its deformations to provide new families of completely integrable systems through the previous construction. On the other hand, we would like to clarify the limitations imposed on this formalism by the choice of the phase-space representation of the dynamical Poisson coalgebra. In particular, we shall analyze the systems coming from a four-dimensional phase space realization of a rank one algebra, showing why, in this case, the complete integrability can also be explicitly proven. On the contrary, we also present some particular examples for which a specific choice of the representation gives rise to either trivial or functionally dependent integrals of the motion.

In Sec. II we recall both classical and quantum Poisson $sl(2)$ coalgebras. In Sec. III the general construction is reviewed through an example based on the Gelfan'd-Dyson realization[9] of $sl(2)$, and in Sec. IV new families of $N=2$ integrable systems are given, together with their standard and non-standard integrable deformations. Among them, we find as (canonically equivalent) examples of two-dimensional coalgebra symmetry the well-known Smorodinsky-Winternitz Hamiltonian[10,11] and the rational Calogero system,[12] as a consequence, two new integrable deformations for them can be constructed. In general, it is interesting to mention that quantum deformations introduce hyperbolic functions of the canonical variables in the Hamiltonian, and the associated integrals of the motion have also such kind of hyperbolic terms depending on positions and/or momenta. Note also that the existence of the N-dimensional generalization of all these systems is, by construction, ensured (although we will not describe their explicit form here).

In Sec. V we present the generalization of this construction to $sl(2)$ systems for which the phase-space realization of $sl(2)$ is defined in terms of two pairs of canonical variables. By using the classical Jordan-Schwinger (JS) realization[13,14] as an outstanding example of this kind of situation, we show how complete integrability is also preserved for the corresponding system, now with $2N$ degrees of freedom. Consequently, the deformation of such systems poses the interesting problem of deforming the JS map. It turns out that coalgebra symmetry is also essential at this point, since we show that the Jordan-Schwinger (JS) realization of $sl(2)$ is canonically equivalent to a reducible representation of $sl(2)$ given by a non-coassociative coproduct. From it, a standard deformation of the JS realization is given and related $2N$ dimensional integrable systems can be defined.

Finally, in Sec. VI we turn to Poisson coalgebras other than $sl(2)$ in order to illustrate the above-mentioned limitations of the formalism for certain phase-space realizations of the symmetry coalgebra. First, we consider an example of non-simple algebra, namely the Heisenberg-Weyl one. In this case, for the usual phase space realization the coalgebra method does not allow to prove the complete integrability of the non-deformed system. Remarkably enough on the contrary, the complete integrability of the systems obtained through one of its q-deformations (compatible with the same phase-space realization) can be explicitly demonstrated through the deformed coproduct. Second, a particular two-particle representation of the Poisson $so(3,2)$ algebra is used as a rank-two benchmark for the coalgebra formalism. In this example, the functional dependence of the coproduct of the two Casimir functions implies that only half of the integrals of the motion can be explicitly derived from the coproduct.

II. $sl(2)$ POISSON COALGEBRAS

Let us consider classical angular momentum variables J_3, $J_\pm$ and the associated $sl(2)$ Poisson-Lie algebra

$$\{J_3,J_\pm\}=\pm 2J_\pm, \quad \{J_+,J_-\}=J_3 \tag{2.1}$$

with Casimir function

$$C(J_3,J_+,J_-)=\tfrac{1}{4}J_3^2+J_+J_-. \tag{2.2}$$

The Poisson algebra (2.1) is endowed with a coalgebra structure by the usual ''primitive'' coproduct defined between $sl(2)$ and $sl(2)\otimes sl(2)$

$$\Delta(J_3)=1\otimes J_3+J_3\otimes 1,\quad \Delta(J_\pm)=1\otimes J_\pm+J_\pm\otimes 1. \tag{2.3}$$

Compatibility between Eqs. (2.3) and (2.1) means that Δ is a Poisson map: the three functions defined through Eq. (2.3) close also a Poisson $sl(2)$ algebra.

There are few deformations of the $sl(2)$ algebra for which there exist compatible deformations of the coproduct [Eq. (2.3)]. In fact, two relevant and distinct structures appeared in quantum group literature during last years, and they can be realized as Poisson algebras as follows:

• The "*standard*" deformation $sl_q(2)$ $(q=e^z)$[5,6,15] given by the following deformed Poisson brackets

$$\{\tilde J_3,\tilde J_+\}=2\,\tilde J_+,\quad \{\tilde J_3,\tilde J_-\}=-2\,\tilde J_-,\quad \{\tilde J_+,\tilde J_-\}=\frac{\sinh(z\tilde J_3)}{z}, \tag{2.4}$$

which are compatible with the deformed coproduct

$$\begin{aligned}
&\Delta_z(\tilde J_3)=1\otimes\tilde J_3+\tilde J_3\otimes 1,\\
&\Delta_z(\tilde J_+)=e^{-(z/2)\tilde J_3}\otimes\tilde J_++\tilde J_+\otimes e^{(z/2)\tilde J_3};\\
&\Delta_z(\tilde J_-)=e^{-(z/2)\tilde J_3}\otimes\tilde J_-+\tilde J_-\otimes e^{(z/2)\tilde J_3};
\end{aligned} \tag{2.5}$$

in the sense that Eq. (2.5) is a Poisson algebra homomorphism with respect to (2.4). The function

$$C_z(\tilde J_3,\tilde J_\pm)=\left(\frac{\sinh((z/2)\tilde J_3)}{z}\right)^2+\tilde J_+\tilde J_-, \tag{2.6}$$

is the deformed Casimir for this Poisson coalgebra.

• The "*non-standard*" deformation $sl_h(2)$[16–18] whose defining relations are

$$\{\tilde J_3,\tilde J_+\}=2\,\frac{\sinh(h\tilde J_+)}{h},\quad \{\tilde J_3,\tilde J_-\}=-2\,\tilde J_-\cosh(h\tilde J_+),\quad \{\tilde J_+,\tilde J_-\}=\tilde J_3. \tag{2.7}$$

$$\begin{aligned}
&\Delta_h(\tilde J_+)=1\otimes\tilde J_++\tilde J_+\otimes 1,\\
&\Delta_h(\tilde J_-)=e^{-h\tilde J_+}\otimes\tilde J_-+\tilde J_-\otimes e^{h\tilde J_+},\\
&\Delta_h(\tilde J_3)=e^{-h\tilde J_+}\otimes\tilde J_3+\tilde J_3\otimes e^{h\tilde J_+}.
\end{aligned} \tag{2.8}$$

The non-standard deformed Casimir is now

$$C_h(\tilde J_3,\tilde J_+,\tilde J_-)=\frac{1}{4}\,\tilde J_3^2+\frac{\sinh(h\tilde J_+)}{h}\tilde J_-. \tag{2.9}$$

Equivalently, an isomorphic non-standard Poisson deformation is obtained by choosing $\tilde J_-$ as the primitive generator. We then find that

$$\{\tilde{J}_3,\tilde{J}_+\}=2\,\tilde{J}_+\cosh(h\tilde{J}_-),\quad \{\tilde{J}_3,\tilde{J}_-\}=-2\,\frac{\sinh(h\tilde{J}_-)}{h},\quad \{\tilde{J}_+,\tilde{J}_-\}=\tilde{J}_3. \tag{2.10}$$

$$\begin{aligned}\Delta_h(\tilde{J}_-)&=1\otimes\tilde{J}_-+\tilde{J}_-\otimes 1,\\ \Delta_h(\tilde{J}_+)&=e^{-h\tilde{J}_-}\otimes\tilde{J}_++\tilde{J}_+\otimes e^{h\tilde{J}_-},\\ \Delta_h(\tilde{J}_3)&=e^{-h\tilde{J}_-}\otimes\tilde{J}_3+\tilde{J}_3\otimes e^{h\tilde{J}_-}.\end{aligned} \tag{2.11}$$

The non-standard deformed Casimir is now

$$C_h(\tilde{J}_3,\tilde{J}_+,\tilde{J}_-)=\frac{1}{4}\,\tilde{J}_3^2+\tilde{J}_+\frac{\sinh(h\tilde{J}_-)}{h}. \tag{2.12}$$

In what follows we shall make use of these coalgebra symmetries in order to construct new integrable systems. Note that the undeformed $sl(2)$ structure is smoothly recovered when deformation parameters vanish. Jacobi identity can be also easily checked for Eqs. (2.4), (2.7), and (2.10).

III. GELFAN'D-DYSON MAP, GAUDIN MAGNET, AND DEFORMATIONS

Let us now recall the general construction[1] through an example provided by the classical phase space analogue of the one-boson (polynomial) Gelfan'd-Dyson (GD) realization of $sl(2)$:

$$J_3=2\,p\,q-b,\quad J_+=p,\quad J_-=-p\,q^2+b\,q, \tag{3.1}$$

where b is a real constant that labels the representation through the Casimir [Eq. (2.2)], which turns out to be $b^2/4$ under Eq. (3.1).

Let us now consider an *arbitrary* function $\mathcal{H}(J_3,J_\pm)$. Since the coproduct [Eq. (2.3)] is an algebra homomorphism, it is immediate to prove that the two-particle Hamiltonian that can be defined through the coproduct of H in the form

$$H^{(2)}=\Delta(\mathcal{H}(J_3,J_\pm))=\mathcal{H}(\Delta(J_3),\Delta(J_\pm)) \tag{3.2}$$

will commute with the coproduct $C^{(2)}$ of the Casimir element:

$$\{H^{(2)},C^{(2)}\}=\{\Delta(\mathcal{H}),\Delta(C)\}=\Delta(\{\mathcal{H},C\})=0. \tag{3.3}$$

Therefore, in this case *any* function of the generators defines a two-site integrable Hamiltonian with $sl(2)$ coalgebra symmetry. In particular, the Casimir itself can be taken as the function $\mathcal{H}$ itself. In that case, the constant of motion will be given by the coproduct of any of the generators of the algebra. Explicitly, in the $sl(2)$ case we have

$$\begin{aligned}H_C^{(2)}&:=C(\Delta(J),\Delta(J_+),\Delta(J_-))=\tfrac{1}{4}(1\otimes J_3+J_3\otimes 1)^2+(1\otimes J_++J_+\otimes 1)(1\otimes J_-+J_-\otimes 1)\\ &=1\otimes C+C\otimes 1+\tfrac{1}{2}J_3\otimes J_3+J_-\otimes J_++J_+\otimes J_-,\end{aligned} \tag{3.4}$$

which is just the two-site hyperbolic Gaudin magnet.[19–21] Once Eq. (3.4) is realized in terms of two copies of Eqs. (3.1) we shall obtain an integrable two-particle Hamiltonian

$$H_C^{(2)}(q_1,q_2,p_1,p_2) := \frac{b^2}{4}+\frac{b^2}{4}+\frac{1}{2}(2\,p_1\,q_1-b)(2\,p_2\,q_2-b)$$
$$+(-p_1\,q_1^2+b\,q_1)\,p_2+p_1\,(-p_2\,q_2^2+b\,q_2)$$
$$=-\,p_1\,p_2\,(q_1-q_2)^2-b\,(p_1-p_2)\,(q_1-q_2)+b^2. \tag{3.5}$$

Since $H_C^{(2)}$ is the coproduct of C, it will commute, for instance, with $\Delta(J_+)$, which is just the total momentum p_1+p_2 and gives us the integral of the motion. The generalization of this result to an N-site Gaudin magnet is straightforward by taking into account the appropriate N-th generalization of the coproduct. By following Ref. 1, we obtain that

$$H^{(N)}=\sum_{i=1}^{N} C_i+\sum_{i<j}^{N}\,(\tfrac{1}{2}J_3^i\,J_3^j+J_-^i\,J_+^j+J_+^i\,J_-^j) \tag{3.6}$$

$$=\sum_{i<j}^{N}\{-\,p_i\,p_j\,(q_i-q_j)^2-b\,(p_i-p_j)\,(q_i-q_j)\}+\frac{b^2}{4}N^2. \tag{3.7}$$

The $m=2,\ldots,N$ Hamiltonians $H^{(m)}$, together with the total momentum $\Delta^{(N)}(J_+)=p_1+p_2+\ldots+p_N$ are again the functionally independent N constants of the motion in involution. Note also that we could have taken a different realization on each lattice site through different b_i constants in Eq. (3.1), and the formalism will guarantee the integrability in the same manner (this kind of realizations will be relevant when the coalgebra symmetry of the Calogero system is analyzed in Sec. IV).

Now, the same construction can be applied to deformed $sl(2)$ coalgebras. We shall consider the non-standard one [Eqs. (2.7)–(2.9)]. The following deformed phase-space realization of Eq. (2.7) can be found

$$\tilde{J}_+=p,\quad \tilde{J}=2\,\frac{\sinh(h\,p)}{h}\,q-b\,\cosh(h\,p),$$
$$\tilde{J}_-=-\,\frac{\sinh(h\,p)}{h}\,q^2+b\,\cosh(h\,p)\,q-b^2\frac{h}{4}\sinh(h\,p), \tag{3.8}$$

which leads again the same $b^2/4$ constant when substituted in the deformed Casimir function [Eq. (2.9)]. Therefore, an integrable deformation of the system [Eq. (3.5)] will be given by the deformed coproduct of the (also deformed) Casimir [Eq. (2.9)]. In terms of two phase-space realizations of the type [Eq. (3.8)], the coproduct [Eq. (2.8)] defines the two-particle functions

$$\tilde{f}_+=\Delta_h(\tilde{J}_+)=p_1+p_2,$$
$$\tilde{f}_-=\Delta_h(\tilde{J}_-)=e^{-h\,p_1}\left\{-\,\frac{\sinh(h\,p_2)}{h}\,q_2^2+b\,\cosh(h\,p_2)\,q_2-b^2\frac{h}{4}\sinh(h\,p_2)\right\}$$
$$+\left\{-\,\frac{\sinh(h\,p_1)}{h}\,q_1^2+b\,\cosh(h\,p_1)\,q_1-b^2\frac{h}{4}\sinh(h\,p_1)\right\}e^{h\,p_2}; \tag{3.9}$$
$$\tilde{f}_3=\Delta_h(\tilde{J}_3)=e^{-h\,p_1}\left\{2\,\frac{\sinh(h\,p_2)}{h}\,q_2-b\,\cosh(h\,p_2)\right\}+\left\{2\,\frac{\sinh(h\,p_1)}{h}\,q_1-b\,\cosh(h\,p_1)\right\}e^{h\,p_2}.$$

The corresponding Hamiltonian is obtained as

$$H_h^{(2)}(q_1,q_2,p_1,p_2)=\Delta_h\left(\frac{1}{4}\,\tilde{J}_3^2+\frac{\sinh(h\tilde{J}_+)}{h}\tilde{J}_-\right)$$

$$=\frac{1}{4}\,(\tilde{f}_3)^2+\frac{\sinh(h\tilde{f}_+)}{h}\tilde{f}_-$$

$$=-\frac{\sinh hp_1}{h}e^{-h(p_1-p_2)}\frac{\sinh hp_2}{h}(q_1-q_2)^2-b\,\frac{1-e^{-2h(p_1-p_2)}}{2h}(q_1-q_2)$$

$$+\frac{b^2}{4}(1+e^{-2h\,p_1}+e^{2h\,p_2}+e^{-2h(p_1-p_2)}). \tag{3.10}$$

This Hamiltonian will commute, by construction, with the coproduct of $\tilde{J}_+$ (i.e., the total momentum p_1+p_2 again) and the limit $h\to 0$ of this expression leads to Eq. (3.5). The N-th dimensional integrable generalization of this system is given by the N-th deformed coproduct of the deformed Casimir, and the integrals of motion will be the lower degree coproducts of such Casimir and the N-th total momenta. Apart from the GD realization [Eq. (3.1)], the essential ingredients for the explicit formulation of such system can be extracted from Ref. 1. We stress that, although the next section will be devoted to systems with two degrees of freedom, their corresponding N-dimensional integrable generalizations will be—by construction—completely defined.

IV. $N=2$ SYSTEMS AND THEIR INTEGRABLE DEFORMATIONS

Let us now use realizations of $sl(2)$ linked to well-known dynamical symmetries of physically relevant potentials like the Morse and the harmonic oscillator with centrifugal term in order to obtain new systems with $sl(2)$ coalgebra symmetry.

A. Morse potential realization

If we consider the following $sl(2)$ phase-space realization

$$J_3=2\,p_1,\quad J_+=\tfrac{1}{2}e^{-q_1},\quad J_-=-2\,p_1^2\,e^{q_1}-a_1\,e^{q_1}. \tag{4.1}$$

The dynamical Hamiltonian

$$H_m=\tfrac{1}{8}J_3^2-4\,s\,J_++4\,s\,J_+^2 \tag{4.2}$$

leads to the Morse one:

$$H_m=\tfrac{1}{2}p_1^2+s\,(e^{-2\,q_1}-2\,e^{-q_1}). \tag{4.3}$$

The corresponding Casimir is

$$C_m=\frac{1}{2}\,J_3^2+J_+\,J_-=-\frac{a_1}{2}. \tag{4.4}$$

The two-body system is obtained by applying the method described previously. The coproduct of the Hamiltonian [Eq. (4.2)] in the realization [Eq. (4.1)] is

$$H_m^{(2)}=\tfrac{1}{2}(p_1+p_2)^2+s\,(e^{-2\,q_1}-2\,e^{-q_1})+s\,(e^{-2\,q_2}-2\,e^{-q_2})+2\,s\,e^{-(\,q_1+q_2)}. \tag{4.5}$$

Note that, in general, we could have performed another coalgebra construction by taking different symplectic realizations on each copy of the algebra [for instance [Eq. (4.1)] and [Eq. (3.1)]. Of course, in order to have a Morse-type Hamiltonian, two realizations [Eq. (4.1)] are needed, though with possibly different Casimir values a_1 and a_2. In this way, the coproduct of the Casimir providess a two-parametric family of constants of the motion in the form:

$$C_m^{(2)} = -\tfrac{1}{2}(a_1+a_2) - (\tfrac{1}{2}a_1 + p_1^2)\, e^{\,q_1-q_2} - (\tfrac{1}{2}a_2 + p_2^2) e^{-(q_1-q_2)} + 2\, p_1\, p_2 . \tag{4.6}$$

The Hamiltonian [Eq. (4.5)] can be diagonalized if we consider a canonical transformation

$$P_1 = p_1 + p_2, \quad P_2 = p_2, \quad Q_1 = q_1 \quad Q_2 = q_2 - q_1 . \tag{4.7}$$

This leads to a Hamiltonian in which P_2 does not appear, and consequently the relative position between the particles $Q_2 = q_2 - q_1$ is a constant of the motion. Namely

$$H_{Q_2}^{(2)} = \tfrac{1}{2}P_1^2 + s(e^{-2\,Q_1}(1+e^{-Q_2})^2 - 2\, e^{-Q_1}(1+e^{-Q_2})). \tag{4.8}$$

Note that Eq. (4.8) is a Morse-type problem depending on the constant parameter Q_2. Actually, in the limit $Q_2 \to \infty$ we recover the original Morse potential. It is worth recalling that this kind of parameter-dependent dynamics was already observed in Ref. 22, where the classical motion on the Poisson-Lie $sl(2)$ group was considered. On the other hand, it is immediate to check that the N-dimensional generalization of the system [Eq. (4.5)] can be reduced to the same type of one-dimensional Morse-type problem (now with $N-2$ parameters) through a canonical transformation containing the new total momenta $P_1 = \Sigma_{i=1}^{N} p_i$.

B. Deformed Morse systems

- The *standard* case. The phase space realization

$$\tilde{J}_3 = 2p_1, \quad \tilde{J}_+ = \tfrac{1}{2}e^{-q_1}, \quad \tilde{J}_- = -2\left(\frac{\sinh(z\,p_1)}{z}\right)^2 e^{q_1} - a\, e^{q_1}, \tag{4.9}$$

leads to the $sl_q(2)$ Poisson algebra [Eq. (2.4)]. Therefore, the one-particle Hamiltonian

$$\mathcal{H}_z = \tfrac{1}{8}\tilde{J}_3^2 - 4\, s\, \tilde{J}_+ + 4\, s\, \tilde{J}_+^2 , \tag{4.10}$$

does not change under deformation:

$$H_z = \tfrac{1}{2}p_1^2 + s\,(e^{-2\,q_1} - 2\, e^{-q_1}), \tag{4.11}$$

and the deformed Casimir element [Eq. (2.6)] is just $-a_1/2$.

Let us now construct the associated two-body integrable deformation. By applying the deformed coproduct onto Eq. (4.10) and with the aid of two copies of the realization [Eq. (4.9)] we get

$$H_z^{(2)} = \tfrac{1}{2}(p_1+p_2)^2 + s\,(e^{-2\,(q_1 - z\,p_2)} - 2\, e^{-(q_1 - z\,p_2)}) + s\,(e^{-2(q_2+zp_1)} - 2\, e^{-(q_2+zp_1)}) + 2\, s\, e^{-\{(q_1 - z\,p_2)+(q_2+zp_1)\}}. \tag{4.12}$$

If we substitute again in terms of P_1, we see that P_2 does appear within the Hamiltonian, and the deformation would imply that Q_2 is no longer a constant of motion (however, note the persistent coupling of the type $q_1 - z\,p_2$ and $q_2 + z\,p_1$). The constant of motion for [Eq. (4.12)] would be just the result of taking the phase-space realization of

$$C_z^{(2)} = \Delta_z(C_z) = \left(\frac{\sinh((z/2)\Delta_z(\tilde{J}_3))}{z}\right)^2 + \Delta_z(\tilde{J}_+)\,\Delta_z(\tilde{J}_-). \tag{4.13}$$

Explicitly, Eq. (4.13) gives the following two-particle function:

$$C_z^{(2)}=\left(\frac{\sinh(z(p_1+p_2))}{z}\right)^2-\left(\left(\frac{\sinh z\,p_2}{z}\right)^2+\frac{a_2}{2}\right)(e^{-2zp_1}+e^{-(q_1-q_2)-z\,(p_1-p_2)})$$
$$-\left(\left(\frac{\sinh z\,p_1}{z}\right)^2+\frac{a_1}{2}\right)(e^{2zp_2}+e^{(q_1-q_2)-z\,(p_1-p_2)}). \tag{4.14}$$

Note that the limit $z\to 0$ of Eq. (4.14) leads to Eq. (4.6).

• The *non-standard* case. The deformed phase-space realization corresponding to the $-a/2$ value of the deformed Casimir is now

$$\tilde{J}_3=2\,\frac{\sinh(h\,e^{-q_1}/2)}{(h\,e^{-q_1}/2)}p_1,\quad \tilde{J}_+=\frac{1}{2}\,e^{-q_1},$$
$$\tilde{J}_-=-2e^{q_1}\frac{\sinh(h\,e^{-q_1}/2)}{(h\,e^{-q_1}/2)}p_1^2-h\,\frac{a_1}{\sinh(h\,e^{-q_1}/2)}. \tag{4.15}$$

Therefore, the one-particle Hamiltonian

$$\mathcal{H}=\tfrac{1}{8}\tilde{J}_3^2-4\,s\,\tilde{J}_++4\,s\,\tilde{J}_+^2, \tag{4.16}$$

leads to:

$$H_h^{(2)}=\frac{1}{2}\left(\frac{\sinh(h\,e^{-q_1}/2)}{(h\,e^{-q_1}/2)}\right)^2p_1^2+s\,(e^{-2\,q_1}-2\,e^{-q_1}). \tag{4.17}$$

The two-particle Hamiltonian is obtained from the deformed coproduct [Eq. (2.8)] of Eq. (4.16):

$$H_h^{(2)}=\frac{1}{4}\left(e^{-\,(h/2)\,e^{-q_1}}2\,\frac{\sinh(h\,e^{-q_2}/2)}{(h\,e^{-q_2}/2)}p_2+2\,\frac{\sinh(h\,e^{-q_1}/2)}{(h\,e^{-q_1}/2)}e^{(h/2)\,e^{-q_2}}p_1\right)^2$$
$$+s\,(e^{-2\,q_1}-2\,e^{-q_1})+s\,(e^{-2\,q_2}-2\,e^{-q_2})+2\,s\,e^{-(\,q_1+q_2)}. \tag{4.18}$$

Again, the role of the p_1+p_2 dynamical variable is no longer relevant under deformation. The two-particle Casimir would be obtained as the phase-space realization of

$$\Delta_h(C_h)=\frac{1}{4}\,(\Delta_h(\tilde{J}_3))^2+\frac{\sinh(h\,\Delta_h(\tilde{J}_+))}{h}\Delta_h(\tilde{J}_-) \tag{4.19}$$

in terms of two copies of the non-standard deformation [Eq. (4.15)].

C. The Smorodinsky-Winternitz system

The following realization of $sl(2)$

$$J_3=p_1\,q_1,\quad J_+=\frac{1}{2}\,p_1^2+\frac{c_1}{q_1^2};\quad J_-=-\frac{1}{2}\,q_1^2 \tag{4.20}$$

underlies the $sl(2)$ dynamical symmetry of the harmonic oscillator potential with centrifugal term ($c_1>0$), since by defining

$$\mathcal{H}_c=J_+-\omega^2\,J_- \tag{4.21}$$

we obtain that

$$H=\frac{1}{2}\,(p_1^2+\omega^2\,q_1^2)+\frac{c_1}{q_1^2}. \tag{4.22}$$

Note that the Casimir function is related to the centrifugal term, since

$$C_c=\frac{1}{4}\,J_3^2+J_+\,J_-=\frac{-c_1}{2}. \tag{4.23}$$

The realization [Eq. (4.20)] exhibits a singularity at $J_-=0$: hence, even if the Poisson vector fields associated with Eq. (4.21) are of course complete, such completeness may not be guaranteed at the level of phase-space dynamics. In this particular example, a finite-time divergence arises when $c_1<0$. Actually, for each concrete symplectic realization, a careful analysis of the relation between the Poisson dynamics and the corresponding description(s) in terms of canonical variables is needed.

A two-particle Hamiltonian with coalgebra symmetry can be immediately derived by computing the coproduct of Eq. (4.21). Since this dynamical Hamiltonian is linear in the generators, we have that

$$H^{(2)}=\frac{1}{2}\,(p_1^2+p_2^2)+\frac{1}{2}\;\omega^2(q_1^2+q_2^2)+\frac{c_1}{q_1^2}+\frac{c_2}{q_2^2}, \tag{4.24}$$

in case we assume both phase-space representations not to be the same ($c_1\neq c_2$). This system is the well-known Smorodinsky-Winternitz Hamiltonian (SW),[10,11] and its Casimir function can be straightforwardly obtained through the coproduct of C_c in the actual representation, which reads

$$\Delta(C_c)=C^{(2)}(q_1,q_2,p_1,p_2)=-\frac{1}{4}\,(p_1q_2-p_2q_1)^2-\frac{(q_1^2+q_2^2)}{2}\left(\frac{c_1}{q_1^2}+\frac{c_2}{q_2^2}\right). \tag{4.25}$$

1. Integrable deformations of the SW system

The very same deformation machinery can be now used provided suitable deformed realizations generalizing Eq. (4.20) are found. Hereafter it will be useful to consider the function

$$I_{(1/2)}[t,x]:=\frac{\sinh(t\,x/2)}{t\,x}. \tag{4.26}$$

Note that $\lim_{t\to 0} I_{(1/2)}[t,x]=1/2$.

• The *standard* case. The deformed realization is

$$\begin{gathered}\tilde{J}_3=p_1\,q_1,\quad \tilde{J}_+=I_{(1/2)}[z,p_1\,q_1]\,p_1^2+\frac{1}{2\,I_{(1/2)}[z,p_1\,q_1]}\,\frac{c_1}{q_1^2},\\ \tilde{J}_-=-I_{(1/2)}[z,p_1\,q_1]\,q_1^2.\end{gathered} \tag{4.27}$$

The one-particle Hamiltonian derived from

$$\mathcal{H}_z=\tilde{J}_+-\omega^2\tilde{J}_- \tag{4.28}$$

that in this realization becomes:

$$H_z=I_{(1/2)}[z,p_1\,q_1](p_1^2+\omega^2q_1^2)+\frac{1}{2\,I_{(1/2)}[z,p_1\,q_1]}\,\frac{c_1}{q_1^2}. \tag{4.29}$$

The deformed Casimir function is again

$$C_z=\left(\frac{\sinh(z\,\tilde{J}_3/2)}{z}\right)^2+\tilde{J}_+\,\tilde{J}_-=\frac{-c_1}{2}. \tag{4.30}$$

When the deformed coproduct of Eq. (4.28) is realized in terms of two-phase space realizations of the type [Eq. (4.27)] it leads to the following integrable two-particle Hamiltonian:

$$\begin{aligned}H_z^{(2)}=&\left(I_{(1/2)}[z,p_1\,q_1](p_1^2+\omega^2q_1^2)+\frac{1}{2\,I_{(1/2)}[z,p_1\,q_1]}\,\frac{c_1}{q_1^2}\right)e^{z\,p_2q_2/2}\\&+\left(I_{(1/2)}[z,p_2\,q_2](p_2^2+\omega^2q_2^2)+\frac{1}{2\,I_{(1/2)}[z,p_2\,q_2]}\,\frac{c_2}{q_2^2}\right)e^{-z\,p_1q_1/2}\\=&H^{(2)}+z\left\{p_2\,q_2\left(\frac{1}{2}\,p_1^2+\frac{1}{2}\;\omega^2q_1^2+\frac{c_1}{q_1^2}\right)-p_1\,q_1\left(\frac{1}{2}\,p_2^2+\frac{1}{2}\;\omega^2q_2^2+\frac{c_2}{q_2^2}\right)\right\}+o[z^2].\end{aligned} \tag{4.31}$$

Note that this power series expansion shows how the undeformed one-particle Hamiltonians arises in the first order of the perturbation. As usual, the constant of the motion wil be given by Eq. (4.13) where we should use two copies of the proper realization Eq. (4.27). As a result, we obtain

$$\begin{aligned}C_z^{(2)}=&\left(\frac{\sinh(z(p_1+p_2)/2)}{z}\right)^2-\left\{e^{-z\,p_1\,q_1}\left(I_{(1/2)}[z,p_2\,q_2]^2\,p_2^2\,q_2^2+\frac{c_2}{2}\right)\right.\\&\left.+e^{z\,p_2\,q_2}\left(I_{(1/2)}[z,p_1\,q_1]^2\,p_1^2\,q_1^2+\frac{c_1}{2}\right)\right\}-I_{(1/2)}[z,p_1\,q_1]\,I_{(1/2)}[z,p_2\,q_2]\\&\times\left\{(\,p_1^2\,q_2^2+\,p_2^2\,q_1^2)+\frac{1}{2}\left(\frac{c_1}{I_{(1/2)}[z,p_1\,q_1]^2}\,\frac{q_2^2}{q_1^2}+\frac{c_2}{I_{(1/2)}[z,p_2\,q_2]^2}\,\frac{q_1^2}{q_2^2}\right)\right\}.\end{aligned} \tag{4.32}$$

A straightforward computation shows that the limit $z\to 0$ of this integral gives the undeformed one [Eq. (4.25)].

• The *non-standard* case. The deformed realization for the non-standard $sl_h(2)$ Poisson algebra with $\tilde{J}_-$ as primitive generator [Eq. (2.10)] is:

$$\tilde{J}_3=2\,I_{(1/2)}[h,q_1^2]\,q_1\,p_1,\quad \tilde{J}_+=I_{(1/2)}[h,q_1^2]\,p_1^2+\frac{c_1}{2\,I_{(1/2)}[h,q_1^2]\,q_1^2},\quad \tilde{J}_-=-\frac{1}{2}\;q_1^2. \tag{4.33}$$

If we consider again the dynamical one-particle Hamiltonian as

$$\mathcal{H}_h=\tilde{J}_+-\omega^2\tilde{J}_-, \tag{4.34}$$

we obtain the following deformation of Eq. (4.22):

$$H_h=p_1^2\,I_{(1/2)}[h,q_1^2]+\frac{1}{2}\;\omega^2\,q_1^2+\frac{c_1}{2\,I_{(1/2)}[h,q_1^2]\,q_1^2}. \tag{4.35}$$

The corresponding two-body system is, as usual, provided by the non-standard coproduct of the dynamical Hamiltonian [Eq. (4.34)], that reads

$$H_h^{(2)}=\left(I_{(1/2)}[h,q_1^2]p_1^2+\frac{c_1}{2\,I_{(1/2)}[h,q_1^2]\,q_1^2}\right)e^{-h\,q_2^2/2}+\left(I_{(1/2)}[h,q_2^2]p_2^2+\frac{c_2}{2\,I_{(1/2)}[h,q_2^2]\,q_2^2}\right)e^{h\,q_1^2/2}$$
$$+\frac{1}{2}\,\omega^2\,(q_1^2+q_2^2)=H^{(2)}+\frac{h}{2}\left\{q_1^2\left(\frac{1}{2}\,p_2^2+\frac{c_2}{q_2^2}\right)-q_2^2\left(\frac{1}{2}\,p_1^2+\frac{c_1}{q_1^2}\right)\right\}+o[h^2]. \tag{4.36}$$

Note that this power series expansion shows the presence of ''crossed'' oscillator and centrifugal terms coming from the deformation. Finally, the associated constant of the motion can be deduced from the coproduct of the non-standard Casimir equation (2.12) under two realizations of the type [Eq. (4.33)]. We recall that that the N-dimensional generalization of this non-standard deformation has been explicitly obtained in Ref. 4.

2. Coalgebra symmetry of the N=2 rational Calogero system

Let us now consider the $N=2$ rational Calogero Hamiltonian[12]

$$H_{\alpha,\beta}^{(2)}(Q,P)=\tfrac{1}{2}(P_1^2+P_2^2)+\Omega^2(Q_1^2+Q_2^2)+\frac{\alpha}{(Q_1-Q_2)^2}+\frac{\beta}{(Q_1+Q_2)^2}. \tag{4.37}$$

It turns out that the canonical transformation

$$Q_1:=(q_1+q_2)/2,\quad Q_2:=(q_2-q_1)/2,\quad P_1:=p_1+p_2,\quad P_2:=p_2-p_1 \tag{4.38}$$

leads to the identification

$$H_{\alpha,\beta}^{(2)}(Q,P)=2\,H^{(2)}(q,p), \tag{4.39}$$

where $H^{(2)}(q,p)$ is given by Eq. (4.24) with $\Omega^2=\omega^2/2$, $\alpha=2\,c_1$, and $\beta=2\,c_2$.

Therefore, the Calogero Hamiltonian [Eq. (4.37)] does have $sl(2)$ coalgebra symmetry, being canonically equivalent to the (non-deformed) coproduct of $\mathcal{H}:=2\,(J_+-\omega^2\,J_-)$ and provided that two appropriate (and in general, different) phase-space realizations of $sl(2)$ are considered. Moreover, an integral of the motion for Eq. (4.37) is immediately deduced from the coalgebra symmetry, since it will be given by the (canonically transformed) coproduct of the $sl(2)$ Casimir given by Eq. (4.25), namely:

$$C_{\alpha,\beta}^{(2)}(Q,P)=-\tfrac{1}{4}(P_1Q_2-P_2Q_1)^2-(Q_1^2+Q_2^2)\left(\frac{\alpha/2}{(Q_1-Q_2)^2}+\frac{\beta/2}{(Q_1+Q_2)^2}\right). \tag{4.40}$$

As a further consequence, the coalgebra symmetry provides a systematic procedure to get integrable deformations of the $N=2$ Calogero system. In particular, a factor two times the deformed Hamiltonians [Eqs. (4.31) and (4.36)] will give rise [respectively, and by using the inverse of the canonical transformation of Eq. (4.38)] to the standard and non-standard deformations of $H_{\alpha,\beta}^{(2)}(Q,P)$. Once again, corresponding deformed integrals would be given by the inverse canonical transformation of the coproduct of the deformed Casimirs in the original (q,p) variables.

V. TWO-PARTICLE REALIZATIONS AND 2 *N* DIMENSIONAL SYSTEMS

So far we have considered one-particle phase-space realizations of coalgebras, but this is not the most general possibility. For instance, the classical analogue of the so-called Jordan-Schwinger (JS) realization of $sl(2)$ would be

$$J_3=a_1^+\,a_1-b_1^+\,b_1=\mathcal{N}_1^a-\mathcal{N}_1^b,\quad J_+=b_1\,a_1^+,\quad J_-=a_1\,b_1^+, \tag{5.1}$$

where $\{a_1,a_1^+\}=\{b_1,b_1^+\}=1$. This realization can be used to construct integrable systems by using the coalgebra approach, but now each $sl(2)$ copy will have two degrees of freedom.

Therefore, Eq. (5.1) would give rise to a $2N$ dimensional system, whose complete integrability will be linked to the existence of $2N$ quantities in involution. N of them are provided from the previous formalism (the m-th coproducts of the Casimir and the N-th coproduct of the dynamical Hamiltonian). However, N more integrals are also available if we take into account that, under Eq. (5.1), the Casimir of $sl(2)$ is no longer a numerical constant, but a two-particle function. Namely,

$$C_i=\tfrac{1}{4}(J_3^i)^2+J_+^i\,J_-^i=\tfrac{1}{4}(a_i^+\,a_i+b_i^+\,b_i)^2=\tfrac{1}{4}(\mathcal{N}_i^a+\mathcal{N}_i^b)^2. \tag{5.2}$$

And we have N of this quantities (in terms of classical number operators) that, by construction, will commute with the N integrals coming from the coproduct. For instance, from Eq. (3.6) we find that the JS classical Gaudin magnet is

$$\begin{aligned}H_{\mathrm{JS}}^{(N)}&=\sum_{i=1}^{N}C_i+\sum_{i<j}^{N}\left(\tfrac{1}{2}J_3^iJ_3^j+J_-^iJ_+^j+J_+^iJ_-^j\right)\\&=\frac{1}{4}\sum_{i=1}^{N}(\mathcal{N}_i^a+\mathcal{N}_i^b)^2+\frac{1}{2}\sum_{i<j}^{N}(\mathcal{N}_i^a-\mathcal{N}_i^b)(\mathcal{N}_j^a-\mathcal{N}_j^b)+\sum_{i<j}^{N}(a_i^+\,b_j^+\,a_j\,b_i+b_i^+\,a_j^+\,b_j\,a_i).\end{aligned} \tag{5.3}$$

Therefore, this Hamiltonian is completely integrable, since it is in involution with both the C_i functions [Eq. (5.2)] and the ''lower dimensional'' Hamiltonians $H_{JS}^{(m)}$. Finally, we remark that the last term in Eq. (5.3) is just the classical counterpart of a long-range interacting system with a four-wave interaction Hamiltonian mixing each pair of sites (see Ref. 23 for related quantum optical integrable systems).

A. Jordan-Schwinger map and coalgebra structure

At this point, it becomes clear that a suitable deformation of the classical JS map [Eq. (5.1)] would give rise to a new class of $2N$ dimensional $sl_q(2)$ invariant Hamiltonians. The answer to this question can be directly related to the study of the reducibility properties of the classical JS map, and it will lead us to a new interesting type of coalgebra structures.

A straightforward computation shows that the $\overline{J_i}$ functions

$$\begin{aligned}\overline{J_3}&=\overline{\Delta}(J_3)=1\otimes J_3+J_3\otimes 1,\\ \overline{J_+}&=\overline{\Delta}(J_+)=1\otimes J_+-J_+\otimes 1,\\ \overline{J_-}&=\overline{\Delta}(J_-)=1\otimes J_--J_-\otimes 1\end{aligned} \tag{5.4}$$

close a $sl(2)$ algebra. We could now consider a pair of ''harmonic oscillator'' realizations-given by Eq. (4.20) with $c=0$-and obtain a realization of Eq. (5.4) on the two-particle phase space in the form

$$\overline{J_3}=p_1\,q_1+p_2\,q_2,\quad \overline{J_+}=\tfrac{1}{2}(p_1^2-p_2^2),\quad \overline{J_-}=-\tfrac{1}{2}(q_1^2-q_2^2). \tag{5.5}$$

Now, the following canonical transformation can be defined

$$p_1 = b_1 + \tfrac{1}{2}a_1^+, \quad q_1 = a_1 - \tfrac{1}{2}b_1^+,$$
$$p_2 = b_1 - \tfrac{1}{2}a_1^+, \quad q_2 = -a_1 - \tfrac{1}{2}b_1^+. \tag{5.6}$$

By substituting Eq. (5.6) into Eq. (5.5) we recover Eq. (5.1). Therefore, the JS realization is canonically equivalent to a ''fermionic coproduct'' [Eq. (5.4)] of two irreps of $sl(2)$. Note that the map $\overline{\Delta}$ defined by Eq. (5.4) is not coassociative since

$$(id \otimes \overline{\Delta}) \circ \Delta \neq (\overline{\Delta} \otimes id) \circ \overline{\Delta}. \tag{5.7}$$

The coalgebra structure allows us to perform the same trick in the deformed case, where we can obtain the deformed realization by setting

$$\overline{\Delta}_z(\tilde{J}_3) = 1 \otimes \tilde{J}_3 + \tilde{J}_3 \otimes 1,$$
$$\overline{\Delta}_z(\tilde{J}_+) = e^{-(z/2)\tilde{J}_3} \otimes \tilde{J}_+ - \tilde{J}_+ \otimes e^{(z/2)\tilde{J}_3}, \tag{5.8}$$
$$\overline{\Delta}_z(\tilde{J}_-) = e^{-(z/2)\tilde{J}_3} \otimes \tilde{J}_- - \tilde{J}_- \otimes e^{(z/2)\tilde{J}_3}.$$

These expressions are compatible with $sl_q(2)$ brackets [Eq. (2.4)] and define a non-cocommutative and non-coassociative homomorphism. From them, the $sl_q(2)$ generators can be expressed in terms of two phase-space realizations [Eq. (4.27)] with $c=0$:

$$\tilde{f}_3 = \overline{\Delta}_z(\tilde{J}_3) = p_1 q_1 + p_2 q_2,$$
$$\tilde{f}_+ = \overline{\Delta}_z(\tilde{J}_+) = e^{-(z/2) p_1 q_1} I_{(1/2)}[z, q_2 p_2]\, p_2^2 - I_{(1/2)}[z, q_1 p_1]\, p_1^2\, e^{(z/2) p_2 q_2}, \tag{5.9}$$
$$\tilde{f}_- = \overline{\Delta}_z(\tilde{J}_-) = -e^{-(z/2) p_1 q_1} I_{(1/2)}[z, q_2 p_2]\, q_2^2 + I_{(1/2)}[z, q_1 p_1]\, q_1^2\, e^{z/2 p_2 q_2}.$$

Now, if we apply the canonical transformation [Eq. (5.6)] onto the functions $\tilde{f}_i$, we shall obtain the appropriate standard deformation of the JS map [Eq. (5.1)], that can be recovered in the limit $z \to 0$.

Note that the q-deformation of the JS map has been treated in the previous literature[24] by making use of a deforming functional approach.[25,26] However, the discovery of its ''internal'' coalgebra structure makes it possible to give an answer in terms of the $su_q(2)$ properties. It is also worthy to stress that the non-standard deformation seems not to be compatible with such ''fermionic'' comultiplication.

Finally, we mention that the construction of a $2N$ dimensional standard deformation of the Gaudin-JS system [Eq. (5.3)] is straightforward by considering N copies of the deformed JS map [Eq. (5.9)] and by representing through them the N-th deformed coproduct of the standard $sl_q(2)$ Casimir [Eq. (2.6)]. The integrals of motion will be given by the M-th coproducts ($M = 2, \ldots, N-1$) of such deformed Casimir and by the N different functions C_i^z defined by the expressions of the $sl_q(2)$ Casimir on each copy of the JS realization.

VI. ON THE ROLE OF THE REPRESENTATION: BEYOND $sl(2)$

The aim of this Section is to emphasize that the coalgebra symmetry of the Hamiltonian can be used to obtain the full set of integrals of the motion provided that the initial phase space representation fulfills the sufficient conditions that have been stated in Sec. I. This has been the case for the examples presented so far, all of them based on $sl(2)$. As we shall see in the sequel, if we consider either non-simple algebras or higher rank ones, it could happen that the initial representation does not satisfy such requirements. In the cases presented here the integrals coming from the coproduct of the Casimirs turn out to be either trivial ones (Heisenberg-Weyl example) or

functionally dependent [$so(3,2)$ representation]. However, it is worth mentioning that certain deformations can help to overcome these restrictions, as we shall see in the Heisenberg-Weyl case.

A. Heisenberg-Weyl coalgebras

The Heisenberg-Weyl Poisson algebra h_3

$$\{A_-,A_+\}=M \quad \{A_-,M\}=0 \quad \{A_+,M\}=0 \tag{6.1}$$

is endowed with a Poisson coalgebra structure by means of the usual primitive coproduct

$$\Delta(M)=1\otimes M+M\otimes 1, \quad \Delta(A_\pm)=1\otimes A_\pm+A_\pm\otimes 1. \tag{6.2}$$

Note that the Casimir function for h_3 is just the central generator M. The natural phase-space realization for h_3 is given by

$$A_-=\omega_1 q_1, \quad A_+=p_1, \quad M=\omega_1. \tag{6.3}$$

If we consider the quadratic function

$$\mathcal{H}=A_+^2+A_-^2, \tag{6.4}$$

the associated one-particle Hamiltonian will be $H^{(1)}=p_1^2+\omega_1^2 q_1^2$, and the Casimir function is just the constant $C^{(1)}=M=\omega_1$. By following the coalgebra picture, the two-particle Hamiltonian $H^{(2)}=\Delta(\mathcal{H})$ reads:

$$H^{(2)}=p_1^2+p_2^2+\omega_1^2 q_1^2+\omega_2^2 q_2^2+2(p_1p_2+\omega_1\omega_2 q_1 q_2). \tag{6.5}$$

The constant of motion $C^{(2)}$ would be the coproduct of the Casimir $C^{(2)}=\Delta(C)=\omega_1+\omega_2$. Obviously, the generalization of this construction to N-particles will give the sum of the constants ω_i as the corresponding integrals. Therefore, the coalgebra symmetry is not able to provide a set of non-trivial constants of motion for this system (which is actually a completely integrable one).

However, this problem is surprisingly removed when we consider a certain quantum deformation of the Heisenberg-Weyl algebra. Let us introduce the quantum algebra $U_z(h_3)$ with deformed coproduct,[27]

$$\begin{aligned}
\Delta_z(A_-)&=1\otimes A_-+A_-\otimes 1\\
\Delta_z(A_+)&=e^{-zA_-}\otimes A_+ + A_+\otimes e^{zA_-}\\
\Delta_z(M)&=e^{-zA_-}\otimes M+M\otimes e^{zA_-}.
\end{aligned} \tag{6.6}$$

This coproduct is compatible with the non-deformed Poisson brakets [Eq. (6.1)]. As a consequence, the Casimir coincides again with M and the one-particle representation [Eq. (6.3)] also holds for the deformed case.

In fact, the deformation is restricted to the coproduct and, consequently, it will become apparent in the two-particle system. Although the phase-space realizations on each space are classical ones, their composition law [Eq. (6.6)] is not, and leads to the following two-particle functions

$$\begin{aligned}
\Delta_z(A_-)&=\omega_1 q_1+\omega_2 q_2\\
\Delta_z(A_+)&=p_2 e^{-z\omega_1 q_1}+p_1 e^{z\omega_2 q_2}\\
\Delta_z(M)&=\omega_2 e^{-z\omega_1 q_1}+\omega_1 e^{z\omega_2 q_2},
\end{aligned} \tag{6.7}$$

whose Poisson brackets will close again the h_3 Poisson algebra. If the function $\mathcal{H}$ given in Eq. (6.4) is considered, these expressions will lead to a deformed two-particle Hamiltonian

$$H_z^{(2)}=\Delta_z(\mathcal{H})=p_1^2\,e^{2z\omega_2 q_2}+p_2^2 e^{-2z\omega_1 q_1}+\omega_1^2 q_1^2+\omega_2^2 q_2^2+2\{p_1\,p_2 e^{-z(\omega_1 q_1-\omega_2 q_2)}+\omega_1\omega_2 q_1 q_2\}. \tag{6.8}$$

But now the deformed two-particle Casimir is no longer a constant:

$$C_z^{(2)}=\Delta_z(\mathcal{C})=\omega_1 e^{z\omega_2 q_2}+\omega_2 e^{-z\omega_1 q_1}. \tag{6.9}$$

Therefore, the non-primitive nature of the coproduct of the Casimir turns out to be an essential difference with respect to the non-deformed coalgebra and provides the non-trivial integral for the system (6.8).

B. A Poisson-$so(3,2)$ coalgebra

Finally, let us consider a representation of the Poisson $so(3,2)$ algebra with generators $\{E_0,E_\pm,F_0,F_\pm,C_\pm,D_\pm\}$ given by the two-particle functions

$$\begin{gathered} E_0=\tfrac{1}{2}p_1\,q_1,\quad E_+=\tfrac{1}{2}p_1^2,\quad E_-=\tfrac{1}{2}q_1^2,\\ F_0=\tfrac{1}{2}p_2\,q_2,\quad F_+=\tfrac{1}{2}p_2^2,\quad F_-=\tfrac{1}{2}q_2^2,\\ C_+=p_1\,q_2,\quad C_-=q_1\,p_2,\quad D_+=p_1\,p_2,\quad D_-=q_1\,q_2. \end{gathered} \tag{6.10}$$

The algebra $so(3,2)$ is of rank two (E_0 and F_0 are the generators of the Cartan sub-algebra) and, consequently, it has two independent Casimir functions,[28,29] that in this Poisson algebra context are given by

$$I_1=2\,(-E_0^2+E_+\,E_-)+2\,(-F_0^2+F_+\,F_-), \tag{6.11}$$

$$I_2=\{C_+,\Phi\}\,\{C_-,\Phi\}-\{D_+,\Phi\}\,\{D_-,\Phi\}-\Phi^2, \tag{6.12}$$

where $\Phi=(-E_0^2+E_+\,E_-)-(-F_0^2+F_+\,F_-)$ and $\{\cdot,\cdot\}$ is the Poisson bracket on $so(3,2)^*$. Note that in the representation [Eq. (6.10)] both Casimir functions vanish.

Obviously, the primitive coproduct $\Delta(X)=1\otimes X+X\otimes 1$ endows the $so(3,2)$ algebra with a coalgebra structure and the representation [Eq. (6.10)] has the same number of degrees of freedom as the rank of the algebra. A straightforward computation of the coproduct of the Casimir I_1 gives the four-particle integral

$$I_1^{(2)}=\Delta(I_1)=\tfrac{1}{2}(p_3\,q_1+p_4\,q_2-p_1\,q_3-p_2\,q_4)^2, \tag{6.13}$$

where the variables (p_3,q_3,p_4,q_4) come from to the second copy of the algebra. However, the coproduct of the second Casimir leads to a non-trivial second integral that is functionally dependent with respect to Eq. (6.13); namely $I_2^{(2)}=-(I_1^{(2)})^2/4$. As a consequence, the realization [Eq. (6.10)] of the $so(3,2)$ coalgebra can be used as the elementary block in order to construct N integrals of the motion in involution for a number of Hamiltonian systems with $2N$ degrees of freedom, but it does not account for the complete integrability of such systems. In this context, an interestingly open problem would be to determine whether some Poisson coalgebra deformation of $so(3,2)$ could break the functional dependence of the second set of corresponding (deformed) integrals.

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Superintegrability in a two-dimensional space of nonconstant curvature

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A Hamiltonian with two degrees of freedom is said to be superintegrable if it admits three functionally independent integrals of the motion. This property has been extensively studied in the case of two-dimensional spaces of constant (possibly zero) curvature when all the independent integrals are either quadratic or linear in the canonical momenta. In this article the first steps are taken to solve the problem of superintegrability of this type on an arbitrary curved manifold in two dimensions. This is done by examining in detail one of the spaces of revolution found by G. Koenigs. We determine that there are essentially three distinct potentials which when added to the free Hamiltonian of this space have this type of superintegrability. Separation of variables for the associated Hamilton–Jacobi and Schrödinger equations is discussed. The classical and quantum quadratic algebras associated with each of these potentials are determined. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1429322]

I. INTRODUCTION

A Hamiltonian system in classical mechanics with n degrees of freedom is described by a Hamiltonian function $H(x_1,\ldots,x_n,p_1,\ldots,p_n)=H(x,p)$. The dynamics of such a system is described by Hamilton's equations

$$\dot{x}_i=\frac{\partial H}{\partial p_i},\quad \dot{p}_i=-\frac{\partial H}{\partial x_i}. \tag{1}$$

The time rate of change of a classical observable $\ell=\ell(x,p)$ is given by

$$\frac{d\ell}{dt}=\{\ell,H\}=\sum_{i=1}^{n}\left(\frac{\partial \ell}{\partial x_i}\frac{\partial H}{\partial p_i}-\frac{\partial \ell}{\partial p_i}\frac{\partial H}{\partial x_i}\right), \tag{2}$$

where $\{,\}$ is the Poisson bracket. A Hamiltonian system is called "Liouville integrable" if it admits n functionally independent integrals of motion $\{X_1,\ldots,X_n\}$ which are mutually in involution, i.e.,

$$\{X_i,X_j\}=0,\quad i,j=1,\ldots,n, \tag{3}$$

where one of these constants can be taken to be the Hamiltonian H.[1,2] The system is superintegrable if a further m integrals $\{Y_1,\ldots,Y_m,1\leqslant m\leqslant n-1\}$ exist such that the set of constants $\{X_1=H,X_2,\ldots,X_n,Y_1,\ldots,Y_m\}$ is functionally independent. The additional integrals have vanishing

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Poisson bracket with H, but not necessarily with each other or with the X_i's. A classical Hamiltonian system is maximally superintegrable if $m=n-1$. There are then $2n-1$ functionally independent integrals of motion. The concepts of complete integrability and superintegrability have their analog in quantum mechanics. In this case a superintegrable quantum mechanical system is described by $n+m$ quantum observables $\{\hat{X}_1=\hat{H},\hat{X}_2,\ldots,\hat{X}_n,\hat{Y}_1,\ldots,\hat{Y}_m\}$ which satisfy the commutation relations

$$[\hat{H},\hat{X}_i]=\hat{H}\hat{X}_i-\hat{X}_i\hat{H}=0,\quad [\hat{H},\hat{Y}_j]=0,\quad [\hat{X}_i,\hat{X}_k]=0, \tag{4}$$

where $i,k=1,...,n$, $j=1,...,m$. For superintegrable classical Hamiltonian systems it is often the case that the elements of our set of constants are polynomial in the canonical momenta. The best known maximally superintegrable systems in Euclidean space E_n are the Kepler problem and the harmonic oscillator. All finite (bounded) trajectories in these two systems are closed. Moreover, these are the only spherically symmetric potentials for which all finite trajectories are closed.[3]

Systematic studies of superintegrable systems have been conducted for spaces of constant curvature in two and three dimensions.[4–10] In particular, a complete classification of all superintegrable systems in the real Euclidean spaces E_2 and E_3 with at most second order integrals of motion was given.[4–8] More recently, a relation between superintegrable systems and generalized Lie symmetries has been established,[11] as well as their relation to exactly solvable problems in quantum mechanics.[12] Recently[13–15] it has been possible to classify all maximally superintegrable systems for spaces of constant curvature (possibly zero) in two dimensions for which all the extra constants of the motion are at most quadratic in the canonical momenta.

A natural question to ask is whether the concept of superintegrability is restricted to spaces of constant curvature. The purpose of this article is to show that this is not so and to start a study of superintegrable systems in more general Riemannian, pseudo-Riemannian and complex Riemannian spaces. More specifically, we consider real two-dimensional spaces and search for Hamiltonian systems allowing additional constants of the motion that are at most quadratic in the momenta.

To make initial progress on this problem we first need to know which Riemannian spaces in two dimensions have associated with them more than one classical quadratic constant of the motion. This is a problem that has been comprehensively solved by Koenigs[16] in a note written in Vol. IV of the treatise of Darboux.[17]

In addition to being of intrinsic interest, additional motivation for this problem comes from the observation that all two-dimensional Riemannian spaces can be embedded in the three-dimensional Euclidean or pseudo-Euclidean space. Consequently, any such two-dimensional classical motion is equivalent to a constrained motion in three dimensions. It is also possible to interpret the motion, via general relativity, as motion in a two-dimensional gravitational field.

Given that we have a Riemannian space in two dimensions with infinitesimal distance

$$ds^2=g_{ij}(u)du^i du^j,\quad i,j=1,2, \tag{5}$$

and $u=(u^1,u^2)$, the classical Hamiltonian has the form

$$H=\tfrac{1}{2}g^{ij}p_i p_j+V(u) \tag{6}$$

and the corresponding Schrödinger equation can be taken to have the form

$$\hat{H}\Psi=-\frac{1}{2\sqrt{g}}\partial_{u^i}(\sqrt{g}g^{ik}\partial_{u^k}\Psi)+V(u)\Psi=E\Psi, \tag{7}$$

where $g=\det(g_{ij})$. For the classical Hamiltonian H our problem is to look for potentials $V(u)$ and Riemannian spaces specified by the metric g_{ij} for which there are at least two extra functionally independent constants of the motion of the form

$$\lambda_1=a^{ij}(u)p_i p_j+b(u) \tag{8}$$

or

$$\lambda_2 = a^i(u)p_i + c(u), \tag{9}$$

other than H. One well known way of solving the corresponding classical problem is to use Hamilton–Jacobi theory. The crucial equation to solve is then the Hamilton–Jacobi equation obtained from the equation $H=E$ via the substitution $p_i = \partial S/\partial u^i$, that is,

$$H = \frac{1}{2} g^{ij} \frac{\partial S}{\partial u^i} \frac{\partial S}{\partial u^j} + V(u) = E. \tag{10}$$

This equation is sometimes solvable by the method of separation of variables using the additive separation ansatz

$$S = S_1(u^1, \alpha, E) + S_2(u^2, \alpha, E). \tag{11}$$

The corresponding Schrödinger equation can also be solved by separation of variables with the product ansatz

$$\Psi = \psi_1(u^1, \lambda, E)\psi_2(u^2, \lambda, E). \tag{12}$$

The quantities λ_i are constants of the motion if

$$\{\lambda_i, H\} = 0. \tag{13}$$

For λ_2 this implies that $a^i(u)$ is a Killing vector and $a^i(u)p_i$ is a symmetry of the free Hamiltonian [H without $V(u)$]. In the case of λ_1 this implies that $a^{ij}(u)$ is a Killing tensor. Such tensors are directly related to the notion of additive separation as described above. We note that for constants of the type λ_2, the condition implies $c(u)=0$. It is also clear that for every constant linear in the momenta, its square is a constant quadratic in the momenta, that is, of the form of λ_1.

As mentioned earlier, Darboux and Koenigs have given a comprehensive analysis of when a two-dimensional Riemannian space admits more than one quadratic constant. In Sec. II we summarize some of these results.[16,17] In the remaining sections we concentrate on a particular space with a Killing vector and two Killing tensors. Section III deals with the free Hamilton–Jacobi equation and we show that the Schrödinger equation allows separation of variables in three different coordinates systems which we determine explicitly. Potentials that allow separation of variables in these systems are then introduced. In Sec. IV we find all potentials with this superintegrability property. We then discuss in Sec. V the various surfaces that may be represented by the infinitesimal distances that we have and the consequent special functions that arise from the corresponding Schrödinger equation.

II. ON GEODESICS WITH QUADRATIC INTEGRALS

In 1889 G. Koenigs[16] wrote a note in the last volume of Darboux's treatise "Théorie générale de surfaces," the title of which coincides with the title of this section. This note contains a summary of results which are the solution of the problem outlined in the Introduction, viz. when does the free Hamiltonian of a two-dimensional Riemannian space admit more than one quadratic constant of the motion. The analysis was performed over the field of complex numbers and must be modified over the reals. What Koenigs did was to write the infinitesimal distance for a general two-dimensional Riemannian space in the form

$$ds^2 = 4f(x,y)dxdy. \tag{14}$$

This can always be done in two dimensions over $\mathbb{C}$. The corresponding free Hamiltonian then has the form

$$H=\frac{1}{2f(x,y)}p_x p_y. \tag{15}$$

By making the requirement that there is a second order Killing tensor of the form

$$\lambda=a^{ij}(u)p_i p_j, \tag{16}$$

Darboux and Koenigs establish the following propositions.

(1) Any two-dimensional Riemannian space that admits more than one Killing vector must be a space of constant curvature and admit three linearly independent Killing vectors.
(2) Any two-dimensional Riemannian space that admits more than three Killing tensors is a space of constant curvature. It then actually admits five linearly independent Killing tensors which are all bilinear expressions in the Killing vectors. The sixth bilinear combination is the Hamiltonian itself.
(3) Any two-dimensional Riemannian space that admits precisely three linearly independent Killing tensors will be a Riemannian space of revolution. In fact, there will be one Killing vector and two Killing tensors.

Two-dimensional Riemannian spaces of this latter type were distinguished to be of four types. The infinitesimal distances of these types are given by

(I) $ds^2=(x+y)dxdy$,
(II) $ds^2=(a/(x-y)^2+b)dxdy$,
(III) $ds^2=(ae^{-(x+y)/2}+be^{-x-y})dxdy$,
(IV) $ds^2=(a(e^{(x-y)/2}+e^{(y-x)/2})+b)/(e^{(x-y)/2}-e^{(y-x)/2})^2\,dxdy$.

It is the first of these infinitesimal distances that we analyze in some detail in the next section. We shall call the spaces ''Darboux spaces'' and denote them by D_1, D_2, D_3 and D_4, respectively.

III. THE FREE PARTICLE AND SEPARATION OF VARIABLES IN A DARBOUX SPACE OF TYPE ONE

If we consider the first space of Darboux's list and look at real forms of this space only, it is convenient to make the new choice of variables

$$x=u+iv, \quad y=u-iv. \tag{17}$$

The corresponding infinitesimal distance can then be taken as

$$ds^2=2u(du^2+dv^2), \tag{18}$$

and the corresponding Hamiltonian has the form

$$H=\frac{1}{4u}(p_u^2+p_v^2). \tag{19}$$

Associated with this Hamiltonian are three integrals of the free motion, two quadratic and one linear:

$$\begin{aligned} K&=p_v, \quad X_1=p_u p_v-\frac{v}{2u}(p_u^2+p_v^2),\\ X_2&=p_v(vp_u-up_v)-\frac{v^2}{4u}(p_u^2+p_v^2). \end{aligned} \tag{20}$$

These three integrals satisfy the polynomial Poisson algebra relations,

$$\{K,X_1\}=2H, \quad \{K,X_2\}=-X_1, \quad \{X_1,X_2\}=2K^3. \tag{21}$$

They cannot be functionally independent and, in fact, satisfy the relation

$$4HX_2+X_1^2+K^4=0. \tag{22}$$

For the analogous quantum problem it is sufficient to consider the operators

$$\hat{H}=-\frac{1}{4u}(\partial_u^2+\partial_v^2), \quad \hat{K}=-i\partial_v,$$
$$\hat{X}_1=-\partial_u\partial_v+\frac{v}{2u}(\partial_u^2+\partial_v^2), \quad \hat{X}_2=-\frac{1}{2}[\partial_v, v\partial_u-u\partial_v]_+ +\frac{v^2}{4u}(\partial_u^2+\partial_v^2), \tag{23}$$

where $[A,B]_+=AB+BA$. The quantum versions of the quadratic constants are obtained via the formula

$$\hat{\lambda}=-\frac{1}{\sqrt{g}}\partial_i(a^{ij}\sqrt{g}\partial_j). \tag{24}$$

These operators have the same commutation relations as for the classical constants with the Poisson bracket replaced by the commutator bracket:

$$[\hat{K},\hat{X}_1]=2i\hat{H}, \quad [\hat{K},\hat{X}_2]=-i\hat{X}_1, \quad [\hat{X}_1,\hat{X}_2]=-2i\hat{K}^3. \tag{25}$$

There is also the operator relation

$$4\hat{H}\hat{X}_2+\hat{X}_1^2+\hat{K}^4=0. \tag{26}$$

The question we address in this section relates to the various possible ways that separation of variables can be achieved in the case of free classical motion or its quantum analogue, the free Schrödinger equation. The criteria for this to occur is the same in either case. Classically, if we have a general quadratic first integral λ and free Hamiltonian

$$H=\tfrac{1}{2}g^{ij}(u)p_ip_j, \tag{27}$$

and if the characteristic equation,

$$|a^{ij}-\rho g^{ij}|=0, \tag{28}$$

has two distinct roots ρ_1 and ρ_2, the Hamiltonian will have Liouville form when written in terms of the new variables ρ_1, ρ_2. That is,

$$H=\frac{\sigma(\rho_1)p_{\rho_1}^2+\tau(\rho_2)p_{\rho_2}^2}{\rho_1+\rho_2}. \tag{29}$$

In this form, both classical and quantum systems can be solved by the separation of variables ansatz.

If we want to classify all different separable coordinate systems for a given Hamiltonian, we need to know how many essentially different quadratic first integrals are possible. To decide on the notion of equivalence we first observe that the variable v does not explicitly appear in the metric tensor, that is, it is an ignorable variable. This means that the transformations $v\to v+b$ form a

one-dimensional Lie group. Accordingly, we determine the notion of equivalence to mean that two quadratic integrals are equivalent if they are related by a motion of this group. Consequently, the most general quadratic constant can be written

$$\lambda = aX_1 + bX_2 + cK^2 \tag{30}$$

to within the addition of a multiple of H. The second order elements X_i transform under the adjoint action according to

$$X_i \to \exp(\alpha K) X_i \exp(-\alpha K) = \exp(\alpha Ad(K)) X_i = X_i + \alpha\{K, X_i\} + \tfrac{1}{2}\alpha^2\{K,\{K,X_i\}\} + \ldots, \tag{31}$$

or specifically

$$X_1 \to X_1 + 2\alpha H, \quad X_2 \to X_2 - \alpha X_1 - \alpha^2 H. \tag{32}$$

There are three classes of possible quadratic first integrals under this equivalence relation. Typical representatives are

$$X_1 + aK^2, \quad X_2 + aK^2, \quad K^2. \tag{33}$$

We can now explicitly demonstrate the separable coordinates in each of these cases.

(1) *Separating coordinates associated with* $X_1 + aK^2$. If we choose a representative to be

$$L = X_1 + \sinh c\, K^2, \tag{34}$$

the corresponding roots of the characteristic equation and hence new variables are

$$r = \rho_1 = -2(Cu + v), \quad s = \rho_2 = \frac{2}{C}(u - Cv), \quad C = e^{-c}. \tag{35}$$

In terms of these coordinates the Hamiltonian has the form

$$H = \frac{2(C^2+1)^2}{C(s-r)}\left(\frac{1}{C^2}p_s^2 + p_r^2\right), \tag{36}$$

and the corresponding quadratic constant in these coordinates is

$$L = 2\frac{(C^2+1)^2}{C(s-r)}\left(\frac{r}{C^2}p_s^2 + s p_r^2\right). \tag{37}$$

(2) *Separating coordinates associated with* $X_2 + aK^2$. Taking the second representative in the list (33), that is, $L = X_2 + aK^2$, a convenient choice of new variables ξ, η is related to the roots ρ_i by

$$\rho_1 = \eta^2(2a - \eta^2), \quad \rho_2 = -\xi^2(2a + \xi^2). \tag{38}$$

The corresponding classical Hamiltonian then has the form

$$H = \frac{p_\xi^2 + p_\eta^2}{2(\xi^2 + \eta^2)(\xi^2 - \eta^2 + 2a)}. \tag{39}$$

The associated constant of the motion in the new coordinates ξ and η is

$$L = \frac{\eta^2(2a - \eta^2)p_\xi^2 - \xi^2(\xi^2 + 2a)p_\eta^2}{2(\xi^2 + \eta^2)(\xi^2 - \eta^2 + 2a)}. \tag{40}$$

The defining coordinates u,v are written in terms of the new coordinates ξ,η via

$$u=\tfrac{1}{2}(\xi^2-\eta^2)+a, \quad v=\xi\eta, \tag{41}$$

which looks like displaced parabolic coordinates in the u,v plane.

(3) *Separating coordinates associated with* K^2. For the last representative, K^2, we need only the coordinates u,v and to recognize the fact that $K=p_v$.

We conclude this section by discussing the solutions to the free particle and free Schrödinger equation in these three cases.

In case 1 above it is more convenient to choose the variables according to

$$u=r\cos\theta+s\sin\theta, \quad v=-r\sin\theta+s\cos\theta. \tag{42}$$

The classical Hamilton–Jacobi equation then has the form

$$H=\frac{(\partial S/\partial r)^2+(\partial S/\partial s)^2}{4(r\cos\theta+s\sin\theta)}=E, \tag{43}$$

which has the general separable solution

$$S=S_1(r)+S_2(s)=\frac{(4Er\cos\theta-\lambda)^{3/2}}{6E\cos\theta}+\frac{(4Es\sin\theta+\lambda)^{3/2}}{6E\sin\theta}. \tag{44}$$

The corresponding free Schrödinger equation

$$\hat{H}\Psi=-\frac{1}{4(r\cos\theta+s\sin\theta)}(\partial_r^2+\partial_s^2)\Psi=E\Psi \tag{45}$$

has the typical product solutions

$$\Psi=\sqrt{\left(r-\frac{\mu}{4E\cos\theta}\right)\left(s+\frac{\mu}{4E\sin\theta}\right)}\,C_{1/3}\left(\frac{2}{3}\sqrt{4E\cos\theta}\left(r-\frac{\mu}{4E\cos\theta}\right)^{3/2}\right)$$
$$\times C_{1/3}\left(\frac{2}{3}\sqrt{4E\sin\theta}\left(s+\frac{\mu}{4E\sin\theta}\right)^{3/2}\right), \tag{46}$$

where $C_\nu(z)$ is a solution of Bessel's equation.

In the second case the classical Hamilton–Jacobi equation is

$$H=\frac{(\partial S/\partial\xi)^2+(\partial S/\partial\eta)^2}{2(\xi^2+\eta^2)(\xi^2-\eta^2+2c)}=E \tag{47}$$

and has a general solution of the form

$$S=\int\sqrt{2E\xi^4+2Ec\xi^2-\lambda}\,d\xi+\int\sqrt{-2E\eta^4+2Ec\eta^2+\lambda}\,d\eta, \tag{48}$$

which can be expressed in terms of elliptic integrals. The corresponding Schrödinger equation has a solution of the form $\Psi=\psi_1(\xi)\psi_2(\eta)$, where the ψ_i satisfy

$$(\partial_\xi^2+2E\xi^4+4Ec\xi^2+\lambda)\psi_1(\xi)=0,$$
$$(\partial_\eta^2-2E\eta^4+4Ec\eta^2-\lambda)\psi_2(\eta)=0. \tag{49}$$

These equations are readily identified as the equations for the anharmonic oscillator.

In the third case the classical Hamilton-Jacobi equation is

$$H=\frac{1}{4u}\left(\left(\frac{\partial S}{\partial u}\right)^2+\left(\frac{\partial S}{\partial v}\right)^2\right)=E, \tag{50}$$

which has separable solutions

$$S=\frac{1}{6E}(4Eu-k^2)^{3/2}+kv. \tag{51}$$

The separable solutions to the corresponding free Schrödinger equation

$$-\frac{1}{4u}(\partial_u^2+\partial_v^2)\Psi=E\Psi \tag{52}$$

have the form

$$\Psi=\sqrt{u-\frac{m^2}{4E}}C_{1/3}\left(\frac{2}{3}\sqrt{4E}\left(u-\frac{m^2}{4E}\right)^{3/2}\right)e^{imv}. \tag{53}$$

It is clear that the actual solutions to the classical motion or the corresponding Schrödinger equation depend on the range of values assumed by the various real variables, that is, on exactly which real manifold we are considering.

IV. INTEGRABLE AND SUPERINTEGRABLE SYSTEMS FOR THE DARBOUX SPACE OF TYPE ONE

In this section we address the problem of superintegrability for the Hamiltonian

$$H=\frac{1}{4u}(p_u^2+p_v^2), \tag{54}$$

that is, look for potentials $V(u,v)$ for which

$$\overline{H}=H+V(u,v) \tag{55}$$

admits at least two extra quadratic integrals. The way to solve this problem is as follows. First we consider that we already have one quadratic first integral

$$\overline{L}=a(u,v)p_u^2+b(u,v)p_up_v+c(u,v)p_v^2+d(u,v). \tag{56}$$

We know that the quadratic part of $\overline{L}$ [i.e., that part obtained by putting $d(u,v)=0$ in (56)] must correspond to one of the three possibilities outlined in the previous section. For each of these possibilities separation of variables is possible in coordinates α,β where $u=u(\alpha,\beta)$, $v=v(\alpha,\beta)$. The addition of a potential implies that separation is preserved. As a consequence of this, $\overline{H}$ can be written as

$$\overline{H}=\frac{p_\alpha^2+p_\beta^2+f(\alpha)+g(\beta)}{\sigma(\alpha)+\tau(\beta)} \tag{57}$$

and the corresponding first integral will be

$$\overline{L}=\frac{\sigma(\alpha)(p_\beta^2+g(\beta))-\tau(\beta)(p_\alpha^2+f(\alpha))}{\sigma(\alpha)+\tau(\beta)}. \tag{58}$$

The next step is to impose the condition that there is a further quadratic first integral and see what conditions this imposes on the functions $f(\alpha)$ and $g(\beta)$. If we do these calculations systematically, we arrive at the following three cases.

(1)

$$H=\frac{p_u^2+p_v^2}{4u}+\frac{b_1(4u^2+v^2)}{4u}+\frac{b_2}{u}+\frac{b_3}{uv^2}. \tag{59}$$

The additional constants of the motion have the form

$$R_1=X_2-\frac{b_1v^4}{4u}-\frac{b_2v^2}{u}-\frac{b_3(4u^2+v^2)}{v^2u},\quad R_2=K^2+b_1v^2+\frac{4b_3}{v^2} \tag{60}$$

and the corresponding quadratic algebra[18,19] relations are determined by

$$\begin{gathered}\{R,R_1\}=8HR_1+6R_2^2+16b_2R_2-32b_1b_3,\\ \{R,R_2\}=-8HR_2-16b_1R_1,\\ R^2=-16HR_1R_2-4R_2^3-16b_2R_2^2-64b_3H^2-16b_1R_1^2+64b_1b_3R_2+256b_1b_2b_3,\end{gathered} \tag{61}$$

where $R=\{R_1,R_2\}$. The Hamiltonian clearly separates in the coordinates u and v as well as the coordinates ξ,η given by $u=\frac{1}{2}(\xi^2-\eta^2)+a$, $v=\xi\eta$. This can be seen from the explicit form

$$H=\frac{p_\xi^2+p_\eta^2}{2(\xi^2+\eta^2)(\xi^2-\eta^2+2a)}+\frac{b_1((\xi^2-\eta^2+2a)^2+\xi^2\eta^2)+4b_2+(4b_3/\xi^2\eta^2)}{2(\xi^2-\eta^2+2a)}. \tag{62}$$

The corresponding quadratic quantum algebra relations are

$$\begin{gathered}[\hat R,\hat R_1]=-6\hat R_2^2-8\hat H\hat R_1+16b_2\hat R_2+2b_1(3+16b_3),\\ [\hat R,\hat R_2]=8\hat H\hat R_2-16b_1\hat R_1,\\ \hat R^2=+4\hat R_2^3-8\hat H[\hat R_1,\hat R_2]_+-16b_2\hat R_2^2-16b_1\hat R_1^2-4b_1(11+16b_3)\hat R_2\\ -4(3+16b_3)\hat H^2+16b_1b_2(3+16b_3),\end{gathered} \tag{63}$$

where $\hat R=[\hat R_1,\hat R_2]$.

(2)

$$H=\frac{p_u^2+p_v^2}{4u}+\frac{a_1}{u}+\frac{a_2v}{u}+\frac{a_3(u^2+v^2)}{u}. \tag{64}$$

The additional constants of the motion have the form

$$\begin{gathered}R_1=X_1-\frac{2a_1v}{u}+\frac{2a_2(u^2-v^2)}{u}+\frac{2a_3v(u^2-v^2)}{u},\\ R_2=K^2+4a_2v+4a_3v^2,\end{gathered} \tag{65}$$

and the corresponding quadratic algebra relations are determined by

$$\{R,R_1\}=-8H^2+16a_3R_2+8(a_2^2+4a_1a_3),$$

$$\{R,R_2\}=16a_2H-16a_3R_1, \tag{66}$$

$$R^2=16H^2R_2-16a_3R_2^2+32a_2HR_1-16a_3R_1^2-16(a_2^2+4a_1a_3)R_2-64a_1a_2^2.$$

If we change the coordinates according to $u=r\cos\theta+s\sin\theta$, $v=-r\sin\theta+s\cos\theta$, the Hamiltonian assumes the form

$$H=\frac{p_r^2+p_s^2+4a_1+4a_2(-r\sin\theta+s\cos\theta)+4a_3(r^2+s^2)}{4(r\cos\theta+s\sin\theta)}, \tag{67}$$

which clearly also separates in these coordinates.

The commutation relations of the corresponding quantum algebra are

$$[\hat{R},\hat{R}_1]=16a_3\hat{R}_2+8\hat{H}^2-8(a_2^2+4a_1a_3),$$

$$[\hat{R},\hat{R}_2]=-16a_3\hat{R}_1+16a_2\hat{H}, \tag{68}$$

$$\hat{R}^2=-16a_3\hat{R}_2^2-16a_3\hat{R}_1^2+16\hat{H}^2\hat{R}_2+32a_2\hat{H}\hat{R}_1-16(a_2^2+4a_1a_3)\hat{R}_2+64(a_3^2-a_1a_2^2).$$

(3) The third potential gives rise to a Hamiltonian of the form

$$H=\frac{p_u^2+p_v^2}{4u}+\frac{a}{u}. \tag{69}$$

There are three extra constants associated with this Hamilonian,

$$R_1=X_1-\frac{2av}{u},\quad R_2=X_2-\frac{av^2}{u}\quad\text{and}\quad K. \tag{70}$$

The associated Poisson bracket relations are

$$\{K,R_1\}=2H,\quad \{K,R_2\}=-R_1,\quad \{R_1,R_2\}=2K(K^2+2a), \tag{71}$$

and the corresponding functional relation among these constants is

$$4HR_2+R_1^2+K^4+4aK^2=0. \tag{72}$$

The commutation relations associated with the corresponding quantum problem have the form

$$[\hat{K},\hat{R}_1]=2i\hat{H},\quad [\hat{K},\hat{R}_2]=-i\hat{R}_1,\quad [\hat{R}_1,\hat{R}_2]=-2i\hat{K}(\hat{K}^2-2a), \tag{73}$$

and the identity amongst the defining operators is

$$4\hat{H}\hat{R}_2+\hat{R}_1^2+\hat{K}^4-4a\hat{K}^2=0. \tag{74}$$

Upon examination of the various superintegrable potentials we have constructed, we see that by multiplying the equation $H=E$ by a suitable factor we essentially recover a variant of one of the superintegrable systems already classified for spaces of constant (or zero) curvature. For the first potential above, the equation $H=E$ may be written

$$p_u^2+p_v^2+b_1(4u^2+v^2)+4b_2+\frac{4b_3}{v^2}-4Eu=0. \tag{75}$$

This equation is known to have separable solutions in coordinates u, v and associated parabolic coordinates ξ,η given by $u=\frac{1}{2}(\xi^2-\eta^2)$, $v=\xi\eta$. With the second potential, $H=E$ becomes

$$p_u^2+p_v^2+4a_3(u^2+v^2)+4a_1+4a_2v-4Eu=0, \tag{76}$$

and the third becomes

$$p_u^2+p_v^2-4Eu+4a=0. \tag{77}$$

This observation is crucial to the whole program that we will undertake which aims at finding all superintegrable systems associated with a curved space in two dimensions and having quadratic constants.

All three of the above systems are special cases of the superintegrable systems found in E_2.[4,11] They were shown to be exactly solvable in Ref. 12.

V. EMBEDDINGS OF A DARBOUX SPACE OF REVOLUTION OF TYPE ONE

It is clear that the infinitesimal distance

$$ds^2=2u(du^2+dv^2) \tag{78}$$

does not uniquely determine a manifold. This then gives rise to the question of just what sort of surfaces can this infinitesimal distance represent. A particular choice of such a surface would determine the range of variation of the parameters u, v which in turn enables the solution of the geodesic equations in the case of classical mechanics and the quantum mechanics of a point particle. It is known that any two-dimensional Riemannian space can be embedded in a three-dimensional Euclidean space of indefinite or definite signature. In this section we look at a number of natural embeddings and discuss their associated geodesics and quantum mechanics. The infinitesimal distance that we are dealing with can be embedded in three-dimensional Euclidean space E_3 via the formulas

$$X=\sqrt{2u}\cos v, \quad Y=\sqrt{2u}\sin v, \tag{79}$$

$$Z=\frac{\sqrt{2}}{3}\left(F\left(\varphi,\frac{1}{\sqrt{2}}\right)+\sqrt{4u^3-u}\right), \tag{80}$$

where $u\geqslant\frac{1}{2}$, $v_0\leqslant v\leqslant 2\pi+v_0$, $\sin\varphi=\sqrt{2u+1}$ and $F(\varphi,k)$ is an elliptic integral of the first kind. This embedding gives the infinitesimal distance

$$dX^2+dY^2+dZ^2=2u(du^2+dv^2). \tag{81}$$

To do quantum mechanics on this surface let us first look for separable solutions to the free Schrödinger equation. A typical solution has already been found in the previous section, viz.

$$\Psi=\sqrt{u-\frac{m^2}{4E}}\,C_{1/3}\left(\frac{2}{3}\sqrt{4E}\left(u-\frac{m^2}{4E}\right)^{3/2}\right)e^{imv}, \tag{82}$$

where m is an integer. As $u\geqslant\frac{1}{2}$ and we see that $u=\frac{1}{2}$ is not a singular point of the separable equation in u, we can impose a condition of the form

$$a\Psi(\tfrac{1}{2},v)+b\Psi_u(\tfrac{1}{2},v)=0 \tag{83}$$

together with the periodic boundary condition $\Psi(u,v)=\Psi(u,v+2\pi)$, which is already satisfied. If we take $a=1$, $b=0$, then $E\geqslant 0$, otherwise there is no solution satisfying the boundary condition at $u=\frac{1}{2}$. If $E\geqslant 0$, then we can find a suitably behaved solution that vanishes as $u\to\infty$ and satisfies the boundary condition at $u=\frac{1}{2}$, viz.

$$\Psi=(UU')^{1/2}(J_{1/3}(U)J_{-1/3}(U')-J_{1/3}(U')J_{-1/3}(U)), \tag{84}$$

where $U=\frac{2}{3}\sqrt{4E}(u-m^2/4E)^{3/2}$ and $U'=\frac{2}{3}\sqrt{4E}(\frac{1}{2}-m^2/4E)^{3/2}$. These solutions are the analog of the scattering states on this manifold subject to the boundary condition we have adopted.

An interesting embedding in pseudo-Euclidean space is given by

$$X=\sqrt{2u}v, \quad Y=\sqrt{u}(\tfrac{4}{5}u^2-v^2+\tfrac{1}{2}), \quad T=\sqrt{u}(\tfrac{4}{5}u^2-v^2-\tfrac{1}{2}), \tag{85}$$

for which $dX^2+dY^2-dT^2=2u(du^2+dv^2)$. In this case the variables vary over the ranges $-\infty<v<\infty$, $0\leqslant u<\infty$. We could indeed do an analysis of the free Schrödinger equation on this surface and come to a similar conclusion if we imposed the condition that the wave function is zero at $u=0$. However, if we consider the first potential (59) and choose $b_1=-\beta^2$, $b_3=\frac{1}{4}(\frac{1}{4}-\gamma^2)$ for real β and $\gamma\geqslant 0$, and if we write the solutions to Schrödinger's equation in the form $\Psi=U(u)V(v)$, then two independent solutions of the separation equation satisfied by V can be taken as

$$V_{\pm}=\exp\left(-\frac{1}{2}\beta v^2\right)v^{\pm\gamma+1/2}{}_1F_1\left(\frac{1}{2}(1\pm\gamma)-\frac{\mu}{\beta},1\pm\gamma,\beta v^2\right). \tag{86}$$

If we wish to interpret these solutions as being associated with an angle variable which varies in the range $0<v_0\leqslant v\leqslant v_0+2\pi$, then we would require the periodic boundary conditions

$$V(v_0)=V(v_0+2\pi), \quad V'(v_0)=V'(v_0+2\pi). \tag{87}$$

The possibility of imposing these boundary conditions depends on whether $v=0$ occurs inside the domain of v. If it does not, then the spectrum is determined from the condition

$$W[V_+(x)-V_+(x+2\pi),V_-(x)-V_-(x+2\pi)]\big|_{x=v_0}=0. \tag{88}$$

If $v=0$ is included, then the same conditions no longer work as this is a regular singular point of the equation. Indeed, if $v_0=0$ and we assume $\gamma>\frac{1}{2}$, then we choose the solution V_+ and impose the condition

$$V_+(2\pi)=0 \tag{89}$$

as $V_+(0)$ is already zero. The quantization condition is then determined by

$${}_1F_1\left(\frac{1}{2}(1+\gamma)-\frac{\mu}{\beta},1+\gamma,4\beta\pi^2\right)=0. \tag{90}$$

For the u separation equation the range of variation of the variable $u>\frac{1}{2}$ is clear and $u=\frac{1}{2}$ is not a singularity of the the separation equation. We can accordingly take typical solutions to be

$$U_{\pm}(u)=a_1D_\nu\left(2\sqrt{\beta}\left(u-\frac{E}{2\beta^2}\right)\right)+a_2D_\nu\left(-2\sqrt{\beta}\left(u-\frac{E}{2\beta^2}\right)\right), \tag{91}$$

where $\nu=(1/4\beta)(E^2/\beta^2+4b_2-\mu)-\frac{1}{2}$. To obtain a solution that vanishes as $u\to\infty$ requires that $a_2=0$. The remaining boundary condition becomes

$$D_\nu\left(2\sqrt{\beta}\left(\frac{1}{2}-\frac{E}{2\beta^2}\right)\right)=0. \tag{92}$$

This condition determines the nature of the discrete spectrum. For large eigenvalues the discrete spectrum is given by

$$E\cong-2\sqrt{\beta^3 n} \tag{93}$$

for suitable large integer n.

If we consider the second potential (64), then putting $a_3=-\alpha^2$ the equation for $V(v)$ has solutions of the form

$$V=d_1D_\nu\left(2\sqrt{\alpha}\left(v-\frac{a_2}{2\alpha^2}\right)\right)+d_2D_\nu\left(-2\sqrt{\alpha}\left(v-\frac{a_2}{2\alpha^2}\right)\right)=d_1V_+ + d_2V_-, \tag{94}$$

where

$$\nu=\frac{1}{4\alpha}\left(4\mu+\frac{a_2^2}{\alpha^2}\right)-\frac{1}{2}. \tag{95}$$

As there are no singularities in v in this equation and we can require that $w_0\leqslant v\leqslant w_0+2\pi$,

$$V(w_0)=V(w_0+2\pi), \quad V'(w_0)=V'(w_0+2\pi), \tag{96}$$

which is equivalent to

$$W[V_+(x)-V_+(x+2\pi),V_-(x)-V_-(x+2\pi)]|_{x=w_0}=0. \tag{97}$$

The solutions for the function $U(u)$ that are well behaved for large u are

$$U(u)=D_\rho\left(2\sqrt{\alpha}\left(u-\frac{E}{2\beta^2}\right)\right), \tag{98}$$

where $\rho=(1/4\beta)(4a_1-4\mu+E^2/\alpha^2)-\frac{1}{2}$.

VI. CONCLUSION

In this article we have examined one of the four spaces of revolution listed by Koenigs.[16] For the space that we have considered, it has been shown that there are three potentials that can be added to give superintegrable Hamiltonian systems of the type we seek. In each of these cases we have exhibited the various inequivalent ways in which a separation of variables can be achieved for both the classical and quantum equations that result. This is equivalent to determining the various inequivalent ways in which a Hamiltonian can be written in Liouville form (57) for suitable separable coordinates α, β. In particular, we note that each of the three superintegrable systems we have examined are such that when we write out the classical equation $H=E$ and factor out the denominator we recover a variant of a superintegrable system corresponding to flat space.[4] This is an example of what is called coupling-constant metamorphosis.[20] It has been proven in Ref. 12 that all of the superintegrable systems in the plane are such that the bound state energies can be calculated algebraically. In all cases the Hamiltonian lies in the enveloping algebra of $sl(3,\mathbb{R})$. We conclude that analogous statements apply to the superintegrable systems that we have found.

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Dark soliton generation for the intermediate nonlinear Schrödinger equation

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The generation of dark solitons due to a small change of the initial data is studied within the framework of the intermediate nonlinear Schrödinger (INLS) equation. In particular, we analyze the spectral problem associated with the INLS equation when the potential consists of a small perturbation imposed on a constant background. We derive a criterion for the perturbation to generate a pair of new discrete eigenvalues as well as their explicit expressions in terms of the perturbation. In addition, we demonstrate that the eigenvalues appear without a threshold on the magnitude of the perturbation. We also consider both the shallow- and deep-water limits of various results obtained for the INLS spectral problem. In the former case, the limiting procedure can be performed smoothly whereas in the latter case, the spectral equation exhibits a new feature of bound states, showing that the eigenvalue is exponentially small compared with the magnitude of the perturbation. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1430623]

I. INTRODUCTION

It is well known that the nonlinear Schrödinger (NLS) equation describes the long-term evolution of a quasiharmonic wave on the surface of a liquid layer.[1] Recently, a similar nonlinear evolution equation was derived in the context of internal (or interfacial) waves.[2,3] It can be written in an appropriate dimensionless form as follows:

$$iu_t = u_{xx} + u(i + \dot{T})(|u|^2)_x . \tag{1.1a}$$

Here, $u = u(x,t)$ is a complex function representing the envelope of the wave, T is an integral operator defined by

$$Tu(x,t) = \frac{1}{2\delta} P \int_{-\infty}^{\infty} \coth\left[\frac{\pi(y-x)}{2\delta}\right] u(y,t)\mathrm{d}y, \tag{1.1b}$$

where δ ia a parameter proportional to the depth of the fluid, the symbol P stands for the Cauchy principal value integral, and the subscripts t and x appended to u denote partial differentiation. It has been demonstrated that the constant state $u = \rho$ is modulationally stable against infinitesimal perturbation[2] and as a result, Eq. (1.1) has a dark soliton solution of the form[2]

$$u = \rho \frac{1 + \dfrac{V - i\kappa}{V + i\kappa} e^{-\kappa(\xi - i\delta)}}{1 + e^{-\kappa(\xi - i\delta)}}, \quad |u|^2 = \rho^2 - \frac{\kappa \sin(\kappa\delta)}{\cosh(\kappa\xi) + \cos(\kappa\delta)}, \tag{1.2}$$

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where $\xi=x-Vt-x_0$ and V is determined by the algebraic equation $V^2+2\rho^2V+\kappa^2=2\rho^2\kappa\cot(\kappa\delta)$ (κ: positive constant, x_0: real constant). The profile of $|u|^2$ shows a dip on a constant background. It is noteworthy that the general N-soliton solution is now available which represents the interaction of N dark solitons.[2,4,5]

In the shallow-water limit $\delta\to 0$, Eq. (1.1) reduces to the defocusing NLS equation

$$iu_{\tilde{t}}=u_{\tilde{x}\tilde{x}}-\tilde{u}(|\tilde{u}|^2-\rho^2),\quad \tilde{u}=\tilde{u}(\tilde{x},\tilde{t}), \tag{1.3}$$

after rescaling the variables x, t, and u according to the relations $x=\sqrt{\delta}\tilde{x}$, $t=\delta\tilde{t}$, and $u(x,t)=\tilde{u}(\tilde{x},\tilde{t})$, respectively, where the expansion $Tf_x=-\delta^{-1}f+O(\delta)$ was used together with the boundary condition $|u|\to\rho,|x|\to\infty$. In the deep-water limit $\delta\to\infty$, on the other hand, Eq. (1.1) reduces simply to the nonlocal NLS equation

$$iu_t=u_{xx}+u(i+H)(|u|^2)_x, \tag{1.4a}$$

with the Hilbert transform operator H defined by

$$Hu(x,t)=\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{u(y,t)}{y-x}\mathrm{d}y. \tag{1.4b}$$

Thus, Eq. (1.1) is an intermediate version of Eqs. (1.3) and (1.4) and hence it is referred to as the intermediate nonlinear Schrödinger (INLS) equation.[2]

The initial value problem of Eq. (1.1) under the boundary condition $|u|\to\rho,|x|\to\infty$ has been solved by means of the inverse scattering transform (IST) method.[5] It turns out that Eq. (1.1) has common properties to completely integrable nonlinear evolution equation such as N-soliton solution, Bäcklund transformation, and infinite number of conservation laws. However, it should be remarked that its complete integrability is still an open problem. Although a number of works have been done for the defocusing NLS equation (1.3),[6,7] many open problems are left for the nonlocal NLS equation (1.4). In particular, the deep-water limit $\delta\to\infty$ of the IST scheme for the INLS equation would exhibit a novel feature to be resolved by a new method. Thus, the initial value problem of Eq. (1.4) is left for a future work. As for exact solutions, however, the multiperiodic and multisoliton solutions have recently been constructed[8] without recourse to the IST and the stability of the latter solution has been proved.[9]

The linear system (or the so-called Lax pair) associated with Eq. (1.1) is given by[5]

$$i\phi_x-\frac{\mu}{2}\phi+u\psi^+=0, \tag{1.5a}$$

$$\psi^+-\lambda\psi^-+u^*\phi=0, \tag{1.5b}$$

$$i\phi_t+i\mu\phi_x+\phi_{xx}-2iu_x\psi^++\nu\phi=0, \tag{1.5c}$$

$$i\psi_t^{\pm}+i\mu\psi_x^{\pm}+\psi_{xx}^{\pm}+[(\pm i+T)(|u|^2)_x+\nu]\psi^{\pm}=0. \tag{1.5d}$$

Here, $\phi=\phi(x,t)$ and $\psi^{\pm}=\psi^{\pm}(x,t)$ are Jost functions and λ, μ, and ν are constants related to a spectral parameter where $\psi^{\pm}(x,t)\equiv\psi(x\mp i\delta,t)$ represent the boundary values of functions analytic in the horizontal strip between $\mathrm{Im}\,x=0$ and $\mathrm{Im}\,x=\pm 2\delta$ and the asterisk appended to u denotes the complex conjugate.

In this paper, we shall deal with the problem of soliton generation within the framework of system (1.5). Our main concern here is as to whether a small initial data can support new eigenvalues. To be more specific, we consider the following initial data:

$$u(x,0)=\rho+\epsilon v(x), \tag{1.6}$$

where $\rho(>0)$ is the boundary value of u as $|x|\to\infty$, $v(x)$ is a complex function decreasing at infinity, and ϵ is a small positive parameter so that ϵv represents a perturbation imposed on a constant background. It is important that the above-noted initial data exhibit no phase change when x varies from $-\infty$ to $+\infty$. However, we can impose the more general boundary condition such that $u(x,0)\to\rho e^{-i\phi}(x\to-\infty)$ and $u(x,0)\to\rho(x\to\infty)$ where ϕ is a real constant. A simple example is given by the initial condition $u(x,0)=\rho e^{-i\phi}(x<0)$, $u(x,0)=\rho(x>0)$, which shows a phase step on a constant background. In this case, we can solve the eigenvalue problem (1.5) explicitly and obtain the equation $\tan(\phi/2)=\kappa/\mu$ that determines the eigenvalue κ where $\mu=\mu(i\kappa)$ satisfies the equation $\mu^2+2\rho^2\mu+\kappa^2=2\rho^2\kappa\cot(\kappa\delta)$. Comparing this equation with (1.2), one sees that $\mu=V=-\rho^2\pm\sqrt{\rho^4-\kappa^2+2\rho^2\kappa\cot(\kappa\delta)}\equiv\mu_{\pm}$. Thus, the above-noted initial data produce a single dark soliton whose amplitude and velocity are determined uniquely by the phase change ϕ. Note in particular that if the phase change is very small, i.e., $0<\phi\ll 1$, then $\kappa\simeq\mu\phi/2$ and $\mu=\mu_{+}\simeq-\rho^2+\sqrt{\rho^4+(2\rho^2/\delta)}$, implying the generation of a small dark soliton with a positive velocity. Another important example of the background field is provided by a single soliton solution (1.2). Obviously, this exhibits a finite phase change when x varies from $-\infty$ to ∞. It turns out that the generation of solitons due to small perturbation is a difficult problem to be handled by means of the Fourier transform method developed in this paper. One needs to solve the eigenvalue equation with variable coefficient. This issue is, however, beyond the scope of the present paper.

We now summarize the main result in this paper as follows: if the condition

$$\int_{-\infty}^{\infty}(v(x)+v^*(x))\mathrm{d}x<0 \tag{1.7}$$

is satisfied, then a small initial data generate a pair of new discrete eigenvalues (i.e., new solitons) in the linear spectral problem (1.5). These eigenvalues are found to emerge from the edge of the continuous spectrum without a *threshold* on the amplitude of the perturbation ϵv. We also show that the similar conclusion holds for both shallow- and deep-water limits. In connection with the problem under consideration, it is worth mentioning that the soliton generation by a small change of the initial date was studied recently in the context of the Benjamin–Ono (BO),[10] intermediate long wave (ILW),[11] and Kadomtsev–Petviashvili (KPI)[12] equations. It was demonstrated that the linear systems associated with the BO and ILW equations exhibit a thresholdless generation of a new eigenvalue whereas for the KPI equation, the corresponding linear system yields a threshold generation.

In Sec. II, we analyze the eigenvalue problem [(1.5a), (1.5b)] with the initial data (1.6). We first transform Eqs. (1.5a) and (1.5b) to an equivalent system of integral equations by using the Fourier transform and then employ a systematic perturbation method to obtain new eigenvalues. The criterion (1.7) is established for the generation of a pair of new eigenvalues. The explicit expressions of new eigenvalues as well as the corresponding eigenfunctions are obtained in terms of the initial disturbance v. In Sec. III, the shallow-water limit $\delta\to 0$ is taken straightforwardly for the expressions of the eigenvalues and eigenfunctions derived in Sec. II. We recover the first-order correction to the eigenvalues which has already been obtained by a different method.[13] We emphasize that the second-order correction is presented here for the first time. In Sec. IV, we consider the deep-water limit $\delta\to\infty$. We find that unlike the shallow-water limit, this limiting procedure yields no meaningful results. In particular, the eigenvalues are shown to vanish identically. This fact would imply that the order of the limits $\epsilon\to 0$ and $\delta\to\infty$ cannot be interchanged. Hence, we start from a system of integral equations equivalent to the eigenvalue problem associated with the nonlocal NLS equation (1.5). By developing the similar analysis to that used for finite δ, we obtain a criterion for a new eigenvalue to emerge from a small change of the initial data. The resulting eigenvalue is found to be exponentially small compared with ϵ. Section V is devoted to concluding remarks. In Appendix A, we describe some properties of a function as well as those of the spectral parameters μ and λ, which play important roles in developing the perturbation analysis. In Ap-

pendix B, we investigate the asymptotic behavior of the two-soliton solution of the INLS equation and show that the solution can be used to simulate a pair of dark solitons produced by a small perturbation.

II. EIGENVALUE PROBLEM ASSOCIATED WITH THE INLS EQUATION

A. Eigenvalue problem

We start our analysis with the system of eigenvalue equations (1.5a) and (1.5b) subjected to the initial data (1.6). It reads in the form

$$i\phi_x - \frac{\mu}{2}\phi + \rho\psi^+ = -\epsilon v\psi^+, \tag{2.1a}$$

$$\psi^+ - \lambda\psi^- + \rho\phi = -\epsilon v^*\phi. \tag{2.1b}$$

In the following, we focus our attention on the spatial part of the Lax pair since the temporal part is used only for determining the time dependence of the spectral parameters. We first specify the asymptotic forms of the Jost functions ϕ and ψ as $\phi \sim e^{\pm ikx/2}$, $\psi \sim e^{\pm ikx/2}$ where k is a spectral parameter. Then, the constants μ and λ are related to k by the following relations:[5]

$$\mu^2 + 2\rho^2\mu = 2\rho^2 k\coth(k\delta) + k^2, \tag{2.2a}$$

$$\lambda = \frac{k}{k\cosh(k\delta) - \mu\sinh(k\delta)}. \tag{2.2b}$$

It has been shown that the nth zero $k_n = i\kappa_n$, $0 < \kappa_n < \kappa_c$ of the scattering data corresponds to the nth soliton[5] where κ_c is a solution of the equation $\kappa_c \tan(\kappa_c\delta/2) = \rho^2$. Hence, we assume $\mu = \mu(i\kappa)$ and $\lambda = \lambda(i\kappa)$ $(0 < \kappa \ll 1)$ in (2.1) and solve it by using a perturbation method.

It is convenient to rewrite Eq. (2.1) into an equivalent system of integral equations. For this purpose, we decompose ϕ and $\psi^{\pm}$ in the form of the Fourier integral as

$$\phi(x) = \int_{-\infty}^{\infty} \alpha(k) e^{ikx/2}\,dk, \tag{2.3a}$$

$$\psi^{\pm}(x) = \int_{-\infty}^{\infty} \beta(k) e^{ik(x \mp i\delta)/2}\,dk. \tag{2.3b}$$

Substituting (2.3) into (2.1) and taking the inverse Fourier transform, we obtain the following system of integral equations for α and β:

$$-\frac{1}{2}\{k + \mu(i\kappa)\}\alpha(k) + \rho e^{k\delta/2}\beta(k) = -\frac{\epsilon}{4\pi}\int_{-\infty}^{\infty} K(k,k')e^{k'\delta/2}\beta(k')dk', \tag{2.4a}$$

$$\rho\alpha(k) + \{e^{k\delta/2} - \lambda(i\kappa)e^{-k\delta/2}\}\beta(k) = -\frac{\epsilon}{4\pi}\int_{-\infty}^{\infty} K^*(k',k)\alpha(k')dk', \tag{2.4b}$$

where we have put

$$K(k,k') = \int_{-\infty}^{\infty} v(x)e^{-i(k-k')x/2}\,dx, \tag{2.4c}$$

for simplicity. If we introduce the new variables A and B according to

$$A(k) = D(k,\kappa)\alpha(k), \tag{2.5a}$$

$$B(k)=D(k,\kappa)\beta(k)e^{k\delta/2}, \tag{2.5b}$$

with

$$D(k,\kappa)=-\tfrac{1}{2}\{k+\mu(i\kappa)\}\{1-\lambda(i\kappa)e^{-k\delta}\}-\rho^2, \tag{2.5c}$$

Eq. (2.4) can be put into the form

$$A(k)=\frac{\epsilon\rho}{4\pi}\int_{-\infty}^{\infty}\frac{K^*(k',k)}{D(k',\kappa)}A(k')\mathrm{d}k'-\frac{\epsilon}{4\pi}\{1-\lambda(i\kappa)e^{-k\delta}\}\int_{-\infty}^{\infty}\frac{K(k,k')}{D(k',\kappa)}B(k')\mathrm{d}k', \tag{2.6a}$$

$$B(k)=\frac{\epsilon}{8\pi}\{k+\mu(i\kappa)\}\int_{-\infty}^{\infty}\frac{K^*(k',k)}{D(k',\kappa)}A(k')\mathrm{d}k'+\frac{\epsilon\rho}{4\pi}\int_{-\infty}^{\infty}\frac{K(k,k')}{D(k',\kappa)}B(k')\mathrm{d}k'. \tag{2.6b}$$

The above-noted system of integral equations for $A(k)$ and $B(k)$ is the starting point of the following analysis. It is crucial to observe that the quantity $D(k',\kappa)$ in the integrand in (2.6) has zeros at $k'=\pm i\kappa$. To show this, we take the limit $|x|\to\infty$ in (2.1), use the asymptotic form ϕ, $\psi\sim e^{ikx/2}$ and obtain the relation

$$1-\lambda(k)e^{-k\delta}=-\frac{2\rho^2}{k+\mu(k)}. \tag{2.7}$$

Combining (2.7) with (2.5c) yields

$$D(k,\kappa)=-\frac{1}{2}\{k+\mu(i\kappa)\}\{\lambda(k)-\lambda(i\kappa)\}e^{-k\delta}-\rho^2\frac{\mu(k)-\mu(i\kappa)}{k+\mu(k)}. \tag{2.8}$$

Since $\mu(k)=\mu(-k)$, $\lambda(k)=\lambda(-k)$ by (2.2), one can see that $D(\pm i\kappa,\kappa)=0$. The function $D(k,\kappa)$ plays an important role in developing the perturbation analysis. Some properties of $D(k,\kappa)$ are summarized in Appendix A for later use. Thus, we see that the integrand in (2.6) exhibits singularities in the limit of $\kappa\to 0$. It turns out that these singularities become the origin of the generation of new eigenvalues, as will be demonstrated in the following. In order to regularize the singular behavior in each integrand, we modify the integral by subtracting the contribution from the two poles $k'=\pm i\kappa$ as

$$\int_{-\infty}^{\infty}\frac{K^*(k',k)}{D(k',\kappa)}A(k')\mathrm{d}k'=\int_{-\infty}^{\infty}\frac{1}{k'^2+\kappa^2}\left[\frac{k'^2+\kappa^2}{D(k',\kappa)}K^*(k',k)A(k')\right.$$
$$\left.-\{C_R(\kappa)k'+C_I(\kappa)\kappa\}K^*(0,k)A(0)\right]\mathrm{d}k'+\pi C_I(\kappa)K^*(0,k)A(0), \tag{2.9a}$$

where

$$C_R(\kappa)=\frac{1}{D_k(i\kappa,\kappa)}+\frac{1}{D_k(-i\kappa,\kappa)}, \tag{2.9b}$$

$$C_I(\kappa)=i\left[\frac{1}{D_k(i\kappa,\kappa)}-\frac{1}{D_k(-i\kappa,\kappa)}\right], \tag{2.9c}$$

$$D_k(\pm i\kappa,\kappa)=\left[\frac{\partial D(k,\kappa)}{\partial k}\right]_{k=\pm i\kappa}. \tag{2.9d}$$

Substituting (2.9) and an analogous expression for B into (2.6), we obtain the system of equations for A and B:

$$A(k)=\frac{\epsilon}{4}C_I(\kappa)[\rho K^*(0,k)A(0)-\{1-\lambda(i\kappa)e^{-k\delta}\}K(k,0)B(0)]$$
$$+\frac{\epsilon\rho}{4\pi}\left[\int_{-\infty}^{\infty}\frac{1}{k'^2+\kappa^2}\left\{\frac{k'^2+\kappa^2}{D(k',\kappa)}K^*(k',k)A(k')\right.\right.$$
$$\left.\left.-(C_R(\kappa)k'+C_I(\kappa)\kappa)K^*(0,k)A(0)\right\}dk'\right]-\frac{\epsilon}{4\pi}\{1-\lambda(i\kappa)e^{-k\delta}\}$$
$$\times\left[\int_{-\infty}^{\infty}\frac{1}{k'^2+\kappa^2}\left\{\frac{k'^2+\kappa^2}{D(k',\kappa)}K(k,k')B(k')\right.\right.$$
$$\left.\left.-(C_R(\kappa)k'+C_I(\kappa)\kappa)K(k,0)B(0)\right\}dk'\right], \tag{2.10a}$$

$$B(k)=\frac{\epsilon}{4}C_I(\kappa)\left[\frac{1}{2}\{k+\mu(i\kappa)\}K^*(0,k)A(0)+\rho K(k,0)B(0)\right]+\frac{\epsilon}{8\pi}\{k+\mu(i\kappa)\}$$
$$\times\left[\int_{-\infty}^{\infty}\frac{1}{k'^2+\kappa^2}\left\{\frac{k'^2+\kappa^2}{D(k',\kappa)}K^*(k',k)A(k')-(C_R(\kappa)k'+C_I(\kappa)\kappa)K^*(0,k)A(0)\right\}dk'\right]$$
$$+\frac{\epsilon\rho}{4\pi}\left[\int_{-\infty}^{\infty}\frac{1}{k'^2+\kappa^2}\left\{\frac{k'^2+\kappa^2}{D(k',\kappa)}K(k,k')B(k')-(C_R(\kappa)k'+C_I(\kappa)\kappa)K(k,0)B(0)\right\}dk'\right]. \tag{2.10b}$$

B. Perturbation analysis

1. Leading-order analysis

Now, we solve (2.10) by means of a perturbation method. We expand A, B, and κ in powers of ϵ as

$$A(k)=A_0(k)+\epsilon A_1(k)+\cdots, \tag{2.11a}$$

$$B(k)=B_0(k)+\epsilon B_1(k)+\cdots, \tag{2.11b}$$

$$\kappa=\epsilon\kappa_1+\epsilon^2\kappa_2+\cdots, \tag{2.11c}$$

substitute these expressions as well as (A1) and (A6) into (2.10), and compare the coefficient of ϵ^n $(n=0,1,\ldots)$ on both sides. At $O(\epsilon^0)$, one obtains

$$A_0(k)=-\frac{1}{2\kappa_1\lambda_0\delta(1-(\delta\mu_0/2))}[\rho K^*(0,k)A_0(0)-(1-\lambda_0e^{-k\delta})K(k,0)B_0(0)], \tag{2.12a}$$

$$B_0(k)=-\frac{1}{2\kappa_1\lambda_0\delta(1-(\delta\mu_0/2))}\left[\frac{1}{2}(k+\mu_0)K^*(0,k)A_0(0)+\rho K(k,0)B_0(0)\right]. \tag{2.12b}$$

The constants λ_0 and μ_0 are given explicitly by (A2a). If we put $k=0$ in (2.12), we have

$$(z+\rho K^*(0,0))A_0(0)-(1-\lambda_0)K(0,0)B_0(0)=0, \tag{2.13a}$$

$$\tfrac{1}{2}\mu_0K^*(0,0)A_0(0)+(z+\rho K(0,0))B_0(0)=0, \tag{2.13b}$$

where

$$z \equiv 2\kappa_1 \lambda_0 \delta (1 - \tfrac{1}{2}\delta\mu_0). \tag{2.13c}$$

The compatibility condition for (2.13) now yields the following algebraic equation for z:

$$(z+\rho K^*(0,0))(z+\rho K(0,0)) + \tfrac{1}{2}\mu_0(1-\lambda_0)K^*(0,0)K(0,0) = 0. \tag{2.14}$$

In view of relation (A3a) as well as the condition $z \neq 0$, we can find the solution of Eq. (2.14) that determines κ_1,

$$z = -\rho(K(0,0)+K^*(0,0)). \tag{2.15}$$

Using (2.13c), (A2a), and (A3b), this expression can be rewritten in an explicit form as

$$\kappa_1 = -\frac{\rho}{2\delta}\frac{1-\delta\mu_0}{1-(\delta\mu_0/2)}(K(0,0)+K^*(0,0)) = -\frac{\rho}{2\delta}\left(1 \mp \frac{1}{\sqrt{1+(2/\delta\rho^2)}}\right)(K(0,0)+K^*(0,0)). \tag{2.16}$$

The condition $\kappa > 0$ implies $\kappa_1 > 0$ when $\epsilon \to 0$ by virtue of (2.11c). Thus, the condition $\kappa_1 > 0$ is equivalent to

$$K(0,0)+K^*(0,0) \equiv \int_{-\infty}^{\infty} (v(x)+v^*(x))\mathrm{d}x < 0. \tag{2.17}$$

Under condition (2.17), the small perturbation on the constant background always generates two discrete eigenvalues whose explicit values are given by (2.16). These correspond to a pair of dark solitons of the form (1.2) with the amplitude parameters $\kappa \equiv \kappa_\pm$ and corresponding velocities $V \equiv V_\pm$ given, respectively, by

$$\kappa \sim \epsilon\kappa_1, \quad V = \mu(i\kappa) \sim \mu_0 + \mu_1(\epsilon\kappa_1)^2 = -\rho^2 \pm \sqrt{\rho^4 + \frac{2\rho^2}{\delta}} \mp \frac{2(1+\frac{2}{3}\rho^2\delta)}{\sqrt{\rho^4+(2\rho^2/\delta)}}(\epsilon\kappa_1)^2. \tag{2.18}$$

Note that the $\pm$ sign in κ and V is ordered vertically. The two solitons thus generated propagate to opposite directions with different amplitudes and velocities. This two-soliton state may be approximated by a two-soliton solution[2,4,5] of the INLS equation with the soliton parameters given by (2.18). See Appendix B for details. It should be stressed that the generation of solitons occurs without a threshold on the magnitude of the perturbation to a constant background. In Fig. 1, we display the three-dimensional plot of a two-soliton solution (B1). The soliton parameters are chosen in accordance with (2.18). Explicitly, $\rho = \delta = 1$, $\epsilon = 0.2$, $k_1 = \kappa_+ = 0.2$, $k_2 = \kappa_- = 0.746$, $v_1 = V_+ = 0.655$, $v_2 = V_- = -1.66$, $x_{10} = x_{20} = 0$. The amplitude of each soliton may be defined as $\kappa \tan(\kappa\delta/2)$, which is equal to the maximum value of the dip of $|u|^2$ [see (1.2)]. In the above-given example, the amplitude ratio is found to be 14.5. In the shallow-limit $\delta \to 0$, this ratio approaches 1 while in the deep-water limit $\delta \to \infty$, it increases indefinitely. As will be demonstrated in Sec. III, the former case represents the generation of two solitons with equal amplitude and opposite velocities.

It now follows from (2.13) and (2.15) that

$$A_0(0) = -\frac{1}{\rho}(1-\lambda_0)B_0(0). \tag{2.19}$$

Substituting (2.19) into (2.12), we obtain the leading terms for the coefficients $A(k)$ and $B(k)$,

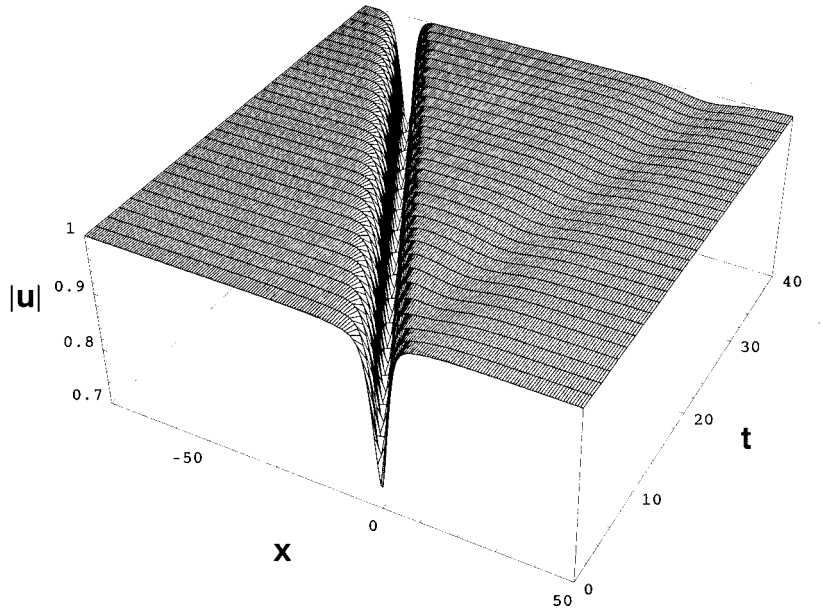

FIG. 1. Plot of a two-soliton solution of the INLS equation. The solution simulates a two-soliton state generated by a small perturbation.

$$A_0(k)=-\frac{1}{z}\left[\rho K^*(0,k)+\rho\frac{1-\lambda_0 e^{-k\delta}}{1-\lambda_0}K(k,0)\right]A_0(0), \tag{2.20a}$$

$$B_0(k)=-\frac{1}{z}\left[\rho K(k,0)-\frac{1}{2\rho}(1-\lambda_0)(k+\mu_0)K^*(0,k)\right]B_0(0). \tag{2.20b}$$

The eigenfunctions corresponding to the eigenvalue $\kappa\sim\epsilon\kappa_1$ are given from (2.3), (2.5), and (2.20) as

$$\phi(x)=-\frac{A_0(0)}{z}\int_{-\infty}^{\infty}\frac{\rho K^*(0,k)+\rho\dfrac{1-\lambda_0 e^{-k\delta}}{1-\lambda_0}K(k,0)}{D(k,\kappa)}e^{ikx/2}\,dk+O(\epsilon), \tag{2.21a}$$

$$\psi^{\pm}(x)=-\frac{B_0(0)}{z}\int_{-\infty}^{\infty}\frac{\rho K(k,0)-\dfrac{1}{2\rho}(1-\lambda_0)(k+\mu_0)K^*(0,k)}{D(k,\kappa)}e^{-k\delta/2}e^{ik(x\mp i\delta)/2}\,dk+O(\epsilon). \tag{2.21b}$$

The unknown constants $A_0(0)$ and $B_0(0)$ are fixed by specifying the asymptotic behavior of these eigenfunctions for large $|x|\sim O(1/\epsilon)$. We first observe that in view of (A4) the function $D(k,\kappa)$ behaves like

$$D(k,\kappa)=-\frac{1}{2}\lambda_0\delta\left(1-\frac{1}{2}\delta\mu_0\right)\left(k^2+\frac{(1-\lambda_0)\mu_1-\lambda_1\mu_0}{\lambda_0\delta(1-(\delta\mu_0/2))}\kappa^2\right)+O(\kappa^2 k), \tag{2.22}$$

for small k and κ. The coefficient of κ^2 in (2.22) is seen to be 1 by (A3c). Thus, we evaluate (2.21) with the aid of the Cauchy residue theorem to obtain

$$\phi(x)=\frac{2\pi A_0(0)}{\epsilon\kappa_1 z}\,\frac{\rho\{K(0,0)+K^*(0,0)\}}{\lambda_0\delta(1-(\delta\mu_0/2))}e^{-\epsilon\kappa_1|x|/2}+O(\epsilon), \tag{2.23a}$$

$$\psi^{\pm}(x)=\frac{2\pi B_0(0)}{\epsilon\kappa_1 z}\,\frac{\rho\{K(0,0)+K^*(0,0)\}}{\lambda_0\delta(1-(\delta\mu_0/2))}e^{-\epsilon\kappa_1|x|/2}+O(\epsilon). \tag{2.23b}$$

If we choose $A_0(0),B_0(0)\sim O(\epsilon)$, then (2.23) represent appropriate asymptotic forms for the bound states corresponding to the eigenvalues $\mu(i\kappa)$ given by (2.18).

2. Second-order analysis

We now proceed to the second-order analysis. The main purpose here is to derive the expression of the second-order correction κ_2 to the eigenvalue κ in terms of the initial data v. It follows from the $O(\epsilon)$ terms of (2.10) that

$$\begin{aligned}A_1(k)=&-\frac{1}{z}\Bigg[\rho K^*(0,k)A_1(0)-(1-\lambda_0e^{-k\delta})K(k,0)B_1(0)\\&-\frac{\kappa_2}{\kappa_1}\{\rho K^*(0,k)A_0(0)-(1-\lambda_0e^{-k\delta})K(k,0)B_0(0)\}\Bigg]\\&+\frac{\rho}{4\pi}\Bigg[P\int_{-\infty}^{\infty}\frac{1}{k'^2}\Bigg\{\frac{k'^2}{D(k',0)}K^*(k',k)A_0(k')\\&+\frac{2}{\lambda_0\delta(1-(\delta\mu_0/2))}K^*(0,k)A_0(0)\Bigg\}\mathrm{d}k'\Bigg]\\&-\frac{1}{4\pi}(1-\lambda_0e^{-k\delta})\Bigg[P\int_{-\infty}^{\infty}\frac{1}{k'^2}\Bigg\{\frac{k'^2}{D(k',0)}K^*(k,k')B_0(k')\\&+\frac{2}{\lambda_0\delta(1-(\delta\mu_0/2))}K^*(0,k)B_0(0)\Bigg\}\mathrm{d}k'\Bigg],\end{aligned} \tag{2.24a}$$

$$\begin{aligned}B_1(k)=&-\frac{1}{z}\Bigg[\frac{1}{2}(k+\mu_0)K^*(0,k)A_1(0)+\rho K(k,0)B_1(0)\\&-\frac{\kappa_2}{\kappa_1}\Bigg\{\frac{1}{2}(k+\mu_0)K^*(0,k)A_0(0)+\rho K(k,0)B_0(0)\Bigg\}\Bigg]+\frac{1}{8\pi}(k+\mu_0)\\&\times\Bigg[P\int_{-\infty}^{\infty}\frac{1}{k'^2}\Bigg\{\frac{k'^2}{D(k',0)}K^*(k',k)A_0(k')+\frac{2}{\lambda_0\delta(1-(\delta\mu_0/2))}K^*(0,k)A_0(0)\Bigg\}\mathrm{d}k'\Bigg]\\&+\frac{\rho}{4\pi}\Bigg[P\int_{-\infty}^{\infty}\frac{1}{k'^2}\Bigg\{\frac{k'^2}{D(k',0)}K(k,k')B_0(k')+\frac{2}{\lambda_0\delta(1-(\delta\mu_0/2))}K(0,k)B_0(0)\Bigg\}\mathrm{d}k'\Bigg],\end{aligned} \tag{2.24b}$$

where

$$D(k,0)=-\tfrac{1}{2}(k+\mu_0)(1-\lambda_0e^{-k\delta})-\rho^2, \tag{2.24c}$$

by (2.5c). We see from (A4) that for small k, $D(k,0)$ behaves like

$$D(k,0)=-\tfrac{1}{2}\lambda_0\delta(1-\tfrac{1}{2}\delta\mu_0)k^2+O(k^3). \tag{2.25}$$

Hence, the principal value should be taken for all the integrals in (2.24) since the integrands behave like k'^{-1} when $k'\to 0$. If we put $k=0$ in (2.24) and eliminate $A_1(0)$ and $B_1(0)$ with use of (2.15) and (A3a), we obtain

$$\frac{\kappa_2 z}{\kappa_1}[\rho K^*(0,0)A_0(0)-(1-\lambda_0)K(0,0)B_0(0)] + \frac{\rho z^2}{4\pi}P\int_{-\infty}^{\infty}\frac{1}{k^2}\left\{\frac{k^2}{D(k,0)}K^*(k,0)A_0(k)+\frac{4\kappa_1}{z}K^*(0,0)A_0(0)\right\}dk - \frac{1-\lambda_0}{4\pi}z^2P\int_{-\infty}^{\infty}\frac{1}{k^2}\left\{\frac{k^2}{D(k,0)}K(0,k)B_0(k)+\frac{4\kappa_1}{z}K(0,0)B_0(0)\right\}dk=0. \quad (2.26)$$

Last, introducing (2.19), (2.20), and (A2) into (2.26), we arrive at an explicit expression of κ_2 as follows:

$$\kappa_2=-\frac{\rho^2\kappa_1}{4\pi z}P\int_{-\infty}^{\infty}\frac{1}{k^2}\left[\frac{k^2}{D(k,0)}\left\{(K(0,k)+K^*(k,0))(K(k,0)+K^*(0,k)) - \frac{1}{\delta\mu_0}(1-e^{-k\delta})K(k,0)K^*(k,0)+\frac{1}{\mu_0}kK(0,k)K^*(0,k)\right\} + \frac{2(1-\delta\mu_0)}{\delta(1-(\delta\mu_0/2))}(K(0,0)+K^*(0,0))^2\right]dk. \quad (2.27)$$

Here, the ratio κ_1/z is obtained from (2.13c). We can express (2.27) in terms of v by substituting the definition (2.4c) of $K(k,k')$. However, the resulting integral with respect to k is too formidable to perform analytically. Thus, the expression (2.11c) with (2.16) and (2.27) gives the second-order approximation to the new eigenvalues generated by a small perturbation imposed on a constant background.

III. SHALLOW-WATER LIMIT

A. Eigenvalue problem

In this section, we consider the shallow-water limit of various formulas derived in Sec. II for the INLS spectral problem. It will be demonstrated that the limiting procedure can be performed smoothly by introducing appropriate scalings for the spectral parameters.

We first scale the variables x,t, and u according to the relations

$$x=\sqrt{\delta}\tilde{x},\quad t=\delta\tilde{t},\quad u=\tilde{u}(\tilde{x},\tilde{t}), \quad (3.1)$$

respectively. In this limit, the INLS equation reduces to the defocusing NLS equation (1.3) and the one-soliton solution (1.2) becomes

$$\tilde{u}=\rho\frac{1+\dfrac{\tilde{V}-i\tilde{\kappa}}{\tilde{V}+i\tilde{\kappa}}e^{-\tilde{\kappa}\tilde{\xi}}}{1+e^{-\tilde{\kappa}\tilde{\xi}}},\quad |\tilde{u}|^2=\rho^2-\frac{\tilde{\kappa}^2/2}{\cosh^2(\tilde{\kappa}\tilde{\xi}/2)}, \quad (3.2a)$$

with the scalings

$$\kappa=\frac{\tilde{\kappa}}{\sqrt{\delta}},\quad V=\frac{\tilde{V}}{\sqrt{\delta}},\quad x_0=\sqrt{\delta}\tilde{x}_0. \quad (3.2b)$$

Here, $\tilde{\xi}=\tilde{x}-\tilde{V}\tilde{t}-\tilde{x}_0$, and the soliton velocity $\tilde{V}$ is now given by $\tilde{V}=\pm\sqrt{2\rho^2-\tilde{\kappa}^2}$ $(0<\tilde{\kappa}<\sqrt{2}\rho)$.

To find the appropriate form of the IST equations corresponding to (2.1), we rescale the wave number k as $k=\tilde{k}/\sqrt{\delta}$. It then turns out that

$$\mu=-\rho^2\pm\sqrt{\frac{2\rho^2}{\delta}+\rho^4+k^2}\sim\pm\frac{1}{\sqrt{\delta}}\sqrt{\tilde{k}^2+2\rho^2}\equiv\frac{s\tilde{\mu}}{\sqrt{\delta}}, \tag{3.3a}$$

$$\lambda=1+\mu\delta+O(\delta^2)\sim1\pm\sqrt{\delta}\sqrt{\tilde{k}^2+2\rho^2}\equiv1+s\sqrt{\delta}\tilde{\mu}, \tag{3.3b}$$

where $s\equiv\pm1$.

Under these scalings, the Jost functions ϕ and $\psi^{\pm}$ take the form

$$\phi(x)\equiv\sqrt{\delta}\tilde{\phi}(\tilde{x}), \tag{3.4a}$$

$$\psi^{\pm}(x)=\psi(x\mp i\delta)=\psi(x)\mp i\delta\psi_x(x)+O(\delta^2)\equiv\tilde{\psi}(\tilde{x})\mp i\sqrt{\delta}\tilde{\psi}_{\tilde{x}}(\tilde{x})+O(\delta). \tag{3.4b}$$

Substituting (3.3) and (3.4) into (2.1) and taking the limit $\delta\to0$, we obtain

$$i\tilde{\phi}_{\tilde{x}}-\frac{\tilde{\mu}}{2}\tilde{\phi}+\tilde{u}\tilde{\psi}=0, \tag{3.5a}$$

$$-i\tilde{\psi}_{\tilde{x}}-\frac{\tilde{\mu}}{2}\tilde{\psi}+\frac{\tilde{u}^*}{2}\tilde{\phi}=0, \tag{3.5b}$$

which coincides with the spatial part of the IST equations[6] for the defocusing NLS equation.

A system of integral equations equivalent to (3.5) can be reduced from (2.6). For this purpose, we introduce the scalings

$$k=\tilde{k}/\sqrt{\delta},\quad k'=\tilde{k}'/\sqrt{\delta},\quad \alpha(k)=\delta\tilde{\alpha}(\tilde{k}),\quad \beta(k)=\sqrt{\delta}\tilde{\beta}(\tilde{k}),\quad A(k)=\delta\tilde{A}(\tilde{k}),\quad B(k)=\sqrt{\delta}\tilde{B}(\tilde{k}), \tag{3.6}$$

$$K(k,k')=\sqrt{\delta}\tilde{K}(\tilde{k},\tilde{k}')=\sqrt{\delta}\int_{-\infty}^{\infty}\tilde{v}(\tilde{x})e^{-i(\tilde{k}-\tilde{k}')\tilde{x}/2}\,d\tilde{x}.$$

At the leading order, (2.5) then become

$$A(k)\sim-\frac{\delta}{2}(\tilde{k}^2+\tilde{\kappa}^2)\tilde{\alpha}(\tilde{k})\equiv\delta\tilde{A}(\tilde{k}), \tag{3.7a}$$

$$B(k)\sim-\frac{\sqrt{\delta}}{2}(\tilde{k}^2+\tilde{\kappa}^2)\tilde{\beta}(\tilde{k})\equiv\sqrt{\delta}\tilde{B}(\tilde{k}), \tag{3.7b}$$

$$D(k,\kappa)\sim-\tfrac{1}{2}(\tilde{k}^2+\tilde{\kappa}^2). \tag{3.7c}$$

Substituting (3.3), (3.6), and (3.7) into (2.6), we obtain the system of integral equations for $\tilde{A}$ and $\tilde{B}$:

$$\tilde{A}(\tilde{k})=-\frac{\epsilon\rho}{2\pi}\int_{-\infty}^{\infty}\frac{\tilde{K}^*(\tilde{k}',\tilde{k})}{(\tilde{k}')^2+\tilde{\kappa}^2}\tilde{A}(\tilde{k}')d\tilde{k}'+\frac{\epsilon}{2\pi}(\tilde{k}-s\sqrt{2\rho^2-\tilde{\kappa}^2})\int_{-\infty}^{\infty}\frac{\tilde{K}(',\tilde{k})}{(\tilde{k}')^2+\tilde{\kappa}^2}\tilde{B}(\tilde{k}')d\tilde{k}', \tag{3.8a}$$

$$\tilde{B}(\tilde{k})=-\frac{\epsilon\rho}{4\pi}(\tilde{K}+s\sqrt{2\rho^2-\tilde{\kappa}^2})\int_{-\infty}^{\infty}\frac{\tilde{K}^*(\tilde{k}',\tilde{k})}{(\tilde{k}')^2+\tilde{\kappa}^2}\tilde{A}(\tilde{k}')\mathrm{d}\tilde{k}'-\frac{\epsilon\rho}{2\pi}\int_{-\infty}^{\infty}\frac{\tilde{K}(\tilde{k}',\tilde{k})}{(\tilde{k}')^2+\tilde{\kappa}^2}\tilde{B}(\tilde{k}')\mathrm{d}\tilde{k}'. \tag{3.8b}$$

B. Perturbation analysis

1. Leading-order analysis

We expand $\tilde{A}$, $\tilde{B}$, and $\tilde{\kappa}$ in powers of ϵ as

$$\tilde{A}(\tilde{k})=\tilde{A}_0(\tilde{k})+\epsilon\tilde{A}_1(\tilde{k})+\cdots, \tag{3.9a}$$

$$\tilde{B}(\tilde{k})=\tilde{B}_0(\tilde{k})+\epsilon\tilde{B}_1(\tilde{k})+\cdots, \tag{3.9b}$$

$$\tilde{\kappa}=\epsilon\tilde{\kappa}_1+\epsilon^2\tilde{\kappa}_2+\cdots. \tag{3.9c}$$

The expressions corresponding to (2.12), (2.16), and (2.19) become

$$2\tilde{\kappa}_1\tilde{A}_0(\tilde{k})=-\rho\tilde{K}^*(0,\tilde{k})\tilde{A}_0(0)+(\tilde{k}-s\sqrt{2}\rho)\tilde{K}(\tilde{k},0)\tilde{B}_0(0), \tag{3.10a}$$

$$2\tilde{\kappa}_1\tilde{B}_0(\tilde{k})=-\tfrac{1}{2}(\tilde{k}+s\sqrt{2}\rho)\tilde{K}^*(0,\tilde{k})\tilde{A}_0(0)-\rho\tilde{K}(\tilde{k},0)\tilde{B}_0(0), \tag{3.10b}$$

$$\tilde{\kappa}_1=-\frac{\rho}{2}\{\tilde{K}(0,0)+\tilde{K}^*(0,0)\}=-\frac{\rho}{2}\int_{-\infty}^{\infty}(\tilde{v}(\tilde{x})+\tilde{v}^*(\tilde{x})\mathrm{d}\tilde{x}, \tag{3.11}$$

$$\tilde{A}_0(0)=\sqrt{2}s\tilde{B}_0(0), \tag{3.12}$$

respectively. Thus, if $\tilde{\kappa}_1>0$, then the new eigenvalues

$$s\tilde{\mu}=\pm\sqrt{2\rho^2-(\epsilon\tilde{\kappa}_1)^2}\sim\pm(\sqrt{2\rho^2}-(\epsilon\tilde{\kappa}_1)^2/(2\sqrt{2\rho^2})), \tag{3.13}$$

with $\tilde{\kappa}_1$ given by (3.11) appear from the small initial data $\epsilon\tilde{v}$ without a threshold. Namely, any small perturbation generates a pair of dark solitons with an equal amplitude and opposite velocities $\pm\tilde{\mu}$. This result is in agreement with the corresponding one derived by a different method.[13] The expressions (2.20) now reduce to

$$\tilde{A}_0(\tilde{k})=-\frac{\rho}{2\tilde{\kappa}_1}\left\{\frac{s}{\sqrt{2}\rho}(-\tilde{k}+s\sqrt{2}\rho)\tilde{K}(\tilde{k},0)\mp K^*(0,\tilde{k})\right\}\tilde{A}_0(0), \tag{3.14a}$$

$$\tilde{B}_0(\tilde{k})=-\frac{\rho}{2\tilde{\kappa}_1}\left\{\tilde{K}(\tilde{k},0)+\frac{s}{\sqrt{2}\rho}(\tilde{k}+s\sqrt{2}\rho)\tilde{K}^*(0,\tilde{k})\right\}\tilde{B}_0(0). \tag{3.14b}$$

The eigenfunctions corresponding to the eigenvalue $\tilde{\kappa}\sim\epsilon\kappa_1$ follow from (2.21) as

$$\tilde{\phi}(\tilde{x})=\frac{2\rho\tilde{A}_0(0)}{\tilde{z}}\int_{-\infty}^{\infty}\frac{\frac{s}{\sqrt{2}\rho}(-\tilde{k}+s\sqrt{2}\rho)\tilde{K}(\tilde{k},0)+\tilde{K}^*(0,\tilde{k})}{\tilde{k}^2+\tilde{\kappa}^2}e^{i\tilde{k}\tilde{x}/2}\mathrm{d}\tilde{k}+O(\epsilon), \tag{3.15a}$$

$$\tilde{\psi}(\tilde{x})=\frac{2\rho\tilde{B}_0(0)}{\tilde{z}}\int_{-\infty}^{\infty}\frac{\tilde{K}(\tilde{k},0)+\frac{s}{\sqrt{2}\rho}(\tilde{k}+s\sqrt{2}\rho)\tilde{K}^*(0,\tilde{k})}{\tilde{k}^2+\tilde{\kappa}^2}e^{i\tilde{k}\tilde{x}/2}\mathrm{d}\tilde{k}+O(\epsilon), \tag{3.15b}$$

where

$$\tilde{z}=-\rho\{\tilde{K}(0,0)+\tilde{K}^*(0,0)\}. \tag{3.15c}$$

If we take $\tilde{A}_0(0),\tilde{B}_0(0)\sim O(\epsilon)$, then we can see that (3.14) represent the appropriate bound states for the eigenvalues $s\tilde{\mu}$ given by (3.13).

2. Second-order analysis

In the limit of $\delta\to 0$, $\lambda_0\sim 1$ and $\mu_0\sim s\sqrt{2\rho^2/\delta}$ $(s=\pm 1)$ as seen from (A7). Substituting these approximate values as well as (3.6) and (3.7c) into (2.27), we find the second-order correction to $\tilde{\kappa}$,

$$\tilde{\kappa}_2=\frac{\rho^2}{4\pi}P\int_{-\infty}^{\infty}\frac{1}{\tilde{k}^2}\Bigg[(\tilde{K}(0,\tilde{k})+\tilde{K}^*(\tilde{k},0))(\tilde{K}(\tilde{k},0)+\tilde{K}^*(0,\tilde{k}))-(\tilde{K}(0,0)+\tilde{K}^*(0,0))^2$$
$$-\frac{s}{\sqrt{2}\rho}\tilde{k}\tilde{K}(\tilde{k},0)\tilde{K}^*(\tilde{k},0)+\frac{s}{\sqrt{2}\rho}\tilde{k}\tilde{K}(0,\tilde{k})\tilde{K}^*(0,\tilde{k})\Bigg]\mathrm{d}\tilde{k}. \tag{3.16}$$

If we use (3.6) for $\tilde{K}(\tilde{k},\tilde{k}')$ and the formulas

$$\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{e^{ikx}-1}{k^2}\mathrm{d}k=-|x|, \tag{3.17a}$$

$$P\int_{-\infty}^{\infty}\frac{e^{ikx}}{k}\mathrm{d}k=\pi i\,\mathrm{sgn}\,x, \tag{3.17b}$$

(3.16) can be rewritten in terms of the perturbation $\tilde{v}$ as

$$\tilde{\kappa}_2=-\frac{\rho^2}{8}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}\tilde{x}\,\mathrm{d}\tilde{y}|\tilde{x}-\tilde{y}|(\tilde{v}(\tilde{x})+\tilde{v}^*(\tilde{x}))(\tilde{v}(\tilde{y})+\tilde{v}^*(\tilde{y}))$$
$$+\frac{i\rho s}{2\sqrt{2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}\tilde{x}\,\mathrm{d}\tilde{y}\,\mathrm{sgn}(\tilde{x}-\tilde{y})\{\tilde{v}(\tilde{x})\tilde{v}^*(\tilde{y})-\tilde{v}^*(\tilde{x})\tilde{v}(\tilde{y})\}. \tag{3.18}$$

This expression for the second-order correction to the new eigenvalue is obtained here for the first time.

IV. DEEP-WATER LIMIT

A. Eigenvalue problem

In the deep-water limit $\delta\to\infty$, we find it appropriate to scale the parameter κ as

$$\kappa=\frac{\pi}{\delta}\left(1-\frac{1}{a\delta}\right),\quad 0<a<\frac{\rho^2}{2}. \tag{4.1}$$

Then, the one-soliton solution (1.2) reduces to the algebraic soliton of the form

$$u=\rho\frac{a\xi+i\left(1+\dfrac{2a}{V}\right)}{a\xi+i},\quad |u|^2=\rho^2-\frac{2a}{(a\xi)^2+1}, \tag{4.2}$$

where $\xi=x-Vt-x_0$ and V is the velocity of the soliton determined by the algebraic equation $V^2+2\rho^2V+2\rho^2a=0$. In the deep-water limit, the eigenvalue derived in Sec. II for the INLS

equation does not yield a nonzero value. Indeed, we can see by using (A2) that both the first-order correction (2.16) and second-order one (2.27) vanish identically. This fact would imply that the limiting procedures $\epsilon \to 0$ and $\delta \to \infty$ cannot be interchanged. We should take the limit $\delta \to \infty$ first and then develop a perturbation expansion in ϵ. It turns out that the eigenvalue problem for the nonlocal NLS equation would exhibit a novel feature when compared with that of the INLS and defocusing NLS equations.

The linear system (2.1) remains the same form

$$i\phi_x - \frac{\mu}{2}\phi + \rho\psi^+ = -\epsilon v\psi^+, \tag{4.3a}$$

$$\psi^+ - \lambda\psi^- + \rho\phi = -\epsilon v^*\phi, \tag{4.3b}$$

but here $\psi^+(\psi^-)$ represents the boundary value of a function analytic in the upper-(lower-)half complex x plane. For the bound states, we impose the boundary conditions $\phi \sim \phi_0/x$, $\psi^\pm \sim \pm 1/x$, $|x| \to \infty$ where ϕ_0 is a constant. Using (2.2), the parameters μ and λ are expanded as

$$\mu(k) = -\rho^2 \pm (\rho^2 + |k|)\left\{1 + \frac{2\rho^2|k|}{(\rho^2+|k|)^2} e^{-2|k|\delta} + \cdots\right\}, \tag{4.4a}$$

$$\lambda(k) = \frac{2|k|}{(|k|-\mu)e^{|k|\delta} + (|k|+\mu)e^{-|k|\delta}}. \tag{4.4b}$$

By virtue of (4.1), the expressions of $\mu(i\kappa)$ and $\lambda(i\kappa)$ which follow from (2.2) become

$$\mu(i\kappa) \sim \rho^2\left(-1 \pm \sqrt{1 - \frac{2a}{\rho^2}}\right) \equiv \mu_\pm, \tag{4.5a}$$

$$\lambda(i\kappa) \sim -\frac{1}{1 + \dfrac{\mu(i\kappa)}{a}}. \tag{4.5b}$$

With $\mu(i\kappa)$ and $\lambda(i\kappa)$ given by (4.5), the function $D(k,\kappa)$ defined by (2.5c) has the following leading-order expression:

$$D(k,\kappa) \sim -\tfrac{1}{2}(k + \mu(i\kappa) + 2\rho^2) \quad (k>0), \tag{4.6a}$$

$$D(k,\kappa) \sim \tfrac{1}{2}(k + \mu(i\kappa))\lambda(i\kappa)e^{-k\delta} \quad (k<0). \tag{4.6b}$$

In order to find an appropriate form of the linear system corresponding to (2.6), we define the new variables $A_\pm$ and $B_\pm$ by the relations

$$A(k) = \theta(k)A_+(k) + \lambda(i\kappa)e^{-k\delta}\theta(-k)A_-(k), \tag{4.7a}$$

$$B(k) = \theta(k)B_+(k) + \theta(-k)\lambda(i\kappa)B_-(k), \tag{4.7b}$$

where $\theta(k)$ is the Heaviside function, i.e., $\theta(k)=1$ for $k>0$, and $\theta(k)=0$ for $k<0$. Substituting (4.6) and (4.7) into (2.6), we obtain, in the limit of $\delta \to \infty$, the following closed system of integral equations for $A_\pm$ and B_+:

$$A_+(k)=-\frac{\epsilon\rho}{2\pi}\int_0^\infty \frac{K^*(k',k)}{k'+\mu(i\kappa)+2\rho^2}A_+(k')\mathrm{d}k'+\frac{\epsilon\rho}{2\pi}\int_{-\infty}^0 \frac{K^*(k',k)}{k'+\mu(i\kappa)}A_-(k')\mathrm{d}k'$$
$$+\frac{\epsilon}{2\pi}\int_0^\infty \frac{K(k,k')}{k'+\mu(i\kappa)+2\rho^2}B_+(k')\mathrm{d}k' \quad (k>0), \tag{4.8a}$$

$$A_-(k)=-\frac{\epsilon}{2\pi}\int_0^\infty \frac{K(k,k')}{k'+\mu(i\kappa)+2\rho^2}B_+(k')\mathrm{d}k' \quad (k<0), \tag{4.8b}$$

$$B_+(k)=\frac{\epsilon}{4\pi}(k+\mu(i\kappa))\left[-\int_0^\infty \frac{K^*(k',k)}{k'+\mu(i\kappa)+2\rho^2}A_+(k')\mathrm{d}k'+\int_{-\infty}^0 \frac{K^*(k',k)}{k'+\mu(i\kappa)}A_-(k')\mathrm{d}k'\right]$$
$$-\frac{\epsilon\rho}{2\pi}\int_0^\infty \frac{K(k,k')}{k'+\mu(i\kappa)+2\rho^2}B_+(k')\mathrm{d}k' \quad (k>0). \tag{4.8c}$$

Note that the equation for $B_-(k)$ $(k<0)$ is obtained simply by replacing $B_+(k)$ by $\lambda(i\kappa)B_-(k)$ on the left-hand side of (4.8c).

The eigenfunctions corresponding to the eigenvalue $\mu(i\kappa)$ follow from (2.3), (2.5), (4.6), and (4.7). Explicitly, they take the form

$$\phi(x)=-2\int_0^\infty \frac{A_+(k)}{k+\mu(i\kappa)+2\rho^2}e^{ikx/2}\,\mathrm{d}k+2\int_{-\infty}^0 \frac{A_-(k)}{k+\mu(i\kappa)}e^{ikx/2}\,\mathrm{d}k, \tag{4.9a}$$

$$\psi^+(x)=-2\int_0^\infty \frac{B_+(k)}{k+\mu(i\kappa)+2\rho^2}e^{ikx/2}\,\mathrm{d}k, \tag{4.9b}$$

$$\psi^-(x)=2\int_{-\infty}^0 \frac{B_-(k)}{k+\mu(i\kappa)}e^{ikx/2}\,\mathrm{d}k. \tag{4.9c}$$

B. Perturbation analysis

1. Leading-order analysis

Now, we shall apply a perturbation method to Eq. (4.8) for two different values $\mu_\pm$ given by (4.5a). The constant a in $\mu_\pm$ should be a small quantity since it represents a dip on the constant background [see (4.2)] induced by a small initial data.

a. $\mu(i\kappa)=\mu_-$. We first consider the case $\mu(i\kappa)=\mu_-=\rho^2(-1-\sqrt{1-(2a/\rho^2)})$. Note that $\mu_-\sim-2\rho^2$, $\mu_+\sim-a$, $\lambda(i\kappa)\sim a/(2\rho^2)$ in the limit of $a\to0$. Hence, the integrand including a factor $(k'-\mu_+)^{-1}$ in Eq. (4.8) becomes singular when $k'\to0$. Indeed, it yields a logarithmic singularity upon integration. We remove this singularity by a similar procedure to that used in Sec. II [see (2.10)]. The resulting integral equations are written in the form

$$A_+(k)=\frac{\epsilon\rho}{2\pi}\left[-\int_0^1 \frac{K^*(0,k)}{k'-\mu_+}A_+(0)\mathrm{d}k'-\int_0^1 \frac{K^*(k',k)A_+(k')-K^*(0,k)A_+(0)}{k'-\mu_+}\mathrm{d}k'\right.$$
$$\left.-\int_1^\infty \frac{K^*(k',k)}{k'-\mu_+}A_+(k')\mathrm{d}k'+\int_{-\infty}^0 \frac{K^*(k',k)}{k'+\mu_-}A_-(k')\mathrm{d}k'\right]$$
$$+\frac{\epsilon}{2\pi}\left[\int_0^1 \frac{K(k,0)}{k'-\mu_+}B_+(0)\mathrm{d}k'+\int_0^1 \frac{K(k,k')B_+(k')-K(k,0)B_+(0)}{k'-\mu_+}\mathrm{d}k'\right.$$
$$\left.+\int_1^\infty \frac{K(k,k')}{k'-\mu_+}B_+(k')\mathrm{d}k'\right] \quad (k>0), \tag{4.10a}$$

$$A_-(k)=-\frac{\epsilon}{2\pi}\left[\int_0^1\frac{K(k,0)}{k'-\mu_+}B_+(0)\mathrm{d}k'+\int_0^1\frac{K(k,k')B_+(k')-K(k,0)B_+(0)}{k'-\mu_+}\mathrm{d}k'\right.$$
$$\left.+\int_1^\infty\frac{K(k,k')}{k'-\mu_+}B_+(k')\mathrm{d}k'\right]\quad(k<0),\tag{4.10b}$$

$$B_+(k)=\frac{\epsilon}{4\pi}(k+\mu_-)\left[-\int_0^1\frac{K^*(0,k)}{k'-\mu_+}A_+(0)\mathrm{d}k'-\int_0^1\frac{K^*(k',k)A_+(k')-K^*(0,k)A_+(0)}{k'-\mu_+}\mathrm{d}k'\right.$$
$$\left.-\int_1^\infty\frac{K^*(k',k)}{k'-\mu_+}A_+(k')\mathrm{d}k'+\int_{-\infty}^0\frac{K^*(k',k)}{k'+\mu_-}A_-(k')\mathrm{d}k'\right]-\frac{\epsilon\rho}{2\pi}\left[\int_0^1\frac{K(k,0)}{k'-\mu_+}B_+(0)\mathrm{d}k'\right.$$
$$\left.+\int_0^1\frac{K(k,k')B_+(k')-K(k,0)B_+(0)}{k'-\mu_+}\mathrm{d}k'+\int_1^\infty\frac{K(k,k')}{k'-\mu_+}B_+(k')\mathrm{d}k'\right]\quad(k>0).\tag{4.10c}$$

We now solve Eq. (4.10) in the form of an asymptotic series in ϵ. By inspecting the magnitude of each term in (4.10), it is legitimate to expand $A_\pm$, B_+, and μ_+ as

$$A_\pm(k)=A_\pm^{(0)}(k)+\epsilon A_\pm^{(1)}(k)+\cdots,\tag{4.11a}$$

$$B_+(k)=B_+^{(0)}(k)+\epsilon B_+^{(1)}(k)+\cdots,\tag{4.11b}$$

$$\ln(-\mu_+)=\frac{1}{\epsilon}\mu_+^{(-1)}+\mu_+^{(0)}+\cdots.\tag{4.11c}$$

Note that the expression of μ_- is simply derived by the relation $\mu_-=-\mu_+-2\rho^2$. At $O(\epsilon^0)$, one obtains

$$A_+^{(0)}(k)=\frac{1}{2\pi}\mu_+^{(-1)}[\rho K^*(0,k)A_+^{(0)}(0)-K(k,0)B_+^{(0)}(0)],\tag{4.12a}$$

$$A_-^{(0)}(k)=\frac{1}{2\pi}\mu_+^{(-1)}K(k,0)B_+^{(0)}(0),\tag{4.12b}$$

$$B_+^{(0)}(k)=\frac{1}{4\pi}\mu_+^{(-1)}[(k-2\rho^2)K^*(0,k)A_+^{(0)}(0)+2\rho K(k,0)B_+^{(0)}(0)].\tag{4.12c}$$

If we put $k=0$ in (4.12), we have

$$\left\{1-\frac{\rho}{2\pi}\mu_+^{(-1)}K^*(0,0)\right\}A_+^{(0)}(0)+\frac{1}{2\pi}\mu_+^{(-1)}K(0,0)B_+^{(0)}(0)=0.\tag{4.13a}$$

$$\frac{\rho^2}{2\pi}\mu_+^{(-1)}K^*(0,0)A_+^{(0)}(0)+\left\{1-\frac{\rho}{2\pi}\mu_+^{(-1)}K(0,0)\right\}B_+^{(0)}(0)=0,\tag{4.13b}$$

which gives the leading-order expression of μ_+,

$$\mu_+^{(-1)}=\frac{2\pi}{\rho}\frac{1}{K(0,0)+K^*(0,0)}.\tag{4.14}$$

This corresponds to the expression (2.16) for the INLS equation and the expression (3.11) for the defocusing NLS equation. To assure the convergence of the expansion (4.11c), one must impose the condition $\mu_+^{(-1)}<0$, which is equivalent to

$$K(0,0)+K^*(0,0)=\int_{-\infty}^{\infty}(v(x)+v^*(x))\mathrm{d}x<0. \tag{4.15}$$

Under this condition, a small eigenvalue would appear from the edge $k=0$ of the continuous spectrum. It is quite interesting to observe that the mechanism of the soliton generation is similar to that of the BO equation.[10] This result may be expected since Eq. (1.4) has been derived from the BO equation by means of an asymptotic multiscale expansion.[2]

It now follows from (4.13) and (4.14) that

$$B_+^{(0)}(0)=-\rho A_+^{(0)}(0). \tag{4.16}$$

Substituting (4.16) into (4.12), one obtains

$$A_+^{(0)}(k)=\frac{\rho}{2\pi}\mu_+^{(-1)}\{K(k,0)+K^*(0,k)\}A_+^{(0)}(0), \tag{4.17a}$$

$$A_-^{(0)}(k)=-\frac{\rho}{2\pi}\mu_+^{(-1)}K(k,0)A_+^{(0)}(0), \tag{4.17b}$$

$$B_+^{(0)}(k)=\frac{1}{4\pi}\mu_+^{(-1)}\{(k-2\rho^2)K(k,0)-2\rho^2K^*(0,k)\}A_+^{(0)}(0). \tag{4.17c}$$

The eigenfunctions corresponding to the eigenvalue $\mu(i\kappa)=\mu_-$ follow from (4.9), (4.17) and the relation $\mu_++\mu_-=-2\rho^2$. They read in the form

$$\phi(x)=-2\int_0^{\infty}\frac{A_+^{(0)}(k)}{k-\mu_+}e^{ikx/2}\,\mathrm{d}k+2\int_{-\infty}^{0}\frac{A_-^{(0)}(k)}{k+\mu_-}e^{ikx/2}\,\mathrm{d}k+O(\epsilon), \tag{4.18a}$$

$$\psi^+(x)=-2\int_0^{\infty}\frac{B_+^{(0)}(k)}{k-\mu_+}e^{ikx/2}\,\mathrm{d}k+O(\epsilon), \tag{4.18b}$$

$$\psi^-(x)=2\int_{-\infty}^{0}\frac{B_-^{(0)}(k)}{k+\mu_-}e^{ikx/2}\,\mathrm{d}k+O(\epsilon). \tag{4.18c}$$

The asymptotic forms of these eigenfunctions for $|x|\to\infty$ can be evaluated easily upon integration by parts and using (4.16) and the relation $\lambda(i\kappa)B_-^{(0)}(0)=B_+^{(0)}(0)$. The resulting expressions are given by

$$\phi(x)\sim\frac{4i}{\mu_+}\frac{A_+^{(0)}(0)}{x}, \tag{4.19a}$$

$$\psi^+(x)\sim-\frac{4i\rho}{\mu_+}\frac{A_+^{(0)}(0)}{x}, \tag{4.19b}$$

$$\psi^-(x)\sim\frac{4i\rho}{\mu_+}\frac{A_+^{(0)}(0)}{x}. \tag{4.19c}$$

The boundary conditions are satisfied if we put $A_+^{(0)}(0)=-\mu_+/(4i\rho)$.

b. $\mu(i\kappa)=\mu_+$. Next, we consider the generation of another eigenvalue $\mu(i\kappa)=\mu_+ =\rho^2(-1+\sqrt{1-(2a/\rho^2)})$. It then follows that $\mu_+\sim -a$, $\mu_-\sim -2\rho^2$, $\lambda(i\kappa)\sim 2\rho^2/a$ when $a\to 0$. This case can be treated following the same procedure as that developed for μ_-.

The linear system (4.8) now becomes

$$A_+(k)=-\frac{\epsilon\rho}{2\pi}\int_0^\infty \frac{K^*(k',k)}{k'-\mu_-}A_+(k')\mathrm{d}k'+\frac{\epsilon\rho}{2\pi}\int_{-\infty}^0 \frac{K^*(k',k)}{k'+\mu_+}A_-(k')\mathrm{d}k' + \frac{\epsilon}{2\pi}\int_0^\infty \frac{K(k,k')}{k'-\mu_-}B_+(k')\mathrm{d}k' \quad (k>0), \tag{4.20a}$$

$$A_-(k)=-\frac{\epsilon}{2\pi}\int_0^\infty \frac{K(k,k')}{k'-\mu_-}B_+(k')\mathrm{d}k' \quad (k<0), \tag{4.20b}$$

$$B_+(k)=\frac{\epsilon}{4\pi}(k+\mu_+)\left[-\int_0^\infty \frac{K^*(k',k)}{k'-\mu_-}A_+(k')\mathrm{d}k'+\int_{-\infty}^0 \frac{K^*(k',k)}{k'+\mu_+}A_-(k')\mathrm{d}k'\right] - \frac{\epsilon\rho}{2\pi}\int_0^\infty \frac{K(k,k')}{k'-\mu_-}B_+(k')\mathrm{d}k' \quad (k>0). \tag{4.20c}$$

The singularity arises from a factor $(k'+\mu_+)^{-1}$ when $k'\to 0$. The balance of the magnitude in ϵ would be satisfied if we assume the following expansions:

$$A_+(k)=A_+^{(0)}(k)+\epsilon A_+^{(1)}(k)+\cdots, \tag{4.21a}$$

$$A_-(k)=\epsilon A_-^{(1)}(k)+\epsilon^2 A_-^{(2)}(k)+\cdots, \tag{4.21b}$$

$$B_+(k)=B_+^{(0)}(k)+\epsilon B_+^{(1)}(k)+\cdots, \tag{4.21c}$$

$$\ln(-\mu_+)=\frac{1}{\epsilon^2}\mu_+^{(-2)}+\frac{1}{\epsilon}\mu_+^{(-1)}+\cdots. \tag{4.21d}$$

We substitute (4.21) into the linear system analogous to (4.10) and compare the coefficients of ϵ^n $(n=0,1,\ldots)$. At the lowest order, we obtain the relations

$$A_+^{(0)}(k)=\frac{\rho}{2\pi}\mu_+^{(-2)}K^*(0,k)A_-^{(0)}(0), \tag{4.22a}$$

$$A_-^{(1)}(k)=-\frac{1}{2\pi}\int_0^\infty \frac{K(k,k')}{k'+2\rho^2}B_+^{(0)}(k')\mathrm{d}k', \tag{4.22b}$$

$$B_+^{(0)}(k)=\frac{k}{4\pi}\mu_+^{(-2)}K^*(0,k)A_-^{(1)}(0). \tag{4.22c}$$

If we introduce (4.22) into (4.9) with $\mu(i\kappa)=\mu_+$, we obtain the lowest-order expressions of the Jost functions. The asymptotic evaluation of the Jost functions for $|x|\to\infty$ reveals that $\phi(x)\sim O(x^{-1})$ and $\psi^{\pm}\sim O(x^{-2})$. The latter expression comes from the fact $B_+^{(0)}(0)=0$ by (4.22c), which may be contrasted with the corresponding value $B_+^{(0)}(0)\neq 0$ derived from (4.17c). Obviously, these asymptotic forms are not consistent with the boundary conditions. Thus, we conclude that the perturbation does not produce a new eigenvalue in the eigenvalue problem (4.3) with $\mu(i\kappa)=\mu_+$.

2. Second-order analysis

We now evaluate the second-order correction to the eigenvalue in the case of $\mu(i\kappa)=\mu_-$. At $O(\epsilon)$, (4.10) and (4.11) yield the following linear system of integral equations for $A_+^{(1)}$, $A_-^{(1)}$ and $B_+^{(1)}$:

$$A_+^{(1)}(k)=\frac{\rho}{2\pi}[\{\mu_+^{(-1)}A_+^{(1)}(0)+\mu_+^{(0)}A_+^{(0)}(0)\}K^*(0,k)-F(k)]$$
$$+\frac{1}{2\pi}[-\{\mu_+^{(-1)}B_+^{(1)}(0)+\mu_+^{(0)}B_+^{(0)}(0)\}K(k,0)+G(k)], \tag{4.23a}$$

$$A_-^{(1)}(k)=\frac{1}{2\pi}[\{\mu_+^{(-1)}B_+^{(1)}(0)+\mu_+^{(0)}B_+^{(0)}(0)\}K(k,0)-F(k)], \tag{4.23b}$$

$$B_+^{(1)}(k)=\frac{1}{4\pi}(k-2\rho^2)[\{\mu_+^{(-1)}A_+^{(1)}(0)+\mu_+^{(0)}A_+^{(0)}(0)\}K^*(0,k)-F(k)]$$
$$-\frac{2\rho}{\pi}[-\{\mu_+^{(-1)}B_+^{(1)}(0)+\mu_+^{(0)}B_+^{(0)}(0)\}K(k,0)+G(k)], \tag{4.23c}$$

with

$$F(k)\equiv\int_0^1\frac{1}{k'}\{K^*(k',k)A_+^{(0)}(k')-K^*(0,k)A_+^{(0)}(0)\}dk'$$
$$+\int_1^\infty\frac{K^*(k',k)A_+^{(0)}(k')}{k'}dk'-\int_{-\infty}^0\frac{K^*(k',k)A_-^{(0)}(k')}{k'-2\rho^2}dk', \tag{4.24a}$$

$$G(k)\equiv\int_0^1\frac{1}{k'}\{K(k,k')B_+^{(0)}(k')-K(k,0)B_+^{(0)}(0)\}dk'+\int_1^\infty\frac{K^*(k,k')B_+^{(0)}(k')}{k'}dk'. \tag{4.24b}$$

If we put $k=0$ in (4.23a) and (4.23b) and eliminate $A_+^{(1)}(0)$ and $B_+^{(1)}(0)$ with use of (4.14), we obtain

$$\frac{1}{2\pi}\{\rho K^*(0,0)A_+^{(0)}(0)-K(0,0)B_+^{(0)}(0)\}\mu_+^{(0)}=\frac{\rho}{2\pi}F(0)-\frac{1}{2\pi}G(0). \tag{4.25a}$$

Substitution of (4.16) into (4.25a) gives

$$\frac{\rho}{2\pi}\{K(0,0)+K^*(0,0)\}A_+^{(0)}(0)\mu_+(0)=\frac{\rho}{2\pi}F(0)-\frac{1}{2\pi}G(0). \tag{4.25b}$$

The specific values $F(0)$ and $G(0)$ are expressed in terms of $K(k,k')$ and $K^*(k,k')$ by introducing (4.17) into (4.24). The resulting expressions are substituted into (4.25b) to obtain the second-order quantity $\mu_+^{(0)}$,

$$\frac{\mu_+^{(0)}}{\mu_+^{(-1)}}=\frac{\rho}{2\pi}\int_0^1\frac{1}{k}\left[\frac{\{K(0,k)+K^*(k,0)\}\{K(k,0)+K^*(0,k)\}}{K(0,0)+K^*(0,0)}-\{K(0,0)+K^*(0,0)\}\right]\mathrm{d}k$$
$$+\frac{\rho^2\mu_+^{(-1)}}{4\pi^2}\int_1^\infty\frac{1}{k}\{K(0,k)+K^*(k,0)\}\{K(k,0)+K^*(0,k)\}\mathrm{d}k$$
$$+\frac{\mu_+^{(-1)}}{8\pi^2}\left[-\int_0^\infty K(0,k)K^*(0,k)\mathrm{d}k+2\rho^2\int_{-\infty}^0\frac{K(k,0)K^*(k,0)}{k-2\rho^2}\mathrm{d}k\right]. \tag{4.26}$$

Lastly, we use the definition (2.4c) for $K(k,k')$ and the formula

$$\int_0^1\frac{e^{izs}-1}{s}\mathrm{d}s+\int_1^\infty\frac{e^{izs}}{s}\mathrm{d}s=-\gamma-\ln|z|+\frac{i\pi}{2}\mathrm{sgn}(z)\quad(\gamma:\text{Euler's constant}), \tag{4.27}$$

to express $\mu_+^{(0)}$ in terms of the initial data v. The result is

$$\mu_+^{(0)}=\left(\frac{\rho\mu_+^{(-1)}}{2\pi}\right)^2\left[-(\gamma-\ln 2)\left\{\int_{-\infty}^\infty(v(x)+v^*(x))\mathrm{d}x\right\}^2\right.$$
$$-\int_{-\infty}^\infty\int_{-\infty}^\infty\mathrm{d}x\,\mathrm{d}y(v(x)+v^*(x))(v(y)+v^*(y))\ln|x-y|$$
$$\left.-\int_{-\infty}^\infty\int_{-\infty}^\infty\mathrm{d}x\,\mathrm{d}yv(x)v^*(y)\int_0^\infty\frac{s+2}{s+1}e^{i\rho^2(x-y)s}\mathrm{d}s\right]. \tag{4.28}$$

Note that if $v(x)$ is an analytic function in the upper-half complex x plane, then the third-term on the right-hand side of (4.28) vanishes identically.

Up to the second-order approximation in ϵ, we thus obtain the expression of a new eigenvalue generated by a small initial data. Actually, it follows from (4.11c) that

$$\mu_+\sim-e^{\mu_+^{(0)}}e^{\mu_+^{(-1)}/\epsilon}, \tag{4.29}$$

where $\mu_+^{(-1)}$ and $\mu_+^{(0)}$ are given, respectively, by (4.14) and (4.28). This implies the generation of a new soliton of the form (4.2) whose amplitude parameter a and velocity V are given, respectively, by the relations $a=-\mu_+(\mu_++2\rho^2)/(2\rho^2)\sim-\mu_+$ and $V=\mu_-\sim-2\rho^2$. The magnitude of a is exponentially small compared with ϵ in contrast to the corresponding result for the INLS and defocusing NLS equations for which the magnitude is comparable to that of the perturbation.

V. CONCLUDING REMARKS

In this paper, we studied the problem of the soliton generation by a small perturbation on the basis of the INLS equation. In particular, we analyzed the spectral problem associated with it by means of the Fourier transform. An important generalization of our approach would be to investigate the mechanism of the soliton generation induced by a small perturbation on the general N-soliton state. This problem has been discussed in the case of the BO[10] and KPI[12] equations where the completeness relations for the Jost functions have played a central role in the perturbation analysis. For the spectral problem associated with the INLS equation, however, the corresponding completeness relation has not been established yet. We also remark that the soliton generation for the nonlocal NLS equation (1.4) has been considered quite recently in conjunction with the linear stability of the N-soliton solution.[9] We have found that any small perturbation on the N-soliton solution would produce a new soliton if the condition $\epsilon\int_{-\infty}^\infty(u_N(x)v^*(x)+u_N^*(x)v(x))\mathrm{d}x<0$ is satisfied where u_N is an N-soliton solution and $\epsilon v(x)$ is a perturbation. If we put $u_N=\rho$ ("0-soliton" state), then the above-given condition reduces to (4.15), which is just

a condition for the generation of a new soliton. One may extract a similar condition for the INLS equation through a full development of the associated spectral problem. Undoubtedly, this will become an important issue in the near future.

APPENDIX A: PROPERTIES OF THE FUNCTION $D(k,\kappa)$

In this Appendix, we describe some properties of the function $D(k,\kappa)$ introduced in (2.8) as well as those of the spectral parameters μ and λ.

By taking into account the fact that the parameters $\mu(i\kappa)$ and $\lambda(i\kappa)$ are even functions of κ, we expand $\mu(i\kappa)$ and $\lambda(i\kappa)$ in powers of κ^2,

$$\mu(i\kappa)=\mu_0+\mu_1\kappa^2+\cdots, \quad \lambda(i\kappa)=\lambda_0+\lambda_1\kappa^2+\cdots. \tag{A1}$$

Substituting these expressions into (2.2) and comparing the coefficient of κ^{2n} $(n=0,1,\ldots)$, one can determine μ_j and λ_j $(j=0,1,\ldots)$ successively. The first two terms of which read in the form

$$\mu_0^2+2\rho^2\mu_0-\frac{2\rho^2}{\delta}=0, \quad \lambda_0=\frac{1}{1-\delta\mu_0}, \tag{A2a}$$

$$\mu_1=-\frac{1+\frac{2}{3}\rho^2\delta}{2(\mu_0+\rho^2)}, \quad \lambda_1=\frac{\delta+\frac{1}{3}\rho^2\delta^2}{2(\mu_0+\rho^2)(\delta\mu_0-1)}. \tag{A2b}$$

Note that μ_0 has two real roots given by $\mu_0=-\rho^2+s\sqrt{\rho^4+(2\rho^2/\delta)}$ $(s\equiv\pm1)$ and the coefficients λ_0, μ_j and λ_j $(j\geqslant1)$ are expressed in terms of μ_0. Direct calculations using (A2) give the relations

$$\mu_0(1-\lambda_0)+2\rho^2=0, \tag{A3a}$$

$$\frac{1-\delta\mu_0}{1-(\delta\mu_0/2)}=1-s\frac{1}{\sqrt{1+(2/\delta\rho^2)}}, \tag{A3b}$$

$$\frac{(1-\lambda_0)\mu_1-\lambda_1\mu_0}{\lambda_0\delta(1-(\delta\mu_0/2))}=1. \tag{A3c}$$

If we introduce (A1)–(A3) into (2.5c), we obtain the Taylor series expansion of $D(k,\kappa)$,

$$\begin{aligned}D(k,\kappa)=&\frac{-1}{2}\{(1-\lambda_0)\mu_1-\lambda_1\mu_0\}\kappa^2-\frac{1}{2}\{\delta(\lambda_0\mu_1+\lambda_1\mu_0)-\lambda_1\}\kappa^2k\\&-\frac{1}{2}\left[\lambda_0\delta-\frac{\delta^2}{2}\lambda_0\mu_0+\left\{\lambda_1\delta-\frac{\delta^2}{2}(\lambda_0\mu_1+\lambda_1\mu_0)\right\}\kappa^2\right]k^2+O(\kappa^2k^3).\end{aligned} \tag{A4}$$

Differentiating (A4) by k and putting $k=\pm ik$, one has

$$D_k(i\kappa,\kappa)=-i\lambda_0\delta(1-\tfrac{1}{2}\delta\mu_0)\kappa-\tfrac{1}{2}\{\delta(\lambda_0\mu_1+\lambda_1\mu_0)-\lambda_1\}\kappa^2+O(\kappa^3), \tag{A5a}$$

$$D_k(-i\kappa,\kappa)=i\lambda_0\delta(1-\tfrac{1}{2}\delta\mu_0)\kappa-\tfrac{1}{2}\{\delta(\lambda_0\mu_1+\lambda_1\mu_0)-\lambda_1\}\kappa^2+O(\kappa^3). \tag{A5b}$$

It follows from (A5) that

$$C_R(\kappa)\equiv\frac{1}{D_k(i\kappa,\kappa)}+\frac{1}{D_k(-i\kappa,\kappa)}=-\frac{\delta(\lambda_0\mu_1+\lambda_1\mu_0)-\lambda_1}{\left(\lambda_0\delta-\frac{\delta^2}{2}\lambda_0\mu_0\right)^2}+O(\kappa^2), \tag{A6a}$$

$$C_I(\kappa)\equiv i\left[\frac{1}{D_k(i\kappa,\kappa)}-\frac{1}{D_k(-i\kappa,\kappa)}\right]=-\frac{2}{\lambda_0\delta(1-\frac{1}{2}\delta\mu_0)\kappa}+O(\kappa). \tag{A6b}$$

The following expansions in δ are useful in taking the shallow-water limit $\delta\to 0$:

$$\mu_0=s\sqrt{\frac{2\rho^2}{\delta}}-\rho^2+\frac{s\rho^3}{4}\sqrt{2\delta}+O(\delta^{3/2}), \tag{A7a}$$

$$\lambda_0=1+s\sqrt{2\rho^2\delta}+O(\delta), \tag{A7b}$$

$$\mu_1=-s\sqrt{\frac{\delta}{2\rho^2}}\left(1+\frac{5}{12}\delta\rho^2\right)+O(\delta^{5/2}), \tag{A7c}$$

$$\lambda_1=-\frac{\delta^{3/2}}{2\sqrt{2\rho^2}}(s+\sqrt{2\rho^2\delta})+O(\delta^{5/2}). \tag{A7d}$$

APPENDIX B: TWO-SOLITON SOLUTION OF THE INLS EQUATION

Here, we investigate the asymptotic properties of the two-soliton solution of the INLS equation. In particular, we show that the solution has a common asymptotic value under appropriate choice of the soliton parameters.

The two-soliton solution may be expressed in the form[2,4,5]

$$u=\rho\frac{G}{F},\quad |u|^2=\rho^2-i\frac{\partial}{\partial x}\ln\left(\frac{F}{F^*}\right), \tag{B1a}$$

where

$$F=1+e^{\eta_1+i\phi_1}+e^{\eta_2+i\phi_2}+e^{\eta_1+\eta_2+i(\phi_1+\phi_2)+A_{12}}, \tag{B1b}$$

$$G=1+e^{\eta_1+i\psi_1}+e^{\eta_2+i\psi_2}+e^{\eta_1+\eta_2+i(\psi_1+\psi_2)+A_{12}}, \tag{B1c}$$

$$\eta_j=k_j(x-v_jt-x_{j0}), \tag{B1d}$$

$$\phi_j=-\delta k_j,\quad \psi_j=-\delta k_j+i\ln\left(\frac{v_j-ik_j}{v_j+ik_j}\right), \tag{B1e}$$

$$e^{A_{ij}}=\frac{(k_i-k_j)^2+(v_i-v_j)^2}{(k_i+k_j)^2+(v_i-v_j)^2}\quad (i\neq j), \tag{B1f}$$

$$v_j^2+2\rho^2v_j+k_j^2=2\rho^2k_j\cot(k_j\delta). \tag{B1g}$$

Note that the soliton parameters k_j and v_j correspond, respectively, to κ and V in (2.18). It follows from (B1g) that the velocity of the jth soliton is determined by

$$\begin{aligned} v_j&=-\rho^2\pm\sqrt{\rho^4-k_j^2+2\rho^2k_j\cot(k_j\delta)}\\ &=-\rho^2\pm\sqrt{\{k_j+\rho^2\tan(k_j\delta/2)\}\{(\rho^2-k_j\tan(k_j\delta/2)\}/\tan(k_j\delta/2)}. \end{aligned} \tag{B2}$$

Hence, if $0<k_j<k_c$ with k_c being a positive solution of the equation $k_c\tan(k_c\delta/2)=\rho^2$, then v_j has two real roots. This inequality is assumed in the following analysis. The asymptotic form of u as $|x|\to\infty$ is easily obtained from (B1). It takes the form

$$u \to \rho, \quad x \to -\infty, \tag{B3a}$$

$$u \to \rho e^{i(\psi_1+\psi_2-\phi_1-\phi_2)} = \rho \frac{v_1+ik_1}{v_1-ik_1}\frac{v_2+ik_2}{v_2-ik_2}, x \to +\infty. \tag{B3b}$$

We can see that the solution exhibits a change of the phase given by (B3b). However, if the condition

$$v_1 k_2 + v_2 k_1 = 0, \tag{B4}$$

is satisfied, then the solution has the same asymptotic value ρ without the phase shift. We now show that (B4) holds for particular values of k_1 and k_2. Note that since both k_1 and k_2 are positive, v_1 and v_2 must have different signs. We may take them as

$$v_1 = -\rho^2 + \sqrt{\rho^4 - k_1^2 + 2\rho^2 k_1 \cot(k_1\delta)}, \tag{B5a}$$

$$v_2 = -\rho^2 - \sqrt{\rho^4 - k_2^2 + 2\rho^2 k_2 \cot(k_2\delta)}, \tag{B5b}$$

so that $v_2 < 0 < v_1$. The positivity of v_1 is assured by imposing the condition

$$k_1 < 2\rho^2 \cot(k_1\delta). \tag{B6}$$

If we substitute (B5) into (B4), condition (B4) is transformed into the form

$$(k_1+k_2)^2 - 2\rho^2(k_1+k_2)\{\cot(k_1\delta)+\cot(k_2\delta)\} + \{k_1\cot(k_2\delta) - k_2\cot(k_1\delta)\}^2 = 0. \tag{B7}$$

It can be verified that there exist pairs (k_1,k_2) $(0<k_1<k_2<k_c)$ that satisfy the conditions (B6) and (B7) simultaneously. We shall demonstrate this statement by a numerical calculation. We take $\rho=\delta=1$ as a typical example. Then, $k_c = 1.307$ and condition (B6) becomes $k_1 < 1.077$. In the following, we shall write down some numerical solutions (k_1,k_2) of (B7):

$$(k_1,k_2) = (0.05,0.186),\ (0.1,0.367),\ (0.2,0.695),\ (0.3,0.958),$$

$$(0.4,1.14),\ (0.5,1.25),\ (0.6,1.30),\ (0.65,1.306). \tag{B8}$$

When both k_1 and k_2 are sufficiently small, (B7) reduces to

$$(k_1-k_2)^2 = 2\rho^2\delta k_1 k_2. \tag{B9}$$

Solving this equation, the ratio k_1/k_2 is found to have a limiting value

$$\frac{k_1}{k_2} = 1 + \rho^2\delta - \sqrt{\rho^2\delta(2+\rho^2\delta)}. \tag{B10}$$

In the above-given example, this ratio is $2-\sqrt{3} \simeq 0.268$, which is in agreement with the numerical values (B8) for small k_j $(j=1,2)$.

It is quite interesting to observe that the two eigenvalues given by (2.16) exactly satisfy condition (B9). Hence, if we approximate a pair of dark solitons with the soliton parameters (2.18) by a two-soliton solution (B1), then we can see that the boundary condition $u \to \rho$, $|x| \to \infty$ is satisfied within the approximation up to order ϵ.

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Remarks on several 2+1 dimensional lattices

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In this paper, five 2+1 dimensional lattices considered by several authors are revisited again. First of all we will show that two lattices proposed by Blaszak and Szum [J. Math. Phys. **42**, 225 (2001)] become the so-called differential-difference KP equation due to Date, Jimbo, and Miwa [J. Phys. Soc. Jpn. **51**, 4116 (1982); **51**, 4125 (1982); **52**, 388 (1983); **52**, 761 (1983); **52**, 766 (1983)] by simple variable transformations, while another lattice found by Blaszak and Szum can be viewed as a higher-dimensional generalization of a lattice given by Wu and Hu [J. Phys. A **32**, 1515 (1999)]. Some integrable properties on these three lattices are derived. Second, it is shown that a 2+1 dimensional Toda-like lattice studied by Cao, Geng, and Wu [J. Phys. A **32**, 8059 (1999)] can be transformed into the bilinear equation given by Hu, Clarkson, and Bullough [J. Phys. A **30**, L669 (1997)]. For this bilinear version we also present some rational solutions and Lie symmetries. Finally, a lattice due to Levi, Ragnisco, and Shabat [Can. J. Phys. **72**, 439 (1994)] is transformed into coupled bilinear equations. It is shown that these coupled bilinear equations do not have two-soliton solutions. This further confirms that the lattice under consideration is not completely integrable. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1430899]

I. INTRODUCTION

The subject of discrete systems described by differential-difference, difference, lattice equations and mappings has undergone remarkable development in recent years. With such development, there has also been an increasing interest in integrable discrete systems. Currently, much progress is being made in the understanding of the mathematical aspects of integrable discrete systems, including integrable dynamical mappings, ordinary and partial difference equations, lattice solitons, discrete versions of the Painlevé equations, and application to numerical analysis, computer science, physics, etc. Several powerful approaches, such as the inverse scattering method, singularity confinement criteria, symmetry approaches, etc., have been proposed to deal with discrete nonlinear systems toward their complete integrability, linearizability, and solvability.

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(See, e.g., Refs. 1–3, and references therein.) Among these approaches, Hirota's bilinear formalism provides us with an efficient tool in the search for exact solutions of discrete systems, and also in the search for new integrable discrete equations.

Until now, much research has been conducted on many 1+1 dimensional lattices such as the Toda lattice

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}u(n)=e^{u(n-1)-u(n)}-e^{u(n)-u(n+1)}$$

and the Lotka–Volterra lattice

$$\frac{\mathrm{d}}{\mathrm{d}t}u(n)=u(n)(u(n+1)-u(n-1)).$$

Comparatively less research has been done on 2+1 dimensional lattices. Recently, the following five 2+1 dimensional lattices have been proposed by several authors:

$$u_t(n)=2u(n)u_y(n)+\mathcal{H}u_{yy}(n), \tag{1}$$

$$v_t(n)=\mathcal{H}v_{yy}(n)-(v(n)\mathcal{H}v(n))_y, \tag{2}$$

$$u_t(n)=u(n)\mathcal{H}^{-1}p(n-1), \tag{3}$$

$$v_t(n)=u(n+1)-u(n)+(E+1)^{-1}p_y(n), \tag{4}$$

$$p_t(n)=v(n+1)-v(n)-p(n)\mathcal{H}^{-1}p(n), \tag{5}$$

$$\frac{\partial^2 Q_n}{\partial x\partial y}=\exp(Q_{n+1}-Q_n)\frac{\partial}{\partial x}(Q_{n+1}+Q_n)-\exp(Q_n-Q_{n-1})\frac{\partial}{\partial x}(Q_n+Q_{n-1}), \tag{6}$$

and

$$\begin{aligned}\chi_{xy}(n)=&e^{\chi(n+2)+\chi(n+1)-2\chi(n)}+e^{2\chi(n+1)-\chi(n)-\chi(n-1)}\\&-e^{\chi(n+1)+\chi(n)-2\chi(n-1)}-e^{2\chi(n)-\chi(n-1)-\chi(n-2)},\end{aligned} \tag{7}$$

where E is a shift operator, i.e., $Eu(n)=u(n+1)$ and $\mathcal{H}=(E+1)/(E-1)$. The lattices (1), (2) and (3)–(5) are constructed by Blaszak and Szum as an application of the so-called ''central extension procedure and operand formalism'' in a very recent paper.[4] Lattice (6) was considered by Cao, Geng, and Wu in a remarkable paper,[5] and lattice (7) was proposed by Levi, Ragnisco, and Shabat in a short but interesting paper.[6] In view of the fact that there are not many integrable 2+1 dimensional lattices available in the literature, it would be of interest for us to revisit the above-mentioned five lattices again.

The purpose of this paper is to study these five 2+1 dimensional lattices in Hirota's bilinear formalism. Several new results, such as rational solutions, Lie symmetries, nonlinear superposition principles, etc., have been obtained on these lattices.

The organization of the paper is as follow. In Sec. II we show that lattices (1) and (2) become the so-called differential-difference KP equation considered in Refs. 7 and 8 by simple variable transformations. In Sec. III, it is shown that lattice (3)–(5) could be viewed as a higher dimensional generalization of a lattice derived in Ref. 9. By a dependent variable transformation, the lattice (3)–(5) is transformed into coupled bilinear equations. A bilinear Bäcklund transformation and its associated nonlinear superposition formula are presented. As a result, soliton solutions and lump solutions to (3)–(5) are obtained. In Sec. IV, we show that the lattice (6) can be transformed into a bilinear equation found by Hu, Clarkson, and Bullough in Ref. 10. Some particular solutions to the bilinear equation are derived by using the corresponding Bäcklund transformation. Finally,

in Sec. V, by a dependent variable transformation, the lattice (7) is transformed into coupled bilinear equations. For these coupled bilinear equations, we have obtained one-solition solution but failed to obtain two-soliton solutions. This further confirms that lattice (7) is not completely integrable.

II. LATTICES (1) AND (2)

It is noted that lattices (1) and (2) are related by the relation $v(n)=(1-E)u(n)$. Therefore in the following we only consider lattice (1). Lattice (1) can be rewritten as

$$u_t(n+1)-u_t(n)=2(u(n+1)u_y(n+1)-u(n)u_y(n))+u_{yy}(n+1)+u_{yy}(n). \tag{8}$$

Setting $u(n)=(\ln f(n+1)/f(n))_y$, Eq. (8) is transformed into the bilinear equation

$$(D_t-D_y^2)e^{(1/2)D_n}f(n)\cdot f(n)=0, \tag{9}$$

where Hirota's bilinear differential operator $D_y^m D_t^k$ and the bilinear difference operator $\exp(\delta D_n)$ are defined by[11]

$$D_y^m D_t^k a\cdot b\equiv\left(\frac{\partial}{\partial y}-\frac{\partial}{\partial y'}\right)^m\left(\frac{\partial}{\partial t}-\frac{\partial}{\partial t'}\right)^k a(y,t)b(y',t')|_{y'=y,t'=t},$$

$$\exp(\delta D_n)a(n)\cdot b(n)\equiv\exp\left[\delta\left(\frac{\partial}{\partial n}-\frac{\partial}{\partial n'}\right)\right]a(n)b(n')|_{n'=n}=a(n+\delta)b(n-\delta).$$

Equation (9) becomes the bilinear form

$$(D_t+2D_y-D_y^2)e^{(1/2)D_n}f(n)\cdot f(n)=0 \tag{10}$$

by the linear transformation $y\to y+2t, t\to t$. Equation (10) is just the bilinear form for the so-called differential-difference KP equation[7,8]

$$\Delta\left(\frac{\partial w}{\partial t}+2\frac{\partial w}{\partial y}-2w\frac{\partial w}{\partial y}\right)=(2+\Delta)\frac{\partial^2 w}{\partial y^2} \tag{11}$$

through the dependent variable transformation given by

$$w=\frac{\partial}{\partial y}\ln\frac{f(n+1)}{f(n)},$$

where $\Delta=E-1$, i.e., $\Delta w(n)=w(n+1)-w(n)$. Besides, it is obvious that (8) and (11) are linked by $u(n)=w(n)-1$. Concerning (9), we can easily obtain its bilinear BT

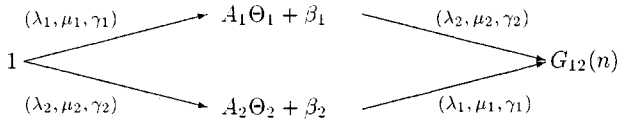
$$(D_y+\lambda^{-1}e^{-D_n}+\mu)f(n)\cdot g(n)=0, \tag{12}$$

$$(D_t-\lambda^{-1}D_y e^{-D_n}-\lambda^{-1}\mu e^{-D_n}-\gamma)f(n)\cdot g(n)=0, \tag{13}$$

and nonlinear superposition formula

$$\exp(-\tfrac{1}{2}D_n)f_0\cdot f_{12}=k[\lambda_1\exp(-\tfrac{1}{2}D_n)-\lambda_2\exp(\tfrac{1}{2}D_n)]f_1\cdot f_2, \tag{14}$$

where λ, μ, and γ are arbitrary constants and k is a nonzero constant. By using these results, we can easily rederive soliton solutions and rational solutions. For example, we have



where

$$G_{12}(n)=A_1A_2\Theta_1\Theta_2+\Theta_1\left(A_1\beta_2+\frac{A_1A_2}{\lambda_1-\lambda_2}\right)+\Theta_2\left(A_2\beta_1-\frac{A_1A_2}{\lambda_1-\lambda_2}\right)+\beta_1\beta_2+\frac{A_2\beta_1-A_1\beta_2}{\lambda_1-\lambda_2}, \tag{15}$$

with

$$\Theta_i\equiv\lambda_i^{-1}n+2\lambda_i^{-3}t+\lambda_i^{-2}y,\quad \mu_i=-\lambda_i^{-1},\quad \gamma_i=\lambda_i^{-2}.$$

Thus we have the following rational solution to (8) or (1):

$$u(n)=\frac{\partial}{\partial y}\ln\frac{G_{12}(n+1)}{G_{12}(n)}.$$

We can obtain a hierarchy of rational solutions for the lattice (9) using the above-mentioned process. In particular, if we choose

$$A_1=A_2,\quad \lambda_1=a+ib,\quad \lambda_2=\lambda_1^*=a-ib\quad (A_1,a,b\in\mathcal{R}),b\neq 0,$$

$$\beta_1=\frac{A_1}{\lambda_1-\lambda_2},\quad \beta_2=\frac{A_2}{\lambda_2-\lambda_1},$$

we have from (15) that

$$G_{12}(n)=A_1^2\Theta_1\Theta_1^*+\frac{A_1^2}{4b^2}-\frac{A_1}{2b^2}, \tag{16}$$

which becomes a one-lump solution when we choose $A_1<0$ or $A_1>2$. Correspondingly, we have the one-lump solution to (8) or (1):

$$u(n)=\frac{\partial}{\partial y}\ln\frac{G_{12}(n+1)}{G_{12}(n)},$$

where $G_{12}(n)$ is given by (16).

Since (9) is an integrable lattice, it would be interesting to derive some other integrable properties. In the following we write down five Lie symmetries for (9):

$$\sigma_0=h(t)f,\quad \sigma_1=yh(t)f,$$

$$\sigma_2=(h(t)n+\tfrac{1}{4}\dot{h}(t)y^2)f,\quad \sigma_3=h(t)f_y+(\tfrac{1}{2}ny\dot{h}+\tfrac{1}{24}y^3\ddot{h})f,$$

$$\sigma_4=h(t)f_t+\tfrac{1}{2}y\dot{h}f_y+(\tfrac{1}{8}ny^2\ddot{h}+\tfrac{1}{192}y^4h^{(3)}+\tfrac{1}{4}n^2\dot{h})f,$$

where $h(t)$ is an arbitrary function of t and $\dot{h}(t)\equiv \mathrm{d}h(t)/\mathrm{d}t$, $\ddot{h}(t)\equiv \mathrm{d}^2h(t)/\mathrm{d}t^2$, $h^{(3)}\equiv \mathrm{d}^3h(t)/\mathrm{d}t^3$.

III. LATTICES (3)–(5)

Setting $w(n)=(E+1)^{-1}p(n)$, lattices (3)–(5) can be rewritten as

$$u_t(n)=u(n)(w(n)-w(n-1)), \tag{17}$$

$$v_t(n)=u(n+1)-u(n)+w_y(n), \tag{18}$$

$$w_t(n+1)+w_t(n)=v(n+1)-v(n)-w^2(n+1)+w^2(n). \tag{19}$$

By the dependent variable transformation

$$u(n)=\frac{f(n+1)f(n-1)}{f^2(n)}, \quad v(n)=\frac{D_t^2 f(n)\cdot f(n+1)}{f(n)f(n+1)}, \quad w(n)=\left(\ln\frac{f(n+1)}{f(n)}\right)_t,$$

Eqs. (17)–(19) become

$$\begin{aligned} &D_t(D_t^2 f(n)\cdot f(n+1))\cdot f(n)f(n+1)\\ &\quad=f(n+2)f^3(n)-f(n-1)f^3(n+1)+D_y(D_t f(n+1)\cdot f(n))\cdot f(n+1)f(n). \end{aligned} \tag{20}$$

By introducing an auxiliary variable z, (20) can be decoupled into the bilinear form:

$$(D_z e^{(1/2)D_n}-D_t^2 e^{(1/2)D_n})f(n)\cdot f(n)=0, \tag{21}$$

$$(D_t D_z-D_t D_y)f(n)\cdot f(n)=4\sinh^2(\tfrac{1}{2}D_n)f(n)\cdot f(n). \tag{22}$$

In particular, if f is independent of y, then (21) and (22) become the bilinear form for a lattice proposed in Ref. 9. Therefore (21) and (22) may be viewed as a two-dimensioal generalization of the lattice in Ref. 9. Concerning (21) and (22), we have the following results:

Proposition 1: The system of bilinear equations (21) and (22) has the Bäcklund transformation

$$(D_t+\lambda^{-1}e^{-D_n}+\mu)f(n)\cdot g(n)=0, \tag{23}$$

$$(D_z e^{-(1/2)D_n}-D_y e^{-(1/2)D_n}-\lambda e^{(1/2)D_n}+\gamma e^{-(1/2)D_n})f(n)\cdot g(n)=0, \tag{24}$$

$$(D_z-\lambda^{-1}D_t e^{-D_n}-\lambda^{-1}\mu e^{-D_n}-\omega)f(n)\cdot g(n)=0, \tag{25}$$

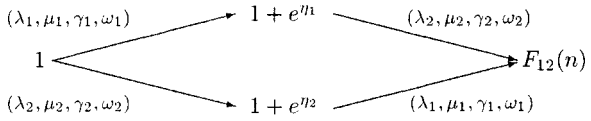
where λ, μ, γ, and ω are arbitrary constants.

Proposition 2: Let f_0 be a solution of (21) and (22). Suppose that $f_i(i=1,2)$ are solutions of (21) and (22), which are related to f_0 under the BT (23)–(25) with parameters $(\lambda_i,\mu_i,\gamma_i,\omega_i)$. Then f_{12} defined by

$$\exp(-\tfrac{1}{2}D_n)f_0\cdot f_{12}=c[\lambda_1\exp(-\tfrac{1}{2}D_n)-\lambda_2\exp(\tfrac{1}{2}D_n)]f_1\cdot f_2 \tag{26}$$

is a new solution related to f_1 and f_2 under the BT (23)–(25) with parameters $(\lambda_2,\mu_2,\gamma_2,\omega_2)$, $(\lambda_1,\mu_1,\gamma_1,\omega_1)$, respectively. Here c is a nonzero constant.

These results can be proved in a way similar to those of Ref. 9. We omit the details. Instead we are going to construct soliton solutions to (21) and (22) by using these results. Choose, for example, $f_0=1$, $c=1/(\lambda_1-\lambda_2)$. It can be easily verified that



where

$$F_{12}(n)=1+\frac{\lambda_1 e^{-p_1}-\lambda_2}{\lambda_1-\lambda_2}e^{\eta_1}+\frac{\lambda_1-\lambda_2 e^{-p_2}}{\lambda_1-\lambda_2}e^{\eta_2}+\frac{\lambda_1 e^{-p_1}-\lambda_2 e^{-p_2}}{\lambda_1-\lambda_2}e^{\eta_1+\eta_2}, \tag{27}$$

with

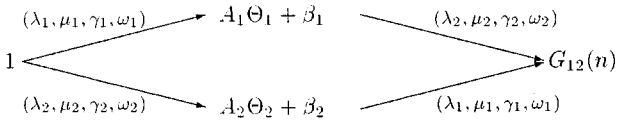
$$\eta_i=p_i n+\lambda_i^{-1}(e^{p_i}-1)t+\lambda_i^{-2}(e^{2p_i}-1)z+[\lambda_i^{-2}(e^{2p_i}-1)+\lambda_i(e^{-p_i}-1)]y+\eta_i^0,$$

$$\mu_i=-\lambda_i^{-1},\quad \gamma_i=\lambda_i,\quad \omega_i=\lambda_i^{-2}.$$

The corresponding two-soliton solution to (17)–(19) is given by

$$u(n)=\frac{F_{12}(n+1)F_{12}(n-1)}{F_{12}^2(n)},\quad v(n)=\frac{D_t^2F_{12}(n)\cdot F_{12}(n+1)}{F_{12}(n)F_{12}(n+1)},\quad w(n)=\left(\ln\frac{F_{12}(n+1)}{F_{12}(n)}\right)_t.$$

In general, along this line, we can obtain multisoliton solutions for the lattice (21) and (22) step by step. Besides, we have



where

$$G_{12}(n)=A_1A_2\Theta_1\Theta_2+\Theta_1\left(A_1\beta_2+\frac{A_1A_2}{\lambda_1-\lambda_2}\right)+\Theta_2\left(A_2\beta_1-\frac{A_1A_2}{\lambda_1-\lambda_2}\right)+\beta_1\beta_2+\frac{A_2\beta_1-A_1\beta_2}{\lambda_1-\lambda_2}, \tag{28}$$

with

$$\Theta_i\equiv\lambda_i^{-1}n+\lambda_i^{-2}t+(2\lambda_i^{-3}-1)y+2\lambda_i^{-3}z,\quad \mu_i=-\lambda_i^{-1},\quad \gamma_i=\lambda_i,\quad \omega_i=\lambda_i^{-2}.$$

The corresponding rational solution to (17)–(19) is given by

$$u(n)=\frac{G_{12}(n+1)G_{12}(n-1)}{G_{12}^2(n)},\quad v(n)=\frac{D_t^2G_{12}(n)\cdot G_{12}(n+1)}{G_{12}(n)G_{12}(n+1)},\quad w(n)=\left(\ln\frac{G_{12}(n+1)}{G_{12}(n)}\right)_t.$$

We can obtain a hierarchy of rational solutions for the lattice (21) and (22) using the above-mentioned process. In particular, if we choose

$$A_1=A_2,\quad \lambda_1=a+ib,\quad \lambda_2=\lambda_1^*=a-ib\quad (A_1,a,b\in\mathcal{R}),\quad b\neq 0,$$

$$\beta_1=\frac{A_1}{\lambda_1-\lambda_2},\quad \beta_2=\frac{A_2}{\lambda_2-\lambda_1},$$

we have from (28) that

$$G_{12}(n)=A_1^2\Theta_1\Theta_1^*+\frac{A_1^2}{4b^2}-\frac{A_1}{2b^2}, \tag{29}$$

which becomes a one-lump solution when we choose $A_1<0$ or $A_1>2$. In this case, the one-lump solution to (17)–(19) is given by

$$u(n)=\frac{G_{12}(n+1)G_{12}(n-1)}{G_{12}^2(n)},\quad v(n)=\frac{D_t^2G_{12}(n)\cdot G_{12}(n+1)}{G_{12}(n+1)},\quad w(n)=\left(\ln\frac{G_{12}(n+1)}{G_{12}(n)}\right)_t,$$

where $G_{12}(n)$ is given by (29). Furthermore, starting from $1 \xrightarrow{(\lambda_i,-\lambda_i^{-1},\lambda_i,\lambda_i^{-2})} A\Theta_i+\beta_i$ $(i=1,2,3,4)$, it is possible to construct two-lump solutions.

IV. THE SPECIAL 2+1 TODA LATTICE (6)

In Ref. 5, Cao *et al.* have considered the special 2+1 Toda lattice (6) and obtained the explicit theta-function solutions by resorting to separation techniques. Here we will show that there is some connection between this special 2+1 Toda lattice (6) and a bilinear equation found in Ref. 10. In fact, by the dependent variable transformation

$$Q_n=-\frac{x}{2}+h(y)+\ln\frac{f(n+1)}{f(n)}$$

with $h(y)$ being an arbitrary function of y, we can transform (6) into the bilinear equation

$$D_xD_yf(n)\cdot f(n)=2[D_xe^{D_n}+e^{D_n}-1]f(n)\cdot f(n), \tag{30}$$

which is a special case of the bilinear equation proposed in Ref. 10. Therefore we have the following bilinear BT for (30):

$$D_yf(n)\cdot g(n)=\left(\lambda e^{-D_n}-\frac{1}{\lambda}e^{D_n}+\mu\right)f(n)\cdot g(n), \tag{31}$$

$$(-4\lambda D_xe^{-(1/2)D_n}-4D_xe^{(1/2)D_n})f(n)\cdot g(n)=\left[\left(4+\frac{\gamma}{\lambda}\right)e^{(1/2)D_n}+\gamma e^{-(1/2)D_n}\right]f(n)\cdot g(n), \tag{32}$$

where λ, μ, and γ are arbitrary constants. Starting from BT (31) and (32), we have obtained explicit soliton solutions to (30).[10] Its Pfaffian solution was given in Ref. 12. Starting from BT (31) and (32), we can also obtain polynomial solutions to (30). For example, starting from the trivial solution $f(n)=1$ and using BT (31) and (32) with

$$\mu=\frac{1}{\lambda}-\lambda,\quad \gamma=-\frac{4\lambda}{1+\lambda},$$

we have

$$g(n)=n-\frac{\lambda}{(1+\lambda)^2}x-\frac{(\lambda^2+1)}{\lambda}y+\alpha.$$

Furthermore, starting from the solution

$$f(n)=n-\frac{\lambda_1}{(1+\lambda_1)^2}x-\frac{(\lambda_1^2+1)}{\lambda_1}y+\alpha$$

and using BT (31) and (32) with $\mu=1/\lambda-\lambda$, $\gamma=-4\lambda/(1+\lambda)$, we have

$$g(n)=n^2+n\left[-\left(\frac{\lambda}{(1+\lambda)^2}+\frac{\lambda_1}{(1+\lambda_1)^2}\right)x-\left(\frac{\lambda^2+1}{\lambda}+\frac{\lambda_1^2+1}{\lambda_1}\right)y+\beta\right]$$
$$+\left[\frac{(\lambda_1^2+1)\lambda}{\lambda_1(1+\lambda)^2}+\frac{(\lambda^2+1)\lambda_1}{\lambda(1+\lambda_1)^2}\right]xy+\frac{(\lambda^2+1)(\lambda_1^2+1)}{\lambda\lambda_1}y^2$$
$$+\frac{\lambda\lambda_1}{(\lambda_1+1)^2(\lambda+1)^2}x^2+y\left[\frac{\lambda^2-1}{\lambda}+\alpha\left(\frac{\lambda_1^2+1}{\lambda_1}-\frac{\lambda^2+1}{\lambda}\right)-\beta\frac{\lambda_1^2+1}{\lambda_1}\right]$$
$$+x\frac{-\alpha\lambda+[(1+\lambda)(-1+\beta+\lambda+\beta\lambda)+\alpha(1+\lambda^2)]\lambda_1-\alpha\lambda\lambda_1^2}{(1+\lambda)^2(1+\lambda_1)^2}$$
$$+\frac{\lambda\lambda_1}{\lambda_1(\lambda^2+1)-\lambda(\lambda_1^2+1)}\left[\frac{\lambda^2+1}{\lambda}(\alpha\beta-\alpha^2-1)+\frac{\lambda^2-1}{\lambda}(-\beta+2\alpha)+\frac{\lambda_1^2+1}{\lambda_1}(\alpha^2-\beta\alpha)\right],$$

where α, β, λ, and λ_1 are constants. The corresponding rational solution to (6) is given by

$$Q_n=-\frac{x}{2}+h(y)+\ln\frac{g(n+1)}{g(n)}.$$

In addition, concerning bilinear equation (30), we have found the following Lie symmetries:

$$\sigma_1=(h_1(x)+h_2(y))f,\quad \sigma_2=nh_2(y)f,$$

$$\sigma_3=h_1(x)f_x+(yh_1(x)+\tfrac{1}{2}nh_1(x))f,$$

$$\sigma_4=h_2(y)f_y+(xh_2(y)+\tfrac{1}{2}\dot{h}_2(y)n^2)f,$$

where $h_1(x)$ and $h_2(y)$ are arbitrary functions of x and y, respectively, and $\dot{h}_2(y)\equiv \mathrm{d}h_2(y)/\mathrm{d}y$.

V. THE LEVI–RAGNISCO–SHABAT LATTICE (7)

In this section, we will consider the Levi–Ragnisco–Shabat lattice (7). In Ref. 6, it was mentioned that (7) can be reduced to a nonintegrable equation under some reduction. This means that (7) is not completely integrable in such a sense. In what follows, we will show that (7) does not have multisoliton solution. To this end, we set $\chi(n)=\ln(f(n+1)/f(n))$. Then (7) can be transformed into the quadrilinear form

$$(D_xD_yf(n)\cdot f(n))f^2(n)=4\cosh(D_n)(e^{D_n}f(n)\cdot f(n))\cdot f^2(n)-4f^4(n). \tag{33}$$

By introducing an auxiliary variable z, (33) may be decoupled into the bilinear equations

$$(D_xD_y+4-4e^{2D_n}+D_ze^{2D_n})f(n)\cdot f(n)=0, \tag{34}$$

$$(D_ze^{D_n}+2-2e^{D_n})f(n)\cdot f(n)=0. \tag{35}$$

We can easily obtain one-soliton solution to (34) and (35):

$$f(n)=1+e^{\eta},\quad \eta=pn+qx+ry+sz+\eta^0,$$

$$s=\frac{2\cosh(p)-2}{\sinh(p)},\quad r=\frac{4\cosh(2p)-4-4\cosh^2(p)+4\cosh(p)}{q}.$$

Now it is natural to go on to seek the following two-soliton solution to (34) and (35):

$$f(n)=1+e^{\eta_1}+e^{\eta_2}+A_{12}e^{\eta_1+\eta_2}, \quad \eta_i=p_in+q_ix+r_iy+s_iz+\eta_i^0,$$

$$s_i=\frac{2\cosh(p_i)-2}{\sinh(p_i)}, \quad r_i=\frac{4\cosh(2p_i)-4-4\cosh^2(p_i)+4\cosh(p_i)}{q_i}.$$

From (34) and (35) we can determine A_{12}, respectively,

$$A_{12}=-\frac{(s_1-s_2)\sinh(p_1-p_2)+2-2\cosh(p_1-p_2)}{(s_1+s_2)\sinh(p_1+p_2)+2-2\cosh(p_1+p_2)}, \tag{36}$$

$$A_{12}=-\frac{(q_1-q_2)(r_1-r_2)+4+(s_1-s_2)\sinh(2(p_1-p_2))-4\cosh(2(p_1-p_2))}{(q_1+q_2)(r_1+r_2)+4+(s_1+s_2)\sinh(2(p_1+p_2))-4\cosh(2(p_1+p_2))}. \tag{37}$$

It is obvious to see that the system (34) and (35) has the above-mentioned two-soliton solution, provided that

$$\frac{(s_1-s_2)\sinh(p_1-p_2)+2-2\cosh(p_1-p_2)}{(s_1+s_2)\sinh(p_1+p_2)+2-2\cosh(p_1+p_2)} \equiv \frac{(q_1-q_2)(r_1-r_2)+4+(s_1-s_2)\sinh(2(p_1-p_2))-4\cosh(2(p_1-p_2))}{(q_1+q_2)(r_1+r_2)+4+(s_1+s_2)\sinh(2(p_1+p_2))-4\cosh(2(p_1+p_2))} \tag{38}$$

for arbitrary constants p_1, p_2, q_1 and q_2 and without any additional condition. But by using MATHEMATICA it turns out that (38) does not hold automatically. Therefore our computations give further evidence that (7) is not completely integrable.

VI. CONCLUSION

In this paper, five 2+1 dimensional lattices studied by several authors have been reviewed in Hirota's bilinear formalism. First, we have shown that two lattices proposed by Blaszak and Szum[4] share the same bilinear form with the so-called differential-difference KP equation due to Date, Jimbo, and Miwa.[7] This means that these two lattices are linked to the differential-difference KP equation by simple variable transformations. We have also transformed another lattice found by Blaszak and Szum[4] into a set of coupled bilinear equations, which is a higher-dimensional generalization of the bilinear form for a lattice given by Wu and Hu.[9] Several integrable properties on these three lattices given by Blaszak and Szum, such as lump solutions, Lie symmetries, etc., have been derived. Second, we have shown that a 2+1 dimensional Toda-like lattice considered by Cao, Geng, and Wu[5] can be transformed into a bilinear equation given by Hu, Clarkson, and Bullough.[10] For this bilinear version, some rational solutions and Lie symmetries have also been obtained. Finally, a lattice due to Levi, Ragnisco, and Shabat is transformed into coupled bilinear equations. Based on the fact that these coupled bilinear equations do not have two-soliton solutions, we further confirm that the lattice under consideration is not completely integrable.

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Euclidean scalar Green function in a higher dimensional global monopole space–time

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We construct the explicit Euclidean scalar Green function associated with a massless field in a higher dimensional global monopole space–time, i.e., a $(1+d)$-space–time with $d\geqslant 3$ which presents a solid angle deficit. Our result is expressed in terms of an infinite sum of products of Legendre functions with Gegenbauer polynomials. Although this Green function cannot be expressed in a closed form, for the specific case where the solid angle deficit is very small, it is possible to develop the sum and obtain the Green function in a more workable expression. Having this expression it is possible to calculate the vacuum expectation value of some relevant operators. As an application of this formalism, we calculate the renormalized vacuum expectation value of the square of the scalar field, $\langle \Phi^2(x)\rangle_{\mathrm{Ren}}$, and the energy-momentum tensor, $\langle T_{\mu\nu}(x)\rangle_{\mathrm{Ren}}$, for the global monopole space–time with spatial dimensions $d=4$ and $d=5$. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421424]

I. INTRODUCTION

In this article we consider the Euclidean scalar Green function associated with a massless field in the higher dimensional global monopole space–time. We define this space–time as a generalization of the previous one given in Ref. 1 (the metric of cosmic string space–time, which is spatially flat, was considered in Ref. 2). The generalization of the Euclidean line element of Ref. 1 for a higher dimensional case is given by

$$ds^2=d\tau^2+\frac{dr^2}{\alpha^2}+r^2d\Omega_{d-1}^2=g_{\mu\nu}(x)dx^\mu dx^\nu, \tag{1}$$

where $\mu,\ \nu=0,1,2,\ldots,d$, with $d\geqslant 3$ and $x^\mu=(\tau,r,\theta_1,\theta_2,\ldots,\theta_{d-2},\phi)$. The coordinates are defined in the intervals $\tau\in(-\infty,\infty)$, $\theta_i\in[0,\pi]$ for $i=1,2,\ldots,d-2$, $\phi\in[0,2\pi]$ and $r\geqslant 0$. The parameter α, which codifies the presence of the global monopole, is smaller than unity. In this coordinate system the metric tensor is explicitly defined as shown:

$$\begin{gathered} g_{00}=1,\quad g_{11}=1/\alpha^2,\quad g_{22}=r^2,\\ g_{jj}=r^2\sin^2\theta_1\sin^2\theta_2\ldots\sin^2\theta_{j-2}, \end{gathered} \tag{2}$$

for $3\leqslant j\leqslant d$, and $g_{\mu\nu}=0$ for $\mu\neq\nu$.

This space–time corresponds to a pointlike global monopole. It is not flat: the scalar curvature $R=(d-1)(d-2)(1-\alpha^2)/r^2$, and the solid angle associated with a hypersphere with unity radius

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is $\Omega=2\pi^{d/2}\alpha^2/\Gamma(d/2)$, so it is smaller than an ordinary one. The energy-momentum tensor associated with this object has a diagonal form and its nonvanishing components read $T_0^0=T_1^1=(\alpha^2-1)(d-2)/r^2$.

The Euclidean scalar Green function associated with a massless field in the geometry defined by (2) should obey the nonhomogeneous second order differential equation

$$(\Box-\xi R)G_E(x,x')=-\delta^n(x,x')=-\frac{\delta^n(x-x')}{\sqrt{g}}, \tag{3}$$

where $n=d+1$, $\Box$ denotes the covariant d'Alembertian in the space–time defined by (2), ξ is an arbitrary coupling constant, $\delta^d(x,x')$ is the bidensity Dirac distribution and R is the scalar curvature.

The vacuum expectation value of the square of the scalar field, $\langle\Phi^2(x)\rangle$, is given by the evaluation of the Green function at the same point which provides a divergent result. So, in order to obtain a finite and well defined one, we should apply some renormalization procedure. The method which we shall adopt here is the point-splitting renormalization procedure. The basic idea of this method consists of subtracting from the Green function all the divergences which appears in the coincidence limit. (As it is well known, this procedure is ambiguous in even dimensions and the ambiguity is a consequence of mass scale parameter μ which is introduced after the renormalization procedure. In this way the final result contains a finite part which depends on the scale μ.)

In Ref. 3 Wald observed that the singular behavior of the Green function in the coincidence limit has the same structure as the Hadamard function, so his proposal was to subtract from the Green function the Hadamard one. In fact, the use of the Hadamard function to renormalize the vacuum expectation value of the energy-momentum tensor in a curved space–time was first introduced by Adler *et al.*[4] In Ref. 3 Wald added a modification to this technique in order to provide the correct result for the trace anomaly. In this way the renormalized vacuum expectation value of the square of the field operator is given by

$$\langle\Phi^2(x)\rangle_{\mathrm{Ren}}=\lim_{x'\to x}[G_E(x,x')-G_H(x,x')]. \tag{4}$$

The renormalized vacuum expectation value of the energy-momentum tensor can also be obtained in a similar way:

$$\langle T_{\mu\nu}(x)\rangle_{\mathrm{Ren}}=\lim_{x'\to x}\mathcal{D}_{\mu\nu'}(x,x')[G_E(x,x')-G_H(x,x')], \tag{5}$$

where $\mathcal{D}_{\mu\nu'}(x,x')$ is a bivector differential operator. Moreover, this vacuum expectation value should be conserved, i.e.,

$$\nabla_\mu\langle T^\mu_\nu(x)\rangle_{\mathrm{Ren}}=0, \tag{6}$$

and gives us the correct conformal trace anomaly,

$$\langle T^\mu_\mu(x)\rangle_{\mathrm{Ren}}=\frac{1}{(4\pi)^{n/2}}a_{n/2}(x) \tag{7}$$

for $n=1+d$ even and

$$\langle T^\mu_\mu(x)\rangle_{\mathrm{Ren}}=0 \tag{8}$$

for $n=1+d$ odd.[5]

In this article we study the quantum field theory associated with a massless scalar field in the background space–time defined by (2). More specifically, we shall specialize in the cases where

the spatial section of our space–time has dimensions $d=4$ and $d=5$. In Sec. II, we construct explicitly the Euclidean Green function for a massless scalar field in a higher dimensional global monopole space–time. We show that this Green function is expressed in terms of an infinite sum of product of the Legendre function with Gegenbauer polynomials. In Sec. III we calculate explicitly the renormalized vacuum expectation value of the square of the scalar field operator for $d=4$ and $d=5$ dimensions in the case where $\eta^2 \ll 1$, where $\eta^2=1-\alpha^2$. The parameter α is related to the energy scale where the global symmetry of the system is spontaneously broken (see Ref. 1). For a typical grand unified theory in a physical $(1+3)$-dimensional space–time, this scale is of order 10^{16} Gev. So, $1-\alpha^2=\eta^2 \sim 10^{-5}$. We show that for six dimensions the expression obtained presents an ambiguity given by the mass scale parameter and that this ambiguity vanishes if we assume for the nonminimal coupling constant its conformal value, $\xi=\frac{1}{5}$. In Sec. IV we present the formal expressions for the vacuum expectation values of the energy-momentum tensor for the cases $d=4$ and $d=5$. For the six dimensional case we present, after a long calculation, an explicit expression for the scale dependent term up to the first order in η^2. We explicitly show that this term is traceless for the conformal coupling. In Sec. V we present our conclusions and some important remarks about this article. Although the formalism developed here is applied only when the dimension of the space section is $d \geqslant 3$, in the Appendix we present an expression for the Green function in a limiting case $d \to 2$.

II. GREEN FUNCTION

In this section we calculate the Euclidean scalar Green function associated with a massless field in the space–time described by (2). This Green function must obey the nonhomogeneous second order differential equation

$$(\Box - \xi R) G_E(x,x') = -\delta^d(x,x') = -\frac{\delta^2(x-x')}{\sqrt{g}}, \tag{9}$$

where we have introduced the nonminimal coupling of the scalar field with the geometry. As we have already said, the scalar curvature for this space–time is $R=(d-1)(d-2)(1-\alpha^2)/r^2$.

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

$$G_E(x,x') = \int_0^\infty ds K(x,x';s), \tag{10}$$

where the heat kernel, $K(x,x';s)$, can be expressed in terms of eigenfunctions of the operator $\Box - \xi R$ as follows:

$$K(x,x';s) = \sum_\sigma \Phi_\sigma(x) \Phi_\sigma^*(x') \exp(-s\sigma^2), \tag{11}$$

σ^2 being the corresponding positively defined eigenvalue. Writing

$$(\Box - \xi R)\Phi_\sigma(x) = \sigma^2 \Phi_\sigma(x), \tag{12}$$

we obtain the complete set of normalized solutions of the above equation:

$$\Phi_\sigma(x) = \sqrt{\frac{\alpha p}{2\pi}} \frac{1}{r^{d/2-1}} e^{-i\omega\tau} J_{\nu_n}(pr) Y(n,m_j;\phi,\theta_j), \tag{13}$$

with

$$\sigma^2 = \omega^2 + \alpha^2 p^2, \tag{14}$$

$Y(n,m_j;\phi,\theta_j)$ being the hyperspherical harmonics of degree n,[6] J_ν the Bessel function of order

$$\nu_n=\alpha^{-1}\sqrt{(n+(d-2)/2)^2+(d-1)(d-2)(1-\alpha^2)(\xi-\overline{\xi})}, \tag{15}$$

with $\overline{\xi}=(d-2)/4(d-1)$. So according to (11) our heat kernel is given by

$$\begin{aligned}K(x,x';s)&=\int_{-\infty}^{\infty}d\omega\int_0^{\infty}dp\sum_{n,m_j}\Phi_\sigma(x)\Phi_\sigma^*(x')e^{-s\sigma^2}\\&=\frac{1}{8\alpha\pi^{(d+1)/2}s^{3/2}}\frac{1}{(rr')^{d/2-1}}\frac{\Gamma(d/2)}{d-2}e^{-(\Delta\tau^2\alpha^2+r^2+r'^2)/4\alpha^2 s}\\&\quad\times\sum_{n=0}^{\infty}[2(n-1)+d]I_{\nu_n}\left(\frac{rr'}{2\alpha^2 s}\right)C_n^{(d-2)/2}(\cos\gamma),\end{aligned} \tag{16}$$

I_ν being the modified Bessel function, $C_n^\mu(x)$ the Gegenbauer polynomial of degree n and order μ and γ is the angle between two arbitrary directions. Our final expression (16) was obtained using the addition theorem for the hyperspherical harmonics[6] and the integral table.[7]

Now we are in position to obtain the Euclidean Green function substituting (16) into (10). Our final result is

$$G_E^{(d)}(x,x')=\frac{1}{4\pi^{d/2+1}}\frac{1}{(rr')^{(d-1)/2}}\frac{\Gamma(d/2)}{d-2}\sum_{n=0}^{\infty}[2(n-1)+d]Q_{\nu_n-1/2}(u)C_n^{(d-2)/2}(\cos\gamma), \tag{17}$$

where

$$u=\frac{\alpha^2\Delta\tau^2+r^2+r'^2}{2rr'} \tag{18}$$

and Q_μ is the Legendre function. Unfortunately because the dependence of the order of the Legendre functions on the parameter α is not a simple one, it is not possible to develop the summation and to obtain a closed expression for the Green function even in the simpler case $d=3$.[8] However, for $\xi=\overline{\xi}$, ν_n becomes equal to $(n+(d-2)/2)/\alpha$ and for $\gamma=0$ it is possible to represent this Green function in an integral form using the integral representation for the Legendre function

$$Q_{\nu-1/2}(\cosh\rho)=\frac{1}{\sqrt{2}}\int_\rho^{\infty}dt\frac{e^{-\nu t}}{\sqrt{\cosh t-\cosh\rho}} \tag{19}$$

and

$$C_n^{(d-2)/2}(1)=\frac{(n+d-3)!}{n!(d-3)!}. \tag{20}$$

Now it is possible to develop the summation and after some intermediate steps we get

$$G_E^{(d)}(r,\tau;r',\tau')=\frac{1}{4\pi^{d/2+1}}\frac{1}{(rr')^{(d-1)/2}}\frac{\Gamma(d/2)}{2^{d-3/2}}\int_\rho^{\infty}dt\frac{1}{\sqrt{\cosh t-\cosh\rho}}\frac{\cosh(t/2\alpha)}{(\sinh(t/2\alpha))^{d-1}}. \tag{21}$$

For the case where $\alpha=\frac{1}{2}$, i.e., a large solid angle deficit, the above expression can be written in a simpler form by performing the integral. Making an appropriate transformation of variable, $t := \operatorname{arccosh}((u-1)/q+1)$, we get

$$G_E^{(d)}(r,\tau;r,\tau')=\frac{1}{4\sqrt{2}\,\pi^{d/2+1}}\,\frac{\Gamma(d/2)}{d-2}\,\frac{(rr')^{(d-3)/2}}{[(r-r')^2+\Delta\tau^2/4]^{d/2-1}}\,\frac{1}{[(r+r')^2+\Delta\tau^2/4]^{d/2-1}}. \tag{22}$$

The next section is devoted to the obtainment of the renormalized vacuum expectation value of the square of the field operator. As an explicit application we shall develop these quantities for the cases where $d=4$ and $d=5$.

III. CALCULATION OF $\langle\Phi^2(x)\rangle_{\mathrm{Ren}}$

The calculation of the vacuum expectation value of the square of the field operator is obtained computing the Green function in the coincidence limit:

$$\langle\Phi^2(x)\rangle=\lim_{x'\to x} G_E(x,x'). \tag{23}$$

However, this procedure provides a divergent result. In order to obtain a finite and well defined result, we must apply in this calculation some renormalization procedure. Here we shall adopt the point-splitting renormalization. This procedure is based upon a divergence subtraction scheme in the coincidence limit of the Green function. In Ref. 3, Wald examined the behavior of the Green function in this limit. He observed that its divergences have the same structure as given by the Hadamard function, which, on the other hand, can be explicitly written in terms of the square of the geodesic distance between the two points. So, we shall adopt the following prescription: we subtract from the Green function the Hadamard one before applying the coincidence limit as shown:

$$\langle\Phi^2(x)\rangle_{\mathrm{Ren}}=\lim_{x'\to x}[G_E(x,x')-G_H(x,x')]. \tag{24}$$

Now let us develop this calculation explicitly. As we have mentioned earlier, it is not possible to proceed exactly with the summation which appears in the Green function. By this reason the best that we can do is to obtain an approximate expression for it, developing a series expansion in powers of the parameter $\eta^2=1-\alpha^2$, which is much smaller than unity for the physical four-dimensional space–time. Moreover, because we want to take the coincidence limit in the Green function, let us take first $\gamma=0$ and $\Delta\tau=0$ in (17). The approximate expression for the order of the Legendre function, up to the first power in η^2, is

$$\nu_n\approx\left(n+\frac{d-2}{2}\right)(1+\eta^2/2)+\frac{(d-1)(d-2)(\xi-\overline{\xi})}{2n+d-2}\,\eta^2+O(\eta^4). \tag{25}$$

We also need to develop the summation

$$S=\sum_{n=0}^{\infty}[2n+d-2]\,\frac{(n+d-3)!}{n!}\,e^{-\nu_n t}. \tag{26}$$

Substituting the approximate expression for ν_n into the summation in (26), we get, after some intermediate steps,

$$S=\frac{(d-2)!}{2^{d-2}}\,\frac{\cosh(t/2)}{\sinh^{d-1}(t/2)}\left[1-\frac{t\,\eta^2(d-1)}{2\sinh(t)}(1+4\xi\sinh^2(t/2))\right]. \tag{27}$$

So the approximate Green function is given by

$$G_E^{(d)}(r,r')=\frac{1}{2^{d+1/2}\pi^{d/2+1}}\frac{\Gamma(d/2)}{(rr')^{(d-1)/2}}\int_\rho^\infty dt\,\frac{1}{\sqrt{\cosh t-\cosh\rho}}$$
$$\times\frac{\cosh(t/2)}{\sinh^{d-1}(t/2)}\left[1-\frac{t\eta^2(d-1)}{2\sinh(t)}(1+4\xi\sinh^2(t/2))\right]. \tag{28}$$

In his beautiful paper Christensen[5] has given a general expression for the Hadamard function for any dimensional space-time, which is expressed in terms of the square of the geodesic distance $2\sigma(x,x')$. Moreover, there he has called attention to the different behavior of this function when the dimension of the space–time is an even or odd number. In the latter case there is no logarithmic term in the expansion of the Hadamard function. So because of this fact we shall develop, separately, the calculation of the renormalized vacuum expectation value of the square of the field operator, for $n=1+d$ odd and even.

Following Ref. 5, next we write down the Hadamard function for the massless case when the dimension of the space–time is an odd number. This function is given by

$$G_H(x,x')=\frac{\Delta^{1/2}(x,x')}{2(2\pi)^{n/2}}\frac{1}{\sigma^{n/2-1}(x,x')}\sum_{k=0}^{(n-3)/2}a_k(x,x')\sigma^k(x,x')\frac{\Gamma(n/2-k-1)}{2^k}, \tag{29}$$

where $\Delta(x,x')$, the Van Vleck–Morette determinant, and the factor $a_k(x,x')$, for $k=0,1,2$, have been computed by many authors. See Refs. 9 and 10.

Now let us apply this formalism for the case $n=5$, i.e., $d=4$. The Euclidean Green function in this case is

$$G_E^{(4)}(r,r')=\frac{1}{16\sqrt{2}\pi^3}\frac{1}{(rr')^{3/2}}\int_\rho^\infty dt\,\frac{1}{\sqrt{\cosh t-\cos\rho}}$$
$$\times\frac{\cosh(t/2)}{\sinh^3(t/2)}\left[1-\frac{3t\eta^2}{2\sinh(t)}(1+4\xi\sinh^2(t/2))\right]. \tag{30}$$

Because we need to evaluate the Hadamard function in the coincidence limit we can write this function exhibiting only its divergent contributions as shown:

$$G_H(x,x')=\frac{1}{16\sqrt{2}\pi^2}\frac{1}{\sigma^{3/2}(x,x')}\left[1+\left(\frac{1}{6}-\xi\right)R(x)\sigma(x,x')\right], \tag{31}$$

where we have substituted the explicit expression for Δ, a_0 and a_1 in the coincidence limit. The scalar curvature in this five-dimensional space–time is $R=6\eta^2/r^2$. The radial one-half of the geodesic distance, $\sigma(x,x')=(1/2\alpha^2)(r-r')^2$, in our approximation is equal to $\sigma\approx(\frac{1}{2})(r-r')^2(1+\eta^2+\cdots)$. Now substituting (30) and (31) into (24) we get, after a long calculation,

$$\langle\Phi^2(x)\rangle_{\mathrm{Ren}}=\frac{3\eta^2}{64\pi r^3}\left(\xi-\frac{3}{16}\right). \tag{32}$$

We can see that for the conformal coupling in five dimensional space–time, $\xi=\frac{3}{16}$, the above expectation vanishes, i.e., the renormalized vacuum expectation value of the operator $\Phi^2(x)$ is zero up to the first order in η^2.

The six dimensional case will be analyzed now. This case, together with the four dimensional one studied in Ref. 8, exhibits explicitly the ambiguity in the renormalization procedure given by a mass subtraction point μ. (Moretti, in Ref. 11, has used the local ζ-function renormalization

technique to show, by a general argument, that the scale ambiguity is present in the calculation of vacuum expectation value of the square of scalar field operator in a curved space–time of dimension even.)

The Hadamard function in even dimensions is explicitly written in the paper by Christensen,[5] so we shall not reproduce it here. The singular behavior of the Hadamard function in the six dimensional space–time is

$$G_H(x,x')=\frac{\Delta^{1/2}(x,x')}{16\pi^3}\left[\frac{a_0(x,x')}{\sigma^2(x,x')}+\frac{a_1(x,x')}{2\sigma(x,x')}-\frac{a_2(x,x')}{4}\ln\left(\frac{\mu^2\sigma(x,x')}{2}\right)\right]. \tag{33}$$

Substituting the expressions for the factors a_k, we get, up to the first order in the parameter η^2, the following result:

$$G_H(r,r')=\frac{1}{2\pi^3}\left[\frac{(1-2\eta^2)}{(r-r')^4}+\frac{(1-6\xi)\eta^2}{2r^2(r-r')^2}-\frac{\eta^2}{4r^4}\left(\xi-\frac{1}{5}\right)\ln\left(\frac{\mu^2(r-r')^2}{4}\right)\right]. \tag{34}$$

Now taking $d=5$ in (28) and substituting the result, together with Eq. (34), into (24), we get, after some calculation, the following expression:

$$\langle\Phi^2(x)\rangle_{\mathrm{Ren}}=-\frac{\eta^2}{96\pi^3r^4}\left(\frac{47}{25}-10\xi\right)+\frac{\eta^2}{8\pi^3r^4}\left(\xi-\frac{1}{5}\right)\ln(\mu r). \tag{35}$$

We can see that for the conformal coupling in six dimensions, $\xi=\frac{1}{5}$, there is no ambiguity, the logarithmic contribution disappears and we get $\langle\Phi^2(x)\rangle_{\mathrm{Ren}}=\eta^2/800\pi^3r^4$. [In order to obtain the above result we expressed the logarithmic term which is present in (33) in terms of the $Q_0(\overline{u})$, $\overline{u}$ being $(r^2+r'^2)/2rr'$, and write this Legendre function in its integral representation (19).]

The next section is devoted to the analysis of the vacuum expectation value of the energy-momentum tensor in five and six dimensional space–time.

IV. VACUUM EXPECTATION VALUE OF THE ENERGY-MOMENTUM TENSOR

In this article we are working with a massless scalar quantum field theory in the metric space–time defined by (2), which does not present any dimensional parameter. Moreover, we are adopting the natural system units where $\hbar=c=1$, so because of these reasons the physical quantities calculated in this model can only depend on the radial coordinate r or on the renormalization mass scale μ. By dimensional point of view we could expect that $\langle\Phi^2(x)\rangle_{\mathrm{Ren}}$ be proportional to $1/r^{n-2}$ and $\langle T_{\mu,\nu}(x)\rangle_{\mathrm{Ren}}$ proportional to $1/r^n$. The factor of proportionality should be given in terms of the parameter η^2 and the nonminimal coupling ξ. As to the square of the scalar field, this calculation has been done in this article for the cases where the dimension of the space–time is 5 and 6 up to the first order in η^2. In this section we want to analyze the vacuum expectation value of the energy-momentum tensor. We start considering the five dimensional case.

The renormalized vacuum expectation value of the energy-momentum tensor in five dimensions does not depend on the subtraction mass parameter. So, there is no logarithmic term, and it can be written in a general form by

$$\langle T^{\nu}_{\mu}(x)\rangle_{\mathrm{Ren}}=\frac{A^{\nu}_{\mu}(\xi,\eta^2)}{r^5}. \tag{36}$$

Because there is no trace anomaly in odd dimension, for $\xi=\frac{3}{16}$, we can write

$$\langle T^{\mu}_{\mu}(x)\rangle_{\mathrm{Ren}}=0, \tag{37}$$

so $A^{\mu}_{\mu}=0$. On the other hand, by symmetry of this space–time, the above vacuum expectation value should be diagonal. Moreover, the conservation condition

$$\nabla_\nu \langle T^\nu_\mu(x)\rangle_{\rm Ren}=0 \tag{38}$$

imposes additional restrictions on the components of the tensor A^ν_μ. So, under these conditions we have

$$A^0_0=A^1_1, A^2_2=A^3_3=A^4_4. \tag{39}$$

Using these relations and the traceless condition we can express all nonzero components of A^ν_μ in terms of one of them. Let us choose A^0_0, so we can write

$$A^\nu_\mu=A^0_0\,\mathrm{diag}(1,\ 1,\ -\tfrac{2}{3},\ -\tfrac{2}{3},\ -\tfrac{2}{3}). \tag{40}$$

The explicit calculation of the component A^0_0 involves an extensive calculation which we shall not do here.

The vacuum expectation value of the energy-momentum tensor in six dimensions requires more details. By the expression obtained for the vacuum expectation value of the square of the field, it is possible to infer that there exists a logarithmic contribution to this tensor. Moreover, by the trace anomaly[5] we have

$$\langle T^\mu_\mu(x)\rangle_{\rm Ren}=\frac{1}{64\pi^3}a_3(x). \tag{41}$$

So, we can conclude that the general expression for this object is

$$\langle T^\nu_\mu(x)\rangle_{\rm Ren}=\frac{1}{64\pi^3 r^6}[A^\nu_\mu(\eta^2,\xi)+B^\nu_\mu(\eta^2,\xi)\ln(\mu r)], \tag{42}$$

where A^ν_μ, in principal, are arbitrary numbers. Because the cutoff factor μ is completely arbitrary, there is an ambiguity in the definition of this renormalized vacuum expectation value. Moreover, the change in this quantity under the change of the renormalization scale is given in terms of the tensor B^ν_μ as shown:

$$\langle T^\nu_\mu(x)\rangle_{\rm Ren}(\mu)-\langle T^\nu_\mu(x)\rangle_{\rm Ren}(\mu')=\frac{1}{64\pi^3 r^6}B^\nu_\mu(\eta^2,\xi)\ln(\mu/\mu'). \tag{43}$$

In Ref. 5, Christensen pointed out that the difference between them is given in terms of the effective action which depends on the logarithmic terms whose final expression, in arbitrary even dimension, is

$$\langle T^\nu_\mu(x)\rangle_{\rm Ren}(\mu)-\langle T^\nu_\mu(x)\rangle_{\rm Ren}(\mu')=\frac{1}{(4\pi)^{n/2}}\frac{1}{\sqrt{g}}\frac{\delta}{\delta g^{\mu\nu}}\int d^n x\sqrt{g}a_{n/2}(x)\ln(\mu/\mu'). \tag{44}$$

In our six dimensional case we need the factor $a_3(x)$. The explicit expression for this factor can be found in the paper by Gilkey[12] and in a more systematic form in the paper by Jack and Parker,[13] for a scalar second order differential operator D^2+X, D_μ being the covariant derivative including gauge field and X an arbitrary scalar function. This expression involves 46 terms and we shall not repeat it here in a complete form. The reason is that our calculation has been developed up to the first order in the parameter η^2 and only the quadratic terms in Riemann and Ricci tensors, and in the scalar curvature, are relevant for us. This reduces to 12 the number of terms which will be considered. Discarding the gauge fields and taking $X=-\xi R$ we get

$$\overline{a}_3(x)=\frac{1}{6}\left(\frac{1}{6}-\xi\right)\left(\frac{1}{5}-\xi\right)R\Box R+\frac{\xi^2}{12}R^{;\mu}R_{;\mu}+\frac{\xi}{90}R^{\mu\nu}R_{;\mu\nu}-\frac{\xi}{36}R^{;\mu}R_{;\mu}-\frac{1}{7!}[28R\Box R$$
$$+17R_{;\mu}R^{;\mu}-2R_{\mu\nu;\rho}R^{\mu\nu;\rho}-4R_{\mu\nu;\rho}R^{\mu\rho;\nu}+9R_{\mu\nu\rho\sigma;\gamma}R^{\mu\nu\rho\sigma;\gamma}-8R_{\mu\nu}\Box R^{\mu\nu}$$
$$+24R_{\mu\nu}R^{\mu\rho;\nu}{}_{\rho}+12R_{\mu\nu\rho\sigma}\Box R^{\mu\nu\rho\sigma}+O(R^3). \tag{45}$$

This expression is of sixth order derivative on the metric tensor. Our next step is to take the functional derivative of $\overline{a}_3(x)$. Using the expressions for the functional derivative of the Riemann and Ricci tensor, together with the scalar curvature,[14] we obtain after a long calculation the following expression for the tensor B_μ^ν:

$$B_\mu^\nu(\eta^2,\xi)=\frac{r^6}{6}\left[-\delta_\mu^\nu\Box^2R\left(\xi^2-\frac{\xi}{3}+\frac{23}{840}\right)+\frac{1}{40}\Box^2R_\mu^\nu+\nabla^\nu\nabla_\mu\Box R\left(\xi^2-\frac{\xi}{3}+\frac{1}{42}\right)\right]+O(R^2). \tag{46}$$

Moreover, developing all the terms which appear in Eq. (46) we obtain, after some calculations,

$$B_\mu^\nu(\eta^2,\xi)=\frac{\eta^2}{225}\,\mathrm{diag}(6,6,-3,-3,-3,-3)+16\eta^2(\xi-1/5)(\xi-2/15)\,\mathrm{diag}(1,-4,2,2,2,2). \tag{47}$$

As in the last case, it is possible to make some restrictions on the tensor A_μ^ν. Again because of the spherical symmetry of the problem, we can infer that this tensor should be diagonal. Moreover, the renormalized vacuum expectation value of the energy-momentum tensor must be conserved, i.e.,

$$\langle T_\mu^\nu(x)\rangle_{\mathrm{Ren};\nu}=0. \tag{48}$$

From these six equations and defining the variable $T=64\pi^3r^6\langle T_\mu^\mu(x)\rangle_{\mathrm{Ren}}$ we obtain

$$A_0^0=T+A_1^1-B_1^1+(B_1^1-B_0^0)\ln(\mu r) \tag{49}$$

and

$$A_2^2=A_3^3=A_4^4=A_5^5=\frac{B_1^1}{4}-\frac{A_1^1}{2}-\left(B_2^2+\frac{B_1^1}{2}\right)\ln(\mu r). \tag{50}$$

When the nonminimal coupling ξ coincides with the conformal one, $\frac{1}{5}$, we get

$$A_0^0=T+A_1^1-B_1^1, \tag{51}$$

$$A_2^2=A_3^3=A_4^4=A_5^5=\frac{B_1^1}{4}-\frac{A_1^1}{2}, \tag{52}$$

with

$$T=r^6a_3(x)=-\frac{1}{4200}\Box^2R+O(R^2)=\frac{8}{350}\frac{\eta^2}{r^6}+O(\eta^4). \tag{53}$$

Again the complete evaluation of $\langle T_\mu^\nu(x)\rangle_{\mathrm{Ren}}$ requires the knowledge of at least one component of the tensor A_μ^ν, say A_1^1. However, we do not attempt to do this straightforward and long calculation here.

V. CONCLUDING REMARKS

In this article we have found a formal expression for the Euclidean scalar Green function associated with a massless field in higher dimensional global monopole space–time defined by (2), i.e., space-time where the dimension is bigger than four and presents a solid angle deficit. The expression for this function is given in terms of an infinite sum of products of Legendre functions with Gegenbauer polynomials or hyperspherical harmonics. Having this Green function in our hands, we can use it to calculate the vacuum expectation value of some physically relevant operators, as the square of the field and the energy-momentum tensor. We have applied this formalism to calculate $\langle\Phi^2(x)\rangle$ and $\langle T_{\mu\nu}(x)\rangle$ in five and six dimensions. However, these calculations become effective only for the case when the parameter α, associated with the solid angle deficit, is close to unity. In this case we can expand the Green function in powers of the parameter $\eta^2=1-\alpha^2$, and obtain closed results for these two quantities.

As it was mentioned, the vacuum expectation values for these quantities are divergent and these divergences are a consequence of the evaluation of the two-point Green functions in the coincidence limit. In order to obtain finite and well defined results we adopted the point-splitting renormalization procedure and eliminated all divergences, subtracting from the Green function the Hadamard one. An interesting result of our calculation was that the renormalized vacuum expectation value of the square of the field in the five dimensional global monopole space–time vanishes when we take for the nonminimal coupling constant ξ the conformal value $\frac{3}{16}$. A similar calculation in the six dimensional case shows that a finite contribution remains for $\xi=\frac{1}{5}$, which is independent of the mass cutoff parameter.

Moreover, in the six dimensional case, there appears in the renormalized vacuum expectation value of the energy-momentum tensor, the function $a_3(x)$. This function, according to Ref. 15 on p. 159, is associated with a purely geometric (divergent) Lagrangian that should renormalize the modified classical Einstein one. When similar terms are inserted into the gravitational action, the field equation is modified by the presence of order six terms proportional to

$$c_1 g_{\mu\nu}\Box^2 R + c_2 \Box^2 R_{\mu\nu} + c_3 \nabla_\mu \nabla_\nu \Box R + O(R^2). \tag{54}$$

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APPENDIX: THE (1+2)-DIMENSIONAL CASE LIMIT

In this appendix we present a nontrivial extension of our Green function (17) for the case where $d=2$. Although this Green function constructed for $d\geqslant 3$ presents a pole at $d=2$, the Gegenbauer polynomial is also not defined when its order is zero. However, it is possible to get such an expression if we admit that (17) is a function of a continuous parameter d. According to Ref. 16, it is possible to obtain a well defined limit for the ratio of the Gegenbauer polynomial by its order when it goes to zero. This limit is given by

$$\lim_{d\to 2}\frac{1}{d-2}C_n^{(d-2)/2}(x)=\frac{T_n(x)}{n}, \tag{A1}$$

where $T_n(x)$ is the Chebychev polynomials type I. Moreover, in the limit $d=2$, $\nu_n=|n|/\alpha$. However, we have to be careful when we try to substitute the above limit into (17). The definition of the Chebychev polynomial type I by its generating function reproduces explicitly the polynomials with order $n\geqslant 1$ in a recurrence equation separated from the $T_0(x)$ (see Ref. 16). Taking into account this fact we have to consider a multiplicity factor in the summation. Finally, we arrive at the following Green function:

$$G^{(2)}(x,x')=\frac{1}{2\pi^2}\frac{1}{\sqrt{rr'}}\sum_{n=0}^{\infty}Q_{n/\alpha-1/2}T_n(\cos\gamma)\epsilon(n), \tag{A2}$$

with $\epsilon(0)=1$ and $\epsilon(n>0)=2$. However, $T_n(\cos\gamma)=\cos(n\gamma)$ (see again Ref. 16, p. 631). Finally, substituting the integral representation for the Legendre function (19), we obtain

$$G^{(2)}(x,x')=\frac{1}{2\pi^2}\frac{1}{\sqrt{2rr'}}\int_{\rho}^{\infty}dt\,\frac{1}{\sqrt{\cosh t-\cosh\rho}}\,\frac{\sinh(t/\alpha)}{\cosh(t/\alpha)-\cos(\gamma)}. \tag{A3}$$

This equation is equivalent with the Euclidean Green function for the three dimensional conical space given in Eq. (2.19) of Ref. 17. We can see that by changing in a compatible way the coordinates r by r/α, γ by γ/α and τ by z.

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Integrable cases of gravitating static isothermal fluid spheres

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It is shown that different approaches toward the solution of the Einstein equations for a static spherically symmetric perfect fluid with a γ-law equation of state lead to an Abel differential equation of the second kind. Its only integrable cases at present are flat space–time, de Sitter solution and its Buchdahl transform, Einstein static universe, and the Klein–Tolman solution. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1431259]

I. INTRODUCTION

The Einstein equations for static and spherically symmetric perfect fluids have been investigated by many authors.[1–3] The metric of a static spherically symmetric space–time reads:

$$ds^2 = e^{2\nu}dt^2 - e^{\lambda}dr^2 - R^2(d\theta^2 + \sin^2\theta\, d\varphi^2), \tag{1}$$

where ν,λ,R depend only on the radial coordinate r. We use units in which $8\pi G = c = 1$. Spherical symmetry requires that the energy–momentum tensor is diagonal, $T^{\nu}_{\mu} = \mathrm{diag}(\rho, -p_r, -p_0, -p_\varphi)$ where $\rho(r)$ is the fluid density, $p_r(r)$ is the radial pressure, and $p_\theta(r), p_\varphi(r)$ are the tangential pressures. It also requires that $p_\theta = p_\varphi$. Perfect fluids, in addition, have no pressure anisotropy, namely $p \equiv p_r = p_\theta = p_\varphi$.

An abundance of solutions has been found when no equation of state is prescribed, since then the unknown functions are more than the equations. The problem becomes very difficult when p is defined as a known function of ρ. A realistic equation of state is provided by the Newtonian polytropes $p = (1/n)\rho^{1+1/k}$, which have been studied for many years.[4,5] In the limit when $k \to \infty$ a softer isothermal equation of state emerges

$$\rho = np, \tag{2}$$

usually called the γ-law, because it is traditionally written as $p = (\gamma - 1)\rho$. Physically realistic perfect fluid solutions should have finite and positive density and pressure and $\rho \geqslant p$, i.e., we impose the weak and dominant energy conditions. The fluid should be causal; the speed of sound $(dp/d\rho)^{1/2}$ must be positive and less than 1, the speed of light. Stability against radial pulsations requires that p should decrease outwards and ρ should not increase outwards.[3] For the equation of state (2) these conditions demand that $n \geqslant 1$ and at least one of the fluid characteristics is finite, positive, and decreasing. Important special cases include dust ($n = \infty$), incoherent radiation ($n = 3$), and stiff fluid ($n = 1$) where the speed of sound equals the speed of light.

Even for such a simple relation, few analytic solutions have been found. When $n = \infty$ and $\rho \neq 0$ the pressure vanishes, giving the case of dust. In fact, the density also vanishes and what remains is trivial flat space–time. When $n = -1$ the pressure and the density are constant and the solution is equivalent to a vacuum solution with a cosmological constant found by de Sitter. We show in this paper that the case $n = -5$ is connected to it by the Buchdahl transformation $n \to -(n+6)$[6–8] and is also soluble. The case $n = -3$ leads to the Einstein static universe.[2] It is

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clear that the unphysical cases ($n<1$) should be studied too since they produce cosmological solutions or are connected to the physical ones by a general transformation, valid also when no equation of state is prescribed.

A simple solution for a general n was hidden among the solutions found by Tolman.[9] In fact, he studied the field equations under simplifying assumptions for the metric components, without imposing an equation of state. The pressure and the density in some of his solutions happen to satisfy Eq. (2) when certain constants are sent to zero or to infinity.[3] The first who systematically investigated relation (2) was Klein. He rediscovered the Tolman solution first for $n=3$ and later for arbitrary n.[10,11] His approach and results, published in a not-readily available journal, remained unnoticed for a long time. Even in Ref. 1 his second work is mentioned as referring to the polytropic equation of state, which is true only for its beginning. For a third time this Klein–Tolman (KT) solution was found by Misner and Zapolsky[12] where its relevance to neutron stars was studied. The radial dependence of the density, however, was omitted due to a misprint, causing additional confusion. Nevertheless, this paper became a standard reference toward which further rediscoveries[13,14] were directed.[15] This solution is singular at the center where ρ and p become infinite.

Klein also found numerically a regular solution for $n=3$, starting in phase space from Minkowski space–time and spiraling toward the KT solution. His work was based on a certain first-order differential equation. This solution was also rediscovered later by numeric studies of two-dimensional autonomous dynamical systems[5,16,17] and generalized for arbitrary realistic n. Its phase space is contaminated by grossly unrealistic solutions with density, vanishing in some finite interval $[0,r_c]$, and metric possessing curvature singularities. Only the exact KT solution and the numerical regular solution are acceptable. Unfortunately, solutions satisfying Eq. (2) are not asymptotically flat and the fluid sphere extends to infinity. Nevertheless they can describe the superdense core of a neutron star and have finite masses when a cutoff is done at some distance, despite the singularity in the KT solution.[12,18] They can be joined smoothly to the exterior Schwarzschild solution with the help of an intermediate layer of perfect fluid with boundary, like the degenerate nonrelativistic neutron gas[12] or the Schwarzschild interior solution.

Another way for the fluid to acquire a boundary is to add to the right-hand side of the scale-invariant Eq. (2) a positive constant ρ_0. The numerical study of a perfect fluid with such linear equation of state[19] stresses once more the importance of the solutions of Eq. (2) which appear as scale-invariant boundaries for all orbits in a three-dimensional compact phase space. All equilibrium points lie on these boundaries, including Minkowski space–time, which is a starting point for the regular subset of solutions. The high pressure limit which probes the relativistic effects lies there too. The KT and the regular scale-invariant solutions, together with some nonregular solution, play a crucial role in the understanding of the structure of solution space for the linear equation of state. Therefore it is desirable to have analytic expressions for these unique solutions. They will allow one to study in detail the qualitative changes in their behavior with respect to the parameter n such as the change of the KT equilibrium point from focus to node when $n=\sqrt{64/7}-3$, the bifurcation point at $n=1$ or the relation to the simple integrable cases for negative n.

The question whether the regular solution to Eq. (2) has an explicit expression has never been answered in a satisfactory way. The persistent closure of analytic methods on the irregular KT solution suggests that there are no more integrable cases except it and the few above-mentioned solutions. On the other hand, similar problems have been completely solved explicitly. For example, static dust solutions are not possible. The dust must be nonstatic or charged. In both cases the general solution has been found.[20–22] The cylindrically symmetric static case has been solved in simple functions, using two different gauges.[23,24] The relation between them was clarified in Ref. 25. The planar case follows easily from the cylindrical one[24] or from the spherical one.[17,26]

The purpose of this paper is to derive the integrable cases in a unified manner and to elucidate the mathematical difficulty of the problem. We show that in its heart stands the Abel equation of the second kind, whose normal form is

$$ww_{,z}-w=f(z). \tag{3}$$

Derivatives are denoted by a comma and subscript. Derivatives with respect to r are also denoted by a prime. The integrable cases of Eq. (3) depend on the shape of $f(z)$ and are tabulated in Ref. 27. The functions that emerge are in general transcendental, but simplify for special values of n. The integrable cases that we find are given by $n=-5,-3,-1,\infty$ and the KT solution with n outside the interval $(-5.83,-0.17)$.

In the following three sections three different approaches are discussed which invariably lead to Eq. (3) with functions $f(z)$ possessing the same general structure but with different coefficients. In Sec. II we start from the well-known Tolman–Oppenheimer–Volkoff (TOV) equation[9,28] written in a general spherical metric. In Sec. III the starting point is a differential equation derived by Klein in curvature coordinates. In Sec. IV we utilize the approach of Haggag and Hajj-Boutros (HH) described in Ref. 14 for a stiff perfect fluid in isotropic coordinates. Section V is dedicated to the Buchdahl transformation which supplies the integrable case $n=-5$. Finally, Sec. VI contains some discussion and conclusions.

II. ANALYSIS OF THE TOV EQUATION

The Einstein equations for the metric (1) and the energy–momentum tensor of a perfect fluid, discussed in Sec. I, are written as[29]

$$\rho=\frac{1}{R^2}-e^{-\lambda}\left(\frac{2R''}{R}+\frac{R'^2}{R^2}\right)-(e^{-\lambda})'\frac{R'}{R}, \tag{4}$$

$$p=-\frac{1}{R^2}+e^{-\lambda}\frac{R'}{R}\left(\frac{R'}{R}+2\nu'\right), \tag{5}$$

$$p=e^{-\lambda}\left[\frac{R''}{R}+\nu''+\left(\nu'-\frac{\lambda'}{2}\right)\left(\nu'+\frac{R'}{R}\right)\right]. \tag{6}$$

The contracted Bianchi identity

$$p'=-(\rho+p)\nu', \tag{7}$$

follows from Eqs. (4)–(6) and usually replaces Eq. (6). Thus Eqs. (4), (5), and (7) determine ν, λ, R, ρ and p. One of the metric functions is redundant and can be used to fix the gauge. Different coordinate systems have been introduced in the literature. Curvature coordinates (also called Schwarzschild coordinates) are obtained when $R=r$. Isotropic coordinates have $R=re^{\lambda/2}$ while polar Gaussian coordinates set $e^{\lambda}=1$. Other coordinates are known as well. Fixing the gauge and the equation of state equals the number of unknowns and equations. For the time being, we proceed in full generality to derive the TOV equation. Let us define the so-called mass function $m(r)$, which is obtained from the sectional curvature of the spherical two-surfaces:

$$m(r)\equiv\tfrac{1}{2}R(1-e^{-\lambda}R'^2). \tag{8}$$

Then Eq. (4) may be written as

$$\rho=\frac{2m'}{R^2R'}, \tag{9}$$

which integrates to

$$m(R)=\frac{1}{2}\int_0^R\rho R^2\,\mathrm{d}R. \tag{10}$$

Passing from r to R dependence, inserting $e^{-\lambda}$ from Eq. (8) and ν_R from Eq. (7) into Eq. (5) results in the general TOV equation

$$p_{,R}=-\frac{(\rho+p)(2m+pR^3)}{2R(R-2m)}. \tag{11}$$

In the case of dust $p=0$. Then Eq. (11) yields $\rho m=0$, which combined with Eqs. (9) and (10) gives $\rho=0$. There is no matter and the solution is trivial flat space–time. In the general case when $p=p(\rho)$, Eq. (9) shows that Eq. (11) is a differential equation for $m(R)$. Let us now introduce the variables $M=m/R$, $D=\frac{1}{2}\rho R^2$ and $P=\frac{1}{2}pR^2$. Then Eq. (11) becomes

$$RD_{,R}=2D-\frac{(D+P)(M+P)}{(1-2M)p_{,\rho}}. \tag{12}$$

Specializing to the γ-law equation of state and introducing $\tau=\ln R$ we obtain from Eqs. (12) and (9) the autonomous system[29]

$$(2M-1)D_{,\tau}=D\left[(n+5)M-2+\frac{n+1}{n}D\right], \tag{13}$$

$$D=M_{,\tau}+M. \tag{14}$$

The case $n=0$ is excluded because it gives vanishing density. This system was derived in polar Gaussian coordinates by Collins[5] and further analyzed by him in Refs. 17 and 30.

Now, let us insert Eq. (14) into Eq. (13) and define $x=M-1/2$. The result is

$$xx_{,\tau,\tau}=\frac{n+1}{2n}x_{,\tau}^2+\left[\frac{(n+1)(n+2)+2n}{2n}x+\frac{(n+1)(n+2)}{4n}\right]x_{,\tau}+A(x), \tag{15}$$

$$A(x)\equiv\left(x+\frac{1}{2}\right)\left[\frac{(n+1)^2+4n}{2n}\left(x+\frac{1}{2}\right)-1\right]. \tag{16}$$

Equation (8) indicates that $x<0$. The solution of Eq. (15) determines M and consequently m as functions of R. Then D is given by Eq. (14) which determines $\rho(R)$. The pressure is given by Eq. (2), while ν follows from Eq. (7) written as

$$(\rho+p)\nu_{,R}=-p_{,R}. \tag{17}$$

Finally, $e^{-\lambda}R'^2$ is found from Eq. (5), written as

$$e^{-\lambda}R'^2=\frac{1+pR^2}{1+2R\nu_{,R}}. \tag{18}$$

In order to determine $\lambda(r)$ one should specify $R(r)$, the most simple choice being $R=r$. In polar Gaussian coordinates Eq. (18) yields an equation for $R(r)$ with separated variables. The same is true in isotropic coordinates.

Equation (15) simplifies enormously when x is constant, becoming

$$M\left[\frac{(n+1)^2+4n}{2n}M-1\right]=0. \tag{19}$$

The choice $M_1=0$ leads to $m=p=\rho=0$, i.e., to flat space–time. The choice

$$M_2=\frac{2n}{(n+1)^2+4n} \tag{20}$$

gives via Eq. (14) $D=M=$const and $\lambda=$const, $\rho=2D/R^2$ which is exactly the KT solution. At the center the density and the pressure have poles and diverge. This solution does not exist when $-5.83=-3-2\sqrt{2}<n<-3+2\sqrt{2}=-0.17$ because then $x_2=M_2-1/2$ is positive or vanishes (when $n=-1$). In the intervals $-0.17<n<0$ and $n<-5.83$ the solution exists but ρ and p have different signs.

When $x_{,\tau}\neq 0$ we can decrease the order of Eq. (15) by the standard change of variables $x_{,\tau}\equiv -y(x)$:

$$xyy_{,x}=\frac{n+1}{2n}y^2-\left[\frac{(n+1)(n+2)+2n}{2n}x+\frac{(n+1)(n+2)}{4n}\right]y+A(x). \tag{21}$$

Equation (21) falls in the class

$$[g_1(x)y+g_0(x)]y_{,x}=f_2(x)y^2+f_1(x)y+f_0(x). \tag{22}$$

There is a standard procedure for the solution of such equations.[27] It consists of two changes of variables which bring them to the Abel equations of the second kind given by Eq. (2) or by

$$ww_{,\zeta}=g(\zeta)w+1. \tag{23}$$

This procedure is much easier when $g_0=0$ and $f_2=$const as in Eq. (21). Namely, we have $w=yE$, $f(z)=f_0E/f_1$, $g(\zeta)=f_1/f_0E$, and

$$E=\exp\left(-\int\frac{f_2}{g_1}\mathrm{d}x\right), \tag{24}$$

$$z(x)=\int\frac{f_1}{g_1}E\mathrm{d}x, \tag{25}$$

$$\zeta(x)=\int\frac{f_0}{g_1}E^2\mathrm{d}x. \tag{26}$$

Since f_1 is a simpler polynomial than f_0 we shall use Eqs. (3) and (25). The use of Eqs. (23) and (26) is more complicated, but does not bring additional integrable cases.

Applied to Eq. (21) the chosen alternative of the general method yields

$$w=yx^{-(n+1)/n}, \tag{27}$$

$$z=-\frac{1}{4n}\int[(n^2+5n+2)2x+(n+1)(n+2)]x^{-(n+1)/2n-1}\mathrm{d}x. \tag{28}$$

The case $n=1$ (stiff fluid) is special because a logarithmic term appears in z,

$$z=-4\ln|x|+\frac{3}{2x}, \tag{29}$$

$$f(z)=-\frac{(2x+1)(4x+1)}{x(8x+3)}. \tag{30}$$

The relation $z(x)$ is transcendental and throws $f(z)$ out of the tables with integrable cases present in Ref. 27. The case $n=-1$ also leads to a logarithmic term but its coefficient vanishes. This case

is integrable. In fact, we may go back directly to Eq. (13) which becomes $D_{,\tau}=2D$ if $M\neq 1/2$ and yields $\rho=-p=\text{const}$. This is the well-known de Sitter solution. When $M=1/2$, Eq. (13) is satisfied identically and we obtain formally the KT solution (20) with $n=-1$, but it has $e^{-\lambda}R'^2=0$ which is unacceptable.

In the generic case $n\neq\pm 1$ and Eq. (28) integrates to

$$z=-\frac{x^{-(n+1)/2n}}{2(n-1)}[(n^2+5n+2)2x-(n-1)(n+2)], \tag{31}$$

$$f(z)=\frac{(n-1)(2x+1)[(n^2+6n+1)2x+(n+1)^2]z}{[(n^2+5n+2)2x-(n-1)(n+2)][(n^2+5n+2)2x+(n+1)(n+2)]}. \tag{32}$$

The $z-x$ connection in Eq. (31) is transcendental, except for special values of n, and Eq. (3) is nonintegrable in general. Let us investigate the special cases.

When $n=-3$, f_1 divides f_0 and $f(z)=8z$, $z=-\frac{1}{2}(2x+1)x^{-1/3}$. This is an integrable case, corresponding to the Einstein static universe. It is discussed in more detail in Sec. III. There is also the formal $n=-3$ case of the KT solution (20). It does not exist since $x=1/4>0$.

One may try to simplify Eq. (31) by nullifying the coefficients on the right-hand side. The condition $n^2+5n+2=0$ gives $n=\frac{1}{2}(-5\pm\sqrt{17})$. This is of no good since the radical enters the power of x. The other possibility $n=-2$ looks more promising. Then Eq. (31) becomes $x^{3/4}=-3z/4$ and Eq. (32) reduces to

$$f(z)=\tfrac{21}{16}z-\tfrac{9}{16}(\tfrac{4}{3})^{4/3}z^{-1/3}+\tfrac{3}{64}(\tfrac{4}{3})^{8/3}z^{-5/3}. \tag{33}$$

This function leads to an integrable equation when the coefficient in front of z is $-3/16$, which is not true here.

There are several n which convert Eq. (31) into an algebraic equation for x of fourth order or lower. It can be solved explicitly for $x(z)$ and the answer replaced in Eq. (32). Third- and fourth-order equations appear when $n=\pm 1/5,\pm 1/7,-1/2,-3/5$. The radical structure of $f(z)$, however, is incompatible with the tables with integrable $f(z)$. Second-order equations appear when $n=\mp 1/3$, respectively,

$$4x=-5\pm\sqrt{25+48z}, \tag{34}$$

$$6zx=17\pm\sqrt{17+42z}. \tag{35}$$

Unfortunately, the only integrable functions with square roots include the term $\sqrt{z^2+z_0}$, which is not present in the above-given relations.

Comparison between Eqs. (31)–(32) and Eq. (20) shows how complex the numerical regular solution must be, which starts in x,y coordinates from flat space–time and focuses on the KT solution, following a spiral around it. The innocent parameter n, introduced in Eq. (2), proliferates like cancer in the process of solution, ending with the intricate coefficients in $z(x)$ and $f(z)$. It even determines the transcendental or algebraic nature of $z(x)$. In conclusion, the only integrable cases found within this approach are $n=\infty$ (trivial dust solution), $n=-1$ (de Sitter solution), $n=-3$ (Einstein static universe), and $M=\text{const}$ (the KT solution).

Finally, let us discuss for comparison the case of planar symmetry, which is solvable. Going to polar Gaussian coordinates, the metric element reads

$$\mathrm{d}s^2=e^{2\nu}\mathrm{d}t^2-\mathrm{d}r^2-R^2(\mathrm{d}x_2^2+F(x_2)^2\mathrm{d}x_3^2), \tag{36}$$

where $F(x_2)=\sin x_2$ for spherical symmetry and $F(x_2)=1$ for planar symmetry.[17,26] It is possible to generalize the TOV equation to encompass both cases. Instead of Eq. (13) one should write

$$(2M-K)D_{,\tau}=D\left[-2K+(n+5)M+\frac{n+1}{n}D\right], \tag{37}$$

where $K=1$ or 0, corresponding to spherical or planar symmetry, respectively. In the second case, Eq. (37) simplifies

$$2MM_{,\tau,\tau}=\frac{n+1}{n}M_{,\tau}^2+bMM_{,\tau}+aM^2, \tag{38}$$

where $a=n+1/n+6$, $b=n+2/n+5$. This is the analog of Eq. (15). Proceeding in the same way we again obtain the Abel equation (3) with $y=-M_{,\tau}$ and

$$w=yM^{-(n+1)/2n}, \tag{39}$$

$$z=\frac{bn}{1-n}M^{(n-1)/2n}, \tag{40}$$

$$f(z)=\frac{(n-1)a}{nb^2}z. \tag{41}$$

As mentioned before, Eq. (3) with $f(z)=\alpha z+\beta$, where α and β are constants, is integrable. The solution, in parametric form, reads

$$z=Ce^T-\frac{\beta}{\alpha}, \tag{42}$$

$$w=C\sigma e^T, \tag{43}$$

$$T=-\int\frac{\sigma \mathrm{d}\sigma}{\sigma^2-\sigma-\alpha}, \tag{44}$$

with C being an arbitrary constant. In Ref. 17 the problem was solved in a different way, by introducing the variable $\tilde{D}=D/M$. Then Eqs. (14) and (37) are equivalent to

$$2\tilde{D}_{,\tau}=\tilde{D}\left(n+7+\frac{1-n}{n}\tilde{D}\right). \tag{45}$$

This is a Bernoulli equation and is easily solved. Further details may be found in Ref. 17 where also a connection with earlier work[31,32] on the particular cases $n=1$ and $n=3$ is established.

III. THE APPROACH OF KLEIN

This approach was developed in curvature coordinates where Eqs. (4), (5), and (7) simplify to

$$p=\frac{2}{r}\nu' e^{-\lambda}-\frac{1}{r^2}(1-e^{-\lambda}), \tag{46}$$

$$\rho=\frac{1}{r}\lambda' e^{-\lambda}+\frac{1}{r^2}(1-e^{-\lambda}), \tag{47}$$

$$p'=-(\rho+p)\nu'. \tag{48}$$

Imposing the γ-law, we can integrate Eq. (48):

$$p = p_0 e^{-(n+1)\nu}. \tag{49}$$

Like before, the case of dust $n=\infty$, $p=0$ gives a trivial solution with constant ν and λ. Supposing that $p \neq 0$, let us introduce the variables $s = p_0 r^2$, $\xi = e^{(n+1)\nu}/s$ and

$$x = \xi e^{-\lambda} = \frac{e^{-\lambda}}{pr^2}. \tag{50}$$

Obviously x and ξ always have the same sign and are positive when the pressure is positive.

We shall derive an equation for x, similar to Eq. (15). In Secs. II–IV the main functions are denoted by x although they are different, in order to simplify notation and to stress the role of Eq. (22) in the whole problem. Let us multiply Eq. (46) by $(n+1)/4$, Eq. (47) by $-1/2$, and sum. The result is

$$4(sx)_{,s} - (n+3)(1-e^{-\lambda})\xi = 1-n. \tag{51}$$

Let us introduce $2\tau = \ln s$. It differs by a constant from the variable in Sec. II, but this is not important since the final equation will be autonomous. Laying temporarily aside the special case $n=-3$, we can express ξ from Eq. (51) as

$$\xi = \frac{1}{n+3}[2x_{,\tau} + (n+7)x + n - 1]. \tag{52}$$

Equation (46) may be written in the following way:

$$4(s\xi)_{,s} - (n+1)(e^{\lambda}-1)\xi = (n+1)e^{\lambda}. \tag{53}$$

The usage of Eqs. (50) and (52) transforms this relation into an autonomous second-order equation for x. The change of variables $x_{,\tau} = -y(x)$ applies again, leading to

$$\begin{aligned} 2(n+3)xyy_{,x} = {} & 2(n+1)y^2 + 2(n+11)xy - (n+1)(3n+1)y - 4(n+7)x^2 \\ & + (n^3+9n^2+11n+11)x + (n+1)^2(n-1). \end{aligned} \tag{54}$$

This is exactly the equation of Klein derived in Refs. 10 and 11, where the notation $n = 2n_{Kl} + 1$ and $x = (n_{Kl}+1)^2 x_{Kl}$ was used. He studied it by series expansion and numerically, and was the first to find its regular solution (see Fig. 1 from Ref. 10). When $x(\tau)$ is known Eq. (52) gives ξ, and Eq. (50) determines both λ and p. Then Eq. (49) becomes an expression for ν and finally ρ is given by Eq. (2). Modulo coefficients, Eq. (54) is the same as Eq. (21) and also falls in the class (22). Therefore, the procedure described in Sec. II can be applied to bring it to the form of Eq. (3) with

$$w = yx^{-(n+1)/(n+3)}, \tag{55}$$

$$z = \tfrac{1}{2}[(n+11)x + 3n + 1]x^{-(n+1)/(n+3)}, \tag{56}$$

$$f(z) = -\frac{2[4x-(n+1)^2][(n+7)x+n-1]z}{[2(n+11)x-(n+1)(3n+1)][(n+11)x+3n+1]}. \tag{57}$$

There are no logarithmic terms in z within this approach. As with Eq. (31), $x(z)$ is transcendental except in special cases.

Equation (54) shows that the KT solution is given here by

$$x_0 = \frac{(n+1)^2}{4}. \tag{58}$$

The other root $x=-(n-1)/(n+7)$ leads to $\xi=0$ and $e^{2\nu}=e^{\lambda}=0$, $\rho=np=\infty$, which is unacceptable. Now, since $x_0\geqslant 0$ for any n, we must ensure that $\xi_0>0$ in order to have positive $e^{-\lambda}$. Equation (52) gives $\xi_0=n^2+6n+1$ and we obtain the same conditions for the existence of the KT solution as Sec. II.

In the case $n=-1$, Eq. (48) yields $p=p_0$, $\rho=-p_0$, while the sum of Eqs. (46) and (47) provides the relation $2\nu=-\lambda$. Equation (47) is a linear equation for $e^{-\lambda}$, its solution being

$$e^{-\lambda}=1-\frac{2m_0}{r}+\frac{p_0}{3}r^2, \tag{59}$$

where m_0 is a constant of integration, identified as the gravitating mass. This is precisely the Kottler solution.[2] It can be used as a regular interior solution when $m_0=0$. Then it becomes the de Sitter solution. The KT solution for $n=-1$ has $x_0=0$ and does not exist.

When $n=-3$, Eq. (51) determines directly x: $x=1+x_1/s$, while Eq. (49) gives $p=p_0e^{2\nu}$. Then we have from Eq. (50) $e^{-2\nu-\lambda}=x_1+s$. Equation (46) becomes a linear equation for $e^{2\nu}$ when these results are taken into account. There are two possibilities. When the constant $x_1=0$, $x=1$, which is the formal KT solution (58) for $n=-3$. In fact, it does not exist. When $x_1\neq 0$ the solution is

$$x_1e^{2\nu}=1+C_1\left(1+\frac{x_1}{s}\right)^{1/2}, \tag{60}$$

where C_1 is another integration constant. A regular solution is obtained when $x_1=1$ and $C_1=0$. Then $\nu=0$ and

$$e^{\lambda}=\frac{1}{1+p_0r^2}. \tag{61}$$

The last two equations represent the metric of the Einstein static universe. The pressure and the density are constant, $p=p_0$, $\rho=-3p_0$.

There are two cases when the coefficients of $z(x)$ are simplified, namely $n=-11$ and $n=-1/3$. In the first case, Eq. (57) reads

$$-320f(z)=75z+16^{8/5}z^{-3/5}+22\times 16^{4/5}z^{1/5}. \tag{62}$$

The function

$$f(z)=c_1z+c_2z^{q_1}+c_3z^{q_2} \tag{63}$$

is integrable for a set of (q_1,q_2) but $(-3/5,1/5)$ is not among them. When $n=-1/3$ we have

$$f(z)=-\tfrac{15}{64}z+\tfrac{7}{96}\left(\tfrac{16}{3}\right)^{4/3}z^{-1/3}-\tfrac{1}{192}\left(\tfrac{16}{3}\right)^{8/3}z^{-5/3}. \tag{64}$$

The set $(-1/3,-5/3)$ is integrable, but only when $c_1=-3/16$, which is not the case here.

Finally, there are few n when Eq. (56) is an algebraic equation up to the fourth order. Only the cases $n=-5,-2,1$ are candidates for integrability because they lead to quadratic equations. Of these, $n=-5,-2$ yield radicals resembling those in Eqs. (34) and (35) and should be rejected. More interesting is the case of stiff fluid when

$$x=\tfrac{1}{72}(z^2-24\pm z\sqrt{z^2-48}), \tag{65}$$

$$f(z)=-\frac{2z[(z^2-60)x-4]}{9[(z^2-24)x-8]}. \tag{66}$$

The radicals in $f(z)$ are of the necessary type, but its structure is too complex to figure in the tables with integrable cases.

Like in Sec. II, the only integrable cases found are $n=-3,-1,\infty$ and $x=x_0$. The unsuccessful candidates for explicit solutions have in general different values of n in the two approaches. When they coincide, as is the case $n=1$, the reasons for rejection are different—a logarithmic term in the TOV–Collins approach and a complicated $f(z)$ in the Klein approach.

It is interesting to compare the main variable in this section $x\equiv x_K$ to the variables in the TOV approach, specialized to curvature coordinates. Equation (8) becomes

$$M=\frac{m}{r}=\frac{1}{2}(1-e^{-\lambda}), \tag{67}$$

and transforms Eq. (50) into

$$x_K=\frac{1-2M}{2nD}. \tag{68}$$

Thus, not only $x=M-1/2$, but also the above-mentioned combination satisfy Abel equations of the second kind. The function x_K resembles $\tilde{D}$, used in the planar case. It is well known that when $\tilde{D}$ satisfies the Bernoulli equation (45), $\tilde{D}^{-1}=M/D$ satisfies a linear equation. This fact stresses once more the conclusion that the spherical case is much more complicated than the planar one.

IV. APPROACH IN ISOTROPIC COORDINATES

One can pass from arbitrary to isotropic coordinates in Eqs. (4)–(6) by putting $R=re^{\lambda/2}$. Let us make also the change $s=\ln r$. Then

$$\rho r^2e^{\lambda}=-\lambda_{,s,s}-\tfrac{1}{4}\lambda_{,s}^2-\lambda_{,s}, \tag{69}$$

$$pr^2e^{\lambda}=\tfrac{1}{4}\lambda_{,s}^2+\lambda_{,s}\nu_{,s}+\lambda_{,s}+2\nu_{,s}, \tag{70}$$

$$pr^2e^{\lambda}=\tfrac{1}{2}\lambda_{,s,s}+\nu_{,s,s}+\nu_{,s}^2. \tag{71}$$

Let us introduce next the variable

$$\frac{1}{t}=\lambda_{,s}+2, \tag{72}$$

and impose the γ-law equation of state. An expression for $\nu_{,s}$ is obtained from Eqs. (69) and (70):

$$\nu_{,s}=\frac{t_{,s}}{nt}-\frac{n+1}{4n}\left(\frac{1}{t}-4t\right). \tag{73}$$

Next, let us combine Eqs. (70) and (71) and replace in them $\lambda_{,s}$ and $\nu_{,s}$ from Eqs. (73) and (74). A long, but straightforward computation produces an autonomous equation for t,

$$\begin{aligned}2ntt_{,s,s}=&-2(1-n)t_{,s}^2+\tfrac{1}{2}(n^2+5n+2)t_{,s}-2(n+1)(n+2)t^2t_{,s}-2(n+1)^2t^4\\&+[(n+1)^2+2n]t^2-\frac{n}{2}-\frac{(n+1)^2}{8}.\end{aligned} \tag{74}$$

A solution of this master equation determines all characteristics of the metric and the fluid.

When $n=1$, Eq. (74) is exactly Eq. (9) from Ref. 14. In this section we generalize the HH approach to arbitrary n and bring it to its logical end—the Abel equation (3). We first lower the order of the polynomial in Eq. (74) by setting $t^2=x/4$ and then perform the change of variables

$$(\sqrt{x})_{,s}=-\tfrac{1}{2}y. \tag{75}$$

The condition $x\geqslant 0$ should be maintained throughout the calculations. Equation (74) acquires its final form

$$2nxyy_{,x}=(n-1)y^2+[(n+1)(n+2)x-(n^2+5n+2)]y+(x-1)[4n+(n+1)^2-(n+1)^2x]. \tag{76}$$

It falls in the class (22) and resembles Eqs. (21) and (54), but its coefficients are different functions of n. Proceeding like before, we get

$$w=yx^{-(n-1)/2n}, \tag{77}$$

$$(n-1)z=[(n-1)(n+2)x+n^2+5n+2]x^{-(n-1)/2n}, \tag{78}$$

$$f(z)=\frac{(n-1)(x-1)[4n+(n+1)^2-(n+1)^2x]z}{[(n+1)(n+2)x-(n^2+5n+2)][(n-1)(n+2)x+n^2+5n+2]}, \tag{79}$$

in the generic case $n\neq\pm 1$.

The stiff fluid case leads to a logarithmic term in $z(x)$, which makes

$$f(z)=-\frac{2(x-1)(x-2)}{3x-4} \tag{80}$$

nonintegrable.

The case $n=-1$ is pseudologarithmic since the coefficient in front of $\ln x$ vanishes. We have $x=1/z$ and $f(z)=2z-2$. This case is integrable and the solution is given by Eqs. (42)–(44) with $\alpha=-\beta=2$.

The case $n=-3$ leads to a gross simplification of $f(z)$ and is also soluble. One obtains $f(z)=2z$, i.e., $\alpha=2$, $\beta=0$.

The other candidate cases may be investigated in the same manner as in Secs. II and III. The values $n=\pm 1/3$ lead to quadratic equations with radicals of the wrong type. The case $n=-2$ yields

$$f(z)=\tfrac{21}{16}z-\tfrac{18}{16}(\tfrac{4}{3})^{4/3}z^{-1/3}-\tfrac{3}{16}(\tfrac{4}{3})^{8/3}z^{-5/3}. \tag{81}$$

This equation belongs to the class (63) but again $c_1\neq -3/16$ and integrability is not gained.

Finally, let us discuss the KT solution in the HH approach. When $x=\text{const}$ Eq. (76) becomes purely algebraic and has two roots: $x_1=1$ and

$$x_2=1+\frac{4n}{(n+1)^2}. \tag{82}$$

When $n=-1$, x_2 does not exist. In fact, the requirement $x_2>0$ shows that n must satisfy the conditions derived in Sec. II. The first root leads to $t_1=\pm 1/2$. In the first subcase Eqs. (72) and (73) give flat space–time. In the second subcase the following line element is obtained

$$\mathrm{d}s^2=\mathrm{d}t^2-r^{-4}(\mathrm{d}r^2+r^2\,\mathrm{d}\Omega^2). \tag{83}$$

The transformation $\tilde{r}=1/r$ converts this element into the usual element for flat space–time.

The second root x_2 represents the KT solution in isotropic coordinates, namely $e^{\lambda}=r^{\alpha_1}$, $e^{2\nu}=r^{\alpha_2}$ where

$$\alpha_1=\pm\frac{2(n+1)}{\sqrt{4n+(n+1)^2}}-2, \tag{84}$$

$$\alpha_2=\pm\frac{4}{\sqrt{4n+(n+1)^2}}. \tag{85}$$

When $n=1$, $\alpha_1=\pm\sqrt{2}-2$ and $\alpha_2=\pm\sqrt{2}$. These values were found in Ref. 14, where the KT solution was discovered for a fifth time.

The integrable cases found in the HH approach coincide with those found in the Klein or the TOV–Collins approaches. In order to make connection with the last one, we must pass in Sec. II to isotropic coordinates. We have

$$R'=e^{\lambda/2}\left(1+\frac{\lambda_{,s}}{2}\right), \tag{86}$$

$$2x=2M-1=-R'^2e^{-\lambda}=-\frac{1}{4t^2}. \tag{87}$$

We cannot obtain Eq. (74) from Eq. (15) by replacing there just x from Eq. (87) because $s=\ln r$, while $\tau=\ln R=s+\lambda/2$. The necessary additional relations are

$$x_{,\tau}=\frac{t_{,s}}{2t^2}, \tag{88}$$

$$x_{,\tau,\tau}=\frac{t_{,s,s}}{t}-\frac{2t_{,s}^2}{t^2}. \tag{89}$$

Therefore, the HH approach combines the TOV equation in isotropic coordinates together with the linear equation (18) for λ.

V. BUCHDAHL TRANSFORMATION AND THE CASE $N=-5$

This transformation was found by Buchdahl[6] and rediscovered by Glass and Goldman.[7] Its general formulation refers to static perfect fluid solutions, not necessarily satisfying an equation of state. In the case of spherical symmetry it states that if

$$\mathrm{d}s^2=e^{2\nu}\,\mathrm{d}t^2-e^{\lambda}(\mathrm{d}r^2+r^2\,\mathrm{d}\Omega^2) \tag{90}$$

is the metric of a perfect fluid solution with pressure p and density ρ then there is a reciprocal solution which has $\nu_b=-\nu$, $\lambda_b=4\nu+\lambda$, and

$$p_b=e^{-4\nu}p, \tag{91}$$

$$\rho_b=-e^{-4\nu}(\rho+6p). \tag{92}$$

The transformation is simplest in isotropic coordinates and may be applied to the results obtained in Sec. IV. When p and ρ satisfy the γ-law, the same is true for p_b and ρ_b but with a different parameter:

$$\rho_b=-(n+6)p_b. \tag{93}$$

Thus, the transformation of the parameter is $n\to-(n+6)$. It is clear that when the starting solution is physically realistic ($n\geqslant 1$), the transformed one is unphysical, $-(n+6)\leqslant -7$. However, when the starting solution is unphysical and $n\leqslant -7$, then the reciprocal one is physical. When n is in the interval $-7<n<1$ both solutions are unphysical. The existence of this transformation teaches that unphysical solutions should not be neglected *a priori* and the whole spectrum of n must be investigated.

Let us apply the transformation to the integrable cases found in Sec. IV. The KT solution is self-reciprocal, i.e., transforms into itself. The reason is that $4n+(n+1)^2$ is invariant under the transformation. Taking α_{1-} and α_{2-} as the powers of r in the starting solution, it is easy to show that $\alpha_{2+}=-\alpha_{2-}$ and $\alpha_{1+}=\alpha_{1-}+2\alpha_{2-}$ when the plus solution is Buchdahl transformed. Solutions with n outside the interval $(-5.83,-0.17)$ transform between themselves.

The case $n=-3$ is also self-reciprocal, as was noticed already by Buchdahl. This explains why $\nu=0$ when the element of the Einstein static universe is written in isotropic coordinates.[33] This is necessary to ensure the equality between the starting and the transformed solution.

The interesting case is the de Sitter solution ($n=-1$) which transforms into an explicit solution with $n=-5$. In isotropic coordinates the de Sitter solution reads[33]

$$e^{2\nu}=\left(\frac{1+cr^2}{1-cr^2}\right)^2, \tag{94}$$

$$e^{\lambda}=(1-cr^2)^{-2}, \tag{95}$$

and $p=12/c$, $\rho=-12/c$, where c is some constant. The transformed solution has

$$e^{2\nu_b}=\left(\frac{1-cr^2}{1+cr^2}\right)^2, \tag{96}$$

$$e^{\lambda_b}=\frac{(1+cr^2)^4}{(1-cr^2)^6}, \tag{97}$$

$$p_b=\left(\frac{1-cr^2}{1+cr^2}\right)^4\frac{12}{c}, \tag{98}$$

and, of course, $\rho_b=-5p_b$. Equation (72) supplies the corresponding t:

$$t=\frac{1-cr^2}{2(1+cr^2)}, \tag{99}$$

$$t_b=\frac{1-c^2r^4}{2(1+10cr^2+c^2r^4)}. \tag{100}$$

From Eq. (75) we get $x=4t^2$ and $y=-4rt_{,r}$. When t_b is plugged in these relations we obtain the parametric solution $x(r)$, $y(r)$ of Eq. (76) for $n=-5$:

$$xyy_{,x}=\tfrac{3}{5}y^2-\tfrac{6}{5}xy+\tfrac{1}{5}y+\tfrac{2}{5}(4x^2-3x-1). \tag{101}$$

Equations (78) and (79) yield in this case

$$-3z=(9x+1)x^{-3/5}, \tag{102}$$

$$f(z)=\frac{6(x-1)(4x+1)}{(6x-1)(9x+1)}z. \tag{103}$$

Equation (102) is a fifth-order equation for x and seems to be transcendental. Obviously $f(z)$ is not among the tabulated integrable functions. Equation (101) does not coincide with any of the equations in Sec. 1.3.4. from Ref. 27 which belong to the class (22). If we use Eq. (23) instead, $g(\zeta)=1/f(z)$ and

$$3\zeta x^{6/5}=6x^2+18x+1. \tag{104}$$

This equation is even more complicated than Eq. (102) and $g(\zeta)$ is not among the few integrable cases listed in Sec. 1.3.2 from the same handbook. Unless some mistake has been made, Eq. (101) is integrable, but is not covered by Ref. 27. This situation is not unique. Recently, nonstatic charged perfect fluid distributions were discovered which, too, are missing in the handbooks with solutions of differential equations.[34]

VI. DISCUSSION AND CONCLUSIONS

In this paper we have discussed explicit solutions of the Einstein equations for a static spherically symmetric perfect fluid with the γ-law equation of state. Three approaches may be found in the literature which, at first sight, have nothing in common. The approach of Collins transforms the TOV equation in polar Gaussian coordinates into a two-dimensional autonomous system of differential equations. He studies it numerically.[5,17,30] This is a representative example of other similar dynamical systems.[16,19] In his approach Klein finds a second-order autonomous master equation, whose solution determines all characteristics of the metric and the fluid. He lowers its order and studies it by series expansion and numerically. Klein also discovers a simple exact but singular solution. This work is done in curvature coordinates.[10,11] Haggag and Hajj-Boutros perform a similar study but in isotropic coordinates and only for a stiff fluid.[14] They also obtain an autonomous second-order equation and transform it into another second-order equation [see Eqs. (9) and (14) in their paper]. Then they look for polynomial solutions and find either flat space–time or the KT solution.

We have generalized these three approaches and pursued them further, to their logical end—an equation, whose integrable cases are tabulated in the handbooks, like Ref. 27. Surprisingly, we invariably reach the Abel equation of the second kind (3). It behaves like a ''strange attractor'' and underlines the common features in the different approaches. The question of integrability is answered by the form of $f(z)$, the known integrable cases being tabulated. For this purpose we have generalized to an arbitrary coordinate system the dynamical system of Collins and to arbitrary n the HH approach. The functions $z(x)$ and $f(x)$ have the same general structure in all approaches but with different coefficients. The relations between the master variables x, x_K, and x_{HH} have been elucidated, the TOV–Collins approach serving as a basis.

The integrable cases found are one and the same and include $n=\infty$ (trivial dust solution), $n=-1$ (de Sitter solution), $n=-3$ (Einstein static universe) and $x=\mathrm{const}$, $n<-5.83$ or $n>-0.17$ (Klein–Tolman solution). They appear either as exceptional cases, when equations simpler than Eq. (3) are to be solved, or as Eq. (2) with $f(z)=\alpha z+\beta$, the simplest integrable case. Some candidate values of n lead to Eq. (63), but at least one of the constants there has the wrong value.

It has been shown that Eq. (3) stands in the center of the problem, independent from the approach or the coordinate system and the integrable cases may be derived in a unified manner. The problem is a very strange mixture of simple integrable cases and extremely difficult nonintegrable ones. Perhaps this gives some explanation why the de Sitter and the Einstein solutions were found in 1917, two years after the appearance of general relativity, and why the next years have brought only a fivefold discovery of the KT solution.

An important point is that the problem has been pushed to the mathematical realm of Abel differential equations and further progress depends on developments in this field. Using the Buchdahl transformation we have shown that the case $n=-5$ is integrable and have given its metric and fluid characteristics. However, its master equation in isotropic coordinates (101) does not seem to be present in the handbooks. This leaves this paper with an open end and one may hope that other integrable cases will be found in the future.

Finally, it is interesting to note that all discrete integrable cases $n=-1,-3,-5$ are regular and fall in the interval where the singular KT solution does not exist. One is tempted to speculate that in this interval there is a regular one-parameter solution, encompassing the discrete cases.

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Inverse scattering theory of the heat equation for a perturbed one-soliton potential

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The inverse scattering theory of the heat equation is developed for a special subclass of potentials nondecaying at space infinity—perturbations of the one-soliton potential by means of decaying two-dimensional functions. Extended resolvent, Green's functions, and Jost solutions are introduced and their properties are investigated in detail. The singularity structure of the spectral data is given and then the inverse problem is formulated in an exact distributional sense. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1427410]

I. INTRODUCTION

The equation of the heat conduction, or heat equation for short,

$$\mathcal{L}\Phi(x)=0, \tag{1.1}$$

where the operator

$$\mathcal{L}(x,\partial_x)=-\partial_{x_2}+\partial_{x_1}^2-u(x), \quad x=(x_1,x_2), \tag{1.2}$$

for more than 25 years has been known[1,2] to be associated to the Kadomtsev–Petviashvili (more precisely, KPII) equation

$$(u_t-6uu_{x_1}+u_{x_1x_1x_1})_{x_1}=-3u_{x_2x_2}. \tag{1.3}$$

The scattering theory for the equation of heat conduction with a real potential $u(x)$ was developed in Refs. 3–5, but only the case of potentials rapidly decaying at large distances on the x-plane was considered. On the other side, it is well known that (1.3) is a $(2+1)$-dimensional generalization of the famous KdV equation: if the function $u_1(t,x_1)$ obeys KdV, then

$$u(t,x_1,x_2)=u_1(t,x_1+\mu x_2-3\mu^2 t) \tag{1.4}$$

solves (1.3) for an arbitrary constant $\mu\in\mathbb{R}$. Thus it is natural to consider solutions of (1.3) that are not decaying in all directions at space infinity but have one-dimensional rays with behavior of the type (1.4). The scattering theory for the operator (1.2) with such potentials is absent in the literature. Moreover, it is easy to observe that, like in the KPI case (see Ref. 6), the standard integral equation for the Jost solution[3] is meaningless for this situation and does not determine the solution itself. In trying to solve this problem for the nonstationary Schrödinger operator, associated to the KPI equation, a new general approach to the inverse scattering theory was introduced, which was called resolvent approach (see Refs. 6–10 and references therein). In Ref. 11 we

developed the scattering theory for the N-soliton solutions given in terms of Bäcklund transformations of the decaying background potential. These results for the simplest case $N=1$ are essentially used below.

Here we apply the resolvent approach to the heat equation (1.2) with a potential $u(x)$ that is a perturbation of a one-dimensional potential $u_1(x)$ of the kind (1.4) by means of a potential $u_2(x)$ rapidly decaying in all directions:

$$u(x)=u_1(x)+u_2(x). \tag{1.5}$$

We introduce and study properties of the resolvent, dressing operators, Jost solutions and scattering data, and formulate the inverse problem relevant to this case. In fact, we consider here the simplified version of (1.4) in which $\mu=0$. The generic case is reconstructed by means of the Galilean invariance of (1.3). Thus in what follows $u_1(x)\equiv u_1(x_1)$ and, moreover, we consider for simplicity the case where u_1 is the one-dimensional soliton potential [see (3.1)].

Thus here we apply the inverse scattering theory to a nonscattering situation since the "obstacle" is infinite. Such extension of the inverse scattering theory results in the new and unexpected properties of familiar objects, like the Jost solutions and the spectral data. We show that they get specific singularities in the complex domain of the spectral parameter. Derivation and description of these singularities are our main results here. The article is organized as follows. In Sec. II we sketch some general aspects of the resolvent approach that are necessary for our construction. In Sec. III we present results of embedding the theory of the one-dimensional one-soliton potential in two dimensions. Presentation here is based on work Ref. 11. We describe in detail properties of the extended resolvent and Green's functions of operator (1.2) with $u(x)=u_1(x_1)$. On this basis in Sec. IV the resolvent of the operator (1.2) now with the generic potential $u(x)$ given in (1.5) is introduced and its properties are described. The departure from analyticity of the resolvent leads us to definitions of the Jost solutions and spectral data and description of their properties (Sec. V). In this way we supply all terms of the inverse problem with proper meaning in terms of distributions. In the Conclusion some generalizations and future developments of these results are discussed. The main results of this article were announced in our earlier work, Ref. 12.

II. EXTENSION OF DIFFERENTIAL OPERATORS AND RESOLVENT

In the framework of the resolvent approach we work in the space $\mathcal{S}'$ of tempered distributions $A(x,x';q)$ of the six real variables $x=(x_1,x_2),x',q\in\mathbb{R}^2$. It is convenient to consider q as the imaginary part of a two-dimensional complex variable $\mathbf{q}=\mathbf{q}_{\Re}+i\mathbf{q}_{\Im}=(\mathbf{q}_1,\mathbf{q}_2)\in\mathbb{C}^2$ and to introduce the "shifted" Fourier transform

$$A(p;\mathbf{q})=\frac{1}{(2\pi)^2}\int dx\int dx'\, e^{i(p+\mathbf{q}_{\Re})x-i\mathbf{q}_{\Re}x'}A(x,x';\mathbf{q}_{\Im}), \tag{2.1}$$

where $p\in\mathbb{R}^2$, $px=p_1x_1+p_2x_2$ and $\mathbf{q}_{\Re}x=\mathbf{q}_{1\Re}x_1+\mathbf{q}_{2\Re}x_2$. We consider the distributions $A(x,x';q)$ and $A(p;\mathbf{q})$ as kernels in two different representations, the x- and p-representation, respectively, of the operator $A(q)$ (A for short). The composition law in the x-representation is defined in the standard way, that is,

$$(AB)(x,x';q)=\int dx''\,A(x,x'';q)\,B(x'',x';q). \tag{2.2}$$

Since the kernels are distributions, this composition is neither necessarily defined for all pairs of operators nor associative. In terms of the p-representation (2.1), this composition law is given by a sort of a "shifted" convolution, $(AB)(p;\mathbf{q})=\int dp'A(p-p';\mathbf{q}+p')B(p';\mathbf{q})$. On the space of these operators we define the conjugation A^*, which in the x-representations reads as

$$A^*(x,x';q)=\overline{A(x,x';q)}, \tag{2.3}$$

where bar denotes complex conjugation, or as $A^*(p;\mathbf{q})=\overline{A(-p;-\overline{\mathbf{q}})}$ in the p-representation. Below we say that the operator $A(q)$ is real if $A^*(q)=A(q)$, which in terms of p-representation means that $\overline{A(p;\mathbf{q})}=A(-p;-\overline{\mathbf{q}})$. The set of differential operators $\mathcal{D}(x,\partial_x)=\Sigma d_n(x)\partial_x^n$ is embedded in the introduced space of operators by considering the operators D with kernel $D(x,x')=\mathcal{D}(x,\partial_x)\delta(x-x')$, where $\delta(x)=\delta(x_1)\delta(x_2)$ is the two-dimensional δ-function and, then, by mapping them in the operators $D(q)$ with kernel

$$D(x,x';q)\equiv e^{-q(x-x')}D(x,x')=\mathcal{D}(x,\partial_x+q)\,\delta(x-x'), \tag{2.4}$$

to which we refer as the **extended** version of the differential operator $\mathcal{D}$. The notion of reality for a differential operator D is exactly the condition that its coefficients $d_n(x)$ are real.

For the operator (1.2) the extension $L(q)$ is given by

$$L=L_0-U, \tag{2.5}$$

where L_0 is the extension of $\mathcal{L}(x,\partial_x)$ in the case of zero potential, i.e., it has kernels

$$L_0(x,x';q)=[-(\partial_{x_2}+q_2)+(\partial_{x_1}+q_1)^2]\delta(x-x'),\quad L_0(p;\mathbf{q})=(i\mathbf{q}_2-\mathbf{q}_1^2)\delta(p), \tag{2.6}$$

and the multiplication operator U can be called the potential since it has kernel

$$U(x,x';q)=u(x)\,\delta(x-x'). \tag{2.7}$$

Below we always suppose that $u(x)$ is real, which by (2.3) means that the operator (1.2) is real also: $L^*=L$.

The main object of our approach is the **extended resolvent** $M(q)$ of the operator $L(q)$, which is defined as the inverse of the operator L, that is,

$$LM=ML=I, \tag{2.8}$$

in the space of operators. Here I is the unity operator, $I(x,x';q)=\delta(x-x')$, $I(p;\mathbf{q})=\delta(p)$. In order to make this inversion uniquely defined we impose the condition that the product

$$\int dp'M(p-p';\mathbf{q}+\mathbf{s}+p')M(p';\mathbf{q}) \tag{2.9}$$

exists as distribution in p and $\mathbf{q}$ and that it is a continuous function of $\mathbf{s}$ in a neighborhood of $\mathbf{s}=0$ when $\mathbf{s}\neq 0$.

Thanks to definitions (2.5), (2.6), and (2.8), M is real and, in particular, the resolvent M_0 of the bare operator L_0 has in the p-representation kernel

$$M_0(p;\mathbf{q})=\delta(p)\,\frac{1}{i\mathbf{q}_2-\mathbf{q}_1^2}. \tag{2.10}$$

As function of $\mathbf{q}$ it is singular when $\mathbf{q}=\not{\ell}(\mathbf{q}_1)$, where the special two-component vector

$$\not{\ell}(k)=(k,-ik^2) \tag{2.11}$$

was introduced. The kernel of M_0 in the x-representation

$$M_0(x,x';q)=\frac{1}{2\pi}\int d\alpha\,[\theta(q_1^2-\alpha^2-q_2)-\theta(x_2-x_2')]\,e^{-(i\not{\ell}(\alpha+iq_1)+q)(x-x')} \tag{2.12}$$

is obtained from (2.10) by using (2.1).

For a generic operator A with kernel $A(x,x';q)$ the operation inverse to the extension procedure, defined in (2.4) for a differential operator, is given by

$$\hat{A}(x,x';q)=e^{q(x-x')}A(x,x';q). \tag{2.13}$$

In contrast with the case of the extended differential operators for which $\hat{D}(x,x';q)=D(x,x')\equiv\mathcal{D}(x,\partial_x)\delta(x-x')$, in general $\hat{A}(x,x';q)$ does depend on q and, moreover, can have an exponential growth at space infinity. Therefore $\hat{A}(x,x';q)$ does not necessarily belong to the space $\mathcal{S}'$ of tempered distributions. The fact that $\hat{A}(x,x';q)$ can depend on q will play a crucial role in the following. For instance, also in the case of the simplest resolvent (2.12), we have that the function $\hat{M}_0(x,x';q)$ depends effectively on the variable q and is exponentially growing at space infinity. More generally from (2.8) we have

$$\mathcal{L}(x,\partial_x)\hat{M}(x,x';q)=\mathcal{L}^{\mathrm{d}}(x',\partial_{x'})\hat{M}(x,x';q)=\delta(x-x'), \tag{2.14}$$

where $\mathcal{L}^{\mathrm{d}}$ is the operator dual to $\mathcal{L}$. The function $\hat{M}(x,x';q)$ can be considered a parametric ($q\in\mathbb{R}^2$) family of Green's functions of the operator $\mathcal{L}$. In what follows we use special notations for the equalities of the type (2.14), writing them as

$$\vec{\mathcal{L}}\hat{M}(q)=\hat{M}(q)\tilde{\mathcal{L}}=I, \tag{2.15}$$

where $\vec{\mathcal{L}}$ denotes the operator $\mathcal{L}$ applied to the x-variable of the function $\hat{M}(x,x';q)$ and $\tilde{\mathcal{L}}$ denotes the operator dual to $\mathcal{L}$ applied to the x'-variable of the same function. Operation (2.13) has no analog in terms of the p-representation. Nevertheless, local properties of the kernels in the x-representation are preserved, and we use the kernels with the hat in what follows intensively.

Thanks to our definitions (2.1) and (2.4) it is easy to see that in terms of the p-representation the dependence on the $\mathbf{q}$-variables of the kernels of the extension of a differential operator is polynomial [like in the example (2.6)]. Correspondingly, the essential role in the study of the properties of the resolvent is played by the investigation of its departure from analyticity, in particular, by its d-bar derivatives with respect to the $\mathbf{q}$-variables. Thus to a generic operator A with kernel $A(p;\mathbf{q})$ in the p-representation we associate two operators $\overline{\partial}_j A$ with kernels

$$(\overline{\partial}_j A)(p;\mathbf{q})=\frac{\partial A(p;\mathbf{q})}{\partial\overline{\mathbf{q}}_j},\quad j=1,2, \tag{2.16}$$

where the derivatives are considered in the sense of distributions. In terms of the objects introduced in (2.13) we get by inversion of (2.1) that

$$\widehat{(\overline{\partial}_j A)}(q)=\frac{i}{2}\frac{\partial\hat{A}(q)}{\partial q_j}. \tag{2.17}$$

Multiplying equalities in (2.8) from the left and right, correspondingly, by M_0 we get, thanks to (2.5),

$$M=M_0+M_0UM,\quad M=M_0+MUM_0. \tag{2.18}$$

Since the resolvent M_0 is explicitly given, these are integral equations determining the solution M of (2.8). In the literature (see, say, Refs. 4 and 5) on the Jost solutions of the heat equation some small norm conditions on the potential u are known to guarantee the existence of the Jost solutions. So it is natural to assume that under such conditions the solution M of the above integral equations exists and is unique (the same for both integral equations). In this case the resolvent M can be considered as a small perturbation of the resolvent M_0 and this bare resolvent determines

the properties of M by means of (2.18). The main problem of construction of the inverse scattering transform for the operator (1.2) is that the potential $u(x)$ in (1.5) does not obey any small norm condition.

In order to overcome this difficulty we use a so-called inverse scattering transform on a nontrivial background.[10] Let us consider a kind of Hilbert identity, known in the standard spectral theory of operators. Precisely, if $M(q)$ is the extended resolvent of the operator $L(q)$ with potential u and $M'(q)$ the extended resolvent of the operator $L'(q)$ with a different potential u', then, by (2.8) we have

$$M'-M=-M'(L'-L)M. \tag{2.19}$$

Strictly speaking, this follows under the assumption that the product on the rhs is associative. This is a natural assumption since $L'(x,x';q)-L(x,x';q)=(u(x)-u(x'))\delta(x-x')$ and M satisfies condition (2.9). Let now $\mathcal{L}_1$ denote the operator (1.2) in the special case where the potential $u(x)$ in (1.5) is purely one-dimensional, i.e., $u_2(x)\equiv 0$. Let L_1 denote its extension and M_1 its resolvent, that is, let [cf. (2.5)]

$$L_1=L_0-U_1, \quad \mathcal{L}_1(x,\partial_x)=-\partial_{x_2}+\partial_{x_1}^2-u_1(x), \tag{2.20}$$

$$L=L_1-U_2, \quad L_1M_1=M_1L_1=I, \tag{2.21}$$

where as in (2.7) $U_j(x,x';q)=u_j(x)\delta(x-x')$. Choosing now in (2.19) $L'=L_1$ we get

$$M=M_1+M_1U_2M, \quad M=M_1+MU_2M_1, \tag{2.22}$$

where the second equality is derived in analogy. These equations generalize (2.18) for the case where M_1 is nontrivial and, if the resolvent M_1 is known, they also can be considered as defining the resolvent M. If we choose U_2 obeying the small norm condition mentioned above, we can assume that the solution M of both Eqs. (2.22) exists and is unique. Then, thanks to (2.21), M obeys (2.8). Contrary to (2.18), now M can be considered a perturbation of the resolvent M_1. So, in the next section, we study the properties of the resolvent M_1 in detail.

III. ONE-DIMENSIONAL POTENTIAL

We already mentioned in the Introduction that in this article we deal with the case where u_1 in (1.5) is the one-dimensional soliton potential

$$u_1(x)=\frac{-2a^2}{\cosh^2[a(x_1-x_0)]}, \tag{3.1}$$

with $a>0$ and x_0 real constants. In this section we consider the case where the perturbation is absent, $u_2\equiv 0$. We reformulate in the two-dimensional space the well known facts about Jost solutions of this one-soliton potential and introduce and study the properties of the resolvent and Green's functions in this case.

The differential equations $\mathcal{L}_1(x,\partial_x)\Phi_1(x,k)=0$, $\mathcal{L}_1^{\mathrm{d}}(x',\partial_{x'})\Psi_1(x',k)=0$ for the Jost solution $\Phi_1(x,k)$ and its dual $\Psi_1(x',k)$, by using the notation introduced in (2.15) and by considering $\Phi_1(x,k)$ and $\Psi_1(x',k)$ as kernel operators independent, respectively, of x' and x, can be rewritten in the operatorial form

$$\vec{\mathcal{L}}_1\Phi_1(k)=0, \quad \Psi_1(k)\vec{\mathcal{L}}_1=0, \tag{3.2}$$

which we will use frequently in the following. These solutions are given explicitly by

$$\Phi_1(x,k)=\frac{k-ia\tanh[a(x_1-x_0)]}{k-ia}e^{-i\not{\ell}(k)x}, \tag{3.3}$$

$$\Psi_1(x,k)=\frac{k+ia\tanh[a(x_1-x_0)]}{k+ia}e^{i\not{x}(k)x}, \tag{3.4}$$

where $k\in\mathbb{C}$ and the two-component vector $\not{x}(k)$ is defined in (2.11). They obey the conjugation properties

$$\overline{\Phi_1(x,k)}=\Phi_1(x,-\bar{k}),\quad \overline{\Psi_1(x,k)}=\Psi_1(x,-\bar{k}) \tag{3.5}$$

that are equivalent to the reality condition for the potential u_1, and are normalized at k-infinity as follows:

$$\lim_{k\to\infty}e^{i\not{x}(k)x}\Phi_1(x,k)=1,\quad \lim_{k\to\infty}e^{-i\not{x}(k)x}\Psi_1(x,k)=1. \tag{3.6}$$

The functions $\Phi_1(x,k)$ and $\Psi_1(x,k)$ are meromorphic in the complex domain of the spectral parameter k with poles at $k=ia$ and $k=-ia$, correspondingly. Thus, these functions obey the d-bar equations

$$\frac{\partial\Phi_1(x,k)}{\partial\bar{k}}=i\pi\Phi_{1,a}(x)\,\delta(k-ia),\quad \frac{\partial\Psi_1(x,k)}{\partial\bar{k}}=i\pi\Psi_{1,-a}(x)\,\delta(k+ia), \tag{3.7}$$

where we introduced the notations

$$\Phi_{1,a}(x)=-i\operatorname*{res}_{k=ia}\Phi_1(x,k),\quad \Psi_{1,-a}(x)=-i\operatorname*{res}_{k=-ia}\Psi_1(x,k). \tag{3.8}$$

Explicitly we have

$$\Phi_{1,a}(x)=\frac{ae^{ax_0+a^2x_2}}{\cosh[a(x_1-x_0)]},\quad \Psi_{1,-a}(x)=-\frac{ae^{ax_0-a^2x_2}}{\cosh[a(x_1-x_0)]}. \tag{3.9}$$

Let

$$c=2ae^{2ax_0} \tag{3.10}$$

and $\Phi_{1,-a}(x)$ and $\Psi_{1,a}(x)$ be the values of the Jost solutions in the conjugated points,

$$\Phi_{1,-a}(x)=\Phi_1(x,-ia),\quad \Psi_{1,a}(x)=\Psi_1(x,ia). \tag{3.11}$$

Then, thanks to (3.3), (3.4), and (3.9), the Jost solutions obey in the complex domain of the spectral parameter the following scalar products:

$$\int dx_1\Psi_1(x,k+p)\Phi_1(x,k)=2\pi\delta(p),\quad p\in\mathbb{R}, \tag{3.12}$$

$$c\int dx_1\,\Phi_{1,-a}(x)\Psi_{1,a}(x)=1, \tag{3.13}$$

$$\int dx_1\,\Psi_{1,a}(x)\Phi_1(x,k)=0,\quad k_\mathfrak{I}^2<a^2, \tag{3.14}$$

$$\int dx_1\,\Phi_{1,-a}(x)\Psi_1(x,k)=0,\quad k_\mathfrak{I}^2<a^2, \tag{3.15}$$

and the completeness relation

$$\frac{1}{2\pi}\int_{x_2=x_2'} dk_{\Re}\,\Phi_1(x,k)\Psi_1(x',k)+c\,\theta(a^2-k_{\Im}^2)\Phi_{1,-a}(x)\Psi_{1,a}(x')\Big|_{x_2=x_2'}=\delta(x_1-x_1'). \tag{3.16}$$

Equations (3.7) can be considered as two inverse problems defining the Jost solution and the dual Jost solution. The formulation of these problems is closed by giving the normalization conditions (3.6) and the following relations:

$$\Phi_{1,a}(x)=c\Phi_{1,-a}(x), \quad \Psi_{1,-a}(x)=-c\Psi_{1,a}(x), \tag{3.17}$$

where $\Phi_{1,-a}(x)$ and $\Psi_{1,a}(x)$ are defined in (3.11).

These formulas show that the embedding in two dimensions of the Jost solutions of the one-soliton potential is trivial and just mimics the one-dimensional construction up to the warning that, due to their exponential dependence on x_2, the functions $\Phi_{1,a}(x)$ and $\Psi_{1,-a}(x)$ are not square integrable with respect to the x-variables and, therefore, are not eigenfunctions of the operator $\mathcal{L}_1$.

On the contrary, the two-dimensional resolvent $M_1(q)$ as well as the Green's function G_1 of the two-dimensional operator $\mathcal{L}_1$ with the one-dimensional potential u_1 are not trivial extensions of the corresponding one-dimensional objects associated to the operator $(k^2+\partial_{x_1}^2-u_1(x_1))$. In terms of the Jost solutions introduced above, we can write the kernel of this resolvent obtained in Ref. 11 as

$$\begin{aligned}\hat{M}_1(x,x';q)=\frac{1}{2\pi}\int_{k_{\Im}=q_1} dk_{\Re}\,[\,\theta(q_1^2-q_2-k_{\Re}^2)-\theta(x_2-x_2')\,]\,\Phi_1(x,k)\Psi_1(x',k)\\ +c\,\theta(a^2-q_1^2)[\,\theta(a^2-q_2)-\theta(x_2-x_2')\,]\Phi_{1,-a}(x)\Psi_{1,a}(x'),\end{aligned} \tag{3.18}$$

where the hat over the kernel is used in the sense of notation (2.13).

Thanks to the equalities (3.2) and (3.16) it is easy to check directly that $\hat{M}_1(q)$ obeys the equations

$$\vec{\mathcal{L}}_1\hat{M}_1(q)=\hat{M}_1(q)\vec{\mathcal{L}}_1=I, \tag{3.19}$$

which means [cf. (2.15)] that $M_1(q)$ obeys (2.21) and is indeed the inverse of the operator $L_1(q)$. Moreover, using the explicit formulas (3.3), (3.4) and (3.9) we get that $M_1(x,x';q)\in\mathcal{S}'(R^6)$, i.e., it belongs to the space of operators under consideration. It can also be proved directly that M_1 obeys condition (2.9), so it is the extended resolvent according to our definition. By means of (3.5) we get also that M_1 is real, $M_1^*=M_1$ according to definition (2.3).

We emphasize that in order to prove these results it is not necessary to use the explicit formulas for Φ_1 and Ψ_1 but only their general properties. In fact, if one considers a one-dimensional potential u_1 which, in addition, has a nontrivial continuous spectrum, one gets the same formula for the resolvent M_1. If the discrete (one-dimensional) spectrum of u_1 contains N solitons with parameters a_j and c_j $(j=1,2,\ldots,N)$, then the last term in (3.18) must be substituted by the sum of similar terms each corresponding to a value of j.

Now we describe in detail the properties of $M_1(x,x';q)$. The first term on the rhs of (3.18) is a continuous function of $q=(q_1,q_2)$ on the q-plane with discontinuities on the lines $q_1=\pm a$ due to the pole singularities of $\Phi_1(k)$ and $\Psi_1(k)$. The second term, thanks to the θ functions, has discontinuities on the lines $q_1=\pm a$ and on the cut $q_2=a^2$, $|q_1|<a$. The singularities on the lines $q_1=\pm a$ are exactly compensated among the two terms. Thus the kernel $M_1(x,x';q)$ is a continuous function of q with a discontinuity on the cut $q_2=a^2$, $|q_1|<a$. This discontinuity is specific of the potential $u_1(x)$, or more generally of a potential with discrete spectrum and it gives the essential difference of M_1 with respect to the bare resolvent M_0 (2.12). Let us underline that, in spite of the fact that $\mathcal{L}_1$ applied to the term with $\theta(a^2-q_2)$ that causes this discontinuity gives

zero, this term cannot be omitted in (3.18), since, only thanks to the fact that $\theta(x_2-x_2')$ and $\theta(a^2-q_2)$ have opposite signs, the kernel $M_1(x,x';q)\equiv e^{-q(x-x')}\hat{M}_1(x,x';q)$ is a tempered distribution with respect to the x-variables.

The kernel $M_1(p;\mathbf{q})$ in the p-representation is not an analytic function of $\mathbf{q}$. By (2.17) the d-bar derivatives of M_1 with respect to $\mathbf{q}_j$ are proportional to $\partial\hat{M}_1/\partial q_j$ and for the latter we get from (3.18) equalities

$$\frac{\partial\hat{M}_1(q)}{\partial q_1}=\frac{i}{\pi}\int_{k_\Im=q_1} dk_\Re\,\overline{k}\,\delta(\mathscr{l}_{2\Im}(k)-q_2)\,\Phi_1(k)\otimes\Psi_1(k), \tag{3.20}$$

$$\frac{\partial\hat{M}_1(q)}{\partial q_2}=\frac{-1}{2\pi}\int_{k_\Im=q_1} dk_\Re\,\delta(\mathscr{l}_{2\Im}(k)-q_2)\,\Phi_1(k)\otimes\Psi_1(k), \tag{3.21}$$

where $(\Phi_1(k)\otimes\Psi_1(k))(x,x')\equiv\Phi_1(x,k)\Psi_1(x',k)$ is the standard direct product, $\mathscr{l}_{2\Im}(k)$ is the imaginary part of the second component of the vector $\mathscr{l}(k)$ defined in (2.11) and where by the above discussion we consider $q_2\neq a^2$. For the discontinuity along this line we get

$$\hat{M}_1(q)|_{q_2=a^2+0}-\hat{M}_1(q)|_{q_2=a^2-0}=-c\,\theta(a^2-q_1^2)\Phi_{1,-a}\otimes\Psi_{1,a}. \tag{3.22}$$

We have to study now the behavior of $M_1(q)$ at the end points of the cut, i.e., when $q\sim(\pm a,a^2)$. First, it is convenient to subtract from $M_1(q)$ its value, say, on the upper or lower edges of the cut:

$$g_1^{\pm}=\lim_{q_2=a^2\pm 0}\hat{M}_1(q)|_{|q_1|<a}. \tag{3.23}$$

Since $\Phi_1(k)$ and $\Psi_1(k)$ are analytic for $|k_\Im|<a$, we deduce from (3.18) that $g_1^{\pm}$ are independent also of q_1 and their kernels equal

$$g_1^{\pm}(x,x')=-\frac{\theta(x_2-x_2')}{2\pi}\int d\alpha\,\Phi_1(x,\alpha)\Psi_1(x',\alpha)\mp c\,\theta(\pm(x_2-x_2'))\Phi_{1,-a}(x)\Psi_{1,a}(x'), \tag{3.24}$$

where $\int d\alpha$ denotes integration along the whole real axis. Now extracting explicitly from the first term on the rhs of (3.18) the contribution coming from the poles of $\Phi_1(k)$ and $\Psi_1(k)$ we get that, say, difference $\hat{M}_1(q)-g_1^-$ behaves at points $q=(\pm a,a^2)$ as

$$\hat{M}_1(q)-g_1^-=-c\left(\frac{\theta(q_1^2-q_2)}{\pi}\operatorname{arccot}\frac{a-|q_1|}{\sqrt{q_1^2-q_2}}+\theta(q_2-q_1^2)\,\theta(q_2-a^2)\right)\Phi_{1,-a}\otimes\Psi_{1,a}+o(1),$$

$$q\sim(\pm a,a^2). \tag{3.25}$$

Thus $\hat{M}_1(q)$ is bounded but discontinuous at $q=(\pm a,a^2)$, while its regular part, g_1^-, is the same for both these points.

Now it is easy to see that the discontinuity of the resolvent along the cut $q_2=a^2$, $|q_1|<a$ and the ill definiteness at the points $q=(\pm a,a^2)$ are the result of embedding the one-dimensional potential in the two-dimensional space. Indeed, the resolvent of the Sturm–Liouville operator $\partial_{x_1}^2-u_1(x_1)-q_2$ is obtained from $M_1(q)$ by means of the operation $\int dx_2\,e^{-q_2(x_2-x_2')}\hat{M}_1(x,x';q)$. By (3.18) and (3.3), (3.4), and (3.9) we get the standard expression for the one-dimensional Green's function with a pole at $q_2=a^2$.

We already noted that $\hat{M}_1(x,x';q)$ defines a family of Green's functions. Among them that we expect should play a special role are those obtained considering the values of q belonging to the support of the defects of analyticity given in (3.20), (3.21) and (3.22). We consider, therefore, the Green's functions

$$G_1(x,x',k)=\hat{M}_1(x,x';q)|_{q=\ell_{\mathfrak{J}}(k)}, \tag{3.26}$$

$$G_1^{\pm}(x,x';k)=\hat{M}_1(x,x';q)|_{q_1=k_{\mathfrak{J}},\, q_2=a^2\pm 0}, \tag{3.27}$$

where $k\in\mathbb{C}$ is the spectral parameter and we denote $q_1=k_{\mathfrak{J}}$ [see (2.11)] in order to meet the standard notation. From these definitions it follows directly that

$$\vec{\mathcal{L}}_1 G_1(k)=G_1(k)\tilde{\mathcal{L}}_1=I, \quad \vec{\mathcal{L}}_1 G_1^{\pm}(k)=G_1^{\pm}(k)\tilde{\mathcal{L}}_1=I, \tag{3.28}$$

$$\overline{G_1(k)}\equiv G_1(-\bar{k})\equiv G_1(k), \tag{3.29}$$

$$G_1(k)|_{k_{\mathfrak{R}}=0}=G_1(0), \quad G_1^{\pm}(k)=G_1^{\pm}(ik_{\mathfrak{J}}), \tag{3.30}$$

i.e., $G_1^{\pm}(k)$ are independent on $k_{\mathfrak{R}}$ and then inside the strip they coincide with $g_1^{\pm}$ introduced in (3.23),

$$G_1^{\pm}(x,x';k)|_{|k_{\mathfrak{J}}|<a}=g_1^{\pm}(x,x'). \tag{3.31}$$

As well from (3.18) we get the representations

$$\begin{aligned} G_1(x,x',k)=\frac{1}{2\pi}\int_{k'_{\mathfrak{J}}=k_{\mathfrak{J}}} dk' \,[\,\theta(|k_{\mathfrak{R}}|-|k'_{\mathfrak{R}}|)-\theta(x_2-x'_2)]\Phi_1(x,k')\Psi_1(x',k') \\ +c\;\theta(a-|k_{\mathfrak{J}}|)\,\theta(x'_2-x_2)\Phi_{1,-a}(x)\Psi_{1,a}(x'), \end{aligned} \tag{3.32}$$

$$\begin{aligned} G_1^{\pm}(x,x',k)=\frac{1}{2\pi}\int_{k'_{\mathfrak{J}}=k_{\mathfrak{J}}} dk'_{\mathfrak{R}}\,[\,\theta((k_{\mathfrak{J}})^2-a^2-(k'_{\mathfrak{R}})^2)-\theta(x_2-x'_2)]\Phi_1(x,k')\Psi_1(x',k') \\ \mp c\;\theta(a^2-k_{\mathfrak{J}}^2)\,\theta(\pm(x_2-x'_2))\Phi_{1,-a}(x)\Psi_{1,a}(x'). \end{aligned} \tag{3.33}$$

The first of these equalities shows that the cut of the resolvent at $q_2=a^2$, $|q_1|<a$ is not inherited by $G_1(k)$ (in contrast to the case of the nonstationary Schrödinger equation, as mentioned in the Introduction) and that $G_1(k)$ is discontinuous only at the points $k=\pm ia$. Its behavior in the neighborhoods of these points follows from (3.25) and reads as

$$G_1(k)=g_1^{-}-\frac{c}{\pi}\left\{\operatorname{arccot}\frac{a-|k_{\mathfrak{J}}|}{|k_{\mathfrak{R}}|}\right\}\Phi_{1,-a}\otimes\Psi_{1,a}+o(1), \quad k\sim\pm ia. \tag{3.34}$$

Also the Green's functions $G_1^{\pm}(k)$ are discontinuous only at $k_{\mathfrak{J}}=\pm a$ and one gets, thanks to (3.25), that for $k\sim ia$ or $k\sim -ia$

$$G_1^{\pm}(k)=g_1^{-}-c\,\frac{1\pm\theta(a-|k_{\mathfrak{J}}|)}{2}\Phi_{1,-a}\otimes\Psi_{1,a}+o(1). \tag{3.35}$$

Notice that these functions $G_1^{\pm}(k)$ coincide when $|k_{\mathfrak{J}}|>a$ and are independent of $k_{\mathfrak{J}}$ [and then of k by (3.30)] when $|k_{\mathfrak{J}}|<a$. On the borders of these strips they have the discontinuity

$$G_1^{\pm}(k)\big|_{\text{outside}} - G_1^{\pm}(k)\big|_{\text{inside}} = \pm\frac{c}{2}\Phi_{1,-a}\otimes\Psi_{1,a}\,. \tag{3.36}$$

Taking into account the discontinuous behavior of the Green's functions we see that equalities of the type $G_1^{\pm}(ia)=G_1(ia)$ and $G_1^{\pm}(-ia)=G_1(-ia)$ have no meaning in our case. Thanks to (3.32) and (3.35) we have only that

$$\lim_{|k_{\Im}|\to a-0}\ \lim_{k_{\Re}\to 0} G_1(k) = g_1^{-}\,, \tag{3.37}$$

where the limiting procedure must be performed in such a way that $|k_{\Re}|/(a-|k_{\Im}|)\to+0$.

In order to complete the study of the Green's functions we mention that $G_1(k)$ obeys the standard equalities

$$\lim_{k\to\infty}(-2ik)\frac{\partial}{\partial x_1}e^{i\not<(k)(x-x')}G_1(x,x',k)=\delta(x-x'), \tag{3.38}$$

$$\frac{\partial G_1(x,x',k)}{\partial\overline{k}}=\frac{\operatorname{sgn}k_{\Re}}{2\pi}\Phi_1(x,-\overline{k})\Psi_1(x',-\overline{k}). \tag{3.39}$$

The first of them follows either from the differential equations (3.28), or from the integral representation (3.32) and properties (3.6). The second one also follows from (3.28), or it can be derived from (3.26) by means of (3.20) and (3.21). This equality must be understood in the sense of distributions and we see that the discontinuity of $G_1(k)$ at points $k=\pm ia$ leads [by (3.3) and (3.4)] to the pole singularities of the rhs at these points. In view of (3.39) in what follows we refer to $G_1(k)$ as the Green's function of the Jost solutions.

IV. RESOLVENT OF THE PERTURBED *L*-OPERATOR

Now we consider the general case of the operator (1.2) with potential given in (1.5), where $u_2(x)$ is a real function of two space variables, smooth and rapidly decaying at space infinity. The extended resolvent $M(q)$ is determined by (one of) Eqs. (2.22) and we need to study its analyticity properties first. The increment $M(p;\mathbf{q}+\mathbf{s})-M(p;\mathbf{q})$ of M can be obtained from the Hilbert identity (2.19) where prime means the increment $\mathbf{s}$ of $\mathbf{q}$. We have $M'-M=-M'(L_1'-L_1)M$ and, then, using (2.21),

$$M'-M=M'L_1'(M_1'-M_1)L_1M. \tag{4.1}$$

Thus for the d-bar derivatives with respect to $\mathbf{q}_j$ we get

$$\overline{\partial}_j M=(ML_1)(\overline{\partial}_j M_1)(L_1M),\quad j=1,2, \tag{4.2}$$

in the region where M_1 is continuous, i.e., for $q_2\neq a^2$. In terms of the objects introduced in (2.13), we obtain

$$\widehat{\overline{\partial}_j M}=\hat{M}\vec{\mathcal{L}}_1(\widehat{\overline{\partial}_j M_1})\vec{\mathcal{L}}_1\hat{M},\quad j=1,2, \tag{4.3}$$

where we used that $\hat{L}_1(x,x';q)=\mathcal{L}_1\delta(x-x')$ and took into account that when kernels with hats are considered, the multiplication by $\mathcal{L}_1$ is no longer associative and it is necessary to use the arrows to indicate the correct order of operations [cf. (2.15)]. Now, thanks to (2.17) and using (3.20) and (3.21) we get for $q_2\neq a^2$

$$\frac{\partial \hat{M}(q)}{\partial q_1} = \frac{i}{\pi} \int_{k_{\Im}=q_1} dk_{\Re}\, \overline{k}\, \delta(\not{\omega}_{2\Im}(k) - q_2)\, \Phi(k) \otimes \Psi(k), \tag{4.4}$$

$$\frac{\partial \hat{M}(q)}{\partial q_2} = \frac{-1}{2\pi} \int_{k_{\Im}=q_1} dk_{\Re}\, \delta(\not{\omega}_{2\Im}(k) - q_2)\, \Phi(k) \otimes \Psi(k), \tag{4.5}$$

where $\Phi(k)$ and $\Psi(k)$ are defined by

$$\Phi(k) = G(k)\vec{\mathcal{L}}_1 \Phi_1(k), \quad \Psi(k) = \Psi_1(k)\vec{\mathcal{L}}_1 G(k), \tag{4.6}$$

with

$$G(x,x',k) = \hat{M}(x,x';q)\big|_{q=\not{\omega}_{\Im}(k)}. \tag{4.7}$$

More explicitly, say, the first of Eqs. (4.6) stands for $\Phi(x,k) = \int dx' (\mathcal{L}_1^{\mathrm{d}}(x', \partial_{x'}) \times G_1(x,x',k)) \Phi_1(x',k)$. The function $G(k)$ with kernel $G(x,x',k)$ defined in (4.6) satisfies the differential equations

$$\vec{\mathcal{L}} G(k) = G(k)\tilde{\mathcal{L}} = I, \tag{4.8}$$

which can be obtained as a direct reduction of (2.15). Therefore, $G(k)$ is a Green's function. Since the reduction is the same used in (3.26) for getting $G_1(k)$ from $\hat{M}_1$ we derive from (2.22) that this Green's function obeys the integral equations

$$G(k) = G_1(k) + G_1(k) U_2 G(k), \quad G(k) = G_1(k) + G(k) U_2 G_1(k). \tag{4.9}$$

Again, as in Sec. III, thanks to (4.7) and (4.4) and (4.5) we get the d-bar derivative of the Green's function in the form

$$\frac{\partial G(k)}{\partial \overline{k}} = \frac{\operatorname{sgn} k_{\Re}}{2\pi} \Phi(-\overline{k}) \otimes \Psi(-\overline{k}), \tag{4.10}$$

where $\Phi(k)$ and $\Psi(k)$ are defined in (4.6). These objects, due to their definition and (4.9), obey the integral equations

$$\Phi(k) = \Phi_1(k) + G_1(k) U_2 \Phi(k), \quad \Psi(k) = \Psi_1(k) + \Psi(k)\, U_2 G_1(k), \tag{4.11}$$

where again the first equation more explicitly reads as $\Phi(x,k) = \Phi_1(x,k) + \int dx' G_1(x,x',k) \times u_2(x') \Phi(x',k)$. It is clear that the differential equations

$$\vec{\mathcal{L}} \Phi(k) = 0, \quad \Psi(k)\tilde{\mathcal{L}} = 0 \tag{4.12}$$

hold and, therefore, we can consider $\Phi(x,k)$ and $\Psi(x,k)$ as the generalization of the Jost solutions to the case where the perturbation $u_2(x)$ is different from zero. Let us mention that thanks to these definitions we succeeded in avoiding the indeterminacy in the definition of the Jost solutions discussed in the Introduction. Later we study the properties of the Green's function and the Jost solutions in more detail and discuss the singular structure of the terms involved in (4.10). Now let us mention the following standard properties

$$-2i \lim_{k\to\infty} k \partial_{x_1} (e^{i\not{\omega}(k)(x-x')} G(x,x',k)) = \delta(x-x'), \tag{4.13}$$

$$\overline{G(k)} = G(-\overline{k}) = G(k), \tag{4.14}$$

$$\overline{\Phi(x,k)}=\Phi(x,-\overline{k}),\quad \overline{\Psi(x,k)}=\Psi(x,-\overline{k}), \tag{4.15}$$

which can be obtained by means of the integral equations (4.9) and properties (3.5), (3.29), and (3.38) for the Green's function $G_1(k)$.

Till now we studied the departure from analyticity of the resolvent in the case $q_2\neq a^2$. Since the resolvent $M_1(q)$ is discontinuous along the line $q_2=a^2$ [see (3.22)], the integral equations (2.22) suggest that also $M(q)$ has a discontinuity. Let us denote the limiting values on the two edges of the line by

$$M^{\pm}(q)=M(q)|_{q_2=a^2\pm 0}. \tag{4.16}$$

Then from the Hilbert identity (4.1) we derive that

$$M^{+}(q)-M^{-}(q)=M^{\pm}(q)L_1(q)(M_1^{+}(q)-M_1^{-}(q))L_1(q)M^{\mp}(q),\quad q_2=a^2, \tag{4.17}$$

where the lhs is independent of the choice of the sign on the rhs. In analogy with (3.27) we introduce the two Green's functions

$$G^{\pm}(x,x';k)=\hat{M}(x,x';q)|_{q_1=k_{\Im},\ q_2=a^2\pm 0} \tag{4.18}$$

and rewrite (4.17) in these terms as $G^{+}(k)-G^{-}(k)=(G^{\pm}(k)\tilde{\mathcal{L}}_1)(G_1^{+}(k)-G_1^{-}(k))\times(\vec{\mathcal{L}}_1G^{\mp}(k))$. Then by (3.22) and (3.27) we get

$$G^{+}(k)-G^{-}(k)=-c\,\theta(a^2-k_{\Im}^2)\Phi^{\pm}(k)\otimes\Psi^{\mp}(k), \tag{4.19}$$

where the new solutions [cf. (4.6)] were introduced:

$$\Phi^{\pm}(k)=G^{\pm}(k)\tilde{\mathcal{L}}_1\Phi_{1,-a},\quad \Psi^{\pm}(k)=\Psi_{1,a}\vec{\mathcal{L}}_1G^{\pm}(k). \tag{4.20}$$

Following properties of $G_1^{\pm}(k)$ it is easy to show that these Green's functions obey the following differential and integral equations and reality condition:

$$\vec{\mathcal{L}}G^{\pm}(k)=G^{\pm}(k)\tilde{\mathcal{L}}=I, \tag{4.21}$$

$$G^{\pm}(k)=G_1^{\pm}(k)+G_1^{\pm}(k)U_2G^{\pm}(k),\quad G^{\pm}(k)=G_1^{\pm}(k)+G^{\pm}(k)U_2G_1^{\pm}(k), \tag{4.22}$$

$$\overline{G^{\pm}(k)}=G^{\pm}(k). \tag{4.23}$$

By definition they are independent of $k_{\Re}$ and by the corresponding properties of $G_1^{\pm}(k)$ we have that $G^{+}(k)=G^{-}(k)$ when $|k_{\Im}|>a$ and they are independent of $k_{\Im}$ when $|k_{\Im}|<a$. By (4.20) and (4.21) we get that $\Phi^{\pm}(k)$ and $\Psi^{\pm}(k)$ are solutions of the heat equation with potential (1.5),

$$\vec{\mathcal{L}}\Phi^{\pm}(k)=0,\quad \Psi^{\pm}(k)\tilde{\mathcal{L}}=0. \tag{4.24}$$

Integral equations for these solutions follow by applying operations (4.20) to the equations (4.22):

$$\Phi^{\pm}=\Phi_{1,-a}+G_1^{\pm}U_2\Phi^{\pm},\quad \Psi^{\pm}=\Psi_{1,a}+\Psi^{\pm}U_2G_1^{\pm}. \tag{4.25}$$

Let us also mention that, thanks to (4.23), these solutions are real and are independent of k inside the strip $|k_{\Im}|<a$, due to the corresponding property of $G^{\pm}(k)$ and (4.20). Since in the following we use intensively the Green's functions and these solutions inside the strip, it is convenient to introduce the following specific notations:

$$g^{\pm}(x,x')=G^{\pm}(x,x',k)|_{|k_{\Im}|<a}, \tag{4.26}$$

and also

$$\phi^{\pm}(x)=\Phi^{\pm}(x,k)\big|_{|k_{\jmath}|<a}, \quad \psi^{\pm}(x)=\Psi^{\pm}(x,k)\big|_{|k_{\jmath}|<a}. \tag{4.27}$$

Equality (4.19) enables us to find relations between solutions (4.20). Let $|k_{\jmath}|<a$. Then applying, say, $\tilde{\mathcal{L}}_1\Phi_{1,-a}$ to this equality from the right and using (4.20) we derive that

$$(1+\lambda)\phi^{+}=\phi^{-}, \tag{4.28}$$

where

$$\lambda=c(\Psi_{1,a}\vec{\mathcal{L}}_1 g^{-}\tilde{\mathcal{L}}_1\Phi_{1,-a}). \tag{4.29}$$

Explicitly $\lambda=c\int dx\int dx'\Psi_{1,a}(x)(\mathcal{L}_1(x,\partial_x)\mathcal{L}_1^{\mathrm{d}}(x',\partial_{x'})g^{-}(x,x')\Phi_{1,-a}(x'))$. By (4.23) this constant is real and, thanks to (4.20), it is also equal to $\lambda=c(\Psi_{1,a}\vec{\mathcal{L}}_1\phi^{-})=c(\psi^{-}\tilde{\mathcal{L}}_1\Phi_{1,-a})$. Inserting here $\mathcal{L}_1=\mathcal{L}+U_2$ we get by (4.21) and (4.24) that

$$\lambda=c\{(\Psi_{1,a}U_2\Phi_{1,-a})+(\Psi_{1,a}U_2 g^{-}U_2\Phi_{1,-a})\}, \tag{4.30}$$

or $\lambda=c(\Psi_{1,a}U_2\phi^{-})=c(\psi^{-}U_2\Phi_{1,-a})$, where we also used $\vec{\mathcal{L}}_1\Phi_{1,-a}=0$ and $\Psi_{1,a}\tilde{\mathcal{L}}_1=0$, which follow from (3.2) and (3.8). Next, applying to (4.28) $\Psi_{1,a}\vec{\mathcal{L}}_1$ from the left and again by (4.20) we get

$$(1+\lambda)[1-c(\Psi_{1,a}\vec{\mathcal{L}}_1 g^{+}\tilde{\mathcal{L}}_1\Phi_{1,-a})]=1, \tag{4.31}$$

where a new constant $(\Psi_{1,a}\vec{\mathcal{L}}_1 g^{+}\tilde{\mathcal{L}}_1\Phi_{1,-a})=(\Psi_{1,a}U_2\Phi_{1,-a})+(\Psi_{1,a}U_2 g^{+}U_2\Phi_{1,-a})$ [cf. (4.30)] appeared. Since we chose u_2 to be rapidly decaying at infinity, all terms must be finite. Then $1+\lambda\neq 0$ and, more precisely, taking into account that for $u_2\to 0$ also $\lambda\to 0$, we have that

$$1+\lambda>0. \tag{4.32}$$

Summarizing, we get the following relations:

$$c(\Psi_{1,a}\vec{\mathcal{L}}_1 g^{+}\tilde{\mathcal{L}}_1\Phi_{1,-a})=\frac{\lambda}{1+\lambda}, \tag{4.33}$$

$$\phi^{+}=\frac{\phi^{-}}{1+\lambda}, \quad \psi^{+}=\frac{\psi^{-}}{1+\lambda}, \tag{4.34}$$

$$G^{+}(k)=G^{-}(k)-\frac{c\,\theta(a-|k_{\jmath}|)}{1+\lambda}\phi^{-}\otimes\psi^{-}. \tag{4.35}$$

Here (4.33) is just (4.31), the first equality in (4.34) is (4.29) and the second equality is derived by analogy, and (4.35) follows from (4.19) thanks to (4.34). In their turn (4.33) and (4.34) follow from (4.35) thanks to (4.20) and (4.28).

We have shown in (3.36) that the Green's functions $G_1^{\pm}(k)$ are discontinuous at $k_{\jmath}=a$ and $k_{\jmath}=-a$. By (4.22) we deduce that $G^{\pm}(k)$ have the same behavior. In order to study this discontinuity we use, as above, the Hilbert identity (4.1) where $M=M(q)$, $M'=M(q')$, etc. We choose $q_2=q_2'=a^2\pm 0$, $q_1=a-\varepsilon$, $q_1'=a+\varepsilon$, and in the limit $\varepsilon\to+0$ we use the hat notation (2.13) and definitions (3.27) and (4.18) of the Green's functions. Then we get $G^{\pm}(i(a+0))-g^{\pm}=G^{\pm}(i(a+0))\tilde{\mathcal{L}}_1(G_1^{\pm}(i(a+0))-g_1^{\pm})\vec{\mathcal{L}}_1 g^{\pm}$, where again (3.31) and (4.26) were used. Now by (3.36) for the discontinuity of the unperturbed Green's functions we obtain

$$G^{\pm}(i(a+0))-g^{\pm}=\pm\frac{c}{2}\Phi^{\pm}(i(a+0))\otimes\psi^{\pm}, \tag{4.36}$$

where notations (4.20), (4.26) and (4.27) were used. Applying $\tilde{\mathcal{L}}_1\Phi_{1,-a}$ from the right and $\Psi_{1,a}\vec{\mathcal{L}}_1$ from the left in analogy with the derivation of (4.35) we get by (4.28) that $c(\Psi_{1,a}\vec{\mathcal{L}}_1G^{\pm}(i(a+0))\tilde{\mathcal{L}}_1\Phi_{1,-a})=2\lambda(2+\lambda)^{-1}$, which is finite due to (4.32). Then omitting details we derive the equalities $G^{\pm}(i(a+0))=G^{\pm}(-i(a+0))=g^{-}-c(2+\lambda)^{-1}\phi^{-}\otimes\psi^{-}$, that, say, for the bottom sign can also be rewritten in the form

$$G^{-}(k)=g^{-}-\frac{c\,\theta(|k_{\mathfrak{I}}|-a)}{2+\lambda}\phi^{-}\otimes\psi^{-}+o(1),\quad k\sim\pm ia, \tag{4.37}$$

where we took (4.26) into account.

V. PROPERTIES OF THE JOST SOLUTIONS AND INVERSE PROBLEM

In this section we complete the investigation of the properties of the Jost solutions by describing their behavior at the points $k=\pm ia$. Formulas (4.6) suggest to study first the behavior of the Green's function $G(k)$. We expect that it is ill defined at these points, so in order to describe this behavior we compare $G(k)$ with some well defined Green's function, say, g^{-}. For this aim, as we have already shown, relations of the type (4.19) can be very useful. In order to derive them we start again from the Hilbert identity (4.1) where $M'=M(q')$ and $M=M(q)$ and we choose $q'=\ell_{\mathfrak{I}}(k)$, $q_1=k_{\mathfrak{I}}$, $q_2=a^2-0$ [see (2.11), (4.7) and (4.16)]. Then, passing to the objects with hats by (2.13), recalling definitions (4.7) and (4.18) and keeping only the leading term in the neighborhood of $k\sim\pm ia$, we get

$$G(k)-G^{-}(k)=G(k)\tilde{\mathcal{L}}_1(G_1(k)-G_1^{-}(k))\vec{\mathcal{L}}_1G^{-}(k)+o(1),\quad k\sim\pm ia.$$

Inserting the explicit singular behaviors of $G_1(k)$, $G_1^{-}(k)$ and $G^{-}(k)$ at $k=\pm ia$ given in (3.34), (3.35) and (4.37), we have

$$G(k)-g^{-}=-\frac{c\,\theta(|k_{\mathfrak{I}}|-a)}{2+\lambda}\phi^{-}\otimes\psi^{-}+c\left(-\frac{1}{\pi}\operatorname{arccot}\frac{a-|k_{\mathfrak{I}}|}{|k_{\mathfrak{R}}|}+\frac{\theta(|k_{\mathfrak{I}}|-a)}{2}\right)G(k)\tilde{\mathcal{L}}_1\Phi_{1,-a}\otimes\Psi^{-}(k)+o(1),$$

where in the last multiplier the definition of $\Psi^{-}(k)$ in (4.20) was used. Again by (4.20) and (4.37) $\Psi^{-}(k)=\{[2+\lambda\,\theta(a-|k_{\mathfrak{I}}|)]/(2+\lambda)\}\psi^{-}$, where as always ψ^{-} denotes $\Psi^{-}(k)$ for $|k_{\mathfrak{I}}|<a$ by (4.27). Then

$$G(k)-g^{-}=\left\{-\frac{c\,\theta(|k_{\mathfrak{I}}|-a)}{2+\lambda}\phi^{-}+c\left(-\frac{1}{\pi}\operatorname{arccot}\frac{a-|k_{\mathfrak{I}}|}{|k_{\mathfrak{R}}|}+\frac{\theta(|k_{\mathfrak{I}}|-a)}{2}\right)\times\frac{2+\lambda\,\theta(a-|k_{\mathfrak{I}}|)}{2+\lambda}G(k)\tilde{\mathcal{L}}_1\Phi_{1,-a}\right\}\otimes\psi^{-}+o(1). \tag{5.1}$$

Thus in order to get the behavior of $G(k)$ we need to find that of $G(k)\tilde{\mathcal{L}}_1\Phi_{1,-a}$, which follows by applying to (5.1) operation $\tilde{\mathcal{L}}_1\Phi_{1,-a}$ from the right and using again (4.20), (4.27) and (4.29). Then

$$G(k)\tilde{\mathcal{L}}_1\Phi_{1,-a}=\frac{\pi\phi^{-}}{A(k)}+o(1),\quad k\sim\pm ia, \tag{5.2}$$

where we denoted for brevity

$$A(k)=\pi+\lambda\ \mathrm{arccot}\frac{a-|k_{\Im}|}{|k_{\Re}|}. \tag{5.3}$$

This function is real positive thanks to (4.32) and discontinuous at $k=\pm ia$. Now inserting (5.2) in (5.1) we derive finally that

$$G(k)=g^{-}-\frac{c}{A(k)}\left(\mathrm{arccot}\frac{a-|k_{\Im}|}{|k_{\Re}|}\right)\phi^{-}\otimes\psi^{-}+o(1),\quad k\sim\pm ia. \tag{5.4}$$

Applying to (5.4) from the left the operation $\Psi_{1,a}\vec{\mathcal{L}}_1$ and recalling the definitions (4.20) and (4.27) we derive

$$\Psi_{1,a}\vec{\mathcal{L}}_1G(k)=\frac{\pi\psi^{-}}{A(k)}+o(1),\quad k\sim\pm ia, \tag{5.5}$$

and by (4.29) also

$$c\Psi_{1,a}\vec{\mathcal{L}}_1G(k)\tilde{\mathcal{L}}_1\Phi_{1,-a}=\frac{\pi\lambda}{A(k)}+o(1),\quad k\sim\pm ia. \tag{5.6}$$

Correspondingly, we get for the behavior of the Jost solutions in the neighborhood of $k=\pm ia$, thanks to (3.3) and (5.2),

$$\Phi(k)=\frac{i\pi c\phi^{-}}{A(k)(k-ia)}+O(1),\quad k\sim ia, \tag{5.7}$$

$$\Phi(k)=\frac{\pi\phi^{-}}{A(k)}+o(1),\quad k\sim -ia \tag{5.8}$$

and analogous relations for $\Psi(k)$.

Now we are ready to consider the d-bar derivative in the sense of distributions of the Jost solution, say, $\Phi(k)$. Let first $k\neq\pm ia$. Then we use (3.3), (4.6), and (4.10) to derive

$$\frac{\partial\Phi(k)}{\partial\overline{k}}=\Phi(-\overline{k})r(k),\quad k\neq\pm ia, \tag{5.9}$$

where the spectral data are defined as follows:

$$r(k)=\frac{\mathrm{sgn}\,k_{\Re}}{2\pi}(\Psi_1(-\overline{k})\vec{\mathcal{L}}_1G(k)\tilde{\mathcal{L}}_1\Phi_1(k)). \tag{5.10}$$

Thanks to (3.3), (3.4) and (5.6) we get the singular behavior of these spectral data in the form

$$r(k)=\frac{i\lambda\ \mathrm{sgn}\,k_{\Re}}{2(k_{\Re}+i|k_{\Im}|-ia)A(k)}+o(1),\quad k\sim\pm ia, \tag{5.11}$$

i.e., in both points it has a pole singularity multiplied by the discontinuous function $A(k)$. Taking into account that the singular behavior of $\Phi(-\overline{k})$ is given by the denominator $\overline{(k-ia)}A(k)$ at point $k=ia$ and by $A(k)$ at point $k=-ia$ we see that the rhs in (5.9) is integrable at the latter point but it has a singularity $\mathrm{sgn}\,k_{\Re}|k-ia|^{-2}A(k)^{-2}$ at point $k=ia$, which is not integrable. On the other hand, $\Phi(k)$ is locally integrable for any k, so $\Phi(x,k)e^{i\not\subset(k)x}$ is a Schwartz distribution with respect to k. Thus its d-bar derivative in the sense of distributions exists and can be defined

in the standard way. Let $f(k)$ be a test function that properly decays at infinity (we are now not interested in the exponential growth due to the multiplier $e^{-i\ell(k)x}$). Then the d-bar derivative of $\Phi(k)$ is defined as

$$\int d^2k \frac{\partial\Phi(k)}{\partial\bar{k}} f(k) = -\int d^2k\, \Phi(k) \frac{\partial f(k)}{\partial\bar{k}} = -\lim_{\varepsilon\to 0}\int_{|k\pm ia|>\varepsilon} d^2k\, \Phi(k) \frac{\partial f(k)}{\partial\bar{k}},$$

where in the last equality we again used the property of local integrability of $\Phi(k)$. Integrating by parts for $\varepsilon>0$ we can use (5.9) and we have

$$-\lim_{\varepsilon\to 0}\int_{|k\pm ia|>\varepsilon} d^2k\, \Phi(k) \frac{\partial f(k)}{\partial\bar{k}} = \frac{f(ia)}{2i}\lim_{\varepsilon\to 0}\oint_{|k-ia|=\varepsilon} dk\, \Phi(k) + \lim_{\varepsilon\to 0}\int_{|k-ia|>\varepsilon} d^2k$$

$$\times\Phi(-\bar{k})r(k)f(k),$$

where we omitted the term $\oint_{|k+ia|>\varepsilon}$ since thanks to (5.8) it gives zero in the limit $\varepsilon\to 0$. Thanks to (5.7) and (5.8) both limits on the rhs exist. To be more precise, let us introduce the distribution

$$\text{p.v.}\int d^2k \frac{\operatorname{sgn} k_{\Re} f(k)}{|k-ia|^2 A(k)^2} = \lim_{\varepsilon\to 0}\int_{|k-ia|>\varepsilon} d^2k \frac{\operatorname{sgn} k_{\Re} f(k)}{|k-ia|^2 A(k)^2}. \tag{5.12}$$

Notice the presence in the numerator of $\operatorname{sgn} k_{\Re}$ that guaranties existence of the limit. We used the principal value (p.v.) notation in analogy with the one-dimensional case. It can be checked directly that

$$\text{p.v.}\int d^2k \frac{\operatorname{sgn} k_{\Re} f(k)}{|k-ia|^2 A(k)^2} = \int d^2k \frac{\operatorname{sgn} k_{\Re}}{|k-ia|^2 A(k)^2}[f(k)-\theta(\delta-|k-ia|)f(ia)]$$

$$= \frac{1}{2}\int d^2k \operatorname{sgn} k_{\Re} \frac{f(k)-f(-\bar{k})}{|k-ia|^2 A(k)^2}, \tag{5.13}$$

where δ is some real positive parameter and the second term in (5.13) is independent of the choice of δ. In the case where a distribution has singularities of this form at some finite number of points a_1, a_2, etc., we use the same notation for the integral assuming that either the cutoff procedure in (5.12) or the subtraction procedure in (5.13) is performed at each point. Of course, the parameters ε_j and δ_j must be chosen in such a way that corresponding discs do not overlap.

Let us denote

$$\Phi_a = -\frac{1}{2\pi}\lim_{\varepsilon\to 0}\oint_{|k-ia|=\varepsilon} dk\, \Phi(k), \tag{5.14}$$

so that $i\Phi_a$ can be considered as an extension of the definition of residuum to the case in which the pole singularity is multiplied by a function discontinuous at the same point. Thanks to (5.7) we get that this limit also exists and equals

$$\Phi_a = c\frac{\log(1+\lambda)}{\lambda}\phi^-. \tag{5.15}$$

Thus, summarizing all above definitions we get that

$$\frac{\partial\Phi(k)}{\partial\bar{k}} = \Phi(-\bar{k})r(k) + i\pi\Phi_a\delta(k-ia), \tag{5.16}$$

where $\Phi(x,-\overline{k})r(k)$ is now a distribution in k defined by the p.v. prescription given above. By (5.7), (5.8) and (5.11) it is integrable at $k=-ia$, but it behaves as $|k-ia|^{-2}A^{-2}(k)$ in the neighborhood of the point $k=ia$.

Equation (5.16) supplies us with the first equation of the inverse problem. In order to close it we need the analog of the first relation in (3.17), where it is stated that the residuum of the function is proportional to its value in the conjugated point. But in our case $\Phi(k)$ is discontinuous at point $k=-ia$, so again some modification of the notion of "value" at this point must be given. Following the procedure used in (5.14) we can define it as

$$\Phi_{-a}=\frac{1}{2\pi i}\lim_{\varepsilon\to 0}\oint_{|k+ia|=\varepsilon}\frac{dk}{k+ia}\Phi(k). \tag{5.17}$$

Thanks to (5.8) this limit also exists and equals

$$\Phi_{-a}=\frac{\log(1+\lambda)}{\lambda}\phi^{-}, \tag{5.18}$$

so that by (5.15) we have

$$\Phi_a=c\Phi_{-a}, \tag{5.19}$$

which shows that the parameter c is not modified by the perturbation. This equality closes the formulation of the inverse problem (5.16). Finally, taking into account the asymptotic behavior of $\Phi(x,k)$ and (5.17) and (5.19), we can formulate the inverse problem as the following system of integral equations:

$$\Phi(x,k)=e^{-i\not{\ell}(k)x}+\frac{1}{\pi}\text{p.v.}\int\frac{d^2k'}{k-k'}e^{i(\not{\ell}(k')-\not{\ell}(k))x}\Phi(x,-\overline{k'})r(k')+i\frac{e^{i(\not{\ell}(ia)-\not{\ell}(k))x}}{k-ia}\Phi_a(x), \tag{5.20}$$

$$\frac{1}{c}\Phi_a(x)=e^{-i\not{\ell}(-ia)x}-\frac{1}{\pi}\text{p.v.}\int d^2k\,\frac{\Phi(x,-\overline{k})r(k)}{k+ia}e^{i(\not{\ell}(k)-\not{\ell}(-ia))x}+\frac{e^{i(\not{\ell}(ia)-\not{\ell}(-ia))x}}{2a}\Phi_a(x). \tag{5.21}$$

The integrands on the rhs of these two equations are not locally integrable, respectively, the first at $k=ia$ and the second at $k=\pm ia$. Correspondingly, their integrals are regularized by means of the principal value prescription, as in (5.12) or (5.13), at $k=ia$ and at $k=\pm ia$.

The potential is reconstructed by means of

$$u(x)=-\frac{2i}{\pi}\text{p.v.}\int d^2k\,\frac{\partial}{\partial x_1}(\,e^{i\not{\ell}(k)x}\Phi(x,-\overline{k})r(k))+2\,\frac{\partial}{\partial x_1}(e^{i\not{\ell}(ia)x}\,\Phi_a(x)). \tag{5.22}$$

VI. CONCLUSION

In this article on the basis of the resolvent approach we gave a detailed presentation of an extension of the inverse scattering theory for the heat operator to the case where the potential (1.5) is a perturbation of the one-dimensional one-soliton potential $u_1(x_1)$ (3.1) by means of a smooth, decaying at infinity function $u_2(x)$ of two space variables. To our knowledge this is the first time that inverse scattering theory is applied to a nonscattering situation, i.e., a situation with an infinite obstacle. As a result of our investigation we proved that under such a perturbation the Jost solutions get specific singularities (5.7) and (5.8) on the complex plane of the spectral parameter k. We demonstrated that the d-bar problem (5.16) and (5.19), while looking familiar for a potential whose spectrum has a discrete and continuous part, needs a substantially modified approach due to the singularity structure of the spectral data given in (5.11). It was necessary to establish the

meaning in the sense of distributions of all terms involved in this problem, in order to be able to formulate the inverse problem as the system of integral equations (5.20) and (5.21). It is easy to check that the singular behavior of the spectral data and Jost solution as given in (5.11) and (5.7) and (5.8) is compatible with this inverse problem. On the other side, it is necessary to prove that the potential $u(x)$ reconstructed by means of (5.22) is of the type (1.5). We plan to address this problem in a forthcoming work.

Another open problem is the application of these results to the KPII equation (1.3) itself. In particular, investigation of the time asymptotics of solutions with initial data of the type (1.5) must be performed. Let us mention only that the singular behavior (5.11) of the spectral data is preserved under evolution (1.3). Indeed,[3] the time dependence of the spectral data is given as

$$r(k,t)=e^{4i(k^3+\bar{k}^3)}. \tag{6.1}$$

Thus we get that

$$a=\text{const}, \quad \lambda=\text{const}, \tag{6.2}$$

also with respect to time.

In Sec. III we mentioned that the above construction can be easily generalized to the case where the potential $u_1(x_1)$ is a pure N-soliton one-dimensional potential. At the same time our approach also admits straightforward generalization to the case where $u_1(x)$ is not a function of one space variable but the result of application of the Bäcklund transformation to a generic background two-dimensional potential $u_0(x)$ decaying on the x-plane. Then the inverse problem is again given by Eqs. (5.20) and (5.21), where the spectral data $r(k)$ are replaced with

$$r(k)+\frac{(k+ia)(\bar{k}+ia)}{(\bar{k}-ia)(k-ia)}r_0(k), \tag{6.3}$$

where $r(k)$ is of the type (5.11) and $r_0(k)$ are the spectral data of the potential $u_0(x)$ (see Ref. 11).

The theory of the heat equation with respect to the nonstationary Schrödinger equation is in some respects simpler and in some other respects unexpectedly more difficult. As we have shown, under perturbation the Jost solution get singularities more complicated than poles, but this solution has no additional cut in the complex domain, in contrast with the nonstationary Schrödinger case as discovered in Ref. 13. On the other hand, the generalization of this scheme to the case of multi-ray structure of the potential $u(x)$ meets with essential problems, first of all due to the fact that the resolvent (or Green's function) of the heat equation even of a two-soliton (generic) potential is unknown in the literature. This problem also needs future development.

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Angle operators on weighted Bergman spaces

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Among the multiplication operators on weighted Bergman Hilbert spaces are those where the multiplying function (operator symbol) depends only on the angular polar coordinate in the unit disk: we call these ''angle operators.'' As these Hilbert spaces carry a CCR representation unitarily equivalent to the Schrödinger representation, angle operators are associated with quantum phase in the same way as are Toeplitz operators, for example. We determine the matrix elements of the angle operators with respect to the natural orthonormal basis on each of these spaces, and also with respect to the appropriate family of coherent states. By using a method of comparison with the corresponding results for Toeplitz operators, asymptotic expressions for the expectations and variances in these two families of states are obtained for the angle operators whose symbols are the polar angle function and its two complex exponentials. Notable is the fact that the asymptotic limit of the variance of the polar angle operator in the natural basis family is $\pi^2/3$, which many authors take to be a requirement for a quantum phase operator. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1423401]

I. INTRODUCTION

In order to understand the phenomena collectively known as ''quantum phase,'' a number of operators have been proposed as a quantum phase observable. These proposals have been described in a number of reviews and book,[1–5] highlighting different points of view, and particularly in a book by the authors together with Smith,[6] whose conventions we shall adopt here.

Among the proposals are the Toeplitz operator X of multiplication by the angle variable in the Hardy space $H^2(\mathbb{T})$, and the operator of multiplication by the angle variable in Bargmann–Segal space (Fock space over $\mathbb{C}$). In addition, functions of these operators (in the sense of spectral theory) have been considered as describing aspects of the quantum phase, and so we take it that there is a respectable pedigree to considering operators of multiplication by functions of an angle on Hilbert spaces of functions whose domain is a subset of the complex plane—notwithstanding that these operators are not diagonal (so that the angle is not the spectral variable which will be measured).

In this paper we add a one-parameter family to the catalog of such operators by considering angle operators on the weighted Bergman spaces (Hilbert spaces associated with the weighted Bergman kernels).

The paper is organized as follows. In Sec. II we set down our conventions for weighted Bergman spaces and general multiplication operators on them. In Sec. III we introduce those Toeplitz–Bergman operators we call angle operators, denoted $B_{\mathfrak{f}}^{(\alpha)}$. These are multiplication operators on the weighted Bergman Hilbert space by functions of the form $(r,\theta)\mapsto \mathfrak{f}(re^{i\theta})$, where $\mathfrak{f}$ is essentially bounded. We determine their matrix elements with respect to the natural basis $\{e_n^{(\alpha)}: n\geqslant 0\}$ on the Hilbert space in Sec. IV, in particular for the expectation and variance in the

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states $e_n^{(\alpha)}$. By interpolation from integer α, we are able to obtain an asymptotic expression (as $n\to\infty$) of the difference between the expectations and variances of the maps $B_{\mathfrak{f}}^{(\alpha)}$ and those of the Toeplitz operators whose symbols are $\mathfrak{f}$. We find this difference to be at least as fast as $O(1/n)$. Knowledge of the asymptotic properties of the variance of Toeplitz operator whose symbol is the angle function on the circle enables us to show that, in the limit $n\to\infty$, the variance of $B_{\varphi}^{(\alpha)}$ is $\pi^2/3$, where φ is the (suitably defined) argument function. This establishes $B_{\varphi}^{(\alpha)}$ as being as closely related to quantum phase as are the Toeplitz and Bargmann–Segal angle operators.

In Sec. V we introduce a family of coherent states on $\mathcal{H}_\alpha$, and consider the expectation of the angle operators with respect to them. Employing a comparison method, we then obtain an asymptotic form for the variance of $B_{\varphi}^{(\alpha)}$. In the final section we note some open mathematical problems.

II. WEIGHTED BERGMAN SPACES

Let $\mathbb{D}$ be the open unit disc and $dA(z)=dxdy/\pi$ the normalized Lebesgue area measure on $\mathbb{D}$. For all $\alpha\in(-1,\infty)$, define the measure

$$d\mu_\alpha(z)=(\alpha+1)(1-|z|^2)^\alpha dA(z). \tag{1}$$

We write $\mathcal{H}_\alpha$ for the Hilbert space of functions F which are both holomorphic in $\mathbb{D}$ and square integrable with respect to $d\mu_\alpha$. If $f, g\in\mathcal{H}_\alpha$, we write $\|f\|_\alpha$ for the norm of f and $\langle g,f\rangle_\alpha$ for the inner product of f and g: the inner product is antilinear in the first variable. The space $\mathcal{H}_\alpha$ is a weighted Bergman space in the terminology of Hendenmalm, Korenblum, and Zhu,[7] whose conventions we adopt (for the most part). The original Bergman space corresponds to $\alpha=0$, but we shall refer to all of the $\mathcal{H}_\alpha$ simply as Bergman spaces.

In several places we shall be using the Hilbert space $L^2(\mathbb{D},d\mu_\alpha)$ as a space in which $\mathcal{H}_\alpha$ is embedded. There will be no possibility of confusion if we use the same symbols for the norm and inner product on both spaces.

The functions,

$$e_n^{(\alpha)}(z)=i^{-n}\sqrt{\binom{n+\alpha+1}{n}}z^n,\quad n\in\mathbb{N}_0,\ z\in\mathbb{D}, \tag{2}$$

constitute an orthonormal basis for $\mathcal{H}_\alpha$. (The binomial coefficients are extended to nonintegral values by use of the Gamma function.) This choice differs from that of Hedenmalm *et al.*[7] and other authors through the appearance of the factor i^{-n}, which is necessary for consistency with the conventions of Dubin *et al.*[6]

The space $\mathcal{H}_\alpha$ is equipped with the reproducing kernel (see Neeb[8] for the general theory) which is the integral kernel of the projection operator,

$$P_\alpha f=\sum_{n=0}^{\infty}\langle e_n^{(\alpha)},P_\alpha f\rangle_\alpha\, e_n^{(\alpha)}, \tag{3a}$$

of $L^2(\mathbb{D},d\mu_\alpha)$ onto $\mathcal{H}_\alpha$. This series converges pointwise on $\mathbb{D}$, uniformly on compact subsets of $\mathbb{D}$, and is norm-convergent in $L^2(\mathbb{D},d\mu_\alpha)$. Its reproducing kernel is then the positive definite kernel,

$$\mathcal{K}_\alpha(z,w)=(1-z\bar{w})^{-(2+\alpha)}, \tag{3b}$$

so that

$$[P_\alpha f](z)=\int_{\mathbb{D}}\mathcal{K}_\alpha(z,w)f(w)d\mu_\alpha(w) \tag{3c}$$

belongs to $\mathcal{H}_\alpha$ for every $f \in L^2(\mathbb{D}, d\mu_\alpha)$. The $\mathcal{K}_\alpha$ are the weighted Bergman kernels; the original kernel of Bergman results from putting $\alpha = 0$.

We mention parenthetically that the Bergman metric is the Kähler metric,

$$ds^2 = \partial^2 \log \mathcal{K}_\alpha(z, \overline{z}) / \partial z \partial \overline{z} dz d\overline{z}.$$

If F is a function which is bounded except on a μ_α-null set (the usual convention of identifying functions which differ only on a null set is in force), pointwise multiplication by F will, in general, take a function f in $\mathcal{H}_\alpha$ to the function Ff in $L^2(\mathbb{D}, d\mu_\alpha)$. If we want an operator on $\mathcal{H}_\alpha$ we must act with the projection operator P_α on Ff. Now $f \mapsto Ff$ is bounded on $L^2(\mathbb{D}, d\mu_\alpha)$ with the bound not greater than the sup norm of F. As P_α is a projection operator, it can only reduce the bound, and so we come to the following result: a function $F \in L^\infty(\mathbb{D})$ determines a bounded operator $B_F^{(\alpha)}$ on $\mathcal{H}_\alpha$ by $B_F^{(\alpha)}(g) = P_\alpha(Fg)$. For the bound we have $\|B_F^{(\alpha)}\| \leqslant \|F\|_\infty$. In accordance with the standard practice in function theory, we shall refer to $B_F^{(\alpha)}$ as the Toeplitz–Bergman operator (on $\mathcal{H}_\alpha$) and F as the *symbol* of $B_F^{(\alpha)}$.

As a last topic in our cursory discussion of weighted Bergman spaces, we wish to note that each $\mathcal{H}_\alpha$ carries a representation of the canonical commutation relation for one degree of freedom which is equivalent to the Schrödinger representation on $L^2(\mathbb{R})$. As such, these representations are irreducible and gauge invariant and, if one has a quantum phase in mind, could be thought of as describing a single mode of the quantized electromagnetic field whose state is the coherent "laser" radiation. For a discussion of these points, see Dubin *et al.*[6]

This representation arises from the fact that the correspondence $h_n \mapsto W_\alpha(h_n) = e_n^{(\alpha)}$, $n \geqslant 0$, extends to a unitary transformation $L^2(\mathbb{R}) \to \mathcal{H}_\alpha$. (Here h_n is the nth Hermite–Gauss vector.) Since the raising operator of the Schrödinger representation is

$$A^+ h_n = \sqrt{n+1}\, h_{n+1}, \quad n \geqslant 0,$$

the raising operator on $\mathcal{H}_\alpha$ is

$$A_\alpha^+ = W_\alpha A^+ W_\alpha^*,$$

with action

$$A_\alpha^+ e_n^{(\alpha)} = \sqrt{n+1}\, e_{n+1}^{(\alpha)}, \quad n \geqslant 0:$$

similarly for the lowering operator. We have no explicit expression for these ladder operators, but we can describe the number operator N_α. From

$$N_\alpha\, e_n^{(\alpha)} = n e_n^{(\alpha)},$$

we obtain

$$N_\alpha = z d/dz.$$

Although every $f \in \mathcal{H}_\alpha$ is analytic, $zf'(z)$ need not belong to $\mathcal{H}_\alpha$, and so N_α is unbounded; similarly, the raising and lowering operators are unbounded. The appropriate domains for working with this representation can be transferred from those for the Schrödinger representation via the map W_α, but we shall have no need of this here. We note that, up to a phase factor, $e_0^{(\alpha)}$ is the only normalized function in $\mathcal{H}_\alpha$ which is invariant under the gauge group generated by N_α.

III. ANGULAR TOEPLITZ–BERGMAN OPERATORS

Our interest is in the class of Toeplitz–Bergman operators obtained by starting from a bounded function of the angle, $\mathfrak{f}: \mathbb{T} \to \mathbb{C}$, and using it to define a function $\mathfrak{f}_{\text{ang}} \in L^\infty(\mathbb{D})$ on $\mathbb{D}$ by the formula

$$\mathfrak{f}_{\mathrm{ang}}(re^{i\theta})=\mathfrak{f}(e^{i\theta}). \tag{4}$$

To avoid excessive notation, the multiplication operator determined by $\mathfrak{f}_{\mathrm{ang}}$ will be written as $B_{\mathfrak{f}}^{(\alpha)}$, but the distinction between $\mathfrak{f}$ and $\mathfrak{f}_{\mathrm{ang}}$ will be otherwise maintained.

We shall be considering the Fourier series for $\mathfrak{f}$, and our convention for the Fourier coefficients is

$$\hat{\mathfrak{f}}_n=\frac{1}{2\pi}\int_{\pi}^{\pi}\mathfrak{f}(e^{i\theta})e^{-in\theta}d\theta. \tag{5}$$

Since $L^{\infty}(\mathbb{T})\subset L^2(\mathbb{T})$, it is clear that the identity,

$$\mathfrak{f}(e^{i\theta})=\sum_{n\in\mathbb{Z}}\hat{\mathfrak{f}}_n e^{in\theta}, \tag{6a}$$

holds in $L^2(\mathbb{T})$. It is elementary to show that the functions

$$re^{i\theta}\mapsto e^{in\theta},\quad n\in\mathbb{Z},$$

form an orthonormal collection in $L^2(\mathbb{D},d\mu_\alpha)$ (but not an orthonormal basis), and so we deduce that $\mathfrak{f}_{\mathrm{ang}}\in L^2(\mathbb{D},d\mu_\alpha)$ for all $\mathfrak{f}\in L^{\infty}(\mathbb{T})$, and that

$$\mathfrak{f}_{\mathrm{ang}}(re^{i\theta})=\sum_{n\in\mathbb{Z}}\hat{\mathfrak{f}}_n e^{in\theta}, \tag{6b}$$

with this series converging in the norm topology on $L^2(\mathbb{D},d\mu_\alpha)$.

In order that our notation not cause any misunderstanding, we note that the function $\mathfrak{f}$ has a smooth harmonic extension $\mathfrak{f}_{\mathrm{ext}}:\mathbb{D}\to\mathbb{C}$ given by

$$\mathfrak{f}_{\mathrm{ext}}(re^{i\theta})=\sum_{n\in\mathbb{Z}}\hat{\mathfrak{f}}_n r^{|n|}e^{in\theta}, \tag{7}$$

but $\mathfrak{f}_{\mathrm{ext}}$ is *not* the same function as $\mathfrak{f}_{\mathrm{ang}}$—which has the unfortunate consequence of our not being able to use the known spectral theory for the harmonic case; cf. McDonald and Sundberg.[9]

In connection with the quantum phase, the exponential and angle function on $\mathbb{D}$ are particularly important. We reserve the symbol φ for the angle (argument) function $\varphi:\mathbb{D}\to\mathbb{C}$ given by

$$\varphi(re^{i\theta})=\begin{cases}\theta, & 0<r\leqslant 1,-\pi\leqslant\theta<\pi,\\ 0, & r=0.\end{cases} \tag{8}$$

If we identify $\mathbb{T}$ with the real interval $[-\pi,\pi)$, then $\varphi=\mathfrak{p}_{\mathrm{ang}}$ for $\mathfrak{p}(e^{i\theta})=\theta$. The function φ is bounded but discontinuous (across the cut).

Similarly, the complex exponential function on $\mathbb{D}$ will be taken to be given by

$$e^{\pm i\varphi}(re^{i\theta})=\begin{cases}e^{\pm i\theta}, & \text{if } 0<r<1,\\ 1, & \text{if } r=0.\end{cases} \tag{9}$$

These definitions are consistent with the complex exponentials of the values of φ.

We shall refer to an operator of the form $B_{\mathfrak{f}}^{(\alpha)}$ as a Toeplitz–Bergman angle operator—more simply, as an angle operator.

IV. MATRIX ELEMENTS FOR THE NATURAL BASIS

For the purposes of application we need the matrix elements of the angle operators: these will determine the quantum expectations and variances in the pure states we shall consider here.

When taking matrix elements $\langle g, B_{\mathfrak{f}}^{(\alpha)} f\rangle_\alpha$, because both f and g belong to $\mathcal{H}_\alpha$ and P_α is Hermitian and idempotent, the projection operator drops out of the integral, and so we have the following.

Lemma 1: For $f, g \in \mathcal{H}_\alpha$, $F \in L^\infty(\mathbb{D})$,

$$\langle g, B_F^{(\alpha)} f\rangle_\alpha = \int_{\mathbb{D}} \overline{g(w)} F(w) f(w) d\mu_\alpha(w), \tag{10}$$

and

$$\|B_F^{(\alpha)} g\|_\alpha^2 = \langle Fg, P_\alpha F g\rangle_\alpha = \int_{\mathbb{D}} \overline{F(z) g(z)} \left(\int_{\mathbb{D}} \mathcal{K}_\alpha(z,w) F(w) g(w) d\mu_\alpha(w) \right) d\mu_\alpha(w). \tag{11}$$

When we apply this lemma to the special case $f = e_n^{(\alpha)}$, $g = e_m^{(\alpha)}$ and $F = \mathfrak{f}_{\text{ang}}$, after a certain amount of calculation we can express the integral in terms of choose and beta functions. This result is basic to the application to quantum mechanics.

Proposition 2: Let $\mathfrak{f} \in L^\infty(\mathbb{T})$. The matrix elements of $B_{\mathfrak{f}}^{(\alpha)}$ with respect to the basis elements $e_n^{(\alpha)}$ and $e_m^{(\alpha)}$ on $\mathcal{H}_\alpha$ are

$$\langle e_m^{(\alpha)}, B_{\mathfrak{f}}^{(\alpha)} e_n^{(\alpha)}\rangle_\alpha = i^{m-n}(\alpha+1) \sqrt{\binom{m+\alpha+1}{m}\binom{n+\alpha+1}{n}} B\left(\frac{1}{2}(m+n)+1, \alpha+1\right) \hat{\mathfrak{f}}_{m-n}. \tag{12}$$

Proof: We have that

$$\begin{aligned}
&\langle e_m^{(\alpha)}, B_{\mathfrak{f}}^{(\alpha)}, e_n^{(\alpha)}\rangle_\alpha \\
&\quad = i^{m-n} \int \int_{\mathbb{D}} \sqrt{\binom{m+\alpha+1}{m}\binom{m+\alpha+1}{n}} \overline{z^m} \mathfrak{f}_{\text{ang}}(z) z^n d\mu_\alpha z \\
&\quad = i^{m-n} \frac{\alpha+1}{\pi} \sqrt{\binom{m+\alpha+1}{m}\binom{n+\alpha+1}{n}} \int_0^{2\pi} d\theta \int_0^1 r dr\, r^{m+n} e^{i(n-m)\theta} \mathfrak{f}(e^{i\theta}) (1-r^2)^\alpha \\
&\quad = i^{m-n} \frac{\alpha+1}{\pi} \sqrt{\binom{m+\alpha+1}{m}\binom{n+\alpha+1}{n}} \int_0^1 r^{m+n+1} (1-r^2)^\alpha dr \int_0^{2\pi} \mathfrak{f}(e^{i\theta}) e^{i(n-m)\theta} d\theta \\
&\quad = 2 i^{m-n} (\alpha+1) \sqrt{\binom{m+\alpha+1}{m}\binom{n+\alpha+1}{n}} \int_0^1 r^{m+n+1} (1-r^2)^\alpha dr \hat{\mathfrak{f}}_{m-n} \\
&\quad = i^{m-n} (\alpha+1) \sqrt{\binom{m+\alpha+1}{m}\binom{n+\alpha+1}{n}} \int_0^1 r^{(m+n)/2} (1-r)^\alpha dr \hat{\mathfrak{f}}_{m-n} \\
&\quad = i^{m-n} (\alpha+1) \sqrt{\binom{m+\alpha+1}{m}\binom{n+\alpha+1}{n}} B\left(\frac{1}{2}(m+n)+1, \alpha+1\right) \hat{\mathfrak{f}}_{m-n},
\end{aligned}$$

completing the proof. □

If we introduce the expression

$$X_{m,n}^{(\alpha)} = (\alpha+1) \sqrt{\binom{m+\alpha+1}{m}\binom{n+\alpha+1}{n}} B\left(\frac{1}{2}(m+n)+1, \alpha+1\right), \tag{13}$$

this last identity reads as

$$\langle e_m^{(\alpha)}, B_{\mathfrak{f}}^{(\alpha)} e_n^{(\alpha)}\rangle_\alpha = i^{m-n} X_{m,n}^{(\alpha)} \hat{\mathfrak{f}}_{m-n}. \tag{14}$$

Our further results depend on a close analysis of these positive real numbers $X_{m,n}^{(\alpha)}$.

We will now show that the limit $\alpha \to -1$ results in the matrix elements of the (usual) Toeplitz operator of multiplication by $\mathfrak{f}$ on $H^2(\mathbb{T})$. To this end we recall that, if P_+ is the projection operator from $L^2(\mathbb{T})$ to $H^2(\mathbb{T})$, the Toeplitz operator $\mathcal{M}(\mathfrak{f})$ with symbol $\mathfrak{f}$ is the bounded operator on $H^2(\mathbb{T})$ defined by

$$\mathcal{M}(\mathfrak{f})(F) = P_+(\mathfrak{f}F), \quad F \in H^2(\mathbb{T}). \tag{15a}$$

If χ_n is the function in $H^2(\mathbb{T})$ taking values $\chi_n(e^{i\theta}) = i^{-n}e^{in\theta}$, $\theta \in \mathbb{T}$, so that the set of vectors $\{\chi_n : n \geqslant 0\}$ forms an orthonormal basis for $H^2(\mathbb{T})$, we see that

$$\langle \chi_m, \mathcal{M}(\mathfrak{f})\chi_n \rangle = i^{m-n}\hat{\mathfrak{f}}_{m-n}. \tag{15b}$$

The precise connection is the following.

Proposition 3: For $\mathfrak{f} \in L^\infty(\mathbb{T})$ and all $m, n \geqslant 0$,

$$\lim_{\alpha \to -1} \langle e_m^{(\alpha)}, B_{\mathfrak{f}}^{(\alpha)} e_n^{(\alpha)} \rangle_\alpha = \langle \chi_m, \mathcal{M}(\mathfrak{f})\chi_n \rangle. \tag{16}$$

Proof: We rewrite $X_{m,n}^{(\alpha)}$ in a form in which the α-dependence is easier to work with; the expression we obtain will be used further on as well:

$$X_{m,n}^{(\alpha)2} = (\alpha+1)^2 \binom{m+\alpha+1}{m} \binom{n+\alpha+1}{n} B\left(\frac{1}{2}(m+n)+1, \alpha+1\right)^2$$

$$= \frac{\Gamma(m+\alpha+2)\Gamma(n+\alpha+2)\Gamma\left(\frac{1}{2}(m+n)+1\right)^2}{\Gamma(m+1)\Gamma(n+1)\Gamma\left(\frac{1}{2}(m+n)+\alpha+2\right)^2} = \frac{\Xi(m+1,n+1)}{\Xi(m+\alpha+2,n+\alpha+2)},$$

where the function $\Xi(r,s)$ is defined for $r, s \geqslant 1$ by the formula

$$\Xi(r,s) = \frac{\Gamma\left(\frac{1}{2}(r+s)^2\right)^2}{\Gamma(r)\Gamma(s)} = \prod_{k \geqslant 0} \left[1 - \left(\frac{r-s}{r+s+2k}\right)^2\right]$$

(see Gradshteyn and Ryzhik,[10] Sec. 8.325).

It follows from this that $X_{m,n}^{(\alpha)} = X_{n,m}^{(\alpha)}$ for all $m, n \geqslant 0$. Clearly, $X_{m,n}^{(\alpha)}$ is a continuous function of $\alpha \in (-1,\infty)$ for all $m, n \geqslant 0$, and $X_{m,n}^{(-1)} = 1$ for all $m, n \geqslant 0$. Consequently the limit $\alpha \to -1$ can be taken from above, and yields the indicated result. □

The expressions for the matrix elements evidently simplify when α is a positive integer. Further analysis of $X_{m,n}^{(\alpha)}$ allows us to interpolate from the integers. The precise estimate we need is the following.

Lemma 4: For all $m, n \geqslant 0$ and $\alpha \in [-1,\infty)$,

$$1 \geqslant X_{m,n}^{(\alpha)} \geqslant 1 - \frac{1}{2}(\lfloor \alpha \rfloor + 2)\left(\frac{m-n}{m+n+2}\right)^2. \tag{17}$$

Proof: We see that

$$\Xi(m+\alpha+2,n+\alpha+2) = \prod_{k \geqslant 0} \left[1 - \left(\frac{m-n}{m+n+2\alpha+4+2k}\right)^2\right],$$

from which it is clear that $\Xi(m+\alpha+2,n+\alpha+2)$ is an increasing function of $\alpha \in [-1,\infty)$, and hence it follows that $X^{(\alpha)}_{m,n}$ is a decreasing function of $\alpha \in [-1,\infty)$.

Restricting α to the non-negative integers, we obtain

$$X^{(\alpha)^2}_{m,n} = \frac{\Pi_{k\geqslant 0}\left[1-\left(\frac{m-n}{m+n+2+2k}\right)^2\right]}{\Pi_{k\geqslant 0}\left[1-\left(\frac{m-n}{m+n+2\alpha+4+2k}\right)^2\right]} = \frac{\Pi_{k\geqslant 0}\left[1-\left(\frac{m-n}{m+n+2+2k}\right)^2\right]}{\Pi_{k\geqslant \alpha+1}\left[1-\left(\frac{m-n}{m+n+2+2k}\right)^2\right]} = \prod_{k=0}^{\alpha}\left[1-\left(\frac{m-n}{m+n+2+2k}\right)^2\right],$$

and so

$$1\geqslant X^{(\alpha)^2}_{m,n}\geqslant \left[1-\left(\frac{m-n}{m+n+2}\right)^2\right]^{\alpha+1}.$$

As the quantity in braces is less than 1, we can sharpen this ''squeeze'' to

$$1\geqslant X^{(\alpha)}_{m,n}\geqslant 1-\frac{1}{2}(\alpha+1)\left(\frac{m-n}{m+n+2}\right)^2,$$

for all m, $n\geqslant 0$.

Since $X^{(\alpha)}_{m,n}$ is decreasing in α generally, extrapolation to $\alpha \in [-1,\infty)$ is immediate, and yields the estimate asserted in the lemma. □

Setting $m=n$ we see that $X^{(\alpha)}_{n,n}=1$, from which we obtain the expectation of the angle operator $B^{(\alpha)}_{\mathfrak{f}}$ in the state $e^{(\alpha)}_n$, and observe that it is identical to the expectation of the Toeplitz operator $\mathcal{M}(\mathfrak{f})$ in the state χ_n. That is, we have the following.

Proposition 5: For all $\mathfrak{f}\in L^\infty(\mathbb{T})$ and $n\geqslant 0$,

$$\mathfrak{Exp}[e^{(\alpha)}_n;B^{(\alpha)}_{\mathfrak{f}}]=\langle e^{(\alpha)}_n,B^{(\alpha)}_{\mathfrak{f}},e^{(\alpha)}_n\rangle=X^{(\alpha)}_{n,n}=\hat{\mathfrak{f}}_0=\mathfrak{Exp}[\chi_n;\mathcal{M}(\mathfrak{f})]. \tag{18}$$

The general form of the variance of $B^{(\alpha)}_{\mathfrak{f}}$ in the state $e^{(\alpha)}_n$ is as a series:

$$\mathfrak{Var}[e^{(\alpha)}_n;B^{(\alpha)}_{\mathfrak{f}}]=\mathfrak{Exp}[e^{(\alpha)}_n;B^{(\alpha)^2}_{\mathfrak{f}}]-\mathfrak{Exp}[e^{(\alpha)}_n;B^{(\alpha)}_{\mathfrak{f}}]^2 \tag{19a}$$

$$=\sum_{m\geqslant 0}|\hat{\mathfrak{f}}_{m-n}|^2X^{(\alpha)^2}_{m,n}-|\hat{\mathfrak{f}}_0|^2. \tag{19b}$$

Things become more tractable if we compare this with the variance for the corresponding Toeplitz operator. Indeed, the comparison allows us to obtain an asymptotic form for the difference.

Proposition 6: For all $\mathfrak{f}\in C^1[-\pi,\pi]$ and $n\geqslant 0$,

$$\mathfrak{Var}[\chi_n;\mathcal{M}(\mathfrak{f})]-\mathfrak{Var}[e^{(\alpha)}_n;B^{(\alpha)}_{\mathfrak{f}}]=O(1/n),\quad n\to\infty. \tag{20}$$

Proof: Starting from the known result, cf. Dubin *et al.*,[6]

$$\mathfrak{Var}[\chi_n;\mathcal{M}(\mathfrak{f})]=\sum_{m\geqslant 0}|\hat{\mathfrak{f}}_{m-n}|^2,$$

the expression

$$\begin{aligned}0&\geqslant\mathfrak{Var}[\chi_n;\mathcal{M}(\mathfrak{f})]-\mathfrak{Var}[e_n^{(\alpha)};B_{\mathfrak{f}}^{(\alpha)}]\\&=\sum_{m\geqslant 0}|\hat{\mathfrak{f}}_{m-n}|^2(1-X_{m,n}^{(\alpha)})^2\\&\geqslant\frac{1}{2}(\lfloor\alpha\rfloor+2)\sum_{m\geqslant 0}\left(\frac{(m-n)}{m+n+2}\right)^2|\hat{\mathfrak{f}}_{m-n}|^2.\end{aligned}$$

(for any $n\geqslant 0$) follows from our two-sided bound on $X_{m,n}^{(\alpha)}$.

At this point we use the assumption that $\mathfrak{f}\in C^1[-\pi,\pi]$, from which standard calculations then show the existence of a constant $K(\mathfrak{f})>0$ such that

$$|k\hat{\mathfrak{f}}_k|\geqslant K(\mathfrak{f}),\quad k\in\mathbb{Z}.$$

This implies that

$$0\leqslant\mathfrak{Var}[\chi_n;\mathcal{M}(\mathfrak{f})^2]-\mathfrak{Var}[e_n^{(\alpha)};B_{\mathfrak{f}}^{(\alpha)^2}]\geqslant\frac{1}{2}(\lfloor\alpha\rfloor+2)k(\mathfrak{f})^2\sum_{m\geqslant n+2}m^{-2}\leqslant\lfloor\alpha\rfloor+2K(\mathfrak{f})^2/2(n+1),$$

for all $n\geqslant 0$. As the right hand side is $O(1/n)$, the proof is complete.

Now we are in a position to use known results for the Toeplitz operators to obtain the asymptotic forms for $B_{\varphi}^{(\alpha)}$, $B_C^{(\alpha)}$ and $B_S^{(\alpha)}$, where $C(e^{i\theta})=\cos\theta$ and $S(e^{i\theta})=\sin\theta$. The latter two operators are preferred to the exponentials because they are (bounded) Hermitian. (Cf. Dubin *et al.*[6] for the relevant Toeplitz asymptotics.) □

Proposition 7: For the expectation and variance of $B_{\varphi}^{(\alpha)}$,

$$\mathfrak{Exp}[e_n^{(\alpha)};B_{\varphi}^{(\alpha)}]=0,\quad n\geqslant 0,\tag{21a}$$

$$\mathfrak{Var}[e_n^{(\alpha)};B_{\varphi}^{(\alpha)}]=\pi^2/3+O(1/n),\quad n\to\infty.\tag{21b}$$

For the trigonometric angle operators,

$$\mathfrak{Exp}[e_n^{(\alpha)};B_C^{(\alpha)}]=\mathfrak{Exp}[e_n^{(\alpha)};B_S^{(\alpha)}]=0,\quad n\geqslant 0,\tag{22a}$$

$$\mathfrak{Var}[e_n^{(\alpha)};B_C^{(\alpha)}]=\mathfrak{Var}[e_n^{(\alpha)};B_S^{(\alpha)}]=1/2+O(1/n^2),\tag{22b}$$

as $n\to\infty$. Taking the limit

$$\lim_{n\to\infty}\mathfrak{Var}[e_n^{(\alpha)};B_{\varphi}^{(\alpha)}]=\pi^2/3,\tag{23}$$

$$\lim_{n\to\infty}\mathfrak{Var}[e_n^{(\alpha)};B_C^{(\alpha)}]=\lim_{n\to\infty}\mathfrak{Var}[e_n^{(\alpha)};B_S^{(\alpha)}]=1/2.\tag{24}$$

The sharpening of the order from $O(1/n)$ to $O(1/n^2)$ results from the fact that C and S have only a finite number of nonzero Fourier coefficients—we omit the details.

These limiting results for $n\to\infty$ are in accord with the feeling of many physicists concerning the distribution law phase operators should obey in the ''classical'' limit, here represented by $n\to\infty$. For a discussion of this point, see Dubin *et al.*[6]

V. ANGLE OPERATORS AND BERGMAN COHERENT STATES

In all of the Hilbert spaces on which the various angle operators (of quantum phase) act, there are distinguished states known as *coherent*. These states characteristically act as classically as the laws of quantum mechanics permit. For example, the coherent states in the Schrödinger representation, they are states of minimal uncertainty (in position and momentum).

We will not need the general theory, and refer the reader to the excellent review of Ali, Antoine, Gazeau, and Mueller,[11] for a mathematical account. It suffices for our purposes simply to define the coherent states for $\mathcal{H}_\alpha$ as

$$\Psi_\zeta^{(\alpha)} = e^{-|\zeta|^2/2} \sum_{n\geqslant 0} \overline{\zeta^n} e_n^{(\alpha)} / \sqrt{n!}. \tag{25}$$

Here $\zeta \in \mathbb{C}$ is a parameter labelling the family of coherent states.

This family forms a weak overcomplete decomposition of the identity in the sense that, for all $f,g \in \mathcal{H}_\alpha$,

$$\int_{\mathbb{C}} \langle g, \Psi_\zeta^{(\alpha)} \rangle_\alpha \langle \Psi_\zeta^{(\alpha)}, f \rangle_\alpha dA(\zeta) = \langle g, f \rangle_\alpha . \tag{26}$$

The ''classical'' region for these coherent states is obtained from restricting ζ by $\zeta = -iR/\sqrt{2}$ and taking R large. For this choice of ζ we simplify the notation by writing $\Psi^{(\alpha,R)}$ for the vector in question, in which case

$$\Psi^{(\alpha,R)} = e^{-R^2/4} \sum_{n\geqslant 0} i^n R^n e_n^{(\alpha)} / \sqrt{2^n n!}. \tag{27}$$

By substituting our result for the matrix elements with respect to the $e_n^{(\alpha)}$, we obtain the expectation of Bergman angle operators with respect to these states.

Proposition 8: For $\mathfrak{f} \in L^\infty(\mathbb{T})$ and $R>0$,

$$\begin{aligned} \mathfrak{Expt}[\Psi^{(\alpha,R)}; B_\mathfrak{f}^{(\alpha)}] &= e^{-R^2/2} \sum_{m,n\geqslant 0} i^{n-m} R^{n+m} \langle e_m^{(\alpha)}, B_\mathfrak{f}^{(\alpha)} e_n^{(\alpha)} \rangle_\alpha / \sqrt{2^{m+n} m! n!} \\ &= e^{-R^2/2} \sum_{m,n\geqslant 0} R^{m+n} X_{m,n}^{(\alpha)} \hat{\mathfrak{f}}_{m-n} / \sqrt{2^{m+n} m! n!}. \end{aligned} \tag{28}$$

If $\mathfrak{f}$ is odd on $[-\pi, \pi]$, this expectation is zero, and so, in particular,

$$\mathfrak{Expt}[\Psi^{(\alpha,R)}; B_\varphi^{(\alpha)}] = 0. \tag{29}$$

Considering only $B_\varphi^{(\alpha)}$, its variance in these states reduces to

$$\mathfrak{Var}[\Psi^{(\alpha,R)}; B_\varphi^{(\alpha)}] = \| B_\varphi^{(\alpha)} \Psi^{(\alpha,R)} \|_\alpha^2. \tag{30}$$

This can be written as a series with terms containing the $X_{m,n}^{(\alpha)}$, but that is not very illuminating. More information is obtained from the large R asymptotic expression, but we will not attempt to compute this directly. Instead, we shall carry over a technique used in Dubin *et al.*[6] to obtain asymptotics for Toeplitz operators with respect to the coherent states on $H^2(\mathbb{T})$.

The first step is to note that the variance is smaller than the expression

$$\| \varphi \cdot \Psi^{(\alpha,R)} \|_\alpha^2 = \langle \Psi^{(\alpha,R)}, B_{|\varphi|^2}^{(\alpha)} \Psi^{(\alpha,R)} \rangle_\alpha = e^{-R^2/2} \sum_{m,n\geqslant 0} R^{m+n} X_{m,n}^{(\alpha)} (|\varphi|^2)\hat{}_{m-n} / \sqrt{2^{m+n} m! n!}.$$

This can be successfully compared to the quantity

$$\Phi(R)=e^{-R^2/2}\sum_{m,n\geqslant 0} R^{m+n}(|\Phi|^2)^{\wedge}_{m-n}/\sqrt{2^{m+n}m!n!}, \tag{31}$$

which is the expectation of the Toeplitz operator with symbol $\mathfrak{p}^2(e^{i\theta})=\theta^2$ with respect to a certain Hardy space coherent state, the details of which will not be needed here.

The asymptotic form for $\Phi(R)$ is[6]

$$\Phi(R)=1/(2R^2)+O(1/R^3). \tag{32}$$

The result is the following.

Proposition 9: The estimate

$$|\Phi(R)-\|\varphi\cdot\Psi^{(\alpha,R)}\|_\alpha^2|\leqslant C/R, \tag{33}$$

holds for some constant C. Hence

$$\mathfrak{Var}[\Psi^{(\alpha,R)};B_\varphi^{(\alpha)}]=O(1/R),\ \text{ as }\ R\to\infty. \tag{34}$$

From our work with Toeplitz operators, we expect that this result could be sharpened to the asymptotic order $O(R^{-2})$.

Proof: Using our estimate for $X_{m,n}^{(\alpha)}$,

$$\begin{aligned}|\Phi(R)-\|\varphi\cdot\Psi^{(\alpha,R)}\|_\alpha^2|&\leqslant e^{-R^2/2}\sum_{m,n\geqslant 0} R^{m+n}(1-X_{m,n}^{(\alpha)})|(|\varphi|^2)^{\wedge}_{m-n}|/\sqrt{2^{m+n}m!n!}\\ &\leqslant\frac{1}{2}(\lfloor\alpha\rfloor+2)e^{-R^2/2}\sum_{m,n\geqslant 0} R^{m+n}\left(\frac{m-n}{m+n+2}\right)^2|(|\varphi|^2)^{\wedge}_{m-n}|/\sqrt{2^{m+n}m!n!}.\end{aligned}$$

The Fourier coefficients of the function $\mathfrak{p}^2(e^{i\theta})=\theta^2$ are

$$(\mathfrak{p}^2)\hat{}_k=\begin{cases}2(-1)^k/k^2, & k\neq 0,\\ \pi^2/3, & k=0.\end{cases}$$

Substituting this back, then applying some manipulations to the result,

$$\begin{aligned}|\Phi(R)-\|\varphi\cdot\Psi^{(\alpha,R)}\|_\alpha^2&\leqslant(\lfloor\alpha\rfloor+2)e^{-R^2/2}\sum_{m\neq n}\frac{R^{m+n}}{\sqrt{2^{m+n}m!n!}}\frac{1}{(m+n+2)^2}\\ &\leqslant(\lfloor\alpha\rfloor+2)e^{-R^2/2}\sum_{m\neq n}\frac{R^{m+n}}{\sqrt{2^{m+n}m!(n+1)!}}\frac{1}{(m+n+2)^{3/2}}\\ &\leqslant(\lfloor\alpha\rfloor+2)e^{-R^2/2}\left(\sum_{m\neq n}\frac{R^{2(m+n)}}{2^{m+n}m!(n+1)!}\right)^{1/2}\left(\sum_{m\neq n}\frac{1}{(m+n+2)^3}\right)^{1/2}\leqslant C/R,\end{aligned}$$

for some constant C. With the asymptotic form for $\Phi(R)$ given above, the variance is seen to be as asserted. □

VI. SUMMARY

The angle operators $B_{\mathfrak{f}}^{(\alpha)}$, and in particular $B_\varphi^{(\alpha)}$, $B_{e^{\pm i\varphi}}^{(\alpha)}$, play the same role in relation to quantum phase theory for $\mathcal{H}_\alpha$ as do the Toeplitz and Bargmann–Segal operators do on their respective Hilbert spaces. The connection to physics relies on the fact that these Hilbert spaces carry (unitarily equivalent) irreducible and gauge invariant representations of the canonical commutation relation for one degree of freedom. The asymptotic variance of the operators with

symbol φ in the natural basis all have the limit $\pi^2/3$. Whether or not this is a convincing argument for the relevance of these operators for the quantum phase is left to the reader to decide: it is often taken so.

There are a number of mathematical questions left unanswered by this work. First, there is the technical question of sharpening the asymptotic order of the variance for $B_{\varphi}^{(\alpha)}$ for the coherent state family. Next, we have not considered all the families of states usually taken to be interesting for the quantum phase. Notably, we have omitted the family

$$\xi_{s;\beta}^{(\alpha)}=\frac{1}{\sqrt{s+1}}\sum_{n=0}^{s} e^{in\beta}e_n^{(\alpha)}, \tag{35}$$

which span the $s+1$-dimensional subspace of $\mathcal{H}_\alpha$ with the alternate basis $\{e^{(\alpha)},\ldots,e_s^{(\alpha)}\}$. Since

$$e^{-i\gamma N}\xi_{s;\beta}^{(\alpha)}=\xi_{s;\beta+\gamma}^{(\alpha)},$$

these states can be interpreted as being uniformly distributed over gauge—though some physicists identify gauge with quantum phase, which we do not believe to be justified. As all sums are finite, there is no particular difficulty in filling this gap in our asymptotic analysis.

There is the question of finding an explicit form for the raising and lowering operators acting on $\mathcal{H}_\alpha$. This is not essential for the quantum phase, but it would be useful to know nonetheless.

Most worrying is that we have no results at all for the spectrum of the $B_{\mathrm{f}}^{(\alpha)}$. This is a problem for Toeplitz–Bergman operators with symbols which do not happen to be special, e.g., harmonic, and any spectral results would be of interest to pure mathematicians as well.

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Subharmonic projections for a quantum Markov semigroup

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This article introduces a concept of subharmonic projections for a quantum Markov semigroup, in view of characterizing the support projection of a stationary state in terms of the semigroup generator. These results, together with those of our previous article [J. Math. Phys. **42**, 1296 (2001)], lead to a method for proving the existence of *faithful stationary states*. This is often crucial in the analysis of ergodic properties of quantum Markov semigroups. The method is illustrated by applications to physical models. © *2002 American Institute of Physics.*
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I. INTRODUCTION

This article continues the investigation on normal stationary states initiated in Ref. 1. Our main goal is to characterize the support projection of a stationary state under the action of a quantum Markov semigroup. This is an important problem in several respects, which is solved here for the first time, in terms of the semigroup generator.

The qualitative analysis of a quantum dynamics usually enquiries whether the evolution eventually goes in the steady state regime. This is information primarily carried by the support projection of a stationary state.

We recall that a normal state ω is called *faithful* if $\omega(a)=0$, for a positive a, implies that $a=0$. In this case its support projection coincides with the identity. The existence of a normal faithful stationary state is often assumed as a crucial hypothesis in the analysis of the ergodic behavior of a quantum Markov semigroup (see, e.g., Refs. 2–4).

The support of a normal stationary state here is characterized through subharmonic projections (see Definition II.1). This name is borrowed from potential and classical Markov processes theories (see Refs. 5 and 6). In the latter, the absence of nontrivial subharmonic projections is equivalent to the concept of *irreducibility*, which roughly means that the dynamics cannot end up eventually in a smaller subspace. In this article (see Corollary III.1 and the related discussion), we compare this notion with its operator-algebraic counterpart (see Refs. 7 and 8).

The article is organized as follows. The next section characterizes the support projection of a stationary state on a semi-finite von Neumann algebra. Then we analyze subharmonic projections for semigroups on the algebra of all linear bounded operators on a given Hilbert space. This is further specialized to a class of quantum Markov semigroups with unbounded infinitesimal generators of Lindblad type. The main result (Theorem III.1) shows that, in this case, the support projection of a stationary state determines an invariant subspace for the coefficient operators of the infinitesimal generator. A full description of invariant subspaces for a family of operators, on an infinite dimensional space, is usually a hard mathematical problem (see Ref. 9). However, this article also provides some useful tools (Theorems IV.1 and IV.2) for actually solving this problem. The last section is devoted to physical applications[10,11] illustrating our method.

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II. THE SUPPORT OF A STATIONARY STATE

Let there be given a semifinite von Neumann algebra $\mathfrak{A}$ of operators over a complex separable Hilbert space $\mathfrak{h}$, endowed with a trace $\mathrm{tr}(\cdot)$ and a unit $\mathbf{1}$. A quantum Markov semigroup (QMS) $\mathcal{T}=(\mathcal{T}_t)_{t\geqslant 0}$ on $\mathfrak{A}$ is a w^*-continuous semigroup of normal, completely positive maps preserving $\mathbf{1}$. Its generator is the operator $\mathcal{L}$ whose domain $D(\mathcal{L})$ is the vector space of all elements $a\in\mathfrak{A}$ for which the w^*-limit of $t^{-1}(\mathcal{T}_t(a)-a)$ exists. For $a\in D(\mathcal{L})$, $\mathcal{L}(a)$ is defined as the limit above.

Throughout this article we will be concerned only with normal states; moreover, we will often identify such states with their density matrices. The *support projection* of a state ρ is the orthogonal projection over the closure of its range. An *invariant (or stationary) state* ρ is characterized through the equation $\mathrm{tr}(\rho\mathcal{T}_t(a))=\mathrm{tr}(\rho a)=\mathrm{tr}(\mathcal{T}_{*t}(\rho)a)$ for any $a\in\mathfrak{A}$, $t\geqslant 0$, where $\mathcal{T}_*$ denotes the predual semigroup.

Definition II.1: A positive operator $a\in\mathfrak{A}$ is subharmonic (resp. superharmonic, resp. harmonic*) for the semigroup if $\mathcal{T}_t(a)\geqslant a$* (resp. $\mathcal{T}_t(a)\leqslant a$, resp $\mathcal{T}_t(a)=a$), *for all $t\geqslant 0$.*

Subharmonic functions play a fundamental role in the potential theory of classical Markov semigroups (see, for instance, Ref. 5). They allow us to establish useful criteria for deciding whether the dynamics scatters or eventually remains in a bounded region. In our framework, we will start by showing a relation between invariant states and subharmonic projections.

Theorem II.1: *The support projection of a normal stationary state for a quantum Markov semigroup is subharmonic.*

This theorem has important consequences like the following proposition.

Proposition II.1: For any quantum Markov semigroup $\mathcal{T}$ the following are equivalent:

(a) *p is subharmonic for $\mathcal{T}_t(\cdot)$, for any $t\geqslant 0$,*
(b) *the subalgebra $p^\perp\mathfrak{A}p^\perp$ is invariant under $\mathcal{T}_t(\cdot)$, for all $t\geqslant 0$, and*
(c) *for any normal state ρ such that $p\rho p=\rho$, we have $\mathrm{tr}(\rho\mathcal{T}_t(p^\perp))=0$, for all $t\geqslant 0$.*

Postponing the proof, we introduce a definition motivated by this result.

Definition II.2: We say that a quantum Markov semigroup is irreducible if there is no nontrivial subharmonic projection.

This notion will be compared with that of *topological irreducibility* (see Ref. 7, Definition 2.3.7) in the next section.

We now proceed to the proofs, starting with a lemma of frequent use in this article.

Lemma II.1: Let p be a projection of the von Neumann algebra $\mathfrak{A}$, and $x\in\mathfrak{A}$ a positive element. If $pxp=0$, then $p^\perp xp=pxp^\perp=0$.

Proof: Suppose $\mathfrak{A}\subseteq\mathcal{B}(\mathfrak{h})$ and let $u,v\in\mathfrak{h}$ with $pu=u$, $pv=0$. Since x is positive, $\langle zu+v,x(zu+v)\rangle=2\Re(z\langle v,xu\rangle)+\langle v,xv\rangle$ is positive for every $z\in\mathbb{C}$. Therefore $\langle v,xu\rangle$ must vanish and the conclusion readily follows. □

Proof (of Theorem II.1): Let p be the support projection of a normal stationary state ρ of $(\mathcal{T}_t)_{t\geqslant 0}$. Thus $\rho p=p\rho=\rho$. Fix $t\geqslant 0$. We first notice that $p\mathcal{T}_t(p)p\leqslant p$, since $p\leqslant\mathbf{1}$. Therefore, $\mathrm{tr}(\rho(p-p\mathcal{T}_t(p)p))=\mathrm{tr}(\rho(p-\mathcal{T}_t(p)))=0$, and, since ρ is faithful on the subalgebra $p\mathfrak{A}p$, it follows

$$p\mathcal{T}_t(p)p=p. \tag{1}$$

On the other hand, $p\mathcal{T}_t(p^\perp)p=p\mathcal{T}_t(\mathbf{1})p-p\mathcal{T}_t(p)p=p-p=0$. Thus, since $\mathcal{T}_t(p^\perp)$ is positive and $\mathcal{T}_t(p)=\mathbf{1}-\mathcal{T}_t(p^\perp)$, Lemma II.1 yields $p\mathcal{T}_t(p^\perp)p^\perp=0=p^\perp\mathcal{T}_t(p^\perp)p$. This identity, together with (1), lead to $\mathcal{T}_t(p)=p+p^\perp\mathcal{T}_t(p)p^\perp$, showing that p is subharmonic. □

Proof (of Proposition II.1): Assume that condition (a) holds. Then (1) yields $p\mathcal{T}_t(p^\perp)p=p\mathcal{T}_t(\mathbf{1})p-p\mathcal{T}_t(p)p=0$. Therefore, for any positive $x\in p^\perp\mathfrak{A}p^\perp$ it follows $p\mathcal{T}_t(x)p=0$ since $0\leqslant p\mathcal{T}_t(x)p\leqslant\|x\|p\mathcal{T}_t(p^\perp)p=0$. From Lemma II.1, $p\mathcal{T}_t(x)p^\perp=p^\perp\mathcal{T}_t(x)p=0$, since $\mathcal{T}_t(x)$ is positive. Thus $\mathcal{T}_t(x)=p^\perp\mathcal{T}_t(x)p^\perp\in p^\perp\mathfrak{A}p^\perp$. The same conclusion holds for any arbitrary $x\in p^\perp\mathfrak{A}p^\perp$ since it is a linear combination of four positive elements of $p^\perp\mathfrak{A}p^\perp$.

We now prove that (b) implies (c). By hypothesis, for any $x\in p^\perp\mathfrak{A}p^\perp$, it holds $\mathcal{T}_t(x)=p^\perp yp^\perp$ for some $y\in\mathfrak{A}$. Clearly, the above equality yields $y=\mathcal{T}_t(x)$ since $\langle v,\mathcal{T}_t(x)u\rangle=\langle v,yu\rangle$

for all vectors u and v belonging to the range of $p^\perp$. Therefore, $\mathcal{T}_t(x)=p^\perp\mathcal{T}_t(x)p^\perp$. In particular, $\mathcal{T}_t(p^\perp)=p^\perp\mathcal{T}_t(p^\perp)p^\perp$. Hence, given a state ρ such that $p\rho=\rho p=\rho$, we have $p^\perp\rho=\rho p^\perp=0$ which yields $\mathrm{tr}(\rho\mathcal{T}_t(p^\perp))=0$.

Finally, (c) implies (a). From (c) we obtain $\mathrm{tr}(\rho p\mathcal{T}_t(p^\perp)p)=0$, thus $p\mathcal{T}_t(p^\perp)p=0$. As a result, by Lemma II.1, $\mathcal{T}_t(p^\perp)=p^\perp\mathcal{T}_t(p^\perp)p^\perp\leqslant p^\perp$, which gives $\mathcal{T}_t(p)=\mathcal{T}_t(\mathbf{1}-p^\perp)\geqslant p$. □

III. SUBHARMONIC PROJECTIONS. THE CASE $\mathfrak{A}=\mathcal{B}(\mathfrak{h})$

We now concentrate on the case $\mathfrak{A}=\mathcal{B}(\mathfrak{h})$. From now on, the QMS is the minimal obtained from an unbounded generator given as a quadratic form (generalizing the representations given by Gorini, Kossakowsky, and Sudharshan,[12] and Lindblad[13] and extended by Davies[14]):

$$\mathfrak{L}(x)[v,u]=\langle Gv,xu\rangle+\sum_{\ell\geqslant 1}\langle L_\ell v,xL_\ell u\rangle+\langle v,xGu\rangle,$$

$(x\in\mathcal{B}(\mathfrak{h}),v,u\in D(G))$, under the following hypotheses:

(1) **(H-min)** The operator G is the generator of a strongly continuous contraction semigroup $(P_t)_{t\geqslant 0}$ on $\mathfrak{h}$. The domain $D(L_\ell)$ of each operator L_ℓ contains the domain $D(G)$ of G and $\mathfrak{L}(\mathbf{1})[v,u]=0$, for all $u,v\in D(G)$.
(2) **(H-Markov)** $\mathcal{T}_t(\mathbf{1})=\mathbf{1}$, for all $t\geqslant 0$.

Thus, for all $x\in\mathcal{B}(\mathfrak{h})$, the quadratic form $\mathfrak{L}(x)$ is defined over the domain $D(G)\times D(G)$.

The main result of this section is the following characterization of subharmonic projections.

Theorem III.1: *Assume* **(H-min)** *and* **(H-Markov)**. *A projection p is subharmonic for $\mathcal{T}$ if and only if the range $R(p)$ of p is invariant for the operators P_t $(t\geqslant 0)$ and*

$$L_\ell u=pL_\ell u, \tag{2}$$

for all $u\in D(G)\cap R(p)$, $\ell\geqslant 1$.

If G and the L_ℓ's are bounded, Theorem III.1 says that a projection p is subharmonic if and only if its range $R(p)$ is an invariant subspace for these operators. In the general case, this needs to be handled more carefully as shows the following lemma.

Lemma III.1: Let $(P_t)_{t\geqslant 0}$ be the semigroup generated by G. A closed subspace $R(p)$ is invariant for the operators P_t $(t\geqslant 0)$ if and only if $D(G)\cap R(p)$ is dense in $R(p)$, $(\lambda-G)(D(G)\cap R(p))=R(p)$ for any $\lambda>0$ and $Gu=pGu$ for any $u\in D(G)\cap R(p)$.

Remark: In other words p is invariant for the operators $P_t(t\geqslant 0)$ if and only if the restriction of G to $R(p)$ is the infinitesimal generator of the semigroup $(P_{t|R(p)})_{t\geqslant 0}$ on $R(p)$.

Proof: Suppose first that $R(p)$ is invariant for the operators P_t $(t\geqslant 0)$. Then $R(p)$ is also invariant for the resolvent operators $R(\lambda;G)$ $(\lambda>0)$. Therefore, for each $u\in R(p)$, the vector $u_\lambda=\lambda R(\lambda;G)u$ belongs to $D(G)\cap R(p)$ and, by the well-known properties of the Yosida approximations, u_λ converges to u as λ goes to infinity. Thus $D(G)\cap R(p)$ is dense in $R(p)$. Moreover, for any $u\in D(G)\cap R(p)$ we have $t^{-1}(P_tu-u)=t^{-1}(P_tpu-pu)=pt^{-1}(P_tu-u)$. Therefore, letting $t\to 0$, we obtain $Gu=pGu$.

Finally, since $R(p)=(\lambda-G)R(\lambda;G)R(p)$ and $R(\lambda;G)(R(p))\subseteq D(G)\cap R(p)$,

$$R(p)\subseteq(\lambda-G)(D(G)\cap R(p))=p(\lambda-G)(D(G)\cap R(p))\subseteq R(p).$$

It follows that $(\lambda-G)(D(G)\cap R(p))=R(p)$.

Conversely, since $R(\lambda;G)R(p)=R(\lambda;G)(\lambda-G)(D(G)\cap R(p))=D(G)\cap R(p)$, the closed subspace $R(p)$ is invariant for $R(\lambda;G)$ for any $\lambda>0$. From the equality

$$P_t=\text{strong}-\lim_{n\to\infty}(nt^{-1}R(nt^{-1};G))^n, \tag{3}$$

(Ref. 15, Cor. 5.45, p. 92) it follows that $R(p)$ is P_t-invariant. □

To proceed with the proof of Theorem III.1 we recall some notations and well-known facts on the minimal QMS (see, e.g., Refs. 16, 1, and 17). Under **(H-min)** and **(H-Markov)**, for any $x \in \mathcal{B}(\mathfrak{h})$, $(\mathcal{T}_t(x))_{t\geqslant 0}$ is the unique w^*-continuous family of operators in $\mathfrak{h}$ such that, for all $u,v \in D(G)$, any of the equivalent equations below holds:

$$\langle v,\mathcal{T}_t(x)u\rangle=\langle P_tv,P_tu\rangle+\sum_{\ell\geqslant 1}\int_0^t\langle L_\ell P_{t-s}v,\mathcal{T}_t(x)L_\ell P_{t-s}u\rangle ds, \tag{4}$$

$$\langle v,\mathcal{T}_t(x)u\rangle=\langle v,xu\rangle+\int_0^t\langle v,\pounds(\mathcal{T}_s(x))u\rangle ds. \tag{5}$$

Moreover, the solution to (4) is obtained as the limit of an approximating sequence $(\mathcal{T}^{(n)})_{n\geqslant 0}$ defined recursively by $\mathcal{T}_t^{(0)}(x)=P_t^*xP_t$ and

$$\langle u,\mathcal{T}_t^{(n+1)}(x)u\rangle=\langle P_tu,xP_tu\rangle+\sum_{\ell\geqslant 1}\int_0^t\langle L_\ell P_{t-s}u,\mathcal{T}_t^{(n)}(x)L_\ell P_{t-s}u\rangle ds,$$

for any $x\in\mathcal{B}(\mathfrak{h})$ and $u\in D(G)$. Given a positive element $x\in\mathcal{B}(\mathfrak{h})$ the above sequence is increasing with n and this allows us to define $\mathcal{T}_t(x)=\sup_n\mathcal{T}_t^{(n)}(x)$, which is the well-known *minimal quantum Markov semigroup* (see, for instance, Ref. 16).

Proof (of Theorem III.1): We start assuming that p is subharmonic, thus $\mathcal{T}_t(p)\geqslant p$ for all $t\geqslant 0$. From Eq. (4) we obtain $p^\perp\geqslant\mathcal{T}_t(p^\perp)\geqslant P_t^*p^\perp P_t$. Therefore, for all $u\in R(p)$ it holds $\langle u,P_t^*p^\perp P_tu\rangle=\|p^\perp P_tu\|^2=0$, that is, $p^\perp P_tp=0$. Thus $P_tp=pP_tp$, for all $t\geqslant 0$, i.e., the range $R(p)$ of p is invariant for the operators P_t $(t\geqslant 0)$. In addition, Eq. (5) yields

$$\int_0^t\left(\langle Gu,\mathcal{T}_s(p^\perp)u\rangle+\sum_{\ell\geqslant 1}\langle L_\ell u,\mathcal{T}_s(p^\perp)L_\ell u\rangle+\langle u,\mathcal{T}_s(p^\perp)Gu\rangle\right)ds\leqslant 0,$$

for all $t\geqslant 0$ and all $u\in D(G)\cap R(p)$. As a result, computing the derivative at 0 of the above equation, we obtain $\langle Gu,p^\perp u\rangle+\Sigma_{\ell\geqslant 1}\langle L_\ell u,p^\perp L_\ell u\rangle+\langle u,p^\perp Gu\rangle\leqslant 0$. Now, $pu=u$ implies $p^\perp Gu=0$. The above inequality yields $\Sigma_{\ell\geqslant 1}\|p^\perp L_\ell pu\|^2\leqslant 0$, that is, $p^\perp L_\ell pu=0$ and (2) follows.

Conversely, we assume condition (2). We will prove that p is subharmonic by an induction argument which relays on the sequence $(\mathcal{T}^{(n)})_{n\geqslant 0}$ used in the construction of $\mathcal{T}$. First, p is subharmonic for $\mathcal{T}^{(0)}$ since $\mathcal{T}_t^{(0)}(p^\perp)=P_t^*p^\perp P_t=p^\perp P_t^*p^\perp P_tp^\perp\leqslant p^\perp$. Second, assume that p is subharmonic for $\mathcal{T}^{(n)}$. We prove that it is subharmonic for $\mathcal{T}^{(n+1)}$, too. Indeed, for all $u\in D(G)\cap R(p)$, the definition of $\mathcal{T}^{(n+1)}$ and the induction hypothesis yield

$$\langle u,\mathcal{T}_t^{(n+1)}(p^\perp)u\rangle\leqslant\langle u,P_t^*p^\perp P_tu\rangle+\sum_{\ell\geqslant 1}\int_0^t\langle L_\ell P_{t-s}u,p^\perp L_\ell P_{t-s}u\rangle ds=0,$$

for any $t\geqslant 0$. It follows that $p\mathcal{T}_t^{(n+1)}(p^\perp)p=0$ and Lemma II.1 implies $p^\perp\mathcal{T}_t^{(n+1)}(p^\perp)p=p\mathcal{T}_t^{(n+1)}(p^\perp)p^\perp=0$. Therefore, $\mathcal{T}_t^{(n+1)}(p^\perp)\leqslant p^\perp$, for all $t\geqslant 0$ and p is subharmonic for $\mathcal{T}^{(n)}$. Hence, p is subharmonic for the minimal semigroup $\mathcal{T}$ and the proof is complete. □

In what follows, given a set $\mathfrak{M}$ of bounded operators on $\mathfrak{h}$, we denote $\mathfrak{M}'$ the commutator algebra. We recall that $\mathfrak{M}$ is called *topologically irreducible* if $\mathfrak{M}'=\mathbb{C}\mathbf{1}$ (see Ref. 7, Definition 2.3.7). This is equivalent to saying that the only closed subspaces of $\mathfrak{h}$ which are invariant under the action of $\mathcal{M}$ are the trivial subspaces $\{0\}$ and $\mathfrak{h}$.

If G and the L_ℓ's are bounded operators, Theorem III.1 implies that *$\mathcal{T}$ is irreducible if and only if $\{G,L_\ell;\ell\geqslant 1\}$ is topologically irreducible.* If G and the L_ℓ's satisfy only **(H-min)**, we can prove the following:

Corollary III.1: Assume that **(H-min)** and **(H-Markov)** *hold and denote by $\mathcal{T}$ the related minimal quantum Markov semigroup. Let*

$$\mathfrak{M}=\{L_\ell\in\mathcal{B}(\mathfrak{h}):\ell\geqslant 1,\exists m\geqslant 1 s.t. L_m=L_\ell^*\}.$$

Then every subharmonic projection belongs to $\mathfrak{M}'$.

If $\mathfrak{M}$ *is topologically irreducible, then* $\mathcal{T}$ *is an irreducible semigroup.*

Moreover, if $\mathcal{T}$ *admits a normal stationary state* ρ*, then* ρ *is the unique normal faithful stationary state and* $\mathcal{T}_{*t}(\sigma)$ *converges in trace-norm to* ρ *as* t *goes to* ∞*, for any normal state* σ.

Proof: Let p be a subharmonic projection. Clearly, by (2) p satisfies $L_\ell p=pL_\ell p$, for all $L_\ell\in\mathfrak{M}$. In addition, if $L_{m*}=L_\ell$, then $pL_\ell=(L_\ell^* p^*)^*=(L_m p)^*=(pL_m p)^*=pL_\ell p=L_\ell p$. This shows that $p\in\mathfrak{M}'$. In particular, if $\mathfrak{M}'$ is trivial, then the semigroup is irreducible.

If $\mathcal{T}$ has a normal stationary state ρ, then Theorems III.1 and II.1 imply that its support projection coincides with the identity, so that this state is faithful.

Now, given any normal state σ, $\mathcal{T}_{*t}(\sigma)$ satisfies $\mathrm{tr}(\mathcal{T}_{*t}(\sigma)x)\to\mathrm{tr}(\rho x)$, by Theorem 2.1 in Ref. 4. Suppose that ρ_0 is another normal stationary state. Then $\mathrm{tr}(\rho_0 x)=\mathrm{tr}(\mathcal{T}_{*t}(\rho_0)x)\to\mathrm{tr}(\rho x)$, for all $x\in\mathcal{B}(\mathfrak{h})$. Then $\rho_0=\rho$.

Finally, notice that for each $t\geqslant 0$ both $\mathcal{T}_{*t}(\sigma)$ and ρ have unit trace norm. This fact, together with the weak convergence of the family $(\mathcal{T}_{*t}(\sigma))_{t\geqslant 0}$, finally implies its trace-norm convergence towards ρ. □

IV. INVARIANT SUBSPACES

The problem of finding *all* the invariant subspaces for a given bounded operator on an infinite dimensional Hilbert space is far from being simple (see, e.g., Ref. 9). Therefore, it is so far unclear how (2) will actually be useful for an unbounded L_ℓ. To overcome this difficulty, we start from the operators P_t and prove that any subharmonic projection is invariant also for semigroups generated by suitable perturbations of G by means of the L_ℓ's.

The first theorem is inspired by Theorem 3.2, on p. 81 of Ref. 15.

Theorem IV.1: *Let* G *be the generator of the strongly continuous contraction semigroup* P *and let* B *an operator on* $\mathfrak{h}$ *such that*

(i) $D(B)\supseteq D(G)$,
(ii) $\|Bu\|\leqslant\alpha\|Gu\|+\beta\|u\|$, *for* $u\in D(G)$, *with* $0\leqslant\alpha<1$ *and* $\beta\geqslant 0$, *and*
(iii) $G+rB$ *is dissipative for each* $r\in[0,1]$.

Then, $G+rB$ *generates a strongly continuous contraction semigroup* $P^{(r)}$.

Moreover, if the range $R(p)$ *of a projection* p *is invariant for the operators* P_t *and* $B(D(G)\cap R(p))\subseteq R(p)$*, then* $R(p)$ *is also invariant for the operators* $P_t^{(r)}$*, for each* $r\in[0,1]$.

Proof: We prove that there exists a $\delta>0$, depending only on α and β, such that if $G+r_0B$ is maximal dissipative (hence its generates a strongly continuous contraction semigroup by the Lumer–Phillips' theorem) and $R(p)$ is invariant for the operators $P_t^{(r_0)}$, then the same conclusion holds for $G+rB$ for $r\in[r_0-\delta,r_0+\delta]\cap[0,1]$. The result follows since every point of $[0,1]$ can be reached from 0 in a finite number of steps of length δ.

Since $G+r_0B$ is maximal dissipative, then $\lambda\mathbf{1}-(G+r_0B)$ is invertible for every $\lambda\geqslant 1$ and its inverse $I(\lambda,r_0)$ satisfies $\|I(\lambda,r_0)\|\leqslant\lambda^{-1}$. The inequality (ii) allows us to show that $BI(\lambda,r_0)$ is a bounded operator. Indeed, for $u\in D(G)$ we have

$$\|Bu\|\leqslant\alpha\|(G+r_0B)u\|+\alpha r_0\|Bu\|+\beta\|u\|\leqslant\alpha\|(G+r_0B)u\|+\alpha\|Bu\|+\beta\|u\|.$$

It follows that $\|Bu\|\leqslant\alpha(1-\alpha)^{-1}\|(G+r_0B)u\|+\beta(1-\alpha)^{-1}\|u\|$. Moreover, since $I(\lambda,r_0):\mathfrak{h}\to D(G)$ and satisfies $(G+r_0B)I(\lambda,r_0)=\lambda I(\lambda,r_0)-\mathbf{1}$, the above inequality implies

$$\|BI(\lambda,r_0)u\|\leqslant\frac{\alpha}{1-\alpha}\|(\lambda I(\lambda,r_0)-\mathbf{1})u\|+\frac{\beta}{1-\alpha}\|I(\lambda,r_0)u\|\leqslant\frac{2\alpha+\beta}{1-\alpha}\|u\|,$$

for all $u\in D(G)$. Therefore $BI(\lambda,r_0)$ $(\lambda\geqslant 1)$ is bounded.

Let $\delta=(1-\alpha)(4\alpha+2\beta)^{-1}$. We show now that, for every $r\in[r_0-\delta,r_0+\delta]\cap[0,1]$, $G+r_0B$ is maximal dissipative by proving that it is invertible so that its range is all of $\mathfrak{h}$. The identity $\lambda\mathbf{1}-(G+rB)=\lambda\mathbf{1}-(G+r_0B)+(r_0-r)B=(\mathbf{1}+(r_0-r)BI(\lambda,r_0))(\lambda\mathbf{1}-(G+r_0B))$ shows that $\lambda\mathbf{1}-(G+rB)$ is invertible if and only if $\mathbf{1}+(r_0-r)BI(\lambda,r_0)$ is invertible. But this operator is indeed invertible for all r such that $\|r-r_0\|<(1-\alpha)(2\alpha+\beta)^{-1}\leqslant\|BI(\lambda,r_0)\|^{-1}$ and its inverse is given by the von Neumann series

$$(\mathbf{1}+(r_0-r)BI(\lambda,r_0))^{-1}=\sum_{n\geqslant 0}(r-r_0)^nBI(\lambda,r_0)^n. \tag{6}$$

This shows that $G+rB$ is maximal dissipative and

$$(\lambda\mathbf{1}-(G+rB))^{-1}=(\lambda\mathbf{1}-(G+r_0B))^{-1}(\mathbf{1}+(r_0-r)BI(\lambda,r_0))^{-1}. \tag{7}$$

If $R(p)$ is invariant for the semigroup generated by $G+r_0B$ and $B(D(G)\cap R(p))\subseteq R(p)$, then $BI(\lambda,r_0)(R(p))\subseteq B(D(G)\cap R(p))\subseteq R(p)$. Therefore, by (6), $R(p)$ is invariant also for $(\mathbf{1}+(r_0-r)BI(\lambda,r_0))^{-1}$. It follows then from (7) that $R(p)$ is invariant also under the resolvent $(\lambda\mathbf{1}-(G+rB))^{-1}$. Finally, the approximation (3) shows that $R(p)$ is invariant also for the operators $P_t^{(r)}$. □

Invariant subspaces are also stable under appropriate multiplicative perturbations of G.

Theorem IV.2: *Let G be the generator of the strongly continuous contraction semigroup P and let $R(p)$ be an invariant subspace under the operators P_t. Let $B\in\mathcal{B}(\mathfrak{h})$ such that*

(i) *the domain of G is invariant under both B and B^*,*
(ii) *the closure of B^*GB generates a strongly continuous contraction semigroup P^B, and*
(iii) *$R(p)$ is an invariant subspace for both B and B^*.*

Then $R(p)$ is an invariant subspace for the operators P_t^B.

Remark: Notice that B^*GB is dissipative, hence it is closable (see, e.g., Ref. 7, Prop. 3.1.15). Moreover, its closure is dissipative, too, therefore the hypothesis (ii) is equivalent to require that B^*GB is maximal dissipative by the Lumer–Phillips theorem.

Proof: We first assume that G is bounded. In this case, for every $\lambda>\|B^*GB\|$, we have

$$(\lambda\mathbf{1}-B^*GB)^{-1}=\sum_{n\geqslant 0}\lambda^{-(n+1)}(B^*GB)^n.$$

It follows then from (iii) that $R(p)$ is invariant under $(\lambda\mathbf{1}-B^*GB)^{-1}$ and, by the approximation (3), we obtain that $R(p)$ is invariant under all the operators P_t^B.

In the general case, with G unbounded, for every $\lambda>0$, let $G^\lambda=\lambda G(\lambda\mathbf{1}-G)^{-1}$. The subspace $R(p)$ is invariant under G^λ, thus, by the first part of the proof, it is also invariant under the operators $P_t^{B,\lambda}$ of the semigroup generated by $B^*G^\lambda B$.

Clearly, for each $u\in D(B^*GB)$ we have $B^*GBu=\lim_{\lambda\to\infty}B^*G^\lambda Bu$, and $D(B^*GB)$ is a core for the closure of B^*GB, i.e., $(\eta\mathbf{1}-B^*GB)(D(B^*GB))$ is dense in $\mathfrak{h}$ for any $\eta>0$. Therefore, by Theorem 4.5 on p. 88 of Ref. 15, $P_t^{B,\lambda}$ converges strongly to P_t^B as $\lambda\to\infty$ uniformly for t in bounded intervals. The conclusion readily follows. □

V. APPLICATIONS

A. A quantum model of absorption and stimulated emission

This example corresponds to a family of models introduced by Gisin and Percival in Ref. 10. The framework is given by the Hilbert space $\mathfrak{h}=l^2(\mathbb{N})$ where, as usual, we call $(e_n)_{n\geqslant 0}$ the canonical orthonormal basis. The operators defining the form-generator $\mathfrak{L}(\cdot)$ are $L_1=\nu a^*a$, $L_2=\mu a$, $H=\xi(a^*+a)$, where $\mu,\nu>0$ and $\xi\in\mathbb{R}$. Thus, $G=-i\xi(a^*+a)-2^{-1}(\nu^2(a^*a)^2+\mu^2a^*a)$, whose domain is $D(G)=D(N^2)$, where $N=a^*a$ is the number operator. We skip the straightforward verification of **(H-min)**. **(H-Markov)** can be checked applying the main result of

Ref. 18. The existence of an invariant state has been proved in Ref. 17 as an application of the main result in Ref. 1. To continue the analysis, we prove its faithfulness and uniqueness.

Corollary V.1: If $\xi\neq 0$, the QMS which corresponds to the model of absorption and stimulated emission here before is Markovian and has a unique faithful stationary state ρ_∞.

Moreover, given any other state σ, $\lim_{t\to\infty}\mathrm{tr}(\mathcal{T}_{*t}(\sigma)x)=\mathrm{tr}(\rho_\infty x)$, for any $x\in\mathcal{B}(\mathfrak{h})$.

Proof: We must characterize *all* common invariant subspaces for P_t, which satisfy additionally (2) We will repeatedly use Theorem IV.1 to obtain the desired classification of invariant subspaces.

Note that, for $u\in D(N^2)$, $L_1^2u=(2G+\mu^2(a^*a)+2i\xi(a^*+a))u$. Hence, a standard computation, using Young's inequality ($2ts\leqslant\epsilon^2t^2+\epsilon^{-2}s^2$) and the canonical commutation relations, yields

$$\begin{aligned}\|L_1^2u\|&\leqslant 2\|Gu\|+\mu^2\nu^{-2}\|L_1u\|+4|\xi|\|a^*u\|\\&\leqslant 2\|Gu\|+\left(\frac{\mu^2}{\nu^2}+\frac{2|\xi|}{\nu^2}\right)\|L_1u\|+4|\xi|\|u\|\\&\leqslant 2\|Gu\|+\frac{\mu^2+2|\xi|}{\nu^2}\|L_1^2u\|^{1/2}\|u\|^{1/2}+4|\xi|\|u\|\\&\leqslant 2\|Gu\|+\epsilon\|L_1^2u\|+\left[\left(\frac{\mu^2+2|\xi|}{\nu^2\epsilon}\right)^2+4|\xi|\right]\|u\|.\end{aligned}$$

Therefore, $(1-\epsilon)\|L_1^2u\|\leqslant 2\|Gu\|+[(\mu^2+2|\xi|)^2\nu^{-4}\epsilon^{-2}+4|\xi|]\|u\|$, for any $u\in D(N^2)$, $0<\epsilon<1$. Thus, for all $0\leqslant\lambda<1$, there exists $0\leqslant\alpha<1$ and $\beta>0$ such that $\|(\lambda/2)L_1u\|\leqslant\alpha\|Gu\|+\beta\|u\|$. Clearly, $G_\lambda=G+(\lambda/2)L_1^2$ is dissipative and generates a semigroup $P^{(\lambda)}$, by Theorem IV.1. Moreover, the same theorem shows that all our invariant subspaces are also invariant under the operators $P_t^{(\lambda)}$.

We now let $\lambda\to 1$. Since $D(N^2)$ is a core for G_1 and $G_\lambda u\to G_1u$ as $\lambda\to 1$ for any $u\in D(N^2)$ it follows from Ref. 15, Theorem 4.5, p. 88, that $P_t^{(\lambda)}u\to P_t^{(1)}u$, uniformly in t for t in bounded intervals. As a result, all our invariant subspaces are $P_t^{(1)}$-invariant as well.

Repeating the above argument, it turns out that the sought invariant subspaces are invariant under the semigroup generated by $G_1+(\mu^2/2\nu)L_1$ too. This generator is a restriction of $-i\xi(a^*+a)$. It follows from Lemma III.1 that $(a^*+a)(D(N)\cap R(p))\subseteq R(p)$. At this point, we can apply again Theorem IV.1, adding $i\xi(a^*+a)$ to G_1, so that the desired invariant subspaces are also invariant under the operators e^{-tN}, for all t. These operators are compact and self-adjoint, therefore their invariant subspaces are generated by eigenvectors (see Ref. 19, Theorem 4), i.e., they are the subspaces $\mathfrak{I}_K$, spanned by $\{e_k:k\in K\}$ where $K\subseteq\mathbb{N}$.

In the above argument we obtained also that, if $\xi\neq 0$, $(a^*+a)(\mathfrak{I}_K\cap D(N))\subseteq\mathfrak{I}_K$. This, together with $a(\mathfrak{I}_K\cap D(N))\subseteq\mathfrak{I}_K$, yields $a^*(\mathfrak{I}_K\cap D(N))\subseteq\mathfrak{I}_K$, for all $K\subseteq\mathbb{N}$, if $\xi\neq 0$. As a result, if $\xi\neq 0$, the only invariant subspaces are $\{0\}$ and $\mathfrak{h}$. If $\xi=0$, it is easy to show that the full collection of invariant subspaces is $\{0\},\mathfrak{h},\mathfrak{I}_{\{0,\ldots,k\}}$, for all $k\in\mathbb{N}$.

To summarize, if $\xi\neq 0$, the QMS has a faithful normal stationary state ρ_∞, say.

Moreover, since the generalized commutator of $\{L_\ell,L_\ell^*,\ell\geqslant 1\}$ is trivial, the semigroup converges towards the equilibrium (cf. Refs. 2 and 4, Theorem 2.1, p. 567) and the set of normal stationary states is reduced to a single element. □

B. A multimode Dicke model in quantum optics

This model has been introduced by Alli and Sewell in Ref. 11. In our previous article,[1] we proved that a stationary state exists for this semigroup. We recall the corresponding notations briefly.

The system consists of N identical two-level atoms coupled with a radiation field corresponding to n modes. Therefore, one can choose $\mathfrak{h}=(\mathbb{C}^2)^{\otimes N}\otimes(l^2(\mathbb{N}))^{\otimes n}$.

Let σ_1, σ_2, σ_3 be the Pauli matrices and define the spin raising and lowering operators $\sigma_\pm=(\sigma_1\pm i\sigma_2)/2$. We denote by $\sigma_{\epsilon,r}$ ($\epsilon=1,2,3,+,-$) the spin component of the atom at the site r. The free evolution of the atoms is described by a generator $\mathcal{L}_{\text{mat}}$:

$$\mathcal{L}_{\text{mat}}(x)=i[H,x]-\frac{1}{2}\sum_{j=1}^{3N}(V_j^*V_jx-2V_j^*xV_j+xV_j^*V_j), \tag{8}$$

where $H=(\varepsilon/2)\Sigma_{r=1}^{N}\sigma_{3,r}$, and the V_j's are the operators $V_j=c_\pm\sigma_{\pm,r}$ if $j=3r\pm1$, and $V_j=c_3\sigma_{3,r}$ if $j=3r$, with $\varepsilon,c_+,c_->0$, $c_3\geqslant0$.

We denote by a_j^*, a_j, the creation and annihilation operators corresponding to the jth mode of the radiation ($j=1,\ldots,n$), which clearly satisfy the CCR: $[a_j,a_k^*]=\delta_{jk}\mathbf{1}$, $[a_j,a_k]=0$.

The free evolution of the radiation is given by the formal generator

$$\mathcal{L}_{\text{rad}}(x)=\sum_{\ell=1}^{n}(\kappa_\ell(-a_\ell^*a_\ell x+2a_\ell^*xa_\ell-xa_\ell^*a_\ell)+i\omega_\ell[a_\ell^*a_\ell,x]), \tag{9}$$

where $\kappa_\ell>0$ and ω_ℓ is real. The operator

$$H_{\text{int}}=\frac{i}{N^{1/2}}\sum_{r=1}^{N}\sum_{\ell=1}^{n}\lambda_\ell(\sigma_{-,r}a_\ell^*e^{-2\pi ik_\ell r}-\sigma_{+,r}a_\ell e^{2\pi ik_\ell r}) \tag{10}$$

(k_ℓ,λ_ℓ real) describes the coupling between radiation and matter.

With the above notations, the generator of the whole dynamics is given by

$$\mathcal{L}(x)=\mathcal{L}_{\text{mat}}(x)+\mathcal{L}_{\text{rad}}(x)+i[H_{\text{int}},x]. \tag{11}$$

Identifying L_ℓ and G in our notations, $L_\ell=\sqrt{\kappa_\ell}a_\ell$ ($\ell=1,\ldots,n$). All the remaining L_ℓ's are bounded. Among them a finite number ($3N$) coincide with some of the V_j's appearing in (8) and the others vanish. The operator G, with domain $D(\Sigma_{\ell=1}^{n}a_\ell^*a_\ell)$, becomes

$$G=-\frac{1}{2}\sum_\ell L_\ell^*L_\ell-i\sum_\ell\omega_\ell a_\ell^*a_\ell-iH-iH_{\text{int}}. \tag{12}$$

In Ref. 1 we checked both **(H-min)**, **(H-Markov)** and proved that a stationary state exists. As a further step we now show the following.

Corollary V.2: The Alli–Sewell QMS has a unique faithful normal stationary state.

Characterizing subharmonic projections p is not a trivial problem at all because the annihilation operators admit plenty of nontrivial invariant subspaces (e.g., the linear span of any finite family of exponential vectors).

Proof: Call $\mathfrak{M}$ the set $\{\sigma_{+,r},\sigma_{-,r}:r=1,\ldots,N\}$. $\mathfrak{M}$ is a self-adjoint set, and by Corollary III.1 any invariant projection is an element of $\mathfrak{M}'$, therefore it is of the form $\mathbf{1}\otimes p$, where p is a projection on $l^2(\mathbb{N})$. Now, $\mathbf{1}\otimes p$ must be invariant under the operators P_t of the semigroup generated by G. We apply Theorem IV.1 as in the previous example to remove $iH+(1/2)\Sigma_{\ell>n}L_\ell^*L_\ell$ from G, to end up with $G_1=-\frac{1}{2}\Sigma_{\ell=1}^{n}(\kappa_\ell+2i\omega_\ell)a_\ell^*a_\ell-iH_{\text{int}}$. Theorem IV.1 shows that $\mathbf{1}\otimes p$ is invariant under the operators $P_t^{(1)}$ of the semigroup generated by G_1, too.

Applying Theorem IV.2 with $B=\sigma_{+,1},\ldots,\sigma_{+,N}$, since $B^*H_{\text{int}}B=0$, the sought projections are also invariant under the operators P_t^B of the semigroup generated by $2B^*G_1B=-B^*B\Sigma_{\ell=1}^{n}(\kappa_\ell+2i\omega)a_\ell^*a_\ell$. Therefore, being of the form $\mathbf{1}\otimes p$, it follows that p is an invariant projection for $\exp(-t\Sigma_{\ell=1}^{n}(\kappa_\ell+2i\omega)a_\ell^*a_\ell)$, for all t. These are normal operators but normality alone does not guarantee that the eigenspaces are generated by eigenvectors (see Ref. 9). However, the above operators are compact, too. Thus, Theorem 4 on p. 272 in Ref. 19 applies, and shows that all the invariant subspaces are generated by eigenvectors.

At this point, since the eigenvectors are explicitly known and $L_\ell = \sqrt{\kappa_\ell} a_\ell$, with $\kappa_\ell > 0$, we can repeat the argument of the previous example to conclude that p must be trivial. □

C. A classical Markov semigroup

Let E be a metric space and let $\mathcal{E}$ its Borel σ-field. Given a positive measure μ on $(E,\mathcal{E})$ call $\mathfrak{A} = L^\infty(E,\mathcal{E},\boldsymbol{\mu})$. Let $M(x,A) = \int_A m(x,y)\mu(dy)$ be a transition function on $E \times \mathcal{E}$. Then (see, for instance, Ref. 6),

$$Lf(x) = \int_E (f(y) - f(x)) M(x,dy)$$

defines a bounded operator on $\mathfrak{A}$ which is the generator of a (classical) Markov semigroup.

In this case, the predual von Neumann algebra $\mathcal{A}_*$ is $L^1(E,\mathcal{E},\boldsymbol{\mu})$ and any normal state is represented by a probability measure ν absolutely continuous with respect to μ.

Proposition V.1: A projection 1_A $(A \in \mathcal{E})$ *is subharmonic for the given Markov semigroup if and only if* $M(x,A^c) = 0$ *for* μ *almost all* $x \in A$.

In particular, the semigroup is irreducible if and only if the support of $M(x,\cdot)$ *coincides with that of* μ *for* μ*-almost all* $x \in E$.

It is worth noticing that the Markov process, starting from a point $x \in A$, can only go inside the support of $M(x,\cdot)$. Then to say that 1_A is subharmonic means that A includes the support of any $M(x,\cdot)$ for $x \in A$, $\mu-$ almost surely. That is, for any $x \in A$, the process cannot jump outside of A.

Proof: Take a projection $p = 1_A \in \mathfrak{A}$. This projection is subharmonic if and only if $L1_A \geqslant 0$. However, for $x \in A$, $L1_A(x) = (M(x,A) - M(x,E)) \leqslant 0$, and for $x \in A^c$, $L1_A(x) = M(x,A)$. Therefore, 1_A is subharmonic if and only if, for μ, almost all $x \in A$, $M(x,A^c) = 0$.

The second assertion now follows easily. □

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Automorphisms of the fine grading of $sl(n,\mathbb{C})$ associated with the generalized Pauli matrices

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We consider the grading of $sl(n,\mathbb{C})$ by the group Π_n of generalized Pauli matrices. The grading decomposes the Lie algebra into n^2-1 one-dimensional subspaces. In the article we demonstrate that the normalizer of grading decomposition of $sl(n,\mathbb{C})$ in Π_n is the group $\mathrm{SL}(2,\mathbb{Z}_n)$, where $\mathbb{Z}_n$ is the cyclic group of order n. As an example we consider $sl(3,\mathbb{C})$ graded by Π_3 and all contractions preserving that grading. We show that the set of 48 quadratic equations for grading parameters splits into just two orbits of the normalizer of the grading in Π_3. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1430046]

I. INTRODUCTION

Among the gradings of reductive Lie algebras over the complex number field and the simultaneous gradings of their representation spaces, by far the most important ones are the gradings by maximal torus. In the case of the Lie algebra it is also called root or Cartan decomposition. Such a grading means a decomposition into eigenspaces of the maximal torus. For a greater part of the past century such gradings have been the workhorses of the theory and applications.

The typical role a Lie algebra plays in physics is the algebra of infinitesimal symmetries of a physical system, which themselves are described in terms of elements of representation spaces, eigenvectors of the maximal torus. The corresponding eigenvalues are then the quantum numbers.

The question about the existence of other gradings, like those by maximal torus (called fine gradings), has been raised systematically in Ref. 1 and solved for the simple Lie algebras of over $\mathbb{C}$ in Refs. 2–4 and recently also for the real number field in Refs. 5 and 6.

Gradings of Lie algebras are closely related to their automorphisms. In a seminal paper[1] in 1989, it was shown that the finest gradings (called fine) of finite-dimensional simple Lie algebras $\mathcal{L}$ can be classified (up to equivalence generated by elements of $\mathrm{Aut}\,\mathcal{L}$) by the maximal Abelian groups of diagonable automorphisms of $\mathcal{L}$, briefly the MAD groups. In general, the MAD groups

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are composed, besides subgroups of the maximal torus, by well-known outer automorphisms,[7] and by elements of finite order (EFO) in the corresponding Lie groups. Since the conjugacy classes of EFO were systematically described in Ref. 8 (see also Ref. 7), it was not difficult to classify the fine gradings in the lowest cases like $sl(2,\mathbb{C})$ and $sl(3,\mathbb{C})$.[9–11]

A prominent role in the grading problem of simple Lie algebras is played by the finite group Π_n of n^3 matrices $\mathbb{C}^{n\times n}$. A subset of Π_n, consisting of n^2-1 traceless matrices, can be taken as a basis of $sl(n,\mathbb{C})$. Since these traceless matrices are used as a basis of a Lie algebra, they can be normalized in any convenient way. In particular, for $n=2$ the Pauli matrices of $sl(2,\mathbb{C})$ are obtained.

Most importantly, the adjoint action of Π_n, though non-Abelian in general, induces an Abelian action on $sl(n,\mathbb{C})$. The fine grading of $sl(n,\mathbb{C})$, which arises in this way, decomposes the algebra into one-dimensional subspaces generated by traceless elements of Π_n.[9]

In further prospect, the gradings are to be used, e.g., for constructing grading preserving contractions (*graded contractions*) of semisimple $\mathcal{L}$.[12,13] For gradings involving a decomposition into a small number of grading subspaces, this is a relatively easy task.[14–16] However for fine gradings of algebras with ranks $\geqslant 3$, the system of quadratic equations for contraction parameters one needs to solve often gets quite large. The task of solving of such a system would be simplified by knowledge of its symmetries. Symmetries that are available are provided by those elements of $\mathrm{Aut}\,\mathcal{L}$ which leave the given grading invariant.

The main goal of this paper is to demonstrate that the decomposition of $sl(n,\mathbb{C})$, as the fine grading by Π_n, is preserved by the finite group $\mathrm{SL}(2,\mathbb{Z}_n)$, acting through its n-dimensional representation on the labels (a,b) of the one-dimensional subspace of $sl(n,\mathbb{C})$. Thus the group $\mathrm{SL}(2,\mathbb{Z}_n)$ plays a role analogous to the Weyl group in the case of root decomposition/grading of $sl(n,\mathbb{C})$. Here $\mathbb{Z}_n$ is the cyclic group of order n. We also illustrate an application of this fact.

The special role of matrices Π_n has been recognized in the physical literature for a long time.[17] In more recent years there were a number of papers where the matrices were used as a basic part of the formalism in the development of quantum mechanics in discrete spaces $\mathbb{Z}_n$. Here, the finite group Π_n plays the role of the discrete Weyl group acting in an n-dimensional complex Hilbert space. See Refs. 18 and 19 and references therein.

The Π_n-grading of $sl(n,\mathbb{C})$ has other special properties. Let us name just two.

(1) All generators are in the same conjugacy class of $\mathrm{SL}(n,\mathbb{C})$. Considered as group elements, they are of order n, belonging to the Costant conjugacy class of finite order elements, specified as $[1,1,\ldots,1]$ in the notation introduced in Ref. 8.

(2) The Π_n-grading makes explicit the decomposition of $sl(n,\mathbb{C})$ into the sum of $n+1$ Cartan subalgebra. Indeed, if the element of $\mathcal{P}_n$ defined by a couple (a,b) (a,b considered $\bmod n$), belongs to one such Cartan subalgebra, that subalgebra is then generated by the $n-1$ elements carrying labels $(a,b),(2a,2b),\ldots,((n-1)a,(n-1)b)$. Clearly such elements commute and have a nonzero determinant.

In Sec. II, the role of automorphisms of the Lie algebra in its gradings is recalled. Grading groups of $sl(n,\mathbb{C})$ which do not involve outer automorphisms are described in Sec. III. Our main result is in Sec. IV, namely the normalizers of the grading groups. Sec. V contains an application to $sl(3,\mathbb{C})$: It is shown that the set of 48 quadratic equations for contraction parameters splits into just two orbits of the normalizer of the grading group Π_3.

II. GRADINGS AND AUTOMORPHISMS OF LIE ALGEBRAS

A grading of Lie algebra $\mathcal{L}$ is a decomposition of $\mathcal{L}$ into direct sum of subspaces

$$\Gamma: \quad \mathcal{L}=\bigoplus_{i\in I}\mathcal{L}_i \tag{1}$$

such that for any pair of indices $i,j\in I$ there exists an index $k\in I$ with the property

$$[\mathcal{L}_i,\mathcal{L}_j]:=\{[X,Y]\,|\,X\in\mathcal{L}_i, Y\in\mathcal{L}_j\}\subseteq\mathcal{L}_k.$$

A grading which cannot be further refined is called *fine*.

Gradings can be obtained by looking at $\mathrm{Aut}\,\mathcal{L}$, the group of all automorphisms of $\mathcal{L}$. It consists of all non-singular linear transformations ϕ of $\mathcal{L}$ as linear space $[\phi \in \mathrm{GL}(\mathcal{L})]$ which preserve the binary operation in $\mathcal{L}$:

$$\phi[X,Y]=[\phi X,\phi Y].$$

If ϕ is *diagonable* and X, Y are its eigenvectors with nonzero eigenvalues λ, μ,

$$\phi X=\lambda X, \quad \phi Y=\mu Y,$$

then clearly

$$\phi[X,Y]=[\phi X,\phi Y]=\lambda\mu[X,Y]. \tag{2}$$

This means that the element $[X,Y]$ is either an eigenvector of ϕ with eigenvalue $\lambda\mu$, or is the zero element. The given automorphism ϕ thus leads to a decomposition of the linear space $\mathcal{L}$ into eigenspaces of ϕ,

$$\mathcal{L}=\bigoplus_{i\in I}\mathrm{Ker}(\phi-\lambda_i\,\mathrm{id}),$$

which, according to (2), satisfies the definition of a grading.

Refinements of a given grading, i.e., further decompositions of the subspaces, can be obtained by adjoining further automorphisms commuting with ϕ. Hence, in general, sets $\phi_1,\ldots,\phi_m$ of mutually commuting automorphisms determine gradings.

Conversely, if a grading (1) of a simple Lie algebra $\mathcal{L}$ is given, it defines a particular Abelian subgroup $\mathrm{Diag}\,\Gamma\subset\mathrm{Aut}\,\mathcal{L}$ consisting of those automorphisms $\phi\in GL(\mathcal{L})$ which

(i) preserve Γ, $\phi(\mathcal{L}_i)=\mathcal{L}_i$,
(ii) are diagonal, $\phi X=\lambda_i X \quad \forall X\in\mathcal{L}_i$, $i\in I$, where $\lambda_i\neq 0$ depends only on ϕ and $i\in I$.

In Ref. 1 an important theorem was proved:

Theorem 1: *Let $\mathcal{L}$ be a finite-dimensional simple Lie algebra over an algebraically closed field of characteristic zero. Then the grading Γ is fine, if and only if the diagonal subgroup* $\mathrm{Diag}\,\Gamma$ *is a maximal Abelian group of diagonable automorphisms (MAD group).*

A general algorithm to construct all MAD groups for the class of simple classical Lie algebras over complex numbers was given in Refs. 2–4. (Further results concerning the real forms can be found in Refs. 5 and 6.) These Lie algebras are Lie subalgebras of $gl(n,\mathbb{C})$, hence their MAD groups can be determined from the MAD groups of $gl(n,\mathbb{C})$ by imposing certain conditions.

The automorphisms of $gl(n,\mathbb{C})$ can be easily written as combinations of inner and outer automorphisms. For all $X\in gl(n,\mathbb{C})$, *inner automorphisms* have the general form

$$\mathrm{Ad}_A X=A^{-1}XA \quad \text{for} \quad \text{any} \quad A\in GL(n,\mathbb{C});$$

outer automorphims have the general form

$$\mathrm{Out}_C X=-(C^{-1}XC)^T=\mathrm{Out}_I\,\mathrm{Ad}_C X, \quad \text{where} \quad C\in GL(n,\mathbb{C}).$$

Relevant properties of inner and outer automorphisms of $gl(n,\mathbb{C})$ are summarized in the following lemma (Ref. 2) which allows one to express MAD groups in $\mathrm{Aut}\,gl(n,\mathbb{C})$ in terms of special elements of $GL(n,\mathbb{C})$:

Lemma 2: Let $A,B,C\in GL(n,\mathbb{C})$.

(1) Ad_A *is diagonable automorphism if and only if the corresponding matrix A is diagonable.*

(2) *Inner automorphisms commute,* $\mathrm{Ad}_A\,\mathrm{Ad}_B=\mathrm{Ad}_B\,\mathrm{Ad}_A$, *if and only if there exists $q\in\mathbb{C}$ such that*

$$AB = qBA, \quad \textit{where } q \textit{ satisfies} \quad q^n = 1. \tag{3}$$

(3) Out_C *is diagonable if and only if* $C(C^T)^{-1}$ *is diagonable.*

(4) *Inner and outer automorphisms commute,* $\mathrm{Ad}_A \mathrm{Out}_C = \mathrm{Out}_C \mathrm{Ad}_A$, *if and only if* $ACA^T = rC$; *since* $\mathrm{Ad}_{\alpha A} = \mathrm{Ad}_A$ *for* $\alpha \neq 0$, *number* r *can be normalized to unity.*

Remark 3: The sets of complex $n \times n$ matrices satisfying (3) were to our knowledge first studied by Weyl.[17]

III. MAD GROUPS WITHOUT OUTER AUTOMORPHISMS

In this contribution we are going to look at the MAD groups in $\mathrm{Aut}\, gl(n,\mathbb{C})$ without outer automorphisms, i.e., generated by inner automorphisms [the Ad action in $GL(n,\mathbb{C})$ only]. It is shown in Ref. 2 that there exists a one-to-one correspondence between MAD groups without outer automorphisms and Ad groups (to be defined in the following) in $GL(n,\mathbb{C})$.

Definition 4: A subgroup of diagonable matrices $G \subset GL(n,\mathbb{C})$ *will be called an* **Ad group** *if*

(1) *for any pair* $A,B \in G$ *the commutator* $q(A,B) = ABA^{-1}B^{-1}$ *lies in the center* $Z = \{\alpha I_n | \alpha \in \mathbb{C}^*\} \subset GL(n,\mathbb{C})$;

(2) G *is maximal, i.e., for each* $M \notin G$ *there exists* $A \in G$ *such that* $q(A,M) \notin Z$.

In order to describe Ad groups we introduce the following notation. The subgroup of $GL(n,\mathbb{C})$ containing all regular diagonal matrices will be denoted by $D(n)$. We also define special $k \times k$ diagonal matrices (for $k=1$ we set $Q_1 = P_1 = 1$)

$$Q_k = \mathrm{diag}(1, \omega_k, \omega_k^2, \ldots, \omega_k^{k-1}),$$

where ω_k is the primitive kth root of unity, $\omega_k = \exp(2\pi i/k)$, and

$$P_k = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & & & \ddots & & \\ 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

The unitary matrices P_k, Q_k appear in the finite-dimensional quantum mechanics (FDQM),[17–20] where their integral powers play the role of exponentiated operators of position and momentum in the position representation. The matrices P_k, Q_k satisfy the identity (3) with $q = \omega_k$,

$$P_k Q_k = \omega_k Q_k P_k, \tag{4}$$

which in FDQM replaces the usual Heisenberg commutation relations. The discrete subgroup of $GL(k,\mathbb{C})$ generated by powers of P_k, Q_k is the *discrete Weyl (or Heisenberg) group* of FDQM in k-dimensional Hilbert space $\mathcal{H}_k$. In Ref. 9 this group was called the *Pauli group*; it consists of k^3 elements

$$\Pi_k = \{\omega_k^l Q_k^i P_k^j | i,j,l = 0,1,\ldots,k-1\}. \tag{5}$$

The classification of Ad groups in $GL(n,\mathbb{C})$ is given by the following theorem[3]

Theorem 5: $G \subset GL(n,\mathbb{C})$ *is an Ad group if and only if* G *is conjugated to one of the finite groups*

$$\Pi_{\pi_1} \otimes \cdots \otimes \Pi_{\pi_s} \otimes D(n/\pi_1 \ldots \pi_s),$$

where $\pi_1, \ldots, \pi_s$ *are powers of primes and their product* $\pi_1 \ldots \pi_s$ *divides* n, *with the exception of the case* $\Pi_2 \cdots \otimes \Pi_2 \otimes D(1)$. (In this case there is an outer automorphism in the MAD group.)

The simplest form of an Ad group is $G=D(n)$. The MAD group corresponding to this Ad group gives the Cartan decomposition of $gl(n,\mathbb{C})$.

In this article we shall focus on the other extremal case, namely on the Ad group

$$\Pi_n \otimes D(1) = \Pi_n .$$

The corresponding fine grading decomposes $gl(n,\mathbb{C})$ into a sum of n^2 one-dimensional subspaces[1,9]

$$\Gamma_\Pi : \quad gl(n,\mathbb{C}) = \bigoplus_{(r,s)\in \mathbb{Z}_n\times\mathbb{Z}_n} \mathcal{L}_{rs}, \tag{6}$$

where $\mathcal{L}_{rs}=\mathbb{C}X_{rs}$ with X_{rs} being the basis elements of $gl(n,\mathbb{C})$ representing n^2 cosets of Π_n with respect to its center $\{\omega^l | l\in\mathbb{Z}_n\}$:

$$X_{rs} = Q^r P^s .$$

Their commutators [henceforth the index k in ω_k, P_k, Q_k as well as explicit notation (mod n) will be omitted]

$$[X_{rs}, X_{r's'}] = Q^r P^s Q^{r'} P^{s'} - Q^{r'} P^{s'} Q^r P^s = (\omega^{sr'} - \omega^{rs'}) X_{r+r',s+s'} \tag{7}$$

clearly satisfy the grading property with the index set I being the Abelian group $\mathbb{Z}_n\times\mathbb{Z}_n$. The binary correspondence $((r,s),(r',s'))\mapsto(r+r',s+s')$, $0\neq[\mathcal{L}_{rs},\mathcal{L}_{r's'}]\subseteq\mathcal{L}_{r+r',s+s'}$ is the group multiplication in $\mathbb{Z}_n\times\mathbb{Z}_n$ written additively modulo n.

The corresponding grading of $sl(n,\mathbb{C})$ contains n^2-1 subspaces

$$sl(n,\mathbb{C}) = \bigoplus_{(r,s)\neq(0,0)} \mathcal{L}_{rs},$$

since $\mathrm{Tr}(X_{rs})=0$ except $r=s=0$.

IV. SYMMETRIES OF THE FINE GRADINGS Γ_Π

In this section we are going to study the symmetries of the fine gradings (6) of $gl(n,\mathbb{C})$. From Sec. III we know that they are induced by the Pauli group $\Pi_n\subset GL(n,\mathbb{C})$.

Generally, the symmetry group or the automorphism group $\mathrm{Aut}\,\Gamma\subset\mathrm{Aut}\,\mathcal{L}$ of the grading (1) consists of those automorphisms ϕ of $\mathcal{L}$ which permute the components of (1),

$$\phi\mathcal{L}_i = \mathcal{L}_{\overline{\phi}(i)} .$$

Here $\overline{\phi}: I\to I$ is a permutation of the elements of I, so we have a permutation representation Δ_Γ of $\mathrm{Aut}\,\Gamma$,

$$\overline{\phi} = \Delta_\Gamma(\phi), \quad \phi\in\mathrm{Aut}\,\Gamma .$$

The kernel of Δ_Γ is the stabilizer of Γ in $\mathrm{Aut}\,\Gamma$,

$$\mathrm{Stab}\,\Gamma = \ker\Gamma = \{\phi\in\mathrm{Aut}\,\mathcal{L} \,|\, \phi\mathcal{L}_i = \mathcal{L}_i \ \forall\, i\in I\}.$$

It is a normal subgroup of $\mathrm{Aut}\,\Gamma$ with quotient group isomorphic to the group of permutations of I,

$$\mathrm{Aut}\,\Gamma/\mathrm{Stab}\,\Gamma \simeq \Delta_\Gamma\,\mathrm{Aut}\,\Gamma .$$

For fine gradings $\mathrm{Stab}\,\Gamma=\mathcal{G}$. The *symmetry group* $\mathrm{Aut}\,\Gamma$ is by definition[1] the normalizer of $\mathcal{G}$ in $\mathrm{Aut}\,gl(n,\mathbb{C})$:

$$\mathcal{N}(\mathcal{G})=\mathrm{Aut}\,\Gamma=\{\phi\in \mathrm{Aut}\,gl(n,\mathbb{C})\,|\,\phi\mathcal{G}\phi^{-1}\subset\mathcal{G}\}.$$

Why do we look for the symmetry group $\mathrm{Aut}\,\Gamma$? We know that

(1) elements of $\mathrm{Aut}\,\Gamma/\mathrm{Stab}\,\Gamma$ permute the grading subspaces,
(2) given a grading subspace, the action of $\mathrm{Aut}\,\Gamma/\mathrm{Stab}\,\Gamma$ will yield some other grading subspaces.

So its knowledge may give us the way to construct the grading decomposition (1) from one or a small number of starting subspaces. $\mathrm{Aut}\,\Gamma/\mathrm{Stab}\,\Gamma$ may also be valuable as a symmetry of the contraction equations which enables one to lower their number and so simplify their solution.

Let us denote the MAD group Ad_{Π_n} by $\mathcal{P}_n$. It is an Abelian subgroup of $\mathrm{Aut}\,gl(n,\mathbb{C})=GL(n^2,\mathbb{C})$ with generators Ad_P, Ad_Q,

$$\mathcal{P}_n=\{\mathrm{Ad}_{Q^iP^j}|(i,j)\in\mathbb{Z}_n\times\mathbb{Z}_n\}.$$

It is obvious that n^2 elements of $\mathcal{P}_n$ stabilize the grading: namely, taking the generators Ad_P, Ad_Q, one has

$$\mathrm{Ad}_P X_{rs}=PQ^rP^sP^{-1}=\omega^r X_{rs},\quad \mathrm{Ad}_Q X_{rs}=QQ^rP^sQ^{-1}=\omega^{-s}X_{rs}$$

and $\mathcal{P}_n=\mathrm{Stab}\,\Gamma_\Pi$ since $\mathcal{P}_n$ is maximal.

In order to describe the quotient group $\mathcal{N}(\mathcal{P}_n)/\mathcal{P}_n$ we note that its elements are classes of equivalence in $\mathcal{N}(\mathcal{P}_n)$ given by

$$\phi\sim\psi \quad \text{if and only if} \quad \phi\psi^{-1}\in\mathcal{P}_n.$$

Let $\phi\sim\psi$, i.e., $\phi\psi^{-1}=\beta$ for some $\beta\in\mathcal{P}_n$. Using the commutativity of $\mathcal{P}_n$ we have

$$\phi^{-1}\alpha\phi=\psi^{-1}\beta^{-1}\alpha\beta\psi=\psi^{-1}\alpha\psi$$

for any $\alpha\in\mathcal{P}_n$. On the other hand, let $\phi^{-1}\alpha\phi=\psi^{-1}\alpha\psi$ for any $\alpha\in\mathcal{P}_n$. Then $\phi\psi^{-1}$ commutes with every element in $\mathcal{P}_n$ and therefore $\phi\psi^{-1}\in\mathcal{P}_n$. It means that

$$\phi\sim\psi \quad \text{if and only if} \quad \phi^{-1}\alpha\phi=\psi^{-1}\alpha\psi \quad \text{for any} \quad \alpha\in\mathcal{P}_n.$$

Since the group $\mathcal{P}_n$ has only two generators Ad_P and Ad_Q, the previous condition can be rewritten

$$\phi\sim\psi \quad \text{if and only if} \quad \phi^{-1}\,\mathrm{Ad}_P\,\phi=\psi^{-1}\,\mathrm{Ad}_P\,\psi \quad \text{and} \quad \phi^{-1}\,\mathrm{Ad}_Q\,\phi=\psi^{-1}\,\mathrm{Ad}_Q\,\psi. \tag{8}$$

If ϕ belongs to the normalizer $\mathcal{N}(\mathcal{P}_n)$, then there exist elements a,b,c,d in the cyclic group $\mathbb{Z}_n$ such that

$$\phi^{-1}\,\mathrm{Ad}_Q\,\phi=\mathrm{Ad}_{Q^aP^b} \quad \text{and} \quad \phi^{-1}\,\mathrm{Ad}_P\,\phi=\mathrm{Ad}_{Q^cP^d}.$$

Thus to any equivalence class a quadruple of indices is assigned. Denote this assignment by Φ. According to (8), quadruples assigned to distinct classes are different. We shall see that it is convenient to write the quadruple as a matrix

$$\Phi(\phi)=\begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \text{with entries from} \quad \mathbb{Z}_n.$$

Suppose that the equivalence classes containing the automorphisms ϕ_1 and ϕ_2 correspond to the quadruples a_1, b_1, c_1, d_1 and a_2, b_2, c_2, d_2, respectively. Computing the quadruple assigned to the composition $\phi_1\phi_2$,

$$(\phi_1\phi_2)^{-1}\,\mathrm{Ad}_Q(\phi_1\phi_2)=(\phi_2^{-1}\,\mathrm{Ad}_Q\phi_2)^{a_1}(\phi_2^{-1}\mathrm{Ad}_P\phi_2)^{b_1}$$
$$=(\mathrm{Ad}_{Q^{a_2}P^{b_2}})^{a_1}(\mathrm{Ad}_{Q^{c_2}P^{d_2}})^{b_1}$$
$$=\mathrm{Ad}_{Q^{a_2a_1}P^{b_2a_1}}\mathrm{Ad}_{Q^{c_2b_1}P^{d_2b_1}}$$
$$=\mathrm{Ad}_{Q^{a_1a_2+b_1c_2}P^{a_1b_2+b_1d_2}},$$

$$(\phi_1\phi_2)^{-1}\,\mathrm{Ad}_P(\phi_1\phi_2)=\mathrm{Ad}_{Q^{a_1a_2+b_1c_2}P^{a_1b_2+b_1d_2}}$$

we see that to the automorphism $\phi_1\phi_2$ the product matrix is assigned,

$$\Phi(\phi_1\phi_2)=\Phi(\phi_1)\Phi(\phi_2).$$

Thus Φ is an injective homomorphism of the quotient group $\mathcal{N}(\mathcal{P}_n)/\mathcal{P}_n$.

Let $\phi\in\mathcal{N}(\mathcal{P}_n)$ be an *inner* automorphism, say Ad_A with the corresponding matrix

$$\Phi(\phi)=\begin{pmatrix}a & b\\ c & d\end{pmatrix}\quad\text{with entries from } \mathbb{Z}_n.$$

Then

$$\mathrm{Ad}_A^{-1}\,\mathrm{Ad}_Q\,\mathrm{Ad}_A=\mathrm{Ad}_{A^{-1}QA}=\mathrm{Ad}_{Q^aP^b}\quad\text{implies}\quad A^{-1}QA=\mu Q^aP^b, \tag{9}$$

$$\mathrm{Ad}_A^{-1}\,\mathrm{Ad}_P\,\mathrm{Ad}_A=\mathrm{Ad}_{A^{-1}PA}=\mathrm{Ad}_{Q^cP^d}\quad\text{implies}\quad A^{-1}PA=\nu Q^cP^d \tag{10}$$

for some $\mu,\nu\in\mathbb{C}^*$. Multiplying Eqs. (9) and (10) by PA and QA from the right, respectively, and using the relation $PQ=\omega QP$, we obtain

$$PQA=\mu\nu AQ^cP^dQ^aP^b=\omega^{ad}\mu\nu Q^{a+c}P^{b+d}$$

and

$$QPA=\mu\nu AQ^aP^bQ^cP^d=\omega^{bc}\mu\nu Q^{a+c}P^{b+d}.$$

Since $PQA=\omega QPA$ we obtain the identity

$$\omega^{ad-1}=\omega^{bc},\quad\text{i.e.,}\quad ad-1=bc(\mathrm{mod}\,n),$$

hence

$$\det\Phi(\phi)=1.$$

A simple computation further shows that for this inner automorphism one has

$$A^{-1}X_{rs}A=\rho X_{r's'},$$

where $|\rho|=1$ and

$$(r',s')=(r,s)\begin{pmatrix}a & b\\ c & d\end{pmatrix}. \tag{11}$$

Consider now the outer automorphism $\mathrm{Out}_I X:=-X^T$. Because of

$$(\mathrm{Out}_I)^{-1}\mathrm{Ad}_Q\mathrm{Out}_I=\mathrm{Ad}_{(Q^{-1})^T}=\mathrm{Ad}_{Q^{-1}}\in\mathcal{P}_n,$$

$$(\mathrm{Out}_I)^{-1}\mathrm{Ad}_P\mathrm{Out}_I=\mathrm{Ad}_{(P^{-1})^T}=\mathrm{Ad}_P\in\mathcal{P}_n,$$

the automorphism Out_I belongs to the normalizer $\mathcal{N}(\mathcal{P}_n)$. The matrix corresponding to Out_I is

$$\Phi(\mathrm{Out}_I)=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix} \quad \text{and} \quad \det\Phi(\mathrm{Out}_I)=-1.$$

Note that

$$\mathrm{Out}_I X_{rs}=-\omega^{-rs}X_{r,-s}$$

corresponds to the permutation of indices

$$(r,s)\mapsto(r,-s).$$

Any other outer automorphism ϕ from $\mathcal{N}(\mathcal{P}_n)$ is the composition of Out_I and an inner automorphism from $\mathcal{N}(\mathcal{P}_n)$ and thus $\det\Phi(\phi)=-1$. We conclude with

Proposition 6: Φ is an injective homomorphism of $\mathcal{N}(\mathcal{P}_n)/\mathcal{P}_n$ into the group

$$H=\left\{\begin{pmatrix}a & b\\ c & d\end{pmatrix}\middle|\, a,b,c,d\in\mathbb{Z}_n, ad-bc=\pm 1 \bmod n,\right\}.$$

The group H contains as its subgroup the group of matrices with determinant $+1$. This group is usually denoted by $\mathrm{SL}(2,\mathbb{Z}_n)$. Note that $\mathbb{Z}_n$ is a field iff n is prime. Clearly

$$H=\mathrm{SL}(2,\mathbb{Z}_n)\cup\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\mathrm{SL}(2,\mathbb{Z}_n).$$

Let us briefly show that for any $n\in\mathbb{N}$, the group $\mathrm{SL}(2,\mathbb{Z}_n)$ is generated by two matrices

$$A=\begin{pmatrix}1 & 0\\ 1 & 1\end{pmatrix} \quad \text{and} \quad B=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}.$$

In order to show it, we have to realize that in the ring $\mathbb{Z}_n$, the matrices A and B are of orders n and 4, respectively. The matrix $C=A^T$ is generated by A and B:

$$C=\begin{pmatrix}1 & 1\\ 0 & 1\end{pmatrix}=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 1 & 1\end{pmatrix}^{n-1}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}^3.$$

Moreover, any matrix of $\mathrm{SL}(2,\mathbb{Z}_n)$ satisfies

$$\begin{pmatrix}a & b\\ c & d\end{pmatrix}=\begin{pmatrix}1 & 0\\ 1 & 1\end{pmatrix}\begin{pmatrix}a & b\\ c-a & d-b\end{pmatrix}=\begin{pmatrix}1 & 1\\ 0 & 1\end{pmatrix}\begin{pmatrix}a-c & b-d\\ c & d\end{pmatrix}. \tag{12}$$

Now recall that Euclid's algorithm for finding the greatest common divisor of integers is based on the trivial fact that $\gcd(x,y)=\gcd(x-y,y)$. By several repetitions of this rule, where we replace the pair of non-negative integers $\{x,y\}, x\geqslant y$, by another pair of non-negative integers $\{x-y,y\}$, the Euclid's algorithm gives finally a pair of integers, where one of them is 0 and the other is $\gcd(x,y)$.

Denote $\gcd(a,c)=s$. Then by suitable applications of (12) we obtain

$$\begin{pmatrix}a & b\\ c & d\end{pmatrix}=A^{k_1}C^{l_1}\ldots A^{k_p}C^{l_p}T,$$

where $k_1,l_1,\ldots,k_p,l_p\in\mathbb{N}_0$ and T is a matrix with $\det T=1$, of the form

$$T=\begin{pmatrix} s & t \\ 0 & u \end{pmatrix} \quad \text{or} \quad T=\begin{pmatrix} 0 & v \\ s & w \end{pmatrix}.$$

But any matrix T of such form is a product of several matrices A,B, and C, since

$$\begin{pmatrix} s & t \\ 0 & u \end{pmatrix}=\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}^{s(t-1)}\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}^{u}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}^{s}$$

$$\begin{pmatrix} 0 & v \\ s & w \end{pmatrix}=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} -s & -w \\ 0 & v \end{pmatrix}.$$

This proves that $\mathrm{SL}(2,\mathbb{Z}_n)$ has two generators, the matrices A and B.

Now we shall present two elements of the normalizer—special unitary $n\times n$ matrices inducing Ad actions which represent generating elements of $\mathrm{SL}(2,\mathbb{Z}_n)$.

Example 7: Since the matrices Q and P have the same spectra, they are similar with a similarity matrix S such that $S^{-1}PS=Q$. Such S is not determined uniquely. We choose for the matrix S the Sylvester matrix defined as follows:

$$S_{ij}=\omega^{-ij}, \quad \text{for } i,j\in\mathbb{Z}_n.$$

It is easy to verify that S^2 is a parity operator

$$S_{ij}^2=\delta_{i,-j} \quad \text{for} \quad i,j\in\mathbb{Z}_n \text{ such that } \quad S^4=I.$$

Note that the indices (and operations on them) are always considered to be elements of the ring $\mathbb{Z}_n$. Let us verify that Ad_S belongs to the normalizer. Note that S is a symmetric matrix and therefore $Q=Q^T=(S^{-1}PS)^T=SP^TS^{-1}=SP^{-1}S^{-1}$, which implies $S^{-1}QS=P^{-1}$. Now we can easily check the conditions on Ad_S to be in the normalizer:

$$(\mathrm{Ad}_S)^{-1}\mathrm{Ad}_Q\mathrm{Ad}_S=\mathrm{Ad}_{S^{-1}QS}=\mathrm{Ad}_{P^{-1}}\in\mathcal{P}_n$$

$$(\mathrm{Ad}_S)^{-1}\mathrm{Ad}_P\mathrm{Ad}_S=\mathrm{Ad}_{S^{-1}PS}=\mathrm{Ad}_Q\in\mathcal{P}_n.$$

By (9) and (10) the matrix corresponding to Ad_S is

$$\Phi(\mathrm{Ad}_S)=\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Example 8: For this example we shall use the similarity of matrices P and PQ. Put $\varepsilon=1$, if n is odd, and $\varepsilon=\sqrt{\omega}$, if n is even. Denote by

$$D=\mathrm{diag}(d_0,d_1,\ldots,d_{n-1}), \text{ where } d_j=\varepsilon^{-j}\omega^{-\binom{j}{2}}, \text{ for } j\in\mathbb{Z}_n.$$

It is easy to see that $Q=D^{-1}QD$ and $PQ=\varepsilon D^{-1}PD$; it implies

$$(\mathrm{Ad}_D)^{-1}\mathrm{Ad}_Q\mathrm{Ad}_D=\mathrm{Ad}_{D^{-1}QD}=\mathrm{Ad}_Q\in\mathcal{P}_n$$

and

$$(\mathrm{Ad}_D)^{-1}\mathrm{Ad}_P\mathrm{Ad}_D=\mathrm{Ad}_{D^{-1}PD}=\mathrm{Ad}_{PQ}\in\mathcal{P}_n,$$

which means that Ad_D belongs to the normalizer. By (9) and (10) the matrix assigned to Ad_D is therefore

$$\Phi(\mathrm{Ad}_D)=\begin{pmatrix}1 & 0\\ 1 & 1\end{pmatrix}.$$

The homomorphism Φ maps three elements of the normalizer Out_I, Ad_S, and Ad_D into three matrices generating the whole group H. This observation together with Proposition 6 gives us

Theorem 10: *The quotient group $\mathcal{N}(\mathcal{P}_n)/\mathcal{P}_n$ is isomorphic to the group*

$$\left\{\begin{pmatrix}a & b\\ c & d\end{pmatrix}\middle| a,b,c,d\in\mathbb{Z}_n,\ ad-bc=\pm 1 \bmod n\right\}=\mathrm{SL}(2,\mathbb{Z}_n)\cup\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\mathrm{SL}(2,\mathbb{Z}_n).$$

The direct consequence of Theorem 10 is

Corollary 11: *The normalizer $\mathcal{N}(\mathcal{P}_n)$ of the group $\mathcal{P}_n$ is generated by*

$$\mathrm{Out}_I,\mathrm{Ad}_S,\mathrm{Ad}_D,\mathrm{Ad}_Q \quad \textit{and} \quad \mathrm{Ad}_P.$$

If n is prime, i.e., $\mathbb{Z}_n$ is a field, we can use the Bruhat decomposition of $\mathrm{SL}(2,\mathbb{Z}_n)$ and explicitly describe the normalizer. It enables us to count the number of its elements. The group $\mathrm{SL}(2,\mathbb{Z}_n)$ is the union of two disjoint sets

$$\left\{\begin{pmatrix}1 & 0\\ a & 1\end{pmatrix}\begin{pmatrix}b & 0\\ 0 & b^{-1}\end{pmatrix}\middle| a\in\mathbb{Z}_n, b\in\mathbb{Z}_n^*\right\}$$

and

$$\left\{\begin{pmatrix}1 & 0\\ a & 1\end{pmatrix}\begin{pmatrix}b & 0\\ 0 & b^{-1}\end{pmatrix}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ c & 1\end{pmatrix}\middle| a,c\in\mathbb{Z}_n, b\in\mathbb{Z}_n^*\right\}.$$

Corollary 12: *Let n be a prime. Any element of the normalizer $\mathcal{N}(\mathcal{P}_n)$ has the form Ad_A or $\mathrm{Out}_I\,\mathrm{Ad}_A$, where $A=D^iM^jQ^kP^l$ or $A=D^iM^jSD^sQ^kP^l$.*

The normalizer $\mathcal{N}(\mathcal{P}_n)$ has therefore $2(n^2-1)n^3$ elements for an odd prime n and 24 elements for $n=2$ (here the outer automorphism does not play any role).

Summarizing, for any natural number n we described the generators of the normalizer $\mathcal{N}(\mathcal{P}_n)/\mathcal{P}_n$. For n prime we moreover were able to determine the cardinality of normalizer, using the Bruhat decomposition of the group $\mathrm{SL}(2,\mathbb{Z}_n)$. For the explicit description of the special n-dimensional representation of $\mathrm{SL}(2,\mathbb{Z}_n)$, where n is prime of the form $n=4K\pm 1$, see Ref. 20.

V. GRADED CONTRACTIONS OF *sl*(3,$\mathbb{C}$)

In this section we want to illustrate how the explicit knowledge of the normalizer of a fine grading can simplify and, indeed, bring further insight into the structure of the problem of finding all graded contractions of $sl(3,\mathbb{C})$. Practically one needs to solve a system of 48 quadratic equations involving 28 contraction parameters. The normalizer is the symmetry group of that system. It turns out that there are only two orbits of the normalizer among the 48 quadratic equations. For more conventional approach to this problem see Refs. 11 and 21.

Let $\mathcal{L}=\oplus_{i\in I}\mathcal{L}_i$ be a grading decomposition of a Lie algebra with the commutator $[\,\cdot\,,\cdot\,]$. Definition of the contracted commutator of the algebra involves the contraction parameters ε_{ij} for $i,j\in I$ and the old commutator. The new bilinear mapping of the form

$$[x,y]_{new}:=\varepsilon_{ij}[x,y] \quad \text{for all } x\in\mathcal{L}_i,\ y\in\mathcal{L}_j$$

is a commutator on the same vector space $\mathcal{L}$.

To satisfy antisymmetry of the commutator we have to choose $\varepsilon_{ij}=\varepsilon_{ji}$. To satisfy the Jacobi identity one has to solve a system of quadratic equations for the unknown contraction parameters ε_{ij}.

Let us illustrate this problem on the graded algebra $sl(3,\mathbb{C})=\oplus_{(i,j)\neq(0,0)}\mathcal{L}_{ij}$, which has 8 one-dimensional graded subspaces $\mathcal{L}_{ij}=\mathbb{C}X_{ij}$, where $0\leqslant i,j\leqslant 2$. For example, for the triple of vectors $X_{(0,1)}$, $X_{(0,2)}$, and $X_{(1,0)}$ the Jacobi identity has the form

$$[X_{(0,1)},[X_{(0,2)},X_{(1,0)}]_{\text{new}}]_{\text{new}}+\text{cyclically}=0.$$

The commutation relations (7) give us

$$\varepsilon_{(02)(10)}\varepsilon_{(01)(12)}(\omega-1)(\omega^2-1)X_{(1,0)}+\varepsilon_{(10)(01)}\varepsilon_{(02)(11)}(1-\omega)(\omega^2-1)X_{(1,0)}=0$$

and therefore

$$\varepsilon_{(02)(10)}\varepsilon_{(01)(12)}-\varepsilon_{(10)(01)}\varepsilon_{(02)(11)}=0. \tag{13}$$

For all possible triples of basis elements $X_{(i,j)}$ we have to write similar equations. There are $\binom{8}{3}=56$ triples. Since triples of the form $X_{(a,b)}$, $X_{(c,d)}$, and $X_{(e,f)}$, with $a+c+e=0(\mathrm{mod}\,3)$ and $b+d+f=0(\mathrm{mod}\,3)$ satisfy $[X_{(a,b)},[X_{(c,d)},X_{(e,f)}]]=0$, we have in fact only 48 equations.

The Jacobi identity for the triple $X_{(0,1)}$, $X_{(1,0)}$, and $X_{(1,1)}$, is the equality

$$\varepsilon_{(10)(11)}\varepsilon_{(01)(21)}-\varepsilon_{(11)(01)}\varepsilon_{(10)(12)}=0. \tag{14}$$

The triple of indices (0,1), (1,0), and (1,1) is distinguished by the property that the indices of any epsilon appearing in (14) are linearly independent over the field $\mathbb{Z}_3$. Quite different are the indices in (13) There the pair of indices (0,1) and (0,2) is linearly dependent over the field $\mathbb{Z}_3$. These two cases exhaust all distinct possibilities for the choice of triples in the Jacobi identity.

Consider now the mappings on the index set I defined by (11)

$$(i,j)\mapsto(i,j)A \quad \text{where} \quad A\in \mathrm{SL}(2,\mathbb{Z}_3).$$

Applying such a mapping with a fixed matrix A to the indices occurring in Eq. (13) we obtain a new equation corresponding to the Jacobi identity for another triple of grading subspaces. If we gradually apply all 24 matrices from $\mathrm{SL}(2,\mathbb{Z}_3)$ to Eqs. (13) and (14), we obtain all 48 quadratic equations which should be satisfied. In this way the symmetries of the system of equations are directly seen.

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Reduction restrictions of Darboux and Laplace transformations for the Goursat equation

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We study Darboux and Laplace transformations of the solutions and potentials of the Goursat equation which is equivalent to one of the Lax pair equations for the 2D-MKdV hierarchy. The reduction restrictions for these transformations are considered. The derived reduction equations are generalizations of the Liouville and sinh-Gordon equation. The integrability of these equations by the ST method is proved. The binary Darboux transformation for the Goursat equation is suggested. We find exact rational nonsingular solutions of the 2D-MKdV equations via the Moutard transformation for the Goursat equation. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1427761]

I. INTRODUCTION

A covariance of general Lax pairs leads to abundant but generally useless integrable systems while reductions of them may have straight applications in mathematical physics.[1] In $2+1$ or higher dimensions there exists the problem of an elaboration of similar or another approach to classification or at least of a choice of invariant subsets by some key rule.[2] Such a rule is directly connected with discrete covariance of Lax equations[3] that appears in the classic Laplace scheme developed by Darboux, Moutard, and Le Roux[4] and investigated recently from different points of view (e.g., Refs. 5 and 6). We consider subclasses of Laplace (Darboux)-covariant ''potentials,'' i.e., introduce a notion of ''reduction equation'' that follows directly from the constraint form invariance. It means that Darboux (Laplace) transforms together with the appropriate partial solutions of a basic equation determine some discrete symmetry and chains of solutions. Let us demonstrate this by an example.

It is known that the Laplace transformation (LT) of the equation

$$\psi_{xy}+a\psi_y+b\psi=0 \tag{1}$$

has the form

$$a\to a_{-1}=a-\partial_x \ln(b-a_y), \quad b\to b_{-1}=b-a_y, \quad \psi\to\psi_{-1}=\psi_x+a\psi, \tag{2}$$

$$a\to a_1=a+\partial_x \ln b, \quad b\to b_1=b+\partial_y(a+\partial_x \ln b), \quad \psi\to\psi_1=\frac{\psi_y}{b}, \tag{3}$$

and plays a significant role in the theory of soliton equation development.

The Goursat equation (GE) has the form[7]

$$\zeta_{xy}=2\sqrt{\lambda\zeta_x\zeta_y},$$

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where $\zeta=\zeta(x,y)$ and $\lambda=\lambda(x,y)$. We call λ a potential function. This equation can be linearized by the substitution $\psi=\sqrt{\zeta_x}$ and $\chi=\sqrt{\zeta_y}$. We get

$$\psi_y=\sqrt{\lambda}\chi, \quad \chi_x=\sqrt{\lambda}\psi$$

or

$$\psi_{xy}=\tfrac{1}{2}(\ln\lambda)_x\psi_y+\lambda\psi, \tag{4}$$

and the similar equation for the χ but we will not need one.

Equation (4) is the particular case of Eq. (1) with two potentials $a=a(x,y)$ and $b=b(x,y)$. This equation has two types of local discrete symmetries:

(1) Laplace transformations (2) and (3), mentioned above, and
(2) Darboux transformations (DT):

$$a\to a_1=a-\partial_x\ln(a+\tau), \quad b\to b_1=b+\tau_y, \quad \psi\to\psi_1=\psi_x-\tau\psi, \tag{5}$$

$$a\to{}_1a=-(\tau+b\rho), \quad b\to{}_1b=b-(b\rho)_y, \quad \psi\to{}_1\psi=\rho\psi_y-\psi, \tag{6}$$

where $\tau=\phi_x/\phi$, $\rho=\phi/\phi_y$, ψ and ϕ are particular solutions of (1) by preassigned a and b, and we call ϕ **the support function** of the DT.

The aim of this work is to study the validity of LT and DT for the GE. It is clear that after single DT or LT the reduction restriction

$$a=-\partial_x\ln b \tag{7}$$

will be true only for the special class of potentials and we will specify it in Sec. II.

Our interest in the GE is connected with the two applications of this equation in geometry and in the solitons theory, respectively.

(1) Let x be the complex coordinate, $y=-\overline{x}$, $\sqrt{\lambda}$ is the real-valued function, and ψ and χ from (1) are complex-valued functions. Then one defines three real-valued functions X_i, $i=1,2,3$, which are the coordinates of surface in R^3:[8]

$$X_1+iX_2=2i\int_\Gamma(\overline{\psi^2}dy'-\overline{\chi^2}dx'),$$

$$X_1-iX_2=-2i\int_\Gamma(\psi^2dy'-\chi^2dx'), \tag{8}$$

$$X_3=-2\int_\Gamma(\overline{\psi}\chi dy'+\overline{\chi}\psi dx'),$$

where Γ is an arbitrary path of integration in the complex plane. The corresponding first fundamental form, the Gaussian curvature K, and the mean curvature H yield

$$ds^2=4U^2dxdy, \quad K=\frac{1}{U^2}\partial_x\partial_y\ln U, \quad H=\frac{\sqrt{\lambda}}{U},$$

where

$$U=|\psi|^2+|\chi|^2,$$

and any analytic surface in R^3 can be globally represented by (8) (see Ref. 9).

(2) The system of the 2D-MKdV equations looks like:

$$4\lambda^2(\lambda_t - A\lambda_x + B\lambda_y - \lambda_{3x} - \lambda_{3y}) + 4\lambda^3[(2\lambda + B)_y + (2\lambda - A)_x]$$
$$+ 6\lambda(\lambda_y\lambda_{yy} + \lambda_x\lambda_{xx}) - 3(\lambda_x^3 + \lambda_y^3) = 0, \tag{9a}$$
$$B_x = 3\lambda_y - \lambda_x, \quad A_y = \lambda_y - 3\lambda_x.$$

Here $\lambda = \lambda(x,y,t)$, $A = A(x,y,t)$, $B = B(x,y,t)$. If we introduce the function $u = \sqrt{\lambda}$ then we can rewrite (9) in the more customary form (see Ref. 10):

$$u_t + 2u^2(u_x + u_y) + \tfrac{1}{2}(B_y - A_x)u + Bu_y - Au_x - u_{3y} - u_{3x} = 0$$
$$B_x = (3\partial_y - \partial_x)u^2, \quad A_y = (\partial_y - 3\partial_x)u^2. \tag{9b}$$

The reduction conditions

$$A = -B = -2u^2, \quad u_y = u_x,$$

lead us to the MKdV equation,

$$u_t + 12u^2u_x - 2u_{3x} = 0,$$

so we call (9a) the 2D-MKdV equations.

The 2D-MKdV equations (9) is the compatibility condition of the linear system (so-called [L, A] pair) which contains Eq. (4) and

$$\psi_t = \psi_{3x} + \psi_{3y} - \frac{3}{2}\frac{\lambda_y}{\lambda}\psi_{yy} + \left[\frac{3}{4}\left(\frac{\lambda_y}{\lambda}\right)^2 - \lambda - B\right]\psi_y + (A - \lambda)\psi_x + \frac{1}{2}(A_x - \lambda_x)\psi.$$

We will study (9a) in the last section (Sec. IV).

Remark 1: In Ref. 11 A. I. Zenchuk studied the discrete transformation (2), (3), (5), and (6) of solutions and potentials in the general case of the linear second order partial differential equation with two independent variables. The simplest ($k=2$) closed chains of these transformations are considered and the author obtain a novel **integrable** equation:

$$\tfrac{1}{2}S_{xy} - e^S - e^{-S}[C_1 - C_2\partial_x^{-1}(e^{-S})_y] = 0, \tag{10}$$

where $C_2 > 0$.

In the present work we use reduction restriction (7) as a (weak) condition of closing. In Sec. II we will obtain a new integrable equation [see (19)] which looks like (10) and it is a somewhat two-dimensional generalization of the sinh-Gordon equation. In Sec. III we suggest the binary DT for a construction of explicit solutions of the GE. These transformations allow one to obtain new solutions of the GE without solving some reduction equation. We also discuss the transformation for Laplace invariants.

II. THE REDUCTION EQUATIONS

The reduction restriction (7) is valid only for special types of potentials. These functions are solutions of the special equations which we call **reduction equations**. In this section we will obtain these equations for the LT and DT.

(I) Let us consider the Laplace transformations (2). The invariance of the reduction constraint means

$$\lambda_{-1} = \lambda - \frac{1}{2}\partial_x\partial_y \ln\lambda = \frac{C}{2\lambda}. \tag{11}$$

It is obvious that Eq. (11) is valid for the LT (3) because the one is inverse to the transformation (2).

It easy to show that the reduction equation for this transformation is the well-known sinh-Gordon equation:

$$\partial_x\partial_y \ln\lambda = 2\lambda - \frac{C}{\lambda}, \tag{12}$$

where $C=\text{const}$, and the new potential λ_{-1} is a solution of (12) too.

Let us remark that in the case of $C=0$ we obtain $\lambda_{-1}=0$ and the Liouville equation instead of (12). In this case the GE may be integrated and

$$\lambda = \frac{f'g'}{(f+g)^2}, \quad \zeta = -\frac{1}{C^2}\partial_y \ln(f+g) + V,$$

where $f=f(x)$ and $g=g(y)$ are arbitrary differentiable functions, $C=\text{const}$, $V=V(y)$ is the function such that

$$V' = \left[\frac{1}{2C}(\ln g')'\right]^2 = \frac{1}{4C^2}\left(\frac{g''}{g'}\right)^2,$$

and

$$\psi = \frac{\sqrt{f'g'}}{C(f+g)}, \quad \chi = \frac{1}{2C}\partial_y \ln\left(-\partial_y \frac{1}{f+g}\right).$$

Proposition 1: Let M and L be two Laplace invariants of Eq. (4). It means that

$$M = \tfrac{1}{2}\partial_x\partial_y \ln\lambda - \lambda, \quad L = -\lambda.$$

Using the reduction equation (11) we get

$$M = -\frac{C}{2\lambda}, \quad L = -\lambda$$

and

$$M_{-1} = M_1 = L, \quad L_{-1} = L_1 = M.$$

(II) Let us consider the DT (5). Inserting both transforms into the reduction condition (7) yields

$$\lambda_{-1} = \lambda - \tau_y = \lambda\left(\tau - \frac{\lambda_x}{2\lambda}\right). \tag{13}$$

Denote now $\alpha=\ln\phi$, $\Lambda=\ln\lambda$. Since

$$\lambda - \tau_y = (-\tfrac{1}{2}\Lambda_x + \alpha_x)\alpha_y,$$

and $\tau=\alpha_x$ one gets from the transform (13) the condition for Λ:

$$(\alpha_x - \tfrac{1}{2}\Lambda_x)[\alpha_y - \exp(\lambda)(\alpha_x - \tfrac{1}{2}\Lambda_x)] = 0. \tag{14}$$

The setting zero for the first parentheses yields

$$\Lambda_{xy} = 2\exp(\Lambda),$$

and $\alpha=\Lambda/2-c(y)$, where $c(y)$ is arbitrary function. But in this case we get $\lambda_1=0$, and the Liouville equation is in the realm of the reduction equation.

Setting equal to zero the square brackets in (14) one arrives at the relevant equation

$$(\exp(-2\alpha)\lambda)_x=(\exp(-2\alpha))_y, \tag{15}$$

therefore

$$\theta_x=\psi^2=\frac{1}{F_x+C_2}, \quad \lambda=\frac{F_y+C_1}{F_x+C_2},$$

where $F=F(x,y)$ is any differentiable function and $C_{1,2}=\text{const}$. Substituting (15) into (4) we get

$$2(C_2+F_x)C_1^2+[(F_{yxx}+4F_y)C_2+F_xF_{yxx}+4F_yF_x-F_{xx}F_{yx}]C_1+(F_{yxx}F_y-\tfrac{1}{2}F_{yx}^2+2F_y^2)C_2$$
$$+2F_y^2F_x-\tfrac{1}{2}F_{yx}^2F_x-F_yF_{xx}F_{yx}+F_xF_yF_{yxx}=0. \tag{16}$$

We define new fields:

$$F_x=P-C_2, \quad F_y=Q-C_1.$$

Then (16) can be split into the system

$$2Q_xQP_x-(2Q_{xx}Q-Q_x^2+4Q^2)P=0, \quad P_y=Q_x. \tag{17}$$

After integration of the first equation we get

$$P=\frac{CQ_x}{\sqrt{Q}}\exp(G), \quad G_x=2\frac{Q}{Q_x},$$

where C is the third constant of integration. It is necessary that the second equation in (17) will be true. Let

$$Q=n^2, \quad G=\ln m,$$

where $m=m(x,y)$ and $n=n(x,y)$. The reduction equation takes the simple form

$$(n^2)_x=2C(mn_x)_y, \quad m_xn_x=mn. \tag{18}$$

This system can be rewritten in more convenient form. Let

$$n_x=n\exp(S), \quad m_x=m\exp(-S),$$

$S=S(x,y)$. After substituting into (18) we get

$$S_y=\frac{1}{C}\frac{n}{m}-\partial_y\ln(mn),$$

therefore

$$S_{xy}=4\sinh S\partial_y\partial_x^{-1}\cosh S. \tag{19}$$

Equation (19) is the reduction equation for the DT (5). It looks like Eq. (10) and it is the generalization of $d=2$ sinh-Gordon equation. We will present the Lax pair analog for Eq. (19) by the following proposition:

Proposition 2: Let us introduce the $[L,A]$ pair for Eq. (19) in the form

$$K\psi=0, \quad K_1 D\psi=0$$

where

$$K=\partial_x\partial_y-\frac{1}{2}\frac{\lambda_x}{\lambda}\partial_y-\lambda, \quad K_1=\partial_x\partial_y-\frac{1}{2}\frac{\lambda_{1,x}}{\lambda_1}\partial_y-\lambda_1, \quad D=\partial_x-\tau,$$

the variables λ and λ_1 are defined by the equalities

$$\lambda=\frac{(S_x+2\cosh S)_y}{4\sinh S}\exp(-S), \quad \lambda_1=\frac{(S_x+2\cosh S)_y}{4\sinh S}\exp(S), \tag{20}$$

and

$$\tau_y\equiv\lambda-\lambda_1.$$

It is possible to check the statement by direct substitution. Thus the reduction equations for the DT (5) has either the form of Eq. (19) or the Liouville equation.

We can study the reduction equations for the DT (6) analogously. As a result we get

$$\lambda=C_1\phi_y\exp(F), \quad {}_1\lambda=-\frac{C_1C_2\phi^2}{\phi_y}\exp(F), \tag{21}$$

where ϕ is the support function of the DT (6) and the reduction equation can be written like the system:

$$\phi_{xy}=\phi_y[F_x+2C_1\phi\exp(F)], \quad F_y\phi_y-C_2\phi.$$

Proposition 3: By the construction (20) for the DT (5) we get

$$M=-\lambda_1, \quad L=-\lambda,$$

and

$$M_1=M\exp(-2S), \quad L_1=L\exp(2S).$$

Quite similar for the DT (6) the use of (21) gives

$$M=-\frac{C_2(-\phi_x+\phi F_x+C_1\phi^2\exp(F))}{\phi_y}, \quad L=-C_1\phi_y\exp(F),$$

and

$${}_1M=-\frac{\phi_y^2}{C_2\phi^2}M, \quad {}_1L=-\frac{C_2\phi^2}{\phi_y^2}L.$$

The multiple of the Laplace invariants ML is invariant in both cases.

III. BINARY DT

In Ref. 12 Ganzha studied the analog of the Moutard transformation for the Goursat equation. This transformation is valid without a reduction restriction and reduction equations. In this section we obtained binary Darboux transformation for the GE with the same property.

We introduce new variables ξ and η:

$$\partial_y=\partial_\eta-\partial_\xi, \quad \partial_x=\partial_\eta+\partial_\xi,$$

and rewrite (4) in the matrix form

$$\Psi_\eta = \sigma_3 \Psi_\xi + U\Psi, \tag{22}$$

where

$$\Psi = \begin{pmatrix} \psi_1 & \psi_2 \\ \chi_1 & \chi_2 \end{pmatrix}, \quad U = \sqrt{\lambda}\sigma_1, \tag{23}$$

$\psi_k = \psi_k(\xi, \eta)$, $\chi_k = \chi_k(\xi, \eta)$ with the $k = 1,2$ particular solutions of (1) with some $\lambda(\xi, \eta)$, and $\sigma_{1,3}$ are the Pauli matrices. Let Ψ_1 some solution of Eq. (22) and $\Psi \neq \Psi_1$. We define a matrix function $\tau \equiv \Psi_{1,\xi}\Psi_1^{-1}$. Equation (22) is covariant with respect to DT:

$$\Phi[1] = \Phi_\xi - \tau\Phi, \quad U[1] = U + [\sigma_3, \tau]. \tag{24}$$

Remark 2: It is not difficult to check that the DT (24) is the superposition formula for the two simpler Darboux transformations given by formulas (5) and (6).

Remark 3: Equation (22) is the spectral problem for the Davey–Stewartson (DS) equations.[13] The LTs produce an explicitly invertible Bäcklund autotransformation for the DS equations. In Ref. 14 we showed that these transformations allow one to construct solutions to the DS equations that fall off in all directions in the plane according to exponential and algebraic law.

Let us consider a closed one-form

$$d\Omega = d\xi \Phi\Psi + d\eta \Phi\sigma_3\Psi, \quad \Omega = \int d\Omega,$$

where a 2×2 matrix function Φ solves the equation

$$\Phi_\eta = \Phi_\xi \sigma_3 - \Phi U. \tag{25}$$

We shall apply the DT for (22). One can verify by immediate substitution that (25) is covariant with respect to the transform if

$$\Phi[+1] = \Omega(\Phi, \Psi_1)\Psi_1^{-1}.$$

Now we can alternatively affect U by the following transformation:

$$U[+1,-1] = U + [\sigma_3, \Psi_1\Omega^{-1}\Phi].$$

The particular solution of Eq. (25) has the form

$$\Phi_1 = \begin{pmatrix} s_1\psi_1 + s_2\psi_2 & -s_1\chi_1 - s_2\chi_2 \\ s_3\psi_1 + s_4\psi_2 & -s_3\chi_1 - s_4\chi_2 \end{pmatrix}, \tag{26}$$

where $s_k = \text{const}$ $(k = 1,...,4)$. It is convenient to choose one in the form

$$\Phi_1 = \Psi_1^T \sigma_3, \tag{27}$$

where Ψ_1^T is the transposed matrix Ψ_1 [(27) is the particular case of (26)].

In this case

$$U[+1,-1] = U - 2A_F, \tag{28}$$

where A_F is the off-diagonal part of the matrix A:

$$A = \Psi_1\Omega^{-1}\Psi_1^T,$$

$\Omega=\Omega(\Phi_1,\Psi_1)$, and

$$A_F^T=A_F=f\sigma_1, \tag{29}$$

where $f=f(\xi,\eta)$ is a some function.

Using (23), (28), and (29) we can see that $U[+1,-1]$ has the same form as the initial matrix U:

$$U[+1,-1]\equiv\begin{pmatrix} 0 & \sqrt{\lambda[+1,-1]} \\ \sqrt{\lambda[+1,-1]} & 0 \end{pmatrix}=\begin{pmatrix} 0 & \sqrt{\lambda}-2f \\ \sqrt{\lambda}-2f & 0 \end{pmatrix},$$

thus the reduction restriction is valid without the reduction equations.

The new function $\Phi[+1,-1]$ has the form

$$\Phi[+1,-1]=\Phi-\Omega(\Phi,\Psi_1)(\Omega(\Psi_1,\Psi_1))^{-1}\Phi_1, \tag{30}$$

where Φ is arbitrary solution of Eq. (25).

Using binary DT (28) and (30) we can construct a new solution of the GE from understanding particular solutions of one.

As a result we get the following theorem (in the old variables x and y):

Theorem: Let

$$\psi_{k,y}=\sqrt{\lambda}\chi_k, \quad \chi_{k,x}=\sqrt{\lambda}\psi_k, \quad \alpha_{k,y}=-\sqrt{\lambda}\beta_k, \quad \beta_{k,x}=-1\sqrt{\lambda}\alpha_k,$$

where $k=1,2$. Then new functions

$$\alpha_1'=\alpha_1-\frac{A_1\psi_1+A_2\psi_2}{D}, \quad \beta_1'=\beta_1+\frac{A_1\chi_1+A_2\chi_2}{D}$$

are solutions of the equations

$$\alpha_{1,y}'=\sqrt{\lambda'}\beta_1', \quad \beta_{1,x}'=\sqrt{\lambda'}\alpha_1',$$

where

$$\sqrt{\lambda'}=-\sqrt{\lambda}+\frac{\psi_1\chi_1\Omega_{22}+\psi_2\chi_2\Omega_{11}-(\psi_1\chi_2+\psi_2\chi_1)\Omega_{12}}{D},$$

and

$$\Omega_{11}=\int dx\psi_1^2+dy\chi_1^2, \quad \Omega_{12}=\Omega_{21}=\int dx\psi_1\psi_2+dy\chi_1\chi_2,$$

$$\Omega_{22}=\int dx\psi_2^2+dy\chi_2^2, \quad D=\Omega_{11}\Omega_{22}-\Omega_{12}^2,$$

$$\Lambda_{11}=\int dx\alpha_1\psi_1+dy\beta_1\chi_1, \quad \Lambda_{12}=\int dx\alpha_1\psi_2+dy\beta_1\chi_2,$$

$$\Lambda_{21}=\int dx\alpha_2\psi_1+dy\beta_2\chi_1, \quad \Lambda_{22}=\int dx\alpha_2\psi_2+\beta_2\chi_2,$$

$$A_1=\Lambda_{11}\Omega_{22}-\Lambda_{12}\Omega_{12}, \quad A_2=\Lambda_{12}\Omega_{11}-\Lambda_{11}\Omega_{12}.$$

Here $\int = \int_\Gamma$ where Γ is an arbitrary path of integration in the plane. It is easy to obtain the expressions for the functions α_2' and β_2', but we will not do it.

Thus the binary DT allows one to construct explicit solutions of the GE without the solving of some reduction equation.

IV. THE MOUTARD TRANSFORMATION FOR THE 2D-MKdV EQUATIONS

The Lax $([L,A])$ pair for the 2D-MKdV equations (9a) has the form

$$\psi_{xy} = \frac{u_x}{u}\psi_y + u^2\psi,$$
$$\psi_t = \psi_{3x} + \psi_{3y} - 3\frac{u_y}{u}\psi_{yy} + \left[3\left(\frac{u_y}{u}\right)^2 - u^2 - B\right]\psi_y + (A-u^2)\psi_x + \frac{1}{2}(A-u^2)_x\psi. \tag{31}$$

In Ref. 12 Ganzha studied the one of analog of the Moutard transformation for the Goursat equation. To use this transformation for obtaining exact solutions of (9a) we must complete a definition of the Moutard transformation. It is easy to do. Let ϕ be the second solution of (31) (the support function). Then we have a closed one-form,

$$d\theta = dx\,\theta_1 + dy\,\theta_2 + dt\,\theta_3, \quad \theta \equiv \int d\theta,$$

where

$$\theta_1 = \phi^2, \quad \theta_2 = \left(\frac{\phi_y}{u}\right)^2,$$

$$\theta_3 = (A-u^2)\phi^2 - \phi_y^2 - \phi_x^2 + 2\phi\phi_{xx} + \frac{(2\phi_{3y}\phi_y - \phi_{yy}^2 - B\phi_y^2)u^2 - 2u\phi_y(u_y\phi_y)_y + 3(u_y\phi_y)^2}{u^4}.$$

We define the **generalized** Moutard transformation in the following way:

$$u \to \tilde{u} = u - \sqrt{(\ln\theta)_x(\ln\theta)_y}, \quad A \to \tilde{A} = A - (\partial_x\partial_y - 3\partial_x^2)\ln\theta,$$
$$B \to \tilde{B} = B + (\partial_x\partial_y - 3\partial_y^2)\ln\theta, \quad \psi \to \tilde{\psi} = \frac{\phi Q}{\theta}, \tag{32}$$

where

$$Q \equiv \int dQ,$$

$$dQ = dx\,Q_1 + dy\,Q_2 + dt\,Q_3,$$

and $(w = \psi/\phi)$

$$Q_1 = \theta w_x, \quad Q_2 = -\frac{\theta^3(1/\theta)_{xy}w_y}{\theta_{xy}},$$

$$Q_3 = \theta w_{3x} + c_1 w_{3y} + c_2 w_{xx} + c_3 w_{yy} + c_4 w_x + c_5 w_y,$$

with

$$c_1=-\frac{\theta_{xy}}{2u^2}+\theta,\quad c_2=\frac{3}{2}\,\theta(\ln\theta_x)_x-\theta_x,\quad c_4=\left(\frac{3\phi_{xx}}{\phi}+A-u^2\right)\theta-\frac{\theta_{xx}}{2},$$

$$c_3=\frac{u_y\theta_{xy}}{2u^3}+\frac{\phi\phi_{yy}}{u^2}-\frac{3u_y\theta}{u}+3\left(\frac{\theta}{2}(\ln\theta_x)_y-\theta_y\right),$$

$$c_5=-\frac{3u_y^2\theta_{xy}}{2u^4}+\frac{1}{u^3}(\theta_{xy}u_{yy}+u_y\phi\phi_{yy})+\frac{1}{u^2}\left(3\theta u_y^2-\phi\phi_{3y}+\frac{1}{2}\left[B-\frac{\phi_{yy}}{\phi}\right]\theta_{xy}\right)$$
$$+\left(\frac{3\phi_{yy}}{\phi}-B\right)+\frac{u_y}{u}\left(2\theta_y-\frac{3\theta\theta_{xy}}{\theta_x}\right)+\frac{\theta_{xy}}{2}-u^2\theta.$$

The one-form dQ is closed,

$$Q_{1,y}=Q_{2,x},\quad Q_{1,t}=Q_{3,x},\quad Q_{2,t}=Q_{3,y}.$$

It is easy to verify that the $[L,A]$ pair (31) is covariant with respect to the generalized Moutard transformation (32).

Now we use these transformations to construct exact solutions of the 2D-MKdV equations (9a). First we would mention the known localized solutions from Ref. 10. Let us choose $u=\text{const}$, $A=B=0$. We will consider two examples.

(1) If we take the solution of (31) as $\phi=\sinh\xi$, where

$$\xi=ax+\frac{u^2}{a}y+\frac{(u^2-a^2)(u^4-a^4)}{a^3}t, \tag{33}$$

with the real $a=\text{const}$, then using (32) we get new solutions of the 2D-MKdV equations,

$$\tilde{u}=\frac{u[2\eta-a^3\sinh(2\xi)]}{2\eta+a^3\sinh(2\xi)},\quad \tilde{A}=\frac{16a^3\sinh\xi[3a^5\sinh\xi-(u^2-3a^2)\eta\cosh\xi]}{(2\eta+a^3\sinh(2\xi))^2},$$

$$\tilde{B}=\frac{16av^2\cosh\xi[3a^3u^2\cosh\xi-(3u^2-a^2)\eta\sinh\xi]}{(2\eta+a^3\sinh(2\xi))^2},$$

where

$$\eta=a^2(u^2y-a^2x)+(u^2-a^2)(3u^4+3a^4+2a^2u^2)t. \tag{34}$$

(2) To construct the algebraic solutions of (9a) we choose the solutions of (31) as

$$\phi=(-1)^n\int_\alpha^\beta dk\zeta(k)\exp(\xi(k))\frac{d^n}{dk^n}\delta(k-k_0),$$

with $\xi(k)$ from (33), $a=a(k)$, $\beta>k_0>\alpha>0$, and $\zeta(k)$ is some arbitrary differentiable function. For $n=1$, $\zeta=1$, we get

$$\tilde{u}=\frac{u(a^6-2\eta^2-2a^3\eta)}{2\eta^2+2a^3\eta+a^6},\quad \tilde{A}=-\frac{8a^6(u^2+3a^2)\eta(\eta+a^3)}{(2\eta^2+2a^3\eta+a^6)^2},$$
$$\tilde{B}=\frac{8u^2a^4(3u^2+a^2)\eta(\eta+a^3)}{(2\eta^2+2a^3\eta+a^6)^2}, \tag{35}$$

with the η from (34) and $a=a(k_0)$. Equation (35) is a simple nonsingular algebraic solution of the 2D-MKdV.

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On analytic properties of higher analogs of the second Painlevé equation

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In the present paper, we investigate value distribution of the higher analogs of the second Painlevé equation $({}_vP_2)$. After getting the precise expression of the dominant term of $({}_vP_2)$, we obtain some value distribution properties for the transcendental meromorphic solutions of $({}_vP_2)$ in the general case which generalize the theorems in Gromak and He [Proc. Math. Inst. Belarus Natl. Acad. Sci. **4**, 37–48 (2000)]. We further get other results for the $({}_vP_2)$ and $({}_4P_2)$. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1420396]

I. INTRODUCTION

It is well known that the Painlevé equations (P_1)–(P_6) are the most important second-order algebraic ordinary differential equations. They were first derived by Painlevé (1897) and by his colleagues at the end of the 19th century from strictly mathematical considerations. In the last few years, there has been considerable interest in the Painlevé equations due to the fact that some of their affinities with mathematical and physical equations, such as (P_2) and the Korteweg–de Vries (KdV) equation, have been found. They arise as reduction of solutions of soliton equations solved by the inverse scattering method.

On the other hand, many works have focused on a variety of properties of Painlevé equations. Recently, Hinkkanen and Laine (1999) completely proved that every local solution of (P_1) and (P_2) admits unrestricted analytic continuation, and hence is a meromorphic function in the complex plane. Steinmets (2001) and Shimomura (2001) proved, by different methods, that the growth order of the solutions of (P_1) and (P_2) are finite. In addition, value distribution properties of the solutions of the Painlevé equations are studied in Baesch (1992), Schubart (1996), Shimomura (2000), Steinmetsz (1989), and Wittich (1968).

In this paper, we are concerned with value distribution of the higher analog of (P_2) which arises as an exact reduction of the higher analog of the KdV equation $({}_m\text{KdV})$. Let L_u be the operator

$$L_u := 2(u + \hat{D}u\hat{D}^{-1}) - \hat{D}^2, \tag{1.1}$$

where $\hat{D} = \partial/\partial x$, $\hat{D}^{-1}$ denotes the integral operator $\int \cdot \, dx$. Consider the higher analog of the KdV equation in the form

$$(2m-1)u_t = X_m u \quad ({}_m\text{KdV})$$

$$X_m u = L_u X_{m-1} u = \hat{D}\frac{\partial H_m}{\partial u}, \tag{1.2}$$

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where $X_1u=\hat{D}u=u_x=\hat{D}(\partial H_1/\partial u)$ and H_m is the Hamiltonian system. Let $z=xt^{-1/(2m-1)}$, $u(x,t)=t^{-2/(2m-1)}q(z)$, then $q(z)$ satisfies the differential equation

$$X_mq+2q+zq'=0,$$

where L_q and X_mq are defined by (1.1) and (1.2) with q and z instead of u and x. If $q(z)=y'(z)+y^2(z)$, and we define the operator $S_y=4y^2+4y'D^{-1}y-D^2$ as in Adler and Moser (1979), we have

$$(2y+D)S_y=L_q(2y+D)$$

and

$$X_mq=(2y+D)S_y^{m-1}(y'). \tag{1.3}$$

Airault (1979) proved that the system

$$y'+y^2=q, \quad y\left(2\frac{\partial H_{m-1}}{\partial q}+z\right)+\alpha=X_{m-1}q$$

is equivalent to the algebraic differential equation

$$({}_vP_2) \quad D^{-1}S_y^{m-1}(y')+zy+\alpha=0,$$

where α is an arbitrary parameter. The order of $({}_vP_2)$ is $v=2m-2$. We call $({}_vP_2)$ the higher analog of the second Painlevé equation. If $m=2$, equations $({}_m\mathrm{KdV})$ and $({}_vP_2)$ become

$$3u_t=6uu_x-u_{xxx}$$

and the second Painlevé equation

$$y''=2y^3+zy+\alpha,$$

respectively, with the connection between the solutions $u(x,t)=t^{-2/3}(y'(z)+y^2(z))$, $z=xt^{-1/3}$, which is the well-known Ablowitz's result. For $m=3$, 4, and 5 in $({}_vP_2)$, we have

$$({}_4P_2) \quad y^{(4)}=10y^2y''+10y(y')^2-6y^5-zy-\alpha,$$

$$({}_6P_2) \quad y^{(6)}=14y^2y^{(4)}+56yy'y^{(3)}+42y(y'')^2-70(y^4-(y')^2)y''-140y^3(y')^2+20y^7+zy+\alpha,$$

$$\begin{aligned}({}_8P_2) \quad y^{(8)}=&18y^2y^{(6)}+108yy'y^{(5)}-6(21y^4-35(y')^2-38yy'')y^{(4)}-138y(y^{(3)})^2\\&-252y'(4y^3-3y'')y^{(3)}+182(y'')^3-756y^3(y'')^2+84y^2(5y^4-37(y')^2)y''\\&-798y(y')^4+1260y^5(y')^2-70y^9-zy-\alpha.\end{aligned}$$

Throughout this paper, we use the standard notations and basic results of the Nevanlinna theory such as $m(r,f)$, $N(r,f)$, $T(r,f)$, $N_1(r,f)=N(r,f)-\overline{N}(r,f)$,

$$\delta(f,c)=\liminf_{r\to\infty}\frac{m\left(r,\frac{1}{f-c}\right)}{T(r,f)}=1-\limsup_{r\to\infty}\frac{N\left(r,\frac{1}{f-c}\right)}{T(r,f)} \quad (c\neq\infty),$$

$$\delta(f,\infty)=\liminf_{r\to\infty}\frac{m(r,f)}{T(r,f)}=1-\limsup_{r\to\infty}\frac{N(r,f)}{T(r,f)},$$

$$\vartheta(f,\infty)=\liminf_{r\to\infty}\frac{N_1(r,f)}{T(r,f)}.$$

And $T(r,1/(f-c))=N(r,1/(f-c))+m(r,1/(f-c))=T(r,f)+O(1)$, $(c\neq\infty)$ is called Nevanlinna's first fundamental theorem.

II. MAIN RESULTS

Theorem 2.1: Let $y(z)$ be a nonrational meromorphic solution of $({}_vP_2)$, then

(i) if $\alpha\neq 0$, then $y(z)$ assumes every complex number $c\in C$ an infinite number of times;

(ii) if $\alpha=0$, then $y(z)$ assumes every nonzero complex number $c\in C\backslash\{0\}$ an infinite number of times. In both of the cases, $y(z)$ has an infinite number of poles and

$$\delta(y,c)=\delta(y,\infty)=0,$$

(iii) if $\alpha=0$, then $\delta(y,\alpha)=\delta(y,0)\leqslant 1/2$,

(iv) $\vartheta(f,\infty)=0$.

Corollary 2.2: Suppose $y(z)$ is a nonrational meromorphic solution of $({}_vP_2)$, then there exists a set E in R with finite linear measure such that for all a, $b\in C$, $a\neq b$ and $(|\alpha|+|a|)(|\alpha|+|b|)\neq 0$, we have

$$\lim_{r\to\infty}\frac{N\left(r,\dfrac{1}{y-a}\right)}{N\left(r,\dfrac{1}{y-b}\right)}=1$$

for $r\notin E$.

Theorem 2.3: Let $y(z)$ be the nonrational meromorphic solution of $({}_vP_2)$, then for $\alpha\neq 0$,

$$\liminf_{r\to\infty}\frac{N\left(r,\dfrac{1}{y'}\right)}{T(r,y)}=2.$$

Theorem 2.4: Suppose $y(z)$ is a nonrational meromorphic solution of $({}_4P_2)$, for $\alpha=(\epsilon/2)$ $(\epsilon^2=1)$, then $y(z)$ has infinite number of poles with residue $-\epsilon$ or 2ϵ, and there is not any pole with residue -2ϵ.

III. PROOF OF THEOREMS

To prove Theorem 2.1, we need the following propositions and lemmas.

Proposition 3.1: The differential polynomial of the left-hand side of $({}_vP_2)$ has only one dominant term in the form $A_m y^{2m-1}$ where

$$A_m=\prod_{j=1}^{m-1}\frac{2(2j-1)}{j}.$$

The degree of other terms is no greater than $2m-3$ and the coefficients are constants except for y whose coefficient is z.

Proof: First, we assert that differentiating or integrating a differential polynomial will neither increase nor decrease the degree of its leading term. In fact, let $y^{l_o}(y')^{l_1}\cdots(y^{(n)})^{l_n}$ be a differential monomial with degree $n_l=l_o+l_1+\cdots+l_n$, then

$$(y^{l_o}(y')^{l_1}\cdots(y^{(n)})^{l_n})'=\sum_{i=0}^{n} l_i y^{l_o}(y')^{l_1}\cdots(y^{(i)})^{l_i-1}(y^{(i+1)})^{l_{i+1}+1}\cdots(y^{(n)})^{l_n}. \tag{3.1}$$

It is obvious that the highest degree of the differential polynomial of the right-hand side of (3.1) is also n_l. On the other hand, if $y^{l_o}(y')^{l_1}\cdots(y^{(n)})^{l_n}$ can be integrated into another differential

polynomial and the highest degree of $\int y^{l_o}(y')^{l_1}\cdots(y^{(n)})^{l_n}dz$ were greater or less than n_l, then the degree of $(\int y^{l_o}(y')^{l_1}\cdots(y^{(n)})^{l_n}dz)'$ is also greater or less than n_l. It is impossible, therefore, that the degree of $\int y^{l_o}(y')^{l_1}\cdots(y^{(n)})^{l_n}dz$ is n_l.

We are going to prove proposition 3.1 by inductive method. For $m=2$, we have

$$\begin{aligned}D^{-1}S_y^{m-1}(y')+zy+\alpha&=D^{-1}S_y(y')+zy+\alpha\\&=D^{-1}(4y^2+4y'D^{-1}y-D^2)(y')+zy+\alpha\\&=D^{-1}(4y^2y'+4y'D^{-1}yy'-y''')+zy+\alpha\\&=\int(6y^2y'-y''')dz+zy+\alpha\\&=2y^3+zy-y''+\alpha.\end{aligned}$$

The dominant term of $D^{-1}S_y(y')$ is $2y^3$ whose degree 3 is greater than the degree of the remaining terms of $D^{-1}S_y(y')$. Therefore, the result holds when $m=2$. For $m=3$, we have

$$\begin{aligned}D^{-1}S_y^2(y')+zy+\alpha&=D^{-1}S_y(6y^2y'-y''')+zy+\alpha\\&=D^{-1}[30y^4y'+y^{(5)}-D12y(y')^2-D6y^2y''-4y^2y^{(3)}-4yy'y''+2(y')^3]\\&\quad+zy+\alpha=6y^5-10y^2y''-10y(y')^2+y^{(4)}+zy+\alpha.\end{aligned}$$

Obviously, the conclusion also holds and $D^{-1}S_y^2(y')$ has only one dominant term $6y^5$. The degree of the remaining term of $D^{-1}S_y^2(y')$ is no greater than $3(=2m-3)$.

Now we may assume that the conclusion in proposition 3.1 holds for $m=k$, i.e., the dominant term of $T=D^{-1}S_y^{k-1}(y')$ is only A_ky^{2k-1} (A_k is a constant only depending on k) and the degree of the remaining monomials is no greater than $2k-3$. We wish to show the result also holds for $m=k+1$. In fact,

$$\begin{aligned}D^{-1}S_y^k(y')+zy+\alpha&=D^{-1}S_yD[D^{-1}S_y^{k-1}(y')]+zy+\alpha\\&=D^{-1}(4y^2+4y'D^{-1}y-D^2)D[T]+zy+\alpha\\&=D^{-1}4y^2D[T]+D^{-1}4y'D^{-1}yD[T]-D^2[T]+zy+\alpha\\&=4y^2(T)-D^{-1}8yy'[T]-D^2[T]+D^{-1}4y'(y[T]-D^{-1}[T]y')+zy+\alpha\\&=-4yD^{-1}[T]y'+4y^2[T]-D^2[T]+zy+\alpha\\&=-4yD^{-1}\left[A_ky^{2k-1}+\sum_{l_o+\cdots+l_{2k-2}\leqslant 2k-3}b_{kl}(y)^{l_o}\cdots(y^{(2k-2)})^{l_{2k-2}}\right]\\&\quad\times Dy+4y^2\left(A_ky^{2k-1}+\sum_{l_o+\cdots+l_{2k-2}\leqslant 2k-3}b_{kl}(y)^{l_o}\cdots(y^{(2k-2)})^{l_{2k-2}}\right)\\&\quad-D^2[T]+zy+\alpha\\&=\frac{4(2k-1)A_k}{2k}y^{2k+1}+4y^2(T-A_ky^{2k-1})\\&\quad-D^2[T]-4yD^{-1}[T-A_ky^{2k-1}]Dy\\&=\frac{4(2k-1)A_k}{2k}y^{2k+1}+\cdots+zy+\alpha+\sum_{l_o+\cdots+l_{2k}\leqslant 2k-1}b_{kl}(y)^{l_o}\cdots(y^{(2k)})^{l_{2k}}.\end{aligned}$$

So the result holds for $m=k+1$. In addition, noting $A_2=2$, from the above-mentioned computing process, we have

$$\begin{aligned}A_{k+1}&=\frac{4(2k-1)A_k}{2k}=\frac{4(2k-1)}{2k}\,\frac{4[2(k-1)-1]}{2(k-1)}A_{k-1}\\&=\frac{4(2k-1)}{2k}\,\frac{4[2(k-1)-1]}{2(k-1)}\cdots\frac{4(4-1)}{4}A_2\\&=A_2\prod_{j=2}^{k}\frac{4(2j-1)}{2j}=\prod_{j=1}^{k}\frac{2(2j-1)}{j}.\end{aligned}$$

Now we can rewrite $({}_vP_2)$ in the following form:

$$\begin{aligned}P(\alpha,z,y,y',\ldots,y^{(2m-2)})&=(A_m y^{2m-1}+\cdots+zy+\alpha)+y^{(2m-2)}\\&\quad+\sum_{l=l_o+\cdots+l_{2m-2}\leqslant 2m-3}B_l(y)^{l_o}\cdots(y^{(2m-2)})^{l_{2m-2}}=0,\end{aligned}\tag{3.2}$$

where $l_o+l_1+\cdots+l_{2m-2}\geqslant 2$, $l_1+\cdots+l_{2m-2}\geqslant 1$ and B_l is constant.

Lemma 3.2 (J. Clunie): Let f be a transcendental meromorphic solution of

$$f^nP(z,f)=Q(z,f),$$

where $P(z,f)$ and $Q(z,f)$ are polynomials in f and its derivatives with meromorphic coefficients, say $\{a_\lambda|\lambda\in I\}$, such that $m(r,a_\lambda)=S(r,f)$ for all $\lambda\in I$. If the total degree of $Q(z,f)$ as a polynomial in f and its derivatives is $\leqslant n$, then

$$m(r,P(z,f))=S(r,f).$$

Lemma 3.3 (A. Z. Mohon'ko and V. D. Mohon'ko): Let

$$P(z,f,f',\ldots,f^{(n)})=0\tag{3.3}$$

be an algebraic differential equation, i.e., $P(z,u_o,u_1,\ldots,u_n)$ is a polynomial in all of its arguments, and let f be a transcendental meromorphic solution of (3.3). If a constant $c\in\mathbf{C}$ does not solve (3.3), then

$$m\left(r,\frac{1}{f-c}\right)=S(r,f).$$

For proofs of the lemmas, see Lemma 2.4.2 and Proposition 9.2.3 in Laine (1993).

Proposition 3.4: Suppose $y(z)$ is a nonrational solution of $({}_vP_2)$. If $\alpha=c=0$, then $m(r,y)\leqslant\frac{1}{2}T(r,y)+S(r,y)$.

Proof: If $\alpha=0$, multiply $({}_vP_2)$ by $2y'$ and integrating, we get

$$\begin{aligned}&\int_{z_o}^{z}2D^{-1}S_y^{m-1}(y')y'\,\mathrm{d}z+\int_{z_o}^{z}2zyy'\,\mathrm{d}z\\&\quad=2yD^{-1}S_y^{m-1}(y')\\&\quad\quad-\int_{z_o}^{z}2yS_y^{m-1}(y')\mathrm{d}z+zy^2-\int_{z_o}^{z}y^2\,\mathrm{d}z=0\ .\end{aligned}\tag{3.4}$$

By (1.2) and (1.3), we have

$$2yS_y^{m-1}(y')=X_m(y'+y^2)-DS_y^{m-1}(y')=D\frac{\partial H_m(q)}{\partial q}-DS_y^{m-1}(y'),$$

where $q=y'+y^2$, H_m is the Hamiltonian system. Therefore

$$\int_{z_o}^{z}2yS_y^{m-1}(y')\mathrm{d}z=\frac{\partial H_m(q)}{\partial q}-S_y^{m-1}(y')$$

is a differential polynomial. Since differentiating or integrating a differential polynomial does not change its total degree, by (3.2), (3.4) can be written in the following form:

$$\int_{z_o}^{z}y^2\,\mathrm{d}z=zy^2+\sum_{l=l_o+\cdots+l_{2m-3}\leqslant 2m-3}C_l(y)^{l_o}\cdots(y^{(2m-3)})^{l_{2m-3}}+C_0$$

with $l_o+l_1+\cdots+l_{2m-3}\geqslant 2$ and C_l, C_0 are constants. Set

$$G(z)=zy^2+\sum_{l=l_o+\cdots+l_{2m-3}\leqslant 2m-3}C_l(y)^{l_o}\cdots(y^{(2m-3)})^{l_{2m-3}}$$

by proposition 3.1 and lemma 3.2, we have $m(r,G)=S(r,y)$.

From $G'(z)=y^2$, it is easy to know that $m(r,G/G')=S(r,y)$. Since $y(z)$ has only simple poles [Gromak and He (2000)], we have

$$N(r,G)=N(r,G')-\overline{N}(r,G')=N(r,y^2)-\overline{N}(r,y^2)=N(r,y)$$

hence $T(r,G)=T(r,y)+S(r,y)$ and $S(r,G)=S(r,y)$. From all the above, we have

$$2m\left(r,\frac{1}{y}\right)=m\left(r,\frac{1}{y^2}\right)=m\left(r,\frac{1}{G'}\right)\leqslant m\left(r,\frac{G}{G'}\right)+m\left(r,\frac{1}{G}\right)=m\left(r,\frac{1}{G}\right)+S(r,y)\leqslant T(r,y)+S(r,y)$$

so we can get the result of proposition 3.4.

Proof of Theorem 2.1: Suppose $y(z)$ is a nonrational solution of $({}_vP_2)$. By (3.2), $({}_vP_2)$ can be written as

$$A_m y y^{2m-2}=\sum_{l=l_o+\cdots+l_{2m-2}\leqslant 2m-3}B_l(y)^{l_o}\cdots(y^{(2m-2)})^{l_{2m-2}}+zy+\alpha$$

then by lemma 3.2 it follows

$$m(r,y)=S(r,y).$$

Therefore, $\delta(y,\infty)=0$ and so y has infinitely many poles. And through computation, it is not difficult to know c does not solve (3.2) in both cases of (i) and (ii). By lemma 4.3, we have $m(r,1/(y-c))=S(r,y)$ for both cases, hence $\delta(y,c)=0$ and y has infinitely many c points.

If $\alpha=0$, by proposition 3.4 and the definition of $\delta(y,0)$, we have $\delta(y,0)\leqslant\frac{1}{2}$.

Note: Especially, for $({}_4P_2)$, the multiplicity of zeros of $y(z)$ is no more than 3. In fact, by $({}_4P_2)$, we have

$$\frac{y^{(4)}}{y}=10yy''+10y(y')^2-6y^4-z. \tag{3.5}$$

If z_o is a zero of $y(z)$ with multiply $k(k\geqslant 4)$, then z_o must be a pole of the left-hand side of (3.5), this contradicts with the right-hand side of (3.5).

(iv) follows from the fact that $y(z)$ has only simple poles.

Proof of Corollary 2.2: If $|\alpha|+|a|\neq 0$, then by Theorem 2.1 and Nevanlinna's first fundamental theorem

$$N\left(r,\frac{1}{y-a}\right)=T(r,y)-m\left(r,\frac{1}{y-a}\right)+O(1)=T(r,y)+S(r,y)$$

and then

$$N\left(r,\frac{1}{y-a}\right)=T(r,y)(1+o(1)),\quad r\notin E_1,$$

where E_1 is a set with finite linear measure. Similarly for $|\alpha|+|b|\neq 0$,

$$N\left(r,\frac{1}{y-b}\right)=T(r,y)(1+o(1)),\quad r\notin E_2,$$

where E_2 is a set with finite linear measure. Set $E=E_1\cup E_2$, then

$$\lim_{r\to\infty}\frac{N\left(r,\frac{1}{y-a}\right)}{N\left(r,\frac{1}{y-b}\right)}=1$$

for $r\notin E$.

Proof of Theorem 2.3: Differentiating (3.2), we get

$$\begin{aligned}y=&-(2m-1)A_m y^{2m-2}y'-\cdots-zy'\\&-\sum_{l\leqslant 2m-3}B_l\sum_{i=0}^{2m-2}l_i y^{l_o}\cdots(y^{(i)})^{l_i-1}(y^{(i+1)})^{l_{i+1}+1}\cdots(y^{(2m-2)})^{l_{2m-2}}\end{aligned}\tag{3.5$'$}$$

dividing (3.5) by y' and rewriting it as the following form:

$$\begin{aligned}\frac{y}{y'}=&-(2m-1)A_m y^{2m-2}-\cdots-z\\&-\sum_{l\leqslant 2m-3}B_l\sum_{i=0}^{2m-2}l_i y^{l_o}(y')^{l_1-1}\cdots(y^{(i)})^{l_i-1}(y^{(i+1)})^{l_{i+1}+1}\cdots(y^{(2m-2)})^{l_2m-2}\\=&L_1(y)+L_2(y)+L_3(y)=L(y)\ ,\end{aligned}$$

where $L_1(y)=-(2m-1)A_m y^{2m-2}-\cdots-z$, $L_2(y)=-\Sigma_{l\leqslant 2m-3}B_l l_o y^{l_o-1}(y')^{l_1}\cdots(y^{(2m-2)})^{l_{2m-2}}$,

$$L_3(y)=-\sum_{l\leqslant 2m-3}B_l\sum_{i=1}^{2m-2}l_i y^{l_o}(y')^{l_1-1}\cdots(y^{(i)})^{l_i-1}(y^{(i+1)})^{l_{i+1}+1}\cdots(y^{(2m-2)})^{l_2m-2}$$

and $l_1+\cdots+l_{2m-2}\geqslant 1$ for $L_3(y)$. Noting $m(r,y)=S(r,y)$ and $m(r,y^{(i+k)}/y^{(i)})=S(r,y)$ outside a set of r with finite linear measure, from the above-mentioned expression, we have

$$m\left(r,\frac{y}{y'}\right)=m(r,L(y))\leqslant M_1 m(r,y)+M_2\sum_{i=1}^{2m-2}m\left(r,\frac{y^{(i)}}{y}\right)+M_3\sum_{i=2}^{2m-2}m\left(r,\frac{y^{(i)}}{y'}\right)=S(r,y),\tag{3.6}$$

where M_1, M_2, and M_3 are constants. Since $m(r,1/y)=S(r,y)$ for $\alpha\neq 0$, we get

$$m\left(r,\frac{1}{y'}\right)\leqslant m\left(r,\frac{y}{y'}\right)+m\left(r,\frac{1}{y}\right)=S(r,y)$$

we know that $y(z)$ just has simple poles, thus

$$T(r,y')=m(r,y')+N(r,y')=2N(r,y)+S(r,y).$$

By Nevanlinna's first fundamental theorem, we have

$$N\left(r,\frac{1}{y'}\right)=T(r,y)-m\left(r,\frac{1}{y'}\right)+O(1)=2T(r,y)+S(r,y)$$

therefore

$$\liminf_{r\to\infty}\frac{N\left(r,\frac{1}{y'}\right)}{T(r,y)}=2.$$

This proves Theorem 2.3.

To prove Theorem 2.4, we need the following proposition:

Proposition 3.5: Suppose $y(z)$ is a nonrational meromorphic solution of $({}_4P_2)$ and z_o is a pole of $y(z)$, then $y(z)$ just has its poles with residues ±1, ±2 and if the residues $a_{-1}=\pm1$, $y(z)$ have the following expression

$$y(z)=\pm(z-z_o)^{-1}+a_1(z-z_o)+a_2(z-z_o)^2+\cdots \tag{3.7}$$

if the residues $a_{-1}=\pm2$, then

$$y(z)=\pm2(z-z_o)^{-1}+a_3(z-z_o)^3+\cdots. \tag{3.8}$$

Proof: Suppose $y(z)=a_{-1}(z-z_o)^{-1}+\Sigma_{n=1}^{\infty}a_n(z-z_o)^n$, substituting it into $({}_4P_2)$, then we have

$$\begin{aligned}
&24a_{-1}(z-z_o)^{-5}+\sum n(n-1)(n-2)(n-3)a_n(z-z_o)^{n-4}\\
&\quad=10\left(a_{-1}(z-z_o)^{-1}+\sum_{n=1}^{\infty}a_n(z-z_o)^n\right)^2\left(2a_{-1}(z-z_o)^{-3}+\sum_{n=1}^{\infty}n(n-1)a_n(z-z_o)^{n-2}\right)\\
&\qquad+10\left(a_{-1}(z-z_o)^{-1}+\sum_{n=1}^{\infty}a_n(z-z_o)^n\right)\left(-a_{-1}(z-z_o)^{-2}+\sum_{n=1}^{\infty}na_n(z-z_o)^{n-1}\right)^2\\
&\qquad-6\left(a_{-1}(z-z_o)^{-1}+\sum_{n=1}^{\infty}a_n(z-z_o)^n\right)^5-z\left(a_{-1}(z-z_o)^{-1}+\sum_{n=1}^{\infty}a_n(z-z_o)^n\right)-\alpha.
\end{aligned}\tag{3.9}$$

Comparing the coefficients of $(z-z_o)^{-5}$, we have $24a_{-1}=20(a_{-1})^3+10(a_{-1})^3-6(a_{-1})^5$, since $a_{-1}\neq0$, we get $a_{-1}=\pm1$ or ±2; comparing the coefficients of $(z-z_o)^{-3}$ of both sides of Eq. (3.9), we get $40a_1(a_{-1})^2-10a_1(a_{-1})^2-30a_1(a_{-1})^4=0$, it follows that $a_1=0$ or $a_{-1}=\pm1$; Similarly from the coefficients of $(z-z_o)^{-2}$, we get $60a_2(a_{-1})^2-30a_2(a_{-1})^2-6C_5^4a_2(a_{-1})^4=0$ and then $a_2=0$ or $a_{-1}=\pm1$. So $y(z)$ has the property shown in the theorem.

Proof of Theorem 2.4: According to Airault (1979) and Gromak and Lukashevich (1990) for $\alpha=\epsilon/2$, $({}_4P_2)$ is equivalent to the system

$$y' = -\epsilon y^2 + w, \quad w'' = 3\epsilon w^2 + \frac{\epsilon z}{2}. \tag{3.10}$$

Let $(w(z),\epsilon) = w_\epsilon(z)$ denote the solution of (3.10) with parameter ϵ; Let z_{-1}, z_1, z_{-2}, and z_2 denote the poles of $y(z)$ with residue -1, 1, -2, and 2, respectively. If $\epsilon = 1$, then by (3.8), (3.9), and the first equation of (3.10), the Laurent expansions of $w(z)$ around z_{-1}, z_2 and z_1 are

$$w_1(z) = \frac{2}{(z-z_{-1})^2} - 2a_3(z-z_{-1})^2 + \cdots,$$

$$w_1(z) = \frac{2}{(z-z_2)^2} + 7a_3(z-z_2)^2 + \cdots,$$

$$w_1(z) = 3a_1 + 4a_2(z-z_1) + \cdots,$$

respectively. These expansions show that $w_1(z)$ has double poles at z_{-1} and z_2 and it is analytic at z_1. For $z = z_{-2}$, from (3.8) and the first equation of (3.10), we have

$$w_1(z) = \frac{6}{(z-z_2)^2} - a_3(z-z_2)^3 + \cdots.$$

It is obvious that $w_1(z)$ is not a solution of (3.10), because it does not satisfy the second equation of (3.10). So in the case $\epsilon = 1$, $y(z)$ has no poles with residue -2. If $\epsilon = -1$, by using the same reasoning, we get the following conclusions: $w_{-1}(z)$ has second-order poles at z_1, z_{-2} and is analytic at z_{-1}; $y(z)$ has no poles with residue 2.

Let E_ϵ denote the set of poles of $y(z)$ with residues $-\epsilon$ and 2ϵ, then E_ϵ is also the set of the poles of $w_\epsilon(z)$. We assert E_ϵ is an infinite set. In fact, from the second equation of (18), we have

$$2m(r,w_\epsilon) = m\left(r, w_\epsilon \frac{w_\epsilon''}{w_\epsilon}\right) + O(\log r) \leqslant m(r,w_\epsilon) + S(r,w_\epsilon)$$

hence, $m(r,w_\epsilon) = S(r,w_\epsilon)$. Then $N(r,w_\epsilon) = T(r,w_\epsilon) + S(r,w_\epsilon)$, and by definition $w_\epsilon(z)$ has an infinite number of poles. This proves Theorem 2.4.

Question: Related to Theorem 2.4, we are not sure whether y has infinitely many poles with residues $-\epsilon$ and infinitely many with $+2\epsilon$, but we believe this to be the case.

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L^p spectral independence of the streaming operator

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The L^p spectrum of the streaming operator in spherical geometry with detailed balancing wall is discussed. First, the L^p-independence of the spectrum is established. Second, the Browder essential spectrum is proved to be empty except for ∞ under the assumption that the wall is nonmultiplying. Finally, we give a simple example to show that the L^p spectral independence of the operator is not valid if the wall is not detailed balancing. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The systematic study of L^p spectral independence of differential operators in L^p spaces was initiated by Simon. He conjectured in Refs. 1 and 2 that the spectrum of the Schrödinger operator $-\Delta+V$ is of L^p independence when V belongs to Kato class. This problem was solved by Hempel and Voigt.[3,4] Since then, the L^p spectral independence for some general and higher order elliptic operators was established by many researchers (see, e.g., Refs. 5–7, and the references therein). On the other hand, Hempel and Voigt[4] gave an interesting example (a second-order singular differential operator on the half line) which shows that the spectrum is L^p dependent. So, generally speaking, the spectra of physical interesting operators are not always L^p independence. Nevertheless, we will show in this paper that the L^p spectral independence of the streaming operator, which is important in physics (especially in gas dynamics,[8] neutron transport,[9,10] and radiative transfer,[11] etc.), is valid if the material wall satisfies the detailed balancing principle.

Roughly speaking, the streaming operator is a first-order singular differential operator equipped with a half range boundary condition which is expressed by an integral operator.[8,12–14] So, we may regard the streaming operator as a differential-integral operator (rather than a differential operator) which is different from the Schrödinger operator in its physical background. Physics suggests that the natural space for Schrödinger operator is L^2 (Refs. 1, 2, and 15) whereas the natural space for streaming operator is L^1.[8,12–14] But the streaming operator is also treated in L^p spaces for some technical reasons (see, e.g., Refs. 8, 16, and 17). Generally speaking, we can calculate the spectrum of an operator more easily in L^2 than in L^1. Then a question arises: Is the L^2 spectrum just the L^1 one? This is the problem of L^p spectral independence. If the answer to the problem is negative, then the dynamics governed by the operator in L^2 may differ greatly from that in L^1 and results obtained in L^2 space do not tell the real story of the original physical problem. So just as in the theory of Schrödinger operators, the problem of L^p spectral independence is also important in the theory of streaming operators. Of course, this problem is also interesting from a pure mathematical point.

This paper is organized as follows: In Sec. II we describe the problem and the main results, and give the equivalent description of the problem. In Sec. III we prepare some auxiliary propositions which will be used in the proof of the main results. Section IV is devoted to the proof of Theorems 2.1 and 2.2, and we will finish the proof by several steps. In Sec. V, a counterexample is given to show that the spectrum is L^p dependent if the wall does not satisfy the detailed balancing principle [condition (2) of Sec. II].

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II. DESCRIPTION OF THE PROBLEM AND MAIN RESULTS

For simplicity, we will restrict ourselves to the one-speed and spherical symmetric case. The spectrum of this operator was discussed in Refs. 12 and 13 in the L^1 setting. The multispeed case was thoroughly studied in Refs. 14 and 18, and we will follow the notations used there. Note that the results obtained in Ref. 14 are also valid for the one-speed case if we let $V_m=V_M=1$. It should be mentioned here that the spectra of the operator in slab geometry were discussed in Refs. 19 and 20 in L^1 space and in Refs. 16 and 17 (more general boundary conditions were considered) in L^p setting, and that more general cases (multidimensional and abstract boundary conditions) were discussed in Refs. 8 and 21 in the L^2 and L^1 spaces. Nevertheless, those authors did not investigate the L^p independent properties of the spectra.

Let $G=[0,R]\times[-1,1]$, $\Omega=[-1,1]$, the streaming operator B_p defined in the space $L^p(G,r^2 dr d\mu)$ for $1\leqslant p\leqslant\infty$ reads:

$$(B_p f)(r,\mu)=-\mu\frac{\partial}{\partial r}f(r,\mu)-\frac{1-\mu^2}{r}\frac{\partial}{\partial\mu}f(r,\mu)-\Sigma(r,\mu)f,\quad (r,\mu)\in[0,R]\times[-1,1]=G.$$

The domain $D(B_p)=\{f|f$ and $B_p f\in L^p(G,r^2\,\mathrm{d}r\,\mathrm{d}\mu)$ such that $f(r,\mu)$ satisfies the diffuse reflection boundary condition, i.e., $f(R,\mu)\in L^p(\Omega,|\mu|\mathrm{d}\mu)$, and $|\mu|f(R,\mu)=\int_0^1\alpha_0(\mu,\mu')\mu' f(R,\mu')\mathrm{d}\mu'$ for $\mu\in[-1,0)\}$. Where $\Sigma(r,\mu)$ is a bounded non-negative and measurable function, and $\alpha_0(\mu,\mu')$ is a non-negative and measurable function defined on $[-1,0)\times(0,1]$ which describes the interaction of particles with the boundary wall, we denote $\inf\{\Sigma(r,\mu)|(r,\mu)\in G\}$ by λ_0.

In the following, we suppose that the boundary wall is bounded multiplying (including conservative and nonmultiplying cases) and satisfies the detailed balancing principle, i.e., $\alpha_0(\mu,\mu')$ satisfies

$$\alpha=\sup\left\{\int_{-1}^{0}\alpha_0(\mu,\mu')\mathrm{d}\mu\,\middle|\,\mu'\in(0,1]\right\}<\infty,\tag{1}$$

$$|\mu'|\alpha_0(\mu,\mu')=|\mu|\alpha_0(-\mu',-\mu),\ (\mu,\mu')\in[-1,0)\times(0,1].\tag{2}$$

Furthermore, we also suppose that for every measurable subset $E\subset[-1,0)$ we have

$$\lim_{\mathrm{mes}\,E\to 0}\sup\left\{\int_E\alpha_0(\mu,\mu')\mathrm{d}\mu\,\middle|\,\mu'\in(0,1]\right\}=0.\tag{3}$$

Now we can write down our main results.

Theorem 2.1: *For every $p\in[1,\infty]$, we have, $\sigma(B_p)=\sigma(B_1)$.*

Theorem 2.2: *If $\alpha\leqslant 1$, then for every $p\in[1,\infty]$, $\sigma_{\mathrm{ess}}(B_p)=\{\infty\}$, where $\sigma_{\mathrm{ess}}(B_p)$ is the Browder essential spectrum of B_p.*

We remark that there exist several definitions of the essential spectrum and the Browder essential spectrum is the largest one among them (see, e.g., Ref. 22, p. 40). We also remark that the Browder essential spectrum is the complement of the discrete spectrum $\sigma_{\mathrm{dis}}(\cdot)$ relative to the spectrum $\sigma(\cdot)$ and the discrete spectrum $\sigma_{\mathrm{dis}}(\cdot)$ consists of all isolated eigenvalues with finite algebraic multiplicity (Ref. 23, pp. 242–243).

As in Refs. 12 and 14, we use the transformation $x=r\mu$, $y=r\sqrt{1-\mu^2}$, then B_p has the following equivalent form:

$$B_p:X_p\to X_p;(B_p\varphi)(x,y)=-\frac{\partial}{\partial x}\varphi(x,y)-\sigma(x,y)\varphi(x,y),$$

$$D(B_p)=\{\varphi|\varphi\ \text{ and }\ B_p\varphi\in X_p\ \text{ such that }\ \varphi(\pm\sqrt{R^2-y^2},y)\in Y_p,$$

and

$$\frac{y}{R^2}\varphi(-\sqrt{R^2-y^2},y)=\int_S \alpha(y,y')\frac{y'}{R^2}\varphi(\sqrt{R^2-y'^2},y')\mathrm{d}y'\},$$

where $X_p=L^p(D,y\,\mathrm{d}x\,\mathrm{d}y)$ and $Y_p=L^p(S,(y/R^2)\,\mathrm{d}y)$ with $D=\{(x,y)|x^2+y^2\leqslant R^2,y\geqslant 0\}$ and $S=[0,R]$. We denote the norms of X_p and Y_p by $\|\cdot\|_p$. Here for simplicity we introduced the following symbols:

$$\sigma(x,y)=\Sigma\left(\sqrt{x^2+y^2},\frac{x}{\sqrt{x^2+y^2}}\right),$$

$$\alpha(y,y')=\frac{y}{R\sqrt{R^2-y^2}}\alpha_0\left(-\frac{\sqrt{R^2-y^2}}{R},\frac{\sqrt{R^2-y'^2}}{R}\right).$$

With those in mind, we can rewrite Eqs. (1)–(3) as the following:

$$\alpha=\sup\left\{\int_S \alpha(y,y')\mathrm{d}y\,\middle|\,y'\in S\right\}<\infty, \tag{4}$$

$$y'\alpha(y,y')=y\alpha(y',y),(y,y')\in S\times S, \tag{5}$$

$$\lim_{\mathrm{mes}\,E\to 0}\sup\left\{\int_E \alpha(y,y')\mathrm{d}y\,\middle|\,y'\in S\right\}=0. \tag{6}$$

We will follow the notations of Ref. 14 and define the following operators:

$$M_{p,\lambda}:Y_p\to Y_p;(M_{p,\lambda}\psi)(y)=\int_S M(\lambda;y,y')\psi(y')\mathrm{d}y',$$

$$H_{p,\lambda}:X_p\to Y_p;(H_{p,\lambda}\varphi)(y)=\int_D H(\lambda;y,x',y')\varphi(x',y')\mathrm{d}x'\,\mathrm{d}y',$$

$$L_{p,\lambda}:Y_p\to X_p;(L_{p,\lambda}\psi)(x,y)=\exp\left(-\int_{-\sqrt{R^2-y^2}}^{x}\Delta(\lambda;z,y)\mathrm{d}z\right)\psi(y),$$

$$P_{p,\lambda}:X_p\to X_p;(P_{p,\lambda}\varphi)(x,y)=\int_{-\sqrt{R^2-y^2}}^{x}\exp\left(-\int_{x'}^{x}\Delta(\lambda;z,y)\mathrm{d}z\right)\varphi(x',y)\mathrm{d}x',$$

where

$$M(\lambda,y,y')=\frac{y'}{y}\alpha(y,y')\exp\left(-\int_{-\sqrt{R^2-y'^2}}^{\sqrt{R^2-y'^2}}\Delta(\lambda;z,y')\mathrm{d}z\right),$$

$$H(\lambda,y,x',y')=\frac{y'}{y}\alpha(y,y')\exp\left(-\int_{x'}^{\sqrt{R^2-y'^2}}\Delta(\lambda;z,y')\mathrm{d}z\right),$$

$$\Delta(\lambda;x,y)=\lambda+\sigma(x,y).$$

Remark 2.1: (i) If we denote the streaming operator defined in X_p with non-reentry boundary condition [i.e., $\alpha_0(\mu,\mu')=0$] by $B_{p,0}$, then $P_{p,\lambda}$ is nothing else but the resolvent of $B_{p,0}$ and the resolvent set $\rho(B_{p,0})=C$ (the whole complex plane).

(ii) The proof of the main theorems, which follows from several properties of the operators $M_{p,\lambda}$, $H_{p,\lambda}$, $L_{p,\lambda}$, and $P_{p,\lambda}$ established in Sec. III, will be given in Sec. IV, at present we want to describe the strategy used in the proof. We will show that (Proposition 4.3)

$$\sigma(B_p)=\{\lambda|1\in\sigma(M_{p,\lambda})\}\cup\{\infty\},p\in[1,\infty].$$

Then the problem reduces to prove the p independence of $\sigma(M_{p,\lambda})\backslash\{0\}$, which will be established in Proposition 4.2. It is worth notice that in proving Proposition 4.3 we also need to use Proposition 4.2. In general, spectra of integral operators (even with positively definite and symmetric kernels) may be dependent upon p.[3] In our situation, the kernel of $M_{p,\lambda}$ is unsymmetrical and very complicated. Nevertheless, we are able to show that it is of power compactness for $p=1,\infty$, which enables us to obtain the conclusions.

III. AUXILIARY THEOREMS

In this section, we prepare some auxiliary results which are useful in the proof of the main theorems. Especially, we will establish some compactness results and the analyticity of $M_{p,\lambda}$ and $H_{p,\lambda}$. In the L^1 setting, those results were obtained in Refs. 12–14, in order to derive those results in the L^p spaces, the detailed balancing principle is needed. In the following, we will denote the adjoint number of p by p'.

Proposition 3.1: The operators $M_{p,\lambda}$, $H_{p,\lambda}$, $L_{p,\lambda}$, and $P_{p,\lambda}$ have the following properties:

(i) *For every $\lambda\in C$ and every $p\in[1,\infty]$, $M_{p,\lambda}$, $H_{p,\lambda}$, $L_{p,\lambda}$, and $P_{p,\lambda}$ are bounded linear operators.*

(ii) *If* $\mathrm{Re}\,\lambda>-\lambda_0$, *then,*

$$r(M_{1,\lambda})<\alpha,\ \|M_{p,\lambda}\|<\alpha\quad\text{for } p\in(1,\infty],$$

where $r(M_{1,\lambda})$ is the spectral radius of $M_{1,\lambda}$.

(iii) *If* $\mathrm{Re}\,\lambda>-\lambda_0$, *then for every $p\in[1,\infty]$,*

$$\|H_{p,\lambda}\|\leqslant(\mathrm{Re}\,\lambda+\lambda_0)^{-1/p'}R^{-2/p}\alpha,\quad \|L_{p,\lambda}\|\leqslant R^{2/p}(p(\mathrm{Re}\,\lambda+\lambda_0))^{-1/p},\quad \|P_{p,\lambda}\|\leqslant\frac{1}{\mathrm{Re}\,\lambda+\lambda_0}.$$

Proof: The case of $p=1$ has been proved in Ref. 14, for $1<p<\infty$ and $\psi\in Y_p$ we have

$$\begin{aligned}\|M_{p,\lambda}\psi\|_p^p&=\int_S|(M_{p,\lambda}\psi)(y)|^p\frac{y}{R^2}\mathrm{d}y\\&=\int_S\left|\int_S M(\lambda;y,y')\psi(y')\mathrm{d}y'\right|^p\frac{y}{R^2}\mathrm{d}y\\&\leqslant\int_S\left(\int_S\frac{y'}{y}\alpha(y,y')\exp(-\sqrt{R^2-y'^2}(\mathrm{Re}\,\lambda+\lambda_0))|\psi(y')|dy'\right)^p\frac{y}{R^2}\mathrm{d}y.\end{aligned}$$

Using Hölder inequality and (5), we obtain,

$$\begin{aligned}\|M_{p,\lambda}\psi\|_p^p\leqslant&\int_S\left(\int_S\alpha(y',y)\exp(-\sqrt{R^2-y'^2}(\mathrm{Re}\,\lambda+\lambda_0))dy'\right)^{p/p'}\\&\times\left(\int_S y'\alpha(y,y')\exp(-\sqrt{R^2-y'^2}(\mathrm{Re}\,\lambda+\lambda_0))|\psi(y')|^p\,\mathrm{d}y'\right)\frac{1}{R^2}dy.\end{aligned}$$

If $\mathrm{Re}\,\lambda>-\lambda_0$, let

$$\alpha_1=\sup\left\{\int_S \alpha(y',y)\exp(-\sqrt{R^2-y'^2}(\mathrm{Re}\,\lambda+\lambda_0))\mathrm{d}y' \,\middle|\, y\in S\right\}$$

since

$$\alpha(y',y)\exp(-\sqrt{R^2-y'^2}(\mathrm{Re}\,\lambda+\lambda_0))<\alpha(y',y),\ (y,y')\in S\times S,$$

hence $\alpha_1<\alpha$, which implies that

$$\|M_{p,\lambda}\psi\|_p^p\leqslant\alpha_1^{p/p'}\alpha\int_S|\psi(y')|^p\frac{y'}{R^2}\mathrm{d}y',$$

i.e., $\|M_{p,\lambda}\|\leqslant\alpha_1^{1/p'}\alpha^{1/p}<\alpha$. Hence, $\|M_{p,\lambda}\|<\alpha$.

If $\mathrm{Re}\,\lambda\leqslant\lambda_0$, by a similar method we get

$$\|M_{p,\lambda}\psi\|_p^p\leqslant\alpha^{(p/p')+1}\exp\left(R|\mathrm{Re}\,\lambda+\lambda_0|\left(\frac{p}{p'}+1\right)\right)\int_S|\psi(y')|^p\frac{y'}{R^2}\mathrm{d}y'$$

so, $\|M_{p,\lambda}\psi\|_p\leqslant\alpha\exp(R|\mathrm{Re}\,\lambda+\lambda_0|)\|\psi\|_p$, which implies that $\|M_{p,\lambda}\|_p\leqslant\alpha\exp(R|\mathrm{Re}\,\lambda+\lambda_0|)$.

If $p=\infty$, then for $\psi\in Y_\infty$ we get from (4) and (5),

$$\begin{aligned}\|M_{\infty,\lambda}\psi\|_\infty&\leqslant\sup_{y\in S}\int_S M(\lambda;y,y')|\psi(y')|\mathrm{d}y',\\&\leqslant\sup_{y\in S}\int_S\frac{y'}{y}\alpha(y,y')\exp(-\sqrt{R^2-y'^2}(\mathrm{Re}\,\lambda+\lambda_0))|\psi(y')|\mathrm{d}y'\\&\leqslant\sup_{y\in S}\int_S\alpha(y',y)\exp(-\sqrt{R^2-y'^2}(\mathrm{Re}\,\lambda+\lambda_0))|\psi(y')|\mathrm{d}y'.\end{aligned}$$

Consequently, we obtain $\|M_{\infty,\lambda}\psi\|_\infty\leqslant\alpha_1\|\psi\|_\infty$ for $\mathrm{Re}\,\lambda>-\lambda_0$ and $\|M_{\infty,\lambda}\psi\|_\infty\leqslant\alpha\exp(R|\mathrm{Re}\,\lambda+\lambda_0|)\|\psi\|_\infty$ for $\mathrm{Re}\,\lambda\leqslant-\lambda_0$. That is to say, $\|M_{\infty,\lambda}\|_\infty\leqslant\alpha_1<\alpha$ for $\mathrm{Re}\,\lambda>-\lambda_0$ and $\|M_{\infty,\lambda}\|_\infty\leqslant\alpha\exp(R|\mathrm{Re}\,\lambda+\lambda_0|)$ for $\mathrm{Re}\,\lambda\leqslant-\lambda_0$.

Hence, (i) and (ii) of the theorem for $M_{p,\lambda}$ are proved. We can manage (i)–(iii) for the other three operators by similar procedures. Q.E.D.

Proposition 3.2: If $p=1$ or ∞, then for every $\lambda\in C$, $M_{p,\lambda}^2$ is compact. If furthermore $1\in\rho(M_{p,\lambda})$ and $\mu\in\rho(P_{p,\lambda})$, then $(L_{p,\lambda}(I-M_{p,\lambda})^{-1}H_{p,\lambda}(\mu I-P_{p,\lambda})^{-1})^2$ is compact.

Proof: It has been proved (see, Ref. 14, Lemma 2.3 and the proof of Theorem 3.2) that for $p=1$, $M_{p,\lambda}^2$ and $(L_{p,\lambda}(I-M_{p,\lambda})^{-1}H_{p,\lambda}(\mu I-P_{p,\lambda})^{-1})^2$ are compact operators for $\lambda\in C$ satisfying the conditions described previously. For $p=\infty$, we consider the following operators:

$$N_{1,\lambda}:Y_1\to Y_1;(N_{1,\lambda}\psi)(y)=\int_S\frac{y'}{y}M(\lambda;y',y)\psi(y')\mathrm{d}y',$$

$$J_{1,\lambda}:Y_1\to X_1;(J_{1,\lambda}\psi)(y)=\int_D\frac{1}{R^2}\frac{y'}{y}H(\lambda;y',x,y)\psi(y')\mathrm{d}y'.$$

Obviously, $M_{\infty,\lambda}=N_{1,\lambda}^\star$ and $H_{\infty,\lambda}=J_{1,\lambda}^\star$, where $\star$ means the adjoint operator. Define vector-valued functions $G_{1,\lambda}$ and $G_{2,\lambda}$ as

$$G_{1,\lambda}:S\to Y_1;G_{1,\lambda}(y')=\frac{y'}{y}M(\lambda;y',y),\quad y'\in S,$$

$$G_{2,\lambda}:S\to X_1;G_{2,\lambda}(y')=\frac{1}{R^2}\frac{y'}{y}H(\lambda;y',x,y),\quad y'\in S,$$

then we have

$$\begin{aligned}\|G_{1,\lambda}(y')\|_1&\leqslant\int_S\alpha(y',y)\exp(-2\sqrt{R^2-y^2}(\operatorname{Re}\lambda+\lambda_0))\frac{y}{R^2}\mathrm{d}y\\&\leqslant\int_S\alpha(y,y')\exp(-2\sqrt{R^2-y^2}(\operatorname{Re}\lambda+\lambda_0))\frac{y'}{R^2}\mathrm{d}y\\&\leqslant\alpha\exp(2R|\operatorname{Re}\lambda+\lambda_0|)\frac{1}{R},\end{aligned}\tag{7}$$

$$\begin{aligned}\|G_{2,\lambda}(y')\|_1&\leqslant\int_D\alpha(y',y)\exp(-(\sqrt{R^2-y^2}-x)(\operatorname{Re}\lambda+\lambda_0))\frac{y}{R^2}\mathrm{d}x\mathrm{d}y\\&\leqslant\int_D\alpha(y,y')\exp(-(\sqrt{R^2-y^2}-x)(\operatorname{Re}\lambda+\lambda_0))\frac{y'}{R^2}\mathrm{d}x\,\mathrm{d}y\\&\leqslant\alpha\exp(2R|\operatorname{Re}\lambda+\lambda_0|)\frac{1}{R}.\end{aligned}\tag{8}$$

Furthermore, for measurable subsets $E\in S$ and $F\in D$ we have

$$\int_E\frac{y'}{y}|M(\lambda;y',y)|\frac{y}{R^2}\mathrm{d}y\leqslant\int_E\alpha(y,y')\exp(2R|\operatorname{Re}\lambda+\lambda_0|)\frac{1}{R^2}\mathrm{d}y,$$

$$\int_F\frac{1}{R^2}\frac{y'}{y}|H(\lambda;y',x,y)|y\,\mathrm{d}x\,\mathrm{d}y\leqslant\int_F\frac{1}{R^2}\alpha(y,y')\exp(2R|\operatorname{Re}\lambda+\lambda_0|)\mathrm{d}x\,\mathrm{d}y.$$

By (6), we obtain that

$$\lim_{\text{mes }E\to0}\sup\left\{\int_E\frac{y'}{y}|M(\lambda;y',y)|\frac{y}{R^2}\mathrm{d}y\,\middle|\,y'\in S\right\}=0,\tag{9}$$

$$\lim_{\text{mes }F\to0}\sup\left\{\int_F\frac{1}{R^2}\frac{y'}{y}|H(\lambda;y',x,y)|y\,\mathrm{d}x\,\mathrm{d}y\,\middle|\,y'\in S\right\}=0.\tag{10}$$

It follows from (7)–(10) and Ref. 24 that $N_{1,\lambda}$ and $J_{1,\lambda}$ are weakly compact operators, consequently, $N_{1,\lambda}^2$ is compact. Hence, $M_{\infty,\lambda}^2=(N_{1,\lambda}^2)^\star$ is a compact operator. If $1\in\rho(M_{\infty,\lambda})$ and $\mu\in\rho(P_{\infty,\lambda})$, we consider the following operators:

$$T_{1,\lambda}:X_1\to Y_1;(T_{1,\lambda}\varphi)(y)=\int_{-\sqrt{R^2-y^2}}^{\sqrt{R^2-y^2}}R^2\exp\left(-\int_{-\sqrt{R^2-y^2}}^{x}\Delta(\lambda;z,y)\mathrm{d}z\right)\varphi(x',y)\mathrm{d}x',$$

$$Q_{1,\lambda}:X_1\to X_1;(Q_{1,\lambda}\varphi)(x,y)=\int_x^{\sqrt{R^2-y^2}}\exp\left(-\int_x^{x'}\Delta(\lambda;z,y)\mathrm{d}z\right)\varphi(x',y)\mathrm{d}x'.$$

Obviously, $T_{1,\lambda}^{\star}=L_{\infty,\lambda}$ and $Q_{1,\lambda}^{\star}=P_{\infty,\lambda}$. So, we have $1\in\rho(N_{1,\lambda})$ and $\mu\in\rho(Q_{1,\lambda})$, furthermore, $(L_{\infty,\lambda}(I-M_{\infty,\lambda})^{-1}H_{\infty,\lambda}(\mu I-P_{\infty,\lambda})^{-1})^2=\{((\mu I-Q_{1,\lambda})^{-1}J_{1,\lambda}(I-N_{1,\lambda})^{-1}T_{1,\lambda})^2\}^{\star}$. But $J_{1,\lambda}$ is weakly compact, so $((\mu I-Q_{1,\lambda})^{-1}J_{1,\lambda}(I-N_{1,\lambda})^{-1}T_{1,\lambda})^2$ is compact.[24] Hence, $(L_{\infty,\lambda}(I-M_{\infty,\lambda})^{-1}H_{\infty,\lambda}(\mu I-P_{\infty,\lambda})^{-1})^2$ is compact. Q.E.D.

Proposition 3.3: For every $p\in[1,\infty]$, the operator-valued functions $M_{p,\lambda}$, $H_{p,\lambda}$, $L_{p,\lambda}$ and $P_{p,\lambda}$ are analytic on the whole complex plane C.

Proof: Define bounded linear operators: $M'_{p,\lambda}:Y_p\to Y_p$, $H'_{p,\lambda}:X_p\to Y_p$, and $L'_{p,\lambda}:Y_p\to X_p$ as

$$(M'_{p,\lambda}\psi)(y)=\int_S -2\sqrt{R^2-y'^2}M(\lambda;y,y')\psi(y')\mathrm{d}y',$$

$$(H'_{p,\lambda}\varphi)(y)=\int_S (x'-\sqrt{R^2-y'^2})H(\lambda;y,x',y')\varphi(x',y')\mathrm{d}x'\,\mathrm{d}y',$$

$$(L'_{p,\lambda}\psi)(x,y)=-(x+\sqrt{R^2-y^2})(L_{p,\lambda}\psi)(x,y).$$

It follows from Ref. 25 that we only need to show that for $\psi\in Y_p$ and $\varphi\in X_p$,

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}M_{p,\lambda}\psi=M'_{p,\lambda}\psi,\quad \frac{\mathrm{d}}{\mathrm{d}\lambda}H_{p,\lambda}\varphi=H'_{p,\lambda}\varphi,\quad \frac{\mathrm{d}}{\mathrm{d}\lambda}L_{p,\lambda}\psi=L'_{p,\lambda}\psi.$$

Let $0<|\Delta\lambda|<1$ and denote $M(\lambda+\Delta\lambda;y,y')-M(\lambda;y,y')$ by $\Delta M(\lambda;y,y')$, then we have

$$|\Delta\lambda^{-1}\Delta M(\lambda;y,y')+2\sqrt{R^2-y'^2}M(\lambda;y,y')|\leqslant\exp(2R)|M(\lambda;y,y')|$$

and

$$\lim_{\Delta\lambda\to 0}(\Delta\lambda^{-1}\Delta M(\lambda;y,y')+2\sqrt{R^2-y'^2}M(\lambda;y,y'))=0.$$

On the other hand, by Hölder inequality we have

$$\begin{aligned}
&\|\Delta\lambda^{-1}(M_{p,\lambda+\Delta\lambda}\psi-M_{p,\lambda}\psi)-M'_{p,\lambda}\psi\|_p\\
&\quad\leqslant\int_S\frac{y}{R^2}\mathrm{d}y\left(\int_S\exp(2R)|M(\lambda;y,y')|\mathrm{d}y'\right)\\
&\qquad\times\left(\int_S|\Delta\lambda^{-1}\Delta M(\lambda;y,y')+2\sqrt{R^2-y'^2}M(\lambda;y,y')||\psi(y')|^p\,\mathrm{d}y'\right)\\
&\quad\leqslant C(\lambda)\int_S\frac{y}{R^2}\mathrm{d}y\int_S|\Delta\lambda^{-1}\Delta M(\lambda;y,y')+2\sqrt{R^2-y'^2}M(\lambda;y,y')||\psi(y')|^p\,\mathrm{d}y',
\end{aligned}$$

where $C(\lambda)=\alpha\exp(2R(1+|\mathrm{Re}\,\lambda+\lambda_0|))$. Using the above-given inequalities and the method used in the proof of Ref. 14, Lemma 2.3 (note that $|\psi|^p\in Y_1$ when $\psi\in Y_p$), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}M_{p,\lambda}\psi=M'_{p,\lambda}\psi.$$

Similarly, we can verify $(\mathrm{d}/\mathrm{d}\lambda)H_{p,\lambda}\varphi=H'_{p,\lambda}\varphi$ and $(\mathrm{d}/\mathrm{d}\lambda)L_{p,\lambda}\psi=L'_{p,\lambda}\psi$. The analyticity of $P_{p,\lambda}$ follows from Remark 2.1(i). Q.E.D.

IV. PROOF OF THE MAIN THEOREMS

We will finish the proof of Theorems 2.1 and 2.2 by the following several propositions:
Proposition 4.1: For every $\lambda \in C$,

$$\sigma(M_{1,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{1,\lambda})\backslash\{0\}=\sigma(M_{\infty,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{\infty,\lambda})\backslash\{0\}.$$

Proof: We have by Proposition 3.2 and Riesz–Schauder theory that

$$\sigma(M_{1,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{1,\lambda})\backslash\{0\}, \tag{11}$$

$$\sigma(M_{\infty,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{\infty,\lambda})\backslash\{0\}. \tag{12}$$

On the other hand, it is easy to verify that the adjoint operator of $M_{1,\lambda}$ is

$$M_{1,\lambda}^{\star}: Y_\infty \to Y_\infty; (M_{1,\lambda}^{\star}\psi)(y)=\int_S \alpha(y',y)\exp\left(-\int_{-\sqrt{R^2-y^2}}^{\sqrt{R^2-y^2}}\Delta(\lambda,z,y)dz\right)\psi(y')\mathrm{d}y'.$$

Define bounded linear operators T_1 and T_2 as follows,

$$T_1: Y_\infty \to Y_\infty; (T_1\psi)(y)=\exp\left(-\int_{-\sqrt{R^2-y^2}}^{\sqrt{R^2-y^2}}\Delta(\lambda,z,y)\mathrm{d}z\right)\psi(y),$$

$$T_2: Y_\infty \to Y_\infty; (T_2\psi)(y)=\int_S \alpha(y',y)\,\psi(y')\mathrm{d}y'$$

obviously, $T_1T_2=M_{1,\lambda}^{\star}$ and $T_2T_1=M_{\infty,\lambda}$. It follows from Ref. 25 that

$$\sigma(M_{1,\lambda}^{\star})\backslash\{0\}=\sigma(M_{\infty,\lambda})\backslash\{0\}. \tag{13}$$

So, the result follows from (11)–(13) and $\sigma(M_{1,\lambda})=\sigma(M_{1,\lambda}^{\star})$. Q.E.D.

Proposition 4.2: For every $\lambda \in C$ *and* $p \in [1,\infty]$,

$$\sigma(M_{p,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{p,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{1,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{\infty,\lambda})\backslash\{0\}.$$

Proof: It follows from Proposition 4.1 that

$$\sigma(M_{1,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{1,\lambda})\backslash\{0\}=\sigma(M_{\infty,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{\infty,\lambda})\backslash\{0\}. \tag{14}$$

By the definition of $M_{p,\lambda}$, the above (14) and $Y_\infty \subset Y_p \subset Y_1$ for $p \in [1,\infty]$, we have

$$\sigma_{\mathrm{dis}}(M_{\infty,\lambda})\backslash\{0\}\subset\sigma_{\mathrm{p}}(M_{p,\lambda})\backslash\{0\}\subset\sigma_{\mathrm{dis}}(M_{1,\lambda})\backslash\{0\}, \tag{15}$$

where $\sigma_{\mathrm{p}}(\cdot)$ represents the point spectrum of an operator.

If $\mu \in \rho(M_{1,\lambda})\backslash\{0\}=\rho(M_{\infty,\lambda})\backslash\{0\}$, then $(\mu I-M_{1,\lambda})^{-1}$ and $(\mu I-M_{\infty,\lambda})^{-1}$ are bounded operators, further,

$$(\mu I-M_{1,\lambda})(\mu I-M_{1,\lambda})^{-1}=(\mu I-M_{1,\lambda})^{-1}(\mu I-M_{1,\lambda})=I,$$

$$(\mu I-M_{\infty,\lambda})(\mu I-M_{\infty,\lambda})^{-1}=(\mu I-M_{\infty,\lambda})^{-1}(\mu I-M_{\infty,\lambda})=I.$$

For every $\psi \in Y_1 \cap Y_\infty = Y_\infty$, we have

$$(\mu I-M_{1,\lambda})(\mu I-M_{1,\lambda})^{-1}\psi=(\mu I-M_{1,\lambda})^{-1}(\mu I-M_{1,\lambda})\psi=\psi,$$

$$(\mu I-M_{\infty,\lambda})(\mu I-M_{\infty,\lambda})^{-1}\psi=(\mu I-M_{\infty,\lambda})^{-1}(\mu I-M_{\infty,\lambda})\psi=\psi,$$

so $(\mu I-M_{1,\lambda})^{-1}|_{Y_\infty}=(\mu I-M_{\infty,\lambda})^{-1}$. By Riesz–Thorin interpolation theorem[15] $(\mu I-M_{\infty,\lambda})^{-1}$ can be extended to any Y_p for $p\in[1,\infty]$. Furthermore, for every $\psi\in Y_\infty$ we have

$$(\mu I-M_{p,\lambda})(\mu I-M_{\infty,\lambda})^{-1}\psi=(\mu I-M_{\infty,\lambda})^{-1}(\mu I-M_{p,\lambda})\psi=\psi.$$

Since Y_∞ is dense in Y_p, hence $\mu\in\rho(M_{p,\lambda})$. This shows that

$$\sigma(M_{p,\lambda})\backslash\{0\}\subset\sigma(M_{1,\lambda})\backslash\{0\}. \tag{16}$$

It follows from (14)–(16) and the trivial inclusion $\sigma_p(M_{p,\lambda})\backslash\{0\}\subset\sigma(M_{p,\lambda})\backslash\{0\}$ that

$$\sigma(M_{p,\lambda})\backslash\{0\}=\sigma_p(M_{p,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{1,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{\infty,\lambda})\backslash\{0\}.$$

The fact that $\sigma_p(M_{p,\lambda})\backslash\{0\}=\sigma_{\mathrm{dis}}(M_{p,\lambda})\backslash\{0\}$ is obvious since $N((\mu I-M_{\infty,\lambda})^k)\subset N((\mu I-M_{p,\lambda})^k)\subset N((\mu I-M_{1,\lambda})^k)$ for every $\mu\in\sigma_p(M_{p,\lambda})$ and every positive integer k, where $N(\cdot)$ is the null space of an operator. Q.E.D.

Proposition 4.3 (Theorem 2.1): For every $p\in[1,\infty]$, $\sigma(B_p)=\sigma(B_1)$. *Furthermore* $\sigma(B_p)=\{\lambda|1\in\sigma(M_{p,\lambda})\}\cup\{\infty\}$ *and* $(\lambda I-B_p)^{-1}=L_{p,\lambda}(I-M_{p,\lambda})^{-1}H_{p,\lambda}+P_{p,\lambda}$ *for* $\lambda\in\rho(B_p)$.

Proof: The proof of $\{\lambda|1\in\rho(M_{p,\lambda})\}\subset\rho(B_p)$ and $(\lambda I-B_p)^{-1}=L_{p,\lambda}(I-M_{p,\lambda})^{-1}H_{p,\lambda}+P_{p,\lambda}$ is the same as that of Ref. 14, Theorem 3.1(i). In the following, we show that $\{\lambda|1\in\sigma(M_{p,\lambda})\}\subset\sigma(B_p)$.

It follows from Propositions 4.1 and 4.2 that $\{\lambda|1\in\sigma(M_{p,\lambda})\}=\{\lambda|1\in\sigma_{\mathrm{dis}}(M_{p,\lambda})\}$. Hence, for every $\lambda\in\{\lambda|1\in\sigma(M_{p,\lambda})\}$ there exists an eigenvector $\psi\in Y_p$ and $\psi\neq0$ such that $M_{p,\lambda}\psi=\psi$. Let

$$f(x,y)=(L_{p,\lambda}\psi)(x,y)=(L_{p,\lambda}M_{p,\lambda}\psi)(x,y);$$

then $f\in X_p$ and $f\neq0$. On the one hand, we have

$$f(-\sqrt{R^2-y^2},y)=(M_{p,\lambda}\psi)(y)=\psi(y),$$

$$f(\sqrt{R^2-y^2},y)=\exp\left(-\int_{-\sqrt{R^2-y^2}}^{\sqrt{R^2-y^2}}\Delta(\lambda,z,y)\,dz\right)\psi(y),$$

so $f\in X_p$ is continuously differentiable with respect to x and satisfies the boundary condition, which shows that $f\in D(B_p)$. On the other hand, it is easy to verify that $(\lambda I-B_p)f=0$. Therefore, we have shown $\{\lambda|1\in\sigma(M_{p,\lambda})\}\subset\sigma(B_p)$. $\sigma(B_p)=\sigma(B_1)$ follows from the above-mentioned result and Propositions 4.1 and 4.2. Q.E.D.

Remark 4.1: It follows from the proof of Proposition 4.3 that $\sigma(B_p)\backslash\{\infty\}=\sigma_p(B_p)\backslash\{\infty\}$ and $L_{p,\lambda}N(I-M_{p,\lambda})\subset N(\lambda I-B_p)$ for $p\in[1,\infty],\lambda\in\sigma_p(B_p)\backslash\{\infty\}$. On the other hand, we can show that $L_{p,\lambda}N(I-M_{p,\lambda})\supset N(\lambda I-B_p)$ (see Ref. 14, Proof of Theorem 3.2). Hence we obtain that $L_{p,\lambda}N(I-M_{p,\lambda})=N(\lambda I-B_p)$.

Proposition 4.4 (Theorem 2.2): If the boundary wall is nonmultiplying or conservative, i.e., $\alpha\leqslant1$, *then for every* $p\in[1,\infty],\sigma_{\mathrm{ess}}(B_p)=\{\infty\}$.

Proof: If $p=1$, the result has been proved [see, Ref. 14, the proof of Theorem 3.2(i)], if $p=\infty$, with Remark 2.1(i) and Propositions 3.1–3.3, we can manage it by the same perturbation method as in Ref. 14 (note that Proposition 3.1 and Ref. 26 show that there exist at most countable $\lambda\in C$ such that $1\in\sigma_p(M_{\infty,\lambda})$). If $1<p<\infty$, let $\lambda\in\sigma(B_p)=\sigma_p(B_p)$ (see Remark 4.1), then for every positive integer n we have

$$N((\lambda I-B_\infty)^n)\subset N((\lambda I-B_p)^n)\subset N((\lambda I-B_1)^n)$$

since $B_\infty\subset B_p\subset B_1$. On the other hand, since $\sigma_{\mathrm{ess}}(B_\infty)=\sigma_{\mathrm{ess}}(B_1)=\{\infty\}$, the closure of $\cap_{n=1}^{\infty}N((\lambda I-B_1)^n)$ is finitely dimensional, so is $\cap_{n=1}^{\infty}N((\lambda I-B_p)^n)$. Hence, $\lambda\in\sigma_{\mathrm{dis}}(B_p)$, that is, $\sigma_{\mathrm{ess}}(B_p)=\{\infty\}$. Q.E.D.

V. DISCUSSION

In this section we shall give an example which shows that when the wall is not detailed balancing the spectrum of B_p is L^p dependent. Let $\Sigma(r,\mu)=\Sigma$ and $\alpha_0(\mu,\mu')=\alpha_0$ be constants, then the detailed balancing condition (2) is not valid: $|\mu'|\alpha_0(\mu,\mu')\neq|\mu|\alpha_0(-\mu',-\mu)$. In this case we have

$$\alpha(y,y')=\frac{\alpha_0 y}{R\sqrt{R^2-y^2}},$$

$$M(\lambda,y,y')=\frac{\alpha_0 y'}{R\sqrt{R^2-y^2}}\exp\left(-\int_{-\sqrt{R^2-y'^2}}^{\sqrt{R^2-y'^2}}\Delta(\lambda;z,y')\mathrm{d}z\right),$$

$$H(\lambda,y,x',y')=\frac{\alpha_0 y'}{R\sqrt{R^2-y^2}}\exp\left(-\int_{x'}^{\sqrt{R^2-y'^2}}\Delta(\lambda;z,y')\mathrm{d}z\right),$$

and it has been proved that

Proposition 5.1 (*Ref. 12, Theorems 1 and 2): If* $p=1$ *and* $\alpha_0\leqslant 1$, *then*

$$\sigma(B_1)=\sigma_{\mathrm{dis}}(\mathrm{B}_1)\cup\{\infty\}=\left\{\lambda\left|\frac{\alpha_0(1-\exp(-2(\lambda+\Sigma)R))}{2(\lambda+\Sigma)R}=1\right.\right\}\cup\{\infty\}$$

and each $\lambda\in\sigma_{\mathrm{dis}}(B_1)$ *is a simple eigenvalue of* B_1.

Remark 5.1: In fact, this result is also valid for every $\alpha_0>0$ (i.e., multiplying boundary wall is covered) and $p\in[1,2)$. The proof is similar to that of Ref. 12, Theorems 1 and 2.

If $p\geqslant 2$, there is a different result. In fact, we have,

Proposition 5.2: If $p\geqslant 2$, *then* $\sigma(B_p)=C\cup\{\infty\}$.

Proof: For every $\lambda\in C$, we shall show $R(\lambda I-B_p)\neq X_p$, i.e., the range of $\lambda I-B_p$ does not equal X_p. Consequently, every $\lambda\in C$ belongs to the spectrum of B_p. We know that Y_p is continuously embedded in X_p. Let $g\in Y_p$, if $\varphi\in D(B_p)$ satisfies $(\lambda I-B_p)\varphi=g$, then we obtain by integrating it,

$$\begin{aligned}\varphi(\sqrt{R^2-y^2},y)=&\exp(-2(\lambda+\Sigma)\sqrt{R^2-y^2})\varphi(-\sqrt{R^2-y^2},y)\\&+(\lambda+\Sigma)^{-1}(1-\exp(-2(\lambda+\Sigma)\sqrt{R^2-y^2}))g(y).\end{aligned}\tag{17}$$

On the other hand, $\varphi(\pm\sqrt{R^2-y^2},y)$ satisfy the boundary condition, i.e., $\varphi(\pm\sqrt{R^2-y^2},y)\in Y_p$ and

$$\frac{y}{R^2}\varphi(-\sqrt{R^2-y^2},y)=\int_S\alpha(y,y')\frac{y'}{R^2}\varphi(\sqrt{R^2-y'^2},y')\mathrm{d}y'.\tag{18}$$

It follows from (17) and (18) that $\varphi(-\sqrt{R^2-y^2},y)=c(R^2-y^2)^{-1/2}$, where c is a constant. So, we have $c=0$, otherwise $\varphi(-\sqrt{R^2-y^2},y)\notin Y_p$ (note that $p\geqslant 2$), i. e., $\varphi(-\sqrt{R^2-y^2},y)=0$. In consideration of (17) and (18), we obtain

$$\int_S(\lambda+\Sigma)^{-1}(1-\exp(-2(\lambda+\Sigma)\sqrt{R^2-y^2}))g(y)y\,\mathrm{d}y=0,$$

which is impossible for many $g\in Y_p$. The proof is complete. Q.E.D.

Remark 5.2: It follows from Propositions 5.1 and 5.2 and Remark 5.1 that the spectrum of B_p is possibly L^p dependent if the material wall is not detailed balancing.

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ERRATA

Erratum: "Exact equation of state for 2-dimensional gravitating system within Tsallis statistical mechanics" [J. Math. Phys. 42, 1148–1153 (2001)]

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On page 1151, Eq. (18) should be replaced by

$$\frac{e^{ab}b^{1-z}}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}t\,\frac{e^{ibt}}{(a+\mathrm{i}t)^{z}}=\begin{cases}\dfrac{1}{\Gamma(z)} & \text{for } b>0\\ 0 & \text{for } b<0\end{cases}.$$

Also on page 1151, in line 4 the equation for b should be replaced by

$$b=\left[1-(1-q)\beta\sum_{i=1}^{N}(P_i^2/2m)\Big/\left(1+(q-1)\beta\sum_{i\neq j}Gm^2\ln|\mathbf{x}_i-\mathbf{x}_j|\right)\right].$$

The relativistic *J*-matrix theory of scattering: An analytic solution

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The relativistic J-matrix is investigated in the case of Coulomb-free scattering for a general short-range spin-dependent perturbing potential and in two different L^2 bases. The resulting recursion relation of the reference problem, in this case, has an analytic solution. The nonrelativistic limit is obtained and shown to be identical to the familiar nonrelativistic J-matrix. © *2002 American Institute of Physics.*
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The J-matrix[1–3] is an algebraic method of quantum scattering whose structure in function space parallels that of the R-matrix method in configuration space. The perturbing short range potential, $\tilde{V}(r)$, in the R-matrix method is confined to an "R-box" in configuration space [i.e., $\tilde{V}(r)=0$ for $r\geqslant R$], while in the J-matrix method it is confined to an "N- box" in function space. That is the matrix representation $\tilde{V}_{nm}=0$ for $n,m\geqslant N$. In the two methods, the unperturbed (reference) problem is solved analytically, enabling scattering calculation over a continuous range of energy despite the fact that confinement in both methods produce discrete energy spectra. The basis of the function space, in the J-matrix method, is chosen such that the matrix representation of the reference Hamiltonian, H_0, is tridiagonal. This has no parallel in the R-matrix method. It restricts the type of L^2 bases and limits reference Hamiltonians to those with this type of symmetry that admits such tridiagonal representations. It turns out that this restriction implies that the reference Hamiltonian must belong to the dynamical symmetry group SO(2,1).[4,5] Recently, a simple and robust numerical scheme was developed that lifts this restriction without compromising any of the advantages offered by the method.[6] The reference wave equation in the J-matrix method gives a symmetric three-term recursion relation for the expansion coefficients of the unperturbed wave function. The regularized analytic solutions of this recursion give the asymptotic scattering states that enable calculation of the phase shift after the introduction of the perturbing potential $\tilde{V}(r)$. The method together with its multi-channel extension[7,8] has been used successfully in a large number of scattering problems in atomic and nuclear physics.

P. Horodecki introduced a relativistic extension of the theory for the Coulomb free interaction.[9] This was followed by a systematic development of the theory for the Dirac–Coulomb problem that includes perturbing short-range potentials with spin-dependent coupling.[10] In this article, we investigate the case where $Z=0$ of the latter development and in two different L^2 bases: the Laguerre-type and oscillator-type functions. The motivation for this treatment comes from the fact that the resulting three-term recursion relation, in this case, has an analytic solution. This is in contrast to the general case, $Z\neq 0$, where the recursion relation was too difficult to solve analytically and a numerical solution is obtained.[10] It turns out that in the Coulomb-free case, the recursion relation is identical to the nonrelativistic one, whose analytic solution is well known,[3] except for a redefinition of the energy variable. The nonrelativistic limit is found and shown to coincide with the familiar nonrelativistic J-matrix. We carry out the detailed analysis of the problem in the two-component Laguerre-type L^2 basis. The extension to the oscillator-type basis,

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which is straightforward, is summarized in Table I that lists all quantities needed for relativistic scattering calculations in this basis.

In atomic units ($m=e=\hbar=1$) and taking the speed of light $c=\alpha^{-1}$, the free radial Dirac equation for a two-component spinor is[10,11]

$$\begin{pmatrix} 1 & \alpha\left(\frac{\kappa}{r}-\frac{d}{dr}\right) \\ \alpha\left(\frac{\kappa}{r}+\frac{d}{dr}\right) & -1 \end{pmatrix}\begin{pmatrix} \phi(r) \\ \theta(r) \end{pmatrix}=\varepsilon\begin{pmatrix} \phi(r) \\ \theta(r) \end{pmatrix}, \tag{1}$$

where α is the fine structure parameter and ε is the relativistic energy. Here κ is the spin-orbit coupling parameter defined by $\kappa=\pm(j+\frac{1}{2})$ for $l=j\pm\frac{1}{2}$, where j is the total angular momentum quantum number. Equation (1) relates the two components of the spinor wave function as

$$\theta(r)=\frac{\alpha}{\varepsilon+1}\left(\frac{\kappa}{r}+\frac{d}{dr}\right)\phi(r). \tag{2}$$

Substituting this back into Eq. (1) gives the following second-order differential equation for the upper component,

$$\left[-\frac{d^2}{dr^2}+\frac{\kappa(\kappa+1)}{r^2}-\frac{\varepsilon^2-1}{\alpha^2}\right]\phi(r)=0, \tag{3}$$

which is analogous to the radial potential-free Schrödinger equation

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}-2E\right]\chi(r)=0 \tag{4}$$

with the substitution $E=(\varepsilon^2-1)/2\alpha^2$ and $l=\kappa$ or $l=-\kappa-1$.

For building the relativistic J-matrix formalism, we need to construct an L^2 discrete representation in which the reference Hamiltonian,

$$H_0=\begin{pmatrix} 1 & \alpha\left(\frac{\kappa}{r}-\frac{d}{dr}\right) \\ \alpha\left(\frac{\kappa}{r}+\frac{d}{dr}\right) & -1 \end{pmatrix},$$

is tridiagonal so that the Dirac operator $J=H_0-\varepsilon$ gives a symmetric three-term recursion relation for the expansion coefficients of the spinor wave function. The solution of this recursion relation, subject to proper initial conditions, gives the two ''regularized'' solutions of the relativistic wave equation (1) that behave asymptotically as $\sin(kr)$ and $\cos(kr)$, where k is the energy-dependent wave number. Therefore, the J-matrix formalism can be applied giving the relativistic S-matrix for a scattering problem with perturbing short-range potential $\tilde{V}(r)$.[3,10] The L^2 space is spanned by the two-component radial spinor wave functions $\{\psi_n(r)\}_{n=0}^{\infty}$ whose upper component is $\phi_n(r)$ and lower component is $\theta_n(r)$. The conjugate space is spanned by $\{\overline{\psi}_n(r)\}_{n=0}^{\infty}$ such that

$$\langle\overline{\psi}_n|\psi_m\rangle=\int_0^{\infty}\overline{\phi}_n(r)\phi_m(r)dr+\int_0^{\infty}\overline{\theta}_n(r)\theta_m(r)dr=\delta_{nm}. \tag{5}$$

Now, the analogy of the second order differential equation (3) to the Schrödinger equation (4) suggests that the upper spinor component can be taken to be either of the Laguerre-type or oscillator-type basis functions of the nonrelativistic J-matrix[3] with $l=\kappa$. We shall work out the

TABLE I. The table gives the oscillator-type spinor basis $\{\phi_n,\theta_n\}_{n=0}^{\infty}$, its J-matrix coefficients $\{s_n,c_n\}$, the matrix elements of the reference Hamiltonian and that of the scattering short range potential. In the table ζ is an arbitrary real parameter, ${}_1F_1(a;c;z)$ is the confluent hypergeometric function, $\eta(\varepsilon)\equiv k(\varepsilon)/\lambda$ where $k(\varepsilon)$ is as defined in Eq. (15), and $G^{\nu}_{nm}\equiv\Sigma_{k=0}^{M-1}\Lambda^{\nu}_{nk}\Lambda^{\nu}_{mk}f[(\xi^{\nu}_k)^{1/2}/\lambda]$, $Q^{\nu}_{nm}\equiv\Sigma_{k=0}^{M-1}(\xi^{\nu}_k)^{-1/2}\Lambda^{\nu}_{nk}\Lambda^{\nu}_{mk}f[(\xi^{\nu}_k)^{1/2}/\lambda]$, where the eigenvalues $\{\xi^{\nu}_n\}_{n=0}^{M-1}$ and corresponding normalized eigenvectors $\{\Lambda^{\nu}_{mn}\}_{n,m=0}^{M-1}$ are associated with the same $M\times M$ tridiagonal matrix (17) but for a different value of the parameter ν.

$\phi_n(r)$	$a_n(\lambda r)^{\kappa+1}e^{-\lambda^2r^2/2}L_n^{\kappa+1/2}(\lambda^2r^2)$
$\theta_n(r)$	$\lambda C a_n(\lambda r)^{\kappa}e^{-\lambda^2r^2/2}[(n+\kappa+\frac{1}{2})L_n^{\kappa-1/2}(\lambda^2r^2)+(n+1)L_{n+1}^{\kappa-1/2}(\lambda^2r^2)]$
a_n	$\sqrt{2\lambda\Gamma(n+1)/\Gamma(n+\kappa+\frac{3}{2})}$
$\overline{\phi_n}(r)$	$\zeta\phi_n(r)+\dfrac{(1-\zeta)/2}{2n+\kappa+\frac{3}{2}}(\lambda r)^2\phi_n(r)$
$\overline{\theta_n}(r)$	$\dfrac{(1-\zeta)/2\lambda^2C^2}{2n+\kappa+\frac{3}{2}}\theta_n(r)$
$(H_0)_{nm}$	$(H_0)_{nn}=1+\lambda^2C^2(-1+2\alpha/C)(2n+\kappa+\frac{3}{2})$ $(H_0)_{n,n-1}=\lambda^2C^2(-1+2\alpha/C)\sqrt{n(n+\kappa+\frac{1}{2})}$ $(H_0)_{n,n+1}=\lambda^2C^2(-1+2\alpha/C)\sqrt{(n+1)(n+\kappa+\frac{3}{2})}$
I_{nm}	$I_{nn}=1+\lambda^2C^2(2n+\kappa+\frac{3}{2})$ $I_{n,n-1}=\lambda^2C^2\sqrt{n(n+\kappa+\frac{1}{2})}$ $I_{n,n+1}=\lambda^2C^2\sqrt{(n+1)(n+\kappa+\frac{3}{2})}$
$\tilde{V}_{nm}$	$\tilde{V}_{nm}\cong\alpha^2\tilde{V}_+G^{\kappa+1/2}_{n,m}+\alpha^2\lambda^2C^2\tilde{V}_-[\sqrt{(n+\kappa+\frac{1}{2})(m+\kappa+\frac{1}{2})}G^{\kappa-1/2}_{n,m}+\sqrt{(n+1)(m+1)}G^{\kappa-1/2}_{n+1,m+1}$ $+\sqrt{(m+1)(n+\kappa+\frac{1}{2})}G^{\kappa-1/2}_{n,m+1}+\sqrt{(n+1)(m+\kappa+\frac{1}{2})}G^{\kappa-1/2}_{m,n+1}]$ $+2\alpha^2\lambda C\tilde{V}_0[\sqrt{(n+\kappa+\frac{1}{2})(m+\kappa+\frac{1}{2})}Q^{\kappa-1/2}_{n,m}-\sqrt{(n+1)(m+1)}Q^{\kappa-1/2}_{n+1,m+1}]$
$c_n(\varepsilon)$	$(-1)^n\dfrac{\Gamma(\kappa+\frac{1}{2})}{\sqrt{2\pi}}\dfrac{a_n}{\lambda}\eta^{-\kappa}e^{-\eta^2/2}\,{}_1F_1(-n-\frac{1}{2}-\kappa;\frac{1}{2}-\kappa;\eta^2)$
$s_n(\varepsilon)$	$\dfrac{(-1)^n}{\lambda}\sqrt{\dfrac{\pi}{2}}a_n\eta^{\kappa+1}e^{-\eta^2/2}L_n^{\kappa+1/2}(\eta^2)$

details in the first basis. The results for the second basis are obtainable the same way and in a straightforward manner. These results are summarized in Table I, which lists all quantities needed for relativistic scattering calculations in this basis.

In the Laguerre-type basis the stated analogy suggests that we can write

$$\phi_n(r)=a_n(\lambda r)^{\kappa+1}e^{-\lambda r/2}L_n^{2\kappa+1}(\lambda r), \tag{6}$$

where λ is the basis scale parameter and $L_n^{2\kappa+1}(x)$ is the generalized Laguerre polynomial. The normalization constant a_n will be determined from the normalization condition (5). Here $\phi_n(r)$ satisfies the following differential equation

$$\left[-\frac{d^2}{dr^2}+\frac{\kappa(\kappa+1)}{r^2}-\frac{\lambda(\kappa+n+1)}{r}+\frac{\lambda^2}{4}\right]\phi_n(r)=0.$$

The requirement that the matrix representation of the reference Hamiltonian and the basis-overlap matrix, $\langle \psi_n | \psi_m \rangle$, be at most tridiagonal is satisfied by the following expression for the lower component,

$$\theta_n(r) = C\left(\frac{\kappa}{r} + \frac{d}{dr}\right)\phi_n(r), \tag{7}$$

where the small component strength parameter, C, is nonzero and independent of n. This expression is also motivated by the solution of the wave equation in (2). Using the differential and recursion properties of the Laguerre polynomials,[12] we can write (7) explicitly as

$$\theta_n(r) = \frac{\lambda C}{2} a_n (\lambda r)^{\kappa} e^{-\lambda r/2}[(2\kappa + n + 1)L_n^{2\kappa}(\lambda r) + (n+1)L_{n+1}^{2\kappa}(\lambda r)]. \tag{8}$$

The orthogonal conjugate representation defined in (5) gives

$$\overline{\phi}_n(r) = \frac{(1-\zeta)/4}{\kappa + n + 1}\phi_n(r) + \frac{\zeta}{\lambda r}\phi_n(r), \quad \overline{\theta}_n(r) = \frac{(1-\zeta)/\lambda^2 C^2}{\kappa + n + 1}\theta_n(r),$$

where ζ is an arbitrary constant parameter. The normalization constant obtained is

$$a_n = \sqrt{\lambda \Gamma(n+1)/\Gamma(2\kappa + n + 2)}.$$

In this basis, which is defined by the set of functions in Eqs. (6) and (8), the matrix representation of the reference Hamiltonian H_0 is tridiagonal and has the following elements:

$$\begin{aligned}
(H_0)_{n,n} &= 2(\kappa + n + 1)[1 - (\lambda C/2)^2(1 - 2\alpha/C)], \\
(H_0)_{n,n+1} &= -\sqrt{(n+1)(2\kappa + n + 2)}[1 + (\lambda C/2)^2(1 - 2\alpha/C)], \\
(H_0)_{n,n-1} &= -\sqrt{n(2\kappa + n + 1)}[1 + (\lambda C/2)^2(1 - 2\alpha/C)].
\end{aligned} \tag{9}$$

The tridiagonal basis-overlap matrix elements, $I_{nm} = \langle \psi_n | \psi_m \rangle$, are

$$\begin{aligned}
I_{n,n} &= 2(\kappa + n + 1)[1 + (\lambda C/2)^2], \\
I_{n,n+1} &= -\sqrt{(n+1)(2\kappa + n + 2)}[1 - (\lambda C/2)^2], \\
I_{n,n-1} &= -\sqrt{n(2\kappa + n + 1)}[1 - (\lambda C/2)^2].
\end{aligned} \tag{10}$$

These will define the matrix elements of the tridiagonal Dirac operator $J_{nm}(\varepsilon) = (H_0)_{nm} - \varepsilon I_{nm}$ that gives the symmetric three-term recursion relation.

The expansion coefficients of the spinor wave function that solves the reference equation (1) satisfy this recursion relation, which reads

$$J_{n,n-1}h_{n-1} + J_{n,n}h_n + J_{n,n+1}h_{n+1} = 0, \quad n \geqslant 1, \tag{11}$$

where h_n stands for either s_n or c_n (the asymptotic sinelike and cosinelike solutions, respectively). The initial relations are[10]

$$J_{00}s_0 + J_{01}s_1 = 0, \quad J_{00}c_0 + J_{01}c_1 = -\alpha^2 W/2s_0,$$

where $W(\varepsilon)$ is the Wronskian of the regular and irregular solutions of the free Dirac problem:

$$W(\varepsilon)=W(\psi_{\rm reg},\psi_{\rm irreg})=\psi_{\rm reg}\frac{d\psi_{\rm irreg}}{dr}-\psi_{\rm irreg}\frac{d\psi_{\rm reg}}{dr}=-\frac{2}{\alpha}\sqrt{\frac{\varepsilon-1}{\varepsilon+1}}.$$

These coefficients also satisfy the Wronskian-like relation

$$J_{n,n-1}(c_n s_{n-1}-c_{n-1}s_n)=-\alpha^2 W/2,\quad n\geqslant 1.$$

Using the matrix elements given in (9) and (10), we can write the homogeneous recursion relation (11) as

$$2(n+\kappa+1)\left\{\frac{(\varepsilon-1)[1+(\lambda C/2)^2]-(\lambda^2C^2/2)(\alpha/C-1)}{(\varepsilon-1)[1-(\lambda C/2)^2]+(\lambda^2C^2/2)(\alpha/C-1)}\right\}h_n(\varepsilon)$$
$$+b_{n-1}h_{n-1}(\varepsilon)+b_n h_{n+1}(\varepsilon)=0, \tag{12}$$

where the recursion coefficient $b_n=\sqrt{(n+1)(2\kappa+n+2)}$. This is to be compared with the well-known analytically solved nonrelativistic J-matrix recursion relation in the Laguerre-type basis[3]

$$2(n+l+1)\left[\frac{E-\lambda^2/8}{E+\lambda^2/8}\right]h_n'(E)+b_{n-1}'h_{n-1}'(E)+b_n'h_{n+1}'(E)=0, \tag{13}$$

where $b_n'=\sqrt{(n+1)(2l+n+2)}$ and h_n' stands for either the sinelike or cosinelike solutions for the nonrelativistic problem. Therefore, by comparing relation (12) with (13) we conclude that

$$h_n(\varepsilon)=h_n'\left(\frac{-1}{2C^2}\frac{\varepsilon-1}{\varepsilon-1+2(1-\alpha/C)}\right)\Bigg|_{l=\kappa}$$

and that the range of the small component strength parameter is $\alpha>C>0$. Using the analytic solution of the nonrelativistic recursion, $h_n'(E)$, derived by Yamani and Fishman,[3] we can write

$$c_n(\varepsilon)=-\frac{2^\kappa}{\sqrt{\pi}}\frac{a_n}{\lambda}\frac{\Gamma(\kappa+1/2)}{(\sin\omega)^\kappa}{}_2F_1\left(-n-1-2\kappa,n+1;1/2-\kappa;\sin^2\frac{\omega}{2}\right),$$
$$s_n(\varepsilon)=\frac{2^\kappa}{\lambda}a_n\Gamma(\kappa+1)(\sin\omega)^{\kappa+1}C_n^{\kappa+1}(\cos\omega), \tag{14}$$

where ${}_2F_1(a,b;c;z)$ is the hypergeometric function and $C_n^\nu(x)$ is the Gegenbauer polynomial. The angle ω is defined by

$$\cos(\omega)=\frac{[k(\varepsilon)/\lambda]^2-\frac{1}{4}}{[k(\varepsilon)/\lambda]^2+\frac{1}{4}},$$

where

$$k(\varepsilon)=\sqrt{\frac{-1}{C^2}\frac{\varepsilon-1}{\varepsilon-1+2(1-\alpha/C)}}. \tag{15}$$

The nonrelativistic limit is achieved by letting $\alpha\to 0$ [i.e., $c(\text{speed of light})\to\infty$], which gives $\varepsilon\cong 1+\alpha^2E$ and $\kappa=l$. Moreover, in the same limit, the small component, $\theta_n(r)$, of the wave function will be negligible compared to the larger component $\phi_n(r)$. That is, the small component strength parameter C in Eq. (7) will be of the order of α. Taking this limit in the relativistic recursion relation (12) gives

$$2(n+l+1)\left[\frac{\alpha^2 E-(\lambda^2 C^2/2)(\alpha/C-1)}{\alpha^2 E+(\lambda^2 C^2/2)(\alpha/C-1)}\right]h_n(\varepsilon)+b_{n-1}h_{n-1}(\varepsilon)+b_n h_{n+1}(\varepsilon)=0.$$

This nonrelativistic limit can be identified with the nonrelativistic recursion relation (13) if we choose $C=+\alpha/2$. Therefore, the nonrelativistic J-matrix limit for the case $Z=0$ is achieved by making the following choice of parameters in the relativistic J-matrix formalism development above:

$$\alpha\to 0,\ \ \kappa=l,\ \ C=\alpha/2$$

with the nonrelativistic energy $E\cong(\varepsilon-1)/\alpha^2$.

The solution (14) gives the J-matrix kinematical coefficients $\{R_n^{\pm}\}_{n=1}^{\infty}$ and $\{T_n\}_{n=0}^{\infty}$ defined by

$$T_n=\frac{c_n-is_n}{c_n+is_n};\quad R_{n+1}^{\pm}=\frac{c_{n+1}\pm is_{n+1}}{c_n\pm is_n};\quad n\geqslant 0.$$

These will be the coefficients that enter in the calculation of the Nth order relativistic S-matrix,[10]

$$S^{(N)}(\varepsilon)=T_{N-1}(\varepsilon)\frac{1+g_{N-1,N-1}(\varepsilon)J_{N-1,N}(\varepsilon)R_N^{-}(\varepsilon)}{1+g_{N-1,N-1}(\varepsilon)J_{N-1,N}(\varepsilon)R_N^{+}(\varepsilon)},\tag{16}$$

where $g_{N-1,N-1}(\varepsilon)$ is the finite Green's function in the conjugate subspace[3,10] spanned by $\{\overline{\psi}_n(r)\}_{n=0}^{N-1}$ and carries the dynamical effects of the short range model potential $\tilde{V}(r)$:

$$g_{N-1,N-1}(\varepsilon)=\langle\overline{\psi}_{N-1}|(H_0+\tilde{V}-\varepsilon)^{-1}|\overline{\psi}_{N-1}\rangle.$$

Due to the fact that the basis of the L^2 space is nonorthogonal, care should be exercised in the calculation of the finite Green's function as outlined in Appendix B of Ref. 10.

Now, for scattering we consider a general short-range perturbing potential, which has spin-dependent coupling, that is, the potential is a 2×2 real symmetric matrix of the following form:

$$\tilde{V}(r)=\begin{pmatrix}\tilde{V}_+(r) & \tilde{V}_0(r)\\ \tilde{V}_0(r) & \tilde{V}_-(r)\end{pmatrix}.$$

Its matrix elements in the spinor basis are, therefore, written as

$$\tilde{V}_{nm}=\alpha^2\int_0^{\infty}\phi_n(r)\tilde{V}_+(r)\phi_m(r)dr+\alpha^2\int_0^{\infty}\theta_n(r)\tilde{V}_-(r)\theta_m(r)dr$$
$$+\alpha^2\int_0^{\infty}\phi_n(r)\tilde{V}_0(r)\theta_m(r)dr+\alpha^2\int_0^{\infty}\theta_n(r)\tilde{V}_0(r)\phi_m(r)dr.$$

We will consider the case where $\tilde{V}(r)=\tilde{A}_0 f(r)$ and $\tilde{A}_0$ is a constant 2×2 real symmetric matrix (i.e., the coupling parameters $\tilde{V}_{\pm},\tilde{V}_0$ are constants). To evaluate these integrals we utilize a scheme based on Gauss quadrature as outlined in Appendix A of Ref. 10 The result of this computation is

$$\tilde{V}_{nm} \cong \alpha^2 \tilde{V}_+ [\sqrt{(2\kappa+n+2)(2\kappa+m+2)}\, G^{2\kappa+2}_{n,m} + \sqrt{nm}\, G^{2\kappa+2}_{n-1,m-1} - \sqrt{m(2\kappa+n+2)}\, G^{2\kappa+2}_{n,m-1}$$
$$- \sqrt{n(2\kappa+m+2)}\, G^{2\kappa+2}_{m,n-1}] + \left(\frac{\alpha\lambda C}{2}\right)^2 \tilde{V}_- [\sqrt{(m+1)(2\kappa+n+1)}\, G^{2\kappa}_{n,m+1}$$
$$+ \sqrt{(n+1)(2\kappa+m+1)}\, G^{2\kappa}_{m,n+1}] + \alpha^2 \lambda C \left(\frac{\lambda C}{4}\tilde{V}_- + \tilde{V}_0\right) \sqrt{(2\kappa+n+1)(2\kappa+m+1)}\, G^{2\kappa}_{n,m}$$
$$+ \alpha^2 \lambda C \left(\frac{\lambda C}{4}\tilde{V}_- - \tilde{V}_0\right) \sqrt{(n+1)(m+1)}\, G^{2\kappa}_{n+1,m+1},$$

where G^{ν}_{nm} is the Gauss quadrature integral approximation

$$G^{\nu}_{nm} \cong \sum_{k=0}^{M-1} \Lambda^{\nu}_{nk} \Lambda^{\nu}_{mk} f(\xi^{\nu}_k/\lambda) = G^{\nu}_{mn}, \quad M > N.$$

The eigenvalues $\{\xi^{\nu}_n\}^{M-1}_{n=0}$ and corresponding normalized eigenvectors $\{\Lambda^{\nu}_{mn}\}^{M-1}_{n,m=0}$ are associated with the $M \times M$ tridiagonal matrix

$$\begin{pmatrix} \hat{a}_0 & \hat{b}_0 & & & & & \\ \hat{b}_0 & \hat{a}_1 & \hat{b}_1 & & 0 & & \\ & \hat{b}_1 & \hat{a}_2 & \hat{b}_2 & & & \\ & & \hat{b}_2 & \times & \times & & \\ & & & \times & \times & \times & \\ & 0 & & & \times & \times & \times \\ & & & & & \times & \times \end{pmatrix} \tag{17}$$

whose recursion coefficients are parametrized by ν and defined as $\hat{a}_n = 2n + \nu + 1$ and $\hat{b}_n = -\sqrt{(n+1)(n+\nu+1)}$.

Finally, with these potential matrix elements for the given problem, we have all the physical quantities that are needed for evaluating the relativistic scattering matrix in (16). Scattering examples have already been worked out where the accuracy of the nonrelativistic limit is verified and the relativistic effects in the phase shift were calculated. However, the present mathematical treatment of the problem may not be suitable for such presentation. These results will be reported shortly elsewhere.

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Stable orbits in a Higgs-Monopole field

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Motion of Yang–Mills particles in Yang–Mills–Higgs fields are studied. By regarding the Higgs field contribution on the particle's motion, a complete set of equations is worked out for the particle and fields. The planar motions as well as three-dimensional bounded motions are studied. Stable orbits are allowed in this scenario. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1433942]

I. INTRODUCTION

In our last article[1] we described the motion of a colored test particle in which the color was coupled only to the Yang–Mills field, and the nonrelativistic real space motion at large distances was stated to be the same as for an electric point particle in a Dirac point monopole field. We introduced planar motion of a non-Abelian particle in field of a BPS monopole. There, a monopole exerts a force on the particle via its non-Abelian charge. We studied various characteristics of orbits and their stabilities. With some numerical analysis we stated that the planar bound motions are not stable, and three-dimensional bound orbits were not observed.

In this work, we introduce the Higgs field to exert a force on the particle in addition to the monopole force. We introduce Wong's equations in five dimensions, and modify the equations of motion for a particle in the Yang–Mills–Higgs fields. We have chosen the extra fifth dimension to have no contribution in the fields, leaving it as a dynamical variable. A close relation between the time evolution of the fifth dimension and the isospace vectors, the Higgs and non-Abelian charge, are observed. Motion of a test particle, now in the presence of a force from the Higgs field, is studied. Three-dimensional bounded orbits are observed, and stable planar orbits are allowed.

Fehér[2] has given a reinvestigation for a classical motion of a colored test particle in the Prasad–Sommerfield monopole field. He has considered coupling of the particle to both the Yang–Mills and the Higgs fields, and mentioned the existence of bounded orbits at nonrelativistic limit at large distances. He has used the Wong equations and regarded the Higgs field as the fifth component of a Yang–Mills vector field in five dimensions (Ref. 3, p. 46), interpreting the motion in the fifth direction as providing an effective mass of the particle. Fehér has supposed an affine parameter on the path of the particle in the five-dimensional manifold to write down the Wong's equations. Then he has reformulated the equations by using the proper time parameter as the projection of the affine parameter in the four-dimensional space–time path of the particle, and interpreted the mass as the derivative of the proper time by this affine parameter. We think this formalism is not a natural generalization of the four-dimensional Wong equations.[4] In addition, the limit of nonrelativistic motion is unclear, so the bounded orbits at far distances are questionable. We have searched the literature but we have not found any other work in this direction. So, we have reformulated the problem again.

II. GENERALIZING EQUATIONS OF MOTION TO FIVE DIMENSIONS

In this section we want to rebuild the equations of motion of a colored particle in a non-Abelian Yang–Mills–Higgs field in a five-dimensional space–time as Wong extracted his equations from a four-dimensional analysis. The Lagrangian regarding to the Kinetic part of the fields (with the usual definition) is

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$$-\tfrac{1}{4}F^{a\mu\nu}F^{a}_{\mu\nu}-\tfrac{1}{2}(\mathbf{D}^{\mu}\mathbf{\Phi})^{a}(\mathbf{D}_{\mu}\mathbf{\Phi})^{a}, \tag{2.1}$$

where $F^{a}_{\mu\nu}$ is the field strengths, $\mathbf{\Phi}^{a}$ is the Higgs's fields and $\mathbf{D}_{\mu}$ is covariant derivative. This field system can be regarded as a pure Yang–Mills system over a five-dimensional flat space–time $\mathcal{M}^{5}$, for which the corresponding connection is invariant with respect to translations of the fifth coordinate. We suggest the fifth coordinate, say x^{5} here, as an internal but dynamical coordinate so that no field variables depend on this internal coordinate. So the field Lagrangian (2.1) can formally be written in pure Yang–Mills fields in five dimensions in a compact form:

$$\mathcal{L}_{f}=-\tfrac{1}{4}F^{aAB}F^{a}_{AB}, \tag{2.2}$$

where $A,B,\ldots=0,1,2,3$ and 5 denote indices in the five-dimensional space–time, and

$$F^{a}_{AB}=\partial_{A}A^{a}_{B}-\partial_{B}A^{a}_{A}+e\,f^{abc}A^{b}_{A}A^{c}_{B} \tag{2.3}$$

is the gauge field strength where f^{abc} are the structure constants, and e is the coupling constant of the particle with the Yang–Mills–Higgs field. We have defined the Higgs field as the fifth component of the Yang–Mills field:

$$\Phi^{a}\equiv A^{a}_{5}, \tag{2.4}$$

$$F^{a}_{\mu 5}=\partial_{\mu}A^{a}_{5}-\partial_{5}A^{a}_{\mu}+e\,f^{abc}A^{b}_{\mu}A^{c}_{5}=(\mathbf{D}_{\mu}\mathbf{\Phi})^{a}, \tag{2.5}$$

where $\mu=0,1,2,3$ shows the usual four-dimensional space–time indices, and a, b, and c shows the isospace indices—that is $=1,2,3$ for SU(2) gauge group.

Now consider the interaction between the Yang–Mills field $\mathbf{A}_{A}(x)$ (x_{0} standing for time component and the rest for spatial components) and a spin-$\frac{1}{2}$ field $\Psi(x)$ which transforms under the fundamental representation of the gauge group with generators χ^{a} [for SU(2) gauge group, $\chi^{a}=\sigma^{a}/2i$ where σ^{a} with $a=1,2,3$ are Pauli matrices]. So we may add the particle-field interaction term to the Lagrangian (2.2) to get

$$\mathcal{L}=-\tfrac{1}{4}F^{aAB}F^{a}_{AB}-\bar{\Psi}(\gamma^{A}\partial_{A}+e\,\gamma^{A}A^{a}_{A}\chi^{a}+m)\Psi, \tag{2.6}$$

where e is the coupling constant, m is the mass of particle and γ^{A} are Dirac gamma matrices, with $\gamma^{5}=\gamma^{0}\gamma^{1}\gamma^{2}\gamma^{3}$. Comparing Lagrangian (2.6) with Wong analysis in four dimension, the extra term

$$-\bar{\Psi}(\gamma^{5}\partial_{5}+e\,\gamma^{5}\Phi^{a}\chi^{a})\Psi=-e\bar{\Psi}\gamma^{5}\Phi^{a}\chi^{a}\Psi$$

appears in five-dimensional generalization, which indicates the interaction between the particle and the Higgs field.[5–7]

The field equations are

$$(\mathbf{D}^{B}\mathbf{F}_{AB})^{a}=-e\bar{\Psi}\gamma_{A}\chi^{a}\Psi, \tag{2.7}$$

$$\gamma^{A}(\partial_{A}+e\chi^{a}A^{a}_{A})\Psi+m\Psi=0. \tag{2.8}$$

This is the usual Dirac-type treatment to find classical equations of motion from quantum recipe, by regarding Eq. (2.8) as a one-particle Dirac equation for a colored particle in a given external field $\mathbf{A}_{A}$. This has been done by Wong[4] in four dimensions. The equations of motion are essentially similar to the Wong equations in four dimensions. The five-dimensional motion of a particle in this pure Yang–Mills field is governed by the following Wong equations:

$$m\frac{d^2x^A}{d\tau^2}=e\frac{dx^B}{d\tau}F^{aA}{}_{B}I^a, \tag{2.9}$$

$$\frac{dI^a}{d\tau}+e\,f^{abc}\frac{dx^A}{d\tau}A^b_A I^c=0, \tag{2.10}$$

where I^a is the charge isovector and τ is proper time.

The fifth dimension is a dynamical variable, so the evolution of this internal coordinate (x^5) is governed by

$$m\frac{d^2x^5}{d\tau^2}=e\frac{dx^B}{d\tau}F^{a5}{}_{B}I^a=-e\frac{dx^\mu}{d\tau}(\mathbf{D}_\mu\mathbf{\Phi})^aI^a. \tag{2.11}$$

For the components of the real four-dimensional space–time, the equations of motion are

$$m\frac{d^2x^\mu}{d\tau^2}=e\frac{dx^B}{d\tau}F^{a\mu}{}_{B}I^a=e\frac{dx^5}{d\tau}F^{a\mu}{}_{5}I^a+e\frac{dx^\nu}{d\tau}F^{a\mu}{}_{\nu}I^a=e\frac{dx^\nu}{d\tau}F^{a\mu}{}_{\nu}I^a+e\frac{dx^5}{d\tau}(\mathbf{D}^\mu\mathbf{\Phi})^aI^a. \tag{2.12}$$

In Fehér's work an extra term appears on the right-hand side of Eq. (2.12) which comes from the difference between the affine parameter in the five dimensions and four dimensions. The Wong equation for non-Abelian charge **I** in five dimensions (2.10) can be expanded as

$$\frac{dI^a}{d\tau}+e\,f^{abc}\frac{dx^\mu}{d\tau}A^b_\mu I^c+e\,f^{abc}\frac{dx^5}{d\tau}\Phi^bI^c=0. \tag{2.13}$$

Multiplying both sides of Eq. (2.13) by I^a, we obtain the same result as in four-dimensional analysis:

$$\frac{d(I^aI^a)}{d\tau}=0,\ \text{ so }\ I^aI^a=\text{const}, \tag{2.14}$$

which indicates conservation of the length of charge isovector. It is in this sense that non-Abelian charge is conserved.

The field equations which arise from the Lagrangian (2.6) are

$$\mathbf{D}_B\mathbf{F}^{AB}=\mathbf{J}^A, \tag{2.15}$$

where $\mathbf{J}^A$ are current due to the colored particle(s). In the matrix representation

$$\mathbf{A}_B\equiv A^a_B\chi^a,\quad \mathbf{\Phi}\equiv\Phi^a\chi^a,\quad \mathbf{F}_{AB}\equiv F^a_{AB}\chi^a,\quad \mathbf{D}_B\equiv\mathbf{1}\partial_B+e[\mathbf{A}_B,\ ]. \tag{2.16}$$

One may simply show the identities

$$\mathbf{D}_A\mathbf{D}_B\mathbf{F}^{AB}=0, \tag{2.17}$$

$$\mathbf{D}_A\mathbf{F}_{BC}+\mathbf{D}_C\mathbf{F}_{AB}+\mathbf{D}_B\mathbf{F}_{CA}=0. \tag{2.18}$$

From Eqs. (2.17) and (2.15) the conservation of the colored (non-Abelian) current $\mathbf{J}^A$ is given by

$$\mathbf{D}_A\mathbf{J}^A=0. \tag{2.19}$$

Expanding Eq. (2.15), the fifth and the space–time components of the current are

$$\mathbf{J}^5=\mathbf{D}_B\mathbf{F}^{5B}=\mathbf{D}_\mu\mathbf{F}^{5\mu}=-\mathbf{D}_\mu\mathbf{D}^\mu\mathbf{\Phi}, \tag{2.20}$$

$$\mathbf{J}^{\mu}=\mathbf{D}_{B}\mathbf{F}^{\mu B}=\mathbf{D}_{\nu}\mathbf{F}^{\mu\nu}+\mathbf{D}_{5}\mathbf{F}^{\mu 5}. \tag{2.21}$$

When the potential $V(\mathbf{A}^5)\equiv V(\Phi^a\Phi^a)=(\lambda/4)\,(\Phi^b\Phi^b-a^2)^2$ is considered in the Lagrangian (2.6), the fifth component of current will be

$$\mathbf{J}^{5}=-\mathbf{D}_{\mu}\mathbf{D}^{\mu}\mathbf{\Phi}+\lambda\mathbf{\Phi}(\Phi^a\Phi^a-a^2).$$

The last term on the right-hand side of Eq. (2.21) is simplified by our initial principles:

$$\mathbf{D}_{5}\mathbf{F}^{\mu 5}=[\mathbf{A}_{5},\mathbf{F}^{\mu 5}]\quad(\partial_{5}\mathbf{F}^{\mu 5}=0).$$

Then

$$\mathbf{J}^{\mu}=\mathbf{D}_{\nu}\mathbf{F}^{\mu\nu}+[\mathbf{\Phi},\mathbf{D}^{\mu}\mathbf{\Phi}], \tag{2.22}$$

which shows the usual current in the four-dimensional space–time has a contribution from the Higgs field.

For a non-Abelian point particle with charge **I**, the current can be defined in five dimensions in the normal way as in Wong's work in four dimensions:

$$\mathbf{J}^{A}(y)=e\int d\tau\,\mathbf{I}(\tau)\,\frac{dx^{A}(\tau)}{d\tau}\,\delta^{5}(y-x(\tau)), \tag{2.23}$$

where $x(\tau)$ is the location (world-line) of the charged particle in the five-dimensional space–time, y is an arbitrary point in the space–time, and δ is the Dirac delta function. The consistency between the above definition and the equations of motion is valid, i.e., from Eqs. (2.19) and (2.23) and the definition of covariant derivative we may obtain Eq. (2.10).

Equations (2.11)–(2.13), (2.20) and (2.22) completely describe the motion of a colored particle in the non-Abelian Yang–Mills–Higgs field. It is possible to find a first integral of Eq. (2.11). The right-hand side of Eq. (2.11) can be expanded as

$$-e\,\frac{dx^{\mu}}{d\tau}\,\frac{d\Phi^{a}}{dx^{\mu}}I^{a}-e^{2}\frac{dx^{\mu}}{d\tau}f^{abc}A_{\mu}^{b}\Phi^{c}I^{a},$$

and then Eq. (2.11) can be written

$$m\,\frac{d^{2}x^{5}}{d\tau^{2}}=-e\,\frac{d\Phi^{a}}{d\tau}I^{a}-e^{2}\frac{dx^{\mu}}{d\tau}f^{abc}I^{a}A_{\mu}^{b}\Phi^{c}. \tag{2.24}$$

Multiplying both sides of Eq. (2.13) by Φ^a, one can show

$$\Phi^{a}\frac{dI^{a}}{d\tau}=e\,\frac{dx^{\mu}}{d\tau}f^{abc}I^{a}A_{\mu}^{b}\Phi^{c}, \tag{2.25}$$

which, if substituted in Eq. (2.24), we have

$$m\,\frac{d^{2}x^{5}}{d\tau^{2}}=-e\,\frac{d\Phi^{a}}{d\tau}I^{a}-e\,\Phi^{a}\frac{dI^{a}}{d\tau}=-e\,\frac{d}{d\tau}(\Phi^{a}I^{a}). \tag{2.26}$$

From this equation we obtain a first order differential equation for the internal coordinate

$$m\,\frac{dx^{5}}{d\tau}=-e\,\Phi^{a}I^{a}+h, \tag{2.27}$$

where h is the constant of integration, which is indeed a constant of motion. As the fields are independent of the fifth dimension x^5, in a Lagrangian approach[8–10] in five dimensions $\partial L/\partial x^5$ vanishes. Therefore $\partial L/\partial \dot{x}^5 = m\dot{x}^5 + e\Phi^a I^a$ is a constant, in agreement with Eq. (2.27). So the momentum conjugate to x^5, h, is a constant of motion. Equation (2.27) presents a relation for the internal component of the particle's momentum. In fact, this is an internal variable, i.e., this variable is only a function of isovectors, the Higgs field and charge isovectors. We called the extra dimension, x^5, an internal dimension, which is now sensible in the same way as the space of symmetry (isospace) is called an internal space. The time variation of the internal direction, x^5, is related to the field and particle internal (isospace) vectors. If we replace dx^5/dt in the equations of motion, it gives a completely four-dimensional equations, which contain terms corresponding to the Higgs interaction with the particle. The only remnant of the fifth dimension in the equations is the free parameter h, which depends on the initial value of dx^5/dt.

The constant, h, in Eq. (2.27) depends on the initial orientation of the two isovectors and the initial value of $dx^5/d\tau$. For example, in the field of the 'tHooft–Polyakov monopole, if the particle starts the motion from the rest, $dx^A/d\tau = 0$, in the Higgs vacuum ($\vec{\Phi} = a\hat{r}$), and if the particle's charge isovector lies in the radial direction, the constant will be eaI, where I is the norm of the charge isovector which is always constant. If the particle starts the motion while the charge isovector lies in a tangential direction, then the constant will be zero. Regardless of the constant, Eq. (2.27) shows the internal component of momentum is proportional to the projection of the Higgs field on the direction of the particle's charge isovector, and the proportionality factor is $-eI$, i.e., the particle's charge. One can replace $dx^5/d\tau$ from Eq. (2.27) in Eqs. (2.12) and (2.13) to obtain a complete set of equations independent of the internal coordinate.

The equations of motion become simpler with some interesting consequences if we use a BPS magnetic monopole as the source of the Yang–Mills–Higgs field.

III. PARTICLE IN THE FIELD OF A BPS MONOPOLE

One of the most important solutions of the Yang–Mills fields is monopoles. Although experimentally no monopole is found yet, but monopole solutions in the field theory are very rich phenomena in theoretical physics. The 'tHooft ansatz is a solution which gives the right behavior of a magnetic monopole at far distances. The BPS monopole is an exact solution which gives the answer everywhere. About the behavior of motion of a particle in a monopole at far distances we may find some results in literature. The goal of this section is to explain some solution not only at far distances, but everywhere. So we have used the BPS monopole to discuss solutions at far and close distances from the origin. In this section we use the procedure described in the previous section and apply the conditions of the BPS monopole for a test particle. With a test particle we mean, relative to the monopole, the particle is so small in mass and charge such that the resulting perturbation due to the particle can be ignored. Therefore, the particle has no contribution in the evolution of the fields, and we ignore the current **J** on the left-hand side of field equations (2.20) and (2.22). Thus the field equations satisfy the BPS monopole conditions,[11] and we can use BPS solution

$$A^{a0} = 0, \quad \partial_0 A^{ia} = \partial_0 \Phi^a = 0,$$

$$A^{ai} = \epsilon^{aij} \frac{x^j}{er^2}(1-K), \quad K = \frac{aer}{\sinh(aer)}, \tag{3.1}$$

$$\Phi^a = \frac{x^a}{er^2} H, \quad H = aer\coth(aer) - 1,$$

for the fields.

Equations (3.1) satisfy the field equations, and in a nonrelativistic framework the equations of motion (2.12) and (2.27) become

$$m\frac{d^2x^i}{dt^2}=e\frac{dx^j}{dt}F^a_{ij}I^a+e\,p\,(\mathbf{D}_i\mathbf{\Phi})^aI^a, \tag{3.2}$$

$$m\,p=-e\,\Phi^aI^a+h, \tag{3.3}$$

where we have substituted τ by $t=x^0$, dropped the equation for x^0 and defined

$$p=\frac{dx^5}{dt}. \tag{3.4}$$

The constant h depends on the initial conditions as we explained after its introduction in Eq. (2.27). A force due to the Higgs field has appeared in the equation of motion, Eq. (3.2), beyond the usual Lorentz force. The equation of evolution of the charge isovector (2.13) becomes

$$\frac{dI^a}{dt}+e\,\epsilon^{abc}\frac{dx^i}{dt}A^b_iI^c+e\,p\,\epsilon^{abc}\,\Phi^bI^c=0. \tag{3.5}$$

By replacing F^a_{ij}, $(\mathbf{D}_i\mathbf{\Phi})^a$, A^a_i and Φ^a from Eqs. (3.1) into Eqs. (3.2)–(3.5), the equations in a convenient form are

$$m\dot{\vec{v}}=e\vec{v}\times\vec{B}^aI^a-e\,p\vec{B}^aI^a=\frac{\vec{r}\cdot\vec{I}}{r^4}(K^2-rK'-1)[(\vec{v}\times\vec{r})-p\vec{r}]+\frac{K'}{r}[(\vec{v}\times\vec{I})-p\vec{I}], \tag{3.6}$$

$$m\,p=-\frac{H}{r^2}(\vec{r}\cdot\vec{I})+h, \tag{3.7}$$

$$\dot{\vec{I}}=\frac{1-K}{r^2}(\vec{r}\times\vec{v})\times\vec{I}-\frac{pH}{r^2}(\vec{r}\times\vec{I}), \tag{3.8}$$

where the magnetic field is

$$B^a_i=\frac{1}{2}\epsilon^{ijk}F^a_{jk}=-(\mathbf{D}_i\mathbf{\Phi})^a=\frac{1}{er^2}\left\{\frac{x^ax^i}{r^2}(K^2-rK'-1)+rK'\,\delta^{ai}\right\}. \tag{3.9}$$

The energy and the total angular momentum are constants of motion. Using the general equation in five dimensions (2.9), multiplying both sides by $dx^A/d\tau$, one can simply find

$$\frac{d}{d\tau}\left[\frac{1}{2}m\left(\frac{dx^A}{d\tau}\right)^2\right]=0,$$

which in a nonrelativistic framework implies

$$E\equiv\tfrac{1}{2}mv^2+\tfrac{1}{2}mp^2=\text{const.} \tag{3.10}$$

Here, $\vec{v}$ is velocity of the particle ($v=|\vec{v}|$), and p is defined in Eq. (3.4). The validity of relation (3.10) can be checked directly by using the equations of motion (3.3), (3.6), and (3.8) to show

$$m\dot{\vec{v}}\cdot\vec{v}+m\dot{p}\,p=0.$$

Another constant is $\vec{J}$, the total angular momentum of particle and fields,[12] which is

$$\vec{J}=m(\vec{r}\times\vec{v})+K\vec{I}+\frac{(1-K)(\vec{I}\cdot\vec{r})}{r^2}\vec{r}. \tag{3.11}$$

Replacing from Eqs. (3.6) and (3.8) in Eq. (3.11), after some algebra, one may easily show $\dot{\vec{J}}=0$ and so

$$\vec{J}=\text{const.} \tag{3.12}$$

In the first view, we find Eqs. (3.6) and (3.8) are too complicated to be solved. Therefore, we consider the asymptotic behavior of the equations at large distances. Because of the different behavior of K and K' with H at large distances we may consider two cases. At large distances $K(r)$ and $K'(r)$ vanish exponentially, and $\vec{B}^a=-(x^a/er^4)\vec{r}$. If r is not too much bigger than 1, $H(r)\to aer-1$, and if $r\gg 1$, then 1 might be ignored and so $H=aer$. So at large distances (but not too far) Eqs. (3.6) and (3.7) become

$$m\dot{\vec{v}}=\frac{\alpha}{r^3}[\vec{r}\times\vec{v}+p\vec{r}], \tag{3.13}$$

$$p=\left(-e\ a\ \alpha+h+\frac{\alpha}{r}\right)/m, \tag{3.14}$$

where we have defined the charge isovector as

$$\vec{I}=\alpha\hat{r}+\beta\hat{w}+\gamma\hat{z}, \tag{3.15}$$

in an orthogonal moving frame along the particle trajectory:

$$\vec{r},\vec{w}=\vec{r}\times\vec{v}\left(\vec{v}=\frac{d\vec{r}}{dt}\right),\vec{z}=\vec{r}\times\vec{w}, \tag{3.16}$$

where hatted letters denote the unit vectors along each axis. Evidently the coefficients α, β, and γ satisfy

$$I\equiv(I^aI^a)^{1/2}=(\alpha^2+\beta^2+\gamma^2)^{1/2}=\text{const.} \tag{3.17}$$

From Eq. (3.8), after a little algebra we find

$$\dot{\alpha}=-\frac{K|\vec{w}|}{r^2}\gamma, \tag{3.18}$$

$$\dot{\beta}=\left\{r\frac{\dot{\vec{v}}\cdot\vec{w}}{|\vec{w}|^2}+\frac{pH}{r}\right\}\gamma,\quad p=\frac{1}{m}\left(-\frac{\alpha H}{r}+h\right), \tag{3.19}$$

$$\dot{\gamma}=\left\{-r\frac{\dot{\vec{v}}\cdot\vec{w}}{|\vec{w}|^2}-\frac{pH}{r}\right\}\beta+\frac{K|\vec{w}|}{r^2}\alpha. \tag{3.20}$$

These equations, by using the asymptotic behaviors of K and H at large distances, and using the asymptotic equation (3.13), become

$$\dot{\alpha}=0, \tag{3.21}$$

$$\dot{\beta}=\left[\frac{\alpha}{mr^2}+p\frac{aer-1}{r}\right]\gamma, \tag{3.22}$$

$$\dot{\gamma}=-\left[\frac{\alpha}{mr^2}+p\frac{aer-1}{r}\right]\beta, \tag{3.23}$$

where p has the asymptotic value in Eq. (3.14). From Eq. (3.21), obviously $\alpha=\alpha_0$ is a constant.

For this asymptotic case, using Eqs. (3.13) and (3.21), the length of the angular momentum $l=|m(\vec{r}\times\vec{v})|$, the total angular momentum vector $\vec{j}=\vec{l}+\alpha_0\hat{r}$, and in addition, $\vec{j}\cdot\hat{r}=\alpha_0$ are constants of motion [in agreement with Eq. (3.11)]. From Eqs. (3.13) and (3.14) one may simply find $m(v^2+p^2)/2$ is also a constant of motion [see Eq. (3.10)]. If $j=|\vec{j}|=0$ so $l=\alpha_0=0$, then the particle moves uniformly in a radial direction (or stays at rest). For $j\neq 0$, the motion will take place on a cone with the axis $\vec{j}$ and the half-angle $\cos^{-1}(\alpha_0/j)$.

We may compare the forces on the right-hand side of the asymptotic equation (3.13) with forces due to certain point objects sitting at the origin. From the components of the isovector charge $\vec{I}$, only α (that is a constant) has appeared in the equation of motion, Eq. (3.13). Therefore, we may assume only the $e\alpha$ portion of the particle's charge, eI, participates in the motion at large distances

$$m\dot{\vec{v}}=-\frac{\alpha}{r^3}(\vec{v}\times\vec{r})+\frac{\alpha(h-e\,a\,\alpha)}{mr^3}\vec{r}+\frac{\alpha^2}{mr^4}\vec{r}. \tag{3.24}$$

The first term on the right-hand side of Eq. (3.24) is a force due to a point magnetic monopole. The second and the third terms are forces exerted from the scalar Higgs field on the colored test particle. The second term corresponds to the force due to an electric point charge on the test particle and the third term has the characteristic of a spherical charge distribution of total charge zero. At close distances the force from the fields on the particle are very complicated, and at far distances the dominant terms are those on the right-hand side of Eq. (3.24). For $r\gg 1$ the dominant forces are the first and second terms on the right-hand side of Eq. (3.24).

For too large distances, i.e., $r\gg 1$, where the Higgs field asymptotically becomes

$$\vec{\Phi}=a\hat{r}, \tag{3.25}$$

we may neglect 1 in the term $aer-1$, and rewrite the equations of motion (3.13), (3.14), and (3.21)–(3.23),

$$m\dot{\vec{v}}=\frac{\alpha}{r^3}[\vec{r}\times\vec{v}+p\,\vec{r}], \tag{3.26}$$

$$p=\frac{(-e\,a\,\alpha+h)}{m}, \tag{3.27}$$

$$\dot{\alpha}=0, \tag{3.28}$$

$$\dot{\beta}=eap\,\gamma, \tag{3.29}$$

$$\dot{\gamma}=-eap\,\beta, \tag{3.30}$$

where now p is a constant and $\dot{\beta}$ and $\dot{\gamma}$ have simpler forms. In this approximation (too large distances) l, α, and $\vec{j}$ (so $\hat{j}\cdot\hat{r}$) are constants of motion (the same as in the large distances approximation). Now p is a constant, so from Eq. (3.26) $mv^2/2+\alpha p/r=\text{const}$ [that can be obtained by expanding $E=m(v^2+p^2)/2=\text{const}$ at large distances using Eq. (3.14) and then dropping the order of $1/r^2$ and redefining p as in Eq. (3.27)].

Equations (3.29) and (3.30) provide a precession motion for the charge isovector $\vec{I}$, around the radial direction of the particle in the isospace

$$\beta(t)=\sqrt{I^2-\alpha^2}\sin(aep\,t+\Omega_0),\ \gamma(t)=\sqrt{I^2-\alpha^2}\cos(aep\,t+\Omega_0), \tag{3.31}$$

where Ω_0 is a constant. The charge isovector moves around a circle of radius $(I^2-\alpha^2)^{1/2}$ with a constant angular frequency $\omega=aep$. Therefore p measures how fast the charge isovector moves around in the isospace, when the particle travels its path in the real space. So p which was defined as the velocity in the fifth-spatial direction [Eq. (3.4)] appears as the velocity of the charge isovector in its precession around the particle's radial direction [note, ae has the dimension of $(\text{length})^{-1}$].

IV. SOLUTIONS OF THE EQUATIONS OF MOTION

In our previous work[1] we observed planar and bounded motions and we presented numerical works in two and three dimensions. There the only force on the particle was the force from the monopole and a force from the Higgs field on the particle was not considered. In the first part of this article we explained the equations of motion containing the Higgs and the particle interaction as well as the monopole force, and in this section we search for some solutions.

A. Planar motions

It is interesting to know if the planar motions occur here. In a planar motion $\vec{r}\times\vec{v}$ is always normal to the plane of motion, so in the equations of motion the coefficient of $\vec{w}=\vec{r}\times\vec{v}$ must be set to zero and we find some consistent solutions. Using the moving frame (3.16), the component of Eq. (3.6) in the $\hat{w}$-direction is

$$-\frac{\alpha(K^2-rK'-1)}{r^3}|\vec{w}|-\frac{K'}{r^2}(\alpha|\vec{w}|+\gamma(\vec{r}\cdot\vec{v}))-\frac{K'}{r}p\,\beta. \tag{4.1}$$

For a planar motion this coefficient must identically be equal to zero, so

$$(K^2-1)|\vec{w}|\alpha+r^2K'\,p\,\beta+rK'(\vec{r}\cdot\vec{v})\,\gamma=0. \tag{4.2}$$

Under these considerations the equations of motion (3.6) and (3.18)–(3.20) become

$$m\dot{\vec{v}}=\left[-\frac{K^2-rK'-1}{r^2}p\alpha+\frac{K'}{r^2}(|\vec{w}|\beta-rp\alpha)\right]\hat{r}+\frac{K'}{r^2}[(\vec{r}\cdot\vec{v})\beta-r\,p\,\gamma]\hat{z}, \tag{4.3}$$

$$\dot{\alpha}=-\frac{K\,w}{r^2}\gamma, \tag{4.4}$$

$$\dot{\beta}=\frac{p\,H}{r}\gamma, \tag{4.5}$$

$$\dot{\gamma}=\frac{K\,w}{r^2}\alpha-\frac{p\,H}{r}\beta, \tag{4.6}$$

and p is unchanged:

$$mp=-\frac{H}{r}\alpha+h. \tag{4.7}$$

Let us first examine the above equations at large distances. At large distances where K and K' vanish, Eq. (4.2) necessitates $\alpha=0$. Replacing this result in Eq. (4.3) shows the particle move on a straight line at large distances [see also Eq. (3.13)]. Also at large distances p is a constant and β and γ have a precessional motion (if $p\neq0$), which are compatible with the asymptotic behavior of equations we studied before.

In fact, Eq. (4.2) is an extra equation and might not be consistent with the equations of motion (4.3)–(4.6) in general. But it might be consistent with equations of motion under some circum-

stances. Finding the conditions where this extra equation might be consistent with the others does not seem to be easy. Looking at Eq. (4.2), one may choose $\alpha=\beta=\gamma=0$, which is, of course, a contradiction (while $\vec{I}$ is a nonzero vector). One acceptable possibility is $\alpha=\gamma=p=0$, which causes Eq. (4.2) to vanish identically. From Eq. (4.7) the condition $p=0$ is equivalent to $h=0$. So,

$$\alpha=\gamma=h=0 \tag{4.8}$$

are conditions for planar motion subject to the validity of equations of motion. Replacing from Eq. (4.8) in Eqs. (4.3)–(4.6) we obtain exactly the planar equations of Ref. 1. So the planar motion and indeed the bounded orbits are allowed in this regime as well. Because the equations of planar motion are the same as in Ref. 1 we skip their solutions in this article. The stability of planar motion must be studied independently. In the planar solutions of Ref. 1 we stated the planar motions were not stable, but in this case the Higgs field might play a role to keep the particle close to the plane and does not let it scatter to infinity. I have not checked this problem.

A proper question is, under what circumstances the force from the Higgs field on the particle fails and the particle feels only a force from the monopole (i.e., the generalized equations of motion we found in this article shrink to the equations of motion of Ref. 1). In fact, it is not possible to ignore the Higgs field interaction with the particle in general. Equating p to zero is an obvious way, but this equation exerts an extra constraint. Setting $p=0$ occasions $\alpha=hr/H$, then from Eq. (3.18) we find γ and from Eq. (3.20) β. So we may replace α, β, and γ in Eqs. (3.19) and (3.6) to find two parallel equations which are too complicated (and I think they are not consistent in general). A possible case (maybe the only one) is the mentioned planar motion, which means in the specified planar motions the Higgs interaction has no contribution.

B. Radial motions

A radial motion is possible if initially the charge isovector and the particle velocity are radial. In this case from Eq. (3.8) the charge isovector remains constant, $\alpha=I$ and $\beta=\gamma=0$, and from Eq. (3.6)

$$m\ddot{r}=\frac{I}{r^2}(K^2-1)p, \tag{4.9}$$

where $p=-IH/r+h$. In the previous case (the monopole interaction only), the right-hand side of Eq. (4.9) was vanishing ($p=0$) and the particle had a uniform radial motion, and could pass through the origin. Equation (4.9) shows a different situation.

Assume the particle is moving along a radial direction, say the z-axis. From Eq. (3.10) we may write

$$E=\tfrac{1}{2}m\dot{r}^2+V(r), \tag{4.10}$$

where

$$V(r)=\frac{1}{2}m\,p^2=\frac{1}{2}m\left(\frac{-IH(r)}{r}+h\right)^2 \tag{4.11}$$

is the one-dimensional potential, and r (is the variable along the z-axis and) takes both negative and positive values. The time derivative of Eq. (4.10) leads to Eq. (4.9). Regardless of mass, a, e, and I, the potential $V(r)$ depends on the constant h. Figure 1 shows the different shapes of $V(r)$ with respect to the different values of h. To see these results one may equate $V'(r)$ to zero and find the roots (that are indeed the roots of $p=0$). For a negative value of h, $V(r)$ is the mirror image of the the potential for $-h$, with respect to the vertical axis.

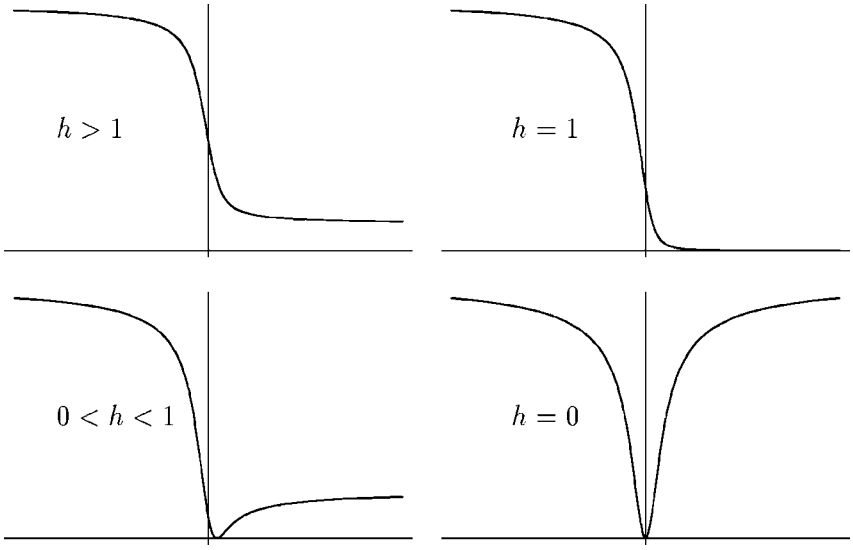

FIG. 1. One-dimensional potential $V(r)$ (vertical axis) vs r (horizontal axis). For a given h, the mirror image of $V(r)$ with respect to the vertical axis gives $V(r)$ for $-h$.

From Fig. 1, if $|h| \geqslant 1$, the particle may be repelled back (before reaching the origin, just at the origin or after passing the origin), or just passes through the origin depending on the energy E. For $0 < |h| < 1$, in addition to the mentioned possibilities for $|h| \leqslant 1$, bounded motions are also possible (in the $h = 0$ case, the particle just passes or is bound).

Referring to Fig. 2, for $E \geqslant E_1$ the particle passes through the origin and travels to infinity. For $E_1 < E \leqslant E_3$, such as E_2, the particle is repelled back (even before reaching the origin or after passing through the origin) in its trajectory and travels to infinity. For $0 < E < E_3$, the orbit is bounded and the particle oscillates along the z-axis. For $h = 0$ the oscillation is symmetric with respect to the origin (the origin is the equilibrium point). But in the other cases, the origin is not the equilibrium point (center of the oscillatory motion) and the amplitude of the motion on the two sides of the origin are not equal (even not equal on either side of the equilibrium point). And, on top of it all, for the energies less than E_4, the particle oscillates only on one side of the origin. At

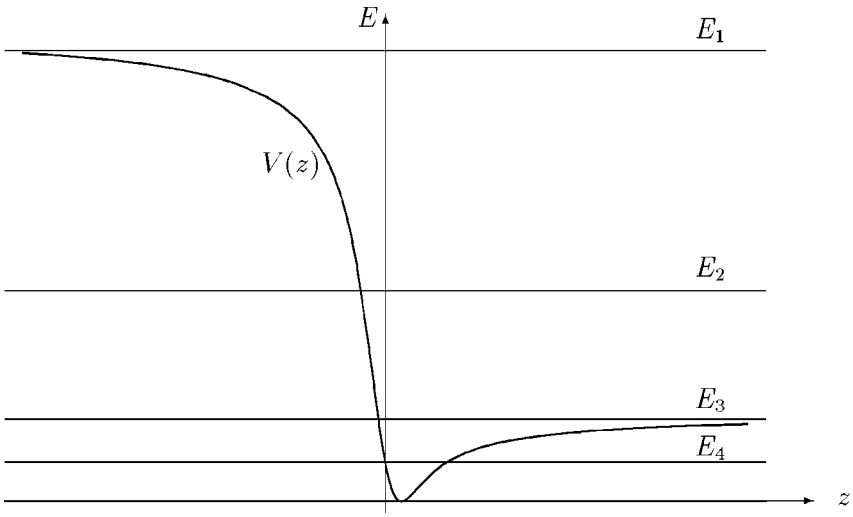

FIG. 2. Different possibilities of motion for $0 < h < 1$.

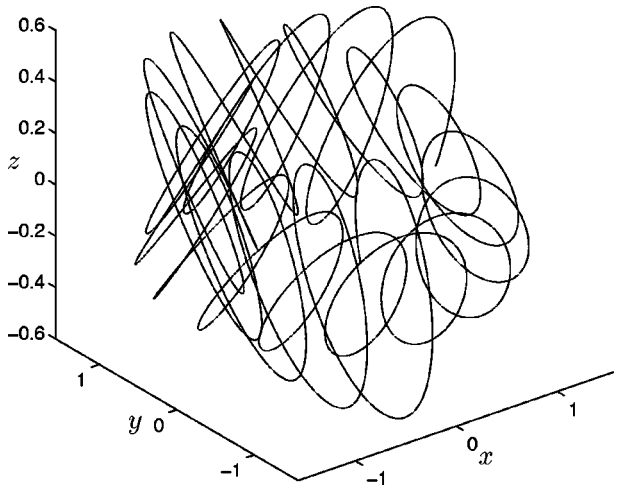

FIG. 3. Bounded orbit in three dimensions.

the equilibrium point $p=0$, the position of equilibrium (with respect to the origin) depends on the constant h. For larger $|h|$, the location of the equilibrium point is more distant.

The role of h in the radial motion is similar to the role of j in the planar motion. As the orientation of the charge isovector and the Higgs field are fixed in the radial motion, the constant h depends only on the initial starting point, r_0, and the initial value of p, p_0. The initial value of p, p_0, is a free parameter in the radial motion and it must be determined by the overall theory of motion. From Eq. (4.10) one may write an integral equation for t and r:

$$t=\pm\int_{r_0}^{r}\frac{dr}{\sqrt{2E/m-[-IH(r)/r+h]^2}}. \tag{4.12}$$

C. Three-dimensional bounded orbits

We studied the planar and radial motions in the previous subsections. In both cases, bounded orbits were allowed. Suppose a particle is moving in a bounded orbit in a plane, say the xy-plane, so that the charge isovector is normal to the plane of motion along the z-axis. Regardless of the motion in the plane, suppose the particle has also a motion in the z-direction such that the particle can oscillate in the z-direction. This is a motivation to believe, if we mix the initial condition of the both motions, we may get a bounded motion in three dimensions. Of course, we do not say that the resulting motion is the superposition of the two previously mentioned motions. It is clear that the equations governing the motion [i.e., Eqs. (3.6) and (3.8)] are not linear, therefore the superposition of the solutions is not necessarily a solution. The above motivation is correct only for the starting point, and for the other instants we must follow the equations of motion. Let us examine an example by numerical solution. Under these circumstances, the planar motion condition requires $h=0$. For example, with $h=0$, if the particle is launched into the fields with the initial values $[\vec{r}_0,\vec{v}_0,\vec{I}_0]=[[1,0,0],[0.1,0,0],[0,0,1]]$, the result is a bounded planar motion in the xy-plane (see plot on the bottom-left of Fig. (2). If the particle is launched in the field with the initial values [[0,0,0],[0,0,0.1],[0,0,1]], the result is a symmetric bounded oscillation along the z-axis around the origin. So we expect, if the particle is launched with the initial values [[1,0,0],[0.1,0,0.1],[0,0,1]], the result will be a bounded orbit in three dimensions. By chance it is right. Using the three-dimensional equations of motion (3.6) and (3.8), a numerical analysis confirms the claim as it is plotted in Fig. (3). We have tested the motion for a remarkable amount of time (10 000 units of time), and numerically a result is obtained.

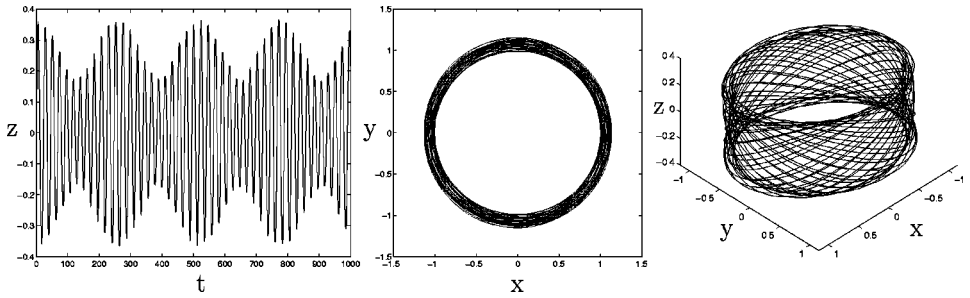

FIG. 4. The left plot shows the variation of z-direction vs time, the middle one shows the intersection of the motion in the xy-plane, and the right plot shows the three-dimensional orbit.

One result that we may get quickly from the above discussion is the stability of the planar motions. In fact, it is sensible to understand the stability of the planar motions in the new scenario. When small perturbations normal to the plane of motion disturb the motion, there is a vertical force to keep the motion oscillating close to the plane so that the pattern of the planar orbit stays unchanged. So, involving the Higgs field interaction makes a significant difference. In Ref. 1 the Higgs field interaction was ignored, so the planar motions were not stable (in the sense of vertical perturbations). We have checked the stability of the planar motions by considering small perturbations in any of the motion's parameters, numerically by using the general equations of motion.

In general the closed orbits are unknown in the nonplanar motions. For example, if we start the motion from the initial values [[1,0,0],[0,0.266,0],[0,0,1]] and $h=0$, we obtain a closed circular motion, and if we start the motion from [[0,0,0],[0,0,0.1],[0,0,1]] we obtain a symmetric radial oscillation. The motion with initial values [[1,0,0],[0,0.266,0.1],[0,0,1]] forms a bounded orbit such that the intersection of the orbits with the xy-axis is bounded between two circles, and the z-direction has an oscillatory motion along the z-axis with the domain changes between a minimum and a maximum periodically [see Fig. (4)]. If the equations of motions were linear, we might say the superposition of two closed orbits is closed if the ratio of periods of two motions is a rational number. But in our case the equations of motion are not linear, so we are not able to use this theorem. We might play with the parameters to gain a closed orbit in three dimensions. Studying the bounded and closed orbits needs an analytic description of the equations of motion, which is not available here.

With $h=0$ we may choose any combination of the initial values (not only a combination of the planar and radial motions initial values) and test the equations of motion by numerical computations. The bounded orbits are observed for different kinds of combinations of the initial values. Of course for many initial values we cannot expect a bounded orbit. For nonzero h's the combination of initial values is too sensitive and for most of them the orbit is unbounded. But still for some initial values bounded orbits are observed. An example is [[1,0,0],[0.1,0,0],[1,0,1]] with $h=0.5$. Now the initial values [[1,0,0],[0.1,0,0],[0,0,1]] with $h=0.5$ is neither a planar motion nor a nonplanar bounded motion, but when it mixes with an oscillatory motion in the x-direction, the resulting three-dimensional motion will be bounded.

At far distances a particle moves on a surface of a cone (see Sec. III). Figure 5 shows the orbit for an initial values [[10,10,0],[0,−0.1,0],[0,0,1]] with $h=1$ in 200 units of time. The variations on x and z are small and of the order 10^{-4} (the unusual ticks in the vertical axis are badly managed by MATLAB, and means the variations in this axis are of order 10^{-4}). The particle, which has started the motion with an initial velocity in the negative y-direction, moves along the y-direction almost uniformly.

V. THE FORCE LAW

In this section we consider further the force on a non-Abelian particle in a BPS monopole field configuration [$\mathbf{B}_i=\pm\mathbf{D}_i\Phi$, $\mathbf{A}_0=0$, $V(\Phi)=0$] which we studied in the previous section. We shall show the force has the form of a ''generalized'' Lorentz force.

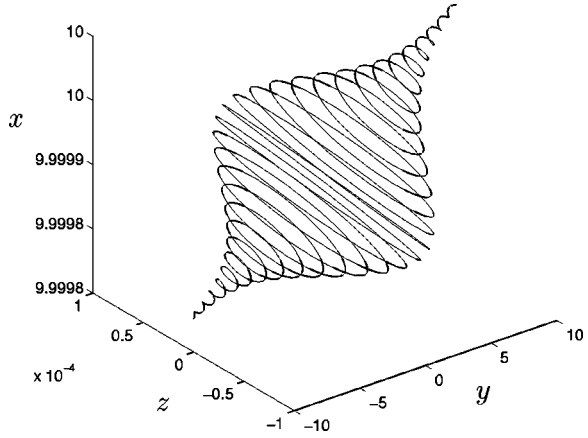

FIG. 5. Three-dimensional motion at large distance.

Looking at the first equality in Eq. (3.6), if we suppose eI^a is an electric charge of the particle (in a non-Abelian sense), then $eI^a\vec{v}\times\vec{B}^a$ is a magnetic force due to a magnetic field $\vec{B}^a$ on the particle, and $eI^a\,p\vec{B}^a$ may be interpreted as an electric force due to an electric field $p\vec{B}^a$ on the particle (regardless of the notation $\vec{B}^a$ that is used for magnetic field).

Let us explain more. In the usual electrodynamics, the force of an electric field $\vec{E}$ on an electric charged particle with the charge q is $q\vec{E}$, and the force of a magnetic field $\vec{B}$ on an electric charged particle with the charge q is $q\vec{v}\times\vec{B}$, where $\vec{v}$ is the velocity of particle. Let us switch to the non-Abelian fields and particles. Assume a field B_i^a in the space and a non-Abelian test particle with charge isovector Y^a in this field. The particle feels only the component of the magnetic field that is projected along its charge isovector. Let us choose a unit vector $\hat{n}$ along the charge isovector (remember in the isospace),

$$\vec{Y}=q\hat{n}, \tag{5.1}$$

where $q=|\vec{Y}|=\text{const}$ is the charge of the particle. Now the effective magnetic field the particle feels is

$$\mathcal{H}_i=\vec{B}_i\cdot\hat{n}, \tag{5.2}$$

or equivalently $\vec{\mathcal{H}}=\vec{B}^a\hat{n}^a$. Now we can write down the equation of motion of the particle, Eq. (3.6), in a familiar form (for positive magnetic charge):

$$m\dot{\vec{v}}=q\vec{v}\times\vec{\mathcal{H}}+p\,q\,\vec{\mathcal{H}}, \tag{5.3}$$

where here $q=eI$.

Equation (5.3) is a generalization of the Lorentz force. Comparing with the usual electrodynamics, two major differences show themselves in Eq. (5.3). The first difference is the following: In Eq. (5.3), rather than a term analogous to the usual Lorentz force (first term on the right-hand side), there is another term that is similar to the Coulomb force in the usual electrodynamics. We should remember that this new term is originally different from the Coulomb force. The Coulomb force is regarded as the zeroth component of the Yang–Mills fields, which in our discussions has been ignored (remember we are working in stationary fields with $\mathbf{A}_0=0$), but here the origin of the Coulomb-like force is the Higgs field. The coefficient p in front of the Coulomb-like force contains some information about the interaction of the Higgs field and the charge isovector. We will say how this generalized equation reduces to the normal Lorentz force when the field and particle can be regarded as a non-Abelian field and particle. The second difference is this:

In the usual Lorentz force, the force vanishes if and only if the nonvanishing magnetic field and the particle's velocity become parallel. But in the non-Abelian case it might happen that neither of the particle's velocity or the non-Abelian magnetic field vanish, nor the particle's velocity and the magnetic field (in any sense, either in the non-Abelian form B_i^a or in the Higgs gauge-invariant form $\mathcal{B}_i$ (Ref. 13) are parallel, but the force vanishes. This happens when the projection of the magnetic field along the charge isovector vanishes, i.e., $\vec{\mathcal{H}}=0$.

We can define a usual (say Abelian) particle in general as a non-Abelian particle whose charge isovector is fixed in the isospace, i.e.,

$$Y^a = q\,\delta^{a3}. \tag{5.4}$$

Now when the charge isovector $\vec{Y}$ takes a radial direction in the isospace, we can transform its direction to the three-direction by a proper gauge transformation.[14] This happens for both the charge isovector and the Higgs field simultaneously when both the isovectors take radial direction in a part of the space. A good example is the regions too far from the core of the fields, where we found the equations of motion asymptotically.

Suppose $\vec{Y}=q\hat{r}$ $(q=eI)$ and $\vec{\Phi}=a\hat{r}$ in the asymptotic case. So, the charge isovector has no components in the directions normal to the radial direction, and therefore $\beta=\gamma=0$. In this case our definitions of $\mathcal{B}$ and $\mathcal{H}$ overlap, and the equation of motion (5.3) transforms to Eq. (3.26) (for self-dual case):

$$m\dot{\vec{v}}=\frac{I}{r^3}[(\vec{v}\times\vec{r})+p\vec{r}], \quad p=(-eaI+h)/m. \tag{5.5}$$

Both of the isovectors can be rotated by a gauge transformation to lie in the three-direction by a gauge transformation, where we expect to have the usual Abelian electrodynamics laws. By the rotation, the particle will be the usual particle that is defined in Eq. (5.4), and the electromagnetic field becomes the usual one. In addition, in the usual space that we are talking about, there should be no trace of the free parameter p which is related to the extra dimension. So, we may have $p=0$, and set the constant h

$$h=eaI. \tag{5.6}$$

Now Eq. (5.5) is reverted to the proper usual Lorentz force. The differences between the generalized force and the usual Lorentz force we enumerated before automatically disappear, because the factor p vanishes and the extra term in the generalized force is gone. Also the Higgs field and the charge isovector have become parallel, therefore the second difference we mentioned can no longer happen.

In general we need 13 initial values $[x^A(t_0),\ \dot{x}^A(t_0),$ and $I^a(t_0)]$ to determine solutions of the equations of motion. In the nonrelativistic framework there are 11 values, 9 of which are position, velocity, and charge isovector that are indeed needed to solve the equations (3.2) and (3.5). The other two initial values are connected to the internal fifth dimension x^5. Because neither the fields nor the equations of motions depend on the internal direction, therefore the initial starting point in the x^5-direction is not important. But the time variation of internal direction dx^5/dt, which was called p, is very important.

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[13] 'tHooft introduced a gauge-invariant electromagnetic tensor which reduces to the usual electromagnetic field tensor when the scalar field, Φ has only third component, i.e., $\Phi^b = a\,\delta^{b3}$, $\mathcal{F}_{\mu\nu} = \partial_\mu(\hat{\Phi}^a A^a_\nu) - \partial_\nu(\hat{\Phi}^a A^a_\mu) - (1/e)\,\epsilon^{abc}\hat{\Phi}^a(\partial_\mu\hat{\Phi}^b) \times(\partial_\nu\hat{\Phi}^c)$, so the magnetic field is $\mathcal{B}^i \equiv \frac{1}{2}\,\epsilon^{ijk}\mathcal{F}_{jk}$.

[14] At each point (r,θ,ϕ) in the real space, the direction $\hat{r}$ in the isospace rotates to the three-direction with the gauge transformation $U^{-1} = \cos(\theta/2) + i\vec{z}\cdot\vec{\sigma}\,\sin(\theta/2)$, $z^i = \epsilon^{ij3}\hat{r}^j/\sin\theta$, where σ^a are Pauli sigma matrices.

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Quantum mechanics of layers with a finite number of point perturbations

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We study spectral and scattering properties of a spinless quantum particle confined to an infinite planar layer with hard walls containing a finite number of point perturbations. A solvable character of the model follows from the explicit form of the Hamiltonian resolvent obtained by means of Krein's formula. We prove the existence of bound states, demonstrate their properties, and find the on-shell scattering operator. Furthermore, we analyze the situation when the system is put into a homogeneous magnetic field perpendicular to the layer; in that case the point interactions generate eigenvalues of a finite multiplicity in the gaps of the free Hamiltonian essential spectrum. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The object of our interest in this article is a spinless quantum particle living in a layer of a fixed width d with the Dirichlet boundary conditions and interacting with a finite number of point perturbations. An obvious motivation for this problem is to find a description for an electron in a semiconductor layer with impurities. However, such physical systems are in reality rather complicated objects which involve a crystal lattice with some alien atoms and an electron gas, so one has to ask first whether such a simple model can reproduce the basic features known from experiments.

It is well known that an electron in an ideally pure bulk semiconductor material can be modeled as a free particle with an effective mass m^* which characterizes the relation between the energy and quasi-momentum at the Fermi level. Properties of the crystalline structure are thus expressed through a single material constant, which may be very different from the ''bare'' mass—recall that for GaAs we have $m^* = 0.067 m_e$.

There are two other assumptions in the ''free'' part of the model. The first is its one-particle character which neglects the interactions between the electrons. There are situations where the repulsion plays an important role, such as the Coulomb blockade in quantum wires. On the other hand, the one-electron model is known to work when the electron-gas density is sufficiently low. Another assumption is the neglection of spin which is also not entirely trivial; recall that spin-dependent effects in nanostructures have been studied recently—see Ref. 1 and references therein. In most situations, however, spinless electrons are a reasonable approximation.

The next question concerns the way in which we model the impurities. Using again a certain idealization, we describe them by point interactions. This method proved rather useful in the last two decades and gave rise to numerous solvable models; our aim here is to add one more class to this family. Intuitively point interactions are understood as sharply localized potentials, but it is

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known that a sophisticated coupling constant renormalization is required to give this concept meaning in terms of a limit of scaled potentials (Ref. 2, Secs. I.1 and I.5). Mathematically such operators can be handled since they differ from the free Hamiltonian H_0 just by a change of the boundary conditions at the interaction sites. However, the counterintuitive features of three-dimensional point interactions are reflected both in the slow way in which they found their place in the theory and in the fact that the parameters appearing in these conditions cannot be interpreted as δ potential coupling constants but rather as the inverse scattering lengths corresponding to the point ''obstacles'' (cf. Ref. 2, Chap. I.3).

Scores of papers discussing point-interaction models in the Euclidean space, both for particles otherwise free or with a background regular potential, are summarized in Ref. 2. Only in the last decade has the attention shifted to systems with point interactions restricted to a certain region of configuration space; the reason clearly was a wide collection of new physical phenomena observed in such spatially restricted systems, mostly mesoscopic objects, but also electromagnetic waveguides, photonic crystals, etc. (see Ref. 3). Here, too, point-interaction Hamiltonians proved a useful tool and yielded some unexpected results such as the existence of a chaotic behavior in systems whose classical counterparts are integrable.[4]

Today there are many papers treating point interaction in restricted areas; a bibliography is given in the introduction of Ref. 5. They typically put emphasis on the description of a specific model rather than a proper handling of the point interaction. Among the few existing rigorous treatments of the problem, it is Ref. 5 which motivates the present study analyzing point interactions in an infinite planar strip with Dirichlet boundary conditions, together with similar systems. There are two ways in which the results can be generalized to dimension three. One is a straight Dirichlet tube in $\mathbb{R}^3$ with a fixed compact cross section discussed in Ref. 6; it is a straightforward extension, a part of a different way of computing the regularized Green's function.

In the present article we are going to study a less trivial generalization, with point interactions situated in a flat layer with a Dirichlet boundary. The free system allows here again a separation of variables, so the free resolvent kernel and all the quantities derived from it such as eigenfunctions, etc., can be written by means of an explicitly given series (in this sense models considered here are little ''less solvable'' than those in the full space when such quantities can be written in terms of elementary or special functions).

Although the model description is simple, it covers many different situations. For the sake of brevity we restrict ourselves in this article to systems with a finite number of point perturbations in the absence of a background potential, leaving other cases to a sequel. We make an exception, however, by devoting a separate section to the case when the particle is under the influence of a homogeneous magnetic field perpendicular to the layer. The spectrum of the unperturbed system is then changed, completely consisting of infinitely degenerate eigenvalues which are sums of the Landau levels and the transverse eigenvalues; for ''rational'' combinations of parameters different Landau levels may lead to the same eigenvalue. A finite number of point perturbations then gives rise to a nontrivial discrete spectrum.

Let us describe briefly the contents. The next section is devoted to the case of a single perturbation. We start from the definition of the point-interaction Hamiltonian by means of boundary conditions coupling generalized boundary values. After that we use Krein's formula to derive the explicit expression for the resolvent; it involves the regularized Green's function which is given by a specific series as mentioned earlier [see (2.14)]. In Sec. II D we use this result to analyze spectral properties of such Hamiltonians. The bound state energies are given by the implicit equation (2.19), and it is just the limits of strong and weak coupling where we are able to write the explicit expressions for the leading term of the asymptotics. In both the extreme cases the eigenvalue behavior can be easily understood: in the strong-coupling situation it goes to $-\infty$ in the same way as if there were no boundaries because the corresponding eigenfunction is strongly localized, while in the weak-coupling case the eigenvalue approaches the threshold of the essential spectrum and the wavefunction is dominated transversally by the lowest mode. We also find that the eigenvalue decreases with the distance from the layer boundary. In the last part of Sec. II we shall discuss the scattering in the presence of a perturbation. If there is a single point interaction,

we can employ the symmetry of the problem with respect to rotation around the axis passing through the perturbation and perpendicular to the layer. The partial wave decomposition in the ''longitudinal'' coordinates shows that the only nontrivial contribution to the scattering comes from the s-wave, i.e., from states with the orbital momentum $m=0$. Within this subspace, the scattering problem is reduced to transitions between transverse modes; the final S-matrix then describes a coupling of the ''open'' channels, i.e., the transverse modes with the energies lower than that of the incoming spherical wave. We also derive the on-shell scattering operator which maps the incoming wave vector and transverse mode into the outgoing ones; the advantage of this approach is that it does employ the symmetry and allows for a generalization to the case with multiple perturbations.

Section III extends the described analysis to any finite number N of point perturbations. The technique remains the same, and since the difference between the two resolvents is of rank N, the essential and absolutely continuous spectra are again preserved. On the other hand, the analysis of the discrete spectrum becomes more complicated. There are n eigenvalues, where $1\leqslant n\leqslant N$, which are found by solving the implicit equation $\det\Lambda(z)=0$ with the $N\times N$ matrix Λ given by (3.8). The number n depends on the coupling strength. In the strong coupling limit there exist exactly N eigenvalues having the same asymptotic behavior as in the one-center case. On the other hand, for weak coupling we find only one eigenvalue approaching the threshold of the essential spectrum; in this sense our system exhibits a behavior typical for all weakly coupled Schrödinger operators.

A new feature for systems with $N\geqslant 2$ is that they can possess eigenvalues embedded in the essential spectrum. This is possible, e.g., when the point perturbations are placed symmetrically with respect to the layer axis and have the same (sufficiently strong) coupling: the corresponding eigenfunction cannot then contain contributions from transverse modes with the energy equal or smaller than this eigenvalue. We will show that this is true for embedded eigenvalues generally: their eigenvectors have to be orthogonal to the subspace spanned by the ''lower'' transverse modes. For $N\geqslant 2$ the system no longer exhibits a rotational symmetry, hence we cannot employ the partial-wave decomposition to describe the scattering. However, the second approach mentioned above is applicable here and we can derive again the on-shell scattering operator. It is similar to that of the one-center case differing just by replacement of a single regularized Green's function by a sum of the elements of the matrix Λ [see (3.34)].

Section IV deals with the situation when the layer is placed into a homogeneous magnetic field perpendicular to its boundary. The Krein's formula is applicable but the free resolvent is substantially different from the nonmagnetic case; this is reflected in the form of the essential spectrum which now consists the ''sum'' of the Landau levels and the transverse mode energies; it, of course, is preserved by a finite number of point perturbations. If there is a single perturbation, we get exactly one eigenvalue in each spectral gap, i.e., between any two neighboring levels. In the strong and weak coupling limits it approaches the upper and lower endpoint of corresponding ''free'' gap, respectively. Only for the lowest gap we find a different behavior in the strong-coupling limit case; the eigenvalue goes to $-\infty$ with the same asymptotics as in the nonmagnetic case. Finally, we present a generalization to the case of N point interactions analogous to the considerations of Sec. III.

II. A SINGLE PERTURBATION

A. The free system

Consider an infinite layer $\Sigma:=\mathbb{R}^2\times[0,d]$ with the coordinates denoted as $\vec{x}=(x,y)$, where $x=(x_1,x_2)\in\mathbb{R}^2$ and $y\in[0,d]$. We consider a single spinless nonrelativistic particle confined to Σ. Since the actual values of physical constants are not essential throughout the article, we put $\hbar=2m=1$ and suppose that the free motion of the particle is governed by the Dirichlet Laplacian $-\Delta_D^{\Sigma}$.

Recall that this operator can be defined for rather general domains in $\mathbb{R}^n$ as the Friedrichs extension of an appropriate quadratic form (Ref. 7, Sec. XIII.15). However, since the boundary of

Σ consists of two disjoint planes and has therefore the segment property, the operator acts simply as $H_0\psi=-\Delta\psi$ on the domain of all ψ of the local Sobolev space $W^{2,2}(\Sigma)$ which satisfy the boundary conditions

$$\psi(x,0)=\psi(x,d)=0 \tag{2.1}$$

for all $x\in\mathbb{R}^2$ (see again Ref. 7, Sec. XIII.15).

We will make use of the fact that the ''longitudinal'' and ''transverse'' variables decouple in the free system. The state Hilbert space of our problem can then be decomposed into traverse modes,

$$L^2(\Sigma)=\bigoplus_{n=1}^{\infty} L^2(\mathbb{R}^2)\otimes\{\chi_n\},\quad \chi_n(y):=\sqrt{\frac{2}{d}}\sin\left(\frac{\pi n y}{d}\right),$$

because the functions $\chi_n(y)$ form an orthonormal basis in $L^2([0,d])$. The free Hamiltonian can be correspondingly written in the form of a direct sum,

$$H_0=\bigoplus_{n=1}^{\infty} h_n\otimes I_n,\quad h_n:=-\frac{\partial^2}{\partial x_1^2}-\frac{\partial^2}{\partial x_2^2}+\left(\frac{\pi n}{d}\right)^2. \tag{2.2}$$

Since the resolvent $(H_0-z)^{-1}$ of the two-dimensional Laplacian is known explicitly, the above decomposition yields in turn the free resolvent kernel

$$G_0(x,y;x',y';z)=\frac{i}{4}\sum_{n=1}^{\infty} H_0^{(1)}(k_n|x-x'|)\chi_n(y)\,\chi_n(y'), \tag{2.3}$$

where $k_n\equiv k_n(z):=\sqrt{z-(\pi n/d)^2}$.

B. Definition of a point interaction

Our first goal is to construct a one-center perturbation supported by a point $\vec{a}:=(a,b)$ with $a\in\mathbb{R}^2$ and $b\in(0,d)$. This can be done in a standard way.[2] We restrict $-\Delta_D^{\Sigma}$ to functions which vanish in a neighborhood of $\vec{a}$; the operator obtained in this way is symmetric but not self-adjoint and we look for the perturbed one among its self-adjoint extensions. Since the restriction has deficiency indices (1,1), the family of extensions is by the standard von Neumann theory (Ref. 7, Sec. X.1) characterized by a single parameter.

What is equally important is that the perturbation is local, and therefore we can characterize the extensions by the usual boundary condition derived in Ref. 2, Chap. I.1, for point interactions in $\mathbb{R}^3$. We introduce the generalized boundary values,

$$L_0(\psi,\vec{a}):=\lim_{|\vec{x}-\vec{a}|\to 0}|\vec{x}-\vec{a}|\,\psi(\vec{x}),\quad L_1(\psi,\vec{a}):=\lim_{|\vec{x}-\vec{a}|\to 0}\left[\psi(\vec{x})-\frac{L_0(\psi,\vec{a})}{|\vec{x}-\vec{a}|}\right],$$

and require

$$L_1(\psi,\vec{a})-4\pi\alpha L_0(\psi,\vec{a})=0. \tag{2.4}$$

For a fixed $\alpha\in\mathbb{R}$ this leads to the self-adjoint operator $H(\alpha,\vec{a})$ acting as

$$(H(\alpha,\vec{a})\psi)(\vec{x})=-(\Delta\psi)(\vec{x}) \tag{2.5}$$

for $\vec{x}\neq\vec{a}$ on the domain

$$D(H(\alpha,\vec{a})):=\{\psi:-\Delta\psi\in L^2(\Sigma\backslash\{\vec{a}\})\ \text{and}\ (2.1)\ \text{and}\ (2.4)\ \text{are satisfied}\} \tag{2.6}$$

in $L^2(\Sigma)$, where $-\Delta\psi$ is, of course, understood in the sense of distributions. The family of self-adjoint extension also includes the case which is formally given by $\alpha=\infty$, which means $L_0(\psi,\vec{a})=0$. It is easy to see that the corresponding $H(\alpha,\vec{a})$ is nothing else than the free Hamiltonian H_0.

C. The resolvent

As usual the spectral properties of the operator $H(\alpha,\vec{a})$ can be studied using its resolvent. Since $H(\alpha,\vec{a})$ and H_0 have a common restriction with deficiency indices (1,1), the kernel of the full resolvent can be obtained by means of Krein's formula (Ref. 2, Appendix A)

$$(H(\alpha,\vec{a})-z)^{-1}(\vec{x}_1,\vec{x}_2)=G_0(\vec{x}_1,\vec{x}_2;z)+\frac{G_0(\vec{x}_1,\vec{a};z)\,G_0(\vec{a},\vec{x}_2;z)}{\alpha-\xi(\vec{a};z)}, \tag{2.7}$$

where

$$\xi(\vec{a};z):=\frac{1}{4\pi}\lim_{\vec{x}\to\vec{a}}\left\{\frac{2\pi i}{d}\sum_{n=1}^{\infty}H_0^{(1)}(k_n|x-a|)\sin\left(\frac{\pi n y}{d}\right)\sin\left(\frac{\pi n b}{d}\right)-\frac{1}{|x-a|}\right\} \tag{2.8}$$

is the regularized Green's function; we have employed here the fact that the resolvent singularity is the same as for the kernel of $-\Delta$ in $L^2(\mathbb{R}^3)$ (see Ref. 8, Sec. 13.5). The form of the denominator in expression (2.7) follows from the boundary condition (2.4) applied to $\psi=(H(\alpha,\vec{a})-z)^{-1}\varphi$, where φ is an arbitrary vector from $L^2(\Sigma)$. However, the above definition does not give a practical way to compute $\xi(\vec{a};z)$. To this end we use first $K_0(z)=(\pi i/2)\,H_0^{(1)}(iz)$ and introduce $\kappa_n:=\sqrt{(\pi n/d)^2-z}=-ik_n$. Then we have

$$\xi(\vec{a};z)=\lim_{\varrho\to 0}\left\{\frac{1}{\pi d}\sum_{n=1}^{\infty}K_0(\kappa_n\varrho)\sin^2\left(\frac{\pi n b}{d}\right)-\frac{1}{4\pi\varrho}\right\}, \tag{2.9}$$

where $\varrho:=|x-a|$ and we have already put $y=b$. We use the asymptotic behavior $\kappa_n\approx\pi n/d$ as $n\to\infty$ to write the identity

$$K_0(\kappa_n\varrho)=K_0\left(n\frac{\pi\varrho}{d}\right)+\left[K_0(\kappa_n\varrho)-K_0\left(n\frac{\pi\varrho}{d}\right)\right] \tag{2.10}$$

and to divide the function ξ into two parts, $\xi(\vec{a};z)=\xi_1+\xi_2$, where

$$\xi_1:=\lim_{\varrho\to 0}\frac{1}{\pi d}\sum_{n=1}^{\infty}\left[K_0(\kappa_n\varrho)-K_0\left(\frac{\pi n\varrho}{d}\right)\right]\sin^2\left(\frac{\pi n b}{d}\right),$$

$$\xi_2:=\lim_{\varrho\to 0}\left\{\frac{1}{2\pi d}\sum_{n=1}^{\infty}\left[K_0\left(\frac{\pi n\varrho}{d}\right)-K_0\left(\frac{\pi n\varrho}{d}\right)\cos\left(\frac{2\pi n b}{d}\right)\right]-\frac{1}{4\pi\varrho}\right\};$$

we have used $2\sin^2\alpha=1-\cos 2\alpha$. To deal with the first term we employ the asymptotic behavior of the Macdonald function (Ref. 9, Sec. 9.6.13) which yields

$$K_0(\kappa_n\varrho)-K_0\left(\frac{\pi n\varrho}{d}\right)=-\ln\sqrt{1-z\left(\frac{d}{\pi n}\right)^2}\,(1+\mathcal{O}(\varrho^2))$$

as $\varrho\to 0$. It shows that the sum converges uniformly wrt ϱ and the limit can be interchanged with the series thus giving

$$\xi_1 = -\frac{1}{\pi d}\sum_{n=1}^{\infty} \ln\sqrt{1-z\left(\frac{d}{\pi n}\right)^2}\,\sin^2\left(\frac{\pi n b}{d}\right). \tag{2.11}$$

The second part can be computed by means of the formula (Ref. 10, II, 5.9.1.4.),

$$\sum_{n=1}^{\infty} K_0(nx)\cos(na) = \frac{\pi}{2\sqrt{x^2+a^2}} + \frac{1}{2}\left(\gamma + \ln\frac{x}{4\pi}\right) + \frac{\pi}{2}\sum_{n=1}^{\infty}\left[\frac{1}{\sqrt{(2n\pi-a)^2+x^2}} - \frac{1}{2n\pi}\right] + \frac{\pi}{2}\sum_{n=1}^{\infty}\left[\frac{1}{\sqrt{(2n\pi+a)^2+x^2}} - \frac{1}{2n\pi}\right].$$

So, introducing $\beta := b/d$ and $\mu := \varrho/d$ and performing the limit $\mu \to 0$, we get

$$\xi_2 = \frac{1}{4\pi d}\left\{-\frac{1}{2\beta} - \sum_{n=1}^{\infty}\frac{\beta^2}{n(n^2-\beta^2)}\right\}. \tag{2.12}$$

The last sum equals Ref. 10, I, 5.1.15.2. expressed by means of the digamma function as $\psi(1) - 1/2\,(\psi(1+\beta)+\psi(1-\beta))$, and since $\psi(1) = -\gamma$, where $\gamma = 0.577\ldots$ is the Euler number, and $\psi(1-\beta) = \psi(\beta) + \pi\cot(\pi\beta)$, $\psi(1+\beta) = \psi(\beta) + 1/\beta$, we arrive at

$$\xi_2 = \frac{\gamma}{4\pi d} + \frac{1}{8\pi d}\,(2\psi(\beta) + \pi\cot(\pi\beta)). \tag{2.13}$$

Putting the results together, we get the sought formula

$$\xi(\vec{a};z) = -\frac{1}{\pi d}\sum_{n=1}^{\infty} \ln\sqrt{1-z\left(\frac{d}{\pi n}\right)^2}\,\sin^2\left(\frac{\pi n b}{d}\right) + \frac{1}{4\pi d}\left[\gamma + \psi\left(\frac{b}{d}\right) + \frac{\pi}{2}\cot\left(\frac{\pi b}{d}\right)\right], \tag{2.14}$$

expressing the regularized Green's function in the form of a series. It is certainly more complicated than an expression of the corresponding quantity for the whole space in terms of elementary functions (Ref. 2, Chap. I.1), but it allows us to derive the needed properties of the function ξ to compute the values of $\xi(\vec{a};z)$ numerically.

Remark 2.1: Notice the scaling behavior with respect to the change of the layer thickness, i.e., the formulas relating properties of the family $\Sigma^\sigma = \mathbb{R}^2 \times [0, d\sigma]$, $\sigma > 0$. Here the dimension of the configuration space is decisive. While for a two-dimensional system the scaling amounts to logarithmic shift of the function ξ as shown in Ref. 5, in three dimensions the transformation is multiplicative. We find easily that the situation is the same as for straight tubes in $\mathbb{R}^3$ studied in Ref. 6, i.e., we have $\xi(\vec{a}^\sigma; z\sigma^{-2}) = \sigma^{-1}\xi(\vec{a};z)$, where $\vec{a}^\sigma := (a\sigma, b\sigma)$. This means, in particular, that the singularities of the resolvent which we will discuss later using Eq. (2.19) are related as follows:

$$\epsilon^\sigma(\alpha^\sigma, \vec{a}^\sigma) = \sigma^{-2}\epsilon(\alpha,\vec{a}), \quad \alpha^\sigma := \sigma^{-1}\alpha. \tag{2.15}$$

Without loss of generality we put therefore $d = \pi$ in the rest of this and the next section.

D. Spectral properties

The explicit form of the resolvent (2.7) allows us to derive information about the spectrum. Since its difference from $(H_0 - z)^{-1}$ is a rank one operator, the essential spectrum remains by Weyl's theorem (Ref. 7, Thm. XIII.14) the same as for the free Hamiltonian H_0, i.e., we have $\sigma_{ess}(H(\alpha,\vec{a})) = [1,\infty)$. At the same time, also the absolutely continuous spectrum is preserved, $\sigma_{ac}(H(\alpha,\vec{a})) = [1,\infty)$, this time by Birman–Kuroda theorem (Ref. 7, Thm. XI.9).

Next we would like to prove the absence of the singularly continuous spectrum. To this aim we have to check that the expression $(\psi,(E_z-E_c)\psi)$ for all $\psi\in L^2(\Sigma)$ is an absolutely continuous function for z from any interval $(c,t)\subset(1,\infty)$; in other words, that it can be written as an integral of a locally integrable function. Since σ_{sc} cannot be supported by discrete points, we may choose the interval (c,t) in such a way that it contains none of the points m^2, $m\in\mathbb{N}$. We exclude these points because the free Green's function $G_0(z)$ diverges at them. For the spectral projection E_t-E_c to the interval (c,t) we employ Stone's formula,

$$(\psi,(E_t-E_c)\psi)=\frac{1}{\pi}\lim_{\varepsilon\to 0_+}\int_c^t(\psi,\mathrm{Im}\,G(u+i\varepsilon)\psi)\,du; \tag{2.16}$$

we have used here the fact which we will establish a little later, namely that $H(\alpha,\vec{a})$ has no eigenvalues in $(1,\infty)$, and therefore the spectral projections to (c,t) and $[c,t]$ are the same. The Green's function (2.7) is analytic for z with $\mathrm{Re}\,z\in(c,t)$ and $\pm\mathrm{Im}\,z\in(0,\varepsilon)$, and, furthermore, its limits when z approaches the real axis from above and from below exist and are continuous functions of z. Recall that by assumptions no thresholds are contained in (c,t) and ξ has nonzero imaginary part for $z\neq m^2$,

$$\mathrm{Im}\,\xi(\vec{a};z)=\frac{1}{2\pi}\sum_{n=1}^{[\sqrt{z}]}\sin^2(nb)>0, \tag{2.17}$$

where we have used $\sqrt{z-m^2}=i\sqrt{m^2-z}$; hence, the denominator of the second term in (2.7) cannot be singular. Consequently, the integrated function is bounded in $(c,t)\times[0,\varepsilon)$, and by the dominated convergence theorem the limits can be interchanged with the integral giving

$$(\psi,(E_t-E_c)\psi)=\frac{1}{\pi}\int_c^t(\psi,\mathrm{Im}\,G(u)\psi)\,du. \tag{2.18}$$

The function under the integral is again continuous in the interval (c,t), hence it is integrable and the statement is proved. If $t=t_0$ would be an isolated eigenvalue embedded in the continuous spectrum and ψ the corresponding eigenfunction, the above relation remains valid for $t\in(t_0-\eta,t_0)\cup(t_0,t_0+\eta)$ with some $\eta>0$, while at the point t_0 the lhs should have a jump, which is clearly impossible due to the continuity of the integrated function.

To determine the discrete spectrum, we have to find the poles of the resolvent. Recall that a perturbation which can be reduced to a self-adjoint extension of a common symmetric restriction with deficiency indices (1,1) can give rise to at most one simple eigenvalue in each gap of the spectrum (Ref. 11, Sec. 8.3, Cor. 1). In our case it means one simple eigenvalue in the interval $(-\infty,1)$. In view of the relation (2.7) one can find it by solving the implicit equation

$$\xi(\vec{a};z)=\alpha \tag{2.19}$$

for $z\in\mathbb{R}$. The series contained in the formula (2.14) converges for all $z\in\mathbb{R}\setminus\{n^2:n\in\mathbb{N}\}$, because its terms decay like n^{-2} as $n\to\infty$ as we can see using the Taylor expansion of $\ln(1-\zeta)$ to the first order. The remaining term ξ_2 is independent of z and finite for any $b\in(0,\pi)$.

The value of $\xi(\vec{a};z)$ is real for any $z\in(-\infty,1)$. In particular, it is easy to compute

$$\xi(\vec{a};z=0)=\frac{1}{4\pi^2}\left[\gamma+\psi\left(\frac{b}{\pi}\right)+\frac{\pi}{2}\cot(b)\right].$$

Differentiating $\xi(\vec{a},\cdot)$ we get

$$\frac{d\xi}{dz}=\frac{1}{2\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2-z}\sin^2(nb)>0, \tag{2.20}$$

so the function is monotonously increasing for $z<1$. Moreover, it diverges at both endpoints. At the continuum threshold we have

$$\xi(\vec{a};z)=-\frac{1}{\pi^2}\ln\sqrt{1-z}\,\sin^2(b)+\mathcal{O}(1)\quad\text{as}\quad z\to 1-, \tag{2.21}$$

while on the opposite side we may employ a simple estimate

$$\xi(\vec{a};z)<-\frac{1}{\pi^2}\ln\sqrt{1-z}\,\sin^2(b)+\xi_2\to-\infty\quad\text{as}\quad z\to-\infty.$$

We will need more precise asymptotics at large negative energies. Below we shall prove that

$$\xi(\vec{a};z)=-\frac{\sqrt{-z}}{4\pi}+\mathcal{O}(e^{-c\sqrt{-z}})\quad\text{as}\quad z\to-\infty \tag{2.22}$$

for any $c<\mathrm{dist}(\vec{a},\mathrm{bd}\,\Omega)=\pi/2-|b-\pi/2|$. In other words, the leading term corresponds to the analogous function for the point-interaction Laplacian in $\mathbb{R}^3$ computed in Ref. 2, Chap. I.1; it corresponds to the heuristic concept that strongly bound states are well localized, and therefore not much influenced by the presence of the boundary. Another property of $\xi(\vec{a},z)$ is its monotonicity across the half-layer,

$$\xi(\vec{a};z)>\xi(\vec{a}';z)\quad\text{if}\quad |b-\pi/2|<|b'-\pi/2|,\ \ a=a'. \tag{2.23}$$

To prove it we employ the relation (2.8) which yields

$$\xi(\vec{a};z)-\xi(\vec{a}';z)=\lim_{|x-a|\to 0}\frac{i}{2\pi}\sum_{n=1}^{\infty}H_0^{(1)}(k_n(z)|x-a|)[\sin^2(nb)-\sin^2(nb')].$$

Since $\sin^2(nb)-\sin^2(nb')=\sin(n(b+b'))\sin(n(b-b'))$ holds for $0<b'<b\leqslant\pi/2$ we arrive at

$$\xi(\vec{a};z)-\xi(\vec{a}';z)=G_0(a,b+b';a,b-b';z); \tag{2.24}$$

the monotonicity then follows from the fact that $z\in(-\infty,1]$ and from the positivity of free resolvent kernel (cf. Ref. 7, Appendix to Sec. XIII.12). This behavior is illustrated in Fig. 1.

This confirms the mentioned general conclusion: it follows from the stated properties of $\xi(\vec{a};\cdot)$ that Eq. (2.19) has for any $\alpha\in\mathbb{R}$ a unique eigenvalue $\varepsilon(\alpha,\vec{a})$ in $(-\infty,1]$ and that the function $\varepsilon(\cdot,\vec{a})$ is monotonously increasing,

$$\varepsilon(\alpha,\vec{a})>\varepsilon(\alpha',\vec{a})\quad\text{if}\quad\alpha>\alpha'.$$

Furthermore, $\xi(\vec{a},\cdot)$ is a real-analytic function because for a fixed $z_1<-1$ it is expressed on a complex neighborhood of $(-\infty,z_1)$ through a uniformly convergent series whose terms are analytic. It follows from the implicit-function theorem that $\varepsilon(\cdot,\vec{a})$ is a C^∞ function (see Ref. 12, Chap. XIV). The function $\varepsilon(\cdot,\vec{a})$ is also monotonous with b:

$$\varepsilon(\cdot,\vec{a})<\varepsilon(\cdot,\vec{a}')\quad\text{if}\quad|b-\pi/2|<|b'-\pi/2|. \tag{2.25}$$

The behavior of the eigenvalue is shown in Fig. 2.

We are also interested in the asymptotic behavior of the eigenvalue in the limits of weak and strong coupling. In the former case we have

$$\varepsilon(\alpha,\vec{a})\approx 1-\exp\left(-\frac{2\pi^2\alpha}{\sin^2(b)}\right)\quad\text{as}\quad\alpha\to\infty, \tag{2.26}$$

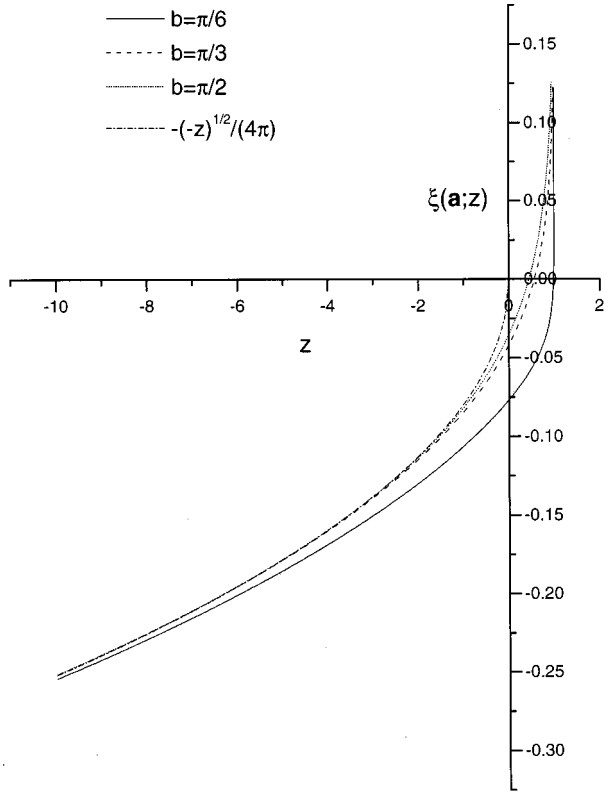

FIG. 1. The function $\xi(\vec{a};\cdot)$ for three different positions of the point interaction. The dash-dotted line is the leading term of the asymptotics (2.22).

where the symbol $\approx$ means that for any $\epsilon>0$ and α large enough the eigenvalue can be squeezed between a pair of expressions from the rhs in which $2\pi^2$ is replaced by $2\pi^2\pm\epsilon$. On the other hand, the strong coupling asymptotics can be proved directly. By Dirichlet bracketing (Ref. 7, Sec. XIII.15) $\varepsilon(\alpha,\vec{a})$ is for $\alpha<0$ bounded from below by $-(-4\pi\alpha)^2$, and from above by the ground state of the Dirichlet Laplacian in a ball of radius c with the point interaction in the center. The latter is easily found: writing $\varepsilon(\alpha,\vec{a})=-\kappa^2$ one has to solve the equation

$$(-4\pi\alpha)^2=\kappa^2(1+\sinh^{-2}\kappa c).$$

It yields the sought asymptotic behavior

$$\varepsilon(\alpha,\vec{a})=-16\pi^2\alpha^2+\mathcal{O}(e^{\alpha c}) \quad \text{as} \quad \alpha\to-\infty, \tag{2.27}$$

which justifies in view of (2.19) *a posteriori* the relation (2.22).

The formula (2.7) provides us with the (non-normalized) wavefunction of the bound state through the residue at the pole, $\psi(\vec{x};\alpha,\vec{a})=G_0(\vec{x},\vec{a};\varepsilon(\alpha,\vec{a}))$, so we have

$$\psi(\vec{x};\alpha,\vec{a})=\frac{i}{2\pi}\sum_{n=1}^{\infty} H_0^{(1)}(\sqrt{\varepsilon(\alpha,\vec{a})-n^2}\ |x-a|)\sin(nb)\sin(ny). \tag{2.28}$$

For $\alpha\to-\infty$ we can write $H_0^{(1)}(u)\approx\sqrt{2/\pi u}\ e^{i(u-\pi/4)}$ so we see that the wavefunction is well

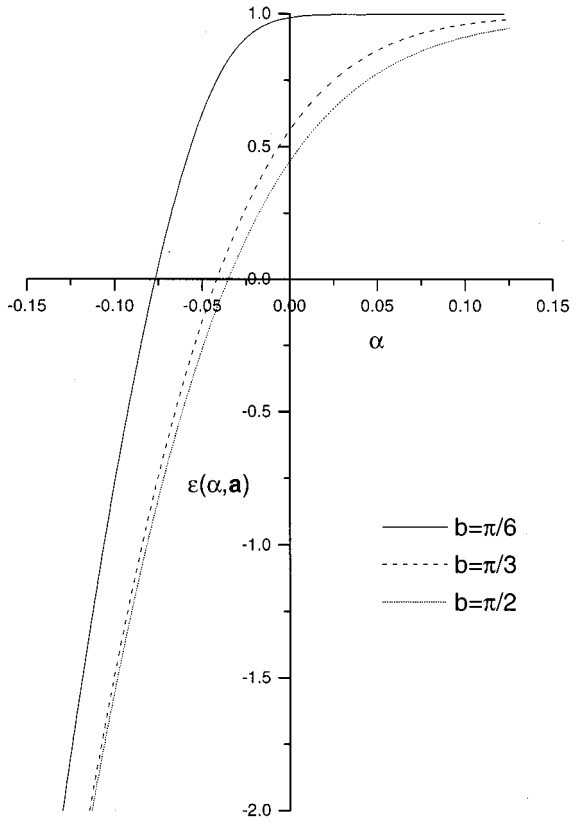

FIG. 2. The dependence of the eigenvalues $\varepsilon(\alpha,\vec{a})$ on the parameter α for three positions of the point interaction.

localized,

$$\psi(\vec{x};\alpha,\vec{a}) \approx \sum_{n=1}^{\infty} \sqrt{\frac{1}{\pi^3\sqrt{16\pi^2\alpha^2+n^2}|x-a|}}\, e^{-\sqrt{16\pi^2\alpha^2+n^2}|x-a|} \sin(nb)\sin(ny); \qquad (2.29)$$

this is illustrated in Fig. 3. On the other hand, in the limit $\alpha\to\infty$ the wavefunction for $|x-a|$ from a compact set behaves as

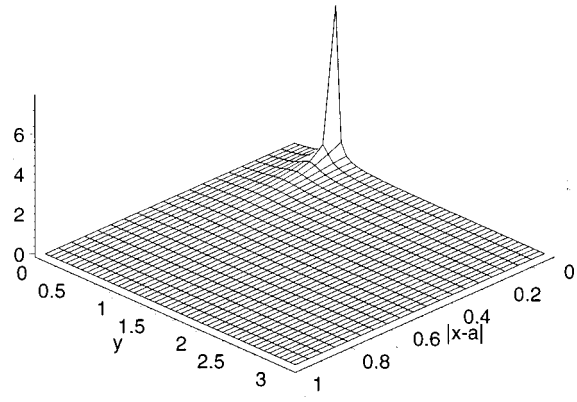

FIG. 3. The non-normalized eigenfunction for $b=\pi/6$ and $\alpha=-0.1$.

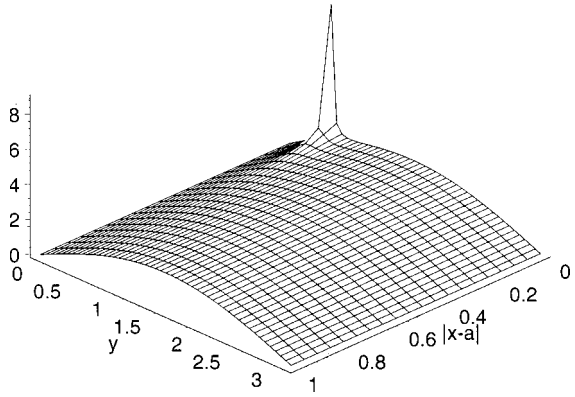

FIG. 4. The unnormalized eigenfunction for $b=\pi/6$ and $\alpha=1$.

$$\psi(\vec{x};\alpha,\vec{a})\approx\alpha\frac{\sin y}{\sin b}-\frac{1}{\pi^2}\ln|x-a|\sin b\sin y+\frac{i}{2\pi}\sum_{n=2}^{\infty}H_0^{(1)}(\sqrt{1-n^2}\ \ |x-a|)\sin(nb)\sin(ny). \tag{2.30}$$

The wavefunction is dominated by the first transverse mode as Fig. 4 shows.

Let us finally return to embedded eigenvalues. We have excluded their existence away from the thresholds. If $z=m^2$, we use Eq. (2.7) again to check that the singularities on the rhs cancel. In the vicinity of $z=m^2$ the free resolvent kernel and the denominator $\alpha-\xi(\vec{a};z)$ behave as

$$G_0(\vec{x}_1,\vec{x}_2;z)=-\frac{1}{\pi^2}\ln\sqrt{m^2-z}\,\sin(my_1)\sin(my_2)(1+\mathcal{O}(\sqrt{m^2-z})),$$

$$\alpha-\xi(\vec{a};z)=\tilde{\alpha}+\frac{1}{\pi^2}\ln\sqrt{m^2-z}\sin^2(mb),$$

where

$$\tilde{\alpha}:=\alpha-\xi_2+\frac{1}{\pi^2}\sum_{n\neq m}\ln\sqrt{1-\frac{m^2}{n^2}}\sin^2(nb)-\frac{1}{\pi^2}\ln\, m\,\sin^2(mb).$$

Then the full-resolvent kernel asymptotically behaves as

$$\left(\tilde{\alpha}+\frac{1}{\pi^2}\ln\sqrt{m^2-z}\,\sin^2(mb)\right)^{-1}\frac{\tilde{\alpha}}{\pi^2}\ln\sqrt{m^2-z}\,\sin(my_1)\sin(my_2)(1+\mathcal{O}(\sqrt{m^2-z}))$$

and cannot thus have a pole-type singularity at $z=m^2$.

Let us summarize the results obtained so far:

Theorem 2.2: *Let $H(\alpha,\vec{a})$ be defined by (2.5) and (2.6) for $d=\pi$. Then*

(a) $\sigma_{ess}(H(\alpha,\vec{a}))=\sigma_{ac}(H(\alpha,\vec{a}))=[1,\infty)$ *and* $\sigma_{sc}(H(\alpha,\vec{a}))=\varnothing$.

(b) *For any $\alpha\in\mathbb{R}$ there is a single eigenvalue $\varepsilon(\alpha,\vec{a})$ in $(-\infty,1)$ which is increasing and infinitely differentiable wrt α. The corresponding eigenfunction is given by (2.28).*

(c) *The eigenvalue is by (2.25) strictly monotonous across the half-layer, $\varepsilon(\alpha,\vec{a})<\varepsilon(\alpha,\vec{a}')$ if $|b-\pi/2|<|b'-\pi/2|$.*

(d) *In the limit $\alpha\to\infty$ the bound state behaves according to (2.26) and (2.30). In the strong coupling case the eigenvalue asymptotic is given by (2.27) and the eigenfunction is described by (2.29).*

(e) *There are no eigenvalues in* $[1,\infty)$.

E. Scattering

Since the Hamiltonian $H(\alpha,\vec{a})$ is invariant under rotations around the axis passing through the point $\vec{a}$ and perpendicular to Σ, we may simplify the treatment of stationary scattering using a partial-wave decomposition. We use the tensor-product representation

$$L^2(\Sigma)=L^2((0,\infty)\times[0,d];r\,dr\,dy)\otimes L^2(S^1), \tag{2.31}$$

where S^1 is the unit circle in $\mathbb{R}^2$ and $r:=|x|$. This can be written as

$$L^2(\Sigma)=\bigoplus_{m=-\infty}^{\infty}\tilde{U}^{-1}L^2((0,\infty)\times[0,d])\otimes\{Y_m\}, \tag{2.32}$$

where $\tilde{U}:L^2((0,\infty)\times[0,d];r\,dr\,dy)\to L^2((0,\infty)\times[0,d])$ is the unitary operator defined by $(\tilde{U}\psi)(r):=r^{1/2}\psi(r)$, the "spherical" functions $Y_m(\omega):=(2\pi)^{-1/2}e^{im\theta}$ with $\omega=(\cos\theta,\sin\theta)$ form a basis in $L^2(S^1)$, and the symbol $\{\cdot\}$ means, as above, the linear envelope. Shifting the point $\vec{a}$ to the origin of the polar coordinates by $T_a:(T_a\phi)(x,y)=\phi(x+a,y)$, we can decompose the corresponding free Hamiltonian $H_0=-\Delta_D^{\Sigma}$ as

$$H_0=T_a^{-1}\left\{\bigoplus_{m=-\infty}^{\infty}\tilde{U}^{-1}h_m^{(0)}\tilde{U}\otimes I\right\}T_a, \tag{2.33}$$

with the partial-wave operators

$$h_m^{(0)}=-\frac{\partial^2}{\partial r^2}-\frac{\partial^2}{\partial y^2}+\frac{4m^2-1}{4r^2},\quad m\in\mathbb{Z}. \tag{2.34}$$

Their domains are given in a standard way (Ref. 13, Sec. 5.7); the only nontrivial part is the radial boundary condition at the origin. As in Ref. 2, Chap. I.5, none are imposed in "higher" partial waves, $m\neq 0$, because the radial part of (2.34) is then limit-point at zero (Ref. 7, Appendix to Sec. X.1). Consequently, this part of the Hamiltonian is trivial from the point of view of the point interaction. On the other hand, for $m=0$ we introduce the generalized boundary values,

$$\ell_0(\phi)(y):=\lim_{r\to 0}\phi(r,y)\sqrt{r},\quad \ell_1(\phi)(y):=\lim_{r\to 0}r^{-1/2}[\phi(r,b)-\ell_0(\phi)(y)r^{-1/2}]. \tag{2.35}$$

The s-wave component of the free Hamiltonian is specified by the condition $\ell_0(\phi)(y)=0$ [for any $y\in(0,d)$], while the s-wave component h_0^{α} of $H(\alpha,\vec{a})$ is given by the same differential expression (2.34) with the boundary condition at $y=b$ changed to

$$\ell_1(\phi)(b)-4\pi\alpha\ell_0(\phi)(b)=0. \tag{2.36}$$

It is also clear from this discussion that the eigenfunction of $H(\alpha,\vec{a})$ analyzed in the previous section exhibits a symmetry, $\psi(R(\varphi)\vec{x};\alpha,\vec{a})=\psi(\vec{x};\alpha,\vec{a})$, where $R(\varphi)$ is the rotation of Σ on an angle φ around the axis passing through the point $\vec{a}$ and perpendicular to Σ.

Let us return to the scattering problem. As in Ref. 2, Chap. I.5, the rotational symmetry means that the S-matrix part corresponding to partial waves with $m\in\mathbb{Z}\setminus\{0\}$ is trivial, i.e., the unit operator. In distinction to Ref. 2, Chap. I.5, however, the s-wave part (we denote it as S again to keep the notation simple) is still in general a complicated operator because the point interaction can couple different transverse modes. Its dimension depends on the number of the "open channels," i.e., of the transverse modes in which the particle of energy z can propagate; for $d=\pi$ the latter is $[\sqrt{z}]$. Using the partial-wave operator (2.34) with $m=0$ it is easy to see that the function

$$\psi^{(0)}_{\alpha,n}(\vec{x};k)=J_0(k_n(z)r)\chi_n(y)+\frac{1}{\alpha-\xi(\vec{a};z)}\,\frac{i}{2\pi}\sum_{j=1}^{\infty}H_0^{(1)}(k_j(z)r)\sin(jb)\sin(nb)\chi_j(y)\,, \tag{2.37}$$

with $r=|x-a|$ satisfies the boundary condition (2.4) and $r^{1/2}\psi^{(0)}_{\alpha,n}(\vec{x};k)$ is a generalized eigenfunction of $h_0^{(0)}\otimes(-\partial^2/\partial y^2)$ with the eigenvalue $z=k^2$. In the limit $r\to\infty$ it behaves as

$$\begin{aligned}\psi^{(0)}_{\alpha,n}(\vec{x};k)\approx{}&\sqrt{\frac{2}{\pi k_n(z)r}}\cos(k_n(z)r-\pi/4)\chi_n(y)\\&+\frac{1}{\alpha-\xi(\alpha;z)}\,\frac{i}{2\pi}\sum_{j=1}^{[\sqrt{z}]}\sqrt{\frac{2}{\pi k_j(z)r}}\,e^{i(k_j(z)r-\pi/4)}\sin(nb)\sin(jb)\chi_j(y).\end{aligned} \tag{2.38}$$

To find the matrix elements S_{nj} one has to compare this with the asymptotics of the outgoing wave in the jth transverse mode expressed by means of the scattering phase shift. For the wave scattered back into the incident nth mode we have

$$\begin{aligned}&\sqrt{\frac{2}{\pi k_n(z)r}}\left[\cos(k_n(z)r-\pi/4)+\frac{1}{\alpha-\xi(\alpha;z)}\,\frac{i}{2\pi}\,e^{i(k_n(z)r-\pi/4)}\sin^2(nb)\right]\\&\quad=\sqrt{\frac{2}{\pi k_n(z)r}}\,e^{i\delta_{nn}}\cos(k_n(z)r-\pi/4+\delta_{nn}(k)),\end{aligned}$$

which yields

$$S_{nn}(k)=e^{2i\delta_{nn}(k)}=1+\frac{i}{\pi}\,\frac{\sin^2(nb)}{\alpha-\xi(\vec{a};z)}.$$

In a similar way scattering to the jth mode, $n\neq j$, requires the identification

$$\frac{1}{\alpha-\xi(\vec{a};z)}\,\frac{i}{2\pi}\,e^{i(k_j(z)r-\pi/4)}\sin(nb)\sin(jb)=e^{i\delta_{nj}(k)}\cos(k_n(z)r-\pi/4+\delta_{nj}(k));$$

together we get

$$S_{nj}(k)=e^{2i\delta_{nj}(k)}=\delta_{nj}+\frac{i}{\pi}\,\frac{\sin(nb)\sin(jb)}{\alpha-\xi(\vec{a};z)}. \tag{2.39}$$

We have to check that the obtained S-matrix is unitary, i.e.,

$$\sum_{j=1}^{[\sqrt{z}]}S_{nj}\overline{S}_{sj}=\delta_{ns}\,. \tag{2.40}$$

Using (2.39) we can write

$$\begin{aligned}\sum_{j=1}^{[\sqrt{z}]}S_{nj}\overline{S}_{sj}&=\sum_{j=1}^{[\sqrt{z}]}(S_{nj}-\delta_{nj})(\overline{S}_{sj}-\delta_{js})+2\,\mathrm{Re}(S_{ns}-\delta_{ns})+\delta_{ns}\\&=\frac{2}{\pi}\,\frac{\sin(nb)\sin(sb)}{|\alpha-\xi(\vec{a};z)|^2}\left(\frac{1}{2\pi}\sum_{j=1}^{[\sqrt{z}]}\sin^2(jb)-\mathrm{Im}\;\xi(\vec{a};z)\right)+\delta_{ns}\,,\end{aligned}$$

so the desired property follows from (2.17).

The scattering problem can be also described in another way—by means of a scattering operator in $L^2(S^1)\otimes L^2([0,d])$. Applying (2.7) to an arbitrary $\phi\in L^2(\Sigma)$ we see that to any $\psi\in D(H(\alpha,\vec{a}))$ and a nonreal z there is $\psi_z\in D(H_0)$ such that

$$\psi(\vec{x})=\psi_z(\vec{x})+\frac{1}{\alpha-\xi(\vec{a},z)}G_0(\vec{x},\vec{a};z)\psi_z(\vec{a}). \tag{2.41}$$

If we choose, in particular, $\psi_z^\varepsilon(\vec{x})=e^{ik_n(z)\omega x-\varepsilon|x|^2}\chi_n(y)$ with ω a unit vector in $\mathbb{R}^2$, then the corresponding $\psi^\varepsilon(\vec{x})\in D(H(\alpha,\vec{a}))$ satisfies the equation

$$((H(\alpha,\vec{a})-z)\psi^\varepsilon)(\vec{x})=4\varepsilon[1-\varepsilon|x|^2+ik_n\omega x]\,\psi_z^\varepsilon(\vec{x}). \tag{2.42}$$

The rhs converges in the L^2 sense as z approaches the real line and the resulting ψ^ε belongs to $D(H(\alpha,\vec{a}))$ for a fixed $z\in[1,\infty)$. Furthermore, the pointwise limit exists as $\varepsilon\to 0+$ and equals

$$\psi_{\alpha,n}(\vec{x};k_n(z)\omega)=e^{ik_n(z)\omega x}\chi_n(y)+\frac{e^{ik_n(z)\omega a}}{\alpha-\xi(\vec{a};z)}\frac{i}{2\pi}\sum_{j=1}^{\infty}H_0^{(1)}(k_j(z)|x-a|)\sin(jb)\sin(nb)\chi_j(y). \tag{2.43}$$

The function defined by the rhs is locally square integrable, solves the equation $(H(\alpha,\vec{a})-z)\psi=0$ and satisfies the appropriate boundary condition, i.e., it is a generalized eigenfunction of $H(\alpha,\vec{a})$. Let us expand it into partial waves. We know already the s-wave eigenfunction (2.37); the remaining ones are trivial, $\psi_n^{(m)}(\vec{x};k_n(z))=J_m(kr)\chi_n(y)$ if $m\neq 0$. Here again, this expression describes an eigenfunction of $h_m^{(0)}\otimes\partial^2/\partial y^2$ in the Hilbert space (2.31); multiplying it with $r^{1/2}$ one obtains an eigenfunction in the Hilbert space (2.32). Using the known identity

$$e^{ik\omega(x-a)}=2\pi\sum_{m=-\infty}^{\infty}i^m J_m(k|x-a|)\overline{Y_m(\omega)}Y_m(\omega_{x-a}), \tag{2.44}$$

where Y_m are the functions introduced above and $\omega_{x-a}:=(x-a)/|x-a|$, we get

$$e^{-ik_n(z)\omega a}\psi_{\alpha,n}(\vec{x};k_n(z)\omega)=\psi_{\alpha,n}^{(0)}(\vec{x};k_n(z))+2\pi\sum_{0\neq l\in\mathbb{Z}}i^l\psi_n^{(l)}(x-a,y;k_n(z))\overline{Y_l(\omega)}Y_l(\omega_{x-a}).$$

Components of the on-shell scattering amplitude $(f_\alpha(k_n(z),\omega_x,\omega))_{jn}$ are then given by $\lim_{|x|\to\infty,x/|x|=\omega_x}|x|^{1/2}e^{-ik_j|x|}[\psi_{\alpha,n}(\vec{x};k_n(z)\omega)-e^{ik_n\omega x}\chi_n(y)]$. Specifically, its part corresponding to the jth transverse mode is

$$(f_\alpha(k_n(z),\omega_x,\omega))_{jn}=\frac{e^{\pi i/4}}{\pi\sqrt{2\pi k_j(z)}}\frac{\sin(jb)\sin(nb)}{\alpha-\xi(\vec{a};z)}e^{ik_n(z)\omega a-ik_j(z)\omega_x a} \tag{2.45}$$

and the on-shell scattering operator $S_\alpha(z)$ on $L^2(S^1)\otimes L^2([0,d])$ has the form

$$S_\alpha(z)=I+\frac{i}{\pi}\sum_{n,j=1}^{[\sqrt{z}]}\frac{\sin(nb)\sin(jb)}{\alpha-\xi(\vec{a};z)}(e^{-ik_n(z)(\cdot)a}Y_0\chi_n,\cdot)e^{-ik_j(z)(\cdot)a}Y_0\chi_j. \tag{2.46}$$

It follows from (2.17) that the denominator is nonzero in $[1,\infty)$. However, we have argued above that $\xi(\vec{a};\cdot)$ can be continued analytically to the complex plane where zeros exist in general. In the weak coupling case there is one resonance pole of $S_\alpha(z)$ close to the threshold of each higher transverse mode similarly as in the two-dimensional case.[5]

III. A FINITE NUMBER OF POINT INTERACTIONS

A. Boundary conditions

Consider now a finite number N of point interactions and suppose that their positions are $\vec{a}_j = (a_j, b_j)$, where $a_j \in \mathbb{R}^2$ and $b_j \in (0,\pi)$. For the sake of brevity we denote $\vec{a} = (\vec{a}_1, \ldots, \vec{a}_N)$ and $\alpha = (\alpha_1, \ldots, \alpha_N)$. The way to define a point interaction is the same as above; now we have N independent boundary conditions

$$L_1(\psi, \vec{a}_j) - 4\pi\alpha_j L_0(\psi, \vec{a}_j) = 0, \quad j = 1, \ldots, N. \tag{3.1}$$

The Hamiltonian $H(\alpha, \vec{a})$ is given again by the formulas (2.5) and (2.6) with the boundary condition (2.4) replaced by (3.1) and $\vec{a}$ understood in the sense mentioned above. Any of the point interactions can be switched off when corresponding coupling constant α_j is formally put equal to infinity.

B. The resolvent

We again use the Krein formula to find the resolvent kernel. Since the deficiency indices of the operator obtained by restriction of the free Hamiltonian to the set of functions which vanish at the vicinity of the points $\vec{a}$ are equal to (N,N), the rhs is a rank N operator expressed in terms of vectors from the corresponding deficiency subspaces,

$$(H(\alpha,\vec{a}) - z)^{-1}(\vec{x}_1, \vec{x}_2) = G_0(\vec{x}_1, \vec{x}_2; z) + \sum_{j,k=1}^{N} \lambda_{jk}(\alpha, \vec{a}; z)\, G_0(\vec{x}_1, \vec{a}_j; z)\, G_0(\vec{a}_k, \vec{x}_2; z). \tag{3.2}$$

Applying this to an arbitrary vector of $L^2(\Sigma)$ we get

$$\psi(\vec{x}) = \psi_0(\vec{x}) + \sum_{j,k=1}^{N} \lambda_{jk}(\alpha, \vec{a}; z)\, G_0(\vec{x}, \vec{a}_j; z)\, \psi_0(\vec{a}_k), \tag{3.3}$$

with $\psi_0 \in D(H_0)$. The generalized boundary values are

$$L_0(\psi, \vec{a}_m) = \sum_{j,k=1}^{N} \frac{\lambda_{jk}}{4\pi}\, \delta_{jm}\, \psi_0(\vec{a}_k), \tag{3.4}$$

$$\begin{aligned} L_1(\psi, \vec{a}_m) = {} & \psi_0(\vec{a}_m) + \sum_{j,k=1}^{N} \lambda_{jk}(1 - \delta_{jm}) G_0(\vec{a}_m, \vec{a}_j; z)\, \psi_0(\vec{a}_k) \\ & + \sum_{j,k=1}^{N} \lambda_{jk}\, \delta_{jm}\, \psi_0(\vec{a}_k) \lim_{|\vec{x} - \vec{a}_m| \to 0} \left(G_0(\vec{x}, \vec{a}_j; z) - \frac{1}{4\pi|\vec{x} - \vec{a}_m|} \right). \end{aligned} \tag{3.5}$$

The limit contained in the expression of $L_1(\psi, \vec{a}_m)$ equals $\xi(\vec{a}_m; z)$. After substituting these boundary values into (3.1) we arrive at the conditions

$$\psi_0(\vec{a}_m) + \sum_{j,k=1}^{N} \lambda_{jk}[\, \delta_{jm}(\xi(\vec{a}_m; z) - \alpha_m) + (1 - \delta_{jm}) G_0(\vec{a}_m, \vec{a}_j; z)\,]\, \psi_0(\vec{a}_k) = 0, \tag{3.6}$$

which should be satisfied for an arbitrary vector ψ_0 belonging to $D(H_0)$, i.e., for any N-tuple $(\psi_0(\vec{a}_1), \ldots, \psi_0(\vec{a}_N))$. This is possible only if the expressions in the square brackets are up to the sign elements of the matrix inverse to $\lambda(\alpha, \vec{a}; z)$, in other words, if the coefficients are

$$\lambda(\alpha, \vec{a}; z) = \Lambda(\alpha, \vec{a}; z)^{-1}, \tag{3.7}$$

where

$$\Lambda_{jj} := \alpha_j - \xi(\vec{a}_j;z) = \alpha_j + \frac{1}{\pi^2}\sum_{n=1}^{\infty} \ln\sqrt{1-\frac{z}{n^2}}\sin^2(nb_j) - \frac{1}{4\pi^2}\left[\gamma + \psi\left(\frac{b_j}{\pi}\right) + \frac{\pi}{2}\cot(b_j)\right],$$
$$\Lambda_{jm} := -G_0(\vec{a}_j,\vec{a}_m;z) = -\frac{i}{2\pi}\sum_{n=1}^{\infty} H_0^{(1)}(\sqrt{z-n^2}|a_j-a_m|)\sin(nb_j)\sin(nb_m), \quad j\neq m. \tag{3.8}$$

The Green's function value $G_0(\vec{a}_j,\vec{a}_m;z)$ is finite for any pair of mutually different vectors $\vec{a}_j$ and $\vec{a}_m$. When the point interactions are arranged vertically, i.e., $a_j = a_m$, the expression through Hankel's functions is useless and the corresponding nondiagonal element Λ_{jm} can be alternatively written as

$$\Lambda_{jm} = \frac{1}{\pi^2}\sum_{n=1}^{\infty} \ln\sqrt{1-\frac{z}{n^2}}\sin(nb_j)\sin(nb_m) - \xi_2\left(\frac{b_j+b_m}{2}\right) + \xi_2\left(\frac{|b_j-b_m|}{2}\right). \tag{3.9}$$

To derive this expression we employ the argument analogous to that leading to the value of the function $\xi(\vec{a};z)$ in Sec. II C.

C. The discrete spectrum

Since a finite rank operator is both compact and trace class, the argument presented at the opening of Sec. II D remains valid. In other words, a finite number of point interaction changes neither the essential nor the absolutely continuous spectrum, $\sigma_{ess}(H(\alpha,\vec{a})) = \sigma_{ac}(H(\alpha,\vec{a})) = \sigma_{ess}(H_0) = [1,\infty)$. The singularly continuous spectrum is empty because the proof given in Sec. II D can be used here again.

The discrete spectrum is determined by poles of the resolvent, which occur if the coefficient matrix $(\lambda_{jk})^{-1}$ becomes singular. This leads to the condition

$$\det \Lambda(\alpha,\vec{a};z) = 0. \tag{3.10}$$

To find the eigenfunctions we use the procedure from Ref. 2, Sec. II.1. Suppose that $H := H(\alpha,\vec{a})$ satisfies the equation $H\varphi = z\varphi$ for some $z\in\mathbb{R}$ and pick an arbitrary $z'\in\varrho(H)$. Then in accordance with (3.3) there is a function $\psi_0 \in D(H_0)$ which makes it possible to write

$$\varphi(\vec{x}) = \psi_0(\vec{x}) + \sum_{j=1}^{N} d_j G_0(\vec{x},\vec{a}_j;z'), \tag{3.11}$$

with the coefficients $d_j := \Sigma_{k=1}^{N}(\Lambda(z')^{-1})_{jk}\psi_0(\vec{a}_k)$. We also see that

$$(H_0 - z')\psi_0 = (H-z')\varphi = (z-z')\varphi. \tag{3.12}$$

Applying the resolvent $(H_0-z')^{-1}$ to the last identity we arrive at the expression

$$\psi_0 = (z-z')\left[(H_0-z')^{-1}\psi_0 + \sum_{j=1}^{N} d_j (H_0-z')^{-1} G_0(\cdot,\vec{a}_j;z')\right], \tag{3.13}$$

which allows us to find the action of (H_0-z) at the vector ψ_0,

$$(H_0-z)\psi_0 = (H_0-z')\psi_0 - (z-z')\psi_0 = (z-z')\sum_{j=1}^{N} d_j G_0(\cdot,\vec{a}_j;z'). \tag{3.14}$$

If $z<1$, the resolvent $(H_0-z)^{-1}$ exists and may be applied to the last relation, giving by means of the first resolvent identity

$$\psi_0=\sum_{j=1}^{N} d_j[G_0(\cdot,\vec{a}_j;z)-G_0(\cdot,\vec{a}_j;z')]. \tag{3.15}$$

Substituting this into (3.11) we get an expression for the eigenfunction,

$$\varphi(\vec{x})=\sum_{j=1}^{N} d_j G_0(\vec{x},\vec{a}_j;z), \tag{3.16}$$

where it remains to determine the coefficients. Equation (3.15) taken at the point $\vec{x}=\vec{a}_j$ can be rewritten using the components of matrix Λ as

$$\psi_0(\vec{a}_j)=\sum_{m=1}^{N} d_m(\Lambda(\alpha,\vec{a};z')_{jm}-\Lambda(\alpha,\vec{a};z)_{jm}). \tag{3.17}$$

We already know that $d_m=\Sigma_{k=1}^{N}(\Lambda(z')^{-1})_{mk}\psi_0(\vec{a}_k)$; taking the inverse we get $\psi_0(\vec{a}_j)=\Sigma_{m=1}^{N}\Lambda(z')_{jm}d_m$. In combination with (3.17) this yields

$$\sum_{m=1}^{N} \Lambda(z)_{jm}d_m=0, \tag{3.18}$$

i.e., $d:=(d_1,\ldots,d_N)$ has to be an eigenvector of the matrix $\Lambda(\alpha,\vec{a};z)$ corresponding to zero eigenvalue. The corresponding system of linear equations is solvable under the condition (3.10), and the sought eigenfunctions of $H(\alpha,\vec{a})$ are given by the formula (3.11).

It remains to check that Eq. (3.10) can have a solution in $(-\infty,1)$. Let us start with the limiting situations of strong and weak coupling. We know from (2.22) how $\xi(\vec{a}_j;z)$ behaves as $-\sqrt{-z}/4\pi$ as $z\to-\infty$. At the same time, the nondiagonal part of matrix Λ vanishes in the limit in view of the asymptotics

$$H_0^{(1)}(\sqrt{z-n^2}|a_j-a_m|)=H_0^{(1)}(i\sqrt{n^2-z}|a_j-a_m|)\approx\sqrt{\frac{2}{i\pi\sqrt{n^2-z}\,|a_j-a_m|}}\,e^{-\sqrt{n^2-z}|a_j-a_m|-i\pi/4}$$

for $z\to-\infty$. This argument is not applicable if $a_j=a_m$ for $j\neq m$. Nevertheless, the nondiagonal matrix elements are up to the sign equal to Green's function values, and thus they are bounded. In this way we get

$$\Lambda(\alpha,\vec{a};z)=\frac{\sqrt{-z}}{4\pi}I+\mathcal{O}(1)\quad\text{as}\quad z\to-\infty \tag{3.19}$$

with the coefficient α_j included into the error term. On the other hand,

$$\Lambda(\alpha,\vec{a};z)=\frac{1}{\pi^2}\ln\sqrt{1-z}\;M+\mathcal{O}(1)\quad\text{as}\quad z\to1-, \tag{3.20}$$

where $M:=(\sin b_j \sin b_m)_{j,m=1}^{N}$. This matrix has zero eigenvalue of multiplicity $N-1$ and the positive eigenvalue $\Sigma_{j=1}^{N}\sin^2 b_j$ corresponding to the eigenvector $(\sin b_1,\ldots,\sin b_N)$. The latter is more important, because it means that one eigenvalue of $\Lambda(\alpha,\vec{a};z)$ tends to $-\infty$ as $z\to1-$. Furthermore, the eigenvalues of $\Lambda(\alpha,\vec{a};z)$ are continuous functions of z, so comparing the last claim with (3.19) we find that at least one of the eigenvalues crosses zero for some z, i.e., that $H(\alpha,\vec{a})$ has at least one isolated eigenvalue.

We may ask whether some of the eigenvalues may be degenerate. For the sake of brevity we rewrite the matrix $\Lambda(\alpha,\vec{a};z)$ as

$$\Lambda(\alpha,\vec{a};z)=\delta_{jm}(\alpha_j-\xi_j(z))+(1-\delta_{jm})g_{jm}(z), \tag{3.21}$$

where $\xi_j(z) := \xi(\vec{a}_j; z)$ and $g_{jm}(z) := -G_0(\vec{a}_j - \vec{a}_m; z)$. Since all g_{jm} are negative, the maximum possible degeneracy is $N-1$, which means that for a pair of point interactions the discrete spectrum is always simple. Let us consider the case $N=3$. Let $z<1$, $\vec{a}_{1,3}=(\pm a, b_1)$ and $\vec{a}_2 = (0, b_2)$. If $b_2 \to 0$, then the value $g_{12}=g_{23}$ approaches zero, thus being smaller than g_{13} for b_2 small enough. On the contrary, if $b_2 = b_1$ we obtain the opposite inequality; this follows from the expression (2.3) and from the monotonicity of the Macdonald function $K_0(u)$ with a positive argument (see Ref. 9, 9.6.24). Hence there exists a $b_2 \in (0, b_1)$ such that all the nondiagonal elements of the matrix are the same, $g_{13}=g_{12}=g_{23}$. Choosing α_j which satisfy $\alpha_j - \xi_j = g_{12}$ we obtain a matrix of rank one, i.e., z is an eigenvalue of multiplicity two.

D. Embedded eigenvalues

We have shown in the previous section, that a single point interaction cannot produce eigenvalues embedded in the continuous spectrum. This is no longer true if $N \geqslant 2$ as the following example shows.

Example 3.1: Consider a pair of perturbations with the same α placed at $\vec{a}_1=(0,0,b)$ and $\vec{a}_2=(0,0,\pi-b)$. We can divide the eigenvalue problem into symmetric and antisymmetric parts with respect to the plane $\{(x, \pi/2): x \in \mathbb{R}^2\}$. We obtain properties of the antisymmetric part by scaling the one-center problem: substituting $\sigma = 1/2$ into the relation (2.15) we see that the antisymmetric part has a single eigenvalue which tends to 4 as $\alpha \to \infty$, hence it is embedded in the continuous spectrum for α large enough.

Thus we cannot exclude existence of embedded eigenvalues in general. We can, however, prove a weaker result. In the example the symmetry was essential, which means in particular that the eigenfunction is dominated by the second transverse mode. We will show that in general *any eigenvalue $z>1$ cannot contain contributions from transverse modes with $n \leqslant [\sqrt{z}]$*. Suppose that $H(\alpha, \vec{a})\varphi = z\varphi$ for $z>1$. We employ the relation (3.11) and take ψ_0 in the form $\psi_0(\vec{x}) = \sum_{n=1}^{\infty} g_n(x)\chi_n(y)$, where $g_n \in L^2(\mathbb{R}^2)$. Substituting this ψ_0 into (3.11) and using the fact that $\{\chi_n\}$ is an orthonormal basis in $L^2((0,\pi))$ we get

$$\left[-\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - z + n^2 \right] g_n(x) = (z - z') \sum_{j=1}^{N} d_j \, \frac{i}{4} H_0^{(1)}(k_n(z')|x - a_j|) \chi_n(b_j)$$

for $n = 1,2,\ldots$. The Fourier–Plancherel operator transforms this into

$$[|p|^2 - z + n^2] \hat{g}_n(p) = \frac{(z - z')}{2\pi} \sum_{j=1}^{N} d_j \, \chi_n(b_j) \frac{e^{-ipa_j}}{|p|^2 - z' + n^2}. \tag{3.22}$$

If $g_n \in L^2(\mathbb{R}^2)$, then $\hat{g}_n$ should also belong to $L^2(\mathbb{R}^2)$. It is not possible if $z > n^2$ and the rhs of (3.22) is nonzero at $p_n\omega$, where $p_n = \sqrt{z - n^2}$ and ω is a unit vector in $\mathbb{R}^2$. Recall that the factor $(|p|^2 - z' + n^2)^{-1}$ has no singularity, because $z' \in \rho(H)$ by assumption.

To avoid the singularity of $\hat{g}_n$ at $|p| = p_n$ we have to require

$$\sum_{j=1}^{N} d_j \chi_n(b_j) e^{-ip_n \omega a_j} = 0 \tag{3.23}$$

for an arbitrary unit vector ω from $\mathbb{R}^2$. If all the a_j's are different, it follows that $d_j \chi_n(b_j) = 0$ for each j. If some of them are the same, the condition changes to $\sum_j d_j \chi_n(b_j) = 0$ where j runs through the a_j's which coincide. In both cases $\hat{g}_n$ is identically zero for $n^2 < z$.

Consider now an arbitrary $g \in L^2(\mathbb{R}^2)$ and $n^2 < z$. Using (3.11) and (2.3) we arrive at

$$(g\chi_n, \varphi) = (\hat{g}, \hat{g}_n) + \sum_{j=1}^{N} d_j \, \chi_n(b_j) \left(g, \frac{i}{4} H_0^{(1)}(k_n(z')|x - a_j|) \right). \tag{3.24}$$

The first scalar product is equal to zero because $\hat{g}_n$ is zero. If all the a_j's are different, then $d_j\chi_n(b_j)=0$ for all j and the whole rhs is equal to zero. If some a_j's are the same, the condition $\Sigma_{j=1}^{N} d_j\chi_n(b_j)=0$ leads to $(g\chi_n,\varphi)=0$ again. The conclusion holds true for all $n=1,\ldots,[\sqrt{z}]$, what we have set out to prove.

E. The limits of strong and weak coupling

Of the two extreme situations, consider first the strong coupling. One can write the matrix $\Lambda(\alpha,\vec{a};z)$ in the form

$$\Lambda(z)=\left(\left(\alpha_j+\frac{\sqrt{-z}}{4\pi}\right)\delta_{jk}\right)\left[I+\left(\left(\alpha_j+\frac{\sqrt{-z}}{4\pi}\right)\delta_{jk}\right)^{-1}\tilde{\Lambda}(z)\right], \tag{3.25}$$

where $\tilde{\Lambda}(z)$ is the remainder matrix, which is independent of α_j and has a bounded norm as $z\to-\infty$. For an arbitrary finite interval $J\subset(-\infty,1)$ we can always choose α_j's large enough negative that no eigenvalues are contained in J and the two matrices in the above product are regular in J. It means that the roots of Eq. (2.19) come from the region where $\Lambda(z)$ is dominated by its diagonal part. Then there are exactly N eigenvalues (including a possible degeneracy), which behave asymptotically as

$$\varepsilon_j(\alpha,\vec{a})\approx-16\pi^2\alpha_j^2 \quad \text{as} \quad \max_{1\leqslant j\leqslant N}\alpha_j\to-\infty. \tag{3.26}$$

As we expect the eigenfunctions in the strong limit are strongly localized and only slightly influenced by the other perturbations. The eigenfunction localized at $\vec{a}_j$ has the same form as in Sec. II D where we put $\vec{a}=\vec{a}_j$.

Consider now on the contrary that all the point interactions are weak, i.e., that all the α_j's are large positive. Denoting $A:=\mathrm{diag}(\alpha_1,\ldots,\alpha_N)$ we can write

$$\Lambda(z)=A+\frac{1}{\pi^2}\ln\sqrt{1-z}M+\tilde{\Lambda}(z), \tag{3.27}$$

where $\tilde{\Lambda}(z)$ is a remainder matrix, which is again independent of α with its norm bounded, $\|\tilde{\Lambda}(z)\|\leqslant C_{\vec{a}}$ for $z\in(z_0,1)$. In Sec. III C we found that $\Lambda(z)$ was asymptotically a rank one operator on $\mathbb{C}^N$. Hence only one isolated eigenvalue of $H(\alpha,\vec{a})$ exists in this asymptotic situation.

To find the leading term of the asymptotic expansion, we have to solve the spectral problem for matrix $M-\eta A-\eta\tilde{\Lambda}(z)$, where $\eta:=-2\pi^2(\ln(1-z))^{-1}$. The largest eigenvalue of this matrix satisfies $\mu_N(\eta)\geqslant\mu_N(0)-(C_{\vec{a}}+\alpha_+)\eta$, where $\alpha_+:=\max\alpha_j$, while for $j=1,\ldots,N-1$ we have $\mu_j(\eta)\leqslant(C_{\vec{a}}-\alpha_-)\eta$, where $\alpha_-:=\min\alpha_j$. Since $\mu_N(0)>0$ we see that for α_- large enough the condition has just one solution for $\eta>0$. One can check directly that without $\tilde{\Lambda}(z)$ the condition is satisfied for $\eta=\Sigma_j\alpha_j^{-1}\sin^2 b_j$. Thus $\eta=\mathcal{O}(\alpha_-^{-1})$ and the eigenvalue expansion follows. Hence the bound-state energy in the weak-coupling case behaves as

$$\varepsilon(\alpha,\vec{a})\approx1-\exp\left\{-2\pi^2\left(\sum_{j=1}^{N}\frac{\sin^2 b_j}{\alpha_j}\right)^{-1}\right\} \tag{3.28}$$

as $\min_{1\leqslant j\leqslant N}\alpha_j\to\infty$. Since the eigenvector of matrix M corresponding to the nonzero eigenvalue is $(\sin b_1,\ldots,\sin b_N)$, the asymptotic expression of the eigenfunction for $\vec{x}$ from a restricted part of Σ is

$$\varphi(\vec{x}) \approx \sin y \left(\frac{\Sigma_{j=1}^{N} \sin^2 b_j}{\Sigma_{j=1}^{N} (\sin^2 b_j)/\alpha_j} - \frac{1}{\pi^2} \sum_{j=1}^{N} \sin^2 b_j \ln|x-a_j| \right) + \frac{1}{\pi^2} \sum_{n=2}^{\infty} \sin(ny) \sum_{j=1}^{N} \sin b_j \sin(nb_j)\, K_0(\sqrt{n^2-1}|x-a_j|). \tag{3.29}$$

Let us summarize the spectral properties of our Hamiltonian in the N-center case derived in the previous three paragraphs.

Theorem 3.2: *Let $H(\alpha,\vec{a})$ be defined by (2.5) and (2.6) for $d=\pi$, where $\vec{a}=(\vec{a}_1,\ldots,\vec{a}_N)$ and $\alpha=(\alpha_1,\ldots,\alpha_N)$ and the boundary condition (2.4) is replaced by (3.1). Then we have the following.*

(a) $\sigma_{ess}(H(\alpha,\vec{a}))=\sigma_{ac}(H(\alpha,\vec{a}))=[1,\infty)$ *and* $\sigma_{sc}(H(\alpha,\vec{a}))=\varnothing$.

(b) *For any $\alpha\in\mathbb{R}^N$ there is at least one eigenvalue $\varepsilon(\alpha,\vec{a})$ in $(-\infty,1)$. The maximum number of eigenvalues is N with the multiplicity taken into account; the maximum multiplicity is $N-1$. The corresponding eigenfunction is given by (3.16), where the coefficients d_m, $m=1,\ldots,N$, are components of a vector solving the equation $\Lambda d=0$ with the matrix Λ given by (3.8).*

(c) *In the limit $\min_{1\leqslant j\leqslant N}\alpha_j\to\infty$ the bound state wave function behaves according to (3.28) and (3.29). On the other hand, in the strong coupling case there are exactly N eigenvalues whose asymptotics is given by (3.26); the corresponding eigenfunctions are strongly localized around the points $\vec{x}=\vec{a}_j$ and given by (2.29) with $\vec{a}=\vec{a}_j$ and $\alpha=\alpha_j$.*

(d) *If an eigenvalue $z\in[1,\infty)$ exists, the corresponding eigenvector is orthogonal to the subspace $\oplus_{n=1}^{[\sqrt{z}]} L^2(\mathbb{R}^2)\otimes\{\chi_n\}$.*

F. Scattering

Comparing to the one-center case, the Hamiltonian $H(\alpha,\vec{a})$ with a finite number of perturbations loses in general the invariance with respect to rotations around an axis perpendicular to Σ. Hence we cannot employ here the partial wave decomposition and we turn directly to the "closed form" of the on-shell scattering amplitude and on-shell scattering operator. By (3.3), to any $\psi\in D(H(\vec{a},\alpha))$ and a nonreal z there exists $\psi_z\in D(H_0)$ such that

$$\psi(\vec{x}) = \psi_z(\vec{x}) + \sum_{j,k=1}^{N} \lambda_{jk}(\alpha,\vec{a};z)\, G_0(\vec{x},\vec{a}_j;z)\, \psi_z(\vec{a}_k). \tag{3.30}$$

We take again $\psi_0^\varepsilon(\vec{x})=e^{ik_n(z)\omega x-\varepsilon|x|^2}\chi_n(y)$ for ψ_z, where ω is a unit vector in $\mathbb{R}^2$. Denoting the lhs of (3.30) as ψ^ε we have $\psi^\varepsilon\in D(H(\alpha,\vec{a}))$ and

$$((H(\alpha,\vec{a})-z)\psi^\varepsilon)(\vec{x}) = 4\varepsilon[1-\varepsilon|x|^2+ik_n\omega x]\,\psi_z^\varepsilon(\vec{x}). \tag{3.31}$$

The rhs converges in $L^2(\mathbb{R}^2)$ as z approaches the real line and the ψ^ε belongs to $D(H(\alpha,\vec{a}))$. The pointwise limit $\varepsilon\to 0+$ exists and equals

$$\psi_{\alpha,n}(\vec{x};k_n(z)\omega) = e^{ik_n(z)\omega x}\chi_n(y) + \sum_{j,k=1}^{N} \lambda_{jk}(\alpha,\vec{a};z)\, G_0(\vec{x},\vec{a}_j;z)\, e^{ik_n(z)\omega a_k}\chi_n(b_k). \tag{3.32}$$

The limiting function is locally square integrable and it thus is a generalized eigenfunction of $H(\alpha,\vec{a})$.

The components $(f_\alpha(k_n(z),\omega_x,\omega))_{mn}$ of the on-shell scattering amplitude are then given by the part of the following expression corresponding to the outgoing mth transverse mode,

$$\lim_{|x|\to\infty, x/|x|=\omega_x} |x|^{1/2} e^{-ik_m|x|}[\psi_{\alpha,n}(\vec{x};k_n(z)\omega) - e^{ik_n\omega x}\chi_n(y)].$$

It yields

$$(f_\alpha(k_n(z),\omega_x,\omega))_{mn} = \frac{e^{i\pi/4}}{\pi\sqrt{2\pi k_m(z)}} \sum_{j,k=1}^{N} e^{-ik_m(z)\omega_x a_j} \lambda_{jk}(\alpha,\vec{a};z)\, e^{ik_n(z)\omega a_k} \sin(mb_j)\sin(nb_k), \tag{3.33}$$

and the on-shell scattering operator $S_\alpha(z)$ on $L^2(S^1)\otimes L^2([0,d])$ is

$$S_\alpha(z) = I + \frac{i}{2\pi^2} \sum_{k,j=1}^{N} \sum_{m,n=1}^{[\sqrt{z}]} \sin(mb_j)\sin(nb_k)\, \lambda_{jk}(\alpha,\vec{a};z)\, (e^{-ik_n(z)(\cdot)a_k}\chi_n, \cdot)\, e^{-ik_m(z)(\cdot)a_j}\chi_m . \tag{3.34}$$

As in the one-center case, resonances are determined by the poles in the meromorphic continuation of the matrix-valued function $(\lambda_{jk}(\alpha,\vec{a};\cdot))$.

IV. A LAYER IN MAGNETIC FIELD

A. The free Hamiltonian

In this section, the layer $\Sigma = \mathbb{R}^2\times(0,d)$ is placed into a homogeneous magnetic field $\vec{B} = (0,0,B)$. As usual the vector potential generating this field can be chosen in different ways, e.g., we can employ the symmetric gauge, $\vec{A} = 1/2\,(-Bx_2, Bx_1, 0)$. We again use the decomposition into transverse modes,

$$\begin{aligned} H_0^B &= \bigoplus_{n=1}^{\infty} h_n^B \otimes I_n , \\ h_n^B &= \left(-i\frac{\partial}{\partial x_1} + \frac{1}{2}Bx_2\right)^2 + \left(-i\frac{\partial}{\partial x_2} - \frac{1}{2}Bx_1\right)^2 + \left(\frac{\pi n}{d}\right)^2 . \end{aligned} \tag{4.1}$$

The first two terms on the rhs denoted as h^B describe a two-dimensional particle in the perpendicular homogeneous field. The resolvent kernel of such an operator is well known:[14]

$$\begin{aligned} (h^B - z)^{-1}(x,x') = \frac{1}{4\pi} \exp\left(\frac{iB}{2}(-x_1x_2' + x_2x_1') - \frac{|B|}{4}|x-x'|^2\right) \\ \times \Gamma\left(\frac{|B|-z}{2|B|}\right) U\left(\frac{|B|-z}{2|B|}, 1; \frac{|B|}{2}|x-x'|^2\right), \end{aligned}$$

where U is the irregular confluent hypergeometric function (Ref. 9, 13.1.33). For the sake of brevity we denote the exponential term in the above formula as $\Phi^B(x,x')$. The decomposition (4.1) then yields the sought resolvent kernel

$$\begin{aligned} G_0^B(\vec{x},\vec{x}';z) &\equiv (H_0^B - z)^{-1}(x,y;x',y') \\ &= \frac{1}{2\pi d} \exp\left(\frac{iB}{2}(-x_1x_2' + x_2x_1') - \frac{|B|}{4}|x-x'|^2\right) \\ &\quad \times \sum_{n=1}^{\infty} \Gamma\left(\frac{|B| - k_n^2(z)}{2|B|}\right) U\left(\frac{|B|-k_n^2(z)}{2|B|}, 1; \frac{|B|}{2}|x-x'|^2\right) \sin\left(\frac{n\pi y}{d}\right)\sin\left(\frac{n\pi y'}{d}\right). \end{aligned} \tag{4.2}$$

B. The perturbed resolvent

As in the nonmagnetic case we start from a single point interaction located at the point $\vec{a} \in \Sigma$ and modify to the present situation the argument of Sec. II C. We employ the fact that *locally* the magnetic field means a regular perturbation of the Schrödinger equation; motivated by this we *define* the one-center Hamiltonian in the same way as in Sec. II: it acts as free

$$(H^B(\alpha,\vec{a})\psi)(\vec{x}) = \left(\left[\left(-i\frac{\partial}{\partial x_1} + \frac{1}{2}Bx_2 \right)^2 + \left(-i\frac{\partial}{\partial x_2} - \frac{1}{2}Bx_1 \right)^2 - \frac{\partial^2}{\partial y^2} \right] \psi \right)(\vec{x}) \tag{4.3}$$

for $\vec{x} \neq \vec{a}$ with the domain changed to

$$\begin{aligned} D(H^B(\alpha,\vec{a})) = \{ \psi \in L^2(\Sigma \setminus \{\vec{a}\}) :\ & H^B(\alpha,\vec{a})\psi \in L^2(\Sigma \setminus \{\vec{a}\}), \\ & \psi(x,0) = \psi(x,d) = 0,\ L_1(\psi,\vec{a}) - 4\pi\alpha L_0(\psi,\vec{a}) = 0 \}, \end{aligned} \tag{4.4}$$

where L_0 and L_1 in the last relation are again the generalized boundary values from Ref. 2, Chap. I.1.

Remark 4.1: To justify such a definition we have to check that the resolvent kernel (4.2) has the same singularity as the nonmagnetic expression (2.3) for $\vec{x}' \to \vec{x}$. We have $G_0^B(\vec{x},\vec{x}';z) \approx c|\vec{x}' - \vec{x}|^{-1}$ by Ref. 15, Thm. III.5.1, with a nonzero c independent of z. To check that the constant has the needed value it is sufficient to find operators H_- and H_β with β from some interval $(\beta_0,1)$ whose resolvent kernels are $\sim(4\pi)^{-1}|\vec{x}' - \vec{x}|$ around the singularity and which satisfy the inequalities

$$H_- \leqslant H_0^B \leqslant \beta^{-1} H_\beta, \tag{4.5}$$

since the last named property implies easily

$$(H_- - z)^{-1} \geqslant (H_0^B - z)^{-1} \geqslant \beta(H_\beta - \beta z)^{-1}$$

for a fixed $z<0$ and $c=(4\pi)^{-1}$ follows by contradiction. For the lower bound we choose the projection to the layer of the magnetic Schrödinger operator $(-i\vec{\nabla} - \vec{A})^2$ in $L^2(\mathbb{R}^3)$ obtained by removing the Dirichlet boundaries of Σ, because the latter is of the form $h_B \otimes I + I \otimes (-\partial_y^2)$ and we may apply the bracketing argument (Ref. 7, Sec. XIII.15) to the nonmagnetic part in the y-direction. Its kernel is known[16,17] to be

$$\tilde{G}_0^B(\vec{x},\vec{x}';z) = \frac{1}{4\pi}\left(\frac{|B|}{2}\right)^{1/2} \Phi^B(x,x') \sum_{l=0}^{\infty} \frac{\exp[-(|B|(2l+1)-z)^{1/2}|y-y'|]}{(l+\frac{1}{2}-z/2|B|)^{1/2}} L_l\left(\frac{B}{2}|x-x'|^2\right), \tag{4.6}$$

where the factor Φ^B is the same as in the relation (4.2) and L_l are the Laguerre polynomials. We want to prove that $|\vec{x}-\vec{x}'|\tilde{G}_0^B(\vec{x},\vec{x}';z)$ tends to $(4\pi)^{-1}$ in the limit $|\vec{x}-\vec{x}'| \to 0$. Putting $|x-x'| = 0$, we can neglect the Laguerre polynomials and the factor Φ^B; it remains to compute the simplified sum. For a given z there exists an integer number l_0 such that $|B|(2l_0-1)-z>0$. Then one could split the series into two parts: the finite sum over $l=0,\ldots,l_0-1$ which is irrelevant for the singularity and the truncated series with $l=l_0,\ldots$. The latter can be estimated as follows,

$$I_- \leqslant \frac{|B|}{4\pi} \sum_{l=l_0}^{\infty} \frac{\exp[-(|B|(2l+1)-z)^{1/2}\varrho]}{(|B|(2l+1)-z)^{1/2}} \leqslant I_+, \tag{4.7}$$

where

$$I_{\pm} := \frac{|B|}{4\pi} \int_{l_0}^{\infty} \frac{\exp[-(|B|(2l\mp 1)-z)^{1/2}\varrho]}{(|B|(2l\mp 1)-z)^{1/2}}\, dl = \frac{1}{4\pi\varrho}\, e^{-(|B|(2l_0\mp 1)-z)^{1/2}\varrho}.$$

Hence the resolvent $\widetilde{G}_0^B$ has the needed singularity.

In the opposite direction we add a Dirichlet boundary at $|x|=R$, cutting thus a finite cylinder of Σ. It is clearly sufficient to find a bound of the type (4.5) for the ''planar'' part of the operator and this task is further reduced to finding bounds for its partial-wave components,

$$\widetilde{h}_m^B = -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \left(\frac{m}{r} - \frac{Br}{2}\right)^2 \tag{4.8}$$

on $L^2(0,R)$ with the boundary condition $\lim_{r\to 0}\phi(r)(r^{1/2}\ln r)^{-1}=0$ at the origin (Ref. 2, Sec. I.5) and Dirichlet at $r=R$. A comparison of the potential terms shows that $\widetilde{h}_m^B \leqslant \beta^{-1}\widetilde{h}_m^0$ holds if $R < ((2/|B|)(\beta^{-1/2}-1))^{1/2}$, so one can choose for H_β the nonmagnetic Dirichlet Laplacian in the cylinder of an arbitrarily small radius. This operator has again the resolvent kernel with the needed singularity.[8] Notice finally that alternative ways to prove this result can be found in Ref. 18 or derived by techniques from the classical theory of partial differential equations (Ref. 19, Thm. 20.6).

Remark 4.2: The previous remark still does not answer the question about the Green's function singularity fully. To explain why it is the case, recall that the requirement of symmetry of the magnetic Hamiltonian yields for any functions ψ_1, ψ_2 from the domain by means of the Gauss theorem the condition[18]

$$\lim_{r\to 0}\int_{S_{\vec{a}}}\left(-\overline{\psi}_1\frac{\partial\psi_2}{\partial r} + \psi_2\frac{\partial\overline{\psi}_1}{\partial r} + 2i\overline{\psi}_1\psi_2\frac{\vec{A}\vec{r}}{r}\right)dS = 0,$$

where $\vec{r}=\vec{x}-\vec{a}$, $r=|\vec{r}|$ and the integral is taken over the surface of the sphere $S_{\vec{a}}$ with center at $\vec{a}$ and radius r. It is satisfied if the functions have the following asymptotic behavior in the vicinity of the point interaction:

$$\psi(\vec{x}) = c_0\frac{1+\vec{A}(\vec{a})(\vec{x}-\vec{a})}{|\vec{x}-\vec{a}|} + c_1 + \mathcal{O}(|\vec{x}-\vec{a}|). \tag{4.9}$$

This motivates us to change the generalized boundary value L_1 to

$$L_1(\psi,\vec{a}) = \lim_{|\vec{x}-\vec{a}|\to 0}\left[\psi(\vec{x}) - L_0(\psi,\vec{a})\frac{1+i\vec{A}(\vec{a})(\vec{x}-\vec{a})}{|\vec{x}-\vec{a}|}\right]. \tag{4.10}$$

This suggests to use for $\xi(B,\vec{a};z)$ the following limit,

$$\xi(B,\vec{a};z) = \lim_{\vec{x}\to\vec{a}}\left[G_0^B(\vec{x},\vec{a};z) - \frac{1+i\vec{A}(\vec{a})(\vec{x}-\vec{a})}{4\pi|\vec{x}-\vec{a}|}\right], \tag{4.11}$$

which has the disadvantage that it is direction dependent and can be altered by a gauge change.

However, it is possible to employ the function $\xi(B,\vec{a};z)$ defined by means of the pole singularity alone. By (4.2) the Green's function $G_0^B(\vec{x},\vec{a};z)$ has the form $\exp(i\vec{A}(\vec{a})(\vec{x}-\vec{a}))F(|\vec{x}-\vec{a}|;z)$ in the symmetric gauge. In Remark 4.1 we have shown that $F(|\vec{x}-\vec{a}|;z)$ has the following asymptotic behavior for small $|\vec{x}-\vec{a}|$,

$$F(|\vec{x}-\vec{a}|;z) = \frac{1}{4\pi|\vec{x}-\vec{a}|} + c(z) + \mathcal{O}(|\vec{x}-\vec{a}|),$$

where $c(z) := \lim_{\varrho\to 0}[F(\varrho;z) - 1/4\pi\varrho]$. The function c defined in this way can be understood as $\xi(B,\vec{a};z)$ obtained for the Green's function without the exponential factor; the corresponding generalized boundary value L_1 does not contain the extra part $\vec{A}(\vec{a})(\vec{x}-\vec{a})$. In the respective asymptotic formula for complete Green's function one has to multiply the last expression by the two first terms of the Taylor series of the exponential factor,

$$G_0^B(\vec{x},\vec{a};z) = \frac{1+i\vec{A}(\vec{a})(\vec{x}-\vec{a})}{4\pi|\vec{x}-\vec{a}|} + c(z) + \mathcal{O}(|\vec{x}-\vec{a}|).$$

Using now the modified boundary value L_1 we find that $\xi(B,\vec{a};z) = c(z)$. This justifies the choice of the generalized boundary values made in the beginning of this section; one has to keep in mind to ignore the exponential term $\Phi^B(x,a)$ when computing $\xi(B,\vec{a};z)$. This argument also remains valid for a finite number of point interactions, hence the functions $\xi(B,\vec{a}_j;z)$ for $j=1,\ldots,N$ contained in matrix $\Lambda(B,\alpha,\vec{a};z)$ in Sec. IV D are computed in the way described here.

After this digression we can return to evaluation of the Green's function of the operator $H^B(\alpha,\vec{a})$. By construction it is given by Krein's formula,

$$G^B(\vec{x},\vec{x}';z) = G_0^B(\vec{x},\vec{x}';z) + \frac{G_0^B(\vec{x},\vec{a};z)G_0^B(\vec{a},\vec{x}';z)}{\alpha - \xi(B,\vec{a};z)}, \tag{4.12}$$

where the regularized Green's function $\xi(B,\vec{a};\cdot)$ is, as we have explained in the above remarks, now given by

$$\begin{aligned}\xi(B,\vec{a};z) &= \lim_{|\vec{x}-\vec{a}|\to 0}\left[G_0^B(\vec{x},\vec{a};z) - \frac{1}{4\pi|\vec{x}-\vec{a}|}\right] \\ &= \lim_{\varrho\to 0}\left[\frac{1}{2\pi d}\sum_{n=1}^{\infty}\Gamma\left(\frac{|B|-k_n^2(z)}{2|B|}\right)U\left(\frac{|B|-k_n^2(z)}{2|B|},1;\frac{|B|}{2}\varrho^2\right)\sin^2\left(\frac{n\pi b}{d}\right) - \frac{1}{4\pi\varrho}\right].\end{aligned} \tag{4.13}$$

One can check directly the consistency requirement

$$\lim_{B\to 0} G^B(\vec{x},\vec{x}';z) = G(\vec{x},\vec{x}';z) \tag{4.14}$$

for fixed α, $\vec{a}$ and $\vec{x}\neq\vec{x}'$, where $G(\cdot,\cdot;z)$ is the non-magnetic Green's function of Sec. II C. It follows easily from a known relation (Ref. 9, 13.3.3) for the confluent hypergeometric function,

$$\lim_{u\to\infty}\Gamma(u)U\left(u,1,\frac{s}{u}\right) = 2K_0(2\sqrt{s}).$$

To make use of the Green's function, we have to evaluate the rhs of (4.13). We employ again the same trick and split a part of the series which can be summed explicitly for a general ϱ while in the remaining series the limit $\varrho\to 0$ can be interchanged with the sum. Since $U(u,1;\cdot)$ and $K_0(\cdot)$ both have a logarithmic singularity at zero, we modify the ansatz of Sec. II C writing $\xi(B,\vec{a};z) = \xi_1 + \xi_2$ with

$$\xi_1 := \lim_{\varrho\to 0}\frac{1}{2\pi d}\sum_{n=1}^{\infty}\left[\Gamma\left(\frac{|B|-k_n^2(z)}{2|B|}\right)U\left(\frac{|B|-k_n^2(z)}{2|B|},1;\frac{|B|}{2}\varrho^2\right) - 2K_0\left(\varrho\frac{\pi n}{d}\right)\right]\sin^2\left(\frac{n\pi b}{d}\right),$$

$$\xi_2 := \lim_{\varrho\to 0}\left[\frac{1}{2\pi d}\sum_{n=1}^{\infty}2K_0\left(\varrho\frac{\pi n}{d}\right)\sin^2\left(\frac{n\pi b}{d}\right) - \frac{1}{4\pi\varrho}\right].$$

The function ξ_2 is evaluated as above: In analogy with (2.13) we have

$$\xi_2=\frac{\gamma}{4\pi d}+\frac{1}{8\pi d}\left(2\psi\left(\frac{b}{d}\right)+\pi\cot\left(\frac{\pi b}{d}\right)\right). \tag{4.15}$$

As for the first part, ξ_1, we employ the small ϱ asymptotics for the confluent hypergeometric and Macdonald functions,

$$U(u,1;s)=-\frac{1}{\Gamma(u)}[\ln s+\psi(u)-2\psi(1)]+\mathcal{O}(|s\ln s|) \quad \text{as} \quad s\to 0,$$

$$K_0(s)=-\left[\ln\frac{s}{2}-\psi(1)\right]+\mathcal{O}(s^2) \quad \text{as} \quad s\to 0$$

(see Ref. 20, 6.7.13 and Ref. 9, 9.6.13). Putting them together we see that the summand behaves for small ϱ as

$$\ln\left(\frac{(\pi n)^2}{2|B|d^2}\right)-\psi\left(\frac{|B|-z+(\pi n/d)^2}{2|B|}\right)+\mathcal{O}(|\varrho^2\ln\varrho|).$$

For large n the digamma function $\psi(s)=\ln(s)-2/s+\mathcal{O}(s^{-2})$, so the above expression can be written for large n as

$$-\ln\left(1+(|B|-z)\left(\frac{d}{\pi n}\right)^2\right)+\frac{1}{2}\,\frac{2|B|}{|B|-z+(\pi n/d)^2}+\mathcal{O}(n^{-4})=z\left(\frac{d}{\pi n}\right)^2+\mathcal{O}(n^{-4}).$$

Hence the series in the definition of ξ_1 converges uniformly and the limit can be interchanged with the sum giving the sought formula for the regularized Green's function,

$$\begin{aligned}\xi(B,\vec{a};z)=\xi_1+\xi_2=\frac{1}{2\pi d}\sum_{n=1}^{\infty}&\left[\ln\left(\frac{(\pi n)^2}{2|B|d^2}\right)-\psi\left(\frac{|B|-z+(\pi n/d)^2}{2|B|}\right)\right]\sin^2\left(\frac{\pi n b}{d}\right)\\&+\frac{1}{4\pi d}\left[\gamma+\psi\left(\frac{b}{d}\right)+\frac{\pi}{2}\cot\left(\frac{\pi b}{d}\right)\right].\end{aligned} \tag{4.16}$$

Remark 4.3: The scaling behavior for the family $\Sigma^\sigma=\mathbb{R}^2\times[0,d\sigma]$, $\sigma>0$, is similar to that of Remark 2.1; however, one has to scale simultaneously the magnetic field by

$$B^\sigma=\sigma^{-2}B. \tag{4.17}$$

In distinction to the previous sections we shall keep a general d in the following discussion.

C. Spectral properties

The essential spectrum of $H^B(\vec{a},\alpha)$ remains the same as that of the free Hamiltonian H_0^B which follows easily from Weyl's theorem (Ref. 7, Thm. XIII.14). The latter is in turn obtained from the essential spectrum of the two-dimensional Landau Hamiltonian, $\sigma(h^B)=\sigma_{ess}(h^B)=\{|B|(2m+1): m\in\mathbb{N}_0\}$ (see, e.g., Ref. 21, Thm. 1). Using the transverse-mode decomposition (4.1) we arrive at

$$\sigma_{ess}(H^B)=\sigma_{ess}(H_0^B)=\left\{|B|(2m+1)+\left(\frac{\pi n}{d}\right)^2:\ m,n-1\in\mathbb{N}_0\right\}. \tag{4.18}$$

Furthermore, the general properties of self-adjoint extensions mentioned in Sec. II D imply that there is at most one eigenvalue in each spectral gap of the unperturbed operator, i.e., between the two neighboring values from $\sigma_{ess}(H^B)$ and in the interval $(-\infty,|B|+(\pi/d)^2)$; to find these eigenvalues one has to solve the equation

$$\xi(B,\vec{a};z)=\alpha. \tag{4.19}$$

We have already checked that the terms of the series expressing $\xi(B,\vec{a};z)$ decay as n^{-2}, so the series converges with the exceptions of the points where the ψ function has a singularity, i.e., for any $z\in\mathbb{R}-\sigma_{ess}(H^B)$. It is also obvious that $\xi(B,\vec{a};z)$ is real for any such z. We have

$$\frac{d}{dz}\xi(B,\vec{a};z)=\frac{1}{4\pi d|B|}\sum_{n=1}^{\infty}\psi'\left(\frac{|B|-z+(\pi n/d)^2}{2|B|}\right)\sin^2\left(\frac{\pi nb}{d}\right), \tag{4.20}$$

where $\psi'(s)=(d/ds)\,\psi(s)$ is the trigamma function. For large n it behaves as

$$\psi'\left(\frac{|B|-z+(\pi n/d)^2}{2|B|}\right)=\frac{2|B|}{|B|-z+(\pi n/d)^2}+\mathcal{O}(n^{-4}),$$

so the series converges for $z\in\mathbb{R}\setminus\sigma_{ess}(H^B)$ and we are allowed to interchange the sum with the derivative. The explicit expression (Ref. 9, 6.4.10) for the digamma derivative,

$$\psi'(s)=\sum_{j=0}^{\infty}\frac{1}{(s+j)^2}\quad\text{for}\quad s\neq 0,-1,-2,\ldots,$$

shows that $\xi(B,\vec{a};z)$ is monotonously growing with respect to z in each gap. Using the relation (Ref. 9, 6.3.16)

$$\psi(1+s)=-\gamma+\sum_{j=1}^{\infty}\frac{s}{j(j+s)},\quad s\neq -1,-2,\ldots,$$

we find that ξ diverges as z approaches any point of the essential spectrum behaving in its vicinity as

$$\xi(B,\vec{a};z)=-\frac{|B|}{\pi d}\frac{\sin^2(\pi nb/d)}{z-|B|(2m+1)-(\pi n/d)^2}+\mathcal{O}(1), \tag{4.21}$$

provided the considered value from $\sigma_{ess}(H_0)$ is "nondegenerate" in the sense that it can be expressed by means of a single pair of indices m,n. This is the generical case since the last name property is valid always if the ratio of the coefficients $|B|$ and $(\pi/d)^2$ is irrational. If it is rational, then to a given $z_0\in\sigma_{ess}(H_0)$ there may exist different pairs m_j,n_j with the index belonging to a family $J(z_0)$ such that $|B|(2m_j+1)+(\pi n_j/d)^2=z_0$ for all $j\in J(z_0)$.

Taking this degeneracy into account we have

$$\xi(B,\vec{a};z)=-\frac{|B|}{\pi d}\frac{1}{z-z_0}\sum_{j\in J(z_0)}\sin^2\left(\frac{\pi n_j b}{d}\right)+\mathcal{O}(1). \tag{4.22}$$

When z approaches z_0 from below, ξ diverges to ∞, while if it approaches z_0 from above, ξ goes to $-\infty$. The formula (4.22) also shows that we can disregard those j for which $\sin(\pi n_j b/d)=0$: as above the system does not "feel" a point perturbation situated at a transverse eigenfunction node.

To find the behavior as $z\to-\infty$, recall that the argument leading to the expression (4.16) shows that the latter differs from the nonmagnetic formula (2.14) by the replacement $z\to z-|B|$ together with the addition of terms which remain bounded as $z\to-\infty$. Consequently, the asymptotics is independent of B and given by the formula

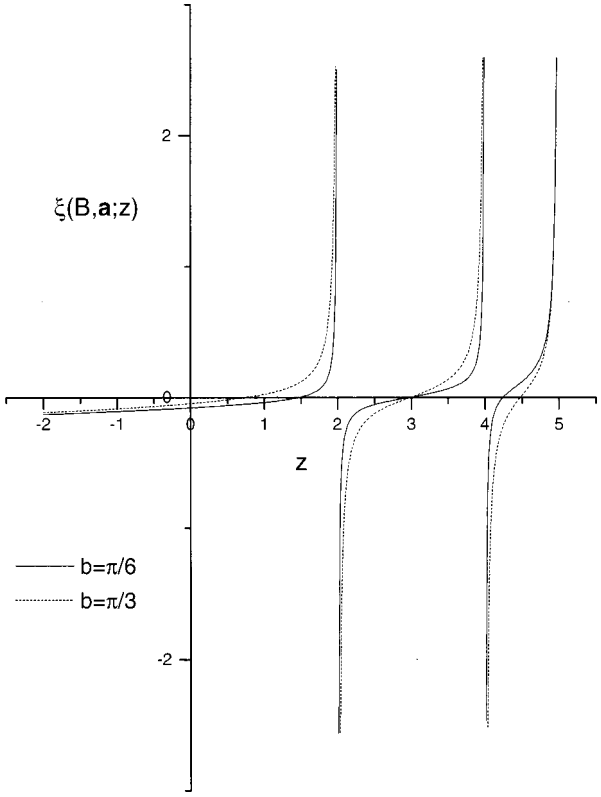

FIG. 5. The function $\xi(B,\vec{a};\cdot)$ for $B=1$, $d=\pi$ and $b=\pi/6,\pi/3$.

$$\xi(B,\vec{a};z)=-\frac{\sqrt{-z}}{4\pi}+\mathcal{O}(1) \quad \text{as} \quad z\to-\infty. \tag{4.23}$$

The behavior of the function $\xi(B,\vec{a};\cdot)$ is illustrated in Fig. 5.

Having discussed the properties of the function ξ, we can apply the conclusions on Eq. (4.19). Since ξ is strictly increasing between every pair of neighboring singularities, there is a unique eigenvalue $\varepsilon_r(B,\alpha,\vec{a})$ in each gap for any $\alpha\in\mathbb{R}$ and it satisfies the inequality

$$\varepsilon_r(B,\alpha,\vec{a})>\varepsilon_r(B,\alpha',\vec{a}) \quad \text{if} \quad \alpha>\alpha', \tag{4.24}$$

where the index r is labeling the gaps of H_0. The value $r=0$ corresponds to the interval $(-\infty,|B|+(\pi/d)^2)$, $r=1$ represents the first finite gap with the left endpoint $|B|+(\pi/d)^2$, etc.

Since we know the behavior of ξ around the singularities, we can write the explicit expression of $\varepsilon_r(B,\alpha,\vec{a})$ in the limits of strong and weak coupling. Suppose that the point $|B|(2m_j+1)+(\pi n_j/d)^2=z_0\in\sigma_{ess}(H_0)$ separates the rth and $(r+1)$th gap. Then, using the implicit-function theorem, we get

$$\begin{aligned}
\varepsilon_r(B,\alpha,\vec{a})&=z_0-\frac{1}{\alpha}\frac{|B|}{\pi d}\sum_{j\in J(z_0)}\sin^2\left(\frac{\pi n_j b}{d}\right)+\mathcal{O}(\alpha^{-2}) \quad \text{as} \quad \alpha\to\infty,\\
\varepsilon_{r+1}(B,\alpha,\vec{a})&=z_0-\frac{1}{\alpha}\frac{|B|}{\pi d}\sum_{j\in J(z_0)}\sin^2\left(\frac{\pi n_j b}{d}\right)+\mathcal{O}(\alpha^{-2}) \quad \text{as} \quad \alpha\to-\infty.
\end{aligned} \tag{4.25}$$

We see that the strong and weak limits are similar in the magnetic case. A different behavior we find only for the lowest eigenvalue for which the asymptotic formula (4.23) gives

$$\varepsilon_0(B,\alpha,\vec{a}) = -16\pi^2\alpha^2(1+\mathcal{O}(\alpha^{-1})) \quad \text{as} \quad \alpha\to-\infty. \tag{4.26}$$

A finer estimate with the error term replaced by $\mathcal{O}(\alpha^{-2})$ can be obtained when the ξ is expressed in terms of the Hurwitz ζ-function (see, e.g., Ref. 17). As in the nonmagnetic case, the residuum of the resolvent pole in the formula (4.12) yields a (non-normalized) eigenfunction

$$\psi(\vec{x};\alpha,\vec{a}) = G_0^B(\vec{x},\vec{a};\varepsilon_r(B,\alpha,\vec{a})) \tag{4.27}$$

corresponding to $\varepsilon_r(B,\alpha,\vec{a})$, where G_0^B is the free resolvent (4.2).

We are naturally interested in the behavior of the eigenfunction in the limit $|\alpha|\to\infty$ for eigenvalues satisfying the asymptotic relations (4.25). In both cases, by Ref. 20, 1.17.11 the gamma functions in the sum (4.2) corresponding to n_j, $j\in J(z_0)$, diverge as

$$\Gamma(-m_j+\epsilon) = \frac{(-1)^{m_j}}{m_j!}\frac{1}{\epsilon}+\mathcal{O}(1) \quad \text{as} \quad \epsilon\to 0.$$

This makes it possible to write the leading term of the asymptotics explicitly,

$$\begin{aligned}\psi(\vec{x};\alpha,\vec{a}) = {} & \frac{\alpha}{\sum_{j\in J(z_0)}\sin^2(\pi n_j b/d)}\Phi^B(x,x') \\ & \times\sum_{j\in J(z_0)} U\left(-m_j+\frac{1}{\alpha}\frac{1}{2\pi d}\sum_{j\in J(z_0)}\sin^2\left(\frac{\pi n_j b}{d}\right),1;\frac{|B|}{2}|x-a|^2\right) \\ & \times\frac{(-1)^{m_j}}{m_j!}\sin\left(\frac{\pi n_j b}{d}\right)\sin\left(\frac{\pi n_j y}{d}\right)+\mathcal{O}(1) \quad \text{as} \quad |\alpha|\to\infty.\end{aligned} \tag{4.28}$$

By Ref. 9, 13.6.27, the hypergeometric function is reduced to a Laguerre polynomial,

$$U(-n,1,u) = (-1)^n n! L_n(u),$$

at positive-integer values of the first index, so the wave function can be rewritten as

$$\psi(\vec{x};\alpha,\vec{a}) \approx \frac{\alpha}{\sum_{j\in J(z_0)}\sin^2(\pi n_j b/d)}\Phi^B(x,a)\sum_{j\in J(z_0)} L_{m_j}\left(\frac{|B|}{2}|x-a|^2\right)\sin\left(\frac{\pi n_j b}{d}\right)\sin\left(\frac{\pi n_j y}{d}\right). \tag{4.29}$$

In the last formula we have not specified the error term which has an extra part coming from the variation of the hypergeometric function $U(\cdot,1,u)$ around integer values.

We stated that the eigenvalue $\varepsilon_0(B,\alpha,\vec{a})$ in the strong coupling limit case has the same behavior as if there were no magnetic field. The same is true for the corresponding eigenfunction which is strongly localized,

$$\begin{aligned}\psi(\vec{x};\alpha,\vec{a}) = {} & \frac{1}{d}\Phi^B(x,a)\sum_{n=1}^{\infty}\left(2\pi\sqrt{|B|+16\pi^2\alpha^2+\left(\frac{\pi n}{d}\right)^2}|x-a|\right)^{-1/2} \\ & \times e^{-\sqrt{|B|+16\pi^2\alpha^2+(\pi n/d)^2}|x-a|}\sin\left(\frac{\pi n y}{d}\right)\sin\left(\frac{\pi n b}{d}\right)+\mathcal{O}(\alpha^{-1}).\end{aligned} \tag{4.30}$$

Let us summarize the results obtained for the layer in the magnetic field with one point interaction.

Theorem 4.4: *Let $H^B(\alpha,\vec{a})$ be defined by (4.3) and (4.4). Then*

(a) $\sigma_{ess}(H^B(\alpha,\vec{a})) = \{|B|(2m+1)+(\pi n/d)^2 : m,n-1\in\mathbb{N}_0\}$.

(b) *For any $\alpha\in\mathbb{R}$ there exists a single eigenvalue $\varepsilon_r(B,\alpha,\vec{a})$ between every two neighboring values from the essential spectrum, with the exception of the case when the leading term coefficient in (4.22) is zero and the eigenvalue coincides with the Landau in question for a particular value of α. Each of these eigenvalues is increasing and infinitely differentiable wrt α. The corresponding eigenfunction is given by (4.27).*

(c) *In both limits $\alpha\to\pm\infty$ the eigenvalue behaves similarly according to (4.25), except for the strong coupling limit for the lowest eigenvalue, where the formula (4.26) is valid. The eigenfunctions corresponding to the eigenvalues (4.25) and (4.26) are given by (4.28) and (4.30), respectively.*

D. Finite number of point interactions

Next we consider a finite number N of point interactions supported by points $\vec{a}_j$, $j=1,\dots,N$. We define the Hamiltonian in a way similar to that of Sec. III, i.e., it will be given by (4.3) and (4.4), where $\vec{a}$, α are again shorthands for $\vec{a}=(\vec{a}_1,\dots,\vec{a}_N)$ and $\alpha=(\alpha_1,\dots,\alpha_N)$, and instead of a single boundary condition there is an N-tuple of them,

$$L_1(\psi,\vec{a}_j)-4\pi\alpha_j L_0(\psi,\vec{a}_j)=0,\quad j=1,\dots,N. \tag{4.31}$$

Accordingly, Krein's formula reads

$$(H^B(\alpha,\vec{a})-z)^{-1}(\vec{x},\vec{x}')=G_0^B(\vec{x},\vec{x}';z)+\sum_{j,k=1}^{N}\lambda_{jk}(B,\alpha,\vec{a};z)\,G_0^B(\vec{x},\vec{a}_j;z)\,G_0^B(\vec{a}_k,\vec{x}';z). \tag{4.32}$$

Repeating the argument of Sec. III B, we find $\lambda(B,\alpha,\vec{a};z)^{-1}=\Lambda(B,\alpha,\vec{a};z)$ with

$$\Lambda_{mj}(B,\alpha,\vec{a};z):=\delta_{jm}(\alpha_m-\xi(B,\vec{a}_m;z))-(1-\delta_{jm})G_0^B(\vec{a}_m,\vec{a}_j;z), \tag{4.33}$$

or, more explicitly by means of (4.16) and (4.2),

$$\begin{aligned}\Lambda_{jj}=\alpha_j&-\frac{1}{2\pi d}\sum_{n=1}^{\infty}\left[\ln\left(\frac{(\pi n)^2}{2|B|d^2}\right)-\psi\left(\frac{|B|-k_n^2(z)}{2|B|}\right)\right]\sin^2\left(\frac{\pi n b_j}{d}\right)\\&-\frac{1}{4\pi d}\left[\gamma+\psi\left(\frac{b_j}{d}\right)+\frac{\pi}{2}\cot\left(\frac{\pi b_j}{d}\right)\right]\end{aligned} \tag{4.34}$$

and

$$\begin{aligned}\Lambda_{mj}=&-\frac{1}{2\pi d}\Phi^B(a_m,a_j)\sum_{n=1}^{\infty}\Gamma\left(\frac{|B|-k_n^2(z)}{2|B|}\right)\\&\times U\left(\frac{|B|-k_n^2(z)}{2|B|},1;\frac{|B|}{2}|a_m-a_j|^2\right)\sin\left(\frac{\pi n b_j}{d}\right)\sin\left(\frac{\pi n b_m}{d}\right)\end{aligned} \tag{4.35}$$

for $j\neq m$. If some perturbations are arranged vertically, $a_j=a_m$ for $j\neq m$, the last expression can be written as

$$\begin{aligned}\Lambda_{mj}=&-\frac{1}{2\pi d}\sum_{n=1}^{\infty}\left[\ln\left(\frac{(\pi n)^2}{2|B|d^2}\right)-\psi\left(\frac{|B|-z+(\pi n/d)^2}{2|B|}\right)\right]\sin\left(\frac{\pi n b_m}{d}\right)\sin\left(\frac{\pi n b_j}{d}\right)\\&-\xi_2\left(\frac{b_j+b_m}{2}\right)+\xi_2\left(\frac{|b_j-b_m|}{2}\right),\end{aligned} \tag{4.36}$$

as we find by a direct modification of the argument yielding $\xi(B,\vec{a};z)$.

Consider again a point $z_0 \in \sigma_{ess}(H_0)$. If z approaches this value, the appropriate contributions to the sums in (4.16) and (4.2) diverge and the matrix elements of Λ behave in the limit $z \to z_0$ as

$$\Lambda_{jj} = \alpha_j - \frac{|B|}{\pi d} \frac{1}{z_0 - z} \sum_{i \in J(z_0)} \sin^2\left(\frac{\pi n_i b_j}{d} \right) + \mathcal{O}(1),$$

$$\Lambda_{mj} = -\frac{|B|}{\pi d} \Phi^B(\vec{a}_m, \vec{a}_j) \frac{1}{z_0 - z} \sum_{i \in J(z_0)} \frac{(-1)^{m_i}}{m_i!} U\left(\frac{|B| + (\pi n_i/d)^2 - z}{2|B|}, 1; \frac{|B|}{2} |a_j - a_m|^2 \right)$$
$$\times \sin\left(\frac{\pi n_i b_j}{d} \right) \sin\left(\frac{\pi n_i b_m}{d} \right) + \mathcal{O}(1) \quad \text{if} \quad j \neq m, \tag{4.37}$$

$$\Lambda_{mj} = -\frac{|B|}{\pi d} \frac{1}{z_0 - z} \sum_{i \in J(z_0)} \sin\left(\frac{\pi n_i b_j}{d} \right) \sin\left(\frac{\pi n_i b_m}{d} \right) + \mathcal{O}(1) \quad \text{if} \quad j \neq m, \ \ a_j = a_m .$$

Moreover, the hypergeometric functions reduce to the Laguerre polynomials in the limit, so

$$\Lambda_{mj} \approx -\frac{|B|}{\pi d} \Phi^B(a_m, a_j) \frac{1}{z_0 - z} \sum_{i \in J(z_0)} L_{m_i}\left(\frac{|B|}{2} |a_m - a_j|^2 \right) \sin\left(\frac{\pi n_i b_j}{d} \right) \sin\left(\frac{\pi n_i b_m}{d} \right). \tag{4.38}$$

For large negative energies, $z \to -\infty$, we employ the asymptotic behavior of ξ given by (4.23), arriving thus at

$$\Lambda_{jj} = \alpha_j + \sqrt{\frac{-z}{4\pi}} + \mathcal{O}(1), \tag{4.39}$$

with B dependence being hidden in the error term. The nondiagonal part of the matrix Λ vanishes in the limit of large negative energy, because by Ref. 9, 13.3.3, one has

$$\Lambda_{mj} \approx -\frac{1}{2\pi d} \Phi^B(\vec{a}_m, \vec{a}_j) \sum_{n=1}^{\infty} K_0\left(\sqrt{|B| - k_n^2(z)} |a_m - a_j| \right) \sin\left(\frac{\pi n b_j}{d} \right) \sin\left(\frac{\pi n b_m}{d} \right),$$

which is exponentially decreasing, $K_0(s) \approx \sqrt{\pi/2s}\ e^{-s}$ as $s \to \infty$. In the case of a vertical arrangement, $a_j = a_m$ for $j \neq m$, we can again claim only that the matrix element Λ_{jm} is bounded.

Having obtained the coefficient matrix $\Lambda(B, \alpha, \vec{a}; z)$ given by (4.34) and (4.35) we proceed with finding the eigenvalues (the essential spectrum is preserved, of course). In the same way as in Sec. III C we check that an eigenvalue z is a solution of the implicit equation

$$\det \Lambda(B, \alpha, \vec{a}; z) = 0, \tag{4.40}$$

and the corresponding eigenfunction can be written as

$$\varphi(\vec{x}) = \sum_{j=1}^{N} d_j G_0^B(\vec{x}, \vec{a}_j; z), \tag{4.41}$$

where $d := (d_1, \ldots, d_N)$ is an eigenvector of the matrix $\Lambda(B, \alpha, \vec{a}; z)$.

As in the Sec. IV C we would like to say something about the number of eigenvalues in each gap. We already know that this number is limited from above by N. Denoting $\alpha_j = \tilde{\alpha}_j + \overline{\alpha}$ we can split the matrix $\Lambda(z, \alpha)$ into two parts,

$$\Lambda(z, \alpha) = \overline{\alpha} I - M(z, \tilde{\alpha}), \tag{4.42}$$

where $\tilde{\alpha}:=(\tilde{\alpha}_1,\ldots,\tilde{\alpha}_N)$. The explicit form of the matrix M can be obtained from the relations (4.34) and (4.35) by changing the signs and substituting α_j by $\tilde{\alpha}_j$. The same can be done for the formulas (4.37) which express the behavior around the singularity. In the limit $z\to z_0$ one can neglect the parameters $\tilde{\alpha}_j$'s. Then it is possible to write

$$M(z,\tilde{\alpha})=\frac{1}{z_0-z}\,\frac{|B|}{\pi d}\,\overline{M}(z_0)+\mathcal{O}(1),$$

where

$$\overline{M}_{jj}(z_0)=\sum_{i\in J(z_0)}\sin^2\left(\frac{\pi n_i b_j}{d}\right),$$

$$\overline{M}_{mj}(z_0)=\Phi_B(\vec{a}_m,\vec{a}_j)\sum_{i\in J(z_0)}L_{m_i}\left(\frac{|B|}{2}|a_m-a_j|^2\right)\sin\left(\frac{\pi n_i b_j}{d}\right)\sin\left(\frac{\pi n_i b_m}{d}\right).$$

Following Ref. 22 the eigenvalues of $\Lambda(z)$ monotonously increase between two neighboring singularities. Then all eigenvalues of $\overline{M}$ are non-negative numbers. For $\Sigma_{j=1}^{N}\Sigma_{i\in J(z_0)}\sin^2(\pi n_i b_j/d)\neq 0$ at least one is positive, hence at least one eigenvalue of the matrix $M(z,\tilde{\alpha})$ diverges to $-\infty$ or to ∞ as $z\to z_{0+}$, $z\to z_{0-}$, respectively. Let us summarize the results:

Theorem 4.5: *Let the operator $H^B(\alpha,\vec{a})$ be defined by (4.3) and (4.4), where $\vec{a}=(\vec{a}_1,\ldots,\vec{a}_N)$ and $\alpha=(\alpha_1,\ldots,\alpha_N)$ and the boundary condition is replaced by (4.31). Then*

(a) $\sigma_{ess}(H^B(\alpha,\vec{a}))=\{|B|(2m+1)+(\pi n/d)^2: m,n-1\in\mathbb{N}_0\}$.

(b) *For any $\alpha\in\mathbb{R}^N$ there exists at most N eigenvalues between every two neighboring values from the essential spectrum with the multiplicity taken into account. The corresponding eigenfunctions are given by (4.41).*

(c) *In the limits $\min_{1\leqslant j\leqslant N}\alpha_j\to\infty$ and $\max_{1\leqslant j\leqslant N}\alpha_j\to-\infty$ at least one eigenvalue converges to each value z_0 from the essential spectrum from below and from above, respectively, with the exception of the case when the leading term coefficients in (4.37) are zero. In the strong limit case there are also N eigenvalues given by (4.26) with corresponding eigenfunctions given by (4.30), where α and $\vec{a}$ is replaced by α_j and $\vec{a}_j$ for $j=1,\ldots,N$.*

Further results on the number of eigenvalues of the Hamiltonian H_0^B can be obtained in the same way as in Ref. 23.

Remark 4.6: If some of the point interactions are vertically arranged, we cannot exclude that eigenvalues are absent in a particular gap for some α.

Consider two point interactions placed at $(0,0,1/4d)$ and $(0,0,2/3d)$ with $\tilde{\alpha}_1=\tilde{\alpha}_2=0$. The numerical calculation for $B=1$ and $d=\pi$ shows that the eigenvalues of matrix $M(z,\tilde{\alpha})$ for $z\in(z_0(1,1),z_0(0,2))$ cover the whole $\mathbb{R}$ except one gap (see Fig. 6). The symbol $z_0(m,n)$ represents the Landau level $z_0=|B|(2m+1)+(\pi n/d)^2$. Hence for $\overline{\alpha}$ from this gap the matrix Λ has no eigenvalue in the interval $(z_0(1,1),z_0(0,2))=(4,5)$.

V. CONCLUSIONS

We have analyzed here spectral and scattering properties of a hard-wall layer with a finite number of point interactions. The results offer one more illustration of the efficiency of Krein's formula which allows us to reduce the task in fact to an algebraic problem. There are other interesting questions related to systems with finitely many perturbations such as relations between the perturbation configurations and the spectra including the nodal structure, etc., positions of resonances including those coming from perturbation of the embedded eigenvalues, and so on. To keep this article within reasonable limits, however, we postpone these questions to a sequel.

The same applies to systems with an infinite number of point obstacles which offer a wider variety of spectral types. Let us briefly mention several problems which we regard as worthy of

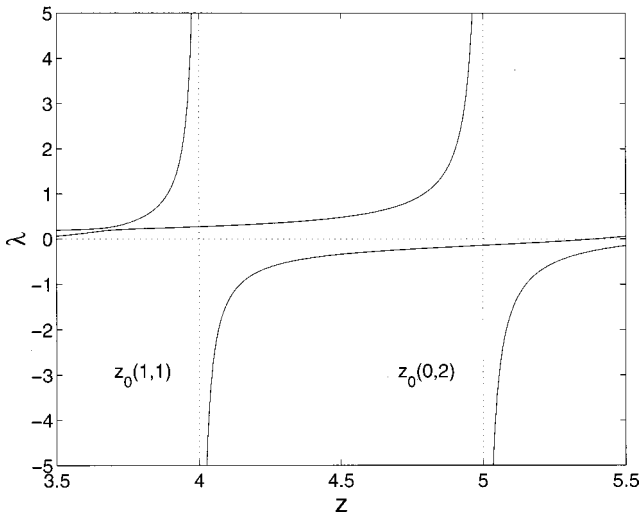

FIG. 6. The behavior of two eigenvalues of the matrix $M(z,\tilde{\alpha})$ for $z\in(4,5)$.

attention. One of them concerns the number of gaps in periodic systems. A periodic layer of point interactions in $\mathbb{R}^3$ has at most one gap (Ref. 2, Sec. III.1, or Ref. 24). On the other hand, it is known that the presence of boundaries can enhance the number of gaps in the two-dimensional case;[5] a similar effect is expected in dimension three: for a thin enough layer there will be many open gaps between the first and the second transverse threshold. A more difficult question concerns the validity of the Bohr–Sommerfeld conjecture in such systems.

Even more interesting are spectral properties of periodically perturbed layers in the presence of a magnetic field. It is well known that a combination of a square lattice of point interactions and a homogeneous magnetic field leads to a very rich spectrum whose properties depend substantially on the number-theoretical properties of the ratio between the lattice spacing and the field intensity (which determines the cyclotronic radius) (see Ref. 2, Sec. III.2.5, or Ref. 25). Putting such a system into a layer brings a third parameter (the layer width d) which will determine how ''thickly'' the transverse-mode component are overlayed in the spectrum.

The same applies to edge-type states. It was shown recently that an equidistant array of point interaction in combination with a homogeneous magnetic field can produce bands of absolutely continuous spectrum away from the Landau levels.[26] One is naturally interested in how the spectrum will change if the array is confined between a pair of hard walls. Other problems concern aperiodic perturbations, external electric field, spin effects, etc.

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Semiclassics in the lowest Landau band

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This article deals with the comparison between the strong Thomas–Fermi theory and the quantum mechanical ground state energy of a large atom confined to lowest Landau band wave functions. Using the tools of microlocal semiclassical spectral asymptotics we derive precise error estimates. The approach presented in this article suggests the definition of a modified strong Thomas–Fermi functional, where the main modification consists in replacing the integration over the variables perpendicular to the magnetic field by an expansion in angular momentum eigenfunctions. The resulting DSTF theory is studied in detail in the second part of the article. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1432776]

I. INTRODUCTION

In this article we study semiclassical theories describing the ground state energies of heavy atoms in strong homogeneous magnetic fields, where additionally the electrons are confined to the lowest Landau band.

An atom with N electrons of charge $-e$ and mass m_e and nuclear charge Ze is described by the nonrelativistic Pauli Hamiltonian operator

$$H_N=\sum_{1\leqslant j\leqslant N}\left\{((-i\nabla^{(j)}+\mathbf{A}(x_j))\cdot\sigma^j)^2-\frac{Z}{|x_j|}\right\}+\sum_{1\leqslant i<j\leqslant N}\frac{1}{|x_i-x_j|}, \tag{I.1}$$

acting on the Hilbertspace $\wedge_{1\leqslant j\leqslant N}L^2(\mathbb{R}^3,\mathbb{C}^2)$ of electrons. The units are chosen such that $\hbar=2m_e=e=1$. The magnetic field is $\mathbf{B}=(0,0,B)$, with vector potential $\mathbf{A}=\frac{1}{2}B(-x_2,x_1,0)$, where B is the magnitude of the field in units of $B_0=m_e^2e^3c/\hbar^3=2.35\times10^9$ G, the field strength for which the cyclotron radius $l_B=(\hbar c/(eB))^{1/2}$ is equal to the Bohr radius $a_0=\hbar^2/(m_ee^2)$. The ground state energy is

$$E^{\mathrm{Q}}(N,Z,B)=\inf\{(\psi,H_N\psi):\psi\in\text{domain } H_N,(\psi,\psi)=1\}. \tag{I.2}$$

Recall that the spectrum of the free Pauli Hamiltonian on $\mathcal{L}^2(\mathbb{R}^3;\mathbb{C}^2)$ for one electron in the magnetic field $\mathbf{B}$,

$$H_{\mathbf{A}}=[\boldsymbol{\sigma}\cdot(-i\nabla+\mathbf{A}(\mathbf{x}))]^2, \tag{I.3}$$

is given by

$$p_z^2+2\nu B,\quad \nu=0,1,2,\ldots,\quad p_z\in\mathbb{R}. \tag{I.4}$$

The projector Π_0 onto the lowest Landau band, $\nu=0$, is represented by the kernel

$$\Pi_0(\mathbf{x},\mathbf{x}')=\frac{B}{2\pi}\exp\left\{\frac{i}{2}(\mathbf{x}_\perp\times\mathbf{x}'_\perp)\cdot\mathbf{B}-\frac{1}{4}(\mathbf{x}_\perp-\mathbf{x}'_\perp)^2B\right\}\delta(z-z')P_\downarrow, \tag{I.5}$$

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where $\mathbf{x}_\perp$ and z are the components of $\mathbf{x}$ perpendicular and parallel to the magnetic field, and $P_\downarrow$ denotes the projection onto the spin-down component.

In this article we are especially interested in the ground state energy,

$$E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B)=\inf_{\|\psi\|=1}(\psi,\Pi_0^N H_N \Pi_0^N \psi), \tag{I.6}$$

where Π_0^N denotes the Nth tensorial power of Π_0. Lieb, Solovej, and Yngvason pointed out that for $B\gg Z^{4/3}$ the electrons are to the leading order confined to the lowest Landau band, which is expressed by the following theorem.

Theorem I.1: *(Ref. 1, Theorem 1.2): For any fixed $\lambda=N/Z$ there is a $\delta(x)$ with $\delta(x)\to 0$ as $x\to\infty$ such that*

$$E^{\mathrm{Q}}_{\mathrm{conf}}\geqslant E^{\mathrm{Q}}\geqslant E^{\mathrm{Q}}_{\mathrm{conf}}(1+\delta(B/Z^{4/3})). \tag{I.7}$$

The energy (I.6) can be approximated by means of the STF-functional (strong Thomas–Fermi),

$$\mathcal{E}^{\mathrm{STF}}[\rho]=\frac{4\pi^4}{3B^2}\int \rho^3-\int V\rho+D(\rho,\rho), \tag{I.8}$$

$V(x)=Z/|x|$ and $D(\rho,\rho)=\frac{1}{2}(\rho,|x|^{-1}*\rho)$. In Ref. 2 it is shown that $E^{\mathrm{Q}}/E^{\mathrm{STF}}\to 1$ if $Z\to\infty$, $B/Z^3\to 0$ and $B/Z^{4/3}\to\infty$, where

$$E^{\mathrm{STF}}(N,Z,B)=\inf\left\{\mathcal{E}^{\mathrm{STF}}[\rho]\,\middle|\,\rho\geqslant 0,\rho\in D^{\mathrm{STF}},\int\rho\leqslant N\right\}, \tag{I.9}$$

with an appropriately chosen domain D^{STF}. Combined with Theorem I.1 this implies Theorem I.2

Theorem I.2: *(Ref. 2) If $Z\to\infty$ with N/Z fixed, $B/Z^3\to 0$ and $B/Z^{4/3}\to\infty$, then*

$$E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B)/E^{\mathrm{STF}}(N,Z,B)\to 1. \tag{I.10}$$

This article contains an intensive study of the STF functional and of related functionals describing lowest Landau band particles. A justification for such studies is the fact that these functionals are of much simpler form than the original MTF (Magnetic Thomas-Fermi) functional (cf. Ref. 2), since the concerning kinetic energy density is the Legendre transform of the Fermi pressure P_B, i.e.

$$\tau_B(t)=\sup_{w\geqslant 0}[tw-P_B(w)], \tag{I.11}$$

with

$$P_B(w)=\frac{B}{3\pi^2}\left(w^{3/2}-2\sum_{i=1}^{\infty}\left|2iB-w\right|_-^{3/2}\right), \tag{I.12}$$

which is probably somewhat harder to deal with than (I.8).

A. Comparing the STF energy with the QM ground state energy in the lowest Landau band

In this article we not only want to give a direct proof of Theorem I, but we want to derive precise error estimates. In this respect our procedure is related to Refs. 3 and 4. Our main theorem is the following:

Theorem I.3: *Let $N\sim Z$ and $Z^{4/3}\leqslant B\leqslant Z^3$. Then*

$$|E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B)-E^{\mathrm{STF}}(N,Z,B)|\leqslant CB^{4/5}Z^{3/5} \tag{I.13}$$

for an appropriate constant C.

Remark I.4: In Ref. 4 Ivrii estimated the difference between the full quantum mechanical energy E^{Q} and the MTF energy, which is given by minimizing the MTF functional (cf. Ref. 2), where all Landau levels are taken into account. The main theorem in Ref. 4 reads as follows.

Theorem I.5: *(Ref. 4, Theorem 0.2): Let $B \leqslant Z^3$ and $N \sim Z$. Then*

$$\left|E^{Q}(N,Z,B) - E^{\mathrm{MTF}}(N,Z,B) - \tfrac{1}{4}Z^2\right| \leqslant R_1 + R_2, \tag{I.14}$$

with

$$R_1 = CZ^{4/3}(N+B)^{1/3} \quad \textit{and} \quad R_2 = CZ^{3/5}B^{4/5}. \tag{I.15}$$

Remark I.6: Although true for all $B \leqslant Z^3$, it should be noted that only for $B < Z^{7/4}$ are the error terms R_1 and R_2 smaller than the Scott term $\frac{1}{4}Z^2$.

One of the main difficulties Ivrii has to cope with in the proof of Theorem I.5 is the fact that the self-consistent MTF potential is not smooth, because it includes all Landau levels. So he has to create an approximating C^{∞} potential in order to apply the tools of microlocal semiclassical spectral asymptotics. Fortunately, in our case of Theorem I.3 we need not care about such problems, since the STF potential [see (I.19)] has all required properties for semiclassical spectral asymptotics.

Moreover, in Theorem I.5 Ivrii already captures (I.13) on the region where only the lowest Landau band is occupied, i.e., on $\{\mathbf{x} \mid |\mathbf{x}| \geqslant C_0 Z/B\}$ with a large constant C_0.

Remark I.7: A good guess cencerning the magnitude of the difference between the physical ground state energy E^{Q} and the confined energy E^{Q}_{conf} is given by

$$\left|E^{Q} - E^{Q}_{\mathrm{conf}}\right| \sim \left|E^{\mathrm{MTF}} - E^{\mathrm{STF}}\right| \lesssim Z^3/B^{1/2}, \tag{I.16}$$

as presented in Ref. 5. Combined with (I.13) this leads to the estimate

$$\left|E^{Q} - E^{\mathrm{STF}}\right| \lesssim Z^3/B^{1/2} + B^{4/5}Z^{3/5}. \tag{I.17}$$

Therefore, the region, where from a physical point of view it is meaningful to use the STF functional intead of the MTF functional, is given by

$$Z^{24/13} \leqslant B \leqslant Z^3, \tag{I.18}$$

which is imposed by the condition $Z^3/B^{1/2} \leqslant B^{4/5}Z^{3/5}$. Nevertheless, E^{STF} produces the right leading order for $Z^{4/3} \ll B \ll Z^3$, which justifies, in some sense, the mathematical analysis of Theorem I.3 on the whole region $Z^{4/3} \leqslant B \leqslant Z^3$.

Next we mention some important steps of the proof of Theorem I.3. Let ϕ^{STF} denote the effective STF potential (for simplicity think of the neutral case $N = Z$)

$$\phi^{\mathrm{STF}}(x) = Z|x|^{-1} - \rho^{\mathrm{STF}} * |x|^{-1}, \tag{I.19}$$

where ρ^{STF} is the minimizer of the STF functional (I.8). We will see in Sec. II.A that the main contribution of (I.13) is given by

$$\left| \mathrm{Tr}[\Pi_0 (H_{\mathbf{A}} - \phi^{\mathrm{STF}}(\mathbf{x}))\Pi_0]_- - \frac{B}{2\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}} \frac{dp\,d\mathbf{x}}{2\pi}[p^2 - \phi^{\mathrm{STF}}(\mathbf{x})]_- \right|, \tag{I.20}$$

with $[t]_- = \min\{0,t\}$. Recall

$$E^{\mathrm{STF}} = \frac{B}{2\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}} \frac{dp\,dx}{2\pi}[p^2 - \phi^{\mathrm{STF}}(\mathbf{x})]_- - D(\rho^{\mathrm{STF}}, \rho^{\mathrm{STF}}). \tag{I.21}$$

With the decomposition $\mathcal{L}^2(\mathbb{R}^3,d\mathbf{x};\mathbb{C}^2)=\mathcal{L}^2(\mathbb{R}^2,d\mathbf{x}_\perp)\otimes\mathcal{L}^2(\mathbb{R},dz)\otimes\mathbb{C}^2$ the projector Π_0 can be written as

$$\Pi_0=\sum_{m\geqslant 0}|\phi_m\rangle\langle\phi_m|\otimes 1\otimes P_\downarrow, \tag{I.22}$$

where ϕ_m denotes the function in the lowest Landau band with angular momentum $-m\leqslant 0$, i.e., using polar coordinates (r,φ),

$$\phi_m(\mathbf{x}_\perp)=\sqrt{\frac{B}{2\pi}}\frac{1}{\sqrt{m!}}\left(\frac{Br^2}{2}\right)^{m/2}e^{-im\varphi}e^{-Br^2/4}. \tag{I.23}$$

Using this and $H_{\mathbf{A}}\Phi_m=0$, we can write

$$\Pi_0 H_{\mathbf{A}}\Pi_0=\sum_{m\geqslant 0}|\phi_m\rangle\langle\phi_m|\otimes(-\partial_z^2)\otimes P_\downarrow. \tag{I.24}$$

By means of the above decompositions one gets the relation (cf. Ref. 5, Theorem 3.13)

$$\mathrm{Tr}[\Pi_0(-\partial_z^2-\phi^{\mathrm{STF}}(\mathbf{x}))\Pi_0]_-=\sum_m \mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}[-\partial_z^2-\phi_m^{\mathrm{STF}}(z)]_-, \tag{I.25}$$

with

$$\phi_m^{\mathrm{STF}}(z)=\int d\mathbf{x}_\perp\,\phi^{\mathrm{STF}}(\mathbf{x})|\phi_m(\mathbf{x}_\perp)|^2. \tag{I.26}$$

Next we multiply the mth term of the right hand side of (I.25) with $(B/2\pi)\,\chi_m(\mathbf{x}_\perp)$, where

$$\chi_m(\mathbf{x}_\perp)=\begin{cases}1 & \text{for } \sqrt{2m/B}\leqslant|\mathbf{x}_\perp|\leqslant\sqrt{2(m+1)/B},\\ 0 & \text{otherwise,}\end{cases} \tag{I.27}$$

and integrate over $\mathbf{x}_\perp$, which is just an identity operation. Since we are allowed to put the sum into the trace as well into the $[\,]_-$ bracket we arrive at

$$\mathrm{Tr}[\Pi_0[-\partial_z^2-\phi^{\mathrm{STF}}(\mathbf{x})]\Pi_0]_-=\frac{B}{2\pi}\int d\mathbf{x}_\perp\,\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}[-\partial_z^2-\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})]_-, \tag{I.28}$$

with

$$\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})=\sum_m \chi_m(\mathbf{x}_\perp)\,\phi_m^{\mathrm{STF}}(z). \tag{I.29}$$

The equation (I.28) follows from the fact that the terms $\chi_m(\mathbf{x}_\perp)\phi_m^{\mathrm{STF}}(z)$ in (I.29) have disjoint supports.

Hence, (I.20) can be written as

$$\left|\frac{B}{2\pi}\int_{\mathbb{R}^2}d\mathbf{x}_\perp\left(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}[-\partial_z^2-\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})]_- -\int_{\mathbb{R}^2}\frac{dzdp}{2\pi}[p^2-\phi^{\mathrm{STF}}(\mathbf{x})]_-\right)\right|. \tag{I.30}$$

We shall estimate (I.30) by splitting into the following two terms:

$$\left|\frac{B}{2\pi}\int_{\mathbb{R}^2}d\mathbf{x}_\perp\left(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}[-\partial_z^2-\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})]_- -\int_{\mathbb{R}^2}\frac{dzdp}{2\pi}[p^2-\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})]_-\right)\right|. \tag{I.31}$$

and

$$\left| \frac{B}{2\pi} \int_{\mathbb{R}^2} d\mathbf{x}_\perp \left(\int_{\mathbb{R}} \frac{dzdp}{2\pi} [p^2 - \widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})]_- - \int_{\mathbb{R}^2} \frac{dzdp}{2\pi} [p^2 - \phi^{\mathrm{STF}}(\mathbf{x})]_- \right) \right|. \tag{I.32}$$

B. Modified STF functionals

From Eqs. (I.25) and (I.28) it is apparent that the STF energy (I.9) is not the most natural semiclassical approximation of $E^{\mathrm{Q}}_{\mathrm{conf}}$. As already argued in Ref. 5, (I.25) suggests the definition of a functional, where the integration over $\mathbf{x}_\perp$, the variables orthogonal to the magnetic field, is replaced by an expansion in angular momentum eigenfunctions in the lowest Landau band. This leads to a *discrete STF functional* (DSTF) depending on a sequence of one-dimensional densities $\rho = (\rho_n)_{n \in \mathbb{N}_0}$, i.e.,

$$\mathcal{E}^{\mathrm{DSTF}}[\rho] = \sum_{m \in \mathbb{N}_0} \left(\kappa \int \rho_m(z)^3 - Z \int V_m(z) \rho_m(z) dz \right) + \overline{D}(\rho, \rho), \tag{I.33}$$

where $\kappa = \pi^2/3$,

$$\overline{D}(\rho, \rho) = \frac{1}{2} \sum_{m,n} \int V_{m,n}(z - z') \rho_m(z) \rho_n(z') dz dz', \tag{I.34}$$

and the potentials V_m and $V_{m,n}$ are given by

$$\begin{aligned} V_m(z) &= \int \frac{1}{|\mathbf{x}|} |\phi_m(\mathbf{x}_\perp)|^2 d\mathbf{x}_\perp, \\ V_{m,n}(z - z') &= \int \frac{|\phi_m(\mathbf{x}_\perp)|^2 |\phi_n(\mathbf{x}_\perp')|^2}{|\mathbf{x} - \mathbf{x}'|} d\mathbf{x}_\perp d\mathbf{x}_\perp'. \end{aligned} \tag{I.35}$$

An equivalent functional, depending on a three-dimensional density ρ, can be obtained as in (I.28), if in STF theory the Coulomb potential is replaced by

$$\widetilde{|\mathbf{x}|^{-1}} = \sum_m \chi_m(\mathbf{x}_\perp) \int_{\mathbb{R}^2} d\mathbf{x}_\perp |\mathbf{x}|^{-1} \phi_m(\mathbf{x}_\perp). \tag{I.36}$$

The resulting *modified* STF functional is given by

$$\mathcal{E}^{\mathrm{MSTF}}[\rho] = \frac{4\pi^4}{3B^2} \int d\mathbf{x} \rho(\mathbf{x})^3 - \int d\mathbf{x} \widetilde{|\mathbf{x}|^{-1}} \rho(\mathbf{x}) + \tilde{D}(\rho, \rho), \tag{I.37}$$

with

$$\tilde{D}(\rho, \rho) = \frac{1}{2} \sum_{m,n} \int d\mathbf{x} d\mathbf{y} V_{m,n}(z - z') \chi_m(\mathbf{x}_\perp) \chi_n(\mathbf{y}_\perp) \rho(\mathbf{x}) \rho(\mathbf{y}). \tag{I.38}$$

Let $\rho^{\mathrm{DSTF}} = (\rho_m^{\mathrm{DSTF}}(z))_m$ and $\rho^{\mathrm{MSTF}} = \rho^{\mathrm{MSTF}}(\mathbf{x})$ be the ground state densities of (I.33) and (I.37), respectively, corresponding to a fixed particle number N. Then the relationship between the densities reads

$$\rho^{\mathrm{MSTF}}(\mathbf{x}) = \frac{B}{2\pi} \sum_m \rho_m^{\mathrm{DSTF}}(z) \chi_m(\mathbf{x}_\perp). \tag{I.39}$$

Furthermore, the energies are equal,

$$E^{\mathrm{MSTF}}(N,Z,B)=E^{\mathrm{DSTF}}(N,Z,B). \tag{I.40}$$

Since a short computation shows that for $B\geqslant Z^{4/3}$ the difference between the D(M)STF energy and the STF energy is smaller than $B^{4/5}Z^{3/5}$, the estimate (I.13) with STF replaced by D(M)STF immediately follows for this region ($B\geqslant Z^{4/3}$).

Theorem I.8: *Let $Z^{4/3}\leqslant B\leqslant Z^3$ and $N\sim Z$. Then*

$$\left|E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B)-E^{\mathrm{D(M)STF}}(N,Z,B)\right|\leqslant CB^{4/5}Z^{3/5}. \tag{I.41}$$

II. PROOF OF THEOREM I.3

A. Derivation of lower and upper bounds to $E^{\mathrm{Q}}_{\mathrm{conf}}$

First of all, recall that the TF equation satisfied by the minimizer of (I.8) under the constraint $\int\rho=N$ is

$$\kappa(\rho^{\mathrm{STF}})^2/B^2=[Z|\mathbf{x}|^{-1}-\rho^{\mathrm{STF}}+\nu]_+=[\phi^{\mathrm{STF}}+\nu]_+, \tag{II.1}$$

where $\nu=\nu(N)$ is the chemical potential corresponding to the electron number N. Using (II.1) one sees that the STF energy (I.9) can be written as

$$E^{\mathrm{STF}}=\frac{B}{2\pi}\int_{\mathbb{R}^2}d\mathbf{x}_\perp\int_{\mathbb{R}}\frac{dzdp}{2\pi}[p^2-\phi^{\mathrm{STF}}(\mathbf{x})-\nu]_-+\nu N-D(\rho^{\mathrm{STF}},\rho^{\mathrm{STF}}). \tag{II.2}$$

This expression will be used for deriving upper and lower bounds to the quantum mechanical ground state energy $E^{\mathrm{Q}}_{\mathrm{conf}}$.

1. Lower bound

Let ψ denote a ground state wave function of H_N. Then we can write $E^{\mathrm{Q}}_{\mathrm{conf}}$ as

$$E^{\mathrm{Q}}_{\mathrm{conf}}=(\psi,\Pi_0^N H_N\Pi_0^N\psi)=\sum_{i=1}^N(\psi,\Pi_0^N[H_A(\mathbf{x}_i)-Z|\mathbf{x}_i|^{-1}+\rho^{\mathrm{STF}}*|\mathbf{x}_i|^{-1}-\nu]\Pi_0^N\psi)$$
$$+N\nu-2D(\rho_\psi,\rho^{\mathrm{STF}})+\sum_{i<j}(\psi,|\mathbf{x}_i-\mathbf{x}_j|^{-1}\psi), \tag{II.3}$$

where we have added and subtracted the term $\rho^{\mathrm{STF}}*|\mathbf{x}|^{-1}-\nu$ and used the definition

$$\rho_\psi(\mathbf{x})=N\sum_{s^i}\int|\psi(\mathbf{x},x_2,\ldots,x_N;s^1,\ldots,s^N)|^2dx_2\cdots dx_N. \tag{II.4}$$

By means of the Lieb–Oxford inequality[6]

$$\sum_{i<j}(\psi,|\mathbf{x}_i-\mathbf{x}_j|^{-1}\psi)\geqslant D(\rho_\psi,\rho_\psi)-1.68\int\rho_\psi^{4/3}, \tag{II.5}$$

(II.3) can be bounded from below by

$$E^{\mathrm{Q}}_{\mathrm{conf}}\geqslant\mathrm{Tr}[\Pi_0(H_{\mathbf{A}}-\phi^{\mathrm{STF}}-\nu)\Pi_0]_--D(\rho^{\mathrm{STF}},\rho^{\mathrm{STF}})+\nu N-1.68\int\rho_\psi^{4/3}, \tag{II.6}$$

where we have used that

$$D(\rho_\psi-\rho^{\mathrm{STF}},\rho_\psi-\rho^{\mathrm{STF}})\geqslant 0. \tag{II.7}$$

Furthermore, by (I.28) and (II.2) we get

$$E^{\mathrm{Q}}_{\mathrm{conf}} \geqslant E^{\mathrm{STF}} - \mathcal{R}_1 - 1.68 \int \rho_\psi^{4/3}, \tag{II.8}$$

with

$$\mathcal{R}_1 = \left| \frac{B}{2\pi} \int_{\mathbb{R}^2} d\mathbf{x}_\perp \left(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})} [-\partial_z^2 - \widetilde{\phi^{\mathrm{STF}}}(\mathbf{x}) - \nu]_- - \int_{\mathbb{R}^2} \frac{dz dp}{2\pi} [p^2 - \phi^{\mathrm{STF}}(\mathbf{x}) - \nu]_- \right) \right|. \tag{II.9}$$

Since ψ is a ground state wave function, or at least an approximate ground state wave function, we can estimate [cf. Ref. 1, (8.5)]

$$\int \rho_\psi^{4/3} \leqslant \left(\int \rho_\psi^3 \right)^{1/6} \left(\int \rho_\psi \right)^{5/6} \leqslant \mathrm{const}(B^2 |E^{\mathrm{STF}}|)^{1/6} N^{5/6} \leqslant \mathrm{const}\, Z^{1/5} N^{14/15} B^{2/5} \leqslant C B^{4/5} Z^{3/5}, \tag{II.10}$$

using $N \sim Z$ and $B \geqslant Z^{4/3}$.

2. Upper bound

For every fixed integer N and a normalized N-particle wave function ψ we have

$$E^{\mathrm{Q}}_{\mathrm{conf}} \leqslant (\psi, \Pi_0^N H_N \Pi_0^N \psi) = \sum_{i=1}^N (\psi, \Pi_0^N [H_A(\mathbf{x}_i) - Z|\mathbf{x}_i|^{-1} + \rho^{\mathrm{STF}} * |\mathbf{x}_i|^{-1} - \nu] \Pi_0^N \psi)$$

$$+ N\nu - 2D(\rho_\psi, \rho^{\mathrm{STF}}) + \sum_{i<j} (\psi, |\mathbf{x}_i - \mathbf{x}_j|^{-1} \psi). \tag{II.11}$$

We set

$$\psi = \frac{1}{\sqrt{N!}} \phi_1 \wedge \cdots \wedge \phi_N, \tag{II.12}$$

where ϕ_i is the eigenvector corresponding to the ith lowest eigenvalue λ_i of the one-particle operator

$$\Pi_0 (H_A - Z|\mathbf{x}|^{-1} + \rho^{\mathrm{STF}} * |\mathbf{x}|^{-1}) \Pi_0. \tag{II.13}$$

By means of the decomposition,

$$\mathrm{Tr}[\Pi_0 (H_A(\mathbf{x}) - \phi^{\mathrm{STF}}(\mathbf{x}) - \nu) \Pi_0]_- = \sum_i [\lambda_i - \nu]_- = \sum_{i=1}^N (\lambda_i - \nu) + \sum_{\lambda_N < \lambda_i < \nu} (\lambda_i - \nu), \tag{II.14}$$

and the equation (II.7) we can estimate (II.11) as

$$E^{\mathrm{Q}}_{\mathrm{conf}} \leqslant \mathrm{Tr}[\Pi_0 (H_A - \phi^{\mathrm{STF}} - \nu) \Pi_0]_- + \nu N - D(\rho^{\mathrm{STF}}, \rho^{\mathrm{STF}})$$

$$+ D(\rho_\psi - \rho^{\mathrm{STF}}, \rho_\psi - \rho^{\mathrm{STF}}) - \sum_{\lambda_N < \lambda_i < \nu} (\lambda_i - \nu), \tag{II.15}$$

which implies

$$E^{\mathrm{Q}}_{\mathrm{conf}} \leqslant \mathcal{R}_1 + R_2 + R_3, \tag{II.16}$$

with

$$R_2 = -\sum_{\lambda_N < \lambda_i < \nu} (\lambda_i - \nu), \tag{II.17}$$

$$R_3 = D(\rho_\psi - \rho^{\mathrm{STF}}, \rho_\psi - \rho^{\mathrm{STF}}). \tag{II.18}$$

Since it is difficult to tackle directly the term R_2, we estimate R_2 by $|\lambda_N - \nu|$ multiplied by the number of eigenvalues of the operator (II.13) between λ_N and ν. We know

$$\frac{B}{2\pi}\int d\mathbf{x}_\perp \int \frac{dzdp}{2\pi}\Theta_-(p^2 - \phi^{\mathrm{STF}}(\mathbf{x}) - \nu) = \int \rho^{\mathrm{STF}} = N, \tag{II.19}$$

with

$$\Theta_-(t) = \begin{cases} 1 & \text{for } t \leqslant 0, \\ 0 & \text{otherwise.} \end{cases} \tag{II.20}$$

So the number of eigenvalues of (II.13) between λ_N and ν can be expressed by

$$\mathrm{Tr}\Theta_-(\Pi_0(-\partial_z^2 - \phi^{\mathrm{STF}}(\mathbf{x}) - \nu)\Pi_0) - \frac{B}{2\pi}\int d\mathbf{x}_\perp \int \frac{dzdp}{2\pi}\Theta_-(p^2 - \phi^{\mathrm{STF}}(\mathbf{x}) - \nu). \tag{II.21}$$

Mimicking the derivation of (I.28), with $[t]_-$ being replaced by $\Theta_-(t)$, leads to

$$(\text{II.21}) = \frac{B}{2\pi}\int_{\mathbb{R}^2} d\mathbf{x}_\perp \left(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}\Theta_-(\tilde{H}_{\mathbf{x}_\perp} - \nu) - \int \frac{dzdp}{2\pi}\Theta_-(h_{\mathbf{x}_\perp} - \nu)\right), \tag{II.22}$$

where we have defined

$$\tilde{H}_{\mathbf{x}_\perp} = -\partial_z^2 - \widetilde{\phi^{\mathrm{STF}}}(\mathbf{x}) \quad \text{and} \quad h_{\mathbf{x}_\perp} = p^2 - \phi^{\mathrm{STF}}(\mathbf{x}). \tag{II.23}$$

Hence, instead of R_2 we estimate the error term

$$\mathcal{R}_2 = |\lambda_N - \nu|\frac{B}{2\pi}\int_{\mathbb{R}^2} d\mathbf{x}_\perp \left(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}\Theta_-(\tilde{H}_{\mathbf{x}_\perp} - \nu) - \int \frac{dzdp}{2\pi}\Theta_-(h_{\mathbf{x}_\perp} - \nu)\right). \tag{II.24}$$

We introduce the notation

$$e(\tilde{H}_{\mathbf{x}_\perp}, \mu) = \Theta_-(\tilde{H}_{\mathbf{x}_\perp} - \mu), \tag{II.25}$$

the projector of the operator $\tilde{H}_{\mathbf{x}_\perp}$ onto the eigenspace corresponding to the eigenvalues smaller or equal to μ. Let ψ be given by (II.12). Then we have

$$\rho_\psi(\mathbf{x}) = \frac{B}{2\pi} e(z, z; \tilde{H}_{\mathbf{x}_\perp}, \lambda_N), \tag{II.26}$$

whereas the semiclassical density ρ^{STF} can be written as

$$\rho^{\mathrm{STF}}(\mathbf{x}) = \frac{B}{2\pi}\int_{\mathbb{R}} dp\,\Theta_-(h_{\mathbf{x}_\perp} - \nu) = \frac{B}{2\pi}[\phi^{\mathrm{STF}}(\mathbf{x}) + \nu]_+^{1/2}. \tag{II.27}$$

Furthermore, we introduce the auxiliary density

$$\overline{\rho}(\mathbf{x}) = \frac{B}{2\pi}[\phi^{\mathrm{STF}}(\mathbf{x}) + \lambda_N]_+^{1/2}. \tag{II.28}$$

In order to bound the error term R_3 from above, we combine the two terms

$$\mathcal{R}_3 = D(\rho_\psi - \overline{\rho}, \rho_\psi - \overline{\rho}), \tag{II.29}$$

$$\mathcal{R}_4 = D(\rho^{\mathrm{STF}} - \overline{\rho}, \rho^{\mathrm{STF}} - \overline{\rho}), \tag{II.30}$$

which are easier to handle than R_3 alone. Observe that by convexity one has $R_3 \leqslant 2\mathcal{R}_3 + 2\mathcal{R}_4$. In the next sections we will separately have to carry out the estimations

$$\mathcal{R}_i \leqslant C B^{4/5} Z^{3/5} \quad \forall i = 1,...,4. \tag{II.31}$$

B. Methods used in the proof

The methods used here in order to estimate the error terms $\mathcal{R}_{1-4}$, have been established in Refs. 3 and 7. For the sake of better understanding we will state here the most important theorem, which we use throughout this section.

Consider the Schrödinger operator

$$H = -\tfrac{1}{2}\Delta - \phi(\mathbf{x}) \text{ on } \mathbb{R}^d. \tag{II.32}$$

Its symbol is denoted by

$$\overline{h} = \tfrac{1}{2}p^2 - \phi(\mathbf{x}). \tag{II.33}$$

In addition there are the following conditions imposed on the real potential ϕ:

There are Lipschitz functions $l(\mathbf{x}) > 0$ and $f(\mathbf{x}) > 0$, such that

$$(i) \quad |\nabla l(\mathbf{x})| \leqslant M, \tag{II.34}$$

$$(ii) \quad c f(\mathbf{y}) \leqslant f(\mathbf{x}) \leqslant C f(\mathbf{y}), \tag{II.35}$$

$$(iii) \quad |\partial^\nu \phi(\mathbf{x})| \leqslant C_\nu f(\mathbf{x})^2 l(\mathbf{x})^{-|\nu|} \forall\, \nu \in \mathbb{N}^d. \tag{II.36}$$

Under these assumptions Ivrii and Sigal have proved the following theorem:

Theorem II.1: *(Ref. 3, Theorem 7.1.): Assume conditions (i)–(iii) are obeyed and let ψ be smooth and obey $|\partial^\nu \psi(\mathbf{x})| \leqslant C_\nu l(\mathbf{x})^{-|\nu|}$ for any ν. Let $g_s(\lambda) = [-\lambda]_+^s$ for some $s \in [0,1]$. Then*

$$\left| \mathrm{Tr}(\psi g_s(H)) - \int \frac{dx dp}{2\pi} \psi g_s(\overline{h}) \right| \tag{II.37}$$

$$\leqslant C \int_{\mathrm{supp}\psi} d\mathbf{x} \max\left[\left(\frac{1}{f(\mathbf{x}) l(\mathbf{x})} \right)^{\alpha - s - d}, 1 \right] l(\mathbf{x})^{-2s-d}. \tag{II.38}$$

Here $\alpha = 1$ if either $d \geqslant 2$ or $d = 1$ and ϕ obeys

$$|\phi(\mathbf{x})| + l(\mathbf{x}) |\nabla \phi(\mathbf{x})| \geqslant \varepsilon f(\mathbf{x})^2 \tag{II.39}$$

on $\{\mathbf{x} | l(\mathbf{x}) f(\mathbf{x}) \geqslant 1\}$, with some $\varepsilon > 0$, and $\alpha = 1/2$ otherwise.

The most important tools for the proof of Theorem II.1 are multiscale analysis and semiclassical spectral asymptotics. First of all, the domain, i.e., the support of ψ, is covered by a countable number of balls. Then on each of these balls $B(\mathbf{y}, l(\mathbf{y}))$, the operator H is transformed into

$$K_h = f^{-2} U(l) H U(l)^{-1} = -\frac{h^2}{2}\Delta - V(\mathbf{x}), \tag{II.40}$$

with $h=l(\mathbf{y})^{-1}f(\mathbf{y})^{-1}$, by means of a unitary scaling transformation $U(l)$, which maps the ball $B(\mathbf{y},l(\mathbf{y}))$ into $B(0,1)$. Next Theorem 6.1 from Ref. 3, which we state below, is applied to the sum of the negative eigenvalues of $g_s(K_h)$. After rescaling and summing over all balls one arrives at Theorem II.1.

The symbol of K_h is given by

$$k(\mathbf{x},p)=p^2/2-V(\mathbf{x}). \tag{II.41}$$

If, furthermore, all derivatives of V are bounded by a constant, i.e.,

$$|\partial^\nu V(\mathbf{x})|\leqslant C_\nu \text{ on } B(0,2)\forall i, \tag{II.42}$$

then the following theorem is valid:

Theorem II.2: *Let $\psi\in C_0^\infty(B(0,1))$ and let 0 be a regular value of the function k_0 restricted to* $\mathrm{supp}\psi\times\mathbb{R}^d$. *Then for $h\leqslant 1$*

$$\mathrm{Tr}(\psi g_s(K_h))=h^{-d}\int\frac{dxdp}{2\pi}\psi g_s(k(x,p))+O(h^{s+1-d}). \tag{II.43}$$

Assume next that the potential V can be written as

$$V(\mathbf{x})=V_0(\mathbf{x})+h\overline{V}(\mathbf{x},h), \tag{II.44}$$

such that the principal symbol of K_h reads $k_0(\mathbf{x},p)=p^2/2-V_0(\mathbf{x})$. Then, if additionally $\overline{V}$ fulfills (II.42) (uniformly in h), Theorem II.2 remains valid for $s=0$ with k replaced by the principal symbol k_0. (cf. Ref. 7, Theorem 4.5.3).

Theorem II.3: *Let $\psi\in C_0^\infty(B(0,1))$ and let 0 be a regular value of the function k_0 restricted to* $\mathrm{supp}\psi\times\mathbb{R}^d$. *Then for $h\leqslant 1$*

$$\mathrm{Tr}(\psi g_0(K_h))=h^{-d}\int\frac{dxdp}{2\pi}\psi g_0(k_0(x,p))+O(h^{1-d}). \tag{II.45}$$

C. Relationship between the potentials ϕ^{STF} and $\widetilde{\phi^{\mathrm{STF}}}$

Next we collect some information about the potentials ϕ^{STF} and $\widetilde{\phi^{\mathrm{STF}}}$.

The scaling functions, which we will use in order to apply Theorem II.1 to the operator $H_{\mathbf{x}_\perp}$, have to be chosen such that the conditions (II.34)–(II.36) hold for the potentials ϕ^{STF} and $\widetilde{\phi^{\mathrm{STF}}}$, at least away from the origin.

Since we will see that ϕ^{STF} behaves like $Z|\mathbf{x}|^{-1}$ for $|\mathbf{x}|\leqslant r_S$, the edge of the STF atom, it is thus natural to define

$$l(\mathbf{x})=(\mathrm{const})|\mathbf{x}| \quad\text{and}\quad f(\mathbf{x})^2=Z|\mathbf{x}|^{-1}. \tag{II.46}$$

If we denote the effective STF potential as

$$V_{\mathrm{eff}}^{\mathrm{STF}}(\mathbf{x})=\phi^{\mathrm{STF}}(\mathbf{x})+\nu, \tag{II.47}$$

then the following lemma is valid:

Lemma II.4: (i) (Ref. 2) The density $\rho^{\mathrm{STF}}(\mathbf{x})$ as well as $[V_{\mathrm{eff}}^{\mathrm{STF}}(\mathbf{x})]_+$ have compact support with radius $r_S\leqslant 3.3\pi^2Z^{1/5}B^{-2/5}$.

(ii) For fixed but arbitrary $\mathbf{x}_\perp$, $\phi^{\mathrm{STF}}(\mathbf{x})$ and $\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})$ are $\in C^\infty(\mathbb{R}-0)$ as a function of z and

$$|\partial_z^\nu\phi^{\mathrm{STF}}(\mathbf{x})|\leqslant C_\nu f(\mathbf{x})^2 l(\mathbf{x})^{-\nu},\quad |\partial_z^\nu\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})|\leqslant C'_\nu f(\mathbf{x})^2 l(\mathbf{x})^{-\nu}, \tag{II.48}$$

for all $\nu \in \mathbb{N}$ *and* $\mathbf{x} \in \mathbb{R}^3$.

Proof: (*ii*) The C^∞ property follows from the TF equation (II.1) and the definition (I.29). Equation (II.48) follows from (II.1) and (I.29) and the fact that

$$|\partial_z^\nu Z|\mathbf{x}|^{-1}| \leqslant f(\mathbf{x})^2 |\mathbf{x}|^{-\nu} \frac{Z}{|\mathbf{x}|} \leqslant f(\mathbf{x})^2 l(\mathbf{x})^{-\nu}. \tag{II.49}$$

The proof of (*i*) is given in Ref. 2, Theorem 4.11. □

Remark II.5: The estimates (II.48) seem to be very crude, especially in the vicinity of r_S, but nevertheless they are good enough to provide precise error estimates. Next let us try to get an idea of how $V_{\text{eff}}^{\text{STF}}$ behaves in the vicinity of the radius r_S. We consider the neutral case $N=Z$. Since $V_{\text{eff}}^{\text{STF}}$ is spherical symmetric, we can make the ansatz $V_{\text{eff}}^{\text{STF}}(\mathbf{x}) = \chi(r)/r$ ($|\mathbf{x}| = r$), which leads by (II.1) to

$$\chi''(r) = B r^{1/2} \chi(r) \quad \text{and} \quad \chi(0) = Z. \tag{II.50}$$

Around each point r_0, this equation has a solution χ that can be expanded in a series of terms $c_i[r_0 - r]^i$ with $i \geqslant 4$. In the vicinity of $r_0 = r_S$ we get the approximate solution

$$V_{\text{eff}}^{\text{STF}} \sim \frac{Z^{1/5} B^{8/5}}{r} [r_S - r]_+^4, \tag{II.51}$$

which shows that $V_{\text{eff}}^{\text{STF}}$ tends to 0 as $[r_S - r]_+^4$ as $r \to r_S$.

Next we fix a point $\mathbf{y} \in \mathbb{R}^3$ and we set $l = l(\mathbf{y})$ and $f = f(\mathbf{y}) = Z^{1/2}|\mathbf{y}|^{1/2}$. (We assume that (II.34)–(II.36) are fulfilled in $B(\mathbf{y}, l(\mathbf{y}))$. This in our case can be done by defining $l(\mathbf{y})$, e.g., as $|\mathbf{y}|/2$.) Furthermore, we define the unitary transformation

$$U(l): \psi(\mathbf{x}) \to l^{3/2} \psi(l\mathbf{x} + \mathbf{y}), \tag{II.52}$$

which maps the ball $B(\mathbf{y}, l(\mathbf{y}))$ to $B(0,1)$ and transforms the operator $-\partial_z^2 - \widetilde{\phi^{\text{STF}}}$ into

$$-l^{-2}\partial_z^2 - \widetilde{\phi^{\text{STF}}}(l\mathbf{x} + \mathbf{y}). \tag{II.53}$$

Introduce the new potential

$$\tilde{W}(\mathbf{x}) = f^{-2} \widetilde{\phi^{\text{STF}}}(l\mathbf{x} + \mathbf{y}). \tag{II.54}$$

The resulting operator is related to the original one (II.23) as

$$U(l) \tilde{H}_{\mathbf{x}_\perp} U(l)^{-1} = f^2 \tilde{K}_h, \tag{II.55}$$

with

$$\tilde{K}_h = -h^2 \partial_z^2 - \tilde{W}(\mathbf{x}) \quad \text{and} \quad h = (lf)^{-1}. \tag{II.56}$$

If we denote $W(\mathbf{x}) = f^{-2}\phi^{\text{STF}}(l\mathbf{x} + \mathbf{y})$, then one easily sees that $\tilde{W}$ can equivalently be defined by applying (I.29), i.e., the operation $\tilde{\cdot}$, to W, with B replaced by $B' = Bl^2$. In other words the unitary transformation $U(l)$ scales the magnetic field strength B to $B' = Bl^2$ and for the difference $\tilde{W} - W$ we get the following lemma.

Lemma II.6: There exists a function $a(\mathbf{x}, \alpha)$ *such that*

$$\tilde{W}(\mathbf{x}) - W(\mathbf{x}) = \alpha a(\mathbf{x}, \alpha), \tag{II.57}$$

where $\alpha = B^{-1/2} l^{-1}$ *and* $a(\mathbf{x}, \alpha)$ *fulfills (II.42) uniformly in* α *for* $\alpha \leqslant 1$.

Proof: Since the potential ϕ^{STF} is spherically symmetric and Eq. (II.48) is fulfilled for derivatives in all directions, we get for $\mathbf{x}\in B(0,2)$

$$|\partial^\nu W(\mathbf{x})| = |f^{-2}\partial^\nu \phi^{\mathrm{STF}}(l\mathbf{x}+\mathbf{y})| \leqslant C_\nu \text{ for all } \quad \nu \in \mathbb{N}^3. \tag{II.58}$$

Hence, $W(\mathbf{x})$, together with all derivatives, is bounded above by a constant on a ball around $\mathbf{x}=0$. Since the operation $\tilde{\cdot}$ smears the potential, for every $\mathbf{x}$, over a region $\sim\alpha$ in the $|\mathbf{x}_\perp|$-direction, the difference $\widetilde{W}-W$ can be expressed by α times a function $a(\mathbf{x},\alpha)$ which is bounded by a constant. Since $\widetilde{\partial_z^n W}(\mathbf{x}) = \partial_z^n \widetilde{W}(\mathbf{x})$ the same argument can be given for all derivatives. □

Let us rewrite the operator K_h in the form

$$K_h = -h^2\partial_z^2 - (W(\mathbf{x}) + \alpha a(\mathbf{x},\alpha)). \tag{II.59}$$

In order to be allowed to apply Theorem II.3 to (II.59), i.e., in order to guarantee that $p^2 - W(x)$ is the principal symbol of K_h, it is necessary, that

$$\alpha \leqslant h \Leftrightarrow B^{-1/2} l^{-1} \leqslant l^{-1} f^{-1}, \tag{II.60}$$

which leads to the condition

$$|\mathbf{y}| \geqslant Z/B. \tag{II.61}$$

Hence, in the sense of Theorem II.3, this implies that in the region $\{\mathbf{x}|\,|\mathbf{x}|\geqslant Z/B\}$ Theorem II.1, with $s=0$, can be applied to the error terms $\mathcal{R}_{2-4}$, with $\widetilde{\phi^{\mathrm{STF}}}$ replaced by ϕ^{STF}. Next we decompose $\mathbb{R}^3$ into $\Omega_1=\{\mathbf{x}||\mathbf{x}|\leqslant Z/B\}$ and $\Omega_2=\{\mathbf{x}|\,|\mathbf{x}|\geqslant Z/B\}$ and estimate the error terms $\mathcal{R}_{1-4}$ on each of these regions separately.

D. Analysis in the region Ω_1

We first assume that $B<Z^2$. This assumption is made in order to be sure that Ω_1 is not completely contained in the non-semiclassical region $\{\mathbf{x}||\mathbf{x}|\leqslant 1/Z\}$, where each term, the quantum mechanical as well as the semiclassical, has to be estimated separately. Furthermore, let $\psi^{(1)}(\mathbf{x})$ be supported in $\{\mathbf{x}|0\leqslant|\mathbf{x}|\leqslant Z/B(1+\epsilon)\}$ and fulfill $\psi^{(1)}(\mathbf{x})=1$ in $\{\mathbf{x}||\mathbf{x}|\leqslant(Z/B)(1-\epsilon)\}$, as well as $|\partial_z^n\psi^{(1)}|\leqslant C_n l(\mathbf{x})^{-n}$ for all $n\in\mathbb{N}$.

With respect to $\mathcal{R}_1$ and $\mathcal{R}_2$, we in particular have to estimate the term

$$\frac{B}{2\pi}\int d\mathbf{x}_\perp \left(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}(\psi^{(1)} g_s(\widetilde{H}_{\mathbf{x}_\perp}-\nu)) - \int \frac{dzdp}{2\pi}\psi^{(1)} g_s(h_{\mathbf{x}_\perp}-\nu)\right), \tag{II.62}$$

with $\widetilde{H}_{\mathbf{x}_\perp}$ and $h_{\mathbf{x}_\perp}$ given by (II.23). Let $\widetilde{h}_{\mathbf{x}_\perp}$ be defined analogously, i.e., $\widetilde{h}_{\mathbf{x}_\perp}=p^2-\widetilde{\phi^{\mathrm{STF}}}$. Adding and subtracting $\int (dzdp/2\pi)\,\psi^{(1)} g_s(\widetilde{h}_{\mathbf{x}_\perp}-\nu)$ in (II.62), we split (II.62) into

$$R_1^s(\psi^{(1)}) = \frac{B}{2\pi}\int d\mathbf{x}_\perp \left(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}(\psi^{(1)} g_s(\widetilde{H}_{\mathbf{x}_\perp}-\nu)) - \int \frac{dzdp}{2\pi}\psi^{(1)} g_s(\widetilde{h}_{\mathbf{x}_\perp}-\nu)\right) \tag{II.63}$$

and the fully semiclassical part

$$R_2^s(\psi^{(1)}) = \frac{B}{2\pi}\int d\mathbf{x}_\perp \left(\int \frac{dzdp}{2\pi}\psi^{(1)} g_s(\widetilde{h}_{\mathbf{x}_\perp}-\nu) - \int \frac{dzdp}{2\pi}\psi^{(1)} g_s(h_{\mathbf{x}_\perp}-\nu)\right). \tag{II.64}$$

Since $l(\mathbf{x})f(\mathbf{x})\geqslant 1$, which is equivalent to $|\mathbf{x}|\geqslant Z^{-1}$, is necessary for being able to apply Theorem II.1, we have to carry out a corresponding decomposition of Ω_1. Let $\psi_1^{(1)}+\psi_2^{(1)}=\psi^{(1)}$ be a partition of unity on Ω_1, with

$$\text{supp } \psi_1^{(1)}=\{\mathbf{x}||\mathbf{x}|\leqslant Z^{-1}(1+\epsilon)\},\ \ \text{supp } \psi_2^{(1)}=\{\mathbf{x}|Z^{-1}(1-\epsilon)\leqslant|\mathbf{x}|\leqslant Z/B(1+\epsilon)\},\quad \text{(II.65)}$$

and $|\partial_z^n\psi_i^{(1)}|\leqslant C_n l(\mathbf{x})^{-n}$ for $i=1,2$, with C_n independent of Z and B.

Lemma II.7: With the above definitions we have for (II.63)

$$R_1^s(\psi^{(1)})\leqslant CB^{(3/2)s-1}Z^{2-(1/2)s}. \quad \text{(II.66)}$$

Proof: On supp $\psi_2^{(1)}$ we apply Theorem II.1 to (II.62) with $\alpha=1$ and $d=1$, which implies for arbitrary but fixed $\mathbf{x}_\perp$ (we may set the chemical potential $\nu=0$ for simplicity; the computations for arbitrary ν are essentially the same)

$$\left|\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}(\psi_2^{(1)}g_s(\tilde{H}_{\mathbf{x}_\perp}))-\int\frac{dzdp}{2\pi}\psi_2^{(1)}g_s(\tilde{h}_{\mathbf{x}_\perp})\right|\leqslant C\int_{\mathrm{supp}\psi_2^{(1)}(\mathbf{x}_\perp,z)}dzl(\mathbf{x})^{-1-s}f(\mathbf{x})^s. \quad \text{(II.67)}$$

Hence, multiplying with $B/2\pi$ and integrating over $\mathbf{x}_\perp$ leads to

$$R_1^s(\psi^{(1)})\leqslant C\frac{B}{2\pi}\int d\mathbf{x}l(\mathbf{x})^{-1-s}f(\mathbf{x})^s\leqslant BZ^{(1/2)s}\int_{Z^{-1}}^{Z/B}r^{1-(3/2)s}dr\leqslant CB^{(3/2)s-1}Z^{2-(1/2)s}. \quad \text{(II.68)}$$

In the case of $r\leqslant Z^{-1}$ the terms of (II.63) have to be estimated separately. The semiclassical part reads

$$\frac{B}{2\pi}\int\frac{d\mathbf{x}dp}{2\pi}\psi_1^{(1)}[\tilde{h}_{\mathbf{x}_\perp}]_-^{1/2+s}\leqslant\frac{B}{2\pi}\int_{|\mathbf{x}|\leqslant Z^{-1}}d\mathbf{x}[\widetilde{\phi^{\mathrm{STF}}}]_+^{1/2+s}\leqslant CBZ^{2s-2}. \quad \text{(II.69)}$$

An analogous estimate is derived for $(B/2\pi)\int d\mathbf{x}_\perp\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}(\psi_1^{(1)}g_s(\tilde{H}_{\mathbf{x}_\perp}))$ by using Ref. 3, Lemma 7.9. □

Lemma II.8: For (II.64) we have

$$R_2^s(\psi^{(1)})\leqslant CZ^{s+1/2}B^{s/2-1/4}. \quad \text{(II.70)}$$

Proof: Obviously, the main contribution to the magnitude of the semiclassical term

$$R_2^s(\psi^{(1)})\leqslant\frac{B}{2\pi}\int_{\mathbb{R}^3}d\mathbf{x}\psi^{(1)}|[\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})]_+^{s+1/2}-[\phi^{\mathrm{STF}}(\mathbf{x})]_+^{s+1/2}| \quad \text{(II.71)}$$

is produced by the Coulomb singularity, i.e.,

$$R_2^s(\psi^{(1)})\leqslant\frac{B}{2\pi}\int_{|\mathbf{x}|\leqslant B^{-1/2}}d\mathbf{x}|\phi^{\mathrm{STF}}(\mathbf{x})|_+^{s+1/2} \quad \text{(II.72)}$$

$$\leqslant CB\int_{|\mathbf{x}|\leqslant B^{-1/2}}d\mathbf{x}\left(\frac{Z}{r}\right)^{s+1/2}$$

$$\leqslant CZ^{s+1/2}B^{s/2-1/4}. \quad \text{(II.73)}$$

□

Hence, we are ready to carry out the estimate of the error terms $\mathcal{R}_{1-4}$, restricted to Ω_1, which we denote as $\mathcal{R}_i(\Omega_1)$.

Proposition II.9: For $Z^{4/3}\leqslant B\leqslant Z^3$ one has

$$\mathcal{R}_1(\Omega_1)=\frac{B}{2\pi}\int_{\mathbb{R}^2}d\mathbf{x}_\perp\left(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}(\psi^{(1)}[\tilde{H}_{\mathbf{x}_\perp}-\nu]_-)-\int\frac{dzdp}{2\pi}\psi^{(1)}[h_{\mathbf{x}_\perp}-\nu]_-\right)\leqslant CB^{4/5}Z^{3/5}. \quad \text{(II.74)}$$

Proof: This is done by putting together Lemmas II.7 and II.8 and setting $s=1$. □

Before turning to $\mathcal{R}_2(\Omega_1)$ we need a preparing lemma.

Lemma II.10: Let λ_N be the Nth eigenvalue of (II.13) and ν the chemical potential of (II.1) belonging to the electron number N. Then

$$|\lambda_N-\nu|\leqslant CB^{3/5}Z^{1/5}. \tag{II.75}$$

Proof: We assume now that we already have the estimate

$$\left|\mathrm{Tr}\Theta_-(\Pi_0(-\partial_z^2-\phi^{\mathrm{STF}})\Pi_0)-\frac{B}{2\pi}\int d\mathbf{x}_\perp\int\frac{dzdp}{2\pi}\Theta_-(p^2-\phi^{\mathrm{STF}})\right|\leqslant CB^{1/5}Z^{2/5}, \tag{II.76}$$

which until now we have only proven on Ω_1, by setting $s=0$ in Lemmas II.7 and II.8. The missing part will be proved in Lemma II.16. Since we know by definition

$$\frac{B}{2\pi}\int_{\mathbb{R}^2}d\mathbf{x}_\perp\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}\Theta_-(\tilde{H}_{\mathbf{x}_\perp}-\lambda_N)=N=\frac{B}{2\pi}\int d\mathbf{x}[\phi^{\mathrm{STF}}(\mathbf{x})+\nu]_+^{1/2}, \tag{II.77}$$

we get

$$B^{1/5}Z^{2/5}\geqslant\frac{B}{2\pi}\int d\mathbf{x}([\phi^{\mathrm{STF}}+\lambda_N]_+^{1/2}-[\phi^{\mathrm{STF}}+\nu]_+^{-1/2}) \tag{II.78}$$

$$\geqslant C|\lambda_N-\nu|B\int_0^{r_S}[\phi^{\mathrm{STF}}+\nu']_+^{-1/2}r^2dr$$

$$\geqslant C|\lambda_N-\nu|(BZ^{-1/2}r_S^{7/2}), \tag{II.79}$$

for some $\nu'\in[\nu,\lambda_N]$. This implies the statement of the lemma. □

Proposition II.11:

$$\mathcal{R}_2(\Omega_1)=\left|\lambda_N-\nu\left|\frac{B}{2\pi}\right|\int_{\mathbb{R}^2}d\mathbf{x}_\perp(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}(\psi^{(1)}\Theta_-(\tilde{H}_{\mathbf{x}_\perp}-\nu))\right| \tag{II.80}$$

$$-\int\frac{dzdp}{2\pi}\psi^{(1)}\Theta_-(h_{\mathbf{x}_\perp}-\nu))\Bigg|$$

$$\leqslant CB^{4/5}Z^{3/5}. \tag{II.81}$$

Proof: By Lemma II.10 and combining the estimations of Lemmas II.7 and II.8 with $s=0$.□

Remarki II.12: We remark here that if one has a partition of unity $\varphi_1+\varphi_2=1$, then the relation

$$D(f,f)\leqslant 2D(f\varphi_1,f\varphi_1)+2D(f\varphi_2,f\varphi_2) \tag{II.82}$$

is valid, which one gets by the simple inequality

$$D(f\varphi_1-f\varphi_2,f\varphi_1-f\varphi_2)\geqslant 0. \tag{II.83}$$

Remark II.12 justifies the notations $\mathcal{R}_3(\Omega_i),\mathcal{R}_4(\Omega_i)$, since (II.82) means that we can consider each region Ω_i separately.

Proposition II.13: For $Z^{4/3}\leqslant B\leqslant Z^3$ we get with (II.28)

$$\mathcal{R}_4(\Omega_1)=D(\psi^{(1)}(\rho^{\mathrm{STF}}-\overline{\rho}),\psi^{(1)}(\rho^{\mathrm{STF}}-\overline{\rho}))\leqslant CB^{4/5}Z^{3/5}. \tag{II.84}$$

Proof: Recall

$$\rho^{\mathrm{STF}}=\frac{B}{2\pi}[\phi^{\mathrm{STF}}+\nu]_+^{1/2} \text{ and } \overline{\rho}=[\phi^{\mathrm{STF}}+\lambda_N]_+^{1/2}. \tag{II.85}$$

By the Hardy–Littlewood–Sobolev inequality we derive

$$\begin{aligned}\mathcal{R}_4(\Omega_1)&=D(\psi^{(1)}(\rho^{\mathrm{STF}}-\overline{\rho}),\psi^{(1)}(\rho^{\mathrm{STF}}-\overline{\rho}))\\&\leqslant CB^2\|\psi^{(1)}(\rho^{\mathrm{STF}}-\overline{\rho})\|_{6/5}^2\\&\leqslant CB^2|\lambda_N-\nu|^2\|\psi^{(1)}(\phi^{\mathrm{STF}}+\nu')^{-1/2}\|_{6/5}^2\\&\leqslant Z^{27/5}B^{-14/5}.\end{aligned} \tag{II.86}$$

□

In the case of $\mathcal{R}_3(\Omega_1)$ we proceed as above, namely we introduce the auxiliary density $\tilde{\rho}(\mathbf{x})=(B/2\pi)[\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})+\lambda_N]_+^{1/2}$ and decompose $\mathcal{R}_3(\Omega_1)$ by using convexity.

Proposition II.14: For $Z^{4/3}\leqslant B\leqslant Z^3$ we have

$$\mathcal{R}_3(\Omega_1)=D(\psi^{(1)}(\rho^{\mathrm{STF}}-\rho_\psi),\psi^{(1)}(\rho^{\mathrm{STF}}-\rho_\psi))\leqslant CB^{4/5}Z^{3/5}. \tag{II.87}$$

Proof: By decomposition we have, on the one hand, the fully semiclassical and easier to handle part

$$\mathcal{R}_4(\Omega_1)=D(\psi^{(1)}(\rho^{\mathrm{STF}}-\tilde{\rho}),\psi^{(1)}(\rho^{\mathrm{STF}}-\tilde{\rho}))\leqslant B^2\|\psi^{(1)}(\rho^{\mathrm{STF}}-\tilde{\rho})\|_{6/5}^2\leqslant B^{4/5}Z^{3/5}. \tag{II.88}$$

On the other hand, there is the more interesting term

$$D(\psi^{(1)}(\rho_\psi-\tilde{\rho}),\psi^{(1)}(\rho_\psi-\tilde{\rho})). \tag{II.89}$$

For $r\leqslant Z^{-1}$ we separately calculate

$$\left(\frac{B}{2\pi}\right)^2 D(\psi_1^{(1)}e(z,z;\tilde{H}_{\mathbf{x}_\perp},\lambda_N),\psi_1^{(1)}e(z,z;\tilde{H}_{\mathbf{x}_\perp},\lambda_N))\leqslant CB^2\|\psi_1^{(1)}e(z,z;\tilde{H}_{\mathbf{x}_\perp},\lambda_N)\|_{6/5}^2 \tag{II.90}$$

and

$$\left(\frac{B}{2\pi}\right)^2 D(\psi_1^{(1)}[\widetilde{\phi^{\mathrm{STF}}}+\lambda_N]_+^{1/2},\psi_1^{(1)}[\widetilde{\phi^{\mathrm{STF}}}+\lambda_N]_+^{1/2})\leqslant CB^2\|\psi_1^{(1)}[\widetilde{\phi^{\mathrm{STF}}}+\lambda_N]_+^{1/2}\|_{6/5}^2. \tag{II.91}$$

Whereas (II.91) can be bounded by

$$CB^2\|\psi_1^{(1)}[Z/|\mathbf{x}|]^{1/2}\|_{6/5}^2\leqslant CB^2/Z^3, \tag{II.92}$$

(II.90) can analogously be estimated by Ref. 3, Lemma 10.7, or Ref. 4, Proposition 4.3.

The term

$$D(\psi_2^{(1)}(\rho_\psi-\tilde{\rho}),\psi_2^{(1)}(\rho_\psi-\tilde{\rho})) \tag{II.93}$$

is a bit more delicate. We can either use Ref. 4, Proposition 4.3, or Ref. 7, Theorem 4.5.4(i), which states that for K_h, given in (II.40), with V fulfilling (II.42) and $|V(\mathbf{x})+\tau|\geqslant\epsilon$,

$$\left|e(x,x;K_h,\tau)-h^{-d}\int\Theta_-(k(\mathbf{x},p)-\tau)\right|\leqslant h^{1-d}\quad\forall\mathbf{x}\in B\left(0,\frac{1}{2}\right). \tag{II.94}$$

Since $|\lambda_N|\leqslant B^{3/5}Z^{1/5}$, we get that $|\widetilde{\phi^{\mathrm{STF}}}+\lambda_N|\geqslant\epsilon f(\mathbf{x})^2$ in Ω_1. Hence, we can apply (II.94) to our case, with $d=1$, yielding

$$|e(z,z;\tilde{H}_{\mathbf{x}_\perp},\lambda_N)-[\widetilde{\phi^{\mathrm{STF}}}(\mathbf{x})+\lambda_N]_+^{1/2}|\leqslant l(\mathbf{x})^{-1}. \tag{II.95}$$

The term l^{-1} stems from rescaling $B(0,1)$ to $B(0,l)$. So,

$$D(\psi_2^{(1)}(\rho_\psi-\tilde{\rho}),\psi_2^{(1)}(\rho_\psi-\tilde{\rho}))\leqslant CB^2\|\psi_2^{(1)}l(\mathbf{x})^{-1}\|_{6/5}^2\leqslant CB^2[Z/B]^3. \tag{II.96}$$

□

In the case $B\geqslant Z^2$, Z/B is smaller than $1/Z$ and in the above calculations only the separate terms have to be taken into account, which yields analog estimates as above.

E. Analysis in the outer region Ω_2

This region has already been treated by Ivrii in Ref. 4, Sec. 4.

Recall first that r_S is the radius of the support of ϕ^{STF}, in the neutral case, and of $[\phi^{\mathrm{STF}}+\nu]_+$ otherwise. In order that Theorem II.1 can be applied ϕ^{STF} and $\widetilde{\phi^{\mathrm{STF}}}$ have to fulfill condition (II.39). We know that $\nabla\phi^{\mathrm{STF}}(r_S)=\phi^{\mathrm{STF}}(r_S)=0$. Hence, we look for a parameter $0<c<1$, and the concerning radius cr_S, such that the separate quantum mechanical as well as semiclassical parts of $\mathcal{R}_{1-4}$ in $\{\mathbf{x}||\mathbf{x}|\geqslant cr_S\}$ do not exceed $CB^{4/5}Z^{3/5}$ and that ϕ^{STF} fulfills (II.39). The existence of such a c is a consequence of the behavior of ϕ^{STF} in the vicinity of r_S [cf. (II.51)]. By means of such a parameter c we decompose the outer region Ω_2 into $\Omega_2^1\cup\Omega_2^2$ and define a concerning partition of unity, i.e.,

$$\mathrm{supp}\,\psi_1^{(2)}=\{\mathbf{x}|\,[Z/B](1+\epsilon)\leqslant|\mathbf{x}|\leqslant cr_S\},\quad \mathrm{supp}\,\psi_2^{(2)}=\{\mathbf{x}|\,|\mathbf{x}|\geqslant cr_S(1-\epsilon)\}, \tag{II.97}$$

with $\psi_1^{(2)}+\psi_2^{(2)}=1$ for $r\geqslant[Z/B](1+\epsilon)$. On Ω_2^2, by definition, all terms separately are bounded above by $CB^{4/5}Z^{3/5}$ and on Ω_2^1 condition (II.39) is fulfilled for ε small enough.

Throughout this section we assume $Z^{4/3}\leqslant B\leqslant Z^3$.

Proposition II.15:

$$\mathcal{R}_1(\Omega_2^1)\leqslant CB^{4/5}Z^{3/5}. \tag{II.98}$$

Proof: First we assume $B<Z^2$. Applying Theorem II.1 with $\alpha=1$ and $d=1$ we get for arbitrary but fixed $\mathbf{x}_\perp$ (we set $\nu=0$)

$$\left|\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}(\psi_1^{(2)}g_1(\tilde{H}_{\mathbf{x}_\perp}))-\int\frac{dzdp}{2\pi}\psi_1^{(2)}g_1(\tilde{h}_{\mathbf{x}_\perp})\right|\leqslant C\int_{\mathrm{supp}\psi_1^{(2)}(\mathbf{x}_\perp,z)}dzl(\mathbf{x})^{-2}f(\mathbf{x}). \tag{II.99}$$

After multiplying with B and integrating over $\mathbf{x}_\perp$ we get

$$(\mathrm{II.99})\leqslant C\frac{B}{2\pi}\int d\mathbf{x}l(\mathbf{x})^{-2}f(\mathbf{x})\leqslant CBZ^{1/2}\int_{Z/B}^{cr_S}r^{-1/2}dr\leqslant CBZ^{1/2}[r_S]^{1/2}. \tag{II.100}$$

In the case of $B>Z^2$ we again have to decompose Ω_2^1, since Z/B is smaller than $1/Z$. So for fixed but arbitrary B, Ω_2^1 is decomposed with respect to $r=1/Z$. For $r\leqslant 1/Z$ we proceed as in the previous section and estimate each term separately and for $r\geqslant 1/Z$ we immediately arrive at (II.100).

The pure semiclassical part

$$\frac{B}{2\pi}\int d\mathbf{x}_\perp\left(\int\frac{dzdp}{2\pi}\psi^{(2)}g_1(\tilde{h}_{\mathbf{x}_\perp}-\nu)-\int\frac{dzdp}{2\pi}\psi^{(2)}g_1(h_{\mathbf{x}_\perp}-\nu)\right) \tag{II.101}$$

can analogously be estimated as in Lemma II.8 □

Denote

$$R^0(\psi_1^{(2)}) = \frac{B}{2\pi}\int d\mathbf{x}_\perp \left(\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}(\psi_1^{(2)}\Theta_-(\tilde{H}_{\mathbf{x}_\perp}-\nu)) - \int \frac{dzdp}{2\pi}\psi_1^{(2)}\Theta_-(h_{\mathbf{x}_\perp}-\nu)\right). \tag{II.102}$$

Lemma II.16:

$$R^0(\psi_1^{(2)}) \leqslant CB^{1/5}Z^{2/5}. \tag{II.103}$$

Proof: As in Proposition II.15 we first assume $B<Z^2$. The other case, where the terms have to be computed separately, works as in Lemma II.7. Applying Theorem II.1 with $\alpha=1$ and $d=1$ we get for arbitrary but fixed $\mathbf{x}_\perp$ (we set $\nu=0$)

$$\left| \mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}(\psi_1^{(2)}\Theta_-(\tilde{H}_{\mathbf{x}_\perp})) - \int \frac{dzdp}{2\pi}\psi_1^{(2)}\Theta_-(h_{\mathbf{x}_\perp}) \right| \leqslant C\int_{\mathrm{supp}\psi_1^{(2)}(\mathbf{x}_\perp,z)} dz\, l(\mathbf{x})^{-1}. \tag{II.104}$$

This implies

$$R^0(\psi_1^{(2)}) \leqslant C\frac{B}{2\pi}\int d\mathbf{x} l(\mathbf{x})^{-1} \leqslant CB\int_{Z/B}^{cr_S} r\,dr \leqslant CB[r_S]^2. \tag{II.105}$$

□

Proposition II.17:

$$\mathcal{R}_2(\Omega_2^1) \leqslant CB^{4/5}Z^{3/5}. \tag{II.106}$$

Proof: Note that by the Lemmas II.7, II.8 and II.16 the estimate (II.76) is proved and the assumption of Lemmas II.10 justified. So by Lemmas II.10 and II.16 we arrive at (II.106). □

Proposition II.18:

$$\mathcal{R}_4(\Omega_2^1), \mathcal{R}_3(\Omega_2^1) \leqslant CB^{4/5}Z^{3/5}. \tag{II.107}$$

Proof: Let us start with

$$\mathcal{R}_4(\Omega_2^1) = D(\psi_1^{(2)}(\rho^{\mathrm{STF}}-\overline{\rho}), \psi_1^{(2)}(\rho^{\mathrm{STF}}-\overline{\rho})). \tag{II.108}$$

By the HLS inequality we get

$$\mathcal{R}_4(\Omega_2^1) \leqslant CB^2 \|\psi_1^{(2)}(\rho^{\mathrm{STF}}-\overline{\rho})\|_{6/5}^2 \leqslant CB^2|\lambda_N-\nu|^2\|\psi_1^{(2)}(\phi^{\mathrm{STF}}+\nu)^{-1/2}\|_{6/5}^2 \leqslant CB^{4/5}Z^{3/5}. \tag{II.109}$$

The term

$$\mathcal{R}_3(\Omega_2^1) = D(\psi_1^{(2)}(\rho^{\mathrm{STF}}-\rho_\psi), \psi_1^{(2)}(\rho^{\mathrm{STF}}-\rho_\psi)) \tag{II.110}$$

is a bit more delicate and we refer to Ref. 4 Propositions 4.2 and 4.3, for a proof of the estimate (II.107).

Note: Proposition 4.3 in Ref. 4 is proved for region $\chi_4=\{\mathbf{x}||\mathbf{x}|\geqslant C_0Z/B\}$ with possibly a very large parameter C_0. This parameter C_0 is chosen in a way such that only the lowest Landau band contributes to Ivrii's calculations. Since we only treat the lowest Landau band case, the assertion of Proposition 4.3 holds in our case on the whole region Ω_2^1.

Furthermore, we remark that if (II.95) would be valid on Ω_2^1, we could immediately conclude by the HLS inequality that $\mathcal{R}_4(\Omega_2^1) \leqslant CB^2[r_S]^3$. But since the validity of (II.95) cannot be guaranteed on Ω_2^1, we have to refer to Ivrii's method. □

Recall that we have made a partition of unity, $\Sigma_{i,j=1}^2 \psi_j^{(i)}(\mathbf{x})=1$. So, collecting all estimations of the Secs. II D and II E, we have finished the proof of Theorem I.3.

III. SEMICLASSICAL THEORIES APPROXIMATING E^{Q}_{conf}

As we have already argued throughout the introduction, the natural semiclassical approximation of E^{Q}_{conf} is given by the DSTF functional

$$\mathcal{E}^{\mathrm{DSTF}}[\rho]=\sum_{m\in\mathbb{N}_0}\left(\kappa\int\rho_m(z)^3-Z\int V_m(z)\rho_m(z)dz\right)+\overline{D}(\rho,\rho). \tag{III.1}$$

Here ρ is a sequence of one-dimensional densities $\rho=(\rho_m(z))_{m\in\mathbb{N}_0}$. Contrary to the usual STF theory, the integration over the variables orthogonal to the magnetic field is replaced by an expansion in angular momentum eigenfunctions in the lowest Landau band. The potentials V_m and $\overline{D}$ are defined in (I.35). The corresponding energy is given by

$$E^{\mathrm{DSTF}}(N,Z,B)=\inf\left\{\mathcal{E}^{\mathrm{DSTF}}[\rho]\,\middle|\,\rho\in\mathcal{D}\ \text{ and }\ \sum_m\int\rho_m\leqslant N\right\}, \tag{III.2}$$

with

$$\mathcal{D}=\left\{\rho\,\middle|\sum_m\int\rho_m^3<\infty,\sum_m\int V_m\rho_m<\infty,\widetilde{D}(\rho,\rho)<\infty\right\}. \tag{III.3}$$

Another semiclassical approximation, where the variables, as in the usual STF theory, are three dimensional densities, is realized by the MSTF functional

$$\mathcal{E}^{\mathrm{MSTF}}[\rho]=\frac{4\pi^4}{3B^2}\int d\mathbf{x}\rho^3(\mathbf{x})-\int d\mathbf{x}\widetilde{|\mathbf{x}|^{-1}}\rho(\mathbf{x})+\widetilde{D}(\rho,\rho), \tag{III.4}$$

with respective energy

$$E^{\mathrm{MSTF}}(N,Z,B)=\inf\left\{\mathcal{E}^{\mathrm{MSTF}}[\rho]\,\middle|\,\rho\in\widetilde{\mathcal{D}}\ \text{ and }\ \int\rho\leqslant N\right\}, \tag{III.5}$$

where

$$\widetilde{\mathcal{D}}=\left\{\rho\,\middle|\,\rho\in\mathcal{L}^3(\mathbb{R}^3),\int\widetilde{|x|^{-1}}\rho<\infty,\widetilde{D}(\rho,\rho)<\infty\right\}. \tag{III.6}$$

First of all, we will show that these two functionals are equivalent.

Lemma III.1: For all $\rho\in\widetilde{\mathcal{D}}$ let

$$\overline{\rho}(\mathbf{x})=\frac{B}{2\pi}\sum_m\chi_m(\mathbf{x}_\perp)\rho_m(z), \tag{III.7}$$

with $\rho_m(z)=\int\rho(\mathbf{x})\chi_m(\mathbf{x}_\perp)d\mathbf{x}_\perp$, and denote $\tilde{\rho}=(\rho_m)_m$. Then one gets

$$\mathcal{E}^{\mathrm{MSTF}}[\rho]\geqslant\mathcal{E}^{\mathrm{MSTF}}[\overline{\rho}]=\mathcal{E}^{\mathrm{DSTF}}[\tilde{\rho}]. \tag{III.8}$$

Proof: By the definition of the MSTF functional, it suffices to show that $\int\rho^3\geqslant\int\overline{\rho}^3$.

For this purpose we note that for every non-negative function f, on a general measure space, one derives from convexity that

$$\frac{1}{\mu(\Omega)}\int f^3d\mu\geqslant\left(\int\frac{1}{\mu(\Omega)}fd\mu\right)^3. \tag{III.9}$$

Hence for every $m\in\mathbb{N}$ and $z\in\mathbb{R}$, we have

$$\frac{1}{|\chi_m|}\int_{\mathrm{supp}\chi_m}\rho(\mathbf{x})^3\chi_m(\mathbf{x}_\perp)d\mathbf{x}_\perp \geqslant \left(\frac{1}{|\chi_m|}\int \rho(\mathbf{x})\chi_m(\mathbf{x}_\perp)d\mathbf{x}_\perp\right)^3. \tag{III.10}$$

Since $|\chi_m| = 2\pi/B$, we arrive at

$$\frac{4\pi^4}{3B^2}\int \rho(\mathbf{x})^3 d\mathbf{x} \geqslant \frac{\pi^2}{3}\sum_m \int \rho_m(z)^3 dz = \frac{4\pi^4}{3B^2}\int \overline{\rho}(\mathbf{x})^3 d\mathbf{x}. \tag{III.11}$$

□

Proposition III.2: For all N,Z,B

$$E^{\mathrm{MSTF}}(N,Z,B) = E^{\mathrm{DSTF}}(N,Z,B). \tag{III.12}$$

Proof: Lemma III.1 immediately implies

$$E^{\mathrm{MSTF}}(N,Z,B) = \inf\left\{\mathcal{E}^{\mathrm{MSTF}}[\rho]\,\middle|\,\rho = \frac{B}{2\pi}\sum_m \rho_m(z)\chi_m(\mathbf{x}_\perp), (\rho_m)_m \in \mathcal{D}\right\}. \tag{III.13}$$

□

For simplicity we first concentrate on the DSTF functional and then apply our results to the MSTF functional.

Lemma III.3: $\mathcal{E}^{\mathrm{DSTF}}[\rho]$ is uniformly bounded from below on $\mathcal{D}$. There exists even a positive constant α and a C, such that

$$\mathcal{E}^{\mathrm{DSTF}}[\rho] \geqslant \alpha\left(\sum_m \int \rho_m^3 + \overline{D}(\rho,\rho)\right) - C \tag{III.14}$$

for all $\rho \in \mathcal{D}$.

Proof: We set $\rho(\mathbf{x}) = \Sigma_m \rho_m(z)|\phi_m(\mathbf{x}_\perp)|^2$ for an arbitrary $(\rho_m)_m \in \mathcal{D}$. We get from Ref. 8, Lemma 2, that for every $\varepsilon > 0$ there exists a C_ε, such that

$$\int |\mathbf{x}|^{-1}\rho \leqslant \varepsilon\|\rho\|_3 + C_\varepsilon D(\rho,\rho)^{1/2}. \tag{III.15}$$

Hence, this implies

$$\sum_m \int V_m\rho_m \leqslant \varepsilon\left(\int d\mathbf{x}\left(\sum_m |\phi_m(\mathbf{x}_\perp)|^2\rho_m(z)\right)^3\right)^{1/3} + C_\varepsilon\overline{D}(\rho,\rho)^{1/2}. \tag{III.16}$$

By convexity of x^3, for $x \geqslant 0$, and by the equation $\Sigma_m|\phi_m|^2 = B/2\pi$, we get

$$\left(\frac{2\pi}{B}\sum_m |\phi_m|^2\rho_m\right)^3 \leqslant \frac{2\pi}{B}\sum_m |\phi_m|^2\rho_m^3. \tag{III.17}$$

Using (III.17) and integrating over the $\mathbf{x}_\perp$-variable, the inequality (III.16) can be written as

$$\sum_m \int V_m\rho_m \leqslant \varepsilon\left(\frac{B}{2\pi}\right)^{2/3}\left(\sum_m \int \rho_m^3\right)^{1/3} + C_\varepsilon\overline{D}(\rho,\rho)^{1/2}. \tag{III.18}$$

Consequently, the functional $\mathcal{E}^{\mathrm{DSTF}}[\rho]$ can be estimated from below by $[\epsilon = \varepsilon(B/2\pi)^{2/3}]$

$$\begin{aligned}\mathcal{E}^{\mathrm{DSTF}}[\rho] &\geq \kappa \sum_m \int \rho_m^3 - \epsilon \left(\sum_m \int \rho_m^3 \right)^{1/3} + \overline{D}(\rho,\rho) - C_\varepsilon \overline{D}(\rho,\rho)^{1/2} \\ &\geq \inf_{X,Y\geq 0} \{\kappa X^3 - \epsilon X + Y^2 - C_\varepsilon Y\} \\ &\geq \alpha(X^3+Y^2) - C, \end{aligned} \tag{III.19}$$

for α, C appropriately chosen, where we used the notations $X=(\Sigma_m \int \rho_m^3)^{1/3}$ and $Y=\overline{D}(\rho,\rho)^{1/2}$. □

Lemma III.4: There exists a $\rho^{(\infty)}$, *which minimizes* $\mathcal{E}^{\mathrm{DSTF}}[\rho]$ *uniquely in* $\mathcal{D}$, *i.e.*, $\inf\{\mathcal{E}^{\mathrm{DSTF}}[\rho] | \rho \in \mathcal{D}\} = \mathcal{E}^{\mathrm{DSTF}}[\rho^{(\infty)}]$.

Proof: Let $\rho^{(i)}$ be a minimizing sequence of $\mathcal{E}^{\mathrm{DSTF}}$. Lemma III.3 yields that there exists a constant C, such that

$$\sum_m \kappa \int (\rho_m^{(i)})^3 \leq C, \quad \overline{D}(\rho^{(i)},\rho^{(i)}) \leq C, \quad \sum_m \rho_m^{(i)} V_m \leq C \tag{III.20}$$

for all $m \in \mathbb{N}_0$. By the Banach–Alaoglu theorem there exists a subsequence, still denoted as $\rho^{(i)}$, and a $\rho^{(\infty)}$, with $\rho_m^{(i)} \in \mathcal{L}^3(\mathbb{R})$ $\forall m \in \mathbb{N}_0$, such that

$$\rho_m^{(i)} \rightharpoonup \rho_m^{(\infty)} \text{ weakly in } \mathcal{L}^3(\mathbb{R}) \quad \forall i \in \mathbb{N}_0. \tag{III.21}$$

Since $\mathcal{L}^p$-norms are weakly lower semicontinuous, we derive for all m

$$\liminf_{i\to\infty} \int (\rho_m^{(i)})^3 \geq \int (\rho_m^{(\infty)})^3, \tag{III.22}$$

and, using Fatou's lemma, we consequently arrive at

$$\liminf_{i\to\infty} \sum_m \int (\rho_m^{(i)})^3 \geq \sum_m \int (\rho_m^{(\infty)})^3. \tag{III.23}$$

Moreover, since $V_m \in \mathcal{L}^{3/2}(\mathbb{R})$ for all m, we conclude by weak convergence

$$\lim_{i\to\infty} \int dz V_m(z) \rho_m^{(i)}(z) \to \int dz V_m(z) \rho_m^{(\infty)}(z) \tag{III.24}$$

for each m. By (III.20) and the dominated convergence theorem we have

$$\lim_{i\to\infty} \sum_m \int dz V_m(z) \rho_m^{(i)}(z) \to \sum_m \int dz V_m(z) \rho_m^{(\infty)}(z). \tag{III.25}$$

In order to show

$$\liminf_{i\to\infty} \overline{D}(\rho^{(i)},\rho^{(i)}) \geq \overline{D}(\rho^{(\infty)},\rho^{(\infty)}), \tag{III.26}$$

we use the fact that for sequences of functions $f=(f_m(z))_m$, $g=(g_m(z))_m$,

$$\langle f,g\rangle_D = \overline{D}(f,g) \tag{III.27}$$

defines a real inner product and, consequently, a real Hilbert-space $\mathcal{H}_D$. Since (III.20) yields $\|\rho^{(i)}\|_D = \sqrt{\langle \rho^{(i)},\rho^{(i)}\rangle_D} \leq C$ for all i, we can extract another subsequence $\rho^{(i)}$, such that

$$\langle f,\rho^{(i)}\rangle \to \langle f,\rho^{(\infty)}\rangle \text{ for all } f \in \mathcal{H}_D. \tag{III.28}$$

Hence, we conclude

$$\overline{D}(\rho^{(\infty)},\rho^{(\infty)}) = \lim_{i\to\infty} \langle \rho^{(i)},\rho^{(\infty)}\rangle \leqslant \langle \rho^{(\infty)},\rho^{(\infty)}\rangle^{1/2} \liminf_{i\to\infty} \langle \rho^{(i)},\rho^{(i)}\rangle^{1/2}$$

$$= \overline{D}(\rho^{(\infty)},\rho^{(\infty)})^{1/2} \liminf_{i\to\infty} \overline{D}(\rho^{(i)},\rho^{(i)})^{1/2}, \tag{III.29}$$

and consequently get (III.26). Altogether we have shown

$$\liminf_{i\to\infty} \mathcal{E}^{\mathrm{DSTF}}[\rho^{(i)}] \geqslant \mathcal{E}^{\mathrm{DSTF}}[\rho^{(\infty)}]. \tag{III.30}$$

The uniqueness follows from the strict convexity of $\mathcal{E}^{\mathrm{DSTF}}$. □

Theorem III.5: Denote $N_c = \Sigma_m \int \rho_m^{(\infty)}$. Then (i) for each $N \leqslant N_c$ there exists a unique minimizer ρ^N for $\mathcal{E}^{\mathrm{DSTF}}$, under the restriction $\Sigma_m \int \rho_m \leqslant N$, i.e., $E^{\mathrm{DSTF}}(N,Z,B) = \mathcal{E}^{\mathrm{DSTF}}[\rho^N]$. Moreover, ρ^N satisfies $\Sigma_m \int \rho_m^N = N$.

(ii) $E^{\mathrm{DSTF}}(N,Z,B)$, as a function of N, is strictly decreasing and strictly convex up to N_c, and constant for $N > N_c$.

Proof: Let $N \leqslant N_c$. Then the same proof as in Lemma III.4 shows that there exists a $\rho^N \in \mathcal{D}$, with $\Sigma_m \int \rho_m^N \leqslant N$ and

$$\mathcal{E}^{\mathrm{DSTF}}[\rho^N] = E^{\mathrm{DSTF}}(N,Z,B). \tag{III.31}$$

Obviously $E^{\mathrm{DSTF}}(N,Z,B)$, as a function of N, is nonincreasing, and the convexity of $\mathcal{E}^{\mathrm{DSTF}}$ implies the convexity of E^{DSTF}. Hence, by definition of N_c and Lemma III.4 it is clear that E^{DSTF} is strictly decreasing up to N_c and constant for $N > N_c$. Furthermore, we get that $\Sigma_m \int \rho_m^N = N$ for $N \leqslant N_c$. (Note that $\Sigma_m \int \rho_m^N < N$ would be a contradiction to $N \leqslant N_c$.) □

Proposition III.6: Let $N \leqslant N_c$. Then for every minimizer ρ^N there exists a parameter $\mu(N)$, the chemical potential, such that ρ^N obeys the coupled TF equations

$$3\kappa(\rho_m^N(z))^2 = \left[ZV_m(z) - \sum_n \int V_{m,n}(z-z')\rho_n^N(z') + \mu(N) \right]_+ \quad \forall (m \in \mathbb{N}_0), \tag{III.32}$$

and $\mu(N)$ fulfills the relation

$$\frac{\partial}{\partial N} E^{\mathrm{DSTF}}(N,Z,B) = \mu(N). \tag{III.33}$$

Proof: The proof works analogously to Ref. 9, Theorem II.10, if the variable perpendicular to the field is replaced by the angular momentum quantum numbers. □

Theorem III.7: All statements of Theorem III.5 and Proposition III.6 are also valid for the MSTF theory, where the minimizing MSTF densities $\rho^N(\mathbf{x})$ and the minimizing DSTF densities $(\rho_m^N(z))_m$ are related as

$$\rho^N(\mathbf{x}) = \frac{B}{2\pi} \sum_m \chi_m(\mathbf{x}_\perp)\rho_m^N(z). \tag{III.34}$$

The corresponding TF equation reads

$$3\kappa(\rho^N(\mathbf{x}))^2 = \left[Z\widetilde{|\mathbf{x}|^{-1}} - \sum_{n,m} \int d\mathbf{x}' \chi_m(\mathbf{x}_\perp) V_{m,n}(z-z')\chi_n(\mathbf{x}'_\perp)\rho^N(\mathbf{x}') + \mu(N) \right]_+ . \tag{III.35}$$

Proof: The existence of a minimizing density $\rho^N(\mathbf{x})$ we get from Theorem III and Lemma III.1. The uniqueness follows from the strict convexity of ρ^3 in ρ. □

Next we try to collect some information about the ''critical'' particle number N_c, which measures the maximal particle number that can be bound to the nucleus in the D(M)STF theory.

Proposition III.8: $N_c \geqslant Z$.

Proof: By definition of N_c, we have $\mu(N_c)=0$, so the TF equation reads ($\rho^{N_c}=\rho$)

$$3\kappa\rho_m(z)=[\varphi_{\text{eff}}^{(m)}(z)]_+ \quad \forall m \in \mathbb{N}_0, \tag{III.36}$$

with

$$\varphi_{\text{eff}}^{(m)}(z)=ZV_m(z)-\sum_n \int V_{m,n}(z-z')\rho_n(z'). \tag{III.37}$$

We assume $N_c<Z$.

References 10 and 11 tell us that the potentials $V_m(z)$ and $V_{n,m}(z-z')$ behave like $1/|z|$ as $z\to\infty$. Hence, we get that for each m

$$\lim_{z\to\infty}|z|[ZV_m(z)]=Z, \tag{III.38}$$

as well as

$$\lim_{z\to\infty}|z|\left[\sum_n \int V_{m,n}(z-z')\rho_n(z')\right]=\sum_n \int \lim_{z\to\infty}|z|V_{m,n}(z-z')\rho_n(z')=\sum_n \int \rho_n=N_c. \tag{III.39}$$

Since we therefore get

$$\lim_{z\to\infty}|z|\varphi_{\text{eff}}^{(m)}(z)=Z-N_c>0, \tag{III.40}$$

we can conclude that there exists an $\varepsilon>0$ and a $\overline{z}>0$, such that

$$\varphi_{\text{eff}}^{(m)}(z)\geqslant\varepsilon|z| \quad \text{for } z\geqslant\overline{z}, \tag{III.41}$$

which by (III.36) is a contradiction to $\rho_m \in \mathcal{L}^1(\mathbb{R})$. □

In the usual STF theory the inequality $N_c\leqslant Z$ is a consequence of Newton's potential theory. Since we miss this powerful tool in our DSTF theory we cannot expect to get an analogous estimate. But if we use methods similar to those applied in Refs. 10, 12, and 13 we at least get the following B-independent upper bound for N_c.

Proposition III.9: $N_c\leqslant 4Z$.

Proof: If we multiply (III.36) with ρ_m/V_m and integrate over z, we get

$$3\kappa\int dz\frac{\rho_m(z)^3}{V_m(z)}=Z\int dz\rho_m(z)-\sum_n \int dzdz'\frac{1}{V_m(z)}\rho_n(z')V_{n,m}(z-z')\rho_m(z). \tag{III.42}$$

Note that by multiplication with ρ_m the $[\,]_+$-bracket can be dropped, since $\rho_m=0$ where $\varphi_{\text{eff}}^{(m)}(z)\leqslant 0$. Clearly $\int\rho_m^3/V_m\geqslant 0$, so after summing over m we arrive at

$$ZN_c\geqslant\sum_{n,m} \int dzdz'\frac{1}{V_m(z)}\rho_n(z')V_{n,m}(z-z')\rho_m(z). \tag{III.43}$$

Moreover, Ref. 13, Lemma 4.1, tells us

$$\left(\frac{1}{V_m(z)}+\frac{1}{V_n(z)}+\frac{1}{V_m(z')}+\frac{1}{V_n(z')}\right)V_{m,n}(z-z')\geqslant 1, \tag{III.44}$$

which we use, together with symmetry, in order to estimate the right side of (III.43):

$$\begin{aligned}\sum_{m,n}\int\frac{1}{V_m(z)}\rho_m(z)V_{m,n}(z-z')\rho_n(z')dzdz'&\\ =\frac{1}{4}\sum_{m,n}\int\left(\frac{1}{V_m(z)}+\frac{1}{V_n(z)}+\frac{1}{V_m(z')}+\frac{1}{V_n(z')}\right)\rho_m(z)V_{m,n}(z-z')\rho_n(z')dzdz'&\\ \geqslant\frac{1}{4}N_c^2.&\end{aligned}\tag{III.45}$$

Inserting into (III.43) finally leads to

$$N_c\leqslant 4Z.\tag{III.46}$$

□

Remark III.10 (The difference between E^{DSTF} and E^{STF}): Obviously, the magnitude of difference between the D(M)STF and the STF energy is given by

$$B\left[\int|\phi^{\mathrm{MSTF}}(\mathbf{x})|^{3/2}-\int|\phi^{\mathrm{STF}}(\mathbf{x})|^{3/2}\right].\tag{III.47}$$

Due to the singularity of the STF potential, (III.47) has to be split into

$$B\int_{|\mathbf{x}|\leqslant B^{-1/2}}\left[|\phi^{\mathrm{MSTF}}(\mathbf{x})|^{3/2}-\int|\phi^{\mathrm{STF}}(\mathbf{x})|^{3/2}\right]+B\int_{|\mathbf{x}|\geqslant B^{-1/2}}\left[|\phi^{\mathrm{MSTF}}(\mathbf{x})|^{3/2}-\int|\phi^{\mathrm{STF}}(\mathbf{x})|^{3/2}\right].\tag{III.48}$$

The magnitude of the first term is proportional to

$$Z^{3/2}B\int_{|\mathbf{x}|\leqslant B^{-1/2}}|\mathbf{x}|^{-3/2}=O(Z^{3/2}B^{1/4}).\tag{III.49}$$

The second term of (III.48) could be estimated by

$$B\int_{|\mathbf{x}|\geqslant B^{-1/2}}|\phi^{\mathrm{STF}}(\mathbf{x})|^{1/2}|\partial_\theta\phi^{\mathrm{STF}}(\mathbf{x})|B^{-1/2}\leqslant Z^{3/2}B^{1/2}[r_S]^{3/2},\tag{III.50}$$

with $\theta=|\mathbf{x}_\perp|$. So we see that the main contribution to (III.47) stems from the $B^{-1/2}$-vicinity of the nucleus, i.e.,

$$E^{\mathrm{DSTF}}-E^{\mathrm{STF}}=O(Z^{3/2}B^{1/4}).\tag{III.51}$$

A. Some notes about the one-dimensional case

If we reduce the DSTF functional to the angular momentum channel with $m=0$, one gets the functional

$$\mathcal{E}^{1\mathrm{DSTF}}[\rho]=\kappa\int dz\rho(z)^3-Z\int dzV_0(z)\rho(z)+\frac{1}{2}\int dzdz'V_{0,0}(z-z')\rho(z)\rho(z'),\tag{III.52}$$

which can be treated analogously to the three dimensional case, and Theorem III.5 and Proposition III.8 are also valid. Concerning the upper bound of N_c, it is not necessary to symmetrize over n and m, and in this case (III.45) reads

$$\int \frac{1}{V_0(z)}\rho(z)V_{0,0}(z-z')\rho(z')dzdz' = \frac{1}{2}\int \left(\frac{1}{V_0(z)}+\frac{1}{V_0(z')}\right)\rho(z)V_{0,0}(z-z')\rho(z')dzdz'$$
$$\geqslant \frac{1}{2}N_c^2.$$

Consequently, one gets $N_c \leqslant 2Z$ for the maximum particle number that can be bound to the nucleus in the one-dimensional theory.

Moreover, let us regard the absolute minimum $\overline{E}^{1\mathrm{DSTF}}(Z,B)$ of the functional $\mathcal{E}^{1\mathrm{DSTF}}[\rho] = \mathcal{E}_{Z,B}[\rho]$. If we use the scaling relations

$$V_0(z) = B^{1/2}V_0^1(B^{1/2}z), \quad V_{0,0}(z) = B^{1/2}V_{0,0}^1(B^{1/2}z), \tag{III.53}$$

and define

$$\overline{\rho}(z) = B^{1/4}Z^{1/2}\rho(B^{1/2}z), \tag{III.54}$$

we get

$$\mathcal{E}_{Z,B}[\overline{\rho}] = B^{1/4}Z^{3/2}\mathcal{E}_{1,1}^{\lambda}[\rho], \tag{III.55}$$

with

$$\mathcal{E}_{1,1}^{\lambda}[\rho] = \kappa\int dz\rho(z)^3 - \int dzV_0^1(z)\rho(z) + \frac{1}{\lambda}\int dzdz' V_{0,0}^1(z-z')\rho(z)\rho(z'), \tag{III.56}$$

and $\lambda = 2B^{1/4}Z^{1/2}$.

Let $E_w^{1D}(Z,B)$ be the minimum of the functional

$$\mathcal{E}_w^{1D}[\rho] = \kappa\int dz\rho(z)^3 - Z\int dzV_0(z)\rho(z), \tag{III.57}$$

where the repulsive energy term is omitted. Using the above scaling (III.54), one immediately gets $E_w^{1D}(Z,B) = Z^{3/2}B^{1/4}E_w^{1D}(1,1)$. So we can formulate the following theorem:

Theorem III.11: *If $Z,B \geqslant 1$ are fixed, then*

$$E_w^{1D}(Z,B) \leqslant \overline{E}^{1\mathrm{DSTF}}(Z,B) \leqslant E_w^{1D}(Z,B) + Z(1+2\ln[BZ^2]^2). \tag{III.58}$$

Proof: The lower bound is obvious.

For the upper bound we use the relation (III.55) and take the TF-solution of $\mathcal{E}_{1,1}^{\infty}$, i.e.,

$$\rho(z) = \frac{1}{\pi}\sqrt{V_0^1(z)}. \tag{III.59}$$

This density is neither in $\mathcal{L}^1$ nor in $\mathcal{L}^2$, so we define a cut-off density $\rho_R(z) = \pi\sqrt{V_0^1(z)}\Theta(R-|z|)$ and use this as comparison density in (III.55), which leads to

$$\mathcal{E}_{1,1}^{\lambda}[\rho_R] = E_w^{1D}(1,1) + \int_R^{\infty}(V_0^1(z))^{3/2} + \frac{1}{\lambda}\int \rho_R(z)V_{0,0}^1(z-z')\rho_R(z')dzdz'. \tag{III.60}$$

Since $V_{0,0}^1(z) \leqslant \min\{1/|x|, \sqrt{\pi/4}\}$ we get by Young's inequality

$$\int \rho_R(z)V_{0,0}^1(z-z')\rho_R(z')dzdz' \leqslant \left[\left(\int \rho_R\right)^2\frac{1}{\beta} + 2\ln(\beta)\int \rho_R^2\right] \quad \forall \beta \geqslant 1. \tag{III.61}$$

After estimating $\int \rho_R$ and $\int \rho_R^2$ we see that the minimum of (III.61) as a function of β is achieved for $\beta = R/\ln(R)$, which implies

$$\int \rho_R(z) V_{0,0}^1(z-z') \rho_R(z') dz dz' \leqslant [\ln(R) + \ln(R)^2]. \tag{III.62}$$

Next, optimizing the last two term on the right side of (III.60) with respect to R and multiplying with $B^{1/4}Z^{3/2}$ yields the statement of the theorem. □

By aid of this theorem we can also prove that $\overline{E}^{1\mathrm{DSTF}}(Z,B)$ is the semiclassical approximation of $\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}[-\partial_z^2 - ZV_0(z)]_-$, the sum of all negative eigenvalues of $-\partial_z^2 - ZV_0(z)$.

Corollary III.12: Let B,Z≥1 and B≤Z². Then there exists a constant C, such that

$$\left|\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}[-\partial_z^2 - ZV_0(z)]_- - \overline{E}^{1\mathrm{DSTF}}(Z,B)\right| \leqslant C \max\{Z \ln[BZ^2], B^{3/4}Z^{1/2}\}. \tag{III.63}$$

Proof: This is an immediate consequence of Theorem III.11 and Ref. 5, Theorem 3.19, which says that

$$\left|\mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}[-\partial_z^2 - ZV_0(z)]_- - E_w^{1D}(Z,B)\right| \leqslant CB^{3/4}Z^{1/2}. \tag{III.64}$$

□

We learn from Theorem 3.10 that in a model of a one dimensional semiclassical atom, where the electrons are forced to stay in the angular momentum channel $m=0$, the repulsive interaction energy does not contribute to the leading order of the energy $\overline{E}^{1\mathrm{DSTF}}(Z,B)$ for large Z and $B \geqslant 1$.

An analogous effect is obtained for the quantum mechanical interaction energy of N particles reduced to the angular momentum $m=0$, i.e.,

$$\Psi = \phi_0 \otimes \cdots \otimes \phi_0 \psi(z_1, \ldots, z_N). \tag{III.65}$$

For ψ a Slater determinant or at least for ψ close to the ground state of the corresponding N-particle Hamiltonian H_0, which is the projection onto the angular momentum eigenspace with angular momentum $m=0$, the interaction energy can be bounded from above by (for a precise lower bound see Ref. 14)

$$\frac{1}{2} \int_{\mathbb{R}^2} \rho_\psi(z) \rho_\psi(z') V_{0,0}(z-z') dz dz', \tag{III.66}$$

which can be estimated by an analogous method to (III.61). This leads to

$$\frac{1}{2} \int_{\mathbb{R}^2} \rho_\psi(z) \rho_\psi(z') V_{0,0}(z-z') dz dz' \leqslant C E_0^{1/2} N^{1/2} [1 + \ln(BN^3/E_0)], \tag{III.67}$$

where we have used that $\langle \Psi, H_N \Psi \rangle \leqslant 0$ and E_0 is the corresponding ground state energy [of wave functions of the form (III.65)], which is of the same order as $\overline{E}^{1\mathrm{DSTF}}$ as long as $B \leqslant Z^2$. Relation (III.67) yields that the quantum mechanical interaction energy in one dimension is $\ll E_0$ as long as $E_0 \gg N$.

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Coherent states on spheres

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We describe a family of coherent states and an associated resolution of the identity for a quantum particle whose classical configuration space is the d-dimensional sphere S^d. The coherent states are labeled by points in the associated phase space $T^*(S^d)$. These coherent states are *not* of Perelomov type but rather are constructed as the eigenvectors of suitably defined annihilation operators. We describe as well the Segal–Bargmann representation for the system, the associated unitary Segal–Bargmann transform, and a natural inversion formula. Although many of these results are in principle special cases of the results of Hall and Stenzel, we give here a substantially different description based on ideas of Thiemann and of Kowalski and Rembieliński. All of these results can be generalized to a system whose configuration space is an arbitrary compact symmetric space. We focus on the sphere case in order to carry out the calculations in a self-contained and explicit way. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1446664]

I. INTRODUCTION

In Ref. 1, Hall introduced a family of coherent states for a system whose classical configuration space is the group manifold of a compact Lie group G. These coherent states are labeled by points in the associated phase space, namely the cotangent bundle $T^*(G)$. The coherent states themselves were originally defined in terms of the *heat kernel* on G, although we will give a different perspective here. One may identify[2] $T^*(G)$ with the complexified group $G_{\mathbb{C}}$, where, for example, if $G=\mathrm{SU}(2)$ then $G_{\mathbb{C}}=\mathrm{SL}(2;\mathbb{C})$. The paper[1] establishes a resolution of the identity for these coherent states, and equivalently, a unitary Segal–Bargmann transform. The Segal–Bargmann representation of this system is a certain Hilbert space of holomorphic functions over the complex group $G_{\mathbb{C}}$. Additional results may be found in Refs. 2–4 and the survey paper.[5]

The coherent states for G (in the form of the associated Segal–Bargmann transform) have been applied to quantum gravity in Ref. 6, with proposed generalizations due to Thiemann.[7] More recently the coherent states themselves have been used by Thiemann and co-authors[8] in an attempt to determine the classical limit of the quantum gravity theory proposed by Thiemann in Ref. 9. In particular, the second entry in Ref. 8 establishes good phase space localization properties (in several different senses) for the coherent states associated to the configuration space $G=\mathrm{SU}(2)$.

In another direction, Wren,[10] using a method proposed by Landsman,[11] has shown that the coherent states for G arise naturally in the canonical quantization of $(1+1)$-dimensional Yang–Mills theory on a space–time cylinder. Here G is the structure group of the theory and plays the role of the reduced configuration space, that is, the space of connections modulo based gauge transformation over the spatial circle. Wren considers first the ordinary canonical coherent states for the unreduced (infinite-dimensional) system. He then shows that after ''projecting'' them into the gauge-invariant subspace (using a suitable regularization procedure) these become precisely the generalized coherent states for G, as originally defined in Ref. 1. Driver and Hall[12] elaborate

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on the results of Wren, using a different regularization scheme. They show in particular how the resolution of the identity for the generalized coherent states can be obtained by projection from the resolution of the identity for the canonical coherent states. See also Ref. 13 for an appearance of the generalized Segal–Bargmann transform in the setting of two-dimensional Euclidean Yang–Mills theory.

Finally, the paper[14] shows that the generalized Segal–Bargmann transform for G can be obtained by means of geometric quantization (see also Ref. 5, Sec. 3.2). This means that the associated coherent states for G are of ''Rawnsley type'' [15] and are thus in the spirit of Berezin's approach to quantization.

We emphasize that the coherent states for G are *not of Perelomov type*.[16] Instead they are realized as the eigenvectors of certain non-self-adjoint ''annihilation operators,'' as will be described in detail in the present paper. (See Sec. X for further comments.)

The coherent states and the resolution of the identity for G ''descend'' in a straightforward way to the case of a system whose configuration space is a compact symmetric space X (Ref. 1, Sec. 11). Compact symmetric spaces are manifolds of the form G/K, where G is a compact Lie group and K is a special sort of subgroup, namely, the fixed-point subgroup of an involution. Examples include the spheres $S^d = \mathrm{SO}(d+1)/\mathrm{SO}(d)$ and the complex projective spaces $\mathbb{C}P^d = \mathrm{SU}(d+1)/\mathrm{SU}(d)$. Compact Lie groups themselves can be thought of as symmetric spaces by identifying G with $(G\times G)/\Delta(G)$ where $\Delta(G)$ is the ''diagonal'' copy of G inside $G\times G$.

We emphasize that in the case $X=S^2$ the 2-sphere is playing the role of the *configuration space* and thus the coherent states discussed here are completely different from the spin coherent states in which the 2-sphere plays the role of the phase space. Whereas the spin coherent states are labeled by points in S^2 itself, our coherent states are labeled by points in the cotangent bundle $T^*(S^2)$.

Although the case of compact symmetric spaces can be treated by descent from the group, it is preferable to give a direct treatment, and such a treatment was given by Stenzel.[17] In particular Stenzel gives a much better description, in the symmetric space case, of the measure that one uses to construct the resolution of the identity (see also Ref. 5, Sec. 3.4). Although Stenzel formulates things in terms of a unitary Segal–Bargmann transform and does not explicitly mention the coherent states, only a notational change is needed to re-express his results as a resolution of the identity for the associated coherent states.

More recently, the coherent states for the 2-sphere S^2 were independently discovered, from a substantially different point of view, by Kowalski and Rembieliński.[18] (Reference 18 builds on earlier work of Kowalski, Rembieliński, and Papaloucas[19] on the S^1 case.) These authors were unaware at the time of the work of Hall and Stenzel. Reference 20 then describes the resolution of the identity for the coherent states on the 2-sphere, showing in a different and more explicit way that the result of Ref. 17, Theorem 3 holds in this case. (See Sec. VII of Ref. 20 for comments on the relation of their work to that of Stenzel.)

The purpose of this paper is to describe the coherent states for a compact symmetric space using the points of view advocated by Thiemann and by Kowalski and Rembieliński. For the sake of concreteness we concentrate in this paper on the case $X=S^d$. In Refs. 1 and 17 the coherent states are defined in terms of the heat kernel on the configuration space, which takes the place of the Gaussian that enters into the description of the canonical coherent states. Here by contrast the coherent states are defined to be the eigenvectors of suitable annihilation operators, and only afterwards does one discover the role of the heat kernel, in the position wave function of the coherent states and in the reproducing kernel. The annihilation operators, meanwhile, are defined by (a special case of) the ''complexifier'' method proposed by Thiemann, which we will show is equivalent to (a generalization of) the polar decomposition method of Kowalski and Rembieliński. We emphasize, though, that the approach described in this paper gives ultimately the same results as the heat kernel approach of Hall and Stenzel.

II. MAIN RESULTS

In this section we briefly summarize the main results of the paper. All results are explained in greater detail in the subsequent sections. Briefly, our strategy is this. First, we construct complex-valued functions $a_1,\ldots,a_{d+1}$ on the classical phase space that serve to define a complex structure on phase space. Second, we construct the quantum counterparts of these functions, operators $A_1,\ldots,A_{d+1}$ that we regard as the annihilation operators. Third, we construct simultaneous eigenvectors for the annihilation operators, which we regard as the coherent states. Fourth, we construct a resolution of the identity for these coherent states.

We consider a system whose classical configuration space is the d-dimensional sphere S^d of radius r. We consider also the corresponding phase space, the cotangent bundle $T^*(S^d)$, which we describe as

$$T^*(S^d)=\{(\mathbf{x},\mathbf{p})\in\mathbb{R}^{d+1}\times\mathbb{R}^{d+1}|x^2=r^2,\mathbf{x}\cdot\mathbf{p}=0\},$$

where $\mathbf{p}$ is the *linear* momentum.

In Sec. III we consider the classical component of Thiemann's method. To apply this method we must choose a constant ω with units of frequency. The classical "complexifier" is then defined to be *kinetic energy function divided by* ω, which can be expressed as

$$\text{complexifier}=\frac{\text{kinetic energy}}{\omega}=\frac{j^2}{2m\omega r^2},$$

where j^2 is the total angular momentum. (Thiemann's method allows other complexifiers; see Sec. III.) We construct complex-valued functions $a_1,\ldots,a_{d+1}$ by taking the position functions $x_1,\ldots,x_{d+1}$ and applying repeated Poisson brackets with the complexifier. Specifically,

$$a_k=e^{i\{\cdot,\text{complexifier}\}}x_k=\sum_{n=0}^{\infty}\left(\frac{i}{2m\omega r^2}\right)^n\frac{1}{n!}\underbrace{\{\cdots\{\{x_k,j^2\},j^2\},\cdots,j^2\}}_{n}. \tag{1}$$

If we let $\mathbf{a}=(a_1,\ldots,a_{d+1})$ then the calculations in Sec. III will give the following explicit formula:

$$\mathbf{a}=\cosh\left(\frac{j}{m\omega r^2}\right)\mathbf{x}+i\frac{r^2}{j}\sinh\left(\frac{j}{m\omega r^2}\right)\mathbf{p}. \tag{2}$$

These complex-valued functions satisfy $a_1^2+\cdots+a_{d+1}^2=r^2$ and $\{a_k,a_l\}=0$. In the case $d=2$ this agrees with Eq. (6.1) of Ref. 18.

In Sec. IV we consider the quantum component of Thiemann's method. We consider the quantum counterpart of the classical complexifier, namely,

$$\text{complexifier}=\frac{\text{kinetic energy}}{\omega}=\frac{J^2}{2m\omega r^2},$$

where J^2 is the total angular momentum operator. Then if $X_1,\ldots,X_{d+1}$ denote the position operators we define, by analogy with (1),

$$A_k=e^{i[\cdot,\text{complexifier}]/i\hbar}X_k=\sum_{n=0}^{\infty}\left(\frac{1}{2m\omega r^2\hbar}\right)^n\frac{1}{n!}\underbrace{[\cdots[[X_k,J^2],J^2],\cdots,J^2]}_{n}. \tag{3}$$

This may also be written as

$$A_k=e^{-J^2/2m\omega r^2\hbar}X_k e^{J^2/2m\omega r^2\hbar}. \tag{4}$$

Equation (30) in Sec. IV gives the quantum counterpart of (2); it is slightly more complicated than (2) because of quantum corrections. The annihilation operators satisfy $A_1^2+\cdots+A_{d+1}^2=r^2$ and $[A_k,A_l]=0$. Applying the same procedure in the $\mathbb{R}^d$ case produces the usual complex coordinates on phase space and the usual annihilation operators (Sec. VIII).

One can easily deduce from (4) a "polar decomposition" for the annihilation operator, given in (33) in Sec. IV. In the case $d=2$ this is essentially the same as what Kowalski and Rembieliński take as the definition of the annihilation operators. This shows that Thiemann's complexifier approach is equivalent to the polar decomposition approach of Kowalski and Rembieliński. Similarly, the polar form of the annihilation operators in the $d=1$ case is essentially the same as what Kowalski, Rembieliński, and Papaloucas take as the definition of the annihilation operator in Ref. 19.

In Sec. V we consider the coherent states, defined to be the simultaneous eigenvectors of the annihilation operators. Using (4) we may immediately write down some eigenvectors for the A_k's, namely, the vectors of the form,

$$|\psi_{\mathbf{a}}\rangle = e^{-J^2/2m\omega r^2\hbar}|\delta_{\mathbf{a}}\rangle, \tag{5}$$

where $|\delta_{\mathbf{a}}\rangle$ is a simultaneous eigenvector for the position operators corresponding to a point $\mathbf{a}$ in S^d. A key result of Sec. V is that one can perform an analytic continuation with respect to the parameter $\mathbf{a}$, thereby obtaining coherent states $|\psi_{\mathbf{a}}\rangle$ corresponding to any point $\mathbf{a}$ in the *complexified* sphere, $S^d_{\mathbb{C}}=\{\mathbf{a}\in\mathbb{C}^{d+1}|\ a^2=r^2\}$. These vectors $|\psi_{\mathbf{a}}\rangle$ are normalizable and satisfy

$$A_k|\psi_{\mathbf{a}}\rangle = a_k|\psi_{\mathbf{a}}\rangle, \quad \mathbf{a}\in S^d_{\mathbb{C}}.$$

Equation (5) shows that the coherent states are expressible in terms of the heat kernel on the sphere, thus demonstrating that Thiemann's definition of the coherent states is equivalent to the definition in Refs. 1, 17 in terms of the heat kernel. The reproducing kernel for these coherent states is also expressed in terms of the heat kernel on the sphere.

In Sec. VI we describe a resolution of the identity for these coherent states. In a suitable coordinate system this takes the form

$$I=\int_{\mathbf{x}\in S^d}\int_{\mathbf{p}\cdot\mathbf{x}=0}|\psi_{\mathbf{a}}\rangle\langle\psi_{\mathbf{a}}|\,\nu(2\tau,2p)\left(\frac{\sinh 2p}{2p}\right)^{d-1}2^d d\mathbf{p}d\mathbf{x}, \tag{6}$$

where $\mathbf{a}$ is a function of $\mathbf{x}$ and $\mathbf{p}$ as in (2). Here ν is the heat kernel for d-dimensional hyperbolic space and τ is the dimensionless quantity given by $\tau=\hbar/m\omega r^2$. Explicit formulas for ν are found in Sec. VI. The resolution of the identity for the coherent states is obtained by a continuous deformation of the resolution of the identity for the position eigenvectors.

In Sec. VII we discuss the Segal–Bargmann representation for this system, namely, the space of holomorphic functions on the complexified sphere that are square-integrable with respect to the density in (6). We think of the Segal–Bargmann representation as giving a sort of *phase space wave function* for any state. There is an inversion formula stating the position wave function can be obtained from the phase space wave function by integrating out the momentum variables, specifically,

$$\langle\delta_{\mathbf{x}}|\phi\rangle=\int_{\mathbf{p}\cdot\mathbf{x}=0}\langle\psi_{\mathbf{a}(\mathbf{x},\mathbf{p})}|\phi\rangle\,\nu(\tau,p)\left(\frac{\sinh p}{p}\right)^{d-1}d\mathbf{p}$$

for any state $|\phi\rangle$. Note that whereas the resolution of the identity involves $\nu(2\tau,2p)$, the inversion formula involves $\nu(\tau,p)$.

In Sec. VIII we show that the complexifier method, when applied to the $\mathbb{R}^d$ case, yields the usual canonical coherent states and their resolution of the identity. In Sec. IX we summarize some of the relevant representation theory for the Euclidean group. Finally, in Sec. X we compare our construction to other constructions of coherent states on spheres.

Although all of the results here generalize to arbitrary compact symmetric spaces X, we concentrate for the sake of explicitness on the case $X=S^d$. We will describe the general case in a forthcoming paper.

III. COMPLEX COORDINATES ON PHASE SPACE

In this section we define Poisson-commuting complex-valued functions $a_1,\ldots,a_{d+1}$ on the classical phase space. In Sec. IV we will introduce the quantum counterparts of these functions, commuting non-self-adjoint operators $A_1,\ldots,A_{d+1}$ which we regard as the annihilation operators for this system. In Sec. V we will consider the coherent states, that is, the simultaneous eigenvectors of the annihilation operators.

Consider the d-dimensional sphere of radius r in $\mathbb{R}^{d+1}$, namely,

$$S^d=\{\mathbf{x}\in\mathbb{R}^{d+1}|x_1^2+\cdots+x_{d+1}^2=r^2\},$$

regarded as the *configuration space* for a classical system ($d\geqslant 1$). Then consider the associated phase space, the cotangent bundle $T^*(S^d)$, which we think of as

$$T^*(S^d)=\{(\mathbf{x},\mathbf{p})\in\mathbb{R}^{d+1}\times\mathbb{R}^{d+1}|x^2=r^2,\ \mathbf{x}\cdot\mathbf{p}=0\}.$$

Here p is the *linear* momentum, which must be tangent to S^d, i.e., perpendicular to $\mathbf{x}$.

We also have the **angular momentum** functions j_{kl}, $1\leqslant k,l\leqslant d+1$, given by

$$j_{kl}=p_kx_l-p_lx_k. \tag{7}$$

We may think of j as a function on $T^*(S^d)$ taking values in the space of $(d+1)\times(d+1)$ skew-symmetric matrices, that is, in the Lie algebra so$(d+1)$. Thinking of j as a matrix we may rewrite (7) as

$$\mathbf{j}(\mathbf{x},\mathbf{p})=\mathbf{p}\otimes\mathbf{x}-\mathbf{x}\otimes\mathbf{p},$$

where $\otimes$ denotes the outer product. [That is, $(\mathbf{a}\otimes\mathbf{b})_{kl}=a_kb_l$.]

For a particle constrained to the sphere it is possible and convenient to express everything in terms of $\mathbf{x}$ and $\mathbf{j}$ instead of $\mathbf{x}$ and $\mathbf{p}$. We may alternatively describe $T^*(S^d)$ as the set of pairs $(\mathbf{x},\mathbf{j})$ in which $\mathbf{x}$ is a vector in $\mathbb{R}^{d+1}$, $\mathbf{j}$ is a $(d+1)\times(d+1)$ skew-symmetric matrix, and $\mathbf{x}$ and $\mathbf{j}$ satisfy

$$x^2=r^2 \tag{8}$$

and

$$r^2j_{kl}=j_{km}x_mx_l-x_kj_{lm}x_m \tag{9}$$

(sum convention). This last condition says that if we *define* $\mathbf{p}$ to be $r^{-2}\mathbf{jx}$, then $\mathbf{j}=\mathbf{p}\otimes\mathbf{x}-\mathbf{x}\otimes\mathbf{p}$. Equation (9) reflects the constraint to the sphere and does not hold for a general particle in $\mathbb{R}^{d+1}$. On $T^*(S^d)$ we have the relations

$$\begin{aligned}\mathbf{jx}&=r^2\mathbf{p},\\ \mathbf{jp}&=-p^2\mathbf{x}.\end{aligned} \tag{10}$$

Recall that $\mathbf{j}$ is a matrix; thus $\mathbf{jx}$ is the vector obtained by applying the matrix $\mathbf{j}$ to the vector $\mathbf{x}$, and similarly for $\mathbf{jp}$.

In the case $d=2$ (S^2 sitting inside $\mathbb{R}^3$) a standard vector identity shows that for any vector $\mathbf{v}\in\mathbb{R}^3$, $\mathbf{jv}=(\mathbf{x}\times\mathbf{p})\times\mathbf{v}$, where $\times$ is the cross-product and $\mathbf{x}\times\mathbf{p}$ is the usual angular momentum vector $\mathbf{l}$. So in the $\mathbb{R}^3$ case $\mathbf{jv}=\mathbf{l}\times\mathbf{v}$.

The symplectic structure on $T^*(S^d)$ may be characterized by the Poisson bracket relations,

$$\{j_{kl},j_{mn}\}=\delta_{kn}j_{lm}+\delta_{lm}j_{kn}-\delta_{km}j_{ln}-\delta_{ln}j_{km},$$
$$\{x_k,j_{lm}\}=\delta_{kl}x_m-\delta_{km}x_l, \tag{11}$$
$$\{x_k,x_l\}=0.$$

These are the commutation relations for the Euclidean Lie algebra, which is the semidirect product $e(d+1)\cong \mathrm{so}(d+1)\ltimes \mathbb{R}^{d+1}$.

Poisson bracket relations involving $\mathbf{p}$ should be derived from (11) using the relation $\mathbf{p}=r^{-2}\mathbf{jx}$. Since the constraint to the sphere alters the dynamics and hence the Poisson bracket relations, we will not get the same formulas as in $\mathbb{R}^{d+1}$. For example, we have

$$\{x_k,p_l\}=\delta_{kl}-\frac{x_kx_l}{r^2}. \tag{12}$$

The complex coordinates on phase space will be constructed from the position functions x_k by means of repeated Poisson brackets with a multiple of the kinetic energy function. In the sphere case it is convenient to express the kinetic energy in terms of the total angular momentum j^2, given by

$$j^2=\sum_{k<l}(j_{kl})^2. \tag{13}$$

The total angular momentum satisfies $j^2=r^2p^2$, and the kinetic energy is $p^2/2m=j^2/2mr^2$.

We now choose a constant ω with units of a frequency. The significance of this constant is that $m\omega$ has the units of momentum divided by position. Thus ω (together with m) allows us to put position and momentum onto the same scale, which is necessary in order to define complex-valued functions that involve both x and p. Ultimately, $m\omega$ will control the ratio of the width in position space of the coherent states to the radius of the sphere.

Kowalski and Rembieliński do not have a parameter comparable to our ω; the only dimensional parameters in Ref. 18 are m, r, and $\hbar$. This affects the interpretation of their Eq. (6.1) for the complex coordinates on phase space (what we call **a**). Equation (6.1) involves $\cosh l$ and $\sinh l$, where l is the classical angular momentum. The argument of cosh and sinh should be dimensionless, and the only way to make l dimensionless using only m, r, and $\hbar$ is to divide l by $\hbar$. Thus in Eq. (6.1) of Ref. 18, l implicitly means $l/\hbar$. In our view it is unnatural in a *classical* formula to insist that the angular momentum be measured in units of Planck's constant. In our approach [see (18) below], angular momentum is measured in units of $m\omega r^2$. Although nothing prevents one from choosing ω so that $m\omega r^2=\hbar$, it seems artificial to us to insist on this. After all, Eq. (6.1) concerns a classical construction that ought to be independent of the value of Planck's constant.

We are now ready to apply the ''complexifier'' method of Thiemann.[7] We take as our classical complexifier the kinetic energy function divided by ω,

$$\text{complexifier}=\frac{\text{kinetic energy}}{\omega}=\frac{j^2}{2m\omega r^2}. \tag{14}$$

We then define complex-valued functions $a_1,\ldots,a_{d+1}$ on $T^*(S^d)$ by

$$a_k(\mathbf{x},\mathbf{p})=\exp\left(i\left\{\cdot,\frac{j^2}{2m\omega r^2}\right\}\right)x_k=\sum_{n=0}^{\infty}\left(\frac{i}{2m\omega r^2}\right)^n\frac{1}{n!}\underbrace{\{\cdots\{\{x_k,j^2\},j^2\},\cdots,j^2\}}_{n}. \tag{15}$$

Note that the a_k's are obtained from the x_k's by means of the classical time-evolution generated by the kinetic energy function, evaluated at the *imaginary* time i/ω. The calculations below will show that the series (15) converges for all $\mathbf{x}$ and $\mathbf{p}$.

In Ref. 7, Thiemann allows *any* function C on the phase space to be the complexifier, provided that $\exp(i\{\cdot,C\})x_k$ converges. (Thiemann also allows any cotangent bundle to be the phase space.) The condition of convergence, however, imposes severe restrictions on the choice of C, even when C is quadratic in the momenta. We consider in this paper only the complexifier (14).

To compute the functions a_k explicitly, we first compute using (11) and (13) that, in vector notation,

$$\left\{\mathbf{x},\frac{j^2}{2m\omega r^2}\right\}=\frac{1}{m\omega r^2}\mathbf{j}\mathbf{x}=\frac{1}{m\omega}\mathbf{p}. \tag{16}$$

On the other hand, it is easily verified that $\{j_{kl},j^2\}=0$, which means that if we compute further Poisson brackets with j^2, the matrix $\mathbf{j}$ gets ignored and we get

$$\left(\frac{1}{2m\omega r^2}\right)^n \underbrace{\{\cdots\{\{\mathbf{x},j^2\},j^2\},\cdots,j^2\}}_{n}=\left(\frac{1}{m\omega r^2}\right)^n \mathbf{j}^n\mathbf{x}.$$

Here $\mathbf{j}^n\mathbf{x}$ means the matrix $\mathbf{j}$ applied n times to the vector $\mathbf{x}$.

We obtain, then, the following "polar coordinates" expression for $\mathbf{a}=(a_1,\ldots,a_{d+1})$

$$\mathbf{a}(\mathbf{x},\mathbf{p})=e^{i\mathbf{j}(x,p)/m\omega r^2}\mathbf{x}. \tag{17}$$

[Compare Eq. (3.37) in the first entry of Ref. 8.] Using (10) we can compute this explicitly as

$$\mathbf{a}(\mathbf{x},\mathbf{p})=\cosh\left(\frac{p}{m\omega r}\right)\mathbf{x}+i\frac{r}{p}\sinh\left(\frac{p}{m\omega r}\right)\mathbf{p}=\cosh\left(\frac{j}{m\omega r^2}\right)\mathbf{x}+i\frac{r^2}{j}\sinh\left(\frac{j}{m\omega r^2}\right)\mathbf{p}. \tag{18}$$

We may at this point check the units: $p/m\omega r=j/m\omega r^2$ is dimensionless and the whole expression has units of position. Note also that $\mathbf{a}(\mathbf{x},-\mathbf{p})=\mathbf{a}(\mathbf{x},\mathbf{p})$.

With $d=2$ (and $r=m\omega=1$) (18) agrees with Eq. (6.1) of Ref. 18. [See also Eq. (3.6) in the second entry of Ref. 8.] In any dimension (18) agrees with the "adapted complex structure" on $T^*(S^d)$ as defined by Lempert and Szőke[21] and Guillemin and Stenzel,[22] which for the special case of rank one symmetric spaces was constructed earlier by Morimoto and Nagano.[23] See, for example, p. 410 of Ref. 24.

It is instructive to consider how this works out in the case of $S^1\subset\mathbb{R}^2$. In that case we have only a single component of angular momentum, $j_{12}=p_1x_2-p_2x_1$, so that $j=|j_{12}|$. Since both terms in (18) are even functions of j, we may replace j by j_{12} there. Then let θ be the usual angular coordinate and let $\rho=-j_{12}/m\omega r^2$, so that ρ is (up to a constant) the canonically conjugate momentum to θ. Our phase space is the set of points (x_1,x_2,p_1,p_2) with $x_1^2+x_2^2=r^2$ and $p_1x_1+p_2x_2=0$. On this set we have the easily verified identity $j_{12}(x_2,-x_1)=r^2(p_1,p_2)$. Upon using this identity and $\mathbf{x}=r(\cos\theta,\sin\theta)$, (18) becomes

$$\mathbf{a}=r(\cosh\rho\cos\theta-i\sinh\rho\sin\theta,\cosh\rho\sin\theta+i\sinh\rho\cos\theta)=r(\cos(\theta+i\rho),\sin(\theta+i\rho)). \tag{19}$$

This result facilitates comparison with the analysis of the S^1 case in Ref. 19 and should be thought of as the "complexification" of the identity $\mathbf{x}=r(\cos\theta,\sin\theta)$.

As is well known, the Poisson bracket satisfies a Leibniz-type product rule, $\{f_1,f_2f_3\}=\{f_1,f_2\}f_3+f_2\{f_1,f_3\}$, and the analogous formula for Poisson brackets, $\{f_1,\{f_2,f_3\}\}=\{\{f_1,f_2\},f_3\}+\{f_2,\{f_1,f_3\}\}$. (This last expression is equivalent to the Jacobi identity.) Suppose then that we define the "complexification" $f_{\mathbb{C}}$ of any function f to be

$$f_{\mathbb{C}}=e^{i\{\cdot,\text{complexifier}\}}f$$

whenever the power series for the exponential converges. Then by a standard power series argument we have

$$(f_1 f_2)_{\mathbb{C}} = (f_1)_{\mathbb{C}} (f_2)_{\mathbb{C}} \tag{20}$$

and

$$\{f_1, f_2\}_{\mathbb{C}} = \{(f_1)_{\mathbb{C}}, (f_2)_{\mathbb{C}}\}. \tag{21}$$

Equation (20) shows that if we "complexify" any polynomial in the variables $x_1, \ldots, x_{d+1}$ we will get simply the same polynomial in $a_1, \ldots, a_{d+1}$. Furthermore, since $\{x_k, x_l\} = 0$, (21) shows that

$$\{a_k, a_l\} = 0, \tag{22}$$

which implies that $\{\overline{a_k}, \overline{a_l}\} = 0$. The formula for $\{a_k, \overline{a_l}\}$, however, is complicated and we will not compute it here.

Equation (20) also shows that

$$a^2(\mathbf{x}, \mathbf{p}) = r^2 \tag{23}$$

for all $\mathbf{x}, \mathbf{p}$, which is also evident from (18). Thus the map $(\mathbf{x}, \mathbf{p}) \to \mathbf{a}(\mathbf{x}, \mathbf{p})$ defines a map of the cotangent bundle $T^*(S^d)$ to the *complexified sphere*,

$$S^d_{\mathbb{C}} = \{\mathbf{a} \in \mathbb{C}^{d+1} | a_1^2 + \cdots + a_{d+1}^2 = r^2\}. \tag{24}$$

It is not hard to see that this map is invertible, indeed a diffeomorphism of $T^*(S^d)$ with $S^d_{\mathbb{C}}$.

IV. THE ANNIHILATION OPERATORS

We now consider the quantum counterpart of the constructions in the previous section. This means that the functions j_{kl} and x_k should be replaced by self-adjoint operators J_{kl} and X_k acting on (suitable domains in) some separable complex Hilbert space. These should satisfy $J_{lk} = -J_{kl}$ and the quantum counterpart of the Poisson-bracket relations (11), namely,

$$\begin{aligned} \frac{1}{i\hbar}[J_{kl}, J_{mn}] &= \delta_{kn} J_{lm} + \delta_{lm} J_{kn} - \delta_{km} J_{ln} - \delta_{ln} J_{km}, \\ \frac{1}{i\hbar}[X_k, J_{lm}] &= \delta_{kl} X_m - \delta_{km} X_l, \\ \frac{1}{i\hbar}[X_k, X_l] &= 0. \end{aligned} \tag{25}$$

We recognize this as a representation of the Euclidean Lie algebra $e(d+1) = \mathrm{so}(d+1) \ltimes \mathbb{R}^{d+1}$. We assume that this representation of $e(d+1)$ comes from an irreducible unitary representation of the associated connected, simply connected Lie group $\tilde{E}(d+1)$. Here $\tilde{E}(d+1) \cong \mathrm{Spin}(d+1) \ltimes \mathbb{R}^{d+1}$ for $d \geq 2$ and $\tilde{E}(2) \cong \mathbb{R} \ltimes \mathbb{R}^2$, where $\ltimes$ denotes a semidirect product with the normal factor on the right.

The irreducible unitary representations of $\tilde{E}(d+1)$ may be classified by the Wigner–Mackey method. One first chooses an orbit of $\mathrm{Spin}(d+1)$ on $\mathbb{R}^{d+1}$, namely, a sphere of some radius $r \geq 0$. Since the case $r = 0$ is presumably unphysical (though mathematically permitted), we assume from now on that $r > 0$. Next one selects any one point in the sphere of radius r and considers the "little group," that is, the stabilizer in $\mathrm{Spin}(d+1)$ of the point. For $r > 0$ the little group is simply $\mathrm{Spin}(d)$. The irreducible representations of $\tilde{E}(d+1)$ are then labeled by the value of r and by an

irreducible unitary representation of the little group. In this paper we will consider only the case in which the representation of the little group is trivial. Nevertheless the definitions of the annihilation operators and of the coherent states make sense in general. Concretely, the representations in which the little group acts trivially may be realized in the Hilbert space $L^2(S^d)$, with the position operators acting as multiplication operators and the angular momentum operators acting as the differential operators given in (52) below.

Choosing a sphere of radius r amounts to requiring that the operators in (25) satisfy

$$X^2 = r^2. \tag{26}$$

We will shortly impose an additional condition among the X's and J's that forces the representation of the little group to be trivial. For now, however, we will assume only the $e(d+1)$ relations (25) and the condition (26).

We define the total angular momentum J^2 as in the classical case by

$$J^2 = \sum_{k<l} J_{kl}^2 . \tag{27}$$

As in the classical case we define

$$\text{complexifier} = \frac{\text{kinetic energy}}{\omega} = \frac{J^2}{2m\omega r^2}.$$

We then define the annihilation operators by replacing $\{\cdot, \text{complexifier}\}$ in (15) with its quantum counterpart, $(1/i\hbar)[\cdot, \text{complexifier}]$,

$$A_k = \exp\left(\frac{i}{i\hbar}\left[\cdot, \frac{J^2}{2m\omega r^2}\right]\right) X_k = \sum_{n=0}^{\infty} \frac{1}{(2m\omega r^2\hbar)^n} \frac{1}{n!} [\cdots[[X_k, J^2], J^2]\cdots, J^2]. \tag{28}$$

By a standard formula from Lie group theory this may be written as

$$A_k = e^{-J^2/2m\omega r^2\hbar} X_k e^{J^2/2m\omega r^2\hbar}. \tag{29}$$

In the general form of Thiemann's method, (29) would be $\exp(-\hat{C}/\hbar)X_k \exp(\hat{C}/\hbar)$, where $\hat{C}$ is the quantum operator corresponding to the classical complexifier C.

For determining the eigenvectors of the annihilation operators (i.e., the coherent states), (29) is the most useful expression for the A_k's. Nevertheless we will give two other formulas, a polar decomposition and an "explicit" formula in terms of the position and momentum operators. The A_k's are unbounded operators and so something must be said about their domains; see the discussion at the end of this section. The annihilation operators satisfy (in analogy to (22) and (23))

$$[A_k, A_l] = 0, \tag{30}$$

$$A^2 = r^2 \tag{31}$$

(since $[X_k, X_l] = 0$ and $X^2 = r^2$).

To compute $\mathbf{A}$ we first compute using (25) and (27) that

$$\frac{1}{i\hbar}[X_k, J^2] = J_{kl}X_l + X_l J_{kl} = 2J_{kl}X_l + i\hbar(\delta_{lk}X_l - \delta_{ll}X_k) = 2J_{kl}X_l - i\hbar d X_k .$$

Here we have chosen to order things with the J's to the left of the X's and we use the sum convention. Thus in vector notation we have

$$\frac{1}{i\hbar}\left[\mathbf{X}, \frac{J^2}{2m\omega r^2}\right] = \frac{1}{m\omega r^2}\left(\mathbf{J} - \frac{i\hbar d}{2}\right)\mathbf{X}. \tag{32}$$

Here the term involving $i\hbar d/2$ is a "quantum correction;" compare (16).

Since $[J_{kl}, J^2]=0$, further brackets will give just another factor of the matrix operator $\mathbf{J}-i\hbar d/2$. Thus the polar coordinates decomposition of $\mathbf{A}$ has just a single quantum correction, namely,

$$\mathbf{A}=\exp\left\{\frac{i\mathbf{J}+\hbar d/2}{m\omega r^2}\right\}\mathbf{X}. \tag{33}$$

In the case $d=2$, a formula very similar to this is taken in Ref. 18 as the definition of the annihilation operators. The only difference is that Kowalski and Rembieliński formulate things in terms of 2×2 matrix operators, whereas in the case $d=2$, (33) is in terms of 3×3 matrix operators. Nevertheless, our expression is equivalent to that of Kowalski and Rembieliński; see below and Eq. (5.9) of Ref. 20. The analog of (33) for the group case is given in Eq. (3.44) of the first entry in Ref. 8 and in Eq. (3.13) of the second entry in Ref. 8.

Note that the definition (28) makes sense in any irreducible representation of $\tilde{E}(d+1)$ (with $X^2=r^2>0$,) and that the formula (33) is valid in this generality. However, to compute $\mathbf{A}$ more explicitly than this we need to further specify the irreducible representation of $\tilde{E}(d+1)$. We limit ourselves to the case in which the representation of the little group Spin(d) is trivial. This corresponds to a quantum particle on the sphere with no internal degrees of freedom. In the case of S^2, this corresponds to taking the "twist" (in the notation of Kowalski and Rembieliński) to be zero. We show in Sec. IX that the little group acts trivially if and only if the following relation holds:

$$X^2 J_{kl}=J_{km}X_m X_l - J_{lm}X_m X_k\,. \tag{34}$$

This is the quantum counterpart of the classical constraint (9).

In computing $\mathbf{A}$ it is convenient to introduce "momentum" operators P_k given by

$$P_k := \frac{J_{kl}X_l}{r^2}.$$

These operators are *not* self-adjoint and we have chosen to put the J's to the left of the X's [because we have put $\mathbf{J}$ to the left of $\mathbf{X}$ in (32) and (33)]. We may rewrite (34) in terms of the P_k's as

$$J_{kl}=P_k X_l - P_l X_k\,. \tag{35}$$

The position and momentum operators satisfy

$$\frac{1}{i\hbar}[X_k, P_l]=\delta_{kl}I-\frac{X_k X_l}{r^2} \tag{36}$$

[compare (12)]. We may also compute using (25) the quantum counterpart of $\mathbf{x}\cdot\mathbf{p}=0$, which is really two relations on the quantum side,

$$\mathbf{P}\cdot\mathbf{X}=0,$$

$$\mathbf{X}\cdot\mathbf{P}=i\hbar d I.$$

We now write down the formulas that allow us to compute $\mathbf{A}$ in terms of $\mathbf{X}$ and $\mathbf{P}$,

$$\begin{aligned}\mathbf{J}\mathbf{X}&=r^2\mathbf{P},\\ \mathbf{J}\mathbf{P}&=-P^2\mathbf{X}+i\hbar(d-1)\mathbf{P}.\end{aligned} \tag{37}$$

The first line is simply the definition of **P**. The second line comes from (34) or (35) and is essential to the explicit calculation of the annihilation operators in terms of **X** and **P**. Note that there is an additional quantum correction here. To verify the second line of (37), write **J** in terms of **P** using (35) and then use (36).

We now treat **J** as a 2×2 matrix acting on the "basis" **X** and **P**, as given in (37). Since all the entries of this 2×2 matrix commute, we can just treat P^2 as a scalar and compute an ordinary 2×2 matrix exponential. So effectively we have

$$\mathbf{J}=\begin{pmatrix} 0 & -P^2 \\ r^2 & i\hbar(d-1) \end{pmatrix}.$$

One can then compute the exponential of this matrix either by hand or using a computer algebra program. A calculation shows that $P^2=r^{-2}J^2$ as in the classical case. It is convenient to express things in terms of the scalar operator,

$$J:=\sqrt{J^2+\hbar^2(d-1)^2/4}.$$

Then after exponentiating **J**, (33) becomes

$$\mathbf{A}=e^{\hbar/2m\omega r^2}\cosh\left(\frac{J}{m\omega r^2}\right)\mathbf{X}+e^{\hbar/2m\omega r^2}\frac{\hbar(d-1)}{2J}\sinh\left(\frac{J}{m\omega r^2}\right)\mathbf{X}+ie^{\hbar/2m\omega r^2}\frac{r^2}{J}\sinh\left(\frac{J}{m\omega r^2}\right)\mathbf{P}. \tag{38}$$

Equation (38) is similar to the corresponding classical expression (18), with only the following differences: (1) there is an overall factor of $\exp(\hbar/2m\omega r^2)$; (2) the quantity j in (18) is replaced by $(J^2+\hbar^2(d-1)^2/4)^{1/2}$; and (3) there is an extra sinh term in the coefficient of **X** that does not occur in the classical formula. Note that the above expression formally coincides with the classical one in the limit $\hbar\to 0$. In the case $d=2$ with $r=m\omega=\hbar=1$, (38) agrees with Eq. (4.16) in Ref. 18. In the case $d=3$ [identifying S^3 with SU(2) and adjusting for minor differences of normalization] (38) agrees with Eq. (3.132) in the last entry in Ref. 8. In the case $d=1$ we get an expression identical to the classical expression (19) except for an overall factor of $\exp(\hbar/m\omega r^2)$ [compare Eqs. (3.3) and (3.4) of Ref. 19].

It is clear from (38) that the A_k's are unbounded operators, as expected since the a_k's are unbounded functions. This means that the A_k's cannot be defined on the whole Hilbert space, but only on some dense subspace, which should be specified. We take the expression (29) as our definition of the annihilation operators. We first define the A_k's on what we will call the "minimal domain," namely, the space of finite linear combinations of spherical harmonics (that is, of eigenvectors for J^2). Expression (29) makes sense on the minimal domain, since each of the three factors making up A_k preserve this space. We consider also a "maximal domain" for the A_k's, defined as follows. Given any vector $|\phi\rangle$ in the Hilbert space, we expand $|\phi\rangle$ in a series expansion in terms of spherical harmonics. Then we apply A_k term-by-term, that is, by formally interchanging A_k with the sum. The result will then be a formal series of spherical harmonics. If this formal series converges in the Hilbert space then we say that $|\phi\rangle$ is in the maximal domain of A_k and that the value of $A_k|\phi\rangle$ is the sum of this series. (It can be shown that the product of x_k and a spherical harmonic of degree n is the sum of a spherical harmonic of degree $n+1$ and a spherical harmonic of degree $n-1$. It follows that the degree l term in the expansion of $A_k|\phi\rangle$ involves only the degree $n-1$ and degree $n+1$ terms of $|\phi\rangle$. So each term in the formal series for $A_k|\phi\rangle$ can be computed by means of a finite sum.)

It can be shown that if one starts with the operator A_k on its minimal domain and then takes its closure (in the functional analytic sense) the result is the operator A_k on its maximal domain. Thus if we want A_k to be a closed operator there is only one reasonable choice for its domain. The coherent states will not be finite linear combinations of spherical harmonics but will be in the maximal domain of all the A_k's.

V. THE COHERENT STATES

We are now ready to introduce the coherent states, which we define to be the simultaneous eigenvectors of the annihilation operators. These coherent states are *not of Perelomov type*. Although we have described the quantum Hilbert space as an irreducible representation of $\tilde{E}(d+1)$, the coherent states are not obtained from one fixed vector by the action of $\tilde{E}(d+1)$. Indeed the only elements of $\tilde{E}(d+1)$ that preserve the set of coherent states are the rotations. See Sec. X for a comparison of these coherent states to the generalized Perelomov-type coherent states for $\tilde{E}(d+1)$, as constructed either by De Bièvre or by Isham and Klauder.

The coherent states will be simultaneous eigenvectors of the annihilation operators A_k, and thus can be thought of as the quantum counterparts of a classical state with definite values for the complex coordinates a_k. On the quantum side, however, $A_k^\dagger$ does not commute with A_k, and thus although the coherent states satisfy $A_k|\psi\rangle = a_k|\psi\rangle$ they do *not* satisfy $A_k^\dagger|\psi\rangle = \overline{a_k}|\psi\rangle$.

We use formula (29) for the annihilation operators. If we introduce the dimensionless form of the total angular momentum,

$$\tilde{J}^2 = \frac{1}{\hbar^2} J^2,$$

then this may be expressed as

$$\mathbf{A} = e^{-\tau \tilde{J}^2/2} \mathbf{X} e^{\tau \tilde{J}^2/2}, \tag{39}$$

where τ is the dimensionless quantity given by

$$\tau = \frac{\hbar}{m\omega r^2}.$$

The parameter τ is a new feature of the sphere case; no such dimensionless quantity arises in the $\mathbb{R}^d$ case. The significance of τ for the coherent states is that it controls the ratio of the spatial width of the coherent states to the radius of the sphere. Specifically, we expect the approximate spatial width ΔX of a coherent state to be $\sqrt{\hbar/2m\omega}$, at least if this quantity is small compared to r. In that case

$$\frac{\Delta X}{r} \approx \frac{\sqrt{\hbar/2m\omega}}{r} = \sqrt{\frac{\tau}{2}}.$$

So if $\tau \ll 1$ we expect the coherent states to be concentrated in a small portion of the sphere, and to look, in appropriate coordinates, approximately Gaussian. This has been proven[8] for the case of $S^3 = \mathrm{SU}(2)$.

Kowalski and Rembieliński implicitly take $\tau = 1$ in their treatment of the $d = 2$ case, since they choose units with $m = r = \hbar = 1$, and since they do not have the parameter ω. (See our comments in Sec. III about the parameter ω.) To us this seems a needless loss of generality, even though it is easy to insert τ in the appropriate places in their formulas.

We now proceed with the construction of the coherent states. For each $\mathbf{a}$ in the *real* sphere S^d, let $|\delta_\mathbf{a}\rangle$ be the (generalized) position eigenfunction with $X_k|\delta_\mathbf{a}\rangle = a_k|\delta_\mathbf{a}\rangle$. Since we assume that the little group acts trivially these position eigenfunctions are (for each $\mathbf{a}$) unique up to a constant and we may normalize them so that the action of the rotation group takes $|\delta_\mathbf{a}\rangle$ to $|\delta_{R\mathbf{a}}\rangle$, $R \in \mathrm{SO}(d+1)$. If we let

$$|\psi_\mathbf{a}\rangle = e^{-\tau \tilde{J}^2/2}|\delta_\mathbf{a}\rangle, \tag{40}$$

then it follows immediately from (39) that $|\psi_\mathbf{a}\rangle$ is a simultaneous eigenvector for each A_k with eigenvalue a_k. Although $|\delta_\mathbf{a}\rangle$ is non-normalizable, the smoothing nature of the operator

$\exp(-\tau\tilde{J}^2/2)$ guarantees that $|\psi_{\mathbf{a}}\rangle$ is normalizable for all $\mathbf{a}\in S^d$. A key result of this section is the following proposition, which asserts that we can analytically continue the coherent states $|\psi_{\mathbf{a}}\rangle$ with respect to $\mathbf{a}$ so as to obtain states labeled by points $\mathbf{a}$ in the *complex* sphere $S^d_{\mathbb{C}}$.

Proposition 1: There exists a unique family of states $|\psi_{\mathbf{a}}\rangle$ *parameterized by* $\mathbf{a}\in S^d_{\mathbb{C}}$ *such that* (1) *the states depend holomorphically on* $\mathbf{a}$, *and* (2) *for* $\mathbf{a}\in S^d$, *they agree with the states in* (40). *These are normalizable states and satisfy*

$$A_k|\psi_{\mathbf{a}}\rangle = a_k|\psi_{\mathbf{a}}\rangle, \quad \mathbf{a}\in S^d_{\mathbb{C}}.$$

We call these states the *coherent states*. Note that we have then one coherent state for each point in $S^d_{\mathbb{C}}$, that is, one coherent state for each point in the classical phase space. It can be shown that these are (up to a constant) the *only* simultaneous eigenvectors of the annihilation operators. These coherent states are *not* normalized to be unit vectors. The proof of Proposition 1 is at the end of this section.

Note that since the operator $\tilde{J}^2$ commutes with rotations, the action of the rotation subgroup $\mathrm{SO}(d+1)$ of $E(d+1)$ will take $|\psi_{\mathbf{a}}\rangle$ to $|\psi_{R\mathbf{a}}\rangle$ for any $R\in\mathrm{SO}(d+1)$. On sufficiently regular states we can analytically continue the action of $\mathrm{SO}(d+1)$ to an action of $\mathrm{SO}(d+1;\mathbb{C})$, which will take $|\psi_{\mathbf{a}}\rangle$ to $|\psi_{R\mathbf{a}}\rangle$ for any $R\in\mathrm{SO}(d+1;\mathbb{C})$. Then any coherent state can be obtained from any other by the action of $\mathrm{SO}(d+1;\mathbb{C})$. Since, however, the action of $\mathrm{SO}(d+1;\mathbb{C})$ is neither unitary nor irreducible, this observation still does not bring the coherent states into the Perelomov framework.

We can give an explicit formula for the coherent states in the position representation in terms of the *heat kernel* on S^d. The heat kernel is the function on $S^d\times S^d$ given by $\rho_\tau(\mathbf{x},\mathbf{y}) = \langle\delta_{\mathbf{x}}|e^{-\tau\tilde{J}^2/2}|\delta_{\mathbf{y}}\rangle$. It can be shown (see Ref. 1 or the formulas below) that the ρ_τ extends (uniquely) to a holomorphic function on $S^d_{\mathbb{C}}\times S^d_{\mathbb{C}}$, also denoted ρ_τ. In terms of the analytically continued heat kernel the coherent states are given by

$$\langle\delta_{\mathbf{x}}|\psi_{\mathbf{a}}\rangle = \rho_\tau(\mathbf{a},\mathbf{x}), \quad \mathbf{a}\in S^d_{\mathbb{C}}, \mathbf{x}\in S^d. \tag{41}$$

Meanwhile, explicit formulas for the heat kernel may be found, for example, in Refs. 25 and 26. For $\mathbf{x}$ and $\mathbf{y}$ in the real sphere, $\rho_\tau(\mathbf{x},\mathbf{y})$ depends only on the angle θ between $\mathbf{x}$ and $\mathbf{y}$, where $\theta=\cos^{-1}(\mathbf{x}\cdot\mathbf{y}/r^2)$. This remains true for $\rho_\tau(\mathbf{a},\mathbf{x})$, with $\mathbf{a}\in S^d_{\mathbb{C}}$, except now $\theta=\cos^{-1}(\mathbf{a}\cdot\mathbf{x}/r^2)$ is complex-valued. Of course the inverse cosine function is multiple-valued, but because the heat kernel is an even, 2π-periodic function of θ, it does not matter which value of θ we use, provided that $\cos\theta=\mathbf{a}\cdot\mathbf{x}/r^2$.

We now record the formulas, writing ρ^d_τ to indicate the dependence on the dimension. For $d=1,2,3$ we have

$$\rho^1_\tau(\mathbf{a},\mathbf{x}) = (2\pi\tau)^{-1/2}\sum_{n=-\infty}^{\infty} e^{-(\theta-2\pi n)^2/2\tau},$$

$$\rho^2_\tau(\mathbf{a},\mathbf{x}) = (2\pi\tau)^{-1}e^{\tau/8}\frac{1}{\sqrt{\pi\tau}}\int_\theta^\pi \frac{1}{\sqrt{\cos\theta-\cos\phi}}\sum_{n=-\infty}^{\infty}(-1)^n(\phi-2\pi n)e^{-(\phi-2\pi n)^2/2\tau}\,d\phi,$$

$$\rho^3_\tau(\mathbf{a},\mathbf{x}) = (2\pi\tau)^{-3/2}e^{\tau/2}\frac{1}{\sin\theta}\sum_{n=-\infty}^{\infty}(\theta-2\pi n)e^{-(\theta-2\pi n)^2/2\tau}.$$

In the formula for ρ^2_τ we may without loss of generality take θ with $0\leqslant\mathrm{Re}\,\theta\leqslant\pi$, in which case the integral is to be interpreted as a contour integral in the strip $0\leqslant\mathrm{Re}\,\phi\leqslant\pi$. The relatively simple formula for the heat kernel on $S^3=\mathrm{SU}(2)$ allows for detailed calculations for the coherent states in this case, as carried out in Ref. 8. To find the formula in higher dimensions we use the inductive formula,

$$\rho_\tau^{d+2}(\mathbf{a},\mathbf{x}) = -e^{d\tau/2}\frac{1}{2\pi\sin\theta}\frac{d}{d\theta}\rho_\tau^d(\mathbf{a},\mathbf{x}).$$

There is also an expression for the heat kernel in terms of spherical harmonics. For example, when $d=2$ we have

$$\rho_\tau^2(\mathbf{a},\mathbf{x}) = \sum_{l=0}^{\infty} e^{-\tau l(l+1)/2}\sqrt{2l+1}P_l(\cos\theta), \tag{42}$$

where the P_l is the Legendre polynomial of degree l. [Compare Eq. (5.3) of Ref. 18.] The earlier expression for ρ_τ^2 is a sort of Poisson-summed version of (42) (see Ref. 26).

We also consider the reproducing kernel, defined by

$$R_\tau(\mathbf{a},\mathbf{b}) = \langle \psi_{\mathbf{b}} | \psi_{\mathbf{a}} \rangle, \quad \mathbf{a},\mathbf{b} \in S_{\mathbb{C}}^d. \tag{43}$$

In terms of the analytically continued heat kernel the reproducing kernel is given by

$$R_\tau(\mathbf{a},\mathbf{b}) = \rho_{2\tau}(\mathbf{a},\overline{\mathbf{b}}), \quad \mathbf{a},\mathbf{b} \in S_{\mathbb{C}}^d.$$

Note that $R_\tau(\mathbf{a},\mathbf{b})$ depends holomorphically on $\mathbf{a}$ and antiholomorphically on $\mathbf{b}$.

In the case of $S^1 = \mathrm{U}(1)$ and $S^3 = \mathrm{SU}(2)$, Thiemann and Winkler have proved in the second and third entries of Ref. 8 that the coherent states defined here satisfy good phase space localization properties and that the Ehrenfest theorem holds infinitesimally. We fully expect that these results hold for all d. This expectation is based on the idea that the heat kernel in (41) will behave for small τ like $c\exp(-\theta^2/2\tau)$, even for complex values of θ. Thiemann and Winkler have verified this in the cases $d=1,3$ and a similar analysis should be possible in general, using the explicit formulas for small d and the inductive formula for ρ^{d+2} in terms of ρ^d.

Proof of Proposition 1: There are two ways to prove this proposition. The simplest way is to use the expression for $\psi_{\mathbf{a}}$ in terms of the heat kernel ρ_τ and the explicit formulas above for ρ_τ. It is easily seen that ρ_τ extends to an entire holomorphic function of θ. Thus the expression $\langle \delta_{\mathbf{x}} | \psi_{\mathbf{a}} \rangle = \rho_\tau(\mathbf{a},\mathbf{x})$ makes sense for any $\mathbf{a}$ in $S_{\mathbb{C}}^d$, with $\cos\theta$ and thus also θ taking complex values. It is not hard to see that the $|\psi_{\mathbf{a}}\rangle$, so defined, is in the (maximal) domain of the annihilation operators and that it depends holomorphically on $\mathbf{a} \in S_{\mathbb{C}}^d$. Since $A_k|\psi_{\mathbf{a}}\rangle = a_k|\psi_{\mathbf{a}}\rangle$ for $\mathbf{a} \in S^d$, an analytic continuation argument will show that this equation remains true for all $\mathbf{a} \in S_{\mathbb{C}}^d$. Alternatively we may use the expansion of the coherent states in terms of spherical harmonics as in (42) and show that this expression can be analytically continued term-by-term in $\mathbf{a}$. (Compare Sec. IV of Ref. 1.) □

VI. THE RESOLUTION OF THE IDENTITY

We now choose a coordinate system in which $r=1$ and $m\omega=1$. This amounts to using the normalized position $\mathbf{x}/r$ and normalized momentum $\mathbf{p}/m\omega r$. Since these choices set our position and momentum scales we cannot also take $\hbar=1$. Note that the dimensionless parameter $\tau = \hbar/m\omega r^2$ equals $\hbar$ in such a coordinate system. We now write $|\psi_{\mathbf{x},\mathbf{p}}\rangle$ for $|\psi_{\mathbf{a}(\mathbf{x},\mathbf{p})}\rangle$.

Theorem 2: *The coherent states have a resolution of the identity of the form,*

$$I = \int_{\mathbf{x}\in S^d}\int_{\mathbf{p}\cdot\mathbf{x}=0} |\psi_{\mathbf{x},\mathbf{p}}\rangle\langle\psi_{\mathbf{x},\mathbf{p}}|\ \nu(2\tau,2p)\left(\frac{\sinh 2p}{2p}\right)^{d-1} 2^d d\mathbf{p}\, d\mathbf{x}, \tag{44}$$

where $\nu(s,R)$ is the solution to the differential equation,

$$\frac{d\nu(s,R)}{ds} = \frac{1}{2}\left[\frac{\partial^2\nu}{\partial R^2} - (d-1)\frac{\cosh R}{\sinh R}\frac{\partial\nu}{\partial R}\right],$$

subject to the initial condition,

$$\lim_{s\downarrow 0} c_d \int_0^\infty f(R)\,\nu(s,R)(\sinh R)^{d-1}\,dR = f(0)$$

for all continuous functions f on $[0,\infty)$ with at most exponential growth at infinity. Here $d\mathbf{x}$ is the surface area measure on S^d, τ is the dimensionless quantity $\tau=\hbar/m\omega r^2$, and c_d is the volume of the unit sphere in $\mathbb{R}^d$.

The operator on the right-hand side of the equation for ν is just the radial part of the Laplacian for d-dimensional hyperbolic space (Ref. 27, Sec. 5.7). This means that $\nu(s,R)$ is the heat kernel for hyperbolic space, that is, the fundamental solution of the heat equation. Hyperbolic space is the noncompact, negatively curved "dual" of the compact, positively curved symmetric space S^d. Note that the function ν is evaluated at "time" 2τ and radius $2p$. The inversion formula for the Segal–Bargmann transform, described in Sec. VII, involves the function ν evaluated at time τ and radius p.

The resolution of the identity for the coherent states will be obtained by continuously varying the dimensionless parameter τ. When $\tau=0$ the coherent states are simply the position eigenvectors, which have a resolution of the identity because the position operators are self-adjoint. We will show that the function ν satisfies the correct differential equation to make the resolution of the identity remain true as we move to nonzero τ.

Theorem 2 is a special case of Theorem 3 of Ref. 17, written out more explicitly and restated in terms of coherent states instead of the Segal–Bargmann transform. However we give below a self-contained and elementary proof. The case $d=2$ is also described (with a different proof) in Ref. 20. Since $S^3=\mathrm{SU}(2)$, the $d=3$ case belongs to the group case, which is found in Ref. 1. See also Sec. IV D of the second entry in Ref. 8 for another proof in the SU(2) case.

We report here the formulas for the function $\nu(s,R)$, which may be found, for example, in Ref. 27 Sec. 5.7 or Ref. 26 Eq. (8.73). Writing $\nu_d(s,R)$ to make explicit the dependence on the dimension we have

$$\nu_1(s,R)=(2\pi s)^{-1/2}e^{-R^2/2s},$$

$$\nu_2(s,R)=(2\pi s)^{-1}e^{-s/8}\frac{1}{\sqrt{\pi s}}\int_R^\infty \frac{\rho e^{-\rho^2/2s}}{(\cosh\rho-\cosh R)^{1/2}}\,d\rho,$$

$$\nu_3(s,R)=(2\pi s)^{-3/2}e^{-s/2}\frac{R}{\sinh R}e^{-R^2/2s},$$

and the recursion relation

$$\nu_{d+2}(s,R)=-\frac{e^{-ds/2}}{2\pi\sinh R}\frac{\partial}{\partial R}\nu_d(s,R).$$

Estimates on the behavior as $R\to\infty$ of ν may be found in Ref. 27, Sec. 5.7 and in Ref. 28. Note the similarities between the formulas for ν and the formulas for the heat kernel ρ_τ on the sphere.

Some care must be taken in the interpretation of the integral (44). Even in the $\mathbb{R}^d$ case this integral is not absolutely convergent in the operator norm sense. Rather the appropriate sense of convergence is the weak sense. This means that for all vectors ϕ_1,ϕ_2 in the Hilbert space we have

$$\langle\phi_1|\phi_2\rangle=\int_{\mathbf{x}\in S^d}\int_{\mathbf{p}\cdot\mathbf{x}=0}\langle\phi_1|\psi_{\mathbf{x},\mathbf{p}}\rangle\langle\psi_{\mathbf{x},\mathbf{p}}|\phi_2\rangle\;\nu(2\tau,2p)\left(\frac{\sinh 2p}{2p}\right)^{d-1}2^d d\mathbf{p}\,d\mathbf{x}, \tag{45}$$

where the integral (45) is an absolutely convergent complex-valued integral. This of course is formally equivalent to (44). We will prove Theorem 2 at first without worrying about convergence or other similar technicalities. Then at the end we will explain how such matters can be dealt with.

Proof of Theorem 2: We now write the coherent states as $|\psi_{\mathbf{a}}^{\tau}\rangle$ to emphasize the dependence on the dimensionless quantity $\tau=\hbar/m\omega r^2$. We regard the coherent states $|\psi_{\mathbf{a}}^{\tau}\rangle$ as living in some fixed (τ-independent) Hilbert space [for example, $L^2(S^d)$] and given heuristically by

$$|\psi_{\mathbf{a}}^{\tau}\rangle = e^{-\tau\tilde{J}^2/2}|\delta_{\mathbf{a}}\rangle, \quad \mathbf{a}\in S_{\mathbb{C}}^d, \tag{46}$$

where $|\delta_{\mathbf{a}}\rangle$ is a position eigenvector. Our strategy is essentially the one proposed by Thiemann in a more general setting in Ref. 7, Sec. 2.3. We begin with two lemmas that allow us to carry out this strategy explicitly in this situation. The proofs of these lemmas are given at the end of the proof of Theorem 2.

Lemma 3: The measure

$$\left(\frac{\sinh 2p}{2p}\right)^{d-1} 2^d d\mathbf{p}\, d\mathbf{x}$$

is invariant under the action of $\mathrm{SO}(d+1;\mathbb{C})$ *on* $S_{\mathbb{C}}^d \cong T^*(S^d)$.

Lemma 4: Let $J_{\mathbf{a}}^2$ *and* $J_{\overline{\mathbf{a}}}^2$ *denote the differential operators on* $S_{\mathbb{C}}^d$ *given by*

$$J_{\mathbf{a}}^2 = -\sum_{k<l}\left(a_l\frac{\partial}{\partial a_k} - a_k\frac{\partial}{\partial a_l}\right)^2,$$

$$J_{\overline{\mathbf{a}}}^2 = -\sum_{k<l}\left(\overline{a}_l\frac{\partial}{\partial \overline{a}_k} - \overline{a}_k\frac{\partial}{\partial \overline{a}_l}\right)^2.$$

Let ϕ *be a smooth, even, real-valued function on* $\mathbb{R}$ *and consider the function on* $S_{\mathbb{C}}^d$ *given by*

$$\phi(2p),$$

where p *is regarded as a function of* $\mathbf{a}$ *by means of (18). Then,*

$$J_{\mathbf{a}}^2\phi(2p) = J_{\overline{\mathbf{a}}}^2\phi(2p) = -\left[\frac{\partial^2\phi}{\partial R^2} + (d-1)\frac{\cosh R}{\sinh R}\frac{\partial\phi}{\partial R}\right]_{R=2p}.$$

Assuming for now the two lemmas, we proceed with the proof of the resolution of the identity. Because the coherent states depend holomorphically on $\mathbf{a}$ they satisfy

$$J_{\overline{\mathbf{a}}}^2|\psi_{\mathbf{a}}^{\tau}\rangle = 0.$$

Furthermore, it follows from the definition of the coherent states that

$$\frac{d}{d\tau}|\psi_{\mathbf{a}}^{\tau}\rangle = \frac{1}{2}J_{\mathbf{a}}^2|\psi_{\mathbf{a}}^{\tau}\rangle.$$

The proof of this is essentially the standard calculation of the action of $\tilde{J}^2$ in the position representation. It then follows that the projection operator $|\psi_{\mathbf{a}}^{\tau}\rangle\langle\psi_{\mathbf{a}}^{\tau}|$ satisfies the operator-valued differential equation,

$$\frac{\partial}{\partial\tau}|\psi_{\mathbf{a}}^{\tau}\rangle\langle\psi_{\mathbf{a}}^{\tau}| = \frac{1}{2}(J_{\mathbf{a}}^2 + J_{\overline{\mathbf{a}}}^2)|\psi_{\mathbf{a}}^{\tau}\rangle\langle\psi_{\mathbf{a}}^{\tau}|.$$

Now we let

$$\beta(p)=2^d\left(\frac{\sinh 2p}{2p}\right)^{d-1}. \tag{47}$$

Since by Lemma 3 the measure $\beta(p)\,d\mathbf{p}\,d\mathbf{x}$ is invariant under the action of $\mathrm{SO}(d+1;\mathbb{C})$ the operators $J_{\mathbf{a}}^2$ and $J_{\bar{\mathbf{a}}}^2$ are self-adjoint in $L^2(S_{\mathbb{C}}^d,\beta(p)\,d\mathbf{p}\,d\mathbf{x})$. Thus differentiating under the integral sign and using the self-adjointness gives

$$\frac{d}{d\tau}\int_{\mathbf{x}\in S^d}\int_{\mathbf{p}\cdot\mathbf{x}=0}|\psi_{\mathbf{a}}^\tau\rangle\langle\psi_{\mathbf{a}}^\tau|\;\nu(2\tau,2p)\beta(p)\,d\mathbf{p}\,d\mathbf{x}$$

$$=\int_{\mathbf{x}\in S^d}\int_{\mathbf{x}\cdot\mathbf{p}=0}|\psi_{\mathbf{a}}^\tau\rangle\langle\psi_{\mathbf{a}}^\tau|\left[\frac{\partial}{\partial\tau}+\frac{1}{2}(J_{\mathbf{a}}^2+J_{\bar{\mathbf{a}}}^2)\nu(2\tau,2p)\right]\beta(p)\,d\mathbf{p}\,d\mathbf{x}.$$

Lemma 4 and the differential equation satisfied by $\nu(s,R)$ tell us that the last integral is zero. Thus the operator on the right-hand side in (44) is independent of τ. On the other hand, the initial conditions for ν imply that as τ tends to zero the measure $\nu(2\tau,2p)\beta(p)\,d\mathbf{p}\,d\mathbf{x}$ "collapses" to the Lebesgue measure $d\mathbf{x}$ on the real sphere, i.e., the set where $\mathbf{p}=0$. Furthermore, if we consider coherent states $|\psi_{\mathbf{x},\mathbf{p}}^\tau\rangle$ with $\mathbf{p}=0$, these become simply $|\delta_{\mathbf{x}}\rangle$ in the $\tau\downarrow 0$ limit. Thus

$$\lim_{\tau\downarrow 0}\int_{\mathbf{x}\in S^d}\int_{\mathbf{p}\cdot\mathbf{x}=0}|\psi_{\mathbf{x},\mathbf{p}}^\tau\rangle\langle\psi_{\mathbf{x},\mathbf{p}}^\tau|\;\nu(2\tau,2p)\beta(p)\,d\mathbf{p}\,d\mathbf{x}=\int_{S^d}|\delta_{\mathbf{x}}\rangle\langle\delta_{\mathbf{x}}|\,d\mathbf{x}=I.$$

Since the value of the first integral is independent of τ this shows that the integral equals the identity for all τ. □

It remains now to prove Lemmas 3 and 4. We begin with the second lemma.

Proof of Lemma 4: Note that expressions such as $\partial/\partial a_k$ do not make sense when applied to a function that is defined only on the complex sphere $S_{\mathbb{C}}^d$. So the operator $a_l\partial/\partial a_k-a_k\partial/\partial a_l$ (and its complex conjugate) should be interpreted as follows. Given a smooth function f on $S_{\mathbb{C}}^d$, extend f smoothly to a neighborhood of $S_{\mathbb{C}}^d$, then apply $a_l\partial/\partial a_k-a_k\partial/\partial a_l$, and then restrict again to $S_{\mathbb{C}}^d$. Since $(a_l\partial/\partial a_k-a_k\partial/\partial a_l)a^2=0$ the derivatives are all in directions tangent to $S_{\mathbb{C}}^d$. This means that the value of the operator on $S_{\mathbb{C}}^d$ is independent of the choice of the extension. It is in this way that $J_{\mathbf{a}}^2$ and $J_{\bar{\mathbf{a}}}^2$ are to be interpreted as operators on $S_{\mathbb{C}}^d$.

Now let $R=2p$ and let $\alpha=|\mathbf{a}|^2=\Sigma|a_k|^2$. Then (18) (with $r=m\omega=1$) tells us that

$$\alpha:=|\mathbf{a}|^2=\cosh^2 p+\sinh^2 p=\cosh 2p.$$

So, $R=2p=\cosh^{-1}\alpha$. We now need to apply $J_{\mathbf{a}}^2$ to a function of the form $\phi(R)$, which we do by using the chain rule

$$\frac{\partial\phi}{\partial a_k}=\frac{d\phi}{dR}\frac{dR}{d\alpha}\frac{\partial\alpha}{\partial a_k}.$$

Calculation shows that (for $k\neq l$),

$$\left(a_l\frac{\partial}{\partial a_k}-a_k\frac{\partial}{\partial a_l}\right)^2\phi(R)=\frac{(a_k\overline{a_l}-a_l\overline{a_k})^2}{|\mathbf{a}|^4-1}\frac{\partial^2\phi}{\partial R^2}-\frac{(|a_k|^2+|a_l|^2)(|\mathbf{a}|^4-1)+|\mathbf{a}|^2(a_k\overline{a_l}-a_l\overline{a_k})^2}{(|\mathbf{a}|^4-1)^{3/2}}\frac{\partial\phi}{\partial R}. \tag{48}$$

We now note that

$$\sum_{k<l}(|a_k|^2+|a_l|^2)=\frac{1}{2}\sum_{k,l}(1-\delta_{kl})(|a_k|^2+|a_l|^2)=\frac{1}{2}[2(d+1)|\mathbf{a}|^2-2|\mathbf{a}|^2]=d\,|\mathbf{a}|^2. \tag{49}$$

We use also the easily verified identity

$$\sum_{k<l} (a_k \overline{a_l} - a_l \overline{a_k})^2 = -(|\mathbf{a}|^4 - |a^2|^2) = -(|\mathbf{a}|^4 - 1), \tag{50}$$

where the first equality is valid everywhere and the second equality is valid on the complex sphere $S^d_{\mathbb{C}} = \{a^2 = 1\}$.

Using (49) and (50) we get, upon summing (48) over $k<l$,

$$\sum_{k<l} \left(a_l \frac{\partial}{\partial a_k} - a_k \frac{\partial}{\partial a_l} \right)^2 \phi(R) = -\frac{\partial^2 \phi}{\partial R^2} - (d-1) \frac{|\mathbf{a}|^2}{\sqrt{|\mathbf{a}|^4 - 1}} \frac{\partial \phi}{\partial R}.$$

Recalling that $|\mathbf{a}|^2 = \cosh R$, so that $\sqrt{|\mathbf{a}|^4 - 1} = \sinh R$, we get the claimed formula. This completes the proof of the second lemma (with the same argument for the conjugated case). □

Proof of Lemma 3: Our proof is indirect and uses Lemma 4. We regard $S^d_{\mathbb{C}}$ as the quotient $\mathrm{SO}(d+1;\mathbb{C})/\mathrm{SO}(d;\mathbb{C})$. Since both $\mathrm{SO}(d+1;\mathbb{C})$ and $\mathrm{SO}(d;\mathbb{C})$ are unimodular, general principles (Ref. 29 Theorem. 8.36) tell us that there is a smooth $\mathrm{SO}(d+1;\mathbb{C})$-invariant measure on $S^d_{\mathbb{C}}$ and that it is unique up to a constant. This measure must be in particular $\mathrm{SO}(d+1)$-invariant, which means that it must be of the form $\gamma(p)\, d\mathbf{p}\, d\mathbf{x}$, since $d\mathbf{p}\, d\mathbf{x}$ is also $\mathrm{SO}(d+1)$-invariant. Now the operator $J^2_{\mathbf{a}}$ must be self-adjoint with respect to the $\mathrm{SO}(d+1;\mathbb{C})$-invariant measure. In particular, $J^2_{\mathbf{a}}$ must be self-adjoint when restricted to the space of $\mathrm{SO}(d+1)$-invariant functions, which can all be written in the form $f(\mathbf{a}) = \phi(2p)$, as in Lemma 4.

Meanwhile, according to Lemma 4, on $\mathrm{SO}(d+1)$-invariant functions $J^2_{\mathbf{a}}$ is just the hyperbolic Laplacian, rescaled by a factor of 2. This operator is therefore self-adjoint [on $\mathrm{SO}(d+1)$-invariant functions] with respect to the measure $\beta(p)\, d\mathbf{p}\, d\mathbf{x}$, which is just hyperbolic volume measure with the same rescaling.

We conclude, then, that on $\mathrm{SO}(d+1)$-invariant functions, $J^2_{\mathbf{a}}$ is self-adjoint with respect to both the measures $\gamma(p)\, d\mathbf{p}\, d\mathbf{x}$ and $\beta(p)\, d\mathbf{p}\, d\mathbf{x}$. From this it follows that

$$\left[\frac{\partial^2 g}{\partial R^2} + (d-1) \frac{\cosh R}{\sinh R} \frac{\partial g}{\partial R} \right]_{R=2p} = 0, \tag{51}$$

where $g(p) = \gamma(p)/\beta(p)$. But since both γ and β are smooth, $\mathrm{SO}(d+1)$-invariant functions on $S^d_{\mathbb{C}}$ we must have $\partial g/\partial R|_{R=0} = 0$. Solving (51) gives $\partial g/\partial R = c \exp[-(d-1)\int \coth S\, dS]$, so we have

$$\left. \frac{\partial g}{\partial R} \right|_{R=0} = c \lim_{\varepsilon \to 0} \exp\left[(d-1) \int_{\varepsilon}^{1} \coth S\, dS \right] = 0,$$

which can occur only if $c=0$, i.e., if g is constant. Thus γ is a constant multiple of β, which is what we want to show. □

We conclude this section with a few remarks about technicalities in the proof of the resolution of the identity. We have already said that the integral in Theorem 2 is to be interpreted in the weak sense, as in (45). We first establish (45) in the case where $|\phi_1\rangle$ and $|\phi_2\rangle$ are finite linear combinations of spherical harmonics. In that case it can be shown that the integrand $\langle \phi_1 | \psi^{\tau}_{\mathbf{x},\mathbf{p}} \rangle \times \langle \psi^{\tau}_{\mathbf{x},\mathbf{p}} | \phi_2 \rangle$ grows only exponentially with $\mathbf{p}$. Since ν has a faster-than-exponential decay (namely, Gaussian) the integral (45) is convergent. In this case there is not much difficulty in justifying the formal manipulations we have made, such as interchanging derivatives with the integral and integrating by parts. Then once (45) is established for such "nice" vectors, a simple passage to the limit will establish it for all $|\phi_1\rangle$ and $|\phi_2\rangle$ in the Hilbert space. See Refs. 1 or 17 for more details on these technicalities.

VII. THE SEGAL–BARGMANN REPRESENTATION

As shown in Sec. IX, any two irreducible unitary representations of $\tilde{E}(d+1)$ satisfying (26) and (34) are equivalent. The simplest concrete realization of such representations is the position

representation, in which the Hilbert space is $L^2(S^d)$, the position operators act by multiplication, and the angular momentum operators act as differential operators given by

$$J_{kl} = -i\hbar\left(x_l \frac{\partial}{\partial x_k} - x_k \frac{\partial}{\partial x_l} \right). \tag{52}$$

The resolution of the identity for the coherent states can be used to give another realization, the (generalized) Segal–Bargmann representation. In the Segal–Bargmann representation the Hilbert space is the space of holomorphic functions on $S^d_{\mathbb{C}}$ that are square-integrable with respect to the density occurring in the resolution of the identity. In this representation the action of the position operators X_k is somewhat complicated, but the action of the creation operators (the adjoints of the annihilation operators) becomes simply multiplication by a_k. The resolution of the identity can be reinterpreted as the unitary intertwining map between these two representations, that is, the generalized Segal–Bargmann transform.

Specifically, given any function f in $L^2(S^d)$ we define the Segal–Bargmann transform Cf of f by

$$Cf(\mathbf{a}) = \langle \overline{\psi_{\mathbf{a}}} | f \rangle. \tag{53}$$

Then for any f, $Cf(\mathbf{a})$ is a holomorphic function of $\mathbf{a} \in S^d_{\mathbb{C}}$. Note that in the interests of consistency with Refs. 1, 17 we have put a complex conjugate on the $\mathbf{a}$ in (53), so that the dependence of Cf on $\mathbf{a} \in S^d_{\mathbb{C}}$ is holomorphic rather than antiholomorphic. The Segal–Bargmann transform can be computed as

$$Cf(\mathbf{a}) = \int_{S^d} \rho_\tau(\mathbf{a},\mathbf{x}) f(\mathbf{x}) d\mathbf{x}, \quad \mathbf{a} \in S^d_{\mathbb{C}}. \tag{54}$$

Here $\rho_\tau(\mathbf{a},\mathbf{x})$ is the heat kernel on S^d, with the $\mathbf{a}$ variable extended by analytic continuation from S^d to $S^d_{\mathbb{C}}$.

Theorem 5 (Segal–Bargmann transform): *The map C defined by (53) or (54) is a unitary map of $L^2(S^d, d\mathbf{x})$ onto $\mathcal{H}L^2(S^d_{\mathbb{C}}, \nu)$, where $\mathcal{H}L^2(S^d_{\mathbb{C}}, \nu)$ denotes the space of holomorphic functions F on $S^d_{\mathbb{C}}$ for which*

$$\int_{\mathbf{x} \in S^d} \int_{\mathbf{p}\cdot\mathbf{x}=0} |F(\mathbf{a}(\mathbf{x},\mathbf{p}))|^2 \nu(2\tau, 2p) \left(\frac{\sinh 2p}{2p} \right)^{d-1} 2^d d\mathbf{p}\, d\mathbf{x} < \infty.$$

The isometricity of the map C as a map from $L^2(S^d)$ into $L^2(S^d_{\mathbb{C}}, \nu)$ is equivalent to the resolution of the identity [compare (45)]. That C maps into the holomorphic subspace of $L^2(S^d_{\mathbb{C}}, \nu)$ follows from the holomorphic dependence of the coherent states on $\mathbf{a}$. It remains only to show that the image of C is *all* of $\mathcal{H}L^2(S^d_{\mathbb{C}}, \nu)$. The proof of this is a fairly straightforward density argument using spherical harmonics, which we omit. (See Sec. IV of Ref. 17 and Sec. VIII of Ref. 1.)

In the Segal–Bargmann space $\mathcal{H}L^2(S^d_{\mathbb{C}}, \nu)$ the angular momentum operators act by the holomorphic analog of (52), namely,

$$J_{kl} = -i\hbar\left(a_l \frac{\partial}{\partial a_k} - a_k \frac{\partial}{\partial a_l} \right).$$

Meanwhile, the *creation* operators, defined as the adjoints of the annihilation operators, are given by

$$A_k^\dagger F(\mathbf{a}) = a_k F(\mathbf{a}).$$

The annihilation operators can be described as *Toeplitz operators*. This means that

$$A_k F = P(\overline{a_k} F),$$

where P is the orthogonal projection from the full L^2-space $L^2(S^d_{\mathbb{C}},\nu)$ onto the holomorphic subspace (see Ref. 33). In the Segal–Bargmann representation the action of the position operators is more complicated.

Another important feature of the Segal–Bargmann representation is the reproducing kernel identity. Recall from Sec. V that the reproducing kernel $R_\tau(\mathbf{a},\mathbf{b})=\langle \psi_{\mathbf{b}} | \psi_{\mathbf{a}} \rangle$ is holomorphic in $\mathbf{a}$ and antiholomorphic in $\mathbf{b}$. We then have the following result, which follows easily from general principles. (See, for example, Sec. IX of Ref. 1.)

Proposition 6 (Reproducing kernel identity): For any $F \in \mathcal{H}L^2(S^d_{\mathbb{C}},\nu)$ we have

$$F(\mathbf{a})=\int_{\mathbf{x}\in S^d}\int_{\mathbf{p}\cdot\mathbf{x}=0} R_\tau(\mathbf{a},\mathbf{b})F(\mathbf{b}(\mathbf{x},\mathbf{p}))\,\nu(2\tau,2p)\left(\frac{\sinh 2p}{2p}\right)^{d-1} 2^d d\mathbf{p}\; d\mathbf{x}.$$

Here $R_\tau(\mathbf{a},\mathbf{b})=\rho_{2\tau}(\mathbf{a},\overline{\mathbf{b}})$ is the reproducing kernel, and the integral is absolutely convergent.

The Segal–Bargmann representation can be thought of as defining a *phase space wave function* for a quantum particle on the sphere, which is related to the position wave function by the Segal–Bargmann transform. This phase space wave function can then be turned into a *phase space probability density* in the usual way: if f is a unit vector in $L^2(S^d)$ then the associated probability density is

$$|Cf(\mathbf{a}(\mathbf{x},\mathbf{p}))|^2\,\nu(2\tau,2p)\left(\frac{\sinh 2p}{2p}\right)^{d-1} 2^d. \tag{55}$$

This is a manifestly non-negative function on the phase space that integrates to one. In the $\mathbb{R}^d$ case,[33] the expression corresponds to the *Husimi function* of f.

If one takes the probability density (55) and integrates out the momentum variables one will *not* get the standard position probability density $|f(\mathbf{x})|^2$ (even in the $\mathbb{R}^d$ case). That is, with this definition, the position probability density cannot be obtained from the phase space probability density by integrating out the momentum variables. On the other hand, there is a nice inversion formula for the generalized Segal–Bargmann transform that can be stated roughly as follows: the position *wave function* can be obtained from the phase space *wave function* by integrating out the momentum variables.

Theorem 7 (Inversion Formula): *Given any function f in $L^2(S^d)$, let $F=Cf$ be the Segal–Bargmann transform of f. Then f may be recovered from F by the formula,*

$$f(\mathbf{x})=\int_{\mathbf{p}\cdot\mathbf{x}=0} F(\mathbf{a}(\mathbf{x},\mathbf{p}))\,\nu(\tau,p)\left(\frac{\sinh p}{p}\right)^{d-1} d\mathbf{p}. \tag{56}$$

This result is a special case of Ref. 17; the group analog of this inversion formula was given in Ref. 3. An analog of this formula holds also in the $\mathbb{R}^d$ case (Ref. 4, Sec. IV), but does not seem to be well known. Note that whereas the resolution of the identity involves $\nu(2\tau,2p)$, the inversion formula involves $\nu(\tau,p)$.

This statement of the inversion formula is a bit imprecise, because we have glossed over the question of the convergence of the integral in (56). The integral cannot always be convergent, since a general function f in $L^2(S^d)$ can have singularities. As shown in Theorems 1 and 2 of Ref. 17, we have the following two precise statements. First, if f is sufficiently smooth, then the integral in (56) is absolutely convergent for all $\mathbf{x}$ and is equal to $f(\mathbf{x})$. Second, for any $f \in L^2(S^d)$ we have

$$f(\mathbf{x})=\lim_{R\to\infty}\int_{\substack{\mathbf{p}\cdot\mathbf{x}=0\\ p\le R}} F(\mathbf{a}(\mathbf{x},\mathbf{p}))\,\nu(\tau,p)\left(\frac{\sinh p}{p}\right)^{d-1} d\mathbf{p},$$

where the limit is in the topology of $L^2(S^d)$.

We will describe the proof of Theorem 7 in greater detail in the setting of general compact symmetric spaces. Here we give only the barest outline. The Cauchy–Riemann equations on $S^d_{\mathbb{C}}$ imply that, when applied to holomorphic functions, the hyperbolic Laplacian in the momentum variables is the negative of the spherical Laplacian in the position variables, just as for holomorphic functions on $\mathbb{C}$ we have $\partial^2 F/\partial y^2 = -\partial^2 F/\partial x^2$. For this result to hold, we must omit the rescaling of the momentum variables that is present in the resolution of the identity; hence the inversion formula involves $\nu(\tau,p)$ rather than $\nu(2\tau,2p)$. The integration in (56) against the hyperbolic heat kernel is computing the forward heat equation in the momentum variables, which for holomorphic functions is then the same as the backward heat equation in the position variables. Since the Segal–Bargmann transform may be computed in terms of the forward heat equation in the position variables, (56) is inverting the Segal–Bargmann transform. Although this is the basic idea of the proof, the convergence questions are more subtle.

Note that there are, besides (56), many other inversion formulas for the Segal–Bargmann transform. The ''overcompleteness'' of the coherent states means that there is a lot of redundant information in the Segal–Bargmann transform, and therefore many different ways that one can recover f from Cf. To look at it another way, it is possible to have many different integrals that all give the same value when applied to holomorphic functions, as in the Cauchy integral formula. Of particular importance is the inversion formula,

$$f(\mathbf{x}') = \int_{S^d_{\mathbb{C}}} \overline{\rho_\tau(\mathbf{a},\mathbf{x}')} F(\mathbf{a}(\mathbf{x},\mathbf{p}))\, \nu(2\tau,2p) \left(\frac{\sinh 2p}{2p}\right)^{d-1} 2^d d\mathbf{p}\, d\mathbf{x},$$

where ρ_τ is the analytical continuation of the heat kernel for S^d. This formula is obtained by noting that C is isometric, and therefore its inverse is its adjoint. One can apply the above integral to any function F in $L^2(S^d_{\mathbb{C}},\nu)$ (not necessarily holomorphic), in which case we have $f = C^{-1}PF$, where PF is the orthogonal projection of F onto the holomorphic subspace of $L^2(S^d_{\mathbb{C}},\nu)$. See Ref. 1, Sec. IX and Ref. 20, Eq. (6.13).

VIII. THE $\mathbb{R}^d$ CASE

We verify in this section that the methods in this paper, when applied to the $\mathbb{R}^d$ case, do indeed reproduce the canonical coherent states. Our ''complexifier'' is $1/\omega$ times the kinetic energy function, namely, $p^2/2m\omega$. (In the $\mathbb{R}^d$ case the kinetic energy cannot be expressed in terms of the angular momentum.) Then we define

$$a_k = e^{i\{\cdot,\text{complexifier}\}} x_k = \sum_{n=0}^{\infty} \left(\frac{i}{2m\omega}\right)^n \frac{1}{n!} \underbrace{\{\ldots\{\{x_k,p^2\},p^2\},\ldots,p^2\}}_{n}.$$

Since $\{x_k,p^2\} = 2p_k$ and $\{\{x_k,p^2\},p^2\} = 0$ we obtain

$$a_k = x_k + i\frac{p_k}{m\omega}.$$

This is, up to an overall constant, the standard complex coordinate on phase space. More generally one can apply the same method to any function of the x_k's, and one will obtain the corresponding function of a_k. For example, it is easily verified by induction that

$$e^{i\{\cdot,\text{complexifier}\}}(x_k^n) = \left(x_k + i\frac{p_k}{m\omega}\right)^n$$

for all positive integers n.

Similarly on the quantum side if we define the complexifier to be $P^2/2m\omega$ and

$$A_k = e^{i[\,\cdot\,,\text{complexifier}]/i\hbar} X_k = \sum_{n=0}^{\infty} \frac{1}{(2m\omega\hbar)^n} \frac{1}{n!} [\cdots[[X_k, P^2], P^2]\cdots, P^2]$$

we get simply

$$A_k = X_k + i\frac{P_k}{m\omega}.$$

This is, up to an overall constant, the usual annihilation operator. Applying the same procedure to any function of the X_k's will give the corresponding function of the A_k's.

Following the same normalization procedure as in the sphere case we obtain coherent states given by

$$|\psi_{\mathbf{a}}\rangle = e^{-P^2/2m\omega\hbar}|\delta_{\mathbf{a}}\rangle,$$

at first for $\mathbf{a} \in \mathbb{R}^d$ and then by analytic continuation for any $\mathbf{a} \in \mathbb{C}^d$. In the $\mathbb{R}^d$ case we have the formula

$$|\psi_{\mathbf{a}}\rangle = e^{i\mathbf{a}\cdot\mathbf{P}/\hbar}|\psi_0\rangle.$$

This normalization coincides with what Hecht[30] calls type I coherent states. In the position representation we have

$$\langle \delta_{\mathbf{x}}|\psi_{\mathbf{a}}\rangle = (2\pi\hbar/m\omega)^{-d/2} \exp\left[-\frac{(\mathbf{x}-\mathbf{a})^2}{2\hbar/m\omega}\right].$$

With this normalization of the coherent states the resolution of the identity takes the form

$$I = \int_{\mathbb{C}^d} |\psi_{\mathbf{a}}\rangle\langle\psi_{\mathbf{a}}|\,\gamma(\mathbf{a})\,d\mathbf{a},$$

where $d\mathbf{a}$ is $2d$-dimensional Lebesgue measure and where γ is the density

$$\gamma(\mathbf{a}) = \left(\frac{\pi\hbar}{m\omega}\right)^{-d/2} \exp\left[-\frac{(\mathrm{Im}\,\mathbf{a})^2}{\hbar/m\omega}\right].$$

The associated Segal–Bargmann space is the space of holomorphic functions on $\mathbb{C}^d$ that are square-integrable with respect to the density γ. This normalization of the Segal–Bargmann space is different from that of Segal[31] and Bargmann,[32] because of the different normalization of the coherent states. See Ref. 33, Sec. VI for comparisons with the conventions of Segal and of Bargmann.

To compare this to what we have in the sphere case, let $\sigma = \hbar/m\omega$ and consider the Euclidean heat kernel in the imaginary directions, given by

$$\nu(\sigma, \mathbf{a}) = (2\pi\sigma)^{-d/2} \exp\left[-\frac{(\mathrm{Im}\,\mathbf{a})^2}{2\sigma}\right].$$

Then $\gamma(\mathbf{a}) = 2^d \nu(2\sigma, 2\mathbf{a})$, similar to what we have in the sphere case. Note that in the Euclidean case $\nu(2\sigma, 2\mathbf{a})$ is the same, up to an overall constant, as $\nu(\sigma/2, \mathbf{a})$. Thus it is hard to see the "correct" scaling of the space and time variables from the Euclidean case.

An inversion formula similar to Theorem 7 holds in the $\mathbb{R}^d$ case; see Ref. 4, Sec. IV.

IX. REPRESENTATION THEORY OF THE EUCLIDEAN GROUP

We consider representations by self-adjoint operators of the commutation relations (25) for the Lie algebra $e(d+1)$. We further assume that these operators are the Lie algebra representation associated to a representation of the corresponding connected, simply connected Lie group $\tilde{E}(d+1)$. It is known that all the irreducible unitary representations of $\tilde{E}(d+1)$ can be realized in spaces of sections of smooth vector bundles with the Lie algebra acting by smooth differential operators. The action of the Lie algebra then extends to an action on distributional sections, including the generalized eigenvectors of the position operators. With this discussion in mind we will make free use of position eigenvectors in what follows.

We apply the Wigner–Mackey method and consider an orbit of Spin$(d+1)$ in $\mathbb{R}^{d+1}$, namely, a sphere of radius r. We consider only the case $r>0$, in which case the little group is Spin(d). Fixing a value for r amounts to assuming that the operators X_k satisfy $\Sigma X_k^2 = r^2$.

The purpose of this section is to show that the little group acts trivially if and if the following relation holds for all k and l,

$$X^2 J_{kl} = J_{km} X_m X_l - J_{lm} X_m X_k \tag{57}$$

(sum convention). This is equivalent to the relation

$$J_{kl} = P_k X_l - P_l X_k , \tag{58}$$

where by definition $P_k = r^{-2} J_{kl} X_l$.

Note that (57) is the quantum counterpart of the constraint to the sphere (9) and therefore representations of $\tilde{E}(d+1)$ satisfying it are closest to the classical motion on a sphere. Nevertheless, other representations are of interest, and describe a quantum particle on a sphere with internal degrees of freedom. We will consider the general case in a future work.

Suppose now that (57) holds. We wish to show that this implies that the representation of the little group is trivial. So we consider the space of generalized eigenvectors for the operators X_k satisfying

$$X_k |\psi\rangle = 0, \quad k = 1,\ldots,d$$

$$X_{d+1} |\psi\rangle = r. \tag{59}$$

This is the space on which the little group acts, where the Lie algebra of the little group is given by the operators J_{kl} with $1 \leqslant k,l \leqslant d$. But now if (57) holds then for $k,l \leqslant d$ we have

$$r^2 J_{kl} |\psi\rangle = 0$$

since in that case $X_k |\psi\rangle = X_l |\psi\rangle = 0$. This shows (for $r>0$) that if (57) holds, then the little group acts trivially.

Consider now the quantity,

$$W_{kl} := X^2 J_{kl} - J_{km} X_m X_l + J_{lm} X_m X_k , \tag{60}$$

which satisfies $W_{lk} = -W_{kl}$. Condition (57) is equivalent to $W_{kl} = 0$. Consider also the quantity

$$C := \sum_{k<l} W_{kl}^2 . \tag{61}$$

As we will show below, C is a Casimir, that is, an element of the universal enveloping algebra of $e(d+1)$. This implies that C acts as cI in each irreducible representation. (The value of the constant c is r^4 times the value of the quadratic Casimir for the little group in each generalized eigenspace for the position operators.)

Let us now assume that the little group acts trivially and determine the value of c in this case. We may compute c by applying C to a position eigenvector as in (59). That the little group acts trivially means that $J_{kl}|\psi\rangle = 0$ for $k<l<d+1$. Since also $X_k|\psi\rangle = X_l|\psi\rangle = 0$ for $k<l<d+1$ we get

$$C|\psi\rangle = c|\psi\rangle = \sum_k \left(X^2 J_{k,d+1} - J_{km}X_m X_{d+1} + J_{d+1,m}X_m X_k\right)^2 |\psi\rangle.$$

But since $X_m|\psi\rangle = 0$ unless and $m = d+1$ (and since $J_{d+1,d+1} = 0$) we get that

$$\begin{aligned}\left(X^2 J_{k,d+1} - J_{km}X_m X_{d+1} + J_{d+1,m}X_m X_k\right)|\psi\rangle &= \left(X^2 J_{k,d+1} - J_{k,d+1}X_{d+1}^2 + 0\right)|\psi\rangle \\ &= \left(r^2 J_{k,d+1} - r^2 J_{k,d+1}\right)|\psi\rangle = 0.\end{aligned}$$

This means that if the representation of the little group is trivial then the constant c must be zero, which means the element C must be zero in that representation. A calculation shows that for each $k<l$, W_{kl} is self-adjoint. Thus C is a sum of squares of self-adjoint operators, and the only way the sum can be zero is if each term is zero, that is, if (57) holds. So if the little group acts trivially, (57) must hold, which is what we want to prove.

In the case $d=2$ (considered in Ref. 18) it is possible to verify that

$$C = X^2 (L \cdot X)^2, \tag{62}$$

where L is the angular momentum *vector*, related to our angular momentum *matrix* by $L = (J_{32}, J_{13}, J_{12})$. One can easily check that at least this relation holds in each irreducible representation (which is all that is really relevant) as follows. Both sides are Casimirs and so it suffices to check (62) on the generalized eigenspace in (59). But for $|\psi\rangle$ in this space we calculate that

$$C|\psi\rangle = X^2 (L \cdot X)^2 |\psi\rangle = X^4 J_{12}^2 |\psi\rangle,$$

and indeed (62) holds. From (62) we see that taking $C=0$ is equivalent in the $d=2$ case to taking $L \cdot X = 0$ as in Ref. 18.

It remains only to show that the element C in (61) is a Casimir. To do this we first compute the commutation relations of W_{kl} with the J's and the X's. These come out to be

$$\frac{1}{i\hbar}[X_k, W_{lm}] = 0, \tag{63}$$

$$\frac{1}{i\hbar}[J_{kl}, W_{mn}] = \delta_{kn} W_{lm} + \delta_{lm} W_{kn} - \delta_{km} W_{ln} - \delta_{ln} W_{km}. \tag{64}$$

Equation (64) is what we expect for a matrix operator—compare this to the formula for $[J_{kl}, J_{mn}]$. Equation (63) implies immediately that C commutes with each X_k, and Eq. (64) implies, after a short calculation, that C commutes with each J_{kl}.

X. CONCLUDING REMARKS

We end this paper by discussing how the coherent states described here compare to other coherent states that have been proposed for systems whose configuration space is a sphere (or homogeneous space). As we have explained in detail above, the coherent states introduced in Ref. 18 are equivalent to those in Refs. 1, 17, but were discovered independently and from a different point of view.

Meanwhile, there are several other generalized Segal–Bargmann transforms for spheres that have been considered. These are similar but not identical to each other and were introduced by Bargmann and Todorov,[34] Rawnsley,[35] Ii,[36] Wada,[37] Thomas and Wassell,[38] and Villegas-Blas.[39] In

most cases the transform is unitary, and this unitarity can be reformulated as a resolution of the identity for the associated coherent states. These constructions all have in common that the coherent states are labeled by points in the cotangent bundle *minus the zero section* (i.e., with the points of zero momentum removed). In these papers the cotangent bundle minus the zero section is identified with the null quadric $\{a \in \mathbb{C}^{d+1} | a^2 = 0\}$. This is to be contrasted with the present paper, in which the full cotangent bundle of the sphere is identified with the quadric $\{a^2 = r^2\}$ with $r > 0$. Thus these constructions are inequivalent to the one considered in this paper. Furthermore these constructions do not generalize to higher-rank symmetric spaces.[40]

Besides these, there have been to our knowledge two other proposed constructions of coherent states on spheres (and other homogeneous spaces). These constructions, inequivalent to Refs. 1, 17 and to each other, are those of De Bièvre[41] and of Isham and Klauder.[42] Both Refs. 41 and 42 are based on extensions of the Perelomov approach, in that their coherent states are all obtained from one fixed vector ψ_0 by the action of the Euclidean group. As explained in those papers, the ordinary Perelomov approach is not applicable in this case, because the irreducible representations of the Euclidean group are not square-integrable. Non-square-integrability means that the usual Perelomov-type integral, which should be a multiple of the identity operator, is in this case divergent.

De Bièvre's approach to this problem is to apply to the fiducial vector ψ_0 only a part of the Euclidean group. We describe just the simplest case of Ref. 41. (This special case was worked out independently in a more elementary way by Torresani.[43]) Specifically, if we work in $L^2(S^d)$ then start with a basic coherent state ψ_0 such that (a) ψ_0 is invariant under rotations about the north pole $\mathbf{n}$ and (b) ψ_0 is supported in the northern half-sphere with a certain rate of decay at the equator. One may think of ψ_0 being concentrated near the north pole and approximating a state whose position is at the north pole and whose momentum is zero. The other coherent states are then of the form,

$$\exp(i\mathbf{k}\cdot\mathbf{x})\psi_0(R^{-1}\mathbf{x}),$$

where we consider only pairs $(\mathbf{k}, R)$ satisfying $\mathbf{k}\cdot R\mathbf{n} = 0$. This last restriction is crucial. Since ψ_0 is invariant under rotations about the north pole, the coherent states are determined by the values of $\mathbf{k}$ and $R\mathbf{n}$ and are thus labeled by points in the cotangent bundle of S^d. The resolution of the identity for these coherent states follows from the general procedure in Ref. 41 but can also be proved in this case by an elementary application of the Plancherel formula. The condition that ψ_0 be supported in the northern half-sphere is crucial to the proof.

It is clear that the coherent states considered in this paper are quite different from those in Ref. 41. First, De Bièvre's coherent states do not depend holomorphically on the parameters. Second, each coherent state must be supported in a half-sphere, hence cannot be real-analytic in the space variable. Third, there does not seem to be any preferred choice for ψ_0 in Ref. 41, whereas for the coherent states considered here the only choice one has to make is the value of the parameter ω.

Meanwhile, Isham and Klauder use a different method of working around the nonsquare-integrability of the irreducible representations of $E(d+1)$. They use reducible representations, corresponding to integration over some small range $[r, r+\varepsilon]$ of radii. This allows for a family of coherent states invariant under the full Euclidean group and allows a more general basic coherent state ψ_0, without any support conditions. On the other hand it seems natural to get back to an irreducible representation by letting ε tend to zero, so that the particle is constrained to a sphere with one fixed radius. Unfortunately, although the representation itself does behave well under this limit (becoming irreducible) the coherent states themselves do not have a limit as ε tends to zero. (See the remarks at the bottom of the first column on p. 609 in Ref. 42.) This seems to be a drawback of this approach.

Finally, we mention that in the group case, the coherent states described in this paper can be obtained by means of geometric quantization, as shown in Ref. 14. This means that in the group case the coherent states are of "Rawnsley type."[15] However, this result does not carry over to the

case of general compact symmetric spaces. In particular the results of Ref. 14 apply only to those spheres that are also groups, namely, $S^1 = \mathrm{U}(1)$ and $S^3 = \mathrm{SU}(2)$.

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Relativistic *N*-boson systems bound by oscillator pair potentials

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We study the lowest energy E of a relativistic system of N identical bosons bound by harmonic-oscillator pair potentials in three spatial dimensions. In natural units $\hbar=c=1$ the system has the semirelativistic (or ''spinless-Salpeter'') Hamiltonian, $H=\Sigma_{i=1}^{N}\sqrt{m^2+\mathbf{p}_i^2}+\Sigma_{j>i=1}^{N}\gamma|\mathbf{r}_i-\mathbf{r}_j|^2$, $\gamma>0$. We derive the following energy bounds: $E(N)=\min_{r>0}[N(m^2+2(N-1)P^2/(Nr^2))^{1/2}+(N/2)(N-1)\gamma r^2]$, $N\geqslant 2$, where $P=1.376$ yields a lower bound and $P=\frac{3}{2}$ yields an upper bound for all $N\geqslant 2$. A sharper lower bound is given by the function $P=P(m)$ which makes the formula for $E(2)$ exact: with this choice of P, the bounds coincide for all $N\geqslant 2$ in the Schrödinger limit defined by $m\to\infty$. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1446245]

I. INTRODUCTION AND MAIN RESULT

Many-body problems form essential links between quantum-theoretical models and real nuclear, atomic, or macroscopic systems. However, even for nonrelativistic quantum theory, there are very few many-body problems that have explicit analytic solutions; the harmonic oscillator and the attractive delta interaction are well-known exceptions. In relativistic quantum theories the situation is even worse, in spite of the fact that the phenomenon of particle creation allowed by quantum field theory would suggest that there is no such thing as a one-body problem in that theory. Therefore, it is of considerable interest to study model N-body systems within the framework of the semirelativistic ''spinless-Salpeter'' equation. For this problem there exists a well-defined nonrelativistic limit which yields a useful consistency check. Specifically, we investigate in this article the relative energy E of a system of N identical bosons represented by a semirelativistic ''spinless-Salpeter'' Hamiltonian[1,2] of the form

$$H=\sum_{i=1}^{N}\sqrt{m^2+\mathbf{p}_i^2}+\sum_{j>i=1}^{N}\gamma|\mathbf{r}_i-\mathbf{r}_j|^2, \tag{1.1}$$

where m is the boson mass, and $\gamma>0$ is a coupling parameter, and we have chosen units in which $\hbar=c=1$. The operators $\mathbf{p}_i$ are defined[3,4] in the momentum-space representation where they become multiplicative operators (c-variables). The present work is an extension to the case of N

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bosons of our earlier study[5] in which we derived energy bounds for the corresponding one-body problem. We may compare H with the corresponding Schrödinger N-body problem with Hamiltonian

$$H_S=\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}+\sum_{j>i=1}^{N}\gamma|\mathbf{r}_i-\mathbf{r}_j|^2. \tag{1.2}$$

Given our goal of investigating the *relative* (that is, binding) energies, both of these Hamiltonians have the unwelcome feature that they include the kinetic energy of the center-of-mass motion. This is easy to remedy for H_S, but a correct form is not so immediate in the relativistic case H. The exact solution to (1.2) is periodically ''rediscovered'' but has been known at least since 1935 when Houston solved the problem.[6,7] The ground-state energy E_S of the nonrelativistic problem is given for $N\geqslant 2$ (in three dimensions) by the simple formula

$$\varepsilon=3v^{1/2},\quad \varepsilon=\frac{mE_S}{N-1},\quad v=\frac{mN\gamma}{2}. \tag{1.3}$$

Thus ε is exactly the bottom of the spectrum of the one-body Hamiltonian $-\Delta+vr^2$. In this article we shall prove the following statement.

Theorem 1: *Bounds on the ground-state energy eigenvalue E of the semirelativistic Hamiltonian (1.1) are provided by the formula*

$$E=\min_{r>0}\left[N\left(m^2+\frac{2(N-1)P^2}{Nr^2}\right)^{1/2}+\frac{N}{2}(N-1)\gamma r^2\right],\quad N\geqslant 2, \tag{1.4}$$

which yields an upper bound on E when $P=\frac{3}{2}$, *and a lower bound on E when* $P=P(m)$, *a function that makes the approximation (1.4) exact in the case* $N=2$. *The function* $P(m)$ *is monotone increasing with m, has bounds*

$$1.376<P(m)<\tfrac{3}{2}, \tag{1.5}$$

and has the limit

$$\lim_{m\to\infty}P(m)=\tfrac{3}{2}. \tag{1.6}$$

In the large-m limit, the upper and lower bounds coalesce to the corresponding exact (nonrelativistic) Schrödinger energy $E_{NR}=E_S+Nm$.

The article is primarily concerned with proving Theorem 1. The main technical difficulties are twofold: to keep the fundamental symmetries of translation invariance and boson permutation symmetry, and to find ways of ''penetrating'' the square-root operator of the Salpeter kinetic energy. Our policy is to work with Jacobi relative coordinates to guarantee translation invariance of the wave functions, and to accept the concomitant complications of permutation symmetry. We discuss the relative coordinates and some of their properties in Sec. II. We shall exploit the necessary permutation symmetry to relate the N-body energy to that of a scaled and reduced two-body problem. The exact solution of the one-body problem is discussed in Sec. III. It is well known that the one-body Salpeter problem is equivalent to a Schrödinger problem with Hamiltonian $-\Delta+\sqrt{m^2+r^2}$.[8,9] We take the position in this article that the lowest eigenvalue $e(m)$ of this problem, which is easy to find numerically, is at our disposal. In Fig. 1 we exhibit graphs of the functions $\{e(m),P(m)\}$. The extension of these results to the two-body problem is treated in Sec. IV. The lower bound discussed in Sec. V is rendered possible by an operator property introduced in Sec. II that allows us, in a sense, to remove certain annihilation operators from inside the square-root operator. For the N-body upper bound discussed in Sec. VI we use a Gaussian wave function and minimize the energy expectation with respect to a scale variable. The

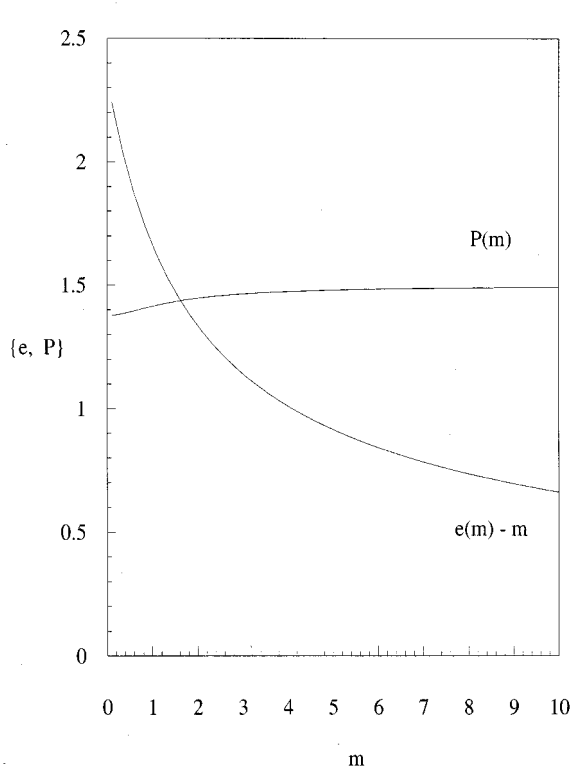

FIG. 1. The monotone energy function $e(m)$ of the one-body problem defined by (3.1), and the monotone function $P(m)$ used in our standard representation (3.8) for $e(m)$; the function $P(m)$ is bounded by $P(0)=1.376\leqslant P(m)\leqslant P(\infty)=\frac{3}{2}$.

calculation is helped by special factoring properties of the Gaussian and by the use of Jensen's inequality. The bounds corresponding to $P=\{1.376,1.5\}$ are depicted in Fig. 2, and the convergence of the bounds $P=\{P(m),\frac{3}{2}\}$ with increasing m is shown in Fig. 3, for $2\leqslant N\leqslant 8$.

II. RELATIVE COORDINATES

Jacobi relative coordinates may be defined with the aid of an orthogonal matrix B relating the column vectors of the new $[\rho_i]$ and old $[\mathbf{r}_i]$ coordinates according to

$$[\rho_i]=B[\mathbf{r}_i]. \tag{2.1}$$

The first row of B defines a center-of-mass variable with every entry $1/\sqrt{N}$, the second row defines a pair distance $\rho_2=(\mathbf{r}_1-\mathbf{r}_2)/\sqrt{2}$, and the kth row, $k\geqslant 2$, has the first $k-1$ entries $B_{ki}=1/\sqrt{k(k-1)}$, the kth entry $B_{kk}=-\sqrt{(k-1)/k}$, and the remaining entries zero. We define the corresponding momentum variables as

$$[\pi_i]=(B^{-1})^t[\mathbf{p}_i]=B[\mathbf{p}_i]. \tag{2.2}$$

These coordinates have some nice properties which we shall need. First, we have

$$k\sum_{i=2}^{k}\rho_i^2=\sum_{j>i=1}^{k}(\mathbf{r}_i-\mathbf{r}_j)^2,\quad k=2,3,...,N, \tag{2.3}$$

and similarly for the momenta

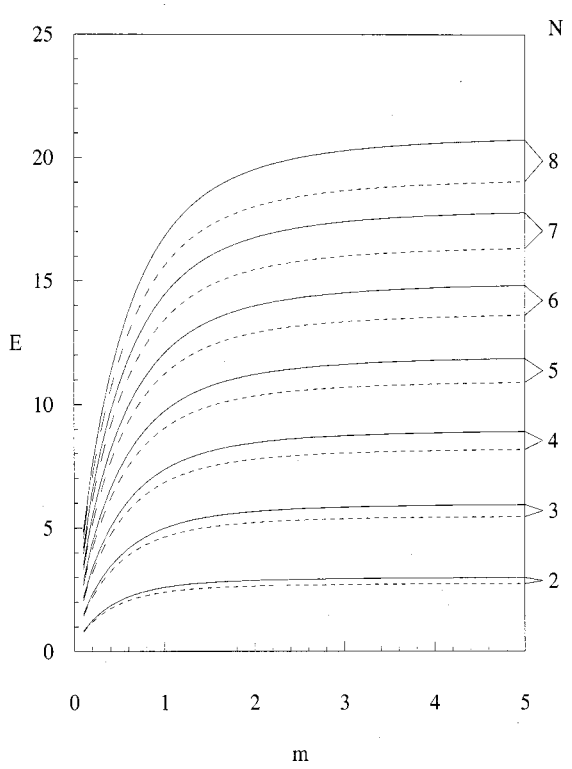

FIG. 2. Upper (full lines) and lower (dashed lines) bounds to the lowest energy $E(m)$ of the N-boson relativistic harmonic-oscillator problem for $N=2,3,...,8$ obtained by employing the constant values $P=1.376$ and $P=1.5$, respectively, in Eq. (1.4) of Theorem 1.

$$k\sum_{i=2}^{k}\pi_i^2=\sum_{j>i=1}^{k}(\mathbf{p}_i-\mathbf{p}_j)^2,\quad k=2,3,...,N. \tag{2.4}$$

It follows immediately that if Ψ is a translation-invariant wave function which is symmetric (or antisymmetric) under the permutation of the individual-particle indices, then it follows that

$$(\Psi,\rho_i^2\Psi)=(\Psi,\rho_2^2\Psi),\quad 2\leqslant i\leqslant N, \tag{2.5}$$

and

$$(\Psi,\pi_i^2\Psi)=(\Psi,\pi_2^2\Psi),\quad 2\leqslant i\leqslant N. \tag{2.6}$$

These expectation symmetries might suggest that the wave function Ψ is symmetric under permutation of the relative coordinates, but this stronger property is only true for Gaussian wave functions. Moreover, Gaussian boson wave functions of Jacobi relative coordinates uniquely[10,11] have the further factoring property that

$$\Phi(\rho_2,\rho_3,\ldots,\rho_N)=\phi(\rho_2)\,\theta(\rho_3,\ldots,\rho_N), \tag{2.7}$$

where ϕ and θ are also Gaussian.

III. THE ONE-BODY PROBLEM

We consider the one-body problem with Hamiltonian

$$H_1=\sqrt{m^2+\mathbf{p}^2}+r^2\rightarrow e(m), \tag{3.1}$$

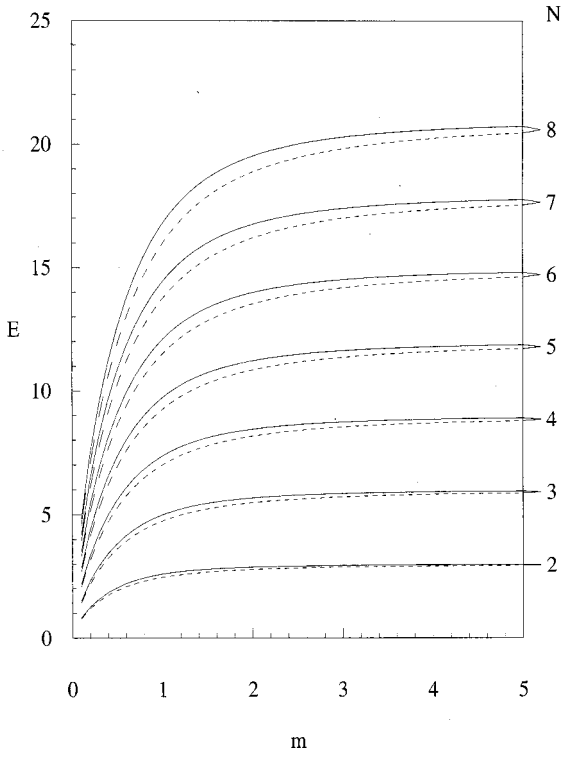

FIG. 3. Upper (full lines) and lower (dashed lines) bounds to the lowest energy $E(m)$ of the N-boson relativistic harmonic-oscillator problem for $N=2,3,...,8$ obtained by employing the values $P=P(m)$ and $P=1.5$, respectively, in Eq. (1.4) of Theorem 1. For $N=2$, the lower bound is exact.

where, for coupling $\gamma=1$, $e(m)$ is the lowest eigenvalue as a function of the mass m. By transforming this problem into momentum space we obtain the equivalent problem

$$\tilde{H}_1=-\Delta+\sqrt{m^2+r^2}\rightarrow e(m). \tag{3.2}$$

Since this Schrödinger problem is easy to solve numerically to arbitrary accuracy, we shall take the position that $e(m)$ is "known" and at our disposal. We note that in the large-m (nonrelativistic or Schrödinger) limit, we have

$$e(m)\simeq e_{\mathrm{NR}}(m)=m+\frac{3}{(2m)^{1/2}}. \tag{3.3}$$

We now define, for a given value of m, the (lowest) "kinetic potential" [12–14] $\overline{h}(s)$ associated with the relativistic-kinetic-energy square-root operator $\sqrt{m^2+\mathbf{p}^2}$ and the harmonic-oscillator potential r^2 by

$$\overline{h}(s)=\inf_{\substack{\psi\in\mathcal{D}(H_1)\\ \|\psi\|=1\\ (\psi,\sqrt{m^2+\mathbf{p}^2}\psi)=s}}(\psi,r^2\psi), \tag{3.4}$$

where $\psi(\mathbf{r})$ is a wave function in the domain $\mathcal{D}(H_1)$ of H_1. That is to say, we find the minimum mean-value of the potential, subject to the constraint that the mean kinetic energy is held constant at the value s. It follows that the eigenvalue may now be recovered from $\overline{h}(s)$ by a further minimization with respect to the kinetic energy s. Thus we have

$$e(m)=\min_{s>m}[s+\overline{h}(s)]. \tag{3.5}$$

An important and useful aspect of this representation for $e(m)$ is that the identical kinetic potential $\overline{h}(s)$ can be used for a more general one-body problem in which the kinetic-energy term is multiplied by the positive factor β, say, and the coupling $\gamma>0$ is returned. We have explicitly

$$\beta\sqrt{m^2+\mathbf{p}^2}+\gamma r^2\to\varepsilon(m,\beta,\gamma)=\min_{s>m}[\beta s+\gamma\overline{h}(s)]. \tag{3.6}$$

However, we still have to find the kinetic potential $\overline{h}(s)$. We do this by changing the minimization variable from $s>m$ to $r>0$ according to the following defining equation for $P(m)$:

$$\overline{h}(s)=r^2,\quad s=\sqrt{m^2+\left(\frac{P(m)}{r}\right)^2}. \tag{3.7}$$

Now, by rewriting (3.5) in terms of the function $P(m)$, we obtain

$$e(m)=\min_{r>0}\left[\sqrt{m^2+\left(\frac{P(m)}{r}\right)^2}+r^2\right], \tag{3.8}$$

and, by solving (3.8), we obtain the following expression for $P(m)$ in terms of the one-body energy $e(m)$:

$$P(m)=\left(\frac{2(e(m)+\sqrt{e^2(m)+3m^2})}{27}\right)^{1/2}(2e(m)-\sqrt{e^2(m)+3m^2}). \tag{3.9}$$

The graphs of $e(m)-m$ and $P(m)$ are shown in Fig. 1: both $e(m)$ and $P(m)$ are monotone increasing with m; $e(m)-m$, however, is monotone *decreasing*, in agreement, for large m, with the Feynman–Hellmann theorem for the corresponding nonrelativistic case. In the (ultrarelativistic) limit $m\to0$ we have $\tilde{H}_1\to-\Delta+r$, that is to say, the operator limit is the Schrödinger operator for the linear potential in three dimensions, with lowest energy $e(0)=2.338\,107\,41$. In the (nonrelativistic) large-m limit we have $H_1\to m-(1/2m)\Delta+r^2$, that is to say, the Schrödinger harmonic oscillator with energy $e(m)\simeq m+3/\sqrt{2m}$. By substituting these "outer" energies in (3.9), we obtain the bounds

$$1.376<P(m)<\tfrac{3}{2}. \tag{3.10}$$

It is clear from Eq. (3.8) that the expression for $e(m)$, as a function of *m and P*, is monotone increasing in P. Thus, by substituting, respectively, the constants $P=1.376$ and $P=1.5$, we obtain from this formula lower and upper bounds on the one-body energy $e(m)$. These bounds agree exactly with the bounds we obtained earlier[5,14] for this one-body harmonic-oscillator problem. In summary—and with the introduction of one more parameter $\lambda>0$, which we shall need later—we have

$$\beta\sqrt{m^2+\lambda\mathbf{p}^2}+\gamma r^2\to\varepsilon(m,\beta,\gamma\lambda)=\min_{r>0}\left[\beta\left(m^2+\lambda\left(\frac{P}{r}\right)^2\right)^{1/2}+\gamma r^2\right]. \tag{3.11}$$

For each $\beta>0$, $\gamma>0$, $\lambda>0$, this formula is exact when $P=P(m)$, is a lower bound when $P=1.376$, and is an upper bound when $P=1.5$. We have chosen to express this result in this form because of the extension to the N-body problem. By elementary scaling arguments we may also express $\varepsilon(m,\beta,\gamma\lambda)$ directly in terms of the energy function $e(m)$ by the explicit formula

$$\varepsilon(m,\beta,\gamma\lambda)=(\beta^2\gamma\lambda)^{1/3}e\left(m\left(\frac{\beta}{\gamma\lambda}\right)^{1/3}\right). \tag{3.12}$$

As we shall see in the next section, the two-body energy is obtained from (3.11) or (3.12) by simply setting $\lambda=1$, $\beta=2$. It is an extension of this reasoning that will allow us, in Sec. V, to obtain also the N-body, $N\geqslant 2$, lower energy bound by using suitable values for β, γ, and λ.

IV. THE TWO-BODY PROBLEM

For the case $N=2$ we have explicitly

$$H=\sqrt{m^2+\mathbf{p}_1^2}+\sqrt{m^2+\mathbf{p}_2^2}+\gamma|\mathbf{r}_1-\mathbf{r}_2|^2. \tag{4.1}$$

Let $\psi(\rho_2)$ be a normalized boson wave function. Then the lowest relative eigenvalue of the operator H is the infimum of expectation values of the form $(\psi,H\psi)$. But the boson symmetry of $\psi(\rho_2)$ means that the two kinetic-energy terms in $(\psi,H\psi)$ must have the same value. Moreover, in terms of relative coordinates, the operator $\mathbf{p}_2^2$ may be written

$$\mathbf{p}_2^2=\frac{(\pi_1-\pi_2)^2}{2}. \tag{4.2}$$

Now, the operator π_1 would immediately annihilate $\psi(\rho_2)$ if it were not contained in the square root. We claim that, inside the expectation value, the operator π_1 may simply be removed; this may be seen as an immediate generalization of the following observation.

Lemma 1: Suppose $\Psi(x,y)=\psi(x)$, *then*

$$\left[1-\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)^2\right]^{1/2}\Psi=\left(1-\frac{\partial^2}{\partial x^2}\right)^{1/2}\Psi. \tag{4.3}$$

Proof of Lemma 1: If $\mathcal{F}$ indicates the two-dimensional Fourier transform and our new variables are $\{p,q\}$, then we find $\mathcal{F}(\Psi)(p,q)=\tilde{\psi}(p)\,\delta(q)$, and, by definition, the Fourier transform of the left-hand side of (4.3) becomes

$$(1+(p-q)^2)^{1/2}\,\tilde{\psi}(p)\,\delta(q)=(1+p^2)^{1/2}\tilde{\psi}(p)\,\delta(q). \tag{4.4}$$

By transforming back to the variables $\{x,y\}$, we obtain the right-hand side of (4.3). □

Applying the generalization of this lemma to our problem in three dimensions, we find, for $\psi=\psi(\rho_2)$,

$$(\psi,H\psi)=(\psi,(2\sqrt{m^2+\tfrac{1}{2}\pi_2^2}+2\gamma\rho_2^2)\psi). \tag{4.5}$$

By defining the pair-distance variable $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2=\sqrt{2}\rho_2$, and the corresponding momentum as $\mathbf{p}=-i\nabla_{\mathbf{r}}=\pi_2/\sqrt{2}$, we may rewrite (4.5) as

$$(\psi,H\psi)=(\psi,(2\sqrt{m^2+\mathbf{p}^2}+\gamma r^2)\psi). \tag{4.6}$$

By using a formal relative coordinate $\mathbf{r}$, we have thus recovered the well-known[15] two-body result: the minimum of the right-hand side of (4.6) is the bottom of the spectrum of H which corresponds precisely to the energy of a one-body problem with the kinetic-energy parameter $\beta=2$. This result may also be expressed in terms of the one-body energy function $e(m)$ by means of Eq. (3.12). Thus we have explicitly for $N=2$

$$E=(4\gamma)^{1/3}e\left(m\left(\frac{2}{\gamma}\right)^{1/3}\right). \tag{4.7}$$

In the next section we shall apply a similar reasoning to the N-body problem; however, for $N>2$ we obtain, instead of the exact energy, a lower energy bound.

V. THE LOWER BOUND

Suppose that $\Psi(\rho_2,\rho_3,\ldots,\rho_N)$ is a normalized translation-invariant N-boson wave function. Boson symmetry and, in particular, formula (2.3) allow us to write

$$E\leqslant(\Psi,H\Psi)=N(\Psi,(m^2+\mathbf{p}_N^2)^{1/2}\Psi)+\binom{N}{2}\gamma(\Psi,2\rho_N^2\Psi). \tag{5.1}$$

Now, from the definition of the relative coordinates, we have

$$\mathbf{p}_N=\frac{1}{\sqrt{N}}\,\pi_1-\sqrt{\frac{N-1}{N}}\,\pi_N. \tag{5.2}$$

Consequently, an application of an immediate generalization of Lemma 1 allows us to ''remove'' the operator π_1 from the square root of the kinetic-energy term and write

$$E\leqslant N\left(\Psi,\left(m^2+\frac{N-1}{N}\,\pi_N^2\right)^{1/2}\Psi\right)+\binom{N}{2}\gamma(\Psi,2\rho_N^2\Psi). \tag{5.3}$$

Adapting the argument presented in Sec. IV for the two-body case $N=2$, we define a relative coordinate $\mathbf{r}=\sqrt{2}\rho_N$, and the corresponding momentum $\mathbf{p}=\pi_N/\sqrt{2}$. The expression for the upper bound to the lowest N-boson energy E then becomes

$$E\leqslant N\left(\Psi,\left(m^2+\frac{2(N-1)}{N}\,\mathbf{p}^2\right)^{1/2}\Psi\right)+\binom{N}{2}\gamma(\Psi,r^2\Psi). \tag{5.4}$$

The inequality (rather than an equality) in (5.4) comes only from the choice of wave function. If we find the infimum of such expressions over all normalized translation-invariant N-boson wave functions, we would obtain the exact energy E; if we find this minimum but without the constraint of boson symmetry, then the right-hand side of (5.4) will in general fall below E but will in any case be bounded from below by the bottom of the spectrum of the one-body semirelativistic Salpeter Hamiltonian

$$H=N\left(m^2+\frac{2(N-1)}{N}\,\mathbf{p}^2\right)^{1/2}+\binom{N}{2}\gamma r^2. \tag{5.5}$$

But this latter problem corresponds precisely to Eq. (3.11) if we make the parameter substitutions

$$\beta=N,\quad \lambda=\frac{2(N-1)}{N},\quad \gamma\to\binom{N}{2}\gamma=\frac{N(N-1)}{2}\,\gamma. \tag{5.6}$$

Thus, in view of the P representation (3.8), it is clear that we have established the lower bound (1.4) of Theorem 1.

It is interesting to note that we can substitute the N-body values (5.6) for the parameters β, γ, and λ into the result (3.12) for the one-body ground-state energy $\varepsilon(m,\beta,\gamma\lambda)$ in order to obtain the following explicit expression for the lower bound:

$$E\geqslant(N^2(N-1)^2\gamma)^{1/3}e\left(m\left(\frac{N}{(N-1)^2\gamma}\right)^{1/3}\right). \tag{5.7}$$

This expression—which is equivalent to the lower bound (1.4) of Theorem 1—gives the exact energy and agrees with Eq. (4.7) when $N=2$. Meanwhile, for all $N\geqslant 2$, in the nonrelativistic large-m (Schrödinger) limit it yields the exact N-body energy

$$E_{\mathrm{NR}}=Nm+3\left(\frac{\gamma}{2m}\right)^{1/2}N^{1/2}(N-1), \tag{5.8}$$

reproducing thus the old result of Houston recalled in Eq. (1.3).

VI. THE UPPER BOUND

For the upper bound we employ a Gaussian wave function of the form

$$\Phi(\rho_2,\rho_3,\ldots,\rho_N)=C\exp\left(-\alpha\sum_{i=2}^{N}\rho_i^2\right),\quad \alpha>0, \tag{6.1}$$

where C is a normalization constant. The factoring property (2.7) of this function and the boson-symmetry reduction leading to (5.4) allows us to write

$$E\leqslant N\left(\phi,\left(m^2+\frac{2(N-1)}{N}\mathbf{p}^2\right)^{1/2}\phi\right)+\binom{N}{2}\gamma(\phi,r^2\phi), \tag{6.2}$$

where the function $\phi(r)$ is given by

$$\phi(r)=\left(\frac{\alpha}{\pi}\right)^{3/4}\exp\left(-\frac{\alpha r^2}{2}\right). \tag{6.3}$$

Since the kinetic-energy operator is a *concave* function of the square $\mathbf{p}^2$ of the momentum, we can use Jensen's inequality[16] to move the expectation value $\langle\mathbf{p}^2\rangle$ inside the square root and thus estimate the mean value of this operator from above and write

$$E\leqslant N\left(m^2+\frac{2(N-1)}{N}(\phi,\mathbf{p}^2\phi)\right)^{1/2}+\binom{N}{2}\gamma(\phi,r^2\phi). \tag{6.4}$$

We shall minimize this upper bound with respect to the scale variable $\alpha>0$. We parametrize the basic kinetic-energy and potential-energy expectation values in terms of a variable $r>0$ by the following relations:

$$(\phi,r^2\phi)=\frac{3}{2\alpha}:=r^2,\quad (\phi,\mathbf{p}^2\,\phi)=\frac{3\alpha}{2}=\left(\frac{P}{r}\right)^2,\quad P:=\frac{3}{2}. \tag{6.5}$$

By substituting these expressions in Eq. (6.4) and minimizing over the variable r, we establish the upper bound (1.4) of Theorem 1.

VII. SUMMARY AND CONCLUSION

This article is devoted to the investigation of the ground-state eigenvalue of the semirelativistic ("spinless-Salpeter") Hamiltonian (1.1) which governs the dynamics of a system of N identical bosons that experience pair interactions described by a harmonic-oscillator potential with coupling strength γ. For a fixed coupling $\gamma=1$, we have represented the exact ground-state energy eigenvalue of the corresponding one-body problem, regarded as a function $e(m)$ of the boson mass m, by a monotone rising function $P(m)$, which is bounded by $1.376=P(0)\leqslant P(m)\leqslant P(\infty)=1.5$. Our bounds (1.4) on the energy of the N-body problem are expressed in terms of a formula which has this function P as a parameter.

In Fig. 2 we have plotted the energy bounds corresponding to fixed lower and upper limiting values of $P(m)$, namely, $P=\{1.376,1.5\}$. In Fig. 3 we have kept the same upper energy bound, obtained with the help of a Gaussian trial wave function and corresponding to $P=1.5$, but added the best lower energy bound of this type, using a ''running'' $P=P(m)$. The lower energy bound of Fig. 3 is identical to the exact energy for the case $N=2$. For higher $N>2$, Fig. 3 shows the approach of both upper and lower bounds to the well-known exact nonrelativistic solution (1.3) in the large-m limit.

A key ingredient in this analysis is the use of relative coordinates: only in such a framework could the upper and lower energy bounds be made to converge in the Schrödinger limit. This study of the semirelativistic harmonic-oscillator problem is a first step towards energy bounds valid for more general central pair interactions.

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Maximization of capacity and l_p norms for some product channels

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It is conjectured that the Holevo capacity of a product channel $\Omega\otimes\Phi$ is achieved when product states are used as input. Amosov, Holevo, and Werner have also conjectured that the maximal l_p norm of a product channel is achieved with product input states. In this article we establish both of these conjectures in the case that Ω is arbitrary and Φ is a CQ or QC channel (as defined by Holevo). We also establish the Amosov, Holevo and Werner conjecture when Ω is arbitrary and either Φ is a qubit channel and $p=2$, or Φ is a unital qubit channel and p is integer. Our proofs involve a new conjecture for the norm of an output state of the half-noisy channel $I\otimes\Phi$, when Φ is a qubit channel. We show that this conjecture in some cases also implies additivity of the Holevo capacity. © *2002 American Institute of Physics.*
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I. INTRODUCTION

A quantum channel is the mathematical description of a device which stores and transmits quantum states. Much work has been devoted to the study of particular quantum channels with highly nonclassical properties, and also to general questions such as the information capacity of classes of channels. In this article we will consider some problems of the second type, concerning additivity and multiplicativity properties that are believed to hold for all product channels.

The basic components of a quantum channel are a Hilbert space $\mathcal{H}$ and a noise operator Φ. The quantum states are positive operators on $\mathcal{H}$, with trace equal to one. The noise operator Φ is a completely positive, trace-preserving map which acts on the set of states. Positivity means that Φ is a positive operator on $B(\mathcal{H})$ (the algebra of bounded operators on $\mathcal{H}$). Complete positivity means that the map $I\otimes\Phi$ is also a positive operator on $B(\mathbf{C}^K\otimes\mathcal{H})$ for every K.

When the channel $(\mathcal{H},\Phi)$ is used to store or transmit information, it is assumed that the information is encoded as a state on the product space $\mathcal{H}^{\otimes n}$ for some n, and that the noise acts on this state through the product operator $\Phi^{\otimes n}$, thereby mimicking the action of a memoryless channel in classical information theory. The basic properties of such quantum memoryless channels have been studied by many authors.[1–5] One outstanding problem is to determine the ultimate rate at which classical information can be transmitted through this channel, when no prior entanglement is available between sender and receiver. The protocol that achieves this capacity may require messages to be encoded using entangled states and/or decoded using collective measurements. It is conjectured that this ultimate capacity is given by the well-known Holevo bound[3]

$$C_{\mathrm{Holv}}(\Phi)=\sup_{\pi,\,\rho}\left[S\left(\sum\ \pi_i\Phi(\rho_i)\right)-\sum\ \pi_i S(\Phi(\rho_i))\right], \tag{1}$$

where $S(\rho)=-\mathrm{Tr}\rho\log\rho$ is the von Neumann entropy, and the sup runs over all probability distributions $\{\pi_i\}$ and collections of states $\{\rho_i\}$ on $\mathcal{H}$. This capacity conjecture is equivalent to the statement that there is no benefit gained when entangled states are used to encode messages for transmission through a quantum channel. As shown by Holevo[3] and Schumacher–Westmoreland,[5]

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the ultimate rate for information transmission using non-entangled coding states is exactly C_{Holv}. Thus the capacity conjecture is implied by the *additivity conjecture* for C_{Holv}, which states that for any channels Ω and Φ

$$C_{\mathrm{Holv}}(\Omega\otimes\Phi)=C_{\mathrm{Holv}}(\Omega)+C_{\mathrm{Holv}}(\Phi). \tag{2}$$

Although the equality (2) has been shown in some special cases,[4–8] it remains a challenging problem to prove this result for a general pair of channels (Ω,Φ). Amosov, Holevo, and Werner introduced a related conjecture, concerning the noncommutative l_p norm of output states from a product channel[6] (this norm is defined later in this work). In this article we report progress toward establishing these conjectures for some special product channels, namely the cases when Ω is arbitrary and either (i) Φ is a CQ or QC channel (these are defined later), or (ii) Φ is a qubit channel. In the first case we establish both conjectures. In the second case we establish the Amosov, Holevo, and Werner conjecture for integer values of p. A principal ingredient in our proof in the second case is a new bound concerning the l_p norm of the output from a ''half-noisy'' channel $I\otimes\Phi$, for integer values of p. We conjecture that this bound holds for all $p\geqslant 1$, and we show that in some cases this conjecture implies additivity of the Holevo bound (2).

The article is organized as follows. Section II contains a precise statement of the results, and the conjectured bound for half-noisy channels. In Sec. III we review the relation of relative entropy and the Holevo bound. In Secs. IV and V we prove the results for CQ and QC channels. Then in Sec. VI we prove the results for qubit channels, and in Sec. VII we prove the corollaries of our new conjecture. In Sec. VIII we give a summary and overview of the results in the paper. Finally, the Appendix contains a proof by Lieb and Ruskai of a special case of the conjecture.

II. STATEMENT OF RESULTS

The noncommutative l_p norm of a matrix A is defined by

$$\|A\|_p=(\mathrm{Tr}|A|^p)^{1/p}=[\mathrm{Tr}(A^*A)^{p/2}]^{1/p}. \tag{3}$$

The corresponding maximal l_p norm for a positive map Φ on $B(\mathcal{H})$ is

$$\nu_p(\Phi)=\sup_{\rho}\|\Phi(\rho)\|_p, \tag{4}$$

where the sup runs over states in $\mathcal{H}$ (this quantity was introduced in Ref. 6, where it was called the ''maximal output purity'' of the channel). It is always true that for any maps Ω and Φ, and any $p\geqslant 1$,

$$\nu_p(\Omega\otimes\Phi)\geqslant\nu_p(\Omega)\,\nu_p(\Phi). \tag{5}$$

The multiplicativity conjecture of Ref. 6 states that for any completely positive trace-preserving maps Ω and Φ, and for all $p\geqslant 1$,

$$\nu_p(\Omega\otimes\Phi)=\nu_p(\Omega)\,\nu_p(\Phi). \tag{6}$$

Equality always holds in (6) for $p=1$. It has been shown in several different ways that (6) holds for all $p\geqslant 1$ and all Ω when $\Phi=I$.[6,9,10] Recently, it has been shown that (6) holds when both Ω and Φ are depolarizing channels, and p is integer.[11] In this article we provide some further examples where it holds.

The first case we consider involves the CQ and QC channels introduced by Holevo,[4] so we recall their definitions now. Let $\{X_b\}$ be a POVM on $\mathcal{H}$ (so $X_b\geqslant 0$ and $\Sigma X_b=I$) and let $\{Q_b\}$ be any collection of states. Then we can define a channel Φ by the formula

$$\Phi(\rho)=\sum\ \mathrm{Tr}(\rho\,X_b)\,Q_b\,. \tag{7}$$

Holevo considered two special cases of (7). First, if $\{X_b=|e_b\rangle\langle e_b|\}$ are projections onto an orthonormal basis $\{|e_b\rangle\}$ in $\mathcal{H}$, then (7) is called a CQ channel. Second, if $\{Q_b=|e_b\rangle\langle e_b|\}$, then (7) is called a QC channel. Holevo proved the additivity result (2) when $\Omega=\Phi$ is either a CQ or QC channel. Our first result generalizes this by allowing one of the channels, Ω, to be arbitrary.

Theorem 1: *Let Φ be a CQ or QC channel. Then for any completely positive trace-preserving map Ω, l_p-multiplicativity* (6) *holds for all $p\geqslant 1$, and Holevo additivity* (2) *holds.*

For our second set of results we restrict to channels on a two-dimensional Hilbert space. For brevity of notation we will say that Φ is a *qubit channel* if it is a completely positive trace-preserving map on $\mathcal{B}(\mathbf{C}^2)$.

Theorem 2: *Let Φ be a qubit channel. Then the equality* (6) *holds for $p=2$, that is, $\nu_2(\Omega\otimes\Phi)=\nu_2(\Omega)\nu_2(\Phi)$ for all channels Ω.*

In order to state the next result we need to recall the classification of qubit maps. Any qubit map Φ can be represented by a real 4×4 matrix with respect to the basis $I,\sigma_1,\sigma_2,\sigma_3$, where σ_i are the Pauli matrices. In Ref. 8 it was explained that by using independent unitary transformations in its domain and range, this matrix can be put into the following form:

$$\Phi=\begin{pmatrix} 1 & 0 & 0 & 0 \\ t_1 & \lambda_1 & 0 & 0 \\ t_2 & 0 & \lambda_2 & 0 \\ t_3 & 0 & 0 & \lambda_3 \end{pmatrix}. \tag{8}$$

This form makes it easy to see how Φ acts on the Bloch sphere. The sphere is first compressed to an ellipsoid with semi-major axes $|\lambda_1|,|\lambda_2|,|\lambda_3|$, and is then translated by the vector $\mathbf{t}=(t_1,t_2,t_3)$. There are constraints on the allowed values of these six parameters (coming from the requirements that Φ be completely positive and trace-preserving), and these constraints have been fully worked out in Ref. 12. If $t_i=0$ for $i=1,2,3$, then $\Phi(I)=I$, in which case Φ is a *unital* qubit map.

Our next result requires a slightly stronger condition on the map Φ, which we now state in terms of these parameters:

$$\text{if } |\lambda_i|<|\lambda_j|<|\lambda_k|, \text{ then } t_it_j=0. \tag{9}$$

This condition can be stated in words as follows: the ellipsoid may be translated only in directions lying in the two planes that are perpendicular to its two smaller axes (if any two axes have equal length, there is no restriction).

Theorem 3: *Let Φ be a qubit channel satisfying the condition* (9). *Then l_p-multiplicativity* (6) *holds for all integer p, that is, $\nu_p(\Omega\otimes\Phi)=\nu_p(\Omega)\,\nu_p(\Phi)$ for all channels Ω and all integers p.*

The proofs of Theorems 2 and 3 make use of a bound for the l_p norm of the output state from the half-noisy channel $I\otimes\Phi$. We believe that this bound holds for all $p\geqslant 1$, however we can prove it only for the cases listed in the theorems. So, we state the general bound as a conjecture.

Conjecture 4: Let Φ be a qubit channel, and let $M\geqslant 0$ be a $2K\times 2K$ matrix. Write M in the form

$$M=\begin{pmatrix} X & Y \\ Y^* & Z \end{pmatrix}, \tag{10}$$

where X, Y and Z are $K\times K$ matrices. Then for all $p\geqslant 1$

$$\|(I\otimes\Phi)(M)\|_p\leqslant\nu_p(\Phi)\,(\|X\|_p+\|Z\|_p). \tag{11}$$

This conjecture has several important consequences, which we list in the next three corollaries. In particular, the first corollary shows that Conjecture 4 implies Theorems 2 and 3.

Corollary 5: Let Φ *be a qubit channel, and suppose that* (11) *holds for all positive* $2K \times 2K$ *matrices* M, *for some* $p \geqslant 1$. *Then for any completely positive map* Ω *on* $B(\mathbf{C}^K)$, l_p*-multiplicativity* (6) *holds for the same value of* p.

In Sec. V we will prove that (11) holds for all qubit maps Φ when $p=2$, and also for the cases listed in Theorem 3. Combining this with Corollary 5 will prove Theorems 2 and 3.

Our next result concerns the additivity of minimal entropy. The minimal entropy of a completely positive trace-preserving map Φ is defined by

$$S_{\min}(\Phi) = \inf_{\rho} S(\Phi(\rho)). \tag{12}$$

The additivity of minimal entropy is the statement that

$$S_{\min}(\Omega \otimes \Phi) = S_{\min}(\Omega) + S_{\min}(\Phi). \tag{13}$$

Corollary 6: Let Φ *be a qubit channel, and suppose that* (11) *holds for all positive* $2K \times 2K$ *matrices* M, *and for all* $p \in [1,s)$ *for some* $s>1$. *Then for any completely positive map* Ω *on* $B(\mathbf{C}^K)$, *additivity of minimal entropy* (13) *holds.*

For our last corollary, recall that a map Φ is unital if $\Phi(I)=I$, which means roughly that Φ leaves unchanged the "noisiest" state through the channel.

Corollary 7: Let Φ *be a unital qubit channel, and suppose that* (11) *holds for all positive* $2K \times 2K$ *matrices* M, *and for all* $p \in [1,s)$ *for some* $s>1$. *Then for any completely positive trace-preserving map* Ω *on* $B(\mathbf{C}^K)$, *Holevo additivity* (2) *holds.*

Remarks:

(1) There are two special cases where it is easy to verify Conjecture 4. First, if M is a one-dimensional projection, then the right side of (11) becomes $\nu_p(\Phi)\,\mathrm{Tr}(M)$, and then the result follows immediately from the definition (4). Second, suppose that Φ is the identity map, so $\nu_p(\Phi)=1$. Define the projections

$$P_0 = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \quad P_1 = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}. \tag{14}$$

Then convexity of the l_p norm for $p \geqslant 1$ implies that

$$\|M\|_p = \|M^{1/2}(P_0+P_1)M^{1/2}\|_p \leqslant \|M^{1/2}P_0M^{1/2}\|_p + \|M^{1/2}P_1M^{1/2}\|_p. \tag{15}$$

Furthermore, for any matrix A, the matrices AA^* and A^*A have the same spectrum, so we deduce that

$$\|M\|_p \leqslant \|P_0MP_0\|_p + \|P_1MP_1\|_p = \|X\|_p + \|Z\|_p \tag{16}$$

(this derivation is a special case of a more general result for POVMs which is described in Ref. 13).

(2) Lieb and Ruskai have recently established Conjecture 4, Eq. (11), for a depolarizing channel in the special case $X=Z$, for all $p \geqslant 1$. Recall that the depolarizing channel is described by the parameter values $\lambda_1=\lambda_2=\lambda_3=\lambda$, and $t_1=t_2=t_3=0$, so that in this case the bound (11) becomes

$$\left\| \begin{pmatrix} X & \lambda Y \\ \lambda Y^* & X \end{pmatrix} \right\|_p \leqslant \nu_p(\Phi)\,(2\|X\|_p), \tag{17}$$

where

$$\nu_p(\Phi) = \left[\left(\frac{1+\lambda}{2} \right)^p + \left(\frac{1-\lambda}{2} \right)^p \right]^{1/p}. \tag{18}$$

Their proof appears as an Appendix to this article.

(3) Theorem 3 was proved in Ref. 8 for unital maps in the case $p=\infty$, and our proof here extends this result to all integer values of p (and to a larger class of maps). The class of qubit maps which satisfy (9) includes all unital qubit maps and many nonunital maps. In particular, our proof applies to any extreme point in the set of qubit maps (this refers to recent work in Ref. 12, and we discuss it more fully in Sec. III).

(4) To prove Corollaries 6 and 7 we need only the derivative of (11) at $p=1$, which we now state as a separate bound. Assume that M has the form (10) with $\mathrm{Tr}(M)=1$, and define the states

$$\xi=\frac{1}{\mathrm{Tr}X}X, \quad \zeta=\frac{1}{\mathrm{Tr}Z}Z. \tag{19}$$

Then taking the derivative of (11) at $p=1$ gives

$$S((I\otimes\Phi)(M))\geqslant S_{\min}(\Phi)+\mathrm{Tr}(X)S(\xi)+\mathrm{Tr}(Z)S(\zeta). \tag{20}$$

(5) When Ω and Φ are both unital qubit maps, the additivity result (2) follows immediately from the additivity of minimal entropy (13), as was discussed in Ref. 8. This is also true if $\Omega=\Phi_1\otimes\cdots\otimes\Phi_n$ is a product of unital qubit maps. Additivity of Holevo capacity (2) for the ''half-noisy'' case $\Phi=I$ was proved by Schumacher and Westmoreland,[10] and their analysis underlies our proof of Corollary 7.

III. RELATIVE ENTROPY AND THE HOLEVO BOUND

The Holevo bound (1) can be reexpressed in terms of relative entropy in several ways (see, for example, the discussion in Ref. 14). Here we will follow the approach of Ohya, Petz, and Watanabe[15] and Schumacher and Westmoreland,[10] who express (1) as an optimization of relative entropy.

Let Φ be a channel, and let $\mathcal{E}=\{\pi_i,\rho_i\}$ be an ensemble of input states for the channel. Define

$$\chi(\Phi;\mathcal{E})=S\left(\sum\ \pi_i\Phi(\rho_i)\right)-\sum\ \pi_i S(\Phi(\rho_i)). \tag{21}$$

Following the notation of Ref. 10, the Holevo capacity of the channel is denoted

$$\chi^*(\Phi)=C_{\mathrm{Holv}}(\Phi)=\sup_{\mathcal{E}}\chi(\Phi;\mathcal{E}). \tag{22}$$

As shown in Ref. 10 there is an ensemble which achieves this supremum. The ensemble may not be unique, however its average input state is unique. We let $\rho^*=\Sigma\pi_i\rho_i$ denote this optimal average input state.

The relative entropy of a state ω with respect to a state ρ is defined by

$$S(\omega|\rho)=\mathrm{Tr}\omega(\log\omega-\log\rho). \tag{23}$$

Relative entropy is non-negative: $S(\omega|\rho)\geqslant 0$, with equality if and only if $\omega=\rho$. There is a useful characterization of the capacity $\chi^*(\Phi)$ in terms of relative entropy, namely

$$\chi^*(\Phi)=\inf_{\rho}\sup_{\omega}S(\Phi(\omega)|\Phi(\rho)). \tag{24}$$

This result was derived in Ref. 15 and also in Ref. 10. For our purposes it is convenient to restate it as follows: for any state ρ,

$$\chi^*(\Phi)\leqslant\sup_{\omega}S(\Phi(\omega)|\Phi(\rho)) \tag{25}$$

and equality holds in (25) if and only if $\rho=\rho^*$.

Our goal is the additivity result (2). By restricting to product states it is clear that

$$\chi^*(\Omega)+\chi^*(\Phi)\leqslant\chi^*(\Omega\otimes\Phi). \tag{26}$$

So, to establish (2) it is sufficient to prove the bound

$$\chi^*(\Omega\otimes\Phi)\leqslant\chi^*(\Omega)+\chi^*(\Phi). \tag{27}$$

For a channel Φ, denote the optimal average *output* state by

$$\rho_\Phi := \Phi(\rho^*). \tag{28}$$

Then (25) implies that

$$\chi^*(\Omega\otimes\Phi)\leqslant\sup_\tau S((\Omega\otimes\Phi)(\tau)|\rho_\Omega\otimes\rho_\Phi). \tag{29}$$

Therefore, in order to prove (27), and hence (2), it is sufficient to show that for any state τ,

$$S((\Omega\otimes\Phi)(\tau)|\rho_\Omega\otimes\rho_\Phi)\leqslant\chi^*(\Omega)+\chi^*(\Phi). \tag{30}$$

IV. PROOF FOR CQ CHANNEL

Let Φ be a CQ channel on $B(\mathbf{C}^N)$, so that

$$\Phi(\rho)=\sum \mathrm{Tr}(\rho X_b)Q_b, \tag{31}$$

where $\{X_b\}$ are one-dimensional orthogonal projections. It follows that for all $b=1,\ldots,N$,

$$Q_b=\Phi(X_b). \tag{32}$$

Let Ω be a completely positive map on $B(\mathbf{C}^K)$. Then for any state τ in $B(\mathbf{C}^K\otimes\mathbf{C}^N)$,

$$(\Omega\otimes\Phi)(\tau)=\sum_b \Omega(\mathrm{Tr}_2[(I\otimes X_b)\tau])\otimes Q_b, \tag{33}$$

where Tr_2 is the trace over the second factor. For each $b=1,\ldots,N$ let

$$n_b=\mathrm{Tr}((I\otimes X_b)\tau), \tag{34}$$

and define the state

$$\tau_b=\frac{1}{n_b}\mathrm{Tr}_2((I\otimes X_b)\tau). \tag{35}$$

Then (33) can be written

$$(\Omega\otimes\Phi)(\tau)=\sum_b n_b\Omega(\tau_b)\otimes Q_b=\sum_b n_b\Omega(\tau_b)\otimes\Phi(X_b), \tag{36}$$

where in the second equality we used (32).

Turning first to the l_p norm result, it follows from (36) and the definition (4) that

$$\|(\Omega\otimes\Phi)(\tau)\|_p\leqslant\sum n_b\,\nu_p(\Omega)\,\nu_p(\Phi)=\nu_p(\Omega)\,\nu_p(\Phi), \tag{37}$$

and this proves (6).

Turning next to the channel capacity result, we will prove that (30) holds. Indeed (36) implies that

$$S((\Omega\otimes\Phi)(\tau)|\rho_\Omega\otimes\rho_\Phi)\leqslant\sum\ n_b\,[S(\Omega(\tau_b)|\rho_\Omega)+S(\Phi(X_b)|\rho_\Phi)], \tag{38}$$

where we used the additivity of relative entropy for product states. Now (24) implies

$$S(\Omega(\tau_b)|\rho_\Omega)\leqslant\chi^*(\Omega),\quad S(\Phi(X_b)|\rho_\Phi)\leqslant\chi^*(\Phi), \tag{39}$$

which proves the result.

V. PROOF FOR QC CHANNEL

Let Φ be a QC channel, so that

$$\Phi(\rho)=\sum\ \mathrm{Tr}(\rho X_b)Q_b\,, \tag{40}$$

where now $\{Q_b\}$ are one-dimensional orthogonal projections. For any state τ,

$$(\Omega\otimes\Phi)(\tau)=\sum\ \Omega(\mathrm{Tr}_2(I\otimes X_b)\tau)\otimes Q_b=\sum\ n_b\Omega(\tau_b)\otimes Q_b\,, \tag{41}$$

where we use the definitions (34) and (35). Now define

$$\theta=\mathrm{Tr}_1(\tau). \tag{42}$$

Then it follows that

$$n_b=\mathrm{Tr}(\theta X_b) \tag{43}$$

and (41) can be written as

$$(\Omega\otimes\Phi)(\tau)=\sum\ \Omega(\tau_b)\otimes(\mathrm{Tr}(\theta X_b)Q_b). \tag{44}$$

First we prove the bound for the l_p norm. Using the fact that $\{Q_b\}$ are orthogonal projections, we get

$$\mathrm{Tr}|(\Omega\otimes\Phi)(\tau)|^p=\sum\ \mathrm{Tr}|\Omega(\tau_b)|^p\ (\mathrm{Tr}(\theta X_b))^p. \tag{45}$$

The definition of the l_p norm implies that for any positive matrix A,

$$\|\Omega(A)\|_p\leqslant\nu_p(\Omega)\ \mathrm{Tr}(A), \tag{46}$$

and hence (45) implies that

$$\mathrm{Tr}|(\Omega\otimes\Phi)(\tau)|^p\leqslant(\nu_p(\Omega))^p\sum\ (\mathrm{Tr}(\theta X_b))^p. \tag{47}$$

Furthermore, from (40) it follows that

$$\mathrm{Tr}|\Phi(\theta)|^p=\sum\ [\mathrm{Tr}(\theta X_b)]^p. \tag{48}$$

Combining (47) and (48) and taking the pth root gives

$$\|\Omega\otimes\Phi(\tau)\|_p \leqslant \nu_p(\Omega)\,\|\Phi(\theta)\|_p \leqslant \nu_p(\Omega)\,\nu_p(\Phi), \tag{49}$$

which then proves the result.

Turning now to the additivity of the channel capacity, we will again establish the bound (30). We claim that the following identity holds:

$$S((\Omega\otimes\Phi)(\tau)|\rho_\Omega\otimes\rho_\Phi) = \sum \mathrm{Tr}(\theta X_b) S(\Omega(\tau_b)|\rho_\Omega) + S(\Phi(\theta)|\rho_\Phi). \tag{50}$$

From the result (25) it follows that

$$S(\Phi(\theta)|\rho_\Phi) \leqslant \chi^*(\Phi), \quad S(\Omega(\tau_b)|\rho_\Omega) \leqslant \chi^*(\Omega). \tag{51}$$

Therefore (50) implies

$$S((\Omega\otimes\Phi)(\tau)|\rho_\Omega\otimes\rho_\Phi) \leqslant \sum \mathrm{Tr}(\theta X_b)\chi^*(\Omega) + \chi^*(\Phi) = \chi^*(\Omega) + \chi^*(\Phi), \tag{52}$$

and this proves the result.

So it remains to verify the identity (50). This follows easily from the definition of relative entropy, and the fact that $\{Q_b\}$ are orthogonal projections.

VI. PROOFS FOR QUBIT CHANNELS

In this section we prove Theorems 2 and 3. We do this by establishing the bound (11), and then using Corollary 5, which will be proved in the next section.

Let Φ be a qubit map, and assume that bases have been chosen in its domain and range so that it has the form (8). Clearly, the maximal l_p norm of Φ is invariant under permutations of the three coordinates. It is also invariant under the following symmetry operations.

Lemma 8: For every p, $\nu_p(\Phi)$ is invariant if the signs of any two of $(\lambda_1,\lambda_2,\lambda_3)$ are reversed, or if the signs of any two of (t_1,t_2,t_3) are reversed.

The proof is easy: first notice that conjugation by σ_1 in the domain of Φ switches the signs of λ_2,λ_3 without any other changes, and similarly for conjugation by σ_2 and σ_3. Then notice that simultaneous conjugation by σ_1 in both the domain and range of Φ switches the signs of t_2,t_3 without any other changes, and similarly for σ_2 and σ_3.

As a consequence, we will assume henceforth without loss of generality that

$$t_1 \geqslant 0, t_2 \geqslant 0 \quad \text{and} \quad \lambda_1 \geqslant \lambda_2 \geqslant 0. \tag{53}$$

Our first goal is to establish Conjecture 4 for $p=2$, for any map Φ. We rewrite (10) more fully as

$$M = \begin{pmatrix} X & Y_1 - iY_2 \\ Y_1 + iY_2 & Z \end{pmatrix}, \tag{54}$$

where $X>0$, $Z>0$ and Y_1, Y_2 are Hermitian. Let $W=(X+Z)/2$. Then using the special form (8) we get

$$(I\otimes\Phi)(M) = \begin{pmatrix} c_{++}X + c_{-+}Z & (t_1W + \lambda_1 Y_1) - i(t_2W + \lambda_2 Y_2) \\ (t_1W + \lambda_1 Y_1) + i(t_2W + \lambda_2 Y_2) & c_{--}X + c_{+-}Z \end{pmatrix}, \tag{55}$$

where

$$c_{++} = (1+\lambda_3+t_3)/2, \quad c_{-+} = (1-\lambda_3+t_3)/2, \tag{56}$$

$$c_{+-}=(1+\lambda_3-t_3)/2, \quad c_{--}=(1-\lambda_3-t_3)/2.$$

Note that since $M\geqslant 0$ and Φ is a qubit map, it follows that $(I\otimes\Phi)(M)\geqslant 0$ for all choices of X and Z. Hence the four coefficients in (56) are positive, for all allowed values of t_3 and λ_3.

Taking the trace of the square of (55) gives

$$\begin{aligned}\mathrm{Tr}|(I\otimes\Phi)(M)|^2=&\mathrm{Tr}(c_{++}X+c_{-+}Z)^2+\mathrm{Tr}(c_{+-}X+c_{--}Z)^2+2\,\mathrm{Tr}(t_1W+\lambda_1Y_1)^2\\&+2\,\mathrm{Tr}(t_2W+\lambda_2Y_2)^2.\end{aligned} \tag{57}$$

Define

$$x=\|X\|_2,\ \ z=\|Z\|_2,\ \ y_1=\|Y_1\|_2,\ \ y_2=\|Y_2\|_2. \tag{58}$$

Then using the Cauchy–Schwarz inequality for the Hilbert–Schmidt norm and our positivity condition (53) we get

$$\begin{aligned}\mathrm{Tr}|(I\otimes\Phi)(M)|^2\leqslant&(c_{++}x+c_{-+}z)^2+(c_{+-}x+c_{--}z)^2+2\left(t_1\frac{(x+z)}{2}+\lambda_1y_1\right)^2\\&+2\left(t_2\frac{(x+z)}{2}+\lambda_2y_1\right)^2.\end{aligned} \tag{59}$$

Define the 2×2 matrix

$$m=\begin{pmatrix}x & y_1-iy_2\\ y_1+iy_2 & z\end{pmatrix}. \tag{60}$$

Then (59) can be rewritten as

$$\|I\otimes\Phi(M)\|_2\leqslant\|\Phi(m)\|_2. \tag{61}$$

The positivity of M implies that

$$y_1^2+y_2^2=\mathrm{Tr}|Y_1-iY_2|^2\leqslant\|X\|_2\|Z\|_2=xz, \tag{62}$$

and hence that m is positive. Therefore

$$\|(I\otimes\Phi)(M)\|_2\leqslant\nu_2(\Phi)\mathrm{Tr}(m)=\nu_2(\Phi)(x+z)=\nu_2(\Phi)(\|X\|_2+\|Z\|_2), \tag{63}$$

which establishes (11) for $p=2$, and hence by Corollary 5 proves Theorem 2.

In order to prove Theorem 3 we will assume that the condition (9) is satisfied. Without loss of generality, this condition can be rewritten as follows:

$$t_1\geqslant 0 \quad \text{and} \quad t_2=0 \quad \text{and} \quad \lambda_1\geqslant\lambda_2\geqslant 0. \tag{64}$$

To see this, suppose first that $|\lambda_i|\neq|\lambda_j|$ for any i,j. Then the condition (9) implies that at least one of the t_i is zero, and also that the corresponding $|\lambda_i|$ is not the largest. Hence by permuting coordinates we can arrange that $t_2=0$ and that $|\lambda_1|>|\lambda_2|$. By switching signs of pairs of parameters we can then restate (9) as (64). Suppose now that $|\lambda_i|=|\lambda_j|$ for some i,j. By permuting coordinates we can assume that $|\lambda_1|=|\lambda_2|$, and by changing signs that $\lambda_1=\lambda_2\geqslant 0$. This allows a further symmetry transformation, namely we can conjugate by a unitary matrix $U=e^{i\theta\sigma_3}$ in the range of Φ without changing $\nu_p(\Phi)$. With such a conjugation we can set $t_2=0$, and then the condition (64) again holds.

The condition (64) is clearly satisfied for all unital maps, since in that case $t_i=0$ for all i. It is also satisfied by all maps in the closure of the set of extreme points of the (convex) set of qubit maps. This fact follows from Theorem 4 in Ref. 12, where it was shown that all such maps have only one of the parameters t_1,t_2,t_3 being nonzero.

In order to prove (11), we rewrite (55) as

$$(I\otimes\Phi)(M)=\begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22}\end{pmatrix}=R_{11}\otimes E_{11}+R_{12}\otimes E_{12}+R_{21}\otimes E_{21}+R_{22}\otimes E_{22}, \tag{65}$$

where E_{ij} is the 2×2 matrix with 1 in position (i,j) and 0 elsewhere, and where

$$\begin{aligned} R_{11}&=c_{++}X+c_{-+}Z,\\ R_{12}&=(t_1W+\lambda_1Y_1)-i\lambda_2Y_2,\\ R_{21}&=(t_1W+\lambda_1Y_1)+i\lambda_2Y_2,\\ R_{22}&=c_{--}X+c_{+-}Z \end{aligned} \tag{66}$$

[we have used the condition (64) to set $t_2=0$].

For integer p we can evaluate $\mathrm{Tr}|(I\otimes\Phi)(M)|^p$ by multiplying the right side of (65) with itself p times, and taking the trace with respect to a product basis $e_i\otimes f_j$ where $\{e_i\}$ span $\mathbf{C}^K$ and f_1,f_2 span $\mathbf{C}^2$. The result is

$$\mathrm{Tr}|(I\otimes\Phi)(M)|^p=\sum \mathrm{Tr}[E_{i_1j_1}E_{i_2j_2}\cdots E_{i_pj_p}]\mathrm{Tr}[R_{i_1j_1}R_{i_2j_2}\cdots R_{i_pj_p}], \tag{67}$$

where the sum runs over all indices $i_1,j_1,\ldots,i_p,j_p=1,2$. The coefficient $\mathrm{Tr}[E_{i_1j_1}E_{i_2j_2}\cdots E_{i_pj_p}]$ in each of these terms is non-negative, since the matrices $\{E_{ij}\}$ are all non-negative. Furthermore, repeated application of Hölder's inequality shows that

$$|\mathrm{Tr}A_1A_2\cdots A_p|\leqslant\|A_1\|_p\|A_2\|_p\cdots\|A_p\|_p \tag{68}$$

for any product of p matrices. Hence the sum in (67) is bounded above by

$$\mathrm{Tr}|(I\otimes\Phi)(M)|^p\leqslant\sum \mathrm{Tr}[E_{i_1j_1}E_{i_2j_2}\cdots E_{i_pj_p}]\|R_{i_1j_1}\|_p\|R_{i_2j_2}\|_p\cdots\|R_{i_pj_p}\|_p. \tag{69}$$

We define the 2×2 matrix

$$m'=\begin{pmatrix} x' & y' \\ y' & z'\end{pmatrix}, \tag{70}$$

where now

$$x'=\|X\|_p,\quad z'=\|Z\|_p,\quad y'=\|Y_1-iY_2\|_p. \tag{71}$$

The matrix m' is positive. This can be seen most easily by noting that the positivity of M implies that $Y_1-iY_2=\sqrt{X}\,T\,\sqrt{Z}$ where T is a contraction,[12] and hence by Hölder's inequality $y'\leqslant\sqrt{x'z'}$. Applying the map Φ gives

$$\begin{aligned}\Phi(m')=&[c_{++}x'+c_{-+}z']\otimes E_{11}+[t_1(x'+z')/2+\lambda_1y']\otimes E_{12}\\ &+[t_1(x'+z')/2+\lambda_1y']\otimes E_{21}+[c_{--}x'+c_{+-}z']\otimes E_{22}.\end{aligned} \tag{72}$$

Applying the same method to evaluate $\mathrm{Tr}|\Phi(m')|^p$ gives

$$\mathrm{Tr}|\Phi(m')|^p=\sum \mathrm{Tr}[E_{i_1j_1}E_{i_2j_2}\cdots E_{i_pj_p}]r_{i_1j_1}r_{i_2j_2}\cdots r_{i_pj_p}, \tag{73}$$

where

$$\begin{aligned} r_{11}&=c_{++}x'+c_{-+}z',\\ r_{12}=r_{21}&=t_1(x'+z')/2+\lambda_1 y',\\ r_{22}&=c_{--}x'+c_{+-}z'. \end{aligned} \tag{74}$$

We now claim that

$$\mathrm{Tr}|(I\otimes\Phi)(M)|^p\leqslant\mathrm{Tr}|\Phi(m')|^p. \tag{75}$$

If we assume for the moment that (75) is valid, then it implies

$$\|(I\otimes\Phi)(M)\|_p\leqslant\|\Phi(m')\|_p\leqslant\nu_p(\Phi)\mathrm{Tr}(m')\leqslant\nu_p(\Phi)(x'+z'). \tag{76}$$

This proves (11), which by Corollary 5 implies Theorem 3.

So, it is sufficient to demonstrate (75). From (69) and (73) it is sufficient to show that

$$\|R_{ij}\|_p\leqslant r_{ij} \tag{77}$$

for all $i,j=1,2$. First, using the positivity of c_{++}, etc., we have

$$\begin{aligned} \|R_{11}\|_p&=\|c_{++}X+c_{-+}Z\|_p\leqslant c_{++}x'+c_{-+}z'=r_{11},\\ \|R_{22}\|_p&=\|c_{+-}X+c_{--}Z\|_p\leqslant c_{+-}x'+c_{--}z'=r_{22}. \end{aligned}$$

The remaining bound also follows easily, since

$$\begin{aligned} \|R_{12}\|_p=\|t_1\frac{(X+Z)}{2}+\lambda_1Y_1-i\lambda_2Y_2\|_p&\leqslant\|t_1\frac{(X+Z)}{2}\|_p+\|(\lambda_1-\lambda_2)Y_1+\lambda_2(Y_1-iY_2)\|_p\\ &\leqslant t_1(x'+z')/2+(\lambda_1-\lambda_2)\|Y_1\|_p+\lambda_2\|Y_1-iY_2\|_p, \end{aligned} \tag{78}$$

where in the last line we used (53). Furthermore,

$$\|Y_1\|_p=\|(Y_1-iY_2)/2+(Y_1+iY_2)/2\leqslant\tfrac{1}{2}\|Y_1-iY_2\|_p+\tfrac{1}{2}\|Y_1+iY_2\|_p=y'.$$

Hence (78) becomes

$$\|R_{12}\|_p\leqslant t_1(x'+z')/2+(\lambda_1-\lambda_2)y'+\lambda_2y'=t_1(x'+z')/2+\lambda_1y'=r_{12}, \tag{79}$$

which establishes the result.

VII. PROOFS OF COROLLARIES

A. Corollary 5

Let Ω be any completely positive map on $\mathcal{B}(\mathbf{C}^K)$, and let τ be a state on $\mathcal{B}(\mathbf{C}^K\otimes\mathbf{C}^2)$ of the form

$$\tau=\begin{pmatrix} A & B\\ B^* & C\end{pmatrix}, \tag{80}$$

where A,B,C are $K\times K$ matrices, with $A\geqslant 0$, $C\geqslant 0$ and $\mathrm{Tr}(A+C)=1$. Then $M=(\Omega\otimes I)(\rho)$ has the form (10) with $X=\Omega(A)$, $Y=\Omega(B)$ and $Z=\Omega(C)$. Hence from the definition of the maximal l_p norm it follows that

$$\|X\|_p\leqslant \nu_p(\Omega)\mathrm{Tr}(A),\ \ \|Z\|_p\leqslant \nu_p(\Omega)\mathrm{Tr}(C). \tag{81}$$

Applying (11) and using the facts that $(I\otimes\Phi)(M)=(\Omega\otimes\Phi)(\rho)$ and $\mathrm{Tr}(A)+\mathrm{Tr}(C)=\mathrm{Tr}(\rho)=1$ we immediately deduce Corollary 5.

B. Corollary 6

Recall that the entropy of a state ρ is defined by

$$S(\rho)=-\mathrm{Tr}\rho\log\rho. \tag{82}$$

Using $\mathrm{Tr}\rho=1$ it follows that

$$\frac{d}{dp}(\|\rho\|_p)_{p=1}=-S(\rho), \tag{83}$$

and hence that

$$\frac{d}{dp}(\nu_p(\Phi))_{p=1}=-S_{\min}(\Phi). \tag{84}$$

Therefore taking the derivative of (6) at $p=1$ yields immediately (13).

C. Corollary 7

From the results of Sec. II, it is sufficient to establish the bound (30). For any states ω and ρ we have

$$\log(\omega\otimes\rho)=\log\omega\otimes I+I\otimes\log\rho. \tag{85}$$

Furthermore, since Φ is a unital qubit map it follows that its optimal average output state is

$$\rho_\Phi=\tfrac{1}{2}I. \tag{86}$$

Since $\log(1/2\,I)=-\log(2)I$ and $\mathrm{Tr}(\Omega\otimes\Phi)(\rho)=1$ it follows that the left side of (30) can be written as

$$-S((\Omega\otimes\Phi)(\tau))-\mathrm{Tr}((\Omega\otimes\Phi)(\tau)\log(\rho_\Omega)\otimes I)+\log(2). \tag{87}$$

Define

$$\omega=\mathrm{Tr}_2\tau. \tag{88}$$

Then the second term in (87) is equal to

$$-\mathrm{Tr}\Omega(\omega)\log(\rho_\Omega). \tag{89}$$

Also, the fact that Φ is unital implies that

$$\chi^*(\Phi)=\log(2)-S_{\min}(\Phi). \tag{90}$$

Hence to prove (30) it is sufficient to prove that

$$-S((\Omega\otimes\Phi)(\tau))-\mathrm{Tr}\Omega(\omega)\log(\rho_\Omega)\leqslant\chi^*(\Omega)-S_{\min}(\Phi). \tag{91}$$

Now we use the bound (20), which is implied by (11). Again let τ have the form (80), so that $M=(\Omega\otimes I)(\tau)$ has the form (10) with $X=\Omega(A)$ and $Z=\Omega(C)$. Let $a=\mathrm{Tr}A=\mathrm{Tr}X$, and define the states

$$\alpha=\frac{1}{\mathrm{Tr}A}A=\frac{1}{a}A, \quad \gamma=\frac{1}{\mathrm{Tr}C}C=\frac{1}{1-a}C. \tag{92}$$

Then using the notation of (19), $\xi=\Omega(\alpha)$ and $\zeta=\Omega(\gamma)$, and (20) can be written

$$S((\Omega\otimes\Phi)(\tau))\geqslant S_{\min}(\Phi)+aS(\Omega(\alpha))+(1-a)S(\Omega(\gamma)). \tag{93}$$

Comparing with (91), it is sufficient to prove that

$$-aS(\Omega(\alpha))-(1-a)S(\Omega(\gamma))-\mathrm{Tr}\,\Omega(\omega)\log(\rho_\Omega)\leqslant\chi^*(\Omega). \tag{94}$$

Since $\omega=a\alpha+(1-a)\gamma$, we can rewrite the left side of (94) as

$$aS(\Omega(\alpha)|\rho_\Omega)+(1-a)S(\Omega(\gamma)|\rho_\Omega). \tag{95}$$

Since ρ_Ω is the optimal output state for the channel Ω, it follows from (24) that

$$S(\Omega(\alpha)|\rho_\Omega)\leqslant\chi^*(\Omega), \tag{96}$$

$$S(\Omega(\gamma)|\rho_\Omega)\leqslant\chi^*(\Omega). \tag{97}$$

Combining (94)–(96) yields the result.

VIII. SUMMARY

The results in this article all concern product channels of the form $\Omega\otimes\Phi$, where in every case Ω is an arbitrary channel. For these product channels we prove a variety of results involving different measures of the purity of output states from the channel.

The first set of results apply when Φ is a CQ or QC channel. Recall that the CQ channel first maps an input state to a letter in a classical alphabet, and then maps this to a quantum state at the output. The QC channel measures the input state with some POVM, and assigns different results to orthogonal output states. In both cases we prove that the output state with maximal l_p norm is a product state, and also that the Holevo capacity is achieved on a product state. In other words, the maximal l_p norm of the product channel is multiplicative and the Holevo capacity is additive. These results were previously shown to be true in the case where Φ is the identity map (and the additivity of the Holevo capacity also when $\Omega=\Phi$).

The second set of results applies when Φ is a qubit map, that is, a map on states in $\mathbf{C}^2$. We prove multiplicativity for the $p=2$ norm, for any qubit map Φ. We also prove multiplicativity for the l_p norm when p is any integer, and with some restrictions on Φ. The class of maps Φ satisfying the restrictions includes all unital qubit maps.

The third set of results revolves around a conjectured bound (11) for the l_p norm of any output state from the half-noisy channel $I\otimes\Phi$, when Φ is a qubit channel. We show that this bound implies multiplicativity of the l_p norm for any product channel $\Omega\otimes\Phi$. We also show that when Φ is *unital* the bound implies additivity of the Holevo capacity of the product channel $\Omega\otimes\Phi$. Therefore we believe that this conjecture provides a new and useful approach to the conjecture that the Holevo capacity is universally additive. In a hopeful sign of future progress on this important problem, Lieb and Ruskai have established Conjecture 4 in one nontrivial case (their proof appears as the Appendix that follows).

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APPENDIX: THEOREM OF LIEB AND RUSKAI

Let $M=\left(\begin{smallmatrix} X & Y \\ Y^* & Z \end{smallmatrix}\right)$ and recall that M is positive semi-definite if and only $Y=\sqrt{X}R\sqrt{Z}$ with R a contraction. Moreover, any contraction can be written as a convex combination of unitary matrices. (See Ref. 16 or 12 for details and further references.) Hence, by the convexity of the p-norm, it suffices to prove (17) under the assumption that $Y=\sqrt{X}V\sqrt{Z}$ with V unitary.

We now consider the special case $X=Z$ and note that we can write

$$(I\otimes\Phi)(M)=\begin{pmatrix} X & \lambda Y \\ \lambda Y^* & X \end{pmatrix}=\sqrt{F}G\sqrt{F} \tag{A1}$$

with $F=\left(\begin{smallmatrix} X & 0 \\ 0 & X \end{smallmatrix}\right)$ and $G=\left(\begin{smallmatrix} I & \lambda V \\ \lambda V^* & I \end{smallmatrix}\right)$. We will use a result of Lieb and Thirring (Appendix B of Ref. 17) that, for $p\geqslant 1$ and $F,G\geqslant 0$,

$$\mathrm{Tr}(F^{1/2}GF^{1/2})^p\leqslant\mathrm{Tr}(F^pG^p). \tag{A2}$$

The critical feature is to note that G has eigenvalues $(1\pm\lambda)$. Moreover,

$$\begin{pmatrix} I & \lambda V \\ \lambda V^* & I \end{pmatrix}=\frac{1}{2}\begin{pmatrix} I & V \\ V^* & -I \end{pmatrix}\begin{pmatrix} (1+\lambda)I & 0 \\ 0 & (1-\lambda)I \end{pmatrix}\begin{pmatrix} I & V \\ V^* & -I \end{pmatrix}. \tag{A3}$$

Thus

$$\begin{aligned}\mathrm{Tr}[(I\otimes\Phi)(M)]^p&\leqslant\frac{1}{2}\mathrm{Tr}\begin{pmatrix} I & V \\ V^* & -I \end{pmatrix}\begin{pmatrix} X^p & 0 \\ 0 & X^p \end{pmatrix}\begin{pmatrix} I & V \\ V^* & -I \end{pmatrix}\begin{pmatrix} (1+\lambda)^pI & 0 \\ 0 & (1-\lambda)^pI \end{pmatrix}\\ &=(1+\lambda)^p\mathrm{Tr}\frac{1}{2}(X^p+VX^pV^*)+(1-\lambda)^p\,\mathrm{Tr}\frac{1}{2}(X^p+V^*X^pV)\\ &=[2\nu_p(\Phi)]^p\|X\|_p^p.\end{aligned}$$

Taking the pth root gives the desired result, $\|(I\otimes\Phi)(M)\|_p\leqslant\nu_p(\Phi)2\|X\|_p$.

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Pinning phenomena near the lower critical field for superconductor

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In this paper, we prove that for fields close to the lower critical field, minimizers of the Ginzburg–Landau functional of an inhomogeneous superconductor have a number of vortices bounded independently from the Ginzburg–Landau parameter. We also locate the vortices. © *2002 American Institute of Physics.*
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I. INTRODUCTION AND STATEMENT OF THE RESULTS

We are interested in describing the global minimizers of the Ginzburg–Landau functional

$$J(u,A)=\frac{1}{2}\int_{\Omega}|\nabla_A u|^2+|h-h_{\mathrm{ex}}|^2+\frac{\kappa^2}{2}(a(x)-|u|^2)^2 \tag{1.1}$$

that corresponds to the free energy of a superconductor[1,2] in a prescribed, constant magnetic field h_{ex}. Here $\Omega\subset\mathbb{R}^2$ is the smooth, bounded, simply connected section of the superconductor and $a(x):\Omega\to\mathbb{R}$ is a given function satisfying $0<\min_{\bar{\Omega}}a(x)\leqslant a(x)\leqslant 1$ in Ω. The unknowns in (1.1) are the complex-valued order parameter $u\in H^1(\Omega,\mathbb{C})$ and the $U(1)$ connection $A\in H^1(\Omega,\mathbb{R}^2)$. Here $h=\mathrm{curl}A=-\partial_2A_1+\partial_1A_2$ is the induced magnetic field and $\nabla_A u=\nabla u-iAu$. The order parameter u indicates the local state of the material: $|u|$ is the density of superconducting electron pairs, so that, when $|u|\simeq 1$, the material is in its superconducting state, whereas when $|u|\simeq 0$, it is in its normal state. $\kappa>0$ is the Ginzburg–Landau parameter depending on the material. The minima of $a(x)$ corresponds to the impurities in the material. It is expected that these minima will be the pinning sites for the vortices.

Minimizers of $J(u,A)$ in $H^1(\Omega,\mathbb{C})\times H^1(\Omega,\mathbb{R}^2)$ solve the Euler equations

$$\begin{cases}-\nabla_A^2 u=\kappa^2 u(a(x)-|u|^2) & \text{in } \Omega,\\ -\nabla^{\perp}h=(iu,\nabla_A u) & \text{in } \Omega,\end{cases} \tag{1.2}$$

with the boundary conditions

$$\begin{cases}h=h_{\mathrm{ex}} & \text{on } \partial\Omega,\\ (\nabla u-iAu)\cdot\nu=0 & \text{on } \partial\Omega.\end{cases} \tag{1.3}$$

Here $\nabla^{\perp}$ denotes $(-\partial_{x_2},\partial_{x_1})$, ν is the unit outer normal vector to $\partial\Omega$, and $(z,w)=\mathrm{Re}(z\bar{w})$ where z and w are in $\mathbb{C}$.

The functional $J(u,A)$ are invariant under $U(1)$ gauge transformations of the type

$$v=ue^{i\varphi},\quad B=A+\nabla\varphi \quad \text{for any } \varphi\in H^2(\Omega,\mathbb{R}). \tag{1.4}$$

It is well known that there are two critical fields H_{c_1} and H_{c_2} for which a phase transition occurs. Above H_{c_2}, superconductivity is destroyed and material is in the normal phase. Below

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H_{c_1}, the material is superconducting everywhere. When $H_{c_1} \leqslant h_{\text{ex}} \leqslant H_{c_2}$, the material is in mixed state. In this state, the minimizers of (1.1) exhibit vortices, i.e., points where the order parameter vanishes. It is of interest to determine where these points are located. We refer to Refs. 3–13 for a discussion of this functional in the case $a(x)=1$.

In this paper, we want to address the question of how the term will modify the properties of the superconductor in the presence of an exterior magnetic field here. In particular, our interest is the pinning phenomena of vortices. First, we recall some results. In Ref. 14, we obtained the asymptotic expansion

$$H_{c_1} \sim \frac{|\log \kappa|}{\max_{\Omega} \left| \frac{\xi_0}{a} \right|} \quad \text{as} \quad \kappa \to \infty, \tag{1.5}$$

where h_0 is the solution of

$$\begin{cases} -\operatorname{div}\left(\frac{1}{a}\nabla h_0\right) + h_0 = 0 & \text{in } \Omega, \\ h_0 = 1 & \text{on } \partial\Omega, \end{cases} \tag{1.6}$$

and

$$\xi_0 = h_0 - 1 < 0. \tag{1.7}$$

In Ref. 15, we prove the following theorem.

Theorem A: *There exist constants $\kappa_0, C>0$ such that for any $\kappa > \kappa_0$ and $h_{\text{ex}} < H_{c_1} - C \log\log \kappa$, the minimizer (u,A) of (1.1) satisfies $|u| \geqslant \frac{1}{2}\min_{\Omega} a > 0$ in $\overline{\Omega}$, that is, the minimizer (u,A) has no vortex.*

In this paper, we are interested in the case $h_{\text{ex}} \leqslant H_{c_1} + C \log\log \kappa$. We prove that the minimizers have bounded vorticity and locate them. Before stating our main results, we recall the construction of vortex balls.

Proposition 1.1: Assume that $\Omega \subset \mathbb{R}^2$ is a smooth simply connected, bounded domain, $a(x):\Omega \to \mathbb{R}_+$ is a C^2--smooth function satisfying $0 < \min_{\Omega} a \leqslant a(x) \leqslant 1$. Then, for any $\kappa > \kappa_0, h_{\text{ex}} < K \log \kappa$, and critical point (u,A) of $J(u,A)$ satisfying the a priori bound $J(u,A) < K(\log \kappa)^2$ the following is true.

There exists a finite family of disjoint balls $\{B_i\}$, where $B_i = B_{r_i}(p_i)$ and

(1) $\{|u| < \sqrt{a} - 1/(\log \kappa)^2\} \subset \cup_i B_i$,
(2) $\Sigma_i r_i < (\log \kappa)^{-10}$.
(3) *Writing $u = \rho e^{i\varphi}$,*

$$\frac{1}{2}\int_{B_i} \rho^2 |\nabla \varphi - A|^2 + |h - h_{\text{ex}}|^2 \geqslant \pi a(p_i)|d_i|(\log \kappa - C \log\log \kappa), \tag{1.8}$$

where d_i is the degree of the map $u/|u|$ restricted to ∂B_i if $B_i \subset \Omega$ and $d_i = 0$ otherwise.

We say that $\{(p_i, d_i)\}$ is a family of vortices associated to (u,A), and we call $\{B_i\}$ the family of vortex balls. It is easily seen by testing J with the configuration $(u \equiv \sqrt{a}, A \equiv 0)$ that a minimizer (u,A) of (1.1) satisfies the *a priori* bound $J(u,A) < \frac{1}{2}(\int_{\Omega} |\nabla \sqrt{a}|^2) h_{\text{ex}}^2$, and therefore can be associated with a family of vortices by the above proposition whenever $h_{\text{ex}} < K \log \kappa$. We may now state our main theorem.

Theorem 1.2: *Let Ω be a smooth, bounded, simply connected domain in $\mathbb{R}^2$. Assume that $a(x):\Omega \to \mathbb{R}$ is an analytic function satisfying $0 < a_0 = \min_{\Omega} a(x) \leqslant a(x) \leqslant 1$ in Ω. For any $K>0$,*

there exist positive constants κ_0, C, α *such that for any* $\kappa>\kappa_0$ *and any* $h_{\text{ex}}<H_{c_1}+K\log\log\kappa$, *if* (u,A) *is a global minimizer of (1.1) and* $\{(p_i,d_i)\}$ *is an associated family of vortices then the following holds:*

(1) $\forall i,\ d_i\geqslant 0$,
(2) $\Sigma_i d_i\leqslant C$,
(3) $\text{dist}(p_i,\Lambda)\leqslant C(\log\kappa)^{-\alpha}$ *for any* i *such that* $d_i\neq 0$, *where*

$$\Lambda=\left\{x\in\Omega:\frac{\xi_0(x)}{a(x)}=\max_\Omega\left|\frac{\xi_0}{a}\right|\right\} \tag{1.9}$$

and $\xi_0=h_0-1$.

Remark: It follows from conclusion (3) of Theorem 1.2 that the distribution of the vortices location is governed both by the term $a(x)$ and by the function ξ_0. This is called the pinning phenomena in superconductor. This conclusion extends the results in Ref. 10.

This paper is organized as follows. In Sec. II, we shall prove Proposition 1.1. In Sec. III, we shall split the energy J. In Sec. IV, we shall prove Theorem 1.2.

II. CONSTRUCTION OF VORTEX BALLS

In this section we will give a proof of Proposition 1.1. We will divide the proof into three steps.

Step 1: Denoting $|u|$ by ρ, since $\int_\Omega|\nabla u|^2\geqslant\int_\Omega|\nabla\rho|^2$, we have from $J(u,A)<K(\log\kappa)^2$,

$$\int_\Omega|\nabla\rho|^2+\frac{\kappa^2}{2}(a-\rho^2)^2\leqslant 2K(\log\kappa)^2.$$

Hence,

$$\int_\Omega|\nabla(\rho-\sqrt{a})|^2+\frac{\kappa^2}{2}(a-\rho^2)^2\leqslant C(\log\kappa)^2.$$

Step 2: For any $t\in\mathbb{R}$, let $\Omega_t=\{x\in\Omega:|\rho-\sqrt{a}|>t\}$ and $\gamma_t=\partial\Omega_t$. Applying the Coarea formula and arguing as in Lemma 4.2 of Ref. 7,

$$C|\log\kappa|^2\geqslant\int_\Omega|\nabla(\rho-\sqrt{a})|^2+\frac{\kappa^2}{2}(a-\rho^2)^2\geqslant C\kappa\int_\Omega|\nabla(\rho-\sqrt{a})||a-\rho^2|\geqslant C\kappa\int_0^{+\infty}r(\gamma_t)\mathrm{d}t. \tag{2.1}$$

Here, as in Ref. 7, $r(\gamma_t)$ is defined as the infimum over all finite covering of γ_t by balls $B_i,\ldots,B_k$ of the sum $r_1+\cdots+r_k$, where r_i is the radius of B_i. Combining the previous inequality with the mean-value theorem, we find that there exists a $t\in[0,1/(\log\kappa)^2]$ such that $r(\gamma_t)<C(\log\kappa)^4/\kappa$.

Step 3: The next step to construct the vortex balls: starting from the chosen γ_t, covered by balls $B_1,\ldots,B_k$, we use the method of growing and merging of balls used in Refs. 16 and 7: one needs to grow these balls B_i, keeping a suitable lower bound on the energy they contain, until the desired size is reached, with the desired lower bound. When some balls happen to intersect during the growth process, they are merged into a large one.[7] Here we only need to apply the result of Proposition 4.1 of Ref. 7 to A and $v=u/|u|=e^{i\varphi}$ in $\Omega\backslash\Omega_t$, $\sigma=(\log\kappa)^{-10}$. We then obtain the existence of balls $B_i=B(p_i,r_i)$ such that conclusions (1), (2) of Proposition 1.1 hold,[17,18] and

$$\frac{1}{2}\int_{B_i\backslash\Omega_t}|\nabla\varphi-A|^2+\frac{1}{2}\int_{B_i}|h-h_{\text{ex}}|^2\geqslant\pi|d_i|\left(\log\frac{\sigma}{r(\gamma_t)}-C\right)\geqslant\pi|d_i|(\log\kappa-C\log\log\kappa), \tag{2.2}$$

with $d_i=(u,\partial B_i)$ if $\overline{B_i}\subset\Omega$, and 0 otherwise. But we also have, from the Ginzburg–Landau equation $-\nabla^\perp h=\rho^2(\nabla\varphi-A)$, and from $\rho\leqslant 1$ (Ref. 1),

$$\int_\Omega |\nabla h|^2=\int_\Omega \rho^4|\nabla\varphi-A|^2\leqslant\int_\Omega |\nabla_A u|^2\leqslant C(\log\kappa)^2, \tag{2.3}$$

hence

$$\int_{B_i}|h-h_{\rm ex}|^2\leqslant Cr_i\|h-h_{\rm ex}\|^2_{L^4(\Omega)}\leqslant Cr_i\|h-h_{ex}\|^2_{H^1(\Omega)}=o(1). \tag{2.4}$$

Thus, by (2.2), we have

$$\frac{1}{2}\int_{B_i\setminus\Omega_t}|\nabla\varphi-A|^2\geqslant\pi|d_i|(\log\kappa-C\log\log\kappa). \tag{2.5}$$

Now, by using conclusion (1) of this proposition,

$$\begin{aligned}\frac{1}{2}\int_{B_i\setminus\Omega_t}\rho^2|\nabla\varphi-A|^2&=\frac{1}{2}\int_{B_i\setminus\Omega_t}a|\nabla\varphi-A|^2+\frac{1}{2}\int_{B_i\setminus\Omega_t}(\rho^2-a)|\nabla\varphi-A|^2\\&\geqslant\frac{1}{2}(\min_{B_i}a)\int_{B_i\setminus\Omega_t}|\nabla\varphi-A|^2-\frac{C}{(\log\kappa)^2}\int_{B_i\setminus\Omega_t}|\nabla\varphi-A|^2.\end{aligned} \tag{2.6}$$

In view of (2.5), we have

$$\frac{1}{2}\int_{B_i\setminus\Omega_t}|\nabla\varphi-A|^2\geqslant\pi(\min_{B_i}a)|d_i|(\log\kappa-C\log\log\kappa). \tag{2.7}$$

Now, using mean-valued theorem and conclusion (2) of this proposition, we have the following lower bound:

$$\frac{1}{2}\int_{B_i\setminus\Omega_t}|\nabla\varphi-A|^2\geqslant\pi(a(p_i)|d_i|(\log\kappa-C\log\log\kappa). \tag{2.8}$$

This proves the conclusion (3) of Proposition 1.1. The proof of Proposition 1.1 is completed. □

III. SPLITTING OF THE ENERGY $J(u,A)$

The proof of Theorem 1.2 relies on an expansion of the energy of a minimizer in terms of the positions and degrees of its vortices. To get this expansion of the energy, we need the following lemma.

Lemma 3.1: (Ref. 1) *We have for any* $q<2$,

$$\left\|-\operatorname{div}\left(\frac{1}{a}\nabla h\right)+h-2\pi\sum_i d_i\delta_{p_i}\right\|_{W^{-1,q}(\Omega)}=o(1). \tag{3.1}$$

Proposition 3.2: For any $K>0$, *there exist positive* κ_0, C *such that for any* $\kappa>\kappa_0$ *and any* $h_{ex}<K\log\kappa$, *if* (u,A) *is a critical point of* $J(u,A)$ *satisfying* $J(u,A)<K(\log\kappa)^2$ and $\{(p_i,d_i)\}$ *is an associated family of vortices then*

$$J(u,A)\geqslant \frac{1}{2}\int_\Omega |\nabla\sqrt{a}|^2+h_{\rm ex}^2J_0+\pi\Big(\sum_i a(p_i)|d_i|\Big)(\log\kappa-C\log\log\kappa)+2\pi h_{\rm ex}\sum_i d_i\xi_0(p_i)$$
$$+\frac{1}{2}\int_{\Omega\setminus\cup_i B_i}\frac{1}{\rho^2}|\nabla(h-h_{\rm ex}h_0)|^2+\frac{1}{2}\int_\Omega |h-h_{\rm ex}h_0|^2-o(1), \tag{3.2}$$

where we have written $h=\mathrm{curl}A$ *and*

$$J_0=\frac{1}{2}\int_\Omega\frac{1}{a}|\nabla h_0|^2+|h_0-1|^2. \tag{3.3}$$

Proof: Since the quantities involved are gauge invariant we may assume we are working in a Coulomb gauge, i.e., that $\mathrm{div}\,A=0$ in Ω and $A\cdot\nu=0$ on $\partial\Omega$. In the Coulomb gauge, the following *a priori* bounds holds (see Refs. 1 and 14),

$$\|A\|_{H^1(\Omega)}\leqslant C\log\kappa,\quad \|A\|_{L^\infty(\Omega)}\leqslant C\log\kappa,\quad \|u\|_{H^1(\Omega)}\leqslant C\log\kappa. \tag{3.4}$$

Let $\tilde\Omega=\Omega\setminus\cup_i B_i$, where $\{B_i\}_{i\in I}$ is the family of vortex balls defined in Proposition 1.1. Writing $u=\rho e^{i\varphi}$, it follows from $-\nabla^\perp h=(iu,\nabla_A u)=\rho^2(\nabla\varphi-A)$ that

$$|\nabla_A u|^2=|\nabla\rho|^2+\rho^2|\nabla\varphi-A|^2=\frac{1}{\rho^2}|\nabla h|^2+|\nabla\rho|^2. \tag{3.5}$$

Thus,

$$J(u,A)\geqslant\frac{1}{2}\int_{\cup_i B_i}\rho^2|\nabla\varphi-A|^2+|h-h_{\rm ex}|^2+\frac{1}{2}\int_\Omega|\nabla\rho|^2+\frac{\kappa^2}{2}(a-\rho^2)^2$$
$$+\frac{1}{2}\int_{\tilde\Omega}\frac{1}{\rho^2}|\nabla h|^2+|h-h_{\rm ex}|^2. \tag{3.6}$$

Note that

$$\frac{1}{2}\int_\Omega|\nabla\rho|^2+\frac{\kappa^2}{2}(a-\rho^2)^2\geqslant\min_{v\in H^1(\Omega,\mathbb{R})}\frac{1}{2}\int_\Omega|\nabla v|^2+\frac{\kappa^2}{2}(a-v^2)^2. \tag{3.7}$$

Now let

$$\frac{1}{2}\int_\Omega|\nabla v_\kappa|^2+\frac{\kappa^2}{2}(a-v_\kappa^2)^2=\min_{v\in H^1(\Omega,\mathbb{R})}\frac{1}{2}\int_\Omega|\nabla v|^2+\frac{\kappa^2}{2}(a-v^2)^2, \tag{3.8}$$

we claim

$$\frac{1}{2}\int_\Omega|\nabla v_\kappa|^2=\frac{1}{2}\int_\Omega|\nabla\sqrt{a}|^2+o(1)\quad\text{as}\quad\kappa\to\infty. \tag{3.9}$$

In fact, for any given sequence $\kappa_n\to\infty$, we have

$$\frac{1}{2}\int_\Omega|\nabla v_{\kappa_n}|^2+\frac{\kappa_n^2}{2}(a-v_{\kappa_n}^2)^2\leqslant\frac{1}{2}\int_\Omega|\nabla\sqrt{a}|^2. \tag{3.10}$$

Hence, there exist a subsequence of $\{v_{\kappa_n}\}$ (still denote $\{v_{\kappa_n}\}$) and $v_0\in H^1(\Omega,\mathbb{R})$ such that $v_{\kappa_n}\rightharpoonup v_0$ weakly in $H^1(\Omega,\mathbb{R})$. From (3.10) we have

$$\int_\Omega (a-v_{\kappa_n}^2)^2 \leqslant \frac{C}{\kappa_n^2} \to 0,$$

which imply that $v_0 = \sqrt{a}$ a.e. in Ω. So, we have

$$\int_\Omega |\nabla \sqrt{a}|^2 = \int_\Omega |\nabla v_0|^2. \tag{3.11}$$

Hence, using (3.10) and (3.11),

$$\begin{aligned}\int_\Omega |\nabla (v_{\kappa_n} - v_0)|^2 &= \int_\Omega |\nabla v_{\kappa_n}|^2 + \int_\Omega |\nabla v_0|^2 - 2\int_\Omega \nabla v_{\kappa_n} \nabla v_0 \\ &\leqslant 2\int_\Omega |\nabla v_0|^2 - 2\int_\Omega \nabla v_{\kappa_n} \nabla v_0 \\ &= o(1). \end{aligned} \tag{3.12}$$

This proves (3.9). Combining (3.7) with (3.9), we have

$$\frac{1}{2}\int_\Omega |\nabla \rho|^2 + \frac{\kappa^2}{2}(a-\rho^2)^2 \geqslant \frac{1}{2}\int_\Omega |\nabla \sqrt{a}|^2 - o(1). \tag{3.13}$$

Also, from Proposition 1.1,

$$\frac{1}{2}\int_{\cup_i B_i} \rho^2 |\nabla \varphi - A| + |h - h_{\mathrm{ex}}^2| \geqslant \pi \sum_i \ (a(p_i)|d_i|)(\log \kappa - C \log\log \kappa)$$

and, letting $h = h_{\mathrm{ex}} h_0 + f$,

$$\begin{aligned}\frac{1}{2}\int_{\tilde{\Omega}} \frac{1}{\rho^2} |\nabla h|^2 + |h - h_{\mathrm{ex}}|^2 &= \frac{1}{2} h_{\mathrm{ex}}^2 \int_{\tilde{\Omega}} \frac{1}{\rho^2} |\nabla h_0|^2 + |h_0 - 1|^2 \\ &\quad + \frac{1}{2}\int_{\tilde{\Omega}} \frac{1}{\rho^2} |\nabla f|^2 + f^2 + h_{\mathrm{ex}} \int_{\tilde{\Omega}} \frac{1}{\rho^2} \nabla f \nabla h_0 + f(h_0 - 1). \end{aligned} \tag{3.14}$$

Note that $J(u,A) \leqslant C(\log \kappa)^2$ and conclusion (1) of Proposition 1.1, we have

$$\begin{aligned} h_{\mathrm{ex}}^2 \int_{\tilde{\Omega}} \frac{1}{\rho^2} |\nabla h_0|^2 &= h_{\mathrm{ex}}^2 \int_{\tilde{\Omega}} \frac{1}{a} |\nabla h_0|^2 + h_{\mathrm{ex}}^2 \int_{\tilde{\Omega}} \frac{a-\rho^2}{a\rho^2} |\nabla h_0|^2 \\ &\geqslant h_{\mathrm{ex}}^2 \int_{\tilde{\Omega}} \frac{1}{a} |\nabla h_0|^2 - \frac{C(\log \kappa)^3}{\kappa} \|\nabla h_0\|_{L^4(\Omega)}^2 \\ &\geqslant h_{\mathrm{ex}}^2 \int_{\tilde{\Omega}} \frac{1}{a} |\nabla h_0|^2 - o(1). \end{aligned} \tag{3.15}$$

From $-\nabla^\perp h = (iu, \nabla_A u)$ and $J(u,A) \leqslant C(\log \kappa)^2$, we have

$$\|\nabla h\|_{L^2(\Omega)} \leqslant C \log \kappa. \tag{3.16}$$

Hence, by $\|\nabla h_0\|_{L^\infty} \leqslant C$, (3.16), $J(u,A) \leqslant C(\log \kappa)^2$ and Holder inequality,

$$\begin{aligned} h_{\mathrm{ex}} \int_{\tilde{\Omega}} \frac{1}{\rho^2} \nabla f \nabla h_0 &= h_{\mathrm{ex}} \int_{\tilde{\Omega}} \frac{1}{a} \nabla f \nabla h_0 + h_{\mathrm{ex}} \int_{\tilde{\Omega}} \frac{a-\rho^2}{a\rho^2} \nabla f \nabla h_0 \\ &\geqslant h_{\mathrm{ex}} \int_{\tilde{\Omega}} \frac{1}{a} \nabla f \nabla h_0 - \frac{C(\log \kappa)^3}{\kappa} \\ &\geqslant h_{\mathrm{ex}} \int_{\tilde{\Omega}} \frac{1}{a} \nabla f \nabla h_0 - o(1). \end{aligned} \tag{3.17}$$

Note that $h_{\mathrm{ex}}^2\int_{\cup_i B_i}(1/a)\,|\nabla h_0|^2+|h_0-1|^2=o(1)$, combining the above relations, we have

$$J(u,A)\geqslant\frac{1}{2}\int_\Omega|\nabla\sqrt{a}|^2+\pi\left(\sum_i\ a(p_i)|d_i|\right)(\log\kappa-C\log\log\kappa)+h_{\mathrm{ex}}^2\int_\Omega\frac{1}{a}|\nabla h_0|^2+|h_0-1|^2$$
$$+\frac{1}{2}\int_{\tilde\Omega}\frac{1}{\rho^2}|\nabla f|^2+f^2+h_{\mathrm{ex}}\int_{\tilde\Omega}\frac{1}{a}\nabla f\nabla h_0+f(h_0-1). \tag{3.18}$$

Since, $f=h_{\mathrm{ex}}h_0-h$ and both h and $h_{\mathrm{ex}}h_0$ are bounded in H^1 norm and therefore in L^4 norm for instance, by $C\log\kappa$. Then, by Holder inequality

$$\left(\int_{\cup_i B_i}f^2\right)^2\leqslant\left(\sum_i\ |B_i|\right)\int_{\cup_i}|f|^4=o(1).$$

Also,

$$h_{\mathrm{ex}}\int_{\cup_i B_i}\frac{1}{a}\nabla f\nabla h_0+f(h_0-1)\leqslant Ch_{\mathrm{ex}}\int_{\cup_i B_i}|\nabla f|+|f|=o(1).$$

Combining these relations with (3.17), we have

$$J(u,A)\geqslant\frac{1}{2}\int_\Omega|\nabla\sqrt{a}|^2+h_{\mathrm{ex}}^2J_0+\pi\left(\sum_i\ a(p_i)|d_i|\right)(\log\kappa-C\log\log\kappa)$$
$$+\frac{1}{2}\int_{\tilde\Omega}\frac{1}{\rho^2}|\nabla f|^2+\frac{1}{2}\int_\Omega f^2+h_{\mathrm{ex}}\int_\Omega\frac{1}{a}\nabla f\nabla h_0+f(h_0-1). \tag{3.19}$$

Moreover,

$$-\mathrm{div}\left(\frac{1}{a}\nabla f\right)+f=-\mathrm{div}\left(\frac{1}{a}\nabla h\right)+h$$

and using Lemma 3.1,

$$\int_\Omega\frac{1}{a}\nabla f\nabla(h_0-1)+f(h_0-1)=2\pi\sum_i\ d_i(h_0-1)(p_i)+o(1),$$

which, together with (3.19), proves Proposition 3.2. □

IV. PROOF OF THEOREM 1.2

In this section, we will give a proof of Theorem 1.2. We need the following lemmas.

Lemma 4.1: For any $\kappa,h_{\mathrm{ex}}>0$, a minimizer (u,A) of (1.1) satisfies

$$J(u,A)\leqslant\frac{1}{2}\int_\Omega|\nabla\sqrt{a}|^2+h_{\mathrm{ex}}^2J_0. \tag{4.1}$$

Proof: Let $A_0=\nabla^\perp h_0$, then,

$$J(u,A)\leqslant J\left(\sqrt{a},\frac{1}{a}h_{\mathrm{ex}}A_0\right)=\frac{1}{a}\int_\Omega|\nabla\sqrt{a}|^2+\frac{1}{2}h_{\mathrm{ex}}^2\int_\Omega\frac{1}{a}|\nabla h_0|^2+|h_0-1|^2$$
$$=\frac{1}{a}\int_\Omega|\nabla\sqrt{a}|^2+h_{\mathrm{ex}}^2J_0. \tag{4.2}$$

This proves Lemma 4.1. □

Lemma 4.2: The set Λ where ξ_0/a attains its minimum is finite and there exist $\delta,N>0$ such that $\xi_0(p)/a(p)\geqslant\min_\Omega(\xi_0/a)+\delta\,\mathrm{dist}(p,\Lambda)^N$ for every $p\in\Omega$.

Proof: Since $a(x)$ is a real analytic function, we have the $\xi_0(x)$ is also a real analytic function. Also, Ω is a simply connected domain in $\mathbb{R}^2$. The standard analytic function theory implies directly the assertion of the lemma. □

Proof of Theorem 1.2: Let (u,A) be a minimizer of (1.1) and $\{(p_i,d_i)\}_{i\in I}$ are associated vortices. We assume that $h_{\text{ex}}<H_{c_1}+K\log\log\kappa$. Using Proposition 3.2 and Lemma 4.1 we have

$$\pi\left(\sum_i a(p_i)|d_i|\right)(\log\kappa - C\log\log\kappa)+2\pi h_{\text{ex}}\sum_i d_i\xi_0(p_i)$$
$$+\frac{1}{2}\int_{\Omega\setminus\cup_i B_i}\frac{1}{\rho^2}|\nabla(h-h_{\text{ex}}h_0)|^2+\frac{1}{2}\int_\Omega|h-h_{\text{ex}}h_0|^2\leqslant o(1). \tag{4.3}$$

We let

$$D=\sum_i a(p_i)|d_i|. \tag{4.4}$$

Step 1: Vortices have mostly positive degrees. Let

$$I_-=\{i\in I: d_i<0\},\quad I_+=I\setminus I_-,$$
$$D_-=\sum_{i\in I_-}a(p_i)|d_i|,\quad D_+=\sum_{i\in I_+}a(p_i)|d_i|, \tag{4.5}$$

so that $D=D_++D_-$. Since ξ_0 is negative in Ω, thus

$$\sum_i d_i\xi_i(p_i)=\sum_i a(p_i)d_i\frac{\xi_0(p_i)}{a(p_i)}\geqslant D_+\min_\Omega\frac{\xi_0}{a}=-D_+\max_\Omega\left|\frac{\xi_0}{a}\right|. \tag{4.6}$$

Since $h_{\text{ex}}\leqslant H_{c_1}+C\log\log\kappa$, using (4.3), we have

$$\pi D(\log\kappa - C\log\log\kappa)-D_+(\pi\log\kappa+C\log\log\kappa)\leqslant o(1),$$

which imply that

$$D_-\leqslant CD\frac{\log\log\kappa}{\log\kappa}+o(1).$$

Hence

$$D_-\leqslant CD_+\frac{\log\log\kappa}{\log\kappa}+o(1).$$

Note that $a(p_i\geqslant a_0)>0$, we have

$$\sum_{i\in I_-}|d_i|\leqslant C\left(\sum_{i\in I_+}|d_i|\right)\frac{\log\log\kappa}{\log\kappa}+o(1).$$

Hence,

$$\sum_{i\in I}|d_i|=\left(\sum_{i\in I_+}|d_i|\right)(1+o(1)). \tag{4.7}$$

Step 2: Vortices are mostly close to Λ. Let

$$I_0=\{i\in I:\mathrm{dist}(p_i,\Lambda)<(\log\kappa)^{-1/2N}\},\quad D_0=\sum_{i\in I_0}a(p_i)|d_i|, \tag{4.8}$$

where N is defined in Lemma 4.2. If $i\notin I_0$, Lemma 4.2 yields

$$\frac{\xi_0}{a}(p_i)\geqslant-\max_\Omega\left|\frac{\xi_o}{a}\right|+\frac{C}{\sqrt{\log\kappa}}, \tag{4.9}$$

while, if $i\in I_0$, we have the obvious inequality $(\xi_0/a)(p_i)\geqslant-\max_\Omega|(\xi_o/a)|$. Combining this relation with (4.3) we have

$$\pi D(\log\kappa-C\log\log\kappa)-2\pi(D-D_0)(H_{c_1}+C\log\log\kappa)\left(\max_\Omega\left|\frac{\xi_0}{a}\right|-\frac{C}{\sqrt{\log\kappa}}\right)$$

$$-2\pi d_0(H_{c_1}+C\log\log\kappa)\max_\Omega\left|\frac{\xi_0}{a}\right|\leqslant o(1). \tag{4.10}$$

From this we have

$$-CD\log\log\kappa+C(D-D_0)\sqrt{\log\kappa}\leqslant o(1)$$

and then

$$D-D_0\leqslant CD\frac{\log\log\kappa}{\sqrt{\log\kappa}}+o(1),$$

which imply that

$$\sum_{i\in I\setminus I_0}|d_i|\leqslant C\left(\sum_{i\in I}|d_i|\right)\frac{\log\log\kappa}{\sqrt{\log\kappa}}+o(1).$$

Hence,

$$\sum_{i\in I}|d_i|=\sum_{i\in I_0}|d_i|+\sum_{i\in I\setminus I_0}|d_i|=\sum_{i\in I_0}|d_i|+\left(\sum_{i\in I}|d_i|\right)o(1), \tag{4.11}$$

which implies

$$\sum_{i\in I_0}|d_i|=\left(\sum_{i\in I}|d_i|\right)(1+o(1)). \tag{4.12}$$

Step 3: To conclude the proof of Theorem 1.2, it suffices to prove that

$$D\leqslant C. \tag{4.13}$$

Let $f=h-h_{\mathrm{ex}}h_0$, $\tilde\Omega=\Omega\setminus\cup_i B_i$. Now we will deal with the term

$$\int_{\tilde\Omega}\frac{1}{\rho^2}|\nabla f|^2+\int_\Omega f^2. \tag{4.14}$$

Let C_t be a circle of radius t lying entirely in $\tilde\Omega$, i.e., not intersecting the vortex balls, and bounding a ball B_t. In $\tilde\Omega$ we write $u=\rho e^{i\varphi}$. Then,

$$-\nabla^{\perp}h=\rho^2(\nabla\varphi-A) \text{ in } \tilde{\Omega}.$$

Also, we have

$$-\operatorname{div}\left(\frac{1}{a}\nabla h_0\right)+h_0=0 \text{ in } \Omega.$$

Hence,

$$\int_{C_t}\frac{1}{a}\frac{\partial h_0}{\partial \nu}=-\int_{B_t}h_0, \quad \int_{C_t}\frac{1}{\rho^2}\frac{\partial h}{\partial \nu}=\int_{C_t}\frac{\partial \varphi}{\partial \tau}-A\cdot\tau=\int_{C_t}\frac{\partial \varphi}{\partial \tau}-\int_{B_t}h,$$

where ν is the inward unit normal vector to B_t and (τ,ν) is a direct frame. We deduce

$$\int_{C_t}\frac{1}{\rho^2}\frac{\partial f}{\partial \nu}+\int_{B_t}f+\int_{C_t}\frac{\rho^2-a}{a\rho^2}\frac{\partial h_0}{\partial \nu}=2\pi d_t, \tag{4.15}$$

where d_t is the winding number of $u:C_t\to S^1$. Equivalently, d_t is the sum of the degrees of vortices included in B_t. Using Holder inequality, we have

$$\frac{1}{2}\int_{C_t}\frac{1}{\rho^2}\left(\frac{\partial f}{\partial \nu}\right)^2+\frac{t}{4}\int_{B_t}f^2\geqslant 2\pi d_t^2-C\int_{C_t}(a-\rho^2)^2. \tag{4.16}$$

Now, Λ is a finite set, we have $\Lambda=\{b_1,\ldots,b_n\}$ where $b_i\in\Omega$. Let $1>\alpha>0$ be such that for all $1\leqslant i\neq j\leqslant n$,

$$\alpha<\frac{|b_i-b_j|}{2}, \quad \alpha<\operatorname{dist}(b_i,\partial\Omega).$$

We denote by $C_{i,t}$ the circle with center b_i and radius t and let E be the set of $0<\alpha<t$ such that for all $1\leqslant i\leqslant n$ we have $C_{i,t}\subset\tilde{\Omega}$. For $t\in E$, we let $d_{i,t}$ be the winding number of u restricted to $C_{i,t}$. From (4.16) we have

$$\frac{1}{2}\int_{C_{i,t}}\frac{1}{\rho^2}\left(\frac{\partial f}{\partial \nu}\right)^2+\frac{t}{4}\int_{B_{i,t}}f^2\geqslant 2\pi d_{i,t}^2-C\int_{C_{i,t}}(a-\rho^2)^2, \tag{4.17}$$

where $B_{i,t}$ is the ball bounded by $C_{i,t}$. Summing over $1\leqslant i\leqslant n$ we find

$$\frac{1}{2}\int_{\cup_i C_{i,t}}\frac{1}{\rho^2}\left(\frac{\partial f}{\partial \nu}\right)^2+\frac{t}{4}\int_{\cup_i B_{i,t}}f^2\geqslant 2\pi\sum_i d_{i,t}^2-C\int_{\cup_i C_{i,t}}(a-\rho^2)^2. \tag{4.18}$$

Now we know from step 2 that most of the vortices are close to Λ in a sense precise enough to imply that if $t\geqslant(\log\kappa)^{-1/2N}$ then

$$\sum_{i=1}^{n}|d_{i,t}|=\sum_{i\in I}|d_i|(1+o(1))+o(1). \tag{4.19}$$

But since step 1 the degrees of the vortices are mostly positive,

$$\sum_{i=1}^{n}d_{i,t}=\sum_{i=1}^{n}|d_{i,t}|(1+o(1))+o(1). \tag{4.20}$$

It follows that if $t\geqslant(\log\kappa)^{-1/2N}$ that

$$\sum_{i=1}^{n} d_{i,t} = \sum_{i \in I} |d_i|(1+o(1))+o(1). \tag{4.21}$$

Using Cauchy–Schawarz's inequality, we have

$$\frac{1}{2}\int_{\cup_i C_{i,t}} \frac{1}{\rho^2}|\nabla f|^2 + \frac{t}{4}\int_{\cup_i B_{i,t}} f^2 \geqslant \frac{C}{t}\left(\sum_{i\in I}|d_i|\right)^2 - C\int_{\cup_i C_{i,t}} (a-\rho^2)^2 \geqslant \frac{C}{t}D^2 - C\int_{\cup_i C_{i,t}} (a-\rho^2)^2 \tag{4.22}$$

for all $t \in E, t \geqslant (\log \kappa)^{-1/2N}$. We now wish to integrate this inequality with respect to t. Since the sum of the radius of the vortex ball is less than $(\log \kappa)^{-10}$ and the function $1/t$ is decreasing, we may bound from below the integral of the right-hand side of (4.22) over $t \in E$,

$$\int_{\{t\in E\}\cap\{t\geqslant(\log\kappa)^{-1/2N}\}} \frac{dt}{t} \geqslant \int_{(\log\kappa)^{-1/2N}+(\log\kappa)^{-10}}^{\alpha} \frac{dt}{t}.$$

This yields the lower bound

$$\begin{aligned}\frac{1}{2}\int_{\tilde{\Omega}} \frac{1}{\rho^2}|\nabla f|^2 + \frac{1}{2}\int_{\Omega} f^2 &\geqslant CD^2 \log\log\kappa - C\int_{\Omega}(a-\rho^2)^2 \\ &\geqslant CD^2\log\log\kappa - \frac{C(\log\kappa)^2}{\kappa^2} \\ &= CD^2\log\log\kappa - o(1).\end{aligned} \tag{4.23}$$

Using (4.23) in (4.3) together with the fact that $\xi_0(p_i)/a(p_i) \leqslant -\max_{\Omega}|\xi_0/a|$ we have

$$-CD\log\log\kappa - CD^2\log\log\kappa \leqslant o(1),$$

which yields

$$D \leqslant C.$$

This relation, step 1, step 2, and $a(x) \geqslant a_0 > 0$ prove the other assertions of Theorem 1.2. □

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On asymptotic perturbation theory for quantum mechanics: Almost invariant subspaces and gauge invariant magnetic perturbation theory

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Singular perturbation theory for quantum mechanics is considered in a framework generalizing the spectral concentration theory. Under very general conditions, asymptotic estimations on the Rayleigh–Schrödinger expansions of the perturbed spectral projections are obtained. As a consequence almost invariant subspaces of exponential order are constructed. The results cover practically all singular perturbations considered in nonrelativistic quantum mechanics. In the magnetic field case, under the condition that the magnetic field does not increase at infinity, a gauge invariant perturbation theory leading to convergent series with field-dependent coefficients is developed. © *2002 American Institute of Physics.*
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I. INTRODUCTION

While the regular perturbation theory achieved its final form in the papers of Sz-Nagy, Rellich and Kato [see Kato (1980), Reed and Simon (1978b), and references therein], in the case of singular perturbations (Stark and Zeeman effects in quantum mechanics are in this class) the progress has been much slower, at least for the degenerate eigenvalues case. In the general framework laid down in Kato's book a systematic theory of asymptotic Rayleigh–Schrödinger perturbation theory for degenerate eigenvalues has been developed fairly recently by Hunziker and co-workers: Vock and Hunziker (1982), Hunziker and Pillet (1983), Hunziker (1988) [see the beautiful review paper by Hunziker (1988) and also the recent book by Hislop and Sigal (1996) for detailed exposition and an extensive bibliography]. The key condition which selects the allowed class of perturbations is the so-called ''stability condition;'' in the cases where the considered eigenvalues are not stable one considers, in the spirit of Aguilar–Balslev–Combes theory [see Aguilar and Combes (1971), Balslev and Combes (1971)], a related (e.g., dilated) Hamiltonian for which the stability condition holds true. The main point of the theory is that the stability condition, together with the exponential decay of unperturbed eigenvectors given by Combes–Thomas (1973) theory [see also Hunziker (1988)], allows one to obtain powerful asymptotic estimates. The price to be paid are strong conditions (e.g., dilation analyticity) on the perturbation. Also, at the technical level the theory is far from being elementary since one has to deal with non-self-adjoint operators, analytic continuation, etc. In addition, as far as we understand, it does not seem easy to obtain information on the perturbed eigenvectors.

In this paper which, with the exception of the last section, is a continuation of Nenciu (1981) we follow a different route, closer in its spirit to the theory of spectral concentration, in which the main objects are the perturbed subspaces. The aim is twofold: First, using the results in Nenciu (1993) we push the estimations in Nenciu (1981), Nenciu and Nenciu (1981) up to exponential order; second, and more important, we extend the analysis to cases where the techniques in Nenciu (1981) and Nenciu (1993), based on adiabatic expansions, do not apply.

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The content of the paper is as follows. In Sec. II we set up the framework. Almost invariant subspaces of families of self-adjoint operators are defined and it is shown that their existence gives (up to some errors) similar spectral and evolution information as the existence of invariant subspaces. In this context we give a very general form of the Hylleraas–Wigner "$2n+1$" theorem: "the knowledge of eigenfunction up to errors of order δ, gives the knowledge of the corresponding eigenvalue up to errors of order δ^2." Section III, again of general nature, is devoted to the construction of almost invariant subspaces out of asymptotic Rayleigh–Schrödinger series of the perturbed projection. Section IV contains one of the main results of the paper: For the Schrödinger operator in $\mathbb{R}^3$ (actually all the arguments work in an appropriate abstract setting), under very general conditions on the perturbing potential, we are able to construct formal Rayleigh–Schrödinger expansions for the perturbed projection [see also Howland (1991)] and to obtain good asymptotic estimates on the coefficients of this expansions. The results (or their easy extensions to $\mathbb{R}^n$) cover the perturbations by polynomially bounded potentials of bound states in atomic, molecular, and solid state physics. Also for perturbing potentials growing up at infinity at most linearly (as in the case of the Stark effect) one can treat the perturbations of the energy bands in solids (the Stark–Wannier problem). In all these cases one obtains that the perturbed subspaces are almost invariant up to exponentially long times, which in the present setting is the analog of the fact that the imaginary part of the corresponding resonances (in the cases when they can be defined) are exponentially small.

Section V concerns perturbations given by magnetic fields which do not grow at infinity (the most important particular case being the Zeeman effect, i.e., the case of constant magnetic field) and can be read independently of the rest of the paper. The main result is that this case is closer to regular perturbation theory. More exactly, one finds that *after factorizing* the so-called "nonintegrable gauge phase factor" on can write down a gauge invariant *convergent* perturbation series for the integral kernel of the perturbed resolvent, with coefficients depending themselves upon the perturbing magnetic field. This dependence comes from *phase factors* containing fluxes through some polygonal contours and the asymptotic nature of the usual expansions comes *solely* from expanding these phase factors. In particular this leads (for the first time to our best knowledge) to a convergent expansion for the usual Zeeman effect. The fact that the factorization of the nonintegrable gauge phase factor makes the perturbation given by magnetic fields less singular has been used many times in the physical literature [see, e.g., Luttinger (1951), Nenciu (1991), and references therein in connection with the Peierls–Onsager problem] and has been fully used recently by Cornean and Nenciu (1998) in connection with decay of eigenfunctions [see also Cornean (2000) for the use of the same idea to control the thermodynamic limit for quantum gases in constant magnetic field].

The results have been announced in Nenciu (2001).

II. ALMOST INVARIANT SUBSPACES: GENERAL THEORY

We start with the definition of almost invariant subspaces (a.i.s.).

Definition II.1: Let H_ϵ, P_ϵ, $\epsilon \in [0,\epsilon_0], \epsilon_0 > 0$ be families of self-adjoint operators and orthogonal projections, respectively, in a separable Hilbert space, $\mathcal{H}$, satisfying the following conditions:

(i)

$$\lim_{\epsilon\to 0} \|P_\epsilon - P_0\| = 0, \tag{2.1}$$

(ii) $P_\epsilon \mathcal{D}(H_\epsilon) \subset \mathcal{D}(H_\epsilon)$ where $\mathcal{D}(H_\epsilon)$ is the domain of H_ϵ and on $\mathcal{D}(H_\epsilon)$,

$$\|[H_\epsilon, P_\epsilon]\| \leq \delta(\epsilon), \quad 0 \leq \delta(\epsilon) < \infty, \quad \lim_{\epsilon\to 0} \delta(\epsilon) = 0. \tag{2.2}$$

Then we say that $P_\epsilon \mathcal{H}$ are almost invariant subspaces of order $\delta(\epsilon)$ for H_ϵ.

The definition implies that $P_0\mathcal{H}$ is an invariant subspace of H_0. In what follows we shall restrict ourselves to the case when P_0 is the spectral projection of H_0 corresponding to a bounded isolated part, σ_0, of $\sigma(H_0)$. That is,

(iii)

$$P_0=\frac{i}{2\pi}\oint_\Gamma (H_0-z)^{-1}\mathrm{d}z, \tag{2.3}$$

where Γ is a contour enclosing σ_0. In particular, we shall not consider the perturbation of embedded eigenvalues.

Remark 2.1: Condition (2.1) implies that for sufficiently small ϵ (for which $\|P_\epsilon-P_0\|<1$), P_ϵ and P_0 are unitarily equivalent; in particular $\dim P_\epsilon\mathcal{H}=\dim P_0\mathcal{H}$. Notice that (2.1) cannot be replaced by $s-\lim_{\epsilon\to 0}P_\epsilon=P_0$ even if $\dim P_0\mathcal{H}<\infty$ and $H_\epsilon\to H_0$ in the strong resolvent sense [see, e.g., Hunziker (1988)].

Remark 2.2: Condition (ii) is equivalent to the following one: $P_\epsilon\mathcal{D}_\epsilon\subset\mathcal{D}(H_\epsilon)$ where $\mathcal{D}_\epsilon$ is a core of H_ϵ and (2.2) holds true on $\mathcal{D}_\epsilon$.

If we write H_ϵ in a matrix form according to the decomposition $\mathcal{H}=P_\epsilon\mathcal{H}\oplus(1-P_\epsilon)\mathcal{H}$ then the off-diagonal part, B_ϵ,

$$B_\epsilon=P_\epsilon H(1-P_\epsilon)+(1-P_\epsilon)HP_\epsilon=(1-2P_\epsilon)[H_\epsilon,P_\epsilon], \tag{2.4}$$

is bounded on $\mathcal{D}(H_\epsilon)$,

$$\|B_\epsilon\|\leqslant\delta(\epsilon). \tag{2.5}$$

It follows that both $P_\epsilon H_\epsilon P_\epsilon$ and $(1-P_\epsilon)H_\epsilon(1-P_\epsilon)$ are self-adjoint on $P_\epsilon\mathcal{D}(H_\epsilon)$ and $(1-P_\epsilon)\mathcal{D}(H_\epsilon)$, respectively. Notice that $P_\epsilon H_\epsilon P_\epsilon$ need not be bounded.

In what follows we shall use the notations:

$$H_{\epsilon,D}\equiv H_\epsilon-B_\epsilon=P_\epsilon H_\epsilon P_\epsilon+(1-P_\epsilon)H_\epsilon(1-P_\epsilon), \tag{2.6}$$

$$h_\epsilon\equiv P_\epsilon H_\epsilon P_\epsilon:P_\epsilon\mathcal{D}(H_\epsilon)\to P_\epsilon\mathcal{H}. \tag{2.7}$$

Taking into account (2.4)–(2.7) the above-given definition of a.s.i. coincides with the definition of asymptotic invariant subspaces in Nenciu (1981).

One expects the existence of a.i.s. to give [up to some errors controlled by $\delta(\epsilon)$] similar spectral information on H_ϵ as the existence of invariant subspaces.

Proposition II.2: If $P_\epsilon\mathcal{H}$ are a.i.s. of order $\delta(\epsilon)$ for H_ϵ then

$$\|(1-P_\epsilon)\exp(-itH_\epsilon)P_\epsilon\|\leqslant|t|\,\delta(\epsilon). \tag{2.8}$$

If h_ϵ has an eigenvalue E_ϵ and

$$h_\epsilon\psi_\epsilon=E_\epsilon\psi_\epsilon \tag{2.9}$$

then

$$\exp(-itH_\epsilon)\psi_\epsilon=\exp(-itE_\epsilon)\psi_\epsilon+\chi_\epsilon(t) \tag{2.10}$$

with

$$\|\chi_\epsilon(t)\|\leqslant|t|\,\delta(\epsilon). \tag{2.11}$$

In particular,

$$|\langle\psi_\epsilon,\exp(-itH_\epsilon)\psi_\epsilon\rangle|\geqslant 1-|t|\,\delta(\epsilon), \tag{2.12}$$

i.e., in the physicists language ψ_ϵ describes a metastable state.

Proof: The direct consequence of the definition and of the formula:

$$\exp(-itH_\epsilon)=\exp(-itH_{\epsilon,D})-i\int_0^t \exp(-itH_{\epsilon,D}(t-s))B_\epsilon \exp(-isH_\epsilon)\mathrm{ds}. \tag{2.13}$$

Remark 2.3: Iterating once (2.13) and taking into account that B_ϵ is off-diagonal one can improve (2.12) to

$$|\langle \psi_\epsilon, \exp(-itH_\epsilon)\psi\epsilon\rangle| \geqslant 1-|t|^2\delta(\epsilon)^2/2. \tag{2.14}$$

Consider now the case when $H_\epsilon \to H_0$ in the strong resolvent sense and $\sigma_0=\{\lambda_0\}$ with λ_0 an isolated, m-degenerate eigenvalue so that

$$\dim P_0\mathcal{H}=m<\infty. \tag{2.15}$$

From (2.1) it follows that for sufficiently small ϵ,

$$\dim P_\epsilon\mathcal{H}=m<\infty. \tag{2.16}$$

In this case the existence of a.i.s. of order $\delta(\epsilon)$ is equivalent [see Nenciu (1981)] to the spectral concentration as defined in Riddell (1967) and Kato (1980). Indeed suppose $P_\epsilon\mathcal{H}$ are a.i.s. of order $\delta(\epsilon)$ for H_ϵ. Since $P_\epsilon\mathcal{H}$ are finite dimensional there exist

$$\phi_{\epsilon,j}\in P_\epsilon\mathcal{H}, \quad \langle \phi_{\epsilon,j},\phi_{\epsilon,k}\rangle=\delta_{j,k}, \quad \tilde{\lambda}_{\epsilon,j}\in\mathbf{R}, \quad j,k=1,2,\ldots,m$$

such that

$$h_\epsilon\phi_{\epsilon,j}=\tilde{\lambda}_{\epsilon,j}\phi_{\epsilon,j}. \tag{2.17}$$

From (2.1), (2.2), and (2.6) it follows that

$$\lim_{\epsilon\to 0}\|(1-P_0)\phi_{\epsilon,j}\|=0, \tag{2.18}$$

$$\|(H_\epsilon-\tilde{\lambda}_{\epsilon,j})\phi_{\epsilon,j}\|\leqslant\delta(\epsilon), \tag{2.19}$$

i.e., $\phi_{\epsilon,j},\tilde{\lambda}_{\epsilon,j}$ are pseudoeigenvectors and pseudoeigenvalues of all orders $p\in\mathbf{N}$ for which $\lim_{\epsilon\to 0}\epsilon^{-p}\delta(\epsilon)=0$ and this is equivalent to the spectral concentration according to Riddel's (1967) theorem. Conversely if $\tilde{\lambda}_{\epsilon,j}$ and $\phi_{\epsilon,j}$ satisfying (2.18) and (2.19) exist then $P_\epsilon\mathcal{H}$ with

$$P_\epsilon=\sum_{j=1}^m \langle \phi_{\epsilon,j},\cdot\rangle\phi_{\epsilon,j} \tag{2.20}$$

are a.i.s. of order $\delta(\epsilon)$ for H_ϵ.

Finally let us consider the case when, in addition, λ_0 is stable [see Hunziker (1988) and also Kato (1980), Hislop and Sigal (1996)]. From the definition of stability there exist $d>0,\epsilon_1>0$ such that for $\epsilon\in[0,\epsilon_1]$, $\Gamma=\{z\|z-\lambda_0|=d\}\subset\rho(H_\epsilon)$, and

$$\inf_{z\in\Gamma}\mathrm{dist}(z,\sigma(H_\epsilon))\geqslant d/2. \tag{2.21}$$

In addition, if

$$Q_\epsilon = \oint_\Gamma (H_\epsilon - z)^{-1} dz \tag{2.22}$$

then

$$\lim_{\epsilon \to 0} \| Q_\epsilon - P_0 \| = 0. \tag{2.23}$$

From (2.1), (2.2), and (2.23) there exist $\epsilon_2 > 0$ such that for all $\epsilon \in [0, \epsilon_2]$ one has

$$\| Q_\epsilon - P_0 \| < 1/6, \quad \| P_\epsilon - P_0 \| < 1/6, \quad \delta(\epsilon) \leqslant d/8. \tag{2.24}$$

As expected Q_ϵ and the spectrum of $Q_\epsilon H_\epsilon Q_\epsilon$ (as an operator in the m-dimensional space $Q_\epsilon \mathcal{H}$) are close to P_ϵ and $\sigma(h_\epsilon)$, respectively.

Proposition II.3: For $\epsilon \in [0, \min\{\epsilon_1, \epsilon_2\}]$,

$$\| P_\epsilon - Q_\epsilon \| \leqslant c_1(d)\, \delta(\epsilon), \tag{2.25}$$

$$\operatorname{dist}(\sigma(Q_\epsilon H_\epsilon Q_\epsilon), \sigma(h_\epsilon) \leqslant c_2(d)\, \delta(\epsilon)^2. \tag{2.26}$$

Remark 2.4: The proof gives the following (nonoptimal) values for $c_i(d)$: $c_1(d) = 16/3d$, $c_2(d) = 512/9d$.

Remark 2.5: The interesting part of Proposition II.3 is (2.26), which is a general form of the so called Hylleraas–Wigner "$2n+1$" theorem in perturbation theory [see Gonze (1995), and references therein]: Knowledge of the perturbed wave function to order $\delta(\epsilon)$ gives the perturbed eigenvalue with errors of order $\delta(\epsilon)^2$. To see the connection, consider the elementary case of regular perturbations of nondegenerate isolated eigenvalues. Let $H_\epsilon \psi_\epsilon = \lambda_\epsilon \psi_\epsilon$ and suppose that one knows an approximate *normalized* wave function $\tilde{\psi}_\epsilon$, $\| \tilde{\psi}_\epsilon \| = 1$ with $\| \tilde{\psi}_\epsilon - \psi_\epsilon \| \leqslant \delta(\epsilon)$, $\| H_\epsilon (\tilde{\psi}_\epsilon - \psi_\epsilon) \| \leqslant M\, \delta(\epsilon)$; M uniformly bounded as $\epsilon \to 0$. Then if

$$P_\epsilon = \langle \tilde{\psi}_\epsilon, \cdot \rangle \tilde{\psi}_\epsilon$$

one has

$$\| [P_\epsilon, H_\epsilon] \| \leqslant 2(M + |\lambda_\epsilon|)\, \delta(\epsilon),$$

which according to Proposition II.3 gives

$$|\lambda_\epsilon - \langle \tilde{\psi}_\epsilon, H_\epsilon \tilde{\psi}_\epsilon \rangle| \leqslant \text{const}\ \delta(\epsilon)^2. \tag{2.27}$$

Actually in this simple case one can obtain (2.27) at once from

$$\begin{aligned} |\lambda_\epsilon - \langle \tilde{\psi}_\epsilon, H_\epsilon \tilde{\psi}_\epsilon \rangle| &= |\langle \tilde{\psi}_\epsilon, (H_\epsilon - \lambda_\epsilon) \tilde{\psi}_\epsilon \rangle| \\ &= |\langle \tilde{\psi}_\epsilon, (H_\epsilon - \lambda_\epsilon)(\tilde{\psi}_\epsilon - \psi_\epsilon) \rangle| \\ &= |\langle (H_\epsilon - \lambda_\epsilon)(\tilde{\psi}_\epsilon - \psi_\epsilon), \tilde{\psi}_\epsilon - \psi_\epsilon \rangle|. \end{aligned}$$

Notice, however, that the above-presented argument cannot be generalized directly to the degenerate case and actually we do not know a reference for the Hylleraas–Wigner theorem in the degenerate case in spite of the fact that it is probably known to experts. The reason for the quadratic estimation in (2.26) is the fact that B_ϵ is an off-diagonal perturbation of $H_{\epsilon,D}$. Let us stress that the condition $P_\epsilon = P_\epsilon^2$ is essential for (2.26) to hold true; actually it replaces the condition that $\tilde{\psi}_\epsilon$, in the above-mentioned proof of Hylleraas–Wigner theorem, is normalized.

Remark 2.6: Proposition II.3 can be easily extended to the case when σ_0 is a stable, bounded isolated part of the spectrum oh H_0 but the constants in (2.25), (2.26) become more complicated and depend also upon the diameter of σ_0.

Proof of Proposition II.3: We apply regular perturbation theory to the pair $H_{\epsilon,D}, H_\epsilon = H_{\epsilon,D} + B_\epsilon$. From (2.5),(2.6), and (2.24),

$$\mathrm{dist}(\Gamma, \sigma(H_{\epsilon,D})) \geqslant 3d/8. \tag{2.28}$$

If

$$T_\epsilon = \frac{i}{2\pi} \oint_\Gamma (H_{\epsilon,D} - z)^{-1} \mathrm{d}z, \tag{2.29}$$

then

$$Q_\epsilon - T_\epsilon = -\frac{i}{2\pi} \oint_\Gamma (H_{\epsilon,D} - z)^{-1} B_\epsilon (H_\epsilon - z)^{-1} \mathrm{d}z, \tag{2.30}$$

which gives

$$\|Q_\epsilon - T_\epsilon\| \leqslant 16\delta(\epsilon)/3d < 2/3. \tag{2.31}$$

From (2.24) and (2.31) one has

$$\|P_\epsilon - T_\epsilon\| < 1. \tag{2.32}$$

Now (2.32) implies that

$$P_\epsilon = T_\epsilon, \tag{2.33}$$

which together with (2.31) gives (2.25). Indeed since P_ϵ, T_ϵ are orthogonal projections commuting with $H_{\epsilon,D}$, in a $L^2(M, d\mu)$ representation of $H_{\epsilon,D}$ they are multiplications with some characteristic functions so $P_\epsilon - T_\epsilon$ is the multiplication with a function taking only the values 0 and ± 1. As the values ± 1 are ruled out by (2.32) the equality (2.33) follows.

For the proof of (2.26) consider the Sz–Nagy transformation matrix [see Kato (1980)] corresponding to the pair P_ϵ, Q_ϵ,

$$U_\epsilon = (1 - (Q_\epsilon - P_\epsilon)^2)^{-1/2} [Q_\epsilon P_\epsilon + (1 - Q_\epsilon)(1 - P_\epsilon)]. \tag{2.34}$$

As is well known U_ϵ is unitary and intertwines Q_ϵ and P_ϵ,

$$Q_\epsilon = U_\epsilon P_\epsilon U_\epsilon^*. \tag{2.35}$$

As a consequence,

$$U_\epsilon^* Q_\epsilon H_\epsilon Q_\epsilon U_\epsilon = P_\epsilon U_\epsilon^* H_\epsilon U_\epsilon P_\epsilon, \tag{2.36}$$

i.e., $Q_\epsilon H_\epsilon Q_\epsilon$ is unitarily equivalent with the ''effective'' Hamiltonian $P_\epsilon U_\epsilon^* H_\epsilon U_\epsilon P_\epsilon$. On the other hand, the analytic perturbation theory [see Kato (1980)] applied to the pair $H_{\epsilon,D}$, $H_\epsilon = H_{\epsilon,D} + B_\epsilon$ gives for $P_\epsilon U_\epsilon^* H_\epsilon U_\epsilon P_\epsilon$:

$$P_\epsilon U_\epsilon^* H_\epsilon U_\epsilon P_\epsilon = h_\epsilon + P_\epsilon B_\epsilon P_\epsilon + \mathcal{O}(B_\epsilon^2) \tag{2.37}$$

so that (since the second terms on the right-hand side vanishes)

$$\|P_\epsilon U_\epsilon^* H_\epsilon U_\epsilon P_\epsilon - h_\epsilon\| \leqslant \mathcal{O}(B_\epsilon^2), \tag{2.38}$$

which in particular implies (2.26). The computation in the following gives a precise form of the error in terms of $\delta(\epsilon)$ and d. Without restricting the generality one can take $\lambda_0=0$. Using

$$Q_\epsilon H_\epsilon Q_\epsilon=\frac{i}{2\pi}\oint_\Gamma z(H_\epsilon-z)^{-1}\mathrm{d}z \tag{2.39}$$

and

$$\begin{aligned}(H_\epsilon-z)^{-1}=&(H_{\epsilon,D}-z)^{-1}-(H_{\epsilon,D}-z)^{-1}B_\epsilon(H_{\epsilon,D}-z)^{-1}\\&+(H_\epsilon-z)^{-1}B_\epsilon(H_{\epsilon,D}-z)^{-1}B_\epsilon(H_{\epsilon,D}-z)^{-1},\end{aligned} \tag{2.40}$$

one has

$$\begin{aligned}P_\epsilon Q_\epsilon H_\epsilon Q_\epsilon P_\epsilon=&P_\epsilon\frac{i}{2\pi}\oint_\Gamma z(H_{\epsilon,D}-z)^{-1}\mathrm{d}z\,P_\epsilon-P_\epsilon\frac{i}{2\pi}\oint_\Gamma z(H_{\epsilon,D}-z)^{-1}B_\epsilon(H_{\epsilon,D}-z)^{-1}\mathrm{d}z\,P_\epsilon\\&+P_\epsilon\frac{i}{2\pi}\oint_\Gamma z(H_\epsilon-z)^{-1}B_\epsilon(H_{\epsilon,D}-z)^{-1}B_\epsilon(H_{\epsilon,D}-z)^{-1}\mathrm{d}zP_\epsilon.\end{aligned} \tag{2.41}$$

Now from (2.39) written for $H_{\epsilon,D}$, the first terms on the right-hand side of (2.41) gives h_ϵ while the second vanishes due to the fact that B_ϵ is off-diagonal and P_ϵ commutes with $H_{\epsilon,D}$. Then estimating brutally the third terms on the right-hand side of (2.41) one obtains

$$\|P_\epsilon Q_\epsilon H_\epsilon Q_\epsilon P_\epsilon-h_\epsilon\|\leqslant 128\delta(\epsilon)^2/9d. \tag{2.42}$$

On the other hand,

$$P_\epsilon U_\epsilon^* H_\epsilon U_\epsilon P_\epsilon-P_\epsilon Q_\epsilon H_\epsilon Q_\epsilon P_\epsilon=(P_\epsilon U_\epsilon^*-P_\epsilon Q_\epsilon)Q_\epsilon H_\epsilon Q_\epsilon U_\epsilon P_\epsilon+P_\epsilon Q_\epsilon H_\epsilon Q_\epsilon(U_\epsilon P_\epsilon-Q_\epsilon P_\epsilon) \tag{2.43}$$

and then

$$\|U_\epsilon^* Q_\epsilon H_\epsilon Q_\epsilon U_\epsilon-P_\epsilon Q_\epsilon H_\epsilon Q_\epsilon P_\epsilon\|\leqslant 2\|U_\epsilon P\epsilon-Q_\epsilon P_\epsilon\|\cdot\|Q_\epsilon H_\epsilon Q_\epsilon\|. \tag{2.44}$$

Now from

$$U_\epsilon P_\epsilon-Q_\epsilon P_\epsilon=[(1-(Q_\epsilon-P_\epsilon)^2)^{-1/2})-1]Q_\epsilon P_\epsilon \tag{2.45}$$

one obtains [see (2.31) and (2.33)]

$$\|U_\epsilon P_\epsilon-Q_\epsilon P_\epsilon\|=\|P_\epsilon U_\epsilon^*-P_\epsilon Q_\epsilon\|\leqslant 128\delta(\epsilon)^2/3d^2. \tag{2.46}$$

Since (remember that we took $\lambda_0=0$)

$$\|Q_\epsilon H_\epsilon Q_\epsilon\|\leqslant d/2, \tag{2.47}$$

putting all together one obtains

$$\|P_\epsilon U_\epsilon^* H_\epsilon U_\epsilon P_\epsilon-h_\epsilon\|\leqslant\frac{512}{9d}\delta(\epsilon)^2, \tag{2.48}$$

which gives in particular (2.26) with the value of c_2 given in Remark 2.4.

III. PERTURBATIVE CONSTRUCTION OF ALMOST INVARIANT SUBSPACES

We turn now to the problem of constructing a.i.s. for families, H_ϵ, of self-adjoint operators. The setting we shall consider, which is sufficiently general to cover practically all physical situations in nonrelativistic quantum mechanics, is as follows: $\epsilon>0$ is a small parameter $\epsilon\in[0,\epsilon_0]$; H_0 and $V(\epsilon)$ are self-adjoint operators such that there exists a dense subspace, $\mathcal{D}$, $\mathcal{D}\subset\mathcal{D}(H_0)\cap\mathcal{D}(V(\epsilon))$ on which $H_0+\epsilon V(\epsilon)$ has self-adjoint extensions [in most examples $H_0+\epsilon V(\epsilon)$ is essentially self-adjoint on $\mathcal{D}$]; we shall denote by H_ϵ any of its self-adjoint extensions with the property $\mathcal{D}(H_\epsilon)\supset\mathcal{D}(H_0)\cap\mathcal{D}(V_\epsilon)$.

We shall consider explicitly only the particular case when $V(\epsilon)=V$ is independent of ϵ, and in this case $\mathcal{D}=\mathcal{D}(H_0)\cap\mathcal{D}(V)$, but all the results generalize as far as $V(\epsilon)$ obeys the needed technical conditions uniformly in ϵ. Indeed in this case one obtains results (uniformly in $\eta\in[0,\epsilon_0]$) for

$$H_{\epsilon,\eta}=H_0+\epsilon V(\eta)$$

and at the end one sets $\eta=\epsilon$.

At the heuristic level the problem of finding a.i.s. for H_ϵ can be viewed as the search for solutions of

$$[H_\epsilon,P_\epsilon]=[H_0,P_\epsilon]+\epsilon[V,P_\epsilon]\simeq 0, \tag{3.1}$$

$$P_\epsilon^2-P_\epsilon\simeq 0. \tag{3.2}$$

Making the ''perturbational'' ansatz

$$P_\epsilon\simeq\sum_j E_j\epsilon^j \tag{3.3}$$

one is led to the problem of solving the following equations for E_j, $j=1,2,...$:

$$P_0=E_0, \tag{3.4}$$

$$[H_0,E_j]=-[V,E_{j-1}], \tag{3.5}$$

$$\sum_{l=0}^{j}E_lE_{j-l}=E_j. \tag{3.6}$$

Equation (3.4) is nothing but (2.1) for $\epsilon=0$ while (3.5) and (3.6) follow from plugging (3.3) into (3.1) and (3.2), respectively.

In the rest of this section we shall outline how the existence of solutions, E_0, $E_1\ldots,E_N$; $N\leqslant\infty$ of (3.4)–(3.6) together with estimates on the norm of E_j and $[V,E_j]$ gives the existence of a.i.s. in the sense of (2.1) and (2.2) with control on the constant $\delta(\epsilon)$. Of course the technical core of the theory is the proof of existence of solutions of (3.4)–(3.6) with bounds on their norms and this question will be addressed in Sec. IV.

Suppose $E_j\mathcal{H}\subset\mathcal{D}(H_0)\cap\mathcal{D}(V)$, $j=0,1,...,N$ and there satisfy (3.4)–(3.6). In addition,

$$\|E_j\|\leqslant e_j, \tag{3.7}$$

$$\|[V,E_j]\|\leqslant f_j, \quad j=1,2...,N. \tag{3.8}$$

Consider

$$T_N(\epsilon)=\sum_{j=0}^{N}E_j\epsilon^j, \tag{3.9}$$

where N can depend upon ϵ. Unfortunately $T_N(\epsilon)$ is not a projection [in particular $T_N(\epsilon)^2 \neq T_N(\epsilon)$ and even if $T_N(\epsilon)$ is self-adjoint $i[(\mathrm{d}/\mathrm{d}\epsilon)\, T_N(\epsilon), T_N(\epsilon)]$ is not self-adjoint; this point has been overlooked in Howland (1991) but without consequences on the result there]. So the first step is to construct out of $T_N(\epsilon)$ a projection operator, $P_N(\epsilon)$, whose expansion in ϵ should coincide with $T_N(\epsilon)$ up to order N. Of course such a ''completion'' is far from being unique; we shall use the method employed in Nenciu (1993) since it gives an easy control on $\|[H_\epsilon, P_N(\epsilon)]\|$.

We need a few elementary facts about projections. Here we consider the self-adjoint case; for the non-self-adjoint case see the Appendix where a more elaborate version of (elementary) Proposition 3 in Nenciu (1993) is given. Let T be a bounded self-adjoint operator satisfying

$$\|T^2 - T\| \leqslant \delta < 1/4. \tag{3.10}$$

Then by the spectral theorem

$$\sigma(T) \subset \left[\frac{1-\sqrt{1+4\delta}}{2}, \frac{1-\sqrt{1-4\delta}}{2}\right] \cup \left[\frac{1+\sqrt{1-4\delta}}{2}, \frac{1+\sqrt{1+4\delta}}{2}\right].$$

In particular $1/2 \in \rho(T)$, $\|T\| \leqslant (1+\sqrt{1+4\delta})/2$, and

$$\sup_{|z-1|=1/2} \|(T-z)^{-1}\| \leqslant \frac{2}{\sqrt{1-4\delta}}. \tag{3.11}$$

Now, if P is the spectral projection of T corresponding to the part of the spectrum around 1:

$$P = \frac{i}{2\pi} \oint_{|z-1|=1/2} (T-z)^{-1} \mathrm{d}z. \tag{3.12}$$

Then again by the spectral theorem

$$\|T-P\| \leqslant \frac{1-\sqrt{1-4\delta}}{2} = \frac{2\delta}{1+\sqrt{1-4\delta}}. \tag{3.13}$$

Consider now $T_N(\epsilon)$. Due to (3.6) and (3.7) $\|T_N(\epsilon)^2 - T_N(\epsilon)\| \sim \mathcal{O}(\epsilon^{N+1})$, i.e., for sufficiently small ϵ,

$$\|T_N(\epsilon)^2 - T_N(\epsilon)\| < 1/4,$$

and one can define $P_N(\epsilon)$ by

$$P_N(\epsilon) = \frac{i}{2\pi} \oint_{|z-1|=1/2} (T_N(\epsilon) - z)^{-1} \mathrm{d}z. \tag{3.14}$$

$P_N(\epsilon)$ is a projection and according to (3.13)

$$\|P_N(\epsilon) - T_N(\epsilon)\| \sim \mathcal{O}(\epsilon^{N+1}). \tag{3.15}$$

We now compute $[H_\epsilon, P_N(\epsilon)]$. Notice first that due to the identity

$$(T-z)^{-1} = z^{-1}(T(T-z)^{-1} - 1),$$

$[H_\epsilon, P_N(\epsilon)]$ is well defined on a dense subspace and the following computation can be done. From (3.5)

$$[H_\epsilon, T_N(\epsilon)] = \epsilon^{N+1}[V, E_N]$$

and then

$$[H_\epsilon,P_N(\epsilon)]=-\frac{i}{2\pi}\oint_{|z-1|=1/2}(T_N(\epsilon)-z)^{-1}[H_\epsilon,T_N(\epsilon)](T_N(\epsilon)-z)^{-1}\mathrm{d}z$$

$$=-\epsilon^{N+1}\frac{i}{2\pi}\oint_{|z-1|=1/2}(T_N(\epsilon)-z)^{-1}[V,E_N](T_N(\epsilon)-z)^{-1}\mathrm{d}z. \tag{3.16}$$

We summarize the above-given discussion in the following lemma:

Lemma III.1: Suppose E_j satisfy (3.4)–(3.8), $T_N(\epsilon)$ is given by (3.9), and let ϵ_N be the positive solution of

$$\sum_{l=N+1}^{2N}\epsilon^l a_l=1/8, \tag{3.17}$$

where

$$a_l=\sum_{j+m=l,0\leqslant j,m\leqslant N}e_j e_m .$$

Then for $0\leqslant\epsilon\leqslant\epsilon_N$:

$$\|T_N(\epsilon)^2-T_N(\epsilon)\|\leqslant\sum_{l=N+1}^{2N}\epsilon^l a_l\equiv\delta_N(\epsilon)\leqslant 1/8 \tag{3.18}$$

and if $P_N(\epsilon)$ is given by (3.14)

$$\|P_N(\epsilon)-T_N(\epsilon)\|\leqslant 2\,\delta_N(\epsilon), \tag{3.19}$$

$$\|[H_\epsilon,P_N(\epsilon)]\|\leqslant 4\epsilon^{N+1}\|[V,E_N]\|. \tag{3.20}$$

Proof: For (3.18) notice that from (3.6)

$$T_N(\epsilon)^2-T_N(\epsilon)=\sum_{l=N+1}^{2N}\epsilon^l\left(\sum_{j+m=l,0\leqslant j,m\leqslant N}E_j E_m\right).$$

Then (3.19) follows from (3.18) and (3.14) while (3.20) follows from (3.16) and (3.19).

Remark 3.1: The main point of the lemma is the estimate (3.20).

Remark 3.2: Notice that in each particular case one has still to prove that $P_\epsilon\mathcal{D}_\epsilon\subset\mathcal{D}(H_\epsilon)$ [see Remark 2.2 and recall that $\mathcal{D}_\epsilon$ is a core of H_ϵ].

At a more elaborate level of perturbation theory the task is to obtain, under specific conditions on H_0, V, and P_0 the dependence on j of e_j, f_j; the rate of increase of these constants "measures" the singularity of the perturbation. The simplest case is when $e_j\leqslant e^j$ for some finite constant e; this corresponds to the well-known regular perturbations and there is no need for further discussion. The most interesting case is when $N=\infty$ and there exist constants $E,F'g<\infty$, $\alpha>0$ such that

$$e_j\leqslant Eg^j(j!)^\alpha,\quad f_j\leqslant Fg^{j+1}((j+1)!)^\alpha,\quad j=1,2,\ldots . \tag{3.21}$$

In this case the series in (3.3) is not convergent and the idea here is to use a best remainder estimate a la Necharosev, i.e., to take N depending on ϵ in (3.9) in order to have the right-hand side of (3.16) as small as possible. This requirement leads to N_ϵ given by

$$N_\epsilon + 1 = \left[\left(\frac{1}{g\epsilon} \right)^{1/\alpha} \right], \tag{3.22}$$

where [ ] means the integer part. Plugging (3.22) into (3.9) one obtains:

Lemma III.2: Let N_ϵ be given by (3.22). Then there exists $\epsilon_0 > 0$ such that for $\epsilon \in [0, \epsilon_0]$, (3.18) holds true and $P_\epsilon \equiv P_{N_\epsilon}$ satisfies (2.2) with

$$\delta(\epsilon) = 4FK^\alpha \frac{1}{(g\epsilon)^{1/2}} \exp\left(- \frac{\alpha}{(g\epsilon)^{1/\alpha}} \right), \tag{3.23}$$

where K is an absolute constant.

Proof: From (3.21)

$$a_l \leqslant \sum_{j=0}^{l} e_j e_{l-j} \leqslant E^2 g^l (l+1)(l!)^\alpha. \tag{3.24}$$

From the Stirling formula there exist $K > \infty$, $\tilde{K} > 0$ such that

$$\tilde{K} j^j e^{-j} \leqslant j! \leqslant K j^{j+1/2} e^{-j} \tag{3.25}$$

and from this and the fact that for all $N_\epsilon + 1 \leqslant k \leqslant 2N_\epsilon$:

$$\alpha \ln k \leqslant \alpha \ln 2N_\epsilon \leqslant \alpha \ln 2 - \ln(g\epsilon) \tag{3.26}$$

one obtains

$$\epsilon^j a_j \leqslant E^2 K^\alpha (j+1)^{1+\alpha/2} e^{-j\alpha(1-\ln 2)}, \tag{3.27}$$

so

$$\delta_N(\epsilon) \leqslant E^2 K^\alpha \sum_{j=N_\epsilon+1}^{\infty} (j+1)^{\alpha+1/2} e^{-\alpha(1-\ln 2)j}. \tag{3.28}$$

Since $N_\epsilon \to \infty$ as $\epsilon \to 0$ the first part of the lemma is proved. Then (3.23) follows from (3.8),(3.20),(3.21), (3.22), and (3.25).

Remark 3.3: If $g\epsilon < 1$, in the limit $\alpha \to 0$ one has $\delta(\epsilon) \to 0$, which fits with the fact that for $\alpha = 0$ the series in (3.3) is convergent for $\epsilon < g^{-1}$.

IV. ASYMPTOTIC ESTIMATIONS

In this section we consider the problem of finding solutions E_j of (3.4)–(3.6) satisfying estimations like (3.7) and (3.8) with e_j, f_j satisfying (3.21). In spite of the fact that all the following arguments work in an appropriate abstract setting (covering in particular N-body Stark and Zeeman effects in atoms and molecules), for definiteness we shall discuss a simple Schrödinger case in $\mathbb{R}^3$,

$$H_\epsilon = -\Delta + V_0(\mathbf{x}) + \epsilon V(\mathbf{x}) \equiv H_0 + \epsilon V(\mathbf{x}), \quad \epsilon > 0, \tag{4.1}$$

with

$$V_0 \in L^2_{\text{uloc}}, \text{ i.e., } \sup_{\mathbf{x} \in \mathbb{R}^3} \int_{|\mathbf{x}-\mathbf{y}| \leqslant 1} |V_0(\mathbf{y})|^2 d\mathbf{y} < \infty, \tag{4.2}$$

$$|V(\mathbf{x})| \leqslant \langle \mathbf{x} \rangle^\beta, \quad \langle \mathbf{x} \rangle = (1 + \mathbf{x}^2)^{1/2}, \quad \beta \in \mathbf{R}, \tag{4.3}$$

and $\epsilon>0$. In particular H_0 is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^3)$ [see Reed and Simon (1978a)]. In what follows H_ϵ is *any* self-adjoint extension of $H_0+\epsilon V(\mathbf{x})$ defined on $\mathcal{D}(H_0)\cap\mathcal{D}(V)\supset\mathcal{C}_0^\infty(\mathbb{R}^3)$. As P_0 we shall take the spectral projection of H_0 corresponding to a bounded isolated part, σ_0, of its spectrum.

The main fact about H_0 we shall use is the following elementary result from Combes–Thomas theory [see Combes and Thomas (1973), Hunziker (1988), Nenciu (1991)]:

Proposition IV.1: Let $K\subset\rho(H_0)$ be compact, λ_0 an isolated finitely degenerate eigenvalue of H_0. Then there exist $\gamma_0>0, M<\infty$ such that for all $\gamma\in[0,\gamma_0]$:

$$\sup_{z\in K}\|R_{0,\gamma}(z)\|\leqslant M, \tag{4.4}$$

$$\|e^{\gamma\langle\cdot\rangle}P_0e^{\gamma\langle\cdot\rangle}\|\leqslant M, \tag{4.5}$$

where

$$R_{0,\gamma}(z)=e^{\gamma\langle\cdot\rangle}(H_0-z)^{-1}e^{-\gamma\langle\cdot\rangle} \tag{4.6}$$

and P_0 is the spectral projection of H_0 corresponding to λ_0.

If $\beta\in[-\infty,0]$ then $VR_0(z)$ $(R_0(z)=(H_0-z)^{-1})$ is bounded and E_j given by the well-known perturbation formula

$$E_j=(-1)^j\frac{i}{2\pi}\oint_\Gamma R_0(z)(VR_0(z))^j\mathrm{d}z, \tag{4.7}$$

where Γ is a contour enclosing σ_0, satisfying (3.4)–(3.6) and the estimations (3.7), (3.8), (3.21) with $\alpha=0$. Now, if $\beta>0$, $VR_0(z)$ is not bounded and one cannot decide at once from (4.7) whether or not E_j are bounded and the main idea in what follows is to find alternative formulas for E_j which coincide with (4.7) for $\beta\leqslant0$ but still make sense for $\beta>0$. Many such formulas, each of them making sense under various assumptions on β and $\dim P_0$, will appear in the following [see (4.12), (4.17), (4.31) and (4.41)]. The need for alternative formulas comes from the fact that a formula covering all interesting cases does not seem to exist; for example, if $\dim P_0<\infty$ one uses the exponential decay of the corresponding eigenvalues (see Proposition IV.1) while for $\dim P_0=\infty$ when (4.5) does not hold true one has to rely on the fact that $[V,R_0(z)]$ might be bounded even for potentials which are unbounded at infinity. Let us stress that although they look different, as far as they make sense, they give the same E_j: For example, if $\beta\leqslant1$ and $\dim P_0<\infty$ (4.12) gives the same E_j as the recurrence formula (4.31). This is due to the fact [see Nenciu (1993)] that as far as it exists and is bounded, the solution of (3.4)–(3.6) is unique.

We prove first that, for all β, E_j is well defined and bounded on $\mathcal{C}_0^\infty(\mathbb{R}^3)$.

Lemma IV.2: For all $\beta\in\mathbb{R}$, E_j given by (4.7) are well defined and satisfy (3.4)–(3.6) on $\mathcal{C}_0^\infty(\mathbb{R}^3)$.

Proof: The key observation [see Hunziker (1988)] is that due to (4.3) and (4.4) expressions like $R_0(z)(VR_0(z))^l$, $VR_0(z)(VR_0(z))^lV$ are well defined on $\mathcal{C}_0^\infty(\mathbb{R}^3)$. In particular from (4.7), for $u\in\mathcal{C}_0^\infty(\mathbb{R}^3)$, E_ju is well defined for all $\gamma\in[0,\gamma_0]$ since

$$E_ju=(-1)^j\frac{i}{2\pi}\oint_\Gamma R_0(z)(Ve^{-(\gamma/j)\langle\cdot\rangle})R_{0,\gamma/j}(z)\cdots R_{0,\gamma}(z)e^{\gamma\langle\cdot\rangle}u\,\mathrm{d}z. \tag{4.8}$$

For all $z\neq z'\in\rho(H_0)$, $j=1,\ldots,$ and $u\in\mathcal{C}_0^\infty(\mathbf{R}^3)$,

$$\frac{1}{z-z'}[R_0(z)(VR_0(z))^j-R_0(z')(VR_0(z'))^j]u=\sum_{l=0}^{j}[R_0(z)(VR_0(z))^l][R_0(z')(VR_0(z'))^{j-l}]u. \tag{4.9}$$

Indeed from the resolvent formula

$$(z-z')\sum_{l=0}^{j}[R_0(z)(VR_0(z))^l][R_0(z')(VR_0(z'))^{j-l}]u$$
$$=(R_0(z)-R_0(z'))VR_0(z')\cdots VR_0(z')u+R_0(z)V(R_0(z)-R_0(z'))VR_0(z')\ldots VR_0(z')u$$
$$+\cdots+R_0(z)VR_0(z)\cdots(R_0(z)-R_0(z'))u=R_0(z)(VR_0(z))^j-R_0(z')(VR_0(z'))^j u.$$

Integrating (4.9) on two contours $\Gamma,\Gamma'\subset\rho(H_0),\Gamma'\subset \mathrm{Int}\,\Gamma$ enclosing σ_0 one obtains

$$E_j u=\sum_{l=0}^{j}E_l E_{j-l}u. \tag{4.10}$$

From $H_0R_0(z)=1+zR_0(z)$, again on $u\in\mathcal{C}_0^\infty(\mathbb{R}^3)$,

$$H_0R_0(z)(VR_0(z))^jVR_0(z)u-R_0(z)(VR_0(z))^jVR_0(z)H_0u$$
$$=(VR_0(z))^jVR_0(z)u-R_0(z)(VR_0(z))^jVu,$$

which after the integration on Γ gives

$$[H_0,E_{j+1}]u=-[V,E_j]u$$

and the proof is finished.

Consider first the case when $\sigma_0=\{\lambda_0\}$ with λ_0 a finite degenerate, isolated eigenvalue of H_0:

$$\mathrm{dist}(\lambda_0,\sigma(H_0)\backslash\lambda_0)=d_0>0,\quad \dim P_0=m<\infty,\Gamma=\{z\|\lambda_0-z|=d_0/2\}. \tag{4.11}$$

By the residue theorem, for all β and $u\in\mathcal{C}_0^\infty(\mathbb{R}^3)$, from (4.7)

$$E_j u=(-1)^{j-1}\sum_{\nu_1,\nu_2\cdots\nu_{j+1};\nu_l\geqslant 0;\sum_{l=1}^{j+1}\nu_l=j}S^{\nu_1}VS^{\nu_2}V\cdots VS^{\nu_{j+1}}u, \tag{4.12}$$

where S is the reduced resolvent at λ_0:

$$S=S(\lambda_0),\quad S(z)=\frac{i}{2\pi}\oint_\Gamma R_0(\zeta)(z-\zeta)^{-1}\mathrm{d}\zeta,|z-\lambda_0|<\frac{d_0}{2} \tag{4.13}$$

and by convention

$$S^0=-P_0. \tag{4.14}$$

Taking $K=\Gamma$ in Proposition IV.1, one obtains from (4.13) that for $|z-\lambda_0|<d_0/4$:

$$\|e^{\gamma\langle\cdot\rangle}S(z)e^{-\gamma\langle\cdot\rangle}\|\leqslant\frac{d_0}{d_0-2|\lambda_0-z|}\leqslant 2M,\quad \text{all}\ \ \gamma\in[0,\gamma_0]. \tag{4.15}$$

The main point about (4.12) is that all terms on its right-hand side contain at *least* one P_0; this together with the decay property (4.5) of P_0 and (4.15), which allows to propagate this decay in order to control the unboundedness of V, implies that E_j defined initially on $\mathcal{C}_0^\infty(\mathbb{R}^3)$ are bounded and their extensions by continuity satisfy (3.5) and (3.6). Consider now the problem of estimating $\|E_j\|$. Estimating as in the proof of Lemma IV.2, one can see directly that each term in (4.12) is bounded by

$$M^{j+1}\|V^j e^{-\gamma_0\langle\cdot\rangle}\|$$

so that

$$\|E_j\| \leq N(j) M^{j+1} \| V^j e^{-\gamma_0 \langle \cdot \rangle} \|, \tag{4.16}$$

where $N(j)$ is the number of terms on the right-hand side of (4.12). Unfortunately, due to the fact that $N(j)$ is at least of order $j!$ (4.16) is much weaker than the expected estimation; for example if $\beta = 1$ one expects $\|E_j\| \leq \text{const}\, e^j j!$ while (4.16) gives at best $\text{const}\, e^j (j!)^2$. In order to overcome this difficulty we shall write down yet another formula for E_j:

Lemma IV.3: For all $\beta \in \mathbb{R}$ and $u \in \mathcal{C}_0^\infty(\mathbb{R}^3)$:

$$E_j u = (-1)^j \frac{i}{2\pi} \int_{|z-\lambda_0| = d_0/4} \frac{1}{\lambda_0 - z} \sum_{k=0}^{j} (S(z)V)^k P_0 (V R_0(z))^{j-k} \mathrm{d}z\, u. \tag{4.17}$$

Proof: Formula (4.17) follows from (4.7) by using repeatedly the decomposition [see Kato (1980)]:

$$R_0(z) = \frac{P_0}{\lambda_0 - z} + S(z)$$

and remarking that due to the analyticity of $S(z)$;

$$\int_{|z-\lambda_0| = d_0/4} (S(z)V)^j S(z) \mathrm{d}z\, u = 0.$$

The advantage of (4.17) over (4.12) is clear: on one hand all terms on the right-hand side of (4.17) still contain one P_0 and on the other hand the number of terms is only $j+1$.

We are now ready to state one of the main results of this section.

Theorem IV.4: *Let β, γ_0, M, d_0 as given by (4.3) and (4.4) with $K = \{z \mid d_0/4 \leq |z - \lambda_0| \leq d_0/2\}$ and (4.11). Then the operators E_j, $j = 0,1,2,\ldots$ defined as extensions by continuity starting from any of the formulas, (4.7), (4.12), (4.17) have the following properties:*

$$E_0 = P_0, \tag{4.18}$$

$$E_j L^2(\mathbb{R}^3) \subset \mathcal{D}(H_0) \cap \mathcal{D}(V), \tag{4.19}$$

$$E_j = \sum_{l=0}^{j} E_l E_{j-l}, \tag{4.20}$$

$$[H_0, E_j] u = -[V, E_j] u \quad all \quad u \in \mathcal{D}(H_0) \cap \mathcal{D}(V), \tag{4.21}$$

and for any $g > 2M(\beta/e\gamma_0)^\beta$ there exist $E < \infty$, $F < \infty$ such that for $j = 1,2,\ldots$:

$$\|E_j\| \leq E g^j j^{\beta j}, \tag{4.22}$$

$$\|[V, E_j]\| \leq F g^{j+1} j^{\beta(j+1)}. \tag{4.23}$$

Proof: The property (4.19) can be read from (4.12) and then (4.20), (4.21) follows from (4.19) and Lemma IV.2.

Writing $(S_\gamma(z) \equiv e^{\gamma \langle \cdot \rangle} S(z) e^{-\gamma \langle \cdot \rangle})$,

$$(S(z)V)^k P_0 (V R_0(z))^{j-k} = S(z) V e^{-\gamma_0 \langle \cdot \rangle / j} S_{\gamma_0/j}(z) \cdots S_{[(k-1)\gamma_0]/j}(z) V e^{-\gamma_0 \langle \cdot \rangle / j} e^{k \gamma_0 \langle \cdot \rangle / j} P_0$$
$$\times e^{(j-k)\gamma_0 \langle \cdot \rangle / j} V e^{-\gamma_0 \langle \cdot \rangle / j} \ldots R_{0,(j-k-1)\gamma_0/j}(z) V e^{-\gamma_0 \langle \cdot \rangle / j} R_0(z),$$

from

$$\|Ve^{-\gamma_0\langle\cdot\rangle/j}\|^j=\|V^je^{-\gamma_0\langle\cdot\rangle}\|\leqslant\sup_{a>0}a^{\beta j}e^{-\gamma_0 a}=(\beta j/e\gamma_0)^{\beta j}, \tag{4.24}$$

(4.17), (4.15) and IV.1 one obtains

$$\|E_j\|\leqslant M(j+1)(2M)^j\left(\frac{\beta}{e\gamma_0}\right)^{\beta j}j^{\beta j}. \tag{4.25}$$

In a similar way,

$$\|[V,E_j]\|\leqslant(j+1)(2M)^{j+1}\left(\frac{\beta}{e\gamma_0}\right)^{(j+1)\beta}(j+1)^{\beta(j+1)}, \tag{4.26}$$

which together with (4.25) gives the needed estimates.

Remark 4.1: One can also prove estimations of the form (4.22) and (4.23) by recurrence using the identity (4.20) in the form:

$$E_j=P_0E_j+E_jP_0+\sum_{l=1}^{j-1}E_lE_{j-l} \tag{4.27}$$

and taking advantage of the extra P_0 in P_0E_j and E_jP_0 which allows one to use (4.7) instead of (4.12).

Remark 4.2: By Stirling's formula $j^{\beta j}\leqslant e^{\beta j}(j!)^\beta$ so (4.22), (4.23) can be rewritten as

$$\|E_j\|\leqslant E\tilde{g}^j(j!)^\beta, \tag{4.28}$$

$$\|[V,E_j]\|\leqslant F\tilde{g}^{j+1}((j+1)!)^\beta \tag{4.29}$$

with

$$\tilde{g}=2M(\beta/\gamma_0)^\beta.$$

Remark 4.3: As already said the result in Theorem IV.4 can be extended in a variety of situations as for example for Zeeman effect

$$H_\epsilon=(\mathbf{P}-\epsilon\mathbf{a})^2+V_0,\quad \mathbf{P}=-i\nabla$$

with (4.3) replaced by

$$|\mathbf{a}|+|\nabla\cdot\mathbf{a}|\leqslant\langle\mathbf{x}\rangle^\beta.$$

Also if $V_0(\mathbf{x})\to\infty$ as $|\mathbf{x}|\to\infty$ one can replace the decay factor $e^{-\gamma_0\langle\cdot\rangle}$ by a better one, e.g., in the "harmonic oscillator" case $V_0(\mathbf{x})\sim|\mathbf{x}|^2$ as $|\mathbf{x}|\to\infty$ one can take [see Hunziker (1988)] $e^{-\gamma_0\langle\cdot\rangle^2}$ instead of $e^{-\gamma_0\langle\cdot\rangle}$ and in this case the asymptotic estimations are in terms of $\|V^je^{-\gamma_0\langle\cdot\rangle^2}\|$. Notice also that even in the case (4.3) one can allow $|V(\mathbf{x})|\leqslant e^{\eta\langle\cdot\rangle}$ with η sufficiently small, but in this case only a finite number of E_j can be controlled.

Remark 4.4: There is another way of proving that E_j given by (4.12) satisfy (4.20) and (4.21) namely starting with a cutoff perturbation, $V_\lambda(\mathbf{x})=V(\mathbf{x})$ if $|V(\mathbf{x})|\leqslant\lambda$ and zero otherwise, for which (4.20) and (4.21) are true (since the series $P_{\epsilon,\lambda}=\Sigma_{j=0}^\infty\epsilon^jE_{j,\lambda}$ is convergent and satisfies $-\epsilon[P_{\epsilon,\lambda},V_\lambda]=[P_{\epsilon,\lambda},H_0]$, $P_{\epsilon,\lambda}=P_{\epsilon,\lambda}^2$) and then taking the limit $\lambda\to\infty$. Yet another proof can be found in Howland (1991).

The proof of Theorem IV.4 rests heavily on exponential decay of eigenfunctions [see (4.5)], that is on the fact that $\dim P_0<\infty$. We consider now the case $\dim P_0=\infty$ when (4.5) does not hold true. Still, as far as $\beta\leqslant 1$ [see (4.3)] one can find solutions of (3.4)–(3.6). More exactly:

Theorem IV.5: *Suppose* $d_0=\mathrm{dist}(\sigma_0,\sigma(H_0)\backslash\sigma_0)>0$, $D_0=\sup_{\lambda,\mu\in\sigma_0}<\infty$ *and*

$$\sup_{\mathbf{x}\in\mathbb{R}^3}|\nabla V(\mathbf{x})|\leqslant 1. \tag{4.30}$$

Then:

(i) E_j *given recurrently by*

$$E_0=P_0,$$

$$E_{j+1}=\frac{i}{2\pi}\oint_\Gamma R_0(z)\{P_0[V,E_j]Q_0-Q_0[V,E_j]P_0\}R_0(z)\mathrm{d}z+S_j-2P_0S_jP_0, \tag{4.31}$$

where

$$Q_0=1-P_0, \tag{4.32}$$

$$S_j=\sum_{k=1}^{k=j}E_kE_{j+1-k} \tag{4.33}$$

have the properties:

$$E_j\mathcal{D}(V)\subset\mathcal{D}(H_0)\cap\mathcal{D}(V), \tag{4.34}$$

$$\|E_j\|\leqslant g^j j!, \tag{4.35}$$

$$\|[V,E_{j-1}]\|\leqslant g^j j! \tag{4.36}$$

for some $g<\infty$ *and satisfy (3.4)–(3.6).*

(ii) Let P_ϵ *as given by (3.14), (3.9), and (3.22) with* $\alpha=1$. *Let* H_ϵ *be the [unique by Faris–Lavine theorem: see Reed and Simon (1978a)] self-adjoint extension of* $H_0+\epsilon V$ *defined on* $\mathcal{D}(H_0)\cap\mathcal{D}(V)$. *Then for sufficiently small* ϵ*:*

$$P_\epsilon\mathcal{D}(H_0)\cap\mathcal{D}(V)\subset\mathcal{D}(H_0)\cap\mathcal{D}(V) \tag{4.37}$$

and on $\mathcal{D}(H_0)\cap\mathcal{D}(V)$

$$\|[H_\epsilon,P_\epsilon]\|\leqslant\frac{K}{(g\epsilon)^{1/2}}\exp\left(-\frac{1}{g\epsilon}\right), \tag{4.38}$$

where K is an absolute constant.

Remark 4.5: In order to see why bounded E_j should however exist consider E_1u with $u\in\mathcal{C}_0^\infty(\mathbb{R}^3)$ as given by (4.7). Then

$$\begin{aligned}E_1u&=-\frac{i}{2\pi}\left(\oint_\Gamma R_0(z)VR_0(z)\mathrm{d}z\right)u\\&=-\frac{i}{2\pi}\left(\oint_\Gamma R_0^2(z)V\mathrm{d}z\right)u-\frac{i}{2\pi}\left(\oint_\Gamma R_0(z)[V,R_0(z)]\mathrm{d}z\right)u.\end{aligned} \tag{4.39}$$

Now for $u\in\mathcal{C}_0^\infty(\mathbb{R}^3)$,

$$[V,R_0(z)]u=iR_0(z)(\mathbf{P}\cdot\nabla V+\nabla V\cdot\mathbf{P})R_0(z)u \tag{4.40}$$

so the operator in the last term on the right-hand side of (4.39) is bounded. On the other hand, by residue theorem, the first term on the right-hand side of (4.39) vanishes. It follows that E_1 as given by (4.39) is bounded on $\mathcal{C}_0^\infty(\mathbb{R}^3)$ and then it has a bounded extension by continuity. In addition it follows that $E_1L^2(\mathbb{R}^3)\subset\mathcal{D}(H_0)$ and one can argue that (see the proof of Lemma 4.2) that $E_1\mathcal{D}(V)\subset\mathcal{D}(V)$. Actually one can prove the existence of E_j "rewriting" (4.7) in a form in which V enters only in multiple commutators $[V,[V\cdots[V,R_0(z)]\cdots]$. This is achieved by the construction of the adiabatic projections based on the theory of pseudodifferential operators [see Sjostrand (1993), Martinez and Nenciu (1995)] which gives yet another recurrence formula for E_j:

$$E_j=\frac{i}{2\pi}\oint_\Gamma q_j(z)\mathrm{d}z, \tag{4.41}$$

where

$$q_0(z)=R_0(z),\quad q_j(z)=R_0(z)[q_{j-1}(z),V]. \tag{4.42}$$

Let us stress once again that various formulas for E_j must coincide since the solution of (3.4)–(3.6) (as far as it exists and is bounded) is unique [see Nenciu (1993)].

Remark 4.6: Actually, the result in Theorem IV.5 holds true for all potentials satisfying (4.3) with $\beta\leqslant 1$ since such a potential can be written as the sum of a potential satisfying (4.30) with a bounded one.

Proof of Theorem IV.5: As already said Theorem 4.4 follows from the treatment of the Stark effect in Nenciu (1981), Nenciu and Nenciu (1981) combined with the adiabatic exponential estimations in Nenciu (1993), so we shall only outline the main points.

Consider the family of self-adjoint operators

$$H(s)=e^{isV}H_0e^{-isV}=(\mathbf{P}-is\nabla V)^2+V_0. \tag{4.43}$$

Let $\Gamma\subset\rho(H_0)$ be a contour of finite length enclosing σ_0. By regular perturbation theory, $(H(s)-z)^{-1}$ is, for all $z\in\Gamma$, analytic in s, in a strip around real axis and uniformly bounded there so we can apply the methods in Nenciu (1993). In the following lemma we collect some results from Nenciu (1993) in an appropriate form.

Lemma IV.6: (*i*) *Let*

$$P_0(s)=e^{isV}P_0e^{-isV},\quad R(s;z)\equiv(H(s)-z)^{-1}=e^{isV}(H_0-z)^{-1}e^{-isV}. \tag{4.44}$$

Then $E_j(s)$ *given by the reccurence formula*

$$E_{j+1}(s)=\frac{1}{2\pi}\oint_\Gamma R(s;z)\left\{P_0(s)\frac{\mathrm{d}}{\mathrm{d}s}E_j(s)Q_0(s)-Q_0(s)\frac{\mathrm{d}}{\mathrm{d}s}E_j(s)P_0(s)\right\}$$
$$\times R(s;z)\mathrm{d}z+S_j(s)-2P_0(s)S_j(s)P_0(s) \tag{4.45}$$

where

$$Q_0(s)=1-P_0(s), \tag{4.46}$$

$$S_j(s)=\sum_{k=1}^{k=j}E_k(s)E_{j+1-k}(s) \tag{4.47}$$

are the unique solution of

$$E_0(s)=e^{isV}P_0e^{-isV}\equiv P_0(s), \tag{4.48}$$

$$i\frac{\mathrm{d}}{\mathrm{d}s}E_j(s)=[H(s),E_{j+1}(s)], \tag{4.49}$$

$$E_j(s)=\sum_{k=0}^{k=j}E_k(s)E_{j-k}(s), \tag{4.50}$$

are norm differentiable, and satisfy

$$E_j(s)L^2(\mathbb{R}^3)\subset\mathcal{D}(H(s)), \tag{4.51}$$

$$\|E_j(s)\|\leqslant g^j j!, \quad \left\|\frac{d}{ds}E_j(s)\right\|\leqslant g^{j+1}(j+1)!, \tag{4.52}$$

for some $g<\infty$.

(*ii*) *Let* $P_\epsilon(s)$ *as given by (3.14), (3.9), and (3.22) with* $\alpha=1$. *Then* $P_\epsilon(s)$ *is norm differentiable*

$$P_\epsilon(s)L^2(\mathbb{R}^3)\subset\mathcal{D}(H(s)) \tag{4.53}$$

and there exists $\epsilon_0>0$ *such that for* $\epsilon\in[0,\epsilon_0]$:

$$\left\|\epsilon\frac{\mathrm{d}}{\mathrm{d}s}P_\epsilon(s)-[H(s),P_\epsilon(s)]\right\|\leqslant\frac{K}{(g\epsilon)^{1/2}}\exp\left(-\frac{1}{g\epsilon}\right), \tag{4.54}$$

where K *is an absolute constant.*

Let A be a bounded operator, such that $A(s)=e^{isV}Ae^{-isV}$ is norm differentiable. Then from Stone's theorem for $f\in\mathcal{D}(V)$ one has $Af\in\mathcal{D}(V)$ and

$$i\frac{\mathrm{d}}{\mathrm{d}s}A(s)f=e^{isV}[A,V]e^{-isV}f. \tag{4.55}$$

Notice that $[A,V]$ is bounded on $\mathcal{D}(V)$. Since $E_0(s)=e^{isV}P_0e^{-isV}$, from (4.45) and (4.55) it follows that $E_j(s)$ are of the form

$$E_j(s)=e^{isV}E_je^{-isV}, \tag{4.56}$$

where E_j have all the properties stated in Theorem IV.5.i.

By the same argument [see (3.14)]

$$P_\epsilon(s)=e^{isV}P_\epsilon e^{-isV}, \quad P_\epsilon\mathcal{D}(V)\subset\mathcal{D}(V), \tag{4.57}$$

and

$$i\epsilon\frac{\mathrm{d}}{\mathrm{d}s}P_\epsilon(s)=\epsilon e^{isV}[P_\epsilon,V]e^{-isV}, \tag{4.58}$$

which together with $P_\epsilon L^2(\mathbb{R}^3)\subset\mathcal{D}(H_0)$ and (4.54) finishes the proof of Theorem IV.5.

V. MAGNETIC SCHRÖDINGER OPERATORS: GAUGE INVARIANT PERTURBATION THEORY

The aim of this section (which can be read independently of the rest of the paper) is to point out how the gauge covariance can be used to control the singularitiy of perturbations given by magnetic fields which do not vanish (or decay very slowly) as $|\mathbf{x}|\to\infty$. In order not to obscure the

main ideas we shall consider here a particular case: a particle in $\mathbb{R}^3$, subjected to a magnetic field $\mathbf{b}(\mathbf{x})$, and an electric potential $V_0(\mathbf{x})$. Also the proofs of some technical lemmas in the following will be given at the end of the section.

Concerning the magnetic field, $\mathbf{b}(\mathbf{x})$, we suppose that

$$|\mathbf{b}(\mathbf{x})|+\sum_{j=1}^{d}|\partial_j\mathbf{b}(\mathbf{x})|\leqslant\langle\mathbf{x}\rangle^{\beta},\quad \beta\leqslant 0 \tag{5.1}$$

and for $V_0(\mathbf{x})$ as before, we suppose to be uniformly L^2_{loc}, i.e.,

$$\sup_{\mathbf{x}\in\mathbb{R}^3}\int_{|\mathbf{x}-\mathbf{y}|\leqslant 1}|V_0(\mathbf{y})|^2\mathrm{d}\mathbf{y}<\infty. \tag{5.2}$$

As is well known [see, e.g., Cycon *et al.* (1986)], for a large class of vector potentials, $\mathbf{a}(\mathbf{x})$, corresponding to $\mathbf{b}(\mathbf{x})$ and $\epsilon\in[0,\infty)$ the Hamiltonian

$$H_{\epsilon,\mathbf{a}}=(\mathbf{P}-\epsilon\mathbf{a})^2+V_0 \tag{5.3}$$

is essentially self-adjoint on $\mathcal{C}_0^{\infty}(\mathbb{R}^3)$ and we shall denote by the same symbol its self-adjoint closure. As before, the unperturbed Hamiltonian (i.e., $\epsilon=0$) is denoted by H_0,

$$H_0=\mathbf{P}^2+V_0. \tag{5.4}$$

The results in the following can be extended in many directions: arbitrary dimensions; more (locally) singular $\mathbf{b}(\mathbf{x})$ and $V(\mathbf{x})$; many particle systems; the presence of a fixed magnetic field which amounts to replacing in (4.4) $\mathbf{P}$ by $(\mathbf{P}-\mathbf{A}_0)$ where $\mathbf{A}_0(\mathbf{x})$ corresponds to a *fixed* magnetic field, $\mathbf{B}_0(\mathbf{x})$; Dirac operators, etc.

Suppose that H_0 has an isolated and bounded part, σ_0, of the spectrum, i.e.,

$$\sigma(H_0)=\sigma_0\cup\sigma_1,\quad \mathrm{dist}(\sigma_0,\sigma_1)=d>0 \tag{5.5}$$

and let P_0 be the spectral projection of H_0 corresponding to σ_0. The problem is to study the "deformation" of σ_0 and P_0 when $\epsilon\neq 0$, $\epsilon\to 0$. If β in (5.1) is less than -1 then there exist magnetic potentials which are uniformly bounded (e.g., the transversal gauge, see the following) there is nothing new to say since in that case

$$H_{\epsilon,\mathbf{a}}=H_0-\epsilon(\mathbf{P}\cdot\mathbf{a}-\mathbf{a}\cdot\mathbf{P}+\epsilon^2|\mathbf{a}|^2)\equiv H_0-\epsilon W_{\epsilon,\mathbf{a}}, \tag{5.6}$$

where $W_{\epsilon,\mathbf{a}}$ is a regular perturbation of H_0 and the analytic perturbation theory works.

On the contrary, if in (5.1), $\beta\geqslant -1$ it is not possible in general to find $\mathbf{a}$ which is uniformly bounded and this implies that $W_{\epsilon,\mathbf{a}}(H_0-z)^{-1}$ is not bounded so one cannot obtain an expansion in ϵ of $(H_{\epsilon,\mathbf{a}}-z)^{-1}$ from

$$(H_{\epsilon,\mathbf{a}}-z)(H_0-z)^{-1}=1-\epsilon W_{\epsilon,\mathbf{a}}(H_0-z)^{-1}. \tag{5.7}$$

If $\sigma_0\subset\sigma_{\mathrm{discr}}(H_0)$ the asymptotic perturbation theory developed in previous sections works for all $\beta\in\mathbb{R}$ and gives asymptotic expansions for perturbed eigenvalues and corresponding eigenvectors. The situation is more involved when σ_0 is not contained in the discrete spectrum of H_0. On the one hand for $\beta\leqslant 0$, i.e., for magnetic fields which are uniformly bounded, it has been proved by Avron and Simon (1985) in a particular case and by Nenciu (1986) and Helffer and Sjostrand (1989) in the general case that the spectrum (as a set) is stable and then for sufficiently small ϵ one can still define the spectral projection $P_{\epsilon,\mathbf{a}}$ of $H_{\epsilon,\mathbf{a}}$ corresponding to the part of $\sigma(H_{\epsilon,\mathbf{a}})$ coinciding with σ_0 in the limit $\epsilon\to 0$. Now the singularity of the perturbation manifests itself in the "nonsmooth" behavior of $P_{\epsilon,\mathbf{a}}$ as $\epsilon\to 0$; There are examples [see Nenciu (1991)] in solid state theory (i.e., V periodic and $\mathbf{b}$ constant) where

$$\lim_{\epsilon\to 0}\|P_{\epsilon,\mathbf{a}}-P_0\|=1 \tag{5.8}$$

(of course one still has $s-\lim_{\epsilon\to 0}P_{\epsilon,\mathbf{a}}=P_0$) so there is no room for a (norm) asymptotic expansion of $P_{\epsilon,\mathbf{a}}$. Since, in contrast to $\sigma(H_{\epsilon,\mathbf{a}})$, $P_{\epsilon,\mathbf{a}}$ is not a gauge invariant quantity, the above-mentioned discussion suggests that, in general, the gauge invariant quantities behave much more smoothly in the limit $\epsilon\to 0$ than the nongauge invariant ones. In other words if one wants to develop a perturbation theory, one has to consider gauge invariant quantities. The problem is that, in almost all perturbation schemes, the basic object is the resolvent which is not a gauge invariant quantity.

Fortunately, one can ''factor'' out the nongauge invariant part. Let $G_{\epsilon,\mathbf{a}}(\mathbf{x},\mathbf{y};z)$, $z\in\rho(H_{\epsilon,\mathbf{a}})$ be the integral kernel (we shall prove in the following that it exists) of $(H_{\epsilon,\mathbf{a}}-z)^{-1}$ and $\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})$ be the famous nonintegrable phase factor corresponding to $\mathbf{a}$, i.e.,

$$\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})=\int_{\mathbf{y}}^{\mathbf{x}}\mathbf{a}(\mathbf{u})\cdot \mathrm{d}\mathbf{u}, \tag{5.9}$$

where the integral is along the straight line joining $\mathbf{x}$ and $\mathbf{y}$. Alternatively one can write (5.9) as

$$\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})=\left(\int_0^1\mathbf{a}(\mathbf{y}+t(\mathbf{x}-\mathbf{y}))\mathrm{d}t\right)\cdot(\mathbf{x}-\mathbf{y}). \tag{5.10}$$

Then as one can easily check

$$K_\epsilon(\mathbf{x},\mathbf{y};z)=e^{-i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}G_{\epsilon,\mathbf{a}}(\mathbf{x},\mathbf{y};z) \tag{5.11}$$

is a gauge invariant quantity. In other words we have to make the ansatz

$$G_{\epsilon,\mathbf{a}}(\mathbf{x},\mathbf{y};z)=e^{i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}K_\epsilon(\mathbf{x},\mathbf{y};z) \tag{5.12}$$

and seek a perturbation expansion for $K_\epsilon(\mathbf{x},\mathbf{y};z)$. The formula (5.12) is crucial for all that follows; it says that the whole gauge noninvariance of the integral kernel of the resolvent (and then for other related objects such as spectral projections, evolution, etc.) is contained in an exponential factor $e^{i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}$. Coming back to perturbation theory, (5.12) suggests to take as the ''zeroth'' approximation for $(H_{\epsilon,\mathbf{a}}-z)^{-1}$ the operator $S_{\epsilon,\mathbf{a}}(z)$, given by the following integral kernel (''twisted'' unperturbed resolvent)

$$(S_{\epsilon,\mathbf{a}}(z)f)(\mathbf{x})=\int_{\mathbf{R}^3}e^{i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}G_0(\mathbf{x},\mathbf{y};z)f(\mathbf{y})\mathrm{d}\mathbf{y}, \tag{5.13}$$

where $G_0(\mathbf{x},\mathbf{y};z)$ is the integral kernel of $(H_0-z)^{-1}$. Let us consider now (5.7) with $(H_0-z)^{-1}$ replaced by $S_{\epsilon,\mathbf{a}}(z)$ and define $T_{\epsilon,\mathbf{a}}(z)$ by

$$(H_{\epsilon,\mathbf{a}}-z)S_{\epsilon,\mathbf{a}}(z)=1-\epsilon T_{\epsilon,\mathbf{a}}(z). \tag{5.14}$$

Before computing $T_{\epsilon,\mathbf{a}}(z)$ let us give the following gauge covariance formula.

Lemma V.1: Let $\mathbf{a}(\mathbf{x})$ *be an arbitrary continuous vector potential corresponding to* $\mathbf{b}(\mathbf{x})$, $\mathbf{c}\in\mathbf{R}^3$ *and* $\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})$ *the corresponding nonintegrable phase factor. Then*

$$e^{-i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})}(\mathbf{P}_{\mathbf{x}}-\epsilon\mathbf{a}(\mathbf{x}))e^{i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})}=(\mathbf{P}_{\mathbf{x}}-\epsilon\mathbf{a}_{\mathbf{c}}(\mathbf{x})) \tag{5.15}$$

where $\mathbf{P}_{\mathbf{x}}=-i\nabla_{\mathbf{x}}$ *and* $\mathbf{a}_{\mathbf{c}}(\mathbf{x})$ *is the vector potential given by the transversal (Poincare) gauge relative to the point* $\mathbf{c}$*:*

$$\mathbf{a}_{\mathbf{c}}(\mathbf{x})=\left(\int_0^1 t\mathbf{b}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))\mathrm{d}t\right)\wedge(\mathbf{x}-\mathbf{c}). \tag{5.16}$$

Notice that $\mathbf{a_0}(\mathbf{x})$ is the usual transversal gauge [see Thaller (1992)]:

$$\mathbf{a_0}(\mathbf{x})=\left(\int_0^1 t\mathbf{b}(t\mathbf{x})\mathrm{d}t\right)\wedge\mathbf{x}. \tag{5.17}$$

The most interesting properties of $\mathbf{a_c}(\mathbf{x})$ and $\phi_{\mathbf{a_c}}(\mathbf{x},\mathbf{y})$ are given in the following:

Lemma V.2: (i)

$$\phi_{\mathbf{a_c}}(\mathbf{x},\mathbf{y})=-\left(\int_0^1 \mathrm{d}t\int_0^1 \mathrm{d}s\, s\mathbf{b}(st(\mathbf{x}-\mathbf{y})+s(\mathbf{y}-\mathbf{c}))\cdot((\mathbf{x}-\mathbf{c})\wedge(\mathbf{y}-\mathbf{c}))\right) \tag{5.18}$$

i.e., $\phi_{\mathbf{a_c}}(\mathbf{x},\mathbf{y})$ *is the flux through the triangle* **x c y**.

(ii)

$$|\mathbf{a_c}(\mathbf{x})|\leqslant|\mathbf{x}-\mathbf{c}|/2, \tag{5.19}$$

$$|\nabla\mathbf{a_c}(\mathbf{x})|\leqslant 2|\mathbf{x}-\mathbf{c}|. \tag{5.20}$$

(iii)

If $\mathbf{b}(\mathbf{x})=\mathbf{b}_0=\mathrm{const}$ *then*

$$\mathbf{a_c}(\mathbf{x})=\mathbf{b}_0\wedge(\mathbf{x}-\mathbf{c})/2, \tag{5.21}$$

$$\phi_{\mathbf{a_c}}(\mathbf{x},\mathbf{y})=-\mathbf{b}_0\cdot((\mathbf{x}-\mathbf{c})\wedge(\mathbf{y}-\mathbf{c}))/2. \tag{5.22}$$

Computing the right-hand side of (5.14) applied to $f\in\mathcal{C}_0^\infty(\mathbb{R}^3)$ by using Lemma V.1 one finds:

$$(T_{\epsilon,\mathbf{a}}(z)f)(\mathbf{x})=\int_{\mathbf{R}^3} e^{i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}M_\epsilon(\mathbf{x},\mathbf{y};z)f(\mathbf{y})\mathrm{d}\mathbf{y}, \tag{5.23}$$

where

$$M_\epsilon(\mathbf{x},\mathbf{y};z)=(-2i\mathbf{a}_{\mathbf{y}}(\mathbf{x})\cdot\boldsymbol{\nabla}_{\mathbf{x}}-i(\nabla_{\mathbf{x}}\mathbf{a}_{\mathbf{y}}(\mathbf{x}))-\epsilon|\mathbf{a}_{\mathbf{y}}(\mathbf{x})|^2)G_0(\mathbf{x},\mathbf{y};z). \tag{5.24}$$

Notice that M_ϵ depends only upon **b**, i.e., is gauge invariant. Up to now the discussion was at the heuristic formal level. The main technical point of this section is contained in:

Theorem V.3: *Suppose: (5.1) and (5.2) hold true,* $z\in\rho(H_0)$, $\epsilon\in[0,\epsilon_0]$, $\epsilon_0<\infty$, $K\subset\rho(H_0)$ *compact. Then (5.23), (5.24) define a bounded operator in* $L^2(\mathbb{R}^3)$ *and there exist* $t(z)<\infty$ *(depending upon V,* **b***, and* ϵ_0 *but not upon* **a***) such that uniformly for* $\epsilon\in[0,\epsilon_0]$ *and* $z\in K$:

$$\|T_{\epsilon,\mathbf{a}}(z)\|\leqslant t(z). \tag{5.25}$$

As a direct consequence we obtain the following perturbation formula for $(H_{\epsilon,\mathbf{a}}-z)^{-1}$:

Lemma V.4: If $\epsilon\in[0,t(z)^{-1}]$ *then* $z\in\rho(H_{\epsilon,\mathbf{a}})$ *and*

$$(H_{\epsilon,\mathbf{a}}-z)^{-1}=S_{\epsilon,\mathbf{a}}(z)\sum_{j=0}^{\infty}\epsilon^j T_{\epsilon,\mathbf{a}}(z)^j \tag{5.26}$$

as a norm convergent series.

Combining (5.13), (5.23), and (5.26) one can write down the expansion for $K_\epsilon(\mathbf{x},\mathbf{y};z)$:

$$K_\epsilon(\mathbf{x},\mathbf{y};z)=G_0(\mathbf{x},\mathbf{y};z)+\sum_{j=1}^{\infty}\epsilon^j K_{\epsilon,j}(\mathbf{x},\mathbf{y};z), \tag{5.27}$$

where

$$K_{\epsilon,j}(\mathbf{x},\mathbf{y};z)=\int\cdots\int \mathrm{d}\mathbf{u}_1\mathrm{d}\mathbf{u}_2\cdots\mathrm{d}\mathbf{u}_j e^{i\epsilon\Phi(\mathbf{x},\mathbf{u}_1,\mathbf{u}_2\ldots\mathbf{u}_j,\mathbf{y})} \times G_0(\mathbf{x},\mathbf{u}_1;z)M_\epsilon(\mathbf{u}_1,\mathbf{u}_2;z)\cdots M_\epsilon(\mathbf{u}_j,\mathbf{y};z) \tag{5.28}$$

and

$$\Phi(\mathbf{x},\mathbf{u}_1,\mathbf{u}_2\ldots\mathbf{u}_j,\mathbf{y})=\phi_{\mathbf{a}}(\mathbf{y},\mathbf{u}_j)+\phi_{\mathbf{a}}(\mathbf{u}_j,\mathbf{u}_{j-1})+\cdots+\phi_{\mathbf{a}}(\mathbf{u}_1,\mathbf{x})+\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y}). \tag{5.29}$$

Notice that Φ is gauge invariant and is the flux through the polygonal contour $\mathbf{y}\mathbf{u}_j\mathbf{u}_{j-1}\ldots\mathbf{x}\mathbf{y}$. In terms of integral kernels, (5.26) rewrites as

$$G_{\epsilon,\mathbf{a}}(\mathbf{x},\mathbf{y};z)=e^{i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}\left\{G_0(\mathbf{x},\mathbf{y};z)+\sum_{j=1}^{\infty}\epsilon^j K_{\epsilon,j}(\mathbf{x},\mathbf{y};z)\right\}. \tag{5.30}$$

Formulas (5.28) and (5.30) are the main result of this section.

Starting from (5.30), as in the analytic perturbations case, one can compute all physical quantities as convergent series in ϵ but with coefficients which depend themselves upon ϵ. For example, if $\sigma_0=\{\lambda_0\}$ where λ_0 is nondegenerate, then for sufficiently small ϵ the perturbed eigenvalue, $\lambda(\epsilon)$, has an expansion:

$$\lambda(\epsilon)=\sum_{j=0}^{\infty}\epsilon^j\lambda_{\epsilon,j},\quad |\lambda_{\epsilon,j}|\leqslant k^j \quad \text{for some } k<\infty. \tag{5.31}$$

The expressions for $\lambda_{\epsilon,j}$ can be obtained from

$$\lambda(\epsilon)=\mathrm{Tr}(H_{\epsilon,\mathbf{a}}P_{\epsilon,\mathbf{a}})=\mathrm{Tr}\frac{i}{2\pi}\oint_\Gamma z(H_{\epsilon,\mathbf{a}}-z)^{-1}\mathrm{d}z,$$

where Γ is a contour enclosing λ_0. Notice that [$\psi_0(\mathbf{x})$ is the eigenfunction of H_0 corresponding to λ_0]

$$\lambda_{\epsilon,0}=\frac{i}{2\pi}\int_{\mathbf{R}^3}\mathrm{d}\mathbf{x}\oint_\Gamma z\frac{|\psi_0(\mathbf{x})|^2}{\lambda_0-z}\mathrm{d}z=\lambda_0. \tag{5.32}$$

For $j\geqslant 1$, due to the fact that $K_{\epsilon,j}(\mathbf{x},\mathbf{x})$ is finite one can write

$$\lambda_{\epsilon,j}=\frac{i}{2\pi}\int_{\mathbf{R}^3}\mathrm{d}\mathbf{x}\oint_\Gamma zK_{\epsilon,j}(\mathbf{x},\mathbf{x};z)\mathrm{d}z. \tag{5.33}$$

In order to see that $\lambda_{\epsilon,j}$ as given by (5.33) are finite and satisfy (5.31) one has to plug the decomposition

$$R_0(z)=\frac{P_0}{\lambda_0-z}+S(z) \tag{5.34}$$

into (5.33), observe that the term containing no P_0 vanishes due to the contour integral and then use the exponential decay of the eigenfunction corresponding to λ_0. Further details and applications of Theorem V.3 will be given elsewhere.

The rest of this section is devoted to the proofs of Lemmas V.1 and V.2 and Theorem V.3.

Proof of Lemma V.1: By the usual computation

$$e^{-i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})}(\mathbf{P}_{\mathbf{x}}-\epsilon\mathbf{a}(\mathbf{x}))e^{i\epsilon\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})}=(\mathbf{P}_{\mathbf{x}}-\epsilon(\mathbf{a}(\mathbf{x})-\nabla\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})). \tag{5.35}$$

To compute $\nabla_{\mathbf{x}}\phi_{\mathbf{a}}$ one uses (5.10) and the vector analysis formula [see Spain (1965)]

$$\nabla(\mathbf{A}(\mathbf{x})\cdot\mathbf{B}(\mathbf{x}))=\mathbf{B}(\mathbf{x})\wedge(\nabla\wedge\mathbf{A}(\mathbf{x}))+\mathbf{A}(\mathbf{x})\wedge(\nabla\wedge\mathbf{B}(\mathbf{x}))+(\mathbf{B}(\mathbf{x})\cdot\nabla)\mathbf{A}(\mathbf{x})+(\mathbf{B}(\mathbf{x})\cdot\nabla)\mathbf{A}(\mathbf{x}) \tag{5.36}$$

with

$$\mathbf{A}(\mathbf{x})=\int_0^1\mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))\mathrm{d}t,$$

$$\mathbf{B}(\mathbf{x})=(\mathbf{x}-\mathbf{c}).$$

One obtains four terms; the first one gives $-\mathbf{a}_{\mathbf{c}}(\mathbf{x})$, the second vanishes, and the fourth gives $\int_0^1\mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))\mathrm{d}t$. Observing that

$$t\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))=((\mathbf{x}-\mathbf{c})\cdot\nabla_{\mathbf{x}})\mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))$$

the third term gives $\int_0^1 t\,(\mathrm{d}/\mathrm{d}t)\,\mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))\mathrm{d}t$ and then, after integration by parts $\mathbf{a}(\mathbf{x})-\int_0^1\mathbf{a}(\mathbf{c}+t(\mathbf{x}-\mathbf{c}))\mathrm{d}t$. Summing up all the terms one obtains (5.15).

Proof of Lemma V.2: The only thing to be proved is (5.18) since (5.19)–(5.22) can be read directly from (5.10),(5.16), and (5.1). Now (5.18) follows, either directly by direct computation from (5.10), and (5.16) or from Stokes's theorem by observing that

$$\int_{\mathbf{c}}^{\mathbf{x}}\mathbf{a}_{\mathbf{c}}(\mathbf{u})\cdot\mathrm{d}\mathbf{u}=\int_{\mathbf{c}}^{\mathbf{y}}\mathbf{a}_{\mathbf{c}}(\mathbf{u})\cdot\mathrm{d}\mathbf{u}=0.$$

Proof of Theorem V.3: We have to estimate $M_{\epsilon}(\mathbf{x},\mathbf{y};z)$. The key fact is that [see (5.19) and (5.20)] $\mathbf{a}_{\mathbf{y}}(\mathbf{x})$ and $\nabla_{\mathbf{x}}\cdot\mathbf{a}_{\mathbf{y}}(\mathbf{x})$ diverge only when $|\mathbf{x}-\mathbf{y}|\to\infty$ and this divergence is canceled by the decay of $G_0(\mathbf{x},\mathbf{y};z)$ and $\nabla_{\mathbf{x}}\cdot G_0(\mathbf{x},\mathbf{y};z)$ as given by the following proposition which is the pointwise analog of Proposition IV.1.

Proposition V.5: (i) For all $z\in\rho(H_0)$, $(H_0-z)^{-1}$ is a Carleman operator; in particular it has an integral kernel $G_0(\mathbf{x},\mathbf{y};z)$.

(ii) Let $K\subset\rho(H_0)$ be compact. Then there exist $C<\infty$, $\gamma>0$ such that uniformly in $z\in K$:

$$|G_0(\mathbf{x},\mathbf{y};z)|\leqslant\frac{C}{|\mathbf{x}-\mathbf{y}|}e^{-\gamma|\mathbf{x}-\mathbf{y}|}, \tag{5.37}$$

$$|\nabla_{\mathbf{x}}G_0(\mathbf{x},\mathbf{y};z)|\leqslant\frac{C}{|\mathbf{x}-\mathbf{y}|^2}e^{-\gamma|\mathbf{x}-\mathbf{y}|}. \tag{5.38}$$

From

$$\sup_{r>0}r^m e^{-\nu r}=M(m,\nu)<\infty,\quad m\geqslant 0,\nu>0, \tag{5.39}$$

(5.19), (5.20), (5.37), (5.38), and (5.24) one obtains that uniformly for $\epsilon\in[0,\epsilon_0]$, $z\in K$,

$$|M_{\epsilon}(\mathbf{x},\mathbf{y};z)|\leqslant\mathrm{const}\frac{1}{|\mathbf{x}-\mathbf{y}|}e^{-\gamma|\mathbf{x}-\mathbf{y}|/2} \tag{5.40}$$

and then by Young inequality

$$\|T_\epsilon f\| \leqslant \text{const}\left(\int_{\mathbb{R}^3} \frac{e^{-\gamma|\mathbf{x}|/2}}{|\mathbf{x}|} d\mathbf{x} \right) \|f\| \tag{5.41}$$

and the proof is finished.

Proof of Proposition V.5: The proposition follows from the results in Simon (1982), so we shall only outline the proof. The fact that $(H_0-z)^{-1}$ is a Carleman operator follows from the fact that V_0 is $-\Delta$ bounded and then $(H_0-z)^{-1} \in \mathcal{B}(L^2(\mathbb{R}^3), L^\infty(\mathbb{R}^3))$ [see Corollary A.1.2 in Simon (1982)]. The inequality (5.37) follows from Theorem B 7.2. in Simon (1982) [actually Theorem B 7.2. in Simon (1982) is stated for a fixed z but the proof covers the given case].

For $z=-a$, $a>0$ and sufficiently large

$$G_0(\mathbf{x},\mathbf{y};-a) = \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} e^{-a^{1/2}|\mathbf{x}-\mathbf{y}|} - \int_{\mathbb{R}^3} \frac{1}{4\pi|\mathbf{x}-\mathbf{u}|} e^{-a^{1/2}|\mathbf{x}-\mathbf{u}|} V(u) G_0(\mathbf{u},\mathbf{y};-a) \mathrm{d}\mathbf{u} \tag{5.42}$$

and then

$$\nabla_{\mathbf{x}} G_0(\mathbf{x},\mathbf{y};-a) = \nabla_{\mathbf{x}} \left(\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} e^{-a^{1/2}|\mathbf{x}-\mathbf{y}|} \right) - \int_{\mathbb{R}^3} \nabla_{\mathbf{x}} \left(\frac{1}{4\pi|\mathbf{x}-\mathbf{u}|} e^{-a^{1/2}|\mathbf{x}-\mathbf{u}|} \right) V(u) G_0(\mathbf{u},\mathbf{y};-a) \mathrm{d}\mathbf{u}, \tag{5.43}$$

which gives (5.38) for $z=-a$. Finally (5.38) is ''carried'' from $-a$ to $z \in K$ via the resolvent equation

$$\nabla_{\mathbf{x}} G_0(\mathbf{x},\mathbf{y};z) = \nabla_{\mathbf{x}} G_0(\mathbf{x},\mathbf{y};-a) \tag{5.44}$$

$$+ (z+a) \int_{\mathbb{R}^3} \nabla_{\mathbf{x}} G_0(\mathbf{x},\mathbf{u};-a) G_0(\mathbf{u},\mathbf{y};z) \mathrm{d}\mathbf{u}. \tag{5.45}$$

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APPENDIX: ALMOST IDEMPOTENT OPERATORS

Although the Proposition 3 in Nenciu (1993) provides the needed construction we shall give below a more aesthetical form of it.

Let P be a bounded idempotent. Then [see, e.g., Kato (1980), Chap. III.4] $\mathcal{H}=\mathcal{M}+\mathcal{N}$ such that if $f=m+n$, $m \in \mathcal{M}$, $n \in \mathcal{N}$ then $Pf=m$, i.e., P is a projection. By direct computation

$$(P-z)(P+z-1) = z(z-1),$$

which in particular implies that $\sigma(P)=\{0,1\}$. Moreover it gives the following formula for the resolvent of P:

$$(P-z)^{-1} = \frac{(P+z-1)}{z(1-z)}.$$

Let T now be bounded and ''almost'' idempotent (but not necessarily self-adjoint). The problem is whether T is close to an idempotent.

Proposition VI.1: Let T be a bounded operator, $\Delta = T^2 - T$.

Then for $\|\Delta\| \equiv \delta \leqslant 1/4$ *one has* $\{|z-1|=1/2\} \subset \rho(T)$ *and*

$$\|T-P\| \leqslant \frac{4\delta(2\|T\|+1)}{1-4\delta},$$

where

$$P = \frac{i}{2\pi} \oint_{|z-1|=1/2} (T-z)^{-1}\, dz.$$

Proof: By direct computation,

$$(T-z)(T+z-1) = z(1-z)[1+\Delta/z(1-z)]$$

whereof for $\|\Delta\|/|z(z-1)| < 1$

$$(T-z)^{-1} = \frac{T+z-1}{z(1-z)}\left[1+\frac{\Delta}{z(1-z)}\right]^{-1} = \left(\frac{T}{z(1-z)} - \frac{1}{z}\right)\left[1 - \frac{\Delta}{z(1-z)}\left(1+\frac{\Delta}{z(1-z)}\right)^{-1}\right],$$

whereof for $\delta < 1/4$

$$P - T = -\Delta \frac{i}{2\pi} \oint_{|z-1|=1/2} \frac{1}{z(1-z)}\left(\frac{T}{z(1-z)} - \frac{1}{z}\right)\left(1+\frac{\Delta}{z(1-z)}\right)^{-1} dz, \tag{A1}$$

which gives the result.

Remark 6.1: If T is self-adjoint then P is also self-adjoint.

Remark 6.2: By performing the integral in the last equation by using the residue theorem one can show that

$$P - T = (T-1/2)[(1+4\Delta)^{-1/2} - 1],$$

which gives the estimation

$$\|P-T\| \leqslant \frac{2\delta(2\|T\|+1)}{1-4\delta}, \tag{A2}$$

which is better than the result in Proposition VI.1 by a factor of 2.

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On the structure of covariant phase observables

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We study the mathematical structure of covariant phase observables. Such observables can alternatively be expressed as phase matrices, as sequences of unit vectors, as sequences of phase states, or as equivalence classes of covariant trace-preserving operations. Covariant generalized operator measures are defined by structure matrices which form a W*-algebra with phase matrices as its subset. The properties of the Radon–Nikodým derivatives of phase probability measures are studied.
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I. INTRODUCTION

Covariant phase observables constitute a particular solution to the problem of quantum phase (see, e.g., Ref. 1, and 2). In this article, we study general mathematical properties of covariant phase observables and represent them as covariant trace-preserving operations (Sec. III). We also analyze the structure matrix W*-algebra of covariant generalized operator measures (Sec. IV) and the pointwise convergence of phase probability densities (Sec. V)

Let $\mathcal{H}$ be a complex Hilbert space with a fixed basis $\{|n\rangle \in \mathcal{H} \mid n \in \mathbb{N}\}$. Define the number operator $N := \Sigma_{n=0}^{\infty} n|n\rangle\langle n|$ with its usual domain $\mathcal{D}(N) := \{\psi \in \mathcal{H} \mid n^2 |\langle n|\psi\rangle|^2 < \infty\}$ and the phase shifter $R(\theta) := e^{i\theta N}$ for all $\theta \in \mathbb{R}$. Let $\mathcal{L}(\mathcal{H})$, $\mathcal{T}(\mathcal{H})$, and $\mathcal{T}(\mathcal{H})_1^+$ denote the sets of bounded operators, trace-class operators, and states (positive trace-one operators) on $\mathcal{H}$, respectively.

Let $\mathcal{B}([0,2\pi))$ denote the σ-algebra of the Borel subsets of $[0,2\pi)$, and consider an operator measure $E: \mathcal{B}([0,2\pi)) \to \mathcal{L}(\mathcal{H})$. The measure E is normalized if $E([0,2\pi)) = I$, positive if $E(X) \geqslant O$ for all $X \in \mathcal{B}([0,2\pi))$, and phase shift covariant if $R(\theta)E(X)R(\theta)^* = E(X \oplus \theta)$ for all $X \in \mathcal{B}([0,2\pi))$ and for all $\theta \in [0,2\pi)$, where $X \oplus \theta := \{x \in [0,2\pi) \mid (x-\theta) (\mathrm{mod}\ 2\pi) \in X\}$. A phase shift covariant normalized positive operator measure is called a *(covariant) phase observable*.

In the next section we collect some known properties of covariant phase observables. The new results are contained in Secs. III–V.

II. THE STRUCTURE OF PHASE OBSERVABLES

Any covariant phase observable is of the (weakly convergent) form

$$E(X) = \sum_{n,m=0}^{\infty} c_{n,m} i_{n-m}(X) |n\rangle\langle m|, \quad X \in \mathcal{B}([0,2\pi)), \tag{1}$$

where $i_k(X) := (2\pi)^{-1} \int_X e^{ik\theta} \mathrm{d}\theta$ for all $k \in \mathbb{Z}$, and where the phase matrix $(c_{n,m})_{n,m \in \mathbb{N}}$ is a positive semidefinite (complex) matrix with $c_{n,n} = 1$, $n \in \mathbb{N}$ (see, e.g., Phase Theorem 2.2 of Ref. 2). A complex matrix $(c_{n,m})$ is a phase matrix if and only if there exists a sequence $(\psi_n)_{n \in \mathbb{N}}$ of unit vectors such that $c_{n,m} = \langle \psi_n | \psi_m \rangle$, $n, m \in \mathbb{N}$.[3] A constant sequence, e.g., $\psi_n = |0\rangle$, $n \in \mathbb{N}$, defines the *canonical phase observable*

$$E_{\mathrm{can}}(X) := \sum_{n,m=0}^{\infty} i_{n-m}(X) |n\rangle\langle m|, \quad X \in \mathcal{B}([0,2\pi)),$$

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whereas any orthonormal sequence, e.g., $\psi_n=|n\rangle$, $n\in\mathbb{N}$, gives the *trivial phase observable*

$$E_{\mathrm{triv}}(X):=i_0(X)\,I,\quad X\in\mathcal{B}([0,2\pi)).$$

Next we show how any phase observable can be constructed by using a sequence of phase states (Theorem 2).

Define $\mathcal{H}_1:=\{\psi\in\mathcal{H}\mid\Sigma_{n=0}^{\infty}|\langle n|\psi\rangle|<\infty\}$. A phase matrix $(c_{n,m})$ can be interpreted as a phase kernel, that is, a positive (possible unbounded in the norm of $\mathcal{H}$) sequilinear form $C:\mathcal{H}_1\times\mathcal{H}_1\to\mathbb{C}$ defined as

$$C(\varphi,\psi):=\sum_{n,m=0}^{\infty}c_{n,m}\langle\varphi|n\rangle\langle m|\psi\rangle,\quad\varphi,\psi\in\mathcal{H}_1,$$

where the sum converges absolutely. Keeping this in mind, we may formally write

$$C=\sum_{n,m=0}^{\infty}c_{n,m}|n\rangle\langle m|.$$

Since $R(\theta)\mathcal{H}_1=\mathcal{H}_1$ for all $\theta\in[0,2\pi)$ we can define a continuous integrable function $[0,2\pi]\to\mathbb{C}$,

$$\theta\mapsto C(R(-\theta)\varphi,R(-\theta)\psi)=\sum_{n,m=0}^{\infty}c_{n,m}e^{i(n-m)\theta}\langle\varphi|n\rangle\langle m|\psi\rangle,$$

for all $\varphi,\psi\in\mathcal{H}_1$, and thus a bounded positive sesquilinear form $\mathcal{H}_1\times\mathcal{H}_1\to\mathbb{C}$,

$$(\varphi,\psi)\mapsto E(X)_{\varphi,\psi}:=\frac{1}{2\pi}\int_X C(R(-\theta)\varphi,R(-\theta)\psi)\mathrm{d}\theta=\sum_{n,m=0}^{\infty}c_{n,m}i_{n-m}(X)\langle\varphi|n\rangle\langle m|\psi\rangle,$$

for all $X\in\mathcal{B}([0,2\pi))$.[4] The form $(\varphi,\psi)\mapsto E(X)_{\varphi,\psi}$ has a unique bounded positive extension to $\mathcal{H}\times\mathcal{H}$ which is determined by a unique bounded operator, say, $E(X)\in\mathcal{L}(\mathcal{H})$. Operators $E(X)$, $X\in\mathcal{B}([0,2\pi))$, constitute a covariant phase observable. The following route to define a phase observable is thus justified:

(1) Take a phase matrix $(c_{n,m})$ and define the phase kernel $\Sigma_{n,m=0}^{\infty}c_{n,m}|n\rangle\langle m|$.

(2) Act on it by $R(\theta)$ to get

$$R(\theta)\sum_{n,m=0}^{\infty}c_{n,m}|n\rangle\langle m|R(\theta)^*=\sum_{n,m=0}^{\infty}c_{n,m}e^{i(n-m)\theta}|n\rangle\langle m|.$$

(3) Integrate it over $X\in\mathcal{B}([0,2\pi))$ to get a bounded sesquilinear form $\mathcal{H}_1\times\mathcal{H}_1\to\mathbb{C}$,

$$\frac{1}{2\pi}\int_X R(\theta)\sum_{n,m=0}^{\infty}c_{n,m}|n\rangle\langle m|R(\theta)^*\mathrm{d}\theta=\sum_{n,m=0}^{\infty}c_{n,m}i_{n-m}(X)|n\rangle\langle m|.$$

(4) This has a unique bounded extension $\mathcal{H}\times\mathcal{H}\to\mathbb{C}$ which defines the phase observable

$$E(X):=\sum_{n,m=0}^{\infty}c_{n,m}i_{n-m}(X)|n\rangle\langle m|.$$

Let $\mathcal{H}_\infty$ be a complex Banach space of vectors $\Sigma_{n=0}^{\infty}g_n|n\rangle$ for which the norm $\|\Sigma_{n=0}^{\infty}g_n|n\rangle\|_\infty:=\sup\{|g_n|\mid n\in\mathbb{N}\}<\infty$.[5] Embedding $\mathcal{H}$ in $\mathcal{H}_\infty$ we get the following triplet:

$$\mathcal{H}_1\subset\mathcal{H}\subset\mathcal{H}_\infty.$$

We have the following theorem.[6]

Theorem 1: *For any phase matrix* $(c_{n,m})$,

$$\sum_{n,m=0}^{\infty} c_{n,m}\langle\varphi|n\rangle\langle m|\psi\rangle=\sum_{k=0}^{\infty}\langle\varphi|F_k)(F_k|\psi\rangle,$$

for all $\varphi,\ \psi\in\mathcal{H}_1$, *that is, briefly,*

$$\sum_{n,m=0}^{\infty} c_{n,m}|n\rangle\langle m|=\sum_{k=0}^{\infty}|F_k)(F_k|,$$

where $|F_k)\in\mathcal{H}_\infty$ *for all* $k\in\mathbb{N}$ *and* $\Sigma_{k=0}^{\infty}|\langle n|F_k)|^2=1$ *for all* $n\in\mathbb{N}$. *Conversely, if* $(|F_k))_{k\in\mathbb{N}}\subset\mathcal{H}_\infty$ *is such that* $\Sigma_{k=0}^{\infty}|\langle n|F_k)|^2=1$, *then* $\Sigma_{k=0}^{\infty}|F_k)(F_k|$ *is a phase kernel.*

Let $|F)\in\mathcal{H}_\infty$ and define $|F;\theta):=R(\theta)|F)$ and $(F;\theta|:=(F|R(\theta)^*$ for all $\theta\in\mathbb{R}$. Since $R(\theta')|F;\theta)=|F;\theta+\theta')$ we say that $|F;\theta)$ is a *phase state*. It is easy to see that the following sesquilinear form $\mathcal{H}_1\times\mathcal{H}_1\to\mathbb{C}$,

$$(\varphi,\psi)\mapsto\frac{1}{2\pi}\int_X\langle\varphi|F;\theta)(F;\theta|\psi\rangle\mathrm{d}\theta,$$

is positive and bounded for all $X\in\mathcal{B}([0,2\pi))$ and it defines a covariant positive operator measure

$$\mathcal{B}([0,2\pi))\ni X\mapsto E_F(X)=\sum_{n,m=0}^{\infty}\langle n|F)(F|m\rangle i_{n-m}(X)|n\rangle\langle m|\in\mathcal{L}(\mathcal{H}). \tag{2}$$

The operator measure E_F is normalized, that is, a phase observable, if and only if $|\langle n|F)|=1$ for all $n\in\mathbb{N}$, that is, when

$$|F)=\sum_{n=0}^{\infty}e^{i\upsilon_n}|n\rangle,$$

where $(\upsilon_n)_{n\in\mathbb{N}}\subset[0,2\pi)$. Let $U:=\Sigma_{n=0}^{\infty}e^{i\upsilon_n}|n\rangle\langle n|$. Then E_F is a phase observable if and only if

$$E_F(X)=UE_{\mathrm{can}}(X)U^*,\quad X\in\mathcal{B}([0,2\pi)).$$

If, for two phase observables E_1 and E_2, the condition $E_1(X)=UE_2(X)U^*$, $X\in\mathcal{B}([0,2\pi))$, holds, we say that E_1 is E_2 up to unitary equivalence, or, briefly, E_1 is E_2 (u.e.). Thus, using Theorem 1 we get a variant of Phase Theorem 2.2 of Ref. 2.

Theorem 2: *E is a phase observable if and only if for all* $X\in\mathcal{B}([0,2\pi))$

$$E(X)=\mathrm{w}\text{-}\lim_{n\to\infty}\sum_{k=0}^{n}E_{F_k}(X),$$

where $E_{F_k}(X)$ *is the bounded operator defined by a sesquilinear form*

$$\frac{1}{2\pi}\int_X|F_k;\theta)(F_k;\theta|\mathrm{d}\theta,$$

where $|F_k)\in\mathcal{H}_\infty$, $k\in\mathbb{N}$, *and* $\Sigma_{k=0}^{\infty}|\langle n|F_k)|^2=1$.

The phase observable E is defined by a single phase state if and only if E is E_{can} *(u.e.).*

Since the sequence $n\mapsto\Sigma_{k=0}^{n}E_{F_k}(X)$ is increasing, $E(X)=\text{s-}\lim_{n\to\infty}\Sigma_{k=0}^{n}E_{F_k}(X)$ also.

III. PHASE OBSERVABLES AS OPERATIONS

A linear mapping $\Phi:\mathcal{T}(\mathcal{H})\to\mathcal{T}(\mathcal{H})$ is a *covariant trace-preserving operation* if it is covariant $[R(\theta)\Phi(T)R(\theta)^*=\Phi(R(\theta)TR(\theta)^*),\quad \theta\in[0,2\pi),\quad T\in\mathcal{T}(\mathcal{H})]$, trace-preserving $[\mathrm{tr}(\Phi(T))=\mathrm{tr}(T),\ T\in\mathcal{T}(\mathcal{H})]$, and positive $[\Phi(\mathcal{T}(\mathcal{H})_1^+)\subseteq\mathcal{T}(\mathcal{H})_1^+]$ (for the theory of operations, see e.g., Refs. 7 and 8). We prove next a theorem essentially due to Hall and Fuss.[9,10]

Theorem 3: *A mapping* $E:\mathcal{B}([0,2\pi))\to\mathcal{L}(\mathcal{H})$ *is a phase observable if and only if*

$$\mathrm{tr}(TE(X))=\mathrm{tr}(\Phi(T)E_{\mathrm{can}}(X)) \tag{3}$$

for all $X\in\mathcal{B}([0,2\pi))$ *and* $T\in\mathcal{T}(\mathcal{H})$ *where* $\Phi:\mathcal{T}(\mathcal{H})\to\mathcal{T}(\mathcal{H})$ *is a covariant trace-preserving operation.*

Proof: Let E be a phase observable with the phase matrix $(c_{n,m})$. For all $T\in\mathcal{T}(\mathcal{H})$ define

$$\Theta(T):=\sum_{n,m=0}^{\infty}c_{m,n}T_{n,m}|n\rangle\langle m|. \tag{4}$$

Since $T=\alpha T_\alpha-\beta T_\beta+i\gamma T_\gamma-i\delta T_\delta$ where T_α, T_β, T_γ, and T_δ are states, and α, β, γ, and δ are non-negative real numbers, it suffices to consider only states. Thus, assume that T is a state. Since $\sup\{|\langle\varphi|\Theta(T)\psi\rangle|\,|\,\|\varphi\|\leqslant1,\|\psi\|\leqslant1\}\leqslant\sup\{\Sigma_{n,m=0}^{\infty}|T_{n,m}|\,|\langle\varphi|n\rangle|\,|\langle m|\psi\rangle|\,|\,\|\varphi\|\leqslant1,\|\psi\|\leqslant1\}\leqslant1$ it follows that $\Theta(T)$ is a bounded operator. Using a decomposition $T=\Sigma_{j=0}^{\infty}|\phi_j\rangle\langle\phi_j|$, $\phi_j\in\mathcal{H}$, $j\in\mathbb{N}$, one sees that $\langle\psi|\Theta(T)\psi\rangle=\Sigma_{j=0}^{\infty}\Sigma_{n,m=0}^{\infty}\overline{\langle m|\phi_j\rangle\langle\psi|m\rangle}c_{m,n}\langle n|\phi_j\rangle\langle\psi|n\rangle\geqslant0$ for all $\psi\in\mathcal{H}_1$ and, thus, Θ is positive. Since $\Sigma_{n=0}^{\infty}\langle n|\Theta(T)|n\rangle=1$, $\Theta(T)$ is a trace-one operator. Moreover, $\mathrm{tr}(TE(X))=\mathrm{tr}(\Theta(T)E_{\mathrm{can}}(X))$, $X\in\mathcal{B}([0,2\pi))$, and Θ is covariant. Thus, Θ is a covariant trace-preserving operation. The converse part is trivial. □

There are many covariant trace-preserving operations Φ which satisfy Eq. (3) for a given E. One such operation Θ is defined in (4). It is the identity operation in the case of the canonical phase whereas for the trivial phase it is of the form $\Theta(T)=\Sigma_{n=0}^{\infty}T_{n,n}|n\rangle\langle n|$. We note also that, in the case of the trivial phase, $T\mapsto T_{0,0}|1\rangle\langle1|+T_{1,1}|0\rangle\langle0|+\Sigma_{n=2}^{\infty}T_{n,n}|n\rangle\langle n|$ is another operation fulfilling Theorem 3. Since the diagonal elements $T_{n,n}$ do not "contain" any phase information of the state T we see that the trivial phase "loses" all phase information. In the general case, if $c_{n,m}=0$ for some $n\neq m$, there are vector states (other than number states) $\psi:=d_n|n\rangle+d_m|m\rangle$, d_n, $d_m\in\mathbb{C}\backslash\{0\}$, $|d_n|^2+|d_m|^2=1$, for which the probability measure $X\mapsto\langle\psi|E(X)\psi\rangle$ is random. Next we study the properties of Θ.

Let E be a phase observable with the phase matrix $(c_{n,m})$, and let $\Theta(T)=\Sigma_{n,m=0}^{\infty}c_{m,n}T_{n,m}|n\rangle\langle m|$ for all $T\in\mathcal{T}(\mathcal{H})$. The dual mapping $\Theta^*:\mathcal{L}(\mathcal{H})\to\mathcal{L}(\mathcal{H})$ of an operation Θ defined by the relation $\mathrm{tr}(T\Theta^*(A))=\mathrm{tr}(\Theta(T)A)$, $A\in\mathcal{L}(\mathcal{H})$, $T\in\mathcal{T}(\mathcal{H})$, is a positive linear mapping, and

$$\Theta^*(A)=\sum_{n,m=0}^{\infty}c_{n,m}A_{n,m}|n\rangle\langle m|,\quad A\in\mathcal{L}(\mathcal{H}).$$

From Theorem 1 one gets (weakly)

$$\Theta(T)=\sum_{k=0}^{\infty}A_kTA_k^*,\quad T\in\mathcal{T}(\mathcal{H}),$$

where $A_k:=\Sigma_{n=0}^{\infty}(F_k|n\rangle)|n\rangle\langle n|$ for all $k\in\mathbb{N}$ showing that Θ is *completely positive* (see the First Representation Theorem of Ref. 8). Note that $\Sigma_{k=0}^{\infty}A_kA_k^*=I$ and $\Theta^*(A)=\Sigma_{k=0}^{\infty}A_k^*AA_k$, $A\in\mathcal{L}(\mathcal{H})$.

Let $\Theta_1^+:\mathcal{T}(\mathcal{H})_1^+\to\mathcal{T}(\mathcal{H})_1^+$ be the restriction of Θ to the set of states.

Theorem 4: (1) Θ *and* Θ_1^+ *are injections if and only if* $c_{n,m}\neq0$ *for all* $n,m\in\mathbb{N}$.

(2) Θ_1^+ *is surjection if and only if* E *is* E_{can} *(u.e.).*

(3) Θ_1^+ *is bijection if and only if* E *is* E_{can} *(u.e.).*

(4) Θ *preserves pure states* $[\Theta(|\psi\rangle\langle\psi|)^2=\Theta(|\psi\rangle\langle\psi|)$ *for all unit vectors* $\psi\in\mathcal{H}]$ *if and only if* E *is* E_{can} *(u.e.).*

Proof: It is easy to see that Θ and Θ_1^+ are injections if and only if $c_{m,n}T_{n,m}=0$ for all $n, m\in\mathbb{N}$ where $T\in\mathcal{T}(\mathcal{H})$ implies that $T=O$. Thus, Θ and Θ_1^+ are injections if and only if $c_{n,m}\neq 0$ for all n, m.

Suppose that Θ_1^+ is a surjection. If $c_{m,n}=0=c_{n,m}$ for some $n\neq m$, then $\Theta_1^+(T)\neq T':=(|n\rangle+|m\rangle)(\langle n|+\langle m|)/2$ for all $T\in\mathcal{T}(\mathcal{H})_1^+$ and, thus, $c_{n,m}\neq 0$ for all n, m and Θ_1^+ is an injection and bijection. If $|c_{n,m}|<1$ for some $n\neq m$, then there is no state T such that $\Theta_1^+(T)=T'$. Thus, $|c_{n,m}|=1$, $n, m\in\mathbb{N}$, and $E=E_{\mathrm{can}}$ (u.e.). This proves items (2) and (3).

Let $\psi:=\Sigma_{n=0}^{\infty}d_n|n\rangle$ where $d_n>0$ for all n and $\Sigma_{n=0}^{\infty}d_n^2=1$. Now $\Theta(|\psi\rangle\langle\psi|)^2=\Theta(|\psi\rangle\langle\psi|)$ implies that $\Sigma_{n=0}^{\infty}|c_{n,m}|^2d_n^2=1$ for all m which shows that $|c_{n,m}|=1$, $n, m\in\mathbb{N}$, and $E=E_{\mathrm{can}}$ (u.e.). This completes the proof. □

IV. COVARIANT GOMS AND PHASE MATRICES

The standard way to represent an observable in quantum mechanics is to find an appropriate self-adjoint operator, or an idempotent POM, which describes that observable. However, in many cases this representation is too narrow and it is convenient to give up the idempotency (see, e.g., Ref. 11). The strength of POMs is that they associate a probability measure to *all* states. If we restrict ourselves to a subset of (vector) states to be called physical states, we can give up the positivity of POM and require that the operator measure gives a probability measure (via trace formula) only for physical states. Actually, we do not have to assume that the observable can even be ''defined'' for other states than physical ones. Hence, define a set of physical states $\mathcal{V}$. It is a linear subspace of the Hilbert space of the physical system. The linearity is assumed because of the possibility to superpose the physical states. Let $\mathcal{SL}(\mathcal{V},\mathcal{V};\mathbb{C})$ be the set of sesquilinear forms from $\mathcal{V}\times\mathcal{V}$ to $\mathbb{C}$ (the first argument is antilinear). A *generalized operator measure*,[12] or a *GOM*, G is the mapping from the σ-algebra $\mathcal{A}$ of the set of measurement outcomes Ω to $\mathcal{SL}(\mathcal{V},\mathcal{V};\mathbb{C})$ such that $\mathcal{A}\ni X\to[G(X)](\varphi,\psi)\in\mathbb{C}$ is a complex measure for all $\varphi, \psi\in\mathcal{V}$. It is *normalized* if $[G(\Omega)](\varphi,\psi)=\langle\varphi|\psi\rangle$, $\varphi, \psi\in\mathcal{V}$.

In the case of phase, it is natural to assume that $\Omega=[0,2\pi)$, $\mathcal{A}=\mathcal{B}([0,2\pi))$, and $\mathcal{V}$ contains number states, coherent states, etc. Since they are elements of $\mathcal{H}_1$ we assume that $\mathcal{V}=\mathcal{H}_1$. If we study the coherent state phase measurements with the associated GOM $E:\mathcal{B}([0,2\pi))\to\mathcal{SL}(\mathcal{H}_1,\mathcal{H}_1;\mathbb{C})$, it is natural to assume the following phase shift covariance condition:

$$[E(X)](|ze^{-\alpha}\rangle,|ze^{-\alpha}\rangle)=[E(X\oplus\alpha)](|z\rangle,|z\rangle) \tag{5}$$

for all $X\in\mathcal{B}([0,2\pi))$, $z\in\mathbb{C}$, and $\alpha\in[0,2\pi)$. The following GOMs are solutions of (5):

$$[E(X)](\varphi,\psi)=\sum_{n,m=0}^{\infty}d_{n,m}i_{n-m}(X)\langle\varphi|n\rangle\langle m|\psi\rangle, \tag{6}$$

where $(d_{n,m})\in\mathbb{C}^{\mathbb{N}\times\mathbb{N}}$, $\sup\{|d_{n,m}|\,|\,n,m\in\mathbb{N}\}<\infty$, $X\in\mathcal{B}([0,2\pi))$, and $\varphi, \psi\in\mathcal{H}_1$. We use the following short notation for E:

$$E(X)=\sum_{n,m=0}^{\infty}d_{n,m}i_{n-m}(X)|n\rangle\langle m|,$$

and we say that E is a *covariant GOM* defined by the *structure matrix* $(d_{n,m})$. Note that $E([0,2\pi))=\Sigma_{n=0}^{\infty}d_{n,n}|n\rangle\langle n|$ can be extended to a unique bounded operator. If $d_{n,n}=1$, $n\in\mathbb{N}$, then E is normalized. If $(d_{n,m})$ is a phase matrix, then E is a phase observable. For all $\varphi, \psi\in\mathcal{H}_1$, the complex measure $X\to[E(X)](\varphi,\psi)$ has a continuous density which is

$$\theta \mapsto \sum_{n,m=0}^{\infty} d_{n,m} e^{i(n-m)\theta} \langle \varphi | n \rangle \langle m | \psi \rangle .$$

Let $\mathcal{M}_\infty$ be a set of structure matrices $(d_{n,m})_{n,m\in\mathbb{N}} \in \mathbb{C}^{\mathbb{N}\times\mathbb{N}}$, $\sup\{|d_{n,m}| \mid n,m \in \mathbb{N}\} < \infty$. Since for all $(d_{n,m}) \in \mathcal{M}_\infty$ we have a unique covariant genaralized operator measure E defined in (6), we can identify $(d_{n,m})$ with E. Now $\mathcal{M}_\infty$ is a W*-algebra (over $\mathbb{C}$) with the norm $\|(d_{n,m})\| := \sup\{|d_{n,m}| \mid n,m \in \mathbb{N}\} < \infty$. The summation, scalar product, and algebra product are defined pointwise. Let $\star$ be the algebra product operation, that is, $(d_{n,m}) \star (e_{n,m}) := (d_{n,m} e_{n,m})$. The identity of $\mathcal{M}_\infty$ is the canonical phase matrix $(c_{n,m})$ with $c_{n,m} = 1$, $n, m \in \mathbb{N}$. The algebra $\mathcal{M}_\infty$ is commutative and the involution is $(d_{n,m}) \mapsto (d_{n,m})^* := (\overline{d_{n,m}})$. The unique predual of $\mathcal{M}_\infty$ is the Banach space $\mathcal{M}_1$ of matrices $(d_{n,m})$ for which $\Sigma_{n,m=0}^{\infty} |d_{n,m}| < \infty$. A matrix $(d_{n,m}) \in \mathcal{M}_\infty$ has an inverse if and only if $d_{n,m} \neq 0$ for all $n, m \in \mathbb{N}$. The inverse is $(d_{n,m}^{-1})$. A matrix $(d_{n,m}) \in \mathcal{M}_\infty$ is positive if $d_{n,m} \geqslant 0$ for all $n, m \in \mathbb{N}$. However, we are not interested in this standard positivity; we rather study positive semidefinitess of matrices.

The positive semidefinite matrices of $\mathcal{M}_\infty$ form a convex cone. We denote it by $\mathcal{M}_\infty^+$. Any $(d_{n,m}) \in \mathcal{M}_\infty^+$ defines a covariant positive operator measure E via Eq. (6). The phase matrices are such matrices of $\mathcal{M}_\infty^+$ whose diagonal elements equal 1. Let $\mathcal{C}$ be the σ-convex set of phase matrices.[13] Phase matrices define phase observables. The phase matrices of phase observables unitarily equivalent to E_{can} are only phase matrices which have phase matrix inverses. Note that $\mathcal{C}^* = \mathcal{C}$, and for all $(c_{n,m}) \in \mathcal{C}$ the norm $\|(c_{n,m})\| = 1$, that is, all phase matrices lie on the unit ball.

We can embed the bounded operators, trace-class operators, and states in $\mathcal{M}_\infty$. We simply define

$$\mathcal{L} := \left\{ (A_{n,m}) \in \mathcal{M}_\infty \,\middle|\, \sum_{n,m=0}^{\infty} A_{n,m} |n\rangle\langle m| \in \mathcal{L}(\mathcal{H}) \right\},$$

$$\mathcal{T} := \left\{ (T_{n,m}) \in \mathcal{M}_\infty \,\middle|\, \sum_{n,m=0}^{\infty} T_{n,m} |n\rangle\langle m| \in \mathcal{T}(\mathcal{H}) \right\},$$

$$\mathcal{T}_1^+ := \left\{ (T_{n,m}) \in \mathcal{M}_\infty \,\middle|\, \sum_{n,m=0}^{\infty} T_{n,m} |n\rangle\langle m| \in \mathcal{T}(\mathcal{H})_1^+ \right\}.$$

Thus, $\mathcal{T}_1^+$ contains such $(T_{n,m}) \in \mathcal{M}_\infty^+$ for which $\Sigma_{n=0}^{\infty} T_{n,n} = 1$. Note that $\mathcal{T} \cap \mathcal{C} = \varnothing$ and $\mathcal{C} \nsubseteq \mathcal{L} \neq \mathcal{M}_\infty$.

As we saw in the previous section, for any phase matrix $(c_{n,m})$ and a state $(T_{n,m})$ the product $(c_{n,m}) \star (T_{n,m})$ is a state. Thus, $\mathcal{C} \star \mathcal{T}_1^+ = \mathcal{T}_1^+$. An operation Θ defined in (4) corresponds a mapping $\mathcal{T} \ni (T_{n,m}) \mapsto (c_{m,n}) \star (T_{n,m}) \in \mathcal{T}$, $(c_{n,m}) \in \mathcal{C}$, which is continuous with respect to the trace-norm. If Θ_1 and Θ_2 are the operations [defined in (4)] of phase observables E_1 and E_2 with $(c_{n,m}^1)$ and $(c_{n,m}^2)$, respectively, then the matrix $(c_{m,n}^1) \star (c_{m,n}^2)$ corresponds to the composition operation $\Theta_1 \circ \Theta_2$. Note that $\Theta_1 \circ \Theta_2 = \Theta_2 \circ \Theta_1$.

Let $(d_{n,m})$ and $(e_{n,m})$ be elements of $\mathcal{M}_\infty^+$. Now there exist vector sequences $(\varphi_n)_{n\in\mathbb{N}}$ and $(\psi_n)_{n\in\mathbb{N}}$ such that $d_{n,m} = \langle \varphi_n | \varphi_m \rangle$ and $e_{n,m} = \langle \psi_n | \psi_m \rangle$ for all $n, m \in \mathbb{N}$.[3] Now $d_{n,m} e_{n,m} = \langle \varphi_n \otimes \psi_n | \varphi_m \otimes \psi_m \rangle$, $n, m \in \mathbb{N}$, and $(d_{n,m}) \star (e_{n,m})$ is positive semidefinite.[14] Hence, $\mathcal{M}_\infty^+ \star \mathcal{M}_\infty^+ = \mathcal{M}_\infty^+$ and $\mathcal{C} \star \mathcal{C} = \mathcal{C}$.

Let $(d_{n,m}) \in \mathcal{M}_\infty^+$. Now we can write $d_{n,m} = \Sigma_{k=0}^{\infty} d_{n,m}^{(k)}$ where $d_{n,m}^{(k)} = \langle n | F_k \rangle \langle F_k | m \rangle$ for all $n, m \in \mathbb{N}$, and $|F_k) \in \mathcal{H}_\infty$, $k \in \mathbb{N}$. Hence, the finite sums of matrices $(\langle n|F)(F|m\rangle)_{n,m\in\mathbb{N}}$, $|F) \in \mathcal{H}_\infty$ form a dense subset of $\mathcal{M}_\infty^+$. Every $|F) \in \mathcal{H}_\infty$ defines a covariant positive operator measure E_F of Eq. (2).

Following Ref. 10, we can define a certain ordering relation on $\mathcal{M}_\infty$ as follows: $(d_{n,m}) \preccurlyeq (e_{n,m})$ if $(d_{n,m}) = (e_{n,m}) \star (f_{n,m})$ for some $(f_{n,m}) \in \mathcal{M}_\infty$. Let $(1)_{n,m\in\mathbb{N}}$ and $(\delta_{n,m})_{n,m\in\mathbb{N}}$ be the

phase matrices of the canonical and the trivial phase observables, respectively. Now $(d_{n,m})_{n,m\in\mathbb{N}} \preccurlyeq (1)_{n,m\in\mathbb{N}}$ for all $(d_{n,m})\in\mathcal{M}_\infty$ and $(\delta_{n,m}) \preccurlyeq (c_{n,m})$ for all $(c_{n,m})\in\mathcal{C}$. Note that $\preccurlyeq$ is not a partial ordering. It does not satisfy the antisymmetry condition.

Define the following equivalence relation in $\mathcal{C}$:

$$(c_{n,m}) \simeq (d_{n,m}) \quad \text{if } (c_{n,m}) = (d_{n,m}) \star (e^{i(v_n - v_m)}), \quad (v_n)_{n\in\mathbb{N}} \subset [0, 2\pi).$$

Denote the equivalence class of $(c_{n,m})\in\mathcal{C}$ by $[(c_{n,m})]$, and define a partial ordering $\preccurlyeq$ in the set of equivalence classes as follows: $[(c_{n,m})] \preccurlyeq [(d_{n,m})]$ if $(c_{n,m}) = (d_{n,m}) \star (e_{n,m})$ for some $(e_{n,m}) \in \mathcal{C}$. Now $[(\delta_{n,m})] \preccurlyeq [(c_{n,m})] \preccurlyeq [(1)]$ for all $(c_{n,m})\in\mathcal{C}$ and, thus, the equivalence class of the canonical phase matrix is the upper bound.

V. ON THE POINTWISE CONVERGENCE OF PHASE KERNELS

As we have seen, a phase observable E is determined uniquely by a phase matrix $(c_{n,m})$ via Eq. (1). For any trace-class operator T we can define a complex measure $X \mapsto p_T^E(X) := \mathrm{tr}(TE(X))$ which is absolutely continuous with respect to the normalized Lebesgue measure and, thus, has a Radon–Nikodým derivative g_T^E such that $p_T^E(X) = (2\pi)^{-1} \int_X g_T^E(\theta)\mathrm{d}\theta$, $X \in \mathcal{B}([0,2\pi))$. Following Eq. (1) it is tempting to write $g_T^E(\theta) = \sum_{n,m=0}^\infty T_{m,n} c_{n,m} e^{i(n-m)\theta}$ where the summation converges pointwise for $\mathrm{d}\theta$-almost all $\theta\in\mathbb{R}$. But is it possible? In this section we study this problem.

Let us start with the simplest case. Let E be the canonical phase, and let $T = |\varphi\rangle\langle\psi|$ where $\varphi, \psi \in \mathcal{H}$. From the Carleson theorem[15] we know that any L^2-Fourier series converges pointwise for almost all $\theta\in\mathbb{R}$. Thus, we get

$$g^{E_{\mathrm{can}}}_{|\varphi\rangle\langle\psi|}(\theta) = \sum_{n=0}^\infty \langle\psi|n\rangle e^{in\theta} \sum_{m=0}^\infty \langle m|\varphi\rangle e^{-im\theta} = \sum_{n,m=0}^\infty \langle m|\varphi\rangle\langle\psi|n\rangle e^{i(n-m)\theta}$$

for almost all $\theta\in\mathbb{R}$. Let then T be an arbitrary trace-class operator, and let E be any phase observable with the covariant trace-preserving operation Φ of Theorem 3. Now we can write $\Phi(T) = T_\alpha - T_\beta + iT_\gamma - iT_\delta$ where the operators T_u are positive trace-class operators with decompositions $T_u = \sum_{k=0}^\infty |\varphi_k^{(u)}\rangle\langle\varphi_k^{(u)}|$, $\varphi_k^{(u)} \in \mathcal{H}$, $k\in\mathbb{N}$, where $u = \alpha, \beta, \gamma, \delta$. Thus,

$$g_T^E(\theta) = g^{E_{\mathrm{can}}}_{T_\alpha}(\theta) - g^{E_{\mathrm{can}}}_{T_\beta}(\theta) + ig^{E_{\mathrm{can}}}_{T_\gamma}(\theta) - ig^{E_{\mathrm{can}}}_{T_\delta}(\theta)$$

and, by monotonic convergence,

$$g^{E_{\mathrm{can}}}_{T_u}(\theta) = \sum_{k=0}^\infty \sum_{n,m=0}^\infty \langle m|\varphi_k^{(u)}\rangle\langle\varphi_k^{(u)}|n\rangle e^{i(n-m)\theta} \tag{7}$$

for all $u = \alpha, \beta, \gamma, \delta$ and for almost all $\theta\in\mathbb{R}$. We will get a similar equation without using the operation Φ. Namely, by using Theorem 2 one gets for any $|\varphi\rangle\langle\varphi|$

$$g^E_{|\varphi\rangle\langle\varphi|}(\theta) = \sum_{k=0}^\infty \sum_{n,m=0}^\infty \langle\varphi|n\rangle\langle n|F_k)(F_k|m\rangle\langle m|\varphi\rangle e^{i(n-m)\theta} \tag{8}$$

for almost all $\theta\in\mathbb{R}$. A problem of Eqs. (7) and (8) is that it is not clear that we can change the order of k- and (n,m)-sums. So we have to consider other methods.

First we prove a simple proposition. Let B be a complex Banach space, and let $S: \mathcal{H}\times\mathcal{H} \to B$ be a bounded sesquilinear form (the first argument is antilinear), that is, $\|S\| := \sup\{\|S(\varphi,\psi)\| \mid \|\varphi\| \leq 1, \|\psi\| \leq 1\} < \infty$. Note that $\mathcal{T}(\mathcal{H})$ is equipped with the trace norm.

Proposition 1: Denote $S_{n,m} := S(|n\rangle, |m\rangle)$ for all $n, m \in \mathbb{N}$. Then for all $\varphi, \psi \in \mathcal{H}$

$$S(\varphi,\psi)=\lim_{s,t\to\infty}\sum_{n=0}^{s}\sum_{m=0}^{t}S_{n,m}\langle\varphi|n\rangle\langle m|\psi\rangle,$$

that is,

$$S=\sum_{n,m=0}^{\infty}S_{n,m}|n\rangle\langle m|$$

weakly, and S can be uniquely extended to a continuous linear mapping $\tilde{S}\colon\mathcal{T}(\mathcal{H})\to B$,

$$T\mapsto\tilde{S}(T):=\sum_{n,m=0}^{\infty}S_{n,m}T_{m,n}:=\lim_{s,t\to\infty}\sum_{n=0}^{s}\sum_{m=0}^{t}S_{n,m}T_{m,n},$$

where $T_{m,n}:=\langle m|T|n\rangle$, $n,m\in\mathbb{N}$. *Clearly,* $\tilde{S}(|\psi\rangle\langle\varphi|)=S(\varphi,\psi)$ *for all* $\varphi,\psi\in\mathcal{H}$.

Proof: For $\varphi,\psi\in\mathcal{H}$ one gets

$$\|S(\varphi,\psi)-S(P_s\varphi,P_t\psi)\|\leqslant\|S\|\,\|\varphi\|\,\|\psi-P_t\psi\|+\|S\|\,\|\varphi-P_s\varphi\|\,\|P_t\psi\|\to 0$$

when $s,t\to 0$, where $P_s:=\Sigma_{n=0}^{s}|n\rangle\langle n|$. Fix $T\in\mathcal{T}(\mathcal{H})_1^+$. One can write $T=\Sigma_{k=0}^{\infty}\lambda_k|\varphi_k\rangle\langle\varphi_k|$ where $\lambda_k\in[0,1]$, $\Sigma_{k=0}^{\infty}\lambda_k=1$, $\varphi_k\in\mathcal{H}$, and $\|\varphi_k\|=1$ for all $k\in\mathbb{N}$. Define $\alpha^T:=\Sigma_{k=0}^{\infty}\lambda_k S(\varphi_k,\varphi_k)$ and $\alpha_{s,t}^T:=\Sigma_{k=0}^{\infty}\lambda_k S(P_s\varphi_k,P_t\varphi_k)=\Sigma_{n=0}^{s}\Sigma_{m=0}^{t}S_{n,m}T_{m,n}$ which exist since $\Sigma_{k=0}^{\infty}\lambda_k=1$ and $\|S(\varphi,\psi)\|\leqslant\|S\|$ for all vectors φ,ψ with $\|\varphi\|\leqslant 1$, $\|\psi\|\leqslant 1$. Also we see that $\|\alpha^T\|\leqslant\|S\|$. By the dominated convergence theorem

$$\|\alpha^T-\alpha_{s,t}^T\|\leqslant\sum_{k=0}^{\infty}\lambda_k\|S(\varphi_k,\varphi_k)-S(P_s\varphi_k,P_t\varphi_k)\|\leqslant\|S\|\sum_{k=0}^{\infty}\lambda_k(\|\varphi_k-P_t\varphi_k\|+\|\varphi_k-P_s\varphi_k\|)\to 0$$

when $s,t\to\infty$. As we can easily see from the beginning of the proof, the matrix elements $T_{n,m}$ define the operator T uniquely and, thus, $\tilde{S}(T):=\alpha^T$ is well-defined. Since any $T\in\mathcal{T}(\mathcal{H})$ can be uniquely written in the form $T=\alpha T_\alpha-\beta T_\beta+i\gamma T_\gamma-i\delta T_\delta$ where T_α, T_β, T_γ, and T_δ are states, and α, β, γ, and δ are non-negative real numbers, we can define $\tilde{S}(T):=\alpha\tilde{S}(T_\alpha)-\beta\tilde{S}(T_\beta)+i\gamma\tilde{S}(T_\gamma)-i\delta\tilde{S}(T_\delta)$. The rest of the proof follows immediately. □

Note that it follows from Proposition 1 that any bounded operator A can be written in the form $A=\Sigma_{n,m=0}^{\infty}A_{n,m}|n\rangle\langle m|$ (weakly) and $\mathrm{tr}(AT)=\Sigma_{n,m=0}^{\infty}A_{n,m}T_{m,n}$ for any $T\in\mathcal{T}(\mathcal{H})$ where $A_{n,m}:=\langle n|A|m\rangle$, $n,m\in\mathbb{N}$.

Let E be a phase observable with $(c_{n,m})$, and let g_T^E be a Radon–Nikodým derivative of the complex measure p_T^E associated to $T\in\mathcal{T}(\mathcal{H})$. The sesquilinear mapping $\mathcal{H}\times\mathcal{H}\ni(\varphi,\psi)\mapsto g_{|\psi\rangle\langle\varphi|}^E\in L^1[0,2\pi)$ is bounded since by using the polarization identity and the parallelogram law $(2\pi)^{-1}\int_0^{2\pi}|g_{|\psi\rangle\langle\varphi|}^E(\theta)|\mathrm{d}\theta\leqslant\|\psi\|^2+\|\varphi\|^2$ for all $\psi,\varphi\in\mathcal{H}$. From Proposition 1 one gets

$$g_T^E=\sum_{n,m=0}^{\infty}T_{m,n}c_{n,m}e_n\overline{e_m},$$

where $e_n(\theta)=e^{in\theta}$ and the double series converges with respect to the L^1-norm. This implies (Ref. 16, Theorem 3.12, p. 68) the following theorem:

Theorem 5: *There exists a subsequence* $\mathbb{N}\ni k\mapsto n_k\in\mathbb{N}$, $n_1<n_2<n_3<\cdots$, *such that*

$$g_T^E(\theta)=\lim_{k\to\infty}\sum_{n,m=0}^{n_k}T_{m,n}c_{n,m}e^{i(n-m)\theta}$$

for almost all $\theta\in\mathbb{R}$.

It can be shown (Ref. 16, Theorem 7.8, p. 140) that

$$g_T^E(\theta)=2\pi\left.\frac{\mathrm{d}p_T^E[0,x)}{\mathrm{d}x}\right|_{x=\theta}$$

for almost all $\theta\in[0,2\pi)$. Thus, by direct calculation, one gets

$$g_T^E(\theta)=\lim_{\epsilon\to 0+}\sum_{n,m=0}^{\infty}T_{m,n}c_{n,m}e^{i(n-m)\theta}f_{n-m}^{(1)}(\epsilon)$$

for almost all $\theta\in\mathbb{R}$ where $f_k^{(1)}(\epsilon):=(e^{ik\epsilon}-1)/(ik\epsilon)$, $k\neq 0$, and $f_0^{(1)}(\epsilon)=1$. Thus, $\lim_{\epsilon\to 0+}f_k^{(1)}(\epsilon)=1$ for all $k\in\mathbb{Z}$. Also, by a theorem of Fatou (Ref. 17, p. 34), one can show that

$$g_T^E(\theta)=\lim_{\epsilon\to 0+}\sum_{n,m=0}^{\infty}T_{m,n}c_{n,m}e^{i(n-m)\theta}f_{n-m}^{(2)}(\epsilon)$$

for almost all $\theta\in\mathbb{R}$ where $f_k^{(2)}(\epsilon):=(1-\epsilon)^{|k|}$ for all $k\in\mathbb{Z}$ and the double series converges absolutely when $\epsilon\in(0,1]$. Also $\lim_{\epsilon\to 0+}f_k^{(2)}(\epsilon)=1$ for all $k\in\mathbb{Z}$.

Since the operators

$$C_\epsilon^{(j)}:=\sum_{n,m=0}^{\infty}c_{n,m}f_{n-m}^{(j)}(\epsilon)|n\rangle\langle m|,\quad j=1,2,$$

are bounded with $\|C_\epsilon^{(1)}\|\leqslant 2\pi/\epsilon$ and $\|C_\epsilon^{(2)}\|\leqslant 2/\epsilon-1$ for each $\epsilon\in(0,1]$ it follows that

$$g_T^E(\theta)=\lim_{\epsilon\to 0+}\mathrm{tr}[TR(\theta)C_\epsilon^{(j)}R(\theta)^*],\quad j=1,2,$$

for almost all $\theta\in\mathbb{R}$.

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[5] Equip $\mathcal{H}_1$ with the norm $\psi\mapsto\|\psi\|_1:=\Sigma_{n=0}^{\infty}|\langle n|\psi\rangle|$. The continuous linear mappings $\mathcal{H}_1\to\mathbb{C}$ form a topological dual $\mathcal{H}_1'$ of $\mathcal{H}_1$. Using the Dirac notation, an element $(F|\in\mathcal{H}_1'$ can be represented in the form $(F|=\underline{\Sigma_{n=0}^{\infty}f_n}\langle n|$ where $(f_n)_{n\in\mathbb{N}}\subset\mathbb{C}$ and $\sup\{|f_n|\mid n\in\mathbb{N}\}<\infty$. Defining a conjugate form $|F)$ of $(F|$ as a mapping $\mathcal{H}_1\ni\psi\mapsto(F|\psi\rangle\in\mathbb{C}$ we may define the linear space $\mathcal{H}_\infty$ of conjugate forms of the elements of $\mathcal{H}_1'$. Thus, using the Dirac formalism, we may write an element $|G)\in\mathcal{H}_\infty$ of the form $|G)=\Sigma_{n=0}^{\infty}g_n|n\rangle$ where $(g_n)_{n\in\mathbb{N}}\subset\mathbb{C}$ and $\sup\{|g_n|\mid n\in\mathbb{N}\}<\infty$. We can define the following norm in $\mathcal{H}_\infty:|G)\mapsto\||G)\|_\infty:=\sup\{|g_n|\mid n\in\mathbb{N}\}$.
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[14] For any sequence $(f_n)_{n\in\mathbb{N}}\subset\mathbb{C}$ for which $f_n\neq 0$ for only finite many $n\in\mathbb{N}$, the sum $\Sigma_{n,m=0}^{\infty}\overline{f_n}d_{n,m}e_{n,m}f_m = \|\Sigma_{n=0}^{\infty} f_n|\varphi_n\otimes\psi_n\rangle\|^2\geqslant 0$. This shows that $(d_{n,m}e_{n,m})$ is positive semidefinite.

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Quantum superintegrability and exact solvability in *n* dimensions

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A family of maximally superintegrable systems containing the Coulomb atom as a special case is constructed in n-dimensional Euclidean space. Two different sets of n commuting second-order operators are found, overlapping in the Hamiltonian alone. The system is separable in several coordinate systems and is shown to be exactly solvable. It is solved in terms of classical orthogonal polynomials. The Hamiltonian and n further operators are shown to lie in the enveloping algebra of a hidden affine Lie algebra. © *2002 American Institute of Physics.*
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I. INTRODUCTION

We shall consider the stationary Schrödinger equation

$$H\psi = E\psi, \quad H = -\frac{1}{2}\sum_{i=1}^{n}\frac{\partial^2}{\partial x_i^2} + V(x_1,\ldots,x_n) \tag{1}$$

in an n-dimensional Euclidean space E_n. By analogy with classical Hamiltonian mechanics, such a system is called integrable if there exist $n-1$ algebraically independent linear operators X_a satisfying

$$[H,X_a]=0, \quad [X_a,X_b]=0, \quad a,b=1,\ldots,n-1. \tag{2}$$

The system is called "superintegrable" if there exist further k operators $\{Y_1,\ldots,Y_k\}$ commuting with the Hamiltonian

$$[H,Y_j], \quad j=1,\ldots,k, \tag{3}$$

such that the set $\{H,X_1,\ldots,X_n,Y_1,\ldots,Y_k\}$ is algebraically independent. Note that the additional operators Y_i need not commute with the operators X_a nor amongst each other. The number of additional operators satisfies

$$1 \leqslant k \leqslant n-1. \tag{4}$$

For $k=1$ we call the system "minimally superintegrable," for $k=n-1$ it is "maximally superintegrable."

The best known superintegrable systems in E_3 (and also in E_n for any $n \geqslant 2$) are the harmonic oscillator and the hydrogen atom (or Kepler system in classical mechanics). The harmonic oscil-

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lator is superintegrable because of the $su(n)$ algebra of first- and second-order operators commuting with the Hamiltonian.[1,2] The hydrogen atom in E_n is superintegrable, because of the $o(n+1)$ Lie algebra of linear operators commuting with the Hamiltonian.[3–7] In both cases it is possible to choose different subsets of n operators commuting with each other and overlapping only in the Hamiltonian. Each subset corresponds to the separation of variables in the Schrödinger equation in a different system of coordinates.[8]

Characteristic features of these two superintegrable systems are as follows.

(1) In classical mechanics all finite (bounded) trajectories are periodic. Moreover, Bertrand's theorem[9,10] tells us that γ/r and γr^2 are the only spherically symmetric potentials for which all finite trajectories are periodic.
(2) In quantum mechanics these two systems are exactly solvable: their energy levels can be calculated algebraically, as can the degeneracies of these levels. Their eigenfunctions are polynomials in the appropriate variables, multiplied by some overall factor.
(3) These systems are extremely important in physical applications, both in classical and quantum physics.

It makes sense to search systematically for superintegrable systems in classical and quantum mechanics, especially for maximally superintegrable ones. It can be safely assumed that they will all have the above-mentioned properties (1) and (2) and hoped that they will also, to some degree, share property (3).

In searches for superintegrable systems restrictions are imposed on the form of the commuting operators X_a and Y_i. A systematic search in E_2 and E_3 was conducted some time ago.[11–16] The restriction was that all operators involved should be at most of second order. All superintegrable systems satisfying this restriction in E_2 and E_3 were found.[11–16] Four classes of them exist in E_2, five maximally superintegrable ($2n-1=5$ operators commuting with H) and eight minimally superintegrable ones ($n+1=4$ operators) in E_3. These results have been recently extended to two- and three-dimensional spaces of constant curvature and to complex spaces[17–20] and also to certain two-dimensional spaces of nonconstant curvature.[21]

With the restriction to second-order operators all superintegrable systems turned out to be multiseparable, that is, separable in at least two different coordinate systems. In two-dimensional spaces they also turned out to be exactly solvable.[22] By this we mean that their energy spectra can be calculated algebraically (by solving algebraic equations only).[22–24] It was also shown that superintegrable systems are obtained by considering non-Abelian algebras of generalized Lie symmetries.[25]

The purpose of this article is to consider a family of integrable systems in n-dimensional Euclidean space for any n. The family, containing the n-dimensional hydrogen atom as a special case, is introduced in Sec. II, together with a set of $2n-1$ algebraically independent operators, commuting with the Hamiltonian. In Sec. III we solve the Schrödinger equation in parabolic and spherical coordinates and show that it is exactly solvable in a precise and well-defined sense.[22–24] Finally, in Sec. IV we introduce parabolic rotational coordinates in E_n and solve the Schrödinger equation in these coordinates and also in spherical ones. We also prove the exact solvability in this case. Some conclusions are drawn in Sec. 5.

II. A FAMILY OF MAXIMALLY SUPERINTEGRABLE SYSTEMS IN E_n CONTAINING THE HYDROGEN ATOM

Let us first consider the hydrogen atom in n-dimensional Euclidean space E_n,

$$H=-\frac{1}{2}\Delta-\frac{\gamma}{r},\quad \Delta=\sum_{i=1}^{n}\frac{\partial^2}{\partial x_i^2},\quad r=(x_1^2+\cdots+x_n^2)^{1/2}. \tag{5}$$

This Hamiltonian commutes with $n(n+1)/2$ linear operators, namely

$$L_{ik}=x_i\frac{\partial}{\partial x_k}-x_k\frac{\partial}{\partial x_i},\quad 1\leqslant i<k\leqslant n,$$
$$A_i=\frac{1}{2}\sum_{a=1}^{n}(p_aL_{ia}+L_{ia}p_a)+\gamma\frac{x_i}{r},\quad 1\leqslant i\leqslant n \tag{6}$$

with $p_i=\partial_{x_i}$. The operators L_{ik} correspond to angular momentum, A_i to the n-dimensional Laplace–Runge–Lenz vector, characterizing the Coulomb or Kepler problem.[6,10] Only $2n-1$ of the operators $\{H,L_{ik},A_i\}$ can be, and are, algebraically independent. They satisfy the commutation relations

$$[H,L_{ik}]=[H,A_i]=0,$$
$$[L_{ij},L_{ab}]=\delta_{ja}L_{ib}+\delta_{ib}L_{ja}-\delta_{ia}L_{jb}-\delta_{jb}L_{ia},$$
$$[L_{ij},A_k]=\delta_{jk}A_i-\delta_{ik}A_j, \tag{7}$$
$$[A_i,A_j]=-2HL_{ij}.$$

The commutation relations (7) in general correspond to a Kac–Moody algebra.[26,27] For a fixed energy, $H=E$ they correspond to the Lie algebra of the rotation group $O(n+1)$, the Lorentz group $O(n,1)$, and the Euclidean group $E(n)$ for $E<0$, $E>0$ and $E=0$, respectively. These symmetries for $n=3$ were discovered implicitly by Pauli[3] and explicitly by Fock[4] and Bargmann.[5]

According to the operator approach to the separation of variables,[28–33] separation of variables in the Schrödinger equation is achieved by looking for eigenfunctions of a complete set of n commuting second-order operators $\{H,X_1,\ldots,X_{n-1}\}$,

$$H\psi=E\psi,\quad X_a\psi=\lambda_a\psi,\quad a=1,\ldots,n-1. \tag{8}$$

The operators X_a will be at most linear in A_i and bilinear in L_{ik}. If more than one inequivalent set of commuting operators exists, the system is multiseparable, i.e., separable in more than one coordinate system.

In view of the commutation relations (7) any set of commuting operators $\{X_i\}$ can contain at most one operator involving A_i:

$$X=\sum_i a_iA_i+\sum_{i,k,j,m}b_{ik,jm}L_{ik}L_{jm},\quad \sum_{i=1}^{n}a_i^2\neq 0. \tag{9}$$

The complete sets of commuting operators can be classified under the action of $O(n)$; in particular we can rotate and normalize so as to have $a_n=1$, $a_k=0$ for $k=1,\ldots,n-1$. Here we just give the example of the case $n=3$. It is easy to verify by a direct calculation that in this case, precisely four inequivalent sets exist: $\{H,X_1,X_2\}$ with

$$X_1=A_3,\quad X_2=L_{12}^2, \tag{10}$$
$$X_1=A_3+a(L_{12}^2+L_{23}^2+L_{31}^2),\quad X_2=L_{12}^2, \tag{11}$$
$$X_1=L_{12}^2+L_{23}^2+L_{31}^2,\quad X_2=L_{12}^2, \tag{12}$$
$$X_1=L_{12}^2+L_{23}^2+L_{31}^2,\quad X_2=L_{23}^2+fL_{31}^2. \tag{13}$$

They correspond to the separation of variables in parabolic rotational coordinates, shifted spheroidal coordinates, spherical coordinates, and spheroconical coordinates, respectively.

In each coordinate system it is possible to add further terms to the potential $-\gamma/r$ in such a manner that the Schrödinger equation still separates. The system will remain integrable and the corresponding operators X_1 and X_2 will only be modified by the addition of a scalar function. It is also possible to preserve superintegrability and to require that the extended potentials should allow separation of variables in at least two coordinate systems.

Here we will be interested in the most general potential allowing separation of variables in the same four coordinate systems as the hydrogen atom itself. In E_3 there is, up to equivalence, only one such Hamiltonian, namely (see Refs. 13 and 14)

$$H=-\frac{1}{2}\Delta-\frac{\gamma}{r}+\frac{\beta_1}{x_1^2}+\frac{\beta_2}{x_2^2}. \tag{14}$$

One triplet of commuting operators for the Hamiltonian (14) consists of

$$\begin{aligned} X&=\frac{1}{2}(p_1L_{31}+L_{31}p_1+p_2L_{32}+L_{32}p_2)+2x_3\left(\frac{\gamma}{2r}-\frac{\beta_1}{x_1^2}-\frac{\beta_2}{x_2^2}\right),\\ Z&=L_{12}^2-2r^2\left(\frac{\beta_1}{x_1^2}+\frac{\beta_2}{x_2^2}\right). \end{aligned} \tag{15}$$

Another triplet can be chosen to be H and

$$\begin{aligned} Y_1&=L_{12}^2+L_{23}^2+L_{31}^2-2r^2\left(\frac{\beta_1}{x_1^2}+\frac{\beta_2}{x_2^2}\right),\\ Y_2&=L_{23}^2-2\beta_2\frac{x_2^2+x_3^2}{x_2^2}. \end{aligned} \tag{16}$$

It is the set of five algebraically independent operators $\{H,X_1,X_2,Y_1,Y_2\}$ which guarantees that the Hamiltonian (14) is maximally superintegrable.

The generalization to the n-dimensional Euclidean space E_n is immediate. Thus, the Hamiltonian will be

$$H=-\frac{1}{2}\Delta-\frac{\gamma}{r}+\sum_{i=1}^{n-1}\frac{\beta_i}{x_i^2} \tag{17}$$

with Δ and r as in Eq. (5). One of the two different complete sets of commuting operators can be chosen to be H and

$$\begin{aligned} X&=\frac{1}{2}\sum_{k=1}^{n-1}(L_{nk}p_k+p_kL_{nk})+2x_n\left(\frac{\gamma}{2r}-\sum_{i=1}^{n-1}\frac{\beta_i}{x_i^2}\right),\\ Z_l&=\sum_{1\leqslant i<k\leqslant l+1}L_{ik}^2-2\left(\sum_{i=1}^{l+1}x_i^2\right)\left(\sum_{k=1}^{l+1}\frac{\beta_k}{x_k^2}\right),\quad 1\leqslant l\leqslant n-2. \end{aligned} \tag{18}$$

Another complete set of commuting operators is again H and

$$Y_p=\sum_{p\leqslant i<k\leqslant n}L_{ik}^2-2\left(\sum_{i=p}^{n}x_i^2\right)\left(\sum_{k=p}^{n-1}\frac{\beta_k}{x_k^2}\right),\quad 1\leqslant p\leqslant n-1. \tag{19}$$

The two sets (18) and (19) are disjoint. If we set $\beta_i=0, 1\leqslant i\leqslant n-1$, then the operator Z_l will be a Casimir operator of the group $O(l+1)$ acting on the coordinates $\{x_1,\ldots,x_{l+1}\}$. The operator Y_p will be a Casimir operator of $O(n+1-p)$ acting on the coordinates $\{x_p,\ldots,x_n\}$.

It is the Hamiltonian (17) that we shall study in the following sections, first for $n=3$, then for arbitrary n.

III. EXACT SOLVABILITY OF THE SUPERINTEGRABLE SYSTEM FOR $n=3$

A. Solution by separation of variables

Let us first consider the Hamiltonian (14) and the complete set of commuting operators (15). We are looking for eigenvalues and common eigenfunctions of the systems:

$$H\psi=E\psi, \quad X\psi=\lambda\psi, \quad Z\psi=k\psi. \tag{20}$$

To do this we introduce parabolic rotational coordinates, putting

$$x_1=\mu\nu\cos\phi, \quad x_2=\mu\nu\sin\phi, \quad x_3=\tfrac{1}{2}(\mu^2-\nu^2). \tag{21}$$

In these coordinates the operators in (20) are

$$\begin{aligned} H&=-\frac{1}{2(\mu^2+\nu^2)}\left(\frac{\partial^2}{\partial\mu^2}+\frac{1}{\mu}\frac{\partial}{\partial\mu}+\frac{\partial^2}{\partial\nu^2}+\frac{1}{\nu}\frac{\partial}{\partial\nu}+4\gamma\right)-\frac{1}{2\mu^2\nu^2}\left(\frac{\partial^2}{\partial\phi^2}-\frac{2\beta_1}{\cos^2\phi}-\frac{2\beta_2}{\sin^2\phi}\right)\\ X&=\frac{1}{2(\mu^2+\nu^2)}\left(-\nu^2\left(\frac{\partial^2}{\partial\mu^2}+\frac{1}{\mu}\frac{\partial}{\partial\mu}\right)+\mu^2\left(\frac{\partial^2}{\partial\nu^2}+\frac{1}{\nu}\frac{\partial}{\partial\nu}\right)+2\gamma(\mu^2-\nu^2)\right)\\ &\quad+\frac{\mu^2-\nu^2}{2\mu^2\nu^2}\left(\frac{\partial^2}{\partial\phi^2}-\frac{2\beta_1}{\cos^2\phi}-\frac{2\beta_2}{\sin^2\phi}\right)\\ Z&=\frac{\partial^2}{\partial\phi^2}-\frac{2\beta_1}{\cos^2\phi}-\frac{2\beta_2}{\sin^2\phi}. \end{aligned} \tag{22}$$

We see immediately that the variables separate and we can solve the corresponding ordinary differential equations to obtain

$$\begin{aligned} \psi_{N_1,N_2,J}&=(\sin\phi)^{p_2}(\cos\phi)^{p_1}(\mu\nu)^m e^{-\sqrt{-E/2}(\mu^2+\nu^2)}\\ &\quad\times P_J^{(p_2-1/2,p_1-1/2)}(\cos 2\phi)L_{N_1}^m(\sqrt{-2E}\,\mu^2)L_{N_2}^m(\sqrt{-2E}\,\nu^2), \end{aligned} \tag{23}$$

where $P_J^{(\alpha,\beta)}(z)$ and $L_N^m(x)$ are Jacobi and Laguerre polynomials, respectively. We have put

$$\beta_i=\tfrac{1}{2}p_i(p_i-1), \quad m=2J+p_1+p_2$$

and the eigenvalues in Eq. (20) are equal to

$$\begin{aligned} E&=-\frac{\gamma^2}{2(N_1+N_2+2J+p_1+p_2+1)^2},\\ \lambda&=-\frac{\gamma(N_1-N_2)}{N_1+N_2+2J+p_1+p_2+1},\\ k&=-m^2=-(2J+p_1+p_2)^2. \end{aligned} \tag{24}$$

We see that the bound state energy is given by a shifted Balmer formula and the only effect of the β_i/x_i^2 terms in the potential is to add a constant p_1+p_2 to the principal quantum number. The

solutions (23) are square integrable and correspond to bound states when J, N_1, and N_2 are integers. They are polynomials multiplied by a factor which, however, is not "universal." It depends on the energy E and also on the angular quantum number J (since we have $m=2J+p_1+p_2$).

The second set of commuting operators, namely (16), also corresponds to the separation of variables, this time in spherical coordinates, chosen as

$$x_1=r\cos\theta, \quad x_2=r\sin\theta\cos\alpha, \quad x_3=r\sin\theta\sin\alpha. \tag{25}$$

In these coordinates we have

$$H\psi=-\frac{1}{2}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\alpha^2}\right)+\frac{2\gamma}{r}-\frac{2}{r^2}\left(\frac{\beta_1}{\cos^2\theta}+\frac{\beta_2}{\sin^2\theta\cos^2\alpha}\right)\right]\psi$$
$$=E\psi,$$

$$Y_1\psi=\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}-\frac{2\beta_1}{\cos^2\theta}+\frac{k_2}{\sin^2\theta}\right)\psi=k_1\psi, \tag{26}$$

$$Y_2\psi=\left(\frac{\partial^2}{\partial\alpha^2}-\frac{2\beta_2}{\cos^2\alpha}\right)\psi=k_2\psi.$$

The coordinates separate and we obtain $\psi=R(r)F(\theta)G(\alpha)$ where F and G can be expressed in terms of Jacobi polynomials and R in terms of Laguerre ones.

The explicit expression for the eigenfunctions in this type of spherical coordinates is

$$\psi_{N,J_1,J_2}(r,\theta,\alpha)=r^{m_1-1/2}e^{-\sqrt{-2E}\,r}L_N^{2m_1}(2\sqrt{-2E}\,r)(\sin\theta)^{m_1}(\cos\theta)^{p_1}(\cos\alpha)^{p_2}$$
$$\times P_{J_1}^{(m_2,p_1-1/2)}(\cos 2\theta)P_{J_2}^{(-1/2,p_2-1/2)}(\cos 2\alpha) \tag{27}$$

with eigenvalues equal to

$$E=-\frac{\gamma^2}{2(N+2J_1+2J_2+p_1+p_2+1)^2},$$
$$k_1=\tfrac{1}{4}-m_1^2, \quad k_2=-m_2^2, \quad m_1=2J_1+2J_2+p_1+p_2+\tfrac{1}{2}, \quad m_2=2J_2+p_2. \tag{28}$$

B. Exact solvability and underlying affine Lie algebra

We have established that the potential (14) provides a Hamiltonian that is maximally superintegrable and multiseparable. Let us now turn to the question of exact solvability. A Hamiltonian is exactly solvable if its spectrum can be calculated algebraically. This occurs if it can be explicitly transformed into block diagonal form where each block is finite dimensional. This in turn means that there exists an infinite flag of finite dimensional subspaces in the Hilbert space $\mathcal{H}$ of bound state solutions that is preserved by the Hamiltonian[22–24]

$$\mathcal{H}_1\subset\mathcal{H}_2\subset\cdots\subset\mathcal{H}, \quad H\mathcal{H}_i\subseteq\mathcal{H}_i. \tag{29}$$

Typically this occurs under the following circumstances.

(1) The bound state wave functions are polynomials in some variables, possible multiplied by some factor g, i.e., $\psi=gP$. We then have

$$h=g^{-1}Hg, \quad hP=EP, \tag{30}$$

that is, there exists a gauge transformation and a change of variables to a new Hamiltonian h that has polynomial eigenfunctions.

(2) The gauge transformed Hamiltonian h is an element of the enveloping algebra of some affine Lie algebra L, a basis of which can be realized by the operators

$$K_i=\frac{\partial}{\partial s_i},\quad M_{ik}=s_i\frac{\partial}{\partial s_k},\quad i,k\in\{1,\ldots,n\} \tag{31}$$

(in some coordinates s_i).

Let us now investigate the Hamiltonian (14) and the commuting set of operators (15) and (16) from this point of view.

Consider the wave function (23) in parabolic coordinates. They do have the required form

$$\psi_{N_1,N_2,J}=gP_{N_1,N_2,J}(s,t,z),\quad s=\sqrt{-2E}\,\mu^2,\quad t=\sqrt{-2E}\,\nu^2,\quad z=\cos 2\phi,$$
$$g=\left(\frac{1+z}{2}\right)^{p_1/2}\left(\frac{1-z}{2}\right)^{p_2/2}\left(\frac{s\,t}{-2E}\right)^{m/2}e^{-(s+t)/2}, \tag{32}$$

where P is a polynomial (a product of three polynomials in one variable each). To proceed further we must get rid of the conformal factor $(\mu^2+\nu^2)^{-1}$ figuring in Eq. (22) and replace the system (20) by

$$Q_0\psi=2\gamma\psi,\quad Q_1\psi=2\lambda\psi,\quad Z\psi=-m^2\psi \tag{33}$$

$$Q_0=(\mu^2+\nu^2)(H-E)+2\gamma=-\frac{1}{2}\left(\frac{\partial^2}{\partial\mu^2}+\frac{1}{\mu}\frac{\partial}{\partial\mu}+\frac{\partial^2}{\partial\nu^2}+\frac{1}{\nu}\frac{\partial}{\partial\nu}\right)+\frac{m^2}{2}\left(\frac{1}{\mu^2}+\frac{1}{\nu^2}\right)-E(\mu^2+\nu^2),$$

$$Q_1=2X+(\mu^2-\nu^2)(H-E)=-\frac{1}{2}\left(\frac{\partial^2}{\partial\mu^2}+\frac{1}{\mu}\frac{\partial}{\partial\mu}-\frac{\partial^2}{\partial\nu^2}-\frac{1}{\nu}\frac{\partial}{\partial\nu}\right)+\frac{m^2}{2}\left(\frac{1}{\mu^2}-\frac{1}{\nu^2}\right)-E(\mu^2-\nu^2),$$

$$Q_2=Z.$$

We see here a phenomenon which has been called ''metamorphosis'' [34] or ''migration'' [22] of the coupling constant. In Eq. (33) the energy E plays the role of the frequency of a harmonic oscillator whereas the Coulomb coupling constant γ plays the role of an eigenvalue of Q_0. The other eigenvalues, λ and m^2, remain eigenvalues (of Q_1 and Z, respectively).

Similarly as in the case of potentials containing the Coulomb atom as a special case in two dimensions, it is the system (33) [rather than the original system (20)] that is exactly solvable in the sense defined above. Indeed, let us gauge rotate the operators Q_0, Q_1, and Q_2 and transform to the variables s, t, and z. We obtain

$$\tilde{Q}_0=g^{-1}Q_0g=-2\sqrt{-2E}(s\partial_s^2+(m+1-s)\partial_s+t\partial_t^2+(m+1-t)\partial_t-m-1),$$

$$\tilde{Q}_1=g^{-1}Q_1g=-2\sqrt{-2E}(s\partial_s^2+(m+1-s)\partial_s-t\partial_t^2-(m+1-t)\partial_t), \tag{34}$$

$$\tilde{Q}_2=g^{-1}Q_2g=4(1-z^2)\partial z^2+4(p_1-p_2-(p_1+p_2+1)z)\partial_z-(p_1+p_2)^2.$$

We see that $\tilde{Q}_\mu$, $\mu=0,1,2$ lie in the enveloping algebra of the direct sum of three affine Lie algebras, $\mathrm{saff}(1,\mathbf{R})\oplus\mathrm{saff}(1,\mathbf{R})\oplus\mathrm{saff}(1,\mathbf{R})$, realized by

$$\{\partial_s,s\partial_s,\partial_t,t\partial_t,\partial_z,z\partial_z\}. \tag{35}$$

Now let us consider the two remaining operators Y_1 and Y_2 of (26). They are not diagonal in the basis that we use (where H,X,Z and equivalently Q_0,Q_1,Q_2 are diagonal). They do, however, commute with the Hamiltonian so they can only mix states of equal energy. We also have

$$[Y_1,Z]=0, \quad [Y_2,Z]\neq 0, \quad [Y_1,X]\neq 0. \tag{36}$$

It follows that Y_1 also preserves the quantum number $k=-m^2$ of Eq. (20), whereas Y_2 mixes all states of a given energy. The gauge factor g depends not only on the energy, but also on m, the eigenvalue of Z. Thus, $\tilde{Y}_1=g^{-1}Y_1g$ should transform polynomials into polynomials, whereas $\tilde{Y}_2=g^{-1}Y_2g$ is not obliged to. Performing the gauge transformation and change of variables we find

$$\tilde{Y}_1=g^{-1}Y_1g=s\,t(\partial_s-\partial_t)^2-(m+1)(s-t)(\partial_s-\partial_t)-m(m+1). \tag{37}$$

The algebra underlying this expression includes $t\partial_s$ and $s\partial_t$, in addition to the elements listed in (35). We recognize this to be the Lie algebra saff(2,**R**)$\oplus$saff(1,**R**)

Superintegrable systems, including the hydrogen atom as special case, in two dimensions were associated with the algebra saff(2,**R**). The extension to $n=3$ is seen to lead to saff(2,**R**) $\oplus$saff(1,**R**), not to saff(3,**R**) as one might have expected. It follows from expression (37) that $\tilde{Y}_1$ will take polynomials into polynomials and indeed we have

$$\begin{aligned}\tilde{Y}_1P_{N_1,N_2,J}=&-[2N_1N_2+(N_1+N_2+m)(m+1)]P_{N_1,N_2,J}+(N_1+m)(N_2+1)P_{N_1-1,N_2+1,J}\\&+(N_1+1)(N_2+m)P_{N_1+1,N_2-1,J}.\end{aligned} \tag{38}$$

The operator $\tilde{Y}_2$ does not take polynomials into polynomials and cannot be written as an element of the enveloping algebra of an affine Lie algebra.

The one-dimensional equations appearing above are easily shown to be related to the standard types in the classification of exact and quasiexact solvable one-dimensional systems.[35,36]

IV. EXACT SOLVABILITY OF THE SUPERINTEGRABLE SYSTEM IN E_n

A. Solution by separation of variables

We now consider the Hamiltonian (17) for arbitrary n. It allows separation of variables in many coordinate systems. We shall use parabolic rotational coordinates corresponding to the set of operators (18) and spherical ones corresponding to the set (19). The parabolic coordinates $(\mu,\nu,\theta_1,\ldots,\theta_{n-2})$ are defined by

$$\begin{aligned}x_1&=\mu\nu\cos\theta_1\cos\theta_2\cdots\cos\theta_{n-3}\cos\theta_{n-2},\\x_2&=\mu\nu\cos\theta_1\cos\theta_2\cdots\cos\theta_{n-3}\sin\theta_{n-2},\\x_3&=\mu\nu\cos\theta_1\cos\theta_2\cdots\sin\theta_{n-3},\\&\vdots\\x_{n-2}&=\mu\nu\cos\theta_1\sin\theta_2,\\x_{n-1}&=\mu\nu\sin\theta_1,\\x_n&=\tfrac{1}{2}(\mu^2-\nu^2).\end{aligned} \tag{39}$$

We put $\beta_i=p_i(p_i-1)/2$ in Eq. (17). The eigenvalue problem that we have to solve is

$$H\psi=E\psi, \quad X\psi=\lambda\psi, \quad Z_l\psi=k_l\psi, \quad 1\leqslant l\leqslant n-2. \tag{40}$$

In parabolic coordinates the operators H and X will involve all variables, the operators Z_l will involve the angles only. Indeed, we have

$$H=-\frac{1}{2(\mu^2+\nu^2)}\left(\frac{\partial^2}{\partial\mu^2}+\frac{n-2}{\mu}\frac{\partial}{\partial\mu}+\frac{\partial^2}{\partial\nu^2}+\frac{n-2}{\nu}\frac{\partial}{\partial\nu}\right)-\frac{2\gamma}{\mu^2+\nu^2}-\frac{1}{2\mu^2\nu^2}\left[\Delta(S_{n-2})\right.$$
$$\left.-\frac{p_1(p_1-1)}{\cos^2\theta_1\cdots\cos^2\theta_{n-2}}-\frac{p_2(p_2-1)}{\cos^2\theta_1\cdots\cos^2\theta_{n-3}\sin^2\theta_{n-2}}-\cdots-\frac{p_{n-1}(p_{n-1}-1)}{\sin^2\theta_1}\right] \tag{41}$$

$$X=\frac{1}{2(\mu^2+\nu^2)}\left[-\nu^2\left(\frac{\partial^2}{\partial\mu^2}+\frac{n-2}{\mu}\frac{\partial}{\partial\mu}\right)+\mu^2\left(\frac{\partial^2}{\partial\nu^2}+\frac{n-2}{\nu}\frac{\partial}{\partial\nu}\right)\right]+\gamma\frac{\mu^2-\nu^2}{\mu^2+\nu^2}+\frac{\mu^2-\nu^2}{2\mu^2\nu^2}$$
$$\times\left[\Delta(S_{n-2})-\frac{p_1(p_1-1)}{\cos^2\theta_1\cdots\cos^2\theta_{n-2}}-\frac{p_2(p_2-1)}{\cos^2\theta_1\cdots\cos^2\theta_{n-3}\sin^2\theta_{n-2}}-\cdots-\frac{p_{n-1}(p_{n-1}-1)}{\sin^2\theta_1}\right], \tag{42}$$

where $\Delta(S_{n-2})$ is the Laplace operator on an $n-2$ dimensional sphere.

The operators Z_l satisfy

$$Z_1\psi=\left(\frac{\partial^2}{\partial\theta_{n-2}^2}-\frac{p_1(p_1-1)}{\cos^2\theta_{n-2}}-\frac{p_2(p_2-1)}{\sin^2\theta_{n-2}}\right)\psi=k_1\psi,$$

$$Z_2\psi=\left(\frac{\partial^2}{\partial\theta_{n-3}^2}-\tan\theta_{n-3}\frac{\partial}{\partial\theta_{n-3}}+\frac{k_1}{\cos^2\theta_{n-3}}-\frac{p_3(p_3-1)}{\sin^2\theta_{n-3}}\right)\psi=k_2\psi,$$

and in general

$$Z_l\psi=\left(\frac{\partial^2}{\partial\theta_{n-l-1}^2}-(l-1)\tan\theta_{n-l-1}\frac{\partial}{\partial\theta_{n-l-1}}+\frac{k_{l-1}}{\cos^2\theta_{n-l-1}}-\frac{p_{l+1}(p_{l+1}-1)}{\sin^2\theta_{n-l-1}}\right)\psi=k_l\psi, \tag{43}$$

$$1\leqslant l\leqslant n-2,\quad k_0=-p_1(p_1-1).$$

We write

$$\psi=M(\mu)N(\nu)\prod_{l=1}^{n-2}F_l(\theta_{n-l-1}) \tag{44}$$

and solve (43) to obtain F_l in terms of Jacobi polynomials

$$F_l(\theta_{n-l-1})=(\sin\theta_{n-l-1})^{p_{l+1}}(\cos\theta_{n-l-1})^{m_{l-1}+1-l/2}P_{J_l}^{(p_{l+1}-1/2,m_{l-1})}(\cos 2\theta_{n-l-1}), \tag{45}$$

$$m_l=2\sum_{i=1}^{l}J_i+\sum_{i=1}^{l+1}p_i+\frac{l-1}{2},\quad k_l=\frac{(l-1)^2}{4}-m_l^2. \tag{46}$$

The equations for $M(\mu)$ and $N(\nu)$ are obtained from Eqs. (41) and (42) once the angular part is replaced by k_{n-2}. The final result is that the wave functions are

$$\psi_{N_1,N_2,J_1,J_2,\ldots,J_{n-2}}(\mu,\nu,\theta_1,\ldots,\theta_{n-2})$$
$$=(\mu\nu)^{\sigma}e^{-\sqrt{-E/2}(\mu^2+\nu^2)}\prod_{l=1}^{n-2}(\sin\theta_{n-l-1})^{p_{l+1}}(\cos\theta_{n-l-1})^{m_{l-1}+1-l/2}L_{N_1}^{m_{n-2}}(\sqrt{-2E}\,\mu^2)$$
$$\times L_{N_2}^{m_{n-2}}(\sqrt{-2E}\,\nu^2)\prod_{l=1}^{n-2}P_{J_l}^{(p_{l+1}-1/2,m_{l-1})}(\cos 2\theta_{n-l-1}),\quad \sigma=2\sum_{i=1}^{n-2}J_i+\sum_{i=1}^{n-1}p_i. \tag{47}$$

The energy is given by a shifted Balmer formula

$$E=-\frac{\gamma^2}{2\left(N_1+N_2+2\Sigma_{i=1}^{n-2}J_i+\Sigma_{i=1}^{n-1}p_i+\dfrac{n-1}{2}\right)^2} \tag{48}$$

and the remaining quantum number is

$$\lambda=-\frac{\gamma(N_1-N_2)}{N_1+N_2+2\Sigma_{i=1}^{n-2}J_i+\Sigma_{i=1}^{n-1}p_i+\dfrac{n-1}{2}}. \tag{49}$$

We see that the case of n arbitrary is a straightforward generalization of $n=3$ and involves the same functions, namely, Jacobi and Laguerre polynomials.

Obviously, one can also solve in spherical coordinates. In fact, formulas (39) can be written as

$$x_a=\mu\nu s_a,\quad x_n=\frac{1}{2}(\mu^2-\nu^2),\quad a=1,\ldots,n-1,\quad \sum_{a=1}^{n-1}s_a^2=1 \tag{50}$$

and we could introduce any coordinates on the S_{n-2} sphere that allow separation of variables in the Laplace–Beltrami equation. For a discussion of such coordinate systems see Refs. 33, 37–40.

We will write for the sake of completeness the explicit expression of the eigenfunctions in the following set of spherical coordinates on the S_{n-1} sphere [which are a generalization to dimension n of those we used in the case $n=3$, see Eq. (25)]:

$$\begin{aligned}
x_1&=r\cos\theta_1\\
x_1&=r\sin\theta_1\cos\theta_2\\
&\vdots\\
x_{n-1}&=r\sin\theta_1\cdots\sin\theta_{n-2}\cos\theta_{n-1}\\
x_n&=r\sin\theta_1\cdots\sin\theta_{n-2}\sin\theta_{n-1}
\end{aligned} \tag{51}$$

and the Hamiltonian can be written in these coordinates as

$$H=-\frac{1}{2}\left[\partial_r^2+\frac{n-1}{r}\partial_r+\frac{2\gamma}{r}\right]-\frac{1}{2r^2}\left\{\left[\partial_{\theta_1}^2+(n-2)\cot\theta_1\partial_{\theta_1}-\frac{p_1(p_1-1)}{\cos^2\theta_1}\right.\right.$$
$$+\frac{1}{\sin^2\theta_1}\left[\partial_{\theta_2}^2+(n-3)\cot\theta_2\partial_{\theta_2}-\frac{p_2(p_2-1)}{\cos^2\theta_2}+\cdots+\frac{1}{\sin^2\theta_{n-3}}\left[\partial_{\theta_{n-2}}^2+\cot\theta_{n-2}\partial_{\theta_{n-2}}\right.\right.$$
$$\left.\left.\left.-\frac{p_{n-2}(p_{n-2}-1)}{\cos^2\theta_{n-2}}+\frac{1}{\sin^2\theta_{n-2}}\left[\partial_{\theta_{n-1}}^2-\frac{p_{n-1}(p_{n-1}-1)}{\cos^2\theta_{n-1}}\right]\cdots\right]\right\}. \tag{52}$$

The set of Y_l, $l=1,\ldots,n-1$ operators are:

$$Y_l=\partial_{\theta_l}^2+(n-l-1)\cot\theta_l\partial_{\theta_l}-\frac{p_l(p_l-1)}{\cos^2\theta_l}+\frac{k_{l+1}}{\sin^2\theta_l},\quad l=1,\ldots,n-2,$$
$$Y_{n-1}=\partial_{\theta_{n-1}}^2-\frac{p_{n-1}(p_{n-1}-1)}{\cos^2\theta_{n-1}} \tag{53}$$

and the eigenvalue equations:

$$H\psi=E\psi,\quad Y_lG_l(\theta_l)=k_lG_l(\theta_l),\quad l=1,\ldots,n-1,\quad \psi=R(r)\prod_{l=1}^{n-1}G_l(\theta_l) \tag{54}$$

can be easily solved. The solution for the angular part is ($m_n=-1/2$):

$$\prod_{l=1}^{n-1}G_l(\theta_l)=\prod_{l=1}^{n-1}(\sin\theta_l)^{m_{l+1}+1-(n-l)/2}(\cos\theta_l)^{p_l}P_{J_l}^{(m_{l+1},p_l-1/2)}(\cos 2\theta_l) \tag{55}$$

and for the radial part:

$$R(r)=r^{m_1-(n-2)/2}e^{-\sqrt{-2E}r}L_{N_r}^{2m_1}(2\sqrt{-2E}r). \tag{56}$$

The energy is written as

$$E=-\frac{\gamma^2}{2\left(N_r+2\Sigma_{i=1}^{n-1}J_i+\Sigma_{i=1}^{n-1}p_{n-i}+\frac{1}{2}(n-1)\right)^2} \tag{57}$$

and the eigenvalues of the operators Y_l are

$$k_l=\frac{1}{4}(n-l-1)^2-m_l^2,\quad m_l=2\sum_{i=l}^{n-1}J_i+\sum_{i=l}^{n-1}p_i+\frac{1}{2}(n-l-1),\quad l=1,\ldots,n-1. \tag{58}$$

Finally, the eigenfunctions are

$$\psi_{N,J_1,\ldots,J_{n-1}}(r,\theta_1,\ldots,\theta_{n-1})=r^{m_1-(n-2)/2}e^{-\sqrt{-2E}r}L_{N_r}^{2m_1}(2\sqrt{-2E}r)$$
$$\times\prod_{l=1}^{n-1}\left[(\sin\theta_l)^{m_{l+1}+1-(n-l)/2}(\cos\theta_l)^{p_l}P_{J_l}^{(m_{l+1},p_l-1/2)}(\cos 2\theta_l)\right]. \tag{59}$$

B. Exact solvability

The exact solvability of the system (17) for general n can be treated in the same way as for $n=3$. We can gauge transform each of the operators in the set (18) separately and transform to the variables

$$s=\sqrt{-2E}\,\mu^2, \quad t=\sqrt{-2E}\,\nu^2, \quad z_{n-l+1}=\cos 2\theta_{n-l+1}, \quad l=1,\ldots,n-2. \tag{60}$$

Before doing this, we again introduce Q_0 and Q_1 as in Eq. (33).

The final result is

$$\begin{aligned}
&\tilde{Q}_0+\tilde{Q}_1=g^{-1}(Q_0+Q_1)g=-2\sqrt{-2E}(2s\partial_s^2+2(1+m_{n-2}-s)\partial_s-m_{n-2}-1),\\
&\tilde{Q}_0-\tilde{Q}_1=g^{-1}(Q_0-Q_1)g=-2\sqrt{-2E}(2t\partial_t^2+2(1+m_{n-2}-t)\partial_t-m_{n-2}-1),
\end{aligned} \tag{61}$$

$$\begin{aligned}
\tilde{Z}_l=g^{-1}Z_lg=4(1-z_{n-l-1}^2)\frac{\partial^2}{\partial z_{n-l-1}^2}+4\left(m_{l-1}-p_{l+1}+\frac{1}{2}-\left(p_{l+1}+m_{l-1}+\frac{3}{2}\right)z_{n-l-1}\right)\partial_{z_{n-l-1}}\\
+\frac{l(l-2)}{4}-(m_{l-1}+p_{l+1})(m_{l-1}+p_{l+1}+1).
\end{aligned}$$

We see that the entire set of operators $\{Q_0,Q_1,Z_1,\ldots,Z_{n-2}\}$ lies in the enveloping algebra of direct product of n special affine Lie algebras saff(1,**R**).

Finally let us turn to the other complete set of commuting operators (19), associated with the separation of variables in spherical coordinates. Among these operators there is just one, namely Y_1, that commutes with all the operators Z_l. We have

$$[Y_1,Z_l]=0, \quad [Y_1,X]\neq 0, \quad [Y_p,Z_l]\neq 0, \quad 1\leqslant l\leqslant n-2, \quad 2\leqslant p\leqslant n-1. \tag{62}$$

Thus, $\tilde{Y}_1$ will take polynomials into polynomials but $\{\tilde{Y}_2,\ldots,\tilde{Y}_{n-1}\}$ will not. We have

$$\tilde{Y}_1=g^{-1}\tilde{Y}_1g=s\,t(\partial_s-\partial_t)^2-(m_{n-2}+1)(s-t)(\partial_s-\partial_t)-m_{n-2}(m_{n-2}+1)+\frac{(n-3)(n-1)}{4}. \tag{63}$$

Finally we see that the ''hidden Lie algebra'' that is not a symmetry algebra of the problem, but underlies its exact solvability is saff(2,**R**)$\oplus$[saff(1,**R**)]$_1\oplus\cdots\oplus$[saff(1,**R**)]$_{n-2}$ generated by

$$\{\partial_s,\partial_t,s\partial_s,t\partial_t,s\partial_t,t\partial_s,\partial_{z_1},z_1\partial_{z_1},\ldots,\partial_{z_n-2},z_{n-2}\partial_{z_{n-2}}\}. \tag{64}$$

V. CONCLUSIONS

Superintegrability and exact solvability were defined in completely different ways, though both have a group theoretical underpinning. Superintegrability for a Hamiltonian system is defined by the requirement that there be more integrals of motion than degrees of freedom.[11] It can be characterized by the fact that the corresponding Schrödinger equation allows a non-Abelian algebra of generalized symmetries, containing an n-dimensional Abelian subalgebra.[25] Exact solvability is defined by the requirement that the energy spectrum can be calculated algebraically.[22–24] It can be characterized by the fact that the Hamiltonian lies in the enveloping algebra of a certain type of finite dimensional affine Lie algebra. It was conjectured[22] that all maximally superintegrable systems are exactly solvable. In this article we have confirmed the conjecture for the considered integrable system in E_n.

The exact connection between superintegrability and exact solvability remains an open problem.

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Fiber bundles in quantum physics

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The theory of fiber bundles provides a natural setting for the description of macroscopic quantum systems, wherein their classical and quantum features are represented by actions on the base manifolds and the fibers, respectively, of the relevant bundles. We provide realizations of this picture in the description of (a) quasiparticle excitations of many-body systems, especially those in superfluid helium, (b) the interplay between the microscopic and macroscopic dynamics in certain irreversible processes, such as that of a laser, and (c) local thermodynamic equilibrium. In particular, (b) involves the treatment of a dynamical system which is defined on a vector bundle. © *2002 American Institute of Physics.*
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I. INTRODUCTION

As pointed out by Bohr, the description of a quantum system, Σ, must have a classical component: otherwise, we could not tell our friends what we have observed! A natural way of expressing this basic fact is to represent the classical and essentially quantum features of Σ by actions on the base space M and the fibers Y, respectively, of a fiber bundle B. In fact, this picture has already been employed in Refs. 1–3 for the description of quasiparticle excitations, such as phonons, magnons, etc., in many-particle systems. In the simplest cases, M was the space of Galilei boosts and Y the single particle Hilbert representation space. The natural action of the Galilei group on the bundle $M\times Y$ permitted a simple description of the quasiparticle spectrum and yielded the noteworthy result that the energy, E, and momentum, $\mathbf{p}$, of a phonon in superfluid helium transformed, under boosts of velocity $\mathbf{v}$, according to Landau's formula

$$\mathbf{p}\to\mathbf{p}, \quad E\to E+\mathbf{p}\cdot\mathbf{v}.$$

The object of this article is to enlarge the above-presented picture in two ways. First, we extend the actions on the bundle from groups to semigroups, in order to accommodate a description of the irreversible dynamics of open dissipative systems; and second we obtain a picture of the interplay between the macroscopic (classical) and microscopic (quantum) dynamics of many-particle systems in terms of these actions.

We shall organize our material as follows. In Sec. II, we present a simple sketch of the theory of fiber bundles. In Sec. III, we formulate the action thereon of both groups and semigroups, and in Sec. IV, we apply the resultant theory to the description of quasiparticle excitations in many-particle systems. Here, the key action is that of the Galilei semigroup, as given by the restriction of the Galilei group to non-negative time translations, and this serves to extend the results of Refs. 1–3 to quasiparticles with finite lifetimes.

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The rest of the article is devoted to a demonstration that the interplay between the macroscopic and microscopic properties of many-particle quantum systems may naturally be expressed in terms of actions on fiber bundles. Since dynamics is perceived as a group or semigroup action but studied by infinitesimal (Hamiltonian) methods, we start in Sec. V by obtaining the infinitesimal form of the action of a one-parameter group or semigroup on a product bundle, provided that the action is fiber-preserving. We continue in Sec. VI with a brief sketch of the operator algebraic description of macroscopic quantum systems, including a formulation of local thermodynamic equilibrium conditions. We then turn, in Sec. VII, to a class of open systems, such as the laser model, in which the microscopic evolution is piloted by the macroscopic dynamics (Refs. 4 and 5). Here we show explicitly that the macroscopic-cum-microscopic dynamics of such a system corresponds to the action of a one-parameter semigroup of transformations of the bundle $B=M\times\mathfrak{A}$, where M, the base, is the space of its macroscopic (classical) variables and $\mathfrak{A}$, the fiber, is the $C^\star$-algebra of its microscopic (quantum) observables. Likewise, in Sec. VIII, we show that the local thermodynamic equilibrium conditions of Sec. VI can also be naturally expressed in terms of actions on a fiber bundle.

We conclude in Sec. IX with a brief discussion of the picture presented here and of its possible further ramifications.

Since some readers might not be conversant with both fiber bundles and operator-algebraic quantum theory, we have included brief sketches of these topics in Secs. II and V, respectively.

II. FIBER BUNDLES

A *fiber bundle* $\mathcal{B}=\{B,X,p,G,Y\}$ is, first and foremost, a topological space B which is locally, but not (necessarily) globally, a product. The notation and terminology are suggestive; one can visualize a fiber bundle as a bunch of fibers ''tied together'' by X, the base space. Y is the (abstract) fiber, and $p:B\to X$ a map called the *projection* and, for $x\in X$, the inverse image $Y_x=p^{-1}(x)$ is called the fiber over x. All fibers Y_x are homeomorphic to each other and to Y. G is a topological group, called the group of the bundle, which has an effective action on the fiber.

The space $B=X\times Y$ is a bundle with base X, fiber Y, and projection $p(x,y)=x$. It is called a *trivial bundle* because it is globally a product of the base and the fiber, and G consists only of the identity. The Euclidean plane is also a product, but one needs a coordinate system to display it as a product $X\times Y$. For this reason, it is said to be *equivalent to the product*, and is sometimes called *trivializable*. However, the mathematical literature is not consistent about the use of these terms.

A simple example of a nontrivial bundle is the *Möbius band*, which may be constructed as follows. Take the rectangular strip B_0 in $\mathbb{R}^2$ delimited by the points

$$(a,1),(a,-1),(-a,-1),\quad(-a,1).$$

It is the topological product $B_0=[-a,a]\times[-1,1]$. Now give this strip a twist and glue the short edges together; mathematically, identify the point $[a,-1]$ with $[-a,1]$, and $[a,1]$ with $[-a,-1]$. The twist flips the fibers, which destroys the global product structure. The Möbius band is a nontrivial bundle, with a circle S_1 as base and a real interval, here $[-1,1]$, as fiber. Observe that if glueing had been done without the twist, we would have obtained the cylinder $S_1\times[-1,1]$, which is again a trivial bundle.

The local product (or local triviality) condition in the bundle $\{B,X,p,G,Y\}$ is expressed as follows. There is an open cover $\{V_\alpha\}_{\alpha\in A}$ of X and, for each $\alpha\in A$, a fiber-preserving homeomorphism $\phi_a:p^{-1}(V_\alpha)\to V_\alpha\times Y$; a map $\psi:B_1\to B_2$ between two bundles or subbundles B_1,B_2 is called fiber-preserving if $b,b'\in B_1$, $p_1(b)=p_1(b')$ implies that $p_2(\psi(b))=p_2(\psi(b'))$. The maps ϕ_a are called local trivializations. The local trivializations are glued together to form the bundle, and this is where the group of the bundle G comes in. We shall omit the details, and refer the reader to the standard text of Steenrod (Ref. 6).

The fact that the Möbius band is locally trivial means that, for any open arc C in S_1, there is a fiber-preserving homeomorphism between $p^{-1}(C)$ and $C\times[-1,1]$. S_1 can be covered by two

such arcs C_1 and C_2. In this case the topological group G is the two-element group $\{e,g\}$, where e is the identity and g acts to flip the fibers on one of the two components of the intersection $C_1 \cap C_2$.

A bundle is equivalent to the product if either (1) the base X is paracompact and contractible, or if (2) the base is paracompact and the group G is contractible. Therefore any Banach bundle (a bundle of Banach spaces) on a paracompact and contractible base is equivalent to the product. A stronger result holds for Hilbert bundles,[7] because the group which preserves the inner product structure of an infinite-dimensional Hilbert space (called the ''big'' unitary group) is contractible (Ref. 8). Therefore any Hilbert bundle on a paracompact base is equivalent to the product. All Hilbert and Banach bundles that we shall consider will be equivalent to the product, and may be written as $X \times \mathfrak{K}$, where $\mathfrak{K}$ is a Hilbert space or a Banach space. Their interest would lie in the fact that they bring together two different structures, the differential or symplectic structure of the base space and the linear inner-product or normed space structure of the fiber.

III. ACTIONS OF GROUPS AND SEMIGROUPS ON PRODUCT BUNDLES

A. Principal and associated bundles; the bundle structure theorem

A bundle $\mathcal{B}=\{B,X,p,G,G\}$ is called a *principal bundle* if the fiber is the same as the group, and the group of the bundle acts upon the fiber by left-translations. A bundle $\mathcal{B}'=\{B',X,p,G,Y\}$ is said to be *associated* with the principal bundle $\mathcal{B}$ if the group G acts effectively upon the topological space Y. Note that changing the fiber changes the total space, and therefore the projection. However, we continue to use the same letter to denote the projection in all associated bundles as well. As the context will always be clear, there will be no confusion.

An important result in fiber bundle theory, known as the *bundle structure theorem*, has the following corollary (see Steenrod, Ref. 6, Secs. 7.4 and 7.5): If G is a Lie group and H a (topologically) closed subgroup of G, then G is a principal bundle over the space G/H of left-cosets with respect to the natural projection $p:G \to G/H$ which sends an element of $g \in G$ to its left-coset gH, with group and fiber H: $\mathcal{G}=\{G,G/H,p,H,H\}$.

B. Actions of groups

Any group acts upon itself by left-translations. Therefore any Lie group G has a natural action upon the principal bundle $\mathcal{G}=\{G,G/H,p,H,H\}$. An important special case is that of an associated Hilbert bundle $\mathcal{B}=\{B,G/H,p,H,\mathfrak{H}\}$, but since the group H will generally have many possible actions on the Hilbert space $\mathfrak{H}$, we shall have to choose a particular action, or representation $D(H)$ of H upon $\mathfrak{H}$, and write the associated bundle accordingly:

$$\mathcal{G}_D=\{B,G/H,p,D(H),\mathfrak{H}\}. \tag{1}$$

However, if G is a Lie group, then G/H is necessarily paracompact, and any Hilbert bundle over the base G/H is necessarily equivalent to the product,

$$\mathcal{G}_D \equiv G/H \times \mathfrak{H}. \tag{2}$$

The action of G upon $\mathcal{G}$ (i.e., upon G) by left-translations is known, and so therefore is its action upon $\mathcal{G}_D$, as given by Eq. (1). We have to derive an explicit formula for this action, and then to rework this formula when the total space of $\mathcal{G}_D$ is given in the product form.

It turns out to be simpler to do it directly. This has the further advantage that the resulting formulas are valid for the action of the group upon *any* product bundle, for example a bundle of Banach spaces or operator algebras. We shall therefore work with the generic product bundle

$$B=G/H \times \mathfrak{F}, \tag{3}$$

where the only demand on $\mathfrak{F}$ is that it be a complete normed linear space, and determine the actions of the group G on it.

Let $g \in G$, $x \in G/H$, $\phi \in \mathfrak{F}$, and $b=(x,\phi) \in B$. Write

$$gb = g(x,\phi) = (gx, u(g,x)\phi), \tag{4}$$

where $u(g,x)$ is an appropriate linear map upon $\mathfrak{F}$ which depends upon g and x. $u(g,x)$ has to satisfy the condition

$$u(g'g,x) = u(g',gx)u(g,x) \tag{5}$$

that arises from the associativity of multiplication in G:

$$(g'g)\cdot b = g'(g\cdot b). \tag{6}$$

Observe that Eq. (6) has to hold even if G is only a semigroup.

The action of G on G/H being known, it only remains to determine the quantity $u(g,x)$ which appears in Eq. (4). $u(g,x)$ must be a linear transformation of $\mathfrak{F}$, and it must satisfy Eq. (5). The method of solving Eq. (5) was devised by Wigner in 1939 (Ref. 9). It is as follows.

Let

$$\eta: G/H \to G \tag{7}$$

be an *algebraic cross section* of the bundle $\mathcal{G}$, i.e., a map which satisfies

$$p \circ \eta = \mathrm{id}, \tag{8}$$

where p is the projection in the bundle $\mathcal{G}$ and id is the identity map. An important theorem in fiber bundle theory states that a *continuous* cross section of a principal bundle $\mathcal{G}$ exists if and only if the bundle is equivalent to the product, $\mathcal{G} \equiv G/H \times H$, so that in general the map η cannot be continuous. We shall presently return to this point. Given η, define the map

$$k: G \times G/H \to G \tag{9}$$

by

$$k(g,x) = \eta(gx)^{-1} g\, \eta(x). \tag{10}$$

Then $k(g,x)$ obviously satisfies

$$k(g'g,x) = k(g',gx)k(g,x), \tag{11}$$

and it is easily seen that $k(g,x) \in H$, i.e., k is actually a map,

$$k: G \times G/H \to H. \tag{12}$$

Finally, choose a linear action $D(H)$ of H on $\mathfrak{F}$, and set

$$u(g,x) = D(k(g,x)). \tag{13}$$

The continuity of the action (4) remains to be established. It follows from the definition of the quotient topology that the action of G on G/H by left translations is continuous. According to a theorem of von Neumann, a unitary Hilbert-space representation of a locally compact group is strongly continuous if it is weakly measurable. If η is a measurable map, so is $k(g,x)$ defined by Eq. (10). Thus, for unitary representations, measurability of η suffices to ensure the continuity of $D(k(g,x))$, and therefore of the action (4). In practice, η can always be chosen to be piecewise-continuous. Finally, it is again a standard result in the theory of infinite-dimensional unitary group

representations that the passage from one section η to another is equivalent to a change of basis in $\mathfrak{H}$. (Detailed treatments of infinite-dimensional unitary group representations may be found in Refs. 9–11.)

The arguments of the previous paragraph do not apply if the fiber $\mathfrak{F}$ is not a Hilbert space and the group H does not act upon it as a unitary representation. In this case the problem of continuity has to be studied separately. In the examples we shall consider, the map η will always be continuous, so that the continuity of $D(H)$ would be a sufficient requirement.

The map k of Eq. (10) is sometimes called a $(G,G/H,H)$ cocycle in the mathematics literature, and sometimes a ''Wigner rotation'' of G into H in the physics literature. In Wigner's language, H is the ''little group.''

C. Actions of semigroups

The results of Sec. III B were based on the bundle structure theorem for Lie groups, and the theory of unitary representations on locally compact groups. Neither is available for an arbitrary semigroup G. However, for physical applications one is mainly interested in a very restricted class of semigroups, those that arise from symmetry groups like the Galilei or the Poincaré group by dropping the requirement of time reversibility. In these cases one may mimic the general theorems by *ad hoc* constructions. We shall illustrate the procedure for the ''Galilei semigroup.''

Let $g=(b,\mathbf{a},\mathbf{v},R)$ be an element of the inhomogeneous Galilei group G, where b is a time translation, $\mathbf{a}$ is a space translation, $\mathbf{v}$ is a (velocity) boost, and R is a rotation. The multiplication law in the group is

$$g'g=(b',\mathbf{a}',\mathbf{v}',R')(b,\mathbf{a},\mathbf{v},R)=(b'+b,\mathbf{a}'+R'\mathbf{a}+\mathbf{v}'b,\mathbf{v}'+R'\mathbf{v},R'R), \tag{14}$$

the identity element is $e=(0,0,0,1)$, and the inverse of g is

$$g^{-1}=(-b,-R^{-1}(\mathbf{a}-b\mathbf{v}),\quad R^{-1}\mathbf{v},R^{-1}). \tag{15}$$

We define the Galilei semigroup G^+ by the condition

$$b\geqslant 0. \tag{16}$$

Then the generic element g does not have an inverse, but group elements with $b=0$ are invertible,

$$(0,\mathbf{a},\mathbf{v},R)^{-1}=(0,-R^{-1}\mathbf{a},R^{-1}\mathbf{v},R^{-1}), \tag{17}$$

and G^+ has an identity which is the same as the identity of the group. Clearly, the one-parameter subsemigroup T^+ of time translations has an identity. Therefore, by the Hille–Yosida theorem (Ref. 12), $T^+(b)$ will be strongly differentiable and will have an infinitesimal generator in any bounded strongly continuous Hilbert space representation. We shall confine our search for representations to these cases.

Now T^+ is also topologically closed. The following facts are readily established:

(1) For any closed subsemigroup H^+ of G^+, the factor space $M=G^+/H^+$ is defined and is identical with G/H.
(2) If H^+ is a normal subsemigroup of G^+, then M is a group, and G^+ is equivalent to the product bundle $M\times H^+$.
(3) If the above-mentioned condition is satisfied, then there exists a self-evident cross section of M in G^+ which is continuous, and invertible in G^+.

In this case the action of the semigroup G^+ on the bundle $M\times\mathfrak{H}$ may be constructed exactly as in the case of the group.

We shall exhibit the above-mentioned procedures by the following simple example. Let G^+ be the Galilei semigroup, and H^+ the subsemigroup of time translations. Then $M=G^+/H^+$ is a group, the semidirect product of the group of boosts V and the Euclidean group E_3 in three dimensions. Write $x\in M$ explicitly as

$$x=(\mathbf{z};\mathbf{w};\rho), \tag{18}$$

where $\mathbf{z}$ is a space translation, $\mathbf{w}$ a boost, and ρ a rotation. The map $\eta: M\to G^+$ defined by

$$\eta(x)=(0,\mathbf{z},\mathbf{w},\rho), \tag{19}$$

is a continuous cross section which is invertible in G^+, and G^+ acts on M as follows:

$$gx= \ (b,\mathbf{a},\mathbf{v},R)\cdot(\mathbf{z};\mathbf{w};\rho)=(\mathbf{a}+R\mathbf{z}-(\mathbf{v}+R\mathbf{w})b;\mathbf{v}+R\mathbf{w};R\rho). \tag{20}$$

The cocycle k takes the simple form

$$k(g,x)=(b,0,0,1). \tag{21}$$

Finally, we choose a bounded representation, D, of H^+ on $\mathfrak{H}$:

$$D(b,0,0,1)\phi=D(k(g,x))\phi=e^{(i\alpha-\beta)b}\phi, \tag{22}$$

where $\phi\in\mathfrak{H}$, $\alpha,\beta\in\mathbb{R}$, and $\beta>0$. Hence, by Eq. (12),

$$u(k(g,x))\phi=e^{(i\alpha-\beta)b}\phi. \tag{23}$$

Equations (20) and (23) provide a representation of G^+ on the bundle $M\times\mathfrak{H}$. To see this representation in a more transparent form, we look at the fiber $(0;0;1)$, in a more familiar notation:

$$g(x_0,\phi)=(t,\mathbf{x},\mathbf{v},R)\cdot(0;0;1)=((\mathbf{x}-\mathbf{v}t;\mathbf{v};R), \ \ e^{(i\alpha-\beta)t}\phi). \tag{24}$$

The representation "decays" as t increases.

IV. ELEMENTARY EXCITATIONS AS BUNDLE REPRESENTATIONS

The description of elementary excitations by bundle representations of the Galilei and Poincaré groups has been discussed at length in earlier works (Refs. 2 and 3). Therefore we shall confine ourselves, in the following, to one particular representation of the Galilei group which seems to describe (stable) nonrelativistic zero-mass excitations, and consider how the representation changes if the Galilei group is replaced by the Galilei semigroup.

A. Case of the Galilei group

Here G is the Galilei group and $H=T\times E_3$, the direct product of the subgroup of time translations T and the Euclidean group E_3. In this case the base space M is just the space of the boosts, and there is a natural invertible cross section:

$$\begin{aligned} x&=\mathbf{w},\\ \eta(x)&=(0,0,\mathbf{w},1). \end{aligned} \tag{25}$$

Easy computations yield the formulas

$$\begin{aligned} gx&=\mathbf{v}+R\mathbf{w},\\ k(g,x)&=(b,\mathbf{a}-(\mathbf{v}+R\mathbf{w})b,0,R). \end{aligned} \tag{26}$$

To construct the bundle representation, we recall that irreducible unitary representations of E_3 are characterized by the invariants $\{\mathbf{p}^2,n\}$, where, loosely speaking, $\mathbf{p}^2$ is the square of the momentum and n is the helicity (a non-negative integer). The irreducible representation space is $L_2(S_2,dS)$, where S_2 is the two-sphere and dS is the rotation-invariant measure on it. For our purposes, it is convenient to use *not* the irreducible unitaries, but the following one, U, on $\mathfrak{H}=L_2(\mathbf{p},d^3p)$, which is the direct integral of copies of $L_2(S_2,dS)$ over two spheres of all radii.

$$U(\mathbf{a},R)\phi(\mathbf{p})=e^{in\sigma(R,\omega)}e^{-i\mathbf{a}\cdot\mathbf{p}}\phi\circ R^{-1}(\mathbf{p}). \tag{27}$$

In the above, $\sigma(R,\omega)$ is an (O_3,S_2,O_2)-cocycle or Wigner rotation, where O_3,O_2 are the orthogonal (rotation) groups in three and two dimensions, respectively, $S_2=O_3/O_2$ is the two sphere, and ω a point on S_2. All component irreducibles in Eq. (27) have the same helicity. Finally, we represent $T\times E_3$ on $\mathfrak{H}$ as follows:

$$U(b,\mathbf{a},R)\phi(\mathbf{p})=e^{iE(\mathbf{p}^2,n)b}U(\mathbf{a},R)\phi(\mathbf{p}). \tag{28}$$

In the previous text, E is a positive, but otherwise arbitrary function of $\mathbf{p}^2$, and n is fixed. By Eqs. (13) and (26), the bundle representations are obtained by taking $D(k(g,x))\phi=U(b,\mathbf{a}-(\mathbf{v}+R\mathbf{w})b),R)\phi$.

On the fiber $\mathbf{w}=0$, the bundle representation takes the explicit form

$$(b,\mathbf{a},\mathbf{v},R)(0,\phi)=(\mathbf{v},e^{i\Lambda}(\phi\circ R^{-1})\mathbf{p}), \tag{29}$$

where

$$\Lambda=-\mathbf{a}\cdot\mathbf{p}+b(E+\mathbf{v}\cdot\mathbf{p})+n\sigma(R,\omega). \tag{30}$$

In the previous text, we have suppressed the arguments in E. Formulas (29) and (30) show that under a boost,

$$\begin{aligned}\mathbf{p}&\to\mathbf{p},\\ E&\to E+\mathbf{p}\cdot\mathbf{v}.\end{aligned} \tag{31}$$

In their analysis of irreducible unitary representations of the Galilei group, Inönü and Wigner (Ref. 13) had concluded that these representations had no physical interpretation because they did not admit either localizable states (since $\mathbf{p}^2$ was constant in an irreducible, not enough momenta were available to form a delta function) or states that were—like the photon—localizable in velocity space. The first argument would not apply to a *reducible* representation which contains all values of $\mathbf{p}^2$ with the same weight. However, the invariance group imposes no relationship between E and $\mathbf{p}^2$, and, as the second equation of (31) shows, in any linear representation, for any value of $\mathbf{p}^2$, the quantity E takes—owing to the boosts—all values between $-\infty$ and $+\infty$. This alone would rule out the possibility of a physical interpretation for these representations.

In the above-constructed *bundle* representations, the boosts are represented not on the fibers but on the base space. Specializing formulas (29) and (30) to the case $\mathbf{a}=0$, $R=1$ and setting $\sigma(1,\omega)=0$ (which can be done without loss of generality), we find that

$$(b,0,\mathbf{v},1)(0,\phi)=(\mathbf{v},e^{ib(E+\mathbf{p}\cdot\mathbf{v})}\phi(\mathbf{p})), \tag{32}$$

i.e., on any given fiber, we are able to assign a value of E to a given $\mathbf{p}^2$, because this assignment will not be disturbed by the boosts. That is, we may choose, arbitrarily, a *dispersion law* $E=E(\mathbf{p}^2)$. Since all values of $\mathbf{p}$ occur with the same weight, it becomes possible to construct localizable states, which may be interpreted as excitations corresponding to the chosen dispersion law. Finally, Eq. (31) shows that these excitations have *zero nonrelativistic mass*.

Equation (31) constitutes the transformations laws, under boosts, of the excitations posited by Landau in his explanation of superfluidity (Refs. 14 and 15).

B. Case of the Galilei semigroup

For the Galilei semigroup G^+, we shall construct a representation that is as close as possible to that previously mentioned, above, without being identical to it. We shall take $H^+ = T^+ \times E_3$, so that G^+/H^+ will again be the space of the boosts. The natural cross section will again be given by the second equation in (25), and formula (26) for $g\mathbf{x}$ and $k(g,\mathbf{x})$ will remain valid, with the proviso that $b \geqslant 0$. We shall represent E_3 on $\mathfrak{H}$ as before, i.e., by formula (27). However, the subsemigroup of time translations will be represented, not by a character $\exp i\epsilon b$, but by a quantity $\exp(i\epsilon - \gamma)b$, where $\gamma \geqslant 0$. Equation (28) will [cf. Eqs. (22) and (23)] accordingly change to the following formula for the relevant representation, Δ, of H^+:

$$\Delta(b,\mathbf{a},R)\phi(\mathbf{p}) = e^{(iE(\mathbf{p}^2,n)-\Gamma(\mathbf{p}^2,n))b} U(\mathbf{a},R)\phi(\mathbf{p}), \tag{33}$$

where Γ is a positive function, n is a fixed positive integer, and $b \geqslant 0$. Formally, the passage from the group to the semigroup is equivalent to replacing E by $E + i\Gamma$ in the representation $U(b,\mathbf{a},R)$. Clearly, $\mathbf{p}, E,$ and Γ will transform under boosts as

$$\begin{aligned} \mathbf{p} &\to \mathbf{p}, \\ E &\to E + \mathbf{p}\cdot\mathbf{v}, \\ \Gamma &\to \Gamma. \end{aligned} \tag{34}$$

The quantity $\Gamma(\mathbf{p}^2)$ may be interpreted as the inverse lifetime of the excitation with momentum $\mathbf{p}$. For large values of $\Gamma(\mathbf{p}^2)$, the excitations become very unstable, and perhaps no longer experimentally detectable. As the last equation in (34) shows, properties of the excitations that depend on Γ are invariant under the boosts.

Since the representation Δ is bounded and continuous, and since the semigroup has an identity, the semigroup of time translations has an infinitesimal generator.

V. DYNAMICS ON BANACH BUNDLES

Symmetries are usually studied via group rather than Lie algebra actions, because they avoid the problems associated with unbounded operators. By contrast, dynamics is usually studied via the infinitesimal generator of the one-parameter group or semigroup of time translations—the Hamiltonian—because the Hamiltonian represents the total energy of the system. In quantum mechanics, the Hamiltonian is an operator on a Hilbert space. In classical mechanics, it is a complete vector field on a manifold of states. From physical considerations, one would expect a one-parameter group or semigroup of time translations of a Banach bundle to possess an infinitesimal generator, which would act like a linear transformation on the fibers and a vector field on the base space. To the best of the authors' knowledge, such mathematical objects have not yet been studied, and there is no generalized ''Stone–Whitney theorem'' which asserts their existence for dynamics on vector bundles. We therefore begin—assuming that time translations indeed act as a one-parameter group or semigroup of fiber-preserving maps on a vector bundle—by defining the two constituents of this generator, one acting on the base space and the other on the fibers. The dynamical systems these pairs define will be seen in Sec. VII to be realized by certain quantum mechanical models.

Let Γ be a dynamical system (B,T), where $B = X \times Y$ is a Banach bundle and $T = \{T_t | t \in \mathbb{R}$ or $\mathbb{R}^+\}$ is a one-parameter group or semigroup of fiber-preserving transformations of B. These maps define a one-parameter group or semigroup of base maps $\{S_t | t \in \mathbb{R}$ or $\mathbb{R}^+\}$, and the action of T on B is analogous to that of g in Eq. (4), i.e.,

$$T_t(x,y)=(S_tx,V(t,x)y)\equiv(x_t,y_t)\forall\ \ x\in X,\ \ y\in Y,\ \ t\in\mathbb{R}\ \text{ or }\ \mathbb{R}^+, \tag{35}$$

where $V(t,x)$ is a linear transformation of Y. Then it follows immediately from the semigroup properties of S and T that

$$\begin{aligned} S_{t+t'}x&=S_t(S_{t'}x),\\ V(t+t',x)&=V(t',S_tx)V(t,x). \end{aligned} \tag{36}$$

Furthermore, assuming that S_tx and $V(t,x)y$ are differentiable with respect to t in the natural topologies of X and Y, respectively, it follows from Eqs. (35) and (36) that the equations of motion for x_t and y_t are

$$\frac{\mathrm{d}x_t}{\mathrm{d}t}=F(x_t) \tag{37}$$

and

$$\frac{\mathrm{d}y_t}{\mathrm{d}t}=L(x_t)y_t, \tag{38}$$

where

$$F(x)=\lim_{h\to 0}h^{-1}(S_h-I)x\ \ \forall\ \ x\in X \tag{39}$$

and

$$L(x)y=\lim_{h\to 0}h^{-1}(V(h,x)-I)y\forall\ \ x\in X,\ \ y\in Y. \tag{40}$$

Thus, Eqs. (37) and (38) signify that the flow $x\to x_t$ in the base space X is not only autonomous but also serves to drive the flow $y\to y_t$ in the fibers.

VI. THE GENERIC OPERATOR ALGEBRAIC QUANTUM MODEL

A. Observables, states, dynamics

In a standard way (cf. Refs. 15–20), we idealize a macroscopic quantum system, Σ, as an infinitely extended assembly of interacting particles living in a space X, which may be either a Euclidean space $\mathbb{R}^d$ or a lattice $\mathbb{Z}^d$. The generic model of Σ is given[21] in the Schrödinger picture,[22] by an algebra of observables $\mathfrak{A}$, a state space Ω of expectation functionals on $\mathfrak{A}$, and a one-parameter group or semigroup τ of transformations of Ω representing the dynamics of the system. The model conforms to the following specifications.

(I) $\mathfrak{A}$ is the $C^\star$-algebra of observables. This has a local structure, which is as follows.

(a) Each bounded region Λ of X carries a $C^\star$-subalgebra $\mathfrak{A}_\Lambda$, comprising the bounded operators in a local Hilbert space $\mathfrak{H}_\Lambda$, whose self-adjoint elements are the observables in Λ.

(b) The algebras $\mathfrak{A}_\Lambda$ satisfy the conditions of isotony and local commutativity, namely

$$\mathfrak{A}_\Lambda\subset\mathfrak{A}_{\Lambda'}\qquad\text{if}\quad\Lambda\subset\Lambda'$$

and

$$[a,a']=0\qquad\text{if}\quad a\in\mathfrak{A}_\Lambda,\ \ a'\in\mathfrak{A}_{\Lambda'}\qquad\text{and}\ \ \Lambda\cap\Lambda'=\emptyset.$$

Furthermore, space translations correspond to a homomorphism, σ, of the additive group X into $\mathrm{Aut}(\mathfrak{A})$, and the local algebras $\mathfrak{A}_\Lambda$ transform covariantly under $\sigma(X)$, i.e.,

$$\sigma(x)\mathfrak{A}_\Lambda = \mathfrak{A}_{\Lambda+x}.$$

The unbounded observables for the region Λ are the unbounded self-adjoint operators in $\mathcal{H}_\Lambda$ (Ref. 23).

(c) $\mathfrak{A}$ is the norm-closure of the union of the local algebras $\mathfrak{A}_\Lambda$. We shall denote this union, which is a subalgebra of $\mathfrak{A}$, by $\mathfrak{A}_{\text{loc}}$.

(II) The state space Ω and the dynamical group or semigroup τ are defined as follows.[21] Ω is a folium[24] of positive, normalized, locally normal[25] linear functionals on $\mathfrak{A}$ that is stable under the dual of σ, while τ is a representation *either* of $\mathbb{R}$ *or* of $\mathbb{R}^+$ in the affine transformations of the state space Ω. The interpretation of the model is that the expectation value of an observable a at time t, subject to the condition that ω is the initial state of the system, is $\langle \tau(t)\omega;a\rangle$, where $\langle \omega;a\rangle \equiv \omega(a)$. We assume that τ and Ω satisfy the following conditions.

(a) τ is the infinite volume limit, in a sense we shall presently specify, of the one-parameter dynamical group or semigroup τ_Λ of the finite volume version, Σ_Λ, of Σ consisting of the particles of the given species confined to the bounded region Λ. Here τ_Λ is the predual of a one-parameter group of automorphisms or a semigroup of completely positive,[26–28] identity preserving transformations of $\mathfrak{A}_\Lambda$, depending on whether Σ_Λ is a conservative system or an open dissipative one. In either case, its form is obtained, by standard constructions, in terms of the interactions between the particles of the system. Denoting now by ω_Λ the restriction of a state ω of Σ to $\mathfrak{A}_\Lambda$, i.e., the state it induces in Σ_Λ, we express our condition that τ is an infinite volume limit of τ_Λ by

$$\langle \tau(t)\omega;a\rangle = \lim_{\Lambda\uparrow X}\langle \tau_\Lambda(t)\omega;a\rangle \forall \quad a\in\mathfrak{A}_{\text{loc}}, \quad \omega\in\Omega, t\in\mathbb{R} \text{ or } \mathbb{R}^+.$$

(b) Ω is the maximal locally normal folium of states that supports the dynamics given by this formula.

It follows from these specifications that Ω and τ, like τ_Λ, are determined by the interactions in the system. We note here that the norm-closed linear span $[\Omega]$ of Ω is a Banach space, whose dual is a $W^\star$-algebra $\hat{\mathfrak{A}}$ (Ref. 29) which in turn is just the weak closure of the representation, Π, of $\mathfrak{A}$ given by the direct sum of the GNS representations of this algebra for all states in the space Ω (Ref. 21). Correspondingly, the transformations $\tau^\star(t)$ of $\hat{\mathfrak{A}}$ dual to $\tau(t)$ form a one-parameter group of automormorphisms of $\hat{\mathfrak{A}}$ or a semigroup of completely positive, identity preserving linear transformations of $\hat{\mathfrak{A}}$, according to whether Σ is a conservative system or an open dissipative one.

B. Macroscopic observables

These are *classical* nonlocalized observables (such as the global space averages of the translates of local ones) that are attached, not to $\mathfrak{A}$, but to certain representations of $\mathfrak{A}$. We define them as follows (cf. Ref. 30). Let π be a representation of $\mathfrak{A}$ in a Hilbert space $\mathfrak{H}$, such that the set, Ω_π, of states on $\mathfrak{A}$ corresponding to the density matrices in $\mathfrak{H}$ is a subset of Ω. Then the macroscopic observables associated with the representation π are defined to be the strong limits, $\hat{F}$, of uniformly bounded sequences $\{\pi(F_n)|n\in\mathbb{N}\}$, where the F_n's are elements of $\mathfrak{A}$ such that

$$\text{norm}-\lim_{n\to\infty}[F_n,A]=0 \quad \forall \quad A\in\mathfrak{A}.$$

It follows easily from these specifications that the macroscopic observables $\hat{F}$ belong the center of the von Neumann algebra $\pi(\mathfrak{A})''$. They therefore form an Abelian $W^\star$-algebra, $\mathfrak{M}$, i.e., an algebra of functions on a classical phase space.[29] Evidently, they may be identified with functionals on the set of states Ω_π according to

$$\hat{F}(\omega) = \lim_{n\to\infty}\omega(F_n) \forall \quad \omega\in\Omega_\pi.$$

A prototype of a macroscopic observable is obtained by choosing

$$F_n = |\Lambda_n|^{-1} \int_{\Lambda_n} \mathrm{d}x\, \sigma(x) f,$$

where $f \in \mathfrak{A}$ and $\{\Lambda_n\}$ is a increasing sequence of bounded spatial regions, whose union is X. $\hat{F}$ is then the global space average of $\pi(\sigma(x)f)$, i.e.,

$$\hat{F} = s - \lim_{n\to\infty} |\Lambda_n|^{-1} \int_{\Lambda_n} \mathrm{d}x\, \pi(\sigma(x) f).$$

We shall now provide a sketch of how the above-mentioned general definition of $\hat{F}$ can be extended, for some representations π, to cases where the local observables F_n are unbounded, e.g., when they correspond to space averages over bounded regions of the locally conserved densities of standard thermodynamic observables (Refs. 14 and 20). Thus, we consider the case where $(\mathfrak{H}, \pi, \Phi)$ is the GNS representation of $\mathfrak{A}$ for a primary,[31] translationally invariant state ω. We assume that $\hat{\xi}$ is a Hermitian quantum field such that $\hat{\xi}(x)$ is a distribution-valued observable for the ball of center x and some x-independent radius a and that $\hat{\xi}$ is covariant with respect to space translations, i.e., $\sigma(x')\hat{\xi}(x) = \hat{\xi}(x+x')$. We define (formally) the derivation δ and the local observable F_n by

$$\delta = i \int_X \mathrm{d}x [\pi(\hat{\xi}(x)), .],$$

where the dot on the right refers to the argument of δ and

$$F_n = |\Lambda^n|^{-1} \int_{\Lambda_n} \mathrm{d}x\, \hat{\xi}(x).$$

We then make the following assumptions concerning $\hat{\xi}$.

(a) $\omega(F_n)$ converges to a limit, $\hat{F}(\omega)$, as $n \to \infty$. In view of the assumed translational invariance of ω, this is equivalent to the condition that $\omega(\hat{\xi}(x))$ is well-defined.

(b) There is a dense subset, $\mathfrak{B}$, of $\mathfrak{A}_{\mathrm{loc}}$ such that Φ lies in the domain of the (possibly unbounded) observable δB, for all $B \in \mathfrak{B}$. Here we note that it follows from the above-mentioned specifications that, in view of the local commutativity property of $\mathfrak{A}$, δB reduces here to $i\int_{\Lambda_n} \mathrm{d}x [\hat{\xi}(x), B]$ for n sufficiently large.

(c) For each $A \in \mathfrak{A}$, the correlation function $\omega(A\hat{\xi}(x)) - \omega(A)\omega(\hat{\xi}(x))$ is of class L_1, in keeping with the standard cluster properties of primary states (Ref. 32).

It follows easily from these specifications that, for all $B \in \mathfrak{B}$, the expectations of the observables F_n in the states $\omega_B(.) := \omega(B^\star(.)B)/\omega(B^\star B)$ satisfy the condition

$$\lim_{n\to\infty} \omega_B(F_n) = \hat{F}(\omega) \quad \forall B \in \mathfrak{B}.$$

This is equivalent to the statement that the sequence $\{\pi(F_n)\}$ converges to $\hat{F}(\omega)I$ as $n \to \infty$, and therefore signifies that the limit of the sequence is a macroscopic observable $\hat{F} := \hat{F}(\omega)I$.

Equilibrium states and thermodynamical variables. In the case where Σ is conservative, its equilibrium states at inverse temperature β comprise the convex set Ω_β of states that satisfy the Kubo–Martin–Schwinger condition, whose general significance was first exposed by Haag, Hugenholtz, and Winnink (Ref. 33). This takes the form

$$\omega(A_t B) = \omega(B A_{t+i\hbar\beta}) \quad \forall A, B \in \mathfrak{A},$$

where, in our Schrödinger picture (cf. Refs. 34 and 21), ω is the canonical extension of the state denoted by the same symbol, and A_t is the element $\tau^\star(t)\pi(A)$ of the von Neumann algebra generated by the corresponding GNS representation, π, of $\mathfrak{A}$. The extremal elements of Ω_β are precisely the primary ones and therefore may naturally be interpreted as the pure thermodynamic phases of the system (Refs. 35 and 36). Furthermore, it follows from their primary property that they may be indexed by an appropriate set of macroscopic observables (Ref. 30); and, in accordance with the demands of classical thermodynamics, we shall assume that the latter observables are the global space averages of locally conserved fields $\hat{q}(x) = (\hat{q}_1(x), .., \hat{q}_n(x))$, such as those representing densities of energy, mass, etc. We shall denote the pure equilibrium phase at inverse temperature β for which these macroscopic variables take the values $(q_1, \ldots, q_n)$ by $\omega_{\beta,q}$.

C. Local equilibrium

The concept of local equilibrium is natural for a hydrodynamic, i.e., large scale, description of Σ, in which a point corresponds to cell containing an enormous number of particles in the microscopic picture. We shall now formulate this concept for the case where Σ is a conservative system, whose algebra of observables, $\mathfrak{A}$, is generated by a quantum field, ψ, that satisfies the canonical commutation or anticommutation relations, according to whether Σ consists of bosons or fermions. Thus,

$$[\psi(x), \psi^\star(y)]_\pm = \delta(x-y); \quad [\psi(x), \psi(y)]_\pm = 0,$$

and the action of the space translational automorphisms is given by

$$\sigma(x)\psi(y) = \psi(x+y).$$

We define $\gamma(L)$ to be the automorphism of $\mathfrak{A}$ representing the distance rescaling $x \to Lx$, i.e.,

$$\gamma(L)\psi(y) = L^{d/2}\psi(Ly),$$

the factor $L^{d/2}$ ensuring that γ preserves the canonical commutation and anticommutation relations. It follows easily from these definitions that $\{\gamma(L) | L \in \mathbb{R}^+\}$ form a group, with $\gamma(L_1)\gamma(L_2) = \gamma(L_1 L_2)$, and that γ and σ satisfy the important equation

$$\gamma(L)\sigma(x) = \sigma(Lx)\gamma(L). \tag{41}$$

Now let $\{\omega^{(L)} | L \in \mathbb{R}^+\}$ be a family of states indexed by L, where the parameter L is a characteristic length governing the spatial variations of $\omega^{(L)}$ in the following sense. For any local observable a, $\omega^{(L)}(\sigma(Lx)a)$ reduces to an L-independent function of x, at least for sufficiently large L. We define $\tilde{\omega}^{(L)}$ to be the version of $\omega^{(L)}$ in the scaling for which the unit of length is L, i.e.,

$$\tilde{\omega}^{(L)}(a) = \omega^{(L)}(\gamma(L)a) \forall \quad a \in \mathfrak{A}. \tag{42}$$

Our hydrodynamic picture of Σ will be based on the structure of this state in the large scale limit where $L \to \infty$.

We now note that, by Eqs. (41) and (42),

$$\tilde{\omega}^{(L)}(\sigma(x)a) = \omega^{(L)}(\gamma(L)\sigma(x)a) = \omega^{(L)}(\sigma(Lx)\gamma(L)a).$$

Hence, replacing a by $\gamma(L^{-1})a$ and defining

$$\alpha(L,x) = \sigma(x)\gamma(L^{-1}), \tag{43}$$

it follows that

$$\tilde{\omega}^{(L)}(\alpha(L,x)a)=\omega^{(L)}(\sigma(Lx)a). \tag{44}$$

In order to see the significance of this equation, we note that it follows from our definitions of the automorphisms σ,γ, and α that

$$\alpha(L,x)\psi(y)=L^{-d/2}\psi(x+L^{-1}y). \tag{45}$$

Thus, for large L, the action of $\alpha(L,x)$ serves to localize the observables around the point x. Hence the left-hand side of our formula for $\tilde{\omega}^{(L)}$ yields the state in the vicinity of x, according to the large scale description.

Suppose now that D is a fixed, bounded spatial region that is sufficiently large to contain an enormous number of particles, in the microscopic description. Thus, the subsystem in D is mesoscopic, in that, on the one hand, it contains a huge number of particles, while, on the other hand, the ratio of its span to the distance, L, vanishes in the limit $L\to\infty$. In other words, D corresponds to a *hydrodynamic point*.

Our local equilibrium condition is that the restriction of $\omega^{(L)}$ to the space translate, $D+Lx$, of D reduces to an equilibrium state corresponding to some position-dependent values, $\beta(x)$ and $q(x)$, of the thermodynamic variables β and q, in the limit $L\to\infty$, i.e., that, if a is an arbitrary observable for the region D, then

$$\lim_{L\to\infty}\omega^{(L)}(\sigma(Lx)a)=\omega_{\beta(x),q(x)}(a), \tag{46}$$

which is consistent with our earlier assertion that $\omega^{(L)}(\sigma(x)a)$ is L independent for L sufficiently large. Evidently, $(\beta(x),q(x))$ is a classical field, representing the local thermodynamic variables in the hydrodynamic description. Further, since D is an arbitrary bounded region, the above-specified local equilibrium condition extends to all elements a of the algebra $\mathfrak{A}$. Moreover, by Eq. (44), it takes a particularly simple form when expressed in terms of the rescaled state, $\tilde{\omega}^{(L)}$, namely

$$\lim_{L\to\infty}\tilde{\omega}^{(L)}(\alpha(L,x)a)=\omega_{\beta(x),q(x)}(a)\quad\forall\quad a\in\mathfrak{A}. \tag{47}$$

In other words, the state as described in the large scale limit reduces, at any spatial point x, to the equilibrium state $\omega_{\beta(x),q(x)}$. In fact, this condition has been proved to be fulfilled by Gibbs states of nonrelativistic gravitational systems (Ref. 37).

Finally, this formulation of local equilibrium may easily be extended to the dynamical situation in the case where the macroscopic equations of motion for the evolutes, $(\beta_t(x),q_t(x))$, of $(\beta(x),q(x))$ are invariant under the transformation $x\to Lx, t\to L^k t$, for some positive constant k, as in the cases of both diffusion or Eulerian hydrodynamics. For then, the space–time generalization of the above-mentioned local equilibrium condition is simply

$$\lim_{L\to\infty}\langle\tau(L^k t)\omega^{(L)};(\sigma(Lx)a)\rangle=\omega_{\beta_t(x),q_t(x)}(a). \tag{48}$$

Equivalently, defining the time-dependent state, $\tilde{\omega}_t^{(L)}$, in the hydrodynamic description by

$$\tilde{\omega}_t^{(L)}(a)=\langle\tau(L^k t)\tilde{\omega}^{(L)};\gamma(L)a\rangle, \tag{49}$$

the local equilibrium condition takes the form

$$\lim_{L\to\infty}\tilde{\omega}_t^{(L)}(\alpha(L,x)a)=\omega_{\beta_t(x),q_t(x)}(a)\quad\forall\quad a\in\mathfrak{A}. \tag{50}$$

This condition has been proved to be satisfied by various classical stochastic models (Ref. 38).

VII. BUNDLE DYNAMICAL MODEL OF MACROSCOPIC-CUM-MICROSCOPIC EVOLUTION

In the generic model of a many-particle system, as formulated in Sec. VI, the microscopic observables are quantum mechanical variables, whereas the macroscopic ones are classical. This dichotomy is essential for the reconciliation of quantum microphysics with the empirical fact that the macroscopic dynamics of ''large'' systems generally conforms to classical laws, such as those of hydrodynamics or heat conduction. Furthermore, it has been established that, at least in particular models (cf. Refs. 39 and 5), the macroscopic dynamics is governed by self-contained deterministic laws and acts so as to ''pilot'' the microdynamics. We shall now show that the macroscopic-cum-microscopic evolution of such systems provides a concrete example of the bundle dynamical model of Sec. V.

We base our treatment on the model Σ of Sec. VI, and for simplicity, we restrict our consideration to the case where this is an open dissipative system, i.e., where τ is a one-parameter semigroup. The treatment of the conservative case can be carried out analogously.

We assume that, as in the laser model of Refs. 4 and 5, τ induces macroscopic and microscopic evolutions that may be described as follows.

(I) Σ has a set of macroscopic observables that are functions on a phase space M and evolve according to a deterministic law given by a one-parameter semigroup $\{S_t | t \in \mathbb{R}^+\}$ of transformations $m \to S_t m = m_t$ of M. Thus, assuming that $S_t m$ is differentiable with respect to t, the macroscopic equation of motion takes the form

$$\frac{\mathrm{d}m_t}{\mathrm{d}t} = F(m_t), \tag{51}$$

where F is a vector field on M.

(II) The microscopic evolution of the system is piloted by its macroscopic dynamics in such a way that the equation of motion for the evolute, a_t, of an observable a at time t has the form

$$\frac{\mathrm{d}a_t}{\mathrm{d}t} = L(m_t)a_t, \tag{52}$$

where $L(m_t)$ acts linearly on $\mathfrak{A}$. To be precise, the microscopic dynamics is given by a two-parameter family, $\{W(t,u;m) | t \geqslant u\}$, of completely positive, identity-preserving linear transformations of $\mathfrak{A}$, such that

$$a_t = W(t,u;m)a_u, \tag{53}$$

and

$$W(t,u;m)W(u,v;m) = W(t,v;m), \tag{54}$$

which is essentially a determinacy condition. Equations (51)–(54) then signify that $L(m_t)$ is the generator of the transformations W, i.e., that

$$L(m_t) = (\partial W(t,u;m)/\partial t)_{t=u} \tag{55}$$

and hence that

$$\frac{\partial}{\partial t} W(t,u;m) = L(m_t)W(t,u;m) \equiv L(S_t m)W(t,u;m), \quad \forall \quad m \in M, \quad t \geqslant u. \tag{56}$$

(III) $L(m_t)$ is indeed a true generator, in that Eq. (56) determines W uniquely, subject to the condition that $W(t,t;m) \equiv I$.

We shall now show that, under assumptions (I)–(III), the macroscopic-cum-microscopic dynamics of Σ reduces to that on a fiber bundle, as formulated in Sec. V. To this end, we start by defining B to be the bundle $M\times\mathfrak{A}$ and $V(t,m)$ and T_t to be the transformations of $\mathfrak{A}$ and B, respectively, given by

$$V(t,m)=W(t,0;m) \quad \forall \quad m\in M, \quad t\in\mathbb{R}^+ \tag{57}$$

and

$$T_t(m,a)=(S_t m, V(t,m)a) \quad \forall \quad m\in M, \quad a\in\mathfrak{A}, \quad t\in\mathbb{R}^+. \tag{58}$$

We then prove the following proposition, which establishes that the transformations T_t form a one-parameter semigroup that satisfies all the conditions of the bundle dynamical model of Sec. V.

Proposition 7.1: Under the above-given assumptions, V satisfies the bundle structure property (sometimes called the *cocycle condition*)

$$V(t+u,m)=V(u,S_t m)V(t,m) \quad \forall \quad m\in M, t,u\in\mathbb{R}^+ \tag{59}$$

and T possesses the semigroup properties

$$T_t T_u = T_{t+u} \qquad \text{and} \qquad T_0 = I \quad \forall t,u\in\mathbb{R}^+. \tag{60}$$

Comment: This proposition establishes that the transformations T_t form a one-parameter semigroup that satisfies all the conditions of the bundle dynamical model of Sec. V. In other words, the macroscopic-cum-microscopic dynamics of the system Σ are completely captured by that model.

Proof of Proposition 7.1: It follows from the replacement of m, t, u by $S_u m$, $t-u$,0, respectively, in Eq. (56) that

$$\frac{\partial}{\partial t}W(t-u,0;S_u m)=L(S_{t-u}S_u m)W(t-u,0;S_u m),$$

which, in view of the semigroup property of S, is equivalent to

$$\frac{\partial}{\partial t}W(t-u,0;S_u m)=L(S_t m)W(t-u,0;S_u m). \tag{61}$$

Hence, $W(t-u,0;S_u m)$, as well as $W(t,u;m)$, is a solution of Eq. (56), and therefore, in view of the uniqueness assumption (III),

$$W(t-u,0;S_u m)=W(t,u;m) \quad \forall \quad m\in M, \quad u,t(\geqslant u)\in\mathbb{R}^+.$$

On replacing t by $t+u$ in this equation, we see that

$$W(t,0;S_u m)=W(t+u,u;m) \quad \forall \quad m\in M, \quad t,u\in\mathbb{R}^+. \tag{62}$$

The bundle structure formula (59) for V now follows immediately from this formula, together with Eqs. (54) and (57). Furthermore, this result, together with the semigroup property of S, implies that the transformations T, defined by Eq. (58), form a one-parameter semigroup.

VIII. FIBER BUNDLE DESCRIPTION OF LOCAL EQUILIBRIUM

We shall now show that local thermodynamic equilibrium (LTE), as formulated in Sec. VI C, may be simply described in terms of actions on a fiber bundle. For notational simplicity, we denote by $\theta(x)$ the $(n+1)$-component hydrodynamic field $(\beta(x),q(x))\equiv(\beta(x),q_1(x),\ldots,q_n(x))$ specified in Sec. VI C. Thus, the LTE formula (47) takes the form

$$\lim_{L\to\infty} \tilde{\omega}^{(L)}(\alpha(L,x)a)) = \omega_{\theta(x)}(a). \tag{63}$$

Evidently, θ is a mapping from X into $\mathbb{R}^{n+1}$ whose range is the Cartesian product of those of the thermodynamic variables $(\beta, q_1, \ldots, q_n)$. We shall denote by Θ the space of kinematically possible forms of the field θ. For present purposes, it is not necessary to specify the topology of Θ. We shall assume that the dynamical group, τ, of Σ induces a phenomenological dynamics given by a semigroup $\{\phi(t) | t \in \mathbb{R}^+\}$ of transformations of Θ. Thus,

$$\phi(t)\theta = \theta_t \equiv (\beta_t, q_t), \tag{64}$$

where β_t, q_t are the time-dependent fields that appear in Eq. (50).

We now define the fiber bundle B, in the notation of Sec. V, to be $X \times \mathfrak{A}$. Its fiber at the spatial point x therefore consists of elements a_x of $\mathfrak{A}$. We then define P to be the mapping $\theta \to P_\theta$ of Θ into the complex-valued functions on B given by

$$P_\theta(x, a_x) = \omega_{\theta(x)}(a_x). \tag{65}$$

On comparing this equation with Eq. (63), we see immediately that P carries a full description of LTE in that, for each $\theta \in \Theta$, P_θ represents the local equilibrium corresponding to the hydrodynamic field θ at each spatial point x. Likewise, defining the evolute P^t of P to be the mapping $\theta \to {P^t}_\theta$ of Θ into the complex functions on B given by

$${P^t}_\theta = P_{\theta_t}, \tag{66}$$

we see from Eqs. (50) and (64) that P^t carries a full representation of the LTE at time t. Moreover, by Eqs. (64) and (66),

$${P^t}_\theta = P_{\phi(t)\theta}, \tag{67}$$

which signifies that the time dependence of the local equilibrium profile is completely determined by the phenomenological semigroup ϕ.

IX. CONCLUDING REMARKS

The purpose of this paper has been to combine the geometric picture of fiber bundles with the operator algebraic one of quantum theory for the purpose of describing macroscopic quantum systems. The combination of these mathematical structures is quite natural in this context, since it offers the means of representing the complementary classical and quantum aspects of complex systems by actions on the bases and the fibers, respectively, of the relevant bundles. Here, we have shown that it serves to provide simple pictures of quasiparticle excitations, of local thermodynamic equilibrium, and of the interplay between the macroscopic (classical) dynamics and microscopic (quantum) dynamics of certain systems, e.g., lasers. In view of its apparent generality, we envisage that the fusion of geometric and operator algebraic concepts presented here should have wider ramifications for the theory of complex systems.

Finally, in view of the results of this paper, it would appear that the mathematical problem of establishing the existence of infinitesimal generators of one-parameter groups of bundle maps of vector bundles is of physical interest as well. We have not addressed this problem in its abstract form, but have given an explicit construction in Sec. V which is of fairly wide applicability.

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Large N limit of $SO(N)$ scalar gauge theory

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In this paper we study the large N_c limit of $SO(N_c)$ gauge theory coupled to a real scalar field following ideas of Rajeev [Int. J. Mod. Phys. A **9**, 5583 (1994)]. We will see that the phase space of this resulting classical theory is $Sp_1(\mathcal{H})/U(\mathcal{H}_+)$ which is the analog of the Siegel disk in infinite dimensions. The linearized equations of motion give us a version of the well-known 't Hooft equation of two dimensional quantum chromodynamics. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Gauge theories are the fundamental theories that describe nature: Quantum chromodynamics (QCD) is the gauge theory of hadrons, and it is believed that one can compute the masses and excitations of all these hadrons from QCD. As yet there is no satisfactory understanding of these bound states. All the hadrons are color singlets, in fact we never see the underlying quarks as asymptotic states. That means QCD should be a confining theory and there should be an independent formulation of it which is expressed completely in terms of these color invariant states.

In Ref. 1, Rajeev has constructed such a theory of mesons in two dimensions in the limit N_c, the number of colors in $SU(N_c)$, goes to infinity. The idea that QCD should simplify while keeping all its essential features in this limit goes back to 't Hooft[2,3] and that this limit should be a kind of classical mechanics to Migdal and Witten. Even this large-N_c theory is quite complicated and 't Hooft looked at a two-dimensional model to understand the meson spectrum in this limit and obtained his bound state equation.[3] It is not so clear how to treat the baryons in the large-N_c limit. Witten suggested that baryons could also be understood (as solitonic excitations) in his classic papers (Refs. 4 and 5). A much more ambitious program was presented by Lee and Rajeev[6] for the large-N_c limit of more complicated gauge theories.

In this paper we study the large N_c limit of $SO(N_c)$ gauge theory coupled to a real scalar field. This theory is not physical, but it is a good model to test some of the ideas about gauge theories. We will apply the methods developed by Rajeev to this toy model. We recommend the lectures of Rajeev for a more detailed exposition of the underlying ideas.[7] Rajeev in his work[1] has shown that the phase space of the two-dimensional QCD is an infinite dimensional Grassmannian, well known from the theory of integrable systems and loop groups.[8] Scalar QCD was worked out using the same methods in Ref. 9, where it was shown that the phase space of the theory is an infinite dimensional disk. Originally scalar two-dimensional QCD was worked out by Shei and Tsao in Ref. 10 following 't Hooft, and later by Tomaras using Hamiltonian methods in Ref. 11. These works obtained the analog of the 't Hooft equation for this case. A natural extension of these would be to look at combined (fermionic) QCD and scalar QCD. This is done in a paper of Aoki,[12] where it is shown that the various types of mesons are possible and they all obey 't Hooft equations. At about the same time, following a path integral approach and bilocal fields, coupled fermions and bosons as well as some other models in two dimensions were worked out in a

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beautiful article by Cavicchi.[13] Recently, Konechny and O.T.T. have extended the methods of Ref. 1 to the above-mentioned case and showed that the underlying large-N_c phase space is a certain kind of super-Grassmannian. The linearized equations agree with the ones found in Ref. 12. The correct equations are nonlinear, and there is a baryon number operator which corresponds to the supertrace of the basic variable.[14]

The real scalar field is an interesting testing ground. There are some ideas in the literature which suggest that gauge theories in two dimensions all behave in a very similar way.[15] In this work we show that the phase space of the resulting classical theory is $Sp_1(\mathcal{H})/U(\mathcal{H}_+)$, which is the analog of the Siegel disk in infinite dimensions. The linearized equations of motion give us a version of the well-known 't Hooft equation of two-dimensional QCD, and this new one is the same equation found in Ref. 10 apart from some numerical factors. That means that we have the same spectral behavior for the mesons of the theory. Since most of the details are very similar to the ones in Rajeev's lectures[7] and various aspects of the geometry of the phase space were given in a few other places[16–18] our treatment will be brief.

II. THE SCALAR $SO(N_c)$ MODEL IN THE LIGHT CONE

Since the basic philosophy was explained in Ref. 1 we will state our conventions and write down the Lagrangian of the theory. We will use the light cone coordinates $x^+=(1/\sqrt{2})\,(t+x)$, $x^-=(1/\sqrt{2})\,(t-x)$ and choose $A_-=0$ gauge,

$$S=\int \mathrm{d}x^+\,\mathrm{d}x^-\left[\frac{1}{2}\,\mathrm{Tr}\,F_{+-}F^{+-}+\frac{1}{2}\,\phi^\alpha(-2\partial_-)\partial_+\phi_\alpha\right.$$
$$\left.+\frac{g}{2}(\partial_-\phi^\alpha A_{+\alpha}^{\ \ \beta}\phi_\beta-\phi^\alpha A_{+\alpha}^{\ \ \beta}\partial_-\phi_\beta)-\frac{m^2}{2}\,\phi^\alpha\phi_\alpha\right]. \tag{1}$$

Here we have $SO(N_c)$ gauge theory for which the matter fields are in the fundamental representation and Tr denotes an invariant inner product in the Lie algebra. The Lie algebra condition implies that $A_+^T=-A_+$. To compute the variations we need the independent degress of freedom, we can expand $A_+=A_+^a T^a$, where T^a are the generators of $SO(N_c)$ Lie algebra. We can choose them such that $\mathrm{Tr}\,T^aT^b=-1/2\,\delta^{ab}$. When we use the light cone approach in $1+1$ dimensions, the gauge fields do not carry dynamical degrees of freedom. We first eliminate the gauge fields and then write the resulting action. Let us find the equation of motion for the gauge field once we rewrite the action,

$$S=\int \mathrm{d}x^+\,\mathrm{d}x^-\left[\frac{1}{2}\,\phi^\alpha(-2\partial_-)\partial_+\phi_\alpha+\frac{g}{2}A_+^a(\partial_-\phi^\alpha T^{a\beta}_{\ \ \alpha}\phi_\beta-\phi^\alpha T^{a\beta}_{\ \ \alpha}\partial_-\phi_\beta)\right.$$
$$\left.+\frac{1}{2}(\partial_-A_+^a)^2-\frac{m^2}{2}\,\phi^\alpha\phi_\alpha\right]. \tag{2}$$

If we define the current $J^a=1/2\,(\phi^\alpha T^{a\beta}_{\ \ \alpha}\partial_-\phi_\beta-\partial_-\phi^\alpha T^{a\beta}_{\ \ \alpha}\phi_\beta)$, we get

$$-\partial_-^2A_+^a=gJ^a, \tag{3}$$

which can be solved formally (an actual solution can be found if we specify some boundary conditions) and by substituting this into our Lagrangian again,

$$S=\int \mathrm{d}x^+\,\mathrm{d}x^-\left(\frac{1}{2}\,\phi^\alpha(-2\partial_-)\partial_+\phi_\alpha+\left[\frac{g^2}{2}J^a\frac{1}{\partial_-^2}J^a+\frac{m^2}{2}\,\phi^\alpha\phi_\alpha\right]\right). \tag{4}$$

Written in this form we immediately see that[1,19] we have the following symplectic form:

$$\omega^{-1}(x^-,y^-)=\langle x^-|(-2\partial_-)^{-1}|y^-\rangle=-\tfrac{1}{4}\,\mathrm{sgn}(x^--y^-) \tag{5}$$

and the Hamiltonian,

$$H=\int \mathrm{d}x^{-}\left[-\frac{g^2}{2}J^a\frac{1}{\partial_{-}^2}J^a+\frac{m^2}{2}\phi^{\alpha}\phi_{\alpha}\right]. \tag{6}$$

The same boundary conditions as the one used to find the symplectic form gives us the more explicit expression,

$$H=\frac{m^2}{2}\int \mathrm{d}x^{-}\ \phi^{\alpha}(x^{-})\phi_{\alpha}(x^{-})-\frac{g^2}{4}\int \mathrm{d}x^{-}\,\mathrm{d}y^{-}J^a(x^{-})|x^{-}-y^{-}|J^a(y^{-}). \tag{7}$$

We note that one needs the properties of the group and its represention to compute the interaction term. This can be achieved due to the identity $\Sigma_a(T^a)_{\alpha\beta}(T^a)_{\lambda\gamma}=-1/2(\delta_{\alpha\gamma}\delta_{\lambda\beta}-\delta_{\alpha\lambda}\delta_{\beta\gamma})$.

It is now possible to compute the equations of motion for the classical variable $\phi(x^{-};x^{+})$ using

$$\frac{\partial\phi}{\partial x^{+}}=\{\phi,H\}. \tag{8}$$

It is a useful exercise to find the equations of motion even for the free field theory (see the beautiful lectures by Heinzl[19]). Another important exercise is to check that the theory is Poincaré invariant written in this new way, by finding the generators.

We will follow Ref. 1 (or Ref. 7) and rewrite the theory in terms of the color invariant bilinears of the field variable ϕ after canonical quantization. In the large N_c limit these will be the only dynamical variables, and the theory has a completely classical formulation in terms of these bilinears. We will see that the remaining global $SO(N_c)$ symmetry we have imposes a constraint for these variables and that means the phase space of the theory is a curved manifold in infinite dimensions.

Canonical quantization is standard, since the theory is super-renormalizable the result is the same as free field theory and the choice of vacuum is exactly the same. The equal ''time'' commutator is given by

$$[\hat{\phi}_{\alpha}(x^{-},x^{+}),\hat{\phi}_{\beta}(y^{-},x^{+})]=-\frac{i}{4}\delta_{\alpha\beta}\,\mathrm{sgn}(x^{-}-y^{-}). \tag{9}$$

This means that it is simpler to introduce creation and annihilation operators, satisfying

$$[a_{\alpha}(p),a_{\beta}(q)]=2\pi\delta(p+q)\delta_{\alpha\beta}\,\mathrm{sgn}(p), \tag{10}$$

such that

$$\hat{\phi}_{\alpha}(x^{-})=\int\frac{\mathrm{d}p}{2\pi}\frac{a_{\alpha}(p)}{\sqrt{2|p|}}e^{-ipx^{-}}. \tag{11}$$

For quantum theory we introduce the Fock vacuum $|0\rangle$:

$$a_{\alpha}(p)|0\rangle=0 \quad \text{when } 0\leqslant p. \tag{12}$$

To get well-defined expressions for various operators—such as the Hamiltonian—we need a normal ordering prescription:

$$:a_{\alpha}(p)a_{\beta}(q):=\begin{cases}a_{\beta}(q)a_{\alpha}(p) & \text{if } q<0,\quad p>0\\ a_{\alpha}(p)a_{\beta}(q) & \text{otherwise.}\end{cases} \tag{13}$$

We note that it is also possible to think about the creation and annihilation operators via a Fourier expansion,

$$\hat{\phi}_\alpha(x^-)=\int_0^\infty \frac{dp}{2\pi\sqrt{2|p|}}(a_\alpha(p)e^{-ipx^-}+a_\alpha^\dagger(p)e^{ipx^-}), \tag{14}$$

manifesting the real valuedness of the field $\hat{\phi}_\alpha^\dagger=\hat{\phi}_\alpha$. This automatically implies that $a_\alpha^\dagger(p)=a_\alpha(-p)$ for $p>0$. In Sec. III we will see that this is a more appropriate way to think about quantization, yet from a calculational point of view the other is better. One notes that this is consistent with the commutation relations of a_α's. (See Refs. 19 and 20 for more details about the light-cone vacuum structure of the real scalar field.)

The normal ordering can be written in terms of the ordinary products of the operators and a vacuum subtraction,

$$:a_\alpha(p)a_\beta(q):=a_\alpha(p)a_\beta(q)-\tfrac{1}{2}(\mathrm{sgn}(p)+1)2\pi\delta(p+q)\delta_{\alpha\beta}. \tag{15}$$

We will make use of this relation quite frequently in Sec. III.

III. ALGEBRA OF COLOR INVARIANT OPERATORS

In this section we will discuss the class of operators we will use to reformulate the gauge theory in the large-N_c limit. Since we have fixed the gauge as $A_-=0$ we are not allowed to make any more space-dependent gauge transformations. (The equations of motion at the quantum level imply that the ''time''-dependent transformations cannot be made arbitrarily but given by the evolution of the scalar field. We do not need to look at these in any case since in the Hamiltonian formalism observables at a fixed ''time'' slice are enough.) Yet there is still a global $SO(N_c)$ symmetry which is left over. To emphasize the contraction we write down the color invariant bilinears with one index up, the other index down,

$$N(x^-,y^-)=\frac{1}{N_c}:\hat{\phi}^\alpha(x^-)\hat{\phi}_\alpha(y^-):. \tag{16}$$

The set of these equal time bilinears constitute the set of all possible color invariant operators for this theory. One may equally look at the Fourier transform of these operators, so the basic bilinears in this case become

$$\hat{T}(p,q)=\frac{2}{N_c}\sum_\alpha :a_\alpha(p)a_\alpha(q):. \tag{17}$$

As we will see in Sec. IV conceptually it is more natural to use the variables

$$\hat{K}(p,q)=-\frac{2}{N_c}\mathrm{sgn}(p)\sum_\alpha :a_\alpha^\dagger(p)a_\alpha(q):, \tag{18}$$

but for calculations it is easier to keep the above-given variables. The basic idea of the large-N_c theory is to write everything in terms of these color invariant bilinears. In the limit N_c becomes large only the color invariant operators survive and furthermore the expectation values of color invariant operators split as a product up to $1/N_c$ corrections. This implies that the set of color invariant operators becomes classical; all color invariant operators should be representable as classical observables. The resulting theory, restricted to the space of color invariant states, therefore becomes a classical theory.[1,7,21] To define this classical theory we compute the commutator of two such color invariant operators and then take the appropriate large-N_c limit. The result will be

postulated as a classical Poisson bracket of these classical variables. We will see later on that this Poisson bracket actually comes from a symplectic form on a very natural infinite dimensional homogeneous symplectic manifold.[17]

When we compute the commutator of such bilinears we get

$$[\hat{T}(p,q),\hat{T}(s,t)]=\frac{2}{N_c}(\mathrm{sgn}(p)\,\delta[p+s]\hat{T}(q,t)+\mathrm{sgn}(q)\,\delta[q+s]\hat{T}(p,t)$$
$$+\mathrm{sgn}(p)\,\delta[p+t]\hat{T}(s,q)+\mathrm{sgn}(q)\,\delta[q+t]\hat{T}(s,p)$$
$$+(\mathrm{sgn}(p)+\mathrm{sgn}(q))(\,\delta[p+s]\delta[q+t]+\delta[p+t]\delta[s+q])),$$

where we defined $\delta[p+q]=2\pi\delta(p+q)$ for convenience.

If we take the limit $N_c\to\infty$ we assume that there are corresponding classical observables and the commutators go to Poisson brackets of these observables. We still denote them by the same letter except we drop the caret on the top. Applying the rule $-(i/\hbar)[A,B]\mapsto\{A,B\}$, as $\hbar=N_c^{-1}\to 0$, we get

$$\{T(p,q),T(s,t)\}=-2i(\mathrm{sgn}(p)\,\delta[p+s]T(q,t)+\mathrm{sgn}(q)\,\delta[q+s]T(p,t)$$
$$+\mathrm{sgn}(p)\,\delta[p+t]T(s,q)+\mathrm{sgn}(q)\,\delta[q+t]T(s,p)$$
$$+(\mathrm{sgn}(p)+\mathrm{sgn}(q))(\,\delta[p+s]\delta[q+t]+\delta[p+t]\delta[s+q])).$$

(There is really no way to determine the correct quantization parameter in this approach. We can only find this when we quantize the theory back again. The most natural method to employ is geometric quantization, due to the natural geometry of the phase space. We will come back to these issues in a separate publication.) We will postulate these to be the basic Poisson brackets of our dynamical variables. It is a good exercise to compute the equations of motion for the free field in this language and write down the solution.

These variables acting on the color invariant sector are not completely independent, there is a constraint coming from the global color invariance. Recall that the global $SO(N_c)$ is generated by the operators acting on the Fock space,

$$\hat{Q}_{\alpha\beta}=\int_0^\infty\frac{\mathrm{d}p}{2\pi}a_\alpha^\dagger(p)a_\beta(p)-\int_0^\infty\frac{\mathrm{d}p}{2\pi}a_\beta^\dagger(p)a_\alpha(p). \tag{19}$$

These operators satisfy $\hat{Q}_{\alpha\beta}|0\rangle=0$ and

$$[\hat{Q}_{\alpha\beta},\hat{Q}_{\lambda\gamma}]=\hat{Q}_{\lambda\alpha}\delta_{\beta\gamma}+\hat{Q}_{\beta\lambda}\delta_{\alpha\gamma}+\hat{Q}_{\gamma\beta}\delta_{\lambda\alpha}+\hat{Q}_{\lambda\alpha}\delta_{\gamma\beta}. \tag{20}$$

One can see that $\hat{Q}_{\alpha\beta}=-\hat{Q}_{\beta\alpha}$. Recall the related set of bilinear variables,

$$\hat{K}(p,q)=-\frac{2}{N_c}\mathrm{sgn}(p):a_\alpha^\dagger(p)a_\alpha(q):, \tag{21}$$

a careful computation shows that when we restrict these variables to the color invariant sector of the Fock space in the large-N_c limit we get

$$\int_{-\infty}^{\infty}K(p,s)K(s,q)[\mathrm{ds}]-\mathrm{sgn}(p)K(p,q)-K(p,q)\mathrm{sgn}(q)=0. \tag{22}$$

This operator equation is now interpreted as an equation for the kernel of an integral operator acting on the one-particle Hilbert space. We can write the same constraint in a more succint manner as

$$(K+\epsilon)^2=I, \tag{23}$$

where $\epsilon(p,q)=-\mathrm{sgn}(p)\delta[p-q]$ and we interpret this as an operator equation again. We will talk about the meaning of this equation from a more geometric point of view in Sec. IV. The important assumption is that when we let $N_c\mapsto\infty$, the above-mentioned constraint translated into a constraint for the classical variables K. So the dynamical variables K satisfy this constraint, which implies a constraint for $T(p,q)$ trivially.

We rewrite the Hamiltonian by redefining the coupling constant as $g^2N_c\mapsto g^2$ and dividing the Hamiltonian by an overall factor of N_c. Thus the Hamiltonian becomes, after mass renormalization,

$$H_0=\frac{1}{8}\left(m_R^2-\frac{g^2}{2\pi}\right)\mathcal{P}\int\frac{[\mathrm{d}p]}{|p|}T(-p,p), \tag{24}$$

where the renormalized mass is given by $m^2=m_R^2+(g^2/4\pi)\ln(\Lambda_U/\Lambda_I)$, Λ_U, Λ_I referring to the ultraviolet and infrared cutoffs, respectively, we also used the shorthand $[\mathrm{d}p]=\mathrm{d}p/2\pi$, and $\mathcal{P}$ denotes the principal value prescription. This is not a simple computation but the essential steps are given in Ref. 7, and the interaction part

$$H_I=\frac{g^2}{64}\mathcal{FP}\int\frac{[\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t]}{\sqrt{|pqst|}}\delta[p+q+s+t]\frac{sq-st+pt-pq}{(p+s)^2}T(p,q)T(s,t), \tag{25}$$

where $\mathcal{FP}$ denotes the finite part, as explained in Ref. 7. For simplicity of notation from now on we will drop the symbols, $\mathcal{P}$ and $\mathcal{FP}$, but the calculations should be performed keeping these in mind. At this point we have the complete formulation of our theory—one can compute the equations of motion using the above-mentioned form of the Hamiltonian and the Poisson brackets of the variables $T(u,v)$. At this stage we will not be able to give an analysis of these nonlinear equations and instead confine ourselves to the linear approximation.

For the linear approximation we follow Ref. 7 and we will write the above-mentioned constraint in terms of the T variables and ignore the second-order term in T. This will be our linearized constraint,

$$[1-\mathrm{sgn}(u)\mathrm{sgn}(v)]T(u,v)=0. \tag{26}$$

In the following we will keep all the equations of motion to this approximation and search for a bound state solution.

We can compute the equations of motion in the linear approximation: this means we look at $T(u,v)$ for $u,v>0$ or $u,v<0$, the other cases imply $T(u,v)=0$ from the constraint equation. Let us look at the $u,v<0$ case and define $P=-(u+v)$ and $x=-u/P$. This means $u=-Px$, $v=-P(1-x)$ and $0<x<1$. If we actually compute the equations of motion $\partial_+T(u,v;x^+)=\{T(u,v;x^+),H\}$, and make an ansatz, $T(u,v)=e^{iP_+x^+}\zeta(x)$, we get

$$\mu^2\zeta(x)=\left(m_R^2-\frac{g^2}{2\pi}\right)\left[\frac{1}{x}+\frac{1}{1-x}\right]\zeta(x)-\frac{g^2}{8\pi}\int_0^1\left[\frac{y(1-x)+x(1-y)+y(1-y)+x(1-x)}{(x-y)^2}\right.$$
$$\left.+\frac{xy+(1-x)(1-y)+y(1-y)+x(1-x)}{(y-(1-x))^2}\right]\frac{\zeta(y)\mathrm{d}y}{\sqrt{x(1-x)y(1-y)}},$$

where $\mu^2=2P_+P$ is the invariant mass of this excitation. We should solve this eigenvalue equation to find the allowed values of μ^2 and the function ζ. This will determine the spectrum of the theory. One notes that the equation is symmetric under $x\mapsto1-x$ and $y\mapsto1-y$, that means we may choose $\zeta(x)=\zeta(1-x)$. This simplifies our equation to

$$\mu^2\zeta(x)=\left(m_R^2-\frac{g^2}{2\pi}\right)\left[\frac{1}{x}+\frac{1}{1-x}\right]\zeta(x)-\frac{g^2}{4\pi}\int_0^1\frac{(x+y)(2-x-y)}{(x-y)^2}\frac{\zeta(y)\mathrm{d}y}{\sqrt{x(1-x)y(1-y)}}. \quad (27)$$

The above-given form is in fact identical to the bound state equation found in Ref. 10 and later on by Tomaras using Hamiltonian methods apart from the numerical factors (this approach is closer to the one in Ref. 1). It is known that this theory has only discrete states, that is we only have bound state solutions and no scattering states.

We may search for the baryons in this theory [from a more standard point of view, we do not have any $U(1)$ symmetry in the classical action; this suggests that there should not be baryon number conservation and no baryons—we will see that the baryon number is indeed not conserved for the gauge theory].

Note that there is no antibaryon. Let us write down a typical baryonic operator,

$$B(p_1,p_2,\ldots,p_{N_c})=\frac{1}{Z}\epsilon_{\alpha_1\alpha_2\ldots\alpha_{N_c}}a^\dagger_{\alpha_1}(p_1)a^\dagger_{\alpha_2}(p_2)\cdots\ a^\dagger_{\alpha_{N_c}}(p_{N_c}), \quad (28)$$

where Z is an appropriate normalization factor. When we take the large-N_c limit these operators become infinite strings which are not representable in a simple way. But we can still detect them if they are present in a physical state. We write a one-baryon state as $B(p_1,p_2,\ldots,p_{N_c})|0\rangle$, and define the baryon operator,

$$\hat{B}=\frac{1}{N_c}\int_0^\infty[\mathrm{d}p]{:}a^\dagger_\alpha(p)a_\alpha(p){:}. \quad (29)$$

In general we have the action of the baryon operator on many baryon states,

$$\frac{1}{N_c}\int_0^\infty[\mathrm{d}p]{:}a^\dagger_\alpha(p)a_\alpha(p){:}B(p_1,p_2,\ldots,p_{N_c})B(q_1,q_2,\ldots,q_{N_c})\ldots B(s_1,s_2,\ldots,s_{N_c})|0\rangle$$
$$=(\textbf{number of baryons})B(p_1,p_2,\ldots,p_{N_c})B(q_1,q_2,\ldots,q_{N_c})\ \cdots B(s_1,s_2,\ldots,s_{N_c})|0\rangle.$$

We may have mesonic parts in general, but in this picture they seem to be of smaller order. Note that this operator will survive the large-N_c limit and can be represented as the half trace of the variable $T(p,q)$ evaluated only for the positive momenta. A natural question is if the baryon number operator is conserved under the evolution of our system—it does not follow from a simple symmetry principle—a direct method is to see if this operator Poisson commutes with a quadratic Hamiltonian. Let us write down a general quadratic Hamiltonian as

$$H=\int[\mathrm{d}p]h(p)T(-p,p)+\int[\mathrm{d}p\ \mathrm{d}q\ \mathrm{d}s\ \mathrm{d}t]G(p,q;s,t)T(p,q)T(s,t). \quad (30)$$

The Poincaré invariance will impose certain restrictions on the choice of functions h, G. There are a few obvious symmetries coming from the properties of the variable T, the considerations of Sec. IV show all the symmetries required on $G(p,q;s,t)$. If we now compute

$$\left\{H,\int_{-\infty}^{\infty}T(-u,u)[\mathrm{d}u]\right\}=2i\int[\mathrm{sgn}(p)+\mathrm{sgn}(q)]G(p,q;s,t)T(p,q)T(s,t)[\mathrm{d}p\ \mathrm{d}q\ \mathrm{d}s\ \mathrm{d}t], \quad (31)$$

the use of the symmetries in general will not give zero: this means that the baryon number is not conserved in general! In our case the computation gives a nonzero result, thus in the conventional sense *we do not have baryons*, yet we may have nonzero values of the trace implying possible baryonic states. We will see more comments on this from the geometry in Sec. IV.

IV. GEOMETRY OF THE PHASE SPACE

In this section we present a somewhat more rigorous approach and provide an interpretation of the underlying phase space of the theory. To do this let us discuss quantization again, for this we closely follow the ideas in the article by Bowick and Rajeev[17] and for a more detailed presentation we refer to the beautiful article by Gracia-Bondia and Varilly.[16] There is also a nice group theoretic presentation in Ref. 22.

When we look at a real scalar field in two dimensions in the light cone formalism, we may formally quantize the system by declaring the existence of operators corresponding to the fields and we replace the Poisson bracket relations of these fields by commutators with an additional factor of i. Of course we assume that there is an underlying *complex* Hilbert space on which these operators act! In this formal process we do not see where the complex structure comes from. In fact there is a natural complex structure: let us assume that the free Hamiltonian is formally written as a quadratic form in the fields, $H_0=\int 1/2\,\phi_\alpha Q_{\alpha\beta}\phi_\beta$, and we have a symplectic structure, ω, $\int 1/2\,\phi_\alpha \omega_{\alpha\beta}\partial_+\phi_\beta$. This symplectic structure defines a skew form on the space of solutions to the classical field equations. The natural operator to introduce is $\tilde{\omega}=\omega^{-1}Q$, this is a real antisymmetric operator(matrix) of type (1,1), and comes from the equations of motion. We use its polar decomposition, $\tilde{\omega}=JS$, where $J^TJ=1$ and $S^T=S$ with $S>0$. Now using the antisymmetry of $\tilde{\omega}$ we see that $J^2=-1$. This defines a complex structure which we can use to complexify our real Hilbert space. If we apply this to our case, the metric coming from the free Hamiltonian, $H_0=(m^2/2)\int dx^-\,\phi_\alpha(x^-)\phi_\alpha(x^-)$, becomes $Q_{\alpha\beta}(x^-,y^-)=m^2\delta(x^--y^-)\,\delta_{\alpha\beta}$, and the symplectic form (see Sec. III) $\omega_{\alpha\beta}(x^-,y^-)=\langle x^-|-2\partial_-|y^-\rangle\,\delta_{\alpha\beta}$. If we write down the polar decomposition, we have

$$J_{\alpha\beta}(x^-,y^-)=\langle x^-|-(\partial_-^T\partial_-)^{1/2}\partial_-^{-1}|y^-\rangle\,\delta_{\alpha\beta}=\langle x^-|-(-\partial_-^2)^{1/2}\partial_-^{-1}|y^-\rangle\,\delta_{\alpha\beta}. \tag{32}$$

Written in this form this is a real operator acting on the L_2 space of initial data on the light cone. We can extend this operator to a complex Hilbert space and it is then possible to diagonalize the above-mentioned J in this complexified space. So we think of a complex L_2 space, $V^{\mathbf{C}}=V\otimes\mathbf{C}=W\oplus\overline{W}$, where W is isomorphic to $\overline{W}$, in the infinite dimensional case they are both separable. The decomposition we use corresponds to the eigenspaces of J. If we write J as a block diagonal on such a decomposition we get

$$J=\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.$$

We know from our experience in physics that this is the form we use. If we decompose the fields into Fourier modes at the initial data surface $x^+=0$,

$$\phi_\alpha(x^-)=\int_0^\infty \frac{[dp]}{\sqrt{2p}}(\overline{z_\alpha}(p)e^{-ipx^-}+z_\alpha(p)e^{ipx^-}) \tag{33}$$

and act upon it by J, we see that we get

$$(J\phi_\alpha)(x^-)=\int_0^\infty \frac{[dp]}{\sqrt{2p}}(-i\overline{z_\alpha}(p)e^{-ipx^-}+iz_\alpha(p)e^{ipx^-}). \tag{34}$$

So we see that the decomposition of the field into its positive and negative frequency modes is the same as using the eigenvalue decomposition of the underlying complex structure. (We note that this decomposition is relativistically invariant, and the division by momentum variable $\sqrt{2p}$ is for convenience.) Now we can also see that the inverse of our skew form transforms under such a change of basis as $R^{-1}\omega^{-1}(R^{-1})^T$, where we represent the Fourier transform as R. Here T refers to the ordinary transpose. Thus we evaluate

$$\int \mathrm{d}x^- \,\mathrm{d}y^- \, e^{iqx^-}\sqrt{2|q|}\left(\frac{-1}{2\partial_-}\right)e^{ipy^-}\sqrt{2|p|} = i\,\mathrm{sgn}(p)\,\delta[p+q], \tag{35}$$

which shows that the symplectic form transforms to the standard form now defined on a complex Hilbert space.

The correct quantization in the infinite dimensional case requires this complex structure, the formal quantization rule,

$$[\hat{\phi}_\alpha(x^-),\hat{\phi}_\beta(y^-)] = -\frac{i}{4}\,\delta_{\alpha\beta}\,\mathrm{sgn}(x^- - y^-), \tag{36}$$

clearly requires a complex space, we assume the real field is a self-adjoint operator, $\hat{\phi}(x^-) = \hat{\phi}(x^-)$. In fact we really think of this system in terms of creation and annihilation operators acting on a complex Hilbert space. This is best done by going into a Fourier decomposition and introducing the creation and annihilation operators corresponding to positive and negative frequency components. Such a decomposition is necessary to make the commutation relations meaningful, a glance at them shows that $[a_\alpha(p),a_\beta(q)] = \mathrm{sgn}(p)\delta[p+q]$ is consistent with the creation and annihilation operator interpretation if we define $a_\alpha(p)$ to be the annihilation and $a_\alpha(-p)$ to be the creation operators for $p>0$. Now we see that what determines this is precisely the complex structure, $J=-i\,\mathrm{sgn}(p)$. This form of the complex structure reveals another important aspect of this problem: there is no dependence on the mass. *If the bare mass changes due to the interactions, this does not change the quasifree representation of our commutation relations that were chosen at the start using the free part only*. The frequencies obviously change but that does not affect the representation. To make the Hamiltonian and various other operators of physical interest well-defined in this Fock space we must introduce a normal ordering prescription.

If we compute the commutator of two normal ordered bilinears of the field operators, that provides a realization of the real symplectic Lie algebra in its standard form. When we switch to the Fourier modes, and use the corresponding creation and annihilation operators we use the embedding of the real symplectic Lie algebra into the complex symplectic Lie algebra. In fact our operators $K(p,q)$, in the large-N_c limit, correspond to the Lie algebra generators with respect to this embedding. We will discuss this in the following. If we define our symplectic form as a matrix $\omega = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$, and the complex structure as $J = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$, we can diagonalize our complex structure in a complex Hilbert space by $R = (1/\sqrt{2})\left(\begin{smallmatrix} i & -i \\ 1 & 1 \end{smallmatrix}\right)$, then $R^{-1}JR = \left(\begin{smallmatrix} -i & 0 \\ 0 & i \end{smallmatrix}\right)$, whereas $R^T\omega R = i\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$. In such an embedding the real symlectic group defined by ω becomes

$$\begin{pmatrix} a & b \\ \overline{b} & \overline{a} \end{pmatrix}, \tag{37}$$

and naturally still preserves the transformed form of ω, but that is the same as the complex symplectic group, since ω as a matrix preserves its form. A general complex symplectic matrix $g = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$, satisfies,

$$a^T c = c^T a, \quad b^T d = d^T b, \quad a^T d - c^T b = 1. \tag{38}$$

In our example we see that the Fourier transform does this transformation: it brings J into diagonal form and ω to the standard form.

The real Lie algebra can be written as

$$1 + i\begin{pmatrix} F & G \\ -\overline{G} & -\overline{F} \end{pmatrix}, \tag{39}$$

where $F^\dagger = F$ and $G^T = G$. In fact one can check that the large-N_c limit operators $K(p,q)$ obey these conditions. Furthermore there will be convergence conditions coming from the super-

renormalizability of our theory. This corresponds to the fact that we require normal ordered bilinears to create finite norm states when they act on any other state constructed from the vacuum by the action of creation operators—of course strictly speaking we should think about smeared out operators but we will ignore this technical part for this work. We can simply say that the off-diagonal components of these operators, that is b parts, should be Hilbert–Schmidt operators. In the same way we demand the same for the Lie algebra elements. (In higher dimensional theories this requirement is not satisfied and one needs a much more sophisticated not completely understood approach. One possibility was proposed by Mickelsson and Rajeev.[23,24])

In this language the constraint should be written as $(iK+i\epsilon)^2=-1$, and $i\epsilon=J$, i.e., it is the diagonal form of the complex structure we were to begin with. There is the skew form which has a matrix form in this basis $\omega=\left(\begin{smallmatrix}0 & 1\\ -1 & 0\end{smallmatrix}\right)$, which defines the symplectic group on $W\oplus\overline{W}$. We will see that the constraint actually defines a homogeneous manifold of the underlying real symplectic group. If we introduce a variable $\Phi=K+\epsilon$, the constraint becomes

$$\Phi^2=1. \tag{40}$$

One can also verify the following condition:

$$\Phi^T=\omega^{-1}\Phi\omega. \tag{41}$$

This is nothing but the Lie algebra condition. In this basis there is no difference as matrices between ω and ω^{-1} but we should remember that they transform differently. Furthermore the convergence condition becomes,

$$[\epsilon,\Phi]\in\text{Hilbert}-\text{Schmidt}. \tag{42}$$

As we will see in the following part these conditions correspond to the infinite dimensional version of the Siegel disk.

We now define a homogeneous manifold which will be denoted by D_1^R. It is essentially a real version of the disk which corresponds to the pseudounitary group. Let us define a Hilbert space $\mathcal{H}_+$, which refers to the positive frequency modes of the theory. We can also say that these are the functions which have only positive modes in their Fourier decomposition. We introduce a set of operators $Z:\mathcal{H}_+\to\mathcal{H}_-$, where $\mathcal{H}_-$ is $\overline{\mathcal{H}_+}$ in the above-given language. (If we use the full complex Hilbert space, $\mathcal{H}=\mathcal{H}_+\oplus\mathcal{H}_-$.) We impose $Z^T=Z$. We have a complex conjugation σ, this intertwines between $\mathcal{H}_+$ and $\mathcal{H}_-$, we define $Z^T=\sigma Z^\dagger\sigma$, note that $Z^\dagger:\mathcal{H}_-\to\mathcal{H}_+$, thus $Z^T:\mathcal{H}_+\to\mathcal{H}_-$. Furthermore $\overline{Z}=\sigma Z\sigma:\mathcal{H}_+\to\mathcal{H}_-$. There is an extra condition on Z: $1-Z^\dagger Z>0$. We also need a convergence condition which comes from the infinite dimensionality of the theory: $Z\in\mathcal{I}_2$, where $\mathcal{I}_2$ denotes the Hilbert–Schmidt ideal.[7,24,25]

We introduce a real restricted symplectic group, Sp_1 embedded into the above-mentioned complex symplectic group, which we precisely define in the following:

$$Sp_1^c(\mathcal{H})=\{g:\mathcal{H}\to\mathcal{H}|g^{-1}\text{ exits},\ \ g^T\omega g=\omega\ \text{ and }\ [\epsilon,g]\in\mathcal{I}_2\}. \tag{43}$$

Here we are using ordinary matrix transpose to be able to write explicit matrix elements. We can see that this is a group and we call it the restricted complex symplectic group, and its subgroup of the form

$$\begin{pmatrix} a & b\\ \overline{b} & \overline{a}\end{pmatrix},\ \text{where } b\in\mathcal{I}_2 \tag{44}$$

corresponds to the restricted real symplectic group $Sp_1(\mathcal{H})$. J itself is a real symplectic matrix and we are using a basis for the complexified Hilbert space in which J becomes diagonal.

The real symplectic group has an action on the space of operators Z, given by

$$g\circ Z=(aZ+b)(\overline{b}Z+\overline{a})^{-1}. \tag{45}$$

We can check that the action obeys the usual rule $g_1\circ(g_2\circ Z)=(g_1g_2)\circ Z$. To prove that the action preserves all the conditions we look at the orbit of $Z=0$, which is obviously in this set D_1^R. We see that the resulting element $b\overline{a}^{-1}$ satisfies all the properties, hence the orbit remains inside the disk. (We should of course see that the inverse of $\overline{a}$ exists, but that is easy using the properties of the group.) Let us assume that a Z is given, we claim that any such element lies in the orbit of $Z=0$. To show this we explicitly construct a group element which does this:

$$g(Z)=\begin{pmatrix} (1-\overline{Z}Z)^{-1/2} & Z(1-\overline{Z}Z)^{-1/2} \\ \overline{Z}(1-Z\overline{Z})^{-1/2} & (1-\overline{Z}Z)^{-1/2} \end{pmatrix}. \tag{46}$$

Note that everything here is well-defined. We leave it to the reader to check that $g(Z)$ is an element of the real group. This shows that the disk is actually a homogeneous space: take any element Z, pull it back to $Z=0$ by $g^{-1}(Z)$ and to reach any element $\tilde{Z}$ use the group element corresponding to this for the orbit of $Z=0$, $g(\tilde{Z})$ and use the compatibility condition, $\tilde{Z}=(g(\tilde{Z})g^{-1}(Z))\circ Z$. It is clear that the action then remains inside the disk.

We see that the disk is actually a complex homogeneous space, the stability subgroup corresponding to $Z=0$ is given by

$$U(\mathcal{H}_+)=\begin{pmatrix} a & 0 \\ 0 & \overline{a} \end{pmatrix}. \tag{47}$$

If we use symplectic condition we get $a^\dagger a=aa^\dagger=1$, which means a is an element of the unitary group of $\mathcal{H}_+$. This means we have

$$D_1^R=\frac{Sp_1(\mathcal{H})}{U(\mathcal{H}_+)}. \tag{48}$$

We will in fact see that the above-mentioned space is a complex homogeneous symplectic manifold, but before this it is useful to introduce a variable $\Phi(Z)$:

$$\Phi(Z)=-1+2\begin{pmatrix} (1-Z\overline{Z})^{-1} & -(1-Z\overline{Z})^{-1}Z \\ \overline{Z}(1-Z\overline{Z})^{-1} & -\overline{Z}(1-Z\overline{Z})^{-1}Z \end{pmatrix}. \tag{49}$$

Using the defining properties of Z we can check that

$$\Phi(Z)^2=1, \quad \Phi(Z)^T=\omega^{-1}\Phi(Z)\omega, \quad [\epsilon,\Phi(Z)]\in\mathcal{I}_2, \tag{50}$$

where we used the explicit standard matrix form of ω. Note that these are the same conditions on our physical variable Φ. We claim that all such $\Phi(Z)$ lie on the orbit of $\epsilon=\Phi(Z=0)$. This is easy to see using

$$\Phi(Z)=-g(Z)\epsilon\omega^{-1}g(Z)^T\omega, \tag{51}$$

which also verifies the above-mentioned conditions once more. One can see using the above-mentioned identification that the action of the group on Z becomes quite simple in terms of Φ,

$$g\circ Z\mapsto g\Phi g^{-1}. \tag{52}$$

We can check that this action preserves all the conditions on Φ.

The manifold we have found is actually symplectic. We may define a natural two form,

$$\Omega = \frac{i}{4} \mathrm{Tr}\, \Phi\, d\Phi \wedge d\Phi. \tag{53}$$

This formal expression should be understood as follows. We look at vector fields at a point Φ, any such thing can be expressed in terms of the Lie algebra elements, $V_u(\Phi) = [u, \Phi]$, where u is an element of the Lie algebra. then the two form becomes.

$$\Omega(V_u, V_v) = \frac{i}{8} \mathrm{Tr}\, \Phi[[u,\Phi],[v,\Phi]] = \frac{i}{8} \mathrm{Tr}\, \epsilon[[\epsilon, g^{-1}ug],[\epsilon, g^{-1}vg]]. \tag{54}$$

The above-mentioned form shows that the trace is well-defined due to the Hilbert–Schmidt conditions.[1,7,9] From this point of view it is easy to see that the above-mentioned form is homogeneous, and it is closed (see Refs. 1 and 7). Nondegeneracy can be proved at $\Phi = \epsilon$ and using homogeneity this is true over the manifold. If we look at the symplectic form at ϵ by using the Z coordinates, we get

$$\Omega|_{\epsilon} = 2i\, \mathrm{Tr}\, d\bar{Z} \wedge dZ. \tag{55}$$

A short computation reveals that when we write $g^{-1}ug = i\left(\begin{smallmatrix} F_1 & G_1 \\ -\bar{G}_1 & -\bar{F}_1 \end{smallmatrix}\right)$ and the same for v, $g^{-1}vg = i\left(\begin{smallmatrix} F_2 & G_2 \\ -\bar{G}_2 & -\bar{F}_2 \end{smallmatrix}\right)$ we get

$$\Omega(V_u, V_v) = -\frac{i}{2} \mathrm{Tr}(G_1 \bar{G}_2 - G_2 \bar{G}_1) = -i\, \Im\mathrm{m}\, \mathrm{Tr}\, G_1 \bar{G}_2. \tag{56}$$

In fact the previous Poisson brackets come from this sympectic form, as can be checked. We will leave the details to the reader. We note an important point about Φ. The reader can verify that

$$\Phi - \epsilon = \begin{pmatrix} 2Z(1-\bar{Z}Z)^{-1}\bar{Z} & -(1-Z\bar{Z})^{-1}Z \\ 2\bar{Z}(1-Z\bar{Z})^{-1} & -2\bar{Z}(1-Z\bar{Z})Z \end{pmatrix} \in \begin{pmatrix} \mathcal{I}_1 & \mathcal{I}_2 \\ \mathcal{I}_2 & \mathcal{I}_1 \end{pmatrix}, \tag{57}$$

where $\mathcal{I}_1$ denotes the ideal of trace class operators, hence a conditional trace for the variable $\Phi - \epsilon$ exists. We may therefore find moment maps which generate the underlying symmetry of the theory. We write down the answer but do not spend much time on it since we will not make use of these maps: $F_u = -1/2 \mathrm{Tr}_{\epsilon}\, u(\Phi - \epsilon)$, here $\mathrm{Tr}_{\epsilon} A = 1/2 \mathrm{Tr}(A + \epsilon A \epsilon)$. These provide a Poisson realization of the Lie algebra.

There could be baryonic states in the finite N_c theory given by

$$\frac{1}{Z} \epsilon_{\alpha_1 \alpha_2 \cdots \alpha_{N_c}} a^{\dagger}_{\alpha_1}(p_1) a^{\dagger}_{\alpha_2}(p_2) \cdots a^{\dagger}_{\alpha_{N_c}}(p_{N_c}) |0\rangle, \tag{58}$$

where all the momenta are positive (see Sec. III). We can measure this baryonic content by the half-trace of the operator K. We iterate again that *this is not a conserved quantity*, hence there is no baryon in the usual sense or a baryon number. The full trace gives zero since there is no antibaryon. Let us see this by looking at the operator Φ. If we evaluate the trace $\mathrm{Tr}_{\epsilon}(\Phi - \epsilon) = 2(\mathrm{Tr}\, bb^{\dagger} - \mathrm{Tr}\, \bar{b}\bar{b}^{T})$, where we used the appropriate group element $g = \left(\begin{smallmatrix} a & b \\ \bar{b} & \bar{a} \end{smallmatrix}\right)$ to write Φ. One can see that $\mathrm{Tr}\, \bar{b}\bar{b}^{T} = \overline{\mathrm{Tr}\, bb^{\dagger}} = \mathrm{Tr} bb^{\dagger}$ since $bb^{\dagger}$ is poisitive Hermitian. This shows that the trace is zero. In fact physically the correct one to take is half of this trace as we have seen in Sec. III, so we define

$$B = \frac{1}{2} \mathrm{Tr}\left[\left(\frac{1+\epsilon}{2} \right) (\Phi - \epsilon) \right]. \tag{59}$$

We see that this is a positive number, which in the large-N_c limit corresponds to the some type of baryonic content. The authors are unable to find a reason for this to be an integer, unlike the case discussed by Rajeev in Ref. 1, where the trace is related to the Fredholm index of the operators, and thus is automatically an integer. Not only is the baryonic content noninteger, it is always nonzero. That is, when there are mesons there are also baryonic states. The limit we use seems to suggest that the baryon content and mesonic states start to mix up, since the above-mentioned trace is zero only for the vacuum ϵ. Another perspective on baryons is to think of the solitonic excitations of the gauge theory, and in our case a nonzero trace perhaps implies these type of excitations. The reader may then question the validity of the linear approximation, since we claim that the baryon number is always nonzero. In the linear approximation the above-mentioned trace should be taken as zero, since it corresponds to a quadratic.

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Quantum Clifford algebra from classical differential geometry

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We show the emergence of Clifford algebras of nonsymmetric bilinear forms as cotangent algebras of Kaluza–Klein (KK) spaces pertaining to teleparallel space–times. These spaces are canonically determined by the horizontal differential invariants of Finsler bundles of the type, $B'(M)\rightarrow S(M)$, where $B'(M)$ is the set of all the tangent frames to a differentiable manifold M, and where $S(M)$ is the sphere bundle. If M is space–time itself, M^4, the ''geometric phase space,'' $S(M^4)$, has dimension seven. This reformulation of the horizontal invariants as pertaining to a KK space removes the mismatch between the dimensionality of the tangent frames to M^4 and the dimensionality of $S(M^4)$. In the KK space, a symmetric tangent metric induces a cotangent metric which is not symmetric in general. An interior covariant derivative in the sense of Kaehler is defined. It involves the antisymmetric part of the cotangent metric, which thus enters electrodynamics and the Dirac equation. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In this paper, we follow Fauser and Ablamowicz in using the term quantum Clifford algebra (QCA) to refer to the Clifford algebra of a bilinear, not necessarily symmetric, metric.[1] The main interest of these algebras is their applicability to problems in quantum field theory, particle physics, and condensed matter physics. Some of the applications that have been suggested are fermion creation and annihilation,[2] regularization,[3] vertex ordering,[4] generating functionals,[5] and composite and multiparticle theory.[1] Also, the relation of QCAs to q-deformations of Clifford algebras[6] allows one to claim for QCA applications such as collective excitations, already claimed for q-deformations of Clifford algebras.[7] The impending issue is: where do these Clifford algebras of nonsymmetric form come from? In this paper, we show that they emerge naturally in the Kaluza–Klein (KK) context intimated in the abstract. But, first, we shall explain the title of the paper.

A more precise, though cumbersome, version of the title could have been as follows: *Quantum Clifford algebra from the differential invariants that are already present in (and are usually but incorrectly thought to be exclusive of) the traditional sector of classical differential geometry*. We use the term ''classical'' to refer to geometry in the tangent bundle, rather than Yang–Mills geometry. The term ''traditional sector'' is used to refer to the part of classical differential geometry that studies connections, metric relations, their interplay, etc. The term ''nontraditional sector'' is used to refer to Kähler's exterior–interior calculus and concomitant theory of Dirac equations.[8] The basic equations of structure of the traditional sector concern clearly the differentials of deeply geometric objects. In the case of the Kähler theory, on the other hand, the equation which plays the central role, the Kähler equation, is

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$$\partial u = a \vee u, \tag{1}$$

where ∂ represents the sum of the exterior and interior covariant derivatives, "a" is a given tensor-valued differential form (TVDF), and "u" is the unknown TVDF. Dirac's original equation is a most simple particular case of Eq. (1). It corresponds to a being given by the scalar-valued differential form $m + eA$, up to universal constants (m is mass, e is charge, and A is electromagnetic potential). The motivation to view the theory of Eq. (1) as an extension of classical differential geometry is enhanced by the possibility of using a geometric object to play the role of a,[9,10] especially since the unknown TVDF u does not make part of the differential invariants which make a and define ∂.

It is legitimate to ask why even bother about classical differential geometry in connection with QCAs, given the success of Yang–Mills theory. The reason is that "the key feature of Yang–Mills theory is that it deals with connections on auxiliary bundles, not directly tied to the geometry of the base manifold." [11] In mathematics, a bundle is auxiliary because we make it to be so as a matter of definition in the context of some geometry, say Riemannian geometry. In physics, on the other hand, the Riemannicity of space–time might in principle be just the geometrically identified part of a deeper classical-geometric reality of the world. For instance, a Riemannian structure can be reconfigured on the Finsler bundle without loss of information but with increased structural richness. A bundle may be auxiliary simply because of our inability to identify it as pertaining to a more sophisticated bundle directly tied to the base manifold, like a Finsler bundle. Weyl geometry was considered—and still is considered—as the first of the Yang–Mills theories, ahead of the times. And yet, Weyl geometry is directly related to the geometry of base manifolds endowed with metric-compatible affine connections of the particular type that Cartan called metric connections (whose fibers contain the rotations, as in Riemannian geometry, plus the dilatations or similarity transformations).[12] For Cartan's related discussions of Weyl's spaces see Refs. 13–15. One thus has to leave open the possibility that some Yang–Mills theories may eventually become part of classical differential geometry of some more general type.

The contents of the paper is organized as follows. In Sec. II, we refer to the evolution of some modern mathematics that are relevant for this work, like the emergence of the concept of quantum Clifford algebra and recent developments in both the exterior–interior calculus of Kähler and in Finsler geometry. It is precisely in the context of these developments that, in Sec. III, nonsymmetric cotangent algebras emerge from symmetric tangent algebras, both pertaining to a Kaluza–Klein (KK) structure that is canonical of Finslerian teleparallelism. However, the same structure arises if one confronts the issue of making the metric, $ds^2 = g_{\mu\nu} dx^\mu \otimes dx^\nu$, fit the mold of Clifford algebras. In Sec. IV, we relate this KK space to standard geometric structures, for the purpose of deriving in Sec. V the expression for the interior covariant derivative in the KK space. In Sec. VI, we discuss issues that should follow this work.

II. RECENT DEVELOPMENTS IN CLIFFORD ALGEBRA AND THE EXTERIOR–INTERIOR CALCULUS

Clifford algebras of nonsymmetric metrics were first considered in implicit form by Chevalley[16] and explicitly by Helmstetter,[17] Crumeyrolle,[18] and Lounesto.[19] Independently of these developments, Oziewicz also suggested new directions in Clifford algebras (algebras of multivectors and algebras of nonsymmetric metrics) and pointed out applications of these algebras to quantum field theory.[2] The physical impact of nonsymmetric metrics was not yet suggested, however. These two lines of development started to come together first in a paper by Ablamowicz and Lounesto,[20] but especially when applications of nonsymmetric metrics to quantum field theory were shown.[1,3–5]

At an even earlier time, Kähler's incorporation of Clifford algebras in the Cartan calculus resulted in a powerful, general theory of harmonic functions and Dirac equations.[8] Kähler's scheme is so clean and general that, in principle, it can be used to extend the concepts of interior derivatives and Laplacian operators to new realms of classical differential geometry, like Finsler geometry, provided that the new spaces have the appropriate algebraic structure. In the case of

Finsler geometry, for example, this requires that it be viewed from the enhanced algebraic perspective that frame bundles and affine connections bring to differential geometry, rather than from the purely metric perspective, as was the case with Riemannian geometry before the Levi-Civita connection.[21] Unfortunately the metric perspective is still dominant in Finsler geometry, which is indeed viewed, more often than not, as the geometry of spaces in which the length of curves is defined. In the alternative perspective, it is the geometry of purely affine (and of metric-compatible affine) connections in bundles where the total space is the same set of vector bases (respectively, orthonormal frames or Euclidean bases) tangent to a differentiable manifold M, but refibrated over the tangent bundle or, better yet, the bundle of directions, $S(M)$.[22]

In Sec. I, we suggested the possibility that the classical geometric reality of the space may be richer than it presently appears to be. It is then worth emphasizing that (a) the Levi-Civita affine connection is two years younger than general relativity itself and (b) although this connection uses the much older Cristoffel symbols, the two should not be identified at the conceptual level. For the enormous significance of this connection as a conceptual breakthrough, see Cartan.[23–25] Eventually, general relativity incorporated the Levi-Civita affine connection, but it might as well have incorporated any other metric compatible affine connection. All such theories share the same metric relations. No experiment has been proposed or performed that would test the affine connection of space–time, as an issue separate from the testing of the metric relations. By virtue of the fact that teleparallel connections—and only they—define an equality of vectors from different tangent spaces to a differentiable manifold, teleparallelism (TP) enhances geometric structure beyond the enhancement already achieved by the use of affine connections and bundles.

The status of the mathematical subjects that we have touched upon is as follows. The Kähler calculus has limitations[9,10] (for minimal background on the Kähler calculus, we refer readers to the appendix of our paper on the adaptation of this calculus to TP[26]). The important issue of the interior derivative remains unresolved in Finsler geometry. We have shown how the problems in these two areas are solved at the same time in a KK type of context corresponding to a teleparallel Finsler structure.[9,10,27] This paper constitutes a new step in the understanding of this KK structure, the arena where the QCA emerges. It can, however, be viewed in a way which does not explicitly resort to those developments. First, reformulate space–time geometry in a Hamilton framework (meaning that we have additional independent coordinates), as opposed to an Euler framework, since this is what our view of a particular sector of Finsler geometry amounts to. Instead of $u^i = \mathrm{d}x^i/\mathrm{d}t$, we now have $\mathrm{d}x^i - u^i\,\mathrm{d}t = 0$. These two sets of equations are equivalent only on curves. Second, further reformulate this Hamiltonian theory in five dimensions so as to include the distance element $\mathrm{d}s$ as an additional differential one-form, which presently it is not.

III. CANONICAL QUANTUM CLIFFORD ALGEBRA

In order to motivate the ''logical necessity,'' or at least the ''naturalness'' of quantum Clifford algebras, we provide a brief introduction to the ''Hamiltonian view'' of the base space for affine and Euclidean (i.e., metric compatible affine) connections. In other words, the affine Finsler bundle and Euclidean Finsler bundle (which we call the metric Finsler bundle, even if we do not include the dilations) provide an alternative arena for the treatment of metric-compatible connections on Lorentzian metrics of the usual pre-Finslerian type. On differentiable manifolds M with no metric yet assumed, denote one of the coordinates as x^0, and let $\mathbf{e}_0$ be its dual basis vector. The $\mathrm{d}x^i/\mathrm{d}x^0$ on curves generates velocity coordinates of the ''phase-space–time manifold'' $S(M)$. Via an isomorphism, one refibrates over $S(M)$, with coordinates (x^0, x^i, u^i), the set of all tangent bases to M. This refibration constitutes a bundle $B(M) \to S(M)$ which we call the affine-Finsler bundle.[22] In the isomorphism, the basis vectors named $\mathbf{e}_0$ play the role of a preferred direction.

Assume that we now put on M a pseudo-Riemannian metric of Lorentzian signature. This restricts the bundle of bases to the bundle of frames, or metric-Finsler bundle, $B'(M) \to S(M)$. If $\mathbf{e}_0$ is timelike, the group on the fibers is $O(3)$. But the group is $O(2,1)$ if $\mathbf{e}_0$ is spacelike. This second choice artificially creates a special role for a spatial direction, rather than assigning the role of the preferred direction that is used in the aforementioned isomorphism to the canonically distinguished time direction. Hence, the Lorentzian signature is distinguished or canonical for the

Finsler bundle, since it is the only one which has a direction to match the preferred direction of the Finslerian structure. The Finsler bundle of space–time with canonical choice of direction is very useful to do geometry of manifolds where the distance on curves is post-Riemannian or Finslerian. Doing Finsler geometry on this bundle complies with Cartan's view of geometry as pertaining to the tangent bundles rather than to the base manifold proper. But this is by no means the only use of this bundle, and it is not the one in which we are interested. When the usual affine connections are formulated on the Finsler bundle, the new formulation is to the old formulation of these connections what the Hamiltonian formalism is to the Euler/Lagrange formalism. Furthermore, Finsler bundles have the advantage of accepting more general connections than the usual bundles.

As in the usual bundles, ω^μ determines the translation part, $\mathrm{d}\mathbf{P}=\omega^\mu\mathbf{e}_\mu$, of the affine connection. When a metric is given, the ω^μ are implicit in the canonical form of the metric, since $\mathrm{d}s^2=(\omega^0)^2-\Sigma_i(\omega^i)^2$. On sections of Finsler bundles, we need to specify, in addition, a number $n-1$ of differential one-forms, ω_0^i, which are linear combinations of $\mathrm{d}x^0,\mathrm{d}x^i$, and $\mathrm{d}u^i$. They determine the derivative of the four-velocity vector through $\mathrm{d}\mathbf{u}=\mathrm{d}\mathbf{e}_0=\omega_0^i\mathbf{e}_i$. The identification of $\mathbf{u}$ with $\mathbf{e}_0$ is due to the fact that, in the refibration, the bases and frames become adapted to $S(M)$: all those at the point of coordinates (t,x^i,u^i) have the common velocity of components u^i and are related just by the $O(3)$ rotations. Correspondingly, the subset $(\omega_0^{\cdot i})$ of the set $(\omega_\mu^{\cdot\nu})$ has left the fibers to sit on the new (larger) base space, for both the affine-Finsler and metric-Finsler connections. The metric determines the dot product $\mathrm{d}x^\mu\cdot\mathrm{d}x^\nu=g^{\mu\nu}$. Equivalently, it determines what are the ω^μ such that $\omega^\mu\cdot\omega^\nu=\delta^{\mu\nu}$. But there is no satisfactory definition of the other dot products, $\omega^\mu\cdot\omega_0^{\cdot i}$ and $\omega_0^j\cdot\omega_0^{\cdot i}$, of the horizontal invariant forms ω^μ and $\omega_0^{\cdot i}$ of the metric-Finsler bundles.

Consider now the direct sum $M^4\oplus M^1$ of a teleparallel space–time M^4, endowed with a metric-compatible connection, and a space M^1 whose mission is to represent space–time curves when lifted to M^4. As in traditional KK, one is limited on the allowed transformations on this space by virtue of its nature as a direct sum. We endow $M^4\oplus M^1$ with connection equations:

$$\mathrm{d}\wp=\mathrm{d}\mathbf{P}+\mathrm{d}\tau\,\mathbf{e}_4,\quad \mathrm{d}\mathbf{e}_A=\omega_A^{\cdot B}\mathbf{e}_B, \tag{2}$$

where $A,B,\ldots=0,1,\ldots,4$ and where $\mathbf{e}_4$ is viewed as a tangent vector on M^1 of square minus one.[27] The $\{\mathbf{e}_\mu\}$ will be chosen to be orthonormal though not necessarily constant. Thus, with g_{AB} defined as $\mathbf{e}_A\cdot\mathbf{e}_B$, the entries $g_{\mu\nu}$ are the $\eta_{\mu\nu}$. The basis $\{\mathbf{e}_A\}$ is not a canonical basis, i.e., not a (pseudo)-orthonormal basis, of the tangent Clifford algebra defined by this dot product since the products $\mathbf{e}_4\cdot\mathbf{e}_\mu=g_{4\mu}=\mathbf{e}_\mu\cdot\mathbf{e}_4$, which evolve into components of the four-velocity on the pullbacks to (curves of) space–time, are assumed to be different from zero. We postulated

$$\omega^A\cdot\omega^B=0\quad for\ \ A\neq B \tag{3}$$

and saw the double dot product of $\mathrm{d}\wp$ with itself become

$$\mathrm{d}\wp(\cdot,\cdot)\mathrm{d}\wp=\omega^A\cdot\omega^B\mathbf{e}_A\cdot\mathbf{e}_B=\omega^0\cdot\omega^0-\omega^1\cdot\omega^1-\ldots-\mathrm{d}\tau\cdot\mathrm{d}\tau. \tag{4}$$

We further postulated $\mathrm{d}\wp(\cdot,\cdot)\mathrm{d}\wp=0$, which yielded the *natural lifting condition*:

$$\mathrm{d}\tau\cdot\mathrm{d}\tau=\mathrm{d}s\cdot\mathrm{d}s, \tag{5}$$

where

$$\mathrm{d}s\cdot\mathrm{d}s\equiv\omega^0\cdot\omega^0-\omega^1\cdot\omega^1-\omega^2\cdot\omega^2-\omega^3\cdot\omega^3. \tag{6}$$

Equations (5) and (6) justify referring to $\mathrm{d}\tau$ and $\mathbf{e}_4$, respectively, as the differential of proper time and as the five-vector whose "differential" plays the role of the acceleration one-form, even if $\mathbf{e}_4$ has projection on but is not contained in space–time (i.e., it is not a linear combination of only the $\mathbf{e}_\mu$'s). We shall now relax the conditions (3) and still obtain Eqs. (4)–(6).

We introduce the symbols "$\dot\wedge$" and "$\cdot$" to refer to the antisymmetric and symmetric parts,

$$a\dot{\wedge}b=\tfrac{1}{2}(a\vee b-b\vee a),\quad a\cdot b=\tfrac{1}{2}(a\vee b+b\vee a),\tag{7}$$

of the Clifford product "$\vee$" of two vectors, a and b, from some vector space. We obviously have $a\vee b=a\dot{\wedge}b+a\cdot b$. It is well known that the usual Clifford algebras are specified when the symmetric products $\gamma^{\mu}\cdot\gamma^{\nu}$ are given, where the (γ^{μ}) constitute a basis of the vector space (or the module) to which the a and b belong. The Clifford algebra can be tangent or cotangent, depending on whether a and b are both tangent vectors or both differential one-forms. As explained elsewhere,[9] our differential r-forms are functions of r-surfaces and not antisymmetric r-linear functions of vectors. Let us illustrate this for one-forms, like the ω^{μ}. These are functions of curves and their exterior derivative in the sense of Kähler is the usual exterior derivative. On the other hand, an element ϕ^{μ} of a field of bases (ϕ^{μ}) of the space of linear functions of vectors, $\phi^{\mu}(\mathbf{e}_{\nu})=\boldsymbol{\delta}^{\mu}_{\nu}$, can be replaced with $\mathbf{e}^{\mu}$ defined by $\mathbf{e}^{\mu}\cdot\mathbf{e}_{\nu}=\boldsymbol{\delta}^{\mu}_{\nu}$. The exterior derivative of $\mathbf{e}^{\mu}$ in the sense of Kähler is the connection-dependent derivative $\mathrm{d}\mathbf{e}^{\mu}=-\omega^{\mu}_{\nu}\mathbf{e}^{\nu}$. Hence the tangent algebra (of the ϕ^{μ} and $\mathbf{e}_{\nu}$) and cotangent algebras (of the ω^{μ}) are intertwined but not identifiable with each other. We assume that the tangent metric is symmetric. The tangent algebra is then defined by $\mathbf{e}_{\mu}\cdot\mathbf{e}_{\nu}+\mathbf{e}_{\nu}\cdot\mathbf{e}_{\mu}=2g_{\mu\nu}$. Equivalently, it is defined by $\mathbf{e}_{\mu}\vee\mathbf{e}_{\nu}+\mathbf{e}_{\nu}\vee\mathbf{e}_{\mu}=2g_{\mu\nu}$ with $g_{\mu\nu}=g_{\nu\mu}$. The symbol $\dot{\wedge}$ is in this case the symbol $\wedge$ of standard Clifford algebra. No other symbols for products are needed in the symmetric case.

Since we have to deal with two algebras at the same time, we need to introduce symbols for pairs of products. Given a pair of symbols for products within parentheseis, the first symbol will refer to the cotangent algebra and the second one to the tangent algebra. As an example, $\alpha\mathbf{a}(\dot{\wedge},\cdot)\beta\mathbf{b}=(\alpha\dot{\wedge}\beta)(\mathbf{a}\cdot\mathbf{b})$. If A and B are vector-valued one-forms, we have

$$A(\vee,\vee)B=A(\dot{\wedge},\dot{\wedge})B+A(\dot{\wedge},\cdot)B+A(\cdot,\dot{\wedge})B+A(\cdot,\cdot)B.\tag{8}$$

When A equals B, mixed products, like $A(\dot{\wedge},\cdot)A$ and $A(\cdot,\dot{\wedge})A$, cancel out. We thus have $\mathrm{d}\varphi(\vee,\vee)\mathrm{d}\varphi=\mathrm{d}\varphi(\wedge,\wedge)\mathrm{d}\varphi$ if $\mathrm{d}\varphi(\cdot,\cdot)\mathrm{d}\varphi=0$.

The key point now is that we let the cotangent algebra emerge as it may, not necessarily with a symmetric inner product even if the inner product of the tangent algebra is. We use closed circle ($\bullet$) to refer to nonsymmetric inner products. Let the center dot ($\cdot$) and the open circle ($\circ$) denote the symmetric and antisymmetric parts of the inner product "$\bullet$" of two differential scalar-valued differential one-forms, i.e., $a\bullet b=a\circ b+a\cdot b$. Since the first equation of (7) is the definition of the $\dot{\wedge}$ product, $a\dot{\wedge}b$ contains the antisymmetric part $a\circ b$ of $a\bullet b$. In other words, $a\dot{\wedge}b$ has bivector and scalar parts, namely $a\wedge b$ and $a\circ b$, respectively,

$$a\dot{\wedge}b=a\wedge b+a\circ b,\tag{9}$$

where the grading is with respect to the undotted product. The definition of $\wedge$ is such that $a\wedge b$ is the suface integrand formed with the one-forms a and b in the given order. We thus have

$$a\vee b=a\wedge b+a\circ b+a\cdot b=a\wedge b+a\bullet b.\tag{10}$$

In the same way as the usual Clifford algebra is specified when a symmetric quadratic form is given, the quantum Clifford algebra is specified when both the $a\circ b$ and $a\cdot b$ products are given

$$\omega^{A}\circ\omega^{B}=A^{AB},\quad \omega^{A}\cdot\omega^{B}=Q^{AB},\tag{11}$$

$$\omega^{A}\bullet\omega^{B}=A^{AB}+Q^{AB}.\tag{12}$$

Hence, a nonsymmetric cotangent algebra is specified by A^{AB} and Q^{AB}. We let A^{AB} be an arbitrary antisymmetric matrix whose entries are numbers or real valued functions. We define the

$\omega^A \cdot \omega^B$, equivalently the Q^{AB}, so that we precisely obtain Eq. (6). In terms of a basis of differential forms, Eq. (6) reads $\mathrm{d}\tau \cdot \mathrm{d}\tau = g_{\mu\nu} \mathrm{d}x^\mu \cdot \mathrm{d}x^\nu$ and means nothing other than $\mathrm{d}\tau\,\mathrm{d}\tau = g_{\mu\nu}\mathrm{d}x^\mu\,\mathrm{d}x^\nu$, usually written as $\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}x^\mu\,\mathrm{d}x^\nu$.

We still need to verify that Eq. (5) is satisfied. This is indeed the case,

$$0 = \mathrm{d}\wp(\cdot,\cdot)\mathrm{d}\wp = Q^{AB} g_{AB} = \omega^\mu \cdot \omega^\nu - \mathrm{d}\tau.\mathrm{d}\tau + 2Q^{\mu 4} g_{\mu 4}, \tag{13}$$

if we require that

$$Q^{\mu 4} g_{\mu 4} = 0. \tag{14}$$

In matrix form, the symmetric part, $\omega^\mu \cdot \omega^\nu$, of the cotangent inner product, $\omega^\mu \bullet \omega^\nu$, is

$$Q^{AB} = \omega^A \cdot \omega^B = \begin{bmatrix} \omega^0 \cdot \omega^0 & 0 & 0 & 0 & Q^0 \\ 0 & \omega^1 \cdot \omega^1 & 0 & 0 & Q^1 \\ 0 & 0 & \omega^2 \cdot \omega^2 & 0 & Q^2 \\ 0 & 0 & 0 & \omega^3 \cdot \omega^3 & Q^3 \\ Q^0 & Q^1 & Q^2 & Q^3 & \mathrm{d}\tau.\mathrm{d}\tau \end{bmatrix}. \tag{15}$$

The matrix Q^{AB} is not to be confused with the matrix g^{AB} inverse to g_{AB}. The conditions (15) are far more general than the conditions (3). There is no restriction on the quantities A^{AB} other than antisymmetry. Hence, the specification of the intertwined tangent and cotangent algebras requires the specification of $g_{\mu\nu}$, $g_{\mu 4}(=g_{4\mu})$, A^{AB} and a Q^μ that satisfies Eq. (14). The $g_{\mu 4}$ will now be interpreted.

IV. RELATION BETWEEN THE KALUZA–KLEIN AND STANDARD GEOMETRIC FORMULATIONS

In this section, we relate the KK formulation to the standard formulation of classical differential geometry by first identifying flat space–time itself in the first of these formulations. In Ref. 27, we produced a KK connection for teleparallel Finsler spaces. We simply assumed metric compatibility and that

$$\omega_\rho^{\cdot\sigma} = 0 \tag{16}$$

and obtained

$$\omega_{4\rho} = \mathrm{d}g_{4\rho}, \tag{17}$$

and

$$\omega_4^{\cdot\rho} = \eta_\rho(\omega_{4\rho} - g_{4\rho}\omega_4^{\cdot 4}), \quad \omega_4^{\cdot 4} = G^{-1}\eta_\rho g_{4\rho}\mathrm{d}g_{4\rho} = \omega_4^{\cdot\rho} g_{4\rho}, \quad \omega_\rho^{\cdot 4} = 0, \tag{18}$$

where η_ρ is $(+1,-1,-1,-1)$ and where

$$G \equiv 1 + (g_{40})^2 - (g_{41})^2 - (g_{42})^2 - (g_{43})^2. \tag{19}$$

We return momentarily to the Finsler bundle. One imposes six conditions among the seven horizontal forms of $S(M^4)$ to obtain curves. Three of these conditions constitute, for instance, the statement that $\mathrm{d}\mathbf{e}_4 = \mathbf{0}$, or, as another important option, the statement of stationary length. Three additional conditions are the "Cartan conditions," $\mathrm{d}x^i - u^i\,\mathrm{d}t = 0$. These six forms together determine the curves of interest in the seven-dimensional $S(M^4)$ space. All differential one-forms become proportional to just one, say $\mathrm{d}t$. In the five-dimensional KK space, we need to impose only four conditions. For example, the statement $\mathrm{d}\mathbf{u} = 0$ achieves this. Although this amounts to the five equations

$$\omega_4^{\cdot A}=0, \tag{20}$$

these equations are not independent since

$$\omega_4^{\cdot 4}=\omega_4^{\cdot \mu}g_{4\mu}. \tag{21}$$

Equation (20) thus provides four independent conditions to determine curves in the KK space.

The condition $\omega_\mu^{\cdot \nu}=0$ (constant frame fields in TP) together with metric compatibility yielded the full set of $\omega_A^{\cdot B}$. These equations then allowed us in turn to reduce the torsion to the form:

$$\Omega'^{\mu}=\mathrm{d}\omega^{\mu}-\mathrm{d}\tau\wedge\omega_4^{\cdot \mu}, \tag{22}$$

$$\Omega'^{4}=-\mathrm{d}\tau\wedge\omega_4^{\cdot 4}. \tag{23}$$

The conditions $\omega_4^{\cdot \mu}=0$ and $\omega_4^{\cdot 4}=0$ that determine the autoparallels are the same conditions that project Ω'^{μ} and Ω'^{4} down to space–time. This opens the door for the interpretation that $\omega_4^{\cdot \mu}$ embodies inertial forces, since they do not affect the space–time structure. In this case, $\omega_4^{\cdot 4}$ also does, by virtue of Eq. (21). Only when the "additional structure" generated by $\omega_4^{\cdot \mu}$ is zero, all the forces are noninertial.[28]

We proceed to unearth in the KK formalism the standard equations of the autoparallels of space–time. For this, we do not assume constant frame fields, where $\omega_\mu^{\cdot \nu}=0$, even if we assume TP. The reason is that, in these fields, we have

$$\mathrm{d}\mathbf{u}=\mathrm{d}(u^{\mu}\mathbf{e}_{\mu})=\mathrm{d}u^{\mu}\mathbf{e}_{\mu}+u^{\mu}\omega_{\mu}^{\cdot \nu}\mathbf{e}_{\nu}=\mathrm{d}u^{\mu}\mathbf{e}_{\mu}. \tag{24}$$

The statement $\mathrm{d}\mathbf{u}=0$ would amount to assuming constant u^{μ}. In the relativistic analog that $\mathbf{u}$ were the four-velocity, this would represent motion under gravitational forces being referred to free-falling comoving reference frames. The problem of finding the equations of the motion has metamorphosed into the problem of finding the relation of the free falling frames to the bases attached to matter (say, the coordinate basis fields). We readily have

$$\mathrm{d}g_{4\rho}=\mathrm{d}(\mathbf{e}_4\cdot\mathbf{e}_{\rho})=\mathrm{d}\mathbf{e}_4\cdot\mathbf{e}_{\rho}+\mathbf{e}_4\cdot\omega_{\rho}^{\cdot \nu}\mathbf{e}_{\nu}-\omega_{\rho}^{\cdot 4}. \tag{25}$$

By virtue of the assumption $\mathrm{d}\mathbf{e}_4=\mathbf{0}$ for the equations of the motion, we further get

$$\mathrm{d}g_{4\rho}=g_{4\nu}\omega_{\rho}^{\cdot \nu}-\omega_{\rho}^{\cdot 4}. \tag{26}$$

With orthonormal frames, we have: $\omega_{\rho}^{\cdot \nu}=\eta_{\nu}\omega_{\rho\nu}=-\eta_{\nu}\omega_{\nu\rho}=-\omega_{\cdot\rho}^{\nu}$. Hence:

$$\mathrm{d}g_{4\rho}+\omega_{\cdot\rho}^{\nu}g_{4\nu}=-\omega_{\rho}^{\cdot 4}. \tag{27}$$

The equations of the autoparallels are present here if the pull-back of $g_{4\rho}$ to space–time curves is interpreted as constituting the components of the four-velocity on those curves, consistently with a previous related discussion.[27] The interpretation of $\omega_{\rho}^{\cdot 4}$ will be dealt with in a paper in preparation. Notice that this equation is not affected by the antisymmetric part of the dot product in the cotangent Clifford algebra. We shall now see the impact of this antisymmetric part on the physics through the interior derivative.

V. IMPACT OF THE QCA ON THE INTERIOR DERIVATIVE

The combined exterior–interior derivative, ∂, of the Kähler calculus is given by

$$\partial\alpha=\omega^{\mu}\vee\mathrm{d}_{\mu}\alpha=\omega^{\mu}\dot{\wedge}\mathrm{d}_{\mu}\alpha+\omega^{\mu}\cdot\mathrm{d}_{\mu}\alpha=\omega^{\mu}\wedge\mathrm{d}_{\mu}\alpha+\omega^{\mu}\bullet\mathrm{d}_{\mu}\alpha \tag{28}$$

where the symbols for the products are as defined in Sec. III and where $\mathrm{d}_\mu\alpha$ is what Kähler denotes as the covariant derivative of α. So far, the relation between the two exterior products may be viewed from the equivalent definitions

$$\omega^\mu \dot{\wedge} \mathrm{d}_\mu\alpha = \omega^\mu \wedge \mathrm{d}_\mu\alpha + \omega^\mu \bigcirc \mathrm{d}_\mu\alpha \tag{29}$$

and

$$\omega^\mu \wedge \mathrm{d}_\mu\alpha = \omega^\mu \dot{\wedge} \mathrm{d}_\mu\alpha - \omega^\mu \bigcirc \mathrm{d}_\mu\alpha. \tag{30}$$

We identify the gradation of "$\wedge$" with the one defined by Stokes theorem. The choice of A^{BC} together with Eq. (9) (viewed as a definition) then fix the $\dot{\wedge}$ product. Kähler's interior derivative must then be taken to be the complement, $\omega^\mu \bullet \mathrm{d}_\mu\alpha$, of the exterior derivative, $\omega^\mu \wedge \mathrm{d}_\mu\alpha$, that enters Stokes' theorem (Kähler conceived the covariant derivative so that $\omega^\mu \wedge \mathrm{d}_\mu\alpha$ coincides with the exterior derivative when α is scalar-valued, and with the exterior covariant derivative when it is a TVDF). The interior derivative so defined has both symmetric and antisymmetric contributions from the "$\bullet$" product.

It is clear that electrodynamics and quantum mechanics will depend on the nonsymmetric part of the metric in this new scenario, since the interior derivative enters both of these theories in an essential way. The relevance of the interior derivative in the case of gravitation, precisely the most geometric of all these theories in the present paradigm, depends on what we assume to be the connection of space–time and the role that this connection is postulated to play in the theory. Indeed, the affine curvature is the exterior covariant derivative $\mathrm{d}(\omega_\mu^{\cdot\nu}\mathbf{e}_\nu)$ of $\omega_\mu^{\cdot\nu}\mathbf{e}_\nu$, i.e.,

$$\mathrm{d}(\omega_\mu^{\cdot\nu}\mathbf{e}_\nu) = (\mathrm{d}\omega_\mu^{\cdot\nu} - \omega_\mu^{\cdot\lambda} \wedge \omega_\lambda^{\cdot\nu})\mathbf{e}_\nu. \tag{31}$$

Einstein's field equations involve only the Einstein tensor and thus fail to involve the full curvature in the field equations. Hence they fail to involve the full exterior derivative of $\omega_\mu^{\cdot\nu}\mathbf{e}_\nu$. The interior derivative is not even mentioned in general relativity. Denoting this derivative with the symbol δ, we have

$$\delta(\omega_\mu^{\cdot\nu}\mathbf{e}_\nu) = \omega^\rho \bullet R_{\mu\cdot\rho\sigma}^{\cdot\nu}\omega^\sigma\mathbf{e}_\nu, \tag{32}$$

which is not zero for general connection. It is, however, zero for teleparallel connections since $R_{\mu\cdot\rho\sigma}^{\cdot\nu}$ itself is then zero. The conclusion is that the cotangent Clifford algebra (QCA) does not impact the gravitational sector of the physical theory canonically determined by TP. It fails to impact general relativity for a completely different reason, namely that this theory does not involve the Kähler derivative of the connection.

We proceed to consider interior derivatives. In order to avoid the clutter produced by connection terms, we shall assume space–time TP, so that we can use frame fields where $\omega_\mu^{\cdot\nu} = 0$. Whether we assume TP or not, we can still neglect the connection terms in the computations and restore them in the final results through replacement of the partial derivatives with covariant derivatives. A connection-dependent result, however, is that $\omega_\mu^{\cdot\nu} = 0$ (TP) implies $\omega_\mu^{\cdot A} = 0$, at least when all the $g_{4\mu}$ are different from zero.[27]

We shall limit ourselves to space–time differential forms on practical grounds, although there may well be deep reasons not to consider differential forms with a term proportional to $\mathrm{d}\tau$ for most purposes. This is reminiscent of the limited form of the transformations allowed in the traditional KK theory. In order to deal with bases ω^μ, we extend the meaning of the comma when used as a subscript. The $f_{,\mu}$ means the coefficients defined by the equation $\mathrm{d}f = f_{,\mu}\omega^\mu$. The $f_{,\mu}$ become the partial derivatives when ω^μ is $\mathrm{d}x^\mu$ itself.

Let α be the one-form $a_\mu\omega^\mu$. We then have:

$$\mathrm{d}(a_\mu\omega^\mu) = \mathrm{I} + \mathrm{II} + \mathrm{III}, \tag{33}$$

where

$$\mathrm{I}=a_{\nu,\mu}\omega^{\mu}\wedge\omega^{\nu}, \tag{34}$$

$$\mathrm{II}=a_{\nu}\Omega^{\nu}, \tag{35}$$

$$\mathrm{III}=a_{\nu}\omega^{C}\wedge\omega_{C}^{\nu}=a_{\nu}\omega^{4}\wedge\omega_{4}^{\nu}. \tag{36}$$

The interior derivative, δ_{I}, resulting from the I term is

$$\delta_{\mathrm{I}}=a_{\nu,\mu}\omega^{\mu}\bullet\omega^{\nu}=a_{\nu,\mu}A^{\mu\nu}+\sum_{\nu}a_{\nu,\nu}\omega^{\nu}\cdot\omega^{\nu}. \tag{37}$$

For the II term, we use that the torsion in KK space is

$$\mathbf{\Omega}'=\mathrm{d}(\mathrm{d}\wp)=\mathrm{d}(\mathrm{d}\mathbf{P}+\mathrm{d}\tau\mathbf{e}_4)=\Omega-\mathrm{d}\tau\wedge\mathrm{d}\mathbf{e}_4. \tag{38}$$

Hence, we have $\Omega'^{\mu}=\Omega^{\mu}-\mathrm{d}\tau\wedge\omega_4^{\mu}$ and $\Omega'^{4}=-\mathrm{d}\tau\wedge\omega_4^{4}$. It follows that

$$\mathrm{II}=a_{\nu}\Omega'^{\nu}=a_{\nu}\Omega^{\nu}-a_{\nu}\,\mathrm{d}\tau\wedge\omega_4^{\nu}. \tag{39}$$

For the above-stated reasons, we drop the term III, or simply compute mod ω_4^{ν}. We thus have

$$\delta_{\mathrm{II}}=a_{\nu}R^{\nu}_{\mu\lambda}\omega^{\mu}\bullet\omega^{\lambda}=a_{\nu}R^{\nu}_{\mu\lambda}A^{\mu\lambda}. \tag{40}$$

The symmetric part of the product has dropped out because $R^{\nu}_{\mu\lambda}=-R^{\nu}_{\lambda\mu}$. The third term disappears mod ω_4^{ν}. Collecting terms, we get

$$\delta(a_{\mu}\omega^{\mu})=\sum_{\nu}a_{\nu,\nu}\omega^{\nu}\cdot\omega^{\nu}+a_{\nu,\mu}A^{\mu\nu}+a_{\nu}R^{\nu}_{\mu\lambda}A^{\mu\lambda}. \tag{41}$$

Consider now a two-form, $\beta=b_{\lambda\rho}\omega^{\lambda}\wedge\omega^{\rho}$, and assume the same simplifying assumptions. We have

$$\mathrm{d}\beta=\mathrm{d}(b_{\lambda\rho}\omega^{\lambda}\wedge\omega^{\rho})=b_{\lambda\rho,\mu}\omega^{\mu}\wedge\omega^{\lambda}\wedge\omega^{\rho}+b_{\sigma\rho}\mathrm{d}\omega^{\sigma}\wedge\omega^{\rho}-b_{\rho\sigma}\omega^{\rho}\wedge\mathrm{d}\omega^{\sigma}. \tag{42}$$

The first term on the right of this equation contributes to the interior derivative $\delta\beta$ with

$$\delta_{\mathrm{I}}=b_{\lambda\rho,\mu}\omega^{\mu}\bullet(\omega^{\lambda}\wedge\omega^{\rho})=b_{\lambda\rho,\mu}\omega^{\mu}\bullet(\omega^{\lambda}\dot{\wedge}\omega^{\rho}-\omega^{\lambda}\bigcirc\omega^{\rho}). \tag{43}$$

We proceed to compute this "$\bullet$" product. For any clifform B, we have

$$\omega^{\mu}\bullet B=\omega^{\mu}\vee B-\omega^{\mu}\wedge B=\omega^{\mu}\dot{\wedge}B+\omega^{\mu}\cdot B-\omega^{\mu}\wedge B. \tag{44}$$

Hence, for $B=\omega^{\lambda}\wedge\omega^{\rho}$, we get

$$\begin{aligned}\omega^{\mu}\bullet(\omega^{\lambda}\wedge\omega^{\rho})&=\omega^{\mu}\bullet(\omega^{\lambda}\dot{\wedge}\omega^{\rho}-\omega^{\lambda}\bigcirc\omega^{\rho})\\&=\omega^{\mu}\dot{\wedge}(\omega^{\lambda}\dot{\wedge}\omega^{\rho}-\omega^{\lambda}\bigcirc\omega^{\rho})+\omega^{\mu}\cdot(\omega^{\lambda}\dot{\wedge}\omega^{\rho}-\omega^{\lambda}\bigcirc\omega^{\rho})-\omega^{\mu}\wedge\omega^{\lambda}\wedge\omega^{\rho}.\end{aligned} \tag{45}$$

Of the five terms that arise from Eq. (45), the first and fifth together yield $\omega^{\mu}A^{\lambda\rho}+\omega^{\lambda}A^{\rho\mu}+\omega^{\rho}A^{\mu\lambda}$. The second term is $-\omega^{\mu}A^{\lambda\rho}$. The third term is $(\omega^{\mu}\cdot\omega^{\lambda})\omega^{\rho}-(\omega^{\mu}\cdot\omega^{\rho})\omega^{\lambda}$. The fourth term is zero, since $\omega^{\lambda}\bigcirc\omega^{\rho}(=A^{\lambda\rho})$ is scalar-valued. All this together yields

$$\omega^{\mu}\bullet(\omega^{\lambda}\wedge\omega^{\rho})=\omega^{\lambda}A^{\rho\mu}+\omega^{\rho}A^{\mu\lambda}+(\omega^{\mu}\cdot\omega^{\lambda})\omega^{\rho}-(\omega^{\mu}\cdot\omega^{\rho})\omega^{\lambda}. \tag{46}$$

Combining the first term with the fourth one and the second with the third, we get

$$\omega^{\mu}\bullet(\omega^{\lambda}\wedge\omega^{\rho})=\omega^{\rho}(\omega^{\mu}\bullet\omega^{\lambda})-\omega^{\lambda}(\omega^{\mu}\bullet\omega^{\rho}). \tag{47}$$

Either Eq. (46) or (47) is to be substituted in Eq. (43).

The second term of Eq. (42) yields, with $\omega_{\mu}^{\cdot\nu}=0$, that $b_{\sigma\rho}\mathrm{d}\omega^{\sigma}\wedge\omega^{\rho}$ equals $b_{\sigma\rho}\Omega^{\sigma}\wedge\omega^{\rho}$. We shall denote as δ_{IV} the contribution to the interior derivative of this term. We readily get

$$\delta_{\mathrm{IV}}=b_{\sigma\rho}R^{\sigma}_{\mu\lambda}\omega^{\mu}\bullet(\omega^{\lambda}\wedge\omega^{\rho}). \tag{48}$$

Finally, the last term on the right-hand side of Eq. (42) can be written as $-b_{\rho\sigma}\mathrm{d}\omega^{\sigma}\wedge\omega^{\rho}$, which equals the second term. The sought $\delta\beta$ then is $\delta_{\mathrm{I}}+2\,\delta_{\mathrm{IV}}$. Using first Eqs. (43) and (48), and then Eq. (46), we obtain

$$\begin{aligned}\delta\beta=\delta(b_{\lambda\rho}\omega^{\lambda}\wedge\omega^{\rho})&=[b_{\lambda\rho,\mu}+2b_{\sigma\rho}R^{\sigma}_{\mu\lambda}]\omega^{\mu}\bullet(\omega^{\lambda}\wedge\omega^{\rho})\\&=b_{\lambda\rho,\mu}(\omega^{\lambda}A^{\rho\mu}+\omega^{\rho}A^{\mu\lambda})+b_{\lambda\rho,\mu}[(\omega^{\mu}\cdot\omega^{\lambda})\omega^{\rho}-(\omega^{\mu}\cdot\omega^{\rho})\omega^{\lambda}]\\&\quad+2b_{\sigma\rho}R^{\sigma}_{\mu\lambda}(\omega^{\lambda}A^{\rho\mu}+\omega^{\rho}A^{\mu\lambda})+2b_{\sigma\rho}R^{\sigma}_{\mu\lambda}[(\omega^{\mu}\cdot\omega^{\lambda})\omega^{\rho}-(\omega^{\mu}\cdot\omega^{\rho})\omega^{\lambda}].\end{aligned} \tag{49}$$

Hence, we finally get

$$\delta\beta=2(b_{\mu\rho,\mu}-b_{\sigma\mu}R^{\sigma}_{\mu\rho})(\omega^{\mu}\cdot\omega^{\mu})\omega^{\rho}+2b_{\lambda\rho,\mu}A^{\rho\mu}\omega^{\lambda}+2(b_{\sigma\rho}R^{\sigma}_{\mu\lambda}-b_{\sigma\lambda}R^{\sigma}_{\mu\rho})A^{\rho\mu}\omega^{\lambda}. \tag{50}$$

The factors $b_{\lambda\rho,\mu}$ go into $b_{\lambda\rho;\mu}$ when the connection is taken into account. The factor of 2 (actually $r!$ if we were dealing with an r-form) disappears when we introduce r-forms with the standard coefficient of $(1/r!)$.

It is now clear what the interior derivative, $\delta\mathbf{T}$, of a vector-valued two-form $\mathbf{T}=(1/2)T^{\pi}_{\lambda\rho}\omega^{\lambda}\wedge\omega^{\rho}\mathbf{e}_{\pi}$ is

$$\delta\mathbf{T}=[(T^{\pi}_{\mu\rho,\mu}-T^{\pi}_{\sigma\mu}R^{\sigma}_{\mu\lambda})(\omega^{\mu}\cdot\omega^{\mu})\omega^{\rho}+T^{\pi}_{\lambda\rho,\mu}A^{\rho\mu}\omega^{\lambda}+(T^{\pi}_{\sigma\rho}R^{\sigma}_{\mu\lambda}-T^{\pi}_{\sigma\lambda}R^{\sigma}_{\mu\rho})A^{\rho\mu}\omega^{\lambda}]\mathbf{e}_{\pi}. \tag{51}$$

The most interesting result happens when the vector-valued two-form is the torsion itself, which, for present purposes, we shall restrict to the space–time type, $\mathbf{\Omega}=(1/2)R^{\pi}_{\lambda\rho}\omega^{\lambda}\wedge\omega^{\rho}\mathbf{e}_{\pi}$. We then have

$$\delta\mathbf{\Omega}=[(R^{\pi}_{\mu\rho,\mu}-R^{\pi}_{\sigma\mu}R^{\sigma}_{.\mu\lambda})(\omega^{\mu}\cdot\omega^{\mu})\omega^{\rho}+R^{\pi}_{\lambda\rho,\mu}A^{\rho\mu}\omega^{\lambda}+(R^{\pi}_{\sigma\rho}R^{\sigma}_{\mu\lambda}-R^{\pi}_{\sigma\lambda}R^{\sigma}_{\mu\rho})A^{\rho\mu}\omega^{\lambda}]\mathbf{e}_{\pi}. \tag{52}$$

In this case, $A^{\rho\mu}$ multiplies linear terms on the torsion's partial derivatives, and quadratic but not linear terms on the torsion itself. This seems to indicate that the effects of $A^{\rho\mu}$ will be the larger in absolute terms the greater the torsion is (the terms $R^{\pi}_{\lambda\rho,\mu}A^{\rho\mu}\omega^{\lambda}$, however, make qualitative arguments nontrivial).

VI. CONCLUDING REMARKS

The issue of the interior derivative is one which typically resists treatment in post-Riemannian contexts, especially when Finsler metrics are involved. In contrast, Finslerian TP on Riemannian metrics yields one such derivative in a canonical way. A better understanding of terms proportional to $\omega^{\mu}\cdot\omega^{\mu}$ and $(\omega^{\mu}\cdot\omega^{\mu})\omega^{\rho}$ is to be sought. It is probably safe to assume, however, that $\omega^{\mu}\cdot\omega^{\mu}$ and $(\omega^{\mu}\cdot\omega^{\mu})\omega^{\rho}$ have to be seen as members of a basis. The coefficients of these basis elements on the left- and right-hand sides of equations would have to be matched. On the right-hand sides, they would arise in the process of obtaining Hodge duals of the three-forms j and $\mathbf{j}$ that constitute the current, in equations such as $\mathrm{d}F=*j$ and $\mathrm{d}\mathbf{\Omega}=*\mathbf{j}$. The process of obtaining this dual should give rise to terms of this type in a natural way, but this is a topic which certainly deserves closer scrutiny.

A second area of research to follow the present work has to do with the possibility of using the equations of structure of the traditional and nontraditional sectors of Finslerian TP as the field equations of the physics.[10] In this regard recall that, in a Finslerian torsion,

$$\Omega^0 = R^0_{\mu\nu}\omega^\mu \wedge \omega^\nu + S^0_{\mu j}\omega^\mu \wedge \omega_0^{\cdot j}, \tag{53}$$

$$\Omega^i = R^i_{\mu\nu}\omega^\mu \wedge \omega^\nu + S^i_{\mu j}\omega^\mu \wedge \omega_0^{\cdot j}. \tag{54}$$

The coefficients $R^0_{\mu\nu}$, $R^i_{\mu\nu}$, and $S^0_{\mu j}$ can tentatively be interpreted as the components of the electromagnetic, strong, and weak fields.[28] One must then associate $S^i_{\mu j}$ with some weak/strong complex. The interpretation of $R^i_{\mu\nu}$ as the weak interaction is already present in Pandres,[29,30] though his context is not Finslerian. One would, therefore, expect that boosts would mix the $R^0_{\mu\nu}$ and $R^i_{\mu\nu}$ components, which does not make sense. The way in which this problem is avoided in the non-Finslerian context is by using tetrads, use which comes accompanied by a separate treatment of the superscript and the subscripts in the tetrads. One further stipulates *ab initio* that the Lorentz transformations (or at least the boosts) only affect the subscripts in the tetrads, equivalently in the components of the torsion. The Finslerian context provides a natural interpretation of this, since the boosts are no longer transformations in the fibers of the Finsler bundles, but rather ''translations'' in the seven-dimensional ''phase-space–time'' manifold $S(M^4)$.

The differential invariants that determine the teleparallel Finslerian classical differential geometry are the same ones as those that determine the KK space. One thus has to assume that the degrees of freedom contained in the S components of the torsion have moved to other places in the KK structure. We thus tentatively associate the A^{BC} entries with $S^0_{\mu j}$ and, therefore, with the strong interaction. It then appears that the Q^μ would have to be associated with the other S quantities, namely with the $S^i_{\mu j}$ interaction, if the basic equations of the physics happen to be a manifestation of a teleparallel Finsler structure of space–time. The association of Q^μ with the weak/strong complex represented by $S^i_{\mu j}$ is suggested by Eq. (13), expressing the orthogonality of the velocity and Q^μ (recall that, from a Finslerian perspective, ''weak'' appears to be associated with orthogonality to the four-velocity[28]). Of course, it would seem that there are too few degrees of freedom in the Q^μ, as compared with the three indices in $S^i_{\mu j}$. This is not, however, the case, for the following reason. The $\omega_i^{\cdot j}$ represents a rotation of both the moving frame (MF) and the reference frame (RF) in standard differential geometry viewed as a theory of moving frames, since the motion of the MF is referred to itself and the MF and RF coincide. In our KK treatment, the boosts of the MF are represented by $d\mathbf{u}$, and the boosts and rotations of the RF are represented by $d\mathbf{e}_\mu$. The rotations of the MF have been removed *ab initio* from our KK construction. This was possible because a standard teleparallel structure is determined once the ω^μ's are given in a constant frame field, and a Finslerian teleparallel structure is determined once the $(\omega^\mu,\ \omega^i_0)$ are given on a constant section $(\omega^i_j = 0)$ of the metric-Finsler bundle. Thus the active rotations must be introduced by hand (say like a direct product) in the KK formalism, which is consistent with, but is not in principle about, MFs. It is in the context of such process that the relation to $S^i_{\mu j}$ of Q^μ (together with the differential invariants of the attached rotations) have to be viewed. The correspondence between the differential invariants in the teleparallel Finsler structure, on the one hand, and in its associated KK structure, on the other hand, thus emerges as an interesting subject for further research.

We conclude with the statement of our main finding, namely that the canonical geometry of Finslerian TP and its ramifications provides a solution to the issue of the interior derivative which is deeply connected with the cutting edge subject of Clifford algebras of nonsymmetric metrics.

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On separable Pauli equations

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We classify $(1+3)$-dimensional Pauli equations for a spin-$\frac{1}{2}$ particle interacting with the electro-magnetic field, that are solvable by the method of separation of variables. As a result, we obtain the 11 classes of vector-potentials of the electro-magnetic field $A(t,\vec{x})=(A_0(t,\vec{x}),\vec{A}(t,\vec{x}))$ providing separability of the corresponding Pauli equations. It is established, in particular, that the necessary condition for the Pauli equation to be separable into second-order matrix ordinary differential equations is its equivalence to the system of two uncoupled Schrödinger equations. In addition, the magnetic field has to be independent of spatial variables. We prove that coordinate systems and the vector-potentials of the electro-magnetic field providing the separability of the corresponding Pauli equations coincide with those for the Schrödinger equations. Furthermore, an efficient algorithm for constructing all coordinate systems providing the separability of Pauli equation with a fixed vector-potential of the electro-magnetic field is developed. Finally, we describe all vector-potentials $A(t,\vec{x})$ that (a) provide the separability of Pauli equation, (b) satisfy vacuum Maxwell equations without currents, and (c) describe non-zero magnetic field. [DOI: 10.1063/1.1436563]

I. INTRODUCTION

A quantum mechanical system consisting of a spin-$\frac{1}{2}$ charged particle, moving with momentum $\vec{p}$ in a time-dependent electro-magnetic field with the four-component vector-potential $(A_0,\vec{A})$, is described in a nonrelativistic approximation by the Pauli equation (see, e.g., Ref. 1)

$$(p_0-eA_0(t,\vec{x})-(\vec{p}-e\vec{A}(t,\vec{x}))^2+e\vec{\sigma}\vec{H})\psi(t,\vec{x})=0. \tag{1}$$

Here $\psi(t,\vec{x})$ is the two-component wave function in three space dimensions $\vec{x}=(x_1,x_2,x_3)$, $\vec{H}=\mathrm{rot}\vec{A}$ is the magnetic field, and $\vec{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ is a vector consisting of three Pauli matrices

$$\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}. \tag{2}$$

Hereafter we use the notations

$$p_0=i\frac{\partial}{\partial t},\quad \vec{p}=-i\vec{\nabla},\quad a=1,2,3, \tag{3}$$

and summation over the repeated Latin indices from 1 to 3 is implied.

As the Pauli equation has variable coefficients, we cannot apply the standard Fourier transformation. The only regular way for solving (1) is the classical method of separation of variables in curvilinear coordinate systems. In this respect, a natural question arises, which equations of the form (1) are separable, namely, which potentials A_0, $\vec{A}$ allow for separability of the Pauli equation

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in some curvilinear coordinate system? One of the principal objectives of the present article is to provide an efficient algorithm for answering these kinds of questions for systems of partial differential equations. It is essentially based on the results of Ref. 2, where the problem of separation of variables in the Schrödinger equation has been analyzed in detail. As the Pauli equation (1) differs from the Schrödinger equation by the term $e\vec{\sigma}\vec{H}$ only, it is natural to attempt modifying the technique employed in Ref. 2 in order to make it applicable to system of partial differential equations (PDEs) (1).

Integrable Hamiltonian systems with velocity-dependent potentials have been studied for the case $n=2$, i.e., in a Euclidean plane by Winternitz with co-authors.[3,4] Recently Benenti with co-authors[5] studied the problem of separation of variables in the stationary Hamilton–Jacobi equation with vector-potential from a geometrical point of view.

The problem of separation of variables for linear systems of first-order partial differential equations such as the Dirac equation has been repeatedly addressed by Shapovalov and Bagrov with co-authors[6,7] and by Kalnins and Miller with co-authors.[8–10] They developed a symmetry approach to the separation of variables in the Dirac equation where separability is characterized by the existence of a complete set of first-order matrix symmetry operators.

Symmetry and supersymmetry properties of the Pauli equations are studied in Ref. 11–13. Let us also mention Ref. 14, where physical aspects of the problem of separation of variables in some $(1+3)$-dimensional Pauli equations with time-dependent potentials are studied, and Ref. 7, where some classes of exact solutions of the Pauli equation are presented.

With all the variety of approaches to separation of variables in PDEs one can notice the three generic principles, namely,

(a) representation of a solution to be found in a separated (factorized) form via several functions of one variable,
(b) requirement that the above mentioned functions of one variable should satisfy some ordinary differential equations, and
(c) dependence of so found solution on several arbitrary (continuous or discrete) parameters, called spectral parameters or separation constants.

By a proper formalizing of the above features we have formulated in Ref. 2 an algorithm for variable separation in the Schrödinger equation with vector-potential. Below we generalize this algorithm for the case of system of PDEs (1).

To have a right to talk about description of *all* potentials and *all* coordinate systems enabling us to separate the Pauli equation, one needs to provide a rigorous definition of separation of variables. The definition we intend to use is based on ideas contained in the paper by Koornwinder.[15]

Let us introduce a new coordinate system t, $\omega_a=\omega_a(t,\vec{x})$, $a=1,2,3$, where ω_a are real-valued functions, functionally independent with respect to the spatial variables x_1, x_2, x_3, i.e.,

$$\det\left\|\frac{\partial\omega_a}{\partial x_b}\right\|_{a,b=1}^{3}\neq 0. \tag{4}$$

For a solution to be found we adopt the following separation ansatz:

$$\psi(t,\vec{x})=Q(t,\vec{x})\varphi_0(t)\prod_{a=1}^{3}\varphi_a(\omega_a(t,\vec{x}),\vec{\lambda})\chi, \tag{5}$$

where Q, φ_μ, $(\mu=0,1,2,3)$ are nonsingular 2×2-matrix functions of the indicated variables and χ is an arbitrary two-component constant column. What is more, the condition of commutativity of the matrices φ_μ is imposed, namely,

$$[\varphi_\mu,\varphi_\nu]=\varphi_\mu\varphi_\nu-\varphi_\nu\varphi_\mu=0,\quad \mu,\nu=0,1,2,3. \tag{6}$$

Note that the restriction (6) is an extra requirement, which narrows the class of separable Pauli equations. However, without this condition an efficient handling of the ansätze of the form (6) seems to be impossible. At least, in all papers devoted to variable separation in a systems of PDEs the condition of commutativity is imposed (explicitly or implicitly).

Definition 1: We say that the Pauli equation (1) admits separation of variables in a coordinate system t, $\omega_a=\omega_a(t,\vec{x})$, $a=1,2,3$, *if there are nonsingular* 2×2 *-matrix function* $Q(t,\vec{x})$ *and four matrix ordinary differential equations*

$$\begin{aligned} i\dot{\varphi}_0 &= -(P_{00}(t)+P_{0b}(t)\lambda_b)\varphi_0, \\ \ddot{\varphi}_a &= (P_{a0}(\omega_a)+P_{ab}(\omega_a)\lambda_b)\varphi_a, \quad a=1,2,3, \end{aligned} \tag{7}$$

jointly depending in an analytic way on three independent complex parameters λ_1, λ_2, λ_3 *(separation constants), such that, for each triplet* $(\lambda_1, \lambda_2, \lambda_3)$ *and for each set of solutions* $\varphi_0(t)$, $\varphi_1(\omega_1)$, $\varphi_2(\omega_2)$, $\varphi_3(\omega_3)$ *of (7), function (5) under condition (6) is a solution of (1).*

In the above formulas $P_{\mu\nu}$, μ, $\nu=0,1,2,3$, are some complex 2×2-matrix functions of the indicated variables.

Definition 2: Three complex parameters λ_1, λ_2, λ_3 *in (7) are called independent if the equality*

$$\operatorname{rank}\|P_{\mu a}\|_{\mu=0}^{3}{}_{a=1}^{3}=6 \tag{8}$$

holds, whenever $\varphi_0(t)\varphi_1(\omega_1)\varphi_2(\omega_2)\varphi_3(\omega_3)\neq 0$.

Condition (8) secures essential dependence of a solution with separated variables on the separation constants $\vec{\lambda}$.

Note that putting $Q=I$, $\omega_a=x_a$, $a=1,2,3$, in (6) yields the standard separation of variables in the Cartesian coordinate system. Next, choosing the spherical coordinates as ω_1, ω_2, ω_3 we arrive at the variable separation in the spherical coordinate system and so on. The principal task is describing all possible forms of the functions Q, ω_a, $a=1,2,3$, that provide separability of the Pauli equation in the sense of the definition given above. Solution of this problem, in its turn, requires describing the functions $A_0,\ldots,A_3$ that enable variable separation in the Pauli equation in the corresponding coordinate system. More precisely, we will need to solve the two mutually connected principal problems:

(i) to describe *all* cases of coefficients, for which the corresponding Pauli equation (1) is separable (in the sense of Definition 1) in at least one coordinate system, and
(ii) to construct *all* coordinate systems that allow for separation of variables (in the sense of Definition 1) in the Pauli equation (1) with some fixed vector-potential $(A_0,\vec{A})$.

Note, that formulas (5)–(8) form the input data of the method. We can change these conditions and thereby modify the definition of separation of variables. For instance, we can change the order of the reduced equations (7) or the number of essential parameters λ_a (a more detailed analysis of this problem for the Schrödinger equation can be found in Ref. 16). So, our claim of obtaining the *complete description* of vector-potentials and coordinate systems providing separation of variables in (1) makes sense only within the framework of Definition 1. If one uses a more general definition, it might be possible to construct new coordinate systems and vector-potentials providing separability of Eq. (1). But all solutions of the Pauli equation with separated variables known to us fit into the above suggested scheme.

Transformations

$$\lambda_a\to\lambda_a'=\Lambda_a(\lambda_1,\lambda_2,\lambda_3), \quad a=1,2,3, \tag{9}$$

under condition

$$\det\left\|\frac{\partial\Lambda_a}{\partial\lambda_b}\right\|_{a,b=1}^{3}\neq 0, \tag{10}$$

preserve the form of relations (5)–(8). So we can regard the corresponding spectral parameters $\vec{\lambda}$ and $\vec{\lambda}'$ as *equivalent* ones. Within the framework of this equivalence relation we can choose $\vec{\lambda}$ in such a way that all matrices $P_{\mu\nu}$, μ, $\nu=0,1,2,3$, in reduced Eqs. (7) are Hermitian ones and parameters λ_1, λ_2, λ_3 are real numbers.

Next, we introduce an equivalence relation on the set of all vector-potentials $A_0(t,\vec{x})$, $\vec{A}(t,\vec{x})$ providing separability of Eq. (1), on the sets of solutions with separated variables and corresponding coordinate systems.

Definition 3: We say that two vector-potentials $A(t,\vec{x})$ and $A'(t,\vec{x})$ are equivalent if they are transformed one into another by the gauge transformation

$$\vec{A}\to\vec{A}'=\vec{A}+\vec{\nabla}f,\quad A_0\to A_0'=A_0-\frac{\partial f}{\partial t}, \tag{11}$$

where $f=f(t,\vec{x})$ is an arbitrary smooth function.

For the Pauli equations to be invariant with respect to the above transformation, the wave function $\psi(t,\vec{x})$ is to be transformed according to the rule

$$\psi\to\psi'=\psi\exp(ief). \tag{12}$$

Indeed, if the transformations (11) and (12) in the Pauli equation (1) are performed one after another, we obtain the initial equation, provided we replace the functions $\vec{A}$, A_0, ψ with $\vec{A}'$, A_0', ψ'.

Note that the system of PDEs (1) admits a wider equivalence group from the point of view of the standard theory of partial differential equations (Shapovalov and Sukhomlin, Ref. 17). However this group cannot be regarded as an equivalence group within the context of quantum mechanics, since allowed transformations of the wave function must preserve the probability density $\psi^*\psi$. And it is straightforward to check the the wider Shapovalov and Sukhomlin equivalence group breaks this rule, because it, generally speaking, does not preserve $\psi^*\psi$. By this very reason, we restrict our considerations to the gauge transformations only.

Definition 4: Two solutions of the Pauli equation with separated variables are called equivalent if they can be transformed one into another by group transformations from the Lie transformation group admitted by Pauli equation (1). Moreover, solutions of the Pauli equation with separated variables having equivalent [in the sense of equivalence relation (9) and (10)] spectral parameters $\vec{\lambda}$ are equivalent.

Definition 5: Two coordinate systems t, ω_1, ω_2, ω_3 and t', ω_1', ω_2', ω_3' are called equivalent if they give equivalent solutions with separated variables. In particular, two coordinate systems are equivalent if the corresponding ansätze (5) are transformed one into another by reversible transformations of the form

$$t\to t'=f_0(t),\quad \omega_a\to\omega_a'=f_a(\omega_a),\quad a=1,2,3, \tag{13}$$

$$Q\to Q'=Ql_0(t)l_1(\omega_1)l_2(\omega_2)l_3(\omega_3), \tag{14}$$

where $f_0,\ldots,f_3$ are some smooth functions and $l_0,\ldots,l_3$ are some smooth 2×2-matrix functions of the indicated variables.

Indeed, transformations (13) and (14) preserve the form of ansätze (5). So, after completing the procedure of separation of variables in these coordinate systems we obtain the same solutions with separated variables.

These equivalence relations reflect the freedom in choice of the functions Q, ω_1, ω_2, ω_3 and separation constants λ_1, λ_2, λ_3 preserving the form of the conditions (5)–(8). They split the set

of all possible vector-potentials, providing separability of Eq. (1), and sets of solutions with separated variables and corresponding coordinate systems into equivalence classes. In a sequel, when presenting the corresponding lists we will give only one representative for each equivalence class.

II. CLASSIFICATION OF SEPARABLE PAULI EQUATIONS (1)

In this section we obtain an exhaustive classification of the Pauli equations solvable within the framework of the approach described in the Introduction. Furthermore, we describe curvilinear coordinate systems enabling separation of variables in (1).

Using the equalities (7) and (6) we get

$$[P_{\mu 0}+P_{\mu a}\lambda_a, P_{\nu 0}+P_{\nu a}\lambda_a]=0.$$

Splitting the expression with respect to λ_a yields

$$[P_{\mu\alpha}, P_{\nu\beta}]+[P_{\mu\beta}, P_{\nu\alpha}]=0, \tag{15}$$

where $\mu,\nu,\alpha,\beta=0,1,2,3$ and henceforth summation over repeated Greek indices is not used. Choosing $\alpha=\beta$ we have

$$[P_{\mu\alpha}, P_{\nu\alpha}]=0.$$

Taking into account this equality and the fact that any Hermitian (2×2)-matrix can be represented as a linear combination of the unit and Pauli matrices (2), we get the following form of $P_{\mu\alpha}$:

$$P_{\mu\alpha}=F_{\mu\alpha}(\omega_\mu)I+G_{\mu\alpha}(\omega_\mu)\vec{s}_\alpha\vec{\sigma}, \tag{16}$$

where $F_{\mu\alpha}$, $G_{\mu\alpha}$ are some smooth scalar functions of the indicated variables, $\omega_0=t$ and $\vec{s}_\alpha$ is a constant three-component vector. Substitution of expression (16) into (15) yields

$$(G_{\mu\alpha}G_{\nu\beta}-G_{\mu\beta}G_{\nu\alpha})[\vec{s}_\alpha\vec{\sigma}, \vec{s}_\beta\vec{\sigma}]=0.$$

From this equality we conclude that there are two distinct cases: either $\vec{s}_\alpha\sim\vec{s}_\beta$ or $G_{\mu\alpha}\sim G_{\mu\beta}$. In view of this fact we get the two possible forms for the Eqs. (7):

$$\begin{aligned} i\dot{\varphi}_0&=-(F_{00}(t)+F_{0b}(t)\lambda_b+(G_{00}(t)+G_{0b}(t)\lambda_b)\vec{s}\vec{\sigma})\varphi_0,\\ \ddot{\varphi}_a&=(F_{a0}(\omega_a)+F_{ab}(\omega_a)\lambda_b+(G_{a0}(\omega_a)+G_{ab}(\omega_a)\lambda_b)\vec{s}\vec{\sigma})\varphi_a, \end{aligned} \tag{17}$$

and

$$\begin{aligned} i\dot{\varphi}_0&=-(F_{00}(t)+F_{0b}(t)\lambda_b+G_0(t)(\vec{s}_0+\vec{s}_b\lambda_b)\vec{\sigma})\varphi_0,\\ \ddot{\varphi}_a&=(F_{a0}(\omega_a)+F_{ab}(\omega_a)\lambda_b+G_a(\omega_a)(\vec{s}_0+\vec{s}_b\lambda_b)\vec{\sigma})\varphi_a, \end{aligned} \tag{18}$$

with $a=1,2,3$.

Definition 1 is quite algorithmic in the sense that it contains a regular algorithm of variable separation in Pauli equation (1). Formulas (5), (17), and (18) form the input data of the method. The principal steps of the procedure of variable separation in Pauli equation (1) are as follows.

(1) We insert the ansatz (5) into the Pauli equation and express the derivatives $\dot{\varphi}_0$, $\ddot{\varphi}_1$, $\ddot{\varphi}_2$, $\ddot{\varphi}_3$ in terms of functions φ_0, φ_1, φ_2, φ_3, using Eqs. (17) and (18).
(2) We regard φ_0, φ_1, φ_2, φ_3, λ_1, λ_2, λ_3 as new independent variables $y_1,\ldots,y_7$. As the functions Q, ω_1, ω_2, ω_3, A_0, A_1, A_2, A_3 are independent on the variables $y_1,\ldots,y_7$, we can demand that the obtained equality is transformed into identity under arbitrary $y_1,\ldots,y_7$. In other words, we should split the equality with respect to these variables under condition of

commutativity (6). After splitting we get an overdetermined system of nonlinear partial differential equations for unknown functions Q, ω_1, ω_2, ω_3, A_0, A_1, A_2, A_3.

(3) After solving the above system we get an exhaustive description of vector-potentials $A(t,\vec{x})$ providing separability of the Pauli equation and corresponding coordinate systems.

Having performed the first two steps of the above algorithm we obtain the system of nonlinear matrix PDEs:

$$(i) \quad \frac{\partial \omega_b}{\partial x_a}\frac{\partial \omega_c}{\partial x_a}=0, \quad b\neq c, \quad b,c=1,2,3.$$

$$(ii) \quad \sum_{a=1}^{3} F_{ab}(\omega_a)\frac{\partial \omega_a}{\partial x_c}\frac{\partial \omega_a}{\partial x_c}=F_{0b}(t), \quad b=1,2,3.$$

(*iiia*) For the case of reduced equations given by (17),

$$\sum_{a=1}^{3} G_{a\mu}(\omega_a)\frac{\partial \omega_a}{\partial x_c}\frac{\partial \omega_a}{\partial x_c}=G_{0\mu}(t), \quad \mu=0,1,2,3.$$

(*iiib*) For the case of reduced equations given by (18),

$$\sum_{a=1}^{3} G_{a}(\omega_a)\frac{\partial \omega_a}{\partial x_c}\frac{\partial \omega_a}{\partial x_c}=G_{0}(t).$$

$$(iv) \quad 2\left(\frac{\partial Q}{\partial x_b}-ieQA_b\right)\frac{\partial \omega_a}{\partial x_b}+Q\left(i\frac{\partial \omega_a}{\partial t}+\Delta\omega_a\right)=0, \quad a=1,2,3.$$

$$(v) \quad Q\sum_{a=1}^{3} F_{a0}(\omega_a)\frac{\partial \omega_a}{\partial x_b}\frac{\partial \omega_a}{\partial x_b}+i\frac{\partial Q}{\partial t}+\Delta Q-2ieA_b\frac{\partial Q}{\partial x_b}$$
$$+\left(-F_{00}(t)-ie\frac{\partial A_b}{\partial x_b}-eA_0-e^2A_bA_b+e\vec{\sigma}\vec{H}\right)Q=0.$$

Thus the problem of variable separation in the Pauli equation reduces to integrating a system of nonlinear PDEs for eight unknown functions A_0, A_1, A_2, A_3, Q, ω_1, ω_2, ω_3 of four variables $t,\vec{x}$. What is more, some coefficients are arbitrary matrix functions which should be determined in the process of integrating of the system of PDEs (i)–(v). We succeeded in constructing the general solution of the latter which yields, in particular, all possible vector-potentials $A(t,\vec{x})=(A_0(t,\vec{x}),\ldots,A_3(t,\vec{x}))$ such that Pauli equation (1) is solvable by the method of separation of variables.

In view of (8) we can always choose from each set of the equations (ii), $(iiia)$, and (ii), $(iiib)$ three such equations that the matrix of coefficients of $\omega_{ax_c}\omega_{ax_c}$ $(a=1,2,3)$ is nonsingular. It is called the Stäckel matrix.[18] The system consisting of these three equations and of the equations (i) was integrated in Ref. 2. Its general solution $\vec{\omega}=\vec{\omega}(t,\vec{x})$ is given implicitly within the equivalence relation (13) by the following formulas:

$$\vec{x}=\mathcal{O}(t)\mathcal{L}(t)(\vec{z}(\vec{\omega})+\vec{v}(t)). \tag{19}$$

Here $\mathcal{O}(t)$ is a time-dependent 3×3 orthogonal matrix with Euler angles $\alpha(t)$, $\beta(t)$, $\gamma(t)$:

$$\mathcal{O}(t)=\begin{pmatrix} \cos\alpha\cos\beta-\sin\alpha\sin\beta\cos\gamma & -\cos\alpha\sin\beta-\sin\alpha\cos\beta\cos\gamma & \sin\alpha\sin\gamma \\ \sin\alpha\cos\beta+\cos\alpha\sin\beta\cos\gamma & -\sin\alpha\sin\beta+\cos\alpha\cos\beta\cos\gamma & -\cos\alpha\sin\gamma \\ \sin\beta\sin\gamma & \cos\beta\sin\gamma & \cos\gamma \end{pmatrix}; \tag{20}$$

$\vec{v}(t)$ stands for the vector-column whose entries $v_1(t)$, $v_2(t)$, $v_3(t)$ are arbitrary smooth functions of t; $\vec{z}=\vec{z}(\vec{\omega})$ is given by one of the eleven formulas

(1) Cartesian coordinate system,

$$z_1=\omega_1,\quad z_2=\omega_2,\quad z_3=\omega_3,$$

$$\omega_1,\omega_2,\omega_3\in\mathbf{R}.$$

(2) Cylindrical coordinate system,

$$z_1=e^{\omega_1}\cos\omega_2,\quad z_2=e^{\omega_1}\sin\omega_2,\quad z_3=\omega_3,$$

$$0\leqslant\omega_2<2\pi,\quad \omega_1,\omega_3\in\mathbf{R}.$$

(3) Parabolic cylindrical coordinate system,

$$z_1=(\omega_1^2-\omega_2^2)/2,\quad z_2=\omega_1\omega_2,\quad z_3=\omega_3,$$

$$\omega_1>0,\quad \omega_2,\omega_3\in\mathbf{R}.$$

(4) Elliptic cylindrical coordinate system,

$$z_1=a\cosh\omega_1\cos\omega_2,\quad z_2=a\sinh\omega_1\sin\omega_2,\quad z_3=\omega_3,$$

$$\omega_1>0,\quad -\pi<\omega_2\leqslant\pi,\quad \omega_3\in\mathbf{R},\quad a>0.$$

(5) Spherical coordinate system,

$$z_1=\omega_1^{-1}\operatorname{sech}\omega_2\cos\omega_3,$$

$$z_2=\omega_1^{-1}\operatorname{sech}\omega_2\sin\omega_3,$$

$$z_3=\omega_1^{-1}\tanh\omega_2,$$

$$\omega_1>0,\quad \omega_2\in\mathbf{R},\quad 0\leqslant\omega_3<2\pi.$$

(6) Prolate spheroidal coordinate system,

$$z_1=a\operatorname{csch}\omega_1\operatorname{sech}\omega_2\cos\omega_3,\quad a>0,$$

$$z_2=a\operatorname{csch}\omega_1\operatorname{sech}\omega_2\sin\omega_3,$$

$$z_3=a\coth\omega_1\tanh\omega_2,$$

$$\omega_1>0,\quad \omega_2\in\mathbf{R},\quad 0\leqslant\omega_3<2\pi. \tag{21}$$

(7) Oblate spheroidal coordinate system,

$$z_1=a\csc\omega_1\operatorname{sech}\omega_2\cos\omega_3,\quad a>0,$$

$$z_2=a\csc\omega_1\operatorname{sech}\omega_2\sin\omega_3,$$

$$z_3 = a \cot \omega_1 \tanh \omega_2,$$

$$0 < \omega_1 < \pi/2, \quad \omega_2 \in \mathbf{R}, \quad 0 \leqslant \omega_3 < 2\pi.$$

(8) Parabolic coordinate system,

$$z_1 = e^{\omega_1 + \omega_2} \cos \omega_3, \quad z_2 = e^{\omega_1 + \omega_2} \sin \omega_3,$$

$$z_3 = (e^{2\omega_1} - e^{2\omega_2})/2,$$

$$\omega_1, \omega_2 \in \mathbf{R}, \quad 0 \leqslant \omega_3 \leqslant 2\pi.$$

(9) Paraboloidal coordinate system,

$$z_1 = 2a \cosh \omega_1 \cos \omega_2 \sinh \omega_3, \quad a > 0,$$

$$z_2 = 2a \sinh \omega_1 \sin \omega_2 \cosh \omega_3,$$

$$z_3 = a(\cosh 2\omega_1 + \cos 2\omega_2 - \cosh 2\omega_3)/2,$$

$$\omega_1, \omega_3 \in \mathbf{R}, \quad 0 \leqslant \omega_2 < \pi.$$

(10) Ellipsoidal coordinate system,

$$z_1 = a \frac{1}{\mathrm{sn}(\omega_1, k)} \mathrm{dn}(\omega_2, k') \, \mathrm{sn}(\omega_3, k), \quad a > 0,$$

$$z_2 = a \frac{\mathrm{dn}(\omega_1, k)}{\mathrm{sn}(\omega_1, k)} \mathrm{cn}(\omega_2, k') \mathrm{cn}(\omega_3, k),$$

$$z_3 = a \frac{\mathrm{cn}(\omega_1, k)}{\mathrm{sn}(\omega_1, k)} \mathrm{sn}(\omega_2, k') \, \mathrm{dn}(\omega_3, k),$$

$$0 < \omega_1 < K, \quad -K' \leqslant \omega_2 \leqslant K', \quad 0 \leqslant \omega_3 \leqslant 4K.$$

(11) Conical coordinate system,

$$z_1 = \omega_1^{-1} \mathrm{dn}(\omega_2, k') \, \mathrm{sn}(\omega_3, k),$$

$$z_2 = \omega_1^{-1} \mathrm{cn}(\omega_2, k') \, \mathrm{cn}(\omega_3, k),$$

$$z_3 = \omega_1^{-1} \mathrm{sn}(\omega_2, k') \, \mathrm{dn}(\omega_3, k),$$

$$\omega_1 > 0, \quad -K' \leqslant \omega_2 \leqslant K', \quad 0 \leqslant \omega_3 \leqslant 4K;$$

and $\mathcal{L}(t)$ is a 3×3 diagonal matrix

$$\mathcal{L}(t) = \begin{pmatrix} l_1(t) & 0 & 0 \\ 0 & l_2(t) & 0 \\ 0 & 0 & l_3(t) \end{pmatrix}, \tag{22}$$

where $l_1(t), l_2(t), l_3(t)$ are arbitrary nonzero smooth functions that satisfy the following conditions:

(i) $l_1(t) = l_2(t)$ for the partially split coordinate systems [cases 2–4 from (21)],

(ii) $l_1(t)=l_2(t)=l_3(t)$ for nonsplit coordinate systems [cases 5-11 from (21)].

Here we use the usual notations for the trigonometric, hyperbolic and Jacobi elliptic functions, number $k\,(0<k<1)$ being the modulus of the latter and $k'=(1-k^2)^{1/2}$.

From a geometric point of view the right-hand side of formula (19) is a result of application to vector $\vec{z}(\vec{\omega})$ of the following time-dependent transformations performed one after another:

(1) translations $\vec{z}\to\vec{z}'=\vec{z}+\vec{v}(t)$,
(2) dilatations $\vec{z}\to\vec{z}'=\mathcal{L}(t)\vec{z}$,
(3) three-dimensional rotations $\vec{z}\to\vec{z}'=\mathcal{O}(t)\vec{z}$ with Euler angles $\alpha(t),\ \beta(t),\ \gamma(t)$.

Together with the rotations the following vector $\vec{\Omega}(t)=(\Omega_1,\Omega_2,\Omega_3)$ is considered (Ref. 19, Sec. 35),

$$\begin{aligned}\Omega_1(t)&=\dot{\gamma}(t)\cos\alpha(t)+\dot{\beta}(t)\sin\alpha(t)\sin\gamma(t),\\ \Omega_2(t)&=\dot{\gamma}(t)\sin\alpha(t)-\dot{\beta}(t)\cos\alpha(t)\sin\gamma(t),\\ \Omega_3(t)&=\dot{\alpha}(t)+\dot{\beta}(t)\cos\gamma(t),\end{aligned}\tag{23}$$

that is directed along momentary axis of rotation and called *angular velocity vector*.

Note that we have chosen the coordinate systems $\omega_1,\ \omega_2,\ \omega_3$ by means of the equivalence relation (13) in such a way that the relations

$$\Delta\omega_a=0,\quad a=1,2,3,\tag{24}$$

hold for all the cases 1–11 in (21).

After integration of system $(i)-(iii)$ it is not difficult to integrate the remaining (iv) and (v) from the system under study, since they can be regarded as algebraic equations for the functions $A_a(t,\vec{x}),(a=1,2,3)$ and $A_0(t,\vec{x})$, correspondingly.

Multiplying (iv) from the right by Q^{-1} we obtain for each component of matrices $(\partial Q/\partial x_b)\,Q^{-1}$, $b=1,2,3$, the systems of three linear algebraic equations. The determinants of the systems do not vanish according to (4). So they have the unique solution

$$\frac{\partial Q}{\partial x_b}Q^{-1}=f_b(t,\vec{x})I,\quad b=1,2,3,\tag{25}$$

where $f_b(t,\vec{x})$ are scalar smooth functions and I is unit 2×2-matrix. From the compatibility conditions

$$\frac{\partial f_a}{\partial x_b}=\frac{\partial f_b}{\partial x_a},\quad a,b=1,2,3,$$

of the above system of PDEs we obtain that there exists such function $g(t,\vec{x})$ that the equalities $f_a=\partial g/\partial x_a$, $a=1,2,3$, hold. So (25) takes the form

$$\frac{\partial Q}{\partial x_b}=\frac{\partial g}{\partial x_b}Q,\quad b=1,2,3.$$

The general solution of this system of matrix PDEs is

$$Q=\mathcal{U}(t)\exp g(t,\vec{x}),\tag{26}$$

where $\mathcal{U}(t)$ is arbitrary 2×2-matrix function of t.

Let us represent the complex-valued function $g(t,\vec{x})$ in (26) as $g=S_1+iS$, where S_1, S are real-valued functions. Now, if we take into account that the components of the vector potential $A(t,\vec{x})$ and functions ω_1, ω_2, ω_3 are real-valued functions, then after inserting (26) into (iv) with the use of (24) we can split the obtained equations into real and imaginary parts:

$$\frac{\partial S_1}{\partial x_b}\frac{\partial \omega_a}{\partial x_b}=0, \quad a=1,2,3; \tag{27}$$

$$2\left(\frac{\partial S}{\partial x_b}-eA_b\right)\frac{\partial \omega_a}{\partial x_b}+\frac{\partial \omega_a}{\partial t}=0, \quad a=1,2,3. \tag{28}$$

Taking into account the equality (4), we obtain from (27) the equalities $\partial S_1/\partial x_b=0$, $b=1,2,3$. It gives that $S_1=S_1(t)$.

Let us denote $e\vec{\mathcal{A}}=e\vec{A}-\vec{\nabla}S$. Then the system (28) takes the form of three linear algebraic equations for functions $\mathcal{A}_1$, $\mathcal{A}_2$, $\mathcal{A}_3$:

$$\frac{\partial \omega_a}{\partial t}=2e\frac{\partial \omega_a}{\partial x_b}\mathcal{A}_b, \quad a=1,2,3.$$

The determinant of this system does not vanish due to (4). Consequently, it has a unique solution. Making in this solution the hodographic transformation

$$t=t, \quad x_a=u_a(t,\omega_1,\omega_2,\omega_3), \quad a=1,2,3, \tag{29}$$

we get the following expressions for $\mathcal{A}_1$, $\mathcal{A}_2$, $\mathcal{A}_3$:

$$\vec{\mathcal{A}}=-\frac{1}{2e}\frac{\partial \vec{u}(t,\vec{\omega})}{\partial t}.$$

After substitution into this formula expression for $\vec{u}(t,\vec{\omega})$ (19), we return to variables t,x_1,x_2,x_3 and thus obtain the following system:

$$2(-e\vec{A}(t,\vec{x})+\vec{\nabla}S)=\mathcal{M}(t)\vec{x}+\mathcal{O}(t)\mathcal{L}(t)\dot{\vec{v}}. \tag{30}$$

Here we use the designation

$$\mathcal{M}(t)=\dot{\mathcal{O}}(t)\mathcal{O}^{-1}(t)+\mathcal{O}(t)\dot{\mathcal{L}}(t)\mathcal{L}^{-1}(t)\mathcal{O}^{-1}(t), \tag{31}$$

where $\mathcal{O}(t)$, $\mathcal{L}(t)$ are variable 3×3 matrices defined by formulas (20) and (22), correspondingly, $\vec{v}=(v_1(t),v_2(t),v_3(t))^T$. Note that $\dot{\mathcal{O}}\mathcal{O}^{-1}$ is antisymmetric and $\mathcal{O}\dot{\mathcal{L}}\mathcal{L}^{-1}\mathcal{O}^{-1}$ is the symmetric part of matrix $\mathcal{M}$.

The direct calculation shows that (v) and (30) are invariant under gauge transformations (11). Thus the function S is transformed by the rule

$$S\to S'=S+ef, \tag{32}$$

which follows from (12). In other words, if the transformations (11) and (32) in (v) and (30) are performed one after another, we obtain the initial equations where functions $\vec{A}$, A_0, S should be replaced with functions $\vec{A}'$, A_0', S'. So, if the Pauli equation (1) with potential $\vec{A}$, A_0 admits separation of variables in some coordinate system, then the Pauli equation with potential $\vec{A}'$, A_0' admits separation of variables in the same coordinate system [the multiplier Q (26) is changed only]. Therefore, it is worthwhile to fix some gauge and to work only with representatives of the equivalence classes of potentials $A(t,\vec{x})$ [in the sense of equivalence relation (11)].

We choose the gauge in a way that the equality

$$2\vec{\nabla}S=\mathcal{O}(t)\dot{\mathcal{L}}(t)\mathcal{L}^{-1}(t)\mathcal{O}^{-1}(t)\vec{x}+\mathcal{O}(t)\mathcal{L}(t)\dot{\vec{v}} \tag{33}$$

holds. After integration of this system of PDEs we obtain the expression for S

$$S=\frac{1}{4}\sum_{a=1}^{3}\left(\frac{\dot{l}_a}{l_a}x'^2_a+2l_a\dot{v}_a x'_a\right), \tag{34}$$

where we use the notations

$$\vec{x}'=\mathcal{O}^{-1}\vec{x}. \tag{35}$$

Next, we obtain from Eq. (30) the explicit form for spacelike components of vector-potential of electromagnetic field

$$\vec{A}(t,\vec{x})=-\frac{1}{2e}\dot{\mathcal{O}}\mathcal{O}^{-1}\vec{x}, \tag{36}$$

where the explicit form of matrix $\dot{\mathcal{O}}\mathcal{O}^{-1}$ is given by the formula

$$\dot{\mathcal{O}}\mathcal{O}^{-1}=\begin{pmatrix} 0 & -(\dot{\alpha}+\dot{\beta}\cos\gamma) & \dot{\gamma}\sin\alpha-\dot{\beta}\cos\alpha\sin\gamma \\ \dot{\alpha}+\dot{\beta}\cos\gamma & 0 & -(\dot{\gamma}\cos\alpha+\dot{\beta}\sin\alpha\sin\gamma) \\ -(\dot{\gamma}\sin\alpha-\dot{\beta}\cos\alpha\sin\gamma) & \dot{\gamma}\cos\alpha+\dot{\beta}\sin\alpha\sin\gamma & 0 \end{pmatrix}, \tag{37}$$

where α,β,γ are arbitrary functions of t.

Thus formula (36) means that the spacelike components of electromagnetic field $A(t,\vec{x})$ are linear with respect of spatial variables. So the magnetic field $\vec{H}=\mathrm{rot}\vec{A}$ should be homogeneous, i.e., independent of spatial variables $\vec{x}$. From formulas (36) and (37) we can obtain its explicit form

$$\begin{aligned} eH_1&=-\dot{\gamma}(t)\cos\alpha(t)-\dot{\beta}(t)\sin\alpha(t)\sin\gamma(t), \\ eH_2&=-\dot{\gamma}(t)\sin\alpha(t)+\dot{\beta}(t)\cos\alpha(t)\sin\gamma(t), \\ eH_3&=-\dot{\alpha}(t)-\dot{\beta}(t)\cos\gamma(t). \end{aligned} \tag{38}$$

Now the spacelike components of the electromagnetic field take the final form

$$\vec{A}(t,\vec{x})=\frac{1}{2}\begin{pmatrix} 0 & -H_3(t) & H_2(t) \\ H_3(t) & 0 & -H_1(t) \\ -H_2(t) & H_1(t) & 0 \end{pmatrix}\vec{x}=\frac{1}{2}\vec{H}(t)\times\vec{x}, \tag{39}$$

where symbol $\times$ denotes cross product.

Within the equivalence relation (14) we can always choose the function $\mathcal{U}(t)$ to be a solution of matrix ODE

$$i\dot{\mathcal{U}}=(-e\vec{\sigma}\vec{H}(t))\mathcal{U} \tag{40}$$

with the initial conditions $\mathcal{U}(0)=I$. Due to the theorem of existence and the uniqueness of the solution of the Cauchy problem for the system of ODEs there is unique solution $\mathcal{U}(t)$ of system (40) for each fixed configuration of magnetic field $\vec{H}(t)$. Moreover, matrix $\mathcal{U}(t)$ is a unitary one. Indeed, taking into account (40), we have the equality

$$\frac{d}{dt}(\mathcal{U}^*\mathcal{U})=\mathcal{U}^*(ie\vec{\sigma}\vec{H})\mathcal{U}+\mathcal{U}^*(-ie\vec{\sigma}\vec{H})\mathcal{U}=0,$$

i.e., $\mathcal{U}^*\mathcal{U}=\text{const}$. The initial conditions give $\mathcal{U}^*\mathcal{U}=I$.

Thus we can consider the following change of variables in the Pauli equation (1),

$$\psi=\mathcal{U}(t)\tilde{\psi}. \tag{41}$$

Due to the unitarity of the matrix $\mathcal{U}$ the quantity $\psi^*\psi$, which is regarded in quantum mechanics as the probability density, is not changed. So the change of variables (41) is the correct one. As a result, the term $e\vec{\sigma}\vec{H}$ in Pauli equation (1) vanishes, and we obtained a system of two Schrödinger equations for the function $\tilde{\psi}$.

Thus we proved the following assertion.

Lemma 1: A necessary condition for the Pauli equation (1) to be separable (in the sense of Definition 1) is that it has to be equivalent [in the sense of equivalence relation (41)] to a system of two uncoupled Schrödinger equations.

Let us substitute the equality (26) into (v), taking into account Eq. (40) and $S_1=S_1(t)$. Splitting the equation obtained into real and imaginary parts (note that all functions F_{00}, F_{a0}, $a=1,2,3$, are real-valued ones), we obtain the equalities

$$\sum_{a=1}^{3} F_{a0}(\omega_a)\frac{\partial\omega_a}{\partial x_b}\frac{\partial\omega_a}{\partial x_b}-\frac{\partial S}{\partial t}-\frac{\partial S}{\partial x_b}\frac{\partial S}{\partial x_b}+2eA_b\frac{\partial S}{\partial x_b}-F_{00}(t)-eA_0-e^2A_bA_b=0, \tag{42}$$

$$\dot{S}_1+\Delta S-e\frac{\partial A_b}{\partial x_b}=0. \tag{43}$$

Inserting into Eq. (42) expressions for S (34) and A_1, A_2, A_3 (39), we obtain the explicit form of A_0:

$$eA_0(t,\vec{x})=\sum_{a=1}^{3} F_{a0}(\omega_a)\frac{\partial\omega_a}{\partial x_b}\frac{\partial\omega_a}{\partial x_b}-F_{00}(t)-e^2A_bA_b-\frac{1}{4}P. \tag{44}$$

Here A_bA_b follows from (39) and (37):

$$4A_bA_b=(H_2x_3-H_3x_2)^2+(H_3x_1-H_1x_3)^2+(H_2x_1-H_1x_2)^2, \tag{45}$$

where H_1, H_2, H_3 are components of magnetic field (38); function P has the form

$$P=\sum_{a=1}^{3}\left(\frac{\ddot{l}_a}{l_a}x'^2_a+2(l_a\ddot{v}_a+2\dot{l}_a\dot{v}_a)x'_a+l_a^2\dot{v}_a^2\right), \tag{46}$$

where x'_1, x'_2, x'_3 are given by formula (35) and $l_a=l_a(t)$, $v_a=v_a(t)$, $a=1,2,3$, are arbitrary smooth functions, which define new coordinate system (19).

Let us emphasize that the expression for A_0 includes arbitrary functions $F_{10}(\omega_1)$, $F_{20}(\omega_2)$, $F_{30}(\omega_3)$, $F_{00}(t)$, where functions $\omega_a=\omega_a(t,\vec{x})$, $a=1,2,3$, belong to one of 11 classes, whose representatives are given implicitly by the formulas (19)–(22).

Below we give explicit forms of the eikonals $R_a^{-2}=(\partial\omega_a/\partial x_b)(\partial\omega_a/\partial x_b)$ for each class of ω_a (see also Ref. 2):

$$(1)\quad R_i^{-2}=h_i^{-2},\quad i=1,2,3;$$

$$(2)\quad R_1^{-2}=R_2^{-2}=h_1^{-2}e^{-2\omega_1},\quad R_3^{-2}=h_3^{-2};$$

$$(3)\quad R_1^{-2}=R_2^{-2}=h_1^{-2}(\omega_1^2+\omega_2^2)^{-1},\quad R_3^{-2}=h_3^{-2};$$

$$(4)\quad R_1^{-2}=R_2^{-2}=h_1^{-2}a^{-2}(\cosh^2\omega_1-\cos^2\omega_2)^{-1},\quad R_3^{-2}=h_3^{-2};$$

$$(5)\quad R_1^{-2}=h_1^{-2}\omega_1^4,\quad R_2^{-2}=R_3^{-2}=h_1^{-2}\omega_1^2\cosh^2\omega_2;$$

$$(6)\quad R_1^{-2}=h_1^{-2}a^{-2}\sinh^2\omega_1(\sinh^{-2}\omega_1+\cosh^{-2}\omega_2)^{-1},$$

$$R_2^{-2}=h_1^{-2}a^{-2}\cosh^2\omega_2(\sinh^{-2}\omega_1+\cosh^{-2}\omega_2)^{-1},$$

$$R_3^{-2}=h_1^{-2}a^{-2}\sinh^2\omega_1\cosh^2\omega_2; \tag{47}$$

$$(7)\quad R_1^{-2}=h_1^{-2}a^{-2}\sin^2\omega_1(\sin^{-2}\omega_1-\cosh^{-2}\omega_2)^{-1},$$

$$R_2^{-2}=h_1^{-2}a^{-2}\cosh^2\omega_2(\sin^{-2}\omega_1-\cosh^{-2}\omega_2)^{-1},$$

$$R_3^{-2}=h_1^{-2}a^{-2}\sin^2\omega_1\cosh^2\omega_2;$$

$$(8)\quad R_1^{-2}=h_1^{-2}e^{-2\omega_1}(e^{2\omega_1}+e^{2\omega_2})^{-1},$$

$$R_2^{-2}=h_1^{-2}e^{-2\omega_2}(e^{2\omega_1}+e^{2\omega_2})^{-1},\quad R_3^{-2}=h_1^{-2}e^{-2(\omega_1+\omega_2)};$$

$$(9)\quad R_1^{-2}=h_1^{-2}a^{-2}(\cosh 2\omega_1-\cos 2\omega_2)^{-1}(\cosh 2\omega_1+\cosh 2\omega_3)^{-1},$$

$$R_2^{-2}=h_1^{-2}a^{-2}(\cosh 2\omega_1-\cos 2\omega_2)^{-1}(\cos 2\omega_2+\cosh 2\omega_3)^{-1},$$

$$R_3^{-2}=h_1^{-2}a^{-2}(\cosh 2\omega_1+\cosh 2\omega_3)^{-1}(\cos 2\omega_2+\cosh 2\omega_3)^{-1};$$

$$(10)\quad R_1^{-2}=h_1^{-2}a^{-2}\left(\frac{\mathrm{dn}^2(\omega_1,k)}{\mathrm{sn}^2(\omega_1,k)}-k'^2\mathrm{cn}^2(\omega_2,k')\right)^{-1}\left(\frac{\mathrm{dn}^2(\omega_1,k)}{\mathrm{sn}^2(\omega_1,k)}+k^2\mathrm{cn}^2(\omega_3,k)\right)^{-1},$$

$$R_2^{-2}=h_1^{-2}a^{-2}\left(\frac{\mathrm{dn}^2(\omega_1,k)}{\mathrm{sn}^2(\omega_1,k)}-k'^2\mathrm{cn}^2(\omega_2,k')\right)^{-1}(k'^2\mathrm{cn}^2(\omega_2,k')+k^2\mathrm{cn}^2(\omega_3,k))^{-1},$$

$$R_3^{-2}=h_1^{-2}a^{-2}\left(\frac{\mathrm{dn}^2(\omega_1,k)}{\mathrm{sn}^2(\omega_1,k)}+k^2\mathrm{cn}^2(\omega_3,k)\right)^{-1}(k'^2\mathrm{cn}^2(\omega_2,k')+k^2\mathrm{cn}^2(\omega_3,k))^{-1};$$

$$(11)\quad R_1^{-2}=h_1^{-2}\omega_1^4,\quad R_2^{-2}=R_3^{-2}=h_1^{-2}\omega_1^2(k'^2\mathrm{cn}^2(\omega_2,k')+k^2\mathrm{cn}^2(\omega_3,k))^{-1}.$$

At last, let us find the multiplier Q. Substituting the formulas (34) and (39) into Eq. (43) gives

$$\dot{S}_1=-\frac{1}{2}\sum_{a=1}^{3}\frac{\dot{l}_a}{l_a},$$

where it follows that

$$S_1=-\frac{1}{2}\sum_{a=1}^{3}\ln l_a. \tag{48}$$

Taking into account expression for S (34), we obtain from formula (26) the explicit form of Q

$$Q=\mathcal{U}(t)\frac{1}{\sqrt{l_1l_2l_3}}\exp\sum_{a=1}^{3}\frac{i}{4}\left(\frac{\dot{l}_a}{l_a}x'^2_a+2l_a\dot{v}_ax'_a\right), \tag{49}$$

where $\mathcal{U}(t)$ is given by Eq. (40), and x'_1,x'_2,x'_3 are given by formula (35).

Thus we have proved the main result of the article:

Theorem 1: *Pauli equation (1) admits separation of variables (in the sense of Definition 1) if and only if it is gauge equivalent to Pauli equation where*

(*i*) *the magnetic field* $\vec{H}=\mathrm{rot}\ \vec{A}$ *is independent of the spatial variables,*
(*ii*) *the spacelike components* A_1, A_2, A_3 *of the vector-potential of the electromagnetic field are given by* (*39*)*, and*
(*iii*) *the timelike component* A_0 *is given by formulas (44)–(47).*

Comparing the components of magnetic field (38) with components of angular velocity vector (23) of rotation of coordinate system (19), we obtain the equality $e\vec{H}=-\vec{\omega}$. So, we prove the following assertion:

Corollary 1: Let Pauli equation (1) admit separation of variables in some nonstationary coordinate system t, $\omega_a=\omega_a(t,\vec{x})$, $a=1,2,3$, *where functions* $\omega_1(t,\vec{x})$, $\omega_2(t,\vec{x})$, $\omega_3(t,\vec{x})$ *are given implicitly by formulas* (*19*)–(*22*). *Then angular velocity vector* (*23*) *of rotation of this coordinate system equals* $-e\vec{H}$, *where* $\vec{H}=\mathrm{rot}\ \vec{A}$ *is magnetic field.*

It follows from the corollary that a necessary condition for the Pauli equation (1) with nonzero magnetic field $\vec{H}$ to be separable (in the sense of our Definition 1) is that the angular velocity vector (23) of rotation of the separation coordinate system (19)–(22) has to be nonzero.

Summing up we conclude that coordinate systems and vector-potentials of the electromagnetic field $A(t,\vec{x})=(A_0(t,\vec{x}),\vec{A}(t,\vec{x}))$ providing separability of the corresponding Pauli equations coincide with those for the Schrödinger equations. Namely, we prove that the magnetic field $\vec{H}=\mathrm{rot}\ \vec{A}$ has to be independent of the spatial variables. Next, we have 11 classes of potentials $A_0(t,\vec{x})$, corresponding to 11 classes of coordinate systems $t,\omega_a=\omega_a(t,\vec{x})$, $a=1,2,3$, where the functions $\omega_1(t,\vec{x}),\omega_2(t,\vec{x}),\omega_3(t,\vec{x})$ are given implicitly by formulas (19)–(22). Pauli equation (1) for each class of the functions $A_0(t,\vec{x}),\vec{A}(t,\vec{x})$ defined by (39), (44) and (47) under arbitrary $F_{00}(t),F_{a0}(\omega_a)$ and fixed arbitrary functions $\alpha(t)$, $\beta(t)$, $\gamma(t)$, $v_a(t)$, $l_a(t)$, $a=1,2,3$, separates in exactly one coordinate system.

The solutions with separated variables are of the form (5), where Q is given by (49). The separation equations read as (17) or (18), where the functions $F_{\mu0}$, $\mu=0,1,2,3$, are arbitrary smooth functions defining the form of the timelike component of the vector-potential $A(t,\vec{x})$ [see (44)]. The explicit forms of other coefficients $F_{\mu a}$, $G_{\mu\nu}$, G_μ of reduced equations can be obtained by splitting relations (*ii*) and (*iii*) with respect to independent variables ω_1, ω_2, ω_3, t for each class of the functions $\vec{z}=\vec{z}(\vec{\omega})$ given in (21). Let us denote

$$S=\begin{pmatrix} T_1 & T_2 & T_3\\ S_{11} & S_{12} & S_{13}\\ S_{21} & S_{22} & S_{23}\\ S_{31} & S_{32} & S_{33}\end{pmatrix}, \tag{50}$$

where the functions $S_{ab}(\omega_a)$ $(a,b=1,2,3)$ are given below as entries of 3×3 Stäckel matrices, whose structure is determined by the choice of the functions $\vec{z}=\vec{z}(\vec{\omega})$:

$$\mathcal{F}_1=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\quad \mathcal{F}_2=\begin{pmatrix}e^{2\omega_1}&-1&0\\0&1&0\\0&0&1\end{pmatrix},\quad \mathcal{F}_3=\begin{pmatrix}\omega_1^2&-1&0\\\omega_2^2&1&0\\0&0&1\end{pmatrix},$$

$$\mathcal{F}_4=\begin{pmatrix} a^2\cosh^2\omega_1 & 1 & 0\\ -a^2\cos^2\omega_2 & -1 & 0\\ 0 & 0 & 1\end{pmatrix},\quad \mathcal{F}_5=\begin{pmatrix} \omega_1^{-4} & -\omega_1^{-2} & 0\\ 0 & \cosh^{-2}\omega_2 & -1\\ 0 & 0 & 1\end{pmatrix},$$

$$\mathcal{F}_6=\begin{pmatrix} a^2\sinh^{-4}\omega_1 & -\sinh^{-2}\omega_1 & -1\\ a^2\cosh^{-4}\omega_2 & \cosh^{-2}\omega_2 & -1\\ 0 & 0 & 1\end{pmatrix},\quad \mathcal{F}_7=\begin{pmatrix} a^2\sin^{-4}\omega_1 & -\sin^{-2}\omega_1 & 1\\ -a^2\cosh^{-4}\omega_2 & \cosh^{-2}\omega_2 & -1\\ 0 & 0 & 1\end{pmatrix},\tag{51}$$

$$\mathcal{F}_8=\begin{pmatrix} e^{4\omega_1} & -e^{2\omega_1} & -1\\ e^{4\omega_2} & e^{2\omega_2} & -1\\ 0 & 0 & 1\end{pmatrix},\quad \mathcal{F}_9=\begin{pmatrix} a^2\cosh^2 2\omega_1 & -a\cosh 2\omega_1 & -1\\ -a^2\cos^2 2\omega_2 & a\cos 2\omega_2 & 1\\ a^2\cosh^2 2\omega_3 & a\cosh 2\omega_3 & -1\end{pmatrix},$$

$$\mathcal{F}_{10}=\begin{pmatrix} a^2\dfrac{\mathrm{dn}^4(\omega_1,k)}{\mathrm{sn}^4(\omega_1,k)} & -\dfrac{\mathrm{dn}^2(\omega_1,k)}{\mathrm{sn}^2(\omega_1,k)} & 1\\ -a^2k'^4\,\mathrm{cn}^4(\omega_2,k') & k'^2\,\mathrm{cn}^2(\omega_2,k') & -1\\ a^2k^4\,\mathrm{cn}^4(\omega_3,k) & k^2\,\mathrm{cn}^2(\omega_3,k) & 1\end{pmatrix},$$

$$\mathcal{F}_{11}=\begin{pmatrix} \omega_1^{-4} & -\omega_1^{-2} & 0\\ 0 & k'^2\mathrm{cn}^2(\omega_2,k') & -1\\ 0 & k^2\mathrm{cn}^2(\omega_3,k) & 1\end{pmatrix}.$$

The functions $T_1(t)$, $T_2(t)$, $T_3(t)$ are expressed in terms of the functions $h_1(t)$, $h_2(t)$, $h_3(t)$:

$$\begin{aligned}&(1)\quad T_i=h_i^{-2},\quad i=1,2,3;\\ &(2)\text{-}(4)\quad T_1=h_1^{-2},\quad T_2=0,\quad T_3=h_3^{-2};\\ &(5)\text{-}(11)\quad T_1=h_1^{-2},\quad T_2=T_3=0.\end{aligned}\tag{52}$$

Let K and M be 3×3 constant matrices. Now, if the reduced equations are given by (17), then

$$F=\|F_{\mu a}\|_{\mu=0}^{3}\ {}_{a=1}^{3},\quad G=\|G_{\mu a}\|_{\mu=0}^{3}\ {}_{a=1}^{3}$$

are block (6×8)-matrices, where $F_{\mu a}$ and $G_{\mu a}$ are 2×2-matrices that are equal to products of the corresponding entries of the matrices SK and SM by the unit (in the case of the matrix F) or $\vec{s}\vec{\sigma}$ (in the case of the matrix G) matrices. Accordingly, Eq. (8) takes the form

$$\mathrm{rank}\,(F+G)=6.\tag{53}$$

If rank $K=3$, then we can always rearrange $\lambda_1,\lambda_2,\lambda_3$ with the use of the equivalence relation (9) in order to get $K=I$. Analogously, without loss of generality we may put $M=I$, provided rank $M=3$ and $\vec{s}^2\neq 0$.

If rank $M=0$, then the column $\|G_{\mu 0}\|_{\mu=0}^{3}$ has necessarily the form $S\vec{g}$, where $\vec{g}$ is a constant three-component column. If rank $M\neq 0$, then we can always kill this column by a proper rearranging of $\lambda_1,\lambda_2,\lambda_3$ with the use of the equivalence relation (9).

Next, if the reduced equations are given by (18), then the matrix F is defined in the same way as in the previous case. Furthermore,

$$G=\|G_\mu\vec{s}_a\vec{\sigma}\|_{\mu=0}^{3}\ {}_{a=1}^{3}$$

is a block (6×8)-matrix, where G_μ are the three-component columns $S\vec{g}_\mu$ ($\vec{g}_\mu$ is a constant three-component column). In addition, in this case identity (53) holds, so that we can put $K=I$, when rank $K=3$. If $\vec{s}_a$, $(1=1,2,3)$ are three linear independent vectors, then we can always put $\vec{s}_0=0$.

We will finish this section with the following remark. It follows from Theorem 1 that a choice of magnetic fields $\vec{H}$ allowing for variable separation in the corresponding Pauli equation is very restricted. Namely, the magnetic field should be independent of spatial variables x_1, x_2, x_3 in order to provide the separability of Pauli equation (1) into three second-order matrix ordinary differential equations of the form (7). However, if we allow for separation equations to be of a lower order, then additional possibilities for variable separation in the Pauli equation arise. As an example, we give the vector potential

$$A(t,\vec{x})=(A_0(\sqrt{x_1^2+x_2^2}),\ 0,\ 0,\ A_3(\sqrt{x_1^2+x_2^2})),$$

where A_0, A_3 are arbitrary smooth functions. The Pauli equation (1) with this vector-potential separates in the cylindrical coordinate system

$$t,\quad \omega_1=\ln(\sqrt{x_1^2+x_2^2}),\quad \omega_2=\arctan(x_1/x_2),\quad \omega_3=x_3$$

into two first-order and one second-order matrix ordinary differential equations. The corresponding magnetic field $\vec{H}=\mathrm{rot}\,\vec{A}$ is evidently x-dependent. In this respect, let us also mention the recent paper by Benenti with co-authors,[5] where the problem of separation of variables in the stationary Hamilton–Jacobi equation with vector-potential has been studied. They have presented a number of vector-potentials, for which the Hamilton–Jacobi equation is separable, and the corresponding magnetic fields are inhomogeneous ones. These potentials allow for separation of variables in the stationary Schrödinger and Pauli equations with vector-potentials as well (see, e.g., Ref. 15 concerning the relationship between the separation of variables in the Schrödinger and Hamilton–Jacobi equations). These facts imply an importance of application of our approach to classify the nonstationary Pauli equations of the form (1), which admit separation of variables into first- and second-order matrix ordinary differential equations. We remind that here we give the classification results for the case, when all the reduced equations are second-order ones. We intend to address this problem in one of our future publications.

III. ALGORITHM OF SEPARATION OF VARIABLES IN THE PAULI EQUATION WITH FIXED POTENTIAL

Theorem 1 gives the solution of the problem of classification of the Pauli equations (1) with variable coefficients that are separable (in the sense of Definition 1) at least in one coordinate system.

Let us consider the problem of classification of coordinate systems that allow for separation of variables (in the sense of Definition 1) in the Pauli equation (1) with fixed vector-potential A_0, $\vec{A}$.

Let some fixed vector-potential $\vec{A}(t,\vec{x})$, $A_0(t,\vec{x})$ be given. The scheme of finding all coordinate systems providing separation of variables is as follows:

(1) With help of gauge transformations (11) we reduce the spacelike components of vector-potential $\vec{A}(t,\vec{x})$ to the form (39). If it is impossible, then Pauli equation (1) with this vector-potential is not solvable by the method of separation of variables in the framework of our approach.

(2) We solve the system of ODE (38) for given magnetic field $\vec{H}(t)$ and obtain the explicit form of functions $\alpha(t)$, $\beta(t)$, $\gamma(t)$.

(3) For each of 11 classes of coordinate systems t, $\omega_a=\omega_a(t,\vec{x})$, $a=1,2,3$, which are given by formulas (19)–(22), taking into account restrictions obtained on the first step of the algorithm, we find the explicit form of

(a) the timelike component A_0 of the vector-potential in terms of $\vec{\omega}$;
(b) function P, substituting in (46) the expression for $\vec{x}'$ in terms of $\vec{\omega}$ [see formulas (35) and (19)]:

$$\vec{x}' = \mathcal{L}(t)(\vec{z}(\vec{\omega}) + \vec{v}(t)); \tag{54}$$

(c) quantity $e^2 A_b A_b$ by the formula

$$4e^2 A_b A_b = (n_2 x_3' - n_3 x_2')^2 + (n_3 x_1' - n_1 x_3')^2 + (n_2 x_1' - n_1 x_2')^2,$$

where x_1', x_2', x_3' are given by the formula (54), and functions n_1, n_2, n_3 are as follows

$$\begin{aligned} n_1 &= \dot{\gamma}(t)\cos\beta(t) + \dot{\alpha}(t)\sin\beta(t)\sin\gamma(t), \\ n_2 &= -\dot{\gamma}(t)\sin\beta(t) + \dot{\alpha}(t)\cos\beta(t)\sin\gamma(t), \\ n_3 &= \dot{\beta}(t) + \dot{\alpha}(t)\cos\gamma(t); \end{aligned} \tag{55}$$

(d) eikonals $(\partial\omega_a/\partial x_b)(\partial\omega_a/\partial x_b) = R_a^{-2}$, $a = 1,2,3$, which are determined from the list (47) for given class of coordinates.

(4) We substitute the equalities obtained into Eq. (44) and obtain 11 equations for each of 11 classes of coordinate systems t, ω_1, ω_2, ω_3. For each of these equalities we find all possible functions $F_{a0}(\omega_a)$, $a = 1,2,3$, $F_{00}(t)$ that reduce it to the identity by the independent variables t, ω_1, ω_2, ω_3 (i.e., we split this equality with respect to these variables). It gives, in its turn, the explicit form of the functions $v_a(t)$, $l_a(t)$, $a = 1,2,3$, and additional restriction on $\alpha(t)$, $\beta(t)$, $\gamma(t)$, giving the form of the coordinate system in question. All obtained coordinates for which the functions $F_{a0}(\omega_a)$, $a = 1,2,3$, $F_{00}(t)$ exist are only coordinate systems providing separability of Pauli equations in the sense of Definition 1.

Example: As illustration of this algorithm consider the problem of separation of variables in Pauli equation (1) for a particle interacting with a constant magnetic field. Without loss of generality we can always choose it as directed along axes OZ: $e\vec{H} = (0,0,c)^T$, where c is a nonzero real constant. The vector-potential of electro-magnetic field has the form

$$2e\vec{A} = \begin{pmatrix} 0 & -c & 0 \\ c & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \vec{x}, \quad eA_0 = \frac{q}{|\vec{x}|} - \frac{c^2}{12}(x_1^2 + x_2^2 - 2x_3^2), \tag{56}$$

where q is a nonzero real constant and $|\vec{x}| = \sqrt{x_1^2 + x_2^2 + x_3^2}$.

A direct check shows this vector-potential satisfies the vacuum Maxwell equations without currents,

$$\begin{aligned} \Box A_0 - \frac{\partial}{\partial t}\left(\frac{\partial A_0}{\partial t} + \operatorname{div}\vec{A}\right) &= 0, \\ \Box \vec{A} + \overrightarrow{\operatorname{grad}}\left(\frac{\partial A_0}{\partial t} + \operatorname{div}\vec{A}\right) &= \vec{0}, \end{aligned} \tag{57}$$

where $\Box = \partial^2/\partial t^2 - \Delta$ is d'Alembert operator. Therefore, it is a natural generalization of the standard Coulomb potential, which is obtained from (56) under $c \to 0$.

Proposition 1: The set of inequivalent coordinate systems providing separability of the Pauli equation (1) with vector potential of electromagnetic field (56) is exhausted by the following ones:

$$\vec{x} = \mathcal{O}(t)\vec{z}, \tag{58}$$

where $\mathcal{O}$ is a time-dependent 3×3 orthogonal matrix (20), *with Euler angles*

$$\alpha(t)=-ct, \quad \beta=\text{const}, \quad \gamma=\text{const}, \tag{59}$$

and $\vec{z}$ is one of the following coordinate systems:

(*1*) *spherical [formula 5 from list (21)]*,
(*2*) *prolate spheroidal II [formula 6 from (21), where one should replace z_3 with $z_3=a(\coth\omega_1\tanh\omega_2\pm 1)$]*,
(*3*) *conical [formula 11 from (21)]*.

Proof: The spacelike component $\vec{A}(t,\vec{x})$ of the given vector-potential (56) is already reduced to form (39).

The system of ODE (38) for given magnetic field takes the form

$$\dot\gamma\ \cos\alpha+\dot\beta\ \sin\alpha\sin\gamma=0, \quad \dot\gamma\ \sin\alpha-\dot\beta\ \cos\alpha\sin\gamma=0, \quad \dot\alpha+\dot\beta\ \cos\gamma=-c.$$

This implies the equivalent system

$$\dot\gamma=0, \quad \dot\beta\ \sin\gamma=0, \quad \dot\alpha+\dot\beta\ \cos\gamma=-c.$$

Its general solution up to translation by t is given by formulas (59) [solution $\alpha\pm\beta=-ct$ for case $\sin\gamma=0$ is included into (59) as a particular case after denoting $\alpha\pm\beta\to\alpha$].

The steps 3 and 4 of the above algorithm will be illustrated by the case of spherical coordinate system 5 from (21) (for other coordinate systems this procedure is an analogous one). For this case the equality (44) in terms ω_1, ω_2, ω_3 takes the form

$$\begin{aligned} &l^{-2}(F_{10}(\omega_1)\omega_1^4+(F_{20}(\omega_2)+F_{30}(\omega_3))\omega_1^2\cosh^2\omega_2)-F_{00}(t)\\ &\quad=\frac{q}{|\vec{x}'|}+\left(\frac{c^2}{6}+\frac{1}{4}\frac{\ddot l}{l}\right)|\vec{x}'|^2+\sum_{a=1}^{3}(2(l\ddot v_a+2\dot l\dot v_a)x_a'+l^2\dot v_a^2), \end{aligned} \tag{60}$$

where $l=l_1=l_2=l_3$, $l\neq 0$ (because of the spherical coordinate system is a nonsplit one), and

$$x_1'=l(\omega_1^{-1}\,\mathrm{sech}\,\omega_2\cos\omega_3+v_1(t)),$$

$$x_2'=l(\omega_1^{-1}\,\mathrm{sech}\,\omega_2\sin\omega_3+v_2(t)),$$

$$x_3'=l(\omega_1^{-1}\tanh\omega_2+v_3(t)).$$

Next we perform on both parts of equality (60) the following step by step operations:

(1) multiplying by ω_1,
(2) differentiation with respect to ω_1,
(3) division by ω_1^2,
(4) differentiation with respect to ω_1,
(5) differentiation with respect to ω_2,
(6) multiplying by $l\omega_1^7|\vec{x}'|^7$,
(7) twice multiplying by ω_1.

As result we get

$$\begin{aligned} &-24q\,\mathrm{sech}^3\omega_2(v_1^2+v_2^2+v_3^2)(v_1\cos\omega_3+v_2\sin\omega_3+v_3\sinh\omega_2)\\ &\quad\times(-v_3+(v_1\cos\omega_3+v_2\sin\omega_3)\sinh\omega_2)=0. \end{aligned}$$

The equality obtained is transformed into an identity with respect to independent variables ω_1, ω_2, ω_3 if and only if the condition $v_1=v_2=v_3=0$ holds. Now the equality (60) takes the form

$$l^{-2}(F_{10}(\omega_1)\omega_1^4+(F_{20}(\omega_2)+F_{30}(\omega_3))\omega_1^2\cosh^2\omega_2)-F_{00}(t)=\frac{q}{l}\omega_1+\left(\frac{c^2}{6}+\frac{1}{4}\frac{\ddot{l}}{l}\right)\frac{l^2}{\omega_1^2}. \quad (61)$$

Performing on both parts of equality (61) the following step by step operations,

(1) differentiation with respect to ω_1,
(2) multiplying by l^2,
(3) differentiation with respect to t,
(4) multiplying by ω_1^3,
(5) differentiation with respect to ω_1,

we get the equality $3q\dot{l}\omega_1^2=0$. This implies $l=\text{const}$ and with the help of dilatations we can put without loss of generality $l=1$. Thus the coordinate system takes the form (58).

The equation (61) yields

$$F_{10}(\omega_1)\omega_1^4+(F_{20}(\omega_2)+F_{30}(\omega_3))\omega_1^2\cosh^2\omega_2-F_{00}(t)=q\omega_1+\frac{c^2}{6}\omega_1^{-2}.$$

We can split the equation obtained by the independent variables ω_1, ω_2, ω_3. As a result we get

$$F_{10}=q\omega_1^{-3}+\frac{c^2}{6}\omega_1^{-6}+k_1\omega_1^{-4}-k_2\omega_1^{-2},$$

$$F_{20}=k_2\,\mathrm{sech}^2\omega_2-k_3, \quad F_{30}=k_3, \quad F_{00}=k_1.$$

The theorem is proved. □

IV. SEPARATION OF VARIABLES IN THE PAULI–MAXWELL SYSTEM

The expressions (39) and (44)–(47) give the most general form of the vector-potential of the electromagnetic field, providing separability of the corresponding Pauli equations. But, because of generality of the results, these expressions are too cumbersome, and their physical interpretation is somewhat difficult. Therefore it would be interesting to know the form of these potentials under certain physical restrictions. The most natural restriction is that the vector-potential satisfies the vacuum Maxwell equations without currents (57).

In this section we describe all explicit forms of the vector-potentials $A(t,\vec{x})$ that

(a) provide separability of Pauli equation,
(b) satisfy vacuum Maxwell equations without currents (57), and
(c) describe the nonzero magnetic field.

Furthermore, we construct inequivalent coordinate systems enabling us to separate variables in the corresponding Pauli equation.

The similar problem with more strong restrictions was analyzed in Ref. 20 for a two-dimensional Schrödinger equation with vector-potential. Note that an analogous problem for the Dirac equation for an electron was analyzed in Ref. 21.

Taking into account the form of $\vec{A}$ (39), the Maxwell equations (57) take the form

$$\Delta A_0=0, \quad (62)$$

and

$$\frac{\partial^2 A_0}{\partial t\partial x_1}=-\ddot{l}_3x_2+\ddot{l}_2x_3,\quad \frac{\partial^2 A_0}{\partial t\partial x_2}=\ddot{l}_3x_1-\ddot{l}_1x_1,\quad \frac{\partial^2 A_0}{\partial t\partial x_3}=-\ddot{l}_2x_1+\ddot{l}_1x_2.$$

From the compatibility conditions of the above system of PDEs we get

$$\begin{gathered}\ddot{l}_1=\ddot{l}_2=\ddot{l}_2=0,\\ \frac{\partial^2 A_0}{\partial t\partial x_a}=0,\quad a=1,2,3.\end{gathered}\tag{63}$$

Inserting expression for potential $A_0(t,\vec{x})$ (44) into (62) with subsequent change of independent variables (19) yields (we use the relations $\Delta\omega_i=0$, $\omega_{ix_a}\omega_{jx_a}=0$, $i\neq j$, $i,j=1,2,3$)

$$\sum_{j=1}^{3}\frac{\partial^2}{\partial\omega_j^2}\left(\sum_{i=1}^{3}F_{i0}(\omega_i)R_i^{-2}\right)R_j^{-2}=\frac{1}{2}\sum_{i=1}^{3}\frac{\ddot{l}_i}{l_i}+e^2(H_1^2+H_2^2+H_3^2),\tag{64}$$

where the eikonals

$$R_i^{-2}=\frac{\partial\omega_i}{\partial x_a}\frac{\partial\omega_i}{\partial x_a},\quad i=1,2,3,\tag{65}$$

are given in the list (47).

Thus we get 11 functional relations $\mathcal{P}_1,\ldots,\mathcal{P}_{11}$ for each class of coordinate system (19), whose form is determined by the form of 1 of the 11 expressions $z_1(\omega_1,\omega_2,\omega_3)$, $z_2(\omega_1,\omega_2,\omega_3)$, $z_3(\omega_1,\omega_2,\omega_3)$ from the list (21). As t, ω_1, ω_2, ω_3 are functionally independent, we can split the above relations with respect to the variables t, ω_1, ω_2, ω_3, thus getting ordinary differential equations for the functions $F_{i0}(\omega_i),l_i(t)$, $i=1,2,3$. After solving them the formula (44) yields the expressions for A_0 in terms of variables t, ω_1, ω_2, ω_3. Returning to variables t, x_1, x_2, x_3 [with the aid of (19)], we should split the expression obtained for $A_0(t,\vec{x})$ with respect to t. Indeed, the general solution of the second equation from the system (63) is

$$A_0(t,\vec{x})=f_1(\vec{x})+f_2(t).$$

At the expense of the gauge invariance of the Pauli equation we may choose $f_2(t)=0$. Thus the potential A_0 should be a function of $\vec{x}$ only. This condition restricts the choice of A_0, thus giving ordinary differential equations for the functions $l_i(t)$, $v_i(t)$, $i=1,2,3$. Solving them we obtain the explicit forms of the function $F_{00}(t)$ and coordinate systems (19). After simplifying these coordinate systems with the aid of equivalence transformations we get a full description of the vector-potentials $A(t,\vec{x})$ and coordinate systems, giving the solution of the problem under study.

Omitting the details of the calculations (they are very cumbersome) we present below the results. Note, when presenting lists of the vector-potentials $A(t,\vec{x})$ and coordinate systems we use invariance of the system of the Pauli and Maxwell equations with respect to the groups of rotations by spatial variables x_1, x_2, x_3 and translations by all variables t, x_1, x_2, x_3 (see, e.g., Ref. 22).

A. Case of nonstationary magnetic field

$$e\vec{H}=(0,0,At+B),$$

$$eA_0=-\frac{k}{2}(x_1^2+x_2^2-2x_3^2)+a_1x_1+a_2x_2+a_3x_3,$$

where A, B, k, a_1, a_2, a_3 are arbitrary real constants.

The coordinate system is

$$\vec{x}=\mathcal{L}\mathcal{O}(\vec{z}+\vec{v}).$$

Here $\mathcal{O}$ is a time-dependent 3×3 orthogonal matrix $\mathcal{O}(\alpha,\beta,\gamma)$, where

$$\alpha=-\tfrac{1}{2}At^2-Bt,\quad \beta=0,\quad \gamma=0;$$

$\vec{z}$ is a cartesian, cylindrical or elliptic cylindrical coordinate system [formulas 1, 2, and 4 from (21)]; $\mathcal{L}$ is the 3×3 diagonal matrix

$$\mathcal{L}=\begin{pmatrix} l(t) & 0 & 0\\ 0 & l(t) & 0\\ 0 & 0 & l_3(t)\end{pmatrix},$$

and $\vec{v}(t)$ is vector-column $\vec{v}(t)=(v_1,v_2,v_3)^T$ where functions $l(t)$, $l_3(t)$, $v_1(t)$, $v_2(t)$, $v_3(t)$ are solutions of the following system of ordinary differential equations:

$$2\frac{c}{l^4}-\frac{1}{2}\frac{\ddot{l}}{l}+k=\frac{1}{2}(At+B)^2,\quad \frac{c_3}{l_3^4}-\frac{1}{4}\frac{\ddot{l}_3}{l_3}=k,$$

$$l\ddot{v}_1+2\dot{l}\dot{v}_1+4c\frac{v_1}{l^3}-2c_{11}\frac{1}{l}=-2(a_1\cos\alpha+a_2\sin\alpha),$$

$$l\ddot{v}_2+2\dot{l}\dot{v}_2+4c\frac{v_2}{l^3}-2c_{12}\frac{1}{l}=-2(-a_1\sin\alpha+a_2\cos\alpha),$$

$$l_3\ddot{v}_3+2\dot{l}_3\dot{v}_3+4c_3\frac{v_3}{l_3^3}-2c_{13}\frac{1}{l_3}=-2a_3.$$

Here c, c_3, c_{11}, c_{12}, c_{13} are arbitrary real constants.

B. Cases of stationary magnetic field

1. Case 1

Here

$$e\vec{H}=(0,0,k),\quad k=\text{const}\neq0;$$

$$eA_0=-\frac{k^2}{12}(x_1^2+x_2^2-2x_3^2)+a_1x_1+a_2x_2+a_3x_3,$$

where $\vec{a}=(a_1,a_2,a_3)$ is constant vector.

The coordinate system is

$$\vec{x}=l\mathcal{O}(\vec{z}+\vec{v}).$$

Here $\mathcal{O}$ is a time-dependent 3×3 orthogonal matrix $\mathcal{O}(\alpha,\beta,\gamma)$, where $\alpha=-kt$, $\beta=\text{const}$, $\gamma=\text{const}$; $\vec{z}$ is one of coordinate system, given by formulas 1–11 from (21); function $l(t)$ is solution of the equation

$$k^2+\frac{3}{2}\frac{\ddot{l}}{l}=\frac{c}{l^4}$$

given by one of the formulas

$$c=\mp 1, \quad l^2=\sqrt{C_1^2\pm\frac{1}{k^2}}\sin\left(2\sqrt{\frac{2}{3}}kt\right)+C_1,$$

for coordinate system $\vec{z}$ given by the formulas 1, 2, 4, 5, 6, 7, 10, and 11 from the list (21) and

$$c=0, \quad l=C_1\sin\left(\sqrt{\frac{2}{3}}kt\right)$$

for coordinate system $\vec{z}$ given by the formulas 1–11 from the list (21). Here C_1 is an arbitrary real constant. Vector $\vec{v}$ is a solution of the following system of ordinary differential equations:

$$3l\ddot{\vec{v}}+6\dot{l}\dot{\vec{v}}+\frac{2c}{l^3}\vec{v}=-6\mathcal{O}^{-1}\vec{a}.$$

2. Case 2

Here

$$e\vec{H}=(0,0,k), \quad k=\text{const}\neq 0;$$

$$eA_0=\frac{a}{\sqrt{x_1^2+x_2^2+x_3^2}}-\frac{k^2}{12}(x_1^2+x_2^2-2x_3^2), \quad a=\text{const}\neq 0.$$

The coordinate system is

$$\vec{x}=\mathcal{O}\vec{z}.$$

Here $\mathcal{O}$ is a time-dependent 3×3 orthogonal matrix $\mathcal{O}(\alpha,\beta,\gamma)$, where $\alpha=-kt$, $\beta=\text{const}$, $\gamma=\text{const}$; and $\vec{z}$ is one of the following coordinate systems:

(1) spherical [formula 5 from (21)],
(2) prolate spheroidal II [formula 6 from (21), where one should replace z_3 with $z_3=a(\coth\omega_1\tanh\omega_2\pm 1)$], and
(3) conical [formula 11 from (21)].

3. Case 3

Here

$$e\vec{H}=(0,0,k), \quad k=\text{const}\neq 0;$$

$$eA_0=-\frac{k^2}{12}(x_1^2+x_2^2-2x_3^2)+\frac{a_1}{r}+a_2\frac{x_3}{r^3}+\frac{a_3}{r^2}\left(\frac{x_3}{2r}\ln\frac{r+x_3}{r-x_3}-1\right),$$

where $r=\sqrt{x_1^2+x_2^2+x_3^2}$ and a_1, a_2, a_3 are real constant numbers.

The coordinate system is

$$\vec{x}=l\mathcal{O}\vec{z}.$$

Here $\mathcal{O}$ is a time-dependent 3×3 orthogonal matrix $\mathcal{O}(\alpha,\beta,\gamma)$, where $\alpha=-kt$, $\beta=\gamma=0$; $\vec{z}$ is the spherical coordinate system, given by formula 5 from (21); and function $l(t)$ is given by

$$l^2=\sqrt{C_1^2\pm\frac{1}{k^2}}\sin\left(2\sqrt{\frac{2}{3}}kt\right)+C_1, \quad \text{or} \quad l=C_1\sin\left(\sqrt{\frac{2}{3}}kt\right)$$

under condition $a_1=0$ and $l=1$ under condition $a_1\neq 0$. Here C_1 is an arbitrary real constant.

4. Case 4

Here

$$e\vec{H}=(0,0,k),\quad k=\text{const}\neq 0;$$

$$eA_0=-\frac{k^2}{12}(x_1^2+x_2^2-2x_3^2)+\frac{a_1}{r^+}+\frac{a_2}{r^-}+a_3\left(\frac{1}{r^+}\operatorname{arctanh}\frac{x_3^+}{r^+}-\frac{1}{r^-}\operatorname{arctanh}\frac{x_3^-}{r^-}\right),$$

where $x_3^{\pm}=x_3\pm a$ and $r^{\pm}=\sqrt{x_1^2+x_2^2+(x_3\pm a)^2}$, and a, a_1, a_2, a_3 are arbitrary real constants. The coordinate system is

$$\vec{x}=\mathcal{O}\vec{z}.$$

Here $\mathcal{O}$ is a time-dependent 3×3 orthogonal matrix $\mathcal{O}(\alpha,\beta,\gamma)$, where $\alpha=-kt$, $\beta=\gamma=0$, and $\vec{z}$ is a prolate spheroidal coordinate system, given by formula 6 from (21).

5. Case 5

Here

$$e\vec{H}=(0,0,k),\quad k=\text{const}\neq 0;$$

$$eA_0=-\frac{k^2}{12}(x_1^2+x_2^2-2x_3^2)+2a_1a\frac{f_1}{f}+2a_2\frac{x_3}{ff_1}-2a_3\left(a\frac{f_1}{f}\operatorname{arccot}f_1-\frac{x_3}{ff_1}\operatorname{arctanh}\frac{x_3}{af_1}\right),$$

where

$$f=\sqrt{(a^2-r^2)^2+4a^2x_3^2},\quad f_1=\sqrt{\frac{-a^2+r^2+f}{2a^2}},\quad r=\sqrt{x_1^2+x_2^2+x_3^2},$$

and a, a_1, a_2, a_3 are arbitrary real constants. The coordinate system is

$$\vec{x}=\mathcal{O}\vec{z}.$$

Here $\mathcal{O}$ is a time-dependent 3×3 orthogonal matrix $\mathcal{O}(\alpha,\beta,\gamma)$, where $\alpha=-kt$, $\beta=\gamma=0$, and $\vec{z}$ is an oblate spheroidal coordinate system, given by formula 7 from (21).

Note that expression for A_0 can be rewritten in the form

$$eA_0=-\frac{k^2}{12}(x_1^2+x_2^2-2x_3^2)+\frac{a_1+ia_2}{\tilde{r}^+}+\frac{a_1-ia_2}{\tilde{r}^-}+ia_3\left(\frac{1}{\tilde{r}^+}\operatorname{arctanh}\frac{\tilde{x}_3^+}{\tilde{r}^+}-\frac{1}{\tilde{r}^-}\operatorname{arctanch}\frac{\tilde{x}_3^-}{\tilde{r}^-}\right),$$

where $\tilde{x}_3^{\pm}=x_3\pm ia$ and $\tilde{r}^{\pm}=\sqrt{x_1^2+x_2^2+(x_3\pm ia)^2}$.

6. Case 6

Here

$$e\vec{H}=(0,0,k),\quad k=\text{const}\neq 0;$$

$$eA_0=-\frac{k^2}{6}(x_1^2+x_2^2-2x_3^2)+\frac{a_1}{r}+a_2x_3+\frac{a_3}{r}\ln\frac{r+x_3}{r-x_3},$$

where $r=\sqrt{x_1^2+x_2^2+x_3^2}$ and a_1, a_2, a_3 are arbitrary real constants.

The coordinate system is

$$\vec{x}=\mathcal{O}\vec{z}.$$

Here $\mathcal{O}$ is a time-dependent 3×3 orthogonal matrix $\mathcal{O}(\alpha,\beta,\gamma)$, where $\alpha=-kt$ and $\beta=\gamma=0$, and $\vec{z}$ is a parabolic coordinate system, given by formula 8 from (21).

7. Case 7

Here

$$e\vec{H}=(0,0,k),\quad k=\text{const}\neq 0;$$

$$eA_0=-\frac{q}{2}(x_1^2+x_2^2-2x_3^2)+a\ln(x_1+x_2)+a_3x_3,$$

where k, a, a_3 are arbitrary real constants.

The coordinate system is

$$x_1=e^{\omega_1}\cos(\omega_1-kt),\quad x_2=e^{\omega_1}\sin(\omega_1-kt),\quad x_3=l_3\omega_3+v_3,$$

where l_3, v_3 are solutions of the system of ordinary differential equations

$$\frac{c_3}{l_3^4}-\frac{1}{4}\frac{\ddot{l}_3}{l_3}=q,\quad l_3\ddot{v}_3+2\dot{l}_3\dot{v}_3+4c_3\frac{v_3}{l_3^3}-2c_{13}\frac{1}{l_3}=-2a_3.$$

Note that some of the potentials obtained have the clear physical meaning. For instance, cases 2 and 3 under condition $k=a_2=a_3=0$ give the standard Coulomb potential. Case 4 under condition $k=a_3=0$ gives the potential for a well-known two-center Kepler problem, i.e., the problem of finding wave functions of electrons moving in the field of two fixed Coulomb centers with charges a_1, a_2 and intercenter distance $2a$ (the model of ionized hydrogen molecule). Coulson and Joseph[23] showed that the corresponding Schrödinger equation admits separation of variables in the prolate coordinate system only. We obtained this potential as a particular case of the more general potential.

V. CONCLUDING REMARKS

Theorem 1 provides the complete solution of the problem of classification of the Pauli equations (1), which are solvable within the framework of the method of separation of variables in the sense of our Definition 1. According to these theorems the coordinate systems and the vector-potentials of the electromagnetic field $A(t,\vec{x})=(A_0(t,\vec{x}),\vec{A}(t,\vec{x}))$ providing separability of the corresponding Pauli equations coincide with those for the Schrödinger equations with vector-potential. So the results obtained in the article are valid for the Schrödinger equation as well.

It is well known that the possibility of variable separation in a system of PDEs is closely connected to its symmetry properties.[9,10] Namely, solutions with separated variables are common eigenfunctions of three matrix mutually commuting symmetry operators of the equation under study. For all the cases of variable separation in Pauli equation (1) such matrix second-order operators can be constructed in the explicit form, by analogy to what has been done in Ref. 24 for the $(1+2)$-dimensional Schrödinger equation. They are expressed in terms of the matrix coefficients of the separation equations (17) and (18).

A promising development of the research is classification and study of superintegrable (admitting sufficiently many higher symmetries) cases of Pauli equation. Notice that the notions of separability and superintegrability are closely related. By now, superintegrable physical systems can be regarded as one of the most intensively developed and significant fields of mathematical physics. The problem of classifying superintegrable stationary Schrödinger equations with scalar

potential has been solved by Winternitz with co-workers[25] and Evans[26] for space dimensions $n=2$ and $n=3$ (see also Ref. 4). They have found all potentials that allow for separability of the corresponding Schrödinger equation in more than one coordinate system. We intend to modify and generalize this approach to $(1+3)$-dimensional Pauli equation (1). A study of the problem is in progress now and will be reported in our future publications.

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High temperature expansion for a chain model

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We consider an arbitrary translationally invariant chain model with nearest neighbors interaction and satisfying periodic boundary condition. The approach developed here allows a thermodynamic description of the chain model directly in terms of grand potential per site. This thermodynamic function is derived from an auxiliary function constructed only from open connected subchains. In order to exemplify its application and how this approach works we consider the Heisenberg XXZ model. We obtain the coefficients of the high temperature expansion of the free energy per site of the model up to third order. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1432484]

I. INTRODUCTION

Chain models, such as the spin-$\frac{1}{2}$ Heisenberg models XYZ and XXZ[1,2] and their extensions,[3,4] the one-dimensional Hubbard model,[5] etc., have attracted intense interest due to their property of integrability. We also have other models like the one-dimensional d-p model[6] and its generalizations,[7,8] employed to simulate a Cu–O linear chain with strong Coulomb repulsion. These models are also relevant because they may explain high temperature superconductivity.

The solution of the XXZ model[9] and the one-dimensional Hubbard model[5] at $T=0$ are examples of the success of the Bethe ansatz. In 1972 Takahashi and Suzuki[10] obtained the exact thermodynamics of the XXZ model. More recently the same results were reobtained by Kuniba *et al.*[11] using the quantum transfer matrix approach. The exact thermodynamics of the one-dimensional Hubbard model was also derived by this same method.[12–14] In all those models the thermodynamic functions are solutions of integral coupled equations, and it is possible to obtain their behavior in the very high temperature limit. However, it is not an easy task to derive a systematic temperature expansion for the thermodynamic functions in such temperature range.

The high temperature limit of any model can be obtained by a standard expansion in terms of the inverse of temperature β,[15] $\beta=1/kT$, where k is the Boltzmann constant and T is the absolute temperature. Sometimes, perturbation theory can be applied to obtain the coefficients of the β-expansion method; this approach is also called the high temperature expansion and it has been applied to the t-J model[16] and to the Hubbard model.[17–19] In all standard high temperature expansions we always need to calculate the weight of each graph in the grand canonical partition function as well as to determine all graphs that contribute at a given β-order term.

Recently, we applied the basic properties of the Grassmann generators to calculate analytically the coefficients of the β-expansion of the grand canonical partition function $\mathcal{Z}(\beta,\mu)$ of self-interacting fermionic fields in any dimension.[20] We applied it to the one-dimensional Hubbard model.[21,22] We have two drawbacks in our method: a large number of graphs must be calculated, as well as counting the number of times each graph contributes to each β-term in the expansion of $\mathcal{Z}(\beta,\mu)$.

In this article restrict ourselves to the study of translationally invariant chain models with first neighbor interactions and subject to periodic boundary condition. Instead of calculating the grand canonical partition function, we derive a β-expansion for the grand potential per site, that is, an intensive quantity. The coefficient of order β^n is exactly obtained for arbitrary values of n. The proposed approach is not restricted to self-interacting fermionic models.

In Sec. II, we expand the grand canonical partition function as a Taylor series around $\beta=0$. In fact, the idea behind this method was previously developed, up to order β^5, in Ref. 20 for fermions only. Here we generalize the expansion for fermionic and bosonic fields to arbitrary orders of β^n. In performing this expansion we write $\mathcal{Z}(\beta,\mu)$ as a sum of traces whose coefficients are known. We obtain the expansion of the grand potential per site, and verify that it is an intensive quantity. In this calculation we do not use the traditional method of quantum transfer matrix. As an illustrative example of the method developed here, in Sec. III we apply it to spin-$\frac{1}{2}$ Heisenberg XXZ model. We calculate the β-expansion of the Helmholtz free energy of the model up to order β^3. Taking $\Delta=h=0$ we recover the β-expansion of this thermodynamic function of the free fermion model[23] whereas when $t=0$ we recover the limiting Ising model.[24] In Sec. IV we draw our main conclusions. In Appendix A we explain our graphic representation of the normalized traces; in Appendix B we extend our results for $\langle \mathbb{K}^n \rangle$ with arbitrary n; in Appendix C we write the grand potential per site in terms of an auxiliary function $\varphi(\lambda)$ that is constructed only from open connected subchains; and finally in Appendix D we write the function $K_{1,m}^{(n)}$ as sums of normalized traces for n up to 4.

II. GRAND CANONICAL PARTITION FUNCTION FOR A CHAIN MODEL

Let us consider a one-dimensional regular lattice (a periodic chain) with N sites, so that the Hilbert space of the chain model is simply $\mathcal{H}^{(N)}=\otimes^N\mathcal{H}$, $\mathcal{H}$ being the irreducible representation at one site, including all its degrees to freedom. The dimension of this Hilbert space is $\dim\mathcal{H}^{(N)}=\mathrm{tr}_N(\mathbb{1})$. The notation tr_N means the trace over all N sites and their internal degrees of freedom, such as spin.

The grand canonical partition function of a quantum system in the chain with N sites is given by

$$\mathcal{Z}_N(\beta,\mu)=\mathrm{tr}_N(\mathrm{e}^{-\beta\mathbb{K}}), \tag{1}$$

where $\mathbb{K}=\mathbb{H}-\mu\mathbb{N}$, with μ being the chemical potential and $\mathbb{N}$ being an operator that acts on $\mathcal{H}^{(N)}$ and that commutes with the Hamiltonian of the system. The expansion of $\mathcal{Z}_N(\beta,\mu)$ around $\beta=0$ is

$$\mathcal{Z}_N(\beta,\mu)=\mathrm{tr}_N(\mathbb{1})+\sum_{n=1}^{\infty}(-\beta)^n\frac{\mathrm{tr}_N(\mathbb{K}^n)}{n!}. \tag{2}$$

Let $\mathbf{A}$ be any operator that acts on $\mathcal{H}^{(M)}$ where $M\leqslant N$. We define $\langle\mathbf{A}\rangle\equiv\mathrm{tr}_M(\mathbf{A})/\mathrm{tr}_M(\mathbf{1})$, for any dimension of $\mathcal{H}^{(M)}$. From now on, we call $\langle\mathbf{A}\rangle$ the *normalized trace* of operator $\mathbf{A}$. The dimension of the subspace $\mathcal{H}^{(M)}$ is determined by the operator $\mathbf{A}$.

Using the definition of normalized trace, Eq. (2) becomes

$$\mathcal{Z}_N(\beta,\mu)=\mathrm{tr}_N(\mathbb{1})\left\{1+\sum_{n=1}^{\infty}(-\beta)^n\frac{\langle\mathbb{K}^n\rangle}{n!}\right\}. \tag{3}$$

Along this section we consider a general Hamiltonian $\mathbb{H}$ subject to two constraints: the interaction is only between first neighbors and the Hamiltonian $\mathbb{H}$ is invariant under translation along the chain. The most general operator $\mathbb{K}$ satisfying both conditions is

$$\mathbb{K}=\sum_{i=1}^{N}\tilde{\mathbf{K}}_{i,i+1}, \tag{4}$$

where $\tilde{\mathbf{K}}_{i,i+1}\in\mathcal{H}^{(N)}$. Each operator $\tilde{\mathbf{K}}_{i,i+1}$ is defined as

$$\tilde{\mathbf{K}}_{1,2}=\mathbf{K}_{1,2}\otimes\mathbf{1}_3\otimes\cdots\otimes\mathbf{1}_N$$

$$\tilde{\mathbf{K}}_{2,3}=\mathbf{1}_1\otimes\mathbf{K}_{2,3}\otimes\mathbf{1}_4\otimes\cdots\otimes\mathbf{1}_N$$

$$\vdots$$

$$\tilde{\mathbf{K}}_{i,i+1}=\mathbf{1}_1\otimes\cdots\otimes\mathbf{1}_{i-1}\otimes\mathbf{K}_{i,i+1}\otimes\mathbf{1}_{i+2}\otimes\cdots\otimes\mathbf{1}_N \tag{5}$$

and $\mathbf{K}_{i,i+1}\in\mathcal{H}_i\otimes\mathcal{H}_{i+1}$. We use the notation $\mathbf{1}_i\in\mathcal{H}_i$ for the identity matrix on the irreducible subspace of the ith particle.

Our aim is to get the coefficients $\langle\mathbb{K}^n\rangle$, on the rhs of Eq. (3), in terms of the normalized traces of products of operators $\mathbf{K}_{i,i+1}$. Let us calculate explicitly the first three coefficients ($n=1$, $n=2$, and $n=3$) of the expansion (3). They will help us to construct the coefficient $\langle\mathbb{K}^n\rangle$ for arbitrary n. We begin with $n=1$.

Since the operator $\mathbf{K}_{i,i+1}$ acts only on the sites i and $i+1$, we have

$$\mathrm{tr}_N(\tilde{\mathbf{K}}_{i,i+1})=\mathrm{tr}_2(\mathbf{K}_{i,i+1})(\mathrm{tr}_1(\mathbf{1}))^{N-2}. \tag{6}$$

We stress out that the traces of the rhs of Eq. (6) are calculated on the subspace $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$ whereas the trace on the lhs is calculated on the complete space $\mathcal{H}^{(N)}$. Dividing both sides of Eq. (6) by $\mathrm{tr}_N(\mathbb{1})$,

$$\frac{\mathrm{tr}_N(\tilde{\mathbf{K}}_{i,i+1})}{\mathrm{tr}_N(\mathbb{1})}=\frac{\mathrm{tr}_2(\mathbf{K}_{i,i+1})}{\mathrm{tr}_2(\mathbf{1}\otimes\mathbf{1})}=\langle\mathbf{K}_{i,i+1}\rangle. \tag{7}$$

Due to the property of the Hamiltonian being translationally invariant we have $\langle\tilde{\mathbf{K}}_{i,i+1}\rangle=\langle\mathbf{K}_{i,i+1}\rangle=\langle\mathbf{K}_{1,2}\rangle$. Taking into account the periodic boundary condition ($\mathbf{K}_{N,N+1}=\mathbf{K}_{N,1}$), we have that $\langle\mathbb{K}\rangle$ is equal to

$$\langle\mathbb{K}\rangle=\sum_{i=1}^{N}\langle\mathbf{K}_{i,i+1}\rangle=N\langle\mathbf{K}_{1,2}\rangle. \tag{8}$$

For $n=2$ on the rhs of expansion (3) we have to calculate the normalized traces of $\langle\mathbb{K}^2\rangle$. From the definition of operator $\mathbb{K}$ [see Eq. (4)], we have

$$\langle\mathbb{K}^2\rangle=\sum_{i,j=1}^{N}\langle\mathbf{K}_{i,i+1}\mathbf{K}_{j,j+1}\rangle. \tag{9}$$

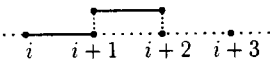
In the normalized trace $\langle\mathbf{K}_{i,i+1}\mathbf{K}_{j,j+1}\rangle$ we have three different cases (in Appendix A we explain our graphic representation):

(i) $i=j$:

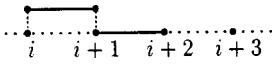
$$\langle\mathbf{K}^2_{i,i+1}\rangle=\langle\mathbf{K}^2_{1,2}\rangle \quad\longrightarrow\quad \cdots\bullet\cdots\bullet\!\!=\!\!\bullet\cdots\bullet\cdots \qquad i-1 \quad i \quad i+1 \quad i+2 \tag{10a}$$

This equality comes from the invariance under translation and the periodic boundary condition satisfied by the model. In the double sum (9) we have N terms of this type.

(*ii*) $i = j \pm 1$:

- $i = j+1:\quad \langle \mathbf{K}_{i,i+1}\mathbf{K}_{i+1,i+2}\rangle \longrightarrow$ 

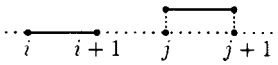
(10b)

- $i = j-1:\quad \langle \mathbf{K}_{i+1,i+2}\mathbf{K}_{i,i+1}\rangle \longrightarrow$ 

(10c)

In the double sum on the rhs of Eq. (9) we have N terms of the type of one of these two previous configurations. Using the cyclic property of traces and translation invariance, we get that the normalized traces (10b) and (10c) are equal. Therefore, we can write $\langle \mathbf{K}_{i,i+1}\mathbf{K}_{i-1,i}\rangle = \langle \mathbf{K}_{i,i+1}\mathbf{K}_{i+1,i+2}\rangle$.

(*iii*) $i \neq j$ and $i \neq j \pm 1$:

$\langle \mathbf{K}_{i,i+1}\mathbf{K}_{j,j+1}\rangle \longrightarrow$ 

(10d)

The normalized trace (10d) can be written as $\langle \mathbf{K}_{i,i+1}\rangle\langle \mathbf{K}_{j,j+1}\rangle = \langle \mathbf{K}_{1,2}\rangle^2$. The number of terms in the double sum in Eq. (9) that satisfies configuration (10d) is equal to $N(N-3)$.

The terms that contribute to $\langle \mathbb{K}^2\rangle$, with respective of number of configurations (weight) in the sum on the rhs of Eq. (9) are

$$\langle \mathbb{K}^2\rangle = N\langle \mathbf{K}_{1,2}^2\rangle + 2N\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\rangle + N(N-3)\langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\rangle. \tag{11}$$

The last term on the rhs of (11) can be written as a product of normalized traces with $n=1$.

The term $\langle \mathbb{K}^3\rangle$ has a richer structure of traces than the two previous ones. Its explicit study will help us to generalize the results for arbitrary n. The expansion of normalized traces in $\langle \mathbb{K}^3\rangle$ is

$$\langle \mathbb{K}^3\rangle = \sum_{i,j,k=1}^{N} \langle \mathbf{K}_{i,i+1}\mathbf{K}_{j,j+1}\mathbf{K}_{k,k+1}\rangle. \tag{12}$$

Similarly to $\langle \mathbb{K}\rangle$ and $\langle \mathbb{K}^2\rangle$, we determine the types of configurations we have in the sum on the rhs of Eq. (12) and their respective weights. For $\langle \mathbb{K}^3\rangle$ we have

$$\begin{aligned}\langle \mathbb{K}^3\rangle = {} & N\langle \mathbf{K}_{1,2}^3\rangle + 3N\left\{\frac{\langle \mathbf{K}_{1,2}^2\mathbf{K}_{2,3}\rangle}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}^2\rangle}{2!}\right\} + 3N\{\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{3,4}\rangle + \langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{2,3}\rangle\} \\ & + 3N(N-3)\left\{\frac{\langle \mathbf{K}_{1,2}^2\mathbf{K}_{3,4}\rangle}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}^2\rangle}{2!}\right\} + 3N(N-4)\{\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{4,5}\rangle + \langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{4,5}\rangle\} \\ & + N(N-4)(N-5)\langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{5,6}\rangle. \end{aligned} \tag{13}$$

From the expressions (8), (11) and (13) we have that each type of normalized trace (in the expression of $\langle \mathbb{K}^3\rangle$ we collect them inside of braces) corresponds to all normalized traces that we

can write for that set of operators. For example, the term: $3\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{3,4}\rangle + 3\langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{2,3}\rangle$ includes all normalized traces that we can write for the set of operators $\{\mathbf{K}_{1,2},\mathbf{K}_{2,3},\mathbf{K}_{3,4}\}$. The factors 3 come from the fact that some of them are equals by the cyclic property of the trace.

To make ours simpler and generalize our results for arbitrary n, we define the *g-trace*:

$$\langle \mathbf{K}^{n_1}_{i_1,i_1+1}\mathbf{K}^{n_2}_{i_2,i_2+1}\cdots\mathbf{K}^{n_m}_{i_m,i_m+1}\rangle_{\mathrm{g}} \equiv \frac{n_1!\cdots\ n_m!}{n!}\sum_{\mathcal{P}}\ \langle \mathcal{P}(\mathbf{K}^{n_1}_{i_1,i_1+1},\mathbf{K}^{n_2}_{i_2,i_2+1},\ldots,\mathbf{K}^{n_m}_{i_m,i_m+1})\rangle, \tag{14}$$

where $\Sigma_{i=1}^{m} n_i = n$ with $n_i \neq 0$ and the indices i_k, $k=1,...,m$ are distinct among themselves. By definition, $\langle \mathcal{P}(\mathbf{K}^{n_1}_{i_1,i_1+1},\mathbf{K}^{n_2}_{i_2,i_2+1},\ldots,\mathbf{K}^{n_m}_{i_m,i_m+1})\rangle$ represents all distinct permutations that we can write the n operators $\{\mathbf{K}_{i_1,i_1+1},\mathbf{K}_{i_2,i_2+1},\ldots,\mathbf{K}_{i_m,i_m+1}\}$. In the particular case when the operators $\{\mathbf{K}_{i_1,i_1+1},\mathbf{K}_{i_2,i_2+1},\ldots,\mathbf{K}_{i_m,i_m+1}\}$ commute among themselves, $\langle \mathbf{K}^{n_1}_{i_1,i_1+1}\mathbf{K}^{n_2}_{i_2,i_2+1}\cdots \mathbf{K}^{n_m}_{i_m,i_m+1}\rangle_g$ reduces to the normalized trace $\langle \mathbf{K}^{n_1}_{i_1,i_1+1}\mathbf{K}^{n_2}_{i_2,i_2+1}\cdots\ \mathbf{K}^{n_m}_{i_m,i_m+1}\rangle$.

The normalized traces $\langle \mathbb{K}\rangle$, $\langle \mathbb{K}^2\rangle$ and $\langle \mathbb{K}^3\rangle$ written in terms of the g-traces become

$$\langle \mathbb{K}\rangle = N\langle \mathbf{K}_{1,2}\rangle_{\mathrm{g}}, \tag{15a}$$

$$\frac{\langle \mathbb{K}^2\rangle}{2!} = N\frac{\langle \mathbf{K}^2_{1,2}\rangle_{\mathrm{g}}}{2!} + N\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\rangle_{\mathrm{g}} + \frac{N(N-3)}{2!}\langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\rangle_{\mathrm{g}}, \tag{15b}$$

and

$$\begin{aligned}\frac{\langle \mathbb{K}^3\rangle}{3!} = {} & N\frac{\langle \mathbf{K}^3_{1,2}\rangle_{\mathrm{g}}}{3!} + N\left\{\frac{\langle \mathbf{K}^2_{1,2}\mathbf{K}_{2,3}\rangle_{\mathrm{g}}}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}^2_{2,3}\rangle_{\mathrm{g}}}{2!}\right\} + N\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{3,4}\rangle_{\mathrm{g}} + \frac{N(N-3)}{2!}\left\{\frac{\langle \mathbf{K}^2_{1,2}\mathbf{K}_{3,4}\rangle_{\mathrm{g}}}{2!}\right. \\ & \left. + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}^2_{3,4}\rangle_{\mathrm{g}}}{2!}\right\} + \frac{N(N-4)}{2!}\{\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{4,5}\rangle_{\mathrm{g}} + \langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{4,5}\rangle_{\mathrm{g}}\} \\ & + \frac{N(N-4)(N-5)}{3!}\langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{5,6}\rangle_{\mathrm{g}}.\end{aligned} \tag{15c}$$

Some of the g-traces at order n can be written as the product of the normalized traces of lower order. The latter are already calculated, which means that we have a smaller number of new normalized traces to be calculated at order n. To distinguish the normalized traces that appear for the first time at order n from the others we use the notation $\mathrm{K}^{(n)}_{r,m}$, where n is the power ($\langle \mathbb{K}^n\rangle$) of the term in expansion (3) to which the g-traces contribute, r is the number of products of the traces that the original trace can be broken and m is the number of distinct $\mathbf{K}_{i,i+1}$ operators that appear in the g-trace. The terms $\mathrm{K}^{(n)}_{r,m}$ with $r=1$ are the g-traces that appear in the expansion for the first time at order β^n.

We begin by defining $\mathrm{K}^{(n)}_{1,m}$ as

$$\mathrm{K}^{(n)}_{1,1} = \frac{\langle \mathbf{K}^n_{1,2}\rangle_{\mathrm{g}}}{n!}, \tag{16a}$$

$$\mathrm{K}^{(n)}_{1,2} = \sum_{\{n_i\}}^{n}{}'' \ \frac{\langle \mathbf{K}^{n_1}_{1,2}\mathbf{K}^{n_2}_{2,3}\rangle_{\mathrm{g}}}{n_1!\quad n_2!}, \tag{16b}$$

$$\vdots$$

$$\mathrm{K}^{(n)}_{1,m} = \sum_{\{n_i\}}^{n}{}'' \ \frac{\langle \mathbf{K}^{n_1}_{1,2}\mathbf{K}^{n_2}_{2,3}\cdots\ \mathbf{K}^{n_m}_{m,m+1}\rangle_{\mathrm{g}}}{n_1!n_2!\cdots\ n_m!}. \tag{16c}$$

From now on we use the notation $\Sigma''_{\{n_i\}}$ to mean the restriction $\Sigma_{i=1}^{n} n_i = n$ and $n_i \neq 0$ for $i = 1,2,...,m$. The index m satisfies the condition: $1 \leqslant m \leqslant \min(n,N)$. In Eq. (16c) we are assuming $m \leqslant n$. However, if $m > n$, we define $\mathrm{K}_{1,m}^{(n)} = 0$.

Since in the definition of the g-traces are included all possible permutations of the n operators, we have

$$\mathrm{K}_{1,m}^{(n)} = \sum_{\{n_i\}}^{n}{}'' \left\langle \prod_{i=1}^{m} \frac{\mathbf{K}_{i,i+1}^{n_i}}{n_i!} \right\rangle_{\mathrm{g}} . \tag{17}$$

For $r = 2$, the natural definition is

$$\mathrm{K}_{2,2}^{(n)} = \sum_{\{n_i\}}^{n}{}'' \frac{\langle \mathbf{K}_{1,2}^{n_1} \mathbf{K}_{3,4}^{n_2} \rangle_{\mathrm{g}}}{n_1! \quad n_2!} = \sum_{\{n_i\}}^{n}{}'' \frac{\langle \mathbf{K}_{1,2}^{n_1} \rangle_{\mathrm{g}}}{n_1!} \frac{\langle \mathbf{K}_{3,4}^{n_2} \rangle_{\mathrm{g}}}{n_2!} = \sum_{\{n_i\}}^{n}{}'' \mathrm{K}_{1,1}^{(n_1)} \mathrm{K}_{1,1}^{(n_2)} , \tag{18a}$$

$$\mathrm{K}_{2,3}^{(n)} = \sum_{\{n_i\}}^{n}{}'' \left(\frac{\langle \mathbf{K}_{1,2}^{n_1} \mathbf{K}_{2,3}^{n_2} \mathbf{K}_{4,5}^{n_3} \rangle_{\mathrm{g}}}{n_1! n_2! n_3!} + \frac{\langle \mathbf{K}_{1,2}^{n_1} \mathbf{K}_{3,4}^{n_2} \mathbf{K}_{4,5}^{n_3} \rangle_{\mathrm{g}}}{n_1! n_2! n_3!} \right) = \sum_{\{n_i\}}^{n}{}'' (\mathrm{K}_{1,1}^{(n_1)} \mathrm{K}_{1,2}^{(n_2)} + \mathrm{K}_{1,2}^{(n_1)} \mathrm{K}_{1,1}^{(n_2)}), \tag{18b}$$

where we took into account the invariance of the model under translations and the fact that

$$[\mathbf{K}_{i,i+1}, \mathbf{K}_{j,j+1}] = \begin{cases} \mathbf{0}, & \text{when } i \neq j \pm 1, \\ \neq \mathbf{0}, & \text{when } i = j \pm 1. \end{cases} \tag{19}$$

To obtain the second equality on the rhs of Eq. (18b) we rearrange the indices in the double sum. We see that these g-traces can always be written as the product of g-traces of lower order which give us

$$\mathrm{K}_{2,m}^{(n)} = \sum_{\{n_i\}}^{n}{}'' \sum_{l=1}^{m-1} \mathrm{K}_{1,l}^{(n_1)} \mathrm{K}_{1,m-l}^{(n_2)} = \sum_{\{n_i\}}^{n}{}'' \sum_{\{m_j\}}^{m}{}'' \mathrm{K}_{1,m_1}^{(n_1)} \mathrm{K}_{1,m_2}^{(n_2)} . \tag{20}$$

The indices n_i satisfy the condition $n_1 + n_2 = n$ while $m_1 + m_2 = m$ and $2 \leqslant m \leqslant \min(n,N)$. We are assuming $m \leqslant n$, otherwise $\mathrm{K}_{2,m}^{(n)} = 0$. For $\mathrm{K}_{3,3}^{(n)}$ and $\mathrm{K}_{3,4}^{(n)}$ we have

$$\mathrm{K}_{3,3}^{(n)} = \sum_{\{n_i\}}^{n}{}'' \mathrm{K}_{1,1}^{(n_1)} \mathrm{K}_{1,1}^{(n_2)} \mathrm{K}_{1,1}^{(n_3)} , \tag{21a}$$

$$\mathrm{K}_{3,4}^{(n)} = \sum_{\{n_i\}}^{n}{}'' (\mathrm{K}_{1,1}^{(n_1)} \mathrm{K}_{1,1}^{(n_2)} \mathrm{K}_{1,2}^{(n_3)} + \mathrm{K}_{1,1}^{(n_1)} \mathrm{K}_{1,2}^{(n_2)} \mathrm{K}_{1,1}^{(n_3)} + \mathrm{K}_{1,2}^{(n_1)} \mathrm{K}_{1,1}^{(n_2)} \mathrm{K}_{1,1}^{(n_3)}). \tag{21b}$$

It follows for arbitrary m, where $3 \leqslant m \leqslant \min(n,N)$,

$$\mathrm{K}_{3,m}^{(n)} = \sum_{\{n_i\}}^{n}{}'' \sum_{\{m_i\}}^{m}{}'' \mathrm{K}_{1,m_1}^{(n_1)} \mathrm{K}_{1,m_2}^{(n_2)} \mathrm{K}_{1,m_3}^{(n_3)} , \tag{22}$$

and $\mathrm{K}_{3,m}^{(n)} = 0$ for $m > n$.

We generalize our definition of $\mathrm{K}_{r,m}^{(n)}$

$$\mathrm{K}_{r,m}^{(n)} \equiv \sum_{\{n_i\}}^{n}{}'' \sum_{\{m_i\}}^{m}{}'' \prod_{j=1}^{r} \mathrm{K}_{1,m_j}^{(n_j)} , \tag{23}$$

where $\{n_i\}\equiv\{n_1,n_2,\ldots,n_r\}$ and $\{m_i\}\equiv\{m_1,m_2,\ldots,m_r\}$. Equation (23) is valid for $r>1$ and it makes possible to write $\mathrm{K}_{r,m}^{(n)}$ as products of $\mathrm{K}_{1,m}^{(n)}$ [see Eq. (16c)]. The indices r and m satisfy the conditions $1\leqslant r\leqslant\min(n,N)$ and $r\leqslant m\leqslant\min(n,N)$. We are assuming $n\geqslant r$ and m, otherwise $\mathrm{K}_{r,m}^{(n)}=0$.

In terms of $\mathrm{K}_{r,m}^{(n)}$, the normalized traces $\langle\mathbb{K}\rangle$, $\langle\mathbb{K}^2\rangle$ and $\langle\mathbb{K}^3\rangle$ are simply

$$\langle\mathbb{K}\rangle=N\mathrm{K}_{1,1}^{(1)}, \tag{24a}$$

$$\frac{\langle\mathbb{K}^2\rangle}{2!}=N\mathrm{K}_{1,1}^{(2)}+N\mathrm{K}_{1,2}^{(2)}+\frac{N(N-3)}{2!}\mathrm{K}_{2,2}^{(2)}, \tag{24b}$$

$$\frac{\langle\mathbb{K}^3\rangle}{3!}=N\mathrm{K}_{1,1}^{(3)}+N\mathrm{K}_{1,2}^{(3)}+N\mathrm{K}_{1,3}^{(3)}+\frac{N(N-3)}{2!}\mathrm{K}_{2,2}^{(3)}+\frac{N(N-4)}{2!}\mathrm{K}_{2,3}^{(3)}+\frac{N(N-4)(N-5)}{3!}\mathrm{K}_{3,3}^{(3)}. \tag{24c}$$

In Appendix B we write $\langle\mathbb{K}^4\rangle$ in terms of $\mathrm{K}_{r,m}^{(4)}$ and the coefficients of $\mathrm{K}_{1,m}^{(n)}$, $\mathrm{K}_{2,m}^{(n)}$ and $\mathrm{K}_{3,m}^{(n)}$ for $n=1,2$ and 3 are rewritten in terms of binomial coefficients. In this appendix we also extend the previous results for arbitrary n.

For arbitrary n, Eq. (B8) gives the expression of $\langle\mathbb{K}^n\rangle$, that is,

$$\frac{\langle\mathbb{K}^n\rangle}{n!}=\sum_{r=1}^{[n,N]}\sum_{m=r}^{[n,N]}\frac{N}{r}\binom{N-m-1}{r-1}\mathrm{K}_{r,m}^{(n)}. \tag{25}$$

The notation $[n,N]$ means the $\min(n,N)$. Differently from our previous work,[20–22] in Eq. (25) we already have the weight of each set of subchain $\mathrm{K}_{r,m}^{(n)}$ in $\langle\mathbb{K}^n\rangle$. The coefficient that multiplies $\mathrm{K}_{r,m}^{(n)}$ in Eq. (25) is independent of the particular Hamiltonian under consideration.

For $n<N$ the trace will be calculated on a maximum subspace given by $\mathcal{H}^{(n+1)}$, whereas for $n\geqslant N$ due to the periodic boundary condition the operators act on the whole Hilbert space $\mathcal{H}^{(N)}$, therefore we can say that the operators act more than one period in the periodic chain.

Rewriting the coefficient of $\mathrm{K}_{r,m}^{(n)}$ in Eq. (25) in a more convenient way,

$$\frac{\langle\mathbb{K}^n\rangle}{n!}=\sum_{r=1}^{[n,N]}\sum_{m=r}^{[n,N]}\sum_{k=1}^{r}(-1)^{r+k}\frac{k}{r}\binom{m+r-k-1}{r-k}\binom{N}{k}\mathrm{K}_{r,m}^{(n)}\equiv\sum_{k=1}^{[n,N]}\binom{N}{k}\mathfrak{K}_{k,n} \tag{26}$$

with

$$\mathfrak{K}_{k,n}\equiv\sum_{r=k}^{[n,N]}\sum_{m=r}^{[n,N]}(-1)^{r+k}\frac{k}{r}\binom{m+r-k-1}{r-k}\mathrm{K}_{r,m}^{(n)}. \tag{27}$$

From Eq. (27) we have that the biggest possible value of k is $\min(n,N)$ while there is no restriction on n. The function $\mathfrak{K}_{k,n}$ has the property,

$$\mathfrak{K}_{k,n}=\sum_{\{n_i\}}^{n}{}''\prod_{i=1}^{k}\mathfrak{K}_{1,n_i}, \tag{28}$$

where $\{n_i\}\equiv\{n_1,n_2,\ldots,n_k\}$. Replacing Eq. (26) in Eq. (3) we get

$$\mathcal{Z}_N(\beta,\mu)=\mathrm{tr}_N(\mathbb{1})\left\{1+\sum_{k=1}^{N}\binom{N}{k}\sum_{n=k}^{\infty}(-\beta)^n\mathfrak{K}_{k,n}\right\}. \tag{29}$$

From property (28) and recombining the summations conveniently, Eq. (29) is finally written for any value of N as

$$\mathcal{Z}_N(\beta,\mu)=\left\{\mathrm{tr}_1(\mathbf{1})\left(1+\sum_{n=1}^{\infty}(-\beta)^n\mathfrak{K}_{1,n}\right)\right\}^N. \tag{30}$$

The grand potential per site $\mathcal{W}(\beta,\mu)$ is

$$\mathcal{W}_N(\beta,\mu)=-\frac{1}{N\beta}\ln\mathcal{Z}_N(\beta,\mu)=-\frac{1}{\beta}\ln\left(\mathrm{tr}_1(\mathbf{1})\left(1+\sum_{n=1}^{\infty}(-\beta)^n\mathfrak{K}_{1,n}\right)\right). \tag{31}$$

This expansion can be used to obtain analytical results of chain models in the high temperature limit.

We can be misled by the notation $\mathfrak{K}_{1,n}$ in Eq. (31) since in it are included not only connected subchains but also disconnected ones. For finite N, Eq. (31) is the simplest form of the grand potential per site since in this case n can be bigger than N which means to go around the chain more than once.

A. The thermodynamic limit

Our main interest is to get the thermodynamical behavior of physical quantities that characterize physical systems. Those are attained only in the thermodynamic limit ($N\to\infty$). We first take the thermodynamic limit and after make the expansion (2), so that we never goes along the chain more than once when we calculate the normalized traces. In this thermodynamic limit the rhs of Eq. (30) is equal to the highest eigenvalue obtained from the associated quantum transfer matrix[24] to the quantum system of interest. From Eq. (31), the grand potential per site $\mathcal{W}(\beta,\mu)$ in this limit is

$$\mathcal{W}(\beta,\mu)=-\lim_{N\to\infty}\frac{1}{N\beta}\ln\mathcal{Z}_N(\beta,\mu)=-\frac{1}{\beta}\ln\left(\mathrm{tr}_1(\mathbf{1})\left(1+\sum_{n=1}^{\infty}(-\beta)^n\mathfrak{K}_{1,n}\right)\right). \tag{32}$$

Equations (31) and (32) look alike. Their difference relies on the fact that in Eq. (32) the biggest subchain that contributes to $\mathfrak{K}_{1,n}$ has at most the length of the chain. Equation (32) confirms that the grand potential is an intensive quantity.

Certainly our aim is to be able to calculate the smallest possible number of open subchains to obtain the grand potential per site. But the definition of $\mathfrak{K}_{1,n}$ [see Eq. (27)] includes connected as well disconnected subchains. In Eq. (32) we have the following sum to calculate:

$$\xi\equiv\sum_{n=1}^{\infty}(-\beta)^n\mathfrak{K}_{1,n}. \tag{33}$$

Let us define

$$\Gamma_m\equiv\sum_{n=m}^{\infty}(-\beta)^n\mathrm{K}_{1,m}^{(n)} \tag{34}$$

as a summation of powers series of β. The expression of $\mathrm{K}_{1,m}^{(n)}$ is given by Eq. (16c). We point out that only connected open subchains contribute to the functions Γ_m. We define the function $\varphi(\lambda)$ in terms of the functions Γ_m as follows:

$$\varphi(\lambda)=\sum_{m=1}^{\infty}\frac{\Gamma_m}{\lambda^m}, \tag{35}$$

where λ is a parameter. In Appendix C we show that the

$$\xi=\sum_{n=0}^{\infty}\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}\left(\frac{\varphi(\lambda)^{n+1}}{(n+1)!}\right)\Bigg|_{\lambda=1}. \tag{36}$$

From Eqs. (27) and (32) we have that the connected and disconnected open subchains contribute to the grand potential per site. In the thermodynamic limit we have from Eqs. (34)–(36) that all these subchains can be derived only from a sum of connected open subchains (for details see Appendix C). We finally write the grand potential per site simply as

$$\mathcal{W}(\beta,\mu)=-\frac{1}{\beta}\{\ln(\mathrm{tr}_1(\mathbf{1}))+\ln(1+\xi)\}. \tag{37}$$

Due to the fact that ξ can be derived from the function $\varphi(\lambda)$, one has the consequence that a much smaller number of terms has to be calculated at each β-order in the β-expansion of $\mathcal{W}(\beta,\mu)$. The weight of each g-trace in Eq. (37) is already included in the definition of ξ.

III. THE HEISENBERG XXZ MODEL

Let us consider the Hamiltonian of the well known anisotropic one-dimensional Heisenberg XXZ model with spin-$\frac{1}{2}$,[1,2]

$$\mathbb{H}=\frac{1}{2}\sum_{j=1}^{N}(\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y+\Delta\sigma_j^z\sigma_{j+1}^z-2h\sigma_j^z), \tag{38}$$

where h is the external magnetic field and $(\sigma_j^x,\sigma_j^y,\sigma_j^z)$ are the Pauli matrices at the jth site on a periodic chain with N space sites and Δ is called the anisotropy parameter. For $\Delta>0$ ($\Delta<0$) we have a repulsive (attractive) interaction core. The case $\Delta=1$ ($\Delta=-1$) corresponds to the isotropic antiferromangetic (ferromagnetic) Heisenberg model with fully polarized ground state.

Through the Jordan–Wigner transformation,[25] the Hamiltonian (38) is mapped on a spinless fermionic model, whose Hamiltonian is

$$\mathbb{H}=\sum_{j=1}^{N}(t(\mathbf{a}_j^{\dagger}\mathbf{a}_{j+1}+\mathbf{a}_{j+1}^{\dagger}+\mathbf{a}_j)+V\mathbf{n}_j\mathbf{n}_{j+1}+E\mathbf{n}_j)+N\left(h+\frac{\Delta}{2}\right), \tag{39}$$

with $V=2\Delta$, $E=-2h-2\Delta$, where $\mathbf{n}_i=\mathbf{a}_i^{\dagger}\mathbf{a}_i$ and $\mathbf{a}_i^{\dagger}(\mathbf{a}_i)$ is the fermionic creation(annihilation) operator at site j. The operators $\mathbf{a}_i^{\dagger}$ and $\mathbf{a}_i$ satisfy the usual anticommutation relations of the fermionic fields. The hopping constant t is included in Hamiltonian (39) only to help us count the powers of the terms that contribute to a given order β^n in the β-expansion of the Helmholtz free energy per site. Throughout our calculations, we take $t=1$. The term $N(h+\Delta/2)$ leads to a shift in the energy of the ground state of the model.

A. High temperature expansion

In this section we calculate the β-expansion of the Helmholtz free energy per site of the XXZ model, whose Hamiltonian is given by Eq. (39), up to order β^3.

In order to apply the method derived in Sec. II, we write Hamiltonian (38) as $\mathbb{H}=\Sigma_{i=1}^{N}\mathbf{H}_{i,i+1}$, where

$$\mathbf{H}_{i,i+1}\equiv\mathbf{E}_{i,i+1}+\mathbf{T}_{i,i+1}^{+}+\mathbf{T}_{i,i+1}^{-}+\mathbf{V}_{i,i+1}, \tag{40}$$

and each term on the rhs of Eq. (40) is defined as $\mathbf{E}_{i,i+1}\equiv\frac{1}{2}E(\mathbf{n}_i+\mathbf{n}_{i+1})$, $\mathbf{T}_{i,i+1}^{-}\equiv t\mathbf{a}_i^{\dagger}\mathbf{a}_{i+1}$, $\mathbf{T}_{i,i+1}^{+}\equiv t\mathbf{a}_{i+1}^{\dagger}\mathbf{a}_i$ and $\mathbf{V}_{i,i+1}\equiv V\mathbf{n}_i\mathbf{n}_{i+1}$.

Our aim is to obtain the Helmholtz free energy per site of the XXZ model in the thermodynamic limit. For doing that we need the auxiliary function $\varphi(\lambda)$ [see Eq. (35)] of the XXZ model. This function is calculated from the functions Γ_m that are written in terms of $\mathrm{K}_{1,m}^{(n)}$ [see Eq. (34)].

Since we intend to calculate the β-expansion of the Helmholtz free energy per site of the XXZ model up to order β^3, we need to obtain the analytical expressions of $\Gamma_1,\ldots,\Gamma_4$, namely,

$$\Gamma_1=-\beta \mathrm{K}_{1,1}^{(1)}+\beta^2\mathrm{K}_{1,1}^{(2)}-\beta^3\mathrm{K}_{1,1}^{(3)}+\beta^4\mathrm{K}_{1,1}^{(4)}+\mathcal{O}(\beta^5), \tag{41a}$$

$$\Gamma_2=\beta^2\mathrm{K}_{1,2}^{(2)}-\beta^3\mathrm{K}_{1,2}^{(3)}+\beta^4\mathrm{K}_{1,2}^{(4)}+\mathcal{O}(\beta^5), \tag{41b}$$

$$\Gamma_3=-\beta^3\mathrm{K}_{1,3}^{(3)}+\beta^4\mathrm{K}_{1,3}^{(4)}+\mathcal{O}(\beta^5), \tag{41c}$$

$$\Gamma_4=\beta^4\mathrm{K}_{1,4}^{(4)}+\mathcal{O}(\beta^5). \tag{41d}$$

In Appendix D the functions $\mathrm{K}_{1,m}^{(n)}$ in Eqs. (41) are written as sums of normalized traces.

In particular, for Hamiltonian (39) the hopping terms ($\mathbf{T}_{i,i+1}^{+}$ and $\mathbf{T}_{i,i+1}^{-}$) in the normalized traces only contribute to those functions $\mathrm{K}_{1,m}^{(n)}$ where we have $\mathbf{H}_{i,i+1}^{l}$ with $l>1$. Since we are calculating traces, the number of $\mathbf{T}_{i,i+1}^{+}$'s in a given normalized trace has to be equal to the number of terms $\mathbf{T}_{i,i+1}^{-}$'s in it. Otherwise, the normalized trace is null.

Calculating explicitly the normalized traces that contribute to $\mathrm{K}_{1,m}^{(n)}$ (see Appendix D) for the XXZ model, we obtain the following.

(*i*) $m=1$:

$$\mathrm{K}_{1,1}^{(1)}=\frac{E}{2}+\frac{V}{4}, \tag{42a}$$

$$\mathrm{K}_{1,1}^{(2)}=\frac{t^2}{4}+\frac{3E^2}{16}+\frac{EV}{4}+\frac{V^2}{8}, \tag{42b}$$

$$\mathrm{K}_{1,1}^{(3)}=\frac{5E^3}{96}+\frac{V^3}{24}+\frac{Et^2}{8}+\frac{VE^2}{8}+\frac{EV^2}{8}, \tag{42c}$$

$$\mathrm{K}_{1,1}^{(4)}=\frac{t^4}{48}+\frac{E^2t^2}{32}+\frac{3E^4}{256}+\frac{VE^3}{24}+\frac{E^2V^2}{16}+\frac{EV^3}{24}+\frac{V^4}{96}. \tag{42d}$$

(*ii*) $m=2$:

$$\mathrm{K}_{1,2}^{(2)}=\frac{5E^2}{16}+\frac{3EV}{8}+\frac{V^2}{8}, \tag{43a}$$

$$\mathrm{K}_{1,2}^{(3)}=\frac{E^3}{4}+\frac{V^3}{8}+\frac{Et^2}{4}+\frac{17VE^2}{32}+\frac{7EV^2}{16}+\frac{Vt^2}{8}, \tag{43b}$$

$$\mathrm{K}_{1,2}^{(4)}=\frac{t^4}{24}+\frac{5E^2t^2}{24}+\frac{95E^4}{768}+\frac{25VE^3}{64}+\frac{33E^2V^2}{64}+\frac{5EV^3}{16}+\frac{7V^4}{96}+\frac{t^2V^2}{24}+\frac{EVt^2}{6}. \tag{43c}$$

(*iii*) $m=3$:

$$\mathrm{K}_{1,3}^{(3)}=\frac{3E^3}{16}+\frac{V^3}{16}+\frac{23VE^2}{64}+\frac{EV^2}{4}, \tag{44a}$$

$$\mathrm{K}_{1,3}^{(4)}=\frac{41E^2t^2}{192}+\frac{59E^4}{256}+\frac{85VE^3}{128}+\frac{101E^2V^2}{128}+\frac{7EV^3}{16}+\frac{7t^2V^2}{96}+\frac{23EVt^2}{96}+\frac{3V^4}{32}. \tag{44b}$$

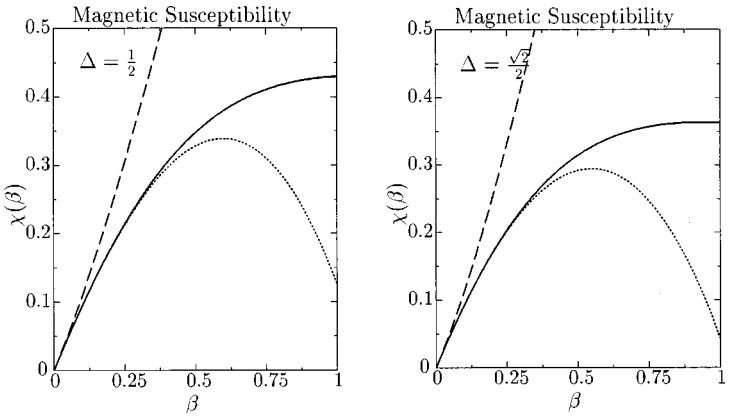


FIG. 1. The pointed line corresponds the β-expansion (46), the dashed line represents the β-expansion obtained by Destri and de Vega (Ref. 27) and the solid line corresponds to the numerical solution of the NLIE in Ref. 23 and 27.

(iv) $m=4$:

$$\mathrm{K}_{1,4}^{(4)}=\frac{29E^4}{256}+\frac{19VE^3}{64}+\frac{5E^2V^2}{16}+\frac{5EV^3}{32}+\frac{V^4}{32}. \tag{45}$$

Substituting those expressions in Eqs. (41) (taking $t=1$) and those in Eq. (35) we obtain the auxiliary function $\varphi(\lambda)$ for the XXZ model. Using the algebraic language MAPLE 5.1 we calculate the Helmholtz free energy per site of the model up to order β^3, that is,

$$\mathcal{W}(\beta)=\frac{\ln(2)}{\beta}+\mathcal{W}_I(\beta)+\mathcal{W}_F(\beta)-\frac{\Delta}{8}\beta^2+\frac{1}{4}\left(h^2+\frac{\Delta^2}{6}\right)\beta^3+\mathcal{O}(\beta^4), \tag{46}$$

where $\mathcal{W}_I(\beta)$ is the Helmholtz free energy per site of the Ising model[24,26] up to order β^3, that is,

$$\mathcal{W}_I(\beta)=-\frac{\ln(2)}{\beta}-\left(\frac{h^2}{2}+\frac{\Delta^2}{8}\right)\beta+\frac{h^2\Delta}{2}\beta^2+\left(\frac{h^4}{12}-\frac{h^2\Delta^2}{4}+\frac{\Delta^4}{192}\right)\beta^3+\mathcal{O}(\beta^4) \tag{47}$$

and $\mathcal{W}_F(\beta)$ is the Helmholtz free energy per site of the free fermion model[23,26] up to same β-order,

$$\mathcal{W}_F(\beta)=-\frac{\ln(2)}{\beta}-\frac{t^2}{4}\beta-\frac{t^4}{32}\beta^3+\mathcal{O}(\beta^4). \tag{48}$$

We rewrite the Helmholtz free energy per site [Eq. (46)] using the constants of Hamiltonian in Ref. 27. Comparing our results with Eq. (6.5) of this reference, we conclude (i) both results agree up to order β; (ii) our coefficient at order β^2 is $-J^3\cos(\gamma)+J\cos(\gamma)h^2$, which means that we have two misprints in Eq. (6.5) of Ref. 27, that is, the sign of $-J^3\cos(\gamma)\beta^2$ and a missing power of J multiplying h^2 [the two terms that contribute to order β^2 in Eq. (6.5) have different dimensions]; (iii) and it is missing the term $-J^2\cos^2(\gamma)h^2\beta^3$ in Eq. (6.5) of Ref. 27 (we point out that without this term we do not recover the limiting case of Ising model[24,26] ($t=0$) from XXZ model). Morever, the other terms at order β^3 in Eq. (6.5) have the following misprints: $-\frac{1}{4}J^4\beta^3$ should be $\frac{1}{2}J^4\beta^3$ and the term $-\frac{1}{6}J^4\cos^2(\gamma)\beta^3$ should be $\frac{2}{3}J^4\cos^2(\gamma)\beta^3$. With the previous corrections we get the Helmholtz free energy per site of the Ising model and the free fermion model as limiting cases of the XXZ model.

In Ref. 27 Destri and de Vega obtained the Helmholtz free energy per site of the XXZ model as a nonlinear integral equation (NLIE), as similarly obtained by Klümper.[23] Once our disagreement with the result of Ref. 27 is proportional h^2 at order β^3, we calculate the β-expansion of the magnetic susceptibility $\chi(\beta)$ $[\chi(\beta)=-\partial^2\mathcal{W}(\beta)/\partial h^2]$, obtained from Eq. (46). In Fig. 1 we plot the curve of the magnetic susceptibility derived from NLIE in Refs. 23 and 27, the β-expansion of

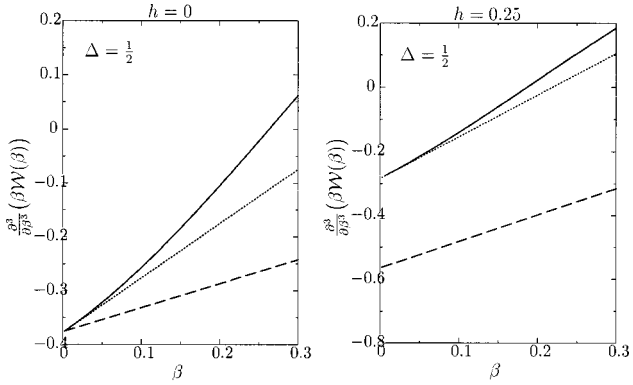


FIG. 2. We plot the function $(\partial^3/\partial\beta^3)(\beta\mathcal{W}(\beta))$ vs β. The pointed line (a straight line) corresponds to the results obtained from (46), the dashed line the β-expansion obtained by Destri and de Vega (Ref. 27) and the solid line the numerical solution of the NLIE (Refs. 23 and 27).

$\chi(\beta)$ derived in Ref. 27 and our own β-expansion of $\chi(\beta)$. From Fig. 1 we see that our result with $\Delta=\frac{1}{2}$ and $\Delta=\sqrt{2}/2$ coincides with the one derived from the NLIE in Refs. 23 and 27 for β up to 0.3, while the β-expansion of Destri and de Vega does not.

As a final check of our β-expansion (46) we plot in Fig. 2 the third partial derivative with respect to β of the function $\beta\mathcal{W}(\beta)$. We compare the numerical solution for this function obtained from the NLIE,[23,27] in the same reference, and our results derived from Eq. (46). In the region $\beta\approx 0$, the function $(\partial^3/\partial\beta^3)(\beta\mathcal{W}(\beta))$ is a straight line. From Fig. 2 we see that the result derived from Eq. (46) is identical to the one from the NLIE for β up to 0.1. For $h\neq 0$ in Fig. 2 we get that the function $(\partial^3/\partial\beta^3)(\beta\mathcal{W}(\beta))$ derived from the β-expansion in Ref. 27 does not even touch the exact curve.

We conclude that even though the NLIE derived in Refs. 23 and 27 gives the exact thermodynamics of the XXZ model with spin-$\frac{1}{2}$ the β-expansion obtained in Ref. 27 is not correct.

IV. CONCLUSIONS

There are several interesting one-dimensional models with translational invariance, with interactions between first neighbors only, satisfying periodic boundary conditions. They are generically called chain models, some of which have the property of integrability and to which the Bethe ansatz has been applied to solve them exactly at $T=0$ and at finite T. Their thermodynamical properties are obtained through coupled integral equations which demand numerical analysis to be solved (as examples see Refs. 10–14).

In this article we present a new analytical method to get the β-expansion coefficients of the grand potential per site, for translationally invariant chain models with nearest-neighbors interactions. Differently from our previous works[20–22] we calculate directly the β-expansion of the grand potential per site $\mathcal{W}(\beta,\mu)$. The weight of each subchain in $\mathcal{W}(\beta,\mu)$ is obtained, and we show explicitly that the grand potential per site is an intensive quantity. In the thermodynamic limit $(N\to\infty)$ we show that $\mathcal{W}(\beta,\mu)$ can be derived from an auxiliary function $\varphi(\lambda)$ that is written only in terms of open connected subchains. The present approach gives a β-expansion of $\mathcal{W}(\beta,\mu)$, whose coefficient of order β^n can be obtained exactly for arbitrary value of n. The existence of this auxiliary function allows us to get higher order terms in the β-expansion of $\mathcal{W}(\beta,\mu)$ than we were able to before, in Refs. 20–22. The coefficient of order β^n is analytically obtained, and it is exact. The number of terms (traces) to be calculated when deriving each coefficient in the β-expansion of $\mathcal{W}(\beta,\mu)$ is much smaller than before.

The present method applies to chains in both real space and momentum space, and the result given by Eq. (37) is valid for both classic and quantum models (bosonic and/or fermionic fields).

As an illustrative application of the method, we consider the spin-$\frac{1}{2}$ Heisenberg XXZ chain model and derive its Helmholtz free energy per site up to order β^3. The exact thermodynamics of the XXZ model is derived in Refs. 23 and 27. Our results in the high temperature region fully agree with the numerical solution of the NLIE derived in those references in this interval of temperature. Our β-expansion (46) recovers the Helmholtz free energy per site in two limiting cases: the Ising model ($t=0$) and the free fermion model ($\Delta=h=0$). We compare our high temperature expansion of the $\mathcal{W}(\beta)$ Eq. (46) of the XXZ model with the one derived by Destri and de Vega.[27] We show that Eq. (6.5) of this last reference has misprints and it is missing a term at order β^3.

As a final word we want to point out that the present approach can be well applied to models that do not have the property of integrability. Besides, once we have closed expressions for the coefficients of the β-expansion of $\mathcal{W}(\beta)$, the method can be implemented through a procedure in an algebraic language to get high β-order terms of the high temperature expansion of $\mathcal{W}(\beta)$ for the model under interest. We hope to report in the future progress in this direction.

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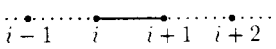
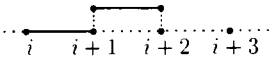
APPENDIX A: GRAPHIC REPRESENTATION OF NORMALIZED TRACES

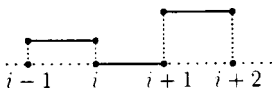
We have a better visualization of the normalized traces that contribute to $\langle \mathbb{K}^n \rangle$ through a graphic representation. In the graph, the operator $\mathbf{K}_{i,i+1}$ is represented by a straight line that links the sites i and $i+1$. In the case where we have a product of operators $\mathbf{K}_{i,i+1}$, for each operator a line is drawn at a different step of the ladder. It is important in the normalized trace the order in which the operators $\mathbf{K}_{i,i+1}$ appear in the string. We take this order into account in our graph representation of the normalized traces. To exemplify how to take into account the order of the operators in the string, we consider the following examples:

$\langle \mathbf{K}_{i,i+1} \rangle \longrightarrow$ 

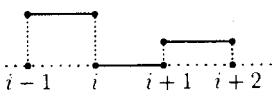
(A1)

$\langle \mathbf{K}_{i,i+1}\mathbf{K}_{i+1,i+2} \rangle \longrightarrow$ 

(A2)

$\langle \mathbf{K}_{i,i+1}\mathbf{K}_{i-1,i}\mathbf{K}_{i+1,i+2} \rangle \longrightarrow$ 

(A3)

$\langle \mathbf{K}_{i,i+1}\mathbf{K}_{i+1,i+2}\mathbf{K}_{i-1,i} \rangle \longrightarrow$ 

(A4)

The graphs (A1)–(A4) are *connected* graphs, which means that the normalized trace cannot be written as a product of normalized traces of smaller number of operators $\mathbf{K}_{i,i+1}$.

APPENDIX B: CALCULATION OF $\langle \mathbb{K}^n \rangle$

In this appendix we give the explicit definition of $K^{(4)}_{r,m}$ in terms of which we write $\langle \mathbb{K}^4 \rangle$. The expression of $\langle \mathbb{K}^4 \rangle$ plus Eqs. (24) will allow us to write down $\langle \mathbb{K}^n \rangle$ for arbitrary n.

We define $K^{(4)}_{1,m}$ as

$$K^{(4)}_{1,1} = \frac{\langle \mathbf{K}^4_{1,2} \rangle_g}{4!}, \tag{B1a}$$

$$K^{(4)}_{1,2} = \frac{\langle \mathbf{K}^3_{1,2}\mathbf{K}_{2,3} \rangle_g}{3!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}^3_{2,3} \rangle_g}{3!} + \frac{\langle \mathbf{K}^2_{1,2}\mathbf{K}^2_{2,3} \rangle_g}{2!2!}, \tag{B1b}$$

$$K^{(4)}_{1,3} = \frac{\langle \mathbf{K}^2_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{3,4} \rangle_g}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}^2_{2,3}\mathbf{K}_{3,4} \rangle_g}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}^2_{3,4} \rangle_g}{2!}, \tag{B1c}$$

$$K^{(4)}_{1,4} = \langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{3,4}\mathbf{K}_{4,5} \rangle_g. \tag{B1d}$$

The other traces can be written as products of traces of lower order and they are

$$K^{(4)}_{2,2} = \frac{\langle \mathbf{K}^3_{1,2}\mathbf{K}_{3,4} \rangle_g}{3!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}^3_{3,4} \rangle_g}{3!} + \frac{\langle \mathbf{K}^2_{1,2}\mathbf{K}^2_{3,4} \rangle_g}{2!2!}, \tag{B2a}$$

$$\begin{aligned} K^{(4)}_{2,3} = {} & \frac{\langle \mathbf{K}^2_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{4,5} \rangle_g}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}^2_{2,3}\mathbf{K}_{4,5} \rangle_g}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}^2_{4,5} \rangle_g}{2!} \\ & + \frac{\langle \mathbf{K}^2_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{4,5} \rangle_g}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}^2_{3,4}\mathbf{K}_{4,5} \rangle_g}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}^2_{4,5} \rangle_g}{2!}, \end{aligned} \tag{B2b}$$

$$K^{(4)}_{2,4} = \langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{3,4}\mathbf{K}_{5,6} \rangle_g + \langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{4,5}\mathbf{K}_{5,6} \rangle_g + \langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{4,5}\mathbf{K}_{5,6} \rangle_g, \tag{B2c}$$

$$K^{(4)}_{3,3} = \frac{\langle \mathbf{K}^2_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{5,6} \rangle_g}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}^2_{3,4}\mathbf{K}_{5,6} \rangle_g}{2!} + \frac{\langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}^2_{5,6} \rangle_g}{2!}, \tag{B2d}$$

$$K^{(4)}_{3,4} = \langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{4,5}\mathbf{K}_{6,7} \rangle_g + \langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{4,5}\mathbf{K}_{6,7} \rangle_g + \langle \mathbf{K}_{1,2}\mathbf{K}_{2,3}\mathbf{K}_{4,5}\mathbf{K}_{6,7} \rangle_g, \tag{B2e}$$

$$K^{(4)}_{4,4} = \langle \mathbf{K}_{1,2}\mathbf{K}_{3,4}\mathbf{K}_{5,6}\mathbf{K}_{7,8} \rangle_g. \tag{B2 f}$$

From those definitions, the normalized trace $\langle \mathbb{K}^4 \rangle$ is written as

$$\begin{aligned} \frac{\langle \mathbb{K}^4 \rangle}{4!} = {} & N K^{(4)}_{1,1} + N K^{(4)}_{1,2} + N K^{(4)}_{1,3} + N K^{(4)}_{1,4} + \frac{N(N-3)}{2!} K^{(4)}_{2,2} + \frac{N(N-4)}{2!} K^{(4)}_{2,3} + \frac{N(N-5)}{2!} K^{(4)}_{2,4} \\ & + \frac{N(N-4)(N-5)}{3!} K^{(4)}_{3,3} + \frac{N(N-5)(N-6)}{3!} K^{(4)}_{3,4} + \frac{N(N-5)(N-6)(N-7)}{4!} K^{(4)}_{4,4}. \end{aligned} \tag{B3}$$

We use the following notations to write the coefficients of Eqs. (24) and (B3):

$$C^N_{1,1} = N,$$

$$C^N_{1,2} = N, \quad C^N_{2,2} = \frac{N(N-3)}{2!}, \tag{B4}$$

$$C_{1,3}^N = N,\quad C_{2,3}^N = \frac{N(N-4)}{2!},\quad C_{3,3}^N = \frac{N(N-4)(N-5)}{3!},$$

$$C_{1,4}^N = N,\quad C_{2,4}^N = \frac{N(N-5)}{2!},\quad C_{3,4}^N = \frac{N(N-5)(N-6)}{3!},\quad C_{4,4}^N = \frac{N(N-5)(N-6)(N-7)}{4!}.$$

Replacing the definitions given by Eqs. (B4) in Eqs. (24) and (B3), we obtain a compact way of writing the normalized traces:

$$\langle \mathbb{K} \rangle = C_{1,1}^N K_{1,1}^{(1)}, \tag{B5a}$$

$$\frac{\langle \mathbb{K}^2 \rangle}{2!} = C_{1,1}^N K_{1,1}^{(2)} + C_{1,2}^N K_{1,2}^{(2)} + C_{2,2}^N K_{2,2}^{(2)}, \tag{B5b}$$

$$\frac{\langle \mathbb{K}^3 \rangle}{3!} = C_{1,1}^N K_{1,1}^{(3)} + C_{1,2}^N K_{1,2}^{(3)} + C_{1,3}^N K_{1,3}^{(3)} + C_{2,2}^N K_{2,2}^{(3)} + C_{2,3}^N K_{2,3}^{(3)} + C_{3,3}^N K_{3,3}^{(3)}, \tag{B5c}$$

$$\begin{aligned}\frac{\langle \mathbb{K}^4 \rangle}{4!} &= C_{1,1}^N K_{1,1}^{(4)} + C_{1,2}^N K_{1,2}^{(4)} + C_{1,3}^N K_{1,3}^{(4)} + C_{1,4}^N K_{1,4}^{(4)} + C_{2,2}^N K_{2,2}^{(4)} + C_{2,3}^N K_{2,3}^{(4)} \\ &\quad + C_{2,4}^N K_{2,4}^{(4)} + C_{3,3}^N K_{3,3}^{(4)} + C_{3,4}^N K_{3,4}^{(4)} + C_{4,4}^N K_{4,4}^{(4)}.\end{aligned} \tag{B5d}$$

From Eqs. (B4) we see that the coefficient that multiplies $K_{r,m}^{(n)}$ is independent of n and it is equal to

$$C_{1,m}^N = N, \quad 1 \leqslant m, \tag{B6a}$$

$$C_{2,m}^N = \frac{N(N-m-1)}{2!}, \quad 2 \leqslant m, \tag{B6b}$$

$$C_{3,m}^N = \frac{N(N-m-1)(N-m-2)}{3!}, \quad 3 \leqslant m, \tag{B6c}$$

$$C_{4,m}^N = \frac{N(N-m-1)(N-m-2)(N-m-3)}{4!}, \quad 4 \leqslant m. \tag{B6d}$$

Afterwards, for any $r \leqslant m \leqslant \min(n,N)$, we obtain a general relation from Eqs. (B6) given by

$$C_{r,m}^N = \frac{N}{r}\binom{N-m-1}{r-1} = \frac{1}{r}\sum_{k=1}^{r} (-1)^{r+k} k \binom{m+r-k-1}{r-k}\binom{N}{k}, \tag{B7}$$

such that

$$\frac{\langle \mathbb{K}^n \rangle}{n!} = \sum_{r=1}^{[n,N]} \sum_{m=r}^{[n,N]} \frac{N}{r}\binom{N-m-1}{r-1} K_{r,m}^{(n)}. \tag{B8}$$

We are using the notation $[n,N] = \min(n,N)$.

APPENDIX C: RELATION BETWEEN THE AUXILIARY FUNCTION $\varphi(\lambda)$ AND ξ

In Eq. (34) we define the function Γ_m,

$$\Gamma_m \equiv \sum_{n=m}^{\infty} (-\beta)^n \mathrm{K}_{1,m}^{(n)}, \tag{C1}$$

and the auxiliary function $\varphi(\lambda)$,

$$\varphi(\lambda) \equiv \sum_{m=1}^{\infty} \frac{\Gamma_m}{\lambda^m}. \tag{C2}$$

In this appendix we show that the grand potential per site, in the thermodynamic limit, can be obtained from derivatives of powers of the function $\varphi(\lambda)$.

To calculate the grand potential per site [see Eq. (32)] we need to perform the sum

$$\sum_{n=0}^{\infty} (-\beta)^n \mathfrak{K}_{1,n} \equiv \xi. \tag{C3}$$

Substituting the expression of $\mathfrak{K}_{1,n}$ [Eq. (27) with $k=1$] in ξ and taking into account that in $\mathrm{K}_{1,m}^{(n)}$ we have to have $n>m$, Eq. (C3) becomes

$$\xi = \sum_{n=1}^{\infty} \sum_{m=1}^{n} (-\beta)^n \mathrm{K}_{1,m}^{(n)} - \frac{1}{2} \sum_{n=2}^{\infty} \sum_{m=2}^{n} (-\beta)^n \binom{m}{1} \mathrm{K}_{2,m}^{(n)} + \frac{1}{3} \sum_{n=3}^{\infty} \sum_{m=3}^{n} (-\beta)^n \binom{m+1}{2} \mathrm{K}_{3,m}^{(n)} + \ldots \tag{C4}$$

$$\equiv \sum_{r=1}^{\infty} \varphi_r, \tag{C5}$$

where φ_r is such that

$$\varphi_r \equiv \frac{(-1)^{r+1}}{r} \sum_{n=r}^{\infty} \sum_{m=r}^{n} (-\beta)^n \binom{m+r-2}{r-1} \mathrm{K}_{r,m}^{(n)}. \tag{C6}$$

We drop the upper limit $[n,N]$ condition in the sum over m [see Eq. (27)] because now we are taking first the thermodynamic limit ($N \to \infty$), which means that we always have $n<N$.

Applying the equality

$$\sum_{n=r}^{\infty} \sum_{m=r}^{n} \cdots = \sum_{m=r}^{\infty} \sum_{n=r}^{\infty} \cdots \tag{C7}$$

on Eq. (C6), we obtain

$$\varphi_r = \frac{(-1)^{r+1}}{r} \sum_{m=r}^{\infty} \binom{m+r-2}{r-1} \sum_{n=r}^{\infty} (-\beta)^n \mathrm{K}_{r,m}^{(n)}. \tag{C8}$$

From Eqs. (C1) and (C2) we have

$$\varphi(\lambda) = \sum_{m=1}^{\infty} \frac{1}{\lambda^m} \sum_{n=1}^{\infty} (-\beta)^n \mathrm{K}_{1,m}^{(n)}. \tag{C9}$$

Our next step is to take powers of the function $\varphi(\lambda)$. We begin with $\varphi(\lambda)^2$:

$$\varphi(\lambda)^2=\sum_{m_1,m_2=1}^{\infty}\frac{1}{\lambda^{m_1+m_2}}\sum_{n_1,n_2=1}^{\infty}(-\beta)^{n_1+n_2}\mathrm{K}_{1,m_1}^{(n_1)}\mathrm{K}_{1,m_2}^{(n_2)}$$

$$=\sum_{m=2}^{\infty}\frac{1}{\lambda^m}\sum_{n=2}^{\infty}(-\beta)^n\sum_{\{n_i\}}^{n}{}''\sum_{\{m_i\}}^{m}{}''\mathrm{K}_{1,m_1}^{(n_1)}\mathrm{K}_{1,m_2}^{(n_2)}$$

$$=\sum_{m=2}^{\infty}\frac{1}{\lambda^m}\sum_{n=2}^{\infty}(-\beta)^n\mathrm{K}_{2,m}^{(n)}. \tag{C10}$$

For arbitrary r we obtain

$$\varphi(\lambda)^r=\sum_{m=r}^{\infty}\frac{1}{\lambda^m}\sum_{n=r}^{\infty}(-\beta)^n\mathrm{K}_{r,m}^{(n)} \tag{C11}$$

and we note that

$$\varphi(\lambda)\big|_{\lambda=1}=\varphi_1, \tag{C12a}$$

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{\varphi(\lambda)^2}{2!}\right)\bigg|_{\lambda=1}=\varphi_2, \tag{C12b}$$

$$\vdots$$

$$\frac{\mathrm{d}^{r-1}}{\mathrm{d}\lambda^{r-1}}\left(\frac{\varphi(\lambda)^r}{r!}\right)\bigg|_{\lambda=1}=\varphi_r. \tag{C12c}$$

Finally we have

$$\xi=\sum_{r=1}^{\infty}\varphi_r=\sum_{r=1}^{\infty}\frac{\mathrm{d}^{r-1}}{\mathrm{d}\lambda^{r-1}}\left(\frac{\varphi(\lambda)^r}{r!}\right)\bigg|_{\lambda=1}, \tag{C13}$$

which shows that the sum (C3) can be obtained from a function that contains only open connected subchains.

APPENDIX D: USEFUL RELATIONS BETWEEN $\mathrm{K}_{1,m}^{(n)}$ AND THE NORMALIZED TRACES

In Sec. III we calculate the β-expansion of the Helmholtz free energy per site of the XXZ model up to order β^3. In order to do so, we need to write the functions $\mathrm{K}_{1,m}^{(n)}$ [see Eq. (16c)] in terms of the normalized traces instead of the g-traces.

For any quantum system driven by a Hamiltonian with interactions between first neighbors only, invariant under translations along the chain, and null chemical potential, we have the following.

(*i*) $m=1$:

$$\mathrm{K}_{1,1}^{(1)}=\langle\mathbf{H}_{1,2}\rangle, \tag{D1a}$$

$$\mathrm{K}_{1,1}^{(2)}=\frac{1}{2!}\langle\mathbf{H}_{1,2}^2\rangle, \tag{D1b}$$

$$\mathrm{K}_{1,1}^{(3)}=\frac{1}{3!}\langle\mathbf{H}_{1,2}^3\rangle, \tag{D1c}$$

$$K_{1,1}^{(4)}=\frac{1}{4!}\langle \mathbf{H}_{1,2}^4\rangle. \tag{D1d}$$

(*ii*) $m=2$:

$$K_{1,2}^{(2)}=\langle \mathbf{H}_{1,2}\mathbf{H}_{2,3}\rangle, \tag{D2a}$$

$$K_{1,2}^{(3)}=\frac{1}{2!}[\langle \mathbf{H}_{1,2}^2\mathbf{H}_{2,3}\rangle+\langle \mathbf{H}_{1,2}\mathbf{H}_{2,3}^2\rangle], \tag{D2b}$$

$$K_{1,2}^{(4)}=\frac{1}{3!}\left[\langle \mathbf{H}_{1,2}^3\mathbf{H}_{2,3}\rangle+\frac{1}{2!}(2\langle \mathbf{H}_{1,2}^2\mathbf{H}_{2,3}^2\rangle+\langle \mathbf{H}_{1,2}\mathbf{H}_{2,3}\mathbf{H}_{1,2}\mathbf{H}_{2,3}\rangle)+\langle \mathbf{H}_{1,2}\mathbf{H}_{2,3}^3\rangle\right]. \tag{D2c}$$

(*iii*) $m=3$:

$$K_{1,3}^{(3)}=\langle \mathbf{H}_{1,2}\mathbf{H}_{2,3}\mathbf{H}_{3,4}\rangle, \tag{D3a}$$

$$K_{1,2}^{(4)}=\frac{1}{2}\left[\langle \mathbf{H}_{1,2}^2\mathbf{H}_{2,3}\mathbf{H}_{3,4}\rangle+\frac{2}{3}\langle \mathbf{H}_{1,2}\mathbf{H}_{2,3}^2\mathbf{H}_{3,4}\rangle+\langle \mathbf{H}_{1,2}\mathbf{H}_{2,3}\mathbf{H}_{3,4}^2\rangle+\frac{1}{3}\langle \mathbf{H}_{1,2}\mathbf{H}_{2,3}\mathbf{H}_{3,4}\mathbf{H}_{2,3}\rangle\right]. \tag{D3b}$$

(*iv*) $m=4$:

$$K_{1,4}^{(4)}=\langle \mathbf{H}_{1,2}\mathbf{H}_{2,3}\mathbf{H}_{3,4}\mathbf{H}_{4,5}\rangle. \tag{D4}$$

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A bi-Hamiltonian formulation for triangular systems by perturbations

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A bi-Hamiltonian formulation is proposed for triangular systems resulting from perturbations around solutions, from which infinitely many symmetries and conserved functionals of triangular systems can be explicitly constructed, provided that one operator of the Hamiltonian pair is invertible. Through our formulation, four examples of triangular systems are exhibited, which also show that bi-Hamiltonian systems in both lower dimensions and higher dimensions are many and varied. Two of four examples give local $2+1$ dimensional bi-Hamiltonian systems and illustrate that multiscale perturbations can lead to higher-dimensional bi-Hamiltonian systems. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1432775]

I. INTRODUCTION

The bi-Hamiltonian formulation is a great success in the Hamiltonian theory of differential equations.[1] It has attracted the attention of a wide audience within both the mathematical community and the physical community due to its importance in producing symmetries and conserved functionals, and has already become one of active research directions in the field of soliton theory and integrable systems.

In this paper, we are concerned with the bi-Hamiltonian formulation of triangular systems resulting from various perturbations around solutions, specific systems of which were furnished in Refs. 2–4. Such triangular systems provide candidates of integrable couplings for given integrable systems.[5,6] A general triangular system reads as

$$\begin{cases} u_t = K(u) = K(u,\ldots,u^{(k)}), \\ v_t = S(u,v) = S(u,v,\ldots,u^{(l)},v^{(l)}), \end{cases} \tag{1.1}$$

where $u=u(t,x)$, $v=v(t,x)$, and $u^{(n)}$ and $v^{(n)}$ are derivatives with respect to the spatial variable x. Such a concrete example by a first-order perturbation is given by

$$\begin{cases} u_t = K(u), \\ v_t = K'(u)[v], \end{cases} \tag{1.2}$$

where $K'(u)[v]$ denotes the Gateaux derivative of $K(u)$ at a direction v, i.e.,

$$K'(u)[v] = \frac{\partial}{\partial \varepsilon}\bigg|_{\varepsilon=0} K(u+\varepsilon v).$$

A mathematical structure called the perturbation bundle has been established in Ref. 5 to study its integrable properties. Note that the second component of the above-mentioned system is just the linearized system of the original system $u_t=K(u)$, and thus the symmetry problem leads to a triangular system together with the original system, which also shows the importance of studying triangular systems (see Ref. 6 for more discussion). Other similar examples of specific triangular

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systems were presented by means of perturbations in Refs. 2–4. However, there is no discussion on the bi-Hamiltonian formulation of general triangular systems by perturbations, even the specific systems mentioned previously.

With a view to exposing integrability, we would like to answer whether there exists any bi-Hamiltonian formulation for triangular systems resulting from various perturbations around solutions. It will be shown that a bi-Hamiltonian formulation of the resulting triangular systems can be inherited from an original bi-Hamiltonian system. The general formulation allows us to present various examples of bi-Hamiltonian systems, in both $1+1$ and $2+1$ dimensions.

The paper is organized as follows. In Sec. II, we shall choose perturbed systems of given bi-Hamiltonian systems as starting systems and introduce our triangular systems by using perturbations around solutions of starting systems, which contain many special triangular systems in Refs. 2–4. Then in Sec. III, a bi-Hamiltonian formulation for the resulting triangular systems will be proposed, based on the bi-Hamiltonian formulation of starting systems. In Sec. IV, we will go on to exhibit four examples of triangular systems through the general bi-Hamiltonian formulation, which also show that bi-Hamiltonian systems in both $1+1$ and $2+1$ dimensions are many and varied. Two of four examples give local $2+1$ dimensional bi-Hamiltonian systems and illustrate that multiscale perturbations can lead to higher-dimensional bi-Hamiltonian systems. Finally in Sec. V, some concluding remarks will be given.

II. TRIANGULAR SYSTEMS BY PERTURBATIONS

A. Bi-Hamiltonian systems

Assume that we have a bi-Hamiltonian system

$$u_t = K(u) = J\frac{\delta \tilde{H}_1}{\delta u} = M\frac{\delta \tilde{H}_0}{\delta u}, \quad \tilde{H}_0 = \int H_0\,\mathrm{d}x, \quad \tilde{H}_1 = \int H_1\,\mathrm{d}x, \tag{2.1}$$

where J and M constitute a Hamiltonian pair (see Refs. 7–9 for more information), t is a single variable but x can be a single or vector variable. If one operator of the Hamiltonian pair is invertible, we can have infinitely many symmetries $\{K_n\}_{n=0}^{\infty}$ and conserved functionals $\{\tilde{H}_n\}_{n=0}^{\infty}$, which can be explicitly computed through

$$\begin{cases} K_n = \Phi^{n-1}K(u) = (MJ^{-1})^{n-1}K(u), \quad n \geqslant 1, \\ \tilde{H} = \int H_n\,\mathrm{d}x, \quad H_n = \int_0^1 \langle u, (J^{-1}\Phi^{n-1}K)(\lambda u)\rangle \mathrm{d}\lambda, \quad n \geqslant 0, \end{cases} \tag{2.2}$$

where $\langle \cdot, \cdot \rangle$ denotes the standard inner product of the corresponding Euclidean space. Moreover, they are related through the bi-Hamiltonian formulation[10]

$$K_n = J\frac{\delta \tilde{H}_n}{\delta u} = M\frac{\delta \tilde{H}_{n-1}}{\delta u}, \quad n \geqslant 1. \tag{2.3}$$

Fuchssteiner and Fokas[11] discovered an important fact that when J and M constitute a Hamiltonian pair and J is invertible, the operator $\Phi = MJ^{-1}$ is hereditary,[12] i.e.,

$$\Phi'[\Phi X]Y - \Phi\Phi'[X]Y = \Phi'[\Phi Y]X - \Phi\Phi'[Y]X$$

holds for any vector fields X and Y, where $\Phi'[X]$ denotes the Gateaux derivative

$$\Phi'[X] = \frac{\partial}{\partial \epsilon}\bigg|_{\varepsilon=0} \Phi(u + \varepsilon X).$$

This condition is actually equivalent to an invariance of Lie derivative of Φ (see, e.g., Refs. 13 and 14). It is the hereditariness of Φ that gives rise to an explanation why soliton systems come in hierarchies.

B. Perturbed systems

Let us now choose a perturbed system with a perturbation parameter ε:

$$u_t = K^{\mathrm{per}}(u) := \sum_{j=0}^{m} \alpha_j \varepsilon^j K_{i_j}(u) = J\frac{\delta \tilde{H}_1^{\mathrm{per}}}{\delta u} = M\frac{\delta \tilde{H}_0^{\mathrm{per}}}{\delta u}, \tag{2.4}$$

where $m \geqslant 0$, the α_j are arbitrary constants, the i_j are arbitrary natural numbers [which means to take arbitrary vector fields $K_{i_j}(u)$ from $\{K_n\}_{n=1}^{\infty}$], and two Hamiltonian functionals read

$$\tilde{H}_0^{\mathrm{per}} = \int H_0^{\mathrm{per}}\,\mathrm{d}x, \quad H_0^{\mathrm{per}} = \sum_{j=0}^{m} \alpha_j \varepsilon^j H_{i_j}, \quad \tilde{H}_1^{\mathrm{per}} = \int H_1^{\mathrm{per}}\,\mathrm{d}x, \quad H_1^{\mathrm{per}} = \sum_{j=0}^{m} \alpha_j \varepsilon^j H_{i_j+1}. \tag{2.5}$$

This system (2.4) is called a starting system, which is nothing but a generalized system of the original bi-Hamiltonian system (2.1). Following the general scheme shown in (2.2), we have infinitely many symmetries and conserved functionals

$$\begin{cases} K_n^{\mathrm{per}} := \Phi^{n-1} K^{\mathrm{per}} = \sum_{j=0}^{m} \alpha_j \varepsilon^j K_{i_j+n-1}(u), \quad n \geqslant 1, \\ \tilde{H}_n^{\mathrm{per}} := \int H_n^{\mathrm{per}}\,\mathrm{d}x, \quad H_n^{\mathrm{per}} = \sum_{j=0}^{m} \alpha_j \varepsilon^j H_{i_j+n}(u), \quad n \geqslant 0, \end{cases} \tag{2.6}$$

for the starting system (2.4), since we can directly check that

$$K_n^{\mathrm{per}} = J\frac{\delta \tilde{H}_n^{\mathrm{per}}}{\delta u} = M\frac{\delta \tilde{H}_{n-1}^{\mathrm{per}}}{\delta u}, \quad n \geqslant 1.$$

C. Triangular systems

For any integers $N \geqslant 0$ and $r \geqslant 0$, take a perturbation series:

$$\hat{u}_N = \sum_{i=0}^{N} \varepsilon^i \eta_i, \quad \eta_i = \eta_i(y_0, y_1, y_2, \ldots, y_r, t), \tag{2.7}$$

where $y_i = \varepsilon^i x$, $0 \leqslant i \leqslant N$, are all slow variables. Now we make a perturbation around solutions of the starting system (2.4) and observe the Nth order perturbation system

$$\hat{u}_{Nt} = K^{\mathrm{per}}(\hat{u}_N) + \mathrm{o}(\varepsilon^N),$$

where u, η_i, $0 \leqslant i \leqslant N$ are supposed to be column vectors of the same dimension. By the Taylor expansion, this leads to an equivalent and bigger system

$$\eta_{it} = \frac{1}{i!}\frac{\partial^i}{\partial \varepsilon^i} K^{\mathrm{per}}(\hat{u}_N)\bigg|_{\varepsilon=0} = \sum_{j=0}^{\min(m,i)} \frac{\alpha_j}{(i-j)!}\frac{\partial^{i-j}}{\partial \varepsilon^{i-j}} K_{i_j}(\hat{u}_N)\bigg|_{\varepsilon=0}, \quad 0 \leqslant i \leqslant N. \tag{2.8}$$

For brevity, we rewrite it as a concise form

$$\hat{\eta}_{Nt} = (\mathrm{per}_N K^{\mathrm{per}})(\hat{\eta}_N) = ((\mathrm{per}_N K^{\mathrm{per}})_0^T, \ldots, (\mathrm{per}_N K^{\mathrm{per}})_N^T)^T, \quad \hat{\eta}_N = (\eta_0^T, \ldots, \eta_N^T)^T, \tag{2.9}$$

where T denotes the matrix transpose. Noting that

$$\hat{u}_N=\hat{u}_i+\varepsilon^{i+1}\sum_{j=0}^{N-i-1}\varepsilon^j\eta_{j+i+1},\quad \hat{u}_i=\sum_{j=0}^{i}\varepsilon^j\eta_j,\quad 0\leqslant i\leqslant N-1,$$

an application of the Taylor expansion tells us that

$$(\mathrm{per}_N K^{\mathrm{per}})_i=\frac{1}{i!}\frac{\partial^i}{\partial\varepsilon^i}K^{\mathrm{per}}(\hat{u}_N)\bigg|_{\varepsilon=0}=\frac{1}{i!}\frac{\partial^i}{\partial\varepsilon^i}K^{\mathrm{per}}(\hat{u}_i)\bigg|_{\varepsilon=0},\quad 0\leqslant i\leqslant N-1,$$

and thus the perturbation system (2.8) is triangular, i.e., the $(i+1)$th component $\eta_{it}=(\mathrm{per}_N K^{\mathrm{per}})_i$ just involves the first $i+1$ dependent variables $\eta_0,\ldots,\eta_i$ but no the other dependent variables $\eta_{i+1},\ldots,\eta_N$.

In our formulation, the superscript ''per'' denotes the perturbed objects such as the perturbed tensor fields and the perturbed functionals as in (2.4) and (2.5), but the prefix ''per_N'' means the perturbation resulting from the Nth order perturbation (2.7) of the dependent variable u. The small parameter ε is involved in both the starting system (2.4) and the perturbation series (2.7), but there is no relation among three integers m, N, and r that we need to take in the starting system (2.4) and the perturbation series (2.7). This demonstrates diversity to formulate our triangular systems. If we take a special choice of $\alpha_0=1$ and $K_{i_0}=K$ in our construction, the triangular system (2.8) becomes a coupling system of $u_t=K(u)$, because its first component is $\eta_{0t}=K(\eta_0)$. This paves a way for constructing integrable couplings of given integrable systems.[4,6] If a starting system is particularly chosen as

$$u_t=K^{\mathrm{per}}(u)=K(u)+\alpha\varepsilon K(u),\quad \alpha=\mathrm{const},\tag{2.10}$$

the following specific triangular system

$$\begin{cases}\eta_{0t}=K(\eta_0),\\ \eta_{1t}=K'(\eta_0)[\eta_1]+\alpha K(\eta_0),\end{cases}\tag{2.11}$$

will be engendered upon making a first-order perturbation. This system looks simple, but it generalizes the triangular system (1.2) resulting from the symmetry problem. The main objective of this paper is to propose a bi-Hamiltonian formulation for the triangular systems determined by (2.8), which contain two specific interesting triangular systems (1.2) and (2.11).

III. BI-HAMILTONIAN FORMULATION

For now on, we focus on the establishment of a bi-Hamiltonian formulation for the triangular systems determined by (2.8). We would actually like to show that a bi-Hamiltonian formulation of the resulting triangular systems can be inherited from an original bi-Hamiltonian system (2.1).

To the end, let us first introduce a new Hamiltonian pair:

$$(\mathrm{per}_N J)(\hat{\eta}_N)\equiv\hat{J}_N(\hat{\eta}_N),\quad (\mathrm{per}_N M)(\hat{\eta}_N)\equiv\hat{M}_N(\hat{\eta}_N),\tag{3.1}$$

which are defined as follows:

$$
\begin{aligned}
(\mathrm{per}_N P)(\hat{\eta}_N) \equiv \hat{P}_N(\hat{\eta}_N) &= [(\hat{P}_N(\hat{\eta}_N))_{ij}]_{(N+1)\times(N+1)} \\
&= \left[\frac{1}{(i+j-N)!} \quad \frac{\partial^{i+j-N} P(\hat{u}_N)}{\partial \varepsilon^{i+j-N}}\bigg|_{\varepsilon=0} \right]_{(N+1)\times(N+1)} \\
&= \begin{bmatrix} 0 & \cdots & 0 & P(\eta_0) \\ \vdots & \iddots & \vdots & \frac{1}{1!}\frac{\partial P(\hat{u}_N)}{\partial \varepsilon}\big|_{\varepsilon=0} \\ 0 & \vdots & \vdots & \vdots \\ P(\eta_0) & \frac{1}{1!}\frac{\partial P(\hat{u}_N)}{\partial \varepsilon}\big|_{\varepsilon=0} & \cdots & \frac{1}{N!}\frac{\partial^N P(\hat{u}_N)}{\partial \varepsilon^N}\big|_{\varepsilon=0} \end{bmatrix}, \quad P = J, M;
\end{aligned} \tag{3.2}
$$

and a new hereditary recursion operator defined by

$$
\begin{aligned}
(\mathrm{per}_N \Phi)(\hat{\eta}_N) \equiv \hat{\Phi}_N(\hat{\eta}_N) &= [(\hat{\Phi}_N(\hat{\eta}_N))_{ij}]_{(N+1)\times(N+1)} \\
&= \left[\frac{1}{(i-j)!} \frac{\partial^{i-j} \Phi(\hat{u}_N)}{\partial \varepsilon^{i-j}}\bigg|_{\varepsilon=0} \right]_{(N+1)\times(N+1)} \\
&= \begin{bmatrix} \Phi(\eta_0) & 0 & \cdots & 0 \\ \frac{1}{1!}\frac{\partial \Phi(\hat{u}_N)}{\partial \varepsilon}\big|_{\varepsilon=0} & \Phi(\eta_0) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \frac{1}{N!}\frac{\partial \Phi(\hat{u}_N)}{\partial \varepsilon}\big|_{\varepsilon=0} & \cdots & \frac{1}{1!}\frac{\partial \Phi(\hat{u}_N)}{\partial \varepsilon}\big|_{\varepsilon=0} & \Phi(\eta_0) \end{bmatrix},
\end{aligned} \tag{3.3}
$$

where $i,j=0,1,\ldots,N$, and $\hat{u}_N$ is defined by (2.7). These operators will be used to establish our new bi-Hamiltonian formulation for the triangular systems by (2.8). The structures of these operators originate from those proposed for single Hamiltonian formulations in Ref. 4. The only difference is the scale of perturbations. In our previous work,[4] single-scale perturbations were considered, but in this paper, multiscale perturbations will need to be considered. Like single-scale perturbations, multiscale perturbations also guarantee that two operators defined by (3.2) constitute a Hamiltonian pair and the operator defined by (3.3) is hereditary. The proofs are direct and very similar to those in the case of single-scale perturbations,[4] although they are rather laborious and much harder (see Ref. 6 for a detailed proof). Obviously, however, new operators still satisfy the following coupled condition:

$$
\hat{\Phi}_N = \hat{M}_N (\hat{J}_N)^{-1}, \quad \hat{J}_N \hat{\Psi}_N = \hat{\Phi}_N \hat{J}_N, \quad \hat{\Psi}_N = (\hat{\Phi}_N)^{\dagger}, \tag{3.4}
$$

where the superscript † means to take the adjoint operation. The existence of the inverse operator $(\hat{J}_N)^{-1}$ is guaranteed by the existence of J^{-1}, following the definition of $\hat{J}_N^{-1}$ as in (3.1) and (3.2). The coupled condition (3.4) ensures[1] that conserved functionals recursively determined by $\hat{\Phi}_N$ commute with each other under two Poisson brackets generated by $\hat{J}_N$ and $\hat{M}_N$.

For the triangular system defined by (2.8), new Hamiltonian functionals can be chosen as

$$
(\mathrm{per}_N \tilde{H}_0^{\mathrm{per}})(\hat{\eta}_N) := \frac{1}{N!} \frac{\partial^N}{\partial \varepsilon^N} \tilde{H}_0^{\mathrm{per}}(\hat{u}_N)\bigg|_{\varepsilon=0} = \sum_{j=0}^{\min(m,N)} \frac{\alpha_j}{(N-j)!} \frac{\partial^{N-j}}{\partial \varepsilon^{N-j}} \tilde{H}_{i_j}(\hat{u}_N)\bigg|_{\varepsilon=0}, \tag{3.5}
$$

$$(\mathrm{per}_N\tilde{H}_1^{\mathrm{per}})(\hat{\eta}_N) := \frac{1}{N!}\frac{\partial^N}{\partial\varepsilon^N}\tilde{H}_1^{\mathrm{per}}(\hat{u}_N)\Big|_{\varepsilon=0} = \sum_{j=0}^{\min(m,N)} \frac{\alpha_j}{(N-j)!}\frac{\partial^{N-j}}{\partial\varepsilon^{N-j}}\tilde{H}_{i_j+1}(\hat{u}_N)\Big|_{\varepsilon=0}, \quad (3.6)$$

where $\tilde{H}_0^{\mathrm{per}}$ and $\tilde{H}_1^{\mathrm{per}}$ are defined by (2.5), and $\hat{u}_N$ is defined by (2.7). They will offer the required Hamiltonian functionals in our bi-Hamiltonian formulation of the triangular system (2.8). The above-mentioned crucial form of the Hamiltonian functionals are motivated by a study of the perturbation system of the KdV equation.[16]

Now a direct computation can show that the triangular system (2.8) has the following bi-Hamiltonian formulation:

$$\hat{\eta}_{Nt} = \hat{J}_N\frac{\delta(\mathrm{per}_N\tilde{H}_1^{\mathrm{per}})}{\delta\hat{\eta}_N} = \hat{M}_N\frac{\delta(\mathrm{per}_N\tilde{H}_0^{\mathrm{per}})}{\delta\hat{\eta}_N}, \quad \hat{\eta}_N = (\eta_0^T, \eta_1^T, \ldots, \eta_N^T)^T. \quad (3.7)$$

Here a Hamiltonian pair of $\hat{J}_N$ and $\hat{M}_N$ is defined by (3.1) and (3.2), and two Hamiltonian functionals $\mathrm{per}_N\tilde{H}_0^{\mathrm{per}}$ and $\mathrm{per}_N\tilde{H}_1^{\mathrm{per}}$ are defined by (3.5) and (3.6). The bi-Hamiltonian formulation (3.7) is what we intend to establish for the triangular system (2.8). It follows that the triangular system (2.8) is a good example of integrable systems.

In fact, let us first introduce

$$\begin{cases} \mathrm{per}_N K_n^{\mathrm{per}} := \left((K_n^{\mathrm{per}}(\hat{u}_N))^T\Big|_{\varepsilon=0}, \frac{1}{1!}\frac{\partial}{\partial\varepsilon}(K_n^{\mathrm{per}}(\hat{u}_N))^T\Big|_{\varepsilon=0}, \ldots, \frac{1}{N!}\frac{\partial^N}{\partial\varepsilon^N}(K_n^{\mathrm{per}}(\hat{u}_N))^T\Big|_{\varepsilon=0}\right)^T, \quad n\geqslant 1, \\ \mathrm{per}_N\tilde{H}_n^{\mathrm{per}} := \frac{1}{N!}\frac{\partial^N}{\partial\varepsilon^N}\tilde{H}_n^{\mathrm{per}}(\hat{u}_N)\Big|_{\varepsilon=0}, \quad n\geqslant 0, \end{cases} \quad (3.8)$$

where K_n^{per} and $\tilde{H}_n^{\mathrm{per}}$ are defined by (2.6), and $\hat{u}_N$ is defined by (2.7). Then it can directly be verified that

$$\begin{cases} \mathrm{per}_N K_n^{\mathrm{per}} = (\hat{\Phi}_N)^{n-1}(\mathrm{per}_N K^{\mathrm{per}}), \quad n\geqslant 1, \\ \mathrm{per}_N\tilde{H}_n^{\mathrm{per}} = \sum_{j=0}^{\min(m,N)} \frac{\alpha_j}{(N-j)!}\frac{\partial^{N-j}}{\partial\varepsilon^{N-j}}\tilde{H}_{i_j+n}(\hat{u}_N)\Big|_{\varepsilon=0}, \quad n\geqslant 0, \end{cases}$$

and further

$$\mathrm{per}_N K_n^{\mathrm{per}} = \hat{J}_N\frac{\delta(\mathrm{per}_N\tilde{H}_n^{\mathrm{per}})}{\delta\hat{\eta}_N} = \hat{M}_N\frac{\delta(\mathrm{per}_N\tilde{H}_{n-1}^{\mathrm{per}})}{\delta\hat{\eta}_N}, \quad n\geqslant 1.$$

Therefore, it follows from the bi-Hamiltonian formulation (3.7) that $\mathrm{per}_N K_n^{\mathrm{per}}$, $n\geqslant 1$, and $\mathrm{per}_N(\tilde{H}_n^{\mathrm{per}}), n\geqslant 0$, defined by (3.8), are symmetries and conserved functionals of the triangular system (2.8), respectively. This implies that the triangular system (2.8) is integrable if we start from a bi-Hamiltonian system (2.1).

Summing up, the above-given manipulation shows how to inherit the bi-Hamiltonian formulation and to compute symmetries and conserved functionals for the triangular system (2.8) while taking perturbations for the starting system (2.4). In Sec. IV, we perform applications of the above-given formulation to four concrete examples, in which new bi-Hamiltonian systems in both $1+1$ dimensions and $2+1$ dimensions will be formulated.

IV. ILLUSTRATIVE EXAMPLES

Let us consider the KdV equation

$$u_t = K(u) = u_{xxx} + 6uu_x. \tag{4.1}$$

It is well known that it has a local bi-Hamiltonian formulation[1,10]

$$u_t = K(u) = J\frac{\delta \tilde{H}_1}{\delta u} = M\frac{\delta \tilde{H}_0}{\delta u}, \tag{4.2}$$

where the Hamiltonian pair and the Hamiltonian functionals are given by

$$J = \partial_x, \quad M = \partial_x^3 + 4u\partial_x + 2u_x, \quad \tilde{H}_0 = \int \frac{1}{2}u^2\,dx, \quad \tilde{H}_1 = \int \left(\frac{1}{2}uu_{xx} + u^3\right) dx. \tag{4.3}$$

Therefore, it has infinitely many symmetries and conserved functionals

$$K_n = \Phi^n u_x, \quad \tilde{H}_n = \int H_n\,dx, \quad H_n = \int_0^1 u(\Psi^n u)(\lambda u)\,d\lambda, \quad n \geqslant 0, \tag{4.4}$$

where the hereditary recursion operator Φ and its adjoint operator Ψ read as

$$\Phi(u) = MJ^{-1} = \partial_x^2 + 4u + 2u_x\partial_x^{-1}, \quad \Psi = \Phi^\dagger = \partial_x^2 + 4u - 2\partial_x^{-1}u_x, \tag{4.5}$$

where $\partial^{-1}\partial = \partial\partial^{-1} = 1$. For example, we can obtain

$$\begin{cases} K_2(u) = u_{5x} + 10uu_{xxx} + 20u_xu_{xx} + 30u^2u_x, \\ H_2(u) = \dfrac{1}{2}uu_{4x} + \dfrac{10}{3}u^2u_{xx} + \dfrac{5}{3}uu_x^2 + \dfrac{5}{2}u^4. \end{cases} \tag{4.6}$$

Note that in (4.4) we added $K_0 = u_x$ to the Abelian symmetry algebra $\{K_n\}_{n=1}^{\infty}$ as defined in (2.2).

If we choose the original KdV equation as a starting equation, taking single-scale perturbations leads to the standard perturbation KdV systems,[15] which were proved to be bi-Hamiltonian.[16] In what follows, we will formulate other examples of integrable couplings for the KdV equation, by choosing proper perturbed equations as starting equations and taking biscale perturbations in Sec. IV B. All examples also show that bi-Hamiltonian systems in both $1+1$ and $2+1$ dimensions are many and varied.

A. The case of single-scale perturbations

We take a special perturbed equation

$$u_t = K^{\mathrm{per}}(u) = K_1(u) + \varepsilon K_1(u) = J\frac{\delta \tilde{H}_1^{\mathrm{per}}}{\delta u} = M\frac{\delta \tilde{H}_0^{\mathrm{per}}}{\delta u} \tag{4.7}$$

with two Hamiltonian functionals

$$\tilde{H}_0^{\mathrm{per}} = \tilde{H}_0 + \varepsilon\tilde{H}_0, \quad \tilde{H}_1^{\mathrm{per}} = \tilde{H}_1 + \varepsilon\tilde{H}_1 \tag{4.8}$$

as a starting equation. Here $K_1 = K, J, M, \tilde{H}_0, \tilde{H}_1$ are given by (4.3), (4.4), and (4.5). The first-order perturbation

$$\hat{u}_1 = \eta_0 + \varepsilon\,\eta_1$$

yields the following triangular system:

$$\begin{cases} \eta_{0t}=K_1(\eta_0)=\eta_{0xxx}+6\,\eta_0\eta_{0x}, \\ \eta_{1t}=K_1'(\eta_0)[\eta_1]+K_1(\eta_1)=\eta_{1xxx}+6(\eta_0\eta_1)_x+\eta_{0xxx}+6\,\eta_0\eta_{0x}. \end{cases} \tag{4.9}$$

According to our scheme of construction in Sec. III, its Hamiltonian pair and corresponding hereditary recursion operator are

$$\hat{J}_1=\begin{bmatrix} 0 & \partial_x \\ \partial_x & 0 \end{bmatrix}, \quad \hat{M}_1=\begin{bmatrix} 0 & M_0 \\ M_0 & M_1 \end{bmatrix}, \quad \hat{\Phi}_1=\begin{bmatrix} \Phi_0 & 0 \\ \Phi_1 & \Phi_0 \end{bmatrix}, \tag{4.10}$$

with the entries of $\hat{M}_1$ and $\hat{\Phi}_1$ being defined by

$$M_i=\delta_{i0}\partial_x^3+4\,\eta_0\partial_x+2\,\eta_{0x}, \quad \Phi_i=\delta_{i0}\partial_x^2+4\,\eta_i+2\,\eta_{ix}\partial_x^{-1}, \quad i=0,1, \tag{4.11}$$

where δ_{0i} is the Kronecker symbol. The triangular system (4.9) has a local bi-Hamiltonian formulation:

$$\hat{\eta}_{1t}=\hat{J}_1\frac{\delta(\mathrm{per}_1\tilde{H}_1^{\mathrm{per}})}{\delta\hat{\eta}_1}=\hat{M}_1\frac{\delta(\mathrm{per}_1\tilde{H}_0^{\mathrm{per}})}{\delta\hat{\eta}_1}, \quad \hat{\eta}_1=(\eta_0,\eta_1)^T, \tag{4.12}$$

with two Hamiltonian functionals

$$\begin{cases} \mathrm{per}_1\tilde{H}_0^{\mathrm{per}}=(\mathrm{per}_1\tilde{H}_0^{\mathrm{per}})(\hat{\eta}_1)=\dfrac{\partial\tilde{H}_0(\hat{u}_1)}{\partial\varepsilon}\Big|_{\varepsilon=0}+\tilde{H}_0(\eta_0) \\ \qquad\qquad =\displaystyle\int\left(\eta_0\eta_1+\frac{1}{2}\eta_0^2\right)\mathrm{d}x, \\ \mathrm{per}_1\tilde{H}_1^{\mathrm{per}}=(\mathrm{per}_1\tilde{H}_1^{\mathrm{per}})(\hat{\eta}_1)=\dfrac{\partial\tilde{H}_1(\hat{u}_1)}{\partial\varepsilon}\Big|_{\varepsilon=0}+\tilde{H}_1(\eta_0) \\ \qquad\qquad =\displaystyle\int\left(\frac{1}{2}\eta_{0xx}\eta_1+\frac{1}{2}\eta_0\eta_{1xx}+3\,\eta_0^2\eta_1+\frac{1}{2}\eta_0\eta_{0xx}+\eta_0^3\right)\mathrm{d}x. \end{cases} \tag{4.13}$$

Noting that in this example, we have

$$K_n^{\mathrm{per}}=K_n+\varepsilon K_n, \quad \tilde{H}_n^{\mathrm{per}}=\tilde{H}_n+\varepsilon\tilde{H}_n, \quad n\geqslant 0,$$

infinitely many symmetries and conserved functionals of the triangular system (4.9) are computed as follows:

$$\begin{cases} \mathrm{per}_1(K_n^{\mathrm{per}})=\begin{bmatrix} K_n(\eta_0) \\ \dfrac{\partial K_n(\hat{u}_1)}{\partial\varepsilon}\Big|_{\varepsilon=0}+K_n(\eta_0) \end{bmatrix}, \quad n\geqslant 0, \\ \mathrm{per}_1(\tilde{H}_n^{\mathrm{per}})=\dfrac{\partial\tilde{H}_n(\hat{u}_1)}{\partial\varepsilon}\Big|_{\varepsilon=0}+\tilde{H}_n(\eta_0), \quad n\geqslant 0. \end{cases} \tag{4.14}$$

Second, we take another special perturbed equation

$$u_t=K^{\mathrm{per}}(u)=K_1(u)+\varepsilon K_2(u), \tag{4.15}$$

as a starting equation, which can be written as a bi-Hamiltonian system

$$u_t = K^{\mathrm{per}}(u) = J\frac{\delta \tilde{H}_1^{\mathrm{per}}}{\delta u} = M\frac{\delta \tilde{H}_0^{\mathrm{per}}}{\delta u}, \quad \tilde{H}_0^{\mathrm{per}} = \tilde{H}_0 + \varepsilon \tilde{H}_1, \quad \tilde{H}_1^{\mathrm{per}} = \tilde{H}_1 + \varepsilon \tilde{H}_2. \tag{4.16}$$

Here $K_1 = K$, J, M, $\tilde{H}_0$, $\tilde{H}_1$, $\tilde{H}_2$, K_2, are determined by (4.1), (4.3), and (4.6). The second-order perturbation yields the following triangular system:

$$\begin{cases} \eta_{0t} = \eta_{0xxx} + 6\eta_0\eta_{0x}, \\ \eta_{1t} = \eta_{1xxx} + 6(\eta_0\eta_1)_x + K_2(\eta_0), \\ \eta_{2t} = \eta_{2xxx} + 6(\eta_0\eta_2)_x + 6\eta_1\eta_{1x} + \left.\dfrac{\partial K_2(\hat{u}_2)}{\partial \varepsilon}\right|_{\varepsilon=0}, \end{cases} \tag{4.17}$$

where

$$\begin{aligned} \left.\frac{\partial K_2(\hat{u}_2)}{\partial \varepsilon}\right|_{\varepsilon=0} &= \eta_{1,5x} + 10\eta_1\eta_{0xxx} + 10\eta_0\eta_{1xxx} + 20\eta_{1x}\eta_{0xx} \\ &\quad + 20\eta_{0x}\eta_{1xx} + 60\eta_0\eta_{0x}\eta_1 + 30\eta_0^2\eta_{1x}. \end{aligned} \tag{4.18}$$

The corresponding Hamiltonian pair and hereditary recursion operator are

$$\hat{J}_2 = \begin{bmatrix} 0 & 0 & \partial_x \\ 0 & \partial_x & 0 \\ \partial_x & 0 & 0 \end{bmatrix}, \quad \hat{M}_2 = \begin{bmatrix} 0 & 0 & M_0 \\ 0 & M_0 & M_1 \\ M_0 & M_1 & M_2 \end{bmatrix}, \quad \hat{\Phi}_2 = \begin{bmatrix} \Phi_0 & 0 & 0 \\ \Phi_1 & \Phi_0 & 0 \\ \Phi_2 & \Phi_1 & \Phi_0 \end{bmatrix}, \tag{4.19}$$

where the entries of $\hat{M}_2$ and $\hat{\Phi}_2$ are given by

$$M_i = \delta_{i0}\partial_x^3 + 4\eta_0\partial_x + 2\eta_{0x}, \quad \Phi_i = \delta_{i0}\partial_x^2 + 4\eta_i + 2\eta_{ix}\partial_x^{-1}, \quad 0 \leqslant i \leqslant 2. \tag{4.20}$$

Through our scheme of construction in Sec. III, the triangular system (4.17) has a local bi-Hamiltonian formulation

$$\hat{\eta}_{2t} = \hat{J}_2\frac{\delta(\mathrm{per}_2\tilde{H}_1^{\mathrm{per}})}{\delta\hat{\eta}_2} = \hat{M}_2\frac{\delta(\mathrm{per}_2\tilde{H}_0^{\mathrm{per}})}{\delta\hat{\eta}_2}, \quad \hat{\eta}_2 = (\eta_0, \eta_1, \eta_2)^T, \tag{4.21}$$

with two Hamiltonian functionals

$$\begin{cases} \mathrm{per}_2\tilde{H}_0^{\mathrm{per}} = (\mathrm{per}_2\tilde{H}_0^{\mathrm{per}})(\hat{\eta}_2) = \dfrac{1}{2}\left.\dfrac{\partial^2\tilde{H}_0(\hat{u}_2)}{\partial\varepsilon^2}\right|_{\varepsilon=0} + \left.\dfrac{\partial\tilde{H}_1(\hat{u}_2)}{\partial\varepsilon}\right|_{\varepsilon=0} \\ \qquad = \displaystyle\int\left(\frac{1}{2}\eta_1^2 + \eta_0\eta_2 + \frac{1}{2}\eta_{0xx}\eta_1 + \frac{1}{2}\eta_0\eta_{1xx} + 3\eta_0^2\eta_1\right)\mathrm{d}x, \\ \mathrm{per}_2\tilde{H}_1^{\mathrm{per}} = (\mathrm{per}_2\tilde{H}_1^{\mathrm{per}})(\hat{\eta}_2) = \dfrac{1}{2}\left.\dfrac{\partial^2\tilde{H}_1(\hat{u}_2)}{\partial\varepsilon^2}\right|_{\varepsilon=0} + \left.\dfrac{\partial\tilde{H}_2(\hat{u}_2)}{\partial\varepsilon}\right|_{\varepsilon=0} \\ \qquad = \displaystyle\int\left(\frac{1}{2}\eta_{0xx}\eta_2 + \frac{1}{2}\eta_1\eta_{1xx} + \frac{1}{2}\eta_0\eta_{2xx} + 3\eta_0\eta_1^2 + 3\eta_0^2\eta_2\right)\mathrm{d}x \\ \qquad\quad + \left.\dfrac{\partial\tilde{H}_2(\hat{u}_2)}{\partial\varepsilon}\right|_{\varepsilon=0}, \end{cases} \tag{4.22}$$

where

$$\left.\frac{\partial \tilde{H}_2(\hat{u}_2)}{\partial \varepsilon}\right|_{\varepsilon=0} = \int \left(\frac{1}{2}\eta_{0,4x}\eta_1 + \frac{1}{2}\eta_0\eta_{1,4x} + \frac{5}{3}\eta_{0x}^2\eta_1 + \frac{10}{3}\eta_0\eta_{0x}\eta_{1x} + \frac{20}{3}\eta_0\eta_{0xx}\eta_1 + \frac{10}{3}\eta_0^2\eta_{1x} + 10\eta_0^3\eta_1 \right) \mathrm{d}x. \tag{4.23}$$

Its infinitely many symmetries and conserved functionals read as

$$\begin{cases} \mathrm{per}_2(K_n^{\mathrm{per}}) = \begin{bmatrix} K_n(\eta_0) \\ \left.\dfrac{\partial K_n(\hat{u}_2)}{\partial \varepsilon}\right|_{\varepsilon=0} + K_{n+1}(\eta_0) \\ \left.\dfrac{1}{2}\dfrac{\partial^2 K_n(\hat{u}_2)}{\partial \varepsilon^2}\right|_{\varepsilon=0} + \left.\dfrac{\partial K_{n+1}(\hat{u}_2)}{\partial \varepsilon}\right|_{\varepsilon=0} \end{bmatrix}, \quad n \geqslant 0, \\ \mathrm{per}_2\tilde{H}_n^{\mathrm{per}} = \left.\dfrac{1}{2}\dfrac{\partial^2 \tilde{H}_n(\hat{u}_2)}{\partial \varepsilon^2}\right|_{\varepsilon=0} + \left.\dfrac{\partial \tilde{H}_{n+1}(\hat{u}_2)}{\partial \varepsilon}\right|_{\varepsilon=0}, \quad n \geqslant 0, \end{cases} \tag{4.24}$$

by using $K_n^{\mathrm{per}} = K_n + \varepsilon K_{n+1}$ and $\tilde{H}_n^{\mathrm{per}} = \tilde{H}_n + \varepsilon \tilde{H}_{n+1}$ in this example.

B. The case of biscale perturbations

We would like to exhibit two examples in the case of biscale perturbations and show that multiscale perturbations can lead to bi-Hamiltonian systems in higher spatial dimensions. A concrete example in $2+1$ dimensions for the KdV equation is the following triangular system:

$$\begin{cases} \eta_{0t_1} = \eta_{0xxx} + 6\eta_0\eta_{0x}, \\ \eta_{1t_1} = \eta_{1xxx} + 3\eta_{0xxy} + 6(\eta_0\eta_1)_x + 6\eta_0\eta_{0y}, \end{cases} \tag{4.25}$$

resulting from the KdV equation (4.1) by a first-order biscale perturbation

$$\hat{u}_1 = \eta_0(t,x,y) + \varepsilon\eta_1(t,x,y), \quad y = \varepsilon x. \tag{4.26}$$

This system was furnished in Ref. 16, and based on our scheme of construction in Sec. III, it has the following local bi-Hamiltonian formulation:

$$\hat{\eta}_{1t} = \hat{J}_1 \frac{\delta(\mathrm{per}_1\tilde{H}_1)}{\delta\hat{\eta}_1} = \hat{M}_1 \frac{\delta(\mathrm{per}_1\tilde{H}_0)}{\delta\hat{\eta}_1}, \quad \hat{\eta}_1 = (\eta_0, \eta_1)^T, \tag{4.27}$$

where the Hamiltonian pair reads as

$$\hat{J}_1 = \begin{bmatrix} 0 & \partial_x \\ \partial_x & \partial_y \end{bmatrix}, \quad \hat{M}_1 = \begin{bmatrix} 0 & \partial_x^3 + 2\eta_{0x} + 4\eta_0\partial_x \\ \partial_x^3 + 2\eta_{0x} + 4\eta_0\partial_x & Q \end{bmatrix}, \tag{4.28}$$

with Q being defined by

$$Q = \left.\frac{\partial}{\partial\varepsilon}M(\hat{u}_1)\right|_{\varepsilon=0} = 3\partial_x^2\partial_y + 2\eta_{1x} + 2\eta_{0y} + 4\eta_1\partial_x + 4\eta_0\partial_y, \tag{4.29}$$

and the Hamiltonian functionals are

$$\begin{cases} \mathrm{per}_1 \tilde{H}_0 = \dfrac{\partial}{\partial \varepsilon} \tilde{H}_0(\hat{u}_1)\Big|_{\varepsilon=0} = \int \int \eta_0 \eta_1 \, \mathrm{d}x \, \mathrm{d}y, \\ \mathrm{per}_1 \tilde{H}_1 = \dfrac{\partial}{\partial \varepsilon} \tilde{H}_1(\hat{u}_1)\Big|_{\varepsilon=0} = \int \int \left(\dfrac{1}{2} \eta_0 \eta_{1xx} + \eta_0 \eta_{0xy} + \dfrac{1}{2} \eta_1 \eta_{0xx} + 3 \eta_0^3 \eta_1 \right) \mathrm{d}x \, \mathrm{d}y. \end{cases} \tag{4.30}$$

Moreover, the above-given Hamiltonian pair yields a hereditary recursion operator in $2+1$ dimensions

$$\hat{\Phi}_1 = \begin{bmatrix} \partial_x^2 + 2\eta_{0x}\partial_x^{-1} + 4\eta_0 & 0 \\ 2\partial_x\partial_y - 2\eta_{0x}\partial_x^{-2}\partial_y + 2(\eta_{1x} + \eta_{0y})\partial_x^{-1} + 4\eta_1 & \partial_x^2 + 2\eta_{0x}\partial_x^{-1} + 4\eta_0 \end{bmatrix}, \tag{4.31}$$

for the triangular system (4.25).

The second example is the following:

$$\begin{cases} \eta_{0t_1} = K_1(\eta_0) = \eta_{0xxx} + 6\eta_0\eta_{0x}, \\ \eta_{1t_1} = \dfrac{\partial K_1(\hat{u}_2)}{\partial \varepsilon}\Big|_{\varepsilon=0} + K_1(\eta_0) \\ \quad = \eta_{1xxx} + 3\eta_{0xxy} + 6(\eta_0\eta_1)_x + 6\eta_0\eta_{0y} + \eta_{0xxx} + 6\eta_0\eta_{0x}, \\ \eta_{2t_1} = \dfrac{1}{2!}\dfrac{\partial^2 K_1(\hat{u}_2)}{\partial \varepsilon^2}\Big|_{\varepsilon=0} + \dfrac{\partial K_1(\hat{u}_2)}{\partial \varepsilon}\Big|_{\varepsilon=0} \\ \quad = \eta_{2xxx} + 3\eta_{1xxy} + 3\eta_{0xyy} + 6(\eta_0\eta_2)_x + 6\eta_1\eta_{1x} + 6(\eta_0\eta_1)_y \\ \qquad + \eta_{1xxx} + 3\eta_{0xxy} + 6(\eta_0\eta_1)_x + 6\eta_0\eta_{0y}, \end{cases} \tag{4.32}$$

which can be generated from a perturbed KdV equation (4.7) under the second-order biscale perturbation

$$\hat{u}_2 = \eta(t,x,y) + \varepsilon\eta_1(t,x,y) + \varepsilon\eta_2(t,x,y), \quad y = \varepsilon x. \tag{4.33}$$

According to our scheme of construction in Sec. III, the corresponding Hamiltonian pair and recursion operator read as

$$\hat{J}_2 = \begin{bmatrix} 0 & 0 & \partial_x \\ 0 & \partial_x & \partial_y \\ \partial_x & \partial_y & 0 \end{bmatrix}, \quad \hat{M}_2 = \begin{bmatrix} 0 & 0 & M_0 \\ 0 & M_0 & M_1 \\ M_0 & M_1 & M_2 \end{bmatrix}, \quad \hat{\Phi}_2 = \begin{bmatrix} \Phi_0 & 0 & 0 \\ \Phi_1 & \Phi_0 & 0 \\ \Phi_2 & \Phi_1 & \Phi_0 \end{bmatrix}, \tag{4.34}$$

where the entries of $\hat{M}_2$ are defined by

$$\begin{cases} M_0 = M(\hat{u}_2)|_{\varepsilon=0} = \partial_x^3 + 2\eta_{0x} + 4\eta_0\partial_x, \\ M_1 = \dfrac{1}{1!}\dfrac{\partial M(\hat{u}_2)}{\partial \varepsilon}\Big|_{\varepsilon=0} = 3\partial_x^2\partial_y + 2\eta_{1x} + 2\eta_{0y} + 4\eta_1\partial_x + 4\eta_0\partial_y, \\ M_2 = \dfrac{1}{2!}\dfrac{\partial^2 M(\hat{u}_2)}{\partial \varepsilon^2}\Big|_{\varepsilon=0} = 3\partial_x\partial_y^2 + 2\eta_{2x} + 2\eta_{1y} + 4\eta_2\partial_x + 4\eta_1\partial_y, \end{cases} \tag{4.35}$$

and the entries of $\hat{\Phi}_2$ by

$$\begin{cases} \Phi_0=\Phi(\hat{u}_2)|_{\varepsilon=0}=\partial_x^2+2\,\eta_{0x}\partial_x^{-1}+4\,\eta_0, \\ \Phi_1=\dfrac{1}{1!}\dfrac{\partial\Phi(\hat{u}_2)}{\partial\varepsilon}\bigg|_{\varepsilon=0}=2\,\partial_x\partial_y+2(\eta_{1x}+\eta_{0y})\partial_x^{-1}-2\,\eta_{0x}\partial_x^{-2}\partial_y+4\,\eta_1, \\ \Phi_2=\dfrac{1}{2!}\dfrac{\partial^2\Phi(\hat{u}_2)}{\partial\varepsilon^2}\bigg|_{\varepsilon=0}=\partial_y^2+2(\eta_{2x}+\eta_{1y})\partial_x^{-1}-2(\eta_{1x}+\eta_{0y})\partial_x^{-2}\partial_y+2\,\eta_{0x}\partial_x^{-3}\partial_y^2+4\,\eta_2. \end{cases} \tag{4.36}$$

The $2+1$ triangular system (4.32) has a local bi-Hamiltonian formulation

$$\hat{\eta}_{2t}=\hat{J}_2\frac{\delta(\mathrm{per}_2\widetilde{H}_1)}{\delta\hat{\eta}_2}=\hat{M}_2\frac{\delta(\mathrm{per}_2\widetilde{H}_0)}{\delta\hat{\eta}_2}, \quad \hat{\eta}_2=(\eta_0,\eta_1,\eta_2)^T, \tag{4.37}$$

with a Hamiltonian pair $\hat{J}_2$ and $\hat{M}_2$ being defined by (4.34), and two Hamiltonian functionals by

$$\begin{cases} \mathrm{per}_2\widetilde{H}_0^{\mathrm{per}}=\dfrac{1}{2!}\dfrac{\partial^2\widetilde{H}_0^{\mathrm{per}}}{\partial\varepsilon^2}\bigg|_{\varepsilon=0}=\dfrac{1}{2!}\dfrac{\partial^2\widetilde{H}_0}{\partial\varepsilon^2}\bigg|_{\varepsilon=0}+\dfrac{\partial\widetilde{H}_0}{\partial\varepsilon}\bigg|_{\varepsilon=0}=\int\int\left(\frac{1}{2}\eta_0\eta_2+\frac{1}{4}\eta_1^2+\eta_0\eta_1\right)\mathrm{d}x\,\mathrm{d}y, \\ \mathrm{per}_2\widetilde{H}_1^{\mathrm{per}}=\dfrac{1}{2!}\dfrac{\partial^2\widetilde{H}_1^{\mathrm{per}}}{\partial\varepsilon^2}\bigg|_{\varepsilon=0}=\dfrac{1}{2!}\dfrac{\partial^2\widetilde{H}_1}{\partial\varepsilon^2}\bigg|_{\varepsilon=0}+\dfrac{\partial\widetilde{H}_1}{\partial\varepsilon}\bigg|_{\varepsilon=0} \\ \qquad=\int\int\left[\frac{1}{4}(\eta_0\eta_{2xx}+\eta_1\eta_{1xx}+\eta_2\eta_{0xx}+2\,\eta_0\eta_{1xx}+2\,\eta_1\eta_{0xx})\right. \\ \qquad\left.+\frac{1}{2}(\eta_0\eta_{1xy}+\eta_1\eta_{0xy}+2\,\eta_0\eta_{0xy})+\frac{1}{4}\eta_0\eta_{0yy}+3(\eta_0\eta_1^2+\eta_0^2\eta_1+\eta_0^2\eta_2)\right]\mathrm{d}x\,\mathrm{d}y. \end{cases} \tag{4.38}$$

Both $2+1$ dimensional triangular systems above have infinitely many symmetries and conserved functionals due to the existence of hereditary recursion operators, and thus they are also integrable in the sense of the existence of the Abelian symmetry algebra.[17] Note that under the biscale perturbation

$$\hat{u}_N=\sum_{i=0}^{N}\varepsilon^i\eta_i(t,x,y), \quad y=\varepsilon x,$$

we have, for example,

$$\partial_x\to\partial_x+\varepsilon\partial_y, \quad \hat{u}_{Nx}\to\sum_{i=0}^{N}\varepsilon^i(\eta_{ix}+\varepsilon\eta_{iy}), \quad \hat{u}_{Nxx}\to\sum_{i=0}^{N}\varepsilon^i(\eta_{ixx}+2\varepsilon\eta_{ixy}+\varepsilon^2\eta_{iyy}).$$

These equalities have been used in the above-mentioned deduction of bi-Hamiltonian systems in $2+1$ dimensions.

V. CONCLUDING REMARKS

We have proposed a bi-Hamiltonian formulation (3.7) for the triangular systems (2.8) resulting from perturbations around solutions of the perturbed systems. The symmetry problem can lead to a special case (1.2) of our triangular systems (2.8), which is generated by the first-order perturbation. However, the perturbation system (1.2) is a little more general than the symmetry problem itself. It is because the second component system of the perturbation system (1.2) needs to hold only for a solution of the original system $u_t=K(u)$, but the same system in the symmetry problem needs to hold for all solutions of $u_t=K(u)$. The resulting formulation gives a way to construct various integrable couplings in both lower dimensions and higher dimensions for bi-

Hamiltonian systems, all of which at least possess infinitely many commuting symmetries and conserved functionals. Four illustrative examples were given for the KdV equation, which contain two $2+1$ dimensional local bi-Hamiltonian systems (4.27) and (4.37).

The triangular system (4.25) was first introduced in Ref. 16, whose Painlevé property and zero curvature representation were discussed by Sakovich.[18] General triangular systems resulting from multiscale perturbations also can possess rich structures of zero curvature representations. If multiscale perturbations are taken into account, the involved spectral parameters, denoted by μ_i, $0 \leqslant i \leqslant N$, may vary with respect to the spatial variables,[18,6] although they need to satisfy some conditions, for example,

$$\mu_{0x}=0, \quad \mu_{ix}+\mu_{i-1,y}=0, \quad 1 \leqslant i \leqslant N,$$

in the case of biscale perturbations

$$\hat{u}_N=\sum_{i=0}^{N} \varepsilon^i \eta_i(x,y,t)=\sum_{i=0}^{N} \varepsilon^i \eta_i(x,\varepsilon x,t).$$

More interestingly, our $2+1$ dimensional bi-Hamiltonian systems (4.27) and (4.37) are local and possess hereditary recursion operators, and thus they enjoy a different feature from known scalar integrable equations in $2+1$ dimensions. To our best knowledge, (4.27) and (4.37) are the first two examples of local $2+1$ dimensional bi-Hamiltonian systems with hereditary recursion operators. They also can provide useful information for classifying integrable systems in $2+1$ dimensions by the symmetry approach.[19]

We remark that our general bi-Hamiltonian formulation in Sec. III can be used to establish bi-Hamiltonian formulations for a hierarchy of coupled KdV systems introduced in Ref. 20, although it does not work for the other two hierarchies of coupled KdV systems furnished in Refs. 21, 22 and 23. Moreover, our triangular systems, especially (2.11), starting from the KdV equation, provide examples of bi-Hamiltonian systems among the integrable coupled KdV systems described by Gürses and Karasu,[24] and general triangular systems can provide new bi-Hamiltonian systems of other types, e.g., bi-Hamiltonian systems of coupled fifth KdV equations and coupled modified KdV equations. Nonlinearization resulting from symmetry constraints also can be manipulated for linking our triangular systems to finite-dimensional integrable Hamiltonian systems.[25]

We finally point out that our general scheme requires a bi-Hamiltonian structure of the starting system. Nevertheless, we can still make the perturbation to get triangular systems from non-Hamiltonian systems such as the KP hierarchy, and study integrable properties for the resulting triangular systems.

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Group invariant classification of separable Hamiltonian systems in the Euclidean plane and the $O(4)$-symmetric Yang–Mills theories of Yatsun

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We present a new and effective method of determining separable coordinate systems for natural Hamiltonians with two degrees of freedom in flat Riemannian space. The method is based on intrinsic properties of the associated Killing tensors and their invariants under the group of rigid motions $E(2)$. Applications to the Hamiltonian systems derived by the late V. A. Yatsun from $O(4)$-symmetric Yang–Mills theories are presented. In addition, an equivalence between separability of two-dimensional Hamiltonian systems and the existence of Pfaffian quasi-bi-Hamiltonian representations is specified. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The aim of this paper is twofold. First, we present a comprehensive and tractable method of classifying orthogonally separable Hamiltonian systems with two degrees of freedom in terms of intrinsic properties of the associated Killing tensors. This leads to a direct algorithm for determining the transformation to separable coordinates which in practice is *completely algebraic*, and hence can be easily implemented in a symbolic computer algebra system. Our second goal is to use the above-mentioned algorithm to solve explicitly the two integrable Hamiltonian systems derived by the late Yatsun[1–5] from $O(4)$-symmetric Yang–Mills theories. Notably, to the best of our knowledge, these two integrable cases (referred throughout this paper as YIC1 and YIC2, respectively) have not been integrated before by quadratures in the most general case.

We consider a general Hamiltonian system defined by a Hamiltonian (total energy) function in the following general form:

$$H(\mathbf{q},\mathbf{p})=\tfrac{1}{2}g^{ij}(\mathbf{q})p_ip_j+V(\mathbf{q}),\quad i,j=1,2, \tag{1}$$

where g^{ij} denote the components of the contravariant metric tensor $\mathbf{g}$ on a pseudo-Riemannian two-dimensional base manifold $\hat{M}$, V is a scalar potential field on $\hat{M}$, and $\mathbf{q}=(q^1,q^2)$ denote local (position) coordinates, while $\mathbf{p}=(p_1,p_2)$ are the corresponding conjugate (momenta) coordinates. This means that the corresponding Hamiltonian vector field $\mathbf{X_H}$ is determined by the equation

$$\mathbf{X_H}=[\mathbf{P_0},H], \tag{2}$$

where $\mathbf{P_0}=\Sigma_{i=1}^{n}\,\partial/\partial q^i\wedge\partial/\partial p_i$ is the standard canonical Poisson bi-vector. Here in the following, unless otherwise indicated, $[\,,\,]$ denotes the Schouten bracket,[6] which generalizes the usual Lie

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bracket of vector fields. In terms of the components X_H^i of the Hamiltonian vector field $\mathbf{X_H}$, formula (2) means that $X_H^i = P_0^{ij}(\partial H/\partial x^j)$, where $\mathbf{x}=(x^1,\ldots,x^4)$ are local coordinates on the cotangent bundle $T\hat{M}$.

The problem of solving the Hamiltonian system defined by (1) by the method of separation of variables can be traced back to Bertrand,[7] who considered the situation when a Hamiltonian system admits an additional integral of motion, yet the external forces acting on the system are unknown. This problem was later resurrected in the study of Hamiltonian systems with two degrees of freedom admitting an additional integral of motion. The fundamental result, commonly known as the *Bertrand–Darboux theorem* (see Ref. 8 and the relevant references therein), is the following: If a Hamiltonian system defined by (1) admits an additional first integral quadratic in the momenta which is functionally independent of H, then there exists a system of coordinates (u,v) with respect to which the Hamiltonian (1) takes the *Liouville form* (see the following). The latter result immediately entails separability of the Hamiltonian system defined by (1) in the framework of the Hamilton–Jacobi theory. This method is still widely used. We note, however, that its main drawback is in having to solve every time a second-order partial differential equation (PDE) for a given V of (1) by the method of characteristics (first used by Darboux in this context[8]), thus transforming V to the form (10) in separable coordinates (u,v). This fact indicates that this analytical technique is not tensorial.

Another approach to this problem was initiated by Eisenhart[9] for the n-dimensional geodesic case and recently generalized by Benenti (Ref. 10, see also references therein) for a general Hamiltonian system with n degrees of freedom defined by a Hamiltonian with potential. As before, the problem of finding a solution to the system of ordinary differential equations corresponding to a general Hamiltonian vector field (2) defined by (1) can be related via Jacobi's theorem to the problem of finding an orthogonally separable complete integral W of the corresponding Hamilton–Jacobi equation

$$\tfrac{1}{2} g^{ij}(\mathbf{q})\partial_i W \partial_j W + V(\mathbf{q}) = E, \tag{3}$$

under the standard separation ansatz:

$$W(\mathbf{q};\mathbf{c}) = W_1(q^1;\mathbf{c}) + W_2(q^2;\mathbf{c}), \tag{4}$$

where $\mathbf{c}=(c_1,c_2)$ is an integration constant. This is possible iff H admits a second first integral F quadratic in momenta:

$$F = K^{ij}(\mathbf{q})p_i p_j + U(\mathbf{q}), \quad i,j=1,2. \tag{5}$$

Here the emphasis is on the quantity $\mathbf{K}$ of (5) rather than the potential V of (1) as is the case in the Bertrand–Darboux theorem. Recall that $\mathbf{K}$ is a symmetric *tensor* with pointwise simple and real eigenvalues satisfying the *Killing tensor equation*:

$$[\mathbf{g},\mathbf{K}] = 0, \tag{6}$$

which in component form may be written as

$$[\mathbf{g},\mathbf{K}]^{ijk} = g^{(ij}{}_{,l}K^{k)l} - K^{(ij}{}_{,l}g^{k)l} = 0. \tag{7}$$

A solution $\mathbf{K}$ of (6) is called a *Killing tensor*. The quantity U in (5) is defined by

$$\mathrm{d}U = \hat{\mathbf{K}}\,\mathrm{d}V, \tag{8}$$

where the (1,1) tensor $\hat{\mathbf{K}}$ is defined by $\hat{\mathbf{K}} := \mathbf{Kg}$, or in terms of its components $\hat{K}_i{}^j := K_{il}g^{lj}$. We note that the integrability condition for (8) gives rise to the *compatibility condition*:

$$\mathrm{d}(\hat{\mathbf{K}}\,\mathrm{d}V) = 0. \tag{9}$$

The Hamiltonian system defined by (1) is Liouville-integrable in this case. Furthermore, it is worth noting that the involutiveness of H and F, namely

$$0=\{H,F\}=P_0^{ij}\frac{\partial H}{\partial x^i}\frac{\partial F}{\partial x^j},$$

is equivalent to (6) and (8). In what follows we use intrinsic properties of the associated Killing tensor $\mathbf{K}$ to recover canonical separable coordinates (u,v) leading to integration by quadratures of the system (1). More specifically, we classify the four separable cases in the Euclidean plane, known to be Cartesian, polar, parabolic, and elliptic-hyperbolic coordinates, according to various combinations afforded by the eigenvalues λ_1 and λ_2 of $\mathbf{K}$. We also classify the Killing tensors corresponding to the four separable cases in terms of their invariants under the group of rigid motions $E(2)$ of the Euclidean plane. Our classification scheme is equivalent to that given by Benenti and Rastelli,[11] who based their treatment on a classification of the singular points of the Killing tensors represented in terms of sums of symmetrized products of the Killing tensors of the Euclidean plane. Our approach allows us to recognize immediately the Liouville-integrable Hamiltonian systems YIC1 and YIC2 as separable in parabolic and translated elliptic-hyperbolic systems of coordinates, respectively. The existence of the canonical coordinates (u,v) in either case leads to the conclusion that both YIC1 and YIC2 are Pfaffian quasi-bi-Hamiltonian (QBH) systems. These are the subjects of the considerations that follow.

II. GEOMETRICAL BACKGROUND

The underlying structure of an orthogonally separable Hamiltonian system with two degrees of freedom (1) defined on a pseudo-Riemannian space is such that in the separable coordinates (u,v) the Hamiltonian function (1) takes on the *Liouville form*:[12]

$$H=(A(u)+B(v))^{-1}[\tfrac{1}{2}(\epsilon_1 p_u^2+\epsilon_2 p_v^2)+C(u)+D(v)], \tag{10}$$

while the second first integral (5) quadratic in momenta enjoys the following representation:

$$F=\frac{\epsilon_1 B(v)p_u^2-\epsilon_2 A(u)p_v^2+2(B(v)C(u)-A(u)D(v))}{A(u)+B(v)}, \tag{11}$$

where $A(u),C(u)$ and $B(v),D(v)$ are arbitrary smooth functions of u and v respectively, and $(\epsilon_1)^2=(\epsilon_2)^2=1$. Liouville[12] showed that the Hamiltonian systems defined by (10) are separable, while Morera[13] established the converse via an ingenious use of local coordinates. More precisely, if a Hamiltonian system defined by (1) admits additive separation of variables, it enjoys the Liouville form (10)–(11) in the canonical separable coordinates (u,v). Alternatively, this equivalence can be established by employing the coordinate-free moving frames method,[14–17] which also leads to additional interpretations of this remarkable fact, namely, the Killing tensor of (5) in this case has real and distinct eigenvalues and the system defined by (1) admits a certain quasi-bi-Hamiltonian (QBH) representation.[18] Formulas (10) and (11) describe separable Hamiltonian systems with two degrees of freedom defined in pseudo-Riemannian manifolds of arbitrary curvature. We note that the metric defined by (10) is the metric of the Liouville surface:

$$ds^2=(A(u)+B(v))(\epsilon_1\,du^2+\epsilon_2\,dv^2). \tag{12}$$

Similarly, the general covariant Killing tensor corresponding to (11) reads

$$K_{ij}^{(L)}=(A(u)+B(v))\,\mathrm{diag}(\epsilon_1 B(v),-\epsilon_2 A(u)). \tag{13}$$

Hence, $B(v)$ and $-A(u)$ are the eigenvalues of the linear operator $\hat{\mathbf{K}}=\mathbf{K}^{(\mathbf{L})}\mathbf{g}^{-1}$. It can be shown by integrating the Killing tensor equations (6) in the moving frame of normalized eigenvectors of $\mathbf{K}$ that the general solution has the form

$$\mathbf{K}=l\mathbf{g}+m\mathbf{K}^{(\mathrm{L})}, \tag{14}$$

where l and m are arbitrary constants. In order to classify the separable coordinate systems for Hamiltonian systems of the type (10) on Liouville surfaces of given curvature one has to impose conditions on the corresponding Riemann curvature tensor R_{ijkl}. Important cases are the spaces of constant curvature for which

$$R_{ijkl}=\kappa g_{i[k}g_{|j|l]}, \tag{15}$$

where κ is constant (see Ref. 19 for more details). The cases $\kappa=0$ and $\kappa\neq 0$ have to be distinguished in addition to the two possible signatures of the pseudo-Riemannian metric. In each case the separable coordinate systems may be determined based on the eigenvalues of $\mathbf{K}$ which are invariants. For more details on this method see Refs. 16 and 18 where the Riemannian and Lorentzian cases have been studied, respectively.

In the present paper we focus attention on the locally flat Riemannian case $\kappa=0$. It is well known that for this case (the Euclidean plane) there exist four separable coordinate systems, namely Cartesian, polar, parabolic, and elliptic-hyperbolic coordinates. The corresponding metrics, coordinate transformations, and associated Killing tensors for each case are listed in the following:

$$\text{Cartesian:}\quad \begin{cases} \mathrm{d}s^2=\mathrm{d}u^2+\mathrm{d}v^2, \\ x=u,\quad y=v, \\ K^{(C)}_{ij}=\mathrm{diag}(1,0), \end{cases} \tag{16}$$

$$\text{Polar:}\quad \begin{cases} \mathrm{d}s^2=\mathrm{d}u^2+u^2\,\mathrm{d}v^2, \\ x=u\cos v,\quad y=u\sin v, \\ K^{(P)}_{ij}=\mathrm{diag}(0,u^4), \end{cases} \tag{17}$$

$$\text{Parabolic:}\quad \begin{cases} \mathrm{d}s^2=(u^2+v^2)(\mathrm{d}u^2+\mathrm{d}v^2), \\ x=\frac{1}{2}(u^2-v^2),\quad y=uv, \\ K^{(\mathrm{PB})}_{ij}=(u^2+v^2)\,\mathrm{diag}(v^2,-u^2), \end{cases} \tag{18}$$

$$\text{Elliptic-Hyperbolic:}\quad \begin{cases} \mathrm{d}s^2=k^2(\cosh^2 u-\cos^2 v)(\mathrm{d}u^2+\mathrm{d}v^2), \\ x=k\cosh u\cos v,\quad y=k\sinh u\sin v, \\ K^{(\mathrm{EH})}_{ij}=k^4(\cosh^2 u-\cos^2 v)\,\mathrm{diag}(\cos^2 v,\cosh^2 u). \end{cases} \tag{19}$$

In (19) the parameter k is assumed positive and is interpretable as half the distance between the foci of the elliptic-hyperbolic coordinate system.

We observe that the metric (17) for polar coordinates is not in Liouville form. However, it can be written in this form by an appropriate coordinate transformation. We further observe that in all the above-mentioned cases except for polar coordinates we can immediately read off the functions $A(u)$ and $B(v)$ appearing in (12) and thus determine the form of the Hamiltonian (10) for which a complete integral of the corresponding Hamilton–Jacobi equation (3) can be obtained by quadratures from the ansatz (4). However, in most physical applications, a given Hamiltonian system (1) is defined in terms of *Cartesian* (usually, position-momenta) coordinates and hence has the form

$$H=\tfrac{1}{2}(p_1^2+p_2^2)+V(q^1,q^2). \tag{20}$$

The following questions are then crucial:

(1) Is the system separable in one of the above-mentioned coordinate systems?
(2) If yes, how does one determine the coordinate transformation to separable coordinates?

An answer to question (1) may be obtained from Benenti's theorem.[10] One first derives the general solution of the Killing tensor equation (7) in Cartesian coordinates obtaining

$$K_{ij}=\begin{pmatrix} A+2\alpha q^2+\gamma(q^2)^2 & C-\alpha q^1-\beta q^2-\gamma q^1 q^2 \\ C-\alpha q^1-\beta q^2-\gamma q^1 q^2 & B+2\beta q^1+\gamma(q^1)^2 \end{pmatrix}, \tag{21}$$

where A, B, C, α, β, γ are arbitrary parameters. These six constants obviously represent the *maximum* dimension of the space of linearly independent Killing tensors in our Riemannian space that can also be computed by employing the Takeuchi–Thompson formula:[20,21]

$$\dim K^p(M,\mathbf{g})=\frac{1}{n}\begin{pmatrix} n+p \\ p+1 \end{pmatrix}\begin{pmatrix} n+p-1 \\ p \end{pmatrix}, \quad p\geqslant 0$$

for the dimension of the space of $(p,0)$ Killing tensors defined in a pseudo-Riemannian manifold $(\hat{M},\mathbf{g})$ of constant curvature. One next imposes the compatibility condition (9), which may restrict the values of the parameters in (21). Finally, one determines whether the eigenvalues of the resulting K_{ij} are distinct. If they are, the system is orthogonally separable. The answer to question (2) is more difficult, due to the fact that Cartesian coordinates are not unique being defined only up to a translation and a rotation. One of the main objectives of this paper is to provide a theoretical framework in which question (2) may be answered based on a set of invariants of the Killing tensor (21) under the group of rigid motions $E(2)$ of the Euclidean plane. We further describe an algorithm for determining the transformation to separable coordinates which is straightforward and easy to apply.

III. SEPARABLE KILLING TENSORS IN CARTESIAN COORDINATES

We begin our study of orthogonal separability in terms of the associated Killing tensors by observing that the canonical Killing tensors corresponding to the four separable metrics (16)–(19) can be easily transformed to *canonical Cartesian coordinates* (x,y), i.e., the Cartesian coordinates centered at the origin and properly aligned with the four separable systems of coordinates defined by (16)–(19). Note that the *given Cartesian coordinates* (q^1,q^2) may differ, namely when they are related to the canonical Cartesian coordinates through a combination of translations and rotations. Indeed, using the standard coordinate transformations from canonical Cartesian coordinates to the separable coordinates, and the appropriate tensor transformation law we easily obtain the components of the four corresponding "separable" Killing tensors $\mathbf{K}^{(\mathbf{C})}$, $\mathbf{K}^{(\mathbf{P})}$, $\mathbf{K}^{(\mathbf{PB})}$, and $\mathbf{K}^{(\mathbf{EH})}$ with respect to canonical Cartesian coordinates (x,y), namely:

$$\begin{aligned} K^{(C)}_{ij} &:= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \text{Cartesian}, \\ K^{(P)}_{ij} &:= \begin{pmatrix} y^2 & -xy \\ -xy & x^2 \end{pmatrix}, \quad \text{Polar}, \\ K^{(\mathrm{PB})}_{ij} &:= \begin{pmatrix} 0 & y \\ y & -2x \end{pmatrix}, \quad \text{Parabolic}, \\ K^{(\mathrm{EH})}_{ij} &:= \begin{pmatrix} k^2+y^2 & -xy \\ -xy & x^2 \end{pmatrix}, \quad \text{Elliptic-hyperbolic}. \end{aligned} \tag{22}$$

It is easy to see that the polar case is a limiting case $(k=0)$ of the elliptic-hyperbolic case, since $\lim_{k\to 0}\mathbf{K}^{(\mathbf{EH})}=\mathbf{K}^{(\mathbf{P})}$.

Cartesian coordinates are determined only up to the transformations that preserve the metric $\mathbf{g}$, namely the isometry group which consists of translations $t_{\mathbf{a}}$, rotations ρ_θ, and reflections of the

Euclidean plane. We consider only the translations and rotations since it can be shown that reflections play no role in the invariant classification scheme to be presented. Thus, the given Cartesian coordinates (q^1,q^2) of the physical situations are related to the canonical Cartesian coordinates (x,y) via the formula:

$$\begin{pmatrix} q^1 \\ q^2 \end{pmatrix} = t_{\mathbf{a}}\rho_\theta \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} a \\ b \end{pmatrix} \tag{23}$$

for some fixed parameters θ, $\mathbf{a}=(a,b)$. The above-mentioned transformation induces the following transformation laws for the parameters appearing in (21):

$$\begin{aligned} \overline{\gamma} &= \gamma, \\ \overline{\alpha} &= \alpha\cos\theta + \beta\sin\theta - \gamma b, \\ \overline{\beta} &= \beta\cos\theta - \alpha\sin\theta - \gamma a, \\ \overline{A} &= A\cos^2\theta - 2C\cos\theta\sin\theta + B\sin^2\theta - 2b\alpha\cos\theta - 2b\beta\sin\theta + \gamma b^2, \\ \overline{B} &= A\sin^2\theta + 2C\cos\theta\sin\theta + B\cos^2\theta - 2a\beta\cos\theta + 2a\alpha\sin\theta + \gamma a^2, \\ \overline{C} &= (A-B)\sin\theta\cos\theta + C(\cos^2\theta - \sin^2\theta) + (a\alpha + b\beta)\cos\theta + (a\beta - b\alpha)\sin\theta - \gamma ab, \end{aligned} \tag{24}$$

where the quantities with a bar refer to the components of the Killing tensor in the (q^1,q^2) coordinates system. It follows that the components of the four separable Killing tensors relative to (q^1,q^2) coordinates are:

$$\begin{aligned} \widetilde{K}_{ij}^{(C)} &:= \begin{pmatrix} \cos^2\theta & \cos\theta\sin\theta \\ \cos\theta\sin\theta & \sin^2\theta \end{pmatrix}, \\ \widetilde{K}_{ij}^{(P)} &:= \begin{pmatrix} (q^2-b)^2 & -(q^1-a)(q^2-b) \\ -(q^1-a)(q^2-b) & (q^1-a)^2 \end{pmatrix}, \\ \widetilde{K}_{ij}^{(\mathrm{PB})} &:= \begin{pmatrix} 2\sin\theta(b-q^2) & (q^2-b)\cos\theta + (q^1-a)\sin\theta \\ (q^2-b)\cos\theta + (q^1-a)\sin\theta & 2\cos\theta(a-q^1) \end{pmatrix}, \\ \widetilde{K}_{ij}^{(\mathrm{EH})} &:= \begin{pmatrix} k^2\cos^2\theta + (q^2-b)^2 & k^2\cos\theta\sin\theta - (q^1-a)(q^2-b) \\ k^2\cos\theta\sin\theta - (q^1-a)(q^2-b) & k^2\sin^2\theta + (q^1-a)^2 \end{pmatrix}. \end{aligned} \tag{25}$$

Suppose $\mathbf{K}^{(\Lambda)}$ (for some $\Lambda = C$, P, PB, or EH) is a compatible Killing tensor whose components with respect to given Cartesian coordinates are of the form $\widetilde{K}_{ij}^{(\Lambda)}$ for fixed parameters k, θ, $\mathbf{a}$. Then the transformation to separable coordinates (u,v) can be realized as

$$\begin{pmatrix} q^1 \\ q^2 \end{pmatrix} = (t_{\mathbf{a}}\rho_\theta \circ T_\Lambda) \begin{pmatrix} u \\ v \end{pmatrix}, \tag{26}$$

where $(x,y)=T_\Lambda(u,v)$ is one of the standard coordinate transformations associated with Λ-coordinates listed in (16)–(19).

Now if every compatible Killing tensor $\mathbf{K}$ had components relative to (q^1,q^2) coordinates in the form $\widetilde{K}_{ij}^{(\Lambda)}$, or a multiple thereof, then we could intrinsically characterize the separable cases using the natural invariants of $\mathbf{K}$. Indeed, the signs of the determinants along with their eigenvalues could be used in a classification scheme as follows:

Cartesian: $\det \mathbf{K}^{(\mathbf{C})} = 0$ and both eigenvalues constant,

$$\text{Polar:} \quad \det \mathbf{K}^{(\mathbf{P})}=0 \quad \text{and one nonconstant eigenvalue,}$$

$$\text{Parabolic:} \quad \det \mathbf{K}^{(\mathbf{PB})}<0, \tag{27}$$

$$\text{Elliptic-hyperbolic:} \quad \det \mathbf{K}^{(\mathbf{EH})}>0.$$

However, if $\mathbf{K}$ is a compatible Killing tensor with components $\tilde{K}_{ij}^{(\Lambda)}$ relative to (q^1,q^2) coordinates, then $l\mathbf{g}+m\mathbf{K}$, where l and $m\neq 0$ are arbitrary constants, is also a compatible Killing tensor whose components are not of the assumed form. Indeed, addition of the metric changes the eigenvalues and the determinant. Hence, a more precise classification is needed.

IV. GROUP INVARIANTS OF KILLING TENSORS

To classify the separable coordinate systems based on their associated Killing tensors, we study invariants of Killing tensors under the three-parameter group of rigid motions $E(2)$. Since the components of a Killing tensor take the form (21) with respect to *any* Cartesian coordinates, the action of $E(2)$ on the space $\mathcal{K}$ of Killing tensors can be represented by the induced change in the six parameters $\sigma=(A,B,C,\alpha,\beta,\gamma)$ given by (24). We will search for real-valued functions of σ that are invariants of $E(2)$.

As a compatible Killing tensor, $\mathbf{g}$ only indicates that the Hamiltonian H is a first integral. Thus, the subspace $G=\{l\mathbf{g}\,|\,l\in\mathbb{R}\}$ generated by the metric is trivial, since it does not give any information concerning the separable coordinates. Hence, if $\mathbf{K}$ is a compatible Killing tensor, then both $\mathbf{K}$ and $\mathbf{K}+l\mathbf{g}$, $\forall l\in\mathbb{R}$, should determine the same separable coordinate systems. These considerations motivate us to focus on the action of $E(2)$ on the quotient space $Q:=\mathcal{K}/G$, in which $\mathbf{K}$ and $\mathbf{K}+l\mathbf{g}$, $\forall l\in\mathbb{R}$ are considered to be the same element. There is a natural bijection between Q and the parameter space $\mathbb{R}^5$ defined by

$$Q\simeq\left\{\begin{pmatrix}(A-B)+2\alpha y+\gamma y^2 & C-\alpha x-\beta y-\gamma xy\\ C-\alpha x-\beta y-\gamma xy & 2\beta x+\gamma x^2\end{pmatrix}\right\}\simeq\{(A-B,C,\alpha,\beta,\gamma)\}\simeq\mathbb{R}^5.$$

Essentially, in this framework we will be searching for invariants of $\mathbf{K}$ with respect to $E(2)$ which are also invariant under ''metric additions.''

The group $E(2)$ is a Lie group whose Lie algebra $\mathfrak{e}(2)$ is the space of Killing vectors. The algebra $\mathfrak{e}(2)$ is generated by the three basis vectors

$$\mathbf{X}=\frac{\partial}{\partial x},\quad \mathbf{Y}=\frac{\partial}{\partial y},\quad \mathbf{R}=y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y},$$

satisfying the commutator relations $[\mathbf{X},\mathbf{Y}]=0$, $[\mathbf{X},\mathbf{R}]=-\mathbf{Y}$, $[\mathbf{Y},\mathbf{R}]=\mathbf{X}$.

Take any vector $\mathbf{v}\in\mathfrak{e}(2)$. Exponentiation of $\mathbf{v}$ gives a connected one-parameter subgroup $T_{\mathbf{v}}=\{\exp(\epsilon\mathbf{v})|\forall\epsilon\in\mathbb{R}\}$ of $E(2)$. The set of transformations $T_{\mathbf{v}}$ induces a family of one-parameter curves in M. Denote the maximal parametrized curve passing through $\sigma\in M$ by $\Psi(\exp(\epsilon\mathbf{v}),\sigma)$, where Ψ is the flow generated by $\mathbf{v}$ in Q.

Definition 4.1: Let $\mathbf{K}$ *be a Killing tensor, whose components with respect to Cartesian coordinates* (x,y) are

$$K_{ij}=\begin{pmatrix}A+2\alpha y+\gamma y^2 & C-\alpha x-\beta y-\gamma xy\\ C-\alpha x-\beta y-\gamma xy & B+2\beta x+\gamma x^2\end{pmatrix}.$$

Then an $E(2)$-invariant *of* $\mathbf{K}$ *is a real-valued function* $F:\mathbb{R}^6\to\mathbb{R}$ *of* $\sigma=(A,B,C,\alpha,\beta,\gamma)$ *such that*

(1) $F(\Psi(m,\sigma))=F(\sigma)$, $\forall m\in E(2)$,
(2) $F(\sigma+l\hat{g})=F(\sigma)$, $\forall l\in\mathbb{R}$, *where* $\hat{g}=(1,1,0,0,0,0)$.

Letting $E(2)$ act on the quotient space Q, we can use standard techniques from the Lie group theory of differential equations to construct the $E(2)$-invariants. In the proof of the following proposition, the notations are consistent with those used in Ref. 22.

Proposition 4.1: Let

$$\Delta=(\alpha^2-\beta^2+\gamma(B-A))^2+4(\gamma C+\alpha\beta)^2. \tag{28}$$

Then every smooth $E(2)$-invariant of $\mathbf{K}$ *is of the form* $F(\Delta,\gamma)$, *where* $F:\mathbb{R}^2\to\mathbb{R}$ *is an arbitrary smooth function.*

Proof: The corresponding infinitesimal action of the Lie algebra $\mathfrak{e}(2)$ on M is given by

$$\psi(\mathbf{v})\Big|_{\sigma}=\frac{\mathrm{d}}{\mathrm{d}\epsilon}\Psi(\exp(\epsilon\mathbf{v}),\sigma)\Big|_{\epsilon=0}$$

for any $\mathbf{v}\in\mathfrak{e}(2)$, $\sigma\in M$. Equivalently, we can write

$$\psi(\mathbf{v})=\pi(\mathcal{L}_{\mathbf{v}}(\mathbf{K})), \tag{29}$$

where $\mathcal{L}_{\mathbf{v}}(\mathbf{K})$ is the Lie derivative of $\mathbf{K}$ with respect to $\mathbf{v}$ and $\pi:\mathcal{K}\to\mathbb{R}^5$ is the projection map defined by

$$\pi\begin{pmatrix} A_0+2\alpha_0 y+\gamma_0 y^2 & C_0-\alpha_0 x-\beta_0 y-\gamma_0 xy \\ C_0-\alpha_0 x-\beta_0 y-\gamma_0 xy & B_0+2\beta_0 x+\gamma_0 x^2 \end{pmatrix}$$
$$=(A_0-B_0)\frac{\partial}{\partial(A-B)}+C_0\frac{\partial}{\partial C}+\alpha_0\frac{\partial}{\partial\alpha}+\beta_0\frac{\partial}{\partial\beta}+\gamma_0\frac{\partial}{\partial\gamma}.$$

Note that π is a linear surjection and $\pi(\mathbf{K^{(1)}})=\pi(\mathbf{K^{(2)}})$ iff $\mathbf{K^{(1)}}=\mathbf{K^{(2)}}+l\mathbf{g}$ for any $l\in\mathbb{R}$. Equation (29) follows from a straightforward application of the definitions of ψ, $\mathcal{L}$, and π.

The corresponding infinitesimal generators in Q are

$$\mathbf{V_1}=\pi(\mathcal{L}_X(K))=-2\beta\frac{\partial}{\partial(A-B)}-\alpha\frac{\partial}{\partial C}+\gamma\frac{\partial}{\partial\beta},$$

$$\mathbf{V_2}=\pi(\mathcal{L}_Y(K))=2\alpha\frac{\partial}{\partial(A-B)}-\beta\frac{\partial}{\partial C}+\gamma\frac{\partial}{\partial\alpha},$$

$$\mathbf{V_3}=\pi(\mathcal{L}_R(K))=-4C\frac{\partial}{\partial(A-B)}+(A-B)\frac{\partial}{\partial C}+\beta\frac{\partial}{\partial\alpha}-\alpha\frac{\partial}{\partial\beta}.$$

Note that $\mathbf{V_1}$, $\mathbf{V_2}$, $\mathbf{V_3}$ satisfy the commutator relations

$$[\mathbf{V_1},\mathbf{V_2}]=0,\quad [\mathbf{V_1},\mathbf{V_3}]=-\mathbf{V_2},\quad [\mathbf{V_2},\mathbf{V_3}]=\mathbf{V_1}.$$

Hence, ψ is a Lie algebra homomorphism from $\mathfrak{e}(2)$ to the Lie algebra of vector fields generated by $\{\mathbf{V_1},\mathbf{V_2},\mathbf{V_3}\}$ on Q.

It is well known that invariance of an object under an entire Lie group is equivalent to infinitesimal invariance under the infinitesimal generators of the corresponding Lie algebra. The image in Q of the Lie algebra $\mathfrak{e}(2)$ has basis $\{\mathbf{V_1},\mathbf{V_2},\mathbf{V_3}\}$. Hence, $F:Q\to\mathbb{R}$ is a smooth $E(2)$-invariant iff $\mathbf{V_i}(F)\equiv 0$ for $i=1,2,3$. This is a system of three homogeneous linear partial differential equations in five variables. Solving this system by the method of characteristics yields the solution $F(\Delta,\gamma)$. □

As a consequence of Proposition IV, we obtain two essential $E(2)$-invariants, Δ and γ. Let

$$\operatorname{sgn}|x| = \begin{cases} 1 & \text{if } x \neq 0 \\ 0 & \text{if } x = 0 \end{cases},$$

and impose the following equivalence relation on $\mathcal{K}$:

$$\mathbf{K}^{(1)} \sim \mathbf{K}^{(2)} \Leftrightarrow \begin{cases} \operatorname{sgn}|\Delta_{\mathbf{K}^{(1)}}| = \operatorname{sgn}|\Delta_{\mathbf{K}^{(2)}}| \\ \operatorname{sgn}|\gamma_{\mathbf{K}^{(1)}}| = \operatorname{sgn}|\gamma_{\mathbf{K}^{(2)}}|. \end{cases}$$

Note that $\sim$ partitions $\mathcal{K} \setminus G$ into four equivalence classes corresponding to whether Δ and γ are zero or nonzero. Take the components of the ''separable'' Killing tensors with respect to canonical Cartesian coordinates listed in (22), and designate them to be representative elements from their respective equivalence classes. Evaluating the $E(2)$-invariants Δ and γ on each produces the following classification scheme:

$$\begin{gathered} \gamma = 0, \quad \Delta = 0: \quad \text{Cartesian}, \\ \gamma = 0, \quad \Delta \neq 0: \quad \text{Parabolic}, \\ \gamma \neq 0, \quad \Delta = 0: \quad \text{Polar}, \\ \gamma \neq 0, \quad \Delta \neq 0: \quad \text{Elliptic-hyperbolic}. \end{gathered} \tag{30}$$

Now recall that the general solution of the Killing tensor equation is given by the *tensor* equation (14). This implies that if $\mathbf{K}$ is linearly independent of $\mathbf{g}$, we have in (q^1, q^2) coordinates,

$$K_{ij} = l g_{ij} + m \tilde{K}_{ij}^{(\Lambda)} \tag{31}$$

for some $l, m \in \mathbb{R}, m \neq 0$, some unique $\Lambda = C$, P, PB, or EH, and where $\tilde{K}_{ij}^{(\Lambda)}$ depends on the parameters θ, a, b, k as in (25). By comparing the components on both sides (31) and using the $E(2)$-invariant classification, we can express θ, a, b, k as functions of the constants A, B, C, α, β, γ for any particular Killing tensor. We illustrate this method for the elliptic-hyperbolic case in the following.

Take a particular Killing tensor $\mathbf{K}$ whose components with respect to Cartesian coordinates (q^1, q^2) are of the form (21) and suppose that $\gamma \neq 0$, $\Delta \neq 0$. $\mathbf{K}$ is of elliptic-hyperbolic type, and so comparing the components on both sides of (31), we obtain

$$A + 2\alpha q^2 + \gamma (q^2)^2 = l + m(k^2 \cos^2 \theta + (q^2 - b)^2), \tag{32}$$

$$C - \alpha q^1 - \beta q^2 - \gamma q^1 q^2 = m(k^2 \cos\theta \sin\theta - (q^1 - a)(q^2 - b)), \tag{33}$$

$$B + 2\beta q^1 + \gamma (q^1)^2 = l + m(k^2 \sin^2 \theta + (q^1 - a)^2). \tag{34}$$

The coefficients of the terms quadratic and linear in q^1, q^2 yield $m = \gamma$, and $a = -\beta/\gamma$, $b = -\alpha/\gamma$, respectively. Simplifying, we now have

$$A - \frac{\alpha^2}{\gamma} - l = \gamma k^2 \cos^2 \theta, \tag{35}$$

$$C + \frac{\alpha\beta}{\gamma} = \gamma k^2 \cos\theta \sin\theta, \tag{36}$$

$$B - \frac{\beta^2}{\gamma} - l = \gamma k^2 \sin^2 \theta, \tag{37}$$

Note that the product of the left-hand sides of (35) and (37) equals the square of the left-hand side of (36). Solving this for l yields

$$l_{\pm}=\frac{1}{2\gamma}(\gamma(A+B)-\alpha^2-\beta^2\pm\sqrt{\Delta}). \tag{38}$$

Adding (35) and (36) and solving for k^2 yields

$$k^2=\frac{\gamma(A+B)-\alpha^2-\beta^2}{\gamma^2}-\frac{2l}{\gamma}=\mp\frac{\sqrt{\Delta}}{\gamma^2}\neq 0, \tag{39}$$

which forces $l=l_{-}$.

Let $\sigma:=\alpha^2-\beta^2+\gamma(B-A)$. To find the rotation angle θ, we have to consider various cases. If $\gamma C+\alpha\beta\neq 0$, then dividing (37) by (36) gives

$$\tan\theta=\frac{\gamma(B+l)-\beta^2}{\gamma C+\alpha\beta}=\frac{\sigma+\Delta}{2(\gamma C+\alpha\beta)}.$$

If $\gamma C+\alpha\beta=0$, then by (36) we have $\sin\theta\cos\theta=0$, since $\gamma\neq 0$. By (35) and (37), this implies that either $\gamma(A-l)-\alpha^2=0$ (if $\cos\theta=0$) or $\gamma(B-l)-\beta^2=0$ (if $\sin\theta=0$). Using (38), (39), and the fact that $l=l_{-}$, we obtain

$$\begin{aligned}&\sigma=+k^2\gamma^2, \quad \text{if}\cos\theta=0, \text{ or}\\ &\sigma=-k^2\gamma^2, \quad \text{if}\sin\theta=0.\end{aligned}$$

Thus if $\sigma>0$, then $\tan\theta=\pm\infty$, and if $\sigma<0$, then $\tan\theta=0$. Clearly, θ is only unique mod π. In a similar fashion, expressions for θ, a, b in terms of the constants $A, B, C, \alpha, \beta, \gamma$ can be found for the Cartesian, polar, and parabolic cases.

The *singular points* of each coordinate system can also be described in this framework. It follows from Benenti[10] that they are characterized as the points where the eigenvalues of the Killing tensor K_{ij} are equal. The conditions for equal roots for the characteristic equation are

$$K_{11}=K_{22}, \quad K_{12}=0, \tag{40}$$

which in view of (21) give rise to

$$\begin{aligned}&A+2\alpha q^2+\gamma(q^2)^2=B+2\beta q^1+\gamma(q^1)^2,\\ &\gamma q^1q^2+\alpha q^1+\beta q^2=C.\end{aligned} \tag{41}$$

We consider the solution of the above-mentioned system for each equivalence class of Killing tensors in $\mathcal{K}\backslash G$:

(1) *Cartesian* ($\gamma=0,\Delta=0$): In this case, $\alpha=\beta=0$, and (41) is equivalent to $A=B$, $C=0$, which is true only for elements in G. Hence, there are no solutions in this case.

(2) *Parabolic* ($\gamma=0,\Delta\neq 0$). One solution:

$$(q^1,q^2)=\left(\frac{\beta(A-B)+2\alpha C}{2(\alpha^2+\beta^2)},\frac{\alpha(B-A)+2\beta C}{2(\alpha^2+\beta^2)}\right).$$

(3) *Polar* ($\gamma\neq 0,\Delta=0$). One solution:

$$(q^1,q^2)=\left(\frac{-\beta}{\gamma},\frac{-\alpha}{\gamma}\right).$$

(4) *Elliptic-hyperbolic* ($\gamma\neq 0,\Delta\neq 0$). Two solutions:

TABLE I. Formulas for transformation to separable coordinates. Transformation to separable coordinates:

$$\begin{pmatrix} q^1 \\ q^2 \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} T_\Lambda \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} a \\ b \end{pmatrix}.$$

Standard coordinate transformations: $T_C: x=u,\ y=v$, $T_P: x=u\cos v,\ y=u\sin v$, $T_{\mathrm{PB}}: x=\frac{1}{2}(u^2-v^2),\ y=uv$, $T_{\mathrm{EH}}: x=k\cosh u\cos v,\ y=k\sinh u\sin v$.

Coordinate type	γ	Δ	a	b	$\tan(\theta)$	k^2	Singular points
Cartesian	0	0	Arbitrary	Arbitrary	$\begin{cases} 0 \quad \text{if } C=0, \\ \dfrac{B-A+\sqrt{(B-A)^2+4C^2}}{2C} \quad \text{if } C\neq 0. \end{cases}$ (θ unique mod $\dfrac{\pi}{2}$)	0/0	Two at ∞
Parabolic	0	$\neq 0$	$\dfrac{\beta(A-B)+2\alpha C}{2(\alpha^2+\beta^2)}$	$\dfrac{\alpha(B-A)+2\beta C}{2(\alpha^2+\beta^2)}$	$\begin{cases} \pm\infty \quad \text{if } \beta=0, \\ \dfrac{\alpha}{\beta} \quad \text{if } \beta\neq 0. \end{cases}$ (θ unique mod π)	∞	One at **a**, One at ∞
Polar	$\neq 0$	0	$-\dfrac{\beta}{\gamma}$	$-\dfrac{\alpha}{\gamma}$	Arbitrary. Define $\sigma=\alpha^2-\beta^2+\gamma(B-A)$.	0	Two coincide at **a**
Elliptic-hyperbolic	$\neq 0$	$\neq 0$	$-\dfrac{\beta}{\gamma}$	$-\dfrac{\alpha}{\gamma}$	$\begin{cases} 0 \quad \text{if } \gamma C+\alpha\beta=0,\ \sigma<0, \\ \pm\infty \quad \text{if } \gamma C+\alpha\beta=0,\ \sigma>0, \\ \dfrac{\sigma+\sqrt{\Delta}}{2(\gamma C+\alpha\beta)} \quad \text{if } \gamma C+\alpha\beta\neq 0. \end{cases}$ (θ unique mod π)	$\dfrac{\sqrt{\Delta}}{\gamma^2}$	Two distinct

$$(q^1,q^2)=\left(\frac{-\beta}{\gamma}+\frac{1}{\gamma}\left(\frac{\sqrt{\Delta}-\sigma}{2}\right)^{1/2},\frac{-\alpha}{\gamma}+\frac{1}{\gamma}\left(\frac{\sqrt{\Delta}+\sigma}{2}\right)^{1/2}\right),$$

$$(q^1,q^2)=\left(\frac{-\beta}{\gamma}-\frac{1}{\gamma}\left(\frac{\sqrt{\Delta}-\sigma}{2}\right)^{1/2},\frac{-\alpha}{\gamma}-\frac{1}{\gamma}\left(\frac{\sqrt{\Delta}+\sigma}{2}\right)^{1/2}\right).$$

In the elliptic-hyperbolic system, there are two singular points corresponding to the foci with k being half the distance between them, as mentioned earlier. The polar system is a limiting case of the elliptic-hyperbolic system when the foci coincide, so here $k^2=\lim_{\Delta\to 0}\sqrt{\Delta}/\gamma^2=0$ and there is one singular point at the center of the polar system. The parabolic system is also a limiting case of the elliptic-hyperbolic system in the sense that there is one finite singular point and one singular point which has been ''pushed'' to infinity, so $k^2=\lim_{\gamma\to 0}\sqrt{\Delta}/\gamma^2=\infty$. Finally, in the Cartesian system, both singular points from the elliptic-hyperbolic system have been ''pushed'' to infinity. Hence, no (finite) singular points exist. The above classification of the singular points is equivalent to that given by Benenti and Rastelli.[11] Our results are summarized in Table I.

V. MAIN ALGORITHM

The above-presented considerations lead to the following systematic and computationally efficient method of determining separable coordinates for the natural Hamiltonian (20):

(1) Using a generic Killing tensor $\mathbf{K}$ of the form (21) in terms of the given Cartesian coordinates (q^1,q^2), impose the compatibility condition (9) to obtain the equivalent conditions on the parameters A, B, C, α, β, γ.

(2) Decompose the general solution obtained in step (1) as follows:

$$\mathbf{K}=l_0\mathbf{g}+l_1\mathbf{K}^{(1)}+\cdots+l_n\mathbf{K}^{(n)}, \tag{42}$$

where l_i, $i=0,1,\ldots,n$ are arbitrary constants and $\{\mathbf{g},\mathbf{K}^{(1)},\ldots,\mathbf{K}^{(n)}\}$ is a pointwise linearly independent set of Killing tensors. Since $\dim\mathcal{K}=6$, then $n\leqslant 5$. If $n=0$, then H is not orthogonally separable. If $n\geqslant 2$, then H is superseparable.

(3) Each $\mathbf{K}^{(i)}$ will characterize separation in some coordinate system. For each $\mathbf{K}^{(i)}$, evaluate the $E(2)$-invariants γ and Δ. Then use Table I to determine: (1) the separable coordinate system type, and (2) the essential parameters θ, a, b, k. The transformation to separable coordinates can be carried out by using Eq. (26).

A main feature of this algorithm is that once an additional Killing tensor is known, the task of finding separable coordinates reduces to simply looking up the appropriate parameters in Table I. *No additional computations are necessary*. Computationally, the most difficult part of the algorithm is finding the general solution of the compatibility condition (9) in step (1). However, using the generic form (21) of $\mathbf{K}$ with respect to Cartesian coordinates, this computation only amounts to solving a system of linear equations in six variables. This method should be contrasted with that which implements the Bertrand–Darboux theorem in which a second-order PDE must be solved by the method of characteristics. Our algorithm is *completely algebraic*, and hence is well suited for implementation in a symbolic computer algebra system. We have implemented such a program in the MAPLE system and it has been used successfully to analyze the Hamiltonian systems discussed in this paper.

As a brief illustration, we discuss the implications of this algorithm on the two known separable cases of the Hénon–Heiles system (see Ref. 23, and references therein) which is defined by the Hamiltonian

$$H_{\mathrm{HH}}=\frac{1}{2}(p_1^2+p_2^2+c(q^1)^2+d(q^2)^2)+aq^1(q^2)^2-\frac{b}{3}(q^1)^3 \tag{43}$$

for some constants a, b, c, and d. Imposing the compatibility condition (9) with a generic Killing tensor (21) and the above-given potential, we can identify all integrable cases which correspond to an additional first integral quadratic in momenta. In particular, the only nontrivial (i.e., $ab\neq 0$) systems we recover are the first and second known integrable cases. We list these in the following, along with the corresponding compatible Killing tensors, and the transformation to separable coordinates obtained by using Table I:

(1) $b=-a$, $c=d$:

$$K_{ij}=l_0 g_{ij}+l_1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},$$

$$q^1=\frac{1}{\sqrt{2}}(u-v),\quad q^2=\frac{1}{\sqrt{2}}(u+v).$$

(2) $b=-6a$, c, d arbitrary:

$$K_{ij}=l_0 g_{ij}+l_1\begin{pmatrix}\dfrac{4d-c}{2a} & -\beta q^2\\ -\beta q^2 & 2\beta q^1\end{pmatrix},$$

$$q^1=\frac{4d-c}{4a}+\frac{1}{2}(u^2-v^2),\quad q^2=uv.$$

The third known integrable case $b=-16a$, $d=16c$ is not recovered by this method. This indicates that the corresponding system does not have an additional first integral quadratic in momenta, and hence is not orthogonally separable.

In step (2) of the algorithm, we remarked that if $n\geqslant 2$, then H is superseparable. An example of such a system is the two-dimensional Calogero–Moser system defined by the Hamiltonian

$$H_{\mathrm{CM}}=\frac{1}{2}(p_1^2+p_2^2)+\frac{1}{(q^1-q^2)^2}. \tag{44}$$

Solving the compatibility condition yields the following general compatible Killing tensor:

$$K_{ij}=l_0 g_{ij}+l_1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}+l_2\begin{pmatrix}(q^2)^2 & -q^1q^2\\ -q^1q^2 & (q^1)^2\end{pmatrix}+l_3\begin{pmatrix}2q^2 & -q^1-q^2\\ -q^1-q^2 & 2q^1\end{pmatrix}, \tag{45}$$

from which we conclude that the system is separable in the following coordinate systems:

(1) Cartesian: $q^1=(1/\sqrt{2})\,(u-v)$, $q^2=(1/\sqrt{2})\,(u+v)$,
(2) Polar: $q^1=u\cos v$, $q^2=u\sin v$,
(3) Parabolic: $q^1=(1/2\sqrt{2})\,(u^2-2uv-v^2)$, $q^2=(1/2\sqrt{2})\,(u^2+2uv-v^2)$,

thus recovering known results. Again, in contrast with previous methods, the algorithm that we have presented is *exhaustive* in the sense that a given system is separable in some system of coordinates iff the associated Killing tensor is a particular solution of the compatibility condition. The general form of the compatible Killing tensor gives us essentially all the information about the separation properties of a given system. We remark that the algorithm can be used in the reverse direction as a method for determining the general forms of the superseparable potentials in the Euclidean plane. In order to classify such potentials, we specify two (or more) Killing tensors linearly independent from the metric, construct the general Killing tensor (42), and then proceed to solve the compatibility condition (9) for the potential V. For example, if we wish to find the potential V which is separable in both polar and parabolic coordinates, let

$$K_{ij}=l_0 g_{ij}+l_1\begin{pmatrix}y^2 & -xy\\ -xy & x^2\end{pmatrix}+l_2\begin{pmatrix}0 & y\\ y & -2x\end{pmatrix}, \tag{46}$$

where l_0, l_1, l_2 are arbitrary parameters. Solving the compatibility condition recovers the known potential

$$V=\frac{1}{\sqrt{x^2+y^2}}\left(c_0+\frac{c_1 x}{y^2}\right)+\frac{c_2}{y^2}, \tag{47}$$

where c_0, c_1, c_2 are arbitrary constants of integration. Note that for any $k\in\mathbb{R}$, if we let $l_0=k^2$, $l_1=1$, $l_2=k$ in (46), we obtain the Killing tensor

$$K_{ij}=\begin{pmatrix}k^2+y^2 & -(x-k)y\\ -(x-k)y & (x-k)^2\end{pmatrix}, \tag{48}$$

which indicates separation in *translated* elliptic-hyperbolic coordinates, with the origin of the polar and parabolic systems located at one of the *foci* of the elliptic-hyperbolic system of coordinates. Hence, the potential (46) which is superseparable in polar and parabolic coordinates is necessarily also separable in these specific coordinates. This is the *only* translated and rotated elliptic-hyperbolic coordinate system for which V is also separable in polar and parabolic coordinates. Although this method is a systematic way of determining superseparable potentials, it is computationally intensive. Solving the compatibility condition for the potential V given $\mathbf{K}$ amounts to solving the associated PDEs satisfied by V. Using this method, we have recovered the known set of superseparable potentials (see Ref. 24, and the relevant references therein).

In Sec. VI, and the remainder of this paper, we will illustrate this algorithm in more detail for the two integrable systems YIC1 and YIC2 derived by Yatsun.[1–5]

VI. SEPARABLE COORDINATES EXHIBITED

Recall that the Yang–Mills theories provide a reasonable model for the unification of electromagnetic and weak forces. Naturally, many aspects of the theory have become active areas of research developed from algebraic, differential geometric, dynamical, etc., points of view. In particular, many integrable models (see, for instance, Ref. 25) have been derived from self-dual Yang–Mills equations by symmetry reductions.

In a series of papers[1–5] Yatsun investigated two SU(2) gauge theories defined in $\mathbb{R}^4$ over the bundle $P(\mathbb{R}^4,\mathrm{SU}(2))$ from this viewpoint.

A. Yatsun's integrable case 1 (YIC1)

The first SU(2) Yang–Mills theory considered has a Lagrangian density of the form

$$\mathcal{L}_1=\frac{1}{4g^2}F^a_{\mu\nu}F^a_{\mu\nu}+\frac{1}{2}\mathcal{D}_\mu\phi_i\mathcal{D}_\mu\phi_i+\frac{1}{4}\lambda(\phi_i\phi_i)^2, \tag{49}$$

for $\phi_i, i=1,\ldots,4$ in vector representations, where under SU(2) gauge transformations $h=u_4+iu_a\sigma_a\phi_i$ transforms into $\tilde{\phi}_i=u_4\phi_i+\overline{\eta}_{aij}u_a\phi_j$ and $\mathcal{D}_\mu\phi_i=\partial_\mu\phi_i-\frac{1}{2}\overline{\eta}_{aij}A^a_\mu\phi_j$, $\overline{\eta}_{aij}=\epsilon_{aij4}+\delta_{i4}\delta_{aj}-\delta_{j4}\delta_{ai}$ is the anti-self-dual 't Hooft tensor. (For the symmetry properties of the Yang–Mills Lagrangians see Fatibene *et al.*[26]). To solve the problem of finding the fields A_μ and ϕ_ν satisfying the equations of motion of the model (49), namely

$$\begin{gathered}\tilde{D}_\mu F^a_{\mu\nu}+\tfrac{1}{2}g^2\overline{\eta}_{a\rho\tau}\phi_\rho\mathcal{D}_\nu\phi_\tau=0,\\ \mathcal{D}_\mu\mathcal{D}_\mu\phi_\mu+\lambda\phi^2\phi_\nu=0,\end{gathered} \tag{50}$$

where $\tilde{D}_\mu F^a_{\mu\nu}=\partial_\mu F^a_{\mu\nu}+\epsilon_{abc}A^b_\mu F^c_{\mu\nu}$, and $\phi^2=\phi_\nu\phi_\nu$ for which the integral of action is bounded, the author employs the $O(4)$-symmetry reduction

$$A^a_\mu=2\psi(x)\overline{\eta}_{a\mu\nu}\frac{x_\nu}{x^2},\quad \phi_\nu=\varphi(x)\frac{x_\nu}{x}, \tag{51}$$

where $x=(x_\nu x_\nu)^{1/2}$. These equations transform the equations of the motion (50) into the following system of second-order ordinary differential equations (ODEs):

$$\begin{gathered}\psi''+\frac{1}{x}\psi'-\frac{4}{x^2}\psi(1-\psi)(1-2\psi)-\frac{g^2}{4}\varphi^2(1-\psi)=0,\\ \varphi''+\frac{3}{x}\varphi'-\frac{3}{x^2}\varphi(1-\psi)^2+\lambda\varphi^3=0.\end{gathered} \tag{52}$$

By the coordinate transformation

$$t=\ln x,\quad q_1=\psi+1,\quad q_2=\left(\frac{g^2}{12}\right)^{1/2}x\varphi,\quad p_i=\frac{\mathrm{d}q_i}{\mathrm{d}t}, \tag{53}$$

where $i=1,2$, Eq. (52) is reduced to the canonical Hamilton equations defined by the Hamiltonian

$$H_1=\tfrac{1}{2}(p_1^2+p_2^2)+V_1, \tag{54}$$

where

$$V_1=-2\left((q^1)^4+\frac{3}{4}(q^1)^2(q^2)^2+\frac{3}{2}\frac{\lambda}{g^2}(q^2)^4\right)+12\left((q^1)^3+\frac{1}{2}q^1(q^2)^2\right)$$
$$-26\left((q^1)^2+\frac{1}{4}(q^2)^2\right)+24q^1. \tag{55}$$

It is shown next that for $g^2=24\lambda$ the Hamiltonian system is completely integrable having the following additional integral of motion independent of H_1:

$$F_1=p_1p_2q_2-p_2^2q^1-(q^2)^2\{(q^1)^3+\tfrac{1}{2}q^1(q^2)^2-6((q^1)^2+\tfrac{1}{4}(q^2)^2)+13q^1-12\}. \tag{56}$$

Note that (56) is quadratic in momenta, hence the system is orthogonally separable. At this point the author uses the technique developed in Ref. 27 which utilizes the Hamilton–Jacobi equation of (55) to find a *particular* solution of (52) by first finding a particular solution to the Hamilton–Jacobi equation in order to reduce the system of second-order ODEs to a system of first-order ODEs in $\psi(x)$ and $\varphi(x)$ that can be solved explicitly. We are able to show that the Hamiltonian system defined by (55) can be solved in full generality by making use of the Hamilton–Jacobi method of separation of variables under the separation ansatz (4) as described previously. Indeed, we observe that any Killing tensor compatible with V_1 [i.e., $\mathrm{d}(\mathbf{K}\,\mathrm{d}V_1)=0$] is of the form $\mathbf{K}=l_0\mathbf{g}+l_1\mathbf{K^{(1)}}$, l_0, l_1 arbitrary parameters, where

$$K_{ij}^{(1)}=\begin{pmatrix}0 & -q^2\\ -q^2 & 2q^1\end{pmatrix}. \tag{57}$$

Comparing $K_{ij}^{(1)}$ with (21), we see that $A=B=C=\alpha=\gamma=0$, $\beta=1$. Table I indicates that the separable coordinates are of parabolic type with $\theta=a=b=0$. Hence, we use the standard transformation to parabolic coordinates:

$$\begin{aligned}q^1&=\tfrac{1}{2}(u^2-v^2),\\ q^2&=uv.\end{aligned} \tag{58}$$

Transforming the momenta and potential accordingly, we obtain the following form of the Hamiltonian H_1 in parabolic coordinates:

$$H_1=\frac{\frac{1}{2}(p_u^2+p_v^2)+h_+(u^2)+h_-(v^2)}{u^2+v^2}, \tag{59}$$

where $p_u=\partial W/\partial u$, $p_v=\partial W/\partial v$, and

$$h_\pm(\eta)=\frac{-\eta^5}{8}+\frac{3\eta^4}{2}-\frac{13\eta^3}{2}\pm 12\eta^2. \tag{60}$$

The Hamiltonian H_1 is separable in u,v coordinates. Setting $H_1=E$, E an arbitrary constant, and seeking a separable solution $W=W_1(u)+W_2(v)-Et$, the Hamilton–Jacobi equation becomes

$$\left(\frac{\mathrm{d}W_1}{\mathrm{d}u}\right)^2+2h_+(u^2)-2Eu^2=-\left(\frac{\mathrm{d}W_2}{\mathrm{d}v}\right)^2-2h_-(v^2)+2Ev^2=\sigma, \tag{61}$$

where σ is the separation constant. Consequently, the separated equations yield the solution up to quadrature:

$$W_1(u)=\int \sqrt{2Eu^2+\sigma-2h_+(u^2)}\,\mathrm{d}u, \tag{62}$$

$$W_2(v)=\int \sqrt{2Ev^2-\sigma-2h_-(v^2)}\,\mathrm{d}v. \tag{63}$$

Next, solving

$$\beta_1=\frac{\partial W}{\partial \sigma}, \quad t-t_0=\frac{\partial W}{\partial E}, \tag{64}$$

where $W(u,v)=W_1(u)+W_2(v)$, one can obtain the general solution to the dynamical system in closed form.

B. Yatsun's integrable case 2 (YIC2)

A similar approach is used to treat the Yang–Mills theory with the Lagrangian density

$$\mathcal{L}_2=\frac{1}{4g^2}F^a_{\mu\nu}F^a_{\mu\nu}+\frac{1}{2}D_\mu\phi^a_i D_\mu\phi^a_i+\frac{1}{4}\lambda[\phi_i,\phi_j]^a[\phi_i,\phi_j]^a, \tag{65}$$

where the real scalar fields $\phi_i, i=1,\ldots,4$ are given in adjoint representation and $D_\mu\phi^a_i=\partial_\mu\phi^a_i+[A_\mu,\phi_i]^a$, thus leading to the Hamiltonian system defined by

$$H_2=\tfrac{1}{2}(p_1^2+p_2^2)+V_2, \tag{66}$$

where

$$V_2=-2\left((q^1)^4+2(q^1)^2(q^2)^2+\frac{2\lambda}{g^2}(q^2)^4\right)+4((q^1)^3+q^1(q^2)^2)-2((q^1)^2+(q^2)^2). \tag{67}$$

It is shown that the Hamiltonian system is completely integrable if $g^2=2\lambda$ enjoying the following additional first integral independent from (66):

$$\begin{aligned}F_2=&((q^2)^2+\tfrac{3}{4})p_1^2-(2q^1-1)q^2p_1p_2+(q^1-1)q^1p_2^2-3(q^1)^4\\&-2(q^1)^2(q^2)^2+(q^2)^4+6(q^1)^3+2(q^1)(q^2)^2-3(q^1)^2.\end{aligned} \tag{68}$$

As in the previous case the integral F_2 is quadratic in momenta, thus confirming orthogonal separability of (66). More specifically, any Killing tensor compatible with V_2 is of the form $\mathbf{K}=l_0\mathbf{g}+l_1\mathbf{K^{(1)}}$, l_0, l_1 arbitrary parameters, where

$$K^{(1)}_{ij}=\begin{pmatrix}\frac{3}{4}+(q^2)^2 & \frac{1}{2}1\,q^2-q^1q^2\\ \frac{1}{2}q^2-q^1q^2 & -q^1+(q^1)^2\end{pmatrix}. \tag{69}$$

Comparing $K^{(1)}_{ij}$ with (21), we see that $A=\frac{3}{4}$, $B=C=\alpha=0$, $\beta=-\frac{1}{2}$, $\gamma=1$. Table I indicates that the separable coordinates are of elliptic-hyperbolic type with $\theta=b=0$, $a=\frac{1}{2}$, $k=1$. We use *translated* elliptic-hyperbolic coordinates:

$$\begin{aligned}q^1&=\tfrac{1}{2}+\cosh(u)\cos(v),\\ q^2&=\sinh(u)\sin(v).\end{aligned} \tag{70}$$

Transforming the momenta and potential accordingly, we obtain the following form of the Hamiltonian H_2 in parabolic coordinates

$$H_2=\frac{\frac{1}{2}(p_u^2+p_v^2)+g(\cos^2(v))-g(\cosh^2(u))}{\cosh^2(u)-\cos^2(v)}, \tag{71}$$

where $p_u=\partial W/\partial u$, $p_v=\partial W/\partial v$, and

$$g(\eta)=2\eta^3-3\eta^2+\tfrac{9}{8}\eta. \tag{72}$$

The Hamiltonian H_2 is separable in u, v coordinates. Setting $H_2=E$, E an arbitrary constant, and seeking a separable solution $W=W_1(u)+W_2(v)-Et$, the Hamilton–Jacobi equation becomes

$$\left(\frac{\mathrm{d}W_1}{\mathrm{d}u}\right)^2-2g(\cosh^2(u))-2E\cosh^2(u)=-\left(\frac{\mathrm{d}W_2}{\mathrm{d}v}\right)^2-2g(\cos^2(v))+2E\cos^2(v)=\sigma, \tag{73}$$

where σ is the separation constant. Consequently, the separated equations yield the solution up to quadrature:

$$W_1(u)=\int \sqrt{2E\cosh^2(u)+\sigma+2g(\cosh^2(u))}\,\mathrm{d}u, \tag{74}$$

$$W_2(v)=\int \sqrt{-2E\cos^2(v)-\sigma-2g(\cos^2(v))}\,\mathrm{d}v. \tag{75}$$

Finding the complete solution $W(u,v)=W_1(u)+W_2(v)$ leads to the general solution of the dynamical system in closed form [see (64)].

VII. QUASI-BI-HAMILTONIAN REPRESENTATIONS

It is instructive to comment on yet another important property of the completely integrable Hamiltonian systems defined by (55) and (66), respectively, considered in Sec. VI. Recall that a Hamiltonian system is said to be quasi-bi-Hamiltonian (QBH) if its vector field X_{H_1,H_2} enjoys the following representations:

$$\mathbf{X_{H_1,H_2}}=[\mathbf{P_1},H_1]=\frac{1}{\rho}[\mathbf{P_2},H_2], \tag{76}$$

where $\mathbf{P_1}$ and $\mathbf{P_2}$ are compatible Poisson bi-vectors (i.e., $[\mathbf{P_1},\mathbf{P_2}]=0$), H_1, H_2 are the corresponding Hamiltonians, and ρ is some function. If $\rho=-\Pi_{i=1}^{n}\lambda_i$, where λ_i, $i=1,\ldots,n$ are eigenvalues of the operator $\mathbf{A}=\mathbf{P_2}\mathbf{P_1}^{-1}$, assuming $\mathbf{A}$ is of minimal degeneracy (i.e., it has exactly n distinct eigenvalues) having real eigenvalues and $\mathbf{P_1}$ is invertible, the QBH system (76) is called *Pfaffian*. For the case of a Hamiltonian system with two degrees of freedom defined by (1) we will show that this property is equivalent to the Hamilton–Jacobi separability.

Theorem 7.1: *The following statements are equivalent:*

(a) *The pseudo-Riemannian manifold* $(\hat{M},\mathbf{g})$ *defined by (1) admits a valence two Killing tensor* $\mathbf{K}$ *with real and distinct eigenvalues satisfying* $\mathrm{d}(\hat{\mathbf{K}}\mathrm{d}V)=0$, *where the* (1,1) *tensor* $\hat{\mathbf{K}}$ *is given by* $\hat{\mathbf{K}}=\mathbf{Kg}$.

(b) *The Hamiltonian system defined by (1) in the pseudo-Riemannian manifold* $(\hat{M},\mathbf{g})$ *can be integrated by separation of variables within the framework of the Hamilton–Jacobi theorem.*

(c) *A Hamiltonian system defined by (1) admits a Pfaffian QBH representation (76), where* $\mathbf{P_1}$ *is canonical and* $\mathbf{A}=\mathbf{P_2}\mathbf{P_1}^{-1}$ *is of minimal degeneracy with real and distinct eigenvalues.*

Proof: We note that a version of this theorem was announced in Ref. 18. The equivalence (a) $\Leftrightarrow$ (b) is simply a restatement of Benenti's theorem.[10] To prove the validity of the implication (b)

$\Rightarrow$ (c), we use the fact that a completely integrable Hamiltonian system defined by (1) that can be integrated by separation of variables admits the Liouville form (10)–(11) in the canonical separable coordinates (u,v)[13] [although it may also be separable in other coordinates related to (u,v)]. Then direct substitution of the functions $H_1=H$, $H_2=F/2$, where H and F are defined by (10) and (11), respectively, $\rho=-A(u)B(v)$ and the Poisson bi-vectors defined by

$$\mathbf{P_1}=\frac{\partial}{\partial u}\wedge\frac{\partial}{\partial p_u}+\frac{\partial}{\partial v}\wedge\frac{\partial}{\partial p_v},$$
$$\mathbf{P_2}=-A(u)\frac{\partial}{\partial u}\wedge\frac{\partial}{\partial p_u}+B(v)\frac{\partial}{\partial v}\wedge\frac{\partial}{\partial p_v}, \tag{77}$$

into the representation formula (76) confirms the claim. We note that the functions $A(u)$ and $B(v)$ are the eigenvalues of both the linear operator $\mathbf{A}=\mathbf{P_2}\mathbf{P_1}^{-1}$ ($\mathbf{A}$ has doubly degenerate eigenvalues) and Killing tensor $\hat{\mathbf{K}}=\mathbf{Kg}$. Next, (c) $\Rightarrow$ (b) can be easily obtained by making use of the principal result of Ref. 28, namely that there is a canonical transformation to the Darboux–Nijenhuis coordinates with respect to which the Poisson bi-vectors P_1 and P_2 are given by (77) (see also Ref. 29). Moreover, the system admits the Gantmakher form in these coordinates. Indeed, it is easy to verify that in our notations the Hamiltonian (1) takes the following form, corresponding to (77):

$$H_1=H=\frac{C_1(u,p_1)+C_2(v,p_2)}{A(u)+B(v)}, \tag{78}$$

where C_1 and C_2 are arbitrary functions, and thus is separable with respect to the coordinates (u,v). □

Remark 7.1: Taking into account that under the assumption of the theorem the linear operators $\hat{\mathbf{K}}$ and $\mathbf{A}$ share the same eigenvalues [$A(u)$ and $B(v)$ in the canonical separable coordinates (u,v)], we conclude that it is possible to classify alternatively the separable cases in terms of the eigenvalues of $\mathbf{A}$ using the Pfaffian QBH representation (76).

The following corollary describes separation of variables with respect to Cartesian coordinates.

Corollary 7.1: A Hamiltonian system defined by (1) is separable in Catesian coordinates iff it admits the Pfaffian QBH representation (76) with the (1,1) *tensor* $\mathbf{A}$: $=\mathbf{P_2}\mathbf{P_1}^{-1}$ *having constant and distinct eigenvalues*.

Separation of variables of two-dimensional Hamiltonian systems and the existence of Pfaffian QBH representations are thus intimately related. In conclusion we observe that the Liouville-integrable Hamiltonian systems investigated in Sec. VI, that is YIC1 and YIC2, are Pfaffian QBH systems, for example, in the canonical separable coordinate systems.

VIII. CONCLUDING REMARKS

In this paper we have developed an algebraic method of determining separable coordinates in the Euclidean plane based on group invariants of Killing tensors. The main advantage of our approach is that once an additional first integral quadratic in momenta is known, no additional nontrivial computations need to be performed. In a forthcoming paper, we will describe a similar algorithm for investigating orthogonal separability in the Minkowski plane based on an analogous set of group invariants. This framework also provides another starting point for investigating orthogonal separability in three-dimensional pseudo-Riemannian manifolds of constant curvature in a systematic and efficient manner. Work in this direction is under way.

We have also demonstrated that separation of variables in Hamiltonian systems with two degrees of freedom is intimately related to the existence of the Pfaffian QBH representations for the Hamiltonian systems in question. As a matter of fact the separable cases can also be classified by considering the eigenvalues of the linear operator $\mathbf{A}=\mathbf{P_2}\mathbf{P_1}^{-1}$ associated with the QBH repre-

sentation. The results presented in the last part of the paper may also lead to generalizations involving Hamiltonian systems defined in three-dimensional pseudo-Rimemannian manifolds.

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Multi-Lagrangians for integrable systems

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We propose a general scheme to construct multiple Lagrangians for completely integrable nonlinear evolution equations that admit multi-Hamiltonian structure. The recursion operator plays a fundamental role in this construction. We use a conserved quantity higher/lower than the Hamiltonian in the potential part of the new Lagrangian and determine the corresponding kinetic terms by generating the appropriate momentum map. This leads to some remarkable new developments. We show that nonlinear evolutionary systems that admit N-fold first order local Hamiltonian structure can be cast into variational form with $2N-1$ Lagrangians which will be local functionals of Clebsch potentials. This number increases to $3N-2$ when the Miura transformation is invertible. Furthermore we construct a new Lagrangian for polytropic gas dynamics in $1+1$ dimensions which is a *free, local* functional of the physical field variables, namely density and velocity, thus dispensing with the necessity of introducing Clebsch potentials entirely. This is a consequence of bi-Hamiltonian structure with a compatible pair of first and third order Hamiltonian operators derived from Sheftel's recursion operator. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1427765]

I. INTRODUCTION

In this paper we shall point out a general technique for the construction of inequivalent solutions to the inverse problem in the calculus of variations. We shall show that completely integrable partial differential equations in $1+1$ dimensions that admit multi-Hamiltonian structure can be cast into variational form with multiple Lagrangians. It is remarkable that all these new Lagrangians can be obtained directly from our present knowledge of complete integrability of the evolutionary system without doing any new calculations.

One of the important properties we expect from a completely integrable system is multi-Hamiltonian structure. A vector evolutionary system can then be cast into Hamiltonian form in more than one way

$$u^i_{t_{\aleph+\alpha-1}}=\{u^i,H_\alpha\}_\aleph=J^{ik}_\aleph\delta_k H_\alpha \quad i=1,2,\ldots,n \quad \aleph=1,2,\ldots N. \quad \alpha=-1,0,1,\ldots,\infty, \quad (1)$$

where the variational derivative is denoted by $\delta_k\equiv\delta/\delta u^k$ and J is a matrix of differential operators satisfying the properties of a Poisson tensor, namely skew-symmetry and Jacobi identity. For integrable systems there exists more than one such Hamiltonian operator and Hamiltonian function as the respective Hebrew and Greek indices indicate. Then, by the theorem of Magri[1] completely integrable systems admit infinitely many conserved Hamiltonian functions which are in involution with respect to Poisson brackets defined by compatible Hamiltonian operators.

The essential element in the multi-Hamiltonian approach to integrability is the construction of the Hamiltonian operators themselves. Fortunately this is a rich subject[2] that can be put to good use. We shall be interested in the consequences of multi-Hamiltonian structure on the Lagrangian formulation of completely integrable evolutionary equations. We shall work in the opposite direc-

tion to the traditional approach of deriving Hamiltonian structure from a Lagrangian. The crucial fact that we shall exploit is the relationship between Hamiltonian operators and Dirac brackets[3] for degenerate Lagrangian systems which was first pointed out by Macfarlane.[4] In the case of completely integrable systems we have much more information on Hamiltonian structure than Lagrangian and it became clear only recently[5–7] how we can construct multiple Lagrangians for systems that admit multi-Hamiltonian structure. We shall now present the general and most simple technique for generating these new Lagrangians.

II. MULTI-LAGRANGIANS

Evolutionary systems (1) cannot be cast into variational form with a local expression for the Lagrangian using the velocity fields u^i alone but require the introduction of Clebsch potentials. In $1+1$-dimensions the general expression for Clebsch potentials is given by

$$u^i=\phi^i_x \tag{2}$$

and in this paper we shall only consider Lagrangians that are local functionals of these potentials. In the time-honored way we shall split the Lagrangian density for Eqs. (1) into two

$$\mathcal{L}=\mathcal{T}-\mathcal{V}. \tag{3}$$

that consist of the kinetic and potential pieces, respectively. For the first Lagrangian density, an enumeration which will become clear presently, the kinetic term is always given by

$$\mathcal{T}_1=g_{ik}\phi^i_t\phi^k_x, \tag{4}$$

where g_{ik} are constants with $\det g_{ik}\neq 0$ and

$$\mathcal{V}_1=2\mathcal{H}_1 \tag{5}$$

is the Hamiltonian density. We note that the Hamiltonian function that appears in (1) is the space integral of the density. We shall number the conserved Hamiltonians by reserving the subscript 1 to the ''usual'' Hamiltonian function but of course there exists conserved quantities such as Casimirs and the momentum which are of lower order. In fact, for complete integrability, an n-component vector evolutionary system (1) must admit n infinite series of conserved Hamiltonians. We shall denote their densities by

$$\mathcal{H}_{\alpha[i]}, \quad i=1,2,...,n, \quad \alpha=-1,...,\infty \tag{6}$$

and recall that each series starts with a Casimir

$$\mathcal{H}_{-1[i]}=g_{ik}u^k \tag{7}$$

which will carry the label minus one. One of these series is distinguished in that it contains the ''usual'' Hamiltonian function which is the one that appears in Eqs. (1). For the two-component systems that we shall discuss in this paper these are the Eulerian and Lagrangian series. We note also that the two series may coincide up to a relabelling dictated by the recursion operator. This is in fact the case for the $\gamma=2$ case of gas dynamics and in most examples of completely integrable dispersive equations except the Boussinesq equation.

The potential part of the Lagrangian does not depend on the velocities and from Eq. (4) it follows that the Hessian

$$\det\left|\frac{\partial^2\mathcal{L}_1}{\partial\phi^i_t\partial\phi^k_t}\right|=0$$

vanishes identically. We have therefore a degenerate Lagrangian system and in order to cast it into Hamiltonian form we must use Dirac's theory of constraints,[3] or the covariant Witten–Zuckerman theory[8,9] of symplectic structure. In particular, the first Hamiltonian operator obtained from the first Lagrangian is given by

$$J_1^{ik}=g^{ik}D, \quad D\equiv\frac{d}{dx}, \tag{8}$$

where g^{ik} is the inverse of the coefficients in the kinetic part of the first Lagrangian (4) which is nondegenerate.

The construction of multiple Lagrangians relies on the use of the Lenard recursion relation which is implicit in Eqs. (1) that in the Greek and Hebrew indices we have a symmetric matrix

$$J^{ik}_{[\aleph}\delta_{|k|}H_{\alpha]}=0 \tag{9}$$

where square brackets denote complete skew-symmetrization and bars enclose indices which are excluded in this process. Provided we can invert these Hamiltonian operators, we can construct recursion operators

$$R^{\aleph_1\ \ i}_{\aleph_2\ \ k}=J^{im}_{\aleph_2}(J^{mk}_{\aleph_1})^{-1} \tag{10}$$

that map gradients of conserved Hamiltonians into each other (9).

For the construction of Lagrangians we start with the crucial observation that the first Lagrangian is of the form

$$\mathcal{L}_1=\mathcal{H}_{-1[i]}\phi_t^i-2\mathcal{H}_1, \tag{11}$$

which is manifest from (4). The original fields that enter into the evolutionary system (1) are Casimirs which is evident from the subscript minus one. The second Lagrangian will be of the same general structure as (11) if we further suppose that Eqs. (1) can be written in bi-Hamiltonian form. Thus there will exist H_2 which is the next conserved Hamiltonian function in the hierarchy and the momentum H_0 which comes after Casimirs. The higher Lagrangian should simply be

$$\mathcal{L}_2=\mathcal{H}_{0[i]}\phi_t^i-2\mathcal{H}_2,$$

but there is an important refinement that we need to insert here. It is not the conserved density but rather the momentum map that enters into the kinetic part of the Lagrangian. The two differ only by total derivatives which is irrelevant in the context of conservation laws and therefore generally skipped over. However, these divergence terms are of crucial interest as the momentum map in the theory of symplectic structure. We shall show that given αth local Hamiltonian structure, the full new Lagrangian is simply given by

$$\mathcal{L}_\alpha=\{\mathcal{H}_{\alpha-2[i]}+(\mathcal{G}_{\alpha-2[i]})_x\}\phi_t^i-2\mathcal{H}_\alpha, \tag{12}$$

where $\mathcal{G}_{\alpha[i]}$ is a functional of the potentials. The coefficient of ϕ_t^i above is the momentum map and this is the only calculation necessary to find the new Lagrangian.

The fact that it is the momentum map rather than the conserved density that plays an important role in the Lagrangian can be seen at the level of the first Lagrangian. Now the Casimirs play the role of the momentum map and they are used to construct the next higher conserved quantity according to the construction of the canonical energy-momentum tensor

$$\mathcal{H}_0=\frac{\partial\mathcal{L}_1}{\partial\phi_t^i}\phi_x^i=\mathcal{H}_{-1[i]}u^i=\frac{1}{2}g^{ik}\mathcal{H}_{-1[i]}\mathcal{H}_{-1[k]},$$

which is the momentum. This classical result for Lagrangians linear in the velocity can be generalized at each level we have a higher Lagrangian. We have

$$2\mathcal{H}_{\alpha-1}=g^{ik}[\mathcal{H}_{\alpha-2[i]}+(\mathcal{G}_{\alpha-2[i]})_x]\mathcal{H}_{-1[k]} \tag{13}$$

ending at the level where a local Lagrangian is no longer possible. In fact the validity of this equation is directly related to the existence of the Lagrangian. If a check of (13) fails for some α, then there exists no local Lagrangian at αth level.

Now we come to an important reservation that our new Lagrangians will necessarily carry. The Euler equations that follow from the variation of the action with the second Lagrangian will be

$$R_2^{1\ i}{}_k[u_t^k-J_1^{km}\delta_m H_1]=0, \tag{14}$$

so that the first variation of the second action will certainly be an extremum for the original equations of motion (1) but the Euler equations (14) require something weaker, namely linear combinations of functionals in the kernel of the recursion operator can be added to the right-hand side of the equations of motion and the new action will still be an extremum.

From this construction it is manifest that for every Hamiltonian function in the infinite hierarchy of conserved Hamiltonians that we have for completely integrable systems, there exists a degenerate Lagrangian (12) that yields the equations of motion as its Euler equation up to functionals in the kernel of the recursion operator. The number of Lagrangians that can be constructed in this way is therefore infinite in number. Given bi-Hamiltonian structure we have two local Hamiltonian operators but the Lenard recursion operator (10) is nonlocal. However, the special form of the first Hamiltonian operator (8) leads to a local expression for the second Lagrangian in terms of Clebsch potentials. But it is clear that the repeated application of the recursion operator will require the introduction of nonlocal terms in higher Lagrangians. Strictly speaking, this is not a problem because the original Lagrangian is itself nonlocal in terms of the velocity fields u^i which are the original variables. We swept this problem under the rug by introducing Clebsch potentials. Higher Lagrangians for evolutionary equations (1) can be written in local form by introducing potentials for the Clebsch potentials themselves. If, however, the equations of motion admit N local Hamiltonian operators, then our construction guarantees the existence of N Lagrangians which are local functionals of the Clebsch potentials. Thus we have the following theorems.

Theorem 1: *A completely integrable system that admits N-fold local first order Hamiltonian structure can be given N different variational formulations with degenerate Lagrangians that are local functionals of the Clebsch potentials.*

By a convenient abuse of language we claim that we have a Lagrangian for an equation that involves fields when the Lagrangian is in fact only a functional of the Clebsch potentials for these fields. Then we have the audacity to put in by hand the expression for the fields in terms of potentials after the variation. This can be at best only a shorthand for the real variational principle where we must impose the relationship between the fields and their potentials through Lagrange multipliers.

So far we have been guilty of this abuse ourselves. But now we must say that the first Lagrangian is actually

$$\mathcal{L}_1^{\text{full}}=\mathcal{L}_1(\phi^i,\phi_x^i,\phi_{xx}^i,\ldots)+\lambda_i(u^i-\phi_x^i) \tag{15}$$

so that upon variation with respect to all the variables ϕ^i, u^i, λ_i we get (2), $\lambda_i=0$ and arrive at the equations of motion (1) expressed in terms of the original fields u^i without fudging.

Now this obvious observation may seem correct but naive, however, we shall now find that it dramatically increases the number of new Lagrangians we can construct for integrable systems.

For every evolutionary equation that admits, say for simplicity, bi-Hamiltonian structure there exists a differential substitution

$$u^i = M^i(r^k, r^k_x, \ldots) \tag{16}$$

that brings the second Hamiltonian operator to the canonical form (8) of Darboux. This differential substitution is a Miura transformation. Strictly speaking the theorem of Darboux remains unproved in field theory where the number of degrees of freedom is infinite but we shall assume it. Miura transformation works in a direction opposite to the usual action of the recursion operator. It leads to Hamiltonian equations

$$r^i_t = \{r^i, H_0\}_1 = g^{ik} D \delta_{r^k} H_0|_{u^m = M^m(r^n)}, \tag{17}$$

where H_0 is the momentum for Eqs. (1) expressed through (16). These are modified equations, different from the original equations, but the two sets are related by

$$u^i_t - J^{ik}_2 \delta_{u^k} H_0(u) = \mathcal{O}^i_j(r^l)[r^j_t - J^{jk}_1 \delta_{r^k} H_0|_{u^m = M^m(r^n)}] \tag{18}$$

up to functions in the kernel of some matrix differential operator $\mathcal{O}^i_j$.

A comparison of Eqs. (14) and Miura's relation (18) shows us that using the differential substitution of Miura we can obtain new Lagrangians for nonlinear evolution equations that admit multi-Hamiltonian structure in the opposite direction to our earlier construction. Transforming to the variables r^i and using new Clebsch potentials

$$r^i = \psi^i_x \tag{19}$$

we can write the classical Lagrangian for the modified system (17)

$$\mathcal{L}^{\text{modified}}_1 = g_{ik} \psi^i_x \psi^k_t - 2\mathcal{H}_0|_{u^m = M^m(\psi_x, \psi_{xx}, \ldots)}, \tag{20}$$

where the labeling of $\mathcal{H}_0$ refers to its expression in the original variables u^i but these need to be substituted for in terms of r^i according to (16) and expressed through the potentials (19). We note that the Casimirs $r^i = \psi^i_x$ for the modified system are absent in the polynomial $\mathcal{H}_\alpha(u)$ hierarchy. We would expect naively that the Euler equations resulting from the first variation of the action with the Lagrangian (20) would result in the modified equations (17). This would indeed be the case if we were to impose the constraint between the fields r^i and their potentials ψ^i as in (15) but now using (19). However, by imposing the constraint through Miura's differential substitution

$$\mathcal{L}^{\text{full}}_0 = \mathcal{L}^{\text{modified}}_1(\psi^i_x, \psi^i_{xx}, \ldots) + \lambda_i[u^i - M^i(\psi^i_x, \psi^i_{xx}, \ldots)] \tag{21}$$

we obtain a new Lagrangian for the original equation (1) in the original variables u^i. We shall use this construction to derive new Lagrangians, in particular for KdV in Sec. III. It is evident that this construction can be extended when there exists multi-Hamiltonian structure but, as we shall find in the example of KdV, sometimes it is possible to arrive at local Lagrangians using nonlocal Hamiltonian operators as well. We conclude with the following.

Theorem 2: *The first Lagrangian of every modified equation obtained through a Miura transformation will serve as a new zeroth Lagrangian for the original equations of motion provided the constraint between the fields and their potentials is imposed through a Miura-type differential substitution. For N-fold Hamiltonian structure there exists* $N-1$ *such new Lagrangians.*

Miura transformation is in general not invertible because it is a differential substitution. But there exist interesting examples where it reduces to a point transformation which is invertible. In that case we can construct $N-1$ further Lagrangians.

We conclude that for an evolutionary system that admits N-fold first order Hamiltonian structure, the number of different variational principles where the first variation will be an extremum by virtue of the original equations of motion is $2N-1$ and in the case Miura transformation is invertible $3N-2$. We illustrate this situation for the case of bi-Hamiltonian structure in Tables I

TABLE I. The hierarchy of local Hamiltonian structures and Lagrangians which are local functionals of Clebsch potentials for evolutionary system $u_t=J_1\delta H_1=J_2\delta H_0$ where J_1 is in the canonical Darboux form.

Equations of motion	$u_t=J_2\delta H_0$	$u_t=J_1\delta H_1$	$J_2J_1^{-1}u_t=-\delta_\phi H_2$
Local Hamiltonian op.	J_2	J_1	no
Local Lagrangian	no	$\mathcal{L}_1$	$\mathcal{L}_2$
Modified equations	$r_t=\tilde{J}_2\delta H_0$	$r_t=\tilde{J}_1\delta H_1$	
Local Hamiltonian op.	$\tilde{J}_2=J_1$	$\tilde{J}_1$	
Local Lagrangian	$\mathcal{L}_0$	no	

and II. The general situation is much more complicated than what these tables would lead us to expect. Starting with tri-Hamiltonian structure the individual entries in each one of these tables will need to be a table by itself because there are inequivalent Hamiltonian operators that yield the same equations of motion with the same Hamiltonian function. We shall discuss this interesting situation in a future publication on the Chaplygin–Born–Infeld equation.

III. KDV

KdV stands as the symbol of completely integrable systems. We think we know it, but it turns out to be so rich that there is still new information to be learned about it. We recall that KdV

$$u_t+6uu_x-u_{xxx}=0 \tag{22}$$

admits the Kruskal sequence of conserved Hamiltonian densities

$$\mathcal{H}_{-1}^{\mathrm{KdV}}=u, \tag{23}$$

$$\mathcal{H}_{0}^{\mathrm{KdV}}=\tfrac{1}{2}u^2, \tag{24}$$

$$\mathcal{H}_{1}^{\mathrm{KdV}}=u^3+\tfrac{1}{2}u_x^2, \tag{25}$$

$$\mathcal{H}_{2}^{\mathrm{KdV}}=\tfrac{5}{2}u^4+5uu_x^2+\tfrac{1}{2}u_{xx}^2, \tag{26}$$

$$\cdots$$

which are in involution with respect to Poisson brackets defined by two Hamiltonian operators

$$J_1=D, \qquad J_2=-D^3+2uD+2Du, \tag{27}$$

that form a Poisson pencil. By introducing the potential

$$u=\phi_x. \tag{28}$$

KdV can be cast into variational form with two Lagrangians

$$\mathcal{L}_1^{\mathrm{KdV}}=\mathcal{H}_{-1}^{\mathrm{KdV}}\phi_t-2\mathcal{H}_1^{\mathrm{KdV}}, \tag{29}$$

TABLE II. When the Miura transformation is invertible we need to include an additional column to the left of Table I.

Equations of motion		$u_t=J_2\delta H_0$	$\cdots$
Local Hamiltonian op.		J_2	$\cdots$
Local Lagrangian		no	$\cdots$
Modified equations	$\tilde{J}_1\tilde{J}_2^{-1}r_t=-\delta_\psi H_{-1}$	$r_t=\tilde{J}_2\delta H_0$	$\cdots$
Local Hamiltonian op.	no	$\tilde{J}_2=J_1$	$\cdots$
Local Lagrangian	$\mathcal{L}_{-1}$	$\mathcal{L}_0$	$\cdots$

$$\mathcal{L}_2^{\mathrm{KdV}}=(\mathcal{H}_0^{\mathrm{KdV}}+\phi_{xxx})\phi_t-2\mathcal{H}_2^{\mathrm{KdV}}, \tag{30}$$

which consist of the classical Lagrangian and the second Lagrangian,[5] respectively. Note that there is a misprint in the potential term of the second Lagrangian reported in Ref. 6 but the results that follow are correct. Here we observe that both (29) and (30) are examples of our general expression (12) for higher Lagrangians.

The second application of Lenard's recursion operator to J_1 results in a third Hamiltonian operator which is nonlocal so we cannot continue to generate higher Lagrangians. But we can use Theorem 2 to generate new lower Lagrangians for KdV. For this purpose we note that in both Lagrangians (29) and (30) we should have added the constraint $\lambda(u-\phi_x)$ and written the full Lagrangian. But following the convenient abuse of language we did not do so because it was manifest. It is, however, necessary to write the full Lagrangian in the case of lower Lagrangians.

According to our general construction of lower Lagrangians we first recall the original Miura transformation

$$u=r^2+r_x \tag{31}$$

that brings J_2 to the canonical form of J_1 in the variable r. The equation of motion for r is mKdV which is different from (22) but under the substitution (31) we have Miura's result

$$u_t+6uu_x-u_{xxx}=(D+2r)(r_t+6r^2r_x-r_{xxx})=0, \tag{32}$$

so that, on shell, if mKdV is satisfied then so is KdV. Now we can introduce the Clebsch potential for the modified field variable

$$r=\psi_x \tag{33}$$

and write the first Lagrangian for mKdV

$$\mathcal{L}_1^{\mathrm{mKdV}}=\psi_x\psi_t+\mathcal{H}_0^{\mathrm{KdV}}|_{u=\psi_x^2+\psi_{xx}} \tag{34}$$

in a straightforward manner. But now enforcing the constraint in the full Lagrangian through the Miura transformation

$$\mathcal{L}_0^{\mathrm{KdV\ full}}=\mathcal{L}_1^{\mathrm{mKdV}}+\lambda(u-\psi_x^2-\psi_{xx}) \tag{35}$$

we shall arrive at a new Lagrangian for KdV because the Euler equation that comes from the first variation of this action will be satisfied by virtue of (32). Unlike (30) which is a higher Lagrangian, (35) is a lower Lagrangian in the sense of the action of the recursion operator on the equations of motion.

And the saga of KdV continues. We consider the third Hamiltonian operator for KdV

$$J_3=R^2J_1 \tag{36}$$

which is nonlocal but the relationship between differential substitutions and Hamiltonian structures of KdV (Ref. 24) enables us to construct another new local Lagrangian for KdV. For this purpose we recall that the differential substitution

$$r=\alpha q+\frac{\varepsilon}{q}+\frac{q_x}{2q}, \tag{37}$$

which transforms mKdV into twice modified KdV

$$q_t=\left(q_{xx}-\frac{3q_x^2}{2q}+\frac{6\varepsilon^2}{q}-2\alpha^2q^3\right)_x \tag{38}$$

is a Miura transformation for (36). This can best be seen by the expression

$$J_3=\tfrac{1}{2}(q^2D+Dq^2)-q_xD^{-1}q_x \tag{39}$$

for the third nonlocal Hamiltonian operator for KdV in terms of the twice modified variable q. We recall that J_3 is fifth order in u. We have the Miura relation

$$r_t+6r^2r_x-r_{xxx}=\left(\alpha-\frac{\varepsilon}{q^2}-\frac{q_x}{2q^2}+\frac{1}{q}D\right)\left[q_t-\left(q_{xx}-\frac{3q_x^2}{2q}+\frac{6\varepsilon^2}{q}-2\alpha^2q^3\right)_x\right]=0 \tag{40}$$

between modified and twice modified KdV's. Introducing the potential for the twice modified variable $q=\chi_x$ we have

$$u=\Phi(\chi_x,\chi_{xx},\chi_{xxx})\equiv\frac{\chi_{xxx}}{\chi_x}-\frac{\chi_{xx}^2}{\chi_x^2}+2\alpha\chi_{xx}+\alpha^2\chi_x^2+2\alpha\varepsilon+\frac{\varepsilon^2}{\chi_x^2} \tag{41}$$

in terms of the original field u. The first Lagrangian for twice modified KdV is simply

$$\mathcal{L}_1^{\mathrm{m}_2\mathrm{KdV}}=\chi_x\chi_t+\mathcal{H}_{-1}^{\mathrm{KdV}}|_{u=\Phi(\chi_x,\chi_{xx},\chi_{xxx})} \tag{42}$$

and therefore the second lower Lagrangian for KdV is given by

$$\mathcal{L}_{-1}^{\mathrm{KdV\ full}}=\mathcal{L}_1^{\mathrm{m}_2\mathrm{KdV}}+\lambda[u-\Phi(\chi_x,\chi_{xx},\chi_{xxx})] \tag{43}$$

which provides another illustration of (21). This process can be continued.

We note that an alternative to the Clebsch potential for KdV is the Schwartzian which was pointed out by Schiff.[10] We shall postpone consideration of Schwartzian potentials to future work.

IV. POLYTROPIC GAS DYNAMICS

The simplest examples for applying our construction of multi-Lagrangians consist of quasi-linear second order hyperbolic equations that Dubrovin and Novikov[11] have called equations of hydrodynamic type. The distinguished example in this set consists of the Eulerian equations of polytropic gas dynamics in $1+1$ dimensions,

$$\rho_t+u\rho_x+\rho u_x=0,\quad u_t+uu_x+\rho^{\gamma-2}\rho_x=0, \tag{44}$$

and in particular for $\gamma=-1$ we have the case of Chaplygin gas, or Born–Infeld equation that was recently shown to have a string theory antecedent.[12] This system can be cast into quadri-Hamiltonian form.[13] For the Chaplygin–Born–Infeld case the complete Hamiltonian structure can be found in Ref. 14 and its symmetries were given in Ref. 15. In the following we shall use the labeling $u^1=\rho$ and $u^2=u$.

First we have three local Hamiltonian structures of first order[16]

$$J_1=\begin{pmatrix}0 & D\\ D & 0\end{pmatrix}=\sigma^1D, \tag{45}$$

$$J_2=\begin{pmatrix}\rho D+D\rho & (\gamma-2)Du+uD\\ Du+(\gamma-2)uD & \rho^{\gamma-2}D+D\rho^{\gamma-2}\end{pmatrix}, \tag{46}$$

$$J_3=\begin{pmatrix} u\rho D+Du\rho & D\left[\frac{1}{2}(\gamma-2)u^2+\frac{1}{\gamma-1}\rho^{\gamma-1}\right]+\left[\frac{1}{2}u^2+\frac{1}{\gamma-1}\rho^{\gamma-1}\right]D \\ D\left[\frac{1}{2}u^2+\frac{1}{\gamma-1}\rho^{\gamma-1}\right]+\left[\frac{1}{2}(\gamma-2)u^2+\frac{1}{\gamma-1}\rho^{\gamma-1}\right]D & u\rho^{\gamma-2}D+Du\rho^{\gamma-2} \end{pmatrix}, \tag{47}$$

which form a Poisson pencil $\mathcal{J}=J_1+c_1J_2+c_2J_3$ with c_1,c_2 constants, i.e., these Hamiltonian operators are compatible. In Eq. (45) σ^1 is the Pauli matrix and this is the canonical Darboux form of first order Hamiltonian operators. The equations of polytropic gas dynamics admit two infinite hierarchies of conserved Hamiltonians which are in involution with respect to Poisson brackets defined by all three of these Hamiltonian operators. In the first set, which is called Eulerian,[13] the Hamiltonian densities are given by

$$\mathcal{H}^E_{-1}=\rho, \tag{48}$$

$$\mathcal{H}^E_0=u\rho, \tag{49}$$

$$\mathcal{H}^E_1=\frac{1}{2}u^2\rho+\frac{1}{\gamma(\gamma-1)}\rho^{\gamma}, \tag{50}$$

$$\mathcal{H}^E_2=\frac{1}{6}u^3\rho+\frac{1}{\gamma(\gamma-1)}u\rho^{\gamma}, \tag{51}$$

$$\mathcal{H}^E_3=\frac{1}{24}u^4\rho+\frac{1}{2\gamma(\gamma-1)}u^2\rho^{\gamma}+\frac{1}{2\gamma(\gamma-1)^2(2\gamma-1)}\rho^{2\gamma-1}, \tag{52}$$

$$\cdots,$$

where (49) is the momentum, (50) is the familiar Hamiltonian function, the Casimir is in (48) and the rest consist of higher Hamiltonians. Therefore, the Euler series is the distinguished one in the terminology of Sec. II. The second series

$$\mathcal{H}^L_{-1}=u, \tag{53}$$

$$\mathcal{H}^L_0=\frac{1}{2}(\gamma-2)u^2+\frac{1}{\gamma-1}\rho^{\gamma-1}, \tag{54}$$

$$\mathcal{H}^L_1=\frac{1}{6}(\gamma-2)u^3+\frac{1}{\gamma-1}u\rho^{\gamma-1}, \tag{55}$$

$$\mathcal{H}^L_2=\frac{1}{24}(\gamma-2)u^4+\frac{1}{4(\gamma-1)}u^2\rho^{\gamma-1}+\frac{1}{2(\gamma-1)^2(2\gamma-3)}\rho^{2(\gamma-1)}, \tag{56}$$

$$\cdots$$

is the Lagrangian series which starts with the Casimir (53). Note that for $\gamma=2$ this series is no longer polynomial as logarithms will enter and the same remark holds for integer and half-integer values of γ in both series.

Finally, we note that the recursion operator $R_2^1=J_2J_1^{-1}$ can be used to write infinitely many Hamiltonian operators by letting it to act n times on J_1. However, in general none of these operators will be local. In particular we note that

$$R_3^1=J_3(J_1)^{-1}\neq(R_2^1)^2, \quad J_3\neq J_2J_1^{-1}J_2, \tag{57}$$

except in the case of shallow water waves where $\gamma=2$ which admits extension to integrable dispersive equations.

Next, there is a third order Hamiltonian operator[17] which was obtained from Sheftel's remarkable recursion operator[18]

$$J_4=DU_x^{-1}DU_x^{-1}\sigma^1D, \tag{58}$$

where

$$U=\begin{pmatrix} u & \rho \\ \dfrac{1}{\gamma-2}\rho^{\gamma-2} & u \end{pmatrix} \tag{59}$$

which is only compatible with J_0. Higher conserved Hamiltonians start with the density[18,19]

$$\hat{\mathcal{H}}_{-1}^{SV(E)}=\frac{\rho_x}{u_x^2-\rho^{\gamma-3}\rho_x^2} \tag{60}$$

and its flux,

$$\mathcal{F}_{-1}^{SV(L)}=-\frac{u_x}{u_x^2-\rho^{\gamma-3}\rho_x^2}, \tag{61}$$

which is the first in an infinite hierarchy of non-polynomial conservation laws for gas dynamics that depend on space derivatives.

We will be interested in the Lagrangian formulation of the equations of polytropic gas dynamics (44) that correspond to all these Hamiltonian structures. Introducing the Clebsch potentials[20]

$$u=\varphi_x, \quad \rho=\psi_x \tag{62}$$

we have the first Lagrangian representation for this system

$$\mathcal{L}_1^\gamma=\mathcal{H}_{-1}^L\psi_t+\mathcal{H}_{-1}^E\varphi_t-2\mathcal{H}_1^E(\varphi_x,\psi_x) \tag{63}$$

but using the recursion operators $J_2J_1^{-1}$ and $J_3J_1^{-1}$ we find two further Lagrangians

$$\mathcal{L}_2^\gamma=\mathcal{H}_0^L\psi_t+\mathcal{H}_0^E\varphi_t-2\mathcal{H}_2^E(\varphi_x,\psi_x), \tag{64}$$

$$\mathcal{L}_3^\gamma=\mathcal{H}_1^L\psi_t+\mathcal{H}_1^E\varphi_t-2\mathcal{H}_3^E(\varphi_x,\psi_x), \tag{65}$$

which are local functionals of the Clebsch potentials. The Lagrangian obtained through the action of the recursion operator $J_4J_1^{-1}$ is the most interesting one. Because J_4 is a third order operator, the fourth Lagrangian

$$\mathcal{L}_4^\gamma=\mathcal{H}_{-1}^{SV(E)}u_t+\mathcal{F}_{-1}^{SV(L)}\rho_t-2\mathcal{H}_{-1}^E(\varphi_x,\psi_x), \tag{66}$$

$$\mathcal{L}_4^\gamma=\frac{\rho_xu_t-u_x\rho_t}{u_x^2-\rho^{\gamma-3}\rho_x^2}-2\rho \tag{67}$$

is *free*, i.e., it does not contain any Lagrange multipliers, and furthermore it is *local in the original fields*, namely the density and velocity. This is the first time it has been possible to write down such a Lagrangian for polytropic gas dynamics. It was made possible only because of bi-Hamiltonian structure with a pair of first and third order Hamiltonian operators. Here we find another remarkable situation in that the number of Lagrangians that we can construct by repeated application of Sheftel's recursion operator $J_4 J_1^{-1}$ is *infinite* in number. All of these Lagrangians will be *free* and *local* in the original field variables ρ and u.

Now we come to lower Lagrangians that will arise from Miura transformations. The Miura transformations that bring the Hamiltonian operators (46) and (47) to the Darboux form of (45) are point transformations for equations of hydrodynamic type. Dubrovin and Novikov had pointed out that first order Hamiltonian operators for equations of hydrodynamic type are given by

$$J^{ik}=g^{ik}D-g^{im}\Gamma^k_{mn}u^n_x \tag{68}$$

where g_{ik} are the components of a Riemannian metric which is flat by virtue of the Jacobi identities. The Miura transformation provides manifestly flat coordinates for this metric. For example from (46) we find the flat metric

$$ds_2^2=\frac{2}{4\rho^{\gamma-1}-(\gamma-1)^2u^2}[\rho^{\gamma-2}\,d\rho^2-(\gamma-1)u\,d\rho\,du+\rho\,du^2] \tag{69}$$

and it can be verified that the Miura transformation

$$\rho=rp, \qquad u=\frac{1}{\gamma-1}(r^{\gamma-1}+p^{\gamma-1}) \tag{70}$$

brings it into the manifestly flat form $2\,dr\,dp$. In these variables we find the first modified equations of gas dynamics

$$\begin{aligned} &r_t+\frac{\gamma}{\gamma-1}(r^{\gamma-1}+p^{\gamma-1})r_x+\gamma rp^{\gamma-2}p_x=0,\\ &p_t+\gamma pr^{\gamma-2}r_x+\frac{\gamma}{\gamma-1}(r^{\gamma-1}+p^{\gamma-1})p_x=0, \end{aligned} \tag{71}$$

and linear combinations of these equations with variable coefficients give Eqs. (44) of gas dynamics. Introducing the potentials

$$r=\chi_x, \quad p=v_x, \tag{72}$$

we have the Lagrangian

$$\mathcal{L}_0^{\gamma\text{full}}=\chi_x v_t+v_x\chi_t-2\mathcal{H}_0^E+\lambda\left(u-\frac{\chi_x^{\gamma-1}+v_x^{\gamma-1}}{\gamma-1}\right)+\sigma(\rho-\chi_x v_x), \tag{73}$$

where $\mathcal{H}_0^E$ is the momentum (49) expressed in terms of the potentials χ and v. Transforming to the first modified variables r, p we get $\tilde{J}_1$, $\tilde{J}_2=J_1$ and $\tilde{J}_3$ defining the tri-Hamiltonian structure of Eqs. (71). Now there is a new lower Lagrangian that we can construct from the recursion operator $\tilde{J}_1\tilde{J}_2^{-1}$. We find

$$\tilde{J}_1=\begin{pmatrix} (1-\gamma)[rp^{\gamma-2}\Delta D+Dp^{\gamma-2}\Delta] & [(\gamma-2)r^{\gamma-1}+p^{\gamma-1}]\Delta D \\ [r^{\gamma-1}+(\gamma-2)p^{\gamma-1}]\Delta D & +D[r^{\gamma-1}+(\gamma-2)p^{\gamma-1}]\Delta \\ +D[(\gamma-2)r^{\gamma-1}+p^{\gamma-1}]\Delta & (1-\gamma)[pr^{\gamma-2}\Delta D+Dpr^{\gamma-2}\Delta] \end{pmatrix}, \tag{74}$$

$$\Delta \equiv \frac{1}{(\gamma-1)(r^{\gamma-1}-p^{\gamma-1})^2},$$

where the labeling of the variables is in the order r and p. The new Lagrangian is given by

$$\mathcal{L}_{-1}^{\gamma\text{full}} = \frac{\chi_x v_t - v_x \chi_t}{\chi_x^{\gamma-1} - v_x^{\gamma-1}} - \mathcal{H}_{-1}^{E} + \lambda\left(u - \frac{\chi_x^{\gamma-1} + v_x^{\gamma-1}}{\gamma-1}\right) + \sigma(\rho - \chi_x v_x), \tag{75}$$

where the momenta do not belong to the polynomial series of conserved Hamiltonians. However, we can identify the lower momenta from this Lagrangian

$$\mathcal{H}_{-2}^{\gamma\pm} = \xi_{\pm}^{(3-\gamma)/(\gamma-1)}(\xi_+\xi_-)^{-1/2}, \quad \xi^2 + (\gamma-1)u\xi + \rho^{\gamma-1} = 0$$

where $\pm$ refers to Eulerian and Lagrangian series as well as the roots of the quadratic equation.

We now turn to the third Hamiltonian structure (47) defined by the flat metric

$$ds_3^2 = -\frac{8(\gamma-1)^2}{[(\gamma-1)^2u^2 - 4\rho^{\gamma-1}]^2}\left\{u\rho^{\gamma-2}\,d\rho^2 - \frac{1}{2(\gamma-1)}[(\gamma-1)^2u^2 + 4\rho^{\gamma-1}]d\rho\,du + u\rho\,du^2\right\}$$
$$= 2\,dq\,dw, \tag{76}$$

and the coordinate transformation that brings it to the manifestly flat form is given by

$$q = [(\gamma-1)^2u^2 - 4\rho^{\gamma-1}]^{[(\gamma-3)/2(1-\gamma)]}, \tag{77}$$

$$w = \int^z \frac{1}{\sqrt{1+\xi^2}}\,\xi^{(\gamma-3)/(1-\gamma)}\,d\xi, \tag{78}$$

$$z = \sinh\left\{\frac{1}{2}\ln\frac{(\gamma-1)u + 2\rho^{(\gamma-1)/2}}{(\gamma-1)u - 2\rho^{(\gamma-1)/2}}\right\},$$

where, in general, the last integral cannot be done in closed form. For some specific values of γ the integral (78) is elementary as in the notable case of Chaplygin–Born–Infeld. But this paper is devoted to the general case of polytropic gas dynamics and we shall not consider inverting (77), (78) to obtain u, ρ as functions of q and w. We shall only remark that after this inversion we can obtain two more new Lagrangians.

The Lagrangians (63), (64), and (65) for polytropic gas dynamics are examples illustrating the general expression (12) for higher Lagrangians. For equations of hydrodynamic type there is no dispersion and hence $\mathcal{G}$ vanishes identically. We have given only two (73), (75) of the four lower Lagrangians because the integral (78) must be carried out before we arrive at the second modified equations of gas dynamics which will lead to two further new Lagrangians. Certainly the Lagrangian (67) which is derived from bi-Hamiltonian structure with a compatible pair of first and third order operators according to (12) is the most remarkable one because this is the first time it has been possible to write an unconstrained Lagrangian for polytropic gas dynamics that is local in the original field variables, namely the density and velocity. Furthermore it is only the first element in an infinite series of such Lagrangians.

V. KAUP–BOUSSINESQ SYSTEM

Gas dynamics with $\gamma=2$ governs the behavior of long waves in shallow water. From the point of view of complete integrability it is a remarkable case, because in this case we find several completely integrable dispersive generalizations of Eqs. (44). Most prominent among them is the well-known Kaup–Boussinesq system[21]

$$u_t=\left(\frac{u^2}{2}+p\right)_x, \quad \rho_t=(u\rho+\varepsilon^2 u_{xx})_x, \tag{79}$$

which admits tri-Hamiltonian structure. The first Hamiltonian structure is given by the Hamiltonian operator (45) and

$$J_2^{KBq}=\begin{pmatrix} D & \frac{1}{2}Du \\ \frac{1}{2}uD & \frac{1}{2}(\rho D+D\rho)+\varepsilon^2 D^3 \end{pmatrix}, \tag{80}$$

where D^{-1} denotes the principal value integral, is the second Hamiltonian operator for the Kaup–Boussinesq system. In the limit $\varepsilon\to 0$ this Hamiltonian operator reduces to (46) with $\gamma=2$. The recursion operator is given by

$$R_2^{1\,KBq}=\begin{pmatrix} \frac{1}{2}u+\frac{1}{2}u_x D^{-1} & 1 \\ \varepsilon^2 D^2+\rho+\frac{1}{2}\rho_x D^{-1} & \frac{1}{2}u \end{pmatrix} \tag{81}$$

and there is a third local Hamiltonian operator obtained by the action of the recursion operator $J_2^{KBq}=(R_2^{1KBq})^2 J_0$ as in the $\gamma=2$ case of gas dynamics.

The conserved Hamiltonians in the Eulerian and Lagrangian series are

$$\mathcal{H}_{-1}^{KBq}=\rho, \tag{82}$$

$$\mathcal{H}_{0}^{KBq}=u\rho, \tag{83}$$

$$\mathcal{H}_{1}^{KBq}=\tfrac{1}{2}(\rho u^2+\rho^2+\varepsilon^2 u u_{xx}), \tag{84}$$

$$\mathcal{H}_{2}^{KBq}=\tfrac{1}{2}[\rho u^3+3\rho^2 u-\varepsilon^2(4u_x\rho_x+3uu_x^2)], \tag{85}$$

$$H_{3}^{KBq}=\tfrac{1}{4}u^4\rho+\tfrac{3}{2}u^2\rho^2+\tfrac{1}{2}\rho^3+\varepsilon^4 u_{xx}^2-\varepsilon^2(\tfrac{5}{2}\rho u_x^2+4uu_x\rho_x+\rho_x^2+\tfrac{3}{2}u^2u_x^2), \tag{86}$$

$$\cdots,$$

and the degeneracy in the $\gamma=2$ case of gas dynamics is repeated in its dispersive generalization. In particular, the Lagrangian and Eulerian series coincide apart from a relabeling

$$\begin{gathered} \mathcal{H}_{-2}^{KBq(E)}=u=\mathcal{H}_{-1}^{KBq(L)}, \\ \mathcal{H}_{-1}^{KBq(E)}=\rho=\mathcal{H}_{0}^{KBq(L)}, \\ \cdots, \\ \mathcal{H}_{-2+n}^{KBq(E)}=\mathcal{H}_{-1+n}^{KBq(L)}, \end{gathered} \tag{87}$$

that is dictated by the recursion operator.

With the aid of the Clebsch potentials

$$u=\varphi_x, \qquad \rho=\psi_x, \tag{88}$$

we obtain

$$\mathcal{L}_1^{KBq}=\mathcal{H}_{-1}^{KBq}\varphi_t+\mathcal{H}_{-2}^{KBq}\psi_t-2\mathcal{H}_1^{KBq}(\varphi_x,\psi_x,\varphi_{xx},\psi_{xx},\ldots) \tag{89}$$

for the first Lagrangian. Using the technique we have presented in Sec. II we shall now construct higher Lagrangians. These three local Hamiltonian structures enable us to construct two new Lagrangians

$$\mathcal{L}_2^{KBq}=(\mathcal{H}_0^{KBq}+\varepsilon^2\varphi_{xxx})\varphi_t+\mathcal{H}_{-1}^{KBq}\psi_t-2\mathcal{H}_2^{KBq}(\varphi_t,\psi_x,\varphi_{xx},\psi_{xx},\ldots) \tag{90}$$

and

$$\mathcal{L}_3^{KBq}=[\mathcal{H}_1^{KBq}+\varepsilon^2(2\psi_{xxx}+\varphi_{xx}^2+\varphi_x\varphi_{xxx})]\varphi_t+(\mathcal{H}_0^{KBq}+\varepsilon^2\varphi_{xxx})\psi_t-2\mathcal{H}_3^{KBq}(\varphi_x,\psi_x,\ldots) \tag{91}$$

for the Kaup–Boussinesq system. The determination of $\mathcal{G}_{\beta;[i]}$ is according to Eq. (12) with $\beta=2,3$ and $[2]=[1]-1$ because of the relabeling difference (87) between the Lagrangian and Eulerian series. Note that the momentum map which is the coefficient of ϕ_t in (90) is exactly the same as the momentum in front of ψ_t in (91). The reason for this goes back to the degeneration of the Eulerian and Lagrangian series into one and the fact that it is the momentum map that is the important element in the general construction (12). In the dispersionless limit the Lagrangians (89), (90), (91) reduce to the gas dynamics Lagrangians (63), (64), and (65) with $\gamma=2$.

VI. KAUP–BROER SYSTEM

There is another completely integrable dispersive version of the $\gamma=2$ case of gas dynamics which is the Kaup–Broer system.[21,22] The triangular invertible differential substitution

$$\rho=\eta+\varepsilon u_x \tag{92}$$

transforms the Kaup–Boussinesq system (79) into the Kaup–Broer system

$$u_t=uu_x+\eta_x+\varepsilon u_{xx},\qquad \eta_t=(\eta u)_x-\varepsilon\eta_{xx}, \tag{93}$$

which also has three local Hamiltonian structures.[23] For the Kaup-Broer system the conserved Hamiltonians in the Eulerian series are given by

$$\mathcal{H}_0^{KBr}=u\eta, \tag{94}$$

$$\mathcal{H}_1^{KBr}=\tfrac{1}{2}[u^2\eta+\eta^2-2\varepsilon\eta u_x], \tag{95}$$

$$\mathcal{H}_2^{KBr}=\tfrac{1}{2}[u^3\eta+3u\eta^2+6\varepsilon\eta uu_x-4\varepsilon^2u_x\eta_x], \tag{96}$$

$$\mathcal{H}_3^{KBr}=\tfrac{1}{4}u^4\eta+\tfrac{3}{2}u^2\eta^2+\tfrac{1}{2}\eta^3+\varepsilon(\tfrac{3}{2}\eta^2u_x-u^3\eta_x)+\varepsilon^2(2u^2\eta_{xx}-\eta u_x^2-\eta_x^2)-2\varepsilon^2\eta_xu_{xx}, \tag{97}$$

which can be obtained from (83)–(85) through the substitution (92). The first Hamiltonian operator for the Kaup–Broer system is given by (45) and the second Hamiltonian operator

$$J_1^{KBr}=\begin{pmatrix} D & \tfrac{1}{2}Du+\varepsilon D^2 \\ \tfrac{1}{2}uD-\varepsilon D^2 & \tfrac{1}{2}(\eta D+D\eta) \end{pmatrix} \tag{98}$$

can be obtained from (80) of the Kaup–Boussinesq system using the substitution (92).

For Kaup–Broer system we introduce the potentials

$$\eta=w_x,\qquad \psi=w+\varepsilon\varphi_x, \tag{99}$$

and arrive at the first Lagrangian

$$\mathcal{L}_1^{KBr}=\mathcal{H}_{-1}^{KBq}\varphi_L+\mathcal{H}_{-2}^{KBr}w_t-2\mathcal{H}_1^{KBr}(w_x,\varphi_x,w_{xx},\varphi_{xx},\ldots), \tag{100}$$

but now we can derive two further Lagrangians using the recursion operator obtained from the Hamiltonian operators (98) and (45). Following our procedure of Sec. II we find the second Lagrangian

$$\mathcal{L}_2^{KBr}=(\mathcal{H}_0^{KBr}-2\varepsilon w_{xx})\varphi_t+\mathcal{H}_{-1}^{KBr}w_t-2\mathcal{H}_2^{KBr}(w_x,\varphi_x,w_{xx},\varphi_{xx},\ldots) \tag{101}$$

which is the same as the Lagrangian of Kaup–Boussinesq system (91) subject to the differential substitution (92). Similarly we find

$$\mathcal{L}_3^{KBr}=(\mathcal{H}_1^{KBr}+2\varepsilon^2 w_{xxx})\varphi_t+(\mathcal{H}_0^{KBr}+\varepsilon\varphi_x\varphi_{xx}+\varepsilon^2\varphi_{xxx})w_t-2\mathcal{H}_3^{KBr}(\varphi_x,w_x,\ldots) \tag{102}$$

for the third Lagrangian for the Kaup–Broer equations (93). As in the case of Kaup–Boussinesq, these Lagrangians reduce to $\gamma=2$ gas dynamics Lagrangians in the dispersionless limit. In the Kaup–Broer Lagrangians we find another example of the general formula (12) for Lagrangians.

VII. NONLINEAR SHRÖDINGER EQUATION

We shall consider the nonlinear Shrödinger equation in the two-component real version

$$v_t=\left[\frac{v^2}{2}+\eta+\varepsilon^2\left(\frac{\eta_{xx}}{\eta}-\frac{\eta_x^2}{2\eta^2}\right)\right]_x,\qquad \eta_t=(\eta v)_x, \tag{103}$$

which is a reaction–diffusion system. Again this reduces to the $\gamma=2$ case of gas dynamics in the dispersionless limit. This version of NLS can be obtained by another triangular differential substitution

$$u=v+\varepsilon\,\eta_x/\eta \tag{104}$$

from the Kaup–Broer system.

NLS has the same first local Hamiltonian structure (45) as in the case of Kaup–Boussinesq or Kaup–Broer systems. Once again the second Hamiltonian operator for NLS can be found by the transformation (104) from the second Hamiltonian operator (98) of the Kaup–Broer system. Thus for the two-component real version of NLS the second Hamiltonian operator is given by

$$J_2^{\mathrm{NLS}}=\begin{pmatrix} D+\varepsilon^2\begin{Bmatrix}\eta^{-1}D^3+D^3\eta^{-1}\\ -\frac{1}{2}[(\eta^{-1})_{xx}D+D(\eta^{-1})_{xx}]\end{Bmatrix} & \frac{1}{2}Dv \\ \frac{1}{2}vD & \frac{1}{2}(\eta D+D\eta)\end{pmatrix} \tag{105}$$

and the conserved Hamiltonians are

$$\mathcal{H}_{-2}^{\mathrm{NLS}}=v, \tag{106}$$

$$\mathcal{H}_{-1}^{\mathrm{NLS}}=\eta, \tag{107}$$

$$\mathcal{H}_0^{\mathrm{NLS}}=v\,\eta, \tag{108}$$

$$\mathcal{H}_1^{\mathrm{NLS}}=\frac{1}{2}\left(\eta v^2+\eta^2-\varepsilon^2\frac{\eta_x^2}{\eta}\right), \tag{109}$$

$$\mathcal{H}_2^{\mathrm{NLS}}=\frac{1}{2}\left[\eta v^2+3v\,\eta^2+\varepsilon^2\left(v_x\eta_x-3\frac{v\,\eta_x^2}{\eta}\right)\right], \tag{110}$$

$$\mathcal{H}_3^{\mathrm{NLS}}=\frac{3}{4}\eta^2v^2+\frac{1}{4}\eta^3+\frac{1}{8}v^4\eta+\varepsilon^4\left(\frac{\eta_{xx}^2}{2\eta}-\frac{5\eta_x^4}{24\eta^3}\right)+\varepsilon^2\left(v^2\eta_{xx}-\frac{5}{4}\eta_x^2-\frac{3}{4}\frac{\eta_x^2}{\eta}v^2-\frac{1}{2}v_x^2\eta\right), \tag{111}$$

$$\cdots$$

which forms an infinite sequence combining both Eulerian and Lagrangian series according to (87).

In order to construct the Lagrangians for NLS we introduce the potentials

$$v=z_x, \quad z=\varphi-\varepsilon\ln w_x, \tag{112}$$

together with the definition (99) and the first Lagrangian

$$\mathcal{L}_1^{\mathrm{NLS}}=\mathcal{H}_{-1}^{\mathrm{NLS}}z_t+\mathcal{H}_{-2}^{\mathrm{NLS}}w_t-2\mathcal{H}_1^{\mathrm{NLS}}(w_x,z_x,\ldots) \tag{113}$$

is the classical result. Once again we shall use the techniques of Sec. II to construct higher Lagrangians with the recursion operator obtained from (105) and (45). We obtain two higher Lagrangians for NLS,

$$\mathcal{L}_2^{\mathrm{NLS}}=\mathcal{H}_0^{\mathrm{NLS}}z_t+\left[\mathcal{H}_{-1}^{\mathrm{NLS}}+\varepsilon^2\left(\frac{w_{xxx}}{w_x}-\frac{w_{xx}^2}{w_x^2}\right)\right]w_t-2\mathcal{H}_2^{\mathrm{NLS}}(w_x,z_x,\ldots) \tag{114}$$

and

$$\mathcal{L}_3^{\mathrm{NLS}}=\left\{\mathcal{H}_0^{\mathrm{NLS}}+\varepsilon^2\left[z_{xxx}+\left(\frac{z_xw_{xx}}{w_x}\right)_x\right]\right\}w_t+(\mathcal{H}_1^{\mathrm{NLS}}+2\varepsilon^2w_{xxx})z_t-2\mathcal{H}_3^{\mathrm{NLS}}(z_x,w_x,\ldots), \tag{115}$$

that are local functionals of the potentials. Here again, in the dispersionless limit we find the $\gamma=2$ gas dynamics Lagrangians. The remarkable strength of the general expression (12) for new Lagrangians is manifest.

VIII. BOUSSINESQ EQUATION

In order to discuss the bi-Hamiltonian structure and the Lagrangians for the Boussinesq equation in a unified framework we first turn to its dispersionless limit. For polytropic gas dynamics we had

$$\rho_t=(\rho u)_x, \quad u_t=\left(\frac{u^2}{2}+\frac{\rho^{\gamma-1}}{\gamma-1}\right)_x \tag{116}$$

with its first nontrivial commuting flow

$$\rho_y=u_x, \quad u_y=\left(\frac{\rho^{\gamma-2}}{\gamma-2}\right)_x, \tag{117}$$

both of which reduce to a second order quasi-linear wave equation.[13] If we express Boussinesq equation in the form

$$\rho_{yy}-(\tfrac{1}{2}\rho^2-\varepsilon^2\rho_{xx})_{xx}=0 \tag{118}$$

or

$$\rho_y = u_x, \quad u_y = \left(\frac{\rho^2}{2} - \varepsilon^2 \rho_{xx} \right)_x \tag{119}$$

as a first order evolutionary system and compare its dispersionless limit to polytropic gas dynamics, we find that it corresponds to the commuting flow for $\gamma = 4$. The completely integrable dispersive equation

$$\rho_t = [\rho u - 2\varepsilon^2 u_{xx}]_x, \quad u_t = \left[\frac{u^2}{2} + \frac{1}{3}\rho^3 - \frac{3}{2}\varepsilon^2 (2\rho\rho_{xx} + \rho_x^2) + 2\varepsilon^4 \rho_{xxxx} \right]_x \tag{120}$$

is the commuting flow to the Boussinesq equation.

This system admits bi-Hamiltonian structure[25] with the Hamiltonian operators (45) and

$$J_2^B = \begin{pmatrix} \rho D + D\rho - 8\varepsilon^2 D^3 & 3uD + 2u_x \\ 3Du - 2u_x & 8(\rho^2 D + D\rho^2) + 8\varepsilon^4 D^5 - \varepsilon^2 [5(\rho D^3 + D^3 \rho) - 3(\rho_{xx} D + D\rho_{xx})] \end{pmatrix} \tag{121}$$

which are compatible. The conserved Hamiltonian densities for the Boussinesq system are given by

$$\mathcal{H}_{-1}^E = \rho, \tag{122}$$

$$\mathcal{H}_0^E = \rho u, \tag{123}$$

$$\mathcal{H}_1^E = \tfrac{1}{4}[2\rho u^2 + \tfrac{1}{3}\rho^4 + \varepsilon^2 (6\rho\rho_x^2 + 4u_x^2) + 4\varepsilon^4 \rho_{xx}^2], \tag{124}$$

$$\begin{aligned} \mathcal{H}_2^E = \tfrac{1}{28}[& \tfrac{14}{3}\rho u^3 + \tfrac{7}{3}\rho^4 u + 14\varepsilon^2 (2uu_x^2 + 4\rho^2 \rho_x u_x + 3u\rho\rho_x^2) \\ & + 28\varepsilon^4 (u\rho_{xx}^2 + \rho_x^2 u_{xx} + 4\rho_{xx} u_{xx}) + 64\varepsilon^6 \rho_{xxx} u_{xxx}] \end{aligned} \tag{125}$$

in the Eulerian sequence and we also have

$$\mathcal{H}_{-1}^L = u, \tag{126}$$

$$\mathcal{H}_0^L = u^2 + \tfrac{1}{3}\rho^3 + \varepsilon^2 \rho_x^2, \tag{127}$$

$$\mathcal{H}_1^L = \tfrac{1}{3}u^3 + \tfrac{1}{3}\rho^3 u - \varepsilon^2 u(4\rho\rho_{xx} + 3\rho_x^2) + \tfrac{16}{5}\varepsilon^4 u_{xx}\rho_{xx}, \tag{128}$$

$$\begin{aligned} \mathcal{H}_2^L = & \tfrac{2}{3}u^4 + \tfrac{4}{3}\rho^3 u^2 + \tfrac{4}{45}\rho^6 + \varepsilon^2 (\tfrac{28}{3}\rho^3 \rho_x^2 + 4u^2 \rho_x^2 + 32\rho u \rho_x u_x + 8\rho^2 u_x^2) + \varepsilon^4 (\tfrac{136}{5}\rho^2 \rho_{xx}^2 - \tfrac{248}{5}\rho_x^4 \\ & + \tfrac{128}{5} u u_{xx} \rho_{xx} + \tfrac{16}{5} u_x^2 \rho_{xx} + \tfrac{96}{5}\rho u_{xx}^2) + \varepsilon^6 (32\rho\rho_{xxx}^2 - \tfrac{592}{15}\rho_{xx}^3 + \tfrac{64}{5} u_{xxx}^2) + \tfrac{64}{5}\varepsilon^8 \rho_{xxxx}^2 \end{aligned} \tag{129}$$

in the Lagrangian sequence. The Hamiltonian function of Boussinesq system with the first order Hamiltonian operator in Darboux form (45) is $\frac{1}{2}H_0^L$. We note that the system (119) for the Boussinesq equation differs from all dispersive integrable examples we encountered earlier in that its familiar Hamiltonian function (128) is in the Lagrangian sequence. This is because Boussinesq equation belongs to the family of commuting flows of the regular gas dynamics hierarchy. The first commuting higher flow for the Boussinesq system (120) has the Hamiltonian function (124) in the Eulerian series.

By introducing potentials

$$u = \varphi_x, \quad \rho = \psi_x \tag{130}$$

we can obtain two local Lagrangian densities for the Boussinesq system. First we have the classical Lagrangians

$$\mathcal{L}_1^{B(L)} = \mathcal{H}_{-1}^{L\ \gamma=4}\psi_y + \mathcal{H}_{-1}^{E\ \gamma=4}\varphi_y - \mathcal{H}_0^{L\ \gamma=4}, \tag{131}$$

$$\mathcal{L}_1^{B(E)} = \mathcal{H}_{-1}^{L\ \gamma=4}\psi_t + \mathcal{H}_{-1}^{L\ \gamma=4}\varphi_t - 2\mathcal{H}_1^{E\ \gamma=4} \tag{132}$$

for Boussinesq system and its first nontrivial commuting flow (120). The second Lagrangians are given by

$$\mathcal{L}_2^{B(L)} = (\mathcal{H}_0^{E\ \gamma=4} - 4\varepsilon^2\varphi_{xxx})\varphi_y + [\mathcal{H}_0^{L\ \gamma=4} - 5\varepsilon^2(\psi_x\psi_{xx})_x + 4\varepsilon^4\psi_{xxxxx}]\psi_y - \mathcal{H}_1^{L\ \gamma=4}, \tag{133}$$

$$\mathcal{L}_2^{B(E)} = (\mathcal{H}_0^{E\ \gamma=4} - 4\varepsilon^2\varphi_{xxx})\varphi_t + [\mathcal{H}_0^{L\ \gamma=4} - 5\varepsilon^2(\psi_x\psi_{xx})_x + 4\varepsilon^4\psi_{xxxxx}]\psi_t - 2\mathcal{H}_2^{E\ \gamma=4}, \tag{134}$$

according to the general construction of Lagrangians in (12). Here we see also that the Lagrangian for the commuting flow is obtained by flipping the Hamiltonian functions between the Lagrangian and Eulerian series while keeping the momenta fixed. In Sec. IV we had constructed Lagrangians for gas dynamics using the Hamiltonians from the Eulerian series in the potential part of the Lagrangian. The general formula (12) can readily be used to construct Lagrangians for the commuting flow (119) by this simple flip in the potential.

IX. CONCLUSION

This is the first time it has been possible to write an unconstrained Lagrangian for polytropic gas dynamics that is local in the original field variables, namely the density and velocity. Earlier variational principles enforced the continuity equation through Lagrange multipliers.[26,27] It is a result of the general expression (12) that serves to identify immediately multi-Lagrangians for completely integrable systems. What is even more remarkable is that this is only the first element in an infinite series of such local Lagrangians for polytropic gas dynamics.

It is worth emphasizing again that the scheme we have presented in Sec. II is a universal one for the construction of multi-Lagrangians appropriate to evolutionary systems. The expressions (12) and (21) for Lagrangians of completely integrable systems has general validity. We note that (12) with $\alpha=1$ is true even in the case of nonintegrable equations, provided the equations are presented in the form of conservation laws and the system admits one further conserved quantity, namely the Hamiltonian. We have discussed in detail the higher Lagrangians for the completely integrable nonlinear evolution equations of polytropic gas dynamics, Kaup–Boussinesq, Kaup–Broer, NLS, and Boussinesq equations all of which bear out the universal applicability of (12) in the construction of higher Lagrangians. We have also presented the lower Lagrangians (21) fully for KdV and partially for gas dynamics owing to the difficulty of writing the second modified variables in closed form.

The invariance group of these multi-Lagrangians and their Noether currents should prove to be of interest in discovering new hidden symmetries of fluid mechanics. We did not discuss this important issue here. Recently Jackiw and co-workers[28] have used hidden symmetries in the classical Lagrangian for fluid mechanics to construct very interesting field theory models of fluid mechanics. Multi-Lagrangians may prove to be of interest in this connection also.

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Perturbation theory for nearly integrable multicomponent nonlinear PDEs

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The Riemann–Hilbert problem associated with the integrable PDE is used as a nonlinear transformation of the nearly integrable PDE to the spectral space. The temporal evolution of the spectral data is derived with account for arbitrary perturbations and is given in the form of exact equations, which generate the sequence of approximate ordinary differential equations in successive orders with respect to the perturbation. For vector nearly integrable PDEs, embracing the vector nonlinear Schrödinger and complex modified Korteweg–de Vries equations, the main result is formulated in a theorem. For a single vector soliton the evolution equations for the soliton parameters and first-order radiation are given in explicit form. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1448135]

I. INTRODUCTION

Multicomponent (or coupled) nonlinear PDEs have been a subject of considerable interest for many years (see, for instance, Ref. 1, and references therein). Recent revival of interest in multicomponent PDEs is due to new discoveries and technological advances in nonlinear optics and physics of condensed matter. An important example is the incoherent spatial optical solitons, or self-trapped spatially incoherent light beams, recently experimentally observed in nonlinear media,[2] which are described by the multicomponent nonlinear Schrödinger (NLS) equations.[3] Another example of possible application of the coupled NLS equations is the creation and dynamics of solitary waves in the multispecies Bose–Einstein condensates.[4] Similar models of coupled nonlinear PDEs appear in the wavelength division multiplexing, i.e., copropagation of pulses in an optical fiber on beams with different wavelengthes[5–7] and in other important applications.[8,9]

Some of the multicomponent models are integrable. Integrable multicomponent PDEs have another specific feature, which makes them important for applications as zero-approximation models for analytical description of the real phenomena. It has been known for quite some time that dimensional reductions of matrix generalizations of the integrable PDEs, such as the NLS and Korteweg–de Vries (KdV) equations, can produce a variety of new integrable equations.[10] For instance, some of the coupled NLS equations are integrable reductions of the general matrix NLS equation. The N-dimensional matrix NLS equation is the simplest integrable PDE associated with the $(N+1)$-dimensional Zakharov–Shabat spectral problem.[11–13] Recently a variety of integrable coupled higher-order NLS equations was discovered,[14–16] which are important in view of applications to the soliton propagation of subpicosecond pulses in optical fiber.[17–19] Some of these integrable PDEs arise as dimensional reductions of the matrix complex modified KdV (cmKdV) equation, which is also associated with the Zakharov–Shabat spectral problem.

In most cases, the multicomponent PDE is not integrable. However, frequently the terms destroying integrability contain small parameters and the nonintegrable equation can be considered as a perturbation of the integrable one. In this case, a perturbation theory is required for analytical description of the effect of small perturbations. For instance, one is especially interested

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in the dynamics of solitons in nearly integrable PDEs. Soliton solutions to multicomponent equations have many parameters, and their evolution may exhibit a variety of new interesting regimes. Therefore, it is necessary to have at hand a perturbation theory for multicomponent nearly integrable equations. Such perturbation theory is developed in the present paper.

Perturbation theory for nearly integrable PDEs has a long history.[20–45] There are two basic approaches in the perturbation theory based on the inverse scattering transform (IST) method. The first one originated in works of Kaup[20] and Karpman and Maslov,[21] where the perturbation theory was developed for nearly integrable PDEs associated in the integrable limit with the 2×2 matrix Zakharov–Shabat spectral problem. A quite different approach originated from other works (Refs. 22–26). It was found that an integro-differential operator, generating the whole hierarchy of integrable PDEs related to a given spectral problem, called the recursion operator, has a complete set of eigenfunctions, which can be used for the perturbation expansion. Several other methods, not related to the IST, were applied for description of the perturbed soliton dynamics. For instance, a method based on the Green functions was developed in Ref. 29. The IST-independent perturbation theories for solitons are usually referred to as the direct perturbation theories (see, e.g., Ref. 40, and references therein). However, notwithstanding the long history of the perturbation theory, with rare exceptions, only the 2×2 matrix spectral problems were considered. It was noted that construction of the perturbation theory for higher-dimensional matrix spectral problems along the standard approach becomes technically more involved.

To overcome technical difficulties of the standard approach when dealing with multicomponent PDEs, the method based on the Riemann–Hilbert (RH) problem was proposed in Ref. 41, where the perturbation theory was developed for the Zakharov–Shabat spectral problem of an arbitrary matrix dimension. The RH problem was used before for construction of the perturbation theory for the Landau–Lifschitz equation,[30] the NLS, and Maxwell–Bloch equations,[34] which are integrable by the 2×2 matrix spectral problem. The approach of Ref. 41 was applied to the Manakov system[42] (i.e., the two-component NLS equation), modified NLS equation,[43] and massive Thirring model.[44] These examples demonstrate that the perturbation theory based on the RH problem always works. Recently, the RH problem was applied to nearly integrable equations on the half line, arising from the singular dispersion relations.[45] In Refs. 41–45 the perturbation-induced evolution equations for the spectral data were derived with the help of some matrix functional [in the following, the evolution functional $\Pi(x,t,k)$]. It is important to emphasize that the form of the evolution functional is invariant under the gauge transformations of the considered PDE.[43] Thus, once constructed, the evolution functional is valid not only for the whole hierarchy of PDEs associated with a given spectral problem, but also for their images under the gauge transformations. Writing the dispersion law, generating the spectral problem, in an abstract form $\Lambda(k)$ (see Sec. II for details) we discover that the form of the evolution functional remains invariant under the change of the *spectral problem* as well. This invariance trivially extends to the general initial-boundary value problems. For instance, for the half-line, where one would expect a difference, we have found that the evolution functional has similar form.[45] Therefore, it seems that the approach based on the evolution functional is universal for construction of the perturbation theories for nearly integrable PDEs. It is also technically simple. Derivation of the perturbation-induced evolution equations for the spectral data using the evolution functional reduces to calculation of integrals.

This paper is a further development of Ref. 41. The previous results are substantially advanced. In particular, the evolution equations for the spectral data are considerably simplified with the help of some identities found for the evolution functional. We start Sec. II with a brief discussion of the multicomponent integrable PDEs associated with the Zakharov–Shabat spectral problem. We consider two examples, the matrix NLS and cmKdV equations, however, our approach is valid for many other multicomponent PDEs. We have not made an attempt to give a complete exposition of the properties of integrable equations. We need only the Lax representation. Hence a way of deriving the Lax pair for an integrable PDE from the dispersion relation of its linearization is briefly indicated. For completeness of the exposition, a detailed derivation of the RH problem is given in Sec. III. Solution of the RH problem for multicomponent equations

involves some technicalities, which are discussed and detailed derivations are provided in the appendices. We derive evolution equations for the spectral data with account for perturbations in Sec. IV. There, for an important special case of the vector nearly integrable PDEs the main result of this paper is formulated in a theorem. In Sec. V the equations of the first-order perturbation theory for a single vector soliton are given in explicit form.

II. PRELIMINARIES: INTEGRABLE MULTICOMPONENT NONLINEAR PDEs

Here we briefly discuss integrable PDEs with emphasis on the multicomponent equations whose reductions are important for applications. In particular, we consider the matrix nonlinear Schrödinger and complex modified Korteweg–de Vries equations. We do not try to review this subject, for general considerations the reader can consult, for instance, Refs. 1, 10–13, 46–53 and the references therein. The purpose of this section is to recall some of the basic notions in the IST method. Though the approach in the following can be applied to any nonlinear PDE solvable by the RH problem, we restrict the consideration to the integrable equations associated with the N-dimensional Zakharov–Shabat spectral problem (1).

Consider the integrable PDEs which arise as the compatibility condition for the following $N\times N$ matrix linear system (Lax pair):

$$\partial_x\Phi = ik[A,\Phi] + iQ(x,t)\Phi \equiv \Phi\Lambda(k) + U(x,t,k)\Phi, \tag{1}$$

$$\partial_t\Phi = i\omega(k)\Phi A + V(x,t,k)\Phi \equiv \Phi\Omega(k) + V(x,t,k)\Phi, \tag{2}$$

with

$$A = \begin{pmatrix} I_n & 0 \\ 0 & -I_{N-n} \end{pmatrix}, \quad Q = \begin{pmatrix} 0 & \mathbf{q} \\ \overline{\mathbf{q}} & 0 \end{pmatrix},$$

$$\mathbf{q} = \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1,N-n} \\ q_{21} & q_{22} & \cdots & q_{2,N-n} \\ \vdots & \vdots & & \vdots \\ q_{n1} & q_{n2} & \cdots & q_{n,N-n} \end{pmatrix}, \quad \overline{\mathbf{q}} = \begin{pmatrix} \overline{q}_{11} & \overline{q}_{21} & \cdots & \overline{q}_{n1} \\ \overline{q}_{12} & \overline{q}_{22} & \cdots & \overline{q}_{n2} \\ \vdots & \vdots & & \vdots \\ \overline{q}_{1,N-n} & \overline{q}_{2n} & \cdots & \overline{q}_{n,N-n} \end{pmatrix},$$

where $\Lambda(k) = -ikA$ and $\Omega = i\omega(k)A$ are the dispersion laws, Q is called the potential. Here the overline does not mean complex conjugation by default, e.g., in general, the functions q_{ij} and $\overline{q}_{ij}$ are not considered as complex conjugate to each other. When the overline does denote complex conjugation in the following text, each time it will be specially indicated. This special case corresponds to the Hermitian potential Q, $Q^\dagger = Q$ or $\mathbf{q}^\dagger = \overline{\mathbf{q}}$, and it will be referred to as the involution. The temporal evolution equation (2) is specified by choice of the dispersion relation $\omega(k)$ in the following manner. For simplicity, let the dispersion relation be polynomial $\omega(k) = \sum_{p=1}^{M} w_p k^p$, then

$$V(k) = -\mathcal{P}\{\Phi\Omega\Phi^{-1}\} \equiv -\Omega(k) + \sum_{p=0}^{M-1} V_p k^p. \tag{3}$$

Here the matrix function $\Phi(k)$ is expanded into the asymptotic series:

$$\Phi(k) = I + k^{-1}\Phi^{(1)} + k^{-2}\Phi^{(2)} + \cdots, \quad k\to\infty,$$

and the operator $\mathcal{P}$ takes the polynomial in k part of $\Phi\Omega\Phi^{-1}$ on the asymptotics. For example, the Zakharov–Shabat spectral problem (1) is derived in this way,

$$U = -\mathcal{P}\{\Phi\Lambda\Phi^{-1}\} = ikA + i[\Phi^{(1)},A],$$

with the obvious relation

$$Q=[\Phi^{(1)},A]. \tag{4}$$

Hence, the Lax pair satisfies the property $\mathrm{Tr}\,U=-\mathrm{Tr}\,\Lambda$ and $\mathrm{Tr}\,V=-\mathrm{Tr}\,\Omega$.

The integrable nonlinear PDE related to the Lax pair (1)–(2) is given by the compatibility condition (in our case, polynomial in k)

$$i\partial_t Q-\partial_x V+[ikA+iQ,V]=0 \tag{5}$$

via setting $k=0$, while the positive powers of k supply the expressions of the coefficients V_p in (3) as functions of the potential Q and its x-derivatives, $V_p=V_p(Q,Q_x,Q_{xx},\dots)$. For instance, choosing $\omega(k)=2k^2$ we obtain the well-known matrix nonlinear Schrödinger equation. Indeed, in this case

$$V=-2ik^2A-2ikQ-AQ_x+iAQ^2$$

and Eq. (5) becomes

$$iAQ_t+Q_{xx}+2Q^3=0. \tag{6}$$

For a complete classification of the matrix integrable NLS equations with various reductions to Hermitian symmetric spaces consult Ref. 10. A particular important case of Eq. (6) is the vector NLS equation, a generalization of the two-component vector NLS, which was shown to be integrable by Manakov.[12] The vector NLS equation corresponds to the Hermitian potential and the reduction $n=N-1$ (see the expression for A.) In this case we have

$$Q=\begin{pmatrix} 0 & \dots & 0 & q_1 \\ \vdots & & \vdots & \vdots \\ 0 & \dots & 0 & q_n \\ \overline{q_1} & \dots & \overline{q_n} & 0 \end{pmatrix} \tag{7}$$

and matrix equation (6) becomes the vector NLS equation:

$$i\partial_t q_l+\partial_x^2 q_l+2\left(\sum_{j=1}^{n}|q_j|^2\right)q_l=0, \quad l=1,\dots,n. \tag{8}$$

Let us consider another important example of multicomponent nonlinear integrable equations. It is given by setting $\omega(k)=4k^3$. After simple computation we get

$$V=-4ik^3A+4ik^2Q+2ikA(iQ_x+Q^2)-iQ_{xx}+[Q,Q_x]-2iQ^3,$$

which produces the matrix cmKdV equation

$$Q_t+Q_{xxx}+3(Q^2Q_x+Q_xQ^2)=0. \tag{9}$$

Combining together the two considered dispersion laws, i.e., letting $\omega(k)=4i\epsilon k^3+2i\beta k^2$, one can obtain

$$iQ_t+\beta A(Q_{xx}+2Q^3)+i\epsilon Q_{xxx}+3i\epsilon(Q^2Q_x+Q_xQ^2)=0,$$

a special case of the (generally, nonintegrable) matrix higher-order NLS equation

$$iE_z+A(\alpha_1E_{\tau\tau}+\alpha_2E^3)+i\{\alpha_3E_{\tau\tau\tau}+\alpha_4(E^3)_\tau+\alpha_5(E^2)_\tau E\}=0. \tag{10}$$

Our examples are just illustrative. There are many other integrable matrix PDEs which we do not mention here. However, the perturbation theory developed in Sec. IV applies to such PDEs also.

III. RIEMANN–HILBERT PROBLEM FOR MULTICOMPONENT PDEs

In this section we derive the RH problem for the multicomponent integrable PDEs and discuss its solution (for more details consult Refs. 46, 54–57). We are interested in the initial-value problem for nonlinear PDEs on the whole real line with the asymptotically vanishing conditions (Cauchy problem) $q_{ij}\to 0$ as $|x|\to\infty$. The vanishing asymptotics allows us to concentrate entirely on the spectral equation (1) in derivation of the RH problem, while t dependence enters parametrically in our approach (for the RH problem for initial-boundary value problems consult Ref. 47). In the following we omit the explicit t dependence for simplicity of the presentation. To begin with, let us summarize the properties of the spectral problem (1). Define the following $N\times N$ matrix projectors:

$$H_1=\mathrm{diag}(I_n,0),\quad H_2=\mathrm{diag}(0,I_{N-n}). \tag{11}$$

Then $A=H_1-H_2$ and any matrix can be decomposed into the sum of two matrices, commuting and anticommuting with A:

$$\Phi=\Phi^{(c)}+\Phi^{(a)},\quad \Phi^{(c)}=H_1\Phi H_1+H_2\Phi H_2,\quad \Phi^{(a)}=H_1\Phi H_2+H_2\Phi H_1, \tag{12}$$

where $[A,\Phi^{(c)}]=0$ and $\{A,\Phi^{(a)}\}=0$. We will use the block-index notations for the decomposition of matrix Φ with respect to the projectors H_1 and H_2:

$$\Phi=\begin{pmatrix}\Phi_{\mathrm{I,I}} & \Phi_{\mathrm{I,II}}\\ \Phi_{\mathrm{II,I}} & \Phi_{\mathrm{II,II}}\end{pmatrix}.$$

The RH problem is a one-to-one mapping (nonlinear Fourier transform) between the set of smooth (e.g., belonging to the Schwartz space) potentials $Q(x)$ and some set of the spectral data. To identify the RH problem one must construct two solutions, one, $\Phi_+(x,k)$, to the spectral equation (1) and the other, $\Phi_-^{-1}(x,k)$, to the adjoint equation [the second function is inverse of some matrix function satisfying (1), hence the "-1" in its definition], holomorphic with respect to the spectral parameter k in some complementary domains covering the whole complex k-plane. Such solutions can be built from the columns and rows of the Jost solutions $J_\pm$, i.e., solutions defined by the asymptotic conditions: $J_\pm(x,k)\to I$ as $x\to\pm\infty$.

As $\mathrm{Tr}\,Q=0$, letting $x\to\pm\infty$ we conclude that $\det J_\pm=1$. Hence, the columns of either of the two Jost solutions give a linear basis in the space of solutions of the spectral equation. The inverse matrices $J_\pm^{-1}$ satisfy the adjoint spectral equation:

$$\partial_x\tilde{\Phi}=ik[A,\tilde{\Phi}]-i\tilde{\Phi}Q. \tag{13}$$

Each column of $J_\pm(x,k)$ and, respectively, row of $J_\pm^{-1}(x,k)$ is holomorphic and bounded in either upper ($\mathrm{Im}\,k\geqslant 0$) or lower ($\mathrm{Im}\,k\leqslant 0$) half of the complex k-plane. Indeed, this can be easily seen from the Volterra integral equations for the Jost matrices written for the two blocks of columns:

$$J_\pm(x,k)H_1=H_1+i\int_{\pm\infty}^{x}\mathrm{d}\xi\, e^{-2ik(x-\xi)H_2}Q(\xi)J_\pm(\xi,k)H_1,$$

$$J_\pm(x,k)H_2=H_2+i\int_{\pm\infty}^{x}\mathrm{d}\xi\, e^{2ik(x-\xi)H_1}Q(\xi)J_\pm(\xi,k)H_2.$$

The columns of $J_+(k)H_1$ and $J_-(k)H_2$ are holomorphic and bounded in the upper half of the complex plane, while columns of $J_+(k)H_2$ and $J_-(k)H_1$ have the same property in the lower half plane. Similarly, the rows of $J_\pm^{-1}$ satisfy integral equations

$$H_1J_\pm^{-1}(x,k)=H_1-i\int_{\pm\infty}^{x}\mathrm{d}\xi\, H_1J_\pm^{-1}(\xi,k)Q(\xi)e^{2ik(x-\xi)H_2},$$

$$H_2J_\pm^{-1}(x,k)=H_2-i\int_{\pm\infty}^{x}\mathrm{d}\xi\, H_2J_\pm^{-1}(\xi,k)Q(\xi)e^{-2ik(x-\xi)H_1},$$

from which we immediately conclude that $H_1J_+^{-1}(k)$ and $H_2J_-^{-1}(k)$ are holomorphic and bounded in the upper half plane, while $H_2J_+^{-1}(k)$ and $H_1J_-^{-1}(k)$ have the same properties in the lower half plane.

On the real line, the Jost solutions are transformed into each other by the scattering matrix $S(k)$,

$$J_-(x,k)=J_+(x,k)e^{ikxA}S(k)e^{-ikxA}. \tag{14}$$

For the Hermitian potential, $Q^\dagger=Q$, the matrix Jost solutions satisfy the involution (here the overline means complex conjugation)

$$J_\pm^\dagger(x,k)=J_\pm^{-1}(x,\overline{k}), \tag{15}$$

where the spectral parameter takes complex values in the upper or lower half plane depending on the considered column of the Jost matrix. In this case, the scattering matrix also satisfies the involution

$$S^\dagger(k)=S^{-1}(k),\quad k\in\mathrm{Re}. \tag{16}$$

The holomorphic matrix functions $\Phi_+(k)$ and $\Phi_-^{-1}(k)$, satisfying Eqs. (1) and (13), respectively, are given in terms of columns and rows of the Jost solutions:

$$\Phi_+=J_+H_1+J_-H_2,\quad \Phi_-^{-1}=H_1J_+^{-1}+H_2J_-^{-1}. \tag{17}$$

The above-defined matrix functions are holomorphic and bounded in the upper and lower half planes, respectively. They have the following asymptotics:

$$\Phi_\pm(x,k)\to I,\quad k\to\infty, \tag{18}$$

which follow from the Volterra integral equations for the Jost solutions. For the involution (15) the matrices $\Phi_+(k)$ and $\Phi_-^{-1}(k)$ are related via

$$\Phi_+^\dagger(k)=\Phi_-^{-1}(\overline{k}). \tag{19}$$

These matrices can be conveniently expressed in terms of only one Jost solution and elements of the scattering matrix $S(k)$. Indeed,

$$\Phi_+=J_+e^{ikxA}(H_1+SH_2)e^{-ikxA}\equiv J_-e^{ikxA}(H_2+S^{-1}H_1)e^{-ikxA},$$

$$\Phi_-^{-1}=e^{ikxA}(H_1+H_2S^{-1})e^{-ikxA}J_+^{-1}\equiv e^{ikxA}(H_2+H_1S)e^{-ikxA}J_-^{-1}.$$

Denote $S_+=H_1+SH_2$, $S_-=H_2+S^{-1}H_1$. These matrices provide a factorization of the scattering matrix: $S_+=SS_-$. Similarly, $\overline{S_+}=H_1+H_2S^{-1}$ and $\overline{S_-}=H_2+H_1S$, which also factorize the scattering matrix: $\overline{S_+}S=\overline{S_-}$. Then

$$\Phi_+ = J_+ e^{ikxA} S_+ e^{-ikxA} \equiv J_- e^{ikxA} S_- e^{-ikxA}, \tag{20a}$$

$$\Phi_-^{-1} = e^{ikxA} \overline{S}_+ e^{-ikxA} J_+^{-1} \equiv e^{ikxA} \overline{S}_- e^{-ikxA} J_-^{-1}. \tag{20b}$$

The factorization matrices have the block-triangular structure. For instance, S_+ and $\overline{S}_+$ are upper and lower block-triangular, respectively:

$$S_+ = \begin{pmatrix} I_n & \mathbf{b} \\ 0 & \mathbf{a} \end{pmatrix}, \quad \overline{S}_+ = \begin{pmatrix} I_n & 0 \\ \overline{\mathbf{b}} & \overline{\mathbf{a}} \end{pmatrix}, \tag{21}$$

where $\mathbf{b} = S_{\mathrm{I,II}}$, $\mathbf{a} = S_{\mathrm{II,II}}$, $\overline{\mathbf{b}} = (S^{-1})_{\mathrm{II,I}}$, and $\overline{\mathbf{a}} = (S^{-1})_{\mathrm{II,II}}$. The following identity follows from these definitions:

$$\overline{\mathbf{b}}\mathbf{b} + \overline{\mathbf{a}}\mathbf{a} = I_{N-n}, \quad k \in \mathrm{Re}. \tag{22}$$

For the involution (19) the factorizations satisfy

$$S_\pm^\dagger(k) = \overline{S}_\pm(k), \quad k \in \mathrm{Re}.$$

Hence, $\overline{\mathbf{b}} = \mathbf{b}^\dagger$ and $\overline{\mathbf{a}} = \mathbf{a}^\dagger$ in the case of involution.

Considering the product $\Phi_-^{-1}\Phi_+$ we obtain the problem of analytic factorization of a matrix $G(k)$ given on the real line, i.e., the matrix RH problem:

$$\Phi_-^{-1}(x,k)\Phi_+(x,k) = e^{ikxA} G(k) e^{-ikxA}, \quad k \in \mathrm{Re} \tag{23}$$

and $\Phi_\pm(x,k) \to I$ for $k \to \infty$. Here the matrix $G = \overline{S}_+ S_+ \equiv \overline{S}_- S_-$ reads

$$G = \begin{pmatrix} I_n & \mathbf{b} \\ \overline{\mathbf{b}} & I_{N-n} \end{pmatrix}. \tag{24}$$

As was mentioned, the RH problem is a nonlinear mapping between the potential $Q(x)$ and the set of the spectral data, which are necessary for unique identification of the solution to (23). For instance, given a potential, one can obtain the spectral data by solving the spectral equation and its adjoint for $\Phi_+(x,k)$ and $\Phi_-^{-1}(x,k)$. Conversely, by asymptotic expansion of $\Phi_\pm(x,k)$ as $k \to \infty$ one recovers the potential. The asymptotic expansion of $\Phi_\pm(x,k)$ can be derived via integration by parts (in the blocks with $e^{\pm 2ikx}$) in the Volterra integral equations for $J_\pm$ and $J_\pm^{-1}$. It reads

$$\Phi_\pm(x,k) = I - \left(AQ(x) + i\int_{-\infty}^{x} \mathrm{d}\xi\, Q^2(\xi) H_2 + i\int_{x}^{\infty} \mathrm{d}\xi\, Q^2(\xi) H_1 \right) \frac{1}{2k} + \mathcal{O}\left(\frac{1}{k^2}\right).$$

Hence, we obtain [cf. with (4)]

$$Q(x) = \lim_{k\to\infty} k[\Phi_+(x,k), A] = \lim_{k\to\infty} k[A, \Phi_-^{-1}(x,k)]. \tag{25}$$

Solution of the RH problem: Normalization. Let us discuss the way of solution of the RH problem. The coordinate dependence is not important for this purpose and is omitted in the following. In general, the determinants $\det \Phi_+(k)$ and $\det \Phi_-^{-1}(k)$ have zeros and the RH problem is said to be nonregular or with zeros. Note that the determinants do not depend on x as readily seen from Eqs. (1) and (13). We consider only the RH problem with zero index, i.e.,

$$\int_{-\infty}^{\infty} \mathrm{d}\ln\{\det G(k)\}=0,$$

assuming that $G(k)$ is nondegenerate. Since $\Phi_{\pm}\to I$ as $k\to\infty$, the index is equal to the difference between the number of zeros in the upper and lower half planes. Let $k_1,\ldots,k_M$ and $\overline{k_1},\ldots,\overline{k_M}$ be zeros (where some may be equal) of $\det\Phi_+(k)$ and $\det\Phi_-^{-1}(k)$, respectively. Two conditions are imposed on the zeros. First, the geometric multiplicity of a zero must be equal to its order (which we will refer to as the algebraic multiplicity). Here the geometric multiplicity of k_j is defined as the dimension d_j of the null space of $\Phi_+(k_j)$, i.e., $d_j=N-\mathrm{rank}\Phi_+(k_j)$. Trivially, the two multiplicities are equal to 1 in the case of simple zeros. In the case of involution zeros of the RH problem come in complex conjugate pairs [due to formula (19)], with coinciding algebraic (and geometric) multiplicities within each pair. (Due to the involution the index is equal to zero, in this case $\det G(k)$ is real and definite.) Second, as we are mainly interested in the Hermitian potentials Q, i.e., in the case of the involution, we will consider only paired zeros k_j and $\overline{k_j}$, $j=1,\ldots,s\leqslant M$, whose algebraic multiplicities are equal, however without assuming them to be complex conjugate to each other. The algebraic multiplicity ν_j of k_j always satisfies the following inequality (see Appendix A):

$$\nu_j\geqslant N-\mathrm{rank}\Phi_+(k_j)=d_j,$$

while $\mathrm{rank}\Phi_+\geqslant\max(n,N-n)$ by construction of Φ_+ (17). For instance, if $n=N-1$, there can be not more than one vector in the null space of $\Phi_+(k)$, i.e., $d_j=1$ for all $j=1,\ldots,s$. Hence, for this reduction, zeros of $\det\Phi_+(k)$ must be simple to satisfy the equal multiplicity condition. Similar for zeros of $\Phi_-^{-1}(k)$. (More detailed consideration of the multiplicities of zeros is placed in Appendix A.)

Let $\det\Phi_+(k)$ and $\det\Phi_-^{-1}(k)$ have zeros $k_1,\ldots,k_s$ and $\overline{k_1},\ldots,\overline{k_s}$, respectively, with the (algebraic and geometric) multiplicities $\nu_1,\ldots,\nu_s$. Exactly ν_j independent vector-columns $|p_l^{(j)}\rangle$ (vector-rows $\langle\overline{p}_l^{(j)}|$), where $l=1,\ldots,\nu_j$, correspond to each zero k_j (respectively, $\overline{k_j}$), such that

$$\Phi_+(k_j)|p_l^{(j)}\rangle=0,\quad \langle\overline{p}_l^{(j)}|\Phi_-^{-1}(\overline{k_j})=0. \tag{26}$$

To specify a unique solution to the RH problem, additionally to the continuous datum $G(k)$, the set of the discrete data $\{k_j,|p_l^{(j)}\rangle,\overline{k_j},\langle\overline{p}_l^{(j)}|,l=1,\ldots,\nu_j,j=1,\ldots,s\}$ must be given. This becomes evident from the fact that the RH problem with zeros (i.e., nonregular) can be regularized, i.e., reduced to a modified RH problem without zeros by factoring them out with some rational matrix $\Gamma(k)$:

$$\Phi_+(k)=\phi_+(k)\Gamma(k),\quad \Phi_-^{-1}(k)=\Gamma^{-1}(k)\phi_-^{-1}(k). \tag{27}$$

The regularized RH problem reads

$$\phi_-^{-1}(k)\phi_+(k)=\Gamma(k)e^{ikxA}G(k)e^{-ikxA}\Gamma^{-1}(k),\quad k\in\mathrm{Re} \tag{28}$$

and $\phi_{\pm}(k)\to I$ as $k\to\infty$.

The rational matrix functions $\Gamma(k)$ and $\Gamma^{-1}(k)$—for details see Appendix B,

$$\Gamma=I-\sum_{j,l;i,m}\frac{|p_m^{(i)}\rangle(D^{-1})_{im,jl}\langle\overline{p}_l^{(j)}|}{k-\overline{k_j}},\quad \Gamma^{-1}=I+\sum_{j,l;i,m}\frac{|p_l^{(j)}\rangle(D^{-1})_{jl,im}\langle\overline{p}_m^{(i)}|}{k-k_j}, \tag{29}$$

where

$$D_{im,jl}=\frac{\langle \overline{p}_m^{(i)}|p_l^{(j)}\rangle}{k_j-\overline{k_i}},$$

have the same zeros as $\Phi_+(k)$ and $\Phi_-^{-1}(k)$, respectively, and the same null spaces:

$$\Gamma(k_j)|p_l^{(j)}\rangle=0, \quad \langle \overline{p}_l^{(j)}|\Gamma^{-1}(\overline{k_j})=0, \quad l=1,\ldots,\nu_j, \quad j=1,\ldots,s.$$

Moreover,

$$\det\Gamma=\Pi_{j=1}^{s}\left(\frac{k-k_j}{k-\overline{k_j}}\right)^{\nu_j}.$$

Precisely these properties allow us to factor out zeros of $\Phi_+(x,k)$ and $\Phi_-^{-1}(x,k)$.

It is important to emphasize that there is a freedom in choice of the basis vectors spanning the null spaces. Indeed, it is easy to verify that the regularization matrix Γ is invariant under the transformations:

$$|p_l^{(j)}\rangle\to\sum_{m=1}^{\nu_j}|p_m^{(j)}\rangle M_{ml}^{(j)}, \quad \langle \overline{p}_l^{(j)}|\to\sum_{m=1}^{\nu_j}\overline{M}_{lm}^{(j)}\langle \overline{p}_m^{(j)}|, \tag{30}$$

where $M^{(j)}$ and $\overline{M}^{(j)}$ are arbitrary nondegenerate $\nu_j\times\nu_j$-matrices. For the involution, due to Eq. (19) we can choose $\langle \overline{p}_l^{(j)}|=|p_l^{(j)}\rangle^\dagger$. This evidently leads to

$$\Gamma^\dagger(k)=\Gamma^{-1}(\overline{k}). \tag{31}$$

The (x,t)-dependence of the RH data can be found in the following way. The t-dependence of the continuous datum (which does not depend on x) can be derived from Eqs. (23) and (2). We obtain

$$\partial_t G=[G,\Omega]. \tag{32}$$

This equation can be cast in a more explicit form:

$$\partial_t\mathbf{b}=-2i\omega(k)\mathbf{b}, \quad \partial_t\overline{\mathbf{b}}=2i\omega(k)\overline{\mathbf{b}}. \tag{33}$$

Recalling that $\operatorname{Tr}Q=0$ and $\operatorname{Tr}V=-\operatorname{Tr}\Omega$, one can verify that the determinants of $\Phi_\pm$ do not depend on the coordinates. Therefore, the zeros are coordinate independent as well:

$$\partial_x k_j=\partial_t k_j=0, \quad \partial_x\overline{k_j}=\partial_t\overline{k_j}=0, \quad j=1,\ldots,s. \tag{34}$$

Now, let us derive the coordinate dependence of the vector-parameters. Differentiating Eq. (26) we obtain

$$\Phi_+(k_j)(\partial_x|p_l^{(j)}\rangle-ik_jA|p_l^{(j)}\rangle)=0, \quad \Phi_+(k_j)(\partial_t|p_l^{(j)}\rangle+\Omega(k_j)|p_l^{(j)}\rangle)=0.$$

Therefore

$$\partial_x|p_l^{(j)}\rangle=ik_jA|p_l^{(j)}\rangle+\sum_{m=1}^{\nu_j}F_{lm}^{(j)}|p_m^{(j)}\rangle, \quad \partial_t|p_l^{(j)}\rangle=-\Omega(k_j)|p_l^{(j)}\rangle+\sum_{m=1}^{\nu_j}K_{lm}^{(j)}|p_m^{(j)}\rangle,$$

where F and K are some matrices. Using a suitable invariance transformation of the type (30) one can put $F=K=0$ without loss of generality. Hence we have

$$\partial_x|p_l^{(j)}\rangle = ik_jA|p_l^{(j)}\rangle, \quad \partial_t|p_l^{(j)}\rangle = -\Omega(k_j)|p_l^{(j)}\rangle. \tag{35}$$

Similarly,

$$\partial_x\langle\overline{p}_l^{(j)}| = -\langle\overline{p}_l^{(j)}|i\overline{k}_jA, \quad \partial_t\langle\overline{p}_l^{(j)}| = \langle\overline{p}_l^{(j)}|\Omega(\overline{k}_j). \tag{36}$$

Some comments are needed on the reconstruction of the potential Q. First of all, the soliton part of the potential is given by the rational matrix function $\Gamma(k)$ (29). The pure soliton potentials are also called reflectionless; they solve the simplest RH problem with $G=I$, i.e., with zero reflection coefficients: $\mathbf{b}(k)=\overline{\mathbf{b}}(k)=0$. The discrete RH data have the following meaning. Zeros provide the amplitudes and velocities of the solitons, while the null vectors give their initial position, polarization, and phase parameters. Second, the radiation part of the potential is given by the solution to the regularized RH problem (28). The continuous RH data $\mathbf{b}(k)$ and $\overline{\mathbf{b}}(k)$ represent the nonlinear spectral densities of radiation. The regular RH problem is equivalent to some matrix integral equation of the Fredholm type (for instance, consult Ref. 46). Though the solution cannot be given in explicit form, its properties can be explored by the standard technique of the theory of Fredholm integral equations.

For the following, it is convenient to introduce x-independent null vectors $|P_l^{(j)}\rangle$ and $\langle\overline{P}_l^{(j)}|$ setting

$$|p_l^{(j)}\rangle = e^{ik_jxA}|P_l^{(j)}\rangle, \quad \langle\overline{p}_l^{(j)}| = \langle\overline{P}_l^{(j)}|e^{-i\overline{k}_jxA}. \tag{37}$$

Then, we have an x-independent set of the RH data, which we will call the spectral data: $\{\mathbf{b}(k),\overline{\mathbf{b}}(k),k_j,|P_l^{(j)}\rangle,\overline{k}_j,\langle\overline{P}_l^{(j)}|, l=1,\ldots,\nu_j, j=1,\ldots,s\}$.

As the illustrative example, consider one-soliton solution. It is given by $\Gamma(k)$ having only one pole, say $k_1=i\eta+\xi$. In this case,

$$Q=(k_1-\overline{k}_1)[A,P_r], \quad P_r=\sum_{l,m=1}^{\nu_1}|p_l\rangle(\Delta^{-1})_{lm}\langle\overline{p}_m|,$$

with $\Delta_{lm}=\langle\overline{p}_l|p_m\rangle$. Here $\langle\overline{p}_l|\Phi_-^{-1}(\overline{k}_1)=0$ and $\Phi_+(k_1)|p_l\rangle=0$. In the particular case of $n=N-1$ and the Hermitian potential we get the vector soliton solution, for which

$$P_r=\frac{|p\rangle\langle p|}{\langle p|p\rangle}, \quad |p\rangle=\exp\{ik_1xA\}|P\rangle.$$

Define complex parameters $C_l=P_l/P_N$. The t-dependence of C_l then follows from Eq. (35). It can be accounted for in a convenient way by introducing real t-dependent parameters $\overline{x}$, and δ_l, $l=1,\ldots,n$, the soliton position and phases of its components. Let $C_l=\theta_le^{2(\eta-i\xi)\overline{x}}$, where $\theta_l=s_le^{i\delta_l}$. The amplitudes s_l, satisfying

$$\sum_{l=1}^{n}s_l^2=1, \tag{38}$$

describe polarization of the multicomponent soliton. Integrating Eq. (35) we obtain

$$\overline{x}=\overline{x}_0+\frac{\mathrm{Im}\{\omega(i\eta+\xi)\}t}{\eta}, \quad \delta_l=\delta_{l0}+\frac{2}{\eta}\mathrm{Im}\{(\xi-i\eta)\omega(i\eta+\xi)\}t. \tag{39}$$

The vector soliton then takes the form

$$q_l=2i\eta\theta_le^{i(\xi/\eta)z}\,\mathrm{sech}\,z \tag{40}$$

with $z=2\eta(x-\overline{x})$. For instance, for the vector NLS equation $\omega(k)=2k^2$ and we arrive at the n-component generalization of the well-known vector soliton solution for the two-component NLS equation.[12]

IV. PERTURBATION-INDUCED EVOLUTION OF THE SPECTRAL DATA

A perturbation of the integrable PDE, following from the Lax representation (1)–(2), can be written in the form

$$iQ_t - V_x + [ikA + iQ, V] = R, \tag{41}$$

where R (which is k-independent in case of the Zakharov–Shabat spectral problem) represents the terms destroying integrablity. The perturbation matrix R, similar to the potential Q, satisfies $[A,R]=0$. For the Hermitian potential $Q^\dagger = Q$ we also get $R^\dagger = -R$.

In the following we derive evolution equations for the spectral data with account for arbitrary perturbation. For simplicity of the presentation we will frequently omit the explicit dependence on x and t. To distinguish between the ''integrable'' and ''perturbation'' contributions to the evolution let us assign the variational derivatives to the latter. For instance, the perturbation-induced evolution in Eq. (41) reads

$$i\frac{\delta Q}{\delta t} = R,$$

or, explicitly

$$i\frac{\delta \mathbf{q}}{\delta t} = \mathbf{r} \quad \text{and} \quad i\frac{\delta \overline{\mathbf{q}}}{\delta t} = -\overline{\mathbf{r}},$$

where $\mathbf{r} = R_{\mathrm{I,II}}$ and $\overline{\mathbf{r}} = -R_{\mathrm{II,I}}$. For Hermitian Q, $\overline{\mathbf{r}} = \mathbf{r}^\dagger$.

We start with derivation of evolution equations for Φ_+ and Φ_-^{-1}, the solution to the RH problem (23). In other terms, we are going to derive the generalized Lax pair [see Eqs. (52) and (53)] for the *perturbed* nonlinear PDE (41). Differentiation of Eq. (1) with respect to t gives

$$\partial_x\left(\frac{\delta\Phi}{\delta t}\right) = ik\left[A, \frac{\delta\Phi}{\delta t}\right] + iQ\frac{\delta\Phi}{\delta t} + R\Phi,$$

and consequently

$$\partial_x\left(\Phi^{-1}\frac{\delta\Phi}{\delta t}\right) = ik\left[A, \Phi^{-1}\frac{\delta\Phi}{\delta t}\right] + \Phi^{-1}R\Phi.$$

Let us integrate the above-given formula for $\Phi = J_\pm$. We get

$$\frac{\delta J_\pm}{\delta t}(x,k) = J_\pm(x,k)e^{ikxA}\left(\int_{\pm\infty}^{x} \mathrm{d}\xi\, e^{-ik\xi A} J_\pm^{-1}(\xi,k) R(\xi) J_\pm(\xi,k) e^{ik\xi A}\right) e^{-ikxA}.$$

Here we have used that $\delta J_\pm \to 0$ as $x \to \pm\infty$. Let us employ the relation between $J_\pm$ and Φ_+ to rewrite this formula in a more convenient form. Using (20a) we get

$$\frac{\delta J_\pm}{\delta t}(x,k) = J_\pm(x,k)e^{ikxA}S_\pm(k)\Upsilon(\pm\infty, x; k)S_\pm^{-1}(k)e^{-ikxA}. \tag{42}$$

In much the same way, using (20b), we derive

$$\frac{\delta J_{\pm}^{-1}}{\delta t}(x,k) = -e^{ikxA}\overline{S_{\pm}^{-1}}(k)\overline{\Upsilon}(\pm\infty,x;k)\overline{S_{\pm}}(k)e^{-ikxA}J_{\pm}^{-1}(x,k). \tag{43}$$

Here we have introduced the notations:

$$\Upsilon(\pm\infty,x;k) = \int_{\pm\infty}^{x} \mathrm{d}\xi\, e^{-ik\xi A}\Phi_{+}^{-1}R\Phi_{+}e^{ik\xi A}, \tag{44}$$

$$\overline{\Upsilon}(\pm\infty,x;k) = \int_{\pm\infty}^{x} \mathrm{d}\xi\, e^{-ik\xi A}\Phi_{-}^{-1}R\Phi_{-}e^{ik\xi A}. \tag{45}$$

These matrix functionals will enter every formula describing perturbation-induced evolution of the spectral data. For the involution, due to formula (19) these matrix functionals satisfy

$$\Upsilon^{\dagger}(\pm\infty,x;k) = -\overline{\Upsilon}(\pm\infty,x,\overline{k}). \tag{46}$$

Using Eqs. (42), (43), and the definition of the scattering matrix S (14) we get

$$\frac{\delta S}{\delta t} = e^{-ikxA}\frac{\delta}{\delta t}(J_{+}^{-1}J_{-})e^{ikxA} = -\overline{S_{+}^{-1}}\overline{\Upsilon}(\infty,x)\overline{S_{+}}S + SS_{-}\Upsilon(-\infty,x)S_{-}^{-1}$$

$$= S_{+}\Upsilon(-\infty,x)S_{-}^{-1} + \overline{S_{+}^{-1}}\overline{\Upsilon}(x,\infty)\overline{S_{-}}.$$

Setting $x\to\pm\infty$ in this formula produces two simple equivalent formulas:

$$\frac{\delta S(k)}{\delta t} = S_{+}(k)\Upsilon(-\infty,\infty;k)S_{-}^{-1}(k) \equiv \overline{S_{+}^{-1}}(k)\overline{\Upsilon}(-\infty,\infty;k)\overline{S_{-}}(k). \tag{47}$$

Now we can easily obtain the perturbation-induced evolution of the solution to the RH problem. Taking into account the definitions of $S_{\pm}$ and $\overline{S_{\pm}}$ and (20) we write:

$$\frac{\delta\Phi_{+}}{\delta t} = \frac{\delta J_{+}}{\delta t}e^{ikxA}S_{+}e^{-ikxA} + J_{+}e^{ikxA}\frac{\delta}{\delta t}(H_1 + SH_2)e^{-ikxA}$$

$$= \Phi_{+}e^{ikxA}(-\Upsilon(x,\infty) + \Upsilon(-\infty,\infty)H_2)e^{-ikxA}$$

$$= \Phi_{+}e^{ikxA}\Pi e^{-ikxA}, \tag{48a}$$

$$\frac{\delta\Phi_{-}^{-1}}{\delta t} = e^{ikxA}\overline{S}_{+}e^{-ikxA}\frac{\delta J_{+}^{-1}}{\delta t} + e^{ikxA}\frac{\delta}{\delta t}(H_1 + H_2S^{-1})J_{+}^{-1}e^{-ikxA}$$

$$= e^{ikxA}(\overline{\Upsilon}(x,\infty) - H_2\overline{\Upsilon}(-\infty,\infty))\Phi_{-}^{-1}e^{-ikxA}$$

$$= -e^{ikxA}\overline{\Pi}\Phi_{-}^{-1}e^{-ikxA}. \tag{48b}$$

The right-hand sides of the above formulas contain the evolution functionals,

$$\Pi(x,k) = -\Upsilon(x,\infty;k)H_1 + \Upsilon(-\infty,x;k)H_2, \tag{49}$$

$$\overline{\Pi}(x,k) = H_1\overline{\Upsilon}(x,\infty;k) - H_2\overline{\Upsilon}(-\infty,x;k), \tag{50}$$

which account for the perturbation-induced evolution of the solution to the RH problem. As follows from formula (46), for the case of the involution the evolution functionals satisfy

$$\Pi^{\dagger}(k) = -\overline{\Pi}(\overline{k}). \tag{51}$$

From the definitions (49), (50) and also (44), (45) it is easy to see that the matrices $e^{ikxA}\Pi(k)e^{-ikxA}$ and $e^{ikxA}\overline{\Pi}(k)e^{-ikxA}$ are meromorphic and bounded in the upper and lower half planes of the k-plane, respectively. They have simple poles, respectively, at zeros of $\det\Phi_+(k)$ and $\det\Phi_-^{-1}(k)$.

Let us write down the generalized Lax representation for the perturbed PDE (41) in terms of $\Phi_+(x,k)$:

$$\partial_x\Phi_+ = ik[A,\Phi_+] + iQ\Phi_+, \tag{52}$$

$$\partial_t\Phi_+ = \Phi_+\Omega + V\Phi_+ + \Phi_+ e^{ikxA}\Pi e^{-ikxA}. \tag{53}$$

It is easy to check by direct calculation that the compatibility condition for the above-given linear system is equivalent to the perturbed equation (41) (indeed, $\partial_x\Pi = e^{-ikxA}\Phi_+^{-1}R\Phi_+e^{ikxA}$).

Now, let us derive the perturbation-induced evolution of the spectral data. From (48) we immediately obtain

$$\frac{\delta G}{\delta t} = \frac{\delta}{\delta t}(e^{-ikxA}\Phi_-^{-1}\Phi_+e^{ikxA}) = G\Pi - \overline{\Pi}G.$$

Hence, the complete evolution of the continuous datum reads

$$\partial_t G = [G,\Omega] + G\Pi - \overline{\Pi}G, \tag{54}$$

where we have taken into account the integrable evolution given by (32). It is important to notice that the left-hand side of (54) does not depend on x. Therefore, we can put $x\to\pm\infty$ in this equation to simplify it. Equation (54) can be rewritten in a more explicit form. Using the definition (24), formulas (49) and (50) we get two equivalent evolution equations for $\mathbf{b}$ corresponding to the two limits $x\to\pm\infty$:

$$\partial_t\mathbf{b} = -2i\omega(k)\mathbf{b} + \mathbf{b}H_2\Upsilon(-\infty,\infty;k)H_2 + H_1\Upsilon(-\infty,\infty;k)H_2, \tag{55a}$$

$$\partial_t\mathbf{b} = -2i\omega(k)\mathbf{b} - H_1\overline{\Upsilon}(-\infty,\infty;k)H_1\mathbf{b} - H_1\overline{\Upsilon}(-\infty,\infty;k)H_2. \tag{55b}$$

Similarly,

$$\partial_t\overline{\mathbf{b}} = 2i\omega(k)\overline{\mathbf{b}} + \overline{\mathbf{b}}H_1\Upsilon(-\infty,\infty;k)H_1 + H_2\Upsilon(-\infty,\infty;k)H_1, \tag{56a}$$

$$\partial_t\overline{\mathbf{b}} = 2i\omega(k)\overline{\mathbf{b}} - H_2\overline{\Upsilon}(-\infty,\infty;k)H_2\overline{\mathbf{b}} - H_2\overline{\Upsilon}(-\infty,\infty;k)H_1. \tag{56b}$$

Evolution of zeros k_j and $\overline{k_j}$ of $\det\Phi_+(k)$ and $\det\Phi_-^{-1}(k)$, respectively, is derived by differentiation of the determinants. In the integrable limit zeros do not depend on t. Then, for instance,

$$\frac{dk_j}{dt} = -\left.\frac{\partial_t\det\Phi_+(k)}{\partial_k\det\Phi_+(k)}\right|_{k=k_j} = -\left.\frac{\mathrm{Tr}\{\Pi(k)\}\det\Phi_+(k)}{\partial_k\det\Phi_+(k)}\right|_{k=k_j}.$$

To calculate the right-hand side in this formula recall that the evolution functional Π has simple pole at $k=k_j$ and that $\det\Phi_+(k)$ can be written as

$$\det\Phi_+(k) = \det\phi_+(k)\det\Gamma(k) = \det\phi_+(k)\prod_{i=1}^{s}\left(\frac{k-k_i}{k-\overline{k_i}}\right)^{\nu_i},$$

where $\det\phi_+(k)\neq 0$. Simple calculations give

$$\frac{\mathrm{d}k_j}{\mathrm{d}t} = -\frac{\mathrm{Tr}\{\mathrm{Res}\,\Pi(k_j)\}}{\nu_j}.$$

Here "Res" denotes the residue of $\Pi(k)$ at $k=k_j$. Noticing that the left-hand side does not depend on x, we simplify the above-mentioned equation setting $x\to\pm\infty$:

$$\frac{\mathrm{d}k_j}{\mathrm{d}t} = -\frac{\mathrm{Tr}\{\mathrm{Res}\,\Upsilon(-\infty,\infty;k_j)H_2\}}{\nu_j} \equiv \frac{\mathrm{Tr}\{\mathrm{Res}\,\Upsilon(-\infty,\infty;k_j)H_1\}}{\nu_j}. \tag{57}$$

Similarly, using $\det\Phi_-^{-1}$, we get

$$\frac{\mathrm{d}\overline{k_j}}{\mathrm{d}t} = -\frac{\mathrm{Tr}\{\mathrm{Res}\,\overline{\Upsilon}(-\infty,\infty;\overline{k_j})H_2\}}{\nu_j} \equiv \frac{\mathrm{Tr}\{\mathrm{Res}\,\overline{\Upsilon}(-\infty,\infty;\overline{k_j})H_1\}}{\nu_j}. \tag{58}$$

In derivation of the perturbation-induced evolution of the null vectors we will use the following remarkable identities [written for the x-independent null vectors; see (37)]:

$$\mathrm{Res}\,\Pi(k_j)|P_l^{(j)}\rangle = -\frac{\delta k_j}{\delta t}|P_l^{(j)}\rangle, \quad \langle\overline{P}_l^{(j)}|\mathrm{Res}\,\overline{\Pi}(\overline{k_j}) = \langle\overline{P}_l^{(j)}|\frac{\delta\overline{k_j}}{\delta t}, \tag{59}$$

as well as other two identities:

$$\Phi_+(k_j)e^{ik_jxA}\mathrm{Res}\,\Pi(k_j)=0, \quad \mathrm{Res}\overline{\Pi}(\overline{k_j})e^{-i\overline{k}_jxA}\Phi_-^{-1}(\overline{k_j})=0, \tag{60}$$

which follow from (48). To verify the identities (59) one can proceed as follows. Introduce functions $F_j^{(+)}(k)=(k-k_j)\Phi_+^{-1}(k)$ and $F_j^{(-)}(k)=(k-\overline{k_j})\Phi_-(k)$. The regularization matrices $\Gamma^{-1}(k)$ and $\Gamma(k)$ have simple poles at $k=k_j$ and $k=\overline{k_j}$, respectively. Hence the introduced matrix functions are holomorphic in some neighborhoods of these points. Now compute the product

$$\left\{F_j^{(+)}(k)\frac{\delta\Phi_+(k)}{\delta t}|p_l^{(j)}\rangle\right\}_{k=k_j} = \{(k-k_j)e^{ikxA}\Pi(k)e^{-ikxA}|p_l^{(j)}\rangle\}_{k=k_j}$$
$$= e^{ik_jxA}\mathrm{Res}\,\Pi(k_j)e^{-ik_jxA}|p_l^{(j)}\rangle.$$

On the other hand,

$$\left\{F_j^{(+)}(k)\frac{\delta\Phi_+(k)}{\delta t}\right\}_{k=k_j} = \left\{\frac{\delta}{\delta t}(k-k_j)I\right\}_{k=k_j} - \left\{\frac{\delta F_j^{(+)}(k)}{\delta t}\Phi_+(k)\right\}_{k=k_j}$$
$$= -\frac{\delta k_j}{\delta t}I - \frac{\delta F_j^{(+)}(k_j)}{\delta t}\Phi_+(k_j).$$

Multiplication by $|p_l^{(j)}\rangle$ of the latter formula and comparison with the former leads to the first identity in (59). The second one can be checked in a similar way.

Now let us derive evolution equations for the x-independent null vectors defined in (37). To this goal we simply differentiate Eq. (26),

$$\frac{\delta}{\delta t}(\Phi_+(k_j)e^{ik_jxA}|P_l^{(j)}\rangle) = \{\Phi_+(k)e^{ikxA}\Pi(k)|P_l^{(j)}\rangle\}_{k=k_j} + \frac{\delta k_j}{\delta t}\frac{\partial\Phi_+(k_j)}{\partial k}e^{ik_jxA}|P_l^{(j)}\rangle$$
$$+ \frac{\delta k_j}{\delta t}\Phi_+(k_j)ixAe^{ik_jxA}|P_l^{(j)}\rangle + \Phi_+(k_j)e^{ik_jxA}\frac{\delta|P_l^{(j)}\rangle}{\delta t} = 0.$$

Denote $\Pi_r(k_j)$ the value of the regular part of $\Pi(k)$ at $k=k_j$,

$$\Pi_r(k_j)=\left\{\Pi(k)-\frac{\mathrm{Res}\,\Pi(k_j)}{k-k_j}\right\}_{k=k_j}. \tag{61}$$

Then, using (59) and (60) to cancel out secular terms, we arrive at

$$\Phi_+(k_j)e^{ik_jxA}\left\{\frac{\delta|P_l^{(j)}\rangle}{\delta t}+\Pi_r(k_j)|P_l^{(j)}\rangle\right\}=0.$$

Using the same arguments as in Sec. III for derivation of the integrable evolution we get, adding the latter,

$$\frac{\mathrm{d}|P_l^{(j)}\rangle}{\mathrm{d}t}=-\Omega(k_j)|P_l^{(j)}\rangle-\Pi_r(k_j)|P_l^{(j)}\rangle. \tag{62}$$

Similarly,

$$\frac{\mathrm{d}\langle\overline{P}_l^{(j)}|}{\mathrm{d}t}=\langle\overline{P}_l^{(j)}|\Omega(\overline{k}_j)+\langle\overline{P}_l^{(j)}|\overline{\Pi}_r(\overline{k}_j), \tag{63}$$

where

$$\overline{\Pi}_r(\overline{k}_j)=\left\{\overline{\Pi}(k)-\frac{\mathrm{Res}\,\overline{\Pi}(k_j)}{k-\overline{k}_j}\right\}_{k=\overline{k}_j}. \tag{64}$$

In the case of the involution equation (63) is Hermitian conjugate to (62). Note that the left-hand sides of Eqs. (62) and (63) do not depend on x. Hence we can send $x\to\pm\infty$ to considerably simplify these equations. Consider, for instance, (62). Letting $x\to\infty$ and introducing the notations

$$|P_l^{(j)}\rangle=H_1|P_l^{(j)}\rangle+H_2|P_l^{(j)}\rangle\equiv|P_l^{(j)},1\rangle+|P_l^{(j)},2\rangle$$

and $\Upsilon^{(1)}=H_1\Upsilon H_2$, $\Upsilon^{(2)}=H_2\Upsilon H_2$ we get the following system;

$$\frac{\mathrm{d}|P_l^{(j)},1\rangle}{\mathrm{d}t}=-i\omega(k_j)|P_l^{(j)},1\rangle-\Upsilon_r^{(1)}(-\infty,\infty;k_j)|P_l^{(j)},2\rangle, \tag{65a}$$

$$\frac{\mathrm{d}|P_l^{(j)},2\rangle}{\mathrm{d}t}=\{i\omega(k_j)-\Upsilon_r^{(2)}(-\infty,\infty;k_j)\}|P_l^{(j)},2\rangle. \tag{65b}$$

Here $\Upsilon_r(k_j)$ is the value of the regular part of the matrix $\Upsilon(k)$ at $k=k_j$:

$$\Upsilon_r(k_j)=\left\{\Upsilon(k)-\frac{\mathrm{Res}\,\Upsilon(k_j)}{k-k_j}\right\}_{k=k_j}. \tag{66}$$

When dealing with vector PDEs, i.e., for $n=N-1$, one can define the polarization-phase parameters of vector solitons as quotients of components of the null vectors (note that the zeros are simple in this particular case). Let $C_l^{(j)}=P_l^{(j)}/P_N^{(j)}$, $l=1,\ldots,n=N-1$, where $|P^{(j)}\rangle=(P_1^{(j)},\ldots,P_N^{(j)})^T$. Then from (65) we obtain

$$\frac{\mathrm{d}C_l^{(j)}}{\mathrm{d}t}=\{-2i\omega(k_j)+\Upsilon_{rNN}(-\infty,\infty;k_j)\}C_l^{(j)}-\Upsilon_{rlN}(-\infty,\infty;k_j),\quad l=1,...,n.$$

This particular case ($n=N-1$) contains the vector NLS (8) and the complex modified KdV (9) equations as examples. In view of the considerable importance of such vector nonlinear PDEs, we formulate the result of this section in the following theorem.

Theorem: *Let*

$$iQ_t+V_0(Q,Q_x,Q_{xx},\ldots)=\epsilon R(x,t,Q,Q_x,Q_{xx},\ldots) \tag{67}$$

be a perturbed nonlinear PDE associated with the $N\times N$ matrix Zakharov–Shabat spectral problem,

$$\partial_x\Phi=ik[A,\Phi]+iQ(x,t)\Phi, \quad A=\mathrm{diag}(I_n,-1), \tag{68}$$

where ($n=N-1$)

$$Q=\begin{pmatrix}0 & \mathbf{q}\\ \mathbf{q}^\dagger & 0\end{pmatrix}, \quad R=\begin{pmatrix}0 & \mathbf{r}\\ -\mathbf{r}^\dagger & 0\end{pmatrix}, \quad \mathbf{q}=(q_1,q_2,\ldots,q_n)^T, \quad \mathbf{r}=(r_1,r_2,\ldots,r_n)^T.$$

Here the matrix function V_0 represents the limiting integrable evolution given by the dispersion relation $\Omega(k)=i\omega(k)A$, while R contains the terms destroying integrability (ϵ is a small parameter). Then the perturbed evolution is equivalent to the following evolution of the spectral data:

$$\frac{dk_j}{dt}=-\epsilon\,\mathrm{Res}\,\Upsilon_{NN}(t,k_j), \tag{69}$$

$$\frac{dC_l^{(j)}}{dt}=\{-2i\omega(k_j)+\epsilon\Upsilon_{rNN}(t,k_j)\}C_l^{(j)}-\epsilon\Upsilon_{rlN}(t,k_j), \quad l=1,\ldots,n, \tag{70}$$

$$\frac{\partial b_l(k)}{\partial t}=\{-2i\omega(k)+\epsilon\Upsilon_{NN}(t,k)\}b_l(k)+\epsilon\Upsilon_{lN}(t,k), \quad l=1,\ldots,n. \tag{71}$$

Here

$$\Upsilon(t,k)=\int_{-\infty}^{\infty}dx e^{-ikxA}\Phi_+^{-1}(x,t,k)R(x,t)\Phi_+(x,t,k)e^{ikxA}, \tag{72}$$

$$\Upsilon_r(t,k_j)=\left\{\Upsilon(t,k)-\frac{\mathrm{Res}\,\Upsilon(t,k_j)}{k-k_j}\right\}_{k=k_j}.$$

The matrix function $\Phi_+(x,t,k)$ solves the spectral problem (68) and the RH problem

$$\Phi_+^\dagger(x,t,k)\Phi_+(x,t,k)=e^{ikxA}G(k,t)e^{-ikxA}, \quad k\in\mathrm{Re},$$

$$\Phi_+(k)\to I, \quad k\to\infty$$

of analytic factorization of matrix $G(k,t)$,

$$G(k,t)=\begin{pmatrix}I_n & \mathbf{b}(k,t)\\ \mathbf{b}^\dagger(k,t) & 1\end{pmatrix}, \quad \mathbf{b}=(b_1,b_2,\ldots,b_n)^T.$$

The Riemann–Hilbert problem has (simple) zeros $k_j(t)$, $j=1,\ldots,s$, given by $a(k_j,t)=\det\Phi_+(x,t,k_j)=0$. The vector-columns $|C^{(j)}(t)\rangle=(C_1^{(j)}(t),C_2^{(j)}(t),\ldots,C_n^{(j)}(t),1)$ are the null vectors of the matrices $\Phi_+(x,t,k_j)e^{ik_jxA}$:

$$\Phi_+(x,t,k_j)e^{ik_jxA}|C^{(j)}(t)\rangle=0, \quad j=1,\ldots,s.$$

The initial spectral data are obtained via solution of the spectral equation (68) and represent the spectral characterization of the potential $Q(x,0)$. *For real* k, *the spectral densities of radiation* $b_l(k,t)$ *and the function* $a(k,t)$ *satisfy the following identity*

$$\overline{a}a = 1 - \sum_{l=1}^{n} \overline{b}_l b_l .$$

The potential $\mathbf{q}(x,t)$ *is reconstructed by the formula*

$$q_l(x,t) = 2 \lim_{k\to\infty} k(\Phi_+)_{l,N}(x,t,k), \quad l = 1,...,n.$$

Some comments are necessary on the use of Eqs. (69)–(71) for the spectral data. These equations are *exact*, i.e., they account for the perturbation exactly. As a consequence, for the nonintegrable PDE (67), these equations are nonclosed ODEs. Equations (69)–(71) are nonclosed because they explicitly contain the matrix $\Phi_+(x,t,k)$, solution of the RH problem. Therefore, Eqs. (69)–(71) serve as the generating equations for the perturbation expansion: expanding the spectral data into the asymptotic power series in ϵ, one obtains the sequence of closed approximate ODEs for the spectral data. In this way, one does not need to solve the RH problem—the computations are algebraic. In Sec V, we consider a single multicomponent soliton as an example.

V. MULTICOMPONENT SOLITON UNDER PERTURBATIONS

In this section we apply the theorem for construction of the perturbation theory for a single multicomponent soliton. This can be done without specifying the dispersion relation $\omega(k)$ determining the evolution of the spectral data in the unperturbed PDE. Hence our results apply to all nearly integrable vector PDEs associated with the Zakharov–Shabat spectral problem. In the following, we derive equations describing the evolution of the soliton parameters and give formulas for the first-order radiation. For a single vector soliton given by formula (40), i.e., $q_l = 2i\eta\theta_l e^{i(\xi/\eta)z}\operatorname{sech} z$, where $z = 2\eta(x - \overline{x})$, the regularization matrix Γ has the form

$$\Gamma = I - \frac{i\eta}{(k-\overline{k}_1)\cosh z} \begin{pmatrix} e^{-z}|\theta\rangle\langle\theta| & e^{i(\xi/\eta)z}|\theta \\ \langle\theta|e^{-i(\xi/\eta)z} & e^{z} \end{pmatrix}. \tag{73}$$

Here $k_1 = \xi + i\eta$ and we have used the vector notations $|\theta\rangle = (\theta_1,\ldots,\theta_n)^T$ and $\langle\theta| = (\overline{\theta}_1,\ldots,\overline{\theta}_n)$. To simplify some of the calculations introduce the following basis (in the n-dimensional subspace):

$$|\theta^{(1)}\rangle = |\theta\rangle, \quad |\theta^{(2)}\rangle, \quad \ldots, \quad |\theta^{(n)}\rangle; \quad \langle\theta^{(l)}|\theta^{(m)}\rangle = \delta_{lm}.$$

The explicit form of the vectors $|\theta^{(l)}\rangle$ for $l = 2,...,n$ will not be needed at all. Also we will use the basis

$$|e_1\rangle = (1,0,...,0)^T, \quad |e_2\rangle = (0,1,0,...,0)^T, \quad \ldots, \quad |e_n\rangle = (0,...,0,1)^T.$$

With the help of the unitary transformation matrix Ξ, defined as

$$\Xi = \begin{pmatrix} B & 0 \\ 0 & 1 \end{pmatrix}, \quad B = \sum_{l=1}^{n} |e_l\rangle\langle\theta^{(l)}|, \tag{74}$$

the regularization matrix Γ can be considerably simplified:

$$\tilde{\Gamma} = \Xi\Gamma\Xi^{-1} = I - \frac{i\eta}{(k-\overline{k}_1)\cosh z} \begin{pmatrix} e^{-z}|e_1\rangle\langle e_1| & e^{i(\xi/\eta)z}|e_1 \\ \langle e_1|e^{-i(\xi/\eta)z} & e^{z} \end{pmatrix}. \tag{75}$$

Note the evident property $\tilde{\Gamma}^{-1}=\tilde{\Gamma}^{\dagger}$.

The transformation matrix Ξ depends on t due to the perturbation-induced time dependence of the θ-parameters, but does not depend on x. This simple fact allows us to use the transformation with Ξ inside the integrals defining Υ (72). Taking into account that $\Phi_{+}=\Gamma$ for the pure soliton solution of the unperturbed PDE, in the first order we get

$$\tilde{\Upsilon}=\Xi\Upsilon\Xi^{-1}=\int_{-\infty}^{\infty}\mathrm{d}x\, e^{-ikxA}\tilde{\Gamma}^{-1}\tilde{R}\tilde{\Gamma}e^{ikxA}.$$

Here we have defined

$$\tilde{R}=\Xi R\Xi^{-1}=\begin{pmatrix}0 & B|r\rangle\\ -\langle r|B^{\dagger} & 0\end{pmatrix}, \tag{76}$$

where, for convenience of the following presentation, we have changed the notation for the perturbation: $|r\rangle=\mathbf{r}=(r_1,\ldots,r_n)^T$.

In fact, we will need only one diagonal element

$$\Upsilon_{NN}=(\Xi^{-1}\tilde{\Upsilon}\Xi)_{NN}=\int_{-\infty}^{\infty}\mathrm{d}x(\tilde{\Gamma}^{\dagger}\tilde{R}\tilde{\Gamma})_{NN}$$

and the following nondiagonal matrix elements:

$$\Upsilon_{lN}=(\Xi^{-1}\tilde{\Upsilon}\Xi)_{lN}=\sum_{m=1}^{n}B^{-1}_{lm}\tilde{\Upsilon}_{mN}=\theta_l\tilde{\Upsilon}_{1N}+\sum_{m=2}^{n}B^{-1}_{lm}\tilde{\Upsilon}_{mN}=\theta_l\tilde{\Upsilon}_{1N}+F_l,$$

where $l=1,\ldots,n$. The second term simplifies as follows:

$$\begin{aligned}F_l&=\int_{-\infty}^{\infty}\mathrm{d}x\, e^{-2ikx}\sum_{m=2}^{n}B^{-1}_{lm}\tilde{R}_{mN}\tilde{\Gamma}_{NN}\\&=\int_{-\infty}^{\infty}\mathrm{d}x\, e^{-2ikx}\tilde{\Gamma}_{NN}\sum_{m=2}^{n}\langle e_l|B^{-1}|e_m\rangle\langle e_m|B|r\rangle\\&=\int_{-\infty}^{\infty}\mathrm{d}x\, e^{-2ikx}\tilde{\Gamma}_{NN}(r_l-\theta_l\langle\theta|r\rangle).\end{aligned} \tag{77}$$

After simple calculations we get

$$\Upsilon_{NN}=\frac{i}{4}\int_{-\infty}^{\infty}\mathrm{d}z\,\mathrm{sech}^2 z\left(\frac{e^{-z}}{k-k_1}+\frac{e^{z}}{k-\overline{k_1}}\right)(r_0(z)+\overline{r_0}(-z)), \tag{78}$$

$$\begin{aligned}\Upsilon_{lN}=&\frac{\theta_l}{8\eta}\int_{-\infty}^{\infty}\mathrm{d}z\,\mathrm{sech}^2 z\,\frac{\exp\{-2ikx+i(\xi/\eta)z\}}{(k-k_1)(k-\overline{k_1})}\\&\times\{-4\eta^2\overline{r_0}(-z)+[e^{-2z}(k-\overline{k_1})+e^{2z}(k-k_1)]^2 r_0(z)\}+F_l.\end{aligned} \tag{79}$$

Here we have used the notation

$$r_0=e^{-i(\xi/\eta)z}\tilde{R}_{1N}=e^{-i(\xi/\eta)z}\langle\theta|r\rangle=e^{-i(\xi/\eta)z}\sum_{l=1}^{n}\overline{\theta_l}r_l. \tag{80}$$

A. Evolution of the soliton parameters

Let us first derive evolution equations for the soliton parameters η, ξ, $\overline{x}$, and θ_l, $l=1,\ldots,n$. Using the identity $-2ik_1x+i(\xi/\eta)z=z+2\eta\overline{x}-2i\xi\overline{x}$ and the definition $C_l=\theta_l e^{2(\eta-i\xi)\overline{x}}$ from Sec. III, we obtain

$$\mathrm{Res}\,\Upsilon_{NN}(k_1)=\frac{i}{4}\int_{-\infty}^{\infty}\mathrm{d}z\, e^{-z}\mathrm{sech}^2\, z(r_0(z)+\overline{r_0}(-z)), \tag{81}$$

$$\Upsilon_{rNN}(k_1)=\frac{1}{8\eta}\int_{-\infty}^{\infty}\mathrm{d}z\, e^{z}\mathrm{sech}^2\, z(r_0(z)+\overline{r_0}(-z)), \tag{82}$$

$$\Upsilon_{rlN}(k_1)=C_l\{-2i\overline{x}\,\mathrm{Res}\{\Upsilon_{NN}(k_1)\}+\Upsilon_{rNN}(k_1)+J_0\}+f_l, \tag{83}$$

where

$$J_0=\frac{1}{4\eta}\int_{-\infty}^{\infty}\mathrm{d}z\,\mathrm{sech}^2\, z(\cosh z+ze^{-z})(r_0(z)-\overline{r_0}(-z))$$

and

$$f_l=F_l(k_1)=\frac{e^{2(\eta-i\xi)\overline{x}}}{4\eta}\int_{-\infty}^{\infty}\mathrm{d}z\,\mathrm{sech}\, z(e^{-i(\xi/\eta)z}r_l-\theta_l r_0).$$

Let us first consider the more involved derivation of equations for $\overline{x}$ and θ_l. From Eqs. (70), (82), and (83) we get

$$\frac{\mathrm{d}C_l}{\mathrm{d}t}=(-2i\omega(k_1)+2\epsilon i\overline{x}\,\mathrm{Res}\,\Upsilon_{NN}(k_1)-\epsilon J_0)C_l-\epsilon f_l, \tag{84}$$

from which it follows that

$$\frac{\mathrm{d}|C_l|^2}{\mathrm{d}t}=[4\,\mathrm{Im}\{\omega(k_1)\}-4\epsilon\overline{x}\,\mathrm{Im}\{\mathrm{Res}\,\Upsilon_{NN}(k_1)\}-2\epsilon\,\mathrm{Re}\{J_0\}]|C_l|^2-2\epsilon\,\mathrm{Re}\{f_l\overline{C_l}\}.$$

Recalling that $\Sigma_{l=1}^{n}|\theta_l|^2=1$ we obtain

$$\frac{\mathrm{d}\overline{x}}{\mathrm{d}t}=\frac{e^{-4\eta\overline{x}}}{4\eta}\sum_{l=1}^{n}\frac{\mathrm{d}|C_l|^2}{\mathrm{d}t}-\frac{\overline{x}}{\eta}\frac{\mathrm{d}\eta}{\mathrm{d}t},$$

$$\frac{\mathrm{d}\theta_l}{\mathrm{d}t}=\theta_l\left(C_l^{-1}\frac{\mathrm{d}C_l}{\mathrm{d}t}-2\frac{\mathrm{d}(\eta\overline{x})}{\mathrm{d}t}+2i\frac{\mathrm{d}(\xi\overline{x})}{\mathrm{d}t}\right).$$

The rest calculations are straightforward substitutions and using the identity $\Sigma_{l=1}^{n}f_l\overline{C_l}=0$, which follows from the definitions of C_l, r_0, and f_l. After simple calculations one gets a system of equations for the soliton parameters:

$$\frac{\mathrm{d}\eta}{\mathrm{d}t}=-\frac{\epsilon}{2}\int_{-\infty}^{\infty}\mathrm{d}z\,\mathrm{sech}\, z\,\mathrm{Re}\{r_0\}, \tag{85}$$

$$\frac{\mathrm{d}\xi}{\mathrm{d}t}=-\frac{\epsilon}{2}\int_{-\infty}^{\infty}\mathrm{d}z\,\mathrm{sech}\, z\tanh z\,\mathrm{Im}\{r_0\}, \tag{86}$$

$$\frac{d\overline{x}}{dt}=\frac{\mathrm{Im}\{\omega(k_1)\}}{\eta}-\frac{\epsilon}{4\eta^2}\int_{-\infty}^{\infty}dz\, z\,\mathrm{sech}\, z\,\mathrm{Re}\{r_0\}, \tag{87}$$

$$\frac{d\theta_l}{dt}=i\theta_l\left\{\frac{2\,\mathrm{Im}\{\overline{k_1}\omega(k_1)\}}{\eta}-\frac{\epsilon}{2\eta^2}\int_{-\infty}^{\infty}dz\,\mathrm{sech}\, z[\xi z\,\mathrm{Re}\{r_0\}+\eta(1-z\tanh z)\mathrm{Im}\{r_0\}]\right\}$$
$$+\frac{\epsilon}{4\eta}\int_{-\infty}^{\infty}dz\,\mathrm{sech}\, z(\theta_l r_0-e^{-i(\xi/\eta)z}r_l). \tag{88}$$

These equations can be compared with the adiabatic equations derived by Karpman[21] for the single scalar soliton. First, it is convenient to introduce the average phase $\overline{\delta}$ of the soliton by setting

$$\overline{\delta}=\sum_{l=1}^{n}|\theta_l|^2\delta_l.$$

The evolution equation for the average phase then follows from Eq. (88):

$$\frac{d\overline{\delta}}{dt}=\frac{2\,\mathrm{Im}\{\overline{k_1}\omega(k_1)\}}{\eta}-\frac{\epsilon}{2\eta^2}\int_{-\infty}^{\infty}dz\,\mathrm{sech}\, z[\xi z\,\mathrm{Re}\{r_0\}+\eta(1-z\tanh z)\mathrm{Im}\{r_0\}]. \tag{89}$$

Remarkably, the slow evolution of the soliton amplitude η, phase gradient ξ, position $\overline{x}$, and average phase $\overline{\delta}$ is given by equations similar to those derived for the single scalar soliton. The only trace of the vector nature of the soliton in Eqs. (85)–(87) and (89) is that the ''scalar'' perturbation r_0 obtains by averaging the original vector perturbation as follows:

$$r_0=e^{-i(\xi/\eta)z}\sum_{l=1}^{n}\overline{\theta_l}r_l.$$

The equation for $\theta_l=s_l e^{i\delta_l}$ can be cast in the form of two separate equations, one for the polarization parameters s_l and the other for the phases δ_l. We get

$$\frac{ds_l}{dt}=\frac{\epsilon}{4\eta}\int_{-\infty}^{\infty}dz\,\mathrm{sech}\, z\,\mathrm{Re}\{s_l r_0-e^{-i(\xi/\eta)z-i\delta_l}r_l\}, \tag{90}$$

$$\frac{d\delta_l}{dt}=\frac{2\,\mathrm{Im}\{\overline{k_1}\omega(k_1)\}}{\eta}-\frac{\epsilon}{2\eta^2}\int_{-\infty}^{\infty}dz\,\mathrm{sech}\, z[\xi z\,\mathrm{Re}\{r_0\}+\eta(1-z\tanh z)\mathrm{Im}\{r_0\}]$$
$$+\frac{\epsilon}{4\eta}\int_{-\infty}^{\infty}dz\,\mathrm{sech}\, z\,\mathrm{Im}\{r_0-s_l^{-1}e^{-i(\xi/\eta)z-i\delta_l}r_l\}. \tag{91}$$

Note that the equation for δ_l contains s_l in the denominator as a reflection of the fact that the phase is not defined for the components which are not excited.

B. First-order radiation

Now let us consider the evolution of the spectral densities $b_l(k)$ of radiation. Taking into account radiation in the first-order approximation amounts to solving the linearized regular Riemann–Hilbert problem (or the jump problem),

$$\phi_+(k)-\phi_-(k)=\Gamma(k)\begin{pmatrix}0 & e^{2ikx}|b(k)\rangle\\ \langle b(k)|e^{-2ikx} & 0\end{pmatrix}\Gamma^{-1}(k),$$

where we have used the notation $|b\rangle=\mathbf{b}=(b_1,\ldots,b_n)^T$. Solution of the above-mentioned jump problem is obtained by integration and using the normalization condition $\phi_{\pm}(k)\to I$ as $k\to\infty$. We obtain

$$\phi(k)=I+\frac{1}{2i\pi}\int_{-\infty}^{\infty}\frac{d\not{\ell}}{\not{\ell}-k}\Gamma(\not{\ell})\begin{pmatrix}0 & e^{2i\not{\ell}x}|b(\not{\ell})\rangle\\ \langle b(\not{\ell})|e^{-2i\not{\ell}x} & 0\end{pmatrix}\Gamma^{-1}(\not{\ell}).$$

The contribution from radiation to the solution follows from the formula (4),

$$q_l^{(\mathrm{rad})}=-2\lim_{k\to\infty}k\phi_{lN}(k)=\frac{1}{i\pi}\int_{-\infty}^{\infty}dk\left\{\Gamma(k)\begin{pmatrix}0 & e^{2ikx}|b(k)\rangle\\ \langle b(k)|e^{-2ikx} & 0\end{pmatrix}\Gamma^{-1}(k)\right\}_{lN}.$$

As in derivation of the equations for the soliton parameters it is convenient to use the transformation with the matrix Ξ. Using this transformation and formula (75) one can easily simplify the formula for radiation contribution. We get $q_l^{(\mathrm{rad})}=q_l^{(\|)}+q_l^{(\perp)}$, where the "parallel" and "perpendicular" parts of radiation are defined as follows:

$$q_l^{(\|)}=\frac{\eta\theta_l e^{i(\xi/\eta)z}}{i\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\lambda^2+1}\{(\lambda+i\tanh z)^2e^{i\lambda z}\langle\theta|g(\lambda)\rangle+\mathrm{sech}^2 z e^{-i\lambda z}\langle g(\lambda)|\theta\rangle\},\quad(92a)$$

$$q_l^{(\perp)}=\frac{\eta e^{i(\xi/\eta)z}}{i\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\lambda-i}e^{i\lambda z}(\lambda+i\tanh z)(g_l(\lambda)-\theta_l\langle\theta|g(\lambda)\rangle).\quad(92b)$$

Here, for convenience, we have introduced the modified spectral parameter by setting $k=\eta\lambda+\xi$ and the modified spectral densities of radiation:

$$g_l(\lambda)=e^{2i(\eta\lambda+\xi)\overline{x}}\overline{b}_l(\eta\lambda+\xi).\quad(93)$$

The separation of radiation into parallel and perpendicular parts is due the following facts. While the perpendicular part $q_l^{(\perp)}$ satisfies the orthogonality property

$$\sum_{l=1}^{n}\overline{\theta}_l q_l^{(\perp)}=0,\quad(94)$$

the parallel part of the radiation is given by the same formula as the radiation of the scalar soliton (multiplied by θ_l), but for the averaged spectral density $\langle\theta|g(\lambda)\rangle$.

Consider the evolution equation (71) for the spectral densities of radiation. In the first-order approximation the term with Υ_{NN} can be neglected. When deriving evolution equations for the modified spectral densities in the first-order approximation one must take into account only the fast (or "integrable") evolution of the soliton parameters involved in the definition of $g(\lambda)$. In particular, the modified spectral parameter λ is t-independent. The only parameter which has the fast t-dependence in (93) is $\overline{x}$. By differentiation of (93) and using (71) and (87) we obtain

$$\frac{\partial g_l(\lambda)}{\partial t}=i\Omega_r(\lambda)g_l(\lambda)+\epsilon\theta_l\Upsilon^{(\|)}(\lambda)+\epsilon\Upsilon_l^{(\perp)}(\lambda),\quad(95)$$

where

$$\Omega_r(\lambda)=2[\lambda\,\mathrm{Im}\{\omega(k_1)\}+\mathrm{Re}\{\omega(k_1)\}-\omega(\eta\lambda+\xi)].\quad(96)$$

The last two terms in Eq. (95) come from Υ_{lN} (79) [the second one is the contribution of F_l (77)]. They read

$$\Upsilon^{(\|)}(\lambda)=\frac{1}{2\,\eta(\lambda^2+1)}\int_{-\infty}^{\infty}\mathrm{d}z\,e^{-i\lambda z}[(\lambda-i\tanh z)^2 r_0-\mathrm{sech}^2\,z\,\overline{r_0}], \tag{97}$$

$$\Upsilon_l^{(\perp)}(\lambda)=\frac{1}{2\,\eta(\lambda+i)}\int_{-\infty}^{\infty}\mathrm{d}z\,e^{-i\lambda z}(\lambda-i\tanh z)(e^{-i(\xi/\eta)z}r_l-\theta_l r_0). \tag{98}$$

Due to the definition of r_0 (80), the perpendicular component satisfies the identity

$$\sum_{l=1}^{n}\overline{\theta_l}\Upsilon_l^{(\perp)}=0. \tag{99}$$

Integrating the equation for $g_l(\lambda)$ with $g_l(\lambda,t=0)=0$ and using the result in (92) we arrive at the first-order correction to initially pure soliton solution. In this case we obtain

$$q_l^{(\|)}=\epsilon\frac{\eta\theta_l e^{i(\xi/\eta)z}}{i\pi}\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{\lambda^2+1}\{(\lambda+i\tanh z)^2 e^{i\lambda z+i\Omega_r(\lambda)t}\gamma^{(\|)}(\lambda)+\mathrm{sech}^2\,z\,e^{-i\lambda z-i\Omega_r(\lambda)t}\overline{\gamma}^{(\|)}(\lambda)\}, \tag{100a}$$

$$q_l^{(\perp)}=\epsilon\frac{\eta e^{i(\xi/\eta)z}}{i\pi}\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{\lambda-i}(\lambda+i\tanh z)e^{i\lambda z+i\Omega_r(\lambda)t}\gamma_l^{(\perp)}(\lambda), \tag{100b}$$

where

$$\gamma^{(\|)}=\frac{1}{2\,\eta(\lambda^2+1)}\int_{-\infty}^{\infty}\mathrm{d}z\,e^{-i\lambda z}[(\lambda-i\tanh z)^2\hat{r}_0^{(+)}-\mathrm{sech}^2\,z\,\hat{r}_0^{(-)}],$$

$$\gamma_l^{(\perp)}=\frac{1}{2\,\eta(\lambda+i)}\int_{-\infty}^{\infty}\mathrm{d}z\,e^{-i\lambda z}(\lambda-i\tanh z)(e^{-i(\xi/\eta)z}\hat{r}_l-\theta_l\hat{r}_0^{(+)}),$$

with

$$\hat{r}_0^{(+)}(z,t,\lambda)=\int_0^t\mathrm{d}\tau\,e^{-i\Omega_r(\lambda)\tau}r_0(z,\tau),\quad \hat{r}_0^{(-)}(z,t,\lambda)=\int_0^t\mathrm{d}\tau\,e^{-i\Omega_r(\lambda)\tau}\overline{r_0}(z,\tau),$$

$$\hat{r}_l(z,t,\lambda)=\int_0^t\mathrm{d}\tau\,e^{-i\Omega_r(\lambda)\tau}r_l(z,\tau).$$

VI. CONCLUSIONS

In construction of the perturbation theory our main idea is to use the Riemann–Hilbert problem associated with the integrable PDE for the nonlinear transformation of the *perturbed* PDE to the spectral space. The evolution equations for the spectral data follow from the evolution functional, an additional object one needs to introduce into the IST theory to account for perturbations. For a single vector soliton, the equations describing evolution of the soliton parameters and first-order radiation are given in explicit form. The method is not restricted to the first order only. For instance, the second-order equations can also be derived. The perturbation theory can be applied for description of dynamics of the spatial optical solitons, soliton pulses in the multispecies Bose–Einstein condensates, soliton propagation in optical fiber with account of the arbitrary polarization of light pulses, and for many other applications of the multicomponent soliton equations.

In this paper we have restricted the consideration to the Zakharov–Shabat spectral problem. However, the approach of this paper was successfully applied to other spectral problems as

well.[41–45] There, the evolution functional was derived and the evolution equations for the spectral data were obtained. The overall result of this and the previous works on the perturbation theory based on the Riemann–Hilbert problem is that this approach *always works*. The explicit form of the evolution functional was the same for all considered spectral problems and, moreover, it undergoes only insignificant changes in the transition from the Cauchy problem to an initial-boundary value problem.[45]

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APPENDIX A: SOME COMMENTS ON MULTIPLICITY OF ZEROS

Here we explore in more detail the algebraic and geometric multiplicities of zeros of $\det \Phi_+(k)$ and $\det \Phi_-^{-1}(k)$. For instance, consider the determinant

$$\det \Phi_+ = J_{+1} \wedge \cdots \wedge J_{+n} \wedge J_{-n+1} \wedge \cdots \wedge J_{-N}. \tag{A1}$$

None of the columns $J_{\pm l}(x,k)$ is equal to zero [otherwise, due to uniqueness of solution to Eq. (1) we would have $J_{\pm l}=0$ for all x]. Moreover, the minors in the wedge products of columns of J_+ and J_- satisfy linear homogeneous equations, which follow from (1), Sec. III,

$$\partial_x J_{+1} \wedge \cdots \wedge J_{+n} = \left\{ ik \left(\hat{A}^{(n)} - \frac{n(n+1)}{2} \hat{I}^{(n)} \right) + i\hat{Q}^{(n)} \right\} J_{+1} \wedge \cdots \wedge J_{+n},$$

$$\partial_x J_{-n+1} \wedge \cdots \wedge J_{-N} = \left\{ ik \left(\hat{A}^{(N-n)} - \frac{(N-n)(N-n+1)}{2} \hat{I}^{(N-n)} \right) + i\hat{Q}^{(N-n)} \right\} \times J_{-n+1} \wedge \cdots \wedge J_{-N}.$$

Here $\hat{M}^{(j)}$ denotes a supermatrix, whose action on the wedge products of vector-columns is defined by the rule

$$\hat{M}^{(j)} \Psi_1 \wedge \cdots \wedge \Psi_j = \sum_{p=1}^{j} \Psi_1 \wedge \cdots \wedge M\Psi_p \wedge \cdots \wedge \Psi_j.$$

Therefore, rank $J_{+1} \wedge \cdots \wedge J_{+n} = \operatorname{rank} e_1 \wedge \cdots \wedge e_n = n$, and rank $J_{-n+1} \wedge \cdots \wedge J_{-N} = \operatorname{rank} e_{n+1} \wedge \cdots \wedge e_{N-n} = N-n$. Hence, the only possibility for $\det \Phi_+(k)=0$ is the linear dependence of the columns in J_+H_1 and J_-H_2, e.g., at least one of the columns of J_-H_2 is given as a linear combination of the columns of J_+H_1.

Let ν_j and d_j be the algebraic and geometric multiplicities of the jth zero k_j, i.e.,

$$\det \Phi_+(k) = (k-k_j)^{\nu_j} \psi(k), \quad \psi(k_j) \neq 0, \quad d_j = N - \operatorname{rank} \Phi_+(k_j).$$

Writing down the Taylor expansion of $\Phi_+(k)$ about $k=k_j$ we immediately conclude that

$$\operatorname{rank} \Phi_+(k_j) \geqslant N - \nu_j. \tag{A2}$$

Therefore, in general, the algebraic multiplicity is greater than the geometric one; trivially, they coincide for simple zeros. Representation (A1) gives

$$\operatorname{rank} \Phi_+(k_j) \geqslant \max(n, N-n).$$

Hence the geometric multiplicity satisfies

$$d_j \leqslant N - \max(n, N-n). \tag{A3}$$

We consider only zeros whose algebraic multiplicity is equal to the geometric one. In particular, if $n=N-1$, there can be only one vector in the null space of Φ_+, i.e., $d_j=1$. Hence, in this case, zeros of $\det\Phi_+(k)$ must be simple to satisfy the equal multiplicity condition. This condition requires that the only case of a multiple zero, $\det\Phi_+(k_j)=0$, of order ν_j is that there are precisely ν_j columns of $J_-(k_j)H_2$ and $J_+(x,k)H_1$ which are linear combinations of the columns of $J_+(k_j)H_1$ and $J_-(k_j)H_2$, respectively.

The equal multiplicity condition can be guaranteed by the following constraint [imposed for some (x,t)]

$$\operatorname{rank}\left(\Phi_+, \frac{\partial\Phi_+}{\partial k}\right)=N. \tag{A4}$$

Indeed, for algebraic multiplicity ν_j, by the Taylor expansion, (A4) gives $\operatorname{rank}\Phi_+(k_j)=N-\nu_j$. Conversely, if $\operatorname{rank}\Phi_+(k_j)=N-\nu_j$, for algebraic multiplicity ν_j, then there are at least ν_j columns in $\partial\Phi_+(k_j)/\partial k$ independent from the columns of $\Phi_+(k_j)$. Hence (A4) also holds. Similar results are valid for multiplicities of zeros $\overline{k_j}$, $j=1,\ldots,s$, of $\det\Phi_-^{-1}(k)$.

APPENDIX B: PROPERTIES OF THE REGULARIZATION MATRIX

Here we derive the regularization matrix $\Gamma(k)$ and prove its properties (in the main, we follow Refs. 13 and 58). Dependence on the coordinates x and t is not important for this purpose and omitted. Consider one pair of zeros, say, k_s and $\overline{k_s}$ of $\det\Phi_+(k)$ and $\det\Phi_-^{-1}(k)$, respectively. Let the vectors $|p_l^{(s)}\rangle$ and $\langle\overline{p}_l^{(s)}|$, $l=1,\ldots,\nu_s$, satisfying

$$\Phi_+(k_s)|p_l^{(s)}\rangle=0, \quad \langle\overline{p}_l^{(s)}|\Phi_-^{-1}(\overline{k_s})=0, \tag{B1}$$

span the respective null spaces. Construct the following rational matrix functions

$$\chi_s(k)=I-\frac{k_s-\overline{k_s}}{k-\overline{k_s}}P_s, \quad \overline{\chi_s}(k)=I+\frac{k_s-\overline{k_s}}{k-k_s}P_s,$$

where

$$P_s=\sum_{l,m=1}^{\nu_s}|p_l^{(s)}\rangle(M^{-1})_{lm}\langle\overline{p}_m^{(s)}|, \quad M_{lm}=\langle\overline{p}_l^{(s)}|p_m^{(s)}\rangle$$

and P_s is a projector: $P_s^2=P_s$, $\operatorname{rank}P_s=\nu_s$. It is easy to verify that $\overline{\chi_s}(k)$ is inverse to $\chi_s(k)$: $\chi_s(k)\overline{\chi_s}(k)=I$.

The determinant of $\chi_s(k)$ is easily computed in some appropriate basis, where the projector is represented by a diagonal matrix with ν_s ones and $N-\nu_s$ zeros on the diagonal. We get

$$\det\chi_s(k)=\left(\frac{k-k_s}{k-\overline{k_s}}\right)^{\nu_s}.$$

Hence, with such rational matrices we can factor out the sth pair of zeros. Indeed, consider the products $\Phi_+(k)\chi_s^{-1}(k)$ and $\chi_s(k)\Phi_-^{-1}(k)$. These matrix functions are holomorphic in the upper and lower half planes, respectively [the poles are removable due to the identities (B1)]. On the other hand, the determinants are nonzero for $k=k_s$ and $k=\overline{k_s}$, respectively; thus one pair of zeros is factored out. By introducing a sequence of such matrices,

$$\chi_j(k)=I-\frac{k_j-\overline{k_j}}{k-\overline{k_j}}P_j, \quad \overline{\chi_j}(k)=I+\frac{k_j-\overline{k_j}}{k-k_j}P_j, \quad j=1,\ldots,s, \tag{B2}$$

where $\overline{\chi_j}(k)=\chi_j^{-1}(k)$, we factor out all zeros using the regularization matrix Γ and its inverse, where

$$\Gamma(k)=\chi_1(k)\chi_2(k)\cdots\chi_s(k). \tag{B3}$$

The projector P_j is given by

$$P_j=\sum_{l,m=1}^{s}|e_l^{(j)}\rangle(M^{-1})_{lm}\langle\overline{e}_m^{(j)}|,\quad M_{lm}=\langle\overline{e}_l^{(j)}|e_m^{(j)}\rangle.$$

Here the vectors $|e_l^{(j)}\rangle$ and $\langle\overline{e}_l^{(j)}|$ are related to the basis vectors of the null spaces of $\Phi_+(k_j)$ and $\Phi_-^{-1}(\overline{k_j})$ by triangular equations (if scanned starting from s down to 1):

$$|p_l^{(j)}\rangle=\chi_s^{-1}(k_j)\cdot\chi_{s-1}^{-1}(k_j)\cdots\chi_{j+1}^{-1}(k_j)|e_l^{(j)}\rangle, \tag{B4}$$

$$\langle\overline{e}_l^{(j)}|\chi_{j+1}(\overline{k_j})\cdot\chi_{j+2}(\overline{k_j})\cdots\chi_s(\overline{k_j})=\langle\overline{p}_l^{(j)}|. \tag{B5}$$

Due to $P_j^2=P_j$, these vectors satisfy the identities:

$$\chi_j(k_j)|e_l^{(j)}\rangle=0,\quad\langle\overline{e}_l^{(j)}|\chi_j^{-1}(k_j)=0,\quad l=1,\ldots,\nu_j. \tag{B6}$$

The regularization matrix $\Gamma(k)$ can be made parametrized entirely by the vectors from the null spaces. Indeed, let us decompose $\Gamma(k)$ and the inverse matrix into the partial fractions:

$$\Gamma(k)=I-\sum_{j=1}^{s}\frac{\overline{B}_j}{k-\overline{k}_j},\quad\Gamma^{-1}(k)=I+\sum_{j=1}^{s}\frac{B_j}{k-k_j}, \tag{B7}$$

where due to (B4) and (B5) we have

$$B_j=\sum_{l=1}^{\nu_j}|p_l^{(j)}\rangle\langle v_l^{(j)}|,\quad\overline{B}_j=\sum_{l=1}^{\nu_j}|\overline{v}_l^{(j)}\rangle\langle\overline{p}_l^{(j)}|. \tag{B8}$$

From (B7) and the identity $\Gamma\Gamma^{-1}=\Gamma^{-1}\Gamma=I$ it follows that

$$\Gamma(k_j)|p_l^{(j)}\rangle=0,\quad\langle\overline{p}_l^{(j)}|\Gamma^{-1}(\overline{k_j})=0,\quad l=1,\ldots,\nu_j,\quad j=1,\ldots,s. \tag{B9}$$

These are the equations defining the unknown vectors $|\overline{v}_l^{(j)}\rangle$ and $\langle v_l^{(j)}|$. Indeed, rewriting (B9) we have

$$|p_l^{(j)}\rangle=\sum_{i=1}^{s}\frac{1}{k_j-\overline{k}_i}\sum_{m=1}^{\nu_i}|\overline{v}_m^{(i)}\rangle\langle\overline{p}_m^{(i)}|p_l^{(j)}\rangle,\quad\langle\overline{p}_l^{(j)}|=-\sum_{i=1}^{s}\frac{1}{\overline{k}_j-k_i}\sum_{m=1}^{\nu_i}\langle\overline{p}_l^{(j)}|p_m^{(i)}\rangle\langle v_m^{(i)}|.$$

Inversion of these formulas gives

$$|\overline{v}_l^{(j)}\rangle=\sum_{i=1}^{s}\sum_{m=1}^{\nu_i}|p_m^{(i)}\rangle(D^{-1})_{im,jl},\quad\langle v_l^{(j)}|=\sum_{i=1}^{s}\sum_{m=1}^{\nu_i}(D^{-1})_{jl,im}\langle\overline{p}_m^{(i)}|. \tag{B10}$$

Here the matrix D is defined by

$$D_{im,jl}=\frac{\langle\overline{p}_m^{(i)}|p_l{}^{(j)}\rangle}{k_j-\overline{k}_i}.$$

Substitution of (B10) into (B7) produces the needed formula (29).

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Euclidean Friedman–Robertson–Walker cosmology in Brans–Dicke-like theories of gravity

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An explicit and tractable form of the complete solution of Brans–Dicke Euclidean Friedman–Robertson–Walker cosmology, in the matter dominated area, is proposed. In this derivation, the (generally imposed) constraint on the Brans–Dicke parameter $\omega > -3/2$ is relaxed. An isolated power-law solution is exhibited, which turns out to describe an accelerated expansion of the universe, without recourse to any cosmological constant or quintessence matter. It appears that this solution can be generalized for all Brans–Dicke-like theories of gravity. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1447589]

I. INTRODUCTION

In the standard cosmological model, the universe is modeled as being isotropic and homogeneous. The metric of such a space–time can always be written in the Friedman–Robertson–Walker form

$$ds^2 = -dt^2 + a(t)^2\left[\frac{dr^2}{1-kr^2} + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)\right], \tag{1}$$

where $a(t)$ (>0) is the universe scale factor. k $(=+1,0,-1$ for a closed, a flat and an open universe, respectively) describes the geometrical properties of spatial sections. The scale factor is determined inserting the metric (1) in the field equation of the considered theory, in which the matter content is described by a perfect fluid stress tensor, $T_{\alpha\beta} = (\rho + p)u_\alpha u_\beta + p g_{\alpha\beta}$, where the density and pressure fields are related by the state equation $p(\rho)$. For cosmological applications, two extreme cases are generally considered: the so-called matter dominated area, described by $p = 0$, and the so-called radiative area, described by $p = \rho/3$. The cosmological model derived from the general relativity theory (GRT) can be completely integrated, in the matter area, whatever the geometry, leading to the well-known Friedman models.

As soon as Brans and Dicke obtained the equations of their scalar-tensor theory of gravity (BDT, for Brans–Dicke theory), they have reconsidered the standard cosmological model.[1] They have considered the matter dominated area only. The geometrical properties of the space–time are described by the metric (1) and by a time-dependent scalar field $\Phi(t)$. The BDT equations, when written for the metric (1) and the scalar field $\Phi(t)$, are

$$\left(\frac{\dot a}{a} + \frac{\dot\Phi}{2\Phi}\right)^2 + \frac{k}{a^2} = \frac{2\omega+3}{12}\left(\frac{\dot\Phi}{\Phi}\right)^2 + \frac{4K}{3\Phi a^3}, \tag{2}$$

$$\frac{d}{dt}(\dot\Phi a^3) = \frac{4K}{2\omega+3}. \tag{3}$$

The upper point represents the time derivative. K is a (positive) constant, corresponding to $2\pi\rho a^3$ in Brans–Dicke (and standard) notations, where ρ is the mass density (ρa^3 being conserved in the

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pressureless case). In the Euclidean case, they have derived an exact solution, where the scale factor and scalar field are power laws of time.[1] The time exponent of the scale factor converges to the GRT value (2/3), when $\omega\to\infty$, while the scalar field, and then the related "effective gravitational constant" (Ref. 1), reduces to a true constant.

Recently, Park and Sin[2] have investigated the Euclidean problem, with a barotropic equation of state $p=(\gamma-1)\rho$, where γ is a constant. They find the solution under a parametric integral form, from which they derive the main properties (singularities, asymptotic forms,...) of the solutions. More recently, Quiros, Bonal, and Cardenas[3] have reinvestigated this problem. As in Park and Sin, the solution is found under a (non easily tractable) parametric integral form. However, these authors point out some divergences between their results and those of Park and Sin, for $-3/2<\omega<-4/3$. Holden and Wands[4] have derived, from a phase-plane analysis, the qualitative properties of the solutions for the elliptic and hyperbolic problems. All these papers are restricted (in the four-dimensional case we are interested in) to the case $\omega>-3/2$.

In this paper, we concentrate on the sole matter dominated case ($p=0$), described by Eqs. (2) and (3). We obtain the complete solution, $a(t)$ and $\Phi(t)$, without the constraint $\omega>-3/2$ (but with the restriction $\omega\neq 3/2$, the scalar Brans–Dicke equation being not defined for $\omega=-3/2$). A power law solution, different from the one considered by Brans and Dicke, is exhibited, in the case $\omega<-3/2$, which describes an accelerated expanding universe. This solution turns out to have its counterpart in the framework of all Brans–Dicke-like theories of gravity.

II. THE GENERAL SOLUTION OF THE EUCLIDEAN CASE IN BRANS–DICKE THEORY

Let us consider the Euclidean case ($k=0$). Equation (2) reduces to

$$\left(\frac{\dot a}{a}+\frac{\dot\Phi}{2\Phi}\right)^2=\frac{3+2\omega}{12}\left(\frac{\dot\Phi}{\Phi}\right)^2+\frac{4K}{3\Phi a^3}, \tag{4}$$

while Eq. (3) can be integrated as

$$\dot\Phi a^3=\frac{4K}{3+2\omega}t. \tag{5}$$

Let us remark that, setting the integration constant to zero in Eq. (5), a choice of the origin of time has been made implicitly. As a consequence, looking for solutions under the form $a\propto t^q$ (and $\Phi\propto t^r$), as made by Brans and Dicke for their exact solution, has the consequence of selecting only solutions with singularity at the so defined origin of time.

Multiplying Eq. (4) by $9\Phi^2a^6$, and using Eq. (5), it turns out that

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\Phi a^3+\frac{Kt^2}{3+2\omega}\right)\right]^2=12K\left(\Phi a^3+\frac{Kt^2}{3+2\omega}\right). \tag{6}$$

Using the new variable $Z=\Phi a^3+Kt^2/(3+2\omega)$, this equation is rewritten as

$$\left[\frac{\mathrm{d}Z}{\mathrm{d}t}\right]^2=12KZ. \tag{7}$$

This equation shows that one has necessarily $Z\geqslant 0$. Let us rewrite this equation under the form

$$\frac{\mathrm{d}Z}{\mathrm{d}t}=\epsilon.2\sqrt{3K}\sqrt{Z}, \tag{8}$$

where $\epsilon=\pm 1$. Since the choice $\epsilon=-1$ corresponds to a mere reversal of time, let us consider the case $\epsilon=+1$ only.

Equation (8) admits the trivial solution $Z=0$, which leads to an isolated family of solutions

$$\Phi = Pt^{-4}, \tag{9}$$

$$a = At^2, \tag{10}$$

where A and P are two constants related by $A^3P = -K/(3+2\omega)$.

If now $Z>0$, Eq. (8) integrates into

$$\Phi a^3 + \frac{Kt^2}{3+2\omega} = \left(\sqrt{3K}t + A\sqrt{\frac{K}{|3+2\omega|}} \right)^2, \tag{11}$$

where A is an integration constant. Combining this equation with Eq. (5), one obtains

$$\frac{\dot{\Phi}}{\Phi} = \frac{4t}{(3+2\omega)\left(\sqrt{3}t + \dfrac{A}{\sqrt{|3+2\omega|}} \right)^2 - t^2}. \tag{12}$$

Now, two cases have to be distinguished, according to the sign of $3+2\omega$.

If $3+2\omega>0$, Eq. (12) leads to

$$\Phi = P|t-t_1|^{-2/(\sqrt{3(3+2\omega)}+1)}|t-t_2|^{2/(\sqrt{3(3+2\omega)}-1)} \tag{13}$$

and Eq. (5) gives

$$a^3 = s\frac{2K}{P}\frac{4+3\omega}{3+2\omega}|t-t_1|^{(\sqrt{3(3+2\omega)}+3)/(\sqrt{3(3+2\omega)}+1)}|t-t_2|^{(\sqrt{3(3+2\omega)}-3)/(\sqrt{3(3+2\omega)}-1)}, \tag{14}$$

where s is the sign of $(t-t_1)(t-t_2)$. t_1 and t_2 are given by

$$t_1 = \frac{-A}{\sqrt{3(3+2\omega)}+1} \tag{15}$$

and

$$t_2 = \frac{-A}{\sqrt{3(3+2\omega)}-1}. \tag{16}$$

This solution corresponds to the case $\gamma=1$ (the pressureless case) given, for instance, in Ref. 4.

Let us remark that this solution is well-defined for all positive value of $3+2\omega$, apart from $\omega=-4/3$, for which t_2 is not defined. This case can be obtained directly from the integration of Eq. (12). This leads to

$$\Phi = P\left|1+\frac{2t}{A}\right|^{-1}\exp\left(\frac{2t}{A}\right) \tag{17}$$

and Eq. (5) gives

$$a^3 = s\frac{3KA^2}{P}\left(1+\frac{2t}{A}\right)^2\exp\left(-\frac{2t}{A}\right), \tag{18}$$

where s is the sign of $1+2t/A$.

If $3+2\omega<0$, Eq. (12) leads to, up to a mere change of time origin,

$$\Phi = P\left\{1+\left(\frac{t}{\tau}\right)^2\right\}^{-1/|4+3\omega|} \exp\left\{2\,\frac{\sqrt{3|3+2\omega|}}{|4+3\omega|}\arctan\left(\frac{t}{\tau}\right)\right\} \tag{19}$$

while a^3, derived from Eq. (5), writes

$$a^3 = \frac{2K}{P}\,\frac{|4+3\omega|}{|3+2\omega|}\,\tau^2\left\{1+\left(\frac{t}{\tau}\right)^2\right\}^{3|1+\omega|/|4+3\omega|} \times \exp\left\{-2\,\frac{\sqrt{3|3+2\omega|}}{|4+3\omega|}\arctan\left(\frac{t}{\tau}\right)\right\}. \tag{20}$$

In these expressions, one has written

$$\tau = \frac{A}{2|4+3\omega|}. \tag{21}$$

Remark that solutions (13), (14); (17), (18); and (19), (20), when time reflected, correspond to the same solutions (respectively), with the integration constant A changed for $-A$, in such a way that both cases $\epsilon = \pm 1$ are described by the solutions (13), (14); (17), (18) and (19), (20).

III. DETAILED PROPERTIES OF THE SOLUTION AND DISCUSSION

Since Φ determines the effective gravitational constant (Ref. 1), which is positive, we will consider, in all the present discussion, only solutions such that $P>0$. The peculiar properties of these solutions are highlighted in this section.

Consider first the case $\omega > -3/2$. If the integration constant A is chosen to be zero, the Brans–Dicke power law solution is recovered.

If $A \neq 0$, two peculiar dates t_1 and t_2 $(\neq 0)$ enter the solution. As pointed out in Sec. II, changing the sign of A is the same as considering the time-reflected solution. Let us then consider the case $A>0$ only. Since $q_1 = (\sqrt{1+2\omega/3}+1)/(3\sqrt{1+2\omega/3}+1) > 0$, t_1 is a date of singularity, while t_2 is a date of singularity if and only if $q_2 = (\sqrt{1+2\omega/3}-1)/(3\sqrt{1+2\omega/3}-1) > 0$, i.e., if and only if $\omega \notin [-4/3, 0]$. The condition $a>0$ shows that $s=+1$ (respectively -1) in the case $\omega > -4/3$ (respectively $< -4/3$).

If $\omega > -4/3$, one then has $t_2 < t_1 < 0$, and the time t is necessarily outside the time interval $[t_2, t_1]$. The solution exhibits two disconnected branches. Let us point out that, in both branches, a varies as $|t|^{q_1+q_2}$ at $\pm\infty$, where $q_1+q_2 = 2(1+\omega)/(4+3\omega)$. Studying the variations of (14), one finds the following.

(1) If $\omega > 0$, a decreases in the first branch from $+\infty$ at $t=-\infty$ to zero at $t=t_2$, and increases in the second branch from zero at $t=t_1$ to $+\infty$ at $t=+\infty$. $\ddot{a}$, the second time derivative of the scale factor, remains negative in both branches.

(2) If $\omega = 0$, one has $q_2 = 0$. The solution takes the form $a \propto |t-t_1|^{1/2}$. Let us point out that it is defined outside the interval $[t_2, t_1]$ $(=[-A/2, -A/4])$ only. a decreases in the first branch from $+\infty$ at $t=-\infty$ to a finite nonzero value at $t=t_2$, and increases in the second branch from zero at $t=t_1$ to $+\infty$ at $t=+\infty$. $\ddot{a}$ remains negative in both branches.

(3) If $-1 < \omega < 0$, a decrease in the first branch from $+\infty$ at $t=-\infty$, reaches a strictly positive minimum value at a date $t_{\min}$, and increases to $+\infty$ at $t=t_2$. In the second branch, a increases from zero at $t=t_1$ to $+\infty$ at $t=+\infty$. In the first branch, $\ddot{a} < 0$ until a date t_{infl} $(< t_{\min})$, and is positive between t_{infl} and t_2. $\ddot{a}$ remains negative in the second branch.

(4) If $\omega = -1$, one has $q_1+q_2 = 0$. The solution takes the form $a \propto |(t-t_1)/(t-t_2)|^{1/\sqrt{3}}$. It reaches asymptotically a constant value when $t \to \pm\infty$.

(5) If $-4/3 < \omega < -1$, a increases in the first branch from 0 at $t=-\infty$ to $+\infty$ at $t=t_2$. In the second branch, a increases from zero at $t=t_1$ to a maximum value at a date $t_{\max}$, and decreases to zero at $t=+\infty$. $\ddot{a}$ is positive in all the first branch, is negative in the second branch between t_1 and a date t_{infl} $(> t_{\max})$, and is positive between t_{infl} and $+\infty$.

If $\omega = -4/3$, the solution is given by (17) and (18). This solution exhibits a singularity at the time $t_1 = -A/2$. Since $a>0$, one has $s=+1$, and then $t/A > -1/2$. The case $A>0$, being under consideration, one finds the following.

(6) If $\omega=-4/3$, the solution has one branch. a increases from zero at $t_1=-A/2$ to $+\infty$ at $t=+\infty$. $\ddot{a}<0$ from t_1 to a date t_{infl}, and is positive after.

If $\omega<-4/3$, $t_1<0<t_2$, and the condition $a>0$ leads to $s=-1$. The time t is then inside the time interval $[t_1,t_2]$, and one has the following.

(7) If $-3/2<\omega<-4/3$, a increases from zero at $t=t_1$, reaches a maximum value at a date $t_{\max}$, and decreases to zero at $t=t_2$. It is remarkable that the singularity at $t=t_1$ is such that $\dot{a}=\infty$, while the singularity at $t=t_2$ is such that $\dot{a}=0$. $\ddot{a}<0$ from t_1 to a date t_{infl} ($>t_{\max}$), and is positive after.

Consider now the case $\omega<-3/2$. In this case, the solution $a(t)$ is defined for all real value of the time, and turns out to be singularity-free. It reaches a minimum value at a time $t_{\min}$. Here again, if the integration constant A is chosen to be (asymptotically) zero, the Brans–Dicke power law solution is recovered. If, besides, $\omega=-2$, one finds $a\sim t$ and $\Phi\sim 1/t$, the linear solution (in t for the scale factor) to which reduces the linear solution exhibited by Banerjee and Pavon, in the Euclidean case.[5]

Here again, since changing the sign of A is the same as considering the time-reflected solution, we consider the case $A>0$. From Eq. (20), one finds the following two cases.

(8) If $-2\leqslant\omega<-3/2$, a decreases from $+\infty$ at $t=-\infty$, reaches a minimum value at $t_{\min}$, and increases to $+\infty$ at $t=+\infty$. $\ddot{a}$ remains positive for all time.

(9) If $\omega<-2$, a decreases from $+\infty$ at $t=-\infty$, reaches a minimum value at $t_{\min}$, and increases to $+\infty$ at $t=+\infty$. $\ddot{a}$ is positive in an interval $[t_{\text{infl1}},t_{\text{infl2}}]$ containing $t_{\min}$, and is negative outside.

The time-reflected cases $(1')-\ldots.(9')$ of the nine previous cases (in the same order) correspond to the same cases, but with negative values of A.

One has to add the isolated solution (9) and (10) to these cases. For this solution, the relation $PA^3=-K/(3+2\omega)$ shows that $\omega<-3/2$ (from $a>0$, A is necessarily >0 for this solution). One then adds the tenth case.

(10) If $\omega<-3/2$, $a\propto t^2$, and $\ddot{a}$ is positive for all time.

Let us insist on the, at first sight, very strange comportment of the solution (2) near the date t_2: the first branch of the solution ends suddenly at t_2, encountering neither a singularity nor a divergence. This can be checked directly inserting the solution (13) and (14), with $\omega=0$, in the field equations (4) and (5). A careful inspection of the transition from the solution (1) to the solution (3) shows, indeed, that it is a reasonable comportment, since the first branches of (1) and (3) become closer and closer to the curve $a\propto|t-t_1|^{1/2}$, but remain outside $[t_2,t_1]$, when $\omega\to 0^+$ or 0^-. The second branch of the time reversed $(2')$ of (2) begins then suddenly at the date $-t_2$ ($>-t_1$), which is neither the date of a singularity nor of an infinite value for the scale factor $a(t)$.

It could seem disturbing that the solution (6) possesses one branch only. In fact, this is the logical continuity of the case (5), since $\lim_{\omega\to-4/3^+}(t_2)=-\infty$.

Let us remark that the solution (7) does not fill the conclusion derived by Quiros, Bonal and Cardenas for the same values of ω. In this case, these authors have concluded that the problem [as well in the pressureless case as in the barotropic perfect fluid case $p=(\gamma-1)\rho$] is singularity-free in the Jordan frame (the frame considered in the current paper), which, from the present approach made directly in this frame, seems not to be correct, at least in the pressureless case.

It is worth pointing out that the solutions (3), $(3')$, (5), $(5')$, (6), $(7')$, (8), $(8')$, (9), $(9')$, and (10) exhibit phases of accelerated expansion without any recourse to quintessence matter (or to cosmological constant). This possibility, which has already been pointed out[5] for some peculiar power law exact solutions, is enforced here, since it appears to be the case for a wide class of solutions.

Besides, let us mention that, when $\omega\gg 1$, both the exponents q_1 and q_2 are close to 1/3, with the consequence that near the singularity (i.e., at dates such that $|t-t_k|\ll t_1-t_2$), one has $a\propto|t-t_k|^{1/3}$ ($\gg|t-t_k|^{2/3}$). The scale factor varies then as the power 1/3 of time, a comportment drastically different from that of the Friedman solution of GRT (power 2/3 of time). Since $\lim_{\omega\to\infty}(t_1-t_2)=0$, this comportment disappears as soon as the limit is reached.

It can easily be checked that both solutions (13) and (14) and (19) and (20) develop in power series of $1/\omega$, and then converge through the analog GRT solution, i.e., $\Phi = P$ (i.e., a constant) and $a \propto t^{2/3}$, when $|\omega| \to \infty$. However, let us point out the pathological comportment of the isolated solution (9), (10) in this limit process. Indeed, the limit of this solution is highly unphysical (whilst the solution itself, i.e., for a finite ω, is physical), since $\lim_{|\omega|\to\infty}(PA^3) = 0$, which means that either $a \to 0$ (no universe) and/or $\Phi \to 0$ (infinitely strong effective gravitational constant).

IV. A SOLUTION FOR ALL BRANS–DICKE-LIKE THEORIES OF GRAVITY

Let us now consider the previous problem in the framework of general scalar-tensor theories (STT) of gravity, where the Brans–Dicke parameter ω is replaced by an arbitrary function $\omega(\Phi)$ (each such function defining a peculiar STT). For a general presentation of these theories, see for instance Ref. 6. Modulo this change, Eq. (4) remains unchanged, while Eq. (3) is replaced by

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\sqrt{|2\omega(\Phi)+3|}\frac{\mathrm{d}\Phi}{\mathrm{d}t}a^3 \right) = \sigma \frac{4K}{\sqrt{|2\omega(\Phi)+3|}}, \tag{22}$$

where σ is the sign of $2\omega(\Phi)+3$. Let us define a new time variable τ by

$$\mathrm{d}t = \mathrm{d}\tau \sqrt{|2\omega(\Phi)+3|} \tag{23}$$

and let us write X^* for $\mathrm{d}X/\mathrm{d}\tau$. Equation (22) can be integrated, and gives

$$a^3\Phi^* = \sigma 4K\tau, \tag{24}$$

while Eq. (4) can be rewritten as

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}(\Phi a^3 + \sigma K\tau^2) \right]^2 = 12K(\Phi a^3 + \sigma K\tau^2), \tag{25}$$

which generalizes Eq. (6). As in the Brans–Dicke case, this equation admits a trivial solution, which verifies $\Phi a^3 + \sigma K\tau^2 = 0$. Since the case $\Phi > 0$ only is considered, one has necessarily $\sigma = -1$, and then $3 + 2\omega(\Phi) < 0$. This leads to the solution under the parametric form

$$\Phi = P\tau^{-4}, \tag{26}$$

$$a = A\tau^2, \tag{27}$$

and

$$t = \int \mathrm{d}\tau \sqrt{-3 - 2\omega\left(\frac{P}{\tau^4}\right)}, \tag{28}$$

where A and P are related by $A^3P = K$. This solution extends the isolated solution (9) and (10) of the Brans–Dicke problem to the general case of STT.

As in the Brans–Dicke case, this solution leads to an accelerated expansion for a large class of STT. For instance, considering gravity theories characterized by $3 + 2\omega(\Phi) \sim \Phi^\lambda$, where λ is a constant, an accelerated expansion is recovered for $-1/2 < \lambda < +1/2$, which includes, of course, the Brans–Dicke case $\lambda = 0$.

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Remarks on the distributional Schwarzschild geometry

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This work is devoted to a mathematical analysis of the distributional Schwarzschild geometry. The Schwarzschild solution is extended to include the singularity; the energy momentum tensor becomes a δ-distribution supported at $r=0$. Using generalized distributional geometry in the sense of Colombeau's (special) construction the nonlinearities are treated in a mathematically rigorous way. Moreover, generalized function techniques are used as a tool to give a unified discussion of various approaches taken in the literature so far; in particular we comment on geometrical issues. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1448684]

I. INTRODUCTION

Since the formulation of the first singularity theorems it is generally conceded that singular space–times are of fundamental importance in general relativity. Geometrically, a singularity is defined via the notion of (geodesic) incompleteness, a viewpoint which fits in the singularity theorems of Hawking and Penrose (see, e.g., Ref. 1, Chap. 8), forcing us to regard a singularity as some kind of singular boundary point of space–time. Recently, as an alternative, it has been suggested to describe (mild) singularities as internal points, where the field equations are satisfied in a weak (probably distributional) sense (cf. Ref. 2). General relativity as a physical theory is governed by particular physical equations; the focus of interest is the breakdown of physics which need not coincide with the breakdown of geometry.

In the context of conical space–times algebras of generalized functions[3,4] have been used to overcome the problem of simultaneously dealing with singular (i.e., distributional) metrics and the nonlinearities of general relativity.[5–7] These techniques allow one to assign to the cone metric a singular energy momentum tensor supported on a submanifold of codimension two, which, by a result of Geroch and Traschen,[8] is not possible within classical (i.e., linear) distribution theory.

The main focus of this work is a (nonlinear) distributional description of the Schwarzschild space–time. Although the nature of the Schwarzschild singularity is much ''worse'' than the quasiregular conical singularity, there are several distributional treatments in the literature (cf. Ref. 9–13), mainly motivated by the following considerations: the physical interpretation of the Schwarzschild metric is clear as long as we consider it merely as an exterior (vacuum) solution of an extended (sufficiently large) massive spherically symmetric body. Together with the interior solution it describes the entire space–time. The concept of point particles—well understood in the context of linear field theories—suggests a mathematical idealization of the underlying physics: one would like to view the Schwarzschild solution as defined on the entire space–time and regard it as generated by a point mass located at the origin and acting as the gravitational source. This of course amounts to the question of whether one can reasonably ascribe distributional curvature quantities to the Schwarzschild singularity at the origin.

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The emphasis of the present work lies on mathematical rigor. We derive the ''physically expected'' result for the distributional energy momentum tensor of the Schwarzschild geometry, i.e., $T_0^0 = 8\pi m \delta^{(3)}(\vec{x})$, in a conceptually satisfactory way. Additionally, we set up a unified language to comment on the respective merits of some of the approaches taken so far. In particular, we discuss questions of differentiable structure as well as smoothness and degeneracy problems of the regularized metrics, and present possible refinements and workarounds. These aims are accomplished using the framework of nonlinear generalized functions (Colombeau algebras)[3,4] and, in particular, the geometric approach taken in Refs. 14 and 15.

The paper is organized in the following way: in Sec. II we discuss the conceptual as well as the mathematical prerequisites. In particular we comment on geometrical matters (differentiable structure, coordinate invariance) and recall the basic facts of nonlinear distributional geometry in the context of algebras of generalized functions. Moreover, we derive sensible regularizations of the singular functions to be used throughout the paper. Section III is devoted to a first approach to the problem; a detailed discussion follows in Sec. IV: we comment on problems and obstacles associated with the direct approach. Finally, in Sec. V, we present a new conceptually satisfactory method to derive the main result. Overly technical calculations are shifted to various appendices. In Sec. VI we investigate the horizon and describe its distributional curvature. Using nonlinear distributional geometry and generalized functions it seems possible to show that the horizon singularity is only a coordinate singularity *without leaving Schwarzschild coordinates*.

II. PREREQUISITES

To begin with, let us have a look at the conceptually much simpler problem of point charges in Maxwell's theory and consider the Coulomb solution $1/r$ of an extended spherically symmetric body. In an idealized picture the charged body is reduced to a point charge, and this way of looking at the problem has proven to be very fruitful, mainly due to the following two reasons: first, the function $1/r \in \mathcal{C}^2(\mathbb{R}^3\backslash\{0\})$, since also in $L^1_{\mathrm{loc}}(\mathbb{R}^3)$, naturally gives rise to a distribution on $\mathbb{R}^3$. Reinserting this distributional potential into the field equation we obtain $\Delta(1/r) = -4\pi\delta$, which has the clear physical interpretation as the charge density of a point charge. Second, also in accordance with physical intuition, the situation may be interpreted in terms of the following sensible regularization scenario: consider a regularization of the ''singular'' potential by any sequence of (say smooth) functions converging weakly to $1/r$. Then, by virtue of linearity of the field equation, distribution theory guarantees that the corresponding sequence of charge densities will converge weakly to $-4\pi\delta$, i.e., the density of the point charge.

The general relativistic case is much more involved. Consider the Schwarzschild metric inside the horizon: extending the space–time to $r=0$ we are confronted with several distinct problems. First—according to the standard picture of general relativity—no manifold structure is given at the singularity $r=0$, since the field equations are meaningless there within the smooth category. In addition, the differentiable structure of the extended manifold cannot be uniquely determined from the differentiable structure of the original space–time. This problem is dealt with in the relevant literature by fixing some differentiable structure by hand, most often the one induced by Cartesians associated with Schwarzschild coordinates.

In analogy to the Maxwell case, we want to regard the metric as a distribution on the whole extended space–time. Now, the second conceptual problem is due to the inherently nonlinear nature of general relativity: no distributional meaning can be given to the field equations, since it is not possible to calculate the curvature from a distributional metric. In the literature, this obstacle is circumvented by using various—more or less—*ad hoc* regularization approaches in order to calculate a regularized Ricci tensor within the smooth category. Eventually, its distributional limit is computed and—via the field equations—a distributional energy momentum tensor is obtained. This tensor may then be interpreted as distributional source of the Schwarzschild geometry.[9–13] However, using ad-hoc regularizations we are confronted with the problem of regularization independence of the results which may not be suitably addressed within this setting.

In this work, while arguing from a related point of view, we are going to use a different

apparatus to deal with the nonlinearities of general relativity: the theory of algebras of generalized functions gives us the additional flexibility and power of a rigorous mathematical framework in which distributions may undergo nonlinear operations. In particular, following the procedure of Ref. 5, we will first model the distributionally extended Schwarzschild metric by a generalized metric obtained by a suitable (and general) regularization procedure. Then, after entering the generalized framework (cf. Ref. 15) we may calculate all the relevant curvature quantities from the generalized metric and subject it to the field equations. Note that within the generalized setting the field equations possess a well-defined meaning. Finally, we may descend to the distributional level for the purpose of interpretation using the concept of association (see the following).

Note that, in general, a regularization procedure depends on the coordinate system it is performed in (for a diffeomorphism invariant notion of regularization using paths of mollifiers see Refs. 16 and 17). However, since we had to fix the differentiable structure beforehand this is no further restriction. Actually, geometric considerations play an important role: as shown in the following, a brute force regularization attempt does not lead to a sensible description of the problem at hand. Indeed, we shall see that a satisfactory treatment of the distributional Schwarzschild space–time has to use the Kerr–Schild form of the Schwarzschild metric (which fixes both the differentiable structure and the coordinates); moreover, it must be retained during the whole regularization process. Note that this is in accordance with physical intuition since in the Kerr–Schild form the radial coordinate retains its spatial character near the singularity which of course is not the case in Schwarzschild coordinates.

In Secs. II A and II B we are going to introduce some mathematical prerequisites. First, we are going to briefly recall generalized tensor analysis and generalized curvature (in Colombeau's so-called special setting). For all further details we refer the reader to Refs. 14 and 15. Second, we explicitly calculate the regularization of the relevant components of the metric tensor to be used throughout the paper.

A. Nonlinear distributional geometry

The basic idea of Colombeau's theory of generalized functions[3,4] is regularization by sequences (nets) of smooth functions and the use of asymptotic estimates in terms of a regularization parameter ϵ. Let $(u_\varepsilon)_{\varepsilon\in(0,1]}$ with $u_\varepsilon\in\mathcal{C}^\infty(M)$ for all ε (M a separable, smooth orientable Hausdorff manifold of dimension n). The algebra of generalized functions on M is defined as the quotient $\mathcal{G}(M):=\mathcal{E}_M(M)/\mathcal{N}(M)$ of the space $\mathcal{E}_M(M)$ of sequences of moderate growth modulo the space $\mathcal{N}(M)$ of negligible sequences. More precisely the notions of moderateness, respectively, negligibility are defined by the following asymptotic estimates [$\mathfrak{X}(M)$ denoting the space of smooth vector fields on M]:

$$\mathcal{E}_M(M):=\{(u_\varepsilon)_\varepsilon:\forall K\subset\subset M,\ \forall k\in\mathbb{N}_0\exists N\in\mathbb{N}\forall \xi_1,\dots,\xi_k\in\mathfrak{X}(M):\sup_{p\in K}|L_{\xi_1}\cdots\ L_{\xi_k}u_\varepsilon(p)|$$
$$=O(\varepsilon^{-N})\},$$
$$\mathcal{N}(M):=\{(u_\varepsilon)_\varepsilon:\forall K\subset\subset M,\ \forall k,q\in\mathbb{N}_0\forall \xi_1,\dots,\xi_k\in\mathfrak{X}(M):\sup_{p\in K}|L_{\xi_1}\cdots\ L_{\xi_k}u_\varepsilon(p)|=O(\varepsilon^q))\}.$$

Elements of $\mathcal{G}(M)$ are denoted by $u=\mathrm{cl}[(u_\varepsilon)_\varepsilon]=(u_\varepsilon)_\varepsilon+\mathcal{N}(M)$. With componentwise operations $\mathcal{G}(M)$ is a fine sheaf of differential algebras with respect to the Lie derivative defined by $L_\xi u:=\mathrm{cl}[(L_\xi u_\varepsilon)_\varepsilon]$. The spaces of moderate, respectively, negligible sequences and hence the algebra itself may be characterized locally, i.e., $u\in\mathcal{G}(M)$ iff $u\circ\psi_\alpha\in\mathcal{G}(\psi_\alpha(V_\alpha))$ for all charts (V_α,ψ_α), where on the open set $\psi_\alpha(V_\alpha)\subset\mathbb{R}^n$ in the respective estimates Lie derivatives are replaced by partial derivatives. Smooth functions are embedded into $\mathcal{G}$ simply by the "constant" embedding σ, i.e., $\sigma(f):=\mathrm{cl}[(f)_\varepsilon]$, hence $\mathcal{C}^\infty(M)$ is a faithful subalgebra of $\mathcal{G}(M)$. On open sets of $\mathbb{R}^n$ compactly supported distributions are embedded into $\mathcal{G}$ via convolution with a mollifier $\rho\in\mathcal{S}(\mathbb{R}^n)$ with unit integral satisfying $\int\rho(x)x^\alpha dx=0$ for all $|\alpha|\geqslant 1$; more precisely setting $\rho_\varepsilon(x)=(1/\varepsilon^n)\rho(x/\varepsilon)$ we have $\iota(w):=\mathrm{cl}[(w*\rho_\varepsilon)_\varepsilon]$. In case $\mathrm{supp}(w)$ is not compact one uses a

sheaf-theoretical construction. However, in the special case of the functions to be treated in the context of the Schwarzschild metric this will not be necessary (see the following). From the explicit formula it is clear that (on open subsets of Euclidean space) embedding commutes with partial differentiation. On a general manifold, however, there is no canonical embedding of $\mathcal{D}'$ available; a suitable replacement (cf. Ref. 14) is provided by physically motivated modeling and the use of the notion of association (see the following). Inserting $p \in M$ into $u \in \mathcal{G}(M)$ yields a well-defined element of the ring of constants (also called generalized numbers) $\mathcal{K}$ (corresponding to $\mathbb{K}=\mathbb{R}$, respectively, $\mathbb{C}$), defined as the set of moderate nets of numbers $((r_\varepsilon)_\varepsilon \in \mathbb{K}^{(0,1]}$ with $|r_\varepsilon| = O(\varepsilon^{-N})$ for some N) modulo negligible nets ($|r_\varepsilon| = O(\varepsilon^m)$ for each m). Finally, generalized functions on M are characterized by their generalized point values, i.e., by their values on points in $\tilde{M}_c$, the space of equivalence classes of compactly supported nets $(p_\varepsilon)_\varepsilon \in M^{(0,1]}$ with respect to the relation $p_\varepsilon \sim p'_\varepsilon :\Leftrightarrow d_h(p_\varepsilon, p'_\varepsilon) = O(\varepsilon^m)$ for all m, where d_h denotes the distance on M induced by any Riemannian metric.

The $\mathcal{G}(M)$-module of generalized sections in vector bundles—especially the space of generalized tensor fields $\mathcal{G}^r_s(M)$—is defined along the same lines using analogous asymptotic estimates with respect to the norm induced by any Riemannian metric on the respective fibers. However, it is more convenient to use the following algebraic description of generalized tensor fields:

$$\mathcal{G}^r_s(M) \cong \mathcal{G}(M) \otimes \mathcal{T}^r_s(M), \tag{1}$$

where $\mathcal{T}^r_s(M)$ denotes the space of smooth tensor fields and the tensor product is taken over the module $\mathcal{C}^\infty(M)$. Hence generalized tensor fields are just given by classical ones with generalized coefficient functions. Many concepts of classical tensor analysis carry over to the generalized setting,[14] in particular Lie derivatives with respect to both classical and generalized vector fields, Lie brackets, exterior algebra, etc. Moreover, generalized tensor fields may also be viewed as $\mathcal{G}(M)$-multilinear maps taking generalized vector and covector fields to generalized functions, i.e., as $\mathcal{G}(M)$-modules we have

$$\mathcal{G}^r_s(M) \cong L_{\mathcal{G}(M)}(\mathcal{G}^0_1(M)^r, \mathcal{G}^1_0(M)^s; \mathcal{G}(M)).$$

In particular a generalized metric is defined to be a symmetric, generalized (0,2)-tensor field $g_{ab} = \mathrm{cl}[(g_{ab\,\varepsilon})_\varepsilon]$ (with its index independent of ε and) whose determinant $\det(g_{ab})$ is invertible in $\mathcal{G}(M)$. The latter condition is equivalent to the following notion called strictly nonzero on compact sets: for any representative $\det(g_{ab\,\varepsilon})_\varepsilon$ of $\det(g_{ab})$ we have $\forall K \subset\subset M \exists m \in \mathbb{N}: \inf_{p \in K} |\det(g_{ab\,\varepsilon})| \geqslant \varepsilon^m$ for all ε small enough. This notion captures the intuitive idea of a generalized metric to be a sequence of classical metrics approaching a singular limit in the following sense: g_{ab} is a generalized metric iff (on every relatively compact open subset V of M) there exists a representative $(g_{ab\,\varepsilon})_\varepsilon$ of g_{ab} such that for fixed ε (small enough) $g_{ab\,\varepsilon}$ (respectively, $g_{ab\,\varepsilon}|_V$) is a classical pseudo-Riemannian metric and $\det(g_{ab})$ is invertible in the algebra of generalized functions. A generalized metric induces a $\mathcal{G}(M)$-linear isomorphism from $\mathcal{G}^1_0(M)$ to $\mathcal{G}^0_1(M)$ and the inverse metric $g^{ab} := \mathrm{cl}[(g^{-1}_{ab\,\varepsilon})_\varepsilon]$ is a well-defined element of $\mathcal{G}^2_0(M)$ [i.e., independent of the representative $(g_{ab\,\varepsilon})_\varepsilon$]. Also the generalized Levi-Civita connection as well as the generalized Riemann, Ricci, and Einstein tensor of a generalized metric are defined simply by the usual coordinate formulas on the level of representatives.

Finally, the above-introduced setting displays maximal consistency (in the light of Schwartz's impossibilty result[18]) with respect to smooth, respectively, distributional geometry most conveniently formalized in terms of the notion of association. A generalized function $u \in \mathcal{G}(M)$ is called associated to zero, $u \approx 0$, if one (hence any) representative $(u_\varepsilon)_\varepsilon$ converges to zero weakly. (In a sloppy fashion we shall often write $u_\varepsilon \approx 0$.) The equivalence relation $u \approx v :\Leftrightarrow u - v \approx 0$ gives rise to a linear quotient of $\mathcal{G}$ that extends distributional equality. Moreover we call a distribution $w \in \mathcal{D}'(M)$ the distributional shadow or macroscopic aspect of u and write $u \approx w$ if for all compactly supported n-forms ν and one (hence any) representative $(u_\varepsilon)_\varepsilon$,

$$\lim_{\varepsilon\to 0}\int_M u_\varepsilon \nu = \langle w,\nu\rangle,$$

where $\langle,\rangle$ denotes the distributional action. By (1) the concept of association extends to generalized tensor fields in a natural way.

B. Regularizations of the singular functions occurring in the Schwarzschild metric

The two most important singular functions we will work with throughout this paper (namely the singular components of the Schwarzschild metric) are $1/r$ and $1/(r-c)$ ($r=\|\vec{x}\|$; c a positive constant). Since $1/r\in L^1_{\mathrm{loc}}(\mathbb{R}^3)$, it gives rise to the regular distribution $1/r\in\mathcal{D}'(\mathbb{R}^3)$. By convolution with a mollifier ρ (adapted to the symmetry of the space–time, thus chosen radially symmetric) we embed it into the Colombeau algebra $\mathcal{G}(\mathbb{R}^3)$,

$$\frac{1}{r}\overset{\iota}{\to}\iota\left(\frac{1}{r}\right)=\left(\frac{1}{r}*\rho_\varepsilon\right)=:\left(\frac{1}{r}\right)_\varepsilon. \tag{2}$$

Using radial symmetry of the convoluted function and inserting $\rho_\varepsilon(r)=(1/\varepsilon^3)\,\rho(r/\varepsilon)$ we obtain

$$\left(\frac{1}{r}\right)_\varepsilon=\frac{4\pi}{r}\int_0^{r/\varepsilon}\mathrm{d}t\,t^2\,\rho(t)+\frac{4\pi}{\varepsilon}\int_{r/\varepsilon}^{\infty}\mathrm{d}t\,t\rho(t). \tag{3}$$

It is easy to confirm that $(1/r)_\varepsilon=\sigma(1/r)_\varepsilon=(1/r)$ on $\mathbb{R}^3\backslash\{0\}$, and at the origin we have $(1/r)_\varepsilon|_{r=0}=(4\pi/\varepsilon)\int_0^\infty dt\,t\rho(t)$.

In contrast to $1/r$, the function $1/(r-c)$ is not in $L^1_{\mathrm{loc}}(\mathbb{R}^3)$. A canonical regularization (in the sense of Gelfand–Shilov[19]) is the principal value $vp(1/(r-c))\in\mathcal{D}'(\mathbb{R}^3)$ which can be embedded into $\mathcal{G}(\mathbb{R}^3)$,

$$\frac{1}{r-c}\to vp\left(\frac{1}{r-c}\right)\in\mathcal{D}'(\mathbb{R}^3)\overset{\iota}{\to}\iota\left(vp\left(\frac{1}{r-c}\right)\right)=:\left(vp\left(\frac{1}{r-c}\right)\right)_\varepsilon. \tag{4}$$

Making use of $vp(1/(r-c))=(\partial/\partial r)\log|r-c|$ we obtain

$$\begin{aligned}\iota\left(vp\left(\frac{1}{r-c}\right)\right)(x)=&\left(1+r\frac{\partial}{\partial r}\right)\int \mathrm{d}^3y\,\frac{1}{|x-y|}\log|\,|x-y|-c|\,\rho_\varepsilon(y)\\&-\frac{\partial}{\partial x^i}\int \mathrm{d}^3y\,y^i\frac{1}{|x-y|}\log|\,|x-y|-c|\,\rho_\varepsilon(y)\end{aligned}$$

and finally for $v\geqslant c$,

$$\begin{aligned}\iota\left(vp\left(\frac{1}{r-c}\right)\right)(x)=&\frac{4\pi}{r-c}\int_0^{r-c}\mathrm{d}s\,\rho_\varepsilon(s)s^2+\frac{4\pi}{r}\int_{r-c}^{\infty}\mathrm{d}s\,\rho_\varepsilon(s)s^2\\&+\frac{4\pi}{r-c}\frac{c}{r}\int_0^{r-c}\mathrm{d}s\,\rho_\varepsilon(s)s^2\sum_{l=1}^{\infty}\frac{1}{2l+1}\left(\frac{s}{r-c}\right)^{2l}\\&+\frac{4\pi}{r-c}\frac{c}{r}\int_{r-c}^{\infty}\mathrm{d}s\,\rho_\varepsilon(s)(r-c)^2\sum_{l=0}^{\infty}\frac{1}{2l+1}\left(\frac{r-c}{s}\right)^{2l}.\end{aligned} \tag{5}$$

For $0<r\leqslant c$ the roles of r and c are interchanged and we obtain $vp(1/(r-c))_\varepsilon|_{r=0}=-1/c+O(\varepsilon)$.

III. A FIRST APPROACH TO THE PROBLEM

In this section we present a first approach to the "Schwarzschild point mass problem," thereby essentially following earlier treatments in the literature (Refs. 9, 11–13). However, we are going to use the language of nonlinear distributional geometry introduced previously in order to obtain a unified view, which will enable us to carry out a detailed analysis of the previous approaches in Sec. IV.

In the usual Schwarzschild coordinates $(t,r>0,\theta,\phi)$ the metric takes the form

$$\mathrm{d}s^2=h(r)\mathrm{d}t^2-h(r)^{-1}\mathrm{d}r^2+r^2\,\mathrm{d}\Omega^2 \quad \text{with} \quad h(r)=-1+\frac{2m}{r}. \tag{6}$$

Following the above-presented discussion we consider the singular metric coefficient $h(r)$ as an element of $L^1_{\mathrm{loc}}(\mathbb{R}^3)\subseteq\mathcal{D}'(\mathbb{R}^3)$ and embed it into $\mathcal{G}(\mathbb{R}^3)$ by convolution with a mollifier. Note that, accordingly, we have fixed the differentiable structure of the manifold: the Cartesian coordinates associated with the spherical Schwarzschild coordinates in (6) are extended through the origin. We have

$$h(r)=-1+\frac{2m}{r}\overset{\iota}{\to}\iota(h(r))=h_\varepsilon(r)=-1+2m\left(\frac{1}{r}\right)_\varepsilon\in\mathcal{G}(\mathbb{R}^3), \tag{7}$$

where $(1/r)_\varepsilon$ is given by (3). Inserting (7) into (6) we obtain a generalized object modeling the singular Schwarzschild metric, i.e.,

$$\mathrm{d}s^2_\epsilon=h_\epsilon(r)\mathrm{d}t^2-h_\epsilon(r)^{-1}\mathrm{d}r^2+r^2\,\mathrm{d}\Omega^2. \tag{8}$$

The generalized Ricci tensor may now be calculated componentwise using the classical formulas

$$(R^0_{\ 0})_\varepsilon=(R^1_{\ 1})_\varepsilon=\frac{1}{2}\left(h''_\varepsilon+\frac{2}{r}h'_\varepsilon\right)=\frac{1}{2}\Delta h_\varepsilon, \tag{9}$$

$$(R^2_{\ 2})_\varepsilon=(R^3_{\ 3})_\varepsilon=\frac{h'_\varepsilon}{r}+\frac{1+h_\varepsilon}{r^2}. \tag{10}$$

Due to the linear structure of $R^0_{\ 0}$ it is evident that it is associated to a constant times the δ-distribution, i.e.,

$$(R^0_{\ 0})_\varepsilon=\frac{1}{2}\Delta h_\varepsilon=m\Delta\left(\frac{1}{r}\right)_\varepsilon\to-4\pi m\,\delta\quad(\varepsilon\to0). \tag{11}$$

Investigating the weak limit of the angular components of the Ricci tensor [using the abbreviation $\tilde{\Phi}(r)=\int\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\Phi(\vec{x})$] we get (cf. Appendix A)

$$\begin{aligned}\int(R^2_{\ 2})_\varepsilon\Phi\,\mathrm{d}^3x&=\int(rh'_\varepsilon+1+h_\varepsilon)\tilde{\Phi}(r)\mathrm{d}r\\&\overset{(3)}{=}8\pi m\int\frac{1}{\varepsilon}\left[\int_{r/\varepsilon}^{\infty}t\rho(t)\mathrm{d}t\right]\tilde{\Phi}(r)\mathrm{d}r\\&=8\pi m\int\mathrm{d}x\,\tilde{\Phi}(\varepsilon x)\int_x^\infty t\rho(t)\mathrm{d}t\\&\to32\pi^2m\,\Phi(0)\int_0^\infty\mathrm{d}x\int_x^\infty t\rho(t)\mathrm{d}t\overset{(A3)}{=}8\pi m\langle\delta|\Phi\rangle\quad(\varepsilon\to0).\end{aligned}$$

Hence, the Ricci tensor and the curvature scalar R are of δ-type, i.e.,

$$R^0_0=R^1_1\approx -4\pi m\ \delta, \quad R^2_2=R^3_3\approx 8\pi m\ \delta, \quad R\approx \pi m\ \delta. \tag{12}$$

Equation (12) is obviously given in spherical coordinates. Strictly speaking this is not sensible, because the basis fields $\{\partial/\partial r, \partial/\partial\phi, \partial/\partial\theta\}$ are not globally defined. Representing distributions concentrated at the origin requires a basis regular at the origin. Transforming the results for $(R^i_j)_\varepsilon$ [i.e., (9) and (10)] into Cartesian coordinates associated with the spherical ones (i.e., $\{r,\theta,\phi\}\leftrightarrow\{x^i\}$) we obtain, e.g., for the Einstein tensor

$$G^i{}_j\approx -8\pi m\ \delta\ \delta^i_0\delta^0_j. \tag{13}$$

Note that the use of the particular regularization (7) is not essential here. We could have replaced (7) by any other smooth *ad hoc* regularization of $h(r)$, as has been done, e.g., in Ref. 11, by setting $h_\varepsilon(r)=-1+2m/(\sqrt{r^2+\varepsilon^2})$. Indeed, we can show that the results (12) hold for all regularizations, i.e., for all sequences of the form $h_\varepsilon(r)=-1+2ms_\varepsilon(r)\to h(r)$ (i.e., $\forall\ s_\varepsilon$ smooth, $s_\varepsilon\to 1/r$ in $\mathcal{D}'$). For the (0,0)- and (1,1)-components of the Ricci tensor the result follows from the special form of (9). For the angular components [cf. (10)] we write

$$2m\int_0^\infty r^2\left(\frac{s'_\varepsilon(r)}{r}+\frac{s_\varepsilon(r)}{r^2}\right)\tilde{\Phi}(r)\,\mathrm{d}r=-2m\int_0^\infty \mathrm{d}r\, r^2 s_\varepsilon\frac{1}{r}\tilde{\Phi}'(r)\to 8\pi m\Phi(0), \tag{14}$$

where in the last step we used the fact that $(1/r)\,\tilde{\Phi}'\in\mathcal{D}(\mathbb{R})$.

IV. COMMENTS AND PROBLEMS

In order to be able to calculate the curvature from the metric we must keep the regularization $h_\varepsilon(r)$ smooth on the entire space–time. This fact—although somewhat hidden because we worked with spherical coordinates—is essential from the conceptual point of view. In fact, choosing a regularization $h_\varepsilon(r)$ which is smooth only on $\mathbb{R}^3\backslash\{0\}$ is not sufficient to derive the result as is explicitly shown by the following counterexample. Set $h_\varepsilon=-1+2ms_\varepsilon$ and $s_\varepsilon=(1/r)\,o_\varepsilon$ (with $o_\varepsilon\to 1$ weakly) consisting of regular distributions, so that $s_\varepsilon\in L^1_{\mathrm{loc}}(\mathbb{R}^3)$ with $s_\varepsilon\to 1/r\in\mathcal{D}'(\mathbb{R}^3)$. Moreover, we may require $o_\varepsilon(r)$ to be smooth on $\mathbb{R}^3\backslash\{0\}$. Summing over (9) and (10) we get $R_\varepsilon=2m((1/r)\,o''_\varepsilon+(2/r^2)\,o'_\varepsilon)$. Choosing $o_\varepsilon(r)=(1+c\,[r^\varepsilon-1])$ we obtain for R_ε different weak limits as the constant c varies, i.e.,

$$R_\varepsilon\to 8\pi mc\ \delta. \tag{15}$$

For $o_\varepsilon=r^{-\varepsilon}$ the situation is even worse. Although $o_\varepsilon\in L^1_{\mathrm{loc}}\ \forall\ \varepsilon$ and $o_\varepsilon\to 1\in\mathcal{D}'$ as $\varepsilon\to 0$, R_ε does not converge weakly, so that we obtain no distributional result whatsoever.

Nonetheless, similar nonsmooth regularizations have been considered in the literature. In these cases the desired result (12) can only be produced by means of a clever choice of explicit formulas; in particular, $o_\varepsilon=r^\varepsilon$ in Ref. 13 and $o_\varepsilon(r)=\Theta(r-\varepsilon)$ in Ref. 12. The authors of Ref. 9 have shown that the result (12) may be reproduced as long as $o_\varepsilon|_{r=0}=0$. However, the conceptual problem remains untouched: $R_\varepsilon[h_\varepsilon]$ can only be derived for smooth regularizations h_ε; distributions cannot be used as an input for nonlinear operations.

Prior to a more detailed investigation of the choice of regularization, we briefly comment on two more attempts in the literature. In Ref. 12 a regularization of the metric using thin shell solutions is investigated. The limit ($\varepsilon\to 0$) corresponds to a shrinking of the shell. However, the shells can only be placed outside the horizon (of a black hole with identical mass). This implies that a shrinking of the shell must be coupled to a decrease in mass: m converges to zero in the limiting process, so the obtained results should either be considered trivial ($R\sim m\delta|_{m=0}=0$) or be rejected completely.

In Ref. 11 the authors claim to have found different results for the curvature quantities by regularizing the Schwarzschild metric in a different coordinate system. They study the interrelations of regularizations and coordinate transformations for this particular problem. However, some details are not overly convincing. If we choose a new radial coordinate $\tilde{r}$ such that $r=\Lambda\tilde{r}+a$ with $a=2m$, then $\tilde{r}=0$ does not describe the Schwarzschild singularity. Instead, $\tilde{r}=0$ corresponds to the coordinate singularity at the horizon $r=2m$, but shrunk to one point. Obviously, we should not compare the outcome of these considerations with our former results.

We now begin with an in-depth analysis of certain aspects of the regularization procedure commencing with the issue of componentwise regularization and invertibility of the regularized metric. According to (1) in Sec. II, regularizing a tensor such as the Schwarzschild metric (6) comes up to regularizing each distribution-valued component separately. Following this rule we obtain a regularized metric slightly different from (8), namely

$$\mathrm{d}s^2_\varepsilon = h_\varepsilon(r)\mathrm{d}t^2-(h^{-1})_\varepsilon(r)\mathrm{d}r^2+r^2\,\mathrm{d}\Omega^2. \tag{16}$$

Since $\mathrm{cl}[h_\varepsilon]\mathrm{cl}[(h^{-1})_\varepsilon]\neq 1\in\mathcal{G}$, the determinant of the regularized metric (16) is no longer identically one. (This, in fact, does not come as a surprise; cf. Schwartz's impossibility result.[18]) However, the product *is* preserved in the sense of association, i.e., $h_\varepsilon(h^{-1})_\varepsilon\approx 1$. Analogous issues arise from the inverse metric: embedding also g^{-1} componentwise into $\mathcal{G}$ we obtain regularized objects, g_ε and $(g^{-1})_\varepsilon$, which are only inverse to each other in the sense of association. Taking a different viewpoint, however, it is comparatively easy to avoid these issues: on the classical level the Schwarzschild geometry is uniquely determined by the set of variables $\{g_{tt},g_{rr},g_{\theta\theta},g_{\varphi\varphi}\}$, or, e.g., equivalently by $\{g_{tt},g_{\theta\theta},g_{\varphi\varphi},\det g\}$. Embedding the second set of variables into $\mathcal{G}$ leads directly to the regularization (8) used previously; no invertibility problems arise at all since $\det g_\varepsilon$ is forced to equal one.

Finally we return to discussing the problem of smoothness of the regularized metric from a different, more geometrical point of view. We regard this problem to be so essential that in Sec. V we propose an approach entirely different form the one taken so far.

In fact, the regularizations used so far (as all the other regularizations in the relevant literature) do *not* provide a *smooth* regularized metric tensor. This fact is hidden again by the use of spherical coordinates. In Cartesian coordinates pertaining to (r,θ,ϕ)—which we used to fix the differentiable structure of the extended manifold at $r=0$—however, it can be explicitly seen from the form of the metric

$$\mathrm{d}s^2 = h(r)\mathrm{d}t^2+\mathrm{d}\vec{x}^2-(1+h(r)^{-1})\frac{x_ix_j}{r^2}\mathrm{d}x^i\,\mathrm{d}x^j. \tag{17}$$

In order to obtain a smooth regularization it is not sufficient to merely regularize $h(r)$. In fact, we must embed the singular coefficient $(1+h(r)^{-1})(x_ix_j/r^2)$ as a whole into $\mathcal{G}$. Apart from technical difficulties this approach should provide a smooth regularized metric $\mathrm{d}s_\varepsilon$. However, we have reached an impasse: the regularized metric will not be invertible at some distinct value r_0 of the radial coordinate, where $r_0\to 0(\varepsilon\to 0)$. This will be shown in the remainder of this section.

As shown in Appendix B, the regularization of (17) takes the form

$$\mathrm{d}s^2_\varepsilon = h_\varepsilon(r)\mathrm{d}t^2+(1-a_\varepsilon(r))\mathrm{d}r^2+(1-b_\varepsilon(r))r^2\,\mathrm{d}\Omega^2, \tag{18}$$

with $a_\varepsilon(0)\to\frac{1}{3}(\varepsilon\to 0)$. This implies that the rr-component of the regularized metric (18) is positive at $r=0$ (at least for small ε), because $(g_{rr})_\varepsilon(0)=(1-a_\varepsilon(0))\to\frac{2}{3}$ $(\varepsilon\to 0)$. On the other hand, $(1-a_\varepsilon)$ approximates $-h^{-1}$, i.e., $(g_{rr})_\varepsilon(r\neq 0)\to -r/(2m-r)<0$ $(\varepsilon\to 0)$. So we conclude that at some value r_0 of r the smooth function $(g_{rr})_\varepsilon(r)$ must have a zero at least for small ε. (Interestingly enough, this is not the case for negative masses since $-r/(2m-r)$ is positive then). In other words, this means that the regularization of the metric (17) degenerates at some radius r_0. Evidently, $r_0\to 0$ as $\varepsilon\to 0$.

Note that the occurrence of this radius of degeneracy is neither due to the fact that we choose the particular regularization (18), nor is it possible to avoid it by giving up spherical symmetry. To see this in some more detail consider the spatial part of (17) [set $\tilde{h}(r) := h^{-1}(r)$] and consider a certain class of regularizations

$$ds_\varepsilon^2 = d\vec{x}^2 - (1+\tilde{h}_\varepsilon(r))\frac{x_i x_j}{r^2}dx^i\,dx^j, \tag{19}$$

where $\tilde{h}_\varepsilon(r)$ denotes an arbitrary regularization of $\tilde{h}(r)$. However, for ds_ε^2 to become smooth, we must require that $\tilde{h}_\varepsilon(r)$ be $-1+O(r^2)$ for $(r\to 0)$. Now, an arbitrary regularization of ds^2 not necessarily respecting spherical symmetry is obtained by adding zero-sequences to (19),

$$ds_\varepsilon^2 = d\vec{x}^2 - (1+\tilde{h}_\varepsilon(r))\frac{x_i x_j}{r^2}dx^i dx^j + (a_{ij})_\varepsilon(\vec{x})\,dx^i\,dx^j. \tag{20}$$

For special cases of $(a_{ij})_\varepsilon$ it is easy to show that (20) is degenerate. Choose, e.g., $(a_{ij})_\varepsilon$ such that only $(a_{12})_\varepsilon =: b_\varepsilon(\vec{x})$ is nonvanishing. The determinant of (20) at $\vec{x}=(0,0,r)$ is equal to $-\tilde{h}_\varepsilon(r)\times(1-b_\varepsilon(\vec{x})^2)$. As $-\tilde{h}_\varepsilon(0)=1$ and $-\tilde{h}_\varepsilon(r)<0$ for small ε and finite r, there exists a radius r_ε (with $r_\varepsilon\to 0$ for $\varepsilon\to 0$), such that $\det(g_\varepsilon)=0$. Again, we observe degeneracy.

V. THE KERR–SCHILD APPROACH

To begin with let us summarize what we have done so far: we considered regularizations of the Schwarzschild metric (using the language of algebras of generalized functions) to calculate the (distributional) curvature at the singularity. The regularizations used were essentially based on Cartesian coordinates associated with the spherical Schwarzschild coordinates. However, it turned out that all these regularizations were either nonsmooth or not invertible. *Smoothness and invertibility mutually exclude each other* in this context. Hence, we are going to take another more geometrical viewpoint in this section. The main idea—following Refs. 20 and 10—is to use the Kerr–Schild form of the Schwarzschild metric. Retaining this preferred structure also during the whole regularization process will enable us to derive the physically desired result in a rigorous manner.

A metric belongs to the so-called Kerr-Schild class[21] if it can be written as

$$g_{ij} = \eta_{ij} + f k_i k_j \quad \text{with} \quad k^i k_i = 0. \tag{21}$$

Here, the null vector field $k \in \mathfrak{X}$ is normalized $(k^0=1)$ and f is a smooth function. Exploiting the Kerr–Schild form, some curvature quantities take a particularly simple form, e.g.,

$$R = \partial_a \partial_b (f k^a k^b). \tag{22}$$

The Schwarzschild metric is a member of the Kerr–Schild class. In fact, transformation to Eddington–Finkelstein coordinates $(\bar{t} = t + 2m\log|2m-r|)$ yields

$$ds^2 = -d\bar{t}^2 + dr^2 + r^2\,d\Omega^2 + \frac{2m}{r}(d\bar{t}-dr)^2. \tag{23}$$

Evidently, (23) is of Kerr–Schild form, $g_{ij} = \eta_{ij} + f k_i k_j$, with

$$k = \frac{\partial}{\partial \bar{t}} + \frac{\partial}{\partial r}, \quad f = \frac{2m}{r}. \tag{24}$$

Analogous to Sec. III, we regard f and k as distributions on $\mathbb{R}^4$. By this we again implicitly fix the differentiable structure: the coordinates $(\overline{t},x^i)$ are extended through the origin.

We now proceed by regularizing *both* f and k. Indeed, this is necessary due to the fact that not only the profile function f is singular, but also the null vector field k is nonsmooth. Recall that, on account of the nonlinearities in $R[g]$, (22) can only be derived for smooth functions; it is inaccessible for distributional input. [Note the analogy of this situation with the one encountered in (8).] Hence, f and k are chosen to be the fundamental variables characterizing the metric (compare with the remarks in Sec. IV). Regularizing the function f as in Sec. III gives

$$f(r)=\frac{2m}{r}\overset{\iota}{\to}\iota(f(r))=f_\varepsilon(r)=2m\left(\frac{1}{r}\right)_\varepsilon. \tag{25}$$

The regularization of k_i is carried out in detail in Appendix C, yielding

$$k_i(r)=\frac{x_i}{r}\overset{\iota}{\to}\iota\left(\frac{x_i}{r}\right)=k_{i\varepsilon}=\left(\frac{x_i}{r}\right)_\varepsilon=x_iF_\varepsilon(r)\quad(i=1,\ldots,3), \tag{26}$$

where F_ε is given by (C3). Note that, for the moment, $k_0=1$ is embedded trivially into $\mathcal{G}$. Collecting the results of (25) and (26) we get the regularized metric

$$\mathrm{d}s^2_\varepsilon=(-1+f_\varepsilon)\mathrm{d}t^2-2rf_\varepsilon F_\varepsilon\,\mathrm{d}t\,\mathrm{d}r+(1+\tilde{f}_\varepsilon)\mathrm{d}r^2+r^2\,\mathrm{d}\Omega^2, \tag{27}$$

where, for simplicity, $\overline{t}$ has been replaced by t again, and $\tilde{f}_\varepsilon$ abbreviates $r^2f_\varepsilon F^2_\varepsilon$. Unfortunately, (27) is no longer of Kerr–Schild form. This can be shown indirectly: assuming that (27) is Kerr–Schild, i.e., assuming that $\mathrm{d}s^2_\varepsilon=-\mathrm{d}t'^2+\mathrm{d}r^2+r^2\,\mathrm{d}\Omega^2+f'_\varepsilon(\mathrm{d}t'-\mathrm{d}r)^2$ can be achieved by a transformation $t\to t'(t,r)$, it follows that $f'_\varepsilon=\tilde{f}_\varepsilon/(1-f_\varepsilon+\tilde{f}_\varepsilon)$ and $(dt/dt')^2=1/(1-f_\varepsilon+\tilde{f}_\varepsilon)$. As a consequence, the denominator $1-f_\varepsilon+\tilde{f}_\varepsilon$ must be a strictly positive function. In fact, in the sense of association, it is equal to one. However, at the origin $r=0$, we obtain $1-f_\varepsilon+\tilde{f}_\varepsilon=1-8\pi m\,1/\varepsilon\int_0^\infty t\rho(t)\mathrm{d}t$, which is negative for small ε as long as $\int_0^\infty t\rho(t)\mathrm{d}t>0$, a contradiction.

The fact that the embedding (27) is no longer of Kerr–Schild form bears a strong relation to the fact that smooth regularizations degenerate at a certain value of r (see Sec. IV): the determinant of (27) contains the factor $1-f_\varepsilon+\tilde{f}_\varepsilon$, which was shown to possess a zero.

Additionally, in analogy to the statements made at the end of Sec. IV, we note that the loss of the Kerr–Schild form does not stem from choosing to regularize the singular coefficient functions via convolution. On the contrary, it may be shown that any regularization of the metric displays this behavior as long as only the spatial components of k are taken into account.

We will now take the announced geometrical viewpoint: we consider regularizations retaining the Kerr–Schild decomposition. This requires, in particular, that the regularized vector k_ε is still null. Thus, we consider the regularization

$$k^i_\varepsilon=rF_\varepsilon k^i\quad(i=0,\ldots,3). \tag{28}$$

While the spatial components of (28) coincide with (26), k^0_ε is only associated to $1(k^0_\varepsilon=rF_\varepsilon\approx 1)$. As required, k_ε satisfies the condition $k^i_\varepsilon k_{\varepsilon i}=0$. Note that, in order to obtain (28), the functions f, $k^i(i=1,\ldots,3)$ and $k\cdot k$ are chosen as fundamental variables determining the geometric structure of the spacetime.

Using (25) and (28) the regularized metric takes the form

$$g_{ij\varepsilon}=\eta_{ij}+f_\varepsilon k_{\varepsilon i}k_{\varepsilon j}=\eta_{ij}+(r^2F^2_\varepsilon f_\varepsilon)k_ik_j=\eta_{ij}+\tilde{f}_\varepsilon k_ik_j. \tag{29}$$

Obviously, (29) is of Kerr–Schild form. Finally we have arrived at a regularization of the Schwarzschild metric which is *both smooth and invertible* (the inverse being $\eta^{ij}-\tilde{f}_\varepsilon k^i k^j$). This allows us to fully exploit the Kerr–Schild form, i.e., to use (22), to obtain

$$R_\varepsilon=\partial_a\partial_b(\tilde{f}_\varepsilon k^a k^b)=\frac{4}{r}\tilde{f}'_\varepsilon+\tilde{f}''_\varepsilon+\frac{2}{r^2}\tilde{f}_\varepsilon\,. \tag{30}$$

To complete our program we calculate the weak limit of R_ε. The technically involved calculations are deferred to Appendix D. Finally we derive

$$(R_\varepsilon)_\varepsilon\approx 8\pi m\,\delta. \tag{31}$$

The Ricci tensor can be treated in complete analogy to obtain the Einstein tensor

$$(G^a_{b\varepsilon})_\varepsilon\approx -8\pi m\,\delta\delta^a_0\delta^0_b\,. \tag{32}$$

VI. THE HORIZON

In this section we leave the neighborhood of the singularity at the origin and turn to the singularity at the horizon. The question we are aiming at is the following: using distributional geometry (thus without leaving Schwarzschild coordinates), is it possible to show that the horizon singularity of the Schwarzschild metric is merely a coordinate singularity? In order to investigate this issue we calculate the distributional curvature at the horizon (in Schwarzschild coordinates).

Examining the Schwarzschild metric (6) in a neighborhood of the horizon, we see that, whereas $h(r)$ is smooth, $h^{-1}(r)$ is not even L^1_{loc} (note that the origin is now always excluded from our considerations; the space we are working on is $\mathbb{R}^3\backslash\{0\}$). Thus, regularizing the Schwarzschild metric amounts to embedding h^{-1} into $\mathcal{G}$ [as done in (5)].

$$\mathrm{d}s^2_\varepsilon=h(r)\mathrm{d}t^2-(h^{-1})_\varepsilon(r)\mathrm{d}r^2+r^2\,\mathrm{d}\Omega^2 \tag{33}$$

with

$$h(r)=-1+\frac{2m}{r},\quad (h^{-1})_\varepsilon(r)=-1-2m\left[vp\left(\frac{1}{r-2m}\right)\right]_\varepsilon. \tag{34}$$

Obviously, (33) is degenerate at $r=2m$, because $h(r)$ is zero at the horizon. However, this does not come as a surprise. Both $h(r)$ and $h^{-1}(r)$ are positive outside of the black hole and negative in the interior. As a consequence *any* (smooth) regularization of $h(r)$ (or h^{-1}) must pass through zero somewhere and, additionally, this zero must converge to $r=2m$ as the regularization parameter goes to zero (note the analogy to the situation in Sec. IV).

Due to the degeneracy of (33), the Levi-Cività connection is not available. Consider, therefore, the following connection $\Gamma^l_{kj}\in\mathcal{G}$:

$$\Gamma^l_{kj}=\tfrac{1}{2}[\iota(g^{-1})]^{lm}[\iota(g)_{mk,j}+\iota(g)_{mj,k}-\iota(g)_{kj,m}]. \tag{35}$$

Clearly, Γ coincides with the Levi-Cività connection on $\mathbb{R}^3\backslash\{r=2m,r=0\}$, as $\iota(g)=g$ and $\iota(g^{-1})=g^{-1}$ there.

Unfortunately, Γ does not respect the regularized metric $\iota(g)$ (33), i.e., $\iota(g)_{ij;k}\neq 0$, e.g., $\iota(g)_{00;1}=(1-h(h^{-1})_\varepsilon)h'$. However, compatibility with the metric $\iota(g)$ is *a priori* ruled out by the following statement: there exists no connection whatsoever under which $\iota(g)$ would be a parallel tensor. To show this, just look at (L^i_{jk} denoting a not necessarily torsion-free connection) $\iota(g)_{00;1}=\iota(g)_{00,1}-2L^0_{10}\iota(g)_{00}$. At the horizon $\iota(g)_{00}=0$, so that $\iota(g)_{00;1}|_{r=2m}=h'(2m)=-(1/2)m\neq 0$. In the sense of association, however, the connection (35) is in fact metric compatible: $\iota(g)_{ij;k}\approx 0$.

We now investigate the curvature pertaining to the connection (35), picking out $R_{00\varepsilon}$ as a characteristic example. The result of the calculations displays the following structure:

$$R_{00\varepsilon}(r)=vp'_\varepsilon\left(-\frac{m^2}{r^2}+4\frac{m^3}{r^3}-4\frac{m^4}{r^4}\right)+vp_\varepsilon\left(2\frac{m^3}{r^4}-4\frac{m^4}{r^5}\right)+\left(-\frac{m^2}{r^4}-2\frac{m^3}{r^5}\right) \tag{36}$$

$$=vp'_\varepsilon(r)\sum_{l=2}^{\infty}c_l x^l+vp_\varepsilon(r)\sum_{l=1}^{\infty}d_l x^l-\frac{1}{8m^2}-\frac{1}{16m^2}\sum_{l=1}^{\infty}e_l x^l. \tag{37}$$

Here, the abbreviations $vp_\varepsilon=[vp(1/(r-2m))]_\varepsilon$ and $x=(r-2m)/2m$ are used; c_l, d_l, and e_l are constants. Equation (37) holds for $|x|<1$; the infinite sums converge in this case.

If the horizon is excluded, $R_{00\varepsilon}=0(\mathrm{mod}\,\mathcal{N})$, because (35) coincides with the Schwarzschild Levi-Cività connection there. In the neighborhood of $r=2m$ we aim at comparing $R_{00\varepsilon}(r)$ with a Colombeau object of the type $f((r-2m)/\varepsilon)$ (f a Schwartz function). To this end we choose a fundamental sequence $r_\varepsilon=2m+\varepsilon^q a_0$ converging to $r=2m$ and examine $R_{00\varepsilon}(r_\varepsilon)$ [use (37) together with (5)].

$q>1$: $R_{00\varepsilon}(r_\varepsilon)=\mathrm{const}+o(\varepsilon^{q-1})$.

$q<1$: Using (5) we find that $vp_\varepsilon(r_\varepsilon)=1/(r_\varepsilon-2m)$ and $vp'_\varepsilon(r_\varepsilon)=-1/(r_\varepsilon-2m)^2$ (in the sense of generalized numbers). Inserting these results into Eq. (36), we obtain $R_{00\varepsilon}(r_\varepsilon)=0$.

$q=1$: $R_{00\varepsilon}(r_\varepsilon)=\mathrm{const}+o(1)$.

Thus, $R_{00\varepsilon}(r_\varepsilon)$ has the same asymptotic behavior as a sequence of the type $f((r_\varepsilon-2m)/\varepsilon)$ (as $\varepsilon\to 0$). As a consequence, the weak limit of $R_{00\varepsilon}(r)$ can be calculated easily, simply by evaluating $\int \mathrm{d}r\, r^2\tilde{\Phi}(r)f((r-2m)/\varepsilon)$. Evidently, this expression vanishes as $\epsilon\to 0$. Since analogous results hold for the other components of the Ricci tensor, we are finally able to state

$$R_{ij\varepsilon}\approx 0. \tag{38}$$

In other words: viewed as a distribution, $R_{ij}=0$ on $\mathbb{R}^3\backslash\{0\}$, i.e., including the horizon. If we were courageous enough we could take this as a proof that the metric singularity at the horizon is only a coordinate singularity.

We conclude this section with a remark on the connection (35). Due to the degeneracy of any regularization of the metric [e.g., (33)] no canonical (Levi-Cività) connection could be defined. The choice of connection (35) bears a strong relation to the regularized metric; however, there seems no way of telling if this choice is canonical in some sense and thus preferred to other choices. Despite this open question, at least it is clear that the connection (35) is a regularization of the Schwarzschild *connection*. Indeed, we could change our viewpoint: we consider the Schwarzschild connection (forgetting where it came from, i.e., forgetting about the metric), regularize its distribution-valued components, and calculate the distributional curvature from it. Proceeding in this manner, we obtain the result (38), i.e., the space–time is weakly Ricci-flat (the origin was excluded from our considerations).

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APPENDIX A: MOLLIFIER INTEGRALS

Throughout this paper we work invariably with radially symmetric mollifiers $\rho(r)$ (cf. Sec. II). Most importantly, we have the properties

$$\int_0^\infty \mathrm{d}t\, t^2\rho(t)=\frac{1}{4\pi},\quad \int_0^\infty \mathrm{d}t\, t^{2k}\rho(t)=0\quad (k>1). \tag{A1}$$

We investigate multiple integrals involving the mollifier $\rho(r)$ and powers of r:

$$\int_x^\infty \mathrm{d}t\, t^n\int_t^\infty s\rho(s)\mathrm{d}s=-\frac{x^{n+1}}{n+1}\int_x^\infty t\rho(t)\mathrm{d}t+\frac{1}{n+1}\int_x^\infty \mathrm{d}t\, t^{n+2}\rho(t). \tag{A2}$$

(A2) holds for $(n,k\neq -1)$, it is proven by simply performing integration by parts. One of the most interesting cases resulting from (A2) is $n=0$ and $x\to 0$:

$$\int_0^\infty \mathrm{d}t\int_t^\infty s\rho(s)\mathrm{d}s=\frac{1}{4\pi}. \tag{A3}$$

APPENDIX B: EMBEDDING OF THE CARTESIAN COMPONENTS

Referring to Sec. IV we investigate

$$\iota\left(\frac{1+h(r)^{-1}}{r^2}x_ix_j\right)\mathrm{d}x^i\,\mathrm{d}x^j=\left(2m\int f(\|\vec{z}\|)z_iz_j\rho_\varepsilon(\|\vec{z}+\vec{x}\|)\mathrm{d}^3z\right)\mathrm{d}x^i\,\mathrm{d}x^j, \tag{B1}$$

where $f(q)=1/(2m-q)(1/q^2)$. In order to simplify (B1) we show the following relation:

$$\iota\left(\frac{1+h(r)^{-1}}{r^2}x_ix_j\right)=x_ix_jc_\varepsilon(\vec{x})\quad \text{for } i\neq j\quad (c_\varepsilon \text{ smooth}). \tag{B2}$$

Proof: Since both $f(\|\vec{z}\|)$ and ρ_ε are even functions in z_i, we observe that

$$\iota\left(\frac{1+h(r)^{-1}}{r^2}x_ix_j\right)\Big|_{x_i=0}=2m\int f(\|\vec{z}\|)z_iz_j\rho_\varepsilon(\ldots,z_i,\ldots)\mathrm{d}^3z=0. \tag{B3}$$

We can conclude that

$$\iota\left(\frac{1+h(r)^{-1}}{r^2}x_ix_j\right)=x_ic'_\varepsilon(\vec{x})\quad (c'_\varepsilon \text{ smooth}). \tag{B4}$$

Also,

$$\iota\left(\frac{1+h(r)^{-1}}{r^2}x_ix_j\right)\Big|_{x_j=0}=0,$$

from which follows that $c'_\varepsilon(\vec{x})=x_jc_\varepsilon(\vec{x})$, yielding (B2). Note, however, that the smooth function $c_\varepsilon(\vec{x})$ in (B2) is not equal to $\iota((1+h(r)^{-1})/r^2)$. ■

In the case $i=j$, Eq. (B2) is no longer valid. We are able to calculate the $ii-$component in the limiting case $\varepsilon\to 0$, i.e.,

$$\iota\left(\frac{1+h(r)^{-1}}{r^2}x_i^2\right)\Big|_{\vec{x}=0}=2m\int f(\|\vec{z}\|)z_i^2\rho_\varepsilon(\|\vec{z}\|)\mathrm{d}^3z\to\frac{1}{3}\quad (\varepsilon\to 0). \tag{B5}$$

Proof: Clearly, $2m\int f(\|\vec{z}\|)z_i^2\rho_\varepsilon(\|\vec{z}\|)\mathrm{d}^3z$ is independent of the choice of the index i, so that we may substitute it by $(2m/3)\int f(\|\vec{z}\|)\|\vec{z}\|^2\rho_\varepsilon(\|\vec{z}\|)\mathrm{d}^3z$. Obviously, this converges to $\frac{1}{3}$ as ε goes to zero. ■

The regularized metric (B1) is radially symmetric, $R^*g_\varepsilon=g_\varepsilon$ (R a rotation), as long as radially symmetric mollifiers are used. Thus, it must be of the form of a general radially symmetric metric $\mathrm{d}s^2=a(r)\mathrm{d}r^2+r^2b(r)\ \mathrm{d}\Omega^2$, hence

$$\iota\left(\frac{1+h(r)^{-1}}{r^2}x_ix_j\right)\mathrm{d}x^i\,\mathrm{d}x^j=(a_\varepsilon-b_\varepsilon)(r)\frac{x_i}{r}\frac{x_j}{r}\mathrm{d}x^i\,\mathrm{d}x^j+b_\varepsilon(r)\mathrm{d}\vec{x}^2. \tag{B6}$$

For the general radially symmetric metric (B6) to be smooth $(a_\varepsilon-b_\varepsilon)(r)=O(r^2)$ is required. We observe consistency with (B2) and conclude

$$a_\varepsilon(r)=b_\varepsilon(r)+c_\varepsilon r^2. \tag{B7}$$

At the origin $r=0$ only the second term $b(r)\mathrm{d}\vec{x}^2$ remains relevant, since

$$(a-b)(r)\frac{x_i}{r}\frac{x_j}{r}\bigg|_{r=0}=c_\varepsilon x_ix_j|_{r=0}=0.$$

Turning Eq. (B5) to good account we obtain

$$b_\varepsilon(0)\to\tfrac{1}{3}\quad(\varepsilon\to0),\quad a_\varepsilon(0)\to\tfrac{1}{3}\quad(\varepsilon\to0). \tag{B8}$$

Combining (17) with (B6), we finally obtain

$$\mathrm{d}s_\varepsilon^2=h_\varepsilon(r)\mathrm{d}t^2+(1-a_\varepsilon(r))\mathrm{d}r^2+(1-b_\varepsilon(r))r^2\,\mathrm{d}\Omega^2. \tag{B9}$$

APPENDIX C: EMBEDDING OF k^i

We explicitly embed the radially outward pointing unit vector field $k_i=(x_i/r)$ $(i=1,\ldots,3)$ into the Colombeau algebra, i.e.,

$$\iota\left(\frac{x_i}{r}\right)=\int\mathrm{d}^3x'\frac{x_i-x_i'}{\|\vec{x}-\vec{x}'\|}\rho_\varepsilon(\|\vec{x}'\|)=-\int\mathrm{d}^3z\frac{z_i}{\|\vec{z}\|}\rho_\varepsilon(\|\vec{x}+\vec{z}\|). \tag{C1}$$

Equation (C1) is of an analogous form to (B1). We may conclude that $\iota(x_i/r)$ is a radially symmetric vector field. Moreover, despite $\iota(x_i/r)\neq x_i\iota(1/r)$, we must still have [repeating (B2)ff.]

$$\iota\left(\frac{x_i}{r}\right)=x_iF_\varepsilon(\vec{x})\quad(i=1,\ldots,3). \tag{C2}$$

Here, $F_\varepsilon(\vec{x})$ is a smooth function and moreover, because this function must be radially symmetric, $F_\varepsilon(\vec{x})=F_\varepsilon(r)$.

This fact makes it possible to calculate $\iota(x_i/r)$ explicitly. Take $x=(0,0,r)$ and investigate $\iota(x_3/r)=x_3F_\varepsilon(r)=rF_\varepsilon(r)$:

$$
\begin{aligned}
rF_\varepsilon(r) &= \int \frac{x_3 - x_3'}{\|\vec{x}-\vec{x}'\|}\rho_\varepsilon(r')\,\mathrm{d}^3x' \\
&= 2\pi \int r'^2\,\mathrm{d}r'\,\rho_\varepsilon(r') \int_{-1}^{1} \mathrm{d}(\cos\theta')\,\frac{r - r'\cos\theta'}{\sqrt{r^2+r'^2-2rr'\cos\theta'}} \\
&= r\left(\frac{1}{r}\right)_\varepsilon - 2\pi \int r'^2\,\mathrm{d}r'\,\rho_\varepsilon\left(\frac{1}{r}(|r-r'|+(r+r'))+\frac{1}{3}\frac{1}{r^2}\frac{1}{r'}(|r-r'|^3-(r+r')^3)\right) \\
&= r\left(\frac{4\pi}{r}\int_0^r \mathrm{d}s\, s^2\rho_\varepsilon(s) + \frac{8\pi}{3}\int_r^\infty \mathrm{d}s\, s\rho_\varepsilon(s) - \frac{4\pi}{3}\frac{1}{r^3}\int_0^r \mathrm{d}s\, s^4\rho_\varepsilon(s)\right).
\end{aligned} \tag{C3}
$$

Clearly, $F_\varepsilon(r) = 1/r$ on $\mathbb{R}^3\backslash\{0\}$ and, moreover, $F_\varepsilon(r) \approx 1/r$ on the whole space. We can write the latter also in the form $rF_\varepsilon(r) \approx 1$.

APPENDIX D: WEAK LIMITS FOR THE KERR–SCHILD CASE

We investigate the distributional limit of (30). Inserting for $\tilde{f}_\varepsilon$, (30) becomes

$$
\begin{aligned}
R_\varepsilon = \frac{128\pi^3 m}{3}\Bigg(& 16[1]_\varepsilon^3 + \frac{4}{r^7}[2]_\varepsilon[4]_\varepsilon^2 + \frac{2}{r^6}[1]_\varepsilon[4]_\varepsilon^2 - \frac{4}{r^5}[4]_\varepsilon[2]_\varepsilon^2 + \frac{32}{r}[2]_\varepsilon[1]_\varepsilon^2 + \frac{14}{r^2}[1]_\varepsilon[2]_\varepsilon^2 \\
& - 3\rho_\varepsilon[2]_\varepsilon^2 - 4r\rho_\varepsilon[1]_\varepsilon[2]_\varepsilon - \frac{4r^2}{3}\rho_\varepsilon[1]_\varepsilon^2 - \frac{1}{3r^4}\rho_\varepsilon[4]_\varepsilon^2 + 2\frac{1}{r^2}\rho_\varepsilon[2]_\varepsilon[4]_\varepsilon + \frac{4}{3r}\rho_\varepsilon[1]_\varepsilon[4]_\varepsilon\Bigg),
\end{aligned} \tag{D1}
$$

where $[1]_\varepsilon := \int_r^\infty \mathrm{d}s\, s\rho_\varepsilon(s)$, $[2]_\varepsilon := \int_0^r \mathrm{d}s\, s^2\rho_\varepsilon(s)$, $[4]_\varepsilon := \int_0^r \mathrm{d}s\, s^4\rho_\varepsilon(s)$.

In order to compute the weak limit of (D1), expressions of the form (D2) and (D3) have to be investigated [note that the negative powers of r are compensated by the integrals so that both (D2) and (D3) are well-defined as $r \to 0$],

$$
r^{-4+2j+3i}\,\rho_\varepsilon(r)\,[1]_\varepsilon^i\,[2]_\varepsilon^j\,[4]_\varepsilon^k \quad (i+j+k=2), \tag{D2}
$$

$$
r^{-9+2j+3i}\,[1]_\varepsilon^i\,[2]_\varepsilon^j\,[4]_\varepsilon^k \quad (i+j+k=3). \tag{D3}
$$

Terms of the forms (D2) and (D3) possess related distributional limits:

$$
\begin{aligned}
(r^{-9+2j+3i}[1]_\varepsilon^i[2]_\varepsilon^j[4]_\varepsilon^k)_\varepsilon \approx & + \frac{i}{2j+3i-6}(r^{-7+2j+3i}\rho_\varepsilon(r)[1]_\varepsilon^{i-1}[2]_\varepsilon^j[4]_\varepsilon^k)_\varepsilon \\
& - \frac{j}{2j+3i-6}(r^{-6+2j+3i}\rho_\varepsilon(r)[1]_\varepsilon^i[2]_\varepsilon^{j-1}[4]_\varepsilon^k)_\varepsilon \\
& - \frac{k}{2j+3i-6}(r^{-4+2j+3i}\rho_\varepsilon(r)[1]_\varepsilon^i[2]_\varepsilon^j[4]_\varepsilon^{k-1})_\varepsilon .
\end{aligned}
$$

In order to show this, consider the distributional action on a test function $\Phi(\vec{x})$, i.e., $\int_0^\infty \mathrm{d}r\tilde{\Phi}(r)r^{-7+2j+3i}[1]_\varepsilon^i[2]_\varepsilon^j[4]_\varepsilon^k$. Here, we have introduced $\tilde{\Phi}(r) := \int \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\ \Phi(\vec{x})$. Integrating by parts and using $\tilde{\Phi}'(0) = 0$, the claim is established.

Taking $(j=2; k=1)$ as an example, we obtain the following weak limit:

$$\int \mathrm{d}r\tilde{\Phi}(r)\frac{1}{r^3}[2]_\varepsilon^2[4]_\varepsilon \overset{\varepsilon\to 0}{\to} \tilde{\Phi}(0)\int \mathrm{d}x\,\rho(x)[2][4]+\frac{1}{2}\tilde{\Phi}(0)\int \mathrm{d}x\,x^2\rho(x)[2]^2$$
$$\overset{(A1)}{=} \tilde{\Phi}(0)\int \mathrm{d}x\,\rho(x)[2][4]+\frac{1}{6}\frac{1}{64\pi^3}\tilde{\Phi}(0).$$

Here,

$$[1]:=\int_x^\infty \mathrm{d}t\,t\rho(t),\quad [2]:=\int_0^x \mathrm{d}t\,t^2\rho(t),\quad [4]:=\int_0^x \mathrm{d}t\,t^4\rho(t).$$

Eventually, we obtain the result (31) for the distributional limit of (D1).

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Adding twist to anisotropic fluids

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We present a solution generating technique for anisotropic fluids which preserves specific Killing symmetries. Anisotropic matter distributions that can be used with the one parameter Ehlers–Geroch transform are discussed. Example space–times that support the appropriate anisotropic stress-energy are found and the transformation applied. The $3+1$ black string solution is one of the space–times with the appropriate matter distribution. Use of the transform with a black string seed is discussed. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1448683]

I. INTRODUCTION

Physically relevant solution generating techniques were developed in the 1960s and 1970s. Ehlers,[1] Harrison,[2] and Geroch[3,4] showed that a projective transform on the norm and twist (λ,ω), of a Killing vector will generate a Killing vector with norm and twist (λ',ω'). Starting with a vacuum space–time and a twist-free Killing vector, their method adds twist. For example, their method applied to the vacuum Schwarzschild metric generates a NUT metric. The generating method can be applied to any vacuum space–time with a Killing vector and has been generalized to the Einstein–Maxwell spaces[5] and to some matter space–times.[6] The extension to matter metrics is restrictive; Stephani[7] has shown that the only two equations of state that can be treated within this formalism are

$$\rho = P, \qquad \rho + 3P = 0. \tag{1}$$

Raca and Zsigrai[8] have also considered solution generating on fluids with this equation of state. The result clearly applies to fluids with isotropic stress. A close examination of the method used to generate the allowed matter distributions shows that it can be generalized to fluids with anisotropic stresses.

There has been increasing interest in general relativistic systems with anisotropic stress. Herrera and Santos[9] have reviewed some of the possible causes and the related general relativistic solutions. Anisotropic fluid spheres have been a useful model for discussing anisotropy since the early work of Bowers and Liang[10] on anisotropic fluid spheres. More recently Corchero[11] has discussed a post-Newtonian approximation to anisotropic fluid spheres. Das *et al.*[12] and Das and Kloster[13] have investigated the spherically symmetric collapse of anisotropic fluid objects into a black hole. Hernandez, Lunez, and Percoco[14] have treated anisotropy and nonlocal equations of state in radiating spheres. Conformally flat anisotropic spheres were examined by Herrera *et al.*[15] Glass and Krisch[16] have discussed diffusion induced anisotropies in a Vaidya atmosphere. Following up the recent interest in dimensional effects, Harko and Mak[17] discussed charged anisotropic fluid spheres in D-dimensions. Anisotropy in cosmological solutions has also been studied by McManus and Coley,[18] vandenHoogen and Coley,[19] Giovannini,[20] and Rainsford.[21] Relative motion as a source of anisotropy in multifluid systems was suggested long ago by Jeans.[22]

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Letelier[23] has shown that two perfect fluids in relative motion can be described as a system with anisotropic pressures and has given the standard two-fluid stress energy form.

Physically, anisotropy is finding increasing application in systems at the density extremes of very compact objects and very diffuse mass clusters. This increasing interest in fluid solutions with anisotropic pressures suggests it would be of interest to extend the solution generating technique to space–times that have anisotropic fluid content. While it is relatively simple to create anisotropic fluid solutions by changing the functional dependence of metric potentials, the generating technique here will preserve specific Killing symmetries while obtaining new anisotropic solutions.

In Sec. II, we briefly review the formalism that leads to the isotropic pressure restrictions on the standard solution generating technique. The extension to anisotropic stresses follows directly from this. Isotropic seed space–times are discussed in Sec. III. Some examples of space–times containing the allowed anisotropies are in Sec. IV. Killing symmetries for the possible anisotropic spaces are covered in Sec. V, and Sec. VI has a discussion of the effect of the Geroch transformation on the fluid description in these spaces.

II. FORMALISM

A. The Killing description

Let (M,g_{ab}) be a solution of the Einstein field equations with energy density ρ and isotropic pressure P. Assume that g_{ab} has a Killing vector ξ^a with norm λ and twist ω^a where

$$\begin{aligned} \lambda &:= \xi^a \xi_a , \\ \omega^a &:= \epsilon^{abcd} \xi_b \nabla_c \xi_d . \end{aligned} \tag{2}$$

The induced metric on the three-dimensional space of vectors orthogonal to the Killing vector is

$$h_{ab} = g_{ab} - \xi_a \xi_b / \lambda . \tag{3}$$

The vacuum field equations can be written in terms of λ, ω and γ_{ab},

$$\begin{aligned} \gamma_{ab} &= |\lambda| h_{ab} , \\ \omega_a &= D_a \omega , \end{aligned} \tag{4}$$

where γ_{ab} is conformally related to h_{ab},[3] ω is the scalar potential associated with the Killing twist, and D_a is the covariant derivative for metric γ_{ab}.

B. Vacuum space–times

Consider the action written in the conformal three-space of γ_{ab},

$$I = \int d^3x \sqrt{\gamma} \left[\mathcal{R} - \frac{1}{2\lambda^2} (D_a \lambda D^a \lambda + D_a \omega D^a \omega) \right]. \tag{5}$$

A projective transform of the complex potential $\tau = \omega + i\lambda$ can be written

$$\tau' = \frac{\tau \cos(\delta) + \sin(\delta)}{\cos(\delta) - \tau \sin(\delta)}, \tag{6}$$

where δ is a transformation parameter. The action is invariant under this transformation, so we have added twist to the Killing vector with γ_{ab} unchanged and can generate the new $3+1$ space–time, g'_{ab}, from the formalism. The development of the transformation method is described in Refs. 3 and 4. We briefly review the transformation method for twist-free Killing vectors.

C. Generating the new space–time from a twist-free seed

The generation method as described by Geroch[3,4] for vacuum will be the same in the matter space–times. Starting with metric g_{ab}, define forms α_a, β_a, and η_a based on a seed Killing vector, ξ_a, with norm λ and transformation parameter δ,

$$\beta_a = \xi_a(\lambda - \lambda^{-1}), \tag{7a}$$

$$2\alpha_{[b,a]} = \varepsilon_{abcd}\nabla^c \xi^d, \tag{7b}$$

$$\eta_a = \lambda^{-1}\xi_a + \alpha_a \sin(2\delta). \tag{7c}$$

The new metric is then given by

$$g'_{ab} = F(g_{ab} - \lambda^{-1}\xi_a\xi_b) + (\lambda/F)\,\eta_a\eta_b \tag{8}$$

with

$$F = \cos^2(\delta) + \lambda^2 \sin^2(\delta). \tag{9}$$

The norm of the Killing vector becomes

$$\lambda' = \lambda/F. \tag{10}$$

The scalar twist potential that has been added to the Killing vector is

$$\omega' = \frac{\sin(\delta)\cos(\delta)(1-\lambda^2)}{F}. \tag{11}$$

These are the equations that will generate the new space–time from static seed metrics.

III. ISOTROPIC MATTER DESCRIPTIONS

A. Isotropic model 1

To find the isotropic matter space–times that can be used with this method, consider the action[24]

$$I = \int \mathrm{d}^3x\sqrt{\gamma}\left[\mathcal{R} - \frac{D_a\lambda D^a\lambda}{2\lambda^2} + \Psi\right] \tag{12}$$

with Ψ a specified function. Stephani[7] has shown that the Ricci tensor in four dimensions is

$$R_{ab} = -\Psi|\lambda|(g_{ab} - \xi_a\xi_b/\lambda) \tag{13}$$

and clearly the action will be invariant under the projective transform on τ. In the isotropic case, this Ricci tensor is associated with a perfect fluid for ξ^a timelike. The fluid has an equation of state $\rho + 3P = 0$, with $8\pi\rho = 3\Psi\lambda/2$.

B. Isotropic model 2

A second action that one can consider is[24]

$$I = \int \mathrm{d}^3x\sqrt{\gamma}\left[\mathcal{R} - \frac{D_a\lambda D^a\lambda}{2\lambda^2} - s_a s^a\right] \tag{14}$$

with

$$s_a \xi^a = 0. \tag{15}$$

The four-dimensional Ricci tensor for this action is

$$R_{ab} = s_a s_b \tag{16}$$

which, in the isotropic case, describes a perfect fluid if the Killing vector is spacelike. The fluid has density and pressure

$$\begin{aligned} 8\pi\rho &= -s^a s_a/2, \\ P &= \rho. \end{aligned} \tag{17}$$

Solution generating with both of these isotropic forms has been examined by Garfinkle, Glass, and Krisch.[25]

IV. ANISOTROPIC MATTER DESCRIPTION

The form of the Ricci tensor will be the same for fluids with nonisotropic stress. The stress-energy content can be written as

$$(1/8\pi) T_{ab} = \rho u_a u_b + p_1 e_a^{(1)} e_b^{(1)} + p_2 e_a^{(2)} e_b^{(2)} + p_3 e_a^{(3)} e_b^{(3)}, \tag{18}$$

where $(u^a, e_a^{(i)}, i = 1,2,3)$ is a convenient orthogonal tetrad. The associated Ricci tensor is

$$R_{ab} = T_{ab} - (T/2) g_{ab}, \tag{19}$$

$$(1/8\pi) R_{ab} = \rho u_a u_b + p_1 e_a^{(1)} e_b^{(1)} + p_2 e_a^{(2)} e_b^{(2)} + p_3 e_a^{(3)} e_b^{(3)} + \left(\frac{\rho - p_\Sigma}{2} \right) g_{ab}, \tag{20}$$

where $p_\Sigma = p_1 + p_2 + p_3$.

A. Anisotropic model 1

Consider Ricci tensor $R_{ab} = -\Psi |\lambda| (g_{ab} - \xi_a \xi_b / \lambda)$. There are two Killing vector possibilities: $\xi_a = \lambda u_a$ and $\xi_a = \lambda e_a^{(1)}$, where we have chosen $e_a^{(1)}$ for convenience. The timelike Killing vector will generate isotropic stress. Consider the spacelike vector $\xi_a = \lambda e_a^{(1)}$. We have

$$-(1/8\pi)\Psi|\lambda|(g_{ab} - e_a^{(1)} e_b^{(1)}) = \rho u_a u_b + p_1 e_a^{(1)} e_b^{(1)} + p_2 e_a^{(2)} e_b^{(2)} + p_3 e_a^{(3)} e_b^{(3)} + \left(\frac{\rho - p_\Sigma}{2} \right) g_{ab}. \tag{21}$$

Multiplying by $e_a^{(1)}$ we have

$$p_1 + \rho = p_2 + p_3. \tag{22}$$

Contracting with u_a we find

$$(1/8\pi) 2\Psi |\lambda| = \rho + p_\Sigma. \tag{23}$$

The other spatial contractions give

$$\begin{aligned} -(1/8\pi) 2\Psi |\lambda| &= p_2 - p_1 - p_3 + \rho, \\ -(1/8\pi) 2\Psi |\lambda| &= p_3 - p_1 - p_2 + \rho. \end{aligned} \tag{24}$$

Comparing, we must have $p_2 = p_3$, and

$$-(1/8\pi)2\Psi|\lambda| = -p_1 + \rho. \tag{25}$$

Combining, we find an anisotropic fluid with density and stress

$$\begin{aligned} 8\pi\rho &= -\Psi\lambda/2, \\ 8\pi p_1 &= 3\Psi\lambda/2, \\ p_2 &= p_3 = -\rho. \end{aligned} \tag{26}$$

B. Anisotropic model 2

Consider Ricci tensor $R_{ab} = s_a s_b$. This Ricci tensor model requires that the vector s^a be orthogonal to the Killing vector. Again there are two choices for the Killing vector, and in this model it is the timelike Killing vector that generates the anisotropic stress energy. Consider $\xi_a = \lambda u_a$. Since s_a is orthogonal to the Killing vector, s_a is spacelike. Choose function Φ and $s_a = \Phi e_a^{(1)}$,

$$\frac{s_a s_b}{8\pi} = \frac{\Phi^2 e_a^{(1)} e_b^{(1)}}{8\pi} = \rho u_a u_b + p_1 e_a^{(1)} e_b^{(1)} + p_2 e_a^{(2)} e_b^{(2)} + p_3 e_a^{(3)} e_b^{(3)} + \left(\frac{\rho - p_\Sigma}{2}\right) g_{ab}. \tag{27}$$

Following the same method used in the previous section, we obtain

$$\begin{aligned} 8\pi\rho &= 8\pi p_1 = \Phi^2/2, \\ 8\pi p_2 &= 8\pi p_3 = -\Phi^2/2. \end{aligned} \tag{28}$$

The indices can be relabeled to describe s_a lying along $e_a^{(2)}$ or $e_a^{(3)}$.

V. SPACE–TIMES FOR THE ANISOTROPIC MATTER DISTRIBUTIONS

In Sec. IV we examined two anisotropic models. One has a timelike Killing vector and one a spacelike Killing vector. We now find examples of space–times that could contain the anisotropic matter distribution.

A. Timelike Killing vector

For density and pressures $\rho = p_1 = -p_2 = -p_3$ consider the metric with function $\chi(z)$:

$$ds^2 = -e^{2n\chi}\,dt^2 + dz^2 + e^{2\chi}(dr^2 + r^2\,d\varphi^2). \tag{29}$$

The field equations are

$$\begin{aligned} 8\pi\rho &= -2\chi_{,zz} - 3\chi_{,z}^2, \\ 8\pi p_z &= \chi_{,z}^2(2n+1), \\ 8\pi p_k &= (n+1)\chi_{,zz} + \chi_{,z}^2(n^2+n+1) \end{aligned} \tag{30}$$

with p_k labeling both p_r and p_φ. Enforcing the stress relations, one finds the solution

$$e^{(n+2)\chi} = az + b$$

with fluid $\rho = p_z = -p_k$

$$8\pi\rho = \frac{(2n+1)a^2}{(n+2)^2(az+b)^2} \tag{31}$$

and metric

$$ds^2 = -(az+b)^{2n/(n+2)}dt^2 + dz^2 + (az+b)^{2/(n+2)}(dr^2 + r^2\, d\varphi^2). \tag{32}$$

For $n=1$, this space–time is conformally flat.

B. Spacelike Killing vector

A simple space–time whose fluid content has the necessary anisotropic structure is the conformally flat space–time with metric

$$ds^2 = e^{2az}(-dt^2 + dr^2 + r^2\, d\varphi^2 + dz^2). \tag{33}$$

The fluid parameters are easily shown to be

$$\begin{aligned} 8\pi\rho &= -a^2 e^{-2az}, \\ 8\pi p_z &= 3a^2 e^{-2az}, \\ 8\pi p_k &= a^2 e^{-2az}, \end{aligned} \tag{34}$$

where p_k are the radial and φ-stresses. The negative density does not readily lend itself to a physical description. An interesting space–time that also has the appropriate anisotropic stress relations is the simple lift of the $2+1$ BTZ black hole space–time[26] describing an infinite black string:[27,28]

$$ds^2 = -(-m+\Lambda_3 r^2)dt^2 + \frac{dr^2}{-m+\Lambda_3 r^2} + r^2\, d\varphi^2 + dz^2. \tag{35}$$

In $2+1$ there is a stress energy

$$T_{ii} = \Lambda_3 g_{ii}$$

with Λ_3 the $2+1$ cosmological constant. When the z coordinate is added the fluid content is

$$\begin{aligned} 8\pi\rho &= -\Lambda_3, \\ 8\pi p_r &= 8\pi p_\varphi = \Lambda_3, \\ 8\pi p_z &= 3\Lambda_3, \end{aligned} \tag{36}$$

which has the required anisotropic stress-energy structure. The relation between the $2+1$ BTZ solution and the $3+1$ black string has been studied by Lemos and Zanchin.[29] The negative density in this case can be physically motivated from the cosmological constant. It will be of interest to apply the Geroch transform to this $3+1$ BTZ lift and then project back down to $2+1$ to examine the effects on the cosmological fluid.

VI. APPLYING THE GEROCH TRANSFORMATION

In this section we will use the Geroch formalism described by Eqs. (7)–(10) to add twist to the Killing vectors of our example space–times. The new space–time will be generated and the effect of the transformation on the fluid parameters examined.

A. Timelike Killing vector

The space–time with a timelike Killing vector that we found had metric

$$ds^2 = -(az+b)^{2n/(n+2)}dt^2 + dz^2 + (az+b)^{2/(n+2)}(dr^2 + r^2\, d\varphi^2).$$

The Geroch transform process can be applied to this space–time adding twist to the timelike Killing vector and vorticity to the fluid. From Eqs. (7) to (9) we have

$$\xi_a^{(t)}\xi^a_{(t)}=\lambda=-(az+b)^{2n/(n+2)}, \tag{37}$$

$$F=\cos^2(\delta)+\lambda^2\sin^2(\delta), \tag{38}$$

$$\alpha_{\varphi,r}-\alpha_{r,\varphi}=-\frac{2nar}{n+2}\eta_{tr\varphi z}, \tag{39}$$

$$\alpha_\varphi=-\frac{nar^2}{n+2}+\alpha_0, \tag{40}$$

where $\eta_{tr\varphi z}=1$. The new metric is

$$ds^2=-\frac{(az+b)^{2n/(n+2)}}{F}[dt+\sin(2\delta)\alpha_\varphi\, d\varphi]^2+F\,dz^2+F(az+b)^{2/(n+2)}(dr^2+r^2\,d\varphi^2). \tag{41}$$

The fluid parameters in this space–times are the original parameters scaled by F:

$$\begin{aligned}\rho'&=\rho/F,\\ p_i'&=p_i/F.\end{aligned} \tag{42}$$

The fluid has acquired vorticity along the z axis

$$\omega^{(z)}=\frac{2na\sin(2\delta)}{(n+2)F^2}(az+b)^{(n-2)/(n+2)}. \tag{43}$$

The projective transform on the Killing parameters that generates the new space–time has two fixed points. For the case where the initial space is twist free, the fixed points of the projective transform are $\lambda=\pm1$. For this example, $F=1$ at the fixed points, and the fluid parameters are the same in both the seed and transformed space–times.

B. Spacelike Killing vector

In this example, we wish to add twist to a spacelike Killing vector. We will consider the lift of the BTZ metric as the seed spacetime. The seed metric is

$$ds^2=-(-m+\Lambda_3 r^2)dt^2+\frac{dr^2}{-m+\Lambda_3 r^2}+r^2\,d\varphi^2+dz^2. \tag{44}$$

There are two Killing vector choices: $\xi_a^{(\varphi)}$ or $\xi_a^{(z)}$. We will work with the φ-Killing vector and assume that the metric remains independent of the z-coordinate. From Eq. (7) we have

$$\xi_a^{(\varphi)}\xi^a_{(\varphi)}=\lambda=r^2, \tag{45}$$

$$\alpha_{t,z}-\alpha_{z,t}=2\,\eta_{tzr\varphi}(-m+\Lambda_3 r^2). \tag{46}$$

Calculating α_a and η_a we have

$$\alpha_z=2(m-\Lambda_3 r^2)t+\alpha_0, \tag{47}$$

$$\eta_a=\xi_a^{(\varphi)}/\lambda+\sin(2\delta)\alpha_a, \tag{48}$$

with $F=\cos^2(\delta)+r^4\sin^2(\delta)$. The new $3+1$ metric is

$$ds^2=F\left[-(-m+\Lambda_3 r^2)dt^2+\frac{dr^2}{-m+\Lambda_3 r^2}+dz^2\right]+\frac{r^2}{F}[d\varphi+\alpha_z\sin(2\delta)dz]^2. \tag{49}$$

This black string solution is an anisotropic member of the cylindrical black hole solution family discussed by Lemos.[30]

Using $\delta=\pi/2$, it is easy to see the effect of the transform on the fluid parameters. For this value, the new $3+1$ space–time becomes

$$ds^2=r^4\left[-(-m+\Lambda_3 r^2)dt^2+\frac{dr^2}{-m+\Lambda_3 r^2}+dz^2\right]+\frac{1}{r^2}d\varphi^2 \tag{50}$$

with a fluid content

$$\begin{aligned} 8\pi\rho&=-\Lambda_3/r^4,\\ 8\pi p_r&=\Lambda_3/r^4,\\ 8\pi p_\varphi&=9\Lambda_3/r^4,\\ 8\pi p_z&=3\Lambda_3/r^4. \end{aligned} \tag{51}$$

The new general space–time can be projected back into $2+1$ with the result

$$\begin{aligned} h_{ab}&=g_{ab}-\xi_a^{(z)}\xi_b^{(z)}/\lambda_z,\\ h_{ab}dx^a\,dx^b&=F\left[-(-m+\Lambda_3 r^2)dt^2+\frac{dr^2}{-m+\Lambda_3 r^2}\right]+\frac{r^2}{F}d\varphi^2, \end{aligned} \tag{52}$$

which can be written as

$$\begin{aligned} h_{ab}dx^a\,dx^b=&-(-m+\Lambda_3 r^2)dt^2+\frac{dr^2}{-m+\Lambda_3 r^2}+r^2d\varphi^2+(r^4-1)\\ &\times\sin^2(\delta)\left[-(-m+\Lambda_3 r^2)dt^2+\frac{dr^2}{-m+\Lambda_3 r^2}+\frac{r^2}{1+(r^4-1)\sin^2(\delta)}d\varphi^2\right]. \end{aligned} \tag{53}$$

For $\delta=0$ the original $2+1$ BTZ space–time is recovered. It is also recovered at the $r^2=1$ fixed point. The fluid content of the $2+1$ space–time is

$$\begin{aligned} 8\pi\rho&=\frac{-\Lambda_3}{F}+\frac{2r^2\sin^2(\delta)}{F^3}\{mF+(-m+\Lambda_3 r^2)[7\cos^2(\delta)-r^4\sin^2(\delta)]\},\\ 8\pi p_r&=\frac{\Lambda_3}{F}-\frac{2r^2\sin^2(\delta)}{F^3}\{mF+2r^4\sin^2(\delta)(-m+\Lambda_3 r^2)\},\\ 8\pi p_\varphi&=\frac{\Lambda_3}{F}+\frac{2r^2\sin^2(\delta)}{F^3}\{2mF+(-m+\Lambda_3 r^2)[5\cos^2(\delta)+r^4\sin^2(\delta)]\}. \end{aligned} \tag{54}$$

The original BTZ solution described a black hole of mass m surrounded by a cosmological fluid with parameters $8\pi\rho=-\Lambda_3$, $8\pi p_r=8\pi p_\varphi=\Lambda_3$. From Eq. (54) it is clear that the cosmological fluid is still present but scaled by F, and that in addition a new fluid has been added. For $\delta=\pi/2$, for example, the fluid parameters are

$$8\pi\rho=(4m-3r^2\Lambda_3)/r^6,$$
$$8\pi p_r=(2m-3r^2\Lambda_3)/r^6, \tag{55}$$
$$8\pi p_\varphi=(2m+3r^2\Lambda_3)/r^6.$$

At infinity, the new solution describes an empty vacuum in contrast to the cosmological vacuum found in the BTZ asymptotic limit. The original BTZ solution had constant negative curvature making it locally isometric to AdS while the new space–time has a nonconstant Ricci scalar

$$R=-\frac{6\Lambda_3}{F}+(-m+\Lambda_3 r^2)\frac{8r^2\sin^2(\delta)\cos^2(\delta)}{F^3}. \tag{56}$$

VII. DISCUSSION

We have shown that the simple one parameter Ehlers–Geroch transform can be applied to space–times with anisotropic matter content for two different stress-energy situations. The formalism broadens the way in which anisotropy can be introduced and studied with relation to the Killing symmetry of the space–time. The formalism was applied to the simple lift of the BTZ solution and when the new $3+1$ solution was projected back to $2+1$, a different static $2+1$ solution was obtained. It describes a $2+1$ black hole with a horizon at the same position as the original BTZ horizon but with an additional fluid atmosphere. The asymptotic structure of the two solutions is very different. This result suggests that it would be useful to develop the formalism in dimensions higher than $3+1$, and use the projection technique to generate and study the resulting anisotropic $3+1$ solutions. Another generalization which could prove interesting is to broaden the fixed point structure of the projective transform. The fixed points described by Eq. (6) are $\lambda=\pm1$, as discussed previously. When using the Ehlers–Geroch method with a spacelike Killing vector, generalizing the projective transform by placing the fixed points at $\lambda=L^2$ offers a better chance of interpreting the fixed points and would broaden the applicability of the method.

In summary, the solution generating method developed here preserves specific Killing symmetries while creating new anisotropic solutions. These solutions may be useful for investigating relativistic behavior at the density extremes.

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The methods of gluing manifolds in general relativity

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Some areas of modern theoretical physics such as modern cosmology contain different manifolds which must be glued together along a common boundary. These boundaries can be spacelike, timelike, or lightlike hypersurfaces. This paper shows how this gluing for different hypersurfaces is possible. Two different approaches are considered and the extent to which these approaches are equivalent are discussed. In particular, we will construct a distributional approach for dynamics of lightlike hypersurfaces in general relativity. Since Einstein's equations are nonlinear PDEs, for discontinuous metrics such as signature changing metrics, product of distributions are unavoidable. To glue two different manifolds which admit signature change, we consider this problem in the context of Colombeau's new theory of generalized functions. Some examples are given for clarification. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1452758]

I. INTRODUCTION

In the inflationary scenario of cosmology, when two phases coexist, the wall separating them can be treated as an infinitely thin bubble or shell, whose history is a timelike surface layer.[1] Analogously, in sudden global phase transition, the transition region can sometimes be considered as an infinitely thin spacelike surface layer.[2,3] Lightlike thin shells arise, for example, when sufficiently large bubbles in a sea of false vacuum are rapidly accelerated toward the speed of light by the imbalance of normal pressures. So the dynamics of bubbles and surface layers in general relativity has been studied extensively in the last two decades.[4–7] There are two different approaches to study these hypersurfaces: the Darmois–Israel (DI)[8–10] and Mansouri–Khorrami (MKh) distributional approach.[11,12]

In the DI approach, the formalism now commonly in use expresses the surface properties in terms of the jump of the extrinsic curvature across the shell wall. In this approach, the properties are obtained directly as functions of the shell's intrinsic coordinates. The intrinsic geometry of the layer must be continuous at the hypersurface, i.e., the intrinsic metric of the hypersurface must be the same determined from either side, and the discontinuity across the hypersurface of its extrinsic curvature (second fundamental form) is related via the Einstein field equations to the stress-energy associated with the surface layer.

This approach must be modified for the case of null hypersurfaces. The extrinsic curvature tensor of a spacelike or timelike hypersurface measures the change in the normal vector to the hypersurface as that vector is transported along the hypersurface. But the normal vector to a null hypersurface is also tangential to it, and the definition of Gaussian normal coordinates cannot be based on a null hypersurface. Since the normal to the null hypersurface declines into tangency with hypersurface, the normal prescription breaks down, because the normal extrinsic curvature is disabled as a carrier of transverse geometrical information. The degeneration of the induced metric

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to the hypersurface is the other complication and definition of the normal distance to the null shell is not simple as the case of timelike or spacelike shells.

On the other hand, the distributional approach of MKh considers the whole space–time, including the singular hypersurface, with a unified metric without bothering about the junction conditions along the hypersurface. These conditions are shown to be automatically fulfilled as part of the field equations. In this approach one chooses special coordinates which are continuous along the singular hypersurface to avoid nonlinear operations of distributions.

The aim of this paper is to compare different approaches to gluing space–time manifolds. To do this we first give an overview of the DI approach for both nonlightlike and lightlike hypersurfaces. Since Mansouri and Khorrami in Ref. 12 constructed their distributional approach for the case of nonlightlike hypersurfaces, here we will show that this approach is applicable for the case of null hypersurfaces also and there is no need for considerable change in their formalism. For examining this claim, we consider the well-known example of spherical lightlike shells in this framework and compare the results with the DI approach. It is shown that two formalism gives the same results and so our distributional approach for the case of a null shell is correct. Since equations of general relativity are nonlinear PDEs, for steplike metrics such as signature changing metrics, nonlinear operations on distributions are unavoidable. Here, using Colombeau algebra, which allows for nonlinear operations of distributions,[13–16] we generalize the MKh method to the special case of signature changing cosmological models. In each case, for clarification, some examples are given.

Notations and Conventions: We use the signature $(-\ +\ +\ +)$, and follow the curvature conventions of Misner, Thorne, and Wheeler.[17] However, our sign convention for extrinsic curvature is that of Israel.[8] The Greek indices run from 0 to 3 and Latin indices i, j, and k from 1 to 3. A semicolon indicates covariant derivatives with respect to either the four-metric of the whole space–time or the three-metric of the layer. $\nabla^{\pm}$ denotes the covariant derivative with respect to either of the metrics of partial manifolds $M^{\pm}$ which are to be glued together. The square brackets, $[F]$, are used to indicate the jump of any quantity F at the layer, and the terms proportional to the δ-function in equations are denoted by $\breve{F}$.

The organization of the paper is as follows: Section II first considers spacelike and timelike hypersurfaces in the DI approach. As we have stated, lightlike hypersurfaces must be studied more carefully and therefore Sec. II B is devoted to this subject. Section III considers dynamics of hypersurfaces in the MKh distributional approach in a unified formalism. Section IV gives an example which shows both the possibility of application of the MKh approach to the case of lightlike hypersurfaces and comparison of its results with respect to the DI method. Section V considers discontinuous metrics, which leads to nonlinear operations on distributions. To perform such operations, we use Colombeau theory of new generalized functions. As an example, we consider signature changing manifolds with steplike metrics and, as a special case, junction conditions for de Sitter space–time in this framework are derived.

II. DARMOIS–ISRAEL FORMALISM

A. Spacelike and timelike hypersurfaces

Assume two space–time manifolds M^+ and M^- with spacelike or timelike boundaries Σ^+ and Σ^-. We want to glue these two space–time manifolds together. Coordinates on the two space–time manifolds are defined independently as x_+^μ and x_-^μ, and the metrics denoted by $g^+_{\alpha\beta}(x_+^\mu)$ and $g^-_{\alpha\beta}(x_-^\mu)$. The induced metrics on the boundaries are called $g^+_{ij}(\xi_+^k)$ and $g^-_{ij}(\xi_-^k)$, where $\xi_\pm^k$ are intrinsic coordinates on $\Sigma^\pm$, respectively. Now to paste the manifolds together, we demand that the boundaries be isometric having the same coordinates, $\xi_-^k=\xi_+^k=\xi^k$. The identification $\Sigma_-=\Sigma_+=:\Sigma$ gives us the single glued manifold $M=M_+\cup M_-$. This condition, which is the minimum requirement for gluing two manifolds together formulated as

$$[g_{ij}]=0, \tag{1}$$

gives, together with the continuity of second fundamental form on Σ,

$$[K_{ij}]=0, \tag{2}$$

the Darmois conditions. Both conditions should be satisfied if Σ is just a boundary surface. But in the case of a thin shell we do not expect the second condition to be satisfied since the matter content of the shell should lead to a jump in the extrinsic curvature K_{ij}. On Σ we define a three-bein

$$e_i=\frac{\partial}{\partial\xi^i} \tag{3}$$

having the component

$$e_i^\mu=\frac{\partial x^\mu}{\partial\xi^i}. \tag{4}$$

The induced metric on Σ is given by the scalar product

$$g_{ij}=e_i\cdot e_j=g_{\mu\nu}e_i^\mu e_j^\nu. \tag{5}$$

Let the parametric equation of the Σ be

$$\Phi(x^\mu(\xi^i))=0 \tag{6}$$

having the unit normal four-vector n^μ given by

$$n_\mu=\alpha^{-1}\partial_\mu\Phi, \tag{7}$$

where

$$\alpha=\pm\sqrt{\left|g^{\mu\nu}\frac{\partial\Phi}{\partial x^\mu}\frac{\partial\Phi}{\partial x^\nu}\right|}. \tag{8}$$

Therefore

$$n_\mu e_i^\mu=0 \tag{9}$$

and

$$n_\mu n^\mu=\epsilon, \tag{10}$$

where

$$\epsilon\equiv\mathrm{sign}(\alpha)=\frac{|\alpha|}{\alpha} \tag{11}$$

and in our case, since Σ is spacelike or timelike, ϵ becomes by definition equal to -1 or $+1$, respectively. The extrinsic curvature of Σ is defined as

$$K_{ij}^\pm=e_i^\mu e_j^\nu\nabla_\mu^\pm n_\nu=K_{ji}^\pm. \tag{12}$$

Now we have all the prerequisites to write Einstein's equations for hypersurface Σ in the Darmois–Israel approach. These are ten equations which will be written in components normal and tangent to the hypersurface. The first and second contracted Gauss–Kodazzi equations are

$$G_{\mu\nu}n^{\mu}n^{\nu}=\tfrac{1}{2}(K^2-K_{ij}K^{ij}-\epsilon^{3}R), \tag{13}$$

$$G_{\mu\nu}e_i^{\mu}n^{\nu}=K_{ij}^{j}-K_{,i}, \tag{14}$$

where $K=K_{ij}K^{ij}$ and ${}^3R$ is the Ricci scalar of the three metric, g_{ij}. Now to discover the effect of the energy–momentum tensor S_{ij} of Σ on space–time geometry, we perform a "pill-box" integration of Einstein's equation across Σ:

$$S_{\mu\nu}=\lim_{\sigma\to 0}\int_{-\sigma}^{\sigma}\left(T_{\mu\nu}-g_{\mu\nu}\frac{\Lambda}{\kappa}\right)dn=\frac{1}{\kappa}\lim_{\sigma\to 0}\int_{-\sigma}^{\sigma}G_{\mu\nu}\,dn, \tag{15}$$

where n is the proper distance through Σ in the direction of the normal n^{μ}. $S_{\mu\nu}$ is the associated four-tensor of energy–momentum of the shell. According to Eqs. (13) and (14), there is no moment associated with the surface layer, flows out of Σ. Therefore $S_{\mu\nu}$ vanishes off the Σ,

$$S_{\mu\nu}n^{\nu}=0. \tag{16}$$

The energy–momentum four- and three-tensors of Σ are related as

$$S^{\mu\nu}=e_i^{\mu}e_j^{\nu}S^{ij}. \tag{17}$$

Similarly we can associate to the three-tensor K_{ij} defined on Σ, the corresponding four-dimensional tensor:

$$K^{\mu\nu}=K^{ij}e_i^{\mu}e_j^{\nu}, \tag{18}$$

satisfying

$$K^{\mu\nu}n_{\nu}=0. \tag{19}$$

The remaining components of Einstein's equations lead to the following nonvanishing result:

$$\lim_{\sigma\to 0}\int_{-\sigma}^{\sigma}G_{\mu\nu}e_i^{\mu}e_j^{\nu}\,\mathrm{d}N=\epsilon([K_{ij}]-g_{ij}[K])=\kappa S_{ij}. \tag{20}$$

This distributional equivalent of Einstein's equation is called the Lanczos equation, which partly determines the dynamics of the thin shell. The other dynamical equations come from the defining equation of the matter contents of the shell.

B. Lightlike hypersurfaces

Now assume two space–time manifolds M^{+} and M^{-} with lightlike boundaries Σ^{+} and Σ^{-}. We want to glue these two manifolds together. In this case, K_{ij} must be defined carefully, since normal prescription breaks down. For this end we proceed as follows. We want to define a coordinate system in the vicinity of a null hypersurface of discontinuity, tied to the geometry of that hypersurface and analogous to Gaussian normal coordinates. Suppose Σ denotes the intended null hypersurface of discontinuity. A well-known theorem says that the null generators of Σ must be geodesics, i.e., if a congruence of curves is both null and hypersurface-orthogonal, then it is also geodesic.[18] Each generator possesses an affine parameter, η, unique up to change of origin on each generator and changes of scale uniform on each generator. Since Σ is a three-dimensional hypersurface, the null generators are labeled by two parameters. These two parameters, x^a where $a=2$, 3 are constant on any given generator, and the affine parameter η along the generators, provide a reasonably natural coordinate system for Σ. The coordinates η and x^a:$a=2$, 3, the coordinate basis vectors $\partial/\partial\eta$ and $\partial/\partial x^a$, and the metric components g_{ij}, on the hypersurface Σ, are components of the intrinsic geometry of Σ. To calculate the curvature associated with any

δ-function surface layers on Σ for the rest of the junction conditions, it is necessary to extend the coordinate system off Σ. One way to do this, in the spirit of Gaussian normal coordinates, is as follows. At each point of Σ, the tangent vectors $\partial/\partial\eta$ and $\partial/\partial x^a$ define a unique null direction off Σ on both sides, i.e., on each side of Σ there exists a unique null vector $\mathbf{N}$ satisfying $\mathbf{N}\cdot(\partial/\partial\eta) = -1$ and $\mathbf{N}\cdot(\partial/\partial x^a) = 0$. At each point of Σ a null geodesic tangent to this direction extends off Σ. Defining these geodesics to be loci of constant η and x^a and using an affine parameter N on each geodesics (with $N=0$ on Σ) as fourth coordinate establishes the desired coordinate system in some neighborhood of Σ. The direction of the vector $\mathbf{N}$ plays the same role here as the normal direction for timelike or spacelike hypersurfaces of discontinuity. Note that for null hypersurface Σ, the normal direction is that of $\partial/\partial\eta$, which is also tangent to Σ. Now, the parametric equation for Σ is

$$\Phi(x^\mu(\xi^i)) = 0, \tag{21}$$

where $\xi^i = (x^a, \eta)$ with $a = 2, 3$. The normal four-vector to Σ is given by

$$n_\mu = \alpha^{-1}\partial_\mu\Phi, \tag{22}$$

where $n_\mu n^\mu = 0$, since Σ is null hypersurface. Here we use the normalization condition,

$$N^\mu n_\mu = -1. \tag{23}$$

We now introduce a slight generalization of the concept of extrinsic curvature by defining

$$K_{ij} = -N_\mu \frac{\delta e_i^\mu}{\delta\xi^j} = K_{ji}, \tag{24}$$

where $\delta/\delta\xi^j$ shows the absolute derivatives and $e_i^\mu = \partial x^\mu/\partial x^i$, where $x^i = (\eta, x^a)$. K_{ij} so defined is called the transverse extrinsic curvature. K_{ij} is not independent of the choice of transversal vector. Now we have all the prerequisites to write Einstein's equations for null hypersurfaces in the Darmois–Israel approach. To do this we define

$$\gamma_{ij} = 2[K_{ij}], \tag{25}$$

which is well defined and free of arbitrariness in the transversal $\mathbf{N}$. γ_{ij} is the projection onto Σ of the $\gamma_{\mu\nu}$, which is defined as

$$\gamma_{\mu\nu} = N^\alpha[\partial_\alpha g_{\mu\nu}], \tag{26}$$

i.e.,

$$\gamma_{ij} = \gamma_{\mu\nu} e^\mu_{(i)} e^\nu_{(j)}. \tag{27}$$

The four vectors $(\mathbf{N}, \mathbf{e_{(i)}})$ form an oblique basis with respect to which the normal vector $\mathbf{n}$ can be decomposed as

$$\mathbf{n} = -\boldsymbol{\epsilon}\mathbf{N} + \mathbf{l}^i\mathbf{e}_i, \tag{28}$$

where l^i are smooth functions and $\boldsymbol{\epsilon} = \mathbf{n}\cdot\mathbf{n} = \mathbf{0}$. This decomposition gives

$$g_{ij}l^j = \boldsymbol{\epsilon}N_i = 0, \tag{29}$$

which shows that the induced metric is degenerate and its inverse cannot be defined. To raising the indices i, j we see that a symmetric matrix g_*^{ij} exists such that

$$g_*^{ik}g_{jk} = \delta^i_j + l^i N_j. \tag{30}$$

In particular g_*^{ij} could be chosen as the contravariant two-metric g^{ab} in convected coordinates ($l^i=\delta_1^i$) with the choice $\mathbf{N}\cdot\mathbf{e_i}=\mathbf{0}$.[9,10] In this case $g_{ij}g_*^{ij}=2$, $g_{ij}l^j=0$ and $\gamma_{ij}l^il^j=0$ and we find for dynamics of the null hypersurface Σ:

$$\kappa S^{ij}=-\tfrac{1}{2}(g_*^{ik}l^jl^l+l^il^kg_*^{jl}-l^il^jg_*^{kl})\gamma_{kl}, \tag{31}$$

which implies that $S^{ij}n_j=0$ where S^{ij} is the singular part of $T^{\mu\nu}$ in the distributional sense.

III. DISTRIBUTIONAL APPROACH

In this section we give a unified distributional approach to glue two different manifolds with boundaries which can be spacelike, timelike, or lightlike hypersurfaces. We assume the metric to be continuous at the hypersurface Σ,

$$[g^{\mu\nu}]=0. \tag{32}$$

Write the metric in the following form:

$$g_{\mu\nu}=g_{\mu\nu}^{+}\Theta(\Phi(x))+g_{\mu\nu}^{-}\Theta(-\Phi(x)), \tag{33}$$

where Θ is the Heaviside step function and

$$g_{\mu\nu}^{+}|_{\Phi(x)=0}=g_{\mu\nu}^{-}|_{\Phi(x)=0}. \tag{34}$$

This condition guarantees the smoothness of the metric on the hypersurface. Should this not be the case we try a coordinate transformation $x=x(x')$ having a jump in the first derivative:

$$\frac{\partial x^\mu}{\partial x'^\rho}=\alpha_\rho^{+\mu}\Theta(\Phi(x))+\alpha_\rho^{-\mu}\Theta(-\Phi(x)). \tag{35}$$

The condition for the new metric to be continuous comes out to be

$$\alpha_\rho^{+\mu}\alpha_\sigma^{+\nu}g_{\mu\nu}^{+}|_{\Phi(x)=0}=\alpha_\rho^{-\mu}\alpha_\sigma^{-\nu}g_{\mu\nu}^{-}|_{\Phi(x)=0}. \tag{36}$$

We assume from now on that the metric is smooth everywhere, C^0 at the hypersurface, and C^∞ on both sides of it. Although the metric is continuous on Σ, its derivatives, and so the corresponding connection coefficients, are discontinuous. The connection coefficients can be written as

$$\Gamma_{\mu\nu}^{\rho}=\tfrac{1}{2}g^{\rho\sigma}(g_{\mu\sigma,\nu}+g_{\nu\sigma,\mu}-g_{\mu\nu,\sigma})=\Theta(\Phi(x))\Gamma_{\mu\nu}^{+\rho}+\Theta(-\Phi(x))\Gamma_{\mu\nu}^{-\rho}, \tag{37}$$

where $\Gamma_{\mu\nu}^{\pm\rho}$ are the ordinary connection coefficients on $M^{\pm}$. The above connection has jump discontinuity on Σ. To write the field equation for the hypersurface Σ, we define the energy–momentum tensor of the hypersurface as

$$\breve{T}_{\mu\nu}=CS_{\mu\nu}\delta(\Phi(x)), \tag{38}$$

where C is a constant which can be calculated as follows. We integrate (38) in the direction normal (transverse in the lightlike case) to the hypersurface Σ,

$$\int \breve{T}_{\mu\nu}\,\mathrm{d}\zeta=CS_{\mu\nu}\int \delta(\Phi(x))\mathrm{d}\zeta=CS_{\mu\nu}\left|\frac{\mathrm{d}\zeta}{\mathrm{d}\Phi}\right|, \tag{39}$$

where ζ is a distance in the direction of n^μ or N^μ for nonlightlike or lightlike Σ, respectively. Now by means of (15), we obtain

$$C=\left|\frac{d\Phi}{d\zeta}\right|=|\zeta^{\mu}\partial_{\mu}\Phi|=|\alpha|, \tag{40}$$

where ζ^{μ} is n^{μ} or N^{μ} for nonlightlike or lightlike Σ, respectively. Therefore (38) can be written as

$$\check{T}_{\mu\nu}=CS_{\mu\nu}\delta(\Phi(x))=S_{\mu\nu}|\zeta^{\rho}\partial_{\rho}\Phi|\,\delta(\Phi(x))=|\alpha|S_{\mu\nu}\delta(\Phi(x)). \tag{41}$$

In order to write field equations, there is no need to change the ordinary concept of covariant derivative. The covariant derivative of the tensor

$$T^{(\rho)}=\Theta(\Phi)T^{+(\rho)}+\Theta(-\Phi)T^{-(\rho)}, \tag{42}$$

where (ρ) stands for any number of indices, is calculated to be

$$T^{(\rho)}_{;\nu}=\nabla_{\nu}T^{(\rho)}+[T^{(\rho)}](\partial_{\nu}\Phi)\,\delta(\Phi). \tag{43}$$

Now to writing Einstein's field equation for hypersurface, Σ, we expect the curvature and Einstein tensor to be proportional to δ. This means that in calculating the connection coefficients and the components of the Ricci tensor we consider only terms proportional to δ. Since

$$R_{\mu\nu}=\Gamma^{\rho}_{\mu\rho,\nu}-\Gamma^{\rho}_{\mu\nu,\rho}+\Gamma^{\sigma}_{\mu\rho}\Gamma^{\rho}_{\sigma\nu}-\Gamma^{\sigma}_{\mu\nu}\Gamma^{\rho}_{\rho\sigma}, \tag{44}$$

the term proportional to δ is

$$\check{R}_{\mu\nu}=\check{\Gamma}^{\rho}_{\mu\rho,\nu}-\check{\Gamma}^{\rho}_{\mu\nu,\rho}. \tag{45}$$

Now,

$$\Gamma^{\rho}_{\mu\rho}=\frac{1}{2g}g_{,\mu}, \tag{46}$$

where g is the determinant of the metric $g_{\mu\nu}$. The δ distribution can only occur in the second derivatives of the metric. Therefore,

$$\check{\Gamma}^{\rho}_{\mu\rho,\nu}=\frac{1}{2g}\check{g}_{,\mu\nu}. \tag{47}$$

For the second term in (45) we have

$$\check{\Gamma}^{\rho}_{\mu\nu,\rho}=\tfrac{1}{2}g^{\rho\sigma}(\check{g}_{\sigma\mu,\nu\rho}+\check{g}_{\sigma\nu,\mu\rho}-\check{g}_{\mu\nu,\sigma\rho}). \tag{48}$$

Having the metric in the form (33), we obtain

$$\check{g}_{\alpha\beta,\mu\nu}=[g_{\alpha\beta,\mu}](\partial_{\nu}\Phi)\,\delta(\Phi(x)) \tag{49}$$

and

$$\check{g}_{,\mu\nu}=[g_{,\mu}](\partial_{\nu}\Phi)\,\delta(\Phi(x)). \tag{50}$$

Therefore we obtain for terms in the Ricci tensor proportional to δ,

$$\begin{aligned}\check{R}_{\mu\nu}&=\left(\frac{1}{2g}[g_{,\mu}]\partial_{\nu}\Phi-g^{\rho\sigma}([g_{\sigma\mu,\nu}]+[g_{\sigma\nu,\mu}]-[g_{\mu\nu,\sigma}])\partial_{\rho}\Phi\right)\delta(\Phi)\\&=\left(\frac{1}{2g}[g_{,\mu}]\partial_{\nu}\Phi-[\Gamma^{\rho}_{\nu\mu}]\partial_{\rho}\Phi\right)\delta(\Phi(x)).\end{aligned} \tag{51}$$

Now we can write Einstein's field equation for the hypersurface Σ as

$$\check{G}_{\mu\nu}=\kappa\check{T}_{\mu\nu}. \tag{52}$$

Defining

$$Q_{\mu\nu}=(\alpha^{-1})\left(\frac{1}{2g}[g_{,\mu}]\delta^{\rho}_{\nu}-[\Gamma^{\rho}_{\mu\nu}]\right)\partial_{\rho}\Phi=\left(\frac{1}{2g}[g_{,\mu}]\delta^{\rho}_{\nu}-[\Gamma^{\rho}_{\mu\nu}]\right)n_{\rho}, \tag{53}$$

we obtain, using Eqs. (41) and (51) for the energy–momentum tensor, the field equations in the four-dimensional form

$$Q_{\mu\nu}-\tfrac{1}{2}g_{\mu\nu}Q=\epsilon\kappa S_{\mu\nu}, \tag{54}$$

where $Q=Q_{\mu\nu}g^{\mu\nu}$ and $\epsilon=|\alpha|/\alpha$. $Q_{\mu\nu}$ is a tensor with support on Σ and this equation describes the dynamics of Σ. Multiplying (53) with n^{μ} we obtain

$$S_{\mu\nu}n^{\nu}=0, \tag{55}$$

which tells us that the components corresponding to $S_{\mu\nu}n^{\mu}n^{\nu}$ and $S_{\mu\nu}n^{\mu}e^{\nu}_{i}$ in the nonlightlike case and $S_{\mu\nu}N^{\mu}n^{\nu}$ and $S_{\mu\nu}n^{\mu}e^{\nu}_{i}$ in the lightlike case identically vanishes. To obtain the proper three-dimensional components we have

$$Q_{ij}=Q_{\mu\nu}e^{\mu}_{i}e^{\nu}_{j}=-[\Gamma^{\rho}_{\mu\nu}]n_{\rho}e^{\mu}_{i}e^{\nu}_{j}=[K_{ij}]. \tag{56}$$

The three-dimensional analoge of (54) is therefore

$$Q_{ij}=\epsilon\kappa(S_{ij}-\tfrac{1}{2}g_{ij}S), \tag{57}$$

where $S=S_{ij}S^{ij}$ and this is equivalent to Lanczos equation (20), (31).

IV. EXAMPLE: SPHERICAL LIGHTLIKE SHELLS

The equivalence of the DI and MKh methods for spacelike and timelike thin shells in general relativity has been shown in Ref. 12. In Sec. III it was shown that the MKh method is applicable for the case of the null shell with few changes. Now to examine our claim, we consider the familiar example of lightlike shells with spherical symmetry. This example has been studied extensively in the DI approach,[9] but we want to consider it in our distributional method. Expressed in terms of Eddington retarded or advanced time u, the metric of a general spherisymmetric geometry is

$$ds^2=-e^{\psi}du(fe^{\psi}du+2\xi\,dr)+r^2\,d\Omega^2, \tag{58}$$

where ψ and f are functions of u and r. The sign factor ξ is $+1$ if r increases toward the future along a ray $u=$constant, i.e., if the light cone $u=$constant is expanding; if it contracts then $\xi=-1$. It is useful to introduce a local mass function $m(u,r)$ defined as $f=1-2m/r$. We consider the case where the geometry on both sides of the lightlike shell is static, i.e., $\psi=0$ and $f=f(r)$ in (58). The Einstein field equations then take the form

$$\begin{aligned} T_{rr}&=0,\\ T^{r}_{u}&=0,\\ \frac{\partial m}{\partial r}&=-4\pi r^2T^{u}_{u}. \end{aligned} \tag{59}$$

We consider a thin shell whose history Σ, a light cone $u=$constant, splits space–time into past and future domains M_- and M_+. The four metric has the form (58) in both M_- and M_+, but with different functions f_- and f_+. We want to glue two space–times M_- and M_+ along the hypersurface Σ defined as $\Phi(x)=u=$const, using the distributional approach. The normal vector to the hypersurface Σ has the component

$$n_\mu=\partial_\mu\Phi=(1,0,0,0). \tag{60}$$

Now using (53) we find

$$Q_{uu}=\frac{1}{2}\left[\frac{\mathrm{d}f}{\mathrm{d}r}\right] \tag{61}$$

and other component of $Q_{\mu\nu}$ are vanishing. The inverse four-metric nonvanishing components are

$$\begin{gathered} g^{ur}=g^{ru}=-1, \\ g^{rr}f, \\ g^{\theta\theta}=\frac{1}{r^2}, \\ g^{\phi\phi}=\frac{1}{r^2\sin^2\theta}. \end{gathered} \tag{62}$$

Therefore it is easy to show that $Q=0$. Now from (54) we find

$$Q_{uu}-\tfrac{1}{2}g_{uu}Q=8\pi S_{uu}, \tag{63}$$

which leads to

$$\frac{1}{2}\left[\frac{\mathrm{d}f}{\mathrm{d}r}\right]=8\pi S_{uu} \tag{64}$$

or in terms of m,

$$[m]=8\pi r^2 S_{uu}. \tag{65}$$

This equation tell us how we can embed Σ in four-dimensional space–time and is the same as Eq. (51) of Ref. 9.

V. DISCONTINUOUS METRICS

In this section we consider the general case of discontinuous metrics. Since Einstein's field equations are nonlinear, with these types of metrics, product of distributions are unavoidable. Classical theory of distributions (the so-called Schwartz–Sobolov theory of distributions) do not allow nonlinear operations on distributions, thus we consider the problem in the context of Colombeau's new theory of generalized functions. We consider the case of signature changing manifolds as an interesting problem in modern cosmology. It is important to note that the MKh distributional approach assumes the continuity of the metric at the hypersurface. Since in the Colombeau algebra, step function and other classically sharp functions become smooth and continuous, it is possible to continue to use the MKh method for classically discontinuous (in the sense of Schwartz–Sobolov) metrics.

A. New generalized functions

Suppose $\Phi \in D(\mathbb{R}^n)$ with $D(\mathbb{R}^n)$ the space of smooth (i.e., C^∞) C-valued test functions on $\mathbb{R}^n$. For $f:\mathbb{R}^n \to C$, not necessarily continuous, we define the smoothing process for f as one of the convolutions

$$\tilde{f}(x) := \int f(y)\Phi(y-x)d^n y, \tag{66}$$

or

$$\tilde{f}_\epsilon(x) := \int f(y)\,\frac{1}{\epsilon^n}\,\Phi\left(\frac{y-x}{\epsilon}\right)d^n y. \tag{67}$$

This smoothing procedure is valid for distributions too. Take the distribution R, then by smoothing of R we mean one of the two convolutions (66) or (67) with f replaced by R. Now we can perform the product Rf of the distribution R with the discontinuous function f through the action of the product on a test function Ψ as follows:

$$(Rf,\psi) = \lim_{\epsilon \to 0} \int \tilde{R}_\epsilon(x)\tilde{f}_\epsilon(x)\Psi(x)d^n x. \tag{68}$$

The multiplication so defined does not coincide with the ordinary multiplication even for continuous functions. To resolve this difficulty consider one-parameter families (f_ϵ) of C^∞ functions used to construct the algebra

$$\mathcal{E}_{\mathcal{M}}(\mathbb{R}^n) = \{(f_\epsilon) | f_\epsilon \in C^\infty(\mathbb{R}^n) \forall K \subset \mathbb{R}^n \text{ compact},$$

$$\forall \alpha \in \mathbb{N}^n \exists N \in \mathbb{N}, \quad \exists \eta > 0, \quad \exists > 0$$

$$\text{such that } \sup_{x \in K} |D^\alpha f_\epsilon(x)| \leqslant c\epsilon^{-N} \forall 0 < \epsilon < \eta\}, \tag{69}$$

where

$$D^\alpha = \frac{\partial^{|\alpha|}}{(\partial x^1)^{\alpha_1} \cdots (\partial x^n)^{\alpha_n}}, \tag{70}$$

and

$$|\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_n .$$

Accordingly, C^∞-functions are embedded into $\mathcal{E}_{\mathcal{M}}(\mathbb{R}^n)$ as constant sequences. Now, we have to identify different embeddings of C^∞ functions. Take a suitable ideal $\mathcal{N}(\mathbb{R}^n)$ defined as

$$\mathcal{N}(\mathbb{R}^n) = \{(f_\epsilon) | (f_\epsilon) \in \mathcal{E}_{\mathcal{M}}(\mathbb{R}^n) \forall K \subset \mathbb{R}^n \text{ compact},$$

$$\forall \alpha \in \mathbb{N}^n, \quad \forall N \in \mathbb{N} \exists \eta > 0, \quad \exists c > 0,$$

$$\text{such that } \sup_{x \in K} |D^\alpha f_\epsilon(x)| \leqslant c \in {}^N \forall 0 < \epsilon < \eta\}, \tag{71}$$

containing negligible functions such as

$$f(x) - \int d^n y\,\frac{1}{\epsilon^n}\,\varphi\left(\frac{y-x}{\epsilon}\right) f(y). \tag{72}$$

Now, the Colombeau algebra $\mathcal{G}(\mathbb{R}^n)$ is defined as

$$\mathcal{G}(\mathbb{R}^n)=\frac{\mathcal{E}_{\mathcal{M}}(\mathbb{R}^n)}{\mathcal{N}(\mathbb{R}^n)}. \tag{73}$$

A Colombeau generalized function is thus a moderate family $(f_\epsilon(x))$ of C^∞ functions modulo negligible families. Two Colombeau objects (f_ϵ) and (g_ϵ) are said to be associated [written as $(g_\epsilon)\approx(f_\epsilon)$] if

$$\lim_{\epsilon\to 0}\int d^n x(f_\epsilon(x)-g_\epsilon(x))\varphi(x)=0,$$
$$\forall\varphi\in D(\mathbb{R}^n). \tag{74}$$

For example, if $\varphi(x)=\varphi(-x)$ then $\delta\theta\approx\frac{1}{2}\delta$, where δ is Dirac delta function and θ is Heaviside step function. Moreover, we have in this algebra $\theta^n\approx\theta$ and not $\theta^n=\theta$.

B. Signature changing manifolds

In distributional formalism of gluing manifolds, the whole space–time, including the singular hypersurface, is treated with a unified metric without bothering about the junction conditions along the hypersurface. These conditions are shown to be automatically fulfilled as part of the field equations.[12] In this approach one chooses special coordinates which are continuous along the singular hypersurface to avoid nonlinear operations of distributions. Here, using Colombeau algebra, which allows for nonlinear operations of distributions, we generalize our distributional method to the special case of signature changing cosmological models.

Consider as a simple model universe a space–time with the following FRW metric containing a steplike lapse function

$$\mathrm{d}s^2=-f(t)\mathrm{d}t^2+a^2(t)\left(\frac{\mathrm{d}r^2}{1-kr^2}+r^2\,\mathrm{d}\theta^2+r^2\sin^2\theta\,\mathrm{d}\rho^2\right), \tag{75}$$

where

$$f(t)=\theta(t)-\theta(-t) \tag{76}$$

and

$$a^2(t)=a_+^2(t)\,\theta(t)+a_-^2(t)\,\theta(-t). \tag{77}$$

We assume $[a]=a_+-a_-=0$ to achieve continuity of the metric on the surface of signature change. Note that we have assumed for simplicity $k_+=k_-=k$. This metric describes a signature changing space–time with the singular surface $t=0$. It describes a Riemannian space for $t<0$ and a Lorentzian space–time for $t>0$. In Colombeau's point of view, $f(t)$ has a microscopic structure around $t=0$ with a jump equal to ϵ as shown in Fig. 1. Since we are going to construct a signature changing model, we choose

$$\theta(t)|_{t=0}=\tau \quad \text{with} \quad \tau>\tfrac{1}{2}. \tag{78}$$

Since $\theta(-t)=1-\theta(t)$, we have $\theta(-t)=1-\tau$ and

$$f(t)|_{t=0}=2\tau-1. \tag{79}$$

This value gives us the correct change of sign in going from $t<0$ to $t>0$. This "regularization" of $f(t)$ at $t=0$ allows us to use operations such as $f(t)^{-1}$, $f^2(t)$, and $|f(t)|^{-1}$.

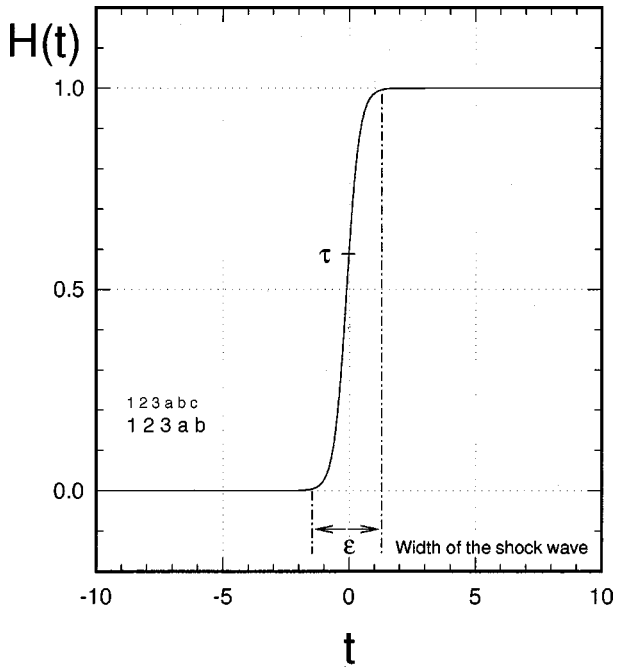

FIG. 1. The profile of Heaviside step function as it is used in Colombeau's theory.

In what follows we consider $f(t)$ to be the regularized function $\tilde{f}_\epsilon$, defined according to Colombeau's algebra. Now, we are prepared to calculate the dynamics of the signature changing hypersurface in the line of distributional procedure.[19] First we calculate the relevant components of the Einstein tensor for the metric (75):

$$G_{tt}=-\frac{-3kf^3f^3}{f^2a^2}-\frac{3f^2(\dot{a}^2)}{f^2a^4}, \tag{80}$$

$$G_{rr}=\frac{1}{1-kr^2}\left(\frac{2a\ddot{a}f}{f^2}-\frac{a\dot{a}\dot{f}}{f^2}+\frac{f(a\dot{a})^2}{a^2f^2}+\frac{kf^2}{f^2}\right), \tag{81}$$

$$G_{\theta\theta}=r^2\left(\frac{2a\ddot{a}f}{f^2}-\frac{a\dot{a}\dot{f}}{f^2}+\frac{f(a\dot{a})^2}{a^2f^2}+\frac{kf^2}{f^2}\right), \tag{82}$$

$$G_{\varphi\varphi}=r^2\sin^2\theta\left(\frac{2a\ddot{a}f}{f^2}-\frac{a\dot{a}\dot{f}}{f^2}+\frac{f(a\dot{a})^2}{a^2f^2}+\frac{kf^2}{f^2}\right). \tag{83}$$

According to standard calculus of distributions, we have

$$\dot{f}(t)=\dot{\theta}(t)-\dot{\theta}(-t)=\delta(t)+\delta(-t)=2\,\delta(t), \tag{84}$$

taking into account $\delta(-t)=\delta(t)$. Now, using Colombeau algebra we can write

$$\theta(t)\,\delta(t)\approx\tfrac{1}{2}\delta(t). \tag{85}$$

Therefore we may write

$$f(t)\,\delta(t)=\theta(t)\,\delta(t)-\theta(-t)\,\delta(t)\approx\tfrac{1}{2}\delta(t)-\tfrac{1}{2}\delta(t)\approx 0. \tag{86}$$

In evaluating (80)–(83) we should take care of the following property of association. Having

$$AB \approx AC,$$

we are not allowed to conclude

$$B \approx C.$$

Since the time derivative of any discontinuous function F is given by

$$\dot{F} = \dot{F}_+ \theta(t) + \dot{F}_- \theta(-t) + [F]\delta(t), \tag{87}$$

using relations (80)–(83) we obtain for the singular parts of these equations:

$$\hat{G}^t_t \approx 0, \tag{88}$$

$$\hat{G}^r_r \approx \left(\frac{f[\dot{a}]}{f^2 a} - \frac{[\dot{a}]}{f^2 a} \right) \delta(t), \tag{89}$$

$$\hat{G}^\theta_\theta \approx \left(\frac{f[\dot{a}]}{f^2 a} - \frac{[\dot{a}]}{f^2 a} \right) \delta(t), \tag{90}$$

$$\hat{G}^\varphi_\varphi \approx \left(\frac{f[\dot{a}]}{f^2 a} - \frac{[\dot{a}]}{f^2 a} \right) \delta(t), \tag{91}$$

where multiplication of the distribution $\delta(t)$ with the generalized functions $1/f^2$ and f/f^2 is defined as in (68).

This is a rigorous calculation which shows definitely that there are nonvanishing terms on the left-hand side of the field equations related to the signature change surface. Now we have to look at the energy–momentum tensor on the right-hand side of the field equations, its possible interpretation, and consequences for the dynamics of the signature change surface.

The complete energy–momentum tensor of space–time (with any kind of matter content) can be written as

$$T_{\mu\nu} = \theta(t) T^+_{\mu\nu} + \theta(-t) T^-_{\mu\nu} + C S_{\mu\nu} \delta(t), \tag{92}$$

where $T^\pm_{\mu\nu}$ are energy–momentum tensors corresponding to Lorentzian and Euclidean regions, respectively, and C is a constant which can be obtained by a little algebra to find

$$C = \left| \frac{\mathrm{d}\Phi}{\mathrm{d}n} \right| = |n^\mu \partial_\mu \Phi| = \frac{1}{|f(t)|}, \tag{93}$$

where $\Phi = t = 0$ defines the singular surface Σ, the vector n_μ is normal to the surface Φ, and n measures the distance along it. The distributional part of the Einstein equations read as follows:

$$\hat{G}_{\mu\nu} = \kappa \hat{T}_{\mu\nu} \tag{94}$$

using Eqs. (88)–(91), (93), (94) we obtain

$$0 \approx \frac{\kappa}{|f(t)|} S^t_t \delta(t), \tag{95}$$

$$\hat{G}^r_r \approx \left(\frac{f[\dot{a}]}{f^2 a} - \frac{[\dot{a}]}{f^2 a} \right) \delta(t) \approx \frac{\kappa}{|f(t)|} S^r_r \delta(t), \tag{96}$$

$$\hat{G}^{\theta}_{\theta}\approx\left(\frac{f[\dot{a}]}{f^2a}-\frac{[\dot{a}]}{f^2a}\right)\delta(t)\approx\frac{\kappa}{|f(t)|}S^{\theta}_{\theta}\delta(t), \tag{97}$$

$$\hat{G}^{\varphi}_{\varphi}\approx\left(\frac{f[\dot{a}]}{f^2a}-\frac{[\dot{a}]}{f^2a}\right)\delta(t)\approx\frac{\kappa}{|f(t)|}S^{\varphi}_{\varphi}\delta(t). \tag{98}$$

Now using Eq. (68), we must define the multiplication of δ-distribution with the discontinuous functions $1/|f|$ and $1/f^2$. To this end we consider them as Colombeau's regularized functions:

$$\tilde{G}_{1\epsilon}(t):=\delta_{\epsilon}(t)\left(\frac{1}{|f(t)|}\right)_{\epsilon}, \tag{99}$$

and

$$\hat{G}_{2\epsilon}(t):=\delta_{\epsilon}(t)\left(\frac{1}{f^2(t)}\right)_{\epsilon}. \tag{100}$$

Now according to (68), these two multiplications are defined as follows:

$$\left(\delta(t)\frac{1}{|f(t)|},\Psi\right):=\lim_{\epsilon\to 0}\int\tilde{G}_{1\epsilon}(t)\Psi(t)\mathrm{d}t, \tag{101}$$

and

$$\left(\delta(t)\frac{1}{f^2(t)},\Psi\right):=\lim_{\epsilon\to 0}\int\tilde{G}_{2\epsilon}(t)\Psi(t)\mathrm{d}t, \tag{102}$$

for any test function, Ψ. Now we argue that $\tilde{G}_{1\epsilon}$ and $\tilde{G}_{2\epsilon}$ are associated in Colombeau's sense, i.e.,

$$\lim_{\epsilon\to 0}\int(\tilde{G}_{1\epsilon}(t)-\tilde{G}_{2\epsilon}(t))\Psi(t)\mathrm{d}t=0. \tag{103}$$

This is correct for any test function Ψ because, although $\tilde{G}_{1\epsilon}$ and $\tilde{G}_{2\epsilon}$ are divergent at a common point, the difference in their ''microscopic structure'' at that point tends to zero for $\epsilon\to 0$. Therefore, we obtain from (95) to (98) the final form of the energy–momentum tensor of the singular surface, or the dynamics of Σ:

$$S^{t}_{t}\approx 0, \tag{104}$$

$$\kappa S^{r}_{r}\approx\left(\frac{f[\dot{a}]}{a}-\frac{[\dot{a}]}{a}\right), \tag{105}$$

$$\kappa S^{\theta}_{\theta}\approx\left(\frac{f[\dot{a}]}{a}-\frac{[\dot{a}]}{a}\right), \tag{106}$$

$$\kappa S^{\varphi}_{\varphi}\approx\left(\frac{f[\dot{a}]}{a}-\frac{[\dot{a}]}{a}\right). \tag{107}$$

Therefore the ''energy–momentum'' tensor of the singular hypersurface is

$$\kappa S_{\mu}^{\nu} = \mathrm{diag}\left(0, \frac{f[\dot{a}]}{a} - \frac{[\dot{a}]}{a}, \frac{f[\dot{a}]}{a} - \frac{[\dot{a}]}{a}, \frac{f[\dot{a}]}{a} - \frac{[\dot{a}]}{a}\right)$$
$$= \mathrm{diag}(0, 2[H_0](\tau - 1), 2[H_0](\tau - 1), 2[H_0](\tau - 1)), \tag{108}$$

where we have used (79). In this equation all quantities are to be taken at $t=0$, and H_0 is defined as

$$H_0 = \frac{\dot{a}}{a}\Big|_{t=0}, \tag{109}$$

which is the familiar Hubble constant at the signature change surface. This is our nontrivial and nonexpected result. One may question the validity of Coloumbeau algebra,[20] although it sounds physically well motivated and based on good physical intuition.[16,21,22] The above-given result is telling us that within this algebra it is not reasonable to assume that the energy–momentum tensor at the singular hypersurface of signature change is vanishing, as is usually assumed in the literature. If we assume that $[\dot{a}]=0$ (as is usually assumed in the literature) then Eq. (108) will give $S_{\mu}^{\nu}=0$, but this is not necessary in general. Therefore the condition $[\dot{a}]=0$ is not compulsory on the singular surface.

We have seen that the requirement of signature change leads to a very specific and nonvanishing form for the $S_{\mu\nu}$. Since the nonvanishing terms of $S_{\mu\nu}$ are related to the extrinsic curvature of the signature change surface, they tell us how it is embedded in the space–time. Therefore one should not be bothered about its matter interpretation. This form of the energy–momentum tensor of the singular hypersurface we have obtained set limits to the possible space–times emerging after signature change. As an example, we will consider in Sec. V C the possibility of the emergence of de Sitter space–time after signature change.

C. Junction conditions for de Sitter space–time

According to the Hartle–Hawking proposal,[23–25] the universe after signature change should be a de Sitter universe (inflationary phase). Let us assume that the space–time after signature change is a de Sitter one. Consider now the following de Sitter metric with appropriate lapse function $f(t)$ in order to contain signature change at $t=0$. The $t=$const sections of this metric are surfaces of constant curvature $k=1$:[26]

$$\mathrm{d}s^2 = -f(t)\mathrm{d}t^2 + a^2(t)(\mathrm{d}\chi^2 + \sin^2\chi(\mathrm{d}\,\theta^2 + \sin^2\theta\,\mathrm{d}\theta^2)) \tag{110}$$

where $f(t)$ is defined as in (77) and

$$a^2(t) = \alpha_+^2 \cosh^2(\alpha_+^{-1}t)\,\theta(t) + \alpha_-^2 \cos^2(\alpha_-^{-1}t)\,\theta(-t). \tag{111}$$

Since $[a]=0$ we will have $\alpha_+ = \alpha_- := R$. Now, the Euclidean sector can be interpreted as a S^4 with S^3 sections defined by $t=$const. The boundary of the Euclidean sector, defined by $t=0$, is an S^3 having the radius $R=\alpha_-=H_0^{-1}$ which is the maximum value of $\alpha_-\cos(\alpha_-^{-1}t)$. In the Lorentzian sector the cosmological constant is given by $\Lambda = 3\alpha_+^{-2} = 3H_0^2$.[26] The $t=$const surfaces are S^3 with radius $\alpha_+\cosh(\alpha_+^{-1}t)$ having the minimum value $R=\alpha_+=H_0^{-1}$.[23] Therefore, the following relation between the cosmological constant and the radius of the boundary is obtained:

$$\Lambda = \frac{3}{R^2}. \tag{112}$$

Following the same procedure as for the metric (75) and again using Colombeau's algebra, or simply using (108), we find for the elements of energy–momentum tensor of the hypersurface

$$\kappa S_{\mu}^{\nu} = \mathrm{diag}(0, \Pi, \Pi, \Pi), \tag{113}$$

where Π is defined as

$$\Pi=\left(\frac{2}{R}\tanh(R^{-1}t)-\frac{2}{R}\tan(R^{-1}t)\right)|_{(t=0)}(\tau-1)=0. \tag{114}$$

We therefore conclude that given the de Sitter metric in the form of (110) the energy–momentum tensor of the hypersurface of signature change defined by $t=0$ vanishes. This is a familiar result the previous authors usually assume from the beginning but we obtain it as a special case depending on the form of the metric of space–time.

It may be useful to look at the Darmois–Israel approach. There we have the following relation between the energy–momentum tensor of the singular hypersurface and the jump of the extrinsic curvature:

$$\kappa S_i^j=[K_i^j]-h_i^j[K], \tag{115}$$

where h_i^j is the three-metric of the singular hypersurface. The extrinsic curvature is defined as

$$K_{ij}=e_i^\mu e_j^\nu \nabla_\mu n_\nu, \tag{116}$$

where e_i, the mutually normal unit four-vectors in signature changing surface Φ, are defined as

$$e_i^\mu=\frac{\partial x^\mu}{\partial \xi^i}, \quad i=1,2,3. \tag{117}$$

ξ^i are coordinates adopted to the signature changing surface Σ and ∇_μ denotes the covariant derivative with respect to the four-geometry. We then find for the nonvanishing components of extrinsic curvature in Lorentzian sector [with $f(t)=+1$]

$$K_i^{+i}=-\frac{1}{\alpha_+}\tanh(\alpha_+^{-1}t), \quad i=1,2,3. \tag{118}$$

The corresponding components in the Euclidean sector are [with $f(t)=-1$]

$$K_i^{-i}=\frac{1}{\alpha_-}\tan(\alpha_-^{-1}t), \quad i=1,2,3. \tag{119}$$

Now we obtain for the jump of the extrinsic curvature on the signature change surface

$$[K_i^i]=(K_i^{+i}-K_i^{-i})|_{t=0}=\left(-\frac{1}{R}\tanh(R^{-1}t)-\frac{1}{R}\tan(R^{-1}t)\right)|_{t=0}=0, \quad i=1,2,3. \tag{120}$$

Within the Darmois–Israel approach to signature change it is used to assume that the energy–momentum tensor of the singular hypersurface vanishes. Therefore, given the above-mentioned result, the junction condition (115) is satisfied and it is concluded that the matching is possible. In contrast to this within the distributional approach, using Coloumbeau algebra, we obtain in general a nonvanishing expression for the energy–momentum tensor $S_{\mu\nu}$ and no explicit junction condition. The Einstein equations written for the whole manifold imply the junction conditions. Only in the special case of the metric (110) does the matching at $t=0$ lead to $S_{\mu\nu}=0$. One could require a matching along other sections corresponding to a nonmaximum radius of the Euclidean sector or a nonminimum radius of the Lorenzian sector. In this case the energy–momentum tensor of the singular surface may not be vanishing anymore, and has to be checked in each case.

VI. CONCLUSIONS

There are two different approaches for gluing manifolds in general relativity: the Darmois–Israel and distributional approaches. In this paper we have shown how these approaches can be used to find dynamics of hypersurfaces in general relativity and modern cosmology. We have discussed the extent to which these approaches are equivalent and it has been shown that lightlike hypersurfaces can be treated in the framework of distributional approach and there is a unified formalism for treating all kinds of hypersurfaces. Also it has been shown that theory of new generalized functions combined with distributional approach is a reasonable framework for treating signature changing manifolds. It is important to note that one of our main results is nonvanishing jump of extrinsic curvature in general signature changing hypersurfaces. This potentially contains interesting results about the nature of space–times emerging after signature change and theory of cosmological perturbations in signature changing space–times.[26] The other main result is the possibility of treating null hypersurfaces in the framework of distributional approach.

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Boost–rotation symmetric vacuum space–times with spinning sources

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Boost–rotation symmetric vacuum space–times with spinning sources which correspond to gravitational field of uniformly accelerated spinning ''particles'' are studied. Regularity conditions and asymptotic properties are analyzed. News functions are derived by transforming the general spinning boost–rotation symmetric vacuum metric to Bondi–Sachs coordinates. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1433941]

I. INTRODUCTION AND SUMMARY

Boost–rotation symmetric space–times correspond to gravitational field of uniformly accelerated ''particles.'' Usually conical singularities, which provide the ''source'' of the acceleration, are also present on the axis of the axial symmetry.

Boost–rotation symmetric space–times have two Killing vectors (the axial ξ and the boost η Killing vectors) and it has been proven that they are the only axially symmetric space–times with an additional symmetry that are radiative and admit global null infinity.[1] This result was generalized for spinning sources, i.e., for nonhypersurface orthogonal Killing vectors, in Ref. 2. Moreover boost–rotation symmetric space–times are the only radiative asymptotically flat space–times known in an analytical form which represent moving sources. While there are several known boost–rotation symmetric solutions with nonrotating sources (see Refs. 3 and 4, and references therein), there is only one known exact solution with spinning sources—the spinning C-metric[5–8] corresponding to two uniformly accelerated Kerr black holes.

Thanks to the rotation of sources there appear torsion singularities besides conical singularities on the axis of the axial symmetry and consequently there can be regions with closed timelike curves (see Ref. 9, Refs. 6, 8 and 10 for examples, and Ref. 10 for references).

The structure of a boost–rotation symmetric space–time with hypersurface orthogonal Killing vectors was studied in Ref. 11 and the general form of its news function was found in Refs. 12, and 13. Recently, news functions for spinning boost–rotation symmetric Petrov-type D space–times were computed in late time approximation in Ref. 14.

The present paper, where some results by Bičák and Bičák and Schmidt from Refs. 11–13 are generalized, is organized as follows. In Sec. II spinning boost–rotation symmetric (brs) vacuum space–times in coordinates adapted to the boost and rotation symmetries and null coordinates are examined, e.g., regularity of the space–time on the roof and on the axis and asymptotic flatness at null infinity are studied. In Sec. III the spinning brs metric is transformed from the coordinates adapted to the boost and rotation symmetries to the Bondi–Sachs coordinates,[15–17] suitable for examining radiation, to find the news functions of spinning brs space–times.

II. SPINNING BOOST–ROTATION SYMMETRIC SPACE–TIMES: REGULARITY CONDITIONS, ASYMPTOTIC BEHAVIOR

The general form of a spinning brs metric in coordinates adapted to the boost and rotation symmetries $\{t,\rho,z,\varphi\}$ is[6]

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$$ds^2=-e^{\lambda}\,d\rho^2-\rho^2e^{-\mu}\,d\varphi^2+2ae^{\mu}(z\,dt-t\,dz)d\varphi+a^2e^{\mu}(z^2-t^2)d\varphi^2$$
$$-\frac{1}{z^2-t^2}[(e^{\lambda}z^2-e^{\mu}t^2)dz^2-2zt(e^{\lambda}-e^{\mu})dz\,dt-(e^{\mu}z^2-e^{\lambda}t^2)dt^2], \tag{1}$$

where μ, λ, and a are functions of

$$A=\rho^2, \quad B=z^2-t^2.$$

It has two Killing vectors

$$\xi=\frac{\partial}{\partial\varphi}, \quad \eta=t\frac{\partial}{\partial z}+z\frac{\partial}{\partial t} \tag{2}$$

with norms

$$\xi^{\alpha}\xi_{\alpha}=g_{\varphi\varphi}=-\rho^2e^{-\mu}+a^2(z^2-t^2)e^{\mu}=-Ae^{-\mu}+a^2Be^{\mu},$$

$$\eta^{\alpha}\eta_{\alpha}=g_{tt}z^2+g_{zz}t^2+2g_{zt}zt=Be^{\mu}.$$

As in the nonspinning case,[11] two null hyperplanes $B=0$, i.e., $z=\pm t$, will be called the "roof," the points with $A=0$ the "axis," the region of the space–time with $B<0$ "above the roof," and finally the region with $B>0$ "below the roof." Notice that the behavior of the boost and axial Killing vectors (2) is more complicated in the spinning case. Below the roof $(B>0)$, the boost Killing vector η is mostly timelike as in the nonspinning case but in the vicinity of spinning sources there may also occur ergoregions where it is spacelike. Due to the presence of spinning strings there may be also regions in their neighborhood with closed timelike curves where the axial Killing vector ξ is timelike. In order to determine if there exist both timelike and spacelike Killing vectors everywhere below the roof $(B>0)$, we study a general linear combination of the boost and the axial Killing vectors with constant coefficients $X=c_1\xi+c_2\eta$. Its norm may be both positive and negative if the product of eigenvalues of the quadratic form $({c_1}^2g_{\phi\phi}+\cdots)$ given by the norm is negative, i.e., if $-\rho^2B<0$, which is satisfied everywhere below the roof, where the space–time is thus stationary and may be transformed to the stationary Weyl metric (A1) (see, e.g., Ref. 6). However, above the roof $(B<0)$, the product is everywhere positive $-\rho^2B>0$ and thus there does not exist a timelike Killing vector and the space–time is nonstationary there. (It is easier to perform these calculations in coordinates $\{\gamma,\rho,\beta,\varphi\}$ and $\{b,\rho,\chi,\varphi\}$, given in Appendix A, for regions below and above the roof, respectively.)

Vacuum Einstein's equations for the spinning brs metric (1) are

$$A\mu_{,AA}+B\mu_{,BB}+\mu_{,A}+\mu_{,B}=-\frac{B}{A}e^{2\mu}(Aa_{,A}{}^2+Ba_{,B}{}^2), \tag{3}$$

$$0=AB(e^{2\mu}a_{,A})_{,A}+(B^2e^{2\mu}a_{,B})_{,B}, \tag{4}$$

$$(A+B)\lambda_{,A}=(A-B)\mu_{,A}-2B\mu_{,B}-B(B\mu_{,B}{}^2-A\mu_{,A}{}^2)+2AB\mu_{,A}\mu_{,B}$$
$$+\frac{B^2}{A}e^{2\mu}(Ba_{,B}{}^2-Aa_{,A}{}^2-2Aa_{,A}a_{,B}), \tag{5}$$

$$(A+B)\lambda_{,B}=(A-B)\mu_{,B}+2A\mu_{,A}+A(B\mu_{,B}{}^2-A\mu_{,A}{}^2)+2AB\mu_{,A}\mu_{,B}$$
$$-Be^{2\mu}(Ba_{,B}{}^2-Aa_{,A}{}^2+2Ba_{,A}a_{,B}). \tag{6}$$

Notice that Eqs. (3) and (4) are integrability conditions for Eqs. (5) and (6).

First let us investigate the regularity of the roof and the axis. From Eq. (5) it follows that on the roof (i.e., for $B=0$)

$$\lambda_{,A}(A,0)=\mu_{,A}(A,0) \quad \rightarrow \quad \lambda(A,0)-\mu(A,0)=K_1=\text{const.}$$

The roof is regular [i.e., g_{zz}, g_{tt}, and g_{tz} in (1) are nonsingular on the roof] if for $B=0$

$$\lambda(A,0)=\mu(A,0), \quad \text{i.e.,} \quad K_1=0. \tag{7}$$

From Eqs. (3), (5), and (6) on the axis ($A=0$) we get

$$a_{,B}(0,B)=0 \quad \rightarrow \quad a=\tilde{a}_0+\tilde{a}_1(B)A+\mathcal{O}(A^2), \quad \tilde{a}_0=\text{const},$$

$$\lambda_{,B}(0,B)+\mu_{,B}(0,B)=0 \quad \rightarrow \quad \lambda(0,B)+\mu(0,B)=K_2=\text{const.}$$

The axis regularity condition

$$\lim_{\rho_0\to 0}\frac{1}{2\pi}\frac{\int_0^{2\pi}\sqrt{g_{\varphi\varphi}|_{\rho_0}}\mathrm{d}\varphi}{\int_0^{\rho_0}\sqrt{g_{\rho\rho}}\mathrm{d}\rho}=1$$

[or equivalently g_{xx}, g_{yy} are nonsingular and $g_{xy}=0$ there, see (A5)] is satisfied if

$$a(0,B)=0 \quad \rightarrow \quad a=\tilde{a}_1(B)A+\mathcal{O}(A^2), \quad \text{i.e.,} \quad \tilde{a}_0=0, \tag{8}$$

$$\lambda(0,B)+\mu(0,B)=0, \quad \text{i.e.,} \quad K_2=0. \tag{9}$$

If $K_2\neq 0$ there is a conical singularity along the axis and if $\tilde{a}_0\neq 0$ a torsion singularity is present there. The regularity condition of the roof (7) is the same as for nonspinning brs space–times,[11] however, a new condition (8) arises for the regularity of the axis except for (9) which also appears in the nonspinning case.[11]

Now let us turn our attention to asymptotic behavior of spinning brs space–times at null infinity. For this purpose we transform (1) to null coordinates in two steps: first transforming it to coordinates $\{b,\rho,\chi,\varphi\}$ by (3.10) in Ref. 11

$$b=\sqrt{-B}=\sqrt{t^2-z^2}, \quad \tanh\chi=\pm\frac{z}{t}$$

we obtain the metric

$$\mathrm{d}s^2=e^{\lambda}(\mathrm{d}b^2-\mathrm{d}\rho^2)-\rho^2e^{-\mu}\,\mathrm{d}\varphi^2-b^2e^{\mu}(\mathrm{d}\chi+a\,\mathrm{d}\varphi)^2. \tag{10}$$

Finally transforming (10) to coordinates $\{\bar{u},\bar{v},\chi,\varphi\}$ by (3.15) in Ref. 11

$$\bar{u}=b-\rho, \quad \bar{v}=b+\rho$$

we obtain

$$\mathrm{d}s^2=e^{\lambda}\,\mathrm{d}\bar{u}\,\mathrm{d}\bar{v}-\frac{(\bar{v}-\bar{u})^2}{4}e^{-\mu}\,\mathrm{d}\varphi^2-\frac{(\bar{v}+\bar{u})^2}{4}e^{\mu}(\mathrm{d}\chi+a\,\mathrm{d}\varphi)^2. \tag{11}$$

Vacuum Einstein's equations for (11) read

$$
\begin{aligned}
&\mu_{,\bar{u}\bar{v}}+\frac{1}{\bar{v}^2-\bar{u}^2}(\bar{v}\mu_{,\bar{u}}-\bar{u}\mu_{,\bar{v}})=\left(\frac{\bar{v}+\bar{u}}{\bar{v}-\bar{u}}\right)^2 e^{2\mu}a_{,\bar{u}}a_{,\bar{v}},\\
&0=a_{,\bar{u}\bar{v}}+a_{,\bar{u}}\left(\mu_{,\bar{v}}+\frac{\bar{v}-2\bar{u}}{\bar{v}^2-\bar{u}^2}\right)+a_{,\bar{v}}\left(\mu_{,\bar{u}}+\frac{2\bar{v}-\bar{u}}{\bar{v}^2-\bar{u}^2}\right),\\
&-\bar{u}\lambda_{,\bar{u}}=\bar{v}\mu_{,\bar{u}}+\frac{\bar{v}^2-\bar{u}^2}{4}\mu_{,\bar{u}}^2+\frac{(\bar{v}+\bar{u})^3}{\bar{v}-\bar{u}}\frac{e^{2\mu}}{4}a_{,\bar{u}}^2,\\
&-\bar{v}\lambda_{,\bar{v}}=\bar{u}\mu_{,\bar{v}}-\frac{\bar{v}^2-\bar{u}^2}{4}\mu_{,\bar{v}}^2-\frac{(\bar{v}+\bar{u})^3}{\bar{v}-\bar{u}}\frac{e^{2\mu}}{4}a_{,\bar{v}}^2.
\end{aligned}
\tag{12}
$$

Assuming the metric functions μ, λ, and a to have expansions in $\bar{v}^{-1}$ for $\bar{v}\to\infty$ ($\mu(\bar{u},\bar{v})=\mu_0(\bar{u})+\mu_1(\bar{u})/\bar{v}+\cdots$) and solving Eqs. (12) at null infinity, i.e., for the limit $\bar{v}\to\infty$ and $\bar{u}$, χ, φ constant, we get

$$
\mu=\mu_0+\frac{\mu_1(\bar{u})}{\bar{v}}+\mathcal{O}(\bar{v}^{-2}),\quad \lambda=\lambda_0(\bar{u})+\frac{\lambda_1(\bar{u})}{\bar{v}}+\mathcal{O}(\bar{v}^{-2}),\quad a=a_0+\frac{a_1(\bar{u})}{\bar{v}}+\mathcal{O}(\bar{v}^{-2}),
\tag{13}
$$

where a_0 and μ_0 are constants and $\lambda_0(\bar{u})$ satisfies

$$
\lambda_{0,\bar{u}}=-\frac{1}{4\bar{u}}(4\mu_{1,\bar{u}}+\mu_{1,\bar{u}}^2+e^{2\mu_0}a_{1,\bar{u}}^2).
$$

The metric (11) with the metric functions (13) is asymptotically Minkowskian at null infinity as in the limit $\bar{v}\to\infty$ and $\bar{u}$, χ, φ constant, it can be transformed to the Minkowski metric using the transformations (3.23) and (3.24) in Ref. 11

$$
\bar{u}'=e^{(1/2)\mu_0}\int e^{\lambda_0(\bar{u})}\,\mathrm{d}\bar{u},\quad \bar{v}'=e^{-(1/2)\mu_0}\bar{v},\quad \chi'=e^{\mu_0}\chi
$$

and

$$
\chi''=\chi'+a_0e^{\mu_0}\varphi.
$$

III. THE BONDI–SACHS COORDINATES AND NEWS FUNCTIONS FOR SPINNING brs SPACE–TIMES

In this section we transform the spinning brs metric (1) into the Bondi–Sachs coordinates $\{u,r,\theta,\phi\}$, in which the metric that does not depend on ϕ because of the axial symmetry, has the form[15–17]

$$
\mathrm{d}s^2=g_{uu}\,\mathrm{d}u^2+2g_{ur}\,\mathrm{d}u\,\mathrm{d}r+2g_{u\theta}\,\mathrm{d}u\,\mathrm{d}\theta+2g_{u\phi}\,\mathrm{d}u\,\mathrm{d}\phi+g_{\theta\theta}\,\mathrm{d}\theta^2+g_{\phi\phi}\,\mathrm{d}\phi^2+2g_{\theta\phi}\,\mathrm{d}\theta\,\mathrm{d}\phi
\tag{14}
$$

with the following expansion for $r\to\infty$ and u, θ, and ϕ constant:

$$g_{uu}=1-\frac{2M}{r}+\mathcal{O}(r^{-2}),$$

$$g_{ur}=1-\frac{c^2+d^2}{2r^2}+\mathcal{O}(r^{-4}),$$

$$g_{u\theta}=-(c_{,\theta}+2c\cot\theta)+\mathcal{O}(r^{-1}),$$

$$g_{u\phi}=-(d_{,\theta}+2d\cot\theta)\sin\theta+\mathcal{O}(r^{-1}), \tag{15}$$

$$g_{\theta\theta}=-r^2-2cr-2(c^2+d^2)+\mathcal{O}(r^{-1}),$$

$$g_{\theta\phi}=-2dr\sin\theta+\mathcal{O}(r^0),$$

$$g_{\phi\phi}=-r^2\sin^2\theta+2cr\sin^2\theta-2(c^2+d^2)\sin^2\theta+\mathcal{O}(r^{-1}),$$

where c, d, and M are functions of u and θ. As a consequence of Einstein's equations, time dependence of the mass aspect M is determined by the news functions $c_{,u}$ and $d_{,u}$ (Refs. 16 and 17),

$$M_{,u}=-(c_{,u}{}^2+d_{,u}{}^2)+\tfrac{1}{2}(c_{,\theta\theta}+3c_{,\theta}\cot\theta-2c)_{,u}.$$

If there is nonvanishing news function, gravitational radiation is present and the total Bondi mass at future null infinity is decreasing.

In order to find the transformation of spinning brs space–times from the coordinates $\{t,\rho,z,\varphi\}$ with the metric (1) into the Bondi–Sachs coordinates $\{u,r,\theta,\phi\}$ with the metric (14) and its expansions (15) we follow Ref. 12 and we first transform the metric (1) to flat-space spherical coordinates $\{R,\Theta,\varphi\}$ and a flat-space retarded time U using the relations

$$t=U+R,\quad \rho=R\sin\Theta,\quad z=R\cos\Theta. \tag{16}$$

We assume the metric functions to have the expansions in powers R^{-1},

$$\lambda(U,\Theta)=\lambda_0(U,\Theta)+\frac{\lambda_1(U,\Theta)}{R}+\mathcal{O}(R^{-2}),$$

$$\mu(U,\Theta)=\mu_0+\frac{\mu_1(U,\Theta)}{R}+\mathcal{O}(R^{-2}), \tag{17}$$

$$a(U,\Theta)=a_0+\frac{a_1(U,\Theta)}{R}+\mathcal{O}(R^{-2}),$$

where μ_0 and a_0 are constants and thus

$$e^{\lambda}=\beta(U,\Theta)\left(1+\frac{\lambda_1(U,\Theta)}{R}+\mathcal{O}(R^{-2})\right),\quad e^{\mu}=\alpha\left(1+\frac{\mu_1(U,\Theta)}{R}+\mathcal{O}(R^{-2})\right) \tag{18}$$

with

$$\beta(U,\Theta)=e^{\lambda_0(U,\Theta)},\quad \alpha=e^{\mu_0}. \tag{19}$$

Now we transform the metric further to the Bondi–Sachs coordinates by an asymptotic transformation

$$
\begin{aligned}
U &= \overset{0}{\pi}(u,\theta) + \frac{\overset{1}{\pi}(u,\theta)}{r} + \frac{\overset{2}{\pi}(u,\theta)}{r^2} + \mathcal{O}(r^{-3}),\\
R &= q(u,\theta)r + \overset{0}{\sigma}(u,\theta) + \frac{\overset{1}{\sigma}(u,\theta)}{r} + \mathcal{O}(r^{-2}),\\
\Theta &= \overset{0}{\tau}(u,\theta) + \frac{\overset{1}{\tau}(u,\theta)}{r} + \frac{\overset{2}{\tau}(u,\theta)}{r^2} + \mathcal{O}(r^{-3}),\\
\varphi &= \phi + \overset{0}{f}(u,\theta) + \frac{\overset{1}{f}(u,\theta)}{r} + \frac{\overset{2}{f}(u,\theta)}{r^2} + \mathcal{O}(r^{-3}).
\end{aligned}
\tag{20}
$$

Comparing the resulting metric expansions with the expansions (15) we obtain differential equations for coefficients entering the asymptotic transformation (20). Since these equations are lengthy we present only their solutions in Appendix B. Their integrability condition [obtained comparing (B4) and (B5)] turns out to be the same as in the nonspinning case[12]

$$
\beta,_{\overset{0}{\pi}}\overset{0}{\pi} + \beta,_{\overset{0}{\tau}}\tan\overset{0}{\tau} = 0, \quad \text{or equivalently} \quad \lambda_{0,U}U + \lambda_{0,\Theta}\tan\Theta = 0,
$$

where the relations $\beta,_u = \beta,_{\overset{0}{\pi}}\overset{0}{\pi},_u$ and $\beta,_\theta = \beta,_{\overset{0}{\tau}}\overset{0}{\tau},_\theta + \beta,_{\overset{0}{\pi}}\overset{0}{\pi},_\theta$ have been used. Solving Eqs. (B1), (B2), (B3), and (B6) one may infer the first-order coefficients in the expansions (20),

$$
\overset{0}{\tau} = 2\arctan[e^{-\nu}(\tan\tfrac{1}{2}\theta)^K], \tag{21}
$$

$$
q = \frac{1}{\sqrt{K}}\sin\frac{1}{2}\theta\cos\frac{1}{2}\theta\left[e^{\nu}\left(\cot\frac{1}{2}\theta\right)^K + e^{-\nu}\left(\tan\frac{1}{2}\theta\right)^K\right], \tag{22}
$$

$$
\overset{0}{f} = \frac{a_0\alpha}{K}\ln\left(\frac{\sin\overset{0}{\tau}}{1+\cos\overset{0}{\tau}}\right), \tag{23}
$$

$$
\overset{0}{\pi},_u = \frac{1}{\beta q}, \tag{24}
$$

where $K \equiv (1+a_0^2\alpha^2)/\alpha$ and ν is an arbitrary constant. The axis (which is the same in both coordinates, i.e., $\Theta = 0$, $\pi \to \theta = 0$, π) is singular for $K \neq 1$ as q goes to 0 for $K<1$ and to ∞ for $K>1$ there. Since the coordinate system $\{t,\rho,z,\varphi\}$ can be chosen in such a way that $a_0 = 0$, we present here news functions for $a_0 = 0$ and the case $a_0 \neq 0$ is given in Appendix B. From Eqs. (B7) and (B8) we obtain the news functions

$$
c,_u = \frac{1}{2}\mu_1,_u - \frac{q,_\theta{}^2}{2q^2} - \frac{q,_\theta\cot\overset{0}{\tau}}{q^2\sqrt{\alpha}} + \frac{1}{2q^2\beta\sin^2\overset{0}{\tau}} - \frac{1}{2} - \frac{\cot^2\overset{0}{\tau}}{2q^2\alpha}, \tag{25}
$$

$$d_{,u} = -\tfrac{1}{2}\alpha a_{1,u}. \tag{26}$$

Having the news functions of the system one can then compute the Bondi mass (see Ref. 2).

For a special case $K=\alpha=1$, i.e., for a regular axis, we get from (21), (22), and (23)

$$\overset{0}{\tau} = 2\arctan(e^{-\nu}\tan\tfrac{1}{2}\theta), \quad q=\cosh\nu+\cos\theta\sinh\nu, \quad \overset{0}{f}=0. \tag{27}$$

Coordinate systems with different ν are connected by Lorentz transformations along the axis belonging to the Bondi–Metzner–Sachs group and thus as in Ref. 12 we may without loss of generality put $\nu=1$ which implies $q=1$ and $\overset{0}{\tau}=\theta$. Then the coefficient $\overset{0}{\tau}$ can be computed from the relation

$$\int e^{\lambda_0(\overset{0}{\pi},\theta)}\,\mathrm{d}\overset{0}{\pi} = u+\omega(\theta) \tag{28}$$

obtained from Eq. (24). The function $\omega(\theta)$ in (28) represents a supertranslation also belonging to the Bondi–Metzner–Sachs group and thus it may be again put equal to zero without loss of generality. Finally the news functions (25) and (26) read

$$c_{,u} = -\frac{1}{2\sin^2\theta}+\frac{1}{2\beta\sin^2\theta}+\frac{1}{2}\mu_{1,u} = \frac{1}{2\beta\sin^2\theta}(1-\beta+\mu_{1,u}\beta\sin^2\theta), \tag{29}$$

$$d_{,u} = -\tfrac{1}{2}a_{1,u}. \tag{30}$$

For $a_1=0$ (29) and (30) reduce to news functions as given in Refs. 12 and 13 for the nonrotating case.

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APPENDIX A: COORDINATE SYSTEMS ADAPTED TO THE BOOST AND ROTATION SYMMETRIES

In the nonradiative stationary region below the roof, a spinning brs metric can be transformed to the stationary Weyl coordinates $\{\overline{t},\overline{\rho},\overline{z},\overline{\varphi}\}$ with the Killing vectors $\xi=\partial_{\overline{\varphi}}$, $\eta=\partial_{\overline{t}}$, and the metric

$$\mathrm{d}s^2 = -e^{-2U}[e^{2\nu}(\mathrm{d}\overline{\rho}^2+\mathrm{d}\overline{z}^2)+\overline{\rho}^2\,\mathrm{d}\overline{\varphi}^2]+e^{2U}(\mathrm{d}\overline{t}+a\,\mathrm{d}\overline{\varphi})^2. \tag{A1}$$

Vacuum Einstein's equations have the form[18]

$$
\begin{aligned}
&U,_{\overline{\rho}\overline{\rho}}+U,_{\overline{z}\overline{z}}+\frac{U,_{\overline{\rho}}}{\overline{\rho}}=-\frac{e^{4U}}{2\overline{\rho}^2}(a,_{\overline{\rho}}^{\ 2}+a,_{\overline{z}}^{\ 2}),\\
&0=\left(e^{4U}\frac{a,_{\overline{\rho}}}{\overline{\rho}}\right),_{\overline{\rho}}+\left(e^{4U}\frac{a,_{\overline{z}}}{\overline{\rho}}\right),_{\overline{z}},\\
&\frac{\nu,_{\overline{\rho}}}{\overline{\rho}}=U,_{\overline{\rho}}^{\ 2}-U,_{\overline{z}}^{\ 2}-\frac{e^{4U}}{4\overline{\rho}^2}(a,_{\overline{\rho}}^{\ 2}-a,_{\overline{z}}^{\ 2}),\\
&\frac{\nu,_{\overline{z}}}{\overline{\rho}}=2U,_{\overline{\rho}}U,_{\overline{z}}-\frac{e^{4U}}{2\overline{\rho}^2}a,_{\overline{\rho}}a,_{\overline{z}}.
\end{aligned}
\tag{A2}
$$

Another appropriate coordinate system in the stationary region below the roof is $\{\gamma,\rho,\beta,\varphi\}$ with Killing vectors $\xi=\partial_\varphi$, $\eta=\partial_\gamma$ and the metric

$$
ds^2=-e^{\lambda}(d\rho^2+d\beta^2)-\rho^2e^{-\mu}\,d\varphi^2+\beta^2e^{\mu}(d\gamma+a\,d\varphi)^2, \tag{A3}
$$

connected with the stationary Weyl coordinates by [see (5.4) and (5.6) in Ref. 11]

$$
\overline{t}=\gamma,\quad \overline{\rho}=\rho\beta,\quad \overline{z}-\overline{z}_0=\frac{\beta^2-\rho^2}{2},\quad \overline{\varphi}=\varphi,\quad \overline{z}_0=\text{const},\quad e^{2U}=\beta^2e^{\mu},\quad e^{2\nu}=\frac{\beta^2}{\rho^2+\beta^2}e^{\mu+\lambda}.
$$

Vacuum Einstein's equations read

$$
\begin{aligned}
&\mu,_{\rho\rho}+\mu,_{\beta\beta}+\frac{\mu,_{\rho}}{\rho}+\frac{\mu,_{\beta}}{\beta}=-\frac{\beta^2}{\rho^2}e^{2\mu}(a,_{\rho}^{\ 2}+a,_{\beta}^{\ 2}),\\
&0=\left(\frac{\beta^3}{\rho}e^{2\mu}a,_{\rho}\right),_{\rho}+\left(\frac{\beta^3}{\rho}e^{2\mu}a,_{\beta}\right),_{\beta},\\
&(\rho^2+\beta^2)\lambda,_{\rho}=(\rho^2-\beta^2)\mu,_{\rho}-2\rho\beta\mu,_{\beta}-\tfrac{1}{2}\rho\beta^2(\mu,_{\beta}^{\ 2}-\mu,_{\rho}^{\ 2})+\rho^2\beta\mu,_{\rho}\mu,_{\beta}\\
&\qquad+\frac{\beta^4}{2\rho}e^{2\mu}\left(a,_{\beta}^{\ 2}-a,_{\rho}^{\ 2}-2\frac{\rho}{\beta}a,_{\rho}a,_{\beta}\right),\\
&(\rho^2+\beta^2)\lambda,_{\beta}=(\rho^2-\beta^2)\mu,_{\beta}+2\rho\beta\mu,_{\rho}+\tfrac{1}{2}\rho^2\beta(\mu,_{\beta}^{\ 2}-\mu,_{\rho}^{\ 2})+\rho\beta^2\mu,_{\rho}\mu,_{\beta}\\
&\qquad-\frac{1}{2}\beta^3e^{2\mu}\left(a,_{\beta}^{\ 2}-a,_{\rho}^{\ 2}+2\frac{\beta}{\rho}a,_{\rho}a,_{\beta}\right).
\end{aligned}
\tag{A4}
$$

The stationary region of a brs space–time, under the roof, is composed of two identical regions ($z>0$, $z>|t|$ and $z<0$, $z<-|t|$) and each of them can be transformed to coordinates $\{\overline{t},\overline{\rho},\overline{z},\overline{\varphi}\}$ or $\{\gamma,\rho,\beta,\varphi\}$.

By further transformation (3.5) in Ref. 11 to coordinates $\{t,\rho,z,\varphi\}$

$$
\tanh\gamma=\pm\frac{t}{z},\quad \beta=\sqrt{z^2-t^2},\quad B\equiv\beta^2,\quad A\equiv\rho^2,
$$

we arrive at the metric (1) where a nonstationary region above the roof (again composed of two identical regions) appears as in the nonspinning case.[11]

For examining regularity of the axis it is convenient to transform (1) to coordinates $\{t,x,y,z\}$, where $x=\rho\cos\varphi$, $y=\rho\sin\varphi$:

$$
\begin{aligned}
ds^2=&-\frac{1}{x^2+y^2}\Big[(e^{\lambda}x^2+e^{-\mu}y^2)dx^2+(e^{\lambda}y^2+e^{-\mu}x^2)dy^2+2xy(e^{\lambda}-e^{-\mu})dx\,dy\\
&-\frac{z^2-t^2}{x^2+y^2}a^2e^{\mu}(-y\,dx+x\,dy)^2-2ae^{\mu}(-yz\,dx\,dt+yt\,dx\,dz+xz\,dy\,dt-xt\,dy\,dz)\\
&-\frac{1}{z^2-t^2}[(e^{\lambda}z^2-e^{\mu}t^2)dz^2-2zt(e^{\lambda}-e^{\mu})dz\,dt-(e^{\mu}z^2-e^{\lambda}t^2)dt^2].
\end{aligned}
\tag{A5}
$$

Let us finally write down vacuum Einstein's equations for the metric (10) with the Killing vectors $\xi=\partial_{\varphi}$, $\eta=\partial_{\chi}$

$$
\begin{aligned}
&\mu_{,\rho\rho}-\mu_{,bb}+\frac{\mu_{,\rho}}{\rho}-\frac{\mu_{,b}}{b}=\frac{b^2}{\rho^2}e^{2\mu}({a_{,\rho}}^2-{a_{,b}}^2),\\
&0=\left(\frac{b^3}{\rho}e^{2\mu}a_{,\rho}\right)_{,\rho}-\left(\frac{b^3}{\rho}e^{2\mu}a_{,b}\right)_{,b},\\
&(\rho^2-b^2)\lambda_{,\rho}=(\rho^2+b^2)\mu_{,\rho}-2\rho b\mu_{,b}-\tfrac{1}{2}\rho b^2({\mu_{,b}}^2+{\mu_{,\rho}}^2)+\rho^2b\mu_{,\rho}\mu_{,b}\\
&\qquad+\frac{b^4}{2\rho}e^{2\mu}\left(-{a_{,b}}^2-{a_{,\rho}}^2+2\frac{\rho}{b}a_{,\rho}a_{,b}\right),\\
&(\rho^2-b^2)\lambda_{,b}=-(\rho^2+b^2)\mu_{,b}+2\rho b\mu_{,\rho}-\tfrac{1}{2}\rho^2b({\mu_{,b}}^2+{\mu_{,\rho}}^2)+\rho b^2\mu_{,\rho}\mu_{,b}\\
&\qquad+\frac{b^3}{2}e^{2\mu}\left(-{a_{,b}}^2-{a_{,\rho}}^2+2\frac{b}{\rho}a_{,\rho}a_{,b}\right).
\end{aligned}
\tag{A6}
$$

The coordinates $\{b,\rho,\chi,\varphi\}$ for the nonstationary region above the roof are analogical to coordinates $\{\gamma,\rho,\beta,\varphi\}$ (A3) in the stationary region below the roof.

As for (3)–(6), in each set of Einstein's equations (A2), (A4), and (A6), the first two are integrability conditions for the other two.

APPENDIX B: TRANSFORMATION OF THE SPINNING brs METRIC TO THE BONDI–SACHS COORDINATES

The spinning brs metric (1) with expansions (17)–(19) being transformed to the Bondi–Sachs coordinates with the metric (14) using transformations (16), (20) and compared with (15) leads to lengthy equations for coefficients of the asymptotic transformation (20) and metric functions from (15). We present here only their solutions:

$$
\begin{aligned}
&(g_{u\phi},r^2)=0 \quad \to \overset{0}{f}{}_{,u}=\overset{0}{\tau}{}_{,u}\frac{a_0\alpha}{K\sin\tau},\\
&(g_{uu},r^2)=0 \quad \to \overset{0}{\tau}{}_{,u}=0=\overset{0}{f}{}_{,u},\\
&(g_{uu},r^1)=0 \quad \to q_{,u}=0,\\
&(g_{\theta\phi},r^2)=0 \quad \to \overset{0}{f}{}_{,\theta}=\overset{0}{\tau}{}_{,\theta}\frac{a_0\alpha}{K\sin\tau},
\end{aligned}
\tag{B1}
$$

$$(g_{\theta\theta},r^2)=-1 \quad \to \overset{0}{\tau}{}_{,\theta}=\pm\frac{\sqrt{K}}{q} \quad \text{(we use the sign +)}, \tag{B2}$$

$$(g_{ur},r^0)=1 \quad \to \overset{0}{\pi}{}_{,u}=\frac{1}{\beta q}, \tag{B3}$$

$$(g_{r\phi},r^0)=0 \quad \to \overset{1}{f}=\frac{a_0\alpha}{q\sin^2\overset{0}{\tau}}\frac{\overset{1}{\tau}q\sin\overset{0}{\tau}+\overset{0}{\pi}\cos\overset{0}{\tau}}{K},$$

$$(g_{r\theta},r^0)=0 \quad \to \overset{1}{\tau}=-\frac{1}{\overset{0}{\tau}{}_{,\theta}q\sin\overset{0}{\tau}}[\overset{0}{\pi}{}_{,\theta}\beta K\sin\overset{0}{\tau}+\overset{0}{\pi}\overset{0}{\tau}{}_{,\theta}\cos\overset{0}{\tau}(1-\beta K)], \tag{B4}$$

$$(g_{r\phi},r^0)=0 \quad \to \overset{1}{f}=\frac{a_0\alpha\beta}{\overset{0}{q}\tau_{,\theta}\sin^2\overset{0}{\tau}}(\overset{0}{\pi}\overset{0}{\tau}{}_{,\theta}\cos\overset{0}{\tau}-\overset{0}{\pi}{}_{,\theta}\sin\overset{0}{\tau}),$$

$$(g_{u\theta},r^1)=0 \quad \to \overset{1}{\tau}{}_{,u}=\frac{1}{\overset{0}{\beta}q^3\overset{0}{\tau}{}_{,\theta}\sin\overset{0}{\tau}}[q_{,\theta}\beta K\sin\overset{0}{\tau}+\overset{0}{\tau}{}_{,\theta}q\cos\overset{0}{\tau}(-1+\beta K)], \tag{B5}$$

$$\begin{aligned}(g_{\theta\theta}g_{\phi\phi},r^3)=0 \quad \to \overset{0}{\sigma}=&\frac{1}{\overset{0}{2}\tau_{,\theta}^3\sin^2\overset{0}{\tau}}\{\overset{0}{\tau}{}_{,\theta}^3(1-2\sin^2\overset{0}{\tau})\overset{0}{\pi}(1-\beta K)+K\sin\overset{0}{\tau}[\beta\overset{0}{\pi}{}_{,\theta}(\overset{0}{\tau}{}_{,\theta}^2\cos\overset{0}{\tau}\\&-\overset{0}{\tau}{}_{,\theta\theta}\sin\overset{0}{\tau})+\overset{0}{\tau}{}_{,\theta}(\beta_{,\theta}(\overset{0}{\pi}{}_{,\theta}\sin\overset{0}{\tau}-\overset{0}{\pi}\overset{0}{\tau}{}_{,\theta}\cos\overset{0}{\tau})+\beta\overset{0}{\pi}{}_{,\theta\theta}\sin\overset{0}{\tau})]\},\end{aligned}$$

$$(g_{\phi\phi},r^2)=-\sin^2\theta \quad \to \sin\overset{0}{\tau}=\pm\frac{\sin\theta}{q\sqrt{K}}, \tag{B6}$$

$$\begin{aligned}&(g_{\phi\phi},r^1)=2c\sin^2\theta\\&\to c=-\frac{1}{2q\sin^2\overset{0}{\tau}(1+a_0^2\alpha^2)}[2\sin\overset{0}{\tau}(1+a_0^2\alpha^2)(\overset{0}{\sigma}\sin\overset{0}{\tau}+\overset{1}{\tau}q\cos\overset{0}{\tau})\\&\quad+\mu_1 q\sin^2\overset{0}{\tau}(-1+a_0^2\alpha^2)+2a_0\alpha^2(a_0\overset{0}{\pi}+a_1 q\sin^2\overset{0}{\tau})]\\&\to c_{,u}=-\frac{a_0\alpha}{K}a_{1,u}+\frac{1-a_0^2\alpha^2}{2(1+a_0^2\alpha^2)}\mu_{1,u}-\frac{q_{,\theta}^2}{2q^2}-\frac{q_{,\theta}\cot\overset{0}{\tau}\sqrt{K}}{q^2}\\&\quad+\frac{1-a_0^2\alpha^2}{2q^2\beta\sin^2\overset{0}{\tau}(1+a_0^2\alpha^2)}-\frac{1}{2}-\frac{K\cot^2\overset{0}{\tau}}{2q^2},\end{aligned} \tag{B7}$$

$$(g_{\theta\phi},r^1)=-2d\sin\theta \quad \rightarrow d=-\frac{1}{2qK\sin^2{}^0\tau}[(1-a_0^2\alpha^2)qa_1\sin^2{}^0\tau+2qa_0\mu_1\sin^2{}^0\tau+2a_0{}^0\pi]$$

$$\rightarrow d_{,u}=-\frac{a_0}{q^2K\beta\sin^2{}^0\tau}-\frac{a_0}{K}\mu_{1,u}-\frac{1-a_0^2\alpha^2}{2K}a_{1,u}. \tag{B8}$$

Equations $(g_{uu},r^0)=1$, $(g_{u\theta},r^2)=0$, $(g_{u\phi},r^1)=0$, $(g_{rr},r^{-1})=0$, $(g_{r\theta},r^1)=0$, $(g_{r\phi},r^1)=0$, and $(g_{\theta\theta},r^1)=-2c$ are satisfied identically.

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The multiple sum formulas for 12*j* coefficients of SU(2) and $u_q(2)$

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The expressions for $12j$ coefficients of the both kinds (without and with braiding) of the SU(2) group and the quantum algebra $u_q(2)$ are considered. Using Dougall's summation formula of the very well-poised hypergeometric ${}_5F_4(1)$ series and its q-generalization, several fourfold sum formulas [with each sum related to the balanced ${}_5F_4(1)$ or ${}_5\phi_4$ series] for the q-$12j$ coefficients of the second kind (without braiding) are derived. Applying q-generalizations of rearrangement formulas of the very well-poised hypergeometric ${}_6F_5(-1)$ series [which correspond to a new expression for the Clebsch–Gordan coefficients of SU(2) and $u_q(2)$], the new expressions with five sums [of the ${}_4F_3(1)$ and ${}_3F_2(1)$ or ${}_4\phi_3$ and ${}_3\phi_2$ type] are derived for the q-$12j$ coefficients of the first kind (with braiding) instead of the usual expansions in terms of q-$6j$ coefficients. Stretched and doubly stretched q-$12j$ coefficients [as triple, double, or single sums, related to composed or separate hypergeometric ${}_4F_3(1)$ and ${}_5F_4(1)$ or ${}_4\phi_3$ and ${}_5\phi_4$ series and, particularly, to q-$9j$ or q-$6j$ coefficients] are considered. © *2002 American Institute of Physics.*
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I. INTRODUCTION AND PRELIMINARIES

The $3nj$ coefficients arise as the recoupling coefficients of several irreducible representations (irreps) of the SU(2) group and play the important role in the quantum mechanical angular momentum theory[1,2] and the Wigner–Racah irreducible tensor calculus, for construction of the complicated matrix elements of the coupled irreducible tensor operators. After the $6j$ (Racah) and $9j$ (Wigner) coefficients (with single and triple sums in expressions, respectively), the $12j$ coefficients of both kinds[1,2] also have many applications as the recoupling coefficients of the five irreps of the SU(2) group.

There are two known types of expressions for $9j$ coefficients: the usual expansion[1,2] of $9j$ coefficients in terms of $6j$ coefficients [including four sums, three in $6j$ coefficients and the last one weighted with factor $(2j+1)$] and the more compact formula, derived originally by Ališauskas and Jucys.[3] Different new expressions (of the second type, i.e., as a triple sum series) for the $9j$ coefficients of the SU(2) group and the quantum algebra $u_q(2)$ were derived recently,[4] generalizing the second Rosengren[5,6] approach to the $9j$ coefficients of the $\mathfrak{su}(1,1)$ algebra, when their expansion in terms of $6j$ coefficients was rearranged using Dougall's summation formula[7] of the very well-poised ${}_4F_3(-1)$ series.

For the quantum algebra $u_q(2)$, the expansion of the q-$9j$ coefficients in terms of q-$6j$ coefficients (Nomura[8–10] and Smirnov *et al.*[11]) was also extended to q-$3nj$ coefficients (particularly, those of the second and the first kinds) by Nomura,[9,10] who discussed their role in frames of the Yang–Baxter relations. The corresponding summation formula of the twisted q-factorial series (generalizing Dougall's summation formula and resembling the very well-poised basic hypergeometric ${}_5\phi_4$ series), depending on three parameters and used in our previous paper,[4] was derived by Ališauskas,[12] when the twisted very well-poised q-factorial series, resembling the basic hypergeometric ${}_7\phi_6$ series (depending on five parameters) appear in a new approach[13] to the Clebsch–Gordan (CG) coefficients of $u_q(2)$. In the $u_q(3)$ context, Ališauskas[12] also used the summation formula of the q-factorial series depending on four parameters which correspond to Dougall's summation formula of the very well-poised hypergeometric ${}_5F_4(1)$ or basic hypergeometric ${}_6\phi_5$ series.[7,14]

The main purpose of the present article is to rearrange expressions for the q-12j and the usual 12j coefficients of both kinds into more convenient forms, with minimal number of sums, or at least without the cumbersome factorial sums weighted with factors $[2j+1]$ or $(2j+1)$, which appear from the compositions of the q-6j or usual 6j coefficients expanded in different forms. We also consider the stretched and doubly stretched 12j and q-12j coefficients, representative for the new types of the higher single and multiple (ordinary and basic) hypergeometric series.

Further in this section, the appropriate expressions for the 6j coefficients of SU(2) and $u_q(2)$ are discussed, which allow one to generalize Rosengren's[6,4] approach. Section II is devoted to rearrangement of the usual expansion formula (in terms of 6j and q-6j coefficients) of 12j and q-12j coefficients of the second kind[1,2,10] (i.e., without braiding[9]) into the fourfold sums, using Dougall's summation formula[7,14] of the very well-poised ${}_5F_4(1)$ and ${}_6\phi_5$ series, depending on four parameters (see Appendix A, where usable Saalschützian and Minton's summation formulas are also presented). Also, specific stretched and doubly stretched 12j and q-12j coefficients of the second kind are studied. As a rule, we present explicitly only those doubly stretched q-12j coefficients, which cannot be derived simply by inserting some fixed values of summation parameters.

In Sec. III, expressions of 12j and q-12j coefficients of the first kind[1,2] (with braiding[10]) in terms of q-6j coefficients are rearranged using the transformation formula[12] of the very well-poised ${}_6F_5(-1)$ series or q-factorial sums (depending on five parameters and weighted with factors $(2j+1)$ or $[2j+1]$), resembling the very well-poised basic hypergeometric ${}_7\phi_6$ series and related to a new expression for the Clebsch–Gordan coefficients of SU(2) and $u_q(2)$ (see Appendix B). Diversity of the stretched and doubly stretched 12j and q-12j coefficients of the first kind are also considered, including the explicit doubly stretched q-12j coefficients, which are proportional to some q-9j and q-6j coefficients.

Here and in what follows $[x]$ and $[x]!$ are, respectively, q-numbers and q-factorials,

$$[x]=(q^x-q^{-x})/(q-q^{-1}),\quad [x]!=[x][x-1]\cdots[2][1],\quad [1]!=[0]!=1, \tag{1.1}$$

which are invariant under substitution $q\to q^{-1}$ and turn into usual integers x and factorials $x!$ for $q=1$.

Only those expressions (see Sec. II of Ref. 4) for the 6j (Racah) coefficients[2,15–17] of SU(2) and $u_q(2)$ are appropriate for our purpose, that include asymmetric triangle coefficients,

$$\nabla[abc]=\left(\frac{[a+b-c]![a-b+c]![a+b+c+1]!}{[b+c-a]!}\right)^{1/2}, \tag{1.2}$$

before the q-factorial sum. They are given by

$$\begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix}_q=\frac{\nabla[acf]\nabla[dbf]}{\nabla[abe]\nabla[dce]}\sum_z \frac{(-1)^{a+b+c+d+z}[c+f-a+z]!}{[z]![a+c-f-z]![b+d-f-z]!}$$
$$\times\frac{[b+f-d+z]![a+d+e-f-z]!}{[e+f-a-d+z]![2f+z+1]!} \tag{1.3a}$$

$$=\frac{\nabla[eab]\nabla[fbd]}{\nabla[ecd]\nabla[fac]}\sum_z \frac{(-1)^{b+c+e+f+z}[2b-z]!}{[z]![b+e-a-z]![b+f-d-z]!}$$
$$\times\frac{[b+e+f-c-z]![b+c+e+f-z+1]!}{[a+b+e-z+1]![b+d+f-z+1]!}, \tag{1.3b}$$

where each parameter $b,c,e,$ or [after some shift of summation parameter, see (2.1b) of Ref. 4] f appears only twice in the factorial arguments under the summation sign in (1.3a), as well as each parameter $a,c,d,$ or [after inversion of summation parameter, see (2.2b) of Ref. 4] b under the summation sign in (1.3b). Hence, the very well-poised series may appear only when the j-type

summation parameters (weighted with factors $[2j+1]$) accept the corresponding position in expansions in terms of q-6j coefficients. Otherwise, the most symmetric (Racah) and the remaining expressions for 6j and q-6j coefficients[1,2,15,16] (which include only usual symmetric triangle coefficients $\Delta[abc]$ in the numerator and denominator before the summation sign, with each parameter appearing four times in the factorial arguments under the summation sign) for this purpose are useless.

It should also be noted that only the expressions presented above (1.3a) and (1.3b) are correlated with the Racah polynomials as introduced by Askey and Wilson,[18,19] (see Ref. 14). In contrast, the most symmetric and the remaining expressions for 6j and q-6j coefficients turn into the Racah polynomials only after some Whipple[20] (Bailey[21]) or Sears[22] transform[14] of the balanced hypergeometric ${}_4F_3(1)$ or ${}_4\phi_3$ series are used.

II. EXPRESSIONS FOR 12j COEFFICIENTS OF THE SECOND KIND OF SU(2) AND $U_q(2)$

A. Generic properties

The 3nj coefficients of the second kind[1,23] ($n\geqslant 4$), whose graphs are planar [hence without braiding,[9,10] in contrast with the 3nj coefficients of the first kind ($n\geqslant 3$), whose graphs are possible only on the Möbius strip] usually are expanded[1,2] in terms of factorized n different 6j coefficients,

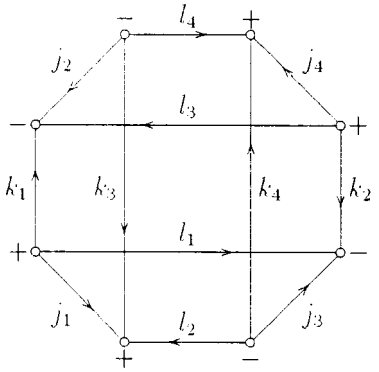
$$\begin{bmatrix} j_1 & & j_2 & & \cdots & & j_n & \\ & l_1 & & l_2 & & \cdots & & l_n \\ k_1 & & k_2 & & \cdots & & k_n & \end{bmatrix} = \sum_x (2x+1)(-1)^{R_n+nx} \begin{Bmatrix} j_1 & k_1 & x \\ k_2 & j_2 & l_1 \end{Bmatrix} \times \begin{Bmatrix} j_2 & k_2 & x \\ k_3 & j_3 & l_2 \end{Bmatrix} \cdots \begin{Bmatrix} j_{n-1} & k_{n-1} & x \\ k_n & j_n & l_{n-1} \end{Bmatrix} \begin{Bmatrix} j_n & k_n & x \\ k_1 & j_1 & l_n \end{Bmatrix}, \tag{2.1}$$

where

$$R_n = \sum_{i=1}^{n} (j_i + k_i + l_i),$$

and the triangular conditions are satisfied by the triplets of the nearest neighbors as l_i, j_i, j_{i+1}, or l_i, k_i, k_{i+1} ($i=1,2,\ldots,n-1$), or l_n, j_n, j_1, or l_i, k_n, k_1, respectively.

The 12j coefficients of the second kind, which may be extracted from the recoupling coefficients of the five irreps without braiding,[9] hence, with the cubic graph[1]



(2.2)

were introduced by Elliott and Flowers[24] and redefined by Vanagas and Čiplys.[25] These $12j$ coefficients and their q-generalizations satisfy 24 symmetries,[1,2,25] generated by the following substitutions:

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{bmatrix}_q = (-1)^{j_1-j_2-j_3+j_4+k_1-k_2-k_3+k_4} \begin{bmatrix} j_1 & & k_1 & & j_2 & & k_3 & \\ & l_1 & & l_3 & & l_4 & & l_2 \\ j_3 & & k_2 & & j_4 & & k_4 & \end{bmatrix}_q \tag{2.3a}$$

$$= \begin{bmatrix} j_4 & j_3 & j_2 & j_1 \\ l_4 & l_3 & l_2 & l_1 \\ k_4 & k_3 & k_2 & k_1 \end{bmatrix}_q = \begin{bmatrix} l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \\ j_1 & j_2 & j_3 & j_4 \end{bmatrix}_q \tag{2.3b}$$

$$= \begin{bmatrix} k_4 & k_2 & k_3 & k_1 \\ l_4 & l_2 & l_3 & l_1 \\ j_4 & j_2 & j_3 & j_1 \end{bmatrix}_q = \begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_2 & l_1 & l_4 & l_3 \\ k_3 & k_4 & k_1 & k_2 \end{bmatrix}_q . \tag{2.3c}$$

Eight triangular conditions may be visualized[2] by means of the extended array

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{bmatrix}$$
$$\begin{matrix} & j_2 & j_3 & \\ & l_2 & l_3 & \end{matrix}$$

and are satisfied by the triplets of parameters in the first and fourth columns, as well as by the skew triplets descending from some parameter of the first or fourth column, e.g., by l_1, k_2, j_3, or by j_4, l_3, k_2.

We restrict ourselves to the following rearrangements of the q-$6j$ coefficients in expressions[1,2,10] for the q-$12j$ coefficients of the second kind:

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{bmatrix}_q = (-1)^{l_1-l_2-l_3+l_4} \sum_x [2x+1] \begin{Bmatrix} k_1 & j_1 & l_1 \\ j_3 & k_2 & x \end{Bmatrix}_q \times \begin{Bmatrix} k_3 & k_4 & x \\ j_3 & j_1 & l_2 \end{Bmatrix}_q \begin{Bmatrix} k_3 & j_2 & l_4 \\ j_4 & k_4 & x \end{Bmatrix}_q \begin{Bmatrix} k_1 & k_2 & x \\ j_4 & j_2 & l_3 \end{Bmatrix}_q \tag{2.4a}$$

$$= (-1)^{l_1-l_2-l_3+l_4} \sum_x [2x+1] \begin{Bmatrix} k_1 & j_1 & l_1 \\ j_3 & k_2 & x \end{Bmatrix}_q \times \begin{Bmatrix} j_3 & x & j_1 \\ k_3 & l_2 & k_4 \end{Bmatrix}_q \begin{Bmatrix} k_3 & k_4 & x \\ j_4 & j_2 & l_4 \end{Bmatrix}_q \begin{Bmatrix} k_1 & x & k_2 \\ j_4 & l_3 & j_2 \end{Bmatrix}_q \tag{2.4b}$$

$$=(-1)^{l_1-l_2-l_3+l_4}\sum_x [2x+1])\begin{Bmatrix} k_1 & j_1 & l_1 \\ j_3 & k_2 & x \end{Bmatrix}_q$$
$$\times\begin{Bmatrix} k_3 & k_4 & x \\ j_3 & j_1 & l_2 \end{Bmatrix}_q\begin{Bmatrix} j_4 & x & j_2 \\ k_3 & l_4 & k_4 \end{Bmatrix}_q\begin{Bmatrix} k_1 & x & k_2 \\ j_4 & l_3 & j_2 \end{Bmatrix}_q \tag{2.4c}$$

$$=(-1)^{l_1-l_2-l_3+l_4}\sum_x [2x+1]\begin{Bmatrix} j_3 & x & j_1 \\ k_1 & l_1 & k_2 \end{Bmatrix}_q$$
$$\times\begin{Bmatrix} k_3 & x & k_4 \\ j_3 & l_2 & j_1 \end{Bmatrix}_q\begin{Bmatrix} j_4 & x & j_2 \\ k_3 & l_4 & k_4 \end{Bmatrix}_q\begin{Bmatrix} l_3 & j_2 & k_1 \\ x & k_2 & j_4 \end{Bmatrix}_q^{(\prime)}. \tag{2.4d}$$

This allows us to cancel the differently distributed asymmetric triangle coefficients depending on the summation parameter x, when all the q-6j coefficients are expressed by means of (1.3a), with exception of the last (primed) q-6j coefficient in (2.4d), in which case (1.3b) should be used. In particular, using expression (1.3a) with shifted summation parameter [see (2.1b) of Ref. 4] for the q-6j coefficients with summation parameter x in the right lower position, then Eq. (1.3a) with inverted summation parameter for the q-6j coefficients with x in the middle column, followed by Eq. (1.3a) in the remaining cases [with exception of the last one in (2.4d)], the summation intervals are ensured, and we may use the summation formula (A1a) for expansion (2.4a) and formula (A1b) (see Ref. 12) for expansions (2.4b)–(2.4d). Again (cf. the rearrangement[4] of expressions for q-6j coefficients) the formal summation intervals may exceed the interval determined by triangular conditions, and we need to consider each case separately. For example, when $\min(j_2+j_4,k_3+k_4)<x\leqslant\min(j_1+j_3,k_1+k_2)$, or $\max(j_1-j_3,k_2-k_1)>x\geqslant\max(|j_2-j_4|,|k_3-k_4|,j_3-j_1,k_1-k_2)$, the definite sum of the type (1.3a) (from two depending on the parameters in the left-hand side of the corresponding inequality) in expansion of (2.4b) turns into 0, in accordance with the q-version[14] of Karlsson's summation formula[26] as presented by Eq. (2.13) of Ref. 4.

B. General expressions with fourfold sums

By carrying out the steps outlined above, we derive four different expressions for the q-12j coefficients of the second kind:

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{bmatrix}_q$$
$$=(-1)^{l_2-l_3+k_1-k_3-j_3+j_4}\frac{\nabla[k_3j_1l_2]\nabla[j_3k_4l_2]\nabla[k_1j_2l_3]\nabla[j_4k_2l_3]}{\nabla[k_1j_1l_1]\nabla[j_3k_2l_1]\nabla[k_3j_2l_4]\nabla[j_4k_4l_4]}$$
$$\times\sum_{z_1,z_2,z_3,z_4}\frac{(-1)^{z_1+z_2+z_3+z_4}[k_2+j_3-l_1+z_1]![k_1+j_1-l_1+z_1]!}{[z_1]![z_2]![z_3]![z_4]![l_1+k_2-j_3-z_1]![j_1+l_1-k_1-z_1]!}$$
$$\times\frac{[2l_1-z_1]![j_1+l_2-k_3+z_2]![l_2-j_3+k_4+z_2]!}{[j_1-l_2+k_3-z_2]![j_3+k_4-l_2-z_2]![2l_2+z_2+1]!}$$
$$\times\frac{[j_4+k_4-l_4+z_3]![j_2+k_3-l_4+z_3]![2l_4-z_3]!}{[k_4+l_4-j_4-z_3]![j_2-k_3+l_4-z_3]![k_1+j_2-l_3-z_4]![2l_3+z_4+1]!}$$
$$\times\frac{[j_2+l_3-k_1+z_4]![k_2+l_3-j_4+z_4]!}{[k_2-l_3+j_4-z_4]![k_1+k_3+j_3+j_4-l_1-l_4+z_1+z_3+1]!}$$

$$\times\frac{[k_1+k_3+j_3+j_4-l_2-l_3-z_2-z_4]!}{[k_1+l_2-l_1-k_3+z_1+z_2]![l_3-l_1+j_3-j_4+z_1+z_4]!}$$

$$\times\frac{[l_2+l_3-l_1-l_4+z_1+z_2+z_3+z_4]!}{[l_2-l_4-j_3+j_4+z_2+z_3]![k_3-k_1+l_3-l_4+z_3+z_4]!} \tag{2.5a}$$

$$=(-1)^{j_1-j_3-k_1+k_2-l_1-l_2-l_3+l_4}\frac{\nabla[j_3k_4l_2]\nabla[k_3j_2l_4]\nabla[k_1j_2l_3]\nabla[j_4k_4l_4]}{\nabla[k_1j_1l_1]\nabla[j_3k_2l_1]\nabla[k_3j_1l_2]\nabla[j_4k_2l_3]}$$

$$\times\sum_{z_1,z_2,z_3,z_4}\frac{(-1)^{z_2+z_3+z_4}[k_2+j_3-l_1+z_1]![k_1+j_1-l_1+z_1]!}{[z_1]![z_2]![z_3]![z_4]![l_1+k_2-j_3-z_1]![j_1+l_1-k_1-z_1]!}$$

$$\times\frac{[2l_1-z_1]![2l_2-z_2]![j_1-l_2+k_3+z_2]!}{[l_2+j_3-k_4-z_2]![j_1+l_2-k_3-z_2]![l_2+j_3+k_4-z_2+1]!}$$

$$\times\frac{[j_2-k_3+l_4+z_3]![k_4+l_4-j_4+z_3]!}{[j_4+k_4-l_4-z_3]![j_2+k_3-l_4-z_3]![2l_4+z_3+1]![k_1-j_2+l_3-z_4]!}$$

$$\times\frac{[2l_3-z_4]![k_2-l_3+j_4+z_4]!}{[k_2+l_3-j_4-z_4]![k_1+j_2+l_3-z_4+1]![k_1+k_3-l_1-l_2+z_1+z_2]!}$$

$$\times\frac{[j_3+j_4+l_2-l_4-z_2-z_3]![k_1+k_3+l_3-l_4-z_3-z_4]!}{[k_1-k_3+j_3-j_4-l_1+l_4+z_1+z_3]![j_3+j_4-l_1-l_3+z_1+z_4]!}$$

$$\times\frac{[j_3-j_4+k_1-k_3+l_2+l_3-z_2-z_4]!}{[l_1+l_2+l_3-l_4-z_1-z_2-z_3-z_4]!} \tag{2.5b}$$

$$=(-1)^{k_1-k_2+l_1-l_2+l_3+l_4-j_2+j_4}\frac{\nabla[k_3j_1l_2]\nabla[j_3k_4l_2]\nabla[j_4k_4l_4]\nabla[k_1j_2l_3]}{\nabla[k_1j_1l_1]\nabla[j_3k_2l_1]\nabla[k_3j_2l_4]\nabla[j_4k_2l_3]}$$

$$\times\sum_{z_1,z_2,z_3,z_4}\frac{(-1)^{z_2+z_3+z_4}[j_3+k_2-l_1+z_1]![j_1+k_1-l_1+z_1]!}{[z_1]![z_2]![z_3]![z_4]![l_1+k_2-j_3-z_1]![j_1-k_1+l_1-z_1]!}$$

$$\times\frac{[2l_1-z_1]![j_1+l_2-k_3+z_2]![l_2-j_3+k_4+z_2]!}{[j_1-l_2+k_3-z_2]![j_3+k_4-l_2-z_2]![2l_2+z_2+1]![j_4-k_4+l_4-z_3]!}$$

$$\times\frac{[2l_4-z_3]![j_2-l_4+k_3+z_3]!}{[j_2-k_3+l_4-z_3]![j_4+k_4+l_4-z_3+1]![k_1-j_2+l_3-z_4]!}$$

$$\times\frac{[2l_3-z_4]![k_2-l_3+j_4+z_4]!}{[k_2+l_3-j_4-z_4]![k_1+j_2+l_3-z_4+1]![k_1-k_3-l_1+l_2+z_1+z_2]!}$$

$$\times\frac{[j_3+j_4-l_2+l_4-z_2-z_3]![j_3-j_4+k_1+k_3-l_2+l_3-z_2-z_4]!}{[j_3-j_4+k_1+k_3-l_1-l_4+z_1+z_3]![j_3+j_4-l_1-l_3+z_1+z_4]!}$$

$$\times\frac{[k_1-k_3+l_3+l_4-z_3-z_4]!}{[l_1-l_2+l_3+l_4-z_1-z_2-z_3-z_4]!} \tag{2.5c}$$

$$=(-1)^{k_3+k_4-l_1+l_2+l_3-l_4-j_1-j_3}\frac{\nabla[j_3k_2l_1]\nabla[k_3j_1l_2]\nabla[j_4k_4l_4]\nabla[k_1j_2l_3]}{\nabla[k_1j_1l_1]\nabla[j_3k_4l_2]\nabla[k_3j_2l_4]\nabla[j_4k_2l_3]}$$

$$\times\sum_{z_1,z_2,z_3,z_4}\frac{(-1)^{z_1+z_2+z_3}[2l_1-z_1]![j_1+k_1-l_1+z_1]!}{[z_1]![l_1-k_2+j_3-z_1]![j_1-k_1+l_1-z_1]![l_1+k_2+j_3-z_1+1]!}$$

$$\times\frac{[2l_2-z_2]![k_4+j_3-l_2+z_2]!}{[z_2]![k_3+l_2-j_1-z_2]![l_2-j_3+k_4-z_2]![j_1+l_2+k_3-z_2+1]!}$$

$$\times\frac{[2l_4-z_3]![j_2+k_3-l_4+z_3]!}{[z_3]![z_4]![j_4+l_4-k_4-z_3]![j_2-k_3+l_4-z_3]![j_4+k_4+l_4-z_3+1]!}$$
$$\times\frac{[2j_2-z_4]![j_2+j_4+k_1-k_2-z_4]![j_2+j_4+k_1+k_2-z_4+1]!}{[k_1+j_2-l_3-z_4]![k_1+j_2+l_3-z_4+1]![j_2+k_3-l_4+z_3-z_4]!}$$
$$\times\frac{[l_1+l_2-k_1+k_3-z_1-z_2]![j_3+j_4-k_3-k_1+l_1+l_4-z_1-z_3]!}{[j_2-j_3+j_4+k_1-l_1+z_1-z_4]![j_2+j_3+j_4-k_3-l_2+z_2-z_4]!}$$
$$\times\frac{[l_2+l_4-j_3+j_4-z_2-z_3]!}{[l_1+l_2+l_4-k_1-j_2-z_1-z_2-z_3+z_4]!}. \tag{2.5d}$$

The numerator–denominator distribution of factorials, depending on the summation parameters z_1,z_2,z_3,z_4, is different in each expression (2.5a)–(2.5d). No single formula exhibites the full symmetry (2.3b)–(2.3c) of the q-12j-symbol, but (2.5a) is invariant with respect to the transition from the main notation to the left array of (2.3c), as well as under transposition

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{bmatrix}_q = \begin{bmatrix} k_2 & k_4 & k_1 & k_3 \\ l_1 & l_3 & l_2 & l_4 \\ j_3 & j_1 & j_4 & j_2 \end{bmatrix}_q, \tag{2.6}$$

which, in turn, is a composition of symmetry relations (2.3b)–(2.3c). Expression (2.5b) is invariant with respect to the same symmetry (2.6), but (2.5c) and (2.5d) do not satisfy any symmetry relations. Since all the sums in these expressions correspond to the balanced hypergeometric functions, the q-phases are also trivial.[9]

All the terms in the first sum of (2.5b) and (2.5c) are of the same sign, as well as in the last sum of (2.5d). Each separate sum corresponds in these expressions to the finite balanced basic hypergeometric series ${}_5F_4[q,1]$ as defined by Eq. (3.2) of Ref. 4, which also appeared in the elementary overlap coefficients of the definite biorthogonal coupled states[12] of $u_q(3)$ and SU(3). The summation intervals are mainly restricted by eight [in (2.5a)–(2.5c)], or seven [in (2.5d)] triangle linear combinations of parameters, respectively. In addition to the correspondence of numerator and denominator factorials, determined by Eq. (A1a) or (A1b), definite correlation between the factorials under summation signs reveals itself in four quintuplets of factorials of each expression (2.5a)–(2.5d), depending on the couples of adjacent summation parameters (z_i and z_{i+1}, where $i=1,2,3$, or z_1 and z_4), although their expansion using the Chu–Vandermonde formulas (cf. Sec. IV of Ref. 4) is not helpful for further rearrangement of the generic expressions.

C. Stretched cases of the q-12j coefficients of the second kind

Let us consider the stretched cases of q-12j coefficients. For definite stretched triangles some summation parameters in (2.5a)–(2.5d) are either fixed (31 times), or expressions are partially summable (in the 11 cases) by means of Minton's summation formulas (A3a) or (A3b) (see Ref. 14). One of three remaining sums turns into the balanced basic hypergeometric series ${}_4F_3[q,1]$, the rearrangement[14] of which enables us to transform a ${}_5F_4[q,1]$ type series into a ${}_4F_3[q,1]$ type series, with only the last one remaining of the ${}_5F_4[q,1]$ type. Particularly, for $j_1+l_1=k_1$ with $z_1=0$, the sum over z_2 in expression (2.5a) corresponds to a q-6j coefficient, which may be reexpressed in such a form (using Regge symmetry and change of the summation parameter) that the sum over z_3 also corresponds to a q-6j coefficient. Hence, we obtain

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ j_1+l_1 & k_2 & k_3 & k_4 \end{bmatrix}_q$$
$$= \frac{(-1)^{j_1+l_2-k_3}\nabla[k_1 j_2 l_3]\nabla[j_4 k_2 l_3]}{\nabla[j_1 l_2 k_3]\nabla[k_4 j_3 l_2]\nabla[k_3 j_2 l_4]\nabla[j_4 k_4 l_4]\nabla[l_1 k_2 j_3]}\left(\frac{[2l_1]![2j_1]!}{[2k_1+1]!}\right)^{1/2}$$
$$\times \sum_{z_1,z_3,z_4} \frac{(-1)^{z_1+z_3}[l_2-j_3+k_4+z_1]![j_1+j_3+k_3-k_4-z_1]!}{[z_1]![z_3]![z_4]![l_2+j_3-k_4-z_1]![j_3-j_4-l_1+l_3+z_4-z_1]!}$$
$$\times \frac{[2j_3-z_1]![j_4+k_4-l_4+z_3]![j_2+k_3-l_4+z_3]![2l_4-z_3]!}{[j_2-k_3+l_4-z_3]![k_3+j_1+j_3+j_4-l_4-z_1+z_3+1]!}$$
$$\times \frac{[j_2+l_3-k_1+z_4]![k_2+l_3-j_4+z_4]!}{[k_4+l_1-l_3+l_4-j_3+z_1-z_3-z_4]![k_3-k_1+l_3-l_4+z_3+z_4]!}$$
$$\times \frac{[k_1+k_3+k_4+j_4-l_3-z_4+1]!}{[k_1+j_2-l_3-z_4]![k_2-l_3+j_4-z_4]![2l_3+z_4+1]!}, \tag{2.7}$$

which is the composition of two balanced ${}_4F_3[q,1]$ series and the third balanced ${}_5F_4[q,1]$ series.

After the summation over z_3 of the balanced ${}_3F_2[q,1]$ series is carried out [see Eqs. (A2a) and (A2b)] in this doubly stretched case of q-12j coefficient with $k_1=j_1+l_1$ and $l_3=k_1+j_2$ [i.e., for adjacent consecutive stretched triangles in graph (2.2)], we recognize some q-6j coefficients, which may also be obtained using the symmetries (2.3b)–(2.3c) and the defining relations (2.4a)–(2.4d) of the q-12j coefficients. In this way, we derive the following relation:

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & k_1+j_2 & l_4 \\ j_1+l_1 & k_2 & k_3 & k_4 \end{bmatrix}_q = \frac{(-1)^{j_1+l_2-k_3+j_4+k_4+l_4}\nabla[l_3 j_4 k_2]\nabla[j_1+j_2,l_2,l_4]}{\nabla[j_1 l_2 k_3]\nabla[j_2 k_3 l_4]\nabla[l_1 k_2 j_3]\nabla[j_1+j_2,j_3,j_4]}$$
$$\times \left(\frac{[2l_1]![2j_1]![2j_2]!}{[2k_1+1][2l_3+1]!}\right)^{1/2} \begin{Bmatrix} j_1+j_2 & l_4 & l_2 \\ k_4 & j_3 & j_4 \end{Bmatrix}. \tag{2.8}$$

In the doubly stretched case of the q-12j coefficient for $j_1=k_1-l_1=l_2-k_3$ [i.e., when the adjacent stretched triangles in graph (2.2) are diverging], we obtain from Eq. (2.5a) or (2.5c), and from Eq. (2.5b) with fixed $z_1=z_2=0$, two different double sum expressions, each depending on ten parameters and corresponding to the q-generalizations of the Kampé de Fériet[27] function $F_{1:3}^{1:4}$, as defined by Eq. (4.6) of Ref. 4. Each separate sum corresponds to the balanced basic hypergeometric ${}_5F_4[q,1]$ series. Again, we may identify the couples of quintuplets of factorials under summation signs in the numerator and denominator, each depending on the summation parameters z_3 and z_4.

Otherwise, in the case of the merging adjacent stretched triangles (e.g., for $k_1=j_1+l_1=j_2+l_3$), the straightforwardly derived expressions include the triple sums; in particular all three sums in (2.8) correspond to the balanced basic hypergeometric ${}_4F_3[q,1]$ series. The ${}_4F_3[q,1]$ type sum over z_4 may be rearranged in analogy with expressions for the q-6j coefficients[2,16] into another form (cf. Ref. 14) in a such way that the sum over z_3 turns into summable balanced basic hypergeometric ${}_3F_2[q,1]$ series. Hence, we obtain the doubly stretched q-12j coefficient in terms of the double sum,

$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & k_1-j_2 & l_4 \\ j_1+l_1 & k_2 & k_3 & k_4 \end{bmatrix}_q$$

$$= \frac{(-1)^{j_1+l_2-k_3}([2l_1]![2j_1]![2j_2]![2l_3]!)^{1/2}\nabla[k_4l_4j_4]}{\nabla[l_3k_2j_4]\nabla[j_1l_2k_3]\nabla[k_4j_3l_2]\nabla[j_2k_3l_4]\nabla[l_1k_2j_3]}$$

$$\times\sum_{z,u}\frac{[l_2-j_3+k_4+z]![l_1+k_2-j_3+z]![j_1+j_3+k_3-k_4-z]!}{[z]![l_2+j_3-k_4-z]![k_2-l_1+j_3-z]![k_3+k_4-j_1-j_3+z]!}$$

$$\times\frac{[2j_3-z]!(-1)^{z+u}[j_4-k_4+l_4+u]![j_4+l_3-k_2+u]!}{[u]![k_4-j_4+l_4-u]![k_3-k_4-j_2+j_4+u]![2j_4+u+1]!}$$

$$\times\frac{[k_3+k_4+j_2-j_4-u]![k_2+l_3+j_4+u+1]!}{[j_1+j_2+j_3-j_4-z-u]![l_1+l_3-j_3+j_4+z+u+1]!}, \tag{2.9}$$

which again depends on ten parameters and corresponds to the q-generalization of the Kampé de Fériet[27] function $F^{1:4}_{1:3}$, with each separate sum corresponding to the balanced basic hypergeometric ${}_5F_4[q,1]$ series. Perhaps this expression is related to the above mentioned special case of (2.5a) with fixed $z_1=z_2=0$ and the adjacent diverging stretched triangles of q-12j coefficient with respect to some composition of the usual and "mirror reflection" ($j\to -j-1$) symmetries.[2]

In the doubly stretched case of the q-12j coefficient with $k_1=j_1+l_1$ and $j_4=k_4+l_4$ [i.e., for antipode stretched triangles of graph (2.2)], we derive from Eq. (2.7), with fixed $z_3=0$ and $z_4=l_1-l_3-j_3+j_4+z_1$, an expression with a single sum, which corresponds to the balanced basic hypergeometric ${}_6F_5[q,1]$ series and depends on ten parameters:

$$\begin{bmatrix} j_1 & j_2 & j_3 & l_4+k_4 \\ l_1 & l_2 & l_3 & l_4 \\ j_1+l_1 & k_2 & k_3 & k_4 \end{bmatrix}_q = \frac{(-1)^{j_1+l_2-k_3}\nabla[k_1j_2l_3]\nabla[j_4k_2l_3]}{\nabla[j_1l_2k_3]\nabla[k_4j_3l_2]\nabla[l_4k_3j_2]\nabla[l_1k_2j_3]}$$

$$\times\left(\frac{[2l_1]![2j_1]![2l_4]![2k_4]!}{[2k_1+1]![2j_4+1]!}\right)^{1/2}$$

$$\times\sum_{z_1}\frac{(-1)^{z_1}[l_2-j_3+k_4+z_1]![j_4-j_3+j_2-j_1+z_1]!}{[z_1]![l_2+j_3-k_4-z_1]![j_1+j_2+j_3-j_4-z_1]!}$$

$$\times\frac{[l_1+k_2-j_3+z_1]![2j_3-z_1]!}{[k_2+j_3-l_1-z_1]![k_3+k_4-j_1-j_3+z_1]!}$$

$$\times\frac{[j_1+j_3+k_3-k_4-z_1]!}{[l_1-l_3-j_3+j_4+z_1]![l_1+l_3-j_3+j_4+z_1+1]!}. \tag{2.10}$$

In the doubly stretched case with $k_1=j_1+l_1$ and $k_4=j_4+l_4$ (again for antipode stretched triangles) from (2.5c), after the summation over z_2 of the balanced ${}_3F_2[q,1]$ series (see Appendix A), we obtain

$$\left[\begin{array}{cccc} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ j_1+l_1 & k_2 & k_3 & j_4+l_4 \end{array}\right]_q = \frac{(-1)^{l_1-l_2-k_2+k_4}\nabla[k_1j_2l_3]\nabla[k_4j_3l_2]}{\nabla[j_1l_2k_3]\nabla[l_4k_3j_2]\nabla[j_4l_3k_2]\nabla[l_1k_2j_3]}$$

$$\times\left(\frac{[2l_1]![2j_1]![2l_4]![2j_4]!}{[2k_1+1]![2k_4+1]!}\right)^{1/2}$$

$$\times\sum_{z_4}\frac{(-1)^{z_4}[j_2+l_3-k_1+z_4]![k_1+k_2-j_2+j_4-z_4]!}{[z_4]![k_1-j_2+l_3-z_4]![k_2+j_2-k_1-j_4+z_4]!}$$

$$\times\frac{[l_4-k_3+j_2+z_4]![j_3-j_4+j_2-j_1+z_4]!}{[j_1-j_2+j_3+j_4-z_4]![l_4-l_2-j_1+j_2+z_4]!}$$

$$\times\frac{[j_2+k_3+l_4+z_4+1]!}{[2j_2+z_4+1]![l_2+l_4-j_1+j_2+z_4+1]!}. \tag{2.11}$$

Again the summation corresponds to the balanced ${}_6F_5[q,1]$ series and depends on ten parameters. Both expressions (2.10) and (2.11) satisfy some Regge type symmetry relations.

Consider also the doubly stretched cases of q-12j coefficients, the case of the remote stretched triangles of graph (2.2) with touching angular momenta forming four-cycles (quadrangles). There are four possible different distributions of the total (maximal) angular momenta of the stretched triangles: both these momenta may be in the same four-cycle, either (a) adjacent, (b) antiparallel, (c) the first angular momentum may be inside and the second one outside of the four-cycle, or (d) both these momenta may be outside of the four-cycle. For q-12j coefficients of the ''adjacent'' (a) type, e.g., with $k_1=j_1+l_1$ and $l_3=k_2+j_4$, we derive from Eq. (2.7) the relation

$$\left[\begin{array}{cccc} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & k_2+j_4 & l_4 \\ j_1+l_1 & k_2 & k_3 & k_4 \end{array}\right]_q = \frac{(-1)^{j_1+l_2-k_3}\nabla[l_3j_2k_1]}{\nabla[j_1l_2k_3]\nabla[k_4j_3l_2]\nabla[k_3j_2l_4]\nabla[j_4k_4l_4]\nabla[l_1k_2j_3]}$$

$$\times\left(\frac{[2l_1]![2j_1]![2k_2]![2j_4]!}{[2k_1+1]![2l_3+1]!}\right)^{1/2}$$

$$\times\sum_{z_1,z_3}\frac{(-1)^{z_1+z_3}[l_2-j_3+k_4+z_1]![j_1+j_3+k_3-k_4-z_1]!}{[z_1]![l_2+j_3-k_4-z_1]![j_3+k_2-l_1-z_1]!}$$

$$\times\frac{[2j_3-z_1]![2l_4-z_3]![j_4+k_4-l_4+z_3]!}{[z_3]![j_2-k_3+l_4-z_3]![k_4+l_1-l_3+l_4-j_3+z_1-z_3]!}$$

$$\times\frac{[j_2+k_3-l_4+z_3]!}{[k_3-k_1+l_3-l_4+z_3]![k_3+j_1+j_3+j_4-l_4-z_1+z_3+1]!}. \tag{2.12}$$

The double sum depends on nine (from ten free) parameters and corresponds to the q-generalization of the Kampé de Fériet[27] function $F^{1:3}_{1:2}$, again defined by Eq. (4.6) of Ref. 4 with $b_1+b_1'=c_1$, and each separate sum corresponding to the balanced ${}_4F_3[q,1]$ or ${}_4\phi_3$ series. Different (i.e., not equivalent) expressions of the (a) type appear also for $k_3=j_1+l_2$ and $j_2=k_1$

$+l_3$ from Eq. (2.5b) and for $j_3=l_1+k_2$ and $k_4=j_4+l_4$ from Eq. (2.5c). Furthermore, the doubly stretched q-12j coefficients of the "antiparallel" (b) type, with $k_1=j_1+l_1$ and $k_3=j_2+l_4$, expressions (2.5a), (2.5c), and (2.5d) (with fixed parameters z_1 and z_3) also turn into (mutually different) double sums again depending on nine (from ten free) parameters and related to the $F_{1:2}^{1:3}$ type functions. This is also the case for expression (2.5b) (with fixed $z_1=z_3=0$) for the doubly stretched q-12j coefficients of the "inside–outside" (c) type, with $k_1=j_1+l_1$ and $l_4=j_2+k_3$ [or, expression (2.5c) with $l_2=j_1+k_3$ and $j_2=k_1+l_3$]. Finally, expression (2.5a) with fixed $z_2=z_4=0$ and $l_2=j_1+k_3$ and $l_3=k_1+j_2$ again turns into the double sums depending on nine (from ten free) parameters and related to the $F_{1:2}^{1:3}$ type function for the doubly stretched q-12j coefficients with the both total angular momenta of the "outside" (d) type. These eight independent expressions should be related to (2.12) by means of some compositions of the usual and "mirror reflection" ($j\rightarrow -j-1$) symmetries.[2] Otherwise, many special versions of (2.5a)–(2.5d) with fixed $z_i=z_{i+1}=0$ ($i=1,2,3$) or $z_1=z_4=0$ give expressions for the doubly stretched q-12j coefficients with remote stretched triangles in terms of the double sums, related to compositions of the balanced ${}_4F_3[q,1]$ and ${}_5F_4[q,1]$ series.

Equation (2.5b) also turns into a single term for $l_1+l_2+l_3-l_4=0$ (when the all summation parameters z_i are fixed),

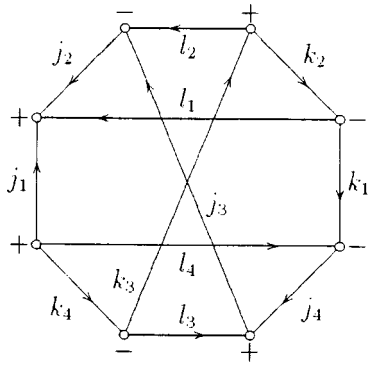
$$\begin{bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_1+l_2+l_3 \\ k_1 & k_2 & k_3 & k_4 \end{bmatrix}_q = \frac{(-1)^{j_1-j_3-k_1+k_2}[2l_1]![2l_2]![2l_3]!\nabla[l_4k_3j_2]\nabla[l_4j_4k_4]}{[2l_4+1]!\nabla[l_1j_1k_1]\nabla[l_1k_2j_3]\nabla[l_2j_1k_3]\nabla[l_2j_3k_4]\nabla[l_3j_2k_1]\nabla[l_3k_2j_4]}. \tag{2.13}$$

For this special q-12j coefficient [as well as in (2.5c) for $l_1-l_2+l_3+l_4=0$ and in (2.5d) for $l_1+l_2-l_3+l_4=0$], four linearly dependent angular momenta appear as disconnected in certain positions on a Hamilton line of graph (2.2). Actually, the single term expression of this virtually stretched case appears in accordance with symmetries (2.3b)–(2.3c) from expansion (2.4a) with $j_1+j_2-j_3+j_4=0$ and fixed $x=j_3-j_1=j_2+j_4$.

III. EXPRESSIONS FOR 12j COEFFICIENTS OF THE FIRST KIND

A. Generic properties

Next, we consider the rearrangement of expressions for the q-12j coefficients of the first kind[1,2,28,29] whose graphs are not planar:



(3.1)

(include some braiding[10]). These coefficients satisfy 16 symmetries, generated by the following substitutions:

$$\begin{Bmatrix} j_1 & j_2 & j_3 & j_4 \\ & l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{Bmatrix}_q = \begin{Bmatrix} j_2 & j_3 & j_4 & k_1 \\ & l_2 & l_3 & l_4 & l_1 \\ k_2 & k_3 & k_4 & j_1 \end{Bmatrix}_q \tag{3.2a}$$

$$= \begin{Bmatrix} k_1 & j_4 & j_3 & j_2 \\ & l_4 & l_3 & l_2 & l_1 \\ j_1 & k_4 & k_3 & k_2 \end{Bmatrix}_q . \tag{3.2b}$$

There expression[1,2,10] in terms of the factorized four differently rearranged q-6j coefficients is

$$\begin{Bmatrix} j_1 & j_2 & j_3 & j_4 \\ & l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{Bmatrix}_q$$

$$= \sum_x (2x+1)(-1)^{R_4-x} q^{x(x+1)+Z_{j_1j_2j_3j_4}+Z_{k_1k_2k_3k_4}} \times \begin{Bmatrix} j_1 & j_2 & l_1 \\ k_2 & k_1 & x \end{Bmatrix}_q \begin{Bmatrix} j_3 & k_3 & x \\ k_2 & j_2 & l_2 \end{Bmatrix}_q \begin{Bmatrix} j_3 & j_4 & l_3 \\ k_4 & k_3 & x \end{Bmatrix}_q \begin{Bmatrix} k_1 & j_1 & x \\ k_4 & j_4 & l_4 \end{Bmatrix}_q \tag{3.3a}$$

$$= \sum_x (2x+1)(-1)^{R_4-x} q^{x(x+1)+Z_{j_1j_2j_3j_4}+Z_{k_1k_2k_3k_4}} \times \begin{Bmatrix} j_1 & j_2 & l_1 \\ k_2 & k_1 & x \end{Bmatrix}_q \begin{Bmatrix} k_2 & x & j_2 \\ j_3 & l_2 & k_3 \end{Bmatrix}_q \begin{Bmatrix} j_3 & k_3 & x \\ k_4 & j_4 & l_3 \end{Bmatrix}_q \begin{Bmatrix} k_1 & x & j_1 \\ k_4 & l_4 & j_4 \end{Bmatrix}_q , \tag{3.3b}$$

where

$$Z_{abcd} = -a(a+1)-b(b+1)-c(c+1)-d(d+1),$$

and the triangular conditions are to be satisfied by all the triplets of the nearest neighbors such as l_i, j_i, j_{i+1}, or l_i, k_i, k_{i+1} $(i=1,2,3)$, or l_4, j_1, k_4, or l_4, k_1, j_4, respectively.

Again, after using expression (1.3a) with shifted summation parameter [see Eq. (2.1b) of Ref. 4] for the q-6j coefficients with summation parameter x in the right lower position, Eq. (1.3a) with inverted summation parameter for q-6j coefficients with x in the middle column, and (1.3a) directly in the remaining cases, the differently distributed asymmetric triangle coefficients (depending on the summation parameter x) cancel in the numerators or denominators of the q-6j coefficients in expansions (3.3a) and (3.3b), with the exception of the factors

$$\frac{\nabla[j_1k_1x]}{\nabla[k_1j_1x]} = \frac{[j_1-k_1+x]!}{[k_1-j_1+x]!}.$$

Then, the sums over x correspond to the q-generalization of the very well-poised classical hypergeometric ${}_6F_5(-1)$ series (resembling the basic hypergeometric ${}_7\phi_6$ series) and may be rearranged into the ${}_3\phi_2$ or ${}_3F_2[q,x]$ type series using the following two formulas:

$$\sum_j \frac{(-1)^{p_2+j+1}q^{j(j+1)}[2j+1][j-p_1-1]![j-p_2-1]![j-p_3-1]!}{[p_1+j+1]![p_2+j+1]![p_3+j+1]![p_4-j]![p_4+j+1]![p_5-j]![p_5+j+1]!}$$

$$=\frac{q^{-(p_4+1)(p_5+1)-p_2(p_4+p_5+1)}[-p_1-p_3-2]!}{[p_1+p_4+1]![p_2+p_5+1]![p_3+p_4+1]!}$$

$$\times\sum_u \frac{(-1)^u q^{u(p_2+p_5+1)}[p_4-p_3-1-u]![p_4-p_1-1-u]!}{[u]![-p_1-p_3-2-u]![p_2+p_4+1-u]![p_4+p_5+1-u]!} \tag{3.4a}$$

with parameters

$$p_1=k_1-j_1-1,\quad p_4=j_1+k_2-l_1+z_1,\quad p_5=j_3+k_4-l_3+z_3,$$

$$p_2=l_2-k_2-j_3+z_2-1,\quad p_3=l_4-k_1-k_4+z_4-1;$$

$$\sum_j \frac{q^{j(j+1)}[2j+1][j-p_1-1]![j-p_2-1]![j-p_3-1]![j-p_5-1]!}{[p_1+j+1]![p_2+j+1]![p_3+j+1]![p_4-j]![p_4+j+1]![p_5+j+1]!}$$

$$=q^{-(p_4+1)(p_5+1)-p_2(p_4+p_5+1)}\frac{[-p_1-p_3-2]![-p_2-p_5-2]!}{[p_1+p_4+1]![p_3+p_4+1]!}$$

$$\times\sum_u \frac{(-1)^u q^{u(p_2+p_5+1)}[p_4-p_3-1-u]![p_4-p_1-1-u]!}{[u]![p_4+p_5+1-u]![p_2+p_4+1-u]![-p_1-p_3-2-u]!} \tag{3.4b}$$

with parameters

$$p_1=k_1-j_1-1,\quad p_2=j_3-k_3-z_2-1,\quad p_3=j_1-k_1-z_4-1,$$

$$p_4=j_1+k_2-l_1+z_1,\quad p_5=l_3-j_3-k_4+z_3-1.$$

Equation (3.4a) may be derived by comparing alternative expressions for the Clebsch–Gordan coefficients of $u_q(2)$ (see Appendix B) and corresponds to Eq. (5.5) [or (5.6), when $q=1$] of Ref. 12, with the right-hand side of (5.5) replaced by the less symmetric (Bandzaitis–Jucys) expression[2,17,30] for the Clebsch–Gordan coefficients of SU(2) and $u_q(2)$, instead of the most symmetric (Van der Waerden) expression[1,2,8,17,31,32] (cf. also Refs. 13 and 33). Relation (3.4b) is derived from (3.4a) using the analytical continuation technique. Summation formulas (A1) and (A2) of Ref. 4 (each depending on three parameters) may be obtained after canceling some factorials in the numerators and denominators of (3.4a) and (3.4b), respectively, for $p_3=-p_1-2$.

B. General expressions with five sums

Substituting the summation parameter u, which appeared after using (3.4a) and (3.4b) in (3.3a) and (3.3b), by $u+z_1$, we obtain the following expressions for the q-12j coefficients of the first kind:

$$
\begin{Bmatrix} j_1 & j_2 & j_3 & j_4 \\ l_1 & l_2 & l_3 & l_4 \\ k_1 & k_2 & k_3 & k_4 \end{Bmatrix}_q
$$

$$
\begin{aligned}
&=(-1)^{k_1+k_2-k_3-j_2+j_3+j_4-l_4}\,\frac{\nabla[j_3j_2l_2]\nabla[k_2k_3l_2]\nabla[k_1j_4l_4]\nabla[k_4j_1l_4]}{\nabla[j_1j_2l_1]\nabla[k_2k_1l_1]\nabla[j_3j_4l_3]\nabla[k_4k_3l_3]}\\
&\quad\times q^{-(j_1+k_2-l_1+1)(k_4-l_3+l_2-k_2)-(l_2-k_2-j_3-1)(j_3+k_4-l_3)+Z_{j_1j_2j_3j_4}+Z_{k_1k_2k_3k_4}}\\
&\quad\times\sum_{z_1,z_2,z_3,z_4,u}\frac{(-1)^{z_3+z_4+u}[j_1+j_2-l_1+z_1]![2l_1-z_1]!}{[z_1]![z_2]![z_3]![z_4]![k_1-k_2+l_1-z_1]![l_1-j_1+j_2-z_1]!}\\
&\quad\times\frac{q^{-z_2(j_1+j_3+k_2+k_4-l_1-l_3+z_3+1)}[l_2+j_2-j_3+z_2]![l_2+k_3-k_2+z_2]!}{[j_2+j_3-l_2-z_2]![k_2+k_3-l_2-z_2]![2l_2+z_2+1]![2l_4+z_4+1]!}\\
&\quad\times\frac{[k_3+k_4-l_3+z_3]![j_3+j_4-l_3+z_3]![2l_3-z_3]!}{[k_3+l_3-k_4-z_3]![l_3-j_3+j_4-z_3]![k_1+j_4-l_4-z_4]!}\\
&\quad\times\frac{q^{z_3(l_1-l_2-j_1+j_3)}[j_4+l_4-k_1+z_4]![j_1+l_4-k_4+z_4]!}{[l_2-l_3-k_2+k_4+z_2+z_3]![j_1-k_1+k_2-k_4-l_1+l_4+z_1+z_4]!}\\
&\quad\times\frac{q^{u(k_4-k_2-l_3+l_2+z_2+z_3)}[j_1+k_1+k_2+k_4-l_1-l_4-z_4-u]!}{[u+z_1]![j_1+k_4-l_4-z_1-z_4-u]![j_1-j_3-l_1+l_2+z_2-u]!}\\
&\quad\times\frac{[2j_1-k_1+k_2-l_1-u]!}{[j_1+j_3+k_2+k_4-l_1-l_3+z_3-u+1]!}
\end{aligned}
\tag{3.5a}
$$

$$
\begin{aligned}
&=(-1)^{j_1+j_3+j_4+k_2-k_3-k_4+l_2-l_3+l_4}\frac{\nabla[j_3j_4l_3]\nabla[k_4k_3l_3]\nabla[k_2k_3l_2]\nabla[k_1j_4l_4]}{\nabla[j_1j_2l_1]\nabla[k_2k_1l_1]\nabla[j_3j_2l_2]\nabla[k_4j_1l_4]}\\
&\quad\times q^{(j_1+k_2-l_1+1)(l_2+k_2-l_3+k_4+1)-(l_2+k_2-j_3+1)(j_3+k_4-l_3+1)+Z_{j_1j_2j_3j_4}+Z_{k_1k_2k_3k_4}}\\
&\quad\times\sum_{z_1,z_2,z_3,z_4,u}\frac{(-1)^{z_2+z_3+z_4+u}[j_1+j_2-l_1+z_1]![2l_1-z_1]!}{[z_1]![z_2]![z_3]![k_1-k_2+l_1-z_1]![l_1-j_1+j_2-z_1]!}\\
&\quad\times\frac{q^{-z_2(j_1-j_3+k_2-k_4-l_1+l_3+z_3)}[j_2+j_3-l_2+z_2]![2l_2-z_2]!}{[l_2+k_2-k_3-z_2]![j_2-j_3+l_2-z_2]![l_2+k_2+k_3-z_2+1]!}\\
&\quad\times\frac{q^{-z_3(j_1+j_3-l_1-l_2)}[k_3-k_4+l_3+z_3]![j_4-j_3+l_3+z_3]!}{[k_3+k_4-l_3-z_3]![j_3+j_4-l_3-z_3]![2l_3+z_3+1]!}\\
&\quad\times\frac{[2l_4-z_4]![j_1+k_4-l_4+z_4]![k_2+k_4+l_2-l_3-z_2-z_3]!}{[z_4]![k_1+l_4-j_4-z_4]![j_1-k_1+k_2+k_4-l_1-l_4+z_1+z_4]!}\\
&\quad\times\frac{q^{-u(k_2+k_4+l_2-l_3-z_2-z_3+1)}[2j_1-k_1+k_2-l_1-u]!}{[k_1+l_4+j_4-z_4+1]![u+z_1]![j_1-k_4+l_4-z_1-z_4-u]!}\\
&\quad\times\frac{[j_1+k_1+k_2-k_4-l_1+l_4-z_4-u]!}{[j_1+j_3-l_1-l_2+z_2-u]![j_1-j_3+k_2-k_4-l_1+l_3+z_3-u]!}.
\end{aligned}
\tag{3.5b}
$$

Each of expressions (3.5a) and (3.5b) includes five summations, with four separate sums (over z_1,z_2,z_3, and z_4) corresponding to the finite (balanced in the first and last cases) basic hypergeometric series ${}_4\phi_3$ or ${}_4F_3[\cdots;q,1]$ [as defined by Eq. (3.2) of Ref. 4], and the fifth sum (over $u+z_1$) corresponding to the finite hypergeometric series ${}_3\phi_2$ or ${}_3F_2(1)$, related in the case of (3.5a) to the Clebsch–Gordan coefficients of $u_q(2)$ or SU(2). However, it is impossible to rearrange all

five sums together into standard basic hypergeometric series ${}_{p+1}\phi_p$. Some correlation between the factorials under the summation signs reveals itself in two quintuplets of factorials of each expression (3.5a) and (3.5b), depending on the couples of summation parameters z_2, z_3 and z_1, z_4. Definite correspondences may be observed in Eqs. (3.5a) and (3.5b) between the q-phase structure and three particular factorial arguments, depending on the couples of summation parameters z_2, z_3, and u, respectively [as well as in q-9j coefficients, presented by Eqs. (3.1a)–(3.1e) of Ref. 4, between the q-phases and three factorial arguments, depending on the couples of summation parameters z_1, z_2, and z_3]. The summation intervals in (3.5a) and (3.5b) are mainly restricted by eight triangle linear combinations of parameters, respectively, but in the stretched cases only (3.5a) for $k_4 = l_4 - j_1$ and (3.5b) for $k_4 = l_4 + j_1$ (with $z_4 = u + z_1 = 0$ in the both cases) turn into the triple sums.

C. Stretched cases of the *q*-12*j* coefficients of the first kind

When the total (maximal) angular momentum in a stretched triangle of the q-12j coefficient of the first kind corresponds to a crossbar of the Möbius strip (3.1) [in the middle row of standard array (3.2a), e.g., for $l_4 = k_4 + j_1$], we obtain the following expression:

$$
\begin{Bmatrix} j_1 & j_2 & j_3 & j_4 \\ & l_1 \quad l_2 \quad l_3 & & k_4 + j_1 \\ k_1 & k_2 & k_3 & k_4 \end{Bmatrix}_q
$$

$$
= (-1)^{k_1 + k_2 - k_3 - j_2 + j_3 + j_4 - l_4}
$$

$$
\times \frac{\nabla[j_3 j_2 l_2]\nabla[k_2 k_3 l_2]\nabla[l_4 j_4 k_1]}{\nabla[j_1 j_2 l_1]\nabla[k_2 k_1 l_1]\nabla[j_3 j_4 l_3]\nabla[k_4 k_3 l_3]} \left(\frac{[2k_4]![2j_1]!}{[2l_4+1]!} \right)^{1/2}
$$

$$
\times q^{-(j_1 + k_2 - l_1 + 1)(k_4 - k_2 + l_2 - l_3) - (l_2 - k_2 - j_3 - 1)(j_3 + k_4 - l_3) + Z_{j_1 j_2 j_3 j_4} + Z_{k_1 k_2 k_3 k_4}}
$$

$$
\times \sum_{z_1, z_2, z_3} \frac{(-1)^{z_1 + z_3}[j_1 + j_2 - l_1 + z_1]![k_1 + k_2 - l_1 + z_1]![2l_1 - z_1]!}{[z_1]![z_2]![z_3]![k_1 - k_2 + l_1 - z_1]![l_1 - j_1 + j_2 - z_1]!}
$$

$$
\times \frac{[l_2 + j_2 - j_3 + z_2]![l_2 + k_3 - k_2 + z_2]!}{[j_2 + j_3 - l_2 - z_2]![k_2 + k_3 - l_2 - z_2]![2l_2 + z_2 + 1]!}
$$

$$
\times \frac{[k_3 + k_4 - l_3 + z_3]![j_3 + j_4 - l_3 + z_3]![2l_3 - z_3]!}{[k_3 + l_3 - k_4 - z_3]![l_3 - j_3 + j_4 - z_3]![j_1 - j_3 - l_1 + l_2 + z_1 + z_2]!}
$$

$$
\times \frac{q^{z_3(l_1 - l_2 - j_1 + j_3) - z_2(j_3 + k_2 - l_1 - l_3 + l_4 + z_3 + 1) - z_1(l_2 - l_3 - k_2 + k_4 + z_2 + z_3)}}{[l_2 - l_3 - k_2 + k_4 + z_2 + z_3]![j_3 + k_2 - l_1 - l_3 + l_4 + z_1 + z_3 + 1]!}. \tag{3.6}
$$

This special case of (3.5a) with three separate sums corresponds to the finite basic hypergeometric series ${}_4F_3[\cdots; q, x]$. Expression (3.6) does not simplify noticeably for two adjacent merging stretched triangles (with $l_4 = k_4 + j_1 = k_1 + j_4$) in the same q-6j coefficient of expansion (3.3a), but one of the sums turns into a ${}_3F_2[\cdots; q, x]$ series for two adjacent diverging stretched triangles (e.g., with $j_1 = l_4 - k_4 = l_1 - j_2$, or with $j_1 = l_4 - k_4 = j_2 - j_1$). The Chu–Vandermonde summation formula [see (B1c) of Ref. 4] may be used in Eq. (3.6) for $j_1 = 0$, $l_1 = j_2$, $k_4 = l_4$ and for $k_4 = 0$, $l_4 = j_1$, $k_3 = l_3$. In these cases, the couples of the q-6j coefficients appear in accordance with Eq. (33.21) of Ref. 2, as well as the consequences of expansions (3.3a)–(3.3b) for fixed x.

When the total angular momentum in a stretched triangle of the q-12j coefficient of the first kind is located along the Möbius strip (3.1) (e.g., for $k_4 = l_4 + j_1$), we obtain from (3.5b), after change of summation parameter $z_2 \to l_2 + k_2 - k_3 - z_2$ the following expression:

$$\left\{\begin{array}{ccccc} j_1 & & j_2 & & j_3 & & j_4 & \\ & l_1 & & l_2 & & l_3 & & l_4 \\ k_1 & & k_2 & & k_3 & & l_4+j_1 & \end{array}\right\}_q$$

$$=\frac{(-1)^{j_3+j_4-l_3+l_2+k_2-k_3}\nabla[j_3j_4l_3]\nabla[k_4k_3l_3]\nabla[k_2k_3l_2]}{\nabla[j_1j_2l_1]\nabla[k_2k_1l_1]\nabla[j_3j_2l_2]\nabla[l_4k_1j_4]}\left(\frac{[2j_1]![2l_4]!}{[2k_4+1]!}\right)^{1/2}$$

$$\times q^{(j_1+k_2-l_1+1)(k_2+k_4+l_2-l_3+1)-(l_2+k_2-j_3+1)(j_3-l_3+k_4+1)+Z_{j_1j_2j_3j_4}+Z_{k_1k_2k_3k_4}}$$

$$\times\sum_{z_1,z_2,z_3}\frac{[j_1+j_2-l_1+z_1]![k_1+k_2-l_1+z_1]![2l_1-z_1]!}{[z_1]![z_2]![z_3]![k_1-k_2+l_1-z_1]![l_1-j_1+j_2-z_1]!}$$

$$\times\frac{(-1)^{z_1+z_2+z_3}[j_2+j_3-l_2+z_2]![2l_2-z_2]!}{[l_2+k_2-k_3-z_2]![j_2-j_3+l_2-z_2]![l_2+k_2+k_3-z_2+1]!}$$

$$\times\frac{q^{z_1(k_2+k_4+l_2-l_3-z_2-z_3+1)}[k_3-k_4+l_3+z_3]![j_4-j_3+l_3+z_3]!}{[k_3+k_4-l_3-z_3]![j_3+j_4-l_3-z_3]![2l_3+z_3+1]!}$$

$$\times\frac{q^{-z_2(k_2-j_3-l_1+l_3-l_4+z_3)-z_3(j_1+j_3-l_1-l_2)}[k_2+k_4+l_2-l_3-z_2-z_3]!}{[j_1+j_3-l_1-l_2+z_1+z_2]![k_2-j_3-l_1+l_3-l_4+z_1+z_3]!}. \tag{3.7}$$

Expression (3.7) does not simplify for two couples of adjacent diverging stretched triangles [with $l_4=k_4-j_1=k_1-j_4$, or with $l_4=k_4-j_1=j_4-k_1$, respectively, again in the same q-6j coefficient of expansion (3.3b)], but for $l_4=0$, $k_4=j_1$, $j_4=k_1$ (after substitution $q\to q^{-1}$) it corresponds to the general expression (3.1a) of Ref. 4 for the q-9j coefficients,

$$([2j_1+1][2k_1+1])^{-1/2}\left\{\begin{array}{ccc} j_1 & l_1 & j_2 \\ k_3 & k_2 & l_2 \\ l_3 & k_1 & j_3 \end{array}\right\}_q$$

[cf. Eq. (33.20) of Ref. 2]. The triple sums in (3.6) and (3.7) resemble expressions for the q-9j coefficients and definite correspondences may be observed between the q-phases and three factorial arguments, depending on the couples of summation parameters z_1,z_2, and z_3, respectively. Expansion of the present couples of the factorial quintuplets (depending on parameters z_1,z_2 and z_2,z_3, respectively), using the Chu–Vandermonde summation formulas enables one to perform the summation over z_2 and thus obtain expressions for the stretched q-12j coefficients of the first kind as fourfold sums, related to compositions of ${}_3F_2[\cdots;q,x]$ series.

Again, one of the sums in (3.7) turns into a ${}_3F_2[\cdots;q,x]$ series for two adjacent diverging stretched triangles in two adjacent q-6j coefficients of expansion (3.3a) (e.g., with $j_1=k_4-l_4=l_1-j_2$, or with $j_1=k_4-l_4=j_2-l_1$), as well as for two adjacent merging stretched triangles (e.g., with $k_4=l_4+j_1=k_3+l_3$). The possible rearrangement of the ${}_3F_2[\cdots;q,x]$ series is not helpful for reducing the remaining ${}_4F_3[\cdots;q,x]$ series.

The doubly stretched q-12j coefficients of the first kind with the adjacent consecutive stretched triangles may be expressed for $k_4=l_4+j_1$ and $j_1=l_1+j_2$ or $l_3=k_3+k_4$ by means of (3.7), as well as for $l_4=k_4+j_1$ and $j_1=l_1+j_2$ or $k_4=k_3+l_3$ by means of (3.6), as the double sums, related to the stretched q-9j coefficients, respectively, of the type (3.1a) or (3.1b) of Ref. 4 (with some "reflected" parameters in the last cases). In this way we derive, for $k_4=l_4+j_1$ and $j_1=l_1+j_2$ [comparing (3.7) with Eq. (3.1a) of Ref. 4], the following relation:

$$\begin{Bmatrix} l_1+j_2 & j_2 & j_3 & j_4 \\ & l_1 \quad & l_2 \quad & l_3 \quad & l_4 \\ k_1 & k_2 & k_3 & l_4+j_1 \end{Bmatrix}_q$$

$$=(-1)^{j_3+j_4-l_3+l_2+k_2-k_3}q^{Z_{j_1j_2j_3j_4}+Z_{k_1k_2k_3k_4}-Z_{l_2,l_3,l_1+l_4}}\frac{\nabla[l_1+l_4,j_4,k_2]}{\nabla[l_1k_1k_2]\nabla[l_4k_1j_4]}$$

$$\times\left(\frac{[2l_1]![2l_4]!}{[2l_1+2l_4]![2j_1+1]}\right)^{1/2}\begin{Bmatrix} k_4 & k_3 & l_3 \\ j_2 & l_2 & j_3 \\ l_1+l_4 & k_2 & j_4 \end{Bmatrix}_{q^{-1}}. \tag{3.8}$$

Similarly, for $k_4=l_4+j_1$ and $l_3=k_3+k_4$ we obtain

$$\begin{Bmatrix} j_1 & j_2 & j_3 & j_4 \\ & l_1 \quad & l_2 \quad & k_3+k_4 & l_4 \\ k_1 & k_2 & k_3 & l_4+j_1 \end{Bmatrix}_q$$

$$=q^{Z_{j_1j_2j_3j_4}+Z_{k_1k_2k_3k_4}-Z_{l_2,j_1+k_3,l_1}}\frac{(-1)^{j_3+j_4-l_4-l_2-k_2-j_2+l_1}\nabla[l_3j_3j_4]}{\nabla[l_4k_1j_4]\nabla[j_1+k_3,j_3,k_1]}$$

$$\times\left(\frac{[2l_4]![2j_1+2k_3+1]!}{[2l_3+1]![2k_4+1]}\right)^{1/2}\begin{Bmatrix} j_1 & k_3 & j_1+k_3 \\ j_2 & l_2 & j_3 \\ l_1 & k_2 & k_1 \end{Bmatrix}_{q^{-1}}. \tag{3.9}$$

We remark that the doubly stretched q-12j coefficients of the first kind for $l_4=k_4+j_1$ and $l_2=j_2+j_3$ or $l_2=k_2+k_3$ as obtained from (3.6), as well as for $k_4=l_4+j_1$ and $j_3=l_2+j_2$ or $k_3=l_2+k_2$ as obtained from (3.7), turn into double sums equivalent to compositions of ${}_4F_3[\cdots;q,x]$ and ${}_3F_2[\cdots;q,x]$ series. However, although the ${}_3F_2[\cdots;q,x]$ series may be rearranged into other forms, these double sums are not equivalent to any composition of two generic ${}_3F_2[\cdots;q,x]$ series and, moreover, they are not related to any q-9j coefficient. Minton's summation formula (A3a) (see Ref. 14) may be helpful in the analogical position of the stretched triangles in (3.6) for $l_4=k_4+j_1$ and $j_2=l_2+j_3$ or $k_3=k_2+l_2$, as well as in (3.7) for $k_4=l_4+j_1$ and $l_2=k_2+k_3$. Otherwise, the ${}_3F_2[\cdots;q,x]$ series appearing in the triple sums, which remain in Eq. (3.6) for $j_3=j_2+l_2$ or $k_2=l_2+k_3$, and in Eq. (3.7) for $j_2=l_2+j_3$ or $k_2=l_2+k_3$, may be rearranged, but it is more reasonable in such a case to use the different expansions of the type (3.3a)–(3.3b) with inserted stretched q-6j coefficients and adapted [e.g., expansion (3.3b) for $l_4=k_4+j_1$ and $j_3=j_2+l_2$ or expansion (3.3a) for $k_4=l_4+j_1$ and $j_2=l_2+j_3$, with transposed the middle and the right columns of the third q-6j coefficients in the both cases] for summation by means of (A2) or (A3) of Ref. 4.

Furthermore, expression (3.6) turns into double sums equivalent to compositions of two ${}_4F_3[\cdots;q,x]$ series for the remote stretched triangles of graph (3.1) $l_4=k_4+j_1$ and $j_3=l_3+j_4$ or $k_2=k_1+l_1$ (when two couples of the touching angular momenta form the four-cycles, or quadrangles), as well as expression (3.7) for $k_4=l_4+j_1$ and $l_3=j_3+j_4$ or $k_2=k_1+l_1$. Again, Minton's summation formula (A3a) may be used in (3.7) for $j_4=j_3+l_3$ and the ${}_3F_2[\cdots;q,x]$ series may be rearranged in the triple sums, which remain in Eq. (3.6) for $l_1=k_1+k_2$ or $l_3=j_3+j_4$ and in Eq. (3.7) for $j_3=l_3+j_4$ or $k_1=k_2+l_1$. Expansion (3.3a) with inserted stretched q-6j coefficients may be used for summation by means of (A1) of Ref. 4 for $l_4=k_4+j_1$ and $l_1=k_1+k_2$, as well as expansion (3.3b) for summation by means of (A2) of Ref. 4 for $k_4=l_4+j_1$ and $k_1=k_2+l_1$, after in the both cases the middle and the right columns of the second q-6j coefficients are transposed.

In general, the triply stretched cases of the q-12j coefficients of the first kind may always be expressed in terms of the double sums, applying some "mirror reflection" ($j\to -j-1$) operations

to the above mentioned expressions, or using the above mentioned rearrangements. In particular, the double sums (compositions of two ${}_3F_2[\cdots;q,x]$ series) related to the most generic Kampé de Fériet[27] functions of the type $F_{1:1}^{0:3}$ (with nine independent parameters) appear instead of (3.7) in the triply stretched cases with $k_4=l_4+j_1=k_3+l_3$ and $j_3=j_2+l_2$, or with $j_1=k_4-l_4=j_2-j_1$ and $k_3=k_2+l_2$.

Let us return to the generic expressions (3.5a) and (3.5b). In both formulas, for $j_2=0$, $l_1=j_1$, $l_2=j_3$, the summation parameters z_1,z_2 and u are fixed, the two remaining separate sums (over z_3,z_4) correspond to the balanced ${}_4F_3[q,1]$ series, and the couples of the q-$6j$ coefficients appear straightforwardly, in accordance with the expansion (3.3a)–(3.3b) for fixed x. Furthermore, in both (3.5a) and (3.5b), the parameters z_1,z_2 and u are also fixed for $j_1+j_2+k_1-k_2=0$, i.e., for the adjacent consecutive stretched triangles $k_2=k_1+l_1=k_1+j_1+j_2$ with the intermediate angular momentum corresponding to a crossbar of the Möbius strip (3.1). Two remaining separate sums (over z_3,z_4) correspond to the balanced (Saalschützian) ${}_4F_3[q,1]$ [related to q-$6j$ coefficient of the type (1.3a)] and summable [see Eq. (A2a)] ${}_3F_2[q,1]$ series. In this way, we derived the following relation:

$$\begin{Bmatrix} j_1 & & j_2 & & j_3 & & j_4 & \\ & j_1+j_2 & & l_2 & & l_3 & & l_4 \\ k_1 & & k_1+l_1 & & k_3 & & k_4 & \end{Bmatrix}_q$$
$$=(-1)^{k_1+j_3-l_3-l_4+2k_3}\frac{q^{2j_1k_1+Z_{j_2j_3j_4}+Z_{k_2k_3k_4}}\nabla[k_2k_3l_2]\nabla[k_1+j_1,j_4,k_4]}{\nabla[j_1k_4l_4]\nabla[j_2l_2j_3]\nabla[k_1j_4l_4]\nabla[k_1+j_1,j_3,k_3]}$$
$$\times\left(\frac{[2j_2]![2j_1]![2k_1]!}{[2k_2+1]![2l_1+1]!}\right)^{1/2}\begin{Bmatrix} j_3 & j_4 & l_3 \\ k_4 & k_3 & k_1+j_1 \end{Bmatrix}_q. \tag{3.10}$$

For 4 mutual positions of the couples of the stretched triangles in the graph of the q-$12j$ coefficient of the first kind, there are 22 different orientations of the total (maximal) angular momenta. In seven cases, the expressions include triple sums, twice they are proportional to the stretched q-$9j$ coefficients, and once to the q-$6j$ coefficient. In the remaining 12 cases, double sums may be obtained. Otherwise, for three mutual positions of the stretched triangles in the q-$12j$ coefficient of the second kind, only nine different orientations of the total angular momenta are possible, and in six cases double sums appear, and in three cases the expressions are single sums (only once proportional to the q-$6j$ coefficient).

Finally, the summation parameters z_1,z_3 and u in (3.5b) are fixed for $j_1-j_3+k_1+k_3=0$, as well as for $x=j_3-k_3=j_1+k_1$ in expansion (3.3a), in which cases four linearly dependent angular momenta appear (disconnected) on the Hamilton line of graph (3.1). In this case, two remaining separate sums (over z_2,z_4) are summable Saalschützian series ${}_3F_2[q,1]$ [see Eqs. (A2a) and (A2b)], and the following expression may be derived:

$$\begin{Bmatrix} j_1 & & j_2 & & j_1+k_1+k_3 & & j_4 & \\ & l_1 & & l_2 & & l_3 & & l_4 \\ k_1 & & k_2 & & k_3 & & k_4 & \end{Bmatrix}_q$$
$$=(-1)^{j_2+j_4-l_1-k_1-j_1-l_4}$$
$$\times\frac{q^{2j_1k_1+Z_{j_2j_3j_4}+Z_{k_2k_3k_4}}[2j_1]![2k_1]![2k_3]!\nabla[j_3j_4l_3]\nabla[j_3j_2l_2]}{[2j_3+1]!\nabla[j_1j_2l_1]\nabla[k_1k_2l_1]\nabla[j_1k_4l_4]\nabla[k_1j_4l_4]\nabla[k_3k_2l_2]\nabla[k_3k_4l_3]}. \tag{3.11}$$

As for (2.13), the virtually stretched triangles are seen only in the q-$6j$ coefficients, which appear in expansion of the q-$12j$ coefficient of the first kind with extreme parameters.

IV. CONCLUDING REMARKS

Using Dougall's summation formula[7] of the very well-poised ${}_5F_4(1)$ series and the transformation formula[12] of the very well-poised ${}_6F_5(-1)$ series, we eliminated the factorial sums weighted with factor $(2j+1)$ and the very well-poised series in the traditional expressions of the $12j$ coefficients of SU(2) in terms of $6j$ coefficients, as well as in the expressions of the q-$12j$ coefficients of $u_q(2)$ weighted with factor $[2j+1]$. Although the obtained generic expressions for the q-$12j$ coefficients of the first kind include fivefold sums and the generic expressions for the q-$12j$ coefficients of the second kind contain fourfold sums, the stretched and doubly stretched q-$12j$ coefficients of both become considerably simpler and present some new versions of triple, double, or single basic hypergeometric series, but more unusual and complicated than appear in the manuals of the angular momentum theory (cf. Ref. 34). The single term expressions for the q-$12j$ coefficients of the both kinds also embrace the virtually stretched cases with four extreme linearly dependent disconnected angular momentum parameters appearing on the Hamilton lines of graphs (2.2) or (3.1).

The symmetry properties and variety of expressions for the $12j$ and q-$12j$ coefficients of the both kinds may inspire new possibilities of rearrangement of the classical and basic hypergeometric series. Expressions for $3nj$ coefficients of SU(2) (with $n>4$) in terms of $6j$ coefficients also may be rearranged using, e.g., Watson's transformation formula of the very well-poised ${}_7F_6(1)$ series [see Eq. (2.5.1) of Ref. 14 or Eq. (6.10) of Ref. 35]. One may also use Eq. (5.3) of Ref. 12 for rearrangement of the very well-poised ${}_8F_7(-1)$ series, or Eqs. (A5) of Ref. 36 for rearrangement of the very well-poised ${}_9F_8(1)$ series. The number of sums in two last cases increases with elimination of the sums dependent on $(2j+1)$.

APPENDIX A: DOUGALL'S, SAALSCHÜTZIAN, AND MINTON'S SUMMATION FORMULAS

In Appendix A of Ref. 4, we presented three summation formulas of the twisted very well-poised q-factorial series as generalizations of Dougall's summation formula (2.3.4.8) of Ref. 7 of the ${}_4F_3(-1)$ series, depending on three parameters. We present here two summation formulas of the very well-poised q-factorial series, depending on four parameters:[12]

$$\sum_j \frac{[2j+1][j-p_1-1]![j-p_2-1]!}{[p_1+j+1]![p_2+j+1]![p_3-j]![p_3+j+1]![p_4-j]![p_4+j+1]!}$$
$$= \frac{[-p_1-p_2-2]![p_1+p_2+p_3+p_4+2]!}{[p_1+p_4+1]![p_2+p_4+1]![p_3+p_4+1]![p_2+p_3+1]![p_1+p_3+1]!}; \tag{A1a}$$

$$\sum_j \frac{(-1)^{p_4-j}[2j+1][j-p_1-1]![j-p_2-1]![j-p_3-1]!}{[p_1+j+1]![p_2+j+1]![p_3+j+1]![p_4-j]![p_4+j+1]!}$$
$$= \frac{[-p_1-p_2-2]![-p_2-p_3-2]![-p_1-p_3-2]!}{[p_1+p_4+1]![p_2+p_4+1]![p_3+p_4+1]![-p_1-p_2-p_3-p_4-3]!}. \tag{A1b}$$

[Cf. Dougall's summation theorem of special very well-poised hypergeometric series ${}_5F_4(1)$ as (2.3.4.5) of Ref. 7 and special very well-poised basic hypergeometric series ${}_6\phi_5$ as (2.4.2) of Ref. 14. Note that the very well-poised basic hypergeometric series ${}_{2k}\phi_{2k-1}$ cannot be expressed in terms of ${}_{2k}F_{2k-1}[\cdots;q,x]$ series.[4,13]]

Under condition $c+d=a+b+e$, we may use also the summation formulas of the balanced (Saalschützian) ${}_3F_2[q,1]$ series [cf. Eq. (2.3.1.4) of Ref. 7 and Eqs. (1.7.1) and (1.7.2) of Ref. 14]:

$$\sum_s \frac{(-1)^s[c+s]![d-s]!}{[s]![a-s]![b-s]![e+s+1]!} = \frac{[c]![d-a]![d-b]![c+d+1]!}{[a]![b]![a+e+1]![b+e+1]![e-c]!} \tag{A2a}$$

for $e-c\geqslant 0$ and

$$\sum_s \frac{(-1)^s[c-s]![d-s]!}{[s]![a-s]![b-s]![e-s+1]!}=\frac{[c-a]![c-b]![d-a]![d-b]!}{[a]![b]![e-c]![e-d]![e+1]!} \tag{A2b}$$

for $e-c\geqslant 0$ and $e-d\geqslant 0$.

It is sometimes useful to implement the q-version of Minton's summation formula[37] or its inverse [cf. Eq. (1.9.6) of Ref. 14]:

$$\sum_s \frac{(-1)^s q^{s(n-\Sigma_{i=1}^r m_i)}}{[s]![n-s]![S+s]}\prod_{j=1}^m (b_j+s|q)_{m_j}=\frac{q^{S(\Sigma_{i=1}^r m_i-n)}}{(S|q)_{n+1}}\prod_{j=1}^m (b_j-S|q)_{m_j}, \tag{A3a}$$

if $S+s\neq 0$ for $s=0,1,\ldots,n$, and $n\geqslant\Sigma_{i=1}^r m_i$;

$$\sum_s \frac{(-1)^s q^{s(a+b-c-m)}[c-s]!}{[s]![a-s]![b-s]![S-s+1]}\prod_{j=1}^m [A_j-s]$$

$$=(-1)^{a+b-c-m}q^{(S+1)(a+b-c-m)}\frac{[S-a]![S-b]!}{[S-c]![S+1]!}\prod_{j=1}^m [S-A_j+1], \tag{A3b}$$

which is valid if $S-s+1\neq 0$ for $s=0,1,\ldots,\min(a,b)$ and $a+b-c-m\geqslant 0$. Note that the analytical continuation of the summation formulas (A3a) and (A3b) of the alternating series to related series with the fixed sign of all terms is impossible.

APPENDIX B: CLEBSCH–GORDAN COEFFICIENTS OF SU(2) AND $u_q(2)$ AND TWISTED VERY WELL-POISED SERIES

The very well-poised ${}_6F_5(-1)$ and ${}_7F_6(1)$ series appear in context of the Clebsch–Gordan and $6j$ coefficients of SU(2) as presented in Ref. 33 (see also Ref. 2), as well as their q-analogs in the CG (cf. Ref. 13, where the dual Hahn q-polynomials are considered) and $6j$ coefficients (cf. Ref. 35) of $u_q(2)$.

We deduce here a new expression for the Clebsch–Gordan coefficients of SU(2) and $u_q(2)$ directly from the recoupling relation:

$$\begin{bmatrix}(j_2+m_2)/2 & (j_2-m_2)/2 & j_2\\ (j_2+m_2)/2 & (m_2-j_2)/2 & m_2\end{bmatrix}_q\begin{bmatrix}j_1 & j_2 & j\\ m_1 & m_2 & m\end{bmatrix}_q$$

$$=\sum_x (-1)^{j_1+j_2+j}([2x+1][2j_2+1])^{1/2}\begin{Bmatrix}(j_2+m_2)/2 & (j_2-m_2)/2 & j_2\\ j & j_1 & x\end{Bmatrix}_q$$

$$\times\begin{bmatrix}j_1 & (j_2+m_2)/2 & x\\ m_1 & (j_2+m_2)/2 & m'\end{bmatrix}_q\begin{bmatrix}x & (j_2-m_2)/2 & j\\ m' & (m_2-j_2)/2 & m\end{bmatrix}_q, \tag{B1}$$

where $m'=m_1+\frac{1}{2}(j_2+m_2)=m+\frac{1}{2}(j_2-m_2)$. Inserting the stretched $6j$ and extreme CG coefficients expressed without sums, we obtain the following expression,

$$\begin{bmatrix}j_1 & j_2 & j\\ m_1 & m_2 & m\end{bmatrix}_q=\nabla[j_2j_1j]\left(\frac{[2j+1][j_2+m_2]![j_2-m_2]![j_1-m_1]![j-m]!}{[j_1+m_1]![j+m]!}\right)^{1/2}$$

$$\times q^{\{j_2(j_2+1)-j_1(j_1+1)-j(j+1)\}/2-m_1j_2-(j_2+m_2)(j_2+m_2+2)/4}$$

$$\times\sum_x \frac{(-1)^{j_1+(j_2+m_2)/2-x}q^{x(x+1)}[2x+1][x+m']!}{\nabla^2[\frac{1}{2}(j_2+m_2),j_1,x]\nabla^2[\frac{1}{2}(j_2-m_2),j,x][x-m']!}, \tag{B2}$$

where the right-hand side is related to the left-hand side of Eq. (3.4a) with parameters

$$p_1=\tfrac{1}{2}(j_2-m_2)-j-1,\quad p_2=-m'-1,\quad p_3=\tfrac{1}{2}(j_2+m_2)-j_1-1,$$

$$p_4=\tfrac{1}{2}(j_2-m_2)+j,\quad p_5=\tfrac{1}{2}(j_2+m_2)+j_1.$$

Expression (B2) is invariant under 12 relations of the Regge symmetry, corresponding to the permutations in the sets p_1,p_2,p_3 or p_4,p_5. After expressing the CG coefficient of $u_q(2)$ by means of Eq. (5.17) of Ref. 30 [which after some cyclic permutation, is equivalent to Eq. (65) of Chapter 3 of Ref. 17 or, for $q=1$, related to Eq. (13.1c) of Ref. 2], and using the symmetry relation (4.13) of Ref. 15 (which allows one to interchange the parameters j_2,m_2 and $j,-m$ in the CG coefficients, cf. Ref. 17), we derive our Eq. (3.4a) straightforwardly. The remaining very well-poised series with different numerator and denominator distributions of q-factorial arguments [e.g., the nonalternating left-hand side of (3.4b) or the nonalternating right-hand side of Eq. (5.3) of Ref. 12 with $p_3=-p_2-2$, and their other analytical continuations] are not related to the Clebsch–Gordan coefficients of $u_q(2)$, although sometimes they may be related to the CG coefficients of $u_q(1,1)$.

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Modified braid equations for $SO_q(3)$ and noncommutative spaces

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General solutions of the $\hat{R}TT$ equation with a maximal number of free parameters in the specrtal decomposition of vector $SO_q(3)$ $\hat{R}$ matrices are implemented to construct modified braid equations (MBE). These matrices conserve the given, standard, group relations of the nine elements of T, but are not constrained to satisfy the standard braid equation (BE). Apart from q and a normalization factor our $\hat{R}$ contains two free parameters, instead of only one such parameter for deformed unitary algebras studied in a previous paper [Math. QA/0009178] where the nonzero right hand side of the MBE had a linear term proportional to $(\hat{R}_{(12)} - \hat{R}_{(23)})$. In the present case the rhs is, in general, nonlinear. Several particular solutions are given (Sec. II) and the general structure is analyzed (Appendix A). Our formulation of the problem in terms of projectors yields also two new solutions of standard (nonmodified) braid equation (Sec. II) which are further discussed (Appendix B). The noncommutative three-spaces obtained by implementing such generalized $\hat{R}$ matrices are studied (Sec. III). The role of coboundary $\hat{R}$ matrices (not satisfying the standard BE) is explored. The MBE and Baxterization are presented as complementary facets of the same basic construction, namely, the general solution of $\hat{R}TT$ equation (Sec. IV). A new solution is presented in this context. As a simple but remarkable particular case a nontrivial solution of BE is obtained (Appendix B) for $q=1$. This solution has no free parameter and is not obtainable by twisting the identity matrix. In the concluding remarks (Sec. V), among other points, generalization of our results to $SO_q(N)$ is discussed. [DOI: 10.1063/1.1413225]

I. INTRODUCTION

In a previous paper[1] a particular class of inhomogeneous, modified, braid equations (MBE) was shown to correspond to general solutions of $\hat{R}TT$ relations. Fundamental 2×2 T matrices and the corresponding 4×4 $\hat{R}(=PR)$ matrices for $GL_{p,q}(2)$, $GL_{g,h}(2)$ and $GL_{q,h}(1/1)$ were used as examples. The inputs were the known group relations of the elements (a,b,c,d) for each of the above cases. Then the most general solution (without imposing the Yang–Baxter (YB) equation for R or, equivalently, the braid equation for $\hat{R}$) was sought, for each case, of the relation

$$\hat{R}T_1T_2 = T_1T_2\hat{R}, \tag{1}$$

where

$$T_1 = T\otimes I_2, \quad T_2 = I_2\otimes T.$$

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The only constraint on $\hat{R}$ was the conservation of the given group relations for (a,b,c,d). In each case $\hat{R}$ was found to depend, apart from the two parameters $((p,q),(g,h),(q,h))$, linearly on a third one (K) such that, for a suitable normalization, one obtains

$$\hat{R}_{(12)}\hat{R}_{(23)}\hat{R}_{(12)}-\hat{R}_{(23)}\hat{R}_{(12)}\hat{R}_{(23)}=\left(\frac{K}{K_1}-1\right)\left(\frac{K}{K_2}-1\right)(\hat{R}_{(23)}-\hat{R}_{(12)}). \tag{2}$$

This is the MBE with

$$(K_1,K_2)=(1,p/q),\quad (1,1),\quad (1,1/q), \tag{3}$$

respectively, for the above-mentioned cases.

It was pointed out in Ref. 1 that (2) reexpressed in terms of R provides a particular, interesting class of modified quantum YB equations (MQYBE) of Gerstenhaber, Giaquinto, and Schack (see Ref. 2 and sources cited therein).

The special features of (2) as indicated in Ref. 1, are as follows.

(1) The explicit stucture on the right carries interesting information. After obtaining the general solution of (1) and the MBE it corresponds to, one obtains the unmodified, standard braid or YB matrices as byproducts. One just sets $K=K_1$ or $K=K_2$, the two solutions being related through

$$\hat{R}(K_2)=\hat{R}(K_1)^{-1}. \tag{4}$$

(2) Setting, as explained in Ref. 1,

$$K=2K_1K_2(K_1+K_2)^{-1}, \tag{5}$$

one obtains

$$(\hat{R}(K))^2=I. \tag{6}$$

Hence the construction of ''triangular'' (or ''unitary'' or ''coboundary'') R matrices is again reduced to the choice of a particular value of K in the general solution. This aspect will be studied further later in this work.

(3) It was pointed out in Ref. 1 that MBE and Baxterization are complementary facets of the same basic construction, namely, the general solution of (1). This links MBE to integrable models. This aspect will be taken up in Sec. IV with new examples.

(4) The parameter K plays an interesting role in noncommutative spaces obtained by implementing the general $\hat{R}(K)$. The detailed discussion in Ref. 1 of this aspect will be generalized to higher dimensions in Sec. III.

A. Spectral decomposition and generalization to higher dimensions

Our construction can be generalized to higher dimensional cases most conveniently by introducing arbitrary constant coefficients in the spectral decomposition of R matrices for *vector representations*. The standard solutions (not ''modified'' in our sense) are well-known.[3,4] Instead of wading through larger and larger numbers of group relations $[n^2(n^2-1)/2$ for n^2 elements of $T]$ one starts with the following results for vector representations.

For $\mathrm{GL}_q(N)$ one has, in terms of the projectors $P^{(\pm)}$,

$$\hat{R}=qP^{(+)}-q^{-1}P^{(-)}, \tag{7}$$

where

$$P^{(+)}P^{(-)}=0,\quad (P^{(\pm)})^2=P^{(\pm)},\quad P^{(+)}+P^{(-)}=I. \tag{8}$$

Here $\hat{R}$ satisfies the braid equation and

$$(\hat{R}-qI)(\hat{R}+q^{-1}I)=0. \tag{9}$$

One has also

$$P^{(+)}=\frac{(\hat{R}+q^{-1}I)}{(q+q^{-1})}, \quad P^{(-)}=-\frac{(\hat{R}-qI)}{(q+q^{-1})}. \tag{10}$$

If one sets, *with the same projectors*,

$$\hat{R}(u,v)=uP^{(+)}+vP^{(-)}, \tag{11}$$

where (u,v) are nonzero, unequal but otherwise arbitrary parameters, one obtains

$$(\hat{R}(u,v)-uI)(\hat{R}(u,v)-vI)=0, \tag{12}$$

$$P^{(+)}=\frac{(\hat{R}(u,v)-vI)}{(u-v)}, \quad P^{(-)}=\frac{(\hat{R}(u,v)-uI)}{(v-u)}. \tag{13}$$

Of the two parameters (u,v) one can be fixed by choosing a suitable normalization, leading effectively to one independent, arbitrary parameter. Apart from differences in notations, our construction of $\hat{R}(K)$ in Ref. 1 (see Sec. 3.2 in Ref. 1), namely,

$$\hat{R}(K)=(1-(K/K_1+K/K_2))P_1+P_2, \tag{14}$$

corresponds directly to (11). This and certain other aspects of our previous formalism *can be directly generalized* to $\mathrm{GL}_q(N)$, though the noncommutative spaces will now be of N dimensions.

For $\mathrm{SO}_q(N)$ [and for $\mathrm{Sp}_q(N)$ which we do not consider here] there is a major change. One has now *three* projectors in the spectral decomposition of $\hat{R}$ matrices for vector representations. The consequences for MBE will be seen to be important.

For $\hat{R}$ satisfying the braid equation one obtains[3,4]

$$(\hat{R}-qI)(\hat{R}+q^{-1}I)(\hat{R}-q^{1-N}I)=0 \tag{15}$$

and

$$\hat{R}=qP^{(+)}-q^{-1}P^{(-)}+q^{1-N}P^{(0)}, \tag{16}$$

where [with (i,j) denoting a pair from $(+,-,0)$]

$$P^{(i)}P^{(j)}=P^{(i)}\delta_{ij}, \quad P^{(+)}+P^{(-)}+P^{(0)}=I. \tag{17}$$

Generalizing as before, we introduce [with nonzero and unequal (u,v,w) and the projectors being the *same* as before, independent of (u,v,w)]

$$\hat{R}(u,v,w)=uP^{(+)}+vP^{(-)}+wP^{(0)}. \tag{18}$$

Now [denoting $\hat{R}(u,v,w)$ as $\hat{R}$],

$$(\hat{R}-uI)(\hat{R}-vI)(\hat{R}-wI)=0 \tag{19}$$

and

$$P^{(+)}=\frac{(\hat{R}-vI)(\hat{R}-wI)}{(u-v)(u-w)},$$

$$P^{(-)}=\frac{(\hat{R}-uI)(\hat{R}-wI)}{(v-u)(v-w)}, \tag{20}$$

$$P^{(0)}=\frac{(\hat{R}-uI)(\hat{R}-vI)}{(w-u)(w-v)}.$$

Here, fixing the normalization, *two* independent parameters are left.

In the next section we will study the MBE corresponding to (18). We will set $N=3$. This will permit us to display explicitly matrices of managaeble size. *The essential new features will, however, be present already for* $N=3$.

Let us now note how the number of coboundary (or unitary) solutions for vector representations changes with the number of projectors.

For $\mathrm{GL}_q(N)$ it is seen from (8) and (11) that

$$(\hat{R}(u,v))^2=u^2P^{(+)}+v^2P^{(-)}=P^{(+)}+P^{(-)} \tag{21}$$

for

$$u^2=v^2=1.$$

Hence, apart from an overall $(\pm)$ sign, the only nontrivial solution is

$$\hat{R}_c=P^{(+)}-P^{(-)}=I-2P^{(-)}=-(I-2P^{(+)}), \quad \hat{R}_c^2=I. \tag{22}$$

For $\mathrm{SO}_q(n)$, from (17) and (18) apart from an overall sign one obtains analogously *three* solutions

$$\hat{R}_c=(I-2P^{(+)}), \quad (I-2P^{(-)}), \quad (I-2P^{(0)}). \tag{23}$$

Each satisfies

$$\hat{R}_c^2=I$$

and the product of any two gives the third one with a change of sign. Thus, for example,

$$(I-2P^{(+)})(I-2P^{(-)})=-(I-2P^{(0)}). \tag{24}$$

If the coefficient (-2) in (23) is replaced by an arbitrary number, $\hat{R}$ still satifies as is easily seen a *quadratic* equation, not the cubic (19).

If complex solutions are considered for real q but with complex coefficients in (18), one obtains the unitarity relation when (u,v,w) are phases in (18). Thus (with real deltas)

$$\hat{R}=e^{i\delta_1}P^{(+)}+e^{i\delta_2}P^{(-)}+e^{i\delta_3}P^{(0)} \tag{25}$$

gives, since the projectors are symmetric for the orhogonal case,

$$\hat{R}^\dagger\hat{R}=I.$$

In (18), (u,v,w) were postulated to be unequal. This permits one to express *all the three* projectors in terms of $\hat{R}$ as in (20). But this is not obligatory. As noted in (23) other cases (with

$u=v=-w=1$ and so on) can indeed be of special interest. For (23) in each case one has *two* mutually orthogonal combinations. Selecting the second case, for example, one obtains

$$P^{(-)}=-\tfrac{1}{2}(\hat{R}_c-I), \quad P^{(+)}+P^{(0)}=\tfrac{1}{2}(\hat{R}_c+I). \tag{26}$$

We conclude with a fully explicit statement of our approach. If one has

$$\hat{R}T_1T_2=T_1T_2\hat{R},$$

then any function $f(\hat{R})$ of $\hat{R}$ satisfies

$$f(\hat{R})T_1T_2=T_1T_2f(\hat{R}). \tag{27}$$

To start with let us suppose (for definiteness, such a starting point not being essential) that $\hat{R}$ satifies BE.

For $\mathrm{GL}_q(N)$, $\hat{R}$ satisfies a quadratic constraint (9). Hence any power series in $\hat{R}$ can be reduced to a linear function in $\hat{R}$. Hence, apart from an overall normalization factor, the most general solution of (27), for a given set of group relations, becomes effectively (14) as studied in Ref. 1. [It is easy to see from (7) and (10) that even fractional powers of $\hat{R}$ can be obtained as a linear funtion of $\hat{R}$ but, in general, with complex coefficients. Having noted this, we will usually implicitly consider real coefficients. An analogous situation will hold for the orthogonal case considered later. Complex coefficients, such as in (25), will not be introduced explicitly. Except when roots of unity are involved, complexification of our formalism is, however, straightforward.]

For $\mathrm{SO}_q(N)$, $\hat{R}$ satisfies a cubic constraint (15). Hence the general solution, using analogous arguments, is seen effectively to be, with constant coefficients c_i,

$$f(\hat{R})=c_1(\hat{R})^2+c_2\hat{R}+c_3I. \tag{28}$$

Using the spectral decomposition (16) along with (17),

$$\begin{aligned} f(\hat{R})=c_1(q^2P^{(+)}+q^{-2}P^{(-)}+q^{2(1-N)}P(0))+c_2(qP^{(+)}-q^{-1}P^{(-)} \\ +q^{(1-N)}P(0))+c_3(P^{(+)}+P^{(-)}+P^{(0)}). \end{aligned}$$

Hence, collecting together the coefficients one obtains the form

$$f(\hat{R})=uP^{(+)}+vP^{(-)}+wP^{(0)}. \tag{29}$$

This is the motivation for (18). The starting point is the most general solution, for a given set of group relations, as given by (29). The right hand side of the MBE will be a *consequence* (see Appendix A). In this larger space one then looks for points with particularly attractive properties (for example, those corresponding to $\hat{R}_c$) and, more generally, explores the consequences of the free parameters in (29) such as in related noncommutative geometries (Sec. III).

II. MBE FOR $\mathrm{SO}_q(3)$

We fix the normalization by choosing the top left element (row 1, col. 1) to be unity. In order to simplify the explicit form of $\hat{R}$ we denote the remaining parameters in (18) as follows:

$$\begin{aligned} \hat{R}&=P^{(+)}+(1+a(1+q^2))P^{(-)}+(1+b(1+q+q^2))P^{(0)} \\ &=I+a(1+q^2)P^{(-)}+b(1+q+q^2)P^{(0)}. \end{aligned} \tag{30}$$

The projectors are given explicitly at the end of Appendix A. The 9×9 symmetric $\hat{R}$ is now

$$\hat{R}(a,b;q)$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & (1+a) & 0 & -aq & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & (1+aq+b) & 0 & (b+a(q-1))\sqrt{q} & 0 & (b-a)q & 0 & 0 \\ 0 & -aq & 0 & (1+aq^2) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & (b+a(q-1))\sqrt{q} & 0 & (1+a(q-1)^2+bq) & 0 & (bq-a(q-1))\sqrt{q} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & (1+a) & 0 & -aq & 0 \\ 0 & 0 & (b-a)q & 0 & (bq-a(q-1))\sqrt{q} & 0 & (1+aq+bq^2) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -aq & 0 & (1+aq^2) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{31}$$

This $\hat{R}(a,b;q)$ satisfies the braid equation for

$$\text{case 1:} \quad a=-q^{-2}, \quad b=-q^{-2}+q^{-3}, \qquad \text{case 2:} \quad a=-1, \quad b=-1+q, \tag{32}$$

the two sets giving mutually inverse matrices.

For this $\hat{R}$ [the parameters (a,b) being implicit and I being the 3×3 unit matrix] we define

$$\hat{R}_{12}=\hat{R}\otimes I, \quad \hat{R}_{23}=I\otimes\hat{R}. \tag{33}$$

The general structure of the MBE is presented in Appendix A. We present here three cases obtained for particular constraints on (a,b). One has

$$\hat{R}_{12}\hat{R}_{23}\hat{R}_{12}-\hat{R}_{23}\hat{R}_{12}\hat{R}_{23}=l_1(\hat{R}_{12}-\hat{R}_{23})+l_2(\hat{R}_{12}{}^2-\hat{R}_{23}{}^2), \tag{34}$$

where for case 1, $a=0$ and arbitrary b,

$$l_2=0, \quad l_1=(1+b(1+q+q^2)+b^2q^2); \tag{35}$$

and for case 2, $b=(1-q)a$,

$$l_2=(1+a), \quad l_1=(3+2(2+q^2)a+(1+2q^2)a^2); \tag{36}$$

Setting $a=-1$ one obtains case 2 of (32) with

$$l_1=0, \quad l_2=0.$$

For case 3, $b=(1-q^{-1})a$,

$$l_2=(1+q^2a), \quad l_1=(3+2(1+2q^2)a+q^2(2+q^2)a^2). \tag{37}$$

Setting $a=-q^{-2}$ one obtains case 1 of (32) with

$$l_1=0, \quad l_2=0.$$

Let us note the following features:

The right hand side of (34) is linear only for $a=0$ (case 1). This is evidently not included in the standard cases (32). *Yet the braid equation is satisfied* for

$$a=0, \quad (b^2q^2+b(1+q+q^2)+1)=0,$$

hence (when $q\neq 0$) for

$$b=-\frac{1}{2q^2}(1+q+q^2)\pm\frac{1}{2q^2}((1+3q+q^2)(1-q+q^2))^{1/2}. \tag{38}$$

This gives real b for $q>0$. (See Appendix B for further discussion.)

To complete the picture, we note that the braid matrix becomes for

$$q=0,\quad a=0,\quad b=-1,$$
$$\hat{R}(0,-1;0)=\mathrm{diag}(1,1,0,1,1,1,1,1,1). \tag{39}$$

When a and b are independent and arbitrary even the quadratic terms of the rhs of (34) do not suffice (Appendix A).

III. NONCOMMUTATIVE THREE-SPACE FROM $\hat{R}(a,b;q)$:

When $\hat{R}$ satisfies the braid equation [for (32)] the quantum vector space is discussed in Refs. 3–5. [See, in particular, Sec. (9.3.2) of Refs. 4 and Ex. (4.1.22) of Ref. 5. Our results below are to be compared to these treatments.] We will treat the more general case with parameters (a,b). The explicit form of the rhs of the MBE (Sec. II) is not directly relevant here. We treat (a,b) as free parameters to start with. With a slight change of notation (with respect to Sec. I) we set in (30)

$$v=a(1+q^2),\quad w=b(1+q+q^2),$$

giving

$$\hat{R}=I+vP^{(-)}+wP^{(0)}=P^{+}+(1+v)P^{(-)}+(1+w)P^{(0)}. \tag{40}$$

The coordinates are denoted (x_-,x_0,x_+). Let $(x\otimes x)$ (without "tilde" for simplicity) denote the nine-component *column* obtained from the tensor product. Let (ξ_-,ξ_0,ξ_+) denote the differentials (dx_-,dx_0,dx_+). Let the columns for the other tensor products be denoted, in evident notations, as $(\xi\otimes\xi)$, $(x\otimes\xi)$, $(\xi\otimes x)$.

As in Ref. 1 we will adopt prescriptions that give commutators of (x_i,x_j) and of (ξ_i,ξ_j) independent of (v,w) while those of (x_i,ξ_j) do depend on them.

Let

$$(\hat{R}-I)(\hat{R}-(1+w)I)(x\otimes x)=0$$

or

$$P^{(-)}(x\otimes x)=0. \tag{41}$$

This agrees with Refs. 3–5. Now set

$$(x\otimes\xi)=M(\xi\otimes x). \tag{42}$$

Exterior derivation gives

$$(\xi\otimes\xi)=-M(\xi\otimes\xi) \tag{43}$$

or

$$(M+I)(\xi\otimes\xi)=0.$$

Now exterior derivation of (41) along with (42) gives the typical constraint

$$(\hat{R}-I)(\hat{R}-(1+w)I)(M+I)=0. \tag{44}$$

Hence one can choose (k being an arbitrary constant parameter)

$$(M+I)=k(\hat{R}-(1+v)I)=k(-vP^{(+)}+(w-v)P^{(0)}). \tag{45}$$

From (43) and (45), due to the orthogonality of the projectors, one obtains (in agreement with Refs. 4 and 5)

$$P^{(+)}(\xi\otimes\xi)=0, \quad P^{(0)}(\xi\otimes\xi)=0. \tag{46}$$

From (41) and (46) one obtains (as in the standard treatments cited earlier)

$$\begin{gathered} x_-x_0=qx_0x_-, \quad x_0x_+=qx_+x_0, \\ x_+x_--x_-x_+=hx_0^2, \end{gathered} \tag{47}$$

with

$$h\equiv\left(\sqrt{q}-\frac{1}{\sqrt{q}}\right)$$

and

$$\begin{gathered} \xi_-^2=0, \quad \xi_+^2=0, \quad \xi_-\xi_++\xi_+\xi_-=0, \\ q\xi_-\xi_0+\xi_0\xi_-=0, \quad q\xi_0\xi_++\xi_+\xi_0=0, \\ \xi_0^2=h\xi_-\xi_+. \end{gathered} \tag{48}$$

Now we come to the part specific to our formalism. We define

$$\begin{gathered} \Phi_-=(\xi_-x_0-q\xi_0x_-), \quad \Phi_+=(\xi_0x_+-q\xi_+x_0), \\ \Phi_0=(\xi_-x_++\sqrt{q}\xi_0x_0+q\xi_+x_-), \quad \Phi_0'=(\xi_-x_++h\xi_0x_0-\xi_+x_-). \end{gathered} \tag{49}$$

Then, implementing the definition of M in terms of $\hat{R}(a,b)$ and the explicit form of the latter one obtains from (42), denoting

$$k_1=-(kv+1)=-(ka(q^2+1)+1),$$

the module structure

$$\begin{gathered} x_-\xi_-=k_1\xi_-x_-, \quad x_-\xi_0=k_1\xi_-x_0+ka\Phi_-, \\ x_-\xi_+=k_1\xi_-x_++kaq\Phi_0'+kb\Phi_0, \quad x_0\xi_-=k_1\xi_0x_--kaq\Phi_-, \\ x_0\xi_0=k_1\xi_0x_0+ka(q-1)\sqrt{q}\Phi_0'+kb\sqrt{q}\Phi_0, \\ x_0\xi_+=k_1\xi_0x_++ka\Phi_+, \quad x_+\xi_-=k_1\xi_+x_--kaq\Phi_0'+kbq\Phi_0, \\ x_+\xi_0=k_1\xi_+x_0-kaq\Phi_+, \quad x_+\xi_+=k_1\xi_+x_+. \end{gathered} \tag{50}$$

One can verify that one obtains the relations given in Ex. 4.1.22 of Ref. 5 (p. 133) on setting

$$k=q^2, \quad a=-q^{-2}, \quad b=-q^{-2}+q^{-3}. \tag{51}$$

For

$$k=1, \quad a=-2(1+q^2)^{-1}, \quad b=0 \tag{52}$$

one obtains the case (26) of $\hat{R}_{(c)}$ (with $\hat{R}_{(c)}{}^2=I$) where

$$P^{(-)}=\tfrac{1}{2}(\hat{R}_{(c)}-1), \quad (M+I)=2(P^{(+)}+P^{(0)}). \tag{53}$$

Hence (47) and (48) are conserved along with a particularly simple form of (50). Here one moves out of the restricted space of solutions of BE (or YBE) to implement the particular simplicity of $\hat{R}_{(c)}$. (See the relevant remarks in Sec. V.)

IV. MBE AND BAXTERIZATION

In Ref. 1 we briefly pointed out that MBE and Baxterization are two complementary aspects of the same basic construction: the general solution of $\hat{R}TT$ equation for a given set of group relations of the elements of T. For the cases considered in Ref. 1 [generalizable to $\mathrm{GL}_q(N)$] the correspondence is relatively simple. In (2) the same, single parameter K appears in each member on the left leading to the nonzero rhs (thus modifying the BE) as shown in (2). In a complementary approach, one can vary K in different members on the left in a prescribed fashion (indicated in Ref. 1) so that the rhs remains zero. This is Baxterization. The *same* parameter that leads to MBE thus leads also to integrable systems in a complementary fashion.

One can make a parallel study for $\mathrm{SO}_q(3)$ [generalizable to $\mathrm{SO}_q(N)$ and $\mathrm{Sp}_q(N)$]. But the presence of three projectors and hence (apart from a normalization factor) of two arbitrary parameters leads to a more complex situation. Even restricted cases give the MBE of (34) with quadratic terms on the right, the general structure being given in Appendix A. Let us now look at the complementary situation, namely, Baxterization.

In Sec. 3.9 of Ref. 6 solutions of

$$\hat{R}_{(12)}(x)\hat{R}_{(23)}(xy)\hat{R}_{(12)}(y)=\hat{R}_{(23)}(y)\hat{R}_{(12)}(xy)\hat{R}_{(23)}(x) \tag{54}$$

are given. In our notations and conventions they can be expressed as

$$\hat{R}(x)=I+v(x)P^{(-)}+w(x)P^{(0)}, \tag{55}$$

where

$$v(x)=-1+\frac{f(x)}{f(x^{-1})}, \quad w(x)=-1+\frac{g(x)}{g(x^{-1})},$$

$$f(x)=(xq-x^{-1}q^{-1})$$

and

$$g(x)=(xq^3+x^{-1})$$

or

$$g(x)=(x^{-1}-qx)(xq-x^{-1}q^{-1}).$$

Here we consider $\mathrm{SO}_q(N)$ for $N=3$. But $f(x)$ is independent of N and N appears in $g(x)$ in a simple! fashion.[6] Above $v(x)$ is assumed to be nonzero. We present a distinct class of solutions which is a Baxterization of the new class of *BE* given by our (38). For

$$\hat{R}(x)=I+w(x)P^{(0)} \tag{56}$$

using (A.15) one finds from (54) the single constraint

$$w(xy)=\frac{w(x)+w(y)+w(x)w(y)}{1-k^2w(x)w(y)}, \tag{57}$$

where

$$k^2=(1+q+q^{-1})^{-2}=(1+[2])^{-2}.$$

For $N>3$, $[2]$ is replaced by $[N-1]$. The solutions are

$$\begin{aligned} w(x)&=-1+\frac{g(x)}{g(x^{-1})}\\ g(x)&=-(x-x^{-1})\pm\sqrt{1-4k^2}(x+x^{-1}). \end{aligned} \tag{58}$$

For real q,

$$(1-4k^2)=\frac{((q^{1/2}+q^{-1/2})^2+1)((q^{1/2}-q^{-1/2})^2+1)}{(1+q+q^{-1})^2}$$

is positive and the square root real. Note that for any $(v(x),w(x))$

$$(\hat{R}(x))^{-1}=I-\frac{v(x)}{1+v(x)}P^{(-)}-\frac{w(x)}{1+w(x)}P^{(0)} \tag{59}$$

provided that the denominators are nonzero. Considering the inverse of both sides of (54) one finds that if $(v(x),w(x))$ are to be general solutions one must have

$$-\frac{v(x)}{1+v(x)}=v(x'),\quad -\frac{w(x)}{1+w(x)}=w(x'), \tag{60}$$

where x' is some suitable function of x. The forms following (55), independently of the explicit expressions for (f,g) assure that

$$x'=x^{-1}$$

and

$$\hat{R}(x)\hat{R}(x^{-1})=I. \tag{61}$$

The same is valid for (58). In (55), respectively, for

$$x\gg 1,\quad x\ll 1$$

one obtains the limits

$$v=-(1+q^{\epsilon 2}),\quad w=-(1-q^{\epsilon 3})$$

(where $\epsilon=\pm 1$) the braid values noted in (A.9), (A.10). Let us finally note that setting

$$\epsilon\sqrt{1-4k^2}=\tanh!ta,\quad x=\exp(\theta)$$

one obtains from (58) the elegant Baxterization

$$w(x)=-1+\frac{\sinh(\eta-\theta)}{\sinh(\eta+\theta)}. \tag{62}$$

For $q=1$ with

$$\text{than}\,\eta=\epsilon\frac{5}{\sqrt{3}}$$

one obtains Baxterization of the case studied in Appendix B.

V. REMARKS

We conclude by noting the following points.

(1) After the introductory remarks (Sec. I) on the spectral decomposition of $\hat{R}$ for vector representations of $GL_q(N)$, $SO_q(N)$ and $Sp_q(N)$, from Sec. II onwards we restricted our study to $SO_q(3)$. But a substantial part of our results are evidently generalizable to $SO_q(N)$ with $N>3$. The crucial feature is the number of projectors in the spectral decomposition. The MBE for $GL_q(2)$ with two projectors and that for $SO_q(3)$ with three exhibit major differences, made explicit here. But in $SO_q(N)$ the number of projectors does not vary with N. Still, a careful study of the case of $SO_q(4)$ and comparison of the results with those for $SO_q(3)$ would be of real interest. This is beyond the scope of this article.

(2) In Ref. 1 we started with the criterion of using the most general solution $\hat{R}$ of the $\hat{R}TT$ relations for a given set of group relations of the elements of T. This, being implemented in the standard trilinear structure of the braid equation, modified the right hand side, making it nonzero but *linear* in the R's as shown in (2). *No a priori postulate was made concerning the rhs of the equation*. The explicit form was a *consequence* of the free parameter K in $\hat{R}$. It was then noted in Ref. 1 that the MBE thus obtained [Eq. (2) of this article] coincided with that introduced in Ref. 2 (and sources cited there). Now this is seen to be a *coincidence* valid for the cases studied in Ref. 1 [generalizable to $GL_q(N)$]. All those cases involved two projectors (the sum being I). As soon as this number increases [such as already for $SO_q(3)$], the rhs has a more complex structure. Our starting point (the general solution of $\hat{R}TT$) is exactly the same here. But only in the very particular case (35) one has a linear structure on the right.

(3) In Sec. III we present all the relations involving the coordinates and the differentials. But much remains to be done to better understand the noncommutative space thus obtained. The properties of the Φ's introduced in (49) deserve study. To render the geometry more transparent one should construct the ''frame basis'' in terms of operators commuting with the algebra. (See Refs. 5 and 7 and sources cited there.) Thus equipped, one can study possible attractive consequences concerning the metric of implementing $\hat{R}_c$ as in (53). We hope to explore these aspects elsewhere.

(4) After Ref. 1 we emphasize here again the complementary nature of MBE and Baxterization. We provide a simple new example of the latter in (57). Let us repeat another point made in Ref. 1. The standard braid equation can be made to correspond to the third Reidemeister move in knot theory. Hence (54) can be viewed as a parametrization of this move. It would be worth exploring in the context of knot theory whether this provides access to a richer class of invariants.

(5) Here we have studied coboundary $\hat{R}$ martices in vector representations in terms of projectors. An approach using Drinfeld's transformation can be found in Ref. 8.

(6) Finally, let us recapitulate the remarkable properties of the solution provided by (38). It satifies the $\hat{R}TT$ equation for the standard group relations of $SO_q(3)$. It satisfies the standard braid equation [(34) with zero rhs]. It continues (as shown in Appendix B) to be nontrivial even for $q=1$. It can be relatively simply Baxterized as shown at the end of Sec. IV. This sets the stage for a full study of the corresponding integrable model. This also suggests a search of analogous new solutions, more generally, for $SO_q(N)$ and $Sp_q(N)$ and also for higher dimensional representations of $SO_q(3)$. We hope to explore such possibilities elsewhere.

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APPENDIX A: GENERAL STRUCTURE OF MBE

In the notation of (30) or (40),

$$\hat{R}=I+vP^{(-)}+wP^{(0)}. \tag{A1}$$

For elucidating the sructure of the consequent MBE we start with a number of definitions and auxiliary relations.

We define

$$X_1=P^{(-)}_{(12)},\quad X_2=P^{(-)}_{(23)},\quad Y_1=P^{(0)}_{(12)},\quad Y_2=P^{(0)}_{(23)}. \tag{A2}$$

The orthonormal properties of the projectors imply [for $i=(1,2)$]

$$X_i^2=X_i,\quad Y_i^2=Y_i,\quad X_iY_i=Y_iX_i=0. \tag{A3}$$

We also define

$$S_1=X_1-X_2,\quad S_2=Y_1-Y_2, \tag{A4}$$

$$S_3=(X_1X_2Y_1+X_1Y_2X_1+Y_1X_2X_1)-(X_2X_1Y_2+X_2Y_1X_2+Y_2X_1X_2), \tag{A5}$$

$$S_4=(Y_1Y_2X_1+Y_1X_2Y_1+X_1Y_2Y_1)-(Y_2Y_1X_2+Y_2X_1Y_2+X_2Y_1Y_2), \tag{A6}$$

$$S_5=(X_1X_2X_1-X_2X_1X_2),\quad S_6=(Y_1Y_2Y_1-Y_2Y_1Y_2). \tag{A7}$$

Using these definitions and the properties (A3) one obtains quite generally,

$$\hat{R}_{12}\hat{R}_{23}\hat{R}_{12}-\hat{R}_{23}\hat{R}_{12}\hat{R}_{23}=(v+v^2)S_1+(w+w^2)S_2+v^2wS_3+vw^2S_4+v^3S_5+w^3S_6. \tag{A8}$$

The S's depend on q *only*. The dependence on (v,w) is explicitly displayed in the coefficients of (A8).

Now we exploit systematically the constraints on the S's provided by the known solutions, namely, (32) and (34)–(37).

The rhs of (A8) must vanish for the braid solutions (32), namely, for

$$v=-(1+q^{-2}),\quad w=-(1-q^{-3}), \tag{A9}$$

and also for

$$v=-(1+q^2),\quad w=-(1-q^3). \tag{A10}$$

Implementing these (for $q\neq 1$) we choose to express (S_3,S_4) as

$$S_3=\frac{q^2}{(q^2+1)(q^2+q+1)}S_1-\frac{q^2}{(q^2+1)^2}S_2-\frac{(q^2+1)}{(q^2+q+1)}S_5-\frac{(q^3-1)^2}{q(q^2+1)^2}S_6, \tag{A11}$$

$$S_4=\frac{q^3}{(q^3-1)^2}S_1+\frac{q^2}{(q^2+1)(q^2+q+1)}S_2-q\frac{(q^2+1)^2}{(q^3-1)^2}S_5+\frac{(q^3-1)(q-1)}{q(q^2+1)}S_6. \tag{A12}$$

Now note that implementing (A3) one can express the rhs of (34) as

$$l_1(\hat{R}_{12}-\hat{R}_{23})+l_2(\hat{R}_{12}{}^2-\hat{R}_{23}{}^2)=(l_1v+l_2(2v+v^2))S_1+(l_1w+l_2(2w+w^2))S_2. \quad \text{(A13)}$$

Combining this result with (case 1) or (35) one obtains (since $v=0$, $l_2=0$)

$$l_1wS_2=\left((w+w^2)+\frac{q^2w^3}{(q^2+q+1)^2}\right)S_2=(w+w^2)S_2+w^3S_6. \quad \text{(A14)}$$

Hence

$$S_6=q^2(q^2+q+1)^{-2}S_2. \quad \text{(A15)}$$

From (A11), (A12) and (A15) one obtains

$$S_3=\frac{q^2}{(q^2+1)(q^2+q+1)}S_1-\frac{q(q^2-q+1)}{(q^2+1)^2}S_2-\frac{(q^2+1)}{(q^2+q+1)}S_5, \quad \text{(A16)}$$

$$S_4=\frac{q^3}{(q^3-1)^2}S_1+\frac{q(q^2-q+1)}{(q^2+1)(q^2+q+1)}S_2-q\frac{(q^2+1)^2}{(q^3-1)^2}S_5. \quad \text{(A17)}$$

Combining all the preceding results one finally obtains

$$\begin{aligned}&\hat{R}_{12}\hat{R}_{23}\hat{R}_{12}-\hat{R}_{23}\hat{R}_{12}\hat{R}_{23}\\&\quad=c_1S_1+c_2S_2+c_5S_5\\&\quad=c_1(P^{(-)}_{(12)}-P^{(-)}_{(23)})+c_2(P^{(0)}_{(12)}-P^{(0)}_{(23)})+c_5(P^{(-)}_{(12)}P^{(-)}_{(23)}P^{(-)}_{(12)}-P^{(-)}_{(23)}P^{(-)}_{(12)}P^{(-)}_{(23)}).\end{aligned} \quad \text{(A18)}$$

Here

$$\begin{aligned}c_1&=v+v^2+\frac{v^2wq^2}{(q^2+1)(q^2+q+1)}+vw^2\frac{q^3}{(q^3-1)^2},\\c_2&=w+w^2+\frac{w^2vq(q^2-q+1)}{(q^2+1)(q^2+q+1)}-wv^2\frac{q(q^2-q+1)}{(q^2+1)^2}+\frac{w^3q^2}{(q^2+q+1)^2},\\c_5&=\frac{v}{(q^3-1)^2}((q^3-1)v+(q^2+1)w)((q^3-1)v-q(q^2+1)w).\end{aligned} \quad \text{(A19)}$$

As checks one verifies that $c_1=c_2=c_5=0$ for (A9) and (A10). Moreover, $c_5=0$ for

$$(q^2+1)w=-(q^3-1)v$$

and

$$q(q^2+1)w=(q^3-1)v.$$

Thus one gets back, respectively, case 2 of (36) and case 3 of (37).

The form (A18) makes the dependence on (v,w) entirely explicit, the c's being given by (A19) and the S's depending only on q. This is particularly suitable for our purpose. The P's can be reexpressed in terms of $\hat{R}(v,w)$ using (20). But only for $c_5=0$ [cases 1–3 of (35)–(37), respectively] one obtains a relatively simple form as in (34). For S_5 there is no crucial simplification as for S_6 in (A15). Setting $w=0$ in (A18) one gets no new simplification but an identity.

Throughout this article the projectors $P^{(-)}$ and $P^{(0)}$ have served as the essential building blocks. They can be easily extracted comparing (30) and (31). But for completeness and convenience they are presented below explicitly.

$$(q^2+1)P^{(-)}=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -q & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q & 0 & (q-1)\sqrt{q} & 0 & -q & 0 & 0 \\ 0 & -q & 0 & q^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & (q-1)\sqrt{q} & 0 & (q-1)^2 & 0 & -(q-1)\sqrt{q} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -q & 0 \\ 0 & 0 & -q & 0 & -(q-1)\sqrt{q} & 0 & q & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -q & 0 & q^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{A20}$$

$$(q^2+q+1)P^{(0)}=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \sqrt{q} & 0 & q & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{q} & 0 & q & 0 & q\sqrt{q} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q & 0 & q\sqrt{q} & 0 & q^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{A21}$$

APPENDIX B: NONTRIVIAL BE FOR $q=1$

We pointed out in Sec. II that for $a=0$ and b satisfying (38) one obtains two solutions of BE (not modified, with vanishing rhs). Setting

$$q=1$$

in (38) one obtains

$$b^2+3b+1=0$$

or

$$b=\tfrac{1}{2}(-3\pm\sqrt{5})\equiv -e^{\mp m}. \tag{B1}$$

[It is amusing to note the relation of b, or rather that of $-(b+1)$ with the famous Golden Mean i.e., $\frac{1}{2}(\sqrt{5}-1)$.]

Now one obtains

$$\hat{R}(\mp m)=I-3e^{\mp m}\hat{P}^{(0)}, \tag{B2}$$

where the projector $\hat{P}^{(0)}$ is obtained from $P^{(0)}$ by setting $q=1$. Thus

$$3\hat{P}^{(0)}=\begin{pmatrix} 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&1&0&1&0&1&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&1&0&1&0&1&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&1&0&1&0&1&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0 \end{pmatrix}.$$

From (B2) one easily obtains the nontrivial Hecke condition

$$(\hat{R}(\mp m)-I)(\hat{R}(\mp m)+(3e^{\mp m}-1)I)=0. \tag{B3}$$

Thus $\hat{R}(\mp m)$ are *not* coboundary matrices. They cannot be obtained by twisting I since

$$(\hat{R}(\mp m))^2\neq I.$$

For

$$q=1, \quad b=0, \quad a=-1 \tag{B4}$$

again [from (30), (36), and (37)] one obtains $\hat{R}$ satifying BE given by

$$\hat{R}=I-2\hat{P}^{(-)}, \tag{B5}$$

where $\hat{P}^{(-)}$ is obtained from $P^{(-)}$ setting $q=1$ in (A20).

But now, in contrast to (B3), one has

$$\hat{R}^2=I.$$

The $R(\mp m)$ satisfying YB (Yang–Baxter equation) can be obtained from (B2) as

$$R(\mp m)=P\hat{R}(\mp m)=P-3e^{\mp m}\hat{P}^{(0)}, \tag{B6}$$

where the matrix P [permuting the rows (2,4), (3,7), (6,8)] leaves $\hat{P}^{(0)}$ invariant.

In Hieterinta's classification[9] of 4×4 R matrices appear examples without free parameters. Such a case has been studied[10] in the context of ''exotic bialgebras.'' Here we have obtained 9×9 examples of such matrices.

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Understanding singularities in Cartan's and null surface formulation geometric structures

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In this work we establish a relationship between Cartan's geometric approach to third-order ordinary differential equations and the three-dimensional null surface formulation. We then generalize both constructions to allow for caustics and singularities that necessarily arise in these formalisms. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1408282]

I. INTRODUCTION

During the first half of the twentieth century, while trying to understand the group of transformations of differential equations, Cartan laid down the foundations of modern differential geometry and established a link between analysis and geometry. One particular example that will be discussed in this work shows Cartan's approach to the classification of solutions of ordinary differential equations (ODEs).[1–3] Consider the two-dimensional (2D) space E^2 with local coordinates (x,y) and the following third-order ODE,

$$y'''=F(x,y,y',y''), \tag{1}$$

with ''prime'' denoting the derivative with respect to the independent variable.

If one performs a coordinate transformation on E^2 one gets another ODE that is trivially related to Eq. (1). Cartan thus considered the issue of how to classify solutions of third-order ODEs into equivalence classes, with two solutions belonging to the same class if the corresponding ODEs were related by a coordinate transformation on E^2. It is clear that one can spend many hours before finding the appropriate coordinate transformation that will turn one ODE into the other. Cartan showed that with the general solution of a given third-order ODE, like that shown previously, one can explicitly construct a connection one form on a four-dimensional (4D) space E^4 with local coordinates (x,y,y',y'') (the details are presented in Sec. II). Furthermore, Cartan showed that two third-order ODEs are equivalent if their corresponding solutions yield the same geometric structure on E^4. Cartan also showed that when F satisfies a given partial differential equation (PDE) on E^4, symbolically written as $M[F]=0$, then the connection is torsion free and a unique conformal structure can be given on the solution space [three-dimensional (3D) parameter space] of the starting ODE.

It is worth mentioning that the same equation $M[F]=0$ arises in the three-dimensional version of the so-called null surface formulation (NSF) of general relativity (GR).[4] As we will see in the following, this is not mere coincidence since we will show that the 3D version of NSF is almost contained in one of Cartan's works.[1] Finding the correspondence between these two constructions was one of the motivations for writing this work.

In the NSF the main variable is a function $u=Z(\phi)$, with $\phi\in S^1$, subject to a third-order ordinary differential equation of the form

$$u'''=\Lambda(\phi,u,u',u''), \tag{2}$$

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where the function Λ is restricted to satisfy the "metricity condition" $M[\Lambda]=0$. The general solution of (2) is given by $u=Z(x^a,\phi)$, with the constants of integration x^a taken as coordinates of the 3D solution manifold E^3. From this solution a space–time metric for E^3 can be constructed such that the level surfaces of Z are null foliations of E^3 for each fixed value of ϕ. Furthermore, the covector $l_a \equiv \partial_a Z$ spans, for fixed values of x^a, the circle of null directions and thus the parameter $\phi \in S^1$. Except for the relabeling of functions and the topology of the starting space E^2, both formulations share many geometric features, with Cartan emphasizing the role of the connection one-form and the NSF the explicit construction of a metric on the solution space of (2).

But a key point arises by noting that, by assumption, both formulations are local constructions in the 2D manifold. It follows from this fact that the solutions to (1) are families of smooth curves and (as we will see in the following) that the level sets $Z(x^a,\phi)=\text{const}$ are smooth null surfaces of the induced metric in the 3D solution space. However, we know that characteristic surfaces develop caustics and singularities as a result of the "focusing" properties of null geodesic congruences established in GR singularity theorems.[5] Moreover, the solutions to (1) that yield these null surfaces with caustics cannot be smooth curves on E^2, so they must develop self-intersections and singular points.

A second motivation for this work is thus to consider the nondiffeomorphic generalization of these geometric constructions in order to account for the folds and nondifferentiable edges of curves on E^2 that yield null congruences with caustics. The first step is to introduce the curves on E^2 according to Arnold's theory of Lagrangian manifolds as[6]

$$u=G(p)-pG'(p), \tag{3}$$

$$\phi=-G'(p); \tag{4}$$

[$G(p)$ is called the generating function]. Although G may be smooth, the curve $(u(p),\phi(p))$ might have self-intersections and singular points if $\phi(p)$ is not injective. The question is how to find the proper G such that (3) and (4) define a null surface by setting u and ϕ constant. As we will show in this work, curves with singular points in E^2 will induce null surfaces with caustics in E^3. Conversely, we will also show that if the null surfaces have conjugate points then the corresponding families of curves on E^2 have singularities.

In this reformulation, Eq. (2) for Z is changed to an equation for G, of the same type,

$$\frac{\mathrm{d}^3 G}{\mathrm{d}p^3}=\tilde{\Lambda}(p,G,G',G'') \tag{5}$$

and the metricity condition $M[\Lambda]=0$, which becomes singular at a caustic point, yields an entirely well-behaved equation $\tilde{M}[\tilde{\Lambda}]=0$ whose solutions are the "appropriate" right-hand side of (5). As we will see in an example, among the solutions of (5) we obtain generating functions of caustics as listed in Ref. 6. This result encounters an immediate application inside the $2+1$ NSF and also in the full theory because, to be in complete agreement with the standard GR formulation, it always remained as an open problem to write the metricity conditions of NSF in a form that explicitly shows the existence of the singular solutions.[7]

The work is organized as follows: In Sec. II we first give an account of Cartan's geometric construction obtained in Ref. 1 starting from the third-order equation (2). This review is presented in modern language since the original reference was written before modern differential geometry was invented and it is very difficult to follow. (It is worth mentioning that one "variation" on Cartan's work has appeared in the literature[8] but it is different from the original construction.) We then give a brief review of the NSF in 3D and show that this formalism is a particular case of Cartan's construction. In Sec. III we proceed to generalize the local analysis of Sec. II and write the regularized metricity condition $\tilde{M}[\tilde{\Lambda}]=0$. We also find a relation between curves with caustics on E^2 and null surfaces with conjugate points on E^3. A simple example shows how to generate

germs of caustics for the solutions to (5). We conclude this work with some comments on the possibility of attaching a similar geometric structure to the original construction of the NSF in four dimensions.

II. GEOMETRIC APPROACHES TO A THIRD-ORDER ODE

In this section we present two geometric constructions that arise from a third-order ordinary differential equation

$$u'''=\Lambda(\phi,u,u',u''), \tag{6}$$

where (ϕ,u) are coordinates on the cylinder $S^1\times\mathbf{R}$. As we will see in the following, it turns out that one of these constructions is almost contained as a particular case of the other.

A. Cartan's construction

We first present Cartan's approach,[1,3] achieved by interpreting the integral curves $u(\phi,x^a)$ as points $x^a(a=1,2,3)$ of the three-dimensional solution space E^3, attaching to it a Lorenztian metric g_{ab} and giving the structure of a one-dimensional fiber bundle over E^3, with $\phi\in[0,2\pi)$ as the coordinate of the fiber. On the base space we attach a ''null frame'' satisfying

$$\mathbf{e}_1\cdot\mathbf{e}_1=\mathbf{e}_1\cdot\mathbf{e}_2=\mathbf{e}_3\cdot\mathbf{e}_3=\mathbf{e}_2\cdot\mathbf{e}_3=0,\quad \mathbf{e}_2\cdot\mathbf{e}_2+\mathbf{e}_1\cdot\mathbf{e}_3=0, \tag{7}$$

where $\mathbf{e}_i\cdot\mathbf{e}_j=g_{ab}\,\mathbf{e}_i{}^a\mathbf{e}_j{}^b=g_{ij}$. In terms of the dual basis $\sigma_a{}^i$ of the null frame, the metric can be written as

$$g_{ab}=g_{ij}\,\sigma_a{}^i\sigma_b{}^i=\sigma_a{}^2\otimes\sigma_b{}^2-2\sigma_a{}^{(1}\otimes\sigma_b{}^{3)},$$

where we have chosen $g_{13}=-1$. Note that for fixed values of ϕ, the three functions

$$(\theta^0,\theta^1,\theta^2)\equiv(u,\omega,r)\equiv(u,u',u''), \tag{8}$$

can be taken as coordinates on the base space of the bundle. Thus, each point of the bundle is locally described by (ϕ,u,ω,r).

Equation (6) yields the associated pfaffian system[9] on the bundle which, written in terms of these coordinates, reads

$$\begin{aligned}\sigma^1&=\mathrm{d}u-\omega\,\mathrm{d}\phi,\\ \sigma^2&=\mathrm{d}\omega-r\,\mathrm{d}\phi,\\ \sigma^3&=\lambda(\mathrm{d}r-\Lambda\,\mathrm{d}\phi-\alpha\,\sigma^1-\beta\,\sigma^2),\end{aligned} \tag{9}$$

where α, β, and λ are functions to be determined. The bundle of null directions is constructed by selecting σ^i as the soldering forms and the $\sigma_a{}^i$ as the projections of (9) to the base space. Note that the solution of (6) will give null surfaces $S\in E^3$ by setting $u(\phi,x^a)=\text{const}$, $\phi=\text{const}$. The bundle constructed in this way will be denoted by $\mathcal{N}(E^3,g)$.

To characterize the geometric structure defined from (6), Cartan introduces a connection and a covariant exterior derivative as

$$D\mathbf{e}_i=\omega_i{}^j\mathbf{e}_j,$$

where D is the covariant exterior derivative with respect to this connection (see Refs. 10–12) and $\omega_i{}^j$ are the connection one-forms. Furthermore, Cartan demands that the connection will be compatible with the metric in the sense that a null frame remains null under parallel transport, i.e.,

$$Dg_{ij}=2\overline{\omega}\,g_{ij},$$

where $\overline{\omega}$ is a one-form on the bundle. Therefore,

$$\omega_{ij}+\omega_{ji}=-2g_{ij}\,\overline{\omega},$$

where $\omega_{ij}=\omega_i{}^k g_{kj}$.

It follows from the above that

$$\omega_{11}=\omega_{33}=0, \quad \omega_{13}+\omega_{31}=-2\overline{\omega},$$

$$\omega_{12}=-\omega_{21}, \quad \omega_{23}=-\omega_{32}, \omega_{22}=\overline{\omega}.$$

Thus, the connection is determined by four arbitrary one-forms, namely

$$\omega_{12}, \omega_{23}, \omega_{31}, \quad \overline{\omega}.$$

Note that σ^i, ω_{23} are linearly independent forms in $\mathcal{N}(E^3, g)$. This assertion can be understood from the geometrical meaning that these forms have.

(1) $\sigma^1=\omega_{23}=0$ is the differential system for null 2 surfaces, since on this surface $D\ \mathbf{e}_3=\omega_{13}\ \mathbf{e}_3$ and $D\ \mathbf{e}_2=-\omega_{22}\ \mathbf{e}_2+\omega_{12}\ \mathbf{e}_3$.
(2) $\sigma^1=\sigma^2=\omega_{23}=0$ is the differential system for null geodesic, since on this curve $D\ \mathbf{e}_3=\omega_{13}\ \mathbf{e}_3$.
(3) $\sigma^1=\sigma^2=\sigma^3=0$ is the differential system for a point of E^3.

Note also that the vanishing of σ^1 and ω_{23} is equivalent to imposing $u=\text{const}$, $\phi=\text{const}$. Thus, ω_{23} can be chosen to be of the form $\omega_{23}=\mu(\mathrm{d}\phi+\gamma\sigma^1)$ with γ and μ being *a priori* arbitrary.

The idea is to write the nontrivial connection one-forms in terms of the basis σ^i, ω_{23} and then to impose certain conditions on the torsion and curvature of the connection to uniquely determine the functions α, β, γ, λ, and μ.

Using Cartan's structure equations,

$$\Theta^i=\mathrm{d}\sigma^i+\omega^i{}_j\wedge\sigma^j, \tag{10}$$

$$\Omega^i{}_j=\mathrm{d}\omega^i{}_j+\omega^i{}_k\wedge\omega^k{}_j, \tag{11}$$

and imposing

$$\Theta^1=\Theta^2=0, \quad \Theta^3=A\ \sigma^1\wedge\omega_{23} \tag{12}$$

on the torsion two-forms, we find that

$$\lambda=\mu=1,$$

$$\alpha=\tfrac{1}{3}\partial_r\Lambda,$$

$$\beta=\alpha^2-\frac{1}{2}\frac{\mathrm{d}\alpha}{\mathrm{d}\phi}+\frac{1}{2}\partial_\omega\Lambda,$$

where

$$\frac{\mathrm{d}F}{\mathrm{d}\phi}(u,\omega,r,\phi)=\partial_\phi F+\omega\ \partial_u F+r\ \partial_\omega F+\Lambda\,\partial_r F \tag{13}$$

for any function $F(u,\omega,r,\phi)$. Equation (12) has the following geometrical meaning: Given a point in E^3 and two vectors, we construct a geodesic parallelogram from that point (see Ref. 13); then in order to come back to the same point, we only need a translation in the null direction $\mathbf{e}_3$. If the parallelogram is on the null surface (when $\sigma^1=0$ and $\omega_{23}=0$), no translation is needed.

Furthermore, if we require

$$\Omega_{23}=B\sigma^1\wedge\sigma^2+C\sigma^1\wedge\sigma^3, \tag{14}$$

we find that

$$\gamma=\tfrac{1}{2}\partial_r\alpha.$$

The geometrical meaning of (14) is that the above-mentioned curvature two-form should vanish when $\mathbf{e}_3$ is parallely transported around a parallelogram with one of its sides being the null geodesic generated by $\mathbf{e}_3$.[1]

Summarizing, conditions (12) and (14) suffice to uniquely determine the non trivial components of the connection one-form. They are given by

$$\begin{aligned}
\omega_{23}&=\mathrm{d}\phi+\gamma\sigma^1,\\
\overline{\omega}&=-\alpha\,\mathrm{d}\phi+\left(2\frac{\mathrm{d}\gamma}{\mathrm{d}\phi}-\partial_\omega\alpha\right)\sigma^1-2\gamma\sigma^2,\\
\omega_{31}&=\alpha\,\mathrm{d}\phi+\left(\frac{\mathrm{d}\gamma}{\mathrm{d}\phi}+\alpha\gamma\right)\sigma^1+\gamma\sigma^2,\\
\omega_{12}&=-\beta\,\mathrm{d}\phi+(\partial_u\alpha-\partial_\omega\beta+3\beta\gamma-\alpha\partial_r\beta)\sigma^1+\left(2\frac{\mathrm{d}\gamma}{\mathrm{d}\phi}-\partial_\omega\alpha\right)\sigma^2-\gamma\sigma^3.
\end{aligned} \tag{15}$$

Using the equations in (15) one determines the remaining coefficients for the torsion and curvature in terms of Λ. In particular, the only nontrivial coefficient of the torsion is given by

$$A=\frac{1}{6}\frac{\mathrm{d}^2\partial_r\Lambda}{\mathrm{d}\phi^2}-\frac{1}{3}\partial_r\Lambda\frac{\mathrm{d}\partial_r\Lambda}{\mathrm{d}\phi}-\frac{1}{2}\frac{\mathrm{d}\partial_\omega\Lambda}{\mathrm{d}\phi}+\frac{2}{27}(\partial_r\Lambda)^3+\frac{1}{3}\partial_\omega\Lambda\partial_r\Lambda+\partial_u\Lambda.$$

A connection compatible with a Lorenztian metric constructed in this way was called by Cartan a normal metric connection. The main result of Cartan can be stated as follows:

Theorem 2.1: *To each third-order ordinary differential equation [up to diffeomorphism in (ϕ,u)] one can associate a null bundle with a unique normal metric connection and vice versa, i.e., to each bundle of null directions with normal metric connection one can associate a third-order ordinary differential equation up to diffeomorphism.*

One special class of Cartan's connection is particularly interesting to us. If we impose $A=0$, the connection is torsion free and Monge's equation

$$g_{ab}Y^aY^b=0$$

is constant along the fiber, since

$$\frac{\mathrm{d}g_{ab}}{\mathrm{d}\phi}=-\frac{2}{3}\partial_r\Lambda g_{ab}+2A\sigma_a{}^1\otimes\sigma_b{}^1. \tag{16}$$

Thus, the condition $A=0$ defines a unique conformal structure on the solution space of (6). Moreover, $A=0$ is also the condition that the third-order ODE must satisfy so that the contact of two neighboring integral curves can be given by a Monge's equation of the second order between the parameters of those curves.[14]

Note that even in the case that the connection is torsion free, the metric so obtained depends on ϕ, i.e., we have a monoparametric family of conformally related metrics.

B. NSF's construction

We now turn our attention to the NSF formulation, in which we have a function $u=Z(\phi)$ satisfying a third-order ODE

$$u'''=\Lambda(\phi,u,u',u''), \tag{17}$$

with $\phi\in S^1$ and Λ a smooth generic function. The solutions to this equation are of the form $u=Z(x^a;\phi)$, with $x^a(a=1,2,3)$ representing three constants of integration which define the 3D manifold of solutions E^3 (equivalent to R^3).

Note that the function $Z(x^a;\phi)$ plays a double role, namely:

(1) For each fixed x^a in E^3, $u=Z(x^a;\phi)$ yields a curve C_x on E^2 with coordinates (u,ϕ); these curves will be called cuts.
(2) Fixing (u,ϕ) in E^2, the relation $u=Z(x^a;\phi)$ now defines a surface $S_{(u,\phi)}$ living in E^3.

It is important to realize that the analysis is merely done at a local level, so that the curve C_x is certainly the graph of a function in E^2 and $S_{(u,\phi)}$ turns out to be a smooth surface in E^3.

The key assumption of NSF comes when we require that, for any value of u and ϕ, $S_{(u,\phi)}$ be indeed a null surface of some space–time metric $g_{ab}(x^a)$ to be attached to E^3. This condition implies that for fixed values of x^a and arbitrary values of ϕ the gradient of Z satisfies

$$g^{ab}(x^a)\nabla_a Z(x^a;\phi)\nabla_b Z(x^a;\phi)=0. \tag{18}$$

Note that as the families of foliations intersect at a single but arbitrary point x^a, the enveloping surface forms the light cone of the point x^a. Thus, the parameter ϕ spans the circle of null directions.

The idea now is to consider (18) as an algebraic equation from which the five components of the conformal metric can be determined in terms of $\nabla_a Z(x^a,\phi)$. Given an arbitrary function Z, the problem has no solution since we have an infinite number of algebraic equations (one for each value of ϕ) for five unknowns. Therefore, we must impose conditions on $Z(x^a,\phi)$ so that a solution exists. The solution and conditions are obtained by repeatedly operating $\mathrm{d}/\mathrm{d}\phi$ on (18). They are best expressed when written in the canonical coordinate system (u,ω,r) given in Eq. (8). The final expression for the metric components reads

$$g^{ij}=\Omega^2\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & -\frac{1}{3}\partial_r\Lambda \\ 1 & -\frac{1}{3}\partial_r\Lambda & -\frac{1}{3}\partial(\partial_r\Lambda)+\frac{1}{9}(\partial_r\Lambda)^2+\partial_\omega\Lambda \end{pmatrix}, \tag{19}$$

where the conformal factor must satisfy the differential equation (see Ref. 4 for details)

$$\frac{\mathrm{d}}{\mathrm{d}\phi}\Omega=\frac{1}{3}\partial_r\Lambda\,\Omega,$$

so that the metric is independent of ϕ. Note that the above-mentioned equation is invariant under $\Omega(x,\phi)\to\Omega'(x,\phi)=f(x)\Omega(x,\phi)$ for an arbitrary $f(x)$. This freedom is a consequence of the conformal invariance of the formulation.

The metricity condition is given by

$$M[\Lambda]\equiv 2\left(\frac{\mathrm{d}(\partial_r\Lambda)}{\mathrm{d}\phi}-\partial_\omega\Lambda-\frac{2}{9}(\partial_r\Lambda)^2\right)\partial_r\Lambda-\frac{\mathrm{d}^2(\partial_r\Lambda)}{\mathrm{d}\phi^2}+3\frac{\mathrm{d}(\partial_\omega\Lambda)}{\mathrm{d}\phi}-6\partial_u\Lambda=0,$$

and constraints the available Λ's that must enter in the differential equation (17), for only if $M[\Lambda]=0$ holds, one is able to construct from the solutions $Z(x^a;\phi)$ to the ODE a metric according to (19) such that the level surfaces $S_{(u,\phi)}$ of Z are its characteristic surfaces. Note that this condition is the one deduced by Cartan imposing the connection in the three-dimensional manifold E^3 to be torsion free $(A=0)$.

Summarizing, one solves $M[\Lambda]=0$, which is a partial differential equation in the variables (u,ω,r,ϕ) and, denoting by $\Lambda_0(u,\omega,r,\phi)$ its solution and using the coordinates definitions (8), Eq. (17) becomes

$$Z'''=\Lambda_0(\phi,Z,Z',Z''), \tag{20}$$

which is the ODE whose solutions $Z(x^a;\phi)$ allow for the construction of a metric g_{ab} on E^3 such that the level surfaces of Z are its null hypersurfaces.

Remark 2.1: It is clear from the above that the NSF construction is the special case of Cartan's geometric structure with vanishing torsion.

III. SINGULARITIES IN TERMS OF SMOOTH MANIFOLDS

By assumption, both Cartan's and the NSF are local constructions in the 2D manifold. It follows from this that the cuts $C_x\subset E^2$ are families of smooth curves and (as we will see in the following) that the level sets $Z=u_0$ are smooth null surfaces of the induced metric in the 3D solution space.

It also follows from the above-mentioned assumption that these formalisms are not capable of including the caustics that null surfaces necessarily possess.[6,15,16] Moreover, one might foresee that the families of cuts that yield these null surfaces with caustics will also fail to be smooth, developing self-intersections and singular points. Thus, in this section, we are faced with the problem of generalizing the geometric constructions presented in Sec. II to include the description of singularities of both, cuts and null hypersurfaces.

Our starting assumption is that the cuts develop caustics in the 2D space. Technically this means that cuts are projections onto E^2 of a (smooth) Legendrian submanifold and the caustics arise where the projection map fails to be one to one. In a similar way as in Ref. 17, we use a generating function to describe a cut in the neighborhood of a caustic. Using this function we will be able to see how Λ diverges at a caustic point. Since the original equation and the metricity condition become useless around that point, we will obtain a regularized metricity condition to select the class of generating functions which yield conformal metrics on the solution space. We will also show that caustics come inseparably paired in the Cartan and NSF constructions, in the sense that the existence of caustics in the cut implies the same singular behavior in the null surfaces of the manifold E^3 (and vice versa). Section III C presents an example of a generating function in a Minkowskian space–time.

A. The generating function

The regular solutions of (17) can be used to define smooth curves on the so-called projective cotangent space of E^2 with local coordinates (u,ϕ,π), where π is the momentum canonically conjugated to ϕ. The curves are given by

$$u=Z(x^a;p),$$

$$\phi=p,$$

$$\pi = \frac{dZ}{dp},$$

with x^a parameters to be interpreted as coordinates in the solution space. These smooth curves are called Legendrian submanifolds and the projection of these submanifolds onto the space (u,ϕ) gives the local description of the cuts of E^2. The above-mentioned equations describe the Legendrian submanifolds in the diffeomorphic region since the coordinate ϕ is used as a parameter to describe these curves.

In order to describe the cuts in regions containing caustic points, we introduce a generating function of the form $G=G(x^a;p)$. In this case the Legendrian submanifold is given locally as

$$\begin{aligned} u &= G - pG', \\ \phi &= -G', \\ \pi &= p, \end{aligned} \tag{21}$$

where G' denotes the derivative of G with respect to p holding x^a fixed. The equations of (21) locally describe smooth curves on the projective cotangent space of E^2. Note that the projection of these curves onto the space (u,ϕ) is not necessarily a diffeomorphism, since ϕ fails to be injective in p when G'' vanishes. Therefore, this description includes caustic points in a natural way. It is easy to see that Λ diverges at the caustic points. For this we analyze the behavior of the coordinates (u,ω,r,ϕ) and the function Λ as we approach a caustic in E^2. These variables, expressed in terms of G and p, become

$$\begin{aligned} u &= G - pG', \\ \omega &= \frac{\mathrm{d}u}{\mathrm{d}\phi} = p, \\ r &= \frac{\mathrm{d}\omega}{\mathrm{d}\phi} = -(G'')^{-1}, \end{aligned} \tag{22}$$

and since $\Lambda = \mathrm{d}^3u/\mathrm{d}^3\phi$ we obtain

$$\Lambda = \frac{-G'''}{(G'')^3}.$$

Since at a caustic point $G''=0$, we see from Eq. (22) that both u and ω are bounded while r and Λ diverge at that point. One might argue that G could be such that G''' also vanishes at a caustic point in such a way that Λ remains finite. However, smoothness requires G to be expandable as a polynomial around a caustic point. Thus G''' is always a polynomial of lower degree than G'' and the previous argument does not apply. It follows from these considerations that (a) the third-order ODE (17) will not be defined around caustic points and (b) the coordinate system, metric construction, and metricity condition will not be regular on the 3D solution space.

We look then for a regular third-order ODE where the right-hand side of this equation satisfies a regularized metricity condition. For this we introduce a new set of coordinates (G,G',G'',p). In terms of these coordinates we have

$$G''' = \tilde{\Lambda}(G,G',G'',p) = -(G'')^3\Lambda(G-pG',p,-(G'')^{-1},-G')$$

and the metricity condition $\tilde{M}[\tilde{\Lambda}]=0$ becomes

$$\tilde{M}[\tilde{\Lambda}]=G''\left(2(\tilde{\Lambda}_p+G'\tilde{\Lambda}_G)\tilde{\Lambda}_{G''}-3\tilde{\Lambda}\frac{\mathrm{d}}{\mathrm{d}p}\tilde{\Lambda}_{G''}-5\frac{\mathrm{d}\tilde{\Lambda}}{\mathrm{d}p}\tilde{\Lambda}_{G''}+2\tilde{\Lambda}(\tilde{\Lambda}_{G''})^2\right)$$
$$+G''\left(3\frac{\mathrm{d}^2\tilde{\Lambda}}{\mathrm{d}p^2}-3\frac{\mathrm{d}}{\mathrm{d}p}(\tilde{\Lambda}_p+G'\tilde{\Lambda}_G)\right)+(G'')^2\left(2\tilde{\Lambda}_{G''}\frac{\mathrm{d}}{\mathrm{d}p}\tilde{\Lambda}_{G''}-6\tilde{\Lambda}_G\right)$$
$$-(G'')^2\left(\frac{4}{9}(\tilde{\Lambda}_{G''})^3+\frac{\mathrm{d}^2}{\mathrm{d}p^2}\tilde{\Lambda}_{G''}\right)+3\tilde{\Lambda}\left((\tilde{\Lambda}_p+G'\tilde{\Lambda}_G)+\tilde{\Lambda}\tilde{\Lambda}_{G''}-\frac{\mathrm{d}\tilde{\Lambda}}{\mathrm{d}p}\right)$$
$$=0, \tag{23}$$

where $\mathrm{d}F/\mathrm{d}p=F_p+G'\ F_G+G''\ F_{G'}+\tilde{\Lambda}\ F_{G''}$ for any function $F(G,G',G'',p)$. Note that Eq. (23) is regular in a neighborhood of the caustic $(G''=0)$.

Finally, to obtain null surfaces and study them near a caustic, we proceed in a similar way as we did in the diffeormophic region, i.e., we first solve $\tilde{M}[\tilde{\Lambda}]=0$. Denoting by $\tilde{\Lambda}_0$ a particular solution to this equation we then generate solutions of the ordinary differential equation

$$G'''=\tilde{\Lambda}_0(G,G',G'',p), \tag{24}$$

and construct families of curves with caustics on E^2.

Remark 3.1: Note that in the (G,p) space the solutions to (24) will generate smooth curves. To construct the families of curves with caustics one must use G as the generating function of the contact transformation (21) and the null surfaces are given by the conditions $u=\text{const}$, $\phi=\text{const}$.

Remark 3.2: Note that the contact transformation (21) induces a coordinate transformation (22) which preserves the metric tensor defined on E^3. Thus, Cartan's theorem 2.1 is immediately generalized to include coordinate and contact transformations on E^2.

B. Caustics on null surfaces and cuts

In this section, we prove that the existence of caustic points in the cuts yields the existence of caustic points in the null surfaces of E^3 and vice versa. As it is known (Ref. 5), the divergence of a congruence of null geodesics $\rho=-\nabla_a l^a$ $(l^a=g^{ab}\nabla_a Z)$ becomes infinite at a caustic. Therefore, to prove our assertions, we will derive a relation between ρ of a congruence contained in the null surface and the scalar $Z''(x^a,\phi)$ constructed from the general solution $u=Z(x^a,\phi)$ to (17).

Let l^a be the tangent vector to a geodesic with affine parameter τ, then

$$l^a=\frac{\mathrm{d}x^a}{\mathrm{d}\tau}=g^{ab}\theta^0{}_b=\Omega^2\theta_2{}^a, \tag{25}$$

where $\theta^i{}_b$ and $\theta_j{}^a$ are the form basis and its corresponding dual vector basis associated with the canonical coordinate system (8).

To this tangent vector we associate a triad $\{l^a,m^a,n^a\}$ parallely propagated along the geodesic satisfying

$$m^a m_a=1,\quad n^a n_a=0,\quad l^a m_a=0,\quad l^a n_a=-1,\quad n^a m_a=0.$$

In this frame the metric tensor and the divergence become

$$g_{ab}=m_a m_b-2n_{(a}l_{b)},\quad \rho=m^a m^b\nabla_a l_b,$$

respectively. Since $\theta_1{}^a$ and $\theta_2{}^a$ are coordinate vectors they satisfy

$$\theta_2{}^a\nabla_a\theta_1{}^b=\theta_1{}^a\nabla_a\theta_2{}^b. \tag{26}$$

Expresing the geodesic deviation vector ${\theta_1}^a$ in terms of the triad

$$ {\theta_1}^a = \xi m^a + \alpha l^a, \tag{27} $$

in (26) gives

$$ l^a \nabla_a \xi = \xi m^a m^b \nabla_a l_b = \xi \rho $$

or equivalently

$$ \rho = \xi^{-1} \frac{\mathrm{d}\xi}{\mathrm{d}\tau}. \tag{28} $$

On the other hand we can easily derive a differential equation for the divergence by considering the geodesic deviation equation as follows:

$$ m_c l^a \nabla_a ({\theta_1}^b \nabla_b l^c) = m_c {\theta_1}^a \nabla_a (l^b \nabla_b l^c) + \xi {R_{abd}}^c l^a m^b l^d m_c . $$

Since l^a is a tangent vector of a null geodesic and the triad is parallely propagated along it, using (27) we obtain

$$ m_c l^a \nabla_a (\xi m^b \nabla_b l^c) = \frac{\mathrm{d}\xi}{\mathrm{d}\tau} \rho + \xi \frac{\mathrm{d}\rho}{\mathrm{d}\tau} = \xi \Phi, $$

with $\Phi = {R_{abd}}^c l^a m^b l^d m_c$. Finally, from (28), we see that ρ must satisfy the differential equation

$$ \frac{\mathrm{d}\rho}{\mathrm{d}\tau} + \rho^2 = \Phi. \tag{29} $$

To prove our claims we start with the general solution $u = Z(x^a, \phi)$ to (17), and we assume that the cut $u = Z(x_0^a, \phi)$ has a caustic at $\phi = \phi_0$. As we have seen in Sec. III A, this is equivalent to saying that the function $Z''(x_0^a, \phi)$ diverges at ϕ_0. To show that there is a caustic in the null surface defined by $Z(x^a, \phi_0) = Z(x_0^a, \phi_0) = u_0$, we must prove that $\lim_{r \to \infty} \rho = \infty$, with $r = Z''(x^a, \phi_0)$.

From (25) it follows that

$$ \frac{\mathrm{d}}{\mathrm{d}\tau} = \Omega^2 \frac{\partial}{\partial r} = -\Omega^2 s^2 \frac{\partial}{\partial s}, $$

with the coordinate $s = r^{-1}$. As $\mathrm{d}/\mathrm{d}\tau$ and $\partial/\partial s$ are regular operators near $s = 0$, the factor $\Omega^2 s^2$ must be a nonzero smooth function of s. Hence $\Omega = \mathcal{O}(s^{-1})$, meaning that the conformal factor Ω diverges when we approach a caustic in the cut.

Finally, noting that $g_{11} = g_{ab} {\theta_1}^a {\theta_1}^b$, we express ξ in terms of the conformal factor in the following manner

$$ g_{11} = \Omega^{-2} = g_{ab} (\xi m^a + \alpha l^a)(\xi m^b + \alpha l^b) = \xi^2, $$

therefore

$$ \rho = \frac{\mathrm{d}}{\mathrm{d}\tau} \ln \Omega = -\Omega^2 s^2 \frac{\partial}{\partial s} \ln \Omega, $$

which yields

$$ \rho = \mathcal{O}(s^{-1}). $$

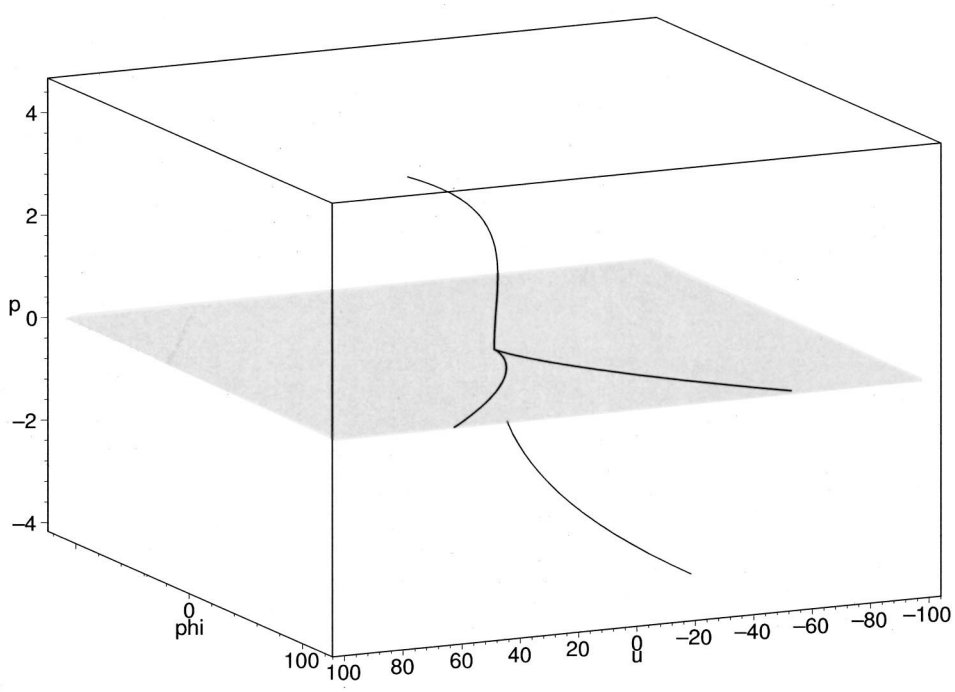

FIG. 1. Legendre submanifold and the corresponding cut for $X^1=X^2=X^3=0$.

We conclude that when s goes to zero (in a singular point of the cut) ρ diverges, i.e., we approach a caustic of the null surface.

It remains now to prove that a caustic in the null surface leads to the same singular behavior in the cut. Suppose that the null surface is defined by $u_0=Z(x^a,\phi_0)$, then near a caustic point x_0^a in the surface the solution of the differential equation (29) in the flat case yields

$$\rho=\frac{1}{\tau-\tau_0},$$

where the singular point x_0^a corresponds to $\tau=\tau_0$. By means of (28) we find $\xi=\Omega^{-1}=\tau-\tau_0$, thus the conformal factor Ω diverges when we approach a caustic in the null surface and since $d\tau=\Omega^{-2}dr$, r diverges (for τ is the affine parameter of the curve and so $d\tau$ is bounded) at x_0^a.

On the other hand, we know that $u=Z(x_0^a,\phi)$ is a solution of (17), then at the singular point x_0^a the function $r=Z''(x_0^a,\phi_0)$ diverges. Thus, the cut $u=Z(x_0^a,\phi)$ also has a caustic point at $\phi=\phi_0$.

Remark 3.3: Note that the spaces E^2 and E^3, used to describe the cuts and null surfaces respectively, are not related in any way. The only tool that was used to prove the above results relating the cuts with null surfaces is the starting ODE (17). This is in contrast with similar results obtained in three and four dimensions where the reciprocity theorem for null congruences and the assumption that E^2 is a hypersurface of E^3 is explicitly used in the proof (Ref. 4).

C. An example: Caustics in flat space

An arbitrary constant function is clearly a solution of the metricity condition $\tilde{M}[\tilde{\Lambda}]=0$, which yields a polynomial of third degree in p for G. Therefore we choose $\tilde{\Lambda}=-1$ and (24) yields

$$G(p,x^a)=-\frac{p^3}{3}+\frac{1}{2}X^1p^2+X^2p+X^3.$$

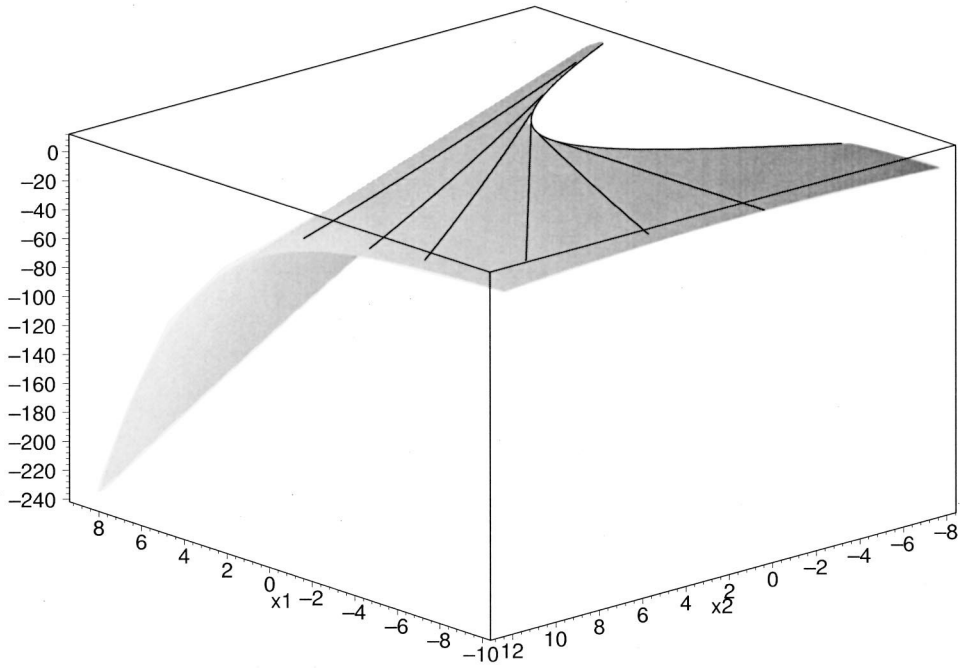

FIG. 2. Null surface for $(u,\phi)=(0,0)$.

With this generating function the Legendre submanifold is given parametrically by

$$u=\tfrac{2}{3}p^3-\tfrac{1}{2}X^1p^2+X^2, \tag{30}$$

$$\phi=p^2-X^1p-X^2, \tag{31}$$

$$p=p. \tag{32}$$

The projection of this submanifold onto E^2, $(u,\phi,p)\rightarrow(u,\phi)$, is the cut and possesses a cusp-like caustic when $p=X^1/2$ (see Fig. 1).

Since ϕ is not an injective function of p, there are two values of p for each ϕ, namely

$$p(\phi)=\tfrac{1}{2}X^1\pm\tfrac{1}{2}\sqrt{(X^1)^2+4\phi+4X^2}. \tag{33}$$

Inserting this expression into Eq. (30) we obtain the corresponding space–time coordinates

$$u=\tfrac{1}{12}((X^1)^2+4\phi+4X^2)^{3/2}+\tfrac{1}{12}(X^1)^3+\tfrac{1}{2}X^1\,\phi+\tfrac{1}{2}X^1\,X^2+X^3,$$

$$\omega=\tfrac{1}{2}X^1+\tfrac{1}{2}\sqrt{(X^1)^2+4\,\phi+4\,X^2}, \tag{34}$$

$$r=\frac{1}{\sqrt{(X^1)^2+4\,\phi+4\,X^2}}.$$

It is clear from (33) that $\sqrt{(X^1)^2+4\phi+4X^2}$ becomes null in the caustic, hence r diverges while u and ω remain bounded at this point.

Figure 2 shows a null surface and null geodesics on it for $(u,\phi)=(0,0)$, which end tangent to the caustic curve. The above-mentioned generating function gives $\Lambda=-r^3$, which yields a flat metric for the conformal factor $\Omega=r$.

IV. CONCLUSIONS

We have shown in this work how the 3D NSF can be recast in terms of a well-known mathematical frame, like Cartan's geometrical theory of differential equations. In this manner, the metricity condition of NSF becomes a simple geometric imposition within Cartan's framework, namely the vanishing of the torsion of the connection in the space E^4.

Moreover, both constructions have been extended from their local scopes to the nondifferentiable regions, in order to account for the singular behavior that null surfaces necessarily possess. As result of this extension,

(1) generalized version of the metricity condition was obtained, whose solutions yield null foliations of a $2+1$ dimensional manifold with caustics and other singularities that the local construction of NSF by definition is not capable of describing.
(2) the singularities of cuts and null surfaces were shown to be closely related in the sense that the singular behavior in one of them induces a similar behavior in the other.

At this point, one can think of applying the same ideas of this work to the original 4D version of NSF.[7,18] This would imply a change from ordinary differential equations over partial ones, since the variable Z now depends on two coordinates (α,β) on S^2 and is subject to the following system of PDEs:

$$Z_{\alpha\alpha}=\Lambda(\alpha,\beta,Z,Z_\alpha,Z_\beta,Z_{\alpha\beta}), \tag{35}$$

$$Z_{\beta\beta}=\Gamma(\alpha,\beta,Z,Z_\alpha,Z_\beta,Z_{\alpha\beta}), \tag{36}$$

where Z_α, Z_β are the partial derivatives of Z with respect to the coordinates. Since the above-given system of equations is integrable, its solution space can be parametrized by four constants x^a, which locally define the 4D solution space M. Thus, one would be able in principle to construct an S^2 bundle over M and attach a similar set of geometric structures that have been presented in this paper.

If this program can be done, the NSF could be described within a well-established context of differential equations; one would be able to give a geometrical interpretation to the metricity conditions (possibly in terms of requirements analogous to the vanishing of the torsion).

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Solution of a second order difference equation using the bilinear relations of Riemann

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A recently proposed technique to solve a class of second order functional difference equations arising in electromagnetic diffraction theory is further investigated by applying it to a case of intermediate complexity. The proposed approach is conceptually simple and relies on first obtaining well-defined branched solutions to a pair of associated first order difference equations. The construction of these branched expressions leads to an equation system whose solution requires relationships akin to Riemann's bilinear relations for differentials of the first and third kinds; their derivation necessitates the application of Cauchy's theorem on Riemann surfaces of, in this particular instance, genera one and three. Branch-free solutions of the second order difference equation are then obtained by taking appropriate linear combinations of the branched solutions of the first order equations. Analysis and computation demonstrate that the resulting expressions have the desired analytical properties and recover known solutions in the appropriate limit. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1445287]

I. INTRODUCTION

The Sommerfeld–Maliuzhinets technique[1,2] remains today the most general approach to solve electromagnetic scattering problems involving wedge-shaped structures with faces characterized by impedance boundary conditions[3] under plane wave illumination. Within its framework solutions are sought by expressing components of the total electric and magnetic fields in terms of unknown plane wave angular spectra, defined here in the complex α plane, which, besides being meromorphic, must satisfy a number of analyticity requirements. In particular, since poles of the spectral functions give rise to plane wave contributions, the spectra are required to be analytic—save for a pole necessary to reproduce the illuminating incident field—in a strip of the complex plane corresponding to the angular opening of the wedge. Additionally, besides the boundary conditions characterizing the surfaces of the wedge, obtaining a unique solution of the wave equation also requires knowledge of the behavior of the fields at the tip of the wedge and enforcement of the resulting edge condition[4] specifies the asymptotic behavior[2,3] of the spectral functions for large imaginary values of α. The imposition of the boundary conditions on the spectral representation of the fields together with a theorem put forward by Maliuzhinets[5] leads to a pair of first order difference equations for the spectra and their periods are related to the open angle of the wedge. The problem is thus reduced to obtaining spectra that satisfy both the difference equations as well as the analyticity requirements outlined above.

In the special case of normal incidence, where the illuminating plane wave is incident perpendicularly to the edge of the structure, the technique leads to uncoupled first order difference equations whose coefficients are rational trigonometric functions and solutions subject to the required constraints are readily obtained in terms of Maliuzhinets functions.[1] At skew (non-normal) incidence, the equation pair is generally coupled and solutions are obtainable for a few particular wedge/angle combinations for which uncoupled first order equations for linear combi-

nations of the spectra can be found. Recent examples of this include the polarization independent wedge studied by Bernard[6] and the right-angled anisotropic impedance wedge with one perfectly conducting face examined by Manara and Nepa.[7] In general the equation pair cannot be uncoupled and we are faced with solving a second order functional difference equation whose coefficients are rational functions of trigonometric polynomials. Its solutions are linear combinations of the desired spectral functions, a consequence of the decoupling procedure, and must therefore satisfy analyticity requirements analogous to those of the spectral functions. A pair of associated first order difference equations can be obtained from the second order one, but these, as we shall see below, typically involve branched functions and Maliuzhinets's technique does not apply.

There have been few attempts published in the literature to solve second order difference equations due to the complicated nature of the problem. A successful example is provided by Gaudin[8] who considers the second order difference equation that arises in the study of the quantum mechanical problem of two electrons interacting with a localized magnetic moment. The particular equation studied is of a high order of complexity and the ensuing analysis is prohibitively complicated. In electromagnetic theory, the second order functional difference equation of form

$$t(\alpha+3\pi)-2\left\{1-2\frac{\cos^2\eta-\cos^2\theta}{\cos^2\alpha-\cos^2\theta}\right\}t(\alpha+\pi)+t(\alpha-\pi)=0 \tag{1}$$

was recently solved by Senior and Legault.[9] It is a generalization of the one considered by Demetrescu *et al.*[10] in their study of the penetrable composite right-angled wedge consisting of abutted resistive and perfectly conducting semi-infinite half-planes. In this particular instance, the parameters η and θ are both related to the resistivity of the wedge. As noted above, the function $t(\alpha)$ represents a combination of the unknown spectral functions and it therefore satisfies requirements related to those imposed on the spectral functions. Accordingly, the solutions $t(\alpha)$ obtained in Ref. 9 are (i) meromorphic, (ii) free of poles and zeros in the strip of analyticity $\mathcal{S}_{2\pi}=\{\alpha:|\mathrm{Re}\,\alpha|\leqslant\pi\}$ (the inclusion of zeros here is a consequence of reciprocal symmetry between solution pairs in certain limits), and, in accordance with the edge condition, (iii) $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha|\to\infty$. Two linearly independent solutions satisfying the above analyticity requirements were constructed by successively eliminating the undesired singularities in the strip $\mathcal{S}_{2\pi}$. The conceptual simplicity of the technique hinges on recognizing that expressions recovered during the course of the analysis are of the same nature as those occurring in Riemann's bilinear relations for differentials of the first and third kinds.[11,12] In contrast, the solution based on a Fourier transform approach proposed in Ref. 10 fails to satisfy requirement (i) above since it is free of branch points only in the strip of analyticity $\mathcal{S}_{2\pi}$ as opposed to the entire α plane.

Equation (1) may be qualified as being of moderate complexity due to the relatively low number of singularities (poles and branch points) which must be eliminated to successfully complete the analysis. In comparison, geometries of contemporary interest such as the right-angled wedge characterized by isotropic impedance boundary conditions on both faces or the anisotropic impedance half-plane (see Ref. 13 for an approximate solution) lead to substantially more complicated equations. To gain insight into the applicability of the technique in such cases and also provide some details on the procedure, as opposed to focusing on a particular physical problem, we examine here a case of intermediate complexity by considering an equation of the same form as (1) but with the period doubled to 4π, viz.

$$t(\alpha+5\pi)-2\left\{1-2\frac{\cos^2\eta-\cos^2\theta}{\cos^2\alpha-\cos^2\theta}\right\}t(\alpha+\pi)+t(\alpha-3\pi)=0, \tag{2}$$

and, consistent with the requirement for (1), a solution is sought which is (i) meromorphic, (ii) free of poles and zeros in the strip of analyticity $\mathcal{S}_{4\pi}=\{\alpha:|\mathrm{Re}\,\alpha|\leqslant 2\pi\}$, and (iii) $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha|\to\infty$. The increase in complexity arises from the doubling of the strip of analyticity as this effectively doubles the number of singularities, both poles and branch points, that must be con-

sidered in the course of the analysis. Consequently, whereas the solution for (1) required analysis on a Riemann surface corresponding to a torus (handlebody of genus one), in the case of (2) it will be seen that we are required to work on Riemann surfaces whose corresponding handlebodies are of genera one and three.

In what follows, Sec. II gives the solution procedure for the branched first order equations associated with (2) and provides the derivation of a system of four equations in four unknowns to be satisfied in order for their solutions to be well-defined. The unknowns consist of two multiplicative constants associated with elliptic integrals of the first kind with periods 2π and 4π, and the location of the logarithmic singularities associated with two elliptic integrals of the third kind also of periods 2π and 4π. Section III shows how to solve for the quantities associated with the 2π periodic elliptic integrals. The analysis, which is carried out on a torus, is of the same nature as that required in Ref. 9 but it is examined here in greater detail. Section IV gives the solution for the quantities associated with the elliptic integrals of period 4π and it is now required to carry out the analysis on a Riemann surface which is the topological equivalent of a handlebody of genus three. The branched solutions to the first order equations are used in Sec. V to construct branch-free solutions to the second order equation. A fully analytic solution that satisfies all of the prescribed requirements is provided. The only shortcoming of the solution is that it vanishes in a certain limit and, in an effort to address this shortcoming, an alternative approach that relies on numerically locating zeros is also examined.

II. FIRST ORDER EQUATIONS AND SOLUTIONS

Since there is no available technique to directly attack the type of second order difference equation with which we are concerned, it must first be recast as an associated pair of more easily handled first order difference equations. Unfortunately the latter generally involve branch points; the price paid for this reduction in order is that the established solution technique for first order equations by Maliuzhinets[1] fails to apply. However, solutions to the first order difference equations can, in principle at least, be obtained by applying a logarithmic derivative and this is the approach taken here. This yields a solution expressed in terms of an initially ill-defined path integral and multiplicative terms of period 4π, corresponding to the period of the difference equation, must be added to rectify this. This ultimately leads to the derivation of a system of four equations in four unknowns which can be partially decoupled into two systems in two unknowns, one involving 2π periodic quantities and the other 4π periodic ones.

A. Reduction to first order equations

The second order functional difference equation (2) can be rewritten in terms of first order difference equations quite straightforwardly by exploiting the periodicity of the functional coefficient. To see this consider the second order difference equation

$$t(\alpha+5\pi)+p(\alpha)t(\alpha+\pi)+\frac{1}{p(\alpha)}\{t(\alpha+\pi)+p(\alpha)t(\alpha-3\pi)\}=0 \tag{3}$$

whose solutions $t(\alpha)$, provided $p(\alpha)$ is 4π periodic, must also explicitly satisfy first order difference equations. Enforcing equality between (3) and (2) then yields the equation pair

$$\frac{t(\alpha+2\pi)}{t(\alpha-2\pi)}=g(\alpha,+u(\alpha))=\frac{u(\alpha)-u(\theta)}{u(\alpha)+u(\theta)}, \tag{4}$$

$$\frac{t(\alpha+2\pi)}{t(\alpha-2\pi)}=g(\alpha,-u(\alpha))=\frac{u(\alpha)+u(\theta)}{u(\alpha)-u(\theta)}, \tag{5}$$

where

$$u(\alpha)=\sqrt{\cos^2\alpha-\cos^2\eta}. \tag{6}$$

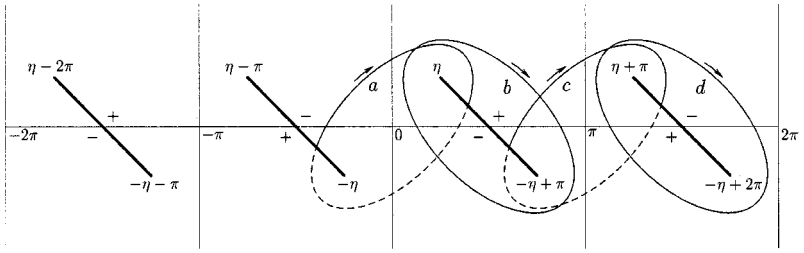


FIG. 1. The strip of analyticity $\mathcal{S}_{4\pi}=\{\alpha:|\mathrm{Re}\,\alpha|\leqslant 2\pi\}$. The thick lines indicate the branch cuts of $u(\alpha)$, the positive and negative signs indicate relative changes in sign of $u(\alpha)$ across the different cuts. The clockwise cycles a, b, c and d used to define the cyclic periods are as indicated. Note that the cycles a and c cross from the upper Riemann sheet (solid line) to the lower Riemann sheet (dashed line) whereas b and d are confined to the upper sheet.

Alternatively, one could also proceed by factoring the associated second order difference operator in (2) into a pair of first order difference operators and recover the same result as above. The first order equations obtained are generally branched owing to the presence of the root $u(\alpha)$ which has branch points at $\alpha=\pm\eta,\pm(\eta-\pi),\pm(\eta+\pi),\pm(-\eta+2\pi)$ in the strip of analyticity $\mathcal{S}_{4\pi}$ and is made well defined in the complex α plane by introducing the cuts shown in Fig. 1. These are such that $u(\alpha)$ has the same symmetry as $\cos\alpha$ so that

$$u(\alpha)=u(-\alpha)=-u(\alpha\pm\pi). \tag{7}$$

Note that the function $t(\alpha)$ is used here to generally denote solutions of the second order equation and each of the first order equations above identifies one such solution. If $t(\alpha)=w(\alpha,u(\alpha))$ is a solution of (4), then $t(\alpha)=w(\alpha,-u(\alpha))$ is a solution of (5), and this follows from the symmetry of the right-hand sides of (4) and (5) with respect to the sign (the branch) of $u(\alpha)$. It is therefore sufficient to consider $w(\alpha,u)$—writing $w(\alpha,u)$ instead of $w(\alpha,u(\alpha))$ for convenience—and, since $g(-\alpha,u)=g(\alpha,u)$, we can construct $w(\alpha,u)$ such that

$$w(-\alpha,u)=\frac{1}{w(\alpha,u)}=w(\alpha,-u). \tag{8}$$

In terms of the solutions of the first order difference equations, solutions to (2) are

$$t(\alpha)=C_1(\alpha)w(\alpha,u)+C_2(\alpha)w(\alpha,-u), \tag{9}$$

where $C_{1,2}(\alpha)$ are 4π periodic functions. This generally conflicts with the requirement for a branch-free solution but there are particular cases of (9) that overcome this difficulty and the simplest two such linearly independent expressions free of branch points are

$$t(\alpha)=w(\alpha,u)+w(\alpha,-u), \quad \text{and} \quad t(\alpha)=\frac{1}{u(\alpha)}\{w(\alpha,u)-w(\alpha,-u)\}. \tag{10}$$

While the branch-free property of these two symmetric forms can be ascertained rigorously by means of Taylor expansions in the neighborhood of branch points of $u(\alpha)$, it can also be appreciated from the fact that both are invariant under a change of the branch of $u(\alpha)$. This crucial feature makes the constructs (10) the fundamental building blocks from which branch-free solutions to the second order difference equation can be assembled once branched solutions of the associated first order equations have been obtained. As we shall soon see, the presence of branch points makes this task quite challenging and the brunt of the subsequent analysis focuses on deriving solutions to the first order equations.

B. Special cases of interest

It is worthwhile to first consider the special cases $\eta=0$ and $\eta=\pi/2$ as the branch points then vanish and known solutions, which are useful when characterizing the behavior of the general solution obtained below, can be obtained in terms of Maliuzhinets functions. The first one when $\eta=\pi/2$ proves to be especially interesting since the branch cuts of $u(\alpha)$, as illustrated in Fig. 1 and chosen so that (7) holds, vanish as $\eta\to\pi/2$. In this instance (4) becomes

$$\frac{w(\alpha+2\pi,u)}{w(\alpha-2\pi,u)}=\frac{\cos\alpha-\cos\theta}{\cos\alpha+\cos\theta},$$

and, despite the fact that the right-hand side is now meromorphic, the dependence of $w(\alpha,u)$ on $u(\alpha)$ is maintained to distinguish it from $w(\alpha,-u)$, the solution to Eq. (5) in the same limit. A solution free of poles and zeros in $\mathcal{S}_{4\pi}$ and $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha|\to\infty$ follows directly from Maliuzhinets.[1] It may be written as

$$\begin{aligned} w(\alpha,u)&=\Psi_1(\alpha)\\ &=\frac{\psi_\pi(\alpha+\pi/2-\theta)}{\psi_\pi(\alpha-\pi/2+\theta)}\\ &=\exp\int_0^\alpha\frac{-(\alpha'/2\pi)\cos\theta\sin\alpha'+\gamma_1+\gamma_2\cos(\alpha'/2)+\gamma_3\cos\alpha'+\gamma_4\cos(3\alpha'/2)}{\cos^2\alpha'-\cos^2\theta}d\alpha', \end{aligned} \tag{11}$$

where

$$\begin{aligned} \gamma_1&=-\tfrac{1}{4}\sin\theta\cos\theta,\\ \gamma_2&=\frac{1}{4}\left(-\cos\frac{\theta}{2}+\sin\frac{\theta}{2}\right)+\frac{1}{2}\cos\frac{\theta}{2}\left(\cos\frac{\theta}{2}+\sin\frac{\theta}{2}\right),\\ \gamma_3&=\left(\frac{\theta}{2\pi}-\frac{1}{4}\right)\sin\theta,\\ \gamma_4&=\frac{1}{4}\left(-\cos\frac{\theta}{2}+\sin\frac{\theta}{2}\right), \end{aligned} \tag{12}$$

and $\psi_\pi(\alpha)$ is the Maliuzhinets function.[1] Since $\Psi_1(-\alpha)=1/\Psi_1(\alpha)$, consistent with (8), two linearly independent solutions of (2) are

$$t_1(\alpha)=\Psi_1(\alpha),\quad t_2(\alpha)=\Psi_1(-\alpha),$$

and these are both $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha|\to\infty$. The other case of interest where the branch points also vanish is $\eta=0$ and in that instance two linearly independent solutions, also $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha|\to\infty$, are provided by

$$t_1(\alpha)=\Psi_2(\alpha)=\cos\frac{\alpha}{4}\,\frac{\psi_\pi^2(\pi/2-\theta)}{\psi_\pi(\alpha+\pi/2-\theta)\psi_\pi(\alpha-\pi/2+\theta)},\quad t_2(\alpha)=\frac{1}{t_1(\alpha)}, \tag{13}$$

and we must now contend with poles or zeros at $\alpha=\pm2\pi$.

C. General case

We now proceed to solve (4) in the general case where $\eta \neq 0$, $\pi/2$ and Maliuzhinets's technique does not apply. The solutions sought should preferably reduce to one or both of the known limiting functions when η goes to the appropriate limit and, consistent with the limiting cases, they must also be $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha| \to \infty$ for all η. As we shall see, while the solution $\Psi_1(\alpha)$ [and $1/\Psi_1(\alpha)$] are easily recovered as $\eta \to \pi/2$, the recovery of $\Psi_2(\alpha)$ [and $1/\Psi_2(\alpha)$] as $\eta \to 0$ proves to be much more difficult. Taking the logarithmic derivative of (4), we obtain

$$\frac{d}{d\alpha}\ln w(\alpha+2\pi,u)-\frac{d}{d\alpha}\ln w(\alpha-2\pi,u)=\frac{d}{d\alpha}\ln g(\alpha,u)=-\frac{u(\theta)}{u(\alpha)}\frac{2\sin\alpha\cos\alpha}{\cos^2\alpha-\cos^2\theta}, \quad (14)$$

and if $v_0(\alpha,u)=d/d\alpha \ln w(\alpha,u)$, then

$$v_0(\alpha+2\pi,u)-v_0(\alpha-2\pi,u)=-\frac{u(\theta)}{u(\alpha)}\frac{2\sin\alpha\cos\alpha}{\cos^2\alpha-\cos^2\theta}$$

and a solution to (4) can tentatively be written as

$$w(\alpha,u)=\exp\int_{\alpha_0}^{\alpha} v_0(\alpha',u)\,d\alpha', \quad (15)$$

with

$$v_0(\alpha,u)=-\frac{\alpha}{2\pi}\frac{u(\theta)}{u(\alpha)}\frac{\sin\alpha\cos\alpha}{\cos^2\alpha-\cos^2\theta}.$$

The form proposed in (15) is, however, ill-defined owing to the presence of the polar and the cyclic periods (we borrow here the terminology used in Ref. 11 when characterizing differentials of the third kind) due to, respectively, the poles and the branch points of $v_0(\alpha,u)$. In order to obtain a single-valued integral expression, we must consider instead

$$w(\alpha,u)=\exp\int_{\alpha_0}^{\alpha}\{v_0(\alpha',u)+v_\Sigma(\alpha',u)\}\,d\alpha', \quad (16)$$

where the added term $v_\Sigma(\alpha,u)$ represents a sum of 4π periodic terms, of even parity like $v_0(\alpha,u)$, specifically selected to remove the offending periods. Not all classes of 4π periodic functions are acceptable: it turns out that $v_\Sigma(\alpha,u)$ must fulfill certain order requirements in order for $\exp\int v_\Sigma(\alpha)d\alpha$ to be a 4π periodic function and a simple analysis shows that, for the case at hand, it is sufficient to consider expressions such that $v_\Sigma(\alpha,u)\to 0$ as $|\mathrm{Im}\,\alpha|\to\infty$. It will be shown below that $v_\Sigma(\alpha,u)$ will consist of five terms: $v_1(\alpha,u)$ to eliminate the polar periods and $v^1_{2\pi}(\alpha,u)$, $v^3_{2\pi}(\alpha,u)$, $v^1_{4\pi}(\alpha,u)$, $v^3_{4\pi}(\alpha,u)$ to eliminate the cyclic periods.

It is worthwhile to discuss the nature of the lower limit α_0 at this juncture as its selection may appear at first glance to be somewhat arbitrary. This is not the case as consideration of the symmetric forms in (10) together with the requirement for continuity reveals that the lower limit α_0 must be a branch point in $\mathcal{S}_{4\pi}$ so that $\alpha_0 \in \{\pm\eta, \pm(\eta-\pi), \pm(\eta+\pi), \pm(2\pi-\eta)\}$. Furthermore, once $v_\Sigma(\alpha,u)$ has been properly defined, the solution is independent of the choice of the particular branch point and this will become more obvious when we consider the elimination of the cyclic periods. We first examine the elimination of the polar periods.

1. Elimination of polar periods

The presence of poles will generally make a path integral such as the one in (16) multivalued. A pole of residue Res will give rise to a polar period equal to $2\pi i\,\mathrm{Res}$ and, depending on the orientation of the integration path and its winding number around the pole, the contribution to the integral will be $2\pi i\mathbb{Z}\mathrm{Res}$. In the case of (15), polar periods arise at the poles of $v_0(\alpha,u)$ at α

$=\pm\theta$, $\pm(\theta-\pi)$, $\pm(\theta+\pi)$, $\pm(2\pi-\theta)$. Elimination of these poles serves two purposes as it not only eliminates their associated polar periods but goes toward fulfilling the requirement for a solution that is pole-free in $\mathcal{S}_{4\pi}$. We eliminate them by introducing the 4π periodic

$$v_1(\alpha,u)=\frac{u(\theta)}{u(\alpha)}\frac{\cos(\alpha)}{\cos(\theta)}\frac{\gamma_1+\gamma_2\cos(\alpha/2)+\gamma_3\cos\alpha+\gamma_4\cos(3\alpha/2)}{\cos^2\alpha-\cos^2\theta},$$

which is even, vanishes as $|\mathrm{Im}\,\alpha|\to\infty$, and has poles coinciding with those of $v_0(\alpha,u)$. The constants γ_n are chosen to eliminate the residues and straightforward algebra yields the coefficients in (12). It then follows from (11) that

$$v_0(\alpha,u)+v_1(\alpha,u)=\frac{u(\theta)}{u(\alpha)}\frac{\cos\alpha}{\cos\theta}\frac{d}{d\alpha}\ln\Psi_1(\alpha),$$

which correctly reduces to $d/d\alpha\ln\Psi_1(\alpha)$ when $\eta=\pi/2$. We therefore recognize that, in the simpler case where the right-hand side of (14) is meromorphic so that (15) is free of cyclic periods, the known solutions expressed in terms of Maliuzhinets can be recovered by following the above procedure of pole elimination. We also note in passing that poles with integer residue $\mathbb{Z}$ do not compromise path independence. Indeed, their capture leads to an additive $2\pi i\mathbb{Z}$ contribution in the exponent of (16) which has no effect on the final value of $w(\alpha,u)$.

2. Elimination of cyclic periods

In a fashion similar to polar periods, a cyclic period arises from the nonzero contribution incurred when integrating along a loop encircling a branch cut in $\mathcal{S}_{4\pi}$, thereby making the path integral multivalued. For example, such a period is obtained when integrating v_0+v_1 along the cycle b, shown in Fig. 1, which encircles the branch cut joining the branch points η and $-\eta+\pi$. As in the case of the polar periods, it is strictly speaking not required for the cyclic periods to vanish identically to avoid jeopardizing single-valuedness since periods equal to $2\pi i\mathbb{Z}$ do not change the value of (16). However, as $\eta\to\pi/2$ the branch points of $1/u(\alpha)$ in $v_{0,1}$ coalesce into poles at $\pm\pi/2$ and $\pm3\pi/2$ and their associated cyclic periods then become polar periods. Consequently, the cyclic periods associated with the cycles b and d in Fig. 1 must be annulled, as opposed to setting them equal to some nonzero integer multiple of $2\pi i$, to eliminate poles that would otherwise arise as $\eta\to\pi/2$. We observe that this requirement is equivalent to annulling the integral of v_0+v_Σ along the cuts between η and $\pi-\eta$ as well as $\pi+\eta$ and $2\pi-\eta$. There is also a similar requirement, which is not obvious when solely considering integration on either of the Riemann sheets, on the cyclic periods associated with the cycles a and c which loop from one Riemann sheet to the other. Its necessity is revealed by examining either of the symmetric forms in (10) together with the requirement for continuity. In short, the above implies, taking advantage of the even parity, the need to annul the cyclic periods of $v_0(\alpha,u)+v_\Sigma(\alpha,u)$ on the clockwise cycles a, b, c and d shown in Fig. 1. Alternatively, this can be thought of as requiring that all branch point to branch point integrals vanish in $\mathcal{S}_{4\pi}$ and, under this condition, the lower limit α_0 can be arbitrarily chosen among any of the branch points located within the strip. This also ensures that the resulting expressions will remain free of poles despite coalescing branch points in the limits $\eta\to0$ and $\eta\to\pi/2$.

Four degrees of freedom are required to annul the cyclic periods of v_0+v_1 on the cycles a, b, c and d. We introduce the following four even 4π periodic terms which, like $v_0(\alpha,u)$ and $v_1(\alpha,u)$, vanish as $|\mathrm{Im}\,\alpha|\to\infty$:

$$v^1_{2\pi}(\alpha,u)=\frac{1}{u(\alpha)},\quad v^3_{2\pi}(\alpha,u)=\frac{u(\zeta_{2\pi})}{u(\alpha)}\frac{\cos\alpha}{\cos\zeta_{2\pi}}\frac{\sin\zeta_{2\pi}}{\cos\alpha-\cos\zeta_{2\pi}},\tag{17}$$

and

$$v^1_{4\pi}(\alpha,u)=\frac{\cos(\alpha/2)}{u(\alpha)},\quad v^3_{4\pi}(\alpha,u)=\frac{u(\zeta_{4\pi})}{u(\alpha)}\frac{\cos\alpha}{\cos\zeta_{4\pi}}\frac{\frac{1}{2}\sin(\zeta_{4\pi}/2)}{\cos(\alpha/2)-\cos(\zeta_{4\pi}/2)}. \tag{18}$$

These all give rise to elliptic integrals with the first pair being 2π periodic and the second 4π periodic. The subscript identifies the periodicity of the term while the superscript identifies the type of elliptic integral to which it gives rise. Hence $v^1_{2\pi}(\alpha,u)$ is 2π periodic and gives rise to an elliptic integral of the first kind while $v^3_{2\pi}(\alpha,u)$, also 2π periodic, gives rise to an elliptic integral of the third kind with logarithmic singularities within $\mathcal{S}_{4\pi}$ at $\pm\zeta_{2\pi},\pm(\zeta_{2\pi}+2\pi)$. Likewise, $v^3_{4\pi}(\alpha,u)$ is 4π periodic and gives rise to an elliptic integral of the third kind with logarithmic singularities at $\pm\zeta_{4\pi}$. The use of expressions associated with integrals of the third kind (with poles having nonvanishing residues) results from the impossibility of introducing the required number of degrees of freedom without violating the order requirement. It must be emphasized that the poles of both $v^3_{2\pi}(\alpha,u)$ and $v^3_{4\pi}(\alpha,u)$ have residues ±1 and their polar periods therefore do not disrupt the single-valuedness of the path integral. Their elimination from the strip of analyticity is the objective of the last step in the construction of the solution and this is carried out in Sec. V. For future reference we define the cyclic periods

$$\begin{aligned}A^{1,3}_{2\pi,4\pi}&=\int_a v^{1,3}_{2\pi,4\pi}(\alpha,u)d\alpha,\quad B^{1,3}_{2\pi,4\pi}=\int_b v^{1,3}_{2\pi,4\pi}(\alpha,u)d\alpha,\\ C^{1,3}_{2\pi,4\pi}&=\int_c v^{1,3}_{2\pi,4\pi}(\alpha,u)d\alpha,\quad D^{1,3}_{2\pi,4\pi}=\int_d v^{1,3}_{2\pi,4\pi}(\alpha,u)d\alpha,\end{aligned} \tag{19}$$

and use similar definitions for $v_{0,1}(\alpha,u)$ [i.e., $A_0=\int_a v_0(\alpha,u)d\alpha$]. Inspection of (17) and (18) reveals that the periods associated with the integrals of the third kind are functions of the poles $\zeta_{2\pi}$ and $\zeta_{4\pi}$, providing two of the four degrees of freedoms required to annul the periods of $v_0(\alpha,u)+v_\Sigma(\alpha,u)$. In contrast, the periods associated with the integrals of the first kind are constant and two multiplicative constants, $\kappa_{2\pi}$ and $\kappa_{4\pi}$, must be introduced to produce the two additional degrees of freedom. The solution to (4) then takes the form

$$\begin{aligned}w(\alpha,u)=\exp\int_{\alpha_0}^{\alpha}\{&v_0(\alpha',u)+v_1(\alpha',u)+\kappa_{2\pi}v^1_{2\pi}(\alpha',u)+\sigma_{2\pi}v^3_{2\pi}(\alpha',u)\\&+\kappa_{4\pi}v^1_{4\pi}(\alpha',u)+\sigma_{4\pi}v^3_{4\pi}(\alpha',u)\}d\alpha',\end{aligned} \tag{20}$$

where the four unknowns to be determined are $\kappa_{2\pi}$, $\zeta_{2\pi}$ and $\kappa_{4\pi}$, $\zeta_{4\pi}$. The quantities $\sigma_{2\pi}=\pm1$ and $\sigma_{4\pi}=\pm1$ have been introduced to avoid loss of generality in the definition of the terms associated with the integrals of the third kind. They account for the eventuality where the sign of the logarithmic residues of $v^3_{2\pi}(\alpha,u)$ or $v^3_{4\pi}(\alpha,u)$ must be changed, thereby swapping poles and zeros of $w(\alpha,u)$ between the two Riemann sheets. Their proper definition will be determined in the course of the analysis and, to reduce clutter, they will be omitted in what follows pending their reintroduction when appropriate.

An equation system consisting of four equations in the four unknowns is obtained by enforcing vanishing cyclic periods on the cycles a, b, c and d. Doing so for the cycle d, for example, leads to

$$\int_{\eta+\pi^-}^{-\eta+2\pi^-}(v_0+v_1+\kappa_{2\pi}v^1_{2\pi}+v^3_{2\pi}+\kappa_{4\pi}v^1_{4\pi}+v^3_{4\pi})d\alpha=0 \tag{21}$$

with the superscript negative sign in the limits indicating the corresponding side of the branch cut (see Fig. 1) along which to integrate. Upon use of (19) this becomes

$$D_0+D_1+\kappa_{2\pi}D^1_{2\pi}+D^3_{2\pi}+\kappa_{4\pi}D^1_{4\pi}+D^3_{4\pi}=0,$$

which is further simplified by exploiting the symmetries $D^1_{2\pi}=-B^1_{2\pi}$, $D^3_{2\pi}=-B^3_{2\pi}$ and $D^1_{4\pi}=B^1_{4\pi}$. Introducing the notation $D_{0+1}=D_0+D_1$, we finally obtain

$$D_{0+1}-\kappa_{2\pi}B^1_{2\pi}-B^3_{2\pi}+\kappa_{4\pi}B^1_{4\pi}+D^3_{4\pi}=0,$$

a relationship equivalent to (21). Repeating the same process for the a, b and c cycles yields

$$A_{0+1}+\kappa_{2\pi}A^1_{2\pi}+A^3_{2\pi}+\kappa_{4\pi}A^1_{4\pi}+A^3_{4\pi}=0, \tag{22a}$$

$$B_{0+1}+\kappa_{2\pi}B^1_{2\pi}+B^3_{2\pi}+\kappa_{4\pi}B^1_{4\pi}+B^3_{4\pi}=0, \tag{22b}$$

$$C_{0+1}-\kappa_{2\pi}A^1_{2\pi}-A^3_{2\pi}+C^3_{4\pi}=0, \tag{22c}$$

$$D_{0+1}-\kappa_{2\pi}B^1_{2\pi}-B^3_{2\pi}+\kappa_{4\pi}B^1_{4\pi}+D^3_{4\pi}=0, \tag{22d}$$

with the explicit unknowns $\kappa_{2\pi}$ and $\kappa_{4\pi}$ and the unknowns $\zeta_{2\pi}$ and $\zeta_{4\pi}$ implied by the presence of cyclic periods associated with the integrals of the third kind. Note that $C^1_{4\pi}$ vanishes since $v^1_{4\pi}(\alpha,u)$, which is odd symmetric with respect to π [see (18)], does not contribute when integrated on cycle c (see Fig. 1). This seemingly intractable system can be fully solved analytically. The quantities associated with the 4π periodic elliptic integrals can be decoupled by adding Eq. (22a) to (22c) and (22b) to (22d) to obtain

$$\kappa_{4\pi}A^1_{4\pi}+A^3_{4\pi}+C^3_{4\pi}=-(A_{0+1}+C_{0+1}), \tag{23a}$$

$$2\kappa_{4\pi}B^1_{4\pi}+B^3_{4\pi}+D^3_{4\pi}=-(B_{0+1}+D_{0+1}), \tag{23b}$$

and the elimination of $\kappa_{4\pi}$ produces

$$A^1_{4\pi}(B^3_{4\pi}+D^3_{4\pi})-2B^1_{4\pi}(A^3_{4\pi}+C^3_{4\pi})=-A^1_{4\pi}(B_{0+1}+D_{0+1})+2B^1_{4\pi}(A_{0+1}+C_{0+1}) \tag{24}$$

in which the only (implicit) unknown $\zeta_{4\pi}$ determines the periods $A^3_{4\pi}$, $B^3_{4\pi}$, $C^3_{4\pi}$ and $D^3_{4\pi}$. Despite appearances, the above equation can be inverted to obtain $\zeta_{4\pi}$ and the technique for doing so is described in Sec. IV. Once $\zeta_{4\pi}$ has been obtained, the value of $\kappa_{4\pi}$ immediately follows either from Eq. (23a) or (23b). One can then proceed to solve for $\zeta_{2\pi}$ by subtracting Eq. (22c) from (22a) and (22d) from (22b) to obtain, respectively,

$$2\kappa_{2\pi}A^1_{2\pi}+2A^3_{2\pi}=-\kappa_{4\pi}A^1_{4\pi}-A^3_{4\pi}+C^3_{4\pi}-A_{0+1}+C_{0+1}, \tag{25a}$$

$$2\kappa_{2\pi}B^1_{2\pi}+2B^3_{2\pi}=-B^3_{4\pi}+D^3_{4\pi}-B_{0+1}+D_{0+1}, \tag{25b}$$

and the elimination of $\kappa_{2\pi}$ gives

$$\begin{aligned}A^1_{2\pi}B^3_{2\pi}-B^1_{2\pi}A^3_{2\pi}=\tfrac{1}{2}\{&A^1_{2\pi}(-B^3_{4\pi}+D^3_{4\pi}-B_{0+1}+D_{0+1})\\&-B^1_{2\pi}(-\kappa_{4\pi}A^1_{4\pi}-A^3_{4\pi}+C^3_{4\pi}-A_{0+1}+C_{0+1})\},\end{aligned} \tag{26}$$

where the only unknown is now $\zeta_{2\pi}$, the value of which determines the periods $A^3_{2\pi}$ and $B^3_{2\pi}$. This equation is of the same form as the one obtained in Ref. 9 and the solution follows the same approach. To set the stage for the comparatively more complicated inversion required for $\zeta_{4\pi}$, we first reexamine the analysis required for $\zeta_{2\pi}$ in more detail.

III. DETERMINATION OF $\zeta_{2\pi}$ AND $\kappa_{2\pi}$

The key to inverting for $\zeta_{2\pi}$ in (26) lies in the application of Cauchy's theorem on the Riemann surface delimited by the contour $\mathcal{C}_1$ shown in Fig. 2. Indeed, by judiciously choosing the integrand it is possible to obtain an alternative expression for the left-hand side of (26) in which

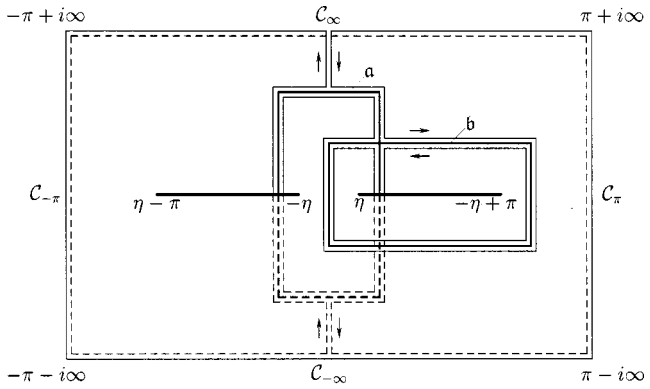


FIG. 2. The contour $\mathcal{C}_1=\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}\cup\mathcal{C}_{\pm\pi}\cup\mathcal{C}_{\pm\infty}$ on the upper (solid line) and lower (dashed line) sheets of the Riemann surface. The thicker inner lines are the dissections $\mathfrak{a}$ and $\mathfrak{b}$ introduced to make the Riemann surface simply connected. The path $\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}$ denotes the portion of the contour enclosing the dissecting cycles $\mathfrak{a}$ and $\mathfrak{b}$.

the unknown $\zeta_{2\pi}$ appears more explicitly as the argument of an elliptic integral of the first kind, paving the way for its inversion by means of the Jacobian elliptic sine function. This follows from recognizing that the relationship between cyclic periods on the left-hand side of (26) is of the same form as the expressions found in Riemann's bilinear relationships for differentials of the first and third kinds;[11,12] these equate expressions involving cyclic periods such as the one on the left-hand side of (26) to sums of residues. To achieve this, we seek to evaluate

$$\int_{\mathcal{C}_1} V^1_{2\pi}(\alpha,u)\,dV^3_{2\pi}(\alpha,u)=2\pi i\sum \text{ Res}, \tag{27}$$

where the elliptic integral $V^1_{2\pi}(\alpha,u)$ of the first kind and $V^3_{2\pi}(\alpha,u)$ of the third kind are defined as

$$V^n_{2\pi}(\alpha,u)=\int_{(\eta,0)}^{(\alpha,u)} v^n_{2\pi}(\alpha',u)\,d\alpha', \quad n\in\{1,3\}.$$

The path of integration $\mathcal{C}_1$, shown in Fig. 2, delimits a strip of width 2π centered at the origin of both Riemann sheets and encloses the dissections and branch cuts contained therein. For 2π periodic functions the enclosed surface is topologically equivalent to a torus (a handlebody of genus 1) as shown in Fig. 3. The canonical dissections $\mathfrak{a}$ and $\mathfrak{b}$ are introduced to make the surface

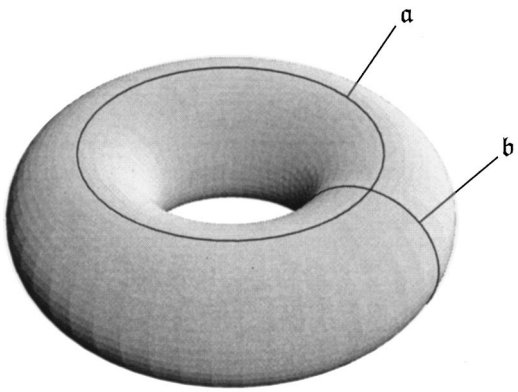


FIG. 3. The torus, handlebody of genus 1, is topologically equivalent to the Riemann surface in Fig. 2. It has been made simply connected by introducing the dissections $\mathfrak{a}$ and $\mathfrak{b}$.

simply connected, a key requirement in order for Cauchy's theorem to apply, and this is more easily appreciated on the dissected torus in Fig. 3. Examination of the integral in (27) shows that only $\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}$, the portion of the path enclosing the branch cuts and dissections, provides a contribution. The rest of the integral vanishes either by symmetry, as for the parts along $\mathrm{Re}\,\alpha=\pm\pi$ on $\mathcal{C}_{\pm\pi}$, or identically, as in the case where $|\mathrm{Im}\,\alpha|=\pm\infty$ on $\mathcal{C}_{\pm\infty}$. Evaluation of the integral along $\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}$ produces[11,12]

$$\int_{\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}} V^1_{2\pi}(\alpha,u)\,dV^3_{2\pi}(\alpha,u)=\mathfrak{A}^1_{2\pi}\mathfrak{B}^3_{2\pi}-\mathfrak{B}^1_{2\pi}\mathfrak{A}^3_{2\pi},$$

where, extending our notation, capitalized letters denote cyclic periods on cycles identified by the correspond lower case letters so that, for example, $\mathfrak{A}^1_{2\pi}=\int_{\mathfrak{a}} v^1_{2\pi}\,d\alpha$. The cycles defined by the dissections $\mathfrak{a}$ and $\mathfrak{b}$ in Fig. 2 are the same as the cycles a and b shown in Fig. 1 so that $\mathfrak{A}^n_{2\pi}=A^n_{2\pi}$ and $\mathfrak{B}^n_{2\pi}=B^n_{2\pi}$. We therefore obtain, in light of (26), the remarkable result

$$\int_{\mathcal{C}_1} V^1_{2\pi}(\alpha,u)\,dV^3_{2\pi}(\alpha,u)=\mathfrak{A}^1_{2\pi}\mathfrak{B}^3_{2\pi}-\mathfrak{B}^1_{2\pi}\mathfrak{A}^3_{2\pi}=A^1_{2\pi}B^3_{2\pi}-B^1_{2\pi}A^3_{2\pi}, \tag{28}$$

which, by virtue of (27), can be expressed as a sum of residues. On the Riemann surface, the residues of the integrand in (27) are given by

$$-\frac{u(\zeta_{2\pi})}{u(\alpha)}\frac{\cos\alpha}{\cos\zeta_{2\pi}}\frac{\sin\zeta_{2\pi}}{\sin\alpha}\int_{(\eta,0)}^{(\alpha,u)} v^1_{2\pi}(\alpha')\,d\alpha'\Bigg|_{\alpha=(\pm\zeta_{2\pi},\pm u)}$$

$$=\begin{cases}\mp\displaystyle\int_{(\eta,0)}^{(\alpha,u)} v^1_{2\pi}(\alpha')\,d\alpha', & \alpha=(\zeta_{2\pi},\pm u),\\ \pm\displaystyle\int_{(\eta,0)}^{(\alpha,u)} v^1_{2\pi}(\alpha')\,d\alpha', & \alpha=(-\zeta_{2\pi},\pm u),\end{cases}$$

and these, after carrying out the integration on the dissected Riemann surface, can be expressed in terms of the elliptic integral $V^1_{2\pi}(\alpha)$ defined on the upper Riemann sheet. Being mindful of the dissections and exploiting the numerous symmetries involved, we obtain

$$\sum \mathrm{Res}=-A^1_{2\pi}\pm 2B^1_{2\pi}-4V^1_{2\pi}(\zeta_{2\pi}),\quad V^1_{2\pi}(\zeta_{2\pi})\in\left\{-\tau'\frac{A^1_{2\pi}}{4}\pm\tau\frac{B^1_{2\pi}}{2}:0\leqslant\tau',\tau\leqslant 1\right\}. \tag{29}$$

It would of course be impossible to obtain a unique expression for the above if the Riemann surface had not previously been made simply connected. Substitution of (28) and (29) in (27) yields

$$V^1_{2\pi}(\zeta_{2\pi})=-\frac{A^1_{2\pi}}{4}\pm\frac{B^1_{2\pi}}{2}-\frac{\sigma_{2\pi}}{8\pi i}(A^1_{2\pi}B^3_{2\pi}-B^1_{2\pi}A^3_{2\pi})=-\frac{A^1_{2\pi}}{4}\pm\frac{B^1_{2\pi}}{2}+\sigma_{2\pi}i\Lambda_{2\pi}, \tag{30}$$

where the only unknown is $\zeta_{2\pi}$ and we have reintroduced $\sigma_{2\pi}$ from Eq. (20). The quantity $\Lambda_{2\pi}$ is, from (26), defined as

$$\Lambda_{2\pi}=\frac{1}{16\pi}\{A^1_{2\pi}(-B^3_{4\pi}+D^3_{4\pi}-B_{0+1}+D_{0+1})-B^1_{2\pi}(-\kappa_{4\pi}A^1_{4\pi}-A^3_{4\pi}+C^3_{4\pi}-A_{0+1}+C_{0+1})\}. \tag{31}$$

This is a known quantity provided equation system (23) has been solved, a procedure carried out in the next section.

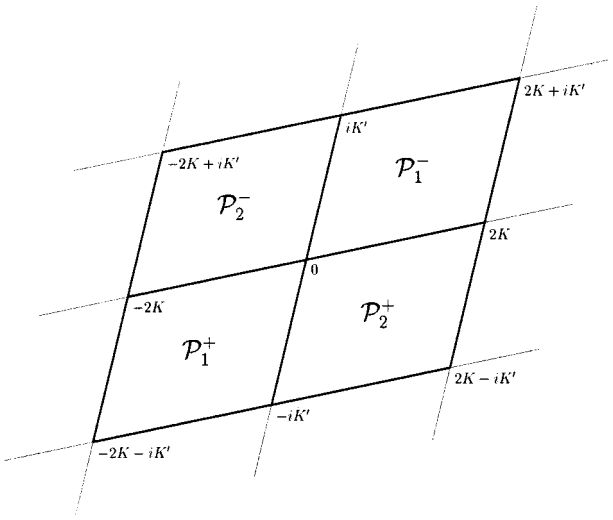


FIG. 4. The regions $\mathcal{P}_1^{\pm}$ and $\mathcal{P}_2^{\pm}$ in terms of the complete integrals of the first kind K and K' with $k=\cos\eta$. The parallelograms $\mathcal{P}$ indicate the various ranges in which $\Lambda_{2\pi}$ must lie when carrying out the inversion for $\zeta_{2\pi}$ with Eq. (34).

A closed-form expression for $\zeta_{2\pi}$ can be found by using the Jacobian elliptic sine function sn to invert the elliptic integral of the first kind in (30). Legendre's standard form for the integral is

$$F(x,k)=\int_0^x \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}},$$

where k is the modulus of the integral and the elliptic sine function is such that

$$\mathrm{sn}[F(x,k),k]=x$$

with x located in the fundamental period parallelogram of dimensions $4K$ and $2iK'$ centered at the origin of the complex plane. The periods K and K' are the standard quantities defined, respectively, by the complete elliptic integrals of the first kind with modulus k and complementary modulus k'. The transformation $x=\cos\alpha/\cos\eta$ then shows that

$$V_{2\pi}^1(\alpha)=\int_\eta^\alpha \frac{d\alpha'}{\sqrt{\cos^2\alpha'-\cos^2\eta}}=i\left\{F\left(\frac{\cos\alpha}{\cos\eta},\cos\eta\right)+i\frac{B_{2\pi}^1}{4}\right\} \tag{32}$$

and we note the following useful relationships:

$$k=\cos\eta,\quad A_{2\pi}^1=4K',\quad B_{2\pi}^1=4iK. \tag{33}$$

Finally, taking into account the definition of $\Sigma\mathrm{Res}$ in terms of the range of $V_{2\pi}^1(\zeta_{2\pi})$ given in (29) and inserting (32) in (30), we obtain after some algebraic manipulations

$$\zeta_{2\pi}=\begin{cases}\arccos[k\,\mathrm{sn}(iK'+3K+\sigma_{2\pi}\Lambda_{2\pi},k)], & \Lambda_{2\pi}\in\mathcal{P}_1^{\sigma_{2\pi}},\\ \arccos[k\,\mathrm{sn}(iK'-K+\sigma_{2\pi}\Lambda_{2\pi},k)], & \Lambda_{2\pi}\in\mathcal{P}_2^{\sigma_{2\pi}},\end{cases} \tag{34}$$

which is an explicit expression for $\zeta_{2\pi}$. The correct expression to use in (34) as well as the correct definition for $\sigma_{2\pi}=\pm1$ follow from locating $\Lambda_{2\pi}$ in the appropriate $\mathcal{P}$ parallelogram in Fig. 4. For instance, if $\Lambda_{2\pi}\in\mathcal{P}_2^-$, then $\sigma_{2\pi}=-1$ and $\zeta_{2\pi}=\arccos[k\,\mathrm{sn}(iK'-K-\Lambda_{2\pi},k)]$. The multiplicative constant $\kappa_{2\pi}$ follows immediately from (25a) or (25b). The period parallelograms in Fig. 4 were obtained by using (30) and (29) to specify the range of $\Lambda_{2\pi}$ in terms of that of $V_{2\pi}^1(\zeta_{2\pi})$. For

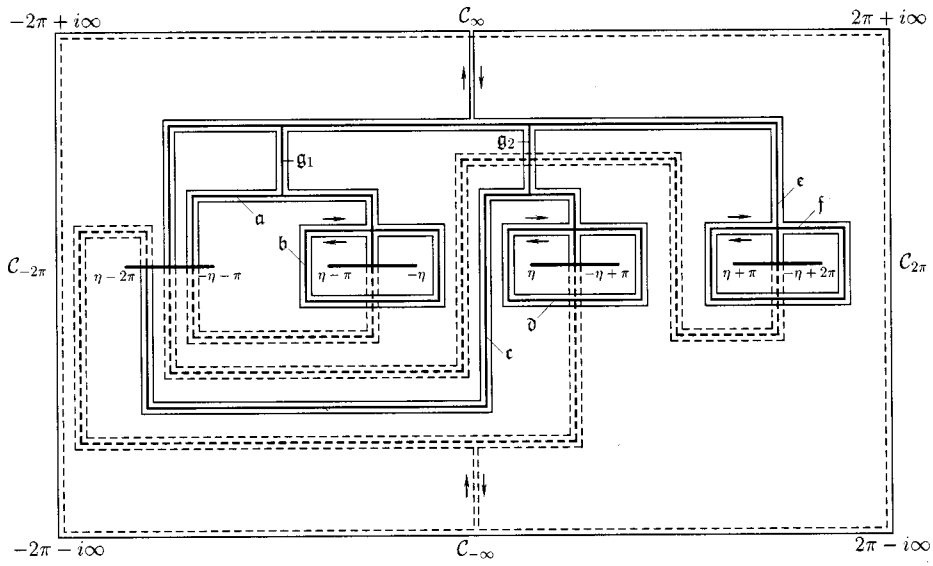


FIG. 5. The contour $\mathcal{C}_2=\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}\cup\mathcal{C}_{\mathfrak{c}\cup\mathfrak{d}}\cup\mathcal{C}_{\mathfrak{e}\cup\mathfrak{f}}\cup\mathcal{C}_{\mathfrak{g}_{1,2}}\cup\mathcal{C}_{\pm 2\pi}\cup\mathcal{C}_{\pm\infty}$ on the upper (solid line) and lower (dashed line) Riemann sheets. The thicker inner lines are the dissections $\mathfrak{a}$, $\mathfrak{b}$, $\mathfrak{c}$, $\mathfrak{d}$, $\mathfrak{e}$, $\mathfrak{f}$ and $\mathfrak{g}_{1,2}$ introduced to make the Riemann surface simply connected. The path $\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}$ denotes, for example, the portion of the contour enclosing the dissecting cycles $\mathfrak{a}$ and $\mathfrak{b}$.

example, if we consider the case of $+2B^1_{2\pi}$, then it follows that $\sigma_{2\pi}\Lambda_{2\pi}\in[-2K,0]\times[-iK',0]$ and, since $\sigma_{2\pi}=\pm 1$, this corresponds to the requirement that $\Lambda_{2\pi}$ lies in either of the parallelograms $\mathcal{P}_1^{\sigma_{2\pi}}$ shown in Fig. 4. One proceeds similarly for the case where we have $-2B^1_{2\pi}$ to obtain the $\mathcal{P}_2^{\sigma_{2\pi}}$ parallelograms in the figure. Taking into account the periodicity of the elliptic sine function, (34) becomes

$$\zeta_{2\pi}=\arccos[k\mathrm{sn}(iK'+3K+\sigma_{2\pi}\Lambda_{2\pi},k)],\quad \Lambda_{2\pi}\in\mathcal{P}_1^{\sigma_{2\pi}}\cup\mathcal{P}_2^{\sigma_{2\pi}},\tag{35}$$

where $\Lambda_{2\pi}$ is given in (31) and the standard periods K and iK' (as well as the parameter k) are given in (33).

IV. DETERMINATION OF $\zeta_{4\pi}$ AND $\kappa_{4\pi}$

A similar procedure to the one given in the previous section is required to successfully invert for $\zeta_{4\pi}$ in (24). However, the cyclic periods appearing on the left-hand side of (24) are now related to 4π periodic expressions and the application of Cauchy's theorem must now be carried out on the Riemann surface delimited by the contour $\mathcal{C}_2$ of width 4π shown in Fig. 5. Proceeding as in Sec. III we consider

$$\int_{\mathcal{C}_2} V^1_{4\pi}(\alpha,u)\,dV^3_{4\pi}(\alpha,u)=2\pi i\sum\ \mathrm{Res},\tag{36}$$

with the elliptic integrals defined as in the previous section but using the 4π periodic terms $v^{1,3}_{4\pi}(\alpha,u)$. For 4π periodic functions, the enclosed surface is now the topological equivalent of a handlebody of genus three (a sphere with three handles) as shown in Fig. 6 and it can be appreciated that making it simply connected involves a larger number of dissections than the torus of the previous section. To make it so, three pairs of canonical dissections $\mathfrak{a},\mathfrak{b}$; $\mathfrak{c},\mathfrak{d}$ and $\mathfrak{e},\mathfrak{f}$ are required as well as the two auxiliary dissections $\mathfrak{g}_1$ and $\mathfrak{g}_2$. They are shown in both Figs. 5 and 6; the simple connectedness is once again better appreciated by examining the handlebody representation of the Riemann surface. To keep the analysis relatively straightforward it is beneficial to draw the dissections such that only members of dissection pairs, $\mathfrak{a}$ and $\mathfrak{b}$, for example, intersect. This,

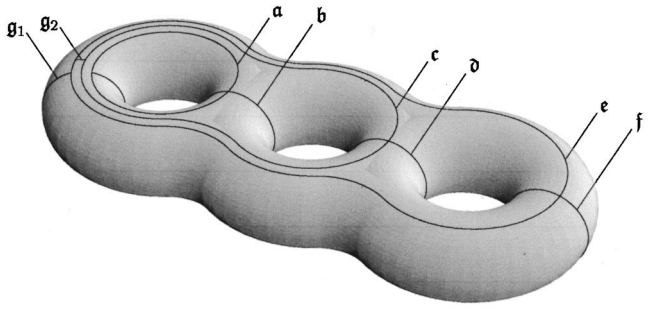


FIG. 6. Handlebody of genus 3, the topological equivalent of the Riemann surface in Fig. 5. It has been made simply connected by introducing the dissections $\mathfrak{a}$, $\mathfrak{b}$, $\mathfrak{c}$, $\mathfrak{d}$, $\mathfrak{e}$, $\mathfrak{f}$ and $\mathfrak{g}_{1,2}$.

while simplifying the evaluation of the path integral around the dissections, entails the rather intricate set of dissections shown in Fig. 5. Carrying out the integration it is seen that only $\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}\cup\mathcal{C}_{\mathfrak{c}\cup\mathfrak{d}}\cup\mathcal{C}_{\mathfrak{e}\cup\mathfrak{f}}$, the portion of the path enclosing the dissection pairs, contributes. The rest of the integral vanishes either by symmetry, as for the parts along $\mathrm{Re}\,\alpha=\pm 2\pi$ on $\mathcal{C}_{\pm 2\pi}$, or identically, as in the case where $|\mathrm{Im}\,\alpha|=\pm\infty$ on $\mathcal{C}_{\pm\infty}$. The contributions from the path enclosing the three dissection pairs, following our previous work, are

$$\int_{\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}} V^1_{4\pi}(\alpha,u)\,dV^3_{4\pi}(\alpha,u)=\mathfrak{A}^1_{4\pi}\mathfrak{B}^3_{4\pi}-\mathfrak{B}^1_{4\pi}\mathfrak{A}^3_{4\pi}, \tag{37}$$

$$\int_{\mathcal{C}_{\mathfrak{c}\cup\mathfrak{d}}} V^1_{4\pi}(\alpha,u)\,dV^3_{4\pi}(\alpha,u)=\mathfrak{C}^1_{4\pi}\mathfrak{D}^3_{4\pi}-\mathfrak{D}^1_{4\pi}\mathfrak{C}^3_{4\pi}, \tag{38}$$

$$\int_{\mathcal{C}_{\mathfrak{e}\cup\mathfrak{f}}} V^1_{4\pi}(\alpha,u)\,dV^3_{4\pi}(\alpha,u)=\mathfrak{E}^1_{4\pi}\mathfrak{F}^3_{4\pi}-\mathfrak{F}^1_{4\pi}\mathfrak{E}^3_{4\pi}. \tag{39}$$

Comparing the canonical cycles defined by the dissections with those defined in Fig. 1, together with symmetry, it is possible to rewrite the above canonical periods in terms of the cyclic periods defined in (19). The cyclic periods are defined on intervals between adjacent branch points and extending these definitions to the negative real axis, by means of the even parity of the expressions, the contributions from the branch point to branch point integrals in $\mathcal{S}_{4\pi}$ can then be identified as shown in Fig. 7(a). The canonical cycles $\mathfrak{a}$, $\mathfrak{b}$, $\mathfrak{c}$, $\mathfrak{d}$, $\mathfrak{e}$ and $\mathfrak{f}$ from Fig. 5 are then partitioned into branch point to branch point contributions, as shown in Figs. 7(b)–7(d). By comparing with Fig. 7(a), they are easily expressed in terms of the cyclic periods and it can thus be shown that

$$\mathfrak{A}=C,\quad \mathfrak{B}=-B,$$

$$\mathfrak{C}=A+B+C+D,\quad \mathfrak{D}=B,$$

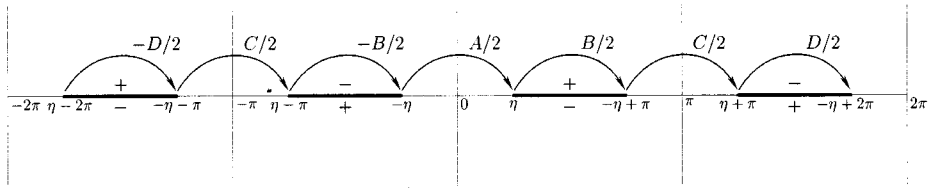
$$\mathfrak{E}=A+B+2C,\quad \mathfrak{F}=D.$$

This yields the following equalities for the right-hand sides of the above equations:

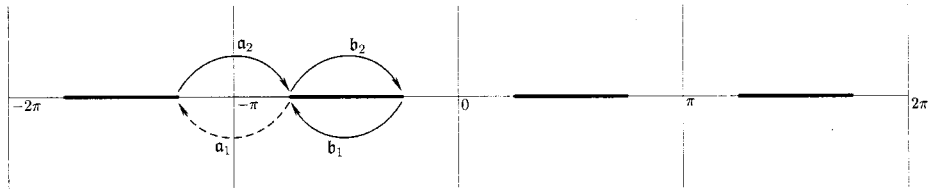
$$\mathfrak{A}^1_{4\pi}\mathfrak{B}^3_{4\pi}-\mathfrak{B}^1_{4\pi}\mathfrak{A}^3_{4\pi}=B^1_{4\pi}C^3_{4\pi}-C^1_{4\pi}B^3_{2\pi},$$

$$\mathfrak{C}^1_{4\pi}\mathfrak{D}^3_{4\pi}-\mathfrak{C}^1_{4\pi}\mathfrak{D}^3_{4\pi}=A^1_{4\pi}B^3_{4\pi}-B^1_{4\pi}A^3_{4\pi}+C^1_{4\pi}B^3_{4\pi}-B^1_{4\pi}C^3_{4\pi}+D^1_{4\pi}B^3_{4\pi}-B^1_{4\pi}D^3_{4\pi},$$

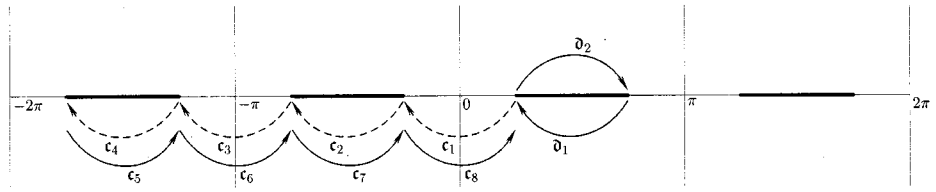
$$\mathfrak{E}^1_{4\pi}\mathfrak{F}^3_{4\pi}-\mathfrak{E}^1_{4\pi}\mathfrak{F}^3_{4\pi}=A^1_{4\pi}D^3_{4\pi}-D^1_{4\pi}A^3_{4\pi}+B^1_{4\pi}D^3_{4\pi}-D^1_{4\pi}B^3_{4\pi}+2(C^1_{4\pi}D^3_{4\pi}-D^1_{4\pi}C^3_{4\pi}).$$



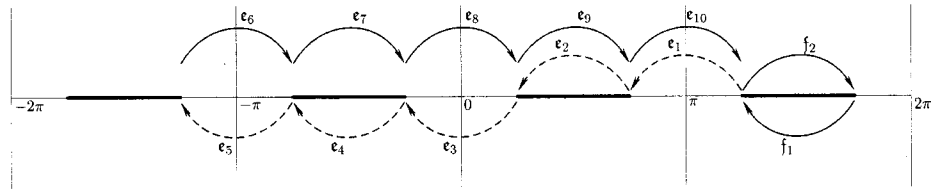
(a) Basic cyclic periods



(b) Canonical cycles $\mathfrak{a}$ and $\mathfrak{b}$



(c) Canonical cycles $\mathfrak{c}$ and $\mathfrak{d}$



(d) Canonical cycles $\mathfrak{e}$ and $\mathfrak{f}$

FIG. 7. Figures used to express the canonical periods in Fig. 5 in terms of the basic cyclic periods in Fig. 1 (e.g., $\mathfrak{A}$ in terms of A, B, C, D). The canonical cycles on the (solid lines) upper and (dashed lines) lower sheets in (b), (c) and (d) are written as chains of branch point to branch point segments—$\mathfrak{e}$ into a sequence of $\mathfrak{e}_n$, for example—which are easily expressed in terms of the basic cyclic periods given in (a).

Summing up these contributions,

$$\begin{aligned}\int_{\mathcal{C}_2} V^1_{4\pi}(\alpha,u)\,dV^3_{4\pi}(\alpha,u) &= \left(\int_{\mathcal{C}_{\mathfrak{a}\cup\mathfrak{b}}} + \int_{\mathcal{C}_{\mathfrak{c}\cup\mathfrak{d}}} + \int_{\mathcal{C}_{\mathfrak{e}\cup\mathfrak{f}}}\right) V^1_{4\pi}(\alpha,u)\,dV^3_{4\pi}(\alpha,u)\\ &= A^1_{4\pi}B^3_{4\pi} - B^1_{4\pi}A^3_{4\pi} + A^1_{4\pi}D^3_{4\pi} - D^1_{4\pi}A^3_{4\pi} + 2(C^1_{4\pi}D^3_{4\pi} - D^1_{4\pi}C^3_{4\pi})\\ &= A^1_{4\pi}(B^3_{4\pi} + D^3_{4\pi}) - 2B^1_{4\pi}(A^3_{4\pi} + C^3_{4\pi}),\end{aligned} \tag{40}$$

where on the last line we have made use of $D^1_{4\pi} = B^1_{4\pi}$ and $C^1_{4\pi} = 0$. This is remarkable in that it reproduces the left-hand side of (24) and can be expressed in terms of residues in accordance with (36). The integrand in (36) has residues

$$-\frac{u(\zeta_{4\pi})}{u(\alpha)}\frac{\cos\alpha}{\cos\zeta_{4\pi}}\frac{\sin(\zeta_{4\pi}/2)}{\sin(\alpha/2)}\int_{(\eta,0)}^{(\alpha,u)} v_{4\pi}^{1}(\alpha')\,d\alpha'\Bigg|_{\alpha=(\pm\zeta_{4\pi},\pm u)}$$

$$=\begin{cases} \mp\displaystyle\int_{(\eta,0)}^{(\alpha,u)} v_{4\pi}^{1}(\alpha')\,d\alpha', & \alpha=(\zeta_{4\pi},\pm u),\\ \pm\displaystyle\int_{(\eta,0)}^{(\alpha,u)} v_{4\pi}^{1}(\alpha')\,d\alpha', & \alpha=(-\zeta_{4\pi},\pm u),\end{cases}$$

which are expressed in terms of $V_{4\pi}^{1}(\zeta_{4\pi})$ and $V_{4\pi}^{1}(2\pi-\zeta_{4\pi})$—both taken on the top Riemann sheet—after carrying out the path integrals on the dissected Riemann surface. Taking advantage of the numerous symmetries and avoiding the crossing of any dissection leads to

$$\sum \text{Res}=\begin{cases} -A_{4\pi}^{1}\pm 4B_{4\pi}^{1}-4V_{4\pi}^{1}(\zeta_{4\pi}), & V_{4\pi}^{1}(\zeta_{4\pi})\in\left\{-\tau'\dfrac{A_{4\pi}^{1}}{4}\pm\tau\dfrac{B_{4\pi}^{1}}{2}:0\leqslant\tau',\tau\leqslant 1\right\},\\ -A_{4\pi}^{1}-4V_{4\pi}^{1}(2\pi-\zeta_{4\pi}), & V_{4\pi}^{1}(2\pi-\zeta_{4\pi})\in\left\{-\tau'\dfrac{A_{4\pi}^{1}}{4}\pm\tau\dfrac{B_{4\pi}^{1}}{2}:0\leqslant\tau',\tau\leqslant 1\right\}.\end{cases} \tag{41}$$

In the short analysis that follows, we restrict for now our attention to the first case given above with the $+4B_{4\pi}^{1}$ term for the sake of brevity. Using (40) and (41) in (36) then produces

$$\begin{aligned} V_{4\pi}^{1}(\zeta_{4\pi}) &= -\frac{A_{4\pi}^{1}}{4}+B_{4\pi}^{1}-\frac{\sigma_{4\pi}}{8\pi i}\{A_{4\pi}^{1}(B_{4\pi}^{3}+D_{4\pi}^{3})-2B_{4\pi}^{1}(A_{4\pi}^{3}+C_{4\pi}^{3})\}\\ &= -\frac{A_{4\pi}^{1}}{4}+B_{4\pi}^{1}+\frac{\sigma_{4\pi}}{\cos(\eta/2)}\Lambda_{4\pi}, \end{aligned} \tag{42}$$

where the only unknown is $\zeta_{4\pi}$ and the sign $\sigma_{4\pi}$ from Eq. (20) has been reintroduced. The $\cos\eta/2$ term is used for future convenience and, in agreement with (24), we have

$$\Lambda_{4\pi}=\frac{\cos(\eta/2)}{8\pi i}\{A_{4\pi}^{1}(B_{0+1}+D_{0+1})-2B_{4\pi}^{1}(A_{0+1}+C_{0+1})\}. \tag{43}$$

In order to use the Jacobian elliptic sine function sn to invert the elliptic integral of the first kind, we recast $V_{4\pi}^{1}(\alpha)$ in terms of Legendre's standard form. The transformation $x=(\sin\alpha/2)/(\sin\eta/2)$, together with the alternative expression to (6),

$$u(\alpha)=2\sqrt{\left(\cos^2\frac{\alpha}{2}-\cos^2\frac{\eta}{2}\right)\left(\cos^2\frac{\alpha}{2}-\sin^2\frac{\eta}{2}\right)},$$

enables us to write

$$V_{4\pi}^{1}(\alpha)=\int_{\eta}^{\alpha}\frac{\cos(\alpha'/2)}{u(\alpha')}d\alpha'=\frac{1}{\cos(\eta/2)}\left\{F\left(\frac{\sin(\alpha/2)}{\sin(\eta/2)},\tan\frac{\eta}{2}\right)-\frac{\cos(\eta/2)}{4}A_{4\pi}^{1}\right\}, \tag{44}$$

and we have the following relationships for the parameter k and the cyclic periods:

$$k=\tan\frac{\eta}{2},\quad A_{4\pi}^{1}=\frac{4K}{\cos(\eta/2)},\quad B_{4\pi}^{1}=\frac{2iK'}{\cos(\eta/2)}. \tag{45}$$

Inserting (44) in (42), solving for $\zeta_{4\pi}$ then produces, after some algebraic manipulations,

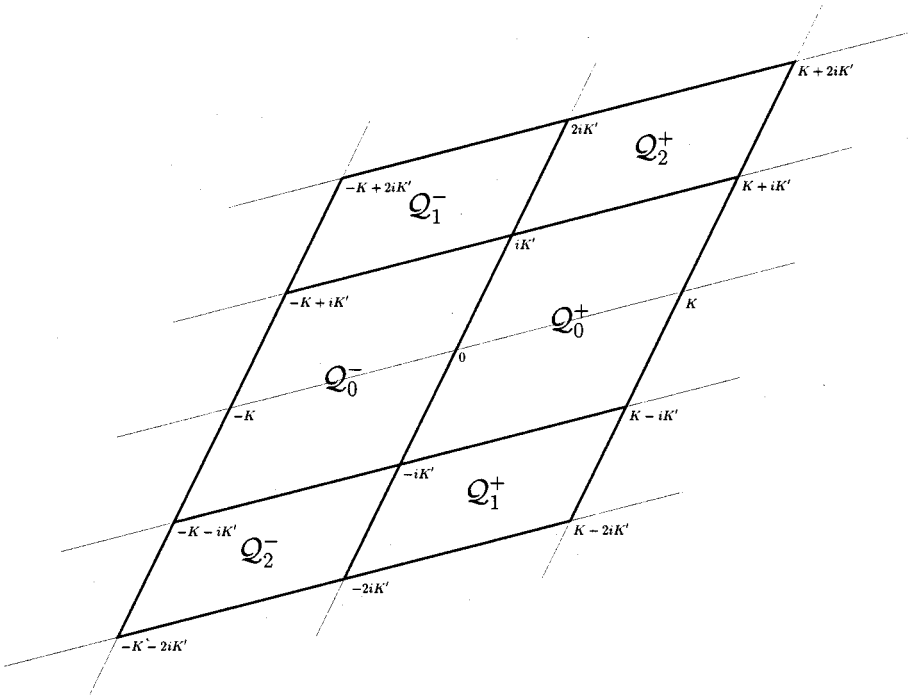


FIG. 8. The regions $\mathcal{Q}_0^{\pm}$, $\mathcal{Q}_1^{\pm}$ and $\mathcal{Q}_2^{\pm}$ in terms of the complete integrals of the first kind K and K' with $k=\tan\eta/2$. The parallelograms $\mathcal{Q}$ indicate the various ranges in which $\Lambda_{4\pi}$ must lie when carrying out the inversion for $\zeta_{4\pi}$ with Eq. (46).

$$\zeta_{4\pi}=2\arcsin\left[\sin\frac{\eta}{2}\,\mathrm{sn}(2iK'+\sigma_{4\pi}\Lambda_{4\pi},k)\right].$$

It follows from (42) and (41) that this holds if $\sigma_{4\pi}\Lambda_{4\pi}$ lies in the period parallelogram $[0,K]\times[-iK',-2iK']$. As $\sigma_{4\pi}=\pm1$, the acceptable range for $\Lambda_{4\pi}$ is therefore $\pm[0,K]\times\pm[-iK',-2iK']$ with the plus sign corresponding to $\sigma_{4\pi}=1$. These regions are identified in Fig. 8 by the period parallelograms $\mathcal{Q}_1^{\sigma_{4\pi}}$. Repeating this process for the other cases in (41), it can be shown that

$$\zeta_{4\pi}=\begin{cases}2\pi-2\arcsin\left[\sin\dfrac{\eta}{2}\,\mathrm{sn}(\sigma_{4\pi}\Lambda_{4\pi},k)\right], & \Lambda_{4\pi}\in\mathcal{Q}_0^{\sigma_{4\pi}},\\ 2\arcsin\left[\sin\dfrac{\eta}{2}\,\mathrm{sn}(2iK'+\sigma_{4\pi}\Lambda_{4\pi},k)\right], & \Lambda_{4\pi}\in\mathcal{Q}_1^{\sigma_{4\pi}},\\ 2\arcsin\left[\sin\dfrac{\eta}{2}\,\mathrm{sn}(-2iK'+\sigma_{4\pi}\Lambda_{4\pi},k)\right], & \Lambda_{4\pi}\in\mathcal{Q}_2^{\sigma_{4\pi}},\end{cases}\tag{46}$$

which is an explicit expression for $\zeta_{4\pi}$. The proper expression and the sign of $\sigma_{4\pi}=\pm1$ are selected by using Fig. 8 in order to determine in which period parallelogram $\mathcal{Q}$ lies the quantity $\Lambda_{4\pi}$. The multiplicative constant $\kappa_{4\pi}$ immediately follows from (23a) or (23b). Note that (46) can be simplified by exploiting the periodicity of the sn function to obtain

$$\zeta_{4\pi}=\begin{cases}2\pi-2\arcsin\left[\sin\dfrac{\eta}{2}\,\mathrm{sn}(\sigma_{4\pi}\Lambda_{4\pi},k)\right], & \Lambda_{4\pi}\in\mathcal{Q}_0^{\sigma_{4\pi}},\\ 2\arcsin\left[\sin\dfrac{\eta}{2}\,\mathrm{sn}(\sigma_{4\pi}\Lambda_{4\pi},k)\right], & \Lambda_{4\pi}\in\mathcal{Q}_1^{\sigma_{4\pi}}\cup\mathcal{Q}_2^{\sigma_{4\pi}},\end{cases}\tag{47}$$

where $\Lambda_{4\pi}$ is given in (43) and k, iK' are given in (45).

V. BRANCH-FREE SOLUTIONS

The determination of the unknowns $\zeta_{2\pi,4\pi}$ and $\kappa_{2\pi,4\pi}$ completes the definition of the solution to the first order difference equations $w(\alpha,u)$ as given in (20). It still has branch points and is therefore multivalued owing to the arbitrariness of the branch of $u(\alpha)$ but its integrand is now such that the path integral is single-valued on either of the Riemann sheets. Meromorphic solutions to the second order difference equation can now be obtained through the use of expressions (10). We recall, however, that solutions free of poles and zeros in the strip $\mathcal{S}_{4\pi}$ are required and therefore seek to use specific linear combinations of (10) to finalize the construction of the solutions. Knowledge of the poles and zeros of $w(\alpha,u)$ is required to successfully complete this endeavor and, since they arise solely due to $v^3_{2\pi}(\alpha,u)$ and $v^3_{4\pi}(\alpha,u)$, it is straightforward to show that in $\mathcal{S}_{4\pi}$

$$w(\alpha,\pm u)\sim\left\{\frac{\alpha+\zeta_{2\pi}}{\alpha-\zeta_{2\pi}}\,\frac{\alpha+(\zeta_{2\pi}-2\pi)}{\alpha-(\zeta_{2\pi}-2\pi)}\,\frac{\alpha+\zeta_{4\pi}}{\alpha-\zeta_{4\pi}}\right\}^{\pm 1}, \tag{48}$$

where $\sigma_{2\pi}=\sigma_{4\pi}=1$ is assumed for simplicity. With this information in hand, the poles of any linear combinations involving (10) are easily determined. Zeros are by nature more elusive and we rely on knowledge of the limiting functions in order to determine their number as well as general location. The cancellation of the poles and zeros is also complicated by the order requirement on the solutions which must be $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha|\to\infty$.

We first present an entirely analytic approach from which two independent solutions are obtained. They satisfy the analyticity requirements, recover the known solutions $\Psi_1(\alpha)$ and $1/\Psi_1(\alpha)$ when $\eta\to\pi/2$, and their only shortcoming is that they vanish as $\eta\to 0$, though knowledge of (13) circumvents this difficulty. In an effort to obtain expressions that also recover the known solution $\Psi_2(\alpha)$ when $\eta\to 0$, a number of approaches relying on numerically locating zeros were explored but, despite producing more desirable behaviors, they fail as $\eta\to 0$ due to inadmissible poles that arise in the strip of analyticity in that limit. An example of such an approach is provided here which nearly succeeds in recovering both limiting functions $\Psi_1(\alpha)$ and $\Psi_2(\alpha)$.

In the following, we use the primed functions $t'_n(\alpha)$ to denote intermediate branch-free solutions of the second order difference equation (2) which still have undesired poles and zeros in the strip $\mathcal{S}_{4\pi}$ whereas the unprimed functions $t_n(\alpha)$ denote the appropriate branch-free and pole/zero-free solutions.

A. Analytical solution

We proceed by constructing two meromorphic solutions of (2), $t'_1(\alpha)$ and $t'_2(\alpha)$, sharing a common pole at $\zeta_{4\pi}$ but having distinct unknown zeros α_1 and α_2, and then use a linear combination to obtain an expression with a known pole/zero pair. Proceeding in a manner similar to the technique presented in Ref. 9, we write

$$t'_1(\alpha)=\frac{T_{2\pi}(\alpha)}{2}\left\{\left(1+\frac{f_1(\alpha)}{u(\alpha)}\right)w(\alpha,u)+\left(1-\frac{f_1(\alpha)}{u(\alpha)}\right)w(\alpha,-u)\right\}, \tag{49}$$

a linear combination of the branch-free forms (10). The functions $f_1(\alpha)$ and $T_{2\pi}(\alpha)$ are 4π periodic; $f_1(\alpha)$ is a trigonometric polynomial used to introduce zeros at appropriate locations in the α plane while the external multiplicative function $T_{2\pi}(\alpha)$ is a rational trigonometric function used to annul poles and zeros. We observe that the introduction of double zeros coincident with the poles of either $w(\alpha,u)$ or $w(\alpha,-u)$ produces, by (48), a simple zero in the term in curly braces above. Thus, if we require

$$1-\frac{f_1(\alpha)}{u(\alpha)}\sim(\alpha+\zeta_{2\pi})^2(\alpha+(\zeta_{2\pi}-2\pi))^2(\alpha+\zeta_{4\pi}), \tag{50}$$

then the second term in braces in (49) has simple zeros coinciding with those of $w(\alpha,u)$ at $\alpha=-\zeta_{2\pi},2\pi-\zeta_{2\pi}$ and is finite at $\alpha=-\zeta_{4\pi}$. This implies

$$\left(1+\frac{f_1(\alpha)}{u(\alpha)}\right)w(\alpha,u)+\left(1-\frac{f_1(\alpha)}{u(\alpha)}\right)w(\alpha,-u)\sim\frac{\alpha+\zeta_{2\pi}}{\alpha-\zeta_{2\pi}}\frac{\alpha+(\zeta_{2\pi}-2\pi)}{\alpha-(\zeta_{2\pi}-2\pi)}\frac{\alpha-\alpha_1}{\alpha-\zeta_{4\pi}},$$

where α_1 is the unknown location of a zero in the $\mathcal{S}_{4\pi}$ strip. While the exact location of α_1 is not easily determined, its general location is known when η is in the neighborhood of $\pi/2$. Indeed, as $\eta\to\pi/2$ we have $f_1(\alpha)/u(\alpha)\to 1$ and

$$\frac{1}{2}\left\{\left(1+\frac{f_1(\alpha)}{u(\alpha)}\right)w(\alpha,u)+\left(1-\frac{f_1(\alpha)}{u(\alpha)}\right)w(\alpha,-u)\right\}\overset{\eta\to\pi/2}{\to}w(\alpha,u),$$

and we conclude, see (48), that when η is in the neighborhood of $\pi/2$, α_1 is in the neighborhood of $-\zeta_{4\pi}$. Choosing $T_{2\pi}(\alpha)$ to eliminate the poles and zeros associated with $\zeta_{2\pi}$ gives

$$T_{2\pi}(\alpha)=\frac{\tan(\zeta_{2\pi}/2)-\tan(\alpha/2)}{\tan(\zeta_{2\pi}/2)+\tan(\alpha/2)}$$

so that

$$t_1'(\alpha)\sim\frac{\alpha-\alpha_1}{\alpha-\zeta_{4\pi}}.$$

The 4π periodic $f_1(\alpha)$ is obtained by letting

$$f_1(\alpha)=\nu_1+\nu_2\cos\alpha+\nu_3\sin\alpha+\nu_4\cos\frac{\alpha}{2}+\nu_5\sin\frac{\alpha}{2}$$

and enforcement of (50) produces

$$\nu_1=\frac{1}{1-\cos(\zeta_{2\pi}-\zeta_{4\pi})}\left\{u(\zeta_{2\pi})-\frac{1}{u(\zeta_{4\pi})}(\sin^2\eta\cos\zeta_{2\pi}\cos\zeta_{4\pi}-\cos^2\eta\sin\zeta_{2\pi}\sin\zeta_{4\pi})\right\},$$

$$\nu_2=\cos\zeta_{2\pi}\left(-\nu_1+\frac{\sin^2\eta}{u(\zeta_{2\pi})}\right),$$

$$\nu_3=\sin\zeta_{2\pi}\left(\nu_1+\frac{\cos^2\eta}{u(\zeta_{2\pi})}\right),$$

with $\nu_4=\nu_5=0$. We note that, in agreement with the analyticity requirements, the function $T_{2\pi}(\alpha)$ and the ratio $f_1(\alpha)/u(\alpha)$ are $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha|\to\infty$. A related meromorphic solution to the second order difference equation sharing the same pole but having a different zero is

$$t_2'(\alpha)=\frac{T_{2\pi}(\alpha)}{2}\left\{\left(1-\frac{f_2(\alpha)}{u(\alpha)}\right)w(\alpha,u)+\left(1+\frac{f_2(\alpha)}{u(\alpha)}\right)w(\alpha,-u)\right\},\tag{51}$$

where $f_2(\alpha)$ is now chosen, following the same kind of procedure as for $f_1(\alpha)$, such that

$$1-\frac{f_2(\alpha)}{u(\alpha)}\sim(\alpha-\zeta_{2\pi})^2(\alpha-(\zeta_{2\pi}-2\pi))^2,$$

$$1+\frac{f_2(\alpha)}{u(\alpha)}\sim(\alpha+\zeta_{4\pi}),$$

and hence

$$t_2'(\alpha)\sim\frac{\alpha-\alpha_2}{\alpha-\zeta_{4\pi}}.$$

By the same reasoning as above, the zero α_2 is also in the neighborhood of $\alpha=-\zeta_{4\pi}$ when η is in the neighborhood of $\pi/2$. The meromorphic solutions $t_1'(\alpha)$ and $t_2'(\alpha)$ then share the same pole and a linear combination can now be used to introduce a zero at $\alpha=-\zeta_{4\pi}$ such that

$$t_1'(\alpha)+\xi t_2'(\alpha)\sim\frac{\alpha+\zeta_{4\pi}}{\alpha-\zeta_{4\pi}} \tag{52}$$

and this requires

$$\xi=-\frac{t_1'(-\zeta_{4\pi})}{t_2'(-\zeta_{4\pi})}=-T_{2\pi}^2(-\zeta_{4\pi})\frac{\sin\zeta_{4\pi}\cos\zeta_{4\pi}-u(\zeta_{4\pi})(\nu_2\sin\zeta_{4\pi}+\nu_3\cos\zeta_{4\pi})}{\sin\zeta_{4\pi}\cos\zeta_{4\pi}+u(\zeta_{4\pi})(\nu_2\sin\zeta_{4\pi}+\nu_3\cos\zeta_{4\pi})}.$$

An acceptable solution of the second order difference equation (2), free of poles and zeros in $\mathcal{S}_{4\pi}$ and $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha|\to\infty$, is then

$$t_1(\alpha)=\frac{\tan(\zeta_{4\pi}/4)-\tan(\alpha/4)}{\tan(\zeta_{4\pi}/4)+\tan(\alpha/4)}\{t_1'(\alpha)+\xi t_2'(\alpha)\}, \tag{53}$$

and

$$t_1(\alpha)\overset{\eta\to\pi/2}{\to}\Psi_1(\alpha),\quad t_1(\alpha)\overset{\eta\to0}{\to}0.$$

The first limit stems from the fact that, as $\eta\to\pi/2$, $1-f_1(\alpha)/u(\alpha)\to0$, $\xi\to0$ and, since in that limit $\kappa_{2\pi,4\pi}\to0$,

$$w(\alpha,u)\overset{\eta\to\pi/2}{\to}\frac{\tan(\zeta_{2\pi}/2)+\tan(\alpha/2)}{\tan(\zeta_{2\pi}/2)-\tan(\alpha/2)}\frac{\tan(\zeta_{4\pi}/4)+\tan(\alpha/4)}{\tan(\zeta_{4\pi}/4)-\tan(\alpha/4)}\Psi_1(\alpha),$$

where we are still assuming that $\sigma_{2\pi}=\sigma_{4\pi}=1$. For the second limit, it is can be shown that $t_1'\to t_2'$ and $\xi\to-1$ as $\eta\to0$, and $t_1(\alpha)$ therefore vanishes in that limit. Following the same prescription as above, a second independent solution $t_2(\alpha)$ can be derived by seeking instead a common pole at $-\zeta_{4\pi}$ and it can easily be shown that

$$t_2(\alpha)=t_1(-\alpha), \tag{54}$$

but we now have, using the same arguments as above,

$$t_2(\alpha)\overset{\eta\to\pi/2}{\to}\frac{1}{\Psi_1(\alpha)},\quad t_2(\alpha)\overset{\eta\to0}{\to}0.$$

The pair of solutions $t_1(\alpha)$ and $t_2(\alpha)$ satisfy the prescribed analyticity requirements listed in Sec. I and recover the known solutions $\Psi_1(\alpha)$ and $1/\Psi_1(\alpha)$ as $\eta\to\pi/2$. However, both vanish as $\eta\to0$ and they therefore fall short of the preferred behavior obtained in Ref. 9 where the solutions are seen to vary smoothly as a function of η between the two known limiting functions when $\eta=\pi/2$ and $\eta=0$. Although undesirable, this is not a serious shortcoming since a pair of linearly independent solutions are known when $\eta=0$ and are given in (13). This vanishing of $t_{1,2}(\alpha)$ when $\eta\to0$ can be attributed to the use of linear combinations [see (52)] in order to create known zeros, a procedure which was not required in Ref. 9. Experience suggests that a purely multiplicative

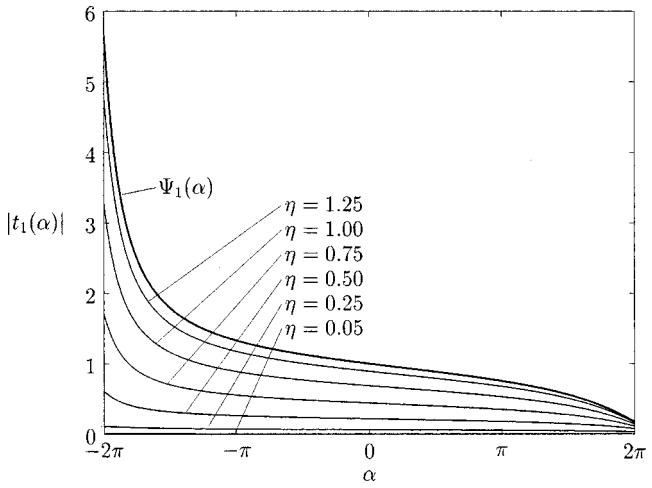


FIG. 9. Magnitude of the branch-free solution $t_1(\alpha)$ given in (53) when $\theta=0.25(1+i)$ for various values of η. The thicker line corresponds to the known limiting function $\Psi_1(\alpha)$, per (11), for $\eta=\pi/2$. The case for $\eta=1.57$ is indistinguishable from $\Psi_1(\alpha)$.

method for eliminating the poles and zeros would likely reproduce the desired behavior, but this so far remains elusive. The continuation of $t_1(\alpha)$ and $t_2(\alpha)$ outside the strip $|\mathrm{Re}\,\alpha|\leqslant 2\pi$ is provided by the first order difference equations (4) and (5), and the results confirm the fact that the solutions are free of branch points everywhere. Indeed, the expressions so obtained are linear combinations of the branch-free forms (10). The technique has been implemented and sample curves for $|t_1(\alpha)|$ are provided in Fig. 9 for various values of η when $\theta=0.25(1+i)$. We observe that $t_1(\alpha)\rightarrow\Psi_1(\alpha)$ as $\eta\rightarrow\pi/2$, and $t_1(\alpha)\rightarrow 0$ as $\eta\rightarrow 0$.

We close this section by summarizing the procedure for computing the solutions $t_1(\alpha)$ and $t_2(\alpha)$. The fundamental building block is $w(\alpha,u)$, given in (20), the solution to the first order equation (4) and its computation requires the quantities $\kappa_{2\pi,4\pi}$, $\zeta_{2\pi,4\pi}$ and $\sigma_{2\pi,4\pi}$. The preliminary step in obtaining those quantities is to first compute the cyclic periods (19) using numerical integration. The quantities $\zeta_{2\pi}$ and $\sigma_{2\pi}$ then follow from (35) and $\kappa_{2\pi}$ from (25). The quantities $\zeta_{4\pi}$, $\sigma_{4\pi}$ and $\kappa_{4\pi}$ are likewise obtained from (47) and (23). The function $w(\alpha,u)$ can then be computed by carrying out numerically the path integral in (20); the functions $t_1'(\alpha)$, $t_2'(\alpha)$ and $t_1(\alpha)$, $t_2(\alpha)$ then respectively follow from (49), (51) and (53), (54).

B. Numerical solution

By foregoing an entirely analytical approach, it is possible to construct solutions that, unlike $t_{1,2}(\alpha)$, do not vanish as $\eta\rightarrow 0$ but we must however resort to the numerical identification of zeros, a somewhat unattractive prospect. The main motivation behind this approach is to proceed with the pole/zero cancellation in a multiplicative fashion and avoid the use of linear combinations of the type (52). Interestingly, it is possible to reproduce in this manner the more desirable behavior obtained in Ref. 9 where Eq. (1) is solved. Therein, the solutions obtained are observed to smoothly vary between two known limiting functions corresponding to, in the case at hand, $\Psi_1(\alpha)$ as $\eta\rightarrow\pi/2$ and $\Psi_2(\alpha)$ as $\eta\rightarrow 0$. This can be achieved here but at the price of having to numerically locate four zeros though, as discussed below, a pole that arises at $\eta\rightarrow 0$ proves to be problematic. Turning once again to the by now familiar form, we write

$$t_3'(\alpha)=\frac{T_{4\pi}(\alpha)}{2}\left\{\left(1+\frac{f_3(\alpha)}{u(\alpha)}\right)w(\alpha,u)+\left(1-\frac{f_3(\alpha)}{u(\alpha)}\right)w(\alpha,-u)\right\}, \tag{55}$$

and examination of the behavior of the solution in Ref. 9 now suggests using

$$f_3(\alpha)=\frac{\cos\zeta_{4\pi}\sin^2\eta\cos\alpha+\sin\zeta_{4\pi}\cos^2\eta\sin\alpha}{u(\zeta_{4\pi})},$$

so that

$$1-\frac{f_3(\alpha)}{u(\alpha)}\sim(\alpha+\zeta_{4\pi})^2(\alpha+(\zeta_{4\pi}-2\pi))^2.$$

The term in braces in (55) is then such that

$$\{\}\sim\frac{\alpha+\zeta_{4_\pi}}{\alpha-\zeta_{4_\pi}}\frac{(\alpha-\alpha_1)(\alpha-\alpha_2)(\alpha-\alpha_3)(\alpha-\alpha_3)}{(\alpha+\zeta_{2\pi})(\alpha-\zeta_{2\pi})(\alpha+(\zeta_{2\pi}-2\pi))(\alpha+(\zeta_{2\pi}+2\pi))}$$

and the pole and zero associated with $\zeta_{4\pi}$ are eliminated by choosing

$$T_{4\pi}(\alpha)=\frac{\tan(\zeta_{4\pi}/4)-\tan(\alpha/4)}{\tan(\zeta_{4\pi}/4)+\tan(\alpha/4)}.$$

In the limit as $\eta\to\pi/2$ we have

$$t_3'(\alpha)\sim\frac{\alpha+\zeta_{2\pi}}{a-\zeta_{2\pi}}\frac{\alpha+(\zeta_{2\pi}-2\pi)}{\alpha-(\zeta_{2\pi}-2\pi)},$$

which implies that, when η is in the neighborhood of $\pi/2$, the poles at $\alpha=-\zeta_{2\pi}$ and $\alpha=-\zeta_{2\pi}+2\pi$ will each have a closely located pair of zeros α_n. Once the location of these zeros has been obtained numerically by evaluating $t_3'(\alpha)$ in (55), the desired solution may be written as

$$t_3(\alpha)=\frac{\cos\alpha-\cos\zeta_{2\pi}}{1-\cos\zeta_{2\pi}}\left(\prod_{n=1}^{4}\frac{\sin(\alpha_n/4)}{\sin\frac{1}{4}(\alpha_n-\alpha)}\right)t_3'(\alpha) \tag{56}$$

so that $t_3(\alpha)$ is free of poles and zeros in $\mathcal{S}_{4\pi}$. It is easily shown that

$$t_3(\alpha)\overset{\eta\to\pi/2}{\to}\Psi_1(\alpha),$$

and since $f_3(\alpha)/u(\alpha)\to\pm1$ as $\eta\to0$, albeit in a branched fashion, it can also be shown (numerically) that

$$t_3(\alpha)\overset{\eta\to0}{\to}\Psi_2(\alpha).$$

Figure 10 provides sample curves for $|t_3(\alpha)|$ for various values of η when $\theta=0.25(1+i)$. The behavior obtained is reminiscent of the one in Ref. 9 since the solution now varies smoothly between the two limiting functions $\Psi_{1,2}(\alpha)$ as a function of η. Once again, a second solution is provided by $t_3(-\alpha)$ and this recovers $1/\Psi_1(\alpha)$ as $\eta\to\pi/2$ and $\Psi_2(\alpha)$ as $\eta\to0$. Despite this, the approach is, however, flawed since one of the numerical zeros strays slightly outside $\mathcal{S}_{4\pi}$ when $\eta\simeq0.001$. This leads to failure of the solution in that limit since the corresponding zero canceling term in (56) gives rise to a pole within the strip of analyticity. It is unclear at this time if this is due to numerical inaccuracies or a fundamental limitation of the approach. It does, however, suggest that the construction procedure based on branch-free combinations of the function $w(\alpha,u)$ has the potential to recover solutions that vary smoothly between the two known limiting functions provided a proper method can be devised for constructing the branch-free solutions.

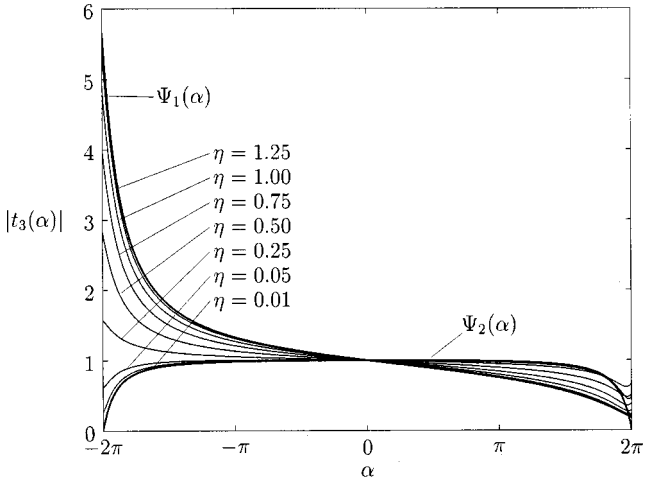


FIG. 10. Magnitude of the branch-free solution $t_3(\alpha)$ given in (56) when $\theta=0.25(1+i)$ for various values of η. The thicker lines corresponds to the known limiting function $\Psi_1(\alpha)$, per (11), for $\eta=\pi/2$ and $\Psi_2(\alpha)$, per (13), for $\eta=0$.

VI. CONCLUSION

A recently proposed solution technique for a class of second order functional difference equations was applied to a case of intermediate complexity in order to assess its potential use for solving certain electromagnetic scattering problems. The essence of this conceptually simple approach lies in the construction of branched solutions to first order difference equations and this is achieved by systematically eliminating singular contributions to produce single-valued expressions. This requirement leads to an equation system whose analytical solution is made possible by obtaining, through the application of Cauchy's theorem on Riemann surfaces, specialized versions of relationships arising in the bilinear relations of Riemann. While the portion of the analysis carried out on a Riemann surface of genus one has the same order of complexity as the one found in Ref. 9, we were also now required to carry out a similar but more intricate analysis on a Riemann surface of genus three in order to obtain well-defined branched solutions to the related first order equations. The final solutions, expressed in terms of branch-free linear combinations of the branched solutions to the first order equations, have all the desired analyticity properties and also recover the known solution $\Psi_1(\alpha)$ as $\eta\rightarrow\pi/2$. The fully analytical approach presented satisfies all of the solution requirements and the fact that it vanishes as $\eta\rightarrow 0$ is not a critical shortcoming since known exact solutions are available in that particular limit. The other variation provided, which requires the numerical identification of zeros in the complex α plane, represents an attempt at resolving this shortcoming and, although it fails when $\eta\sim 0$, it otherwise recovers a solution which varies smoothly between the two known limiting functions $\Psi_1(\alpha)$ and $\Psi_2(\alpha)$. This is encouraging since it suggests that the proposed approach has the potential to produce a solution that smoothly recovers the two known limiting functions provided a proper method for constructing branch-free solutions can be found.

The results obtained demonstrate the promise of the proposed technique but there are still a large number of interesting issues to be addressed. Indeed, while the procedure for constructing branch-free solutions is fairly well understood, the construction of such meromorphic solutions free of poles and zeros in particular regions of the complex α plane, the strip $\mathcal{S}_{4\pi}$ in this instance, remains challenging. Consequently, a fully analytical solution displaying the more desirable behavior obtained for the numerical approach, where the solutions recovers $\Psi_1(\alpha)$ and $\Psi_2(\alpha)$ in the appropriate limits, is still sought. The success of this endeavor is apparently dependent on gaining more insight into the behavior of the zeros of the meromorphic functions constructed. Additionally, a better understanding of the dependency of the quantities $\Lambda_{2\pi,4\pi}$ on the problem parameters η and θ is required. Ideally, this would take the form of specific requirements on, for instance, the

impedances characterizing the structure and would provide a range over which the procedure for determining the values $\zeta_{2\pi,4\pi}$ can be carried out. Indeed, it is not inconceivable that under certain circumstances $\Lambda_{2\pi,4\pi}$ might lie outside the $\mathcal{P}$ and $\mathcal{Q}$ parallelograms, leading to a failure of the technique. Another highly interesting item is the application of the approach when solutions of different orders (i.e., not $\mathcal{O}(1)$ as $|\mathrm{Im}\,\alpha|\to\infty$) are required since in such cases the integrand of $w(\alpha,u)$ is required not to vanish as $|\mathrm{Im}\,\alpha|\to\infty$. It is, however, apparent that, unless beneficial symmetries can be found in cases of higher complexity, a sufficiently large number of singularities in the strip of analyticity, while not precluding a solution in principle, may well make such an approach impractical. Despite this and some of the currently unresolved issues mentioned above, the technique proposed in Ref. 9, as demonstrated herein, can be applied relatively straightforwardly to cases of intermediate complexity. Current efforts focus on its application to cases of higher complexity such as the diffraction from an anisotropic impedance half-plane illuminated at skew incidence.

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Invariant algebraic surfaces of the Lorenz system

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In this paper we provide a complete classification of the Darboux invariants, of the irreducible Darboux polynomials, of the rational first integrals and of the algebraic integrability for the classical Lorenz system $\dot{x}=s(y-x)$, $\dot{y}=rx-y-xz$, $\dot{z}=-bz+xy$. In the proofs, we use the weight homogeneous polynomials and the method of characteristic curves for solving linear partial differential equations. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1435078]

I. INTRODUCTION AND DEFINITIONS

The Lorenz system:

$$\begin{aligned}\dot{x}&=s(y-x)=P(x,y,z),\\ \dot{y}&=rx-y-xz=Q(x,y,z),\\ \dot{z}&=-bz+xy=R(x,y,z),\end{aligned}\tag{1}$$

is a famous dynamical model (see, e.g., Lorenz, 1963), where x, y, and z are real variables; and s, r, and b are real parameters. This system has been thoroughly investigated as a dynamical system (see, e.g., Sparrow, 1982). From the point of view of integrability it was also intensively studied using different integrability theories (see, e.g., Cairó and Hua, 1993; Giacomini, Repetto, and Zandron, 1991; Goriely, 1996; Gupta, 1993; Kús, 1983; Schwarz, 1985; Segur, 1982; Steeb, 1982; and Strelcyn and Wojciechowski, 1988).

The problem involving the algebraic integrability and the Darboux polynomials is classical and difficult. It mainly received contributions from Darboux (1878), and Poincaré (1981, 1987). The former gave a link between algebraic geometry and the search of first integrals, and showed how to construct the first integrals of a planar polynomial vector field having sufficient number of invariant algebraic curves. The latter was mainly interested in rational first integrals and noticed the difficulty for obtaining an algorithm to compute Darboux polynomials. For three-dimensional systems, Labrunie (1996) and Moulin Ollagnier (1997) characterized all polynomial first integrals of the (a,b,c) Lotka–Volterra system. Moulin Ollagnier (1999) studied its homogeneous rational first integrals. Giacomini, Repetto, and Zandron (1991) investigated the integrals of motion for three-dimensional non-Hamiltonian dynamical systems. Llibre and Zhang (2000) characterized all the invariant algebraic surfaces, the polynomial first integrals, the rational first integrals, the invariants, and the algebraic integrability for the Rikitake system.

For the Lorenz system only six independent Darboux invariants had been found:

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Darboux invariant	Parameters
$(x^2-2sz)e^{2st}$	$b=2s$
$(-rx^2+\frac{1}{3}y^2+\frac{2}{3}xy+x^2z-\frac{3}{4}x^4)e^{4t/3}$	$b=0,\ s=\frac{1}{3}$
$(y^2+z^2)e^{2t}$	$b=1,\ r=0$
$(4(1-r)z+rx^2+y^2-2xy+x^2z-\frac{1}{4}x^4)e^{4t}$	$b=4,\ s=1$
$(-rx^2+y^2+z^2)e^{2t}$	$b=1,\ s=1$
$\left(\frac{1}{s}(2s-1)^2x^2+sy^2-(4s-2)xy+x^2z-\frac{1}{4s}x^4\right)e^{4st}$	$b=6s-2,\ r=2s-1.$

The first three invariants were found by Segur (1982) using the Painlevé method (see also Steeb, 1982; Tabor and Weiss, 1981). The last three invariants were found by Kús (1983) using the method of Carlemann embedding. Furthermore, it is easy to prove that the function $H=(y^2+z^2)/(x^2-z)^2$ is a rational first integral under the conditions $b=1$, $s=1/2$, and $r=0$.

Using these invariants, Giacomini and Neukirch (1997) constructed families of two-dimensional surfaces transverse to the flow of the Lorenz system, in which everyone separates the phase space $\mathbb{R}^3$ and hence can be used to describe the location of the global attractor of the flow.

In this paper, by using the weight homogeneous polynomials and the method of characteristics, we obtain the classification of all the irreducible invariant algebraic surfaces, of the invariants, of the rational first integrals and of the algebraic integrability for the Lorenz system. Before presenting our main results, we first recall some definitions.

A real polynomial $f(x,y,z)$ is called a *Darboux polynomial* for the Lorenz system if

$$\frac{\partial f}{\partial x}P+\frac{\partial f}{\partial y}Q+\frac{\partial f}{\partial z}R=kf \tag{2}$$

for some real polynomial $k(x,y,z)$, which is called a *cofactor* of f. It is easy to prove that the degree of k is less than or equal to 1. Therefore, we can assume that the cofactor is of the form

$$k(x,y,z)=k_1x+k_2y+k_3z+c. \tag{3}$$

If $f(x,y,z)$ is a Darboux polynomial of the Lorenz system, then the algebraic surface $f=0$ in $\mathbb{R}^3$ is called an *invariant algebraic surface*. The name is due to the fact that if a solution of (1) has a point on the invariant algebraic surface, then the whole solution is contained in it.

We say that a nonconstant real function $H(x,y,z,t):\mathbb{R}^3\times\mathbb{R}\to\mathbb{R}$, is an *invariant* of the Lorenz system, if it is constant on all solution curves $(x(t),y(t),z(t))$ of the Lorenz system, i.e., $H(x(t),y(t),z(t),t)\equiv$constant for all values of t for which the solution $(x(t),y(t),z(t))$ is defined on $\mathbb{R}^3$. Obviously, if H is differentiable on $\mathbb{R}^3\times\mathbb{R}$, then H is an invariant of the Lorenz system if and only if along every solution of the Lorenz system we have

$$\frac{\partial H}{\partial t}+\frac{\partial H}{\partial x}P+\frac{\partial H}{\partial y}Q+\frac{\partial H}{\partial z}R\equiv 0. \tag{4}$$

If the invariant H is independent on the time, then it is called a *first integral*. If the first integral H is a polynomial (respectively, a rational function), then it is called a *polynomial first integral* (respectively, a *rational first integral*). If the invariant H is of the form $f(x,y,z)\exp(\sigma t)$ with f a polynomial in x,y and z, and σ a real constant, then H is called a *Darboux invariant*. We remark that a Darboux invariant is also called an *integral of motion* by some physicists. Moreover, it is easy to prove that $H=f(x,y,z)\exp(\sigma t)$ is a Darboux invariant if and only if f is a Darboux polynomial with the cofactor $-\sigma$. If H is a Darboux invariant, then σ is called an *exponent* of H.

Let $\mathcal{S}$ be the set of all Darboux polynomials (or Darboux invariants) for the Lorenz system. If $\mathcal{J}$ is a minimum subset of $\mathcal{S}$ such that every element of $\mathcal{S}$ is obtained by doing finitely many product of the elements of $\mathcal{J}$ and the addition of finitely many these new elements having the same cofactor (or having the same exponent), then we say that every element of $\mathcal{J}$ is a *generator* of $\mathcal{S}$.

Two first integrals $H_1(x,y,z)$ and $H_2(x,y,z)$ are said to be *independent*, if their gradients are linearly independent vectors for all points $(x,y,z)\in\mathbb{R}^3$ except perhaps for a set of zero Lebesgue measure. If the Lorenz system has two independent first integrals, then we say that it is *completely integrable*. We note that in this case the orbits of the Lorenz system are contained in the curves $\{H_1(x,y,z)=h_1\}\cap\{H_2(x,y,z)=h_2\}$ when h_1 and h_2 vary in $\mathbb{R}$.

An *algebraic function* $H(x,y,z)=C$ is a solution of the algebraic equation

$$f_0+f_1C+f_2C^2+\cdots+f_{n-1}C^{n-1}+C^n=0,$$

where $f_i(x,y,z)$ are rational functions, and n is the smallest positive integer for which such a relation holds. Obviously, any rational function is algebraic. The Lorenz system is said to be *algebraically integrable* if it has two independent algebraic first integrals.

This paper is organized as follows. In Sec. II, we state our main results and recall some tools we will need later on. In Sec. III, we prove Theorem 1. The proof of Corollary 2 is given in Sec. IV.

II. STATEMENT OF THE MAIN RESULTS AND SOME PRELIMINARY TOOLS

Our main results are the following.

Theorem 1: *When $s\neq 0$, a set of generators for the set of all Darboux polynomials of the Lorenz system consists of the following six ones:*

Darboux polynomial	Cofactor	Parameters
x^2-2sz	$-2s$	$b=2s$
$x^4-\frac{4}{3}x^2z-\frac{4}{9}y^2-\frac{8}{9}xy+\frac{4}{3}rx^2$	$-\frac{4}{3}$	$b=0,\ s=\frac{1}{3}$
y^2+z^2	-2	$b=1,\ r=0$
$x^4-4x^2z-4y^2+8xy-4rx^2-16(1-r)z$	-4	$b=4,\ s=1$
$y^2+z^2-rx^2$	-2	$b=1,\ s=1$
$x^4-4sx^2z-4s^2y^2+4s(4s-2)xy-(4s-2)^2x^2$	$-4s$	$b=6s-2,\ r=2s-1$

Corollary 2: For the Lorenz system, if $s\neq 0$ then the following statements hold:

(a) The cofactor corresponding to every Darboux polynomial of the Lorenz system is a constant.

(b) The generators of Darboux invariants for the Lorenz system are the known six ones of the previous list.

(c) The Lorenz system has no polynomial first integrals.

(d) The Lorenz system has a rational first integral if and only if $b=1$, $s=1/2$, and $r=0$. The rational first integrals are of the form

$$\frac{\displaystyle\sum_{i+2j=K} a_{ij}(x^2-z)^i(y^2+z^2)^j}{\displaystyle\sum_{i_1+2j_1=K} b_{i_1j_1}(x^2-z)^{i_1}(y^2+z^2)^{j_1}},$$

where $a_{ij},b_{i_1j_1}\in\mathbb{R}$ and $i,j,i_1,j_1,K\in\mathbb{N}$.

(e) The Lorenz system is not algebraically integrable.

We remark that when $s=0$, the Lorenz system has the first integral $H(x,y,z)=x$, and then on each plane $x=$constant the system becomes linear.

In the proof of Theorem 1 we will use the following notions and tools.

A polynomial $g(\mathbf{x})$ with $\mathbf{x}\in\mathbb{R}^n$ is said to be *weight homogeneous* if there exist $\mathbf{s}=(s_1,\ldots,s_n)\in\mathbb{N}^n$ and $m\in\mathbb{N}$ such that for all $\alpha\in\mathbb{R}\backslash\{0\}$,

$$g(\alpha^{\mathbf{s}}\mathbf{x})=g(\alpha^{s_1}x_1,\alpha^{s_2}x_2,\ldots,\alpha^{s_n}x_n)=\alpha^m g(\mathbf{x}),$$

where $\mathbb{R}$ denotes the set of real numbers, and $\mathbb{N}$ the set of positive integers. We shall refer $\mathbf{s}$ to the *weight* of g, m the *weight degree*, and $\mathbf{x}\to\alpha^{\mathbf{s}}\mathbf{x}$ the weight change of the variables.

Now we recall the method of characteristic curves for solving linear partial differential equations [for instance, see Bleecker and Csordas (1992), Chap. 2].

Consider the following first-order linear partial differential equation:

$$a(x,y,z)A_x+b(x,y,z)A_y+c(x,y,z)A_z+d(x,y,z)A=f(x,y,z), \tag{5}$$

where $A=A(x,y,z)$, a, b, c, d, and f are C^1 maps.

A curve $(x(t),y(t),z(t))$ in the xyz space is a *characteristic curve* for the partial differential equation (5), if at each point (x_0,y_0,z_0) on the curve, the vector $(a(x_0,y_0,z_0)$, $b(x_0,y_0,z_0),c(x_0,y_0,z_0))$ is tangent to the curve. So, a characteristic curve is a solution of the system

$$\frac{\mathrm{d}x}{\mathrm{d}t}=a(x(t),y(t),z(t)),\quad \frac{\mathrm{d}y}{\mathrm{d}t}=b(x(t),y(t),z(t)),\quad \frac{\mathrm{d}z}{\mathrm{d}t}=c(x(t),y(t),z(t)).$$

In practice, for convenience we treat z as the independent variable instead of t, then the above system is reduced to the system [assuming $c(x,y,z)\neq 0$]

$$\frac{\mathrm{d}x}{\mathrm{d}z}=\frac{a(x,y,z)}{c(x,y,z)},\quad \frac{\mathrm{d}y}{\mathrm{d}z}=\frac{b(x,y,z)}{c(x,y,z)}. \tag{6}$$

This ordinary differential equation is known as the *characteristic equation* of (5).

Suppose that (6) has a solution in the implicit form $g(x,y,z)=c_1$, $h(x,y,z)=c_2$, where c_1 and c_2 are arbitrary constants. We consider the change of the variables

$$u=g(x,y,z),\quad v=h(x,y,z),\quad w=z, \tag{7}$$

and write its inverse transformation as $x=p(u,v,w)$, $y=q(u,v,w)$, and $z=r(u,v,w)$ (of course, sometimes the explicit inverse transformation cannot be obtained, or it is not well defined). Then the linear partial differential equation (5) becomes the following ordinary differential equation in w (for fixed u and v):

$$\overline{c}(u,v,w)\overline{A}_w+\overline{d}(u,v,w)\overline{A}=\overline{f}(u,v,w), \tag{8}$$

where $\overline{c}$, $\overline{d}$, $\overline{A}$, and $\overline{f}$ are c, d, A, and f, are written in terms of u, v, and w.

If $\overline{A}=\overline{A}(u,v,w)$ is a solution of (8), then by transformation (7) we get that

$$A(x,y,z)=\overline{A}(g(x,y,z),h(x,y,z),z)$$

is a solution of the linear partial differential equation (5). Moreover, the general solution of (8) is also the general solution of (5) when, using (7), we write u, v, and w in function of x, y, and z.

III. PROOF OF THEOREM I

In order that readers can follow our proof easily, and use our method to other systems, we state the global strategy of the proof for a general system. Consider the polynomial system

$$\dot{\mathbf{x}}=\mathbf{g}(\mathbf{x}),\quad \mathbf{x}\in\mathbb{R}^n. \tag{9}$$

Step 1. We select a suitable weight change of the variables, denoted by $\mathbf{X}=\alpha^{\mathbf{s}}\mathbf{x}$ $=(\alpha^{s_1}x_1,\ldots,\alpha^{s_n}x_n)$, and rescale the time by $T=\alpha^{-s_0}t$, where $s_i\in\mathbb{N}$ for $i=0,1,\ldots,n$, such that system (9) is transformed to

$$\mathbf{X}' = \sum_{j=0}^{r} \alpha^j \mathbf{g}_{m-j}(\mathbf{X}), \quad r \leqslant m, \tag{10}$$

where the prime denotes the derivative with respect to T, $\mathbf{g}_{m-j}$ is a polynomial vector, such that every component is a weight homogeneous polynomial. Obviously, system (10) with $\alpha=0$ is invariant by the selected transformation.

Step 2. Suppose that $f(\mathbf{x})$ is a Darboux polynomial of (9) with a cofactor $k(\mathbf{x})$. Set

$$F(\mathbf{X}) = \alpha^l f(\alpha^{-\mathbf{s}}\mathbf{X}) = \sum_{i=0}^{p} \alpha^i F_i(\mathbf{X}),$$

$$K(\mathbf{X}) = \alpha^h k(\alpha^{-\mathbf{s}}\mathbf{X}) = \sum_{j=0}^{q} \alpha^j K_j(\mathbf{X}),$$

where $\alpha^{-\mathbf{s}}\mathbf{X} = (\alpha^{-s_1}X_1, \ldots, \alpha^{-s_n}X_n)$, $p,q \in \mathbb{N}$, l and h are the highest weight degrees of the weight homogeneous components for f and k, respectively, and F_i and K_j are weight homogeneous polynomials. Then $F(\mathbf{X})$ is a Darboux polynomial of system (10) with the cofactor $\alpha^{s_0-h}K(\mathbf{X})$. From

$$\left\langle \sum_{j=0}^{r} \alpha^j \mathbf{g}_{m-j}, \frac{\partial F}{\partial \mathbf{X}} \right\rangle = \alpha^{s_0-h} K F, \tag{11}$$

and by equating the terms with α^j in (11), i.e., the weight homogeneous components with the same weight degree, we get

$$L[F_i] = G_i(F_i) + H_i(F_0, \ldots, F_{i-1}), \tag{12}$$

with $i=0,1,\ldots,\max\{r+p, s_0-h+q+p\}$, where G_i is a linear function in F_i, H_i is known by induction, and L a linear partial differential operator of the form

$$L = \left\langle \mathbf{g}_m, \frac{\partial}{\partial \mathbf{X}} \right\rangle.$$

Step 3. Solving (12) we obtain the weight homogeneous polynomial solution F_i. The main tool is the method of characteristic curves for solving linear partial differential equations.

First we transfer Eq. (12) with $i=0$ to an ordinary differential equation. By solving the ordinary differential equation we get a general solution F_0^* of (12) with $i=0$. Generally, F_0^* is not a weight homogeneous polynomial with the given degree. So we must let the components with nonweight homogeneous polynomials of the given degree be equal to zero. Then we get F_0 and the corresponding conditions.

Second, introducing F_0 into (12) with $i=1$ and working in a similar way to solve F_0, we can obtain F_1 and some conditions which must be satisfied. Then introducing F_0 and F_1 into (12) with $i=2$, we obtain F_2. According to this process we obtain all the weight homogeneous polynomial solutions F_i for (12) and the conditions on the coefficients of system (12).

Step 4. From $f(\mathbf{x}) = F(\mathbf{X})|_{\alpha=1} = \Sigma_{i=1}^{p} F_i$, we get all the Darboux polynomials for system (9).

We remark that there is a double aim using the weight change of the variables. First, the general solution of the characteristic equations for $L[F_i] = G_i + H_i$ is easy to obtain, because the reduction process from the linear partial differential equation to the ordinary differential equations becomes simpler. Second, the computation for solving F_i becomes easier.

Proof of Theorem 1: We make the change of the variables

$$x = \alpha^{-1}X, \quad y = \alpha^{-2}Y, \quad z = \alpha^{-2}Z, \quad t = \alpha T, \tag{13}$$

then the Lorenz system (1) becomes

$$X' = s(Y - \alpha X),$$

$$Y' = -XZ - \alpha Y + r\alpha^2 X, \tag{14}$$

$$Z' = XY - b\alpha Z,$$

where the prime denotes the derivative with respect to T. We note that this transformation is almost equivalent to the one introduced by Robbins (1979), but the aim for introducing the changes is different. In Robbins (1979), by rescaling the variables the author changes the Lorenz model with a high valued parameter R to a system with a small parameter ϵ. Then, he uses the first integrals of the new system for $\epsilon = 0$ to construct a solution in power series of ϵ for the new system. In this way the author investigated the behavior of the orbits for the Lorenz model. In our change of the variables, we introduce the auxiliary parameter α and the weight homogeneous polynomials in order that the computations for searching the Darboux polynomials becomes easier.

Suppose that $f(x,y,z)$ is a Darboux polynomial of the Lorenz system (1) with a cofactor $k(x,y,z)$. Using transformation (13), and setting $F(X,Y,Z) = \alpha^l f(\alpha^{-1}X, \alpha^{-2}Y, \alpha^{-2}Z)$, and $K(X,Y,Z) = \alpha^2 k(\alpha^{-1}X, \alpha^{-2}Y, \alpha^{-2}Z)$, where l is the highest weight degree in the weight homogeneous components of f in x, y, and z with weight (1,2,2).

We claim that F is a Darboux polynomial of system (14) with the cofactor $\alpha^{-1}K$. Indeed, along the flow of system (14) we have

$$\frac{\mathrm{d}F}{\mathrm{d}T} = \frac{\partial F}{\partial X}\frac{\mathrm{d}X}{\mathrm{d}T} + \frac{\partial F}{\partial Y}\frac{\mathrm{d}Y}{\mathrm{d}T} + \frac{\partial F}{\partial Z}\frac{\mathrm{d}Z}{\mathrm{d}T} = \alpha^{l+1}\left(\frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t} + \frac{\partial f}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t}\right) = \alpha^{l+1}\frac{\mathrm{d}f}{\mathrm{d}t} = \alpha^{l+1}kf = \alpha^{-1}KF.$$

Assume that $F = F_0 + \alpha F_1 + \alpha^2 F_2 + \cdots + \alpha^m F_m$, where F_i is a weight homogeneous polynomial in X, Y, and Z with the weight degree $l-i$ for $i = 0,1,\ldots,m$, and $l \geqslant m$. Obviously, $f = F|_{\alpha=1}$. From the definition of a Darboux polynomial, we have

$$s(y - \alpha x)\sum_{i=0}^{m} \alpha^i \frac{\partial F_i}{\partial x} + (-xz - \alpha y + r\alpha^2 x)\sum_{i=0}^{m} \alpha^i \frac{\partial F_i}{\partial y} + (xy - b\alpha z)\sum_{i=0}^{m} \alpha^i \frac{\partial F_i}{\partial z}$$

$$= (k_1 x + k_2 \alpha^{-1} y + k_3 \alpha^{-1} z + c\alpha)\sum_{i=0}^{m} \alpha^i F_i,$$

where we still use x,y and z instead of X, Y, and Z. Equating the terms with α^{-1} we can prove that $k_2 = k_3 = 0$. Equating the terms with α^i for $i = 0,1,\ldots,m+2$, we get

$$L[F_0] = k_1 x F_0,$$

$$L[F_1] = k_1 x F_1 + cF_0 + sx\frac{\partial F_0}{\partial x} + y\frac{\partial F_0}{\partial y} + bz\frac{\partial F_0}{\partial z}, \tag{15}$$

$$L[F_j] = k_1 x F_j + cF_{j-1} + sx\frac{\partial F_{j-1}}{\partial x} + y\frac{\partial F_{j-1}}{\partial y} + bz\frac{\partial F_{j-1}}{\partial z} - rx\frac{\partial F_{j-2}}{\partial y}$$

for $j = 2, 3,\ldots,m+2$, where $F_j = 0$ for $j > m$ and L is the linear partial differential operator of the form

$$L = sy\frac{\partial}{\partial x} - xz\frac{\partial}{\partial y} + xy\frac{\partial}{\partial z}.$$

The characteristic equations associated with the first linear partial differential equation of system (15) are

$$\frac{dx}{dz}=\frac{sy}{xy},\quad \frac{dy}{dz}=-\frac{xz}{xy}.$$

This system of equations has the general solution

$$x^2-2sz=d_1,\quad y^2+z^2=d_2,$$

where d_1 and d_2 are constants of integration.

According with the method of characteristics, we make the change of the variables

$$u=x^2-2sz,\quad v=y^2+z^2,\quad w=z. \tag{16}$$

Its inverse transformation is

$$x=\pm\sqrt{u+2sw},\quad y=\pm\sqrt{v-w^2},\quad z=w. \tag{17}$$

In the following, for simplicity we only consider the case $x=\sqrt{u+2sw}$, $y=\sqrt{v-w^2}$, and $z=w$. Under changes (16) and (17), the first equation of (15) becomes the following ordinary differential equation (for fixed u,v):

$$\sqrt{v-w^2}\frac{d\overline{F_0}}{dw}=k_1\overline{F_0},$$

where $\overline{F_0}$ is F_0, written in u, v, and w. In what follows, we always use $\overline{\theta}$ to denote a function $\theta(x,y,z)$ written in terms of u, v, and w. The above equation has the general solution

$$\overline{F_0}=\overline{G_0}(u,v)\exp\left(k_1\arcsin\frac{w}{\sqrt{v}}\right),$$

where $\overline{G_0}$ is an arbitrary smooth function in u and v. So,

$$F_0(x,y,z)=\overline{F_0}(u,v,w)=\overline{G_0}(x^2-2sz,y^2+z^2)\exp\left(k_1\arcsin\frac{z}{\sqrt{x^2+y^2}}\right).$$

In order that F_0 be a weight homogeneous polynomial, we must have $k_1=0$ and $\overline{G_0}$ a polynomial in u and v. Consequently, the cofactor of every Darboux polynomial for the Lorenz system is a constant. Since u and v are weight homogeneous polynomials in x, y, and z of weight degrees 2 and 4, respectively, F_0 should be weight degree either $l=4n$, or $l=4n-2$ for some convenient $n\in\mathbb{N}$. So, F_0 has the form $\Sigma_{i=0}^{n}a_iu^{2i}v^{n-i}$, or $\Sigma_{i=1}^{n}a_iu^{2i-1}v^{n-i}$. Therefore, we have

$$F_0=\sum_{i=0}^{n}a_i(x^2-2sz)^{2i}(y^2+z^2)^{n-i}, \tag{18}$$

with the weight degree $4n$, or

$$F_0=\sum_{i=1}^{n}a_i(x^2-2sz)^{2i-1}(y^2+z^2)^{n-i}, \tag{19}$$

with the weight degree $4n-2$.

Accordingly, with these two different cases, we divide the proof into two subsections.

A. F_0 has the form (19)

Substituting F_0 into the second equation of (15) and doing some computations, we obtain that

$$L[F_1]=\sum_{i=1}^{n}[c+2(2i-1)s+2(n-i)]a_i(x^2-2sz)^{2i-1}(y^2+z^2)^{n-i}$$
$$+\sum_{i=1}^{n}(4s^2-2sb)(2i-1)a_i(x^2-2sz)^{2i-2}(y^2+z^2)^{n-i}z$$
$$+\sum_{i=1}^{n}2(n-i)(b-1)a_i(x^2-2sz)^{2i-1}(y^2+z^2)^{n-i-1}z^2.$$

Using transformations (16) and (17) and working in a similar way to solve $\overline{F}_0$, we get the following ordinary differential equation (for fixed u and v):

$$\sqrt{u+2sw}\,\sqrt{v-w^2}\frac{d\overline{F}_1}{dw}=\sum_{i=1}^{n}[c+2(2i-1)s+2(n-i)]a_iu^{2i-1}v^{n-i}$$
$$+\sum_{i=1}^{n}(4s^2-2sb)(2i-1)a_iu^{2i-2}v^{n-i}w$$
$$+\sum_{i=1}^{n}2(n-i)(b-1)a_iu^{2i-1}v^{n-i-1}w^2.$$

Integrating this equation with respect to w and using formula (A1) from Appendix A, we get

$$\overline{F}_1=\sum_{i=1}^{n}\frac{1}{s}[c+2(2i-1)s+2(n-i)]a_iu^{2i-1}v^{n-i-1}\sqrt{u+2sw}\,\sqrt{v-w^2}$$
$$+\sum_{i=0}^{n}\left\{(4s^2-2sb)(2i+1)a_{i+1}+\frac{1}{s}[c+2(2i-1)s+2(n-i)]a_i\right\}$$
$$\cdot u^{2i}v^{n-i-1}\int\frac{w\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\sum_{i=1}^{n}[3c+6(2i-1)s+(2b+4)$$
$$\times(n-i)]a_iu^{2i-1}v^{n-i-1}\int\frac{w^2\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\overline{G}_1(u,v),$$

where $\overline{G}_1(u,v)$ is an arbitrary smooth function in u and v.

Since $G_1(x,y,z)=\overline{G}_1(u,v)=\overline{G}_1(x^2-2sz,y^2+z^2)$, in order that F_1 be a weight homogeneous polynomial of weight degree $4n-3$, from (A2) and (A3) we have $\overline{G}_1(u,v)=0$, and

$$(4s^2-2sb)(2i+1)a_{i+1}+\frac{1}{s}[c+2(2i-1)s+2(n-i)]a_i=0,\quad i=0,1,\ldots,n$$
$$[3c+6(2i-1)s+(n-i)(2b+4)]a_i=0,\quad i=1,2,\ldots,n \tag{20}$$

where $a_0=a_{n+1}=0$. We claim that conditions (20) are equivalent to one of the following conditions:

(i) $b=1$, $s=1/2$, $c=-(2n-1)$ and there exists an $i_0\in\{1,\ldots,n-1\}$ such that $a_{i_0}\neq 0$,
(ii) $b=2s$, $c=-2(2n-1)s$, and $F_0=a_n(x^2-2sz)^{2n-1}$,

(iii) $b\neq 2s$ and $F_0=0$.

Indeed, we first assume that $b=2s$. Then, conditions (20) can be reduced to

$$(b-1)(n-i)a_i=0,\quad [c+2(2i-1)s+2(n-i)]a_i=0,\quad i=1,\ldots,n.$$

If there exists an $i_0\in\{1,\ldots,n-1\}$ such that $a_{i_0}\neq 0$, then $b=1$. So, we have $s=1/2$ and $c=-(2n-1)$. If $a_i=0$ for $i=1,\ldots,n-1$, then $a_n\neq 0$ (otherwise, $F_0=0$). Thus, we have $c=-2(2n-1)s$. Next, we assume that $b\neq 2s$. Then, by induction, from the first equation of (20) we get that $a_i=0$ for $i=1,\ldots,n$. This proves the claim.

Case (i): $b=1$, $s=1/2$, $c=-(2n-1)$ and there exists an $i_0\in\{1,\ldots,n-1\}$ such that $a_{i_0}\neq 0$. Then $F_1=0$. From (15) with $j=2$ we get

$$L[F_2]=-\sum_{i=1}^{n} 2r(n-i)a_i xy(x^2-2sz)^{2i-1}(y^2+z^2)^{n-1-i}.$$

Using transformations (16) and (17), we get the following ordinary differential equation:

$$\frac{d\overline{F}_2}{dw}=-\sum_{i=1}^{n-1} 2r(n-i)a_i u^{2i-1}v^{n-1-i}.$$

Integrating this equation with respect to w, we have

$$\overline{F}_2=-\sum_{i=1}^{n-1} 2r(n-i)a_i u^{2i-1}v^{n-1-i}w+\overline{G}_2(u,v),$$

where $\overline{G}_2(u,v)$ is an arbitrary smooth function. In order that $F_2(x,y,z)=\overline{F}_2(u,v,w)$ be a weight homogeneous polynomial of weight degree $4n-4$, it must have the form

$$F_2=-\sum_{i=1}^{n-1} 2r(n-i)a_i(x^2-2sz)^{2i-1}(y^2+z^2)^{n-1-i}z+\sum_{i=0}^{n-1} a_i^{(2)}(x^2-2sz)^{2i}(y^2+z^2)^{n-1-i},$$

where $a_i^{(2)}$ are real constants for $i=0,1,\ldots,n-1$.

Substituting F_1 and F_2 into (15) with $j=3$ and working in a similar way to solve F_1 and F_2, we can obtain that

$$\begin{aligned}F_3(x,y,z)&=\overline{F}_3(u,v,w)\\&=-\sum_{i=0}^{n-1} a_i^{(2)}u^{2i}v^{n-1-i}\int\frac{dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}\\&\quad+\sum_{i=1}^{n-1} 2r(n-i)a_i u^{2i-1}v^{n-1-i}\int\frac{w\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\overline{G}_3(u,v).\end{aligned}$$

Since F_3 is a weight homogeneous polynomial of weight degree $4n-5$, we get that $\overline{G}_3=0$, and

$$a_i^{(2)}=0\quad\text{for } i=0,1,\ldots,n-1;\quad r(n-i)a_i=0\quad\text{for } i=1,2,\ldots,n-1.$$

This means that $r=0$ (because there exists an $i_0\in\{1,\ldots,n-1\}$ such that $a_{i_0}\neq 0$). Furthermore, we have $F_2=F_3=0$. By recursive calculations, we can prove that $F_i=0$ for $i=4,\ldots,m$. Hence, the Darboux polynomial is

$$\sum_{i=1}^{n} a_i(x^2-z)^{2i-1}(y^2+z^2)^{n-i}.$$

Its generators are x^2-z and y^2+z^2, which are two Darboux polynomials of the Lorenz system.

Case (ii): $b=2s$, $c=-2(2n-1)s$, and $F_0=(x^2-2sz)^{2n-1}$. Here, we set $a_n=1$, because $a_n\neq 0$ otherwise $F_0=0$ and consequently $F=0$. So, $F_1=0$. From (15) with $j=2$, we can easily prove that

$$F_2=\sum_{i=0}^{n-1} a_i^{(2)}(x^2-2sz)^{2i}(y^2+z^2)^{n-1-i},$$

where $a_i^{(2)}$ are real constants for $i=0,1,\ldots,n-1$.

Working in a similar way to solve F_1 and F_3 as in case (i), we get from (15) with $j=3$ that

$$\begin{aligned}F_3(x,y,z)&=\overline{F}_3(u,v,w)\\&=\sum_{i=0}^{n-1}[-2(2n-1)s+4si+2(n-1-i)]\\&\quad\times a_i^{(2)}u^{2i}v^{n-1-i}\int\frac{dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\sum_{i=0}^{n-1}(n-1-i)(4s-2)\\&\quad\times a_i^{(2)}u^{2i}v^{n-2-i}\int\frac{w^2\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\overline{G}_3(u,v).\end{aligned}$$

Since F_3 is a weight homogeneous polynomial of weight degree $4n-5$, we should have $\overline{G}_3=0$ and

$$[-(2n-1)s+2si+(n-1-i)]a_i^{(2)}=0,\quad (n-1-i)(4s-2)a_i^{(2)}=0,\quad i=0,1,\ldots,n-1.$$

This implies that $F_3=0$. The above-mentioned conditions are equivalent to $a_i^{(2)}=0$ for $i=0,1,\ldots,n-1$, that is, $F_2=0$. By recursive calculations, we can prove that $F_i=0$ for $i=4,\ldots,m$. Hence, the Darboux polynomial is $(x^2-2sz)^{2n-1}$ with the cofactor $-2(2n-1)s$.

Case (iii): $b\neq 2s$ and $F_0=0$. Obviously, the Lorenz system has no Darboux polynomials of the given form.

B. F_0 has the form (18)

Substituting F_0 into the second equation in (15), we get that

$$\begin{aligned}L[F_1]=&\sum_{i=0}^{n}[c+4si+2(n-i)]a_i(x^2-2sz)^{2i}(y^2+z^2)^{n-i}\\&+\sum_{i=0}^{n}4s(2s-b)ia_iz(x^2-2sz)^{2i-1}(y^2+z^2)^{n-i}\\&+\sum_{i=0}^{n}2(b-1)(n-i)a_iz^2(x^2-2sz)^{2i}(y^2+z^2)^{n-i-1}.\end{aligned}$$

Working in a similar way as in Sec. III A we obtain that

$$\overline{F_1}=\sum_{i=0}^{n}\frac{1}{s}[c+4si+2(n-i)]a_i u^{2i}v^{n-i-1}\sqrt{u+2sw}\,\sqrt{v-w^2}$$
$$+\sum_{i=0}^{n-1}\left\{\frac{1}{s}[c+4si+2(n-i)]a_i+4s(2s-b)(i+1)a_{i+1}\right\}$$
$$\cdot u^{2i+1}v^{n-i-1}\int\frac{w\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\frac{1}{s}(c+4sn)a_n u^{2n+1}v^{-1}$$
$$+\sum_{i=0}^{n-1}[3c+12si+2(b+2)(n-i)]a_i u^{2i}v^{n-i-1}\int\frac{w^2\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\overline{G_1}(u,v).$$

In order that $F_1(x,y,z)=\overline{F_1}(u,v,w)$ be a weight homogeneous polynomial of weight degree $4n-1$, we should have $\overline{G_1}(u,v)=0$ and

$$(c+4sn)a_n=0,$$
$$(c+4si+2(n-i))a_i+4s^2(2s-b)(i+1)a_{i+1}=0, \tag{21}$$
$$(3c+12si+2(b+2)(n-i))a_i=0,$$

with $i=0,1,\ldots,n-1$. We claim that conditions (21) are equivalent to one of the following conditions:

(i) $b=2s$, $c=-4sn$, $a_n\neq 0$, and $a_i=0$ for $i=0,1,\ldots,n-1$,
(ii) $b=1$, $s=1/2$, $c=-2n$, and $a_i\neq 0$ for some $i\in\{0,1,\ldots,n-1\}$,
(iii) $b=1$, $c=-2n$, $s\neq 1/2$, $a_0\neq 0$, and $a_i=0$ for $i=1,2,\ldots,n$,
(iv) $b=6s-2$, $c=-4sn$, $s\neq 1/2$, $a_{n-i}=(-4s^2)^i\binom{n}{i}a_n$, and $a_n\neq 0$.

Indeed, we first assume that $b=2s$. Then conditions (21) are reduced to

$$(c+4sn)a_n=0,\quad (c+4si+2(n-i))a_i=0,\quad (3c+12si+4(s+1)(n-i))a_i=0,$$

with $i=0,1,\ldots,n-1$. If $a_i=0$ for $i=0,1,\ldots,n-1$, then $a_n\neq 0$. Otherwise, $F_0=0$. So, $c=-4sn$. This is condition (i). If there exists an $i_0\in\{0,1,\ldots,n-1\}$ such that $a_{i_0}\neq 0$, then we have $c+4si_0+2(n-i_0)=0$ and $3c+12si_0+4(s+1)(n-i_0)=0$. This means that $s=1/2$ and $c=-2n$. Hence, we get condition (ii).

Now we assume that $b\neq 2s$. From the second equality of (21), we get that $a_0\neq 0$. Otherwise, $a_i=0$ for $i=0,1\ldots,n$. Hence, from the third equality of (21) we have

$$3c+2(b+2s)n=0. \tag{22}$$

If $c+2n=0$, then $b=1$ and $c=-2n$. Since $b\neq 2s$, we have $s\neq 1/2$. So, from the first and third equalities of (21) we get that $a_i=0$ for $i=1,\ldots,n$. This is condition (iii). If $c+2n\neq 0$, since $a_0\neq 0$, we obtain from the second equality of (21) that $a_1\neq 0$. So, we have $3c+12s+2(b+2)(n-1)=0$, by the third equality of (21). From equality (22) we have $b=6s-2$ and $c=-4sn$. So, $s\neq 1/2$. Moreover, from the second equality of (21) we get that $a_{n-i}=(-4s^2)^i\binom{n}{i}a_n$. This proves the claim.

In what follows we study the four cases.

Case (i): $b=2s$, $c=-4sn$, $a_n\neq 0$, and $a_i=0$ for $i=0,1,\ldots,n-1$. Then we have $F_0=a_n(x^2-2sz)^{2n}$ and $F_1=0$. Substituting F_0 and F_1 into (15) with $j=2$, we get that $L[F_2]=0$. It is easy to prove that

$$F_2=\sum_{i=1}^{n} a_i^{(2)}(x^2-2sz)^{2i-1}(y^2+z^2)^{n-i},$$

where $a_i^{(2)}$ for $i=1,2,\ldots,n$, are real constants.

From (15) with $j=3$ and doing some computations as in Sec. III A we obtain that

$$\begin{aligned}\overline{F}_3=&\sum_{i=1}^{n}\frac{1}{s}[-4sn+2s(2i-1)+2(n-i)]a_i^{(2)}u^{2i-1}v^{n-i-1}\sqrt{u+2sw}\,\sqrt{v-w^2}\\&+\sum_{i=1}^{n}\frac{1}{s}[-4sn+2s(2i-1)+2(n-i)]a_i^{(2)}u^{2i}v^{n-i-1}\int\frac{w\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}\\&+\sum_{i=1}^{n}[-12sn+6s(2i-1)+6(n-i)+(4s-2)(n-i)]\\&\cdot a_i^{(2)}u^{2i-1}v^{n-i-1}\int\frac{w^2dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\overline{G}_3(u,v),\end{aligned}$$

where $\overline{G}_3$ is an arbitrary smooth function in u and v. In order that $F_3(x,y,z)=\overline{F}_3(u,v,w)$ be a weight homogeneous polynomial of weight degree $4n-3$, we would have $\overline{G}_3=0$ and

$$[-4sn+2s(2i-1)+2(n-i)]a_i^{(2)}=0,\quad (4s-2)(n-i)a_i^{(2)}=0,\quad i=1,2,\ldots,n.$$

This implies that $F_3=0$. The above conditions are equivalent to $a_i^{(2)}=0$ for $i=1,2,\ldots,n$. This means that $F_2=0$.

By induction we can prove that $F_i=0$ for $i=4,\ldots,m$. Therefore, the Darboux polynomial is $F=F_0=a_n(x^2-2sz)^{2n}$ with the cofactor $-4sn$. The corresponding irreducible Darboux polynomial is $f=x^2-2sz$ with the cofactor $-2s$.

Case (ii): $b=1$, $s=1/2$, and $c=-2n$. Then $F_1=0$. From (15) with $j=2$, we can prove that the weight homogeneous polynomial F_2 with the weight degree $4n-2$ has the form

$$F_2=-\sum_{i=0}^{n-1}2r(n-i)a_i(x^2-z)^{2i}(y^2+z^2)^{n-i-1}z+\sum_{i=1}^{n}a_i^{(2)}(x^2-z)^{2i-1}(y^2+z^2)^{n-i}.$$

Similarly, from (15) with $j=3$ we get

$$\begin{aligned}\overline{F}_3=&\sum_{i=0}^{n-1}2r(n-i)a_iu^{2i}v^{n-i-1}\int\frac{w\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}\\&-\sum_{i=1}^{n}a_i^{(2)}u^{2i-1}v^{n-i}\int\frac{w\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\overline{G}_3(u,v).\end{aligned}$$

In order that $F_3(x,y,z)=\overline{F}_3(u,v,w)$ be a weight homogeneous polynomial of weight degree $4n-3$, we should have $\overline{G}_3(u,v)=0$, $r(n-i)a_i=0$ for $i=0,1,\ldots,n-1$ and $a_i^{(2)}=0$ for $i=1,\ldots,n$. This means that $r=0$, $F_2=0$, and $F_3=0$.

By induction, we obtain that the Darboux polynomial is

$$F=F_0=\sum_{i=0}^{n}a_i(x^2-z)^{2i}(y^2+z^2)^{n-i},$$

with the cofactor $-2n$. The corresponding generators are two Darboux polynomials $f_1=x^2-z$ with the cofactor -1 and $f_2=y^2+z^2$ with the cofactor -2.

Case (iii): $b=1$, $c=-2n$, $s\neq 1/2$, and $F_0=a_0(y^2+z^2)^n$. Since $F_1=0$, solving (15) with $j=2$ we get

$$F_2=-2rna_0(y^2+z^2)^{n-1}z+\sum_{i=1}^{n} a_i^{(2)}(x^2-2sz)^{2i-1}(y^2+z^2)^{n-i}.$$

Substituting F_1 and F_2 into (15) with $j=3$ we can prove that

$$\overline{F_3}=2rna_0v^{n-1}\int \frac{w\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\sum_{i=1}^{n}[2i(2s-1)-2s]a_i^{(2)}u^{2i-1}v^{n-i}\int \frac{\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}$$
$$+\sum_{i=1}^{n}(4s^2-2s)(2i-1)a_i^{(2)}u^{2i-2}v^{n-i}\int \frac{w\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\overline{G}_3(u,v).$$

In order that $F_3(x,y,z)=\overline{F_3}(u,v,w)$ be a weight homogeneous polynomial of weight degree $4n-3$ in x,y, and z, we should have $\overline{G_3}(u,v)=0$ and

$$[2i(2s-1)-2s]a_i^{(2)}=0,\quad i=1,2,\ldots,n,$$

$$2rna_0+(4s^2-2s)a_1^{(2)}=0,\quad (4s^2-2s)(2i-1)a_i^{(2)}=0,\quad i=2,\ldots,n.$$

This means that $F_3=0$. These last conditions are equivalent to

(1) $r=0$ and $a_i^{(2)}=0$ for $i=1,2,\ldots,n$, i.e., $F_2=0$.
(2) $r\neq 0$, $s=1$, $a_1^{(2)}=-rna_0\neq 0$ and $a_i^{(2)}=0$ for $i=2,\cdots,n$.

Subcase (1): $r=0$ and $F_2=0$. By induction, we can prove that $F_i=0$ for $i=4,\ldots,m$. Hence, the Darboux polynomial is $f=a_0(y^2+z^2)^n$ with the cofactor $-2n$. The irreducible Darboux polynomial is y^2+z^2 with the cofactor -2.

Subcase (2): $r\neq 0$ and $s=1$. Then we have

$$\begin{aligned}F_2&=-2rna_0(y^2+z^2)^{n-1}z-rna_0(x^2-2z)(y^2+z^2)^{n-1}\\&=-rna_0(y^2+z^2)^{n-1}x^2\\&=a_0\binom{n}{1}(y^2+z^2)^{n-1}(-rx^2).\end{aligned}$$

Substituting F_2 and F_3 into (15) with $j=4$, we get that

$$F_4=2r^2n(n-1)a_0(x^2-z)(y^2+z^2)^{n-2}z+\sum_{i=0}^{n-1} a_i^{(4)}(x^2-2z)^{2i}(y^2+z^2)^{n-i-1},$$

where $a_i^{(4)}$ for $i=0,1,\ldots,n-1$, are arbitrary real constants.

From (15) with $j=5$ we obtain that

$$\overline{F_5}=\left[\sum_{i=0}^{n-1}4ia_i^{(4)}u^{2i-1}v^{n-i-1}-2r^2n(n-1)a_0uv^{n-2}\right]\int \frac{w\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}$$
$$+\sum_{i=0}^{n-1}2(i-1)a_i^{(4)}u^{2i}v^{n-i-1}\int \frac{\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\overline{G}_5(u,v),$$

where $\overline{G}_5(u,v)$ is an arbitrary smooth function. In order that $F_5(x,y,z)=\overline{F}_5(u,v,w)$ be a weight homogeneous polynomial with the weight degree $4n-5$ in x,y, and z, we must have $\overline{G}_5(u,v)=0$ and

$$(i-1)a_i^{(4)}=0, \quad i=0,1,\ldots,n-1,$$

$$\sum_{i=0}^{n-1} 4ia_i^{(4)}u^{2i-1}v^{n-i-1}-2r^2n(n-1)a_0uv^{n-2}=0.$$

This reduces to

$$a_1^4=\frac{n(n-1)}{2}r^2a_0, \quad a_i^{(4)}=0, \quad j=0,2,\ldots,n-1.$$

Therefore, we have

$$F_4=\binom{n}{2}a_0(y^2+z^2)^{n-2}(-rx^2)^2, \quad F_5=0.$$

By recursive calculations, we can prove that

$$F_{2i}=\binom{n}{i}a_0(y^2+z^2)^{n-i}(-rx^2)^i, \quad F_{2i+1}=0, \quad i\geqslant 5, \quad 2i\leqslant m.$$

Hence, the Darboux polynomial of the Lorenz system is

$$f=\sum_{i=0}^{n}\binom{n}{i}a_0(y^2+z^2)^{n-i}(-rx^2)^i=a_0(y^2+z^2-rx^2)^n$$

with the cofactor $-2n$. Moreover, the irreducible Darboux polynomial is $y^2+z^2-rx^2$ with the cofactor -2.

Case (iv): $b=6s-2$, $c=-4sn$, and $s\neq 1/2$. Since $a_{n-i}=(-4s^2)^i\binom{n}{i}a_n$ for $i=1,2,\ldots,n$ and $a_n\neq 0$, without loss of generality, we set $a_n=1$, then we have

$$F_0=[(x^2-2sz)^2-4s^2(y^2+z^2)]^n.$$

Moreover, we have

$$\begin{aligned}
F_1&=\sum_{i=0}^{n-1}\frac{1}{s}[-4sn+4si+2(n-i)]a_i(x^2-2sz)^{2i}(y^2+z^2)^{n-i-1}xy\\
&=-\frac{4s-2}{s}\sum_{j=1}^{n}j(-4s^2)^j\binom{n}{j}(x^2-2sz)^{2(n-j)}(y^2+z^2)^{j-1}xy\\
&=4s(4s-2)\sum_{j=0}^{n-1}(-4s^2)^jn\binom{n-1}{j}(x^2-2sz)^{2(n-1-j)}(y^2+z^2)^jxy\\
&=\binom{n}{1}[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-1}4s(4s-2)xy.
\end{aligned}$$

Substituting F_0 and F_1 into the second equation of (15), we get that

$$F_2=[(4s-2)(4s-12s^2)+8rs^2]n[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-1}z$$
$$+16s^3(4s-2)^2n(n-1)(y^2+z^2)[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-2}z-8s^2(4s-2)^2n(n-1)$$
$$\times x^2[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-2}z^2+\sum_{i=1}^{n} a_i^{(2)}(x^2-2sz)^{2i-1}(y^2+z^2)^{n-i},$$

where $a_i^{(2)}$ are real constants for $i=1,2,\ldots,n$.

From (15) with $j=3$ and working in a similar way to solve F_1, we can prove that

$$\overline{F}_3=-\sum_{i=1}^{n}[(4s-2)(n-i)+2s]a_i^{(2)}u^{2i-1}v^{n-i}\int\frac{dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$-\sum_{i=1}^{n}2s(4s-2)(2i-1)a_i^{(2)}u^{2i-2}v^{n-i}\int\frac{w\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$+\sum_{i=1}^{n}3(4s-2)(n-i)a_i^{(2)}u^{2i-1}v^{n-1-i}\int\frac{w^2\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$-4s(4s-2)rnu(u^2-4s^2v)^{n-1}\int\frac{dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$+32s^3(4s-2)rn(n-1)uv(u^2-4s^2v)^{n-2}\int\frac{dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$+16s[(s-1)(2s-1)(1-3s)-s^2r]n(u^2-4s^2v)^{n-1}\int\frac{w\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$+16s^3[(4s-2)^2(1-5s)+6s(4s-2)r]n(n-1)v\cdot(u^2-4s^2v)^{n-2}\int\frac{w\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$+64s^5(4s-2)^3n(n-1)(n-2)v^2(u^2-4s^2v)^{n-3}\int\frac{w\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$+16s^2[(4s-2)^2-4s(4s-2)r]n(n-1)u\cdot(u^2-4s^2v)^{n-2}\int\frac{w^2\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$-96s^4(4s-2)^3n(n-1)(n-2)uv(u^2-4s^2v)^{n-3}\int\frac{w^2\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$+16s^3(4s-2)n(n-1)[2(4s-2)^2(n-2)+5(3s-1)(4s-2)-10sr](u^2-4s^2v)^{n-2}$$
$$\times\int\frac{w^3\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}-128s^5(4s-2)^3n(n-1)(n-2)v(u^2-4s^2v)^{n-3}$$
$$\times\int\frac{w^3\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}+160s^4(4s-2)^3n(n-1)(n-2)u(u^2-4s^2v))^{n-3}$$
$$\times\int\frac{w^4\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}+192s^5(4s-2)^3n(n-1)(n-2)(u^2-4s^2v)^{n-3}$$
$$\times\int\frac{w^5\,dw}{\sqrt{u+2sw}\sqrt{v-w^2}}+\overline{G}_3(u,v).$$

Using formulas (A4)–(A6), $\overline{F}_3$ can be simplified to

$$\begin{aligned}\overline{F}_3=&\left\{8s(4s-2)[-2(4s-2)r(u+2sw)+(6s-2)(4sr-2s(4s-2))w]\binom{n}{2}\cdot(u^2-4s^2v)^{n-2}\right.\\&\left.+64s^3(4s-2)^3\binom{n}{3}(u+2sw)(v-w^2)(u^2-4s^2v)^{n-3}\right\}\cdot\sqrt{u+2sw}\sqrt{v-w^2}+16s(3s-1)\\&\times(s-1)[r-(2s-1)]n\binom{n-1}{i}(-4s^2)^{n-i-i}\cdot u^{2i}v^{n-1-i}\int\frac{w\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}\\&-6s\sum_{i=1}^{n}\left\{a_i^{(2)}+2(4s-2)n\left[r\binom{n-1}{i-1}+(4s-2)(n-1)\cdot\binom{n-2}{i-1}\right](-4s^2)^{n-i}\right\}u^{2i-1}v^{n-1-i}\\&\times\int\frac{w^2dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\overline{G}_3(u,v).\end{aligned}$$

For details, see Appendix B.

Since $F_3(x,y,z)=\overline{F}_3(u,v,w)$ is a weight homogeneous polynomial with weight degree $4n-3$ in x,y and z, we should have $\overline{G}_3(u,v)=0$ and

$$(3s-1)(s-1)[r-(2s-1)]=0,$$

$$a_i^{(2)}=-2(4s-2)n\left[r\binom{n-1}{i-1}+(4s-2)(n-1)\binom{n-2}{i-1}\right](-4s^2)^{n-i},$$

for $i=1,2,\ldots,n$. Furthermore, we have

$$\begin{aligned}F_2=&[(4s-2)(4s-12s^2)+8rs^2]n[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-1}z+16s^3(4s-2)^2n(n-1)(y^2\\&+z^2)[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-2}z-8s^2(4s-2)^2n(n-1)x^2[(x^2-2sz)^2-4s^2(y^2\\&+z^2)]^{n-2}z^2-2(4s-2)rn(x^2-2sz)[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-1}+8s^2(4s-2)^2n(n-1)\\&\times(x^2-2sz)(y^2+z^2)[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-2}\\=&\binom{n}{2}[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-2}[4s(4s-2)xy]^2+\binom{n}{1}[(x^2-2sz)^2\\&-4s^2(y^2+z^2)]^{n-1}\cdot\{-2(4s-2)rx^2+[(4s-2)(4s-12s^2)+4s(6s-2)r]z\},\end{aligned}$$

$$\begin{aligned}F_3=&\binom{n}{3}[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-3}[4s(4s-2)xy]^3\\&+\binom{n}{2}[(x^2-2sz)^2-4s^2(y^2+z^2)]^{n-2}2[4s(4s-2)xy]\\&\cdot\{-2(4s-2)rx^2+[(4s-2)(4s-12s^2)+4s(6s-2)r]z\}.\end{aligned}$$

If $s=1/3$, then $b=0$, $c=-4n/3$. It is known that the polynomial

$$f_2=x^4-\tfrac{4}{3}x^2z-\tfrac{4}{9}y^2-\tfrac{8}{9}xy+\tfrac{4}{3}rx^2,$$

is a Darboux polynomial with the cofactor $-4/3$. It is easy to prove that F_0, F_1, F_2, and F_3 are the terms of

$$(x^4-\tfrac{4}{3}x^2z-\tfrac{4}{9}y^2-\tfrac{8}{9}xy+\tfrac{4}{3}rx^2)^n=[(x^2-\tfrac{2}{3}z)^2-\tfrac{4}{9}(y^2+z^2)-\tfrac{8}{9}xy+\tfrac{4}{3}rx^2]^n,$$

with weight degrees $4n$, $4n-1$, $4n-2$ and $4n-3$ associated with the weight $\mathbf{s}=(1,2,2)$, respectively. This last function, denoted by f^*, is also a Darboux polynomial with the cofactor $-4n/3$. We claim that $f=F|_{\alpha=1}$ is equal to f^*. Indeed, if not, then $f-f^*$ $(\neq 0)$ is a Darboux polynomial of the Lorenz system with the cofactor $-4n/3$, and the highest weight degree less than $4n-3$ in the weight homogeneous components of $f-f^*$. It is in contradiction with the fact that under the condition $b\neq 2s$, the highest weight degree of the weight homogeneous components of a Darboux polynomial for the Lorenz system is $4h$ for some positive integer h, and that the Darboux polynomial has the cofactor $-4hs$. This proves the claim. Therefore, the irreducible Darboux polynomial is the known one, i.e., f_2.

If $s=1$, then $b=4$ and $c=-4n$. Working in a similar way as in the proof of the previous paragraph, we get that the Darboux polynomial is

$$(x^4-4x^2z-4y^2+8xy-4x^2-16(1-r)z)^n,$$

with the cofactor $-4n$.

If $r=2s-1$, since $c=-4sn$ and $b=6s-2$ with $s\neq 1/2$, we can prove that the Darboux polynomial is

$$(x^4-4sx^2z-4s^2y^2+4s(4s-2)xy-4(2s-1)^2x^2)^n,$$

with the cofactor $-4sn$. This completes the proof of the theorem. ■

IV. THE PROOF OF COROLLARY 2

Proof of statement (a): It is made inside the proof of Theorem 1. ■

Proof of statement (b): The proof of this statement follows from the following result, whose proof is easy.

Lemma 3: Let $\mathbf{X}$ *be an n-dimensional polynomial vector field. Then* $f\in\mathbb{R}[\mathbf{x}]$ *with* $\mathbf{x}\in\mathbb{R}^n$ *is a Darboux polynomial of* $\mathbf{X}$ *with a constant cofactor* k *if and only if the function* $H(\mathbf{x},t)=f(\mathbf{x})e^{-kt}$ *is an invariant.* ■

Proof of statement (c): Since every polynomial first integral is a Darboux polynomial with the cofactor $k=0$, statement (c) follows from Theorem 1 and its proof. ■

Proof of statement (d): In order to prove this statement, we need the following results.

Lemma 4: Let $\mathbf{X}$ *be a polynomial vector field in* $\mathbb{R}^n$. *Then the following statements hold.*

(1) Assume that f_i *for* $i=1,\ldots,m$, *is the Darboux polynomial of* $\mathbf{X}$ *with a cofactor* k_i. *If there exist* $\lambda_i\in\mathbb{R}$ *not all equal to zero such that* $\Sigma_{i=1}^m\lambda_i k_i\equiv 0$, *then* $H=\Pi_{i=1}^m f_i^{k_i}$ *is a first integral of the field* $\mathbf{X}$.

(2) Assume that $f(\mathbf{x})$ *is a polynomial function. Let* $f=f_1^{n_1}\ldots f_m^{n_m}$ *be the factorization of* f *in irreducible factors over* $\mathbb{R}[\mathbf{x}]$. *Then* f *is a Darboux polynomial with a cofactor* k_f *of* $\mathbf{X}$ *if and only if each* f_i *is a Darboux polynomial with a cofactor* k_{f_i} *for* $i=1,\ldots,m$. *Moreover,* $k_f=n_1k_{f_1}+\cdots+n_mk_{f_m}$.

The first statement was proved by Darboux (1878). We call such a first integral a *Darboux first integral*. The second statement was proved in Christopher and Llibre (2000).

From Theorem 1 it is easy to check that the values of the parameters in the Lorenz system in order to have two different generators for the Darboux polynomials are $s=1/2$, $b=1$, and $r=0$. Then, the generators of the Darboux polynomials are x^2-z with the cofactor -1, and y^2+z^2 with the cofactor -2. From statement (1) of Lemma 4, it follows easily that $(x^2-z)^2/((y^2+z^2)$ is a rational first integral. Moreover, from statement (2) of Lemma 4 we obtain that any Darboux polynomial has the form

$$\sum_{i+2j=K} a_{ij}(x^2-z)^i(y^2+z^2)^j,$$

with the cofactor $-K$, where $i,j,K\in\mathbb{N}$. This proves statement (d) using again Lemma (1). ■

Proof of statement (e): We first recall the following result.

Lemma 5: A vector field $\mathbf{X}$ *in* $\mathbb{R}^n$ *has* l $(1\leqslant l<n)$ *independent algebraic first integrals if and only if it has* l *independent rational first integrals.*

It was obtained by Bruns in 1887 [for a proof, see Forsyth (1900) or Goriely (1996)]. This lemma means that the vector field $\mathbf{X}$ is algebraically integrable if and only if it has $n-1$ independent rational first integrals. Therefore, from statement (d) and taking into account that any two rational first integrals given in (d) are dependent we obtain that statement (e) holds. ■

This completes the proof of the corollary.

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APPENDIX A: SOME ELLIPTIC INTEGRALS

The following formulas are used in the proof of Theorem 1:

$$\int \frac{\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}} = \frac{1}{sv}\sqrt{u+2sw}\,\sqrt{v-w^2} + \frac{u}{sv}\int \frac{w\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}} + \frac{3}{v}\int \frac{w^2\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}. \tag{A1}$$

The following two integrating formulas are obtained by using the change $w=\sqrt{v}\sin\theta$ for $\theta\in[-\pi/2,\pi/2)$ and formulas 2.571.2 and 2.571.3 of Gradshteyn and Ryzhik (1980).

$$\int \frac{w\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}$$

$$= \int \frac{\sqrt{v}\sin\theta}{\sqrt{u+2s\sqrt{v}\sin\theta}}\mathrm{d}\theta$$

$$= \begin{cases} \dfrac{u}{s\sqrt{u+2s\sqrt{v}}}W(\delta,\gamma) - \dfrac{\sqrt{u+2s\sqrt{v}}}{s}E(\delta,\gamma), & \text{for } u>2s\sqrt{v}>0, \quad -\dfrac{\pi}{2}\leqslant\theta<\dfrac{\pi}{2}, \\ \sqrt{v}\sqrt{\dfrac{1}{s\sqrt{v}}}\left[W\left(\beta,\dfrac{1}{\gamma}\right)-2E\left(\beta,\dfrac{1}{\gamma}\right)\right], & \text{for } 0<|u|<2s\sqrt{v}, \quad -\arcsin\dfrac{u}{2s\sqrt{v}}<\theta<\dfrac{\pi}{2}, \end{cases} \tag{A2}$$

$$\int \frac{w^2\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}$$

$$=v\int \frac{\sin^2\theta}{\sqrt{u+2s\sqrt{v}\sin\theta}}\mathrm{d}\theta$$

$$=\begin{cases} \dfrac{u\sqrt{u+2s\sqrt{v}}}{3s^2}E(\delta,\gamma)-\dfrac{u^2+2s^2v}{3s^2\sqrt{u+2s\sqrt{v}}}W(\delta,\gamma)-\dfrac{1}{3s}\sqrt{v-w^2}\sqrt{u+2sw}, \\ \qquad \text{for } u>2s\sqrt{v}>0, \quad -\dfrac{\pi}{2}\leqslant\theta<\dfrac{\pi}{2}, \\ \sqrt{\dfrac{1}{s\sqrt{v}}}\left[\dfrac{2u\sqrt{v}}{3s}E\left(\beta,\dfrac{1}{\gamma}\right)-\dfrac{\sqrt{v}(u+s\sqrt{v})}{3s}W\left(\beta,\dfrac{1}{\gamma}\right)\right]-\dfrac{1}{3s}\sqrt{v-w^2}\,\sqrt{u+2sw}, \\ \qquad \text{for } 0<|u|<2s\sqrt{v}, \quad -\arcsin\dfrac{u}{2s\sqrt{v}}<\theta<\dfrac{\pi}{2}, \end{cases} \tag{A3}$$

where

$$\beta=\arcsin\sqrt{\frac{2s\sqrt{v}(1-\sin\theta)}{u+2s\sqrt{v}}}=\arcsin\sqrt{\frac{2s(\sqrt{v}-w)}{u+2s\sqrt{v}}},$$

$$\gamma=\sqrt{\frac{4s\sqrt{v}}{u+2s\sqrt{v}}}, \quad \delta=\arcsin\sqrt{\frac{1-\sin\theta}{2}}=\arcsin\sqrt{\frac{\sqrt{v}-w}{2\sqrt{v}}},$$

and

$$W(\phi,k)=\int_0^{\phi}\frac{\mathrm{d}\zeta}{\sqrt{1-k^2\sin^2\zeta}}=\int_0^{\sin\phi}\frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}},$$

$$E(\phi,k)=\int_0^{\phi}\sqrt{1-k^2\sin^2\zeta}\,\mathrm{d}\zeta=\int_0^{\sin\phi}\frac{\sqrt{1-k^2x^2}}{\sqrt{1-x^2}}\mathrm{d}x,$$

are elliptic integrals of the first and second kind in the Legendre normal form [see, for instance, formulas 8.111.2 and 8.111.3 of Gradshteyn and Ryzhik (1980)]:

$$\int \frac{w^3\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}=\left(\frac{u}{5s^2}-\frac{w}{5s}\right)\sqrt{u+2sw}\,\sqrt{v-w^2}+\left(\frac{u^2}{5s^2}+\frac{3}{5}v\right)\int\frac{w\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}$$
$$+\frac{u}{5s}\int\frac{w^2\,\mathrm{d}w}{\sqrt{u+2sw}\,\sqrt{v-w^2}}, \tag{A4}$$

$$\int \frac{w^4\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}=\left(-\frac{3u^2}{35s^3}+\frac{3uw}{35s^2}-\frac{w^2}{7s}\right)\sqrt{u+2sw}\,\sqrt{v-w^2}+\left(\frac{uv}{35s}-\frac{3u^3}{35s^3}\right)\int\frac{w\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\left(\frac{5}{7}v-\frac{3u^2}{35s^2}\right)\int\frac{w^2\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}},\tag{A5}$$

$$\int \frac{w^5\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}=\left(\frac{7uv}{45s^2}-\frac{7vw}{45s}+\frac{4u^3}{105s^4}-\frac{4u^2w}{105s^3}+\frac{4uw^2}{63s^2}-\frac{w^3}{9s}\right)\sqrt{u+2sw}\,\sqrt{v-w^2}+\left(\frac{u^2v}{7s^2}+\frac{21}{45}v^2+\frac{4u^4}{105s^4}\right)\int\frac{w\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}+\left(\frac{6uv}{35s}+\frac{4u^3}{105s^3}\right)\int\frac{w^2\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}}.\tag{A6}$$

APPENDIX B: THE COEFFICIENTS C_1, C_2, AND C_3

In this appendix we compute the coefficients, denoted by C_1, C_2, and C_3, of

$$\sqrt{u+2sw}\,\sqrt{v-w^2}\int\frac{w\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}},\quad \int\frac{w^2\,dw}{\sqrt{u+2sw}\,\sqrt{v-w^2}},$$

in the expression of $\overline{F_3}$ for case (iv) of Sec. III B.

From the formulas of Appendix A and the expression of $\overline{F_3}$, we have

$$\begin{aligned}C_3=&-\sum_{i=1}^{n}3[(4s-2)(n-i)+2s]a_i^{(2)}u^{2i-1}v^{n-1-i}+\sum_{i=1}^{n}3(4s-2)(n-i)a_i^{(2)}u^{2i-1}v^{n-1-i}\\&-12s(4s-2)rnuv^{-1}(u^2-4s^2v)^{n-1}+96s^3(4s-2)rn(n-1)u(u^2-4s^2v)^{n-2}\\&+16s^2[(4s-2)^2-4s(4s-2)r]n(n-1)u(u^2-4s^2v)^{n-2}-96s^4(4s-2)^3\\&\times n(n-1)(n-2)uv(u^2-4s^2v)^{n-3}+\frac{16}{5}s^2(4s-2)n(n-1)[2(4s-2)^2(n-2)+5(3s-1)\\&\times(4s-2)-10sr]u(u^2-4s^2v)^{n-2}-\frac{128}{5}s^4(4s-2)^3n(n-1)(n-2)uv(u^2-4s^2v)^{n-3}\\&+160s^4(4s-2)^3n(n-1)(n-2)u\left(\frac{5}{7}v-\frac{3u^2}{35s^2}\right)(u^2-4s^2v)^{n-3}\\&+192s^5(4s-2)^3n(n-1)(n-2)\left(\frac{6uv}{35s}+\frac{4u^3}{105s^3}\right)(u^2-4s^2v)^{n-3}\\=&-\sum_{i=1}^{n}6sa_i^{(2)}u^{2i-1}v^{n-1-i}-12s(4s-2)rnuv^{-1}(u^2-4s^2v)^{n-1}\\&+48s^3(4s-2)^2n(n-1)u(u^2-4s^2v)^{n-2}\end{aligned}$$

$$
\begin{aligned}
&=-6s\Bigg[\sum_{i=1}^{n} a_i^{(2)}u^{2i-1}v^{n-i}+2(4s-2)rnu\sum_{i=0}^{n-1}\binom{n-1}{i}(-4s^2)^{n-1-i}u^{2i}v^{n-1-i}\\
&\quad+2(4s-2)^2n(n-1)u\sum_{i=0}^{n-2}\binom{n-2}{i}(-4s^2)^{n-1-i}u^{2i}v^{n-1-i}\Bigg]v^{-1}\\
&=-6s\Bigg\{\sum_{i=1}^{n} a_i^{(2)}u^{2i-1}v^{n-i}+\sum_{i=1}^{n} 2(4s-2)n\Bigg[r\binom{n-1}{i-1}+(4s-2)(n-1)\binom{n-2}{i-1}\Bigg]\\
&\quad\times(-4s^2)^{n-i}u^{2i-1}v^{n-i}\Bigg\}v^{-1},
\end{aligned}
$$

$$
\begin{aligned}
C_2=&-\sum_{i=1}^{n}\frac{1}{s}[(4s-2)(n-i)+2s]a_i^{(2)}u^{2i}v^{n-1-i}-\sum_{i=1}^{n} 2s(4s-2)(2i-1)a_i^{(2)}u^{2i-2}v^{n-i}\\
&-4(4s-2)rnu^2v^{-1}(u^2-4s^2v)^{n-1}+32s^2(4s-2)rn(n-1)u^2(u^2-4s^2v)^{n-2}\\
&+16s[(s-1)(2s-1)(1-3s)-rs^2]n(u^2-4s^2v)^{n-1}+16s^3[(4s-2)^2(1-5s)\\
&+6s(4s-2)r]n(n-1)v(u^2-4s^2v)^{n-2}+64s^5(4s-2)^3n(n-1)(n-2)v^2(u^2-4s^2v)^{n-3}\\
&+16s^3(4s-2)n(n-1)[2(4s-2)^2(n-2)+5(3s-1)(4s-2)-10sr](u^2-4s^2v)^{n-2}\\
&\times\left(\frac{u^2}{5s^2}+\frac{3}{5}v\right)-128s^5(4s-2)^3n(n-1)(n-2)v(u^2-4s^2v)^{n-3}\left(\frac{u^2}{5s^2}+\frac{3}{5}v\right)\\
&+160s^4(4s-2)^3n(n-1)(n-2)u(u^2-4s^2v)^{n-3}\left(\frac{uv}{35s}-\frac{3u^3}{35s^3}\right)\\
&+192s^5(4s-2)^3n(n-1)(n-2)(u^2-4s^2v)^{n-3}\left(\frac{u^2v}{7s^2}+\frac{21}{45}v^2+\frac{4u^4}{105s^4}\right)\\
=&-\sum_{i=0}^{n}\left\{\frac{1}{s}[(4s-2)(n-i)+2s]a_i^{(2)}+2s(4s-2)(2i+1)a_{i+1}^{(2)}\right\}u^{2i}v^{n-1-i}-4(4s-2)\\
&\times rnu^2v^{-1}(u^2-4s^2v)^{n-1}+16s[(s-1)(2s-1)(1-3s)-rs^2]n(u^2-4s^2v)^{n-1}\\
&+\frac{16}{5}s(4s-2)^2n(n-1)[2(4s-2)(n-2)+5(3s-1)]u^2(u^2-4s^2v)^{n-2}+16s^3(4s\\
&-2)^3n(n-1)\left[\frac{6}{5}(n-2)+1\right]v(u^2-4s^2v)^{n-2}+\frac{384}{5}s^5(4s-2)^3n(n-1)(n-2)\\
&\times v^2(u^2-4s^2v)^{n-3}+\frac{32}{5}s^3(4s-2)^3n(n-1)(n-2)u^2v(u^2-4s^2v)^{n-3}\\
&-\frac{32}{5}s(4s-2)^3n(n-1)(n-2)u^4(u^2-4s^2v)^{n-3}\\
=&-\sum_{i=0}^{n}\left\{\frac{1}{s}[(4s-2)(n-i)+2s]a_i^{(2)}+2s(4s-2)(2i+1)a_{i+1}^{(2)}\right\}u^{2i}v^{n-1-i}-4(4s\\
&-2)rnu^2v^{-1}(u^2-4s^2v)^{n-1}+16s[(s-1)(2s-1)(1-3s)-rs^2]n(u^2-4s^2v)^{n-1}+16s(3s\\
&-1)(4s-2)^2n(n-1)(u^2-4s^2v)^{n-1}+16s^3(4s-2)^2(16s-6)n(n-1)v(u^2-4s^2v)^{n-2}
\end{aligned}
$$

$$
\begin{aligned}
&=-\sum_{i=0}^{n-1}\left[\frac{1}{s}(4s-2)(n-i)a_i^{(2)}+2s(4s-2)(2i+1)a_{i+1}^{(2)}\right]u^{2i}v^{n-1-i}-16s^2(4s-2)^2n(n\\
&\quad-1)u^2(u^2-4s^2v)^{n-2}+16s[(s-1)(2s-1)(1-3s)-rs^2]n(u^2-4s^2v)^{n-1}+16s(3s-1)\\
&\quad\times(4s-2)^2n(n-1)(u^2-4s^2v)^{n-1}+16s^3(4s-2)^2(16s-6)n(n-1)v(u^2-4s^2v)^{n-2}\\
&=-\sum_{i=0}^{n-1}\left[\frac{1}{s}(4s-2)(n-i)a_i^{(2)}+2s(4s-2)(2i+1)a_{i+1}^{(2)}\right]u^{2i}v^{n-1-i}+8s(4s-2)^3n(n-1)\\
&\quad\times(u^2-4s^2v)^{n-1}+16s[(s-1)(2s-1)(1-3s)-rs^2]n(u^2-4s^2v)^{n-1}\\
&\quad+48s^3(4s-2)^3n(n-1)v(u^2-4s^2v)^{n-2}\\
&=-\sum_{i=0}^{n-1}4s(4s-2)^2\left[-rn\binom{n-1}{i}+2(4s-2)in\binom{n-1}{i}-(4s-2)n(n-1)\binom{n-2}{i}\right]\\
&\quad\times(-4s^2)^{n-1-i}u^{2i}v^{n-1-i}+\sum_{i=0}^{n-1}\left\{8s(4s-2)^3n(n-1)\binom{n-1}{i}+16s[(s-1)(2s-1)\right.\\
&\quad\left.\times(1-3s)-s^2r]n\binom{n-1}{i}-12s(4s-2)^3n(n-1)\binom{n-2}{i}\right\}(-4s^2)^{n-1-i}u^{2i}v^{n-1-i}\\
&=\sum_{i=0}^{n-1}16s(3s-1)(s-1)[r-(2s-1)]n\binom{n-1}{i}(-4s^2)^{n-1-i}u^{2i}v^{n-1-i},
\end{aligned}
$$

where we use $C_3=0$, that is, the following formulas

$$
\begin{aligned}
&-4(4s-2)rnu^2v^{-1}(u^2-4s^2v)^{n-1}\\
&\quad=2\sum_{i=1}^{n}a_i^{(2)}u^{2i}v^{n-1-i}-16s^2(4s-2)^2n(n-1)u^2(u^2-4s^2v)^{n-2},
\end{aligned}
$$

$$
a_i^{(2)}=-\left[2(4s-2)rn\binom{n-1}{i-1}+2(4s-2)^2n(n-1)\binom{n-2}{i-1}\right](-4s^2)^{n-i},
$$

and

$$
\begin{aligned}
C_1&=-\sum_{i=1}^{n}\frac{1}{s}[(4s-2)(n-i)+2s]a_i^{(2)}u^{2i-1}v^{n-1-i}-4(4s-2)rnuv^{-1}(u^2-4s^2v)^{n-1}\\
&\quad+32s^2(4s-2)rn(n-1)u(u^2-4s^2v)^{n-2}+16s^3(4s-2)n(n-1)[2(4s-2)^2(n-2)\\
&\quad+5(3s-1)(4s-2)-10sr]\cdot\left(\frac{u}{5s^2}-\frac{w}{5s}\right)(u^2-4s^2v)^{n-2}-128s^5(4s-2)^3n(n-1)(n-2)\\
&\quad\times v\left(\frac{u}{5s^2}-\frac{w}{5s}\right)(u^2-4s^2v)^{n-3}+160s^4(4s-2)^3n(n-1)(n-2)u\left(-\frac{3u^2}{35s^3}+\frac{3uw}{35s^2}-\frac{w^2}{7s}\right)\\
&\quad\times(u^2-4s^2v)^{n-3}+192s^5(4s-2)^3n(n-1)(n-2)\\
&\quad\times\left(\frac{7uv}{45s^2}-\frac{7vw}{45s}+\frac{4u^3}{105s^4}-\frac{4u^2w}{105s^3}+\frac{4uw^2}{63s^2}-\frac{w^3}{9s}\right)(u^2-4s^2v)^{n-3}\\
&=-\sum_{i=1}^{n}\frac{1}{s}(4s-2)(n-i)a_i^{(2)}u^{2i-1}v^{n-1-i}+8s(4s-2)^3n(n-1)u(u^2-4s^2v)^{n-2}
\end{aligned}
$$

$$
\begin{aligned}
&-16s^2(4s-2)[(3s-1)(4s-2)-2sr]n(n-1)w(u^2-4s^2v)^{n-2}\\
&-\frac{64}{3}s^3(4s-2)^3n(n-1)(n-2)uv(u^2-4s^2v)^{n-3}+\frac{64}{3}s^4(4s-2)^3n(n-1)\\
&\times(n-2)vw(u^2-4s^2v)^{n-3}-\frac{32}{3}s^3(4s-2)^3n(n-1)(n-2)uw^2(u^2-4s^2v)^{n-3}\\
&-\frac{64}{3}s^4(4s-2)^3n(n-1)(n-2)w^3(u^2-4s^2v)^{n-3}\\
=&-8s(4s-2)^2rn(n-1)u(u^2-4s^2v)^{n-2}-16s^2(3s-1)(4s-2)^2n(n-1)w(u^2-4s^2v)^{n-2}\\
&+32s^3(4s-2)rn(n-1)w(u^2-4s^2v)^{n-2}+64s^3(4s-2)^3\binom{n}{3}uv(u^2-4s^2v)^{n-3}\\
&+128s^4(4s-2)^3\binom{n}{3}vw(u^2-4s^2v)^{n-3}-64s^3(4s-2)^3\binom{n}{3}uw^2(u^2-4s^2v)^{n-3}\\
&-128s^4(4s-2)^3\binom{n}{3}w^3(u^2-4s^2v)^{n-3}\\
=&-8s(4s-2)[2(4s-2)r(u+2sw)+(4s-2)(12s^2-4s)w-4s(6s-2)rw]\\
&\times\binom{n}{2}(u^2-4s^2v)^{n-2}+64s^3(4s-2)^3\binom{n}{3}(u+2sw)(v-w^2)(u^2-4s^2v)^{n-3},
\end{aligned}
$$

where we use the formula

$$
\begin{aligned}
&-\sum_{i=1}^{n}\frac{1}{s}(4s-2)(n-i)a_i^{(2)}u^{2i-1}v^{n-1-i}\\
&\quad=-8s(4s-2)^2\sum_{i=1}^{n-1}(n-i)\left[rn\binom{n-1}{i-1}+(4s-2)n(n-1)\binom{n-2}{i-1}\right]u^{2i-1}(-4s^2v)^{n-1-i}\\
&\quad=-8s(4s-2)^2r\sum_{i=0}^{n-2}n(n-1)\binom{n-2}{i}u^{2i+1}(-4s^2v)^{n-2-i}-8s(4s-2)^3\sum_{i=0}^{n-2}n(n-1)^2\\
&\qquad\times\binom{n-2}{i}u^{2i+1}(-4s^2v)^{n-2-i}+8s(4s-2)^3\sum_{i=2}^{n-1}n(n-1)(n-2)\\
&\qquad\times\binom{n-3}{i-2}u^{2i-1}(-4s^2v)^{n-1-i}\\
&\quad=-8s(4s-2)^2rn(n-1)u(u^2-4s^2v)^{n-2}-8s(4s-2)^3n(n-1)^2u(u^2-4s^2v)^{n-2}\\
&\qquad+8s(4s-2)^3n(n-1)(n-2)u(u^2-4s^2v)^{n-2}+32s^3(4s-2)^3n(n-1)(n-2)\\
&\qquad\times uv(u^2-4s^2v)^{n-3}.
\end{aligned}
$$

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Jacobson generators of the quantum superalgebra $U_q[sl(n+1|m)]$ and Fock representations

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As an alternative to Chevalley generators, we introduce Jacobson generators for the quantum superalgebra $U_q[sl(n+1|m)]$. The expressions of all Cartan–Weyl elements of $U_q[sl(n+1|m)]$ in terms of these Jacobson generators become very simple. We determine and prove certain triple relations between the Jacobson generators, necessary for a complete set of supercommutation relations between the Cartan–Weyl elements. Fock representations are defined, and a substantial part of this paper is devoted to the computation of the action of Jacobson generators on basis vectors of these Fock spaces. It is also determined when these Fock representations are unitary. Finally, Dyson and Holstein–Primakoff realizations are given, not only for the Jacobson generators, but for all Cartan–Weyl elements of $U_q[sl(n+1|m)]$. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The quantization of simple Lie algebras[1,2] or Lie superalgebras[3–7] as quasitriangular Hopf (super)algebras has been carried out more than a decade ago. Since then, these structures have received much attention both in the mathematical and physical literature. In a physical context, one is mostly dealing with representations or realizations of these quantized algebras. This is in fact the main topic of the present paper: Certain special representations (Fock representations) and related realizations (Dyson and Holstein–Primakoff) of the quantum superalgebra $U_q[sl(n+1|m)]$ are presented.

The Lie superalgebra $sl(n+1|m)$ is one of the basic classical simple Lie superalgebras in Kac's classification.[8] It can be considered as the superanalogue of the special linear Lie algebra $sl(n+1)$. The quantum superalgebra $U_q[sl(n+1|m)]$ is a Hopf superalgebra deformation of the associative superalgebra $U[sl(n+1|m)]$, the universal enveloping superalgebra of $sl(n+1|m)$. At this point, it is already worth observing that the more familiar case of $sl(n+1)$ and $U_q[sl(n+1)]$ just follows by putting $m=0$. The readers who are interested in this case only can still use all formulas presented in this paper, simply taking m equal to 0.

For a definition of the quantum superalgebra $U_q[sl(n+1|m)]$, we refer to Refs. 3–7. Usually, $U_q[sl(n+1|m)]$ is defined by its Chevalley generators (often denoted by e_i, f_i, and h_i, with

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$i=1,\ldots,n+m$), subject to the Cartan–Kac relations and the Serre relations.[5–7] Besides these defining relations, also the other Hopf superalgebra maps (comultiplication, co-unit, and antipode) are part of the definition. In this paper, however, we do not use these other Hopf superalgebra maps; so we shall concentrate on $U_q[sl(n+1|m)]$ as an associative superalgebra.

The definition in terms of Chevalley generators has the advantage that the comultiplication, co-unit and antipode are easy to give. Furthermore, certain representations can be constructed explicitly (e.g., for the essentially typical representations a Gelfand–Zetlin basis exist for which the action of the Chevalley generators is known[9]). Having certain physical applications in mind, however, it is sometimes more useful to work with a different set of generators for $U_q[sl(n+1|m)]$.

The different set of generators for $U_q[sl(n+1|m)]$ given here are the Jacobson generators (denoted by a_i^+, a_i^- and H_i, with $i=1,\ldots,n+m$). For the case of $sl(n+1)$, such generators were originally introduced by Jacobson.[10,11] The use of Jacobson generators has a number of advantages.

First of all, in certain applications it is necessary to have a complete basis of $U_q[sl(n+1|m)]$ (following from the Poincaré–Birkhoff–Witt theorem). Such a basis is given in terms of the Cartan–Weyl elements. Although it is possible to express all Cartan–Weyl elements in terms of the Chevalley generators, such expressions soon become rather unmanageable. In terms of the Jacobson generators, the description of all Cartan–Weyl elements is very easy.

Secondly, the Jacobson generators allow for the construction of a class of irreducible $U_q[sl(n+1|m)]$ modules W_p, $p\in\mathbb{C}$, called Fock representations. The Fock representations corresponding to different p are inequivalent. For p a positive integer they provide an explicit construction (basis and transformation of the basis under the action of the generators) of (deformations of) atypical representations of $U_q[sl(n+1|m)]$. This is an interesting mathematical result, since even in the nondeformed case all atypical representations of $sl(n+1|m)$ were not explicitly constructed so far (e.g., even a dimension formula is unknown).

A disadvantage of the Jacobson generators compared to the Chevalley generators is that the explicit expressions for the other Hopf (super)algebra maps (comultiplication, co-unit and antipode) become very lengthy and complicated.

The results of the present paper provide a mathematical background for further studies of noncanonical quantum statistics initiated in Ref. 12 (see also Refs. 11 and 13 for further references). The approach is based on the concept of creation and annihilation operators (CAO's) of a simple Lie (super)algebra $\mathcal{A}$ and its Fock representations.[14] The CAO's of $\mathcal{A}$ provide a description of $\mathcal{A}$ in terms of generators and relations, which are different from the Chevalley generators. In this terminology any n pairs of para-Fermi operators[15] are CAO's of so$(2n+1)$[16] and any n pairs of para-Bose operators[15] are CAO's of the orthosymplectic Lie superalgebra osp$(1|2n)$.[17] The CAO's of $sl(n+1)$[12] and of $sl(1|n)$[14] lead to new quantum statistics. Generalizing the results of Jacobson on Lie triple systems,[10] Okubo has reformulated all above statistics in terms of Lie supertriple systems.[18] In this setting the CAO's of the Lie (super)algebras mentioned above are generators of the related (super)triple systems. This is another reason to call them Jacobson generators (JG's). The link between the JG's and the simple Lie superalgebras provides a natural background for their q-deformations (we refer to Ref. 19 for more discussion in this respect).

The representations of (quantum) superalgebras have certainly wider applications. These algebras (and in particular $U_q[gl(n+1|m)]$[20]) play a role for finding new solutions of the quantum Yang–Baxter equations and for the construction of solvable models. As examples we mention the supersymmetric solvable $t-J$ models of correlated electrons[21] and their quantum analogue.[22] Some other potential physical applications are mentioned in the last section.

In Sec. II we define the Jacobson generators of $U_q[sl(n+1|m)]$, as a special subset of the Cartan-Weyl elements. The description of all Cartan–Weyl elements in terms of the Jacobson generators becomes very simple (Theorem 1). However, in order to apply these results (e.g., in representations) one must have a list of all (super)commutation relations between these Cartan–Weyl elements; in terms of Jacobson generators, this means one has to determine certain triple relations. These are also given in Theorem 1, together with their proof.

In Sec. III we define Fock representations for $U_q[sl(n+1|m)]$, related to the earlier defined Jacobson generators. The main part of this section is devoted to the proof of Theorem 2, describing the action of the Jacobson generators on a basis of the Fock representation. This proof is rather technical and lengthy, and has been divided in a number of lemmas. The essential result is that these Fock representations are labeled by a number p; when p is a nonnegative integer, the Fock representation is finite-dimensional.

The Fock representations determined in Sec. III are further analyzed in Sec. IV. In particular, following conditions required in a physical context, it is determined when these Fock representations are unitary (or unitarizable, or Hermitian), see Theorem 6. In that case, an orthonormal basis of the Fock space is given, together with the action of the Jacobson generators on these basis elements.

Inspired by the Fock representations, we can give new expressions for the Dyson and Holstein–Primakoff realizations of $U_q[sl(n+1|m)]$ (Sec. V). In Ref. 23, the Dyson and Holstein–Primakoff realizations for the Chevalley generators of $U_q[gl(n|m)]$ was already given. Here, we give Dyson and Holstein–Primakoff realizations for the Jacobson generators of $U_q[sl(n+1|m)]$ (Theorems 7 and 8); from these, the corresponding realization for all Cartan–Weyl elements are deduced. All these realizations are in terms of n pairs of Bose and m pairs of Fermi creation and annihilation operators. The Holstein–Primakoff realization becomes particularly simple when expressed in terms of q-deformed Bose and Fermi creation and annihilation operators.

Unless otherwise stated, we consider in this paper $U_q[sl(n+1|m)]$ as a module over the algebra $\mathbb{C}[[h]]$ (with $q=e^h$) of formal power series over an indeterminate h. It is important to note, however, that all considerations remain true if one replaces h by a complex number such that $q=e^h$ is not a root of unity. In fact, most of our results hold also for q being a root of 1, including the unitary Fock representations and the Dyson and Holstein–Primakoff realizations.

Throughout the paper we use the notation: JGs for Jacobson generators; $\mathbb{Z}$ (resp. $\mathbb{Z}_+$) for the set of all integers (resp. of all nonnegative integers); $\mathbb{Z}_2=\{\overline{0},\overline{1}\}$ for the ring of all integers modulo 2; $\mathbb{C}$ for all complex numbers. Furthermore

$$[x]=\frac{q^x-q^{-x}}{q-q^{-1}}, \quad \text{when} \quad x\in\mathbb{C}, \tag{1.1}$$

$$[r;s]=\{r,r+1,r+2,\ldots,s-1,s\}, \quad \text{for} \quad r\leqslant s\in\mathbb{Z}; \tag{1.2}$$

$$\theta_i=\begin{cases}\overline{0} & \text{if} \quad i\in[0;n]\\ \overline{1} & \text{if} \quad i\in[n+1;n+m]\end{cases}; \quad \theta_{ij}=\theta_i+\theta_j; \tag{1.3}$$

$$[a,b]=ab-ba, \quad \{a,b\}=ab+ba, \quad [\![a,b]\!]=ab-(-1)^{\deg(a)\deg(b)}ba; \tag{1.4}$$

$$[a,b]_x=ab-xba, \quad \{a,b\}_x=ab+xba, \quad [\![a,b]\!]_x=ab-(-1)^{\deg(a)\deg(b)}xba, \tag{1.5}$$

where $\deg(a)\in\mathbb{Z}_2$ refers to the degree (or grading) of a when a is a homogeneous element of a superalgebra.

II. JACOBSON GENERATORS OF $U_q[sl(n+1|m)]$

Although the quantization (q-deformation) of simple Lie algebras and basic Lie superalgebras is usually carried out in terms of their Chevalley generators, there exist alternative descriptions in terms of so-called deformed creation and annihilation operators for the q-deformation of $\mathrm{osp}(1|2n)$,[24] $\mathrm{so}(2n+1)$,[25] $\mathrm{osp}(2n+1|m)$,[19] $sl(n+1)$,[26] and $sl(n+1|m)$.[27] These alternative generators have the advantage that in some natural interpretation they have a direct physical significance; furthermore, they allow the definition and construction of a mathematically interesting and physically important class of irreducible representations, the Fock representations.

The Hopf superalgebra $U_q[sl(n+1|m)]$ is defined in the sense of Drinfeld,[1] as a topologically free $\mathbb{C}[[h]]$ module. As a superalgebra, $U_q[sl(n+1|m)]$ is usually defined by means of its Chevalley generators, subject to the Cartan–Kac relations and the Serre relations.[5–7] Unlike the Lie algebra case, there is an ''extra Serre relation'' involving the generator associated with an odd simple root.[5–7,28] This property was investigated further by Yamane.[29,30] Indeed, for the basic classical Lie superalgebras there exist many nonisomorphic simple root systems;[8] one of these, having only one odd simple root, is known as the distinguished simple root system.[8] The classical description of $U_q[sl(n+1|m)]$ is in terms of relations and generators associated with this distinguished simple root system. Yamane[29,30] studied Hopf superalgebras in terms of relations and generators associated with other simple root systems. Apparently, this gives rise to more involved extra Serre relations. Moreover, the structure of the Hopf superalgebra seems to depend on the choice of simple root system.[29,30] In this paper, $U_q[sl(n+1|m)]$ stands for the usual Hopf superalgebra associated with the distinguished simple root system. But we shall be dealing with an alternative set of generators (and relations) for $U_q[sl(n+1|m)]$.

In this Sec. we shall recall the definition of deformed creation and annihilation operators of $U_q[sl(n+1|m)]$, and refer to them as Jacobson generators (JGs) since they are closely related to generators in the sense of a Lie supertriple system[18] (and for Lie triple systems, such generators were originally introduced by Jacobson[10,11]). The definition of JGs can be best presented in the framework of a set of Cartan–Weyl elements of $U_q[sl(n+1|m)]$. Furthermore, in order to construct the Fock representations explicitly, it is necessary to have a complete list of so-called triple relations between the JGs. Such relations can be deduced from the supercommutation relations between all Cartan–Weyl elements. So we begin this section by recalling some properties of Cartan–Weyl elements of $U_q[gl(n+1|m)]$, deduced in Ref. 31, which are then easily restricted to the case of $U_q[sl(n+1|m)]$.

Although a set of generators, such as the Chevalley generators, is sufficient for the definition of $U_q[gl(n+1|m]$ as an associative algebra, it is not sufficient for describing a basis of $U_q[gl(n+1|m]$. For this purpose, the construction of a set of Cartan–Weyl elements is necessary. For $U_q[gl(n+1|m]$, a set of Cartan–Weyl elements is given by elements e_{ij}, with $i,j \in [0;n+m]$; for an explicit expression of these elements e_{ij} in terms of the standard Chevalley generators, see Ref. 31. Finding a set of Cartan–Weyl elements, and their (super)commutation relations, is necessary for the construction of a Poincaré–Birkhoff–Witt basis of $U_q[gl(n+1|m]$. The elements e_{ij} are the q-analogues of the defining basis of $gl(n+1|m)$; their grading is given by $\deg(e_{ij})=\theta_{ij}$. We shall refer to e_{ij} as a positive root vector (resp. negative root vector) if $i<j$ (resp. $i>j$). For the formulation of the Poincaré–Birkhoff–Witt theorem, it is necessary to fix a total order for the set of elements e_{ij}. Among the positive root vectors, this order is given by

$$e_{ij}<e_{kl}, \text{ if } i<k \text{ or } i=k, \text{ and } j<l, \tag{2.1}$$

for the negative root vectors e_{ij} one takes the same rule (2.1), and total order is fixed by choosing

$$\text{positive root vectors} < \text{negative root vectors} < e_{ii}.$$

The order among the elements e_{ii} is of no real importance since they commute. A complete set of relations between the Cartan–Weyl elements e_{ij} is given by (2.2)–(2.7) [see Eqs. (3.10)–(3.15) of Ref. 31]

$$[e_{ii},e_{jj}]=0, \tag{2.2}$$

$$[e_{ii},e_{jk}]=(\delta_{ij}-\delta_{ik})e_{jk}, \tag{2.3}$$

$$(e_{ij})^2=0 \text{ if } \theta_{ij}=1, \tag{2.4}$$

for two positive root vectors $e_{ij}<e_{kl}$:

$$[\![e_{ij},e_{kl}]\!]_{q^{(-1)^{\theta_j}\delta_{jl}-(-1)^{\theta_j}\delta_{jk}+(-1)^{\theta_i}\delta_{ik}}}=\delta_{jk}e_{il}+(q-q^{-1})(-1)^{\theta_k}\theta(l>j>k>i)e_{kj}e_{il}, \tag{2.5}$$

for two negative root vectors $e_{ij}>e_{kl}$

$$[\![e_{ij},e_{kl}]\!]_{q^{-(-1)^{\theta_j}\delta_{jl}+(-1)^{\theta_j}\delta_{jk}-(-1)^{\theta_i}\delta_{ik}}}=\delta_{jk}e_{il}-(q-q^{-1})(-1)^{\theta_k}\theta(i>k>j>l)e_{kj}e_{il}, \quad (2.6)$$

and finally for a positive root vector e_{ij} and a negative root vector e_{kl}

$$\begin{aligned}[\![e_{ij},e_{kl}]\!]=&\frac{\delta_{il}\delta_{jk}}{q-q^{-1}}(q^{e_{ii}-(-1)^{\theta_{ij}}e_{jj}}-q^{-e_{ii}+(-1)^{\theta_{ij}}e_{jj}})+((q-q^{-1})\theta(j>k>i>l)(-1)^{\theta_k}e_{kj}e_{il}\\&-\delta_{il}\theta(j>k)(-1)^{\theta_{kl}}e_{kj}+\delta_{jk}\theta(i>l)e_{il})q^{(-1)^{\theta_k}e_{kk}-(-1)^{\theta_i}e_{ii}}+q^{(-1)^{\theta_l}e_{ll}-(-1)^{\theta_j}e_{jj}}\\&\times(-(q-q^{-1})\theta(k>j>l>i)(-1)^{\theta_j}e_{il}e_{kj}-\delta_{il}\theta(k>j)(-1)^{\theta_{ij}}e_{kj}+\delta_{jk}\theta(l>i)e_{il}). \quad (2.7)\end{aligned}$$

Herein,

$$\theta(i_1>i_2>\cdots>i_r)=\begin{cases}1, & \text{if } i_1>i_2>\cdots>i_r,\\ 0, & \text{otherwise.}\end{cases} \quad (2.8)$$

The difference between $U_q[sl(n+1|m)]$ and $U_q[gl(n+1|m)]$ lies in the elements of the Cartan subalgebra. For $U_q[gl(n+1|m)]$ the Cartan subalgebra is generated by e_{ii} ($i\in[0;n+m]$). For $U_q[sl(n+1|m)]$ the Cartan subalgebra is generated by the elements H_i, with

$$H_i=e_{00}-(-1)^{\theta_i}e_{ii}, \quad i\in[1;n+m]. \quad (2.9)$$

Sometimes, it will be useful to work with the elements L_i and $\overline{L_i}$, where

$$L_i=q^{H_i}, \quad \overline{L_i}=q^{-H_i}, \quad i\in[1;n+m]. \quad (2.10)$$

The Cartan–Weyl elements of $U_q[sl(n+1|m)]$ are now given by $\{H_i;i\in[1;n+m]\}\cup\{e_{ij};i\neq j\in[0;n+m]\}$. The complete set of supercommutation relations between these Cartan–Weyl elements is given by

$$[H_i,H_j]=0, \quad (2.11)$$

$$[H_i,e_{jk}]=(\delta_{0j}-\delta_{0k}-(-1)^{\theta_i}(\delta_{ij}-\delta_{ik}))e_{jk}, \quad (2.12)$$

(2.4)–(2.6) and finally the relation between a positive root vector e_{ij} and a negative root vector e_{kl}:

$$\begin{aligned}[\![e_{ij},e_{kl}]\!]=&\frac{\delta_{il}\delta_{jk}}{q-q^{-1}}(L_j^{(-1)^{\theta_i}}\overline{L_i}^{(-1)^{\theta_i}}-\overline{L_j}^{(-1)^{\theta_i}}L_i^{(-1)^{\theta_i}})+((q-q^{-1})\theta(j>k>i>l)(-1)^{\theta_k}e_{kj}e_{il}\\&-\delta_{il}\theta(j>k)(-1)^{\theta_{kl}}e_{kj}+\delta_{jk}\theta(i>l)e_{il})L_i\overline{L_k}+L_j\overline{L_l}(-(q-q^{-1})\theta(k>j>l>i)\\&\times(-1)^{\theta_j}e_{il}e_{kj}-\delta_{il}\theta(k>j)(-1)^{\theta_{ij}}e_{kj}+\delta_{jk}\theta(l>i)e_{il}). \quad (2.13)\end{aligned}$$

The Jacobson generators of $U_q[sl(n+1|m)]$ are now defined as the Cartan elements H_i ($i\in[1;n+m]$) together with the elements

$$a_i^-=e_{0i}, \quad a_i^+=e_{i0}, \quad i\in[1;n+m]. \quad (2.14)$$

From (2.13) it is easy to deduce that

$$[\![a_i^-,a_j^+]\!]=-(-1)^{\theta_i}L_ie_{ji}, \quad (i<j); \quad [\![a_i^-,a_j^+]\!]=-(-1)^{\theta_j}e_{ji}\overline{L_j}, \quad (i>j). \quad (2.15)$$

However, these relations are not complete in order to reshuffle all Cartan–Weyl elements in an arbitrary expression in the right order. For this purpose, we have the following result:

Theorem 1: *A set of Cartan–Weyl elements of* $U_q[sl(n+1|m)]$ *is given by* H_i, $a_i^{\pm}$, $[\![a_i^+,a_j^-]\!]$ $(i\neq j\in[1;n+m])$. *A complete set of supercommutation relations between these elements is given by*

$$[H_i,H_j]=0;\quad [H_i,a_j^{\pm}]=\mp(1+(-1)^{\theta_i}\delta_{ij})a_j^{\pm}, \tag{2.16}$$

$$[\![a_i^-,a_i^+]\!]=\frac{L_i-\overline{L_i}}{q-q^{-1}}, \tag{2.17}$$

$$[\![a_i^{\eta},a_j^{\eta}]\!]_q=0\quad (i<j);\quad (a_i^{\pm})^2=0\quad (i\in[n+1;n+m]), \tag{2.18}$$

$$\begin{aligned}[\![[\![a_i^{\eta},a_j^{-\eta}]\!],a_k^{\eta}]\!]_{q^{\xi(1+(-1)^{\theta_i}\delta_{ik})}}&=\eta^{\theta_j}\delta_{jk}L_k^{-\xi\eta}a_i^{\eta}+(-1)^{\theta_k}\epsilon(j,k,i)(q-\overline{q})[\![a_k^{\eta},a_j^{-\eta}]\!]a_i^{\eta}\\&=\eta^{\theta_j}\delta_{jk}L_k^{-\xi\eta}a_i^{\eta}+(-1)^{\theta_k\theta_j}\epsilon(j,k,i)q^{\xi}(q-\overline{q})a_i^{\eta}[\![a_k^{\eta},a_j^{-\eta}]\!],\end{aligned} \tag{2.19}$$

where $(j-i)\xi>0$, ξ, $\eta=\pm$

$$and\quad \epsilon(j,k,i)=\begin{cases}1, & \text{if } j>k>i;\\ -1, & \text{if } j<k<i;\\ 0, & \textit{otherwise},\end{cases}$$

and we have used the notation $\overline{q}=q^{-1}$.

Proof: The first part of the statement is obvious. Relation (2.16) follows from (2.11) and (2.12); (2.17) follows from (2.13) with $l=i<j=k$; the first relation in (2.18) follows from (2.5) with $i=k<j<l$ and from (2.6) with $l=j<k<i$, whereas the second relation in (2.18) comes from (2.4). Finally, it remains to prove (2.19). There are four similar cases to consider, according to $\eta=\pm$ and $\xi=\pm$. For $\eta=-$ and $\xi=+$, we use the first relation in (2.15) and find

$$\begin{aligned}[\![[\![a_i^-,a_j^+]\!],a_k^-]\!]_{q^{1+(-1)^{\theta_i}\delta_{ik}}}&=-(-1)^{\theta_i}[\![L_ie_{ji},a_k^-]\!]_{q^{1+(-1)^{\theta_i}\delta_{ik}}}=-(-1)^{\theta_i}L_i[\![e_{ji},a_k^-]\!]\\&=-(-1)^{\theta_i}L_i[\![e_{ji},e_{0k}]\!]=(-1)^{\theta_i+\theta_{ij}\theta_k}L_i[\![e_{0k},e_{ji}]\!].\end{aligned}$$

Herein, we have used the last equation of (2.16) to change the order of L_i and a_k^-. For the last supercommutator, we use (2.13)

$$[\![[\![a_i^-,a_j^+]\!],a_k^-]\!]_{q^{1+(-1)^{\theta_i}\delta_{ik}}}=(-1)^{\theta_i+\theta_{ij}\theta_k}L_iL_k\overline{L_i}(-(q-\overline{q})\,\theta(j>k>i)(-1)^{\theta_k}e_{0i}e_{jk}+\delta_{kj}e_{0i}).$$

Using trivial properties of the θ_i-symbols, the second term in the right-hand side (rhs) of this expression becomes $(-1)^{\theta_j}\delta_{jk}L_ka_i^-$; for the first term we use similar properties and replace according to (2.15) e_{jk} by $-(-1)^{\theta_k}\overline{L_k}[\![a_k^-,a_j^+]\!]$, so there comes

$$(-1)^{\theta_k}q(q-\overline{q})\,\theta(j>k>i)a_i^-[\![a_k^-,a_j^+]\!].$$

This coincides with the second expression in (2.19). Exchanging indices i and k, and using the relation just obtained, one shows that also the first expression in (2.19) is valid.

For the remaining choices of η and ξ, the proof is similar. □

Finally, we wish to remark that in order to construct $U_q[sl(n+1|m)]$ by means of the JGs subject to a set of relations, not all relations of Theorem 1 are needed. Such a minimal set of relations was determined in Ref. 27.

III. FOCK REPRESENTATIONS

In this section we shall construct so-called Fock representations of $U_q[sl(n+1|m)]$. The representations considered here are diagonal with respect to the Cartan elements H_i. So it will be convenient to fix q (or h) as a complex number in this and in the following section.

The Fock representations, or modules, can be defined by means of an induced module construction. First observe that $G=U_q[sl(n+1|m)]$, with Cartan–Weyl elements H_i, $a_i^{\pm}$ and $[\![a_i^+,a_j^-]\!]$ $(i\neq j\in[1;n+m])$, has a subalgebra $H=U_q[gl(n|m)]$ with Cartan–Weyl elements H_i and $[\![a_i^+,a_j^-]\!]$ $(i\neq j\in[1;n+m])$. A trivial one-dimensional H module is defined as follows:

$$[\![a_i^-,a_j^+]\!]|0\rangle=0, \quad (i\neq j\in[1;n+m]), \tag{3.1}$$

$$H_i|0\rangle=p|0\rangle, \tag{3.2}$$

where p is any complex number. Let P be the (associative) subalgebra of $G=U_q[sl(n+1|m)]$ generated by the elements of H and $\{a_i^-;i\in[1;n+m]\}$. The one-dimensional module $\mathbb{C}|0\rangle$ can be extended to a one-dimensional module of P by requiring

$$a_i^-|0\rangle=0, \quad i\in[1;n+m]. \tag{3.3}$$

Now the G module $\overline{W}_p$ is defined as

$$\overline{W}_p=\mathrm{Ind}_P^G\ \mathbb{C}|0\rangle.$$

By construction, this means that $\overline{W}_p$ is freely generated by the generators a_i^+ $(i\in[1;n+m])$ acting on $|0\rangle$. In other words, a basis for $\overline{W}_p$ is given by

$$|p;r_1,r_2,\ldots,r_{n+m}\rangle\equiv(a_1^+)^{r_1}(a_2^+)^{r_2}\cdots(a_n^+)^{r_n}(a_{n+1}^+)^{r_{n+1}}(a_{n+2}^+)^{r_{n+2}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle, \tag{3.4}$$

where

$$r_i\in\mathbb{Z}_+ \ \text{ for } \ i\in[1;n] \ \text{ and } \ r_i\in\{0,1\} \ \text{ for } \ i\in[n+1;n+m].$$

So $\overline{W}_p$ is an infinite-dimensional G module. The main part of this section is devoted to the computation of the action of the JGs on the basis vectors (3.4) of $\overline{W}_p$. This, of course, completely determines the action of $U_q[sl(n+1|m)]$ on $\overline{W}_p$.

Theorem 2: *The transformation of the basis (3.4) of $\overline{W}_p$ under the action of the JGs reads:*

$$H_i|p;r_1,r_2,\ldots,r_{n+m}\rangle=\left(p-(-1)^{\theta_i}r_i-\sum_{j=1}^{n+m}r_j\right)|p;r_1,r_2,\ldots,r_{n+m}\rangle, \tag{3.5}$$

$$a_i^-|p;r_1,r_2,\ldots,r_{n+m}\rangle=(-1)^{\theta_1r_1+\theta_2r_2+\cdots+\theta_{i-1}r_{i-1}}q^{r_1+\cdots+r_{i-1}}[r_i]\left[p-\sum_{j=1}^{n+m}r_j+1\right]$$
$$\times|p;r_1,r_2,\ldots,r_{i-1},r_i-1,r_{i+1},\ldots,r_{n+m}\rangle, \tag{3.6}$$

$$a_i^+|p;r_1,r_2,\ldots,r_{n+m}\rangle=(-1)^{\theta_1r_1+\theta_2r_2+\cdots+\theta_{i-1}r_{i-1}}\overline{q}^{r_1+\cdots+r_{i-1}}(1-\theta_ir_i)|p;r_1,r_2,\ldots,r_{i-1},r_i$$
$$+1,r_{i+1},\ldots,r_{n+m}\rangle, \tag{3.7}$$

where $i\in[1;n+m]$.

Proof: Equation (3.5) is an immediate consequence of $[H_i,a_j^+]=-(1+(-1)^{\theta_i}\delta_{ij})a_j^+$, which is one of the last relations in (2.16). Also the action of a_i^+ on the basis vectors is easy: (3.7) follows directly from (2.18). The hard work lies in the proof of (3.6). For this purpose, we shall use a number of technical lemmas.

Lemma 3: The following relations hold:

(i) $$[\![A,B_1B_2\cdots B_{i-1}B_iB_{i+1}\cdots B_j]\!]_{q^{b_1+b_2+\ldots+b_j}}$$
$$=\sum_{i=1}^{j} q^{b_1+b_2+\cdots+b_{i-1}}(-1)^{\alpha(\beta_1+\cdots+\beta_{i-1})}B_1B_2\cdots B_{i-1}[\![A,B_i]\!]_{q^{b_i}}B_{i+1}\cdots B_j,$$

$$\text{where}\quad \alpha=\deg(A)\quad \text{and}\quad \beta_i=\deg(B_i), \tag{3.8}$$

(ii) $$[\![a_i^-,(a_j^+)^r]\!]=\begin{cases}\dfrac{\overline{q}^{2r}-1}{\overline{q}^2-1}(a_j^+)^{r-1}[\![a_i^-,a_j^+]\!] & \text{when}\quad i<j\\ \dfrac{q^{2r}-1}{q^2-1}(a_j^+)^{r-1}[\![a_i^-,a_j^+]\!] & \text{when}\quad i>j\end{cases}, \tag{3.9}$$

(iii) $$[\![a_i^-,(a_i^+)^r]\!]=\frac{(a_i^+)^{r-1}}{q-\overline{q}}\left(\frac{\overline{q}^{2r}-1}{\overline{q}^2-1}L_i-\frac{q^{2r}-1}{q^2-1}\overline{L}_i\right), \tag{3.10}$$

(iv) $$[\![[\![a_i^-,a_j^+]\!],(a_i^+)^r]\!]_{q^r}=-(-1)^{\theta_j}\frac{\overline{q}^{2r}-1}{\overline{q}^2-1}\overline{L}_ia_j^+(a_i^+)^{r-1},\quad i>j, \tag{3.11}$$

(v) $$[\![[\![a_i^-,a_j^+]\!],(a_k^+)^r]\!]_{q^r}=(-1)^{\theta_j}(q^{2r}-1)a_j^+(a_k^+)^{r-1}[\![a_i^-,a_k^+]\!],\quad i>k>j. \tag{3.12}$$

Proof: Equation (3.8) follows by direct calculation. We need to prove Eq. (3.9) only when $r>1$, i.e., only when $\theta_j=\overline{0}$. Then one writes, using (3.8)

$$[\![a_i^-,(a_j^+)^r]\!]=[\![a_i^-,(a_j^+)^{r-1}a_j^+]\!]=[\![a_i^-,(a_j^+)^{r-1}]\!]a_j^++(a_j^+)^{r-1}[\![a_i^-,a_j^+]\!].$$

Now the result follows using induction on r and using the triple relation (2.19) with $k=j$ and $\eta=-$. The proof of (3.10) is similar, using (3.8), induction on r, and (2.17). Also the proof of (3.11) goes along the same line: First one writes $(a_i^+)^r$ as $a_i^+(a_i^+)^{r-1}$ (for $r>1$); using (3.8) this yields two terms: On the first term one applies (2.19), and on the second term one applies (3.11) by induction; then the result follows. The proof of (3.12) is essentially the same. □

Lemma 4: For $i>1$ the following relation holds:

$$\begin{aligned}&[\![a_i^-,a_1^+]\!](a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle\\ &\quad=-(-1)^{\theta_1+\theta_2r_2+\theta_3r_3+\cdots+\theta_{i-1}r_{i-1}}q^{2r_2+\cdots+2r_{i-1}+r_i+\cdots+r_{n+m}-p}[r_i]\\ &\qquad\times a_1^+(a_2^+)^{r_2}\cdots(a_{i-1}^+)^{r_{i-1}}(a_i^+)^{r_i-1}(a_{i+1}^+)^{r_{i+1}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle.\end{aligned} \tag{3.13}$$

Proof: Consider first $i=2$. Using (3.8), one finds

$$\begin{aligned}[\![a_2^-,a_1^+]\!](a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle&=[\![[\![a_2^-,a_1^+]\!],(a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}]\!]_{q^{r_2+\cdots+r_{n+m}}}|0\rangle\\ &=[\![[\![a_2^-,a_1^+]\!],(a_2^+)^{r_2}]\!]_{q^{r_2}}(a_3^+)^{r_3}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle\\ &\quad+(-1)^{(\theta_1+\theta_2)r_2\theta_2}q^{r_2}(a_2^+)^{r_2}\\ &\quad\times[\![[\![a_2^-,a_1^+]\!],(a_3^+)^{r_3}\cdots(a_{n+m}^+)^{r_{n+m}}]\!]_{q^{r_3+\cdots+r_{n+m}}}|0\rangle.\end{aligned} \tag{3.14}$$

From (3.8) and (2.19) it follows that the second term in the rhs of (3.14) is zero. For the first term, apply (3.11) and use the action of $\overline{L_2}$ as given by (3.5) and (2.10). Then the result follows.

Next we shall use induction on i to prove (3.13) in general. So suppose (3.13) holds for all $j=2,3,\ldots,i-1$, i.e.,

$$\begin{aligned}&[\![a_j^-,a_1^+]\!](a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle\\&\quad=-(-1)^{\theta_1+\theta_2 r_2+\theta_3 r_3+\cdots+\theta_{j-1}r_{j-1}}q^{2r_2+\cdots+2r_{j-1}+r_j+\cdots+r_{n+m}-p}[r_j]\\&\quad\times a_1^+(a_2^+)^{r_2}\cdots(a_{j-1}^+)^{r_{j-1}}(a_j^+)^{r_j-1}(a_{j+1}^+)^{r_{j+1}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle.\end{aligned}\tag{3.15}$$

Making a shift of indices in (3.15) (thereby putting the last r_k-values equal to zero), leads to the following equivalent equation:

$$\begin{aligned}&[\![a_i^-,a_j^+]\!](a_{j+1}^+)^{r_{j+1}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle\\&\quad=-(-1)^{\theta_j+\theta_{j+1}r_{j+1}+\theta_{j+2}r_{j+2}+\cdots+\theta_{i-1}r_{i-1}}q^{2r_{j+1}+\cdots+2r_{i-1}+r_i+\cdots+r_{n+m}-p}[r_i]\\&\quad\times a_j^+(a_{j+1}^+)^{r_{j+1}}\cdots(a_{i-1}^+)^{r_{i-1}}(a_i^+)^{r_i-1}(a_{i+1}^+)^{r_{i+1}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle,\quad(j<i).\end{aligned}\tag{3.16}$$

Now consider the left-hand side (lhs) of (3.13) and apply (3.8)

$$\begin{aligned}[\![a_i^-,a_1^+]\!](a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle&=[\![[\![a_i^-,a_1^+]\!],(a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}]\!]_{q^{r_2+\cdots+r_{n+m}}}|0\rangle\\&=\sum_{k=2}^{n+m}q^{r_2+\cdots+r_{k-1}}(-1)^{(\theta_i+\theta_1)(\theta_2 r_2+\theta_3 r_3+\cdots+\theta_{k-1}r_{k-1})}\\&\quad\times(a_2^+)^{r_2}\cdots(a_{k-1}^+)^{r_{k-1}}[\![[\![a_i^-,a_1^+]\!],(a_k^+)^{r_k}]\!]_{q^{r_k}}\\&\quad\times(a_{k+1}^+)^{r_{k+1}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle.\end{aligned}\tag{3.17}$$

In this last sum, all terms with $k>i$ are easily seen to vanish. For the terms with $k<i$, we apply (3.12), and for the term with $k=i$, we apply (3.11). Then there comes

$$\begin{aligned}&\sum_{k=2}^{i-1}(-1)^{\theta_1+\theta_2 r_2+\theta_3 r_3+\cdots+\theta_{k-1}r_{k-1}}(q^{2r_k}-1)a_1^+(a_2^+)^{r_2}\cdots(a_{k-1}^+)^{r_{k-1}}(a_k^+)^{r_k-1}[\![a_i^-,a_k^+]\!]\\&\quad\times(a_{k+1}^+)^{r_{k+1}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle-(-1)^{\theta_1+\theta_2 r_2+\theta_3 r_3+\cdots+\theta_{i-1}r_{i-1}}q^{-p+\Sigma_{l=i}^{n+m}r_l}[r_i]\\&\quad\times a_1^+(a_2^+)^{r_2}\cdots(a_{i-1}^+)^{r_{i-1}}(a_i^+)^{r_i-1}(a_{i+1}^+)^{r_{i+1}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle.\end{aligned}\tag{3.18}$$

For the terms in (3.18) with $k<i$, we can apply (3.16). Then it is a matter of appropriately summing all contributions, which leads finally to the rhs of (3.13). □

Proof of Theorem 2: There remains to prove Eq. (3.6). First, assume that $i=1$ in (3.6); then we have according to (3.8)

$$\begin{aligned}a_1^-|p;r_1,r_2,\ldots,\ldots,r_{n+m}\rangle&=[\![a_1^-,(a_1^+)^{r_1}(a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}]\!]|0\rangle\\&=[\![a_1^-,(a_1^+)^{r_1}]\!](a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle\\&\quad+\sum_{j=2}^{n+m}(-1)^{\theta_1(\theta_1 r_1+\theta_2 r_2+\cdots+\theta_{j-1}r_{j-1})}\\&\quad\times(a_1^+)^{r_1}\cdots(a_{j-1}^+)^{r_{j-1}}[\![a_1^-,(a_j^+)^{r_j}]\!](a_{j+1}^+)^{r_{j+1}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle.\end{aligned}\tag{3.19}$$

The terms with $j \geqslant 2$ in the rhs of (3.19) are found to be zero using (3.9) and (2.19). So only the first term in the rhs of (3.19) gives a contribution; using (3.10) this is

$$[r_1]\left[p-\sum_{j=1}^{n+m} r_j+1\right]|p;r_1-1,r_2,\ldots,r_{n+m}\rangle,$$

so the case $i=1$ is proved. Now we use again induction on i. So the following equation holds for $j<i$:

$$a_j^-(a_1^+)^{r_1}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle=(-1)^{\theta_1 r_1+\theta_2 r_2+\cdots+\theta_{j-1}r_{j-1}}q^{r_1+\cdots+r_{j-1}}[r_j] \times\left[p-\sum_{l=1}^{n+m} r_l+1\right]|p;r_1,r_2,\ldots,r_{j-1},r_j-1,r_{j+1},\ldots,r_{n+m}\rangle. \tag{3.20}$$

In this equation, put $r_{n+m}=0$ and raise all indices by 1. Then the following (equivalent) equation holds:

$$a_i^-(a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle=(-1)^{\theta_2 r_2+\theta_3 r_3+\cdots+\theta_{i-1}r_{i-1}}q^{r_2+\cdots+r_{i-1}}[r_i] \times\left[p-\sum_{l=2}^{n+m} r_l+1\right] \times(a_2^+)^{r_2}\cdots(a_{i-1}^+)^{r_{i-1}}(a_i^+)^{r_i-1}(a_{i+1}^+)^{r_{i+1}}\cdots(a_{n+m}^+)^{r_{n+m}}|0\rangle. \tag{3.21}$$

Now consider

$$\begin{aligned} a_i^-|p;r_1,r_2,\ldots,r_{n+m}\rangle&=[\![a_i^-,(a_1^+)^{r_1}\cdots(a_{n+m}^+)^{r_{n+m}}]\!]|0\rangle\\ &=[\![a_i^-,(a_1^+)^{r_1}]\!](a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}]\!]|0\rangle\\ &\quad+(-1)^{\theta_i\theta_1 r_1}(a_1^+)^{r_1}[\![a_i^-,(a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}]\!]|0\rangle\\ &=\frac{q^{2r_1-1}}{q^2-1}(a_1^+)^{r_1-1}[\![a_i^-,a_1^+]\!](a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}]\!]|0\rangle\\ &\quad+(-1)^{\theta_i\theta_1 r_1}(a_1^+)^{r_1}[\![a_i^-,(a_2^+)^{r_2}\cdots(a_{n+m}^+)^{r_{n+m}}]\!]|0\rangle. \end{aligned} \tag{3.22}$$

This was obtained by applying (3.9) on the first term. The rhs of (3.22) can now be determined as follows: For the first term we use (3.13), and for the second term, we use (3.21) in which both sides have been multiplied (on the left) by $(a_1^+)^{r_1}$. Adding both contributions leads to the desired result. □

The action of the elements H_i and $a_i^{\pm}$ $(i\in[1;n+m])$ on the basis vectors of $\overline{W}_p$, determined in Theorem 2, clearly imply that $\overline{W}_p$ has an invariant submodule when p is a nonnegative integer. From now on we shall assume that $p\in\mathbb{Z}_+$. Then we have

Corollary 5: The $U_q[sl(n+1|m)]$ module $\overline{W}_p$ has an invariant submodule V_p with basis vectors

$$|p;r_1,r_2,\ldots,r_{n+m}\rangle,\ \textit{with}\ \sum_{i=1}^{n+m} r_i>p.$$

The quotient module $W_p=\overline{W}_p/V_p$ is an irreducible representation for $U_q[sl(n+1|m)]$. The basis vectors of W_p are given by (*the representatives of*)

$$|p;r_1,r_2,\ldots,r_{n+m}\rangle, \ \ with \ \sum_{i=1}^{n+m} r_i \leqslant p. \tag{3.23}$$

These finite-dimensional irreducible $U_q[sl(n+1|m)]$ modules W_p are referred to as the Fock modules or Fock representations of $U_q[sl(n+1|m)]$. Also in the Fock modules, the action of the elements H_i and $a_i^{\pm}$ $(i\in[1;n+m])$ on the basis vectors (3.23) is essentially given by the equations of Theorem 2.

One can verify that the irreducible Fock representations W_p are so-called atypical representations of $U_q[sl(n+1|m)]$. Atypicality is usually defined for highest weight representations of simple Lie superalgebras,[32] but it can be extended to highest weight representations of the corresponding Hopf superalgebras.[33] In the standard basis, the Dynkin labels of W_p (or of its highest weight) are given by $(p,0,\ldots,0)$. This means that in general the representation W_p is multiply atypical.[32,34] More precisely, if $n\geqslant m$, then W_p is m-fold atypical; if $n<m$, then W_p is $(n+1)$-fold atypical for $p<m-n$ and n-fold atypical for $p\geqslant m-n$. Observe that in this way we have obtained the action of a set of generators of $U_q[sl(n+1|m)]$ on a class of atypical irreducible representations, i.e., the Fock modules. In general, an explicit basis for atypical representations is not known, not even in the case of $sl(n+1|m)$. For typical representations of $U_q[sl(n+1|m)]$, it is easier to construct a basis. For a subclass of these, the so-called essentially typical representations, a (Gelfand–Zetlin) basis has been constructed together with the action of the Chevalley generators.[9]

IV. UNITARY FOCK REPRESENTATIONS

In this section we select a class of Fock modules important for physical applications. These are the ones for which the standard Fock metric is positive definite, and for which the representatives of $a_i^{\pm}$ and H_i $(i\in[1;n+m])$ satisfy the Hermiticity conditions

$$(a_i^+)^\dagger = a_i^-, \quad (a_i^-)^\dagger = a_i^+, \quad (H_i)^\dagger = H_i. \tag{4.1}$$

In quantum mechanics, including its generalization to the noncommutative case (see, for instance Refs. 35 and 36), (4.1) follows from the relations $a_k^{\pm}=\text{const}(x_k\mp ip_k)$ and the requirement that the position operators x_k and the momentum operators p_k should be self-adjoint operators. By definition, representations for which (4.1) holds are said to be unitary (with respect to the antiinvolution in $U_q[sl(n+1|m)]$ defined by (4.1), and the Fock space scalar product).

For the Fock representation W_p, we can define a Hermitian form $(,)$ by requiring

$$(|0\rangle, |0\rangle) = \langle 0|0\rangle = 1, \tag{4.2}$$

and by postulating that the Hermiticity conditions (4.1) should be satisfied, i.e.,

$$(a_i^{\pm}v,w) = (v,a_i^{\mp}w), \quad \forall v,w\in W_p. \tag{4.3}$$

It is now easy to determine that any two vectors $|p;r_1,r_2,\ldots,r_{n+m}\rangle$ and $|p;r_1',r_2',\ldots,r_{n+m}'\rangle$ with $(r_1,r_2,\ldots,r_{n+m})\neq(r_1',r_2',\ldots,r_{n+m}')$ are orthogonal. Furthermore, one can compute

$$(|p;r_1,r_2,\ldots,r_{n+m}\rangle,|p;r_1,r_2,\ldots,r_{n+m}\rangle) = \frac{[p]!}{[p-R]!}\prod_{i=1}^{n+m}[r_i]! = \frac{[p]!}{[p-R]!}\prod_{i=1}^{n}[r_i]!, \tag{4.4}$$

where $R=r_1+r_2+\cdots+r_{n+m}$. Clearly, it holds for $R=0$; then use induction on R together with (3.6) and (3.7).

Assume now that $1\leqslant i<j\leqslant n+m$. According to (4.4) we have

$$(a_i^+a_j^+|0\rangle, a_i^+a_j^+|0\rangle) = [p][p-1]. \tag{4.5}$$

From (2.18) we have $a_i^+ a_j^+ = (-1)^{\theta_i\theta_j} q a_j^+ a_i^+ = (-1)^{\theta_i} q a_j^+ a_i^+$ [since $(-1)^{\theta_i\theta_j} = (-1)^{\theta_i}$ for $i < j$]; thus we find

$$(a_j^+ a_i^+|0\rangle, a_i^+ a_j^+|0\rangle) = ((-1)^{\theta_i}\overline{q} a_i^+ a_j^+|0\rangle, a_i^+ a_j^+|0\rangle) = (-1)^{\theta_i}\overline{q}^*[p][p-1], \tag{4.6}$$

where $\overline{q}^*$ is the complex conjugate of $\overline{q} = q^{-1}$. On the other hand, using (3.6),

$$\begin{aligned}(a_j^+ a_i^+|0\rangle, a_i^+ a_j^+|0\rangle) &= (a_i^+|0\rangle, a_j^-|p;0,\ldots,0,1_i,0,\ldots,0,1_j,0,\ldots,0\rangle)\\ &= (a_i^+|0\rangle, (-1)^{\theta_i} q[p-1]|p;0,\ldots,0,1_i,0,\ldots,0\rangle)\\ &= (-1)^{\theta_i} q[p-1](a_i^+|0\rangle, a_i^+|0\rangle) = (-1)^{\theta_i} q[p][p-1].\end{aligned} \tag{4.7}$$

Herein, 1_i stands for a number 1 at the position i. When $p \geqslant 2$, the comparison of (4.6) and (4.7) yields $|q|^2 = 1$. Hence a necessary condition for the Fock space to be unitary is that q must be a phase, i.e.,

$$q = e^{i\phi}, \quad (-\pi < \phi < \pi). \tag{4.8}$$

Let us now further investigate when the Fock module is unitary, i.e., when the Hermitian form (,) is an inner product. This means that for every $(r_1,\ldots,r_{n+m})$ with $0 \leqslant R \leqslant p$, the value in (4.4) should be positive. In particular, this implies that all the numbers

$$[p],\ [p-1],\ [p-2],\ldots,[2],\ [1],$$

should be positive. However, since $q = e^{i\phi}$ is a phase, we have

$$[k] = \frac{q^k - q^{-k}}{q - q^{-1}} = \frac{\sin(k\phi)}{\sin(\phi)}.$$

So we are left with the following question: let $p > 1$, find the values of ϕ $(-\pi < \phi < \pi)$ where all of the following functions:

$$\frac{\sin(2\phi)}{\sin(\phi)}, \frac{\sin(3\phi)}{\sin(\phi)}, \ldots, \frac{\sin(p\phi)}{\sin(\phi)},$$

are positive. For each of these functions $\sin(k\phi)/\sin(\phi)$, the zeros and hence the signs are easy to determine. So the common domain where all of these functions are positive is given by

$$\frac{-\pi}{p} < \phi < \frac{\pi}{p}.$$

Thus we have

Theorem 6: *The irreducible Fock module W_p $(p \geqslant 2)$ is unitary if and only if q is a phase, i.e., $q = e^{i\phi}$, with $-\pi/p < \phi < \pi/p$.*

Observe that whether q is a root of unity or not does not have any effect on the irreducibility or unitarity of the Fock module W_p, as long as the conditions of Theorem 6 are satisfied. Indeed, suppose that $q = e^{i\phi}$ is a root of unity with ϕ a rational multiple of π and $-\pi/p < \phi < \pi/p$. Then the smallest integer N for which $q^N = -1$ is greater than p. As a consequence, the rhs in (4.4) is never zero. This implies that there are no singular vectors among the weight vectors $|p;r_1,\ldots,r_{n+m}\rangle$, and thus irreducibility holds.

Under the conditions of Theorem 6, we can define an orthonormal basis of W_p

$$|p;r_1,r_2,\ldots,r_{n+m}) = \sqrt{\frac{[p-\Sigma_{l=1}^{n+m} r_l]!}{[p]![r_1]!\ldots[r_{n+m}]!}}\,|p;r_1,r_2,\ldots,r_{n+m}\rangle, \tag{4.9}$$

where $0 \leqslant \Sigma_{i=1}^{n+m} r_i \leqslant p$. In the new basis (4.9) the transformation formulas (3.5)–(3.7) read ($i \in [1;n+m]$)

$$H_i|p;r_1,r_2,\ldots,r_{n+m}) = \left(p-(-1)^{\theta_i} r_i - \sum_{j=1}^{n+m} r_j \right) |p;r_1,r_2,\ldots,r_{n+m}), \tag{4.10}$$

$$a_i^-|p;r_1,\ldots,r_{n+m}) = (-1)^{\theta_1 r_1+\cdots+\theta_{i-1}r_{i-1}} \times q^{r_1+\cdots+r_{i-1}} \sqrt{[r_i]\left[p-\sum_{l=1}^{n+m} r_l+1 \right]}\ |p;r_1,\ldots r_{i-1},r_i-1,r_{i+1},\ldots,r_{n+m}), \tag{4.11}$$

$$a_i^+|p;r_1,\ldots,r_{n+m}) = (-1)^{\theta_1 r_1+\cdots+\theta_{i-1}r_{i-1}} \overline{q}^{r_1+\cdots+r_{i-1}}(1-\theta_i r_i) \times \sqrt{[r_i+1]\left[p-\sum_{l=1}^{n+m} r_l \right]}\ |p;r_1,\ldots r_{i-1},r_i+1,r_{i+1},\ldots,r_{n+m}). \tag{4.12}$$

From (2.15) it is now easy to determine the action of the remaining Cartan–Weyl generators e_{ji} on the basis elements of W_p

$$e_{ji}|p;r_1,\ldots,r_{n+m}) = (-1)^{\theta_i(r_i+1)+\theta_{i+1}r_{i+1}+\cdots+\theta_{j-1}r_{j-1}} \overline{q}^{r_{i+1}+\cdots+r_{j-1}-2\theta_i(1-r_i)}(1-\theta_j r_j) \times \sqrt{[r_i][r_j+1]}\ |p;r_1,\ldots r_{i-1},r_i-1,r_{i+1},\ldots,r_{j-1},r_j+1,r_{j+1},\ldots,r_{n+m}), \quad (i<j), \tag{4.13}$$

$$e_{ji}|p;r_1,\ldots,r_{n+m}) = (-1)^{\theta_j r_j+\cdots+\theta_{i-1}r_{i-1}} q^{2\theta_j r_j+r_{j+1}+\cdots+r_{i-1}}(1-\theta_j r_j) \times \sqrt{[r_i][r_j+1]}\ |p;r_1,\ldots r_{j-1},r_j+1,r_{j+1},\ldots,r_{i-1},r_i-1,r_{i+1},\ldots,r_{n+m}), \quad (i>j). \tag{4.14}$$

In particular, it is possible to extend W_p to a $U_q[gl(n+1|m)]$ module, the actions being given by (4.11)–(4.14) and

$$e_{00}|p;r_1,\ldots,r_{n+m}) = \left(p-\sum_{l=1}^{n+m} r_l \right) |p;r_1,\ldots,r_{n+m}), \tag{4.15}$$

$$e_{ii}|p;r_1,\ldots,r_{n+m}) = r_i|p;r_1,\ldots,r_{n+m}), \quad i \in [1;n+m]. \tag{4.16}$$

V. DYSON AND HOLSTEIN–PRIMAKOFF REALIZATIONS OF $U_q[sl(n+1|m)]$

Consider $(n+m)$ $\mathbb{Z}_2$-graded indeterminates $c_i^{\pm}$ ($i \in [1;n+m]$) with

$$\deg(c_i^{\pm}) = \theta_i. \tag{5.1}$$

Denote by $W(n|m)$ the free $\mathbb{C}[[h]]$ module (completed in the h-adic topology) generated by the elements $c_i^{\pm}$ subject to the relations

$$[\![c_i^-, c_j^+]\!] = \delta_{ij}, \quad [\![c_i^+, c_j^+]\!] = [\![c_i^-, c_j^-]\!] = 0. \tag{5.2}$$

As usual, let

$$N_i = c_i^+ c_i^- , \quad N = \sum_{j=1}^{n+m} N_j . \tag{5.3}$$

The algebra $W(n|m)$ of n pairs of Bose and m pairs of Fermi CAO's has a natural action in the Fock space $\mathcal{F}(n|m)$, defined as follows. Let $\mathcal{F}(n|m)$ be the free $W(n|m)$ module generated by a vector $|0\rangle$ subject to the relations

$$c_i^- |0\rangle = 0, \text{ for all } i \in [1;n+m].$$

Then it follows easily that a basis of $\mathcal{F}(n|m)$ is given by

$$(c_1^+)^{l_1}(c_2^+)^{l_2}\cdots(c_{n+m}^+)^{l_{n+m}}|0\rangle \equiv |l_1, l_2, \ldots, l_{n+m}\rangle, \tag{5.4}$$

where

$$l_i \in \mathbb{Z}_+ \text{ for } i \in [1;n] \text{ and } l_i \in \{0,1\} \text{ for } i \in [n+1;n+m].$$

The Dyson[37] and Holstein–Primakoff[38] realizations of $U_q[sl(n+1|m)]$ are two different algebra homomorphisms of $U_q[sl(n+1|m)]$ into $W(n|m)$.[23] Since $W(n|m)$ has the natural Fock representation $\mathcal{F}(n|m)$, these realizations will provide representations of $U_q[sl(n+1|m)]$ in $\mathcal{F}(n|m)$.

Theorem 7 (Dyson realization): *Let p be any complex number. The linear map $\rho: U_q[sl(n+1|m)] \to W(n|m)$, defined on the Jacobson generators by*

$$\rho(H_i) = p - (-1)^{\theta_i} c_i^+ c_i^- - \sum_{j=1}^{n+m} c_j^+ c_j^- = p - (-1)^{\theta_i} N_i - N,$$

$$\rho(a_i^-) = q^{N_1+\cdots+N_{i-1}} \frac{[N_i+1]}{N_i+1} [p-N] c_i^- , \tag{5.5}$$

$$\rho(a_i^+) = \overline{q}^{N_1+\cdots+N_{i-1}} c_i^+ ,$$

is a (associative algebra) homomorphism of $U_q[sl(n+1|m)]$ into $W(n|m)$.

The inspiration of this mapping comes from Theorem 2. The actual proof of Theorem 7 is straightforward but tedious: one has to verify that all relations in Theorem 1 are satisfied under the substitution of H_i and $a_i^\pm$ by $\rho(H_i)$ and $\rho(a_i^\pm)$. These computations are lengthy and based upon easy relations such as

$$f(N_i) c_j^\pm = c_j^\pm f(N_i \pm \delta_{ij}), \quad i,j \in [1;n+m]; \quad q^{N_i} = 1 - N_i + qN_i \text{ for } i > n,$$

or simple q-identities such as $[x+1][y] - [x][y+1] = [y-x]$.

The Dyson realization of the JGs of $U_q[sl(n+1|m)]$ leads to an explicit realization of all Cartan–Weyl elements of $U_q[sl(n+1|m)]$ in terms of the Bose and Fermi CAO's. Indeed, using (2.15) and (5.5) one obtains

$$\rho(e_{ji}) = q^{2\theta_j(N_j-1)+N_{j+1}+N_{j+2}+\cdots+N_{i-1}} \frac{[N_i+1]}{N_i+1} c_j^+ c_i^- , \quad (j<i) \tag{5.6}$$

$$\rho(e_{ji}) = \overline{q}^{2\theta_i N_i + N_{i+1}+N_{i+2}+\cdots+N_{j-1}} \frac{[N_i+1]}{N_i+1} c_j^+ c_i^- , \quad (j>i). \tag{5.7}$$

In (5.6), the convention is that the summation (in the power of q) is 0 when $j = i-1$ [and similarly for (5.7)]. Since $\mathcal{F}(n|m)$ is a $W(n|m)$ module, the Dyson realization provides a representation of

$U_q[sl(n+1|m)]$ into $\mathcal{F}(n|m)$. It is easy to see that the action of every $\rho(H_i)$ and $\rho(a_i^{\pm})$ upon $|l_1,\ldots,l_{n+m}\rangle$ is the same as the action of H_i and $a_i^{\pm}$ in the representation on $\overline{W}_p$ given by Theorem 2, under the identification

$$|l_1,\ldots,l_{n+m}\rangle \equiv |p;l_1,\ldots,l_{n+m}\rangle.$$

Therefore, it follows that the representation ρ of $U_q[sl(n+1|m)]$ into $\mathcal{F}(n|m)$ (under the Dyson realization) is irreducible when $p \notin \mathbb{Z}_+$. When $p \in \mathbb{Z}_+$, the representation ρ is indecomposable. The subspace $\mathcal{F}_1(n|m)$, spanned on the vectors

$$|l_1,\ldots,l_{n+m}\rangle \quad \text{with} \quad l_1+\cdots+l_{n+m}>p$$

is clearly invariant under the action of $U_q[sl(n+1|m)]$. We denote the (finite dimensional) quotient module by $\mathcal{F}_0(n|m)=\mathcal{F}(n|m)/\mathcal{F}_1(n|m)$, and (by abuse of notation) its vectors are denoted by

$$|l_1,\ldots,l_{n+m}\rangle \quad \text{with} \quad l_1+\cdots+l_{n+m}\leqslant p.$$

For h an indeterminate ($q=e^h$), the representation of $U_q[sl(n+1|m)]$ into $\mathcal{F}_0(n|m)$ is irreducible. It is obvious how to identify $\mathcal{F}_0(n|m)$ with W_p.

In order to turn $\mathcal{F}_0(n|m)$ into a unitary $U_q[sl(n+1|m)]$ module, we introduce the Holstein–Primakoff realization.

Theorem 8 (Holstein–Primakoff realization): *Let $p \in \mathbb{C}$. The linear map $\varrho: U_q[sl(n+1|m)] \to W(n|m)$, defined on the Jacobson generators by*

$$\varrho(H_i)=p-(-1)^{\theta_i}c_i^+c_i^- - \sum_{j=1}^{n+m} c_j^+c_j^- = p-(-1)^{\theta_i}N_i - N,$$

$$\varrho(a_i^-)=q^{N_1+\cdots+N_{i-1}}\sqrt{\frac{[N_i+1]}{N_i+1}[p-N]}\,c_i^-, \tag{5.8}$$

$$\varrho(a_i^+)=\overline{q}^{N_1+\cdots+N_{i-1}}\sqrt{\frac{[N_i]}{N_i}[p-N+1]}\,c_i^+,$$

is a homomorphism of $U_q[sl(n+1|m)]$ into $W(n|m)$.

Let us now also consider the special case that p is a positive integer. Just as in the previous case, the subspace $\mathcal{F}_1(n|m)$ is invariant for the action of $U_q[sl(n+1|m)]$ under ϱ when $p \in \mathbb{Z}_+$. It is clearly invariant under the action of $U_q[sl(n+1|m)]$. Let us consider the following basis of the (finite dimensional) quotient module $\mathcal{F}_0(n|m)$:

$$\frac{(c_1^+)^{l_1}(c_2^+)^{l_2}\cdots(c_{n+m}^+)^{l_{n+m}}}{\sqrt{l_1!l_2!\cdots l_{n+m}!}}|0\rangle \equiv |l_1,l_2,\ldots,l_{n+m}), \quad l_1+\cdots+l_{n+m}\leqslant p. \tag{5.9}$$

It is easy to verify that the action of every $\varrho(H_i)$ and $\varrho(a_i^{\pm})$ upon $|l_1,\ldots,l_{n+m})$ is the same as the action of H_i and $a_i^{\pm}$ in the representation on W_p given by (4.11)-(4.12), under the identification

$$|l_1,\ldots,l_{n+m}) \equiv |p;l_1,\ldots,l_{n+m}).$$

Therefore, it follows that the representation ϱ of $U_q[sl(n+1|m)]$ into $\mathcal{F}_0(n|m)$ (under the Holstein–Primakoff realization with $p \in \mathbb{Z}_+$) is an irreducible unitary module when

$$q=e^{i\phi} \quad \text{with} \quad -\frac{\pi}{p}<\phi<\frac{\pi}{p}.$$

From (2.15) and (5.8), one obtains the Holstein–Primakoff realization of the remaining Cartan–Weyl elements of $U_q[sl(n+1|m)]$

$$\varrho(e_{ji})=q^{2\theta_j(N_j-1)+N_{j+1}+N_{j+2}+\cdots+N_{i-1}}\sqrt{\frac{[N_j][N_i+1]}{N_j(N_i+1)}}c_j^+c_i^-,\quad (j<i),$$

$$\varrho(e_{ji})=\overline{q}^{2\theta_iN_i+N_{i+1}+N_{i+2}+\cdots+N_{j-1}}\sqrt{\frac{[N_j][N_i+1]}{N_j(N_i+1)}}c_j^+c_i^-,\quad (j>i). \tag{5.10}$$

Observe that there is an alternative description of the Holstein–Primakoff realization, in terms of deformed Bose[39–42] and Fermi[43] CAO's $\tilde{c}_i^{\pm}$ defined as

$$\tilde{c}_i^-=\sqrt{\frac{[N_i+1]}{N_i+1}}c_i^-,\quad \tilde{c}_i^+=\sqrt{\frac{[N_i]}{N_i}}c_i^+,\quad \tilde{N}_i=N_i,\quad i\in[1;n+m]. \tag{5.11}$$

These elements of $W(n|m)$ satisfy the relations

$$[\![\tilde{c}_i^-,\tilde{c}_j^+]\!]_{q^{\delta_{ij}}}=\delta_{ij}\overline{q}^{(-1)^{\theta_i}\tilde{N}_i},\quad [\tilde{N}_i,\tilde{c}_j^{\pm}]=\pm\delta_{ij}\tilde{c}_j^{\pm},\quad [\![\tilde{c}_i^{\pm},\tilde{c}_j^{\pm}]\!]=[\tilde{N}_i,\tilde{N}_j]=0. \tag{5.12}$$

The Holstein–Primakoff realization can be rewritten in terms of these deformed Bose and Fermi operators $\tilde{c}_i^{\pm}$. We give it here for all Cartan–Weyl elements

$$\begin{aligned}
\varrho(H_i)&=p-(-1)^{\theta_i}\tilde{N}_i-\tilde{N},\\
\varrho(a_i^-)&=q^{\tilde{N}_1+\cdots+\tilde{N}_{i-1}}\sqrt{[p-\tilde{N}]}\tilde{c}_i^-,\\
\varrho(a_i^+)&=\overline{q}^{\tilde{N}_1+\cdots+\tilde{N}_{i-1}}\sqrt{[p-\tilde{N}+1]}\tilde{c}_i^+,\\
\varrho(e_{ji})&=q^{2\theta_j(\tilde{N}_j-1)+\tilde{N}_{j+1}+\tilde{N}_{j+2}+\cdots+\tilde{N}_{i-1}}\tilde{c}_j^+\tilde{c}_i^-,\quad (j<i),\\
\varrho(e_{ji})&=\overline{q}^{2\theta_i\tilde{N}_i+\tilde{N}_{i+1}+\tilde{N}_{i+2}+\cdots+\tilde{N}_{j-1}}\tilde{c}_j^+\tilde{c}_i^-,\quad (j>i).
\end{aligned} \tag{5.13}$$

Furthermore, this is easy to extend to a Holstein–Primakoff realization of $U_q[gl(n+1|m)]$ by

$$\varrho(e_{00})=p-\tilde{N},\quad \varrho(e_{ii})=\tilde{N}_i. \tag{5.14}$$

The Holstein–Primakoff realization has given us a realization in terms of oscillators [in (5.8) and (5.10)] or q-oscillators [in (5.13)]. Observe that this oscillator realization is different from the one given by Floreanini *et al.*:[43] In Ref. 43 only the Chevalley generators are realized in terms of oscillators or q-oscillators. Furthermore all generators are bilinear expressions in the oscillators, whereas here the JGs are linear expressions in the oscillators.

VI. CONCLUSIONS

We have constructed a class of representations of the quantum superalgebra $U_q[sl(n+1|m)]$, which was also extended to $U_q[gl(n+1|m)]$. Our approach is entirely along the lines of Fock representations of parastatistics of order p, for which the defining relations are given by (3.1)–(3.3). The analogy with parastatistics goes further: Within the Fock representations, the JGs $a_i^{\pm}$ can be interpreted as operators creating or annihilating (quasi)particles, or excitations of a new kind of quantum statistics.

In order to be more concrete consider a Hamiltonian $H=\Sigma_{i=1}^{n+m}\ \varepsilon_ie_{ii}$. Then, see (4.16),

$$H|p;r_1,\ldots,r_{n+m})=\sum_{i=1}^{n+m}\varepsilon_ir_i|p;r_1,\ldots,r_{n+m}).$$

Therefore the vector $|p;r_1,\ldots,r_{n+m})$ can be interpreted as a state consisting of r_1 particles with energy ε_1, r_2 particles with energy ε_2, and so on, r_{n+m} particles with energy ε_{n+m}. Moreover,

according to (4.11) and (4.12) any operator a_i^+ (resp. a_i^-) creates (resp. annihilates) a particle on the orbital i. Since $r_i \in \mathbb{Z}_+$ for $i \in [1;n]$ and $r_i \in \{0,1\}$ for $i \in [n+1;m]$ the particles on the first n orbitals behave like bosons, and the particles on the next orbitals like fermions. This is, however, not quite the case if $p<n+m$, since $\Sigma_{i=1}^{n+m} r_i \leqslant p$. In other words the system cannot accommodate more than p particles. Therefore, the statistics falls in the group of exclusion statistics in the broad sense:[44] The number of particles to be accommodated on a certain orbital depends on the number of particles already accommodated in the system. What are the properties of the underlying statistics is a question still to be answered.

Another property worthy of study is to analyze what happens if $p \to \infty$ and $q \to 1$. Having in mind the results from Ref. 11 we expect that in this limit the operators $A(p,q)_i^{\pm} = a_i^{\pm}/\sqrt{p}$ become genuine Bose CAO's for $i \in [1;n]$ and genuine Fermi CAO's for $i \in [n+1;n+m]$. If so, then for large p and values of q close to 1 the operators $A(p,q)_i^{\pm}$ describe small deviations from the canonical quantum statistics. Moreover these CAO's are defined in a state space with positive definite scalar product. Among the various noncanonical statistics (Gentile intermediate statistics,[45] parastatistics,[15] infinite statistics,[46] parons,[47] quons[48]) only the quons have the same property. Therefore, parallel to quons the $A(p,q)_i^{\pm}$ operators may appear as another candidate to describe eventual small violations of canonical quantum statistics (see Ref. 47 where also experiments for detecting small violations of statistics are discussed).

We believe also (having in mind again the results in Ref. 11) that the CAO's of $U_q[sl(n+1|m)]$ and their Fock representations will be natural "building blocks" for any multicomponent $t-J$ supersymmetric lattice model. To this end we note that at each site i the Hubbard operators X^{0k} and X^{k0},[49] (we suppress the site index) are nothing but nondeformed Jacobson generators a_k^- and a_k^+, respectively. Then the representations with $p=1$ satisfy the hard-core condition forbidding configurations with two or more particles to be accommodated simultaneously on each lattice site.

Some of the results related to this quantum statistics were already published in an earlier paper.[50] Let us underline the new contributions in the present paper. Theorem 1 (Sec. II) was already stated without proof in Ref. 50, since it is the main ingredient to describe the quantum statistics; here we have given its relevant background and a complete proof. Sections III and IV contain our key results; all of them are original. We have constructed a class of representations of $U_q[sl(n+1|m)]$ labeled by an arbitrary number p. When p is a positive integer, this representation is indecomposable and the corresponding quotient module is finite dimensional. The derivation of the action of the JGs on basis elements of these representations is highly nontrivial. In Sec. IV we have selected the unitary representations, with respect to the (in physics) natural Hermiticity condition (4.1) considered as an anti-involution, and the requirement that the usual Fock space metric should be positive definite. It is interesting to note that the selected representations remain irreducible when q is a root of unity.

The Dyson and Holstein–Primakoff realizations of $U_q[sl(n+1|m)]$ were given in an earlier paper by one of us,[23] but only for the Chevalley generators. Here, in Sec. V, we give the realization for all Cartan–Weyl elements of $U_q[sl(n+1|m)]$. Such realizations are relevant since also in the classical case ($q=1$) the realization of all Cartan–Weyl generators (Bargmann–Schwinger realizations, ladder representations) are of physical importance. Observe that it is far from trivial to deduce the realization for all Cartan–Weyl elements from those of the realization for the Chevalley generators. This would be rather hard because the expressions of all Cartan–Weyl elements in terms of the Chevalley generators are very involved and difficult to manage, see e.g., Ref. 31. In the present case, the problem was overcome because we were able to give the Dyson and Holstein–Primakoff realizations of the Jacobson generators of $U_q[sl(n+1|m)]$. Since the expressions of the remaining Cartan–Weyl elements in terms of the Jacobson generators is simple, the Dyson and Holstein–Primakoff realizations of all Cartan–Weyl elements followed without too much trouble.

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Analytic Coulomb matrix elements in the lowest Landau level in disk geometry

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Using Darling's theorem on products of generalized hypergeometric series, an analytic expression is obtained for the Coulomb matrix elements in the lowest Landau level in the representation of angular momentum. The result is important in the studies of fractional quantum Hall effect (FQHE) in disk geometry. Matrix elements are expressed as simple finite sums of positive terms, eliminating the need to approximate these quantities with slowly convergent series. As a by-product, an analytic representation for certain integrals of products of Laguerre polynomials is obtained. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1446244]

I. INTRODUCTION

The following integrals,

$$M^l_{mn}=(m+l,n|r_{12}^{-1}|m,n+l)=\int\int d^2r_1 d^2r_2 \psi^*_{m+l}(\mathbf{r}_1)\psi^*_n(\mathbf{r}_2)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\psi_m(\mathbf{r}_1)\psi_{n+l}(\mathbf{r}_2), \quad (1)$$

represent the Coulomb interaction matrix elements in the lowest Landau level. These are the basic quantities for studies of correlated two-dimensional systems in quantizing magnetic fields.[1–7] The single-particle wave functions in the angular momentum representation are given by

$$\psi_m(\mathbf{r})=(2\pi 2^m m!)^{-1/2} r^m e^{im\phi-r^2/4}, \quad (2)$$

where r and ϕ are polar coordinates in the plane, and the magnetic length $\sqrt{\hbar c/eH}$ is taken as a unit of length. The axial gauge for the vector potential $\mathbf{A}=\frac{1}{2}[\mathbf{H},\mathbf{r}]$ is chosen.

Full Coulomb interaction has been shown to play a crucial role in edge effects in fractional quantum Hall systems, not captured by Laughlin's wave function.[1,2] The results of Refs. 1 and 2 would have been difficult to obtain without an analytic formula for M^l_{mn}, the derivation of which is the subject of this work. Use of well-known expressions by Girvin and Jach[3] is prohibitive at moderately large m and n because of large cancellations. The problem was addressed in Ref. 8, where slowly convergent series to approximate M^l_{mn} have been derived.

Here we present analytic formulas for M^l_{mn} that contain simple finite sums of positive terms, which can be easily evaluated for any m, n, and l. Moreover, the symmetry with respect to interchanging m and n is explicitly preserved.

II. FORMULA FOR MATRIX ELEMENTS

We start with the result, which reads

$$M^l_{mn}=\sqrt{\frac{(m+l)!(n+l)!}{m!n!}}\frac{\Gamma(l+m+n+\frac{3}{2})}{\pi 2^{l+m+n+2}}[A^l_{mn}B^l_{nm}+B^l_{mn}A^l_{nm}], \quad (3)$$

where

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$$A^l_{mn}=\sum_{i=0}^{m}\binom{m}{i}\frac{\Gamma(\frac{1}{2}+i)\Gamma(\frac{1}{2}+l+i)}{(l+i)!\Gamma(\frac{3}{2}+l+n+i)}, \tag{4a}$$

and

$$B^l_{mn}=\sum_{i=0}^{m}\binom{m}{i}\frac{\Gamma(\frac{1}{2}+i)\Gamma(\frac{1}{2}+l+i)}{(l+i)!\Gamma(\frac{3}{2}+l+n+i)}(\tfrac{1}{2}+l+2i). \tag{4b}$$

The rest of the article presents the derivation of Eqs. (3) and (4). First, we substitute

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}=\int\frac{d^2q}{2\pi q}\exp[i\mathbf{q}(\mathbf{r}_1-\mathbf{r}_2)] \tag{5}$$

into Eq. (1). The two separate integrals over $\mathbf{r}_1$ and $\mathbf{r}_2$ can be evaluated in terms of Laguerre polynomials $L^l_m(q^2/2)$.[9] Substituting $q^2/2=x$ we obtain

$$M^l_{mn}=\sqrt{\frac{m!n!}{2(m+l)!(n+l)!}}\int dx x^{l-1/2}e^{-2x}L^l_m(x)L^l_n(x). \tag{6}$$

The above integral can be expressed[10] using generalized hypergeometric function[11,12]

$$M^l_{mn}=\sqrt{\frac{(l+m)!}{2\pi m!n!(l+n)!}}\frac{\Gamma(n+\frac{1}{2})\Gamma(l+\frac{1}{2})}{l!}F\left(\left.\begin{matrix}1/2, & l+\frac{1}{2}, & l+m+1\\ & -n+\frac{1}{2}, & l+1\end{matrix}\right|z\right) \tag{7}$$

in the limit $z\to-1$, approached from the right. The function F is defined as

$$F\left(\left.\begin{matrix}a, & b, & c\\ & d, & e\end{matrix}\right|z\right)=\sum_{i=0}^{\infty}\frac{z^i(a)_i(b)_i(c)_i}{i!(d)_i(e)_i}, \tag{8}$$

where $(z)_i=z(z+1)\cdots(z+i-1)=\Gamma(z+i)/\Gamma(z)$. Taking the limit avoids problems at $z=-1$, which is at the radius of convergence of the power series (8). For $|z|<1$ the right-hand side of Eq. (7) gives a more general integral of $x^{l-1/2}e^{(z-1)x}L^l_m(-zx)L^l_n(x)$, which is analytic in z.

When one of the upper parameters is a negative integer, the series (8) terminate yielding a finite sum. At $z=-1$ we have

$$F\left(\left.\begin{matrix}-k, & b, & c\\ & d, & e\end{matrix}\right|-1\right)=\sum_{i=0}^{k}\binom{k}{i}\frac{(b)_i(c)_i}{(d)_i(e)_i}. \tag{9}$$

Since none of the upper parameters of F in Eq. (7) are negative integers, the series is infinite. However, it appears possible to transform Eq. (7) in such a way that the result contains only terminating hypergeometric series. Using Darling's theorem on products,[13] the infinite series (7) are brought into a sum of products of generalized hypergeometric series that each have at least one negative integer upper argument, therefore, representing a finite sum. Darling's theorem for the function F reads

$$(1-z)^{a+b+c-d-e}F\left(\begin{matrix}a, & b, & c\\ & d, & e\end{matrix}\middle| z\right)$$
$$=\frac{e-1}{e-d}F\left(\begin{matrix}d-a, & d-b, & d-c\\ & d, & d+1-e\end{matrix}\middle| z\right)F\left(\begin{matrix}e-a, & e-b, & e-c\\ & e-1, & e+1-d\end{matrix}\middle| z\right)$$
$$+\frac{d-1}{d-e}F\left(\begin{matrix}e-a, & e-b, & e-c\\ & e, & e+1-d\end{matrix}\middle| z\right)F\left(\begin{matrix}d-a, & d-b, & d-c\\ & d-1, & d+1-e\end{matrix}\middle| z\right). \quad (10)$$

Using Eq. (10) and setting $z=-1$ in the end we obtain

$$M^l_{mn}=\sqrt{\frac{(l+m)!}{\pi m!n!(l+n)!}}\frac{\Gamma(n+\frac{1}{2})\Gamma(l+\frac{1}{2})}{2^{l+m+n+1}(l+n+\frac{1}{2})l!}$$
$$\times\left\{(n+\tfrac{1}{2})F\left(\begin{matrix}-m, & \frac{1}{2}, & l+\frac{1}{2}\\ & l+1, & l+n+\frac{3}{2}\end{matrix}\middle| -1\right)F\left(\begin{matrix}-n, & -n-l, & -n-l-m-\frac{1}{2}\\ & -n-\frac{1}{2}, & -n-l+\frac{1}{2}\end{matrix}\middle| -1\right)\right.$$
$$\left.+lF\left(\begin{matrix}-m, & \frac{1}{2}, & l+\frac{1}{2}\\ & l, & l+n+\frac{3}{2}\end{matrix}\middle| -1\right)F\left(\begin{matrix}-n, & -n-l, & -n-l-m-\frac{1}{2}\\ & -n+\frac{1}{2}, & -n-l+\frac{1}{2}\end{matrix}\middle| -1\right)\right\}. \quad (11)$$

Further, we prove the following hypergeometric identity, valid for any positive integer k:

$$F\left(\begin{matrix}-k, & -k-a, & -k-b\\ & -k-c, & -k-d\end{matrix}\middle| -1\right)=\frac{(1+a)_k(1+b)_k}{(1+c)_k(1+d)_k}F\left(\begin{matrix}-k, & 1+c, & 1+d\\ & 1+a, & 1+b\end{matrix}\middle| -1\right). \quad (12)$$

The proof is obtained by reversing the order of summation in the (finite) sum, $i\to k-i$, using the symmetry of the binomial coefficients with respect to this substitution, and noticing that $(-k-a)_{k-i}=(-1)^{k-i}(1+a)_k/(1+a)_i$. Using identity (12) to transform the second hypergeometric function in each of the two terms in Eq. (11), we get

$$M^l_{mn}=\sqrt{\frac{(l+m)!(l+n)!}{m!n!}}\frac{\Gamma(l+m+n+\frac{3}{2})}{\pi 2^{l+m+n+1}(l+n+\frac{1}{2})}$$
$$\times\left\{\sum_{i=0}^{m}\binom{m}{i}\frac{\Gamma(\frac{1}{2}+i)\Gamma(\frac{1}{2}+l+i)}{(l+i-1)!\Gamma(\frac{3}{2}+l+n+i)}\sum_{j=0}^{n}\binom{n}{j}\frac{\Gamma(\frac{1}{2}+j)\Gamma(\frac{1}{2}+l+j)}{(l+j)!\Gamma(\frac{3}{2}+l+m+j)}\right.$$
$$\left.+\sum_{i=0}^{m}\binom{m}{i}\frac{\Gamma(\frac{1}{2}+i)\Gamma(\frac{1}{2}+l+i)}{(l+i)!\Gamma(\frac{3}{2}+l+n+i)}\sum_{j=0}^{n}\binom{n}{j}\frac{\Gamma(\frac{3}{2}+j)\Gamma(\frac{1}{2}+l+j)}{(l+j)!\Gamma(\frac{3}{2}+l+m+j)}\right\}. \quad (13)$$

The two terms in Eq. (13) can be brought together, restoring the symmetry with respect to m and n:

$$M^l_{mn}=\sqrt{\frac{(l+m)!(l+n)!}{m!n!}}\frac{\Gamma(l+m+n+\frac{3}{2})}{\pi 2^{l+m+n+1}(l+n+\frac{1}{2})}\sum_{i=0}^{m}\sum_{j=0}^{n}(l+i+j+\tfrac{1}{2})$$
$$\times\binom{m}{i}\frac{\Gamma(\frac{1}{2}+i)\Gamma(\frac{1}{2}+l+i)}{(l+i)!\Gamma(\frac{3}{2}+l+n+i)}\binom{n}{j}\frac{\Gamma(\frac{1}{2}+j)\Gamma(\frac{1}{2}+l+j)}{(l+j)!\Gamma(\frac{3}{2}+l+m+j)}. \quad (14)$$

Finally, regrouping the terms to split the double sum back into a product of single sums while preserving the $m \leftrightarrow n$ symmetry we arrive at Eqs. (3) and (4).

We note that Eqs. (3) and (4) also represent a useful analytic representation for the integrals of products of Laguerre polynomials (6).

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Braided oscillators

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A generalized oscillator algebra is proposed and the braided Hopf algebra structure for this generalized oscillator is investigated. Using the solutions for the braided Hopf algebra structure, two types of braided Fibonacci oscillators are introduced. This leads to two types of braided Biedenharn–Macfarlane oscillators as special cases of the Fibonacci oscillators. We also find the braided Hopf algebra solutions for the three dimensional braided space. One of these, as a special case, gives the Hopf algebra given in the literature. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The harmonic oscillator has a wide variety of applications from quantum optics to the realizations of the angular momentum algebra and hence the deformations of the oscillator algebra play an important role in q-deformed theories. The realization of the q-deformed angular momentum algebra by Biedenharn–Macfarlane oscillators[1] and the realization of the Hermitian braided matrices by a pair of q-oscillators[2] are some of the examples. The two parameter deformations and some of their applications can be found in Ref. 3. Braided group theory (a self-contained review can be found in Ref. 4) deforms the notion of tensor product (called braided tensor product) and hence deforms the independence of the objects. Although braided groups arise in the formulation of quantum group covariant structures, the idea of braiding can be used without any reference to quantum groups to generalize the statistics.[5]

The permutation map π (π:$A\otimes B\rightarrow B\otimes A$) in the tensor product algebra of boson algebras

$$(a\otimes b)(c\otimes d)=a\,\pi(b\otimes c)d=ac\otimes bd$$

is replaced by a generalized map called braiding ψ (ψ:$A\otimes B\rightarrow B\otimes A$) such that

$$(a\otimes b)(c\otimes d)=a\,\psi(b\otimes c)d.$$

This generalization leads to the generalization of the Hopf algebra called braided Hopf algebra[6] whose axioms in algebraic (not diagrammatic) form read as

$$m\circ(id\otimes m)=m\circ(m\otimes id),$$

$$m\circ(id\otimes\eta)=m\circ(\eta\otimes id)=id,$$

$$(id\otimes\Delta)\circ\Delta=(\Delta\otimes id)\circ\Delta,$$

$$(\epsilon\otimes id)\circ\Delta=(id\otimes\epsilon)\circ\Delta=id,$$

$$m\circ(id\otimes S)\circ\Delta=m\circ(S\otimes id)\circ\Delta=\eta\circ\epsilon,$$

$$\psi\circ(m\otimes id)=(id\otimes m)\circ(\psi\otimes id)\circ(id\otimes\psi),$$

$$\psi\circ(id\otimes m)=(m\otimes id)\circ(id\otimes\psi)\circ(\psi\otimes id), \tag{1}$$

$$(id\otimes\Delta)\circ\psi=(\psi\otimes id)\circ(id\otimes\psi)\circ(\Delta\otimes id),$$

$$(\Delta\otimes id)\circ\psi=(id\otimes\psi)(\psi\otimes id)\circ(id\otimes\Delta),$$

$$\Delta\circ m=(m\otimes m)(id\otimes\psi\otimes id)\circ(\Delta\otimes\Delta),$$

$$S\circ m=m\circ\psi\circ(S\otimes S),$$

$$\Delta\circ S=(S\otimes S)\circ\psi\circ\Delta,$$

$$\epsilon\circ m=\epsilon\otimes\epsilon,$$

$$(\psi\otimes id)\circ(id\otimes\psi)\circ(\psi\otimes id)=(id\otimes\psi)\circ(\psi\otimes id)\circ(id\otimes\psi),$$

where $m:A\otimes A\to A$ is the multiplication map, $\Delta:A\to A\otimes A$ is the comultiplication map, $\eta:K\to A$ is the unit map, $\epsilon:A\to K$ is the counit map, $S:A\to A$ is the antipode map and $\psi:A\otimes A\to A\otimes A$ is the braiding map. The consistency of the relations (1) requires that

$$\Delta(1_A)=1_A\otimes 1_A,\quad \psi(1_A\otimes a)=a\otimes 1_A,\quad \psi(a\otimes 1_A)=1_A\otimes a\quad \forall a\in A, \tag{2}$$

where 1_A is the identity of the algebra A. From now on we will drop the subscript and write 1 for the identity of the algebra. All these maps are linear. Note that in the limit $\psi\to\pi$ the braided Hopf algebra axioms reduce to the ordinary Hopf algebra axioms. The braided Hopf algebra axioms[7] reduce to the axioms given above when the counit map (ϵ) is an algebra homomorphism. The $*$-structure for a braided algebra B is different[8] from the nonbraided one such that

$$\Delta\circ *=\pi\circ(*\otimes *)\circ\Delta,$$

$$S\circ *=*\circ S, \tag{3}$$

$$(a\otimes b)^*=b^*\otimes a^*,\quad \forall a,b\in B.$$

II. GENERALIZED OSCILLATOR

We propose a generalized oscillator algebra generated by a, a^*, q^N and 1 satisfying

$$aq^N=qq^Na,$$

$$q^Na^*=qa^*q^N, \tag{4}$$

$$aa^*-Q_1a^*a=Q_2q^{2N}+Q_3q^N+Q_4,$$

where q,Q_1,Q_2,Q_3,Q_4 are real constants whose values determine the type of the oscillator. For example, if Q_1 is a free parameter, then the $Q_2=1$, $Q_3=Q_4=0$ case and the $Q_3=1$, $Q_2=Q_4=0$ case define two different Fibonacci oscillators. For the $*$-structure we impose $(q^N)^*=q^N$, $(a^*)^*=a$. The actions of the generators on the Hilbert space are given by

$$a|n\rangle=a_n|n-1\rangle,$$

$$a^*|n\rangle=a^*_{n+1}|n+1\rangle, \tag{5}$$

$$q^N|n\rangle=q^n|n\rangle.$$

Using the fact that for a given algebra the Hopf algebra structure is not unique, we write the general forms of the coproducts

$$\Delta(q^N)=A_1q^N\otimes q^N+A_2a\otimes a^*+A_3a^*\otimes a+A_4 1\otimes q^N+A_5q^N\otimes 1+A_6 1\otimes 1,$$
$$\Delta(a)=B_1q^N\otimes a+B_2a\otimes q^N+B_3 1\otimes a+B_4a\otimes 1, \tag{6}$$
$$\Delta(a^*)=B_1a^*\otimes q^N+B_2q^N\otimes a^*+B_3a^*\otimes 1+B_4 1\otimes a^*,$$

the counits

$$\epsilon(q^N)=e_1,\quad \epsilon(a)=\epsilon(a^*)=e_2, \tag{7}$$

the antipodes

$$S(q^N)=k_1q^N+k_2a+k_3a^*+k_4,$$
$$S(a)=m_1q^N+m_2a+m_3a^*+m_4, \tag{8}$$
$$S(a^*)=m_1q^N+m_2a^*+m_3a+m_4,$$

and the braidings

$$\psi(q^N\otimes q^N)=g_1q^N\otimes q^N+g_2a\otimes a^*+g_3a^*\otimes a+g_4 1\otimes q^N+g_5q^N+g_6 1\otimes 1,$$
$$\psi(q^N\otimes a)=d_1a\otimes q^N+d_2q^N\otimes a+d_3 1\otimes a+d_4a\otimes 1,$$
$$\psi(a^*\otimes q^N)=d_1q^N\otimes a^*+d_2a^*\otimes q^N+d_3a^*\otimes 1+d_4 1\otimes a^*,$$
$$\psi(q^N\otimes a^*)=f_1a^*\otimes q^N+f_2q^N\otimes a^*+f_3 1\otimes a^*+f_4a^*\otimes 1,$$
$$\psi(a\otimes q^N)=f_1q^N\otimes a+f_2a\otimes q^N+f_3a\otimes 1+f_4 1\otimes a, \tag{9}$$
$$\psi(a\otimes a)=z_1a\otimes a,$$
$$\psi(a^*\otimes a^*)=z_1a^*\otimes a^*,$$
$$\psi(a\otimes a^*)=b_1q^N\otimes q^N+b_2a\otimes a^*+b_3a^*\otimes a+b_4 1\otimes q^N+b_5q^N\otimes 1+b_6 1\otimes 1,$$
$$\psi(a^*\otimes a)=c_1q^N\otimes q^N+c_2a\otimes a^*+c_3a^*\otimes a+c_4 1\otimes q^N+c_5q^N\otimes 1+c_6 1\otimes 1,$$

where symbols with a subscript are the constants to be determined.

III. BRAIDED HOPF ALGEBRA STRUCTURE OF THE GENERALIZED OSCILLATOR

To find the general braided Hopf algebra structure for the oscillator algebra given by (4) we substitute these general forms into the braided Hopf algebra axioms (1) and find the solutions using the computer programming Maple V. The constants which are the same for all solutions read as

$$Q_4=A_1=A_6=B_1=B_2=0,\quad A_4=A_5=B_3=B_4=1, \tag{10}$$
$$k_2=k_3=k_4=m_1=m_3=m_4=e_1=e_2=0,\quad m_2=-1, \tag{11}$$
$$b_4=b_5=b_6=c_4=c_5=c_6=g_4=g_5=g_6=d_3=d_4=f_3=f_4=0. \tag{12}$$

The solutions for the other parameters are given in the tables. The constants given by (10)–(12) show that the antipodes and the counits of all generators and the coproducts of raising/lowering

TABLE I. Braided Fibonacci oscillator of the first type.

$aa^*-Q_1a^*a=q^{2N},\ aq^N=qq^Na,\ q^Na^*=qa^*q^N$

	sol1	sol2	sol3	sol4	sol5	sol6
$k_1=$	-1	-1	-1	-1	-1	-1
$b_1=$	1	$1-\frac{q}{\sqrt{Q_1}}$	$1+\frac{q}{\sqrt{Q_1}}$	$\frac{Q_1}{q^2}$	0	0
$b_2=$	$\frac{q^2-Q_1}{Q_1}$	$\frac{(q^2-Q_1)(\sqrt{Q_1}+q)}{qQ_1}$	$\frac{(Q_1-q^2)(\sqrt{Q_1}-q)}{qQ_1}$	0	0	0
$b_3=$	Q_1	Q_1	Q_1	$\frac{Q_1^2}{q^2}$	Q_1	Q_1
$z=$	$\frac{q^2}{Q_1}$	$\frac{q^2}{Q_1}$	$\frac{q^2}{Q_1}$	$\frac{Q_1}{q^2}$	$\frac{Q_1}{q^2}$	$\frac{Q_1}{q^2}$
$c_1=$	$-\frac{q^2}{Q_1^2}$	0	0	$\frac{-1}{Q_1}$	$-\frac{q+\sqrt{Q_1}}{qQ_1}$	$\frac{\sqrt{Q_1}-q}{qQ_1}$
$c_2=$	$\frac{q^2}{Q_1^2}$	$\frac{1}{Q_1}$	$\frac{1}{Q_1}$	$\frac{1}{Q_1}$	$\frac{1}{Q_1}$	$\frac{1}{Q_1}$
$c_3=$	0	0	0	$\frac{Q_1-q^2}{q^2}$	$\frac{(q^2-Q_1)(q-\sqrt{Q_1})}{q^2\sqrt{Q_1}}$	$\frac{(Q_1-q^2)(q+\sqrt{Q_1})}{q^2\sqrt{Q_1}}$
$d_1=$	$\frac{q}{Q_1}$	$\frac{q}{Q_1}$	$\frac{q}{Q_1}$	q^{-1}	q^{-1}	q^{-1}
$d_2=$	0	0	0	$\frac{Q_1-q^2}{q^2}$	$\frac{Q_1-q^2}{q^2}$	$\frac{Q_1-q^2}{q^2}$
$f_1=$	q	q	q	$\frac{Q_1}{q}$	$\frac{Q_1}{q}$	$\frac{Q_1}{q}$
$f_2=$	$\frac{q^2-Q_1}{Q_1}$	$\frac{q^2-Q_1}{Q_1}$	$\frac{q^2-Q_1}{Q_1}$	0	0	0
$g_1=$	$\frac{q^2}{Q_1}$	$-\frac{q}{\sqrt{Q_1}}$	$\frac{q}{\sqrt{Q_1}}$	$\frac{Q_1}{q^2}$	$\frac{\sqrt{Q_1}}{q}$	$-\frac{\sqrt{Q_1}}{q}$
$g_2=$	0	$\frac{(q^2-Q_1)(\sqrt{Q_1}+q)}{qQ_1}$	$\frac{(Q_1-q^2)(\sqrt{Q_1}-q)}{qQ_1}$	0	0	0
$g_3=$	0	0	0	0	$-\frac{Q_1(Q_1-q^2)^2}{q^2(Q_1+q\sqrt{Q_1})}$	$\frac{Q_1(Q_1-q^2)^2}{q^2(q\sqrt{Q_1}-Q_1)}$

$A_2=A_3=0$ for all solutions

operators are uniquely determined. We also found that for a free deformation parameter Q_1 at most one of the other deformation parameters, namely Q_2 or Q_3, is nonzero. For $Q_2\neq 0$, we have

$$aa^*-Q_1a^*a=Q_2q^{2N}. \tag{13}$$

Without loss of generality we can take $Q_2=1$ or by rescaling a and a^* the oscillator relation (13) can be reduced to

$$aa^*-Q_1a^*a=q^{2N}. \tag{14}$$

We found that there are only six possible braided Hopf algebra solutions for this two-parameter oscillator which are given in Table I. Defining the free deformation parameter $Q_1\equiv p^{-2}$ the algebra (14) can be rewritten as

$$aa^*-p^{-2}a^*a=q^{2N}, \tag{15}$$

which is the more familiar form of the q, p oscillator algebra (Fibonacci oscillator) which we call the first-type Fibonacci oscillator. Using the actions (5) the eigenvalue of the operator a^*a on the state $|n\rangle$ is found to be

$$a_n^* a_n = \frac{p^{-2n} - q^{2n}}{p^{-2} - q^2}. \tag{16}$$

Substituting $Q_1 = q^{-2}$ into (14) we obtain the Biedenharn–Macfarlane oscillator algebra which we call the first-type Biedenharn–Macfarlane oscillator defined by

$$aa^* - q^{-2}a^*a = q^{2N}. \tag{17}$$

The eigenvalue of the operator a^*a on the state $|n\rangle$ is found to be

$$a_n^* a_n = \frac{q^{2n} - q^{-2n}}{q^2 - q^{-2}}. \tag{18}$$

There are only six braided Hopf algebra solutions for the first-type Biedenharn–Macfarlane oscillator (17) which can be obtained by substituting $Q_1 = q^{-2}$ into the solutions given in Table I. Similarly, for $Q_3 \neq 0$ the oscillator relation

$$aa^* - Q_1 a^*a = Q_3 q^N \tag{19}$$

can again be reduced to

$$aa^* - Q_1 a^*a = q^N, \tag{20}$$

which we call the second-type Fibonacci oscillator. Setting the free deformation $Q_1 \equiv p^{-1}$ the eigenvalue of the operator a^*a on the state $|n\rangle$ is found to be

$$a_n^* a_n = \frac{p^{-n} - q^n}{p^{-1} - q}. \tag{21}$$

The second-type Fibonacci oscillator (20) has only two braided Hopf algebra solutions which are given in Table II. The second-type Biedenharn–Macfarlane oscillator can be obtained simply by substituting $Q_1 = q^{-1}$ into (20) and the same substitution into Table II gives braided Hopf algebra solutions.

A wide variety of one-parameter oscillators can be obtained by assigning $Q_1 = f(q)$ in the algebras (14) and (20). The braided Hopf algebra solutions for these oscillators can be obtained by substituting $Q_1 = f(q)$ into the Tables I and II. However, there are extra solutions for some values Q_1 which are given in Table III.

The braided Hopf algebra structure of the quantum space (called braided space) defined by

$$x_i x_j = q x_j x_i, \quad i > j, \tag{22}$$

determines the structure of the braided integration, derivation and Fourier transform defined on that space.[9] For $Q_1 = q$, $Q_2 = 0$, $Q_3 = 0$, $Q_4 = 0$ the algebra (4) reduces to the three dimensional quantum space with the identifications

$$x_1 \equiv a^*, \quad x_2 \equiv q^N, \quad x_3 \equiv a. \tag{23}$$

The braided Hopf algebra solutions for the three dimensional braided space are given in Table IV. Setting the free parameter $g_1 = q^2$ in the sol5 of Table IV gives the braided Hopf algebra given in Ref. 10 and references therein) as a special case.

TABLE II. Braided Fibonacci oscillator of the second type.

$aa^*-Q_1a^*a=q^N,\ aq^N=qq^Na,\ q^Na^*=qa^*q^N$	sol1	sol2
$A_2=$	$\frac{q-Q_1}{q}$	$\frac{Q_1-q}{Q_1}$
$A_3=$	$\frac{Q_1(Q_1-q)}{q}$	$q-Q_1$
$k_1=$	$-\frac{Q_1}{q}$	$-\frac{q}{Q_1}$
$b_2=$	0	$\frac{Q_1^2-q^2}{qQ_1}$
$b_3=$	q	q
$z=$	$\frac{q}{Q_1}$	$\frac{Q_1}{q}$
$c_2=$	q^{-1}	q^{-1}
$c_3=$	$\frac{q^2-Q_1^2}{qQ_1}$	0
$d_1=$	$\frac{1}{Q_1}$	$\frac{Q_1}{q^2}$
$f_1=$	$\frac{q^2}{Q_1}$	Q_1
$g_1=$	$\frac{q^2}{Q_1^2}$	$\frac{Q_1^2}{q^2}$
$b_1=c_1=d_2=f_2=g_2=g_3=0$ for both solutions		

IV. CONCLUSION

The braidings imply the relations between independent copies of algebras. For example, the implication of the braiding $\psi(a\otimes a)$ can be found by using the identifications $a_1\equiv a\otimes 1$ and $a_2\equiv 1\otimes a$ such that

$$a_2a_1=(1\otimes a)(a\otimes 1)=\psi(a\otimes a)=za\otimes a=za_1a_2.$$

TABLE III. Other braided oscillator solutions

$aa^*-Q_1a^*a=Q_2q^{2N}+Q_3q^N,\ aq^N=qq^Na,\ q^Na^*=qa^*q^N$	sol1	sol2	sol3	sol4	sol5
$Q_1=$	q^2	$-q^2$	$-q^2$	q^2	$-q$
$Q_2=$	1	1	1	1	0
$Q_3=$	0	0	0	0	1
$k_1=$	-1	-1	-1	-1	-1
$b_1=$	0	0	$2-q^2c_1$	$2+q^2c_1$	0
$b_3=$	q^2	$-q^2$	$-q^2$	q^2	$-q$
$z=$	1	-1	-1	1	-1
$c_1=$	0	0	c_1	c_1	0
$c_2=$	q^{-2}	$-q^{-2}$	$-q^{-2}$	q^{-2}	$-q^{-1}$
$d_1=$	q^{-1}	q^{-1}	q^{-1}	q^{-1}	q^{-1}
$f_1=$	q	q	q	q	q
$g_1=$	-1	-1	1	1	1
$A_2=A_3=b_2=c_3=d_2=f_2=g_2=g_3=0$ for all solutions					

TABLE IV. Three dimensional braided space.

	$aa^*=qa^*a,\ aq^N=qq^Na,\ q^Na^*=qa^*q^N$						
	sol1	sol2	sol3	sol4	sol5	sol6	sol7
$A_2=$	A_2	A_2	0	0	0	0	0
$A_3=$	$-qA_2$	qA_2	0	0	0	0	0
$k_1=$	-1	1	-1	-1	-1	-1	-1
$b_2=$	0	0	0	0	$-1+g_1$	$-1+qc_2$	0
$b_3=$	q	q	qg_1	q	q	q	qz
$z=$	1	1	g_1	z	g_1	qc_2	z
$c_2=$	q^{-1}	q^{-1}	q^{-1}	q^{-1}	$q^{-1}g_1$	c_2	q^{-1}
$c_3=$	0	0	g_1-1	0	0	0	$z-1$
$d_1=$	q^{-1}	q^{-1}	q^{-1}	q^{-1}	$q^{-1}g_1$	q^{-1}	q^{-1}
$d_2=$	0	0	g_1-1	0	0	0	0
$f_1=$	q	q	qg_1	q	q	q	q
$f_2=$	0	0	0	0	$-1+g_1$	0	0
$g_1=$	1	1	g_1	g_1	g_1	g_1	g_1
	$b_1=c_1=g_2=g_3=0$ for all solutions						

Thus the braiding relations imply a two-body system of oscillators which can be extended to n-body oscillators using the n-fold braided tensor product as done by Baskerville and Majid in the context of the braided version of the q-Heisenberg algebra.[11] The Fock space representations of the n-fold braided tensor product of oscillators can also be found. This requires the braidings of the generators of the algebra with the states. All these constructions depend on the braiding relations of the generators of the algebra. Since each solution for the braiding gives a different system of oscillators, the solutions we found may provide a general framework for the interacting oscillators and hence for the statistical mechanical quantities calculated by using these oscillators.

Because of the connection between symmetry and statistics it is interesting to investigate the underlying symmetry transformations of the braided oscillators which gives rise to the braiding relations given in the tables. It may also be interesting to find the unbraiding transformations[12] or the decoupling of the braided oscillators. The generalization of supersymmetry to fractional supersymmetry requires the deformation parameter to be a root of unity[13] and this case deserves to be discussed on a seperate study.

The braided Hopf algebra solutions we present for the oscillators and for the three dimensional braided space may provide a general frame on which other structures can be defined.

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Centers of mass and rotational kinematics for the relativistic *N*-body problem in the rest-frame instant form

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A relativistic kinematics for the *N*-body problem which solves all the problems raised until now on this topic is constructed by exploting the Wigner-covariant *rest-frame instant form of dynamics* in the context of *parametrized Minkowski theories*. The Wigner hyperplanes, orthogonal to the total timelike four-momentum of any *N*-body configuration, define the intrinsic rest frame and realize the separation of the center-of-mass motion. The point chosen as origin in each Wigner hyperplane can be made to coincide with the covariant noncanonical Fokker–Pryce *center of inertia*. As is well known, the latter is distinct from the *canonical* pseudo-four-vector describing the decoupled motion of the center of mass (which possess the same Euclidean covariance as the quantum Newton–Wigner three-position operator) and from the noncanonical pseudo-four-vector known as Møller's *center of energy*. Our approach leads to the splitting of the notion of center of mass into an *external* one, defined in terms of an external Poincaré group realization, and an *internal* one defined in terms of an internal unfaithful realization of the group inside the Wigner hyperplane. Because of the first class constraints defining the rest frame (vanishing of the *internal* three-momentum), the latter three *internal* concepts of center of mass weakly *coincide*. The resulting unique *internal* center of mass is thereby a gauge variable which, by a suitable gauge fixing, can be localized at the origin of the Wigner hyperplane. An adapted canonical basis of relative variables is constructed by means of the classical counterpart of the Gartenhaus–Schwartz transformation. The invariant mass of the *N*-body configuration is the Hamiltonian for the relative motions. Within this general framework, the rotational kinematics can be developed in terms of the same *dynamical body frames, orientation-shape* variables, *spin frame*, and *canonical spin bases* already introduced in the case of the nonrelativistic *N*-body problem.
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I. INTRODUCTION

The separation of the *absolute translational motion* of the center of mass from the relative motions for the nonrelativistic *N*-body problem can be easily carried out due to the Abelian character of the translation symmetry group. This character implies that the associated Noether constants of motion (the conserved total three-momentum) are in involution, so that the center-

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of-mass degrees of freedom decouple. Moreover, the fact that the nonrelativistic kinetic energy of the relative motions is a quadratic form in the relative velocities allows for the introduction of special sets of relative coordinates, the *Jacobi normal relative coordinates*, that diagonalize the quadratic form and correspond to different patterns of clustering of the centers of mass of the particles. Each set of Jacobi coordinates arrange the N particles into a *hierarchy of clusters*, in which each cluster of two or more particles has a mass given by an eigenvalue (*reduced mass*) of the quadratic form; the Jacobi normal coordinates join the centers of mass of cluster pairs.

On the other hand, the non-Abelian nature of the rotational symmetry, whose associated Noether constants of motion (the conserved total angular momentum) are not in involution, prevents the possibility of a global separation of *absolute rotations* from the relative motions, so that there is no global definition of *absolute vibrations*. This has the consequence that an *isolated* deformable body can undergo rotations by changing its own shape (as shown by the *falling cat* and the *diver*). It was just to deal with these problems that the theory of the *orientation-shape* $SO(3)$ *principal bundle*[1] has been developed in the context of molecular physics, emphasizing the *gauge* nature of a *static* (i.e., velocity-independent) definition of *body frame* for a deformable body. Both the laboratory and body frame angular velocities as well as the orientational variables of the static body frame thereby become *unobservable gauge* variables. This approach is associated with a set of point canonical transformations, which allow one to define the body frame components of relative motions in a velocity-independent way.

In a previous paper[2] we showed that a more general class of nonpoint canonical transformations exists for $N \geqslant 3$, which allows one to identify a family of *canonical spin bases* connected to the patterns of the possible *clusterings of the spins* associated with relative motions (namely the components of the center-of-mass angular momenta). The definition of these *spin bases* is independent of the use of Jacobi normal relative coordinates, just as the patterns of spin clustering are independent of the patterns of center-of-mass Jacobi clustering.

Two basic frames associated with each spin basis exist: the *spin frame* and the *dynamical body frame*. Their construction is guaranteed by the fact that, besides the existence of a Hamiltonian symmetry *left* action of $SO(3)$[3] on the relative phase space, it is possible to define as many Hamiltonian non-symmetry *right* actions of SO(3) as the possible patterns of spin clustering. While the generators of the left action are the components of the center-of-mass angular momentum (Noether constants of motion), the generators of the right actions are not constants of motion. For $N=3$ the unique canonical *spin basis* coincides with a special class of global cross sections of the trivial orientation-shape SO(3) principal bundle. On the other hand, for $N \geqslant 4$ the existing *spin bases* and *dynamical body frames* turn out to be unrelated to the local cross sections of the *static* nontrivial orientation-shape SO(3) principal bundle, and *evolve* in a dynamical way dictated by the equations of motion. Both the orientation variables and the angular velocities become *measurable* quantities in each canonical spin basis.

For each N, we get a finite number of physically well-defined separations between *rotational* and *vibrational* degrees of freedom. The unique *body frame* of rigid bodies is replaced here by a discrete number of *evolving dynamical body frames* and of *spin canonical bases*. Both of them are grounded on patterns of spin couplings which are the direct analogues of the coupling of quantum angular momenta. Let us note that these results might be useful in nonrelativistic nuclear and molecular physics.

Besides translations and rotations, every isolated nonrelativistic system admits the internal energy, the total mass, and the (time-dependent) Galilei boosts (which amounts essentially to the inertial motion of the center of mass) as constants of the motion. All together, there are 11 constants of motion (the total mass being a central charge) which generate a realization of the kinematical extended Galilei algebra.[4,5]

We want to see what happens when we replace Galilean space–time with Minkowski space–time. More precisely, to see what can be said in this case about the separation of the center of mass from the relative motions and about the rotations, already for the simple model-system of N free scalar positive-energy particles.

First of all we have to describe a relativistic scalar particle. Among the various possibilities

(see Ref. 6 for a review of the various options) we will choose the manifestly Lorentz covariant approach based on Dirac's first class constraints[7]

$$p_i^2 - \epsilon m_i^2 \approx 0. \tag{1.1}$$

The associated Lagrangian description is based on the four-vector positions $x_i^\mu(\tau)$ and the action $S = \int d\tau(-\epsilon \Sigma_i m_i \sqrt{\epsilon \dot{x}_i^2(\tau)})$, where τ is a Lorentz scalar *mathematical* time parameter, i.e., an affine parameter for the particle timelike worldlines. Then Lorentz covariance implies singular Lagrangians and the associated Dirac's theory of constraints for the Hamiltonian description. The individual time variables $x_i^0(\tau)$ are the *gauge variables* associated with the mass-shell constraints, which have the two topologically disjoint solutions $p_i^0 \approx \pm \sqrt{m_i^2 + \vec{p}_i^2}$. As discussed in Refs. 8 and 9 this implies that:

(i) a combination of the time variables may be identified to the clock of one arbitrary observer labeling the evolution of the isolated system;
(ii) the $N-1$ relative times are related to the observer's freedom of looking at the N particles either at the same time or with any prescribed relative delay.

These two gauge arbitrariness describe the *generalized inertial effects* arising from the conventions adopted to quantify the temporal evolution of the particles.

Introducing interactions in this picture without destroying the first class nature of the constraints[10] is a well-known difficult problem. It originated, in the two-particle case, the DrozVincent–Komar–Todorov model.[11] On the other hand, *its extension to N particles has never been given in closed form.*

When the particle is charged and interacts with a dynamical electromagnetic field a *problem of covariance* reappears. The standard description is based on the action

$$S = -\epsilon m \int d\tau \sqrt{\epsilon \dot{x}^2(\tau)} - e \int d\tau \int d^4 z\, \delta^4(z - x(\tau)) \dot{x}^\mu(\tau) A_\mu(z) - \frac{1}{4} \int d^4 z F^{\mu\nu}(z) F_{\mu\nu}(z). \tag{1.2}$$

By evaluating the canonical momenta of the isolated system, *charged particle plus electromagnetic field*, we find two primary constraints:

$$\chi(\tau) = (p - eA(x(\tau)))^2 - \epsilon m^2 \approx 0, \quad \pi^0(z^0, \vec{z}) \approx 0. \tag{1.3}$$

It is immediately seen that, since there is no concept of *equal time*, it is impossible to evaluate the Poisson bracket of these constraints. Also, due to the same reason, the Dirac Hamiltonian which would be $H_D = H_c + \lambda(\tau)\chi(\tau) + \int d^3 z \lambda^0(z^0, \vec{z}) \pi^0(z^0, \vec{z})$ with H_c the canonical Hamiltonian and with $\lambda(\tau)$, $\lambda^0(z^0, \vec{z})$ Dirac's multipliers, does not make sense. This problem is present even at the level of the Euler–Lagrange equations: how to formulate a *Cauchy problem* for a system of coupled equations some of which are ordinary differential equations in the affine parameter τ along the particle worldline, while the others are partial differential equations depending on Minkowski coordinates z^μ? Since the problem is due to the lack of a covariant concept of *equal time* between field and particle variables, a new formulation of the problem is needed. In Ref. 9, after a discussion of the many time formalism, a solution of the problem was found within a context suited to incorporate the gravitational field. The starting point is an arbitrary $3+1$ splitting of Minkowski space–time with spacelike hypersurfaces, which is equivalent to a congruence of timelike accelerated observers. This is essentially Dirac's reformulation[12] of classical field theory (suitably extended to particles) on arbitrary spacelike hypersurfaces (*equal time* or simultaneity Cauchy surfaces). Note incidentally that it is also the classical basis of the Tomonaga–Schwinger formulation of quantum field theory. Given any isolated system (containing any combination of particles, strings, and fields) one is lead to a reformulation of it as a *parametrized Minkowski theory*,[9] with the extra bonus that the theory is already prepared for the coupling to gravity in its ADM formulation. The price to be paid is that the functions $z^\mu(\tau, \vec{\sigma})$ describing the embedding of

the spacelike hypersurface in Minkowski space–time become *additional configuration variables* of the action principle. Since the action is invariant under separate τ-reparametrizations and space-diffeomorphisms, first class constraints appear to ensure the independence of the description from the choice of the $3+1$ splitting. The embedding configuration variables $z^\mu(\tau,\vec{\sigma})$ are the *gauge* variables associated with this kind of general covariance and describe all the possible *inertial effects* compatible with special relativity.

Let us come back to the discussion of the free case within the parametrized Minkowski theory approach. Since the intersection of a timelike worldline with a spacelike hypersurface corresponding to a value τ of the time parameter is identified by three numbers $\vec{\sigma}=\vec{\eta}(\tau)$ and *not by four*, each particle must have a well-defined sign of the energy. Therefore, we cannot describe the two topologically disjoint branches of the mass hyperboloid simultaneously as in the standard manifestly Lorentz-covariant approach. Then, there are no more mass-shell constraints. Each particle with a definite sign of the energy is described by the canonical coordinates $\vec{\eta}_i(\tau)$, $\vec{\kappa}_i(\tau)$ with the derived four-position of the particles given by $x_i^\mu(\tau)=z^\mu(\tau,\vec{\eta}_i(\tau))$. The derived four-momenta $p_i^\mu(\tau)$ are $\vec{\kappa}_i$-dependent solutions of $p_i^2-\epsilon m_i^2=0$ with the given sign of the energy.

Because of the independence from the $3+1$ splitting of Minkowski space–time in parametrized theories, the foliation can be restricted to spacelike hyperplanes. In particular, for each configuration of the isolated system with timelike four-momentum, the leaves are best chosen as the hyperplanes orthogonal to the conserved total four-momentum (*Wigner hyperplanes*). Note that this special foliation is intrinsically determined by the configuration of the isolated system alone. This leads to the definition of the *Wigner-covariant rest-frame instant form of dynamics*,[9] for every isolated system whose configurations have well-defined and finite Poincaré generators with timelike total four-momentum.[13,14]

Such formulation allows one to clarify the roles of the various relativistic centers of mass. This is a long-standing problem which arose just after the foundation of special relativity in the first decade of the last century. In the next 90 years it became clear that the problem of the relativistic center of mass is highly nontrivial: no definition can enjoy all the properties of the ordinary nonrelativistic center of mass. See Refs. 15–20 for a partial bibliography of all the existing attempts and Ref. 21 for reviews.

Let us now summarize some relevant points of the rest-frame instant form on Wigner hyperplanes (see Appendix A). Only four first class constraints survive in this case so that the original configurational variables $z^\mu(\tau,\vec{\sigma})$, $\vec{\eta}_i(\tau)$ and their conjugate momenta $\rho_\mu(\tau,\vec{\sigma})$, $\vec{\kappa}_i(\tau)$ are reduced to the following.

(i) A decoupled point $\tilde{x}_s^\mu(\tau)$, p_s^μ (the only remnant of the spacelike hypersurface) with a positive mass $\epsilon_s=\sqrt{\epsilon p_s^2}$ determined by the first class constraint $\epsilon_s-M_{\rm sys}\approx 0$ ($M_{\rm sys}$ is the invariant mass of the isolated system). Its rest-frame Lorentz scalar time $T_s=(\tilde{x}_s\cdot p_s)/\epsilon_s$ is put equal to the mathematical time by the gauge fixing $T_s-\tau\approx 0$ for the previous constraint. Here, $\tilde{x}_s^\mu(\tau)$ is a *noncovariant canonical variable for the four-center of mass*. After the elimination of T_s and ϵ_s with the previous pair of second class constraints, we are left with a decoupled free point (*point particle clock*) of mass $M_{\rm sys}$ and canonical three-coordinates $\vec{z}_s=\epsilon_s(\vec{\tilde{x}}_s-(\vec{p}_s/p_s^0)\tilde{x}^0)$, $\vec{k}_s=\vec{p}_s/\epsilon_s$. The position $\vec{q}_s=\vec{z}_s/\epsilon_s$ is the classical analog of the Newton–Wigner three-position operator[16] and shares the reduced covariance under the Euclidean subgroup of the Poincaré group. The unit timelike four-vector $u^\mu(p_s)=p_s^\mu/\epsilon_s$ is orthogonal to the Wigner hyperplanes and describes their orientation in the chosen inertial frame. Note that the noncovariant canonical $\tilde{x}_s^\mu(\tau)$ should not be confused with the four-vector $x_s^\mu(\tau)=z^\mu(\tau,\vec{\sigma}=0)$ identifying the origin of the three-coordinates $\vec{\sigma}$ inside the Wigner hyperplanes. The worldline $x_s^\mu(\tau)$ is arbitrary since it depends on $x_s^\mu(0)$, while its four-velocity $\dot{x}_s^\mu(\tau)$ depends on the Dirac multipliers associated with the four first class constraints (see the following). This worldline may be considered as an arbitrary *centroid* for the isolated system.

(ii) The particle canonical variables $\vec{\eta}_i(\tau)$, $\vec{\kappa}_i(\tau)$ *inside* the Wigner hyperplanes. They are restricted by the three first class constraints (the *rest-frame conditions*) $\vec{\kappa}_+=\Sigma_{i=1}^N\vec{\kappa}_i\approx 0$. They are Wigner spin-one three-vectors, like the coordinates $\vec{\sigma}$.

Let us stress that *our approach leads to a doubling of the usual concepts.*

(1) The concepts defined according to the *external* viewpoint of an arbitrary inertial Lorentz observer, describing the Wigner hyperplanes as leaves of a foliation of Minkowski space–time and determined by the timelike configurations of the isolated system. A Lorentz transformation rotates the Wigner hyperplanes and induces a Wigner rotation of the three-vectors inside each Wigner hyperplane. Each such hyperplane inherits an induced *internal Euclidean structure* while the *external* realization of the Poincaré group induces an *internal* unfaithful Euclidean action (the internal translations are generated by the first class constraints $\vec{\kappa}_+ \approx 0$, so that they are eliminable gauge variables).

As stated previously, an arbitrary worldline, the *centroid* $x_s^\mu(\tau)$, is chosen as origin of the *internal* three-coordinates on the Wigner hyperplanes; its velocity $\dot{x}_s^\mu(\tau)$ is determined only after the introduction of four gauge fixings for the four first class constraints (one of them is $T_s - \tau \approx 0$).

Then, three *external* concepts of four-center of mass can be defined (each having an *internal* three-location inside the Wigner hyperplanes) starting from the kinematics of the Wigner hyperplanes and from known concepts of three-centers of mass.[15]

(a) The *external* noncovariant canonical *four-center of mass* $\tilde{x}_s^\mu$ (with three-location $\vec{\tilde{\sigma}}$), extension of the *canonical three-position vector* $\vec{q}_s$ (also named *center of spin*[19]). $\vec{q}_s$ is the classical analog of the Newton–Wigner position operator[16] (Foldy–Wouthuysen mean position operator[22] for Dirac equation). $\tilde{x}_s^\mu$ is not a four-vector ($\vec{q}_s$ does not satisfy the *world line condition*[15]), but it is canonical: $\{\tilde{x}_s^\mu, \tilde{x}_s^\nu\} = 0$.

(b) The *external* noncovariant and noncanonical Møller *four-center of energy* R_s^μ (with three-location $\vec{\sigma}_R$), extension of the Møller three-center of mass $\vec{R}_s$,[17] which corresponds to the standard nonrelativistic definition of center of mass of a system of particles with masses replaced by energies. $\vec{R}_s$ does not satisfy the world line condition, so that R_s^μ is not a four-vector and moreover it satisfies $\{R_s^\mu, R_s^\nu\} \neq 0$.

(c) The *external* noncanonical but covariant Fokker–Pryce *four-center of inertia* Y_s^μ (with three-location $\vec{\sigma}_Y$), extension of the Fokker–Pryce three-center of inertia.[18,19] Y_s^μ is a four-vector by construction: it is the Lorentz transform of the rest-frame pseudo-worldline $R_s^{(\mathrm{rest})\,\mu}$ of the Møller center of energy to an arbitrary frame. It holds $\{Y_s^\mu, Y_s^\nu\} \neq 0$.

Note that while the Fokker–Pryce Y_s^μ is the only four-vector by construction, only $\tilde{x}_s^\mu(\tau)$ can be an adapted coordinate in a Hamiltonian treatment with Dirac constraints,

(2) The concepts defined according to the *internal* viewpoint associated with the Wigner hyperplanes, corresponding to an unfaithful *internal* realization of the Poincaré algebra: the *internal* three-momentum $\vec{\kappa}_+$ vanishes due to the rest-frame conditions. The *internal* energy and angular momentum are given by the invariant mass M_{sys} and by the spin [angular momentum with respect to $\tilde{x}_s^\mu(\tau)$] of the isolated system, respectively.

In analogy with the external viewpoint, we can define three *internal* three-centers of mass: the *internal* canonical three-center of mass $\vec{q}_+$, the *internal* Møller three-center of energy $\vec{R}_+$, and the *internal* Fokker–Pryce three-center of inertia $\vec{y}_+$. However, due to the rest-frame conditions, they *coincide* ($\vec{q}_+ \approx \vec{R}_+ \approx \vec{y}_+$) and become essentially a unique *gauge* variable conjugate to $\vec{\kappa}_+$. As a natural gauge fixing for the rest-frame conditions $\vec{\kappa}_+ \approx 0$, we can add the vanishing of the *internal* Lorentz boosts: this is equivalent to locating the internal canonical three-center of mass $\vec{q}_+$ in $\vec{\sigma} = 0$, i.e., in the external centroid $x_s^\mu(\tau) = z^\mu(\tau, \vec{0})$ origin of the internal three-coordinates in each Wigner hyperplane. With these gauge fixings and with $T_s - \tau \approx 0$, the world-line $x_s^\mu(\tau)$ of the centroid becomes uniquely determined except for the arbitrariness in the choice of $x_s^\mu(0)$ [$u^\mu(p_s) = p_s^\mu / \epsilon_s$,]

$$x_s^\mu(\tau) = x_s^\mu(0) + u^\mu(p_s) T_s, \tag{1.4}$$

and coincides with the *external* covariant noncanonical Fokker–Pryce four-center of inertia, $x_s^\mu(\tau) = x_s^\mu(0) + Y_s^\mu$.

This doubling of concepts *replaces* the separation of the nonrelativistic three-center of mass due to the Abelian translation symmetry. The nonrelativistic conserved three-momentum is replaced by the *external* $\vec{p}_s = \epsilon_s \vec{k}_s$, while the *internal* three-momentum vanishes, $\vec{\kappa}_+ \approx 0$, as a definition of the rest frame.

In the final gauge we have $\epsilon_s \equiv M_{\rm sys}$, $T_s \equiv \tau$, and the canonical basis $\vec{z}_s$, $\vec{k}_s$, $\vec{\eta}_i$, $\vec{\kappa}_i$ restricted by the three pairs of second class constraints $\vec{\kappa}_+ = \Sigma_{i=1}^N \vec{\kappa}_i \approx 0$, $\vec{q}_+ \approx 0$. Therefore the N particles are described by $6N$ canonical variables like in the nonrelativistic case: 6 $(\vec{z}_s, \vec{k}_s)$ for the external decoupled center of mass and $6(N-1)$ for the relative motions. We still need a canonical transformation $\vec{\eta}_i$, $\vec{\kappa}_i \mapsto \vec{q}_+ [\approx 0]$, $\vec{\kappa}_+ [\approx 0]$, $\vec{\rho}_a$, $\vec{\pi}_a$ $(a = 1,...,N-1)$ in order to identify a set of relative canonical variables. The final $6N$-dimensional canonical basis is $\vec{z}_s$, $\vec{k}_s$, $\vec{\rho}_a$, $\vec{\pi}_a$. In order to get this result we exploit a *highly nonlinear* canonical transformation obtained from the Gartenhaus–Schwartz singular transformation.[23]

In the end, we obtain the Hamiltonian for relative motions as *a sum of N square roots*, each one containing a squared mass and a quadratic form in the relative momenta. Such Hamiltonian goes over its nonrelativistic counterpart in the limit $c \to \infty$. This result has the following implications.

(a) If one tries to make the inverse Legendre transformation to find the associated Lagrangian, it turns out that, due to the presence of square roots, the Lagrangian is a hyperelliptic function of $\dot{\vec{\rho}}_a$ already in the free case. A closed form exists only for $N=2$, $m_1 = m_2 = m$: $L = -\epsilon m \sqrt{4 - \dot{\vec{\rho}}^2}$. This exceptional case already shows that the existence of the limiting velocity c *forbids the traditional linear relation between the spin and the angular velocity*. Moreover, determining the allowed range of the relative velocities is a difficult task (for $N=2$, $m_1 = m_2 = m$, we get $|\dot{\vec{\rho}}| \leq 2c$).

(b) The N quadratic forms in the relative momenta which appear in the relative Hamiltonian *cannot* be diagonalized simultaneously. In any case, the Hamiltonian is a sum of square roots, so that concepts like *reduced masses*, *Jacobi normal relative coordinates*, and *tensor of inertia* cannot be extended to special relativity. This entails that the orientation-shape SO(3) principal bundle of Ref. 1 we would like to exploit can be defined only by using unspecified relative coordinates. Therefore:

(c) The best way of studying rotational kinematics is based on the *canonical spin bases* of Ref. 2 with their *spin frames* and *dynamical body frames*. The important point is that *such frames can be constructed in the same way as in the nonrelativistic case starting from the canonical basis* $\vec{\rho}_a$, $\vec{\pi}_a$.

Finally, once this program has been fulfilled in the free case, the introduction of mutual action-at-a-distance interactions among the particles can be done without extra complications.

The paper is organized as follows. In Sec. II we review the rest-frame instant form on the Wigner hyperplane of N positive energy free scalar particles. In Sec. III we discuss the *internal* realization of the Poincaré algebra and define the *internal center-of-mass* concepts. In Sec. IV we discuss the *external* realization of the Poincaré algebra and define the *external center-of-mass* concepts. In Sec. V we construct the relative canonical variables associated with the canonical *internal* center of mass. In Sec. VI we analyze the relativistic rotational kinematics of relative motions inside the Wigner hyperplane using the Hamiltonian methods for the construction of the spin bases introduced in Ref. 2. Some final comments on open problems are given in Sec. IV.

Appendix A contains a review of parametrized Minkowski theories. The results of Sec. V are extended to spinning particles in Appendix B.

Glossary of symbols: $z^\mu(\tau, \vec{\sigma}) = x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\, \sigma^r$—embedding of a Wigner hyperplane in M^4 $(u^\mu(p_s) = p_s^\mu / \sqrt{\epsilon\, p_s^2})$; $x_s^\mu(\tau)$—arbitrary four-vector (centroid), chosen as origin of the *internal* three-coordinates $\vec{\sigma}$; $x_i^\mu(\tau) = x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\, \eta_i^r(\tau)$—world line of particle i, with *internal* three-position $\vec{\eta}_i(\tau)$ and three-momentum $\vec{\kappa}_i(\tau)$; $\tilde{x}_s^\mu(\tau) = (\tilde{x}_s^0; \vec{q}_s + \tilde{x}_s^0 \vec{p}_s / p_s^0) = x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\, \tilde{\sigma}^r$—*external* canonical noncovariant four- and three-center of mass; $R_s^\mu(\tau) = (\tilde{x}_s^0; \vec{R}_s) = x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\, \sigma_R^r$—*external* noncanonical noncovariant Møller four- and three-

center of energy; $Y^\mu_s(\tau)=(\tilde{x}^0_s;\vec{Y}_s)=x^\mu_s(\tau)+\epsilon^\mu_r(u(p_s))\,\sigma^r_Y$—*external* noncanonical covariant Fokker–Pryce four- and three-center of inertia; $T_s=u(p_s))\cdot x_s=u(p_s)\cdot\tilde{x}_s=u(p_s)\cdot Y_s=u(p_s)\cdot R_s$—rest frame time; $\vec{\kappa}_+=\Sigma_i\,\vec{\kappa}_i\approx 0$—rest frame conditions; $\vec{q}_+$, $\vec{R}_+$, $\vec{y}_+$—*internal* canonical three-center of mass, Møller three-center of energy, Fokker–Pryce three-center of inertia; $\vec{q}_+\approx\vec{R}_+\approx\vec{y}_+$ due to $\vec{\kappa}_+\approx 0$; and $\vec{q}_+\approx 0$ implies $x^\mu_s(\tau)=x^\mu_s(0)+Y^\mu_s(\tau)$.

II. THE REST-FRAME INSTANT FORM OF *N* FREE SCALAR RELATIVISTIC PARTICLES

Let us consider a system of N free scalar positive-energy particles in the framework of parametrized Minkowski theory (see Appendix A).

The configuration variables are a three-vector $\vec{\eta}_i(\tau)$ for each particle $[x^\mu_i(\tau)=z^\mu(\tau,\vec{\eta}_i(\tau))]$.[9,24] The sign of the energy must be chosen for each particle, because there is no mass-shell constraint (like $\epsilon p_i^2-m_i^2\approx 0$) at our disposal (there are only three degrees of freedom for particle, determined by the intersection of a timelike trajectory and of the spacelike hypersurface Σ_τ). For each choice of the sign of the energy of the N particles, we describe only one of the 2^N branches of the mass spectrum of the manifestly covariant approach based on the coordinates $x^\mu_i(\tau)$, $p^\mu_i(\tau)$, $i=1,...,N$, and on the constraints $\epsilon p_i^2-m_i^2\approx 0$ (in the free case). In this way, we get a description of relativistic particles with a given sign of the energy with consistent couplings to fields.[25–27]

The system of N free scalar and positive energy particles is described by the action[9,24,26]

$$S=\int \mathrm{d}\tau\,\mathrm{d}^3\sigma\,\mathcal{L}(\tau,\vec{\sigma})=\int \mathrm{d}\tau\,L(\tau),$$

$$\mathcal{L}(\tau,\vec{\sigma})=-\sum_{i=1}^N\,\delta^3(\vec{\sigma}-\vec{\eta}_i(\tau))m_i\sqrt{g_{\tau\tau}(\tau,\vec{\sigma})+2g_{\tau\check{r}}(\tau,\vec{\sigma})\,\dot{\eta}^{\check{r}}_i(\tau)+g_{\check{r}\check{s}}(\tau,\vec{\sigma})\,\dot{\eta}^{\check{r}}_i(\tau)\,\dot{\eta}^{\check{s}}_i(\tau)},$$

$$L(\tau)=-\sum_{i=1}^N\,m_i\sqrt{g_{\tau\tau}(\tau,\vec{\eta}_i(\tau))+2g_{\tau\check{r}}(\tau,\vec{\eta}_i(\tau))\,\dot{\eta}^{\check{r}}_i(\tau)+g_{\check{r}\check{s}}(\tau,\vec{\eta}_i(\tau))\,\dot{\eta}^{\check{r}}_i(\tau)\,\dot{\eta}^{\check{s}}_i(\tau)},\tag{2.1}$$

where the configuration variables are $z^\mu(\tau,\vec{\sigma})$ and $\vec{\eta}_i(\tau)$, $i=1,...,N$. The action is invariant under separate τ- and $\vec{\sigma}$-reparametrizations.

The canonical momenta are

$$\rho_\mu(\tau,\vec{\sigma})=-\frac{\partial\mathcal{L}(\tau,\vec{\sigma})}{\partial z^\mu_\tau(\tau,\vec{\sigma})}=\sum_{i=1}^N\,\delta^3(\vec{\sigma}-\vec{\eta}_i(\tau))m_i$$
$$\times\frac{z_{\tau\mu}(\tau,\vec{\sigma})+z_{\check{r}\mu}(\tau,\vec{\sigma})\,\dot{\eta}^{\check{r}}_i(\tau)}{\sqrt{g_{\tau\tau}(\tau,\vec{\sigma})+2g_{\tau\check{r}}(\tau,\vec{\sigma})\,\dot{\eta}^{\check{r}}_i(\tau)+g_{\check{r}\check{s}}(\tau,\vec{\sigma})\,\dot{\eta}^{\check{r}}_i(\tau)\,\dot{\eta}^{\check{s}}_i(\tau)}}$$
$$=[(\rho_\nu l^\nu)l_\mu+(\rho_\nu z^\nu_{\check{r}})\gamma^{\check{r}\check{s}}z_{\check{s}\mu}](\tau,\vec{\sigma}),$$

$$\kappa_{i\check{r}}(\tau)=-\frac{\partial L(\tau)}{\partial\dot{\eta}^{\check{r}}_i(\tau)}=m_i\frac{g_{\tau\check{r}}(\tau,\vec{\eta}_i(\tau))+g_{\check{r}\check{s}}(\tau,\vec{\eta}_i(\tau))\,\dot{\eta}^{\check{s}}_i(\tau)}{\sqrt{g_{\tau\tau}(\tau,\vec{\eta}_i(\tau))+2g_{\tau\check{r}}(\tau,\vec{\eta}_i(\tau))\,\dot{\eta}^{\check{r}}_i(\tau)+g_{\check{r}\check{s}}(\tau,\vec{\eta}_i(\tau))\,\dot{\eta}^{\check{r}}_i(\tau)\,\dot{\eta}^{\check{s}}_i(\tau)}},$$

$$\{z^\mu(\tau,\vec{\sigma}),\rho_\nu(\tau,\vec{\sigma}')\}=-\eta^\mu_\nu\delta^3(\vec{\sigma}-\vec{\sigma}'),\tag{2.2}$$

$$\{\eta^{\check{r}}_i(\tau),\kappa_{j\check{s}}(\tau)\}=-\delta_{ij}\delta^{\check{r}}_{\check{s}}.$$

The canonical Hamiltonian H_c is zero, the Dirac Hamiltonian is given by Eq. (A9) [there are no other system-dependent primary constraints] and Eq. (A8) becomes

$$\mathcal{H}_\mu(\tau,\vec{\sigma})=\rho_\mu(\tau,\vec{\sigma})-l_\mu(\tau,\vec{\sigma})\sum_{i=1}^{N}\delta^3(\vec{\sigma}-\vec{\eta}_i(\tau))\sqrt{m_i^2-\gamma^{\check{r}\check{s}}(\tau,\vec{\sigma})\kappa_{i\check{r}}(\tau)\kappa_{i\check{s}}(\tau)}$$

$$-z_{\check{r}\mu}(\tau,\vec{\sigma})\gamma^{\check{r}\check{s}}(\tau,\vec{\sigma})\sum_{i=1}^{N}\delta^3(\vec{\sigma}-\vec{\eta}_i(\tau))\kappa_{i\check{s}}\approx 0. \tag{2.3}$$

The conserved Poincaré generators are

$$p_s^\mu=\int \mathrm{d}^3\sigma\rho^\mu(\tau,\vec{\sigma}),$$

$$J_s^{\mu\nu}=\int \mathrm{d}^3\sigma[z^\mu(\tau,\vec{\sigma})\rho^\nu(\tau,\vec{\sigma})-z^\nu(\tau,\vec{\sigma})\rho^\mu(\tau,\vec{\sigma})]. \tag{2.4}$$

After the restriction to spacelike hyperplanes, the Dirac Hamiltonian is reduced to Eq. (A13) with the surviving ten constraints given by

$$\tilde{\mathcal{H}}^\mu(\tau)=\int \mathrm{d}^3\sigma\mathcal{H}^\mu(\tau,\vec{\sigma})=p_s^\mu-l^\mu\sum_{i=1}^{N}\sqrt{m_i^2+\vec{\kappa}_i^2(\tau)}+b_{\check{r}}^\mu(\tau)\sum_{i=1}^{N}\kappa_{i\check{r}}(\tau)\approx 0,$$

$$\tilde{\mathcal{H}}^{\mu\nu}(\tau)=b_{\check{r}}^\mu(\tau)\int \mathrm{d}^3\sigma\sigma^{\check{r}}\mathcal{H}^\nu(\tau,\vec{\sigma})-b_{\check{r}}^\nu(\tau)\int \mathrm{d}^3\sigma\sigma^{\check{r}}\mathcal{H}^\mu(\tau,\vec{\sigma})=S_s^{\mu\nu}(\tau)-[b_{\check{r}}^\mu(\tau)b_\tau^\nu$$

$$-b_{\check{r}}^\nu(\tau)b_\tau^\mu]\sum_{i=1}^{N}\eta_i^{\check{r}}(\tau)\sqrt{m_i^2+\vec{\kappa}_i^2(\tau)}-[b_{\check{r}}^\mu(\tau)b_{\check{s}}^\nu(\tau)-b_{\check{r}}^\nu(\tau)b_{\check{s}}^\mu(\tau)]\sum_{i=1}^{N}\eta_i^{\check{r}}(\tau)\kappa_i^{\check{s}}(\tau)\approx 0. \tag{2.5}$$

Here $S_s^{\mu\nu}$ is the spin part of the Lorentz generators

$$J_s^{\mu\nu}=x_s^\mu p_s^\nu-x_s^\nu p_s^\mu+S_s^{\mu\nu},$$

$$S_s^{\mu\nu}=b_{\check{r}}^\mu(\tau)\int \mathrm{d}^3\sigma\ \sigma^{\check{r}}\rho^\nu(\tau,\vec{\sigma})-b_{\check{r}}^\nu(\tau)\int \mathrm{d}^3\sigma\ \sigma^{\check{r}}\rho^\mu(\tau,\vec{\sigma}). \tag{2.6}$$

On the Wigner hyperplane, we obtain the following constraints and Dirac Hamiltonian:[9,26]

$$\tilde{\mathcal{H}}^\mu(\tau)=p_s^\mu-u^\mu(p_s)\sum_{i=1}^{N}\sqrt{m_i^2+\vec{\kappa}_i^2}+\epsilon_r^\mu(u(p_s))\sum_{i=1}^{N}\kappa_{ir}$$

$$=u^\mu(p_s)\left[\epsilon_s-\sum_{i=1}^{N}\sqrt{m_i^2+\vec{\kappa}_i^2}\right]+\epsilon_r^\mu(u(p_s))\sum_{i=1}^{N}\kappa_{ir}\approx 0,$$

or

$$\epsilon_s-M_{\mathrm{sys}}\approx 0,\quad M_{\mathrm{sys}}=\sum_{i=1}^{N}\sqrt{m_i^2+\vec{\kappa}_i^2},$$

$$\vec{p}_{\mathrm{sys}}=\vec{\kappa}_+=\sum_{i=1}^{N}\vec{\kappa}_i\approx 0,$$

$$H_D=\lambda^\mu(\tau)\tilde{\mathcal{H}}_\mu(\tau)=\lambda(\tau)[\epsilon_s-M_{\rm sys}]-\vec{\lambda}(\tau)\sum_{i=1}^N \vec{\kappa}_i,$$

$$\lambda(\tau)\approx-\dot{x}_{s\mu}(\tau)u^\mu(p_s),$$

$$\lambda_r(\tau)\approx-\dot{x}_{s\mu}(\tau)\epsilon^\mu_r(u(p_s)),\quad \dot{\tilde{x}}^\mu_s(\tau)=-\lambda(\tau)u^\mu(p_s),$$

$$\dot{x}^\mu_s(\tau)\approx-\tilde{\lambda}^\mu(\tau)=-\lambda(\tau)u^\mu(p_s)+\epsilon^\mu_r(u(p_s))\lambda_r(\tau). \tag{2.7}$$

While the Dirac multiplier $\lambda(\tau)$ is determined by the gauge fixing $T_s-\tau\approx0$, the three Dirac's multipliers $\vec{\lambda}(\tau)$ describe the *classical zitterbewegung* of the centroid $x^\mu_s(\tau)$ which is the origin of the three-coordinates on the Wigner hyperplane: each gauge-fixing $\vec{\chi}(\tau)\approx0$ to the three first class constraints $\vec{\kappa}_+\approx0$ (defining the *internal rest-frame*) gives a different determination of the multipliers $\vec{\lambda}(\tau)$ and therefore identifies a different world-line $x^{(\vec{\chi})\mu}_s(\tau)$ for the covariant non-canonical centroid.

The embedding describing Wigner hyperplanes is $z^\mu(\tau,\vec{\sigma})=x^\mu_s(\tau)+\epsilon^\mu_r(u(p_s))\sigma^r$, with the $\epsilon^\mu_r(u(p_s))$ defined in Eqs. (A24).

The various spin tensors and vectors are[9]

$$J^{\mu\nu}_s=x^\mu_s p^\nu_s-x^\nu_s p^\mu_s+S^{\mu\nu}_s=\tilde{x}^\mu_s p^\nu_s-\tilde{x}^\nu_s p^\mu_s+\tilde{S}^{\mu\nu}_s,$$

$$\begin{aligned}S^{\mu\nu}_s&=[u^\mu(p_s)\epsilon^\nu(u(p_s))-u^\nu(p_s)\epsilon^\mu(u(p_s))]\overline{S}^{\tau r}_s+\epsilon^\mu(u(p_s))\epsilon^\nu(u(p_s))\overline{S}^{rs}_s\\&\equiv[\epsilon^\mu_r(u(p_s))u^\nu(p_s)-\epsilon^\nu(u(p_s))u^\mu(p_s)]\sum_{i=1}^N \eta^r_i\sqrt{m^2_ic^2+\vec{\kappa}^2_i}\\&\quad+[\epsilon^\mu_r(u(p_s))\epsilon^\nu_s(u(p_s))-\epsilon^\nu_r(u(p_s))\epsilon^\mu_r(u(p_s))]\sum_{i=1}^N \eta^r_i\kappa^s_i,\end{aligned}$$

$$\overline{S}^{AB}_s=\epsilon^A_\mu(u(p_s))\epsilon^B_\nu(u(p_s))S^{\mu\nu}_s, \tag{2.8}$$

$$\overline{S}^{rs}_s\equiv\sum_{i=1}^N(\eta^r_i\kappa^s_i-\eta^s_i\kappa^r_i),\quad \overline{S}^{\tau r}_s\equiv-\sum_{i=1}^N\eta^r_i\sqrt{m^2_ic^2+\vec{\kappa}^2_i},$$

$$\tilde{S}^{\mu\nu}_s=S^{\mu\nu}_s+\frac{1}{\sqrt{\epsilon p^2_s}(p^0_s+\sqrt{\epsilon p^2_s})}[p_{s\beta}(S^{\beta\mu}_s p^\nu_s-S^{\beta\nu}_s p^\mu_s)+\sqrt{p^2_s}(S^{0\mu}_s p^\nu_s-S^{0\nu}_s p^\mu_s)],$$

$$\tilde{S}^{ij}_s=\delta^{ir}\delta^{js}\overline{S}^{rs}_s,\quad \tilde{S}^{0i}_s=-\frac{\delta^{ir}\overline{S}^{rs}_s p^s_s}{p^0_s+\sqrt{\epsilon p^2_s}},$$

$$\vec{\tilde{S}}\equiv\vec{\tilde{S}}=\sum_{i+1}^N\vec{\eta}_i\times\vec{\kappa}_i\approx\sum_{i=1}^N\vec{\eta}_i\times\vec{\kappa}_i-\vec{\eta}_+\times\vec{\kappa}_+=\sum_{a=1}^{N-1}\vec{\rho}_a\times\vec{\pi}_a.$$

Note that while $L^{\mu\nu}_s=x^\mu_s p^\nu_s-x^\nu_s p^\mu_s$ and $S^{\mu\nu}_s$ are not constants of the motion due to the *classical zitterbewegung*, both $\tilde{L}^{\mu\nu}_s=\tilde{x}^\mu_s p^\nu_s-\tilde{x}^\nu_s p^\mu_s$ and $\tilde{S}^{\mu\nu}_s$ are conserved.

The only remaining canonical variables describing the Wigner hyperplane in the final Dirac brackets are the noncovariant canonical coordinates $\tilde{x}^\mu_s(\tau)$ and p^μ_s. The point with coordinates $\tilde{x}^\mu_s(\tau)$ is the decoupled canonical *external four-center of mass*, playing the role of a kinematical

external four-center of mass and of a decoupled observer with his parametrized clock (*point particle clock*). Its velocity $\dot{\tilde{x}}^\mu_s(\tau)$ is parallel to p^μ_s, so that it has no *classical zitterbewegung*. The connection between the centroid $x^\mu_s(\tau)$ and $\tilde{x}^\mu_s(\tau)$ is given in Eq. (4.1).

After the separation of the relativistic canonical noncovariant *external* four-center of mass $\tilde{x}^\mu_s(\tau)$, on the Wigner hyperplane the N particles are described by the $6N$ Wigner spin-one-three-vectors $\vec{\eta}_i(\tau)$, $\vec{\kappa}_i(\tau)$ restricted by the rest-frame condition $\vec{\kappa}_+ = \Sigma_{i=1}^N \vec{\kappa}_i \approx 0$.

The canonical variables $\tilde{x}^\mu_s$, p^μ_s for the *external* four-center of mass may be replaced by the canonical pairs[28]

$$T_s = \frac{p_s \cdot \tilde{x}_s}{\epsilon_s} = \frac{p_s \cdot x_s}{\epsilon_s}, \quad \epsilon_s = \pm\sqrt{\epsilon p_s^2},$$
$$\vec{z}_s = \epsilon_s \left(\vec{\tilde{x}}_s - \frac{\vec{p}_s}{p^0_s} \tilde{x}^0_s \right), \quad \vec{k}_s = \frac{\vec{p}_s}{\epsilon_s}, \tag{2.9}$$

with the inverse transformation

$$\tilde{x}^0_s = \sqrt{1+\vec{k}_s^2} \left(T_s + \frac{\vec{k}_s \cdot \vec{z}_s}{\epsilon_s} \right), \quad p^0_s = \epsilon_s \sqrt{1+\vec{k}_s^2},$$
$$\vec{\tilde{x}}_s = \frac{\vec{z}_s}{\epsilon_s} + \left(T_s + \frac{\vec{k}_s \cdot \vec{z}_s}{\epsilon_s} \right) \vec{k}_s, \quad \vec{p}_s = \epsilon_s \vec{k}_s . \tag{2.10}$$

This nonpoint canonical transformation in the rest-frame instant form can be summarized as $[\epsilon_s - M_{\rm sys} \approx 0,\ \vec{\kappa}_+ = \Sigma_{i=1}^N \vec{\kappa}_i \approx 0]$

$$\left| \begin{array}{c|c|c} \tilde{x}^\mu_s & \vec{\eta}_i \\ \hline p^\mu_s & \vec{\kappa}_i \end{array} \right| \longrightarrow \left| \begin{array}{c|c|c} \epsilon_s & \vec{z}_s & \vec{\eta}_i \\ \hline T_s & \vec{k}_s & \vec{\kappa}_i \end{array} \right| \quad . \tag{2.11}$$

The invariant mass $M_{\rm sys}$ of the system, which is also its *internal* energy, replaces the nonrelativistic Hamiltonian $H_{\rm rel}$ for the relative degrees of freedom, after the addition of the gauge-fixing $T_s - \tau \approx 0$.[29] This recalls the frozen Hamilton–Jacobi theory, in which the time evolution can be reintroduced by using the energy generator of the Poincaré group as Hamiltonian (see Refs. 30 for a different derivation of this result).

After the gauge fixings $T_s - \tau \approx 0$, the final Hamiltonian and the embedding of the Wigner hyperplane into Minkowski space–time become

$$H_D = M_{\rm sys} - \vec{\lambda}(\tau) \cdot \vec{\kappa}_+ ,$$
$$z^\mu(\tau, \vec{\sigma}) = x^\mu_s(\tau) + \epsilon^\mu_r(u(p_s))\sigma^r = x^\mu_s(0) + u^\mu(p_s)\tau + \epsilon^\mu_r(u(p_s))\sigma^r,$$

with

$$\dot{x}^\mu_s(\tau) = \frac{\overset{\circ}{\mathrm{d}} x^\mu_s(\tau)}{\mathrm{d}\tau} + \{x^\mu_s(\tau), H_D\} = u^\mu(p_s) + \epsilon^\mu_r(u(p_s))\lambda_r(\tau), \tag{2.12}$$

where $x^\mu_s(0)$ is an arbitrary point and $\epsilon^\mu_r(u(p_s)) = L^\mu{}_r(p_s, \mathring{p}_s)$. This equation visualizes the role of the Dirac multipliers as sources of the *classical zitterbewegung* and consequently the *gauge nature* of the latter. Let us remark that the constant $x^\mu_s(0)$ [and $\tilde{x}^\mu_s(0)$] is arbitrary, reflecting the arbitrariness in the absolute location of the origin of the *internal* coordinates on each hyperplane in Minkowski space–time.

The particles' world lines in Minkowski space–time and the associated momenta are then

$$\begin{aligned} &{}^{\mu}_{i}(\tau)=z^{\mu}(\tau,\vec{\eta}_i(\tau))=x^{\mu}_{s}(\tau)+\epsilon^{\mu}_{r}(u(p_s))\,\eta^{r}_{i}(\tau),\\ &p^{\mu}_{i}(\tau)=\sqrt{m^2_i+\vec{\kappa}^2_i(\tau)}\,u^{\mu}(p_s)+\epsilon^{\mu}_{r}(u(p_s))\,\kappa_{ir}(\tau)\Rightarrow \epsilon p^2_i=m^2_i\,. \end{aligned} \tag{2.13}$$

Inside the Wigner hyperplane three degrees of freedom of the isolated system, describing an *internal* center-of-mass three-variable $\vec{\sigma}_{\rm com}$ conjugate to $\vec{\kappa}_+$ (when the $\vec{\sigma}_{\rm com}$ are canonical variables they are denoted $\vec{q}_+$), are *gauge* variables. The natural gauge fixing in order to eliminate the three first class constraints $\vec{\kappa}_+\approx 0$ is $\vec{\chi}=\vec{q}_+\approx 0$, which implies $\lambda_r(\tau)=0$: in this way the *internal* three-center of mass gets located in the centroid $x^{\mu}_s(\tau)=z^{\mu}(\tau,\vec{\sigma}=0)$ of the Wigner hyperplane. The determination of $\vec{q}_+$ for the N particle system will be carried through by the group theoretical methods of Ref. 31 in the next section.[32–34]

It turns out that the Wigner hyperplane is the natural setting for the study of the Dixon multipoles of extended relativistic systems[35] (Dixon's multipoles for the N-body problem are studied in Ref. 36) and the definition of their canonical relative variables with respect to the center of mass. Note, incidentally, that the Euclidean metric structure of the Wigner hyperplane offers a natural solution to the problem of boost for lattice gauge theories and explicitly realizes the Machian view of dynamics according to which only relative motions are relevant.

The *external* rest-frame instant form realization of the Poincaré generators[37] with nonfixed invariants $\epsilon p^2_s=\epsilon^2_s\approx M^2_{\rm sys}$ and $W^2=-\epsilon p^2_s\vec{\bar{S}}^2_s\approx -\epsilon M^2_{\rm sys}\vec{\bar{S}}^2$, is obtained from Eq. (2.8):

$$\begin{aligned} &p^{\mu}_s\,,\quad J^{\mu\nu}_s=\tilde{x}^{\mu}_s p^{\nu}_s-\tilde{x}^{\nu}_s p^{\mu}_s+\tilde{S}^{\mu\nu}_s\,,\\ &p^0_s=\sqrt{\epsilon^2_s+\vec{p}^2_s}=\epsilon_s\sqrt{1+\vec{k}^2_s}\approx\sqrt{M^2_{\rm sys}+\vec{p}^2_s}=M_{\rm sys}\sqrt{1+\vec{k}^2_s},\\ &\vec{p}_s=\epsilon_s\vec{k}_s\approx M_{\rm sys}\vec{k}_s\,,\\ &J^{ij}_s=\tilde{x}^i_s p^j_s-\tilde{x}^j_s p^i_s+\delta^{ir}\delta^{js}\sum_{i=1}^{N}\,(\eta^r_i\kappa^s_i-\eta^s_i\kappa^r_i)=z^i_s k^j_s-z^j_s k^i_s+\delta^{ir}\delta^{js}\epsilon^{rsu}\bar{S}^u_s\,, \end{aligned} \tag{2.14}$$

$$\begin{aligned} K^i_s=J^{0i}_s=\tilde{x}^0_s p^i_s-\tilde{x}^i_s\sqrt{\epsilon^2_s+\vec{p}^2_s}-\frac{1}{\epsilon_s+\sqrt{\epsilon^2_s+\vec{p}^2_s}}\,\delta^{ir}p^s_s\sum_{i=1}^{N}\,(\eta^r_i\kappa^s_i-\eta^s_i\kappa^r_i)=-\sqrt{1+\vec{k}^2_s}\,z^i_s-\frac{\delta^{ir}k^s_s\epsilon^{rsu}\bar{S}^u_s}{1+\sqrt{1+\vec{k}^2_s}}\\ \approx\tilde{x}^0_s p^i_s-\tilde{x}^i_s\sqrt{M^2_{\rm sys}+\vec{p}^2_s}-\frac{\delta^{ir}p^s_s\epsilon^{rsu}\bar{S}^u_s}{M_{\rm sys}+\sqrt{M^2_{\rm sys}+\vec{p}^2_s}}\,. \end{aligned}$$

On the other hand, the *internal* realization of the Poincaré algebra is built inside the Wigner hyperplane by using the expression of $\bar{S}^{AB}_s$ given by Eq. (2.8)

$$\begin{aligned} &M_{\rm sys}=H_M=\sum_{i=1}^{N}\,\sqrt{m^2_i+\vec{\kappa}^2_i},\\ &\vec{\kappa}_+=\sum_{i=1}^{N}\,\vec{\kappa}_i(\approx 0),\\ &\vec{J}=\sum_{i=1}^{N}\,\vec{\eta}_i\times\vec{\kappa}_i\,,\quad J^r=\bar{S}^r=\frac{1}{2}\,\epsilon^{ruv}\bar{S}^{uv}\equiv\bar{S}^r_s\,,\\ &\vec{K}=-\sum_{i=1}^{N}\,\sqrt{m^2_i+\vec{\kappa}^2_i}\,\vec{\eta}_i\,,\quad K^r=J^{0r}=\bar{S}^{\tau r}_s\,, \end{aligned}$$

$$\Pi = M_{\rm sys}^2 - \vec{\kappa}_+^2 \approx M_{\rm sys}^2 > 0, \quad W^2 = -\epsilon (M_{\rm sys}^2 - \vec{\kappa}_+^2)\vec{S}_s^2 \approx -\epsilon M_{\rm sys}^2 \vec{S}_s^2 . \tag{2.15}$$

The meaning of the constraints $\epsilon_s - M_{\rm sys} \approx 0$, $\vec{\kappa}_+ \approx 0$ is the following.

(i) The constraint $\epsilon_s - M_{\rm sys} \approx 0$ is the bridge connecting the *external* and *internal* realizations. The external spin coincides with the internal angular momentum due to Eq. (A16).

(ii) The constraints $\vec{\kappa}_+ \approx 0$, together with $\vec{K} \approx 0$, leads to an unfaithful *internal* realization in which the only non-null generators are the conserved energy and the spin of the isolated system. As we shall see in the next section, $\vec{K} \approx 0$ is implied by the natural gauge fixing $\vec{q}_+ \approx 0$: this makes the internal realization even more unfaithful.

For isolated systems the constraint manifold[38] is a stratified manifold with each stratum corresponding to a type of Poincaré orbit. The main stratum (dense in the constraint manifold) corresponds to all configurations of the isolated system belonging to timelike Poincaré orbits with $\epsilon p_s^2 \approx \epsilon M_{\rm sys}^2 > 0$. As said in Ref. 39, this implies that the center-of-mass coordinates have been adapted to the co-adjoint orbits of the Poincaré group. But, since the second Poincaré invariant (the Pauli–Lubanski invariant $\vec{W}_s^2 = -p_s^2 \vec{S}_s^2$) does not appear among the canonical variables, this canonical basis is not adapted, as yet, to a typical form of canonical action of the Poincaré group[31] on the phase space of the isolated system. As shown in Ref. 39, it possible to construct a canonical basis including both Poincaré invariants in such a way that all of the coordinates are adapted to the co-adjoint action of the group and the new relative variables are thereby adapted to the SO(3) group.

Let us now make here a first simplified attempt to construct the relative variables: the complete solution is in Sec. V. In Ref. 9 a naive *internal* center-of-mass variable $\vec{\eta}_+ = 1/N \sum_{i=1}^N \vec{\eta}_i$ has been introduced together with the definition of relative variables $\vec{\rho}_a$, $\vec{\pi}_a$ based on the following point canonical transformation:

$$\begin{array}{|c|} \hline \vec{\eta}_i \\ \hline \vec{\kappa}_i \\ \hline \end{array} \longrightarrow \begin{array}{|c|c|} \hline \vec{\eta}_+ & \vec{\rho}_a \\ \hline \vec{\kappa}_+ & \vec{\pi}_a \\ \hline \end{array} \quad , \qquad a = 1,\ldots, N-1$$

$$\vec{\eta}_i = \vec{\eta}_+ + \frac{1}{\sqrt{N}} \sum_{a=1}^{N-1} \gamma_{ai} \vec{\rho}_a , \quad \vec{\kappa}_i = \frac{1}{N} \vec{\kappa}_+ + \sqrt{N} \sum_{a=1}^{N-1} \gamma_{ai} \vec{\pi}_a ,$$

$$\vec{\eta}_+ = \frac{1}{N} \sum_{i=1}^{N} \vec{\eta}_i , \quad \vec{\kappa}_+ = \sum_{i=1}^{N} \vec{\kappa}_i \approx 0,$$

$$\vec{\rho}_a = \sqrt{N} \sum_{i=1}^{N} \gamma_{ai} \vec{\eta}_i , \quad \vec{\pi}_a = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \gamma_{ai} \vec{\kappa}_i ,$$

$$\{\eta_i^r, \kappa_j^s\} = \delta_{ij} \delta^{rs}, \quad \{\eta_+^r, \kappa_+^s\} = \delta^{rs}, \quad \{\rho_a^r, \pi_b^s\} = \delta_{ab} \delta^{rs},$$

$$\sum_{i=1}^{N} \gamma_{ai} = 0, \quad \sum_{a=1}^{N-1} \gamma_{ai} \gamma_{aj} = \delta_{ij} - \frac{1}{N}, \quad \sum_{i=1}^{N} \gamma_{ai} \gamma_{bi} = \delta_{ab} . \tag{2.16}$$

This is a family of canonical transformations depending on $\frac{1}{2}(N-1)(N-2)$ free parameters (the independent parameters in the γ_{ai} of Ref. 6).

In the gauge

$$T_s - \tau \approx 0, \tag{2.17}$$

[which entails $0\approx\dot{T}_s-1=\dot{x}_s\cdot u(p_s)-1=-\lambda(\tau)-1$; after going to Dirac brackets we get $T_s\equiv\tau$ and $\epsilon_s\equiv\pm M_{\rm sys}$], the Hamiltonian and the rest-frame constraints become

$$H_D=M_{\rm sys}-\vec{\lambda}(\tau)\cdot\vec{\kappa}_+,\quad \vec{\kappa}_+\approx 0, \tag{2.18}$$

with the invariant mass given by

$$M_{\rm sys}=H_M=\sum_{i=1}^{N}\sqrt{m_i^2+\vec{\kappa}_i^2}=\sum_{i=1}^{N}\sqrt{m_i^2+\left[\frac{1}{N}\vec{\kappa}_+ +\sqrt{N}\sum_{a=1}^{N-1}\gamma_{ai}\vec{\pi}_a\right]^2}$$
$$\approx\sum_{i=1}^{N}\sqrt{m_i^2+N\sum_{a,b}^{1..N-1}\gamma_{ai}\gamma_{bi}\vec{\pi}_a\cdot\vec{\pi}_b}. \tag{2.19}$$

The centroid, origin of the three-coordinates, results

$$x_s^\mu(T_s)=x_s^\mu(0)+u^\mu(p_s)T_s+\epsilon_r^\mu(u(p_s))\int_0^{T_s}d\tau\,\lambda_r(\tau). \tag{2.20}$$

It can be checked that, if we add the gauge fixings $\vec{\eta}_+\approx 0$ and use Hamilton's equations, their time constancy does not imply $\vec{\lambda}(\tau)=0$. *Therefore* $\vec{\sigma}_{\rm sys}=\vec{\eta}_+$ *is not the searched natural gauge fixing* $\vec{q}_+\approx 0$ *for the separation of the center-of-mass motion.*

In Sec. III we construct the natural canonical *internal* three-center-of-mass variable $\vec{q}_+$ (replacing the naive $\vec{\eta}_+$): its vanishing implies $\vec{\lambda}(\tau)=0$. It will be seen that, unlike in the nonrelativistic theory, $\vec{q}_+$ is not a linear combination of the $\vec{\eta}_i$'s with coefficients depending on the masses, but is connected to the Møller *internal* three-center of energy, with the masses replaced by the particle energies.

III. THE *INTERNAL* RELATIVISTIC CENTER-OF-MASS VARIABLES ON THE WIGNER HYPERPLANE

As we have seen, in the relativistic case of N free scalar particles with positive energy, the Hamiltonian kinetic energy is not a quadratic form in the momenta and the Lagrangian form is unknown. The first problem is to separate the global translations: this is the old problem of the definition of a relativistic center of mass. As already said, the rest-frame instant form of dynamics allows one to clarify the problem by splitting the concept of relativistic center of mass into an *external* one (a pseudo-four-vector) and an *internal* one (a Wigner spin-one-three-vector).

The determination of the *internal* three-center of mass can be achieved using the group theoretical methods of Ref. 31 (see also Ref. 15). Given a canonical realization of the ten Poincaré generators, only three three-position variables are definable in terms of them alone, namely:

(i) a canonical *internal* center of mass (or *center of spin*) $\vec{q}_+$; it is the classical analog[19,20] of the Newton–Wigner position operator;[16]
(ii) a noncanonical *internal* Møller *center of energy* $\vec{R}_+$;[17]
(iii) a noncanonical *internal* Fokker–Pryce *center of inertia* $\vec{y}_+$.[18,19]

We shall see that on Wigner hyperplanes, due to $\vec{\kappa}_+\approx 0$, all of them coincide: $\vec{q}_+\approx\vec{R}_+\approx\vec{y}_+$.

Following Ref. 31 we shall determine $\vec{R}_+$, $\vec{q}_+$, $\vec{y}_+$ starting from the *internal* realization (2.15) of the Poincaré algebra. We get the following Wigner spin-one three-vectors:

(i) The *internal* Møller three-center of energy and the associated spin vector

$$\vec{R}_+ = -\frac{1}{M_{\rm sys}}\vec{K} = \frac{\Sigma_{i=1}^N \sqrt{m_i^2+\vec{\kappa}_i^2}\,\vec{\eta}_i}{\Sigma_{k=1}^N \sqrt{m_k^2+\vec{\kappa}_k^2}},$$

$$\vec{S}_R = \vec{J} - \vec{R}_+ \times \vec{\kappa}_+ ,$$

$$\{R_+^r, \kappa_+^s\} = \delta^{rs}, \quad \{R_+^r, M_{\rm sys}\} = \frac{\kappa_+^r}{M_{\rm sys}}, \quad \{R_+^r, R_+^s\} = -\frac{1}{M_{\rm sys}^2}\epsilon^{rsu} S_R^u , \tag{3.1}$$

$$\{S_R^r, S_R^s\} = \epsilon^{rsu}\left(S_R^u - \frac{1}{M_{\rm sys}^2}\vec{S}_R\cdot\vec{\kappa}_+\,\kappa_+^u \right), \quad \{S_R^r, M_{\rm sys}\} = 0.$$

Note that the gauge fixing $\vec{R}_+ \approx 0$ gives

$$\vec{R}_+ \approx 0 \Rightarrow \mathring{\vec{R}}_+ = \{\vec{R}_+, H_D\} = \frac{\vec{\kappa}_+}{\Sigma_{k=1}^N \sqrt{m_k^2+\vec{\kappa}_k^2}} - \vec{\lambda}(\tau)\frac{\Sigma_{i=1}^N \sqrt{m_i^2+\vec{\kappa}_i^2}}{\Sigma_{k=1}^N \sqrt{m_k^2+\vec{\kappa}_k^2}} \approx -\vec{\lambda}(\tau) \approx 0. \tag{3.2}$$

Furthermore, the *internal* boost generator of Eq. (2.15) may be rewritten as $\vec{K} = -M_{\rm sys}\vec{R}_+$, so that $\vec{R}_+ \approx 0$ implies $\vec{K} \approx 0$.

(ii) The canonical *internal* three-center of mass[41] and the associated spin vector

$$\vec{q}_+ = \vec{R}_+ - \frac{\vec{J}\times\vec{\Omega}}{\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}(M_{\rm sys}+\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2})} = -\frac{\vec{K}}{\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}} + \frac{\vec{J}\times\vec{\kappa}_+}{\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}(M_{\rm sys}+\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2})}$$

$$+ \frac{\vec{K}\cdot\vec{\kappa}_+\,\vec{\kappa}_+}{M_{\rm sys}\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}(M_{\rm sys}+\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2})} \approx \vec{R}_+ \quad \text{for} \quad \vec{\kappa}_+ \approx 0, \quad \{\vec{q}_+, M_{\rm sys}\} = \frac{\vec{\kappa}_+}{M_{\rm sys}},$$

$$\vec{S}_q = \vec{J} - \vec{q}_+\times\vec{\kappa}_+ = \frac{M_{\rm sys}\vec{J}}{\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}} + \frac{\vec{K}\times\vec{\kappa}_+}{\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}} - \frac{\vec{J}\cdot\vec{\kappa}_+\,\vec{\kappa}_+}{\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}(M_{\rm sys}+\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2})} \approx \vec{\vec{S}} = \vec{J},$$

$$\{\vec{S}_q, \vec{\kappa}_+\} = \{\vec{S}_q, \vec{q}_+\} = 0, \quad \{S_q^r, S_q^s\} = \epsilon^{rsu} S_q^u . \tag{3.3}$$

Let us recall that the *scheme A* for the *internal* realization of the Poincaré group[31] contains the canonical pairs $\vec{\kappa}_+$, $\vec{q}_+$, S_q^3, $\mathrm{arctg}\,(S_q^2/S_q^1)$, and the two Casimirs invariants $|\vec{S}_q| = \sqrt{-W^2/M_{\rm sys}^2}$, $M_{\rm sys} = \Sigma_{i=1}^N \sqrt{m_i^2+\vec{\kappa}_i^2}$ [see Eq. (3.4)].

(iii) The *internal* noncanonical Fokker–Pryce center of inertia $\vec{y}_+$,

$$\vec{y}_+ = \vec{q}_+ + \frac{\vec{S}_q\times\vec{\kappa}_+}{\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}(M_{\rm sys}+\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2})} = \vec{R}_+ + \frac{\vec{S}_q\times\vec{\kappa}_+}{M_{\rm sys}\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}},$$

$$\vec{q}_+ = \vec{R}_+ + \frac{\vec{S}_q\times\vec{\kappa}_+}{M_{\rm sys}(M_{\rm sys}+\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2})} = \frac{M_{\rm sys}\vec{R}_+ + \sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}\,\vec{y}_+}{M_{\rm sys}+\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}},$$

$$\{y_+^r, y_+^s\} = \frac{1}{M_{\rm sys}\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}}\epsilon^{rsu}\left[S_q^u + \frac{\vec{S}_q\cdot\vec{\kappa}_+\kappa_+^u}{\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2}(M_{\rm sys}+\sqrt{M_{\rm sys}^2-\vec{\kappa}_+^2})}\right], \tag{3.4}$$

$$\vec{\kappa}_+ \approx 0 \Rightarrow \vec{q}_+ \approx \vec{R}_+ \approx \vec{y}_+ .$$

We see that the gauge fixings $\vec{q}_+ \approx \vec{R}_+ \approx \vec{y}_+ \approx 0$ imply $\vec{\lambda}(\tau) \approx 0$ and force the three *internal* collective variables to coincide with the centroid, origin of the three-coordinates, which now becomes

$$x_s^{(\vec{q}_+)\mu}(T_s) = x_s^\mu(0) + u^\mu(p_s) T_s \,. \tag{3.5}$$

It can also be shown that the *centroid* $x_s^\mu(\tau)$ coincides with the *Dixon center of mass* of an extended object[42] as well as with the *Pirani*[43] and the *Tulczyjew*[44] *centroids* (the Dixon multipoles for the *N*-body problem on the Wigner hyperplane are studied in Ref. 36).

We are left with the construction of a canonical transformation bringing from the basis $\vec{\eta}_i$, $\vec{\kappa}_i$, to a new canonical basis $\vec{q}_+$, $\vec{\kappa}_+ (\approx 0)$, $\vec{\rho}_{q,a}$, $\vec{\pi}_{q,a}$, in which $\vec{S}_q = \Sigma_{a=1}^{N-1} \vec{\rho}_{q,a} \times \vec{\pi}_{q,a}$:

$$\begin{array}{|c|}\hline \vec{\eta}_i \\ \hline \vec{\kappa}_i \\ \hline \end{array} \longrightarrow \begin{array}{|c|c|}\hline \vec{q}_+ & \vec{\rho}_{qa} \\ \hline \vec{\kappa}_+ & \vec{\pi}_{qa} \\ \hline \end{array} \quad . \tag{3.6}$$

Let us stress that this cannot be a point transformation, because of the momentum dependence of the relativistic internal center of mass $\vec{q}_+$, realizing the effective separation of the center of mass from the relative motions in the kinetic energy.

The canonical transformation (3.6) will be constructed in Sec. V by using the method of Gartenhaus–Schwartz[23] as delineated in Ref. 45 (see Refs. 31, 45, and 23 for the $N=2$ case).

In Ref. 46 there is the nonrelativistic limit of the rest-frame Lagrangian. This allows to define the rest-frame nonrelativistic Hamiltonian. These quantities have been used in Ref. 2 [see Eq. (2.1) of Ref. 2] to describe the relative motions in the nonrelativistic rest frame. Note that in the nonrelativistic limit $\vec{q}_+$ tends to the nonrelativistic center of mass

$$\vec{q}_{\rm nr} = \frac{\Sigma_{i=1}^N m_i \vec{\eta}_i}{\Sigma_{i=1}^N m_i} .$$

In conclusion, the nonrelativistic Abelian translation symmetry generating the nonrelativistic Noether constants $\vec{P} = \text{const}$ is split at the relativistic level into the two following symmetries: (i) the *external* Abelian translation symmetry whose Noether constants of motion are $\vec{p}_s = \epsilon_s \vec{k}_s \approx M_{\rm sys} \vec{k}_s = \text{const}$ (its conjugate variable being the *external* three-center of mass $\vec{z}_s$); (ii) the *internal* Abelian gauge symmetry generating the three first class constraints $\vec{\kappa}_+ \approx 0$ (rest-frame conditions) inside the Wigner hyperplane (the conjugate *gauge* variable being the *internal* three-center of mass $\vec{q}_+ \approx \vec{R}_+ \approx \vec{y}_+$). Of course, its nonrelativistic counterpart is the nonrelativistic rest-frame condition $\vec{P} \approx 0$.

IV. THE *EXTERNAL* CENTER-OF-MASS VARIABLES ON THE WIGNER HYPERPLANE

We turn now to the localization of the *external* center-of-mass variables on the Wigner hyperplane. Recall first of all[9] that the *external* canonical noncovariant point of coordinates

$$\tilde{x}_s^\mu(\tau) = (\tilde{x}_s^0(\tau); \vec{\tilde{x}}_s(\tau)) = z^\mu(\tau, \vec{\tilde{\sigma}}) = x_s^\mu(\tau) - \frac{1}{\epsilon_s (p_s^0 + \epsilon_s)} \left[p_{s\nu} S_s^{\nu\mu} + \epsilon_s \left(S_s^{0\mu} - S_s^{0\nu} \frac{p_{s\nu} p_s^\mu}{\epsilon_s^2} \right) \right], \tag{4.1}$$

lies on the Wigner hyperplane $z^\mu(\tau, \vec{\sigma}) = x_s^\mu(\tau) + \epsilon_r^\mu(u(p_s))\sigma^r$ at some three-position $\tilde{\sigma}^r$, just like the centroid, origin of the three-coordinates, $x_s^\mu(\tau) = z^\mu(\tau, \vec{0})$, because $p_s \cdot \tilde{x}_s = p_s \cdot x_s$, see Ref. 9.

As in Eqs. (3.1), (3.3), and (3.4) one can build[31] three *external* three-variables, the canonical $\vec{q}_s$, the Møller $\vec{R}_s$, and the Fokker–Pryce $\vec{Y}_s$ by using the rest-frame realization of the Poincaré algebra given in Eq. (2.14),

$$\vec{R}_s = -\frac{1}{p_s^0}\vec{K}_s = \left(\vec{\tilde{x}}_s - \frac{\vec{p}_s}{p_s^0}\tilde{x}_s^0\right) - \frac{\vec{\bar{S}}_s \times \vec{p}_s}{p_s^0(p_s^0+\epsilon_s)},$$

$$\vec{q}_s = \vec{\tilde{x}}_s - \frac{\vec{p}_s}{p_s^0}\tilde{x}_s^0 = \frac{\vec{z}_s}{\epsilon_s} = \vec{R}_s + \frac{\vec{\bar{S}}_s \times \vec{p}_s}{p_s^0(p_s^0+\epsilon_s)} = \frac{p_s^0 \vec{R}_s + \epsilon_s \vec{Y}_s}{p_s^0+\epsilon_s},$$

$$\vec{Y}_s = \vec{q}_s + \frac{\vec{\bar{S}}_s \times \vec{p}_s}{\epsilon_s(p_s^0+\epsilon_s)} = \vec{R}_s + \frac{\vec{\bar{S}}_s \times \vec{p}_s}{p_s^0 \epsilon_s},$$

$$\{R_s^r, R_s^s\} = -\frac{1}{(p_s^0)^2}\epsilon^{rsu}\Omega_s^u, \quad \vec{\Omega}_s = \vec{J}_s - \vec{R}_s \times \vec{p}_s, \tag{4.2}$$

$$\{q_s^r, q_s^s\} = 0, \quad \{Y_s^r, Y_s^s\} = \frac{1}{\epsilon_s p_s^0}\epsilon^{rsu}\left[\bar{S}_s^u + \frac{\vec{\bar{S}}_s \cdot \vec{p}_s\, p_s^u}{\epsilon_s(p_s^0+\epsilon_s)}\right],$$

$$\vec{p}_s \cdot \vec{q}_s = \vec{p}_s \cdot \vec{R}_s = \vec{p}_s \cdot \vec{Y}_s = \vec{k}_s \cdot \vec{z}_s,$$

$$\vec{p}_s = 0 \Rightarrow \vec{q}_s = \vec{Y}_s = \vec{R}_s.$$

All of these have the same velocity and coincide in the Lorentz rest frame where $\mathring{p}_s^\mu = \epsilon_s(1;\vec{0})$.

We can now construct the following *external* four-vectors on the Wigner hyperplane:

(i) the *external* canonical noncovariant four-center of mass $\tilde{x}_s^\mu$;
(ii) the *external* noncanonical and noncovariant Møller four-center of energy R_s^μ;
(iii) the *external* covariant noncanonical Fokker–Pryce four-center of inertia Y_s^μ. It will be shown that the gauge fixings $\vec{q}_+ \approx 0$ force them to coincide with the centroid x_s^μ.

In Ref. 31, within a one-time framework without constraints and at a fixed time, it is shown that the three-vector $\vec{Y}_s$ (but not $\vec{q}_s$ and $\vec{R}_s$) satisfies the world-line condition $\{K_s^r, Y_s^s\} = (1/c^2)\, Y_s^r \{Y_s^s, p_s^0\}$ and is therefore the space part of a four-vector Y_s^μ. On the other hand, within the enlarged canonical approach including time variables, it is not clear which are the time components to be added to $\vec{q}_s$, $\vec{R}_s$, $\vec{Y}_s$, in order to rebuild four-dimensional quantities $\tilde{x}_s^\mu$, R_s^μ, Y_s^μ, in an arbitrary Lorentz frame Γ having the origin of the Wigner hyperplane coincident with the centroid four-vector $x_s^\mu = (x_s^0; \vec{x}_s)$. From Eq. (2.10), we obtain the following expressions of the noncovariant (frame-dependent) canonical four-center of mass and its conjugate momentum:

$$\tilde{x}_s^\mu(\tau) = (\tilde{x}_s^0(\tau); \vec{\tilde{x}}_s(\tau)) = x_s^\mu - \frac{1}{\epsilon_s(p_s^0+\epsilon_s)}\left[p_{s\nu} S_s^{\nu\mu} + \epsilon_s\left(S_s^{0\mu} - S_s^{0\nu}\frac{p_{s\nu}p_s^\mu}{\epsilon_s^2}\right)\right], \quad p_s^\mu,$$

$$\tilde{x}_s^0 = \sqrt{1+\vec{k}_s^2}\left(T_s + \frac{\vec{k}_s \cdot \vec{z}_s}{\epsilon_s}\right) = \sqrt{1+\vec{k}_s^2}(T_s + \vec{k}_s \cdot \vec{q}_s) \neq x_s^0, \quad p_s^0 = \epsilon_s\sqrt{1+\vec{k}_s^2}, \tag{4.3}$$

$$\vec{\tilde{x}}_s = \frac{\vec{z}_s}{\epsilon_s} + \left(T_s + \frac{\vec{k}_s \cdot \vec{z}_s}{\epsilon_s}\right)\vec{k}_s = \vec{q}_s + (T_s + \vec{k}_s \cdot \vec{q}_s)\vec{k}_s, \quad \vec{p}_s = \epsilon_s \vec{k}_s.$$

Each Wigner hyperplane intersects the world line of the arbitrary centroid four-vector $x_s^\mu(\tau) = z^\mu(\tau, \vec{0})$ in $\vec{\sigma} = 0$, the pseudo-world-line of $\tilde{x}_s^\mu(\tau) = z^\mu(\tau, \vec{\tilde{\sigma}})$ in some $\vec{\tilde{\sigma}}$ and the world line of the Fokker–Pryce four-vector $Y_s^\mu(\tau) = z^\mu(\tau, \vec{\sigma}_Y)$ in some $\vec{\sigma}_Y$; one also has $R_s^\mu = z^\mu(\tau, \vec{\sigma}_R)$. Since we have $T_s = u(p_s) \cdot x_s = u(p_s) \cdot \tilde{x}_s \equiv \tau$ on the Wigner hyperplane labeled by τ, we will also require

Y_s^μ, R_s^μ to have time components such that $u(p_s)\cdot Y_s = u(p_s)\cdot R_s = T_s \equiv \tau$. It is reasonable therefore to assume that, consistently with Eqs. (4.2) and (4.3), $\tilde{x}_s^\mu$, Y_s^μ, and R_s^μ satisfy the following equations:

$$\tilde{x}_s^\mu = (\tilde{x}_s^0;\vec{\tilde{x}}_s) = \left(\tilde{x}_s^0;\vec{q}_s + \frac{\vec{p}_s}{p_s^0}\tilde{x}_s^0\right) = \left(\tilde{x}_s^0;\frac{\vec{z}_s}{\epsilon_s} + \left(T_s + \frac{\vec{k}_s\cdot\vec{z}_s}{\epsilon_s}\right)\vec{k}_s\right) = x_s^\mu + \epsilon_u^\mu(u(p_s))\tilde{\sigma}^u,$$

$$Y_s^\mu = (\tilde{x}_s^0;\vec{Y}_s) = \left(\tilde{x}_s^0;\frac{1}{\epsilon_s}\left[\vec{z}_s + \frac{\vec{\overline{S}}_s\times\vec{p}_s}{\epsilon_s[1+u^0(p_s)]}\right] + \left(T_s + \frac{\vec{k}_s\cdot\vec{z}_s}{\epsilon_s}\right)\vec{k}_s\right)$$

$$= \tilde{x}_s^\mu + \eta_r^\mu\frac{(\vec{\overline{S}}_s\times\vec{p}_s)^r}{\epsilon_s[1+u^0(p_s)]} = x_s^\mu + \epsilon_u^\mu(u(p_s))\sigma_Y^u,$$

$$R_s^\mu = (\tilde{x}_s^0;\vec{R}_s) = \left(\tilde{x}_s^0;\quad \frac{1}{\epsilon_s}\left[\vec{z}_s - \frac{\vec{\overline{S}}_s\times\vec{p}_s}{\epsilon_s u^0(p_s)[1+u^0(p_s)]}\right] + \left(T_s + \frac{\vec{k}_s\cdot\vec{z}_s}{\epsilon_s}\right)\vec{k}_s\right)$$

$$= \tilde{x}_s^\mu - \eta_r^\mu\frac{(\vec{\overline{S}}_s\times\vec{p}_s)^r}{\epsilon_s u^0(p_s)[1+u^0(p_s)]} = x_s^\mu + \epsilon_u^\mu(u(p_s))\sigma_R^u,$$

$$T_s = u(p_s)\cdot x_s = u(p_s)\cdot\tilde{x}_s = u(p_s)\cdot Y_s = u(p_s)\cdot R_s,$$

$$\tilde{\sigma}^r = \epsilon_{r\mu}(u(p_s))[x_s^\mu - \tilde{x}_s^\mu] = \frac{\epsilon_{r\mu}(u(p_s))[u_\nu(p_s)S_s^{\nu\mu} + S_s^{0\mu}]}{[1+u^0(p_s)]} = -\overline{S}_s^{\tau r} + \frac{\overline{S}_s^{rs}p_s^s}{\epsilon_s[1+u^0(p_s)]} \tag{4.4}$$

$$= \epsilon_s R_+^r + \frac{\overline{S}_s^{rs}u^s(p_s)}{1+u^0(p_s)} \overset{\vec{q}_+\approx 0}{\approx} \epsilon_s q_+^r + \frac{\overline{S}_s^{rs}u^s(p_s)}{1+u^0(p_s)} \approx \frac{\overline{S}_s^{rs}u^s(p_s)}{1+u^0(p_s)},$$

$$\sigma_Y^r = \epsilon_{r\mu}(u(p_s))[x_s^\mu - Y_s^\mu] = \tilde{\sigma}^r - \epsilon_{ru}(u(p_s))\frac{(\vec{\overline{S}}_s\times\vec{p}_s)^u}{\epsilon_s[1+u^0(p_s)]} = \tilde{\sigma}^r + \frac{\overline{S}_s^{rs}u^s(p_s)}{1+u^0(p_s)}$$

$$= \epsilon_s R_+^r \approx \epsilon_s q_+^r \overset{\vec{q}_+\approx 0}{\approx} 0,$$

$$\Rightarrow x_s^{(\vec{q}_+)\mu}(\tau) = x_s^\mu(0) + Y_s^\mu, \quad when \quad \vec{q}_+ \approx 0,$$

$$\sigma_R^r = \epsilon_{r\mu}(u(p_s))[x_s^\mu - R_s^\mu] = \tilde{\sigma}^r + \epsilon_{ru}(u(p_s))\frac{(\vec{\overline{S}}_s\times\vec{p}_s)^u}{\epsilon_s u^0(p_s)[1+u^0(p_s)]} = \tilde{\sigma}^r - \frac{\overline{S}_s^{rs}u^s(p_s)}{u^0(p_s)[1+u^0(p_s)]}$$

$$= \epsilon_s R_+^r + \frac{[1-u^0(p_s)]\overline{S}_s^{rs}u^s(p_s)}{u^0(p_s)[1+u^0(p_s)]} \overset{\vec{q}_+\approx 0}{\approx} \frac{[1-u^0(p_s)]\overline{S}_s^{rs}u^s(p_s)}{u^0(p_s)[1+u^0(p_s)]}.$$

It is seen that *the external Fokker–Pryce noncanonical center of inertia coincides with the centroid* $x_s^{(\vec{q}_+)\mu}(\tau)$ *carrying the internal three-center of mass.* Let us recall that the centroid $x_s^\mu(\tau)$ corresponds to the *unique* special-relativistic center-of-mass-like world line of Ref. 47.

In each Lorentz frame one has different pseudo-world-lines describing R_s^μ and $\tilde{x}_s^\mu$: the canonical four-center of mass $\tilde{x}_s^\mu$ lies in between Y_s^μ and R_s^μ in every (nonrest)-frame. In an arbitrary Lorentz frame, the pseudo-world-lines associated with $\tilde{x}_s^\mu$ and R_s^μ fill a world tube[17] around the world line Y_s^μ of the covariant noncanonical Fokker–Pryce four-center of inertia Y_s^μ. The *invariant radius* of the tube is $\rho = \sqrt{-\epsilon W^2}/p^2 = |\vec{S}|/\sqrt{\epsilon p^2}$ where ($W^2 = -\epsilon p^2\vec{S}^2$ is the Pauli–Lubanski invariant when $\epsilon p^2 > 0$). This classical intrinsic radius delimits the noncovariance effects (the pseudo-world lines) of the canonical four-center of mass $\tilde{x}_s^\mu$. See Ref. 38 for a discussion of the

properties of the *Møller radius*. At the quantum level ρ becomes the Compton wavelength of the isolated system times its spin eigenvalue $\sqrt{s(s+1)}$, $\rho \mapsto \hat{\rho} = \sqrt{s(s+1)}\hbar/M = \sqrt{s(s+1)}\lambda_M$ with $M = \sqrt{\epsilon p^2}$ the invariant mass and $\lambda_M = \hbar/M$ its Compton wavelength. The criticism to classical relativistic physics argued from quantum pair production concerns testing of distances where, due to the Lorentz signature of space–time, intrinsic classical covariance problems emerge: the canonical four-center of mass $\tilde{x}^\mu_s$ adapted to the first class constraints of the system cannot be localized in a frame-independent way.

Finally, recall[9] that ρ is likewise a remnant of the energy conditions of general relativity in flat Minkowski space–time: since the Møller noncanonical, noncovariant four-center of energy R^μ has noncovariance properties localized inside the same world tube with radius ρ,[17] it turns out that for an extended relativistic system with a material radius smaller than its intrinsic radius ρ one has: (i) its peripheral rotation velocity can exceed the velocity of light; (ii) its classical energy density cannot be positive definite everywhere in every frame.

V. GETTING THE INTERNAL RELATIVE VARIABLES FROM A GARTENHAUS–SCHWARTZ TRANSFORMATION

Given $\vec{\eta}_i$, $\vec{\kappa}_i$, we must find the canonical basis $\vec{q}_+$, $\vec{\kappa}_+$, $\vec{\rho}_{qa}$, $\vec{\pi}_{qa}$ of Eq. (3.6).

We shall exploit the classical analog of the Gartenhaus–Schwartz singular transformation[23] following the scheme used in Ref. 45 in order to find the center-of-mass subspace of phase space defined by $\vec{\kappa}_+ = 0$ (see Ref. 48)

$$U(\alpha) = e^{\alpha\{.,\vec{q}_+ \cdot \vec{\kappa}_+\}},$$

$$\vec{q}_+ \cdot \vec{\kappa}_+ = -\frac{|\vec{\kappa}_+|}{\sum_{k=1}^N \sqrt{m_k^2 + \vec{\kappa}_k^2}} \vec{n}_+ \cdot \vec{K}, \quad \vec{n}_+ = \frac{\vec{\kappa}_+}{|\vec{\kappa}_+|}, \quad \vec{K} = -\sum_{i=1}^N \sqrt{m_i^2 + \vec{\kappa}_i^2}\, \vec{\eta}_i,$$

$$\vec{\kappa}_+(\alpha) = U(\alpha)\vec{\kappa}_+ = e^{-\alpha}\vec{\kappa}_+ \to_{\alpha\to\infty} 0, \tag{5.1}$$

$$\vec{q}_+(\alpha) = U(\alpha)\vec{q}_+ = e^{\alpha}\vec{q}_+ \to_{\alpha\to\infty} \infty, \quad U(-\alpha)\vec{q}_+ = e^{-\alpha}\vec{q}_+ \to_{\alpha\to\infty} 0,$$

$$\Rightarrow \vec{\kappa}_+(\alpha) \cdot \vec{q}_+(\alpha) = \vec{\kappa}_+ \cdot \vec{q}_+, \quad \vec{n}_+(\alpha) = \vec{n}_+.$$

Therefore, $\lim_{\alpha\to\infty} U(\alpha)$ can only be applied to the set of functions on phase space which have vanishing Poisson bracket with $\vec{\kappa}_+$, namely to

$$\vec{\kappa}_i \left[\text{or } \vec{\pi}_a = \frac{1}{\sqrt{N}} \sum_{i=1}^N \gamma_{ai} \vec{\kappa}_i \right] \text{ and to } \vec{\rho}_a = \sqrt{N} \sum_{i=1}^N \gamma_{ai} \vec{\eta}_i$$

of Eq. (2.16). Such a canonical transformation does not identify a good internal center of mass but nevertheless provides a canonical set of relative variables suitable for the application of the Gartenhaus–Schwartz transformation.

Since, for finite α, $U(\alpha)$ is a canonical transformation, the Poisson brackets are preserved even in the limit $\alpha\to\infty$:$[\{f(\alpha), g(\alpha)\} = U(\alpha)\{f,g\}]$.

Let $f = f(\vec{\eta}_i, \vec{\kappa}_i)$ have zero Poisson bracket with $\vec{\kappa}_+$, $\{f, \vec{\kappa}_+\} = 0$, and let be $f(\alpha) = U(\alpha)f$. Then, it follows

$$\{\vec{\kappa}_+, f(\alpha)\} = e^{\alpha}\{\vec{\kappa}_+(\alpha), f(\alpha)\} = e^{\alpha}(U(\alpha)\{\vec{\kappa}_+, f\}) = 0. \tag{5.2}$$

Since the Jacobi identity $\{\vec{\kappa}_+, \{\vec{q}_+, f\}\} + \{f, \{\vec{\kappa}_+, \vec{q}_+\}\} + \{\vec{q}_+, \{f, \vec{\kappa}_+\}\} \equiv 0$ implies $\{\vec{\kappa}_+, \{\vec{q}_+, f\}\} \equiv 0$ [namely also $\{\vec{q}_+, f\}$ has zero Poisson bracket with $\vec{\kappa}_+$ if $\{f, \vec{\kappa}_+\} = 0$, so that $U(\alpha)\{\vec{q}_+, f\}$ has a well-defined limit for $\alpha\to\infty$] one also has

$$\{\vec{q}_+, f(\alpha)\} = e^{-\alpha}\{\vec{q}_+(\alpha), f(\alpha)\} = e^{-\alpha}(U(\alpha)\{\vec{q}_+, f\}) \to_{\alpha\to\infty} 0. \tag{5.3}$$

Moreover it holds

$$\frac{\mathrm{d}f(\alpha)}{\mathrm{d}\alpha}=\{f(\alpha),\vec{\kappa}_+\cdot\vec{q}_+\}=\{f(\alpha),\vec{\kappa}_+(\alpha)\cdot\vec{q}_+(\alpha)\}. \tag{5.4}$$

Therefore, the relative variables $\vec{\pi}_a=(1/\sqrt{N})\,\Sigma_{i=1}^N\gamma_{ai}\vec{\kappa}_i$ and $\vec{\rho}_a=\sqrt{N}\,\Sigma_{i=1}^N\,\gamma_{ai}\vec{\eta}_i$, which commute with $\vec{\kappa}_+$ [see Eq. (2.16)], satisfy

$$\begin{aligned}\vec{\pi}_a(\alpha)&=U(\alpha)\vec{\pi}_a\to_{\alpha\to\infty}\vec{\pi}_a(\infty)\overset{\text{def}}{=}\vec{\pi}_{qa},\\ \vec{\rho}_a(\alpha)&=U(\alpha)\vec{\rho}_a\to_{\alpha\to\infty}\vec{\rho}_a(\infty)\overset{\text{def}}{=}\vec{\rho}_{qa},\end{aligned} \tag{5.5}$$

where $\vec{\rho}_{qa}$, $\vec{\pi}_{qa}$, is a pair of canonical vectors having zero Poisson bracket with $\vec{q}_+$, $\vec{\kappa}_+$. The searched canonical transformation (3.6) is thereby obtained.

First evaluate $\vec{\pi}_{qa}$ following the scheme of Ref. 45. From Eq. (5.4) we get

$$\frac{\mathrm{d}\vec{\kappa}_i(\alpha)}{\mathrm{d}\alpha}=\{\vec{\kappa}_i(\alpha),\vec{\kappa}_+(\alpha)\cdot\vec{q}_+(\alpha)\}=-\frac{\vec{\kappa}_+(\alpha)}{H_M(\alpha)}H_i(\alpha), \tag{5.6}$$

with the notations

$$M_{\text{sys}}=\sum_{i=1}^N H_i,\quad H_M(\alpha)=\sum_{i=1}^N H_i(\alpha)\to_{\alpha\to\infty}H_M(\infty)\overset{\text{def}}{=}H_{(\text{rel})},$$

$$H_i=\sqrt{m_i^2+\vec{\kappa}_i^2},\quad H_i(\alpha)=\sqrt{m_i^2+\vec{\kappa}_i^2(\alpha)}\to_{\alpha\to\infty}H_i(\infty)\overset{\text{def}}{=}H_{(\text{rel})i}, \tag{5.7}$$

$$\Pi=M_{\text{sys}}^2-\vec{\kappa}_+^2\approx M_{\text{sys}}^2.$$

From $m_i^2=H_i^2(\alpha)-\vec{\kappa}_i^2(\alpha)$, it follows

$$\frac{\mathrm{d}H_i(\alpha)}{\mathrm{d}\alpha}H_i(\alpha)=\frac{\mathrm{d}\vec{\kappa}_i(\alpha)}{\mathrm{d}\alpha}\cdot\vec{\kappa}_i(\alpha),$$

$$\Rightarrow\frac{\mathrm{d}H_i(\alpha)}{\mathrm{d}\alpha}=-\vec{\kappa}_i(\alpha)\cdot\frac{\vec{\kappa}_i(\alpha)}{H_M(\alpha)},$$

$$\Rightarrow\frac{\mathrm{d}H_M(\alpha)}{\mathrm{d}\alpha}=\sum_{i=1}^N\frac{\mathrm{d}H_i(\alpha)}{\mathrm{d}\alpha}=-\frac{\vec{\kappa}_+^2(\alpha)}{H_M(\alpha)},$$

$$\Rightarrow\Pi=H_M^2-\vec{\kappa}_+^2=H_M^2(\alpha)-\vec{\kappa}_+^2(\alpha)\to_{\alpha\to\infty}M_{\text{sys}}^2(\infty)=H_{(\text{rel})}^2,$$

$$or\quad\frac{\mathrm{d}\Pi}{\mathrm{d}\alpha}=0. \tag{5.8}$$

Let us now introduce $\theta(\alpha)$ such that $[\mathrm{ch}^2\,\theta(\alpha)-\mathrm{sh}^2\,\theta(\alpha)=1$ also for $\alpha\to\infty]$

$$\text{sh}\,\theta(\alpha)=\frac{|\vec{\kappa}_+|H_M(\alpha)-|\vec{\kappa}_+(\alpha)|M_{\rm sys}}{\Pi}\to_{\alpha\to\infty}\frac{|\vec{\kappa}_+|}{\sqrt{\Pi}},$$

$$\text{ch}\,\theta(\alpha)=\frac{M_{\rm sys}H_M(\alpha)-|\vec{\kappa}_+||\vec{\kappa}_+(\alpha)|}{\Pi}\to_{\alpha\to\infty}\frac{M_{\rm sys}}{\sqrt{\Pi}},\tag{5.9}$$

$$\theta(\alpha)=\tanh^{-1}\frac{|\vec{\kappa}_+|}{M_{\rm sys}}-\tanh^{-1}\frac{|\vec{\kappa}_+(\alpha)|}{H_M(\alpha)}\to_{\alpha\to 0}0,\quad\to_{\alpha\to\infty}\tanh^{-1}\frac{|\vec{\kappa}_+|}{M_{\rm sys}}.$$

Since we have

$$\frac{d\theta(\alpha)}{d\alpha}=\frac{|\vec{\kappa}_+(\alpha)|}{H_M(\alpha)},\quad\frac{d\vec{n}_+(\alpha)}{d\alpha}=0\Rightarrow\vec{n}_+(\alpha)=\vec{n}_+,\tag{5.10}$$

we obtain the coupled equations

$$\frac{d\vec{\kappa}_i(\alpha)}{d\theta}=-H_i(\alpha)\vec{n}_+,\quad\frac{dH_i(\alpha)}{d\theta}=-\vec{\kappa}_i(\alpha)\cdot\vec{n}_+,\tag{5.11}$$

whose integration gives

$$\begin{aligned}\vec{\kappa}_i(\alpha)&=\vec{\kappa}_i+([\text{ch}\,\theta(\alpha)-1]\vec{n}_+\cdot\vec{\kappa}_i-\text{sh}\,\theta(\alpha)H_i)\vec{n}_+\to_{\alpha\to\infty}\vec{\kappa}_i(\infty)\\&=\vec{\kappa}_i+\left[\left(\frac{M_{\rm sys}}{\sqrt{\Pi}}-1\right)\vec{n}_+\cdot\vec{\kappa}_i-\frac{|\vec{\kappa}_+|}{\sqrt{\Pi}}H_i\right]\vec{n}_+\approx\vec{\kappa}_i,\end{aligned}$$

$$\begin{aligned}H_i(\alpha)&=\sqrt{m_i^2+\vec{\kappa}_i^2(\alpha)}=\text{ch}\,\theta(\alpha)H_i-\text{sh}\,\theta(\alpha)\vec{n}_+\cdot\vec{\kappa}_i\to_{\alpha\to\infty}H_i(\infty)\\&=\sqrt{m_i^2+\vec{\kappa}_i^2(\infty)}=\frac{1}{\sqrt{\Pi}}(M_{\rm sys}H_i-\vec{\kappa}_+\cdot\vec{\kappa}_i)\approx H_i,\end{aligned}$$

$$\begin{aligned}\Rightarrow H_i&=\sqrt{m_i^2+\vec{\kappa}_i^2}=H_i(\alpha)\text{ch}\,\theta(\alpha)+\vec{n}_+\cdot\vec{\kappa}_i(\alpha)\text{sh}\,\theta(\alpha)\\&=\frac{1}{\sqrt{\Pi}}[H_i(\infty)\,M_{\rm sys}+\vec{n}_+\cdot\vec{\kappa}_i(\infty)|\vec{\kappa}_+|\approx H_i(\infty),\end{aligned}$$

$$\text{with}\quad\sum_{i=1}^{N}H_i(\infty)=H_M(\infty)=\sqrt{\Pi}\overset{\text{def}}{=}H_{(\text{rel})},$$

$$\vec{\kappa}_i=\vec{\kappa}_i(\alpha)+[\text{ch}\,\theta(\alpha)-1]\vec{n}_+\cdot\vec{\kappa}_i(\alpha)\vec{n}_++\text{sh}\,\theta(\alpha)H_i(\alpha).\tag{5.12}$$

Therefore, we get

$$\vec{\pi}_a(\alpha)=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\gamma_{ai}\vec{\kappa}_i(\alpha),$$

$$\vec{\pi}_{qa}\overset{\text{def}}{=}\vec{\pi}_a(\infty)=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\vec{\kappa}_i(\infty)=\vec{\pi}_a+\frac{\vec{n}_+}{\sqrt{\Pi}}[(M_{\text{sys}}-\sqrt{\Pi})\vec{n}_+\cdot\vec{\pi}_a-|\vec{\kappa}_+|H_a]$$

$$=\vec{\pi}_a-\frac{\vec{\kappa}_+}{\sqrt{M_{\text{sys}}^2-\vec{\kappa}_+^2}}\left[H_a-\frac{M_{\text{sys}}-\sqrt{M_{\text{sys}}^2-\vec{\kappa}_+^2}}{\vec{\kappa}_+^2}\vec{\kappa}_+\cdot\vec{\pi}_a\right]\approx\vec{\pi}_a,$$

$$H_a=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\gamma_{ai}H_i,$$

$$\vec{\kappa}_i(\infty)=\sqrt{N}\sum_{a=1}^{N-1}\gamma_{ai}\vec{\pi}_{qa},$$

$$H_{(\text{rel})i}=H_i(\infty)=\sqrt{m_i^2+N\sum_{ab}^{1..N-1}\gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}},$$

$$M_{\text{sys}}=\sum_{i=1}^{N}H_i=\sqrt{\Pi+\vec{\kappa}_+^2}\approx H_{(\text{rel})}=H_M(\infty)=\sqrt{\Pi}=\sum_{i=1}^{N}H_i(\infty)$$

$$=\sum_{i=1}^{N}\sqrt{m_i^2+N\sum_{ab}^{1..N-1}\gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}}. \tag{5.13}$$

Let us turn to $\vec{\rho}_{qa}$. Let us remark first of all that the following two quantities are invariant under the canonical transformation $U(\alpha)$:

$$\begin{aligned}I_i^{(1)}&=M_{\text{sys}}H_i-\vec{\kappa}_+\cdot\vec{\kappa}_i=H_M(\alpha)\,H_i(\alpha)-\vec{\kappa}_+(\alpha)\cdot\vec{\kappa}_i(\alpha),\quad\Rightarrow\frac{\mathrm{d}I_i^{(1)}}{\mathrm{d}\alpha}=0,\\ I^{(2)}&=\frac{\vec{\kappa}_+\cdot\vec{K}}{M_{\text{sys}}}=-\sum_{i=1}^{N}|\vec{\kappa}_+|\left(\vec{n}_+\cdot\frac{\vec{\eta}_iH_i}{M_{\text{sys}}}\right)=\frac{\vec{\kappa}_+(\alpha)\cdot\vec{K}(\alpha)}{H_M(\alpha)},\quad\Rightarrow\frac{\mathrm{d}I^{(2)}}{\mathrm{d}\alpha}=0,\end{aligned} \tag{5.14}$$

and that we have

$$\frac{1}{H_M(\alpha)|\vec{\kappa}_+(\alpha)|}=\frac{\mathrm{d}J^{(1)}(\alpha)}{\mathrm{d}\alpha},\quad\text{with}\quad J^{(1)}(\alpha)=\frac{\operatorname{sh}\theta(\alpha)}{|\vec{\kappa}_+(\alpha)||\vec{\kappa}_+|},$$

$$\frac{\vec{\kappa}_i(\alpha)}{H_i^2(\alpha)}=\frac{\mathrm{d}\vec{J}_i^{(2)}(\alpha)}{\mathrm{d}\theta(\alpha)}$$

with

$$\vec{J}_i^{(2)}(\alpha)=\frac{\vec{\kappa}_i(\alpha)\operatorname{sh}\theta(\alpha)}{H_iH_i(\alpha)}+(\operatorname{ch}\theta(\alpha)-1)\frac{\vec{n}_+}{H_i}. \tag{5.15}$$

Since we also have

$$n^r_+ \frac{\partial}{\partial \kappa^r_i} n^s_+ = \frac{n^r_+}{|\vec{\kappa}_+|}(\delta^{rs} - n^r_+ n^s_+) = 0, \tag{5.16}$$

we get preliminarly, for $\vec{n}_+ \cdot \vec{\eta}_i(\alpha)$,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\alpha}\vec{n}_+ \cdot \vec{\eta}_i(\alpha) &= \{\vec{n}_+ \cdot \vec{\eta}_i(\alpha), \vec{\kappa}_+(\alpha)\cdot\vec{q}_+(\alpha)\} \\ &= -n^r_+ \frac{\partial}{\partial \kappa^r_i(\alpha)} \frac{\vec{n}_+ \cdot \vec{K}(\alpha)|\vec{\kappa}_+(\alpha)|}{H_M(\alpha)} \\ &= -n^r_+ n^s_+ \frac{\partial}{\partial \kappa^r_i(\alpha)} \frac{|\vec{\kappa}_+(\alpha)| K^s(\alpha)}{H_M(\alpha)}.\end{aligned} \tag{5.17}$$

Then, since

$$n^r_+ \frac{\partial}{\partial \kappa^r_i(\alpha)} \frac{|\vec{\kappa}_+(\alpha)|}{H_M(\alpha)} = \frac{I^{(1)}_i}{H^2_M(\alpha) H_i(\alpha)}, \quad \frac{\partial}{\partial \kappa^r_i(\alpha)} K^s(\alpha) = -\frac{\kappa^r_i(\alpha)\eta^s_i(\alpha)}{H_i(\alpha)}, \tag{5.18}$$

we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\alpha}\vec{n}_+ \cdot \vec{\eta}_i(\alpha) &= -\frac{I^{(2)} I^{(1)}_i}{H_M(\alpha) H_i(\alpha) |\vec{\kappa}_+(\alpha)|} + \frac{\vec{n}_+ \cdot \vec{\eta}_i(\alpha) \vec{n}_+ \cdot \vec{\kappa}_i(\alpha)}{H_i(\alpha)} \frac{|\vec{\kappa}_+(\alpha)|}{H_M(\alpha)} \\ &= -\frac{\vec{n}_+ \cdot \vec{\eta}_i(\alpha)}{H_i(\alpha)} \frac{\mathrm{d}H_i(\alpha)}{\mathrm{d}\alpha} - \frac{I^{(1)}_i I^{(2)}}{H_i(\alpha)} \frac{\mathrm{d}J^{(1)}(\alpha)}{\mathrm{d}\alpha}.\end{aligned} \tag{5.19}$$

These equations have the solution

$$\vec{n}_+ \cdot \vec{\eta}_i(\alpha) = \frac{H_i}{H_i(\alpha)} \vec{n}_+ \cdot \vec{\eta}_i - \frac{I^{(1)}_i I^{(2)}}{H_i(\alpha)} \frac{\mathrm{sh}\,\theta(\alpha)}{|\vec{\kappa}_+(\alpha)||\vec{\kappa}_+|} = \frac{H_i}{H_i(\alpha)} \vec{n}_+ \cdot \vec{\eta}_i - \frac{I^{(2)}}{|\vec{\kappa}_+|}\left(e^{\alpha} - \frac{H_i}{H_i(\alpha)}\right). \tag{5.20}$$

For $\vec{\eta}_i(\alpha)$ we have

$$\begin{aligned}\frac{\mathrm{d}\eta^r_i(\alpha)}{\mathrm{d}\alpha} &= \{\eta^r_i(\alpha), \vec{\kappa}_+(\alpha)\cdot\vec{q}_+(\alpha)\} = -n^s_+ \frac{\partial}{\partial \kappa^r_i(\alpha)} \frac{|\vec{\kappa}_+(\alpha)| K^s(\alpha)}{H_M(\alpha)} = \vec{n}_+ \cdot \vec{\eta}_i(\alpha) \frac{|\vec{\kappa}_+(\alpha)| \kappa^r_i(\alpha)}{H_i(\alpha) H_M(\alpha)} \\ &+ \frac{\sum_{j=1}^N H_j(\alpha) \vec{n}_+ \cdot \vec{\eta}_j(\alpha)}{H_M(\alpha)} \left[\frac{|\vec{\kappa}_+(\alpha)| \kappa^r_i(\alpha)}{H_i(\alpha) H_M(\alpha)} - n^r_+\right].\end{aligned} \tag{5.21}$$

By putting Eq. (5.20) in Eq. (5.21) we get the equations determining $\vec{\eta}_i(\alpha)$.

Instead of integrating these equations, let us study the equations for $\vec{\rho}_a(\alpha) = \sqrt{N}\sum_{i=1}^N \gamma_{ai}\vec{\eta}_i(\alpha)$, since for interactions depending on $\vec{\eta}_i - \vec{\eta}_j$ we have $\vec{\eta}_i(\alpha) - \vec{\eta}_j(\alpha) = (1/\sqrt{N})\sum_{a=1}^{N-1}(\gamma_{ai} - \gamma_{aj})\vec{\rho}_a(\alpha)$. Equations (5.21) and (5.20) imply

$$\frac{\mathrm{d}\vec{\rho}_a(\alpha)}{\mathrm{d}\alpha} = -\sum_{i,j=1}^N \sum_{b=1}^{N-1} \vec{n}_+ \cdot \vec{\rho}_b \frac{H_i H_j}{M_{\mathrm{sys}}} \gamma_{aj}(\gamma_{bi} - \gamma_{bj}) \frac{\vec{\kappa}_j(\alpha)|\vec{\kappa}_+(\alpha)|}{H^2_j(\alpha) H_M(\alpha)},$$

$$\Downarrow$$

$$\frac{\mathrm{d}\vec{\rho}_a(\alpha)}{\mathrm{d}\theta(\alpha)} = -\sum_{i,j=1}^N \sum_{b=1}^{N-1} \vec{n}_+ \cdot \vec{\rho}_b \frac{H_i H_j}{M_{\mathrm{sys}}} \gamma_{aj}(\gamma_{bi} - \gamma_{bj}) \frac{\mathrm{d}\vec{J}^{(2)}_j(\alpha)}{\mathrm{d}\theta(\alpha)}, \tag{5.22}$$

whose solution is

$$\vec{\rho}_a(\alpha)=\vec{\rho}_a-\sum_{i,j=1}^{N}\sum_{b=1}^{N-1}\vec{n}_+\cdot\vec{\rho}_b\frac{H_iH_j}{M_{\rm sys}}\gamma_{aj}(\gamma_{bi}-\gamma_{bj})\vec{J}_j^{(2)}(\alpha). \tag{5.23}$$

For $\alpha\to\infty$ we get

$$\begin{aligned}\vec{\rho}_{qa}\overset{\rm def}{=}\vec{\rho}_a(\infty)&=\vec{\rho}_a-\sum_{i,j=1}^{N}\sum_{b=1}^{N-1}\gamma_{aj}(\gamma_{bi}-\gamma_{bj})\frac{H_i}{M_{\rm sys}}\left[\frac{|\vec{\kappa}_+|\vec{\kappa}_j(\infty)}{H_j(\infty)\sqrt{\Pi}}+\left(\frac{M_{\rm sys}}{\sqrt{\Pi}}-1\right)\vec{n}_+\right]\vec{n}_+\cdot\vec{\rho}_b\\&=\vec{\rho}_a-\sum_{i,j=1}^{N}\sum_{b=1}^{N-1}\gamma_{aj}(\gamma_{bi}-\gamma_{bj})\frac{H_i}{M_{\rm sys}}\frac{\vec{\kappa}_j(\infty)}{H_j(\infty)\sqrt{\Pi}}\vec{\kappa}_+\cdot\vec{\rho}_b\approx\vec{\rho}_a\,.\end{aligned} \tag{5.24}$$

One can check that for $N=2$ and $\gamma_1=-\gamma_2=1/\sqrt{2}$ the results of Ref. 45 are reobtained.

Let us now consider the spin vector $\vec{S}_q=\vec{\tilde{S}}_s-\vec{q}_+\times\vec{\kappa}_+=[\vec{\eta}_+-\vec{q}_+]\times\vec{\kappa}_++\Sigma_{a=1}^{N-1}\vec{\rho}_a\times\vec{\pi}_a$. For arbitrary α we have $\vec{S}_q(\alpha)=\Sigma_{a=1}^{N-1}\vec{\rho}_a(\alpha)\times\vec{\pi}_a(\alpha)+[\vec{\eta}_+(\alpha)-\vec{q}_+(\alpha)]\times\vec{\kappa}_+(\alpha)$ and, since $\vec{q}_+(\alpha)\cdot\vec{\kappa}_+(\alpha)$ is a scalar, $\{\vec{S}_q(\alpha),\vec{q}_+(\alpha)\cdot\vec{\kappa}_+(\alpha)\}=0$. Since $\lim_{\alpha\to\infty}\vec{\kappa}_+(\alpha)=0$, we get

$$\vec{S}_q(\alpha)\to_{\alpha\to\infty}\vec{S}_q=\sum_{a=1}^{N-1}\vec{\rho}_{qa}\times\vec{\pi}_{qa}\,, \tag{5.25}$$

if we can show that $\vec{\eta}_+(\alpha)-\vec{q}_+(\alpha)\to_{\alpha\to\infty}$ *finite value*. Now, since the boost generator may be written as

$$\begin{aligned}\vec{K}(\alpha)&=-\sum_{i=1}^{N}\vec{\eta}_i(\alpha)H_i(\alpha)=-\vec{\eta}_+(\alpha)H_M(\alpha)+\sum_{a=1}^{N-1}\vec{\rho}_a(\alpha)H_a(\alpha),\\H_a(\alpha)&=\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\gamma_{ai}H_i(\alpha),\end{aligned} \tag{5.26}$$

we get

$$\begin{aligned}\vec{\eta}_+(\alpha)-\vec{q}_+(\alpha)&=\frac{\Sigma_{a=1}^{N}\vec{\rho}_a(\alpha)H_a(\alpha)}{H_M(\alpha)}+\frac{\vec{\kappa}_+(\alpha)\times(\Sigma_{a=1}^{N-1}\vec{\rho}_a(\alpha)\times\vec{\pi}_a(\alpha))}{\sqrt{\Pi}(\sqrt{\Pi}+M_{\rm sys})}\\&\quad+\frac{\vec{\kappa}_+(\alpha)\times(\vec{\kappa}_+(\alpha)\times\Sigma_{a=1}^{N-1}\vec{\rho}_a(\alpha)H_a(\alpha))}{H_M(\alpha)\sqrt{\Pi}(\sqrt{\Pi}+M_{\rm sys})}\to_{\alpha\to\infty}\frac{1}{\sqrt{\Pi}}\sum_{a=1}^{N}\vec{\rho}_a(\infty)H_a(\infty)\\&=\frac{1}{\sqrt{\Pi}}\sum_{a=1}^{N-1}\vec{\rho}_{qa}\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\gamma_{ai}\sqrt{m_i^2+N\sum_{ab}^{1,\ldots,N-1}\gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}},\end{aligned}$$

$$\Downarrow$$

$$\begin{aligned}\vec{q}_+=\vec{\eta}_+-\frac{1}{\sqrt{N}}\frac{\Sigma_{a=1}^{N-1}\vec{\rho}_a}{\sqrt{(\Sigma_{i=1}^{N}\sqrt{m_i^2+\vec{\kappa}_i^2})^2-\vec{\kappa}_+^2}}\sum_{i=1}^{N}\gamma_{ai}\sqrt{m_i^2+\vec{\kappa}_i^2}+(\text{terms}\to_{\alpha\to\infty}0,i.e.,\\\approx 0\ \text{ due to }\ \vec{\kappa}_+\approx 0),\end{aligned} \tag{5.27}$$

to be compared with Eq. (2.14).

In this way, although it is not known how to get the inverse transformation, we have successfully achieved the searched canonical transformation (3.6)

$$\boxed{\begin{array}{c}\vec{\eta}_i\\ \vec{\kappa}_i\end{array}} \longrightarrow \boxed{\begin{array}{c|c}\vec{q}_+ & \vec{\rho}_{qa}\\ \vec{\kappa}_+ & \vec{\pi}_{qa}\end{array}} \quad . \tag{5.28}$$

Adding the gauge fixings $\vec{q}_+ \approx 0$ for $\vec{\kappa}_+ \approx 0$ and going to Dirac brackets, we finally obtain

$$\vec{\rho}_{qa} \equiv \vec{\rho}_a\,, \quad \vec{\pi}_{qa} \equiv \vec{\pi}_a\,, \quad \vec{S}_q = \sum_{a=1}^{N-1} \vec{\rho}_{qa} \times \vec{\pi}_{qa} \stackrel{\text{def}}{=} \sum_{a=1}^{N-1} \vec{\rho}_a \times \vec{\pi}_a\,,$$

$$H_{(\text{rel})} = H_M(\infty) = \sum_{i=1}^{N} \sqrt{m_i^2 + N \sum_{ab}^{1,\ldots,N-1} \gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}} \equiv \sqrt{\Pi} \equiv M_{\text{sys}}\,. \tag{5.29}$$

$H_{(\text{rel})}$ replaces the nonrelativistic one $H_{\text{rel,nr}} = \frac{1}{2}\Sigma_{a,b=1}^{N-1} k_{ab}^{-1}[m_i, \gamma_{ai}]\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}$ of Eq. (2.9) of Ref. 2 for $c \to \infty$.

See Appendix B for the case of spinning particles.

VI. RELATIVISTIC ROTATIONAL KINEMATICS

Each square root in the Hamiltonian equation (5.29) for the relative motions in the rest frame instant form contains a $(N-1)\times(N-1)$ matrix $K_{(i)ab}^{-1} = N\gamma_{ai}\gamma_{bi} = K_{(i)ba}^{-1}$.[49] The existence of relativistic normal Jacobi coordinates would require the simultaneous diagonalization of these N matrices. This is impossible, however, because

$$[K_{(i)}^{-1}, K_{(j)}^{-1}]_{ab} = G_{(ij)ab} = -G_{(ij)ba} = -G_{(ji)ab} = -N[\gamma_{ai}\gamma_{bj} - \gamma_{aj}\gamma_{bi}]. \tag{6.1}$$

There are $\frac{1}{2}N(N-1)$ matrices G_{ij}, each one with $\frac{1}{2}(N-1)(N-2)$ independent elements. While the conditions $G_{(ij)ab} = 0$ are $\frac{1}{4}N(N-1)^2(N-2)$, the free parameters at our disposal in the γ_{ai} are only $\frac{1}{2}(N-1)(N-2)$. For $N=3$, there are three conditions and only one parameter; for $N=4$, eighteen conditions and three parameters.

In conclusion, it is impossible to diagonalize the N quadratic forms under the square roots simultaneously: *there are no relativistic normal Jacobi coordinates, and no definition of reduced masses and inertia tensor is allowed.*

In order to find the analog of $L_{rel,nr} = \frac{1}{2}\Sigma_{a,b=1}^{N-1} k_{ab}[m_i, \gamma_{ai}]\dot{\vec{\rho}}_a\cdot\dot{\vec{\rho}}_b$ [Eq. (2.9) of Ref. 2], we should perform an inverse Legendre transformation. The first half of Hamilton equations gives

$$\dot{\rho}_{qa}^r \stackrel{\circ}{=} \{\rho_{qa}^r, H_{(\text{rel})}\} = \sum_{i=1}^{N} \frac{N\gamma_{ai}\Sigma_{b=1}^{N-1}\gamma_{bi}\pi_{qb}^r}{\sqrt{m_i^2 + N\Sigma_{ab}^{1..N-1}\gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}}},$$

$$\Downarrow$$

$$\dot{\vec{\rho}}_{qa}\cdot\dot{\vec{\rho}}_{qb} = \sum_{i,j}^{1,\ldots,N} \frac{N\gamma_{ai}\Sigma_{e=1}^{N-1}\gamma_{ei}\vec{\pi}_{qe}}{\sqrt{m_i^2 + N\Sigma_{a_1b_1}^{1..N-1}\gamma_{a_1i}\gamma_{b_1i}\vec{\pi}_{qa_1}\cdot\vec{\pi}_{qb_1}}} \cdot \frac{N\gamma_{bj}\Sigma_{f=1}^{N-1}\gamma_{fj}\vec{\pi}_{qf}}{\sqrt{m_j^2 + N\Sigma_{a_2b_2}^{1..N-1}\gamma_{a_2j}\gamma_{b_2j}\vec{\pi}_{qa_2}\cdot\vec{\pi}_{qb_2}}}. \tag{6.2}$$

However, in order to get $\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}$ in terms of $\dot{\vec{\rho}}_{qa}\cdot\dot{\vec{\rho}}_{qb}$ we should solve higher order algebraic equations. As already pointed out, this implies that $L_{\text{rel}}(\vec{\rho}_{qa}, \dot{\vec{\rho}}_{qa}) = \Sigma_{a=1}^{N-1}\vec{\pi}_{qa}\cdot\dot{\vec{\rho}}_{qa} - H$ is a hyperelliptic function already in the free case. This in turn means that, unlike the nonrelativistic case, it

is not even possible to define either an Euclidean or a Riemannian metric on the space of velocities from the kinetic energy (see Ref. 2). A Lagrangian dynamics cannot be made explicit as in the nonrelativistic case. The form of the canonical momenta

$$\pi^r_{qa}=\frac{\partial L_{\rm rel}}{\partial \dot\rho^r_{qa}}=\sum_{b=1}^{N-1} f_{ab}(\dot{\vec\rho}_{qc}\cdot\dot{\vec\rho}_{qd})\dot\rho^r_{qb}, \tag{6.3}$$

can only be given in implicit form. Also the restrictions upon the relative velocities $\dot{\vec\rho}_{qa}(\tau)$ resulting from the existence of the limiting light velocity c cannot be evaluated.

We could tentatively try to follow the nonrelativistic pattern of the *static* orientation-shape bundle approach (see Ref. 2). We would get[50]

$$\rho^r_{qa}=R^{rs}(\theta^\alpha)\check\rho^s_{qa}(q),$$

$$\dot\rho^r_{qa}\overset{\rm def}{=}R^{rs}(\theta^\alpha)\check v^s_{qa},\quad \vec v_{qa}=\vec\omega\times\vec\rho_{qa}+\frac{\partial\vec\rho_{qa}}{\partial q^\mu}\dot q^\mu,$$

$$\dot\rho^r_{qa}\overset{\circ}{=}\{\rho^r_{qa},H_{\rm rel}\},$$

$$\pi^r_{qa}=\sum_{b=1}^{N-1} f_{ab}(\dot{\vec\rho}_{qc}\cdot\dot{\vec\rho}_{qd})\dot\rho^r_{qb}=R^{rs}(\theta^\alpha)\check\pi^s_{qa},\quad \check\pi^r_{qa}=\sum_{b=1}^{N-1} f_{ab}(\check{\vec v}_{qc}\cdot\check{\vec v}_{qd})\check v^r_{qb},$$

$$S^r_q=R^{rs}(\theta^\alpha)\check S^s_q=\sum_{a=1}^{N-1}[\vec\rho_{qa}\times\vec\pi_{qa}]^r,$$

$$\vec S_q=\sum_{ab}^{1,\dots,N-1} f_{ab}\left[\left(\vec\omega\times\vec\rho_{qc}+\frac{\partial\vec\rho_{qc}}{\partial q^\mu}\dot q^\mu\right)\cdot\left(\vec\omega\times\vec\rho_{qd}+\frac{\partial\vec\rho_{qd}}{\partial q^\mu}\dot q^\mu\right)\right]\vec\rho_{qa}\times\left(\vec\omega\times\vec\rho_{qb}+\frac{\partial\vec\rho_{qb}}{\partial q^\mu}\dot q^\mu\right), \tag{6.4}$$

$$\check S^r_q=\sum_{ab}^{1,\dots,N-1} f_{ab}[\check I^{uv}_{(cd)}(q)(\check\omega^u+\check A^u_{(cd)\mu}(q)\dot q^\mu)(\check\omega^v+\check A^v_{(cd)\nu}(q)\dot q^\nu)]\check I^{rs}_{(ab)}(q)(\check\omega^s+\check A^s_{(ab)\mu}(q)\dot q^\mu),$$

$$\check{\mathcal I}^{rs}(\check{\vec\omega},q,m)=\sum_{ab}^{1,\dots,N-1} f_{ab}(\vec v_{qc}\cdot\vec v_{qd})\check I^{rs}_{(ab)}(q),$$

$$\check I^{rs}_{(ab)}(q)=\vec\rho_{qa}\cdot\vec\rho_{qb}\delta^{rs}-\frac{1}{2}(\check\rho^r_{qa}\check\rho^s_b+\check\rho^r_{qb}\check\rho^s_{qa}),$$

$$\check a^u_{(ab)\mu}(q)=\frac{1}{2}\left[\vec\rho_{qa}\times\frac{\partial\vec\rho_{qb}}{\partial q^\mu}+\vec\rho_{qb}\times\frac{\partial\vec\rho_{qa}}{\partial q^\mu}\right]^u\overset{\rm def}{=}\check I^{uv}_{(ab)}(q)\check A^v_{(ab)\mu}(q).$$

It is seen, however, that *there is no more a linear relation* between the body frame spin and angular velocity. By expanding $f_{ab}(x)$ in a power series around $x=0$, we see that $\check S^r_q$ is an infinite series containing all the powers of the body frame angular velocity. The lowest term is $\check S^r_{q(0)}=\Sigma^{N-1}_{a,b} f_{ab}(0)\check I^{rs}_{(ab)}(q)(\check\omega^s+\check A^s_{(ab)\mu}(q)\dot q^\mu)$ with $f_{ab}(0)$ playing the role of the nonrelativistic k_{ab}.

Therefore, the tensor of inertia loses a clear identification: only *its building blocks* $\check I^{rs}_{(ab)}$, which appear at the nonrelativistic level, survive within the relativistic construction.

The relative Lagrangian can be worked out in the special case of $N=2$ with equal masses $m_1=m_2=m$. It results in

$$L_{\rm rel}(\vec{\rho},\dot{\vec{\rho}}) = -m\sqrt{4-\dot{\vec{\rho}}^2}. \tag{6.5}$$

so that the relative velocity is bounded by $|\dot{\vec{\rho}}| \leq 2$.

Let us write $\vec{\rho} = \rho\hat{\rho}$ with $\rho = |\vec{\rho}|$ and $\hat{\rho} = \vec{\rho}/|\vec{\rho}|$. With a single relative variable the three Euler angles θ^α are redundant: there are only two independent angles, identifying the position of the unit three-vector $\hat{\rho}$ on S^2. We shall use the parametrization (Euler angles $\theta^1 = \phi,\ \theta^2 = \theta,\ \theta^3 = 0$)

$$\hat{\rho}^r = R^{rs}(\theta,\phi)\,\hat{\rho}_0^s = (R_z(\theta)R_y(\phi))^{rs}\,\hat{\rho}_0^s, \quad \hat{\rho}_0 = (0,0,1). \tag{6.6}$$

By continuing the attempt to follow the *static* orientation-shape bundle approach, we get the following body frame velocity and angular velocity (ρ is the only shape variable for $N=2$):

$$\begin{aligned} &\check{v}^r = R^{T\,rs}\dot{\rho}^s = \rho(R^T\dot{R})^{rs}\hat{\rho}_0^s + \dot{\rho}\hat{\rho}_0^r = \rho\epsilon^{ru3}\check{\omega}^u + \dot{\rho}\hat{\rho}_0^r = \rho(\vec{\omega}\times\hat{\rho}_0)^r + \dot{\rho}\hat{\rho}_0^r, \\ &\vec{\omega} = (\tfrac{1}{2}\epsilon^{urs}(R^T\dot{R})^{rs}) = (\check{\omega}^1 = -\sin\theta\dot{\phi}, \check{\omega}^2 = \dot{\theta}, 0), \\ &\vec{v}^2 = \check{I}(\rho)\vec{\omega}^2 + \dot{\rho}^2, \quad \check{I}(\rho) = \rho^2. \end{aligned} \tag{6.7}$$

The nonrelativistic inertia tensor of the dipole $\check{I}_{\rm nr} = \mu\rho^2$ ($\mu = m_1m_2/m_1+m_2$ is the reduced mass) is replaced by $\check{I} = \check{I}_{\rm nr}/\mu = \rho^2$. The Lagrangian in anholonomic variables becomes

$$\tilde{L}(\vec{\omega},\rho,\dot{\rho}) = -m\sqrt{4-\check{I}(\rho)\vec{\omega}^2-\dot{\rho}^2}. \tag{6.8}$$

It is clear that the bound $|\dot{\vec{\rho}}| \leq 2$ puts upper limitations upon the kinetic energy of both the rotational and vibrational motions.

The canonical momenta are

$$\begin{aligned} \vec{S} &= \frac{\partial\tilde{L}}{\partial\vec{\omega}} = \frac{m\check{I}(\rho)\vec{\omega}}{\sqrt{4-\check{I}(\rho)\vec{\omega}^2-\dot{\rho}^2}}, \\ \pi &= \frac{\partial\tilde{L}}{\partial\dot{\rho}} = \frac{m\dot{\rho}}{\sqrt{4-\check{I}(\rho)\vec{\omega}^2-\dot{\rho}^2}}. \end{aligned} \tag{6.9}$$

When $|\dot{\vec{\rho}}|$ varies between 0 and 2 the momenta vary between 0 and ∞, so that in phase space there is no bound from the limiting light velocity. This shows once more that in special relativity it is convenient to work in the Hamiltonian framework avoiding relative and angular velocities.

Since we have

$$\sqrt{4-\check{I}(\rho)\vec{\omega}^2-\dot{\rho}^2} = \frac{2m}{\sqrt{m^2+\check{I}^{-1}(\rho)\vec{S}^2+\pi^2}},$$

the inversion formulas become

$$\begin{aligned} \vec{\omega} &= \frac{\vec{S}}{m\check{I}(\rho)}\sqrt{4-\check{I}(\rho)\vec{\omega}^2-\dot{\rho}^2} = \frac{2\check{I}^{-1}(\rho)\vec{S}}{\sqrt{m^2+\check{I}^{-1}(\rho)\vec{S}^2+\pi^2}}, \\ \dot{\rho} &= \frac{\pi}{m}\sqrt{4-\check{I}(\rho)\vec{\omega}^2-\dot{\rho}^2} = \frac{2\pi}{\sqrt{m^2+\check{I}^{-1}(\rho)\vec{S}^2+\pi^2}}. \end{aligned} \tag{6.10}$$

On the other hand, the Hamiltonian results

$$\tilde{H}=\pi\dot{\rho}+\vec{S}\cdot\vec{\omega}-\tilde{L}=2\sqrt{m^2+\check{I}^{-1}(\rho)\vec{S}^2+\pi^2}. \tag{6.11}$$

It is seen that the special case we are discussing leads to a point-canonical transformation followed by a transformation to an anholonomic basis, as in the nonrelativistic treatment

$$\begin{array}{|c|}\hline \vec{\rho} \\ \hline \vec{\pi}_q \\ \hline \end{array} \longrightarrow \begin{array}{|ccc|}\hline \theta & \phi & \rho \\ \hline \pi_\theta & \pi_\phi & \pi \\ \hline \end{array} \overset{non\ can.}{\longrightarrow} \begin{array}{|ccc|}\hline \theta & \phi & \rho \\ \hline \check{S}^1 & \check{S}^2 & \pi \\ \hline \end{array} ,$$

$$\rho^r=\rho R^{rs}(\theta,\phi)\hat{\rho}_0^s=\rho(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta),$$

$$\pi_q^r=R^{rs}(\theta,\phi)\,\check{\pi}_q^s=R^{rs}(\theta,\phi)\,\frac{m\check{v}^s}{\sqrt{4-\vec{v}^2}}$$

$$=R^{rs}(\theta,\phi)\,\frac{m[\rho\vec{\omega}\times\hat{\rho}_o+\dot{\rho}\hat{\rho}_o]^s}{\sqrt{4-\check{I}(\rho)\vec{\omega}^2-\dot{\rho}^2}}=R^{rs}(\theta,\phi)[\rho\check{I}^{-1}(\rho)\vec{S}\times\hat{\rho}_o+\pi\hat{\rho}_o]^s. \tag{6.12}$$

In conclusion, because of the lack of a workable Lagrangian approach, we are forced to try to define everything at the Hamiltonian level. Correspondingly, in order to get an extension for arbitrary N, abandoning the *static* orientation-shape bundle approach, we shall exploit the *canonical spin bases* technique utilized in the nonrelativistic case of Ref. 2. We will have to guess in some way a set of nonpoint canonical transformations getting from the canonical variables $\vec{\rho}_{qa}$, $\vec{\pi}_{qa}$ to a basis in which the results of the special case $N=2$ and equal masses can be explicitly generalized.

The nonrelativistic non-Abelian rotational symmetry generating the Noether constants of motion $\vec{S}=$constant will be replaced by the *internal* non-Abelian rotational symmetry generating the constants of motion $\vec{S}_q$ inside the Wigner hyperplane, with the rest-frame conditions $\vec{\kappa}_+\approx 0$.

VII. CANONICAL SPIN BASES

Because of the group-theoretical nature of our technique, the relativistic construction of the *canonical spin bases* with the associated *spin frame* and *evolving dynamical body frames*, starting from the relative canonical variables $\vec{\rho}_{qa}$, $\vec{\pi}_{qa}$, $a=1,..,N-1$, is identical to that proposed in Ref. 2 for the nonrelativistic case. More precisely, this occurs since the total conserved rest-frame spin maintains its nonrelativistic form $\vec{S}_q=\Sigma_{a=1}^{N-1}\vec{\rho}_{qa}\times\vec{\pi}_{qa}=\Sigma_{a=1}^{N-1}\vec{S}_{qa}$ and the construction is essentially based on the *spin clusterings* built from the individual $\vec{S}_{qa}$. Only the Hamiltonian for relative motions turns out to be different.

We shall report here the main results for $N=2$, $N=3$, and $N\geqslant 4$ by referring to Ref. 2 for the relevant calculations.

A. Two-body systems

Consider the initial transformation for the case $N=2$, $i=1,2$,

$$\begin{array}{|c|}\hline \vec{\eta}_i \\ \hline \vec{\kappa}_i \\ \hline \end{array} \longrightarrow \begin{array}{|cc|}\hline \vec{q}_+ & \vec{\rho}_q \\ \hline \vec{\kappa}_+ & \vec{\pi}_q \\ \hline \end{array} . \tag{7.1}$$

After the elimination of the internal center-of-mass degrees of freedom by means of the gauge fixings $\vec{q}_+\approx 0$, the rest-frame dynamics of the relative motions is ruled by the Hamiltonian

$$H_{(\mathrm{rel})}=\sqrt{m_1^2+\vec{\pi}_q^2}+\sqrt{m_2^2+\vec{\pi}_q^2}\equiv M_{\mathrm{sys}}. \tag{7.2}$$

The spin is $\vec{S}_q=\vec{\rho}_q\times\vec{\pi}_q$ $[S_q=\sqrt{\vec{S}_q^2}]$. Define the following decomposition (the notation $\hat{R}$ for the unit vector $\hat{\rho}_q$ is used for comparison with Ref. 39)

$$\vec{\rho}_q=\rho_q\hat{R},\quad \rho_q=\sqrt{\vec{\rho}_q^2},\quad \hat{R}=\frac{\vec{\rho}_q}{\rho_q}=\hat{\rho}_q,\quad \hat{R}^2=1, \tag{7.3}$$

$$\vec{\pi}_q=\tilde{\pi}_q\hat{R}-\frac{S_q}{\rho_q}\hat{R}\times\hat{S}_q=\tilde{\pi}_q\hat{\rho}_q-\frac{S_q}{\rho_q}\hat{\rho}_q\times\hat{S}_q,\quad \tilde{\pi}_q=\vec{\pi}_q\cdot\hat{R}=\vec{\pi}_q\cdot\hat{\rho}_q,\quad \hat{S}_q=\frac{\vec{S}_q}{S_q},\quad \hat{S}_q\cdot\hat{R}=0.$$

The *spin frame* of R^3 is defined by $\hat{S}_q$, $\hat{R}$, $\hat{R}\times\hat{S}_q$ with $\{S_q^i,S_q^j\}=\epsilon^{ijk}S_q^k$, $\{\hat{R}^i,\hat{R}^j\}=0$, $\{\hat{R}^i,S_q^j\}=\epsilon^{ijk}\hat{R}^k$. The vectors $\vec{S}_q$ and $\hat{R}$ are the generators of an E(3) group containing SO(3) as a subgroup.

Consider the canonical transformation adapted to the *spin*

$$\left[\begin{array}{c}\vec{\rho}_q\\ \vec{\pi}_q\end{array}\right]\quad\longrightarrow\quad\left[\begin{array}{cc|c}\alpha & \beta & \rho_q\\ S_q & S_q^3 & \tilde{\pi}_q\end{array}\right]\quad, \tag{7.4}$$

where

$$\alpha=\mathrm{tg}^{-1}\frac{1}{S_q}\left(\vec{\rho}_q\cdot\vec{\pi}_q-\frac{(\rho_q)^2}{\rho_q^3}\pi_q^3\right),\quad \beta=\mathrm{tg}^{-1}\frac{S_q^2}{S_q^1}. \tag{7.5}$$

It holds

$$S_q^1=\sqrt{(S_q)^2-(S_q^3)^2}\cos\beta,\quad S_q^2=\sqrt{(S_q)^2-(S_q^3)^2}\sin\beta,\quad S_q^3, \tag{7.6}$$

$$\hat{R}^1=\hat{\rho}_q^1=\sin\theta\cos\varphi=\sin\beta\sin\alpha-\frac{S_q^3}{S_q}\cos\beta\cos\alpha,$$

$$\hat{R}^2=\hat{\rho}_q^2=\sin\theta\sin\varphi=-\cos\beta\sin\alpha-\frac{S_q^3}{S_q}\sin\beta\cos\alpha,$$

$$\hat{R}^3=\hat{\rho}_q^3=\cos\theta=\frac{1}{S_q}\sqrt{(S_q)^2-(S_q^3)^2}\cos\alpha,$$

$$(\hat{S}_q\times\hat{R})^1=\hat{S}_q^2\hat{R}^3-\hat{S}_q^3\hat{R}^2=\sin\beta\cos\alpha+\frac{S_q^3}{S_q}\cos\beta\sin\alpha,$$

$$(\hat{S}_q\times\hat{R})^2=\hat{S}_q^3\hat{R}^1-\hat{S}_q^1\hat{R}^3=-\cos\beta\cos\alpha+\frac{S_q^3}{S_q}\sin\beta\sin\alpha, \tag{7.7}$$

$$(\hat{S}_q\times\hat{R})^3=-\hat{S}_q^1\hat{R}^2-\hat{S}_q^2\hat{R}^1=\frac{1}{S_q}\sqrt{(S_q)^2-(S_q^3)^2}\sin\alpha,$$

with the inverse canonical transformation

$$\vec{\rho}_q=\rho_q\hat{R}(\alpha,\beta,S_q,S_q^3),$$

$$\vec{\pi}_q=\tilde{\pi}_q\hat{R}(\alpha,\beta,S_q,S_q^3)-\frac{S_q}{\rho_q}\hat{R}(\alpha,\beta,S_q,S_q^3)\times\hat{S}_q(\beta,S_q,S_q^3),$$

$$\Rightarrow\vec{\pi}_q^2=\tilde{\pi}_q^2+\frac{S_q^2}{\rho_q^2},\quad \hat{S}_q\times\hat{R}(\alpha)=\frac{\partial\hat{R}(\alpha)}{\partial\alpha}=\hat{R}\left(\alpha+\frac{\pi}{2}\right),$$

$$\Rightarrow\alpha=-\operatorname{tg}^{-1}\frac{(\hat{S}_q\times\hat{R})^3}{[\hat{S}_q\times(\hat{S}_q\times\hat{R})]^3}. \tag{7.8}$$

From the last line of this equation it is seen that the angle α can be expressed in terms of $\hat{S}_q$ and $\hat{R}$.

The conjugate variables ρ_q, $\tilde{\pi}_q$ will be called *dynamical shape variables*: they describe the vibration of the dipole.

The rest-frame Hamiltonian for the relative motion becomes

$$H_{(\mathrm{rel})}=H_M(\infty)=\sqrt{m_1^2+\vec{\pi}_q^2}+\sqrt{m_2^2+\vec{\pi}_q^2}=\sqrt{m_1^2+\frac{1}{\breve{I}}(S_q)^2+\tilde{\pi}_q^2}+\sqrt{m_2^2+\frac{1}{\breve{I}}(S_q)^2+\tilde{\pi}_q^2},$$

$$\Rightarrow\breve{\omega}\overset{\circ}{=}\frac{\partial H_{(\mathrm{rel})}}{\partial S_q}=\frac{S_q}{\breve{I}}\left(\frac{1}{\sqrt{m_1^2+\frac{1}{\breve{I}}(S_q)^2+\tilde{\pi}_q^2}}+\frac{1}{\sqrt{m_2^2+\frac{1}{\breve{I}}(S_q)^2+\tilde{\pi}_q^2}}\right),$$

$$\dot{\rho}_q\overset{\circ}{=}\frac{\partial H_{(\mathrm{rel})}}{\partial\tilde{\pi}_q}=\tilde{\pi}_q\left(\frac{1}{\sqrt{m_1^2+\frac{1}{\breve{I}}(S_q)^2+\tilde{\pi}_q^2}}+\frac{1}{\sqrt{m_2^2+\frac{1}{\breve{I}}(S_q)^2+\tilde{\pi}_q^2}}\right),$$

$$\tilde{\pi}_q\big|_{\dot{\rho}_q=0}=0,$$

$$H_{(\mathrm{rel})}^{(S)}=H_{(\mathrm{rel})}\big|_{\dot{\rho}_q=0}=\sqrt{m_1^2+\frac{1}{\breve{I}}(S_q)^2}+\sqrt{m_2^2+\frac{1}{\breve{I}}(S_q)^2}, \tag{7.9}$$

$$H_{(\mathrm{rel})}^{(S=0)}=H_{(\mathrm{rel})}\big|_{S_q=0}=\sqrt{m_1^2+\tilde{\pi}_q^2}+\sqrt{m_2^2+\tilde{\pi}_q^2},$$

where $\breve{I}=\rho_q^2=\breve{I}_{\mathrm{nr}}/\mu$ is the nonrelativistic baricentric inertia tensor $\breve{I}_{\mathrm{nr}}$ of the dipole divided by the reduced mass $\mu=m_1m_2/(m_1+m_2)$. The quantities $H_{(\mathrm{rel})}^{(S)}$ and $H_{(\mathrm{rel})}^{(S=0)}$ are the purely rotational and purely vibrational Hamiltonians, respectively.

For equal masses, by making the identifications $\pi=\tilde{\pi}_q$, $\rho=\rho_q$, and $\hat{R}^r=R^{rs}(\theta,\phi)\hat{\rho}_0^s$, we get formally the same results of the previous section but in a different canonical basis. Only after a nonpoint transformation α, S_q, β, $S_q^3\mapsto\theta$, π_θ, ϕ, π_ϕ [i.e. from Eqs. (7.7) to (7.4)], Eq. (7.11) becomes Eq. (6.12).

B. Three-body systems

For $N=3$ the range of the indices is $i=1,2,3$, $a=1,2$. The spin is $\vec{S}_q=\Sigma_{a=1}^{2}\vec{\rho}_{qa}\times\vec{\pi}_{qa}=\Sigma_{a=1}^{2}\vec{S}_{qa}$ after the canonical transformation which separates the internal center of mass

$$\boxed{\begin{array}{|c|}\hline \vec{\eta}_i \\ \hline \vec{\kappa}_i \\ \hline \end{array}} \longrightarrow \boxed{\begin{array}{|c|c|}\hline \vec{q}_+ & \vec{\rho}_{qa} \\ \hline \vec{\kappa}_+ & \vec{\pi}_{qa} \\ \hline \end{array}} \quad . \tag{7.10}$$

Upon the gauge fixings $\vec{q}_+\approx 0$, the relative motions in the rest-frame instant form are ruled by the Hamiltonian

$$H_{(\mathrm{rel})}=H_M(\infty)=\sum_{i=1}^{3}\sqrt{m_i^2+3\sum_{a,b=1}^{2}\gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}}\equiv M_{\mathrm{sys}}. \tag{7.11}$$

We shall assume $\vec{S}_q\neq 0$, because the exceptional SO(3) orbit $S_q=0$ has to be studied separately.[2]

For each value of $a=1,\ 2$ consider the canonical transformation (7.7)

$$\boxed{\begin{array}{|c|}\hline \vec{\rho}_{qa} \\ \hline \vec{\pi}_{qa} \\ \hline \end{array}} \longrightarrow \boxed{\begin{array}{|c|c|c|}\hline \alpha_a & \beta_a & \rho_{qa} \\ \hline S_{qa} & S_{qa}^3 & \tilde{\pi}_{qa} \\ \hline \end{array}} \quad , \tag{7.12}$$

where

$$\alpha_a=\mathrm{tg}^{-1}\frac{1}{S_{qa}}\left(\vec{\rho}_{qa}\cdot\vec{\pi}_{qa}-\frac{(\rho_{qa})^2}{\rho_{qa}^3}\pi_{qa}^3\right),$$

$$\beta_a=\mathrm{tg}^{-1}\frac{S_{qa}^2}{S_{qa}^1},\quad \sin\beta_a=\frac{S_{qa}^2}{\sqrt{(S_{qa})^2-(S_{qa}^3)^2}},\quad \cos\beta_a=\frac{S_{qa}^1}{\sqrt{(S_{qa})^2-(S_{qa}^3)^2}}, \tag{7.13}$$

$$\vec{\rho}_{qa}=\rho_{qa}\hat{R}_a,\quad \rho_{qa}=\sqrt{\vec{\rho}_{qa}^2},\quad \hat{R}_a=\frac{\vec{\rho}_{qa}}{\rho_{qa}}=\hat{\rho}_{qa},\quad \hat{R}_a^2=1,$$

$$\vec{\pi}_{qa}=\tilde{\pi}_{qa}\hat{R}_a-\frac{S_{qa}}{\rho_{qa}}\hat{R}_a\times\hat{S}_{qa},\quad \tilde{\pi}_{qa}=\vec{\pi}_{qa}\cdot\hat{R}_a. \tag{7.14}$$

We now have *two* unit vectors $\hat{R}_a$ and *two* E(3) realizations generated by $\vec{S}_{qa}$, $\hat{R}_a$, respectively, with fixed invariants $\hat{R}_a^2=1$, $\vec{S}_{qa}\cdot\hat{R}_a=0$ (*nonirreducible, type 2*[39]).

Now, we want to implement a SO(3) *Hamiltonian right action* in analogy with the rigid body theory. To this aim, we must construct an orthonormal triad or *body frame* $\hat{N}$, $\hat{\chi}$, $\hat{N}\times\hat{\chi}$. The decomposition $\vec{S}=\check{S}^1\hat{\chi}+\check{S}^2\hat{N}\times\hat{\chi}+\check{S}^3\hat{N}\equiv\check{S}^r\hat{e}_r$, identifies the SO(3) scalar generators $\check{S}^r$ of the right action provided they satisfy $\{\check{S}^r,\check{S}^s\}=-\epsilon^{rsu}\check{S}^u$. This latter condition together with the obvious requirement that $\hat{N}$, $\hat{\chi}$, $\hat{N}\times\hat{\chi}$ be SO(3) vectors $[\{\hat{N}^r,S^s\}=\epsilon^{rsu}\hat{N}^u,\ \{\hat{\chi}^r,S^s\}=\epsilon^{rsu}\hat{\chi}^u,\ \{\hat{N}\times\hat{\chi}^r,S^s\}=\epsilon^{rsu}\hat{N}\times\hat{\chi}^u]$ entails the equations $\{\hat{N}^r,\hat{N}^s\}=\{\hat{N}^r,\hat{\chi}^s\}=\{\hat{\chi}^r,\hat{\chi}^s\}=0$.

To each solution of these equations is associated a couple of canonical realizations of the E(3) group (*nonirreducible, type 2*): one with generators $\vec{S}$, $\vec{N}$ and nonfixed invariants $\check{S}^3=\vec{S}\cdot\hat{N}$ and $|\vec{N}|$; another with generators $\vec{S}$, $\vec{\chi}$ and nonfixed invariants $\check{S}^1=\vec{S}\cdot\hat{\chi}$ and $|\vec{\chi}|$. These realizations contain the relevant information for constructing the angle α and the new canonical pair $\check{S}^3$, $\gamma=\mathrm{tg}^{-1}\check{S}^2/\check{S}^1$ of SO(3) scalars. Since $\{\alpha,\check{S}^3\}=\{\alpha,\gamma\}=0$ must hold, it follows that the vector $\vec{N}$ necessarily belongs to the $\vec{S}-\hat{R}$ plane. The three canonical pairs S, α, S^3, β, $\check{S}^3$, γ will describe

the *orientational* variables of our Darboux basis, while $|\vec{N}|$ and $|\vec{\chi}|$ will belong to the *shape* variables. Alternatively, an anholonomic basis can be constructed by replacing the above-mentioned six variables by $\check{S}^r$ and three uniquely determined Euler angles $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$.

In the $N=3$ case it turns out that a solution of the previous equation exists corresponding to a *body frame* determined by the three-body system configuration only, as in the *rigid body* case. This solution is completely identified once two orthonormal vectors $\vec{N}$ and $\vec{\chi}$, functions of the relative coordinates and independent of the momenta, are found such that $\vec{N}$ lies in the $\vec{S}-\hat{R}$ plane.[51]

The *simplest choice* for the orthonormal vectors $\vec{N}$ and $\vec{\chi}$, functions of the coordinates alone, is

$$\vec{N}=\frac{1}{2}(\hat{R}_1+\hat{R}_2)=\frac{1}{2}(\hat{\rho}_{q1}+\hat{\rho}_{q2}),\quad \hat{N}=\frac{\vec{N}}{|\vec{N}|},\quad |\vec{N}|=\sqrt{\frac{1+\hat{\rho}_{q1}\cdot\hat{\rho}_{q2}}{2}},$$

$$\vec{\chi}=\frac{1}{2}(\hat{R}_1-\hat{R}_2)=\frac{1}{2}(\hat{\rho}_{q1}-\hat{\rho}_{q2}),\quad \hat{\chi}=\frac{\vec{\chi}}{|\vec{\chi}|},\quad |\vec{\chi}|=\sqrt{\frac{1-\hat{\rho}_{q1}\cdot\hat{\rho}_{q2}}{2}}=\sqrt{1-\vec{N}^2},$$

$$\vec{N}\times\vec{\chi}=-\frac{1}{2}\hat{\rho}_{q1}\times\hat{\rho}_{q2},\quad |\vec{N}\times\vec{\chi}|=|\vec{N}||\vec{\chi}|=\frac{1}{2}\sqrt{1-(\hat{\rho}_{q1}\cdot\hat{\rho}_{q2})^2}, \tag{7.15}$$

$$\vec{N}\cdot\vec{\chi}=0,\quad \{N^r,N^s\}=\{\chi^r,\chi^s\}=\{N^r,\chi^s\}=0,$$

$$\hat{R}_1=\hat{\rho}_{q1}=\vec{N}+\vec{\chi},\quad \hat{R}_2=\hat{\rho}_{q2}=\vec{N}-\vec{\chi},\quad \hat{R}_1\cdot\hat{R}_2=\hat{\rho}_{q1}\cdot\hat{\rho}_{q2}=\vec{N}^2-\vec{\chi}^2.$$

Likewise, we have for the spins

$$\vec{S}_q=\vec{S}_{q1}+\vec{S}_{q2},\quad \vec{W}_q=\vec{S}_{q1}-\vec{S}_{q2},\quad \{W_q^r,W_q^s\}=\epsilon^{rsu}S_q^u,$$
$$\vec{S}_{q1}=\tfrac{1}{2}(\vec{S}_q+\vec{W}_q),\quad \vec{S}_{q2}=\tfrac{1}{2}(\vec{S}_q-\vec{W}_q). \tag{7.16}$$

In this way, we succeeded in constructing an orthonormal triad (the *dynamical body frame*) and two E(3) realizations: one with generators $\vec{S}_q$, $\vec{N}$ and nonfixed invariants $|\vec{N}|$ and $\vec{S}\cdot\hat{N}$, the other with generators $\vec{S}_q$ and $\vec{\chi}$ and nonfixed invariants $|\vec{\chi}|$ and $\vec{S}_q\cdot\hat{\chi}$. As said in Ref. 2 this is equivalent to the determination of the nonconserved generators $\check{S}_q^r$ of a Hamiltonian *right action* of SO(3): $\check{S}_q^1=\vec{S}_q\cdot\hat{\chi}=\vec{S}_q\cdot\hat{e}_1$, $\check{S}_q^2=\vec{S}_q\cdot\hat{N}\times\hat{\chi}=\vec{S}_q\cdot\hat{e}_2$, $\check{S}_q^3=\vec{S}_q\cdot\hat{N}=\vec{S}_q\cdot\hat{e}_3$.

The realization of the E(3) group with generators $\vec{S}_q$, $\vec{N}$ and nonfixed invariants $\mathcal{I}_1=\vec{N}^2$, $\mathcal{I}_2=\vec{S}_q\cdot\vec{N}$ leads to the final canonical transformation

$$\left|\begin{array}{c}\vec{\rho}_{qa}\\ \vec{\pi}_{qa}\end{array}\right| \longrightarrow \left|\begin{array}{cccc|c}\alpha_1 & \beta_1 & \alpha_2 & \beta_2 & \rho_{qa}\\ S_{q1} & S_{q1}^3 & S_{q2} & S_{q2}^3 & \tilde{\pi}_{qa}\end{array}\right| \longrightarrow \left|\begin{array}{ccc|c|c}\alpha & \beta & \gamma & |\vec{N}| & \rho_{qa}\\ S_q=\check{S}_q & S_q^3 & \check{S}_q^3=\vec{S}_q\cdot\hat{N} & \xi & \tilde{\pi}_{qa}\end{array}\right|, \tag{7.17}$$

where

$$|\vec{N}| = \sqrt{\frac{1+\hat{\rho}_{q1}\cdot\hat{\rho}_{q2}}{2}},$$

$$\check{S}^3_q = \vec{S}_q\cdot\hat{N} = \frac{1}{\sqrt{2}}\sum_{a=1}^{2}\vec{\rho}_{qa}\times\vec{\pi}_{qa}\cdot\frac{\hat{\rho}_{q1}+\hat{\rho}_{q2}}{\sqrt{1+\hat{\rho}_{q1}\cdot\hat{\rho}_{q2}}} \equiv S_q\cos\psi,$$

$$\cos\psi = \hat{S}_q\cdot\hat{N} = \frac{\check{S}^3_q}{S_q}, \quad \sin\psi = \frac{1}{S_q}\sqrt{(S_q)^2-(\check{S}^3_q)^2},$$

$$S_q = \check{S}_q = \left|\sum_{a=1}^{2}\vec{\rho}_{qa}\times\vec{\pi}_{qa}\right|, \quad S^3_q = \sum_{a=1}^{2}(\vec{\rho}_{qa}\times\vec{\pi}_{qa})^3,$$

$$\alpha = -\mathrm{tg}^{-1}\frac{(\hat{S}_q\times\hat{N})^3}{[\hat{S}_q\times(\hat{S}_q\times\hat{N})]^3} = -\mathrm{tg}^{-1}\frac{[\hat{S}_q\times(\hat{\rho}_{q1}+\hat{\rho}_{q2})]^3}{[\hat{S}_q\times(\hat{S}_q\times[\hat{\rho}_{q1}+\hat{\rho}_{q2}])]^3},$$

$$\beta = \mathrm{tg}^{-1}\frac{S^2_q}{S^1_q},$$

$$\gamma = \mathrm{tg}^{-1}\frac{\vec{S}_q\cdot(\hat{N}\times\hat{\chi})}{\vec{S}_q\cdot\hat{\chi}} = \mathrm{tg}^{-1}\frac{\check{S}^2_q}{\check{S}^1_q},$$

$$\xi = \frac{\vec{W}_q\cdot(\hat{N}\times\hat{\chi})}{|\vec{\chi}|} = \frac{\sqrt{2}\Sigma^2_{a=1}(-)^{a+1}\vec{\rho}_{qa}\times\vec{\pi}_{qa}\cdot(\hat{\rho}_{q2}\times\hat{\rho}_{q1})}{[1-\hat{\rho}_{q1}\cdot\hat{\rho}_{q2}]\sqrt{1+\hat{\rho}_{q1}\cdot\hat{\rho}_{q2}}}. \tag{7.18}$$

For $N=3$ the *dynamical shape variables*, functions of the relative coordinates alone $\vec{\rho}_{qa}$, are $|\vec{N}|$, $\hat{\rho}_{qa}$, while the conjugate shape momenta are ξ, $\tilde{\pi}_{qa}$.

The final array (7.17) is nothing else than a *scheme* B[40] of a realization of an E(3) group with generators $\vec{S}_q$, $\vec{N}$ (*nonirreducible, type 3*). In particular, the two canonical pairs S^3_q, β, S_q, α, constitute the irreducible kernel of the E(3) *scheme A*, whose invariants are $\check{S}^3_q$, $|\vec{N}|$; γ and ξ are the so-called *supplementary variables* conjugated to the invariants; finally, the two pairs ρ_{qa}, $\tilde{\pi}_{qa}$ are so-called *inessential variables*. Let us remark that S^3_q, β, S_q, α, γ, ξ, are a local coordinatization of every E(3) coadjoint orbit with $\check{S}^3_q=$const, $|\vec{N}|=$const and fixed values of the inessential variables, present in the three-body phase space.

By using Eqs. (7.6), (7.7) and adopting the prescription of Eq. (7.10), we can reconstruct $\vec{S}_q$ and define a *new* unit vector $\hat{R}$ orthogonal to $\vec{S}_q$ and satisfying $\{\hat{R}^r,\hat{R}^s\}=0$.

The vectors $\hat{S}_q$, $\hat{R}$, $\hat{S}_q\times\hat{R}$ build up the *spin frame* for $N=3$. The angle α conjugate to S_q is explicitly given by[52]

$$\alpha = -\mathrm{tg}^{-1}\frac{(\hat{S}_q\times\hat{N})^3}{[\hat{S}_q\times(\hat{S}_q\times\hat{N})]^3} = -\mathrm{tg}^{-1}\frac{(\hat{S}_q\times\hat{R})^3}{[\hat{S}_q\times(\hat{S}_q\times\hat{R})]^3}. \tag{7.19}$$

As a consequence of this definition of $\hat{R}$, we get the following expressions for the *dynamical body frame* $\hat{N}$, $\hat{\chi}$, $\hat{N}\times\hat{\chi}$ in terms of the final canonical variables (see Ref. 2 for the explicit expressions and a geometric visualization)

$$\hat{N} = \cos\psi \hat{S}_q + \sin\psi \hat{R} = \hat{N}[S_q, \alpha; S^3_q, \beta; \check{S}^3_q, \gamma],$$

$$\hat{\chi} = \sin\psi \cos\gamma \hat{S}_q - \cos\psi \cos\gamma \hat{R} + \sin\gamma \hat{S}_q \times \hat{R} = \hat{\chi}[S_q, \alpha; S^3_q, \beta; \check{S}^3_q, \gamma],$$

$$\hat{N} \times \hat{\chi} = \sin\psi \sin\gamma \hat{S}_q - \cos\psi \sin\gamma \hat{R} - \cos\gamma \hat{S}_q \times \hat{R} = (\hat{N} \times \hat{\chi})[S_q, \alpha; S^3_q, \beta; \check{S}^3_q, \gamma],$$

$$\Downarrow$$

$$\hat{S}_q = \sin\psi \cos\gamma \hat{\chi} + \sin\psi \sin\gamma \hat{N} \times \hat{\chi} + \cos\psi \hat{N} \stackrel{\text{def}}{=} \frac{1}{S_q}[\check{S}^1_q \hat{\chi} + \check{S}^2_q \hat{N} \times \hat{\chi} + \check{S}^3_q \hat{N}],$$

$$\hat{R} = -\cos\psi \cos\gamma \hat{\chi} - \cos\psi \sin\gamma \hat{N} \times \hat{\chi} + \sin\psi \hat{N},$$

$$\hat{R} \times \hat{S}_q = -\sin\gamma \hat{\chi} + \cos\gamma \hat{N} \times \hat{\chi}. \tag{7.20}$$

While ψ is the angle between $\hat{S}_q$ and $\hat{N}$, γ is the angle between the plane $\hat{N}-\hat{\chi}$ and the plane $\hat{S}_q - \hat{N}$. As in the case $N=2$, α is the angle between the plane $\hat{S}_q - \hat{f}_3$ and the plane $\hat{S}_q - \hat{R}$, while β is the angle between the plane $\hat{S}_q - \hat{f}_3$ and the plane $\hat{f}_3 - \hat{f}_1$.

Owing to the results of Appendix C of Ref. 2, which allow one to reexpress

$$S_{qa} = |\vec{S}_{qa}|, \quad S^3_{qa}, \quad \beta_a = \mathrm{tg}^{-1}\frac{S^2_{qa}}{S^1_{qa}}, \quad \text{and} \quad \alpha_a = -\mathrm{tg}^{-1}\frac{(\hat{S}_{qa} \times \hat{R}_a)^3}{(\hat{S}_{qa} \times (\hat{S}_{qa} \times \hat{R}_a))^3}$$

in terms of the final variables, we can reconstruct the inverse canonical transformation.

The existence of the *spin frame* and of the *dynamical body frame* allows one to define two decompositions of the relative variables, which make the inverse canonical transformation explicit. For the relative coordinates, from Eq. (7.15) and Appendix C of I, we obtain

$$\begin{aligned}
\vec{\rho}_{qa} &= \rho_{qa}\hat{R}_a = \rho_{qa}[\vec{N} + (-)^{a+1}\vec{\chi}] = \rho_{qa}[|\vec{N}|\hat{N} + (-)^{a+1}\sqrt{1-\vec{N}^2}\hat{\chi}] \\
&= [\vec{\rho}_{qa} \cdot \hat{S}_q]\hat{S}_q + [\vec{\rho}_{qa} \cdot \hat{R}]\hat{R} + [\vec{\rho}_{qa} \cdot \hat{S}_q \times \hat{R}]\hat{S}_q \times \hat{R} \\
&= \frac{\rho_{qa}}{S_q}\Bigg[(|\vec{N}|\check{S}^3_q + (-)^{a+1}\sqrt{1-\vec{N}^2}\,\check{S}^1_q)\hat{S}_q + \Bigg(|\vec{N}|\sqrt{(S_q)^2 - (\check{S}^3_q)^2} \\
&\quad - (-)^{a+1}\sqrt{1-\vec{N}^2}\frac{\check{S}^1_q \check{S}^3_q}{\sqrt{(S_q)^2 - (\check{S}^3_q)^2}} \Bigg)\hat{R} \\
&\quad - (-)^{a+1}\sqrt{1-\vec{N}^2}\,\frac{\check{S}^2_q}{\sqrt{(S_q)^2 - (\check{S}^3_q)^2}}\hat{S}_q \times \hat{R} \Bigg] \\
&= \vec{\rho}_{qa}[S_q, \alpha; S^3_q, \beta; \check{S}^3_q, \gamma; \rho_{qa}, |\vec{N}|].
\end{aligned} \tag{7.21}$$

The results of Appendix C of Ref. 2 give the analogous formulas for the relative momenta.

As shown in Ref. 2, it is possible to perform a sequence of a canonical transformation to Euler angles $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ with their conjugate momenta, followed by a transition to the anholonomic basis used in the orientation-shape bundle approach[1]

$$\boxed{\begin{array}{|ccc|}\hline \alpha & \beta & \gamma \\ S_q = \check{S}_q & S_q^3 & \check{S}_q^3 \\ \hline\end{array}} \longrightarrow \boxed{\begin{array}{|ccc|}\hline \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} \\ p_{\tilde{\alpha}} & p_{\tilde{\beta}} & p_{\tilde{\gamma}} \\ \hline\end{array}} \overset{non\ can.}{\longrightarrow} \boxed{\begin{array}{|ccc|}\hline \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} \\ \check{S}_q^1 & \check{S}_q^2 & \check{S}_q^3 \\ \hline\end{array}} ,$$

$$S_q = \check{S}_q = \sqrt{(\check{S}_q^1)^2 + (\check{S}_q^2)^2 + (\check{S}_q^3)^2},$$

$$S_q^3 = -\sin\tilde{\beta}\cos\tilde{\gamma}\check{S}_q^1 + \sin\tilde{\beta}\sin\tilde{\gamma}\check{S}_q^2 + \cos\tilde{\beta}\check{S}_q^3,$$

$$\alpha = \mathrm{arctg}\frac{p_{\tilde{\beta}} tg\,\tilde{\beta}}{\check{S}_q - \dfrac{p_{\tilde{\alpha}} p_{\tilde{\gamma}}}{\check{S}_q \cos\tilde{\beta}}}, \quad \beta = \tilde{\alpha} + \mathrm{arctg}\frac{\mathrm{ctg}\,\tilde{\beta} p_{\tilde{\alpha}} - \dfrac{p_{\tilde{\gamma}}}{\sin\tilde{\beta}}}{p_{\tilde{\beta}}} - \frac{\pi}{2},$$

$$\gamma = \frac{\pi}{2} - \tilde{\gamma} - \mathrm{arctg}\frac{\mathrm{ctg}\,\tilde{\beta} p_{\tilde{\gamma}} - \dfrac{p_{\tilde{\alpha}}}{\sin\tilde{\beta}}}{p_{\tilde{\beta}}},$$

(7.22)

with the *dynamical orientation variables* $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ determined in terms of $\vec{\rho}_{qa}$, $\vec{\pi}_{qa}$. Let us stress that, while in the orientation-shape bundle approach the orientation variables θ^α are gauge variables, the Euler angles $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ we are using here are *uniquely determined* in terms of the original variables.

In conclusion, the complete transition to the anholonomic basis used in the *static* theory of the orientation-shape bundle is

$$\boxed{\begin{array}{|ccc|c|c|}\hline \alpha & \beta & \gamma & |\vec{N}| & \rho_{qa} \\ S_q = \check{S}_q & S_q^3 & \check{S}_q^3 & \xi & \tilde{\pi}_{qa} \\ \hline\end{array}} \overset{non\ can.}{\longrightarrow} \boxed{\begin{array}{|ccc|c|c|}\hline \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} & |\vec{N}| & \rho_{qa} \\ \check{S}_q^1 & \check{S}_q^2 & \check{S}_q^3 & \xi & \tilde{\pi}_{qa} \\ \hline\end{array}} ,$$

(7.23)

with the three pairs of conjugate canonical dynamical shape variables: ρ_{qa}, $\tilde{\pi}_{qa}$, $|\vec{N}|$, ξ and with

$$\rho_{qa}^r = \mathcal{R}^r{}_s(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{\rho}_{qa}^s(q),$$

with

$$\check{\rho}_{qa}^1(q) = (-)^{a+1}\rho_{qa}\sqrt{1-\vec{N}^2}, \quad \check{\rho}_{qa}^2(q) = 0, \quad \check{\rho}_{qa}^3(q) = \rho_{qa}|\vec{N}|,$$
$$S_q^r = \mathcal{R}^r{}_s(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\check{S}_q^s.$$

(7.24)

The final visualization of our sequence of transformations is

$$\boxed{\begin{array}{|c|}\hline \vec{\rho}_{qa} \\ \vec{\pi}_{qa} \\ \hline\end{array}} \overset{non\ can.}{\longrightarrow} \boxed{\begin{array}{|ccc|c|}\hline \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} & q^\mu(\vec{\rho}_{qa}) \\ \check{S}_q^1 & \check{S}_q^2 & \check{S}_q^3 & p_\mu(\vec{\rho}_{qa},\vec{\pi}_{qa}) \\ \hline\end{array}} .$$

(7.25)

Note incidentally that we have $\check{\rho}_{qa}^2 = \vec{\rho}_{qa}\cdot\hat{N}\times\hat{\chi} = 0$ by construction, and this entails that using our *dynamical body frame* is equivalent to a convention (*xxzz gauge*) about the body frame of the type of *xxz* and similar gauges quoted in Ref. 1.

The kinematical calculations of Appendix E of Ref. 46 allow one to obtain the following expression of the Hamiltonian for the relative motions in terms of the anholonomic Darboux basis (7.22):

$$H_{(\mathrm{rel})} \equiv M_{\mathrm{sys}} = H_M(\infty) = \sum_{i=1}^{3} \sqrt{m_i^2 + 3 \sum_{a,b=1}^{2} \gamma_{ai}\gamma_{bi}\vec{\pi}_{qa}\cdot\vec{\pi}_{qb}} = \sum_{i=1}^{3} \Bigg(m_i^2 + \frac{3}{\vec{N}^2}\Bigg[\frac{(\gamma_{1i})^2}{2\rho_{q1}^2} + \frac{(\gamma_{2i})^2}{2\rho_{q2}^2}$$
$$+ \frac{\gamma_{1i}\gamma_{2i}}{\rho_{q1}\rho_{q2}}\Bigg](\check{S}_q^1)^2 + 3\Bigg[\frac{(\gamma_{1i})^2}{2\rho_{q1}^2} + \frac{(\gamma_{2i})^2}{2\rho_{q2}^2} + \frac{\gamma_{1i}\gamma_{2i}(2\vec{N}^2-1)}{\rho_{q1}\rho_{q2}}\Bigg](\check{S}_q^2)^2 + \frac{3}{1-\vec{N}^2}\Bigg[\frac{(\gamma_{1i})^2}{2\rho_{q1}^2} + \frac{(\gamma_{2i})^2}{2\rho_{q2}^2}$$
$$- \frac{\gamma_{1i}\gamma_{2i}}{\rho_{q1}\rho_{q2}}\Bigg](\check{S}_q^3)^2 + 3\sqrt{1-\vec{N}^2}\Bigg[\xi\Bigg(\frac{(\gamma_{1i})^2}{2\rho_{q1}^2} - \frac{(\gamma_{2i})^2}{2\rho_{q2}^2}\Bigg) + 4\gamma_{1i}\gamma_{2i}|\vec{N}|\sqrt{1-\vec{N}^2}\Bigg(\frac{\tilde{\pi}_{q1}}{\rho_{q2}} - \frac{\tilde{\pi}_{q2}}{\rho_{q1}}\Bigg)\Bigg]\check{S}_q^2$$
$$- \frac{3}{|\vec{N}|\sqrt{1-\vec{N}^2}}\Bigg(\frac{(\gamma_{1i})^2}{\rho_{q1}^2} - \frac{(\gamma_{2i})^2}{\rho_{q2}^2}\Bigg)\check{S}_q^1\check{S}_q^3 + 6(\gamma_{1i})^2\Bigg[\tilde{\pi}_{q1}^2 + \frac{\xi^2(1-\vec{N}^2)}{4\rho_{q1}^2}\Bigg] + 6(\gamma_{2i})^2\Bigg[\tilde{\pi}_{q2}^2$$
$$+ \frac{\xi^2(1-\vec{N}^2)}{4\rho_{q2}^2}\Bigg] + 12\gamma_{1i}\gamma_{2i}\Bigg[(2\vec{N}^2-1)\tilde{\pi}_{q1}\tilde{\pi}_{q2} - |\vec{N}|(1-\vec{N}^2)\xi\Bigg(\frac{\tilde{\pi}_{q1}}{\rho_{q2}} + \frac{\tilde{\pi}_{q2}}{\rho_{q1}}\Bigg)$$
$$+ \frac{\xi^2(1-\vec{N}^2)(2\vec{N}^2-1)}{4\rho_{q1}\rho_{q2}}\Bigg]\Bigg)^{1/2} = \sum_{i=1}^{3} H_{(\mathrm{rel})i}, \tag{7.26}$$

where $q^\mu = (\rho_{q1}, \rho_{q2}, |\vec{N}|)$, $p_\mu = (\tilde{\pi}_{q1}, \tilde{\pi}_{q2}, \xi)$ are the dynamical shape variables.

In Ref. 46, this Hamiltonian is put in a form reminiscent of the nonrelativistic orientation-shape bundle approach. It is also shown how to recover the nonrelativistic Hamiltonian (with its splitting in rotational and vibrational parts) and the tensor of inertia in the nonrelativistic limit. We could also define rotational and vibrational relativistic Hamiltonians, but the total Hamiltonian would not result to be their sum.

C. *N*-body systems

Finally, we shall discuss the general case with $N \geqslant 4$. Unlike the method of the Jacobi coordinates, based on coupling the *center-of-mass clusters*, our method of the *canonical spin bases* is based on coupling the spins of the two-body subsystems (*relative particles*) $\vec{\rho}_{qa}$, $\vec{\pi}_{qa}$, $a = 1,..,N-1$, defined in Eq. (3.6), in all possible ways (*spin clusters* from the addition of angular momenta). Let us stress that we can build a *spin basis* with a pattern of *spin clusters* which is completely unrelated to a possible pre-existing *center-of-mass clustering.*

Consider the case $N=4$ as a prototype of the general construction. We have now three relative variables $\vec{\rho}_{q1}$, $\vec{\rho}_{q2}$, $\vec{\rho}_{q3}$ and related momenta $\vec{\pi}_{q1}$, $\vec{\pi}_{q2}$, $\vec{\pi}_{q3}$. In the following formulas we use the convention that the subscripts a, b, c mean any permutation of 1,2,3.

As in Ref. 2, we define a sequence of canonical transformations corresponding to the *spin clustering* pattern $abc \mapsto (ab)c \mapsto ((ab)c)$: first build the spin cluster (ab), then the spin cluster $((ab)c)$, (assume $S_q \neq = 0$; $S_{qA} \neq = 0$, $A = a, b, c$):

$$
\begin{array}{l}
\boxed{\begin{array}{|ccc|}\hline \vec{\rho}_{qa} & \vec{\rho}_{qb} & \vec{\rho}_{qc} \\ \vec{\pi}_{qa} & \vec{\pi}_{qb} & \vec{\pi}_{qc} \\ \hline\end{array}} \longrightarrow \\
\longrightarrow \boxed{\begin{array}{|cc|cc|cc|ccc|}\hline \alpha_a & \beta_a & \alpha_b & \beta_b & \alpha_c & \beta_c & \rho_{qa} & \rho_{qb} & \rho_{qc} \\ S_{qa} & S^3_{qa} & S_{qb} & S^3_{qb} & S_{qc} & S^3_{qc} & \tilde{\pi}_{qa} & \tilde{\pi}_{qb} & \tilde{\pi}_{qc} \\ \hline\end{array}} \longrightarrow \\
\xrightarrow{(ab)c} \boxed{\begin{array}{|ccc|cc|ccc|}\hline \alpha_{(ab)} & \beta_{(ab)} & \gamma_{(ab)} & \alpha_c & \beta_c & |\vec{N}_{(ab)}| & \rho_{qa} & \rho_{qb} & \rho_{qc} \\ S_{q(ab)} & S^3_{q(ab)} & \check{S}^3_{q(ab)} = \vec{S}_{q(ab)} \cdot \hat{N}_{(ab)} & S_{qc} & S^3_{qc} & \xi_{(ab)} & \tilde{\pi}_{qa} & \tilde{\pi}_{qb} & \tilde{\pi}_{qc} \\ \hline\end{array}} \longrightarrow \\
\longrightarrow \boxed{\begin{array}{|ccc|ccc|ccc|}\hline \alpha_{((ab)c)} & \beta_{((ab)c)} & \gamma_{((ab)c)} & |\vec{N}_{((ab)c)}| & \gamma_{(ab)} & |\vec{N}_{(ab)}| & \rho_{qa} & \rho_{qb} & \rho_{qc} \\ S_q = \check{S}_q & S^3_q & \check{S}^3_q = \vec{S}_q \cdot \hat{N}_{((ab)c)} & \xi_{((ab)c)} & \vec{S}_{q(ab)} \cdot \hat{N}_{(ab)} & \xi_{(ab)} & \tilde{\pi}_{qa} & \tilde{\pi}_{qb} & \tilde{\pi}_{qc} \\ \hline\end{array}} \longrightarrow \\
\xrightarrow{non\,can.} \boxed{\begin{array}{|ccc|ccc|ccc|}\hline \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} & |\vec{N}_{((ab)c)}| & \gamma_{(ab)} & |\vec{N}_{(ab)}| & \rho_{qa} & \rho_{qb} & \rho_{qc} \\ \check{S}^1_q & \check{S}^2_q & \check{S}^3_q & \xi_{((ab)c)} & \Omega_{(ab)} = \vec{S}_{q(ab)} \cdot \hat{N}_{(ab)} & \xi_{(ab)} & \tilde{\pi}_{qa} & \tilde{\pi}_{qb} & \tilde{\pi}_{qc} \\ \hline\end{array}}
\end{array}
\tag{7.27}
$$

See Appendix F of Ref. 2 for the explicit construction of the canonical transformations.

The first nonpoint canonical transformation is based on the existence of the three unit vectors $\hat{R}_A$, $A=a,\ b,\ c$, and of three E(3) groups with fixed values ($\hat{R}^2_A=1$, $\vec{S}_A\cdot\hat{R}_A=0$) of their invariants. Use Eqs. (7.13) and (7.14).

In the next canonical transformation the spins of the *relative particles a* and *b* are coupled to form the spin cluster (ab), leaving the *relative particle c* as a spectator. As said in Ref. 2 the cluster (ab) has a unit vector $\hat{R}_{(ab)}$ with $\vec{S}_{(ab)}\cdot\hat{R}_{(ab)}=0$, $\{\hat{R}^r_{(ab)},\hat{R}^s_{(ab)}\}=0$. This unit vector identifies the *spin cluster* (ab) in the same way as the unit vectors $\hat{R}_A=\hat{\vec{\rho}}_{qA}$ identify the *relative particles A*.

The next step is the coupling of the *spin cluster* (ab) with unit vector $\hat{R}_{(ab)}$ with the *relative particle c* with unit vector $\hat{R}_c$ and described by α_c, S_{qc}, β_c, S^3_{qc}: this builds the *spin cluster* $((ab)c)$. As shown in Ref. 2 it is possible to define the vectors $\vec{N}_{((ab)c)}$, $\vec{\chi}_{((ab)c)}$, $\vec{S}_q=\vec{S}_{q((ab)c)}$ $=\vec{S}_{q(ab)}+\vec{S}_{qc}$, $\vec{W}_{q((ab)c)}=\vec{S}_{q(ab)}-\vec{S}_{qc}$. Since $\vec{N}_{((ab)c)}\cdot\vec{\chi}_{((ab)c)}=0$ and $\{N^r_{((ab)c)},N^s_{((ab)c)}\}$ $=\{N^r_{((ab)c)},\chi^s_{((ab)c)}\}=\{\chi^r_{((ab)c)},\chi^s_{((ab)c)}\}=0$ because of $\{\hat{R}^r_{(ab)},\hat{R}^s_c\}=0$, a new E(3) group generated by $\vec{S}_q$ and $\vec{N}_{((ab)c)}$ with nonfixed invariants $|\vec{N}_{((ab)c)}|$, $\vec{S}_q\cdot\vec{N}_{((ab)c)}=\check{S}^3_q|\vec{N}_{((ab)c)}|$ emerges. Again it is possible to define $\alpha_{((ab)c)}$ and $\beta_{((ab)c)}$, and then to identify a final unit vector $\hat{R}_{((ab)c)}$ with $\vec{S}_q\cdot\hat{R}_{((ab)c)}=0$ and $\{\hat{R}^r_{((ab)c)},\hat{R}^s_{((ab)c)}\}=0$.

In conclusion, when $S_q\neq 0$, we construct both a *dynamical body frame* $\hat{\chi}_{((ab)c)}$, $\hat{N}_{((ab)c)}$ $\times\hat{\chi}_{((ab)c)}$, $\hat{N}_{((ab)c)}$, and a *spin frame* $\hat{S}_q$, $\hat{R}_{((ab)c)}$, $\hat{R}_{((ab)c)}\times\hat{S}_q$ as in the three-body case. There is an *important difference*, however: *the orthonormal vectors* $\vec{N}_{((ab)c)}$ and $\vec{\chi}_{((ab)c)}$ *depend on the momenta of the relative particles a and b through* $\hat{R}_{(ab)}$, *so that our results do not share any relation with the* $N=4$ *nontrivial SO(3) principal bundle of the orientation-shape bundle approach.*

The final six *dynamical shape variables* are $q^\mu=\{|\vec{N}_{((ab)c)}|,\gamma_{(ab)},|\vec{N}_{(ab)}|,\rho_{qa},\rho_{qb},\rho_{qc}\}$. While the last four depend only on the original relative coordinates $\vec{\rho}_{qA}$, $A=a,\ b,\ c$, the first two also depend on the original momenta $\vec{\pi}_{qA}$: therefore they are *generalized shape variables*. It follows

$$
\rho^r_{qA}=\mathcal{R}^{rs}(\tilde{\alpha},\tilde{\beta},\tilde{\gamma})\,\check{\rho}^s_{qA}(q^\mu,p_\mu,\check{S}^r_q),\quad A=a,b,c. \tag{7.28}
$$

It is seen that for $N=4$ the dynamical body frame components $\check{\rho}^r_{qA}$ also depend on the dynamical shape momenta and on the dynamical body frame components of the spin. It is clear that this result stands completely outside the orientation-shape bundle approach.

The price to be paid for the existence of three global *dynamical body frames* for $N=4$ is a more complicated form of the Hamiltonian kinetic energy. On the other hand, *dynamical vibrations* and *dynamical angular velocity* are measurable quantities in each dynamical body frame.

For $N=5$ we can repeat the previous construction with either the sequence of spin clusterings $abcd \mapsto (ab)cd \mapsto ((ab)c)d) \mapsto (((ab)c)d)$ or with the sequence $abcd \mapsto (ab)(cd) \mapsto ((ab) \times (cd))$ $[a,b,c,d$ any permutation of 1,2,3,4]. Each *spin cluster* $(\ldots)$ is identified by the unit vector $\hat{R}_{(\ldots)}$, axis of the *spin frame* of the cluster. All the final *dynamical body frames* built with this construction have their axes depending on both the original configurations and momenta.

This construction is trivially generalized to any N: we have only to classify all the possible *spin clustering patterns*.

In conclusion, for $N \geq 4$ our sequence of canonical and noncanonical transformations leads to the following result [compare with Eq. (7.22) of the three-body case]:

$$\boxed{\begin{array}{c}\vec{\rho}_{qA} \\ \vec{\pi}_{qA}\end{array}} \xrightarrow{non\ can.} \boxed{\begin{array}{c|c}\tilde{\alpha}\ \ \tilde{\beta}\ \ \tilde{\gamma} & q^{\mu}(\vec{\rho}_{qA}, \vec{\pi}_{qA}) \\ \tilde{S}_q^1\ \tilde{S}_q^2\ \tilde{S}_q^3 & p_{\mu}(\vec{\rho}_{qA}, \vec{\pi}_{qA})\end{array}} \quad . \tag{7.29}$$

This state of affairs tells us that for $N \geq 4$ and with $S_q \neq 0$, $S_{qA} \neq 0$, $A=a,\ b,\ c$, viz. when the standard $(3N\text{-}3)$-dimensional orientation-shape bundle is not trivial, the original $(6N\text{-}6)$-dimensional relative phase space admits the definition of as many *dynamical body frames* as spin canonical bases,[53] which are globally defined (apart isolated coordinate singularities) for the nonsingular N-body configurations with $\vec{S}_q \neq 0$ (and with nonzero spin for each spin subcluster). Such *dynamical body frames* do not correspond to local cross sections of the static nontrivial orientation-shape SO(3) principal bundle and the spin canonical bases do not coincide with the canonical bases associated with the static theory.

VIII. THE CASE OF INTERACTING PARTICLES

As shown in Ref. 26 and its bibliography, the action-at-a-distance interactions inside the Wigner hyperplane may be introduced either under the square roots (scalar and vector potentials) or outside (scalar potential like the Coulomb one) appearing in the free Hamiltonian (2.19).

In the rest-frame instant form the most general Hamiltonian with action-at-a-distance interactions is

$$H = \sum_{i=1}^{N} \sqrt{m_i^2 + U_i + [\vec{k}_i - \vec{V}_i]^2} + V, \tag{8.1}$$

where $U = U(\vec{\kappa}_k, \vec{\eta}_h - \vec{\eta}_k)$, $\vec{V}_i = \vec{V}_i(\vec{k}_{j\neq i}, \vec{\eta}_i - \vec{\eta}_{j\neq i})$, $V = V_o(|\vec{\eta}_i - \vec{\eta}_j|) + V'(\vec{k}_i, \vec{\eta}_i - \vec{\eta}_j)$.

The rest frame Hamiltonian for the relative motion becomes

$$H_{(\mathrm{rel})} = \sum_{i=1}^{N} \sqrt{m_i^2 + \tilde{U}_i + \left[\sqrt{n}\sum_{a=1}^{N-1} \gamma_{ai}\vec{\pi}_{qa} - \tilde{\vec{V}}_i\right]^2} + \tilde{V}, \tag{8.2}$$

where

$$\begin{aligned}
\tilde{U}_i &= U\left(\sqrt{n}\sum_{a=1}^{N-1} \gamma_{ak}\vec{\pi}_{qa}, \frac{1}{\sqrt{N}}\sum_{a=1}^{N-1}(\gamma_{ah} - \gamma_{ak})\vec{\rho}_{qa}\right), \\
\tilde{\vec{V}}_i &= \vec{V}_i\left(\sqrt{n}\sum_{a=1}^{N-1} \gamma_{aj\neq i}\vec{\pi}_{qa}, \frac{1}{\sqrt{N}}\sum_{a=1}^{N-1}(\gamma_{ai} - \gamma_{aj\neq i})\vec{\rho}_{qa}\right), \\
\tilde{V} &= V_o\left(\left|\frac{1}{\sqrt{N}}\sum_{a=1}^{N-1}(\gamma_{ai} - \gamma_{aj})\vec{\rho}_{qa}\right|\right) + V'\left(\sqrt{n}\sum_{a=1}^{N-1} \gamma_{ai}\vec{\pi}_{qa}, \frac{1}{\sqrt{N}}\sum_{a=1}^{N-1}(\gamma_{ai} - \gamma_{aj})\vec{\rho}_{qa}\right).
\end{aligned} \tag{8.3}$$

The price to be paid for the existence of three global *dynamical body frames* for $N=4$ is:

(i) a more complicated form of the Hamiltonian kinetic energy (it allows, however, for a definition of measurable *dynamical vibrations* and *dynamical angular velocity* in each dynamical body frame);

(ii) the fact that a potential $V(\vec{\eta}_{ij}\cdot\vec{\eta}_{hk})$ with $\vec{\eta}_{ij}=\vec{\eta}_i-\vec{\eta}_j$ becomes shape-momenta dependent, since

$$V(\vec{\eta}_{ij}\cdot\vec{\eta}_{hk})=V\left[\frac{1}{N}\sum_{a,b}^{1,..,N-1}(\Gamma_{ai}-\Gamma_{aj})(\Gamma_{bh}-\Gamma_{bk})\vec{\rho}_{qa}\cdot\vec{\rho}_{qb}\right]. \tag{8.4}$$

For $N=4$, in the pattern $((ab)c)$, it follows

$$V=\tilde{V}_{((ab)c)}[\rho_{qa},\rho_{qb},\rho_{qc},|\vec{N}_{((ab)c)}|,\gamma_{(ab)},|\vec{N}_{(ab)}|;\xi_{((ab)c)},\Omega_{(ab)};\check{S}^r_q]. \tag{8.5}$$

For more general potentials $V(\vec{\eta}_{ij}\cdot\vec{\eta}_{hk},\vec{\kappa}_i\cdot\vec{\eta}_{hk},\vec{\kappa}_i\cdot\vec{\kappa}_j)$, such as that appearing in the nonrelativistic limit of the relativistic Darwin potential of Ref. 26, more complicated expressions emerge.

IX. CONCLUSIONS

In this paper we have explored the relativistic kinematics of a system of N scalar positive-energy particles. In the framework of the rest-frame instant form of dynamics it is possible to find the relativistic extension of the Abelian translational and non-Abelian rotational symmetries whose associated Noether constants of motion are fundamental for the study of isolated systems. In the relativistic case the rest-frame description on the Wigner hyperplanes allows one to clarify all the problems by virtue of a doubling of all the concepts: they can be either *external* (namely observed by an arbitrary inertial Lorentz frame) or *internal* (namely observed by an inertial observer at rest inside the Wigner hyperplane). Correspondingly, two realizations of the Poincaré algebra are naturally defined.

After a clarification of the possible *external* and *internal* definitions of relativistic center of mass, we have shown that it is possible to define a family of canonical transformations leading to the construction of relative canonical variables. The rest-frame Hamiltonian can be expressed in terms of these variables. It turns out that, due to the presence of multiple square roots in the Hamiltonian, the nonrelativistic concepts of *Jacobi normal relative coordinates*, *reduced masses*, and *barycentric tensor of inertia* cannot be extended to the relativistic formulation.

On the other hand, the rest-frame description (Wigner hyperplanes) allows one to exploit the nonrelativistic formalism developed in Ref. 2 for the analysis of the rotational kinematics, being independent of Jacobi coordinates. It is possible, therefore, to extend the concepts of *canonical spin bases*, *spin frames*, and *dynamical body frames* to the relativistic level. It follows again that, because of the non-Abelian nature of rotations, a global separation of rotations from vibrations is *not* possible.

In a future paper[36] we will conclude the discussion of relativistic kinematics by defining Dixon's multipoles[35] for the relativistic N-body problem in the rest-frame instant form of dynamics. It will be shown that concepts like the *tensor of inertia* can be recovered by using the quadrupole moment.

The final task should be the extension of all these results to relativistic extended (*continua*) isolated systems.

APPENDIX A: PARAMETRIZED MINKOWSKI THEORIES

We review here the main features of *parametrized Minkowski theories* and of the canonical reduction of gauge systems, following Refs. 9, 26, and 38, where a complete treatment for N scalar charged positive energy particles plus the electromagnetic field is given.

The starting point is Dirac's[12] reformulation of classical field theory on spacelike hypersurfaces foliating Minkowski space–time M^4. The foliation is defined by an embedding $R\times\Sigma \to M^4$, $(\tau,\vec{\sigma})\mapsto z^\mu(\tau,\vec{\sigma})$, with Σ an abstract three-surface diffeomorphic to R^3.

Let $\{\Sigma_\tau\}$ be the resulting one-parameter family of spacelike hypersurfaces. We use the notations $\sigma^{\check{A}}=(\sigma^\tau=\tau;\vec{\sigma}=\{\sigma^{\check{r}}\})$[54] and $\partial_{\check{A}}=\partial/\partial\sigma^{\check{A}}$. Define the cotetrads

$$z^\mu_{\check{A}}(\tau,\vec{\sigma})=\partial_{\check{A}}z^\mu(\tau,\vec{\sigma}),\quad \partial_{\check{B}}z^\mu_{\check{A}}-\partial_{\check{A}}z^\mu_{\check{B}}=0, \tag{A1}$$

so that the metric on Σ_τ is

$$\begin{aligned} &g_{\check{A}\check{B}}(\tau,\vec{\sigma})=z^\mu_{\check{A}}(\tau,\vec{\sigma})\,\eta_{\mu\nu}z^\nu_{\check{B}}(\tau,\vec{\sigma}),\quad \epsilon g_{\tau\tau}(\tau,\vec{\sigma})>0,\\ &g(\tau,\vec{\sigma})=-\det\|\,g_{\check{A}\check{B}}(\tau,\vec{\sigma})\,\|=(\det\|\,z^\mu_{\check{A}}(\tau,\vec{\sigma})\,\|)^2,\\ &\gamma(\tau,\vec{\sigma})=-\det\|g_{\check{r}\check{s}}(\tau,\vec{\sigma})\|=\det\|{}^3g_{\check{r}\check{s}}(\tau,\vec{\sigma})\|, \end{aligned} \tag{A2}$$

where $g_{\check{r}\check{s}}=-\epsilon\,{}^3g_{\check{r}\check{s}}$, with ${}^3g_{\check{r}\check{s}}$ having positive signature $(+++)$.

If $\gamma^{\check{r}\check{s}}(\tau,\vec{\sigma})=-\epsilon^3g^{\check{r}\check{s}}$ is the inverse of the three-metric $g_{\check{r}\check{s}}(\tau,\vec{\sigma})$ $[\gamma^{\check{r}\check{u}}(\tau,\vec{\sigma})g_{\check{u}\check{s}}(\tau,\vec{\sigma})=\delta^{\check{r}}_{\check{s}}]$, the inverse $g^{\check{A}\check{B}}(\tau,\vec{\sigma})$ of $g_{\check{A}\check{B}}(\tau,\vec{\sigma})$ $[g^{\check{A}\check{C}}(\tau,\vec{\sigma})g_{\check{C}\check{b}}(\tau,\vec{\sigma})=\delta^{\check{A}}_{\check{B}}]$ is given by

$$\begin{aligned} &g^{\tau\tau}(\tau,\vec{\sigma})=\frac{\gamma(\tau,\vec{\sigma})}{g(\tau,\vec{\sigma})},\\ &g^{\tau\check{r}}(\tau,\vec{\sigma})=-\left[\frac{\gamma}{g}g_{\tau\check{u}}\gamma^{\check{u}\check{r}}\right](\tau,\vec{\sigma})=\epsilon\left[\frac{\gamma}{g}g_{\tau\check{u}}\,{}^3g^{\check{u}\check{r}}\right](\tau,\vec{\sigma}),\\ &g^{\check{r}\check{s}}(\tau,\vec{\sigma})=\gamma^{\check{r}\check{s}}(\tau,\vec{\sigma})+\left[\frac{\gamma}{g}g_{\tau\check{u}}g_{\tau\check{v}}\gamma^{\check{u}\check{r}}\gamma^{\check{v}\check{s}}\right](\tau,\vec{\sigma})=-\epsilon\,{}^3g^{\check{r}\check{s}}(\tau,\vec{\sigma})+\left[\frac{\gamma}{g}g_{\tau\check{u}}g_{\tau\check{v}}\,{}^3g^{\check{u}\check{r}}\,{}^3g^{\check{v}\check{s}}\right](\tau,\vec{\sigma}), \end{aligned} \tag{A3}$$

so that $1=g^{\tau\check{C}}(\tau,\vec{\sigma})g_{\check{C}\tau}(\tau,\vec{\sigma})$ is equivalent to

$$\frac{g(\tau,\vec{\sigma})}{\gamma(\tau,\vec{\sigma})}=g_{\tau\tau}(\tau,\vec{\sigma})-\gamma^{\check{r}\check{s}}(\tau,\vec{\sigma})g_{\tau\check{r}}(\tau,\vec{\sigma})g_{\tau\check{s}}(\tau,\vec{\sigma}). \tag{A4}$$

We have

$$z^\mu_\tau(\tau,\vec{\sigma})=\left(\sqrt{\frac{g}{\gamma}}l^\mu+g_{\tau\check{r}}\gamma^{\check{r}\check{s}}z^\mu_{\check{s}}\right)(\tau,\vec{\sigma}), \tag{A5}$$

and

$$\eta^{\mu\nu}=z^\mu_{\check{A}}(\tau,\vec{\sigma})g^{\check{A}\check{B}}(\tau,\vec{\sigma})z^\nu_{\check{B}}(\tau,\vec{\sigma})=(l^\mu l^\nu+z^\mu_{\check{r}}\gamma^{\check{r}\check{s}}z^\nu_{\check{s}})(\tau,\vec{\sigma}), \tag{A6}$$

where

$$l^\mu(\tau,\vec{\sigma})=\left(\frac{1}{\sqrt{\gamma}}\epsilon^\mu{}_{\alpha\beta\gamma}z^\alpha_{\check{1}}z^\beta_{\check{2}}z^\gamma_{\check{3}}\right)(\tau,\vec{\sigma}),\quad l^2(\tau,\vec{\sigma})=1,\quad l_\mu(\tau,\vec{\sigma})z^\mu_{\check{r}}(\tau,\vec{\sigma})=0, \tag{A7}$$

is the unit (future pointing) normal to Σ_τ at $z^\mu(\tau,\vec{\sigma})$.

The price to be paid for carrying out this approach is the necessity of *adding* the embeddings $z^\mu(\tau,\vec{\sigma})$ identifying the points of the spacelike hypersurface Σ_τ as new configuration variables, as a matter of fact the only ones carrying Lorentz indices. A scalar parameter τ labels the leaves of

the foliation and $\vec{\sigma}$ are curvilinear coordinates on Σ_τ. It is then possible to redefine the fields on Σ_τ so that they *know* the whole hypersurface Σ_τ of τ-simultaneity. For a Klein–Gordon field $\phi(x)$, this new field is $\tilde{\phi}(\tau,\vec{\sigma})=\phi(z(\tau,\vec{\sigma}))$: it contains the nonlocal information about the embedding and the associated notion of *equal time*. This is a parametrized field theory with a covariant $3+1$ splitting of flat space–time which is set in a form already suited for the transition to general relativity in its ADM canonical formulation.

The Lagrangian of a isolated system can be rewritten in the form required by the coupling to an external gravitational field, the $3+1$ splitting of Minkowski space–time can be introduced and all the fields of the system can replaced by new fields on Σ_τ, which are Lorentz scalars, carrying only surface indices. Instead of considering the four-metric as describing a gravitational field, one replaces the four-metric by the induced metric $g_{\check{A}\check{B}}[z]=z^\mu_{\check{A}}\eta_{\mu\nu}z^\nu_{\check{B}}$ on Σ_τ (a functional of z^μ), and considers the embedding coordinates $z^\mu(\tau,\vec{\sigma})$ as independent fields. We use the notation $\sigma^{\check{A}}=(\tau,\sigma^{\check{r}})$ of Refs. 9 and 26. The $z^\mu_{\check{A}}(\sigma)=\partial z^\mu(\sigma)/\partial\sigma^{\check{A}}$ are flat cotetrad fields on Minkowski space–time with the $z^\mu_{\check{r}}$'s tangent to Σ_τ [note that in metric gravity the $z^\mu_{\check{A}}\neq\partial z^\mu/\partial\sigma^{\check{A}}$ are not cotetrad fields since no holonomic coordinates $z^\mu(\sigma)$ exist].

From the rewritten Lagrangian [see Eq. (2.3) for the case of N free scalar particles], it follows that: (i) the possible constraints of the system are Lorentz scalars; (ii) four primary first class constraints are added to assure the independence of the description from the choice of the foliation with spacelike hypersufaces:

$$\mathcal{H}_\mu(\tau,\vec{\sigma})=\rho_\mu(\tau,\vec{\sigma})-l_\mu(\tau,\vec{\sigma})T^{\tau\tau}_{\rm system}(\tau,\vec{\sigma})-z_{\check{r}\mu}(\tau,\vec{\sigma})T^{\tau\check{r}}_{\rm system}(\tau,\vec{\sigma})\approx 0. \tag{A8}$$

Here $T^{\tau\tau}_{\rm system}(\tau,\vec{\sigma})$, $T^{\tau\check{r}}_{\rm system}(\tau,\vec{\sigma})$, are the components of the energy–momentum tensor in the holonomic coordinate system on Σ_τ corresponding to the energy– and momentum–density of the isolated system. These four constraints satisfy an Abelian Poisson algebra since they are solved in the four-momenta $\rho_\mu(\tau,\vec{\sigma})$ conjugate to the embedding variables $z^\mu(\tau,\vec{\sigma})$: $\{\mathcal{H}_\mu(\tau,\vec{\sigma}),\mathcal{H}_\nu(\tau,\vec{\sigma}')\}=0$. This shows that the embedding fields $z^\mu(\tau,\vec{\sigma})$ are the *gauge* variables associated with this kind of general covariance.

The Dirac Hamiltonian is

$$H_D=H_{(c)}+\int \mathrm{d}^3\sigma\lambda^\mu(\tau,\vec{\sigma})\mathcal{H}_\mu(\tau,\vec{\sigma})+(\text{system-dependent primary constraints}), \tag{A9}$$

with $\lambda^\mu(\tau,\vec{\sigma})$ arbitrary Dirac multipliers and with $H_{(c)}$ the canonical Hamiltonian (it is either zero or weakly vanishing due to system-dependent secondary constraints). By using Eq. (A6) we can write

$$\begin{aligned}\lambda_\mu(\tau,\vec{\sigma})\mathcal{H}^\mu(\tau,\vec{\sigma})&=[(\lambda_\mu l^\mu)(l_\nu\mathcal{H}^\nu)-(\lambda_\mu z^\mu_{\check{r}})({}^3g^{\check{r}\check{s}}z_{\check{s}\nu}\mathcal{H}^\nu)](\tau,\vec{\sigma})\\ &\overset{\text{def}}{=}N_{(\rm flat)}(\tau,\vec{\sigma})(l_\mu\mathcal{H}^\mu)(\tau,\vec{\sigma})-N_{(\rm flat)\check{r}}(\tau,\vec{\sigma})({}^3g^{\check{r}\check{s}}z_{\check{s}\nu}\mathcal{H}^\nu)(\tau,\vec{\sigma}),\end{aligned} \tag{A10}$$

with the (nonholonomic form of the) constraints $\tilde{\mathcal{H}}(\tau,\vec{\sigma})=(l_\mu\mathcal{H}^\mu)(\tau,\vec{\sigma})\approx 0$, $\tilde{\mathcal{H}}_{\check{r}}(\tau,\vec{\sigma})=(z_{\check{r}\mu}\mathcal{H}^\mu)(\tau,\vec{\sigma})\approx 0$, satisfying the universal Dirac algebra like the ADM super-Hamiltonian and supermomentum constraints.

We have thereby defined new flat lapse and shift functions

$$\begin{aligned}N_{(\rm flat)}(\tau,\vec{\sigma})&=\lambda_\mu(\tau,\vec{\sigma})l^\mu(\tau,\vec{\sigma}),\\ N_{(\rm flat)\check{r}}(\tau,\vec{\sigma})&=\lambda_\mu(\tau,\vec{\sigma})z^\mu_{\check{r}}(\tau,\vec{\sigma}).\end{aligned} \tag{A11}$$

which have the same content of the arbitrary Dirac multipliers $\lambda_\mu(\tau,\vec{\sigma})$: they multiply primary first class constraints satisfying the Dirac algebra. In Minkowski spacetime they are quite distinct from the lapse and shift functions $N_{[z](\mathrm{flat})}(\tau,\vec{\sigma})=\sqrt{g(\tau,\vec{\sigma})/\gamma(\tau,\vec{\sigma})}$, $N_{[z](\mathrm{flat})\check{r}}(\tau,\vec{\sigma})={}^4g_{\tau\check{r}}(\tau,\vec{\sigma})$, defined by starting from the metric (they are functionals of the embeddings). Only by using the Hamilton equations $z^\mu_\tau(\tau,\vec{\sigma})\overset{\circ}{=}\{z^\mu(\tau,\vec{\sigma}),H_D\}=\lambda^\mu(\tau,\vec{\sigma})$ it follows that $N_{[z](\mathrm{flat})}(\tau,\vec{\sigma})\overset{\circ}{=}N_{(\mathrm{flat})}(\tau,\vec{\sigma})$, $N_{[z](\mathrm{flat})\check{r}}(\tau,\vec{\sigma})\overset{\circ}{=}N_{(\mathrm{flat})\check{r}}(\tau,\vec{\sigma})$.

Therefore, when we consider arbitrary $3+1$ splittings of space–time with arbitrary spacelike hypersurfaces, the descriptions of metric gravity plus matter and the parametrized Minkowski description of the same matter do not seem to follow the same pattern. The situation changes, however, if the allowed $3+1$ splittings of space–time in ADM metric gravity are restricted to have the leaves approaching Minkowski spacelike hyperplanes at spatial infinity and if parametrized Minkowski theories are restricted to spacelike hyperplanes.

The restriction of parametrized Minkowski theories to flat hyperplanes in Minkowski space–time is done by adding the gauge-fixings[9]

$$z^\mu(\tau,\vec{\sigma})-x^\mu_s(\tau)-b^\mu_{\check{r}}(\tau)\sigma^{\check{r}}\approx 0. \tag{A12}$$

Here $x^\mu_s(\tau)$ denotes a point on the hyperplane Σ_τ chosen as an arbitrary origin for the three-coordinates; the $b^\mu_{\check{r}}(\tau)$'s form an orthonormal triad at $x^\mu_s(\tau)$, and the τ-independent normal to the family of spacelike hyperplanes is $l^\mu=b^\mu_\tau=\epsilon^\mu{}_{\alpha\beta\gamma}b^\alpha_{\check{1}}(\tau)b^\beta_{\check{2}}(\tau)b^\gamma_{\check{3}}(\tau)$. Each hyperplane is described by ten configuration variables, $x^\mu_s(\tau)$ and the six independent degrees of freedom contained in the triad $b^\mu_{\check{r}}(\tau)$, and by the ten conjugate momenta: p^μ_s and six variables hidden in a spin tensor $S^{\mu\nu}_s$.[9] With these twenty canonical variables it is possible to build ten Poincaré generators $\overline{p^\mu_s}=p^\mu_s$, $\overline{J^{\mu\nu}_s}=x^\mu_s p^\nu_s-x^\nu_s p^\mu_s+S^{\mu\nu}_s$.

After the restriction to spacelike hyperplanes, the part $\int \mathrm{d}^3\sigma\lambda^\mu(\tau,\vec{\sigma})\mathcal{H}_\mu(\tau,\vec{\sigma})$ of the Dirac Hamiltonian is reduced to

$$\tilde{\lambda}^\mu(\tau)\tilde{\mathcal{H}}_\mu(\tau)-\tfrac{1}{2}\tilde{\lambda}^{\mu\nu}(\tau)\tilde{\mathcal{H}}_{\mu\nu}(\tau), \tag{A13}$$

because the time constancy of the gauge-fixings $z^\mu(\tau,\vec{\sigma})-x^\mu_s(\tau)-b^\mu_{\check{r}}(\tau)\sigma^{\check{r}}\approx 0$ implies (the overdot means $d/d\tau$)

$$\lambda_\mu(\tau,\vec{\sigma})=\tilde{\lambda}_\mu(\tau)+\tilde{\lambda}_{\mu\nu}(\tau)b^\nu_{\check{r}}\sigma^{\check{r}}, \tag{A14}$$

with

$$\tilde{\lambda}^\mu(\tau)=-\dot{x}^\mu_s(\tau),\quad \tilde{\lambda}^{\mu\nu}(\tau)=-\tilde{\lambda}^{\nu\mu}(\tau)=\frac{1}{2}\sum_{\check{r}}\,[\dot{b}^\mu_{\check{r}}b^\nu_{\check{r}}-b^\mu_{\check{r}}\dot{b}^\nu_{\check{r}}](\tau).$$

Since at this stage we have $z^\mu_{\check{r}}(\tau,\vec{\sigma})\approx b^\mu_{\check{r}}(\tau)$, we get

$$\begin{aligned} z^\mu_\tau(\tau,\vec{\sigma})&\approx N_{[z](\mathrm{flat})}(\tau,\vec{\sigma})l^\mu(\tau,\vec{\sigma})+N^{\check{r}}_{[z](\mathrm{flat})}(\tau,\vec{\sigma})b^\mu_{\check{r}}(\tau,\vec{\sigma})\\ &\approx\dot{x}^\mu_s(\tau)+\dot{b}^\mu_{\check{r}}(\tau)\sigma^{\check{r}}=-\tilde{\lambda}^\mu(\tau)-\tilde{\lambda}^{\mu\nu}(\tau)b_{\check{r}\nu}(\tau)\sigma^{\check{r}}. \end{aligned} \tag{A15}$$

Note that the coincidence of the two definitions of flat lapse and shift functions, independently of the equations of motion, is recovered at this stage only; actually

$$N_{[z](\mathrm{flat})}(\tau,\vec{\sigma})\approx N_{(\mathrm{flat})}(\tau,\vec{\sigma}),\quad N_{[z](\mathrm{flat})\check{r}}(\tau,\vec{\sigma})\approx N_{(\mathrm{flat})\check{r}}(\tau,\vec{\sigma}). \tag{A16}$$

The independence of our description on arbitrary foliations with spacelike hyperplanes, from the choice of the particular foliation, is assured by the remaining ten first class constraints

$$\tilde{\mathcal{H}}^{\mu}(\tau)=\int \mathrm{d}^3\sigma\,\mathcal{H}^{\mu}(\tau,\vec{\sigma})=p_s^{\mu}-p_{\rm sys}^{\mu}=p_s^{\mu}$$
$$-[\text{total momentum of the system inside the hyperplane}]^{\mu}\approx 0,$$
$$\tilde{\mathcal{H}}^{\mu\nu}(\tau)=b_{\check{r}}^{\mu}(\tau)\int d^3\sigma\,\sigma^{\check{r}}\mathcal{H}^{\nu}(\tau,\vec{\sigma})-b_{\check{r}}^{\nu}(\tau)\int d^3\sigma\,\sigma^{\check{r}}\mathcal{H}^{\mu}(\tau,\vec{\sigma})=S_s^{\mu\nu}-S_{sys}^{\mu\nu}=S_s^{\mu\nu}$$
$$-[\text{intrinsic angular momentum of the system inside the hyperplane}]^{\mu\nu},\tag{A17}$$

so that it follows

$$N_{(\rm flat)}(\tau,\vec{\sigma})=\lambda_{\mu}(\tau,\vec{\sigma})l^{\mu}(\tau,\vec{\sigma})\mapsto N_{(\rm flat)}(\tau,\vec{\sigma})=N_{[z](\rm flat)}(\tau,\vec{\sigma})=-\tilde{\lambda}_{\mu}(\tau)l^{\mu}-l^{\mu}\tilde{\lambda}_{\mu\nu}(\tau)b_{\check{s}}^{\nu}(\tau)\sigma^{\check{s}}$$
$$=-\lambda(\tau)-\tfrac{1}{2}\lambda_{\tau\check{s}}(\tau)\sigma^{\check{s}},$$

$$N_{(\rm flat)\check{r}}(\tau,\vec{\sigma})=\lambda_{\mu}(\tau,\vec{\sigma})z_{\check{r}}^{\mu}(\tau,\vec{\sigma})\mapsto N_{(\rm flat)}(\tau,\vec{\sigma})=N_{[z](\rm flat)\check{r}}(\tau,\vec{\sigma})=-\tilde{\lambda}_{\mu}(\tau)b_{\check{r}}^{\mu}(\tau)$$
$$-b_{\check{r}}^{\mu}(\tau)\tilde{\lambda}_{(\mu)(\nu)}(\tau)b_{\check{s}}^{\nu}(\tau)\sigma^{\check{s}}=-\lambda_{\check{r}}(\tau)-\tfrac{1}{2}\lambda_{\check{r}\check{s}}(\tau)\sigma^{\check{s}},$$

$$\lambda_A(\tau)=\tilde{\lambda}_{\mu}(\tau)b_A^{\mu}(\tau),\quad \tilde{\lambda}_{\mu}(\tau)=b_{\mu}^{A}(\tau)\lambda_A(\tau),\tag{A18}$$

$$\lambda_{AB}(\tau)=\tilde{\lambda}_{\mu\nu}(\tau)[b_A^{\mu}b_B^{\nu}-b_A^{\nu}b_B^{\mu}](\tau)=2[\tilde{\lambda}_{\mu\nu}b_A^{\mu}b_B^{\nu}](\tau),$$

$$\tilde{\lambda}_{\mu\nu}(\tau)=\tfrac{1}{4}[b_{\mu}^{A}b_{\nu}^{B}-b_{\mu}^{B}b_{\nu}^{A}](\tau)\lambda_{AB}(\tau)=\tfrac{1}{2}[b_{\mu}^{A}b_{\nu}^{B}\lambda_{AB}](\tau).$$

This is the main difference of the present approach with respect to the treatment of parametrized Minkowski theories given in standard references: there, no configuration action is defined but only a phase space action, in which people use, wrongly, $N_{[z](\rm flat)}$, $N_{[z](\rm flat)\check{r}}$ instead of $N_{(\rm flat)}$, $N_{(\rm flat)\check{r}}$ not only on spacelike hyperplanes but also on arbitrary spacelike hypersurfaces.

The embedding canonical variables $z^{\mu}(\tau,\vec{\sigma})$, $\rho_{\mu}(\tau,\vec{\sigma})$ are reduced to:

(i) $x_s^{\mu}(\tau),p_s^{\mu}$ with $\{x_s^{\mu},p_s^{\nu}\}=-{}^4\eta^{\mu\nu}$, parametrizing the arbitrary origin of the coordinates on the family of spacelike hyperplanes. The four constraints $\mathcal{H}^{\mu}(\tau)\approx p_s^{\mu}-p_{\rm sys}^{\mu}\approx 0$ mean that p_s^{μ} is determined by the four-momentum of the isolated system.

(ii) $b_A^{\mu}(\tau)$ [momentarily we do not identify the τ-dependent $b_{\tau}^{\mu}(\tau)$ with the normal l^{μ}] and $S_s^{\mu\nu}=-S_s^{\nu\mu}$, with the orthonormality constraints $b_A^{\mu}\,{}^4\eta_{\mu\nu}b_B^{\nu}={}^4\eta_{AB}$. The nonvanishing Dirac brackets enforcing the orthonormality constraints[55,9] for the b_A^{μ}'s are

$$\{b_A^{\rho},S_s^{\mu\nu}\}={}^4\eta^{\rho\mu}b_A^{\nu}-{}^4\eta^{\rho\nu}b_A^{\mu},$$
$$\{S_s^{\mu\nu},S_s^{\alpha\beta}\}=C_{\gamma\delta}^{\mu\nu\alpha\beta}S_s^{\gamma\delta},\tag{A19}$$

with $C_{\gamma\delta}^{\mu\nu\alpha\beta}$ the structure constants of the Lorentz algebra.

Then p_s^{μ}, $J_s^{\mu\nu}=x_s^{\mu}p_s^{\nu}-x_s^{\nu}p_s^{\mu}+S_s^{\mu\nu}$, satisfy the algebra of the Poincaré group, with $S_s^{\mu\nu}$ playing the role of the spin tensor. The other six constraints $\mathcal{H}^{\mu\nu}(\tau)\approx S_s^{\mu\nu}-S_{\rm sys}^{\mu\nu}\approx 0$ entail that $S_s^{\mu\nu}$ coincides with the spin tensor of the isolated system.

The velocity of the origin $x_s^{\mu}(\tau)$ is

$$\dot{x}_s^\mu(\tau) \overset{\circ}{=} \{x_s^\mu(\tau), H_D\} = \tilde{\lambda}_\nu(\tau)\{x_s^\mu(\tau), \mathcal{H}^\mu(\tau)\} = -\tilde{\lambda}^\mu(\tau) = [u^\mu(p_s)u^\nu(p_s) - \epsilon_r^\mu(u(p_s))\epsilon_r^\nu(u(p_s))]\dot{x}_{s\nu}(\tau) = -u^\mu(p_s)\lambda(\tau) + \epsilon_r^\mu(u(p_s))\lambda_r(\tau),$$

$$\dot{x}_s^2(\tau) = \lambda^2(\tau) - \vec{\lambda}^2(\tau) > 0, \quad \dot{x}_s \cdot u(p_s) = -\lambda(\tau),$$

$$U_s^\mu(\tau) = \frac{\dot{x}_s^\mu(\tau)}{\sqrt{\epsilon \dot{x}_s^2(\tau)}} = \frac{-\lambda(\tau)u^\mu(p_s) + \lambda_r(\tau)\epsilon_r^\mu(u(p_s))}{\sqrt{\lambda^2(\tau) - \vec{\lambda}^2(\tau)}}, \tag{A20}$$

$$\Rightarrow x_s^\mu(\tau) = x_s^\mu(0) - u^\mu(p_s)\int_0^\tau d\tau_1\, \lambda(\tau_1) + \epsilon_r^\mu(u(p_s))\int_0^\tau d\tau_1\, \lambda_r(\tau_1).$$

For each configuration of an isolated system with timelike total four-momentum there is a privileged family of Wigner hyperplanes orthogonal to p_s^μ ($\epsilon p_s^2 > 0$), namely that corresponding to the *intrinsic rest-frame* of the isolated system. If we choose these hyperplanes by means of suitable gauge fixings for the constraints $\tilde{\mathcal{H}}^{\mu\nu}(\tau) \approx 0$,[9] we are left with the four constraints $\mathcal{H}^\mu(\tau) \approx 0$, which can be rewritten as

$$\epsilon_s = \sqrt{\epsilon p_s^2} \approx [\text{invariant mass of the isolated system under investigation}] = M_{\text{sys}},$$

$$\vec{p}_{\text{sys}} = [3 - \text{momentum of the isolated system inside the Wigner hyperplane}] \approx 0, \tag{A21}$$

$$H_D = H_{(c)} + \tilde{\lambda}^\mu(\tau)\tilde{\mathcal{H}}_\mu(\tau) + (\text{system-dependent primary constraints}) = H_{(c)} + \lambda(\tau)[\epsilon_s - M_{\text{sys}}] - \vec{\lambda}(\tau)\cdot\vec{p}_{\text{sys}} + (\text{system-dependent primary constraints}).$$

There is no other restriction on p_s^μ, because $u_s^\mu(p_s) = p_s^\mu/\sqrt{\epsilon p_s^2}$ gives the orientation of the Wigner hyperplanes containing the isolated system, with respect to an arbitrarily given external inertial observer.

In this special gauge, after the projection to Dirac brackets, we have $b_A^\mu \equiv L^\mu{}_A(p_s, \mathring{p}_s)$ (the standard Wigner boost for timelike Poincaré orbits) and $S_s^{\mu\nu} \equiv S_{sys}^{\mu\nu}$, $\tilde{\lambda}_{\mu\nu}(\tau) \equiv 0$. The origin $x_s^\mu(\tau)$ does not belong to the canonical basis for these Dirac brackets anymore and is replaced by the noncovariant canonical variable[9]

$$\tilde{x}_s^\mu(\tau) = x_s^\mu(\tau) - \frac{1}{\epsilon_s(p_s^0 + \epsilon_s)}\left[p_{s\nu}S_s^{\nu\mu} + \epsilon_s\left(S_s^{0\mu} - S_s^{0\nu}\frac{p_{s\nu}p_s^\mu}{\epsilon_s^2}\right)\right].$$

In general, we have the problem that in the gauges where $\tilde{\lambda}_{\mu\nu}(\tau)$ or $\tilde{\lambda}_{AB}(\tau)$ are different from zero, the foliations with leaves Σ_τ associated with arbitrary $3+1$ splittings of Minkowski space–time are geometrically *ill-defined* at spatial infinity. Therefore, the variational principle describing the isolated system can make sense only for those $3+1$ splittings having these parts of Dirac's multipliers vanishing. The problem is that, since on hyperplanes $\dot{l}^\mu = 0$ and $l^\mu b_{\check{r}\mu}(\tau) = 0$ imply $l^\mu \dot{b}_{\check{r}\mu}(\tau) = 0$, Eq. (A15) implies $\lambda_{\tau\check{r}}(\tau) = 0$ [i.e., only three $\tilde{\lambda}_{\mu\nu}(\tau)$ are independent] on spacelike hyperplane, because otherwise Lorentz boosts could generate crossing of the foliation leaves. This suggests that, to avoid inconsistencies, the reduction be done from arbitrary spacelike hypersurfaces either directly to the Wigner hyperplanes or to spacelike hypersurfaces approaching Wigner hyperplanes asymptotically.[56] Therefore, the $3+1$ splittings of Minkowski space–time whose leaves are Wigner hyperplanes are the only ones for which the foliation is well defined at spatial infinity: both the induced proper time interval and shift functions are finite there.

In this way we have obtained a new kind of instant form of the dynamics, the *Wigner-covariant one-time rest-frame instant form*.[9,38] For any isolated system, all the variables become

Wigner covariant except for the *external* canonical center of mass $\tilde{x}^\mu_s$, which loses Lorentz covariance. This does not matter, however, being a completely decoupled variable. Our approach realizes the special relativistic generalization of the nonrelativistic separation of the center of mass from the relative motion $[H=\vec{P}^2/2M+H_{\rm rel}]$. The role of the center of mass is taken by the Wigner hyperplane, identified by a point $\tilde{x}^\mu(\tau)$ and its normal p^μ_s.

Let us close the Appendix quoting some notions concerning the *standard Wigner boosts for timelike Poincaré orbits*.

The rest frame form of a timelike four-vector p^μ is $\mathring{p}^\mu=\eta\sqrt{\epsilon p^2}(1;\vec{0})=\eta^{\mu 0}\eta\sqrt{\epsilon p^2}$, $\mathring{p}^2=p^2$, where $\eta=\mathrm{sign}\,p^0$. The standard Wigner boost transforming $\mathring{p}^\mu$ into p^μ is

$$\begin{aligned}
L^\mu{}_\nu(p,\mathring{p}) &= \epsilon^\mu_\nu(u(p)) \\
&= \eta^\mu_\nu + 2\frac{p^\mu \mathring{p}_\nu}{\epsilon p^2} - \frac{(p^\mu+\mathring{p}^\mu)(p_\nu+\mathring{p}_\nu)}{p\cdot\mathring{p}+\epsilon p^2} \\
&= \eta^\mu_\nu + 2u^\mu(p)u_\nu(\mathring{p}) - \frac{(u^\mu(p)+u^\mu(\mathring{p}))(u_\nu(p)+u_\nu(\mathring{p}))}{1+u^o(p)}, \\
&\nu=0, \quad \epsilon^\mu_0(u(p))=u^\mu(p)=p^\mu/\eta\sqrt{\epsilon p^2}, \\
&\nu=r, \quad \epsilon^\mu_r(u(p))=\left(-u_r(p);\delta^i_r-\frac{u^i(p)u_r(p)}{1+u^o(p)}\right).
\end{aligned} \tag{A22}$$

The inverse of $L^\mu{}_\nu(p,\mathring{p})$ is $L^\mu{}_\nu(\mathring{p},p)$, the standard boost to the rest frame, defined by

$$L^\mu{}_\nu(\mathring{p},p)=L_\nu{}^\mu(p,\mathring{p})=L^\mu{}_\nu(p,\mathring{p})|_{\vec{p}\to-\vec{p}}. \tag{A23}$$

Therefore, we can define the following cotetrads and tetrads:[57]

$$\begin{aligned}
&\epsilon^\mu_A(u(p))=L^\mu{}_A(p,\mathring{p}), \\
&\epsilon^A_\mu(u(p))=L^A{}_\mu(\mathring{p},p)=\eta^{AB}\eta_{\mu\nu}\epsilon^\nu_B(u(p)), \\
&\bar{\epsilon^o_\mu}(u(p))=\eta_{\mu\nu}\epsilon^\nu_o(u(p))=u_\mu(p), \quad \epsilon^A_o(u(p))=u_A(p), \\
&\epsilon^r_\mu(u(p))=-\delta^{rs}\eta_{\mu\nu}\epsilon^\nu_r(u(p))=\left(\delta^{rs}u_s(p);\delta^r_j-\delta^{rs}\delta_{jh}\frac{u^h(p)u_s(p)}{1+u^o(p)}\right), \\
&\epsilon^A_\mu(u(p))\epsilon^\nu_A(u(p))=\eta^\mu_\nu, \quad \epsilon^A_\mu(u(p))\epsilon^\mu_B(u(p))=\eta^A_B, \\
&\eta^{\mu\nu}=\epsilon^\mu_A(u(p))\eta^{AB}\epsilon^\nu_B(u(p))=u^\mu(p)u^\nu(p)-\sum_{r=1}^3\epsilon^\mu_r(u(p))\epsilon^\nu_r(u(p)).
\end{aligned} \tag{A24}$$

The *Wigner rotation* corresponding to the Lorentz transformation Λ is

$$\begin{aligned}
&R^\mu{}_\nu(\Lambda,p)=[L(\mathring{p},p)\Lambda^{-1}L(\Lambda p,\mathring{p})]^\mu{}_\nu=\begin{pmatrix}1 & 0\\ 0 & R^i{}_j(\Lambda,p)\end{pmatrix}, \\
&R^i{}_j(\Lambda,p)=(\Lambda^{-1})^i{}_j-\frac{(\Lambda^{-1})^i{}_o p_\beta(\Lambda^{-1})^\beta{}_j}{p_\rho(\Lambda^{-1})^\rho{}_o+\eta\sqrt{\epsilon p^2}}-\frac{p^i}{p^o+\eta\sqrt{\epsilon p^2}}\left[(\Lambda^{-1})^o{}_j-\frac{((\Lambda^{-1})^o{}_o-1)p_\beta(\Lambda^{-1})^\beta{}_j}{p_\rho(\Lambda^{-1})^\rho{}_o+\eta\sqrt{\epsilon p^2}}\right].
\end{aligned} \tag{A25}$$

The polarization vectors transform under the Poincaré transformations (a,Λ) as

$$\epsilon_r^\mu(u(\Lambda p))=(R^{-1})_r{}^s\Lambda^\mu{}_\nu\epsilon_s^\nu(u(p)). \tag{A26}$$

APPENDIX B: THE GARTENHAUS–SCHWARTZ TRANSFORMATION FOR SPINNING PARTICLES

Reference 58 contains the rest-frame instant form description of a system of N spinning positive-energy particles with the intrinsic spin described by Grassmann variables.

The N spinning particles are described on the Wigner hyperplane by a canonical basis including the center-of-mass variables $\tilde{x}_s^\mu$, p_s^μ, the pairs $\vec{\eta}_i$, $\vec{\kappa}_i$, $i=1,..,N$, of Eq. (2.16) and three Grassmann variables $\xi_i^r\equiv\epsilon_\mu^r(u(p_s))\xi_i^\mu$[58] satisfying $\{\xi_i^r,\xi_j^s\}=-i\delta^{rs}\delta_{ij}$ for each spin, and having vanishing Poisson bracket with all of the other variables.

The rest-frame *external* realization of the Poincaré algebra is built in analogy to Eq. (2.14) but with a modified spin tensor $\tilde{S}_s^{\mu\nu}$,

$$\begin{aligned}&\vec{\overline{S}}_s=\sum_{i=1}^N(\vec{\eta}_i\times\vec{\kappa}_i+\vec{\overline{S}}_{i\xi}),\\ &\overline{S}_{i\xi}^r=-\frac{i}{2}\epsilon^{ruv}\xi_i^u\xi_i^v,\quad \{\overline{S}_{i\xi}^r,\overline{S}_{j\xi}^s\}=\delta_{ij}\epsilon^{rsu}\overline{S}_{i\xi}^u.\end{aligned} \tag{B1}$$

In the absence of interactions Eqs. (2.7), (2.8), and (2.16) remain valid.

By using the expression of $\overline{S}_s^{\mu\nu}$ on the Wigner hyperplane given in Ref. 58 and the methodology of Ref. 31, the *internal* realization (2.15) of the Poincaré algebra becomes

$$\begin{aligned}&M_{\rm sys}=\sum_{i=1}^N\sqrt{m_i^2+\vec{\kappa}_i^2}=\sum_{i=1}^N H_i,\quad H_i=\sqrt{m_i^2+\vec{\kappa}_i^2},\\ &\vec{\kappa}_+=\sum_{i=1}^N\vec{\kappa}_i\quad(\approx 0),\\ &\vec{J}=\vec{\overline{S}}_s=\sum_{i=1}^N(\vec{\eta}_i\times\vec{\kappa}_i+\vec{\overline{S}}_{i\xi})=\vec{J}_B+\vec{J}_S,\quad \vec{J}_S=\sum_{i=1}^N\vec{\overline{S}}_{i\xi},\\ &\vec{K}=-\sum_{i=1}^N\vec{\eta}_iH_i+\sum_{i=1}^N\frac{\vec{\overline{S}}_{i\xi}\times\vec{\kappa}_i}{m_i+H_i}=\vec{K}_B+\vec{K}_s,\quad \vec{K}_B=-\sum_{i=1}^N\vec{\eta}_iH_i.\end{aligned} \tag{B2}$$

If, following Ref. 31, we put

$$\begin{aligned}&\vec{K}=-M_{\rm sys}\vec{q}_+ +\frac{\vec{S}_q\times\vec{\kappa}_+}{\sqrt{\Pi}+M_{\rm sys}},\quad \Pi=H_M^2-\vec{\kappa}_+^2,\\ &\vec{S}_q=\vec{J}-\vec{q}_+\times\vec{\kappa}_+,\end{aligned} \tag{B3}$$

we get consistently the expression of the *internal* canonical center of mass $\vec{q}_+$ given in Eq. (4.4), with $\vec{S}_q$ as the associated spin vector.

As in Sec. VI, we apply the Gartenhaus–Schwartz transformation leading from the internal canonical basis $\vec{\eta}_i$, $\vec{\kappa}_i$, $\vec{\xi}_i$ (with $\vec{\kappa}_+\approx 0$) to the center-of-mass basis $\vec{q}_+$, $\vec{\kappa}_+$, $\vec{\rho}_{qa}$, $\vec{\pi}_{qa}$, $\vec{\xi}_{qi}$ (being again $\vec{\kappa}_+\approx 0$) with $\vec{\overline{S}}_{i\xi}\mapsto\vec{S}_{qi\xi}$. Using Eqs. (5.1) and (5.4) with $\vec{K}=\vec{K}_B+\vec{K}_S$ of Eq. (B2), it is possible to find the differential equations for the α-dependence of the various quantities.

Since $\{\vec{\pi}_a,\vec{K}_S\}=0$, $\vec{\pi}_{qa}=\lim_{\alpha\to\infty}\vec{\pi}_a(\alpha)$ is the same as in the spinless case; the $\vec{\pi}_{qa}$'s are given in Eq. (5.13). Here too Π is an invariant and it holds $\sqrt{\Pi}=H_M(\infty)=H_{(\mathrm{rel})}=\Sigma_{i=1}^N H_i(\infty)$ with $H_i(\infty)=(M_{\mathrm{sys}}H_i-\vec{\kappa}_+\cdot\vec{\kappa}_i)/\sqrt{\Pi}$. Moreover, $\vec{n}_+=\vec{\kappa}_+/|\vec{\kappa}_+|$ is invariant.

For the spin variables $\vec{\vec{S}}_{i\xi}$ we obtain

$$\begin{aligned}\frac{\mathrm{d}\overline{S}^r_{i\xi}(\alpha)}{\mathrm{d}\alpha}&=\{\overline{S}^r_{i\xi}(\alpha),\vec{q}_+(\alpha)\cdot\vec{\kappa}_+(\alpha)\}=\left\{\frac{\vec{K}(\alpha)\cdot\vec{\kappa}_+(\alpha)}{H_M(\alpha)},\overline{S}^r_{i\xi}\right\}=\frac{\kappa^s_+(\alpha)}{H_M(\alpha)}\{K^s_S(\alpha),\overline{S}^r_{i\xi}(\alpha)\}\\&=\frac{[(\vec{\kappa}_+(\alpha)\times\vec{\kappa}_i(\alpha))\times\vec{\vec{S}}_{i\xi}(\alpha)]^r}{H_M(\alpha)(m_i+H_i(\alpha))},\\&\Rightarrow\frac{\mathrm{d}\vec{\vec{S}}_{i\xi}(\alpha)}{\mathrm{d}\theta(\alpha)}=\frac{(\vec{n}_+\times\vec{\kappa}_i(\alpha))\times\vec{\vec{S}}_{i\xi}(\alpha)}{m_i+H_i(\alpha)}.\end{aligned}\tag{B4}$$

This equation coincides with Eq. (3.10) of Ref. 45. By using Eq. (3.11) of Ref. 45, its integration provides the *Thomas precession* of the spin variable $\vec{\vec{S}}_{i\xi}$ about an axis $\vec{\kappa}_i\times\vec{n}_+$ in the instantaneous center-of-mass frame:[59]

$$\begin{aligned}&\vec{\vec{S}}_{i\xi}(\alpha)=\cos\gamma(\alpha)\vec{\vec{S}}_{i\xi}+[1-\cos\gamma(\alpha)](\vec{v}_i\cdot\vec{\vec{S}}_{i\xi})\vec{v}_i-\sin\gamma(\alpha)\vec{v}_i\times\vec{\vec{S}}_{i\xi},\\&\vec{v}_i=\frac{\vec{\kappa}_i\times\vec{n}_+}{|\vec{\kappa}_i\times\vec{n}_+|},\\&\mathrm{tg}\frac{\gamma(\alpha)}{2}=\frac{1-\cos\gamma(\alpha)}{\sin\gamma(\alpha)}=\frac{|\vec{\kappa}_i\times\vec{n}_+|}{(m_i+H_i)\mathrm{ctgh}\frac{\theta(\alpha)}{2}-\vec{\kappa}_i\cdot\vec{n}_+}\\&\quad\to_{\alpha\to\infty}\frac{|\vec{\kappa}_i\times\vec{\kappa}_+|}{(m_i+H_i)(M_{\mathrm{sys}}+\sqrt{\Pi})-\vec{\kappa}_i\cdot\vec{\kappa}_+}\approx 0,\quad\left[\mathrm{tg}\frac{\gamma(\infty)}{2}=\frac{M_{\mathrm{sys}}+\sqrt{\Pi}}{|\vec{\kappa}_+|}\right],\\&\sin\gamma(\alpha)=2\frac{(m_i+H_i)\mathrm{ctgh}\frac{\theta(\alpha)}{2}-\vec{\kappa}_i\cdot\vec{n}_+}{|\vec{\kappa}_i\times\vec{n}_+|^2+\left[(m_i+H_i)\mathrm{ctgh}\frac{\theta(\alpha)}{2}-\vec{\kappa}_i\cdot\vec{n}_+\right]^2}|\vec{\kappa}_i\times\vec{n}_+|,\\&\cos\gamma(\alpha)=1-2\frac{|\vec{\kappa}_i\times\vec{n}_+|^2}{|\vec{\kappa}_i\times\vec{n}_+|^2+\left[(m_i+H_i)\mathrm{ctgh}\frac{\theta(\alpha)}{2}-\vec{\kappa}_i\cdot\vec{n}_+\right]^2}.\end{aligned}\tag{B5}$$

Therefore, we obtain

$$\begin{aligned}\vec{S}_{qi\xi}=\lim_{\alpha\to\infty}\vec{\vec{S}}_{i\xi}(\alpha)&=\left[1-\frac{|\vec{\kappa}_i\times\vec{\kappa}_+|^2}{(m_i+H_i)(m_i+H_i(\infty))(M_{\mathrm{sys}}+\sqrt{\Pi})\sqrt{\Pi}}\right]\vec{\vec{S}}_{i\xi}\\&+\frac{\vec{\kappa}_i\times\vec{\kappa}_+\cdot\vec{\vec{S}}_{i\xi}\vec{\kappa}_i\times\vec{\kappa}_+}{(m_i+H_i)(m_i+H_i(\infty))(M_{\mathrm{sys}}+\sqrt{\Pi})\sqrt{\Pi}}-\frac{(m_i+H_i)(M_{\mathrm{sys}}+\sqrt{\Pi})-\vec{\kappa}_i\cdot\vec{\kappa}_+}{(m_i+H_i)(m_i+H_i(\infty))(M_{\mathrm{sys}}+\sqrt{\Pi})\sqrt{\Pi}}(\vec{\kappa}_i\\&\times\vec{\kappa}_+)\times\vec{\vec{S}}_{i\xi}\approx\vec{\vec{S}}_{i\xi}.\end{aligned}\tag{B6}$$

For the Grassmann variables $\vec{\xi}_i$, we get the same differential equation

$$\frac{d\xi_i^r(\alpha)}{d\alpha}=\{\xi_i^r(\alpha),\vec{q}_+(\alpha)\cdot\vec{\kappa}_+(\alpha)\}=\frac{[(\vec{\kappa}_+(\alpha)\times\vec{\kappa}_i(\alpha))\times\vec{\xi}_i]^r}{H_M(\alpha)(m_i+H_i(\alpha))},$$

$$\Rightarrow\frac{d\vec{\xi}_i(\alpha)}{d\theta(\alpha)}=\frac{(\vec{n}_+\times\vec{\kappa}_i(\alpha))\times\vec{\xi}_i(\alpha)}{m_i+H_i(\alpha)},\tag{B7}$$

$$\Downarrow$$

$$\vec{\xi}_{qi}=\lim_{\alpha\to\infty}\vec{\xi}_i(\alpha)=\left[1-\frac{|\vec{\kappa}_i\times\vec{\kappa}_+|^2}{(m_i+H_i)(m_i+H_i(\infty))(M_{\rm sys}+\sqrt{\Pi})\sqrt{\Pi}}\right]\vec{\xi}_i$$
$$+\frac{\vec{\kappa}_i\times\vec{\kappa}_+\cdot\vec{\xi}_i\vec{\kappa}_i\times\vec{\kappa}_+}{(m_i+H_i)(m_i+H_i(\infty))(M_{\rm sys}+\sqrt{\Pi})\sqrt{\Pi}}$$
$$-\frac{(m_i+H_i)(M_{\rm sys}+\sqrt{\Pi})-\vec{\kappa}_i\cdot\vec{\kappa}_+}{(m_i+H_i)(m_i+H_i(\infty))(M_{\rm sys}+\sqrt{\Pi})\sqrt{\Pi}}(\vec{\kappa}_i\times\vec{\kappa}_+)\times\vec{\xi}_i\approx\vec{\xi}_i\,.$$

Let us remark that now, besides the invariants $I_i^{(1)}$ and $I^{(2)}$ of Eqs. (5.14) of the spinless case (we have $I^{(2)}=I_B^{(2)}+I_S^{(2)}$ since $\vec{K}=\vec{K}_B+\vec{K}_S$), we have the additional invariants

$$I_i^{(3)}=(\vec{\kappa}_i\times\vec{n}_+)\cdot\vec{\bar{S}}_{i\xi},$$
$$I^{(2)}=I_B^{(2)}+I_S^{(2)},\quad I_S^{(2)}=\frac{|\vec{\kappa}_+|}{H_M}\sum_{i=1}^N\frac{I_i^{(3)}}{m_i+H_i}.\tag{B8}$$

Consider now the position vectors. As in the spinless case, the preliminary calculations for Eq. (5.19) now give

$$\frac{d}{d\alpha}\vec{n}_+\cdot\vec{\eta}_i(\alpha)=-\frac{\vec{n}_+\cdot\vec{\eta}_i(\alpha)}{H_i(\alpha)}\frac{dH_i(\alpha)}{d\alpha}-\frac{I_i^{(1)}I^{(2)}}{H_i(\alpha)}\frac{dJ^{(1)}(\alpha)}{d\alpha}-\frac{1}{H_i(\alpha)}\frac{dH_i(\alpha)}{d\alpha}\frac{I_i^{(3)}}{(m_i+H_i(\alpha))^2}.\tag{B9}$$

These equations have the solution

$$\vec{n}_+\cdot\vec{\eta}_i(\alpha)=\frac{H_i}{H_i(\alpha)}\vec{n}_+\cdot\vec{\eta}_i-\frac{I^{(2)}}{|\vec{\kappa}_+|}\left(e^\alpha-\frac{H_i}{H_i(\alpha)}\right)+\frac{I_i^{(3)}}{H_i(\alpha)}\left(\frac{1}{m_i+H_i(\alpha)}-\frac{1}{m_i+H_i}\right).\tag{B10}$$

For $\vec{\eta}_i(\alpha)$ it follows

$$\frac{\mathrm{d}\vec{\eta}_i(\alpha)}{\mathrm{d}\alpha}=\{\vec{\eta}_i(\alpha),\vec{\kappa}_+(\alpha)\cdot\vec{q}_+(\alpha)\}=-n^s_+\frac{\partial}{\partial\vec{\kappa}_i(\alpha)}\frac{|\vec{\kappa}_+(\alpha)|K^s(\alpha)}{H_M(\alpha)}=\vec{n}_+\cdot\vec{\eta}_i(\alpha)\frac{|\vec{\kappa}_+(\alpha)|\vec{\kappa}_i(\alpha)}{H_i(\alpha)H_M(\alpha)}$$
$$+\frac{\Sigma^N_{j=1}H_j(\alpha)\vec{n}_+\cdot\vec{\eta}_j(\alpha)}{H_M(\alpha)}\left[\frac{|\vec{\kappa}_+(\alpha)|\vec{\kappa}_i(\alpha)}{H_i(\alpha)H_M(\alpha)}-\vec{n}_+\right]+\frac{\vec{n}_+\cdot(\vec{\vec{S}}_{i\xi}(\alpha)\times\vec{\kappa}_i(\alpha))|\vec{\kappa}_+(\alpha)|\vec{\kappa}_i(\alpha)}{H_M(\alpha)H_i(\alpha)(m_i+H_i(\alpha))^2}$$
$$-\frac{|\vec{\kappa}_+(\alpha)|\vec{n}_+\times\vec{\vec{S}}_{i\xi}(\alpha)}{H_M(\alpha)(m_i+H_i(\alpha))}=\frac{H_i|\vec{\kappa}_+(\alpha)|\vec{\kappa}_i(\alpha)}{H_i^2(\alpha)H_M(\alpha)}\left[\vec{n}_+\cdot\vec{\eta}_i+\frac{I^{(2)}}{|\vec{\kappa}_+|}\right]-\frac{\vec{n}_+\cdot\vec{K}(\alpha)\vec{n}_+}{H_M(\alpha)}$$
$$+\frac{\vec{\kappa}_i(\alpha)|\vec{\kappa}_+(\alpha)|}{H_i(\alpha)H_M(\alpha)}\frac{\vec{n}_+\cdot(\vec{\vec{S}}_{i\xi}(\alpha)\times\vec{\kappa}_i(\alpha))}{(m_i+H_i(\alpha))^2}+\frac{I^{(3)}_i}{H_i(\alpha)}\left[\frac{1}{m_i+H_i(\alpha)}-\frac{1}{m_i+H_i}\right]$$
$$-\frac{|\vec{\kappa}_+(\alpha)|\vec{n}_+\times\vec{\vec{S}}_{i\xi}(\alpha)}{H_M(\alpha)(m_i+H_i(\alpha))}. \tag{B11}$$

The equations for $\vec{\rho}_a(\alpha)=\sqrt{N}\Sigma^N_{i=1}\gamma_{ai}\vec{\eta}_i(\alpha)$ are [see Eq. (3.21) of Ref. 45]

$$\frac{\mathrm{d}\vec{\rho}_a(\alpha)}{\mathrm{d}\alpha}=\sqrt{N}\sum_{i=1}^N\gamma_{ai}\frac{\mathrm{d}\vec{\eta}_i(\alpha)}{\mathrm{d}\alpha}=\sqrt{N}\sum_{i=1}^N\gamma_{ai}\frac{H_i|\vec{\kappa}_+(\alpha)|\vec{\kappa}_i(\alpha)}{H_i^2(\alpha)}\left(\vec{n}_+\cdot\vec{\eta}_i+\frac{I^{(2)}}{|\vec{\kappa}_+|}\right)$$
$$+\sqrt{N}\sum_{i=1}^N\gamma_{ai}\frac{\vec{\kappa}_i(\alpha)}{H_i(\alpha)}\left[\frac{|\vec{\kappa}_+(\alpha)|}{H_M(\alpha)}\frac{\vec{n}_+\cdot(\vec{\vec{S}}_{i\xi}\times\vec{\kappa}_i(\alpha))}{(m_i+H_i(\alpha))^2}+\frac{I^{(3)}_i|\vec{\kappa}_+(\alpha)|}{H_iH_M(\alpha)}\left(\frac{1}{m_i+H_i(\alpha)}\right.\right.$$
$$\left.\left.-\frac{1}{m_i+H_i}\right)\right]+\sqrt{N}\sum_{i=1}^N\gamma_{ai}\frac{|\vec{\kappa}_+(\alpha)|\vec{n}_+\times\vec{\vec{S}}_{i\xi}(\alpha)}{H_M(\alpha)(m_i+H_i(\alpha))}. \tag{B12}$$

By using the results contained in Ref. 45 this equation can be integrated and the final result is

$$\vec{\rho}_a(\alpha)=\vec{\rho}_a-\sum_{i,j=1}^N\sum_{b=1}^{N-1}\gamma_{aj}(\gamma_{bi}-\gamma_{bj})\frac{H_iH_j}{M_{\mathrm{sys}}}\vec{J}^{(2)}_j(\alpha)\vec{n}_+\cdot\vec{\rho}_b$$
$$+\sqrt{N}\sum_{i=1}^N\frac{I^{(3)}_i}{M_{\mathrm{sys}}(m_i+H_i)}\sum_{j=1}^N\gamma_{aj}\frac{\vec{k}_j(\alpha)}{H_j(\alpha)}\,\mathrm{sh}\,\theta(\alpha)$$
$$+\sqrt{N}\sum_{i=1}^N\frac{\gamma_{ai}}{(m_i+H_i(\alpha))(m_i+H_i)}\left[\frac{I^{(3)}_i(\vec{\kappa}_i-|\vec{n}_+\cdot\vec{\kappa}_i|\vec{n}_+\mathrm{sh}\,\theta(\alpha)}{H_i(\alpha)}+\frac{I^{(3)}_i[H_i-H_i(\alpha)]\vec{n}_+}{H_i(\alpha)}\right.$$
$$\left.+[\mathrm{ch}\,\theta(\alpha)-1]\vec{n}_+\cdot\vec{\vec{S}}_{i\xi}\vec{\kappa}_i\times\vec{n}_+-\mathrm{sh}\,\theta(\alpha)\frac{(m_i+H_i)[\mathrm{ch}\,\theta(\alpha)+1]-\vec{n}_+\cdot\vec{k}_i\mathrm{sh}\,\theta(\alpha)}{\mathrm{ch}\,\theta(\alpha)+1}\right]. \tag{B13}$$

Finally we get

$$\vec{\rho}_{qa}=\lim_{\alpha\to\infty}\vec{\rho}_a(\alpha)=\vec{\rho}_a-\sum_{i,j=1}^{N}\sum_{b=1}^{N-1}\gamma_{aj}(\gamma_{bi}-\gamma_{bj})\frac{H_i}{M_{\rm sys}}\left[\frac{|\vec{\kappa}_+|\vec{\kappa}_j(\infty)}{H_j(\infty)\sqrt{\Pi}}+\left(\frac{M_{\rm sys}}{\sqrt{\Pi}}-1\right)\vec{n}_+\right]\vec{n}_+\cdot\vec{\rho}_b$$

$$+\sqrt{N}\sum_{i=1}^{N}\frac{I_i^{(3)}}{M_{\rm sys}(m_i+H_i)}\sum_{j=1}^{N}\gamma_{aj}\frac{|\vec{\kappa}_+|\vec{\kappa}_j(\infty)}{H_j(\infty)\sqrt{\Pi}}+\sqrt{N}\sum_{i=1}^{N}\frac{\gamma_{ai}}{(m_i+H_i)(m_i+H_i(\infty))}\left[\frac{|\vec{\kappa}_+|I_i^{(3)}}{H_i(\infty)\sqrt{\Pi}}(\vec{\kappa}_i\right.$$

$$-\vec{n}_+\cdot\vec{\kappa}_i\vec{n}_+)+\frac{I_i^{(3)}(H_i-H_i(\infty))}{H_i(\infty)}+\frac{(M_{\rm sys}-\sqrt{\Pi})\vec{n}_+\cdot\vec{\vec{S}}_{i\xi}}{\sqrt{\Pi}}\vec{\kappa}_i\times\vec{n}_+$$

$$\left.-\frac{|\vec{\kappa}_+|}{\sqrt{\Pi}}\frac{(m_i+H_i)(M_{\rm sys}+\sqrt{\Pi})-|\vec{\kappa}_+|\vec{n}_+\cdot\vec{\kappa}_i}{M_{\rm sys}-\sqrt{\Pi}}\vec{n}_+\times\vec{\vec{S}}_{i\xi}\right]\approx\vec{\rho}_a\,. \tag{B14}$$

In the same way we obtain, as in the spinless case:

$$\vec{J}_S(\alpha)=\sum_{i=1}^{N}\left[\vec{\eta}_i(\alpha)\times\vec{\kappa}_i(\alpha)+\vec{\vec{S}}_{i\xi}(\alpha)\right]$$

$$\to_{\alpha\to\infty}\vec{S}_q=\sum_{a=1}^{N-1}\vec{\rho}_{qa}\times\vec{\pi}_{qa}+\sum_{i=1}^{N}\vec{S}_{qi\xi}\,. \tag{B15}$$

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Path integrals for boundaries and topological constraints: A white noise functional approach

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Using the Streit–Hida formulation where the Feynman path integral is realized in the framework of white noise analysis, we evaluate the quantum propagator for systems with boundaries and topological constraints. In particular, the Feynman integrand is given as generalized white noise functionals for systems with flat wall boundaries and periodic constraints. Under a suitable Gauss–Fourier transform of these functionals the quantum propagator is obtained for: (a) the infinite wall potential; (b) a particle in a box; (c) a particle constrained to move in a circle; and (d) the Aharonov–Bohm system. The energy spectrum and eigenfunctions are obtained in all four cases. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In 1983, Streit and Hida[1] used white noise analysis[2–4] to provide a more rigorous basis for the Feynman path integral.[5] This approach, where the Feynman integrand is identified as a generalized white noise functional, was subsequently developed[6] and applied to various quantum mechanical systems including time-dependent potentials.[7–12] In this paper, we shall employ the same white noise functional approach[1] to evaluate the Feynman path integral for systems with constraints brought about by specified boundary and topological conditions. We begin with a brief review of the white noise functional approach in Sec. II. The free particle propagator is then evaluated as an example and basic tool in the treatment of the constrained systems. Section III presents the evaluation of the propagator for flat wall boundaries such as a quantum particle in a region bounded by an infinite wall. Then the Feynman integral for a particle in a one-dimensional box[13,14] is examined, where we employ the Poisson sum formula to evaluate the propagator. Section IV considers systems with periodic constraints exemplified by the quantum particle constrained to move in a circle.[15] Here we again utilize the Poisson sum formula instead of introducing smeared wave packets as done in Ref. 16, where a white noise approach was also used. In the Aharonov–Bohm setup, a charged particle is constrained to move in a circle around a solenoid containing a magnetic flux Φ situated at the center. We obtain the propagator for this system which readily yields the Aharonov–Bohm energy spectrum and eigenfunctions. In the limit where the flux Φ vanishes, one obtains the expected result for a quantum particle in a circle.[15,16]

II. BRIEF REVIEW

A. The Feynman path integral

The quantum mechanical propagator, $\langle x_1|\exp(-iHt)|x_0\rangle = K(x_1,t|x_0,0)$, in nonrelativistic quantum mechanics can be calculated using Feynman's prescription of summing over all possible paths or ''histories'' of the particle which start at x_0 and end at x_1. This prescription is symbolically written as

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$$K(x_1,t|x_0,0)=\int \exp\left(\frac{i}{\hbar}S\right)D[x], \tag{2.1}$$

where S is the classical action for a particle of mass μ subjected to a potential $V(x)$ given by

$$S=\int_0^t\left[\frac{1}{2}\mu\dot{x}^2-V(x)\right]\mathrm{d}t. \tag{2.2}$$

A useful procedure in the explicit calculation of the path integral equation (2.1) is to slice the time interval N times, i.e., $t/N=t_j-t_{j-1}=\epsilon_j(j=1,\ldots,N)$, to obtain the time-sliced form,[5]

$$K(x_1,t|x_0,0)=\lim_{N\to\infty}\int\prod_{j=1}^{N}A_j\exp\left(\frac{i}{\hbar}S_j\right)\prod_{j=1}^{N-1}\mathrm{d}[x_j], \tag{2.3}$$

where, $x_j=x(t_j)$, S_j is the short-time action, and $A_j=\sqrt{\mu/2\pi i\hbar\epsilon_j}$ is the normalization. Although numerous quantum mechanical problems are solved using this prescription of Feynman,[17] there is still continuing effort to investigate the mathematical meaning of the Feynman path integral. Specifically, the integral, Eq. (2.1) or Eq. (2.3), with its infinite-dimensional flat ''measure'' $D[x]$ or $\Pi\mathrm{d}[x_j]$ is not mathematically well defined. There are several approaches for providing the Feynman integral with a more solid mathematical foundation,[18] but what we shall follow in this paper is the approach of Streit and Hida,[1] which utilizes the infinite-dimensional white noise calculus.

B. White noise analysis and the Feynman integral

What is referred to as white noise $\omega(t)$ is a random process defined as the time derivative of the Brownian motion $B(t)$, i.e.,

$$\omega(t)=\mathrm{d}B(t)/\mathrm{d}t. \tag{2.4}$$

Therefore, the white noise $\omega(t)$ may be viewed as the ''velocity'' of a Brownian motion. Alternatively, Wiener's Brownian motion $B(t)$ is represented by

$$B(t)=\int_0^t\omega(\tau)\mathrm{d}\tau. \tag{2.5}$$

White noise calculus was introduced by Hida in 1975[19] as a novel approach to infinite dimensional analysis. The basic idea was to take the collection of infinitely many independent random variables, $\{\omega(t);t\in\mathbf{R}\}$, and treat them as the coordinate system of an infinite dimensional space. One then proceeds to investigate generalized white noise functionals, $\Phi(\omega(t);t\in\mathbf{R})$, instead of functionals of Brownian motion, $f(B(t);t\in\mathbf{R})$.

In the framework of white noise analysis, the Feynman integral is treated as the ''average over all paths'' with a well-defined generalized white noise functional, or Hida distribution, as the weight.[2,6] The paths $x(t)$ which start at x_0 are parametrized as

$$x(t)=x_0+\left(\frac{\hbar}{\mu}\right)^{1/2}\int_0^t\omega(\tau)\mathrm{d}\tau, \tag{2.6}$$

in terms of the white noise random variable $\omega(t)$. Here, μ is the mass of the particle. With this, the velocity of the particle becomes $(\mathrm{d}x/\mathrm{d}t)=\sqrt{\hbar/\mu}\omega$, enabling us to write the exponential of $(i/\hbar)S_0$, where S_0 is the action for the free particle, as

$$\exp\left(\frac{i}{\hbar}S_0\right)=\exp\left[\frac{i}{\hbar}\int_0^t\left(\frac{1}{2}\mu\dot{x}^2\right)\mathrm{d}\tau\right]=\exp\left[\frac{i}{2}\int_0^t\omega(\tau)^2\,\mathrm{d}\tau\right]. \tag{2.7}$$

The next step is to interpret the Feynman integration over all paths, $\lim_{N\to\infty}\Pi\mathrm{d}[x_j]$ or $\mathrm{d}^\infty x$, in terms of integration over the Gaussian white noise measure $\mathrm{d}\mu(\omega)$:[2,6]

$$\mathrm{d}\mu(\omega)=N_\omega \exp\left(-\frac{1}{2}\int \omega(\tau)^2\,\mathrm{d}\tau\right)\mathrm{d}^\infty\omega. \tag{2.8}$$

We observe that, in the framework of white noise analysis, Feynman's flat "measure" $\mathcal{N}\mathrm{d}^\infty x$ would correspond to $N_\omega \mathrm{d}^\infty\omega=\exp[(1/2)\int\omega(\tau)^2\,\mathrm{d}\tau]\mathrm{d}\mu(\omega)$. With this, we also get the correspondence ($\hbar=1$),

$$\exp(iS_0)D[x]\rightarrow N\exp\left[\left(\frac{i+1}{2}\right)\int_0^t \omega(\tau)^2\,\mathrm{d}\tau\right]\mathrm{d}\mu(\omega), \tag{2.9}$$

where N is a suitable normalization factor.

The paths in the Feynman integral begin at x_0 and end at x_1. However, the parametrization of the paths $x(t)$ in Eq. (2.6) shows that only the initial point x_0 is fixed from where the random Brownian motion begins. We, therefore, fix the end point of the trajectories by means of the Donsker delta function,[2,16] $\delta(x(t)-x_1)$, where $x(t)$ is given by Eq. (2.6), such that at time t the particle is at the final point x_1. The Feynman integrand can now be represented by

$$I(x_1,t|x_0,0)=N\exp\left[\left(\frac{i+1}{2}\right)\int_0^t \omega(\tau)^2\,\mathrm{d}\tau\right]\delta\left(x_0+(\hbar/\mu)^{1/2}\int_0^t \omega(\tau)\mathrm{d}\tau-x_1\right), \tag{2.10}$$

in terms of the Gauss kernel,

$$I_0=N\exp\left[\left(\frac{i+1}{2}\right)\int_0^t \omega(\tau)^2\,\mathrm{d}\tau\right]. \tag{2.11}$$

Equipped with the Feynman integrand as a generalized white noise functional, and the measure in white noise space, the path integral is obtained by performing a "T-transform" of the Feynman integrand. Explicitly, this is defined as[2–4]

$$(T\Phi)(\xi)=\int \exp\left(i\int \omega(\tau)\xi(\tau)\mathrm{d}\tau\right)\Phi(\omega)\mathrm{d}\mu(\omega), \tag{2.12}$$

with $\xi\in S$, $\Phi\in S^*$, for the triple $S\subset L^2(\mu)\subset S^*$, the S^* being the white noise measure space. Here $\mathrm{d}\mu(\omega)$ is the Gaussian white noise measure[2–4] characterized by its Fourier transform,

$$\int \exp(i\langle\omega,\xi\rangle)d\mu(\omega)=\exp\left(-\frac{1}{2}\int \xi^2\,\mathrm{d}\tau\right)=C(\xi), \tag{2.13}$$

where $C(\xi)$ is the characteristic functional. For example, the T-transform of I_0, Eq. (2.11), is[2,6]

$$(TI_0)(\xi)=\exp\left(-\frac{i}{2}\int \xi^2\,\mathrm{d}\tau\right). \tag{2.14}$$

Similarly, the T-transform of the functional $I(x_1,t|x_0,0)$, Eq. (2.10), is given by $(\hbar=\mu=1)$[2]

$$(TI)(\xi)=\frac{1}{(2\pi it)^{1/2}}\exp\left[-\frac{i}{2}\int_0^t \xi^2(\tau)\mathrm{d}\tau\right]\times\exp\left[\frac{i}{(2t)}\left(\int_0^t \xi(\tau)\mathrm{d}\tau+x_1-x_0\right)^2\right]. \tag{2.15}$$

The $I(x_1,t|x_0,0)$, identified as the Feynman integrand, exists as a Hida distribution.[2,6] For $\xi=0$, this yields the free particle propagator,

$$K(x_1,t|x_0,0)=(TI)(0)=\frac{1}{(2\pi it)^{1/2}}\exp\left[\frac{i}{(2t)}(x_1-x_0)^2\right]. \tag{2.16}$$

We shall now employ this white noise approach to problems with boundaries and systems involving topologically inequivalent paths.

III. FLAT WALL BOUNDARIES

A. Infinite wall

We first consider a quantum particle of mass μ in a potential which describes an infinite wall at the origin, i.e.,

$$V(x)=\infty \quad \text{for } x\leqslant 0$$
$$=0 \quad \text{for } x>0. \tag{3.1}$$

Classically, for a particle which goes from x_0 to x_1 there are two possible paths: the first is a path that goes directly from the initial to the final point, and the second describes a path from x_0 that is reflected by the wall before arriving at x_1. Quantum mechanically, the particle propagator should satisfy the boundary condition,

$$K(x_1,x_0)=0$$
$$\text{at } x_1=0 \text{ or } x_0=0, \tag{3.2}$$

together with

$$\lim_{t\to 0} K(x_1,x_0;t)=\delta(x_1-x_0). \tag{3.3}$$

To obtain the propagator for the infinite wall problem we use the path parametrization of Eq. (2.6) and write the linear combination of white noise functionals,

$$I^W(x_1,t|x_0,0)=I_0\delta\left(x_0+(1/\mu)^{1/2}\int_0^t\omega(\tau)\mathrm{d}\tau-x_1\right)-I_0\delta\left(-x_0+(1/\mu)^{1/2}\int_0^t\omega(\tau)\mathrm{d}\tau-x_1\right), \tag{3.4}$$

where I_0 is the Gauss kernel given by Eq. (2.11). For a propagator which satisfies the boundary condition, Eq. (3.2), the combination of the type given by Eq. (3.4) has been discussed in the literature,[15,20,21] where the second term arises from particle trajectories originating from an image point, $-x_0$, and arriving at x_1.

Writing the delta function in terms of its Fourier representation we express the functional in Eq. (3.4) as ($\hbar=1$)

$$I^W(x_1,t|x_0,0)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\{\exp[ik(x_0-x_1)]-\exp[-ik(x_0+x_1)]\}$$
$$\times I_0\exp\left[(ik/\sqrt{\mu})\int_0^t\omega(\tau)\mathrm{d}\tau\right]\mathrm{d}k. \tag{3.5}$$

We then perform the T-transform of Eq. (3.5) following the definition in Eq. (2.12),

$$(TI^W)(\xi)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\{\exp[ik(x_0-x_1)]-\exp[-ik(x_0+x_1)]\}T\left(I_0\left(\xi+\frac{k}{\sqrt{\mu}}\right)\right)\mathrm{d}k$$
$$=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\{\exp[ik(x_0-x_1)]-\exp[-ik(x_0+x_1)]\}\exp\left(-\frac{i}{2}\int_0^t[\xi+(k/\sqrt{\mu})]^2\,\mathrm{d}\tau\right)\mathrm{d}k. \tag{3.6}$$

With $\xi=0$, the usual quantum propagator $(TI^W)(0)=K^W(x_1,t|x_0,0)$ can be obtained:

$$K^W(x_1,t|x_0,0)=\int_{-\infty}^{+\infty}\Psi_k(x_0)\Psi_k(x_1)\exp(-iE_kt)\mathrm{d}k, \tag{3.7}$$

where the energy is, $E_k=(k^2/2\mu)$, and the eigenfunction is given by $\Psi_k(x)=(1/\sqrt{\pi})\sin(kx)$.

B. Particle in a box

We next consider the Feynman integral for a particle of mass μ confined to move in a one-dimensional box of length L, with sides located at $x=0$ and $x=L$. Classically, the paths of the particle in a box can be categorized into four classes.[15] The first goes directly from x_0 to x_1 without hitting the walls; the second type of path hits the wall at $x=0$ before arriving at x_1; the third leaves x_0 and is reflected from the wall at $x=L$ before reaching x_1; and the fourth class describes a path which bounces once from the boundary at $x=0$ and also once from the wall at $x=L$ before reaching x_1. The other paths belonging to any of the four classes describe a particle bouncing back and forth inside the box of length L and, therefore, traveling an additional distance of $2Ln(n=0,1,2,\ldots)$.

Quantum mechanically, the particle propagator $K(x_1,x_0;t)$ has to satisfy the boundary conditions

$$K(x_1,0;t)=K(x_1,L;t)=K(0,x_0;t)=K(L,x_0;t)=0, \tag{3.8}$$

aside from the requirement

$$\lim_{t\to 0}K(x_1,x_0;t)=\delta(x_1-x_0). \tag{3.9}$$

Using the form of the Feynman functional for a free particle, Eq. (2.10), the white noise functional for a particle in a box can be written as

$$I^B(x_1,t|x_0,0)=\sum_{n=-\infty}^{+\infty}I_0C_n(x_1,t|x_0,0), \tag{3.10}$$

where[14]

$$\begin{aligned}2C_n(x_1,t|x_0,0)=&\,\delta(x(t)-x_1+2Ln)+\delta(-x(t)+x_1+2Ln)-\delta(x(t)+x_1+2Ln)\\&-\delta(-x(t)-x_1+2Ln)\end{aligned} \tag{3.11}$$

with $x(t)$ given by Eq. (2.6). The $(2Ln)$ in the delta function describes the fact that the particle leaving x_0 can bounce back and forth inside the box of length L before arriving at x_1. In Eq. (3.11) we observe that the first two terms, as well as the last two terms can be combined, respectively, so that Eq (3.10) can be written as

$$\begin{aligned}I^B(x_1,t|x_0,0)=\sum_{n=-\infty}^{+\infty}I_0\Bigg\{&\,\delta\Bigg(x_0+(1/\mu)^{1/2}\int_0^t\omega(\tau)\,\mathrm{d}\tau-x_1+2Ln\Bigg)\\&-\delta\Bigg(x_0+(1/\mu)^{1/2}\int_0^t\omega(\tau)\,\mathrm{d}\tau+x_1+2Ln\Bigg)\Bigg\}.\end{aligned} \tag{3.12}$$

We now write $\delta(x(t)-x_1+2Ln)=(\pi/L)\,\delta((\pi/L)[x(t)-x_1]+2\pi n)$, where $x(t)$ is given by Eq. (2.6). We can then apply the Poisson sum formula,[22]

$$\sum_{n=-\infty}^{\infty}\delta(\phi+2\pi n)=(1/2\pi)\sum_{m=-\infty}^{\infty}\exp(im\phi), \tag{3.13}$$

and write Eq. (3.12) as

$$I^B(x_1,t|x_0,0)=(1/2L)\sum_{m=-\infty}^{+\infty} I_0 \exp\left[(im\pi/L\sqrt{\mu})\int_0^t \omega(\tau)\,d\tau\right] \times\{\exp[(im\pi/L)(x_0-x_1)]-\exp[(im\pi/L)(x_0+x_1)]\}. \tag{3.14}$$

Taking the T-transform of the functional in Eq. (3.14) we get

$$\begin{aligned}(TI^B)(\xi)&=(1/2L)\sum_{m=-\infty}^{+\infty}(TI_0)(\xi+(m\pi/L\sqrt{\mu})) \times\{\exp[(im\pi/L)(x_0-x_1)]-\exp[(im\pi/L)(x_0+x_1)]\}\\ &=(1/2L)\sum_{m=-\infty}^{+\infty}\exp\left[-\frac{i}{2}\int_0^t\left(\xi+\frac{m\pi}{L\sqrt{\mu}}\right)^2 d\tau\right] \times\{\exp[(im\pi/L)(x_0-x_1)]-\exp[(im\pi/L)(x_0+x_1)]\}.\end{aligned} \tag{3.15}$$

Taking $\xi=0$, we obtain the propagator,

$$\begin{aligned}K^B(x_1,t|x_0,0)=(TI^B)(0)&=(1/2L)\sum_{m=-\infty}^{+\infty}\exp[-(i/2)(m\pi/L\sqrt{\mu})^2t] \times\{\exp[(im\pi/L)(x_0-x_1)]-\exp[(im\pi/L)(x_0+x_1)]\}\\ &=(1/2L)\sum_{m=-\infty}^{+\infty}\exp[-(i/2)(m\pi/L\sqrt{\mu})^2t] \times\left[\cos\left(\frac{m\pi}{L}(x_0-x_1)\right)-\cos\left(\frac{m\pi}{L}(x_0+x_1)\right)\right],\end{aligned} \tag{3.16}$$

with the sum over terms such as $\sin((m\pi/L)(x_0-x_1))$ giving a zero contribution. Equation (3.16) can be written in the symmetrized form,

$$K^B(x_1,t|x_0,0)=\sum_{m=-\infty}^{+\infty}\phi_m(x_0)\,\phi_m(x_1)\exp(-iE_mt), \tag{3.17}$$

where $E_m=m^2\pi^2/2\mu L^2$ and $\phi_m(x)=(1/\sqrt{L})\sin(m\pi x/L)$ are the energy eigenvalues and eigenfunctions for a quantum particle in a one-dimensional box.

IV. SYSTEMS WITH TOPOLOGICAL CONSTRAINTS

A. Quantum particle in a circle

In this section, we consider white noise functionals for a quantum system in a space which is multiply connected.[15,23–25] In particular, we treat the case of a particle constrained to move in a circle. This has been examined in the context of white noise analysis using smeared wave packets in Ref. 16. In contrast to this earlier work, we shall employ the Poisson sum formula, Eq. (3.13), to facilitate the evaluation of the propagator.

Let us begin by expressing the paths of the particle in a circle as ($\hbar=1;\ t_0=0$),

$$\vartheta(t)=\vartheta_0+\frac{1}{\sqrt{I}}\int_0^t\omega(\tau)\,d\tau, \tag{4.1}$$

where $I=\mu R^2$, for a particle of mass μ and a circle of radius R. We then note that the particle starting at a point ϑ_0 can move clockwise, or counterclockwise, before reaching a final point ϑ_1. The particle may even wind around the circle n times counterclockwise (for n positive), or $|n+1|$ times clockwise (for n negative) before stopping at ϑ_1. In contrast to Eq. (2.10) for the free particle, we must sum over all possible paths with different winding numbers and utilize the winding number decomposition of the propagator[15,23,24] to write

$$I^C(\vartheta_1,t|\vartheta_0,0)=\sum_{n=-\infty}^{+\infty} I_0\,\delta\left(\vartheta_0+\frac{1}{\sqrt{I}}\int_0^t\omega(\tau)\,d\tau-\vartheta_1+2\pi n\right), \tag{4.2}$$

where n is the winding number, and the kinetic part I_0 is given by Eq. (2.11).

Use of the Poisson sum formula, Eq. (3.13), in the functional Eq. (4.2) gives

$$I^C(\vartheta_1,t|\vartheta_0,0)=(1/2\pi)\sum_{m=-\infty}^{+\infty} I_0\exp\left[im\left(\vartheta_0+\frac{1}{\sqrt{I}}\int_0^t\omega(\tau)\,d\tau-\vartheta_1\right)\right]. \tag{4.3}$$

Taking the T-transform we get

$$\begin{aligned}(TI^C)(\xi)&=(1/2\pi)\sum_{m=-\infty}^{+\infty}\exp[im(\vartheta_0-\vartheta_1)]\left(T\left[I_0\exp\left((im/\sqrt{I})\int_0^t\omega(\tau)\,d\tau\right)\right]\right)(\xi)\\&=(1/2\pi)\sum_{m=-\infty}^{+\infty}\exp[im(\vartheta_0-\vartheta_1)]\,[(TI_0)(\xi+(m/\sqrt{I}))]\\&=(1/2\pi)\exp\left(\frac{-i}{2}\int\xi^2\,d\tau\right)\sum_{m=-\infty}^{+\infty}\exp[im(\vartheta_0-\vartheta_1)]\exp\left[\frac{-im^2t}{2I}-\frac{im}{\sqrt{I}}\int_0^t\xi(\tau)d\tau\right].\end{aligned} \tag{4.4}$$

For $\xi=0$, this yields the propagator for a charged particle constrained to move in a circle,

$$K(\vartheta_1,t|\vartheta_0,0)=(TI^C)(0)=(1/2\pi)\sum_{m=-\infty}^{+\infty}\exp[im(\vartheta_0-\vartheta_1)-iE_mt], \tag{4.5}$$

where the energy is $E_m=m^2/2\mu R^2$ in terms of the angular quantum number, m.

B. The Aharonov–Bohm set up

The Aharonov–Bohm setup[26–28] can be described by a charged particle which moves in a space with an impenetrable solenoid of radius R_0 that carries a flux Φ. For a solenoid oriented along the z axis, we can make use of the symmetry of the problem and look at the cross section, or the $(x-y)$ plane, where the Lagrangian for the particle is given by

$$L=\frac{1}{2}\mu\dot{\vec{r}}^2+\frac{e}{c}\vec{A}\cdot\dot{\vec{r}}. \tag{4.6}$$

Here, μ is the mass of the particle, $\dot{\vec{r}}=(d\vec{r}/dt)$, and the vector potential is given by

$$\vec{A}=\frac{\Phi}{2\pi}\frac{(-y\hat{i}+x\hat{j})}{x^2+y^2},\quad x^2+y^2>R_0, \tag{4.7}$$

such that the magnetic field is, $\vec{B}=\vec{\nabla}\times\vec{A}=0$, outside the solenoid. In polar coordinates, $\vec{r}=(r,\vartheta)$, the potential in the Lagrangian has the form

$$\frac{e}{c}\vec{A}\cdot\dot{\vec{r}}=\frac{e\Phi}{2\pi c}\,\dot{\vartheta}. \tag{4.8}$$

By constraining the particle to move in a circle with the solenoid at the center and located at the origin, the Lagrangian, Eq. (4.6), acquires the following form:

$$L=\frac{1}{2}I\dot{\vartheta}^2+\frac{e\Phi}{2\pi c}\,\dot{\vartheta}, \tag{4.9}$$

where, $I=\mu R^2$. The problem can now be cast in the language of white noise by modeling the paths of the particle using Eq. (4.1), such that Eq. (4.9) can be written as

$$L=\frac{1}{2}\omega^2+\frac{e\Phi}{2\pi c\sqrt{I}}\omega. \tag{4.10}$$

As in the case of a particle in a circle discussed previously, we can again use the winding number decomposition of the propagator,[15,23,24] with n being the winding number, and use the Lagrangian, Eq. (4.10), for the Aharonov–Bohm setup to write

$$I^{\mathrm{AB}}(\vartheta_1,t|\vartheta_0,0)=\sum_{n=-\infty}^{+\infty}I_0\,\delta\left(\vartheta_0+\frac{1}{\sqrt{I}}\int_0^t\omega(\tau)\,d\tau-\vartheta_1+2\pi n\right)\exp\left[i(\alpha/\sqrt{I})\int_0^t\omega(\tau)\,\mathrm{d}\tau\right], \tag{4.11}$$

where I_0 is given by Eq. (2.11) and the last factor contains the potential term with the magnetic flux, $\alpha=e\Phi/2\pi c$. Using the Poisson sum formula, Eq. (3.13), the functional, Eq. (4.11), becomes

$$I^{\mathrm{AB}}(\vartheta_1,t|\vartheta_0,0)=(1/2\pi)\sum_{m=-\infty}^{+\infty}I_0\exp[im(\vartheta_0-\vartheta_1)]\exp\left[i[(m+\alpha)/\sqrt{I}]\int_0^t\omega(\tau)\mathrm{d}\tau\right], \tag{4.12}$$

whose T-transform gives us

$$\begin{aligned}(TI^{\mathrm{AB}})(\xi)&=(1/2\pi)\sum_{m=-\infty}^{+\infty}\exp[im(\vartheta_0-\vartheta_1)]\left(T\left[I_0\exp\left(\frac{i(m+\alpha)}{\sqrt{I}}\int_0^t\omega(\tau)\,\mathrm{d}\tau\right)\right]\right)(\xi)\\&=(1/2\pi)\sum_{m=-\infty}^{+\infty}\exp[im(\vartheta_0-\vartheta_1)]\left[(TI_0)\left(\xi+\frac{(m+\alpha)}{\sqrt{I}}\right)\right]\\&=(1/2\pi)\exp\left(\frac{-i}{2}\int\xi^2\,\mathrm{d}\tau\right)\sum_{m=-\infty}^{+\infty}\exp[im(\vartheta_0-\vartheta_1)]\\&\quad\times\exp\left[\frac{-i(m+\alpha)^2t}{2I}-\frac{i(m+\alpha)}{\sqrt{I}}\int_0^t\xi(\tau)\mathrm{d}\tau\right].\end{aligned} \tag{4.13}$$

For $\xi=0$, this yields the Aharonov–Bohm propagator for a charged particle constrained to move in a circle,

$$K^{\mathrm{AB}}(\vartheta_1,t|\vartheta_0,0)=(TI^{\mathrm{AB}})(0)=(1/2\pi)\sum_{m=-\infty}^{+\infty}\exp[im(\vartheta_0-\vartheta_1)-iE_mt], \tag{4.14}$$

where the energy is $E_m=[m+(e\Phi/2\pi c)]^2/2\mu R^2$, with m the angular quantum number modified by the magnetic flux $e\Phi/2\pi c$. For the case where the magnetic flux $\Phi=0$, the Aharonov–Bohm propagator reduces to that of the particle in a circle discussed in the previous section.

V. CONCLUSION

In this paper, Feynman integrals for some systems with boundaries or constraints have been explicitly evaluated using the white noise functional approach. This approach was first introduced by Streit and Hida in Ref. 1, where they constructed the Feynman integral in the framework of white noise analysis. This infinite dimensional calculus provides a natural setting for the ''sum over all trajectories'' while quantum analysis is done in real time without resort to time slicing.[5] Several quantum systems have been treated explicitly using this method,[7–12] and this paper adds topologically constrained systems to the list. These solvable examples should shed more light on the true mathematical meaning of the Feynman integral, as well as pave the way for the treatment of more complicated systems with boundaries and nontrivial non-Gaussian systems.

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The fuzzy sphere ⋆-product and spin networks

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We analyze the expansion of the fuzzy sphere noncommutative product in powers of the noncommutativity parameter. To analyze this expansion we develop a graphical technique that uses spin networks. This technique is potentially interesting in its own right as introducing spin networks of Penrose into noncommutative geometry. Our analysis leads to a clarification of the link between the fuzzy sphere noncommutative product and the usual deformation quantization of the sphere in terms of the ⋆-product. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1456255]

I. INTRODUCTION

This paper originated from an observation that manipulating with functions on the fuzzy sphere is equivalent to manipulating with certain SU(2) spin networks. Although this observation is nothing more than a reinterpretation of the construction[1] of noncommutative sphere spherical harmonics, it does bring spin networks of Penrose[2] into the subject of noncommutative geometry, and is thus interesting as providing an unusual perspective on noncommutative manifolds.

In this paper we would like to illustrate the usage of spin networks by deriving some facts about the noncommutative product on the fuzzy sphere. The fuzzy sphere of Ref. 3 gives one of the simplest examples of noncommutative spaces. In this reference the fuzzy sphere is constructed by replacing the algebra of polynomials on the sphere by the noncommutative algebra generated by Pauli matrices taken in a fixed irreducible representation of SU(2). More precisely, the algebra of functions from $L^2(S^2)$ is thought of as the algebra of polynomials in $x_i \in \mathbb{R}^3$ modulo the relation $\|x\|^2=1$. We set the radius of the sphere to be 1. One then quantizes the coordinates x_i via

$$x_i \to \hat{X}^i := \frac{\hat{J}^i}{\sqrt{\frac{N}{2}\left(\frac{N}{2}+1\right)}}, \tag{1.1}$$

where $\hat{J}^i$ are the generators of $\mathfrak{su}(2)$, satisfying $[\hat{J}^i,\hat{J}^j]=i\epsilon^{ijk}\hat{J}^k$, taken in the $(N+1)$-dimensional irreducible representation of SU(2). The factor in (1.1) is adjusted precisely in such a way that the "quantized" coordinates $\hat{X}^i$ square to one. The rule (1.1) gives quantization of the monomials of order one in coordinates. Monomials of order up to N are quantized by replacing the products of the coordinates x_i by the symmetrized products of matrices $\hat{X}^i$ (see more on this map in Sec. III). Monomials of order $(N+1)$ and higher become linearly dependent of lower order monomials, so that the algebra of functions on the fuzzy sphere is finite dimensional. The integral over S^2 is replaced by the trace:

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$$\int_{S^2} \to \frac{1}{(N+1)} \mathrm{Tr}. \tag{1.2}$$

When $1/N$, which plays the role of the parameter of noncommutativity, is taken to zero, the commutator of $\hat{X}^i$ vanishes, and the algebra of functions on the noncommutative sphere reduces to the commutative algebra. The trace (1.2) then reduces to the usual integral. It is in this sense that the fuzzy sphere reduces to the usual S^2 when the noncommutativity parameter is sent to zero. For more details on this construction see, e.g., Ref. 3.

In practice one would like to have a more explicit description of the above-noted quantization map. In particular, any function on the sphere can be decomposed into the basis of spherical harmonics, and one would like to know the matrices into which the spherical harmonics are sent under the quantization map. This was described in Ref. 1, where it was realized that the components of these matrices are given by certain Clebsch–Gordan coefficients. Interestingly, Ref. 1 appeared before the introduction of the notion of fuzzy sphere in Ref. 3, and contained essentially all the ingredients of the construction.

Let us now explain why one should expect the appearance of Clebsch–Gordan coefficients, or $3j$-symbols, as the result of the quantization map. Consider the following simple chain of isomorphisms:

$$\mathrm{End}(V^{N/2}) \sim V^{N/2} \times (V^{N/2})^* \sim \oplus_{l=1}^{N} V^l. \tag{1.3}$$

Here V^l is the space of the irreducible representation of SU(2) of the dimension $(2l+1)$. The Clebsch–Gordan coefficients relate a basis on the right-hand side of (1.3) to a basis on the left-hand side. A particular basis in V^l is given by the usual spherical harmonics $Y_{lm}(\theta, \phi)$. Thus, the isomorphism in (1.3) implies that every Y_{lm}, $l \leqslant N$ must be representable as an element of $\mathrm{End}(V^{N/2})$, that is, as an $(N+1)\times(N+1)$ matrix. The components of this matrix are given by the corresponding Clebsch–Gordan coefficients. We shall write down the corresponding formulas in Sec. II.

The appearance of the Clebsch–Gordan coefficients, or $3j$-symbols, as components of the matrices representing the spherical harmonics indicates that spin networks must play some role. Indeed, spin networks are exactly the quantities constructed from $3j$-symbols, corresponding to their vertices, with their indices contracted in some way, the contraction being represented by the spin network edges. As we shall see, the problem of calculation of the noncommutative analog of the integral of a product of a number of spherical harmonics always reduces to the evaluation of a particular spin network. One of the goals of the present paper is to develop the corresponding techniques. We do this by studying in some detail the $\star$-product on the fuzzy sphere.

Our paper partially overlaps with Ref. 4. In particular, the formula for the $\star$-product on the fuzzy sphere in terms of the $6j$-symbol is also contained in Ref. 4. What is new in this paper is the expression for the expansion of this $\star$-product in powers of the noncommutativity parameter. Our approach also allows us to clarify the link between the fuzzy sphere product and the deformation quantization $\star$-product. Finally, we would like to mention Ref. 5, which also studies the quantization of the space of functions on S^2.

A large part of the paper deals with the expansion of the $\star$-product in powers of the noncommutativity parameter. As we have already mentioned, the role of noncommutativity parameter is played by $1/N$: the commutative limit corresponds to $N \to \infty$. The limit of large size matrices also plays a key role[6] in the at first seemingly unrelated subject of SU(N) Yang–Mills theories. It is tempting to speculate that this is not a coincidence and that there are some relations between the two subjects. Glimpses of such a relation have started appearing in work on noncommutative geometry in string theory, see, e.g., Ref. 7. Unfortunately, we do not have more to say about this in the present paper.

II. SETUP

Under the quantization map the spherical harmonics $Y_{lm}(x)$, $x \in S^2$ are mapped into certain $(N+1)\times(N+1)$ matrices, and, as explained in Sec. I, components of these matrices are given by the Clebsch–Gordan coefficients. Before we spell out what these matrices are, let us fix our conventions as to what basis of spherical harmonics is used. Let us introduce, for integer l,

$$\overline{\Theta}^l_m(x) := i^{-m}\langle l,m|T_g|\omega\rangle, \tag{2.1}$$

where the bar denotes the complex conjugation, $|l,m\rangle$ form a highest weight normalized basis in the irreducible representation of the dimension $(2l+1)$, and $|\omega\rangle$ is the vector (unique up to a phase) that is invariant under the action of some fixed SO(2) subgroup of SO(3). It is given by $|\omega\rangle = |l,0\rangle$. Then (2.1) is a function on the homogeneous space $\mathrm{SO}(3)/\mathrm{SO}(2) \sim S^2$. Using formula (A1) for the integral of a product of two matrix elements, one gets the orthogonality relation for Θ:

$$\int_{S^2} \mathrm{d}x\, \overline{\Theta}^l_m \Theta^{l'}_{m'} = \frac{\delta^{ll'}\delta_{mm'}}{\dim_l}, \tag{2.2}$$

where $\mathrm{d}x$ is the normalized measure on the sphere. The presence of the factor of $\dim_l = (2l+1)$ in this formula (and also the usage of the normalized measure $\mathrm{d}x$) is what makes our Θ^l_m different from the usual spherical harmonics Y_{lm}. The basis (2.1) satisfies

$$\overline{\Theta}^l_m = (-1)^m \Theta^l{}_{-m}. \tag{2.3}$$

Note that the same relation is satisfied by the usual Y_{lm}, so our basis is indeed only different by a normalization.

Along with the orthogonality relation (2.2), we will need the value of the integral of a product of three spherical harmonics. It is easily computed using formula (A2) for the integral of a product of three matrix elements and definition (2.1) of the spherical harmonics. We have

$$\int_{S^2} \mathrm{d}x\, \overline{\Theta^{l_3}_{m_3}(x)} \Theta^{l_1}_{m_1}(x) \Theta^{l_2}_{m_2}(x) = \overline{\hat{C}^{l_3 l_1 l_2}_{0\,0\,0}} \hat{C}^{l_3 l_1 l_2}_{m_3 m_1 m_2}. \tag{2.4}$$

Here $\hat{C}$ are Clebsch–Gordan coefficients, and we have used the fact that the right-hand side is only nonzero when $m_1 + m_2 = m_3$. Our choice of normalization for Clebsch–Gordan's is such that the so-called theta-symbol is always equal to one, see (2.12). For reference, let us mention that our coefficients $\hat{C}^l$ are given by $1/\sqrt{\dim_l}$ times the Clebsch–Gordan coefficients used by Vilenkin and Klimyk.[8] The caret over the symbol of the coefficient is used precisely to indicate this difference in normalizations. It is now not hard to see that (2.4), together with (2.2), implies that

$$\Theta^{l_1}_{m_1}(x) \Theta^{l_2}_{m_2}(x) = \sum_{l_3 = |l_1 - l_2|}^{l_1 + l_2} \sum_{m_3} \dim_{l_3} \hat{\Theta}^{l_3}_{m_3}(x) \overline{\hat{C}^{l_3 l_1 l_2}_{0\,0\,0}} \hat{C}^{l_3 l_1 l_2}_{m_3 m_1 m_2}. \tag{2.5}$$

Note that, in this formula, the commutativity of the product comes from the symmetry relations for the Clebsch–Gordan, namely:

$$\hat{C}^{l_3 l_2 l_1}_{m_3 m_2 m_1} = (-1)^{l_3 - l_1 - l_2} \hat{C}^{l_3 l_1 l_2}_{m_3 m_1 m_2}. \tag{2.6}$$

The group SO(3) acts on functions on S^2 by left shifts $T_g f(x) = f(g^{-1}x)$, and the functions $\Theta^l_m(x)$ for fixed l span the vector space V^l, in which the representation by shifts is irreducible. In view of the isomorphisms (1.3), functions $\Theta^l_m(x)$, $l \leqslant N$ can be mapped to $(N+1)\times(N+1)$ matrices, whose components must be given by Clebsch–Gordan coefficients. These matrices are

$$[\hat{\Theta}^{l}_{m}]_{ij}=\sqrt{N+1}\,\hat{C}^{l(N/2)(N^*/2)}_{mij}, \tag{2.7}$$

where $\hat{C}^{l(N/2)(N^*/2)}_{mij}$ are Clebsch–Gordan coefficients with properties:

$$\sum_{mij}\overline{\hat{C}^{l(N/2)(N^*/2)}_{mij}}\hat{C}^{(N/2)(N^*/2)}_{mij}=1, \tag{2.8}$$

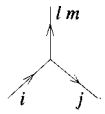
$$\overline{\hat{C}^{l(N/2)(N^*/2)}_{mji}}=(-1)^m\hat{C}^{l(N/2)(N^*/2)}_{-mij}. \tag{2.9}$$

Here $(N/2)^*$ is the conjugate representation to $N/2$. The first of these properties is a normalization condition that will be explained in the following, while the second is a ''quantum'' analog:

$$(\hat{\Theta}^{l}_{m})^{\dagger}=\widehat{\overline{\Theta^{l}_{m}}} \tag{2.10}$$

of the classical property (2.3).

We are now in the position to introduce the graphic notations that will lead us to spin networks and somewhat explain the normalization choices made previously. We shall denote Clebsch–Gordan's by a tri-valent vertex, with its three edges representing the three pairs of indices of $\hat{C}$, so that

$[\hat{\Theta}^{l}_{m}]_{ij}=\sqrt{N+1}$ 

. (2.11)

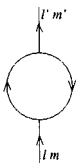
Each edge corresponds to a pair of indices: an irreducible representation (spin) and a basis vector in this representation. If no spin is indicated, as for the bottom edges in (2.11), then $N/2$ is assumed. Edges are oriented. The operation of complex conjugation is represented by changing the orientation of all the edges. The origin of the graphic notation (2.11) is evident: the Clebsch–Gordan coefficients it represents are just the matrix elements of the intertwiner between the tensor product of $V^{N/2}\times(V^{N/2})^*$ and the representation V^l; this intertwiner is represented by a trivalent vertex.

Using the graphical notation introduced, the normalization condition (2.8) is a statement about the value of the so-called theta graph:

$=1.$ (2.12)

This graph is constructed taking the product of two $3j$-symbols and summing over the ''internal'' indices, as in (2.8). The theta graph is the simplest spin network, and the $3j$ symbols we use are normalized in precisely such a way that the value of this graph is always one.

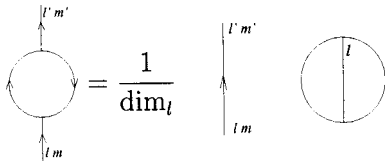
As we mentioned in Sec. I, for the noncommutative sphere, the integral over S^2 goes into the trace. Let us now find the quantum analog of the orthogonality relation (2.2). The corresponding quantity is graphically represented as

$$\frac{1}{N+1}\mathrm{Tr}\left(\hat{\Theta}^{l}_{m}\right)^{\dagger}\hat{\Theta}^{l'}_{m'}=$$ 

. (2.13)

Here † denotes the operation of taking the Hermitian conjugation, and its effect is exactly such that all ''internal'' indices are contracted as in the above-given diagram. Now using an elementary

fact that



(2.14)

where a straight line represents the matrix element of the intertwiner between representations l and l', that is, a product of Kronecker deltas, we see that the "quantum" spherical harmonics $\hat{\Theta}$ satisfy exactly the same orthogonality relation (2.2) as the classical ones. The factor of $\sqrt{N+1}$ in (2.7) was adjusted precisely in such a way that this property holds.

We hope that the reader has already started appreciating the convenience of our graphical notations. Using these notations, complicated expressions are calculated by using elementary facts from representation theory. Thus, the property (2.14) is proved by noticing that the left-hand side of this equation is an intertwiner between representations l and l'. Such an intertwiner only exists when $l=l'$, which means that the result must be proportional to the straight line. The proportionality coefficient can be calculated by taking the trace of the whole expression, which is graphically represented by "closing" the open ends of the diagram. Performing this operation on the left-hand side, one gets the theta graph. The right-hand side gives a loop, whose value is just the dimension of the corresponding representation. We shall see other examples of such proofs in the sequel.

Let us now, before we go to our discussion of the ⋆-product on the fuzzy sphere, prove that the quantization rule (2.7) does give the correct quantization of the sphere, that is, the one given by (1.1). To this end, we must calculate the commutator of the noncommuting coordinates $\hat{X}^i$. Recall that classically the coordinates x_i are just the spherical harmonics corresponding to $l=1$:

$$x_1=\frac{1}{\sqrt{2}}(\Theta^1_1-\Theta^1_{-1}),\quad x_2=\frac{1}{i\sqrt{2}}(\Theta^1_1+\Theta^1_{-1}),\quad x_3=\Theta^1_0. \tag{2.15}$$

In the quantum case we replace the harmonics Θ^1 by the corresponding matrices (2.7). We then must have

$$[\hat{X}^i,\hat{X}^j]=i\epsilon^{ijk}\hat{X}^k\frac{1}{\sqrt{\frac{N}{2}\left(\frac{N}{2}+1\right)}}. \tag{2.16}$$

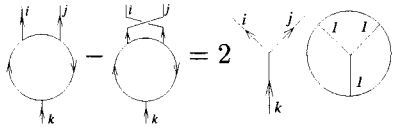
Let us show that this property indeed holds. We have

$$\frac{1}{N+1}[\hat{X}^i,\hat{X}^j]=$$

(2.17)

where the spin 1 is assumed on the vertical lines, and

$$\frac{1}{(N+1)^{3/2}}\mathrm{Tr}\left((\hat{X}^k)^\dagger[\hat{X}^i,\hat{X}^j]\right)=$$



. (2.18)

To get the last equality we used the fact that each of the two terms is an intertwiner from a single representation of spin 1 to the tensor product of two such representations. Such an intertwiner must be proportional to the unique intertwiner that is given by the tri-valent vertex on the right-hand side of (2.18). The proportionality coefficient is easily determined by closing all the open

edges, and is given by the $6j$-symbol on the right-hand side. The second term equals minus the first one, see (2.5), which explains the factor of 2. The $3j$-symbol is given by

$$= \frac{(-i)}{\sqrt{3!}}\epsilon^{ijk}, \tag{2.19}$$

and the $6j$-symbol can be calculated using formula (A3). The result is

$$= (-1)\frac{1}{\sqrt{3!}}\frac{1}{\sqrt{N+1}}\frac{1}{\sqrt{\frac{N}{2}(\frac{N}{2}+1)}}. \tag{2.20}$$

Combining all this together, we see that (2.16) indeed holds.

We thus learn that the quantization rule (2.7) coincides with the standard quantization map (1.1), at least for the spherical harmonics of the first order. Interestingly, the result of the commutator in the quantum case turns out to be expressed through the $6j$-symbol. In the case considered when all the spins were taken to be $l=1$, the commutator coincides with the classical result. However, for higher modes l one expects a deviation from the classical expressions. This is summarized in the notion of the $\star$-product. We shall now illustrate the described spin network techniques by deriving some facts about this $\star$-product.

III. THE $\star_N$-PRODUCT

As we have stated in Sec. I, our aim is to illustrate the spin network construction by deriving some facts about the fuzzy sphere noncommutative product. However, before we introduce and study this product, let us review the usual $\star$-product that arises in the deformation quantization of $\mathbb{R}^3$ equipped with Poisson structure invariant under the rotation group. We will then discuss a relation between this, and the fuzzy sphere product.

Let us start by recalling some general facts about $\star$-products. A $\star$-product gives a noncommutative deformation of the usual (pointwise) multiplication of functions. Let $\mathcal{A}=\mathcal{C}^\infty(M)$ be the space of smooth functions on a manifold M, and suppose that M is equipped with a Poisson bracket $\{\cdot,\cdot\}$. Let us denote by $A[[\hbar]]$ the space of formal power series with coefficients in $\mathcal{A}$. A star product on $\mathcal{A}$ is an associative, $\mathbb{R}[[\hbar]]$-linear product on $A[[\hbar]]$. The product of two functions on M is given by

$$\phi\star\psi=\sum_n \hbar^n B_n(f,g), \tag{3.1}$$

$B_n(\cdot,\cdot)$ being bidifferential operators. The first term in the expansion is the usual commutative product $B_0(f,g)=fg$, while the first term in the commutator is the Poisson bracket $B_1(f,g)-B_1(g,f)=\{f,g\}$. The Poisson bracket therefore gives the germ of deformation of the commutative product towards the $\star$-product. There is a notion of gauge transformation that can be defined on the set of $\star$-products and Poisson brackets. The group of these gauge transformations consists of linear automorphisms of $\mathcal{A}[[\hbar]]$ of the following form:

$$f\to U(f)=f+\hbar U_1(f)+\cdots\hbar^n U_n(f), \tag{3.2}$$

where $U_i(f)$ are differential operators. It acts on the set of star product as

$$\phi\star_U\psi=U^{-1}(U(\phi)\star U(\psi)). \tag{3.3}$$

Products related by such a transformation are called equivalent.

As is well known, when M is the dual of a Lie algebra $M=\mathfrak{g}^*$, there is the so-called Kirillov–Lie Poisson structure on it, whose symplectic leaves are coadjoint orbits. The bracket is

$$\{\phi,\psi\}(x)=x^k C_k^{ij}\partial_i\phi(x)\partial_j\psi(x), \tag{3.4}$$

where x^i are the components of $x\in\mathfrak{g}^*$. Using the natural identification between linear functions on $\mathfrak{g}^*$ and $\mathfrak{g}$ one can equivalently view x^i as a basis e^i in $\mathfrak{g}$. Then C_k^{ij} are the structure constants with respect to this basis. This identification extends to a natural isomorphism between the space $\mathrm{Pol}(\mathfrak{g}^*)$ of polynomials in x^i and symmetric algebra $\mathrm{Sym}(\mathfrak{g}^*)$. There are several equivalent ways to introduce a deformation quantization of the Kirillov bracket. We shall refer to the arising ⋆-product as Kirillov ⋆-product.

A. Universal enveloping algebra

The standard way to introduce a ⋆-product in $\mathfrak{g}^*$ is by using the universal enveloping algebra $\mathfrak{U}(\mathfrak{g})$. Recall that the universal enveloping algebra $\mathfrak{U}(\mathfrak{g})$ of the Lie algebra $\mathfrak{g}$ with generators e^i satisfying

$$[e^i,e^j]=\hbar C_k^{ij}e^k, \tag{3.5}$$

where C_k^{ij} are the structure constants, is the algebra generated by all polynomials in the generators e^i modulo the relation $XY-YX=[X,Y]$ for all $X,\ Y\in\mathfrak{g}$. The Poincare–Birkhoff–Witt theorem states that $\mathfrak{U}$ is isomorphic to the algebra $\mathrm{Sym}(\mathfrak{g})\sim\mathrm{Pol}(\mathfrak{g}^*)$ generated by all completely symmetrized polynomials in the generators: $\mathfrak{U}(\mathfrak{g})\sim\mathrm{Sym}(\mathfrak{g})$. Since the algebra $\mathrm{Sym}(\mathfrak{g})$ is naturally isomorphic to the algebra $\mathrm{Pol}(\mathfrak{g}^*)$ of polynomial functions on the dual space $\mathfrak{g}^*$, we have the one-to-one map

$$\sigma:\mathrm{Pol}(\mathfrak{g}^*)\to\mathfrak{U}(\mathfrak{g}),$$

$$x^{k_1}\cdots x^{k_n}\to\frac{1}{n!}\sum_s\ e^{k_{s(1)}}\cdots e^{k_{s(n)}},$$

where the sum is taken over all permutations s of n integers, x^i are linear functionals on $\mathfrak{g}^*$, and e^i are the corresponding elements in $\mathfrak{g}$. Using the map σ, one can define the following noncommutative product on $\mathrm{Pol}(\mathfrak{g}^*)$:

$$(\phi\star\psi)(x)=\sigma^{-1}[\sigma(\phi)\sigma(\psi)]. \tag{3.6}$$

Note that this ⋆-product explicitly depends on the deformation parameter $\hbar$ because the latter enters the commutator (3.5). What is not so straightforward to see is that this product can be expanded in terms of differential operators. For example, one can prove the following formula:

$$(e^X\star Y)(x)=e^{X(x)}\left[\frac{\mathrm{ad}\,X}{1-e^{-\mathrm{ad}\,X}}\cdot Y\right](x). \tag{3.7}$$

B. Baker–Campbell–Haussdorf formula

The Baker–Campbell–Haussdorf formula states that, given two Lie algebra elements X,Y, the product of the corresponding group elements can be expressed as

$$e^X\cdot e^Y=e^{X+Y+\Psi(X,Y)}, \tag{3.8}$$

where $X,Y,\ \Psi(X,Y)\in\mathfrak{g}$ and

$$X+Y+\Psi(X,Y)=\sum_{m=1}^{\infty}\frac{(-1)^{(m-1)}}{m}\sum_{\substack{k_i+l_i\geqslant 1\\ k_i\geqslant 0,l_i\geqslant 0}}\frac{[X^{k_1}Y^{l_1}\cdots X^{k_m}Y^{l_m}]}{k_1!l_1!\cdots k_m!l_m!},\tag{3.9}$$

and $[X_1\cdots X_n]$, $X_i\in\mathfrak{g}$ denotes $(1/n)[\cdots[[X_1,X_2],X_3],\ldots,X_n]$. This is the so-called Campbell–Hausdorff formula in the Dynkin form, see, e.g., Ref. 9. Representing the commutator as $[X,Y]=XY-YX$, one can think of $\Psi(X,Y)$ as a complicated sum of polynomials in the components X_i, Y_i:

$$\Psi_i(X,Y)=\sum_{i\vec{n}j\vec{m}}A_i^{i\vec{n}j\vec{m}}X_{i_1}\cdots X_{i_n}Y_{j_1}\cdots Y_{j_m}.\tag{3.10}$$

One then defines a $\star$-product on the space of functions on $\mathbb{R}^3=\mathfrak{g}^*$ by

$$(\phi\star\psi)(x)=\phi e^{(1/\hbar)(x|\Psi(\hbar\partial,\hbar\partial))}\psi,\tag{3.11}$$

where we have replaced the argument X_i of $\Psi(X,Y)$ by $\hbar$ times the derivative $\partial/\partial x^i$ acting on the left on ϕ, and the argument Y_i by the derivative acting on the right on ψ. The quantity $(x|\Psi)$ in the exponential stands for the contraction $x^i\Psi_i$. One can prove that the product (3.11) is, in fact, the same as (3.6). A good exposition of the relation between these two quantizations, and also of the relation of both to the Kontsevich deformation quantization, is given in Ref. 10.

C. Path integral

The third way to define the Kirillov $\star$-product uses a version of the Cattaneo–Felder[11] path integral. For the case in question, the function $\alpha^{ij}(x)$ that determines the Poisson structure:

$$\{\phi,\psi\}=\sum_{ij}\alpha^{ij}(x)\partial_i\phi(x)\partial_j\psi(x),\tag{3.12}$$

is linear in x, and the action used in Ref. 11 can be given a simple form of the action of the so-called BF theory. Thus, let us consider the following theory on the unit disk. It has two dynamical fields: the field B_i, which is $\mathfrak{g}^*$ valued, this field is the analog of the field X^i of Ref. 11, and the G-connection A^i, with curvature $F^i(A)$. This connection is the analog of the one-form field η of Ref. 11. The action is then given by

$$S[B,A]=\int_U B_iF^i(A),\tag{3.13}$$

where the integral is taken over the unit disk U. The $\star$-product is then given by the following path integral:

$$(\phi\star\psi)(x)=\langle\phi(B(0))\psi(B(1))\rangle_x\equiv\int_{B(\infty)=x}\mathcal{D}B\mathcal{D}A\,\phi(B(0))\psi(B(1))\exp\left(\frac{1}{\hbar}\int \mathrm{BF}\right).\tag{3.14}$$

Thus, the $\star$-product is obtained by computing the correlation function of two operators in this theory. The operators are given by functions ϕ, ψ on the values of the B field at two boundary points $0,1\in\partial U$. The value of B at the third boundary point ∞ is kept fixed in the path integral. One also has the boundary conditions for the connection: it is required that the connection one-form vanishes on ∂U on vectors tangent to the boundary. Then the perturbative expansion of the path integral (3.14) gives a noncommutative product in $\mathbb{R}^3$, which can be checked to be associative, and, thus, is a $\star$-product. Since the BF action (3.13) is essentially the one used by Cattaneo and Felder[11] product (3.14) is the Kontsevich product.[12] It can then be shown, see Ref. 10, that this product is equivalent to the one defined using the Campbell–Hausdorff formula.

D. $\star_N$-product

Having reviewed the usual ⋆-product, let us introduce the noncommutative product that is relevant in the context of the fuzzy sphere. The square integrable functions on S^2 can be decomposed into the basis of spherical harmonics:

$$\phi(x)=\sum_{lm}\ \phi^l_m\Theta^l_m(x). \tag{3.15}$$

We have a quantization map, which sends spherical harmonics Θ^l_m, $l\leqslant N$ to matrices (2.11). Under this map, functions are sent to matrices:

$$\phi(x)\to\hat{\phi}=\sum_{l=0}^{N}\ \sum_m\ \phi^l_m\hat{\Theta}^l_m \tag{3.16}$$

Note that this map is insensitive to the ''high frequency'' behavior of the function, for it cuts off all the harmonics with $l>N$.

Let us also construct the inverse map. To this end, we introduce a noncommutative analog of the δ function:

$$\hat{\delta}_x=\sum_{l=0}^{N}\ \sum_m\ \dim_l(\hat{\Theta}^l_m)^\dagger\Theta^l_m(x). \tag{3.17}$$

Thus, the ''quantum'' δ-function is a matrix that in addition depends on a point $x\in S^2$. Note that the δ-function is ''real'': $\hat{\delta}^\dagger=\hat{\delta}$. Given an arbitrary operator (matrix) $\hat{\phi}$ one can construct from it a square integrable function:

$$\hat{\phi}\to\phi(x)=\frac{1}{N+1}\mathrm{Tr}(\hat{\delta}_x\hat{\phi}). \tag{3.18}$$

The resulting functions, of course, contain only the modes with $l\leqslant N$. Using the δ-function (3.17) one can give another expression for the quantization rule (3.16). Indeed, we have

$$\hat{\phi}=\int_{S^2}\mathrm{d}x\ \hat{\delta}_x\phi(x). \tag{3.19}$$

One can easily check that the composition of the quantization map (3.16) and its inverse (3.18) give, back the function one started from with all its modes $l>N$ cut off. Let us formalize this introducing the notion of the projector $\mathcal{P}_N$:

$$\phi\to\hat{\phi}\to\frac{1}{N+1}\mathrm{Tr}(\hat{\delta}_x\hat{\phi})=\mathcal{P}_N\phi. \tag{3.20}$$

Thus, the maps (3.16) and (3.18) are one-to-one on the space of functions that only contain modes up to N. Let us denote this space by $\mathcal{A}^N$. Note that $\mathcal{A}^N=\mathcal{A}^\infty/\mathrm{Ker}\,\mathcal{P}_N$, where $\mathcal{A}^\infty$ is the algebra of all L^2 functions on S^2.

Having defined the quantization map, we can use it to define a noncommutative product on the space $\mathcal{A}^N$ via

$$\widehat{\phi\star_N\psi}=\hat{\phi}\hat{\psi}. \tag{3.21}$$

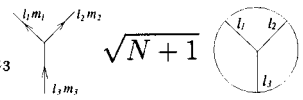
Let us emphasize that this is well defined only in $\mathcal{A}^N$ since $\hat{\phi}=\widehat{\mathcal{P}_N\phi}$ and the product $\star_N$ does not coincide with the usual ⋆-product reviewed previously, because they are defined on different

spaces. While $\star_N$ is the product on the space of functions $\mathcal{A}^N$, the "real" $\star$-product acts on the space of all square integrable functions $\mathcal{A}^\infty$. However, we are going to show that the $\star_N$-product is related to the usual $\star$-product via

$$\phi \star_N \psi = \mathcal{P}_N[\phi \star_\hbar \psi]|_{\hbar = 2/(N+1)}. \tag{3.22}$$

Let us note that the interplay between the noncommutative product and deformation quantization was studied before, see, e.g., Ref. 13. What is new in this paper is the justification for formula (3.22) coming from an explicit expression for the asymptotic expansion of the $\star_N$-product in powers of the noncommutativity parameter. To find this expansion we consider the $\star_N$-product of the modes. The product of two matrices $\hat{\Theta}$ can be decomposed into a sum of $\hat{\Theta}$. A simple calculation, similar to the one performed in (2.17), (2.18), gives

$$\Theta^{l_1}_{m_1} \star_N \Theta^{l_2}_{m_2} = \sum_{l_3=0}^{N} \sum_{m_3} \dim_{l_3} \Theta^{l_3}_{m_3}$$



$$\sqrt{N+1}$$

. (3.23)

Let us notice that the right-hand side depends on N only through the $6j$-symbol (and the square root), and the cutoff in the sum. Therefore, the nontrivial information about the $1/N$ expansion of the $\star_N$-product is all contained in the $6j$-symbol. Thus, the fuzzy sphere gives us an interesting example of a noncommutative manifold for which the $\star$-product is not only known in terms of its $1/N$ derivative expansion, but also in closed form, in terms of the $6j$-symbol in (3.23).

Let us note that (3.23) can also be written as

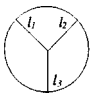
$$\Theta^{l_1}_{m_1} \star_N \Theta^{l_2}_{m_2} = \sum_{l_3=0}^{N} \mathcal{P}^{(l_3)}(\Theta^{l_1}_{m_1} \cdot \Theta^{l_2}_{m_2}) \Psi_{(N)}(l_1, l_2, l_3), \tag{3.24}$$

where $\mathcal{P}^{(l)}$ is the projector on the lth representation

$$\mathcal{P}_N = \sum_{l \leqslant N} \mathcal{P}^{(l)}, \tag{3.25}$$

and

$$\Psi_{(N)}(l_1, l_2, l_3) := \frac{\sqrt{N+1}}{\hat{C}^{l_3 l_1 l_2}_{000}}$$



. (3.26)

As we show below

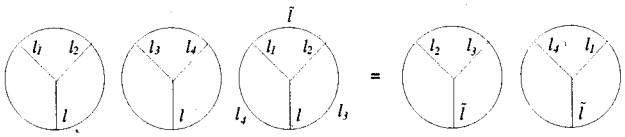
$$\lim_{N\to\infty} \sqrt{N+1}$$

$$= \hat{C}^{l_3 l_1 l_2}_{000}. \tag{3.27}$$

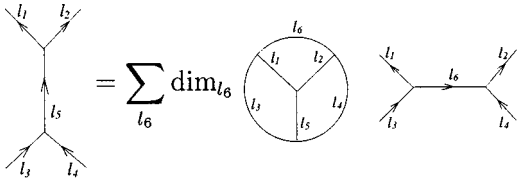
This implies that the expansion of the function $\Psi_{(N)}(l_1, l_2, l_3)$ in powers of $1/N$ starts from unity. This fact, together with relation (2.5) means that the zeroth-order term in the $1/N$ expansion of the $\star_N$-product of two modes Θ is given by the usual product, which is what one expects.

Before we look more closely into the details of the asymptotic expansion, let us show that the noncommutative product defined by (3.23) is indeed an associative product. Interestingly, the

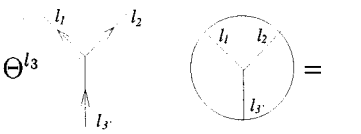
associativity follows from the so-called Biedenharn–Elliott (or pentagon) identity, which reads

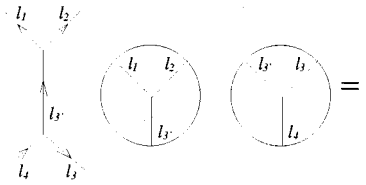
$$\sum_l \dim_l$$  (3.28)

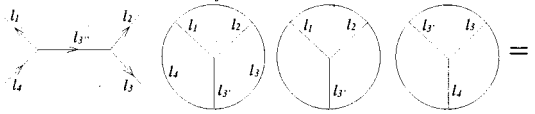
Note that although one has to sum over all l in this formula, only the terms with $l \leqslant N$ survive. We are also going to use the following recoupling identity:

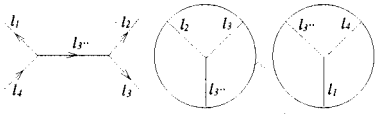
 (3.29)

Here the sum is taken over all l_6. A proof of the associativity is then as follows:

$$\left(\Theta^{l_1} \star_N \Theta^{l_2}\right) \star_N \Theta^{l_3} = \sum_{l_3'} \dim_{l_3'} \Theta^{l_3'} \star_N \Theta^{l_3}$$ 

$$\sum_{l_3' l_4} \dim_{l_3'} \dim_{l_4} \Theta^{l_4}$$ 

$$\sum_{l_3' l_3'' l_4} \dim_{l_3'} \dim_{l_3''} \dim_{l_4} \Theta^{l_4}$$ 

$$\sum_{l_3'' l_4} \dim_{l_3''} \dim_{l_4} \Theta^{l_4}$$  $= \Theta^{l_1} \star_N \left(\Theta^{l_2} \star_N \Theta^{l_3}\right).$ (3.30)

Here we used the recoupling identity (3.29) to get the third line, and the pentagon identity (3.28) to get the last line. Note that, although in the third line the sum is taken over all l_3'', in the last line, after we used the pentagon identity, only the terms with $l_3'' \leqslant N$ are nonzero. Thus, the associativity of the product $\star_N$ is intimately related to the associativity in the category of irreducible representations of SU(2), of which the Biedenharn–Elliot identity is a manifestation.

Let us now study the asymptotic expansion of the $\star_N$-product more closely. To this end, let us rewrite formula (A3) for the $6j$-symbol in a form that is convenient for taking the large N-limit. It is convenient to introduce, for $N+a \geqslant 0$:

$$\gamma(a;N) = \frac{(N+a)!}{N!(N+1)^a}. \tag{3.31}$$

[It is not hard to recognize this function as related to the one appearing in the infinite limit Euler definition of the Γ function. Indeed, $\gamma(z;n) = \Gamma(z-1)/F(z-1,n+1)$, where $F(z,n) = n^z n!/(z(z+1)\cdots(z+n)) = n^z \int_0^1 (1-u)^n u^{z-1} du$, and $\lim_{n\to\infty} F(z,n) = \Gamma(z)$]. Since, for $a > 0$

$$\gamma(a;N)=\prod_{k=1}^{a}\left(1+\frac{k-1}{N+1}\right), \tag{3.32}$$

this function is analytic in $1/(N+1)$, and, for positive a, is a polynomial of degree $a-1$. We have

$$\gamma(a;N)=1+\frac{1}{N+1}\frac{a(a-1)}{2}+\cdots+\left(\frac{1}{N+1}\right)^{a-1}(a-1)! \tag{3.33}$$

One can similarly rewrite the function $\gamma(-a;N)$, $a>0$ as one over a polynomial of degree a:

$$\gamma(a;N)=\frac{1}{\Pi_{k=1}^{a}\left(1-\frac{k}{N+1}\right)}. \tag{3.34}$$

Using this function, the $6j$-symbol can be rewritten as

$$= (-1)^{l_1}(N+1)^{-1/2} l_3! \left[\frac{(l_1+l_2-l_3)!}{(l_1-l_2+l_3)!(l_2-l_1+l_3)!(l_1+l_2+l_3+1)!}\right]^{1/2}$$
$$\left[\frac{\gamma(-l_1;N)\gamma(l_1+1;N)\gamma(l_3+1;N)}{\gamma(-l_2;N)\gamma(-l_3;N)\gamma(l_2+1;N)}\right]^{1/2}$$
$$\sum_k \frac{(-1)^k}{k!}\frac{(l_1+k)!(l_2+l_3-k)!}{(l_1-k)!(l_2-l_3+k)!(l_3-k)!}\frac{\gamma(-l_3+k;N)}{\gamma(k+1;N)}. \tag{3.35}$$

The sum here is restricted to those k for which the quantities inside the factorials are non-negative. Using the representations (3.32), (3.34) for the γ function, it is not hard to deduce the analyticity properties of the $6j$-symbol as a function of $1/(N+1)$. We will need these properties in the following, when we discuss the relation between $\star_N$ and the usual $\star$-product. Function $\gamma(a+1;N)$, $a>0$, viewed as a function of $1/(N+1)$, has simple zeros on the negative axes, with the closest to origin zero located at $1/(N+1)=-1/a$. Function $\gamma(-a;N)$, a has simple poles on the positive axes, with the closest to the origin pole located at $1/(N+1)=1/a$. Then, the expression under the square root in (3.35) can be shown to have at most simple poles and zeros on the positive axes and at most second-order zeros on the negative axes. The function inside the sum in (3.35) has simple poles both on the positive and negative axes. The proves that the $6j$-symbol times $\sqrt{N+1}$ (3.35) is an analytic function of $1/(N+1)$ in the open disk of radius $\min(1/l_1,1/l_2,1/l_3)$ around zero. Moreover, all singularities are located on the positive and negative axes. This means that the function $\Psi_{(N)}(l_1,l_2,l_3)$ introduced in (3.26) can be analytically continued, as a function of $1/(N+1)$, to the whole complex plane. Introducing $\hbar=2/(N+1)$ we shall denote the analytic continuation of $\Psi_{(N)}(l_1,l_2,l_3)$ by $\Psi(l_1,l_2,l_3:\hbar)$.

It is not hard to find first terms of the expansion of $6j$ in powers of $1/(N+1)$. We get

$$\sqrt{N+1}\ \begin{Bmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{Bmatrix} = \hat{C}^{l_1 l_2 l_3}_{0\,0\,0}\left(1+\frac{1}{(N+1)}\frac{1}{2}\left(C_{l_1}-C_{l_2}+C_{l_3}\right)\right)$$
$$-\frac{(-1)^{l_1}}{(N+1)}(l_3+1)!\left[\frac{(l_1+l_2-l_3)!}{(l_1-l_2+l_3)!(l_2-l_1+l_3)!(l_1+l_2+l_3+1)!}\right]^{1/2}$$
$$\sum_k \frac{(-1)^k}{k!}k\frac{(l_1+k)!(l_2+l_3-k)!}{(l_1-k)!(l_2-l_3+k)!(l_3-k)!}+O(1/N^2), \tag{3.36}$$

where we have introduced a notation $C_l=l(l+1)$ and we have used expression (A4) for $C^{l_3 l_1 l_2}_{0\,0\,0}$. This proves that the zeroth-order term is given by the usual commutative product.

Let us introduce a notation for the prefactor in front of the sum in (3.36):

$$\rho(l_3,l_1,l_2)=(-1)^{l_2}l_3!\left[\frac{(l_1+l_2-l_3)!}{(l_1-l_2+l_3)!(l_2-l_1+l_3)!(l_1+l_2+l_3+1)!}\right]^{1/2}. \tag{3.37}$$

It can be noted that the sum in (3.36) is related to a certain Clebsch–Gordan coefficient. Namely,

$$\hat{C}^{l_3 l_1 l_2}_{1\,1\,0}=\frac{1}{l_3}\left(\frac{C_3}{C_1}\right)^{1/2}\rho(l_3,l_1,l_2)\sum_k \frac{(-1)^k}{k!}\frac{(l_1+k)!(l_2+l_3-k)!}{(l_1-k)!(l_2-l_3+k)!}\frac{k}{(l_3-k)!}. \tag{3.38}$$

Therefore, the first-order term in the expansion, that is, the coefficient of $1/(N+1)$ term in (3.36) can be written as

$$\tfrac{1}{2}(C_1-C_2+C_3)\hat{C}^{l_3 l_1 l_2}_{0\,0\,0}-(C_1C_3)^{1/2}\hat{C}^{l_3 l_1 l_2}_{1\,1\,0}. \tag{3.39}$$

It is now possible to prove the following two identities on Clebsch–Gordan coefficients.

$$(C_1-C_2+C_3)\hat{C}^{l_3 l_1 l_2}_{0\,0\,0}=(C_1C_3)^{1/2}(\hat{C}^{l_3 l_1 l_2}_{1\,1\,0}+\hat{C}^{l_3 l_1 l_2}_{-1\,-1\,0}). \tag{3.40}$$

$$\hat{C}^{l_3 l_1 l_2}_{1\,1\,0}=(-1)^{l_1+l_2+l_3}\hat{C}^{l_3 l_1 l_2}_{-1\,-1\,0}.$$

The first equality is just the expression of the intertwining property of the Clebsch–Gordan coefficient, and the second is a symmetry relation.

These two identities imply that (3.39) is equal to zero if $l_1+l_2+l_3$ is even. It is also clear that for odd $l_1+l_2+l_3$ it equals

$$-(C_1C_3)^{1/2}\hat{C}^{l_3 l_1 l_2}_{1\,1\,0}. \tag{3.41}$$

However, as is shown in the Appendix, this quantity is just $P(l_1,l_2,l_3)$, which is the coefficient that appears in the decomposition of the Poisson bracket of two spherical harmonics. This proves that the first-order term is given by the Poisson bracket.

We can summarize all of the above-mentioned results in a form of the following theorem.

Theorem 1: *There exists a function* $\Psi(l_1,l_2,l_3;\hbar)$*, given by the analytic continuation of the function* $\Psi_{(N)}(l_1,l_2,l_3)$ *introduced in (3.26), which is analytic in* $\hbar$ *in the open disk of radius* $\min(1/l_1,1/l_2,1/l_3)$ *around zero, and*

$$\Psi(l_1,l_2,l_3;\hbar)=1+\hbar\Psi_1(l_1,l_2,l_3)+(\hbar)^2\Psi_2(l_1,l_2,l_3)+\cdots. \tag{3.42}$$

For $N\geqslant l_1,l_2,l_3$,

$$\Psi(l_1,l_2,l_3;\hbar)|_{\hbar=2(N+1)}=\Psi_{(N)}(l_1,l_2,l_3). \tag{3.43}$$

The product defined via

$$\Theta^{l_1}_{m_1}\star_\hbar\Theta^{l_2}_{m_2}=\sum_{l_3=0}^{N}\mathcal{P}^{(l_3)}(\Theta^{l_1}_{m_1}\cdot\Theta^{l_2}_{m_2})\Psi(l_1,l_2,l_3;\hbar), \tag{3.44}$$

is an associative product. Moreover,

$$\begin{aligned}&\phi\star_\hbar\psi-\psi\star_\hbar\phi=\hbar\{\phi,\psi\}+o(\hbar),\\ &\mathcal{P}_N[\phi]\star_N\mathcal{P}_N[\psi]=\mathcal{P}_N[\phi\star_\hbar\psi]|_{\hbar=2/(N+1)}.\end{aligned} \tag{3.45}$$

The associativity follows from an analytic continuation of the Biedenharn–Elliot identity, see (3.28). What we did not prove is that the noncommutative product (3.44) is indeed a $\star$-product, that is given by an expansion in terms of derivatives. This is, in principle, possible with our techniques by considering the higher terms in the expansion of the $6j$-symbol. Thus, modulo this caveat, the $\star_\hbar$-product gives a deformation quantization of Kirillov bracket, and must thus be equivalent to the usual Kirillov $\star$-product. Formula (3.45) then establishes a relation between the fuzzy sphere product and Kirillov product.

We conclude by observing that expressions (3.23), (3.24) for the $\star_N$-product can be used to define a noncommutative product on the so-called q-deformed fuzzy sphere. While the usual fuzzy sphere is defined as the structure covariant under the action of the group SU(2), its q-deformed analog is covariant under the action of the quantum group $U_q(su(2))$. For a definition of the q-deformed fuzzy sphere see, e.g., Ref. 14. Expression (3.23) can then be used to get a product on the q-deformed sphere. To this end, one should replace all objects appearing on the right-hand side of (3.23)—the dimension, the $3j$ and $6j$-symbols—by the corresponding q-deformed quantities. One gets a q-deformed product. This product is still associative, for the proof (3.30) of associativity based on the pentagon identity holds for the quantum group as well. This q-deformed product was discussed in Ref. 4, where the usual fuzzy sphere version (3.23) is also mentioned. It would be quite interesting to obtain an analog of our asymptotic formula for the q-deformed product.

ACKNOWLEDGMENTS

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APPENDIX A: SOME FORMULAS

In the main text we use values of the integrals of a product of two and three matrix elements. These are given by

$$\int_G \mathrm{d}g\overline{\langle l_1,m_1|T_g|l_1,m_1'\rangle}\langle l_2,m_2|T_g|l_2,m_2'\rangle=\frac{\delta^{l_1l_2}\delta_{m_1m_2}\delta_{m_1'm_2'}}{\dim_{l_1}}, \tag{A1}$$

and

$$\int_G \mathrm{d}g\overline{\langle l_3,m_3|T_g|l_3,m_3'\rangle}\langle l_1,m_1|T_g|l_1,m_1'\rangle\langle l_2,m_2|T_g|l_2,m_2'\rangle=\hat{C}^{l_3l_1l_2}_{m_3'm_1'm_2'}\overline{\hat{C}^{l_3l_1l_2}_{m_3m_1m_2}}. \tag{A2}$$

Let us now give some explicit formulas for the $3j$- and $6j$-symbols. All these formulas are from Ref. 8, with normalizations properly adjusted to match our conventions. We have

$$= (-1)^{l_1}l_3!\left[\frac{(l_1+l_2-l_3)!}{(l_1-l_2+l_3)!(l_2-l_1+l_3)!(l_1+l_2+l_3+1)!}\right]^{1/2}$$
$$\left[\frac{(N-l_1)!(N+l_1+1)!(N+l_3+1)!}{(N+l_2+1)!(N-l_2)!(N-l_3)!}\right]^{1/2}$$
$$\sum_k \frac{(-1)^k}{k!}\frac{(l_1+k)!(l_2+l_3-k)!}{(l_1-k)!(l_2-l_3+k)!(l_3-k)!}\frac{(N-l_3+k)!}{(N+k+1)!}. \tag{A3}$$

Here the sum is taken over all k such that the factorials are taken of non-negative integers. Using this formula it is not hard to get the value (2.20) of the $6j$-symbol for all spins being equal to 1. In this case the sum in (A3) is taken only over two values $k=0$, 1 and the calculation leading to (2.20) is straightforward.

Let us also give an expression for the $3j$-symbol $C^{l_3 l_1 l_2}_{0\,0\,0}$. It can be obtained from the general expression for the $3j$-symbol (in terms of a finite sum) given in Ref. 8. Taking into account the difference in normalizations, we get

$$\hat{C}^{l_3 l_1 l_2}_{0\,0\,0} = \rho(l_3, l_1, l_2) \sum_k \frac{(-1)^k}{k!} \frac{(l_1+k)!(l_2+l_3-k)!}{(l_1-k)!(l_2-l_3+k)!(l_3-k)!}, \tag{A4}$$

where

$$\rho(l_3, l_1, l_2) = (-1)^{l_1} l_3! \left[\frac{(l_1+l_2-l_3)!}{(l_1-l_2+l_3)!(l_2-l_1+l_3)!(l_1+l_2+l_3+1)!} \right]^{1/2}. \tag{A5}$$

We should also note the formula:

$$\hat{C}^{l l_1 l_2}_{0\,0\,0} = \frac{(-1)^{g-1} g! \Delta(l_1, l_2, l)}{(g-l_1)!(g-l_2)!(g-l)!}, \tag{A6}$$

where $l_1+l_2+l=2g$, $g \in \mathbb{Z}$, and $\Delta(l_1, l_2, l)$ is given by

$$\Delta(l_1, l_2, l) = \left[\frac{(l_1+l_2-l)!(l_1-l_2+l)!(l_2-l_1+l)!}{(l_1+l_2+l+1)!} \right]^{1/2}. \tag{A7}$$

APPENDIX B: POISSON BRACKET OF SPHERICAL HARMONICS

In this section we calculate the Poisson bracket of two spherical harmonics. The result we obtain here is compared in Sec. III with the first-order term in the expansion of the $6j$-symbol in powers of $1/N$. We were not able to find a result for this Poisson bracket in the literature, so we sketch the calculation here.

We begin with some notations. Let J_i be generators of the Lie algebra of SU(2): $[J_i, J_j] = i\epsilon_{ijk} J_k$. These generators can be realized as vector fields in $\mathbb{R}^3$. Denoting by x_i the usual Cartesian coordinates in $\mathbb{R}^3$, we get

$$J_i = \frac{1}{i} \epsilon_i{}^{jk} x_j \partial_k. \tag{B1}$$

To calculate the Poisson bracket, it is convenient to introduce a set of complex coordinates in $\mathbb{R}^3$. We define $z = (x_1 + i x_2)/\sqrt{2}$, $x = x_3$ and $J_\pm = (J_1 \pm i J_2)/\sqrt{2}$, $J = J_3$. These new generators can be expressed in terms of the complex vector fields ∂_z, $\partial_{\overline{z}}$, ∂_x. We have

$$J_+ = x\partial_{\overline{z}} - z\partial_x, \quad J_- = \overline{z}\partial_x + x\partial_z, \quad J = z\partial_z - \overline{z}\partial_{\overline{z}}. \tag{B2}$$

These vector fields satisfy

$$[J_+, J_-] = J, \quad [J, J_\pm] = \pm J_\pm, \tag{B3}$$

and

$$\overline{J_+} = -J_-, \quad \overline{J} = -J. \tag{B4}$$

The spherical harmonics Θ^l_m are given by

$$\Theta^l_m = \alpha^l_m J_-^{l-m} v, \tag{B5}$$

where v is the highest weight vector $v = z^l$. To calculate the normalization factor α^l_m let us consider the norm $\|J_-^{l-m} v\|^2$. Using

$$[J_+, J_-^n]v = \frac{n}{2}(2l-n+1)J_-^{n-1}v, \tag{B6}$$

we get

$$\|J_-^{l-m}v\|^2 = (-1)^{l-m}\langle v|J_+^{l-m}J_-^{l-m}|v\rangle = (-1)^{l-m}\frac{1}{2^{l-m}}\frac{(l-m)!}{(l+m)!}(2l)!\|v\|^2. \tag{B7}$$

An explicit calculation, using the normalized measure on S^3, gives

$$\|v\|^2 = \|z^l\|^2 = \int \sin^{2l}\theta = \frac{1}{(2l+1)}\frac{l!}{(2l-1)!!}. \tag{B8}$$

Combining these two facts, and taking into account the normalization of Θ_m^l (2.2), we see that α_m^l is, up to a phase, given by

$$\frac{1}{l!}\left(\frac{(l+m)!}{2^m(l-m)!}\right)^{1/2}. \tag{B9}$$

We choose the phase factor in such a way that Θ_m^l coincide with the ones given by (2.1). This gives

$$\alpha_m^l = \frac{(-1)^{l-m}}{l!}\left(\frac{(l+m)!}{2^m(l-m)!}\right)^{1/2}. \tag{B10}$$

It is now straightforward to work out the action of vector fields ∂_z, $\partial_{\bar z}$, ∂_x on Θ_m^l. We get

$$\begin{aligned}
\partial_z\Theta_m^l &= \sqrt{\frac{1}{2}(l+m)(l+m-1)}\,\Theta_{m-1}^{l-1},\\
\partial_{\bar z}\Theta_m^l &= -\sqrt{\frac{1}{2}(l-m)(l-m-1)}\,\Theta_{m+1}^{l-1},\\
\partial_x\Theta_m^l &= \sqrt{(l+m)(l-m)}\,\Theta_m^{l-1}.
\end{aligned} \tag{B11}$$

We will also need the action of SU(2) generators on Θ_m^l:

$$\begin{aligned}
J_+\Theta_m^l &= -\sqrt{\frac{1}{2}(l-m)(l+m+1)}\,\Theta_{m+1}^l,\\
J_-\Theta_m^l &= -\sqrt{\frac{1}{2}(l+m)(l-m+1)}\,\Theta_{m-1}^l,\\
J\Theta_m^l &= m\Theta_m^l.
\end{aligned} \tag{B12}$$

The Poisson bracket is given by

$$\{f,g\} = \frac{i}{\sin\theta}\left(\frac{\partial f}{\partial\theta}\frac{\partial g}{\partial\varphi} - \frac{\partial g}{\partial\theta}\frac{\partial f}{\partial\varphi}\right). \tag{B13}$$

It is normalized so that $\{x_1, x_2\} = ix_3$. It can be expressed in terms of vector fields and generators as

$$\{f,g\} = \partial_z f J_+ g + \partial_{\bar z} f J_- g + \partial_x f J g. \tag{B14}$$

Using expressions (B11) and (B12) it is now straightforward to compute the Poisson bracket of two spherical harmonics. We have

$$\{\Theta^{l_1}_{m_1},\Theta^{l_2}_{m_2}\}=-\frac{1}{2}\Big(\sqrt{(l_1+m_1)(l_1+m_1-1)(l_2-m_2)(l_2+m_2+1)}\,\Theta^{l_1-1}_{m_1-1}\Theta^{l_2}_{m_2+1}$$
$$-\sqrt{(l_1-m_1)(l_1-m_1-1)(l_2+m_2)(l_2-m_2+1)}\,\Theta^{l_1-1}_{m_1+1}\Theta^{l_2}_{m_2-1}$$
$$-2\sqrt{(l_1+m_1)(l_1-m_1)}\,m_2\Theta^{l_1-1}_{m_1}\Theta^{l_2}_{m_2}\Big). \tag{B15}$$

Thus, using (2.4) we have

$$\int\{\Theta^{l_1}_{m_1},\Theta^{l_2}_{m_2}\}\overline{\Theta^{l}_{m}}=-\frac{1}{2}\overline{\hat{C}^{ll_1-1l_2}_{0\,0\,0}}\Big(\sqrt{(l_1+m_1)(l_1+m_1-1)(l_2-m_2)(l_2+m_2+1)}\,\hat{C}^{ll_1-1l_2}_{m\,m_1-1\,m_2+1}$$
$$-\sqrt{(l_1-m_1)(l_1-m_1-1)(l_2+m_2)(l_2-m_2+1)}\,\hat{C}^{l\,l_1-1\,l_2}_{m\,m_1+1\,m_2-1}$$
$$-2\sqrt{(l_1+m_1)(l_1-m_1)}\,m_2\hat{C}^{l\,l_1-1\,l_2}_{m\,m_1m_2}\Big). \tag{B16}$$

The requirement of gauge invariance implies that the quantity in brackets is proportional to the Clebsch–Gordan coefficient $\hat{C}^{l\,l_1l_2}_{m\,m_1m_2}$, with the proportionality coefficient depending only on l_1, l_2, l. In other words, we must have

$$\int\{\Theta^{l_1}_{m_1},\Theta^{l_2}_{m_2}\}\overline{\Theta^{l}_{m}}=P(l_1,l_2,l)\hat{C}^{l\,l_1l_2}_{m\,m_1m_2}. \tag{B17}$$

The coefficient $P(l_1,l_2,l)$ is proportional to $\hat{C}^{l\,l_1-1l_2}_{0\,0\,0}$ and thus is nonzero only when $l_1+l_2+l=2g-1$, $g\in\mathbb{Z}$. Since

$$\hat{C}^{l\,l_2l_1}_{m\,m_2m_1}=(-1)^{l-l_1-l_2}\hat{C}^{l\,l_1l_2}_{m\,m_1m_2}, \tag{B18}$$

for values of l_1, l_2, l summing up to an odd integer the Clebsch–Gordan coefficient changes sign under the exchange of l_1 with l_2. Because the Poisson bracket must be antisymmetric, the coefficient $P(l_1,l_2,l)$ must be symmetric under the exchange of l_1 with l_2. Let us now determine this coefficient. It can be determined, for example, by choosing $l=m$ and using

$$\hat{C}^{ll_1l_2}_{ljl-j}=(-1)^{l_1-j}\frac{(l_1+l_2-l)!}{(l_1+l_2+l+1)!\Delta(l_1,l_2,l)}\left[\frac{(l_1+j)!(l_2+l-j)!}{(l_1-j)!(l_2-l+j)!}\right]^{1/2}, \tag{B19}$$

where

$$\Delta(l_1,l_2,l)=\left[\frac{(l_1+l_2-l)!(l_1-l_2+l)!(l_2-l_1+l)!}{(l_1+l_2+l+1)!}\right]^{1/2}. \tag{B20}$$

After some algebraic manipulations this gives

$$P(l_1,l_2,l)=(-1)^{(l_1+l_2-l_{+1}/2)}(2g+2)\,\frac{g!\Delta(l_1,l_2,l)}{(g-l_1)!(g-l_2)!(g-l)!}. \tag{B21}$$

Here $2g+1=l_1+l_2+l$ and we have used formula (A6) for $\hat{C}^{ll_1\,-1l_2}_{0\,0\,0}$. Expression (B17) together with (B21) is our final result for the Poisson bracket of two spherical harmonics. Let us also note that $P(l_1,l_2,l)$ can be written as a certain Clebsch-Gordan coefficient:

$$P(l_1,l_2,l)=-\sqrt{l_1(l_1+1)l(l+1)}\hat{C}^{ll_1l_2}_{1\,1\,0}. \tag{B22}$$

This equality is analogous to formula (A6).

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Observable effects and parametrized scaling limits of a model in nonrelativistic quantum electrodynamics

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Scaling limits of the Hamiltonian H of a system of N charged particles coupled to a quantized radiation field are considered. Ultraviolet cutoffs, $\hat{\lambda}_1,\ldots,\hat{\lambda}_N$, are imposed on the radiation field and the Coulomb gauge is taken. It is the so-called Pauli–Fierz model in nonrelativistic quantum electrodynamics. We mainly consider two cases: (i) all the ultraviolet cutoffs are identical, $\hat{\lambda}_1=\cdots=\hat{\lambda}_N$, (ii) supports of ultraviolet cutoffs have no intersection, $\mathrm{supp}\,\hat{\lambda}_i\cap\mathrm{supp}\,\hat{\lambda}_j=\varnothing$, $i\neq j$. The Hamiltonian acts on $L^2(\mathbb{R}^{dN})\otimes\mathcal{F}$, where $\mathcal{F}$ is a symmetric Fock space, and has the form $H=H_{\mathrm{el}}\otimes 1+B+1\otimes H_{\mathrm{quad}}$. Here H_{el} denotes a particle Hamiltonian, H_{quad} a quadratic field operator, and B an interaction term. The scaling is introduced as $H(\kappa)=H_{\mathrm{el}}\otimes 1+\kappa^l B+\kappa^2 1\otimes H_{\mathrm{quad}}$, where κ is a scaling parameter and $l\leqslant 2$ a parameter of the scaling. Performing a mass renormalization we consider the scaling limit of $H(\kappa)$ as $\kappa\to\infty$ in the strong resolvent sense. Then effective Hamiltonians H_{eff} in $L^2(\mathbb{R}^{dN})$ infected with reaction of effect of the radiation field is derived. In particular (1) effective Hamiltonians with an effective potential for $l=2$, and (2) effective Hamiltonians with an observed mass for $l=1$, are obtained. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1447590]

I. PRELIMINARIES

A. Observable effects and scaling limits

In this paper we consider the Hamiltonian H of a system of N nonrelativistic charged particles interacting with a quantized radiation field. Ultraviolet cutoffs are imposed on the radiation field and recoil of the particles and the radiation field (photons) are excluded, i.e., the dipole approximation is made. Taking scaling limits of the Hamiltonian, we derive effective Hamiltonians. The main idea is to diagonalize H by a canonical transformation derived from a symplectic structure.

The Schrödinger Hamiltonian of one charged particle with external potential V is of the form

$$\frac{1}{2m}p^2+V, \tag{1.1}$$

where p denotes the momentum operator and m the bare mass of the particle. To interpret the Lamb shift[1] intuitively, Welton[2] formally derived an effective Schrödinger Hamiltonian taking into account effects of a radiation field. He expected that a position fluctuation of a particle by a radiation field will effectively modify the external potential V. A fluctuation was thought of as a Gaussian random variable Δx, then a effective potential is formally given by the mean value of $V(x+\Delta x)$,

$$V_{\mathrm{eff}}(x):=\langle V(x+\Delta x)\rangle_{\mathrm{AVE}}=(2\pi)^{-3/2}\int_{\mathbb{R}^3}\hat{V}(k)e^{ikx}\langle e^{ik\Delta x}\rangle_{\mathrm{AVE}}=(2\pi C)^{-3/2}\int_{\mathbb{R}^3}V(y)e^{-|x-y|^2/2C}\,dy,$$

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with a certain positive constant C. Then (1.1) effectively turns out to be the effective Hamiltonian, Welton's Hamiltonian, given by

$$\frac{1}{2m}p^2+V_{\mathrm{eff}}. \tag{1.2}$$

He gave an interpretation of the Lamb shift as the difference of the spectrum between the original Hamiltonian and the effective one.

On the other hand it was found in Ref. 3 that photons enhance the bare mass m. Then m amounts to an observed mass $m+\delta m$, $\delta m>0$, through a coupling to a radiation field. Then (1.1) formally turns out to be

$$\frac{1}{2(m+\delta m)}p^2+V. \tag{1.3}$$

In this paper performing a mass renormalization to eliminate a divergence contribution, we present a rigorous derivation of (1.2) and (1.3) by parametrized scaling limits of Hamiltonians describing an interaction between particles and radiation fields. Thus we interpolate (1.2) and (1.3). We suppose that N particles move in the d-dimensional space and a radiation field has the helicity $d-1$. Throughout this paper we assume

$$d\geqslant 3.$$

$\mathcal{F}$ denotes the Boson Fock space over $W:=\oplus^{d-1}L^2(\mathbb{R}^d)$, which is defined by

$$\mathcal{F}:=\bigoplus_{n=0}^{\infty}[\otimes_s^n W],$$

where $\otimes_s^n W$ denotes the n-fold symmetric tensor product of W, and $\otimes_s^0 W:=\mathbb{C}$. The bare vacuum Ω is defined by

$$\Omega:=\{1,0,0,\ldots\}.$$

Hamiltonians under consideration are of the form

$$H:=H_{\mathrm{el}}\otimes 1+B+1\otimes H_{\mathrm{quad}}$$

acting on the Hilbert space

$$\mathcal{H}:=L^2(\mathbb{R}^{dN})\otimes\mathcal{F}.$$

Here H_{el} describes the particle Hamiltonian of the form

$$H_{\mathrm{el}}:=\sum_{j=1}^{N}\frac{1}{2m_j}p_j^2+V.$$

Here $p_j:=-i\hbar\vec{\nabla}_j$ denotes the momentum operator of the jth particle canonically conjugate to the position operator x_j, $V:\mathbb{R}^{dN}\to\mathbb{R}$ an external potential, $\hbar$ the Planck constant divided by 2π, m_j the mass of the jth particle. H_{quad} a quadratic field operator in $\mathcal{F}$, and B an interaction term. We scale H as follows:

$$H(\kappa):=H_{\mathrm{el}}\otimes 1+\kappa^l B+\kappa^2 1\otimes H_{\mathrm{quad}}.$$

Davies[4,5] considered the scaling limit $\kappa\to\infty$ of the case of

$$l=1$$

for certain simple models to derive N-body Schrödinger Hamiltonians. He called this scaling limit *the weak coupling limit*. See also Refs. 6 and 7. On the other hand Arai[8] considered the case of

$$l=2$$

for the one particle Pauli–Fierz model in the dipole approximation without the self-interacting term A^2. Then he derived effective Hamiltonians with an effective potential. In this paper we consider scaling limits of

$$l\leqslant 2$$

for the N-particle Pauli–Fierz model in the dipole approximation. In particular, performing a mass renormalization, subtracting from $H(\kappa)$ some energy reset, and taking $\kappa\to\infty$ in the resolvent sense, we derive, for $l=2$, Welton's Hamiltonians, and for $l=1$, Hamiltonians with an observed mass.

B. Nonrelativistic models

Let $a^\dagger(f)$ and $a(f)$, $f\in W$, denote the smeared creation and annihilation operators acting on $\mathcal{F}$, respectively. $a^\sharp$ stands for a or $a^\dagger$. We set

$$a^{\sharp r}(f):=a^\dagger(\underbrace{0\oplus 0\cdots\oplus}_{d-1\,\text{times}}\overset{r_{\text{th}}}{f}\oplus\cdots 0\oplus 0).$$

They satisfy the canonical commutation relations,

$$[a^r(g),a^{\dagger s}(f)]=\delta_{rs}\int_{\mathbb{R}^d} f(k)g(k)\mathrm{d}k,$$

$$[a^{\dagger r}(f),a^{\dagger s}(g)]=[a^r(f),a^s(g)]=0$$

on the finite particle subspace of $\mathcal{F}$. We take the Coulomb gauge. The radiation field with the ultraviolet cutoff $\hat{\lambda}_j\in L^2(\mathbb{R}^d)$ is defined by

$$A_{j\mu}(x_j):=A_\mu(x_j,\hat{\lambda}_j):=\frac{1}{\sqrt{2}}\sum_{r=1}^{d-1}\{a^{\dagger r}(e^r_\mu e^{-ikx_j}\tilde{\hat{\lambda}}_j)+a^r(e^r_\mu e^{ikx_j}\hat{\lambda}_j)\},$$

where $e^r(k)=(e^r_1(k),\ldots,e^r_d(k))$ denotes polarization vectors satisying $e^r(k)\cdot e^s(k)=\delta_{rs}$ and $e^r(k)\cdot k=0$,

$$\tilde{\hat{\lambda}}_j(k):=\hat{\lambda}_j(-k),$$

and $\hat{f}$ denotes the Fourier transform of f. We assume

$$\hat{\lambda}_j(k)=\hat{\lambda}_j(-k),\quad j=1,...,N,$$

to ensure that $A_{j\mu}(x_j)$ is symmetric for each $x_j\in\mathbb{R}^d$. The physically reasonable choice of the ultraviolet cutoff is

$$\hat{\lambda}_j(k)=\frac{\sqrt{c}\hbar\hat{\rho}_j(k)}{\sqrt{(2\pi)^d\omega(k)}},$$

where $\hat{\rho}_j$ denotes the Fourier transform of the charge distribution ρ_j of the jth particle and c denotes the speed of the light. The dispersion relation $\omega(k)$ is given by

$$\omega(k) := |k|.$$

The free Hamiltonian H_f in $\mathcal{F}$ is defined by

$$H_f := \hbar c \sum_{r=1}^{d-1} \int \omega(k) a^{\dagger r}(k) a^r(k) \mathrm{d}k,$$

where $a^{\dagger r}(k)$ and $a^r(k)$ denote the kernels of $a^{\dagger r}(f)$ and $a^r(f)$, respectively. The total Hamiltonian is given by

$$H_{\text{total}} := \sum_{j=1}^{N} \frac{1}{2m_j} \left(p_j \otimes 1 - \frac{\alpha_j}{c} A_j(x_j) \right)^2 + 1 \otimes H_f + V \otimes 1,$$

where α_j's are nonzero coupling constants. We take the dipole approximation, i.e., we replace $A_j(x_j)$ with

$$A_j := A_j(0).$$

Then the Hamiltonian in the dipole approximation is given by

$$H := \sum_{j=1}^{N} \frac{1}{2m_j} \left(p_j \otimes 1 - \frac{\alpha_j}{c} 1 \otimes A_j \right)^2 + 1 \otimes H_f + V \otimes 1.$$

We work with the unit $c = \hbar = 1$ in what follows. Since

$$[p_{j\mu}, A_{j\nu}] = 0,$$

we have

$$H = H_{\text{el}} \otimes 1 - \sum_{j=1}^{N} \frac{\alpha_j}{m_j} p_j \otimes A_j + 1 \otimes \left(\sum_{j=1}^{N} \frac{\alpha_j^2}{2m_j} A_j^2 + H_f \right).$$

It is of mathematical interest to see A_j^2-corrections in scaling limits. Then we define, for $\epsilon \geqslant 0$,

$$H_\epsilon := H_{\text{el}} \otimes 1 - \sum_{j=1}^{N} \frac{\alpha_j}{m_j} p_j \otimes A_j + 1 \otimes \left(\sum_{j=1}^{N} \frac{\epsilon \alpha_j^2}{2m_j} A_j^2 + H_f \right)$$

with the domain

$$D(H_\epsilon) = D(H_{\text{el}} \otimes 1) \cap D(1 \otimes H_f) \cap D\left(1 \otimes \sum_{j=1}^{N} \frac{\epsilon \alpha_j^2}{2m_j} A_j^2 \right).$$

Actually, for $\epsilon < 1$, H_ϵ turns out to be an unphysical Hamiltonian for sufficiently large coupling constants, since in this case H_ϵ is unbounded from below. See Remark 3.10 for details. Let

$$\kappa > 1$$

be a scaling parameter. We introduce the scaled Hamiltonian $H_\epsilon(\kappa)$ as follows:

$$H_\epsilon(\kappa) := H_{\text{el}} \otimes 1 - \kappa^l \sum_{j=1}^{N} \frac{\alpha_j}{m_j} p_j \otimes A_j + \kappa^2 1 \otimes \left(\sum_{j=1}^{N} \frac{\epsilon \alpha_j^2}{2m_j} A_j^2 + H_f \right),$$

where

$$l \leqslant 2.$$

In particular we set

$$H(\kappa) := H_1(\kappa).$$

Unless confusion arises we omit $\otimes 1$ and $1 \otimes$ for simplicity in what follows. Throughout this paper we suppose that V satisfies Hypothesis **V**:

Hypothesis **V**: V is infinitesimally small with respect to $\Sigma_{j=1}^{N}(p_j^2/2m_j)$.

First of all we have to establish self-adjointness of $H_\epsilon(\kappa)$. Note that if we assume that $\hat{\lambda}_j/\sqrt{\omega}, \hat{\lambda}_j, \omega\hat{\lambda}_j \in L^2(\mathbb{R}^d)$, then

$$\left\| \left(-\sum_{j=1}^{N} \frac{\alpha_j}{m_j} p_j A_j + \sum_{j=1}^{N} \frac{\epsilon \alpha_j^2}{2m_j} A_j^2 \right) \Psi \right\| \leqslant a' \left\| \left(\sum_{j=1}^{N} \frac{p_j^2}{2m_j} + H_f \right) \Psi \right\| + b' \|\Psi\|$$

for $\Psi \in D(H_f)$ with some a' and b'. Let

$$\mathcal{D} := D\left(\sum_{j=1}^{N} \frac{p_j^2}{2m_j} \otimes 1 \right) \cap D(1 \otimes H_f).$$

Proposition 1.1: Let $\epsilon = 1$. *We suppose that* $\hat{\lambda}_j/\sqrt{\omega}, \hat{\lambda}_j, \omega\hat{\lambda}_j \in L^2(\mathbb{R}^d)$. *(1)* H_{total} *and* H *are self-adjoint on* $\mathcal{D}$ *and bounded from below. (2) Let* $l = 1$. *Then* $H(\kappa)$ *is self-adjoint on* $\mathcal{D}$ *and bounded from below for all* κ.

Proof: See Refs. 9 and 10 for (1). In the case of $l = 1$, $H(\kappa)$ is derived from the scaling $\alpha_j \to \kappa\alpha_j$ and $\omega \to \kappa\omega$ in H. Thus the self-adjointness follows from (1) □

Proposition 1.2: Let $\epsilon \neq 1$ *and* $V = 0$. *Suppose* $\hat{\lambda}_j/\sqrt{\omega}, \hat{\lambda}_j, \omega\hat{\lambda}_j \in L^2(\mathbb{R}^d)$. *Then* $H_\epsilon(\kappa)$ *is essentially self-adjoint on any core of* $\Sigma_{j=1}^{N} p_j^2/(2m_j) + H_f$.

Proof: The proof is due to Arai (Ref. 11 Theorem 2.2). Let $L := \Sigma_{j=1}^{N} p_j^2/(2m_j) + H_f + 1$. Then we see that

$$\|H_\epsilon(\kappa)\Psi\| \leqslant c\|L\Psi\|,$$

and

$$|(H_\epsilon(\kappa)\Psi, L\Psi) - (L\Psi, H_\epsilon(\kappa)\Psi)| \leqslant c'\|L^{1/2}\Psi\|\|L^{1/2}\Psi\|$$

with some constants c and c'. Thus, by the Nelson commutator theorem (Ref. 12, Theorem X.36), $H_\epsilon(\kappa)$ is essentially self-adjoint on any core of L. Thus the proposition follows. □

Self-adjointness of $H_\epsilon(\kappa)$ for $\epsilon < 1$ or $l \neq 1$ is discussed later (Theorem 3.11) in this paper. Since H_ϵ and $H_\epsilon(\kappa)$ are essentially self-adjoint, we take their self-adjoint extensions and denote them by the same symbols.

C. Problems

For the case of $N \geqslant 2$ we have to take care of the choice of ultraviolet cutoffs. For simplicity we mainly consider two cases: identical case, $\hat{\lambda}_1 = \cdots = \hat{\lambda}_N := \hat{\lambda}$, and independent case, $\operatorname{supp}\hat{\lambda}_j \cap \operatorname{supp}\hat{\lambda}_i = \varnothing$ for $i \neq j$.

Arai[8] considered the scaling limit of the case of $l = 2$, $\epsilon = 0$, and $N = 1$. Moreover in Refs. 13 and 14 distinct scaling limits were studied, but unfortunately A^2-corrections did not appear in scaling limits. In this paper we want to improve it and to see the relationship between Davies' scaling limit and Arai's one. As was seen in Sec. I A, Davies' scaling limits correspond to $l = 1$.

We set

$$H_\epsilon^0 := H_\epsilon \restriction_{V=0}.$$

Since H_ϵ^0 commutes with $p_{j\mu}$, H_ϵ is decomposable with respect to the spectrum of the particle momentum operators,

$$H_\epsilon^0 = \int_{\mathbb{R}^{dN}}^{\oplus} H_\epsilon^0(q)\mathrm{d}q.$$

$H_\epsilon^0(q)$ acts on $\mathcal{F}$. The ground state energy for each $q \in \mathbb{R}^{dN}$ is denoted by

$$E(q) := \inf \sigma(H_\epsilon^0(q)).$$

Then we call

$$m^*(\mu,\nu,j) := \left(\frac{\partial^2}{\partial q_{j\mu}\partial q_{j\nu}} E(q) \restriction_{q=0} \right)^{-1}$$

an *observed mass*. In this paper we explicitly give the ground state energy of H_ϵ^0 and its observed mass.

Thus the list of problems considered in this paper is epitomized as follows.

(1) Explicit ground state energy, $\inf \sigma(H_\epsilon^0)$.
(2) Observed mass, $m^*(\mu,\nu,j)$.
(3) Deriving effective Hamiltonians H_{eff} through scaling limits of $H_\epsilon(\kappa)$ subtracting a divergent contribution $E_{\mathrm{ren}}(\kappa)$: $s-\lim_{\kappa\to\infty}(H_\epsilon(\kappa)-E_{\mathrm{ren}}(\kappa)-z)^{-1} = (H_{\mathrm{eff}}-z)^{-1}\otimes P_\epsilon$ for $z \in \mathbb{C}\backslash\mathbb{R}$, where P_ϵ denotes a projection to the subspace spanned by ground states of $\Sigma_{j=1}^N \epsilon\alpha_j^2 A_j^2/(2m_j) + H_f$.
(4) What is a reasonable choice of $E_{\mathrm{ren}}(\kappa)$?
(5) l-dependence of H_{eff}.
(6) A_j^2-dependence (i.e., ϵ-dependence) of H_{eff}.
(7) Ultraviolet cutoff dependence of H_{eff}.

We give answers for (1) in Lemma 3.3, (2) in Corollary 3.7, (3) in Theorems 4.9–4.12, (4) in (4.5), (5), (6), and (7) in (4.7).

This paper is organized as follows. In Sec. II we discuss symplectic group structures of H_ϵ^0. In Sec. III we construct a canonical transformation and diagonalize H_ϵ^0. In Sec. IV we derive effective Hamiltonians by scaling limits. In Sec. V we give a remark on g-factor shift. Sections VI and VII are appendices.

II. SYMPLECTIC GROUP STRUCTURES

A. Unitary representations

$B(W)$ denotes the set of bounded operators on W. We define for $K \in B(W)$,

$$\overline{K}f := \overline{Kf}.$$

We introduce a notation. For $A,B,C,D \in B(W)$ we define

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} a(f) \\ a^\dagger(g) \end{pmatrix} := \begin{pmatrix} a(Af)+a^\dagger(Bg) \\ a(Cf)+a^\dagger(Dg) \end{pmatrix}.$$

Set

$$^{T}\begin{pmatrix} A & B \\ C & D \end{pmatrix} := \begin{pmatrix} A & C \\ B & D \end{pmatrix}.$$

Definition 2.1: Let $S,T \in B(W)$ *and set*

$$\xi := \begin{pmatrix} S & \overline{T} \\ T & \overline{S} \end{pmatrix} : W \oplus W \to W \oplus W.$$

(1) We say that ξ *is of symplectic group* Σ *if*

$$\xi^* J \xi = \xi J \xi^* = J, \tag{2.1}$$

where

$$\xi^* = \begin{pmatrix} S^* & T^* \\ \overline{T}^* & \overline{S}^* \end{pmatrix}, \quad J := \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.$$

(2) We say that ξ *is of* Σ_{B} *if (i)* $\xi \in \Sigma$ *and (ii)* T *is a Hilbert–Schmidt operator.*

Σ_{B} is a subgroup of Σ. We define

$$\mathcal{H}_m := L^2(\mathbb{R}^m) \otimes \mathcal{F} \cong \int_{\mathbb{R}^m}^{\oplus} \mathcal{F} \mathrm{d}q.$$

Suppose that

$$\xi = \begin{pmatrix} S & \overline{T} \\ T & \overline{S} \end{pmatrix} \in \Sigma_{\mathrm{B}},$$

and

$$L = (L_1, \ldots, L_m) \in \oplus^m W.$$

For $f \in W$ we let

$$\begin{pmatrix} b(f) \\ b^{\dagger}(f) \end{pmatrix} := {}^{T}\begin{pmatrix} S & \overline{T} \\ T & \overline{S} \end{pmatrix} \begin{pmatrix} a(f) \\ a^{\dagger}(f) \end{pmatrix}$$

and

$$B(f) := 1 \otimes b(f) + \sum_{l=1}^{m} (L_l, f) p_l \otimes 1,$$

$$B^{\dagger}(f) := 1 \otimes b^{\dagger}(f) + \sum_{l=1}^{m} (\overline{L_l, f}) p_l \otimes 1,$$

where p_l, $l = 1, \ldots, m$, denote the momentum operators in $L^2(\mathbb{R}^m)$. It follows that

$$[b(f), b^{\dagger}(g)] = (\overline{f}, g),$$

$$[b(f), b(g)] = [b^{\dagger}(f), b^{\dagger}(g)] = 0.$$

Moreover since

$$\xi^{-1}=J\xi^{*}J=\begin{pmatrix} S^{*} & -T^{*} \\ -\overline{T}^{*} & \overline{S}^{*} \end{pmatrix},$$

we have

$$\begin{pmatrix} a(f) \\ a^{\dagger}(f) \end{pmatrix}={}^{T}\begin{pmatrix} S^{*} & -T^{*} \\ -\overline{T}^{*} & \overline{S}^{*} \end{pmatrix}\begin{pmatrix} b(f) \\ b^{\dagger}(f) \end{pmatrix} \tag{2.2}$$

and

$$\begin{pmatrix} 1\otimes a(f) \\ 1\otimes a^{\dagger}(f) \end{pmatrix}={}^{T}\begin{pmatrix} S^{*} & -T^{*} \\ -\overline{T}^{*} & \overline{S}^{*} \end{pmatrix}\begin{pmatrix} B(f) \\ B^{\dagger}(f) \end{pmatrix}-\sum_{l=1}^{m}\begin{pmatrix} (SL_l-\overline{TL_l},f)p_l\otimes 1 \\ (\overline{SL_l}-TL_l,f)p_l\otimes 1 \end{pmatrix}. \tag{2.3}$$

Define

$$R_l:=TL_l-\overline{SL_l},$$

and

$$\theta(q,\xi,L):=\exp\left\{\sum_{l=1}^{m} q_l\{a^{\dagger}(R_l)-a(\overline{R}_l)\}\right\},\quad q=(q_1,\ldots,q_m)\in\mathbb{R}^m.$$

Furthermore set

$$\theta(\xi,L):=\int_{\mathbb{R}^m}^{\oplus}\theta(q,\xi,L)\,dq=\exp\left\{\sum_{l=1}^{m} p_l\otimes\{a^{\dagger}(R_l)-a(\overline{R}_l)\}\right\},$$

where p_l, $l=1,...m$, denote the momentum operators.

Proposition 2.2: Suppose $\xi=\left(\begin{smallmatrix} S & \overline{T} \\ T & \overline{S} \end{smallmatrix}\right)\in\Sigma_{\mathrm{B}}$. *Then there exists a unitary operator* $U(\xi)$ *of* $\mathcal{F}$ *such that for all* $f\in W$

(1) $U(\xi)^{-1}b^{\sharp}(f)U(\xi)=a^{\sharp}(f)$,
(2) $U(\xi)^{-1}\theta(\xi,L)^{-1}B^{\sharp}(f)\theta(\xi,L)U(\xi)=a^{\sharp}(f)$.

Proof: See Refs. 15–17 for details. [We easily see that for $\xi_1:=\left(\begin{smallmatrix} S & \overline{T} \\ T & \overline{S} \end{smallmatrix}\right)\in\Sigma_{\mathrm{B}}$ and $\xi_2:=\left(\begin{smallmatrix} U & \overline{V} \\ V & \overline{U} \end{smallmatrix}\right)\in\Sigma_{\mathrm{B}}$: $U(\xi_2)U(\xi_1)a(f)U(\xi_1)^{-1}U(\xi_2)^{-1}=a((US+\overline{VT})f)+a^{\dagger}((VS+\overline{UT})f)$; $U(\xi_2)U(\xi_1)a^{\dagger}(f)U(\xi_1)^{-1}U(\xi_2)^{-1}=a((U\overline{T}+\overline{VS})f)+a^{\dagger}((V\overline{T}+\overline{US})f)$; and $\xi_2\cdot\xi_1=\left(\begin{smallmatrix} US+\overline{VT} & U\overline{T}+\overline{VS} \\ VS+\overline{UT} & V\overline{T}+\overline{US} \end{smallmatrix}\right)$. Then $U(\xi_2)U(\xi_1)=\omega(\xi_2\xi_1)U(\xi_2\xi_1)$, where $\omega(\xi_2\xi_1)$ is a constant. Hence the map $\Sigma_{\mathrm{B}}\ni\xi\mapsto U(\xi)$ defines a projective unitary representation of Σ_{B}.] □

We set

$$\mathcal{U}(q,\xi,L):=\theta(q,\xi,L)U(\xi):\mathcal{F}\to\mathcal{F},$$

and

$$\mathcal{U}(\xi,L):=\theta(\xi,L)U(\xi):\mathcal{H}_m\to\mathcal{H}_m.$$

We call $\mathcal{U}(\xi,L)$ the canonical transformation associated with $\{\xi,L\}\in\Sigma_{\mathrm{B}}\times\oplus^{m}W$.

B. Average of fluctuations

Define

$$\pi(f) := i\{a^\dagger(\overline{f}) - a(f)\}, \quad f \in W.$$

We want to obtain the average of fluctuation $F_{\xi L}$ of a function $F: \mathbb{R}^m \to \mathbb{C}$;

$$F_{\xi L} := \mathcal{U}(\xi, L)^{-1} F \mathcal{U}(\xi, L) = U(\xi)^{-1} F(x_1 + \pi(R_1), \ldots, x_m + \pi(R_m)) U(\xi),$$

with respect to the bare vacuum. Let Γ be the $m \times m$ symmetric matrix defined by

$$\Gamma := ((L_\mu, L_\nu)_W)_{1 \leqslant \mu, \nu \leqslant m},$$

and $\langle a, b \rangle$ denote the scalar product on $\mathbb{C}^m$. Suppose

$$\text{Rank } \Gamma = n \leqslant m$$

and T is a unitary matrix such that

$$T \Gamma T^{-1} = \text{diag}\{\mu_1, \ldots, \mu_n, 0, \ldots, 0\}, \quad \mu := \mu_1 \cdots \mu_n \neq 0.$$

Let

$$F_{T^{-1}}(x) := F(T^{-1}x), \quad x \in \mathbb{R}^m.$$

We define

$$F_{\text{eff}}(x) := (2\pi\mu)^{-m/2} \int_{\mathbb{R}^n} F_{T^{-1}}(y_1, \ldots, y_n, (Tx)_{n+1}, \ldots, (Tx)_m) \times \exp\left(-\sum_{j=1}^{n} |(Tx)_j - y_j|^2/(2\mu) \right) dy.$$

In particular if Rank $\Gamma = n$, then

$$F_{\text{eff}}(x) = (2\pi \det \Gamma)^{-m/2} \int_{\mathbb{R}^m} F(y) e^{-|x-y|^2/(2 \det \Gamma)} dy.$$

Lemma 2.3: Let $\xi = \begin{pmatrix} S & \overline{T} \\ T & \overline{S} \end{pmatrix} \in \Sigma_B$ *and* $(L_1, \ldots, L_m) \in \oplus^m W$. *Suppose that* F *is such that*

$$\int_{\mathbb{R}^n} |F_{T^{-1}}|(y_1, \ldots, y_n, (Tx)_{n+1}, \ldots, (Tx)_m) \exp\left(-\sum_{j=1}^{n} |(Tx)_j - y_j|^2/(2\mu) \right) dy \in L^1_{\text{loc}}(\mathbb{R}^m, dx).$$

Then for $f \in L^2(\mathbb{R}^m)$, *and* $g \in L^2(\mathbb{R}^m)$ *such that* $\mathcal{U}(\xi, L) g \otimes \Omega \in D(F)$, *we see that* $g \in D(F_{\text{eff}})$ *and*

$$(f \otimes \Omega, F_{\xi L} g \otimes \Omega)_{\mathcal{H}_m} = (f, F_{\text{eff}} g)_{L^2(\mathbb{R}^m)}. \tag{2.4}$$

Proof: We see that by (2.2)

$$a(\overline{R_l}) = b(S^* \overline{R_l}) - b^\dagger(\overline{T}^* \overline{R_l}),$$

$$a^\dagger(R_l) = -b(T^* R_l) + b^\dagger(\overline{S}^* R_l).$$

Thus we have

$$a^\dagger(R_l)-a(\overline{R_l})=b^\dagger(\overline{S}^*R_l+\overline{T}^*\overline{R_l})-b(T^*R_l+S^*\overline{R_l}):=b^\dagger(R_l')-b(\overline{R_l'}).$$

It follows from $\xi^*J\xi=\xi J\xi^*$ that

$$R_l'=\overline{S}^*(TL_l-\overline{SL_l})+\overline{T}^*(\overline{TL_l}-SL_l)=(\overline{S}^*T-\overline{T}^*S)L_l+(\overline{T}^*\overline{T}-\overline{S}^*\overline{S})\overline{L_l}=-\overline{L_l}.$$

Hence

$$\pi(R_l)=i\{a^\dagger(R_l)-a(\overline{R_l})\}=i\{b(L_l)-b^\dagger(\overline{L_l})\}.$$

Then we have

$$U(\xi)^{-1}\pi(R_l)U(\xi)=i\{a(L_l)-a^\dagger(\overline{L_l})\}=-\pi(L_l). \tag{2.5}$$

Let

$$F_N(x):=\begin{cases}F(x), & |x|<N,\\ 0, & |x|\geqslant N.\end{cases}$$

Moreover

$$F_{N\epsilon}:=\rho_\epsilon * F_N, \quad \epsilon>0,$$

where $\rho_\epsilon(x):=\rho(x/\epsilon)/\epsilon^m$, $\rho(x)\geqslant 0$, $\operatorname{supp}\rho\subset\{x\in\mathbb{R}^m||x|\leqslant 1\}$, and $\int_{\mathbb{R}^m}\rho(x)\mathrm{d}x=1$. (2.5) leads to

$$\begin{aligned}(f\otimes\Omega,(F_{N\epsilon})_{\xi L}g\otimes\Omega)&=(2\pi)^{-m/2}\int_{\mathbb{R}^m}\mathrm{d}k\, e^{ikx}\check{F}_{N\epsilon}(k)(f\otimes\Omega,U(\xi)^{-1}e^{i\langle k,x+\pi(R)\rangle}U(\xi)g\otimes\Omega)\\ &=(2\pi)^{-m/2}\int_{\mathbb{R}^d}\mathrm{d}k\, e^{ikx}\check{F}_{N\epsilon}(k)(f\otimes\Omega,e^{i\langle k,x-\pi(\overline{L})\rangle}g\otimes\Omega)\\ &=(2\pi)^{-m/2}\int_{\mathbb{R}^m}\mathrm{d}k\, e^{ikx}\check{F}_{N\epsilon}(k)\overline{f(x)}g(x)e^{-\langle k,\Gamma k\rangle/2}=(f,(F_{N\epsilon})_{\mathrm{eff}}g).\end{aligned}$$

Taking $\epsilon\to 0$, we have $(F_{N\epsilon})_{\mathrm{eff}}(x)\to(F_N)_{\mathrm{eff}}(x)$, and $(F_{N\epsilon})_{\xi L}\to(F_N)_{\xi L}$ strongly. Then the lemma follows for F_N. Let $f\in C_0^\infty(\mathbb{R}^m)$. Then taking $N\to\infty$, we also have $(f,(F_N)_{\xi L}g)\to(f,F_{\xi L}g)$ and $(f,(F_N)_{\mathrm{eff}}g)\to(f,F_{\mathrm{eff}}g)$ by the dominated convergence theorem. Hence the lemma follows. □

Remark 2.4: F_{eff} is independent of ξ.

C. Physical vacuum

Let $\xi=\left(\begin{smallmatrix}S & \overline{T}\\ T & \overline{S}\end{smallmatrix}\right)\in\Sigma_{\mathrm{B}}$ and $L\in\oplus^{dN}W$. We define

$$\Omega(q,\xi,L):=\mathcal{U}(q,\xi,L)\Omega.$$

Let K be a Hilbert–Schmidt operator. Then there exist complete orthonormal systems (CONS) $\{\psi_i\}$, $\{\phi_i\}$, and a positive sequence $\{\mu_i\}$ such that

$$Kf=\sum_{i=1}^\infty \mu_i(\psi_i,f)\phi_i, \quad f\in\mathcal{H}_m,$$

with

$$\sum_{i=1}^\infty \mu_i^2=\|K\|_{\mathrm{HS}}^2,$$

where $\|\cdot\|_{\mathrm{HS}}$ denotes the Hilbert–Schmidt norm. We define for a finite particle vector Ψ,

$$\langle a^\dagger|K|a^\dagger\rangle\Psi := s-\lim_{n\to\infty}\sum_{i=1}^{n}\mu_i a^\dagger(\overline{\psi_i})a^\dagger(\phi_i)\Psi.$$

The above-presented strong limit actually exists. It is well known that if

$$(1)K \text{ is a Hilbert–Schmidt operator,}\quad (2)\overline{K}^*=K,\quad (3)\|K\|<1,$$

then

$$U_0(K) := s-\lim_{N\to\infty}\sum_{n=1}^{N}\frac{1}{n!}\left(-\frac{1}{2}\langle a^\dagger|K|a^\dagger\rangle\right)^n\Psi$$

exists for a finite particle vector Ψ. See Ref. 18.

Lemma 2.5: We have

$$\Omega(q,\xi,L)=\det(1-(TS^{-1})^*TS^{-1})^{1/4}\theta(q,\xi,L)U_0(TS^{-1})\Omega.$$

Proof: See Ref. 13 for details. □

III. CANONICAL TRANSFORM OF THE HAMILTONIANS

A. Fixed particle-momentum Hamiltonians

We define the fixed particle-momentum Hamiltonian by

$$H_\epsilon^0(q) := \sum_{j=1}^{N}\frac{1}{2m_j}q_j^2-\sum_{j=1}^{N}\frac{\alpha_j}{m_j}q_j\cdot A_j+\sum_{j=1}^{N}\frac{\epsilon\alpha_j^2}{2m_j}A_j^2+H_f.$$

Here q is a fixed particle-momentum:

$$q=(q_1,\ldots,q_N)\in\mathbb{R}^{dN}.$$

By a canonical transformation $\mathcal{U}(q)$, we will diagonalize $H_\epsilon^0(q)$ as

$$\mathcal{U}(q)^{-1}H_\epsilon^0(q)\mathcal{U}(q)=E(q)+H_f \tag{3.1}$$

with some constant $E(q)$. In Ref. 13, (3.1) was established for $N=1$, in Ref. 14 for $N\geqslant 1$ but sufficiently small $|\alpha_j|$'s. In this section we improve it as follows:

(1) we extend (3.1) to $N\geqslant 1$ and arbitrary α_j's,
(2) we derive an explicit form of $E(q)$,
(3) we show analytic properties of $E(q)$ in each α_j's.

Proposition 3.1: Suppose that $\hat{\lambda}_j/\sqrt{\omega},\hat{\lambda}_j,\omega\hat{\lambda}_j\in L^2(\mathbb{R}^d)$ *for* $j=1,\ldots,N$. *Then for all* $\{\alpha_1,\ldots,\alpha_N\}$ *and all* $q\in\mathbb{R}^{dN}$, $H_\epsilon^0(q)$ *is self-adjoint on* $D(H_f)$ *and bounded from below.*

Proof: The proof is similar to Proposition 1.2. Let $L:=H_f+1$. Then we easily have

$$\|H_\epsilon^0(q)\Psi\|\leqslant c\|L\Psi\|,$$

and

$$|(H_\epsilon^0(q)\Psi,L\Phi)-(L\Psi,H_\epsilon^0(q)\Phi)|\leqslant c'\|L^{1/2}\Psi\|\|L^{1/2}\Phi\|$$

with some constants c and c' for $\Psi,\ \Phi\in D(H_f)$. Hence $H_\epsilon^0(q)$ is essentially self-adjoint on $D(H_f)$ by the Nelson commutator theorem. Moreover it is seen that

$$c''\left(\|H_f\Psi\|^2+\left\|\sum_{j=1}^N\left(\frac{q_j^2}{2m_j}-\frac{\alpha_j}{m_j}q_j\cdot A_j+\frac{\epsilon\alpha_j}{2m_j}A_j^2\right)\Psi\right\|^2\right)\leqslant\|H_\epsilon^0(q)\Psi\|^2+c'''\|\Psi\|^2$$

with some constants c'' and c'''. Then $H_\epsilon^0(q)$ is closed on $D(H_f)$. Thus $H_\epsilon^0(q)$ is self-adjoint on $D(H_f)$. □

B. Assumptions on ultraviolet cutoffs and coupling constants

In this section we introduce assumptions on $\hat{\lambda}_j$ and α_j. We suppose the following assumptions on $\hat{\lambda}_j$'s.

(A.1) $\hat{\lambda}_j$ is rotation invariant, i.e., there exists a function $\varphi_j:[0,\infty)\to\mathbb{R}$ such that $\hat{\lambda}_j(k)=\varphi_j(|k|)$,

(A.2) $\hat{\lambda}_j/\omega,\omega\hat{\lambda}_j\in L^2(\mathbb{R}^d)$,

(A.3) $\varphi_{ij}(s):=\varphi_i(\sqrt{s})\varphi_j(\sqrt{s})s^{(d-1)/2}\in L^\delta([0,\infty),\mathrm{d}s)$ for some $0<\delta<1$, and there exists $0<C_{ij}<1$ such that, for arbitrary $s,t\geqslant 0$, $|\varphi_{ij}(s)-\varphi_{ij}(t)|\leqslant C_{ij}|s-t|$,

(A.4) $\|\hat{\lambda}_j\omega^{(d-2)/2}\|_\infty<\infty$ and $\|\hat{\lambda}_j\omega^{d/2}\|_\infty<\infty$, where $\|g\|_\infty:=\sup_{x\in\mathbb{R}^d}|g(x)|$.

The above-mentioned assumptions are sufficient conditions to construct a canonical transformation. Let

$$m_{ab}:=\begin{cases}m_j, & a=b=j\\ 0, & a\neq b\end{cases}.$$

Define

$$\begin{aligned}D_{ij}(k)&:=m_{ij}-\epsilon\alpha_i\alpha_jK\lim_{\eta\downarrow 0}\int_{\mathbb{R}^d}\frac{\omega(k')\hat{\lambda}_i(k')\hat{\lambda}_j(k')}{\omega(k)^2-\omega(k')^2+i\eta}\mathrm{d}k'\\&=m_{ij}-\epsilon\alpha_i\alpha_j\frac{K}{2}S_{d-1}\left(\lim_{\eta\downarrow 0}\int_{|\omega(k)^2-x|>\eta,x>0}\frac{\varphi_{ij}(x)}{\omega(k)^2-x}\mathrm{d}x-2\pi i\varphi_{ij}(\omega(k)^2)\right),\end{aligned}\tag{3.2}$$

where S_{d-1} denotes the volume of the $(d-1)$-dimensional unit sphere and

$$K:=\frac{d-1}{d}.$$

We define

$$D:=D(k)=(D_{ij}(k))_{1\leqslant i,j\leqslant N}:\overset{N}{\oplus}L^2(\mathbb{R}^d)\to\overset{N}{\oplus}L^2(\mathbb{R}^d).$$

We introduce two assumptions of ultraviolet cutoffs, I_λ and II_λ, as follows:

Hypothesis I_λ*:* $\hat{\lambda}_1=\cdots=\hat{\lambda}_N:=\hat{\lambda}$ and $\Im\hat{\lambda}(k)\neq 0$ for all $k\in\mathbb{R}^d$.

Hypothesis II_λ*:* Each $\hat{\lambda}_j$ has a compact support such that $\mathrm{supp}\,\hat{\lambda}_j\cap\mathrm{supp}\,\hat{\lambda}_i=\varnothing$ for $i\neq j$, and $|\hat{\lambda}_j(k)/D_{jj}(k)|\to 0$ as k converges to the boundary of $\mathrm{supp}\,\hat{\lambda}_j$.

In what follows we mainly study above two cases. The next assumptions are needed to see the boundedness of the Hamiltonians from below.

Hypothesis $I_\lambda^\alpha(\epsilon)$*:* Ultraviolet cutoffs satisfy I_λ, and $\{\alpha_1,\cdots,\alpha_N\}$ satisfy that

$$\begin{cases}\displaystyle\sum_{j=1}^N\frac{\alpha_j^2}{m_j}<\frac{1}{\|\hat{\lambda}/\sqrt{\omega}\|^2}\frac{1}{1-\epsilon}, & 0\leqslant\epsilon<1,\\ \{\alpha_1,\ldots,\alpha_N\}\in\mathbb{R}^N, & \epsilon\geqslant 1.\end{cases}$$

Hypothesis $II_\lambda^\alpha(\epsilon)$*:* Ultraviolet cutoffs satisfy II_λ, and $\{\alpha_1,\ldots,\alpha_N\}$ satisfy that

$$\begin{cases} \dfrac{\alpha_j^2}{m_j} \leqslant \dfrac{1}{\|\hat{\lambda}_j/\sqrt{\omega}\|^2}\dfrac{1}{1-\epsilon}, \quad j=1,\ldots,N, \quad 0\leqslant\epsilon<1, \\ \{\alpha_1,\ldots,\alpha_N\}\in\mathbb{R}^N, \quad \epsilon\geqslant 1. \end{cases}$$

C. Diagonalization of $H_\epsilon^0(q)$

Since

$$D_{ij}(0)=m_{ij}+\epsilon\alpha_i\alpha_j\frac{K}{2}S_{d-1}\int_0^\infty\frac{\varphi_{ij}(x)}{x}\mathrm{d}x,$$

we easily see that $D(0)^{-1}$ exists as an $N\times N$ matrix for I_λ and II_λ. Set

$$\begin{pmatrix} R_1 \\ \vdots \\ R_N \end{pmatrix} := \sqrt{\omega}D(0)^{-1}\begin{pmatrix} \hat{\lambda}_1 \\ \vdots \\ \hat{\lambda}_N \end{pmatrix}.$$

We define

$$\theta(q):=\exp\left(\sum_{j=1}^N\sum_{r=1}^{d-1}\sum_{\mu=1}^d\frac{\alpha_j q_{j\mu}}{\sqrt{2}}\left\{a^r\left(\overline{\frac{e_\mu^r R_j}{\omega^{3/2}}}\right)-a^{\dagger r}\left(\frac{e_\mu^r R_j}{\omega^{3/2}}\right)\right\}\right).$$

Proposition 3.2: Suppose I_λ *or* II_λ.

(1) *There exist* $\mathbb{W}\in\Sigma_{\mathrm{B}}$ *and* Q_j, $j=1,\ldots,N$, *such that*

$$\theta(q,\mathbb{W},L)=\theta(q),$$

where $L=(L_1^1,\ldots,L_1^d,\ldots,L_N^1,\ldots,L_N^d)\in\oplus^{dN}W$ *with*

$$L_j^\mu:=\frac{\alpha_j}{\sqrt{2}}\oplus_{r=1}^{d-1}\frac{e_\mu^r Q_j}{\omega^{3/2}}.$$

(2) *Let*

$$\mathcal{U}(q):=\theta(q)U(\mathbb{W}).$$

Then $\mathcal{U}(q)$ *maps* $D(H_f)$ *onto itself, and*

$$\mathcal{U}(q)^{-1}H_\epsilon^0(q)\mathcal{U}(q)=E(q)+H_f$$

with some $E(q)$.

(3) $E(q)$ *can be analytically continued to a neighborhood* $\mathcal{O}$ *of* $\mathbb{R}$ *in each* α_j*'s*.

Proof: See Sec. VI. □

D. Ground state energy

In this section we show an explicit form of $E(q)$ for both cases I_λ and II_λ. In the case of $N=1$ it is shown in Ref. 19. For the case of $N\geqslant 2$ one needs a slight modification of Ref. 19. We do not, however, need to go into the minor details for the moment. So a proof of the following lemma is taken up in Sec. VII.

Lemma 3.3: (1) Suppose I_λ. *Then we have*

$$E(q)=\frac{1}{2}\sum_{j=1}^{N}\frac{q_j^2}{m_j}-\frac{1}{2}E_{\mathrm{I}}\left|\sum_{j=1}^{N}\frac{\alpha_j}{m_j}q_j\right|^2+g_{\mathrm{I}}(m),$$

where

$$E_{\mathrm{I}}:=\frac{K\|\hat{\lambda}/\sqrt{\omega}\|^2}{1+\epsilon\rho\|\hat{\lambda}/\sqrt{\omega}\|^2},$$

$$g_{\mathrm{I}}(m):=\frac{d}{2\pi}\int_{-\infty}^{\infty}\frac{\epsilon\rho s^2\|\sqrt{\omega}\hat{\lambda}/(s^2+\omega^2)\|^2}{1+\epsilon\rho\|\sqrt{\omega}\hat{\lambda}/\sqrt{s^2+\omega^2}\|^2}\mathrm{d}s,$$

$$\rho:=K\sum_{j=1}^{N}\frac{\alpha_j^2}{m_j}.$$

(2) Suppose II_λ *. Then we have*

$$E(q)=\frac{1}{2}\sum_{j=1}^{N}\frac{q_j^2}{m_j}-\frac{1}{2}\sum_{j=1}^{N}\frac{q_j^2}{m_j}E_{\mathrm{II}}^{j}+g_{\mathrm{II}}(m),$$

where

$$E_{\mathrm{II}}^{j}:=\frac{\rho_j\|\hat{\lambda}_j/\sqrt{\omega}\|^2}{1+\epsilon\rho_j\|\hat{\lambda}_j/\sqrt{\omega}\|^2},$$

$$g_{\mathrm{II}}(m):=\sum_{j=1}^{N}\frac{d}{2\pi}\int_{-\infty}^{\infty}\frac{\epsilon\rho_j s^2\|\sqrt{\omega}\hat{\lambda}_j/(s^2+\omega^2)\|^2}{1+\epsilon\rho_j\|\sqrt{\omega}\hat{\lambda}_j/\sqrt{s^2+\omega^2}\|^2}\mathrm{d}s,$$

$$\rho_j:=K\frac{\alpha_j^2}{m_j}.$$

Proof: See Sec. VII. □

It is an interesting case where $\epsilon=1$.

Corollary 3.4: (1) Suppose II_λ *and* $\epsilon=1$*. Then*

$$E(q)=\sum_{j=1}^{N}\frac{1}{2m_j^{\mathrm{eff}}}q_j^2+\sum_{j=1}^{N}\frac{d}{2\pi}\int_{-\infty}^{\infty}\frac{\rho_j s^2\|\sqrt{\omega}\hat{\lambda}_j/(s^2+\omega^2)\|^2}{1+\rho_j\|\sqrt{\omega}\hat{\lambda}_j/\sqrt{s^2+\omega^2}\|^2}\mathrm{d}s,$$

where

$$m_j^{\mathrm{eff}}:=m_j+\alpha_j^2K\|\hat{\lambda}_j/\sqrt{\omega}\|^2.$$

(2) Suppose $N=1$ *and* $\epsilon=1$*. Then*

$$E(q)=\frac{1}{2m^{\mathrm{eff}}}q^2+\frac{d}{2\pi}\int_{-\infty}^{\infty}\frac{K\alpha_1^2s^2\|\sqrt{\omega}\hat{\lambda}_1/(s^2+\omega^2)\|^2}{m+K\alpha_1^2\|\sqrt{\omega}\hat{\lambda}_1/(s^2+\omega^2)\|^2}\mathrm{d}s,$$

where

$$m^{\mathrm{eff}}:=m_1+\alpha_1^2K\|\hat{\lambda}_1/\sqrt{\omega}\|^2.$$

Lemma 3.5: (1) Suppose $\mathrm{I}_\lambda^\alpha(\epsilon)$. *Then for all* $q\in\mathbb{R}^{dN}$,

$$\sum_{j=1}^N \frac{q_j^2}{2m_j}-\frac{1}{2}E_{\mathrm{I}}\left|\sum_{j=1}^N \frac{\alpha_j}{m_j}q_j\right|^2>0.$$

(2) Suppose $\mathrm{II}_\lambda^\alpha(\epsilon)$. *Then for all* $q\in\mathbb{R}^{dN}$,

$$\sum_{j=1}^N \frac{q_j^2}{2m_j}-\frac{1}{2}\sum_{j=1}^N \frac{q_j^2}{m_j}E_{\mathrm{II}}^j>0.$$

Proof: By the Schwartz inequality we have

$$\frac{1}{2}E_{\mathrm{I}}\left|\sum_{j=1}^N \frac{\alpha_j}{m_j}q_j\right|^2\leqslant\frac{\rho\|\hat{\lambda}/\sqrt{\omega}\|^2}{1+\epsilon\rho\|\hat{\lambda}/\sqrt{\omega}\|^2}\sum_{j=1}^N \frac{q_j^2}{2m_j}.$$

Hence

$$\sum_{j=1}^N \frac{q_j^2}{2m_j}-\frac{1}{2}E_{\mathrm{I}}\left|\sum_{j=1}^N \frac{\alpha_j}{m_j}q_j\right|^2\geqslant\frac{1}{2}\left(1-\frac{\rho\|\hat{\lambda}/\sqrt{\omega}\|^2}{1+\epsilon\rho\|\hat{\lambda}/\sqrt{\omega}\|^2}\right)\sum_{j=1}^N \frac{q_j^2}{2m_j}.$$

Since Hypothesis $\mathrm{I}_\lambda^\alpha(\epsilon)$ implies that

$$1-\frac{\rho\|\hat{\lambda}/\sqrt{\omega}\|^2}{1+\epsilon\rho\|\hat{\lambda}/\sqrt{\omega}\|^2}>0,$$

(1) follows. (2) is similarly proven. □

E. Observed mass

We define the observed mass by

$$m^*(\mu,\nu,j):=\left(\frac{\partial^2}{\partial q_{j\mu}\partial q_{j\nu}}E(q)\bigg|_{q=0}\right)^{-1}.$$

Put

$$m^*(\mu,\mu,j):=m^*(\mu,j).$$

By Lemma 3.3 we have the following corollaries.

Corollary 3.6: (1) Suppose I_λ. *Then*

$$m^*(\mu,\nu,j)=\delta_{\mu\nu}m_j\left(\frac{1+K\left(\epsilon\Sigma_{i=1}^N\frac{\alpha_i^2}{m_i}-\frac{\alpha_j^2}{m_j}\right)\|\hat{\lambda}/\sqrt{\omega}\|^2}{1+\epsilon K\Sigma_{j=1}^N\frac{\alpha_j^2}{m_j}\|\hat{\lambda}/\sqrt{\omega}\|^2}\right)^{-1}.$$

In particular for the case of $\epsilon=1$,

$$m^*(\mu,\nu,j)=\delta_{\mu\nu}m_j\left(\frac{1+K\Sigma_{i\neq j}\dfrac{\alpha_i^2}{m_i}\|\hat{\lambda}/\sqrt{\omega}\|^2}{1+K\Sigma_{j=1}^N\dfrac{\alpha_j^2}{m_j}\|\hat{\lambda}/\sqrt{\omega}\|^2}\right)^{-1}.$$

(2) Suppose II_λ. *Then*

$$m^*(\mu,\nu,j)=\delta_{\mu\nu}\frac{m_j+\epsilon K\alpha_j^2\|\hat{\lambda}_j/\sqrt{\omega}\|^2}{1+(\epsilon-1)K\dfrac{\alpha_j^2}{m_j}\|\hat{\lambda}_j/\sqrt{\omega}\|^2}.$$

In particular for the case of $\epsilon=1$,

$$m^*(\mu,\nu,j)=\delta_{\mu\nu}(m_j+K\alpha_j^2\|\hat{\lambda}_j/\sqrt{\omega}\|^2).$$

Proof: It is a direct calculation. □

It is interesting to compare the sizes of observed masses for I_λ and II_λ.

Corollary 3.7: Suppose $\epsilon=1$. *Let* $m_{\mathrm{I}}^*(\mu,j)$ *be the observed mass for* I_λ *and* $m_{\mathrm{II}}^*(\mu,j)$ *for* II_λ. *Suppose that* $\|\hat{\lambda}/\sqrt{\omega}\|\leqslant\|\hat{\lambda}_j/\sqrt{\omega}\|$ *for a certain* j. *Then*

$$m_{\mathrm{I}}^*(\mu,j)<m_{\mathrm{II}}^*(\mu,j).$$

Proof: Note that

$$f(x)=\frac{x}{a+x},\quad a\geqslant 0,$$

is a monotonously increasing function of x. Directly we have

$$\frac{1}{m_{\mathrm{I}}^*(\mu,j)}=\frac{1}{m_j}\left(\frac{1+K\Sigma_{i\neq j}\dfrac{\alpha_i^2}{m_i}\|\hat{\lambda}/\sqrt{\omega}\|^2}{1+K\Sigma_{j=1}^N\dfrac{\alpha_j^2}{m_j}\|\hat{\lambda}/\sqrt{\omega}\|^2}\right)>\frac{1}{m_j}\left(\frac{1}{1+K\dfrac{\alpha_j^2}{m_j}\|\hat{\lambda}/\sqrt{\omega}\|^2}\right)$$
$$\geqslant\frac{1}{m_j}\left(\frac{1}{1+K\dfrac{\alpha_j^2}{m_j}\|\hat{\lambda}_j/\sqrt{\omega}\|^2}\right)=\frac{1}{m_{\mathrm{II}}^*(\mu,j)}.$$

Hence the corollary follows. □

F. Diagonalization of H_ϵ^0 and its self-adjointness

We define

$$\theta:=\exp\left(\sum_{j=1}^N\sum_{r=1}^{d-1}\sum_{\mu=1}^d\frac{\alpha_j}{\sqrt{2}}p_{j\mu}\otimes\left\{a^r\left(\overline{\frac{e_\mu^rR_j}{\omega^{3/2}}}\right)-a^{\dagger r}\left(\frac{e_\mu^rR_j}{\omega^{3/2}}\right)\right\}\right)$$

and

$$\mathcal{U}:=\theta U(\mathbb{W}).$$

Note that $\mathcal{U}$ maps $\mathcal{D}$ onto itself:

$$\mathcal{U}:\mathcal{D}\to\mathcal{D}.$$

Moreover we define $E(p)$ by the pseudodifferential operator with the kernel $E(q)$ in $L^2(\mathbb{R}^{dN})$.

Lemma 3.8: Suppose I_λ *or* II_λ. *Then for* $\Phi\in C_0^\infty(\mathbb{R}^{dN})\hat{\otimes}D(H_f)$,

$$\mathcal{U}^{-1}H_\epsilon^0\mathcal{U}\Phi=(E(p)\otimes 1+1\otimes H_f)\Phi. \tag{3.3}$$

Proof: Let $\Phi=g\otimes\psi$ *and* $\Psi=f\otimes\phi$, $g,\ f\in C_0^\infty(\mathbb{R}^{dN})$, $\psi,\phi\in D(H_f)$. We note that $\mathcal{U}\Phi\in\mathcal{D}$. Then the left-hand side of (3.3) is well defined. We have by Proposition 3.2

$$\begin{aligned}(\Psi,\mathcal{U}^{-1}H_\epsilon^0\mathcal{U}\Phi)_{\mathcal{H}}&=\int_{\mathbb{R}^{dN}}(\widehat{\mathcal{U}\Psi}(q),\widehat{H_\epsilon^0\mathcal{U}\Phi}(q))_{\mathcal{F}}\,dq\\&=\int_{\mathbb{R}^{dN}}(\mathcal{U}(q)\,\hat{\Psi}(q),H_\epsilon^0(q)\mathcal{U}(q)\,\hat{\Phi}(q))_{\mathcal{F}}\,dq\\&=\int_{\mathbb{R}^{dN}}\overline{\hat{f}}(q)\hat{g}(q)(\mathcal{U}(q)\psi,H_\epsilon^0(q)\mathcal{U}(q)\phi)_{\mathcal{F}}\,dq\\&=\int_{\mathbb{R}^{dN}}\hat{f}(q)\hat{g}(q)(\psi,(E(q)+H_f)\phi)_{\mathcal{F}}\,dq=(\Psi,(E(q)\otimes 1+1\otimes H_f)\Phi)_{\mathcal{H}}.\end{aligned}$$

Thus the lemma follows. □

Lemma 3.9: Suppose $\mathrm{I}_\lambda^\alpha(\epsilon)$ *or* $\mathrm{II}_\lambda^\alpha(\epsilon)$. *Then*

$$\mathcal{U}^{-1}H_\epsilon^0\mathcal{U}=E(p)\otimes 1+1\otimes H_f \tag{3.4}$$

holds on $\mathcal{D}$. *In particular* H_ϵ *is self-adjoint on* $\mathcal{D}$ *and bounded from below*.

Proof: By the assumption on $\{\alpha_1,\ldots,\alpha_N\}$, $E(p)$ is non-negative. Then $E(p)+H_f$ is self-adjoint on $\mathcal{D}$ and bounded from below. For $\Phi\in\mathcal{D}$, we can take a sequence $\Phi_n\in C_0^\infty(\mathbb{R}^{dN})\,\hat{\otimes}D(H_f)$ such that $\Phi_n\to\Phi$ and $(E(p)\otimes 1+1\otimes H_f)\Phi_n\to(E(p)\otimes 1+1\otimes H_f)\Phi$ strongly as $n\to\infty$. Since H_ϵ is closed, $H_\epsilon^0\mathcal{U}\Phi_n\to H_\epsilon^0\mathcal{U}\Phi$ as $n\to\infty$. Thus (3.4) holds. Since $\mathcal{U}$ maps $\mathcal{D}$ onto itself, H_ϵ^0 is self-adjoint on $\mathcal{D}$ and bounded from below. □

Remark 3.10: Let $\epsilon<1$. *Then* $E(p)$ *is unbounded from below for sufficiently large coupling constants. Actually in the case of* $N=1$, *for*

$$\alpha_1^2\geqslant m_1(\|\hat{\lambda}_1/\sqrt{\omega}\|^2(1-\epsilon))^{-1},$$

$E(p)$ *is unbounded from below. Hence* H_ϵ^0 *is unbounded from below for sufficiently large coupling constants. We should not overlook that the approximation of neglecting the self-interaction* A^2 *in* H *is not reasonable for sufficiently large coupling constants*.

Theorem 3.11: *Suppose* $\mathrm{I}_\lambda^\alpha(\epsilon)$ *or* $\mathrm{II}_\lambda^\alpha(\epsilon)$. *Then* H_ϵ *is self-adjoint on* $\mathcal{D}$ *and bounded from below*.

Proof: By Lemma 3.9 and the closed graph theorem there exists a constant c such that

$$\left\|\left(\sum_{j=1}^N\frac{p_j^2}{2m_j}+H_f\right)\Psi\right\|\leqslant c(\|H_\epsilon^0\Psi\|+\|\Psi\|),\quad \Psi\in\mathcal{D}.$$

Thus

$$\|V\Psi\|\leqslant ac(\|H_\epsilon^0\Psi\|+\|\Psi\|)+b\|\Psi\|$$

with some sufficiently small a, and some b, the Kato–Rellich theorem leads to the lemma. □

Corollary 3.12: Suppose I_λ. *Then*

$$\inf\sigma(H_\epsilon^0)=g_{\rm I}(m)=\frac{d}{2\pi}\int_{-\infty}^{\infty}\frac{\epsilon K\Sigma_{j=1}^N\frac{\alpha_j^2}{m_j}s^2\|\sqrt{\omega}\hat{\lambda}/(s^2+\omega^2)\|^2}{1+\epsilon K\Sigma_{j=1}^N\frac{\alpha_j^2}{m_j}\|\sqrt{\omega}\hat{\lambda}/\sqrt{s^2+\omega^2}\|^2}{\rm d}s.$$

Suppose II_λ. *Then*

$$\inf\sigma(H_\epsilon^0)=g_{\rm II}(m)=\sum_{j=1}^N\frac{d}{2\pi}\int_{-\infty}^{\infty}\frac{\epsilon K\frac{\alpha_j^2}{m_j}s^2\|\sqrt{\omega}\hat{\lambda}_j/(s^2+\omega^2)\|^2}{1+\epsilon K\frac{\alpha_j^2}{m_j}\|\sqrt{\omega}\hat{\lambda}_j/\sqrt{s^2+\omega^2}\|^2}{\rm d}s.$$

Proof: It follows from Lemmas 3.3 and 3.8. □

IV. EFFECTIVE HAMILTONIAN

A. Scaled Hamiltonians

Here we recall the scaled Hamiltonian $H_\epsilon(\kappa)$,

$$H_\epsilon(\kappa):=H_{\rm el}\otimes 1-\kappa^l\sum_{j=1}^N\frac{\alpha_j}{m_j}p_j\otimes A_j+\kappa^2 1\otimes\left(\sum_{j=1}^N\frac{\epsilon\alpha_j^2}{2m_j}A_j^2+H_f\right).$$

$H_\epsilon(\kappa)$ is derived from H_ϵ scaled as

$$\omega\to\kappa^2\omega, \tag{4.1}$$

$$\alpha_j\to\kappa^l\alpha_j, \tag{4.2}$$

$$\epsilon\to\kappa^{2-2l}\epsilon. \tag{4.3}$$

Replacing ω,α_j,ϵ as in (4.1)–(4.3), we see that

$$\theta\to\exp\left(\kappa^{l-2}\sum_{j=1}^N\sum_{r=1}^{d-1}\sum_{\mu=1}^d\frac{\alpha_j}{\sqrt{2}}p_{j\mu}\otimes\left\{a^r\left(\frac{\overline{e_\mu^r R_j}}{\omega^{3/2}}\right)-a^{\dagger r}\left(\frac{e_\mu^r R_j}{\omega^{3/2}}\right)\right\}\right), \tag{4.4}$$

$$-\frac{1}{2}E_{\rm I}\left|\sum_{j=1}^N\frac{\alpha_j}{m_j}q_j\right|^2\to-\kappa^{2l-2}\frac{1}{2}E_{\rm I}\left|\sum_{j=1}^N\frac{\alpha_j}{m_j}q_j\right|^2,$$

$$-\frac{1}{2}\sum_{j=1}^N\frac{q_j^2}{m_j}E_{\rm II}^j\to-\kappa^{2l-2}\frac{1}{2}\sum_{j=1}^N\frac{q_j^2}{m_j}E_{\rm II}^j,$$

$$g_{\rm I}(m)\to g_{\rm I}(m/k^2),$$

$$g_{\rm II}(m)\to g_{\rm II}(m/k^2).$$

Lemma 4.1: $U(\mathbb{W})$ *leaves invariant under the scaling* (4.1), (4.2), *and* (4.3).
Proof: See Lemma 6.5. □
Let

$$E_{\mathrm{ren}}(p) := \begin{cases} -\frac{1}{2} E_{\mathrm{I}} \left| \sum_{j=1}^{N} \frac{\alpha_j}{m_j} p_j \right|^2 & \text{for } \mathrm{I}_\lambda \\ -\frac{1}{2} \sum_{j=1}^{N} \frac{p_j^2}{m_j} E_{\mathrm{II}}^j & \text{for } \mathrm{II}_\lambda . \end{cases} \tag{4.5}$$

Moreover we set

$$g(m) := \begin{cases} g_{\mathrm{I}}(m) & \text{for } \mathrm{I}_\lambda \\ g_{\mathrm{II}}(m) & \text{for } \mathrm{II}_\lambda . \end{cases}$$

We define $\mathcal{U}_\kappa$ by $\mathcal{U}$ with ω, α_j, and ϵ replaced as in (4.1),(4.2), and (4.3), respectively.

Lemma 4.2: Suppose $\mathrm{I}_\lambda^\alpha(\kappa^{2l-2}\epsilon)$ *or* $\mathrm{II}_\lambda^\alpha(\kappa^{2l-2}\epsilon)$. *Then*

$$\mathcal{U}_\kappa^{-1} H_\epsilon(\kappa) \mathcal{U}_\kappa = \frac{1}{2} \sum_{j=1}^{N} \frac{p_j^2}{m_j} + \kappa^{2l-2} E_{\mathrm{ren}}(p) + \kappa^2 H_f + g(m/\kappa^2) + \mathcal{U}_\kappa^{-1} V \mathcal{U}_k .$$

In particular $H_\epsilon(\kappa)$ *is self-adjoint on* $\mathcal{D}$ *and bounded from below.*

Proof: It follows from Lemma 3.9. □

Lemma 4.3: Suppose I_λ *or* II_λ. *Then there exists the unique ground state* Ω_ϵ *of* $\Sigma_{j=1}^N \epsilon \alpha_j^2 A_j^2/(2m_j) + H_f$. *Moreover*

$$P_\epsilon := U(\mathbb{W}) P_\Omega U(\mathbb{W})^{-1} \tag{4.6}$$

is the projection to the eigenspace spanned by Ω_ϵ.

Proof: Set $q=0$ in Lemma 3.2 (2). Then

$$\mathcal{U}(0)^{-1} \left(\epsilon \sum_{j=1}^{N} \frac{\alpha_j^2}{2m_j} A_j^2 + H_f \right) \mathcal{U}(0) = H_f + g(m).$$

The right-hand side has the unique ground state Ω. Thus $\mathcal{U}(0)\Omega = U(\mathbb{W})\Omega = \Omega_\epsilon$ is the unique ground state of $\Sigma_{j=1}^N \epsilon \alpha_j^2 A_j^2/(2m_j) + H_f$. Hence the lemma follows. □

Lemma 4.4: (1) Suppose $l=2$. *Then* $\mathcal{U}_\kappa$ *is independent of* κ. (2) *Suppose* $l<2$. *Then s* $-\lim_{\kappa\to\infty} \mathcal{U}_\kappa = U(\mathbb{W})$.

Proof: It follows from (4.1) and (4.4). □

We write as

$$\mathcal{U}_\infty := \begin{cases} \mathcal{U}, & l=2, \\ U(\mathbb{W}), & l<2 . \end{cases}$$

B. Effective potentials

Define V_{eff} acting on $L^2(\mathbb{R}^{dN})$ by

$$(f, V_{\mathrm{eff}} g)_{L^2(\mathbb{R}^{dN})} := (f \otimes \Omega, (\mathcal{U}_\infty^{-1} V \mathcal{U}_\infty) g \otimes \Omega)_{\mathcal{H}} .$$

Note

$$D(V_{\mathrm{eff}}) \supset D\left(\sum_{j=1}^{N} \frac{p_j^2}{2m_j} \right).$$

We define the $N \times N$ correlation matrix $\Delta = (\Delta_{ij})_{1 \le i,j \le N}$ by

$$\Delta_{ij} := \frac{1}{2}\alpha_i\alpha_j K\left(\frac{Q_i}{\omega^{3/2}}, \frac{Q_j}{\omega^{3/2}}\right).$$

Note that

$$(L_i^\mu, L_j^\nu) = \frac{\alpha_i\alpha_j}{2} K\delta_{\mu\nu}\left(\frac{Q_i}{\omega^{3/2}}, \frac{Q_j}{\omega^{3/2}}\right) = \delta_{\mu\nu}\Delta_{ij}.$$

Suppose that $\mathrm{Rank}\Delta = M$ and $T = T_\Delta$ is an $N\times N$ unitary matrix such that

$$T\Delta T^{-1} = \mathrm{diag}\{\mu_1,\ldots,\mu_M,0,\ldots,0\}, \quad \mu = \mu_1\cdots\mu_M \neq 0.$$

Let

$$\tilde{T} := \begin{pmatrix} T_{11}1_d & \cdots & T_{1N}1_d \\ \vdots & & \vdots \\ T_{N1}1_d & \cdots & T_{NN}1_d \end{pmatrix}.$$

Here 1_d denotes the $d\times d$ identity matrix.

Lemma 4.5: Let $l=2$. Suppose

$$\int_{\mathbb{R}^{dM}} |V_{\tilde{T}^{-1}}|(y_1,\ldots,y_M,(\tilde{T}x)_{M+1},\ldots,(\tilde{T}x)_N)\exp\left(-\sum_{j=1}^K |(\tilde{T}x)_j - y_j|^2/(2\mu)\right)dy \in L^1_{\mathrm{loc}}(\mathbb{R}^{dN}).$$

(1) Suppose that $\mathrm{Rank}\Delta = N$. *Then we have*

$$V_{\mathrm{eff}}(x) = (2\pi)^{-dN/2}(\det\Delta)^{-d/2}\int_{\mathbb{R}^{dN}} e^{-|x-y|^2/(2\,\det\Delta)}V(y)dy.$$

(2) *Suppose that* $\mathrm{Rank}\Delta = M < N$. *Then we have*

$$V_{\mathrm{eff}}(x) = (2\pi)^{-dN/2}\mu^{-d/2}\int_{\mathbb{R}^{dM}} V_{\tilde{T}^{-1}}(y_1,\ldots,y_M,(\tilde{T}x)_{M+1},\ldots,(\tilde{T}x)_N)$$
$$\times\exp\left(-\sum_{j=1}^K |(\tilde{T}x)_j - y_j|^2/(2\mu)\right)dy.$$

Proof: It follows from Lemma 2.3. □

Lemma 4.6: Let $l<2$. Then $V_{\mathrm{eff}} = V$.

Proof: Since $\mathcal{U}_\infty$ and V is commutative, the lemma follows. □

C. Scaling limits

Let

$$V_\kappa := \mathcal{U}_\kappa^{-1} V \mathcal{U}_\kappa.$$

We define

$$H_\epsilon^{\mathrm{ren}}(\kappa) := \begin{cases} H_\epsilon(\kappa) - \kappa^{2l-2}E_{\mathrm{ren}}(p) - g(m/\kappa^2), & 1 < l \leqslant 2, \\ H_\epsilon(\kappa) - g(m/\kappa^2), & l \leqslant 1, \end{cases}$$

and

$$H_{\mathrm{eff}}:=\begin{cases}\displaystyle\sum_{j=1}^{N}\frac{p_j^2}{2m_j}+V_{\mathrm{eff}}, & l=2,\\ \displaystyle\sum_{j=1}^{N}\frac{p_j^2}{2m_j}+V, & 1<l<2,\\ \displaystyle\sum_{j=1}^{N}\frac{p_j^2}{2m_j}+E_{\mathrm{ren}}(p)+V, & l=1,\\ \displaystyle\sum_{j=1}^{N}\frac{p_j^2}{2m_j}+V, & l<1.\end{cases}\tag{4.7}$$

Lemma 4.7: Let κ be sufficiently large. Define

$$H_{\mathrm{eff}}(\kappa):=\begin{cases}\displaystyle\sum_{j=1}^{N}\frac{p_j^2}{2m_j}+\kappa^2H_f+V, & 1<l\leqslant 2,\\ \displaystyle\sum_{j=1}^{N}\frac{p_j^2}{2m_j}+\kappa^{2l-2}E_{\mathrm{ren}}(p)+\kappa^2H_f+V, & l\leqslant 1.\end{cases}$$

(1) Suppose I_λ *and* II_λ, *and* $l\neq 1$. *Then*

$$\mathcal{U}_\kappa H_\epsilon^{\mathrm{ren}}(\kappa)\mathcal{U}_\kappa=H_{\mathrm{eff}}(\kappa).\tag{4.8}$$

In particular, for all $\{\alpha_1,\ldots,\alpha_N\}$, $H_\epsilon^{\mathrm{ren}}(\kappa)$ *is self-adjoint on* $\mathcal{D}$ *and bounded from below. (2) Suppose* $\mathrm{I}_\lambda^\alpha(\epsilon)$ *or* $\mathrm{II}_\lambda^\alpha(\epsilon)$, *and* $l=1$. *Then* (4.8) *holds. In particular* $H_\epsilon^{\mathrm{ren}}(\kappa)$ *is self-adjoint on* $\mathcal{D}$ *and bounded from below.*

Proof: By Hypothesis **V** we see that for $\Psi\in\mathcal{D}$,

$$\|V_\kappa\Psi\|\leqslant a\left\|\sum_{j=1}^{N}\frac{p_j^2}{2m_j}\Psi\right\|+b\|\Psi\|.$$

Thus by the Kato–Rellich theorem $H_{\mathrm{eff}}(\kappa)$ for $1<l\leqslant 2$ is self-adjoint on $\mathcal{D}$ and bounded from below. For $l<1$, since κ is sufficiently large, we have $\Sigma_{j=1}^N(p_j^2/2m_j)+\kappa^{2l-2}E_{\mathrm{ren}}(p)$ is positive and

$$\left\|\left(\sum_{j=1}^{N}\frac{p_j^2}{2m_j}+\kappa^{2l-2}E_{\mathrm{ren}}(p)\right)f\right\|\geqslant\epsilon(\alpha_1,\ldots,\alpha_N)\left\|\sum_{j=1}^{N}\frac{p_j^2}{2m_j}f\right\|$$

with some $\epsilon(\alpha_1,\ldots,\alpha_N)>0$ independent of large κ. Then

$$\|V_\kappa\Psi\|\leqslant\frac{a}{\epsilon(\alpha_1,\ldots,\alpha_N)}\left\|\left(\sum_{j=1}^{N}\frac{p_j^2}{2m_j}+\kappa^{2l-2}E_{\mathrm{ren}}(p)\right)\Psi\right\|+b\|\Psi\|.\tag{4.9}$$

Hence $H_{\mathrm{eff}}(\kappa)$ for $l\neq 1$ is self-adjoint on $\mathcal{D}$ and bounded from below. By (3.8), (4.8) holds on $C_0^\infty(\mathbb{R}^{dN})\hat{\otimes}D(H_f)$, and $\mathcal{U}_\kappa$ maps $\mathcal{D}$ onto itself. Then (4.8) holds on $\mathcal{D}$ by a limiting argument. Thus (1) follows. For $l=1$, $\Sigma_{j=1}^N p_j^2/(2m_j)+E_{\mathrm{ren}}(p)$ is a nonnegative self-adjoint operator. Thus $H_{\mathrm{eff}}(\kappa)$ is self-adjoint on $\mathcal{D}$ and bounded from below. Thus (2) follows. □

Lemma 4.8: (1) Suppose $\mathrm{I}_\lambda^\alpha(\epsilon)$ *or* $\mathrm{II}_\lambda^\alpha(\epsilon)$, *and* $l=1$. *Then* H_{eff} *is self-adjoint on* $D(\Sigma_{j=1}^N p_j^2/(2m_j))$ *and bounded from below. (2) Let* $l\neq 1$. *Then* H_{eff} *is self-adjoint on* $D(\Sigma_{j=1}^N p_j^2/(2m_j))$ *and bounded from below.*

Proof: It is clear. We omit it. □

TABLE I. Effective Hamiltonians.

	$H_\epsilon^{\mathrm{ren}}(\kappa)+g(m/\kappa^2)$	H_{eff}
$l=2$, I_λ	$H_\epsilon(\kappa)+\frac{\kappa^2}{2}E_{\mathrm{I}}\left\vert\Sigma_{j=1}^N\frac{\alpha_j}{m_j}p_j\right\vert^2$	$\frac{1}{2m}p^2+V_{\mathrm{eff}}$
$l=2$, II_λ	$H_\epsilon(\kappa)+\frac{\kappa^2}{2}\Sigma_{j=1}^N\frac{p_j^2}{m_j}E_{\mathrm{II}}^j$	$\frac{1}{2m}p^2+V_{\mathrm{eff}}$
$1<l<2$, I_λ	$H_\epsilon(\kappa)+\frac{\kappa^{2l-2}}{2}E_{\mathrm{I}}\left\vert\Sigma_{j=1}^N\frac{\alpha_j}{m_j}p_j\right\vert^2$	$\frac{1}{2m}p^2+V$
$1<l<2$, II_λ	$H_\epsilon(\kappa)+\frac{\kappa^{2l-2}}{2}\Sigma_{j=1}^N\frac{p_j^2}{m_j}E_{\mathrm{II}}^j$	$\frac{1}{2m}p^2+V$
$l=1$, I_λ	$H_\epsilon(\kappa)$	$\Sigma_{j=1}^N\frac{p_j^2}{2m_j}-\frac{1}{2}E_{\mathrm{I}}\left\vert\Sigma_{j=1}^N\frac{\alpha_j}{m_j}p_j\right\vert^2+V$
$l=1$, II_λ	$H_\epsilon(\kappa)$	$\Sigma_{j=1}^N\frac{p_j^2}{2m_j}-\frac{1}{2}\Sigma_{j=1}^N\frac{p_j^2}{m_j}E_{\mathrm{II}}^j+V$
$l<1$	$H_\epsilon(\kappa)$	$\frac{1}{2m}p^2+V$

Let P_ϵ denote the projection to the subspace spanned by the unique ground state of $\Sigma_{j=1}^N\epsilon\alpha_j^2/2m_jA_j^2+H_f$. Note $P_0:=P_\Omega$ is the projection to Ω.

Theorem 4.9: *Let $l=2$. Suppose I_λ or II_λ. Moreover suppose $\vert V_{\mathrm{eff}}\vert\in L^1_{\mathrm{loc}}(\mathbb{R}^{dN})$. Then for all $\{\alpha_1,\ldots,\alpha_N\}$ and $z\in\mathbb{C}\backslash\mathbb{R}$,*

$$s-\lim_{\kappa\to\infty}(H_\epsilon^{\mathrm{ren}}(\kappa)-z)^{-1}=\theta\{(H_{\mathrm{eff}}-z)^{-1}\otimes P_\epsilon\}\theta^{-1}.$$

Theorem 4.10: *Let $1<l<2$. Suppose I_λ or II_λ. Then for all $\{\alpha_1,\ldots,\alpha_N\}$ and $z\in\mathbb{C}\backslash\mathbb{R}$,*

$$s-\lim_{\kappa\to\infty}(H_\epsilon^{\mathrm{ren}}(\kappa)-z)^{-1}=(H_{\mathrm{eff}}-z)^{-1}\otimes P_\epsilon. \tag{4.10}$$

Theorem 4.11: *Let $l=1$. Suppose $\mathrm{I}_\lambda^\alpha(\epsilon)$ or $\mathrm{II}_\lambda^\alpha(\epsilon)$. Then* (4.10) *holds.*

Theorem 4.12: *Let $l<1$. Suppose I_λ or II_λ. Then for all $\{\alpha_1,\ldots,\alpha_N\}$ and $z\in\mathbb{C}\backslash\mathbb{R}$,* (4.10) *holds. (See Table I).*

Before proving Theorems 4.9–4.12 we show a lemma.

Lemma 4.13: Suppose $z\in\mathbb{C}\backslash\mathbb{R}$.

(1) *Let $l=2$. Suppose $\vert V\vert_{\mathrm{eff}}\in L^1_{\mathrm{loc}}(\mathbb{R}^{dN})$, and I_λ or II_λ. Then for all $\{\alpha_1,\ldots,\alpha_N\}$,*

$$s-\lim_{\kappa\to\infty}(H_{\mathrm{eff}}(\kappa)-z)^{-1}=(H_{\mathrm{eff}}-z)^{-1}\otimes P_\Omega. \tag{4.11}$$

(2) *Let $1<l<2$. Suppose I_λ or II_λ. Then for all $\{\alpha_1,\ldots,\alpha_N\}$,* (4.11) *holds.*

(3) *Let $l=1$. Suppose $\mathrm{I}_\lambda^\alpha(\epsilon)$ or $\mathrm{II}_\lambda^\alpha(\epsilon)$. Then* (4.11) *holds.*

(4) *Let $l<1$. Suppose I_λ or II_λ. Then for all $\{\alpha_1,\ldots,\alpha_N\}$,* (4.11) *holds.*

Proof: By an abstract theorem in [Ref. 8 p. 2654, (i),(ii),(iii)] it is enough to prove that

(1) $D(V_\kappa)\supset D(H_{\mathrm{eff}})$ and $V_\kappa(H_{\mathrm{eff}}-z)^{-1}$ is a bounded operator for sufficiently large $-z$ with $\lim_{z\to-\infty}\Vert V_\kappa(H_{\mathrm{eff}}-z)^{-1}\Vert=0$ uniformly in κ,

(2) $V_\kappa(H_{\mathrm{eff}}-z)^{-1}$ is strongly continuous in κ and $s-\lim_{\kappa\to\infty}V_\kappa(H_{\mathrm{eff}}-z)^{-1}=V_{\mathrm{eff}}(H_{\mathrm{eff}}-z)^{-1}$.

By the definition of V_{eff} and Hypothesis **V**, we have

$$\Vert V_{\mathrm{eff}}f\Vert\leq a'\left\Vert\sum_{j=1}^N\frac{p_j^2}{2m_j}f\right\Vert+b'\Vert f\Vert$$

with some positive a' and b'. Together with (4.9) we get

$$\|V_\kappa f\| \leqslant a''\|H_{\mathrm{eff}} f\| + b''\|f\|$$

with some positive a'' and b''. Moreover

$$\|V_\kappa (H_{\mathrm{eff}} - z)^{-1} f\| \leqslant a''\|H_{\mathrm{eff}}(H_{\mathrm{eff}} - z)^{-1} f\| + b''\|(H_{\mathrm{eff}} - z)^{-1} f\|.$$

Hence $V_\kappa (H_{\mathrm{eff}} - z)^{-1} f \to 0$ as $z \to -\infty$. Then (1) follows. Since $\mathcal{U}_\kappa$ is continuous in κ and $s - \lim_{\kappa\to\infty} \mathcal{U}_k = \mathcal{U}_\infty$, we have

$$\begin{aligned}
\|(V_\kappa - V_{\kappa'})f\| &\leqslant \|\mathcal{U}_\kappa^{-1} V \mathcal{U}_k f - \mathcal{U}_\kappa^{-1} V \mathcal{U}_{\kappa'} f\| + \|\mathcal{U}_\kappa^{-1} V \mathcal{U}_{\kappa'} f - \mathcal{U}_{\kappa'}^{-1} V \mathcal{U}_{\kappa'} f\| \\
&\leqslant \|V(\mathcal{U}_\kappa - \mathcal{U}_{\kappa'})f\| + \|(\mathcal{U}_\kappa^{-1} - \mathcal{U}_{\kappa'}^{-1}) V \mathcal{U}_{\kappa'} f\| \\
&\leqslant a \left\| (\mathcal{U}_\kappa - \mathcal{U}_{\kappa'}) \sum_{j=1}^{N} \frac{p_j^2}{2m_j} f \right\| + b\|(\mathcal{U}_\kappa - \mathcal{U}_{\kappa'})f\| + \|(\mathcal{U}_\kappa^{-1} - \mathcal{U}_{\kappa'}^{-1}) V \mathcal{U}_{\kappa'} f\|.
\end{aligned}$$

Here in the third inequality we use that $\mathcal{U}_k$ and $p_j, j = 1,...,N$ are commutative. Then the first statement of (2) follows. The second statement is also proven similarly. □

Proof of Theorems 4.9–4.12: Suppose $l = 2$. Then $\mathcal{U}_\kappa = \mathcal{U}$ is independent of κ. We have by (4.8)

$$(H_\epsilon^{\mathrm{ren}}(\kappa) - z)^{-1} = \mathcal{U}(H_{\mathrm{eff}}(\kappa) - z)^{-1} \mathcal{U}^{-1}.$$

Taking $\kappa \to \infty$, we have

$$\lim_{\kappa\to\infty} (H_\epsilon^{\mathrm{ren}}(\kappa) - z)^{-1} = \mathcal{U}\{(H_{\mathrm{eff}} - z)^{-1} \otimes P_\Omega\}\mathcal{U}^{-1} = \theta\{(H_{\mathrm{eff}} - z)^{-1} \otimes U(\mathbb{W}) P_\Omega U(\mathbb{W})^{-1}\}\theta^{-1}.$$

Since $U(\mathbb{W}) P_\Omega U(\mathbb{W})^{-1} = P_\epsilon$, Theorem 4.9 follows. Next suppose $l = 1$,

$$(H_\epsilon^{\mathrm{ren}}(\kappa) - z)^{-1} = \mathcal{U}_\kappa (H_{\mathrm{eff}}(\kappa) - z)^{-1} \mathcal{U}_\kappa^{-1}.$$

Since

$$s - \lim_{\kappa\to\infty} \mathcal{U}_\kappa = U(\mathbb{W}),$$

taking $k \to \infty$, we have

$$\lim_{\kappa\to\infty} (H_\epsilon^{\mathrm{ren}}(\kappa) - z)^{-1} = U(\mathbb{W})\{(H_{\mathrm{eff}} - z)^{-1} \otimes P_\Omega\} U(\mathbb{W})^{-1}.$$

Hence Theorem 4.11 follows. Theorems 4.10 and 4.12 are proven similarly. □

D. Examples

In this section we assume that $|V_{\mathrm{eff}}| \in L^1_{\mathrm{loc}}(\mathbb{R}^{dN})$. A typical example is for $N = 1$ and $\epsilon = 1$. Put $A_1 = A$, $m_1 = m$, $p_1 = p$, $\alpha_1 = \alpha$.

Corollary 4.14: Let $N = 1$ and $\epsilon = 1$. Suppose I_λ *or* II_λ. *Then for all $\alpha \in \mathbb{R}$ and $z \in \mathbb{C}\backslash\mathbb{R}$:* ($l = 2$)

$$s - \lim_{\kappa\to\infty} \left(H(\kappa) + \kappa^2 \frac{1}{2(m + \delta m)} \frac{\delta m}{m} p^2 - g(m/\kappa^2) - z \right)^{-1} = \theta \left\{ \left(\frac{1}{2m} p^2 + V_{\mathrm{eff}} - z \right)^{-1} \otimes P_1 \right\} \theta^{-1};$$

$(1<l<2)$

$$s-\lim_{\kappa\to\infty}\left(H(\kappa)+\kappa^{2l-2}\frac{1}{2(m+\delta m)}\frac{\delta m}{m}p^2-g(m/\kappa^2)-z\right)^{-1}=\left(\frac{1}{2m}p^2+V-z\right)^{-1}\otimes P_1;$$

$(l=1)$

$$s-\lim_{\kappa\to\infty}(H(\kappa)-g(m/\kappa^2)-z)^{-1}=\left(\frac{1}{2(m+\delta m)}p^2+V-z\right)^{-1}\otimes P_1;$$

$(l<1)$

$$s-\lim_{\kappa\to\infty}(H(\kappa)-g(m/\kappa^2)-z)^{-1}=\left(\frac{1}{2m}p^2+V-z\right)\otimes P_1.$$

By virtue of Corollary 4.14 we see that in the case of $l=2$ the Welton Hamiltonian does appear and in the case of $l=1$ the Hamiltonian with observed mass does. (See Table II.)

Corollary 4.15: Suppose I_λ *and* $l=2$. *Moreover we assume that* $\alpha_1=\cdots=\alpha_N:=\alpha$ *and* $m_1=\cdots=m_N:=m$. *Then*

$$V_{\mathrm{eff}}=(2\pi C)^{-d/2}\int_{\mathbb{R}^d}V_{\tilde{T}^{-1}}(y,(\tilde{T}x)_2,\ldots,(\tilde{T}x)_N))e^{-|(\tilde{T}x)_1-y|^2/2C}\mathrm{d}y,$$

where

$$C:=\frac{N\alpha^2}{2}\frac{d-1}{d}\left\|\frac{Q}{\omega^{3/2}}\right\|^2,$$

Proof: Since the correlation matrix is given by

$$\Delta=\frac{\alpha^2}{2}\left\|\frac{Q}{\omega^{3/2}}\right\|^2K\begin{pmatrix}1&\cdots&1\\ \vdots&\ddots&\vdots\\ 1&\cdots&1\end{pmatrix},$$

where

$$Q=\sqrt{\omega}D^{-1}\begin{pmatrix}\hat{\lambda}\\ \vdots\\ \hat{\lambda}\end{pmatrix},$$

we have Rank $\Delta=1$. Thus the corollary follows. □

Corollary 4.16: Suppose II_λ *and* $l=2$. *Then*

$$V_{\mathrm{eff}}=(2\pi C)^{-d/2}\int_{\mathbb{R}^{dN}}V(y)e^{-|x-y|^2/2C}\mathrm{d}y,$$

where

$$C:=\Pi_{j=1}^N\left(\frac{d-1}{2d}\frac{\alpha_j^2}{m_j}\int_{\mathbb{R}^d}\frac{|\hat{\lambda}_j(k)|^2}{\omega(k)^2(m_j-\epsilon\delta C_j)}\mathrm{d}k\right),$$

TABLE II. Effective Hamiltonians for $N=1$ and $\epsilon=1$.

	$H^{\mathrm{ren}}(\kappa)+g(m/\kappa^2)$	H_{eff}
$l=2$	$H(\kappa)+\kappa^2\frac{1}{2(m+\delta m)}\frac{\delta m}{m}p^2$	$\frac{1}{2m}p^2+V_{\mathrm{eff}}$
$1<l<2$	$H(\kappa)+\kappa^{2l-2}\frac{1}{2(m+\delta m)}\frac{\delta m}{m}p^2$	$\frac{1}{2m}p^2+V$
$l=1$	$H(\kappa)$	$\frac{1}{2(m+\delta m)}p^2+V$
$l<1$	$H(\kappa)$	$\frac{1}{2m}p^2+V$

Proof: Since the correlation matrix is given by

$$\Delta=\mathrm{diag}\left\{\frac{1}{2}\alpha_1^2K\left\|\frac{Q_1}{\omega^{3/2}}\right\|^2,\ldots,\frac{1}{2}\alpha_N^2K\left\|\frac{Q_N}{\omega^{3/2}}\right\|^2\right\},$$

where

$$Q_j=\frac{\sqrt{\omega}\hat{\lambda}_j}{D_{jj}},$$

the corollary follows. □

V. CONCLUDING REMARKS (*g*-FACTOR SHIFT)

For simplicity we set $\epsilon=1$, $N=1$, and $d=3$. Put $A_1=A$, $m_1=m$, $p_1=p$, $\alpha_1=\alpha$. We suppose that spin 1/2 is included in the particle and an external vector potential $a(x)$ is imposed. Thus the Hamiltonian is read

$$H_{\mathrm{spin}}:=\frac{1}{2m}\{\sigma\cdot(p-a(x)-\alpha A)\}^2+V+H_f$$

acting on the Hilbert space

$$\mathbb{C}^2\otimes L^2(\mathbb{R}^3)\otimes\mathcal{F}.$$

Here $\sigma=(\sigma_1,\sigma_2,\sigma_3)$ denotes the Pauli matrices:

$$\sigma_1:=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2:=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_3:=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

We have

$$H_{\mathrm{spin}}=\frac{1}{2m}(p-\alpha A)^2+H_f+V-\frac{g}{4m}\sigma\cdot\ \mathrm{curl}\,a+H_{\mathrm{I}},$$

where

$$g=2$$

and

$$H_{\mathrm{I}} := -\frac{1}{2m}\{(p-\alpha A)\cdot a - a\cdot(p-\alpha A)\} + \frac{1}{2m}a^2 - \frac{\alpha}{2m}\sigma\cdot\mathrm{curl}\,A,$$

and

$$\mathrm{curl}\,A := \frac{-i}{\sqrt{2}}\sum_{r=1}^{2}\{a^{\dagger r}((k\times e^r)\,\tilde{\lambda}) + a^r((-k\times e^r)\hat{\lambda})\}.$$

For simplicity we neglect H_{I}. Then our Hamiltonian is defined by

$$H = \frac{1}{2m}(p-\alpha A)^2 + H_f + V - \frac{g}{4m}\sigma\cdot\mathrm{curl}\,a.$$

Let $l=1$. Then the scaled Hamiltonian is given by

$$H(\kappa) := \frac{1}{2m}(p-\kappa\alpha A)^2 + \kappa^2 H_f + V - \frac{g}{4m}\sigma\cdot\mathrm{curl}\,a.$$

Corollary 5.1: Suppose that a is sufficiently smooth and that a is infinitesimally small with respect to p^2. Then $H(\kappa)$ is self-adjoint on $\mathcal{D}$ and bounded from below. Furthermore for $z \in \mathbb{C}\backslash\mathbb{R}$,

$$s-\lim_{\kappa\to\infty}(H(\kappa) - g(m/\kappa^2) - z)^{-1} = (H_{\mathrm{eff}} - z)^{-1}\otimes P_1.$$

Here

$$H_{\mathrm{eff}} = \frac{1}{2(m+\delta m)}p^2 - \frac{g_{\mathrm{eff}}}{4(m+\delta m)}\sigma\cdot\mathrm{curl}\,a + V,$$

and

$$g_{\mathrm{eff}} := \frac{m+\delta m}{m}g > 2.$$

Proof: The self-adjointness follows from Proposition 1.1. Since σ_j and $\mathcal{U}_k$ are commutative, by Theorem 4.11, we have

$$s-\lim_{\kappa\to\infty}(H(\kappa) - g(m/\kappa^2) - z)^{-1} = \left(\frac{1}{2(m+\delta m)}p^2 - \frac{g}{4m}\sigma\cdot\mathrm{curl}\,a + V - z\right)^{-1}\otimes P_1.$$

Hence the corollary follows. □

VI. PROOF OF PROPOSITION 3.2

A. Construction of canonical transformations

We recall

$$D_{ij} := m_{ij} - \epsilon\alpha_i\alpha_j\frac{K}{2}S_{d-1}\left(\lim_{\eta\downarrow 0}\int_{|\omega(k)^2-x|>\eta, x>0}\frac{\varphi_{ij}(x)}{\omega(k)^2-x}\mathrm{d}x - 2\pi i\varphi_{ij}(\omega(k)^2)\right).$$

Lemma 6.1: Suppose I_λ *or* II_λ. *Then* $\|D_{ij}\|_\infty < \infty$.

Proof: Set

$$\tilde{\varphi}_{ij}(s) := \lim_{\eta \downarrow 0} \int_{|s-x|>\eta, x>0} \frac{\varphi_{ij}(x)}{s-x} \mathrm{d}x.$$

Then by (A.3) and Ref. 20 we see that for $s,t \geqslant 0$,

$$|\tilde{\varphi}_{ij}(s) - \tilde{\varphi}_{ij}(t)| \leqslant C_{ij}|s-t|.$$

Hence $\tilde{\varphi}_{ij}$ is continuous. Since

$$\lim_{|s|\to\infty} \tilde{\varphi}_{ij}(s) = 0,$$

it follows that $\|D_{ij}\|_\infty < \infty$. □

Lemma 6.2: Suppose I_λ. *Then there exists*

$$Q = \begin{pmatrix} Q_1 \\ \vdots \\ Q_N \end{pmatrix} \in \oplus^N L^2(\mathbb{R}^d)$$

such that

$$(1)\ DQ = \sqrt{\omega}\begin{pmatrix} \hat{\lambda}_1 \\ \vdots \\ \hat{\lambda}_N \end{pmatrix},\ (2)\ \|\omega^{(d-1)/2} Q_j\|_\infty < \infty,\ and\ \|\omega^{(d-3)/2} Q_j\|_\infty < \infty,\ (3)\ Q_j/\omega^{3/2} \in L^2(\mathbb{R}^d).$$

Proof: We set

$$D(k) := M - \epsilon K g(k) A(\alpha_1, \ldots, \alpha_N),$$

where

$$M := \mathrm{diag}\{m_1, \ldots, m_N\},$$

$$A(\alpha_1, \ldots, \alpha_N) := \begin{pmatrix} \alpha_1\alpha_1 & \cdots & \alpha_1\alpha_N \\ \vdots & \ddots & \vdots \\ \alpha_N\alpha_1 & \cdots & \alpha_N\alpha_N \end{pmatrix},$$

and

$$g(k) := \lim_{\eta \downarrow 0} \int_{\mathbb{R}^d} \frac{\omega(k')|\hat{\lambda}(k')|^2}{\omega(k)^2 - \omega(k')^2 + i\eta} \mathrm{d}k'.$$

A is a positive definite matrix and we denote its eigenvalues by

$$\{a_1, \ldots, a_M, 0, \ldots, 0\}, \quad a_j > 0, \quad j = 1, \ldots, M, \tag{6.1}$$

with some $M \leqslant N$. A_M denotes the M-dimensional space spanned by eigenvectors with eigenvalues $a_1, \ldots, a_M$, and its orthogonal complement by $A_M^\perp$. Set $m = \min\{m_1, \ldots, m_N\}$, $a = \min\{a_1, \ldots, a_M\}$. For $z \in A_M^\perp$ we have

$$(z, D(k)z) = (z, Mz) \geqslant m|z|^2.$$

For $z \in A_M$, we have

$$|(z, D(k)z)| \geqslant \epsilon K |\Im g(k)||(z, Az)| \geqslant \epsilon a K |\Im g(k)||z|^2.$$

Hence for $\epsilon_0<|k|<\epsilon_1$ with $0<\epsilon_0$ and $0<\epsilon_1$ there exists $d'=d'(\epsilon_0,\epsilon_1)>0$ such that

$$|(z,D(k)z)|\geqslant d'|z|^2.$$

For $k=0$ it follows that

$$(z,D(0)z)=(z,Mz)-\epsilon Kg(0)(z,Az)\geqslant m|z|^2, \tag{6.2}$$

and as $|k|\to\infty$,

$$(z,D(k)z)\to(z,Mz)\geqslant m|z|^2. \tag{6.3}$$

Combining (6.2) with (6.3) we see that for $|k|\leqslant\epsilon_0$ or $|k|\geqslant\epsilon_1$ with some sufficiently small ϵ_0 and sufficiently large ϵ_1 there exists d'' such that

$$|(z,D(k)z)|>d''|z|^2.$$

Hence for all $k\in\mathbb{R}^d$,

$$|(z,D(k)z)|>\min\{d',d''\}|z|^2.$$

In particular the inverse D^{-1} of D exists as a bounded operator of $\oplus^N L^2(\mathbb{R}^d)$. Putting

$$Q:=\sqrt{\omega}D^{-1}\begin{pmatrix}\hat{\lambda}_1\\ \vdots\\ \hat{\lambda}_N\end{pmatrix},$$

we see that Q satisfies (1). It is seen that

$$\|\omega^n Q_j\|_\infty\leqslant\|D^{-1}\|\|\omega^{n+(1/2)}\hat{\lambda}_j\|_\infty.$$

From $\|\hat{\lambda}_j\omega^{(d-2)/2}\|_\infty<\infty$ and $\|\hat{\lambda}_j\omega^{d/2}\|_\infty<\infty$ [see (A.4)], (2) follows. Moreover from

$$\|\omega^n Q_j\|_{L^2(\mathbb{R}^d)}\leqslant\|D^{-1}\|\|\omega^{n+(1/2)}\hat{\lambda}_j\|_{L^2(\mathbb{R}^d)},$$

(3) follows, since $\hat{\lambda}/\omega\in L^2(\mathbb{R}^d)$ [see (A.2)]. Thus the lemma follows. □

Lemma 6.3: Suppose II_λ. *Then there exists Q such that (1)–(3) in Lemma 6.2 are satisfied.*

Proof: Note that

$$D_{jj}(k)\neq 0,\quad \text{for } k\in\{k\in\mathbb{R}^d|\hat{\lambda}_j(k)\neq 0\}.$$

Hence we can define $Q=(Q_1,\ldots,Q_N)$ by

$$Q_j(k):=\begin{cases}\dfrac{\sqrt{\omega(k)}\hat{\lambda}_j(k)}{D_{jj}(k)}, & k\in\{k\in\mathbb{R}^d|\hat{\lambda}_j(k)\neq 0\}\\ 0, & k\notin\mathrm{supp}\hat{\lambda}_j.\end{cases}$$

Since $|\hat{\lambda}_j(k)/D_{jj}(k)|\to 0$ as k converges to the boundary of $\mathrm{supp}\hat{\lambda}_j$, $Q(k)$ is well defined for all $k\in\mathbb{R}^d$, and we can easily check that Q satisfies (1)–(3). Thus the lemma follows. □

Let

$$R_j:=\sqrt{\omega}D(0)^{-1}\begin{pmatrix}\hat{\lambda}_1\\ \vdots\\ \hat{\lambda}_N\end{pmatrix}.$$

Define

$$Gf(k) := \lim_{\eta \downarrow 0} \int_{\mathbb{R}^d} \frac{f(k')}{(\omega(k)^2 - \omega(k')^2 + i\eta)(\omega(k)\omega(k'))^{(d-2)/2}} \mathrm{d}k'.$$

G is a skew symmetric bounded operator of $L^2(\mathbb{R}^{dN})$. Let

$$T_{\mu\nu} f := \delta_{\mu\nu} f + \epsilon \sum_{j=1}^{N} \alpha_j^2 Q_j \omega^{(d-2)/2} G \omega^{(d-2)/2} d_{\mu\nu} \sqrt{\omega} \hat{\lambda}_j f.$$

Lemma 6.4: Suppose I_λ *or* II_λ. *Then the following algebraic relations hold:*

(1) $\Sigma_{\beta=1}^{d} T^*_{\mu\beta} d_{\beta\nu} (1/\omega^2) Q_j = d_{\mu\nu} R_j / \omega^{3/2}$.
(2) $[\omega^2, T^*_{\mu\nu}] f = -\Sigma_{j=1}^{N} \alpha_j^2 (Q_j, f)_{L^2(\mathbb{R}^d)} d_{\mu\nu} \sqrt{\omega} \hat{\lambda}_j$.
(3) $T_{\mu\nu} \sqrt{\omega} \hat{\lambda}_j = \delta_{\mu\nu} m_j Q_j$.
(4) $T^*_{\mu\nu} d_{\nu\beta} T_{\beta\gamma} = d_{\mu\gamma}$.
(5) $e^r_\mu T_{\mu\nu} d_{\nu\beta} T_{\beta\gamma} e^s_\gamma = \delta_{rs}$.

Proof: By (1) of Lemmas 6.2 and 6.3, it is proven. See (Ref. 13, Lemma 2.6) for details. □

We define the bounded operator $W_\pm = (W^{rs}_\pm)_{1 \leqslant r,s \leqslant d-1} : W \to W$ by

$$W^{rs}_+ f := \tfrac{1}{2} e^r_\mu (\omega^{-1/2} T^*_{\mu\nu} \omega^{1/2} + \omega^{1/2} T^*_{\mu\nu} \omega^{-1/2}) e^s_\nu f,$$

$$W^{rs}_- f := \tfrac{1}{2} e^r_\mu (\omega^{-1/2} T^*_{\mu\nu} \omega^{1/2} - \omega^{1/2} T^*_{\mu\nu} \omega^{-1/2}) \widetilde{e^s_\nu f}.$$

It is checked by (A.4), Lemmas 6.2 and 6.3 that

$$\|W^{rs}_\pm f\| \leqslant c \|f\|,$$

where

$$c = 1 + \tfrac{1}{2} \sum_{j=1}^{d} (\|\omega^{(d-3)/2} Q_j\|_\infty \|\omega^{d/2} \hat{\lambda}_j\|_\infty + \|\omega^{(d-1)/2} Q_j\|_\infty \|\omega^{(d-2)/2} \hat{\lambda}_j\|_\infty) \|G\|.$$

We define

$$\mathbb{W} := \begin{pmatrix} W_+ & \overline{W_-} \\ W_- & \overline{W_+} \end{pmatrix}.$$

Lemma 6.5: Suppose I_λ or II_λ. *Then* $\mathbb{W} \in \Sigma_{\mathrm{B}}$. *Moreover* $\mathbb{W}$ *is invariant under the scaling* $\omega \to \kappa^2 \omega$, $\alpha_j \to \kappa^l \alpha_j$, and $\epsilon \to \kappa^{2l-2} \epsilon$.

Proof: It follows from Lemmas 6.4 (4) and (5). □

We define

$$\begin{pmatrix} b(f) \\ b^\dagger(f) \end{pmatrix} := {}^T\mathbb{W} \begin{pmatrix} a(f) \\ a^\dagger(f) \end{pmatrix}.$$

Let

$$L(q) := \sum_{j=1}^{N} \sum_{\mu=1}^{d} q_{j\mu} L^\mu_j \in W$$

with

$$L_j^\mu := \frac{\alpha_j}{\sqrt{2}} \overset{d-1}{\underset{r=1}{\oplus}} \frac{e_\mu^r Q_j}{\omega^{3/2}}.$$

L_j^μ is well defined by Lemmas 6.2 and 6.3. We define

$$\begin{pmatrix} B_q(f) \\ B_q^\dagger(f) \end{pmatrix} := \begin{pmatrix} b(f) \\ b^\dagger(f) \end{pmatrix} + \begin{pmatrix} (L(q),f)_W \\ \overline{(L(q),f)_W} \end{pmatrix}.$$

By (2.2) we have

$$\begin{pmatrix} a(f) \\ a^\dagger(f) \end{pmatrix} = {}^T(\mathbb{W}^{-1}) \begin{pmatrix} B_q(f) \\ B_q^\dagger(f) \end{pmatrix} - \begin{pmatrix} (W_+ L(q) - \overline{W_- \overline{L(q)}}, f)_W \\ \overline{(W_+ L(q) - \overline{W_- \overline{L(q)}}, f)_W} \end{pmatrix}.$$

By Proposition 2.2 there exists a unitary operator $U(\mathbb{W})$ such that

$$U(\mathbb{W})^{-1} b^\sharp(f) U(\mathbb{W}) = a^\sharp(f).$$

Recall

$$\theta(q) := \exp\left(\sum_{j=1}^N \sum_{r=1}^{d-1} \sum_{\mu=1}^d \frac{\alpha_j q_{j\mu}}{\sqrt{2}} \left\{ a^r\left(\overline{\frac{e_\mu^r R_j}{\omega^{3/2}}} \right) - a^{\dagger r}\left(\frac{e_\mu^r R_j}{\omega^{3/2}} \right) \right\} \right)$$

and

$$\mathcal{U}(q) := \theta(q) U(\mathbb{W}).$$

A proof of Proposition 3.2 (1): By Lemma 6.4 (1), we have

$$W_- L(q) - \overline{W_+ L(q)} = -\sum_{j=1}^N \sum_{\mu=1}^d q_{j\mu} \frac{\alpha_j}{\sqrt{2}} \oplus_{r=1}^{d-1} \frac{e_\mu^r R_j}{\omega^{3/2}}.$$

Hence $\theta(q, \mathbb{W}, L) = \theta(q)$ follows. □

A proof of Proposition 3.2 (2): It is seen that by Lemmas 6.4 (2) and (3), for $f \in W$,

$$[H_\epsilon^0(q), B_q(f)] = -B_q((\overset{d-1}{\oplus} \omega) f),$$

$$[H_\epsilon^0(q), B_q^\dagger(f)] = B_q^\dagger((\overset{d-1}{\oplus} \omega) f)$$

on some dense domain. Using these commutation relations we can prove that

$$e^{itH_\epsilon^0(q)} B^\dagger(f) e^{-itH_\epsilon^0(q)} = B^\dagger(e^{it\oplus^{d-1}\omega} f), \tag{6.4}$$

$$e^{itH_\epsilon^0(q)} B(f) e^{-itH_\epsilon^0(q)} = -B(e^{it\oplus^{d-1}\omega} f). \tag{6.5}$$

Then we have

$$B(f) e^{itH_\epsilon^0(q)} \mathcal{U}(q)\Omega = 0,$$

for all $f \in W$. It implies that $e^{itH_\epsilon^0(q)} \mathcal{U}(q)\Omega = \text{constant} \times \mathcal{U}(q)\Omega$. Since $e^{itH_\epsilon^0(q)}$ is one parameter unitary group,

$$e^{itH_\epsilon^0(q)}\mathcal{U}(q)\Omega = e^{itE(q)}\mathcal{U}(q)\Omega \tag{6.6}$$

with some constant $E(q)$. Hence by (6.4),(6.5), and (6.6) we obtain that

$$\mathcal{U}(q)^{-1}e^{itH_\epsilon^0(q)}\mathcal{U}(q)a^\dagger(f_1)\cdots a^\dagger(f_n)\Omega = e^{it(H_f-E(q))}a^\dagger(f_1)\cdots a^\dagger(f_n)\Omega.$$

Then

$$\mathcal{U}(q)^{-1}e^{itH_\epsilon^0(q)}\mathcal{U}(q) = e^{it(H_f-E(q))}.$$

Since $H_\epsilon^0(q)$ is self-adjoint on $D(H_f)$, we see that $\mathcal{U}(q)$ maps $D(H_f)$ onto itself and $\mathcal{U}(q)^{-1}H_\epsilon^0(q)\mathcal{U}(q) = H_f - E(q)$ holds by Stone's theorem. □

B. Analytic continuation

Lemma 6.6: Suppose I_λ. *Let* $f \in L^2(\mathbb{R}^d)$. *Then* $Q_j f$ *can be strongly analytically continued to a neighborhood* $\mathcal{O}$ of $\mathbb{R}$ *in each* α_i's.

Proof: We fix j. We can find a neighborhood $\mathcal{O}$ of $\mathbb{R}$ such that, for $z_j \in \mathcal{O}$,

$$D(z_j) = D(z_j,k) := M - \epsilon K g(k) A(\alpha_1,\ldots,z_j,\ldots,\alpha_N)$$

is a strongly analytic bounded operator on $\oplus^N L^2(\mathbb{R}^d)$, and

$$\inf_{k\in\mathbb{R}^d} |(w, D(z_j,k)w)| > \delta |w|^2, \quad \text{for } w \in \mathbb{C}^N,$$

with some positive constant δ. Hence $D(z_j)^{-1}$ exists as a bounded operator for $z_j \in \mathcal{O}$ and

$$\|D(z_j)^{-1}\| \leqslant \frac{1}{\delta}.$$

We can take a sufficiently small neighborhood $\mathcal{O}(z_j) \subset \mathcal{O}$ of z_j such that

$$\inf_{z_j \in \mathcal{O}(z_j)} \|D(z_j)^{-1}\| < \infty. \tag{6.7}$$

Since

$$\frac{D(z_j)^{-1} - D(z_j')^{-1}}{z_j - z_j'} = D(z_j)^{-1}\left(\frac{D(z_j') - D(z_j)}{z_j - z_j'}\right)D(z_j')^{-1},$$

by (6.7) we conclude that $D(z_j)^{-1}$ is strongly differentiable in $\mathcal{O}$. Thus $D(z_j)^{-1}$ is a strongly analytic bounded operator. Hence the lemma follows. □

Lemma 6.7: Suppose II_λ. *Let* $f \in L^2(\mathbb{R}^d)$. *Then* $Q_j f$ *can be strongly analytically continued to a neighborhood* $\mathcal{O}$ *of* $\mathbb{R}$ *in each* α_i's.

Proof: Note

$$Q_j(k) = \frac{1}{\epsilon K \alpha_j^2}\,\frac{1}{\dfrac{m_j}{\epsilon K \alpha_j^2} - g_j(k)}.$$

Here

$$g_j(k) := \lim_{\eta \downarrow 0} \int_{\mathbb{R}^d} \frac{\omega(k')|\hat{\lambda}_j(k')|^2}{\omega(k)^2 - \omega(k')^2 + i\eta}\,dk'.$$

It is seen that

(1) $g_j(0)<0$, (2) $\Im g_j(k)<0$ for $k\in \mathrm{supp}\hat{\lambda}_j$, (3) $g_j(k)=0$ for $k\notin \mathrm{supp}\hat{\lambda}_j$,
(4) g_j is continuous.

Hence, for arbitrary $\delta>0$,

$$\mathrm{dist}(\mathrm{Ran} g_j,[\delta,\infty))>M$$

with some positive constant M. Thus $Q_j f$ can be analytically continued to

$$\mathcal{O}' := \{a+ib, a\in\mathbb{R}, b\in\mathbb{R} \,|\, |a|>\delta, |b|<M\}$$

in $z_j := m_j/(\epsilon K \alpha_j^2)$. Thus $Q_j f$ can be strongly analytically continued in a neighborhood $\mathcal{O}$ of $\mathbb{R}$ in each α_j. □

A proof of Lemma 3.2 (3): Note that

$$E(q)=\frac{(\Omega, H_\epsilon(q)\mathcal{U}(q)\Omega)}{(\Omega,\mathcal{U}(q)\Omega)}. \tag{6.8}$$

It is proven in Refs. 11 and 13 that by Lemma 2.5 $E(q)$ can be expressed as

$$E(q)=\sum_{j=1}^{N}\frac{1}{2m_j}(q_j+\tilde{q}_j)^2+\Delta,$$

where

$$\tilde{q}_{j\nu} := \sum_{i=1}^{N}\sum_{r=1}^{d-1}\sum_{s=1}^{d-1}\sum_{\mu=1}^{d}\frac{1}{2}q_{\mu i}\alpha_i\alpha_j(e_\mu^r R_j/\omega^{3/2}, (1+W_-W_+^{-1})_{rs}e_\nu^s\hat{\lambda}_i),$$

$$\Delta=\sum_{j=1}^{N}\sum_{r=1}^{d-1}\sum_{\mu=1}^{d}\frac{\alpha_j^2}{4m_j}(e_\mu^r\hat{\lambda}_j,(1-W_-W_+^{-1})_{rs}e_\mu^s\hat{\lambda}_j).$$

By Lemmas 6.6 and 6.7 we see that $T_{\mu\nu}$ can be strongly analytically continued to some $\mathcal{O}\subset\mathbb{R}$ in each α_j's. Moreover $W_\pm$ also can be done. By the identities derived from the symplectic structure,

$$W_+^* W_+ - \overline{W_-^* W_-} = I,$$

$$W_+ W_+^* - \overline{W_- W_-^*} = I,$$

taking a sufficiently small neighborhood $\mathcal{O}'\subset\mathcal{O}$, we see that W_+^{-1} can be extended to $\alpha_j\in\mathcal{O}'$ as a bounded operator $W_+^{-1}(\alpha_j)$. Moreover it is seen that $\sup_{\alpha_j\in\mathcal{O}(\alpha_j)}\|W_+^{-1}(\alpha_j)\|<\infty$ for sufficiently small neighborhood $\mathcal{O}(\alpha_j)$ of α_j. Thus $W_+^{-1}(\alpha_j)$ is strongly differentiable in α_j, and hence strongly analytic on $\mathcal{O}'$. □

VII. PROOF OF LEMMA 3.3

A proof of Lemma 3.3 (1): We take a momentum lattice approximation. The momentum lattice approximated Hamiltonian (7.1) can be identified with a harmonic oscillator. Then its ground state energy can be explicitly obtained. By a limiting argument we get $E(q)$. First we assume that $|\alpha_j|$'s are sufficiently small and replace $\omega(k)$ with

$$\omega_\delta(k) := \omega(k)+\delta, \quad \delta>0.$$

Let $1/a>0$ be the width of the momentum lattice, and some $L>0$ be fixed. For

$$l=(l^1,\ldots,l^d)\in(2\pi\mathbb{Z}/a)^d$$

we define

$$\Gamma(l):=\left[l^1,l^1+\frac{2\pi}{a}\right)\times\cdots\times\left[l^d,l^d+\frac{2\pi}{a}\right).$$

Let $|l|:=\max_r|l^r|$. Suppose

$$|l|\leqslant 2\pi L.$$

Set

$$D:=(2[aL]+1)^d,$$

where $[z]$ denotes the integer part of z. We named the lattice points of the rectangle with width $2[aL]$ centered at the origin as

$$l_1,l_2,\ldots,l_D.$$

We set

$$\vec{q}:=\frac{1}{\sqrt{2}}\frac{1}{\sqrt{\omega_\delta(l)}}\{a^{\dagger r}(\chi_{\Gamma(l)})+a^r(\chi_{\Gamma(l)})\}_{1\leqslant r\leqslant d-1,|l|\leqslant 2\pi L},$$

$$\vec{p}:=\frac{i}{\sqrt{2}}\sqrt{\omega_\delta(l)}\{a^{\dagger r}(\chi_{\Gamma(l)})-a^r(\chi_{\Gamma(l)})\}_{1\leqslant r\leqslant d-1,|l|\leqslant 2\pi L},$$

where χ_I denotes the characteristic function of $I\subset\mathbb{R}^d$. Define

$$H_\epsilon(q,\delta,a,L):=\sum_{j=1}^N\left\{\frac{1}{2m_j}q_j^2-\frac{\alpha_j}{m_j}\sum_{\mu=1}^d(q_{j\mu}v_\mu^j,\vec{q})+\epsilon\sum_{\mu=1}^d\frac{\alpha_j^2}{2m_j}(\vec{q},v_\mu^j)(v_\mu^j,\vec{q})\right\}$$
$$+\frac{1}{2}\{(\vec{p},\vec{p})+(\vec{q},A_0\vec{q})\}-\frac{1}{2}\operatorname{tr}\sqrt{A_0}. \tag{7.1}$$

Here A_0 is the $(d-1)D\times(d-1)D$ symmetric matrix defined by

$$A_0:=(1_{(d-1)}\delta_{ll'}\omega_\delta(l)^2)_{|l|,|l'|\leqslant 2\pi L}=\begin{pmatrix}\omega_\delta(l_1)1_{(d-1)} & & & \\ & \omega_\delta(l_2)1_{(d-1)} & & \\ \vdots & \cdots & \ddots & \vdots \\ & & & \omega_\delta(l_D)1_{(d-1)}\end{pmatrix}, \tag{7.2}$$

and

$$v_\mu := \begin{pmatrix} \sqrt{\omega_\delta(l_1)}\hat{\lambda}(l_1)e^1_\mu(l_1) \\ \vdots \\ \sqrt{\omega_\delta(l_1)}\hat{\lambda}(l_1)e^{(d-1)}_\mu(l_1) \\ \vdots \\ \vdots \\ \sqrt{\omega_\delta(l_D)}\hat{\lambda}(l_D)e^1_\mu(l_D) \\ \vdots \\ \sqrt{\omega_\delta(l_D)}\hat{\lambda}(l_D)e^{(d-1)}_\mu(l_D) \end{pmatrix} \in \mathbb{R}^{(d-1)D}.$$

Here $1_{(d-1)}$ denotes the $(d-1)\times(d-1)$ identity matrix. It is seen that

$$(H_\epsilon(q,\delta,a,L)-z)^{-1} \to (H_\epsilon(q,\delta)-z)^{-1} \tag{7.3}$$

uniformly as $a\to\infty$ and then $L\to\infty$. Here $H_\epsilon(q,\delta)$ denotes $H^0_\epsilon(q)+\delta N$. We define the projection P by

$$P := \epsilon \sum_{j=1}^{N} \sum_{\mu=1}^{d} \frac{\alpha_j^2}{m_j} |v_\mu\rangle\langle v_\mu|.$$

Then

$$H_\epsilon(q,\delta,a,L) = \sum_{j=1}^{N} \left\{ \frac{1}{2m_j} q_j^2 - \frac{\alpha_j}{m_j} \sum_{\mu=1}^{d} (q_{j\mu} v_\mu, \vec{q}) \right\} + \frac{1}{2}(\vec{q}, P\vec{q}) + \frac{1}{2}(\vec{p},\vec{p}) + \frac{1}{2}(\vec{q}, A_0\vec{q}) - \frac{1}{2}\mathrm{tr}\sqrt{A_0}.$$

Set

$$A := A_0 + P.$$

Since $\omega_\delta(k) \geqslant \delta > 0$, the inverse of A_0 exists, and hence A also has the inverse, and it is symmetric. Then we have

$$= \sum_{j=1}^{N} \frac{1}{2m_j} q_j^2 - \sum_{j=1}^{N} \sum_{\mu=1}^{d} \frac{\alpha_j}{m_j} (AA^{-1} q_{j\mu} v_\mu, \vec{q}) + \frac{1}{2}(\vec{q}, A\vec{q}) + \frac{1}{2}(\vec{p},\vec{p}) - \frac{1}{2}\mathrm{tr}\sqrt{A_0}$$

$$= \sum_{j=1}^{N} \frac{1}{2m_j} q_j^2 + \frac{1}{2}((\vec{q}-\vec{f}), A(\vec{q}-\vec{f})) - \frac{1}{2}(\vec{f}, A\vec{f}) + \frac{1}{2}(\vec{p},\vec{p}) - \frac{1}{2}\mathrm{tr}\sqrt{A_0}.$$

Here we put

$$f := \sum_{j=1}^{N} \sum_{\mu=1}^{d} \frac{\alpha_j}{m_j} A^{-1} q_{j\mu} v_\mu.$$

By the commutation relation on $e^{is\vec{p}}$ and $e^{it\vec{q}}$:

$$e^{is\vec{p}_{rl_n}} e^{it\vec{q}_{r'l'_n}} = e^{its\delta_{rr'}\delta_{l_n l'_n}} e^{it\vec{q}_{r'l'_n}} e^{is\vec{p}_{rl_n}},$$

and the von Neumann uniqueness theorem, we can identify $\vec{p}$ and $\vec{q}$ with the momentum and position operators, respectively,

$$\vec{p}_{t,l_n} \cong -i\frac{\partial}{\partial x_{r,n}}, \quad \vec{q}_{r,l_n} \cong x_{r,n},$$

for $r=1,\ldots,d-1$ and $n=1,\ldots,D$. Hence we identify $H_\epsilon(q,\delta,a,L)$ as a harmonic oscillator in $L^2(\mathbb{R}^{(d-1)D})$. Generally for the harmonic oscillator

$$H_T := \tfrac{1}{2}(\vec{p},\vec{p}) + \tfrac{1}{2}(\vec{q},T\vec{q})$$

with non-negative symmetric matrix T, we have

$$\inf\sigma(H_T) = \operatorname{tr}\sqrt{T}.$$

Then it follows that

$$\begin{aligned} E(q) &= \inf\sigma(H_\epsilon(q,\delta,a,L)) \\ &= \inf\sigma\left(\frac{1}{2}(\vec{p},\vec{p}) + \frac{1}{2}((\vec{q}-\vec{f}),A(\vec{q}-\vec{f}))\right) + \sum_{j=1}^{N}\frac{1}{2m_j}q_j^2 - \frac{1}{2}(\vec{f},A\vec{f}) - \frac{1}{2}\operatorname{tr}\sqrt{A_0} \\ &= \sum_{j=1}^{N}\frac{1}{2m_j}q_j^2 - \frac{1}{2}(f,Af) + \frac{1}{2}\operatorname{tr}(\sqrt{A}-\sqrt{A_0}). \end{aligned}$$

Separately we calculate

(1) $\Sigma_{j=1}^{N}(1/2m_j)\,q_j^2 - 1/2(f,Af)$,
(2) $\frac{1}{2}\operatorname{tr}(\sqrt{A}-\sqrt{A_0})$.

First we calculate (1). We give a remark. Let

$$d_{\mu\nu}(k) := \sum_{r=1}^{d-1} e_\mu^r(k)e_\nu^r(k) = \left(1 - \frac{k}{|k|}\otimes\frac{k}{|k|}\right)_{\mu\nu} = \delta_{\mu\nu} - \frac{k_\mu k_\nu}{|k|^2}.$$

For rotation invariant functions f and g it follows that

$$(d_{\mu\nu}f,g) = \delta_{\mu\nu}K(f,g).$$

We have

$$(f,Af) = \sum_{i,j=1}^{N}\sum_{\mu,\nu=1}^{d}\frac{\alpha_i}{m_i}\frac{\alpha_j}{m_j}q_{i\mu}q_{j\nu}(A^{-1}v_\mu,v_\nu).$$

Note that we assume that $|\alpha_j|^2$ are sufficiently small. Then

$$A^{-1} = \sum_{n=1}^{\infty}(-1)^{n-1}A_0^{-1}(PA_0^{-1})^{n-1}.$$

Hence

$$\begin{aligned} (A^{-1}v_\mu,v_\nu) &= \sum_{n=1}^{\infty}(-1)^{n-1}(A_0^{-1}(PA_0^{-1})^{n-1}v_\mu,v_\nu) \\ &= \sum_{n=1}^{\infty}(-1)^{n-1}\sum_{j_1,\ldots,j_{n-1}=1}^{N}\sum_{\mu_1,\ldots,\mu_{n-1}=1}^{d}\epsilon^{n-1}\frac{\alpha_{j_1}^2}{m_{j_1}}\cdots\frac{\alpha_{j_{n-1}}^2}{m_{j_{n-1}}}(v_\mu A_0^{-1}v_{\mu_1}) \\ &\quad\times(v_{\mu_1},A_0^{-1}v_{\mu_2})(v_{\mu_2},A_0^{-1}v_{\mu_3})\cdots(v_{\mu_{n-2}},A_0^{-1}v_{\mu_{n-1}})(v_{\mu_{n-1}},A_0^{-1}v_\nu) \end{aligned}$$

$$= \delta_{\mu\nu} \sum_{n=1}^{\infty} (-1)^{n-1} \sum_{j_1,\ldots,j_{n-1}=1}^{N} \sum_{\mu_1,\ldots,\mu_{n-1}=1}^{d} \epsilon^{n-1} K^n \frac{\alpha_{j_1}^2}{m_{j_1}} \cdots \frac{\alpha_{j_{n-1}}^2}{m_{j_{n-1}}} \xi^n,$$

where

$$\xi := \sum_{|l| \leqslant 2\pi L} \frac{|\hat{\lambda}(l)|^2}{\omega_\delta(l)}.$$

Then it follows that

$$(A^{-1} v_\mu, v_\nu) = \delta_{\mu\nu} \sum_{n=1}^{\infty} (-1)^{n-1} K\xi \left\{ \epsilon K \xi \sum_{j=1}^{N} \frac{\alpha_j^2}{m_j} \right\}^{n-1}$$

$$= \delta_{\mu\nu} \frac{K\xi}{1 + \epsilon K \xi \Sigma_{j=1}^{N} \frac{\alpha_j^2}{m_j}}.$$

We have

$$(f, Af) = \sum_{i,j=1}^{N} \sum_{\mu,\nu=1}^{d} \delta_{\mu\nu} \frac{\alpha_i}{m_i} \frac{\alpha_j}{m_j} q_{i\nu} q_{j\mu} \frac{K\xi}{1 + \epsilon K \xi \Sigma_{j=1}^{N} \frac{\alpha_j^2}{m_j}} = \frac{K\xi}{1 + \epsilon K \xi \Sigma_{j=1}^{N} \frac{\alpha_j^2}{m_j}} \left| \sum_{j=1}^{N} \frac{\alpha_j}{m_j} q_j \right|^2.$$

Hence we have

$$(1) = \frac{1}{2} \sum_{j=1}^{N} \frac{q_j^2}{m_j} - \frac{1}{2} \frac{K\xi}{1 + \epsilon K \xi \Sigma_{j=1}^{N} \frac{\alpha_j^2}{m_j}} \left| \sum_{j=1}^{N} \frac{\alpha_j}{m_j} q_j \right|^2.$$

Next we calculate (2). Using the formula for non-negative self-adjoint operator B,

$$\sqrt{B} = \frac{1}{\pi} \int_{-\infty}^{\infty} B(s^2 + B)^{-1} \, \mathrm{d}s,$$

we see that

$$(2) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{tr}\{A(s^2 + A)^{-1} - A_0(s^2 + A_0)^{-1}\} \mathrm{d}s.$$

Since

$$(s^2 + A)^{-1} = (s^2 + A_0)^{-1} \sum_{n=1}^{\infty} (-1)^{n-1} \{P(s^2 + A_0)^{-1}\}^{n-1},$$

we have

$$A(s^2 + A)^{-1} - A_0(s^2 + A_0)^{-1} = (\mathrm{I}) + (\mathrm{II}).$$

Here we put

$$(\mathrm{I}) := A_0(s^2+A_0)^{-1}\sum_{n=1}^{\infty}(-1)^n\{P(s^2+A_0)^{-1}\}^n, \tag{7.4}$$

$$(\mathrm{II}) := P(s^2+A)^{-1}. \tag{7.5}$$

It follows that

$$\mathrm{tr}(\mathrm{I}) = \sum_{n=1}^{\infty}(-1)^n \sum_{\varphi:\mathrm{CONS}} (\varphi, A_0(s^2+A_0)^{-1}\{P(s^2+A_0)^{-1}\}^n\varphi),$$

where $\Sigma_{\varphi:\mathrm{CONS}}$ means to sum up vectors in a complete orthonormal system. Then

$$= \sum_{n=1}^{\infty}(-1)^n \sum_{\varphi:\mathrm{CONS}} (\varphi, A_0(s^2+A_0)^{-1}\underbrace{P(s^2+A_0)^{-1}P(s^2+A_0)^{-1}\cdots P(s^2+A_0)^{-1}}_{n \text{ times}}\varphi)$$

$$= \sum_{n=1}^{\infty}(-1)^n \sum_{\varphi:\mathrm{CONS}} \sum_{j_1,\ldots,j_n=1}^{N} \sum_{\mu_1,\ldots,\mu_n=1}^{d} \epsilon^n \frac{\alpha_{j_1}^2}{m_{j_1}}\cdots\frac{\alpha_{j_n}^2}{m_{j_n}} (\varphi, A_0(s^2+A_0)^{-1}v_{\mu_1})$$
$$\times (v_{\mu_1}, (s^2+A_0)^{-1}v_{\mu_2})\times\cdots\times(v_{\mu_{n-1}}, (s^2+A_0)^{-1}v_{\mu_n})(v_{\mu_n}, (s^2+A_0)^{-1}\varphi).$$

We take as a CONS

$$\left\{\varphi_1 := \frac{(s^2+A_0)^{-1}v_{\mu_n}}{\|(s^2+A_0)^{-1}v_{\mu_n}\|}, \varphi_2, \varphi_3, \ldots,\right\}.$$

Then

$$\mathrm{tr}(\mathrm{I}) = \sum_{n=1}^{\infty}(-1)^n \sum_{j_1,\ldots,j_n=1}^{N} \sum_{\mu_1,\ldots,\mu_n=1}^{d} \epsilon^n \frac{\alpha_{j_1}^2}{m_{j_1}}\cdots\frac{\alpha_{j_n}^2}{m_{j_n}} (v_{\mu_n}, A_0(s^2+A_0)^{-2}v_{\mu_1})$$
$$\times (v_{\mu_1}, (s^2+A_0)^{-1}v_{\mu_2})\times\cdots\times(v_{\mu_{n-1}}, (s^2+A_0)^{-1}v_{\mu_n})\frac{(v_{\mu_n}, (s^2+A_0)^{-2}v_{\mu_n})}{\|(s^2+A_0)^{-1}v_{\mu_n}\|^2}$$
$$= d\sum_{n=1}^{\infty}(-1)^n\left(\sum_{j=1}^{N}\frac{\alpha_j^2}{m_j}\right)^n \epsilon^n K^n \xi(s)^{n-1}\eta(s),$$

where

$$\xi(s) := \sum_{|l|\leqslant 2\pi L} \frac{\omega_\delta(l)|\hat{\lambda}(l)|^2}{s^2+\omega_\delta(l)^2},$$

and

$$\eta(s) := \sum_{|l|\leqslant 2\pi L} \frac{\omega_\delta(l)^3|\hat{\lambda}(l)|^2}{(s^2+\omega_\delta(l)^2)^2}.$$

Hence

$$\mathrm{tr}(\mathrm{I}) = d\sum_{n=1}^{\infty}(-1)^n\left(\epsilon K\xi(s)\sum_{j=1}^{N}\frac{\alpha_j^2}{m_j}\right)^n \frac{\eta(s)}{\xi(s)}$$

$$= d\frac{-\epsilon K\xi(s)\Sigma_{j=1}^{N}\dfrac{\alpha_j^2}{m_j}}{1+\epsilon K\xi(s)\Sigma_{j=1}^{N}\dfrac{\alpha_j^2}{m_j}}\frac{\eta(s)}{\xi(s)} = d\frac{-\epsilon\rho\,\eta(s)}{1+\epsilon\rho\xi(s)}.$$

Next we see that

$$\begin{aligned}\mathrm{tr}(\mathrm{II}) &= \sum_{\varphi:\mathrm{CONS}}(\varphi,P(s^2+A)^{-1}\varphi) = \sum_{n=1}^{\infty}(-1)^{n-1}\sum_{\varphi:\mathrm{CONS}}(\varphi,P(s^2+A_0)^{-1}(P(s^2+A_0)^{-1})^{n-1}\varphi)\\ &= \sum_{n=1}^{\infty}(-1)^{n-1}\sum_{\varphi:\mathrm{CONS}}\sum_{j_1,\ldots,j_n=1}^{N}\sum_{\mu_1,\ldots,\mu_n=1}^{d}\frac{\alpha_{j_1}^2}{m_{j_1}}\cdots\frac{\alpha_{j_n}^2}{m_{j_n}}\epsilon^n\\ &\quad\times(\varphi,v_{\mu_1})(v_{\mu_1},(s^2+A_0)^{-1}v_{\mu_2})\cdots(v_{\mu_{n-1}},(s^2+A_0)^{-1}v_{\mu_n})(v_{\mu_n},(s^2+A_0)^{-1}\varphi).\end{aligned}$$

Take as a CONS

$$\left\{\varphi_1 := \frac{(s^2+A_0)^{-1}v_{\mu_n}}{\|(s^2+A_0)^{-1}v_{\mu_n}\|},\varphi_2,\varphi_3,\ldots,\right\}.$$

Then we have

$$\begin{aligned}\mathrm{tr}(\mathrm{II}) &= \sum_{n=1}^{\infty}(-1)^{n-1}\sum_{j_1,\ldots,j_n=1}^{N}\sum_{\mu_1,\ldots,\mu_n=1}^{d}\frac{\alpha_{j_1}^2}{m_{j_1}}\cdots\frac{\alpha_{j_n}^2}{m_{j_n}}\epsilon^n\times(v_{\mu_n},(s^2+A_0)^{-1}v_{\mu_1})\\ &\quad\times(v_{\mu_1},(s^2+A_0)^{-1}v_{\mu_2})\times\cdots\times(v_{\mu_{n-1}},(s^2+A_0)^{-1}v_{\mu_n})\frac{(v_{\mu_n},(s^2+A_0)^{-2}v_{\mu_n})}{\|(s^2+A_0)^{-1}v_{\mu_n}\|^2}\\ &= \sum_{n=1}^{\infty}(-1)^{n-1}\sum_{j_1,\ldots,j_n=1}^{N}\sum_{\mu_1,\ldots,\mu_n=1}^{d}\frac{\alpha_{j_1}^2}{m_{j_1}}\cdots\frac{\alpha_{j_n}^2}{m_{j_n}}\epsilon^n K^n\,\mathrm{d}\xi(s)^n\\ &= d\sum_{n=1}^{\infty}(-1)^{n-1}\left(\epsilon K\xi(s)\sum_{j=1}^{N}\frac{\alpha_j^2}{m_j}\right)^n = d\frac{\epsilon\rho\xi(s)}{1+\epsilon\rho\xi(s)}.\end{aligned}$$

Hence

$$\mathrm{tr}((\mathrm{I})+(\mathrm{II})) = \frac{d\epsilon\rho}{1+\epsilon\rho\xi(s)}(\xi(s)-\eta(s)).$$

From

$$\xi(s)-\eta(s) = \sum_{|l|\leqslant 2\pi L}\left\{\frac{|\hat{\lambda}(l)|^2\omega_\delta(l)}{s^2+\omega_\delta(l)^2}-\frac{\omega_\delta(l)^3|\hat{\lambda}(l)|^2}{(s^2+\omega_\delta(l)^2)^2}\right\} = \sum_{|l|\leqslant 2\pi L}\frac{s^2|\hat{\lambda}(l)|^2\omega_\delta(l)}{(s^2+\omega_\delta(l)^2)^2} := \eta'(s),$$

it follows that

$$(2) = \frac{\epsilon}{2\pi}\int_{-\infty}^{\infty}\frac{\epsilon\rho\,\eta'(s)}{1+\epsilon\rho\xi(s)}\mathrm{d}s.$$

As was mentioned in (7.3), as $a\to\infty$ and then $L\to\infty$, $H_\epsilon(q,\delta,a,L)$ uniformly converges to $H_\epsilon^0(q)+\delta N$ in the resolvent sense. Thus as $a\to\infty$ and then $L\to\infty$, it follows that

$$E(q,\delta,a,L)\to\inf\sigma(H_\epsilon(q)+\delta N)\coloneqq E(q,\delta).$$

Since $N\geqslant 0$, we have

$$\liminf_{\delta\to 0} E(q,\delta)\geqslant E(q)$$

and the strong resolvent convergence of $H^0_\epsilon(q)+\delta N$ to $H_\epsilon(q)$ as $\delta\to 0$ implies that

$$E(q)\geqslant\limsup_{\delta\to 0}E(q,\delta).$$

Thus

$$E(q,\delta)\to E(q)$$

as $\delta\to 0$. Thus the lemma follows for sufficiently small $|\alpha_j|$'s. By Proposition 3.2(3), $\inf\sigma(H^0_\epsilon(q))$ can be analytically continued in each α_j's to $\mathcal{O}$, and clearly $E(q)$ also can be done. Hence the lemma follows for all α_j's in $\mathbb{R}$. □

A proof of Lemma 3.3(2): The proof is similar to Lemma 3.3. Define the projection operator

$$P\coloneqq\epsilon\sum_{j=1}^{N}\sum_{\mu=1}^{d}\frac{\alpha_j^2}{m_j}|v^j_\mu\rangle\langle v^j_\mu|,$$

and

$$A\coloneqq A_0+P,$$

where A_0 is defined in (7.2). Here

$$v^j_\mu\coloneqq\begin{pmatrix}\sqrt{\omega_\delta(l_1)}\hat{\lambda}_j(l_1)e^1_\mu(l_1)\\ \vdots\\ \sqrt{\omega_\delta(l_1)}\hat{\lambda}_j(l_1)e^{(d-1)}_\mu(l_1)\\ \vdots\\ \vdots\\ \sqrt{\omega_\delta(l_D)}\hat{\lambda}_j(l_D)e^1_\mu(l_D)\\ \vdots\\ \sqrt{\omega_\delta(l_D)}\hat{\lambda}_j(l_D)e^{(d-1)}_\mu(l_D)\end{pmatrix}\in\mathbb{R}^{(d-1)D}.$$

Let

$$f\coloneqq\sum_{j=1}^{N}\sum_{\mu=1}^{d}\frac{\alpha_j}{m_j}A^{-1}q_{j\mu}v^j_\mu.$$

Similarly to Lemma 3.3 it is enough to calculate

(1) $\Sigma_{j=1}^{N}(1/2)m_jq_j^2-1/2(Af,f)$,
(2) $\frac{1}{2}\mathrm{tr}(\sqrt{A}-\sqrt{A_0})$.

First we calculate (1). We have

$$(A^{-1}v^i_\mu,v^j_\nu)=\delta_{\mu\nu}\delta_{ij}\sum_{n=1}^{\infty}(-1)^{n-1}K^n\epsilon^{n-1}\left(\frac{\alpha_j^2}{m_j}\right)^{n-1}\xi_j^n=\delta_{\mu\nu}\delta_{ij}\frac{K\xi_j}{1+\epsilon K\xi_j\dfrac{\alpha_j^2}{m_j}},$$

where

$$\xi_j := \sum_{|l| \leqslant 2\pi L} \frac{|\hat{\lambda}_j(l)|^2}{\omega_\delta(l)}.$$

Note that, for function g,

$$(\hat{\lambda}_j, g\hat{\lambda}_i) = \delta_{ij}(\hat{\lambda}_j, g\hat{\lambda}_j).$$

Then

$$\begin{aligned}(Af,f) &= \sum_{i,j=1}^{N} \sum_{\mu,\nu=1}^{d} (A^{-1}v_\mu^i, v_\nu^j) \\ &= \sum_{i,j=1}^{N} \sum_{\mu,\nu=1}^{d} \delta_{\mu\nu}\delta_{ij} \frac{\alpha_i}{m_i}\frac{\alpha_j}{m_j} q_{i\nu}q_{j\mu} \frac{K\xi_j}{1+\epsilon K\xi_j \dfrac{\alpha_j^2}{m_j}} \\ &= \sum_{j=1}^{N} \left(\frac{\alpha_j}{m_j}\right)^2 q_j^2 \frac{K\xi_j}{1+\epsilon K\xi_j \dfrac{\alpha_j^2}{m_j}}.\end{aligned}$$

Then

$$\frac{1}{2}\sum_{j=1}^{N} \frac{q_j^2}{m_j} - \frac{1}{2}(Af,f) = \frac{1}{2}\sum_{j=1}^{N} \frac{q_j^2}{m_j}\left(\frac{m_j - (1-\epsilon)K\alpha_j^2\xi_j}{m_j + \epsilon K\alpha_j^2\xi_j}\right).$$

Next we calculate (2). Let (I) and (II) be as in (7.4) and (7.5), respectively. We define

$$\xi_j(s) := \sum_{|l| \leqslant 2\pi L} \frac{\omega_\delta(l)|\hat{\lambda}_j(l)|^2}{s^2 + \omega_\delta(l)^2},$$

$$\eta_j(s) := \sum_{|l| \leqslant 2\pi L} \frac{\omega_\delta(l)^3|\hat{\lambda}_j(l)|^2}{(s^2 + \omega_\delta(l)^2)^2},$$

and

$$\eta_j'(s) := \sum_{|l| \leqslant 2\pi L} \frac{s^2|\hat{\lambda}_j(l)|^2\omega_\delta(l)}{(s^2 + \omega_\delta(l)^2)^2}.$$

We have

$$\begin{aligned}\mathrm{tr(I)} &= d\sum_{j=1}^{N} \sum_{n=1}^{\infty} (-1)^n \left(\frac{\alpha_j^2}{m_j}\right)^n \epsilon^n K^n \xi_j(s)^{n-1}\eta_j(s) \\ &= -d\sum_{j=1}^{N} \eta_j(s)\epsilon\frac{\alpha_j^2}{m_j}K\frac{1}{1+\epsilon\xi_j(s)K\dfrac{\alpha_j^2}{m_j}} \\ &= -d\sum_{j=1}^{N} \frac{\epsilon\rho_j\eta_j(s)}{1+\epsilon\rho_j\xi_j(s)}.\end{aligned}$$

Moreover

$$\mathrm{tr}(\mathrm{II})=\sum_{j=1}^{N}\sum_{n=1}^{\infty}(-1)^{n-1}\frac{\alpha_j^2}{m_j}\epsilon^n K^n \xi_j(s)^n = d\sum_{j=1}^{N}\frac{\epsilon\rho_j\xi_j(s)}{1+\epsilon\rho_j\xi_j(s)}.$$

Hence

$$(\mathrm{I})+(\mathrm{II})=d\sum_{j=1}^{N}\frac{\epsilon\rho_j}{1+\epsilon\rho_j\xi_j(s)}(\xi_j(s)-\eta_j(s))=d\sum_{j=1}^{N}\frac{\epsilon\rho_j}{1+\epsilon\rho_j\xi_j(s)}\eta_j'(s).$$

Then

$$\frac{1}{2}\mathrm{tr}(\sqrt{A}-\sqrt{A_0})=\frac{1}{2}\mathrm{tr}((\mathrm{I})+(\mathrm{II}))=\sum_{j=1}^{N}\frac{d}{2\pi}\int_{-\infty}^{\infty}\frac{\epsilon\rho_j\eta_j'(s)}{1+\epsilon\rho_j\xi_j(s)}\mathrm{d}s.$$

The same limiting argument on a, L, δ as in Lemma 3.3 leads to the desired results. □

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On the Gauss law and global charge for quantum chromodynamics

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The local Gauss law of quantum chromodynamics (QCD) on a finite lattice is investigated. It is shown that it implies a gauge invariant, additive law giving rise to a gauge invariant $\mathbb{Z}_3$-valued global charge in QCD. The total charge contained in a region of the lattice is equal to the flux through its boundary of a certain $\mathbb{Z}_3$-valued, additive quantity. Implications for continuum QCD are discussed. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1447310]

I. INTRODUCTION

Quantum chromodynamics (QCD) is one of the basic building blocks of the standard model for describing elementary particle interactions. During the last decades QCD was quite successful, e.g., in describing deep inelastic scattering processes within the framework of perturbation theory on the one hand and ''measuring'' certain types of observables using (nonperturbative) lattice approximation techniques on the other hand. Nonetheless, we are still facing the basic challenge, which consists in constructing an effective microscopic theory of interacting hadrons out of this gauge theory. For this purpose, nonperturbative methods for describing the low energy regime should be developed. In particular, the observable algebra and the superselection structure of this theory should be investigated. The present paper is a step in this direction.

We stress that standard methods from algebraic quantum field theory for models which do not contain massless particles, see Ref. 1, do not apply here. Some progress toward an implementation of similar ideas for theories with massless particles has been made; for the case of quantum electrodynamics (QED) see Refs. 2 and 3 and further references therein. In particular, Buchholz developed the concept of so-called charge classes and found a criterion for distinguishing between the electric charge (carried by massive particles) and additional superselection sectors corresponding to inequivalent asymptotic infrared clouds of photons. For some attempts to deal with the non-Abelian case we refer to papers by Strocchi and Wightman, see Refs. 4 and 5.

In QED, the notion of *global* (electric) charge is easy to understand. This is due to the fact that in this theory we have a *local* Gauss law, which is built from gauge invariant operators and which is linear. Thus, one can ''sum up'' the local Gauss laws over all points of a given (spacelike) hyperplane in space–time yielding the following gauge invariant conservation law: The global electric charge is equal to the electric flux through a two-sphere at infinity. On the contrary, in QCD the local Gauss law is neither built from gauge invariant operators nor is it linear. The main point of the present paper is to show that it is possible to extract from the local Gauss equation of QCD a gauge invariant, additive law for operators with eigenvalues in $\mathbb{Z}_3$ [which is canonically identified with the dual of the center of SU(3)]. This implies—as in QED—a gauge invariant conservation law: The global $\mathbb{Z}_3$-valued charge is equal to a $\mathbb{Z}_3$-valued gauge invariant quantity obtained from the color electric flux at infinity.

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This color charge, often called *triality*, was invented a long time ago. On the level of lattice gauge theories, this notion is already implicitly contained in a paper by Kogut and Susskind, see Ref. 6. In particular, Mack[7] used it to propose a certain (heuristic) scheme of color screening and quark confinement, based upon a dynamical Higgs mechanism with Higgs fields built from gluons. For similar ideas we also refer to papers by 'tHooft, see Ref. 8, and references therein. This concept was also used in a paper by Borgs and Seiler,[9] where the confinement problem for Yang–Mills theories with static quark sources at nonzero temperature was discussed. In this context, also the Gauss law for color charge was analyzed. Finally, we mention a paper by Fredenhagen and Marcu, see Ref. 10, dealing with a $\mathbb{Z}_2$-gauge theory (with $\mathbb{Z}_2$-valued matter fields) on the lattice. These authors were able to construct the ground state and charged states of this model. For some regions in the space of coupling constants, the thermodynamic limit of charged states was controlled.

In this paper, we consider QCD (with fermions) in the Hamiltonian approach. To be rigorous we restrict ourselves to its approximation on a finite (regular cubic) lattice. For basic notions concerning lattice gauge theories (including fermions) we refer to Ref. 11. The Hamiltonian formulation of lattice gauge theories was first proposed in Refs. 12 and 6. The paper is organized as follows: In Sec. II, we define the algebra of field operators. Since, to our knowledge, this has never been published, we discuss it in some detail. Next, by imposing the local Gauss law and gauge invariance, we obtain the observable algebra $\mathcal{O}(\Lambda)$ for lattice QCD, see Sec. III. In Sec. IV we analyze the local Gauss law and invent the gauge invariant notion of the local charge densitiy. We prove that there exists an operator function, built from the Casimir invariants of the theory under consideration, which—applied to the Gauss law—yields the additive, gauge invariant Gauss law for color charge. Using this notion, in Sec. V the global charge is defined and the flux law for QCD is discussed. Finally, we discuss some perspectives of this approach, including heuristic remarks concerning the continuum case.

For an analogous investigation of QED on the lattice, including its charge superselection structure, we refer to Refs. 13 and 14.

II. THE FIELD ALGEBRA FOR LATTICE QCD

We consider QCD in the Hamiltonian framework on a finite, regular three-dimensional lattice Λ. We denote the set of oriented, i-dimensional elements of Λ by Λ^i, $i=0,1,2,3$. Such elements are (in increasing order of i) called sites, links, plaquettes, and cubes. The set of nonoriented i-dimensional elements will be denoted by $|\Lambda|^i$. If, for instance, $(x,y)\in\Lambda^1$ is an oriented link, then by $|(x,y)|\in|\Lambda|^1$ we mean the corresponding nonoriented link. Instead of using a concrete Hilbert space representation (e.g., the Schrödinger representation), we give an abstract definition of the field algebra in terms of generators and defining relations.

The basic fields of lattice QCD are quarks living at lattice sites and gluons living on links. The field algebra is thus, by definition, the tensor product of local fermionic and bosonic algebras:

$$\mathcal{F}(\Lambda) := \bigotimes_{x\in|\Lambda|^0} \mathcal{F}_x \bigotimes_{|(x,y)|\in|\Lambda|^1} \mathcal{F}_{|(x,y)|}\,. \tag{2.1}$$

We impose locality of the lattice quantum fields by postulating that the local algebras corresponding to different elements of Λ commute with each other.

The fermionic field algebra $\mathcal{F}_x$ associated with a lattice site x is generated from the algebra $\mathcal{L}_x$ of canonical anticommutation relations of quarks. In terms of coordinates, the quark field is given by

$$|\Lambda|^0 \ni x \to (\psi^{aA}(x)) \in \mathcal{L}_x\,, \tag{2.2}$$

where a stands for bispinorial and (possibly) flavor degrees of freedom and $A=1,2,3$ is the color index corresponding to the fundamental representation of SU(3). The conjugate quark field is

denoted by $\psi^{*a}{}_A(x)$, where we raise and lower indices by the help of the canonical Hermitian metric tensor g_{AB} in $\mathbb{C}^3$. Finally, the (nontrivial) canonical anticommutation relations for elements of $\mathcal{L}_x$ read

$$[\psi^{*a}{}_A(x), \psi^{bB}(x)]_+ = \delta^B{}_A \delta^{ab}. \tag{2.3}$$

Passing to self-adjoint generators (real and imaginary parts of ψ), we observe that $\mathcal{F}_x$ is a Clifford algebra.

The bosonic field algebra $\mathcal{F}_{|(x,y)|}$ associated with the nonoriented link $|(x,y)|$ will be constructed in terms of its equivalent copies $\mathcal{F}_{(x,y)}$ and $\mathcal{F}_{(y,x)}$, corresponding to the two orientations of the link (x,y). We will see that there is a natural identification of these two algebras, induced from the vector character of both the gluonic potential A and the color electric field E of the underlying continuum theory: under the change of orientation of the kth axis both A_k and E^k change their signs.

The bosonic field algebra $\mathcal{F}_{(x,y)}$ is, by definition, the tensor product

$$\mathcal{F}_{(x,y)} := \tilde{\mathcal{E}}_{(x,y)} \otimes \mathcal{A}_{(x,y)}, \tag{2.4}$$

where $\tilde{\mathcal{E}}_{(x,y)}$ is the enveloping algebra of the (real) Lie algebra $\mathcal{E}_{(x,y)} \cong \mathrm{su}(3)$ and $\mathcal{A}_{(x,y)} \cong C^\infty(\mathrm{SU}(3))$ is the commutative $*$-algebra of smooth functions on the Lie group SU(3). We note that the above-mentioned tensor product is naturally endowed with the structure of a crossed product of Hopf algebras, given by the action of generators of $\tilde{\mathcal{E}}_{(x,y)}$ on functions, see Ref. 15. We identify the tensor product of elements of $\tilde{\mathcal{E}}_{(x,y)}$ and functions with their product as differential operators on SU(3). This way, $\mathcal{F}_{(x,y)}$ gets identified with the algebra of differential operators on the group manifold. For our purposes, we endow $\mathcal{F}_{(x,y)}$ with a Lie algebra structure. Thus, we have to define the commutator between a generator $e \in \mathcal{E}_{(x,y)}$ of $\tilde{\mathcal{E}}_{(x,y)}$ and a function $f \in \mathcal{A}_{(x,y)}$,

$$[e,f] := e^R(f), \tag{2.5}$$

where $e^R(f)$ denotes the derivative of f with respect to the right-invariant vector field e^R generated by e,

$$e^R(f)(g) := \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} f(\exp(se)\cdot g), \quad g \in \mathrm{SU}(3). \tag{2.6}$$

Now we give an explicit description of $\mathcal{F}_{(x,y)}$ in terms of generators and defining relations. The algebra $\mathcal{A}_{(x,y)}$ is generated by matrix elements of the gluonic gauge potential on the link (x,y),

$$\Lambda^1 \ni (x,y) \to U^A{}_B(x,y) \in \mathcal{A}_{(x,y)}, \tag{2.7}$$

where $A,B = 1,2,3$ are color indices. Being functions on SU(3), these generators fulfill the following relations:

$$(U^A{}_B(x,y))^* U_A{}^C(x,y) = \delta^C{}_B \mathbf{1}, \tag{2.8}$$

$$\epsilon_{ABC} U^A{}_D(x,y) U^B{}_E(x,y) U^C{}_F(x,y) = \epsilon_{DEF} \mathbf{1}. \tag{2.9}$$

The algebra $\tilde{\mathcal{E}}_{(x,y)}$ is generated by color electric fields, spanning the Lie algebra $\mathcal{E}_{(x,y)}$. Choosing a basis $\{t_i\}$, $i = 1,\ldots,8$, of su(3) we denote by $\{E_i(x,y)\}$ the corresponding basis of $\mathcal{E}_{(x,y)}$,

$$\Lambda^1 \ni (x,y) \to E_i(x,y) := t_i \in \mathcal{E}_{(x,y)}. \tag{2.10}$$

These generators are self-adjoint (real), $E_i^* = E_i$. In the sequel we take as the basis the Hermitean, traceless Gell–Mann matrices ${t_i}^A{}_B$, normalized as follows:

$$\sum_i {t_i}^A{}_B {t_i}^C{}_D = \delta^A_D \delta^C_B - \frac{1}{3}\delta^A_B \delta^C_D, \tag{2.11}$$

or, equivalently, ${t_i}^A{}_B\, {t_j}^B{}_A = \delta_{ij}$. We will also use the following traceless matrix built from these fields:

$$E^A{}_B(x,y) = \sum_i E_i(x,y) {t_i}^A{}_B. \tag{2.12}$$

Since the coefficients ${t_i}^A{}_B$ are complex, these fields are no longer self-adjoint:

$$(E^A{}_B(x,y))^* = E_B{}^A(x,y). \tag{2.13}$$

The commutation relations between elements of su(3) translated to the language of these fields read

$$[E^A{}_B(x,y), E^C{}_D(x,y)] = \delta^C{}_B E^A{}_D(x,y) - \delta^A{}_D E^C{}_B(x,y), \tag{2.14}$$

whereas the commutation relations (2.5) between Lie algebra elements and functions, rewritten in terms of generators, take the following form:

$$[E^A{}_B(x,y), U^C{}_D(x,y)] = \delta^C{}_B U^A{}_D(x,y) - \tfrac{1}{3}\delta^A{}_B U^C{}_D(x,y). \tag{2.15}$$

Observe that, for every link (x,y), we have a model of quantum mechanics with configuration space being the group manifold SU(3). The matrix elements of the gluonic potential play the role of functions of position variables, whereas the color electric fields play the role of (noncommuting) canonically conjugate momenta. Formula (2.15) is the analog of the canonical commutation relation $[p,q] = -i$.

Now, we describe the transformation law of these objects under the change of the link orientation. The vector character of the continuum gauge potential implies that the (classical) SU(3)-valued parallel transporter $g(x,y)$ on (x,y) transforms to $g^{-1}(x,y)$ under the change of orientation. Thus, the change of orientation on (x,y) induces the transformation

$$\mathrm{SU}(3) \ni g \to i(g) = g^{-1} \in \mathrm{SU}(3) \tag{2.16}$$

on configuration space. This transformation lifts naturally to a mapping

$$\mathcal{I}_{(x,y)} : \mathcal{F}_{(x,y)} \to \mathcal{F}_{(y,x)} \tag{2.17}$$

of field algebras, defined by

$$\mathcal{I}_{(x,y)}(e,f) := (-i_*(e), i^*(f)). \tag{2.18}$$

We have $i^*(f)(g) \equiv \check{f}(g) := f(g^{-1})$ and $-i_*(e) = e^L$, where e^L is the left invariant vector field on SU(3) generated by $-e$. It acts on functions in the following way:

$$e^L(f)(g) = \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} f(g \cdot \exp(-se)). \tag{2.19}$$

Observe that e^L is not an element of $\mathcal{E}_{(y,x)}$, but it can be expanded with respect to right-invariant vector fields with coefficients being functions on the group. Actually, the following formula is easily proved:

$$e^L = -\sum_{i=1}^{8} \mathrm{Tr}(geg^{-1}t_i)t_i^R, \tag{2.20}$$

where t_i is any orthonormal basis of su(3).

Lemma 1: The mapping $\mathcal{I}_{(x,y)}$ is an isomorphism of algebras.

Proof: We observe that $\mathcal{I}_{(x,y)}$ is obviously a bijective mapping between generators. It extends to an isomorphism of field algebras if we prove that it preserves the commutator. This is obvious for elements, which either belong both to $\mathcal{A}_{(x,y)}$ or to $\mathcal{E}_{(x,y)}$. Thus, it is sufficient to consider the commutator of a Lie algebra element e with a function f. Using the identity

$$e^R(f)(g) = \frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} f(\exp(se)\cdot g) = \frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} \check{f}(g^{-1}\cdot\exp(-se)) = e^L(\check{f})(g^{-1}), \tag{2.21}$$

and applying $\mathcal{I}_{(x,y)}$ to the functions on both sides, we obtain due to (2.5) and (2.18)

$$\mathcal{I}_{(x,y)}([e,f]) = \mathcal{I}_{(x,y)}(e^R(f)) = e^L(\check{f}) = [\mathcal{I}_{(x,y)}(e), \mathcal{I}_{(x,y)}(f)]. \tag{2.22}$$

This ends the proof. □

Field configurations, which are related under $\mathcal{I}_{(x,y)}$ will be identified as different representations of the same object. Thus, the bosonic field algebra $\mathcal{F}_{|(x,y)|}$, associated with the nonoriented link $|(x,y)|$, is defined as the subalgebra of $\mathcal{F}_{(x,y)}\times\mathcal{F}_{(y,x)}$, obtained by this identification:

$$\mathcal{F}_{|(x,y)|} := \{(l_{(x,y)}, k_{(y,x)}) \in \mathcal{F}_{(x,y)}\times\mathcal{F}_{(y,x)} : k_{(y,x)} = \mathcal{I}_{(x,y)}(l_{(x,y)})\}. \tag{2.23}$$

Projection onto the first (respectively, second) component gives us an isomorphism of $\mathcal{F}_{|(x,y)|}$ with $\mathcal{F}_{(x,y)}$ (respectively, $\mathcal{F}_{(y,x)}$).

The above-mentioned transformation law yields relations between generators of the two algebras. For functions on SU(3), formula (2.8) enables us to rewrite (2.18) as follows:

$$U^A{}_B(y,x) = (U_B{}^A(x,y))^*. \tag{2.24}$$

For Lie algebra elements, formula (2.20) applied to $e = t_i$ reads

$$E_j(y,x) = -\sum_{i=1}^{8} U^A{}_B(x,y)t_j{}^B{}_C U^C{}_D(y,x)t_i{}^D{}_A E_i(x,y), \tag{2.25}$$

or, in terms of generators $E^A{}_B(x,y)$,

$$E^A{}_B(y,x) = -U^A{}_D(y,x)U^C{}_B(x,y)E^D{}_C(x,y). \tag{2.26}$$

To summarize, the field algebra $\mathcal{F}(\Lambda)$ is the $*$-algebra, generated by elements

$$\{\psi^{aA}(x), U^A{}_B(x,y), E^A{}_B(x,y)\},$$

fulfilling relations (2.8), (2.9), (2.13), (2.24), and (2.26), together with canonical (anti) commutation relations

$$[\psi^{*a}{}_A(x), \psi^{bB}(y)]_+ = \delta(x-y)\,\delta^B{}_A\,\delta^{ab},$$

$$[E^A{}_B(x,y), E^C{}_D(u,z)] = \delta(x-u)\,\delta(y-z)(\delta^C{}_B E^A{}_D(x,y) - \delta^A{}_D E^C{}_B(x,y)),$$

$$[E^A{}_B(x,y), U^C{}_D(u,z)] = +\delta(x-u)\,\delta(y-z)(\delta^C{}_B U^A{}_D(x,y) - \tfrac{1}{3}\delta^A{}_B U^C{}_D(x,y)) - \delta(x-z)\,\delta(y-u)$$
$$\times(\delta^A{}_D U^C{}_B(y,x) - \tfrac{1}{3}\delta^A{}_B U^C{}_D(y,x)).$$

III. THE OBSERVABLE ALGEBRA

The observable algebra $\mathcal{O}(\Lambda)$ is defined by imposing the local Gauss law and gauge invariance.

The group of local gauge transformations acts on $\mathcal{F}(\Lambda)$ by automorphisms $x \to g^A{}_B(x)$ as follows:

$$\psi^{aA}(x) \to g^A{}_B(x)\psi^{aB}(x), \tag{3.1}$$

$$U^A{}_B(x,y) \to g^A{}_C(x)U^C{}_D(x,y)(g^{-1})^D{}_B(y), \tag{3.2}$$

$$E^A{}_B(x,y) \to g^A{}_C(x)E^C{}_D(x,y)(g^{-1})^D{}_B(x). \tag{3.3}$$

It is easy to check that these transformations are generated by

$$\mathcal{G}^A{}_B(x) := \rho^A{}_B(x) - \sum_y E^A{}_B(x,y), \tag{3.4}$$

where

$$\rho^A{}_B(x) = \sum_a \left(\psi^{*aA}(x)\psi^a{}_B(x) - \frac{1}{3}\delta^A_B \psi^{*aC}(x)\psi^a{}_C(x) \right) \tag{3.5}$$

is the local matter charge density. Observe that $\rho^A{}_A(x) = 0$.

To implement gauge invariance we have to take those elements of $\mathcal{F}(\Lambda)$, which commute with all generators $\mathcal{G}^A{}_B(x)$. Thus, the subalgebra of gauge invariant fields is, by definition, the commutant $\mathcal{A}(\mathcal{G})'$ of the algebra $\mathcal{A}(\mathcal{G})$, generated by the set $\{\mathcal{G}^A{}_B(x)\}$.

The local Gauss law at $x \in \Lambda^0$ has the form

$$\sum_y E^A{}_B(x,y) = \rho^A{}_B(x), \tag{3.6}$$

with the sum taken over all points y adjacent to x. Imposing it on the subalgebra $\mathcal{A}(\mathcal{G})'$ of gauge invariant fields means factorizing the latter with respect to $\mathcal{I}(\Lambda) \cap \mathcal{A}(\mathcal{G})'$, where $\mathcal{I}(\Lambda)$ is the ideal generated by (3.6). Thus, the observable algebra is defined as follows:

$$\mathcal{O}(\Lambda) := \mathcal{A}(\mathcal{G})'/\{\mathcal{I}(\Lambda) \cap \mathcal{A}(\mathcal{G})'\}. \tag{3.7}$$

Obviously, every element of $\mathcal{O}(\Lambda)$ is represented by a gauge invariant element of $\mathcal{F}(\Lambda)$ and $\mathcal{O}(\Lambda)$ can be viewed as a $*$-subalgebra of $\mathcal{F}(\Lambda)$ generated by gauge invariant bosonic combinations of U and E and by gauge invariant combinations of ψ and ψ^* of mesonic and baryonic type, with the Gauss law inducing some identities between those generators.

It will be shown in Sec. IV that there is a (gauge invariant), *additive* law, obtained by combining these two equations, which characterizes the local color charge density carried by the lattice quantum fields. Additivity will allow us to obtain the global color charge by adding up the local Gauss laws. In a subsequent paper we will show that the irreducible representations of $\mathcal{O}(\Lambda)$ are labeled by this global charge. This way, we get the physical Hilbert space $\mathcal{H}^{\text{phys}}$ as a direct sum of color charge superselection sectors. The similar problem for QED on the lattice was solved in Ref. 13.

IV. THE LOCAL CHARGE DENSITY

In this section we are going to analyze the local Gauss law (3.6). Suppose, for that purpose, that we are given a collection of operators $F^A{}_B$ in a Hilbert space $\mathcal{H}$, fulfilling $F^A{}_A = 0$ and $(F^A{}_B)^* = F_B{}^A$, realizing the canonical commutation relations for the Lie algebra su(3):

$$[F^A{}_B, F^C{}_D] = \delta^C{}_B F^A{}_D - \delta^A{}_D F^C{}_B . \tag{4.1}$$

The field algebra $\mathcal{F}(\Lambda)$ provides us with two basic examples of this type: the electric field $E^A{}_B(x,y)$ on each lattice link, see (2.14), and the charge operator $\rho^A{}_B(x)$ at each lattice site, given by formula (3.5). Indeed, due to canonical anticommutation relation (2.3), the latter fulfills (4.1). Thus, the operators occurring on both sides of the local Gauss law fulfill (4.1).

Throughout this paper, we assume integrability of the Lie algebra representations under consideration. This means that for each F there exists a unitary representation of the group SU(3),

$$\mathrm{SU}(3) \ni g \to \overline{F}(g) \in B(\mathcal{H}), \tag{4.2}$$

associated with F.

It is easy to check that if F and G are two commuting representations of su(3) then so is $F+G$. Indeed, if $\overline{F}(g)$ and $\overline{G}(g)$ are representations of SU(3) corresponding to F and G, then $F+G$ may be obtained by differentiating the representation $\mathrm{SU}(3) \ni g \to \overline{F}(g)\overline{G}(g) \in B(\mathcal{H})$, where $B(\mathcal{H})$ denotes the C^*-algebra of bounded operators on $\mathcal{H}$. Moreover, $-F^*$ is also a representation of su(3), corresponding to the following representation of SU(3): $\mathrm{SU}(3) \ni g \to (\overline{F}(g^{-1}))^* \in B(\mathcal{H})$.

Such a collection of operators is an *operator domain* in the sense of Woronowicz (see Ref. 16). We are going to construct an operator function on this domain, i.e., a mapping $F \to \varphi(F)$ which satisfies $\varphi(UFU^{-1}) = U\varphi(F)U^{-1}$ for an arbitrary isometry U. This function will be built from the two gauge-invariant, self-adjoint and commuting (Casimir) operators K_2 and K_3 of F:

$$K_2 = F^A{}_B F^B{}_A , \tag{4.3}$$

$$K_3 = \tfrac{1}{2}(F^A{}_B F^B{}_C F^C{}_A + F^A{}_B F^C{}_A F^B{}_C). \tag{4.4}$$

The Hilbert space $\mathcal{H}$ splits into the direct sum of subspaces $\mathcal{H}_\alpha$ on which F acts irreducibly. Each of these subspaces is a common eigenspace of K_2 and K_3. Denoting the highest weight characterizing a given irreducible representation by (m,n), with m and n being non-negative integers, the eigenvalues k_2 and k_3 of K_2 and K_3 are given by

$$k_2 = \tfrac{2}{3}(m^2 + mn + n^2 + 3m + 3n), \tag{4.5}$$

$$k_3 = \tfrac{1}{9}(m-n)(3+2m+n)(3+m+2n). \tag{4.6}$$

It is easy to check that the above-given formulas may be uniquely solved with respect to m and n yielding

$$\begin{aligned} m &= M(k_2,k_3) \\ &:= \sqrt{\frac{2}{3}(k_2+2)}\left(\cos\left(\frac{1}{3}\arccos\frac{\sqrt{6}k_3}{\sqrt{(k_2+2)^3}} + \frac{2}{3}\pi\right)\right. \\ &\quad \left. + 2\cos\left(\frac{1}{3}\arccos\frac{\sqrt{6}k_3}{\sqrt{(k_2+2)^3}}\right)\right) - 1, \end{aligned} \tag{4.7}$$

$$
\begin{aligned}
n &= N(k_2,k_3) \\
&:= -\sqrt{\frac{2}{3}(k_2+2)}\left(2\cos\left(\frac{1}{3}\arccos\frac{\sqrt{6}k_3}{\sqrt{(k_2+2)^3}}+\frac{2}{3}\pi\right)\right. \\
&\quad \left.+\cos\left(\frac{1}{3}\arccos\frac{\sqrt{6}k_3}{\sqrt{(k_2+2)^3}}\right)\right)-1. \qquad (4.8)
\end{aligned}
$$

Using these functions we may define a function with values in $\mathbb{Z}_3$, which will be identified with the dual to the center $\mathcal{C}$ of the gauge group SU(3):

$$f(k_2,k_3) := (M(k_2,k_3)-N(k_2,k_3)) \mod 3. \qquad (4.9)$$

For our purposes it is convenient to use the parametrization $\mathbb{Z}_3=(-1,0,1)$. Obviously, we have

$$f(k_2,-k_3) = -f(k_2,k_3). \qquad (4.10)$$

Since K_2 and K_3 are commuting and self-adjoint, there exists an operator-valued function:

$$\varphi(F) = f(K_2(F),K_3(F)). \qquad (4.11)$$

This means that $\varphi(F)$ may take eigenvalues $-1,0,1$ and that every irreducible subspace $\mathcal{H}_\alpha$ is an eigenspace of $\varphi(F)$ with eigenvalue $m-n \mod 3$.

Theorem 1: *The operator function φ has the following properties:*

$$\varphi(-F^*) = -\varphi(F), \qquad (4.12)$$

$$\varphi(F+G) = \varphi(F)+\varphi(G), \qquad (4.13)$$

for F and G commuting.

Proof: To show property (4.12) observe that $K_2(-F^*)=K_2(F)$, whereas $K_3(-F^*) = -K_3(F)$. Consequently, due to (4.5) and (4.6), we have $M(k_2,-k_3)=N(k_2,k_3)$ and $N(k_2,-k_3)=M(k_2,k_3)$ which implies (4.12). It remains to prove property (4.13). Let there be given two commuting representations, F and G, of su(3) in $\mathcal{H}$. Denote the irreducible components of F by $\{\mathcal{H}^F_\alpha\}$ and of G by $\{\mathcal{H}^G_\beta\}$. The irreducible spaces may be chosen in such a way that $\mathcal{H}$ decomposes as follows:

$$\mathcal{H} = \bigoplus_{\alpha,\beta} \mathcal{H}^F_\alpha \cap \mathcal{H}^G_\beta. \qquad (4.14)$$

Take $0 \neq x \in \mathcal{H}^F_\alpha \cap \mathcal{H}^G_\beta$ and consider the space $\mathcal{H}^{F+G}_x \subset \mathcal{H}$ generated by vectors $\{\overline{F}(g)\overline{G}(g)x\}$, $g \in \mathrm{SU}(3)$, where $\overline{F}$ and $\overline{G}$ are the corresponding (''integrated'') representations of SU(3). By construction, $\mathcal{H}^{F+G}_x$ carries an irreducible representation of $\overline{FG}$. There exists a canonical embedding

$$\mathcal{H}^{F+G}_x \ni y \to T(y) \in \mathcal{H}^F_\alpha \otimes \mathcal{H}^G_\beta, \qquad (4.15)$$

given by

$$T(\overline{F}(g)\overline{G}(g)x) := \overline{F}(g)x \otimes \overline{G}(g)x, \qquad (4.16)$$

intertwining the representation $\overline{FG}$ with $\overline{F}\otimes\overline{G}$. This means that $\overline{FG}$, acting on $\mathcal{H}^{F+G}_x$, is equivalent to one of the irreducible components of $\overline{F}\otimes\overline{G}$. Passing again to representations of the Lie

algebra su(3), we conclude that $F+G$, acting on $\mathcal{H}_x^{F+G}$, is equivalent to one of the irreducible components of $F\otimes\mathbf{1}+\mathbf{1}\otimes G$, acting on $\mathcal{H}_\alpha^F\otimes\mathcal{H}_\beta^G$. Now, property (4.13) follows from the following

Lemma 2: Let there be given two irreducible representations (m,n) *and* (m',n') *of* $su(3)$, *together with the decomposition of their tensor product into irreducible components,*

$$(m,n)\otimes(m',n')=(m_1,n_1)\oplus\cdots\oplus(m_p,n_p). \tag{4.17}$$

Then we have

$$(m-n)\mod 3+(m'-n')\mod 3=(m_i-n_i)\mod 3, \tag{4.18}$$

for every $i=1,\ldots,p$.

Proof: We use the classification of irreducible representations in terms of Young-tableaux. For su(3), the following two equations hold:

(1) The number of boxes constituting the Young-tableau of (m_i,n_i) equals the sum of boxes of the tableaux corresponding to (m,n) and (m',n') minus $3p$, where p is a non-negative integer.
(2) The number of boxes of an arbitrary irreducible representation of su(3) is equal to $m+2n\equiv m-n+3n$.

Taking the first equation modulo three and using the second equation yields the thesis. This ends the proof of the Lemma and of the Theorem. □

Applying the operator function φ to the local Gauss law (3.6) and using additivity (4.13) of φ we obtain

$$\sum_y \varphi(E(x,y))=\varphi(\rho(x)). \tag{4.19}$$

This is a gauge invariant equation for operators with eigenvalues in $\mathbb{Z}_3$, valid at every lattice site x. The quantity on the right-hand side is the (gauge invariant) local color charge density carried by the quark field.

We complete this section by giving another definition[17] of the function φ. Consider the center $\mathcal{C}=\{\rho\cdot\mathbf{1}_3;\rho^3=1,\rho\in\mathbb{C}\}$ of SU(3), where $\mathbf{1}_3$ is the unit matrix. If $\overline{F}$ is a representation of SU(3), then the center $\mathcal{C}$ acts as a multiple of the identity on each irreducible subspace $\mathcal{H}_\alpha$: $\mathcal{C}\ni c\to\overline{F}(c)|_{\mathcal{H}_\alpha}=f(c)\cdot\mathbf{1}_{\mathcal{H}_\alpha}$. Obviously, f is a character and, therefore, $(f(c))^3=1$. The formula $f(\rho\cdot\mathbf{1}_3)=\rho^k$, $k=-1,0,1$, gives an identification of the group of characters on $\mathcal{C}$ with $\mathbb{Z}_3$. Hence, there exists an operator function φ, whose values on every $\mathcal{H}_\alpha$ belong to $\mathbb{Z}_3$, defined by

$$f(\rho\cdot\mathbf{1}_3)=:\rho^{\varphi(F)}|_{\mathcal{H}_\alpha}. \tag{4.20}$$

To prove that this definition coincides with the previous one we use the equivalence of the irreducible representation (n,m) of SU(3) with the tensor representation in the space $\mathbb{T}_n^m(\mathbb{C}^3)$ of m-contravariant, n-covariant, completely symmetric and traceless tensors over $\mathbb{C}^3$. The center acts here as a multiple of the unit matrix and it is obvious that

$$f(\rho\cdot\mathbf{1}_3)=\rho^{m-n}. \tag{4.21}$$

The advantage of this formulation is that the above-mentioned properties of φ follow directly from the group properties of the characters. On the other hand, expression (4.11) for φ in terms of the fields F is explicit and gives deeper insight into the relation between the global charge and the invariants (Casimirs) of the theory.

V. THE GLOBAL CHARGE AND THE FLUX LAW

Using the commutation relation between E and U, transformation law (2.26) for $E(x,y)$ may be rewritten in three equivalent ways:

$$E^A{}_B(y,x) = U^A{}_D(y,x)E^D{}_C(x,y)U^C{}_B(x,y) + \tfrac{8}{3}\delta^A_B \tag{5.1}$$

$$= -U^C{}_B(x,y)E^D{}_C(x,y)U^A{}_D(y,x) - \tfrac{8}{3}\delta^A_B \tag{5.2}$$

$$= -E^D{}_C(x,y)U^A{}_D(y,x)U^C{}_B(x,y). \tag{5.3}$$

These equations imply that

$$K_2(E(x,y)) = K_2(E(y,x)), \quad K_3(E(x,y)) = -K_3(E(y,x)). \tag{5.4}$$

Hence, due to (4.10), we have

$$\varphi(E(x,y)) + \varphi(E(y,x)) = 0, \tag{5.5}$$

for every lattice bond (x,y).

Now we take the sum of Eq. (4.19) over all lattice sites $x \in \Lambda$. Due to the above-given identity, all terms on the left-hand side cancel, except for contributions coming from the boundary. This way we obtain the total flux through the boundary $\partial\Lambda$ of Λ:

$$\Phi_{\partial\Lambda} := \sum_{x \in \partial\Lambda} \varphi(E(x,\infty)), \tag{5.6}$$

where by $E(x,\infty)$ we denote the color electric charge along the external link, connecting the point x on the boundary of Λ with the ''rest of the world.'' On the right-hand side we get the (gauge invariant) global color charge, carried by the matter field

$$Q_\Lambda = \sum_{x \in \Lambda} \varphi(\rho(x)). \tag{5.7}$$

Both quantities appearing in the global Gauss law

$$\Phi_{\partial\Lambda} = Q_\Lambda, \tag{5.8}$$

take values in the center $\mathbb{Z}_3$ of SU(3). The ''sum modulo three'' is the composition law in $\mathbb{Z}_3$.

In the above-presented discussion we have admitted nonzero values of $E(x,\infty)$ at boundary points $x \in \partial\Lambda$. In the remainder of this section we make some heuristic remarks on the nature of these objects.

(1) One may treat Λ as a piece of a bigger lattice $\tilde{\Lambda}$. Then the boundary flux operators $E(x,\infty)$ belong to $\mathcal{F}(\tilde{\Lambda})$ and commute with $\mathcal{F}(\Lambda)$ [and also with $\mathcal{O}(\Lambda)$]. They are external from the point of view of $\mathcal{F}(\Lambda)$ and measure the ''violation of the local Gauss law'' on the boundary $\partial\Lambda$:

$$E(x,\infty) := \rho(x) - \sum_y E(y,x). \tag{5.9}$$

Nonvanishing of this element is equivalent to gauge dependence of quantum states under the action of boundary gauges $g(x) \in \mathrm{SU}(3)$, $x \in \partial\Lambda$. Let us discuss this point in more detail. Every irreducible representation of SU(3) is equivalent to some tensor representation. More precisely, denote by $T^m_n(\mathbb{C}^3)$ the space of m-contravariant, n-covariant tensors over $\mathbb{C}^3$, endowed with the

natural scalar product induced by the scalar product on $\mathbb{C}^3$. Let $\mathbb{T}^m_n(\mathbb{C}^3) \subset T^m_n(\mathbb{C}^3)$ be the subspace of *irreducible*, i.e., completely symmetric and traceless tensors. These tensors form a Hilbert space $\mathcal{T}(\mathbb{C}^3)$ defined as the direct sum

$$\mathcal{T}(\mathbb{C}^3) := \bigoplus_{m,n} \mathbb{T}^m_n(\mathbb{C}^3). \tag{5.10}$$

Under gauge transformations at $x \in \partial\Lambda$, physical states of QCD on Λ behave like elements of $\mathcal{T}(\mathbb{C}^3)$, whereas the subspaces $\mathbb{T}^m_n(\mathbb{C}^3)$ correspond to eigenspaces of the invariant operators $N(E(x,\infty))$ and $M(E(x,\infty))$, constructed from external fluxes (5.9). If one wants to include all these gauge invariant operators into an axiomatic formulation, as given in Sec. II, one has different options. The remarks at the beginning of this point suggest to postulate that these operators commute with all elements of the observable algebra $\mathcal{O}(\Lambda)$. This corresponds to treating external fluxes as purely *classical objects*, describing extra superselection rules (cf. Refs. 3–5).

(2) Our results concerning the charge superselection structure of QED on a finite lattice[13] suggest, however, a second option. In Ref. 13 all irreducible representations of the observable algebra were classified in terms of the global electric charge Q_Λ contained in Λ. Representations differing only by the local electric flux distribution over the boundary $\partial\Lambda$, but having the same value of the global flux $\Phi_{\partial\Lambda}$ were proved to be equivalent. The redistribution of fluxes is obtained by the action of certain unitary operators, see Ref. 13, acting on the quantum state under consideration. Such a *redistribution operator* has the following (heuristic) counterpart in continuum QED:

$$U(n) := \exp\left(\frac{i}{\hbar} \int_\Sigma n(x) \cdot A(x) \mathrm{d}^3x \right), \tag{5.11}$$

where $n=(n^k)$ is a divergence-free (i.e., fulfilling $\partial_k n^k \equiv 0$) vector-density on $\Sigma \subset \mathbb{R}^3$. Formally, we have

$$\tilde{E}^k(x) := (U^*(n) E(x) U(n))^k = E^k(x) + n^k(x). \tag{5.12}$$

It is obvious that replacing the field E by $\tilde{E}$ and leaving all other observables unchanged gives an equivalent representation of the observable algebra. Nevertheless, the flux field on the boundary $\partial\Sigma$ of the domain Σ is changed by $n^\perp(x)$, where "$\perp$" denotes the component orthogonal to $\partial\Sigma$.

In a subsequent paper we are going to present a similar result for lattice QCD. We shall prove that all irreducible representations of the observable algebra $\mathcal{O}(\Lambda)$ of QCD on a finite lattice are classified by the value of the global color charge Q_Λ, yielding three different superselection sectors labeled by elements of $\mathbb{Z}_3$. However, the local distribution of the (gauge invariant) gluon and antigluon fluxes $M(E(x,\infty))$ and $N(E(x,\infty))$ over the boundary $\partial\Lambda$ may be arbitrarily changed within one sector. The redistribution of fluxes is obtained by the following procedure. Take an arbitrary pair of points $\xi, \eta \in \partial\Lambda$ at the boundary and a path (collection of lattice links) $\gamma = \{(\xi, x_1), (x_1, x_2), \ldots, (x_k, \eta)\}$, connecting them. Define the following operator-valued matrix $U(\gamma) = (U^A{}_B(\gamma))$, where

$$U^A{}_B(\gamma) := \frac{1}{\sqrt{3}} U^A{}_{C_1}(\xi, x_1) U^{C_1}{}_{C_2}(x_1, x_2) \ldots U^{C_k}{}_B(x_k, \eta). \tag{5.13}$$

The action of $U(\gamma)$ on a quantum state ψ is, by definition, a collection $(U^A{}_B(\gamma)\psi)$ with an extra contravariant index A at ξ and an extra covariant index B at η. In general, the new state does not belong to any irreducible representation of SU(3) at ξ and η, even if ψ did. This means that $U(\gamma)\psi$ *is not* an eigenstate of operators $M(E(\xi,\infty))$, $N(E(\xi,\infty))$, $M(E(\eta,\infty))$, and $N(E(\eta,\infty))$, even if ψ was. Decomposing it into irreducible representations, we observe, however, that the value of $\varphi(E(\xi,\infty))$ has been changed by plus one and the value of $\varphi(E(\eta,\infty))$ has been changed by

minus one by this procedure. This suggests that these objects could also be treated as *quantum* and not as classical quantities. Then, only their sum, the global flux $\Phi_{\partial\Lambda}$, would be a classical object proportional to the identity on every superselection sector. This point of view was strongly advocated by Staruszkiewicz already a decade ago (see Ref. 18). We also refer to Ref. 19, where decoherence phenomena in QED in terms of *quantum* fluxes at infinity were discussed. We underline, however, that at the moment it is unclear, whether and if, then in which sense, intertwining operators of the type (5.13) survive in the thermodynamic limit.

(3) Finally, we stress that it does not make sense to attribute any physical meaning to the external gluon or antigluon fluxes M and N themselves. It is only the quantity $(M-N)$ ''modulo three'' which makes sense. This would hold also for the continuum theory, provided such a theory would be constructed in the future. Assume, for a moment, that a rigorous continuum QCD has been obtained as a limit of lattice theories, with surface fluxes $E^A{}_B(\Sigma) := \int_S E^A{}_B$ defined via the projective limit of finite sums corresponding to appropriate lattice approximations. Then it would not make sense to calculate quantities $N(E(\Sigma))$ or $M(E(\Sigma))$, because of the nonadditivity of functions (4.7) and (4.8). Indeed, if S has been divided into small portions, $S=\cup_\alpha S_\alpha$, we have

$$\int_S E = \sum_\alpha \int_{S_\alpha} E, \tag{5.14}$$

but the functions M, N [or even $(M-N)$] give, in general, different results when applied to both sides of Eq. (5.14). On the other hand, the function φ is additive and gives the same result when applied to both sides. This suggests that, in principle, the $\mathbb{Z}_3$-valued flux through S (equal to the sum of fluxes corresponding to its small portions S_α) could possibly survive in the continuum limit. The same argument applies to the color charge density $\varphi(\rho)$. We would then expect that the global $\mathbb{Z}_3$-valued Gauss law (5.8) could possibly survive in this ''would be'' continuum theory.

VI. DISCUSSION

We add some remarks concerning the perspectives of our approach, in which the notion of the observable algebra plays a central role. Often, one defines the observable algebra as the algebra of gauge invariant operators and imposes the Gauss law as a constraint to be fulfilled by physical states. If one discusses, for instance, the quark confinement problem in the somewhat simplified setting of QCD with infinitely heavy external charges, then this seems to be the appropriate choice. However, in our approach, we start with dynamical quarks and our final goal is a quantum theory of interacting hadrons, built from gluons and quarks. Within this strategy, all relations between (composite) physical fields, including the Gauss constraint, should be implemented on the level of the observable algebra. This point of view is strongly supported by our results for lattice QED, see Refs. 13, 14, and 20. The same strategy, applied there, yields exactly the charge superselection sectors of the theory. In these papers, we found that the observable algebra is generated by a certain Lie algebra, $u(2N)$ for spinorial QED and $u(N,N)$ for scalar QED. QCD seems to be generated by a certain Lie superalgebra—a conjecture we are actually working on. The characterization of the observable algebra in terms of a Lie (super)algebra is extremely helpful for the classification of its irreducible representations. It should be also helpful for constructing the thermodynamic limit, because for taking the limit $N\to\infty$ in the generating Lie (super)algebras there seems to exist appropriate mathematical tools for studying the resulting representations, see Ref. 21.

Finally, we stress that this work is part of a larger program, which includes both the study of gauge theoretical models in terms of gauge invariants within the functional integral approach, see Ref. 22, and the investigation of the structure of the full gauge orbit space, including singular strata, see Ref. 23. In the future, a rigorous study of singular strata within the lattice quantum theory discussed previously is also planned.

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Renormalization of Poincaré transformations in Hamiltonian semiclassical field theory

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Semiclassical Hamiltonian field theory is investigated from the axiomatic point of view. A notion of a semiclassical state is introduced. An ''elementary'' semiclassical state is specified by a set of classical field configurations and quantum states in this external field. ''Composed'' semiclassical states viewed as formal superpositions of ''elementary'' states are nontrivial only if the Maslov isotropic condition is satisfied; the inner product of ''composed'' semiclassical states is degenerate. The mathematical proof of Poincaré invariance of semiclassical field theory is obtained for ''elementary'' and ''composed'' semiclassical states. The notion of semiclassical field is introduced; its Poincaré invariance is also mathematically proved. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1453497]

I. INTRODUCTION

Different approaches to semiclassical field theory have been developed. Most of them were based on the functional integral technique: physical quantities were expressed via functional integrals which were evaluated with the help of saddle-point or stationary-phase technique. Since energy spectrum and *S*-matrix elements can be found from the functional integral,[1,2] this approach appeared to be useful for the soliton quantization theory.[1–5]

Another important partial case of the semiclassical field theory is the theory of quantization in a strong external background classical field[6] or in curved space–time:[7] one decomposes the field as a sum of a classical *c*-number component and a quantum component. Then the theory is quantized.

The one-loop approximation,[8–11] the time-dependent Hartree–Fock approximation,[8,9,12,13] and the Gaussian approximation developed in Refs. 14–17 may also be viewed as examples of applications of semiclassical conceptions.

On the other hand, the axiomatic field theory[18–20] tells us that the main objects of quantum field theory (QFT) are states and observables. The Poincaré group is represented in the Hilbert state space, so that evolution, boosts, and other Poincaré transformations are viewed as unitary operators.

The purpose of this paper is to introduce the semiclassical analogs of such QFT notions as states, fields, and Poincaré transformations. The analogs of Wightman Poincaré invariance and field axioms for the semiclassical field theory are to be formulated and checked.

Unfortunately, ''exact'' QFT is mathematically constructed for a restricted class of models only (see, e.g., Refs. 21–24). Therefore, formal approximate methods such as perturbation theory seem to be ways to quantize the field theory rather than to construct approximations for the exact solutions of QFT equations. The conception of field quantization within the perturbation framework is popular.[25,26] One can expect that the semiclassical approximation plays an analogous role.

To construct the semiclassical formalism based on the notion of a state, one should use the equation-of-motion formulation of QFT rather than the usual *S*-matrix formulation. It is well-known that additional difficulties such as Stueckelberg divergences[27] and problems associated with the Haag theorem[28,19,20] arise in the equation-of-motion approach. There are some ways to

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overcome them. The vacuum divergences can be eliminated in the perturbation theory with the help of the Faddeev transformation.[29] Stueckelberg divergences can be treated analogously[30] (exactly solvable models with Stueckelberg divergences have been suggested recently[31,32]). These investigations are important for the semiclassical Hamiltonian field theory.[33]

The semiclassical approaches are formally applicable to the quantum field theory models if the Lagrangian depends on the fields φ and the small parameter λ as follows (see, for example, Ref. 4):

$$\mathcal{L}=\frac{1}{2}\partial_\mu\varphi\partial_\mu\varphi-\frac{m^2}{2}\varphi^2-\frac{1}{\lambda}V(\sqrt{\lambda}\varphi), \tag{1.1}$$

where V is an interaction potential. To illustrate the *formal* semiclassical ansatz for the state vector, use the functional Schrödinger representation (see, e.g., Refs. 12, 13, 16, and 17). States at fixed moment of time are represented as functionals $\psi[\varphi(\cdot)]$ depending on fields $\varphi(\mathbf{x})$, $\mathbf{x}\in\mathbf{R}^d$, the field operator $\hat{\varphi}(\mathbf{x})$ is the operator of multiplication by $\varphi(\mathbf{x})$, while the canonically conjugated momentum $\hat{\pi}(\mathbf{x})$ is represented as a differentiation operator $-i\delta/\delta\varphi(\mathbf{x})$. The functional Schrödinger equation reads

$$i\frac{\mathrm{d}\psi^t}{\mathrm{d}t}=\mathcal{H}\psi^t, \tag{1.2}$$

where

$$\mathcal{H}=\int \mathrm{d}\mathbf{x}\left[-\frac{1}{2}\frac{\delta^2}{\delta\varphi(\mathbf{x})\,\delta\varphi(\mathbf{x})}+\frac{1}{2}(\nabla\varphi)^2(\mathbf{x})+\frac{m^2}{2}\varphi^2(\mathbf{x})+\frac{1}{\lambda}V(\sqrt{\lambda}\varphi(\mathbf{x}))\right].$$

The simplest semiclassical state corresponds to the Maslov theory of complex germ in a point.[34–36] It depends on the small parameter λ as

$$\begin{aligned}\psi^t[\varphi(\cdot)]&=\exp\left(\frac{i}{\lambda}S^t\right)\exp\left(\frac{i}{\lambda}\int \mathrm{d}x\,\Pi^t(\mathbf{x})[\varphi(\mathbf{x})\sqrt{\lambda}-\Phi^t(\mathbf{x})]\right)f^t\left(\varphi(\cdot)-\frac{\Phi^t(\cdot)}{\sqrt{\lambda}}\right)\\&\equiv(K_{S^t,\Pi^t,\Phi^t}f^t)[\varphi(\cdot)],\end{aligned} \tag{1.3}$$

where S^t, $\Pi^t(\mathbf{x})$, $\Phi^t(\mathbf{x})$, $t\in\mathbf{R}$, $\mathbf{x}\in\mathbf{R}^d$ are smooth real functions which rapidly damp with all their derivatives as $\mathbf{x}\to\infty$, $f^t[\phi(\cdot)]$ is a t-dependent functional.

As $\lambda\to 0$, the substitution (1.3) satisfies Eq. (1.2) in the leading order in λ if the following relations are obeyed. First, for the ''action'' S^t one finds

$$\frac{\mathrm{d}S^t}{\mathrm{d}t}=\int \mathrm{d}\mathbf{x}\left[\Pi^t(\mathbf{x})\dot{\Phi}^t(\mathbf{x})-\frac{1}{2}(\Pi^t(\mathbf{x}))^2-\frac{1}{2}(\nabla\Phi^t(\mathbf{x}))^2-\frac{m^2}{2}(\Phi^t(\mathbf{x}))^2-V(\Phi^t(\mathbf{x}))\right]. \tag{1.4}$$

Second, Π^t, Φ^t obeys the classical Hamiltonian system

$$\dot{\Phi}^t=\Pi^t,\ -\dot{\Pi}^t=(-\Delta+m^2)\Phi^t+V'(\Phi^t). \tag{1.5}$$

Finally, the functional f^t satisfies the functional Schrödinger equation with the quadratic Hamiltonian

$$i\dot{f}^t[\phi(\cdot)]=\int \mathrm{d}\mathbf{x}\left[-\frac{1}{2}\frac{\delta^2}{\delta\phi(\mathbf{x})\,\delta\phi(\mathbf{x})}+\frac{1}{2}(\nabla\phi(\mathbf{x}))^2+\frac{m^2}{2}\phi^2(\mathbf{x})+\frac{1}{2}V''(\Phi^t(\mathbf{x}))\phi^2(\mathbf{x})\right]f^t[\phi(\cdot)]. \tag{1.6}$$

There are more complicated semiclassical states that also approximately satisfy the functional Schrödinger equation (1.2). These ansatzes correspond to the Maslov theory of Lagrangian manifolds with complex germs.[34–36] They are discussed in Sec. V.

However, the QFT divergences lead to the following difficulties.

It is not evident how one should specify the class of possible functionals f and introduce the inner product on such a space via functional integral. This class was constructed in Ref. 33. In particular, it was found when the Gaussian functional

$$f[\phi(\cdot)]=\text{const}\exp\left(\frac{i}{2}\int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}\,\phi(x)\,\phi(\mathbf{y})\mathcal{R}(\mathbf{x},\mathbf{y})\right) \tag{1.7}$$

belongs to this class. The condition on the quadratic form $\mathcal{R}$ which was obtained in Ref. 33 depends on Φ, Π and differs from the analogous condition in the free theory. This is in agreement with the statement of Refs. 37 and 38 that nonequivalent representations of the canonical commutation relations at different moments of time should be considered if QFT in the strong external field is investigated in the leading order in λ. However, this does not lead to nonunitarity of the exact theory: the simple example has been presented in Ref. 32.

Another problem is to formulate the semiclassical theory in terms of the axiomatic field theory. Section II deals with formulation of axioms of relativistic invariance and field for the semiclassical theory. Section III is devoted to construction of Poincaré transformations. In Sec. IV the notion of semiclassical field is investigated. More complicated semiclassical states are constructed in Sec. V. Section VI contains concluding remarks.

II. AXIOMS OF SEMICLASSICAL FIELD THEORY

In the Wightman axiomatic approach the main object of QFT is a notion of a state space.[18–20] Formula (1.3) shows us that in the semiclassical field theory a state at fixed moment of time should be viewed as a set $(S,\Pi(\cdot),\Phi(\cdot),f[\phi(\cdot)])$ of a real number S, real functions $\Pi(\mathbf{x})$, $\Phi(\mathbf{x})$, $\mathbf{x}\in\mathbf{R}^d$, and a functional $f[\phi(\cdot)]$ from some class. This class depends on Π and Φ. Superposition of semiclassical states (S_1,Π_1,Φ_1,f_1) and (S_2,Π_2,Φ_2,f_2) is of the semiclassical type (1.3) if and only if $S_1=S_2$, $\Phi_1=\Phi_2$, $\Pi_1=\Pi_2$.

Thus, one introduces[39,40] the structure of a vector bundle (called a ''semiclassical bundle'' in Ref. 40) on the set of semiclassical states of the type (1.3). The base of the bundle being a space of sets (S,Π,Φ) (''extended phase space'' [39]) will be denoted as $\mathcal{X}$. The fibers are classes of functionals which depend on Φ and Π. Making use of the result concerning the class of functionals,[33] one makes the bundle trivial as follows. Consider the Φ, Π-dependent mapping V, which defines a correspondence between functionals f and elements of the Fock space $\mathcal{F}$:

$$V:\Psi\mapsto f,\quad \Psi\in\mathcal{F},\quad f=f[\phi(\cdot)],$$

as follows (see, e.g., Ref. 41). Let $\tilde{\mathcal{R}}(x,y)$ be an Φ, Π-dependent symmetric function such that its imaginary part is a kernel of a positively definite operator and the condition of Ref. 33 [see Eq. (3.41) in Sec. III F] is satisfied. By $\hat{\mathcal{R}}$ we denote the operator with kernel $\tilde{\mathcal{R}}$, while $\hat{\Gamma}$ has a kernel $i^{-1}(\tilde{\mathcal{R}}-\tilde{\mathcal{R}}^*)$. The vacuum vector of the Fock space corresponds to the Gaussian functional (1.7). The operator V is uniquely defined from the relations

$$\begin{aligned} V^{-1}\phi(\mathbf{x})V&=i(\hat{\Gamma}^{-1/2}(A^+-A^-))(\mathbf{x}),\\ V^{-1}\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}V&=i(\hat{\mathcal{R}}\hat{\Gamma}^{-1/2}A^+-\hat{\mathcal{R}}^*\hat{\Gamma}^{-1/2}A^-)(\mathbf{x}).\end{aligned} \tag{2.1}$$

Here $A^{\pm}(\mathbf{x})$ are creation and annihilation operators in the Fock space.

Definition 2.1: A semiclassical state is a point on the trivial bundle $\mathcal{X}\times\mathcal{F}\to\mathcal{X}$.

An important postulate of QFT is Poincaré invariance. This means that a representation of the Poincaré group in the state space should be specified. For each Poincaré transformation of the form

$$x'^{\mu}=\Lambda^{\mu}_{\nu}x^{\nu}+a^{\mu}, \quad \mu,\nu=\overline{0,d}, \tag{2.2}$$

which is denoted as (a,Λ), the unitary operator $\mathcal{U}_{a,\Lambda}$ should be specified. The group property

$$\mathcal{U}_{(a_1,\Lambda_1)}\mathcal{U}_{(a_2,\Lambda_2)}=\mathcal{U}_{(a_1,\Lambda_1)(a_2,\Lambda_2)}$$

with

$$(a_1,\Lambda_1)(a_2,\Lambda_2)=(a_1+\Lambda_1 a_2,\Lambda_1\Lambda_2)$$

should be satisfied.

Formulate an analog of the Poincaré invariance axiom for the semiclassical theory. Suppose that the Poincaré transformation $\mathcal{U}_{a,\Lambda}$ takes any semiclassical state (X,f) to a semiclassical state $(\tilde{X},\tilde{f})$ in the leading order in $\lambda^{1/2}$. Denote $\tilde{X}=u_{a,\Lambda}X$, $\tilde{f}=U(u_{a,\Lambda}X\leftarrow X)f$.

Axiom 1 (Poincaré invariance):

(*a*) *The mappings* $u_{a,\Lambda}\colon \mathcal{X}\to\mathcal{X}$ *are specified, the group properties for them* $u_{a_1,\Lambda_1}u_{a_2,\Lambda_2}=u_{(a_1,\Lambda_1)(a_2,\Lambda_2)}$ *are satisfied*;

(*b*) *for all* $X\in\mathcal{X}$ *the unitary operators* $U_{a,\Lambda}(u_{a,\Lambda}X\leftarrow X)\colon \mathcal{F}\to\mathcal{F}$, *obeying the group property*

$$\begin{aligned}&U_{a_1,\Lambda_1}(u_{(a_1,\Lambda_1)(a_2,\Lambda_2)}X\leftarrow u_{(a_2,\Lambda_2)}X)U_{a_2,\Lambda_2}(u_{(a_2,\Lambda_2)}X\leftarrow X)\\&\quad=U_{(a_1,\Lambda_1)(a_2,\Lambda_2)}(u_{(a_1,\Lambda_1)(a_2,\Lambda_2)}X\leftarrow X)\end{aligned} \tag{2.3}$$

are specified.

An important feature of QFT is the notion of a field: it is assumed that an operator distribution $\hat{\varphi}(\mathbf{x},t)$ is specified. Investigate it in the semiclassical theory. Applying the operator $\varphi(\mathbf{x})$ to the semiclassical state (1.3), we obtain an analogous state:

$$\exp\left(\frac{i}{\lambda}S^t\right)\exp\left(\frac{i}{\lambda}\int d\mathbf{x}\Pi^t(\mathbf{x})[\varphi(\mathbf{x})\sqrt{\lambda}-\Phi^t(\mathbf{x})]\right)\tilde{f}^t\left(\varphi(\cdot)-\frac{\Phi^t(\cdot)}{\sqrt{\lambda}}\right),$$

where

$$\tilde{f}^t[\phi(\cdot)]=(\lambda^{-1/2}\Phi^t(\mathbf{x})+\phi(\mathbf{x}))f^t[\phi(\cdot)].$$

As $\lambda\to 0$, one has

$$\hat{\varphi}(\mathbf{x},t)=\lambda^{-1/2}\Phi^t(\mathbf{x})+\hat{\phi}(\mathbf{x},t{:}X),$$

where $\hat{\phi}(\mathbf{x},t{:}X)$ is a Π,Φ-dependent operator in $\mathcal{F}$, $\Phi^t(\mathbf{x})\equiv\Phi(x{:}X)$ is a solution to the Cauchy problem for Eq. (1.5). The field axiom can be reformulated as follows.

Axiom 2: For each $X\in\mathcal{X}$ *the operator distribution* $\phi(\mathbf{x},t;X)\colon \mathcal{F}\to\mathcal{F}$ *is specified.*

An important feature of the relativistic quantum field theory is the property of Poincaré invariance of fields. The operator distribution $\hat{\varphi}(\mathbf{x},t)$ should obey the following property:

$$\mathcal{U}_{a,\Lambda}\hat{\varphi}(x)=\hat{\varphi}(\Lambda x+a)\mathcal{U}_{a,\Lambda}.$$

Apply this identity to a semiclassical state (X,f). In leading orders in $\lambda^{1/2}$, one obtains

$$\lambda^{-1/2}\Phi(x{:}X)(u_{a,\Lambda}X, U_{a,\Lambda}(u_{a,\Lambda}X{\leftarrow}X)f)+(u_{a,\Lambda}X, U_{a,\Lambda}(u_{a,\Lambda}X{\leftarrow}X)\hat{\phi}(x{:}X)f)$$
$$=\lambda^{-1/2}\Phi(\Lambda x+a{:}u_{a,\Lambda}X)(u_{a,\Lambda}X, U_{a,\Lambda}(u_{a,\Lambda}X{\leftarrow}X)f)$$
$$+(u_{a,\Lambda}X, \hat{\phi}(\Lambda x+a{:}u_{a,\Lambda}X)U_{a,\Lambda}(u_{a,\Lambda}X{\leftarrow}X)f).$$

Therefore, we formulate the following axiom.

Axiom 3 (Poincaré invariance of fields): The following properties are satisfied:

$$\Phi(x{:}X)=\Phi(\Lambda x+a{:}u_{a,\Lambda}X), \tag{2.4}$$

$$\hat{\phi}(\Lambda x+a{:}u_{a,\Lambda}X)U_{a,\Lambda}(u_{a,\Lambda}X{\leftarrow}X)=U_{a,\Lambda}(u_{a,\Lambda}X{\leftarrow}X)\hat{\phi}(x{:}X). \tag{2.5}$$

III. SEMICLASSICAL POINCARÉ TRANSFORMATIONS

A. Construction of Poincaré transformations in the functional representation

(1) Let us construct the mappings $u_{a,\Lambda}$ and unitary operators $U_{a,\Lambda}(u_{a,\Lambda}X{\leftarrow}X)$. Since any Poincaré transformation is a composition of time and space translations, boost and spatial rotations,

$$(a,\Lambda)=(a^0,1)(\mathbf{a},1)(0,\exp(\alpha^k I^{0k}))(0,\exp(\tfrac{1}{2}\theta_{sm}I^{sm}))$$

with $\theta_{sm}=-\theta_{ms}$,

$$(I^{\lambda\mu})^{\alpha}_{\beta}=-g^{\lambda\alpha}\delta^{\mu}_{\beta}+g^{\mu\alpha}\delta^{\lambda}_{\beta},$$

it is sufficient to specify operators $U_{a,\Lambda}$ for these special cases and then apply a group property.

In the ''exact'' theory, the operator $\mathcal{U}_{a,\Lambda}$ has the form

$$\mathcal{U}_{a,\Lambda}=\exp[i\mathcal{P}^0a^0]\exp[-i\mathcal{P}^ja^j]\exp[i\alpha^k\mathcal{M}^{0k}]\exp\left[\frac{i}{2}\mathcal{M}^{lm}\theta_{lm}\right]. \tag{3.1}$$

The momentum and angular momentum operators entering to formula (3.1) have the well-known form (see, e.g., Ref. 25)

$$\mathcal{P}^{\mu}=\int d\mathbf{x}\, T^{\mu 0}(\mathbf{x}), \quad \mathcal{M}^{\mu\lambda}=\int d\mathbf{x}[x^{\mu}T^{\lambda 0}(\mathbf{x})-x^{\lambda}T^{\mu 0}(\mathbf{x})], \tag{3.2}$$

where formally

$$T^{00}=\frac{1}{2}\hat{\pi}^2+\frac{1}{2}\partial_i\hat{\varphi}\partial_i\hat{\varphi}+\frac{m^2}{2}\hat{\varphi}^2+\frac{1}{\lambda}V(\sqrt{\lambda}\hat{\varphi}), \quad T^{k0}=-\partial_k\hat{\varphi}\hat{\pi}.$$

We are going to apply the operator (3.1) to the semiclassical state (1.3). Note that the operators $\mathcal{P}^{\mu}$ and $\mathcal{M}^{\mu\nu}$ (3.2) depend on field $\hat{\varphi}$ and momentum $\hat{\pi}$ semiclassically,

$$\mathcal{P}^{\mu}=\frac{1}{\lambda}P^{\mu}(\sqrt{\lambda}\hat{\pi}(\cdot),\sqrt{\lambda}\hat{\varphi}(\cdot)), \quad \mathcal{M}^{\mu\nu}=\frac{1}{\lambda}M^{\mu\nu}(\sqrt{\lambda}\hat{\pi}(\cdot),\sqrt{\lambda}\hat{\varphi}(\cdot)),$$

It is convenient to consider the more general problem (cf. Ref. 35). Let us find as $\lambda\to 0$ the state

$$\exp(-i\mathcal{A})K_{S^0,\Pi^0,\Phi^0}f^0, \tag{3.3}$$

where $K_{S,\Pi,\Phi}$ has the form (1.3),

$$\mathcal{A}=\frac{1}{\lambda}A(\sqrt{\lambda}\,\hat{\pi}(\cdot),\sqrt{\lambda}\,\hat{\varphi}(\cdot)).$$

Note that the state functional (3.3) may be viewed as a solution to the Cauchy problem of the form

$$\begin{gathered} i\frac{\partial\Psi^{\tau}}{\partial\tau}=\frac{1}{\lambda}A\left(\frac{\sqrt{\lambda}}{i}\frac{\delta}{\delta\varphi(\cdot)},\sqrt{\lambda}\,\varphi(\cdot)\right)\Psi^{\tau}, \\ \Psi^{0}[\varphi(\cdot)]=(K_{S^0,\Pi^0,\Phi^0}f^0)[\varphi(\cdot)] \end{gathered} \tag{3.4}$$

at $\tau=1$. Let us look for the asymptotic solution to Eq. (3.4) in the following form:

$$\Psi^{\tau}[\varphi(\cdot)]=(K_{S^{\tau},\Pi^{\tau},\Phi^{\tau}}f^{\tau})[\varphi(\cdot)]. \tag{3.5}$$

Substitution of functional (3.5) to Eq. (3.4) gives us the following relation:

$$\begin{aligned} &\left[-\frac{1}{\lambda}\left(\dot{S}^{\tau}-\int \mathrm{d}x\,\Pi^{\tau}(\mathbf{x})\dot{\Phi}^{\tau}(\mathbf{x})\right)-\frac{1}{\sqrt{\lambda}}\int \mathrm{d}\mathbf{x}\left(\dot{\Pi}^{\tau}(\mathbf{x})\phi(\mathbf{x})+\dot{\Phi}^{\tau}(\mathbf{x})i\frac{\delta}{\delta\phi(\mathbf{x})}\right)+i\frac{\partial}{\partial\tau}\right]f^{\tau}[\phi(\cdot)] \\ &\quad=\frac{1}{\lambda}A\left(\Pi^{\tau}(\cdot)-i\sqrt{\lambda}\frac{\delta}{\delta\phi(\cdot)},\Phi^{\tau}(\cdot)+\sqrt{\lambda}\,\phi(\cdot)\right)f^{\tau}[\phi(\cdot)]. \end{aligned} \tag{3.6}$$

Considering the terms of the orders $O(\lambda^{-1})$, $O(\lambda^{-1/2})$ and $O(1)$ in Eq. (3.6), we obtain

$$\dot{S}^{\tau}=\int \mathrm{d}\mathbf{x}(\Pi^{\tau}(\mathbf{x})\dot{\Phi}^{\tau}(\mathbf{x})-A(\Pi^{\tau}(\cdot),\Phi^{\tau}(\cdot)), \tag{3.7}$$

$$\dot{\Phi}^{\tau}(\mathbf{x})=\frac{\delta A(\Pi^{\tau}(\cdot),\Phi^{\tau}(\cdot))}{\delta\Pi(\mathbf{x})},\quad \dot{\Pi}^{\tau}(\mathbf{x})=-\frac{\delta A(\Pi^{\tau}(\cdot),\Phi^{\tau}(\cdot))}{\delta\Phi(\mathbf{x})}, \tag{3.8}$$

$$\begin{aligned} i\frac{\partial f^{\tau}[\Phi(\cdot)]}{\partial\tau}=&\left(\int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}\left[\frac{1}{2}\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}\frac{\delta^2A}{\delta\Pi(\mathbf{x})\delta\Pi(\mathbf{y})}\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{y})}+\phi(\mathbf{x})\frac{\delta^2A}{\delta\Phi(\mathbf{x})\delta\Pi(\mathbf{y})}\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{y})}\right.\right. \\ &\left.\left.+\frac{1}{2}\phi(\mathbf{x})\frac{\delta^2A}{\delta\Phi(\mathbf{x})\delta\Phi(\mathbf{y})}\phi(\mathbf{y})\right]+A_1\right)f^{\tau}[\phi(\cdot)]. \end{aligned} \tag{3.9}$$

Here A_1 is a c-number quantity which depends on the ordering of the operators $\hat{\varphi}$ and $\hat{\pi}$ and is relevant to the renormalization problem.

We see that for the cases $\mathcal{A}=-\mathcal{P}^0a^0$, $\mathcal{A}=\mathcal{P}^ja^j$, $\mathcal{A}=-\alpha^k\mathcal{M}^{0k}$, $\mathcal{A}=(1/2)\theta_{sm}\mathcal{M}^{sm}$ the mapping $u_{a,\Lambda}$ takes the initial condition for the system (3.7), (3.8) to the solution of the Cauchy problem for this system at $\tau=1$. The operators $\tilde{U}_{a,\Lambda}$ transform the initial condition for Eq. (3.9) to the solution at $\tau=1$.

(2) The classical mappings $u_{a,\Lambda}$ for our partial cases are presented in Table I.

One can write down the following general formula. Let (a,Λ) be an arbitrary Poincaré transformation. It happens that the mapping $u_{a,\Lambda}:(S,\Pi,\Phi)\mapsto(\tilde{S},\tilde{\Pi},\tilde{\Phi})$ has the following form. Let $\Phi(\mathbf{x},t)\equiv\Phi(x)$ be a solution of the Cauchy problem

$$\begin{gathered} \partial_{\mu}\partial^{\mu}\Phi(x)+m^2\Phi(x)+V'(\Phi(x))=0, \\ \Phi(\mathbf{x},0)=\Phi(\mathbf{x}),\quad \frac{\partial}{\partial t}\Phi(\mathbf{x},t)\big|_{t=0}=\Pi(\mathbf{x}). \end{gathered} \tag{3.10}$$

Denote

TABLE I. Poincaré transformations in classical theory.

Element of Poincaré group (a_τ,Λ_τ)	Classical Poincaré transformation $u_{a_\tau,\Lambda_\tau}:(S^0,\Pi^0,\Phi^0)\mapsto(S^\tau,\Pi^\tau\Phi^\tau)$	Classical Lie derivative $\delta F(S,\Pi,\Phi)=\frac{\mathrm{d}}{\mathrm{d}\tau}\Big\vert_{\tau=0} F(S^\tau,\Pi^\tau,\Phi^\tau)$
$a_\tau=0$	$\Phi^\tau(\mathbf{x})=\Phi^0\left(\exp\left(-\frac{\tau}{2}l^{sm}\theta_{sm}\right)\mathbf{x}\right)$	$\frac{1}{2}\theta_{lm}\delta^{lm}_M=\frac{1}{2}\theta_{lm}\int \mathrm{d}\mathbf{x}\left((x^l\partial_m-x^m\partial_l)\Phi(\mathbf{x})\frac{\delta}{\delta\Phi(\mathbf{x})}+(x^l\partial_m-x^m\partial_l)\Pi(\mathbf{x})\frac{\delta}{\delta\Pi(\mathbf{x})}\right)$
$\Lambda_\tau=\exp\left(\frac{\tau}{2}l^{sm}\theta_{sm}\right)$	$\Pi^\tau(\mathbf{x})=\Pi^0\left(\exp\left(-\frac{\tau}{2}l^{sm}\theta_{sm}\right)\mathbf{x}\right)$	
Spatial rotaion	$S^\tau=S^0$	
$a^0_\tau=0$, $\Lambda_\tau=1$	$\Phi^\tau(\mathbf{x})=\Phi^0(\mathbf{x}-\mathbf{b}\tau)$	$-b^k\delta^k_P=-b^k\int \mathrm{d}\mathbf{x}\left(\partial_k\Phi(\mathbf{x})\frac{\delta}{\delta\Phi(\mathbf{x})}+\partial_k\Pi(\mathbf{x})\frac{\delta}{\delta\Pi(\mathbf{x})}\right)$
$\mathbf{a}_\tau=\mathbf{b}\tau$	$\Pi^\tau(\mathbf{x})=\Pi^0(\mathbf{x}-\mathbf{b}\tau)$	
Spatial translation	$S^\tau=S^0$	
$a^0=-\tau\,\mathbf{a}=0$	Resolving operator for the Cauchy problem $\dot\Phi^\tau=\Pi^\tau$	$-\delta_H=\int \mathrm{d}\mathbf{x}\left[\Pi(\mathbf{x})\frac{\delta}{\delta\Phi(\mathbf{x})}-(-\Delta\Phi(\mathbf{x})+m^2\Phi(\mathbf{x})+V'(\Phi(\mathbf{x})))\frac{\delta}{\delta\Pi(\mathbf{x})}\right]-i\mathrm{d}\mathbf{x}\left[\frac{1}{2}\Pi^2(\mathbf{x})-\frac{1}{2}(\nabla\Phi(\mathbf{x}))^2-\frac{m^2}{2}\Phi^2(\mathbf{x})-V(\Phi(\mathbf{x}))\right]\frac{\partial}{\partial S}.$
$\Lambda=1$	$-\dot\Pi^\tau=(-\Delta+m^2)\Phi^\tau+V'(\Phi^\tau)$	
Evolution	$\dot S^\tau=\int \mathrm{d}\mathbf{x}\left[\Pi^\tau\dot\Phi^\tau-\frac{1}{2}(\Pi^\tau)^2-\frac{1}{2}(\nabla\Phi_\tau)^2-\frac{m^2}{2}(\Phi^\tau)^2-V(\Phi^\tau)\right].$	
$a_\tau=0$	Resolving operator for the Cauchy problem $\dot\Phi^\tau=n^kx^k\Pi^\tau$	$-n^m\delta^m_B=n^m\int \mathrm{d}\mathbf{x}\left[x^m\Pi(\mathbf{x})\frac{\delta}{\delta\Phi(\mathbf{x})}-(-\partial_ix^m\partial_i\Phi(\mathbf{x})+x^mm^2\Phi(\mathbf{x})+x^mV'(\Phi(\mathbf{x})))\frac{\delta}{\delta\Pi(\mathbf{x})}\right]+n^m\int \mathrm{d}\mathbf{x}\,x^m\left[\frac{1}{2}\Pi^2(\mathbf{x})-\frac{1}{2}(\nabla\Phi(\mathbf{x}))^2-\frac{m^2}{2}\Phi^2(\mathbf{x})-V(\Phi(\mathbf{x}))\right]\frac{\partial}{\partial S}.$
$\Lambda_\tau=\exp[-\pi m^kl^{k0}]$	$-\dot\Pi^\tau=-\nabla x^kn^k\nabla\Phi^\tau+x^kn^k(m^2\Phi^\tau+V'(\Phi^\tau))$	
Boost	$\dot S^\tau=\int \mathrm{d}\mathbf{x}\left[\Pi^\tau\dot\Phi^\tau-x^kn^k\frac{1}{2}(\Pi^\tau)^2+\frac{1}{2}(\nabla\Phi^\tau)^2+\frac{m^2}{2}(\Phi^\tau)^2+V(\Phi^\tau)\right]$	

$$\check{\Phi}(x)=\Phi(\Lambda^{-1}(x-a)).$$

It appears that

$$\tilde{\Phi}(\mathbf{x})=\check{\Phi}(\mathbf{x},0),\quad \tilde{\Pi}(\mathbf{x})=\frac{\partial}{\partial t}\check{\Phi}(\mathbf{x},t)\big|_{t=0},$$

$$\tilde{S}=S+\int \mathrm{d}x[\,\theta(x^0)\,\theta(-(\Lambda x+a)^0)-\theta(-x^0)\,\theta((\Lambda x+a)^0)]$$
$$\times\left[\frac{1}{2}\,\partial_\mu\Phi(x)\partial^\mu\Phi(x)-\frac{m^2}{2}\Phi^2(x)-V(\Phi(x)).\right. \tag{3.11}$$

For spatial translations, rotations, and evolution, agreement between (3.11) and Table I is evident. Consider the x^1-boost case, $n^k=(1,0,...,0)$. One has

$$\tilde{\Phi}_\tau(\mathbf{x})=\Phi(x^1\cosh\tau+x^0\sinh\tau,x^2,\ldots,x^d,x^0\cosh\tau+x^1\sinh\tau)\big|_{x^0=0},$$

$$\tilde{\Pi}_\tau(\mathbf{x})=\frac{\partial}{\partial x^0}\Phi(x^1\cosh\tau+x^0\sinh\tau,x^2,\ldots,x^d,x^0\cosh\tau+x^1\sinh\tau)\big|_{x^0=0}.$$

The functions Φ_τ, Π_τ obey the system presented in Table I. For the integral for $\tilde{S}$, consider the substitution $x^0=y^1\sinh\tilde{\tau}$, $x^1=y^1\cosh\tilde{\tau}$, $x^2=y^2,\ldots,x^d=y^d$. One finds

$$\tilde{S}^\tau=S+\int_0^\tau \mathrm{d}\tilde{\tau}y^1\,\mathrm{d}\mathbf{y}\left[\frac{1}{2}(\tilde{\Pi}_\tau(y))^2-\frac{1}{2}(\nabla\tilde{\Phi}_\tau(\mathbf{y}))^2-\frac{m^2}{2}\tilde{\Phi}_\tau^2(\mathbf{y})-V(\tilde{\Phi}_\tau(\mathbf{y}))\right],$$

which agrees with Table I.

One can also notice that the group property for Eq. (3.11) is satisfied.

Let us make more precise the definition of the space χ.

Definition 3.1: χ *is a space of sets* (S,Π,Φ) *of a number S and functions* $\Pi,\Phi\in S(\mathbf{R}^d)$ *such that there exists a unique solution of the Cauchy problem (3.10) such that the functions* $\Phi(\Lambda x+a)\big|_{x^0=0}$ *and* $\partial_\mu\Phi(\Lambda x+a)\big|_{x^0=0}$ *are of the class* $S(\mathbf{R}^d)$ *for all* $a.\Lambda$.

We see that the transformation $u_{a,\Lambda}:\chi\to\chi$ is defined.

(3) The operators $\tilde{U}_{a,\Lambda}(u_{a,\Lambda}X\leftarrow X)$ are presented in Table II.

However, it is not easy to check the group property (2.3). It is much more convenient to investigate the infinitesimal Poincaré transformations and check the algebraic analog of (2.3).

It happens that operators $\tilde{U}_{a,\Lambda}(u_{a,\Lambda}X\leftarrow X)$ induce a Poincaré group representation in a specific space. It is a space of sections $f(x;\phi(\cdot))$ of the semiclassical bundle. The operators $\check{\tilde{U}}_{a,\Lambda}$ act as

$$(\check{\tilde{U}}_{a,\Lambda}f)(X)=\tilde{U}_{a,\Lambda}(X\leftarrow u_{a,\Lambda}^{-1}X)f(u_{a,\Lambda}^{-1}X). \tag{3.12}$$

The group property for the operators $\check{\tilde{U}}$ is equivalent to relation (2.3). Let $(a_{\mathrm{tau}},\Lambda_\tau)$ be a one-parametric subgroup of the Poincaré group with the tangent vector A being an element of the Poincaré algebra. Since the operator $\tilde{U}_{a_\tau,\Lambda_\tau}(u_{a_\tau,\Lambda_\tau}X\leftarrow X)$ takes the initial condition for the Cauchy problem for

$$i\dot{f}_\tau=\tilde{H}(A:u_{a_\tau\Lambda_\tau}X)f_\tau$$

to the solution of this equation, therefore, the generator of representation (3.12) is

TABLE II. Semiclassical Poincaré transformations in functional representation.

Element of Poincaré group (a_τ,Λ_τ)	Semiclassical operator $U_{a_\tau,\Lambda_\tau}(u_{a_\tau,\Lambda_\tau}X\leftarrow X)$: $f_0\mapsto f_\tau$ in the functional representation takes the initial condition for the Cauchy problem to the solution of the Cauchy problem for the equation:
$a_\tau=0$	$i\dot{f}^\tau[\phi(\cdot)]=-\frac{1}{2}\theta_{sm}\tilde{M}^{sm}(X_\tau)f_\tau[\phi(\cdot)]$
$\Lambda_\tau=\exp\left(\frac{\tau}{2}I^{sm}\theta_{sm}\right)$;	$\tilde{M}^{sm}=-\int d\mathbf{x}[(x^s\partial_m-x^m\partial_s)\phi(\mathbf{x})]\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}$
Spatial rotation	
$a^0_\tau=0\ \Lambda_\tau=1$	$i\dot{f}^\tau[\phi(\cdot)]=b^k\tilde{P}^k(X_\tau)f_\tau[\phi(\cdot)]$
$\mathbf{a}_\tau=\mathbf{b}\tau$	$\tilde{P}^k=-\int d\mathbf{x}\,\partial_k\phi(\mathbf{x})\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}$
Spatial translation	
$a^0=-\tau\ \mathbf{a}=0$	$i\dot{f}^\tau[\phi(\cdot)]=\tilde{H}(X_\tau)f_\tau[\phi(\cdot)]$
$\Lambda=1$	$\tilde{H}=\int d\mathbf{x}\left[-\frac{1}{2}\frac{\delta^2}{\delta\phi(\mathbf{x})\delta\phi(\mathbf{x})}+\frac{1}{2}(\nabla\phi)^2(\mathbf{x})+\frac{m^2}{2}\phi^2(\mathbf{x})+\frac{1}{2}V''(\Phi(\mathbf{x}))\phi^2(\mathbf{x})\right]$
Evolution	
$a_\tau=0$	$i\dot{f}^\tau[\phi(\cdot)]=n^m\tilde{B}^m(X_\tau)f_\tau[\phi(\cdot)]$
$\Lambda_\tau=\exp[-\tau n^k l^{k0}]$;	$\tilde{B}^m=\int d\mathbf{x}\,x^m\left[-\frac{1}{2}\frac{\delta^2}{\delta\phi(\mathbf{x})\delta\phi(\mathbf{x})}+\frac{1}{2}(\nabla\phi)^2(\mathbf{x})+\frac{m^2}{2}\phi^2(\mathbf{x})+\frac{1}{2}V''(\Phi(\mathbf{x}))\phi^2(\mathbf{x})\right]$
Boost	

$$(\check{\tilde{H}}(A)f)(X)=i\frac{d}{d\tau}|_{\tau=0}(\check{\tilde{u}}_{a_\tau,\Lambda_\tau}f)(X)=[\tilde{H}(A:X)-i\delta[A]]f(X),$$

where

$$\delta[A]=\frac{d}{d\tau}|_{\tau=0}f(u_{a_\tau,\Lambda_\tau}X)$$

is a Lie derivative presented in Table I. Therefore, the infinitesimal analog of the group property (2.3) is

$$[\tilde{H}(A_1:X)-i\delta[A_1];\tilde{H}(A_2:X)-i\delta[A_2]]=i(\tilde{H}([A_1;A_2]:X)-i\delta[A_1;A_2]]). \tag{3.13}$$

It follows from the notations of Tables I and II that relation (3.13) can be rewritten for the Poincaré algebra as

$$\begin{gathered}[\check{\tilde{P}}^\lambda,\check{\tilde{P}}^\mu]=0,\quad [\check{\tilde{M}}^{\lambda\mu},\check{\tilde{P}}^\sigma]=i(g^{\mu\sigma}\check{\tilde{P}}^\lambda-g^{\lambda\sigma}\check{\tilde{P}}^\mu)\\ [\check{\tilde{M}}^{\lambda\mu},\check{\tilde{M}}^{\rho\sigma}]=-i(g^{\lambda\rho}\check{\tilde{M}}^{\mu\sigma}-g^{\mu\rho}\check{\tilde{M}}^{\lambda\sigma}+g^{\mu\sigma}\check{\tilde{M}}^{\lambda\rho}-g^{\lambda\sigma}\check{\tilde{M}}^{\mu\rho})\end{gathered} \tag{3.14}$$

for operators

$$\check{\tilde{M}}^{ms}=\tilde{M}^{ms}+i\delta^{ms}_M,\quad \check{\tilde{P}}^m=\tilde{P}^m+i\delta^m_P,\quad \check{\tilde{P}}^0=\check{H}+i\delta_H,\quad \check{M}^{k0}=\tilde{B}^k+i\delta^k_B.$$

It is checked by direct calculations that Eq. (3.14) is *formally* satisfied. However, there is a problem of divergences and renormalization which requires more careful investigations.

B. Semiclassical Poincaré transformations in Fock space

For renormalization, let us construct the semiclassical Poincaré transformations in the Fock space. They are related with the constructed operators $\tilde{U}_{a,\Lambda}(u_{a,\Lambda}X \leftarrow X)$ by

$$\tilde{U}_{a,\Lambda}(u_{a,\Lambda}X \leftarrow X) = V_{u_{a,\Lambda}X} U_{a,\Lambda}(u_{a,\Lambda}X \leftarrow X) V_X^{-1}. \tag{3.15}$$

The operator V taking the Fock space vector $\Psi \in \mathcal{F}$ to the functional $f[\phi(\cdot)]$ is defined from the relation

$$V: |0\rangle \mapsto c \exp\left[\frac{i}{2}\int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}\tilde{\mathcal{R}}(\mathbf{x},\mathbf{y})\phi(\mathbf{x})\phi(\mathbf{y})\right] \tag{3.16}$$

and from formula (2.1), which can be rewritten as

$$\begin{aligned} VA^+(\mathbf{x})V^{-1} &= \mathcal{A}^+(\mathbf{x}) \equiv \left(\hat{\Gamma}^{-1/2}\hat{\mathcal{R}}^*\phi - \hat{\Gamma}^{-1/2}\frac{1}{i}\frac{\delta}{\delta\phi}\right)(\mathbf{x}), \\ VA^-(\mathbf{x})V^{-1} &= \mathcal{A}^-(\mathbf{x}) \equiv \left(\hat{\Gamma}^{-1/2}\hat{\mathcal{R}}_\phi - \hat{\Gamma}^{-1/2}\frac{1}{i}\frac{\delta}{\delta\phi}\right)(\mathbf{x}). \end{aligned} \tag{3.17}$$

$|c|$ can be formally found from the normalization condition

$$|c|^2 \int D\phi \left|\exp\left[\frac{i}{2}\int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}\phi(\mathbf{x})\tilde{\mathcal{R}}(\mathbf{x},\mathbf{y})\phi(\mathbf{y})\right]\right|^2 = 1. \tag{3.18}$$

The argument can be chosen to be arbitrary, for example,

$$\operatorname{Arg} c = 0. \tag{3.19}$$

Notice that the operator V is defined from the relations (3.16)–(3.19) uniquely.

Namely, any element of the Fock space can be presented[42] via its components, vacuum state and creation operators as

$$\Psi = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \int \mathrm{d}\mathbf{x}_1 \cdots \mathrm{d}\mathbf{x}_n \Psi_n(\mathbf{x}_1,\ldots,\mathbf{x}_n) A^+(\mathbf{x}_1)\cdots A^+(\mathbf{x}_n)|0\rangle$$

Specify

$$V\Psi = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \int \mathrm{d}\mathbf{x}_1 \cdots \mathrm{d}\mathbf{x}_n \Psi_n(\mathbf{x}_1,\ldots,\mathbf{x}_n) \mathcal{A}^+(\mathbf{x}_1)\cdots\mathcal{A}^+(\mathbf{x}_n)V|0\rangle.$$

The problem of divergence of the series is related with the problem of correctness of the functional Schrödinger representation. It is not investigated here.

Since the operators $\mathcal{A}^\pm(\mathbf{x})$ satisfy usual canonical commutation relations and $\mathcal{A}^-(\mathbf{x})|0\rangle = 0$, we obtain $VA^\pm(\mathbf{x}) = \mathcal{A}^\pm(\mathbf{x})V$.

The operator V depends on $\mathcal{R}$. It is useful to find an explicit form of the operator $V^{-1}\delta V$.

It happens that the following property is satisfied:

$$\begin{aligned} V^{-1}\delta V = &-\frac{i}{2}A^+\hat{\Gamma}^{-1/2}\delta\hat{\mathcal{R}}\hat{\Gamma}^{-1/2}A^+ - \frac{i}{2}A^-\hat{\Gamma}^{-1/2}\delta\hat{\mathcal{R}}^*\hat{\Gamma}^{-1/2}A^- \\ &+ A^+[\hat{\Gamma}^{1/2}\delta\hat{\Gamma}^{-1/2} + i\hat{\Gamma}^{-1/2}\delta\hat{\mathcal{R}}^*\hat{\Gamma}^{-1/2}]A^- + \frac{i}{4}\operatorname{Tr}[\delta(\hat{\mathcal{R}}+\hat{\mathcal{R}}^*)\hat{\Gamma}^{-1}]. \end{aligned} \tag{3.20}$$

The notations of the type $A^+\hat{\mathcal{B}}A^-$ are used for the operators like $\int d\mathbf{x}\,d\mathbf{y}A^+(\mathbf{x})\tilde{\mathcal{B}}(\mathbf{x},\mathbf{y})A^-(\mathbf{y})$, where $\tilde{\mathcal{B}}(\mathbf{x},\mathbf{y})$ is a kernel of the operator $\hat{\mathcal{B}}$.

To check formula (3.20), consider the variation of the formula (2.1) if $\mathcal{R}$ is varied:

$$[A^{\pm}(\mathbf{x});V^{-1}\delta V]=(\hat{\Gamma}^{1/2}\delta\hat{\Gamma}^{-1/2}A^{\pm})(\mathbf{x})-i(\hat{\Gamma}^{-1/2}\delta\hat{\mathcal{R}}\hat{\Gamma}^{-1/2}A^{+})(\mathbf{x})+i(\hat{\Gamma}^{-1/2}\delta\hat{\mathcal{R}}^{*}\hat{\Gamma}^{-1/2}A^{-})(\mathbf{x}).$$

Therefore, formula (3.20) is correct up to an additive constant. To find it, note that

$$\delta V|0\rangle=\left[\frac{i}{2}\int d\mathbf{x}\,d\mathbf{y}\;\phi(\mathbf{x})\,\delta\tilde{\mathcal{R}}(\mathbf{x},\mathbf{y})\,\phi(\mathbf{y})+\delta\ln c\right]V|0\rangle.$$

This relation and formula (2.1) imply

$$\langle 0|V^{-1}\delta V|0\rangle=\frac{i}{2}\mathrm{Tr}(\delta\hat{\mathcal{R}}\hat{\Gamma}^{-1})+\delta\ln c.$$

It follows from the normalization conditions (3.18) and (3.19) that $c=(\det\hat{\Gamma})^{1/4}$. Therefore, $\delta\ln c=\frac{1}{4}\mathrm{Tr}\,\delta\hat{\Gamma}\hat{\Gamma}^{-1}$. Thus, $\langle 0|V^{-1}\delta V|0\rangle=(i/4)\mathrm{Tr}\,\delta(\hat{\mathcal{R}}+\hat{\mathcal{R}}^{*})\Gamma^{-1}$. Formula (3.20) is checked.

It follows from formula (3.15) that the generators $H(A:X)$ in the Fock representation are related with $\tilde{H}(A:X)$ by the following relation:

$$\breve{H}(A:X)=H(A:X)-i\,\delta[A]=V_x^{-1}(\tilde{H}[A:X]-i\,\delta[A])V_x.$$

We see that commutation relations (3.13) are invariant under change of representation.

An explicit form of operators $H(A:X)$ will be simplified if we consider the case when the quadratic form $\mathcal{R}$ is invariant under spatial translations and rotations:

$$\tilde{\mathcal{R}}(\mathbf{x},\mathbf{y}:u_{(\mathbf{a},L)}X)=\tilde{\mathcal{R}}(L^{-1}(\mathbf{x}-\mathbf{a}),L^{-1}(\mathbf{y}-\mathbf{a}):X). \tag{3.21}$$

This property implies that

$$\begin{gathered}[\partial_k;\hat{\mathcal{R}}]=\delta_P^k\hat{\mathcal{R}},\quad [\partial_k;\hat{\Gamma}^{1/2}]=\delta_P^k\hat{\Gamma}^{1/2},\\ [(x^k\partial_l-x^l\partial_k);\hat{\mathcal{R}}]=\delta_M^{kl}\hat{\mathcal{R}},\quad [(x^k\partial_l-x^l\partial_k);\hat{\Gamma}^{1/2}]=\delta_M^{kl}\hat{\Gamma}^{1/2}.\end{gathered} \tag{3.22}$$

The generators $H(A:X)$ are presented in Table III.

We see that renormalization is necessary since the evolution and boost generators contain divergent terms $\frac{1}{4}\mathrm{Tr}\,\hat{\Gamma}$ and $\frac{1}{4}\mathrm{Tr}\,x^k\hat{\Gamma}$ which are to be changed by finite renormalizaed terms $\frac{1}{4}\mathrm{Tr}_R\hat{\Gamma}$ and $\frac{1}{4}\mathrm{Tr}_R x^k\hat{\Gamma}$.

Let us check the commutation relations between $\breve{H}(A:X)$. Since the divergences arise in terms $\overline{B^k}$ and $\overline{H}$ only, we suppose them to be arbitrary and then find the conditions that provide Poincaré invariance.

Let

$$\breve{H}_k=\tfrac{1}{2}A^+\mathcal{H}_k^{++}A^++A^+\mathcal{H}^{+-}A^-+\tfrac{1}{2}A^-\mathcal{H}^{--}A^-+\overline{H_k+}\,i\,\delta_k$$

be arbitrary quadratic Hamiltonians. Then the property $[\breve{H}_1,\breve{H}_2]=i\breve{H}_3$ under condition $[i\,\delta_1,i\,\delta_2]=i^2\delta_3$ means that

$$\mathcal{H}_3^{++}=-i[\mathcal{H}_1^{+-}\mathcal{H}_2^{++}+\mathcal{H}_2^{++}(\mathcal{H}_1^{+-})^{*}-\mathcal{H}_1^{++}(\mathcal{H}_2^{+-})^{*}-\mathcal{H}_2^{+-}\mathcal{H}_1^{++}]+\delta_1\mathcal{H}_2^{++}-\delta_2\mathcal{H}_1^{++}, \tag{3.23}$$

TABLE III. Semiclassical Poincaré transformations in Fock representation.

Element of Poincaré group (a_τ,Λ_τ)	Semiclassical operator $U_{a_\tau,\Lambda_\tau}(u_{a_\tau,\Lambda_\tau}X\leftarrow X):\Psi_0\mapsto\Psi_\tau$ in the Fock representation takes the initial condition for the Cauchy problem to the solution of the Cauchy problem for the equation:
$a_\tau=0$	$i\dot{\Psi}^\tau=-\frac{1}{2}\theta_{sm}M^{sm}\Psi_\tau$
$\Lambda_\tau=\exp\left(\frac{\tau}{2}I^{sm}\theta_{sm}\right)$	$M^{kl}=-iA^+(x^k\partial_l-x^l\partial_k)A^-$
Spatial rotation	
$a_\tau^0=0\ \Lambda_\tau=1$	$i\Psi^\tau=b^kP^k\Psi_\tau$
$\mathbf{a}_\tau=\mathbf{b}\tau$	$P^k=-iA^+\partial_kA^-$
Spatial translation	
$a^0=-\dot{\tau},\ \mathbf{a}=0$	$i\dot{\Psi}^\tau=H(X_\tau)\Psi_\tau$
$\Lambda=1$	$H(X)=\frac{1}{2}A^-\mathcal{H}^{--}(X)A^-+A^+(\hat{\omega}+\mathcal{H}(X))A^-+\frac{1}{2}A^+\mathcal{H}^{++}(X)A^++\overline{H}$
	$\mathcal{H}^{++}(X)=\hat{\Gamma}^{-1/2}[\delta_H\hat{\mathcal{R}}-\hat{\mathcal{R}}\hat{\mathcal{R}}-(-\Delta+m^2+V''(\Phi(\mathbf{x}))]\hat{\Gamma}^{-1/2}$
	$\mathcal{H}^{--}(X)=(\mathcal{H}^{++})^+$
	$\mathcal{H}(X)=\hat{\Gamma}^{-1/2}(\hat{\mathcal{R}}\hat{\mathcal{R}}^*+(-\Delta+m^2+V'')\Phi(\mathbf{x}))-\frac{1}{2}\delta_H(\hat{\mathcal{R}}+\hat{\mathcal{R}}^x)$ $+\frac{i}{2}[\delta_H\hat{\Gamma}^{1/2};\hat{\Gamma}^{1/2};\hat{\Gamma}^{1/2}])\hat{\Gamma}^{-1/2}-\hat{\omega}$
	$\hat{\omega}=\sqrt{-\Delta+m^2}$
	Formally $\overline{H}=\overline{H}_{\mathrm{reg}}+\frac{1}{4}\mathrm{Tr}\hat{\Gamma}$
	$\overline{H}_{\mathrm{reg}}=-\frac{1}{4}\mathrm{Tr}[\mathcal{H}^{++}+\mathcal{H}^{--}]$
	$i\dot{\Psi}^\tau=n^mB^m(X_\tau)\Psi_\tau$
Evolution	
$a_\tau=0$	$B^k(X)=\frac{1}{2}A^-\mathcal{B}^{k--}(X)A^-+A^+(L_k+\mathcal{B}^k(X))A^-+\frac{1}{2}A^+\mathcal{B}^{k++}(X)A^++\overline{B^k}$
$\Lambda_\tau=\exp[-\tau m^kl^{k0}];$	$\mathcal{B}^{k++}(X)=\hat{\Gamma}^{-1/2}[\delta_k^B\hat{\mathcal{R}}-\hat{\mathcal{R}}x^k\hat{\mathcal{R}}-(-\partial_ix^k\partial_i+x^km^2+x^kV''(\Phi(\mathbf{x})))]\hat{\Gamma}^{-1/2}$
	$\mathcal{B}^{k--}=(\mathcal{B}^{++})^+$
	$\mathcal{B}^k=\hat{\Gamma}^{-1/2}\Big[\hat{\mathcal{R}}x^k\hat{\mathcal{R}}^*+(-\partial_ix^k\partial_i+x^km^2+x^kV''(\Phi(\mathbf{x})))$ $-\frac{1}{2}\delta_B^k(\hat{\mathcal{R}}+\hat{\mathcal{R}}^*)+\frac{i}{2}[\delta_k^B\hat{\Gamma}^{1/2},\hat{\Gamma}^{1/2}]\Big]\hat{\Gamma}^{-1/2}-L_k$
	$L_k=\frac{1}{2}\hat{\omega}^{-1/2}[\hat{\omega}x^k\hat{\omega}+(-\partial_ix^k\partial_i+x^km^2)]\hat{\omega}^{-1/2}$
	Formally $\overline{B^k}=\overline{B^k_{\mathrm{reg}}}+\frac{1}{4}\mathrm{Tr}\,x^k\hat{\Gamma}$
	$\overline{B^k_{\mathrm{reg}}}=-\frac{1}{4}\mathrm{Tr}[\mathcal{B}^{k++}+\mathcal{B}^{k--}]$
Boost	

$$\mathcal{H}_3^{+-}=-i\{\mathcal{H}_2^{++}(\mathcal{H}_1^{++})^*-\mathcal{H}_1^{++}(\mathcal{H}_2^{++})^*+[\mathcal{H}_1^{+-};(\mathcal{H}_2^{+-})]\}+\delta_1\mathcal{H}_2^{+-}-\delta_2\mathcal{H}_1^{+-},\quad(3.24)$$

$$\overline{H_3}=-\frac{i}{2}\mathrm{Tr}[\mathcal{H}_2^{++}(\mathcal{H}_1^{++})^*-\mathcal{H}_1^{++}(\mathcal{H}_2^{++})^*]+\delta_1\overline{H_2}-\delta_2\overline{H_1}.\quad(3.25)$$

Relations (3.23)–(3.25) are treated in sense of bilinear forms on $D(T)$.

Consider now the commutation relations.

(1) The relations

$$[\check{P}^k,\check{P}^l]=0, \quad [\check{M}^{lm},\check{P}^s]=i(g^{ms}\check{P}^l-g^{ls}\check{P}^m)$$

are satisfied automatically since

$$[\partial_k,\partial_l]=0, \quad -[x^l\partial_m-x^m\partial_l,\partial_s]=g^{ms}\partial_l-g^{ls}\partial_m.$$

(2) The relation

$$[\check{M}^{lm},\check{M}^{rs}]=-i(g^{lr}\check{M}^{ms}-g^{mr}\check{M}^{ls}+g^{ms}\check{M}^{lr}-g^{ls}\check{M}^{mr})$$

is also satisfied.

(3) For the relation

$$[\check{P}^k,\check{P}^0]=0$$

Eqs. (3.23)–(3.25) take the form

$$\delta_P^k\mathcal{H}^{++}-[\partial_k;\mathcal{H}^{++}]=0, \quad \delta_P^k\mathcal{H}^{+-}-[\partial_k;\mathcal{H}^{+-}]=0, \tag{3.26}$$

$$\delta_P^k\overline{H}=0. \tag{3.27}$$

(4) For the relation

$$[\check{M}^{kl},\check{P}^0]=0,$$

Eqs. (3.23)–(3.25) are written as

$$\delta_M^{kl}\mathcal{H}^{++}-[x^k\partial_l-x^l\partial_k;\mathcal{H}^{++}]=0, \quad \delta_M^{kl}\mathcal{H}^{+-}-[x^k\partial_l-x^l\partial_k;\mathcal{H}^{+-}]=0, \tag{3.28}$$

$$\delta_M^{kl}\overline{H}=0. \tag{3.29}$$

(5) Consider the relation

$$[\check{M}^{k0},\check{P}^s]=-ig^{ks}\check{P}^0.$$

We write Eqs. (3.23)–(3.25) as follows:

$$[\partial_s,\mathcal{B}^{k++}]-\delta_P^s\mathcal{B}^{k++}=-g^{ks}\mathcal{H}^{++}, \quad [\partial_s,\mathcal{B}^{k+-}]-\delta_P^s\mathcal{B}^{k+-}=-g^{ks}\mathcal{H}^{+-}, \tag{3.30}$$

$$\delta_P^s\overline{B^k}=g^{ks}\overline{H}. \tag{3.31}$$

(6) The commutation relation

$$[\check{M}^{lm},\check{M}^{k0}]=-i(g^{lk}\check{M}^{m0}-g^{mk}\check{M}^{l0})$$

is equivalent to

$$\begin{aligned}&[x^l\partial_m-x^m\partial_l;\mathcal{B}^{k++}]-\delta_M^{lm}\mathcal{B}^{k++}=g^{lk}\mathcal{B}^{m++}-g^{mk}\mathcal{B}^{l++},\\&[x^l\partial_m-x^m\partial_l;\mathcal{B}^{k+-}]-\delta_M^{lm}\mathcal{B}^{k+-}=g^{lk}\mathcal{B}^{m+-}-g^{mk}\mathcal{B}^{l+-},\end{aligned} \tag{3.32}$$

$$-\delta_M^{kl}\overline{B^k}=g^{lk}\overline{B^m}-g^{mk}\overline{B^l}. \tag{3.33}$$

(7) The most nontrivial commutation relations are

$$[\check{M}^{k0};\check{P}^{0}]=i\check{P}^{k},\quad [\check{M}^{k0};\check{M}^{l0}]=-i\check{M}^{kl}.$$

They can be rewritten as follows:

$$\begin{aligned}0&=-i\{\mathcal{B}^{k+-}\mathcal{H}^{++}+\mathcal{H}^{++}(\mathcal{B}^{k+-})^{*}-\mathcal{B}^{k++}(\mathcal{H}^{+-})^{*}-\mathcal{H}^{+-}(\mathcal{B}^{k++})\}+\delta_{B}^{k}\mathcal{H}^{++}-\delta_{H}\mathcal{B}^{k++},\\ -i\partial_{k}&=-i\{\mathcal{H}^{++}\mathcal{B}^{k++}-\mathcal{B}^{k++}(\mathcal{H}^{++})^{*}+[\mathcal{B}^{k+-};\mathcal{H}^{+-}]\}+\delta_{B}^{k}\mathcal{H}^{+-}-\delta_{H}\mathcal{B}^{k+-},\end{aligned}\tag{3.34}$$

$$0=-\frac{i}{2}\mathrm{Tr}[\mathcal{H}^{++}(\mathcal{B}^{k++})^{*}-\mathcal{B}^{k++}(\mathcal{H}^{++})^{*}]+\delta_{B}^{k}\overline{H}-\delta_{H}\overline{B^{k}},\tag{3.35}$$

and

$$\begin{aligned}0&=-i\{\mathcal{B}^{k+-}\mathcal{B}^{l++}+\mathcal{B}^{l++}(\mathcal{B}^{k+-})^{*}-\mathcal{B}^{k++}(\mathcal{B}^{l+-})^{*}-\mathcal{B}^{l+-}(\mathcal{B}^{k++})\}+\delta_{B}^{k}\mathcal{B}^{l++}-\delta_{B}^{l}\mathcal{B}^{k++},\\ i(x^{k}\partial_{l}-x^{l}\partial_{k})&=-i\{\mathcal{B}^{l++}\mathcal{B}^{k++}-\mathcal{B}^{k++}(\mathcal{B}^{l++})^{*}+[\mathcal{B}^{k+-};\mathcal{B}^{l+-}]\}+\delta_{B}^{k}\mathcal{B}^{l+-}-\delta_{B}^{l}\mathcal{B}^{k+-},\end{aligned}\tag{3.36}$$

$$0=-\frac{i}{2}\mathrm{Tr}[\mathcal{B}^{l++}(\mathcal{B}^{k++})^{*}-\mathcal{B}^{k++}(\mathcal{B}^{l++})^{*}]+\delta_{B}^{k}\overline{B^{l}}-\delta_{B}^{l}\overline{B^{k}}.\tag{3.37}$$

(3) Properties (3.26), (3.28), (3.30), and (3.32) are obvious corollaries of relation (3.22). Properties (3.34) and (3.36) are checked by nontrivial but also direct computations.

Properties (3.27), (3.29), (3.31), (3.33), (3.35), (3.37) will be satisfied if the renormalized trace satisfies the following properties:

$$\begin{gathered}\delta_{k}^{P}\,\mathrm{Tr}_{R}\hat{\Gamma}=0,\quad \delta_{kl}^{M}\,\mathrm{Tr}_{R}\hat{\Gamma}=0,\\ \delta_{l}^{P}\,\mathrm{Tr}_{R}x^{k}\hat{\Gamma}=-\delta^{kl}\,\mathrm{Tr}_{R}\hat{\Gamma},\quad \delta_{kl}^{M}\,\mathrm{Tr}_{R}x^{k}\hat{\Gamma}=\delta^{kl}\,\mathrm{Tr}_{R}x^{m}\hat{\Gamma}-\delta^{mk}\,\mathrm{Tr}_{R}x^{l}\hat{\Gamma},\\ \mathrm{Tr}[x^{l}(\delta_{k}^{B}\hat{\Gamma}-\hat{\mathcal{A}}x^{k}\hat{\Gamma}-x^{k}\hat{\mathcal{A}})-x^{k}(\delta_{l}^{B}\hat{\Gamma}-\hat{\mathcal{A}}x^{l}\hat{\Gamma}-\hat{\Gamma}x^{l}\hat{\mathcal{A}})]+\delta_{l}^{B}\,\mathrm{Tr}_{R}x^{k}\hat{\Gamma}-\delta_{k}^{B}\,\mathrm{Tr}_{R}x^{l}\hat{\Gamma}=0,\\ \mathrm{Tr}[x^{l}(\delta^{H}\hat{\Gamma}-\hat{\mathcal{A}}\hat{\Gamma}-\hat{\Gamma}\hat{\mathcal{A}})-(\delta_{l}^{B}\hat{\Gamma}-\hat{\mathcal{A}}x^{l}\hat{\Gamma}-\hat{\Gamma}x^{l}\hat{\mathcal{A}})]+\delta_{l}^{B}\,\mathrm{Tr}_{R}\hat{\Gamma}-\delta^{H}\mathrm{Tr}_{R}x^{l}\hat{\Gamma}=0,\end{gathered}\tag{3.38}$$

where $\hat{\mathcal{A}}=\frac{1}{2}(\hat{\mathcal{R}}+\hat{\mathcal{R}}^{*})$.

Thus, algebraic commutation relations are checked.

C. Conditions of integrability

The problem of reconstructing a representation of a local Lie group from a representation of a Lie algebra (''integrability problem'') is mathematically nontrivial. Different conditions of integrability were presented in Refs. 43–47.

The problem of reconstructing the operators $U_{g}(u_{g}X\leftarrow X)$ and checking the group property was discussed in detail in Ref. 48. It has been shown that the operators $U_{g}(u_{g}X\leftarrow X)$ are correctly defined under the following sufficient conditions.

Let $h(\alpha)$ be an arbitrary smooth curve on the Poincaré group.

P1. *For self-adjoint operators*

$$A_{k}=L_{k},\quad A_{d+k}=-i\partial_{k},\quad A_{2d+kd+l}=-i(x^{k}\partial_{l}-x^{l}\partial_{k}),\quad A_{2d+d^{2}+1}=\hat{\omega}$$

there exists such a positively definite operator T that

(1) $\|T^{-1/2}A_{j}T^{-1/2}\|<\infty$, $\|A_{j}T^{-1}\|<\infty$,

(2) *for all* t_{1} *there exists such a constant C that* $\|T^{1/2}e^{iA_{j}t}T^{-1/2}\|\leqslant C$, $\|Te^{-iA_{j}t}T^{-1}\|\leqslant C$, $t\in[-t_{1},t_{1}]$.

P2. *The α-dependent operator functions $T\mathcal{B}^{k++}(u_{h(\alpha)}X)$ and $T\mathcal{H}^{++}(u_{h(\alpha)}X)$ are continuous in the Hilbert–Schmidt topology $\|\cdot\|_2$.*

P3. *The α-dependent operator functions $\mathcal{B}^{k++}(u_{h(\alpha)}X)$ and $\mathcal{H}^{++}(u_{h(\alpha)}X)$ are continuously differentiable with respect to α in the Hilbert–Schmidt topology.*

P4. *The α-dependent operator functions $\mathcal{B}^{k}(u_{h(\alpha)}X)$, $\mathcal{H}(u_{h(\alpha)}X)$, $T\mathcal{B}^{k}(u_{h(\alpha)}X)T^{-1}$, $T^{1/2}\mathcal{B}^{k}(u_{h(\alpha)}X)T^{-1/2}$, $T\mathcal{H}(u_{h(\alpha)}X)T^{-1}$, $T^{1/2}\mathcal{H}(u_{h(\alpha)}X)T^{-1/2}$ are strongly continuous.*

P5. *The α-dependent operator functions $T^{-1/2}\mathcal{H}(u_{h(\alpha)}X)T^{-1/2}$, $T^{-1/2}\mathcal{B}^{k}(u_{h(\alpha)}X)T^{-1/2}$, $\mathcal{H}(u_{h(\alpha)}X)T^{-1}$, $\mathcal{B}^{k}(u_{h(\alpha)}X)T^{-1}$ are continuously differentiable with respect to α in the operator norm $\|\cdot\|$ topology.*

P6. *The functions $\overline{H}(u_{h(\alpha)}X)$ and $\overline{B^{k}}(u_{h(\alpha)}X)$ are continuous.*

The property P6 can be substituted by the following property.

P6′. (*a*) *The operators $\mathcal{B}^{k++}$ and $\mathcal{H}^{++}$ are of the trace class and* $\mathrm{Tr}\,\mathcal{B}^{k++}(u_{h(\alpha)}X)$ *and* $\mathrm{Tr}\mathcal{H}^{++}(u_{h(\alpha)}X)$ *are continuous functions of α.*

(*b*) *The functions* $\mathrm{Tr}_R\Gamma(u_{h(\alpha)}X)$ *and* $\mathrm{Tr}_R x^k\Gamma(u_{h(\alpha)}X)$ *are continuous.*

Let us first justify property P1.

Let

$$\hat{K}=\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}.$$

This is a bounded self-adjoint positively definite operator without zero eigenvalues. Therefore, $\hat{K}^{-1}\equiv T^{1/2}$ is a (nonbounded) self-adjoint operator and

$$T=\hat{\omega}^{1/4}(\mathbf{x}^2+1)\hat{\omega}^{1/2}(\mathbf{x}^2+1)\hat{\omega}^{1/4};$$

$T\geqslant c>0$ for some c.

The first part of property P1 is justified as follows. One should check that the following norms are finite:

$$\|\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\hat{\omega}\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\|,$$

$$\|\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\hat{\omega}x^s\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\|,$$

$$\|\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}(\hat{k}^jx^s-\hat{k}^sx^j)\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\|,$$

$$\|\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\hat{k}^j\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\|,$$

$$\|\hat{\omega}\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\|,$$

$$\|\hat{\omega}x^s\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\|,$$

$$\|(\hat{k}^jx^s-\hat{k}^sx^j)\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\|,$$

$$\|\hat{k}^j\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\hat{\omega}^{-1/4}(\mathbf{x}^2+1)^{-1}\hat{\omega}^{-1/4}\|,$$

where $\hat{k}^j=-i\partial/\partial x^j$.

To check this statement, it is sufficient to notice that lemma A6 implies that the operators

$$[\hat{\omega}^{\alpha};(x^2+1)^{-1}],\quad [\hat{\omega}^{\alpha};x^s(\mathbf{x}^2+1)^{-1}],\quad [\hat{\omega}^{\alpha};x^lx^s(\mathbf{x}^2+1)^{-1}] \tag{3.39}$$

are bounded if $\alpha\leqslant 1$.

To prove the second part of P1, represent it in the following form:

$$\|e^{iA_j+}T^{1/2}e^{-iA_jt}T^{-1/2}\|\equiv\|T_j^{1/2}(t)T^{-1/2}\|\leqslant C,\quad \|T_j(t)T^{-1}\|\leqslant C. \tag{3.40}$$

It is necessary to investigate the Poincaré transformation properties of the operators $\hat{x}^j$ and $\hat{k}^j$.

Notice that the following relations are satisfied:

$$e^{i\hat{\omega}t}\hat{x}^l e^{-i\tilde{\omega}t}=\hat{x}^l+\hat{k}^l\hat{\omega}^{-1}t,\quad e^{i\tilde{\omega}t}\hat{k}^l e^{-i\tilde{\omega}t}=\hat{k}^l,$$

$$e^{i\hat{k}^s a^s}\hat{x}^l e^{-i\hat{k}^s a^s}=\hat{x}^l+a^l,\quad e^{i\hat{k}^s a^s}\hat{k}^l e^{-i\hat{k}^s a^s}=\hat{k}^l,$$

$$\exp\left(\frac{i\tau}{2}\theta_{\mathrm{ms}}(\hat{x}^m\hat{k}^s-\hat{x}^s\hat{k}^m)\right)\hat{x}^l\exp\left(-\frac{i\tau}{2}\theta_{\mathrm{ms}}(\hat{x}^m\hat{k}^s-\hat{x}^s\hat{k}^m)\right)=(e^{-\tau\theta}\hat{x})^l,$$

$$\exp\left(\frac{i\tau}{2}\theta_{\mathrm{ms}}(\hat{x}^m\hat{k}^s-\hat{x}^s\hat{k}^m)\right)\hat{k}^l\exp\left(-\frac{i\tau}{2}\theta_{\mathrm{ms}}(\hat{x}^m\hat{k}^s-\hat{x}^s\hat{k}^m)\right)=(e^{-\tau\theta}\hat{k})^l;$$

$$e^{iL^1\tau}\hat{k}^l e^{-iL^1\tau}=\hat{k}^l,\quad l\geqslant 2;\quad e^{iL^1\tau}\hat{k}^1 e^{-iL^l\tau}=\hat{k}^l\cosh\tau-\hat{\omega}\sinh\tau.$$

The operators $\hat{X}^l(\tau)=e^{iL^1\tau}\hat{x}^l e^{-iL^1\tau}$ have the following Weyl symbols:

$$X^1=\frac{\omega_{\mathbf{k}}}{\omega_{\mathbf{k}}\cosh\tau-k^1\sinh\tau}x^1,\quad X^\alpha=x^\alpha+\frac{k^\alpha\sinh\tau x^1}{\omega_{\mathbf{k}}\cosh\tau-k^1\sinh\tau}.$$

To check the properties, it is sufficient to show that they are satisfied at $\tau=0$ and show that the derivatives of the left-hand and right-hand sides of these relations coincide.

Making use of commutation relations $[x^s,f(\hat{k})]=i(\partial_f/\partial k^s)(\hat{k})$ and boundedness of the operators (3.39), we find that operators (3.40) are bounded uniformly with respect to $t\in[0,t_1]$. Property P1 is checked.

D. Choice of the operator $\mathcal{R}$

Let us choose operator $\mathcal{R}$ in order to satisfy properties P1–P5, P7. We will use the notions of Appendix A. First, we construct such an asymptotic expansion of a Weyl symbol $\underset{\sim}{\mathcal{R}}_N$ that for $\underset{\sim}{\mathcal{R}}=\underset{\sim}{\mathcal{R}}_N$,

$$\begin{gathered}\deg[\,\delta_B^l\underset{\sim}{\mathcal{R}}-\underset{\sim}{\mathcal{R}}*x^l*\underset{\sim}{\mathcal{R}}-x^l(\omega_k^2+V''(\Phi(\mathbf{x})))]\rangle\max\{d/2,d-1\},\\ \deg[\,\delta_H\underset{\sim}{\mathcal{R}}-\underset{\sim}{\mathcal{R}}*\underset{\sim}{\mathcal{R}}-(\omega_k^2+V''(\Phi(\mathbf{x})))]\rangle\max\{d/2,d-1\}.\end{gathered}\tag{3.41}$$

Next, we will construct another asymptotic expansion of a Weyl symbol $\mathcal{R}$ which obeys the condition $\mathrm{Im}\,\underset{\sim}{\mathcal{R}}>0$ and approximately equals to $\underset{\sim}{\mathcal{R}}_N$ at large, $|k|$ so that Eqs. (3.41) are satisfied. This will imply that properties P2–P5, P6′ are satisfied.

Let us define the expansions $\underset{\sim}{\mathcal{R}}_N$ with the help of the following recursive relations. Set

$$\begin{gathered}\underset{\sim}{\mathcal{R}}_0=i\omega_k,\\ \underset{\sim}{\mathcal{S}}_n=-\delta_H\underset{\sim}{\mathcal{R}}_n+\underset{\sim}{\mathcal{R}}_n*\underset{\sim}{\mathcal{R}}_n+\omega_k^2+V''(\Phi(\mathbf{x})),\\ \underset{\sim}{\mathcal{R}}_{n+1}=\underset{\sim}{\mathcal{R}}_n+\frac{i}{2\omega_k}\underset{\sim}{\mathcal{S}}_n.\end{gathered}\tag{3.42}$$

Lemma 3.1: The following relation is satisfied:

$$\deg\underset{\sim}{\mathcal{S}}_n=n.$$

Proof: For $n=0$, $\underset{\sim}{\mathcal{S}}_0=V''(\Phi(\mathbf{x}))$, so that statement of lemma is satisfied. Suppose that statement of lemma is justified for $n<N$. Check it for $n=N$. One has

$$\underline{\mathcal{S}}_N=\underline{\mathcal{S}}_{N-1}+\underline{\mathcal{R}}_N*\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)+\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)*\underline{\mathcal{R}}_N+\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)*\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)-\frac{i}{2\omega_k}\delta_H\underline{\mathcal{S}}_{N-1}.$$

Since

$$\deg\left[\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)*\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)-\frac{i}{2\omega_k}\delta_H\underline{\mathcal{S}}_{N-1}\right]\geqslant\deg\underline{\mathcal{S}}_{N-1}+1=N$$

and

$$\begin{aligned}\underline{\mathcal{S}}_N&=\underline{\mathcal{S}}_{N-1}+\underline{\mathcal{R}}_N*\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)+\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)*\underline{\mathcal{R}}_N\\&\approx\underline{\mathcal{S}}_{N-1}+\underline{\mathcal{R}}_N\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)+\left(\frac{i}{2\omega_k}\underline{\mathcal{S}}_{N-1}\right)\underline{\mathcal{R}}_N=0\end{aligned}$$

up to terms of the degree N, one finds

$$\deg\underline{\mathcal{S}}_N=N.$$

Lemma 3.1 is proved.

Denote

$$\underline{X}^l_n=-\delta^l_B\underline{\mathcal{R}}_n+\underline{\mathcal{R}}_n*x^l*\underline{\mathcal{R}}_n+x^l(\omega_k^2+V''(\Phi(\mathbf{x}))).$$

Lemma 3.2: The following property is obeyed:

$$\delta^l_B\underline{\mathcal{S}}_n-\delta_H\underline{X}^l_n=-\underline{X}^l_n*\underline{\mathcal{R}}_n-\underline{\mathcal{R}}_n*\underline{X}^l_n+\underline{\mathcal{S}}_n*x^l*\underline{\mathcal{R}}_n+\underline{\mathcal{R}}_n*x^l*\underline{\mathcal{S}}_n. \tag{3.43}$$

Proof: Denote

$$\underline{F}^l_n=\delta^l_B\underline{\mathcal{S}}_n-\delta_H\underline{X}^l_n+\underline{X}^l_n*\underline{\mathcal{R}}_n+\underline{\mathcal{R}}_n*\underline{X}^l_n-\underline{\mathcal{S}}_n*x^l*\underline{\mathcal{R}}_n-\underline{\mathcal{R}}_n*x^l*\underline{\mathcal{S}}_n.$$

One has

$$\begin{aligned}\underline{F}^l_n=&(\delta^l_B-x^l\delta_H)V''(\Phi(\mathbf{x}))+[\delta_H;\delta^l_B]\underline{\mathcal{R}}_n-[x^l(\omega_k^2+V''(\Phi(\mathbf{x}))-(\omega_k^2+V''(\Phi(\mathbf{x}))*x^l]*\underline{\mathcal{R}}_n\\&+\underline{\mathcal{R}}_n*[x^l(\omega_k^2+V''(\Phi(\mathbf{x}))-x^l*(\omega_k^2+V''(\Phi(\mathbf{x}))].\end{aligned}$$

It follows from the definition of the Weyl symbol that

$$x^l*f(x,k)=\left(x^l+\frac{i}{2}\frac{\partial}{\partial k^l}\right)f(x,k).$$

One also has

$$(\delta^l_B-x^l\delta_H)V''(\Phi(\mathbf{x}))=0.$$

Thus,

$$\underline{F}^l_n=[\delta_H;\delta^l_B]\underline{\mathcal{R}}_n+ik^l*\underline{\mathcal{R}}_n-\underline{\mathcal{R}}_n*ik^l=\frac{\partial\underline{\mathcal{R}}_n}{\partial x^l}-\delta^l_P\underline{\mathcal{R}}_n.$$

However, the property

$$\frac{\partial \underline{\mathcal{R}}_n}{\partial x^l} = \delta_P^l \underline{\mathcal{R}}_n ,$$

which means that Eq. (3.21) is satisfied as checked by induction. Lemma 3.2 is proved.

Lemma 3.3: The following properties are satisfied:

(1) $\deg \underline{X}_n^l = n$.
(2) $\deg (\underline{X}_n^l - x^l \underline{\mathcal{S}}_n) \geqslant n+1$.

Proof: It follows from the results of the Appendix that X_n^l is an asymptotic expansion of a Weyl symbol. Let $\deg \underline{X}_n^l = \alpha$.

Suppose that $\alpha < n$. Then the left-hand side of Eq. (3.43) is of the degree α, the degree of the right-hand side of Eq. (3.43) is greater than or equal to $\alpha - 1$. In the leading order in $1/|k|$ the right-hand side has the form one has $(-2i\omega_k \underline{X}_n^l)$ and its degree should be greater than or equal to α. Therefore, $\deg \underline{X}_n^l \geqslant \alpha + 1$. We obtain a contradiction.

Suppose $\alpha > n$. Then the left-hand side of Eq. (3.43) is of the degree n, the right-hand side in the leading order in $1/|k|$ has the form $2i\omega_k x^l \underline{\mathcal{S}}_n$. So that $\deg \underline{\mathcal{S}}_n$ should obey the inequality $\deg \underline{\mathcal{S}}_n \geqslant n+1$. We also obtain a contradiction.

Thus, $\alpha = n$. In the leading order in $1/|k|$ one has

$$0 \approx -2i\omega_k (\underline{X}_n^l - x^l \underline{\mathcal{S}}_n)$$

up to terms of the degree n, so that $\deg(\underline{X}_n^l - x^l \underline{\mathcal{S}}_n) \geqslant n+1$. Lemma 3.3 is proved.

We see that for $N \geqslant \max\{d/2, d-1\}$ the properties (3.41) are satisfied.

Lemma 3.4: Let $\underline{\mathcal{R}}^{(1)}$ *and* $\underline{\mathcal{R}}^{(2)}$ *be asymptotic expansions of Weyl symbols,* $\deg \underline{\mathcal{R}}^{(1)} = \deg \underline{\mathcal{R}}^{(2)} = -1$ *and* $\deg(\underline{\mathcal{R}}^{(1)} - \underline{\mathcal{R}}^{(2)}) = N+1$. *Then*

$$\deg(\underline{X}^{(1)l} - \underline{X}^{(2)l}) = N$$

and

$$\deg(\underline{\mathcal{S}}^{(1)} - \underline{\mathcal{S}}^{(2)}) = N.$$

Proof: Denote $\underline{\mathcal{R}} - \underline{\mathcal{R}}^{(2)} = \underline{D}$. Then

$$\underline{X}^{(1)l} - \underline{X}^{(2)l} = -\delta_B^l \underline{D} + \underline{\mathcal{R}}^{(1)} * x^l * \underline{D} + \underline{D} * x^l * \underline{\mathcal{R}}^{(1)} + \underline{D} * \underline{D} * x^l * \underline{D}.$$

We see that $\deg(\underline{X}^{(1)l} - \underline{X}^{(2)l}) = N$. The second statement is checked analogously. Lemma 3.4 is proved.

Let us construct such an asymptotic expansion $\underline{\mathcal{R}}$ that $\deg(\underline{\mathcal{R}} - \underline{\mathcal{R}}_N) = N+1$ and $\operatorname{Im} \underline{\mathcal{R}} > 0$. We will look for $\underline{\mathcal{R}}$ as follows (cf. Ref. 36),

$$\underline{\mathcal{R}} = \underline{\mathcal{A}} + i\omega_k^{1/4} * \exp \underline{\mathcal{B}} * \omega_k^{1/4} * \exp \underline{\mathcal{B}} * \omega_k^{1/4},$$

where $\underline{\mathcal{A}}$ and $\underline{\mathcal{B}}$ are *real* asymptotic expansions. Then

$$\underline{\Gamma}^{1/2} = \omega_k^{1/4} * \exp \underline{\mathcal{B}} * \omega_k^{1/4},$$

$$\underline{\Gamma}^{-1/2} = \omega_k^{-1/4} * \exp(-\underline{\mathcal{B}}) * \omega_k^{-1/4},$$

are also asymptotic expansions of Weyl symbols. Choose $\underline{\mathcal{A}}$ and $\underline{\mathcal{B}}$ to be polynomials,

$$\underline{\mathcal{A}} = \sum_{s=1}^{S_1} \frac{A_s(\mathbf{x}, \mathbf{k}/\omega_{\mathbf{k}})}{\omega_{\mathbf{k}}^{2s}}, \quad \underline{\mathcal{B}} = \sum_{s=1}^{S_2} \frac{B_s(\mathbf{x}, \mathbf{k}/\omega_{\mathbf{k}})}{\omega_{\mathbf{k}}^{2s}},$$

where $S_1=[N/2]$, $S_2=[(N+1)/2]$.

Lemma 3.5: There exists unique functions $A_1,\ldots,A_{S_1},B_1,\ldots,B_{S_2}$ *such that* $\deg(\underline{\mathcal{R}}-\underline{\mathcal{R}}_N)=N+1$.

Proof: It follows from recursive relations (3.42) that

$$\operatorname{Re}\underline{\mathcal{R}}_N=\sum_{s=1}^{\infty}\frac{A_{N,s}(\mathbf{x},\mathbf{k}/\omega_{\mathbf{k}})}{\omega_{\mathbf{k}}^{2s}},$$

$$\operatorname{Im}\underline{\mathcal{R}}_N=\omega_{\mathbf{k}}+\sum_{s=1}^{\infty}\frac{C_{N,s}(\mathbf{x},\mathbf{k}/\omega_{\mathbf{k}})}{\omega_{\mathbf{k}}^{2s}}.$$

Therefore, $A_s=A_{N,s}$, so that $\underline{\mathcal{A}}$ is uniquely defined. Denote

$$\underline{\mathcal{B}_s}=\frac{B_s(\mathbf{x},\mathbf{k}/\omega_{\mathbf{k}})}{\omega_{\mathbf{k}}^{2s}}.$$

Show that $\underline{\mathcal{B}_s}$ is uniquely defined. In the leading order in $1/|\mathbf{k}|$, one has

$$\operatorname{Im}\underline{\mathcal{R}}\approx\omega_{\mathbf{k}}+2\underline{\mathcal{B}_1}\omega_{\mathrm{k}},$$

so that $B_1=C_{N,1}/2$. Suppose that one can choose $\underline{\mathcal{B}_1},\ldots,\underline{\mathcal{B}_{s-1}}$ in such a way that the degree of the asymptotic expansion of a Weyl symbol

$$\underline{F}_{N,s}=\operatorname{Im}\underline{\mathcal{R}}_N-\omega_{\mathbf{k}}^{1/4}*\exp(\underline{\mathcal{B}_1}+\cdots+\underline{\mathcal{B}_{s-1}})*\omega_{\mathbf{k}}^{1/2}*\exp(\underline{\mathcal{B}_1}+\ldots+\underline{\mathcal{B}_{s-1}})*\omega_{\mathbf{k}}^{1/4}$$

satisfies the inequality

$$\deg\underline{F}_{N,s}\geqslant 2s-1.$$

Choose $\underline{\mathcal{B}_s}$ in such a way that $\deg\underline{F}_{N,s}\geqslant 2s-1$. One has

$$\underline{F}_{N,s+1}=\operatorname{Im}\underline{\mathcal{R}}_N-\omega_{\mathbf{k}}^{1/4}*\sum_{l_1=0}^{\infty}\frac{(\underline{\mathcal{B}_1}+\cdots+\underline{\mathcal{B}_{s-1}}+\underline{B_s})^{l/1}}{l_1!}*\omega_{\mathbf{k}}^{1/2}*\sum_{l_2=0}^{\infty}\frac{(\underline{\mathcal{B}_1}+\cdots+\underline{\mathcal{B}_{s-1}}+\underline{\mathcal{B}_s})^{1/2}}{l_2!}*\omega_{\mathbf{k}}^{1/4}.$$

Up to terms of the degree $2s+1$, one has

$$\begin{aligned}\underline{F}_{N,s+1}&\approx\operatorname{Im}\underline{\mathcal{R}}_N\\&\quad-\omega_{\mathbf{k}}^{1/4}*\left(\sum_{l_1=0}^{\infty}\frac{(\underline{\mathcal{B}_1}+\cdots+\underline{\mathcal{B}_{s-1}})^{l/1}}{l_1!}+\underline{\mathcal{B}_s}\right)*\omega_{\mathbf{k}}^{1/2}*\left(\sum_{l_2=0}^{\infty}\frac{(\underline{\mathcal{B}_1}+\cdots+\underline{\mathcal{B}_{s-1}})^{l/2}}{l_2!}+\underline{\mathcal{B}_s}\right)*\omega_{\mathbf{k}}^{1/4}\\&\approx\underline{F}_{N,s}-2\underline{\mathcal{B}_s}\omega_{\mathbf{k}}.\end{aligned}$$

Since

$$\underline{F}_{N,s}=\frac{1}{\omega_{\mathbf{k}}^{2s-1}}\sum_{l=0}^{\infty}\frac{F_{N,s,l}(\mathbf{x},\mathbf{k}/\omega_{\mathbf{k}})}{\omega_{\mathbf{k}}^{l}},$$

one finds that

$$\underline{\mathcal{B}_s}=\frac{1}{2\omega_k^{2s}}F_{N,s,0}(\mathbf{x},\mathbf{k}/\omega_{\mathbf{k}})$$

is uniquely defined. Lemma 3.5 is proved.

Thus, we have constructed the operator $\mathcal{R}$ such that properties (3.41) are satisfied. We obtain the following theorem.

Theorem 3.6: *Properties* (3.21), $P2-P5$, $P6'(a)$ *are satisfied.*

This theorem is a direct corollary of the results of the Appendix. Property P1 is satisfied because of construction of the operator $\mathcal{R}$. Properties $P2-P5$, $P6'(a)$ are corollaries of Theorems A8, A9, A10, properties (3.41) and theorem A2.

E. Regularization and renormalization of a trace

The purpose of this section is to specify functionals $\mathrm{Tr}_R\Gamma$ and $\mathrm{Tr}_R x^k\Gamma$ of arguments Φ, Π in order to satisfy properties $P6'(b)$, (3.38). We want the renormalized trace to satisfy properties like these:

(i) $\mathrm{Tr}_R\hat{A}=\mathrm{Tr}\,\hat{A}$ if $\hat{A}$ is of the trace class,
(ii) $\mathrm{Tr}_R(\hat{A}+\lambda\hat{B})=\mathrm{Tr}_R\hat{A}+\lambda\,\mathrm{Tr}_R\hat{B}$,
(iii) $\mathrm{Tr}_R[\hat{A};\hat{B}]=0$,
(iv) $\mathrm{Tr}_R\hat{A}_n\to 0$ if $A_n\to 0$

for such class of operators that is as wide as possible. Under these conditions, properties $P6'(b)$ and (3.38) are satisfied. However, one cannot specify such a renormalized trace. Namely, one should have

$$\mathrm{Tr}_R\left[\hat{x}_j;\mathcal{W}\left(\frac{k_j}{\omega_{\mathbf{k}}^l}f(\mathbf{x})\right)\right]=0, \tag{3.44}$$

where $f\in S(\mathbf{R}^d)$. $\mathcal{W}(A)$ is a Weyl quantization of the function A (see the appendix). Property (3.44) means that

$$\mathrm{Tr}_R\mathcal{W}\left(i\frac{\partial}{\partial k_i}\frac{k_j}{\omega_{\mathbf{k}}^l}f(\mathbf{x})\right)=0.$$

Therefore,

$$\delta_{ij}\,\mathrm{Tr}_R\mathcal{W}\left(\frac{f(\mathbf{x})}{\omega_{\mathbf{k}}^l}\right)-l\,\mathrm{Tr}_R\mathcal{W}\left(\frac{k_ik_j}{\omega_{\mathbf{k}}^{l+2}}f(\mathbf{x})\right)=0. \tag{3.45}$$

Choose $l=d$. Consider $i=j$ in Eq. (3.45) and perform the summation over i. Making use of the relation $\omega_{\mathbf{k}}^2-k_ik_i=m^2$, we find

$$\mathrm{Tr}_R\mathcal{W}(m^2\omega_{\mathbf{k}}^{-d-2}f(\mathbf{x}))=0.$$

However, the operator with Weyl symbol $m^2f(\mathbf{x})\omega_{\mathbf{k}}^{-d-2}$ is of the trace class. Its trace is nonzero, provided that $\int d\mathbf{x}\,f(x)\neq 0$.

However, we can introduce a notion of a trace for *asymptotic expansions of Weyl symbols*. The trace will be specified not only by operator but also by its asymptotic expansion which is not unique (see the remark after definition A6).

Let $\underline{A}=(A,\check{A})$ be asymptotic expansion of a Weyl symbol. Suppose that the coefficients A_l of the formal asymptotic expansion

$$\check{A}\equiv\sum_{l=0}^{\infty}\omega_{\mathbf{k}}^{-\alpha-l}A_l(x,\mathbf{k}/\omega_{\mathbf{k}})$$

are polynomial in $\mathbf{k}/\omega_{\mathbf{k}}$. One formally has

$$\mathrm{Tr}_R \underline{A} = \sum_{l=0}^{l_0} \int \frac{\mathrm{d}\mathbf{k}\, d\mathbf{x}}{(2\pi)^d} \frac{1}{\omega_{\mathbf{k}}^{\alpha+l}} A_l(\mathbf{x}, \mathbf{k}/\omega_{\mathbf{k}}) + \int \frac{\mathrm{d}\mathbf{k}\, \mathrm{d}\mathbf{x}}{(2\pi)^d} \left(A(\mathbf{x}, \mathbf{k}) - \sum_{l=0}^{l_0} \frac{1}{\omega_{\mathbf{k}}^{\alpha+l}} A_l(\mathbf{x}, \mathbf{k}/\omega_{\mathbf{k}}) \right). \tag{3.46}$$

For $\alpha + l_0 + 1 > d$, the last integral on the right-hand side of Eq. (3.46) converges. To specify trace, it is sufficient then to specify values of integrals

$$I^{s,n}_{i_1 \ldots i_n} = \int \frac{\mathrm{d}\mathbf{k}}{\omega_{\mathbf{k}}^s} \frac{k_{i_1}}{\omega_{\mathbf{k}}} \cdots \frac{k_{i_n}}{\omega_{\mathbf{k}}} \tag{3.47}$$

for $s \leqslant d$ which are divergent. We will define the quantities (3.47), making use of the following argumentation.

(1) We are going to specify trace in such a way that

$$\mathrm{Tr}_R \frac{\partial}{\partial k_i} \underline{A} = 0. \tag{3.48}$$

Let

$$\underline{A} = \frac{1}{\omega_{\mathbf{k}}^{s-1}} \frac{k_{j_1}}{\omega_{\mathbf{k}}} \cdots \frac{k_{j_{n+1}}}{\omega_{\mathbf{k}}},$$

property (3.48) implies the following recursive relations:

$$\sum_{s=1}^{n+1} \delta_{ij_s} I^{s,n}_{j_1 \ldots j_{s-1} j_{s+1} \ldots j_{n+1}} = (s+n) I^{s,n+2}_{i j_1 \ldots j_{n+1}}. \tag{3.49}$$

Therefore, $I^{s,n} = 0$ for odd n, while for even n $I^{s,n}$ is defined from Eq. (3.49), for example, $I^{s,2}_{ij} = (1/s)\, \delta_{ij} I^{s,0}$. Therefore, it is sufficient to define integrals

$$I^{s,0} = \int \mathrm{d}\mathbf{k}\, \omega_{\mathbf{k}}^{-s}. \tag{3.50}$$

Let us use the approach based on the dimensional regularization.[49,50] It is based on considering integrals (3.50) at arbitrary dimensionality of space–time. Expression (3.50) appears to be a meromorphic function of d. Subtracting the poles corresponding to sufficiently small positive integer values of d, we obtain a finite expression.

Formally, one has

$$I^{s,0} = \frac{1}{\Gamma(s/2)} \int_0^\infty \mathrm{d}\alpha\, \alpha^{s/2-1} \int \mathrm{d}\mathbf{k}\, e^{-\alpha(\mathbf{k}^2 + m^2)} = \frac{\pi^{d/2}}{\Gamma(s/2)} \frac{\Gamma\left(\frac{s-d}{2}\right)}{m^{s-d}}.$$

If $(s-d)/2 = -N$ is a nonpositive integer number, one should modify the definition of $I^{s,0}$. Change $d \to d - 2\varepsilon$. One finds

$$\begin{aligned} I^{s,0} &= \frac{\pi^{d/2}}{\Gamma(s/2) m^{s-d}} \frac{\Gamma(1+\varepsilon)(\pi m^2)^{-\varepsilon}}{(-N+\varepsilon)\cdots(-1+\varepsilon)\varepsilon} \\ &\approx \frac{\pi^{d/2}(-1)^N}{\Gamma(s/2) m^{s-d} N! \varepsilon} (1 + \varepsilon(-\ln(\pi m^2) + \Gamma'(1) + 1 + \cdots + N^{-1})) + O(\varepsilon). \end{aligned}$$

In the *MS* renormalization scheme,[50] one should omit the term $O(\varepsilon^{-1})$. There is also an $\overline{MS}$ renormalization scheme in which one omits also a fixed term of order $O(1)$. Let us omit the term $-\ln(\pi m^2)+\Gamma'(1)$. We obtain the following renormalized value of the integral:

$$I^{s,0}_{\mathrm{ren}}=\frac{\pi^{d/2}}{\Gamma(s/2)m^{s-d}}\frac{(-1)^N}{N!}(1+\cdots+1/N),$$

provided that $N=(d-s)/2$ is a non-negative integer number.

Therefore, we have defined the renormalized trace of an asymptotic expansion of a Weyl symbol by formula (3.46), provided that the coefficient functions are polynomials in $\mathbf{k}/\omega_{\mathbf{k}}$.

Let us investigate properties of the renormalized trace. Some properties are direct corollaries of definition (3.46).

Lemma 3.7: The following properties are satisfied:

(i) $\mathrm{Tr}_R(\underline{A}+\lambda\underline{B})=0$.
(ii) $\mathrm{Tr}_R(\partial\underline{A}/\partial k_i)=0$, $\mathrm{Tr}_R(\partial\underline{A}/\partial x_i)=0$.
(iii) *Let* $E-\lim_{n\to\infty}\underline{A}_n=\underline{A}$. *Then* $\lim_{n\to\infty}\mathrm{Tr}_R\underline{A}_n=\mathrm{Tr}_R\underline{A}$.
(iv) *Let* $\deg\underline{A}>d$. *Then* $\mathrm{Tr}_R\underline{A}=\mathrm{Tr}A$.

Corollary: The property P9 is satisfied.

Let us check that $\mathrm{Tr}_R(\underline{A}*\underline{B}-\underline{B}*\underline{A})=0$. First of all, prove the following statement.

Lemma 3.8: $\mathrm{Tr}_R\underline{A}*\underline{B}=\mathrm{Tr}_RAB$.

Proof: Making use of Eq. (A2), we find

$$\begin{aligned}
&(A*B)(\mathbf{x},\mathbf{k})-(AB)(\mathbf{x},\mathbf{k})\\
&\quad=\int\frac{d\mathbf{P}_1d\mathbf{p}_2d\mathbf{y}_1d\mathbf{y}_2}{(2\pi)^{2d}}\int_0^1 d\alpha\frac{\partial}{\partial\alpha}\left[A\left(\mathbf{x}+\mathbf{y}_1;\mathbf{k}+\alpha\frac{\mathbf{p}_2}{2}\right)B\left(\mathbf{x}+\mathbf{y}_2,\mathbf{k}_2-\alpha\frac{\mathbf{p}_1}{2}\right)\right]e^{-i\mathbf{p}_1\mathbf{y}_1-i\mathbf{p}_2\mathbf{y}_2}\\
&\quad=-\frac{i}{2}\int\frac{d\mathbf{p}_1d\mathbf{P}_2d\mathbf{y}_1d\mathbf{y}_2}{(2\pi)^{2d}}\int_0^1 d\alpha\left[\frac{\partial}{\partial k^i}A\left(\mathbf{x}+\mathbf{y}_1;\mathbf{k}+\alpha\frac{\mathbf{p}_2}{2}\right)\frac{\partial}{\partial x^i}B\left(\mathbf{x}+\mathbf{y}_2,\mathbf{k}_2-\alpha\frac{\mathbf{p}_1}{2}\right)\right.\\
&\qquad\left.-\frac{\partial}{\partial x^i}A\left(\mathbf{x}+\mathbf{y}_1;\mathbf{k}+\alpha\frac{\mathbf{p}_2}{2}\right)\frac{\partial}{\partial k^i}B\left(\mathbf{x}+\mathbf{y}_2,\mathbf{k}_2-\alpha\frac{\mathbf{p}_1}{2}\right)\right]e^{-i\mathbf{p}_1\mathbf{y}_1-i\mathbf{p}_2\mathbf{y}_2}\\
&\quad=-\frac{i}{2}\frac{\partial C^i(\mathbf{x},\mathbf{k})}{\partial k^i}
\end{aligned}$$

with

$$\begin{aligned}
C^i(\mathbf{x},\mathbf{k})=f\frac{d\mathbf{p}_1d\mathbf{p}_2d\mathbf{y}_1d\mathbf{y}_2}{(2\pi)^{2d}}\int_0^1 d\alpha\left[A\left(\mathbf{x}+\mathbf{y}_1;\mathbf{k}+\alpha\frac{\mathbf{p}_2}{2}\right)\frac{\partial}{\partial x^i}B\left(\mathbf{x}+\mathbf{y}_2,\mathbf{k}_2-\alpha\frac{\mathbf{p}_1}{2}\right)\right.\\
\left.-B\left(\mathbf{x}+\mathbf{y}_2,\mathbf{k}_2-\alpha\frac{\partial}{\partial x^i}A\left(\mathbf{x}+\mathbf{y}_1;\mathbf{k}+\alpha\frac{\mathbf{p}_2}{2}\right)\frac{\mathbf{p}_1}{2}\right)\right]e^{-i\mathbf{p}_1\mathbf{y}_1-i\mathbf{p}_2\mathbf{y}_2}.
\end{aligned}$$

One also has

$$\check{A}*\check{B}-\check{A}\check{B}=-\frac{i}{2}\frac{\partial\check{C}^j}{\partial k^j}$$

with

$$\check{C}^j(\mathbf{x},\mathbf{k})=\sum_{s=0}^{\infty}\sum_{l_1 l_2\geqslant 0;l_1+l_2=s}\frac{(-i)^{l_1}}{2l_1 l_1!}\frac{i^{l_2}}{2^{l/2}l_2!}\frac{1}{l_1+l_2+1}$$
$$\times\left[\frac{\partial^{l_1+l_2}\check{A}}{\partial k^i 1\ldots\partial k^{il_1}\partial x^{j1}\ldots\partial x^{jl_2}}\frac{\partial}{\partial x^i}\frac{\partial^{l_1+l_2}\check{B}}{\partial k^j 1\ldots\partial k^{jl_2}\partial x^{i_1}\ldots\partial x^{i_{l_1}}}\right.$$
$$\left.-\frac{\partial_{l_1}+l_2\check{B}}{\partial k^{j_1}\ldots\partial k^{j_{i_2}}\partial x^{i_1}\ldots\partial x^{i_{l_1}}}\frac{\partial}{\partial x^i}\frac{\partial^{l_1+l_2}\check{A}}{\partial k^{i_1}\ldots\partial k^{i_{l_1}}\partial x^{j_1}\ldots\partial x^{jl_2}}\right].$$

Analogously to the Appendix, one finds that $(C^j,\check{C}^j)\equiv\check{C}^j$ is an asymptotic expansion of a Weyl symbol. It follows from lemma 3.7 that $\mathrm{Tr}_R(\partial\underline{C}^j/\partial k^j)=0$. We obtain statement of lemma 3.8.

Lemma 3.9: For $\deg\underline{B}\geqslant 2$, $\mathrm{Tr}_R x^k\omega_{\mathbf{k}}*\underline{B}=\mathrm{Tr}_R x^k\omega_{\mathbf{k}}\underline{B}$ *and* $\mathrm{Tr}_R\omega_{\mathbf{k}}*\underline{B}=\mathrm{Tr}_R\omega_{\mathbf{k}}\underline{B}$. The proof is analogous.

Corollary 1: The following relations are satisfied:

(1) $\mathrm{Tr}_R(\underline{A}*\underline{B}-\underline{B}*\underline{A})=0$,
(2) $\mathrm{Tr}_R(x^k\omega_{\mathbf{k}}*\underline{B}-\underline{B}x^k\omega_{\mathbf{k}})=0$,
(3) $\mathrm{Tr}_R(\omega_{\mathbf{k}}*\underline{B}-\underline{B}*\omega_{\mathbf{k}})=0$.

Corollary 2: Property (3.38) *is satisfied.*

Thus, we have constructed functionals $\mathrm{Tr}_R x^k\hat{\Gamma}\equiv\mathrm{Tr}_R x^k\underline{\Gamma}$ and $\mathrm{Tr}_R\hat{\Gamma}\equiv\mathrm{Tr}_R\underline{\Gamma}$ such that properties (3.38) and P6′(b) are satisfied.

Note that the "finite renormalization"[25] can also be made. One can add quantities $\Delta\,\mathrm{Tr}_R x^k\hat{\Gamma}$ and $\Delta\,\mathrm{Tr}_R\hat{\Gamma}$ to renormalized traces in such a way that

$$\delta_k^P\Delta\,\mathrm{Tr}_R\hat{\Gamma}=0,\quad \delta_{kl}^M\Delta\,\mathrm{Tr}_R\hat{\Gamma}=0,$$

$$\delta_P^l\Delta\,\mathrm{Tr}_R x^k\hat{\Gamma}=-\delta^{kl}\Delta\,\mathrm{Tr}_R\hat{\Gamma},\quad \delta_{kl}^M\Delta\,\mathrm{Tr}_R x^k\hat{\Gamma}=\delta^{kl}\Delta\,\mathrm{Tr}_R x^m\hat{\Gamma}-\delta^{mk}\Delta\,\mathrm{Tr}_R x^l\hat{\Gamma},$$

$$\delta_l^B\Delta\,\mathrm{Tr}_R x^k\hat{\Gamma}-\delta_k^B\Delta\,\mathrm{Tr}_R x^l\hat{\Gamma}=0,$$

$$\delta_l^B\Delta\,\mathrm{Tr}_R\hat{\Gamma}-\delta^H\Delta\,\mathrm{Tr}_R x^l\hat{\Gamma}=0.$$

This corresponds to the possibility of adding the finite one-loop counterterm to the Lagrangian.

IV. SEMICLASSICAL FIELD

An important feature of QFT is a notion of field. In this section we introduce the notion of a semiclassical field and check its Poincaré invariance.

A. Definition of semiclassical field

First of all, introduce the notion of a semiclassical field $\tilde{\phi}(\mathbf{x},t:X)$ in the functional Schrödinger representation. At $t=0$, this is the operator of multiplication by $\phi(\mathbf{x})$. For arbitrary t, one has

$$\tilde{\phi}(\mathbf{x},t:X)=\tilde{U}_{-t}(X\leftarrow u_t X)\,\phi(\mathbf{x})\,\tilde{U}_t(u_t X\leftarrow X),$$

where $\tilde{U}_t(u_t X\leftarrow X)$ is the operator transforming the initial condition for the Cauchy problem for Eq. (1.6) to the solution to the Cauchy problem.

The field operator in the Fock representation is related to $\tilde{\phi}$ by the transformation (2.1),

$$\tilde{\phi}(\mathbf{x},t:X)=V_X^{-1}\tilde{\phi}(\mathbf{x},t:X)V_X.$$

Making use of Eq. (3.15), one finds

$$\hat{\phi}(\mathbf{x},t:X)=(U_H^t(X))^{-1}\tilde{\phi}(\mathbf{x},u_tX)U_H^t(X). \tag{4.1}$$

Here $\hat{\phi}(\mathbf{x}:X)=i(\Gamma^{-1/2}(A^+-A^-))(\mathbf{x})$, while

$$U_H^t(X)\equiv U_{a,\Lambda}(u_{a,\Lambda}X\leftarrow X),\quad \Lambda=1,\quad \mathbf{a}=0,\quad a^0=-t.$$

Let us define $\hat{\phi}$ mathematically as an operator distribution.

Let $S(\mathbf{R}^d)$ be a space of complex smooth functions $u:\mathbf{R}^d\to\mathbf{C}$ such that

$$\|u\|_{l,m}=\max_{\alpha_1+\cdots+\alpha_d\leqslant l}\sup_{\mathbf{x}\in\mathbf{R}^d}(1+|\mathbf{x}|)^m\left|\frac{\partial^{\alpha_1+\cdots+\alpha_d}}{\partial x^{\alpha_1}\cdots\partial x^{\alpha_d}}u(\mathbf{x})\right|\to_{k\to\infty}0.$$

We say that the sequence $\{u_k\}\in S(\mathbf{R}^n)$, $k=\overline{1,\infty}$ tends to zero if $\|u_k\|_{l,m}\to_{k\to\infty}0$ for all l,m.

Denote $\mathcal{D}=\{\Psi\in\mathcal{F}\|A^+TA^-\Psi\|<\infty\}$ (cf. Ref. 48).

Definition 4.1 (cf. Ref. 20): (1) An operator distribution ϕ defined on $\mathcal{D}\in\mathcal{F}$ is a linear mapping taking functions $f\in S(\mathbf{R}^d)$ to the linear operator $\phi[f]:\mathcal{D}\to\mathcal{F}$,

$$\phi:f\in S(\mathbf{R}^d)\mapsto\phi[f]:\mathcal{D}\to\mathcal{F},$$

such that $\|\phi[f_n]\Phi\|\to_{n\to\infty}0$ if $f_n\to_{n\to\infty}0$.

(2) Λ sequence of operator distributions ϕ_n is called convergent to the operator distribution ϕ if

$$\|\phi_n[f]\Phi-\phi[f]\Phi\|\to_{n\to\infty}0$$

for all $\Phi\in\mathcal{D}$, $f\in S(\mathbf{R}^d)$.

We will write

$$\phi[f]\equiv\int \mathrm{d}\mathbf{x}\phi(\mathbf{x})f(\mathbf{x}),\quad \mathbf{x}\in\mathbf{R}^d.$$

Consider the mapping $f\mapsto\phi_t\{f\}$, $f\in S(\mathbf{R}^d)$ of the form

$$\phi_t\{f:X\}=\int \mathrm{d}\mathbf{x}\,\hat{\phi}(\mathbf{x},t:X)f(\mathbf{x}).$$

It follows from the results of Ref. 48 that ϕ_t is an operator distribution being continuous with respect to t.

Consider the mapping $f\mapsto\phi[f]$, $f\in S(\mathbf{R}^{d+1})$ of the form

$$\phi[f:X]=\int \mathrm{d}t\,\phi_t\{f(\cdot,t):X\}.$$

Analogously, note also that ϕ is an operator distribution.

B. Poincaré invariance of the semiclassical field

1. Algebraic properties

To check the property of Poincaré invariance, notice that it is sufficient to check it for partial cases: spatial translations, rotations, evolution, boost, since any Poincaré transformation can be presented as a composition of these transformations. Let $g_B(\tau)=(a(\tau),\Lambda(\tau))$ be a one-parametric subgroup of Poincaré group corresponding to the element B of the Poincaré algebra. The Poincaré invariance property can be rewritten as

$$\hat{\phi}[f:X]=(U_B^\tau(X))^+\phi[v_{g_B(\tau)}f:U_{g_B(\tau)}X]U_B^\tau[X], \tag{4.2}$$

where

$$(v_{g_B(\tau)}f)(x)=f(\Lambda^{-1}(\tau)(x-a(\tau))).$$

Obviously, $v_{g_1}v_{g_2}=v_{g_1g_2}$.

Let us check relation (4.2). It is convenient to reduce the group property to an algebraic property. The formal derivative with respect to τ of the right-hand side of Eq. (4.2) is

$$(U_B^\tau(X))^+\left\{i[H(B:u_{g_B(\tau)}X);\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X]]+\frac{\partial}{\partial\tau}\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X]\right\}U_B^\tau(X). \tag{4.3}$$

If the quantity (4.3) vanishes, the property (4.2) will be satisfied since it is obeyed at $\tau=0$. Making use of the group property $g_B(\tau+\delta\tau)=g_B(\delta\tau)g_B(\tau)$, we find that vanishing of expression (4.3) is equivalent to the property:

$$\left.\frac{\partial}{\partial\tau}\right|_{\tau=0}\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X]-i[\phi[f:X];H(B:X)]=0. \tag{4.4}$$

We obtain the following lemma.

Lemma 4.1: Let the bilinear form (4.4) vanish on $\mathcal{D}$. Then the property (4.2) is satisfied on $\mathcal{D}$.

Proof: Consider the matrix element

$$\chi^\tau=(U_B^\tau(X)\Psi_1,\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X]U_B^\tau(X)\Psi_2)-(\Psi_1,\hat{\phi}[f:X]\Psi_2),$$

where Ψ_1, $\Psi_2\in\mathcal{D}$. Show it to be differentiable with respect to τ. Let us check that for $\Psi\in\mathcal{D}$, the vector $\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X]\Psi$ is strongly continuously differentiable with respect to τ.

One has

$$\frac{\phi[v_{g_B(\tau+\delta\tau)}f:u_{g_B(\tau+\delta\tau)}X]-\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X]}{\delta\tau}\Psi$$

$$=\phi\left[\frac{v_{g_B(\delta\tau)}-1}{\delta\tau}v_{g_B(\tau)}f:u_{g_B(\tau+\delta\tau)}X\right]\Psi+\frac{\phi[v_{g_B(\tau)}f:u_{g_B(\delta\tau)g_B(\tau)}X]-\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X]}{\delta\tau}\Psi.$$

It follows from Ref. 48 that the first term tends to $\phi[(\partial/\partial t)|_{t=0}v_{g_B(t)}v_{g_B(\tau)}f:u_{g_B(\tau)}X]\Psi$, while the second term tends to $\delta[B]\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X]\Psi$.

Notice that

$$\frac{\chi^{\tau+\delta\tau}-\chi^\tau}{\delta\tau}=\left(\phi[v_{g_B(\tau+\delta\tau)}f:u_{g_B(\tau+\delta\tau)}X]U_B^{\tau+\delta\tau}(X)\Psi_1;\frac{U_B^{\tau+\delta\tau}(X)-U_B^\tau}{\delta\tau}\Psi_2\right)$$
$$+(U_B^{\tau+\delta\tau}(X)\Psi_1;(\phi[v_{g_B(\tau+\delta\tau)}f:u_{g_B(\tau+\delta\tau)}X]-\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X])U_B^\tau(X)\Psi_2)$$
$$+((U_B^{\tau+\delta\tau}(X)-U_B^\tau(X))\Psi_1;\phi[v_{g_B(\tau)}f:u_{g_B(\tau)}X]U_B^\tau(X)\Psi_2).$$

This quantity tends as $\delta\tau\to0$ to the matrix element of the bilinear form (4.3) and vanishes under condition (4.4). Lemma 4.1 is proved.

2. Check of invariance

One should check property (4.2) for spatial translations and rotations, evolution, and boost transformations.

For spatial translations and rotations, property (4.2) reads

$$\hat{\phi}(\mathbf{x},t:X)=U_{0,\mathbf{a},L}^{-1}\hat{\phi}(L\mathbf{x}+\mathbf{a},t:u_{0,\mathbf{a},L}X)U_{0,\mathbf{a},L}\,. \tag{4.5}$$

It follows from commutativity of $U_{0,\mathbf{a},L}$ and U_t and Table III that property (4.5) is satisfied.

For evolution operator, property (4.2) is rewritten as

$$\hat{\phi}(\mathbf{x},t:X)=(U_H^{\tau}(X))^{-1}\hat{\phi}(\mathbf{x},t-\tau:u_{\tau}X)U_H^{\tau}(X). \tag{4.6}$$

Relation (4.6) is a direct corollary of definition (4.1) and group property for evolution operators.

Consider now the **n**-boost transformation. Check property (4.4). It can be presented as

$$[\check{B}^k;\hat{\phi}(\mathbf{x},t;X)]=-i\left(x^k\frac{\partial}{\partial t}+t\frac{\partial}{\partial x^k}\right)\hat{\phi}(\mathbf{x},t:X)$$

or

$$\begin{aligned}&[B^k(X);(U_H^t(X))^{-1}\phi(\mathbf{x}:u_tX)U_H^t(X)]+i\delta_B^k\{(U_H^t(X))^{-1}\phi(\mathbf{x}:u_tX)U_H^t(X)\}\\&\quad=-i\left(x^k\frac{\partial}{\partial t}+t\frac{\partial}{\partial x^k}\right)(U_H^t(X))^{-1}\phi(\mathbf{x}:u_tX)U_H^t(X).\end{aligned} \tag{4.7}$$

Let us make use of the property

$$U_H^t(X)B^K(X)=i(\delta_B^kU_H^t)(X)+[B^k(u_tX)-tP^k(u_tX)]U_H^t(X), \tag{4.8}$$

which can be checked by multiplication by $(U_H^t(X))^{-1}$ and differentiation with respect to t in a weak sense (cf. Ref. 48). We take relation (4.7) to the form

$$[\check{B}^k(Y)-\check{P}^k(Y)t;\phi(\mathbf{x}:Y)]=x^k[\check{H}(Y);\phi(\mathbf{x}:Y)]-it\frac{\partial\phi(\mathbf{x}:Y)}{\partial x^k},$$

where $Y=u_tX$. The property

$$i\frac{\partial\phi(\mathbf{x}:Y)}{\partial x^k}=[\check{P}^k(Y);\phi(\mathbf{x}:Y)]$$

is a corollary of relation (3.22). The relation

$$[\check{B}^k(Y)-x^k\check{H}(Y);\phi(\mathbf{x}:Y)]=0$$

is also checked by direct calculation.

Thus, we have obtained that the invariance property (2.5) is satisfied.

V. REMARKS ON COMPOSED SEMICLASSICAL STATES

In the soliton quantization theory and in gauge field theories, the zero-mode problem arises.[2] To resolve it, one can consider the superposition of the ''elementary'' quantum field semiclassical states (1.3) of the form (cf. Ref. 36)

$$\psi[\varphi(\cdot)]=\int\frac{\mathrm{d}\alpha}{\lambda^{k/4}}\exp\left(\frac{i}{\lambda}S(\alpha)\right)\exp\left(\frac{i}{\lambda}\Pi(\alpha;\mathbf{x})[\varphi(\mathbf{x})\sqrt{\lambda}-\Phi(\alpha,\mathbf{x})]\right)g\left(\alpha,\varphi(\cdot)-\frac{\Phi(\alpha,\cdot)}{\sqrt{\lambda}}\right), \tag{5.1}$$

where $\alpha\in\mathbf{R}^k$, $S(\alpha)$, $\Pi(\alpha;\mathbf{x})$, $\Phi(\alpha;\mathbf{x})$ are smooth functions. Calculate (formally) the functional integral for (ψ,ψ):

$$(\psi,\psi)=\int \frac{\mathrm{d}\alpha\,\mathrm{d}\gamma}{\lambda^{k/2}}\int D\varphi\exp\left(-\frac{i}{\lambda}S(\alpha)\right)\exp\left(-\frac{i}{\lambda}\Pi(\alpha;\mathbf{x})[\varphi(\mathbf{x})\sqrt{\lambda}-\Phi(\alpha,\mathbf{x})]\right)g^*\left(\alpha,\varphi(\cdot)-\frac{\Phi(\alpha,\cdot)}{\sqrt{\lambda}}\right)\exp\left(\frac{i}{\lambda}S(\gamma)\right)\exp\left(\frac{i}{\lambda}\Pi(\gamma;\mathbf{x})[\varphi(\mathbf{x})\sqrt{\lambda}-\Phi(\gamma,\mathbf{x})]\right)g\left(\gamma,\varphi(\cdot)-\frac{\Phi(\gamma,\cdot)}{\sqrt{\lambda}}\right).$$

After substitution $\gamma=\alpha+\sqrt{\lambda}\beta$, $\varphi(\cdot)=\Phi(\alpha,\cdot)/\sqrt{\lambda}+\phi(\cdot)$ we obtain as $\lambda\to 0$:

$$(\psi,\psi)\simeq\int d\alpha d\beta e^{(i/\sqrt{\lambda})\beta_s(\partial S/\partial g a_s-\int dx\Pi(a,\mathbf{x})\partial\Phi(\alpha,\mathbf{x})/\partial\alpha_s)}e^{(i/2)\beta_s(\partial/\partial\alpha_s)(\partial S/\partial\alpha_l-\int d\mathbf{x}\Pi(\alpha,\mathbf{x})\partial\Phi(\alpha,\mathbf{x})/\partial\alpha_l)\beta_l}$$
$$\times\int D\phi g^*(a,\phi(\cdot))e^{i\beta_l\int d\mathbf{x}((\partial\Pi(\alpha,\mathbf{x})/\partial\alpha_l)\phi(\mathbf{x})-(\partial\Phi(\alpha,\mathbf{x})/\partial\alpha_l)1/i\,(\delta/\delta\phi(\mathbf{x}))}g(\alpha,\phi(\cdot)). \tag{5.2}$$

The condition

$$\frac{\partial S}{\partial\alpha_s}=\int \mathrm{d}\mathbf{x}\,\Pi(\alpha,\mathbf{x})\frac{\partial\Phi(\alpha,\mathbf{x})}{\partial\alpha_s} \tag{5.3}$$

should be satisfied. Otherwise, the integral (5.2) will be exponentially small as $\lambda\to 0$, so that state (5.1) will be trivial. Under condition (5.3), one has

$$(\psi,\psi)\to_{\lambda\to 0}\int \mathrm{d}\alpha\,\mathrm{d}\beta\int D\phi g^*(\alpha,\phi(\cdot))$$
$$\times\exp\left(i\beta_l\int d\mathbf{x}\left(\frac{\partial\Pi(\alpha,\mathbf{x})}{\partial\alpha_l}\phi(\mathbf{x})-\frac{\partial\Phi(\alpha,\mathbf{x})}{\partial\alpha_l}\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}\right)\right)g(\alpha,\phi(\cdot)). \tag{5.4}$$

To specify the composed semiclassical state in the functional representation, one should:

(i) specify the smooth functions $(S(\alpha),\Pi(\alpha,\mathbf{x}),\Phi(\alpha,\mathbf{x}))\equiv X(\alpha)$ obeying Eq. (5.3) (determine the k-dimensional isotropic manifold in the extended phase space $\mathcal{X}$);
(ii) specify the α-dependent functional $g(\alpha,\phi(\cdot))$.

The inner product of composed semiclassical states is given by expression (5.4).

Since the inner product (5.4) may vanish for nonzero g, one should factorize the space of composed semiclassical states. Such functional g that obey the property

$$\int \mathrm{d}\alpha\left(g^*(\alpha,\cdot)\prod_l\delta\left[\int d\mathbf{x}\left(\frac{\partial\Pi(\alpha,\mathbf{x})}{\partial\alpha_l}\phi(\mathbf{x})-\frac{\partial\Phi(\alpha,\mathbf{x})}{\partial\alpha_l}\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}\right)\right]g(\alpha,\cdot)=0 \tag{5.5}$$

should be set to be equal to zero, $g\sim 0$.

One can define the Poincaré transformation of the composed semiclassical state as follows. The transformation of $(S(\alpha),\Pi(\alpha,\cdot),\Phi(\alpha,\cdot))$ is $u_{a,\Lambda}(S(\alpha),\Pi(\alpha,\cdot),\Phi(\alpha,\cdot))$. The transformation of $g(\alpha,\phi(\cdot))$ is

$$\tilde{U}_{a,\Lambda}(u_{a,\Lambda}(S,\Pi,\Phi)\leftarrow(S,\Pi,\Phi))g(\alpha,\phi(\cdot)).$$

One should check that the inner product entering to Eq. (5.5) is invariant under Poincaré transformations. This will also imply that equivalent states are taken to equivalent.

Since the functional Schrödinger representation is not well-defined, let us consider the Fock representation. One should then specify the α-dependent Fock vector $Y(\alpha)=V^{-1}g(\alpha,\cdot)$ instead of the α-dependent functional $g(\alpha,\phi(\cdot))$. Making use of formulas (2.1), we find that the inner product (5.4) takes the form

$$\left(\begin{pmatrix}\Lambda^k\\ Y(\cdot)\end{pmatrix},\begin{pmatrix}\Lambda^k\\ Y(\cdot)\end{pmatrix}\right)=\int \mathrm{d}\alpha\,\mathrm{d}\beta\left(Y(\alpha),\exp\left(\beta_s\int \mathrm{d}\mathbf{x}(B_s(\alpha,\mathbf{x})A^+(\mathbf{x})-B_s^*(\alpha,\mathbf{x})A_s^-(\mathbf{x}))\right)Y(\alpha)\right), \tag{5.6}$$

where

$$B_s(\alpha,\cdot)=\hat{\Gamma}^{-1/2}\left(\hat{\mathcal{R}}\frac{\partial\Phi(\alpha,\cdot)}{\partial\alpha_s}-\frac{\partial\Pi(\alpha,.)}{\partial\alpha_s}\right), \tag{5.7}$$

$\hat{\Gamma}=\hat{\Gamma}(\Phi(\alpha,\cdot),\Pi(\alpha,\cdot))$, $\hat{\mathcal{R}}=\hat{\mathcal{R}}(\Phi(\alpha,\cdot),\Pi(\alpha,\cdot))$. If the isotropic manifold $(\Phi(\alpha,\cdot),\Pi(\alpha,\cdot))$ is nondegenerate, the functions $B_s(\alpha,\mathbf{x})$ are linearly independent.

The Poincaré transformation of the composed semiclassical state

$$\begin{pmatrix}\{X(\alpha)\}\\ Y(\alpha)\end{pmatrix}$$

is

$$\begin{pmatrix}\{u_{a,\Lambda}X(\alpha)\}\\ U_{a,\Lambda}(u_{a,\Lambda}X(\alpha)\leftarrow X(\alpha))Y(\alpha)\end{pmatrix}.$$

Consider the quantity

$$\begin{aligned}(B_s,B_l)-(B_l,B_s)&=\left(\frac{\partial\Phi}{\partial\alpha_s},(\hat{\mathcal{R}}^*-\hat{\mathcal{R}})\hat{\Gamma}^{-1}\frac{\partial\Pi}{\partial\alpha_l}\right)-\left(\frac{\partial\Phi}{\partial\alpha_l},(\hat{\mathcal{R}}^*-\hat{\mathcal{R}})\hat{\Gamma}^{-1}\frac{\partial\Pi}{\partial\alpha_s}\right)\\&=i\int \mathrm{d}\mathbf{x}\left(\frac{\partial\Phi(\alpha,\mathbf{x})}{\partial\alpha_l}\frac{\partial\Pi(\alpha,\mathbf{x})}{\partial\alpha_s}-\frac{\partial\Phi(\alpha,\mathbf{x})}{\partial\alpha_s}\frac{\partial\Pi(\alpha,\mathbf{x})}{\partial\alpha_l}\right).\end{aligned} \tag{5.8}$$

Differentiating (5.3) with respect to α_l, we obtain that quantity (5.8) vanishes. Thus, operators $\beta_s\int \mathrm{d}\mathbf{x}(B_s(\alpha,\mathbf{x})A^+(\mathbf{x})-B_s^*(\alpha,\mathbf{x})A_s^-(\mathbf{x}))$ commute each other.

It follows from the results of Ref. 48 that the inner product (5.7) is correctly defined, while Poincaré transformations of composed semiclassical states satisfy the group property and conserve the inner product (5.7).

VI. CONCLUSIONS

In this paper a notion of a semiclassical state is introduced. ''Elementary'' semiclassical state are specified by a set (X,Ψ) of classical field configuration X (point on the infinite-dimensional manifold $\mathcal{X}$, see Sec. II and III B and element Ψ of the space $\mathcal{F}$. The set of all ''elementary'' semiclassical states may be viewed as a semiclassical bundle.

The physical meaning of classical field X is evident. Discuss the role of Ψ. In the soliton quantization language[1,2] Ψ specifies whether the quantum soliton is in the ground or excited state. For the Gaussian approach,[14–17] Ψ specifies the form of the Gaussian functional, while for QFT in the strong external classical field[6,7] Ψ is a state of a quantum field in the classical background.

The ''composed'' semiclassical states have also been introduced (Sec. V). They can be viewed as superpositions of ''elementary'' semiclassical states and are specified by the functions $(X(\tau),\Psi(\tau))$ defined on some domain of $\mathbf{R}^k$ with values on the semiclassical bundle.

Not arbitrary superposition of elementary semiclassical states is nontrivial. The isotropic condition (5.3) should be satisfied. Moreover, the inner product of the ''composed'' semiclassical states [Eq. (5.6)] is degenerate, so that there is a ''gauge freedom'' (5.5) in specifying composed semiclassical states.

The composed semiclassical states are used[36] in soliton quantization, since there are translation zero modes and solitons can be shifted. They are useful if there are conserved integrals of

motion like charges. The correspondence between composed and elementary semiclassical states in QFT resembles the relationship between WKB and wave packet approximations in quantum mechanics.

An important feature of QFT is the property of Poincaré invariance. In this paper an explicit check of this property is presented for semiclassical QFT. The Poincaré transformations of elementary and composed semiclassical states have been constructed as follows. First, the simplest Poincaré transformations like spatial translations and rotations, evolution and boost are considered. The infinitesimal transformations are investigated, the Lie algebraic commutation relations have been checked and the group properties have been justified.

For the ''composed'' states, conservation of the degenerate inner product and isotropic condition under Poincaré transformation have been checked.

An important feature of QFT is a notion of field. In this paper this notion is introduced for semiclassical QFT. The property of Poincaré invariance of semiclassical field is checked.

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APPENDIX: WEYL CALCULUS

The purpose of this appendix is to formulate some properties of Weyl symbols of operators which are useful in justification of properties P1–P6. The detailed proofs can be found in Ref. 51.

1. Definition and some properties of Weyl symbols

First of all, recall the definition of the Weyl symbol of operator (Refs. 52–54, for reviews see e.g., Refs. 34 and 55). Let $A(x,k)$, $x,k\in\mathbf{R}^d$ be a classical observable depending on coordinates $x=(x_1,\ldots,x_d)$ and momenta $k=(k_1,\ldots,k_d)$. To specify the corresponding quantum observable $\hat{A}$ (to ''quantize'' the observable A), one should present it as a superposition of exponents,

$$A(x,k)=\int \mathrm{d}\alpha\,\mathrm{d}\beta\tilde{A}(\alpha,\beta)e^{i\alpha k+i\beta x}$$

and set

$$\hat{A}=\int \mathrm{d}\alpha\,\mathrm{d}\beta\tilde{A}(\alpha,\beta)e^{i\alpha\hat{k}+i\beta\hat{x}}.$$

Applying the formula for the inverse Fourier transformation, we find

$$(\hat{A}f)(x)=\int \frac{\mathrm{d}\alpha\,\mathrm{d}p}{(2\pi)^d}A\left(x+\frac{\alpha}{2};p\right)e^{-i\alpha p}f(x+\alpha). \tag{A1}$$

We denote the operator $\hat{A}$ of the form (A1) as $\hat{A}=\mathcal{W}(A)$. We will also write $A=\overline{\mathcal{W}}(\hat{A})$ if $\hat{A}=\mathcal{W}(A)$.

Definition A1: The operator $\mathcal{W}(A)$ is called a Weyl quantization of the function A. The function $\overline{\mathcal{W}}(\hat{A})$ is called a Weyl symbol of the operator $\hat{A}$.

For investigations of QFT ultraviolet divergences, we are interested in the behavior of Weyl symbols of operators at large values of momenta. Let us introduce some important spaces. Let $\omega_k=\sqrt{k^2+m^2}$ for some m.

Definition A2: (1) We say that a smooth function $A(x,k)$ is of the class $\mathcal{B}_N$ if and only if the functions $\omega_k^{N+s}(\partial^s A/\partial k^{i_1}\cdots\partial k^{i_s})$ are bounded for all $s,i_1,\ldots,i_s$.

(2) Let $A_n\in\mathcal{B}_N$, $n=1,\infty$, $A\in\mathcal{B}_N$. We say that $\mathcal{B}_N-\lim_{n\to\infty}A_n=A$ if and only if $\lim_{n\to\infty}\max_{k,x}\omega_k^{N+s}(\partial^s(A_n-A)/\partial k^{i_1}\ldots\partial k^{i_s})=0$ for all $s,i_1,\ldots,i_s$.

(3) We say that a function $A\in\mathcal{B}_N$ *is of the class* $\mathcal{A}_N$ *if and only if* $x_{j_1}\ldots x_{j_R}(\partial/\partial x_{s_1})\ldots(\partial/\partial x_{s_P})A\in\mathcal{B}_N$ *for all R, P,* $j_1,\ldots,j_R$, $s_1,\ldots,s_P$.

(4) Let $A_n\in\mathcal{A}_N$, $A\in\mathcal{A}_N$. *We say that* $\mathcal{A}_N-\lim_{n\to\infty}A_n=A$ *if and only if* $\mathcal{B}_N-\lim_{n\to\infty}x_{j_1}\cdots x_{j_R}(\partial/\partial x_{s_1})\cdots(\partial/\partial x_{s_P})\,(A_n-A)=0$ *for all R, P,* $j_1,\ldots,j_R$, $s_1,\ldots,s_P$.

The introduced classes $\mathcal{A}_N$ and $\mathcal{B}_N$ obey the following properties.

Lemma A1: (1) $\mathcal{A}_{N+R}\subseteq\mathcal{A}$, $\mathcal{B}_{N+R}\subseteq\mathcal{B}$ *for* $R\geqslant 0$.

(2) Let $\mathcal{A}_{N+R}-\lim_{n\to\infty}A_n=A$ and $R\geqslant 0$. *Then* $\mathcal{A}_N-\lim_{n\to\infty}A_n=A$.

(3) Let $\mathcal{B}_{N+R}-\lim_{n\to\infty}A_n=A$ *and* $R\geqslant 0$. *Then* $\mathcal{B}_N-\lim_{n\to\infty}A_n=A$.

(4) Let $A\in\mathcal{B}_N$. *Then* $(\partial/\partial k_i)A\in\mathcal{B}_{N+1}$.

(5) Let $A\in\mathcal{A}_N$. *Then* $x_iA\in\mathcal{A}_N$, $(\partial A/\partial x_i)\in\mathcal{A}_N$, $(\partial/\partial k_i)A\in\mathcal{A}_{N+1}$, $f(x)A\in\mathcal{A}_N$ *for smooth bounded function* $f(x)$.

(6) Let $\mathcal{B}_N-\lim_{n\to\infty}A_n=A$. *Then* $\mathcal{B}_{N+1}-\lim_{n\to\infty}(\partial/\partial k_i)A_n=(\partial/\partial k_i)A$.

(7) Let $\mathcal{A}_N-\lim_{n\to\infty}A_n=A$. *Then* $\mathcal{A}_N-\lim_{n\to\infty}x_iA_n=x_iA$, $\mathcal{A}_N-\lim_{n\to\infty}(\partial A_n/\partial x_i)=\partial A/\partial x_i$, $\mathcal{A}_{N+1}-\lim_{n\to\infty}(\partial/\partial k_i)A_n=(\partial/\partial k_i)A$, $\mathcal{A}_N-\lim_{n\to\infty}f(x)A_n=f(x)A$ *for smooth bounded function* $f(x)$.

(8) Let $A_1\in\mathcal{B}_{N_1}$, $A_2\in\mathcal{B}_{N_2}$. *Then* $A_1A_2\in\mathcal{B}_{N_1N_2}$.

(9) The following properties are satisfied: $k_i\in\mathcal{B}_{-1}$, $\omega_k^{\alpha}\in\mathcal{B}_{-\alpha}$.

(10) Let $A\in\mathcal{B}_N$. *Then* $k_iA\in\mathcal{B}_{N-1}$, $\omega_k^{-\alpha}A\in\mathcal{B}_{N+\alpha}$, $(\partial A/\partial k_i)\in\mathcal{B}_{N+1}$.

(11) Let $A\in\mathcal{A}_N$. *Then* $k_iA\in\mathcal{A}_{N-1}$, $\omega_k^{-\alpha}A\in\mathcal{A}_{N+\alpha}$, $\partial A/\partial k_i\in\mathcal{A}_{N+1}$.

(12) Let $\mathcal{B}_N-\lim_{n\to\infty}A_n=A$. *Then* $\mathcal{B}_{N-1}-\lim_{n\to\infty}k_iA_n=k_iA$, $\mathcal{B}_{N+\alpha}-\lim_{n\to\infty}\omega_k^{-\alpha}A_n=\omega_k^{-\alpha}A$, $\mathcal{B}_{N+1}-\lim_{n\to\infty}(\partial A_n/\partial k_i)=\partial A/\partial k_i$.

(13) Let $\mathcal{A}_N-\lim_{n\to\infty}A_n=A$. *Then* $\mathcal{A}_{N-1}-\lim_{n\to\infty}k_iA_n=k_iA$, $\mathcal{A}_{N+\alpha}-\lim_{n\to\infty}\omega_k^{-\alpha}A_n=\omega_k^{-\alpha}A$, $\mathcal{A}_{N+1}-\lim_{n\to\infty}(\partial A_n/\partial k_i)=\partial A/\partial k_i$.

(14) Let $A_1\in\mathcal{A}_{N_1}$, $A_2\in\mathcal{A}_{N_2}$. *Then* $A_1A_2\in\mathcal{A}_{N_1+N_2}$.

(15) Let $\mathcal{A}_{N_1}-\lim_{n\to\infty}A_{1,n}=A_1$, $\mathcal{A}_{N_2}-\lim_{n\to\infty}A_{2,n}=A_2$. *Then* $\mathcal{A}_{N_1+N_2}-\lim_{n\to\infty}A_{1,n}A_{2,n}=A_1A_2$.

Theorem A.2: *(1) Let* $A\in\mathcal{A}_0$. *Then the operator* $\mathcal{W}(A)$ (A1) *is bounded.*

(2) Let $\mathcal{A}_0-\lim_{n\to\infty}A_n=0$. *Then* $\lim_{n\to\infty}\|\mathcal{W}(A_n)\|=0$.

(3) Let $A\in\mathcal{A}_N$, $N>d/2$. *Then* $\mathcal{W}(A)$ *is a Hilbert–Schmidt operator.*

(4) Let $\mathcal{A}_N-\lim_{n\to\infty}A_n=0$, $N>d/2$. *Then* $\lim_{n\to\infty}\|\mathcal{W}(A_n)\|_2=0$.

(5) Let $A\in\mathcal{A}_N$, $N>d$. *Then* $\mathcal{W}(A)$ *is of the trace class.*

(6) Let $\mathcal{A}_N-\lim_{n\to\infty}A_n=0$, $N>d$. *Then* $\lim_{n\to\infty}\mathrm{Tr}\,\mathcal{W}(A_n)=0$.

Recall that the Weyl symbol of the product of operators

$$A*B=\overline{\mathcal{W}}(\mathcal{W}(A)\mathcal{W}(B))$$

can be presented as[34,55]

$$(A*B)(x,k)=\int\frac{\mathrm{d}\beta_1\,\mathrm{d}\beta_2\,\mathrm{d}\xi_1\,\mathrm{d}\xi_2}{(2\pi)^{2d}}A\left(x+\xi_1,k+\frac{\beta_2}{2}\right)B\left(x+\xi_2,k-\frac{\beta_1}{2}\right)e^{-\beta_1\xi_1-i\beta_2\xi_2}. \quad \text{(A2)}$$

Formula (A2) can be obtained from definition (A1).

Let us investigate some properties of formula (A2). Let us find an expansion of formula (A2) as $|k|\to\infty$. Formally, one has

$$A\left(x+\xi_1,k+\frac{\beta_2}{2}\right)=\sum_{n_2=0}^{\infty}\frac{1}{2^{n_2}n_2!}\frac{\partial^{n_2}A(x+\xi_1,k)}{\partial k^{i_1}\cdots\partial k^{i_{n_2}}}\beta_2^{i_1}\cdots\beta_2^{i_{n_2}};$$

$$B\left(x+\xi_2,k-\frac{\beta_1}{2}\right)=\sum_{n_1=0}^{\infty}\frac{(-1)^{n_1}}{2^{n_1}n_1!}\frac{\partial^{n_1}B(x+\xi_2,k)}{\partial k^{j_1}\cdots\partial k^{j_{n_1}}}\beta_1^{j_1}\cdots\beta_1^{j_{n_1}}.$$

Therefore,

$$(A^*B)(x,k)=\sum_{n_1n_2=0}^{\infty}\frac{(-1)^{n_1}}{2^{n_1+n_2}n_1!n_2!}\int\frac{d\beta_1\,d\beta_2\,d\xi_1\,d\xi_2}{(2\pi)^{2d}}e^{-i\beta_1\xi_1-i\beta_2\xi_2}\frac{\partial^{n_2}A(x+\xi_1,k)}{\partial k^{i_1}\cdots\partial k^{i_{n_2}}}\beta_2^{i_1}\cdots\beta_2^{i_{n_2}}$$
$$\times\frac{\partial^{n_1}B(x+\xi_2,k)}{\partial k^{j_1}\cdots\partial k^{j_{n_1}}}\beta_1^{j_1}\cdots\beta_1^{j_{n_1}}$$
$$=\sum_{n_1n_2=0}^{\infty}\frac{i^{n_1-n_2}}{2^{n_1+n_2}n_1!n_2!}\frac{\partial^{n_1+n_2}A(x,k)}{\partial k^{i_1}\cdots\partial k^{i_{n_2}}\partial x^{j_1}\cdots\partial x^{j_{n_1}}}\frac{\partial^{n_1+n_2}B(x,k)}{\partial x^{i_1}\cdots\partial x^{i_{n_2}}\partial k^{j_1}\cdots\partial k^{j_{n_1}}}. \tag{A3}$$

Denote

$$(A\overset{K}{*}B)(x,k)=\sum_{n_1n_2\geqslant 0,n_1+n_2\leqslant K}\frac{i^{n_1-n_2}}{2^{n_1+n_2}n_1!n_2!}\frac{\partial^{n_1+n_2}A(x,k)}{\partial k^{i_1}\cdots\partial k^{i_{n_2}}\partial x^{j_1}\cdots\partial x^{i_{n_1}}}\frac{\partial^{n_1+n_2}B(x,k)}{\partial x^{i_1}\cdots\partial x^{i_{n_2}}\partial k^{j_1}\cdots\partial k^{j_{n_1}}}.$$

This is an asymptotic expansion in $1/|k|$ as $|k|\to\infty$. One can estimate an accuracy of the asymptotic series.

Definition A3: We say that the function $f(x)$, $x\in\mathbf{R}^d$ is of the class $\mathcal{C}$ if f is a smooth function such that for each set $(i_1,\ldots,i_l)$ there exists $m>0$ such that the function $(x^2+1)^{-m}(\partial^l/\partial x^{i_1}\ldots\partial x^{i_l})f$ is bounded.

Theorem A3: *(1) Let $f\in\mathcal{C}$, $B\in\mathcal{A}_N$. Then $f^*B=f\overset{K}{*}B+R_K$ with $R_K\in\mathcal{A}_{N+K+1}$.*

(2) Let $f\in\mathcal{C}$, $\mathcal{A}_N-\lim_{n\to\infty}B_n=0$. Then $\mathcal{A}_{N+K+1}-\lim_{n\to\infty}(f^*B_n-f\overset{K}{*}B_n)=0$.

(3) Let $A=A(k)$, $A\in\mathcal{B}_{M_1}$, $B\in\mathcal{A}_{M_2}$. Then $A^*B=A\overset{K}{*}B+R_K$ with $R_K\in\mathcal{A}_{M_1+M_2+K+1}$.

(4) Let $A=A(k)$, $A\in\mathcal{B}_{M_1}$, $\mathcal{A}_{M_2}-\lim_{n\to\infty}B_n=B$. Then $\mathcal{A}_{M_1+M_2+K+1}-\lim_{n\to\infty}(A^*B_n-A\overset{K}{*}B_n)=0$.

(5) Let $A\in\mathcal{A}_{M_1}$, $B\in\mathcal{A}_{M_2}$. Then $A^*B=A\overset{K}{*}B+R_K$ with $R_K\in\mathcal{A}_{M_1+M_2+K+1}$.

(6) Let $A_n\in\mathcal{A}_{M_1}$, $B_n\in\mathcal{A}_{M_2}$. Then $\mathcal{A}_{M_1+M_2+K+1}-\lim_{n\to\infty}(A_n{}^*B_n-A_n\overset{K}{*}B_n)=A^*B-A\overset{K}{*}B$.

Let us now investigate the properties of the exponent of the operator $\exp\mathcal{W}(A)\equiv\mathcal{W}(*\exp A)$. It is convenient to consider the Fourier transformations of Weyl symbols,

$$\tilde{A}(\gamma,k)=\int\frac{dx}{(2\pi)^d}e^{-i\gamma x}A(x,k).$$

Introduce the following norms for Weyl symbols,

$$\|A\|_{I,K}=\max_{J+M+N\leqslant K}\max_{\gamma,K}\left|\omega_k^{I+J}\frac{\partial^J}{\partial k_{j_1}\cdots\partial k_{jj}}\gamma_{m_1}\cdots\gamma_{m_M}\frac{\partial^N\tilde{A}}{\partial\gamma_{n_1}\cdots\partial\gamma_{n_N}}\right|. \tag{A4}$$

Lemma A4: (1) $A\in\mathcal{A}_1$ if and only if $\|A\|_{1,K}<\infty$ for all $k=\overline{0,\infty}$.

(2) For arbitrary integer numbers K, $L>d/2$ there exists such a constant b_K that $\|A^*B\|_{0,K}\leqslant b_K\|A\|_{0,K+2L}\|B\|_{0,K}$.

Consider the Weyl symbol of the exponent

$$*\exp At-1=\sum_{n=1}^{\infty}\frac{A^{*n}t^n}{n!} \tag{A5}$$

with $A^{*n}=A^*\cdots^*A$.

Lemma A5: (1) Let $A\in\mathcal{A}_M$, $M>0$. *Then the expansion* (A5) *is convergent in the* $\|\cdot\|_{0,K}$*-norm. The estimation* $\|*\exp At-1\|_{0,K}\leqslant C_K$ *is satisfied for* $t\in[0,T]$.

(2) Let $A\in\mathcal{A}_M$, $M>0$. *Then* $\Sigma_{m=N}^{\infty}(A^{*m}/m!)\in\mathcal{A}_{MN}$.

(3) Let $A_n\in\mathcal{A}_M$, $M>0$ *and* $\mathcal{A}_M-\lim_{n\to\infty}A_n=A$. *Then* $\mathcal{A}_{MN}-\lim_{n\to\infty}\Sigma_{m=N}^{\infty}(A_n^{*m}/m!)=\Sigma_{m=N}^{\infty}(A^{*m}/m!)$.

Let $\hat{A}=f(\hat{x})$, $\hat{B}=g(\hat{k})$. Investigate the properties of the commutator $\hat{K}=[\hat{A};\hat{B}]$.

Lemma A6: Let $\partial^n f/\partial x^{i_1}\cdots\partial x^{i_n}$, $\partial^n g/\partial k^{i_n}\ldots\partial k^{i_n}$ *be bounded functions,* $m,n=\overline{1,L}$, *while*

$$\frac{\partial^{L+1}f}{\partial x^{i_1}\cdots\partial x^{i_{L+1}}}\in L^2,\quad \frac{\partial^{L+1}g}{\partial k^{i_1}\cdots\partial k^{i_{L+1}}}\in L^2.$$

Then $[f(\hat{x}),g(\hat{k})]$ *is a bounded operator.*

2. Asymptotic expansions of Weyl symbol

To check the property of Poincaré invariance, it is important to investigate the large-k expansion of the Weyl symbols. Introduce the corresponding definitions.

Definition A4: (1) We say that a smooth function $A(x,n)$, x, $n\in\mathbf{R}^d$, $|n|<1$, *is of the class* $\mathcal{L}$ *if the functions*

$$\frac{\partial^I}{\partial n_{i_1}\cdots\partial n_{i_I}}x_{j_1}\cdots x_{j_J}\frac{\partial^M}{\partial x_{m_1}\cdots\partial x_{m_M}}A \tag{A6}$$

are bounded.

(2) *Let* $A_s\in\mathcal{L}$, $s=\overline{1,\infty}$. *We say that* $\mathcal{L}-\lim_{s\to\infty}A_s=0$ *if*

$$\sup_{|n|\leqslant 1}\lim_{s\to\infty}\left|\frac{\partial^I}{\partial n_{i_1}\cdots\partial n_{i_I}}x_{j_1}\cdots x_{j_J}\frac{\partial^M}{\partial x_{m_1}\cdots\partial x_{m_M}}A\right|=0.$$

Definitions A2 and A4 imply the following statement.

Lemma A.7: (1) Let $A\in\mathcal{L}$. *Then the function* $B(x,k)=A(x,k/\omega_k)$ *is of the class* $\mathcal{B}_0$.

(2) *Let* $\mathcal{L}-\lim_{s\to\infty}A_s=0$. *Then* $\mathcal{B}_0-\lim_{s\to\infty}A_s(x,k/\omega_k)=0$.

Making use of definition A2 and lemma A5, we obtain the following corollary.

Corollary: (1) Let $A\in\mathcal{L}$. *Then the function* $\omega_k^{-\alpha}A(x,k/\omega_k)$ *is of the class* $\mathcal{A}_\alpha$.

(2) *Let* $\mathcal{L}-\lim_{s\to\infty}A_s=0$. *Then* $\mathcal{A}_\alpha-\lim_{s\to\infty}\omega_k^{-\alpha}A_s(x,k/\omega_k)=0$.

Definition A5: (1) A formal asymptotic expansion is a set $\breve{A}$ $\alpha\in\mathbf{R}$ *and functions* $A_0,A_1,\ldots\in\mathcal{L}$. *We say that the formal asymptotic expansions* $\breve{A}=(\alpha,A_0,A_1,\ldots)$ *and* $\breve{B}=(\beta,B_0,B_1,\ldots)$ *are equivalent if* $\alpha-\beta$ *is an integer number and* $A_{l-\alpha+\beta}=B_l$ *for all* $l=\overline{-\infty,+\infty}$ (*we assume* $A_l=0$ *and* $B_l=0$ *for* $l<0$. *We denote formal asymptotic expansions of Weyl symbols as*

$$\breve{A}\equiv\sum_{n=0}^{\infty}\omega_k^{-n-\alpha}A_n(x,k/\omega_k).$$

If $A_0=0,\ldots,A_{l-1}=0$, $A_l\neq 0$, *the quantity* $\deg\breve{A}\equiv\alpha+n$ *is called a degree of a formal asymptotic expansion* $\breve{A}$.

(2) *Let* $\breve{A}_s$, $s=\overline{1,\infty}$ *and* $\breve{A}$ *be formal asymptotic expansions of Weyl symbols. We say that* $F.E-\lim_{s\to\infty}\breve{A}_s=A$ *if* $\alpha_s=\alpha$ *and* $\mathcal{L}-\lim_{s\to\infty}(A_{s,n}-A_s)=0$.

The summation and multiplication by numbers are obviously defined:

$$\breve{A}+\lambda\breve{B}=\sum_{n=0}^{\infty}\omega_k^{-n-\alpha}(A_n(x,k\omega_k)+\lambda B_n(x,k/\omega_k)).$$

The product of formal asymptotic expansions of Weyl symbols

$$\check{A}\equiv\sum_{n=0}^{\infty}\omega_k^{-n-\alpha}A_n(x,k/\omega_k),\quad \check{B}\equiv\sum_{n=0}^{\infty}\omega_k^{-n-\beta}B_n(x,k/\omega_k)$$

is defined as

$$\check{A}\check{B}\equiv\sum_{n=0}^{\infty}\omega_k^{-n-\alpha-\beta}\sum_{s,l\geqslant 0;s+l=n}A_s(x,k/\omega_k)B_l(x,k/\omega_k).$$

Let $f=f(x), f\in\mathcal{C}$. Then

$$f(x)\check{A}\equiv\sum_{n=0}^{\infty}\omega_k^{-n-\alpha}f(x)A_n(x,k/\omega_k).$$

One also defines

$$\omega_k^{-\beta}\check{A}\equiv\sum_{n=0}^{\infty}\omega_k^{-n-\alpha-\beta}A_n(x,k/\omega_k)$$

and

$$\frac{\partial\check{A}}{\partial k_s}=\sum_{l=0}^{\infty}\omega_k^{-l-\alpha-1}\left[-(l+\alpha)A_l(x,n)+\frac{\partial A_l}{\partial n_p}(x,n)(\delta_{ps}-n_pn_s)\right]_{|n=k/\omega_k}.$$

The *-product of formal asymptotic expansions is introduced as

$$\check{A}*\check{B}\equiv\sum_{K=0}^{\infty}\sum_{n_1n_2\geqslant 0,n_1+n_2=K}\frac{i^{n_1-n_2}}{n_1!n_2!2^{n_1+n_2}}\frac{\partial^{n_1+n_2}}{\partial x^{i_1}\cdots\partial x^{i_{n_2}}\partial k^{j_1}\cdots\partial k^{j_{n_1}}}\sum_{l_1=0}^{\infty}\omega_k^{-l_1-\alpha_1}A_{l_1}(x,k/\omega_k)$$
$$\times\frac{\partial^{n_1+n_2}}{\partial x^{j_1}\cdots\partial x^{j_{n_1}}\partial k^{i_1}\cdots\partial k^{i_{n_2}}}\sum_{l_2=0}^{\infty}\omega_k^{-l_2-\alpha_2}A_{l_2}(x,k/\omega_k).$$

The formal asymptotic expansions $\check{A}*\omega_k^{\alpha}$, $\check{A}*f(x)$ are defined analogously. The *-exponent of a formal asymptotic expansion $\check{A}$ is defined as

$$*\exp\check{A}-1=\sum_{n=1}^{\infty}\frac{\check{A}^{*n}}{n!}$$

provided that $\deg A$ is a positive integer number.

Definition A6: (1) An asymptotic expansion of the Weyl symbol is a set $\underline{A}\equiv(A,\check{A})$ *of the Weyl symbol A and a formal asymptotic expansion* $\check{A}$ *such that*

$$A(x,k)-\sum_{l=0}^{n-1}\frac{A_l(x,k/\omega_k)}{\omega_k^{l+\alpha}}\in\mathcal{A}_{n+\alpha}$$

for all $n=\overline{0,\infty}$.

(2) We say that $E-\lim_{s\to\infty}\underline{A_s}=\underline{A}$ *if* $F.E-\lim_{s\to\infty}\check{A}_s=\check{A}$ *and*

$$\mathcal{A}_{n+\alpha}-\lim_{s\to\infty}\left(A_s(x,k)-\sum_{l=0}^{n-1}\frac{A_{s,l}(x,k/\omega_k)}{\omega_k^{l+\alpha}}\right)=A(x,k)-\sum_{l=0}^{n-1}\frac{A_l(x,k/\omega_k)}{\omega_k^{l+\alpha}}$$

for all $n=\overline{0,\infty}$.

Remark: For given Weyl symbol A, the asymptotic expansion is not unique. For example, let

$$A(x,k)=m^2 f(x)/\omega_k .$$

One can choose $\alpha=2$, $A_0(x,n)=m^2 f(x)$ and find $A(x,k)=\omega_k^{-2}A_0(x,k/\omega_k)$. On the other hand, one can set $\alpha=0$, $A_0(x,n)=f(x)(1-n_i n_i)$ and obtain $A(x,k)=A_0(x,k/\omega_k)$ since $\omega_k^2-k_i k_i=m^2$. We see that a degree is a characteristic feature of an expansion rather than of a symbol.

Let $\underline{A}=(A,\check{A})$, $\underline{B}=(B,\check{B})$. Denote $\underline{A}*\underline{B}\equiv(A*B,\check{A}*\check{B})$, $\omega_k^\alpha*\underline{A}\equiv(\omega_k^\alpha*A,\omega_k^\alpha*\check{A})$, $f(x)*\underline{A}\equiv(f(x)*A,f(x)*\check{A})$, $*\exp\underline{A}-1\equiv(*\exp A-1,*\exp\check{A}-1)$.

Theorem A3 and lemma A5 imply the following statements.

Theorem A8: *(1) Let* $\underline{A}$ *be an asymptotic expansion of a Weyl symbol. Then* $\omega_k^\alpha*\underline{A}$ *and* $f(x)*\underline{A}$ *are asymptotic expansions of Weyl symbols under conditions of theorem A3, while* $*\exp\underline{A}-1$ *is an asymptotic expansion of a Weyl symbol, provided that* $\deg\check{A}$ *is a positive integer number.*

(2) Let $\underline{A}$ *and* $\underline{B}$ *be asymptotic expansions of Weyl symbols. Then* $\underline{A}*\underline{B}$ *is an asymptotic expansion of a Weyl symbol.*

Theorem A9: *(1) Let* $E-\lim_{n\to\infty}\underline{A}_n=\underline{A}$. *Then:*

(*a*) $E-\lim_{n\to\infty}\omega_k^\alpha*\underline{A}_n\omega_k^\alpha*\underline{A}$,
(*b*) $E-\lim_{n\to\infty}f(x)*\underline{A}_n f(x)*\underline{A}$ *under conditions of theorem A3,*
(*c*) $E-\lim n\to\infty(*\exp\underline{A}_n-1)=*\exp\underline{A}-1$ *if* $\deg\check{A}_n$, $\deg\check{A}$ *are positive integer numbers.*

(2) Let $E-\lim_{n\to\infty}\underline{A}_n=\underline{A}$ *and* $E-\lim_{n\to\infty}\underline{B}_n=\underline{B}$. *Then* $E-\lim_{n\to\infty}\underline{A}_n*\underline{B}_n=\underline{A}*\underline{B}$.

The time derivative of the asymptotic expansion $\underline{A}(t)$ with respect to t is defined in a standard way

$$E-\lim_{\delta t\to 0}\frac{\underline{A}(t+\delta t)-\underline{A}(t)}{\delta t}=\frac{\mathrm{d}\underline{A}(t)}{\mathrm{d}t}.$$

The integral $\int_{t_1}^{t_2}\underline{A}(t)\mathrm{d}t$ is also defined in a standard way.

Theorem A9 implies the following statement.

Theorem A10: (1) *Let* $\underline{A}(t)$ *be a continuously differentiable asymptotic expansion of a Weyl symbol. Then*

(*a*) $(\mathrm{d}/\mathrm{d}t)(\omega_k^\alpha*\underline{A})=\omega_k^\alpha*(\mathrm{d}A/\mathrm{d}t)$,
(*b*) $(\mathrm{d}/\mathrm{d}t)(f(x)*\underline{A})=f(x)*(\mathrm{d}A/\mathrm{d}t)$ *under conditions of theorem A3.*
(*c*) $(\mathrm{d}/\mathrm{d}t)(*\exp\underline{A}-1)=\int_0^1\mathrm{d}\tau e^{\underline{A}(t-\tau)}*\mathrm{d}\underline{A}/\mathrm{d}t*e^{\underline{A}\tau}$,
(*d*) $(\mathrm{d}/\mathrm{d}t)(\underline{A}*\underline{B})=(\mathrm{d}/\mathrm{d}t)\underline{A}*\underline{B}+\underline{A}*(\mathrm{d}/\mathrm{d}t)\underline{B}$.

The only nontrivial statement is (c). It is proved by using the identity[55]

$$*\exp\underline{A}_1-*\exp\underline{A}_2=\int_0^1\mathrm{d}\tau*\exp(\underline{A}_1(1-\tau))*(\underline{A}_1-\underline{A}_2)*\exp(\underline{A}_2\tau).$$

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On the spectral properties of Hamiltonians without conservation of the particle number

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We consider quantum systems with variable but finite number of particles. For such systems we develop geometric and commutator techniques. We use these techniques to find the location of the spectrum, to prove absence of singular continuous spectrum, and identify accumulation points of the discrete spectrum. The fact that the total number of particles is bounded allows us to give relatively elementary proofs of these basic results for an important class of many-body systems with nonconserved number of particles. © *2002 American Institute of Physics.*
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I. INTRODUCTION

This paper is a contribution toward a geometrical theory of quantum systems with variable number of particles. Such systems occur naturally in quantum field theory, condensed matter physics, and the theory of chemical reactions. Though often, as in cases involving photons (see, e.g., Ref. 1), the number of particles can take arbitrary large values, in other cases such as scattering of spin waves on defects, scattering of massive particles and chemical reactions, there are only a few participants at any given time, though their number can change. It is the situations of the second kind that are addressed in this paper. Having the limitation on the total number of particles involved allows us to apply more sophisticated geometrical and positive commutative techniques than is usually the case (see, e.g., Ref. 1), while keeping the proof rather simple and obtaining stronger results. In this paper we obtain some basic results for the above-described systems by developing for them the method of conjugate operators.

The conjugate operator method consists in obtaining diverse spectral properties of a self-adjoint operator H in the Hilbert $\mathcal{H}$ assuming the existence of a self-adjoint operator A such that the commutator $[iH, A]$ has a definite sign when localized in a small spectral interval of H. More precisely, if τ is a closed subset of $\mathbf{R}$ then A is called locally conjugate for H on $\mathbf{R}\backslash\tau$ if and only if for every $\lambda \in \mathbf{R}\backslash\tau$ there is $c>0$ and a compact operator K such that the Mourre estimate

$$E_{[\lambda-c,\lambda+c]}(H)[iH,A]E_{[\lambda-c,\lambda+c]}(H) \geqslant cE_{[\lambda-c,\lambda+c]}(H)+K \tag{1.1}$$

holds, where $E_Z(H)$ denotes the spectral projector of H on a Borel set $Z\subset\mathbf{R}$ and the intersection of domains $D(H)\cap D(A)$ is assumed dense in $\mathcal{H}$ allowing one to understand the left-hand side as a quadratic form.

The method has appeared to be a remarkably fruitful tool in many recent investigations in spectral and scattering theory of many-body Hamiltonians, cf. Refs. 2–4, see also Refs. 5 and 6.

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If X is a finite-dimensional Euclidean space and H_X is the Schrödinger operator in $L^2(X)$ of the form

$$H_X = -\Delta_X + V_X, \tag{1.2}$$

where Δ_X is the Beltrami–Laplace operator on X and V_X has a many-body structure with interaction potentials satisfying some regularity and decay hypotheses, then there exists a closed, countable set $\tau(H_X) \subset \mathbf{R}$ [called the threshold set of H_X] such that the dilation generator

$$A_X = x \cdot D_x + D_x \cdot x \tag{1.3}$$

is locally conjugate for H_X in $\mathbf{R} \setminus \tau(H_X)$. Moreover the eigenvalues of H_X may accumulate (with multiplicities) only at $\tau(H_X)$ and the singular continuous spectrum of H_X is empty. It is also useful to adopt the convention that $H_X = 0$ in $L^2(X) = \mathbf{C}$ in the case $X = \{0\}$.

The aim of this paper is to obtain similar results for a class of Hamiltonians acting in the Hilbert space

$$\mathcal{H} = \bigoplus_{1 \leqslant n \leqslant N} L^2(X(n)), \tag{1.4}$$

where $\mathbf{X} = \{X(n)\}_{1 \leqslant n \leqslant N}$ is a family of configuration spaces which are finite dimensional Euclidean spaces. The Hamiltonians we consider,

$$\mathbf{H_X} = \mathbf{H_X^{diag}} + \mathbf{W_X}, \tag{1.5}$$

are perturbations of the diagonal operator formed by many-body Schrödinger operators in $L^2(X(n))$,

$$\mathbf{H_X^{diag}} = \bigoplus_{1 \leqslant n \leqslant N} H_{X(n)} = \bigoplus_{1 \leqslant n \leqslant N} (-\Delta_{X(n)} + V_{X(n)}). \tag{1.6}$$

Such Hamiltonians describe a quantum system of at most N particles and the interaction terms can change the number of particles between 1 and N. Hence $\mathbf{H_X}$ acts on the Fock subspace $\mathcal{H}$. In the second-quantized formulation the above-given interaction can contain any power of creation and annihilation operators leaving the above-mentioned Fock subspace invariant:

$$\mathbf{W_X} = P_N \mathbf{W_X} P_N,$$

where P_N is the projection of the Fock subspace of at most N particles. The locally conjugate operator for $\mathbf{H_X}$ is the diagonal operator

$$\mathbf{A_X} = \bigoplus_{1 \leqslant n \leqslant N} A_{X(n)}, \tag{1.7}$$

where $A_{X(n)}$ are dilation generators in $X(n)$ [defined in (1.3)].

The model is motivated by field theoretical and solid state systems, where the particle number is not conserved. This type of problem has recently attracted much attention, see, e.g., Refs. 7, 1, 8, 9, and 10. In Ref. 9 the two state atom coupled to a massive free field was studied, spectral and scattering theory was developed using conjugate operators and other N-body techniques. Previously the authors of Ref. 7 considered a truncated model of the two state atom where, like in this work, the total number of particles is at most $N < \infty$. The work of Ref. 9 was then generalized to a general molecule in a bound state, replacing the two-state atom in Ref. 8.

References 1 and 10 deal with the massless photon/boson field interacting with a bound atom. References 1, 8, and 9 use the dilation as conjugate operator; Refs. 7 and 10 use dilations modified by terms depending on the interaction.

In this work we generalize some of the above-mentioned models in that we allow the ''boson'' system to be interacting. We also allow the interaction between the atomic and boson field to be of general nature. (In all of the above-mentioned models the interaction is linear in the boson fields.)

Our construction of the conjugate operator is different from the above-noted works as it is more geometric in spirit. Our construction uses the geometry of N-body systems as the guiding principle; in particular we can modify the dilation generator using Graf's construction to allow local singularities in the interactions.[11,12] Furthermore our interactions are of a more general nature, and so we can cover the case of pair annihilation in some cases, e.g., the positronium system, when a bound electron and positron pair are annihilated when coupled to a field.

If X, X' are Euclidean spaces then $X' \subseteq X$ denotes the inclusion together with the fact that the Euclidean structure of X' is inherited from the structure of X and $X' \subset X$ denotes the strict inclusion, i.e., $X' \subset X \Leftrightarrow (X' \subseteq X$ and $X' \neq X)$.

Further on we assume that Euclidean spaces $X(n)$ satisfy[13]

$$X(N) \subset \cdots \subset X(2) \subset X(1). \tag{1.8}$$

The configuration space of the system, $X(1)$, is assumed to be Euclidean space, and corresponds to N particles, of various types or masses, e.g.,

$$X(1) = \{x = \{x_1, \ldots, x_N\} \,|\, x_i \in \mathbf{R}^m, i = 1, \ldots, N\},$$

endowed with the metric

$$x, y \in X(1), x \cdot y = \sum_{i=1}^{N} m_i x_i y_i, \quad m_i > 0.$$

$X' \subseteq X(1)$ then denotes a subspace of $X(1)$ endowed with the induced metric of $X(1)$.

Then we take $X(j)$ to denote the subspace of $X(1)$ with the $j-1$ particles x_N to x_{n-j+1} removed (namely, the corresponding coordinates are set to zero)

$$X(j) = \{x = (x_1, \ldots, x_{N-j+1})\}.$$

We then have subspaces $X(j)$ such that

$$X(N) \subset X(N-1) \subset \cdots X(2) \subset X(1).$$

This notation, while nonstandard, will allow us to do the inductive proofs in a standard way, and also emphasizes the generality of the N-body type systems involved: the subspaces $X(j)$ can be chosen more generally for X, so we can cover the generalized N-body systems of Agmon.[14]

To describe the many-body structure of the considered operators we assume that $\mathbf{Y}_0$ is a finite subset of Euclidean spaces contained in $X(1)$ (with inherited Euclidean structures) and for every $Y \in \mathbf{Y}_0$ the associated interaction potential $v_Y \in L^2_{\mathrm{loc}}(Y)$ is real-valued and satisfies some regularity and decay hypotheses (to be described later). For every $X \subseteq X(1)$ we define $V_X : H^2(X) \to L^2(X)$ as the operator of multiplication by

$$V_X(x) = \sum_{Y \in \mathbf{Y}_0, Y \subseteq X} v_Y(\pi^Y x), \tag{1.9}$$

where $x \in X$, π^Y is the orthogonal projection onto Y and $H^s(X)$ denotes the Sobolev space on X.

To describe the perturbation $\mathbf{W}_\mathbf{X}$ we also consider operators $W : H^2(X') \to L^2(X)$ with $X' \subset X$, saying that W is the operator of multiplication by $w \in L^2_{\mathrm{loc}}(X)$ if

$$(W\varphi)(x) = w(x)\varphi(\pi^{X'} x). \tag{1.10}$$

Such interaction terms allow quite general nonparticle number conserving terms. The decay assumptions on $w(x)$ imply that the created particle by the interaction have localized wave function. This is natural as local field theories of massive particles satisfy this condition. It may be violated by massless theories with (strong) infrared interactions.

The simplest case is when the interaction creates "one particle" (linear in the creation/annihilation term):

$$w(x)=f(x_\alpha),x_\alpha\in\mathbf{R}^3,f\in L^2(\mathbf{R}^3)\cap L^\infty(\mathbf{R}^3),$$

$$X'=\mathbb{R}^3\oplus\cdots\mathbb{R}^3,n-times,$$

$$X=X'\oplus\mathbb{R}^3.$$

In this case,

$$(W_\varphi)(x)=f(x_\alpha)\varphi(\Pi^{X'}x)$$

is the operator that creates a particle with wave function $f(x_\alpha)$, acting on the space of n particles into the space of $n+1$ particles.

The construction (1.10) allows much more general type of interactions, e.g., creating pairs of particles in some subspaces of other particles, this can be achieved by choosing

$$w(x)=f(x_\alpha,x_\beta),x_\alpha,x_\beta\in\mathbf{R}^3,$$

which corresponds to a (sum of) products of two creation operators.

We define $\tilde{\mathbf{X}}=\{\tilde{X}(n)\}_{2\leqslant n\leqslant N}$ by

$$X(n-1)=X(n)\oplus\tilde{X}(n)\ \text{ for }\ 2\leqslant n\leqslant N. \tag{1.11}$$

We assume that for $2\leqslant n\leqslant N$ and $Y\in\mathbf{Y}_0$ such that $Y\subseteq X(n)$ we have $w_{n-1,Y}\in L^2_{\mathrm{loc}}(Y\oplus\tilde{X}(n))$ satisfying some regularity and decay hypotheses [to be described later] and $W_{n-1}:H^2(X(n))\to L^2(X(n-1))$ is the operator of multiplication by $w_{n-1}\in L^2_{\mathrm{loc}}(X(n-1))$ of the form

$$w_{n-1}(x(n),\tilde{x}(n))=\sum_{Y\in Y_0,\{0\}\subset Y\subseteq X(n)} w_{n-1,Y}(\pi^Y x(n),\tilde{x}(n)), \tag{1.12}$$

where $(x(n),\tilde{x}(n))\in X(n)\oplus\tilde{X}(n)=X(n-1)$. We assume that $\mathbf{W}_\mathbf{X}$ is the self-adjoint operator in $\mathcal{H}$ defined by the quadratic form

$$\mathbf{W}_{\mathbf{X}[\varphi,\varphi]}=(\mathbf{W}^+_\mathbf{X}\varphi,\varphi)+(\varphi,\mathbf{W}^+_\mathbf{X}\varphi), \tag{1.13}$$

where $\mathbf{W}^+_\mathbf{X}(\varphi)=(W_1\varphi_2,\ldots,W_{N-1}\varphi_N,0)$ for $\varphi=(\varphi_1,\ldots,\varphi_N)\in\mathcal{H}$.

We shall prove:

Theorem I.1: *Let* $\mathbf{H}_\mathbf{X}$ *be defined as previously, let* $\mu>0$ *and* $\mu(n)>\dim\tilde{X}(n)/2$ *for* $2\leqslant n\leqslant N$. *We assume that for all*

$$Y\in Y_0,$$

$$\langle y\rangle^{\mu+|\alpha|}\partial_y^\alpha v_Y(y)(I-\Delta_Y)^{-1} \tag{1.14}$$

are compact operators on $L^2(Y)$ *for* $|\alpha|\leqslant 1$ *and*

$$\langle\tilde{x}(n)\rangle^{\mu(n)+|\tilde{\alpha}|}\langle y\rangle^{\mu+|\alpha|}\partial_y^\alpha\partial^{\tilde{\alpha}}_{\tilde{x}(n)}\omega_{n-1,Y}(y,\tilde{x}(n))(I-\Delta_{Y\oplus\tilde{X}(n)})^{-1} \tag{1.15}$$

are compact operators on $L^2(Y\oplus\tilde{X}(n))$ *for* $|\alpha|+|\tilde{\alpha}|\leqslant 1$, *where we denote* $\langle x\rangle=(1+|x|^2)^{1/2}$. *Then there exists a closed, countable set* $\tau(\mathbf{H_X})\subset\mathbf{R}$ *such that* $\mathbf{A_X}$ *is locally conjugate for* $\mathbf{H_X}$ *in* $\mathbf{R}\backslash\tau(\mathbf{H_X})$ *and the eigenvalues of* $\mathbf{H_X}$ *may accumulate (with multiplicities) only at* $\tau(\mathbf{H_X})$.

Theorem I.2: *We make the same hypotheses as in Theorem I.1 and assume moreover that the operators given by (1.14) are compact for* $|\alpha|\leqslant 2$ *and the operators given by (1.15) are compact for* $|\alpha|+|\tilde{\alpha}|\leqslant 2$. *Then the singular continuous spectrum of* $\mathbf{H_X}$ *is empty. Moreover, the point spectrum outside the threshold set consists of discrete eigenvalues of finite multiplicities. The operator* $\mathbf{H_X}$ *satisfies the limiting absorption principle with respect to either the operator* $\mathbf{A_X}$ *or the operator* $\langle x\rangle$.

II. DESCRIPTION OF THE LATTICE AND ASSOCIATED SUB-HAMILTONIANS

For Banach spaces X_1, X_2 we denote by $B(X_1,X_2)$ and $B_\infty(X_1,X_2)$ the set of bounded and compact operators $X_1\to X_2$, respectively, and $B(X_1)=B(X_1,X_1)$, $B_\infty(X_1)=B_\infty(X_1,X_1)$.

For every $X\subseteq X(1)$ we denote by $X^\perp$ the orthogonal complement of X in $X(1)$, i.e.,

$$X(1)=X\oplus X^\perp. \tag{2.1}$$

Without any loss of generality we may replace $\mathbf{Y}_0$ by $\mathbf{Y}$ being a larger finite family of subspaces of $X(1)$ (it suffices to set $v_Y=0$, $w_{n-1,Y}=0$ identically for $Y\in\mathbf{Y}\backslash\mathbf{Y}_0$). Setting

$$\begin{aligned}\mathbf{Y}_1&=\{Y_1+\cdots+Y_n: n\in\mathbf{N} \text{ and } Y_1,\ldots,Y_n\in\mathbf{Y}_0\cup\mathbf{X}\cup\tilde{\mathbf{X}}\cup\{0\}\},\\ \mathbf{Y}&=\{\pi^{X(1)}Y_1+\cdots+\pi^{X(N)}Y_N: Y_1,\cdots,Y_n\in\mathbf{Y}_1\},\end{aligned} \tag{2.2}$$

we have the following properties:

$$X(n)\in\mathbf{Y} \text{ for } 1\leqslant n\leqslant N,\quad \tilde{X}(n)\in\mathbf{Y} \text{ for } 2\leqslant n\leqslant N, \tag{2.3i}$$

$$Y_1,Y_2\in\mathbf{Y}\Rightarrow Y_1+Y_2\in\mathbf{Y}, \tag{2.3ii}$$

$$Y\in\mathbf{Y}\Rightarrow\pi^{X(n)}Y\in\mathbf{Y} \text{ for } 1\leqslant n\leqslant N. \tag{2.3iii}$$

If $Y\subseteq X\subseteq X(1)$, $Y\in\mathbf{Y}$, then we denote

$$\sharp_X Y=\max\{n\in\mathbf{N}: Y\subseteq Y_1\subset Y_2\subset\cdots\subset Y_n\subseteq X \text{ for some } Y_1,\ldots,Y_n\in\mathbf{Y}\}. \tag{2.4}$$

We denote by $S^m_{\mathrm{hg}}(X)$ the set of smooth functions which are homogeneous of degree m outside a bounded region, i.e.,

$$\begin{aligned}S^m_{\mathrm{hg}}(X)=\{&f\in C^\infty(X): \text{there is } R>0 \text{ such that}\\ &f(\lambda x)=\lambda^m f(x) \text{ hold for } \lambda>1 \text{ and } |x|>R\}.\end{aligned} \tag{2.5}$$

For $r>0$, $\tilde{r}>0$, $X'\in\mathbf{Y}$, $X'\subset X$, we define

$$\begin{aligned}U_X^{X'}(r,\tilde{r})=\{&x\in X: |\pi^{X'}x|<r|x| \text{ and}\\ &|\pi^Y x|>\tilde{r}|x| \text{ for all } Y\in\mathbf{Y} \text{ satisfying } Y\subset X, Y\not\subset X'\}\end{aligned} \tag{2.6}$$

if $X'\neq\{0\}$ and $U_X^{\{0\}}(r,\tilde{r})=U_X^{\{0\}}(\tilde{r})$ with

$$U_X^{\{0\}}(\tilde{r})=\{x\in X: |x|<1\}\cup\{x\in X: |\pi^Y x|>\tilde{r}|x| \text{ for all } Y\in\mathbf{Y} \text{ satisfying } Y\subset X\}. \tag{2.7}$$

If $X'\in\mathbf{Y}$, $X'\subseteq X$ then we may define the following self-adjoint operators in $L^2(X)$:

$$V_X^{X'}(x)=\sum_{Y\in\mathbf{Y},Y\subseteq X'} v_Y(\pi^Y x), \tag{2.8}$$

$$H_X^{X'}=-\Delta_X+V_X^{X'}, \tag{2.8'}$$

where in the case $X'=\{0\}$ we adopt the convention that $V_X^{X'}=0$ and $H_X^{X'}=-\Delta_X$.

Let $J_X^{X'}\in S^0_{\mathrm{hg}}(X)$ be such that supp $J_X^{X'}\subset U_X^{X'}(r,\tilde{r})$ for certain $r>0$, $\tilde{r}>0$. Then

$$(V_X^X-V_X^{X'})J_X^{X'}\in B_\infty(H^2(X),L^2(X)). \tag{2.9}$$

For $X'\in\mathbf{Y}$, $X'\subseteq X(n)$, $2\leqslant n\leqslant N$, we define $W_{n-1}^{X'}:H^2(X(n))\to L^2(X(n-1))$ as the operators of multiplication by

$$w_{n-1}^{X'}(x(n),\tilde{x}(n))=\sum_{Y\in\mathbf{Y},Y\subseteq X'} w_{n-1,Y}(\pi^Y x(n),\tilde{x}(n)) \tag{2.10}$$

and we adopt the convention that $W_{n-1}^{X'}=0$ if $X'=\{0\}$.

Let $J_{X(n)}^{X'}\in S^0_{\mathrm{hg}}(X(n))$ be such that supp $J_{X(n)}^{X'}\subset U_{X(n)}^{X'}(r,\tilde{r})$ for certain $r>0$, $\tilde{r}>0$. Then

$$(W_{n-1}-W_{n-1}^{X'})J_{X(n)}^{X'}\in B_\infty(H^2(X(n)),L^2(X(n-1))). \tag{2.11}$$

For $X'\in\mathbf{Y}$, $X'\subseteq X(N)$ we denote $\mathbf{X}(X')=\{X'(n)\}_{1\leqslant n\leqslant N}$ taking $X'(N)=X'$ and defining successively $X'(N-1)$, $X'(N-2),\ldots,X'(1)\in\mathbf{Y}$ by

$$X'(n-1)=X'(n)\oplus\tilde{X}(n) \quad \text{for} \quad 2\leqslant n\leqslant N. \tag{2.12}$$

Assume moreover $X'\neq\{0\}$ and introduce

$$\mathbf{H}_{\mathbf{X}}^{X'\mathrm{diag}}=\bigoplus_{1\leqslant n\leqslant N} H_{X(n)}^{X'(n)}. \tag{2.13}$$

Still assuming $X'\neq\{0\}$ we define $\mathbf{W}_{\mathbf{X}}^{X'}$ as the self-adjoint operator in $\mathcal{H}$ given by the quadratic form

$$\mathbf{W}_{\mathbf{X}}^{X'}[\varphi,\varphi]=(\mathbf{W}_{\mathbf{X}}^{X'+}\varphi,\varphi)+(\varphi,\mathbf{W}_{\mathbf{X}}^{X'+}\varphi), \tag{2.14}$$

where for $\varphi=(\varphi_1,\ldots,\varphi_N)\in\mathcal{H}$ we have

$$\mathbf{W}_{\mathbf{X}}^{X'+}(\varphi_1,\ldots,\varphi_N)=(W_1^{X'(2)}\varphi_2,\ldots,W_{N-1}^{X'(N)}\varphi_N,0)$$

and set

$$\mathbf{H}_{\mathbf{X}}^{X'}=\mathbf{H}_{\mathbf{X}}^{X'\mathrm{diag}}+\mathbf{W}_{\mathbf{X}}^{X'}. \tag{2.15}$$

In the case $X'\neq\{0\}$ we define $\mathbf{H}_{\mathbf{X}}^{\{0\}}$ according to (2.15), where we set

$$\mathbf{H}_{\mathbf{X}}^{\{0\}\mathrm{diag}}=\left(\bigoplus_{1\leqslant n\leqslant N-1} H_{X(n)}\right)\oplus(-\Delta_{X(N)}) \tag{2.13'}$$

and $\mathbf{W}_{\mathbf{X}}^{\{0\}}$ defined by (2.14), where for $\varphi=(\varphi_1,\ldots,\varphi_N)\in\mathcal{H}$ we take

$$\mathbf{W}_{\mathbf{X}}^{\{0\}+}(\varphi_1,\ldots,\varphi_N)=(W_1^{X'(2)}\varphi_2,\ldots,W_{N-2}^{X'(N-1)}\varphi_{N-1},0,0).$$

The next aim is to construct a suitable partition of unity described in

Proposition II.1: There exists a family $\{\mathbf{J}_{\mathbf{X}}^{X'}\}_{X'\in\mathbf{Y},X'\subset X(N)}$ *of operators of the form*

$$\mathbf{J}_{\mathbf{X}}^{X'}=\bigoplus_{1\leqslant n\leqslant N} J_n^{X'}, \tag{2.16}$$

where every $J_n^{X'}$ *is an operator of multiplication by real-valued* $J_n^{X'}\in S^0_{\mathrm{hg}}(X(n))$, *satisfying*

$$\sum_{X'\in\mathbf{Y},X'\subset X(N)} (\mathbf{J}_{\mathbf{X}}^{X'})^2=I \tag{2.17}$$

and such that for every X', $X''\in\mathbf{Y}$, X', $X''\subset X(N)$, *the following operators*

$$(i+\mathbf{H}_{\mathbf{X}})^{-1}[\mathbf{J}_{\mathbf{X}}^{X'},\mathbf{H}_{\mathbf{X}}^{X''}], \tag{2.18i}$$

$$(i+\mathbf{H}_{\mathbf{X}})^{-1}(\mathbf{H}_{\mathbf{X}}-\mathbf{H}_{\mathbf{X}}^{X'})\mathbf{J}_{\mathbf{X}}^{X'}, \tag{2.18ii}$$

$$(i+\mathbf{H}_{\mathbf{X}})^{-1}[\mathbf{J}_{\mathbf{X}}^{X'},[\mathbf{H}_{\mathbf{X}}^{X''},\mathbf{A}_{\mathbf{X}}]](i+\mathbf{H}_{\mathbf{X}})^{-1}, \tag{2.18iii}$$

$$(i+\mathbf{H}_{\mathbf{X}})^{-1}[\mathbf{H}_{\mathbf{X}}-\mathbf{H}_{\mathbf{X}}^{X'},\mathbf{A}_{\mathbf{X}}]\mathbf{J}_{\mathbf{X}}^{X'}(i+\mathbf{H}_{\mathbf{X}})^{-1} \tag{2.18iv}$$

are compact.

III. PROOF OF PROPOSITION II.1

If $r>0$, then $F(\cdot\leqslant r)$ denotes a smoothed characteristic function of $]-\infty,r]$, i.e., $\lambda\to F(\lambda\leqslant r)$ is a non-negative, smooth function on $\mathbf{R}$ which equals 1 on $]-\infty,r/2]$ and equals 0 on $[r,\infty[$.

Lemma III.1: Let $X'\in\mathbf{Y}$, $\{0\}\subset X'\subset X(N)$ *and* $J_N^{X'}\in S^0_{\mathrm{hg}}(X(N))$. *If* $r>0$ *then the relation*

$$J_{n-1}^{X'}(x(n),\tilde{x}(n))=J_n^{X'}(x(n))F\left(\frac{|\tilde{x}(n)|}{|x(n-1)|}\leqslant r\right) \tag{3.1}$$

allows one to define successively $J_{N-1}^{X'}\in S^0_{\mathrm{hg}}(X(N-1))$, $J_{N-2}^{X'}\in S^0_{\mathrm{hg}}(X(N-2)),\ldots,J_1^{X'}\in S^0_{\mathrm{hg}}(X(1))$. *If moreover* $\mathrm{supp}\ J_N^{X'}\subset U_{X(N)}^{X'}(r_{X'},\tilde{r}_{X'})$ *and* $r_{X'}>0$, $r>0$ *are small enough, then*

$$\mathrm{supp}\ J_n^{X'}\subset U_{X(N)}^{X'(n)}(r_{X'}+(N-n)r,\tilde{r}_{X'}/(1+N-n)) \tag{3.2n}$$

holds for every $1\leqslant n\leqslant N$.

Proof: We assume (3.2n) for a certain $2\leqslant n\leqslant N$ and we show (3.2n−1). Due to (3.2n), for $(x(n),\tilde{x}(n))\in\mathrm{supp}\ J_{n-1}^{X'}$ we have

$$|\tilde{x}(n)|\leqslant r|x(n)| \quad\text{and}\quad |\pi^{X'(n)}x(n)|<(r_{X'}+(N-n)r|x(n)|, \tag{3.3}$$

which implies

$$\begin{aligned}|\pi^{X'(n-1)}x(n-1)|&\leqslant|\pi^{X'(n)}x(n)|+|\tilde{x}(n)|\\&<(r_{X'}+(N-n)r+r)|x(n)|\leqslant(r_{X'}+(N-n+1)r)|x(n-1)|.\end{aligned} \tag{3.4}$$

Now we fix $Y\in\mathbf{Y}$ satisfying $Y\subset X(n-1)$, $Y\not\subseteq X'(n-1)$, and it remains to show that

$$|\pi^{Y}x(n-1)|>\frac{\tilde{r}_{X'}}{2+N-n}|x(n-1)|. \tag{3.5}$$

We define $Y_1 \in \mathbf{Y}$, $Y_1 \subseteq X(n)$ by

$$Y_1 = \pi^{X(n)} Y + X'(n) \tag{3.6}$$

and $Y_2 \subseteq X(n)$ by

$$X(n) = Y_1 \oplus Y_2 . \tag{3.7}$$

We note that $x \in X(n) \cap Y^{\perp} \Leftrightarrow (0 = (x,y) = (x, \pi^{X(n)} y)$ for all $y \in Y) \Leftrightarrow x \in X(n) \cap (\pi^{X(n)} Y)^{\perp}$. Therefore

$$Y_2 = Y_1^{\perp} \cap X(n) = (\pi^{X(n)} Y)^{\perp} \cap X'(n)^{\perp} \cap X(n) = Y^{\perp} \cap X''(n) \tag{3.8}$$

with $X''(n) = X'(n)^{\perp} \cap X(n)$, i.e., with $X''(n)$ satisfying

$$X(n) = X'(n) \oplus X''(n). \tag{3.9}$$

Clearly $Y_2 \subseteq X''(n)$ and we are going to check that the inclusion is strict. Indeed, $Y_2 = X''(n) \Rightarrow Y_1 = X'(n) \Rightarrow \pi^{X(n)} Y \subseteq X'(n) \Rightarrow Y = \pi^{X(n)} Y + \pi^{\tilde{X}(n)} Y \subseteq X'(n) + \tilde{X}(n) \subseteq X'(n-1)$, which is in contradiction with the assumption made on Y.

Thus we have $Y_2 \subset X''(n)$, which implies $X'(n) \subset Y_1$, hence $Y_1 \not\subseteq X'(n)$ and due to (3.2n),

$$|\pi^{Y_1} x(n)|^2 > \left(\frac{\tilde{r}_{X'}}{1+N-n} \right)^2 |x(n)|^2 \tag{3.10}$$

and since $|\pi^{Y_1} x(n)|^2 + |\pi^{Y_2} x(n)|^2 = |x(n)|^2$, (3.10) is equivalent to

$$|\pi^{Y_2}(n)|^2 < \left(1 - \left(\frac{\tilde{r}_{X'}}{1+N-n} \right)^2 \right) |x(n)|^2 . \tag{3.11}$$

Therefore using (3.8), (3.11), and (3.3) we obtain

$$\begin{aligned} |\pi^{Y^{\perp}} x(n-1)| &\leq |\pi^{Y^{\perp} \cap X''(n)} x(n-1)| + |\pi^{Y^{\perp} \cap X'(n)} x(n-1)| + |\pi^{Y^{\perp} \cap \tilde{X}(n)} x(n-1)| \\ &\leq |\pi^{Y_2} x(n)| + |\pi^{X'(n)} x(n)| + |\tilde{x}(n)| \Bigg(\left(1 - \left(\frac{\tilde{r}_{X'}}{1+N-n} \right)^2 \right)^{1/2} \\ &\quad + r_{X'} + (N-n+1) r \Bigg) |x(n)| \end{aligned} \tag{3.12}$$

and taking $r_{X'} > 0$, $r > 0$ small enough, we have

$$\left(1 - \left(\frac{\tilde{r}_{X'}}{1+N-n} \right)^2 \right)^{1/2} + r_{X'} + (N-n+1) r \leq \left(1 - \left(\frac{\tilde{r}_{X'}}{2+N-n} \right)^2 \right)^{1/2} . \tag{3.13}$$

Now it is clear that (3.12) and (3.13) give

$$|\pi^{Y^{\perp}} x(n-1)|^2 < \left(1 - \left(\frac{\tilde{r}_{X'}}{2+N-n} \right)^2 \right) |x(n-1)|^2 , \tag{3.14}$$

which gives (3.5) due to $|\pi^{Y} x(n-1)|^2 + |\pi^{Y^{\perp}} x(n-1)|^2 = |x(n-1)|^2$. □

Lemma III.2: Let $X' \in \mathbf{Y}$, $\{0\} \subset X' \subset X(N)$ *and assume that* $\{J_n^{X'}\}_{1 \leq n \leq N}$ *are as in Lemma 3.1 and (3.2n) holds for* $1 \leq n \leq N$. *If* $\mathbf{J}_{\mathbf{X}}^{X'}$ *is given by* (2.16), *then the operators (2.18i,ii,iii,iv) are compact*.

Proof: (i) Clearly it suffices to consider $\mathbf{H}_{\mathbf{X}}$ instead of $\mathbf{H}_{\mathbf{X}}^{X''}$ in (2.18i). Since the commutators $[J_n^{X'},\Delta_{X(n)}]$ are first-order differential operators with coefficients in $S_{\mathrm{hg}}^{-1}(X(n))$, i.e., $\Delta_{X(n)}$-compact operators, it is clear that

$$[\mathbf{J}_{\mathbf{X}}^{X'},\mathbf{H}_{\mathbf{X}}^{\mathrm{diag}}]=\bigoplus_{1\leqslant n\leqslant N}[J_n^{X'},-\Delta_{X(n)}] \tag{3.15}$$

is $\mathbf{H}_{\mathbf{X}}$-compact. In order to prove that $[\mathbf{J}_{\mathbf{X}}^{X'},\mathbf{W}_{\mathbf{X}}]$ is $\mathbf{H}_{\mathbf{X}}$-compact, it suffices to show that for $2\leqslant n\leqslant N$ one has

$$J_{n-1}^{X'}W_{n-1}-W_{n-1}J_n^{X'}\in B_\infty(H^2(X(n)),L^2(X(n-1))). \tag{3.16}$$

However $J_{n-1}^{X'}W_{n-1}-W_{n-1}J_n^{X'}$ is the operator of multiplication by

$$g(x(n),\tilde{x}(n))=\left(F\left(\frac{|\tilde{x}(n)|}{|x(n-1)|}\leqslant r\right)-1\right)w_{n-1}(x(n),\tilde{x}(n))J_n^{X'}(x(n)) \tag{3.17}$$

and we may write $g=g_3g_2g_1$ with

$$g_1(x(n),\tilde{x}(n))=\langle\tilde{x}(n)\rangle^{-\mu(n)+\epsilon}J_n^{X'}(x(n)), \tag{3.18i}$$

$$g_2(x(n),\tilde{x}(n))=\langle x(n)\rangle^{-\epsilon}\langle\tilde{x}(n)\rangle^{\mu(n)}w_{n-1}(x(n),\tilde{x}(n)), \tag{3.18ii}$$

$$g_3(x(n),\tilde{x}(n))=\left(F\left(\frac{|\tilde{x}(n)|}{|x(n-1)|}\leqslant r\right)-1\right)\langle x(n)\rangle^{\epsilon}\langle\tilde{x}(n)\rangle^{-\epsilon}, \tag{3.18iii}$$

where $\epsilon>0$ is chosen such that $\mu(n)-\epsilon>\dim\tilde{X}(n)/2$, which implies that the multiplication by g_1 is a bounded operator $H^2(X(n))\to H^2(X(n-1))$. Next the compactness hypotheses concerning the operators (1.15) guarantee that the multiplication by g_2 is a compact operator $H^2(X(n-1))\to L^2(X(n-1))$ and we complete the proof noting that the multiplication by g_3 is a bounded operator in $L^2(X(n-1))$ due to the definition of F.

(ii) Clearly (2.9) implies that $(\mathbf{H}_{\mathbf{X}}^{\mathrm{diag}}-\mathbf{H}_{\mathbf{X}}^{X'\,\mathrm{diag}})\mathbf{J}_{\mathbf{X}}^{X'}$ is $\mathbf{H}_{\mathbf{X}}$-compact. For $1\leqslant n\leqslant N$ let $\tilde{J}_n^{X'}\in S_{\mathrm{hg}}^0(X(n))$ be such that $\tilde{J}_n^{X'}=1$ on supp $J_n^{X'}$ and supp $\tilde{J}_n^{X'}\subset U_{X(n)}^{X'(n)}(r_{(n)}^{X'},\tilde{r}_n^{X'})$ for certain $r_n^{X'}>0$, $\tilde{r}_n^{X'}>0$. Setting

$$\tilde{\mathbf{J}}_{\mathbf{X}}^{X'}=\bigoplus_{1\leqslant n\leqslant N}\tilde{J}_n^{X'}, \tag{3.19}$$

it is clear that (2.11) implies the fact that $\tilde{\mathbf{J}}_{\mathbf{X}}^{X'}(\mathbf{W}_{\mathbf{X}}-\mathbf{W}_{\mathbf{X}}^{X'})\mathbf{J}_{\mathbf{X}}^{X'}$ is $\mathbf{H}_{\mathbf{X}}$-compact. Since $(I-\tilde{\mathbf{J}}_{\mathbf{X}}^{X'})\mathbf{J}_{\mathbf{X}}^{X'}=0$, it suffices to note that the operator

$$(I-\tilde{\mathbf{J}}_{\mathbf{X}}^{X'})(\mathbf{W}_{\mathbf{X}}-\mathbf{W}_{\mathbf{X}}^{X'})\mathbf{J}_{\mathbf{X}}^{X'}=(I-\tilde{\mathbf{J}}_{\mathbf{X}}^{X'})[\mathbf{W}_{\mathbf{X}}-\mathbf{W}_{\mathbf{X}}^{X'},\mathbf{J}_{\mathbf{X}}^{X'}] \tag{3.20}$$

is $\mathbf{H}_{\mathbf{X}}$-compact due to (i).

(iii) and (iv) We may define $\tilde{V}_X^{X'}$, $\tilde{H}_X^{X'}$, $\tilde{W}_{n-1}^{X'}$ according to (2.8), (2.10), where v_Y, $w_{n-n,Y}$ are replaced by

$$\tilde{v}_Y(y)=-y\cdot\Delta_y v_Y(y), \tag{3.21}$$

$$\tilde{w}_{n-1,Y}(y,\tilde{x}(n))=-\left(y\cdot\Delta_y+\tilde{x}(n)\cdot\Delta_{\tilde{x}(n)}+\frac{\dim\tilde{X}(n)}{2}\right)w_{n-1,Y}(y,\tilde{x}(n)). \tag{3.21$'$}$$

It is clear we still have

$$(\tilde{V}_X^X - \tilde{V}_X^{X'}) J_X^{X'} \in B_\infty(H^2(X), L^2(X)), \tag{3.22}$$

$$(\tilde{W}_{n-1} - \tilde{W}_{n-1}^{X'}) J_{X(n)}^{X'} \in B_\infty(H^2(X)(n)), L^2(X(n-1))), \tag{3.23}$$

where $\tilde{V}_X = \tilde{V}_X^X$, $\tilde{W}_{n-1} = \tilde{W}_{n-1}^X$.

Thus it suffices to follow the proof of (i) and (ii) noting that

$$\frac{i}{2}[\mathbf{H}_\mathbf{X}^{X'}, \mathbf{A}_\mathbf{X}] = \tilde{\mathbf{H}}_\mathbf{X}^{X'} = \tilde{\mathbf{H}}_\mathbf{X}^{X' \text{ diag}} + \tilde{\mathbf{W}}_\mathbf{X}^{X'}, \tag{3.24}$$

where $\tilde{\mathbf{H}}_\mathbf{X}^{X' \text{ diag}}$ and $\tilde{\mathbf{W}}_\mathbf{X}^{X'}$ are defined according to (2.13), (2.14) with $H_{X(n)}^{X'(n)}$, $W_{n-1}^{X'(n)}$ replaced by $\tilde{H}_{X(n)}^{X'(n)}$, $\tilde{W}_{n-1}^{X'(n)}$. □

Proof of Proposition II.1: Fix $0 < \tilde{r}_2 < 1$, set $\tilde{r}_{X'} = \tilde{r}_2$ for every X' such that $\sharp_{X(N)} X' = 2$ and choose $r_2 = r_2(\tilde{r}_2) > 0$ small enough to guarantee (3.2n) for $1 \leqslant n \leqslant N$ with $r_{X'} = r_2$. Assuming that we have chosen $r_{X'} = r_{\sharp_{X(N)} X'} > 0$, $\tilde{r}_{X'} = \tilde{r}_{\sharp_{X(N)} X'} > 0$ for every X' such that $\sharp_{X(N)} X' \leqslant k$, we choose sufficiently small $\tilde{r}_{k+1} = \tilde{r}_{k+1}(\tilde{r}_2, r_2, \ldots, \tilde{r}_k, r_k) > 0$ and $r_{k+1} = r_{k+1}(\tilde{r}_2, r_2, \ldots, \tilde{r}_k, r_k, \tilde{r}_{k+1}) > 0$ small enough to guarantee (3.2n) for $1 \leqslant n \leqslant N$ with $\tilde{r}_{X'} = \tilde{r}_{k+1}$, $r_{X'} = r_{k+1}$ for every X' such that $\sharp_{X(N)} X' = k+1$. A simple geometric reasoning based on the fact that for $X' \subset X$ and $r > 0$ small, $\{x \in X : |\pi^{X'} x| < r|x|\}$ is a small conical neighborhood of $X'^{\perp} \cap (X \setminus \{0\})$ in $X \setminus \{0\}$, allows one to find $\tilde{r}_{\{0\}} = r_{\{0\}} > 0$ such that $\{U_{X(N)}^{X'}(r_{X'}, \tilde{r}_{X'})\}_{X' \in \mathbf{Y}, X' \subset X(N)}$ is a covering of $X(N)$. Therefore there exists a partition of unity

$$\sum_{X' \in \mathbf{Y}, X' \subset X(N)} \tilde{J}_N^{X'} = 1 \tag{3.25}$$

composed of $\tilde{J}_N^{X'} \in S_{\text{hg}}^0(X(N))$ such that $\operatorname{supp} \tilde{J}_N^{X'} \subset U_{X(N)}^{X'}(r_{X'}, \tilde{r}_{X'})$ and $\tilde{J}_N^{X'} \geqslant 0$.

For $X' \neq \{0\}$ we define successively $\tilde{J}_{N-1}^{X'} \in S_{\text{hg}}^0(X(N-1))$, $\tilde{J}_{N-2}^{X'} \in S_{\text{hg}}^0(X(N-2)), \ldots, \tilde{J}_1^{X'} \in S_{\text{hg}}^0(X(1))$, using relation (3.1) with $\tilde{J}_n^{X'}$ instead of $J_n^{X'}$ and let $\tilde{\mathbf{J}}_\mathbf{X}^{X'}$ be defined as in (3.19). Due to the assertion of Lemma 2.1 we may assume that (3.2n) holds for $1 \leqslant n \leqslant N$ with $\tilde{J}_n^{X'}$ instead of $J_n^{X'}$ and due to Lemma 3.2 the commutator $[\tilde{\mathbf{J}}_\mathbf{X}^{X'}, \mathbf{H}_\mathbf{X}]$ is $\mathbf{H}_\mathbf{X}$-compact.

Defining $\tilde{\mathbf{J}}_\mathbf{X}^{\{0\}}$ by

$$\sum_{X' \in \mathbf{Y}\{0\} \subset X' \subset X(N)} \tilde{\mathbf{J}}_\mathbf{X}^{X'} = 1 - \tilde{\mathbf{J}}_\mathbf{X}^{\{0\}}, \tag{3.26}$$

it is clear that $[\tilde{\mathbf{J}}_\mathbf{X}^{\{0\}}, \mathbf{H}_\mathbf{X}]$ is still $\mathbf{H}_\mathbf{X}$-compact and

$$\tilde{\mathbf{J}}_\mathbf{X}^{\{0\}} = \bigoplus_{1 \leqslant n \leqslant N} \tilde{J}_n^{\{0\}}, \tag{3.27}$$

with $\tilde{J}_n^{\{0\}} \in S_{\text{hg}}^0(X(n))$ for $1 \leqslant n \leqslant N$ and $\operatorname{supp} \tilde{J}_N^{\{0\}} \subset U_{X(N)}^{\{0\}}(\tilde{r}_{\{0\}})$, hence the operators (2.18ii), (2.18iv) are compact for $X' = \{0\}$ as well.

It is clear that (3.26) implies existence of a constant $c_0 > 0$ such that

$$\mathbf{S}_\mathbf{X} = \sum_{X' \in \mathbf{Y}, X' \subset X(N)} (\tilde{\mathbf{J}}_\mathbf{X}^{X'})^2 \geqslant c_0 I \tag{3.28}$$

and then clearly $[\mathbf{S}_\mathbf{X}, \mathbf{H}_\mathbf{X}]$ is $\mathbf{H}_\mathbf{X}$-compact. Hence

$$[f(\mathbf{S_X}),\mathbf{H_X}](i+\mathbf{H_X})^{-1}\in B_\infty(\mathcal{H}) \tag{3.29}$$

if $f(\lambda)=(\lambda\pm i)^{-1}$ and Stone–Weierstrass theorem (see, e.g., Ref. 4) allows one to affirm that (3.26) still holds for every $f\in C(\mathbf{R})$ such that $f(\lambda)\to 0$ when $\lambda\to\infty$. We complete the proof noting that all assertions of Proposition 2.1 are satisfied if we set $\mathbf{J}_\mathbf{X}^{X'}=\tilde{\mathbf{J}}_\mathbf{X}^{X'}\mathbf{S}_\mathbf{X}^{-1/2}$. □

IV. PROOFS OF THEOREMS 1.1 AND 1.2

Let $\mathbf{X}=\{X(n)\}_{1\leqslant n\leqslant N}$ be as before a finite family of Euclidean spaces satisfying (1.8) and let $\mathbf{X}'=\{X'(n)\}_{1\leqslant n\leqslant N'}$ be another finite family of Euclidean spaces satisfying

$$X'(N')\subset\cdots\subset X'(2)\subset X'(1). \tag{4.1}$$

We shall write $\mathbf{X}'\leqslant\mathbf{X}$ if and only if the following three conditions hold:

$$\text{(i)}\quad N'\leqslant N,$$

$$\text{(ii)}\quad X'(1)\subseteq X(1),$$

$$\text{(iii)}\quad \tilde{X}'(n)=\tilde{X}(n)\ \text{ for }\ 2\leqslant n\leqslant N',$$

where $\tilde{X}(n)$ is given by (1.11) and $\tilde{X}'(n)$ by

$$X'(n-1)=X'(n)\oplus\tilde{X}'(n)\ \text{ for }\ 2\leqslant n\leqslant N'. \tag{4.2}$$

Moreover we shall write $\mathbf{X}'<\mathbf{X}\Leftrightarrow(\mathbf{X}'\leqslant\mathbf{X}$ and $\mathbf{X}'\neq\mathbf{X})$.

The idea of the proof of Theorem 1.1 is to show the assertion for $\mathbf{H_X}$ with

$$\tau(\mathbf{H_X})=\bigcup_{\mathbf{X'}<\mathbf{X}}\overline{\sigma_{pp}(\mathbf{H}_{X'})} \tag{4.3}$$

[where $\sigma_{pp}(H)$ denotes the set of eigenvalues of H], assuming that the analogical statement holds for every $\mathbf{H}_{\mathbf{X}'}$ with $\mathbf{X}'<\mathbf{X}$. We note first that Proposition 2.1 has the following

Corollary IV.1: Assume that $\mathbf{J}_\mathbf{X}^{X'}$ satisfies the assertions of Proposition 2.1. If $f\in C_0^\infty(\mathbf{R})$ then for every X', $X''\in\mathbf{Y}$, X', $X''\subset X(N)$, the operators

$$(i+\mathbf{H_X})[\mathbf{J}_\mathbf{X}^{X'},f(\mathbf{H}_\mathbf{X}^{X''})], \tag{4.4}$$

$$(i+\mathbf{H_X})(f(\mathbf{H_X})-f(\mathbf{H}_\mathbf{X}^{X'}))\mathbf{J}_\mathbf{X}^{X'}, \tag{4.4'}$$

are compact. Moreover there exist compact operators K_1, K_2, such that

$$f(\mathbf{H_X})=\sum_{X'\in\mathbf{Y},X'\subset X(N)}\mathbf{J}_\mathbf{X}^{X'}f(\mathbf{H}_\mathbf{X}^{X'})\mathbf{J}_\mathbf{X}^{X'}+K_1, \tag{4.5}$$

$$f(\mathbf{H_X})[i\mathbf{H_X},\mathbf{A_X}]f(\mathbf{H_X})=\sum_{X'\in\mathbf{Y},X'\subset X(N)}\mathbf{J}_\mathbf{X}^{X'}f(\mathbf{H}_\mathbf{X}^{X'})[i\mathbf{H}_\mathbf{X}^{X'},\mathbf{A_X}]f(\mathbf{H}_\mathbf{X}^{X'})\mathbf{J}_\mathbf{X}^{X'}+K_2. \tag{4.6}$$

Indeed, Proposition 2.1 allows one to get the compactness of operators (4.4)–(4.4′) for $f(\lambda)=(\lambda\pm i)^{-1}$ and the general case follows as before via Stone–Weierstrass theorem (cf. Ref. 4). Using (2.18) and (4.4)–(4.4′) we get (4.5–6) as in Ref. 4. We note first that the assertion of Theorem 1.1 holds in the case $N=1$ corresponding to the case of a standard scalar many-body operator treated in Ref. 3 or 4, where

$$\tau(H_X)=\bigcup_{X'\subset X}\overline{\sigma_{pp}(H_{X'})}. \tag{4.7}$$

Consider now the case $N\geqslant 2$ and assume that the assertion of Theorem 1.1 with (4.3) holds for all $\mathbf{X}'$ such that $\mathbf{X}'<\mathbf{X}$. Clearly we may exclude the case $X(N)=\{0\}$, because the corresponding operator may be replaced by $\mathbf{H}_{\mathbf{X}(N-1)}$ with

$$\mathbf{X}(N-1)=\{X(n)\}_{1\leqslant n\leqslant N-1}<\mathbf{X} \tag{4.8}$$

for which the assertion of Theorem 1.1 holds due to our induction hypothesis. It remains to consider the case $X(N)\neq\{0\}$ applying Corollary 4.1 similarly as in Ref. 4. Then for every $X'\in\mathbf{Y}$, $\{0\}\subset X'\subset X(N)$, we use the direct decomposition

$$\mathbf{H}_{\mathbf{X}}^{X'}=\int_{\xi\in X''}^{\oplus}\mathbf{H}_{\mathbf{X}(X')}(\xi)\mathrm{d}\xi, \tag{4.9}$$

where X'' is such that $X(N)=X'\oplus X''$ and

$$\mathbf{H}_{\mathbf{X}(X')}(\xi)=\xi^2+\mathbf{H}_{\mathbf{X}(X')}, \tag{4.9$'$}$$

where $\mathbf{H}_{\mathbf{X}(X')}$ is the Hamiltonian associated with the family of Euclidean subspaces $\mathbf{X}(X')$ defined by (2.12) with $X'(N)=X'$. Thus for $X'\in\mathbf{Y}$, $\{0\}\subset X'\subset X(N)$ we have $\mathbf{X}(X')<\mathbf{X}$ and the assertion of Theorem 1.1 holds for $\mathbf{H}_{\mathbf{X}(X')}$ due to our induction hypothesis. It remains to note that in the case $X'=\{0\}$,

$$\mathbf{H}_{\mathbf{X}}^{\{0\}}=\mathbf{H}_{\mathbf{X}(N-1)}\oplus(-\Delta_{X(N)}), \tag{4.10}$$

with $\mathbf{X}(N-1)$ given by (4.8), hence satisfies the assertion of Theorem 1.1. Therefore we may complete the proof similarly as in the reasoning described in Ref. 4. Here we point out that compactness is (in general) used in the Fock space with differing number of particles. So compactness of the relevant contribution from the W terms is between two spaces. Smallness of the remainder terms, after fibration, follows as in the usual case. The assertion of Theorem 1.2 follows from Theorem 1 and from the boundedness of $[[\mathbf{H}_{\mathbf{X}},\mathbf{A}_{\mathbf{X}}],\mathbf{A}_{\mathbf{X}}](i+\mathbf{H}_{\mathbf{X}})^{-1}$ (cf. Refs. 2 and 13).

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SU(N) skyrmions from harmonic maps $S^2 \to \mathrm{Gr}(2,N)$

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We construct multiskyrmion fields of the SU(N) Skyrme models by using harmonic maps of S^2 to the Grassmannian Gr(2,N), which we express in terms of rank-2 projectors. Within this construction we derive some approximate spherically symmetric solutions of SU(N) Skyrme models and show that their energies are marginally higher than those for the rank-one cases. We also discuss the possibility of generating exact spherically symmetric solutions using this construction. In particular, we present arguments which suggest that the only solutions obtained in this way are embeddings. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The SU(N) Skyrme models are minimal generalizations of the SU(N) chiral models in (3 +1)-dimensional space–time which possess static finite energy solutions called multiskyrmions. They are examples of topological solitons in three spatial dimensions. Recently, they have received a great deal of attention, especially for the $N=2$ case, since, it has been argued[1,2] that they describe, at a classical level, low energy states of nuclei.

The SU(N) Skyrme models are described by SU(N) group valued functions U of space–time coordinates $x^\mu=(\vec{x},t)$. Their dynamics is determined by the Lagrangian density

$$\mathcal{L}=-\frac{F^2}{16}\mathrm{Tr}(L_\mu L^\mu)+\frac{1}{32a^2}\mathrm{Tr}([L_\mu,L_\nu][L^\mu,L^\nu])+\frac{F^2}{16}M_\pi^2\,\mathrm{Tr}(U^{-1}+U-2I), \tag{1}$$

where

$$L_\mu=U^{-1}\partial_\mu U \tag{2}$$

are the SU(N) algebra valued currents, $F\cong 189\,\mathrm{MeV}$ is the pion decay constant, and a is a dimensional constant. The last term in (1) describes the mass term where M_π is the pion mass.

Multiskyrmions are stationary points (minima or saddle points) of the corresponding static energy functional. The requirement of the finiteness of the multiskyrmions energy imposes the condition that the field $U(\vec{x},t)$ goes to a constant matrix U_0 at spatial infinity. As by a global SU(N) transformation, this U_0 can be brought to the identity matrix I, so without the loss of generality we can impose the following boundary condition on U: $U\to I$ as $|\vec{x}|\to\infty$.

As this boundary condition is effectively a mapping from $S^3\to\mathrm{SU}(N)$ we see that each multiskyrmion configuration can be classified by an integer valued winding number

$$B=\frac{1}{24\pi^2}\int_{R^3}\epsilon_{ijk}\mathrm{Tr}(L_iL_jL_k)\mathrm{d}^3\vec{x}. \tag{3}$$

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This number is a topological invariant, i.e., an element of the third homotopy group $\pi_3(\mathrm{SU}(N))\equiv Z$, which classifies the solitonic sectors of the model. Following Skyrme[1] and Witten,[2,3] B is identified with the baryon number of the multiskyrmion configuration.

In what follows we express the energy in the same units as the baryon number B. This is achieved by rescaling the spatial coordinates[4,5] $\vec{x}\to 2\vec{x}/aF$ and by taking $F/4a=1/12\pi^2$. In these units the energy functional is given by

$$E=\frac{1}{12\pi^2}\int_{R^3}\left[-\frac{1}{2}\mathrm{Tr}(L_i^2)-\frac{1}{16}\mathrm{Tr}([L_i,L_j]^2)-\frac{m_\pi^2}{2}\mathrm{Tr}(U^{-1}+U-2I)\right]\mathrm{d}^3\vec{x}, \tag{4}$$

where $m_\pi=2M_\pi/aF$. From (4) we find the equation for the stationary points:

$$\partial_i\left(L_i-\frac{1}{4}[L_j,[L_i,L_j]]\right)-\frac{m_\pi^2}{2}(U-U^{-1})=0. \tag{5}$$

The first exact solution of (5), in the SU(2) case, was found by Skyrme.[1] This solution, also known as a hedgehog solution, describes a spherically symmetric energy lump and has the baryon number $B=1$. Since Witten's suggestion that the Skyrme model arises in the large N_c limit of QCD,[2] most of the studies involving SU(N) for $N>2$ considered configurations which were embeddings of the SU(2) fields.

The first nonembedding solution, for $N=3$, was presented by Balachandran *et al.*,[6] who found an SO(3) subgroup soliton which has baryon number $B=2$. Another configuration, which has a large strangeness content was then found by Kopeliovich *et al.*[7]

A more systematic study, using the harmonic map ansatz method, for any N, was then carried out by Ioannidou *et al.*[8,9] This method enabled the construction of new static spherically symmetric solutions. The method was, in fact, a generalization of the rational map approach of Houghton *et al.*[10] In their seminal work,[10] Houghton *et al.* have shown how to use rational maps of $S^2\to S^2$ to construct field configurations for the SU(2) Skyrme model which have arbitrary baryon number B and, for low values of B, are close to the exact solutions of the model. In Ref. 9, Ioannidou *et al.* took the SU(2) ansatz of Houghton *et al.* and rewrote it in terms of a projector of $S^2\to CP^1$ and then generalized it to more general projectors of $S^2\to CP^{N-1}$ of rank-one.

In this paper we generalize the method of Ioannidou *et al.* further by considering projectors of S^2 into the Grassmannian Gr(2,N), i.e., using projectors of higher rank (we concentrate our attention on the rank-2 projectors). We find that, in contradistinction to the rank-1 case, in which exact spherically symmetric solutions can be found (numerically) by using the Veronese sequence of N mutually orthogonal vector fields in CP^{N-1}, such a construction is now more involved.

In Sec. II, we discuss the harmonic maps of R^2 into the Grassmannian Gr(n,N) in terms of the ($N\times N$) projectors of rank-n, with $1<n<N$ and then present our generalization of the harmonic map ansatz. In Sec. III we rewrite various quantities of the SU(N) Skyrme models in spherical polar coordinates and then, using the harmonic map ansatz, reexpress them in terms of rank-n projectors. Next, in Sec. IV, we derive the stationary equations of the approximate energy functional which we then use to study various field configurations for the $N=3$, 4, and 5 cases using one and two rank-2 projectors in Secs. V and VI, respectively. Then, in Sec. VII, we formulate a condition on the sequence of N mutually orthogonal ($N\times n$) matrix fields in Gr(n,N) which would give exact spherically symmetric solutions of the SU(N) Skyrme models. In Secs. VIII and IX, we analyze this condition further, consider some special configurations, and present arguments suggesting that its only solutions are embeddings.

II. HARMONIC MAPS INTO GRASSMANN MANIFOLDS

Let $\xi\in C$ be a complex variable and $M_k=M_k(\xi,\overline{\xi})$, $k=0,1,...,\lambda$ where $\lambda\leqslant(N-1)$, be a set of $(\lambda+1)$ mutually orthogonal $(N\times n)$ matrices $(n<N)$, i.e.,

$$M_k^\dagger M_l=|M_k|^2\delta_{kl}, \tag{6}$$

where δ_{kl} is the Kronecker's delta, and where

$$|M_k|^2 = M_k^\dagger M_k \tag{7}$$

are $(n\times n)$ nonsingular matrices. Then the corresponding projector $P_k(n)$ onto each matrix M_k is given by

$$P_k(n) = M_k |M_k|^{-2} M_k^\dagger . \tag{8}$$

Clearly, $\mathrm{Tr}\, P_k(n) = \mathrm{Tr}\, I_n = n$, where I_n is an $(n\times n)$ unit matrix which means that each projector $P_k(n)$ has rank-n. From (8), we see that the projectors $P_k(n)$ are mutually orthogonal, i.e., $P_k(n)P_l(n) = \delta_{kl}P_l(n)$, and are Hermitian, i.e., $P_k(n)^\dagger = P_k(n)$, as by definition M_k are mutually orthogonal and, by construction (7), $|M_k|^2$ are Hermitian.

In the following we want to present a generalized harmonic map ansatz. To do this we use a sequence of mutually orthogonal matrices $(M_0, M_1, \ldots, M_\lambda)$ obtained from a sequence of holomorphic (analytic) matrices $(M, \partial_\xi M, \ldots, \partial_\xi^\lambda M), \partial_{\bar\xi} M = 0$, via the Gram–Schmidt orthogonalization process.

We can do this using the operator P_+ (Ref. 11) defined by its action on any matrix $M \in C^{N\times n}$ as

$$P_+ M = \partial_\xi M - M|M|^{-2}(M^\dagger \partial_\xi M). \tag{9}$$

Then we have

$$M_0 = M, \quad M_1 = P_+ M, \quad \ldots, \quad M_k = P_+^k M = P_+(P_+^{k-1} M), \quad \ldots, \quad M_\lambda = P_+^\lambda M. \tag{10}$$

With this construction the following properties of the matrices M_k hold when M_0 is holomorphic:[11]

$$\partial_{\bar\xi} M_k = -M_{k-1}|M_{k-1}|^{-2}|M_k|^2, \tag{11}$$

$$\partial_\xi (M_k |M_k|^{-2}) = M_{k+1}|M_k|^{-2}. \tag{12}$$

Geometrically, the matrices M_k define harmonic maps $R^2 \to \mathrm{Gr}(n,N)$, i.e., in terms of the projectors $P_k(n)$, where $\mathrm{Gr}(n,N)$ is the Grassmann manifold of n-dimensional planes in C^N.[11]

For rank-2 projectors which we are considering in this paper, the matrix M_k is given by

$$M_k = (M_{k1}, M_{k2}), \tag{13}$$

where M_{k1} and M_{k2} are two N-component column vector fields and $|M_k|^2$ is a (2×2) matrix.

Using this column vector notation the entries of the projector $P_k(2)$ are given by

$$(P_k(2))_{ab} = \frac{1}{D_k}[|M_k|^2_{22}(M_{k1})_a(\overline{M}_{k1})_b + |M_k|^2_{11}(M_{k2})_a(\overline{M}_{k2})_b - |M_k|^2_{12}(M_{k1})_a(\overline{M}_{k2})_b - |M_k|^2_{21}(M_{k2})_a(\overline{M}_{k1})_b], \tag{14}$$

where $a,b = 1,2,\ldots,N$, $(\overline{M}_{kj})_a$, $j = 1,2$ is the complex conjugate of $(M_{kj})_a$, and where

$$D_k = \mathrm{Det}|M_k|^2. \tag{15}$$

Clearly, $\mathrm{Tr}\, P_k(2) = 2$. Furthermore, if we let

$$P_{kj}(1) = M_{kj}|M_{kj}|^{-2} M_{kj}^\dagger , \tag{16}$$

then from (14) it follows that

$$P_k(2)=P_{k1}(1)+\tilde{P}_{k2}(1), \tag{17}$$

where

$$\tilde{P}_{k2}(1)=\tilde{M}_{k2}|\tilde{M}_{k2}|^{-2}\tilde{M}_{k2}^{\dagger}, \tag{18}$$

with

$$\tilde{M}_{k2}=[I-P_{k1}(1)]M_{k2}, \tag{19}$$

which is orthogonal to M_{k1}, i.e., $M_{k1}^{\dagger}\tilde{M}_{k2}=0$. Thus, we see from (17) that each projector of $\mathrm{Gr}(2,N)$ is really a sum of two mutually orthogonal rank-1 projectors.

Note that for some cases this construction does not work. To see this take the case where the initial $(N\times 2)$ matrix M_0 is chosen to be given by

$$M_0=(M_{01},\partial_{\xi}M_{01}), \tag{20}$$

i.e., M_{02} is a derivative of M_{01}. Then it follows from (10) that

$$M_1=(0,M_{12}). \tag{21}$$

Thus, in this special case, $|M_1|^2$ is singular, and so the projector $P_1(2)$ does not exist.

Let ξ now be related to the θ, φ, which locally parameterize S^2, via $\xi=\tan(\theta/2)e^{i\varphi}$. Then the matrices M_k define harmonic maps $S^2\to\mathrm{Gr}(n,N)$. Taking our sequence of projectors $P_k(n)=P_k$ in (8) we can now formulate our generalized harmonic map ansatz for the SU(N) Skyrme fields in three dimensions. Namely, we take the matrix $U\in\mathrm{SU}(N)$ of the form

$$U=\exp\left[i\sum_{k=0}^{\lambda-1}g_k\left(P_k-\frac{nI}{N}\right)\right]=\exp\left(-ni\sum_{k=0}^{\lambda-1}g_k/N\right)\left(I+\sum_{l=0}^{\lambda-1}A_lP_l\right), \tag{22}$$

where $g_k=g_k(r)$ for $k=0,...,\lambda-1$ are the profile functions and

$$A_k=(e^{ig_k}-1). \tag{23}$$

The profile functions $g_k(r)$ are required to satisfy the boundary conditions: $g_k(\infty)=0$ and $g_k(0)=2\alpha\pi$, where $\alpha=0$ or ± 1.

III. SU(N) MODEL-FOR THE GENERALIZED HARMONIC MAP ANSATZ

In this section, we first rewrite the energy (4) and the topological charge (3) in the spherical polar coordinates (r,θ,φ). Later we introduce the harmonic map ansatz—so it is convenient to replace the angular coordinates by the complex (or holomorphic) coordinates $(\xi,\bar{\xi})$.

A. Energy

The energy (4), when written in the spherical (holomorphic) coordinates $(r,\xi,\bar{\xi})$, takes the form

$$E=-\frac{i}{12\pi^2}\int \mathrm{d}\xi\,\mathrm{d}\bar{\xi}\,\mathrm{d}r\,r^2\,\mathrm{Tr}\left[\frac{1}{(1+|\xi|^2)^2}L_r^2+\frac{1}{r^2}L_{\xi}L_{\bar{\xi}}+\frac{1}{4r^2}[L_r,L_{\xi}][L_r,L_{\xi}]\right.$$
$$\left.-\frac{(1+|\xi|^2)^2}{16r^4}[L_{\xi},L_{\bar{\xi}}]^2\right], \tag{24}$$

where, for simplicity, we have put the pion (meson) mass $m_{\pi}=0$.

With the matrix $U \in \mathrm{SU}(N)$ given by the harmonic map ansatz (22), the currents L_a''s in (2) take the following form:

$$L_r = i \sum_{k=0}^{\lambda-1} \dot{g}_k \left(P_k - \frac{nI}{N} \right), \tag{25}$$

where $\dot{g}_k = \mathrm{d}g_k/\mathrm{d}r$ and

$$L_\xi = \left[I + \sum_{k=0}^{\lambda-1} (e^{-ig_k} - 1) P_k \right] \left[\sum_{l=0}^{\lambda-1} (e^{ig_l} - 1) P_{l\xi} \right] = \sum_{k=0}^{\lambda-1} [e^{i(g_k - g_{k+1})} - 1](M_{k+1}|M_k|^{-2} M_k^\dagger), \tag{26}$$

where by definition $g_\lambda = 0$, and that $L_{\bar{\xi}} = -(L_\xi)^\dagger$.

Using the expressions for L_r and L_ξ in (25) and (26), respectively, we find that the traces in the energy functional (24) become

$$\mathrm{Tr}(L_r^2) = \frac{n^2}{N} \left(\sum_{k=0}^{\lambda-1} \dot{g}_k \right)^2 - n \sum_{k=0}^{\lambda-1} \dot{g}_k^2, \tag{27}$$

$$\mathrm{Tr}(L_\xi L_{\bar{\xi}}) = -2 \sum_{k=0}^{\lambda-1} S_k \, \mathrm{Tr}(|M_{k+1}|^2 |M_k|^{-2}), \tag{28}$$

$$\mathrm{Tr}([L_r, L_\xi][L_r, L_{\bar{\xi}}]) = -2 \sum_{k=0}^{\lambda-1} (\dot{g}_k - \dot{g}_{k+1})^2 S_k \, \mathrm{Tr}(|M_{k+1}|^2 |M_k|^{-2}), \tag{29}$$

$$\mathrm{Tr}([L_\xi, L_{\bar{\xi}}]^2) = 8 \sum_{k=0}^{\lambda-1} [S_k^2 \, \mathrm{Tr}([|M_{k+1}|^2 |M_k|^{-2}]^2) - S_k S_{k-1} \, \mathrm{Tr}(|M_{k+1}|^2 |M_{k-1}|^{-2})], \tag{30}$$

where by definition $S_{-1} = 0$ and for $k = 0, \ldots, \lambda - 1$:

$$S_k = [1 - \cos(g_k - g_{k+1})]. \tag{31}$$

B. Topological charge

The topological charge (3) in the spherical (holomorphic) coordinate system takes the form

$$B = \frac{1}{8\pi^2} \int \mathrm{d}r \, \mathrm{d}\xi \, \mathrm{d}\bar{\xi} \, \mathrm{Tr}(L_r [L_\xi, L_{\bar{\xi}}]). \tag{32}$$

Using the expression for L_ξ in (26) we find that

$$[L_\xi, L_{\bar{\xi}}] = 2 \sum_{k=0}^{\lambda-1} S_k (M_k |M_k|^{-2} |M_{k+1}|^2 |M_k|^{-2} M_k^\dagger - M_{k+1} |M_k|^{-2} M_{k+1}^\dagger), \tag{33}$$

and so, using this commutator and L_r as given in (25), the topological charge (32) becomes

$$B = -\frac{1}{2\pi} \int \mathrm{d}r \sum_{k=0}^{\lambda-1} (\dot{g}_k - \dot{g}_{k+1})(1 - \cos(g_k - g_{k+1})) \mathcal{N}_k, \tag{34}$$

where

$$\mathcal{N}_k=\frac{i}{2\pi}\int \mathrm{d}\xi\,\mathrm{d}\bar{\xi}\,\mathrm{Tr}(|M_{k+1}|^2|M_k|^{-2}). \tag{35}$$

As $g_k(\infty)=0$, we finally obtain

$$B=\frac{1}{2\pi}\sum_{k=0}^{\lambda-1}\mathcal{N}_k(g_k(0)-g_{k+1}(0)), \tag{36}$$

and so we see that the only contributions to the topological charge comes from $g_k(0)$.

In Appendix A we show that if $D_k=\mathrm{Det}|M_k|^2$ is nonsingular in the whole complex ξ plane, then $\mathcal{N}_k$ obey the recurrence relations

$$\mathcal{N}_k-\mathcal{N}_{k-1}=\omega_k, \tag{37}$$

where ω_k is the highest degree of $|\xi|^2$ in D_k, i.e.,

$$\lim_{|\xi|\to\infty}D_k\to(|\xi|^2)^{\omega_k}, \tag{38}$$

and where by definition $\mathcal{N}_{-1}=0$.

Thus, if we know ω_k then we can determine $\mathcal{N}_k$. In fact, if

$$H_0=M_{01}\wedge M_{02}\wedge\cdots\wedge M_{0n} \tag{39}$$

is the exterior product of the column vectors of M_0 which form the n-dimensional subspace of C^N, then

$$\omega_0=\deg(H_0), \tag{40}$$

i.e., is the highest degree of ξ in H_0.

IV. APPROXIMATE FORMULATIONS

In this section, we derive field equations for the profile functions g_k from the energy (24) into which we have inserted the expressions of the generalized harmonic map ansatz.

To do this we, first of all, take a holomorphic matrix $M_0=M(\xi)$ and then evaluate the sequence $(M_1,M_2,\ldots,M_\lambda)$ using the formulation of Sec. II. Then we compute the angular integrals $\mathcal{N}_k$ in (35),

$$\mathcal{I}_k=\frac{i}{2\pi}\int \mathrm{d}\xi\,\mathrm{d}\bar{\xi}(1+|\xi|^2)^2\,\mathrm{Tr}([|M_{k+1}|^2|M_k|^{-2}]^2), \tag{41}$$

and

$$\mathcal{H}_k=\frac{i}{2\pi}\int \mathrm{d}\xi\,\mathrm{d}\bar{\xi}(1+|\xi|^2)^2\,\mathrm{Tr}(|M_{k+1}|^2|M_{k-1}|^{-2}) \tag{42}$$

for $k=0,\ldots,\lambda-1$, where by definition $\mathcal{H}_0=0$.

In terms of $\mathcal{N}_k$, $\mathcal{I}_k$, and $\mathcal{H}_k$, the energy (24), for our ansatz (22), reduces to

$$E=\frac{1}{6\pi}\int \mathrm{d}r\left(r^2\left[-\frac{n^2}{N}\left(\sum_{k=0}^{\lambda-1}\dot{g}_k\right)^2+n\sum_{k=0}^{\lambda-1}\dot{g}_k^2\right]+2\sum_{k=0}^{\lambda-1}\mathcal{N}_k\left[1+\frac{1}{4}(\dot{g}_k-\dot{g}_{k+1})^2\right]S_k\right.$$
$$\left.+\frac{1}{2r^2}\sum_{k=0}^{\lambda-1}[\mathcal{I}_kS_k^2-\mathcal{H}_kS_kS_{k-1}]\right). \tag{43}$$

Introducing

$$F_k = g_k - g_{k+1}, \tag{44}$$

with $g_\lambda = 0$ we find that, in terms of F_k, the energy integral (43) becomes

$$E = \frac{1}{6\pi}\int \mathrm{d}r\Bigg(r^2\Bigg[-\frac{n^2}{N}\Bigg(\sum_{k=0}^{\lambda-1}(k+1)\dot{F}_k\Bigg)^2 + n\sum_{k=0}^{\lambda-1}\Bigg(\sum_{l=k}^{\lambda-1}\dot{F}_l\Bigg)^2\Bigg] + \frac{1}{2}\sum_{k=0}^{\lambda-1}\mathcal{N}_k(4+\dot{F}_k^2)(1-\cos F_k)$$
$$+ \frac{1}{2r^2}\sum_{k=0}^{\lambda-1}\left[\mathcal{I}_k(1-\cos F_k)^2 - \mathcal{H}_k(1-\cos F_k)(1-\cos F_{k-1})\right]\Bigg), \tag{45}$$

and the topological charge (36) becomes

$$B = \frac{1}{2\pi}\sum_{k=0}^{\lambda-1}\mathcal{N}_k F_k(0). \tag{46}$$

To derive the equations for the profile functions g_k from (45) we note that

$$\frac{\partial \mathcal{E}}{\partial \dot{F}_l} = r^2\Bigg[-\frac{2n^2(l+1)}{N}\sum_{i=0}^{\lambda-1}(i+1)\dot{F}_i + 2n\sum_{i=0}^{l}\Bigg(\sum_{j=i}^{\lambda-1}\dot{F}_j\Bigg)\Bigg] + \mathcal{N}_l\dot{F}_l(1-\cos F_l), \tag{47}$$

where $\mathcal{E}$ denotes the integrand of E.

Thus our field equations for the functions F_i and so also for g_i are given by

$$\Bigg[-\frac{2n^2(l+1)}{N}\sum_{i=0}^{\lambda-1}(i+1)\ddot{F}_i + 2n\sum_{i=0}^{l}\sum_{j=i}^{\lambda-1}\ddot{F}_j\Bigg] + \frac{1}{r^2}\mathcal{N}_l\ddot{F}_l(1-\cos F_l)$$
$$+ \frac{2}{r}\Bigg[-\frac{2n^2(l+1)}{N}\sum_{i=0}^{\lambda-1}(i+1)\dot{F}_i + 2n\sum_{i=0}^{l}\sum_{j=i}^{\lambda-1}\dot{F}_j\Bigg] + \frac{\sin F_l}{2r^2}\Bigg[\mathcal{N}_l(\dot{F}_l^2-4) - \frac{2\mathcal{I}_l(1-\cos F_l)}{r^2}$$
$$+ \frac{\mathcal{H}_l(1-\cos F_{l-1})}{r^2} + \frac{\mathcal{H}_{l+1}(1-\cos F_{l+1})}{r^2}\Bigg]$$
$$= 0. \tag{48}$$

Now a question arises: what is the best choice of the initial matrix M_0 that would yield low energy field configurations which, hopefully, are close to the exact solutions of the full equations of the model, i.e., Eq. (5)? To answer this question we note that each $\mathcal{N}_k$ is, in fact, the energy of the Grassmannian $\mathrm{Gr}(n,N)$ models. Thus in order to have minimal $\mathcal{N}_k$, and so also energy to be close to the exact multiskyrmion energy, the entries of the matrix M_0 must be *polynomials* in ξ.[11,12]

In the following sections we make this choice for M_0 and consider various fields for the SU(3), SU(4), and SU(5) cases with one and two rank-2 projector approximations. Our choices are dictated by simplicity and they lead to energy density distributions which are spherically symmetric. Moreover, looking at the general case we see that they also correspond to setting some g_i functions in (22) equal to zero.

V. ONE PROJECTOR APPROXIMATIONS

In this case, we take only one profile function $g_0 = F_0 = F$, i.e., $\lambda = 1$, and so the approximate energy (45) with the mass term reduces to

$$E=\frac{1}{6\pi}\int \mathrm{d}r\left(\frac{1}{2}\dot{F}^2[A_N(n)r^2+\mathcal{N}_0(1-\cos F)]+2\mathcal{N}_0(1-\cos F)+\frac{\mathcal{I}_0(1-\cos F)^2}{2r^2}\right.$$
$$\left.+m_\pi^2\left[(N-n)\left(1-\cos\left[\frac{nF}{N}\right]\right)+n\left(1-\cos\left[\frac{(N-n)F}{N}\right]\right)\right]\right), \tag{49}$$

where

$$A_N(n)=\frac{2n(N-n)}{N}, \tag{50}$$

and the field equation for the approximate function F becomes

$$\ddot{F}\left[A_N(n)+\frac{\mathcal{N}_0(1-\cos F)}{r^2}\right]+\frac{2A_N(n)}{r}\dot{F}+\frac{\sin F}{2r^2}\left[\mathcal{N}_0(\dot{F}^2-4)-\frac{2\mathcal{I}_0(1-\cos F)}{r^2}\right]$$
$$-m_\pi^2A_N(n)\left[\sin\left(\frac{nF}{N}\right)+\sin\left(\frac{(N-n)F}{N}\right)\right]=0. \tag{51}$$

In the following we restrict our attention to the rank-2 case only, i.e., $n=2$. To solve (51) we impose the boundary conditions: $F(0)=2\pi$ and $F(\infty)=0$. Thus, the baryon number of these configurations is $B=\mathcal{N}_0$. Finally, we compare the approximate energies of each subcase with the corresponding energies of the one rank-1 projector approximations.[8]

As a first attempt to solve (51), let us take the initial matrix $M_0=(M_{01},M_{02})$, where both column vectors are given by the following Veronese type form:

$$M_{01}=(1,\sqrt{C_1^{N-1}}\xi,\ldots,\sqrt{C_k^{N-1}}\xi^k,\ldots,\xi^{N-1})^T,\quad M_{02}=\partial_\xi M_{01}, \tag{52}$$

where C_k^{N-1} denotes the binomial coefficients, and the superscript T denotes transposition.

This special form of M_0 enables us to express the determinant D_0 of $|M_0|^2$ in the following closed form:

$$D_0=(N-1)(1+|\xi|^2)^{2(N-2)}. \tag{53}$$

Then from (38) we conclude that $\mathcal{N}_0=2(N-2)$, which is consistent with (40). This result can be verified explicitly using definition (35) with the help of the recurrence relations (A4), which yields

$$\mathrm{Tr}(|M_1|^2|M_0|^{-2})=\frac{2(N-2)}{(1+|\xi|^2)^2}. \tag{54}$$

For this case, according to (21), $D_1=0$, and so according to formula (B3), $\mathcal{I}_0=\mathcal{N}_0^2=4(N-2)^2$.

In the SU(3) case, we find that $A_3(2)=\frac{4}{3}$, $\mathcal{N}_0=2$, and so $\mathcal{I}_0=4$, which all coincide with the values of the corresponding quantities in the rank-1 projector approximation.[8] Thus, we conclude that their energies also coincide, i.e., $E=2.444\,04$ $(m_\pi=0)$. This equality holds for $m_\pi\neq 0$ as well. This is to be expected as in this case our rank-2 projector is really a sum of two rank-1 projectors constructed from the first two vectors of the Veronese sequence.

It is clear that, for SU(N) with $N>3$ we have: $A_N(2)>A_N(1)$, $\mathcal{N}_0>(N-1)$, and $\mathcal{I}_0>(N-1)^2$. Thus, this Veronese type configuration for $N>3$ will lead to energies higher in comparison with those for the rank-1 projector approximations.[8]

So, in the following, we look only at M_0 with $\mathcal{N}_0=(N-1)$ and $\mathcal{I}_0<(N-1)^2$ in order to compensate $A_N(2)>A_N(1)$ in the energy integral (49). More specifically, we look at the following two subcases for which the determinant of $|M_0|^2$ is of the form,

$$D_0=c(1+|\xi|^2)^{N-1}, \tag{55}$$

or

$$D_0 = c(1+\sigma|\xi|^2)^{N-3}(1+|\xi|^2)^2, \tag{56}$$

where c and σ are some constants. For the subcase (56) we choose the column vector M_{01} to have the Veronese type form (52) while $M_{02} = \partial_\xi^{N-2} M_{01}$.

A. SU(3)

As here we have $N=3$, so subcase (56) is the same with the Veronese type subcase that we have discussed previously. Thus in this section we consider only subcase (55).

In this subcase, we can choose the initial matrix M_0 to be given by

$$M_0 = \begin{bmatrix} 1 & \sqrt{a}\xi & \sqrt{b}\xi^2 \\ 0 & 1 & \sqrt{c}\xi \end{bmatrix}^T. \tag{57}$$

If we now require that $D_0 = (1+|\xi|^2)^2$, then $c=2$ while there is an infinite number of solutions for a and b as here we have only one equation for a and b. In the following we restrict our attention to the solution: $a=0$ and $b=1$.

Starting from the corresponding initial matrix M_0 we find that

$$M_1 = \frac{\sqrt{2}}{D_0}\begin{bmatrix} \sqrt{2}\xi(-\bar{\xi}^2 - \sqrt{2}\bar{\xi}1) \\ -\bar{\xi}^2 - \sqrt{2}\bar{\xi}1 \end{bmatrix}^T, \tag{58}$$

which is orthogonal to M_0, i.e., $M_0^\dagger M_1 = 0$. Note that $|M_1|^2$ is singular, i.e., $D_1 = 0$.

Using these two basis matrices, M_0 and M_1, we find from (35) that $\mathcal{N}_0 = 2$, and from (41) $\mathcal{I}_0 = 4$. These results coincide with the corresponding numbers in the one rank-1 projector approximation of the SU(3) case described by the initial vector field[8]

$$f_0 = (1, \sqrt{2}\xi, \xi^2)^T. \tag{59}$$

As $A_3(2) = \frac{2}{3} = A_3(1)$ both rank-1 and rank-2 projector approximations have equal energy, i.e., $E = 2.444\,04$ $(m_\pi = 0)$. This equality holds for $m_\pi \neq 0$ as well.

The result $D_1 = 0$ that we have encountered previously is in fact a general property for SU(3) case with rank-2 projectors ansatz, which can be seen as follows. Using the splitting relation (17) we see that

$$M_1 = ([I - P_{01}(1) - \tilde{P}_{02}(1)]\partial_\xi M_{01}, [I - P_{01}(1) - \tilde{P}_{02}(1)]\partial_\xi M_{02}). \tag{60}$$

As the case $\partial_\xi M_{02} = 0$ is trivial so we will only consider the nonzero case. We observe that

$$\begin{aligned} V_0 &= M_{01}, \\ V_1 &= [I - P_{01}(1)]M_{02}, \\ V_2 &= [I - P_{01}(1) - \tilde{P}_{02}(1)]\partial_\xi M_{02} \end{aligned} \tag{61}$$

are mutually orthogonal and so they span C^3. Thus,

$$\partial_\xi M_{01} = \alpha V_0 + \beta V_1 + \gamma V_2, \tag{62}$$

where α, β, and γ are expansion coefficients which depend on ξ and $\bar{\xi}$. As

$$[I - P_{01}(1) - \tilde{P}_{02}(1)][\alpha V_0 + \beta V_1 + \gamma V_2] = \gamma V_2, \tag{63}$$

TABLE I.

m_π	$E(1)$	$E(2)$
0.0	3.644 10	3.813 87
0.2	3.682 91	3.861 58
1.0	4.172 41	4.420 30
2.23	5.001 86	5.334 05
7.0	7.471 87	8.023 36
30.0	14.339 3	15.428 7

so

$$M_1=(\gamma V_2, V_2), \tag{64}$$

and it clearly follows that $|M_1|^2$ has a vanishing determinant.

B. SU(4)

1. $D_0=c(1+|\xi|^2)^3$

In this subcase we can choose the initial matrix M_0 to be given by

$$M_0=\begin{bmatrix} 1 & 0 & \sqrt{a}\,\xi & \sqrt{b}\,\xi^2 \\ 0 & 1 & \sqrt{c}\,\xi & \sqrt{d}\,\xi^2 \end{bmatrix}^T. \tag{65}$$

If we require $D_0=(1+|\xi|^2)^3$, then there is an infinite number of solutions for a, b, c and d as here we have only three equations for the four parameters a, b, c, and d. In the following we consider the solution: $a=2$, $b=1$, $c=1$, $d=2$.

Then, starting from M_0 in (65) we have computed the corresponding mutually orthogonal matrix M_1 and by using these two basis matrices, M_0 and M_1, we have computed explicitly the integrals $\mathcal{N}_0$ and $\mathcal{I}_0$ in expressions (35) and (41), respectively and we have found that $\mathcal{N}_0=3$ and $\mathcal{I}_0=\frac{23}{3}$. We note that, in the one projector rank-1 case with initial vector field

$$f_0=(1,\sqrt{3}\,\xi,\sqrt{3}\,\xi^2,\xi^3)^T, \tag{66}$$

$\mathcal{I}_0=9$ which is larger than the above-given result. However, as $A_4(2)=2$ while $A_4(1)=\frac{3}{4}$ it is not clear which energy is larger. To assess this we have solved numerically Eq. (51) for F. In Table I we present our results for the energies $E(2)$ and compare them with the results using one rank-1 projector, $E(1)$,[8] for different values of the mass m_π.

From Table I we see that for all the masses (at least to $m_\pi=30.0$) we always have $E(2)>E(1)$. When we have solved (51) for the approximate profile function $F=g_0$, we found that it is very close to that found in Ref. 8 using rank-1 projector ansatz.

2. $D_0=c(1+\sigma|\xi|^2)(1+|\xi|^2)^2$

In this subcase, we choose the initial matrix M_0 to be given by the following Veronese type form:

$$M_0=\begin{bmatrix} 1 & \sqrt{3}\,\xi & \sqrt{3}\,\xi^2 & \xi^3 \\ 0 & 0 & 2\sqrt{3} & 6\,\xi \end{bmatrix}^T, \tag{67}$$

which has $D_0=12(1+4|\xi|^2)(1+|\xi|^2)^2$. For this configuration, we have found that it has $\mathcal{N}_0=3$ but $\mathcal{I}_0=7.143\,57$ and its energy is $E=3.769\,29$ ($m_\pi=0$), which is a little lower than the energy of Sec. V B 1, but it is still higher than the energy of the one rank-1 projector approximation, i.e., $E=3.644\,10$.

C. SU(5)

1. $D_0 = c(1+|\xi|^2)^4$

In this subcase we can choose the initial matrix M_0 to be

$$M_0 = \begin{bmatrix} 1 & \sqrt{a}\xi & \sqrt{b}\xi^2 & \sqrt{c}\xi^3 & \sqrt{d}\xi^4 \\ 0 & 0 & 0 & 1 & \sqrt{e}\xi \end{bmatrix}^T. \tag{68}$$

If we require $D_0 = (1+|\xi|^2)^4$, then there is an infinite number of solutions for a, b, c, d, and e as here we have only four equations for these five parameters. Here we consider only the solution: $a = b = c = e = \sqrt{2}$ and $d = 1$.

For this configuration, we have found that $\mathcal{N}_0 = 4$ but $\mathcal{I}_0 = 12.2667$, which is much lower than 16. However, as $A_5(2) = \frac{12}{5}$, we see that its energy is $E = 5.105\,80$ $(m_\pi = 0)$, which is still higher than $E = 4.837\,92$ in the rank-1 projector approximation.[13] When we have solved the equations for the approximate profile function $F = g_0$ for each rank (1 and 2), we found that their difference is very small.

2. $D_0 = c(1+\sigma|\xi|^2)^2(1+|\xi|^2)^2$

In this subcase we choose the initial matrix M_0 to have the following Veronese type form:

$$M_0 = \begin{bmatrix} 1 & 2\xi & \sqrt{6}\xi^2 & 2\xi^3 & \xi^4 \\ 0 & 0 & 0 & 12 & 24\xi \end{bmatrix}^T, \tag{69}$$

which has $D_0 = 144(1+3|\xi|^2)^2(1+|\xi|^2)^2$.

We have found that this configuration has $\mathcal{N}_0 = 4$ but $\mathcal{I}_0 = 12.4444$ and its energy is $E = 5.118\,75$ $(m_\pi = 0)$ which is higher than the energy of the case in Sec. V C 1.

VI. TWO PROJECTOR APPROXIMATIONS

Now we consider the case of two projectors. Here we have two profile functions: F_0 and F_1, i.e., $\lambda = 2$, and so the energy integral (45) becomes

$$E = \frac{1}{12\pi}\int \mathrm{d}r\Big(r^2[A_N(n)\dot{F}_0^2 + A_N(2n)\dot{F}_0\dot{F}_1 + A_N(2n)\dot{F}_1^2] + \mathcal{N}_0(4+\dot{F}_0^2)(1-\cos F_0) + \mathcal{N}_1(4+\dot{F}_1^2)$$
$$\times(1-\cos F_1) + \frac{1}{r^2}[\mathcal{I}_0(1-\cos F_0)^2 - \mathcal{H}_1(1-\cos F_0)(1-\cos F_1) + \mathcal{I}_1(1-\cos F_1)^2]\Big), \tag{70}$$

where now, for simplicity, we have set $m_\pi = 0$.

The field equations for F_0 and F_1 are

$$\ddot{F}_0\left[A_N(n) + \frac{\mathcal{N}_0(1-\cos F_0)}{r^2}\right] + \frac{1}{2}A_N(2n)\ddot{F}_1 + \frac{2}{r}\left[A_N(n)\dot{F}_0 + \frac{1}{2}A_N(2n)\dot{F}_1\right]$$
$$+ \frac{\sin F_0}{2r^2}\left[\mathcal{N}_0(\dot{F}_0^2 - 4) - \frac{2\mathcal{I}_0(1-\cos F_0)}{r^2} + \frac{\mathcal{H}_1(1-\cos F_1)}{r^2}\right] = 0, \tag{71}$$

$$\frac{1}{2}A_N(2n)\ddot{F}_0 + \ddot{F}_1\left[A_N(2n) + \frac{\mathcal{N}_1(1-\cos F_1)}{r^2}\right] + \frac{2}{r}\left[\frac{1}{2}A_N(2n)\dot{F}_0 + A_N(2n)\dot{F}_1\right]$$
$$+ \frac{\sin F_1}{2r^2}\left[\mathcal{N}_1(\dot{F}_1^2 - 4) - \frac{2\mathcal{I}_1(1-\cos F_1)}{r^2} + \frac{\mathcal{H}_1(1-\cos F_0)}{r^2}\right] = 0. \tag{72}$$

In the following, we take $n=2$ and solve these equations (numerically) by imposing the boundary conditions: $F_0(0)=2\pi$, $F_1(0)=0$, and $F_0(\infty)=F_1(\infty)=0$. Thus, the baryon number of these configurations is $B=\mathcal{N}_0$. We then compare the approximate energies of each of these cases with the corresponding energies of the one rank-1 projector approximations.[8]

For the SU(3) configurations, we have shown that $|M_1|^2$ is singular. Thus for this case the projector P_1 does not exist. As for the SU(4) and SU(5) cases that we have considered previously, $|M_1|^2$ is nonsingular, so in this section we consider these two cases only.

A. SU(4)

Starting from the initial matrix M_0 in (65), we find that

$$M_2=0, \tag{73}$$

so from (35), (41), and (42) we have $\mathcal{N}_1=0$, $\mathcal{I}_1=0$, and $\mathcal{H}_1=0$. As for this case, $N=4$ and $n=2$, the energy integral (70) reduces to the energy integral (49) for the corresponding one projector of rank-2 projector approximation.

We note that $M_2=0$ is in fact a general property for SU(4) with rank-2 projectors ansatz. To prove this it is convenient to note that $M_k=P_+^k M_0$ is given by

$$M_k=[I-P_0-P_1-\cdots-P_{k-1}]\partial_\xi^k M_0. \tag{74}$$

Then using the splitting relation (17) in (74) for M_2 gives

$$\begin{aligned} M_2&=[I-P_0(2)-P_1(2)]\partial_\xi^2 M_0,\\ &=[I-(P_{01}(1)+\tilde{P}_{02}(1))-(P_{11}(1)+\tilde{P}_{12}(1))]\partial_\xi^2 M_0. \end{aligned} \tag{75}$$

Now, $M_2=0$ follows from the completeness relation for the rank-1 projectors in C^4, i.e.,

$$P_{01}(1)+\tilde{P}_{02}(1)+P_{11}(1)+\tilde{P}_{12}(1)=I. \tag{76}$$

B. SU(5)

As Sec. V C 1 in the one projector approximation has lower energy, we restrict our attention to this subcase. Starting from the matrix M_0 in (69), we have computed the corresponding matrices M_1 and M_2, and we have found that $\mathcal{N}_1=2.0$, $\mathcal{I}_1=4.289\,89$, and $\mathcal{H}_1=3.573\,57$.

Solving Eq. (72) with the correct values for $\mathcal{N}_k$, $\mathcal{I}_k$, and $\mathcal{H}_k$, $k=0$ and 1, we have found that, as $A_5(2)=\frac{12}{5}$ and $A_5(4)=\frac{8}{5}$, this configuration has energy: $E=5.024\,69$. This is higher than the energy of the one rank-1 projector approximation case, i.e., $E=4.837\,92$; however, they are marginally higher than the exact energy of the SU(2) case with $B=4$, i.e., $E=4.464$.[5]

VII. CONDITION FOR AN EXACT SPHERICALLY SYMMETRIC SOLUTION

In this section we consider whether one could also construct exact spherically symmetric solutions of the SU(N) Skyrme field equations (5) using λ rank-2 projectors. When written in the spherical (holomorphic) coordinates, Eq. (5) without the mass term becomes

$$\begin{aligned} &\partial_r\left[r^2 L_r+\frac{(1+|\xi|^2)^2}{8}([L_{\bar\xi},[L_r,L_\xi]]+[L_\xi,[L_r,L_{\bar\xi}]])\right]+\frac{(1+|\xi|^2)^2}{2}(\partial_{\bar\xi}L_\xi+\partial_\xi L_{\bar\xi})\\ &\quad+\frac{(1+|\xi|^2)^2}{8}(\partial_\xi([L_r,[L_{\bar\xi},L_r]])+\partial_{\bar\xi}([L_r,[L_\xi,L_r]]))+\frac{(1+|\xi|^2)^2}{16r^2}[\partial_{\bar\xi}((1\\ &\quad+|\xi|^2)^2[L_\xi,[L_\xi,L_{\bar\xi}]])-\partial_\xi((1+|\xi|^2)^2[L_{\bar\xi},[L_\xi,L_{\bar\xi}]])]=0. \end{aligned} \tag{77}$$

Now, let us look in detail at all the terms in these equations in our generalized harmonic map ansatz (22) case. We find that

$$\partial_{\bar{\xi}} L_{\xi} + \partial_{\xi} L_{\bar{\xi}} = 2i \sum_{l=0}^{\lambda-1} \sin F_l [M_{l+1} |M_l|^{-2} M_{l+1}^{\dagger} - M_l |M_l|^{-2} |M_{l+1}|^2 |M_l|^{-2} M_l^{\dagger}], \tag{78}$$

$$[L_{\bar{\xi}}, [L_r, L_{\xi}]] = -2i \sum_{l=0}^{\lambda-1} S_l \dot{F}_l [M_{l+1} |M_l|^{-2} M_{l+1}^{\dagger} - M_l |M_l|^{-2} |M_{l+1}|^2 |M_l|^{-2} M_l^{\dagger}], \tag{79}$$

$$[L_r, [L_{\xi}, L_r]] = \sum_{l=0}^{\lambda-1} \dot{F}_l^2 b_l M_{l+1} |M_l|^{-2} M_l^{\dagger}, \tag{80}$$

$$\begin{aligned} [L_{\xi}, [L_{\xi}, L_{\bar{\xi}}]] = 2 \sum_{l=0}^{\lambda-1} & [2 S_l b_l M_{l+1} |M_l|^{-2} |M_{l+1}|^2 |M_l|^{-2} M_l^{\dagger} - S_l b_{l+1} M_{l+2} |M_l|^{-2} M_{l+1}^{\dagger} \\ & - S_{l+1} b_l M_{l+1} |M_{l+1}|^{-2} |M_{l+2}|^2 |M_l|^{-2} M_l^{\dagger}], \end{aligned} \tag{81}$$

where S_l is given by (31) and where

$$b_l = (e^{iF_l} - 1). \tag{82}$$

We have checked that none of the configurations that we have considered so far in this paper is an exact solution of (77). This can be seen as follows. First, we multiply (77) by M_l from the right, which results in a set of equations for M_l. As the terms $\partial_r (r^2 L_r) M_l$ are proportional to M_l while the others are not, the contracted equations have the following general structure:

$$a_l M_l + \sum_{k=0}^{\lambda-1} M_k A_{kl} = 0, \tag{83}$$

where a_l depend only on N, n, $\dot{g}_i$, $\ddot{g}_i$, and r while the $(n \times n)$ matrices A_{kl} depend on g_i, ξ, and $\bar{\xi}$ as well. Clearly, these equations are inconsistent, unless each matrix A_{kl} is proportional to the $(n \times n)$ unit matrix I_n, i.e., $A_{kl} = b_{kl} I_n$, where each b_{kl} is independent of ξ and $\bar{\xi}$.

Armed with this observation we can now ask the following question: for which forms of the matrices M_k do the SU(N) Skyrme field equations (77) have exact solutions? In Appendix C, we have looked at the SU(N) chiral models and we found that, if we are able to find the matrices M_k which satisfy the condition

$$|M_{k+1}|^2 |M_k|^{-2} = \mathcal{K}_k (1 + |\xi|^2)^{-2} I_n, \tag{84}$$

where $\mathcal{K}_k$ are some constants which depend on N, n, and k, then this configuration could possibly give exact solutions for the profile functions g_k.

To see how this may work in our case we have put the condition (84) into (78)–(81), which has turned the field equations (77) into the following reduced set

$$\sum_{k=0}^{\lambda-1} \left[\left(P_k - \frac{nI}{N} \right) \alpha_k + (P_{k+1} - P_k) \beta_k + (P_{k+2} - P_{k+1}) \gamma_k \right] = 0, \tag{85}$$

where α_k, β_k, and γ_k are some functions of the profile functions g_i and their derivatives, r and $\mathcal{K}_k$. In the appendix of Ref. 13 we have analyzed this type of equation for the case of the rank-1 projectors [for the alternative SU(N) Skyrme model in Ref. 13, $\gamma_k = 0$] and we have found that these equations do, indeed, yield consistent and compatible equations for the corresponding profile functions g_l.

To show whether this is also true for the case of rank-n projectors, we put the condition (84) into (35), (41), and (42), which yields the following relations:

$$\mathcal{N}_k = n\mathcal{K}_k, \tag{86}$$

$$\mathcal{I}_k = n\mathcal{K}_k^2, \tag{87}$$

$$\mathcal{H}_k = n\mathcal{K}_k\mathcal{K}_{k-1}. \tag{88}$$

Using these relations in (85) and following the procedure of the appendix of Ref. 13, we have found that the resulting equations for the profile functions g_k do, indeed, coincide with (48). This also means that the energy integral (24), in this case, is exact (i.e., not an approximation).

VIII. FURTHER ANALYSIS OF THE CONDITION (84)

As the matrices M_k for $k\neq 0$ are generated from the initial matrix M_0, so in this section, we derive the conditions that M_0 should satisfy in order for condition (84) to hold. To do so, we put (84) into (A3) and (A4) with $k=0$, and obtain

$$\partial_{\bar{\xi}}[(\partial_{\bar{\xi}}|M_0|^2)|M_0|^{-2}] = \mathcal{K}_0(1+|\xi|^2)^{-2}I_n, \tag{89}$$

and

$$\partial_\xi\partial_{\bar{\xi}}[\log D_0] = n\mathcal{K}_0(1+|\xi|^2)^{-2}, \tag{90}$$

respectively.

The general solution of Eq. (89) is

$$|M_0|^2 = (1+|\xi|^2)^{\mathcal{K}_0}G(\bar{\xi},\xi), \tag{91}$$

where $G(\bar{\xi},\xi)$ is an $(n\times n)$ Hermitian matrix satisfying

$$\partial_{\bar{\xi}}[(\partial_{\bar{\xi}}G)G^{-1}] = 0. \tag{92}$$

Equation (92) has the general solution[14]

$$G(\bar{\xi},\xi) = \bar{H}(\bar{\xi})H(\xi), \tag{93}$$

where H and $\bar{H}=H^\dagger$ are arbitrary $(n\times n)$ matrices of one variable.

Thus, with $G(\bar{\xi},\xi)$ given by (93), solution (91) becomes

$$|M_0|^2 = (1+|\xi|^2)^{\mathcal{K}_0}\bar{H}(\bar{\xi})H(\xi), \tag{94}$$

and from condition (84) it follows that (for $l\geqslant 1$)

$$|M_l|^2 = \mathcal{K}_0\mathcal{K}_1\cdots\mathcal{K}_{l-1}(1+|\xi|^2)^{\mathcal{K}_0-2l}\bar{H}(\bar{\xi})H(\xi). \tag{95}$$

Furthermore, from (91) it follows that

$$D_0 = (1+|\xi|^2)^{n\mathcal{K}_0}\mathrm{Det}[\bar{H}(\bar{\xi})]\mathrm{Det}[H(\xi)] \tag{96}$$

is a solution of (90). By putting D_0 into (A6) we have found that $\mathcal{N}_0=n\mathcal{K}_0$, as we have assumed that $\mathrm{Det}[H(\xi)]$ is holomorphic (and $\mathrm{Det}[\bar{H}(\bar{\xi})]$ is antiholomorphic) with the only singularity at $|\xi|\to\infty$, which is consistent with (86). Thus, we can choose $\mathrm{Det}[G(\bar{\xi},\xi)]=1$, and so from (95) it follows that

$$D_l=(\mathcal{K}_0\mathcal{K}_1\cdots\mathcal{K}_{l-1})^n(1+|\xi|^2)^{n(\mathcal{K}_0-2l)}, \tag{97}$$

from which, according to (38),

$$\omega_l=n(\mathcal{K}_0-2l). \tag{98}$$

Using the recurrence relations (37), with ω_l given by (98), we derive

$$\mathcal{N}_l=(l+1)(\mathcal{N}_0-nl). \tag{99}$$

Now, with $|M_0|^2$ given by (94), the projector $P_0(n)=M_0|M_0|^{-2}M_0^\dagger$ becomes

$$P_0(n)=(1+|\xi|^2)^{-\mathcal{K}_0}\tilde{M}_0\tilde{M}_0^\dagger, \tag{100}$$

where $\tilde{M}_0=M_0H^{-1}$. Using (94) then it follows that the matrix $\tilde{M}_0$ satisfies

$$|\tilde{M}_0|^2=\overline{H}^{-1}|M_0|^2H^{-1}=(1+|\xi|^2)^{\mathcal{K}_0}I_n. \tag{101}$$

Equation (101) implies that the column vectors of the matrix $\tilde{M}_0=(\tilde{M}_{01},\tilde{M}_{02},\ldots,\tilde{M}_{0n})$ are mutually orthogonal. Thus, using the SU(N) global symmetry, we can bring the column vectors $\tilde{M}_{0j}$, $(j=1,2,...,n)$ to live in n-disjoint subspaces. In this case, the projector $P_0(n)$ has a block diagonal form. For example, in the rank-2 projector ansatz, i.e., $n=2$, for $N=even$, we have

$$P_0(2)=\begin{bmatrix} P_{01}(1) & 0 \\ 0 & P_{02}(1) \end{bmatrix}, \tag{102}$$

where

$$P_{0s}(1)=\frac{\tilde{M}_0\tilde{M}_0^\dagger}{|\tilde{M}_0|^2}, \tag{103}$$

$s=0$, 1, are rank-1 projectors. For $N=odd$, still in the rank-2 projector ansatz, Eq. (101) requires that one of the entries of $\tilde{M}_{0j}$ should be zero, so if we choose $(\tilde{M}_{0j})_N=0$, then the $((N-1)\times(N-1))$ submatrix of $P_0(2)$ has the block form (102) while $P_0(2)_{NN}=0$.

Thus, as far as condition (84) is concerned, it seems that the only exact spherically symmetric solutions of the SU(N) Skyrme models using projectors of rank-2 are embeddings of a pair of SU($[N]/2$) solutions of rank-1 projector ansatz, where $[N]=N$, or $(N-1)$ for N even or odd, respectively.

IX. SOME SPECIFIC CONFIGURATIONS

In this final section we consider only the rank-2 projector ansatz, i.e., $n=2$. Thus, here, the SU(3) case should be excluded, as from our analysis in Sec. V A, $|M_1|^2$ is singular so it is automatically not proportional to the nonsingular matrix $|M_0|^2$ as required by (84). For the same reason, we also exclude the case $M_{02}=\partial_\xi M_{01}$, i.e., Eq. (21). Next, we have a look at some specific forms of the initial matrix M_0, for the $N=4$ and 6 cases.

A. SU(4)

In this case, we can choose the initial matrix M_0 to be given by

$$M_0=\begin{bmatrix} 1 & \xi & f(\xi) & \xi f(\xi) \\ 0 & 0 & 1 & \xi \end{bmatrix}^T, \tag{104}$$

where $f(\xi)$ is an arbitrary polynomial function of only ξ. Then

$$|M_0|^2=(1+|\xi|^2)\begin{bmatrix}1 & \overline{f(\xi)}\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\ f(\xi) & 1\end{bmatrix}, \tag{105}$$

which is of the form (94).

For the corresponding projector $P_0(2)$, we have found by direct evaluation that it has the block form (102) with

$$P_{0s}(1)=\frac{1}{(1+|\xi|^2)}\begin{bmatrix}1 & \overline{\xi}\\ \xi & |\xi|^2\end{bmatrix}, \tag{106}$$

$s=0$, 1, which clearly are the rank-1 projectors of a one skyrmion SU(2) solution. As $D_0=(1+|\xi|^2)^2$, this configuration has $\mathcal{N}_0=2$, or $\mathcal{K}_0=1$, and so according to (87), $\mathcal{I}_0=2$. Then from (99) we obtained $\mathcal{N}_1=0$ or $\mathcal{K}_1=0$ [according to (86)] so from (95) we conclude that $M_l=0$, for $l\geqslant 2$, which is consistent with our general result in Sec. VI A. Thus, this configuration has only one projector, i.e., $P_0(2)$.

Substituting $\mathcal{N}_0=\mathcal{I}_0=A_4(2)=2$ in the 1-projector energy integral (49) we found that it has energy: $E=2E_{\mathrm{SU}(2)}$, where $E_{\mathrm{SU}(2)}$ is the energy of the SU(2) Skyrme model,[9] as we would have been expected.

B. SU(6)

In this case, we can choose the initial matrix M_0 to be given by

$$M_0=\begin{bmatrix}1 & \sqrt{2}\xi & \xi^2 & f(\xi) & \sqrt{2}\xi f(\xi) & \xi^2 f(\xi)\\ 0 & 0 & 0 & 1 & \sqrt{2}\xi & \xi^2\end{bmatrix}^T, \tag{107}$$

from which it follows that $|M_0|^2$ is of the form (94) as well with $\mathcal{K}_0=2$.

We have also found that the corresponding projector, $P_0(2)$, has the block form (102) with $P_{0s}(1)$, $s=0$, 1, are the rank-1 projectors of the SU(3) solution.[9] As $D_0=(1+|\xi|^2)^4$, this configuration has $\mathcal{N}_0=4$, from which we derived that $\mathcal{I}_0=8$, $\mathcal{N}_1=4$, $\mathcal{I}_1=8$, $\mathcal{H}_1=8$, but $\mathcal{N}_2=0$ or $\mathcal{K}_2=0$ and so $M_l=0$ for $l\geqslant 3$. Thus, this configuration has only two projectors, i.e., $P_0(2)$ and $P_1(2)$.

Substituting the correct values for $\mathcal{N}_k$, $\mathcal{I}_k$, and $\mathcal{H}_k$, $k=0$, 1, into the 2 projectors energy integral (70) we have found that, as $A_6(2)=A_6(4)=\frac{8}{3}$, this configuration has energy: $E=2E_{\mathrm{SU}(3)}$, where $E_{\mathrm{SU}(3)}$ is the energy of the SU(3) Skyrme model.[9]

X. CONCLUSIONS

In this paper we have studied the SU(N) Skyrme models by constructing SU(N) multiskyrmions fields using the harmonic mappings method where we have generalized the method of Ioannidou *et al.*[9] by considering projectors of S^2 into the Grassmannian Gr(n,N), i.e., using projectors of rank $n>1$. In this approach a rank-n projector $P_k(n)$ is constructed from a member of a set of mutually orthogonal $(N\times n)$ matrix fields M_k. In particular, here we have concentrated our attention only on the rank-2 projectors.

Using our construction we have studied some approximate spherically symmetric configurations of SU(N) Skyrme models. When we have solved the equations for the profile functions for configurations with baryon number $B=(N-1)$ we found that they are very close to those for the rank-1 cases and that they have marginally higher energies. These results indicate that the rank-1 projector ansatz[8] is the best way to approximate energy minima of the SU(N) Skyrme models.

We have also discussed the possibility of generating exact spherically symmetric solutions using this construction. However, we have found that, in contradistinction to the rank-1 projector ansatz in which exact spherically symmetric solutions can be found (numerically) by using the Veronese sequence of N mutually orthogonal vector fields in CP^{N-1}, such a construction is more involved in our case. In particular, we have found that if the sequence of the $(N\times n)$ matrix fields

M_k satisfy condition (84) then it seems that the only possible exact solutions are embeddings. For example, for the rank-2 projector ansatz these are embeddings of a pair of SU($[N]/2$) solutions of rank-1 projector ansatz, where $[N]=N$, or $(N-1)$ for N even or odd, respectively.

It is not clear whether there exist other conditions than (84) for the $(N\times n)$ matrix fields M_k that might lead to nonembedding solutions.

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APPENDIX A: RECURRENCE RELATIONS FOR Tr($|M_k|^2|M_{k-1}|^{-2}$) AND $\mathcal{N}_k$

In this appendix, we derive recurrence relations for $\mathrm{Tr}(|M_k|^2|M_{k-1}|^{-2})$ appearing in the integral $\mathcal{N}_k$ of (35). To do this we rewrite the definition of M_{k+1} in (10) as follows:

$$\partial_\xi M_k = M_{k+1} + M_k|M_k|^{-2}(M_k^\dagger \partial_\xi M_k). \tag{A1}$$

As $\partial_{\bar\xi} M_k$ is given by (11) so from the integrability condition

$$\partial_\xi \partial_{\bar\xi} M_k = \partial_{\bar\xi}\partial_\xi M_k, \tag{A2}$$

we derive the recurrence relations

$$\partial_\xi[(\partial_{\bar\xi}|M_k|^2)|M_k|^{-2}] = |M_{k+1}|^2|M_k|^{-2} - |M_k|^2|M_{k-1}|^{-2}. \tag{A3}$$

We note that for the $n=1$ case, i.e., when M_k are a sequence of N-component vector fields, Eq. (A3) gives the celebrated *Toda equation*.[15] Thus, for $n\neq 1$ our Eq. (A3) could be considered as its generalization to the *non-Abelian* case.[16]

Furthermore, taking the trace of Eq. (A3) we obtain

$$\partial_\xi\partial_{\bar\xi}[\log \mathrm{Det}|M_k|^2] = \mathrm{Tr}(|M_{k+1}|^2|M_k|^{-2}) - \mathrm{Tr}(|M_k|^2|M_{k-1}|^{-2}), \tag{A4}$$

i.e., our recurrence relations for $\mathrm{Tr}(|M_k|^2|M_{k-1}|^{-2})$.

Next, if $D_k = \mathrm{Det}|M_k|^2 \neq 0$ in the whole complex plane C then by applying Stokes' theorem in the plane to (A4), i.e.,

$$\int \mathrm{d}\xi\,\mathrm{d}\bar\xi(\psi)_{\bar\xi\xi} = \frac{1}{2}\oint_{|\xi|\to\infty}[\mathrm{d}\bar\xi\,\psi_{\bar\xi} - \mathrm{d}\xi\,\psi_\xi], \tag{A5}$$

we obtain

$$\frac{i}{4\pi}\oint_{|\xi|\to\infty}\left[\mathrm{d}\bar\xi\frac{\partial_{\bar\xi}D_k}{D_k} - \mathrm{d}\xi\frac{\partial_\xi D_k}{D_k}\right] = \mathcal{N}_k - \mathcal{N}_{k-1}. \tag{A6}$$

Thus, if ω_k is the highest degree of $|\xi|^2$ in D_k, i.e., $\lim_{|\xi|\to\infty} D_k \to |\xi|^{2\omega_k}$, then (A6) reduces to the following simple recurrence relations for $\mathcal{N}_k$, i.e.:

$$\omega_k = \mathcal{N}_k - \mathcal{N}_{k-1}. \tag{A7}$$

However, if $D_k = 0$ at some points, these recurrence relations cease to hold.

APPENDIX B: REDUCED FORMULA FOR EVALUATING Tr($[|M_{k+1}|^2|M_k|^{-2}]^2$)

In this appendix, we derive a formula for simplifying the calculation of the trace in $\mathcal{I}$ for the case $n=2$. Using the formula,

$$\mathrm{Tr}(H^2)=(\mathrm{Tr}H)^2-2\,\mathrm{Det}\,H, \tag{B1}$$

which is true for any (2×2) matrix H we note that for $D_k=\mathrm{Det}|M_k|^2\neq 0$, we have

$$\mathrm{Tr}([|M_{k+1}|^2|M_k|^{-2}]^2)=(\mathrm{Tr}[|M_{k+1}|^2|M_k|^{-2}])^2-2\,\frac{D_{k+1}}{D_k}. \tag{B2}$$

Thus, if $D_{k+1}=0$, then from (B2) we have

$$\mathrm{Tr}([|M_{k+1}|^2|M_k|^{-2}]^2)=(\mathrm{Tr}[|M_{k+1}|^2|M_k|^{-2}])^2. \tag{B3}$$

APPENDIX C: CONDITION (84) FROM THE SU(N) CHIRAL MODELS

To simplify our search for finding a condition for exact solution of the SU(N) Skyrme model Eqs. (77), in this appendix, we look at the corresponding SU(N) chiral model equations,

$$\partial_r(r^2L_r)+\frac{(1+|\xi|^2)^2}{2}(\partial_{\bar{\xi}}L_{\xi}+\partial_{\xi}L_{\bar{\xi}})=0, \tag{C1}$$

i.e., (77) without the Skyrme terms. In terms of the rank-n projectors P_k, Eq. (C1), after we have put in (25) and (78), becomes

$$\sum_{k=0}^{\lambda-1}\left[\left(P_k-\frac{nI}{N}\right)\partial_r(r^2\dot{g}_k)+(1+|\xi|^2)^2\sin F_k(M_{l+1}|M_l|^{-2}Mk_{l+1}^{\dagger}-M_l|M_l|^{-2}|M_{l+1}|^2|M_l|^{-2}M_l^{\dagger})\right]$$
$$=0, \tag{C2}$$

where $F_k=g_k-g_{k+1}$, $g_\lambda=0$.

Next we multiply Eq. (C2) from the right by M_s, and noting that M_s are independent matrix fields, we obtain

$$\partial_r\left[r^2\left(\dot{g}_s-\frac{n}{N}\sum_{k=0}^{\lambda-1}\dot{g}_k\right)\right]I_n+(1+|\xi|^2)^2(|M_{s-1}|^{-2}|M_s|^2\sin F_{s-1}-|M_s|^{-2}|M_{s+1}|^2\sin F_s)=0. \tag{C3}$$

Finally, summing over s from 0 to l, and noting that $M_{-1}=0$ (by definition), we find that (C3) gives us

$$\partial_r\left[r^2\left(\sum_{p=0}^{l}\sum_{q=p}^{\lambda-1}\dot{F}_q-\frac{n(l+1)}{N}\sum_{p=0}^{\lambda-1}(p+1)\dot{F}_p\right)\right]I_n-(1+|\xi|^2)^2|M_l|^{-2}|M_{l+1}|^2\sin F_l=0. \tag{C4}$$

Thus, in order to have a compatible and a consistent set of equations for the functions F_l in (C4), the matrices M_l must satisfy

$$|M_l|^{-2}|M_{l+1}|^2=\mathcal{K}_l(1+|\xi|^2)^{-2}I_n, \tag{C5}$$

i.e., condition (84).

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A parabolic approximation method with application to global wave propagation

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Motivated by the difficulty in using the splitting matrix method to obtain parabolic approximations to complicated wave equations, we have developed an alternative method. It is three dimensional, does not *a priori* assume a preferred direction or path of propagation in the horizontal, determines spreading factors, and results in equations that are energy conserving. It is an extension of previous work by several authors relating parabolic equations to the horizontal ray acoustics approximation. Unlike previous work it applies the horizontal ray acoustics approximation to the propagator rather than to the Green's function or the homogenous field. The propagator is related to the Green's function by an integral over the famous ''fifth parameter'' of Fock and Feynman. Methods for evaluating this integral are equivalent to narrow-angle approximations and their wide-angle improvements. When this new method is applied to simple problems it gives the standard results. In this paper it is described by applying it to a problem of current interest—the development of a parabolic approximation for modeling global underwater and atmospheric acoustic propagation. The oceanic or atmospheric waveguide is on an Earth that is modeled as an arbitrary convex solid of revolution. The method results in a parabolic equation that is energy conserving and has a spreading factor that describes field intensification for antipodal propagation. Significantly, it does not have the singularities in its range-sliced version possessed by many parabolic equations developed for global propagation. We then discuss two extensions of the method; first to propagation along refracted geodesics and second to a description involving discrete, local, normal modes. [DOI: 10.1063/1.1458060]

I. INTRODUCTION

In the years following the introduction of the parabolic equation method and the split-step Fourier algorithm to wave propagation [Tappert and Hardin (1973); Hardin and Tappert (1973)], a great deal of work was done not only in applying it to propagation problems in the ocean and atmosphere but also in developing improvements on the method. Approximations and computational schemes were developed that more realistically account for the characteristics of the propagation medium and its boundaries and reduce the restriction to narrow-angle propagation. Fortunately several excellent early [Tappert (1977)] and recent [Brekhovskikh and Godin (1999); Lee and Pierce (1995)] reviews are available since the literature is too large to provide citations to all the relevant work.

A common technique for deriving the standard parabolic equation and improvements to it has been the splitting matrix method where a wave equation is factored into two contributions representing forward and backward propagating waves. This method was first developed by Bremmer (1951) for the one-dimensional problem and the latter generalized to three dimensions by Corones (1975) and Tappert (1977). In this approach it is assumed a particular direction in the ocean

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medium is singled out by the nature of the source excitation and the dominant portion of the acoustic energy propagates in this direction without significant backscatter. For a discussion of this point of view, see Corones, DeFacio, and Krueger (1982). The square-root differential operator in the forward-propagating one is then approximated in some fashion to obtain a useful parabolic equation. Many times this approximation is done so as to reduce the dependence of the solution on the reference wave speed thus relaxing the narrow-angle approximation. The appropriate mathematical formalism for analysis of the one-way equation is in terms of pseudodifferential and Fourier integral operators. For a review, see Fishman (1992), where this mathematical formalism is applied to various equations having an index of refraction quadratic in a subset of the coordinate variables.

Most of these early studies applied the parabolic approximation to the Helmholtz equation

$$[\nabla^2 + k_0^2 n^2(\vec{x})]\, p(\vec{x}) = 0 \tag{1}$$

in Cartesian coordinates. Here a source radiates at angular frequency ω, where $k_0 = \omega/c_0$ with c_0 some reference wave speed, $n(\vec{x}) = c_0/c(\vec{x})$ is the index of refraction, and $c(\vec{x})$ is the wave speed at the point $\vec{x} = (x,y,z)$ in the medium. Sometimes the Laplacian was modified to account for a variable density field, $\nabla^2 \to \rho(\vec{x})\vec{\nabla}\cdot((1/\rho(\vec{x}))\vec{\nabla})$, and sometimes currents were included by introducing an effective wave speed equal to the actual speed shifted by the component of the current in the direction of propagation.

When one considers more complicated wave equations, however, progress has been slow in developing useful parabolic approximations using the splitting matrix method. We illustrate this with three examples. First is the problem of obtaining parabolic approximations to the elastic wave equation [Corones, DeFacio, and Krueger (1982); Hudson (1980); Landers and Claerbout (1972); Wales and McCoy (1983); Greene (1985); Wetton and Brooke (1990); Collins (1991); Collins (1993a)]. Although considerable effort has been devoted to this problem, parabolic equations have only been developed under limiting conditions that include consideration of a two-dimensional rather than a three-dimensional medium, Lamé parameters that are range independent or have very small spatial gradients, or very special types of propagation.

Second is the problem of obtaining parabolic equations for propagation in a moving inhomogeneous fluid. As a result of the work by Brekhovskikh and Godin (1999) and Godin (1987), it is now known that many of the earlier approximations, including the use of an effective wave speed, cannot adequately account for the effects of the motion in many important and practical situations. The appropriate wave equation, correct to first order in the Mach number, is complicated and considerable ingenuity has been devoted developing parabolic approximations that are wide angle, conserve energy, obey the flow reversal theorem and boundary conditions consistent with the parabolic approximation (a requirement ignored in most studies) [Godin (1991); Godin and Mokhov (1992); Godin (1998a); (1998b); (1999)]. Most progress on this problem was obtained using the multiple-scales approach (see the following) rather than with the splitting matrix method because of the problems associated with the splitting matrix method discussed here (Godin, private conversation).

A final example is the problem of developing parabolic approximations for wave equations in curvilinear coordinates with the purpose of modeling global wave propagation [Collins (1993b); McDonald *et al.* (1994); Collins *et al.* (1995a); (1995b); (1996)]. It is common to reduce the problem to a two-dimensional one by introducing local normal modes and by ignoring, to some degree, mode coupling. The matrix splitting method is then applied to the resulting equation in the horizontal coordinates to obtain a forward-propagating parabolic equation. The range-sliced version of this equation, needed to obtain a marching algorithm, has singularities [Collins *et al.* (1996)]. These singularities result from the fact that the commutators in the Baker–Campbell–Hausdorff formula used to develop the range-sliced expression cannot be dropped for small range intervals. They actually become more singular with order, regardless of the size of the range interval. The range-sliced marching algorithm, as well as the closely-related range-sliced path integral representation, are only valid in Cartesian coordinates. This point has been discussed in

detail by Kleinert (1995), who refers to this type of singularity as ''path collapse'' and who has developed techniques for dealing with it by scaling variables. These scaling techniques are only now being applied to wave propagation problems. This problem of singularities would exist even if the three-dimensional wave equation had been considered rather than the reduced two-dimensional one.

For these complicated wave equations, the splitting matrix method is not very easy to apply. It is not always obvious how the factorization should be done nor is it obvious how the resulting differential operators should be approximated to obtain wide-angle equations. Normalizations and spreading factors are not easy to obtain. [The quantity $1/\sqrt{r}$ in Eq. (2) in the following is a spreading factor.] With few exceptions, e.g., Tappert, Spiesberger, and Boden (1995), studies that use the splitting matrix method ignore the determination of the spreading factor.

It seems worthwhile then to consider new approaches to developing parabolic approximations that might have application to complicated wave equations. In developing them we are guided by four principles (prejudices actually).

(A) One should start with equations that are three dimensional. By starting with two-dimensional equations one has already made an assumption about the nature of the propagation. One has assumed there is no significant scattering of the wave field out of the surface defined by the two coordinates. If this is a valid assumption, it should be a consequence of the process of making the parabolic approximation and not something imposed on the problem from the outset and considered as a separate, unjustified approximation. One should also not approach the three-dimensional problem by patching together solutions to the two-dimensional one. One should be able to start with the three-dimensional problem and show that its solution can be written, with appropriate approximations, in terms of solutions to the two-dimensional problem if this patching process is valid.

(B) One should not assume any preferred horizontal direction or path for the propagation. In Corones, DeFacio and Krueger (1982), one reads, ''*...the parabolic approximation is used when a particular direction is singled out in the medium by the nature of the excitation*..... *The direction is distinguished by the excitation, not by the medium*.'' While this statement may be valid for laser propagation through the atmosphere where the radiation is emitted in a narrow beam, it cannot be valid in general. In particular, it cannot be valid for low-frequency sound propagation in the ocean because low-frequency sources (excitations) are essentially omnidirectional. It is possible for either the source or the medium to determine a preferred direction. In this paper we consider that class of problems for which the preferred direction or path, if it exists, is determined by the characteristics of the medium and defined in the process of making the parabolic approximation.

When one writes a wave equation in terms of cylindrical coordinates (r,φ,z) and discards derivatives with respect to φ, one has already assumed a preferred direction. It is the direction of the straight line along the radial connecting the source to the receiver. When one writes

$$p(r,\varphi,z)=\frac{e^{ik_0 r}}{\sqrt{r}}\psi(r,\varphi,z) \tag{2}$$

for the pressure field and assumes ψ varies slowly with r, one has also defined a preferred direction. This is an important point because more complicated wave equations may not have a preferred direction along the radial but in some other direction in the horizontal plane. If horizontal multipaths are present the preferred direction is not unique or it is undefined.

(C) The approach should provide a way for determining spreading factors. While for some applications spreading factors are not important, it is difficult to imagine a systematic, general method for developing parabolic equations that only determines part of the field.

(D) A general parabolic approximation method should consist of two distinct types of approximations: those related to horizontal variation; a preferred direction of propagation along a horizontal multipath, no backscattering, no out-of-plane propagation, etc., and those related to vertical variation; narrow-angle and wide-angle approximations. When one considers the application of the parabolic method to simple problems these two types of approximations are distinct. For example,

only the first type is needed to develop a parabolic equation for the propagation of a single adiabatic mode in a range-dependent waveguide while only the second type is needed for propagation of a field in a range-independent waveguide described by a modal sum. One might expect that a method applicable to more complicated problems as well as these simple ones would not mix the two types of approximations.

In developing an alternative to the splitting matrix method based on the above-mentioned considerations we are motivated by three observations. First, by working order-by-order in perturbation theory in the range-dependent part of the index of refraction, it was found many years ago [Palmer (1976)] that the solution to the Helmhotz equation can be written in terms of the solution to the standard parabolic equation by making a horizontal eikonal approximation followed by the stationary-phase approximation of an integral over the ''fifth parameter'' of Fock (1937) and Feynman (1951). The stationary-phase approximation was shown to be equivalent to the narrow-angle approximation. A completely different approach, based on the use of path integrals rather than perturbation theory, gave the same result [Palmer (1979)]. (In this case, horizontal ray theory was assumed rather than the closely related horizontal eikonal approximation.) Second, an alternative to the splitting matrix method is the method of multiple scales in which the horizontal variables are scaled differently from the depth variable [Tappert (1977); Siegmann, Kreigsmann, and Lee (1985); Kreigsmann (1985); Orchard, Siegmann, and Jacobson (1992)]. This method leads to the factorization of the field into a function that obeys the parabolic equation (e.g., ψ) and a kinematic factor that is dependent on only the horizontal coordinates [e.g., $\exp(ik_0 r)/\sqrt{r}$]. The multiple scales method is closely related to the method used by Brekhovskikh and Godin (1999, Sec. 7.2) to develop horizontal ray theory for a weakly range-dependent, three-dimensional medium. Finally, it is well known that there is a close relationship between ray theory (geometric optics) and parabolic equations [Myers and McAninch (1978); McAninch (1986); Babič and Buldyrev (1991), Chap. 6].

The method we propose then amounts to a horizontal ray theory approximation followed by the approximation of the integral over the Fock–Feynman parameter. It satisfies the four principles we discussed previously. Its validity is based on the fact that horizontal scales of variability in the ocean and atmosphere are much greater than vertical ones. The only aspect of this method that is different from what others have done is that we apply the horizontal ray theory approximation not to the wave equation but to the equation satisfied by the propagator. The two are related by an integral over the Fock–Feynman parameter. This is the key aspect of the method because this propagator obeys (exactly) a four-coordinate parabolic equation. Approximations such as the horizontal ray theory approximation essentially reduce its dimensionality.

Our procedure then for developing parabolic approximations is to express the solution to the wave equation as a one-dimensional integral transform and to apply the horizontal ray acoustics approximation to the transform function. It is worth noting that the work by Klauder (1987), and earlier, Maslov and Fedoriuk (1981) demonstrates that this procedure also has great advantage in avoiding the caustic singularities associated with the ray acoustics approximation, which in a quantum mechanic context is referred to as the semiclassical approximation.

In this paper we apply this method to the problem of developing a parabolic approximation for the wave equation in curvilinear coordinates appropriate for modeling global wave propagation. Our primary interest is acoustic propagation in the ocean although the analysis has application to ultrasonic propagation in the atmosphere. We do not assume the Earth is spherical or even ellipsoidal but only that it is a convex solid of revolution.

This paper is organized as follows. In Sec. II we characterize the waveguide on an Earth modeled as a solid of revolution. In Sec. III the propagator for the Helmholtz equation (modified to include a depth-dependent density variation) and the Fock–Feynman parameter are introduced. In Sec. IV we factor the propagator and apply the horizontal ray theory approximation. The eikonal and transport equations are derived and solved. We provide a detailed solution to the transport equation that determines the spreading factor for this problem. Section V treats the vertical equation and the stationary phase approximation. When applied to the simple Helmhotz equation in Cartesian coordinates it produces the standard narrow-angle parabolic equation. In

many situations one wants to do better. One extension would be to include the possibility of horizontal refraction and horizontal multipaths. Another extension would be the description of the depth dependence of the pressure field by use of normal modes. Section VI contains a discussion of these possibilities. Finally, in Sec. VII we summarize the approach used in the paper.

II. THE EARTH AS A SOLID OF REVOLUTION

The Earth is assumed to be a solid of revolution with, when viewed from space, a convex surface everywhere. The origin of the Cartesian coordinate system is centered in the Earth with the axis of rotation the z axis. The position vector from the origin of this coordinate system to a point on the Earth's surface is

$$\vec{x}_S = x_S\hat{x} + y_S\hat{y} + z_S\hat{z}, \tag{3}$$

where $\hat{x}$, $\hat{y}$, and $\hat{z}$ are unit vectors along the coordinate axes. Since the axis of rotation is the z axis, one can write

$$x_S = \rho_S(\varphi_g)\cos\lambda,$$

$$y_S = \rho_S(\varphi_g)\sin\lambda$$

where φ_g is the *geocentric latitude*

$$\varphi_g \equiv \arctan\left(\frac{z_S}{\sqrt{x_S^2+y_S^2}}\right)$$

and λ is the longitude.

Consider the directed line segment from the point on the surface with coordinates (φ_g,λ) to the nearby point $(\varphi_g+\delta\varphi_g,\lambda+\delta\lambda)$,

$$\delta\vec{x}_S = \delta x_S\hat{x} + \delta y_S\hat{y} + \delta z_S\hat{z}, \tag{4}$$

where $\delta x_S = x_S(\varphi_g+\delta\varphi_g,\lambda+\delta\lambda) - x_S(\varphi_g,\lambda)$, etc. To second order in the quantities $\delta\varphi_g$ and $\delta\lambda$ we have

$$\begin{aligned}
\delta x_S &= \rho_S'\cos\lambda\,\delta\varphi_g - \rho_S\sin\lambda\,\delta\lambda \\
&\quad + \tfrac{1}{2}\rho_S''\cos\lambda(\delta\varphi_g)^2 - \tfrac{1}{2}\rho_S\cos\lambda(\delta\lambda)^2 - \rho_S'\sin\lambda\,\delta\varphi_g\delta\lambda, \\
\delta y_S &= \rho_S'\sin\lambda\,\delta\varphi_g + \rho_S\cos\lambda\,\delta\lambda \\
&\quad + \tfrac{1}{2}\rho_S''\sin\lambda(\delta\varphi_g)^2 - \tfrac{1}{2}\rho_S\sin\lambda(\delta\lambda)^2 + \rho_S'\cos\lambda\,\delta\varphi_g\delta\lambda, \\
\delta z_S &= z_S'\delta\varphi_g + \tfrac{1}{2}z_S''(\delta\varphi_g)^2,
\end{aligned}$$

where a prime indicates differentiation with respect to φ_g. The terms linear in the infinitesimals are used to derive expressions for unit vectors and the quadratic terms are used to derive expressions for radii of curvature.

The unit vector tangent to the surface and in the direction of increasing λ is

$$\hat{\lambda} = \frac{\partial\vec{x}_S}{\partial\lambda} \Big/ \left|\frac{\partial\vec{x}_S}{\partial\lambda}\right| = -\sin\lambda\,\hat{x} + \cos\lambda\,\hat{y}. \tag{5}$$

It is convenient to define a second unit vector in the $x-y$ plane orthogonal to $\hat{\lambda}$,

$$\hat{\rho}_S = \cos\lambda\,\hat{x} + \sin\lambda\,\hat{y}. \tag{6}$$

The unit vector tangent to the surface in the direction of increasing φ_g is

$$\hat{\varphi}_g = \frac{\partial \vec{x}_S}{\partial \varphi_g} \Big/ \left|\frac{\partial \vec{x}_S}{\partial \varphi_g}\right| = \frac{\rho_S' \hat{\rho}_S + z_S' \hat{z}}{\xi} \tag{7}$$

with

$$\xi \equiv \sqrt{(\rho_S')^2 + (z_S')^2}. \tag{8}$$

Finally, the unit vector normal to the surface is

$$\hat{n} = \hat{\lambda} \times \hat{\varphi}_g = \frac{z_S' \hat{\rho}_S - \rho_S' \hat{z}}{\xi}. \tag{9}$$

In terms of these unit vectors we have

$$\vec{x}_S = \rho_S(\varphi_g)\hat{\rho}_S + z_S(\varphi_g)\hat{z}, \tag{10}$$

$$\hat{x}_S = \frac{\vec{x}_S}{|\vec{x}_S|} = \cos\varphi_g \hat{\rho}_S + \sin\varphi_g \hat{z}, \tag{11}$$

and

$$\begin{aligned}\delta\vec{x}_S = {} & \xi\,\delta\varphi_g \hat{\varphi}_g + (\rho_S + \rho_S'\delta\varphi_g)\,\delta\lambda\,\hat{\lambda} \\ & + \frac{1}{2\xi}[(\rho_S'\rho_S'' + z_S' z_S'')(\delta\varphi_g)^2 - \rho_S \rho_S'(\delta\lambda)^2]\hat{\varphi}_g \\ & + \frac{1}{2\xi}[(z_S'\rho_S'' - \rho_S' z_S'')(\delta\varphi_g)^2 - \rho_S z_S'(\delta\lambda)^2]\hat{n}.\end{aligned} \tag{12}$$

The differential line segment tangent to the surface is

$$\mathrm{d}\vec{x}_S = \xi\,\mathrm{d}\varphi_g\,\hat{\varphi}_g + \rho_S\,\mathrm{d}\lambda\,\hat{\lambda} \tag{13}$$

and the differential arc length is

$$\mathrm{ds} \equiv |d\vec{x}_S| = \sqrt{\xi^2(\mathrm{d}\varphi_g)^2 + \rho_S^2(\mathrm{d}\lambda)^2}. \tag{14}$$

At a point on the surface (φ_g, λ), there are two principal radii of curvature; the *meridional*, describing curvature in the $\hat{\varphi}_g - \hat{n}$ plane and the *prime vertical*, describing curvature in the $\hat{\lambda} - \hat{n}$ plane. We discuss first the meridional. Consider two points in the meridional plane at (φ_g, λ) and at $(\varphi_g + \delta\varphi_g, \lambda)$. The directed line segment from the first point to the second can be written as

$$\delta\vec{x}_S = \delta x_\varphi \hat{\varphi}_g + \delta x_n \hat{n}. \tag{15}$$

The meridional radius of curvature μ is given by

$$\mu = -\frac{1}{2}\,\mathrm{Lim}_{\delta\varphi_g \to 0}\frac{(\delta x_\varphi)^2}{\delta x_n} \tag{16}$$

provided the limit exists. If $\mu>0$ the surface is convex at the point (φ_g,λ) with respect to the origin (like a sphere's outer surface) and if $\mu<0$ the surface is concave. By setting $\delta\lambda=0$ in Eq. (12) we find

$$\delta x_\varphi=\xi\delta\varphi_g+\frac{1}{2\xi}(\rho_S'\rho_S''+z_S'z_S'')(\delta\varphi_g)^2$$

and

$$\delta x_n=\frac{1}{2\xi}(z_S'\rho_S''-\rho_S'z_S'')(\delta\varphi_g)^2.$$

Substituting into Eq. (16) gives

$$\mu=\frac{\xi^3}{\rho_S'z_S''-z_S'\rho_S''}. \tag{17}$$

The prime vertical radius of curvature is determined in a similar fashion to be

$$\nu=\frac{\rho_S\xi}{z_S'}. \tag{18}$$

The differential line segment, Eq. (13), can now be written

$$d\vec{x}_S=\frac{\mu}{\xi^2}(\rho_S'z_S''-z_S'\rho_S'')d\varphi_g\,\hat{\varphi}_g+\frac{\nu z_S'}{\xi}d\lambda\,\hat{\lambda}. \tag{19}$$

The geocentric latitude is the angle between the position vector and the equatorial plane

$$\varphi_g=\arcsin(\hat{x}_S\cdot\hat{z}). \tag{20}$$

The *geodetic latitude* φ is defined to be the angle the normal to the surface makes with respect to the equatorial plane

$$\varphi=\arcsin(\hat{n}\cdot\hat{z}). \tag{21}$$

Clearly

$$\sin\varphi=-\frac{\rho_S'}{\xi},\quad \cos\varphi=\frac{z_S'}{\xi}. \tag{22}$$

The geocentric and geodetic latitudes are equal only if the Earth is modeled as a sphere. In terms of the geodetic latitude,

$$\hat{\varphi}_g=-\sin\varphi\hat{\rho}_S+\cos\varphi\hat{z}$$

and

$$\hat{n}=\cos\varphi\hat{\rho}_S+\sin\varphi\hat{z}.$$

From Eq. (13),

$$\frac{d\vec{x}_S}{d\varphi}=\frac{\xi}{\varphi'}\hat{\varphi}_g,$$

so

$$\hat{\varphi} = \pm \hat{\varphi}_g , \tag{23}$$

where the sign is determined by the sign of $\varphi' = d\varphi/d\varphi_g$ since $\xi > 0$. This derivative can be expressed in terms of the derivatives of ρ_S and z_S by differentiating both sides of the equation $\tan\varphi = -\rho_S'/z_S'$ with respect to φ_g. That is

$$\varphi' = -\frac{\sin\varphi z_S'' + \cos\varphi \rho_S''}{\xi} = \frac{\rho_S' z_S'' - \rho_S'' z_S'}{\xi^2}$$

or

$$\mu\varphi' = \xi. \tag{24}$$

We are assuming the Earth has a convex surface everywhere, $\mu > 0$. Therefore $\varphi' > 0$, $\hat{\varphi} = \hat{\varphi}_g$, and there is a one-to-one relationship between the two latitudes enabling us to replace φ_g with φ as the independent variable. This is an advantage since geophysical data are referenced to the geodetic rather than the geocentric latitude.

The basic coordinate transformation equations can be rewritten as

$$x_S = \nu \cos\varphi \cos\lambda, \tag{25}$$

$$y_S = \nu \cos\varphi \sin\lambda, \tag{26}$$

$$z_S = \chi \sin\varphi. \tag{27}$$

The differential line segment is

$$d\vec{x}_S = \mu\, d\varphi\, \hat{\varphi} + \nu \cos\varphi\, d\lambda\, \hat{\lambda}. \tag{28}$$

Observing from this relation that

$$\mu^2 = \left| \frac{d\vec{x}_S}{d\varphi} \right|^2$$

we obtain

$$\mu^2 = \left(\frac{d}{d\varphi}(\nu\cos\varphi) \right)^2 + \left(\frac{d}{d\varphi}(\chi\sin\varphi) \right)^2. \tag{29}$$

Since

$$z_S' \sin\varphi + \rho_S' \cos\varphi = 0$$

we have

$$\sin\varphi \frac{d(\chi\sin\varphi)}{d\varphi} + \cos\varphi \frac{d(\nu\cos\varphi)}{d\varphi} = 0.$$

These equations yield

$$\mu = \nu \left| 1 - \frac{\cot\varphi}{\nu} \frac{d\nu}{d\varphi} \right| \tag{30}$$

and the useful relations

$$\frac{\mathrm{d}}{\mathrm{d}\varphi}(\nu\cos\varphi)=-\mu\sin\varphi,\quad \frac{\mathrm{d}}{\mathrm{d}\varphi}(\chi\sin\varphi)=+\mu\cos\varphi. \tag{31}$$

The arclength is

$$\mathrm{d}s=\sqrt{\mu^2(\mathrm{d}\varphi)^2+\nu^2\cos^2\varphi(\mathrm{d}\lambda)^2}. \tag{32}$$

The unit vector directed from the point with coordinates (φ, λ) to the one with coordinates $(\varphi+\mathrm{d}\varphi,\lambda+\mathrm{d}\lambda)$ is

$$\hat{s}=\frac{\mathrm{d}\vec{x}_S}{\mathrm{d}s}=\mu\frac{\mathrm{d}\varphi}{\mathrm{d}s}\hat{\varphi}+\nu\cos\varphi\frac{\mathrm{d}\lambda}{\mathrm{d}s}\hat{\lambda}. \tag{33}$$

The unit vector $\hat{s}$ can also be written in terms of the angle α the differential line segment makes with respect to $\hat{\varphi}$, i.e., the angle between $\mathrm{d}\vec{x}_S$ and "north"

$$\hat{s}=\cos\alpha\hat{\varphi}+\sin\alpha\hat{\lambda}, \tag{34}$$

where $\cos\alpha=\mu(\mathrm{d}\varphi/\mathrm{d}s)$ and $\sin\alpha=\nu\cos\varphi(\mathrm{d}\lambda/\mathrm{d}s)$.

We define

$$R(\varphi)\equiv\sqrt{\mu(\varphi)\nu(\varphi)}. \tag{35}$$

The length $R(\varphi)$ will play an important role in the development of the parabolic approximation. Since the Earth is almost spherical, it is possible to write

$$\frac{1}{R(\varphi)}=\frac{1}{\overline{R}}(1+\eta g(\varphi)), \tag{36}$$

where $\overline{R}$ is the mean radius of the Earth and g is a function of order unity. The small parameter η is a measure of the deviation of the solid from a sphere. If the Earth is taken to be an ellipsoid, η would be the eccentricity squared, $\eta\approx 1/150$ [see, e.g., Dworski and Mercer (1990)].

We summarize here the unit vectors that have been introduced with their differentials. We have

$$\hat{\varphi}=-\sin\varphi\hat{\rho}_S+\cos\varphi\hat{z}, \tag{37}$$

$$\hat{\lambda}=-\sin\lambda\hat{x}+\cos\lambda\hat{y}, \tag{38}$$

$$\hat{n}=\cos\varphi\hat{\rho}_S+\sin\varphi\hat{z}, \tag{39}$$

$$\begin{aligned}\hat{\rho}_S&=\cos\lambda\hat{x}+\sin\lambda\hat{y},\\ &=\cos\varphi\hat{n}-\sin\varphi\hat{\varphi}.\end{aligned} \tag{40}$$

For the differentials we have

$$\mathrm{d}\hat{\varphi}=-\sin\varphi\hat{\lambda}\,\mathrm{d}\lambda-\hat{n}\,\mathrm{d}\varphi, \tag{41}$$

$$\mathrm{d}\hat{\lambda}=-\hat{\rho}_S\,\mathrm{d}\lambda, \tag{42}$$

$$\mathrm{d}\hat{n}=\cos\varphi\hat{\lambda}\,\mathrm{d}\lambda+\hat{\varphi}\,\mathrm{d}\varphi, \tag{43}$$

and

$$d\hat{\rho}_S = \hat{\lambda}\, d\lambda. \tag{44}$$

The position vector to a general point in the ocean, below the surface, is

$$\vec{x} = \vec{x}_S - \zeta \hat{n},$$

where $\vec{x}_S$ is the position vector of the point on the surface directly over the point of interest, ζ ($\geqslant 0$) is the depth at that point. Propagation in the atmosphere can be considered by simply changing the sign of ζ. The differential line element is

$$d\vec{x} = d\vec{x}_S - d\zeta\, \hat{n} - \zeta\, d\hat{n} = (\mu - \zeta) d\varphi\, \hat{\varphi} + (\nu - \zeta)\cos\varphi\, d\lambda \hat{\lambda} - d\zeta\, \hat{n},$$

where we have used Eq. (43). The differential volume element is

$$d^3\vec{x} = (\mu - \zeta)(\nu - \zeta)\cos\varphi\, d\varphi\, d\lambda\, d\zeta.$$

Also

$$\nabla^2 = \frac{1}{(\mu-\zeta)(\nu-\zeta)\cos\varphi} \frac{\partial}{\partial\varphi}\left(\frac{\nu-\zeta}{\mu-\zeta}\cos\varphi \frac{\partial}{\partial\varphi}\right) + \frac{1}{(\mu-\zeta)^2\cos^2\varphi}\frac{\partial^2}{\partial\lambda^2} + \frac{1}{(\mu-\zeta)(\nu-\zeta)}\frac{\partial}{\partial\zeta}\left((\mu-\zeta)(\nu-\zeta)\frac{\partial}{\partial\zeta}\right) \tag{45}$$

and

$$\delta^{(3)}(\vec{x} - \vec{x}_0) = \frac{1}{(\mu-\zeta)(\nu-\zeta)}\delta(\sin\varphi - \sin\varphi_0)\,\delta(\lambda - \lambda_0)\,\delta(\zeta - \zeta_0).$$

In writing these relations we have used the fact that ν and μ are functions of φ but not of λ and ζ. For many problems it is not ∇^2 which is of concern but rather $\rho\nabla\cdot(\rho^{-1}\nabla)$, where ρ is the density of the medium. Because of stratification ρ is usually assumed to depend only on the depth variable ζ. If this is the case, the last term in Eq. (45) is replaced with

$$\frac{\rho(\zeta)}{(\mu-\zeta)(\nu-\zeta)}\frac{\partial}{\partial\zeta}\left(\frac{(\mu-\zeta)(\nu-\zeta)}{\rho(\zeta)}\frac{\partial}{\partial\zeta}\right).$$

In most work on global propagation, a ''thin-medium'' approximation is made. That is, since the thickness or depth of the medium is much less than the radii of curvature, $\zeta \ll \nu$ and $\zeta \ll \mu$, it is valid to replace $\nu - \zeta$ with ν and $\mu - \zeta$ with μ everywhere in the above-mentioned expressions, even before differentiation with respect to ζ or φ. With this approximation, we have

$$d\vec{x} = \mu d\varphi\hat{\varphi} + \nu\cos\varphi\, d\lambda\, \hat{\lambda} - d\zeta\, \hat{n} \tag{46}$$

and

$$d^3\vec{x} = J(\varphi) d\varphi\, d\lambda\, d\zeta, \tag{47}$$

where

$$J(\varphi) \equiv \mu\nu\cos\varphi. \tag{48}$$

Moreover

$$\rho\nabla\cdot(\rho^{-1}\nabla) = \nabla_S^2 + \rho\frac{\partial}{\partial\zeta}\left(\frac{1}{\rho}\frac{\partial}{\partial\zeta}\right), \tag{49}$$

where

$$\nabla_S^2 = \frac{1}{J(\varphi)}\left[\frac{\partial}{\partial\varphi}\left(\frac{\nu\cos\varphi}{\mu}\frac{\partial}{\partial\varphi}\right)+\frac{\mu}{\nu\cos\varphi}\frac{\partial^2}{\partial\lambda^2}\right] \tag{50}$$

and

$$\delta^{(3)}(\vec{x}-\vec{x}_0)=\frac{1}{J(\varphi)}\,\delta(\varphi-\varphi_0)\,\delta(\lambda-\lambda_0)\,\delta(\zeta-\zeta_0). \tag{51}$$

The thin-medium approximation can be relaxed by scaling and redefining the index of refraction, see, e.g., Tappert (1977) or Collins (1993b). If we had done this scaling the analysis would be unchanged; we would have simply ended up with expressions involving the redefined index of refraction.

III. GREEN'S FUNCTION AND THE PROPAGATOR

The equation for G the Green's function or impulse response function for the time-independent problem is

$$\left[\rho(\vec{x})\vec{\nabla}\cdot\left(\frac{1}{\rho(\vec{x})}\vec{\nabla}\right)+k_0^2 n^2(\vec{x})\right]G(\vec{x}|\vec{x}_0)=-\delta^{(3)}(\vec{x}-\vec{x}_0) \tag{52}$$

for a point source located at $\vec{x}_0=(x_0,y_0,z_0)$. The Green's function will also satisfy appropriate boundary conditions at the top and bottom of the ocean or atmosphere. In developing parabolic approximations, many authors begin with the wave equation appropriate for a source-free region of space [e.g., Eq. (1)]. We prefer to begin with Eq. (52) so that a separate analysis is not needed to account for a source. This analysis involves solving for the field on a surface close to the source and then matching boundary conditions on that surface. It should be noted in this regard that general, linear equations for wave propagation were derived in Brekhovskikh and Godin (1999) [Eqs. (4.1.9)–(4.1.11)] by including source terms from the outset.

It is not Green's functions, however, that obey parabolic equations and marching algorithms, but propagators. The two are related by an integral over τ, the Fock–Feynman parameter [Fock (1937); Feynman (1951)]

$$G(\vec{x}|\vec{x}_0)=\frac{i}{2k_0}\int_0^\infty d\tau\, e^{i\tau k_0/2}\Phi(\tau;\vec{x}). \tag{53}$$

The propagator function Φ is defined by

$$\left[2ik_0\frac{\partial}{\partial\tau}+\rho\vec{\nabla}\cdot\left(\frac{1}{\rho}\vec{\nabla}\right)-2k_0^2V(\vec{x})\right]\Phi(\tau;\vec{x})=0,\quad \tau>0, \tag{54}$$

and

$$\mathrm{Lim}_{\tau\to0}\Phi(\tau;\vec{x})=\delta^{(3)}(\vec{x}-\vec{x}_0), \tag{55}$$

where the wave speed variation is

$$V(\vec{x})\equiv-\tfrac{1}{2}[n^2(\vec{x})-1].$$

In terms of the curvilinear coordinates introducted in Sec. II, Eqs. (54) and (55) become

$$\left[2ik_0\frac{\partial}{\partial\tau}+\nabla_S^2+\rho\frac{\partial}{\partial\zeta}\left(\frac{1}{\rho}\frac{\partial}{\partial\zeta}\right)-2k_0^2V(\varphi,\lambda,\zeta)\right]\Phi(\tau;\varphi,\lambda,\zeta)=0 \tag{56}$$

and

$$\mathrm{Lim}_{\tau\to 0}\Phi(\tau;\varphi,\lambda,\zeta)=\frac{1}{J(\varphi)}\,\delta(\varphi-\varphi_0)\,\delta(\lambda-\lambda_0)\,\delta(\zeta-\zeta_0) \tag{57}$$

with ∇_S^2 given by Eq. (50).

IV. HORIZONTAL RAY THEORY

We write Φ as the product of two factors,

$$\Phi=H\Psi, \tag{58}$$

and require that H be independent of the depth coordinate and obey a parabolic equation in the horizontal coordinates

$$\left[2ik_0\frac{\partial}{\partial\tau}+\nabla_S^2\right]H(\tau,\varphi,\lambda)=0, \tag{59}$$

$$\mathrm{Lim}_{\tau\to 0}H(\tau,\varphi,\lambda)=\frac{1}{J(\varphi_0)}\,\delta(\varphi-\varphi_0)\,\delta(\lambda-\lambda_0). \tag{60}$$

As we shall see, the field H will determine spreading factors and the path along which the field Ψ propagates. The field Ψ, on the other hand, will reflect the dynamic effects associated with a variable wave speed. The factorization in Eq. (58) of the solution to a wave equation into functions having different coordinate dependencies has been used by many authors in the development of parabolic approximations [Myers and McAninch (1978); McAninch (1986); Babič and Buldyrev (1991)]. It is analogous to the factorization of the solution to the Helmholtz equation [Eq. (2)] that is often the starting point in the development of the standard parabolic approximation for the two-dimensional propagation problem in range and depth. In the path integral approach [Palmer (1978); (1979)] where it is as easy to develop ray theory approximations in one or two of the three coordinates as in all three, the factorization is not an *ansätz* but rather a consequence of making the horizontal ray theory approximation.

We assume horizontal spatial scales are large enough compared to the wavelength that the ray theory approximation is valid when considering horizontal wave motion. We do not make any assumption about the vertical scales of variability. Following Weinberg's (1962) matrix approach, we write Eq. (59) as a system of first-order equations,

$$\begin{bmatrix} 2ik_0J\partial/\partial\tau & \partial/\partial\varphi & \partial/\partial\lambda \\ \partial/\partial\varphi & -\mu/(\nu\cos\varphi) & 0 \\ \partial/\partial\lambda & 0 & -(\nu\cos\varphi)/\mu \end{bmatrix}\begin{bmatrix} H \\ H_\varphi \\ H_\lambda \end{bmatrix}=0, \tag{61}$$

and assume a common exponential factor

$$\begin{bmatrix} H \\ H_\varphi \\ H_\lambda \end{bmatrix}=\begin{bmatrix} \hat{H} \\ \hat{H}_\varphi \\ \hat{H}_\lambda \end{bmatrix}\exp(ik_0A), \tag{62}$$

so that

$$\begin{bmatrix} 2ik_0J(ik_0\partial A/\partial\tau+\partial/\partial\tau) & ik_0\partial A/\partial\varphi+\partial/\partial\varphi & ik_0\partial A/\partial\lambda+\partial/\partial\lambda \\ ik_0\partial A/\partial\varphi+\partial/\partial\varphi & -\mu/(\nu\cos\varphi) & 0 \\ ik_0\partial A/\partial\lambda+\partial/\partial\lambda & 0 & -\nu\cos\varphi/\mu \end{bmatrix}\times\begin{bmatrix} \hat{H} \\ \hat{H}_\varphi \\ \hat{H}_\lambda \end{bmatrix}=0. \tag{63}$$

Consider one element in the above-presented square array, say the element in the top row and middle column, $ik_0\partial A/\partial\varphi+\partial/\partial\varphi$. This element will contribute to the differential equation the expression

$$\hat{H}\left(ik_0\frac{\partial A}{\partial\varphi}+\frac{\partial\ln\hat{H}}{\partial\varphi}\right).$$

In this matrix approach, the rule for developing the lowest-order ray theory approximation is to ignore in the matrix elements gradients of $\hat{H}$ (or $\hat{H}_\varphi$ and $\hat{H}_\lambda$) in comparison to terms involving k_0 times the corresponding gradients of A. This rule is justified by using the traditional approach, i.e., writing the matrix equation as a single equation, expanding the $\hat{H}$ in a series in $1/k_0$, separating real and imaginary parts, and equating like powers of k_0. It cannot be justified by considering individual matrix elements such as the one above because the terms involving A and $\hat{H}$ are in general complex. In the present case the advantage of using the matrix approach over the traditional approach is that it is very easy to apply the ray theory approximation to individual coordinates.

Applying this rule to Eq. (63), we obtain, in lowest order,

$$\begin{bmatrix} -2k_0^2J\partial A/\partial\tau & ik_0\partial A/\partial\varphi & ik_0\partial A/\partial\lambda \\ ik_0\partial A/\partial\varphi & -\mu/(\nu\cos\varphi) & 0 \\ ik_0\partial A/\partial\lambda & 0 & -\nu\cos\varphi/\mu \end{bmatrix}\begin{bmatrix}\hat{H}\\ \hat{H}_\varphi\\ \hat{H}_\lambda\end{bmatrix}=0 \tag{64}$$

and

$$[\hat{H}\quad\hat{H}_\varphi\quad\hat{H}_\lambda]\begin{bmatrix} 2ik_0J\partial/\partial\tau & \partial/\partial\varphi & \partial/\partial\lambda \\ \partial/\partial\varphi & 0 & 0 \\ \partial/\partial\lambda & 0 & 0 \end{bmatrix}\begin{bmatrix}\hat{H}\\ \hat{H}_\varphi\\ \hat{H}_\lambda\end{bmatrix}=0. \tag{65}$$

Equation (64) gives the *eikonal equation*

$$\frac{\partial A}{\partial\tau}+\frac{1}{2\mu^2}\left(\frac{\partial A}{\partial\varphi}\right)^2+\frac{1}{2\nu^2\cos^2\varphi}\left(\frac{\partial A}{\partial\lambda}\right)^2=0, \tag{66}$$

which determines A. The factor $\hat{H}$ is determined by the *transport equation*

$$\left(\frac{\partial}{\partial\tau}+\frac{1}{\mu^2}\frac{\partial A}{\partial\varphi}\frac{\partial}{\partial\varphi}+\frac{1}{\nu^2\cos^2\varphi}\frac{\partial A}{\partial\lambda}\frac{\partial}{\partial\lambda}\right)\ln\hat{H}^2+\nabla_S^2A=0, \tag{67}$$

which follows from Eq. (65) after Eq. (64) is used to express $\hat{H}_\varphi$ and $\hat{H}_\lambda$ in terms of $\hat{H}$,

$$\hat{H}_\varphi=ik_0\frac{\nu\cos\varphi}{\mu}\frac{\partial A}{\partial\varphi}\hat{H},\quad \hat{H}_\lambda=ik_0\frac{\mu}{\nu\cos\varphi}\frac{\partial A}{\partial\lambda}\hat{H}. \tag{68}$$

The eikonal equation, Eq. (66), is solved in the usual way by introducing ray path coordinates, i.e., auxilliary functions $q_\tau(\sigma)$, $q_\varphi(\sigma)$, $q_\lambda(\sigma)$ and their conjugate momenta $p_\tau(\sigma)$, $p_\varphi(\sigma)$, $p_\lambda(\sigma)$ of a variable σ defined on an interval, $\sigma_0\leqslant\sigma\leqslant\sigma_1$, that satisfy the end-point conditions

$$q_\tau(\sigma_0)=0,\quad q_\tau(\sigma_1)=\tau, \tag{69}$$

$$q_\varphi(\sigma_0)=\varphi_0,\quad q_\varphi(\sigma_1)=\varphi, \tag{70}$$

$$q_\lambda(\sigma_0)=\lambda_0,\quad q_\lambda(\sigma_1)=\lambda, \tag{71}$$

$$p_\tau(\sigma_1)=\frac{\partial A}{\partial \tau}, \tag{72}$$

$$p_\varphi(\sigma_1)=\frac{\partial A}{\partial \varphi}, \tag{73}$$

$$p_\lambda(\sigma_1)=\frac{\partial A}{\partial \lambda}. \tag{74}$$

The initial values for the momenta are picked so that $\mathcal{E}(\sigma_0)=0$ where

$$\mathcal{E}(\sigma)\equiv p_\tau(\sigma)+\frac{1}{2}\frac{1}{h_\varphi^2(\sigma)}(p_\varphi(\sigma))^2+\frac{1}{2}\frac{1}{h_\lambda^2(\sigma)}(p_\lambda(\sigma))^2 \tag{75}$$

is the Hamiltonian function. Here we introduce the notation

$$h_\varphi(\sigma)\equiv\mu(q_\varphi(\sigma)),\quad h_\lambda(\sigma)\equiv\nu(q_\varphi(\sigma))\cos(q_\varphi(\sigma)). \tag{76}$$

The eikonal equation is equivalent to $\mathcal{E}(\sigma_1)=0$ and will be satisfied provided

$$\frac{\mathrm{d}\mathcal{E}(\sigma)}{\mathrm{d}\sigma}=0.$$

This condition, in turn, is assured if the path variables satisfy Hamilton's equations

$$\frac{\mathrm{d}q_\tau}{\mathrm{d}\sigma}=1, \tag{77}$$

$$\frac{\mathrm{d}q_\varphi}{\mathrm{d}\sigma}=\frac{1}{h_\varphi^2}p_\varphi, \tag{78}$$

$$\frac{\mathrm{d}q_\lambda}{\mathrm{d}\sigma}=\frac{1}{h_\lambda^2}p_\lambda \tag{79}$$

and

$$\frac{\mathrm{d}p_\tau}{\mathrm{d}\sigma}=0, \tag{80}$$

$$\frac{\mathrm{d}p_\varphi}{\mathrm{d}\sigma}=-\frac{1}{2}\left[\frac{\partial}{\partial q_\varphi}\left(\frac{1}{h_\varphi^2}\right)p_\varphi^2+\frac{\partial}{\partial q_\varphi}\left(\frac{1}{h_\lambda^2}\right)p_\lambda^2\right], \tag{81}$$

$$\frac{\mathrm{d}p_\lambda}{\mathrm{d}\sigma}=0. \tag{82}$$

From Eqs. (69) and (77) we have

$$q_\tau(\sigma)=\sigma-\sigma_0,\quad \sigma_1-\sigma_0=\tau. \tag{83}$$

In general, the eikonal A is given by the integral

$$A=\int_{\sigma_0}^{\sigma_1}\mathrm{d}\sigma\left[p_\tau\frac{\mathrm{d}q_\tau}{\mathrm{d}\sigma}+p_\varphi\frac{\mathrm{d}q_\varphi}{\mathrm{d}\sigma}+p_\lambda\frac{\mathrm{d}q_\lambda}{\mathrm{d}\sigma}\right]. \tag{84}$$

According to Eqs. (77)–(80), this integral can be rewritten as

$$A=\tau p_\tau+\int_{\sigma_0}^{\sigma_1}\mathbf{v}^2\,\mathrm{d}\sigma, \tag{85}$$

where

$$\mathbf{v}=\frac{\mathrm{d}s}{\mathrm{d}\sigma}=\sqrt{\frac{1}{h_\varphi^2}p_\varphi^2+\frac{1}{h_\lambda^2}p_\lambda^2}. \tag{86}$$

Because $\mathcal{E}=0$,

$$-2p_\tau=\mathbf{v}^2=\text{constant}.$$

Therefore

$$A=-\tau p_\tau. \tag{87}$$

Consider now the path length

$$s(\sigma)=\int_{\sigma_0}^{\sigma}\mathrm{d}s=\int_{\sigma_0}^{\sigma}\mathbf{v}(\sigma')\mathrm{d}\sigma'=(\sigma-\sigma_0)\sqrt{-2p_\tau}\,. \tag{88}$$

Equation (87) becomes

$$A=\frac{S^2}{2\tau}. \tag{89}$$

Here $S=s(\sigma_1)$ is the total path length along the ray path. This expression gives the functional dependence of A on τ since S is independent of τ.

Consider a function $f=f(q_\tau,q_\varphi,q_\lambda,\zeta)$ of the depth variable ζ and the path variables. The derivative of f along the path is

$$\frac{\mathrm{d}f}{\mathrm{d}\sigma}=\frac{\mathrm{d}q_\tau}{\mathrm{d}\sigma}\frac{\partial f}{\partial q_\tau}+\frac{\mathrm{d}q_\varphi}{\mathrm{d}\sigma}\frac{\partial f}{\partial q_\varphi}+\frac{\mathrm{d}q_\lambda}{\mathrm{d}\sigma}\frac{\partial f}{\partial q_\lambda}=\frac{\partial f}{\partial q_\tau}+\frac{1}{h_\varphi^2}p_\varphi\frac{\partial f}{\partial q_\varphi}+\frac{1}{h_\lambda^2}p_\lambda\frac{\partial f}{\partial q_\lambda}.$$

If this expression is evaluated at the end point $\sigma=\sigma_1$, we have

$$\frac{\mathrm{d}f}{\mathrm{d}\sigma}\Big|_{\sigma=\sigma_1}=\frac{\partial f(\tau,\varphi,\lambda,\zeta)}{\partial\tau}+\frac{1}{\mu^2}\frac{\partial A}{\partial\varphi}\frac{\partial f(\tau,\varphi,\lambda,\zeta)}{\partial\varphi}+\frac{1}{\nu^2\cos^2\varphi}\frac{\partial A}{\partial\lambda}\frac{\partial f(\tau,\varphi,\lambda,\zeta)}{\partial\lambda}. \tag{90}$$

One can change the independent variable in the ray paths from σ to the path length s since $\mathbf{v}(s)=\mathrm{d}s/\mathrm{d}\sigma$ does not change sign. It is, in fact, a constant equal to S/τ. Equation (88) is first solved for σ in terms of s,

$$\sigma(s)=\sigma_0+\int_0^s\frac{1}{\mathbf{v}}\mathrm{d}s'=\sigma_0+s\frac{\tau}{S} \tag{91}$$

and new ray path coordinates are introduced

$$\tau_{\mathrm{ray}}(s)\equiv q_\tau(\sigma(s)),$$

$$\varphi_{\mathrm{ray}}(s)\equiv q_\varphi(\sigma(s)),$$

$$\lambda_{\mathrm{ray}}(s)\equiv q_\lambda(\sigma(s))$$

defined on the interval, $0 \leqslant s \leqslant S$, that satisfies the same end-point conditions satisfied by q_τ, q_φ, and q_λ. In terms of these new path variables, a function $f(s,\zeta)=f(\tau_{\text{ray}}(s),\varphi_{\text{ray}}(s),\lambda_{\text{ray}}(s),\zeta)$ has a derivative with respect to path length given by

$$\mathbf{v}\frac{\partial f}{\partial s}=\left[\frac{\mathrm{d}q_\tau}{\mathrm{d}\sigma}\frac{\partial f}{\partial \tau_{\text{ray}}}+\frac{\mathrm{d}q_\varphi}{\mathrm{d}\sigma}\frac{\partial f}{\partial \varphi_{\text{ray}}}+\frac{\mathrm{d}q_\lambda}{\mathrm{d}\sigma}\frac{\partial f}{\partial \lambda_{\text{ray}}}\right],$$

where the derivatives with respect to σ are evaluated at $\sigma(s)$. At the end point of the path this expression becomes

$$\frac{S}{\tau}\left[\frac{\partial f}{\partial s}\right]_{s=S}=\frac{\partial f(\tau,\varphi,\lambda,\zeta)}{\partial \tau}+\frac{1}{\mu^2}\frac{\partial A}{\partial \varphi}\frac{\partial f(\tau,\varphi,\lambda,\zeta)}{\partial \varphi}+\frac{1}{\nu^2\cos^2\varphi}\frac{\partial A}{\partial \lambda}\frac{\partial f(\tau,\varphi,\lambda,\zeta)}{\partial \lambda}. \tag{92}$$

We have reverted to using a partial derivative on the left-hand side of this equation to remind ourselves that f can be a function of depth as well as of the path variables. By making this change in the independent variable, we will end up with equations that, unlike Eqs (59) and (67), involve τ as a parameter rather than as an independent variable, thus simplifying the evaluation of Eq. (53).

The unit vector along the ray path can be constructed from Eq. (33),

$$\hat{s}(\sigma)=\left(h_\varphi(\sigma)\frac{\mathrm{d}q_\varphi(\sigma)}{\mathrm{d}\sigma}\hat{\varphi}+h_\lambda(\sigma)\frac{\mathrm{d}q_\lambda(\sigma)}{\mathrm{d}\sigma}\hat{\lambda}\right)\Big/\frac{\mathrm{d}s}{\mathrm{d}\sigma}, \tag{93}$$

which at the end point of the path becomes

$$\frac{S}{\tau}\hat{s}(\sigma_1)=\frac{1}{\mu^2}\frac{\partial A}{\partial \varphi}\hat{\varphi}+\frac{1}{\nu^2\cos^2\varphi}\frac{\partial A}{\partial \lambda}\hat{\lambda}. \tag{94}$$

If we make the identification in Eq. (90)

$$f(\sigma_1)=f(\tau,\varphi,\lambda)=\ln \hat{H}^2,$$

Eq. (67) becomes

$$\frac{\mathrm{d}f}{\mathrm{d}\sigma}\Big|_{\sigma=\sigma_1}+\nabla_S^2 A=0. \tag{95}$$

For this expression to be useful, we must write $\nabla_S^2 A$ in terms of path variables evaluated at the end point $\sigma=\sigma_1$. To this end we define

$$A_\varphi(\sigma)\equiv\frac{h_\lambda(\sigma)}{h_\varphi(\sigma)}p_\varphi(\sigma)$$

and

$$A_\lambda(\sigma)\equiv\frac{h_\varphi(\sigma)}{h_\lambda(\sigma)}p_\lambda(\sigma),$$

so that

$$\nabla_S^2 A=\frac{1}{J(\varphi)}\left[\frac{\partial A_\varphi(\sigma_1)}{\partial \varphi}+\frac{\partial A_\lambda(\sigma_1)}{\partial \lambda}\right].$$

Because $\nabla_S^2 A$ involves derivatives with respect to φ and λ, the end-point values of the path coordinates q_φ and q_λ, it is clear it cannot be written as a function of the path (evaluated at the

end point). What is needed, in addition, is a perturbed path whose coordinates differ at the end point from φ and λ by infinitesimal amounts $\delta\varphi$ and $\delta\lambda$. The perturbations δA_φ and δA_λ evaluated at the end points will involve derivatives of A_φ and A_λ with respect to φ and λ. These derivatives can be used to construct $\nabla_S^2 A$. In addition, since $\nabla_S^2 A$ does not involve a derivative with respect to τ, it can be held fixed.

There is some freedom in the choice of how the path is perturbed. The perturbation can be induced by changes in any set of parameters that, together with φ_0 and λ_0, characterize the ray. Here we will use a set that exploits the fact that p_τ and p_λ are constant along the ray path

$$W \equiv \sqrt{-2p_\tau}, \quad P = \frac{p_\lambda}{W}. \tag{96}$$

The derivatives of the paths can be written in terms of W and P as follows:

$$\frac{\mathrm{d}q_\varphi}{\mathrm{d}\sigma} = \frac{A_\varphi}{J} = \frac{W}{J}\sqrt{h_\lambda^2 - P^2}, \quad \frac{\mathrm{d}q_\lambda}{\mathrm{d}\sigma} = \frac{A_\lambda}{J} = \frac{WP}{h_\lambda^2}. \tag{97}$$

Now $A_\varphi(\sigma_1)$ and $A_\lambda(\sigma_1)$ depend on φ and λ (as well as τ) so we can write the matrix equation

$$\begin{bmatrix} \partial A_\varphi(\sigma_1)/\partial W & \partial A_\varphi(\sigma_1)/\partial P \\ \partial A_\lambda(\sigma_1)/\partial W & \partial A_\lambda(\sigma_1)/\partial P \end{bmatrix} = \begin{bmatrix} \partial A_\varphi(\sigma_1)/\partial \varphi & \partial A_\varphi(\sigma_1)/\partial \lambda \\ \partial A_\lambda(\sigma_1)/\partial \varphi & \partial A_\lambda(\sigma_1)/\partial \lambda \end{bmatrix} Q(\sigma_1), \tag{98}$$

where

$$Q(\sigma) \equiv \begin{bmatrix} \partial q_\varphi(\sigma)/\partial W & \partial q_\varphi(\sigma)/\partial P \\ \partial q_\lambda(\sigma)/\partial W & \partial q_\lambda(\sigma)/\partial P \end{bmatrix}. \tag{99}$$

Equation (98) can be inverted provided that the determinant of Q,

$$\det(Q(\sigma)) = \frac{\partial q_\varphi(\sigma)}{\partial W}\frac{\partial q_\lambda(\sigma)}{\partial P} - \frac{\partial q_\varphi(\sigma)}{\partial P}\frac{\partial q_\lambda(\sigma)}{\partial W}, \tag{100}$$

does not vanish at $\sigma = \sigma_1$. (Caustics are located where $\det Q = 0$.) By taking the trace after inverting Eq (98) we obtain

$$\nabla_S^2 A = \frac{1}{J(\varphi)}\mathrm{trace}\left\{ \begin{bmatrix} \partial A_\varphi(\sigma_1)/\partial \varphi & \partial A_\varphi(\sigma_1)/\partial \lambda \\ \partial A_\lambda(\sigma_1)/\partial \varphi & \partial A_\lambda(\sigma_1)/\partial \lambda \end{bmatrix} \right\} = \frac{\mathrm{d}\ln D(\sigma)}{\mathrm{d}\sigma}\Big|_{\sigma=\sigma_1}, \tag{101}$$

where

$$D(\sigma) \equiv J(q_\varphi(\sigma))\det(Q(\sigma)). \tag{102}$$

This result was arrived at by using the relation

$$\frac{\mathrm{d}D}{\mathrm{d}\sigma} = \frac{\partial A_\varphi}{\partial W}\frac{\partial q_\lambda}{\partial P} - \frac{\partial A_\lambda}{\partial W}\frac{\partial q_\varphi}{\partial P} - (W \leftrightarrow P), \tag{103}$$

which follows from the equations of motion. Except for the presence of the function $J(q_\varphi)$, the derivation of Eq. (101) is identical to the usual derivation for the Cartesian problem using Liousville's formula [see, e.g., Brekhovskikh and Godin (1999), Sec. 5.1].

Combining Eq. (101) with Eq. (95) gives

$$\left.\frac{df}{d\sigma}\right|_{\sigma=\sigma_1}+\left.\frac{d}{d\sigma}\ln D(\sigma)\right|_{\sigma=\sigma_1}=0.$$

This equation can be solved by solving the more general one

$$\frac{df(\sigma)}{d\sigma}+\frac{d}{d\sigma}\ln D(\sigma)=0$$

and evaluating the result at $\sigma=\sigma_1$,

$$\hat{H}=\mathcal{C}\sqrt{\frac{1}{D(\sigma_1)}},$$

where $\mathcal{C}$ is an integration constant. It can be determined by considering the solution to the parabolic equation at a point $(\varphi',\lambda',\tau')$ where φ' and λ' are located in a neighborhood of the source at φ_0 and λ_0 taken small enough so that μ and $\nu\cos\varphi$ can be considered constant within it. The solution to the horizontal parabolic equation at $(\varphi',\lambda',\tau')$ that satisfies Eq. (60) is simply

$$H(\tau';\varphi',\lambda')=\left(\frac{k_0}{2\pi i\tau'}\right)\exp\left\{\frac{ik_0}{2\tau'}[\mu_0^2(\varphi'-\varphi_0)^2+\nu_0^2\cos^2\varphi_0(\lambda'-\lambda_0)^2]\right\},$$

where $\mu_0=\mu(\varphi_0)$ and $\nu_0=\nu(\varphi_0)$. We take the point $(\varphi',\lambda',\tau')$ to be along the ray path from $(\varphi_0,\lambda_0,0)$ to (φ,λ,τ),

$$\varphi'=q_\varphi(\sigma'),\quad \lambda'=q_\lambda(\sigma'),\quad \tau'=\sigma'-\sigma_0.$$

The variable $\sigma'-\sigma_0\lesssim\tau'$ is necessarily small enough so that the ray paths can be approximated by straight lines,

$$q_\varphi(\sigma')-\varphi_0=(\sigma'-\sigma_0)\frac{dq_\varphi}{d\sigma}(\sigma_0)=(\sigma'-\sigma_0)\frac{W}{J(\varphi_0)}\sqrt{\nu_0^2\cos^2\varphi_0-P^2},$$

$$q_\lambda(\sigma')-\lambda_0=(\sigma'-\sigma_0)\frac{dq_\lambda}{d\sigma}(\sigma_0)=(\sigma'-\sigma_0)\frac{WP}{\nu_0^2\cos^2\varphi_0}.$$

It is clear from these expressions that $D(\sigma')$ can be written in the form

$$D(\sigma')=\frac{1}{2}(\sigma'-\sigma_0)^2\frac{d^2D}{d\sigma^2}(\sigma_0). \tag{104}$$

[The second derivative in this expression is, in fact, equal to $2W^2/A_\varphi(\sigma_0)$.] Since

$$\hat{H}(\sigma')=\frac{k_0}{2\pi i(\sigma'-\sigma_0),}$$

we have

$$\mathcal{C}=\hat{H}(\sigma')\sqrt{D(\sigma')}=\frac{k_0}{2\pi i}\sqrt{\frac{1}{2}\frac{d^2D}{d\sigma^2}(\sigma_0)}.$$

The amplitude factor is, therefore,

$$\hat{H}=\frac{k_0}{2\pi i}\sqrt{\frac{1}{2D(\sigma_1)}\frac{d^2D}{d\sigma^2}(\sigma_0)}.$$

If both sides of Eq. (97) are differentiated with respect to W and P, we obtain

$$\frac{\partial A_\varphi}{\partial W}=\frac{A_\varphi}{W}+J\Omega\frac{\partial q_\varphi}{\partial W}, \tag{105}$$

$$\frac{\partial A_\varphi}{\partial P}=-\frac{W^2P}{A_\varphi}+J\Omega\frac{\partial q_\varphi}{\partial P}, \tag{106}$$

$$\frac{\partial A_\lambda}{\partial W}=\frac{A_\lambda}{W}+\frac{\partial A_\lambda}{\partial q_\varphi}\frac{\partial q_\varphi}{\partial W}, \tag{107}$$

$$\frac{\partial A_\lambda}{\partial P}=\frac{A_\lambda}{P}+\frac{\partial A_\lambda}{\partial q_\varphi}\frac{\partial q_\varphi}{\partial P}, \tag{108}$$

with

$$\Omega=\frac{1}{J}\frac{\partial A_\varphi}{\partial q_\varphi}=\frac{W^2}{2A_\varphi}\frac{\partial h_\lambda^2}{\partial q_\varphi} \tag{109}$$

and

$$\frac{\partial A_\lambda}{\partial q_\varphi}=A_\lambda\frac{\partial}{\partial q_\varphi}\ln\left(\frac{J}{h_\lambda^2}\right). \tag{110}$$

Substituting these expressions into Eq. (103) yields

$$\frac{\mathrm{d}}{\mathrm{d}\sigma}\left(\frac{D}{A_\varphi}\right)=\frac{D_1}{A_\varphi}+\frac{D_2}{A_\varphi}, \tag{111}$$

where

$$D_1=\frac{1}{W}\left(\frac{W^2(h_\lambda^2-P^2)}{A_\varphi}\frac{\partial q_\lambda}{\partial P}-A_\lambda\frac{\partial q_\varphi}{\partial P}\right) \tag{112}$$

and

$$D_2=\frac{1}{P}\left(\frac{W^2P^2}{A_\varphi}\frac{\partial q_\lambda}{\partial W}+A_\lambda\frac{\partial q_\varphi}{\partial W}\right). \tag{113}$$

The derivatives of D_1 and D_2 with respect to σ can be calculated by again using Eqs. (97) and (105)–(108) with the result

$$\frac{\mathrm{d}}{\mathrm{d}\sigma}\left(\frac{D_1}{A_\varphi}\right)=\frac{W^2}{A_\varphi^2} \tag{114}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}\sigma}(A_\varphi D_2)=W. \tag{115}$$

Equation (115) can be solved for D_2:

$$D_2=(\sigma-\sigma_0)\frac{W^2}{A_\varphi}. \tag{116}$$

Using Eqs. (114) and (116) one sees that $(\sigma-\sigma_0)D_1$ obeys the same equation obeyed by D [Eq. (111)]. Since D and $(\sigma-\sigma_0)D_1$ satisfy the same initial conditions, we have

$$D(\sigma)=(\sigma-\sigma_0)D_1(\sigma). \tag{117}$$

Differentiating both sides of Eq. (114) gives

$$\frac{\mathrm{d}^2 D_1}{\mathrm{d}\sigma^2}-\left(\frac{\mathrm{d}\Omega}{\mathrm{d}\sigma}+\Omega^2\right)D_1=0. \tag{118}$$

The term in parentheses can be written in a particularly convenient form by differentiating Ω using the relations $\mathrm{d}A_\varphi/\mathrm{d}\sigma=-W^2\sin(q_\varphi)$ and $\partial h_\lambda^2/\partial q_\varphi=-2J\sin(q_\varphi)$, which follow from Eqs. (97) and (31). One finds

$$-\left(\frac{\mathrm{d}\Omega}{\mathrm{d}\sigma}+\Omega^2\right)=\frac{W^2}{\mu\nu}>0. \tag{119}$$

Referring to Eq. (35), we can write Eq. (118) as

$$\frac{\mathrm{d}^2 D_1}{\mathrm{d}\sigma^2}+\frac{W^2}{R^2}D_1=0. \tag{120}$$

If the Earth is modeled as a sphere, both μ and ν would be equal to its radius, $\overline{R}$, and the solution for D_1 is immediately found without approximation to be

$$D_1(\sigma)=\frac{1}{2}\frac{\mathrm{d}^2 D}{\mathrm{d}\sigma^2}(\sigma_0)\frac{\overline{R}}{W}\sin\left[\frac{W}{\overline{R}}(\sigma-\sigma_0)\right].$$

At the end of the path the argument of the sine function becomes $S/\overline{R}$, which is easily seen to be the angle at the center of the Earth subtended by the arc that ends at source and receiver positions

$$\cos\left(\frac{S}{\overline{R}}\right)=\cos\varphi\cos\varphi_0\cos(\lambda-\lambda_0)+\sin\varphi\sin\varphi_0.$$

Equation (120) cannot be solved exactly for an arbitrary volume of revolution. However, if

$$\frac{1}{W}\left|\frac{\mathrm{d}R}{\mathrm{d}\sigma}\right|\ll 1, \tag{121}$$

we can approximate D_1 with its WKB solution

$$D_1(\sigma)\approx D_1^{\mathrm{WKB}}(\sigma)=\frac{1}{2W}\frac{\mathrm{d}^2 D}{\mathrm{d}\sigma^2}(\sigma_0)\sqrt{R(\sigma)R(\sigma_0)}\sin\left(W\int_{\sigma_0}^{\sigma}\frac{\mathrm{d}\sigma'}{R(\sigma')}\right). \tag{122}$$

The overall normalization has been determined using Eq. (104).

To explore the validity of condition (121), we use the parametrization equation (36) to find

$$\frac{\mathrm{d}R}{\mathrm{d}\sigma}=-\frac{\overline{R}\eta}{2(1+\eta g(q_\varphi))^{3/2}}\frac{\partial g(q_\varphi)}{\partial q_\varphi}\frac{\mathrm{d}q_\varphi}{\mathrm{d}\sigma}.$$

Since

$$\left|\frac{dq_\varphi}{d\sigma}\right| \leqslant \frac{W}{h_\varphi} \approx \frac{W}{\bar{R}},$$

we have

$$\frac{1}{W}\left|\frac{dR}{d\sigma}\right| \lesssim \frac{1}{2}\eta\left|\frac{\partial g(q_\varphi)}{\partial q_\varphi}\right|. \tag{123}$$

Condition (121) will be satisfied if the smallest scale of variability in latitude of the surface is larger than the deviation of the Earth's shape from that of a sphere. If we (arbitrarily) require that the right-hand side of Eq. (123) be less than 1/10, the condition is satisfied provided one can consider the Earth spherical on horizontal scales of order $10(\bar{R}\eta/2) \approx 210$ km. Clearly Eq. (121) is valid since over distances of a few hundred kilometers it is safe to assume the Earth is flat—one does not need to even assume it is spherical.

Collecting expressions gives

$$\hat{H} = \frac{k_0\sqrt{W}}{2\pi i(R(\sigma_1)R(\sigma_0))^{1/4}}\left[(\sigma_1-\sigma_0)\sin\left(W\int_{\sigma_0}^{\sigma_1}\frac{d\sigma'}{R(\sigma')}\right)\right]^{-1/2}.$$

Changing the independent variable from σ to s and introducing the path-averaged quantity

$$\frac{1}{R_{\text{ave}}} = \frac{1}{S}\int_0^S \frac{ds'}{R(s')} = \frac{1}{S}\int_0^S \frac{ds'}{\sqrt{\mu(\varphi_{\text{ray}}(s'))\,\nu(\varphi_{\text{ray}}(s'))}} \tag{124}$$

results in

$$\hat{H} = \frac{k_0}{2\pi i\tau}\left(\frac{R_{\text{ave}}}{R(S)}\,\frac{R_{\text{ave}}}{R(0)}\right)^{1/4}\left[\frac{S/R_{\text{ave}}}{\sin(S/R_{\text{ave}})}\right]^{1/2}. \tag{125}$$

The ray theory approximation to Eq. (59) is therefore

$$H \simeq H_{\text{ray}} = \frac{k_0}{2\pi i\tau}\left(\frac{R_{\text{ave}}}{R(S)}\,\frac{R_{\text{ave}}}{R(0)}\right)^{1/4}\left[\frac{S/R_{\text{ave}}}{\sin(S/R_{\text{ave}})}\right]^{1/2}\exp\left(\frac{ik_0}{2\tau}S^2\right). \tag{126}$$

V. THE VERTICAL EQUATION AND STATIONARY PHASE

The horizontal ray theory approximation for Φ is slightly more involved than for H because no assumptions are made about the magnitude of the scales of variability of the depth coordinate. For Eqs. (56) and (59) to be satisfied, Ψ must satisfy the matrix equation

$$\begin{bmatrix} 2ik_0J(ik_0V+\partial/\partial\tau) & 2ik_0\partial A/\partial\varphi+\partial/\partial\varphi & 2ik_0\partial A/\partial\lambda+\partial/\partial\lambda & J\rho\partial/\partial\zeta \\ \partial/\partial\varphi & -\mu/(\nu\cos\varphi) & 0 & 0 \\ \partial/\partial\lambda & 0 & -(\nu\cos\varphi)/\mu & 0 \\ J\rho\partial/\partial\zeta & 0 & 0 & -J\rho^2 \end{bmatrix} \times \begin{bmatrix} \Psi \\ \Psi_\varphi \\ \Psi_\lambda \\ \Psi_\zeta \end{bmatrix} = 0 \tag{127}$$

and the initial condition

$$\text{Lim}_{\tau\to 0}\Psi(\tau;\varphi,\lambda,\zeta) = \delta(\zeta-\zeta_0). \tag{128}$$

Just as before we drop the horizontal gradients of the amplitude factors in comparison to the corresponding gradients of A, multiplied by k_0. While the derivative $\partial/\partial\tau$ can be dropped in the matrix in Eq. (63) we are not justified in dropping it in Eq. (127). The result is

$$\begin{bmatrix} 2ik_0J(ik_0V+\partial/\partial\tau) & 2ik_0\partial A/\partial\varphi & 2ik_0\partial A/\partial\lambda & J\rho\partial/\partial\zeta \\ \partial/\partial\varphi & -\mu/(\nu\cos\varphi) & 0 & 0 \\ \partial/\partial\lambda & 0 & -(\nu\cos\varphi)/\mu & 0 \\ J\rho\partial/\partial\zeta & 0 & 0 & -J\rho^2 \end{bmatrix} \times \begin{bmatrix} \Psi \\ \Psi_\varphi \\ \Psi_\lambda \\ \Psi_\zeta \end{bmatrix} = 0,$$

which is equivalent to the single second-order equation

$$\left[2ik_0\left(\frac{\partial}{\partial\tau}+\frac{1}{\mu^2}\frac{\partial A}{\partial\varphi}\frac{\partial}{\partial\varphi}+\frac{1}{\nu^2\cos^2\varphi}\frac{\partial A}{\partial\lambda}\frac{\partial}{\partial\lambda}\right)+\rho\frac{\partial}{\partial\zeta}\left(\frac{1}{\rho}\frac{\partial}{\partial\zeta}\right)-2k_0^2V\right]\Psi=0. \tag{129}$$

Comparison of Eqs. (129) and (92) gives

$$2ik_0\frac{S}{\tau}\left[\frac{\partial\Psi(\tau;\varphi_{\text{ray}}(s),\lambda_{\text{ray}}(s),\zeta)}{\partial s}\right]_{s=S} + \left[\rho\frac{\partial}{\partial\zeta}\left(\frac{1}{\rho}\frac{\partial}{\partial\zeta}\right)-2k_0^2V(\varphi_{\text{ray}}(S),\lambda_{\text{ray}}(S),\zeta)\right]\Psi(\tau;\varphi_{\text{ray}}(S),\lambda_{\text{ray}}(S),\zeta)=0.$$

This equation can be solved by solving the more general one

$$\left[2ik_0\frac{S}{\tau}\frac{\partial}{\partial s}+\rho\frac{\partial}{\partial\zeta}\left(\frac{1}{\rho}\frac{\partial}{\partial\zeta}\right)-2k_0^2V(\varphi_{\text{ray}}(s),\lambda_{\text{ray}}(s),\zeta)\right]\Psi(\tau;\varphi_{\text{ray}}(s),\lambda_{\text{ray}}(s),\zeta)=0 \tag{130}$$

and evaluating the result at $s=S$.

If we require that

$$\text{Lim}_{s\to0}\Psi(\tau;\varphi_{\text{ray}}(s),\lambda_{\text{ray}}(s),\zeta)=\delta(\zeta-\zeta_0), \tag{131}$$

then the initial condition, Eq. (128), will be satisfied because of relation (91). In fact, independent of the ray theory approximation, it is not difficult to see that Ψ has support only in a small neighborhood of ζ about ζ_0 and τ about 0 as $s\to0$.

Collecting expressions and substituting into Eq. (53) give

$$G(\vec{x}|\vec{x}_0)\approx\frac{1}{4\pi}\left(\frac{R_{\text{ave}}}{R(S)}\frac{R_{\text{ave}}}{R(0)}\right)^{1/4}\left[\frac{S/R_{\text{ave}}}{\sin(S/R_{\text{ave}})}\right]^{1/2} \times\int_0^\infty\frac{d\tau}{\tau}\exp\frac{ik_0}{2}\left(\tau+\frac{S^2}{\tau}\right)\Psi(\tau;\varphi,\lambda,\zeta). \tag{132}$$

One can evaluate the integral over the Fock–Feynman parameter in Eq. (132) using the method of stationary phase. The single stationary phase point is at $\tau=S$. If $\Psi(\tau;\varphi,\lambda,\zeta)$ has a phase which is a slowly varying function of τ at $\tau=S$, justifying the stationary phase approximation, then the wave number spectrum of $\Psi(S;\varphi,\lambda,\zeta)$ in path length—the horizontal wave number spectrum—will be dominated by values near the reference wave number k_0. That is, the stationary-phase approximation is equivalent to the narrow-angle approximation [Palmer (1976)].

The stationary phase approximation yields

$$G(\vec{x}|\vec{x}_0)\approx \frac{1}{4\pi}\left(\frac{R_{\rm ave}}{R(S)}\,\frac{R_{\rm ave}}{R(0)}\right)^{1/4}\left[\frac{2\pi i}{k_0 R_{\rm ave}\sin(S/R_{\rm ave})}\right]^{1/2} e^{ik_0 S}\psi(S,\zeta), \tag{133}$$

where

$$\psi(s,\zeta)\equiv\Psi(S;\varphi_{\rm ray}(s),\lambda_{\rm ray}(s),\zeta)$$

satisifies the two-dimensional parabolic equation

$$\left[2ik_0\frac{\partial}{\partial s}+\rho\frac{\partial}{\partial\zeta}\left(\frac{1}{\rho}\,\frac{\partial}{\partial\zeta}\right)-2k_0^2V(s,\zeta)\right]\Psi(s,\zeta)=0 \tag{134}$$

and the initial condition

$$\mathrm{Lim}_{s\to 0}\psi(s,\zeta)=\delta(\zeta-\zeta_0). \tag{135}$$

It being understood that s is measured along the ray path and that

$$V(s,\zeta)=V(\varphi_{\rm ray}(s),\lambda_{\rm ray}(s),\zeta). \tag{136}$$

If the Earth is modeled as a sphere with radius $\overline{R}$, Eq. (133) reduces to

$$G(\vec{x}|\vec{x}_0)\approx \frac{1}{4\pi}\left[\frac{2\pi i}{k_0\overline{R}\sin(S/\overline{R})}\right]^{1/2} e^{ik_0 S}\psi(S,\zeta)\quad(\text{sphere}).$$

It is worth noting that $\psi(s,\zeta)$ does not depend on the total path length S because $\Psi(\tau;\varphi_{\rm ray}(s),\lambda_{\rm ray}(s),\zeta)$ depends on S and τ only through the ratio S/τ. Equation (134) is clearly energy conserving and can be solved numerically using a standard range-sliced marching algorithm. Moreover, it does not possess any kinematic singularities of the type experienced by Collins *et al.* (1996). Caustics in the horizontal are located at $S\approx\pi R_{\rm ave}$ and correspond to the focusing that occurs for near antipodal propagation.

VI. REFRACTED GEODESICS AND NORMAL MODES

In this section we consider two extensions of the method we have presented.

A. Refracted geodesics

The factorization of Φ, Eq. (58), into a term H that depends on the horizontal coordinates and a remainder is not unique. One can always define H by

$$\left[2ik_0\frac{\partial}{\partial\tau}+\nabla_\perp^2-2k_0^2U(\varphi,\lambda)\right]H(\tau;\varphi,\lambda)=0, \tag{137}$$

where

$$U(\varphi,\lambda)=-\tfrac{1}{2}[n_{\rm refr}^2(\varphi,\lambda)-1] \tag{138}$$

is a function of φ and λ but not of the depth coordinate ζ. In Eq. (127) and all subsequent equations $V(\varphi,\lambda,\zeta)$ would be replaced with $\tilde{V}(\varphi,\lambda,\zeta)$ where

$$\tilde{V}(\varphi,\lambda,\zeta)=V(\varphi,\lambda,\zeta)-U(\varphi,\lambda). \tag{139}$$

We want to indicate how the above-presented analysis is modified by the presence of the function U.

The horizontal ray-theory approximation for H now involves a ray path that is a refracted geodesic. The eikonal equation and the expression for the Hamiltonian function become, respectively,

$$\frac{\partial A}{\partial \tau}+\frac{1}{2\mu^2}\left(\frac{\partial A}{\partial \varphi}\right)^2+\frac{1}{2\nu^2\cos^2\varphi}\left(\frac{\partial A}{\partial \lambda}\right)^2+U=0 \tag{140}$$

and

$$\mathcal{E}=p_\tau+\tfrac{1}{2}\mathbf{v}^2+U=0, \tag{141}$$

where $\mathbf{v}$ is now no longer a constant. The equations for p_φ and p_λ become

$$\frac{\mathrm{d}p_\varphi}{\mathrm{d}\sigma}=-\frac{1}{2}\left[\frac{\partial}{\partial q_\varphi}\left(\frac{1}{h_\varphi^2}\right)p_\varphi^2+\frac{\partial}{\partial q_\varphi}\left(\frac{1}{h_\lambda^2}\right)p_\lambda^2\right]-\frac{\partial U}{\partial q_\varphi}$$

and

$$\frac{\mathrm{d}p_\lambda}{\mathrm{d}\sigma}=-\frac{\partial U}{\partial q_\lambda}.$$

The equations for all the other ray-path variables are unchanged. The eikonal is now

$$A=\tau p_\tau+\tilde{A}, \tag{142}$$

where $\tilde{A}$ is the horizontal eikonal function

$$\tilde{A}=\int_{\sigma_0}^{\sigma_1}\mathbf{v}^2\,\mathrm{d}\sigma=\int_0^S\mathbf{v}\,\mathrm{d}s. \tag{143}$$

Since Eq. (142) can be written as

$$A-\tau\frac{\partial A}{\partial \tau}=\tilde{A} \tag{144}$$

it defines a Legendre transform which can be used to change the independent variables from (φ,λ,τ) to (φ,λ,p_τ). The variable τ is then given by

$$\tau=-\frac{\partial \tilde{A}}{\partial p_\tau}=\int_0^S\frac{\mathrm{d}s}{\sqrt{(-2)(p_\tau+U(s))}}.$$

The exponent in Eq. (132) is now

$$ik_0\left(\frac{\tau}{2}+A\right)$$

instead of $ik_0(\tau+S^2/\tau)/2$. At the stationary-phase point $\tau=\tau_{\mathrm{sp}}$ we have

$$\frac{\partial A}{\partial \tau}=p_\tau=-\frac{1}{2} \tag{145}$$

so

$$\mathbf{v}|_{\tau=\tau_{\mathrm{sp}}}=\sqrt{1-2U}=n_{\mathrm{refr}}$$

and

$$\tau_{\mathrm{sp}}=\int_0^S \frac{\mathrm{ds}}{n_{\mathrm{refr}}}.$$

We then have

$$ik_0\left(\frac{\tau}{2}+A\right)_{\tau=\tau_{\mathrm{sp}}}=ik_0\tilde{A}_{\tau=\tau_{\mathrm{sp}}}=ik_0\int_0^S n_{\mathrm{refr}}\,\mathrm{ds}.$$

The stationary-phase approximation then gives

$$\begin{aligned}G(\vec{x}|\vec{x}_0)&\propto\int_0^\infty \hat{H}\exp\left[ik_0\left(\frac{\tau}{2}+A\right)\right]\Psi(\tau;\varphi,\lambda,\zeta)\\&\propto\left[\hat{H}\left(\frac{\partial^2 A}{\partial\tau^2}\right)^{-1/2}\right]_{\tau=\tau_{\mathrm{sp}}}\exp\left[ik_0\int_0^S n_{\mathrm{refr}}\,\mathrm{ds}\right]\Psi(\tau_{\mathrm{sp}};\varphi,\lambda,\zeta).\end{aligned}\tag{146}$$

In calculating $\hat{H}$ it is no longer useful to use the set W and P to characterize ray-path variations. Instead we use

$$v_\varphi\equiv p_\varphi(\sigma_0)=-\frac{\partial A}{\partial\varphi_0},\tag{147}$$

$$v_\lambda\equiv p_\lambda(\sigma_0)=-\frac{\partial A}{\partial\lambda_0}.\tag{148}$$

The relationship between these initial values for the momenta and the derivatives of the eikonal with respect to the coordinates of the source position follow easily from the defining equation, Eq. (84). We still have

$$\hat{H}\propto\sqrt{\frac{1}{D(\sigma_1)}},$$

but now

$$D(\sigma)\equiv J(q_\varphi(\sigma))\det\begin{bmatrix}\partial q_\varphi(\sigma)/\partial v_\varphi & \partial q_\varphi(\sigma)/\partial v_\lambda\\ \partial q_\lambda(\sigma)/\partial v_\varphi & \partial q_\lambda(\sigma)/\partial v_\lambda\end{bmatrix}.$$

We next consider the variation in the ray path due to a change in receiver position

$$\begin{bmatrix}\partial q_\varphi(\sigma)/\partial\varphi & \partial q_\varphi(\sigma)/\partial\lambda\\ \partial q_\lambda(\sigma)/\delta\varphi & \partial q_\lambda(\sigma)/\partial\lambda\end{bmatrix}=-O\times\begin{bmatrix}\partial q_\varphi(\sigma)/\partial v_\varphi & \partial q_\varphi(\sigma)/\partial v_\lambda\\ \partial q_\lambda(\sigma)/\partial v_\varphi & \partial q_\lambda(\sigma)/\partial v_\lambda\end{bmatrix},$$

where

$$O=\begin{bmatrix}\partial^2 A/\partial\varphi_0\partial\varphi & \partial^2 A/\partial\varphi_0\partial\lambda\\ \partial^2 A/\partial\lambda_0\partial\varphi & \partial^2 A/\partial\lambda_0\partial\lambda\end{bmatrix}.\tag{149}$$

(We have used $\partial v_\varphi/\partial\varphi=-\partial^2 A/\partial\varphi_0\partial\varphi$, etc.) At $\sigma=\sigma_1$ the left-hand side of this equation becomes equal to the identity matrix and we have

$$D(\sigma_1)=\frac{J(\varphi)}{\det O}.$$

We now turn to consideration of $\partial^2 A/\partial\tau^2$ in Eq. (146). At $\sigma=\sigma_0$, Eq. (141) becomes

$$p_\tau+\frac{1}{2h_\varphi^2(\varphi_0)}v_\varphi^2+\frac{1}{2h_\lambda^2(\varphi_0)}v_\lambda^2+U(\varphi_0,\lambda_0)=0.$$

Differentiating with respect to τ gives

$$\frac{\partial^2 A}{\partial\tau^2}+\frac{\partial v_\varphi}{\partial\tau}\frac{dq_\varphi}{d\sigma}(\varphi_0)+\frac{\partial v_\lambda}{\partial\tau}\frac{dq_\lambda}{d\sigma}(\varphi_0)=0.$$

The change in the eikonal equation due to a change in source location, keeping the receiver location fixed, is given by

$$\frac{\partial^2 A}{\partial\varphi_0\partial\varphi}\frac{dq_\varphi}{d\sigma}(\varphi)+\frac{\partial^2 A}{\partial\varphi_0\partial\lambda}\frac{dq_\lambda}{d\sigma}(\varphi)=\frac{\partial v_\varphi}{\partial\tau}$$

and

$$\frac{\partial^2 A}{\partial\lambda_0\partial\varphi}\frac{dq_\varphi}{d\sigma}(\varphi)+\frac{\partial^2 A}{\partial\lambda_0\partial\lambda}\frac{dq_\lambda}{d\sigma}(\varphi)=\frac{\partial v_\lambda}{\partial\tau}.$$

Combining these last three equations gives

$$\frac{\partial^2 A}{\partial\tau^2}=e(\sigma_0)^T\cdot O\cdot e(\sigma_1), \tag{150}$$

where

$$e(\sigma)=\begin{bmatrix} dq_\varphi(\sigma)/d\sigma \\ dq_\lambda(\sigma)/d\sigma \end{bmatrix}.$$

Therefore

$$\left[\hat{H}\left(\frac{\partial^2 A}{\partial\tau^2}\right)^{-1/2}\right]_{\tau=\tau_{sp}}=\left(\frac{1}{J(\varphi)}\frac{\det O}{e(\sigma_0)\cdot O\cdot e(\sigma_1)}\right)^{1/2}_{\tau=\tau_{sp}}. \tag{151}$$

[For an alternative way of writing this amplitude factor see Gutzwiller (1990), Eq. (2.10).]

The evaluation of the derivatives of A with respect to source and receiver coordinates that make up the components of O are done at the stationary-phase point

$$A_{\tau=\tau_{sp}}=\frac{1}{2}\int_0^S\left[\frac{2n_{refr}^2-1}{n_{refr}}\right]ds \tag{152}$$

The derivatives can be performed once Hamilton's equations have been solved for the refracted geodesic and the variation of n_{refr} along the path is determined. Collecting expressions gives

$$G(\vec{x}|\vec{x}_0)\propto\left(\frac{1}{J(\varphi)}\frac{\det O}{e(\sigma_0)\cdot O\cdot e(\sigma_1)}\right)^{1/2}_{\tau=\tau_{sp}}\exp\left[ik_0\int_0^S n_{refr}ds\right]\Psi(s,\zeta), \tag{153}$$

where

$$\left[2ik_0 n_{\text{refr}}\frac{\partial}{\partial s}+\rho\frac{\partial}{\partial\zeta}\left(\frac{1}{\rho}\frac{\partial}{\partial\zeta}\right)-2k_0^2\tilde{V}(s,\zeta)\right]\Psi(s,\zeta)=0. \tag{154}$$

This parabolic equation differs from Eq. (134) in two respects—the s-dependent scale factor n_{refr} and the replacement of V with $\tilde{V}$.

B. Modal analysis

Much of the work done to model global propagation has assumed a description involving discrete, local, normal modes propagating without coupling [see, e.g., Munk, Worcester, and Wunsch (1995)]. In this section we discuss how this description can be incorporated into the formalism presented in the previous sections.

We begin with some preliminaries. The local modes satisfy

$$\left[\rho(\zeta)\frac{\partial}{\partial\zeta}\left(\frac{1}{\rho(\zeta)}\frac{\partial}{\partial\zeta}\right)+k_0^2 n^2(\varphi,\lambda,\zeta)\right]Z_m(\varphi,\lambda,\zeta)=k_0^2\varkappa_m^2(\varphi,\lambda)Z_m(\varphi,\lambda,\zeta), \tag{155}$$

where $\varkappa_m$ is the (dimensionless) normal-mode wave number. As a result of the self-adjoint nature of Eq. (155), we have the orthogonal relation

$$\int\frac{d\zeta}{\rho(\zeta)}Z_n(\varphi,\lambda,\zeta)Z_m(\varphi,\lambda,\zeta)=\delta_{nm} \tag{156}$$

and the completeness relation

$$\sum_m Z_m(\varphi,\lambda,\zeta)Z_m(\varphi,\lambda,\zeta_0)=\rho(\zeta_0)\,\delta(\zeta-\zeta_0).$$

We expand Φ in Eq. (56) in terms of these modes

$$\Phi(\tau;\varphi,\lambda,\zeta)=\frac{1}{\rho(\zeta_0)}\sum_m \mathcal{C}_m(\tau;\varphi,\lambda)Z_m(\varphi,\lambda,\zeta)Z_m(\varphi,\lambda,\zeta_0)$$

so that

$$\text{Lim}_{\tau\to 0}\mathcal{C}_m(\tau;\varphi,\lambda)=\frac{1}{J(\varphi)}\,\delta(\varphi-\varphi_0)\,\delta(\lambda-\lambda_0)$$

independent of the index m. We have for the Green's function

$$G(\vec{x}\,|\,\vec{x}_0)=\frac{1}{\rho(\zeta_0)}\sum_m Z_m(\varphi,\lambda,\zeta)Z_m(\varphi,\lambda,\zeta_0)G_m(\varphi,\lambda\,|\,\varphi_0,\lambda_0), \tag{157}$$

where

$$G_m=\frac{i}{2k_0}\int_0^\infty d\tau\, e^{i\tau k_0/2}\mathcal{C}_m(\tau;\varphi,\lambda). \tag{158}$$

The equation satisfied by the model coefficients is

$$\left[2ik_0\frac{\partial\mathcal{C}_m}{\partial\tau}+\nabla_S^2\mathcal{C}_m-2k_0^2W_m\mathcal{C}_m\right]Z_m(\varphi,\lambda,\zeta_0)+\sum_l\left[B_{ml}\mathcal{C}_l+2\vec{F}_{ml}\cdot\nabla_S\mathcal{C}_l\right]=0, \tag{159}$$

where

$$W_m(\varphi,\lambda) = -\tfrac{1}{2}[\varkappa_m^2(\varphi,\lambda) - 1],$$

$$B_{ml} = \int \frac{d\zeta}{\rho} Z_m \nabla_S^2 (Z_l(\varphi,\lambda,\zeta) Z_l(\varphi,\lambda,\zeta_0)),$$

and

$$\vec{F}_{ml} = \int \frac{d\zeta}{\rho} Z_m \nabla_S (Z_l(\varphi,\lambda,\zeta) Z_l(\varphi,\lambda,\zeta_0)).$$

Generally speaking, a modal analysis for the types of wave propagation problems we are considering is useful only if mode coupling can be ignored. If this is the case, then $B_{ml}=0$ and $\vec{F}_{ml}=0$ and Eq. (159) reduces to

$$\left[2ik_0 \frac{\partial}{\partial \tau} + \nabla_S^2 - 2k_0^2 W_m\right] \mathcal{C}_m = 0. \tag{160}$$

With preliminaries out of the way, we develop a method for solving Eq. (160) based on the ideas introduced earlier. We write

$$\mathcal{C}_m(\tau;\varphi,\lambda) = \Psi_m(\tau;\varphi,\lambda) H(\tau;\varphi,\lambda), \tag{161}$$

where H obeys

$$\left[2ik_0 \frac{\partial}{\partial \tau} + \nabla_S^2\right] H = 0$$

and

$$\mathrm{Lim}_{\tau\to 0} H(\tau;\varphi,\lambda) = \frac{1}{J(\varphi)} \delta(\varphi-\varphi_0)\,\delta(\lambda-\lambda_0).$$

The ray theory solution for H is given by Eq. (126). The equation satisfied by Ψ_m is

$$2ik_0 \frac{\partial \Psi_m}{\partial \tau} + \nabla_S^2 \Psi_m + 2\frac{\nabla_S H}{H} \cdot \nabla_S \Psi_m - 2k_0^2 W_m \Psi_m = 0 \tag{162}$$

and

$$\mathrm{Lim}_{\tau\to 0} \Psi_m(\tau;\varphi,\lambda) = 1.$$

We know

$$\frac{2}{H}\nabla_S H = \frac{2ik_0 S}{\tau}\left[\mu \frac{dq_\varphi}{ds}(\sigma_1)\hat{\varphi} + \nu \cos\varphi \frac{dq_\lambda}{ds}(\sigma_1)\hat{\lambda}\right] = \frac{2ik_0 S}{\tau}\hat{s}(\sigma_1) \tag{163}$$

and

$$\frac{S}{\tau}\frac{\partial}{\partial s} = \frac{\partial}{\partial \tau} + \frac{S}{\tau}\hat{s}(\sigma_1)\cdot\nabla_\perp, \tag{164}$$

so that

$$2ik_0 \frac{S}{\tau}\frac{\partial \Psi_m}{\partial s} + \nabla_S^2 \Psi_m - 2k_0^2 W_m \Psi_m = 0. \tag{165}$$

Consistently apply the horizontal ray approximation and replace Eq. (165) with

$$2ik_0\frac{S}{\tau}\frac{\partial\Psi_m}{\partial s}-2k_0^2W_m\Psi_m=0 \tag{166}$$

giving

$$\Psi_m=\exp\left[-ik_0\frac{\tau}{S}\int_0^S \mathrm{d}s\ W_m\right). \tag{167}$$

Combining terms

$$G_m=\frac{1}{4\pi}\left(\frac{R_{\mathrm{ave}}}{R(S)}\frac{R_{\mathrm{ave}}}{R(0)}\right)^{1/4}\left[\frac{S/R_{\mathrm{ave}}}{\sin(S/R_{\mathrm{ave}})}\right]^{1/2}\int_0^\infty\frac{\mathrm{d}\tau}{\tau}\exp\left[\frac{ik_0}{2}\left(\frac{S^2}{\tau}+\tau\langle\varkappa_m^2\rangle\right)\right],$$

where $\langle\varkappa_m^2\rangle$ is the mean-square-average of $\varkappa_m$ over the horizontal ray path

$$\langle\varkappa_m^2\rangle=\frac{1}{S}\int_0^S \mathrm{d}s\ \varkappa_m^2. \tag{168}$$

For $k_0S\gg1$ the integral over τ is approximately equal to

$$\left(\frac{2\pi i}{k_0S^2}\right)^{1/2}\left(\frac{\langle\varkappa_m^2\rangle}{S^2}\right)^{1/4}\exp[ik_0S\sqrt{\langle\varkappa_m^2\rangle}],$$

so that

$$G_m=\frac{1}{4\pi}\left(\frac{R_{\mathrm{ave}}}{R(S)}\frac{R_{\mathrm{ave}}}{R(0)}\frac{\langle\varkappa_m^2\rangle}{S^2}\right)^{1/4}\left[\frac{2\pi i}{k_0SR_{\mathrm{ave}}\sin(S/R_{\mathrm{ave}})}\right]^{1/2}\exp[ik_0S\sqrt{\langle\varkappa_m^2\rangle}]. \tag{169}$$

Alternative approaches to the modal problem are discussed in Burridge and Weinberg (1977); Collins (1993b); McDonald *et al.* (1994); and Collins *et al.* (1995a); (1995b); (1996).

VII. SUMMARY

In this paper we have proposed a method for obtaining parabolic approximations consisting of the following steps

(1) The Green's function for the problem of interest is written as a Laplace or Mellon transform over the corresponding propagator. The transform variable is the Fock–Feynman parameter.

(2) The propagator is factored into a term that is assumed to be a rapidly varying function of the horizontal coordinates and obeys a parabolic equation in those coordinates, and an envelope function that is assumed to be a slowly varying function of the horizontal coordinates.

(3) The dependence on the horizontal coordinates is determined using the ray theory approximation.

(4) The equation for the envelop function is cast into the form of a parabolic equation with the horizontal direction of propagation along the ray path determined in step (3).

(5) The integral over the Fock–Feynman parameter is approximated using the method of stationary phase.

If one applies this method to the Helmhotz equation in Cartesian coordinates, one obtains the standard narrow-angle parabolic equation in two coordinate variables. One can easily derive improved approximations because the proposed method separates the parabolic approximation into two separate approximations: one involving the characteristics of the field in the horizontal and the other its characteristics in the vertical. The horizontal ray-theory approximation can be relaxed in

any number of ways. One possibility is to use the Rytov approximation instead of the ray-theory one [Palmer (1976)]. This results in replacing the index of refraction by an effective one that is constructed by integration over the Fresnel ray tube surrounding the ray path. Another possibility is to allow for horizontal refraction and horizontal multipaths. In Sec. VI we indicate how this might be done.

There are many ways of relaxing the narrow-angle approximation by improving on the stationary-phase approximation. One possibility is to evalute the integral numerically in the same way that the integral over frequency is evaluated in the Fourier representation of the solution to the parabolic equation for a broadband source. One obtains the solution to Eq. (92) for a range of values of τ using a marching algorithm. The integral in Eq. (92) is then evaluated using a fast Fourier transform. Other than those relating to the numerical evaluation, the only approximations made in the development of the global problem considered here are the horizontal ray theory approximation and, of less importance, the WKB approximation for the amplitude.

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Integration of a generalized Hénon–Heiles Hamiltonian

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The generalized Hénon–Heiles Hamiltonian $H=1/2(P_X^2+P_Y^2+c_1X^2+c_2Y^2)+aXY^2-bX^3/3$ with an additional nonpolynomial term μY^{-2} is known to be Liouville integrable for three sets of values of $(b/a,c_1,c_2)$. It has been previously integrated by genus two theta functions only in one of these cases. Defining the separating variables of the Hamilton–Jacobi equations, we succeed here, in the two other cases, to integrate the equations of motion with hyperelliptic functions. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1456948]

I. INTRODUCTION

The generalization of the Hénon–Heiles Hamiltonian defined by

$$H\equiv\frac{1}{2}(P_X^2+P_Y^2+c_1X^2+c_2Y^2)+aXY^2-\frac{b}{3}X^3+\frac{1}{32a^2}\frac{\mu}{Y^2},\quad a\neq 0, \tag{1}$$

$$X'=P_X,\quad Y'=P_Y, \tag{2}$$

$$X''=-aY^2+bX^2-c_1X, \tag{3}$$

$$Y''=-2aXY-c_2Y+\frac{1}{16a^2}\frac{\mu}{Y^3},\quad \mu \text{ arbitrary}, \tag{4}$$

is integrable in the sense of Liouville in three cases,[1–3] namely,

$$\frac{b}{a}=-1,\quad c_1=c_2, \tag{5}$$

$$\frac{b}{a}=-6,\quad c_1,c_2 \text{ arbitrary}, \tag{6}$$

$$\frac{b}{a}=-16,\quad c_1=16c_2, \tag{7}$$

and is equivalent to the reduction $\xi=x-ct$ of three fifth order soliton equations,[4] respectively the Sawada–Kotera (SK), KdV_5 and Kaup–Kupershmidt (KK) equations, by applying the translation

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$$\text{SK:}\quad u=X+\frac{c_2}{2a},\quad c=c_1c_2, \tag{8}$$

$$\text{KdV}_5\text{:}\quad u=X+\frac{c_1+4c_2}{20a},\quad c=\frac{1}{10}(-3c_1^2-16c_1c_2+48c_2^2), \tag{9}$$

$$\text{KK:}\quad u=X+\frac{c_2}{2a},\quad c=c_1c_2. \tag{10}$$

The reduced partial differential equations (PDEs) are respectively

$$\text{SK:}\quad u^{(4)}+10auu''+\frac{20}{3}a^2u^3-cu+4aE-\frac{c_1c_2^2}{3a}=0, \tag{11}$$

$$\text{KdV}_5\text{:}\quad u^{(4)}+20auu''+40a^2u^3+10au'^2-cu+4aE+\frac{1}{100a}(c_1+4c_2)(c_1^2-12c_1c_2+16c_2^2)=0, \tag{12}$$

$$\text{KK:}\quad u^{(4)}+40auu''+\frac{320}{3}a^2u^3+30au'^2-cu+4aE-\frac{c_1c_2^2}{3a}=0, \tag{13}$$

in which E is the constant value of the Hamiltonian H. Therefore we will further use these names for referring to the respective integrable cases of the Hamiltonian.

The problem which we address is to find the separating variables and to explicitly integrate.

The general solution for the KdV_5 case has been obtained in terms of hyperelliptic functions[5–7] by separation of the variables of the Hamilton–Jacobi equation in parabolic coordinates.

For $\mu=0$, the equations of motion for the SK and KK cases have been integrated[8–10] in terms of elliptic functions.

In this article we give the general solution of the equations of motion for the SK and KK cases in terms of hyperelliptic functions. This is achieved by separation of the variables of the Hamilton–Jacobi equation, where the canonical transformation between SK and KK[11] plays an important role.

In Sec. II, we consider the SK case with $\mu=0$ as a starting point to treat the general case (μ arbitrary). In Sec. III, we recover the canonical transformation between SK and KK, starting from the factorization of the scattering operator associated with these equations and using the link with the Fordy–Gibbons equation.[12] In Sec. IV, we give the general solution for KK, using the canonical transformation previously obtained. In Sec. V, we use the fact that the canonical transformation is invertible for obtaining the general solution of the SK case. In both cases, in the limit $\mu\to 0$, we recover the previous results.[9,10] In Sec. VI, we compare the present method of integration, starting from the Hamiltonian system, with the method used by Cosgrove[13] for integrating the fourth order ODEs (11) and (13).

II. PARTICULAR CASE: SAWADA–KOTERA FOR $\mu=0$

This is the simplest case and it will be our starting point to define the separation of variables of the Hamilton–Jacobi equation for KK.

Consider the Hamiltonian in the SK case derived from (1) by setting $a=\frac{1}{2}$ and defining $U=X+c_2$, $V=Y$, $c=c_1c_2$,

$$H\equiv K_{1,0}=\frac{1}{2}(P_U^2+P_V^2)+\frac{1}{2}UV^2+\frac{1}{6}U^3-\frac{c}{2}U, \tag{14}$$

which is a constant of motion of the equations

$$U''=-\frac{1}{2}(V^2+U^2)+\frac{c}{2},$$
$$V''=-UV, \tag{15}$$

where U,V and the derivatives $U'=P_U$, $V'=P_V$ are functions of the independent variable ξ ($'\equiv \mathrm{d}/\mathrm{d}\xi$).

This system possesses a second constant of motion[9]

$$K_{2,0}=-2P_UP_V-U^2V-\frac{V^3}{3}+cV, \tag{16}$$

which is in involution with the Hamiltonian, i.e., $\{K_{1,0},K_{2,0}\}=0$.

The separation of variables is defined as

$$Q_1=U+V, \quad Q_2=U-V,$$
$$P_1=\tfrac{1}{2}(P_U+P_V), \quad P_2=\tfrac{1}{2}(P_U-P_V), \tag{17}$$

and in those new variables the expressions of $K_{1,0}$ and $K_{2,0}$ are

$$K_{1,0}=P_1^2+P_2^2+\frac{1}{12}(Q_1^3+Q_2^3)-\frac{c}{4}(Q_1+Q_2), \tag{18}$$

$$K_{2,0}=2(P_2^2-P_1^2)+\frac{1}{6}(Q_2^3-Q_1^3)-\frac{c}{2}(Q_2-Q_1), \tag{19}$$

such that the equations of motion become

$$Q_1'^2=-\tfrac{1}{3}Q_1^3+cQ_1-K_{2,0}+2K_{1,0},$$
$$Q_2'^2=-\tfrac{1}{3}Q_2^3+cQ_2+K_{2,0}+2K_{1,0}. \tag{20}$$

They possess the general solution

$$Q_1=-12\wp\left(\xi-\xi_1,\frac{c}{12},-\frac{1}{144}(2K_{1,0}-K_{2,0})\right)\equiv-12\wp_1(\xi),$$
$$Q_2=-12\wp\left(\xi-\xi_2,\frac{c}{12},-\frac{1}{144}(2K_{1,0}+K_{2,0})\right)\equiv-12\wp_2(\xi), \tag{21}$$

in terms of the Weierstrass elliptic function $\wp(x-x_0,g_2,g_3)$, solution of the first order differential equation

$$\wp'^2=4\wp^3-g_2\wp-g_3, \tag{22}$$

such that the solutions become

$$U=-6(\wp_1(\xi)+\wp_2(\xi)),$$
$$V=-6(\wp_1(\xi)-\wp_2(\xi)). \tag{23}$$

III. CANONICAL TRANSFORMATION BETWEEN SK AND KK

Let us consider, for μ arbitrary, the equations and the constants of motion associated with the SK and KK Hamiltonians[14,15]

$$\text{SK:}\quad U'=P_U,\quad V'=P_V, \tag{24}$$

$$U''=-\frac{1}{2}(V^2+U^2)+\frac{c}{2},\quad V''=-UV+\frac{\mu}{4V^3}, \tag{25}$$

$$K_1=\frac{1}{2}(P_U^2+P_V^2)+\frac{1}{2}UV^2+\frac{1}{6}U^3-\frac{c}{2}U+\frac{\mu}{8V^2}, \tag{26}$$

$$K_2^2=K_{2,0}^2+\frac{2}{3}\mu U+\mu\frac{P_U^2}{V^2}, \tag{27}$$

$$\text{KK:}\quad a=\tfrac{1}{4},\quad c_1=16c_2,\quad c=c_1c_2,\quad u=X+2c_2,\quad v=Y, \tag{28}$$

$$u'=p_u,\quad v'=p_v, \tag{29}$$

$$u''=-\frac{1}{4}v^2-4u^2+c,\quad v''=-\frac{1}{2}uv+\frac{\mu}{v^3}, \tag{30}$$

$$k_1=\frac{1}{2}(p_u^2+p_v^2)+\frac{1}{4}uv^2+\frac{4}{3}u^3-cu+\frac{1}{2}\frac{\mu}{v^2}, \tag{31}$$

$$k_{2,0}^2=p_v^4-\frac{1}{72}v^6-\frac{1}{12}u^2v^4+up_v^2v^2-\frac{1}{3}p_up_vv^3+\frac{c}{12}v^4, \tag{32}$$

$$k_2^2=k_{2,0}^2+\frac{\mu}{3}u+2\mu\frac{p_v^2}{v^2}+\frac{\mu^2}{v^4}. \tag{33}$$

The reason why the expressions $k_{2,0}$ and k_2 are defined by their square will appear soon.

The two nonlinear partial differential equations SK and KK,

$$\text{SK:}\quad U_t+(U_{xxxx}+5UU_{xx}+\tfrac{5}{3}U^3)_x=0, \tag{34}$$

$$\text{KK:}\quad u_t+(u_{xxxx}+10uu_{xx}+\tfrac{20}{3}u^3+\tfrac{15}{2}u_x^2)_x=0, \tag{35}$$

whose reductions $\xi=x-ct$ are (11) and (13), respectively obtained from the systems (25)–(26) and (30)–(31) by elimination of the variables V and v, possess a Lax pair with a third order scattering problem $(L\psi=\lambda\psi)$.[16,17] The scattering operators can be factorized in the following way,

$$\text{SK:}\quad L\equiv\partial_x^3+U\partial_x=(\partial_x-w)(\partial_x+w)\partial_x, \tag{36}$$

$$\text{KK:}\quad L\equiv\partial_x^3+2u\partial_x+u_x=(\partial_x+w)(\partial_x)(\partial_x-w), \tag{37}$$

such that the solutions of the PDEs are related through a Bäcklund transformation

$$\text{SK:}\quad U=w_x-w^2, \tag{38}$$

$$\text{KK:}\quad u=-w_x-\tfrac{1}{2}w^2 \tag{39}$$

with the solution w of the Fordy–Gibbons equation[12]

$$w_t+(w_{xxxx}-5w_xw_{xx}-5w^2w_{xx}-5ww_x^2+w^5)_x=0. \tag{40}$$

The reduction $\xi=x-ct$ of this equation can be solved for $w(\xi)$, either by eliminating U and w' between (38) and the equations of motion (25),

$$w=\frac{1}{2}\frac{\sqrt{-\mu}}{V^2}-\frac{V'}{V}, \tag{41}$$

or by eliminating u and w' between (39) and the equations of motion (30),

$$w=2\frac{\sqrt{-\mu}}{v^2}+2\frac{v'}{v}, \tag{42}$$

such that, defining $\lambda^2=-\mu$ and

$$\Gamma=6(VK_{2,0}+\lambda P_U), \tag{43}$$

$$\Omega=48(3v^4k_{2,0}^2+6\lambda uv^5p_v+12\lambda p_v^3v^3-\lambda v^6p_u+3\lambda^2uv^4+18\lambda^2v^2p_v^2+12\lambda^3vp_v+3\lambda^4), \tag{44}$$

the canonical transformation is given by[11,18]

$$u=-\frac{3}{2}\left(-\frac{P_V}{V}+\frac{\lambda}{2V^2}\right)^2-U,\quad v^2=\frac{\Gamma}{V^2}, \tag{45}$$

$$p_u=\frac{1}{V^3}(3P_V^3+3UV^2P_V-P_UV^3)-\frac{3\lambda}{2V^6}\left(UV^4+3V^2P_V^2-\frac{3}{2}\lambda VP_V+\frac{\lambda^2}{4}\right),$$

$$p_v=\frac{1}{4V^2}\left(-2P_V+\frac{\lambda}{V}\right)\sqrt{\Gamma}-\lambda\frac{V}{\sqrt{\Gamma}}, \tag{46}$$

$$U=-6\left(\frac{p_v}{v}+\frac{\lambda}{v^2}\right)^2-u,\quad V^2=\frac{\Omega}{4v^8}, \tag{47}$$

$$P_U=\frac{1}{v^3}(12p_v^3+6uv^2p_v-v^3p_u)+\frac{3\lambda}{v^6}(2uv^4+12v^2p_v^2+12\lambda vp_v+4\lambda^2),$$

$$P_V=-\frac{1}{v^5}\left(p_v+\frac{\lambda}{v}\right)\sqrt{\Omega}+\lambda\frac{v^4}{\sqrt{\Omega}}. \tag{48}$$

IV. GENERAL SOLUTION OF THE KAUP–KUPERSHMIDT CASE

Starting from the separation of variables (17) and the canonical transformation (47) and (48) in the case $\mu=0$, we consider the transformation defined by Ref. 10 on the basis of Painlevé analysis

$$
\begin{aligned}
q_1 &= -6\frac{p_v^2 - k_{2,0}}{v^2} - u,\\
q_2 &= -6\frac{p_v^2 + k_{2,0}}{v^2} - u,\\
p_1 &= \frac{1}{2v^3}(12p_v^3 + 6uv^2p_v - v^3p_u - 12p_vk_{2,0}),\\
p_2 &= \frac{1}{2v^3}(12p_v^3 + 6uv^2p_v - v^3p_u + 12p_vk_{2,0}).
\end{aligned}
\tag{49}
$$

This inverts to

$$
\begin{aligned}
u &= -6\left(\frac{p_2 - p_1}{q_2 - q_1}\right)^2 - \frac{1}{2}(q_1 + q_2),\\
v^2 &= \frac{12k_{2,0}}{q_1 - q_2},\\
p_u &= 24\left(\frac{p_1 - p_2}{q_1 - q_2}\right)^3 + 2(p_1 - p_2)\frac{q_1 + q_2}{q_1 - q_2} + 2\frac{p_1q_2 - p_2q_1}{q_1 - q_2},\\
p_v^2 &= 12k_{2,0}\frac{(p_2 - p_1)^2}{(q_1 - q_2)^3}.
\end{aligned}
\tag{50}
$$

Taking account that $k_{2,0}$ is no longer a constant of motion, this change of variables will appear to be useful to find the general solution for KK. In those new variables, the Hamiltonian system (31) becomes

$$
H \equiv k_1 = p_1^2 + p_2^2 + \frac{1}{12}(q_1^3 + q_2^3) - \frac{c}{4}(q_1 + q_2) + \frac{\mu}{24}\frac{q_1 - q_2}{k_{2,0}}, \tag{51}
$$

$$
k_{2,0} = 2(p_2^2 - p_1^2) + \frac{1}{6}(q_2^3 - q_1^3) - \frac{c}{2}(q_2 - q_1), \tag{52}
$$

$$
q_1' = 2p_1 + \frac{\mu}{6}\frac{(q_1 - q_2)p_1}{k_{2,0}^2}, \tag{53}
$$

$$
q_2' = 2p_2 - \frac{\mu}{6}\frac{(q_1 - q_2)p_2}{k_{2,0}^2}. \tag{54}
$$

Therefore, defining $f(q_i, p_i) \equiv p_i^2 + \frac{1}{12}q_i^3 - (c/4)\,q_i$ $(i = 1,2)$, the Hamilton–Jacobi equation is separated

$$
k_1(f(q_1, p_1) - f(q_2, p_2)) = f^2(q_1, p_1) - f^2(q_2, p_2) + \frac{\mu}{48}(q_1 - q_2), \tag{55}
$$

$$
p_i = \frac{\partial S}{\partial q_i}. \tag{56}
$$

We can express the second constant of motion k_2^2 in two equivalent ways

$$k_2^2=-\frac{\mu}{3}q_1+\left(k_{2,0}+\frac{\mu}{12}\frac{q_1-q_2}{k_{2,0}}\right)^2, \tag{57}$$

or

$$k_2^2=-\frac{\mu}{3}q_2+\left(k_{2,0}-\frac{\mu}{12}\frac{q_1-q_2}{k_{2,0}}\right)^2, \tag{58}$$

so that the elimination of $\mu(q_1-q_2)/k_{2,0}$ between (51), (57) and (51), (58) yields

$$k_2^2=-\frac{\mu}{3}q_1+\left(-4p_1^2-\frac{q_1^3}{3}+cq_1+2k_1\right)^2, \tag{59}$$

or

$$k_2^2=-\frac{\mu}{3}q_2+\left(4p_2^2+\frac{q_2^3}{3}-cq_2-2k_1\right)^2. \tag{60}$$

The elimination of p_1 between (59) and (53), and of p_2 between (60) and (54), yields

$$q_1'=\sqrt{2k_1-\frac{q_1^3}{3}+cq_1-\sqrt{k_2^2+\frac{\mu}{3}q_1}}\left(1+\frac{\mu}{3}\frac{q_1-q_2}{(\sqrt{k_2^2+(\mu/3)\,q_2}+\sqrt{k_2^2+(\mu/3)\,q_1})^2}\right), \tag{61}$$

$$q_2'=\sqrt{2k_1-\frac{q_2^3}{3}+cq_2+\sqrt{k_2^2+\frac{\mu}{3}q_2}}\left(1-\frac{\mu}{3}\frac{q_1-q_2}{(\sqrt{k_2^2+(\mu/3)\,q_2}+\sqrt{k_2^2+(\mu/3)\,q_1})^2}\right). \tag{62}$$

In the case $\mu=0$, the differential equations for q_1 and q_2 are separated and their solution is expressed in terms of the Weierstrass elliptic function

$$q_{1,0}=-12\wp\left(\xi-\xi_1,\frac{c}{12},-\frac{1}{144}(2k_{1,0}-k_{2,0})\right)\equiv-12\wp_1(\xi), \tag{63}$$

$$q_{2,0}=-12\wp\left(\xi-\xi_2,\frac{c}{12},-\frac{1}{144}(2k_{1,0}+k_{2,0})\right)\equiv-12\wp_2(\xi), \tag{64}$$

so that the solution for (30) in the case $\mu=0$ is[10]

$$u=-\frac{3}{2}\left(\frac{\wp_1'(\xi)-\wp_2'(\xi)}{\wp_1(\xi)-\wp_2(\xi)}\right)^2+6(\wp_1(\xi)+\wp_2(\xi)), \tag{65}$$

$$v^2=\frac{k_{2,0}}{\wp_2(\xi)-\wp_1(\xi)}. \tag{66}$$

In the case $\mu\neq0$, let us introduce the new variables

$$s_1=\sqrt{3\frac{k_2^2}{\mu}+q_1},\quad s_2=-\sqrt{3\frac{k_2^2}{\mu}+q_2}, \tag{67}$$

which transform Eqs. (61) and (62) into

$$s_1' = \sqrt{2k_1 - \frac{1}{3}\left(s_1^2 - 3\frac{k_2^2}{\mu}\right)^3 + c\left(s_1^2 - 3\frac{k_2^2}{\mu}\right) - \sqrt{\frac{\mu}{3}}s_1}\left(\frac{1}{s_1 - s_2}\right), \tag{68}$$

$$s_2' = -\sqrt{2k_1 - \frac{1}{3}\left(s_2^2 - 3\frac{k_2^2}{\mu}\right)^3 + c\left(s_2^2 - 3\frac{k_2^2}{\mu}\right) - \sqrt{\frac{\mu}{3}}s_2}\left(\frac{1}{s_1 - s_2}\right). \tag{69}$$

Defining

$$P(s) = 2k_1 - \frac{1}{3}\left(s^2 - 3\frac{k_2^2}{\mu}\right)^3 + c\left(s^2 - 3\frac{k_2^2}{\mu}\right) - \sqrt{\frac{\mu}{3}}s, \tag{70}$$

the system (68) and (69) can be solved by inversion of the hyperelliptic integrals

$$\int_\infty^{s_1} \frac{ds}{\sqrt{P(s)}} + \int_\infty^{s_2} \frac{ds}{\sqrt{P(s)}} = k_3, \tag{71}$$

$$\int_\infty^{s_1} \frac{s\,ds}{\sqrt{P(s)}} + \int_\infty^{s_2} \frac{s\,ds}{\sqrt{P(s)}} = \xi + k_4, \tag{72}$$

which define s_1 and s_2 as multivalued functions of ξ.[19,20]

The general solution of the equations of motion (30) in the case $\mu \neq 0$ is

$$u = -\frac{1}{2}(s_1^2 + s_2^2) + \frac{3}{\mu}k_2^2 - \frac{3}{2}\left(\frac{s_1' + s_2'}{s_1 + s_2}\right)^2, \tag{73}$$

$$v^2 = \frac{2\sqrt{3\mu}}{s_1 + s_2}. \tag{74}$$

As they are rational symmetric combinations of s_1 and s_2 and their derivatives, u and v^2 are single-valued functions of ξ.

In the variables q_1, q_2 this solution is expressed as

$$u = -\frac{3}{2}\left(\frac{\sqrt{2k_1 - (q_1^3/3) + cq_1 - \sqrt{k_2^2 + (\mu/3)q_1}} - \sqrt{2k_1 - (q_2^3/3) + cq_2 + \sqrt{k_2^2 + (\mu/3)q_2}}}{q_1 - q_2}\right)^2 - \frac{1}{2}(q_1 + q_2), \tag{75}$$

$$v^2 = 6\frac{\sqrt{k_2^2 + (\mu/3)q_1} + \sqrt{k_2^2 + (\mu/3)q_2}}{q_1 - q_2}, \tag{76}$$

which clearly goes to (65) and (66) in the limit $\mu \to 0$.

V. GENERAL SOLUTION OF THE SAWADA–KOTERA CASE

We start from the general solution (73) and (74) for KK and apply the canonical transformation (47) to obtain the general solution for the SK Hamiltonian system

$$U = \sqrt{-3}(s_1' + s_2') + s_1^2 + s_1 s_2 + s_2^2 - \frac{3}{\mu}K_2^2, \tag{77}$$

$$V^2=-2\sqrt{-3}(s_1+s_2)(s_1s_1'+s_2s_2')+2(s_1+s_2)^2\left(s_1^2+s_2^2-\frac{9K_2^2}{2\mu}\right). \tag{78}$$

Let us check that the limit of this solution when $\mu\to 0$ is (23). The expression (77) for U can also be written as

$$U=\frac{1}{2}(s_1^2+s_2^2)-\frac{3}{\mu}K_2^2+\frac{3}{2}\left(\frac{s_1'+s_2'}{s_1+s_2}\right)^2-\frac{3}{2}\left(\frac{s_1'+s_2'}{s_1+s_2}+\sqrt{-\frac{1}{3}}(s_1+s_2)\right)^2. \tag{79}$$

Since in the limit $\mu\to 0$

$$s_1+s_2=\mathcal{O}(\sqrt{\mu}),$$

$$\frac{s_1'+s_2'}{s_1+s_2}\to\frac{\wp_1'(\xi)-\wp_2'(\xi)}{\wp_1(\xi)-\wp_2(\xi)},$$

one has

$$\lim_{\mu\to 0} U=\tfrac{1}{2}(Q_1+Q_2). \tag{80}$$

Next, for V^2, the expansions

$$2(s_1+s_2)^2\left(s_1^2+s_2^2-\frac{9K_2^2}{2\mu}\right)=\frac{1}{4}(Q_1-Q_2)^2+\mathcal{O}(\mu),\quad \mu\to 0,$$

$$(s_1+s_2)(s_1s_1'+s_2s_2')=\mathcal{O}(\sqrt{\mu}),\quad \mu\to 0,$$

provide the limit of V^2 in (78). Therefore,

$$\lim_{\mu\to 0} V^2=\tfrac{1}{4}(Q_1-Q_2)^2. \tag{81}$$

VI. COMPARISON WITH THE RESULTS OF COSGROVE

Cosgrove[13] recently integrated the ODEs (11) and (13) with hyperelliptic functions, using the postmultiplier method.

To compare the two different ways of integration, let us recall the vocabulary introduced in Painlevé analysis of nonlinear differential equations, making the distinction between fixed and movable constants. A constant is called *fixed* if it appears explicitly in the differential equation, while it is *movable* if it is a constant of integration and therefore depends on the initial data.

In the Hamiltonian formalism, described by the system (28)–(33) and (24)–(27), k_1 (resp. K_1) and k_2 (resp. K_2) are movable constants, while μ is fixed (it appears in the equations of motion).

In Cosgrove's paper, the first integrals of the fourth order equation he obtained in formulas (4.3)–(4.4) and (5.6)–(5.7), which are therefore movable constants, correspond in the Hamiltonian formalism to k_2 (resp. K_2) and μ, respectively introduced as movable and fixed constants. In order to integrate the resulting second order sixth degree differential equation and transform it in a coupled system of first order equations for applying the postmultiplier method, Cosgrove defined ''suitable'' auxiliary variables chosen in a ''subjective'' way. Here the link between the canonical variables and its expressions (4.5)–(4.6) and (5.3)–(5.4) can be clearly established. Those expressions, which are ''hidden'' variables for the fourth order differential equation, are nothing else than the canonical variables v^2 (resp. V^2) and p_v^2 (resp. P_V^2) explicitly defined in the Hamiltonian formalism.

VII. CONCLUSION

We proved that the three integrable cases (SK, KdV_5, and KK) of the Hénon–Heiles Hamiltonian can be integrated in terms of hyperelliptic functions.

We will take advantage of the method developed here to integrate other Hamiltonian systems with two degrees of freedom and additional nonpolynomial terms.

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Generalized sine-Gordon/massive Thirring models and soliton/particle correspondences

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We consider a real Lagrangian off-critical submodel describing the soliton sector of the so-called conformal affine $sl(3)^{(1)}$ Toda model coupled to matter fields. The theory is treated as a constrained system in the context of Faddeev–Jackiw and the symplectic schemes. We exhibit the parent Lagrangian nature of the model from which generalizations of the sine-Gordon (GSG) or the massive Thirring (GMT) models are derivable. The dual description of the model is further emphasized by providing the relationships between bilinears of GMT spinors and relevant expressions of the GSG fields. In this way we exhibit the strong/weak coupling phases and the (generalized) soliton/particle correspondences of the model. The $sl(n)^{(1)}$ case is also outlined. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Integrable theories in two dimensions have been an extraordinary laboratory for the understanding of basic nonperturbative aspects of physical theories and various aspects, relevant in more realistic four-dimensional models, have been tested.[1] In particular the conformal affine Toda models coupled to (Dirac) matter fields (CATM)[2] for the $sl(2)^{(1)}$ and $sl(3)^{(1)}$ cases are discussed in Refs. 3, 4, and 5, respectively. The interest in such models comes from their integrability and duality properties,[2,4] which can be used as toy models to understand some phenomena; such as a confinement mechanism in quantum chromodynamics (QCD)[3,5] and the electric–magnetic duality in four-dimensional gauge theories, conjectured in Ref. 6 and developed in Ref. 7. The affine Toda model coupled to matter field (ATM) type systems may also describe some low dimensional condensed matter phenomena, such as self-trapping of electrons into solitons, see, e.g., Ref. 8, tunneling in the integer quantum Hall effect,[9] and, in particular, polyacteline molecule systems in connection with fermion number fractionization.[10]

Off-critical submodels, such as the $sl(2)$ ATM, can be obtained at the classical or quantum mechanical level through some convenient reduction processes starting from CATM.[4,11] In the $sl(2)$ case, using bosonization techniques, it has been shown that the classical equivalence between the $U(1)$ vector and topological currents holds true at the quantum level, and then leads to a bag model like mechanism for the confinement of the spinor fields inside the solitons; in addition, it has been shown that the $sl(2)$ ATM theory decouples into a sine-Gordon model (SG) and a free scalar.[3,12] These facts indicate the existence of a sort of duality in these models involving solitons and particles.[6] The symplectic structure of the $sl(2)$ ATM model has recently been studied[11] in the context of Faddeev–Jackiw (FJ)[13] and (constrained) symplectic methods.[14,15] Imposing the equivalence between the $U(1)$ vector and topological currents as a constraint there have been obtained the SG or the massive Thirring (MT) model.

One of the difficulties with generalizations of complex affine Toda field theories, beyond $su(2)$ and its associated SG model, has to do with unitarity. Whereas for practical applications

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such as low dimensional condensed matter systems (see Ref. 16 and references therein) and N-body problems in nuclear physics,[17] the properties of interest are usually integrability and nonperturbative results of multifield Lagrangians. Therefore, integrable quantum field theories with several fields (bosons and/or fermions) are of some importance.

In this paper we construct many field generalizations of SG/MT models based on soliton/particle duality and unitarity. Beyond the well-known $sl(2)$ case the related $sl(n)^{(1)}$ CATM model does not possess a local Lagrangian, therefore we resort to an off-critical submodel Lagrangian with well behaved classical solutions making use of the results of Ref. 5. In Ref. 5 the authors studied the $sl(3)^{(1)}$ CATM soliton solutions and some of their properties up to general two-soliton. Using the FJ and symplectic methods we show the parent Lagrangian[18] nature of the $sl(3)$ ATM model from which the generalized sine-Gordon (GSG) or the massive Thirring (GMT) models are derivable. We thus show that there are (at least classically) two equivalent descriptions of the model, by means of either the Dirac or the Toda type fields. The duality exchange of the coupling regimes $g \to 1/g$ and the generalized soliton/particle correspondences in each $sl(2)$ ATM submodel will also be clear, which we uncover by providing explicit relationships between the GSG and GMT fields. We also outline the steps toward the $sl(n)$ affine Lie algebra generalizations. In this way we give a precise field content of both sectors; namely, the correct GMT/GSG duality, first undertaken in Ref. 19.

The paper is organized as follows. In Sec. II we define the $sl(3)$ ATM model. Section III deals with the model in the FJ framework, the outcome is the GMT model. In Sec. IV, we attack the same problem from the point of view of symplectic quantization[14,15] giving the Poisson brackets of the GMT and GSG models. Section V deals with the soliton/particle and strong/weak coupling correspondences. Section VI outlines the relevant steps toward the generalization to $sl(n)$ ATM. In the appendix we present the construction of $sl(3)^{(1)}$ CATM model and its relationship to the (two-loop) Wess–Zumino–Novikov–Witten (WZNW) model.

II. DESCRIPTION OF THE MODEL

In affine Toda type theories the question of whether all mathematical solutions are physically acceptable deserves a careful analysis, especially if any consistent quantization of the models is discussed. The requirement of real energy density leads to certain reality conditions on the solutions of the model. In general, a few soliton solutions survive the reality constraint, if in addition one also demands positivity. These kind of issues are discussed in Refs. 20. Here we follow the prescription to restrict the model to a subspace of classical solutions which satisfy the physical principles of reality of energy density and soliton/particle correspondence.

In CATM models associated with the principal gradation of an affine Lie algebra we have a one-soliton solution (real Toda field) for each pair of Dirac fields ψ^i and $\tilde{\psi}^i$.[2] This fact allows us to make the identifications $\tilde{\psi}^i \sim (\psi^i)^*$, and take real Toda fields. In the case of $sl(2)^{(1)}$ CATM theory, this procedure does not spoil the particle–soliton correspondence.[3,4]

We consider the $sl(3)^{(1)}$ CATM theory (see the Appendix) with the conformal symmetry gauge fixed[21] by setting $\eta = 0$ and the reality conditions

$$\tilde{\psi}^j = -(\psi^j)^*, \quad (j = 1,2,3), \quad \varphi_a^* = \varphi_a \quad (a = 1,2), \tag{2.1}$$

or

$$\tilde{\psi}^j = (\psi^j)^*, \quad j = 1,2, \quad \tilde{\psi}^3 = -(\psi^3)^*,$$

$$\varphi_{1,2} \to \varphi_{1,2} - \pi \ \text{(the new } \varphi_a\text{'s being real fields)}, \tag{2.2}$$

where an asterisk means complex conjugation. The condition (2.2) must be supplied with $x^\mu \to -x^\mu$. Moreover, for consistency of the equations of motion (A15)–(A23) under the reality conditions (2.1) and (2.2), from Eqs. (A16) to (A18), (A20), (A21), and (A23), we get the relationships

$$\tilde{\psi}_L^j \psi_R^3 - \tilde{\psi}_R^j \psi_L^3 e^{-3i\varphi_j} = 0, \quad j = 1,2, \quad \psi_L^1 \psi_R^2 e^{-3i\varphi_1} - \psi_L^2 \psi_R^1 e^{-3i\varphi_2} = 0. \tag{2.3}$$

Then, the above-given reality conditions and constraints allow us to define a suitable physical Lagrangian. Equations (A13), (A15)–(A23), supplied with (2.1) [or (2.2)] and (2.3), follow from the Lagrangian

$$\frac{1}{k}\mathcal{L} = \sum_{j=1}^{3} \left[\frac{1}{24} \partial_\mu \phi_j \partial^\mu \phi_j + i \overline{\psi^j} \gamma^\mu \partial_\mu \psi^j - m_\psi^j \overline{\psi^j} e^{i\phi_j \gamma_5} \psi^j \right], \tag{2.4}$$

where $\overline{\psi^j} \equiv (\psi^j)^\dagger \gamma_0$, $\phi_1 \equiv 2\varphi_1 - \varphi_2$, $\phi_2 \equiv 2\varphi_2 - \varphi_1$, $\phi_3 \equiv \phi_1 + \phi_2$, $m_\psi^3 = m_\psi^1 + m_\psi^2$, k is an overall coupling constant and the φ_j are real fields.

Equation (2.4) defines the $sl(3)$ *affine Toda theory coupled to matter fields* (ATM). Notice that the space of solutions of $sl(3)^{(1)}$ CATM model satisfying conditions (2.1)–(2.3) must be solutions of the $sl(3)$ ATM theory (2.4). Indeed, it is easy to verify that the three species of one-soliton solutions [$S \equiv 1$-soliton($\overline{S} \equiv 1$-antisoliton)]:[5] $\{(\varphi_1, \psi^1)_{S/\overline{S}}, \varphi_2 = 0, \psi^2 = 0, \psi^3 = 0\}$, $\{(\varphi_2, \psi^2)_{S/\overline{S}}, \varphi_1 = 0, \psi^1 = 0, \psi^3 = 0\}$, and $\{(\varphi_1 + \varphi_2, \psi^3)_{S/\overline{S}}, \varphi_1 = \varphi_2, \psi^1 = 0, \psi^2 = 0\}$ satisfy the equations of motion, i.e., each positive root of $sl(3)$ reproduces the $sl(2)$ ATM case.[3,4] Moreover, these solutions satisfy the above-given reality conditions and constriants (2.1)–(2.3) [with (2.1) and (2.2) for S and $\overline{S}$, respectively], and the equivalence between the $U(1)$ vector and topological currents (A29). Then, the soliton/particle correspondences survive the above-given reduction processes performed to define the $sl(3)$ ATM theory.

The class of two-soliton solutions of $sl(3)^{(1)}$ CATM[5] behave as follows: (i) they are given by six species associated with the pair (α_i, α_j), $i \leqslant j$; $i,j = 1,2,3$; where the α's are the positive roots of $sl(3)$ Lie algebra. Each species (α_i, α_i) solves the $sl(2)$ CATM submodel;[22] (ii) satisfy the $U(1)$ vector and topological currents equivalence (A29).

III. THE GENERALIZED MASSIVE THIRRING MODEL (GMT)

Let us consider the following Lagrangian:

$$\frac{1}{k}\mathcal{L} = \sum_{j=1}^{3} \left[\frac{1}{24} \partial_\mu \phi_j \partial^\mu \phi_j + i \overline{\psi^j} \gamma^\mu \partial_\mu \psi^j - m_\psi^j \overline{\psi^j} e^{i\phi_j \gamma_5} \psi^j + \lambda_\mu^j (m^j \overline{\psi^j} \gamma^\mu \psi^j - \epsilon^{\mu\nu} \partial_\nu (q_j \phi_j)) \right], \tag{3.1}$$

where the ATM Lagrangian (2.4) is supplied with the constraints, $(m^l \overline{\psi^l} \gamma^\mu \psi^l + (m^3/2) \overline{\psi^3} \gamma^\mu \psi^3 - \epsilon^{\mu\nu} \partial_\nu \phi_l)$, $(l = 1,2)$, with the help of the Lagrange multipliers λ_μ^j ($\lambda_\mu^3 \equiv (\lambda_\mu^1 + \lambda_\mu^2)/2$, $q_1 \equiv q_2 \equiv 1$, $q_3 \equiv 0$). Their total sum bears an intriguing resemblance to the $U(1)$ vector and topological currents equivalence (A29); however, the m^j's here are some arbitrary parameters. The same procedure has been used, for example, to incorporate the left-moving condition in the study of chiral bosons in two dimensions.[23] The constraints in (3.1) will break the left–right local symmetries (A25)–(A28) of $sl(3)$ ATM (2.4). In order to apply the FJ method we should write (3.1) in the first-order form in time derivative, so let us define the conjugated momenta

$$\begin{gathered} \pi_1 \equiv \pi_{\phi_1} = \tfrac{1}{12}(2\dot{\phi}_1 + \dot{\phi}_2) + \lambda_1^1, \quad \pi_2 \equiv \pi_{\phi_2} = \tfrac{1}{12}(2\dot{\phi}_2 + \dot{\phi}_1) + \lambda_1^2, \\ \pi_{\lambda_\mu^1} = 0, \quad \pi_{\lambda_\mu^2} = 0, \quad \pi_R^j \equiv \pi_{\psi_R}^j = -i\tilde{\psi}_R^j, \quad \pi_L^j \equiv \pi_{\psi_L}^j = -i\tilde{\psi}_L^j. \end{gathered} \tag{3.2}$$

We are assuming that Dirac fields are anticommuting Grasmannian variables and their momenta variables defined through *left* derivatives. Then, as usual, the Hamiltonian is defined by (sum over repeated indices is assumed)

$$\mathcal{H}_c = \pi_1 \dot{\phi}_1 + \pi_2 \dot{\phi}_2 + \dot{\psi}_R^j \pi_R^j + \dot{\psi}_L^j \pi_L^j - \mathcal{L}. \tag{3.3}$$

Explicitly the Hamiltonian density becomes

$$\mathcal{H}_c = 2(\pi_j)^2 + 4(\lambda_1^1)^2 + 4(\lambda_1^2)^2 - \lambda_1^1 \mathcal{J}_1 - \lambda_1^2 \mathcal{J}_2 - 4(\lambda_1^1 \lambda_1^2) + \tfrac{1}{24}(\phi_{j,x})^2 - \pi_R^j \psi_{R,x}^j + \pi_L^j \psi_{L,x}^j + i m_\psi^j (e^{-\phi_j} \tilde{\psi}_R^j \psi_L^j - e^{\phi_j} \tilde{\psi}_L^j \psi_R^j) + \lambda_0^1 [J_1^0 - \phi_{1,x}] + \lambda_0^2 [J_2^0 - \phi_{2,x}], \tag{3.4}$$

where $\pi_3 \equiv \pi_1 - \pi_2$, $\mathcal{J}_1 \equiv J_1^1 + 4(2\pi_1 - \pi_2)$, $\mathcal{J}_2 \equiv J_2^1 + 4(2\pi_2 - \pi_1)$, and

$$J_1^\mu = m^1 j_l^\mu + \frac{m^3}{2} j_3^\mu, \quad J_2^\mu = m^2 j_2^\mu + \frac{m^3}{2} j_3^\mu, \quad j_l^\mu \equiv \overline{\psi^l} \gamma^\mu \psi^l, \quad l = 1,2,3. \tag{3.5}$$

Let us observe that each $U(1)$ Noether current of the $sl(3)$ ATM theory defined in (2.4) is conserved separately, i.e., $\partial_\mu j_l^\mu = 0$, $l = 1,2,3$.

Next, the same Legendre transform (3.3) is used to write the first-order Lagrangian

$$\mathcal{L} = \pi_1 \dot{\phi}_1 + \pi_2 \dot{\phi}_2 + \dot{\psi}_R^j \pi_R^j + \dot{\psi}_L^j \pi_L^j - \mathcal{H}_c. \tag{3.6}$$

Our starting point for the FJ analysis will be this first-order Lagrangian. Then the Euler–Lagrange equations for the Lagrange multipliers allow one to solve two of them

$$\lambda_1^1 = \frac{2\mathcal{J}_1 + \mathcal{J}_2}{12}, \quad \lambda_1^2 = \frac{2\mathcal{J}_2 + \mathcal{J}_1}{12} \tag{3.7}$$

and the remaining equations lead to two constraints,

$$\Omega_1 \equiv J_1^0 - \phi_{1,x} = 0, \quad \Omega_2 \equiv J_2^0 - \phi_{2,x} = 0. \tag{3.8}$$

The Lagrange multipliers λ_1^1 and λ_1^2 must be replaced back in (3.6) and the constraints (3.8) solved. First, let us replace the λ_1^1 and λ_1^2 multipliers into $\mathcal{H}_c$, then one gets

$$\mathcal{H}_c' = 2(\pi_j)^2 - \tfrac{1}{12}\{(\mathcal{J}_1)^2 + (\mathcal{J}_2)^2 + (\mathcal{J}_1 \mathcal{J}_2)\} + \tfrac{1}{24}(\phi_{j,x})^2 + i \tilde{\psi}_R^j \psi_{R,x}^j - i \tilde{\psi}_L^j \psi_{L,x}^j + i m_\psi^j (e^{-i\phi_j} \tilde{\psi}_R^j \psi_L^j - e^{i\phi_j} \tilde{\psi}_L^j \psi_R^j). \tag{3.9}$$

The new Lagrangian becomes

$$\mathcal{L}' = \pi_1 \dot{\phi}_1 + \pi_2 \dot{\phi}_2 + \dot{\psi}_R^j \pi_R^j + \dot{\psi}_L^j \pi_L^j - \mathcal{H}_c'. \tag{3.10}$$

We implement the constraints (3.8) by replacing in (3.10) the fields ϕ_1, ϕ_2 in terms of the space integral of the current components J_1^0, J_2^0. Then we get the Lagrangian

$$\mathcal{L}'' = \pi_1 \partial_t \int^x J_1^0 + \pi_2 \partial_t \int^x J_2^0 + \dot{\psi}_R^j \pi_R^j + \dot{\psi}_L^j \pi_L^j - i \tilde{\psi}_R^j \psi_{R,x}^j + i \tilde{\psi}_L^j \psi_{L,x}^j - i m_\psi^j (e^{-i\int^x J_j^0} \tilde{\psi}_R^j \psi_L^j - e^{i\int^x J_j^0} \tilde{\psi}_L^j \psi_R^j) - \tfrac{1}{12}((J_1)^2 + (J_2)^2 + J_1 . J_2) + \pi_1 J_1^1 + \pi_2 J_2^1, \tag{3.11}$$

where $J_3^0 \equiv J_1^0 + J_2^0$. Observe that the terms containig the π_a's in Eq. (3.11) cancel to each other if one uses the current conservation laws. Notice the appearances of various types of current–current interactions. The following Darboux transformation:

$$\psi_R^j \to \exp\left(-\frac{i}{2}\int^x J_j^0\right) \psi_R^j, \quad \psi_L^j \to \exp\left(\frac{i}{2}\int^x J_j^0\right) \psi_L^j, \quad j = 1,2,3 \tag{3.12}$$

is used to diagonalize the canonical one-form. Then, the kinetic terms will give additional current–current interactions, $-\frac{1}{2}[J_1\cdot(j_1+j_3)+J_2\cdot(j_2+j_3)]$. We are, thus, after defining $k\equiv 1/g$, and rescaling the fields $\psi^j\to 1/\sqrt{k}\,\psi^j$, left with the Lagrangian

$$\mathcal{L}[\psi,\overline{\psi}]=\sum_{j=1}^{3}\{i\overline{\psi^j}\gamma^\mu\partial_\mu\psi^j+m_\psi^j\,\overline{\psi^j}\psi^j\}-\sum_{\substack{k,l=1\\k\leqslant l}}^{3}[\overline{a_{kl}}j_k\cdot j_l], \tag{3.13}$$

where $\overline{a_{kl}}=g\,a_{kl}$, with

$$a_{33}=\frac{1}{2}\left(\frac{(m^3)^2}{8}+m^3\right),\quad a_{12}=\frac{1}{12}m^1m^2,\quad a_{ii}=\frac{1}{2}\left(\frac{(m^i)^2}{6}+m^i\right),$$

$$a_{i3}=\frac{1}{2}\left(\frac{m^im^3}{4}+m^i+\frac{m^3}{2}\right),\quad i=1,2.$$

This defines the *generalized massive Thirring model* (GMT). The canonical pairs are $(-i\tilde{\psi}_R^j,\psi_R^j)$ and $(-i\tilde{\psi}_L^j,\psi_L^j)$.

IV. THE SYMPLECTIC FORMALISM AND THE ATM MODEL

A. The (constrained) symplectic formalism

We give a brief overview of the basic notations of symplectic approach.[24] The geometric structure is defined by the closed (pre)symplectic two-form

$$f^{(0)}=\tfrac{1}{2}f_{ij}^{(0)}(\xi^{(0)})\mathrm{d}\xi^{(0)i}\wedge\mathrm{d}\xi^{(0)j}, \tag{4.1}$$

where

$$f_{ij}^{(0)}(\xi^{(0)})=\frac{\partial}{\partial\xi^{(0)i}}\mathbf{a}_j^{(0)}(\xi^{(0)})-\frac{\partial}{\partial\xi^{(0)j}}\mathbf{a}_i^{(0)}(\xi^{(0)}) \tag{4.2}$$

with $\mathbf{a}^{(0)}(\xi^{(0)})=\mathbf{a}_j^{(0)}(\xi^{(0)})\mathrm{d}\xi^{(0)j}$ being the canonical one-form defined from the original first-order Lagrangian

$$L^{(0)}\mathrm{d}t=\mathbf{a}^{(0)}(\xi^{(0)})-V^{(0)}(\xi^{(0)})\mathrm{d}t. \tag{4.3}$$

The superscript (0) refers to the original Lagrangian, and is indicative of the iterative nature of the computations. The constraints are imposed through Lagrange multipliers which are velocities, and in such case one has to extend the configuration space.[14,15] The corresponding Lagrangian gets modified and consequently the superscript also changes. The algorithm terminates once the symplectic matrix turns out to be nonsingular.

B. The generalized massive Thirring model (GMT)

Next, we will consider our model in the framework of the symplectic formalism. Let $\mathcal{L}'$, Eq. (3.10), be the zeroth-iterated Lagrangian $\mathcal{L}^{(0)}$. Then the first iterated Lagrangian will be

$$\mathcal{L}^{(1)}=\pi_1\dot{\phi}_1+\pi_2\dot{\phi}_2+\dot{\psi}_R^j\pi_R^j+\dot{\psi}_L^j\pi_L^j+\dot{\eta}^1\Omega_1+\dot{\eta}^2\Omega_2-\mathcal{V}^{(1)}, \tag{4.4}$$

where the once-iterated symplectic potential is defined by

$$\mathcal{V}^{(1)}=\mathcal{H}_c'|_{\Omega_1=\Omega_2=0}, \tag{4.5}$$

and the stability conditions of the symplectic constraints, Ω_1 and Ω_2, under time evolution have been implemented by making $\lambda_0^1 \to \dot{\eta}^1$ and $\lambda_0^2 \to \dot{\eta}^2$. Consider the once-iterated set of symplectic variables in the following order

$$\xi^{(1)} = (\eta^1, \eta^2, \phi_1, \phi_2, \psi_R^1, \psi_L^1, \psi_R^2, \psi_L^2, \psi_R^3, \psi_L^3, \pi_1, \pi_2, \pi_R^1, \pi_L^1, \pi_R^2, \pi_L^2, \pi_R^3, \pi_L^3), \tag{4.6}$$

and the components of the canonical one-form

$$\mathbf{a}^{(1)} = (\Omega_1, \Omega_2, \pi_1, \pi_2, -\pi_R^1, -\pi_L^1, -\pi_R^2, -\pi_L^2, -\pi_R^3, -\pi_L^3, 0,0,0,0,0,0,0,0,0). \tag{4.7}$$

These result in the singular symplectic two-form 18×18 matrix

$$f_{AB}^{(1)}(x,y) = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \delta(x-y), \tag{4.8}$$

where the 9×9 martices are

$$a_{11} = \begin{pmatrix} 0 & 0 & \partial_x & 0 & im^1\tilde{\psi}_R^1 & im^1\tilde{\psi}_L^1 & 0 & 0 & \frac{im^3}{2}\tilde{\psi}_R^3 \\ 0 & 0 & 0 & \partial_x & 0 & 0 & im^2\tilde{\psi}_R^2 & im^2\tilde{\psi}_L^2 & \frac{im^3}{2}\tilde{\psi}_R^3 \\ \partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ im^1\tilde{\psi}_R^1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ im^1\tilde{\psi}_L^1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & im^2\tilde{\psi}_R^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & im^2\tilde{\psi}_L^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_R^3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$a_{12} = \begin{pmatrix} \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & m^1\psi_R^1 & m^1\psi_L^1 & 0 & 0 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\ \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & m^2\psi_R^2 & m^2\psi_L^2 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \vdots & 0 & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix},$$

$$a_{21}=\begin{pmatrix} \frac{im^3}{2}\tilde{\psi}^3_L & \frac{im^3}{2}\tilde{\psi}^3_L & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ m^1\psi^1_R & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ m^1\psi^1_L & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & m^2\psi^2_R & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & m^2\psi^2_L & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ \frac{m^3}{2}\psi^3_R & \frac{m^3}{2}\psi^3_R & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ \frac{m^3}{2}\psi^3_L & \frac{m^3}{2}\psi^3_L & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$a_{22}=\begin{pmatrix} 0 & 0 & \cdots & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

This matrix has the zero modes

$$\mathbf{v}^{(1)T}(x)=\left(\frac{-u}{m^1},\frac{-v}{m^2},0,0,u\psi^1_R,u\psi^1_L,v\psi^2_R,v\psi^2_L,\frac{m^3}{2}\left(\frac{u}{m^1}+\frac{v}{m^2}\right)\psi^3_R,\frac{m^3}{2}\left(\frac{u}{m^1}+\frac{v}{m^2}\right)\psi^3_L,-\frac{u'}{m^1},\right.$$
$$\left.-\frac{v'}{m^2},iu\tilde{\psi}^1_R,iu\tilde{\psi}^1_L,iv\tilde{\psi}^2_R,iv\tilde{\psi}^2_L,i\frac{m^3}{2}\left(\frac{u}{m^1}+\frac{v}{m^2}\right)\tilde{\psi}^3_R,\frac{im^3}{2}\left(\frac{u}{m^1}+\frac{v}{m^2}\right)\tilde{\psi}^3_L\right), \tag{4.9}$$

where u and v are arbitrary functions. The zero-mode condition gives

$$\int \mathrm{d}x\mathbf{v}^{(1)T}(x)\frac{\delta}{\delta\xi^{(1)}(x)}\int \mathrm{d}y\mathcal{V}^{(1)}\equiv 0. \tag{4.10}$$

Thus, the gradient of the symplectic potential happens to be orthogonal to the zero-mode $\mathbf{v}^{(1)}$. Since the equations of motion are automatically validated no symplectic constraints appear. This happens due to the presence of the symmetries of the action

$$\delta\xi^{(1)}_A=\mathbf{v}^{(1)}_{\mathbf{A}}(x),\quad A=1,2,\ldots,18. \tag{4.11}$$

So, in order to deform the symplectic matrix into an invertible one, we have to add some gauge fixing terms to the symplectic potential. One can choose any consistent set of gauge fixing conditions.[15] In our case we have two symmetry generators associated with the parameters u and v, so there must be two gauge conditions. Let us choose

$$\Omega_3\equiv\phi_1=0,\quad \Omega_4\equiv\phi_2=0. \tag{4.12}$$

These conditions gauge away the fields ϕ_1 and ϕ_2, so only the remaining field variables will describe the dynamics of the system. Other gauge conditions, which eventually gauge away the spinor fields ψ^i, will be considered in Sec. IV C.

Implementing the consistency conditions by means of Lagrange multipliers η^3 and η^4 we get the twice-iterated Lagrangian

$$\mathcal{L}^{(2)}=\pi_1\dot{\phi}_1+\pi_2\dot{\phi}_2+\dot{\psi}_R\pi_R^j+\dot{\psi}_L\pi_L^j+\dot{\eta}^1\Omega_1+\dot{\eta}^2\Omega_2+\dot{\eta}^3\Omega_3+\dot{\eta}^4\Omega_4-\mathcal{V}^{(2)}, \tag{4.13}$$

where

$$\mathcal{V}^{(2)}=\mathcal{V}^{(1)}|_{\Omega_3=\Omega_4=0}.$$

Assuming now that the new set of symplectic variables is given in the following order,

$$\xi^{(2)}=(\eta^1,\eta^2,\eta^3,\eta^4,\phi_1,\phi_2,\psi_R^1,\psi_L^1,\psi_R^2,\psi_L^2,\psi_R^3,\psi_L^3,\pi_1,\pi_2,\pi_R^1,\pi_L^1,\pi_R^2,\pi_L^2,\pi_R^3,\pi_L^3), \tag{4.14}$$

and the nonvanishing components of the canonical one-form

$$\mathbf{a}^{(2)}=(\Omega_1,\Omega_2,\Omega_3,\Omega_4,\pi_1,\pi_2,-\pi_R^1,-\pi_L^1,-\pi_R^2,-\pi_L^2,-\pi_R^3,-\pi_L^3,0,0,0,0,0,0,0,0), \tag{4.15}$$

one obtains the singular twice-iterated symplectic 20×20 matrix

$$f_{AB}^{(2)}(x,y)=\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}\delta(x-y), \tag{4.16}$$

where the 10×10 matrices are

$$a_{11}=\begin{pmatrix}
0 & 0 & 0 & 0 & \partial_x & 0 & im^1\tilde{\psi}_R^1 & im^1\tilde{\psi}_L^1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \partial_x & 0 & 0 & im^2\tilde{\psi}_R^2 & im^2\tilde{\psi}_L^2 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
\partial_x & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \partial_x & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
im^1\tilde{\psi}_R^1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
im^1\tilde{\psi}_L^1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & im^2\tilde{\psi}_R^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & im^2\tilde{\psi}_L^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},$$

$$a_{12}=\begin{pmatrix}
\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & m^1\psi_R^1 & m^1\psi_L^1 & 0 & 0 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & m^2\psi_R^2 & m^2\psi_L^2 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0
\end{pmatrix},$$

$$a_{21}=\begin{pmatrix}
\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_R^3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{im^3}{2}\tilde{\psi}_L^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
m^1\psi_R^1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
m^1\psi_L^1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & m^2\psi_R^2 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & m^2\psi_L^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
\frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_R^3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{m^3}{2}\psi_L^3 & \frac{m^3}{2}\psi_L^3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},$$

$$a_{22}=\begin{pmatrix}
0 & 0 & 0 & \cdots & 0 & -1 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & -1 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
\multicolumn{7}{c}{\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots} \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
-1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & -1 & 0 & \cdots & 0 & 0 & 0
\end{pmatrix}.$$

The zero-modes are

$$\mathbf{v}^{(2)T}(x)=\Big(u,\ v,\ \omega,\ \chi,\ 0,\ 0,\ m^1u\psi_R^1,\ m^1u\psi_L^1,\ m^2v\psi_R^2,\ m^2v\psi_L^2,\ \frac{m^3}{2}(u+v)\psi_R^3,$$
$$\frac{m^3}{2}(u+v)\psi_L^3,\ u'+\omega,\ v'+\chi,\ im^1\tilde{\psi}_R^1u,\ im^1\tilde{\psi}_L^1u,\ im^2\tilde{\psi}_R^2v,im^2\tilde{\psi}_L^2v,$$
$$\frac{im^3}{2}\tilde{\psi}_R^3(u+v),\ i\frac{m^3}{2}\tilde{\psi}_L^3(u+v)\Big). \tag{4.17}$$

The zero-mode condition gives no constraints, implying the symmetries of the action

$$\delta\xi_{\mathbf{A}}^{(2)}=\mathbf{v}_{\mathbf{A}}^{(2)}(x),\quad A=1,2,\ldots,20. \tag{4.18}$$

Now, let us choose the gauge conditions

$$\Omega_5\equiv\pi_1J_1^1+\tfrac{1}{2}J_1\cdot(j_1+j_3)=0,\quad \Omega_6\equiv\pi_2J_2^1+\tfrac{1}{2}J_2\cdot(j_2+j_3)=0, \tag{4.19}$$

and impose the consistency conditions with the Lagrange multipliers η^5,η^6, then

$$\mathcal{L}^{(3)}=\pi_1\dot{\phi}_1+\pi_2\dot{\phi}_2+\dot{\psi}_R\pi_R^j+\dot{\psi}_L\pi_L^j+\dot{\eta}^1\Omega_1+\dot{\eta}^2\Omega_2+\dot{\eta}^3\Omega_3+\dot{\eta}^4\Omega_4+\dot{\eta}^5\Omega_5+\dot{\eta}^6\Omega_6-\mathcal{V}^{(3)}, \tag{4.20}$$

where

$$\mathcal{V}^{(3)}=\mathcal{V}^{(2)}|_{\Omega_5=\Omega_6=0}, \tag{4.21}$$

or explicitly

$$\mathcal{V}^{(3)}=\tfrac{1}{12}((J_1)^2+(J_2)^2+J_1\cdot J_2)+\tfrac{1}{2}[J_1\cdot(j_1+j_3)+J_2\cdot(j_2+j_3)]+i\tilde{\psi}_R^j\psi_{R,x}^j-i\tilde{\psi}_L^j\psi_{L,x}^j+im_\psi^j\overline{\psi^j}\psi^j. \tag{4.22}$$

The symplectic two-form for this Lagrangian is a nonsingular matrix, then our algorithm has come to an end. Collecting the canonical part and the symplectic potential $\mathcal{V}^{(3)}$ one has

$$\mathcal{L}[\psi,\overline{\psi}]=\sum_{j=1}^{3}\{i\overline{\psi^j}\gamma^\mu\partial_\mu\psi^j+m_\psi^j\overline{\psi^j}\psi^j\}-\sum_{\substack{k,l=1\\k\leqslant l}}^{3}[\overline{a}_{kl}j_k.j_l]+\sum_{l=1}^{3}m^l\nu_lj_l^0, \tag{4.23}$$

where $\nu_3\equiv(\nu_1+\nu_2)/2$. We have made the same choice, $k=1/g$, and the field rescalings $\psi^j\to1/\sqrt{k}\,\psi^j$ as in the last section. This is the same GMT Lagrangian as (3.13). As a bonus, we get the chemical potentials $\mu_l\equiv m^l\nu_l$ ($\dot{\eta}^{1,2}\to\nu_{1,2}$) times the charge densities. These terms are related to the charges $Q_F^l=1/2\pi\int_{-\infty}^{+\infty}dx\,j_l^0(t,x)$, and their presence is a consequence of the symplectic method.[11]

C. The generalized sine-Gordon model (GSG)

One can choose other gauge fixings, instead of (4.12), to construct the twice-iterated Lagrangian. Let us make the choice

$$\Omega_3\equiv J_1^0=0,\quad \Omega_4\equiv J_2^0=0, \tag{4.24}$$

which satisfies the nongauge invariance condition as can be verified by computing the brackets $\{\Omega_a,J_b^0\}=0$; $a,b=1,2$. The twice-iterated Lagrangian is obtained by bringing back these constraints into the canonical part of $\mathcal{L}^{(1)}$, then

$$\mathcal{L}^{(2)}=\pi_1\dot{\phi}_1+\pi_2\dot{\phi}_2+\dot{\psi}_R\pi_R^j+\dot{\psi}_L\pi_L^j+\dot{\eta}^1\Omega_1+\dot{\eta}^2\Omega_2+\dot{\eta}^3\Omega_3+\dot{\eta}^4\Omega_4-\mathcal{V}^{(2)}, \tag{4.25}$$

where the twice-iterated symplectic potential becomes

$$\mathcal{V}^{(2)}=\mathcal{V}^{(1)}\big|_{\Omega_3=\Omega_4=0}. \tag{4.26}$$

Considering the set of symplectic variables in the following order:

$$\xi_A^{(2)}=(\eta^1,\eta^2,\eta^3,\eta^4,\phi_1,\phi_2,\psi_R^1,\psi_L^1,\psi_R^2,\psi_L^2,\psi_R^3,\psi_L^3,\pi_1,\pi_2,\pi_R^1,\pi_L^1,\pi_R^2,\pi_L^2,\pi_R^3,\pi_L^3) \tag{4.27}$$

and the components of the canonical one-form

$$a_A^{(2)}=(\Omega_1,\Omega_2,\Omega_3,\Omega_4,\pi_1,\pi_2,-\pi_R^1,-\pi_L^1,-\pi_R^2,-\pi_L^2,-\pi_R^3,-\pi_L^3,0,0,0,0,0,0,0,0), \tag{4.28}$$

the (degenerated) 20×20 symplectic matrix is found to be

$$f_{AB}^{(2)}(x,y)=\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}\delta(x-y), \tag{4.29}$$

where

$$a_{11}=\begin{pmatrix}
0 & 0 & 0 & 0 & \partial_x & 0 & im^1\tilde{\psi}_R^1 & im^1\tilde{\psi}_L^1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \partial_x & 0 & 0 & im^2\tilde{\psi}_R^2 & im^2\tilde{\psi}_L^2 \\
0 & 0 & 0 & 0 & 0 & 0 & im^1\tilde{\psi}_R^1 & im^1\tilde{\psi}_L^1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & im^2\tilde{\psi}_R^2 & im^2\tilde{\psi}_L^2 \\
\partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
im^1\tilde{\psi}_R^1 & 0 & im^1\tilde{\psi}_R^1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
im^1\tilde{\psi}_L^1 & 0 & im^1\tilde{\psi}_L^1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & im^2\tilde{\psi}_R^2 & 0 & im^2\tilde{\psi}_R^2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & im^2\tilde{\psi}_L^2 & 0 & im^2\tilde{\psi}_L^2 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},$$

$$a_{12}=\begin{pmatrix}
\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & m^1\psi_R^1 & m^1\psi_L^1 & 0 & 0 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & m^2\psi_R^2 & m^2\psi_L^2 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & m^1\psi_R^1 & m^1\psi_L^1 & 0 & 0 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & m^2\psi_R^2 & m^2\psi_L^2 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0
\end{pmatrix},$$

$$a_{21}=\begin{pmatrix}
\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_R^3 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{im^3}{2}\tilde{\psi}_L^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0\\
m^1\psi_R^1 & 0 & m^1\psi_R^1 & 0 & 0 & 0 & -1 & 0 & 0 & 0\\
m^1\psi_L^1 & 0 & m^1\psi_L^1 & 0 & 0 & 0 & 0 & -1 & 0 & 0\\
0 & m^2\psi_R^2 & 0 & m^2\psi_R^2 & 0 & 0 & 0 & 0 & -1 & 0\\
0 & m^2\psi_L^2 & 0 & m^2\psi_L^2 & 0 & 0 & 0 & 0 & 0 & -1\\
\frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_R^3 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{m^3}{2}\psi_L^3 & \frac{m^3}{2}\psi_L^3 & \frac{m^3}{2}\psi_L^3 & \frac{m^3}{2}\psi_L^3 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},$$

$$a_{22}=\begin{pmatrix}
0 & 0 & 0 & \cdots & 0 & -1 & 0\\
0 & 0 & 0 & \cdots & 0 & 0 & -1\\
0 & 0 & 0 & \cdots & 0 & 0 & 0\\
\multicolumn{7}{c}{\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots}\\
0 & 0 & 0 & \cdots & 0 & 0 & 0\\
-1 & 0 & 0 & \cdots & 0 & 0 & 0\\
0 & -1 & 0 & \cdots & 0 & 0 & 0
\end{pmatrix}.$$

Its zero modes are

$$\begin{aligned}\mathbf{v}^{(2)T}(x)=\Big(&u,\ v,\ \omega,\ \chi,\ 0,\ 0,\ m^1(u+\omega)\psi_R^1,\ m^1(u+\omega)\psi_L^1,\ m^2(v+\chi)\psi_R^2,\ m^2(v+\chi)\psi_L^2,\\
&\frac{m^3}{2}(u+v+\omega+\chi)\psi_R^3,\ \frac{m^3}{2}(u+v+\omega+\chi)\psi_L^3,\ u',\ v',\ im^1\tilde{\psi}_R^1(u+\omega),\\
&im^1\tilde{\psi}_L^1(u+\omega),\ im^2\tilde{\psi}_R^2(v+\chi),\ im^2\tilde{\psi}_L^2(v+\chi),\ \frac{im^3}{2}\tilde{\psi}_R^3(u+v+\omega+\chi),\\
&\frac{im^3}{2}\tilde{\psi}_L^3(u+v+\omega+\chi)\Big),\end{aligned}\tag{4.30}$$

where u, v, ω, and χ are arbitrary functions. The zero-mode condition becomes

$$\int \mathrm{d}x\,\mathbf{v}^{(2)T}(x)\frac{\delta}{\delta\xi^{(2)}}\int \mathrm{d}y'\,\mathcal{V}^{(2)}=\int \mathrm{d}x\,J_a^1\,\partial_x f_a\equiv 0,\quad f_a\equiv(\omega,\chi),\quad a=1,2.$$

Since the functions f_a are arbitrary we end up with the following constraints:

$$\Omega_5\equiv J_1^1=0,\quad \Omega_6\equiv J_2^1=0.\tag{4.31}$$

Notice that by solving the constraints, $\Omega_3=\Omega_4=\Omega_5=\Omega_6=0$, Eqs. (4.24) and (4.31), we may obtain

$$\tilde{\psi}_R^j = \psi_R^j, \quad \tilde{\psi}_L^j = \psi_L^j. \tag{4.32}$$

So, at this stage, we have Majorana spinors, the scalars ϕ_1 and ϕ_2, and the auxiliary fields. Next, introduce a third set of Lagrange multipliers into $\mathcal{L}^{(2)}$, then

$$\mathcal{L}^{(3)} = \pi_1\dot{\phi}_1 + \pi_2\dot{\phi}_2 + \dot{\psi}_R\pi_R^j + \dot{\psi}_L\pi_L^j + \dot{\eta}^1\Omega_1 + \dot{\eta}^2\Omega_2 + \dot{\eta}^3\Omega_3 + \dot{\eta}^4\Omega_4 + \dot{\eta}^5\Omega_5 + \dot{\eta}^6\Omega_6 - \mathcal{V}^{(3)}, \tag{4.33}$$

where

$$\mathcal{V}^{(3)} = \mathcal{V}^{(2)}|_{\Omega_5=\Omega_6=0} \tag{4.34}$$

or

$$\mathcal{V}^{(3)} = \tfrac{1}{24}\phi_{j,x}^2 + i\psi_R^j\psi_{R,x}^j - i\psi_L^j\psi_{L,x}^j + im_\psi^j\psi_R^j\psi_L^j(e^{-i\phi_j} + e^{i\phi_j}). \tag{4.35}$$

The new set of symplectic variables is assumed to be ordered as

$$\xi_A^{(3)} = (\eta^1, \eta^2, \eta^3, \eta^4, \eta^5, \eta^6, \phi_1, \phi_2, \psi_R^1, \psi_L^1, \psi_R^2, \psi_L^2, \psi_R^3, \psi_L^3, \pi_1, \pi_2, \pi_R^1, \pi_L^1, \pi_R^2, \pi_L^2, \pi_R^3, \pi_L^3).$$

The components of the canonical one-form are

$$a_A^{(3)} = (\Omega_1, \Omega_2, \Omega_3, \Omega_4, \Omega_5, \Omega_6, \pi_1, \pi_2, -\pi_R^1, -\pi_L^1, -\pi_R^2, -\pi_L^2, -\pi_R^3, -\pi_L^3, 0,0,0,0,0,0,0,0).$$

After some algebraic manipulations we get the third-iterated 22×22 symplectic two-form

$$f_{AB}^{(3)}(x,y) = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \delta(x-y), \tag{4.36}$$

where

$$a_{11} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & \partial_x & 0 & im^1\tilde{\psi}_R^1 & im^1\tilde{\psi}_L^1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \partial_x & 0 & 0 & im^2\tilde{\psi}_R^2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & im^1\tilde{\psi}_R^1 & im^1\tilde{\psi}_L^1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & im^2\tilde{\psi}_R^2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -im^1\tilde{\psi}_R^1 & im^1\tilde{\psi}_L^1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -im^2\tilde{\psi}_R^2 \\
\partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
im^1\tilde{\psi}_R^1 & 0 & im^1\tilde{\psi}_R^1 & 0 & -im^1\tilde{\psi}_R^1 & 0 & 0 & 0 & 0 & 0 & 0 \\
im^1\tilde{\psi}_L^1 & 0 & im^1\tilde{\psi}_L^1 & 0 & im^1\tilde{\psi}_L^1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & im^2\tilde{\psi}_R^2 & 0 & im^2\tilde{\psi}_R^2 & 0 & -im^2\tilde{\psi}_R^2 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},$$

$$a_{12}=\begin{pmatrix}
0 & \frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & m^1\psi_R^1 & m^1\psi_L^1 & 0 & 0 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
im^2\tilde{\psi}_L^2 & \frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & m^2\psi_R^2 & m^2\psi_L^2 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
0 & \frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & m^1\psi_R^1 & m^1\psi_L^1 & 0 & 0 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
im^2\tilde{\psi}_L^2 & \frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & m^2\psi_R^2 & m^2\psi_L^2 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
0 & -\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & -m^1\psi_R^1 & m^1\psi_L^1 & 0 & 0 & -\frac{m^2}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
im^2\tilde{\psi}_L^2 & -\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & -m^2\psi_R^2 & m^2\psi_L^2 & -\frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_L^3 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0
\end{pmatrix},$$

$$a_{21}=\begin{pmatrix}
0 & im^2\tilde{\psi}_L^2 & 0 & im^2\tilde{\psi}_L^2 & 0 & im^2\tilde{\psi}_L^2 & 0 & 0 & 0 & 0 & 0 \\
\frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_R^3 & \frac{im^3}{2}\tilde{\psi}_R^3 & -\frac{im^3}{2}\tilde{\psi}_R^3 & -\frac{im^3}{2}\tilde{\psi}_R^3 & 0 & 0 & 0 & 0 & 0 \\
\frac{im^3}{2}\tilde{\psi}_L^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & \frac{im^3}{2}\tilde{\psi}_L^3 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
m^1\psi_R^1 & 0 & m^1\psi_R^1 & 0 & -m^1\psi_R^1 & 0 & 0 & 0 & -1 & 0 & 0 \\
m^1\psi_L^1 & 0 & m^1\psi_L^1 & 0 & m^1\psi_L^1 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & m^2\psi_R^2 & 0 & m^2\psi_R^2 & 0 & -m^2\psi_R^2 & 0 & 0 & 0 & 0 & -1 \\
0 & m^2\psi_L^2 & 0 & m^2\psi_L^2 & 0 & m^2\psi_L^2 & 0 & 0 & 0 & 0 & 0 \\
\frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_R^3 & \frac{m^3}{2}\psi_R^3 & -\frac{m^3}{2}\psi_R^3 & -\frac{m^3}{2}\psi_R^3 & 0 & 0 & 0 & 0 & 0 \\
\frac{m^3}{2}\psi_L^3 & \frac{m^3}{2}\psi_L^3 & \frac{m^3}{2}\psi_L^3 & \frac{m^3}{2}\psi_L^3 & \frac{m^3}{2}\psi_L^3 & \frac{m^3}{2}\psi_L^3 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},$$

$$a_{22}=\begin{pmatrix}
0 & 0 & 0 & 0 & \cdots & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
 & & & & \cdots\cdots & & & & \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0
\end{pmatrix}.$$

It can be checked that this matrix has the zero modes

$$\mathbf{v}^{(3)}(x)=\Big(u,\ v,\ \omega,\ \chi,\ y,\ z,\ 0,\ 0,\ m^1a_1^-\psi_R^1,\ m^1a_1^+\psi_L^1,\ m^2a_2^-\psi_R^2,\ m^2a_2^+\psi_L^2,\ \frac{m^3}{2}a_3^-\psi_R^3,$$
$$\frac{m^3}{2}a_3^+\psi_L^3,\ u',\ v',\ im^1a_1^-\tilde{\psi}_R^1,\ im^1a_1^+\tilde{\psi}_L^1,\ im^2a_2^-\tilde{\psi}_R^2,\ im^2a_2^+\tilde{\psi}_L^2,$$
$$i\frac{m^3}{2}a_3^-\tilde{\psi}_R^3,\ i\frac{m^3}{2}a_3^+\tilde{\psi}_L^3\Big), \tag{4.37}$$

where $a_1^+\equiv u+\omega+y$, $a_2^+\equiv v+\chi+z$, $a_3^+\equiv u+\omega+y+v+\chi+z$, $a_1^-\equiv u+\omega-y$, $a_2^-\equiv v+\chi-z$, $a_3^+\equiv u+\omega+y+v-\chi-z$, and u, v, ω, χ, y, and z are arbitrary functions. The relevant zero-mode condition gives no constraints. Then the action has the following symmetries:

$$\delta\xi_A^{(3)}=\mathbf{v_A^{(3)}}(x),\quad A=1,2,\ldots,22. \tag{4.38}$$

These symmetries allow us to fix the bilinears $i\psi_R^j\psi_L^j$ to be constants. By taking $\psi_R^j=-iC_j\overline{\theta}_j$ and $\psi_L^j=\theta_j$ $(j=1,2,3)$ with C_j being real numbers, we find that $i\psi_R^j\psi_L^j$ indeed becomes a constant. Note that θ_j and $\overline{\theta}_j$ are Grassmannian variables, while $\overline{\theta}_j\theta_j$ is an ordinary commuting number.

The two form $f_{AB}^{(3)}(x,y)$, Eq. (4.36), in the subspace $(\phi_1,\phi_2,\pi_{\phi_1},\pi_{\phi_2})$ defines a canonical symplectic structure modulo canonical transformations. The coordinates ϕ_a and π_{ϕ_a} $(a=1,2)$ are not unique. Consider a canonical transformation from (ϕ_a,π_{ϕ_a}) to $(\hat{\phi}_a,\hat{\pi}_{\hat{\phi}_a})$ such that $\phi_a=\partial F/\partial\pi_{\phi_a}$ and $\hat{\phi}_a=\partial F/\partial\hat{\pi}_{\hat{\phi}_a}$. Then, in particular if $\phi_a=\hat{\phi}_a$ one can, in principle, solve for the function F such that a manifestly covariant kinetic term appears in the new Lagrangian.

Then choosing $k=1/g$ as the overall coupling constant, we are left with

$$\mathcal{L}''=\sum_{j=1}^{3}\left[\frac{1}{24g}\partial_\mu\phi_j\partial^\mu\phi_j+\frac{M_j}{g}\cos\phi_j\right]+\mu_1\partial_x\phi_1+\mu_2\partial_x\phi_2, \tag{4.39}$$

where $M_j=m_\psi^jC_j$. This defines the *generalized sine-Gordon model* (GSG). In addition we get the terms multiplied by chemical potentials μ_1 and μ_2 $(\dot{\eta}^{1,2}\rightarrow-\mu_{1,2})$. These are just the topological charge densities, and are related to the conservation of the number of kinks minus antikinks $Q^a_{\text{topol}}=1/\pi\int_{-\infty}^{+\infty}\mathrm{d}x\,\partial_x\phi_a$.

In the above-mentioned gauge fixing procedures the possibility of Gribov-type ambiguities deserves a careful analysis. See Ref. 11 for a discussion in the $sl(2)$ ATM case. However, in Sec. V, we provide indirect evidence of the absence of such ambiguities, at least for the soliton sector of the model.

V. THE SOLITON/PARTICLE CORRESPONDENCES

The $sl(2)$ ATM theory contains the sine-Gordon (SG) and the massive Thirring (MT) models describing the soliton/particle correspondence of its spectrum.[3,11,12] The ATM one-(anti)soliton solution satisfies the remarkable SG and MT classical correspondence in which, apart from the Noether and topological currents equivalence, MT spinor bilinears are related to the exponential of the SG field.[25] The last relationship was exploited in Ref. 4 to decouple the $sl(2)$ ATM equations of motion into the SG and MT ones. Here we provide a generalization of that correspondence to the $sl(3)$ ATM case. In fact, consider the relationships

$$\frac{\psi_R^1\tilde{\psi}_L^1}{i}=-\frac{1}{4\Delta}[(m_\psi^1p_1-m_\psi^3p_4-m_\psi^2p_5)e^{i(\varphi_2-2\varphi_1)}+m_\psi^2p_5e^{3i(\varphi_2-\varphi_1)}+m_\psi^3p_4e^{-3i\varphi_1}-m_\psi^1p_1], \tag{5.1}$$

$$\psi_R^2\tilde{\psi}_L^2=-\frac{1}{4\Delta}[(m_\psi^2p_2-m_\psi^1p_5-m_\psi^3p_6)e^{i(\varphi_1-2\varphi_2)}+m_\psi^1p_5e^{3i(\varphi_1-\varphi_2)}-m_\psi^3p_6e^{-3i\varphi_2}-m_\psi^2p_2], \tag{5.2}$$

$$\frac{\tilde{\psi}_R^3\psi_L^3}{i}=-\frac{1}{4\Delta}[(m_\psi^3p_3-m_\psi^1p_4+m_\psi^2p_6)e^{i(\varphi_1+\varphi_2)}+m_\psi^1p_4e^{3i\varphi_1}-m_\psi^2p_6e^{3i\varphi_2}-m_\psi^3p_3], \tag{5.3}$$

where $\Delta\equiv\overline{a}_{11}\overline{a}_{22}\overline{a}_{33}+2\overline{a}_{12}\overline{a}_{23}\overline{a}_{13}-\overline{a}_{11}(\overline{a}_{23})^2-(\overline{a}_{12})^2\overline{a}_{33}-(\overline{a}_{13})^2\overline{a}_{22}$; $p_1\equiv(\overline{a}_{23})^2-\overline{a}_{22}\overline{a}_{33}$; $p_2\equiv(\overline{a}_{13})^2-\overline{a}_{11}\overline{a}_{33}$; $p_3\equiv(\overline{a}_{12})^2-\overline{a}_{11}\overline{a}_{22}$; $p_4\equiv\overline{a}_{12}\overline{a}_{23}-\overline{a}_{22}\overline{a}_{13}$; $p_5\equiv\overline{a}_{13}\overline{a}_{23}-\overline{a}_{12}\overline{a}_{33}$; $p_6\equiv\overline{a}_{11}\overline{a}_{23}-\overline{a}_{12}\overline{a}_{13}$ and the $\overline{a}_{ij}$'s being the current–current coupling constants of the GMT model (3.13). Relationships (5.1)–(5.3) supplied with the conditions (2.1)–(2.3) and conveniently substituted into Eqs. (A13) and (A15)–(A23) decouple the $sl(3)^{(1)}$ CATM equations into the GSG (4.39) and GMT (3.13) equations of motion, respectively.

Moreover, one can show that the GSG (4.39) M_j parameters and the GMT (3.13) couplings $\overline{a}_{ij}$ are related by

$$\frac{2\Delta M_1}{g(m_\psi^1)^2}=\overline{a}_{22}\left(-\frac{m_\psi^3}{m_\psi^1}\overline{a}_{13}+\overline{a}_{33}\right)+\overline{a}_{23}\left(-\overline{a}_{23}+\frac{m_\psi^3}{m_\psi^1}\overline{a}_{12}\right), \tag{5.4}$$

$$\frac{2\Delta M_2}{g(m_\psi^2)^2}=\overline{a}_{11}\left(-\frac{m_\psi^3}{m_\psi^2}\overline{a}_{23}+\overline{a}_{33}\right)+\overline{a}_{13}\left(-\overline{a}_{13}+\frac{m_\psi^3}{m_\psi^2}\overline{a}_{12}\right), \tag{5.5}$$

$$\frac{2\Delta M_3}{g(m_\psi^3)^2}=-\frac{m_\psi^1m_\psi^2}{(m_\psi^3)^2}(\overline{a}_{12}\overline{a}_{33}-\overline{a}_{13}\overline{a}_{23})-\overline{a}_{11}\overline{a}_{22}+(\overline{a}_{12})^2. \tag{5.6}$$

Various limiting cases of the relationships (5.1)–(5.3) and (5.4)–(5.6) are possible. First, let us consider

$$\overline{a}_{jk}\to\begin{cases}\infty & j=k\neq l \quad (\text{for a given } l)\\ \text{finite} & \text{other cases}\end{cases} \tag{5.7}$$

then one has

$$\frac{\psi_R^l\tilde{\psi}_L^l}{i}=\frac{m_\psi^l}{4}(e^{-i\phi_l}-1), \quad \psi_R^j\tilde{\psi}_L^j=0, \quad j\neq l \tag{5.8}$$

for $\overline{a}_{ll}=\delta_l g$ ($\delta_{1,2}=1$, $\delta_3=-1$). The three species of one-soliton solutions of the $sl(3)$ ATM theory (2.4), found in Ref. 5 and described in Sec. II, satisfy the relationship (5.8).[4] Moreover, from Eqs. (5.4) to (5.6) taking the same limits as in (5.7) one has

$$M_l=\frac{(m_\psi^l)^2}{2}, \quad M_j=0, \quad j\neq l. \tag{5.9}$$

Therefore, relationships (5.1)–(5.3) incorporate each $sl(2)$ ATM submodel (particle/soliton) weak/strong coupling phases, i.e., the MT/SG correspondence.[4,11]

Then, the currents equivalence (A29), relationships (5.1)–(5.3), and conditions (2.1)–(2.3) satisfied by the one-soliton sector of CATM theory allowed us to establish the correspondence between the GSG and GMT models, thus extending the MT/SG result.[25] It could be interesting to obtain the counterpart of Eqs. (5.1)–(5.3) for the $N_S\geqslant 2$ solitons, e.g., along the lines of Ref. 25. For $N_S=2$, Eq. (A29) still holds;[5] and Eqs. (2.1)–(2.3) are satisfied for the species (α_i,α_i).

Second, consider the limit

$$\overline{a}_{ik}\to\begin{cases}\infty & i=k=j \quad (\text{for a chosen } j;\ j=1,2)\\ \text{finite} & \text{other cases}\end{cases}, \tag{5.10}$$

one gets $M_j=0$ and

$$4\overline{\Delta}\frac{\psi_R^l\tilde{\psi}_L^l}{i}=(m_\psi^3\overline{a}_{l3}-m_\psi^l\overline{a}_{33})e^{-i\phi_l}-m_\psi^3\overline{a}_{l3}e^{-3i\varphi_l}+m_\psi^l\overline{a}_{33}, \quad l\neq j,$$
$$4\overline{\Delta}\frac{\psi_R^3\tilde{\psi}_L^3}{i}=(m_\psi^3\overline{a}_{ll}-m_\psi^l\overline{a}_{l3})e^{-i\phi_3}+m_\psi^l\overline{a}_{l3}e^{-3i\varphi_l}+m_\psi^3\overline{a}_{ll}, \tag{5.11}$$

$$\psi_R^j\tilde{\psi}_L^j=0, \tag{5.12}$$

where $\overline{\Delta}\equiv 4(\overline{a}_{ll}\overline{a}_{33}-(\overline{a}_{l3})^2)$. The parameters are related by $(m_\psi^3)^2\overline{a}_{ll}M_l=m_\psi^l(m_\psi^3\overline{a}_{l3}-m_\psi^l\overline{a}_{33})M_3$. In the case $M_l=M_3=M$ and redefining the fields as $\phi_l=\sqrt{12g}(A+B)$, $\phi_j=-\sqrt{12g}B$ in the GSG sector, one gets the Lagrangian

$$\mathcal{L}_{\mathrm{BL}}=\frac{1}{2}(\partial_\mu A)^2+\frac{1}{2}(\partial_\mu B)^2+2\frac{M}{g}\cos\sqrt{24g}A\cos\sqrt{72g}B, \tag{5.13}$$

which is a particular case of the Bukhvostov–Lipatov model (BL).[26] It corresponds to a GMT-type theory with two Dirac spinors. The BL model is not classically integrable,[27] and some discussions have appeared in the literature about its quantum integrability.[28]

Alternatively, if one allows the limit $\overline{a}_{33}\to\infty$ one gets $\psi_R^3\tilde{\psi}_L^3=0$, and additional relations for the ψ^1,ψ^2 spinors and the φ_a scalars. The parameters are related by

$$\frac{M_1}{(m_\psi^1)^2\overline{a}_{22}}=\frac{M_2}{(m_\psi^2)^2\overline{a}_{11}}=-\frac{M_3}{m_\psi^1m_\psi^2\overline{a}_{12}}.$$

Then we left with two Dirac spinors in the GMT sector and all the terms of the GSG model. The later resembles the 2-cosine model studied in Ref. 29 in some submanifold of its renormalized parameter space.

VI. GENERALIZATION TO HIGHER RANK LIE ALGEBRA

The procedures presented so far can directly be extended to the CATM model for the affine Lie algebra $sl(n)^{(1)}$ furnished with the principal gradation. According to the construction of Ref. 2, these models have soliton solutions for an off-critical submodel, possess a $U(1)$ vector current proportional to a topological current, apart from the conformal symmetry they exhibit a $(U(1)_R)^{n-1}\otimes(U(1)_L)^{n-1}$ left–right local gauge symmetry, and the equations of motion describe the dynamics of the scalar fields φ_a, η, $\tilde{\nu}$ $(a=1,\ldots,n-1)$ and the Dirac spinors ψ^{α_j}, $\tilde{\psi}^{\alpha_j}$ $(j=1,\ldots,N;\ N\equiv(n/2)\ (n-1)=$number of positive roots α_j of the simple Lie algebra $sl(n))$ with one-(anti)soliton solution associated with the field $\alpha_j\cdot\vec{\varphi}$ $(\vec{\varphi}=\Sigma_{a=1}^{n-1}\varphi_a\alpha_a$, $\alpha_a=$simple roots of $sl(n))$ for each pair of Dirac fields $(\psi^{\alpha_j},\ \tilde{\psi}^{\alpha_j})$.[2] Therefore, it is possible to define the off-critical real Lagrangian $sl(n)$ ATM model for the solitonic sector of the theory. The reality conditions would generalize Eqs. (2.1)–(2.3), i.e., the new φ's real and the identifications $\tilde{\psi}^{\alpha_j}\sim(\psi^{\alpha_j})^*$ (up to $\pm$ signs). To apply the symplectic analysis of $sl(n)$ ATM one must impose $(n-1)$ constraints in the Lagrangian, analogous to (3.1), due to the above-given local symmetries. The outcome will be a parent Lagrangian of a generalized massive Thirring model (GMT) with N Dirac fields and a generalized sine-Gordon model (GSG) with $(n-1)$ fields. The decoupling of the Toda fields and Dirac fields in the equations of motion of $sl(n)^{(1)}$ CATM, analogous to (A13) and (A15)–(A23), could be performed by an extension of the relationships (5.1)–(5.3) and (2.1)–(2.3).

VII. DISCUSSIONS AND OUTLOOK

We have shown, in the context of FJ and symplectic methods, that the $sl(3)$ ATM (2.4) theory is a parent Lagrangian[18] from which both the GMT (3.13) and the GSG (4.39) models are derivable. From (3.13) and (4.39), it is also clear the duality exchange of the couplings: $g \to 1/g$. The various soliton/particle species correspondences are uncovered. The soliton sector satifies the $U(1)$ vector and topological currents equivalence (A29) and decouples the equations of motion into both dual sectors, through the relationships (5.1)–(5.3) [supplied with (2.1)–(2.3)]. Relationships (5.1)–(5.3) contain each $sl(2)$ ATM submodel soliton solution. In connection to these points, recently a parent Lagrangian method was used to give a generalization of the dual theories concept for non-p-form fields.[30] In Ref. 30, the parent Lagrangian contained both types of fields, from which each dual theory was obtained by eliminating the other fields through the equations of motion.

On the other hand, in non-Abelian bosonization of massless fermions,[31] the fermion bilinears are identified with bosonic operators. Whereas, in Abelian bosonization[32] there exists an identification between the massive fermion operator (charge nonzero sector) and a nonperturbative bosonic soliton operator.[33] Recently, it has been shown that symmetric space sine-Gordon models bosonize the massive non-Abelian (free) fermions providing the relationships between the fermions and the relevant solitons of the bosonic model.[34] The ATM model allowed us to establish these types of relationships for interacting massive spinors in the spirit of particle/soliton correspondence. We hope that the quantization of the ATM theories and the related WZNW models, and in particular relationships (A34), would provide the bosonization of the nonzero charge sectors of the GMT fermions in terms of their associated Toda and WZNW fields. In addition, the above-given approach to the GMT/GSG duality may be useful to construct the conserved currents and the algebra of their associated charges in the context of the CATM $\to$ ATM reduction. These currents in the MT/SG case were constructed treating each model as a perturbation on a conformal field theory (see Ref. 35 and references therein).

Moreover, two-dimensional models with four-fermion interactions have played an important role in the understanding of QCD (see, e.g., Ref. 36 and references therein). Besides, the GMT model contains explicit mass terms: most integrable models such as the Gross–Neveu, SU(2), and U(1) Thirring models all present spontaneous mass generation, the exception being the massive Thirring model. A GMT submodel with $a_{ii}=0$, $a_{ij}=1$ $(i>j)$ and equal m_{ψ}^{j}'s defines the so-called extended Bukhvostov–Lipatov model (BL) and has recently been studied by means of a bosonization technique.[37] Finally, BL type models were applied to N-body problems in nuclear physics.[17]

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APPENDIX: THE $sl(3)^{(1)}$ CATM MODEL

We summarize the construction and some properties of the CATM model relevant to our discussions.[38] More details can also be found in Ref. 5. Consider the zero curvature condition $\partial_+ A_- - \partial_- A_+ + [A_+, A_-] = 0$. The potentials take the form

$$A_+ = -BF^+B^{-1}, \quad A_- = -\partial_- BB^{-1} + F^-, \tag{A1}$$

with

$$F^+ = E^3 + F_1^+ + F_2^+, \quad F^- = E^{-3} + F_1^- + F_2^-, \tag{A2}$$

where $E^{\pm 3}\equiv \mathbf{m}\cdot H^{\pm}=\frac{1}{6}[(2m^1_\psi+m^2_\psi)H_1^{\pm 1}+(2m^2_\psi+m^1_\psi)H_2^{\pm 1}]$ and the $F_i^{\pm}$'s and B contain the spinor fields and scalars of the model, respectively,

$$F_1^+=\sqrt{im^1_\psi}\psi^1_R E^0_{\alpha_1}+\sqrt{im^2_\psi}\psi^2_R E^0_{\alpha_2}+\sqrt{im^3_\psi}\tilde{\psi}^3_R E^1_{-\alpha_3}, \tag{A3}$$

$$F_2^+=\sqrt{im^3_\psi}\psi^3_R E^0_{\alpha_3}+\sqrt{im^1_\psi}\tilde{\psi}^1_R E^1_{-\alpha_1}+\sqrt{im^2_\psi}\tilde{\psi}^2_R E^1_{-\alpha_2}, \tag{A4}$$

$$F_1^-=\sqrt{im^3_\psi}\psi^3_L E^{-1}_{\alpha_3}-\sqrt{im^1_\psi}\tilde{\psi}^1_L E^0_{-\alpha_1}-\sqrt{im^2_\psi}\tilde{\psi}^2_L E^0_{-\alpha_2}, \tag{A5}$$

$$F_2^-=\sqrt{im^1_\psi}\psi^1_L E^{-1}_{\alpha_1}+\sqrt{im^2_\psi}\psi^2_L E^{-1}_{\alpha_2}-\sqrt{im^3_\psi}\tilde{\psi}^3_L E^0_{-\alpha_3}, \tag{A6}$$

$$B=e^{i\varphi_1 H_1^0+i\varphi_2 H_2^0}e^{\tilde{\nu}C}e^{\eta Q_{ppal}}, \tag{A7}$$

where $E^n_{\alpha_i}$, H_1^n, H_2^n, and C $(i=1,2,3;\ n=0,\pm 1)$ are some generators of $sl(3)^{(1)}$; Q_{ppal} being the principal gradation operator. The commutation relations for an affine Lie algebra in the Chevalley basis are

$$[H_a^m,H_b^n]=mC\frac{2}{\alpha_a^2}K_{ab}\delta_{m+n,0}, \tag{A8}$$

$$[H_a^m,E^n_{\pm\alpha}]=\pm K_{\alpha a}E^{m+n}_{\pm\alpha}, \tag{A9}$$

$$[E^m_\alpha,E^n_{-\alpha}]=\sum_{a=1}^{r} l_a^\alpha H_a^{m+n}+\frac{2}{\alpha^2}mC\delta_{m+n,0}, \tag{A10}$$

$$[E^m_\alpha,E^n_\beta]=\varepsilon(\alpha,\beta)E^{m+n}_{\alpha+\beta};\quad \text{if } \alpha+\beta \text{ is a roo}, \tag{A11}$$

$$[D,E^n_\alpha]=nE^n_\alpha,\quad [D,H^n_a]=nH^n_a, \tag{A12}$$

where $K_{\alpha a}=2\alpha.\alpha_a/\alpha_a^2=n_b^\alpha K_{ba}$, with n_a^α and l_a^α being the integers in the expansions $\alpha=n_a^\alpha\alpha_a$ and $\alpha/\alpha^2=l_a^\alpha\alpha_a/\alpha_a^2$, and $\varepsilon(\alpha,\beta)$ the relevant structure constants.

Take $K_{11}=K_{22}=2$ and $K_{12}=K_{21}=-1$ as the Cartan matrix elements of the simple Lie algebra $sl(3)$. Denoting by α_1 and α_2 the simple roots and the highest one by $\psi(=\alpha_1+\alpha_2)$, one has $l_a^\psi=1(a=1,2)$, and $K_{\psi 1}=K_{\psi 2}=1$. Take $\varepsilon(\alpha,\beta)=-\varepsilon(-\alpha,-\beta)$, $\varepsilon_{1,2}\equiv\varepsilon(\alpha_1,\alpha_2)=1$, $\varepsilon_{-1,3}\equiv\varepsilon(-\alpha_1,\psi)=1$ and $\varepsilon_{-2,3}\equiv\varepsilon(-\alpha_2,\psi)=-1$.

One has $Q_{ppal}\equiv\Sigma_{a=1}^2\mathbf{s}_a\lambda_a^v.H+3D$, where λ_a^v are the fundamental co-weights of $sl(3)$, and the principal gradation vector is $\mathbf{s}=(1,1,1)$.[39]

The zero curvature condition gives the following equations of motion

$$\frac{\partial^2\varphi_a}{4i\,e^\eta}=m^1_\psi[e^{\eta-i\phi_a}\tilde{\psi}^l_R\psi^l_L+e^{i\phi_a}\tilde{\psi}^l_L\psi^l_R]+m^3_\psi[e^{-i\phi_3}\tilde{\psi}^3_R\psi^3_L+e^{\eta+i\phi_3}\tilde{\psi}^3_L\psi^3_R],\quad a=1,2, \tag{A13}$$

$$-\frac{\partial^2\tilde{\nu}}{4}=im^1_\psi e^{2\eta-\phi_1}\tilde{\psi}^1_R\psi^1_L+im^2_\psi e^{2\eta-\phi_2}\tilde{\psi}^2_R\psi^2_L+im^3_\psi e^{\eta-\phi_3}\tilde{\psi}^3_R\psi^3_L+\mathbf{m}^2e^{3\eta}, \tag{A14}$$

$$-2\partial_+\psi^1_L=m^1_\psi e^{\eta+i\phi_1}\psi^1_R,\quad -2\partial_+\psi^2_L=m^2_\psi e^{\eta+i\phi_2}\psi^2_R, \tag{A15}$$

$$2\partial_-\psi^1_R=m^1_\psi e^{2\eta-i\phi_1}\psi^1_L+2i\left(\frac{m^2_\psi m^3_\psi}{im^1_\psi}\right)^{1/2}e^\eta(-\psi^3_R\tilde{\psi}^2_L e^{i\phi_2}-\tilde{\psi}^2_R\psi^3_L e^{-i\phi_3}), \tag{A16}$$

$$2\partial_- \psi_R^2 = m_\psi^2 e^{2\eta - i\phi_2}\psi_L^2 + 2i\left(\frac{m_\psi^1 m_\psi^3}{i m_\psi^2}\right)^{1/2} e^{\eta}(\psi_R^3 \tilde{\psi}_L^1 e^{i\phi_1} + \tilde{\psi}_R^1 \psi_L^3 e^{-i\phi_3}), \tag{A17}$$

$$-2\partial_+ \psi_L^3 = m_\psi^3 e^{2\eta + i\phi_3}\psi_R^3 + 2i\left(\frac{m_\psi^1 m_\psi^2}{i m_\psi^3}\right)^{1/2} e^{\eta}(-\psi_L^1 \psi_R^2 e^{i\phi_2} + \psi_L^2 \psi_R^1 e^{i\phi_1}), \tag{A18}$$

$$2\partial_- \psi_R^3 = m_\psi^3 e^{\eta - i\phi_3}\psi_L^3, \quad 2\partial_- \tilde{\psi}_R^1 = m_\psi^1 e^{\eta + i\phi_1}\tilde{\psi}_L^1, \tag{A19}$$

$$-2\partial_+ \tilde{\psi}_L^1 = m_\psi^1 e^{2\eta - i\phi_1}\tilde{\psi}_R^1 + 2i\left(\frac{m_\psi^2 m_\psi^3}{i m_\psi^1}\right)^{1/2} e^{\eta}(-\psi_L^2 \tilde{\psi}_R^3 e^{-i\phi_3} - \tilde{\psi}_L^3 \psi_R^2 e^{i\phi_2}), \tag{A20}$$

$$-2\partial_+ \tilde{\psi}_L^2 = m_\psi^2 e^{2\eta - i\phi_2}\tilde{\psi}_R^2 + 2i\left(\frac{m_\psi^1 m_\psi^3}{i m_\psi^2}\right)^{1/2} e^{\eta}(\psi_L^1 \tilde{\psi}_R^3 e^{-i\phi_3} + \tilde{\psi}_L^3 \psi_R^1 e^{i\phi_1}), \tag{A21}$$

$$2\partial_- \tilde{\psi}_R^2 = m_\psi^2 e^{\eta + i\phi_2}\tilde{\psi}_L^2, \quad -2\partial_+ \tilde{\psi}_L^3 = m_\psi^3 e^{\eta - i\phi_3}\tilde{\psi}_R^3, \tag{A22}$$

$$2\partial_- \tilde{\psi}_R^3 = m_\psi^3 e^{2\eta + i\phi_3}\tilde{\psi}_L^3 + 2i\left(\frac{m_\psi^1 m_\psi^2}{i m_\psi^3}\right)^{1/2} e^{\eta}(\tilde{\psi}_R^1 \tilde{\psi}_L^2 e^{i\phi_2} - \tilde{\psi}_R^2 \tilde{\psi}_L^1 e^{i\phi_1}), \tag{A23}$$

$$\partial^2 \eta = 0, \tag{A24}$$

where $\phi_1 \equiv 2\varphi_1 - \varphi_2$, $\phi_2 \equiv 2\varphi_2 - \varphi_1$, $\phi_3 \equiv \varphi_1 + \varphi_2$.

Apart from the *conformal invariance* the above-presented equations exhibit the $(U(1)_L)^2 \otimes (U(1)_R)^2$ *left–right local gauge symmetry*

$$\varphi_a \to \varphi_a + \theta_+^a(x_+) + \theta_-^a(x_-), \quad a = 1,2, \tag{A25}$$

$$\tilde{\nu} \to \tilde{\nu}, \quad \eta \to \eta, \tag{A26}$$

$$\psi^i \to e^{i(1+\gamma_5)\Theta_+^i(x_+) + i(1-\gamma_5)\Theta_-^i(x_-)}\psi^i, \tag{A27}$$

$$\tilde{\psi}^i \to e^{-i(1+\gamma_5)(\Theta_+^i)(x_+) - i(1-\gamma_5)(\Theta_-^i)(x_-)}\tilde{\psi}^i, \quad i = 1,2,3, \tag{A28}$$

$$\Theta_\pm^1 \equiv \pm\theta_\pm^2 \mp 2\theta_\pm^1, \quad \Theta_\pm^2 \equiv \pm\theta_\pm^1 \mp 2\theta_\pm^2, \quad \Theta_\pm^3 \equiv \Theta_\pm^1 + \Theta_\pm^2.$$

One can get global symmetries for $\theta_\pm^a = \mp\theta_\mp^a =$ constants. For a model defined by a Lagrangian these would imply the presence of two vector and two chiral conserved currents. However, it was found only half of such currents.[5] This is a consequence of the lack of a Lagrangian description for the $sl(3)^{(1)}$ CATM; however see the following.

The gauge fixing of the conformal symmetry, by setting the field η to a constant, is used to stablish the $U(1)$ vector, $J^\mu = \Sigma_{j=1}^3 m_\psi^j \overline{\psi^j}\gamma^\mu \psi^j$, and topological currents equivalence.[2,11] Moreover, it has been shown that the soliton solutions are in the orbit of the solution $\eta = 0$. The remarkable equivalence is

$$\sum_{j=1}^{3} m_\psi^j \overline{\psi^j}\gamma^\mu \psi^j \equiv \epsilon^{\mu\nu}\partial_\nu(m_\psi^1 \varphi_1 + m_\psi^2 \varphi_2), \quad m_\psi^3 = m_\psi^1 + m_\psi^2, \quad m_\psi^i > 0. \tag{A29}$$

The CATM theory has a local Lagrangian in terms of the B and the (two-loop) WZNW fields.[2] The relations between their fields can be obtained from

$$F^- = B\partial_- M M^{-1} B^{-1}, \quad F^+ = B^{-1} N^{-1}\partial_+ N B, \tag{A30}$$

where

$$M=\exp\left(\sum_{s>0}\zeta_s\right),\quad N=\exp\left(\sum_{s>0}\xi_{-s}\right), \tag{A31}$$

provided that the following constraints are imposed:

$$(\partial_- MM^{-1})_{-3}=B^{-1}(\mathbf{m}\cdot H^{-1})B,\quad (\partial_- MM^{-1})_{<-3}=0. \tag{A32}$$

and

$$(N^{-1}\partial_+ N)_3=B\,(\mathbf{m}\cdot H^1)B^{-1},\quad (N^{-1}\partial_+ N)_{>3}=0. \tag{A33}$$

In (A31) and (A32) and (A33) s and the subscripts denote the principal gradation structure of the relevant group elements.

The relationships are

$$\sqrt{im_\psi^3}\psi_L^3=e^{-\eta+i\phi_3}\partial_-\xi_{-1}^3,\quad -\sqrt{im_\psi^1}\tilde{\psi}_L^1=e^{-\eta-i\phi_1}\partial_-\xi_{-1}^1,$$

$$-\sqrt{im_\psi^2}\tilde{\psi}_L^2=e^{-\eta-i\phi_2}\partial_-\xi_{-1}^2,\quad \sqrt{im_\psi^3}\psi_R^1=e^{\eta-i\phi_1}\partial_+\zeta_1^1,$$

$$\sqrt{im_\psi^2}\psi_R^2=e^{\eta-i\phi_2}\partial_+\zeta_1^2,\quad \sqrt{im_\psi^3}\tilde{\psi}_R^3=e^{\eta+i\phi_3}\partial_+\zeta_1^3,$$

$$\sqrt{im_\psi^1}\psi_L^1e^{2\eta}=e^{i\phi_1}\partial_-\xi_{-2}^1+\tfrac{1}{2}(\xi_{-1}^3\partial_-\xi_{-1}^2\epsilon_{3,-2}+\xi_{-1}^2\partial_-\xi_{-1}^3\epsilon_{-2,3})e^{i\phi_1},$$

$$\sqrt{im_\psi^2}\psi_L^2e^{2\eta}=e^{i\phi_2}\partial_-\xi_{-2}^2+\tfrac{1}{2}(\xi_{-1}^3\partial_-\xi_{-1}^1\epsilon_{3,-1}+\xi_{-1}^1\partial_-\xi_{-1}^3\epsilon_{-1,2})e^{i\phi_2}, \tag{A34}$$

$$-\sqrt{im_\psi^3}\tilde{\psi}_L^3e^{2\eta}=e^{-i\phi_3}\partial_-\xi_{-2}^3+\tfrac{1}{2}(\xi_{-1}^1\partial_-\xi_{-1}^2\epsilon_{-1,-2}+\xi_{-1}^2\partial_-\xi_{-1}^1\epsilon_{-2,-1})e^{-i\phi_3},$$

$$\sqrt{im_\psi^3}\psi_R^3e^{-2\eta}=e^{-i\phi_3}\partial_+\zeta_2^3-\tfrac{1}{2}(\zeta_1^1\partial_+\zeta_1^2\epsilon_{1,2}+\zeta_1^2\partial_+\zeta_1^1\epsilon_{2,1})e^{-i\phi_3},$$

$$\sqrt{im_\psi^1}\tilde{\psi}_R^1e^{-2\eta}=e^{i\phi_1}\partial_+\zeta_2^1-\tfrac{1}{2}(\zeta_1^3\partial_+\zeta_1^2\epsilon_{-3,2}+\zeta_1^2\partial_+\zeta_1^3\epsilon_{2,-3})e^{i\phi_1},$$

$$\sqrt{im_\psi^2}\tilde{\psi}_R^2e^{-2\eta}=e^{i\phi_2}\partial_+\zeta_2^2-\tfrac{1}{2}(\zeta_1^3\partial_+\zeta_1^1\epsilon_{-3,1}+\zeta_1^1\partial_+\zeta_1^3\epsilon_{1,-3})e^{i\phi_2}.$$

We observe that the WZNW fields ξ_{-1}^i, ξ_{-2}^i, ζ_1^i, ζ_2^i $(i=1,2,3)$ are nonlocal in terms of the spinors and scalars $\{\psi_i, \widetilde{\psi}_i, \varphi_1, \varphi_2, \tilde{\nu}, \text{ and } \eta\}$. Then the CATM model Lagrangian must be nonlocal when written in terms of its fields.

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[22] $sl(2)$ ATM 2-solitons satisfy an analogous equation to (A29); for φ real and $\tilde{\psi}=\pm(\psi)^*$ [constraints (2.1)–(2.2); (2.3) is trivially satisfied since $\tilde{\psi}_j=\psi_j=0$ for $j\neq i$] one has, soliton–soliton SS, SS bounds, and no $S\bar{S}$ bounds (Ref. 3).
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The Lund–Regge surface and its motion's evolution equation

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The system of evolution equations for general motion of surfaces in orthogonal coordinates is analyzed to reduce the number of variables as well as equations. The explicit expression of the Lund–Regge surface is obtained. When the surface corresponds to the Lund–Regge equation, we prove that some components of velocity satisfy the linearizations of the Lund–Regge equation. The soliton solution is derived and one special case of the Lund–Regge surface is studied.
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I. INTRODUCTION

Dynamics of surfaces, interfaces, and front is an important ingredient of numerous nonlinear phenomena in classical physics.[1–4] In some cases, many dynamics can be modeled by the nonlinear partial differential equations which describe an evolution of surfaces in time.[3–5] Moreover, a local evolution law may be established in terms of a velocity field on the surface.[4] In addition, interesting papers by Nakayama *et al.*,[5,6] Mclachlan and Segur,[7] Konopelchenko,[8,9] and Szwabowicz[10] concerned the motion of surfaces and linked it to solitonic equations. Among them, Nakayama and Wadati[5] discussed the motion of surfaces. They calculated time evolutions for sphere, surface of revolution, and developable surface in details. In the appendix, they derived the Lund–Regge (LR) equation, but because of over-restrictions on the metric and the curvature tensor, they did not solve the time evolution of this system by using their theory. It is known that the LR equation is one soliton equation.[11–13] Sym *et al.*[14–16] developed the theory of the soliton surface which provided a geometrical interpretation for many integrable physical systems and is very useful to explicitly construct large classes of surfaces. Bobenko[17] reformulated it in a form familiar to the soliton theory which made it easier to apply the analytical method of this theory to integrable cases. Fokas *et al.*[18] show that the problem of the immersion of a two-dimensional surface into a three-dimensional Euclidean space is related to the problem of studying surfaces in Lie groups and Lie algebras, and proposed a more general formula for surface immerse into Lie algebra. Cieslinski *et al.*[19] generalized it and proved that many results concerning immersion on Lie algebra can be reduced to or interpreted within the soliton surfaces approach. We find that the above-mentioned method can be used to study the motion of surfaces and integrable system. So, we identify R^3 with su(2) and use the soliton theory to discuss the surfaces associated with the LR equation. Making use of one coordinate's transformation and spin transformation, we calculated the explicit expression of the surface.

In Ref. 20, Li suggested one approach to consider the motion of surfaces with constant negative curvature in asymptotic coordinates. Then in Refs. 21 and 22 we generalized this approach to discuss the evolution of surfaces in geodesic coordinates. In this paper, we will use this method to consider the system of evolution equation for general motion of surfaces in orthogonal

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coordinates, especially for the surfaces associated with the LR equation. We shall prove that when the surface corresponds to the LR equation, some components of velocity satisfy the linearizations of the LR equation. The evolution equation associated with the motion of this surface is derived as $2+1$ dimensional integrable equations.

In Sec. II, we describe the correspondence between R^3 and su(2). The explicit expression of the surface corresponding to the LR equation is obtained. In Sec. III, we analyze the system of evolution equations for general motion of surfaces in orthogonal coordinates and obtain one system with eight functions and twelve equations. So, under suitable conditions, we prove a fundamental theorem: this system can be reduced to an equivalent system with eight functions and eight equations. In Sec. IV, we prove that some velocity components of the motion of the LR surface should satisfy the linearization equation of the LR equation. Its corresponding motion equation is also derived. In Sec. V, given special velocity, $2+1$ dimensional integrable equations are obtained, which recovers the relations between the motion of surfaces and the soliton equations, the soliton solution is derived too. In Sec. VI, we study one special case of the LR surface. We conclude and give some remarks in Sec. VII.

II. THE SURFACES IN ORTHOGONAL COORDINATES AND THE LR EQUATION

Let $F(x,y)$ be a smooth surface in a three-dimensional Euclidean space, which is given by a vector-valued function

$$F=(F_1,F_2,F_3):R^2\to R^3.$$

To construct and investigate the surface in R^3 by analytical methods, we use 2×2 matrices instead of 3×3 matrices. More explicitly, we characterize the surface in terms of su(2). Let $\{e_1,e_2,e_3\}$ be the orthonormal bases of R^3 and $\{f_1,f_2,f_3\}$ be the orthonormal bases of su(2),

$$f_1=\frac{1}{2}\begin{pmatrix}0 & i\\ i & 0\end{pmatrix},\quad f_2=\frac{1}{2}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix},\quad f_3=\frac{1}{2}\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix}.$$

Then $\sigma_j=-2if_j(j=1,2,3)$ are Pauli matrices. Map the vector space R^3 with su(2),

$$F=\sum_{j=1}^{3}F_je_j\mapsto\sum_{j=1}^{3}F_jf_j$$

(the inner product $\langle F,G\rangle=-2\,\mathrm{tr}\,F\cdot G$ defines a Euclidean scalar product in R^3 and the Lie bracket corresponds to the vector product in R^3). So we identify three-dimensional Euclidean space with su(2). In the sequel we will follow the notation of Ref. 18.

Similarly to the method which Fokas and Gelfand mentioned in Ref. 18, in orthogonal coordinates, the first fundamental form of surfaces can be expressed by

$$Ih^2\,\mathrm{d}x^2+g^2\,\mathrm{d}y^2,$$

where

$$F_x=\psi^{-1}hf_1\psi,\quad F_y=\psi^{-1}gf_2\psi,\quad bfN=\psi^{-1}f_3\psi \tag{1}$$

and $\psi\in\mathrm{SU}(2)$ satisfies

$$\psi_x=U\psi,\quad \psi_y=V\psi, \tag{2}$$

$$U=\sum_{j=1}^{3}u_jf_j,\quad V=\sum_{j=1}^{3}v_jf_j, \tag{3}$$

where u_j, v_j, $(j=1, 2, 3)$ are functions of (x,y). Then the second fundamental form of surface can be obtained

$$II = L\,\mathrm{d}x^2 + 2M\,\mathrm{d}x\,\mathrm{d}y + N\mathrm{d}y^2,$$

$$L = -\langle F_x, \mathbf{N}_x\rangle = hu_2, \quad N = -\langle F_y, \mathbf{N}_y\rangle = -gv_1,$$

$$M = -\langle F_x, \mathbf{N}_y\rangle = -\langle F_y, \mathbf{N}_x\rangle = hv_2.$$

From the compatibility condition $F_{xy}=F_{yx}$, it yields

$$u_3 = \frac{h_y}{g}, \quad v_3 = -\frac{g_x}{h}, \quad hv_2 = -gu_1 \tag{4}$$

and from the compatibility condition $\psi_{xy}=\psi_{yx}$, we can derive that

$$u_{1y} - v_{1x} - \frac{g_x}{h}u_2 + \frac{h_y}{h}u_1 = 0, \tag{5}$$

$$u_{2y} + \left(\frac{g}{h}u_1\right)_x + \frac{h_y}{g}v_1 + \frac{g_x}{h}u_1 = 0, \tag{6}$$

$$\left(\frac{h_y}{g}\right)_y + \left(\frac{g_x}{h}\right)_x - \frac{g}{h}u_1^2 - u_2v_1 = 0. \tag{7}$$

It is the Gauss–Codazzi equation. Same as the appendix of Ref. 5, let

$$h = \cos\theta, \quad g = \sin\theta \tag{8}$$

and

$$L = p_x\cot\theta + \cos\theta\sin\theta,$$

$$M = p_y\cot\theta, \tag{9}$$

$$N = p_x\cot\theta - \cos\theta\sin\theta,$$

then from (4),

$$u_3 = -\theta_y, \quad v_3 = -\theta_x, \quad v_2 = -u_1\tan\theta.$$

Meanwhile, we have

$$u_1 = -p_y\frac{\cot\theta}{\sin\theta}, \quad v_1 = -p_x\frac{\cot\theta}{\sin\theta} + \cos\theta,$$

$$u_2 = p_x\frac{1}{\sin\theta} + \sin\theta, \quad v_2 = p_y\frac{1}{\sin\theta}.$$

Then from the Gauss–Codazzi equation, it can be derived that θ and p satisfy the LR equation[5,12,13]

$$\theta_{xx}-\theta_{yy}+\frac{\cos\theta}{\sin^3\theta}(p_x^2-p_y^2)=\cos\theta\sin\theta,$$
$$\frac{\partial}{\partial x}(p_x\cot^2\theta)=\frac{\partial}{\partial y}(p_y\cot^2\theta). \tag{10}$$

Gauss curvature and mean curvature are

$$K=-\frac{\theta_{xx}-\theta_{yy}}{\sin\theta\cos\theta},$$
$$H=\frac{p_x}{\sin^3\theta\cos\theta}-2\cot(2\theta),$$

respectively.

We call the surface associated with the LR equation the LR surface. It is known that the LR equation is a one soliton equation. To prove the LR surface is a one soliton surface[14,15] and calculate the explicit expression of the surfaces, we need to introduce one spectral parameter and prove F can be expressed by ψ. So, we do the coordinate transformation

$$\bar{x}=\frac{1}{2\lambda}(x-y),\quad \bar{y}=\frac{\lambda}{2}(x+y) \tag{11}$$

at that time, the LR equation (10) is changed to

$$\theta_{\bar{x}\bar{y}}+\frac{\cos\theta}{\sin^3\theta}p_{\bar{x}}p_{\bar{y}}=\cos\theta\sin\theta,$$
$$\frac{\partial}{\partial\bar{x}}(p_{\bar{y}}\cot^2\theta)+\frac{\partial}{\partial\bar{y}}(p_{\bar{x}}\cot^2\theta)=0. \tag{12}$$

It is another form of the LR equation.[11] Its Gauss curvature and mean curvature are

$$K=-\frac{\theta_{\bar{x}\bar{y}}}{\sin\theta\cos\theta},$$
$$H=\frac{p_{\bar{x}}+\lambda^2 p_{\bar{y}}}{2\lambda\sin^3\theta\cos\theta}-2\cot(2\theta),$$

respectively. Meanwhile Eqs. (2) and (3) can be rewritten as

$$\psi_{\bar{x}}=\bar{M}\psi=\frac{1}{2}\begin{pmatrix} i\theta_{\bar{x}} & -i\lambda e^{-i\theta}+ip_{\bar{x}}\dfrac{\cos\theta}{\sin^2\theta}-\dfrac{p_{\bar{x}}}{\sin\theta} \\ -i\lambda e^{-i\theta}+ip_{\bar{x}}\dfrac{\cos\theta}{\sin^2\theta}+\dfrac{p_{\bar{x}}}{\sin\theta} & -i\theta_{\bar{x}} \end{pmatrix}\psi,$$
$$\psi_{\bar{y}}=\bar{N}\psi=\frac{1}{2}\begin{pmatrix} -i\theta_{\bar{y}} & i\dfrac{e^{i\theta}}{\lambda}-ip_{\bar{y}}\dfrac{\cos\theta}{\sin^2\theta}-\dfrac{p_{\bar{y}}}{\sin\theta} \\ i\dfrac{e^{-i\theta}}{\lambda}-ip_{\bar{y}}\dfrac{\cos\theta}{\sin^2\theta}+\dfrac{p_{\bar{y}}}{\sin\theta} & i\theta_{\bar{y}} \end{pmatrix}\psi, \tag{13}$$

and the tangent vectors Eq. (1) are

$$F_{\bar{x}}=\frac{i\lambda}{2}\psi^{-1}\begin{pmatrix}0 & e^{-i\theta}\\ e^{i\theta} & 0\end{pmatrix}\psi,\quad F_{\bar{y}}=\frac{i}{2\lambda}\psi^{-1}\begin{pmatrix}0 & e^{i\theta}\\ e^{-i\theta} & 0\end{pmatrix}\psi. \tag{14}$$

Let $\lambda=e^{\Lambda}$, then we have

Proposition 1: Let

$$F=-\psi^{-1}\psi_{\Lambda}. \tag{15}$$

If ψ satisfies Eq. (13), then F satisfies Eq. (14).

Proof: It is easy to calculate that

$$F_{\bar{x}}=-\psi^{-1}\bar{M}_{\Lambda}\psi,\quad F_{\bar{y}}=-\psi^{-1}\bar{N}_{\Lambda}\psi$$

So, Eq. (14) can be obtained. □

So, if θ and p is a solution of the LR equation (12), the spectral problem of Eq. (13) can be solved, i.e., we can get the solution ψ in explicit form. Furthermore, the exact expression of the motion of the LR surface can be calculated from expression (15).

Similar to Ref. 20, using the spin transformation

$$T:\psi\rightarrow\varphi=T\psi,\quad T=\frac{1}{\sqrt{2}}\begin{pmatrix}e^{-i/2\,\theta} & e^{-i/2\,\theta}\\ -e^{i/2\,\theta} & e^{i/2\,\theta}\end{pmatrix}, \tag{16}$$

we map the spectral problem (13) to the Ablowitz–Kaup–Newell–Seger (AKNS) system

$$\begin{aligned}\varphi_{\bar{x}}&=\frac{1}{2}\begin{pmatrix} i\left(\lambda-p_{\bar{x}}\frac{\cos(2\theta)}{\sin^2\theta}\right) & 2i\theta_{\bar{x}}-2p_{\bar{x}}\cot\theta\\ 2i\theta_{\bar{x}}+2p_{\bar{x}}\cot\theta & -i\left(\lambda-p_{\bar{x}}\frac{\cos(2\theta)}{\sin^2\theta}\right)\end{pmatrix}\varphi,\\ \varphi_{\bar{y}}&=\frac{1}{2}\begin{pmatrix} -i\left(\frac{\cos 2\theta}{\lambda}-\frac{p_{\bar{y}}}{\sin^2\theta}\right) & -\frac{\sin 2\theta}{\lambda}\\ \frac{\sin 2\theta}{\lambda} & i\left(\frac{\cos 2\theta}{\lambda}-\frac{p_{\bar{y}}}{\sin^2\theta}\right)\end{pmatrix}\varphi.\end{aligned} \tag{17}$$

Given one soliton solution of the LR equation (12),[11,13]

$$\theta=\arcsin[d\,\mathrm{sec}\,h(d\alpha)],\quad p=\arctan\left[\frac{d}{A}\tanh(d\alpha)\right],$$

$$\alpha=c\bar{x}+\frac{\bar{y}}{c},\quad d^2+A^2=1,$$

the basic solution of the spectral problem (17) can be calculated that

$$\varphi=\begin{pmatrix}\varphi_1 & -\varphi_2^{\star}\\ \varphi_2 & \varphi_1^{\star}\end{pmatrix},$$

$$\varphi_1=[\lambda-cA+icd\tanh(d\alpha)]\exp\left[\frac{i}{2}(p+2\beta)\right],$$

$$\varphi_2=-icd\,\mathrm{sec}\,h(d\alpha)\exp\left[\frac{i}{2}(2\beta-p)\right],\quad \beta=\frac{\lambda-cA}{2}\bar{x}+\left(\frac{A}{2c}-\frac{1}{2\lambda}\right)\bar{y}.$$

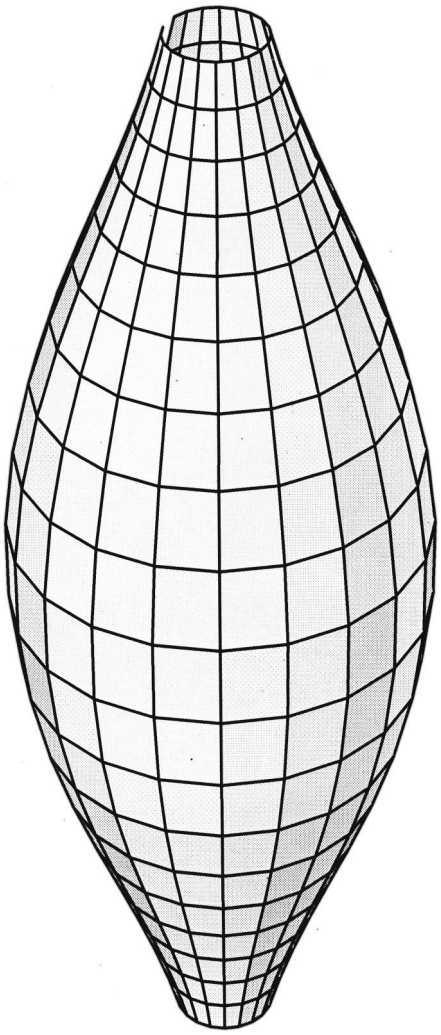

FIG. 1. $c=\lambda=\frac{1}{2}$; $A=\sqrt{2}/2$; $x\in[-3,3]$; $y\in[-10,10]$.

So making use of Eqs. (15) and (16), it can be derived that $F(\overline{x},\overline{y})$ is

$$F(\overline{x},\overline{y})=\frac{1}{2}\begin{pmatrix} iF_3(\overline{x},\overline{y}) & iF_1(\overline{x},\overline{y})-F_2(\overline{x},\overline{y}) \\ iF_1(\overline{x},\overline{y})+F_2(\overline{x},\overline{y}) & -iF_3(\overline{x},\overline{y}) \end{pmatrix},$$

$$F_1(\overline{x},\overline{y})=-\frac{2cd\lambda}{\lambda^2-2cA+c^2}\sec h(d\alpha)\cos(2\beta),$$

$$F_2(\overline{x},\overline{y})=\frac{2cd\lambda}{\lambda^2-2cA+c^2}\sec h(d\alpha)\sin(2\beta), \tag{18}$$

$$F_3(\overline{x},\overline{y})=\frac{2cd\lambda\tanh(d\alpha)}{\lambda^2-2cA+c^2}-\left(\frac{\lambda}{2}\overline{x}+\frac{\overline{y}}{2\lambda}\right).$$

Substituting (11) into (18), the surface corresponding to the first and second fundamental quantities (8) and (9) can be obtained. It is displayed in Figs. 1–5.

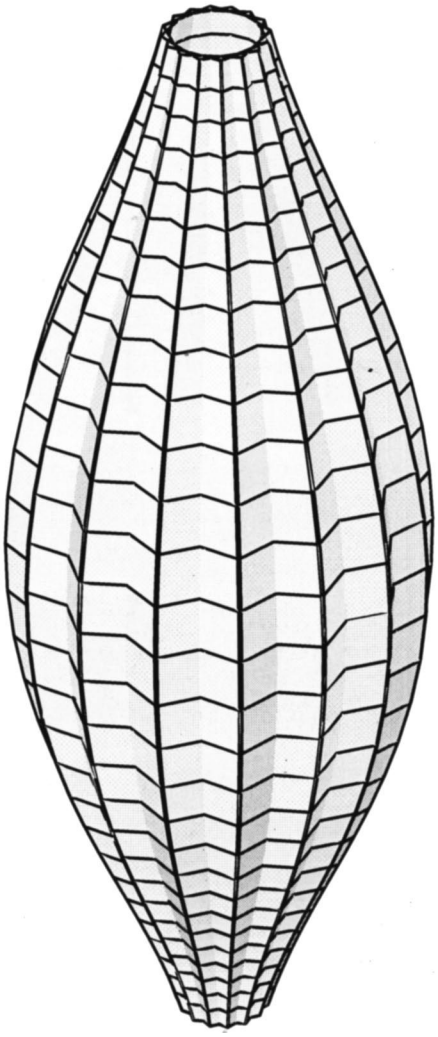

FIG. 2. $c=-\lambda=\frac{1}{2}$; $A=\sqrt{2}/2$; $x\in[-3,3]$; $y\in[-10,10]$.

III. THE MOTION OF SURFACE IN ORTHOGONAL COORDINATES

To discuss the motion of surfaces, we assume the velocity of the motion as

$$F_t=\psi^{-1}C\psi=uF_x+vF_y+w\mathbf{N}$$

and ψ satisfies

$$\psi_t=W\psi,\quad W=\sum_{j=1}^{3}w_jf_j, \tag{19}$$

where u, v, w are functions of (x,y,t) and are projections of F_x, F_y, $\mathbf{N}$, respectively. Then from the compatibility conditions of F_x, F_y, F_t, ψ_x, ψ_y, and ψ_t, it can be calculated that w_1, w_2, w_3 satisfy

$$w_1=-\frac{w_y}{g}+u_1u+v_1v,$$

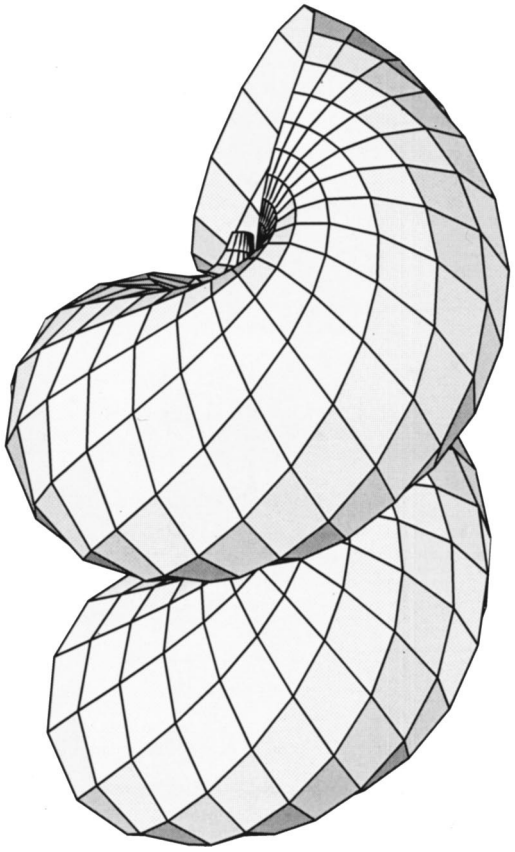

FIG. 3. $c=\frac{1}{2}$; $\lambda=\frac{3}{4}$; $A=\sqrt{2}/2$; $x\in[-10,10]$, $y\in[-15,15]$.

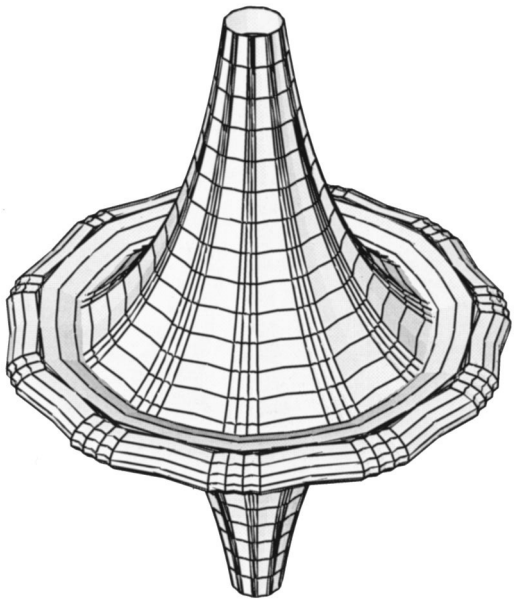

FIG. 4. $c=\lambda=1$; $A=\frac{1}{4}$; $x\in[-3,3]$, $y\in[-15,15]$.

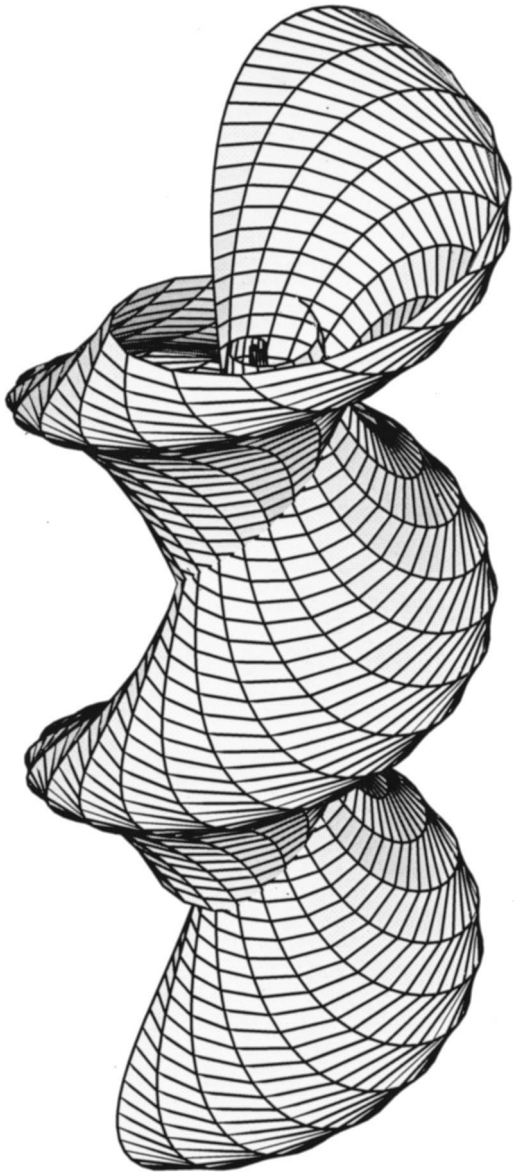

FIG. 5. $c=\frac{1}{2}$; $\lambda=-1$; $A=\sqrt{2}/2$; $x\in[-3,3]$, $y\in[-5,5]$.

$$
\begin{aligned}
w_2&=\frac{1}{h}(w_x+uu_2h-u_1vg),\\
w_3&=-\frac{1}{h}\left[(vg)_x-u\frac{hh_y}{g}+wu_1\right],\\
&=\frac{1}{g}\left[(uh)_y-v\frac{gg_x}{h}+wu_1\frac{g}{h}\right]
\end{aligned}
\tag{20}
$$

and besides the Gauss–Codazzi equation (5)–(7), the eight functions u, v, w, h, g, u_1, u_2, v_1 should satisfy the following equations:

$$h_t=(uh)_x+vh_y-wu_2, \tag{21}$$

$$h^2u_y=-g^2v_x-2gwu_1, \tag{22}$$

$$g_t=(vg)_y+ug_x+wv_1, \tag{23}$$

$$u_{1t}-w_{1x}+u_2w_3-\frac{h_y}{h}w_2=0, \tag{24}$$

$$u_{2t}-w_{2x}+\frac{h_y}{g}w_1-u_1w_3=0, \tag{25}$$

$$\left(\frac{g}{h}u_1\right)_t+w_{2y}+\frac{g_x}{h}w_1+v_1w_3=0, \tag{26}$$

$$\left(\frac{g_x}{h}\right)_t+w_{3y}-v_1w_2-\frac{g}{h}u_1w_1=0, \tag{27}$$

$$\left(\frac{h_y}{g}\right)_t-w_{3x}+u_1w_2-u_2w_1=0, \tag{28}$$

$$v_{1t}-w_{1y}-\frac{h}{g}u_1w_3+\frac{g_x}{h}w_2=0. \tag{29}$$

Among them, Eq. (22) is deduced from the two expressions of w_3 Eq. (20). In the following, we will discuss the reduction of this problem and clarify the relation between the velocities and the surfaces.

Theorem 1: *If $u_2\neq 0$, and w_1, w_2, w_3 are defined by Eq. (20), then Eqs. (26)–(29) can be derived from the Gauss–Codazzi equation (5)–(7) and Eqs. (21)–(25), i.e., in orthogonal coordinates, the motion of surfaces depends on eight functions u, v, w, h, g, u_1, u_2, and v_1, which satisfy the eight fundamental equations (5)–(7), (21)–(25).*

Lemma 1: Equation (26) can be derived from Eqs. (21) to (24).

Proof: By direct calculation, it can be deduced from Eqs. (23) and (24) that

$$\begin{aligned}\left(\frac{gu_1}{h}\right)_t=&\frac{u_1}{h}[(vg)_y+ug_x+wv_1]+\frac{gu_2}{h^2}[wu_1+v_xg+vg_x]\\&+\frac{g}{h}\left(u_{1x}u+u_1u_x+v_{1x}v-v_1v_x-\frac{w_{xy}}{g}+\frac{w_yg_x}{g^2}\right)\\&+\frac{h_y}{h^2}(w_x-vgu_1)-\frac{gu_1}{h^2}[(uh)_x+vh_y-wu_2].\end{aligned} \tag{30}$$

Meanwhile, from Eq. (20), it yields that

$$-w_{xy}=-hw_{2y}-h_yw_2+u_yu_{2y}h+uu_{2y}h+uu_2h_y-u_1(vg)_y-u_{1y}vg.$$

So, by using Eqs. (5), (6), and (22), it can be rewritten as

$$-w_{xy}=-hw_{2y}+\frac{u_2}{h}(-g^2v_x-2gwu_1)+uh\left[-u_1\frac{g_x}{h}-\left(\frac{gu_1}{h}\right)_x-\frac{h_y}{g}v_1\right]$$
$$-vg\left(v_{1x}+u_2\frac{g_x}{h}-\frac{h_y}{h}u_1\right)-u_1(vg)_y-h_yw_2+uu_2h_y.$$

Substituting it into Eq. (30), it yields that

$$\left(\frac{gu_1}{h}\right)_t=-w_{2y}+\frac{g_x}{h}\left(\frac{w_y}{g}-uu_1-v_1v\right)+\frac{v_1}{h}\left(wu_1+gv_x+g_xv-uh\frac{h_y}{g}\right).$$

So, Eq. (26) is obtained and this lemma is proved. □

Lemma 2: Equation (27) can be derived from Eqs. (5), (7), (21)–(23).

Proof: From Eqs. (21) and (23), g_t and h_t can be expressed. So, from Eqs. (7) and (22), it can be calculated that

$$h\left[\left(\frac{g_x}{h}\right)_t+w_{3y}-v_1w_2-\frac{g}{h}u_1w_1\right]=ug_{xx}+(wv_1)_x+v_1(w_x+uhu_2)+guu_1^2+wu_{1y}$$
$$+\frac{1}{h}(wu_1h_y+gv_xh_y)+\frac{g_x}{h}wu_2+\frac{hh_yu_y}{g}+hu\left(\frac{h_y}{g}\right)_y$$
$$=w\left[v_{1x}-u_{1y}+u_1\frac{h_y}{h}+u_1\frac{g_x}{h}-wu_1\frac{h_y}{h}\right].$$

Substituting Eq. (5) into it, the right-hand side of the above-given expression is zero, so Eq. (27) is obtained. This lemma is proved. □

Lemma 3: Equation (28) can be derived from Eqs. (6), (7) and (21)–(25).

Proof: By using Eqs. (6), (21), and (23), the left-hand side of Eq. (28) can be rewritten as

$$\left(\frac{h_y}{g}\right)_t-w_{3x}+u_1w_2-u_2w_1$$
$$=\frac{1}{g}\left[vh_{yy}-wu_{2y}+\left(\frac{gv}{h}g_x-wu_1\frac{g}{h}\right)_x\right]-\frac{h_y}{g}(vg_y+ug_x+wv_1)+\frac{u_1}{h}(w_x-vgu_1)$$
$$+\frac{g_x}{g}\left(uh_y+u_yh-vg\frac{g_x}{h}+wu_1\frac{g}{h}\right)+\frac{h_y}{g^2}(g_yv+g_xu)$$
$$=\frac{1}{g}\left(vh_{yy}+wu_1\frac{g_x}{h}+g_xw_3\right)+\frac{(vg_x)_x}{h}-\frac{vu_1^2g}{h}-\frac{vg_xh_x}{h^2}+\frac{vg_x^2}{gh}. \tag{31}$$

Then from Eq. (27), it yields that

$$\frac{h_{yy}}{g}=\frac{h_xg_x}{h^2}+\frac{gu_1^2}{h}-\frac{g_{xx}}{h}+u_2v_1.$$

Substituting it into Eq. (31), the left-hand side of Eq. (28) is equal to zero, so this lemma is proved. □

Lemma 4: If $u_2\neq 0$, Eq. (29) can be derived from Eqs. (5)–(7) and (21)–(23).

Proof: From Lemmas 1–3, Eqs. (26)–(28) yield. So they can be used to prove this lemma. From Eqs. (24) to (28), Eq. (7) can be rewritten as

$$(u_2w_1-u_1w_2)_y+\left(v_1w_2+\frac{g}{h}u_1w_1\right)_x-\left(\frac{g}{h}\right)_t u_1^2-u_2v_{1t}+2u_1\frac{g}{h}\left(u_2w_3-w_{1x}-\frac{h_y}{g}w_2\right)$$
$$+v_1\left(\frac{h_y}{g}w_1-w_{2x}-u_1w_3\right)=0.$$

Substituting h_t, g_t into it and using Eqs. (5) and (6), we have

$$u_1\left[\frac{g}{h}(u_2w_3-w_{1x})-\frac{g_x}{h}w_1-w_{2y}-\frac{g_t}{h}u_1+\frac{gh_t}{h^2}-v_1w_3\right]\times u_2\left(w_{1y}+\frac{g}{h}u_1w_2+\frac{g_x}{h}u_2w_2-v_{1t}\right)=0.$$

Then using (24) and (26), it can be directly calculated that if $u_2\neq 0$, (29) yields. This lemma is proved. □

From Lemmas 1–4, the theorem is proved.

Remark 1: Note that, among the eight equations, Eqs. (21)–(23) are derived from the compatibility conditions of F_x, F_y, F_t, Gauss–Codazzi equations are from $\psi_{xy}=\psi_{yx}$ and the remaining two are from the compatibility conditions $\psi_{xt}=\psi_{tx}$.

IV. THE MOTION OF THE LUND–REGGE SURFACE

To decide the equations of the surface evolution, we should clarify the relation between the velocity and the surface. First of all, from Eq. (20), we know

$$\begin{aligned}
w_1&=-\frac{w_y}{\sin\theta}-p_yu\frac{\cot\theta}{\sin\theta}+\left(\cos\theta-p_x\frac{\cot\theta}{\sin\theta}\right)v,\\
w_2&=\frac{w_x}{\cos\theta}+p_x\frac{u}{\sin\theta}+\sin\theta u+p_y\frac{v}{\sin\theta},\\
w_3&=-v_x\tan\theta-v\,\theta_x-u\,\theta_y+p_y\frac{w}{\sin^2\theta},\\
&=u_y\cot\theta-v\,\theta_x-u\,\theta_y-p_y\frac{w}{\sin^2\theta}.
\end{aligned}\tag{32}$$

Proposition 2: If the surface satisfies Eqs. (8) and (9), then besides the LR equation, θ and p should satisfy

$$\begin{aligned}
\theta_t&=-u_x\cot\theta+u\,\theta_x+v\,\theta_y+w\left(1+\frac{p_x}{\sin^2\theta}\right),\\
&=v_y\tan\theta+u\,\theta_x+v\,\theta_y+w\left(1-\frac{p_x}{\sin^2\theta}\right),
\end{aligned}\tag{33}$$

$$\left(p_y\frac{\cot\theta}{\sin\theta}\right)_t+w_{1x}-u_2w_3-\theta_yw_2=0.\tag{34}$$

In fact Eq. (34) is just Eq. (24), and from Eq. (21) or (23), it is easy to know that θ_t satisfies Eq. (33).

Proposition 3: The velocity u, v, and w should satisfy

$$\cos^2\theta u_y+\sin^2\theta v_x=2p_yw\frac{\cos\theta}{\sin\theta},\tag{35}$$

$$\cos^2\theta u_x+\sin^2\theta v_y=2wp_x\cot\theta, \tag{36}$$

$$w_{xx}-w_{yy}-w(p_x^2-p_y^2)\left(\csc^2\theta+3\frac{\cos^2\theta}{\sin^4\theta}\right)+2\frac{\cos\theta}{\sin^3\theta}(p_xu_x-p_yu_y)=w\cos 2\theta. \tag{37}$$

Proof: Equation (35) follows from Eq. (32) or (22). And from Eq. (33), Eq. (36) yields. In the following, we should prove that Eq. (37) is satisfied. From Eqs. (32) and (33), Eq. (25) can be rewritten as

$$p_{xt}\cot\theta-w_{xx}-w_x\theta_x\tan\theta-p_{xx}u\cot\theta-2p_yv_x\cot\theta+\theta_yw_y\cot\theta+w(p_y^2-p_x^2)\frac{\cos^2\theta}{\sin^4\theta}+w\cos^2\theta$$
$$+p_xu_x\cot\theta\frac{\cos 2\theta}{\sin^2\theta}-u_x\cot\theta=0. \tag{38}$$

Similarly, by direct calculation, Eq. (29) can be rewritten as

$$-p_{xt}\cot\theta+w_{yy}+w_x\theta_x\tan\theta-\theta_yw_y\cot\theta+p_{yy}u\cot\theta+2p_yu_y\cot\theta+p_{xy}v\cot\theta-wp_y^2\frac{1}{\sin^2\theta}$$
$$-p_x^2w\frac{1}{\sin^2\theta}(1+2\cot\theta)-w\sin^2\theta-2p_y\theta_yu\frac{1}{\sin^2\theta}-v_y\tan\theta+p_xv_y(\tan\theta+3\cot\theta)$$
$$+2wp_x\frac{1}{\sin^2\theta}+2p_x\theta_xu\frac{1}{\sin^2\theta}=0. \tag{39}$$

Then from Eqs. (38) and (39) and noting that θ, p satisfy the LR equation, it follows that

$$w_{yy}-w_{xx}+w\cos 2\theta-w(p_x^2-p_y^2)\frac{3+\cos^2\theta}{\sin^2\theta}+2(\tan\theta+\cot\theta)(p_xv_y-p_yv_x)=0. \tag{40}$$

On the other hand, by using Eqs. (35) and (36), it follows that

$$p_xv_y-p_yv_x=2w\frac{\cos\theta}{\sin^3\theta}(p_x^2-p_y^2)-\cot^2\theta(u_xp_x-u_yp_y).$$

Substituting it into Eq. (40), it yields Eq. (37). □

Then from Eqs. (35) and (36), v_y and v_x can be expressed by u, w, θ, and p. The compatibility condition of $v_{xy}=v_{yx}$ can be written as

$$\frac{\partial}{\partial y}\left(2wp_x\frac{\cos\theta}{\sin^3\theta}-u_x\cot^2\theta\right)=\frac{\partial}{\partial x}\left(2wp_y\frac{\cos\theta}{\sin^3\theta}-u_y\cot^2\theta\right). \tag{41}$$

Proposition 4: u, w satisfy the linearization of the LR equation.

Proof: Replacing θ and p with $\theta+\varepsilon w$, $p+\varepsilon u$ in the LR equation and then keep the $O(\varepsilon)$ terms. It is just Eqs. (37) and (41), that is, u w satisfy the linearization of the LR equation. □

So, if θ, p are a solution of LR equation, then θ_x, p_x are the solution of Eqs. (37) and (41), and θ_y, p_y are too.

V. EVOLUTION EQUATION OF THE LR SURFACE UNDER SPECIAL VELOCITY

Based on the previous text, for p not a constant, we can take the normal velocity component w and the tangent velocity component u as follows:

$$w=a_1\theta_x+a_2\theta_y,\quad u=a_1p_x+a_2p_y, \tag{42}$$

where a_1 and a_2 are constants. From Eqs. (35) and (36) we find that

$$v=-(a_1p_y+a_2p_x)\cot^2\theta. \tag{43}$$

Substituting u, v and w into Eqs. (33) and (34), the evolution equation of surface related to the time can be derived that

Proposition 5: The evolution equation of the LR equation for the velocity equations (42) and (43) is

$$\theta_t=a_1[\theta_x(p_x+1)-(p_x\cot\theta)_x-p_y\theta_y\cot^2\theta]+a_2[\theta_y(p_x+1)+\theta_xp_y-p_{xy}\cot\theta], \tag{44}$$

$$\begin{aligned}p_{yt}=&a_1\left[\theta_{xxy}\tan\theta+\theta_y\theta_{xx}\tan^2\theta-\theta_x\theta_{xy}+p_{xy}+4p_y^2\theta_y\frac{\cos\theta}{\sin^3\theta}+p_xp_{xy}(2-\cot^2\theta)-3p_yp_{yy}\cot^2\theta\right]\\&+a_2\left[\theta_{xyy}\tan\theta+\theta_y\theta_{xy}\tan^2\theta-\theta_x\theta_{yy}+p_{yy}+4p_yp_x\theta_y\frac{\cos\theta}{\sin^3\theta}\right.\\&\left.+(1-2\cot^2\theta)(p_xp_{yy}+p_yp_{xy})\right].\end{aligned} \tag{45}$$

It is 2+1 dimensional nonlinear integrable equations.

Proposition 6:

$$\begin{gathered}\theta=\arcsin[d\sec h(d\eta)],\quad p=\arctan\left[\frac{d}{A}\tanh(d\eta)\right],\\ \eta=c_1x+c_2y+c_3t,\quad c_1=\frac{c}{2\lambda}+\frac{\lambda}{2c},\quad c_2=-\frac{c}{2\lambda}+\frac{\lambda}{2c},\\ c_3=\frac{\lambda}{2c^2}(c-A\lambda)(a_1+a_2)-\frac{c}{2\lambda^2}(Ac-\lambda)(a_1-a_2)\end{gathered} \tag{46}$$

is one soliton solution of the LR equations (10), (44), and (45).

Proof: From the relation among Eqs. (10), (11), and (12), it is easy to know that Eq. (46) satisfies the LR equation (10). So we only need to prove that Eq. (46) satisfies (44) and (45),

$$\theta_x=-\frac{d^2c_1\sec h(d\eta)\tanh(d\eta)}{\sqrt{1-d^2\sec h^2(d\eta)}},\quad p_x=\frac{d^2c_1\sec h^2(d\eta)}{A\left[1+\frac{d^2}{A^2}\tanh^2(d\eta)\right]},$$

$$\cos\theta=\sqrt{1-d^2\sec h^2(d\eta)},\quad \sin\theta=d\sec h(d\eta),$$

$$p_{xy}=-\frac{4Ad^3c_1c_2\sinh(2d\eta)}{[2A^2-1+\cosh(2d\eta)]^2}.$$

So,

$$\theta_xp_x-(p_x\cot\theta)_x-p_y\theta_y\cot^2\theta+\theta_x=\frac{\sqrt{2}d^2(Ac_1^2+Ac_2^2-c_1)\sec h(d\eta)\tanh(d\eta)}{\sqrt{(2A^2-1+\cosh(2d\eta)\sec h^2(d\eta)}},$$

$$\theta_xp_y+\theta_yp_x-p_{xy}\cot\theta+\theta_y=\frac{\sqrt{2}d^2(2Ac_1-1)c_2\sec h(d\eta)\tanh(d\eta)}{\sqrt{[2A^2-1+\cosh(2d\eta)]\sec h^2(d\eta)}}.$$

Meanwhile,

$$[2A^2-1+\cosh(2d\eta)]\sec h^2(d\eta)=2[1-d^2\sec h^2(d\eta)].$$

So, by calculation, it can be proved that Eq. (46) satisfies Eq. (44). Moreover,

$$p_{yt}=-\frac{4Ad^3c_2c_3\sinh(2d\eta)}{[2A^2-1+\cos h(2d\eta)]^2},$$

$$\theta_{xxy}\tan\theta+\theta_y\theta_{xx}\tan^2\theta-\theta_x\theta_{xy}=\frac{16A^2d^5c_1^2c_2\sinh(2d\eta)}{[2A^2-1+\cosh(2d\eta)]^3},$$

$$p_{xy}-3p_yp_{yy}\cot^2\theta=\frac{4Ad^3c_2(3Ac_2^2-c_1)\sinh(2d\eta)}{[2A^2-1+\cosh(2d\eta)]^2},$$

$$4p_y^2\theta_y\frac{\cos\theta}{\sin^3\theta}+p_xp_{xy}(2-\cot^2\theta)$$
$$=-\frac{4A^2d^3c_2[(5-6A^2)c_1^2+2(2A^2-1)c_2^2-(c_1^2-2c_2^2)\cosh(2d\eta)]\sinh(2d\eta)}{[2A^2-1+\cosh(2d\eta)]^3},$$

$$\theta_{xyy}\tan\theta+\theta_y\theta_{xy}\tan^2\theta-\theta_x\theta_{yy}=\frac{16A^2d^5c_1c_2^2\sinh(2d\eta)}{[2A^2-1+\cosh(2d\eta)]^3},$$

$$p_{yy}+4p_yp_x\theta_y\frac{\cos\theta}{\sin^3\theta}=-\frac{4Ad^3(1+2Ac_1)c_2^2\sinh(2d\eta)}{[2A^2-1+\cosh(2d\eta)]^2},$$

$$(1-2\cot^2\theta)(p_xp_{yy}+p_yp_{xy})=\frac{16A^2d^3c_1c_2^2[-2+3A^2\cosh(2d\eta)]\sinh(2d\eta)}{[2A^2-1+\cosh(2d\eta)]^3}.$$

Then substituting them into Eq. (45), this proposition is proved. □

VI. SPECIAL CASE OF *p* BEING CONSTANT

For the LR equation (10), if p is constant, it is just Sine–Gorden (SG) equation

$$\theta_{xx}-\theta_{yy}=\cos\theta\sin\theta \tag{47}$$

and Gauss curvature $K=-1$, mean curvature $H=\tan\theta-\cot\theta$. It is the surface with constant negative curvature. At that time, the equations that velocity u, v, and w satisfy should change and we can not take the velocity at that case. So in the following, we clarify the relation between the velocity and the surface, and give an other set of velocity. From Eq. (37), it yields

$$w_{xx}-w_{yy}=w\cos 2\theta,$$

it is just the linearization of the SG equation. So we can take the normal velocity component w as

$$w=b_1\theta_x+b_2\theta_y.$$

To find the tangent velocity, we should clarify the relation between u, v and w further. From Eqs. (35) and (36), it is easy to know that u, v satisfy

$$\cos^2\theta u_y+\sin^2\theta v_x=0,$$

$$\cos^2\theta u_x+\sin^2\theta v_y=0.$$

And from Eq. (38), it is easy to know that u_x and w satisfy

$$w_{xx}+w_x\theta_x\tan\theta-w_y\theta_y\cot\theta+u_x\cot\theta=w\cos^2\theta.$$

From Eq. (39), it can be derived that v_y and w satisfy

$$w_{yy}+w_x\theta_x\tan\theta-w_y\theta_y\cot\theta-v_y\tan\theta=w\sin^2\theta.$$

So we find the tangent velocity u, v,

$$u=b_1\left(\frac{\theta_x^2}{2}+\frac{\theta_y^2}{2}-\frac{\cos 2\theta}{4}-\theta_{xx}\tan\theta\right)+b_2(\theta_x\theta_y-\theta_{xy}\tan\theta),$$

$$v=b_2\left(\frac{\theta_x^2}{2}+\frac{\theta_y^2}{2}+\frac{\cos 2\theta}{4}+\theta_{yy}\cot\theta\right)+b_1(\theta_x\theta_y+\theta_{xy}\cot\theta).$$

From Eq. (33), the time evolution of θ reads

$$\begin{aligned}\theta_t=&b_1\left[\frac{3}{4}\theta_{xxx}+\frac{1}{4}\theta_{xyy}+\sin^2\theta\theta_x+\frac{\theta_x}{2}(\theta_x^2+3\theta_y^2)\right]\\&+b_2\left[\frac{5}{4}\theta_{xxy}-\frac{1}{4}\theta_{yyy}+\sin^2\theta\theta_y+\frac{\theta_y}{2}(3\theta_x^2+\theta_y^2)\right].\end{aligned}\tag{48}$$

It is one $2+1$ dimensional integrable equation.

Proposition 7:

$$\begin{aligned}\theta&=2\arctan(\exp\delta),\\\delta&=\frac{x}{\sin a}+\frac{\cos a}{\sin a}y+\frac{t\csc^3 a}{4}[b_1(3+\cos^2 a)+b_2\cos a(4+\sin^2 a)]\end{aligned}\tag{49}$$

is one soliton solution of Eqs. (47) and (48), where a is constant.

Proof: Note that

$$\cos\theta=\frac{1-\exp 2\delta}{1+\exp 2\delta},\quad \sin\theta=\frac{2\exp 2\delta}{1+\exp 2\delta},$$

$$\theta_x=\frac{2\csc a\exp\delta}{1+\exp 2\delta},\quad \theta_y=\frac{2\cot a\exp\delta}{1+\exp 2\delta},$$

$$\theta_{xx}=\frac{2\csc^2 a\exp\delta}{1+\exp 2\delta}\left(1-\frac{2\exp 2\delta}{1+\exp 2\delta}\right),$$

$$\theta_{yy}=\frac{2\cot^2 a\exp\delta}{1+\exp 2\delta}\left(1-\frac{2\exp 2\delta}{1+\exp 2\delta}\right),$$

so

$$\theta_{xx}-\theta_{yy}=2\exp\delta\frac{\exp 2\delta-1}{(1+\exp 2\delta)^2}=\cos\theta\sin\theta.$$

Equation (49) is one soliton solution of Eq. (47). Continuously, by direct calculation,

$$w=b_1\theta_x+b_2\theta_y=\frac{2\exp\delta}{1+\exp 2\delta}(b_1\csc a+b_2\cot a)$$

$$u=-\frac{b_1}{4},\quad v=\frac{b_1\cos a}{\sin^2 a}+b_2\cot^2 a+\frac{b_2}{4}.$$

Substituting them into Eq. (33), it yields that

$$\theta_t=\frac{\exp\delta\csc^3 a}{2(1+\exp(2\delta))}[b_1(3+\cos^2 a)+b_2\cos a(4+\sin^2 a)].$$

So, Eq. (48) is satisfied. This proposition is proved. □

VII. CONCLUSION AND REMARKS

In this paper, we discussed the LR surface and its evolution equation. We calculated the explicit expression of the LR surface when θ and p are chosen as solition solution of the LR equation. We obtained the motion equation from the compatibility conditions of some linear equations. Because there are many compatibility equations among them, we reduced the number of equations in orthogonal coordinates and proved Theorem 1. Based on this theorem, it is proved that some velocity components satisfy the linearization of the LR equation. But because the Sym formulation fails in the t term, it is difficult to calculate the explicit expression for the evolution equations of the LR surface. As the special case of the LR surface, we mentioned the surface with $K=-1$, which is the case of the LR equation with p being constant. Comparing this case with Ref. 20, it can be found that we studied a different form of the SG equation with different coordinates. Moreover, when $h=1$, this coordinate is geodesic and this reduction related to Theorem 1 includes the reduction of that Theorem 1 in Ref. 21 in some degree. However, there are many questions deserving further investigation, for instance, solving the spectral problem (19), (32) and obtaining the explicit expression of the motion of LR surface.

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k-constraint for the modified Kadomtsev–Petviashvili system

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By imposing constraint $(L^k)_- = q\partial^{-1}r\partial$ on the pseudo-differential operator L^k, the k constrained modified Kadomtsev–Petviashvili (KP) hierarchy and their corresponding Lax pair are obtained from the linear problem and its adjoint of the modified KP system. Especially, the modified KdV system, the GNS system with derivative coupling, the Burgers system, and a new 3×3 integrable system are presented as examples. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Many integrable equations important in physics can be generated from the Kadomtsev–Petviashvili (KP) hierarchy by imposing some restrictions on the pseudo-differential operator,[1–3]

$$L=\partial+u_2\partial^{-1}+u_3\partial^{-2}+\cdots+u_j\partial^{-j+1}+\cdots. \tag{1.1}$$

The k constraint $(L^k)_- = q\partial^{-1}r$ is a typical example, which leads the KP hierarchy to the so-called k constrained KP equations.[4] Such a reduced approach has an advantage that from this reduction, one can obtain directly the spectral problems of constrained systems with the help of the linear problem of the KP hierarchy. Consequently, the correspondent recursion operator, the bi-Hamiltonian structure, and other some features characteristic of the integrability of soliton equations are also derived.

In this letter, we would like to consider one kind of constraint on a general pseudo-differential operator,

$$L=\partial+u_1+u_2\partial^{-1}+\cdots+u_j\partial^{-j+1}+\cdots, \tag{1.2}$$

which is analogous to the above "k-constraint." If we redefine $(L^n)_-$ [or $(L^n)_+$] as the residual part with the functional term (or pure differential part) of operator L^n [see (2.1) in Sec. II], such a constraint can be expressed as $(L^k)_- = q\partial^{-1}r\partial$ and it makes the modified KP isospectral hierarchy the k constrained modified KP equations. These equations include a lot of interesting soliton hierarchies, such as the modified KdV hierarchy, the generalized nonlinear Schrödinger (GNS) hierarchy with derivative coupling, the Burgers hierarchy for one-constraint, and a new 3×3 integrable hierarchy for two-constraints. Moreover, the associated spectral problems and recursion operators for constrained systems are also obtained from the reduced theory.

II. SATO THEORY OF THE MODIFIED KP SYSTEM

Let $x,y,t_j(j=1,2,\ldots)\in R$, and $S(R^\infty)$ denote the Schwartz space composed of all rapidly decreasing functions $u=u(x,y,t)$ with infinitely many variables $(x,y,t)=(x,y,t_1,t_2,\ldots)$. For $u_j \in S(R^\infty)(j=1,2,\ldots)$, we take the pseudo-differential operator (1.2). Write

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$$L^n=\sum_{j\leqslant n} p_{nj}(u)\partial^j, \tag{2.1a}$$

$$A_n=(L^n)_+=\sum_{j=1}^{n} p_{nj}(u)\partial^j, \tag{2.1b}$$

$$(L^n)_-=L^n-(L^n)_+, \tag{2.1c}$$

namely, $(L^n)_+$ is the pure differential part of L^n and $(L^n)_-$ is the residual part with the functional term.[5] The coefficients $p_{nj}(u)$ in (2.1a) are uniquely determined by the coordinates u_j,$(j=1,2,\ldots)$ and their derivatives. The first few explicit forms of the operators A_n are listed below,

$$A_1=\partial, \tag{2.2}$$

$$A_2=\partial^2+2u_1\partial, \tag{2.3}$$

$$A_3=\partial^3+3u_1\partial^2+3(u_2+u_{1,x}+u_1^2)\partial, \tag{2.4}$$

$$A_4=\partial^4+4u_1\partial^3+(4u_2+6u_{1,x}+6u_1^2)\partial^2+(4u_3+6u_{2,x}+4u_{1,xx}+12u_1u_2+12u_1u_{1,x}+4u_1^3)\partial. \tag{2.5}$$

Consider the linear problem,

$$L\phi=\eta\phi, \tag{2.6a}$$

$$\phi_{t_m}=A_m\phi, \tag{2.6b}$$

where ϕ is an eigenfunction and η is a spectral parameter. If $\eta_{t_m}=0$, then the compatibility condition of (2.6) gives rise to the Lax equation for A_m,

$$L_{t_m}=[A_m,L], \tag{2.7}$$

or equivalent zero-curvature equation

$$A_{m,t_n}-A_{n,t_m}=[A_n,A_m]. \tag{2.8}$$

The modified KP hierarchy is obtained from (2.7) or from (2.8). For example, from (2.7) with $m=2,\ 3$, we have

$$u_{1,t_2}=2u_{2,x}+u_{1,xx}+2u_1u_{1,x}, \tag{2.9a}$$

$$u_{2,t_2}=2u_{3,x}+u_{2,xx}+2(u_1u_2)_x, \tag{2.9b}$$

$$u_{3,t_2}=2u_{4,x}+u_{3,xx}+2u_1u_{3,x}+4u_{1,x}u_3-2u_{1,xx}u_2, \tag{2.9c}$$

$$\ldots,$$

$$u_{1,t_3}=3u_{3,x}+3u_{2,xx}+u_{1,xxx}+6(u_1u_2)_x+3(u_1u_{1,x})_x+3u_1^2u_{1,x}, \tag{2.10a}$$

$$u_{2,t_3}=3u_{4,x}+3u_{3,xx}+u_{2,xxx}+6(u_1u_3)_x+3(u_1u_{2,x})_x+6u_2u_{2,x}+3(u_1^2u_2)_x, \tag{2.10b}$$

$$\ldots.$$

Eliminating u_2, u_3 from (2.9a), (2.9b), and (2.10a), we obtain the modified KP equation ($u_1 = u$),[6]

$$u_{t_3} = \tfrac{1}{4} u_{xxx} - \tfrac{3}{2} u^2 u_x + \tfrac{3}{2} u_x \partial^{-1} u_{t_2} + \tfrac{3}{4} \partial^{-1} u_{t_2 t_2}. \tag{2.11}$$

Equation (2.11) can also be obtained from (2.8) with $n=2$, $m=3$.

III. NOTION OF THE *K*-CONSTRAINT

Let L be the pseudo-differential operator (1.2) and A_m be the differential operator (2.1b). Set $\psi = \partial^{-1}\phi^*$, then it satisfies

$$\overline{L}\psi = \eta\psi, \tag{3.1a}$$

$$\psi_{t_m} = -\overline{A}_m \psi, \tag{3.1b}$$

where

$$\overline{L} = \partial^{-1} L^* \partial, \tag{3.2a}$$

$$\overline{A}_m = \partial^{-1} A_m^* \partial, \tag{3.2b}$$

in which operators L^* and A_m^* denote the adjoint of L and A_m, respectively. The linear problem (3.1) is called the generalized adjoint of (2.6). Its compatibility condition is

$$\overline{L}_{t_m} = [\overline{A}_m, \overline{L}], \tag{3.3}$$

or equivalently

$$\overline{A}_{m,t_n} - \overline{A}_{n,t_m} = [\overline{A}_m, \overline{A}_n]. \tag{3.4}$$

After introducing the adjoint of (2.6), we can turn to two kinds of k reductions for the modified KP system. The starting point of our method is to consider the more general linear problem,

$$L^k \phi = \lambda \phi, \tag{3.5a}$$

$$\phi_m = A_m \phi, \tag{3.5b}$$

for a fixed positive integer k and $\lambda = \eta^k$. If we impose the condition $L^k = A_k$ or $(L^k)_- = 0$ upon operator L^k, then the linear problem (3.5) becomes

$$A_k \phi = \lambda \phi, \tag{3.6a}$$

$$\phi_{t_m} = A_m \phi, \quad m \neq 0 \ (\mathrm{mod}\, k), \tag{3.6b}$$

and the modified KP hierarchy is reduced to the integrable system which is the compatibility condition of (3.6). When $k=2$, one obtains the modified KdV system.

In order to introduce the concept of another reduction, let us recall the linear problem of the modified KP equation,[7]

$$\phi_{t_2} = \phi_{xx} + 2u\phi_x, \tag{3.7a}$$

$$\phi_{t_3} = \phi_{xxx} + 3u\phi_{xx} + \tfrac{3}{2}(u_x + u^2 - \partial^{-1} u_{t_2})\phi_x, \tag{3.7b}$$

and its adjoint

$$\psi_{t_2} = -\psi_{xx} + 2u\psi_x, \tag{3.8a}$$

$$\psi_{t_3} = \psi_{xxx} - 3u\psi_{xx} - \tfrac{3}{2}(u_x - u^2 - \partial^{-1}u_{t_2})\psi_x. \tag{3.8b}$$

If the potential u is subject to the symmetry,

$$u = \phi\psi = qr, \tag{3.9}$$

where $\phi = q$, $\psi = r$, for convenience, then (3.7a) and (3.8a) become

$$q_{t_2} = q_{xx} + 2qrq_x, \tag{3.10a}$$

$$r_{t_2} = -r_{xx} + 2qrr_x, \tag{3.10b}$$

which is the GNS equation with derivative coupling given by Chen *et al.* in Ref. 8. Also (3.7b) and (3.8b) become

$$q_{t_3} = q_{xxx} + 3qrq_{xx} + 3(q_x r + q^2 r^2)q_x, \tag{3.11a}$$

$$r_{t_3} = r_{xxx} - 3qrr_{xx} - 3(qr_x - q^2 r^2)r_x, \tag{3.11b}$$

which is the higher order equation of (3.10). As a result, one can obtain the special solutions of the modified KP equation by solving both (3.10) and (3.11).

Substituting constraint (3.9) ($u_1 = u$) into (2.9), and by using (3.10) and (3.11), we can easily obtain

$$u_2 = -qr_x, \quad u_3 = qr_{xx}, \quad \ldots. \tag{3.12}$$

In this way, the pseudo-differential operator (1.2) becomes

$$L = \partial + q\partial^{-1}r\partial, \tag{3.13}$$

and here the following formula

$$\partial^{-1}\theta = \sum_{j=0}^{\infty} (-1)^j (\partial^j \theta)\partial^{-(j+1)} \tag{3.14}$$

is used. Conversely, with L given by (3.13), we construct the family of equations as

$$q_{t_m} = A_m q = (\partial + q\partial^{-1}r\partial)_+^m q, \tag{3.15a}$$

$$r_{t_m} = -\overline{A_m} r = -(-\partial + r\partial^{-1}q\partial)_+^m r. \tag{3.15b}$$

It can be verified that for $m = 2,3$, (3.15) is just (3.10) and (3.11). In Sec. IV we will prove the coincidence of (3.15) with the whole GNS hierarchy with derivative coupling.

Expression (3.13) (or $L_- = q\partial^{-1}r\partial$) is named as the one constraint of the pseudo-differential operator L. The above idea can be extended to the operator L^k, which leads to the notion of the k constraint.

Now we impose a general restraint on L^k by

$$L^k = A_k + q\partial^{-1}r\partial \quad \text{or} \quad (L^k)_- = q\partial^{-1}r\partial, \tag{3.16}$$

such that the coordinates $u_{k+1},u_{k+2},\ldots$ in L can be expressed by the coordinates $u_1,u_2,\ldots,u_k,q,r$ and their derivatives. Then we take the coupled linear problem,

$$L^k\phi=A_k\phi+q\psi=\lambda\phi, \tag{3.17a}$$

$$\psi_x=r\phi_x, \tag{3.17b}$$

and

$$\phi_{t_m}=A_m\phi, \tag{3.18a}$$

$$\psi_{t_m}=C_m\phi, \tag{3.18b}$$

with a finite number of coordinates $u_1,u_2,\ldots,u_k$, q, and r. Here $\lambda=\eta^k$ and C_m is the polynomial in ∂ satisfying

$$\partial C_m=r\partial A_m-\overline{A}_m r\partial. \tag{3.19}$$

The compatibility conditions of (3.17a) and (3.18a), also (3.17b) and (3.18b) with (3.19), yield, respectively,

$$L^k_{t_m}=[A_m,L^k] \tag{3.20a}$$

and

$$r_{t_m}=-\overline{A}_m r. \tag{3.20b}$$

Substituting (3.16) into (3.20a), and comparing the coefficient of the functional term we have

$$q_{t_m}=A_m q, \tag{3.20c}$$

where formulas (3.14) and (3.20b) are used. For the different time variables, the compatibility conditions of (3.18a), or (3.18b), are just Eq. (2.8).

Expression (3.16) is called the k constraint of the pseudo-differential operator L defined by (1.2). When $q=r=0$, (3.16) is reduced to $L^k=A_k$.

IV. ONE-CONSTRAINT AND RELATED EVOLUTION EQUATIONS

In this case, the pseudo-differential operator L is in the form of (3.13), and the spectral problem (3.17) can be written as

$$\phi_x-\lambda q\psi=-\lambda^2\phi, \tag{4.1a}$$

$$-\lambda\psi_x=r\phi_x, \tag{4.1b}$$

or equivalently

$$\phi_x=-\lambda^2\phi+\lambda q\psi, \tag{4.2a}$$

$$\psi_x=\lambda r\phi-qr\psi. \tag{4.2b}$$

By letting

$$\phi=e^{-1/2(\lambda^2 x+\partial^{-1}qr)}\phi_1, \tag{4.3a}$$

$$\psi=e^{-1/2(\lambda^2 x+\partial^{-1}qr)}\psi_1, \tag{4.3b}$$

(4.2) becomes

$$\phi_{1,x}=-\tfrac{1}{2}(\lambda^2-qr)\phi_1+\lambda q\psi_1, \tag{4.4a}$$

$$\psi_{1,x}=\lambda r\phi_1+\tfrac{1}{2}(\lambda^2-qr)\psi_1. \tag{4.4b}$$

After replacing derivatives with respect to x by using (4.4) repeatedly, we can suppose the time evolution for ϕ_1 and ψ_1 in (3.18) with (4.3) as follows:

$$\phi_{1,t_n}=A\phi_1+B\psi_1, \tag{4.5a}$$

$$\psi_{1,t_n}=C\phi_1-A\psi_1, \tag{4.5b}$$

where A, B, and C are polynomials in λ. From the compatibility conditions of (4.4) and (4.5), we can obtain the evolution equations,

$$\begin{pmatrix} q \\ r \end{pmatrix}_{t_n}=\Phi^n\begin{pmatrix} q \\ -r \end{pmatrix}. \tag{4.6a}$$

Here,

$$\Phi=\begin{pmatrix} \partial+qr+q_x\partial^{-1}r-q\partial^{-1}r_x & q_x\partial^{-1}q+q\partial^{-1}q_x \\ r_x\partial^{-1}r+r\partial^{-1}r_x & -\partial+qr+r_x\partial^{-1}q-r\partial^{-1}q_x \end{pmatrix}, \tag{4.6b}$$

and (4.6) is just the GNS hierarchy with the derivative coupling, while (4.4) is its standard spectral problem. When $n=2,3$, (4.6) becomes (3.10) and (3.11).

In what follows, we shall verify that Eq. (3.15) obtained by one constraint coincides with the hierarchy (4.6) indeed. To this end, we require two auxiliary formulas.

Lemma 1: Let the differential operator A_m be defined by (2.1b), and $\overline{A}_m=\partial^{-1}A_m^*\partial$, then

$$(q\partial^{-1}rA_m)_+=q\partial^{-1}rA_m+q\partial^{-1}\overline{A}_m(\partial^{-1}r)\partial. \tag{4.7}$$

Proof: By use of (3.14), we obtain easily

$$\begin{aligned}(q\partial^{-1}rA_m)_-&=\left(q\sum_{j=1}^{m}\partial^{-1}rp_{mj}(u)\partial^j\right)_- \\ &=q\sum_{j=1}^{m}\sum_{i=j}^{\infty}(-1)^{i-1}(\partial^{i-1}rp_{mj}(u))\partial^{j-i} \\ &=-q\sum_{l=0}^{\infty}(-1)^l[\partial^l(\overline{A}_m\partial^{-1}r)]\partial^{-l} \\ &=-q\partial^{-1}\overline{A}_m(\partial^{-1}r)\partial. \end{aligned} \tag{4.8}$$

Therefore, (4.7) holds.

Lemma 2: Let q and r satisfy Eq. (3.20b) and (3.20c), then the functional term $p_{m0}(u)$ of $(L^m)_-$ in (2.1c) can be expressed as

$$p_{m0}(u)=\partial^{-1}(-q\overline{A}_mr+rA_mq). \tag{4.9}$$

Proof: In Eq. (3.20a) with $k=1$,

$$L_{t_m}=[A_m,L]=-[(L^m)_-,L], \tag{4.10}$$

by equating the functional term yields

$$u_{1t_m}=(qr)_{t_m}=p_{m0,x}(u). \tag{4.11}$$

Inserting (3.20b) and (3.20c) into (4.11), one can easily know that (4.9) holds.

Let us now return to verify the coincidence of (3.15) and (4.6).

For $m=1$, the conclusion obviously holds. If it is also true for general m, then for $m+1$ we have

$$A_{m+1}=[(\partial+q\partial^{-1}r\partial)(A_m+p_{m0}(u))]_+=\partial A_m+qrA_m+p_{m0}(u)\partial-(q\partial^{-1}r_xA_m)_+. \tag{4.12}$$

By use of (4.7) and (4.9) yields

$$A_{m+1}q=(\partial+qr+q_x\partial^{-1}r-q\partial^{-1}r_x)A_mq-(q_x\partial^{-1}q+q\partial^{-1}q_x)\overline{A}_mr. \tag{4.13}$$

Similarly,

$$\overline{A}_{m+1}r=-(r_x\partial^{-1}r+r\partial^{-1}r_x)A_mq+(-\partial+qr+r_x\partial^{-1}q-r\partial^{-1}q_x)\overline{A}_mr. \tag{4.14}$$

The above two equalities are just the desired coincidence for $m+1$.

We make the following remarks:

(1) If we choose $r=1$, then the one constraint is reduced to

$$L=\partial+q, \tag{4.15}$$

and the constrained Eq. (3.15) are reduced to

$$q_{t_n}=(\partial+q)^n_+q, \tag{4.16}$$

which is the Burgers hierarchy. In fact, its spectral problem is

$$\phi_x+q\phi=\lambda\phi, \tag{4.17}$$

so, (4.16) can also be written as the following explicit formula:

$$q_{t_n}=(\partial+q+q_x\partial^{-1})^nq_x. \tag{4.18}$$

(2) Setting

$$\phi_1=e^{1/2\,\partial^{-1}qr}\phi_2, \qquad \psi_1=e^{-1/2\,\partial^{-1}qr}\psi_2, \tag{4.19}$$

(4.4) becomes the Kaup–Newell (KN) spectral problem, so we can prove that two kinds of evolution equations [GNS hierarchy (4.6) and KN hierarchy[9]] associated with these spectral problems are equivalent.

V. TWO-CONSTRAINT AND RELATION EVOLUTION EQUATIONS

In this case, the pseudo-differential operator L^2 takes the form,

$$L^2=\partial^2+2u_1\partial+q\partial^{-1}r\partial, \tag{5.1}$$

from which we find that the coordinates $u_2,u_3,\ldots$ in L can be determined by the coordinates u_1, q, r and their x derivatives as

$$u_2=-\tfrac{1}{2}(u_{1,x}+u_1^2-qr), \tag{5.2a}$$

$$u_3=\tfrac{1}{4}(u_{1,xx}+4u_1u_{1,x}+2u_1^3-2qru_1-q_xr-3qr_x), \tag{5.2b}$$

....

Consider the spectral problems given by

$$\phi_{xx}+2u\phi_x+q\psi=\lambda\phi, \tag{5.3a}$$

$$\psi_x=r\phi_x, \tag{5.3b}$$

where $u=u_1$ and $\lambda=\eta^2$. If we replace the x derivatives which are higher than one by (5.3a) repeatedly, then the time evolution for ϕ and ψ in (3.18) can be written as

$$\phi_{t_n}=A\phi_x+B\phi+C\psi, \tag{5.4a}$$

$$\psi_{t_n}=D\phi_x+E\phi+F\psi, \tag{5.4b}$$

where A, B, C, D, E, and F are certain undetermined polynomials in λ. The compatibility of (5.3) and (5.4) requires that $A,B,\ldots,F$ satisfy $(t=t_n)$,

$$2u_t+A_{xx}-2uA_x-(2u_x+qr)A+2B_x+2rC_x+r_xC+qD=0, \tag{5.5a}$$

$$q_t-2qA_x-q_xA-qB+C_{xx}+2uC_x-qrC-\lambda C+qF=0, \tag{5.5b}$$

$$r_t+rA_x-2ruA+rB+r^2C-D_x+2uD-E-rF=0, \tag{5.5c}$$

and

$$2\lambda A_x+B_{xx}+2uB_x+\lambda rC+qE=0, \tag{5.6a}$$

$$\lambda rA+rB_x-\lambda D-E_x=0, \tag{5.6b}$$

$$qrA-rC_x-qD+F_x=0. \tag{5.6c}$$

From these equations one finds that all $A,B,\ldots,F$ can be taken as the nth-order polynomials. Let $a_j,b_j,\ldots,f_j$ be their coefficients of λ^{n-j}, respectively, then by equating the same powers of λ in (5.5) and (5.6), we obtain for $b_n=e_n=0$,

$$g_t=\theta\begin{pmatrix} a_n \\ c_n \\ d_n \end{pmatrix}, \tag{5.7a}$$

$$\begin{pmatrix} a_{j+1} \\ c_{j+1} \\ d_{j+1} \end{pmatrix}=J\theta\begin{pmatrix} a_j \\ c_j \\ d_j \end{pmatrix} \quad (j=0,1,2,\ldots,n-1), \tag{5.7b}$$

and

$$(a_0,c_0,d_0)=(1,0,r), \tag{5.7c}$$

where

$$g=(2u,q,r)^T, \tag{5.8a}$$

$$\theta=\begin{pmatrix} -\partial^2+2u\partial+2u_x+qr & -2r\partial-r_x & -q \\ 2q\partial+q_x+q\partial^{-1}qr & -\partial^2-2u\partial+q\partial^{-1}r_x & -q\partial^{-1}q \\ -r\partial+2ur-r\partial^{-1}qr & -r\partial^{-1}r_x & \partial-2u+r\partial^{-1}q \end{pmatrix}, \tag{5.8b}$$

$$J=\frac{1}{4}\begin{pmatrix} -(1+2\partial^{-1}u) & 2\partial^{-1}r & 2\partial^{-1}q \\ -2q\partial^{-1} & -4 & 0 \\ -(r+2r_x\partial^{-1}+2r\partial^{-1}u) & 2r\partial^{-1}r & 2r\partial^{-1}q+4\partial \end{pmatrix}. \tag{5.8c}$$

The coefficients b_j, e_j $(j=0,1,\ldots,n-1)$ and f_j $(j=0,1,\ldots,n)$ can be determined by a_j, c_j, and d_j according to (5.5) and (5.6). From (5.7), the evolution equations with odd time variables can be given by

$$g_{t_{2n+1}}=\Phi^n g_x, \tag{5.9}$$

where

$$\Phi=\theta J=(\omega_{ij})_{3\times 3}, \tag{5.10}$$

with

$$\omega_{11}=\tfrac{1}{4}\partial^2+\partial qr\partial^{-1}-\partial u\partial^{-1}u, \quad \omega_{12}=\tfrac{3}{2}r\partial+\tfrac{1}{2}r_x+\partial u\partial^{-1}r,$$

$$\omega_{13}=-\tfrac{3}{2}q\partial-\tfrac{1}{2}q_x+\partial u\partial^{-1}q, \quad \omega_{21}=\tfrac{3}{4}q_x+\tfrac{1}{2}q_{xx}\partial^{-1}-\tfrac{1}{2}q_x\partial^{-1}u+uq_x\partial^{-1},$$

$$\omega_{22}=\partial^2+2u\partial+qr-q\partial^{-1}r_x+\tfrac{1}{2}q_x\partial^{-1}r, \quad \omega_{23}=\tfrac{1}{2}q_x\partial^{-1}q+q\partial^{-1}q_x,$$

$$\omega_{31}=-\tfrac{3}{4}r_x-\tfrac{1}{2}r_{xx}\partial^{-1}-\tfrac{1}{2}r_x\partial^{-1}u+ur_x\partial^{-1}, \quad \omega_{32}=\tfrac{1}{2}r_x\partial^{-1}r+r\partial^{-1}r_x,$$

$$\omega_{33}=\partial^2-2u\partial+qr-r\partial^{-1}q_x+\tfrac{1}{2}r_x\partial^{-1}q. \tag{5.11}$$

Especially, when $n=0,1$ we have

$$u_{t_1}=u_x, \quad q_{t_1}=q_x, \quad r_{t_1}=r_x, \tag{5.12}$$

and

$$u_{t_3}=\tfrac{1}{4}u_{xxx}-\tfrac{3}{2}u^2u_x+\tfrac{3}{2}(uqr)_x+\tfrac{3}{4}(q_xr-qr_x)_x, \tag{5.13a}$$

$$q_{t_3}=q_{xxx}+3uq_{xx}+\tfrac{3}{2}(u_x+u^2+qr)q_x, \tag{5.13b}$$

$$r_{t_3}=r_{xxx}-3ur_{xx}-\tfrac{3}{2}(u_x-u^2-qr)r_x. \tag{5.13c}$$

If one takes that A, C, and D are the nth-order polynomials, while B, E, and F, are the $n+1$th-order polynomials in λ, then the evolution equations with the even time variables can be deduced by comparing the coefficient's method from (5.5) and (5.6),

$$g_{t_{2n}}=\Phi^n\theta g_0, \quad g_0=-(0,q,r_x)^T, \tag{5.14}$$

where Φ and θ are defined by (5.10) and (5.8b), respectively. When $n=0$, Eq. (5.14) becomes

$$u_{t_2}=(qr)_x, \tag{5.15a}$$

$$q_{t_2}=q_{xx}+2uq_x, \tag{5.15b}$$

$$r_{t_2}=-r_{xx}+2ur_x. \tag{5.15c}$$

Similar to that in the one constraint, Eqs. (5.9) and (5.14) obtained by linear problems (5.3) and (5.4) coincide with the equations defined by formula (3.20) for $k=2$.

To our knowledge, the constrained Eqs. (5.9) and (5.14) have not been reported in any literature.

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Shear-free relativistic fluids and the absence of movable branch points

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The problem of determining the metric for a nonstatic shear-free spherically symmetric fluid (either charged or neutral) reduces to the problem of determining a one-parameter family of solutions to a second-order ordinary differential equation (ODE) containing two arbitrary functions f and g. Choices for f and g are determined such that this ODE admits a one-parameter family of solutions that have poles as their only movable singularities. This property is strictly weaker than the Painlevé property and it is used to identify classes of solvable models. It is shown that this procedure systematically generates many exact solutions including the Vaidya metric, which does not arise from the standard Painlevé analysis of the second-order ODE. Interior solutions are matched to exterior Reissner–Nordstrøm metrics. Some solutions given in terms of second Painlevé transcendents are described. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1455688]

I. INTRODUCTION

Several authors have shown that the problem of finding a nonstatic solution of the Einstein–Maxwell equations for a shear-free spherically symmetric charged fluid is equivalent to the problem of finding a t-dependent solution to the equation

$$\frac{\partial^2 y(x,t)}{\partial x^2} = f(x)y^2(x,t) + g(x)y^3(x,t), \tag{1}$$

where f and g are arbitrary functions of x only[1,2] (see also Ref. 3 and the references therein). Given a solution y of Eq. (1), define $r=\sqrt{x}$, $Y(r,t)=1/y(x,t)$, and

$$T(r,t) = h(t)\frac{\partial}{\partial t}\ln y(r^2,t), \tag{2}$$

where h is an arbitrary nonvanishing function of t. In terms of these variables, the metric for the fluid is given by

$$ds^2 = T^2(r,t)dt^2 - Y^2(r,t)\{dr^2 + r^2 d\Omega^2\}, \tag{3}$$

where $d\Omega^2 = d\theta^2 + \sin^2\theta d\phi^2$ is the standard metric on the two-sphere. The density ρ and pressure p are given by

$$8\pi\rho = 3h^{-2} - 12xy_x^2 + 12yy_x + 8xfy^3 + 6xgy^4, \tag{4}$$

$$8\pi p = 4y(y-2xy_x)\frac{y_{xt}}{y_t} + 12xy_x^2 - 8yy_x + 2xgy^4 - 2h^{-3}h_t\frac{y}{y_t} - 3h^{-2}. \tag{5}$$

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The only nonvanishing components of the electromagnetic field are

$$F_{01}=-F_{10}=-h(t)E(r)\frac{\partial y}{\partial t},$$

where $E^2(r)=2xg(x)$.

Although y is a function of two variables x and t, Eq. (1) is essentially an ODE for y as a function of x. As an ODE, the general solution of Eq. (1) contains two arbitrary constants. The general solution of Eq. (1) viewed as a partial differential equation (PDE) is obtained by replacing these arbitrary constants with arbitrary functions of t. Since T is a metric coefficient, it cannot be identically zero, so from Eq. (2) we see that y must have a nonconstant t-dependence. This leads us to the problem of finding families of solutions to Eq. (1) viewed as an ODE which depend on (at least) one parameter.

The connection between integrable systems (equations that are solvable, either explicitly or via a related linear problem) was first used by Kowlevskaya in her work on spinning tops.[4,5] She considered the equations of motion for a spinning top which depend on six parameters (the center of mass and the moments of inertia). Kowalevskaya noticed that in the known cases for which the equations could be integrated, the general solution was a meromorphic function of time when extended to the complex plane. She used local series analysis to determine all choices of the parameters for which the general solution was a meromorphic function of time and found a new set of values for the parameters for which she was then able to solve the equations in terms of ratios of hyper-elliptic functions.

The requirement that all solutions are meromorphic throughout the complex plane may be replaced with the requirement that all solutions be meromorphic on the covering space of **C** with a discrete set of points removed. In this way, branching of solutions is allowed at fixed singularities (singularities of the solutions that cannot occur at arbitrary locations in the complex plane but only at locations at which the equation itself is in some sense singular). An ODE is said to possess the Painlevé property if all movable singularities of all solutions are poles. This property is closely connected with the integrability (solvability) of the ODE. All ODEs that are known to possess the Painlevé property are integrable, either explicitly in terms of classically known functions, or via an associated linear problem. In particular, Painlevé, Gambier, and Fuchs classified all equations of the form

$$\frac{d^2y}{dx^2}=F\left(x;y,\frac{dy}{dx}\right), \tag{6}$$

where F is rational in y and dy/dx and analytic in x, that have the Painlevé property. They showed that each such equation could be transformed via a change of independent variable and an x-dependent Möbius transformation of y to 1 of 50 canonical equations. With the exception of six equations (the Painlevé equations P_I–P_{VI}) each of these canonical equations were solved in terms of classically known functions (see, e.g., Refs. 6 and 7). The first two Painlevé equations are

$$\frac{d^2\eta}{d\zeta^2}=6\eta^2+\zeta, \tag{7}$$

$$\frac{d^2\eta}{d\zeta^2}=2\eta^3+\zeta\eta+\alpha, \tag{8}$$

where α is an arbitrary complex constant. It was later shown that each Painlevé equation is the compatibility condition for a (linear) spectral problem. The Painlevé equations are considered to be integrable because of the underlying structure that emerges from these isomonodromy problems.[7,8]

It is important to note that the transformation of one the equations of the form (6) that possesses the Painlevé property to one of the canonical forms is itself determined by the solutions of a system of differential equations. A weaker definition of the Painlevé property is that all solutions are single-valued about all movable singularities. However, for equations of the form (6) this definition yields the same class of equations.

Shah and Vaidya,[1] Wyman,[9,10] Chatterjee,[11] Maharaj, Leach, and Maartens[12] and Srivastava[13] have studied Eq. (1) to determine choices of f and g for which the general solution has no movable critical points. In particular, Wyman[9] determined all choices of f in the uncharged ($g=0$) case. In Ref. 14 the author found all choices of f and g such that Eq. (1) possesses the Painlevé property. In particular, we have the following.

Proposition 1.1: Equation (1) possesses the Painlevé property (as an ODE in x) if and only if either

(1)

$$f(x)=6w^5(z), \quad g(x)=0, \tag{9}$$

where $w\neq 0$ and v are any solutions of

$$\frac{d^2v}{dz^2}=6v^2+az+b/2, \tag{10}$$

$$\frac{d^2w}{dz^2}=12vw, \tag{11}$$

where a, b are constants and z is given by

$$x=\int w^{-2}(z)dz, \tag{12}$$

or

(2)

$$f(x)=6v(z)w^5(z), \quad g(x)=2w^6(z), \tag{13}$$

where $w\neq 0$ and v are any solutions of

$$\frac{d^2v}{dz^2}=2v^3+(az+b)v+c/2, \tag{14}$$

$$\frac{d^2w}{dz^2}=(6v^2+az+b)w, \tag{15}$$

where a, b, c are constants and z is given by Eq. (12).

Furthermore, in both the above cases, the general solution of Eq. (1) is given by

$$y(x,t)=\frac{u(z,t)-v(z)}{w(z)}, \tag{16}$$

where u (in which t is treated as a parameter) is the general solution of the same second-order equation as v [i.e., in case 1, $u(z,t_0)$, where t_0 is a constant, solves Eq. (10) and in case 2 it solves Eq. (14)].

Note that Eq. (11) [resp. (15)] is the linearization of Eq. (10) [resp. (14)]. So if $v(z)=V(z;\epsilon)$ is a one-parameter family of solutions to Eq. (10) [resp. (14)], then $w(z):=V_\epsilon(z;\epsilon)$ is a solution to Eq. (11) [resp. (15)]. A second independent solution to Eq. (11) [resp. (15)] then

follows by reduction of order. Equation (12) shows that $x=\hat{w}(z)/w(z)$, where $\hat{w}$ is a second solution of Eq. (11) [resp. (15)] satisfying the Wronskian condition $W(w,\hat{w})=w\hat{w}_z-\hat{w}w_z=1$.

If $a=0$, then the general solution to Eq. (10) [resp. (14)] can be given explicitly in terms of elliptic functions. In particular, the case in which $a=0$ and the fixed solution v of Eq. (14) is a constant corresponds to the large class of solutions found by Sussman.[15] In fact, most of the solutions that have appeared in the literature to date are special cases of Sussman's solutions. The case in which v is not constant is solved explicitly in Ref. 14. If $a\neq 0$, then Eq. (10) [resp. (14)] can be mapped to Eq. (7) [resp. (8)]. A class of solutions to Eq. (1) corresponding to the Airy function solutions to Eq. (8) is also described in Ref. 14.

Recall that we wish to find one-parameter families of solutions to Eq. (1). When f and g are chosen so that Eq. (1) possesses the Painlevé property then the equation is integrable and we can find a two-parameter family of solutions. In the present article a property, weaker than the Painlevé property but still complex-analytic in nature, is considered. Namely, we wish to find all one-parameter families of solutions $\mathcal{F}$ to Eq. (1) such that all movable singularities of all solutions in $\mathcal{F}$ are poles. In Sec. II we will find all solutions to Eq. (1) that are simultaneously solutions of a Riccati equation. This class of solutions contains the well-known solutions due to Shah and Vaidya,[16] which does not arise in a regular Painlevé analysis of Eq. (1). A class of solutions that generalizes that due to Shah and Vaidya which is given in terms of solutions to linear equations is also derived.

Sections III and IV address the question of whether the solutions found in Sec. II exhaust the set of all one-parameter families of solutions $\mathcal{F}$ described above. In Sec. V, boundary conditions are determined such that the Riccati solutions can be matched to the Reissner–Nordstrøm external solution. In Sec. VI we find solutions to Eq. (1) corresponding to $a\neq 0$ but $v\equiv 0$ in Eq. (14). In this case the general solution to Eq. (15) is given in terms of Airy functions. From this solution, families of solutions are obtained using the Bäcklund transformation of the second Painlevé equation.

II. RICCATI SOLUTIONS

One way of finding a one-parameter family of solutions to Eq. (1) such that the only movable singularities are poles is to find a family of solutions that are also solutions of a first-order equation of Painlevé type. In this section, solutions to Eq. (1) are found that are also solutions to a first-order differential equation of the form

$$\frac{dy}{dx}=R(x,y), \tag{17}$$

where R is rational in y and locally analytic in x. Fuchs[17] showed that the only equation of the form (17) with the Painlevé property is the Riccati equation,

$$\frac{dy}{dx}=\alpha(x)y^2+\beta(x)y+\gamma(x), \tag{18}$$

where α, β, and γ are (locally) analytic functions of x. The general solution of Eq. (18) is given by

$$y(x)=-\frac{1}{\alpha(x)}\frac{d}{dx}\ln\Phi(x),$$

where Φ is the general solution of the linear equation

$$\frac{d^2\Phi}{dx^2}-\left(\beta+\frac{\alpha_x}{\alpha}\right)\frac{d\Phi}{dx}+\alpha\gamma\Phi=0. \tag{19}$$

Differentiating Eq. (18) with respect to x and again using Eq. (18) to eliminate dy/dx in the resulting expression gives

$$\frac{d^2y}{dx^2}=2\alpha^2y^3+(\alpha_x+3\alpha\beta)y^2+(\beta_x+\beta^2+2\alpha\gamma)y+(\gamma_x+\beta\gamma). \tag{20}$$

It follows that every solution of Eq. (18) is a solution of Eq. (1) if and only if the equations

$$\gamma_x+\beta\gamma=0, \tag{21}$$

$$\beta_x+\beta^2+2\alpha\gamma=0, \tag{22}$$

$$\alpha_x+3\alpha\beta=f, \tag{23}$$

$$2\alpha^2=g, \tag{24}$$

are satisfied.

Solving Eqs. (21)–(24) gives three classes of Riccati equations.

Case 1: $\beta\equiv 0$, $\gamma\equiv 0$. The Riccati equation (18) becomes

$$\frac{dy}{dx}=\alpha y^2,$$

which has the general solution

$$y(x,t)=\frac{1}{H(x)+G(t)}, \tag{25}$$

where $H'(x)=-\alpha(x)$ and G is an arbitrary function of t.

Case 2: $\beta\not\equiv 0$, $\gamma\equiv 0$. The Riccati equation (18) becomes

$$\frac{dy}{dx}=\alpha y^2+\frac{1}{x+C}y,$$

where C is an arbitrary constant, which has the general solution

$$y(x,t)=\begin{cases}\dfrac{x}{H(x)+G(t)}, & H'(x)=-x\alpha(x), \quad \text{if } C=0,\\[2ex] \dfrac{1+kx/4}{H(x)+G(t)}, & H'(x)=-(1+kx/4)\alpha(x), \quad \text{if } C=4/k\neq 0,\end{cases} \tag{26}$$

where G is an arbitrary function of t.

Case 3: $\gamma\not\equiv 0$. The Riccati equation (18) becomes

$$\frac{dy}{dx}+\frac{1}{2}(\gamma^{-1})_{xx}y^2+\frac{\gamma'}{\gamma}y-\gamma=0. \tag{27}$$

In Sec. V, these Riccati solutions will be matched to an external Reissner–Nordstrøm metric.

Note that Eq. (25) corresponds to setting $k=0$ in Eq. (26b). Under the transformation

$$\tilde{r}=\frac{r}{1+kr^2/4}$$

(recall $x=r^2$) the solutions corresponding to Eq. (26b) give rise to the metric

$$ds^2=[F(\tilde{r})+G(t)]^{-2}dt^2-[F(\tilde{r})+G(t)]^2\left[\frac{d\tilde{r}^2}{1-k\tilde{r}^2}+\tilde{r}^2d\Omega^2\right], \tag{28}$$

where $F(\tilde{r})=H(r^2)$ and we have set $h(t)=1/\dot{G}(t)$. The metric (28) was obtained by Shah and Vaidya.[16] This metric does not arise from the standard Painlevé analysis of Eq. (1).

Solutions found in this section will be referred to as Riccati solutions.

III. LOCAL SERIES ANALYSIS

In this section we will analyze Eq. (1) as an ODE in the complex domain. In particular, we will determine necessary conditions that Eq. (1) possesses a one-parameter family of Laurent series solutions. We begin by considering the case in which $g=0$. Under the transformation (16) in which w is given by Eq. (9), v is given by Eq. (11), and z is given implicitly by Eq. (12), Eq. (1) becomes

$$\frac{d^2u}{dz^2}=6u^2+A(z), \tag{29}$$

where

$$A(z)=\frac{d^2v}{dz^2}-6v^2.$$

We will only consider a one-parameter family of solutions $\mathcal{G}$ such that there exists an open connected bounded set $\Omega\in\mathbf{C}$ such that at each point $z_0\in\Omega$ there is a function $u\in\mathcal{G}$ with a pole at $z=z_0$. We will now find a necessary condition on the function A such that Eq. (29) admits a formal Laurent series solution with a pole at a point $z_0\in\Omega$, where A is analytic. Substituting the Laurent series

$$u(z)=\sum_{n=0}^{\infty}a_n(z-z_0)^{n-p}, \tag{30}$$

where p is a positive integer and $a_0\neq 0$, into Eq. (29) gives, to leading order,

$$p(p+1)a_0(z-z_0)^{-(p+2)}+\ldots=6a_0^2(z-z_0)^{-2p}+\ldots.$$

Equating the powers and coefficients of these leading-order terms gives

$$p=2,\quad a_0=1. \tag{31}$$

Using Eqs. (30) and (31) in Eq. (29) and equating coefficients of like powers of $z-z_0$ gives

$$(n+1)(n-6)a_n=P_n(a_0,a_1,\ldots,a_{n-1}), \tag{32}$$

where

$$P_n(a_0,a_1,\ldots,a_{n-1})=6\sum_{m=1}^{n-1}a_ma_{n-m}+\alpha_n(z_0),$$

and

$$\alpha_n(z_0)=\begin{cases}0, & n<4,\\ \dfrac{A^{(n-4)}(z_0)}{(n-4)!}, & n\geqslant 4,\end{cases}$$

is polynomial in its arguments and we have expanded A as a power series about $z=z_0$. The recurrence relation (32) shows that a_n is uniquely determined in terms of $\{a_0,\ldots,a_{n-1}\}$, except in the case when $n=6$. In this case, the left side of Eq. (32) vanishes while the right side is a known function of $(a_0,\ldots,a_5)$. If the right side does not vanish, then there is no solution to Eq. (29) with a pole of any order at $z=z_0$. If the right side of Eq. (32) does vanish, then a formal Laurent series solution exists in which z_0 and a_6 are arbitrary constants. A direct calculation shows that the right side of Eq. (32) vanishes if and only if

$$A''(z_0)=0. \tag{33}$$

Now since Eq. (33) must be satisfied for all z_0 in the open set Ω, this implies that $A(z)=az+b/2$, for some constants a and b. So, we reproduce precisely those solutions given in case 1 of Proposition 1.1.

Now we consider the local series analysis of Eq. (1) when g is not identically zero. In particular, g does not vanish identically on Ω. From Sec. 2 we see that the requirement that there is a one-parameter family of solutions such that all movable singularities are poles yields more solutions than requiring that Eq. (1) possesses the Painlevé property.

Let v and w be defined by Eq. (13) where z is given by Eq. (12). [Note that we are not assuming that Eqs. (14) and (15) hold.] The transformation (16) gives

$$\frac{d^2u}{dz^2}=2u^3+B(z)u+C(z), \tag{34}$$

where

$$B(z)=\frac{w_{zz}}{w}-6v^2, \quad C(z)=v_{zz}-vB(z)-2v^3.$$

We now look for a local Laurent series solution to Eq. (34) with a pole at $z=z_0\in\Omega$. Leading order analysis shows that any such solution u must have a simple pole at $z=z_0$ with residue ±1. Hence we substitute the series

$$u(z)=\sum_{n=0}^{\infty}a_n(z-z_0)^{n-1}, \quad a_0=\varepsilon=\pm1,$$

into Eq. (34) and equate coefficients of like powers of $z-z_0$ to obtain the recurrence relation

$$(n+1)(n-4)a_n=Q_n(a_0,\ldots,a_{n-1}), \tag{35}$$

where

$$Q_n(a_0,\ldots,a_{n-1})=2\left[\sum_{m=0}^{n}\sum_{m'=0}^{n-m}a_ma_{m'}a_{n-m-m'}-3a_n\right]+\beta_n(z_0)+\gamma_n(z_0),$$

and

$$\beta_n(z_0)=\begin{cases}0, & n<2,\\ \displaystyle\sum_{m=0}^{n-2}\frac{B^{(n-m-2)}(z_0)}{(n-m-2)!}a_m, & n\geqslant2,\end{cases} \qquad \gamma(z_0)=\begin{cases}0, & n<3,\\ \dfrac{C^{(n-3)}(z_0)}{(n-3)!}, & n\geqslant3.\end{cases}$$

Note that Q is polynomial in its arguments. The left side of Eq. (35) shows that a necessary and sufficient condition for the existence of a formal Laurent series solution with a pole at $z=z_0$ is $Q_4(a_0,a_1,a_2,a_3)=0$, which is equivalent to $B''(z_0)=-2\varepsilon C'(z_0)$, where $\varepsilon=\pm1=a_0$.

Now the general solution of Eq. (34) will have movable singularities with leading order behaviors that include both $+1$ and -1 residue poles (although, in general, these solutions will not be meromorphic and the Laurent series will have to be augmented by logarithm terms). So if we demand that all movable singularities of all solutions are poles [i.e., if we demand that Eq. (34) possess the Painlevé property], then $B''(z_0)=2'C(z_0)$ and $B''(z_0)=-2C'(z_0)$, for all $z_0\in\Omega$, leading to $B(z)=az+b$, and $C(z)=c/2$, where a, b, and c are arbitrary constants. So u satisfies Eq. (14).

Rather than demand that all movable singularities of all solutions of Eq. (34) are poles, we restrict our consideration to a subset of solutions $\mathcal{G}$ such that given any $z_0\in\Omega$, there is a solution in $\mathcal{G}$ with a pole at $z=z_0$. The above analysis shows that either we are left with Eq. (14) or we must consider the class of solutions where all movable singularities are poles and all but a finite number of these poles in ω have the same residue $\varepsilon=\pm 1$. A necessary condition in this case is the differential equation $B''(z)=-2\varepsilon C'(z)$. In terms of $q(z):=B(z)/2$, we now restrict ourselves to the study of the subset of solutions to the equation

$$\frac{d^2u}{dz^2}=2u^3+2qu+(\kappa-\varepsilon q_z),\quad \varepsilon=\pm 1, \tag{36}$$

where κ is an arbitrary constant, that admit only poles with residue ε in Ω.

IV. THE UNIQUENESS OF THE RICCATI SOLUTIONS

The only Riccati equation for which all solutions u are also solutions of Eq. (36) is

$$\frac{du}{dz}+\varepsilon(u^2+q)=0,\quad \kappa=0. \tag{37}$$

The general solution of equation (37) is given by

$$u=\varepsilon\frac{d}{dz}\ln\Phi, \tag{38}$$

where Φ is the general solution of the linear equation

$$\frac{d^2\Phi}{dz^2}+q\,\Phi=0. \tag{39}$$

We will show that these Riccati type solutions are identical to those found in Sec. II. All movable singularities of any solution to Eq. (37) are simple poles with residue ε. So the general solution to Eq. (37) is a one-parameter family of solutions to Eq. (36) of the kind considered at the end of the previous section. The perturbation argument described below suggests that this is the only such one-parameter family. We will then provide a proof based on Wiman–Valiron theory for the case in which q is a polynomial. Wiman–Valiron theory is particularly useful for finding entire solutions of analytic differential equations.[18]

We will now show how the Riccati equations derived in Sec. II are related to the solutions of Eq. (36) described at the end of Sec. III. It may be verified that the identity

$$w(u_z+\varepsilon[u^2+q])=y_x+\varepsilon w^3y^2+w(w_z+2\varepsilon vw)y+w(v_z+\varepsilon[v^2+q]) \tag{40}$$

follows from Eqs. (12) and (16). Furthermore, given Eqs. (12) and (13), where v and w satisfy

$$v_{zz}=2v^3+2qv-\varepsilon q_z \tag{41}$$

and

$$w_{zz}=(6v^2+2q)w, \tag{42}$$

respectively, it can be shown that Eqs. (21)–(24) are equivalent to

$$\alpha=-\varepsilon w^3, \tag{43}$$

$$\beta=-w(w_z+2\varepsilon v w), \tag{44}$$

$$\gamma=-w(v_z+\varepsilon[v^2+q]). \tag{45}$$

Equations (40) and (43)-(45) show that the Riccati solutions found in Sec. II are the same as those constructed using (16) where u is the general solution of Eq. (37) and v, w satisfy Eqs. (41) and (42), respectively. It is interesting to note that the solution by Shah and Vaidya discussed in Sec. II corresponds to the case in which v also satisfies the Ricatti equation (37). The $\gamma\neq 0$ case (case 3 in Sec. II) corresponds to a non-Ricatti solution v of Eq. (41) (although u still satisfies a Riccati equation).

Next we address the question of whether the class $\mathcal{G}$ consists only of Riccati solutions. Consider Eq. (36) with $q(z)=q_0+hQ(z)$, where q_0 is a complex constant and h is a small complex parameter. To leading order in h, Eq. (36) is

$$\frac{d^2u}{dz^2}=2u^3+2q_0u+\kappa.$$

If u is not constant, then

$$\left(\frac{du}{dz}\right)^2=u^4+2q_0u^2+2\kappa u+C, \tag{46}$$

where C is an integration constant. The nonconstant solutions of Eq. (46) are elliptic functions with simple poles of residue ± 1. The only solutions with poles of residue $\varepsilon=\pm 1$ but no poles of residue $-\varepsilon=\mp 1$ correspond to the case in which $\kappa=0$ and $C=q_0^2$ in which case Eq. (46) factors into two Riccati equations and u satisfies

$$\frac{du}{dz}+\varepsilon(u^2+q_0)=0.$$

The arguments given above assume that the one-parameter family of solutions $\mathcal{G}$ have poles in an open set Ω. In the following we show rigorously that we have found all one-parameter families of solutions that have only poles as their movable singularities under the assumption that q is a polynomial.

Consider the system of first-order equations

$$\frac{du}{dz}=\tilde{u}-\varepsilon u^2-\varepsilon q, \tag{47}$$

$$\frac{d\tilde{u}}{dz}=\kappa+2\varepsilon u\tilde{u}. \tag{48}$$

Differentiating Eq. (47) with respect to z and using Eq. (48) to eliminate $d\tilde{u}/dz$ gives Eq. (36). We wish to show that if there is a one-parameter family of solutions u having only movable poles with residue ε, then $\tilde{u}$ is identically zero. Note that if $\tilde{u}$ is identically zero, then Eq. (47) becomes Eq. (37) and Eq. (48) implies that $\kappa=0$. If $\tilde{u}$ does not vanish identically, then we can solve Eq. (48) for u and substitute it into Eq. (47) to give

$$2\tilde{u}\frac{d^2\tilde{u}}{dz^2}=\left(\frac{d\tilde{u}}{dz}\right)^2+4\tilde{u}^2(\varepsilon\tilde{u}-q)-\kappa^2. \tag{49}$$

We will prove the following.

Proposition 4.1: If q is a polynomial, then either any entire solution of Eq. (49) is a constant or

$$q=q_0+q_1z+q_2z^2,$$

where

$$q_1^2-4q_0q_2=\kappa^2 \tag{50}$$

and

$$\tilde{u}=\varepsilon q. \tag{51}$$

Note that if $\tilde{u}$ is one of the solutions given in Proposition 4.1 but $\tilde{u}\not\equiv 0$, then since $\tilde{u}$ contains no free parameters (i.e., no parameters other than those in the equation itself) u is given by Eq. (48) and so does not represent a one-parameter family of solutions to Eq. (36).

Proof: We will begin by showing that any polynomial solution of Eq. (49) is either a constant or the solution (51). We will then use the central index from Wiman–Valiron theory to show that there are no transcendental (i.e., nonpolynomial) solutions.

Let q and $\tilde{u}$ be polynomials of degree M and N, respectively. Furthermore, we assume that $\tilde{u}$ is not constant (i.e., $N\geqslant 1$ and $\tilde{a}_N\neq 0$). Then q and $\tilde{u}$ have expansions of the form

$$q(z)=\sum_{m=0}^{M}q_mz^m,\quad \tilde{u}(z)=\sum_{n=0}^{N}\tilde{a}_nz^n. \tag{52}$$

Substituting the expansions (52) into Eq. (49) and balancing the dominant terms for large z gives $M=N$. Equation (49) then becomes

$$\sum_{i,j=0}^{N}i(2i-j-2)\tilde{a}_i\tilde{a}_jz^{i+j-2}+\kappa^2=\sum_{i,j,k=0}^{N}4\tilde{a}_i\tilde{a}_j(\varepsilon\tilde{a}_k-q_k)z^{i+j+k}. \tag{53}$$

Now the polynomial on the left side of Eq. (53) is of degree at most $2N-2$ while the degree of the polynomial on the right side is of degree at most $3N$. Since $\tilde{a}_N\neq 0$, then the coefficient of z^{3N} in Eq. (49) gives $\tilde{a}_N=\varepsilon q_N$. Arguing by induction, equating the coefficients of $z^{3M-1},z^{3M-2},\ldots,z^{2N+1}$ to zero gives $\tilde{a}_{N-n}=\varepsilon q_{N-n}$, $n=1,\ldots,N$. Hence $\tilde{u}=\varepsilon q$ and the right side of Eq. (53) vanishes identically. On equating all coefficients of powers of z to zero on the left side of Eq. (49) we find that $N=2$ and q_0, q_1, and q_2 satisfy Eq. (50).

Now we will use Wiman–Valiron theory to show that all entire solutions to Eq. (49) are polynomials. Since $\tilde{u}$ is entire it has an expansion of the form

$$\tilde{u}(z)=\sum_{n=0}^{\infty}\tilde{a}_nz^n.$$

The *central index* $\nu(r,\tilde{u})$ is the greatest non-negative integer m such that

$$|\tilde{a}_m|r^m=\max_{n\geqslant 0}|\tilde{a}_n|r^n.$$

If $\tilde{u}$ is nonpolynomial, then $\nu(r,\tilde{u})$ is increasing, piecewise constant, right-continuous, and tends to $+\infty$ as $r\to+\infty$.

In terms of the central index we have the following lemma (see, e.g., Ref. 19).

Lemma 4.2: Let $\tilde{u}$ be a nonpolynomial entire function, and $\nu=\nu(r,\tilde{u})$ be its central index. Let $0<\delta<1/4$ and z be such that $|z|=r$ and

$$|\tilde{u}(z)|>\nu(r,\tilde{u})^{-(1/4)+\delta}\max_{|z|=r}|\tilde{u}(z)| \tag{54}$$

holds. Then there exists a set $F\subset\mathbf{R}$ of finite logarithmic measure, i.e., $\int_F dt/t<+\infty$ such that

$$\tilde{u}^{(m)}(z)=\left(\frac{\nu(r,\tilde{u})}{z}\right)^m(1+o(1))\tilde{u}(z) \tag{55}$$

holds for all $m\geqslant 0$ and $r\notin F$.

Lemma 4.2 says that for all positive r outside of the set F (which has finite logarithmic measure), the estimate (55) holds near the maximum of $|\tilde{u}|$ on the circle $|z|=r$ [where "near the maximum" means the set of z satisfying Eq. (54)].

Assume that there is a nonpolynomial solution $\tilde{u}$ of Eq. (49). Applying the estimate (55) to Eq. (49) gives

$$\left(\frac{\nu(r,\tilde{u})}{z}\right)^2\tilde{u}^2\sim 4\varepsilon\tilde{u}^3. \tag{56}$$

Since $\nu(r,\tilde{u})$ grows much slower than $\tilde{u}$,[20] it follows that Eq. (56) cannot be balanced. Thus the only entire solutions to Eq. (49) are polynomials. ■

V. BOUNDARY CONDITIONS FOR THE RICCATI SOLUTIONS

In this section we will match the Riccati solutions introduced in Sec. II to an external Reissner–Nordstrøm metric

$$ds^2=\hat{\Gamma}d\hat{t}^2-\hat{\Gamma}^{-1}d\hat{r}^2-\hat{r}^2d\Omega^2, \tag{57}$$

where $d\Omega^2$ is the standard metric on the two-sphere and

$$\hat{\Gamma}=1-\frac{2m}{\hat{r}}+\frac{4\pi e^2}{\hat{r}^2},$$

and m and e are constants. Let Σ_0 be the interface $r=r_0$ between the two solutions. The two metrics (3) and (57) can be matched across Σ_0 provided

$$p(r_0,t)=0, \tag{58}$$

$$g(r_0^2)=2\pi\left(\frac{e}{r_0^3}\right)^2, \tag{59}$$

$$2m=\left[\frac{4\pi e^2}{r}y+\frac{r^3}{h^2y^3}+2\frac{r^2}{y^2}y_r-\frac{r^3}{y^3}y_r^2\right]_{r=r_0}, \tag{60}$$

for all t.[2]

Equation (59) is equivalent to

$$\alpha^2(r_0^2)=\pi\left(\frac{e}{r_0^3}\right)^2. \tag{61}$$

Using Eq. (18) to eliminate y_x and $y_{xt}=(2\alpha y+\beta)y_t$ from Eq. (5) gives

$$8\pi p = 4\{(\beta^2 + 2\alpha\gamma)x - \beta)y^2 + 2\gamma(2\beta x - 1)y + 3x\gamma^2\} - 3h^{-2} - 2h^{-3}h_t\frac{y}{y_t}. \tag{62}$$

Using Eq. (18) to eliminate $y_r = 2ry_x$ from Eq. (60) and using Eq. (62) in Eq. (58), we see that Eqs. (58) and (60) are equivalent to

$$h^{-2}(t) = 4\left[r^2\gamma + \gamma(2r^2\beta - 1)y + \{(\beta^2 + 2\alpha\gamma)r^2 - \beta\}y^2 + \left(\frac{m}{2r^3} + 2r^2\alpha\beta - \alpha\right)y^3\right]_{r=r_0}. \tag{63}$$

A. Dust solutions

Setting p identically zero in Eq. (62) and solving for h^{-2} gives

$$h^{-2} = 4[x\gamma + \gamma(2x\beta - 1)y + \{(\beta^2 + 2\alpha\gamma)x - \beta\}y^2 + \delta y^3], \tag{64}$$

where δ is a function of x only. Recall that h is a function of t only. Differentiating Eq. (64) with respect to x and using Eqs. (21) and (22) gives

$$3\alpha\delta y^2 + \{\delta_x + 3\beta\delta + 2\alpha[(\beta^2 + 2\alpha\gamma)x - \beta]\}y + \gamma\{2x\alpha_x + 3[\alpha + \delta]\} = 0, \tag{65}$$

for all t. Since y must have nonconstant t-dependence, the coefficients of different powers of y in Eq. (65) must vanish identically. If $\alpha = 0$, then $g = 0$ and there are no Riccati solutions. Therefore the coefficient of y^2 in Eq. (65) shows that δ is identically zero. The constant term in Eq. (65) shows that either $\gamma \equiv 0$ or $\alpha(x) = \kappa x^{-3/2}$, where κ is a constant.

If $\gamma = 0$, then the coefficient of y in Eq. (65) shows that either $\beta = 0$ or $\beta = 1/x$. These solutions correspond to the solutions (25) and (26), respectively. Finally, if $\gamma \neq 0$ and $\alpha \neq 0$, then recall from Sec. II (case 3) that for any Riccati solution we must have $\alpha = -(\gamma^{-1})_{xx}$ and $\beta = -\gamma_x/\gamma$. It follows that the coefficient of y and the constant term in Eq. (65) cannot both vanish identically.

VI. BÄCKLUND TRANSFORMATIONS AND SPECIAL SOLUTIONS

In this section we will construct what is perhaps the simplest solution of Eq. (1) involving a genuine transcendent of the second Painlevé equation. It is simple in the sense that we have an explicit formula for the dependence of x on z. We will then use the well-known Bäcklund transformation of the second Painlevé equation to construct a countable family of equations of the form (1) together with their general solutions in terms of second Painlevé transcendents.

If $a \neq 0$, then, after rescaling z and v, Eqs. (14) and (15) become

$$\frac{d^2v}{dz^2} = 2v^3 + zv + \alpha, \tag{66}$$

$$\frac{d^2w}{dz^2} = (6v^2 + z)w, \tag{67}$$

where α is an arbitrary constant. Equation (66) is the standard form of the second Painlevé equation. We will denote the general solution of Eq. (66) by $v(z) = P_{II}(z;\alpha;c_1,c_2)$, where c_1 and c_2 are independent parameters (e.g., $c_1 = v(0)$ and $c_2 = v'(0)$).

Recall that, apart from the solution due to Shah and Vaidya [(Eq. (28)], many of the solutions that appear in the literature are special cases of the solutions of Sussman,[15] which correspond to the special case of Proposition 1.1 in which $a = 0$ and v is a constant. Note that if $a \neq 0$, then Eq. (66) [which is a rescaled version of Eq. (14)] admits a constant solution if and only if $\alpha = 0$. In this case the constant solution is $v \equiv 0$, which is equivalent to the case $f \equiv 0$.

If $v \equiv 0$, then Eq. (67) has the general solution

$$w(z)=\mu \mathrm{Ai}(z)+\nu \mathrm{Bi}(z),$$

where Ai and Bi are the Airy functions and μ and ν are arbitrary constants which are not both zero. From Eq. (12) we have

$$x=\pi \frac{\rho \mathrm{Ai}(z)+\sigma \mathrm{Bi}(z)}{\mu \mathrm{Ai}(z)+\nu \mathrm{Bi}(z)},$$

where ρ and σ are arbitrary constants satisfying $\mu\sigma-\nu\rho=1$. [Note the identity $\mathrm{Ai}(z)\mathrm{Bi}'(z)-\mathrm{Bi}(z)\mathrm{Ai}'(z)=\pi^{-1}$.] In particular, choosing $\mu=\sigma=1$ and $\nu=\rho=0$, we see that the general solution of $y_{xx}=\mathrm{Bi}^6(z)y^3$ is

$$y(x)=\frac{P_{II}(z;0;c_1,c_2)}{\mathrm{Bi}(z)},$$

where c_1 and c_2 are arbitrary constants (or functions of t, viewing the equation as a PDE) and z is given by

$$\frac{\mathrm{Bi}(z)}{\mathrm{Ai}(z)}=\frac{x}{\pi}.$$

Now we will see how to generate other solutions from the $v=0$ case just described. Let v be a solution of Eq. (66) where $\alpha\neq-\frac{1}{2}$. Then it is well known[21] that

$$\tilde{v}:=-v-\frac{1+2\alpha}{2v_z+2v^2+z} \tag{68}$$

satisfies Eq. (66) with α replaced by $\alpha+1$. Equation (68) is the standard Bäcklund transformation of Eq. (66). Let $V(z;\epsilon)$ be a one-parameter (i.e., ϵ) family of solutions to Eq. (66). Since Eq. (67) is the linearization of Eq. (66), it follows that $W(z;\epsilon):=V_\epsilon(z;\epsilon)$ is a solution to Eq. (67). Substituting $v=V(z;\epsilon)$ into Eq. (68) and differentiating with respect to ϵ shows that

$$\tilde{w}:=-w+2(1+2\alpha)\frac{w_z+2vw}{(2v_z+2v^2+z)^2} \tag{69}$$

satisfies Eq. (67) with v replaced by $\tilde{v}$, whenever w satisfies Eq. (67).

Applying the Bäcklund transformations (68) and (69) to $v(z)=0$, $w(z)=\mathrm{Ai}(z)$, described above, yields $\tilde{v}(z)=-z^{-1}$ and $\tilde{w}(z)=2z^{-2}\mathrm{Ai}'(z)-\mathrm{Ai}(z)$. It follows that

$$y(x)=\frac{z^2P_{II}(z;1;c_1,c_2)+z}{2\mathrm{Ai}'(z)-z^2\mathrm{Ai}(z)}$$

is the general solution of Eq. (1) with $f(x)=6\tilde{v}(z)\tilde{w}^5(z)$ and $g(x)=2\tilde{w}^6(z)$, where

$$\frac{2\mathrm{Bi}'(z)-z^2\mathrm{Bi}(z)}{2\mathrm{Ai}'(z)-z^2\mathrm{Ai}(z)}=\frac{x}{\pi}.$$

Repeated application of the Bäcklund transformations (68) and (69) will generate a countable family of equations of the form (1) and solutions in which v is a rational function of z and w is a rational function of z, the Airy functions Ai and Bi and their first derivatives.

VII. DISCUSSION

The search for metrics modeling nonstatic shear-free spherically symmetric charged fluids naturally leads to the problem of finding one-parameter families of solutions to Eq. (1). The

Painlevé property is a very powerful detector of the integrability of ODEs. Indeed, most of the solutions to Eq. (1) that have appeared in the literature to date arise naturally from the Painlevé analysis of Eq. (1) (see Ref. 14). However, since Eq. (1) is second-order while we only require a one-parameter family of solutions, it is not necessary for us to describe the general solution. From this point of view, requiring the Painlevé property is too restrictive.

In this article we have considered the problem of determining one-parameter families of solutions to Eq. (1) whose only movable singularities are poles. Besides the solutions covered by Proposition 1.1 [which corresponds to the cases in which Eq. (1) possesses the full Painlevé property] we found one-parameter families of solutions that satisfy Riccati equations. In particular, this class of solutions contains those of Shah and Vaidya, which do not arise in the standard Painlevé analysis of Eq. (1). The procedure for matching the Riccati solutions to an external Reissner–Nordstrøm metric was also described.

Finally, a special subclass of solutions that arise in Proposition 1.1 were described. In general, when $a \neq 0$, the transformation between x and z involves derivatives of a second Painlevé transcendent. In the class of solutions described in Sec. VI, v, w, and x are given explicitly in terms of Airy functions and there first derivatives—only u is a genuine Painlevé transcendent. Presumably this is the simplest class of solutions characterized by Proposition 2 that contains a genuine Painlevé transcendent.

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Associated Lamé and various other new classes of elliptic potentials from sl(2,$\mathbb{R}$) and related orthogonal polynomials

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Using representations of sl(2,$\mathbb{R}$) generators which yield associated Lamé Hamiltonians we obtain new classes of elliptic potentials. We explicitly calculate eigenstates and spectra for these potentials and construct the associated orthogonal polynomials. We show that in the proper limit these potentials reduce to well-known exactly solvable potentials. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The study of band-edge energies and wave functions for the class of periodic potentials plays an important role in quantum mechanics.[1–6] Recently, it was shown[1] within the framework of supersymmetric quantum mechanics[2] that the bosonic and fermionic sectors for a periodic superpotential $W(x)$ possess an identical spectra (including the zero mode) provided $\int_{\text{period}} W(x)\,dx = 0$. A wide class of solvable periodic potentials was obtained[3] by applying supersymmetry transformations on Lamé and associated Lamé equation,[7,8] and it turned out that the superpartners of Lamé potentials are not physically identical except for some particular cases. On the other hand, periodic potentials belonging to the quasi-exactly solvable (QES) class have also been well studied in the literature.[9–19] It is useful to note that an early treatment on the noncompact sl(2,$\mathbb{R}$) Lie-algebraic scheme is due to Turbiner who formulated the basics of this formalism, gave the first classification of one-dimensional QES, and proposed multidimensional generalizations. Indeed, in Ref. 12 the connection between one-dimensional QES problems and the sl(2,$\mathbb{R}$) algebra was discovered (see also the review by Shifman[13]). Later in this formalism Lamé equation was algebraized[14,15] for integer as well as half-integer values of the potential parameter. Here it may be mentioned that a connection of periodic QES Hamiltonian within a compact Lie-algebraic approach was made by Alhassid *et al.*[16] by expressing the Hamiltonian as a quadratic in su(2) generators.

Recently we have proposed[17] an algebraization of the associated Lamé equation, namely

$$-\psi''(x)+[m(m+1)sn^2x+l(l+1)cn^2x/dn^2x]k^2\psi(x)=E\psi(x) \tag{1.1}$$

for $m,\ l\in\mathbb{R}$ and (m,l) lying in at least one algebraic line (AL) in the m-l plane. Here $snx \equiv sn(x,k)$, $cnx\equiv cn(x,k)$, $dnx\equiv dn(x,k)$ are three Jacobian elliptic functions of real modulus $k(0<k^2<1)$ and $k'^2=1-k^2$ is the complementary modulus. An associated Lamé equation provides a more general class of periodic potentials due to the presence of two parameters m,l and reduces to an ordinary Lamé equation when either of l and m takes the value 0 or -1. The explicit solutions were obtained by us for two cases: (i) m, l are both non-negative integers and (ii) m is a half-integer and l is an integer or half-integer. One of the aims of the present work is to extend our method of algebraization to the third new case when m is an integer but l is a half-integer. To the

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best of our knowledge, our solutions of associated Lamé equation for integer and half-integer combinations of the parameters m and l are new. We also generate two new classes of elliptic potentials and discuss their implications to the exactly solvable class. We also calculate band-edge eigenstates and energies for these new potentials.

The organization of the article is as follows. In Sec. II we discuss the basic method of generating a wide range of families of elliptic potentials within sl(2,$\mathbb{R}$), thereby obtaining three new classes of potentials. In Sec. III we algebraize the associated Lamé equation as a special case of one of them and make a systematic analysis to find the effective combination of two parameters m and l. Section IV is devoted to the construction of associated orthogonal polynomials. In Sec. V the solutions of associated Lamé equations are obtained for various values of m and l. Several new solutions are obtained here. In Sec. VI we calculate band-edge eigenstates and spectra for the two new classes of potentials obtained in Sec. II and show their connection to the known exactly solvable potentials. Finally, our conclusions are presented in Sec. VII.

II. VARIOUS FAMILIES OF ELLIPTIC POTENTIALS GENERATED BY sl(2,$\mathbb{R}$) ALGEBRA

QES models have been studied mainly from the point of view of two approaches. One approach is to find out a suitable Lie-algebraic representation of a QES Hamiltonian[12,13] and then to compute a finite part of the spectrum by diagonalizing a matrix having finite block structure. A slight variation of this approach has been proposed in Ref. 19 where a class of QES rational potentials with normalizable zero energy state is generated from standard so(2,1) representation of an exactly solvable model through a suitable coordinate transformation. Another approach, first suggested by Bender and Dunne,[20,21] is to generate an orthogonal family of polynomials $\{P_j(E)\}$ in the energy variable E and then to find the roots of a critical polynomial $P_n(E)$ (where n is some positive integer) giving the energy eigenvalues of the QES Hamiltonian. In fact, the existence of such a critical polynomial is evidence for a Hamiltonian to be QES.

Let us briefly recall the basic setup within an sl(2,$\mathbb{R}$) Lie algebra to generate the Schrödinger potential. The sl(2,$\mathbb{R}$) algebra is governed by the commutation relations

$$[T^+, T] = -2T^0, \quad [T^0, T^\pm] = \pm T^\pm, \tag{2.1}$$

where the three generators $T^\pm$, T^0 may be realized as

$$T^+ = \xi^2 \partial_\xi - n\xi, \quad T^0 = \xi \partial_\xi - \tfrac{1}{2}n, \quad T^- = \partial_\xi, \tag{2.2}$$

n being a non-negative integer. These generators act on polynomials in real variable ξ of degree $\leqslant n$.

The gauged Hamiltonian is taken as general quadratic combination of the generators in the form

$$H_G = -\sum_{a,b=0,\pm} C_{ab} T^a T^b - \sum_{a=0,\pm} C_a T^a - d, \tag{2.3}$$

which, using (2.2), can be expressed as

$$H_G(\xi) = -\sum_{j=2}^{4} B_j(\xi) \partial_\xi^{j-2}. \tag{2.4}$$

$B_j(\xi)$ are the jth degree polynomials in ξ given by

$$B_4(\xi)=C_{++}\xi^4+2C_{+0}\xi^3+C_{00}\xi^2+2C_{0-}\xi+C_{--},$$

$$B_3(\xi)=2(1-n)C_{++}\xi^3+\{3(1-n)C_{+0}+C_+\}\xi^2+\{(1-n)C_{00}+C_0\}\xi+(1-n)C_{0-}+C_-, \tag{2.5}$$

$$B_2(\xi)=n(n-1)C_{++}\xi^2+n\{(n-1)C_{+0}-C_+\}\xi+\frac{n^2}{4}C_{00}-\frac{1}{2}nC_0+d.$$

Here the numerical parameters C_{ij} $(i,j=0,\pm)$ are symmetric with $C_{+-}=C_{-+}=0$ and d is a suitably chosen constant.

Let us now convert H_G to the form

$$H_G(x)=-\partial_x{}^2+\left.\frac{B'_4-2B_3}{2\sqrt{B_4}}\right|_{\xi=\xi(x)}\partial_x-B_2|_{\xi=\xi(x)}, \tag{2.6}$$

through a coordinate transformation

$$x(\xi)=\int^{\xi}\frac{d\tau}{\sqrt{B_4(\tau)}}, \tag{2.7}$$

where the prime denotes derivative with respect to ξ.

Now the Schrödinger Hamiltonian with potential $V(x)$,

$$H(x)\psi(x)\equiv[-\partial_x{}^2+V(x)]\psi(x)=E\psi(x), \tag{2.8}$$

can be gauge transformed to the form

$$H_G(x)\chi(x)\equiv\left[-\partial_x{}^2+2\mathcal{A}\partial_x+\frac{d\mathcal{A}}{dx}-\mathcal{A}^2+V\right]\chi(x)=E\chi(x), \tag{2.9}$$

through an imaginary phase transformation

$$\psi(x)=e^{-\int\mathcal{A}(x)\,dx}\chi(x). \tag{2.10}$$

Comparing Eqs. (2.6) and (2.9), the potential $V(x)$ is obtained as

$$V(x)=\mathcal{A}^2-\left.\frac{d\mathcal{A}}{dx}-B_2\right|_{\xi=\xi(x)}, \tag{2.11}$$

where the gauge function $\mathcal{A}(x)$ is

$$\mathcal{A}(x)=\left.\frac{B'_4-2B_3}{4\sqrt{B_4}}\right|_{\xi=\xi(x)}. \tag{2.12}$$

The Schrödinger potential $V(x)$ can be written in terms of $B_j(\xi)$ in the following form:

$$V(x)=\left.\left[\frac{(B'_4-2B_3)(3B'_4-2B_3)}{16B_4}-\frac{1}{4}(B''_4-2B'_3+4B_2)\right]\right|_{\xi=\xi(x)}. \tag{2.13}$$

It is clear that the polynomial $B_4(\xi)$ determines the functional relation between ξ and x through Eq. (2.7). Table I contains all 12 forms of $B_4(\xi)$ which relate ξ to x through the elliptic functions.[22,23] Since our goal is to generate elliptic potentials these forms will facilitate our

TABLE I. Different coordinate transformations based on the choice of $B_4(\xi)$ and path of integration giving $\xi=\xi(x)$ in terms of three Jacobi elliptic functions $snx\equiv sn(x,k)$, $cnx\equiv cn(x,k)$ and $dnx\equiv dn(x,k)$ of real modulus $k(0<k^2<1,k'^2=1-k^2)$ are given.

Transformation no.	$B_4(\xi)$	Zeros of $B_4(\xi)$	ξ_0	$x(\xi)=\int_{\xi_0}^{\xi} B_4^{-1/2}(\tau)\,d\tau$ gives $\xi=\xi(x)$	$B_4(\xi(x))$
1	$(1+\xi^2)(1+k'^2\xi^2)$	$\pm i,\pm i/k'$	0	snx/cnx	dn^2x/cn^4x
2	$(1-\xi^2)(1-k^2\xi^2)$	$\pm 1,\pm 1/k$	0	snx	cn^2xdn^2x
3	$(1-\xi^2)(k'^2+k^2\xi^2)$	$\pm 1,\pm ik'/k$	1	$-cnx$	sn^2xdn^2x
4	$(1-\xi^2)(\xi^2-k'^2)$	$\pm 1,\pm k'$	1	$-dnx$	$k^4sn^2xcn^2x$
5	$(1+k^2\xi^2)(1-k'^2\xi^2)$	$\pm i/k,\pm 1/k'$	0	snx/dnx	cn^2x/dn^4x
6	$(\xi^2-1)(\xi^2-k^2)$	$\pm 1,\pm k$	$-\infty$	$-1/snx$	cn^2xdn^2x/sn^4x
7	$(\xi^2-1)(k'^2\xi^2+k^2)$	$\pm 1,\pm ik/k'$	1	$1/cnx$	sn^2xdn^2x/cn^4x
8	$(\xi^2-1)(1-k'^2\xi^2)$	$\pm 1,\pm 1/k'$	1	$1/dnx$	$k^4sn^2xcn^2x/dn^4x$
9	$(1+\xi^2)(k'^2+\xi^2)$	$\pm i,\pm ik'$	$-\infty$	$-cnx/snx$	dn^2x/sn^4x
10	$(\xi^2+k^2)(\xi^2-k'^2)$	$\pm ik,\pm k'$	$-\infty$	$-dnx/snx$	cn^2x/sn^4x
11	$(1-\xi^2)(1-k^2\xi^2)$	$\pm 1,\pm 1/k$	-1	$-cnx/dnx$	k'^4sn^2x/dn^4x
12	$(\xi^2-1)(\xi^2-k^2)$	$\pm 1,\pm k$	-1	dnx/cnx	k'^4sn^2x/cn^4x

purpose. Note that once B_4 is chosen, Eq. (2.13) gives various families of elliptic potentials containing four parameters C_+, C_-, C_0, and n. In particular, for the transformation 1 of Table I we get a new class of periodic potentials

$$V(x)=Psn^2x+Qsnxcnx+R\frac{snx\ \ cnx}{dn^2x}+S\frac{cn^2x}{dn^2x}, \tag{2.14}$$

where

$$\begin{aligned} P&=\frac{k^2}{4}n(n+2)-\frac{C_0}{2}(n+1)+\frac{1}{4k^2}[C_0{}^2-(C_+-C_-)^2],\\ Q&=\frac{1}{2k^2}(C_+-C_-)[k^2(n+1)-C_0],\\ R&=\frac{1}{2k^2}(C_+-k'^2C_-)[k^2(n+1)+C_0],\\ S&=\frac{k^2}{4}n(n+2)+\frac{C_0}{2}(n+1)+\frac{1}{4k^2}\left[C_0{}^2-\frac{1}{k'^2}(C_+-k'^2C_-)^2\right]. \end{aligned} \tag{2.15}$$

Here the constant d is chosen as

$$d=\frac{1}{4k^2}\left[C_-{}^2-(C_0{}^2+2C_+C_-)+\left(\frac{C_+}{k'}\right)^2\right]-\frac{n(n+2)}{2}. \tag{2.16}$$

Again, for the second and third choices of $B_4(\xi)$ from Table I, we are led to

$$V(x)=\begin{cases} k'^2\left[\dfrac{2}{cn^2x}-\dfrac{(n+3)(n+2)}{dn^2x}\right], & (2.17)\\[2ex] \dfrac{2}{sn^2x}-\dfrac{k'^2(n+3)(n+2)}{dn^2x}, & (2.18) \end{cases}$$

where we have taken

TABLE II. The solutions of a system of four nonlinear equations for four parameters n, $C_\pm$ and C_0 given by (3.1) are provided. Proper restrictions on m, l are essential to restrict the spin parameter n to a non-negative integer. It is interesting to note that the solutions 7–12 can be obtained from 1–6 under the translations $m\to m'=-m-1$, $l\to l'=-l-1$.

Solution no.	n	C_+	C_-	C_0	Restrictions on m,l
1	$l+m$	0	0	$k^2(l-m)$	$l+m\in\mathbb{N}-1$
2	$m-l-1$	0	0	$-k^2(l+m+1)$	$m-l\in\mathbb{N}$
3	$m-1/2$	$ik'(2l+1)$	$ik'(2l+1)$	$-k^2(m+1/2)$	$m\in\mathbb{N}-1/2, l\in\mathbb{R}$
4	$m-1/2$	$-ik'(2l+1)$	$-ik'(2l+1)$	$-k^2(m+1/2)$	$m\in\mathbb{N}-1/2, l\in\mathbb{R}$
5	$l-1/2$	$ik'^2(2m+1)$	$i(2m+1)$	$k^2(l+1/2)$	$l\in\mathbb{N}-1/2, m\in\mathbb{R}$
6	$l-1/2$	$-ik'^2(2m+1)$	$-i(2m+1)$	$k^2(l+1/2)$	$l\in\mathbb{N}-1/2, m\in\mathbb{R}$
7	$-(l+m+2)$	0	0	$-k^2(l-m)$	$-(l+m)\in\mathbb{N}+1$
8	$l-m-1$	0	0	$k^2(l+m+1)$	$l-m\in\mathbb{N}$
9	$-(m+3/2)$	$ik'(2l+1)$	$ik'(2l+1)$	$k^2(m+1/2)$	$-m\in\mathbb{N}+1/2, l\in\mathbb{R}$
10	$-(m+3/2)$	$-ik'(2l+1)$	$-ik'(2l+1)$	$k^2(m+1/2)$	$-m\in\mathbb{N}+1/2, l\in\mathbb{R}$
11	$-(l+3/2)$	$ik'^2(2m+1)$	$i(2m+1)$	$-k^2(l+1/2)$	$-l\in\mathbb{N}+1/2, m\in\mathbb{R}$
12	$-(l+3/2)$	$-ik'^2(2m+1)$	$-i(2m+1)$	$-k^2(l+1/2)$	$-l\in\mathbb{N}+1/2, m\in\mathbb{R}$

$$C_+=C_-=0,\quad C_0=\begin{cases}-k'^2(n+4)\\ -(n+4)\end{cases},\quad d=\begin{cases}\dfrac{1}{4}[3n^2+12n+8-k^2(n^2+8n+8)], & (2.19)\\[2mm] \dfrac{1}{4}(3n^2+12n+8)-\dfrac{k^2}{2}n(n+2). & (2.20)\end{cases}$$

Other choices of $B_4(\xi)$ can be similarly used. Later we will show that the families of elliptic potentials (2.14), (2.17), and (2.18) coincide with certain known potentials in the proper limit.

We now discuss the boundary conditions in the corresponding spectral problem. We see that the Schrödinger equation (2.8) for the potential (2.14) can be defined over the entire x axis. It follows from the oscillation theorem[8] that for a periodic potential of period $2K$ (where $K=\int_o^{\pi/2}d\alpha/\sqrt{1-k^2\sin^2\alpha}$) there exists a sequence $\{E_j\}_{j\geq 0}$ such that $E_o<E_1\leqslant E_2<E_3\leqslant E_4\ldots$, which are called the characteristic values of the energy parameter E and the periodic solutions of period $2K$ (or $4K$) exist for $E=E_j$. The intervals of stability of the solutions are (E_{2j},E_{2j+1}). For the $2K$-periodic potentials (2.17) and (2.18) which are singular at $x=\pm K$ and $x=0$, $2K$, respectively, the domains of corresponding equations may be taken as $(-K,K)$ and $(0,2K)$. Our choice of parameters guarantees that the wave functions vanish at boundary points.

III. ALGEBRAIZATION OF ASSOCIATED LAMÉ EQUATION

Associated Lamé potential (1.1) is a special case of the family of elliptic potentials (2.14) where

$$P=k^2m(m+1),\quad Q=R=0,\quad S=k^2l(l+1). \tag{3.1}$$

Equation (3.1) gives the system of constraints determining the four parameters C_+, C_-, C_0, and n. Table II contains the exhaustive list of 12 sets of solutions for them. Since the spin parameter n is restricted to be a non-negative integer, the sixth column of Table II gives the corresponding restrictions on m,l for validity of the solutions. Now 12 solutions for n represent four systems of parallel lines (see Fig. 1) in the $m-l$ plane: in the following these lines will be referred to as algebraic lines (ALs). Each point (m,l) on an ith AL gives (η_i+1) algebraic eigenstates, where η_i is a non-negative integer given by the numerical value of the spin parameter n associated with ith AL. Clearly, if a point lies in the intersection of r ALS, we get $\Sigma_{i=1}^{r}(\eta_i+1)$ eigenstates, all of which are not necessarily distinct. [It should be mentioned that the oblique ALs are discontinuous at half-integer points that is, they do not meet axis-parallel ALs for the reason explained in Sec. IV (see Table IV).]

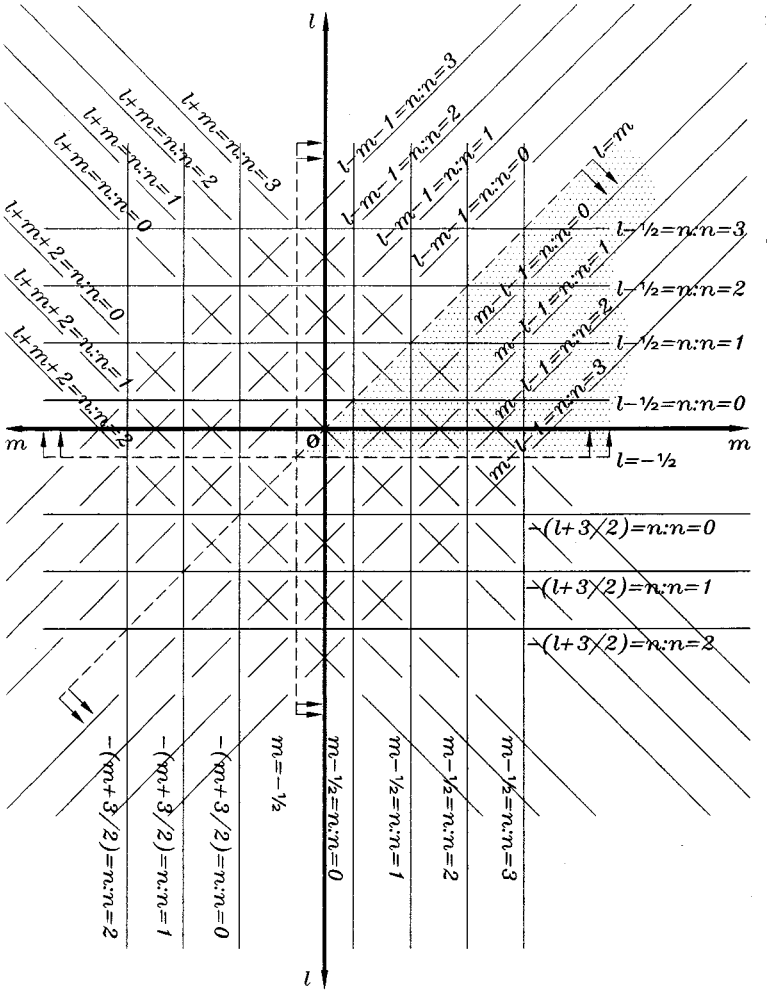

FIG. 1. Algebraic lines (ALs) for the associated Lamé equation are drawn in the $m-l$ plane for some non-negative integer values of n. Three dashed lines determine a triangular infinite region as effective region (shaded area). Oblique ALs are discontinuous at half-integer points.

We now determine the effective region in the $m-l$ plane. Denoting $p\equiv m(m+1)$ and $q\equiv l(l+1)$, we see that p,q are invariant under the translation $m,\ l\to m',\ l'$ where $m'=-m-1$, $l'=-l-1$. Thus it is sufficient to take $l,\ m\geqslant-\frac{1}{2}$. In Fig. 1 these two inequations give a square infinite region. Further, due to the relations $sn(x+2K)=-snx,\ sn(x+K)=cnx/dnx$ ($K=\int_0^{\pi/2}d\alpha/\sqrt{1-k^2\sin^2\alpha}$ is called complete elliptic integral of first kind), we can consider only $p\geqslant q$ without loss of generality. The restriction $p\geqslant q$ in turn implies that $m\geqslant l$. In Fig. 1 this inequation gives a triangular infinite region in the $m-l$ plane. For any point outside this triangular region there exists a point in the region giving the same associated Lamé potential. We call this region (shaded area in Fig. 1) as an effective region. Clearly the ALs lying entirely outside the effective region are not required for our purpose. It is easy to verify that those ALs correspond the solutions 7–12 of Table II. It turns out that we need to consider the first six solutions of Table II: indeed the solutions 7–12 can be generated from the solutions 1–6 by the translation $l,\ m\to l',\ m'$ where $l'=-l-1,\ m'=-m-1$.

The analysis discussed so far reveals that the three-parameter family of associated Lamé potentials $V(x;m,l,k)=m(m+1)k^2sn^2x+l(l+1)k^2cd^2x$ (we use the customary notation $cdx\equiv cnx/dnx$) are generated from sl(2, $\mathbb{R}$) algebra for $0<k^2<1$ and (m,l) lying in at least one AL in the effective region of the $m-l$ plane. We call the points in the effective region not lying in any

TABLE III. Lie-algebraic representations of the linear part H_{linear} of associated Lamé Hamiltonian H_G are given for different solutions of n, in terms of the three sl(2,$\mathbb{R}$) generators $T^{\pm},T^0$. The quadratic part is given by $H_{\text{quadratic}} = -k'^2T^{+2}-(1+k'^2)T^{02}-T^{-2}$.

Solution no.	n	H_{linear}
1	$m+l$	$-k^2(l-m)T^0+\frac{k^2}{4}(l-m)^2+\frac{n(n+2)}{2}$
2	$m-l-1$	$k^2(l+m+1)T^0+\frac{k^2}{4}(l+m+1)^2+\frac{n(n+2)_-}{2}$
3	$m-\frac{1}{2}$	$-ik'(2l+1)(T^+-T^-)+k^2\left(m+\frac{1}{2}\right)T^0+\frac{(2l+1)^2}{4}+\frac{k^2}{4}\left(m+\frac{1}{2}\right)^2+\frac{n(n+2)}{2}$
4	$m-\frac{1}{2}$	$ik'(2l+1)(T^+-T^-)+k^2\left(m+\frac{1}{2}\right)T^0+\frac{(2l+1)^2}{4}+\frac{k^2}{4}\left(m+\frac{1}{2}\right)^2+\frac{n(n+2)}{2}$
5	$l-\frac{1}{2}$	$-i(2m+1)(k'^2T^+-T^-)-k^2\left(l+\frac{1}{2}\right)T^0+\frac{(2m+1)^2}{4}+\frac{k^2}{4}\left(l+\frac{1}{2}\right)^2+\frac{n(n+2)}{2}$
6	$l-\frac{1}{2}$	$i(2m+1)(k'^2T^+-T^-)-k^2\left(l+\frac{1}{2}\right)T^0+\frac{(2m+1)^2}{4}+\frac{k^2}{4}\left(l+\frac{1}{2}\right)^2+\frac{n(n+2)}{2}$

AL as critical points. For instance, though the point $(-\frac{1}{2},-\frac{1}{2})$ lies in the effective region, we cannot algebraize the corresponding associated Lamé equation $-\psi''(x)-(sn^2x+cd^2x)k^2\psi(x)/4=E\psi(x)$ in this scheme, as no ALs pass through this point. In the following sections we consider four cases namely when (i) m and l are both integers, (ii) m is an integer and l is a half-integer, (iii) m and l are both half integers, and (iv) m is a half-integer and l is an integer.

The gauge Hamiltonian can be written in terms of sl(2, $\mathbb{R}$) generators in the form

$$H_G=H_{\text{quadratic}}+H_{\text{linear}}, \tag{3.2}$$

where

$$H_{\text{quadratic}}=-k'^2T^{+^2}-(1+k'^2)T^{0^2}-T^{-^2}, \tag{3.3}$$

and for each of six solutions 1–6 of Table II, H_{linear} is given in Table III. It is to be noted that the generators $T^{\pm}$, T^0 are computed from (2.2) for the corresponding n in Table III.

Before concluding the section, we wish to remark that the associated Lamé potential has two interesting limits:

$$V(x)\xrightarrow[k\to 0]{} 0 \quad (\text{free particle}),$$

$$V(x)\xrightarrow[k\to 1]{} -m(m+1)\text{sech}^2x+l(l+1)+m(m+1) \quad (\text{Pöschl–Teller potential}).$$

In above we have used the following limiting results:

$$sn(x,k)\xrightarrow[k\to 0]{k\to 1}\begin{cases}\tanh x\\ \sin x\end{cases},\quad cn(x,k)\xrightarrow[k\to 0]{k\to 1}\begin{cases}\text{sech}x\\ \cos x\end{cases},\quad dn(x,k)\xrightarrow[k\to 0]{k\to 1}\begin{cases}\text{sech}x\\ 1\end{cases}. \tag{3.4}$$

It may be mentioned that the present results are related to the ones obtained recently by Shifman and Turbiner.[24] Indeed the Hamiltonians 1 and 2 of Table III possess the so-called energy-reflection symmetry.

IV. ORTHOGONAL POLYNOMIALS IN ENERGY VARIABLE GENERATED BY EIGENSTATES OF A QES POTENTIAL

It is well known[15,20,21] that eigenfunctions of almost every one-dimensional QES Hamiltonian generate a family of orthogonal polynomials $\{P_j(E)\}$ in the energy variable E satisfying a three-term recursion relation of the form

$$P_{j+1}(E)=(\alpha_j E+\beta_j)P_j+\gamma_j P_{j-1}, \quad j\geqslant 0, \tag{4.1}$$

where α_j, β_j, γ_j are independent of E, and $\alpha_j\neq 0$, and $\gamma_0=0$, and $\gamma_n=0$ for some positive integer n, provided we expand the algebraic eigenfunction (2.10) as power series in terms of suitable variable $y=y(\xi)$. Simple observation of Eq. (2.5) shows that we can separate the numerical parameters C_{ij} and C_i in $B_3(\xi)$ and $B_2(\xi)$ by rewriting them as

$$B_3(\xi)=\frac{1-n}{2}B_4'(\xi)+A_2(\xi), \quad B_2(\xi)=\frac{n(n-1)}{12}B_4''(\xi)-\frac{n}{2}A_2'(\xi)+\frac{n(n+2)}{12}C_{00}+d, \tag{4.2}$$

where $A_2(\xi)$ is a second degree polynomial in ξ given by

$$A_2(\xi)=C_+\xi^2+C_0\xi+C_-. \tag{4.3}$$

Now, due to the GL(2) symmetry, the form of $H_G(\xi)$ in (2.4) remains invariant under the coordinate transformation

$$\xi=\frac{ey+f}{gy+h}, \quad \begin{pmatrix} e & f \\ g & h \end{pmatrix}\in \mathrm{GL}(2,\mathbb{C}), \tag{4.4}$$

accompanied by the gauge transformation

$$\hat{\chi}(y)=\hat{\mu}(y)\chi\left(\frac{ey+f}{gy+h}\right), \quad \hat{\mu}(y)=(gy+h)^n. \tag{4.5}$$

The transformed Hamiltonian $\hat{H}_G(y)$ can be written as

$$-\hat{H}_G(y)=\hat{B}_4(y)\partial_y^2+\left[\frac{1-n}{2}\hat{B}_4'(y)+\hat{A}_2(y)\right]\partial_y+\frac{n(n-1)}{12}\hat{B}_4''(y)-\frac{n}{2}\hat{A}_2'(y)+\frac{n(n+2)}{12}\hat{C}_{00}+d_1, \tag{4.6}$$

where the prime now denotes derivative wrt y. The transformed polynomials $\hat{B}_4(y)$ and $\hat{A}_2(y)$ are respectively of fourth and second degree and may be written as

$$\hat{B}_4(y)=\hat{C}_{++}y^4+2\hat{C}_{+0}y^3+\hat{C}_{00}y^2+2\hat{C}_{0-}y+\hat{C}_{--}, \qquad \hat{A}_2(y)=\hat{C}_+y^2+\hat{C}_0y+\hat{C}_-. \tag{4.7}$$

In (4.7) the transformed numerical parameters $\hat{C}_{ij}$, $\hat{C}_i$ are determined from the relations

$$\hat{B}_4(y)=\frac{(gy+h)^4}{(eh-fg)^2}B_4\left(\frac{ey+f}{gy+h}\right), \quad \hat{A}_2(y)=\frac{(gy+h)^2}{eh-fg}A_2\left(\frac{ey+f}{gy+h}\right), \tag{4.8}$$

while the constant d_1 in (4.6) is given by

$$d_1=d+\frac{n(n+2)}{12}(C_{00}-\hat{C}_{00}). \tag{4.9}$$

Let us now consider the eigenvalue equation

$$\hat{H}_G(y)\hat{\chi}(y)=E\hat{\chi}(y), \tag{4.10}$$

which is the transformed version of original gauged eigenvalue equation

$$H_G(\xi)\chi(\xi)=E\chi(\xi), \tag{4.11}$$

Here we have identified $\chi(\xi(x))\equiv\chi(x)$ in (2.10). The transformed eigenfunction $\hat{\chi}(y)$ may be taken as power series in y, namely

$$\hat{\chi}(y)=\sum_{j=0}^{\infty} P_j(E)\frac{y^j}{j!}. \tag{4.12}$$

It is straightforward to check that the coefficients $\{P_j(E)\}$, in general, satisfy a five-term recursion relation and to reduce this to a useful three-term recursion relation of the form (4.1), we require $\hat{C}_{++}=\hat{C}_{--}=0$. This means that $\hat{B}_4(y)$ must vanish at 0 and ∞. It is clear from Eq. (4.8) that our problem remains to choose e,f,g,h in (4.4) in such a manner that the two distinct roots ξ_1, ξ_2 of $B_4(\xi)$ are mapped to 0, ∞ of $\hat{B}_4(y)$. Our choice corresponds to the set $e=\xi_2$, $f=-\xi_1$, $g=1$, $h=-1$ so that $eh-fg=\xi_1-\xi_2\neq 0$. We are then led to a three-term recursion relation satisfied by $\{P_j(E)\}$,

$$\begin{aligned}&-[(2j-n+1)\hat{C}_{0-}+\hat{C}_{-}]P_{j+1}\\&\quad=\left[E+d_1+\hat{C}_0\left(j-\frac{n}{2}\right)+\hat{C}_{00}\left(j-\frac{n}{2}\right)^2\right]P_j+j(j-1-n)[(2j-n-1)\hat{C}_{+0}+\hat{C}_{+}]P_{j-1},\quad j\geqslant 0,\end{aligned} \tag{4.13}$$

where $P_{-1}\equiv 0$, $P_0\equiv 1$. Note that the relation (4.13) is of the form (4.1) provided that

$$(2j-n+1)\hat{C}_{0-}+\hat{C}_{-}\neq 0,\quad \forall j\geqslant 0. \tag{4.14}$$

We now examine whether (4.14) trivially holds or some additional restrictions need to be imposed on the spin parameter n. Clearly three cases are relevant which we discuss below.

A. Case 1. Associated Lamé potential (1.1)

This case corresponds to transformation 1 of Table I where $B_4(\xi)$ has four distinct complex roots $\pm i$, $\pm i/k'$. Once the pair of the roots ξ_1, ξ_2 is chosen, the transformed numerical parameters $\hat{C}_{ij}$, $\hat{C}_i$ can be computed from (4.7) and (4.8) corresponding to each of the six solutions 1–6 of Table II as follows:

Solutions 1 and 2: For the choice $\xi_1=-i$, $\xi_2=i$,

$$\hat{C}_{++}=0,\quad \hat{C}_{+0}=k^2/2,\quad \hat{C}_{00}=2(k^2-2),\quad \hat{C}_{0-}=k^2/2,\quad \hat{C}_{--}=0,$$

$$\hat{C}_{+}=\begin{cases}k^2(m-l)/2,\\ k^2(l+m+1)/2,\end{cases}\quad C_0=0,\quad \hat{C}_{-}=\begin{cases}k^2(l-m)/2,\\ -k^2(l+m+1)/2.\end{cases}$$

Then Eq. (4.14) gives

$$\tfrac{1}{2}k^2(2m-2j-1)\neq 0,\quad \forall j\geqslant 0.$$

We thus impose an additional restrictions on m as

$$m\neq \tfrac{1}{2},\tfrac{3}{2},\ldots\ . \tag{4.15}$$

Solutions 3 and 4: For the choice $\xi_1=\pm i/k'$, $\xi_2=\mp i/k'$,

$$\hat{C}_{++}=0,\quad \hat{C}_{+0}=-k^2/2,\quad \hat{C}_{00}=2(k^2-2),\quad \hat{C}_{0-}=-k^2/2,\quad \hat{C}_{--}=0$$

$$\hat{C}_{+}=k^2(m-2l-\tfrac{1}{2})/2,\quad \hat{C}_{0}=(2l+1)(k^2-2),\quad \hat{C}_{-}=-k^2(2l+m+\tfrac{3}{2})/2.$$

Then Eq. (4.14) gives

$$k^2(2j+2l+3)/2\neq 0,\quad \forall j\geqslant 0$$

This is always true in our effective region in the $m-l$ plane (see Fig. 1).

Solutions 5 and 6: For the choice $\xi_1=\pm i$, $\xi_2=\mp i$,

$$\hat{C}_{++}=0,\quad \hat{C}_{+0}=k^2/2,\quad \hat{C}_{00}=2(k^2-2),\quad \hat{C}_{0-}=k^2/2,\quad \hat{C}_{--}=0,$$

$$\hat{C}_{+}=k^2(2m-l+\tfrac{1}{2})/2,\quad \hat{C}_{0}=(2m+1)(k^2-2),\quad \hat{C}_{-}=k^2(2m+l+\tfrac{3}{2})/2.$$

Then Eq. (4.14) gives

$$-k^2(2j+2m+3)/2\neq 0,\quad \forall j\geqslant 0.$$

This is also true in our effective region.

B. Case 2. Potential (2.17)

This case corresponds to transformation 2 of Table I and the solution (2.19). Here $B_4(\xi)$ has four distinct real roots ± 1, $\pm 1/k$. For the choice $\xi_1=1$, $\xi_2=-1$,

$$\hat{C}_{++}=0,\quad \hat{C}_{+0}=-k'^2/2,\quad \hat{C}_{00}=2(1+k^2),\quad \hat{C}_{0-}=-k'^2/2,\quad \hat{C}_{--}=0,$$

$$\hat{C}_{+}=\frac{k'^2}{2}(n+4),\quad \hat{C}_{0}=0,\quad \hat{C}_{-}=-\frac{k'^2}{2}(n+4).$$

Then Eq. (4.14) gives

$$-\frac{k'^2}{2}(2j+5)\neq 0,\quad \forall j\geqslant 0. \tag{4.16}$$

C. Case 3. Potential (2.18)

This case corresponds to transformation 3 of Table I and solution (2.10). The polynomial $B_4(\xi)$ has two real and two complex roots ± 1, $\pm ik'/k$. For the choice $\xi_1=1$, $\xi_2=-1$,

$$\hat{C}_{++}=0,\quad \hat{C}_{+0}=-\tfrac{1}{2},\quad \hat{C}_{00}=2(1-2k^2),\quad \hat{C}_{0-}=-\tfrac{1}{2},\quad \hat{C}_{--}=0,$$

$$\hat{C}_{+}=\tfrac{1}{2}(n+4),\quad \hat{C}_{0}=0,\quad \hat{C}_{-}=-\tfrac{1}{2}(n+4).$$

Then Eq. (4.14) gives

$$-\tfrac{1}{2}(2j+5)\neq 0,\quad \forall_j\geqslant 0. \tag{4.17}$$

Hence we have proved that in every case the eigenfunction generates a family of orthogonal polynomials, provided an additional restriction (4.15) is imposed on potential parameters for case 1 and the roots ξ_1, ξ_2 of the polynomial $B_4(\xi)$ are suitably chosen. The family $\{P_j(E)\}$ can be expressed in terms of monic polynomials $\{\tilde{P}_j(E)\}$ satisfying a recurrence relation of the type

TABLE IV. The coefficients ρ_j, λ_j, and ω_j of the recurrence relation (4.17) and (4.18) are given for different cases. The choice of roots ξ_1, ξ_2 and the restrictions on m,l are also provided for each case.

Solution no.	n	ρ_j	λ_j	ω_j	(ξ_1,ξ_2)	Restrictions on m,l
1	$m+l$	$(\frac{1}{2}k^2)^2 j(l+m+1-j)(2j-2l-1)\times(2m-2j+1)$	$\frac{1}{2}k^2\{l(l+1)+m(m+1)\}+\frac{1}{2}(2-k^2)(l+m-2j)^2$	$\dfrac{(k^2/2)^j\Pi_{i=0}^{m-1}(2m-2i-1)}{\Pi_{i=0}^{m-1-j}(2m-2j-2i-1)}$	$(-i,i)$	$m\notin\mathbb{N}-\frac{1}{2}, l\in\mathbb{R}$ $m+l\in\mathbb{N}-1$
2	$m-l-1$	$(\frac{1}{2}k^2)^2 j(m-l-j)(2m-2j+1)\times(2j+2l+1)$	$\frac{1}{2}k^2\{l(l+1)+m(m+1)\}+\frac{1}{2}(2-k^2)(m-l-1-2j)^2$	$''$	$(-i,i)$	$m\notin\mathbb{N}-\frac{1}{2}, l\in\mathbb{R}$ $m-l\in\mathbb{N}$
3	$m-\frac{1}{2}$	$(\frac{1}{2}k^2)^2 j(j-m-\frac{1}{2})(2j-2m+2l)\times(2j+2l+1)$	$\dfrac{k^2}{4}\left(2m^2+2m-\frac{1}{2}\right)+\dfrac{(2l+1)^2}{4}+\dfrac{1}{2}(2-k^2)\left(2j-m+\dfrac{1}{2}\right)\times\left(2j-m+2l+\dfrac{3}{2}\right)$	$\dfrac{(k^2/2)^j\Pi_{i=1}^{m+3/2}(2l+2i+1)}{\Pi_{i=1}^{m+3/2-j}(2l+2j+2i+1)}$	$\left(\dfrac{i}{k'},\dfrac{-i}{k'}\right)$	$m\in\mathbb{N}-\frac{1}{2}, l\in\mathbb{R}$
4	$m-\frac{1}{2}$	$''$	$''$	$''$	$\left(\dfrac{-i}{k'},\dfrac{i}{k'}\right)$	$m\in\mathbb{N}-\frac{1}{2}, l\in\mathbb{R}$
5	$l-\frac{1}{2}$	$(\frac{1}{2}k^2)^2 j(j-l-\frac{1}{2})(2j-2l+2m)\times(2j+2m+1)$	$\dfrac{k^2}{4}\left(2l^2+2l-\dfrac{1}{2}\right)+\dfrac{(2m+1)^2}{4}+\dfrac{1}{2}(2-k^2)\left(2j-l+\dfrac{1}{2}\right)\times\left(2j-l+2m+\dfrac{3}{2}\right)$	$\dfrac{(-k^2/2)^j\Pi_{i=1}^{l+3/2}(2m+2i+1)}{\Pi_{i=1}^{l+3/2-j}(2m+2j+2i+1)}$	$(i,-i)$	$l\in\mathbb{N}-\frac{1}{2} m\in\mathbb{R}$
6	$l-1/2$	$''$	$''$	$''$	$(-i,i)$	$l\in\mathbb{N}-\frac{1}{2} m\in\mathbb{R}$
7		$(\frac{1}{2}k'^2)^2 j(j-n-1)(2j-2n-5)\times(2j+3)$	$-\dfrac{k'^2}{2}(n+1)(n+4)-\dfrac{1}{2}(1+k^2)(n-2j)^2$	$\dfrac{(k'^2/2)^j\Pi_{i=0}^{j+1}(2j+3-2i)}{3}$	$(1,-1)$	$n\in\mathbb{N}-1$
8		$\frac{1}{4}j(j-n-1)(2j-2n-5)(2j+3)$	$-\dfrac{1}{2}(n+1)(n+4)-\dfrac{1}{2}(1-2k^2)(n-2j)^2$	$\dfrac{(\frac{1}{2})^j\Pi_{i=0}^{j+1}(2j+3-2i)}{3}$	$(1,-1)$	$n\in\mathbb{N}-1$

$$\tilde{P}_{j+1}=(E-\lambda_j)\tilde{P}_j-\rho_j\tilde{P}_{j-1}, \tag{4.18}$$

$$\tilde{P}_j=\omega_j P_j, \quad j\geqslant 0. \tag{4.19}$$

The explicit expressions of ρ_j, λ_j, ω_j together with the choice of roots (ξ_1,ξ_2) and overall restrictions on potential parameters for all cases are contained in Table IV. Note that the last two rows correspond to the potential (2.17) and (2.18). Further restriction (4.15) is reflected in Fig. 1 showing discontinuities of oblique ALs at half-integer points. We see that $\rho_0=0$ and $\rho_{n+1}=0$, so that the critical polynomial is $\tilde{P}_{n+1}$ and the energy eigenvalues of a QES Hamiltonian are precisely the zeros of $\tilde{P}_{n+1}$, provided all the zeros are real and simple.

Let us now turn to the construction of wave functions. From (2.10) and (4.5), the Schrödinger wave function $\psi(x)$ reads

$$\psi(x)=\mu(x)\frac{1}{\hat{\mu}(y)}\hat{\chi}(y)\big|_{y=y(\xi(x))}, \tag{4.20}$$

where

$$\mu(x)=e^{-\int \mathcal{A}(x)\,dx}. \tag{4.21}$$

The gauge function $\mathcal{A}(x)$ can be computed from (2.12) and by using (4.2)

$$\mu(x)=B_4^{-n/4}(\xi)\exp\left[\int^{\xi}\frac{A_2(\tau)}{2B_4(\tau)}d\tau\right]\Bigg|_{\xi=\xi(x)}. \tag{4.22}$$

Finally, the $(n+1)$ eigenfunctions can be computed from (4.4), (4.5), (4.12), and (4.20) at the roots $E=E_i$ $(i=0,1,...,n)$ of $\tilde{P}_{n+1}$ giving the final form

$$\psi_{E_i}(x)=\mu(x)(\xi(x)-\xi_2)^n\sum_{j=0}^{n}\frac{P_j(E_i)}{j!}\left(\frac{\xi(x)-\xi_1}{\xi(x)-\xi_2}\right)^j \quad (i=0,1,...,n). \tag{4.23}$$

It should be mentioned that the infinite power series expansion in (4.12) terminates after $(n+1)$ terms since the coefficients $P_j(E_i)$ vanishes for $j>n$.

V. ALGEBRAIC EIGENFUNCTIONS AND ENERGY SPECTRA OF ASSOCIATED LAMÉ POTENTIAL

Let us recall that here $B_4(\xi(x))=dn^2x/cn^4x$ where $\xi=snx/cnx$ (transformation 1 of Table I). We have already obtained the explicit expression [cf. Eq. (4.23)] of the eigenfunctions. It remains to calculate the gauge factor $\mu(x)$ for each of the six solutions 1–6 of Table II. From (4.22) and (4.3), $\mu(x)$ is given by

$$\mu(x)=\begin{cases} cn^{m+l}x\ dn^{-l}x, \quad n=m+l, & (5.1)\\ cn^{m-l-1}x\ dn^{l+1}x, \quad n=m-l-1, & (5.2)\\ \left.\begin{array}{l} cn^{m-1/2}x\ dn^{-l}x(cnx+ik'snx)^{l+1/2}\\ cn^{m-1/2}x\ dn^{-l}x(cnx-ik'snx)^{l+1/2}\end{array}\right\}, \quad n=m-\frac{1}{2}, & \begin{array}{l}(5.3a)\\(5.3b)\end{array}\\ \left.\begin{array}{l} cn^{l-1/2}x\ dn^{-l}x(cnx+isnx)^{m+1/2}\\ cn^{l-1/2}x\ dn^{-l}x(cnx-isnx)^{m+1/2}\end{array}\right\}, \quad n=l-\frac{1}{2}. & \begin{array}{l}(5.4a)\\(5.4b)\end{array}\end{cases}$$

Besides the elliptic modulus parameter $k(0<k^2<1)$, the associated Lamé potential depends on two other real parameters m, l. In Sec. III we have shown that it is sufficient to consider the points (m, l) in effective region (see Fig. 1). The associated Lamé equation for any point (m, l) lying in at least one AL in the effective region thus gives an algebraic QES potential. In the following we

shall confine ourselves to the case where $m,l \in (\mathbb{N}-1)\cup(\mathbb{N}-\frac{1}{2})$. This can be decomposed into the following four categories. It is to be noted that all points in the m axis give Lamé potential.

A. Case 1: *m* and *l* are both non-negative integers

For $m \neq l$, the point (m, l) lies in two ALs belonging to two different systems given by $m+l=n$ and $m-l-1=n$ and for $m=l$, the point lies in one AL belonging to the system $m+l=2m=n$, for $n=0,1,2,\ldots$. Each AL gives (η_i+1) algebraic eigenstates, where η_i is the numerical value of the spin parameter n associated with the particular AL. Hence in either case, associated Lamé Hamiltonian possesses $(2m+1)$ band-edge eigenstates corresponding to $(2m+1)$ band-edge energies. This emphasizes the fact that the associated Lamé potential is a periodic QES and when m, l are both non-negative integers there are m bound bands followed by a continuum band. The eigenstates for $m \neq l$ generate two distinct families of orthogonal polynomials of the form (4.18) where ρ_j, λ_j, ω_j are given by the entries 1 and 2 of Table IV. The solutions for $m=1,2$ where l is restricted to take $(m+1)$ values $0,1,\ldots,m$, have been obtained by us elsewhere[17] and it has been shown that the so-called Lamé potential is contained in the scheme as a particular case for $l=0$.

B. Case 2: *m* and *l* are both half an odd positive integer

The point (m, l) lies in the intersection of two ALs belonging to two different systems given by $m-\frac{1}{2}=n$ and $l-\frac{1}{2}=n$. Since these two systems correspond to two pairs of algebraizations [see solutions 3–6 of Table II], Eqs. (4.23), (5.3), and (5.4) imply that each of the two algebraizations for each system gives $(m+\frac{1}{2})$ and $(l+\frac{1}{2})$ complex eigenstates, respectively, which are conjugate to one another. Further, the expressions of ρ_j, λ_j, ω_j [see entries 3–6 of Table IV] imply that the complex eigenstates arising from two algebraizations of each system generate the same families of orthogonal polynomials in the energy variable E. It turns out that there are $(m+\frac{1}{2})$ and $(l+\frac{1}{2})$ characteristic values of E for each of which we get two linearly independent solutions given by real and imaginary parts of the complex eigenstates. But we see that the solutions obtained from the system $l-\frac{1}{2}=n$ are included in the solutions obtained from the system $m-\frac{1}{2}=n$ (note that $m \geqslant l$ in the effective region). Hence when m and l are both half-integers, there are $(m+\frac{1}{2})$ characteristics values of E which are doubly degenerate. It may be mentioned that the point (m, l) in this case does not lie in the ALs belonging to the systems $m+l=n$ and $m-l-1=n$ due to the discontinuities of oblique ALs at half-integer points (see Fig. 1). The solutions for $(\frac{1}{2}, \frac{1}{2})$, $(\frac{3}{2}, \frac{1}{2})$, and $(\frac{3}{2}, \frac{3}{2})$ have already been reported.[17] However, for some half-integer combinations of m, l, for instance, $(\frac{3}{2}, \frac{1}{2})$, we notice that only highest energy is doubly degenerate.

C. Case 3: *m* is half an odd positive integer and *l* is a non-negative integer

The point (m, l) lies in one AL belonging to the system $m-\frac{1}{2}=n$. Thus, as before, there are $(m+\frac{1}{2})$ characteristics values of E which are doubly degenerate. The solutions for $(\frac{1}{2}, 0)$, $(\frac{3}{2}, 0)$, and $(\frac{3}{2}, 1)$ are explicitly obtained by us in Ref. 17 and the first two give Lamé potentials.

D. Case 4: *m* is a non-negative integer and *l* is half an odd positive integer

This case is new and corresponds to the system $l-\frac{1}{2}=n$. Two algebraizations given by entires 5 and 6 of Table IV yield $(l+\frac{1}{2})$ characteristics values of E for each of which there are two linearly independent solutions. Here l takes values $\frac{1}{2}, \frac{3}{2},\ldots$ and for each of them m is allowed to take an infinite set of values $l+\frac{1}{2}, l+\frac{3}{2},\ldots$ in the effective region.

From the above discussions it is clear that in the effective region when $m \in \mathbb{N}\cup\mathbb{N}-\frac{1}{2}$, l is restricted to take $(2m+1)$ values $0,\frac{1}{2},1,\frac{3}{2},\ldots,m-\frac{1}{2},m$. In the following examples $\phi_r(x)$ and e_r denote the ordered levels of eigenstates and energy spectra. Note that in the half-integer cases, the parenthesized superscript in the eigenstate indicates the degeneracy of the eigenvalues.

We now consider the following examples.

(a) $m=1$. l is allowed to take three values 0, $\frac{1}{2}$, 1. Solutions for $l=0$, 1 were reported in Ref. 17. The new case corresponds $m=1$, $l=\frac{1}{2}$ and gives the associated Lamé potential as

$$V(x)=2k^2sn^2x+\tfrac{3}{4}k^2cd^2x. \tag{5.5}$$

The wave functions and energy are

$$\phi_0{}^{(1)}(x)=\frac{\sqrt{1+cnx}}{\sqrt{dnx}}(2cnx-1),\quad \phi_0{}^{(2)}(x)=\frac{\mathrm{sgn}(snx)\sqrt{1-cnx}}{\sqrt{dnx}}(2cnx+1),\quad e_0=\frac{1}{4}(k^2+9).$$

(b) $m=2$. l is allowed to take five values 0, $\frac{1}{2}$, 1, $\frac{3}{2}$, 2. The integer values of l have already been given in Ref. 17.

(i) $l=\frac{1}{2}$: Associated Lamé potential

$$V(x)=6k^2sn^2x+\tfrac{3}{4}k^2cd^2x,$$

$$\phi_0{}^{(1)}(x)=\frac{\sqrt{1+cnx}}{\sqrt{dnx}}(4cn^2x-2cnx-1),\quad \phi_0{}^{(2)}(x)=\frac{\mathrm{sgn}(snx)\sqrt{1-cnx}}{\sqrt{dnx}}(4cn^2x+2cnx-1), \tag{5.6}$$

$$e_0=(k^2+25)/4.$$

(ii) $l=\frac{3}{2}$: Associated Lamé potential

$$V(x)=6k^2sn^2x+\frac{15}{4}k^2cd^2x,$$

$$e_{0,1}=\tfrac{1}{4}[49-5k^2+2f_{\mp}(k)],\quad f_{\pm}(k)=5(k^2-2)\pm\sqrt{k^4+25k'^2}, \tag{5.7}$$

$$\phi_{0,1}{}^{(1)}(x)=\frac{\sqrt{1+cnx}}{dn^{3/2}x}[8f_{\pm}(k)cn^3x-4f_{\pm}(k)cn^2x-2\{2f_{\pm}(k)+7k^2\}cnx+\{f_{\pm}(k)+7k^2\}],$$

$$\phi_{0,1}{}^{(2)}(x)=\frac{\mathrm{sgn}(snx)\sqrt{1-cnx}}{dn^{3/2}x}[8f_{\pm}(k)cn^2x+4f_{\pm}(k)cn^2x-2\{2f_{\pm}(k)+7k^2\}cnx$$
$$-\{f_{\pm}(k)+7k^2\}].$$

(c) $m=3$. l is allowed to take seven values 0, $\frac{1}{2}$, 1, $\frac{3}{2}$, 2, $\frac{5}{2}$, 3.

(i) $l=0$: Lamé potential

$$V(x)=12k^2sn^2x,$$

$$\phi_{0,4}(x)=dnx[5k^2sn^2x-f_{\pm}(k)],\quad e_{0,4}=2f_{\mp}(k)+k^2,$$

$$\phi_{1,5}(x)=cnx[5k^2sn^2x-g_{\pm}(k)],\quad e_{1,5}=2g_{\mp}(k)+1, \tag{5.8}$$

$$\phi_{2,6}(x)=snx[5k^2sn^2x-\eta_{\pm}(k)],\quad e_{2,6}=\eta_{\mp}(k)+3(1+k^2),$$

$$\phi_3(x)=snx\ \ cnx\ \ dnx,\quad e_3=4(1+k^2),$$

where $f_{\pm}(k)=2k^2+1\pm\sqrt{4k^4+k'^2}$, $g_{\pm}(k)=k^2+2\pm\sqrt{4-k^2k'^2}$, and $\eta_{\pm}(k)=2(k^2+1)\pm\sqrt{4k^4-7k^2+4}$.

(ii) $l=\frac{1}{2}$: Associated Lamé potential

$$V(x)=12k^2sn^2x+\tfrac{3}{4}k^2cd^2x,$$

$$\phi_0{}^{(1)}(x)=\frac{\sqrt{1+cnx}}{\sqrt{dnx}}[8cn^3x-4cn^2x-4cnx+1],\quad e_0=\frac{1}{4}(k^2+49),\tag{5.9}$$

$$\phi_0{}^{(2)}(x)=\frac{\mathrm{sgn}(snx)\sqrt{1-cnx}}{\sqrt{dnx}}[8cn^3x+4cn^3x-4cnx-1].$$

(iii) $l=1$: Associated Lamé potential

$$\begin{aligned}V(x)&=12k^2sn^2x+2k^2cd^2x,\\ \phi_0(x)&=cnx\ \ dn^2x,\quad e_0=1+4k^2,\\ \phi_1(x)&=snx\ \ dn^2x,\quad e_1=1+9k^2,\\ \phi_{2,3}(x)&=\frac{snx\ \ cnx}{dnx}\left[sn^2x-\frac{1}{5k^2}(k^2+3\pm\sqrt{k^4+9k'^2})\right],\quad e_{2,3}=10+2k^2\mp2\sqrt{k^4+9k'^2}.\end{aligned}\tag{5.10}$$

The remaining three eigenstates can be expressed as

$$\begin{aligned}\phi_i(x)=\frac{1}{dnx}\Bigg[&sn^4x-\frac{1}{10k^2}(9k^2+16-e_i)sn^2x\\&+\frac{1}{15k^4}\{e_i{}^2-2(5k^2+18)e_i+(9k^4+156k^2+320)\}\Bigg],\end{aligned}$$

where the eigenvalues e_i $(i=4,5,6)$ are the roots of the cubic

$$e^3-(11k^2+20)e^2+(19k^4+216k^2+64)e-(9k^6+388k^4+448k^2)=0.$$

(iv) $l=\frac{3}{2}$: Associated Lamé potential

$$\begin{aligned}V(x)&=12k^2sn^2x+\tfrac{15}{4}k^2cd^2x,\\ e_{0,1}&=\tfrac{1}{4}[81-9k^2+2h_{\mp}(k)],\quad h_{\pm}(k)=7(k^2-2)\pm2\sqrt{k^4+49k'^2}\\ \phi_{0,1}{}^{(1)}&=\frac{\sqrt{1+cnx}}{dn^{3/2}x}[16h_{\pm}(k)cn^4x-8h_{\pm}(k)cn^3x-12\{h_{\pm}(k)+3k^2\}cn^2x\\&\quad+2\{2h_{\pm}(k)+9k^2\}cnx+\{h_{\pm}(k)+9k^2\}],\\ \phi_{0,1}{}^{(2)}(x)&=\frac{\mathrm{sgn}(snx)\sqrt{1-cnx}}{dn^{3/2}x}[16h_{\pm}(k)cn^4x+8h_{\pm}(k)cn^3x-12\{h_{\pm}(k)+3k^2\}cn^2x\\&\quad-2\{2h_{\pm}(k)+9k^2\}cnx+\{h_{\pm}(k)+9k^2\}].\end{aligned}\tag{5.11}$$

(v) $l=2$: Associated Lamé potential

$$\begin{aligned}V(x)&=12k^2sn^2x+6k^2cd^2x,\\ \phi_0(x)&=dn^3x,\quad e_0=9k^2.\end{aligned}\tag{5.12}$$

The three eigenstates can be expressed as

$$\phi_i(x)=\frac{cnx}{dn^2x}\left[sn^4x-\frac{1}{10k^2}(4k^2+25-e_i)sn^2x\right.$$
$$\left.+\frac{1}{120k^4}\left\{e_i^2-2(2k^2+17)e_i-\frac{75}{2}k^4+156k^2+225\right\}\right],$$

where the three energies e_i are the roots of the cubic

$$2e^3-2(8k^2+35)e^2-(43k^4-640k^2-518)e+(525k^6-1365k^4-3312k^2-450)=0.$$

The remaining three energies e_r are the roots of the cubic

$$2e^3-2(11k^2+35)e^2-(37k^4-844k^2-518)e+732k^6-1851k^4-4662k^2-450=0,$$

and the three eigenstates are given by

$$\phi_r(x)=\frac{snx}{dn^2x}\left[sn^4x-\frac{1}{10k^2}(9k^2+25-e_r)sn^2x\right.$$
$$\left.+\frac{1}{120k^4}\left\{e_r{}^2-2(5k^2+17)e_r-\frac{57}{2}k^4+306k^2+225\right\}\right].$$

(vi) $l=\frac{5}{2}$: Associated Lamé potential

$$V(x)=12k^2sn^2x+\tfrac{35}{4}k^2cd^2x. \tag{5.13}$$

Three eigenvalues e_i are the roots of the cubic

$$64e^3-16(35k^2+179)e^2+4(39k^4+7398k^2+7459)e+(7915k^6-66871k^4-229507k^2-53361)=0,$$

and two linearly independent solutions for each e_i are

$$\phi_i^{(1)}(x)=\frac{\sqrt{1+cnx}}{dn^{5/2}x}[32\beta_icn^5x-16\beta_icn^4x-16(\gamma_i+2\beta_i)cn^3x+4(2\gamma_i+3\beta_i)cn^2x$$
$$+2(4\gamma_i+3\beta_i+792k^4)cnx-(2\gamma_i+\beta_i+792k^4)],$$

$$\phi_i^{(2)}(x)=\frac{\mathrm{sgn}(snx)\sqrt{1-cnx}}{dn^{5/2}x}[32\beta_icn^5x+16\beta_icn^4x-16(\gamma_i+2\beta_i)cn^3x-4(2\gamma_i+3\beta_i)cn^2x$$
$$+2(4\gamma_i+3\beta_i+792k^4)cnx+(2\gamma_i+\beta_i+792k^4)],$$

where

$$\gamma_i(k)=22k^2(37k^2+9-4e_i),$$

$$\beta_i(k)=16e_i{}^2-8(27k^2+29)e_i+845k^4+1966k^2+441.$$

(vii) $l=3$: Associated Lamé potential

$$V(x)=12k^2sn^2x+12k^2cd^2x. \tag{5.14}$$

Three band-edge eigenstates are given by

$$\phi_i(x)=\frac{snx\ cnx}{dn^3x}\left[sn^4x-\frac{1}{10k^2}(4k^2+36-e_i)sn^2x\right.$$
$$\left.+\frac{1}{120k^4}\{e_i{}^2-4(k^2+13)e_i+24(11k^2+24)\}\right]\quad(i=0,1,2)$$

where the three eigenvalues e_i are the roots of the cubic

$$e^3-8(k^2+7)e^2+16(k^4+35k^2+49)e-192(7k^4+31k^2+12)=0.$$

In particular, for $k^2=\frac{2}{3}$, the energies and eigenvalues can be obtained in exact form:

$$\phi_0(x)=\frac{snx\ cnx}{dn^3x}\left[sn^4x-4sn^2x+\frac{9}{2}\right],\quad e_0=12,$$

$$\phi_1(x)=\frac{snx\ cnx}{dn^3x}\left[sn^4x-3sn^2x+\frac{3}{2}\right],\quad e_1=\tfrac{56}{3},$$

$$\phi_2(x)=\frac{snx\ cnx}{dn^3x}\left[sn^4x-\frac{6}{5}sn^2x+\frac{3}{10}\right],\quad e_2=\tfrac{92}{3}.$$

The remaining four energies e_r are the roots of the biquadratic

$$e^4-4(5k^2+14)e^3+2(59k^4+616k^2+392)e^2-12(15k^6+698k^4+1280k^2+192)e$$
$$+9k^2(9k^6+1824k^4+8320k^2+3072)=0,$$

and the corresponding four eigenstates can be expressed as

$$\phi_r(x)=\frac{1}{dn^3x}\left[sn^6x-\frac{1}{10k^2}(9k^2+36-e_r)sn^4x+\frac{1}{120k^4}\right.$$
$$\times\{e_r{}^2-2(5k^2+26)e_r+9k^4+480k^2+576\}sn^2x+\frac{1}{720k^6}$$
$$\left.\times\{e_r{}^3-(11k^2+56)e_r{}^2+(19k^4+716k^2+784)e_r-3(3k^6+604k^4+2560k^2+768)\}\right].$$

Higher values of m and l can be similarly considered, in principle. But, in practice, as m,l increases, calculations become very complicated due to the fact that the analytical solutions of higher degree critical polynomials are quite lengthy. However, it may be mentioned that our algebraization scheme discovers several new families of associated Lamé potentials for integer and half-integer combinations of m,l, e.g., the potentials (5.5)–(5.7), (5.9), (511), and (5.13), whose solutions can be written analytically.

VI. ELLIPTIC GENERALIZATIONS OF GENDENSHTEIN AND OTHER EXACTLY SOLVABLE PERIODIC POTENTIALS

In Sec. II we have obtained two new families of potentials (2.17) and (2.18) for the second and third choices (transformations 2 and 3 of Table I) of $B_4(\xi)$. For the choice $B_4(\xi)=(1-\xi^2)\times(1-k^2\xi^2)$, we get

$$V(x)=k'^2\left[\frac{2}{cn^2x}-\frac{(n+3)(n+2)}{dn^2x}\right].\tag{6.1}$$

Here $V(x)$ depends on two parameters k $(0<k^2<1, k'^2=1-k^2)$ and n $(\in \mathbb{N}-1)$. Further, we choose the domain $(-K,K)$ where $2K$ is the period of the potential and given by $K=\int_0^{\pi/2} d\alpha/\sqrt{1-k^2\sin^2\alpha}$. We may note that as $k\to 1$, 0 the domain reduces to $(-\infty,\infty)$ and $(-\pi/2, \pi/2)$. It is interesting to observe following two limits:

$$V(x) \xrightarrow[k\to 1]{} 0, \quad x\in(-\infty,\infty) \quad \text{(free particle)}, \tag{6.2}$$

$$V(x) \xrightarrow[k\to 0]{} 2\tan^2 x-(n+1)(n+4), \quad x\in(-\pi/2,\pi/2), \tag{6.3}$$

which is an exactly solvable periodic potential.[25]

Again, for the choice $B_4(\xi)=(1-\xi^2)(k'^2+k^2\xi^2)$ (transformation 3 of Table I), we obtain

$$V(x)=\frac{2}{sn^2x}-\frac{k'^2(n+3)(n+2)}{dn^2x}, \quad x\in(0,2K), \tag{6.4}$$

where n $(\epsilon\mathbb{N}-1)$ and k $(0<k^2<1)$ are two parameters. The following two limits of (6.4) are noted:

$$V(x) \xrightarrow[k\to 1]{} 2\,\text{cosech}^2 x+2, \quad x\in(0,\infty), \tag{6.5}$$

which is singular Gendenshtein potential[26] and

$$V(x) \xrightarrow[k\to 0]{} 2\cot^2 x-(n+1)(n+4), \quad x\in(0,\pi), \tag{6.6}$$

which also belongs to the exactly solvable class. Note that in the above we have used the limiting results (3.4).

The elliptic potentials (6.1) and (6.4) are thus new families of periodic potentials belonging to QES class and can be considered as generalized versions of exactly solvable $\tan^2 x$, $\cot^2 x$, and $\text{cosech}^2 x$ potentials. These potentials are generated from a standard homogeneous quadratic combination of $\text{sl}(2,\mathbb{R})$ generators plus a linear operator. The gauged Hamiltonian can be written explicitly in terms of $\text{sl}(2,\mathbb{R})$ generators as

$$\begin{aligned}\text{Potential (6.1):} \quad H_G=&-k^2T^{+^2}+(1+k^2)T^{0^2}-T^{-^2}+k'^2(n+4)T^0\\ &-\tfrac{1}{4}[3n^2+12n+8-k^2(n^2+8n+8)],\end{aligned} \tag{6.7}$$

$$\begin{aligned}\text{Potential (6.4):} \quad H_G=&k^2T^{+^2}+(1-2k^2)T^{0^2}-k'^2T^{-^2}+(n+4)T^0\\ &-\tfrac{1}{4}[3n^2+12n+8-2k^2n(n+2)],\end{aligned} \tag{6.8}$$

where the generators $T^{\pm}$, T^0 are computed from (2.2) for $n\in\mathbb{N}-1$. The gauge factor $\mu(x)$ is obtained from (4.22), (2.19), and (2.20) for the corresponding choice of $B_4(\xi)$ (transformation 2 and 3 of Table I) as

$$\text{Potential (6.1):} \quad \mu(x)=cn^2x/dn^{n+2}x, \tag{6.9}$$

$$\text{Potential (6:4):} \quad \mu(x)=sn^2x/dn^{n+2}x. \tag{6.10}$$

The $(n+1)$ band-edge eigenstates and spectra can now be easily computed by constructing orthogonal polynomials using entries 7 and 8 of Table IV.

We now consider the following examples.

(a) The class of potentials given by Eq. (6.1)

(i) $n=0$:

$$V(x)=2k'^2\left(\frac{1}{cn^2x}-\frac{3}{dn^2x}\right),$$
$$\phi_0(x)=\frac{cn^2x}{dn^2x},\quad e_0=-2k'^2. \tag{6.11}$$

(ii) $n=1$:

$$V(x)=2k'^2\left(\frac{1}{cn^2x}-\frac{6}{dn^2x}\right),$$
$$\phi_0(x)=\frac{cn^2x}{dn^3x},\quad e_0=7k^2-8, \tag{6.12}$$
$$\phi_1(x)=\frac{snxcn^2x}{dn^3x},\quad e_1=2k^2-3.$$

(b) The class of potentials given by Eq. (6.4)
(i) $n=0$:

$$V(x)=\frac{2}{sn^2x}-\frac{6k'^2}{dn^2x},$$
$$\phi_0(x)=\frac{sn^2x}{dn^2x},\quad e_0=-2. \tag{6.13}$$

(ii) $n=1$:

$$V(x)=\frac{2}{sn^2x}-\frac{12k'^2}{dn^2x},$$
$$\phi_0(x)=\frac{sn^2x}{dn^3x},\quad e_0=k^2-8, \tag{6.14}$$
$$\phi_1(x)=\frac{sn^2xcnx}{dn^3x},\quad e_1=k^2-3.$$

Higher values of m can be similarly considered. We have thus found two new families of QES periodic potentials, which in the proper limit reduce to well-known exactly, solvable class.

VII. CONCLUSION

In this article we have systematically studied the basic method of generating various classes of elliptic potentials within an sl(2,$\mathbb{R}$) Lie-algebraic formulation. We have given a wide range of choice of coordinate transformation in Table I. Using transformations 1–3 of Table I we have obtained three new classes of QES periodic potentials, which, in the limits $k\to 0,1$, reduce to Pöschl–Teller, singular Gendenshtein and other known exactly solvable classes. Other choices from Table I can be similarly used to generate various new classes of elliptic potentials. Further, we have shown that the associated Lamé potential can be derived as a special case. This certainly adds an important member in the list of algebraic QES. We have explicitly obtained the eigenstates and spectra for these potentials. In fact, our algebraic approach discovers a new class of associated Lamé potential when either of the two parameters m and l are integers and other half-integers. It is shown that the eigenfunctions of our QES Hamiltonians generate a family of orthogonal poly-

nomials $\{Pj(E)\}$ satisfying a three-term recurrence relation of the form (4.18). It is to be mentioned that the coefficients ρ_j are not strictly positive for $1 \leqslant j \leqslant n$, in contrast to the cases discussed in Ref. 15. However, the $(n+1)$ roots of the critical polynomial are all real and simple.

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Irreducible modules of finite dimensional quantum algebras of type *A* at roots of unity

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Properly specializing the parameters contained in the maximal cyclic representation of the nonrestricted *A*-type quantum algebra at roots of unity, we find the unique primitive vector in it. In this case, the representation is no longer irreducible. We show that the submodule generated by the primitive vector is the unique irreducible submodule and can be identified with an irreducible highest weight module of the finite dimensional *A*-type quantum algebra, which is defined as the subalgebra of the restricted quantum algebra at roots of unity. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1453498]

I. INTRODUCTION

The quantum group $U_q(\mathfrak{g})$ associated with a simple Lie algebra $\mathfrak{g}$ is an associative algebra over the rational function field $\mathbf{C}(q)$ (q is an indeterminate) and we can define its ''integral'' form over the Laurant polynomial ring $\mathbf{C}[q,q^{-1}]$, which enables us to specialize q to any nonzero complex number ε. We are going to see two types of such integral forms and accordingly, we obtain two types of specializations; one is called the ''restricted specialization,'' denoted by $U_\varepsilon^{\mathrm{res}}$, and the other is called the ''nonrestricted specialization,'' denoted by U_ε. Both coincide if ε is transcendental. But we are interested in the case where ε is the lth primitive root of unity, l being an odd integer greater than 1. In this case, they do not. The former is initiated by Lusztig[1,2] and the latter is introduced in Ref. 3 by DeConcini and Kac. Their representation theories are quite different: Irreducible $U_\varepsilon^{\mathrm{res}}$-modules are highest weight modules in some sense and the classification of the irreducible modules is same as for simple Lie algebras or ordinary quantum algebras (see Theorem 3.5). Furthermore, irreducible modules possess the remarkable property ''tensor product theorem'' (see Theorem 3.6), which claims that the arbitrary irreducible highest weight module $V(\lambda)$ with the highest weight λ is divided into the tensor product of two irreducible modules, $V(\lambda^{(0)})$ and $V(l\lambda)^{(1)}$, where $\lambda^{(0)}$ and $\lambda^{(1)}$ are as in Theorem 3.6. Here the module $V(\lambda^{(0)})$ is identified with the irreducible $U_\varepsilon^{\mathrm{fin}}$-module, where $U_\varepsilon^{\mathrm{fin}}$ is some finite dimensional subalgebra of $U_\varepsilon^{\mathrm{res}}$ (see Sec. II B) and the module $V(l\lambda^{(1)})$ can be identified with the irreducible highest weight $U(\mathfrak{g})$-module $V(\lambda^{(1)})$, whose structure is known very well. Thus, if the structure of $V(\lambda^{(0)})$ is clarified, we can analyze the detailed feature of $V(\lambda)$. Indeed, the character of $V(\lambda)$ is given by the famous Kazhdan–Lusztig formula. But structures as a module, e.g., explicit descriptions of basis vectors or actions of the generators on them, are still unclear.

On the other hand, irreducible U_ε-modules are not necessarily highest or lowest weight modules. They are characterized by many continuous parameters and if they are ''generic,'' their dimensions are all same (see Refs. 3 and 4). But if we specialize the parameters properly, the modules become reducible. In Ref. 5, Date *et al.*, explicitly constructed such U_ε-modules for A_n-type, which is called the ''maximal cyclic representations'' that are realized in the vector space $\mathcal{V}:=(\mathbf{C}^l)^{(1/2)n(n+1)}$. They contains the continuous parameters and it is shown that if those parameters are generic, they are irreducible. Here we consider certain nongeneric specialization of the parameters so that $\mathcal{V}$ becomes a reducible U_ε-module. Moreover, we shall observe that such a module includes the unique primitive vector (see Proposition 4.9). The submodule generated by

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this primitive vector can be seen as an irreducible $U_\varepsilon^{\mathrm{fin}}$-module and isomorphic to $V(\lambda^{(0)})$ for some λ (Theorem 5.5).

From the physical point of view, the cyclic representations at roots of 1 are deeply related to certain physical models, e.g., chiral Potts models,[6,7] via *R*-matrices obtained as intertwining operators of tensor product.[8–10] On the other hand, the algebra $U_\varepsilon^{\mathrm{fin}}$ has the corresponding universal *R*-matrix.[11] So, we can consider its image on $\mathcal{V}$ or the irreducible submodule. The explicit form of the universal *R*-matrix for $U_\varepsilon^{\mathrm{fin}}$ cannot be directly deduced from the usual formula of the universal *R*-matrix for $U_q(\mathfrak{g})$. So, it might be interesting to see whether the image of the universal *R*-matrix of $U_\varepsilon^{\mathrm{fin}}$ can be obtained by specializing the parameters of the *R*-matrix related to the chiral Potts type models.

The organization of the paper is as follows. In Sec. II we review the quantum algebras at roots of unity. In Sec. III, we see the maximal cyclic representations of the *A*-type following Ref. 5 and review the representation theory of $U_\varepsilon^{\mathrm{res}}$. In Sec. IV, we specialize the parameters properly and show that under the specialization, there exists a unique primitive vector in the module. Finally, in Sec. V, it is shown that the representation space becomes the module of the finite dimensional algebra $U_\varepsilon^{\mathrm{fin}}$ and the submodule generated by the primitive vector is irreducible.

II. ALGEBRAS AT ROOTS OF UNITY

In the following, we review the algebras treated in this article.

A. Restricted integral forms and specializations

Let $\mathbf{C}(q)$ be the rational function field in an indeterminate q and denote the ring $\mathbf{C}[q,q^{-1}]$ by $\mathcal{A}$. We use the following notations:

$$[a]_q := \frac{q^a - q^{-a}}{q - q^{-1}}, \quad [a]_q! := [a]_q[a-1]_q \cdots [2]_q[1]_q, \quad \begin{bmatrix} m \\ k \end{bmatrix}_q := \frac{[m]_q!}{[k]_q![m-k]_q!}.$$

Let $I := \{1,2,\ldots,n\}$ be the index set and $(a_{ij})_{i,j\in I}$ be the Cartan matrix of type A_n, i.e., $a_{ii}=2$ $(1 \leqslant i \leqslant n)$, $a_{ii+1}=a_{i+1i}=-1$ $(1 \leqslant i \leqslant n-1)$, and $a_{ij}=0$ otherwise. Let us denote the set of roots (respectively, positive roots) by Δ (respectively, Δ_+). Let $\{h_i\}_{i\in I}$ be the set of simple co-roots and $\{\alpha_i\}_{i\in I}$ the set of simple roots. Define the weight lattice $P := \{\lambda \mid \langle h_i, \lambda \rangle \in \mathbf{Z}\}$ (respectively, the set of dominant integral weights $P_+ := \{\lambda \mid \langle h_i, \lambda \rangle \in \mathbf{Z}_{\geqslant 0}\}$). Let $\{\Lambda_i\}_{i\in I}$ be the fundamental weights which satisfy $\langle h_i, \Lambda_j \rangle = \delta_{ij}$ and then $P = \oplus_i \mathbf{Z}\Lambda_i$. Let W be the Weyl group of type A_n, which is generated by the simple reflections s_i $(i \in I)$. The *quantum algebra* $U_q(\mathfrak{g})$ is the associative algebra generated by e_i, f_i, $t_i^{\pm 1}$ $(i \in I)$ and the following relations:

$$t_i t_i^{-1} = t_i^{-1} t_i = 1, \quad t_i t_j = t_j t_i, \tag{2.1}$$

$$t_i e_j t_i^{-1} = q^{a_{ij}} e_j, \tag{2.2}$$

$$t_i f_j t_i^{-1} = q^{-a_{ij}} f_j, \tag{2.3}$$

$$e_i f_j - f_j e_i = \delta_{ij} \frac{t_i - t_i^{-1}}{q - q^{-1}} \tag{2.4}$$

$$\sum_{k=0}^{1-a_{ij}} (-1)^k e_i^{(k)} e_j e_i^{(1-a_{ij}-k)} = \sum_{k=0}^{1-a_j} (-1)^k f_i^{(k)} f_j f_i^{(1-a_{ij}-k)} = 0 \quad (i \neq j), \tag{2.5}$$

where $e_i^{(k)} := e_i^k/[k]_q!$ and $f_i^{(k)} := f_i^k/[k]_q!$.
Here we set

$$\begin{bmatrix} t_i,p \\ r \end{bmatrix}_q := \prod_{s=1}^{r} \frac{t_i q^{p+1-s} - t_i^{-1} q^{s-p-1}}{q^s - q^{-s}}.$$

The algebra $U_{\mathcal{A}}^{\mathrm{res}}$ is the $\mathcal{A}$-subalgebra of $U_q(\mathfrak{g})$ generated by $e_i^{(k)}$, $f_i^{(k)}$, $t_i^{\pm 1}$, and $\begin{bmatrix} t_{i,p} \\ k \end{bmatrix}$ ($i \in I$, p, $k \in \mathbf{Z}$, and $k \geqslant 0$), which is called the restricted integral form.

Here we can define the *restricted specializations* for any $\varepsilon \in \mathbf{C}^{\times}$;

$$U_{\varepsilon}^{\mathrm{res}} := U_{\mathcal{A}}^{\mathrm{res}} \otimes_{\mathcal{A}} \mathbf{C}_{\varepsilon}, \tag{2.6}$$

where $\mathcal{A}$ acts on $\mathbf{C}_{\varepsilon} := \mathbf{C}$ by $f(q)c := f(\varepsilon)c$ ($c \in \mathbf{C}$).

B. Finite dimensional quantum algebra

For $\varepsilon \in \mathbf{C}^{\times}$ we use

$$[a] := \frac{\varepsilon^a - \varepsilon^{-a}}{\varepsilon - \varepsilon^{-1}}, \quad [a]! := [a][a-1]\cdots[2][1], \quad \begin{bmatrix} m \\ k \end{bmatrix} := \begin{bmatrix} m \\ k \end{bmatrix}_{q=\varepsilon}.$$

Since $\begin{bmatrix} m \\ k \end{bmatrix}_q \in \mathbf{C}[q, q^{-1}]$, the definition of $\begin{bmatrix} m \\ k \end{bmatrix}$ is valid.

As for the specializations of q, we shall be interested in the case where ε is a root of unity. So in what follows, suppose that l is the odd integer greater than 1 and ε is the primitive lth root of unity.

Under this setting, we can find an interesting finite dimensional subalgebra $U_{\varepsilon}^{\mathrm{fin}}$ of $U_{\varepsilon}^{\mathrm{res}}$. $U_{\varepsilon}^{\mathrm{fin}}$ is defined as the subalgebra of $U_{\varepsilon}^{\mathrm{res}}$ generated by e_i, f_i, and $t_i^{\pm 1}$ ($i \in I$). We know that this algebra is finite dimensional over $\mathbf{C}$ with the dimension $2^n l^{n^2+2n}$ (see Proposition 2.2).

This $U_{\varepsilon}^{\mathrm{fin}}$ is also defined by "generators and relations" as follows:

Proposition 2.1 (Refs. 1 and 4): The algebra $U_{\varepsilon}^{\mathrm{fin}}$ is isomorphic to the associative $\mathbf{C}$*-algebra with generators e_α, f_α ($\alpha \in \Delta_+$), and $t_i^{\pm 1}$ ($1 \leqslant i \leqslant n$) satisfying the following relations;*

$$t_i t_i^{-1} = t_i^{-1} t_i = 1, \quad t_i t_j = t_j t_i, \tag{2.7}$$

$$t_i e_j t_i^{-1} = \varepsilon^{a_{ij}} e_j, \tag{2.8}$$

$$t_i f_j t_i^{-1} = \varepsilon^{-a_{ij}} f_j, \tag{2.9}$$

$$e_i f_j - f_j e_i = \delta_{ij} \frac{t_i - t_i^{-1}}{\varepsilon - \varepsilon^{-1}}. \tag{2.10}$$

If $(\alpha_i, \alpha) = 0$ and $i < g(\alpha)$,

$$e_i e_\alpha = e_\alpha e_i, \tag{2.11}$$

$$f_i f_\alpha = f_\alpha f_i. \tag{2.12}$$

If $(\alpha_i, \alpha) = -1$ and $i < g(\alpha)$,

$$e_{\alpha+\alpha_i} = \varepsilon^{-1} e_i e_\alpha - e_\alpha e_i, \tag{2.13}$$

$$\varepsilon e_i e_{\alpha+\alpha_i} = e_{\alpha+\alpha_i} e_i, \tag{2.14}$$

$$\varepsilon e_{\alpha+\alpha_i} e_\alpha = e_\alpha e_{\alpha+\alpha_i}, \tag{2.15}$$

$$f_{\alpha+\alpha_i} = \varepsilon f_\alpha f_i - f_i f_\alpha, \tag{2.16}$$

$$\varepsilon f_i f_{\alpha+\alpha_i} = f_{\alpha+\alpha_i} f_i, \tag{2.17}$$

$$\varepsilon f_{\alpha+\alpha_i} f_\alpha = f_\alpha f_{\alpha+\alpha_i}. \tag{2.18}$$

$$e_\alpha^l = f_\alpha^l = 0 \quad for\ \ any\ \ \alpha \in \Delta_+, \tag{2.19}$$

$$t_i^{2l} = 1 \quad for\ \ any\ \ i \in I, \tag{2.20}$$

where we define $g(\alpha)$ $(\alpha \in \Delta_+)$ *to be the largest index satisfying* $c_i \neq 0$ *if we write* $\alpha = \Sigma_i c_i \alpha_i$ *and set* $e_i := e_{\alpha_i}$ *and* $f_i := f_{\alpha_i}$.

Define $(U_\varepsilon^{\mathrm{fin}})^+$ [respectively $(U_\varepsilon^{\mathrm{fin}})^-$, $(U_\varepsilon^{\mathrm{fin}})^0$] to be the subalgebra of $U_\varepsilon^{\mathrm{fin}}$ generated by e_i (respectively, f_i, $t_i^{\pm 1}$). Fix a reduced expression $w_0 = s_{i_1} s_{i_2} \cdots s_{i_N}$ of the longest element of the Weyl group W and set $\beta_k := s_{i_1} s_{i_2} \cdots s_{i_{k-1}} (\alpha_{i_k})$ for $k \in \{1,...,N\}$ where $N := \frac{1}{2} n(n+1)$ is the number of positive roots. Here we have the following Poincaré–Birkhoff–Witt type theorem:

Proposition 2.2 (Refs. 1 and 4): (*i*) *The algebra* $(U_\varepsilon^{\mathrm{fin}})^+$ *is a finite dimensional* **C***-vector space with the basis*

$$\{e_{\beta_N}^{r_N} e_{\beta_{N-1}}^{r_{N-1}} \cdots e_{\beta_1}^{r_1}\}_{0 \leqslant r_1,\ldots,r_N < l}. \tag{2.21}$$

(*ii*) *The algebra* $(U_\varepsilon^{\mathrm{fin}})^-$ *is a finite dimensional* **C***-vector space with the basis*

$$\{f_{\beta_N}^{r_N} f_{\beta_{N-1}}^{r_{N-1}} \cdots f_{\beta_1}^{r_1}\}_{0 \leqslant r_1,\ldots,r_N < l}. \tag{2.22}$$

(*iii*) *The algebra* $(U_\varepsilon^{\mathrm{fin}})^0$ *is a finite dimensional* **C***-vector space with the basis*

$$\{t_n^{r_n} t_{n-1}^{r_{n-1}} \cdots t_1^{r_1}\}_{0 \leqslant r_l,\ldots,r_n < 2l}. \tag{2.23}$$

(*iv*) *Multiplication defines an isomorphism of* **C***-vector space,*

$$(U_\varepsilon^{\mathrm{fin}})^- \otimes (U_\varepsilon^{\mathrm{fin}})^0 \otimes (U_\varepsilon^{\mathrm{fin}})^+ \xrightarrow{\sim} U_\varepsilon^{\mathrm{fin}}. \tag{2.24}$$

C. Nonrestricted specializations

Here we see another type of specialization of q to a root of unity.

Introduce the elements

$$[t_i; m] := \frac{t_i q^m - t_i^{-1} q^{-m}}{q - q^{-1}} \in U_q(\mathfrak{g}).$$

The algebra $U_{\mathcal{A}}$ is the $\mathcal{A}$-subalgebra of $U_q(\mathfrak{g})$ generated by the elements e_i, f_i, $t_i^{\pm 1}$, and $[t_i; 0]$ $(1 \leqslant i \leqslant n)$.

Remark: The defining relations for $U_{\mathcal{A}}$ are as in Sec. II A, but replacing (2.4) by

$$e_i f_j - f_j e_i = \delta_{ij} [t_i; 0] \tag{2.25}$$

and adding the relation $(q - q^{-1})[t_i; 0] = t_i - t_i^{-1}$.

Now for the lth root of unity ε we define the **C**-algebra

$$U_\varepsilon := U_{\mathcal{A}} \otimes_{\mathcal{A}} \mathbf{C}_\varepsilon,$$

where $\mathcal{A}$ acts on $\mathbf{C}_\varepsilon = \mathbf{C}$ by $f(q)c = f(\varepsilon)c$ $(c \in \mathbf{C})$. This U_ε is called the *nonrestricted specialization*.

III. REPRESENTATIONS

A. Maximal cyclic representations of U_ε

The representation theory of U_ε is discussed in Ref. 3 in which the maximal dimension of irreducible representations for A_n-type is given by $l^{(1/2)n(n+1)}$ in the case where ε is the lth root of unity, and in Ref. 5 it is constructed explicitly and called the ''maximal cyclic representations.'' Here we subtly modify the presentations in Ref. 5 in order to simplify the arguments in Sec. IV.

Let H be the group generated by $\{x_{ij},z_{ij}\}_{1\leqslant i\leqslant j\leqslant n}$ and the center ε with the relations $z_{ij}x_{ij}=\varepsilon x_{ij}z_{ij}$ and all others commute each other, and set $\mathcal{W}:=\mathbf{C}[H]$ the group ring of H. For $r:=(r_1,\ldots,r_n)$, $s:=(s_1,\ldots,s_n)\in(\mathbf{C}^\times)^n$, we define the map $\varphi_{r,s}: U_\varepsilon\to\mathcal{W}$ by (see Ref. 5)

$$\varphi_{r,s}(e_i):=\sum_{k=i}^{n} x_{ik}x_{ik+1}\cdots x_{in}\{r_i z_{ik}z_{ik-1}z_{i-1\,k-1}^{-1}z_{i+1\,k}^{-1}\}, \tag{3.1}$$

$$\varphi_{r,s}(f_i):=\sum_{k=1}^{i} x_{i+1-k\,n+1-k}^{-1}x_{i+2-k\,n+2-k}^{-1}\cdots x_{in}^{-1} \times\{s_i z_{i+1-k\,n-k}z_{i+1-k\,n+1-k}^{-1}z_{i-k\,n+1-k}z_{i-k\,n-k}^{-1}\}, \tag{3.2}$$

$$\varphi_{r,s}(t_i):=\frac{r_i}{s_i}z_{in}^2 z_{i-1\,n}^{-1}z_{i+1\,n}^{-1}, \tag{3.3}$$

where we use the notation $\{z\}=(z-z^{-1})/(\varepsilon-\varepsilon^{-1})$ and set $x_{ij}^{\pm1}=z_{ij}^{\pm1}=1$ unless $1\leqslant i\leqslant j\leqslant n$.

Let $*:\mathcal{W}\to\mathcal{W}$ be the $\mathbf{C}$-linear involution defined by

$$x_{jk}^*:=x_{k+1-j\,k}^{-1},\quad z_{jk}^*:=z_{k+1-j\,k}^{-1},$$

and set

$$A_{ik}:=x_{ik}x_{ik+1}\cdots x_{in},\quad B_{ik}:=z_{ik}z_{ik-1}z_{i-1\,k-1}^{-1}z_{i+1\,k}^{-1}.$$

Then, (3.1) and (3.2) can be written in the following forms:

$$\varphi_{r,s}(e_i)=\sum_{k=i}^{n} A_{ik}\{r_i B_{ik}\},\quad \varphi_{r,s}(f_i)=\sum_{k=1}^{i} A_{n+1-i\,n+1-k}^*\{s_i B_{n+1-i\,n+1-k}^*\}. \tag{3.4}$$

Proposition 3.1: The map $\varphi_{r,s}$ defines a $\mathbf{C}$-linear algebra homomorphism from U_ε to $\mathcal{W}$.

Lemma 3.2: The following commutation relations hold [see Ref. 5, (2.5)]:

$$\begin{aligned} A_{ij}B_{ik}&=\varepsilon^{-2}B_{ik}A_{ij}\quad \text{if } j<k\\ &=\varepsilon^{-1}B_{ik}A_{ij}\quad \text{if } j=k\\ &=B_{ik}A_{ij}\quad \text{if } j>k. \end{aligned}$$

Proof of Proposition 3.1: We have $A_{ik}B_{ik}=\varepsilon^{-1}B_{ik}A_{ik}$ and then

$$\varphi_{r,s}(e_i)=\sum_{k=i}^{n}\{r_i\varepsilon^{-1}B_{ik}\}A_{ik},\quad \varphi_{r,s}(f_i)=\sum_{k=1}^{i}\{s_i\varepsilon^{-1}B_{n+1-i\;n+1-k}^*\}A_{n+1-i\;n+1-k}^*.$$

This implies $\varphi_{r,s}=\rho_{\varepsilon^{-1}r,\varepsilon^{-1}s}$ ($\rho_{r,s}$ is given in Ref. 5). Thus, by Theorem 2.2 in Ref. 5, we obtained the desired result. □

Proposition 3.3: For any $m\in\mathbf{Z}_{>0}$, we have

$$\varphi_{r,s}(e_i^m)=[m]!\sum_{p=1}^{m}\sum_{\substack{i\leqslant k_p<\cdots<k_1\leqslant n\\ 1\leqslant\nu_p<\cdots<\nu_1=m}}\prod_{r=1}^{p}A_{ik_r}^{\nu_r-\nu_{r+1}}\prod_{r=1}^{p}\begin{Bmatrix} r_iB_{ik_r};\nu_r-1\\ \nu_r-\nu_{r+1}\end{Bmatrix},\tag{3.5}$$

$$\varphi_{r,s}(f_i^m)=[m]!\sum_{p=1}^{m}\sum_{\substack{i\leqslant k_p<\cdots<k_1\leqslant n\\ 1\leqslant\nu_p<\cdots<\nu_1=m}}\prod_{r=1}^{p}A^{*\nu_r-\nu_{r+1}}_{n+1-i\ n+1-k_r}\prod_{r=1}^{p}\begin{Bmatrix} s_iB^*_{n+1-i\ n+1-k_r};\nu_r-1\\ \nu_r-\nu_{r+1}\end{Bmatrix},\tag{3.6}$$

where $\nu_{p+1}=0$ and we set

$$\begin{Bmatrix} a;b\\ c\end{Bmatrix}:=\frac{\{a\varepsilon^b\}\{a\varepsilon^{b-1}\}\cdots\{a\varepsilon^{b-c+1}\}}{[c]!}.$$

Remark: The definition of $\{{a;b\atop c}\}$ is invalid for ε such that $[c]!=0$. But on the right-hand side of (3.5) and (3.6) we see that the term

$$\frac{[m]!}{\Pi_{r=1}^{p}[\nu_r-\nu_{r+1}]!}\quad(1\leqslant\nu_p<\cdots<\nu_1=m)$$

is valid since $[m]_q!/\Pi_{r=1}^{p}[\nu_r-\nu_{r+1}]_q!\in\mathbf{Z}[q,q^{-1}]$.

Proof: In Ref. 5, the following formula is given:

$$\rho_{r,s}(e_i^m)=[m]!\sum_{p=1}^{m}\sum_{\substack{i\leqslant k_p<\cdots<k_1\leqslant n\\ 1\leqslant\nu_p<\cdots<\nu_1=m}}\prod_{r=1}^{p}\begin{Bmatrix} r_iB_{ik_r};-\nu_{r+1}\\ \nu_r-\nu_{r+1}\end{Bmatrix}\prod_{r=1}^{p}A_{ik_r}^{\nu_r-\nu_{r+1}},\tag{3.7}$$

where $\nu_{p+1}=0$. Since $\varphi_{r,s}=\rho_{\varepsilon^{-1}r,\varepsilon^{-1}s}$, it follows from (3.7)

$$\varphi_{r,s}(e_i^m)=\rho_{\varepsilon^{-1}r,\varepsilon^{-1}s}(e_i^m)=[m]!\sum_{p=1}^{m}\sum_{\substack{i\leqslant k_p<\cdots<k_1\leqslant n\\ 1\leqslant\nu_p<\cdots<\nu_1=m}}\prod_{r=1}^{p}\begin{Bmatrix} \varepsilon^{-1}r_iB_{ik_r};-\nu_{r+1}\\ \nu_r-\nu_{r+1}\end{Bmatrix}\prod_{r=1}^{p}A_{ik_r}^{\nu_r-\nu_{r+1}}.\tag{3.8}$$

Here by Lemma 3.2 we obtain for $i\leqslant k_p<\cdots<k_1\leqslant n$ and $1\leqslant r\leqslant p$,

$$\begin{Bmatrix} \varepsilon^{-1}r_iB_{ik_r};-\nu_{r+1}\\ \nu_r-\nu_{r+1}\end{Bmatrix}\left(\prod_{r=1}^{p}A_{ik_r}^{\nu_r-\nu_{r+1}}\right)=\left(\prod_{r=1}^{p}A_{ik_r}^{\nu_r-\nu_{r+1}}\right)\begin{Bmatrix} \varepsilon^{-1+\nu_r+\nu_{r+1}-2\nu_{p+1}}r_iB_{ik_r};-\nu_{r+1}\\ \nu_r-\nu_{r+1}\end{Bmatrix}$$
$$=\left(\prod_{r=1}^{p}A_{ik_r}^{\nu_r-\nu_{r+1}}\right)\begin{Bmatrix} r_iB_{ik_r};\nu_r-1\\ \nu_r-\nu_{r+1}\end{Bmatrix},$$

where we use $\nu_{p+1}=0$. Thus, we obtain (3.5). Similarly we also get (3.6). □

Let V_{ij} $(1\leqslant i\leqslant j\leqslant n)$ be a copy of the vector space $\mathbf{C}^l$ and set $\mathcal{V}:=\otimes_{1\leqslant i\leqslant j\leqslant n}V_{ij}$. Let $u_0,\ldots,u_{l-1}$ be the standard basis of $\mathbf{C}^l$. Now we define the representation $(\psi_{a,b},\mathcal{V})$ of $\mathcal{W}$ as follows: Let Z_{jk}, $X_{jk}\in\mathrm{End}(\mathcal{V})$ be the matrices defined as

$$Z_{jk}u_i=\varepsilon^iu_i,\quad X_{jk}u_i=u_{i+1}$$

on the component V_{jk} and as the identity on the other component. For nonzero parameters $a:=(a_{ij})_{1\leqslant i\leqslant j\leqslant n}$ and $b:=(b_{ij})_{1\leqslant i\leqslant j\leqslant n}\in(\mathbf{C}^\times)^{n(n+1)/2}$, define $\psi_{a,b}(x_{ij})$, $\psi_{a,b}(z_{ij})\in\mathrm{End}(\mathcal{V})$ to be

$$\psi_{a,b}(x_{ij})=a_{ij}X_{ij},\quad \psi_{a,b}(z_{ij})=b_{ij}Z_{ij}.\tag{3.9}$$

We can easily check that these define the representation of $\mathcal{W}$:

$$\psi_{a,b};\mathcal{W}\to\mathrm{End}(\mathcal{V}). \tag{3.10}$$

Composing $\varphi_{r,s}$ and $\psi_{a,b}$,

$$\Phi_{r,s,a,b}:=\psi_{a,b}\circ\varphi_{r,s}:U_\varepsilon\overset{\varphi_{r,s}}{\to}\mathcal{W}\overset{\psi_{a,b}}{\to}\mathrm{End}(\mathcal{V}),$$

we obtain the representation of U_ε denoted by $(\Phi_{r,s,a,b},\mathcal{V})$. The representation introduced in Ref. 5 is just as $(\Phi_{\varepsilon r,\varepsilon s,a,b},\mathcal{V})$ in our notation since we have $\varphi_{r,s}=\rho_{\varepsilon^{-1}r,\varepsilon^{-1}s}$ in the proof of Proposition 3.1.

It is shown in Ref. 5 that the representation $(\Phi_{r,s,a,b},\mathcal{V})$ is irreducible for generic parameters *r, s, a, b*. We are interested in specializations of these parameters so that the representation $(\Phi_{r,s,a,b},\mathcal{V})$ is not necessarily irreducible.

B. Representations of $U_\varepsilon^{\mathrm{res}}$ and $U_\varepsilon^{\mathrm{fin}}$

We review the representation theory of $U_\varepsilon^{\mathrm{res}}$. The classification of the irreducible representations of $U_\varepsilon^{\mathrm{res}}$ is given by Lusztig.[2] Before seeing it, let us recall the notions of highest weight modules. A $U_\varepsilon^{\mathrm{res}}$ or $U_\varepsilon^{\mathrm{fin}}$-module M is said to be of type **1**, if $t_i^l=1$ $(i\in I)$ on M.

Definition 3.4: Let V be a $U_\varepsilon^{\mathrm{res}}$-module of type **1**.

(*i*) *The weight spaces V_λ $(\lambda=\Sigma_i m_i\Lambda_i\in P)$ of V are defined by*

$$V_\lambda:=\left\{v\in V\,\middle|\,t_iv=\varepsilon^{m_i^{(0)}}v,\quad \begin{bmatrix}t_i;0\\ l\end{bmatrix}v=\begin{bmatrix}m_i^{(1)}\\ l\end{bmatrix}v\right\}, \tag{3.11}$$

where $m_i=m_i^{(0)}+lm_i^{(1)}$ and $0\leqslant m_i^{(0)}<l$.

(*ii*) *V is a highest weight module if V is generated by a primitive vector, i.e., a vector $v\in V_\lambda$ for some $\lambda\in P$, such that $e_iv=e_i^{(l)}v=0$ for any $i\in I$. In that case, λ is called the highest weight and v is called the highest weight vector of V.*

Let $V(\lambda)$ be the irreducible highest weight $U_q(\mathfrak{g})$-module given by $V(\lambda)=U_q(\mathfrak{g})/\mathcal{I}$ where $\lambda\in P_+$ and $\mathcal{I}$ is the left ideal generated by e_i, $f_i^{1+\langle h_i,\lambda\rangle}$, and $t_i-q^{\langle h_i,\lambda\rangle}$ $(1\leqslant i\leqslant n)$. Here denote the generator of $V(\lambda)$ by v_λ. Let $V_{\mathcal{A}}^{\mathrm{res}}(\lambda)$ be the $U_{\mathcal{A}}^{\mathrm{res}}$-submodule of $V(\lambda)$ generated by v_λ. Set $W_\varepsilon^{\mathrm{res}}(\lambda):=V_{\mathcal{A}}^{\mathrm{res}}(\lambda)\otimes_{\mathcal{A}}\mathbf{C}_\varepsilon$, which is naturally $U_\varepsilon^{\mathrm{res}}$-module. Note that $W_\varepsilon^{\mathrm{res}}(\lambda)$ is not necessarily irreducible. So, let Y be its maximal proper submodule and define $V_\varepsilon^{\mathrm{res}}(\lambda):=W_\varepsilon^{\mathrm{res}}(\lambda)/Y$ to be the irreducible quotient, which is type **1** highest weight module with the highest weight λ.

Theorem 3.5 (Ref. 2): *Arbitrary finite-dimensional irreducible $U_\varepsilon^{\mathrm{res}}$-module V of type* **1** *is isomorphic to $V_\varepsilon^{\mathrm{res}}(\lambda)$ for a unique $\lambda\in P_+$.*

Note that arbitrary finite-dimensional irreducible $U_\varepsilon^{\mathrm{res}}$-module V of type **1** is a direct sum of its weight spaces.

Here we call a weight $\lambda\in P_+$ satisfying $0\leqslant\langle h_i,\lambda\rangle<l$ for $i\in I$ an *l-restricted weight*.

Theorem 3.6 (Refs. 2 and 4, Proposition 11.2.10): (*i*) *For $\lambda=\Sigma_i m_i\Lambda_i\in P_+$, define $\lambda^{(0)}:=\Sigma_i m_i^{(0)}\lambda_i$ and $\lambda^{(1)}:=\Sigma_i m_i^{(1)}\lambda_i$ where $m_i=m_i^{(0)}+lm_i^{(1)}$ with $0\leqslant m_i^{(0)}<l$ (and then $\lambda=\lambda^{(0)}+l\lambda^{(1)}$). The $U_\varepsilon^{\mathrm{res}}$-module $V_\varepsilon^{\mathrm{res}}(\lambda)$ is isomorphic to $V_\varepsilon^{\mathrm{res}}(\lambda^{(0)})\otimes V_\varepsilon^{\mathrm{res}}(l\lambda^{(1)})$.*

(*ii*) *By restricting to $U_\varepsilon^{\mathrm{fin}}$, we obtain the one-to-one correspondence between the family of the finite-dimensional irreducible $U_\varepsilon^{\mathrm{res}}$-modules of type* **1** *with l-restricted highest weight and the family of irreducible $U_\varepsilon^{\mathrm{fin}}$-modules of type* **1**.

As we have stated in Sec. I, the module $V_\varepsilon^{\mathrm{res}}(\lambda^{(0)})$ is an irreducible $U_\varepsilon^{\mathrm{fin}}$-module and $V_\varepsilon^{\mathrm{res}}(l\lambda^{(1)})$ is identified with the irreducible highest weight $\mathfrak{sl}_{n+1}$-module $V(\lambda^{(1)})$. Since we know the structure of the irreducible $\mathfrak{sl}_{n+1}$-module well, this theorem implies that the structure of the module $V_\varepsilon^{\mathrm{res}}(\lambda)$ can be clarified if we shall make clear the one for $V_\varepsilon^{\mathrm{res}}(\lambda^{(0)})$.

IV. PRIMITIVE VECTORS

Let l and ε be same as in Sec. III.

A. Specializations of parameters

Let $M:=\{\mathrm{m}=(m_{jk})_{1\leqslant j\leqslant k\leqslant n} | 0\leqslant m_{jk}\leqslant l-1\}$ be the index set of the standard basis of $\mathcal{V}$. We can consider the additive structure on M via the natural identification $M\cong(\mathbf{Z}/l\mathbf{Z})^{(1/2)n(n+1)}$. For $\mathrm{m}\in M$ we write $u_{\mathrm{m}}:=\otimes_{1\leqslant j\leqslant k\leqslant n}u_{m_{jk}}(u_{m_{jk}}\in V_{jk})$.

We consider the following specialization of parameters *r, s, a, b*:

$$a_{ik}a_{ik+1}\cdots a_{in}=1, \tag{4.1}$$

$$r_i b_{ik}b_{ik-1}b^{-1}_{i-1k-1}b^{-1}_{i+1k}=1 \quad (1\leqslant i\leqslant k\leqslant n), \tag{4.2}$$

$$\frac{r_i}{s_i}b^2_{in}b^{-1}_{i-1n}b^{-1}_{i+1n}=\dot{\varepsilon}^{\lambda_i}, \tag{4.3}$$

where integers $\{\lambda_i\}_{1\leqslant i\leqslant n}$ satisfy $0\leqslant\lambda_i<l$. Here we set $a_{ik}=b_{ik}=1$ unless $1\leqslant i\leqslant k\leqslant n$.

Remark: Note that the set of parameters satisfying (4.1)–(4.3) is never empty. Indeed, if we set $a_{jk}=b_{jk}=1$ for any (j,k) and $r_i=1$ and $s_i=\varepsilon^{-\lambda_i}$ for any i, it is trivial to see that these satisfy (4.1)–(4.3). [By (4.1), we have $a_{jk}=1$ for all $1\leqslant j\leqslant k\leqslant n$].

Lemma 4.1: Under the specialization (4.2) and (4.3), we have

$$s_i b_{i+1-k\ n-k}b^{-1}_{i+1-k\ n+1-k}b_{i-k\ n+1-k}b^{-1}_{i-k\ n-k}=\varepsilon^{-\lambda_i}(1\leqslant k\leqslant i\leqslant n). \tag{4.4}$$

Proof: Using (4.2), we have $r_i b_{ik}b_{ik-1}b^{-1}_{i-1k-1}b^{-1}_{i+1k}=1=r_i b_{ik-1}b_{ik-2}b^{-1}_{i-1k-2}b^{-1}_{i+1k-1}$ and then $b_{i+1k-1}b^{-1}_{i+1k}=b_{ik-2}b^{-1}_{ik}b_{i-1k-1}b^{-1}_{i-1k-2}$. Changing $i\to i-k$ and $k\to n-k+1$, we get

$$b_{i+1-k\ n-k}b^{-1}_{i+1-k\ n+1-k}=b_{i-k\ n-k-1}b^{-1}_{i-k\ n+1-k}b_{i-k-1\ n-k}b^{-1}_{i-k-1\ n-k-1}. \tag{4.5}$$

By (4.2) with $k=n$ and (4.3), we have $s_i b_{in-1}b^{-1}_{in}b_{i-1n}b^{-1}_{i-1n-1}=\varepsilon^{-\lambda_i}$ which is (4.4) in the case $k=1$. Suppose that (4.4) holds and substitute (4.5) into (4.4). Then we obtain

$$s_i b_{i-k\ n-k-1}b^{-1}_{i-k\ n-k}b_{i-k-1\ n-k}b^{-1}_{i-k-1\ n-k-1}=\varepsilon^{-\lambda_i}.$$

Thus, the induction on k proceeds and then we prove (4.4) for any $k\in\{1,2,...,i\}$.

□

Under conditions (4.1)–(4.3), by this lemma we have

$$\Phi_{r,s,a,b}(e_i):=\sum_{k=i}^{n}X_{ik}X_{ik+1}\cdots X_{in}\{Z_{ik}Z_{ik-1}Z^{-1}_{i-1k-1}Z^{-1}_{i+1k}\}, \tag{4.6}$$

$$\Phi_{r,s,a,b}(f_i):=\sum_{k=1}^{i}X^{-1}_{i+1-k\ n+1-k}X^{-1}_{i+2-k\ n+2-k}\cdots X^{-1}_{in}$$
$$\times\{\varepsilon^{-\lambda_i}Z_{i+1-k\ n-k}Z^{-1}_{i+1-k\ n+1-k}Z_{i-k\ n+1-k}Z^{-1}_{i-k\ n-k}\}, \tag{4.7}$$

$$\Phi_{r,s,a,b}(t_i):=\varepsilon^{\lambda_i}Z^2_{in}Z^{-1}_{i-1n}Z^{-1}_{i+1n}, \tag{4.8}$$

B. Primitive vectors in $\mathcal{V}$

Under the specialization in Sec. IV A, we get the following:

Proposition 4.2: Under the specialization (4.1) and (4.2), $v\in\mathcal{V}$ satisfies the condition

$$e_i v=0 \quad \text{for any } i=1,...,n, \tag{4.9}$$

if and only if $v=cu_{\vec{0}}(c\in\mathbf{C})$ *where* $\vec{0}=(0,0,...,0)\in M$.

Proof: By (4.1) and (4.2), the action of e_i on $u_{\mathrm{m}}\in\mathcal{V}\,(\mathrm{m}=(m_{gh})\in M)$ is given by

$$e_iu_{\mathrm{m}}=\sum_{i\leqslant k\leqslant n}[m_{ik}+m_{ik-1}-m_{i-1k-1}-m_{i+1k}]u_{\mathrm{m}+\epsilon_{ik}+\cdots\epsilon_{in}}, \tag{4.10}$$

where $\epsilon_{jk}\in M$ satisfies that the (j,k)-entry is 1 and all others are 0. If $\mathrm{m}=\vec{0}$, we have $m_{ik}+m_{ik-1}-m_{i-1k-1}-m_{i+1k}=0$ for all $i\leqslant k\leqslant n$, which implies that $e_iu_{\vec{0}}=0$ for any i.

Conversely, assume that $v=\Sigma_{\mathrm{m}\in M}c_{\mathrm{m}}u_{\mathrm{m}}$ $(c_{\mathrm{m}}\in\mathbf{C})$ satisfies (4.9). First, we have

$$0=e_nv=X_{nn}\{Z_{n-1n-1}^{-1}Z_{nn}\}v=\sum_{\mathrm{m}\in M}c_{\mathrm{m}}[m_{nn}-m_{n-1n-1}]u_{m+\epsilon_{nn}} \tag{4.11}$$

This implies that

$$m_{n-1n-1}\neq m_{nn}\Rightarrow c_{\mathrm{m}}=0, \tag{4.12}$$

and then we have $v=\Sigma_{\mathrm{m}\in M,m_{n-1n-1}=m_{nn}}c_{\mathrm{m}}v_{\mathrm{m}}$.

Next, by $e_{n-1}v=0$ we have

$$\begin{aligned}0=e_{n-1}v&=(X_{n-1n-1}X_{n-1n}\{Z_{n-1n-1}Z_{n-2n-2}^{-1}\}+X_{n-1n}\{Z_{n-1n}Z_{n-1n-1}Z_{n-2n-1}^{-1}Z_{nn}^{-1}\})v\\&=\sum_{\substack{\mathrm{m}\in M.\\ m_{n-1n-1}=m_{nn}}}c_{\mathrm{m}}[m_{n-1n-1}-m_{n-2n-2}]u_{m+\epsilon_{n-1n-1}+\epsilon_{n-1n}}\\&\quad+c_{\mathrm{m}}[m_{n-1n}+m_{n-1n-1}-m_{n-2n-1}-m_{nn}]u_{m+\epsilon_{n-1n}}.\end{aligned}$$

This implies that

$$c_{\mathrm{m}}[m_{n-1n-1}-m_{n-2n-2}]=c_{\mathrm{m}}[m_{n-1n}+m_{n-1n-1}-m_{n-2n-1}-m_{nn}]=0 \tag{4.13}$$

for any $\mathrm{m}\in M$ satisfying $m_{n-1n-1}=m_{nn}$ since all vectors appearing in the summation are linearly independent under the condition $m_{n-1n-1}=m_{nn}$, that is, the indices $\mathrm{m}+\epsilon_{n-1n-1}+\epsilon_{n-1n}$ and $\mathrm{m}'+\varepsilon_{n-1n}$ never coincide for arbitrary m, m′ under the conditions $m_{n-1n-1}=m_{nn}$ and $m'_{n-1n-1}=m'_{nn}$. Thus, by (4.12) and (4.13) we have $c_{\mathrm{m}}=0$ unless

$$m_{n-2n-2}=m_{n-1n-1}=m_{nn},$$

$$m_{n-2n-1}=m_{n-1n}.$$

Here we assume that $c_{\mathrm{m}}=0$ in v unless

$$\begin{aligned}&m_{ii}=m_{i+1i+1}=\cdots=m_{nn},\\&m_{ii+1}=m_{i+1i+2}=\cdots=m_{n-1n},\\&\vdots\\&m_{in-1}=m_{i+1n}.\end{aligned} \tag{4.14}$$

By $e_iv=0$ we get

$$
\begin{aligned}
0 &= \sum_{k=i}^{n} X_{ik}X_{ik+1}\cdots X_{in}\{Z_{ik}Z_{ik-1}Z_{i-1k-1}^{-1}Z_{i+1k}^{-1}\}v \\
&= \sum_{\substack{\mathrm{m}\in M. \\ \mathrm{m}\ \text{satisfies}\ (4.14)}} \sum_{k=i}^{n} c_{\mathrm{m}}[m_{ik}+m_{ik-1}-m_{i-1k-1}-m_{i+1k}]u_{\mathrm{m}+\epsilon_{ik}+\cdots+\epsilon_{in}} \\
&= \sum_{\substack{\mathrm{m}\in M, \\ \mathrm{m}\ \text{satisfies}\ (4.14)}} (c_{\mathrm{m}}[m_{ii}-m_{i-1i-1}]u_{m+\epsilon_{ii}+\cdots+\epsilon_{in}} \\
&\quad + c_{\mathrm{m}}[m_{ii+1}+m_{ii}-m_{i-1i}-m_{i+1i+1}]u_{m+\epsilon_{i+1}+\cdots+\epsilon_{in}} \\
&\quad + \cdots + c_{\mathrm{m}}[m_{in}+m_{in-1}-m_{i-1n-1}-m_{i+1n}]u_{\mathrm{m}+\epsilon_{in}}).
\end{aligned} \tag{4.15}
$$

It follows from (4.14) that all vectors appearing in the summation (4.15) are linearly independent. Therefore, we obtain that $c_{\mathrm{m}}=0$, unless

$$
\begin{gathered}
m_{ii}-m_{i-1i-1}=0, \\
m_{ii+1}+m_{ii}-m_{i-1i}-m_{i+1i+1}=0, \\
\vdots \\
m_{in}+m_{in-1}-m_{i-1n-1}-m_{i+1n}=0.
\end{gathered}
$$

Thus, from this and (4.14) we get $c_{\mathrm{m}}=0$ unless

$$
\begin{gathered}
m_{i-1i-1}=m_{ii}=m_{i+1i+1}=\cdots=m_{nn}, \\
m_{i-1i}=m_{ii+1}=m_{i+1i+2}=\cdots=m_{n-1n}, \\
\vdots \\
m_{i-1,n-2}=m_{in-1}=m_{i+1n}, \\
m_{i-1n-1}=m_{in}.
\end{gathered} \tag{4.16}
$$

Thus, using $e_2v=e_3v=\cdots=e_{n-1}v=e_nv=0$ we have $c_{\mathrm{m}}=0$ unless

$$
\begin{gathered}
m_{11}=m_{22}=m_{33}=\cdots=m_{nn}, \\
m_{12}=m_{23}=m_{34}=\cdots=m_{n-1n}, \\
\vdots \\
m_{1,n-2}=m_{2n-1}=m_{3n}, \\
m_{1n-1}=m_{2n}.
\end{gathered} \tag{4.17}
$$

Finally, using $e_1v=0$, we have

$$
\begin{aligned}
0 &= \sum_{k=1}^{n} X_{1k}X_{1k+1}\cdots X_{1n}\{Z_{1k}Z_{1k-1}Z_{2k}^{-1}\}v \\
&= \sum_{\substack{\mathrm{m}\in M,\\ \mathrm{m}\ \text{satisfies}\ (4.17)}} \sum_{k=1}^{n} c_{\mathrm{m}}[m_{1k}+m_{1k-1}-m_{2k}]u_{\mathrm{m}+\epsilon_{1k}+\cdots+\epsilon_{1n}} \\
&= \sum_{\substack{\mathrm{m}\in M,\\ \mathrm{m}\ \text{satisfies}\ (4.17)}} (c_{\mathrm{m}}[m_{11}]u_{m+\epsilon_{11}+\cdots+\epsilon_{1n}} + c_{\mathrm{m}}[m_{12}+m_{11}-m_{22}]u_{m+\epsilon_{12}+\cdots+\epsilon_{1n}} \\
&\quad +\cdots+c_{\mathrm{m}}[m_{1n}+m_{1n-1}-m_{2n}]u_{\mathrm{m}+\epsilon_{1n}}). \qquad (4.18)
\end{aligned}
$$

Under the condition (4.17), we get that $c_{\mathrm{m}}=0$, unless

$$0=m_{11}=m_{12}=\cdots=m_{1n}. \qquad (4.19)$$

Therefore, it follows from (4.17) and (4.19) that $c_{\mathrm{m}}=0$ unless

$$
\begin{gathered}
0=m_{11}=m_{22}=m_{33}=\cdots=m_{nn}, \\
0=m_{12}=m_{23}=m_{34}=\cdots=m_{n-1n}, \\
\vdots \qquad (4.20) \\
0=m_{1,n-2}=m_{2n-1}=m_{3n}, \\
0=m_{1n-1}=m_{2n}, \\
0=m_{1n},
\end{gathered}
$$

which implies that $v=cu_{\vec{0}}(c\in\mathbf{C})$.

Remark: In the proof of the proposition, we easily see that we do not need (4.1) essentially. It is required for simplification of the proof or the presentations. So it is possible to proceed with the same argument for generic a_{jk}'s.

The primitive vector $u_{\vec{0}}$ possesses the following property:

Proposition 4.3: Under the conditions (4.1), (4.2) *and* (4.3), *we have* $t_iu_{\vec{0}}=\varepsilon^{\lambda_i}u_{\vec{0}}$ *and* $f_i^{\lambda_i+1}u_{\vec{0}}=0$.

Proof: The first formula is the immediate consequence of (4.8). We obtain the explicit form of $f_i^{\lambda_i+1}$ on $\mathcal{V}$ by (3.6) in Proposition 3.3 taking $m=\lambda_i+1$. By Lemma 4.1, under the specialization (4.1), (4.2), and (4.3), we have $s_ib_{i+1-kn-k}b_{i+1-kn+1-k}^{-1}b_{i-kn+1-k}b_{i-kn-k}^{-1}=\varepsilon^{-\lambda_i}$. Thus, on $u_{\vec{0}}$ we have

$$f_i^{\lambda_i+1}u_{\vec{0}}=[\lambda_i+1]!\sum_{p=1}^{\lambda_i+1}\sum_{\substack{i\leqslant k_p<\cdots<k_1\leqslant n\\ 1\leqslant\nu_p<\cdots<\nu_1=\lambda_i+1}}\prod_{r=1}^{p}A^{*\nu_r-\nu_r+1}_{n+1-i\ \ n+1-k_r}\prod_{r=1}^{p}\begin{Bmatrix}\varepsilon^{-\lambda_i};\nu_r-1\\ \nu_r-\nu_{r+1}\end{Bmatrix}u_{\vec{0}}.$$

For any $p\in\{1,2,...,\lambda_i+1\}$ and any $\nu_p,\ldots,\nu_1$ satisfying $1\leqslant\nu_p<\cdots<\nu_1=\lambda_i+1$, there exists $r\in\{1,2,...,p\}$ such that $\nu_{r+1}\leqslant\lambda_i<\nu_r$. Therefore, for such r we have

$$\begin{Bmatrix}\varepsilon^{-\lambda_i};\nu_r-1\\ \nu_r-\nu_{r+1}\end{Bmatrix}=\frac{\{\varepsilon^{-\lambda_i+\nu_r-1}\}\{\varepsilon^{-\lambda_i+\nu_r-2}\}\cdots\{\varepsilon^{-\lambda_i+\nu_{r+1}}\}}{[\nu_r-\nu_{r+1}]!}=0.$$

Thus, we obtain $f_i^{\lambda_i+1}u_{\vec{0}}=0$. □

Here for $\lambda:=(\lambda_1,\ldots,\lambda_n)$ $(0\leqslant\lambda_i<l)$ we define the U_ε-submodule $L(\lambda)$ of $\mathcal{V}$ by $L(\lambda):=U_\varepsilon u_{\vec{0}}$.

Let $V(\lambda)$ be the irreducible highest weight $U_q(\mathfrak{g})$-module as in Sec. III B. Let $V_{\mathcal{A}}(\lambda)$ be the $U_{\mathcal{A}}$-submodule of $V(\lambda)$ generated by v_λ. Set $V_\varepsilon(\lambda)$ be the U_ε-submodule of $V_{\mathcal{A}}(\lambda)\otimes_{\mathcal{A}}\mathbf{C}_\varepsilon$ generated by v_λ. Note that $V_\varepsilon(\lambda)$ is not necessarily irreducible. By Proposition 4.3, $t_i u_0^{\vec{}} = \varepsilon^{\lambda_i} u_0^{\vec{}}$ and $f_i^{\langle h_i,\lambda\rangle+1} u_0^{\vec{}} = 0$ $(i\in I)$, so we hope to have the surjective U_ε-linear map $\pi: V_\varepsilon(\lambda)\to L(\lambda)$ given by $\pi: v_\lambda \mapsto u_0^{\vec{}}$. It seems that the module $L(\lambda)$ is in the similar stream of the theory of $U_\varepsilon^{\mathrm{res}}$-modules. Here we expect that $L(\lambda)$ is an irreducible highest weight U_ε-module. Surprisingly, in Sec. IV C we will obtain the more interesting results that $L(\lambda)$ can be seen as an irreducible $U_\varepsilon^{\mathrm{fin}}$-module. By Theorem 3.6 this means that we get irreducible $U_\varepsilon^{\mathrm{res}}$ (or $U_\varepsilon^{\mathrm{fin}}$)-modules directly from U_ε-modules.

C. Shifts of parameters

Let $r^{(0)}=(r_j^{(0)})$, $s^{(0)}=(s_j^{(0)})\in(\mathbf{C}^\times)^n$ and $a^{(0)}=(a_{jk}^{(0)})$, $b^{(0)}=(b_{jk}^{(0)})\in(\mathbf{C}^{\mathrm{x}})^N$ be the parameters satisfying (4.1)–(4.3).

Fix a basis vector $u_\xi\in\mathcal{V}(\xi=(\xi_{jk})\in M)$ arbitrarily and set $b^{(\xi)}=(b_{jk}^{(\xi)}):=(\varepsilon^{-\xi_{jk}}b_{jk}^{(0)})\in(\mathbf{C}^\times)^N$. In this setting we obtain the following:

Proposition 4.4: For any $\mu=(\mu_{jk})\in M$ and any $X\in U_\varepsilon$, set

$$\Phi_{r^{(0)}s^{(0)},a^{(0)},b^{(0)}}(X)u_\mu=\sum_{\mathrm{m}\in M} C_{\mathrm{m}}u_{\mathrm{m}}. \tag{4.21}$$

Then we have

$$\Phi_{r^{(0)},s^{(0)},a^{(0)},b^{(\xi)}}(X)u_{\mu+\xi}=\sum_{\mathrm{m}\in M} C_{\mathrm{m}}u_{\mathrm{m}+\xi}. \tag{4.22}$$

Proof: It is shown easily from the formula

$$\psi_{a^{(0)},b^{(0)}}(x_{jk})u_\mu=a_{jk}^{(0)}u_{\mu+\varepsilon_{jk}}\quad \psi_{a^{(0)},b^{(0)}}(z_{jk})u_\mu=b_{jk}^{(0)}\varepsilon^{\mu_{jk}}u_\mu,$$

$$\psi_{a^{(0)},b^{(\xi)}}(x_{jk})u_{\mu+\xi}=a_{jk}^{(0)}u_{\mu+\xi+\varepsilon_{jk}},$$

$$\psi_{a^{(0)},b^{(\xi)}}(z_{jk})u_{\mu+\xi}=b_{jk}^{(\xi)}\varepsilon^{\mu_{jk}+\xi_{jk}}u_{\mu+\xi}=b_{jk}^{(0)}\varepsilon^{\mu_{jk}}u_{\mu+\xi}.$$

□

By Proposition 4.2, Proposition 4.3, and Proposition 4.4, we have the following result.

Proposition 4.5: We consider the representation $(\Phi_{r^{(0)},s^{(0)},a^{(0)},b^{(\varepsilon)}},\mathcal{V})$.

(*i*) *A vector $v\in\mathcal{V}$ satisfies the condition*

$$e_i v=0\quad \text{for any } i=1,\ldots,n, \tag{4.23}$$

if and only if $v=cu_\xi$ $(c\in\mathbf{C})$ where $u_\xi\in\mathcal{V}$ is the fixed basis vector as above.

(*ii*) *We have $t_i u_\xi=\varepsilon^{\lambda_i}u_\xi$ and $f_i^{\lambda_i+1}u_\xi=0$ $(i\in I)$.*

By this proposition, if we take the parameters properly, any basis vector $u_\xi\in\mathcal{V}$ can be the unique (up to constant) primitive vector in $\mathcal{V}$.

V. IRREDUCIBLE $U_\varepsilon^{\mathrm{fin}}$-MODULE

Suppose that parameter *r, s, a, b* satisfy conditions (4.1)–(4.3). In this case $u_0^{\vec{}}$ is the unique (up to constant) primitive vector in $\mathcal{V}$. As we defined in Sec. IV, set $L(\lambda):=U_\varepsilon u_0^{\vec{}}(\lambda=(\lambda_1,\lambda_2,\ldots,\lambda_n),0\leqslant\lambda_i\leqslant l-1)$, which is a U_ε-submodule of $\mathcal{V}$. In this section we shall see several properties of this module and it amounts to an irreducible $U_\varepsilon^{\mathrm{fin}}$-module.

A. Root vectors

First, we see higher root vectors in U_ε. There are several definitions for them. We shall introduce two of them here and discuss their relations.

The first one is defined by using (2.13) and (2.16) inductively. We also denote them by e_α and f_α $(\alpha\in\Delta_+)$.

Lemma 5.1: The root vectors e_α and $f_\alpha\in U_\varepsilon$ $(\alpha\in\Delta_+)$ defined by (2.13) *and* (2.16) *satisfy the relations* (2.11), (2.12), (2.14), (2.15), (2.17), *and* (2.18) *in* U_ε.

Proof: This lemma is easily obtained by using the results in, e.g., Refs. 12, 13, Sec. 3. Indeed, as for the element E_α $(\alpha\in\Delta_+)$ in Ref. 12, Chap. 4, we have the simple relation

$$e_\alpha=(q^{\mathrm{height}(\alpha)-1}E_\alpha)|_{q=\varepsilon^{-1}}. \tag{5.1}$$

Thus, the relations (2.11), (2.14), and (2.15) are immediate from Ref. 12, Proposition 3.2. The remaining relations are also derived similarly.

We introduce the alternative definition of root vectors:[5] For roots $\alpha=\alpha_i+\alpha_{i+1}+\cdots\alpha_j$ and $\beta=\alpha_{j+1}+\alpha_{j+2}+\cdots+\alpha_k$ $(i<j<k)$, we define

$$\overline{e}_{\alpha+\beta}=\overline{e}_\alpha\overline{e}_\beta-\varepsilon\overline{e}_\beta\overline{e}_\alpha, \tag{5.2}$$

$$\overline{f}_{\alpha+\beta}=\overline{f}_\alpha\overline{F}_\beta-\varepsilon^{-1}\overline{f}_\beta\overline{f}_\alpha, \tag{5.3}$$

where we set $\overline{e}_{\alpha_i}:=e_i$ and $\overline{f}_{\alpha_i}:=f_i$. Note that these definitions are well-defined, that is, these do not depend on the choice of j.

Those two types of the root vectors possess the following simple relations:

Lemma 5.2: For any $\alpha\in\Delta_+$, we have

$$\overline{e}_\alpha=\varepsilon^{\mathrm{height}(\alpha)-1}e_\alpha,\quad \overline{f}_\alpha=\varepsilon^{-\mathrm{height}(\alpha)+1}f_\alpha, \tag{5.4}$$

$$\overline{e}_\alpha^{\,l}=e_\alpha^l,\quad \overline{f}_\alpha^{\,l}=f_\alpha^l. \tag{5.5}$$

Proof: The proof of (5.4) is done by using induction on the height of roots and (5.5) is an immediate consequence of (5.4) since $\varepsilon^l=1$. □

B. $U_\varepsilon^{\mathrm{fin}}$-module structure on $\mathcal{V}$

For $\alpha\in\Delta_+$ we define the actions of e_α and f_α recursively by using the formulas (2.13) and (2.16) as in Sec. V A.

Proposition 5.3: For any $\alpha\in\Delta_+$ and $i\in I$, we have

$$e_\alpha^l=f_\alpha^l=0\ \text{ and }\ t_i^l=1\ \text{ on }\ \mathcal{V}. \tag{5.6}$$

Proof: Since $\Phi_{r,s,a,b}(t_i)=\varepsilon^{\lambda_i}Z_{in}^2Z_{i-1n}^{-1}Z_{i+1n}^{-1}$ on $\mathcal{V}$ and $Z_{ij}^l=1$, it is trivial that $t_i^l=1$.

To show the nilpotency of e_α and f_α, we need the following lemma:

Lemma 5.4 (Ref. 5, Proposition 3.4): For $\alpha=\alpha_i+\alpha_{i+1}+\cdots+\alpha_j$, the actions of $\overline{e}_\alpha^{\,l}$ and $\overline{f}_\alpha^{\,l}$ on $\mathcal{V}$ are given by

$$\overline{e}_\alpha^{\,l}=\frac{1}{(\varepsilon-\varepsilon^{-1})^l}\Bigg(\sum_{k_1\geqslant i,\ldots,k_{j-i+1}\geqslant j}\ \sum_{p=1}^{j-i+1}(-1)^{p-1}\theta(k_1\geqslant\cdots\geqslant k_p<\cdots<k_{j-i+1})$$

$$\times C_{ik_1\ldots k_{p-1}}(C_{i+p-1k_p}-C_{i+p-1k_p}^{-1})C_{i+pk_{p+1}\ldots k_{j-i+1}}^{-1}D_{ik_i\ldots k_{j-i+1}}\Bigg)\cdot\mathrm{id},$$

$$\overline{f}^{l}_{\alpha}=\frac{-1}{(\varepsilon-\varepsilon^{-1})^{l}}\Bigg(\sum_{k_1\geqslant n+1-j,\ldots,k_{j-1+1}\geqslant n+1-i}\ \sum_{p=1}^{j-i+1}(-1)^{p-1}\theta(k_1\geqslant\cdots\geqslant k_p<\cdots<k_{j-i+1})$$

$$\times\overline{C}_{n+1-j\ k_1\cdots k_{p-1}}(\overline{C}_{n-j+p\ k_p}-\overline{C}^{-1}_{n-j+p\ k_p})\overline{C}^{-1}_{n-j+p+1k_{p+1}\cdots k_{j-i+1}}\overline{D}_{n-j+1k_1\cdots k_{j-i+1}}\Bigg)\cdot\mathrm{id},$$

where $\theta(X)=1$ *if* X *is true and* $\theta(X)=0$ *otherwise, and we set*

$$C_{i\ k}:=(\varepsilon^{-1}r_ib_{ik}b_{ik-1}b^{-1}_{i-1k-1}b^{-1}_{i+1k})^{l}, \tag{5.7}$$

$$\overline{C}_{ik}:=(\varepsilon^{-1}s_{n-i+1}b_{k+1-i\ k}b_{k-i\ k-1}b^{-1}_{k+1-i\ k-1}b^{-1}_{k-i\ k})^{l}, \tag{5.8}$$

$$D_{ik}:=\prod_{p=k}^{n}(a_{ip})^{l},\overline{D}_{ik}:=\prod_{p=k}^{n}(a^{-1}_{p+1-ip})^{l}, \tag{5.9}$$

and $\phi_{ik_1\cdots k_p}:=\phi_{ik_1}\cdots\phi_{ik_p}$ *for* $\phi=C,\ \overline{C},\ D,\ \overline{D}$.
(Note that in the definition of $\overline{\eta}_{ik}$ [5], s_i must be changed to s_{n+1-i}.).

Applying the specializations of the parameters (4.2) and (4.4) to C_{ik} and $\overline{C}_{ik}$ we have $C_{ik}=\overline{C}_{ik}=1$ for all $1\leqslant i\leqslant k\leqslant n$, which implies that $C_{i+p-1k_p}-C^{-1}_{i+p-1k_p}=\overline{C}_{n-j+p\ k_p}-\overline{C}^{-1}_{n-j+p\ k_p}=0$ and then $\overline{e}^{l}_{\alpha}=\overline{f}^{l}_{\alpha}=0$. Since we have $e^{l}_{\alpha}=\overline{e}^{l}_{\alpha}$ and $f^{l}_{\alpha}=\overline{f}^{l}_{\alpha}$ by Lemma 5.2, we obtain that $e^{l}_{\alpha}=f^{l}_{\alpha}=0$ on $\mathcal{V}$. □

Theorem 5.5: *(i) If we define the actions of* e_α *and* f_α $(\alpha\in\Delta_+)$ *by using* (2.13) *and* (2.16), *the vector space* $\mathcal{V}$ *becomes* $U^{\mathrm{fin}}_{\varepsilon}$*-module of type 1.*

(*ii*) *The subspace* $L(\lambda)$ $(\lambda=(\lambda_1,\ldots,\lambda_n),\ \lambda_i\in\{0,1,...,l-1\})$ *is the unique irreducible* $U^{\mathrm{fin}}_{\varepsilon}$*-submodule of* $\mathcal{V}$.

Proof: To show (i), it suffices to check the relations (2.7)–(2.20) in Proposition 2.1. Relations (2.7)–(2.10) are satisfied since $\mathcal{V}$ is originally U_ε-module. Relations (2.11)–(2.18) are obtained from Lemma 5.1. We have (2.19), $t^{l}_{i}=1$ on $\mathcal{V}$ and then (2.20) from Proposition 5.3. Thus, $\mathcal{V}$ becomes a $U^{\mathrm{fin}}_{\varepsilon}$-module of type **1**.

C. Proof of irreducibility

In order to show the irreducibility of $L(\lambda)$, we need the following:

Proposition 5.6: Any finite dimensional $U^{\mathrm{fin}}_{\varepsilon}$*-module contains a primitive vector.*

To prove this proposition, we shall show the following lemma

Lemma 5.7: Let $L>0$ *be a sufficiently large integer. For any* $i_1,i_2,\ldots,i_L\in I$ *we have in* $U^{\mathrm{fin}}_{\varepsilon}$,

$$e_{i_L}\cdots e_{i_2}e_{i_1}=0. \tag{5.10}$$

Proof: We define a **Z**-gradation on $(U^{\mathrm{fin}}_{\varepsilon})^{+}$ by the following way: As we have seen in Proposition 2.2, $(U^{\mathrm{fin}}_{\varepsilon})^{+}$ has the basis

$$\{e^{r_N}_{\beta_N}e^{r_{N-1}}_{\beta_{N-1}}\cdots e^{r_1}_{\beta_1}\}_{0\leqslant r_1,\ldots r_N<l}.$$

Using this, we define

$$(U^{\mathrm{fin}}_{\varepsilon})^{+}_{d}:=\bigoplus_{r_1\,ht(\beta_1)+\cdots+r_N\,ht(\beta_N)=d}\mathbf{C}e^{r_N}_{\beta_N}e^{r_{N-1}}_{\beta_{N-1}}\cdots e^{r_1}_{\beta_1}, \tag{5.11}$$

where $ht(\beta)$ is the height of a root $\beta\in\Delta_+$. We have

$$(U^{\mathrm{fin}}_{\varepsilon})^{+}=\bigoplus_{d}(U^{\mathrm{fin}}_{\varepsilon})^{+}_{d}.$$

Since all the relations in $(U_\varepsilon^{\mathrm{fin}})^+$, that is, (2.11), (2.13), (2.14), (2.15), and (2.19) are homogeneous, this gradation is well-defined. We call an element in $(U_\varepsilon^{\mathrm{fin}})_d^+$ a *homogeneous element of degree d*. We have $(U_\varepsilon^{\mathrm{fin}})_d^+(U_\varepsilon^{\mathrm{fin}})_e^+ \subset (U_\varepsilon^{\mathrm{fin}})_{d+e}^+$ for $d, e \in \mathbf{Z}_{\geqslant 0}$ and then $e_{i_L}\cdots e_{i_2}e_{i_1}$ is a homogeneous element of degree L. It immediately follows from Proposition 2.2 that the maximum degree is $(l-1)\ \Sigma_{i=1}^N \mathrm{ht}(\beta_i) := J$, which implies that if $L>J$, $(U_\varepsilon^{\mathrm{fin}})_L^+ = 0$. Thus, if L is sufficiently large, a homogeneous element $e_{i_L}\ldots e_{i_2}e_{i_1}$ must vanish. □

Proof of Proposition 5.6: Suppose that a finite dimensional $U_\varepsilon^{\mathrm{fin}}$-module V does not have any primitive vector. So for any nonzero $v \in V$ there exists an infinite sequence $i_1, i_2, \ldots, i_k, \ldots (i_j \in I)$ such that all vectors v, $e_{i_1}v$, $e_{i_2}e_{i_1}v, \ldots, e_{i_k}\cdots e_{i_2}e_{i_1}v, \ldots$ never vanish. But this contradicts to Lemma 5.7. Therefore, V contains a primitive vector. □

Proof of Theorem 5.5 (ii): Let W be a nonzero submodule of $L(\lambda)$. By Proposition 5.6, W contains a primitive vector. By the uniqueness of the primitive vector in $\mathcal{V}$ (Proposition 4.2), W has to contain $u_0^{\sim}$. Therefore, $W = L(\lambda)$ and then $L(\lambda)$ is the unique irreducible submodule in $\mathcal{V}$. Here we completed the proof of Theorem 5.5(ii). □

By Theorem 3.6 (ii), for "l-restricted weight" $\lambda \in P_+$, the $U_\varepsilon^{\mathrm{res}}$-module $V_\varepsilon^{\mathrm{res}}(\lambda)$ (see Sec. III B) is identified with the irreducible $U_\varepsilon^{\mathrm{fin}}$-module, which is isomorphic to $L(\lambda)$. Accordingly, by Theorem 5.5 we realize the irreducible highest weight $U_\varepsilon^{\mathrm{res}}$-module $V_\varepsilon^{\mathrm{res}}(\lambda)$ with the l-restricted highest weight λ in the vector space $\mathcal{V}$.

In Ref. 14, for the B_n, C_n, and D_n cases the analogous presentations of the maximal cyclic representations are given explicitly. Thus, we can apply the procedure adopted here to them and might hope to obtain the irreducible $U_\varepsilon^{\mathrm{fin}}(B_n)$ $(U_\varepsilon^{\mathrm{fin}}(C_n), U_\varepsilon^{\mathrm{fin}}(D_n))$-modules, which will be discussed elsewhere.

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The real geometry of holomorphic four-metrics

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The real geometry of holomorphic four-metrics is investigated. The almost product and complex structures, associated with the real eight-metrics corresponding to the real and imaginary parts of the holomorphic metrics, are studied. It is shown that half-flat holomorphic metrics, and the corresponding real eight-metrics, are associated with integrable almost product, complex and hyper-Kähler structures. Real and complex local coordinate descriptions are presented. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1456947]

I. INTRODUCTION

In the approximately 25 years since the original work by Newman, Penrose and Plebánski on holomorphic half-flat four-metrics,[1–3] there have been many developments of their results.[4–6] There have also been numerous applications of this and related work to real four-metrics of Riemannian and neutral (Kleinian or ultrahyperbolic) signature.[7–9] However, the extension of the original ideas to real four-metrics of Lorentzian signature and Ricci-flat Lorentzian four-metrics remains to be fully realized, although some interesting results have been obtained. There have been promising developments in both the twistorial approach to this problem,[10,11] and in the approach of Newman and his collaborators.[12,13] There have also been some isolated results on combining self-dual and anti-self-dual solutions to obtain Ricci flat and real metrics by using Plebánski's formalism.[14–18] More references to aspects of these various lines of research can be found in a recent review.[19] This article aims to provide further background for research into the construction of real metrics from holomorphic ones by exploring, in greater detail than previously, certain aspects of the real geometry associated with holomorphic four-metrics on complex four-manifolds.

The focus in this article is on the geometry of the underlying eight dimensional real manifold and the two real eight-metrics defined by the real and imaginary parts of holomorphic four-metrics. Most research on such four-metrics focuses on their holomorphic properties. While this is clearly the natural thing to do, different and interesting insights can be obtained from the study of the geometry on the real eight-manifold. Investigations of this type were initiated in the 1970s by Rozga and Woodhouse.[20,21] This article includes an extension of that line of work, with particular attention being paid to half-flat holomorphic four-metrics and the important real structures and geometry which are related to them.

The content of the article is as follows. The Sec. II is devoted to a discussion of the complex and almost complex structures associated with a holomorphic four-metric, g, on a complex four-manifold M. All the real metrics discussed explicitly in this article will have indefinite signature, but in the interests of simplicity the term ''pseudo-'' as in, for example ''pseudo-Kähler'' will be avoided. Here, where complex four dimensional (eight real dimensional) manifolds and holomorphic four-metrics g are considered, the real metrics, $h=\mathrm{Re}\,g$ and $k=\mathrm{Im}\,g$, have neutral signature (4,4) and this simplification in terminology is unambiguous. Some previously obtained results[21–23] are included in this section for the sake of completeness. Examples are the exhibition of the anti-Kähler structure of the real metrics, h and k, and the fact that these real metrics may inherit the Einstein property of a holomorphic Einstein metric g. In the particular case of four complex dimensions being considered here, additional structures occur naturally. The real metrics, h and k, obtained from a holomorphic metric g are almost hyper-Kähler, in two distinct ways. That is, there

are two sets of three almost complex structures, which are compatible with the real metrics, so they are, in fact, almost Hermitian structures with respect to h and k, and which also satisfy quaternionic relations. These structures are determined from the holomorphic metric, certain bases of self-dual (respectively anti self-dual) holomorphic two-forms, and their complex conjugates. Together with the complex structure of the complex four-manifold these almost complex structures also determine two sets of almost product structures satisfying related, but different, algebraic relations. These almost hyper-Kähler and almost product structures, together with the real metrics, encode certain of the information contained in the holomorphic metric. Further aspects of the latter are exposed when differential, in addition to algebraic, relations are considered. In the third section half-flat holomorphic four-metrics are investigated. Since these are necessarily Ricci flat the corresponding real metrics h and k are also Ricci flat. In addition, each self-dual or anti-self-dual holomorphic metric determines bases (respectively anti-self-dual and self-dual) of three holomorphic two-forms with zero covariant exterior derivative. Hence, in the half-flat case there are triples of (covariantly constant) complex structures satisfying quaternionic relations and h and k are in fact hyper-Kähler. Furthermore, there are now triples of almost product structures which are integrable. Unified real descriptions of these structures are presented. The particular case that is dealt with focuses on anti-self-dual metrics and their real parts. However, analogous constructions apply to the imaginary parts of anti-self-dual metrics and the real or imaginary parts of self-dual four-metrics.

In Sec. IV local coordinates, adapted to an integrable almost product metric structure, (P,h), of the type discussed in Sec. III, are introduced. This coordinate formulation is like a real version of the standard local coordinate description of a Kähler metric. Next an integrable and compatible almost complex structure I is added, the system (P,h,I) is described in adapted complex coordinates, and a holomorphic metric g is naturally defined. When the condition of Ricci flatness is imposed on h, the description of g is seen to coincide with a description of half-flat holomorphic four-metrics introduced by Plebánski.[3] Hence an alternative approach to holomorphic four-metrics, via the structure (P,h,I). is provided here.

An appendix contains a brief outline of the relationship between the construction of twistor spaces for the real hyper-Kahler eight-metrics on M,[24,25] and holomorphic half-flat four-metrics.

Lower case, Latin indices $a, b, c,\ldots,i, j, k\ldots$ range and sum from 1 to 4; barred indices $\overline{a},\overline{b}, \overline{c},\ldots$ from $4+1$ to $4+4$; bold lower case Latin indices, **i**, **j**, **k** from 1 to 3; Greek indices from 1 to 8; upper-case Latin indices A,B,... from 1 to 2 and barred upper case Latin indices $\overline{A},\overline{B},\ldots$ from $2+1$ to $2+2$. Complex conjugates (c.c.) are denoted with a bar over the kernel letter. Geometrical considerations are essentially local.

II. HOLOMORPHIC FOUR-METRICS

Let M be a complex manifold with $\dim_{\mathbb{C}} M$ equal to four, and let g be a holomorphic metric on M, with line element given in complex coordinates z^i by

$$ds^2 = g_{ij}\, dz^i \otimes dz^j, \tag{1}$$

with $\partial g_{ij}/\partial \overline{z}^{\overline{k}} = 0$.

Let I denote the (real) complex structure tensor satisfying $I^2 = -1$ and $I dz^i = i dz^i$. Then

$$g(IX, IY) = -g(X, Y) \tag{2}$$

for all vector fields X and Y tangent to M.[26,27] Since $g(X,Y)$ is zero whenever X or Y is a (0,1) vector field, the metric g is degenerate. Nevertheless, when the holomorphic category only is considered, it determines in the usual way, a unique torsion free metric connection, the holomorphic Levi-Civita connection with holomorphic curvature. It is convenient here to present this metric geometry in terms of the holomorphic Cartan structure equations, using conventions which will be used later when real Lorentzn metrics are considered. These conventions are naturally adapted to two component spinor and anti-self-dual formulations.[28]

Let χ^a be a basis of holomorphic one-forms, a Cartan co-frame for g, so that the line element for g is given by

$$ds^2 = \eta_{ab}\chi^a \otimes \chi^b, \tag{3}$$

where

$$\eta_{ab} = \begin{bmatrix} 0 & \epsilon_{AB} \\ -\epsilon_{AB} & 0 \end{bmatrix}, \qquad \epsilon_{AB} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{4}$$

The complex volume element is given by

$$V = i\chi^1 \wedge \chi^2 \wedge \chi^3 \wedge \chi^4. \tag{5}$$

The first and second Cartan structure equations are given by

$$d\chi^a - \chi^b \wedge A^a_b = 0, \qquad A_{ab} + A_{ba} = 0, \tag{6}$$

and

$$dA^a_b + A^a_c \wedge A^c_b = -\tfrac{1}{2} F^a_{bcd} \chi^c \wedge \chi^d. \tag{7}$$

Here A^a_b denotes the holomorphic Levi-Civita connection one-form (with covariant derivative ∇), and F^a_{bcd} are the components of its curvature two-form F^a_b. The structure group is SO(4,C) and the connection and curvature forms, which take values in the Lies algebra so(4,C), can be written as the sum of their self-dual and anti-self-dual parts, ${}^+A^a_b, {}^-A^a_b, {}^+F^a_b, {}^-F^a_b$, respectively. Here, $*{}^+F^a_b = i\,{}^+F^a_b$, $*{}^-F^a_b = -i\,{}^-F^a_b$. In 4×4 matrix form

$${}^+A^a_b = \begin{bmatrix} \varpi^{0'}_{0'} 1 & \varpi^{0'}_{1'} 1 \\ \varpi^{1'}_{0'} 1 & -\varpi^{0'}_{0'} 1 \end{bmatrix}, \tag{8}$$

where here 1 is the unit 2×2 matrix and $\varpi^{0'}_{0'}$, $\varpi^{0'}_{1'}$, $\varpi^{1'}_{0'}$ denote the independent components of ${}^+A^a_b$. Similarly,

$${}^-A^a_b = \begin{bmatrix} \omega^A_B & 0 \\ 0 & \omega^A_B \end{bmatrix}, \tag{9}$$

where the trace of the 2×2 matrix (ω^A_B) is zero. Other self-dual and anti-self-dual objects can be written similarly, for instance,

$${}^-F^a_b = \begin{bmatrix} \Omega^A_B & 0 \\ 0 & \Omega^A_B \end{bmatrix}, \tag{10}$$

where

$$\Omega^A_B = d\omega^A_B + \omega^A_C \wedge \omega^C_B. \tag{11}$$

The structure group SO(4,C) is isomorphic to $\{\mathrm{SL}(2,\mathrm{C})_L \times \mathrm{SL}(2,\mathrm{C})_R\}/Z_2$. The self-dual connection and curvature take values in the Lie algebra $\mathrm{sl}(2,C)_R$ and the anti-self-dual connection and curvature take values in the Lie algebra $\mathrm{sl}(2,\mathrm{C})_L$.

The basis of self-dual holomorphic two-forms, given by

$$
\begin{aligned}
{}^{+}\Sigma^{\mathbf{1}} &= \chi^2 \wedge \chi^1 + \chi^4 \wedge \chi^3, \\
{}^{+}\Sigma^{\mathbf{2}} &= i(\chi^1 \wedge \chi^4 + \chi^3 \wedge \chi^2), \\
{}^{+}\Sigma^{\mathbf{3}} &= i(\chi^1 \wedge \chi^2 + \chi^4 \wedge \chi^3),
\end{aligned}
\tag{12}
$$

defines three holomorphic tensor fields ${}^{+}\mathbb{J}^{\mathbf{i}}$ by

$$
g(X, {}^{+}\mathbb{J}^{\mathbf{i}}(Y)) = {}^{+}\Sigma^{\mathbf{i}}(X,Y) \tag{13}
$$

for any holomorphic vector fields X and Y. It is a straightforward matter to show that

$$
({}^{+}\mathbb{J}^{\mathbf{1}})^2 = ({}^{+}\mathbb{J}^{\mathbf{2}})^2 = ({}^{+}\mathbb{J}^{\mathbf{3}})^2 = -\mathbb{I}, \tag{14}
$$

where $\mathbb{I}$ is the unit operator, and

$$
{}^{+}\mathbb{J}^{\mathbf{1}} {}^{+}\mathbb{J}^{\mathbf{2}} = {}^{+}\mathbb{J}^{\mathbf{3}}, \quad {}^{+}\mathbb{J}^{\mathbf{2}} {}^{+}\mathbb{J}^{\mathbf{3}} = {}^{+}\mathbb{J}^{\mathbf{1}}, \quad {}^{+}\mathbb{J}^{\mathbf{3}} {}^{+}\mathbb{J}^{\mathbf{1}} = {}^{+}\mathbb{J}^{\mathbf{2}}, \tag{15}
$$

$$
g({}^{+}\mathbb{J}^{\mathbf{1}}X, {}^{+}\mathbb{J}^{\mathbf{1}}Y) = g({}^{+}\mathbb{J}^{\mathbf{2}}X, {}^{+}\mathbb{J}^{\mathbf{2}}Y) = g({}^{+}\mathbb{J}^{\mathbf{3}}X, {}^{+}\mathbb{J}^{\mathbf{3}}Y) = g(X,Y), \tag{16}
$$

for all holomorphic vector fields X and Y. The basis of anti-self-dual holomorphic two-forms given by

$$
\begin{aligned}
{}^{-}\Sigma^{\mathbf{1}} &= \chi^3 \wedge \chi^1 + \chi^4 \wedge \chi^2, \\
{}^{-}\Sigma^{\mathbf{2}} &= i(\chi^4 \wedge \chi^1 + \chi^3 \wedge \chi^2), \\
{}^{-}\Sigma^{\mathbf{3}} &= i(\chi^2 \wedge \chi^4 + \chi^3 \wedge \chi^1),
\end{aligned}
\tag{17}
$$

define, as above, three holomorphic tensor fields, ${}^{-}\mathbb{J}^{\mathbf{i}}$, by

$$
g(X, {}^{-}\mathbb{J}^{\mathbf{i}}(Y)) = {}^{-}\Sigma^{\mathbf{i}}(X,Y), \tag{18}
$$

and these satisfy equations of the same form as Eqs. (14)–(16).

The real and imaginary parts, h and k, of the holomorphic metric $g = h + ik$ are two real metrics on the real eight dimensional manifold M. In terms of the complex co-frame of eight one-forms $(\chi^a, \overline{\chi}^a)$ on M, the line element of h is given by

$$
{}_h ds^2 = \tfrac{1}{2}\, \eta_{ab}(\chi^a \otimes \chi^b + \overline{\chi}^a \otimes \overline{\chi}^b), \tag{19}
$$

and the line element of k is given by

$$
{}_k ds^2 = \frac{i}{2}\, \eta_{ab}(-\chi^a \otimes \chi^b + \overline{\chi}^a \otimes \overline{\chi}^b). \tag{20}
$$

The two real metrics have Kleinian (neutral or ultrahyperbolic) signatures (4,4). The covariant derivatives corresponding to the Levi-Civita connections of h and k, ${}_h\nabla$ and ${}_k\nabla$, respectively, are each determined by the same connection one-forms[21]

$$
\begin{bmatrix} A^a_b & 0 \\ 0 & \overline{A}^a_b \end{bmatrix}. \tag{21}
$$

When g is Einstein, that is, when

$$F^{a}_{bad} = \tfrac{1}{4} F \eta_{bd}\,, \tag{22}$$

then h is Einstein if and only if $\mathrm{Im}\, F$ is zero and k is Einstein if and only if $\mathrm{Re}\, F$ is zero, cf. Refs. 22 and 23.

Both real metrics are anti-Hermitian with respect to the complex structure I, that is, for all real vector fields X and Y on M,

$$h(IX,IY) = -h(X,Y); k(IX,IY) = -k(X,Y). \tag{23}$$

Moreover, since

$${}_h\nabla I = {}_k\nabla I = 0, \tag{24}$$

the two real metrics are, in fact, anti-Kähler[21–23] with respect to the complex structure I. They are, of course, related, with the metric k in the anti-Kähler case replacing the two-form of the Kähler case; for any two real vector fields X and Y

$$k(X,Y) = -h(IX,Y). \tag{25}$$

The holomorphic tensor fields ${}^{+}\mathbb{J}^{\mathbf{i}}$ and ${}^{-}\mathbb{J}^{\mathbf{i}}$ defined above can be naturally extended to real tensor fields which satisfy relations like those in Eqs. (14)–(16) above. Define the real tensor fields ${}^{+}J^{\mathbf{i}}$ by

$$h(X, {}^{+}J^{\mathbf{i}}(Y)) = \tfrac{1}{2}({}^{+}\Sigma^{\mathbf{i}} + {}^{+}\overline{\Sigma^{\mathbf{i}}})(X,Y) \tag{26}$$

for X and Y any vector fields tangent to M. Here, and in the following, ${}^{+}\overline{\Sigma^{\mathbf{i}}}$ denotes the complex conjugate of ${}^{+}\Sigma^{\mathbf{i}}$. Then, if α and X are, respectively, a real one-form and vector field on M, with (1,0) parts denoted respectively by $\alpha_{(1,0)}$ and $X_{(1,0)}$, so that $\alpha = \alpha_{(1,0)} + \text{c.c.}$ and $X = X_{(1,0)} + \text{c.c.}$,

$${}^{+}J^{\mathbf{i}}(\alpha, X) = {}^{+}\mathbb{J}^{\mathbf{i}}(\alpha_{(1,0)}, X_{(1,0)}) + \text{c.c.} \tag{27}$$

When h is replaced by k in the left hand side of Eq. (25) the result is the following equation:

$$k(X, {}^{+}J^{\mathbf{i}}(Y)) = \frac{i}{2}(-{}^{+}\Sigma^{\mathbf{i}} + {}^{+}\overline{\Sigma^{\mathbf{i}}})(X,Y). \tag{28}$$

The holomorphic tensor fields ${}^{-}\mathbb{J}^{\mathbf{i}}$ can be extended to the real tensor fields ${}^{-}J^{\mathbf{i}}$ in a similar way.

Both ${}^{+}J^{\mathbf{i}}$ and ${}^{-}J^{\mathbf{i}}$ are triplets of almost complex structures and both h and k are Hermitian with respect to each of these almost complex structures. Furthermore, the almost complex structures satisfy a quaternionic algebra; that is, each of the triplets ${}^{+}J^{\mathbf{i}}$ and ${}^{-}J^{\mathbf{i}}$ separately satisfies the set of equations

$$\begin{gathered}
(J^{\mathbf{1}})^2 = (J^{\mathbf{2}})^2 = (J^{\mathbf{3}})^2 = -1, \\
J^{\mathbf{1}}J^{\mathbf{2}} = J^{\mathbf{3}}, \quad J^{\mathbf{2}}J^{\mathbf{3}} = J^{\mathbf{1}}, \quad J^{\mathbf{3}}J^{\mathbf{1}} = J^{\mathbf{2}}, \\
h(J^{\mathbf{1}}X, J^{\mathbf{1}}Y) = h(J^{\mathbf{2}}X, J^{\mathbf{2}}Y) = h(J^{\mathbf{3}}X, J^{\mathbf{3}}Y) = h(X,Y), \\
k(J^{\mathbf{1}}X, J^{\mathbf{1}}Y) = k(J^{\mathbf{2}}X, J^{\mathbf{2}}Y) = k(J^{\mathbf{3}}X, J^{\mathbf{3}}Y) = k(X,Y).
\end{gathered} \tag{29}$$

In other words, the eight dimensional real manifold M is almost quaternion and each of $(M,h,J^{\mathbf{i}})$ and $(M,k,J^{\mathbf{i}})$ are almost quaternionic metric structures.[27,29]

By interchanging h and k in Eqs. (26) and (28) a second set of real tensor fields, ${}^{+}P^{\mathbf{i}}$ and ${}^{-}P^{\mathbf{i}}$ which are almost product, almost anti-Hermitian structures, rather than almost complex, almost-Hermitian structures, can be defined. Let ${}^{+}P^{\mathbf{i}}$ be defined by

$$k(X,{}^{+}P^{\mathbf{i}}(Y))=\tfrac{1}{2}({}^{+}\Sigma^{\mathbf{i}}+{}^{+}\overline{\Sigma}^{\mathbf{i}})(X,Y) \tag{30}$$

or, equivalently,

$${}^{+}P^{\mathbf{i}}(\alpha,X)=i\,{}^{+}J^{\mathbf{i}}(\alpha_{(1,0)},X_{(1,0)})+\text{c.c.} \tag{31}$$

with the notation as above. It then follows, analogously to Eq. (28), that

$$h(X,{}^{+}P^{i}(Y))=\frac{i}{2}({}^{+}\Sigma^{\mathbf{i}}-{}^{+}\overline{\Sigma}^{\mathbf{i}})(X,Y). \tag{32}$$

Here ${}^{-}P^{\mathbf{i}}$ can be defined in a similar way and satisfies equations parallel to Eqs. (30)–(32). In terms of their components with respect to the co-frame $(\chi^{a},\chi^{\overline{a}})$ and its dual basis of vector fields, these operators are given by

$$I=i\begin{bmatrix}\delta^{a}_{b} & 0\\ 0 & -\delta^{a}_{b}\end{bmatrix},\quad {}^{+}J^{\mathbf{i}}=\begin{bmatrix}{}^{+}\mathbb{J}^{\mathbf{i}} & 0\\ 0 & {}^{+}\overline{\mathbb{J}^{\mathbf{i}}}\end{bmatrix},\quad {}^{+}P^{i}=i\begin{bmatrix}{}^{+}\mathbb{J}^{\mathbf{i}} & 0\\ 0 & -{}^{+}\overline{\mathbb{J}^{\mathbf{i}}}\end{bmatrix}, \tag{33}$$

and similarly for ${}^{-}J^{\mathbf{i}}$ and ${}^{-}P^{\mathbf{i}}$. The algebraic relationships between these real tensors, for short I, $J^{\mathbf{i}}$ and $P^{\mathbf{i}}$, can be summarized in the following equations,

$$\begin{gathered}IJ^{\mathbf{i}}=J^{\mathbf{i}}I=P^{\mathbf{i}},\\ IP^{\mathbf{i}}=-J^{\mathbf{i}},\\ J^{\mathbf{i}}P^{\mathbf{j}}=P^{\mathbf{i}}J^{\mathbf{j}}=-I\delta^{\mathbf{ij}}+\varepsilon^{\mathbf{ijk}}P^{\mathbf{k}},\end{gathered} \tag{34}$$

where in each equation $J^{\mathbf{i}}$ and $P^{\mathbf{i}}$ are both self-dual or both anti-self-dual. The self-dual and anti-self-dual operators commute. Both ${}^{+}P^{\mathbf{i}}$ and ${}^{-}P^{\mathbf{i}}$ are almost product rather than almost complex structures,[27] and satisfy algebraic equations which are generalizations of the quaternionic equations. They also satisfy almost anti-Hermitian rather than almost-Hermitian relations with the real metrics; altogether

$$\begin{gathered}(P^{\mathbf{1}})^{2}=(P^{\mathbf{2}})^{2}=(P^{\mathbf{3}})^{2}=1,\\ P^{1}P^{\mathbf{2}}=IP^{\mathbf{3}},\quad P^{\mathbf{2}}P^{\mathbf{3}}=IP^{\mathbf{1}},\quad P^{\mathbf{3}}P^{\mathbf{1}}=IP^{\mathbf{2}},\\ h(P^{\mathbf{1}}X,P^{\mathbf{1}}Y)=h(P^{\mathbf{2}}X,P^{\mathbf{2}}Y)=h(P^{\mathbf{3}}X,P^{\mathbf{3}}Y)=-h(X,Y),\\ k(P^{\mathbf{1}}X,P^{\mathbf{1}}Y)=k(P^{\mathbf{2}}X,P^{\mathbf{2}}Y)=k(P^{\mathbf{3}}X,P^{\mathbf{3}}Y)=-k(X,Y).\end{gathered} \tag{35}$$

Since g is a *four-metric*, it always follows that

$$\nabla\,{}^{+}\mathbb{J}^{\mathbf{1}}=-{}^{+}\mathcal{A}^{\mathbf{1}}_{\mathbf{i}}\,{}^{+}\mathbb{J}^{\mathbf{i}},\quad \nabla\,{}^{+}\mathbb{J}^{\mathbf{2}}=-{}^{+}\mathcal{A}^{\mathbf{2}}_{\mathbf{i}}\,{}^{+}\mathbb{J}^{\mathbf{i}},\quad \nabla\,{}^{+}\mathbb{J}^{\mathbf{3}}=-{}^{+}\mathcal{A}^{\mathbf{3}}_{\mathbf{i}}\,{}^{+}\mathbb{J}^{\mathbf{i}}, \tag{36}$$

where the so(3,C) -valued one-form ${}^{+}\mathcal{A}^{\mathbf{i}}_{\mathbf{j}}$, is the so(3,C)-valued representation of the self-dual part of the Levi-Civita spin connection. Similar equations holds for the anti-self-dual objects. From these equations it follows that, for $\mathbf{i}=1,2,3$ separately,

$${}_{h}\nabla_{\gamma}({}^{+}J^{\mathbf{i}\alpha}_{\beta})={}_{k}\nabla_{\gamma}({}^{+}J^{\mathbf{i}\alpha}_{\beta})=\begin{bmatrix}-{}^{+}\mathcal{A}^{\mathbf{i}}_{\mathbf{j}\gamma}\,{}^{+}\mathbb{J}^{\mathbf{j}a}_{b} & 0\\ 0 & \text{c.c.}\end{bmatrix} \tag{37}$$

[in components with respect to the complex bases and where c.c. denotes the complex conjugate of $-({}^{+}\mathcal{A}^{\mathbf{i}}_{\mathbf{j}\gamma}\ {}^{+}\mathbb{J}^{\mathbf{j}a}_{b})$]. Similar results hold in the anti-self-dual case. Hence when a gauge can be found in which the components of ${}^{+}\mathcal{A}^{\mathbf{i}}_{\mathbf{j}}$ are real (and hence constant) so that ${}^{+}\mathcal{A}^{\mathbf{i}}_{\mathbf{j}}$ takes values in so(3,R), the triples (M, h, ${}^{+}J^{\mathbf{i}}$) and (M, k, ${}^{+}J^{\mathbf{i}}$) constitute a quaternion Kähler structure and the metrics are Einstein metrics.[29,30] Similar results hold, of course, when the anti-self-dual case is considered.

III. HALF-FLAT ANTI-SELF-DUAL FOUR-METRICS

In this section half-flat, anti-self-dual four-metrics, g, on M will be considered. (In both the self-dual and the anti-self-dual case, the Levi-Civita connection of the corresponding real metrics h and k is determined by the real so(1,3) connection given by twice the real part of the holomorphic Levi-Civita connection of g. There is only one real connection.) Since the self-dual part of the curvature of a holomorphic half-flat anti-self-dual metric is zero, ${}^{+}F^{a}_{b}=0$, a co-frame can be chosen in which ${}^{+}A^{a}_{b}=0$. In this gauge $d^{+}\Sigma^{\mathbf{i}}=0$, and the tensors, defined by Eq. (13), are covariantly constant,

$$\nabla^{+}\mathbb{J}^{\mathbf{i}}=0. \tag{38}$$

It then follows from Eqs. (36) and (37), and then (24) and (34), that the real tensors, defined by Eqs. (26) and (30), are covariantly constant with respect to the Levi-Civita covariant derivatives of the Ricci flat eight-metrics h and k. Relationships between the various structures discussed in this section can be summarized in three propositions which it is a straightforward matter to prove. The first is due to Woodhouse.[21–23]

Proposition 1: Let h be a real eight-metric of signature (4,4) on a real eight dimensional manifold M. Let h be anti-Hermitian with respect to an almost complex structure I. Then I is a complex structure and the tensor g given by the equation

$$g(X,Y)=h(X,Y)-ih(IX,Y)$$

is holomorphic (a holomorphic metric) with respect to the complex structure I if and only if ${}_{h}\nabla I=0$.

Proposition 2: If the conditions and conclusions of Lemma 1 hold, and in addition there is a hyper-Kähler structure (M, h, $J^{\mathbf{i}}$) with $IJ^{\mathbf{i}}=J^{\mathbf{i}}I$, then

(a) $J^{\mathbf{i}}=\mathbb{J}^{\mathbf{i}j}_{k}\partial/\partial z^{j}\otimes dz^{k}+$c.c., for some complex $\mathbb{J}^{\mathbf{i}j}_{k}$, where $I\partial/\partial z^{j}=i\partial/\partial z^{j}$.
(b) For each $\mathbf{i}=1,2,3$, ${}_{g}\nabla\mathbb{J}^{\mathbf{i}}=0$, and $g(\mathbb{J}^{\mathbf{i}}\partial/\partial z^{j},\mathbb{J}^{\mathbf{i}}\partial/\partial z^{k})=g(\partial/\partial z^{j},\partial/\partial z^{k})$.
(c) The holomorphic metric g is half-flat.
(d) (M, $k=\mathrm{Im}\,g$,$J^{\mathbf{i}}$) is also hyper-Kähler, $\nabla_{k}J^{\mathbf{i}}=0$.
(e) The hyper-Kähler structures are Ricci flat.

The results of Proposition 2 can be reformulated in terms of three almost product structures $P^{\mathbf{i}}$.

Proposition 3: If the conditions and conclusions of Lemma 1 hold, and in addition there are three almost product structures $P^{\mathbf{i}}$ which satisfy the conditions $P^{\mathbf{i}}P^{\mathbf{j}}=\epsilon^{\mathbf{ijk}}IP^{\mathbf{k}}$, $h(P^{\mathbf{i}}X,P^{\mathbf{i}}Y)=-h(X,Y)$, $\nabla_{h}P^{\mathbf{i}}=0$ and $IP^{\mathbf{i}}=P^{\mathbf{i}}I$, then the tensors $J^{\mathbf{i}}=-IP^{\mathbf{i}}$ satisfy the conditions of Lemma 2 and hence determine a holomorphic half-flat metric g and Ricci-flat hyper-Kähler structures (M, h, $J^{\mathbf{i}}$) and (M, k, $J^{\mathbf{i}}$) on the eight dimensional real manifold M.

Results from this and the previous section will be used later and it is useful to summarize them in a convenient form, which starts here with the almost product structures. For the sake of explicitness structures arising from anti-self-dual half-flat holomorphic metrics, $g=h+ik$, will be given, but there are similar equations for self-dual holomorphic metrics.

First consider the almost product structures ${}^{+}P^{\mathbf{i}}$, with components given in Eq. (33),

$$ {}^{+}P^{\mathbf{i}} = i\begin{bmatrix} {}^{+}\mathbb{J}^{\mathbf{i}} & 0 \\ 0 & -\overline{{}^{+}\mathbb{J}^{\mathbf{i}}} \end{bmatrix}. \tag{39} $$

Let P denote the almost product structure (strictly the two complex parameter family of almost product structures)

$$ P = i\begin{bmatrix} a_{\mathbf{i}}{}^{+}\mathbb{J}^{\mathbf{i}} & 0 \\ 0 & -\overline{a_{\mathbf{i}}{}^{+}\mathbb{J}^{\mathbf{i}}} \end{bmatrix} \tag{40} $$

for any *complex* numbers $a_{\mathbf{i}}$ satisfying the equation

$$ (a_{\mathbf{1}})^2 + (a_{\mathbf{2}})^2 + (a_{\mathbf{3}})^2 = 1. \tag{41} $$

Then the results given in the propositions above for almost product structures ${}^{+}P^{\mathbf{i}}$, and complex structure I, associated with an anti-self-dual holomorphic half-flat metric g, can be summarized by the equations

$$ (P)^2 = 1, \tag{42} $$

$$ h(PX,PY) = -h(X,Y), \quad k(PX,PY) = -k(X,Y), \tag{43} $$

$$ {}_{h}\nabla P = 0, \quad {}_{k}\nabla P = 0, \tag{44} $$

$$ (I)^2 = -1, \quad PI = IP, \tag{45} $$

$$ h(IX,IY) = -h(X,Y), \quad k(IX,IY) = -k(X,Y), \tag{46} $$

$$ {}_{h}\nabla I = 0, \quad {}_{k}\nabla I = 0, \tag{47} $$

where X and Y are any vectors tangent to M. Furthermore, h and k are Ricci flat. Conversely, Eqs. (42)–(47) imply that the complex metric $g = h + ik$ is a holomorphic four-metric and half-flat, and the eight-metrics h and k are Ricci flat. A local coordinate description of the geometry determined by a single triple consisting of an almost product structure P, an almost complex structure I and a metric h, satisfying Eqs. (42)–(47), will be given in Sec. IV.

It follows from Eqs. (42)–(47) that the almost complex structure J (here strictly a two complex parameter family) defined by

$$ J = -IP, \tag{48} $$

satisfies the equations

$$ \begin{gathered} J^2 = -1, \\ JP = PJ, \quad JI = IJ, \\ h(JX,JY) = h(X,Y), \quad k(JX,JY) = k(X,Y), \\ {}_{h}\nabla J = 0, \quad {}_{k}\nabla J = 0. \end{gathered} \tag{49} $$

A two complex parameter family of Kähler structures, (J,h), so defined, determines the hyper-Kähler structures mentioned above. These results, with the parameters $a_{\mathbf{i}}$ real, are used in the twistor construction reviewed in the Appendix.

Finally, it is interesting to note that all Eqs. (42)–(49) can be rewritten in terms of a four real parameter family of tensors $T(\alpha_{\mathbf{i}},\beta_{\mathbf{j}})$. Define this family of real tensors by

$$T \equiv (\alpha_{\mathbf{i}} + \beta_{\mathbf{i}} I) J^{\mathbf{i}}, \tag{50}$$

where $\alpha_{\mathbf{i}}$ and $\beta_{\mathbf{i}}$ are real parameters satisfying the conditions

$$\alpha_{\mathbf{i}} \beta_{\mathbf{j}} \delta^{\mathbf{ij}} = 0,$$

$$\varepsilon \equiv \alpha_{\mathbf{i}} \alpha_{\mathbf{j}} \delta^{\mathbf{ij}} - \beta_{\mathbf{i}} \beta_{\mathbf{j}} \delta^{\mathbf{ij}},$$

for fixed ε, or, equivalently, the conditions

$$\text{if } a_{\mathbf{i}} = \alpha_{\mathbf{i}} + i \beta_{\mathbf{i}}, \text{ then} (a_{\mathbf{1}})^2 + (a_{\mathbf{2}})^2 + (a_{\mathbf{3}})^2 = \varepsilon. \tag{51}$$

Equations (41)–(49) imply, for all vector fields X and Y, that

$$\begin{gathered} T^2 = -\varepsilon, \\ h(TX, TY) = \varepsilon h(X, Y), \\ k(TX, TY) = \varepsilon k(X, Y), \\ {}_h\nabla T = 0, \quad {}_k\nabla T = 0. \end{gathered} \tag{52}$$

It follows from these equations that, when ε is nonzero, that

$$\begin{gathered} I = -\varepsilon^{-1} T(\alpha_{\mathbf{i}}, \beta_{\mathbf{j}}) T(-\beta_{\mathbf{i}}, \alpha_{\mathbf{j}}), \\ \text{for each } \mathbf{i}\text{: } J^{\mathbf{i}} = T(\alpha^{\mathbf{i}} = 1, \beta^{\mathbf{i}} = 0) = -IT(\alpha^{\mathbf{i}} = 0, \beta^{\mathbf{i}} = 1). \end{gathered} \tag{53}$$

Structures of similar types have been considered by Dunajski.[31,32]

IV. LOCAL COORDINATE DESCRIPTION OF A STRUCTURE (P, h, I)

In this section local coordinate descriptions are given of the geometry represented by a *single* triple (P, h, I) which satisfies Eqs. (42)–(47) of Sec. III. It is shown that when the Ricci tensor of h is zero, such a geometry defines a holomorphic half-flat metric. The aim here is to show, using local coordinates, the effect of a sequential introduction of these structures and the implementation of the equations. Equations (42)–(44) are used first to introduce coordinates adapted to the almost product structure P, and to derive a description of the integrable almost product structure P, and the eight-metric h, in these coordinates. Equations (45)–(47) are then used to introduce complex coordinates adapted to both P and I, and then the triple (P, h, I) is expressed in terms of these coordinates. (Similar calculations could be carried out using the metric k and/or the parallel results associated with self-dual holomorphic metrics.) Finally, a holomorphic half-flat metric is identified.

Equation (44), the vanishing of the covariant derivative of the almost product structure P, implies that the Nijenhuis tensor of P is also zero.[27,33] Hence P is integrable. Standard arguments, analogous to those which can be used for Kähler metrics, can now be applied to construct a local coordinate system adapted to the geometrical structure determined by Eqs. (42)–(44). First, it follows from Eqs. (42) that the eigenvalues of P are 1 or -1. At each point of M the eigenvectors corresponding respectively to the eigenvalues 1 and -1 span complementary distributions, D_1 and D_2, of dimensions d_1 and d_2 say, where $d_1 + d_2 = \dim \mathrm{M}$. The dimensions of the two distributions can be different but here it suffices to consider the case where they are equal. The ideas then apply to even dimensional manifolds but here of course dim M equal eight. Let $(e_\alpha) = (e_a, e_{\bar{a}})$ be a basis of real tangent vectors to M, adapted to the almost product structure so that (e_a) span D_1 and $(e_{\bar{a}})$ span D_2; lower case barred Latin indices range and sum over $4+1$ to $4+4$. It follows from Eqs. (42) and (43) that a real two-form, Π, is defined by the equations

$$\Pi(X,Y)=h(X,PY), \tag{54}$$

for all vector fields X and Y, and that the components of h, with respect to the basis of vector fields $(e_a,e_{\bar a})$, are given by

$$h=\begin{bmatrix} 0 & h_{a\bar b} \\ h_{\bar a b} & 0 \end{bmatrix} \tag{55}$$

where $h_{\bar a b}=h_{b\bar a}$. The vanishing of the Nijenhuis tensor of P is equivalent to integrability of the two complementary distributions,[27,33] D_1 and D_2. Hence adapted local coordinates $u^\alpha=(u^a,u^{\bar a})$ can be introduced on M and the adapted bases chosen to be coordinate bases so that $e_a=\partial/\partial u^a$ and $e_{\bar a}=\partial/\partial u^{\bar a}$. The vanishing of the covariant derivative of P implies that Π is closed and therefore a local potential function, H, exists such that

$$h_{a\bar b}=\partial^2 H/\partial u^a \partial u^{\bar b}\equiv H_{,a\bar b}. \tag{56}$$

Consequently, the line element of h is given, in these coordinates, by

$${}_h ds^2=h_{\alpha\beta}du^\alpha\otimes du^\beta=H_{,a\bar b}(du^a\otimes du^{\bar b}+du^{\bar b}\otimes du^a). \tag{57}$$

Neither the coordinates nor the potential are unique. In these coordinates

$$\Pi=-2H_{,a\bar b}du^a\wedge du^{\bar b}, \tag{58}$$

and

$$P^\alpha_\beta=\begin{bmatrix} \delta^a_b & 0 \\ 0 & -\delta^{\bar a}_{\bar b} \end{bmatrix}. \tag{59}$$

It is a straightforward matter to compute the curvature tensor of the metric given by Eq. (57). Here it is convenient to employ the first and second sets of Cartan structure equations using the adapted coordinate basis of one-forms $du^\alpha=(du^a,du^{\bar a})$. The first set of Cartan structure equations,

$$\begin{aligned} \Gamma^\alpha_{\beta\gamma}du^\gamma&=\Gamma^\alpha_{\gamma\beta}du^\gamma, \\ dh_{\alpha\beta}&=h_{\alpha\sigma}\Gamma^\sigma_\beta+h_{\sigma\beta}\Gamma^\sigma_\alpha, \end{aligned} \tag{60}$$

reduces to the equation

$$dh_{a\bar b}=h_{c\bar b}\Gamma^c_a+h_{a\bar c}\Gamma^{\bar c}_{\bar b}, \tag{61}$$

and the only nonzero Levi-Civita connection one-forms are

$$\begin{aligned} \Gamma^a_b&=\Gamma^a_{bc}du^c=h^{a\bar d}H_{,bc\bar d}du^c, \\ \Gamma^{\bar a}_{\bar b}&=\Gamma^{\bar a}_{\bar b c}du^{\bar c}=h^{d\bar a}H_{,d\bar b\bar c}du^{\bar c}. \end{aligned} \tag{62}$$

Here $h^{a\bar d}=h^{\bar d a}$, and $h^{a\bar d}h_{\bar d b}=\delta^a_b$, $h^{d\bar a}h_{\bar b d}=\delta^{\bar a}_{\bar b}$.

The second set of Cartan structure equations,

$$d\Gamma^\alpha_\beta+\Gamma^\alpha_\sigma\wedge\Gamma^\sigma_\beta=-\tfrac{1}{2}R^\alpha_{\beta\gamma\delta}du^\gamma\wedge du^\delta, \tag{63}$$

reduces to

$$d\Gamma^a_b+\Gamma^a_c\wedge\Gamma^c_b=-R^a_{bc\bar{d}}du^c\wedge du^{\bar{d}},$$
$$d\Gamma^{\bar{a}}_{\bar{b}}+\Gamma^{\bar{a}}_{\bar{c}}\wedge\Gamma^{\bar{c}}_{\bar{b}}=-R^{\bar{a}}_{\bar{b}c\bar{d}}du^{\bar{c}}\wedge du^d. \tag{64}$$

The nonzero components of the curvature tensor in this basis are given by

$$R^a_{bc\bar{d}}=-R^a_{b\bar{d}c}=\Gamma^a_{bc,\bar{d}},$$
$$R^{\bar{a}}_{\bar{b}c\bar{d}}=-R^{\bar{a}}_{\bar{b}d\bar{c}}=\Gamma^{\bar{a}}_{\bar{b}\bar{c},d}. \tag{65}$$

The only components of the Ricci tensor, $R_{\beta\delta}=R^\alpha_{\beta\alpha\delta}$, of this curvature tensor which are not identically zero are

$$R_{b\bar{d}}=R^a_{ba\bar{d}}=[h^{a\bar{c}}(H,_{a\bar{c}b})],_{\bar{d}}=[\ln|\det(H,_{a\bar{c}})|],_{b\bar{d}},$$
$$R_{\bar{b}d}=R^{\bar{a}}_{\bar{b}a\bar{d}}=[h^{\bar{a}d}(H,_{\bar{a}d\bar{b}})],_d=[\ln|\det(H,_{a\bar{c}})|],_{d\bar{b}}. \tag{66}$$

In the Ricci flat case the function H must satisfy a Monge–Ampère equation, $\det(H,_{a\bar{b}})=\exp[B(u^{\bar{a}})+C(u^a)]$, where B and C are arbitrary functions of their arguments. By choice of coordinates the right hand side can be set equal to a constant so that the condition of Ricci flatness of the metric h becomes

$$\det(H,_{a\bar{b}})=\text{const.} \tag{67}$$

It should be noted that the condition that the covariant derivative of P be zero is now also satisfied.

[It is also interesting to note, as an aside, the following. Let N be a four dimensional real submanifold of M, given locally by the level sets $u^a-u^{\bar{a}}=0$. It follows from Eqs. (60) that the connection one-forms Γ^a_b and $\Gamma^{\bar{a}}_{\bar{b}}$ both pull back to define symmetric affine connections on N. When the holonomy group of the pulled-back connections is contained in $\mathrm{SO}(p,q)$, the connections are the Levi-Civita connections of four-metrics on N of signature (p,q).[34] Furthermore, Eqs. (64)–(66), and the appropriate pullbacks to N, imply that these connections are Ricci flat when h is Ricci flat. In the special cases where H is a function only of the four real variables $u^a+u^{\bar{a}}$, that is, h has four Killing vector fields, $\partial/\partial u^a-\partial/\partial u^{\bar{a}}$, and h is also Ricci flat, the eight-metric h pulls back to four-metrics on N given, in local coordinates u^a on N, by ${}_hds^2_N=(\partial^2H/\partial u^a\partial u^b)(du^a\otimes du^b+du^b\otimes du^a)$, where $\det(\partial^2H/\partial u^a\partial u^b)$ is a constant which can be chosen to be one. Such four-metrics belong to a class first considered by Calabi,[35,36] and are formally similar to a class of metrics which are of interest in stochastic geometry.[37] In general, they will not be Ricci flat.]

So far only Eqs. (42)–(44) have been used in the main discussion in this section. Now consider the implementation of Eqs. (45)–(47). It follows from Eq. (45) that, in adapted local coordinates, the almost complex structure I must have components of the form

$$I^\alpha_\beta=\begin{bmatrix} I^a_b & 0 \\ 0 & I^{\bar{a}}_{\bar{b}} \end{bmatrix}, \tag{68}$$

where $I^a_bI^b_c=-\delta^a_c$ and $I^{\bar{a}}_{\bar{b}}I^{\bar{b}}_{\bar{c}}=-\delta^{\bar{a}}_{\bar{c}}$. It follows from Eq. (46) that $h_{\alpha\gamma}I^\gamma_\beta=I_{\alpha\beta}=I_{\beta\alpha}$, where

$$I_{\alpha\beta}=\begin{bmatrix} 0 & I^c_ah_{c\bar{b}} \\ I^{\bar{c}}_{\bar{a}}h_{\bar{c}b} & 0 \end{bmatrix}. \tag{69}$$

Equations (47) now imply that the four dimensional integral manifolds of D_1 and D_2 each admit integrable complex structures I_1 and I_2 with components given respectively by I^a_b and $I^{\bar{a}}_{\bar{b}}$. In fact, Eqs. (47) take the form

$$\begin{aligned} &\partial_c I^a_b - I^a_s \Gamma^s_{bc} + I^s_b \Gamma^a_{sc} = 0, \quad \partial_{\bar{c}} I^a_b = 0, \\ &\partial_{\bar{c}} I^{\bar{a}}_{\bar{b}} - I^{\bar{a}}_{\bar{s}} \Gamma^{\bar{s}}_{\bar{b}\bar{c}} + I^{\bar{s}}_{\bar{b}} \Gamma^{\bar{b}}_{\bar{s}c} = 0, \quad \partial_c I^{\bar{a}}_{\bar{b}} = 0. \end{aligned} \tag{70}$$

Hence the four coordinates on each of D_1 and D_2 can respectively be chosen to be pairs of complex coordinates, $(z^A, \overline{z^{A'}})$ and $(z^{\bar{A}}, \overline{z^{\bar{A}'}})$, where $I_1 \partial/\partial z^A = i\partial/\partial z^A$ and $I_2 \partial/\partial z^{\bar{A}} = i\partial/\partial z^{\bar{A}}$, and $\overline{z^{A'}}$ and $\overline{z^{\bar{A}'}}$ denote the complex conjugate of z^A and $z^{\bar{A}}$ respectively. In order to fully satisfy Eqs. (42)–(47), Eqs. (69) and (70) must now be completely implemented. Equation (69) and the requirement that the matrix $(I_{\alpha\beta})$ be symmetric imply that

$$H_{,A\bar{B}'} = H_{,A'\bar{B}} = 0. \tag{71}$$

It follows that, without loss of generality in this context, the function H can be taken to be of the form

$$H = \mathbb{H} + \text{c.c.}, \tag{72}$$

where $\mathbb{H}$ is a holomorphic function of z^A and $z^{\bar{A}}$ only. In these adapted complex coordinates, the metric h can now be written

$${}_h ds^2 = \mathbb{H}_{,A\bar{B}} (dz^A \otimes dz^{\bar{B}} + dz^{\bar{B}} \otimes dz^A) + \text{c.c.}, \tag{73}$$

and the components of the complex structure I take the form

$$I^\alpha_\beta = \begin{bmatrix} i\delta^A_B & 0 & 0 & 0 \\ 0 & -i\delta^{A'}_{B'} & 0 & 0 \\ 0 & 0 & i\delta^{\bar{A}}_{\bar{B}} & 0 \\ 0 & 0 & 0 & -i\delta^{\bar{A}'}_{\bar{B}'} \end{bmatrix}. \tag{74}$$

It follows from Eq. (70) that, in these complex coordinates, the only nonzero components of the Christoffel symbols Γ^a_{bc} and $\Gamma^{\bar{a}}_{\bar{b}c}$ are the respective pairs of components $(\Gamma^A_{BC}, \Gamma^{A'}_{B'C'})$ and $(\Gamma^{\bar{A}}_{\bar{B}\bar{C}}, \Gamma^{\bar{A}'}_{\bar{B}'\bar{C}'})$, where

$$\begin{aligned} \Gamma^A_B &= h^{A\bar{D}} \mathbb{H}_{,B\bar{D}C} dz^C, \\ \Gamma^{\bar{A}}_{\bar{B}\bar{C}} &= h^{\bar{A}D} \mathbb{H}_{,\bar{B}D\bar{C}} dz^{\bar{C}}, \\ h^{A\bar{D}} \mathbb{H}_{,B\bar{D}} &= \delta^A_B, \quad h^{\bar{A}D} \mathbb{H}_{,D\bar{B}} = \delta^{\bar{A}}_{\bar{B}}, \end{aligned} \tag{75}$$

and similarly for the complex conjugates $\overline{\Gamma^{A'}_{B'C'}}$ and $\overline{\Gamma^{\bar{A}'}_{\bar{B}'\bar{C}'}}$. The curvature of the connection can be simply computed from these expressions as in Eqs. (64)–(66).

Since, by Eq. (25), the components of the metric k, $k_{\alpha\beta}$, are equal to $-I_{\alpha\beta}$, the metric k is given by

$$_k ds^2 = -i\mathbb{H}_{,A\bar{B}}(dz^A \otimes dz^{\bar{B}} + dz^{\bar{B}} \otimes dz^A) + \text{c.c.}, \tag{76}$$

and $g = h + ik$ is a holomorphic metric with line element

$$ds^2 = 2\mathbb{H}_{,A\bar{B}}(dz^A \otimes dz^{\bar{B}} + dz^{\bar{B}} \otimes dz^A). \tag{77}$$

When the condition of Ricci flatness, Eq. (67), is imposed on the metric h, it follows that

$$\det(\mathbb{H}_{,A\bar{B}}) = \text{const.} \tag{78}$$

Hence, as expected, g is also Ricci flat. In fact, the last two equations correspond to a description of holomorphic half-flat four-metrics given by Plebanski.[3] Therefore, it follows that a triple (P,h,I) which satisfies Eqs. (42)–(47) and the condition of Ricci flatness of h imply that the metric $g = h + ik$ is a holomorphic half-flat four-metric.

Finally, here, note the description of the Kähler structure $(J = -IP, h)$, implied by the structure (P,h,I), in these complex coordinates. It follows from Eqs. (59) and (74) that the components of J are given by

$$J^{\alpha}_{\beta} = \begin{bmatrix} -i\delta^{A}_{B} & 0 & 0 & 0 \\ 0 & i\delta^{A'}_{B'} & 0 & 0 \\ 0 & 0 & i\delta^{\bar{A}}_{\bar{B}} & 0 \\ 0 & 0 & 0 & -i\delta^{\bar{A}'}_{\bar{B}'} \end{bmatrix}. \tag{79}$$

Consequently, the Kähler two-form is given by $[i(\mathbb{H}_{,A\bar{B}} dz^A \wedge dz^{\bar{B}}) + \text{c.c.}]$; the metric h is given by Eq. (73).

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APPENDIX: TWISTOR SPACES

In this appendix the relation between twistor spaces for hyper-Kähler metrics eight-metrics on M and half-flat holomorphic metrics on M is outlined.

Salamon's generalization of Penrose's nonlinear graviton construction[24] (see also Ref. 25) to hyper-Kähler structures can be used to encode the hyper-Kähler structures presented in Sec. III in the complex structure of a twistor space, Z, where $\dim_{\mathbb{C}} Z$ is five. As a real manifold Z is $\mathrm{M} \times \mathrm{S}^2$. In the case of the real or imaginary parts of the anti-self-dual half-flat metrics on M, considered above, the complex structure on the corresponding twistor space Z_{ASD} is given by

$$I_{ASD} = (a_{\mathbf{i}}({}^{+}J^{\mathbf{i}}),\ I_0),$$

$$(a_{\mathbf{1}})^2 + (a_{\mathbf{2}})^2 + (a_{\mathbf{3}})^2 = 1,$$

and, following Refs. 24 and 25, $\{a_{\mathbf{i}}\} \in \mathbb{R}$ here.

Here the tangent space at the point (m,ς) in Z_{ASD} has been expressed as the direct sum $T_m \oplus T_\varsigma$, and I_0 is the operation of multiplication by i on the tangent space T_ς of $\varsigma \in \mathrm{S}^2$. Furthermore, S^2 is identified with CP^1, with local complex coordinate ζ, so that at $(a_{\mathbf{1}},a_{\mathbf{2}},a_{\mathbf{3}}) \in \mathrm{S}^2$, $(a_{\mathbf{1}},a_{\mathbf{2}},a_{\mathbf{3}}) = ((1-\varsigma\bar{\varsigma})/(1+\varsigma\bar{\varsigma}), (\varsigma+\bar{\varsigma})/(1+\varsigma\bar{\varsigma}), i(\varsigma-\bar{\varsigma})/(1+\varsigma\bar{\varsigma}))$. It is shown in detail in Refs. 24 and 25 that the integrability conditions for the tensor I_{ASD} to define a complex structure

on $M\times S^2$ are indeed satisfied, and furthermore, that the hyper-Kähler structure on M can be recovered from the holomorphic properties of Z_{ASD}. The twistor space Z_{ASD} can also be identified with the primed projective spin bundle over M.

In a similar way, now using $^{-}J^{\mathbf{i}}$, the hyper-Kahler structures associated with any half-flat self-dual holomorphic metric on M can be encoded in, and extracted from, a complex structure, I_{SD} say on $M\times S^2$ (this time the unprimed projective spin bundle over M), and the holomorphic properties of the resulting twistor space, Z_{SD}. As before, the latter can be extracted from the former.

Although the results contained in Refs. 24 and 25 enable real hyper-Kähler metrics to be derived from the structure of a twistor space Z, this is not quite the same as deriving a holomorphic half-flat metric g from the properties of a twistor space of the above type. An additional complex structure on M satisfying certain properties is also required, as was noted in Propositions 1 and 2 of Sec. III. In summary, the holomorphic structure on the five complex dimensional twistor space Z [which determines a hyper-Kähler structure, say, $(M,J^{\mathbf{i}},h)$], and a complex structure I, on the four complex dimensional manifold M, which together satisfy the compatibility relations $h(IX,IY)=-h(X,Y)$, ${}_h\nabla I=0$ and $IJ^i=J^{\mathbf{i}}I$, determine a half-flat holomorphic metric g. Hence they also determine the real metric k and the hyper-Kähler structure $(M,J^{\mathbf{i}},k)$.

By using results from Sec. III these statements can be reexpressed in terms of (integrable) almost product structures.

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Quantum enveloping superalgebras and link invariants

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Corresponding to each finite dimensional simple basic classical Lie superalgebra, a new quantum enveloping superalgebra is introduced, which has the structure of a braided quasi-Hopf superalgebra. In the case of $\mathfrak{osp}(1|2n)$, this quantum enveloping superalgebra is shown to be isomorphic to the standard Drinfeld–Jimbo quantum superalgebra $U_q(\mathfrak{osp}(1|2n))$ as braided quasi Hopf superalgebras. The new quantum enveloping superalgebras are applied to construct link invariants, from which Vassiliev invariants can be readily extracted. This, in particular, provides a useful construction for the Vassiliev invariants associated with $U_q(\mathfrak{osp}(1|2n))$. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The Drinfeld–Jimbo quantum superalgebras[1–3] were introduced in the early 1990s to describe supersymmetries exhibited by statistical mechanics models such as the Perk–Schultz models. By now a considerable body of theory for the quantum superalgebras[2,4] and the associated quantum supergroups[5,6] exists, and their applications to integrable models[1,7] and low dimensional topology[8–10] have been extensively explored. It has also long been known[11] that there is a deep connection between quantum supergroups and noncommutative geometry. This has been further explored lately and applied to the study of the representation theory,[5] leading to Borel–Weil type theorems for induced representations of quantum $SL(m|n)$ and $OSP(1|2n)$.

A Drinfel–Jimbo quantum superalgebra is a quasi-triangular Hopf superalgebra, which is a deformation (in the sense of Gerstenhaber[12]) of the corresponding enveloping superalgebra.[13] Deformation theory thus lies at the foundation of the theory of quantum superalgebras and quantum supergroups. The broad aim of the article is to develop the deformation theory of enveloping superalgebras following the general strategy of Ref. 14, and to explore its applications in low dimensional topology.

As we have already alluded to, low dimensional topology is one of the areas where quantum superalgebras have major applications. There exists a supersymmetric version[8] of the Reshetikhin–Turaev theory,[15,16] which provides a powerful machinery for generating topological invariants of links and three-manifolds using the representation theory[4] of quantum superalgebras.[1–3] Due to the vast difference between the representations of Lie algebras and Lie superalgebras in the quantum setting,[4] invariants arising from the supersymmetric Reshetikhin–Turaev theory exhibit very different features from those constructed from ordinary quantum algebras.

We may formally regard a quantum superalgebra invariant ν_q of links at generic $q=\exp(h)$ as a power series in h: $\nu_q=\Sigma_{i=0}^{\infty}h^i\nu^{(i)}$. Following the strategy of Birman and Lin,[17] one can show that *each coefficient* $\nu^{(k)}$ *is a Vassiliev invariant*[18,19] *of degree less than or equal to* k. However, it is very difficult to gain any understanding of such Vassiliev invariants within the framework of the Drinfeld–Jimbo superalgebras. Also, there exists no satisfactory quantum Chern–Simons theory formulation[20] for the quantum superalgebra invariants of links and three-manifolds, thus

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perturbative techniques of quantum field theory are not useful for studying the Vassiliev invariants arising from quantum superalgebras. As we shall see later, deformation theory provides a way to the problem at hand.

Let us now briefly describe the main results of this article. Corresponding to each finite dimensional simple basic classical Lie superalgebra,[13] we introduce a new quantum enveloping superalgebra with braiding (i.e., with a universal R-matrix), which is a quasi-Hopf superalgebra with a nontrivial associator. The underlying algebraic structure of the new quantum enveloping superalgebra is identical to that of the corresponding enveloping superalgebra over the power series ring $\mathbb{C}[[h]]$. Its universal R-matrix takes a particularly simple form and is explicitly given. The associator, however, is a highly complicated object, which is constructed by using a Knizhnik–Zamolodchikov equation following the work of Drinfeld.[14] In the case of the Lie superalgebra $\mathfrak{osp}(1|2n)$, we prove, using results of Ref. 21 that the new quantum enveloping superalgebra is isomorphic to the Drinfeld–Jimbo superalgebra as braided quasi-Hopf superalgebras.

The Reshetikhin–Turaev functor[15,16] from the category $\mathcal{H}$ of colored ribbon graphs to the module category of a ribbon Hopf superalgebra is generalized to a functor from $\mathcal{H}$ to the module category of a ribbon quasi-Hopf superalgebra. It is then applied to the new quantum enveloping superalgebras to construct topological invariants of (framed) links. The advantage of the resulting invariants is that the associated Vassiliev invariants (i.e., the coefficients in their power series expansions) can, in principle, be extracted, as the universal R-matrix and the associator are known. This enables us to construct large classes of Vassiliev invariants. This in particular provides us with a practical construction of the Vassiliev invariants associated with $\mathrm{U}_q(\mathfrak{osp}(1|2n))$.

The organization of the article is as follows. In Sec. II we discuss general properties of quasi-Hopf superalgebras. In Sec. III we introduce the new class of quantum enveloping algebras with braiding. In Sec. IV we prove the isomorphism (as quasi-Hopf superalgebras with braiding) between the new quantum enveloping algebra and the standard Drinfeld–Jimbo quantum superalgebra in the special case of $\mathfrak{osp}(1|2n)$. Section V studies link invariants.

This article makes extensive use of results in Refs. 14 and 22 and Kassel's book.[23]

Before closing this Introduction, we mention that there is no systematic study of deformations (e.g., within the category of braided quasi-Hopf superalgebras) of enveloping superalgebras except in the case $\mathfrak{osp}(1|2n)$. Even the relationship among the different Drinfeld–Jimbo quantum superalgebras associated with Weyl group inequivalent simple root systems of a given simple basic classical Lie superalgebra (see Subsec. III A 2) has not been studied in any depth. We hope to give a thorough treatment of the deformation theory of enveloping superalgebras in a future publication.

II. QUASI-HOPF SUPERALGEBRAS

A. Quasi-Hopf superalgebras

We explain the notion of quasi Hopf superalgebras here. In the fundamental paper[24] by Milnor and Moore, a version of graded quasi-Hopf algebras was introduced. Such algebras are similar to graded Hopf algebras but with the coassociativity requirement on the comultiplications removed altogether. In the earlier 1990s, Drinfeld[14] reignited the subject quite independently of Ref. 24 aiming at applications to quantum groups. He arrived at a notion of quasi-Hopf algebras which is more restrictive than that of Ref. 24, but structurally more interesting in that the comultiplications are quasi-coassociative. We shall consider $\mathbb{Z}_2$-graded generalizations of Drinfeld quasi-Hopf algebras here.

Let A be a $\mathbb{Z}_2$-graded associative algebra, i.e., an associative superalgebra, over a commutative ring $\mathbb{K}$, which admits two algebra homomorphisms, $\Delta: A \to A \otimes A$ and $\epsilon: A \to \mathbb{K}$. These homomorphisms will be called the comultiplication and counit, respectively. The algebra A will be called a $\mathbb{Z}_2$-graded quasi-bi-algebra, or a quasi-bi-superalgebra, if there exists an invertible even element $\Phi \in A \otimes A \otimes A$, called the associator, satisfying the following relations:

$$(\mathrm{id}\otimes\Delta)\Delta(x)=\Phi(\Delta\otimes\mathrm{id})\Delta(x)\Phi^{-1},$$

$$(\epsilon\otimes\mathrm{id})\Delta(x)=x,$$

$$(\mathrm{id}\otimes\epsilon)\Delta(x)=x,\quad \forall x\in A, \tag{2.1}$$

$$(\mathrm{id}\otimes\mathrm{id}\otimes\Delta)(\Phi)(\Delta\otimes\mathrm{id}\otimes\mathrm{id})(\Phi)=\Phi_{234}(\mathrm{id}\otimes\Delta\otimes\mathrm{id})(\Phi)\Phi_{123},$$

$$(\mathrm{id}\otimes\epsilon\otimes\mathrm{id})\Phi=1.$$

Here the second to last equation is usually referred to as the pentagon relation.

We use the following notation for $\Delta(x)$,

$$\Delta(x)=\sum_{(x)} x_{(1)}\otimes x_{(2)},\quad x\in A,$$

which will not lead to confusion, even though the standard Sweedler notation becomes ambiguous for $(\Delta\otimes\mathrm{id})\Delta$ and $(\mathrm{id}\otimes\Delta)\Delta$. A quasi-bi-superalgebra A will be called a $\mathbb{Z}_2$-graded quasi-Hopf algebra, or a quasi-Hopf superalgebra, if there exist invertible even elements $\alpha,\beta\in A$, and an algebra anti-automorphism S satisfying the following relations:

$$\sum_{(x)} S(x_{(1)})\alpha x_{(2)}=\epsilon(x)\alpha,\quad \sum_{(x)} x_{(1)}\beta S(x_{(2)})=\epsilon(x)\beta,\quad \forall x\in A,$$

$$\sum_t X_t\beta S(Y_t)\alpha Z_t=1=\sum_t S(\overline{X}_t)\alpha\overline{Y}_t\beta S(\overline{Z}_t), \tag{2.2}$$

where

$$\Phi=\sum_t X_t\otimes Y_t\otimes Z_t,\quad \Phi^{-1}=\sum_t \overline{X}_t\otimes\overline{Y}_t\otimes\overline{Z}_t.$$

Similar to the case of Hopf superalgebras, (S,α,β) will be called the antipode. It immediately follows from the definition that

$$\epsilon(\alpha)\epsilon(\beta)=1,\quad \epsilon S=\epsilon.$$

Note the following freedom in the definition of the antipode: Let (S,α,β) be an antipode of A. Then for any invertible element $g\in A$, the conditions (2.2) are also satisfied by $(\tilde{S},\tilde{\alpha},\tilde{\beta})$, where

$$\tilde{S}(a)=gS(a)g^{-1},\quad \tilde{\alpha}=g\alpha,\quad \tilde{\beta}=\beta g^{-1}. \tag{2.3}$$

Lemma 2.1: If (S,α,β) *and* $(\tilde{S},\tilde{\alpha},\tilde{\beta})$ *are antipodes of the quasi-Hopf superalgebra* A*, then there exists a unique invertible* $g\in A$ *transforming* (S,α,β) *to* $(\tilde{S},\tilde{\alpha},\tilde{\beta})$ *through (2.3).*

The antipode enables one to turn the dual $V^*=\mathrm{Hom}_{\mathbb{K}}(V,\mathbb{K})$ of a left A-module V into a left A-module, with the action

$$A\otimes V^*\to V^*,\quad x\otimes v^*\mapsto xv^*,$$

defined for homogeneous elements by

$$xv^*(w)=v^*((-1)^{[x][v^*]}S(x)w),\quad \forall w\in V,$$

and extending to inhomogeneous elements by linearity. Here $[x]=0$ if x is even, and $[x]=1$ if odd, and $[v^*]$ is similarly defined. However, it should be observed that while the following linear map defines a module homomorphism,

$$V^*\otimes V\to\mathbb{K},\quad v^*\otimes w\mapsto v^*(\alpha w),$$

even though the natural dual space pairing $v^*\otimes w\mapsto v^*(w)$ is no longer a module map if $\alpha\neq 1$.

A quasi-Hopf superalgebra A is called braided if there exists an even and invertible element $R\in A\otimes A$, called the universal R-matrix, which satisfies the following relations

$$R\Delta(x)=\Delta'(x)R,\quad \forall x\in A,$$

$$(\mathrm{id}\otimes\Delta)R=(\Phi_{231})^{-1}R_{13}\Phi_{213}R_{12}(\Phi_{123})^{-1}, \tag{2.4}$$

$$(\Delta\otimes\mathrm{id})R=\Phi_{312}R_{13}(\Phi_{132})^{-1}R_{23}\Phi_{123}.$$

Here $\Delta'=\tau\Delta$, with $\tau: A\otimes A\to A\otimes A$ being the flip $x\otimes y\mapsto(-1)^{[x][y]}y\otimes x$. It immediately follows from the defining relations of the universal R-matrix that we have the following generalized Yang–Baxter equation

$$R_{12}\Phi_{312}R_{13}(\Phi_{132})^{-1}R_{23}\Phi_{123}=\Phi_{321}R_{23}(\Phi_{231})^{-1}R_{13}\Phi_{213}R_{12}. \tag{2.5}$$

Write $R=\Sigma_r a_r\otimes b_r$, and let

$$u=\sum_{r,t}(-1)^{[\overline{X}_t]}S(b_r\overline{Y}_t\beta S(\overline{Z}_t))\alpha a_r\overline{X}_t.$$

Then u is invertible and for all $x\in A$,

$$S^2(x)=uxu^{-1}.$$

Furthermore, $uS(u)=S(u)u$ belongs to the center of A. We shall call A a ribbon quasi-Hopf superalgebra if there exists an even v belonging to the center of A such that

$$v^2=uS(u). \tag{2.6}$$

In studying deformation quantizations of enveloping superalgebras, we will work on the power series ring $\mathbb{C}[[h]]$. The quasi Hopf superalgebras encountered are topological in the sense that the underlying $\mathbb{C}[[h]]$-modules are completed with respect to the h-adic topology, and the structure maps are continuous.

B. Gauge transformations

Let $(A,m,\Delta,\epsilon,\Phi,S,R,\alpha,\beta)$ be a braided quasi-Hopf superalgebra, where m denotes the multiplication of A. Let $F\in A\otimes A$ be an invertible even element $F\in A\otimes A$ satisfying

$$(\epsilon\otimes\mathrm{id})F=(\mathrm{id}\otimes\epsilon)F=1. \tag{2.7}$$

Write $F=\Sigma f_i\otimes g_i$, $F^{-1}=\Sigma\overline{f}_i\otimes\overline{g}_i$, and set

$$\Delta_F=F\cdot\Delta\cdot F^{-1}: A\to A\otimes A,\quad x\mapsto F\Delta(x)F^{-1};$$

$$\Phi_F=F_{23}(\mathrm{id}\otimes\Delta)(F)\Phi(\Delta\otimes\mathrm{id})(F^{-1})F_{12}^{-1}$$

$$R_F=F_{21}RF^{-1}, \tag{2.8}$$

$$\alpha_F=\sum_i S(\overline{f_i})\alpha\overline{g_i},$$

$$\beta_F=\sum_i f_i\beta S(g_i).$$

Lemma 2.2: $(A,m,\Delta_F,\epsilon,\Phi_F,S,R_F,\alpha_F,\beta_F)$ *is a braided quasi-Hopf superalgebra.*

Equation (2.8) is called a gauge transformation by F on the braided quasi-Hopf superalgebra $(A,m,\Delta,\epsilon,\Phi,S,R,\alpha,\beta)$.

Let

$$\mathbf{A}=(A,m^{(A)},\Delta^{(A)},\epsilon^{(A)},\Phi^{(A)},S^{(A)},R^{(A)},\alpha^{(A)},\beta^{(A)}),$$

$$\mathbf{B}=(B,m^{(B)},\Delta^{(B)},\epsilon^{(B)},\Phi^{(B)},S^{(B)},R^{(B)},\alpha^{(B)},\beta^{(B)})$$

be braided quasi Hopf superalgebras. A homomorphism $(f,F):\mathbf{A}\to\mathbf{B}$ between them consists of an algebra homomorphism $f:(A,m^{(A)})\to(B,m^{(B)})$ and a gauge transformation $F\in B\otimes B$ such that

$$(f\otimes f)\Delta^{(A)}=F\cdot(\Delta^{(B)}f)\cdot F^{-1},$$

$$\{F_{23}(\mathrm{id}\otimes\Delta^{(B)})(F)\}(f\otimes f\otimes f)(\Phi^{(A)})=\Phi^{(B)}F_{12}(\Delta^{(B)}\otimes\mathrm{id})F,$$

$$(f\otimes f)R^{(A)}=F_{21}R^{(B)}F^{-1}.$$

If f is an algebra isomorphism, then (f,F) is called an isomorphism between the braided quasi-Hopf superalgebras **A** and **B**. An isomorphism of braided quasi-Hopf superalgebras strictly preserves the algebraic structure, but only preserves the coalgebraic structure, the associator and the braiding up to a gauge transformation. If $(f,F):\mathbf{A}\to\mathbf{B}$ is an isomorphism, then it follows from Lemma 2.1 that there exists a unique invertible $g\in B$ such that

$$f\circ S^{(A)}\circ f^{-1}=g\circ S^{(B)}\circ g^{-1},$$

$$f(\alpha^{(A)})=g\alpha_F^{(B)},$$

$$f(\beta^{(A)})=\beta_F^{(B)}g^{-1}.$$

We mention that the category of left A-modules has the structure of a braided tensor category, where Φ provides the associativity constraint, and the universal R-matrix gives the braiding. If two braided quasi-Hopf superalgebras are isomorphic, then their module categories are equivalent as braided tensor categories

C. Associative tensor product

Let $(A,m,\Delta,\epsilon,\Phi,S,R,\alpha,\beta)$ be a quasi-Hopf superalgebra. Tensor products of A-modules are not strictly associative, but for any A-modules U, V, and W, there exists the module isomorphism

$$\begin{aligned}&(U\otimes V)\otimes W\to U\otimes(V\otimes W),\\&(u\otimes v)\otimes w\mapsto\Phi((u\otimes v)\otimes w)=u\otimes(v\otimes w),\end{aligned}\tag{2.9}$$

where Φ is the associator of A. The nonassociativity of tensor products is a cause of inconvenience in applications of quasi-Hopf superalgebras, but there is a way to get around the problem (See Remark XI.1.4, p. 496 of Ref. 16 and Section XI.5 of Ref. 23).

Let $\mathbf{V}=\{V_1,V_2,\ldots,V_m\}$ be a sequence of A-modules. We denote

$$(\mathbf{V})=(\ldots((V_1\otimes V_2)\otimes V_3)\otimes\ldots\otimes V_{n-1})\otimes V_n.$$

All the tensor products of the V_i's in this order but with parentheses positioned in different ways are isomorphic to $(\mathbf{V})$. Let us introduce the subsequences

$$\mathbf{V}_r^{(k)}=\{V_1,V_2,\ldots,V_k\},$$

$$\mathbf{V}_l^{(k)}=\{V_k,V_{k-1},\ldots,V_m\}.$$

If $\mathbf{W}=\{W_1,W_2,\ldots,W_n\}$ is also a sequence of A-modules, by joining $\mathbf{V}$ with $\mathbf{W}$ we obtain another sequence $\{V_1,V_2,\ldots,V_m,W_1,W_2,\ldots,W_n\}$. We denote by $(\mathbf{V},\mathbf{W})$ the tensor product $(\{V_1,V_2,\ldots,V_m,W_1,W_2,\ldots,W_n\})$.

Now we introduce a new tensor product $\odot$ for A-modules defined by

$$(\mathbf{V})\odot(\mathbf{W})=(\mathbf{V},\mathbf{W}). \tag{2.10}$$

This is clearly associative. The problem is to find an associative tensor product of maps consistent with this tensor product of A-modules. Consider linear maps

$$f:(\mathbf{V})\to(\mathbf{S}),\quad g:(\mathbf{W})\to(\mathbf{T}).$$

Let $J_{(\mathbf{V}),(\mathbf{W})}:(\mathbf{V})\odot(\mathbf{W})\to(\mathbf{V})\otimes(\mathbf{W})$ be the natural A-module isomorphism

$$J_{(\mathbf{V}),(\mathbf{W})}=(\Phi^{-1}_{(\mathbf{V}),(\mathbf{W}_r^{(1)}),W_2}\otimes\mathrm{id}_{W_3}\otimes\ldots\otimes\mathrm{id}_{W_n})(\Phi^{-1}_{(\mathbf{V}),(\mathbf{W}_r^{(2)}),W_3}\otimes\mathrm{id}_{W_4}\otimes\ldots\otimes\mathrm{id}_{W_n})$$
$$\ldots\Phi^{-1}_{(\mathbf{V}),(\mathbf{W}_r^{(n-1)}),W_n}.$$

Similarly we have the A-module isomorphism $J_{(\mathbf{S}),(\mathbf{T})}:(\mathbf{S})\odot(\mathbf{T})\to(\mathbf{S})\otimes(\mathbf{T})$. An associative tensor product, also denoted by $\odot$, of the maps consistent with the associative tensor product of A-modules is then given by the composition

$$(\mathbf{V})\odot(\mathbf{W})\xrightarrow{J_{(\mathbf{V}),(\mathbf{W})}}(\mathbf{V})\otimes(\mathbf{W})\xrightarrow{f\otimes g}(\mathbf{S})\otimes(\mathbf{T})\xrightarrow{J^{-1}_{(\mathbf{S}),(\mathbf{T})}}(\mathbf{S})\odot(\mathbf{T}).$$

Explicitly, we have

$$f\odot g=J^{-1}_{(\mathbf{S}),(\mathbf{T})}(f\otimes g)J_{(\mathbf{V}),(\mathbf{W})}.$$

More formally, one can always turn the tensor category $\mathrm{Mod}(A)$ of A-modules into a strict tensor category $\mathrm{Mod}_s(A)$ with objects being the $(\mathbf{V})$ for all finite sequences of A-modules, and the morphisms $(\mathbf{V})\to(\mathbf{V}')$ being $\mathrm{Hom}((\mathbf{V}),(\mathbf{V}'))$. The strictly associative tensor product is the $\odot$ just defined above.

D. Gauge transformations on modules

Let $(A,m,\Delta,\epsilon,\Phi,S,\alpha,\beta)$ be a quasi-Hopf superalgebra. Let $V_1,\ldots,V_n$ be A-modules. Denote by $(\mathbf{V})$ the ordered tensor product of the modules. For convenience we shall only consider gauge transformations on ordered tensor product of modules and their homomorphisms. Because of the isomorphism (2.9), the discussions below also apply to the nonassociative tensor product.

Let $\Delta^{(k)}$ be defined inductively by

$$\Delta^{(k)}=(\Delta\otimes\mathrm{id}^{\odot(n-1)})\Delta.$$

Under a gauge transformation $F=\Sigma f_i\otimes g_i$ as defined by (2.8), Δ is transformed to $\Delta_F=F\Delta F^{-1}$, and $\Delta^{(k)}$ to $\Delta_F^{(k)}$, which is defined in exactly the same way as $\Delta^{(k)}$ but with Δ replaced by Δ_F.

Let $(\mathbf{V}_F)$ be the A-module with the same underlying $\mathbb{K}$-module as the A-module $(\mathbf{V})$, but with the A-action defined by

$$x\otimes\mathbf{v}_F\mapsto\Delta_F^{(n)}(x)\mathbf{v}_F, \quad x\in A, \ \mathbf{v}_F\in(\mathbf{V}_F).$$

There exists an A-module isomorphism $(\mathbf{V})\to(\mathbf{V}_F)$ defined by

$$\mathbf{v}\mapsto F^{(n)}\mathbf{v}, \quad \mathbf{v}\in(\mathbf{V}),$$

where

$$F^{(n)}=\sum_{i_2,\ldots,i_n}(\cdots((F\Delta(f_{i_2})\otimes g_{i_2})\Delta^{(2)}(f_{i_3})\otimes g_{i_3})\cdots)\Delta^{(n-1)}(f_{i_n})\otimes g_{i_n}.$$

This is indeed an A-module isomorphism as confirmed by the following relation:

$$\Delta_F^{(n)}(x)(F^{(n)}\mathbf{v})=F^{(n)}\Delta^{(n)}(x)\mathbf{v}, \quad \mathbf{v}\in(\mathbf{V}).$$

Let $W_1,\ldots,W_m$ be another set of A-modules. Assume we have the linear map $\psi:(\mathbf{V})\to(\mathbf{W})$. Then F transforms ψ to $\psi_F:(\mathbf{V}_F)\to(\mathbf{W}_F)$, which is defined by the following commutative diagram

$$\begin{array}{ccc}(\mathbf{V})&\to&(\mathbf{W})\\ \downarrow&&\downarrow\\ (\mathbf{V}_F)&\to&(\mathbf{W}_F).\end{array} \tag{2.11}$$

Consider also the transformation (2.3) on the antipode. It affects only the definition of dual modules. Let V be an A-module, and denote by V_S^* and $V_{\tilde{S}}^*$ the dual A-modules defined by using S and $\tilde{S}$, respectively. Then we have the following A-module isomorphism

$$S^{-1}(g):V_{\tilde{S}}^*\to V_S^*.$$

For $\epsilon_i\in\{1,-1\}$, let $V_i^{\epsilon_i}$ be V_i if $\epsilon_i=1$ and $V_i^{\epsilon_i}=V_i^*$ if $\epsilon_i=-1$. Let $(\mathbf{V}^{\epsilon})=(\{V_1^{\epsilon_1},\ldots,V_n^{\epsilon_n}\})$. The isomorphism $G:(\mathbf{V}_S^{\epsilon})\to(\mathbf{V}_{\tilde{S}}^{\epsilon})$ then is given by

$$G=(\ldots((S^{-1}(g^{(1-\epsilon_1)/2})\otimes S^{-1}(g^{(1-\epsilon_2/2)}))\otimes S^{-1}(g^{(1-\epsilon_3/2)}))\otimes\ldots)\otimes S^{-1}(g^{(1-\epsilon_n/2)}).$$

Let $(\mathbf{W}_{\tilde{S}}^{\epsilon'})$ be another A-module and assume we have the linear map $\psi:(\mathbf{V}_S^{\epsilon})\to(\mathbf{W}_S^{\epsilon'})$. Then the antipode transformation changes ψ to $\tilde{\psi}:(\mathbf{V}_{\tilde{S}}^{\epsilon})\to(\mathbf{W}_{\tilde{S}}^{\epsilon'})$, which is defined by the following commutative diagram:

$$\begin{array}{ccc}(\mathbf{V}_S^{\epsilon})&\to&(\mathbf{W}_S^{\epsilon'})\\ \downarrow&&\downarrow\\ (\mathbf{V}_{\tilde{S}}^{\epsilon})&\to&(\mathbf{W}_{\tilde{S}}^{\epsilon'})\end{array}. \tag{2.12}$$

To summarize, tensor product functors $\odot:\mathrm{Mod}_s(A)\times\mathrm{Mod}_s(A)\to\mathrm{Mod}_s(A)$ defined with respect to gauge equivalent comultiplications of A are naturally isomorphic, and so are also the duality functors of $\mathrm{Mod}_s(A)$ defined with respect to gauge equivalent antipodes of A.

III. QUANTUM ENVELOPING SUPERALGEBRAS

In this section we shall work over the power series ring $\mathbb{C}[[h]]$ exclusively. All superalgebras and quasi-Hopf superalgebras should be understood as topological. The main result is contained in Sec. III B, where a new type of quantum enveloping superalgebras with braiding are constructed. For the purpose of studying the relationship amongst different deformations of enveloping superalgebras, we also discuss the standard Drinfeld–Jimbo quantum superalgebras.[1–3] In the next section, we shall show that the new quantum enveloping superalgebra is isomorphic to the Drinfeld–Jimbo quantum superalgebra in the case of $\mathfrak{osp}(1|2n)$.

A. Drinfeld–Jimbo quantum superalgebras

1. Drinfeld-Jimbo quantum superalgebras

The Drinfeld–Jimbo quantum superalgebras[1–3] were studied quite extensively in the last decade. Here we shall summarize some of their main properties.

Let $\mathfrak{g}$ be a simple basic classical Lie superalgebra[13] (all such Lie superalgebras are assumed to be finite dimensional.). Denote by H^* the dual of its Cartan subalgebra with the nondegenerate symmetric bilinear form $(\ ,\ )$. Let $\phi=\{\alpha_i|i=1,2,\ldots,r\}$ be a chosen simple root system. Denote the set of the even simple roots by ϕ_0 and that of the odd simple roots by ϕ_1. Set

$$[\alpha_i]=\begin{cases}0, & \alpha_i\in\phi_0,\\ 1, & \alpha_i\in\phi_1.\end{cases}$$

If $(\alpha_i,\alpha_i)\neq 0$, we define $a_{ij}=2(\alpha_i,\alpha_j)/(\alpha_i,\alpha_i)$ for all j. If $(\alpha_i,\alpha_i)=0$, and this can only happen if $\alpha_i\in\phi_1$, we set

$$a_{ij}=\begin{cases}-1, & (\alpha_i,\alpha_j)\neq 0,\\ 0, & (\alpha_i,\alpha_j)=0.\end{cases}$$

Corresponding to the given data, a Drinfeld–Jimbo quantum superalgebra $\mathrm{U_q}(\mathfrak{g})$ has been introduced. We shall work in the Drinfeld setting, where $\mathrm{U_q}(\mathfrak{g},\phi)$ is a Hopf superalgebra over the power series ring $\mathbb{C}[[h]]$ completed with respect to the h-adic topology. As is well known, $\mathrm{U_q}(\mathfrak{g},\phi)$ is a deformation of the enveloping superalgebra $\mathrm{U}(\mathfrak{g})[[h]]$.

Now we describe $\mathrm{U_q}(\mathfrak{g},\phi)$ in terms of generators and relations. Recall that $\mathrm{U_q}(\mathfrak{g})$ is generated by the identity and the elements e_i,f_i,h_i, $i=1,2,\ldots,r$, subject to the relations

$$[h_i,h_j]=0,$$

$$[h_i,e_j]=(\alpha_i,\alpha_j)e_j,$$

$$[h_i,f_j]=-(\alpha_i,\alpha_j)f_j,$$

$$[e_i,f_j]=\delta_{ij}(q^{h_i}-q^{-h_i})/(q_i-q_i^{-1}),$$

$$(e_s)^2=(f_i)^2=0,\quad (\alpha_s,\alpha_s)=0,$$

$$ad_{e_i}^{1-a_{ij}}(e_j)=0,\quad i\neq j,$$

$$ad_{f_i}^{1-a_{ij}}(f_j)=0,\quad i\neq j,$$

plus higher order Serre-relations.

The higher order Serre relations can be found in Ref. 2 and thus will not be spelled out explicitly here. It suffices to mention that they depend very much on the Lie superalgebra $\mathfrak{g}$ itself and also on the chosen simple root system ϕ.

Some explanations are now in order. Here q is the power series $q=\exp(h)$, and

$$q_i=\begin{cases} q^{(\alpha_i,\alpha_i)/2}, & (\alpha_i,\alpha_i)\neq 0, \\ q, & (\alpha_i,\alpha_i)=0. \end{cases}$$

The $\mathbb{Z}_2$-gradation of the superalgebra is defined in such a way that all h_i and e_j, f_j with $[\alpha_j]=0$ are even, while all e_s, f_s with $[\alpha_s]=1$ are odd. For a homogeneous element $x\in \mathrm{U_q}(\mathfrak{g},\phi)$, we set $[x]=0$ if x is even and $[x]=1$ if x is odd. Then the graded bracket is defined by $[x,y]=xy-(-1)^{[x][y]}yx$. The notation $ad_{e_i}(x)$ and $ad_{f_i}(x)$ are defined by

$$ad_{e_i}(x)=e_ix-(-1)^{[e_i][x]}q^{h_i}xq^{-h_i}e_i,$$

$$ad_{f_i}(x)=f_ix-(-1)^{[f_i][x]}q^{-h_i}xq^{h_i}f_i.$$

Finally, we note that if $(\alpha_s,\alpha_s)=0$ and $a_{sj}\neq 0$, then the relations $(ad_{e_s})^{1-a_{sj}}(e_j)=(ad_{f_s})^{1-a_{sj}}(f_j)=0$ are implied by $e_s^2=f_s^2=0$.

The $\mathrm{U_q}(\mathfrak{g},\phi)$ has the structures of a Hopf superalgebra, with the coassociative comultiplication

$$\Delta_q(h_i)=h_i\otimes 1+1\otimes h_i,$$

$$\Delta_q(e_i)=e_i\otimes q^{h_i}+1\otimes e_i,$$

$$\Delta_q(f_i)=f_i\otimes 1+q^{-h_i}\otimes f_i,$$

counit

$$\epsilon_q(h_i)=\epsilon_q(e_i)=\epsilon_q(f_i)=0,$$

and antipode

$$S_q(h_i)=-h_i,$$

$$S(e_i)=-e_iq^{-h_i},$$

$$S(f_i)=-q^{h_i}f_i.$$

Let 2ρ be the sum of the even positive roots minus the sum of the odd positive roots of $\mathfrak{g}$. Let $2h_\rho$ denote the linear combination of the h_i such that $[h_\rho,e_i]=(\rho,\alpha_i)e_i$ for all i. Set

$$K=q^{2h_\rho}.$$

Then it can be immediately shown that

$$S^2(x)=KxK^{-1},\quad \forall x\in \mathrm{U_q}(\mathfrak{g},\phi).$$

We shall regard $\mathrm{U_q}(\mathfrak{g},\phi)$ as a quasi-Hopf superalgebra with

$$\Phi=1\otimes 1\otimes 1,\quad \alpha=\beta=1.$$

One of the most important properties of $\mathrm{U_q}(\mathfrak{g},\phi)$ is its braiding, that is, the existence of a universal R-matrix R_q.[3] The explicit form of R_q in terms of the generators of $\mathrm{U_q}(\mathfrak{g},\phi)$ is, in principle, known. However, for the purpose of studying the Vassiliev invariants arising from quantum superalgebras, we are interested in the expansion of R_q into a power series in h. The coefficients of this expansion are in $\mathrm{U}(\mathfrak{g})$ as $\mathrm{U_q}(\mathfrak{g},\phi)$ is a deformation of $\mathrm{U}(\mathfrak{g})$. It is easy to see that

$$R_q = 1 \otimes 1 + h r_c + o(h^2), \tag{3.1}$$

where r_c is the classical r-matrix discussed in Ref. 25. However, there exists no method, even in principle, for computing the higher order terms.

2. The choice of simple root systems

We consider very briefly the dependence of the quantum superalgebra $U_q(\mathfrak{g}, \phi)$ on the chosen simple root system ϕ. Recall that a Lie superalgebra in general admits Weyl group inequivalent simple root systems. The quantum superalgebra $U_q(\mathfrak{g}, \phi)$ is defined in terms of simple and Cartan generators subject to some defining relations. The simple roots thus play a special role. One expects $U_q(\mathfrak{g}, \phi)$ to depend on ϕ nontrivially. This is indeed true, even in the simplest case of $\mathfrak{sl}(2|1)$.

The two simple root systems for $\mathfrak{sl}(2|1)$ are, in terms of Dynkin diagrams,

$$\phi: \bigcirc - - - \otimes, \quad \phi': \otimes - - - \otimes.$$

It is known that the definitions of $U_q(\mathfrak{sl}(2|1), \phi)$ and $U_q(\mathfrak{sl}(2|1), \phi')$ do not involve higher order Serre relations. Now it is a simple matter to check that the square of the antipode of $U_q(\mathfrak{sl}(2|1), \phi)$ is nontrivial, while that of $U_q(\mathfrak{sl}(2|1), \phi')$ is the identity map. This immediately shows that the two Hopf superalgebras are not isomorphic,[26] although it is known that the underlying algebraic structures of $U_q(\mathfrak{sl}(2|1), \phi)$ and $U_q(\mathfrak{sl}(2|1), \phi')$ are the same.[21]

B. Braided structure for enveloping superalgebras

Let $U(\mathfrak{g})$ be the enveloping superalgebra of the Lie superalgebra $\mathfrak{g}$ defined over the complex field. Let $U(\mathfrak{g})[[h]]$ be the $\mathbb{C}[[h]]$-module consisting of formal power series in h with coefficients in $U(\mathfrak{g})$. By $\mathbb{C}[[h]]$-linearly extending the structure maps of the complex Hopf superalgebra $U(\mathfrak{g})$ to $U(\mathfrak{g})[[h]]$, one obtains a natural Hopf superalgebra structure on $U(\mathfrak{g})[[h]]$. We denote the multiplication by m, the comultiplication by Δ, the counit by ϵ, and the antipode by S. Then

$$\begin{aligned} \Delta(X) &= X \otimes 1 + 1 \otimes X, \\ \epsilon(X) &= 0, \\ S(X) &= -X, \quad \forall X \in \mathfrak{g}. \end{aligned} \tag{3.2}$$

Let C denote the quadratic Casimir operator of $\mathfrak{g}$, that is, the central element of $U(\mathfrak{g})$ which takes the eigenvalue $(\lambda + 2\rho, \lambda)$ in any irreducible $U(\mathfrak{g})$-module with highest weight λ. Set

$$t = \tfrac{1}{2}(\Delta(C) - C \otimes 1 - 1 \otimes C).$$

The following results are straightforward to prove, but will be of crucial importance for the remainder of this section.

Lemma 3.1:

$$\begin{aligned} (\mathrm{id} \otimes \Delta) t &= t_{12} + t_{13}, \\ (\Delta \otimes \mathrm{id}) t &= t_{13} + t_{23}, \\ [t_{12}, \; t_{13} + t_{23}] &= 0. \end{aligned}$$

The last equation will be referred to as the "four-term relation."

Now we introduce a braided structure on $U(\mathfrak{g})[[h]]$. We shall take as the universal R-matrix the following power series

$$R = \exp(ht/2). \tag{3.3}$$

As $U(\mathfrak{g})[[h]]$ is cocommutative and t belongs to the commutant of $\Delta(U(\mathfrak{g})[[h]])$, we immediately see that

$$R\Delta(x)=\Delta'(x)R, \quad \forall x\in U(\mathfrak{g})[[h]].$$

However, R requires a nontrivial associator Φ to satisfy the defining relations of a universal R-matrix.

Because of Lemma 3.1, Cartier's work[22] on infinitesimal symmetric categories applies to the problem at hand. This in particular tells us that Drinfeld's construction (second paper of Ref. 14) of associators for enveloping algebras of semi-simple Lie algebras can be generalized to the present context to construct the desired associator. Consider the following differential equation on $\mathbb{C}\backslash\{0,1\}$,

$$\frac{dG(z)}{dz}=\frac{h}{2\pi i}\left(\frac{t_{12}}{z}+\frac{t_{23}}{z-1}\right) \tag{3.4}$$

for the analytic function $G:\mathbb{C}\backslash\{0,1\}\to U(\mathfrak{g})^{\otimes 3}[[h]]$. This is a special case of the celebrated Knizhnik–Zamolodchikov equations, which first arose in the context of Wess–Zumino–Witten models of two dimensional conformal quantum field theory. The classical theory of Fuchsian differential equations guarantees the existence and uniqueness of solutions G_0 and G_1 of the Knizhnik–Zamolodchikov equation with the asymptotics

$$G_0(z)\cong z^{ht_{12}/2\pi i}, \quad z\to 0,$$

$$G_1(z)\cong (1-z)^{ht_{23}/2\pi i}, \quad z\to 1.$$

Furthermore, the two solutions can only differ by a z independent factor

$$\Phi_{KZ}:=(G_0(z))^{-1}G_1(z). \tag{3.5}$$

Φ_{KZ} can be expressed as a power series in h with coefficients being linear combinations of Lie words in t_{12} and t_{23}, where the coefficients involve Chen's iterated integrals. We refer to Ref. 27 by Le and Murakami for details.

It follows from Lemma 3.1 and Cartier's work[22]

Theorem 3.1: *Φ_{KZ} satisfies the relations (2.1) and (2.4), and thus yields the desired associator.*

Furthermore, we can also show that for the given comultiplication Δ and universal R-matrix $R=\exp(ht/2)$, Φ_{KZ} is the unique associator.

The complete quasi-Hopf superalgebra structure of $U(\mathfrak{g})[[h]]$ includes α and β. The relationship between α and β with the antipode S requires both of them be central, while the relationship with the associator Φ involves $\alpha\beta$ only. Therefore, we have the freedom to choose $\alpha=1$. Then

$$\beta^{-1}=m(m\otimes \mathrm{id})(\mathrm{id}\otimes S\otimes \mathrm{id})\Phi_{KZ},$$

where m is the multiplication of $U(\mathfrak{g})[[h]]$.

Remark: A natural question is how the Drinfeld–Jimbo superalgebras are related to the new quantum enveloping superalgebras. More generally, we want to classify all quantisations of the enveloping superalgebras. We will address the problem for the superalgebra $\mathfrak{osp}(1|2n)$ in the next section, and results are used in the study of the Vassiliev invariants associated with $U_q(\mathfrak{osp}(1|2n))$.

IV. THE CASE OF $\mathfrak{osp}(1|2n)$

We now consider the Lie superalgebra $\mathfrak{osp}(1|2n)$. We shall set

$$\mathfrak{g}=\mathfrak{osp}(1|2n)$$

in this section.

Recall that all simple root systems of $\mathfrak{osp}(1|2n)$ are equivalent under the Weyl group, thus we can drop ϕ from the notation of the quantum superalgebra of $\mathfrak{osp}(1|2n)$.[28] $\mathrm{U}_q(\mathfrak{osp}(1|2n))$ is the best studied[28] among all the quantum superalgebras. Its finite dimensional representations at generic q are thoroughly understood. This quantum superalgebra also has an unexpected but very interesting application[29] to the study of a Duflo theorem for $\mathrm{U}(\mathfrak{osp}(1|2n))$ at the classical level.

For $\mathrm{U}(\mathfrak{g})[[h]]$, the structure maps m,Δ,ϵ,S are the standard ones of the universal enveloping superalgebra; the associator Φ_{KZ} is that constructed from the KZ equation; $R=\exp(ht/2)$, and $\alpha=1$, $\beta^{-1}=m(m\otimes\mathrm{id})(\mathrm{id}\otimes S\otimes\mathrm{id})\Phi_{KZ}$.

One of the main results of this section is the following theorem.

Theorem 4.1: $(\mathrm{U}_q(\mathfrak{g}),m_q,\Delta_q,\epsilon_q,S_q,R_q)$ *and* $(\mathrm{U}(\mathfrak{g})[[h]],m,\Delta,\epsilon,\Phi_{KZ},S,\alpha,\beta,R)$ *are isomorphic as braided quasi-Hopf superalgebras on* $\mathbb{C}[[h]]$ *in the case* $\mathfrak{g}=\mathfrak{osp}(1|2n)$.

We break the proof of Theorem 4.1 into a series of lemmas and propositions. Recall that $\mathfrak{osp}(1|2n)$ has many remarkable properties not shared by the other Lie superalgebras. We mention in particular that an analog of Whitehead's lemma holds,[21] i.e., for any finite dimensional $\mathfrak{osp}(1|2n)$-module V, the Lie superalgebra cohomology groups $H^1(\mathfrak{g},V)$ and $H^2(\mathfrak{g},V)$ are trivial. The vanishing of $H^1(\mathfrak{g},V)$ for all finite dimensional $\mathfrak{g}$-modules implies that all such modules are completely reducible.

The universal enveloping algebra $\mathrm{U}(\mathfrak{g})$ forms an $\mathfrak{osp}(1|2n)$-module under the adjoint action. Furthermore, it can be decomposed into a direct sum of finite dimensional $\mathfrak{osp}(1|2n)$-modules. Similarly, $\mathrm{U}(\mathfrak{g})\otimes\mathrm{U}(\mathfrak{g})$ as an $\mathfrak{osp}(1|2n)$-module can also be decomposed into a direct sum of finite dimensional modules. Therefore,[21]

$$H^1(\mathfrak{g},\mathrm{U}(\mathfrak{g})\otimes\mathrm{U}(\mathfrak{g}))=0,\quad H^2(\mathfrak{g},\mathrm{U}(\mathfrak{g}))=0. \tag{4.1}$$

Let M be a two-sided $\mathrm{U}(\mathfrak{g})$-module. Then M forms a left $\mathfrak{g}$-module under the action

$$X\otimes v\mapsto Xv-(-1)^{[X][v]}vX. \tag{4.2}$$

Denote by $H_H^k(\mathrm{U}(\mathfrak{g}),M)$ the kth Hochschild cohomology group of $\mathrm{U}(\mathfrak{g})$ with coefficients in M. It can be shown that there exist vector space embeddings

$$H_H^k(\mathrm{U}(\mathfrak{g}),M)\to H^k(\mathfrak{g},M),\quad k=1,2.$$

Combining these results we have the following.

Lemma 4.1:

$$H_H^1(\mathrm{U}(\mathfrak{g}),\mathrm{U}(\mathfrak{g})\otimes\mathrm{U}(\mathfrak{g}))=0,$$

$$H_H^2(\mathrm{U}(\mathfrak{g}),\mathrm{U}(\mathfrak{g}))=0.$$

Observe that $\mathrm{U}_q(\mathfrak{g})$ in the Drinfeld setting is a deformation of $\mathrm{U}(\mathfrak{g})$ in the sense of Gerstenhaber.[12] The deformations of $\mathrm{U}(\mathfrak{g})$ as an associative superalgebra are classified, up to obstructions, by the even part of the Hochschild cohomology group $H^2(\mathrm{U}(\mathfrak{g}),\mathrm{U}(\mathfrak{g}))$. The vanishing of $H_H^2(\mathrm{U}(\mathfrak{g}),\mathrm{U}(\mathfrak{g}))$ thus implies the following.

Proposition 4.1: The algebraic structure of $\mathrm{U}(\mathfrak{g})$ *is rigid, that is, all Gerstenhaber type deformations of* $\mathrm{U}(\mathfrak{g})$ *are isomorphic to* $\mathrm{U}(\mathfrak{g})[[h]]$ *as associative superalgebras over* $\mathbb{C}[[h]]$.

In particular, as associative superalgebras $\mathrm{U}_q(\mathfrak{g})$ and $\mathrm{U}(\mathfrak{g})[[h]]$ are isomorphic. We denote by $H_h:\mathrm{U}_q(\mathfrak{g})\to\mathrm{U}(\mathfrak{g})[[h]]$ the isomorphism. Define

$$\tilde{\Delta}_q=(H_h\otimes H_h)\circ\Delta_q\circ H_h^{-1},$$

$$\tilde{S}_q=H_h\circ S_q\circ H_h^{-1},$$

$$\tilde{\epsilon}_q = \epsilon_q \circ H_h^{-1},$$

$$\tilde{R}_q = (H_h \otimes H_h) R_q.$$

Consider the Drinfeld operator $v_q \in \mathrm{U_q}(\mathfrak{g})$. Its image under H_q gives rise to a central element $\tilde{v}$ of $\mathrm{U}(\mathfrak{g})[[h]]$, which can be expanded into a power series

$$\tilde{v} = 1 + h\tilde{v}_1 + h^2\tilde{v}_2 + \cdots,$$

where each $\tilde{v}_i$ belongs to the center of $\mathrm{U}(\mathfrak{g})$. If V is an irreducible highest weight $\mathrm{U}(\mathfrak{g})$-module, we denote by $\chi_V(C)$ the eigenvalue of C on V. Then $\tilde{v}$ takes the eigenvalue $\exp(h\chi_V(C))$ on the $\mathrm{U}(\mathfrak{g})[[h]]$-module $V[[t]]$. By using Harish–Chandra's homomorphism for the Lie superalgebra $\mathfrak{g}$, one obtains $\tilde{v}_n = C^n/n!$, i.e., the following lemma.

Lemma 4.2: $\tilde{v} = \exp(hC)$.

Also by using $\Delta_q(v_q^{-1}) = R_{21}R(v_q^{-1} \otimes v_q^{-1})$, one obtains

$$(\tilde{R}_q)_{21}\tilde{R}_q = (\tilde{v} \otimes \tilde{v})\tilde{\Delta}_q(\tilde{v}).$$

For any $w = 1^{\otimes n} + hw_1 + h^2w_2 + h^3w_3 + \cdots$ in $\mathrm{U}(\mathfrak{g})^{\otimes n}[[h]]$, we define $w^{1/2}$ to be the power series $x = 1^{\otimes n} + hx_1 + h^2x_2 + \cdots$ such that $x^2 = w$. Then $w^{1/2}$ is uniquely defined. From the above equation, we obtain

$$((\tilde{R}_q)_{21}\tilde{R}_q)^{1/2} = (\tilde{v}^{1/2} \otimes \tilde{v}^{1/2})\tilde{\Delta}_q(\tilde{v}^{-1/2}). \tag{4.3}$$

Now

$$\tilde{A}_q = (\mathrm{U}(\mathfrak{g})[[h]], m, \tilde{\Delta}_q, \tilde{\epsilon}_q, \tilde{S}_q, \tilde{R}_q)$$

forms a braided Hopf superalgebra isomorphic to A_q.

Proposition 4.2: There exists a gauge transformation $F = 1 \otimes 1 + o(h)$ *such that*

$$\Delta = F\tilde{\Delta}_q F^{-1},$$

$$R = F_{21}\tilde{R}_q F^{-1},$$

$$\Phi_{KZ} = F_{23}(\mathrm{id} \otimes \tilde{\Delta}_q)(F)(\tilde{\Delta}_q \otimes \mathrm{id})(F^{-1})F_{12}^{-1},$$

where Δ *is the standard comultiplication for enveloping superalgebras,* $R = \exp(ht/2)$ *and* Φ_{KZ} *is given by (3.5).*

Proof: The deformations of the coalgebraic structure of $\mathrm{U}(\mathfrak{g})$ within the category of quasi-Hopf superalgebras are determined by $H_H^1(\mathrm{U}(\mathfrak{g}), \mathrm{U}(\mathfrak{g}) \otimes \mathrm{U}(\mathfrak{g}))$. Since for $\mathfrak{g} = \mathfrak{osp}(1|2n)$, $H_H^1(\mathrm{U}(\mathfrak{g}), \mathrm{U}(\mathfrak{g}) \otimes \mathrm{U}(\mathfrak{g})) = 0$, one can always find an $f = 1 \otimes 1 + o(h) \in (\mathrm{U}(\mathfrak{g}) \otimes \mathrm{U}(\mathfrak{g}))[[h]]$ with $(\epsilon \otimes \mathrm{id})f = (\mathrm{id} \otimes \epsilon)f = 1$ such that

$$f\tilde{\Delta}_q f^{-1} = \Delta.$$

Then $R^{(f)} = f_{21}\tilde{R}_q f^{-1}$ commutes with $\Delta(\mathrm{U}(\mathfrak{g})[[h]])$. Let

$$f' = (R^{(f)}(R_{21}^{(f)}R^{(f)})^{-1/2})^{1/2}.$$

It is easy to show that $(f'_{21})^2(f')^2 = 1$. Thus it follows from the uniqueness of the square root that $f'_{21} = (f')^{-1}$. Set

$$F = f'f.$$

We claim that F provides the desired gauge transformation.

Consider the effect of the further gauge transformation f' after f. The comultiplication Δ remains unchanged. The transformed R-matrix reads

$$R^{(F)}=f'_{21}R^{(f)}(f')^{-1}.$$

One can show that

$$R^{(F)}_{21}=R^{(F)}=f'(R^{(f)}_{21}R^{(f)})^{1/2}(f')^{-1}.$$

Thus $R^{(F)}$ is symmetric, and

$$(R^{(F)})^2=R^{(F)}_{21}R^{(F)}=f'R^{(f)}_{21}R^{(f)}(f')^{-1}=\Delta(\tilde{v}^{-1})(\tilde{v}\otimes\tilde{v}).$$

Upon taking the square root, we obtain $R^{(F)}=R$. Obviously

$$\Phi=F_{23}(\mathrm{id}\otimes\tilde{\Delta}_q)(F)(\tilde{\Delta}_q\otimes\mathrm{id})(F^{-1})F^{-1}_{12}$$

provides the associator for the braided quasi-Hopf superalgebra $\mathrm{U}(\mathfrak{g})[[h]]$ with the comultiplication Δ and universal R-matrix $\exp(ht/2)$. But with Δ and $R=\exp(ht/2)$ given, Φ_{KZ} is the unique associator, hence we must have $\Phi=\Phi_{KZ}$.

Finally we consider the antipode. Let

$$\alpha_F=m(\tilde{S}_q\otimes id)F^{-1},$$

$$\beta_F=m(id\otimes\tilde{S}_q)F,$$

$$A'_h=(\mathrm{U}(\mathfrak{g})[[h]],\Delta,\epsilon,R,\Phi_{KZ},\tilde{S}_q,\alpha_F,\beta_F).$$

Needless to say, $(\tilde{S}_q,\alpha_F,\beta_F)$ defines an antipode for A'_h. Applying Lemma 2.1 with $g=\alpha_F^{-1}$, we arrive at the antipode $(S,\alpha=1,\beta)$ with $\beta^{-1}=m(m\otimes\mathrm{id})(\mathrm{id}\otimes S\otimes\mathrm{id})\Phi_{KZ}$.

V. FRAMED LINK INVARIANTS

A. Colored ribbon graphs

We briefly discuss colored ribbon graphs here. Standard references on the subject are Refs. 15 and 16. Note that each (0,0) ribbon graph gives rise to a framed oriented link and vice versa.

By a ribbon we mean the square $[0,1]\times[0,1]$ smoothly embedded in $\mathbf{R}^3$. The images of $[0,1]\times 0$ and $[0,1]\times 1$ are the bases, and that of $\frac{1}{2}\times[0,1]$ is called the core of the ribbon. Similarly an annulus is the cylinder $S^1\times[0,1]$ embedded in $\mathbf{R}^3$, and the image of $S^1\times\frac{1}{2}$ under the embedding is called the core of the annulus. Ribbons and annuli are oriented as surfaces and their cores are directed.

Given k, $l\in\mathbb{Z}_+$. A (k,l) ribbon graph is an oriented surface consisting of ribbons and annuli such that ribbons and annuli never meet, and this surface intersects $(\mathbf{R}^2\times 0)\cup(\mathbf{R}^2\times 1)$ in the bases of the ribbons, where the collection of these bases are the collection of segments

$$\{[i-\tfrac{1}{4},i+\tfrac{1}{4}]\times 0\times 0|i=1,2,\ldots,k\}\cup\{[j-\tfrac{1}{4},j+\tfrac{1}{4}]\times 0\times 1|j=1,2,\ldots,l\}.$$

For simplicity, we will represent a ribbon or an annulus by its directed core.

Remark: Our notion of ribbon graphs is more restrictive than that of Refs. 15 and 16 in that coupons are not allowed.

We introduce two operations, composition and juxtaposition, to manufacture new ribbon graphs from given ones. Given (k,l) graph Γ_1, (l,m) graph Γ_2, and (k',l') graph Γ_3, the composition of $\Gamma_1\circ\Gamma_2$ is defined in the following way: shift Γ_2 by the vector (0,0,1) into

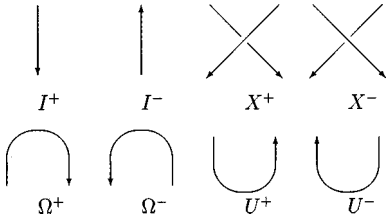

FIG. 1. Generators of ribbon graphs.

$\mathbf{R}^2\times[1,2]$, glue the bottom end of Γ_2 to the top end of Γ_1 in such a way that the core of the ribbons glued together should have the same direction as the core of the resultant ribbon (if this is not possible, then the composition is not defined), then reduce the size of the resultant picture by a factor of 2, leading to a (k, m) graph. The juxtaposition $\Gamma_1\otimes\Gamma_3$ is to position Γ_3 on the right of Γ_1, leading to a $(k+k', l+l')$ graph.

By repeatedly applying these two operations to the set of ribbon graphs depicted in Fig. 1, we can generate all the ribbon graphs.

We associate to each (k,l) graph Γ two sequences $\epsilon_*(\Gamma)=(\epsilon_1,\epsilon_2,\ldots,\epsilon_k)$ and $\epsilon^*(\Gamma)=(\epsilon^1,\epsilon^2,\ldots,\epsilon^l)$, ϵ^i, $\epsilon_j\in\{1,-1\}$, in the following way. For a ribbon of Γ with a base $[i-\frac{1}{4},i+\frac{1}{4}]\times 0\times 0$ (resp. $[j-\frac{1}{4},j+\frac{1}{4}]\times 0\times 1$), if its core is directed towards this base, then $\epsilon_i=1$ (resp. $\epsilon^j=-1$), and $\epsilon_i=-1$ (resp. $\epsilon^j=1$) otherwise.

Let $I=\{1,2,\ldots,N\}$ be a finite index set. We introduce the set $\mathcal{N}$ consisting of finite sequences of the form $((i_1,\epsilon_1),(i_2,\epsilon_2),\ldots,(i_k,\epsilon_k))$, $i_k\in I$, $k\in\mathbb{Z}_+$, $\epsilon_t\in\{1,-1\}$. A coloring of a ribbon graph Γ is a map associating with each ribbon or annulus of Γ an index $i\in I$. The category $\mathcal{H}$ of ribbon graphs is defined to have as objects the elements of $\mathcal{N}$, and as morphisms the ribbon graphs, where we require that if the ribbon graph Γ is a morphism $\eta\to\eta'$, $\eta,\eta'\in\mathcal{N}$, then the sequences of colors and directions of cores of the bottom and top ribbons must be equal to η and η', respectively. $\mathcal{H}$ is provided with a tensor product structure $\otimes:\mathcal{H}\times\mathcal{H}\to\mathcal{H}$, such that the tensor product of objects η and η' is to position the latter on the right of η to form one sequence, and the tensor product of morphism is simply the juxtaposition of ribbon graphs defined earlier.

B. Generalized Reshetikhin–Turaev functor

In Ref. 30, Altschuler and Coste extended the construction of Reshetikhin and Turaev[15,16] to braided quasi-Hopf algebras, obtaining a covariant functor from the category of colored ribbon graphs to the module category (with the strictly associative tensor product) of any ribbon quasi-Hopf algebra. Their result can be directly extended to the supersymmetric setting, leading to the following generalization of Theorem 1 of Ref. 8.

Theorem 5.1: *Let A be a ribbon quasi-Hopf superalgebra. Let $\{V_i|i\in I\}$ be a set of A-modules, which are free $\mathbb{K}$-modules of finite ranks. There exists a unique covariant functor F from the category $\mathcal{H}$ of colored ribbon graphs to the module category of A with the strictly associative tensor product such that*

(1) F transforms any object $\eta=((i_1,\epsilon_1),(i_2,\epsilon_2),\ldots,(i_k,\epsilon_k))$ of $\mathcal{H}$ into the A-module $(\mathbf{V}(\eta))=(\cdots(V_{i_1}^{\epsilon_1}\otimes V_{i_2}^{\epsilon_2})\otimes\cdots)\otimes V_{i_k}^{\epsilon_k}$, where $V_i^{+1}=V_i$, $V_i^{-1}=V_i^*$, and if $k=0$, then $V(\eta)$ is defined as the trivial A module.

(2) For any two colored ribbon graphs Γ and Γ',

$$F(\Gamma\otimes\Gamma')=F(\Gamma)\odot F(\Gamma'), \tag{5.1}$$

that is, F preserves the tensor product $\odot$.

(3) Color the bottom left ribbons of X^+ and X^- by i and the bottom right ones by j, and denote the resultant colored ribbon graphs by X_{ij}^+ and X_{ij}^- respectively. Then

$$F(X_{ij}^{+})=\tau R:\quad V_i\odot V_j\to V_j\odot V_i,$$
$$F(X_{ij}^{-})=R^{-1}\tau:\quad V_i\odot V_j\to V_j\odot V_i, \tag{5.2}$$

where R is the universal R matrix of A, and τ is the flipping map. Similarly, we have

$$F(I_i^{+})=id:V_i\to V_i,$$
$$F(I_i^{-})=id:V_i^{*}\to V_i^{*},$$
$$F(\Omega_i^{+}):V_i^{*}\odot V_i\to\mathbb{K},$$
$$x^{*}\otimes y\mapsto x^{*}(\alpha y),$$
$$F(\Omega_i^{-}):V_i\odot V_i^{*}\to\mathbb{K},$$
$$x\otimes y^{*}\mapsto(-1)^{[x]}y^{*}(S(\alpha)uv^{-1}x),$$
$$F(U_i^{+}):\mathbb{K}\to V_i\odot V_i^{*},$$
$$c\mapsto c\sum_t \beta b_t\otimes b_t^{*},$$
$$F(U_i^{-}):\mathbb{K}\to V_i^{*}\odot V_i,$$
$$c\mapsto c\sum_t (-1)^{[b_t]}b_t^{*}\otimes u^{-1}vS(\beta)b_t, \tag{5.3}$$

where $\{b_t\}$ is a basis for V_i, and $\{b_t^{*}\}$ a basis for V_i^{*}, which are dual to each other in the sense that $b_s^{*}(b_t)=\delta_{st}$.

Let $\eta=((i_1,\epsilon_1),(i_2,\epsilon_2),\ldots,(i_k,\epsilon_k))$. Consider the (k,k) colored ribbon graph $\Gamma_c:\eta\to\eta$. We joint the top and bottom right-most ends to get the following $(k-1,k-1)$ colored ribbon graph

$$(I^{\epsilon_1}\otimes\cdots\otimes I^{\epsilon_{k-1}}\otimes U^{\epsilon_k})(\Gamma_c\otimes I^{-\epsilon_k})(I^{\epsilon_1}\otimes\cdots\otimes I^{\epsilon_{k-1}}\otimes\Omega^{-\epsilon_k}).$$

Iterating this process we will arrive at the (0,0) colored ribbon graph $\hat{\Gamma}_c$, which we call the closure of Γ_c. Now $F(\Gamma_c)$ is a module map from $(\mathbf{V}(\eta))=V_{i_1}^{\epsilon_1}\odot\cdots\odot V_{i_k}^{\epsilon_k}$ to itself, and

$$F(\hat{\Gamma}_c)=\mathrm{str}[\beta S(\alpha)uv^{-1}F(\Gamma_c)],$$

where the supertrace is taken over $(\mathbf{V}(\eta))$. In particular, for a (1,1) graph Γ_c with the open strand colored by an A-module V, there exists a central element γ of A such that

$$F(\Gamma_c)=\gamma:V\to V.$$

If we assume that the A-module V admits central characters, i.e., all central elements of A act by scalars, then

$$F(\Gamma_c)=\chi_V(\gamma)\,\mathrm{id}_V:V\to V,$$
$$F(\hat{\Gamma}_c)=\chi_V(\gamma)SD_q(V),$$

where $\chi_V(\gamma)$ is the eigenvalue of γ in V, and $SD_q(V)=\mathrm{str}_V(\beta S(\alpha)uv^{-1})$ is the quantum superdimension of V. It follows that for any (0,0) graph, if any of its components is colored with an A-module (on which central elements of A act on as scalars), which has a vanishing quantum superdimension, then the Reshetikhin–Turaev functor yields zero when applied to the ribbon graph.

For any colored ribbon graph Γ_c, consider the A-module homomorphism $F(\Gamma_c)$. Under a gauge transformation as defined by (2.8), $F(\Gamma_c)$ transforms according to (2.11). Under a transformation (2.3) on the antipode, $F(\Gamma_c)$ transforms as (2.12). In particular, if Γ_c is a (0,0) colored ribbon graph, $F(\Gamma_c)$ is an A-module map $\mathbb{K}\to\mathbb{K}$. In this case, (2.11) and (2.12) dictate that $F(\Gamma_c)$ is not changed. We state this observation as follows.

Lemma 5.1: For any (0,0) *colored ribbon graph* Γ_c, $F(\Gamma_c)$ *remains intact under gauge transformations and antipode transformations*.

C. Drinfeld–Jimbo quantum superalgebras versus braided enveloping superalgebras

For convenience, we set

$$A_q=(\mathrm{U_q}(\mathfrak{g}),m_q,\Delta_q,\epsilon,S_q,R_q,v_q),$$

$$A[[h]]=(\mathrm{U}(\mathfrak{g})[[h]],m,\Delta,\epsilon,S,\Phi=\Phi_{KZ},R,\alpha,\beta,v),$$

where v is the Drinfeld operator defined by (2.6). For $A[[h]]$, $\alpha=1$ and $v=u$.

Equipped with Theorem 5.1, we can easily construct link invariants from the new braided enveloping superalgebras $A[[h]]$. Such link invariants should be closely related to the link invariants obtained by using the standard Drinfeld–Jimbo quantum superalgebras A_q. We shall formulate a conjecture on their relationship and prove it in the case of $\mathfrak{osp}(1|2n)$.

Consider a set of non-isomorphic $\mathrm{U_q}(\mathfrak{g},\phi)$-modules, $\{V_i[[h]]=V_i\otimes_{\mathbb{C}}\mathbb{C}[[h]]|i\in I\}$, which satisfies the following conditions:

(1) all $V_i[[h]]$ are free $\mathbb{C}[[h]]$-modules of finite ranks;
(2) as $\mathrm{U_q}(\mathfrak{g},\phi)$-modules, the $V_i[[h]]$ are indecomposable and
(3) admit central characters, i.e., the central elements of $\mathrm{U_q}(\mathfrak{g},\phi)$ act on each $V_i[[h]]$ by scalar multiplications; and
(4) for each $i\in I$, there exists a unique $i^*\in I$ such that $V_{i*}[[h]]=(V_i[[h]])^*$.

Now we can use $\{V_i[[h]]|i\in I\}$ to color ribbon graphs, and to construct the RT functor following the general procedure of subsection V.B, but with $\Phi=1\otimes 1\otimes 1$ and $\alpha=\beta=1$. This reproduces the result of Theorem 1 of Ref. 8.

Let Γ be a ribbon graph with m components labeled by the integers $1,2,\ldots,m$. For each k, we color the kth component of the ribbon graph with the $\mathrm{U_q}(\mathfrak{g},\phi)$-module $V_{i_k}[[h]]$, and denote the resultant colored ribbon graph by Γ_c. Applying the generalized RT functor to the colored ribbon graph leads to a $\mathrm{U_q}(\mathfrak{g},\phi)$-module homomorphism

$$F_{A_q,\{V_i[[h]]|i\in I\}}(\Gamma_c):\mathbb{C}[[h]]\to\mathbb{C}[[h]].$$

Each $\mathrm{U_q}(\mathfrak{g})$-module $V_i[[h]]$ gives rise to a finite dimensional $\mathrm{U}(\mathfrak{g})$-module

$$V_i=V_i[[h]]/hV_i[[h]]$$

over $\mathbb{C}$. We assume that as $\mathrm{U}(\mathfrak{g})$-modules, the V_i, $i\in I$, are non-isomorphic and have the following properties: (a) the V_i are indecomposable and (b) admit central characters; and (c) for each $i\in I$, there exists a unique $i^*\in I$ such that $V_{i*}=V_i^*$.

Remark: There always exist $\mathrm{U_q}(\mathfrak{g})$-modules $V_i[[h]]$, $i\in I$, satisfying the conditions (1)–(4), such that the associated $\mathrm{U}(\mathfrak{g})$-modules V_i, $i\in I$, meet the conditions (a)–(c).

Now $V_i\otimes_{\mathbb{C}}\mathbb{C}[[h]]$ admits a $U(\mathfrak{g})[[h]]$-module structure in the obvious way. As $V_i[[h]]$ is free over $\mathbb{C}[[h]]$, we have $V_i[[h]]=V_i\otimes_{\mathbb{C}}\mathbb{C}[[h]]$. We shall apply the construction of Sec. V B to the braided quasi-Hopf superalgebra $A[[h]]$ with the set $\{V_i[[h]]|i\in I\}$ of $U(\mathfrak{g})[[h]]$-modules. Because of the special forms of α and v in the present context, Eq. (5.3) is considerably simplified.

For a (0,0) ribbon graph Γ with m components labeled by the integers $1,2,\ldots,m$, we color its kth component by the $U(\mathfrak{g})[[h]]$-module $V_{i_k}[[h]]$ for each k, and denote by Γ_c the resultant colored ribbon graph. Applying the generalized RT functor to the colored ribbon graph leads to a $U(\mathfrak{g})[[h]]$-module homomorphism

$$F_{A[[h]],\{V_i[[h]]|i\in I\}}(\Gamma_c):\mathbb{C}[[h]]\to\mathbb{C}[[h]].$$

It is important for the purpose of studying link invariants to understand the relationship between $F_{A_q,\{V_i[[h]]|i\in I\}}(\Gamma_c)$ and $F_{A[[h]],\{V_i[[h]]|i\in I\}}(\Gamma_c)$. We conjecture that

$$F_{A_q,\{V_i[[h]]|i\in I\}}(\Gamma_c)=F_{A[[h]],\{V_i[[h]]|i\in I\}}(\Gamma_c) \tag{5.4}$$

for all the simple basic classical Lie superalgebras but a few exceptions. We do not have a proof at hand (A proof probably requires a thorough understanding of the Drinfeld–Jimbo quantum superalgebras from a deformation theoretical point of view.) However, we can show the following.

Theorem 5.2: *Equation (5.4) holds when* $\mathfrak{g}=\mathfrak{osp}(1|2n)$.

Proof: Let $\mathfrak{g}=\mathfrak{osp}(1|2n)$ in the proof. Consider the A_q-module $V_i[[h]]$. The inverse of the Hopf superalgebra isomorphism H_h induces a natural $\tilde{A}_q$-module structure on $V_i[[h]]$, defined by

$$\tilde{A}_q\otimes V_i[[h]]\to V_i[[h]],$$

$$\tilde{x}\otimes v\mapsto H_h^{-1}(\tilde{x})v.$$

Clearly, $F_{A_q,\{V_i[[h]]|i\in I\}}(\Gamma_c)=F_{\tilde{A}_q,\{V_i[[h]]|i\in I\}}(\Gamma_c)$.

As we have shown in the last section, a gauge transformation turns the ribbon Hopf superalgebra $\tilde{A}_q$ into a ribbon quasi-Hopf superalgebra A_h'. Under this gauge transformation, $F_{\tilde{A}_q,\{V_i[[h]]|i\in I\}}(\Gamma_c)$ transforms to $F_{A_h',\{V_i[[h]]|i\in I\}}(\Gamma_c)$. Because Γ_c is a (0,0) colored ribbon graph, it follows Lemma 5.1 that

$$F_{\tilde{A}_q,\{V_i[[h]]|i\in I\}}(\Gamma_c)=F_{A_h',\{V_i[[h]]|i\in I\}}(\Gamma_c).$$

Finally we consider the transformation $g=\alpha_F^{-1}$ on the antipode $(\tilde{S}_q,\alpha_F,\beta_F)$ of A_h'. This transformation also turns $F_{A_h',\{V_i[[h]]|i\in I\}}(\Gamma_c)$ to $F_{A[[h]],\{V_i[[h]]|i\in I\}}(\Gamma_c)$. Using Lemma 5.1 again we have

$$F_{A_h',\{V_i[[h]]|i\in I\}}(\Gamma_c)=F_{A[[h]],\{V_i[[h]]|i\in I\}}(\Gamma_c).$$

This proves the theorem.

D. Vassiliev invariants

Each framed link can be represented as a (0,0)-ribbon graph Γ. Let us color all the components of Γ by the same finite dimensional indecomposable A_q-module $V[[h]]$. Then $F_{A_q,\{V_i[[h]]|i\in I\}}$ gives rise to a framed link invariant, which we denote by ν_q. We may formally regard ν_q as a power series in h,

$$\nu_q=\sum_{k=0}^{\infty}h^k\nu^{(k)}, \tag{5.5}$$

where $\nu^{(k)}:\{\text{framed links}\}\to\mathbb{C}$ are framed link invariants themselves. As we have already mentioned, each $\nu^{(k)}$ is a Vassiliev invariant of degree $\leqslant k$. We now explain this point following Birman and Lin.[17] A framed link invariant ν can be extended to an invariant of singular framed links in the following way. If L is a singular framed link, we may replace any one of its double point by an over crossing to get L_+, or by an under crossing to get L_-. Then $\nu(L)$ is defined inductively by

$$\nu(L)=\nu(L_+)-\nu(L_-).$$

It is easy to see that the definition is independent of the order in which the singular points are resolved. A (framed) link invariant is a Vassiliev invariant of degree $\leqslant k$ if it vanishes on all singular (framed) links with more than k double points.

Consider ν_q applied to a singular framed link L with $(k+1)$ double points. Because of (3.1),

$$\nu_q(L)\in h^{k+1}\mathbb{C}[[h]].$$

Therefore, $\nu^{(i)}(L_c)=0$, $\forall i\leqslant k$.

Remark: Equation (5.5) is of little use for computing the Vassiliev invariants $\nu^{(k)}$, as there is no known way to expand the universal R-matrix R_q into a power series in h.

On the other hand, we may use the $A[[h]]$-module $V[[h]]$ to color all the components of Γ to obtain a framed link invariant from $F_{A[[h]],\{V_i[[h]]|i\in I\}}$, which we will denote by $\mu[[h]]$. Clearly, $\mu[[h]]$ is a powers series in h,

$$\mu[[h]]=\sum_{k=0}^{\infty}h^k\mu^{(k)},$$

and each $\mu^{(k)}$ is a Vassiliev invariant of framed links. Now both the associator and R-matrix of $A[[h]]$ are known as power series in h, thus the $\mu^{(k)}$ are computable.

Thus we have the following from Theorem 5.4 that

Corollary 5.1. In the case of $\mathfrak{osp}(1|2n)$, $\nu^{(k)}=\mu^{(k)}$, *for all* k.

This provides us with a more accessible construction of the Vassiliev invariants $\nu^{(k)}$ associated with the Drinfeld–Jimbo quantum superalgebra $\mathrm{U}_q(\mathfrak{osp}(1|2n))$.

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Controllability of quantum mechanical systems by root space decomposition of $\mathfrak{su}(N)$

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The controllability property of the unitary propagator of an N-level quantum mechanical system subject to a single control field is described using the structure theory of semisimple Lie algebras. Sufficient conditions are provided for the vector fields in a generic configuration as well as in a few degenerate cases. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1467611]

I. INTRODUCTION

The question of controllability for a finite level quantum system, see Dahlen *et al.* (1996), Schirmer *et al.* (2001a), Turinici and Rabitz (2001) is studied in this paper by analyzing the structure of the semisimple Lie algebra of its time evolution operator. The system dynamics is determined by its internal Hamiltonian and by an external Hamiltonian describing the interaction with a control field. Of the several different aspects of controllability that can be defined for a closed system of such type [overviewed in Albertini and D'Alessandro (2001); Schirmer *et al.* (2001b)] we consider here the more direct and important in practical applications, namely the controllability of its unitary propagator which, in control terms, is governed by a bilinear system with drift and a single control input and evolves on $\mathrm{SU}(N)$. For a compact semisimple Lie group like $\mathrm{SU}(N)$, the testing of global controllability is the simplest of all noncommutative Lie groups. In fact, compactness implies that the accessibility property collapses into (global) controllability and semisimplicity implies that almost all pairs of vector fields span the corresponding Lie algebra. The first property means that purely algebraic tools, like the *Lie algebra rank condition* normally used in control theory provides necessary and *sufficient* conditions for controllability, while the second property affirms that controllability is generically verified even in the single control case. The main scope of this paper is to give the interpretation of these properties in terms of structure theory of semisimple Lie algebras, see Cornwell (1997), Gilmore (1974), Sattinger (1986), and to provide alternative tests to the exhaustive computation of commutators that the Lie algebra rank condition requires. So genericity is interpreted in terms of regularity of the roots of the Lie algebra $\mathfrak{su}(N)$ and another property, regularity along the control vector field, immediately follows. Replacing the Lie algebra rank condition means seeking alternative conditions that guarantee the maximal nonintegrability of the pair of vector fields. The main tool we use, together with the regularity of the roots, is the connectivity of the graph of the control vector field. Both properties were classically used to analyze controllability of vector fields on semisimple Lie algebras (especially the noncompact ones, see Jurdjevic and Kupka (1981), Gauthier and Bonnard (1982), El Assoudi *et al.* (1995), Silva Leite and Crouch (1988). For the same type of problem as ours, the properties of the graph were recently used also in Turinici *et al.* (2001). The conditions we obtain, based only on the *a priori* knowledge of the two vector fields, are only sufficient but they allow us to avoid any computation of Lie brackets. From the generic case, physically representing a quantum system with all different transition values between its (nondegenerate) energy levels, these tools carry on to the singular case, where some of these levels might be equispaced.

The paper is organized as follows: the structure theory of semisimple Lie algebras is recalled

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in Sec. II and it is applied to the quantum system in Sec. III, where all the needed control concepts are given. The sufficient conditions for a generic pair of vector fields are given in Sec. IV, while in Sec. V the simplest among the singular cases are analyzed.

II. ROOT SPACE DECOMPOSITION FOR $\mathfrak{su}(N)$

Consider the classical Lie algebra A_{N-1}, complexification of $\mathfrak{su}(N)$ according to Cartan's notation. The subindex $N-1$ is the rank of the *Cartan subalgebra* $\mathfrak{h}$ of A_{N-1}, i.e., of the maximal Abelian subalgebra such that the endomorphism ad_H of A_{N-1} is semisimple for all $H \in \mathfrak{h}$.

Definition 1: An element $H \in A_{N-1}$ is said to be regular if the multiplicity of the zero eigenvalue of ad_H *is equal to the rank of A_{N-1}, i.e.,* $\dim(\ker \mathrm{ad}_H) = \mathrm{rank}\, A_{N-1} = N-1$.

The set of regular elements H is open and dense in A_{N-1}. Choose one such H and consider the corresponding Cartan subalgebra $\mathfrak{h} = \mathfrak{g}_0(H) = \{B \in A_{N-1} | \mathrm{ad}_H B = 0\}$.

The *roots* of A_{N-1} are the functionals α on $\mathfrak{h}$ such that, for $H \in \mathfrak{h}$, $\mathrm{ad}_H B = \alpha(H)B$, $B \in A_{N-1}$, i.e., α give the eigenvalues of ad_H for each choice of H. Denote by Δ the set of nonzero roots of A_{N-1} with respect to $\mathfrak{h}$, by Δ^+ the subset of positive roots with respect to the lexicographic order on the dual of $\mathfrak{h}$, and by Φ the set of *fundamental roots*, i.e., the set of positive roots that cannot be written as sums of two other positive roots.

We need a stronger version of the regularity property, see Jurdjevic (1996)—p. 187.

Definition 2: A regular $H \in A_{N-1}$ is said to be strongly regular if all nonzero eigenvalues $\alpha(H)$ are distinct and have multiplicity 1.

Also the set of strongly regular elements is open and dense in A_{N-1}. For all strongly regular H, the decomposition induced by the roots has the same structure: A_{N-1} can be written as a direct sum of *root spaces* $\mathfrak{g}_\alpha = \{B \in A_{N-1} | \mathrm{ad}_H B = \alpha(H)B\}$:

$$A_{N-1} = \mathfrak{h} + \bigoplus_{\alpha \in \Delta} \mathfrak{g}_\alpha .$$

Each $\mathfrak{g}_\alpha$ is invariant for ad_H and satisfies $[\mathfrak{g}_\alpha, \mathfrak{g}_\beta] = \mathfrak{g}_{\alpha+\beta}$ where $\mathfrak{g}_{\alpha+\beta} = 0$ if $\alpha + \beta \notin \Delta$. Furthermore, calling K the Killing form, i.e., the bilinear form $K : A_{N-1} \times A_{N-1} \to \mathbb{R}$, $X, Y \mapsto \mathrm{trace}(\mathrm{ad}_X \mathrm{ad}_Y)$, the restriction of K to $\mathfrak{h}$ is nondegenerate and for each root $\alpha \in \Delta$ there exists a unique $H_\alpha \in \mathfrak{h}$ such that $\alpha(H) = K(H, H_\alpha)$, so that $\alpha(H_\alpha) = K(H_\alpha, H_\alpha) \neq 0$. If $\alpha \in \Delta$, so does $-\alpha$ and for $X \in \mathfrak{g}_\alpha$ and $Y \in \mathfrak{g}_{-\alpha}$ $[X, Y] = K(X, Y)H_\alpha$. Therefore, by normalizing, we can choose *root vectors* $E_\alpha \in \mathfrak{g}_\alpha$ such that

$$[H, E_\alpha] = \alpha(H)E_\alpha \quad \text{for } H \in \mathfrak{h},$$

$$[E_\alpha, E_{-\alpha}] = H_\alpha ,$$

$$[E_\alpha, E_\beta] = \begin{cases} 0 & \text{if } \alpha + \beta \notin \Delta \\ N_{\alpha\beta} E_{\alpha+\beta} & \text{if } \alpha + \beta \in \Delta, \end{cases} \tag{1}$$

where $N_{\alpha\beta}$ are real constants and $N_{\alpha\beta} = -N_{(-\alpha)(-\beta)}$ From (1), one obtains a *Weyl basis* for A_{N-1}:

$$\{H_\alpha, \alpha \in \Phi\} \cup \{E_\alpha, \alpha \in \Delta\}. \tag{2}$$

Since $\{\mathrm{ad}_H \mid H \in \mathfrak{h}\}$ is a commuting family of semisimple operators, there is a basis of A_{N-1} in which these operators are simultaneously diagonalizable. Fix $\overline{H} \in \mathfrak{h}$ to be one such $N \times N$ diagonal traceless matrices, $\overline{H} = \mathrm{diag}(\lambda_1, \ldots, \lambda_N)$ such that $\Sigma_{i=1}^N \lambda_i = 0$ where the λ_i are assumed to be ordered: $\lambda_1 > \ldots > \lambda_N$. Let E_{ij} be the matrix with 1 in the (ij) slot and 0 elsewhere. Since $\mathrm{ad}_{\overline{H}} E_{ij} = (\lambda_i - \lambda_j)E_{ij}$, the E_{ij} are the root vectors and the roots are the functionals α_{ij} such that

$\alpha_{ij}(\overline{H})=\lambda_i-\lambda_j$. The sum $\alpha_{ij}+\alpha_{kl}$ is a root if and only if $j=k$ or $i=l$ (if both, then it is the zero root). In fact, from $E_{ij}E_{kl}=\delta_{jk}E_{il}$ where δ_{ij} is the Kroneker delta, $[E_{ij},E_{kl}]=\delta_{jk}E_{il}-\delta_{li}E_{kj}$, i.e.,

$$[E_{ij},E_{kl}]=\begin{cases}0 & \text{if } j\neq k \text{ and } i\neq l\\ E_{il} & \text{if } j=k\\ -E_{kj} & \text{if } i=l\\ E_{ii}-E_{jj} & \text{if } j=k \text{ and } i=l.\end{cases} \tag{3}$$

The roots α_{ij} are real and such that if α_{ij} is a root so is $-\alpha_{ij}$. $\overline{H}$ is a strongly regular element if $\alpha_{ij}\neq\alpha_{kl}$, for indexes i, j, k, l such that $(i,j)\neq(k,l)$, $i\neq j$ and $k\neq l$. Thus $\overline{H}$ is strongly regular if and only if $\lambda_i-\lambda_j\neq\lambda_k-\lambda_l$. The fundamental roots are α_{12}, $\alpha_{23},\ldots,\alpha_{N-1,N}$ and a basis of A_{N-1} corresponding to (2) is given by

$$\{H_i=E_{ii}-E_{i+1,i+1},i=1,\ldots,N-1\}\cup\{E_{ij},i,j=1,\ldots,N,i\neq j\} \tag{4}$$

$\mathfrak{su}(N)$ is the *compact real form* of A_{N-1} since it corresponds to a negative definite Killing form. The basis of $\mathfrak{su}(N)$ corresponding to (2) is

$$\{iH_\alpha,\alpha\in\Phi\}\cup\{X_\alpha=E_\alpha-E_{-\alpha},\alpha\in\Delta^+\}\cup\{Y_\alpha=i(E_\alpha+E_{-\alpha}),\alpha\in\Delta^+\} \tag{5}$$

or, after diagonalization of the Cartan subalgebra

$$\{iH_i,i=1,\ldots,N-1\}\cup\{X_{ij}=E_{ij}-E_{ji},\ 1\leqslant i<j\leqslant N\}\cup\{Y_{ij}=i(E_{ij}+E_{ji}),\ 1\leqslant i<j\leqslant N\}. \tag{6}$$

Indeed, this skew-Hermitian basis forms a real Lie algebra as all the structure constants are real:

$$\begin{aligned}
[X_{ij},X_{kl}]&=\delta_{jk}X_{il}+\delta_{il}X_{jk}+\delta_{jl}X_{ki}+\delta_{ik}X_{lj},\\
[Y_{ij},Y_{kl}]&=\delta_{jk}X_{li}+\delta_{il}X_{kj}+\delta_{jl}X_{ki}+\delta_{ik}X_{lj},\\
[X_{ij},Y_{kl}]&=\delta_{jk}Y_{il}-\delta_{il}Y_{kj}+\delta_{jl}Y_{ik}-\delta_{ik}Y_{lj},\\
[iH_i,X_{jk}]&=\delta_{ij}Y_{ik}-\delta_{ik}Y_{ji}-\delta_{i+1,j}Y_{i+1,k}+\delta_{k,i+1}Y_{j,i+1},\\
[iH_i,Y_{jk}]&=\delta_{ij}X_{ki}+\delta_{ik}X_{ji}+\delta_{i+1,j}X_{i+1,k}+\delta_{k,i+1}X_{i+1,j}.
\end{aligned} \tag{7}$$

The basis (5) corresponds to the direct sum, orthogonal with respect to the Killing form:

$$\mathfrak{su}(N)=\bigoplus_{\alpha\in\Phi}i\mathbb{R}H_\alpha\bigoplus_{\alpha\in\Delta^+}\mathbb{R}X_\alpha\bigoplus_{\alpha\in\Delta^+}\mathbb{R}Y_\alpha. \tag{8}$$

If A is in the Cartan subalgebra of $\mathfrak{su}(N)$, then $A=iH$ with $H\in\mathfrak{h}$. Since the values of the roots at H, $\alpha(H)$, are real, $\alpha(A)$ will be imaginary and, from (7),

$$\begin{aligned}
\mathrm{ad}_A X_\alpha&=\alpha(H)Y_\alpha,\\
\mathrm{ad}_A Y_\alpha&=-\alpha(H)X_\alpha,
\end{aligned} \tag{9}$$

thus the vector space $\mathfrak{f}_\alpha=\mathbb{R}X_\alpha+\mathbb{R}Y_\alpha$ is invariant for ad_A. Furthermore, the vector spaces corresponding to the fundamental roots are enough to generate all the α-strings and therefore

Lemma 1: $\{\oplus_{\alpha\in\Phi}\mathfrak{f}_\alpha\}_{L.A.}=\mathfrak{su}(N)$

Proof: Similar to (3), in the basis (6) we obtain [using (7)]:

$$[\mathfrak{f}_{ij},\mathfrak{f}_{kl}]=\begin{cases}\varnothing & \text{if } j\neq k \quad \text{and } i\neq l\\ \mathfrak{f}_{il} & \text{if } j=k\\ \mathfrak{f}_{kj} & \text{if } i=l\\ \in\mathfrak{h} & \text{if } j=k \quad \text{and } i=l.\end{cases} \tag{10}$$

Thus from $\{\oplus_{\alpha\in\Phi}\mathfrak{f}_\alpha\}$ it is possible to generate $\{\oplus_{\alpha\in\Delta^+}\mathfrak{f}_\alpha\}$. Moreover, $[X_{i,i+1},Y_{i,i+1}]=2iH_i$, $i=1,\ldots,N-1$, therefore also $i\mathfrak{h}$ is generated. ■

On the other hand, a proper subset of fundamental roots cannot generate $\mathfrak{su}(N)$.

Lemma 2: If $\Phi'\subsetneq\Phi$ *then* $\{\oplus_{\alpha\in\Phi'}\mathfrak{f}_\alpha\}_{L.A.}\subsetneq\mathfrak{su}(N)$.

Proof: Trivial since by its very definition a fundamental root cannot be written as a sum of other positive roots, therefore if $\overline{\alpha}$ is a missing fundamental root, $\nexists\ \alpha,\beta\in\Phi$ such that $[E_\alpha,E_\beta]=N_{\alpha,\beta}E_{\overline{\alpha}}$. Thus $X_{\overline{\alpha}}$ and $Y_{\overline{\alpha}}$ are not spanned by any bracket. ■

III. QUANTUM CONTROL SYSTEM

Consider a finite level quantum system described by a state $|\psi\rangle$ evolving according to the time-dependent Schrödinger equation

$$i\hbar|\dot{\psi}(t)\rangle=(\hat{H}_0+u(t)\hat{H}_1)|\psi(t)\rangle, \tag{11}$$

where the traceless Hermitian matrices $\hat{H}_0$ and $\hat{H}_1$ are, respectively, the internal (or free) Hamiltonian and the external Hamiltonian, the latter representing the interaction of the system with a single control field $u(t)$. In the N-level approximation, the state $|\psi\rangle$ is expanded with respect to a basis of N orthonormal eigenstates $|\varphi_i\rangle$: $|\psi\rangle=\Sigma_{i=1}^N c_i|\varphi_i\rangle$ where the c_i are complex coefficients that satisfy the normalization condition $\Sigma_{i=1}^N|c_i|^2=1$. If we write the initial condition of (11) as $|\psi_0\rangle=\Sigma_{i=1}^N c_{0i}|\varphi_i\rangle$, then also the vector $c=[c_1\cdots c_N]^T$ satisfies a differential equation similar to (11):

$$\begin{gathered}i\hbar\dot{c}(t)=(\tilde{H}_0+u(t)\tilde{H}_1)c(t),\\ c(0)=c_0,\end{gathered} \tag{12}$$

where now the traceless Hermitian matrix $\tilde{H}_0$ is diagonal. The real coefficients $\mathcal{E}_i$, $\mathcal{E}_1\leqslant\cdots\leqslant\mathcal{E}_N$, appearing along the diagonal of $\tilde{H}_0$ are eigenvalues, $\tilde{H}_0|\varphi_i\rangle=\mathcal{E}_i|\varphi_i\rangle$, and represent the energy levels of the system. If $\mathcal{E}_i=\mathcal{E}_j$ for some $i\neq j$, then the system is said to be *degenerate*. If, instead, some of the levels are equispaced, $\mathcal{E}_i-\mathcal{E}_j=\mathcal{E}_k-\mathcal{E}_l$ for $(i,j)\neq(k,l)$, $i\neq j$, $k\neq l$, then the system is said to have *degenerate transitions* (or resonances). The solution of (12) is $c(t)=X(t)c(0)$ with the unitary matrix $X(t)$ representing the time evolution operator. If we use atomic units ($\hbar=1$), then instead of (12) we can study the right invariant bilinear control system evolving on the Lie group SU(N) and characterized by the skew-Hermitian vector fields $A=-i\tilde{H}_0$ and $B=-i\tilde{H}_1$:

$$\begin{gathered}\dot{X}(t)=(A+u(t)B)X(t),\quad X(t)\in SU(N),\quad A,B\in\mathfrak{su}(N),\\ X(0)=I.\end{gathered} \tag{13}$$

The system (13) is said to be (globally) *controllable* if the reachable set

$$\mathcal{R}_{\{A,B\}}=\{\overline{X}\in SU(N)|\ \text{there exists an admissible input } u(\cdot) \text{ such that the integral curve of (13) satisfies } X(0)=I,\ X(t)=\overline{X} \text{ for some } t\geqslant 0\}$$

is all of the Lie group: $\mathcal{R}_{\{A,B\}}=\mathrm{SU}(N)$. Given (any) $A,B\in\mathfrak{su}(N)$, call $\{A,B\}_{L.A.}$ the Lie algebra generated by A and B with respect to the Lie bracket. The literature on the subject of quantum control, see D'Alessandro (2001), Ramakrishna *et al.* (1995), Albertini and D'Alessandro (2001), has relied essentially on the condition of the following Theorem [originally due to Jurdjevic and Sussmann (1972)]:

Theorem 1: *The system (13) is controllable if and only if* $\{A,B\}_{L.A.}=\mathfrak{su}(N)$.

Theorem 1 is a consequence of the following Lemma, which affirms that subsemigroups of compact groups are always subgroups:

Lemma 3: [Lemma 1, Chap. 6 of Jurdjevic (1996)]: *For the compact semisimple Lie group* $\mathrm{SU}(N)$,

$$\mathrm{cl}(\exp(tA,t<0))\subset\mathrm{cl}(\exp(tA,t\geqslant 0)),\quad \forall A\in\mathfrak{su}(N),$$

where $\exp:\mathfrak{su}(N)\rightarrow\mathrm{SU}(N)$ *is the Lie group exponential map (and* cl *means closure*).

Consequently, the drift vector field A of (13) is not hampering controllability on the large and thus Theorem 1 follows. Since the controllability in this case is obtained for ''large times'' the situation would be different if ''small time local controllability'' were of interest, see D'Alessandro (2001). Furthermore, the semisimple character of $\mathfrak{su}(N)$ implies the following:

Lemma 4: [Theorem 12, Chap. 6 of Jurdjevic (1996)]: *The set of pairs* $A,B\in\mathfrak{su}(N)$ *such that* $\{A,B\}_{L.A.}=\mathfrak{su}(N)$ *is open and dense in* $\mathfrak{su}(N)$.

Putting together Theorem 1 and Lemma 4 then we have:

Corollary 1: The system (13) is controllable for almost all pairs $A,B\in\mathfrak{su}(N)$.

In spite of the above mentioned generic result, there is still some interest in the controllability problem, especially

(1) characterizing the algebraic set in which controllability may fail,

(2) determining alternative procedures for testing controllability, other than exhaustive computation of Lie brackets,

(3) finding sufficient conditions for controllability based on the *a priori* knowledge of the vector fields A and B.

This paper is dedicated to the last two items of the list.

Roots and graphs. B is expressed in terms of the components of the $\mathfrak{su}(N)$ basis (5) as

$$B=B_0+\sum_{\alpha\in\Gamma^+\subseteq\Delta^+}(b_\alpha^{\Re}X_\alpha+b_\alpha^{\Im}Y_\alpha),\tag{14}$$

where $B_0\in i\mathfrak{h}$, $b_\alpha^{\Re}$ and $b_\alpha^{\Im}$ are real and $\Gamma^+\subseteq\Delta^+$ is the subset of roots ''touched'' by B.

In this case, it is possible to use the connectivity properties of the graph of B to draw conclusions about controllability in the same spirit as is done in Gauthier and Bonnard (1982), Silva Leite and Crouch (1988) for *normal* (or *split*) *real forms* and, more recently, in Turinici and Rabitz (2001) for the same quantum control problem. Consider the *graph* $\mathcal{G}_B$ associated with a square matrix $B=[b_{ij}]$, i.e., the pair $\mathcal{G}_B=(\mathcal{N}_B,\mathcal{C}_B)$ where $\mathcal{N}_B$ represents a set of N ordered nodes $\mathcal{N}_B=\{1,\ldots,n\}$ and $\mathcal{C}_B$ the set of oriented arcs joining the nodes: $\mathcal{C}_B=\{(i,j)|b_{ij}\neq 0\}$. The graph $\mathcal{G}_B$ is said to be *strongly connected* if for all pairs of nodes in $\mathcal{N}_B$ there exists an oriented path in $\mathcal{C}_B$ connecting them. A matrix P is said to be a permutation matrix if it has elements that are 0 or 1, see Varga (1962). $\mathcal{G}_B$ is strongly connected if and only if B is permutation-irreducible (P-irreducible), i.e., there exists no permutation matrix P such that

$$P^{-1}BP=\begin{bmatrix}B_1 & *\\ 0 & B_2\end{bmatrix}.$$

A square matrix is P-irreducible if and only if its graph does not contain any strongly disconnected subgraph. As long as we consider matrices B that are Hermitian or skew-Hermitian, the adjective ''strong'' (referring to the path being oriented) is irrelevant since $b_{ij}\neq 0$ if and only if $b_{ji}\neq 0$.

Remark 1: For B Hermitian or skew-Hermitian, $\mathcal{G}_B$ *connected*$\Leftrightarrow\mathcal{G}_B$ *strongly connected.*

This is not anymore true if B belongs to a noncompact real form. Working with the complexification A_{N-1} and considering the graphs associated with the elements E_α, $\alpha\in\Delta^+$, of the Weyl basis (4), a unique $\mathcal{G}_{E_\alpha}$ is associated with each positive root. $\mathcal{G}_{E_\alpha}$ are called *elementary root graphs*. If $b_\alpha=b_\alpha^{\Re}+ib_\alpha^{\Im}$, rewriting B as

$$B=B_0+B_1=B_0+\sum_{\alpha\in\Gamma^+}(b_\alpha E_\alpha-b_\alpha^* E_{-\alpha}), \tag{15}$$

where the asterisk is complex conjugate, then the (positive) *root graph* of B is $\mathcal{G}_B^+=\cup_{\alpha\in\Gamma^+}\mathcal{G}_{E_\alpha}$ and $\mathcal{G}_{B-B_0}$ is "twice" $\mathcal{G}_B^+$.

For the quantum system on $\mathfrak{su}(N)$, the roots admit the interpretation of transitions between energy levels of the system. According to our definitions, $\lambda_i=-\mathcal{E}_i$ and the roots are $\alpha_{ij}=\mathcal{E}_j-\mathcal{E}_i$ $(i<j\Rightarrow\alpha_{ij}\geqslant 0)$.

The concepts of regular and strongly regular roots correspond to those of degenerate system and of system with degenerate transitions in the following way:

(i) if a system is degenerate then it has nonregular roots;
(ii) if a system is nondegenerate but has degenerate transitions then it has regular but not all strongly regular roots;
(iii) if a system is nondegenerate and has no degenerate transitions then it has only strongly regular roots.

In the basis (6), $b_\alpha=b_{ij}$, $1\leqslant i<j\leqslant N$ and B_0 is simply the diagonal

$$B_0=\sum_{k=1}^{N} b_{kk}E_{kk}=\sum_{k=1}^{N-1}\left(\sum_{j=1}^{k} ib_{jj}\right)(iH_K) \tag{16}$$

since $B_0\in\mathfrak{su}(N)$ has to be traceless. The b_{jj} (which must be purely imaginary) correspond to loops on $\mathcal{G}_B$, i.e., to arcs beginning and ending on the same node. Thus they are irrelevant for the connectivity property. In the basis (6), A and B are

$$A=\sum_{k=1}^{N-1}\left(\sum_{j=1}^{k}\mathcal{E}_j\right)(iH_k), \tag{17}$$

$$B=B_0+\sum_{(i,j)\in\mathcal{C}_B^+}(b_{ij}^{\Re}X_{ij}+b_{ij}^{\Im}Y_{ij}). \tag{18}$$

The following lemma is the adaptation to our situation of Theorem 2 and Corollary 2 of Silva Leite and Crouch (1988).

Lemma 5: B is P-irreducible $\Leftrightarrow$ $\{\mathfrak{f}_\alpha,\alpha\in\Gamma^+\}_{L.A.}=\mathfrak{su}(N)$

Proof: If B is P-irreducible, then $B-B_0$ is P-irreducible and $\mathcal{G}_B^+$ is connected. Therefore, every pair of nodes (i,j), $i\neq j$, can be joined by a path made up of elementary root graphs belonging to $\mathcal{G}_B^+$, or, in terms of roots, each positive root of A_{N-1}, $\alpha_{ij}\in\Delta^+$, can be written as a sum of the roots of Γ^+: $\alpha_{ij}=\Sigma_{(k,l)\in\mathcal{C}_B^+}\lambda_{k,l}\alpha_{k,l}$ for positive rationals λ_{kl}. The situation is specular for negative roots. From the commutation relations (10), for some vector spaces $\mathfrak{f}_{k_i,l_i}$ of indexes $(k_i,l_i)\in\mathcal{C}_B^+$ we have

$$[\mathfrak{f}_{k_1,l_1},[\mathfrak{f}_{k_2,l_2},\ldots[\mathfrak{f}_{k_{m-1},l_{m-1}},\mathfrak{f}_{k_m,l_m}]\ldots]=\mathfrak{f}_{i,j}. \tag{19}$$

Then also the Cartan subalgebra can be generated, see (7), and the result follows. On the other direction, $\{\mathfrak{f}_\alpha,\alpha\in\Gamma^+\}_{L.A.}=\mathfrak{su}(N)$ means that repeated brackets like (19) span all the subspaces

$\mathfrak{f}_{ij}$, $1 \leqslant i < j \leqslant N$, and therefore touch all the roots $\alpha_{ij} \in \Delta$. But this is equivalent to $\mathcal{G}_B$ connected. ■

Lemma 1 and Lemma 2 tell us that the condition of Lemma 5 is "minimally" satisfied by a set of fundamental roots, although due to the nonuniqueness of the selection of the fundamental roots, not all the $\alpha \in \Phi$ have to be in Γ^+ for $\mathcal{G}_B$ to be connected.

Corollary 2: If $\Phi \subseteq \Gamma^+$ then B is P-irreducible.

IV. SUFFICIENT CONDITIONS FOR CONTROLLABILITY IN THE GENERIC CASE

Considerations similar to those used in the controllability analysis of normal real forms of classical Lie algebras [see Jurdjevic and Kupka (1981), Gauthier and Bonnard (1982), El Assoudi *et al.* (1995), Silva Leite and Crouch (1988)] can be employed for our compact real form as well. In the case of free Hamiltonian of diagonal type, the connectivity property of the graph of the forced term B can replace the Lie algebraic rank condition, see Gauthier (1982).

Lemma 6: If A is diagonal, a necessary condition for controllability is that $\mathcal{G}_B$ connected.

Proof: If B is P-reducible, then there exist nontrivial invariant subspaces of $\mathfrak{su}(N)$ that are simultaneously A-invariant and B-invariant. Thus the system cannot be controllable. ■

In the case of $\mathcal{G}_B$ disconnected, the quantum system is decomposable into noninteracting subsystems. In Turinici *et al.* (2001) it is required that $\tilde{H}_1$ is off-diagonal. The interpretation in terms of root decomposition offered here shows that this assumption is irrelevant for controllability: the diagonal terms of $\tilde{H}_1$ belong to the Cartan subalgebra and as such they commute with A.

The equivalence between $\{A,B\}_{L.A.} = \mathfrak{su}(N)$ and $\mathcal{G}_B$ connected is not exact: while $\mathcal{G}_B$ connected is a necessary condition for controllability, alone it is not a sufficient condition, but requires extra assumptions to be made on the diagonal matrix A. The simplest case corresponds to the drift term A being strongly regular and corresponds to all nondegenerate transitions.

Theorem 2: *Given A and B as in (17) and (18), assume that $\mathcal{G}_B$ is connected. If A is strongly regular, then the system (13) is controllable.*

Proof: Since ad_A is invariant on each $\mathfrak{f}_\alpha$, $\alpha \in \Delta^+$, the level one bracket $C = \mathrm{ad}_A \Sigma_{\alpha \in \Gamma^+}(b_\alpha^{\Re} X_\alpha + b_\alpha^{\Im} Y_\alpha)$ allows one to reach $\oplus_{\alpha \in \Gamma^+} \mathfrak{f}_\alpha$ as $b_\alpha = b_\alpha^{\Re} + i b_\alpha^{\Im} \neq 0$ for all $\alpha \in \Gamma^+$. Using an argument similar to the proof of Theorem 3 in Silva Leite and Crouch (1988), we compute as many "A-brackets" (like $[A,B]$, $[A,[A,B]]$, etc.) as the number of roots in Γ^+, say $2m$ (with $m \geqslant N-1$). For simplicity of bookkeeping, it is convenient to number roots α and coefficients b_α cardinally from 1 to $2m$: $\{\alpha_1,\ldots,\alpha_{2m}\} = \Gamma^+$, $b_\alpha = b_i$, $i = 1,\ldots,2m$ and $E_\alpha = E_i$, $i = 1,\ldots,2m$,

$$\begin{bmatrix} \mathrm{ad}_A B \\ \mathrm{ad}_A^2 B \\ \vdots \\ \mathrm{ad}_A^{2m} B \end{bmatrix} = \begin{bmatrix} \alpha_1 b_1 & \alpha_2 b_2 & \cdots & \alpha_m b_m & \alpha_1 b_1^* & \cdots & \alpha_m b_m^* \\ \alpha_1^2 b_1 & \alpha_2^2 b_2 & \cdots & \alpha_m^2 b_m & -\alpha_1^2 b_1^* & \cdots & -\alpha_m^2 b_m^* \\ \alpha_1^3 b_1 & \alpha_2^3 b_2 & \cdots & \alpha_m^3 b_m & \alpha_1^3 b_1^* & \cdots & \alpha_m^3 b_m^* \\ & & & \vdots & & & \\ & & & \vdots & & & \\ \alpha_1^{2m} b_1 & \alpha_2^{2m} b_2 & \cdots & \alpha_m^{2m} b_m & -\alpha_1^{2m} b_1^* & \cdots & -\alpha_m^{2m} b_m^* \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ \vdots \\ E_m \\ E_{-1} \\ \vdots \\ E_{-m} \end{bmatrix}$$

$$= M \begin{bmatrix} E_1 \\ E_2 \\ \vdots \\ E_m \\ E_{-1} \\ \vdots \\ E_{-m} \end{bmatrix}. \tag{20}$$

M can be written as

$$M=S_1\left[\begin{array}{ccc|ccc} \alpha_1 & \cdots & \alpha_m & \alpha_1 & \cdots & \alpha_m \\ \alpha_1^3 & \cdots & \alpha_m^3 & \alpha_1^3 & \cdots & \alpha_m^3 \\ \alpha_1^{2m-1} & \cdots & \alpha_m^{2m-1} & \alpha_1^{2m-1} & \cdots & \alpha_m^{2m-1} \\ \hline \alpha_1^2 & \cdots & \alpha_m^2 & 0 & \cdots & 0 \\ \alpha_1^4 & \cdots & \alpha_m^4 & 0 & \cdots & 0 \\ \alpha_1^{2m} & \cdots & \alpha_m^{2m} & 0 & \cdots & 0 \end{array}\right] S_2\left[\begin{array}{ccc|ccc} b_1 & & & & & \\ & \ddots & & & & \\ & & b_m & & & \\ \hline & & & b_1^* & & \\ & & & & \ddots & \\ & & & & & b_m^* \end{array}\right]$$

with

$$S_1=\left[\begin{array}{ccc|ccc} 1 & & & -1 & & \\ & \ddots & & & \ddots & \\ & & 1 & & & -1 \\ \hline & & & 2 & & \\ & & & & \ddots & \\ & & & & & 2 \end{array}\right],\quad S_2=\left[\begin{array}{cccc|ccc} 1 & 0 & & & 0 & & \\ 0 & 0 & & & 1 & 0 & \\ 0 & 1 & 0 & & 0 & 0 & \\ 0 & 0 & 0 & & 0 & 1 & \\ 0 & 0 & 1 & & 0 & 0 & \\ & & & \ddots & & & \ddots \\ & & & 1 & & & 0 \\ & & & 0 & & & 1 \end{array}\right].$$

Straightforward computations give the determinant of M:

$$\det M=(-1)^{m+1}2^m\prod_{i=1}^{m}\alpha_i^m\prod_{1\leqslant i<j\leqslant m}(\alpha_j^2-\alpha_i^2)^2\prod_{i=1}^{m}|b_i|^2\neq 0.$$

Therefore $\{A,B\}_{L.A.}\supseteq\{\mathfrak{f}_\alpha,\alpha\in\Gamma^+\}_{L.A.}$, and controllability follows from P-irreducibility of B (Lemma 5). ■

A weaker property than strong regularity is B-strong regularity, introduced in Silva Leite and Crouch (1988).

Definition 3: Given B as in (14), *A is said to be B*-strongly regular *if the elements* $\alpha(\tilde{H}_0)$, $\alpha\in\Gamma^+$, *are nonzero and distinct.*

Unlike strong regularity, which requires all roots of Δ to be non-null and distinct when computed in A, B-strong regularity requires the root decomposition determined by A to be strongly regular only along the roots Γ^+ entering into the decomposition of B: $\alpha_{ij}(\tilde{H}_0)=\mathcal{E}_j-\mathcal{E}_i\neq 0$ if $b_{ij}\neq 0$. Obviously, A strongly regular means A is B-strongly regular for all B.

Theorem 2 is a particular case of the following:

Theorem 3: *Given A and B as in (17) and (18), assume that* $\mathcal{G}_B$ *is connected. If A is B-strongly regular, then the system (13) is controllable.*

Proof: The only difference with Theorem 2 is that ad_A is invariant only on $\mathfrak{f}_\alpha$, $\alpha\in\Gamma^+$ (rather than Δ^+). However, Lemma 5 is true regardless of this assumption (as it is concerned with B alone) and, using the same construction of the proof of Theorem 2, $\det M\neq 0$ still holds true. ■

An alternative extension of Theorem 2 is mentioned in Turinici and Rabitz (2001). If Π_A^+ is the set of positive roots $\alpha(\tilde{H}_0)$ that are strongly regular for A, call $\Theta_A^+=\Gamma^+\cap\Pi_A^+$ the subset of positive strongly regular roots of Γ^+ when computed in A and Ω_A^+ the corresponding complementary set in Γ^+ (i.e., the set of nonstrongly regular roots of Γ^+): $\Omega_A^+=\Gamma^+\backslash\Theta_A^+$. So B splits into $B=B_r+B_s$ with $B_r=B_0+\Sigma_{\alpha\in\Theta_A^+}(b_\alpha^{\Re}X_\alpha+b_\alpha^{\Im}Y_\alpha)$, the intersection of B with the strongly regular roots, and $B_s=\Sigma_{\alpha\in\Omega_A^+}(b_\alpha^{\Re}X_\alpha+b_\alpha^{\Im}Y_\alpha)$.

Theorem 4: *Given A and B as in* (17) *and* (18), *assume that* $\mathcal{G}_B$ *is connected. If* $\mathcal{G}_{B_r}$ *is connected, then the system* (13) *is controllable.*

Proof: The pair A, B_r is such that A is B_r-strongly regular. If $\mathcal{G}_{B_r}$ is connected, Theorem 3 applies to the pair (A,B_r). We can use an argument similar to the proof of Theorem 2. If $m_r \geqslant N$ are the strongly regular roots and m_s the degenerate ones, instead of the ordering of the root vector used in (20) $E=[E_1\cdots E_m E_{-1}\cdots E_{-m}]^T$ we can use a splitting corresponding to strongly regular and degenerate roots $E=[E^{rt}E^{sT}]^T=[E^r_1\cdots E^r_{m_r}E^r_{-1}\cdots E^r_{-m_r}E^s_1\cdots E^s_{m_s}E^s_{-1}\cdots E^s_{-m_s}]^T$. Then

$$\begin{bmatrix} \mathrm{ad}_A B \\ \mathrm{ad}_A^2 B \\ \vdots \\ \mathrm{ad}_A^{2m_r} B \end{bmatrix} = \begin{bmatrix} \mathrm{ad}_A B_r \\ \mathrm{ad}_A^2 B_r \\ \vdots \\ \mathrm{ad}_A^{2m_r} B_r \end{bmatrix} + \begin{bmatrix} \mathrm{ad}_A B_s \\ \mathrm{ad}_A^2 B_s \\ \vdots \\ \mathrm{ad}_A^{2m_r} B_s \end{bmatrix} = [M_r \;\; 0]E + [0 \;\; M_s]E = M_r E^r + M_s E^s,$$

where the $2m_r\times 2m_r$ matrix M_r is nonsingular and M_s is a rectangular matrix of dimensions $2m_r\times 2m_s$. Since $\det M_r \neq 0$, we have

$$E^r = M_r^{-1}\left(\begin{bmatrix} \mathrm{ad}_A B \\ \vdots \\ \mathrm{ad}_A^{2m_r} B \end{bmatrix} - M_s E^s \right),$$

i.e., the Lie algebra generated by A and B contains a complete set of generators. Thus the statement again follows from Lemma 5 and the B_s part of B is not influencing the controllability property. ■

For controllability, it is sufficient that Θ_A^+ contains the fundamental roots, as in this case $\mathcal{G}_{B_r}$ is connected by Corollary 2.

Corollary 3: If $\Phi\subseteq\Theta_A^+$, *then the system (13) is controllable*.

Notice that the condition of Theorem 2 is the one traditionally used in the literature to show that a generic pair of vector fields on compact semisimple Lie algebras are generating, see Kuranishi (1951), Boothby (1975), Bonnard *et al.* (1980). For this purpose, given A strongly regular, B is constructed such that ad_A is cyclic on $\oplus_{\alpha\in\Delta^+}\mathfrak{f}_\alpha$, for example by having $b_\alpha\neq 0 \;\; \forall\alpha\in\Delta^+$. This means that $\oplus_{\alpha\in\Delta^+}\mathfrak{f}_\alpha$ can be spanned by ''A-brackets'' and thus all $\mathfrak{su}(N)$ is generated by adding the elements of the Cartan subalgebra [bracketing according to the last row of (10)]. However, here the method is not directly applicable because some of the b_{ij} elements of B are allowed to be zero. In this case, from $\oplus_{\alpha\in\Gamma^+}\mathfrak{f}_\alpha$, the missing subspaces must be reached by means of ''B-brackets'' $[C,B]$, $[[C,B],B]$, etc., and then their span completed by single ''A-brackets'' $[A,[C,B]]$, $[A,[[C,B],B]]$, etc.

V. SUFFICIENT CONDITIONS FOR CONTROLLABILITY IN A FEW SINGULAR CASES

The use of ''B-brackets'' is the *leitmotif* of all other sufficient conditions which are based on properties weaker than the strong regularity and B-strong regularity of the diagonal vector field A. These conditions belong to the first two cases of the classification of Sec. III and, from Corollary 3, they correspond to at least a pair of fundamental roots being equal. If new diagonal terms can be provided to compensate for the degenerate transitions, then controllability can be recovered. From (15), writing C as $C=\Sigma_{\Gamma^+}\alpha(A)(b_\alpha E_\alpha + b_\alpha^* E_{-\alpha})$, the level two bracket $[C,B]$ is

$$
\begin{aligned}
D=[C,B]&=[C,B_0]+[C,B_1]\\
&=\left[\sum_{\Gamma^+}\alpha(A)b_\alpha E_\alpha,B_0\right]+\left[\sum_{\Gamma^+}\alpha(A)b_\alpha^* E_{-\alpha},B_0\right]+\left[\sum_{\Gamma^+}\alpha(A)b_\alpha E_\alpha,\sum_{\Gamma^+}b_\alpha E_\alpha\right]\\
&\quad+\left[\sum_{\Gamma^+}\alpha(A)b_\alpha^* E_{-\alpha},\sum_{\Gamma^+}b_\alpha E_\alpha\right]-\left[\sum_{\Gamma^+}\alpha(A)b_\alpha E_\alpha,\sum_{\Gamma^+}b_\alpha^* E_{-\alpha}\right]\\
&\quad-\left[\sum_{\Gamma^+}\alpha(A)b_\alpha^* E_{-\alpha},\sum_{\Gamma^+}b_\alpha^* E_{-\alpha}\right].
\end{aligned}
\tag{21}
$$

If B_0 is non-null and linearly independent from A, it constitutes the simplest candidate to provide the missing fundamental roots. From (16), the fundamental roots at B_0, $\alpha(B_0)$, are equal to $\beta_{i,i+1}=b_{ii}-b_{i+1,i+1}$ when expressed in the basis (6). Restricting to the case (ii) of Sec. III A, i.e., assuming that the system is nondegenerate but with possibly degenerate transitions, equivalent versions of Theorems 2 and 3 hold for B_0 and C instead of A and B.

Theorem 5: *If A is regular and $\mathcal{G}_B$ connected, then either of the following conditions is sufficient for controllability of (13):*
(1) B_0 is strongly regular,
(2) B_0 is C-strongly regular.

Proof: A regular means $\mathcal{E}_i\neq\mathcal{E}_j$ for $i\neq j$, i.e., $\alpha_{ij}\neq 0\ \forall 1\leqslant i<j\leqslant N$. Then in case of $\mathcal{G}_B$ connected also $\mathcal{G}_C$ is connected. Therefore, B_0 strongly regular or C-strongly regular satisfy, respectively, Theorems 2 and 3 for the pair (B_0,C). Since $B=B_0+B_1$ (not B_0) is the available vector field, in order to complete the proof one has to verify that the (B_1,C) pair is not spoiling the maximal nonintegrability property of (B_0,C), i.e., $A\oplus\{B_0,C\}_{L.A.}=A\oplus\{B,C\}_{L.A.}=\mathfrak{su}(N)$ (neglecting the trivial case of A and B_0 linearly dependent). But this follows from Eq. (21): while $[B_0,C]\in\{\mathfrak{f}_\alpha,\alpha\in\Gamma^+\}$, whenever $\Gamma^+\subsetneq\Delta^+$, $[B_1,C]\in\{\mathfrak{f}_\alpha,\alpha\in\tilde{\Gamma}^+\supseteq\Gamma^+\}$ because components along $E_{\pm\alpha\pm\beta}$, $\alpha,\beta\in\Gamma^+$ are produced by the last four terms of (21) [see (1)]. If $\tilde{\Gamma}^+\subsetneq\Gamma^+$, then $[B_0,C]$ and $[B_1,C]$ are automatically linearly independent. If, instead, $\tilde{\Gamma}^+=\Gamma^+$, then from (21) it has to be $\alpha+\beta\in\Gamma^+$ for all roots $\alpha,\beta\in\Gamma^+$ such that $\alpha+\beta$ is a root and $\alpha b_\alpha^* E_{-\alpha}b_\beta E_\beta-\beta b_\beta E_\beta b_\alpha^* E_{-\alpha}=0$ for all $\alpha,\beta\in\Gamma^+$ such that $\alpha-\beta\in\Delta$, $\alpha-\beta\notin\Gamma$. But the only case of roots $\alpha,\beta\in\Gamma^+$ with $\alpha-\beta\in\Delta$ and satisfying $(\alpha-\beta)b_\alpha^* b_\beta[E_{-\alpha},E_\beta]=0$ is the case of all equal (and non-null since A regular) roots. Linear independence of $[B_0,C]$ and $[B_1,C]$ then follows from the fact that $[B_1,C]$ has terms on the diagonal which are certainly non-null for the case of all equal roots [they are computed in detail in the following, see Eqs. (22) and (23)], while $[B_0,C]$ is off-diagonal. Thus, in both cases, the basis elements obtained from $[B_0,C]$, $[B_0,[B_0,C]]$, etc., are not canceled by the remaining parts of the brackets $[B_1,C]$, $[B_0,[B_1,C]]+[B_1,[B_0,C]]+[B_1,[B_1,C]]$, etc. ■

One can think of weakening further the hypothesis of Theorem 5 by combining together strongly regular pieces from both A and B_0. To this end, analogously to what was done for the diagonal matrix A, call Θ_B^+ the set of positive strongly regular roots $\alpha(B_0)$ of Γ^+ and C_r the corresponding part of C: $C_r=\Sigma_{\Theta_B^+}\alpha(A)(b_\alpha E_\alpha+b_\alpha^* E_{-\alpha})$.

Theorem 6: *Assume A regular and $\mathcal{G}_B$ connected. If $\mathcal{G}_{B_r}\cup\mathcal{G}_{C_r}$ is connected then the system (13) is controllable.*

Proof: In this case it is necessary to use both "A-brackets" for the pair $[A,B]$ and "B-brackets" for $[B_0,C]$. Since "A-brackets" and "B-brackets" yield independent new generators, the proof follows by combining the arguments used in proving Theorem 4 and Theorem 5. ■

As last, we treat the case of Cartan subalgebras from level two brackets of A and B. Since C is off-diagonal, the only useful bracket in this respect is $[C,B]$. By looking at the commutators for the Weyl basis (1), new diagonal terms appear only on the fourth and fifth terms of the expression (21) for D. By isolating them

$$D_0=-2\sum_{\Gamma^+}\alpha(A)|b_\alpha|^2[E_\alpha,E_{-\alpha}]=-2\sum_{\Gamma^+}\alpha(A)|b_\alpha|^2H_\alpha$$

or, in terms of the basis (6)

$$D_0=-2\sum_{(i,j)\in\mathcal{C}_B^+}\alpha_{ij}(A)|b_{ij}|^2(H_i+H_{i+1}+\cdots+H_{j-1}).$$

Thus $D=[C,B]=D_0+D_1$ with D_0 diagonal and D_1 off-diagonal. It is convenient to sum over Δ^+ rather than Γ^+ (if $(i,j)\notin\mathcal{C}_B^+$ then $b_{ij}=0$):

$$\begin{aligned}D_0&=-2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\alpha_{ij}(A)|b_{ij}|^2(E_{ii}-E_{jj})\\&=2\sum_{k=1}^{N}\left(\sum_{i=1}^{k-1}\alpha_{ik}|b_{ik}|^2-\sum_{i=k+1}^{N}\alpha_{ki}|b_{ki}|^2\right)E_{kk}\\&=\sum_{k=1}^{N}d_kE_{kk},\end{aligned}\tag{22}$$

where it is intended that $\Sigma_{i=1}^{k-1}\alpha_{ik}|b_{ik}|^2=0$ if $k=1$ and $\Sigma_{i=k+1}^{N}\alpha_{ki}|b_{ki}|^2=0$ if $k=N$. The diagonal elements d_k of D_0 can be expressed in terms of the energy levels $\mathcal{E}_k$ of the quantum system (11) as

$$\begin{aligned}d_k=&2\mathcal{E}_k(|b_{1,k}|^2+\cdots+|b_{k-1,k}|^2+|b_{k,k+1}|^2+\cdots+|b_{k,N}|^2)\\&-2(\mathcal{E}_1|b_{1,k}|^2+\cdots+\mathcal{E}_{k-1}|b_{k-1,k}|^2+\mathcal{E}_{k+1}|b_{k,k+1}|^2+\cdots+\mathcal{E}_N|b_{k,N}|^2)\end{aligned}\tag{23}$$

from which it is straightforward to check that $\Sigma_{k=1}^{N}d_k=0$ (thus that $D_0\in\mathfrak{su}(N)$).

Now we can reformulated Theorem 5 with D_0 replacing B_0.

Theorem 7: *If A is regular and $\mathcal{G}_B$ connected, then any of the following conditions is sufficient for controllability of (13):*
(1) D_0 is strongly regular,
(2) D_0 is B-strongly regular,
(3) D_0 is C-strongly regular.

Proof: The proof is completely analogous to that of Theorem 5, with the extra simplification that now D_1, when $\neq 0$, is linearly independent from both B and C regardless of the regularity of the roots computed in A and B, respectively. ■

The practical situations in which Theorems 5–7 apply are when the system has resonant modes [which, again, corresponds to the case (ii) in the classification of Sec. III]. The extreme case is when $\mathcal{E}_{i+1}-\mathcal{E}_i=\text{const}\ \forall\ i=1,\ldots,n-1$ (nondegenerate system with all equally spaced energy levels).

Often a case-by-case analysis provides less strict sufficient conditions than those discussed in this paper. As an example, consider the completely harmonic system mentioned previously. If $b_{i,j}=0$ for $j\neq i\pm1$ (dipole approximation) and $b_{i,i\pm1}=b_{i,i\pm1}^{\mathfrak{I}}$, we are exactly in the situation described in Fu *et al.* (2001)—Sec. 2.3 (since $\Gamma^+=\Phi^+$, such pair of vector fields A and B is minimal among the generating pairs, in the sense of Lemma 2, which implies that methods like Theorem 4 are inapplicable). In this case, all the fundamental roots are equal, $\alpha_{i,\,i+1}=\mu, i=1,\ldots,N-1$, $B=\Sigma_{i=1}^{N-1}b_{i,i+1}Y_{i,i+1}$ $(B_0=0)$ and $C=\mu\Sigma_{i=1}^{N-1}b_{i,i+1}X_{i,i+1}$. Thus $D=-2\mu\Sigma_{i=1}^{N-1}b_{i,i+1}^2(iH_i)$ and the "new fundamental roots" are $-2\mu(b_{i,\,i+1}^2-b_{i+1,\,i+2}^2)$, which are not necessarily distinct for $i=1,\ldots,N-1$. Thus Theorem 7 needs not be verified. For the same system, Theorem 3 of Fu *et al.* (2001) provides an alternative sufficient condition that is

weaker than any of the items of Theorem 7, obtained by making use of the special structure of the system to compute a full set of generating brackets explicitly. The drawback of this method is that whenever the structure of B or the values of the fundamental roots are modified, the algorithm needs to be redesigned.

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Generalized coherent and squeezed states based on the $h(1)\oplus su(2)$ algebra

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States which minimize the Schrödinger–Robertson uncertainty relation are constructed as eigenstates of an operator which is an element of the $h(1)\oplus su(2)$ algebra. The relations with supercoherent and supersqueezed states of the supersymmetric harmonic oscillator are given. Moreover, we are able to compute general Hamiltonians which behave like the harmonic oscillator Hamiltonian or are related to the Jaynes–Cummings Hamiltonian. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Minimum uncertainty states (MUSs) are usually understood through the minimization of the Heisenberg uncertainty relation (HUR). These states are well-known[1] since they are long associated with the so-called coherent states (CSs)[2] and squeezed states (SSs)[3]. But, it has been observed[4–6] that a more accurate uncertainty relation may be used to construct generalized CSs and SSs. Indeed, this relation known as the Schrödinger–Robertson uncertainty relation (SRUR)[7] can be minimized and gives rise to new classes of CSs and SSs which have received different names in the literature, such as correlated states[4] or intelligent states.[5] There are two main reasons to consider such last states. First, when the two Hermitian operators entering in the SRUR are noncanonical operators, i.e., their commutator is not a multiple of the identity, the HUR could be redundant while the SRUR not. Second, the MUSs that minimize the SRUR are shown to be eigenstates of a linear combination of the two Hermitian operators entering in the SRUR.

Recently[8] a connection has been made with the CS and SS based on group theoretic approaches[9] and the concept of algebra eigenstates (AESs). In particular, AESs have been constructed for the algebras su(2) and su(1,1). This concept constitutes a unification of different definitions of CS and SS.

In this article, we give a general construction of AESs based on the direct sum $h(1)\oplus su(2)$. The Heisenberg algebra $h(1)$ being relevant for the problem of the harmonic oscillator and the algebra su(2) for particles with spin, we have a procedure to find general CSs and SSs for supersymmetric systems, for example. These are clearly MUSs for which the dispersions of corresponding operators may be calculated easily. We show finally how to use these states in the construction of particularly relevant Hamiltonians and in the calculation of their dispersions.

In Sec. II, we put the emphasis on the SRUR and its relevancy with respect to the determination of MUSs. The application to the position and momentum operators MUS leads to the well-known CS and SS of the harmonic oscillator while when the angular momentum operators MUS are considered we have in mind the su(2) CS and SS. These particular applications are given to bring a new light on these states and also to facilitate the treatement of the $h(1)\oplus su(2)$ CS and SS. In Sec. III, we construct the AES based on the $h(1)\oplus su(2)$ algebra and show how this gives CSs and SSs which generalize the supercoherent and supersqueezed states obtained in other approaches.[10,11] Finally, in Sec. IV, we construct general Hamiltonians similar to the one of the

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harmonic oscillator but where the so-called annihilation operator is now an element of the algebra $h(1)\oplus su(2)$. This permits us to use our CS and SS to compute the mean value and the dispersions of the corresponding energies. We show also how the well-known Jaynes–Cummings Hamiltonian enters in this scheme.

II. COHERENT AND SQUEEZED STATES AS MINIMUM UNCERTAINTY STATES

This section will be concerned by the general definition and properties of MUS (Sec. II A). They are explicitly constructed when the usual position and momentum operators are considered (Sec. II B) as well as when the angular momentum operators are taken (Sec. II C). The connection is made with already known results.

A. Minimum uncertainty relation

It is well-known[7] that, for two Hermitian operators A and B such that the commutator is

$$[A,B]=iC, \quad C\neq 0, \tag{2.1}$$

the HUR

$$(\Delta A)^2(\Delta B)^2\geqslant \frac{\langle C\rangle^2}{4} \tag{2.2}$$

is satisfied. The mean value and dispersion of a given operator X are defined, as usual, by

$$\langle X\rangle=\langle\psi|X|\psi\rangle, \quad (\Delta X)^2=\langle X^2\rangle-\langle X\rangle^2, \tag{2.3}$$

for a normalized state $|\psi\rangle$ describing the evolution of a quantum system. As observed by Puri,[6] for noncanonical operators, i.e., such that C is not a multiple of the identity I, we can have $\langle C\rangle=0$ and the relation (2.2) is then redundant. The SRUR[1,7] is never redundant and writes

$$(\Delta A)^2(\Delta B)^2\geqslant \tfrac{1}{4}(\langle C\rangle^2+\langle F\rangle^2), \tag{2.4}$$

where $\langle F\rangle$ is a measure of the correlation between A and B. The operator F is Hermitian and given by

$$F=\{A-\langle A\rangle I, B-\langle B\rangle I\}, \tag{2.5}$$

where $\{\ ,\ \}$ denotes the anticommutator. If there is no correlation between the operators A and B, i.e., if $\langle F\rangle=0$, the SRUR reduces to the usual HUR.

We are interested here in the description of states which minimize the SRUR (2.4). A necessary and sufficient condition to get them is to solve the eigenvalues equation:

$$[A+i\lambda B]|\psi\rangle=\beta|\psi\rangle, \tag{2.6}$$

where

$$\beta=[\langle A\rangle+i\lambda\langle B\rangle], \quad \lambda\in\mathbb{C}, \ \lambda\neq 0. \tag{2.7}$$

Note that, if $\mathrm{Re}\,\lambda\neq 0$, once we know the value of β, this last relation may be inverted to give the mean values

$$\langle A\rangle=\mathrm{Re}\,\beta+\frac{\mathrm{Im}\,\lambda}{\mathrm{Re}\,\lambda}\mathrm{Im}\,\beta, \quad \langle B\rangle=\frac{\mathrm{Im}\,\beta}{\mathrm{Re}\,\lambda} \tag{2.8}$$

and, if $\mathrm{Re}\,\lambda=0$, we get

$$\langle A\rangle=\mathrm{Re}\,\beta+\mathrm{Im}\,\lambda\langle B\rangle. \tag{2.9}$$

As a consequence of (2.6), one has

$$(\Delta A)^2=|\lambda|\Delta, \quad (\Delta B)^2=\frac{1}{|\lambda|}\Delta, \tag{2.10}$$

with

$$\Delta=\tfrac{1}{2}\sqrt{\langle C\rangle^2+\langle F\rangle^2}. \tag{2.11}$$

So the states $|\psi\rangle$ satisfying (2.6) with $|\lambda|=1$ will be called **coherent** because they satisfy

$$(\Delta A)^2=(\Delta B)^2=\Delta, \tag{2.12}$$

i.e., the dispersions in A and B are the same and minimized in the sense of SRUR. The states $|\psi\rangle$ satisfying (2.6) with $|\lambda|\neq 1$ will be called **squeezed** because if $|\lambda|<1$, we have $(\Delta A)^2<\Delta<(\Delta B)^2$ and if $|\lambda|>1$, we have $(\Delta B)^2<\Delta<(\Delta A)^2$.

Some other relations are also useful for our considerations. The direct computation of $(\Delta A)^2$ and $(\Delta B)^2$ is usually complicated but in the MUSs that satisfy (2.6), we can write

$$(\Delta A)^2=\tfrac{1}{2}|\mathrm{Re}\,\lambda\langle C\rangle+\mathrm{Im}\,\lambda\langle F\rangle|, \tag{2.13}$$

$$(\Delta B)^2=\frac{1}{2|\lambda|^2}|\mathrm{Re}\,\lambda\langle C\rangle+\mathrm{Im}\,\lambda\langle F\rangle|, \tag{2.14}$$

with

$$\mathrm{Im}\,\lambda\langle C\rangle=\mathrm{Re}\,\lambda\langle F\rangle. \tag{2.15}$$

For $\mathrm{Re}\,\lambda=0$, we have $\langle C\rangle=0$, which corresponds to the case where the HUR is redundant. The MUSs satisfy the minimum SRUR (MSRUR)

$$(\Delta A)^2(\Delta B)^2=\Delta^2, \tag{2.16}$$

with

$$(\Delta A)^2=\frac{1}{2}|\mathrm{Im}\,\lambda\langle F\rangle|, \quad (\Delta B)^2=\frac{1}{2}\left|\frac{\langle F\rangle}{\mathrm{Im}\,\lambda}\right| \tag{2.17}$$

and

$$\Delta=\tfrac{1}{2}|\langle F\rangle|. \tag{2.18}$$

For $\mathrm{Re}\,\lambda\neq 0$, from (2.15), we have

$$\langle F\rangle=\frac{\mathrm{Im}\,\lambda}{\mathrm{Re}\,\lambda}\langle C\rangle. \tag{2.19}$$

Moreover, from (2.13) and (2.14), we get

$$(\Delta A)^2=\left|\frac{|\lambda|^2}{2\,\mathrm{Re}\,\lambda}\langle C\rangle\right|, \quad (\Delta B)^2=\left|\frac{1}{2\,\mathrm{Re}\,\lambda}\langle C\rangle\right|, \tag{2.20}$$

and, then,

$$\Delta = \left| \frac{|\lambda|}{2 \operatorname{Re} \lambda} \langle C \rangle \right|. \tag{2.21}$$

In this case, it is sufficient to compute the mean value of C to deduce that of F and the dispersions. The particular case where $\operatorname{Im} \lambda = 0$ corresponds to the fact that the MSUR coïncides with the minimum HUR (MHUR).

B. Position and momentum coherent and squeezed states

Let us apply the preceding considerations to the special case of the usual position x and momentum p operators of a given quantum system. The canonical commutation relation (if $\hbar = 1$) being

$$[x,p] = iI, \tag{2.22}$$

the SRUR writes

$$(\Delta x)^2 (\Delta p)^2 \geqslant \tfrac{1}{4}(1 + \langle F \rangle^2). \tag{2.23}$$

The MUSs $|\psi, \lambda, \beta\rangle$ satisfy the eigenvalues equation:

$$[x + i\lambda p]|\psi, \lambda, \beta\rangle = \beta |\psi, \lambda, \beta\rangle. \tag{2.24}$$

If we introduce the usual creation $a^\dagger$ and annihilation a operators,

$$a^\dagger = \frac{x - ip}{\sqrt{2}}, \quad a = \frac{x + ip}{\sqrt{2}}, \tag{2.25}$$

such that $[a, a^\dagger] = I$, the equation (2.24) becomes

$$\frac{1}{\sqrt{2}}[(1-\lambda)a^\dagger + (1+\lambda)a]|\psi, \lambda, \beta\rangle = \beta |\psi, \lambda, \beta\rangle. \tag{2.26}$$

The general resolution of Eq. (2.26) is obtained by expressing the state $|\psi, \lambda, \beta\rangle$ as a superposition of the energy eigenstates $\{|n\rangle, n = 0,1,2, \ldots\}$ of the usual harmonic oscillator Hamiltonian

$$H_0 = w(a^\dagger a + \tfrac{1}{2}). \tag{2.27}$$

Let us recall that these eigenstates satisfy

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger |n\rangle = \sqrt{n+1}|n+1\rangle \tag{2.28}$$

and we can write them as

$$|n\rangle = \frac{a^{\dagger n}}{\sqrt{n!}}|0\rangle, \quad n = 0,1,2, \ldots . \tag{2.29}$$

So, if we insert

$$|\psi, \lambda, \beta\rangle = \sum_{n=0}^{\infty} C_{\lambda,\beta,n}|n\rangle, \quad C_{\lambda,\beta,n} \in \mathbb{C}, \tag{2.30}$$

in Eq. (2.26), using the expressions (2.28), we get the recurrence system

$$\frac{1}{\sqrt{2}}[\sqrt{n}(1-\lambda)C_{\lambda,\beta,n-1}+\sqrt{n+1}(1+\lambda)C_{\lambda,\beta,n+1}]=\beta C_{\lambda,\beta,n},\quad n=1,2,3,\ldots,$$
$$\frac{(1+\lambda)}{\sqrt{2}}C_{\lambda,\beta,1}=\beta C_{\lambda,\beta,0}. \tag{2.31}$$

The case $\lambda=-1$ does not give any solution and must be eliminated. If we set

$$\left(\frac{1-\lambda}{1+\lambda}\right)=\delta e^{i\phi},\quad \delta\in \mathrm{R}_+,\phi\in\left[-\frac{\pi}{2},\frac{3\pi}{2}\right[, \tag{2.32}$$

the resolution of the recurrence system (2.31) leads to the general solution of Eq. (2.26):

$$|\psi,\lambda,\beta\rangle=C_{\lambda,\beta,0}\exp\left(-\delta e^{i\phi}\frac{a^{\dagger 2}}{2}\right)\exp\left(\frac{\beta}{\sqrt{2}}(1+\delta e^{i\phi})a^{\dagger}\right)|0\rangle. \tag{2.33}$$

The special case $\lambda=1$ corresponds to $\delta=0$ and gives rise to the usual expression of the CS of the harmonic oscillator. These states (2.33) can also be obtained as the action of two unitary operators on the fundamental state. The first one[9] is the usual displacement operator D associated with an irreducible representation of the Heisenberg–Weyl group $H(1)$ with algebra $h(1)=\{a,a^{\dagger},I\}$. The second one is the squeezed operator S associated with an irreducible representation of SU(1,1) with algebra $su(1,1)=\{a^2,(a^{\dagger})^2,aa^{\dagger}+a^{\dagger}a\}$. This is a known fact[12] when squeezed states of the harmonic oscillator are studied. We have explicitly

$$|\psi,\lambda,\beta\rangle=S(\chi(\delta,\phi))D(\eta)|0\rangle, \tag{2.34}$$

where

$$D(\eta)=\exp(\eta a^{\dagger}-\overline{\eta}a)\ \text{ and }\ S(\chi)=\exp\left(\chi\frac{a^{\dagger 2}}{2}-\overline{\chi}\frac{a^2}{2}\right) \tag{2.35}$$

with

$$\eta=\frac{\beta}{\sqrt{2}}\frac{(1+\delta e^{i\phi})}{\sqrt{1-\delta^2}}\ \text{ and }\ \chi(\delta,\phi)=-\tanh^{-1}(\delta)e^{i\phi}. \tag{2.36}$$

The condition for having normalizable states is that $0\leqslant\delta<1$. Let us insist here on the fact that these SSs already obtained in the literature as eigenstates of a linear combination of a and $a^{\dagger}$ are also MUSs such that $(\Delta x)^2(\Delta p)^2=\Delta^2=(1+\langle F\rangle^2)/4$. From Eq. (2.19) and the fact that $\langle C\rangle=1$, we get

$$\langle F\rangle=\frac{\mathrm{Im}\,\lambda}{\mathrm{Re}\,\lambda}=\frac{-2\delta\sin\phi}{(1-\delta^2)} \tag{2.37}$$

and the factor Δ is

$$\Delta(\delta,\phi)=\sqrt{\frac{1}{4}(1+\langle F\rangle^2)}=\sqrt{\frac{1}{4}+\frac{\delta^2\sin^2\phi}{(1-\delta^2)^2}}. \tag{2.38}$$

Moreover, from (2.13) and (2.14), the dispersions are

$$(\Delta x)^2=\frac{|\lambda|^2}{2|\mathrm{Re}\,\lambda|}=\frac{(1-2\delta\cos\phi+\delta^2)}{2(1-\delta^2)} \tag{2.39}$$

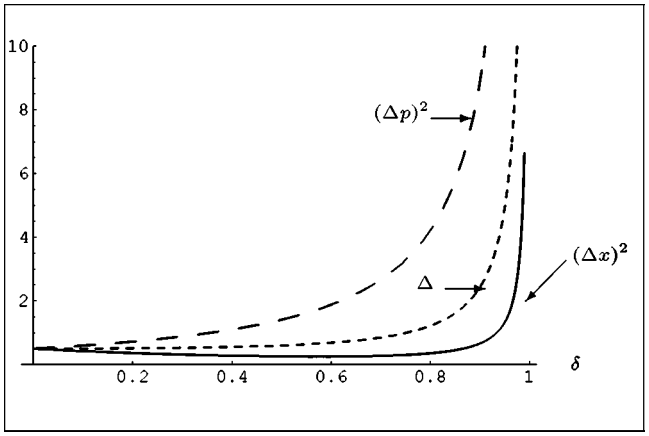

FIG. 1. Graphs of the dispersions $(\Delta x)^2$, $(\Delta p)^2$ and the Δ factor as functions of δ for $\phi=\pi/6$.

and

$$(\Delta p)^2=\frac{1}{2|\mathrm{Re}\,\lambda|}=\frac{(1+2\delta\cos\phi+\delta^2)}{2(1-\delta^2)}. \tag{2.40}$$

Let us recall now that the CSs are not only the one for $\lambda=1$ but also all the states where $|\lambda|=1$. From the relation (2.32), we deduce that

$$\lambda=\frac{1-\delta e^{i\phi}}{1+\delta e^{i\phi}}=\frac{(1-\delta^2)-2i\delta\sin\phi}{(1+2\delta\cos\phi+\delta^2)} \tag{2.41}$$

and then

$$|\lambda|^2=\frac{1-2\delta\cos\phi+\delta^2}{1+2\delta\cos\phi+\delta^2}. \tag{2.42}$$

This means that CSs occur also for $\phi=-\pi/2$ or $\phi=\pi/2$ and $\delta\neq 0$. The other values of λ describe x-squeezed states when $\phi\in\,]-\pi/2,\pi/2[$ and p-squeezed states when $\phi\in\,]\pi/2,3\pi/2[$. On the other hand, for fixed values of ϕ the expression (2.38) attains its minimum value $\frac{1}{2}$ when $\delta=0$ and when $\phi=0$ and $\phi=\pi$ for fixed values of δ. In the first of these cases, we have $\lambda=1$ and we are in the standard CSs of the harmonic oscillator, i.e., eigenstates of the a operator. In the second case, λ is a positive real quantity equal to $(1-\delta)/(1+\delta)\leqslant 1$ if $\phi=0$ and to $(1+\delta)/(1-\delta)\geqslant 1$ if $\phi=\pi$. We are in the special SSs that are eigenstates of the $(a+\delta a^\dagger)$ and $(a-\delta a^\dagger)$ operators, respectively.

Figure 1 shows the behavior of $(\Delta x)^2$, $(\Delta p)^2$ and Δ as functions of δ for $\phi=\pi/6$. In this region $(\Delta x)^2[(\Delta p)^2]$ is always less (greater) than Δ, as expected. For $\delta=0$, the three curves coïncide, and the intersection point corresponds to the CS $|\psi,1,\beta\rangle$. The value of $\Delta=(2.38)$ when $\delta=0$ is also the minimum value $\frac{1}{2}$ which corresponds to the MHUR. Figure 2 shows the behavior of the same quantities as functions of ϕ for $\delta=0.5$. The points where the three curves intersect are the CS.

C. Angular momentum coherent and squeezed states

Let us now take the angular momentum operators J_k for $k=1,2,3$, which satisfy the usual su(2) commutations relations

$$[J_k,J_l]=i\varepsilon_{klm}J_m,\quad k,l,m=1,2,3. \tag{2.43}$$

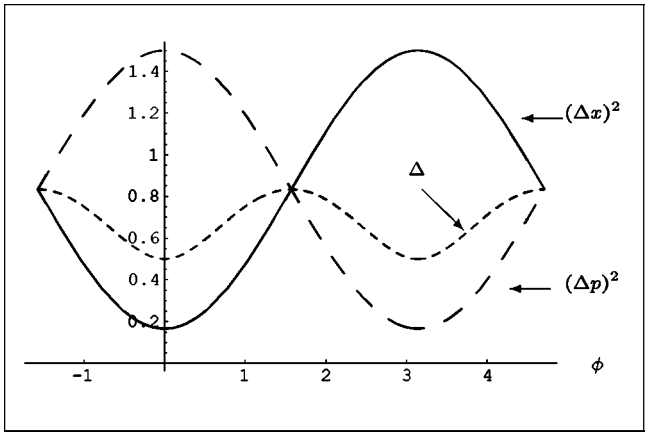

FIG. 2. Graphs of the dispersions $(\Delta x)^2$, $(\Delta p)^2$ and the Δ factor as functions of ϕ for $\delta=0.5$.

Here we want to solve the eigenvalues equation

$$(J_1+i\lambda J_2)|\psi,\lambda,\beta\rangle=\beta|\psi,\lambda,\beta\rangle, \tag{2.44}$$

where $\beta=[\langle J_1\rangle+i\lambda\langle J_2\rangle]$. On the contrary of the preceding example where the HUR is never redundant (because x and p are canonical), here the commutator of J_1 and J_2 is not a multiple of the identity and then $\langle J_3\rangle$ may be equal to zero for some special cases. Some of these cases have been discussed elsewhere.[6,13–15] Here we give the general solution of the equation (2.44), for all possible values of λ and β.

It would be better to work with the operators $J_\pm=J_1\pm iJ_2$ instead of J_1 and J_2, so that the equation (2.44) becomes

$$\tfrac{1}{2}[(1+\lambda)J_+ +(1-\lambda)J_-]|\psi,\lambda,\beta\rangle=\beta|\psi,\lambda,\beta\rangle. \tag{2.45}$$

Using the usual complete set of angular momentum states $\{|j,r\rangle\}$, j integer or half-odd integer and $r\in\{-j,-(j-1),\ldots,j-1,j\}$, we know that

$$J^2|j,r\rangle=(J_1^2+J_2^2+J_3^2)|j,r\rangle=j(j+1)|j,r\rangle, \tag{2.46}$$

$$J_3|j,r\rangle=r|j,r\rangle \tag{2.47}$$

and

$$J_\pm|j,r\rangle=\sqrt{(j\mp r)(j\pm r+1)}|j,r\pm1\rangle. \tag{2.48}$$

This means that for each j fixed, the eigenstates $|\psi,\lambda,\beta\rangle^j$ of Eq. (2.45) may be written as

$$|\psi,\lambda,\beta\rangle^j=\sum_{r=-j}^{j} C^j_{\lambda,\beta,r}|j,r\rangle, \quad C^j_{\lambda,\beta,r}\in\mathbb{C}, \tag{2.49}$$

where the coefficients $C^j_{\lambda,\beta,r}$ satisfy a recurrence system of the form

$$(1+\lambda)\sqrt{(j+r)(j-r+1)}C^j_{\lambda,\beta,r-1}+(1-\lambda)\sqrt{(j-r)(j+r+1)}C^j_{\lambda,\beta,r+1}=2\beta C^j_{\lambda,\beta,r}, \tag{2.50}$$

for $r=-j,\ldots,j$ and $C^j_{\lambda,\beta,j+1}=C^j_{\lambda,\beta,-(j+1)}=0$.

For $\lambda=\pm1$, the unique eigenstates are $|\psi,\pm1,0\rangle^j=|j,\pm j\rangle$. For $\lambda\neq\pm1$ and $\beta=0$, the recurrence relation (2.50) is solved to give

$$|\psi,\lambda,0\rangle^j = C^j_{\lambda,0,j} e^{i(j\phi/2)} \sum_{k=0}^{j} (-1)^k \frac{\binom{j}{k}}{\sqrt{\binom{2j}{2k}}} \delta^k e^{-i(j-2k)\phi/2} |j, j-2k\rangle, \quad j \text{ integer}, \tag{2.51}$$

where we have used the formula (2.32) to express λ in terms of the δ and ϕ. It is again possible to express such a state from the action of unitary operators associated with an irreducible representation of a group which is here SU(2). Indeed, we have

$$|\psi,\lambda,0\rangle^j = C^j_{\lambda,0} \exp[-\tfrac{1}{2}\ln(\delta) J_3] U |j,0\rangle, \tag{2.52}$$

where

$$U = \exp\left(-\frac{\pi}{4}(e^{-i\phi/2} J_+ - e^{i\phi/2} J_-) \right). \tag{2.53}$$

For the general case $\lambda \neq \pm 1$, the analysis of the system (2.50) shows that for each j, there exist $(2j+1)$ possible values for the eigenvalue β, which are

$$\beta^j_m = m\sqrt{1-\lambda^2}, \quad m = -j, \ldots, j. \tag{2.54}$$

If we use the relation

$$[J_1 + i\lambda J_2][\exp(-\tfrac{1}{2}\ln(\delta) J_3) U] = [\exp(-\tfrac{1}{2}\ln(\delta) J_3) U][\sqrt{1-\lambda^2} J_3], \tag{2.55}$$

we see immediately that the corresponding eigenstate $|\psi,\lambda,\beta^j_m\rangle^j$ is

$$|\psi,\lambda,\beta^j_m\rangle^j \equiv |\psi,\lambda,m\rangle^j = C^j_{\lambda,m} \exp[-\tfrac{1}{2}\ln(\delta) J_3] U |j,m\rangle, \quad m = -j, \ldots, j, \tag{2.56}$$

where $U \equiv (2.53)$. They can be written in terms of the Jacobi polynomials as

$$\begin{aligned} |\psi,\lambda,m\rangle^j = {} & C^j_{\lambda,m} \\ & \times \exp\left(-\frac{1}{2}\ln(\delta) J_3 \right) e^{im\phi/2} e^{-i(\phi/2)J_3} \\ & \times \sum_{r=-j}^{j} 2^r \sqrt{\frac{(j+r)!(j-r)!}{(j-m)!(j+m)!}} P^{-r+m,-r-m}_{j+r}(0) |j,r\rangle. \end{aligned} \tag{2.57}$$

In these last states, we want to compute now the mean values and dispersions of some operators in order to exhibit their behavior in the CS and SS.

If $\mathrm{Re}\,\lambda \neq 0$, the mean values of J_1 and J_2 in the states (2.57) are obtained using (2.8) and (2.54). In terms of δ and ϕ as defined by (2.32), we get

$$\langle J_1 \rangle^j_m = 2m \frac{\delta^{1/2}}{(\delta+1)} \cos\left(\frac{\phi}{2}\right), \quad \langle J_2 \rangle^j_m = 2m \frac{\delta^{1/2}}{(\delta+1)} \sin\left(\frac{\phi}{2}\right). \tag{2.58}$$

The relations (2.19)–(2.21) applied to our case tell us that $(\Delta J_1)^2$, $(\Delta J_2)^2$, Δ and $\langle F \rangle$ are all obtained from the mean value of J_3, i.e.,

$$((\Delta J_1)^2)^j_m=\frac{|\lambda|^2}{2\,\mathrm{Re}\,\lambda}\langle J_3\rangle^j_m,\quad ((\Delta J_2)^2)^j_m=\frac{1}{2\,\mathrm{Re}\,\lambda}\langle J_3\rangle^j_m,$$
$$\Delta^j_m=\frac{|\lambda|}{2\,\mathrm{Re}\,\lambda}\langle J_3\rangle^j_m,\quad \langle F\rangle^j_m=\frac{\mathrm{Im}\,\lambda}{\mathrm{Re}\,\lambda}\langle J_3\rangle^j_m. \tag{2.59}$$

The mean values of J_3 in the states (2.57) or equivalently in the states (2.56) are given by

$$\langle J_3\rangle^j_m=-\frac{\partial}{\partial q}\ln(\langle j,m|U^\dagger e^{-qJ_3}U|j,m\rangle), \tag{2.60}$$

where $q=\ln\delta$. After some computations, we get

$$\langle J_3\rangle^j_m=-|m|\tanh\left(\frac{q}{2}\right)-\frac{1}{2}\sinh(q)(j+|m|+1)\,\frac{P^{1,1+2|m|}_{j-|m|-1}(\cosh q)}{P^{0,2|m|}_{j-|m|}(\cosh q)}. \tag{2.61}$$

Inserting (2.61) into the expression (2.59), we get

$$((\Delta J_1)^2)^j_m=(1-2\delta\cos\phi+\delta^2)\Lambda^j_m(\delta),\quad ((\Delta J_2)^2)^j_m=(1+2\delta\cos\phi+\delta^2)\Lambda^j_m(\delta), \tag{2.62a}$$

$$(\Delta)^j_m=\sqrt{1-2\delta^2\cos(2\phi)+\delta^4}\,\Lambda^j_m(\delta),\quad \langle F\rangle^j_m=-4\delta\sin\phi\Lambda^j_m(\delta), \tag{2.62b}$$

where

$$\Lambda^j_m(\delta)=\left[\frac{|m|}{2(1+\delta)^2}+\frac{(j+|m|+1)}{8\delta}\,\frac{P^{1,1+2|m|}_{j-|m|-1}((1+\delta^2)/2\delta)}{P^{0,2|m|}_{j-|m|}((1+\delta^2)/2\delta)}\right]. \tag{2.63}$$

The case $\mathrm{Re}\,\lambda=0$ may be obtained as the limit case of the preceding one by taking $\delta=1$ in the expressions (2.62a), (2.62b) and (2.63). Let us recall that it corresponds to $\langle J_3\rangle=0$ and $\lambda=-i\tan\phi/2$. We get

$$((\Delta J_1)^2)^j_m=\frac{1}{2}[j(j+1)-m^2]\sin^2\left(\frac{\phi}{2}\right),\quad ((\Delta J_2)^2)^j_m=\frac{1}{2}[j(j+1)-m^2]\cos^2\left(\frac{\phi}{2}\right), \tag{2.64a}$$

$$(\Delta)^j_m=\frac{1}{4}[j(j+1)-m^2]|\sin\phi|\ \text{ and }\ \langle F\rangle^j_m=-\frac{1}{2}[j(j+1)-m^2]\sin\phi, \tag{2.64b}$$

using the fact that

$$P^{\alpha,\beta}_n(1)=\frac{(\alpha+1)(\alpha+2)\cdots(\alpha+n)}{n!}. \tag{2.65}$$

These are exactly the results given by Puri.[6]

To illustrate these considerations by a concrete example, let us take the "spin–$\frac{1}{2}$" case, i.e., $j=\frac{1}{2}$. The expressions (2.62a) and (2.62b) thus reduce to

$$((\Delta J_1)^2)_\pm=\frac{(1-2\delta\cos\phi+\delta^2)}{4(1+\delta)^2},\quad ((\Delta J_2)^2)_\pm=\frac{(1+2\delta\cos\phi+\delta^2)}{4(1+\delta)^2} \tag{2.66}$$

and

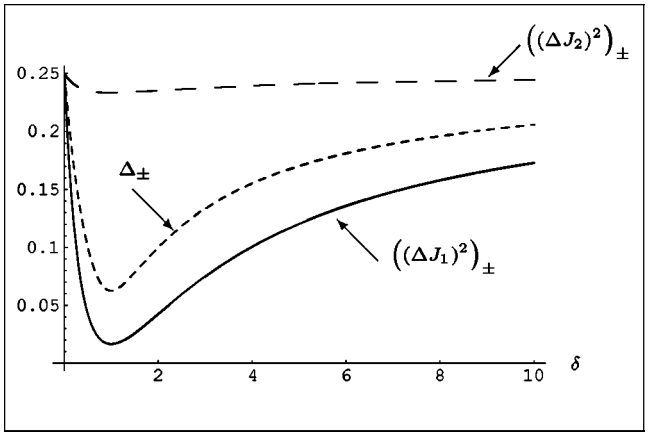

FIG. 3. Graphs of the dispersions $((\Delta J_1)^2)_\pm$, $((\Delta J_2)^2)_\pm$ and the $\Delta_\pm$ factor as functions of δ for $\phi=\pi/6$ and $j=\frac{1}{2}$.

$$\Delta_\pm(\delta,\phi)=\frac{1}{4}\sqrt{1+4\left(\frac{\delta^2\sin^2\phi-\delta(1+\delta)^2}{(1+\delta)^4}\right)}, \tag{2.67}$$

where we have used the $\pm$ sign for the values of $m=\pm\frac{1}{2}$. The MSRUR thus writes

$$((\Delta J_1)^2)_\pm((\Delta J_2)^2)_\pm=(\Delta_\pm)^2(\delta,\phi)=\frac{1}{16}\left[1+4\left(\frac{\delta^2\sin^2\phi-\delta(1+\delta)^2}{(1+\delta)^4}\right)\right]. \tag{2.68}$$

For fixed values of $\phi\neq 0$ and π, the expression (2.67) attains its minimum value $|\sin\phi|/8$ when $\delta=1$. On the other hand, for fixed values of δ such that $\delta\in[0,1[\cup]1,\infty]$, the minimum of (2.67) is $(\frac{1}{4})\sqrt{[1-(4\delta)/(1+\delta)^2]}$ when $\phi=0$ or $\phi=\pi$. In the first case we have $\lambda=-i(\sin\phi)/(1+\cos\phi)$, which means that we have some special classes of SSs from which we recognize CSs with $\lambda=-i$ (eigenstates of the J_1+J_2 operator) and with $\lambda=i$ (eigenstates of the J_1-J_2 operator). In the second case, we have $\lambda=(1-\delta)/(1+\delta)\leqslant 1$ if $\phi=0$ and $\lambda=(1+\delta)/(1-\delta)\geqslant 1$ if $\phi=\pi$, i.e., the minimum $\Delta_\pm(\delta,0)=\Delta_\pm(\delta,\pi)$ values occur for the special states which are eigenstates of the operators $(J_+\pm\delta J_-)$ and $(J_+-\delta J_-)$, respectively. Let us recall that the CSs with $\lambda=1$ occur when $\delta=0$ and those with $\lambda=-1$ when $\delta\mapsto\infty$. They correspond to the eigenstates of J_+ and J_- operators, respectively. For such states, according to Eq. (2.68), we have $((\Delta J_1)^2)_\pm=((\Delta J_2)^2)_\pm=(\Delta_\pm(0,\phi))^2=\lim_{\delta\mapsto\infty}(\Delta_\pm(\delta,\phi))^2=\frac{1}{4}$.

Figure 3 shows the behavior of the dispersions $((\Delta J_1)^2)$, $((\Delta J_2)^2)$ and Δ as functions of δ for $\phi=\pi/6$ and $j=\frac{1}{2}$. The minimum value of $\Delta_\pm$ is here 0,0625. In Fig. 4, we see that the graphs as a function of ϕ are very similar to ones for the preceding example of x and p.

III. ALGEBRA EIGENSTATES ASSOCIATED TO $h(1)\oplus su(2)$

This section begins (Sec. III A) with a review of the SUSY harmonic oscillator and its super-coherent states (SCSs) studied by Aragone and Zypman.[10] We follow (Sec. III B) by the general construction of AES based on the algebra $h(1)\oplus su(2)$. These states are defined as eigenstates of an arbitrary linear combination of the generators of the considered algebra.[8] Then we consider special solutions to CSs and SSs for the so-called super-position and super-momentum operators (Sec. III C).

A. The SUSY harmonic oscillator and its super-coherent states

Let us recall that the quantum SUSY harmonic oscillator is defined as a combination of a bosonic and a fermionic oscillators. Its Hamiltonian is given by

$$H_{\mathrm{SUSY}}=w(a^\dagger a-f^\dagger f), \tag{3.1}$$

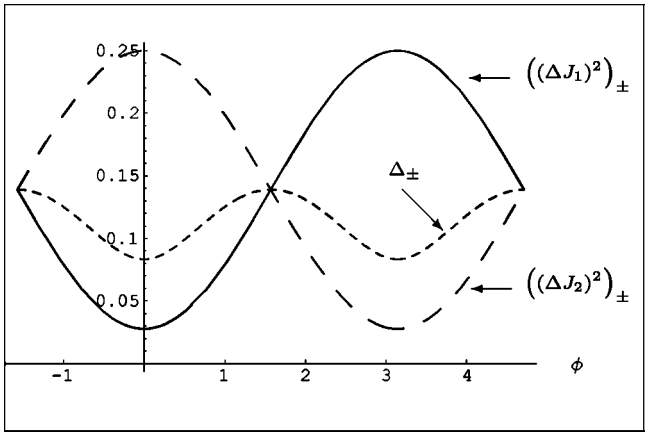

FIG. 4. Graphs of the dispersions $((\Delta J_1)^2)_\pm$, $((\Delta J_2)^2)_\pm$ and the $\Delta_\pm$ factor as functions of ϕ for $\delta=0.5$ and $j=\frac{1}{2}$.

where the bosonic creation and annihilation operators $a^\dagger$ and a are defined as in (2.25) and the corresponding fermionic operators $f^\dagger$ and f are defined as

$$f^\dagger=\sigma_+=\tfrac{1}{2}(\sigma_1+i\sigma_2),\quad f=\sigma_-=\tfrac{1}{2}(\sigma_1-i\sigma_2), \tag{3.2}$$

(the σ_i, $i=1,2$, being the usual Pauli matrices) for the spin $\frac{1}{2}$ fermion. We can thus write

$$H_{\mathrm{SUSY}}=w\left(a^\dagger a-\frac{1}{2}\right)-\frac{w}{2}\sigma_3. \tag{3.3}$$

The representation space we are working with in this context is nothing else than the direct product

$$\begin{aligned}\mathcal{F}=\mathcal{F}_b\otimes\mathcal{F}_f&=\{|n\rangle,n=0,1,2,\ldots\}\otimes\left\{\left|\frac{1}{2},\frac{1}{2}\right\rangle=|+\rangle,\left|\frac{1}{2},\frac{-1}{2}\right\rangle=|-\rangle\right\}\\&=\{|n,+\rangle,|n,-\rangle,n=0,1,2,\ldots\}.\end{aligned} \tag{3.4}$$

Following Aragone and Zypman,[10] SCSs may be constructed as eigenstates of a SUSY annihilation operator $[\sqrt{2}(a+\sigma_+)]$. They are shown to be given as a linear combination of the following normalized pure states:

$$|\psi\rangle_+=D\left(\frac{z}{\sqrt{2}}\right)|0,+\rangle \tag{3.5}$$

and

$$|\psi\rangle_-=D\left(\frac{z}{\sqrt{2}}\right)\frac{[a^\dagger|0,+\rangle-|0,-\rangle]}{\sqrt{2}}, \tag{3.6}$$

in terms of the displacement operator D given in (2.35) and where we recognize in (3.5) the usual CS of the harmonic oscillator. A discussion[10,11] of the properties of such states has led to the observation that, except for the state $|\psi_+\rangle\equiv$ (3.5), no other linear combination of (3.5) and (3.6) will minimize the usual HUR. This means that these states satisfy $(\Delta x)^2(\Delta p)^2\geqslant\frac{1}{4}$, the equality between the position x and the momentum p being realized only for $|\psi_+\rangle\equiv$(3.5).

Such a fact can be clarified from our discussion of Sec. II A. The SCSs (3.5) and (3.6) are in fact MUS for the SRUR (2.4) with

$$A=\frac{1}{\sqrt{2}}[(a^{\dagger}+a)+\sigma_1]=\left[x+\frac{\sigma_1}{\sqrt{2}}\right] \quad \text{and} \quad B=\frac{1}{\sqrt{2}}[i(a^{\dagger}-a)+\sigma_2]=\left[p+\frac{\sigma_2}{\sqrt{2}}\right], \tag{3.7}$$

these operators being different from x and p. The SCSs are coherent in the sense that they satisfy Eq. (2.6) with $\lambda=1$.

Clearly, in such a context, through the group theory level, we are combining the information coming from both the Heisenberg–Weyl $h(1)$ and the su(2) algebras realized in terms of the Pauli matrices in the spin $\frac{1}{2}$ case. It is then natural to ask the questions of determining the general CS and SS for the direct sum $h(1)\oplus \mathrm{su}(2)$ which will indeed include the special SCS we just discussed.

B. Algebra eigenstates

We are working with the $h(1)\oplus \mathrm{su}(2)$ algebra generated by $\{a,a^{\dagger},I;J_+,J_-,J_3\}$ as defined in the preceding sections. The AESs[8] for this algebra are defined as eigenstates corresponding to a complex combination of the associated generators. A general Hermitian operator A constructed from a combination of these generators is

$$A=A_1a+\overline{A}_1a^{\dagger}+A_2I+A_3J_+ +\overline{A}_3J_-+A_4J_3, \quad A_2,A_4\in\mathbb{R}, \ A_1,A_3\in\mathbb{C}. \tag{3.8}$$

Two such operators, called A and B, satisfy the commutation relation (2.1) with

$$C=[i(\overline{A}_1B_1-A_1\overline{B}_1)I+2i(B_3\overline{A}_3-\overline{B}_3A_3)J_3+i(A_3B_4-A_4B_3)J_+ +i(A_4\overline{B}_3-\overline{A}_3B_4)J_-]. \tag{3.9}$$

Once we search for states satisfying (2.6), i.e., for eigenstates of $A+i\lambda B$ ($\lambda\in\mathbb{C},\lambda\neq 0$), we are in fact considering AESs and we know from Sec. II A that they minimize the SRUR (2.4). Let us then study the solutions of such a general eigenstate equation (2.6) for A and B on the form (3.8).

It is convenient to rewrite this equation as

$$[\alpha_-a+\alpha_+a^{\dagger}+\alpha_3I+\beta_-J_+ +\beta_+J_- +\beta_3J_3]|\psi\rangle=z|\psi\rangle, \tag{3.10}$$

where

$$\begin{aligned} &\alpha_-=A_1+i\lambda B_1, \quad \alpha_+=\overline{A}_1+i\lambda\overline{B}_1, \quad \alpha_3=A_2+i\lambda B_2,\\ &\beta_-=A_3+i\lambda B_3, \quad \beta_+=\overline{A}_3+i\lambda\overline{B}_3, \quad \beta_3=A_4+i\lambda B_4. \end{aligned} \tag{3.11}$$

To solve (3.10), we express $|\psi\rangle$ as a superposition of fundamental states $|n;j,m\rangle$ which constitute a generalization of the Fock space (3.4) for spin j. We write

$$|\psi\rangle^j=\sum_{m=-j}^{j}\sum_{n=0}^{\infty}C_{n,m}^{j}|n;j,m\rangle, \tag{3.12}$$

for fixed j, integer or half-odd integer. Let us recall that we have

$$\begin{aligned} a|n;j,m\rangle&=\sqrt{n}|n-1;j,m\rangle,\\ a^{\dagger}|n;j,m\rangle&=\sqrt{n+1}|n+1;j,m\rangle,\\ J_{\pm}|n;j,m\rangle&=\sqrt{(j\mp m)(j\pm m+1)}|n;j,m\pm 1\rangle, \end{aligned} \tag{3.13}$$

with

$$\langle n;j,m|l;j,r\rangle=\delta_{nl}\delta_{mr}. \tag{3.14}$$

Inserting (3.12) into (3.10) and taking into account the relations (3.13) and (3.14), we get a recurrence system which becomes more and more complicated as j increases. We also notice that the case where $\alpha_-=0$ with $\alpha_+\neq 0$ does not give any solution and must be eliminated. Here two ways of solving it completely are presented. The first one uses the results obtained in Sec. II B and Appendix A where AESs of su(2) are explicitly constructed. It is described explicitly in this section using operators acting on a fundamental state. The second one is based on the method of resolution of a first order system of linear differential equations and is described in Appendix B.

With respect to the discussion in Appendix A, we have mainly two types of eigenvalues for z. The first type is given by

$$z=\rho_m^j+\alpha_3+mb, \quad \rho_m^j\in\mathbb{C}, \tag{3.15}$$

for fixed j and where $m=-j,\ldots,j$ and

$$b=\sqrt{4\beta_+\beta_-+\beta_3^2}\neq 0. \tag{3.16}$$

If we compare equations (2.26) and (A5) and their respective solutions (2.33) and (A15), we find the set of solutions

$$|\psi\rangle_m^j=(C_m^j)^{-1/2}\exp\left[-\frac{\alpha_+}{2\alpha_-}a^{\dagger 2}+\frac{\rho_m^j}{\alpha_-}a^\dagger\right]T_{\text{eff}}|0;j,m\rangle, \tag{3.17}$$

when $\alpha_-\neq 0$. Here T_{eff} is given by (A14) when $\{\beta_+\neq 0,\beta_-\neq 0\}$, (A18) when $\{\beta_+=0,\beta_3\neq 0\}$, (A20) when $\{\beta_-=0,\beta_3\neq 0\}$ and finally the identity when $\{\beta_-=\beta_+=0,\beta_3\neq 0\}$.

The second type corresponds to the so-called degenerate case ($b=0$) where $z=\rho+\alpha_3$. The sets of independent solutions are now given by

$$\begin{aligned}|\psi\rangle_m^j=(C_m^j)^{-1/2}&\exp\left[-\frac{\alpha_+}{2\alpha_-}a^{\dagger 2}+\frac{\rho}{\alpha_-}a^\dagger\right]\\&\times\sum_{k=0}^{j-m}(-1)^k\binom{j-m}{k}\frac{(2j-k)!}{(2j)!}(a^\dagger)^{j-m-k}\left(\frac{\alpha_-J_-}{\beta_-}\right)^k|0;j,j\rangle\end{aligned} \tag{3.18}$$

when $\beta_+=\beta_3=0$,

$$\begin{aligned}|\psi\rangle_m^j=(C_m^j)^{-1/2}&\exp\left[-\frac{\alpha_+}{2\alpha_-}a^{\dagger 2}+\frac{\rho}{\alpha_-}a^\dagger\right]\\&\times\sum_{k=0}^{j-m}(-1)^k\binom{j-m}{k}\frac{(2j-k)!}{(2j)!}(a^\dagger)^{j-m-k}\left(\frac{\alpha_-J_+}{\beta_+}\right)^k|0;j,-j\rangle\end{aligned} \tag{3.19}$$

when $\beta_-=\beta_3=0$, and

$$\begin{aligned}|\psi\rangle_m^j=(C_m^j)^{-1/2}&\exp\left[-\frac{\alpha_+}{2\alpha_-}a^{\dagger 2}+\frac{\rho}{\alpha_-}a^\dagger\right]\\&\times\left[\sum_{k=0}^{j-m}(-1)^k\binom{j-m}{k}\frac{(2j-k)!}{(2j)!}(a^\dagger)^{j-m-k}\left(\frac{\alpha_-}{\beta_+}\right)^k\frac{d^k e^{\vartheta J_+}}{d\vartheta^k}\right]|0;j,-j\rangle\end{aligned} \tag{3.20}$$

when β_+,β_- and β_3 are different from zero and for $\vartheta=\beta_3/(2\beta_+)=-2\beta_-/\beta_3$.

C. Coherent and squeezed states for the super-position and super-momentum operators

Let us consider the eigenstates of Eq. (3.10) corresponding to the following special values of the parameters

$$A_4=B_4=A_2=B_2=0,\quad A_1=iB_1=\frac{\mu}{\sqrt{2}},\quad (\mu\neq 0),\quad A_3=iB_3=\frac{\tau}{\sqrt{2}}, \tag{3.21}$$

so that A will be called the super-position operator denoted by X and B the super-momentum operator denoted by P. We have

$$X=\frac{1}{\sqrt{2}}[(\mu a+\overline{\mu}a^{\dagger})+(\tau J_{+}+\overline{\tau}J_{-})],\quad P=\frac{i}{\sqrt{2}}[(\overline{\mu}a^{\dagger}-\mu a)+(\overline{\tau}J_{-}-\tau J_{+})]. \tag{3.22}$$

We see that the operators (3.7) associated to the SCS are then a special case where $\mu=\overline{\mu}=\tau=\overline{\tau}=1$ in the spin-$\frac{1}{2}$ case.

The eigenstate equation (3.10) now writes

$$[X+i\lambda P]|\psi\rangle=z|\psi\rangle \tag{3.23}$$

and the operator C in (3.9) is diagonal and takes the form

$$C=|\mu|^2I+2|\tau|^2J_3. \tag{3.24}$$

Since we have

$$\begin{aligned}&\alpha_{-}=\frac{\mu(1+\lambda)}{\sqrt{2}},\quad \alpha_{+}=\frac{\overline{\mu}(1-\lambda)}{\sqrt{2}},\quad \alpha_3=0,\\ &\beta_{-}=\frac{\tau(1+\lambda)}{\sqrt{2}},\quad \beta_{+}=\frac{\overline{\tau}(1-\lambda)}{\sqrt{2}},\quad \beta_3=0,\end{aligned} \tag{3.25}$$

and finally

$$b=\sqrt{2}|\tau|\sqrt{1-\lambda^2}, \tag{3.26}$$

we can use the preceding solutions to give all the solutions of Eq. (3.23).

For $\lambda=1$, we have $\alpha_{+}=\beta_{+}=b=0$ and the eigenstate equation is

$$[\mu a+\tau J_{+}]|\psi\rangle=\frac{z}{\sqrt{2}}|\psi\rangle. \tag{3.27}$$

The normalized solutions are obtained from (3.18) and take the form

$$|\psi\rangle_m^j=(C_m^j(\mu,\tau))^{-1/2}D\left(\frac{z}{\mu\sqrt{2}}\right)\left[\sum_{k=0}^{j-m}(-1)^k\binom{j-m}{k}\frac{(2j-k)!}{(2j)!}(a^{\dagger})^{j-m-k}\left(\frac{\mu J_{-}}{\tau}\right)^k\right]|0;j,j\rangle, \tag{3.28}$$

where the normalization constant is given by

$$C_m^j(\mu,\tau)=(j-m)!\left[\sum_{k=0}^{j-m}\binom{j-m}{k}\frac{(2j-k)!}{(2j)!}\left(\frac{|\mu|^2}{|\tau|^2}\right)^k\right]. \tag{3.29}$$

Let us recall that in this case we have CSs for which

$$(\Delta X)=(\Delta P)=\Delta=\tfrac{1}{2}\langle C\rangle. \tag{3.30}$$

The mean value of C is easy to compute and we have

$$\langle C\rangle_m^j=|\mu|^2+2|\tau|^2\left[j+|\tau|^2\frac{\partial}{\partial|\tau|^2}\ln(C_m^j(\mu,\tau))\right]. \tag{3.31}$$

In the special case $j=\frac{1}{2}$, we find the normalized and orthogonal states

$$|\psi\rangle^+=D\left(\frac{z}{\mu\sqrt{2}}\right)|0;+\rangle,\quad |\psi\rangle^-=D\left(\frac{z}{\mu\sqrt{2}}\right)\frac{|\tau|}{\sqrt{|\mu|^2+|\tau|^2}}\left[a^\dagger|0;+\rangle-\frac{\mu}{\tau}|0;-\rangle\right], \tag{3.32}$$

where D is again given by (2.35). In those states, we have

$$\langle C\rangle^+=|\mu|^2+|\tau|^2,\quad \langle C\rangle^-=\left[(|\mu|^2+|\tau|^2)-\frac{2|\mu|^2|\tau|^2}{(|\mu|^2+|\tau|^2)}\right]. \tag{3.33}$$

This is clearly a generalization of SCSs considered by Aragone and Zypman[10] and recalled in (3.5) and (3.6).

From (3.33), we see that the dispersions of ΔX and ΔP given by (3.30) computed in the CS $|\psi\rangle^-$ are smaller than in the states $|\psi\rangle^+$. The states $|\psi\rangle^-$ thus are the closest to classical states for the SUSY harmonic oscillators (this means with respect to the super-position and the super-momentum) while $|\psi\rangle^+$ are indeed the ones closest to classical states of the standard harmonic oscillator (i.e., they minimize the HUR for X and P). Let us mention that if we take $\mu=1$, we see that $\langle C\rangle^+$ has its minimum value equal to 1 for $\tau\mapsto 0$ and in this case $X=x$ and $P=p$. For the same value of μ, we see that $\langle C\rangle^-$ takes the form

$$\langle C\rangle^-=\frac{1+|\tau|^4}{1+|\tau|^2}, \tag{3.34}$$

which has a minimum value $\langle C\rangle^-_{\min}=2(\sqrt{2}-1)<1$ for $|\tau|^2=\sqrt{2}-1$.

For $\lambda\neq\pm 1$, from Eq. (3.17) and $T_{\text{eff}}\equiv$ (A13), using also (2.35) and (2.36), we get the states

$$\begin{aligned}|\psi\rangle_m^j=&(C_m^j)^{-1/2}S(\chi(\delta,\phi-2\phi_u))D(\eta_m(z,\delta,\phi,\mu,\tau))\\&\times\exp\left(\frac{-\tau\delta^{-1/2}e^{-i\phi/2}}{|\tau|}J_+\right)\exp\left(\frac{\bar{\tau}\delta^{1/2}e^{i\phi/2}}{2|\tau|}J_-\right)|0;j,m\rangle,\end{aligned} \tag{3.35}$$

where

$$\eta_m(z,\delta,\phi,\mu,\tau)=\frac{1}{\mu}\left\{\frac{z(1+\delta e^{i\phi})}{\sqrt{2}}-2m|\tau|\delta^{1/2}e^{i\phi/2}\right\},\quad \mu=|\mu|e^{i\phi_u} \tag{3.36}$$

and where we have used instead of λ the parameters δ and ϕ as given in (2.32). Let us mention that this general expression (3.35) clearly shows the presence of the unitary operators D and S associated with $h(1)$ and su(1,1), respectively, which is the contribution of the bosonic part of our SUSY model. Moreover, the fermionic contribution appears through the action of a unitary operator associated with su(2).

Now these states satisfy the MUR

$$(\Delta X)_m^j(\Delta P)_m^j=\Delta_m^j=\frac{1}{2}\sqrt{1+\frac{4\delta^2\sin^2\phi}{(1-\delta^2)^2}}|\langle C\rangle_m^j|. \tag{3.37}$$

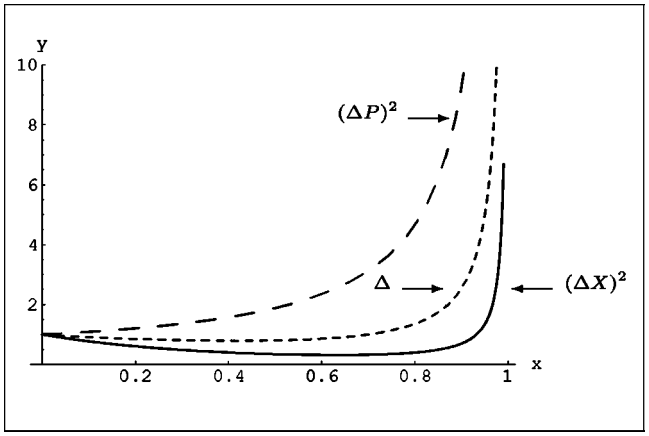

FIG. 5. Graphs of the dispersions $(\Delta X)^2$, $(\Delta P)^2$ and the factor Δ as functions of $x \equiv \delta$ for $\phi = \pi/6$. $|\tau| = |\mu| = 1$, $j = \frac{1}{2}$.

The mean value of C is

$$\langle C \rangle_m^j = |\mu|^2 + 2|\tau|^2 \frac{(1-\delta)}{(1+\delta)} \left(j - \frac{4(j+|m|)\delta}{(1+\delta)^2} \Omega \right), \tag{3.38}$$

where Ω is expressed in terms of Jacobi polynomials (see Appendix A),

$$\Omega = \frac{P_{j-|m|-1}^{(-2j,1)}(1-(8\delta/(1+\delta)^2))}{P_{j-|m|}^{(-2j-1,0)}(1-(8\delta/(1+\delta)^2))}, \tag{3.39}$$

for $m = -j+1, \ldots, j-1$ and $\Omega = 0$ for $m = \pm j$. In fact, we see that in these last cases, we have

$$\langle C \rangle_{\pm j}^j = |\mu|^2 + 2j|\tau|^2 \frac{(1-\delta)}{(1+\delta)}. \tag{3.40}$$

It is now interesting to examine the behavior of the dispersions ΔX and ΔP in these states for the spin $\frac{1}{2}$ case. Using (2.20) with (3.40) for $j = \frac{1}{2}$, we get

$$\begin{aligned} ((\Delta X)^2)_\pm &= \frac{(1-2\delta\cos\phi+\delta^2)}{2(1-\delta^2)} \left[|\mu|^2 + |\tau|^2 \frac{(1-\delta)}{(1+\delta)} \right], \\ ((\Delta P)^2)_\pm &= \frac{(1+2\delta\cos\phi+\delta^2)}{2(1-\delta^2)} \left[|\mu|^2 + |\tau|^2 \frac{(1-\delta)}{(1+\delta)} \right], \end{aligned} \tag{3.41}$$

with

$$\Delta_\pm = \frac{\sqrt{(1-\delta^2)^2 + 4\delta^2 \sin^2\phi}}{2(1-\delta^2)} \left[|\mu|^2 + |\tau|^2 \frac{(1-\delta)}{(1+\delta)} \right]. \tag{3.42}$$

If we take $\delta = 0$ (i.e., $\lambda = 1$) in these last expressions, we find only the values of the dispersions of X and P in the usual coherent states $|\psi\rangle^+$ as given by (3.32) and not the ones in the CS $|\psi\rangle^-$, which is the reason why that case has been treated separately.

Figures 5 and 6 show the behavior of $((\Delta X)^2)_\pm$ and $((\Delta P)^2)_\pm$ and $\Delta_\pm$ as functions of δ for $\phi = \pi/6$ and as functions of ϕ for $\delta = 0.5$, respectively. We notice a similar behavior as for the position and momentum operators.

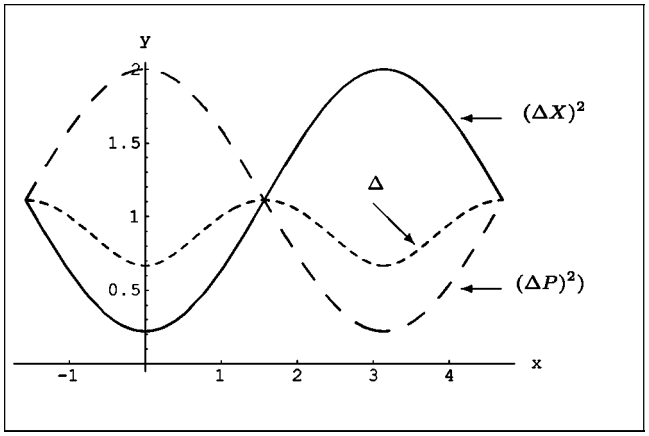

FIG. 6. Graphs of the dispersions $(\Delta X)^2$, $(\Delta P)^2$ and the factor Δ as functions of $x\equiv\phi$, $\delta=0.5$, $|\tau|=|\mu|=1$, $j=\frac{1}{2}$.

IV. CONSTRUCTION OF $h(1)\oplus su(2)$ HAMILTONIANS

An application of our CS and SS based on the algebra $h(1)\oplus su(2)$ will be the study of possible Hamiltonians which can be written as $\mathcal{H}=w\mathcal{A}^\dagger\mathcal{A}$, where $\mathcal{A}$ is a linear combination of the generators of $h(1)\oplus su(2)$. It is clear that the usual harmonic oscillator Hamiltonian will enter in the scheme as a special case (Sec. IV A) but also the Jaynes–Cummings[16] one in the strong coupling limit (Sec. IV B and C).

Moreover, since the CSs and SSs already constructed in the preceding section are in fact eigenstates of the operator $\mathcal{A}$, we would be able to find easily some properties of the mean value and the dispersion of the associated energies in those states.

A. Isospectral $h(1)\oplus su(2)$ harmonic oscillator Hamiltonians

We are interested in systems for which the Hamiltonian is expressed in the form

$$\mathcal{H}=w\mathcal{A}^\dagger\mathcal{A}, \tag{4.1}$$

where

$$\mathcal{A}=\alpha_- a+\alpha_+ a^\dagger+\alpha_3 I+\beta_- J_+ +\beta_+ J_- +\beta_3 J_3, \quad \alpha_-\neq 0, \tag{4.2}$$

is an element of the $h(1)\oplus su(2)$ algebra. The commutator of the operators $\mathcal{A}$ and $\mathcal{A}^\dagger$ is

$$[\mathcal{A},\mathcal{A}^\dagger]=(|\alpha_-|^2-|\alpha_+|^2)I+(|\beta_-|^2-|\beta_+|^2)J_3+(\beta_3\overline{\beta}_+-\overline{\beta}_3\beta_-)J_+ +(\overline{\beta}_3\beta_+-\beta_3\overline{\beta}_-)J_- . \tag{4.3}$$

If $|Z\rangle$ is an eigenstate of the operator $\mathcal{A}$ with eigenvalue z, i.e.,

$$\mathcal{A}|Z\rangle=z|Z\rangle, \tag{4.4}$$

then the mean value of the energy in this state will always be given by

$$\langle Z|\mathcal{H}|Z\rangle=w|z|^2 \tag{4.5}$$

and the dispersion by

$$(\Delta\mathcal{H})^2=w^2|z|^2\langle Z|[\mathcal{A},\mathcal{A}^\dagger]|Z\rangle. \tag{4.6}$$

First, let us consider the special case where

$$[\mathcal{A},\mathcal{A}^{\dagger}]=I. \tag{4.7}$$

This imposes the following conditions on the parameters:

$$|\alpha_-|^2-|\alpha_+|^2=1, \quad |\beta_-|=|\beta_+| \quad \text{and} \quad \beta_3\overline{\beta}_+-\overline{\beta}_3\beta_-=0, \tag{4.8}$$

i.e.,

$$\alpha_-=\cosh\alpha e^{i\theta_-}, \quad \alpha_+=\sinh\alpha e^{i\theta_+}, \quad \beta_\pm=\beta e^{i\varphi_\pm}, \tag{4.9}$$

and

$$\beta_3=\begin{cases} re^{i(\varphi_++\varphi_-)/2}, r\in\mathbb{R}_+\cup\{0\}, & \text{if } \beta\neq 0, \\ re^{i\varphi_3}, r\in\mathbb{R}_+\cup\{0\}, & \text{if } \beta=0. \end{cases} \tag{4.10}$$

When $\beta\neq 0$, the operator $\mathcal{A}$ then takes the form

$$\mathcal{A}=\cosh\alpha e^{i\theta_-}a+\sinh\alpha e^{i\theta_+}a^{\dagger}+\alpha_3 I+\beta(e^{i\varphi_-}J_++e^{i\varphi_+}J_-)+re^{i(\varphi_++\varphi_-)/2}J_3. \tag{4.11}$$

The parameter b given in (3.16) becomes $b=\sqrt{4\beta^2+r^2}e^{i(\varphi_++\varphi_-)/2}$ and is different from zero. Therefore in this case, according to the equation (3.17), the normalized solutions of the eigenstate equation (4.4) are given by

$$|Z\rangle_m^j=S(\Lambda)D(\zeta_m(\alpha_3,1))TD(ze^{-i\theta_-})|0;j,m\rangle, \tag{4.12}$$

where

$$\Lambda=-\alpha e^{i(\theta_+-\theta_-)}, \quad \zeta_m(\alpha_3,\epsilon)=-[\alpha_3+\epsilon m\sqrt{4\beta^2+r^2}e^{i(\varphi_++\varphi_-)/2}]e^{-i\theta_-}, \tag{4.13}$$

and

$$T=\exp\left(-\frac{\tilde{\theta}}{2}[e^{-i(\varphi_+-\varphi_-)/2}J_+-e^{i(\varphi_+-\varphi_-)/2}J_-]\right), \tag{4.14}$$

with

$$\frac{\tilde{\theta}}{2}=\tan^{-1}\left(\sqrt{1-\frac{r}{2\beta^2}(\sqrt{4\beta^2+r^2}-r)}\right). \tag{4.15}$$

This means that T is a unitary operator.

We remark that, if we define the new operator

$$\begin{aligned}\mathcal{A}_0&=D^{\dagger}(-\alpha_3e^{-i\theta_-})S^{\dagger}(\Lambda)\mathcal{A}S(\Lambda)D(-\alpha_3e^{-i\theta_-})\\&=e^{i\theta_-}a+\beta(e^{i\varphi_-}J_++e^{i\varphi_+}J_-)+re^{i(\varphi_++\varphi_-)/2}J_3,\end{aligned} \tag{4.16}$$

which is simpler than the original $\mathcal{A}$, then the new Hamiltonian $\mathcal{H}_0=w\mathcal{A}_0^{\dagger}\mathcal{A}_0$ is isospectral to the Hamiltonian $\mathcal{H}\equiv$ (4.1).

The dispersion of $\mathcal{H}$ calculated on the states (4.12) is, from (4.6) and (4.7), given by $(\Delta\mathcal{H})^2=w^2|z|^2$ and is the same as the one of $\mathcal{H}_0$ calculated on the states $D(\zeta_m(-z,1))T|0;j,m\rangle$. This value is exactly the dispersion of the harmonic oscillator in the usual CS.

On the other hand, due to (4.7) we have $[\mathcal{H},\mathcal{A}]=-w\mathcal{A}$, so we have a complete analogy with the harmonic oscillator. The CSs associated to the Hamiltonian $\mathcal{H}$, called generalized harmonic oscillator, are those given by the equation (4.12) and, thus, one can write them in the form

$$|Z\rangle_m^j = \mathcal{D}(z)|\tilde{0}\rangle_m^j, \quad \text{where} \quad \mathcal{D}(z) = \exp(z\mathcal{A}^\dagger - \bar{z}\mathcal{A}) \tag{4.17}$$

and $|\tilde{0}\rangle_m^j$, $m=-j,\ldots,j$, are the fundamental states of the system $\mathcal{H}$, that is, the eigenstates of $\mathcal{H}$ corresponding to the $(2j+1)$ degenerate eigenvalue 0. They are also eigenstates of $\mathcal{A}$ corresponding to the eigenvalue 0. So, they can be written

$$|\tilde{0}\rangle_m^j = S(\Lambda)D(\zeta_m(\alpha_3,1))T|0;j,m\rangle. \tag{4.18}$$

Furthermore, the SSs associated with $\mathcal{H}$ are given by

$$|\tilde{\psi}\rangle_m^j = \mathcal{S}(\chi)\mathcal{D}(z)|\tilde{0}\rangle_m^j, \tag{4.19}$$

where the super-squeezed operator $\mathcal{S}(\chi)$ is given by $\exp(\chi\mathcal{A}^{\dagger 2}/2 - \bar{\chi}\mathcal{A}^2/2)$ and the super-displacement operator $\mathcal{D}(z)$ is given in (4.17). If we define $\mathcal{X}=(\mathcal{A}+\mathcal{A}^\dagger)/\sqrt{2}$ and $\mathcal{P}=i(\mathcal{A}^\dagger - \mathcal{A})/\sqrt{2}$, these states (4.19) minimize the SRUR $(\Delta\mathcal{X})^2(\Delta\mathcal{P})^2=(1+\langle F\rangle^2)/4$, i.e., they are solutions of the eigenstate equation $[(1-\lambda)\mathcal{A}^\dagger+(1+\lambda)\mathcal{A}]|\psi\rangle=\sqrt{2}|\psi\rangle$.

The eigenstates of $\mathcal{H}$ corresponding to the $(2j+1)$ degenerate energy eigenvalue $E_n=nw$ are now given by

$$|\tilde{n}\rangle_m^j = \frac{\mathcal{A}^{\dagger n}}{\sqrt{n!}}|\tilde{0}\rangle_m^j. \tag{4.20}$$

These states may be obtained as the action of a unitary operator on the states $|n;j,m\rangle$. Indeed, if we introduce the unitary operator

$$U_n^m = e^{-in\theta_-}S(\Lambda)D(\zeta_m(\alpha_3,1))T, \tag{4.21}$$

we see that, from (4.20), we have

$$\begin{aligned}
|\tilde{n}\rangle_m^j &= \frac{e^{in\theta_-}}{\sqrt{n!}}(\mathcal{A}^\dagger)^n U_n^m|0;j,m\rangle, \\
&= \frac{e^{in\theta_-}}{\sqrt{n!}}U_n^m((U_n^m)^\dagger\mathcal{A}^\dagger U_n^m)^n|0;j,m\rangle, \\
&= \frac{e^{in\theta_-}}{\sqrt{n!}}U_n^m(e^{-i\theta_-}a^\dagger + \sqrt{4\beta^2+r^2}e^{-i(\varphi_+ + \varphi_-)/2}(J_3-m))^n|0;j,m\rangle.
\end{aligned} \tag{4.22}$$

Since we have $(J_3-m)|0;j,m\rangle=0$, we finally find

$$|\tilde{n}\rangle_m^j = U_n^m|n;j,m\rangle. \tag{4.23}$$

In the case $\beta=0$, the operator $\mathcal{A}$ is given by

$$\mathcal{A} = \cosh\alpha e^{i\theta_-}a + \sinh\alpha e^{i\theta_+}a^\dagger + \alpha_3 I + re^{i\varphi_3}J_3. \tag{4.24}$$

Then, if $r\neq 0$, one has the same results as above, except that it is necessary to replace T by I and b by $\beta_3=re^{i\varphi_3}$. If $r=0$, $\mathcal{A}$ is an element of the algebra $h(1)$ and then the results are the ones obtained in Sec. II A for the standard harmonic oscillator after applying the unitary transformation $S(\Lambda)D(-\alpha_3 e^{-i\theta_-})$.

B. Strong-coupling limit of the Jaynes–Cummings Hamiltonian as limit of $h(1)\oplus su(2)$ Hamiltonians

We are going to consider now the case where

$$[\mathcal{A},\mathcal{A}^\dagger]=I+2xJ_3, \quad x\in\mathbb{R}. \tag{4.25}$$

This imposes the following conditions on the parameters:

$$|\alpha_-|^2-|\alpha_+|^2=1, \quad |\beta_-|^2-|\beta_+|^2=x \quad \text{and} \quad \beta_3\overline{\beta}_+-\overline{\beta}_3\beta_-=0. \tag{4.26}$$

We already know the results when $x=0$. When $x\neq 0$, the conditions (4.26) imply

$$\alpha_-=\cosh\alpha e^{i\theta_-}, \quad \alpha_+=\sinh\alpha e^{i\theta_+}, \quad \beta_3=0, \tag{4.27}$$

and

$$\beta_-=\begin{cases} x^{1/2}\cosh\beta e^{i\varphi_-}, & \text{if } x>0,\\ |x|^{1/2}\sinh\beta e^{i\varphi_-}, & \text{if } x<0,\end{cases} \tag{4.28}$$

$$\beta_+=\begin{cases} x^{1/2}\sinh\beta e^{i\varphi_+}, & \text{if } x>0,\\ |x|^{1/2}\cosh\beta e^{i\varphi_+}, & \text{if } x<0.\end{cases} \tag{4.29}$$

The parameter $b\equiv$ (3.16) becomes $b=|x|^{1/2}\sqrt{2\sinh(2\beta)}e^{i(\varphi_++\varphi_-)/2}$. This means that $b=0$ if and only if $\beta=0$.

In the case $\beta\neq 0$, according to the equations (3.17), (A7), (A11), and (A12), the normalized eigenstates of the operator $\mathcal{A}$ are given by

$$|Z(x)\rangle_m^j=(C_m^j(x))^{-1/2}S(\Lambda)D(-\alpha_3e^{-i\theta_-})D(\eta_m(z,x))\exp\left[-\frac{x}{2|x|}\ln(\tanh\beta)J_3\right]U|0;j,m\rangle, \tag{4.30}$$

where

$$\eta_m(z,x)=[z-m|x|^{1/2}\sqrt{2\sinh(2\beta)}e^{i(\varphi_++\varphi_-)/2}]e^{-i\theta_-}, \tag{4.31}$$

$$U=\exp\left[-\frac{\pi}{4}(e^{-i(\varphi_+-\varphi_-)/2}J_+-e^{i(\varphi_+-\varphi_-)/2}J_-)\right] \tag{4.32}$$

and

$$\begin{aligned} C_m^j(x)&=\langle j,m|U^\dagger\exp\left[-\frac{x}{|x|}\ln(\tanh\beta)J_3\right]U|j,m\rangle\\ &=\left(\frac{1+\tanh\beta}{2\sqrt{\tanh\beta}}\right)^{\mp 2m}P_{j\pm m}^{0;\mp 2m}\left(\frac{1+\tanh^2\beta}{2\tanh\beta}\right). \end{aligned} \tag{4.33}$$

From (4.6) and (4.25), the dispersion of the $\mathcal{H}\equiv$ (4.1) in the states (4.30) can be calculated explicitly. We get

$$(\Delta\mathcal{H})^2)_m^j=w^2|z|^2(1+2x_m^j\langle Z(x)|J_3|Z(x)\rangle_m^j). \tag{4.34}$$

In the last expression, the mean value of J_3 is obtained in a similar way then to get (2.61). The result is

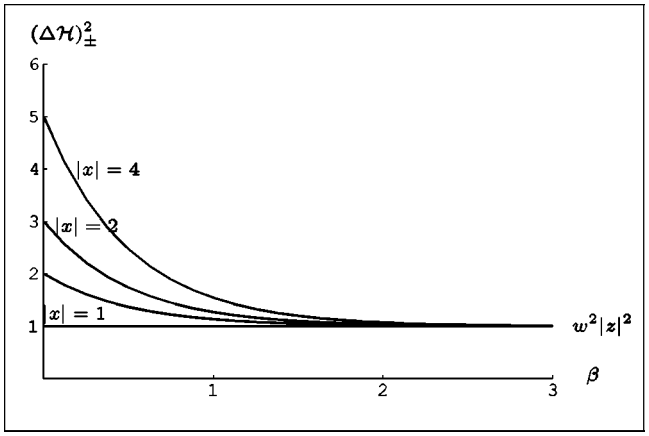

FIG. 7. Graphs of the dispersions $((\Delta\mathcal{H})^2)_{\pm} \equiv$ (4.37) as functions of $\beta>0$ for $|x|=0,1,2,4$.

$$ {}^{j}_{m}\langle Z(x)|J_3|Z(x)\rangle^{j}_{m} = \frac{x}{|x|}\left\{ |m|e^{-2\beta} + \frac{(j+|m|+1)}{2\sinh(2\beta)} \frac{P^{1;2|m|}_{j-|m|-1}(\coth(2\beta))}{P^{0;2|m|}_{j-|m|}(\coth(2\beta))} \right\}. \tag{4.35} $$

If we take $m=\pm j$, the dispersion of $\mathcal{H}$ is

$$ ((\Delta\mathcal{H})^2)^{j}_{\pm j} = w^2|z|^2(1+2j|x|e^{-2\beta}), \tag{4.36} $$

and, in particular, when $j=\frac{1}{2}$, we get

$$ ((\Delta\mathcal{H})^2)_{\pm} = w^2|z|^2(1+|x|e^{-2\beta}). \tag{4.37} $$

Figure 7 shows the graphs of $((\Delta\mathcal{H})^2)_{\pm}$ as functions of β for different values of $|x|$ when $w^2|z|^2$ is taken equal to 1.

Let us compute the new operator $\mathcal{A}_0$ defined as (4.16). We get

$$ \mathcal{A}_0 = \begin{cases} e^{i\theta_-}a + x^{1/2}\cosh\beta e^{i\varphi_-}J_+ + x^{1/2}\sinh\beta e^{i\varphi_+}J_-, & \text{if } x>0, \\ e^{i\theta_-}a + |x|^{1/2}\sinh\beta e^{i\varphi_-}J_+ + |x|^{1/2}\cosh\beta e^{i\varphi_+}J_-, & \text{if } x<0, \end{cases} \tag{4.38} $$

and a new Hamiltonian $\mathcal{H}_0 = w\mathcal{A}_0^{\dagger}\mathcal{A}_0$ isospectral to the Hamiltonian $\mathcal{H}$ which takes the form

$$ \begin{aligned} \mathcal{H}_0 = w\{ & a^{\dagger}a + |x|[\sinh^2(\beta)J_-J_+ + \cosh^2(\beta)J_+J_-] + |x|^{1/2}\cosh\beta[e^{i(\varphi_+-\theta_-)}a^{\dagger}J_- \\ & + e^{-i(\varphi_+-\theta_-)}aJ_+] + |x|^{1/2}\sinh\beta[e^{i(\varphi_--\theta_-)}a^{\dagger}J_+ + e^{-i(\varphi_--\theta_-)}aJ_-] \\ & + |x|\sinh\beta\cosh\beta[e^{i(\varphi_+-\varphi_-)}J_-^2 + e^{-i(\varphi_+-\varphi_-)}J_+^2]\}, \end{aligned} \tag{4.39} $$

if $x<0$. If $x>0$, we get a similar expression except that we must make the change $\sinh\beta \leftrightarrow \cosh\beta$.

In the spin-$\frac{1}{2}$ representation, we have

$$ J_-^2 = J_+^2 = 0, \quad J_+J_- = \frac{I}{2} + J_3 \quad \text{and} \quad J_-J_+ = \frac{I}{2} - J_3, \tag{4.40} $$

hence (4.39) becomes

$$\mathcal{H}_0 = w\left\{\left(a^\dagger a + \frac{I}{2}\right) - xJ_3 + |x|^{1/2}\cosh\beta[e^{i(\varphi_+ - \theta_-)}a^\dagger J_- + e^{-i(\varphi_+ - \theta_-)}aJ_+] \right.$$
$$\left. + |x|^{1/2}\sinh\beta[e^{i(\varphi_- - \theta_-)}a^\dagger J_+ + e^{-i(\varphi_- - \theta_-)}aJ_-] + (|x|\cosh(2\beta) - 1)\frac{I}{2}\right\} \quad (4.41)$$

and a similar expression when $x>0$, making the literal change $\sinh\beta \leftrightarrow \cosh\beta$. If we take $x = -w_0/w$, $\varphi_+ = \theta_-$ and the limit $\beta \mapsto 0$, then $\mathcal{H}_0 \equiv$ (4.41) becomes

$$\mathcal{H}_0 = w\left(a^\dagger a + \frac{1}{2}\right) + w_0 J_3 + \sqrt{ww_0}(a^\dagger J_- + aJ_+) + \frac{w - w_0}{2}I, \quad (4.42)$$

which is the Jaynes–Cummings Hamiltonian[16] up to a constant term and for a coupling constant given by $\kappa = \sqrt{ww_0}$. Let us recall that this Hamiltonian describes the interaction of a cavity mode (with frequency w) with a two level-system (w_0 being the atomic frequency). When $x=-1$, i.e., for $w=w_0$, (4.42) becomes the strong-coupling limit of the Jaynes–Cummings Hamiltonian.

In the case $\beta=0$, the new operator $\mathcal{A}_0 \equiv$ (4.16) reduces now to

$$\mathcal{A}_0(x) = \begin{cases} e^{i\theta_-}a + |x|^{1/2}e^{i\varphi_+}J_-, & \text{if } x<0, \\ e^{i\theta_-}a + |x|^{1/2}e^{i\varphi_-}J_+, & \text{if } x>0. \end{cases} \quad (4.43)$$

As we have here $b=0$, according to the expressions (3.18) and (3.19), the orthonormalized eigenstates of $\mathcal{A}_0$ are given by

$$|Z(x)\rangle_m^j = (\tilde{C}_m^j(x))^{1/2}D(ze^{-i\theta_-}) \times \sum_{k=0}^{j-m}(-1)^k\binom{j-m}{k}\frac{(2j-k)!}{(2j)!}(e^{-i\theta_-}a^\dagger)^{j-m-k}\left(J_\mp\frac{e^{-i\varphi_\mp}}{\sqrt{|x|}}\right)^k\left|0;j,\frac{x}{|x|}j\right\rangle, \quad (4.44)$$

where the $-$ sign refers to $x>0$ and the sign $+$ to $x<0$ and

$$\tilde{C}_m^j(x) = (j-m)!\sum_{k=0}^{j-m}\binom{j-m}{k}\frac{(2j-k)!}{(2j)!}\left(\frac{1}{|x|}\right)^k. \quad (4.45)$$

Since, in this case, we have

$${}_m^j\langle Z(x)|J_3|Z(x)\rangle_m^j = \frac{x}{|x|}\left[j + |x|\frac{\partial}{\partial|x|}\ln(\tilde{C}_m^j(x))\right], \quad (4.46)$$

the dispersion of $\mathcal{H}_0 = w\mathcal{A}_0^\dagger\mathcal{A}_0$ in the states (4.44) is given by

$$((\Delta\mathcal{H}_0)^2)_m^j = w^2|z|^2\left[1 + 2|x|j + 2|x|^2\frac{\partial}{\partial|x|}\ln(\tilde{C}_m^j(x))\right]. \quad (4.47)$$

When $m=j$, we have $\tilde{C}_m^j(x)=1$, so that we get

$$((\Delta\mathcal{H}_0)^2)_j^j = w^2|z|^2(1 + 2|x|j). \quad (4.48)$$

For example, when $j=\frac{1}{2}$, the dispersion corresponding to $m=\frac{1}{2}$ is given by

$$((\Delta\mathcal{H}_0)^2)_+ = w^2|z|^2(1 + |x|) \quad (4.49)$$

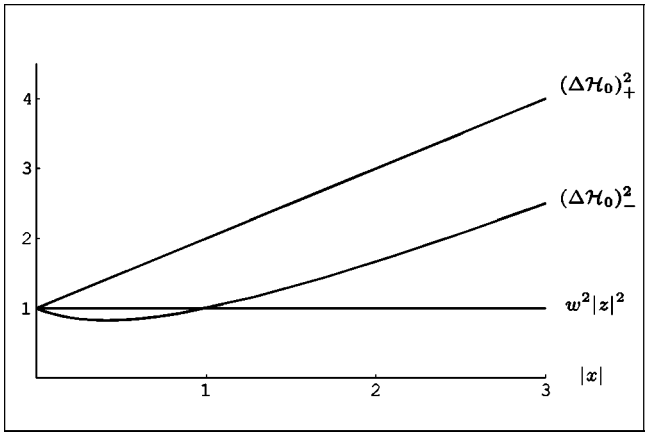

FIG. 8. Graphs of the dispersions $((\Delta\mathcal{H}_0)^2)_\pm$ as given by (4.49) and (4.50) as functions of $|x|$.

and one obtains the same result as in the preceding case when we take the limit $\beta\mapsto 0$. On the other hand, for $m=-1/2$, we get

$$((\Delta\mathcal{H}_0)^2)_-=w^2|z|^2\left[1+|x|\frac{(|x|-1)}{(|x|+1)}\right] \tag{4.50}$$

and it is always smaller than $((\Delta\mathcal{H}_0)^2)_+$. In this last case, we see that if $|x|>1$, the dispersion is bigger than $w^2|z|^2$, while if $|x|<1$ it is smaller than $w^2|z|^2$, and if $|x|=1$, it is equal to $w^2|z|^2$. Furthermore, the dispersion reaches its minimum $0.83w^2|z|^2$ when $|x|=(\sqrt{2}-1)$. Figure 8 shows the behavior of dispersions $((\Delta\mathcal{H}_0)^2)_\pm$ as function of $|x|$.

Let us finally mention that the Hamiltonian $\mathcal{H}_0$ in this case and for $j=\frac{1}{2}$ corresponds to (4.41) when $\beta=0$. A special case is again the Jaynes–Cummings Hamiltonian (4.42) so we get eigenstates of $\mathcal{A}_0\equiv$ (4.43) such that the dispersion of this Hamiltonian is minimized and lower than $w^2|z|^2$.

C. Generalized $h(1)\oplus su(2)$ noncanonical commutation relation

In the case where we have

$$[\mathcal{A},\mathcal{A}^\dagger]=I+\gamma J_+ +\overline{\gamma}J_-, \quad \gamma\in\mathbb{C}, \quad \gamma\neq 0. \tag{4.51}$$

According to (4.3), the necessary conditions on the original parameters are

$$|\alpha_-|^2-|\alpha|_+{}^2=1, \quad |\beta_-|=\beta_+, \quad \beta_3\overline{\beta}_+-\overline{\beta}_3\beta_-=\gamma=\rho e^{i\nu}, \tag{4.52}$$

where $\rho\in\mathbb{R}_+$. A suitable choice of the parameters is

$$\alpha_-=\cosh\alpha e^{i\theta_-}, \quad \alpha_+=\sinh\alpha e^{i\theta+}, \quad \beta_\pm=\beta e^{i\varphi_\pm}, \quad \beta_3=re^{i\varphi_3}, \quad \beta\neq 0, \ r\neq 0, \tag{4.53}$$

such that

$$r\beta[e^{i(\varphi_3-\varphi_+)}-e^{-i(\varphi_3-\varphi_+)}]=\rho e^{i\nu}. \tag{4.54}$$

Equation (4.54) implies that

$$\rho=2r\beta\left|\sin\left(\varphi_3-\frac{(\varphi_++\varphi_-)}{2}\right)\right| \tag{4.55}$$

and the following conditions on the phases: $\varphi_3 \neq (\varphi_+ + \varphi_-)/2$, $\varphi_3 \neq (\varphi_+ + \varphi_-)/2 + \pi$ and $\varphi_+ - \varphi_- = \pi - 2\nu, \nu \in [0, 3\pi/2]$ or $\varphi_+ - \varphi_- = 3\pi - 2\nu$, $\nu \in [\pi/2, 2\pi]$. Thus, the operator $\mathcal{A}$ compatible with all the previous conditions is

$$\mathcal{A} = \cosh \alpha e^{i\theta_-} a + \sinh \alpha e^{i\theta_+} a^\dagger + \alpha_3 I + e^{i(\varphi_- - \nu)} \left[\beta (e^{i\nu} J_+ - e^{-i\nu} J_-) + \frac{\rho}{2\beta |\cos\theta|} e^{i\theta} J_3 \right], \tag{4.56}$$

where

$$\theta = \varphi_3 - (\varphi_- - \nu), \quad -\frac{\pi}{2} < \theta < 3\frac{\pi}{2}. \tag{4.57}$$

The new operator $\mathcal{A}_0$ defined in (4.16) is then given by

$$\mathcal{A}_0 = e^{i\theta_-} a + e^{i(\varphi_- - \nu)} \left[-\beta (e^{i\nu} J_+ - e^{-i\nu} J_-) + \frac{\rho}{2\beta |\cos\theta|} e^{i\theta} J_3 \right]. \tag{4.58}$$

The parameter $b \equiv$ (3.16) is now $b = i\sqrt{16\beta^2 \cos^2(\theta) - \rho^2 e^{2i\theta}} e^{i(\varphi_- - \nu)}/(2\beta|\cos\theta|)$, i.e., $b = 0$ if and only if $\beta = \sqrt{\rho}/2$ and $\theta = \pi$.

Here we can proceed as before, that is, when $b = 0$, find, by means of the equation (3.20) the eigenstates of $\mathcal{A}_0$ and, when $b \neq 0$, find the solutions by means of the equation (3.17) and then calculate the dispersions of $\mathcal{H}_0$.

But, we will follow another treatment which teaches us about the similarities between the canonical and the noncanonical cases. Indeed, seen in another perspective, the commutation relation (4.51) can be expressed in the form

$$[\mathcal{A}_0, \mathcal{A}_0^\dagger] = I + 2\rho \mathbb{J}_3, \tag{4.59}$$

where we have set

$$\mathbb{J}_3 = \frac{(e^{i\nu} J_+ + e^{-i\nu} J_-)}{2}. \tag{4.60}$$

Thus, when $b = 0$, $\mathcal{A}_0$ becomes

$$\mathcal{A}_0 = e^{i\theta_-} a + \sqrt{\rho} e^{i(\varphi_- - \nu)} \mathbb{J}_+, \tag{4.61}$$

with

$$\mathbb{J}_\pm = \pm \frac{(e^{i\nu} J_+ - e^{-i\nu} J_-)}{2} - J_3. \tag{4.62}$$

The operators $\mathbb{J}_3$, $\mathbb{J}_\pm$ satisfy the su(2) algebra and let us denote by $|J, M\rangle$ the eigenstates of both $\mathbb{J}^2$ and $\mathbb{J}_3$. We have again

$$\mathbb{J}_3 |J, M\rangle = M |J, M\rangle, \quad \mathbb{J}_\pm |J, M\rangle = \sqrt{(J \mp M)(J \pm M + 1)} |J, M\rangle. \tag{4.63}$$

Now, it is clear that the resolution of the problem to find the eigenstates of $\mathcal{A}_0$ is similar to the canonical case. Indeed, the normalized eigenstates of $\mathcal{A}_0$ are given by

$$|Z(\rho)\rangle_M^J=(\tilde{C}_M^J(\rho))^{1/2}D(ze^{-i\theta_-})\times\sum_{k=0}^{J-M}(-1)^k\binom{J-M}{k}\frac{(2J-k)!}{(2J)!}(e^{-i\theta_-}a^\dagger)^{J-M-k}\left(\frac{\mathbb{J}_-e^{-i(\varphi_--\nu)}}{\sqrt{\rho}}\right)^k|0;J,J\rangle, \tag{4.64}$$

where $\tilde{C}_M^J(\rho)$ is given as in (4.45).

As before, the dispersion of $\mathcal{H}_0$ in the states (4.64) is given by

$$((\Delta\mathcal{H}_0)^2)_M^J=w^2|z|^2\left[1+2J\rho+2\rho^2\frac{\partial}{\partial\rho}\ln(\tilde{C}_M^J(\rho))\right]. \tag{4.65}$$

For example, when $J=\frac{1}{2}$, we have

$$((\Delta\mathcal{H}_0)^2)_+=w^2|z|^2(1+\rho),\quad((\Delta\mathcal{H}_0)^2)_-=w^2|z|^2\left[1+\rho\frac{(\rho-1)}{(\rho+1)}\right]. \tag{4.66}$$

Evidently, the behavior of these dispersions as functions of ρ is identical to that described in the last paragraph of the previous section.

In the general case where $b\neq0$, $\mathcal{A}_0$ can be expressed in the form

$$\mathcal{A}_0=e^{i\theta_-}a+e^{i(\varphi_--\nu)}\left\{\left[\frac{4\beta^2|\cos\theta|-\rho e^{i\theta}}{4\beta|\cos\theta|}\right]\mathbb{J}_+-\left[\frac{4\beta^2|\cos\theta|+\rho e^{i\theta}}{4\beta|\cos\theta|}\right]\mathbb{J}_-\right\}. \tag{4.67}$$

From (3.17), we see that the eigenstates of $\mathcal{A}_0$ are

$$|Z\rangle_M^J=(C_m^j)^{-1/2}D(ze^{-i\theta_-})T_{\text{eff}}|0;J,M\rangle, \tag{4.68}$$

where

$$T_{\text{eff}}=e^{\Phi_-\mathbb{J}_+}e^{\Phi_+\mathbb{J}_-}, \tag{4.69}$$

with

$$\Phi_-=i\frac{[4\beta^2|\cos\theta|-\rho e^{i\theta}]}{R^{1/2}e^{i\tilde{\varphi}/2}},\quad\Phi_+=i\frac{[4\beta^2|\cos\theta|+\rho e^{i\theta}]}{2R^{1/2}e^{i\tilde{\varphi}}/2}. \tag{4.70}$$

The dispersion of $\mathcal{H}_0$ in these states is

$$((\Delta\mathcal{H}_0)^2)_M^J=w^2|z|^2[1+2\rho_M^J\langle Z|\mathbb{J}_3|Z\rangle_M^J], \tag{4.71}$$

where[17]

$${}_M^J\langle Z|\mathbb{J}_3|Z\rangle_M^J=M\left(\frac{1-|\Phi_-|^2}{1+|\Phi_-|^2}\right)+\frac{(J-M+1)}{2}\frac{P_{J+M-1}^{1,-2M+1}(\Lambda)}{P_{J+M}^{0,-2M}(\Lambda)}\tilde{\Lambda}, \tag{4.72}$$

with

$$\Lambda=1+2|\Phi_-+\bar{\Phi}_+(1+|\Phi_-|^2)|^2 \tag{4.73}$$

and

$$\tilde{\Lambda}=2[|\Phi_-|^2(1+\Phi_-\Phi_++\bar{\Phi}_-\bar{\Phi}_+)+|\Phi_+|^2(|\Phi_-|^4-1)]. \tag{4.74}$$

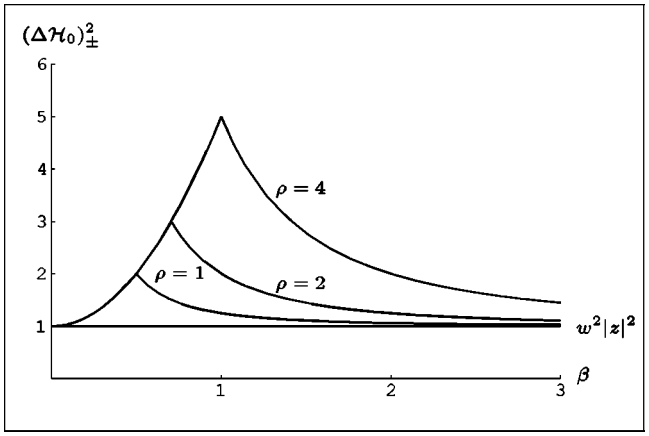

FIG. 9. Graphs of the dispersions $((\Delta\mathcal{H}_0)^2)_\pm \equiv$ (4.76) as functions of $\beta>0$, $\theta=\pi$ and $\rho=1,2,4$.

Thus, in the spin-$\frac{1}{2}$ representation, we get

$$ {}_\pm\langle Z|\mathbb{J}_3|Z\rangle_\pm = \frac{1}{2}\left(\frac{|\Phi_-|^2-1}{1+|\Phi_-|^2}\right). \tag{4.75}$$

Finally, by direct computation, we find

$$((\Delta\mathcal{H}_0)^2)_\pm = w^2|z|^2\left[1+\rho\frac{[16\beta^4\cos^2(\theta)+\rho^2-8\rho\beta^2\cos\theta|\cos\theta|]-R}{[16\beta^4\cos^2(\theta)+\rho^2-8\rho\beta^2\cos\theta|\cos\theta|]+R}\right], \tag{4.76}$$

where

$$R=\sqrt{[16\beta^4\cos^2(\theta)-\rho^2\cos(2\theta)]^2+\rho^4\sin^2(2\theta)}. \tag{4.77}$$

We see that, for fixed value of ρ, Eq. (4.76) as a function of β is symmetric around $\theta=\pi$.

Figure 9 shows the behavior of the dispersions (4.76) as functions of $\beta>0$ when $\theta=\pi$ and for different values of parameter ρ. Let us notice the similarity between these curves starting from a certain value of β and the curves for the canonical case showed in Fig. 7.

Figure 10 shows the behavior of the same functions as functions of $\beta>0$, for different values

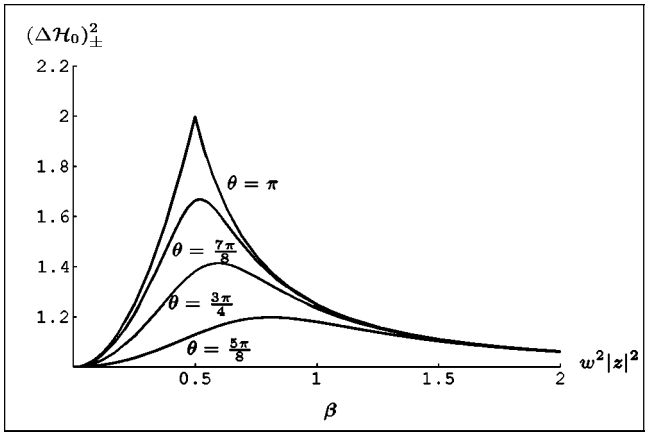

FIG. 10. Graphs of the dispersions $((\Delta\mathcal{H}_0)^2)_\pm \equiv$ (4.76) as functions of $\beta>0$ for $\rho=1$. $\theta=5\pi/8$, $3\pi/4$, $7\pi/8$ and π.

of θ when $\rho=1$. We observe that when the angle θ is different from π the curves have a continuous derivative with respect to β but, when the angle $\theta=\pi$, the derivative of the curve at the point $\beta=0.5=\sqrt{\rho}/2$ is not continuous.

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APPENDIX A: ALGEBRA EIGENSTATES ASSOCIATED TO su(2)

In this appendix we want to solve the eigenvalue equation

$$[\vec{\beta}\cdot\vec{J}]|\psi\rangle=[\beta_1 J_1+\beta_2 J_2+\beta_3 J_3]|\psi\rangle=\Gamma|\psi\rangle,\quad \beta_1,\beta_2,\beta_3\in\mathbb{C}, \tag{A1}$$

where J_1, J_2 and J_3 are the su(2) generators which have already been given in Sec. II C. The eigenvalue equation (A1) can also be written as

$$[\beta_- J_+ +\beta_+ J_- +\beta_3 J_3]|\psi\rangle=\Gamma|\psi\rangle, \tag{A2}$$

where J_1 and J_2 have been expressed in terms of the usual operators $J_\pm$ and

$$\beta_\pm=\frac{\beta_1\pm i\beta_2}{2}. \tag{A3}$$

We see that Eq. (2.45) is just a particular case of Eq. (A2). The eigenvalue equation (A2) has already been solved by Brif[8] by expanding the state $|\psi\rangle$ in the standard coherent-state basis[9], introducing in this way analytic functions and asking for solving a first order differential equation. Here, we consider a different method based on the operator algebra technique.

For j fixed, we can show that (A2) admits the eigenvalues

$$\Gamma^j_m=mb, \tag{A4}$$

with $m=-j,\ldots,j$ and $b=\sqrt{\beta_1^2+\beta 0_2^2+\beta_3^2}=\sqrt{4\beta_+\beta_-+\beta_3^2}$. We then solve

$$[\beta_- J_+ +\beta_+ J_- +\beta_3 J_3]|\psi\rangle^j_m=\Gamma^j_m|\psi\rangle^j_m, \tag{A5}$$

by using

$$|\psi\rangle^j_m=(N^j_m)^{-1/2}T|j,m\rangle, \tag{A6}$$

where the N^j_m are normalization constants and T is an operator that has to be determined. We take it as

$$T=\exp\left(-\frac{\tilde{\theta}}{2}[e^{-i\tilde{\phi}}J_+ -e^{i\tilde{\phi}}J_-]\right),\quad \tilde{\phi},\tilde{\theta}\in\mathbb{C}. \tag{A7}$$

Inserting (A6) with (A7) into (A5) leads to

$$[\vec{\beta}\cdot\vec{J}]T|j,m\rangle=mbT|j,m\rangle. \tag{A8}$$

Using the usual decomposition

$$T=\exp\left(-e^{-i\tilde{\phi}}\tan\left(\frac{\tilde{\theta}}{2}\right)J_+\right)\quad \exp\left(\ln\sec^2\left(\frac{\tilde{\theta}}{2}\right)J_3\right)\quad \exp\left(e^{i\tilde{\phi}}\tan\left(\frac{\tilde{\theta}}{2}\right)J_-\right) \tag{A9}$$

and the relations

$$e^{\eta J_3} J_\pm e^{-\eta J_3} = e^{\pm \eta} J_\pm, \quad e^{\eta J_\pm} J_3 e^{-\eta J_\pm} = J_3 \mp \eta J_\pm, \quad e^{\eta J_\pm} J_\mp e^{-\eta J_\pm} = J_\mp \pm 2\eta J_3 - \eta^2 J_\pm, \tag{A10}$$

we can show that, for $\beta_+ \neq 0$, $\beta_- \neq 0$ and $b \neq 0$, we have

$$e^{i\tilde{\phi}} = \sqrt{\frac{\beta_+}{\beta_-}}, \tag{A11}$$

and

$$\frac{\tilde{\theta}}{2} = \arctan\left(\sqrt{\frac{b-\beta_3}{b+\beta_3}} \right). \tag{A12}$$

Inserting the results (A11) and (A12) in (A9), we obtain

$$T = \exp\left(-\frac{2\beta_-}{b+\beta_3} J_+ \right) \exp\left(\ln\left(\frac{2b}{b+\beta_3} \right) J_3 \right) \exp\left(\frac{2\beta_+}{b+\beta_3} J_- \right). \tag{A13}$$

The original form (A7) of the T operator allows us to look easily for the special cases studied in Refs. 6, and 9 and in the preceding sections while the form (A13) allows us to calculate directly the explicit form of the eigenstates (A6). Indeed, the first relation (A10) allows us to pass the exponential term $\exp(\ln(2b/(b+\beta_3))J_3)$ to the right in (A13) and this without changing essentially the operator action on the pure states $|j,m\rangle$ because $|j,m\rangle$ is an eigenstate of the operator J_3. Thus, in Eq. (A6), we can replace the operator T by the operator

$$T_{\text{eff}} = \left(\frac{b}{\beta_+} \right)^{j+m} \sqrt{\frac{(j+m)!(j-m)!}{(2j)!}} \exp\left(-\frac{2\beta_-}{b+\beta_3} J_+ \right) \exp\left(\frac{\beta_+}{b} J_- \right), \tag{A14}$$

such that

$$|\psi\rangle_m^j = (\tilde{N}_m^j)^{-1/2} T_{\text{eff}} |j,m\rangle, \tag{A15}$$

where $\tilde{N}_m^j$ are new normalization constants. Redefining the summation indices, we get

$$|\psi\rangle_m^j = (\tilde{N}_m^j)^{-1/2} \sum_{u=-j}^{j} \sqrt{\frac{(j+u)!(j-u)!}{(2j)!}} \left(\frac{b}{\beta_+} \right)^{j+u} \frac{(j+m)!}{(j-u)!} \times \sum_{n=0}^{j+u} (-1)^n \frac{(j-u+n)!}{n!(m-u+n)!(j+u-n)!} \left(\frac{(1-\beta_3/b)}{2} \right)^n |j,u\rangle. \tag{A16}$$

We also have an expression in terms of the Jacobi polynomials (see Ref. 18):

$$|\psi\rangle_m^j = (\tilde{N}_m^j)^{-1/2} \sum_{u=-j}^{j} \sqrt{\frac{(j+u)!(j-u)!}{(2j)!}} \left(\frac{b}{\beta_+} \right)^{j+u} P_{j+u}^{-u+m,-u-m} \left(\frac{\beta_3}{b} \right) |j,u\rangle, \tag{A17}$$

which is the result obtained by Brif.[8]

For the special case where $\beta_+ = 0$, $\beta_3 \neq 0$ so that, in connection with (A4), we have $b = \beta_3$, we find the operator

$$T_{\text{eff}} = \exp\left(-\frac{\beta_-}{\beta_3} J_+ \right). \tag{A18}$$

The eigenstates are

$$|\psi\rangle_m^j=(C_m^j)^{-1/2}\sum_{u=m}^{j}\sqrt{\frac{(j+u)!}{(j-u)!}}\frac{1}{(u-m)!}\left(-\frac{\beta_-}{\beta_3}\right)^{u-m}|j,u\rangle, \tag{A19}$$

and become the standard CS of SU(2) (Ref. 9) when $m=-j$.

For the special case where $\beta_-=0$, $\beta_3\neq 0$, we have similar results. Indeed, the new operator T_{eff} is

$$T_{\text{eff}}=\exp\left(\frac{\beta_+}{\beta_3}J_-\right) \tag{A20}$$

and the eigenstates write

$$|\psi\rangle_m^j=(C_m^j)^{-1/2}\sum_{u=-j}^{m}\sqrt{\frac{(j-u)!}{(j+u)!}}\frac{1}{(m-u)!}\left(\frac{\beta_+}{\beta_3}\right)^{u-m}|j,u\rangle, \tag{A21}$$

which become the standard CS of SU(2) (Ref. 9) when $m=j$.

Now, for the case $\beta_+=0$ and $\beta_3=0$ ($\beta_-=0$ and $\beta_3=0$), the only normalizable solution is $|j,-j\rangle$ ($|j,j\rangle$). For $\beta_+=\beta_-=0$ and $\beta_3\neq 0$, the AES are evidently the pure states $|j,m\rangle$.

Finally, the degenerate case $b=0$ leads to the solution $|\psi\rangle_{-j}^j=(C_{-j}^j)^{-1/2}T_{\text{eff}}|j,-j\rangle$ with $T_{\text{eff}}=\exp(-2(\beta_-/\beta_3)J_+)$, that is the standard CS of SU(2).

The mean value of J_3 in the states (A17) has already been calculated by Brif.[8] We have

$$\langle J_3\rangle_m^j=\frac{jY+m(S_+-S_-)}{S_+S_-}-\frac{(j+|m|)Yt}{S_+^2S_-^2}\Omega, \tag{A22}$$

where

$$S_\pm=1+\left|\frac{2\beta_-}{\beta_3\mp b}\right|^2,\quad t=\left|\frac{b}{\beta_+}\right|^2,\quad Y=S_+S_--S_+-S_- \tag{A23}$$

and

$$\Omega=\frac{P_{j-|m|-1}^{(-2j,1)}(1-(2t/S_+S_-))}{P_{j-|m|}^{(-2j-1,0)}(1-(2t/S_+S_-))},\quad \text{if } |m|<j;\quad \Omega=0,\quad \text{if } |m|=j. \tag{A24}$$

APPENDIX B: RESOLUTION OF A FIRST ORDER SYSTEM OF DIFFERENTIAL EQUATIONS

Let us recall that a realization[9] of the Fock space $\mathcal{F}_b=\{|n\rangle,n=0,1,2,\dots\}$ of energy eigenstates of the harmonic oscillator as a space $\mathcal{H}$ of analytic functions $f(\zeta)$ is obtained by expanding this function in the basis of analytic functions $\{\varphi_n(\zeta)=\zeta^n/\sqrt{n!},n=0,1,2,\dots\}$, that is,

$$f(\zeta)=\sum_{n=0}^{\infty}c_n\varphi_n(\zeta)=\sum_{n=0}^{\infty}c_n\frac{\zeta^n}{\sqrt{n!}},\quad \zeta\in\mathbb{C}. \tag{B1}$$

The scalar product is

$$(f_1,f_2)=\int_C\overline{f_1}(\zeta)f_2(\zeta)e^{-|\zeta|^2}\frac{d\zeta\,d\overline{\zeta}}{2\pi i},\quad \forall f_1,f_2\in\mathcal{H}, \tag{B2}$$

the integral being extended to the complex plane. The action of the creation $a^\dagger$ and annihilation a operators on the $\mathcal{H}$ space is then given by

$$a^\dagger \equiv \zeta, \quad a \equiv \frac{d}{d\zeta}. \tag{B3}$$

The eigenvalue equation (2.26) thus becomes a first order differential equation

$$\frac{1}{\sqrt{2}}\left((1+\lambda)\frac{d}{d\zeta}+(1-\lambda)\zeta\right)f(\zeta)=\beta f(\zeta), \tag{B4}$$

for which normalized solutions are obtained for $\lambda \neq -1$. The general solution of (B4) is

$$f(\zeta)=f(0)\exp\left(\frac{2\sqrt{2}\beta\zeta-(1-\lambda)\zeta^2}{2(1+\lambda)}\right). \tag{B5}$$

With respect to the scalar product (B2), the normalization constant $f(0)$ is computed by imposing

$$\int_C |f(\zeta)|^2 e^{-|\zeta|^2}\frac{d\zeta\, d\overline{\zeta}}{2\pi i}=1, \tag{B6}$$

and we find the normalized solution of (B4) as

$$f(\zeta)=(1-|\eta_1|^2)^{1/4}\exp\left(-\frac{1}{2}\left[\frac{|\eta_2|^2-\mathrm{Re}(\overline{\eta}_1\eta_2^2)}{1-|\eta_1|^2}\right]\right)\exp\left(\eta_2\zeta-\frac{\eta_1}{2}\zeta^2\right), \tag{B7}$$

with

$$\eta_1=\frac{(1-\lambda)}{(1+\lambda)}=\delta e^{i\phi} \quad \text{and} \quad \eta_2=\frac{\sqrt{2}\beta}{(1+\lambda)}=\frac{\beta}{\sqrt{2}}(1+\delta e^{i\phi}). \tag{B8}$$

This corresponds to the states (2.33) after normalization.

Now we are concerned with the algebra eigenstates satisfying the equation (3.10) in the Fock space $\mathcal{F}\equiv$ (3.4). A realization of $\mathcal{F}$ can be easily given from the preceding considerations and the expression (3.12) of a state $|\psi\rangle$ for a fixed j. Indeed, we have

$$\psi^j_m(\zeta)=\langle \zeta; j,m|\psi\rangle \tag{B9}$$

and the eigenvalue equation (3.10) then becomes a system of first order differential equations

$$\begin{aligned}\left(\alpha_- \frac{d}{d\zeta}+\alpha_+\zeta+\alpha_3\right)\psi^j_m(\zeta)+[\beta_-\sqrt{(j-m+1)(j+m)}\,\psi^j_{m-1}(\zeta)\\ +\beta_+\sqrt{(j+m+1)(j-m)}\,\psi^j_{m+1}(\zeta)+\beta_3 m\,\psi^j_m(\zeta)]=\beta\psi^j_m(\zeta),\end{aligned} \tag{B10}$$

where j is fixed but m takes the values $-j,\ldots,j$. Let us now solve this system by first introducing the differential operator

$$L=\alpha_-\frac{d}{d\zeta}+\alpha_+\zeta+\alpha_3-\beta \tag{B11}$$

and, second, defining the vector

$$\Psi=\begin{pmatrix}\psi^j_{-j}\\ \psi^j_{-j+1}\\ \vdots\\ \psi^j_{j-1}\\ \psi^j_j\end{pmatrix}. \tag{B12}$$

The system (B10) thus becomes a matrix differential system

$$L\Psi=-A\Psi, \tag{B13}$$

with A a $(2j+1)\times(2j+1)$ matrix given by

$$A=\begin{pmatrix}
-j\beta_3 & \sqrt{2j}\beta_+ & 0 & 0 & \cdots & 0\\
\sqrt{2j}\beta_- & (-j+1)\beta_3 & \sqrt{(2j-1)2}\beta_+ & 0 & \cdots & 0\\
0 & \sqrt{(2j-1)2}\beta_- & (-j+2)\beta_3 & \sqrt{(2j-2)3}\beta_+ & \cdots & 0\\
\vdots & \vdots & \vdots & \ddots & \cdots & \vdots\\
0 & 0 & \sqrt{(2j-2)3}\beta_- & (j-2)\beta_3 & \sqrt{(2j-1)2}\beta_+ & 0\\
0 & 0 & 0 & \sqrt{(2j-1)2}\beta_- & (j-1)\beta_3 & \sqrt{2j}\beta_+\\
0 & 0 & 0 & 0 & \sqrt{2j}\beta_- & j\beta_3
\end{pmatrix}. \tag{B14}$$

If we can find a nonsingular matrix S that diagonalizes A on the form $D=S^{-1}AS$ where

$$D=\mathrm{diag}(\lambda^j_{-j},\lambda^j_{-j+1},\cdots,\lambda^j_j), \tag{B15}$$

the system (B13) will reduce to

$$L\tilde{\Psi}=-D\tilde{\Psi},\quad \tilde{\Psi}=S^{-1}\Psi. \tag{B16}$$

Thus, for $\alpha_-\neq 0$, the direct integration of (B16) will lead to

$$\tilde{\psi}^j_m=\tilde{\psi}^j_m(0)\exp\left(\frac{\beta-\alpha_3-\lambda^j_m}{\alpha_-}\zeta-\frac{\alpha_+}{2\alpha_-}\zeta^2\right) \tag{B17}$$

and the general solution Ψ will be obtained as

$$\begin{pmatrix}\psi^j_{-j}\\ \psi^j_{-j+1}\\ \vdots\\ \psi^j_{j-1}\\ \psi^j_j\end{pmatrix}=S\begin{pmatrix}\tilde{\psi}^j_{-j}\\ \tilde{\psi}^j_{-j+1}\\ \vdots\\ \tilde{\psi}^j_{j-1}\\ \tilde{\psi}^j_j\end{pmatrix}=\sum_{m=-j}^{j}\tilde{\psi}^j_m(0)\exp\left(\frac{\beta-\alpha_3-\lambda^j_m}{\alpha_-}\zeta-\frac{\alpha_+}{2\alpha_-}\zeta^2\right)\begin{pmatrix}S_{-j,m}\\ S_{-j+1,m}\\ \vdots\\ S_{j-1,m}\\ S_{j,m}\end{pmatrix}, \tag{B18}$$

where S is assumed to be of the form

$$S=\begin{pmatrix} S_{-j,-j} & S_{-j,-j+1} & \cdots & S_{-j,j-1} & S_{-j,j} \\ S_{-j+1,-j} & S_{-j+1,-j+1} & \cdots & S_{-j+1,j-1} & S_{-j+1,j} \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ S_{j-1,-j} & S_{j-1,-j+1} & \cdots & S_{j-1,j-1} & S_{j-1,j} \\ S_{j,-j} & S_{j,-j+1} & \cdots & S_{j,j-1} & S_{j,j} \end{pmatrix}. \tag{B19}$$

Computing the eigenvalues of A, we find that we have to distinguish two cases, i.e., the one with $b=\sqrt{4\beta_+\beta_-+\beta_3^2}\neq 0$ and the one with $b=0$. For the first case $b\neq 0$, all eigenvalues are different and given by

$$\lambda_m^j=mb, \quad m=-j,\cdots,j. \tag{B20}$$

The system is diagonalizable and the general solution is given by (B18) with

$$S_{u,m}=\sqrt{\frac{(j+u)!(j-u)!}{(2j)!}}\left(\frac{b}{\beta_+}\right)^{j+u}P_{j+u}^{-u+m,-u-m}\left(\frac{\beta_3}{b}\right), \quad u=-j,\cdots,j, \tag{B21}$$

when $\beta_-\neq 0$, $\beta_+\neq 0$ and $\beta_3\neq 0$,

$$S_{u,m}=\sqrt{\frac{(j-u)!}{(j+u)!}}\frac{1}{(m-u)!}\left(\frac{\beta_+}{\beta_3}\right)^{u-m}, \quad -j\leqslant u\leqslant m, \quad S_{u,m}=0, \quad m<u\leqslant j, \tag{B22}$$

when $\beta_-=0$, $\beta_+\neq 0$ and $\beta_3\neq 0$ and

$$S_{u,m}=\sqrt{\frac{(j+u)!}{(j-u)!}}\frac{1}{(u-m)!}\left(-\frac{\beta_-}{\beta_3}\right)^{u-m}, \quad m\leqslant u\leqslant j, \quad S_{u,m}=0, \quad -j\leqslant u<m, \tag{B23}$$

when $\beta_-\neq 0$, $\beta_+=0$ and $\beta_3\neq 0$.

In the Fock space representation, the solutions (B18) with (B21), (B22) and (B23) correspond, apart from a superfluous change of notation, exactly to the states (3.17) with T_{eff} given by (A14), (A18), and (A20), respectively.

For the second case $b=0$, the matrix A can not be diagonalized. We could use the Jordan form or start from the differential equation system again and include this condition. Taking the second way, we can express the $\psi_m^j(\zeta)$ components in the form

$$\psi_m^j(\zeta)=\exp\left[-\frac{\alpha_+}{2\alpha_-}\zeta^2+\frac{(\beta-\alpha_3-m\beta_3)}{\alpha_-}\zeta\right]\tilde{\psi}_m^j(\zeta), \tag{B24}$$

and insert these in Eq. (B10). We get to the following system:

$$\alpha_-\frac{d}{d\zeta}\tilde{\psi}_m^j(\zeta)+\beta_-\sqrt{(j-m+1)(j+m)}e^{\beta_3\zeta/\alpha_-}\tilde{\psi}_{m-1}^j(\zeta) + \beta_+\sqrt{(j+m+1)(j-m)}e^{-\beta_3\zeta/\alpha_-}\tilde{\psi}_{m+1}^j(\zeta)=0, \tag{B25}$$

when $m=-j,\ldots,j$. By handling these equations suitably we can, for example, obtain an ordinary differential equation of the $2j+1$ order for $\tilde{\psi}_{-j}^j(\zeta)$, namely

$$\left[\prod_{-j}^{j}\left(\frac{d}{d\zeta}-\mu_m^j\right)\right]\tilde{\psi}_{-j}^j(\zeta)=0, \tag{B26}$$

where

$$\mu_m^j = -j\frac{\beta_3}{\alpha_-} + m\frac{b}{\alpha_-}. \tag{B27}$$

When $b=0$, we have $2j+1$ equal roots. This means that the solutions for $\tilde{\psi}^j_{-j}(\zeta)$ take the form:

$$\tilde{\psi}^j_{-j}(\zeta) = \exp\left(\frac{-j\beta_3\zeta}{\alpha_-}\right)\sum_{q=0}^{2j} A_q\zeta^q. \tag{B28}$$

Then, we can insert (B28) in (B25) and thus obtain, in an iterative way, all solutions $\tilde{\psi}^j_m(\zeta)$ and, thereafter, using (B24), all solutions $\psi^j_m(\zeta)$.

For example, in the case $\beta_+=\beta_3=0$ and $\beta_-\neq 0$, we have

$$\tilde{\psi}^j_{-j}(\zeta) = \psi^j_{-j}(0), \tag{B29}$$

i.e., a constant and, consequently, by integrating one by one the equations of the system (B25), we obtain

$$\tilde{\psi}^j_m(\zeta) = \sum_{k=0}^{j+m}\left(-\frac{\beta_-}{\alpha_-}\right)^k\frac{\zeta^k}{k!}\sqrt{\frac{(j+m)!(j-m+k)!}{(j-m)!(j+m-k)!}}\,\psi^j_{m-k}(0), \tag{B30}$$

when $m=-j,\ldots,j$. The general solution (B12) is then given by

$$\Psi = \exp\left[-\frac{\alpha_+}{2\alpha_-}\zeta^2 + \frac{(\beta-\alpha_3)}{\alpha_-}\zeta\right]\sum_{m=-j}^{j}\psi^j_m(0)$$
$$\times\left[\sum_{k=0}^{j-m}\frac{(-1)^k}{k!}\sqrt{\frac{(j-m)!(j+m+k)!}{(j-m-k)!}}\left(\frac{\beta_-}{\alpha_-}\right)^k\zeta^k\begin{pmatrix}0\\ \vdots\\ 0\\ 1\\ 0\\ \vdots\\ 0\end{pmatrix}\right], \tag{B31}$$

where, in each sum, the 1 in the vector column is placed in the $(j+m+k+1)$ row. We thus obtain the $(2j+1)$ independent solutions of the system of differential equations.

In the Fock space representation, we can show that the independent solutions given by Eq. (B31) correspond, apart from a superfluous change of notation, to the states (3.18). In the case $\beta_-=\beta_3=0$ with $\beta_+\neq 0$, following a similar procedure, one finds the expression (3.19).

Finally, when β_+, β_-, $\beta_3\neq 0$, by inserting (B28) in (B25) and ordering the independent solutions with respect to the arbitrary constants A_q, one finds

$$\Psi(\zeta) = \exp\left[-\frac{\alpha_+}{2\alpha_-}\zeta^2 + \frac{(\beta-\alpha_3)}{\alpha_-}\zeta\right]\sum_{q=0}^{2j}A_q$$
$$\times\left[\sum_{k=0}^{q}(-1)^k\binom{q}{k}\frac{(2j-k)!}{(2j)!}\zeta^{q-k}\left(\frac{\alpha_-}{\beta_+}\right)^k\left[\frac{d^k}{d\vartheta^k}\sum_{r=0}^{2j}\sqrt{\frac{(2j)!}{(2j-r)!r!}}\,\vartheta^r\right]\begin{pmatrix}0\\ \vdots\\ 1\\ \vdots\\ 0\end{pmatrix}\right], \tag{B32}$$

where $\vartheta=\beta_3/2\beta_+=-2\beta_-/\beta_3$ and, in each sum, the 1 in the vector column is placed in the $r+1$ row. In the Fock space representation, these solutions, with a slight change of notation, correspond to Eq. (3.20).

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Reversing quantum dynamics with near-optimal quantum and classical fidelity

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We consider the problem of reversing quantum dynamics, with the goal of preserving an initial state's quantum entanglement or classical correlation with a reference system. We exhibit an approximate reversal operation, adapted to the initial density operator and the ''noise'' dynamics to be reversed. We show that its error in preserving either quantum or classical information is no more than twice that of the optimal reversal operation. Applications to quantum algorithms and information transmission are discussed. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Counteracting the effects on quantum systems of noise generated by interaction with an environment is a central problem for the emerging field of quantum information processing. Its solution can be expected to have applications in quantum computation, precision measurement, and information transmission. In this paper we exhibit a reversal operation which takes account of both the noise and the initial density operator, to achieve near-optimal preservation of the initial density operator's quantum entanglement or classical correlation with a reference system. We work throughout with finite-dimensional systems although we expect that the results generalize to infinite-dimensional ones, at least those with separable Hilbert spaces.

Section II reviews some of the theory of completely positive (CP) linear maps on spaces of operators on finite-dimensional Hilbert spaces. When these are trace-nonincreasing, they are also known in the quantum information/computation community as ''quantum operations.'' Readers familiar with these matters may wish to skip Sec. II, or skim it for notation. [The only notation not standard in quantum information theory is our writing $\mathcal{A}\sim\{A_i\}$ to indicate that a CP-map acts as $\mathcal{A}(\rho)=\Sigma_i A_i\rho A_i^\dagger$.] Section III reviews measures of fidelity commonly used in quantum information theory to quantify the effect of noise and information-processing operations on a system's state, or an ensemble of system states. In addition, it motivates the particular measures we use, and indicates their connection to fidelity measures used in classical information-transmission theory. It also explains why, although our measures of quantum fidelity concentrate on preserving the correlation or entanglement of a mixed state, subjected to noise, with a reference system, it is relevant to the preservation of an ensemble of pure states as well. This section includes several formal definitions required in the rest of the paper. Sections IV and VI are the core of the paper, containing the two main results. In Sec. IV the near-optimal reversal operation is defined, and we prove one of our main results: that its error is no worse than twice that of the optimal reversal operation, for either quantum or classical information. Section V discusses the relationship of the reversal operation to a known near-optimal method of recovering classical information encoded in an ensemble of density operators, the ''pretty good measurement.'' When the noise can be viewed as encoding classical information in a completely decohered ensemble of density operators, our reversal operation can be viewed as performing the pretty-good measurement to distinguish these density operators. But when the noise operation may be viewed as encoding classical information

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into these density operators in a way which leaves some coherence between them, our reversal operation writes a nearly optimal estimate of the density operator into a set of orthogonal states *without* decohering these states as a measurement would. Section VI proves the other main result of the paper: a useful lower bound on the fidelity with which the reversal operation recovers classical information. This bound can be more tractable than the reversal operation's fidelity itself, and has proven useful, for example, in discovering upper bounds on quantum query complexity. This and other applications are touched on in the concluding section.

II. QUANTUM NOISE OPERATIONS

We model quantum noise in a system Q by the most general dynamics that can arise via a unitary interaction U^{QE} with an environment E initially independent of the system, in the sense that the initial joint density matrix of system and environment is a product $\rho^Q \otimes \sigma^E$. We also model operations performed on a system in an attempt to counteract noise by such dynamics. For our purposes, where we ultimately care about the effect of operations on the system, and perhaps on its entanglement with systems other than the environment, we may model these with the environment starting in a pure state because the effect *on the system* of interaction with a mixed state σ of E via U^{QE} can be replicated by an interaction $U^{QE_1} \otimes I^{E_2}$ with a pure state $|0\rangle$ of an environment $E = E_1 \otimes E_2$, whose partial trace onto E_1 is equal to σ.

The dynamics thus obtained are trace-preserving completely positive maps $\mathcal{A}: \rho \mapsto \Sigma_i A_i \rho A_i^\dagger$, on the space of linear operators on Q. They are also trace-preserving; equivalently, $\Sigma_i A_i^\dagger A_i = I$. Here

$$A_i := \langle i^E | U^{QE} | 0^E \rangle \tag{1}$$

are the ''operator matrix elements'' of the unitary interaction, between the environment initial state and states $|i^E\rangle$ forming an orthonormal basis for the environment. It should be clear what this means, but to be explicit, we define the operator matrix element $\langle \chi^A | O^{AB} | \psi^{AB} \rangle$ of an operator O^{AB} on the tensor product space $A \otimes B$. Let the matrix elements of O in some tensor product basis $|i^A\rangle |j^B\rangle$ be $O_{ij,i'j'}$, and let χ_i and ψ_i be the components of $|\chi\rangle$ and $|\psi\rangle$ in the basis $|i^A\rangle$. Then the operator matrix element just mentioned is the operator X on B whose matrix elements in the basis $|j^B\rangle$ are given by

$$\langle j | X | j' \rangle = \sum_{i,i'} \chi_i^* \psi_{i'} O_{ij,i'j'}. \tag{2}$$

$A_i |\psi\rangle$ is what is often called the (unnormalized) ''relative state'' of the system Q—relative, that is, to the environment basis state $|i^E\rangle$. The overall evolution of system and environment is $|\psi^Q\rangle |0^E\rangle \to U^{QE} |\psi^Q\rangle |0^E\rangle = \Sigma_i A_i^Q |\psi^Q\rangle |i^E\rangle$. The fact that the overall state remains normalized (so that the density matrix's trace is preserved) results in the requirement $\Sigma_i A_i^\dagger A_i = I$ on a trace-preserving quantum operation.

If the environment were considered as a measuring apparatus, and the states of the basis $|i^E\rangle$ the ''pointer variable'' of that apparatus, so that each value of $|i\rangle$ corresponded to a different measurement result, then $A_i |\psi\rangle$ would be the state of the system conditional on the measurement outcomes i, and their squared norms, the probabilities of the measurement outcomes. The overall operation $\mathcal{A}$ represents the dynamics of the measurement, averaged over measurement results. Of course, a trace-preserving operation need not arise from a measurement in this manner, but it may always be viewed this way, in terms of averaging over a notional readout of the environment in some ''pointer basis,'' if desired.

The A_i are said to form a *decomposition* of $\mathcal{A}$, for which we use the notation $\mathcal{A} \sim \{A_i\}$. Using a different orthonormal ''pointer basis'' [1] for the environment in (1) results in a different decomposition of the same operation. Two such pointer bases are related by a unitary transformation. The corresponding decompositions of the operation are related by the complex conjugate of that unitary (taken in either of the bases):

$$B_i = \sum_j (U_{ij})^* A_j , \tag{3}$$

where U takes the pointer basis used to define the A_j to that used to define the B_i.

III. QUANTIFYING THE EFFECTS OF NOISE

Let us consider how to quantify the effects of a "noise" operation on information which we consider to be contained in a quantum system, using the classical Shannon theory of information transmission as a guide. The information we have about a set of classical alternatives indexed by i of a local system T is usually measured by the entropy of the probabilities we ascribe to the alternatives: $H(\mathbf{p}) := -\Sigma_i p_i \log p_i$. Suppose we want to be able to transmit or store the states i, which will be presented to us with the probabilities p_i. We encode them on a system T, while keeping a reference copy with us, on a system R. T is then affected by noise. We might define perfect success as the preservation of the initial perfect correlation between R and T. In terms of the probability measures, we want the initial and final joint *mixed* states of reference R and system T both to be $p(i^R, j^T) = p_i \delta_{iRjT}$. If our actual, noise-affected transmission results in the state $q(i^R, j^T)$, we could measure how well we have succeeded by looking at the distance between $p(i^R, j^T)$ and $q(i^R, j^T)$ using some standard measure of distance between probability distributions. To give examples of such distances, let $\mathbf{r} = [r_1, \ldots, r_n]$, $\mathbf{s} = [s_1, \ldots, s_n]$ be probabilities on a common set of classical alternatives labeled $1, \ldots, n$. We might, for example, measure the distance between $\mathbf{r}$ and $\mathbf{s}$ by the Bhattacharyya distance $B(\mathbf{r}, \mathbf{s}) := 1 - (\Sigma_k r_k^{1/2} s_k^{1/2})^2$. The L_1-norm distance (also called total variation or Kolmogorov distance) would be another reasonable choice. We will assume $q(i,j) = p_i t(j|i)$, where $t(j|i)$ is a stochastic matrix of transition probabilities describing the noise. Using the Bhattacharyya distance to measure how well the original correlation has been preserved in the above-given example

$$1 - \left(\sum_{i,j} \delta_{ij} p_i^{1/2} q(i,j)^{1/2} \right)^2 = 1 - \left(\sum_i p_i^{1/2} q(i,i)^{1/2} \right)^2 = 1 - \left(\sum_i p_i t(i|i)^{1/2} \right)^2 . \tag{4}$$

Using the L_1-norm distance gives

$$(1/2) \sum_{ij} |\delta_{ij} p_i - \delta_{ij} p_i t(j|i)| = (1/2) \sum_i p_i |1 - t(i|i)| = \sum_i p(R = i \& T \neq i). \tag{5}$$

This is the familiar "error probability" criterion for channel transmission: the average, over messages i, of the probability that i is sent but a different message is received. This is an average pure-state fidelity, but we have shown that it can be rewritten as the fidelity for a *mixed* state representing perfect initial correlation. The measure defined using the Bhattacharyya distance, while not identical to error probability, is equivalent to it as an error criterion for use in Shannon-type block coding theorems. (It goes to zero with the error probability, and with similar speed and dimensional dependence.)

We have gone through this analysis to indicate that there is a classical analog of the approach we here take to quantum as well as classical fidelity: investigating the effects of noise on a channel, which we may want to use to transmit *pure* states, by looking at its effect on a state whose marginal distribution on the noise-affected system is a *mixed* state corresponding to the ensemble of possible pure-state messages. Thus an approach which might if incompletely understood be viewed as perversely concerned with the fidelity of mixed states, provides a good fidelity criterion for the problem of transmitting pure states which are supplied to the channel with probabilities p_i, in terms of the idea of preservation of correlation with a (possibly notional) reference system. And this is not a bit of peculiarly quantum weirdness: the approach can be taken in the classical case, too.

We now present our similar approach to the problem of transmitting *quantum* information, or more generally of evaluating the fidelity with which a given operation preserves quantum infor-

mation. We resume consideration of the trace-preserving completely positive "noise" operation $\mathcal{A}$ which is the analog of the classical stochastic channel matrix $t(i|j)$ presented earlier. But now, rather than preservation of the noise-affected system's correlation with a reference system, we require preservation of its *entanglement*. Just as the classical reference system could be completely notional, introduced because high-fidelity preservation of correlation with a notional reference system implies high-fidelity preservation of states on the noise-affected system when they are supplied to the channel with the marginal distribution p_i, so the quantum reference system may also be taken to be completely notional. When $\mathcal{A}$ acts on Q, an entangled state $|\psi_0^{RQ}\rangle := \Sigma_i \sqrt{p_i}|i^R\rangle|i^Q\rangle$ of Q with a reference system R evolves as

$$|\Psi_0\rangle := \sum_i \sqrt{p_i}|i^R\rangle|i^Q\rangle|0^E\rangle \rightarrow |\Psi_f\rangle := \sum_{ij} \sqrt{p_i}|i^R\rangle A_j|i^Q\rangle|j^E\rangle. \tag{6}$$

The entanglement fidelity $F_e(\rho,\mathcal{A})$ is defined as $||P_0|\Psi_f\rangle||^2$, where $P_0 := |\psi_0^{RQ}\rangle\langle\psi_0^{RQ}| \otimes I^E$.[2] Thus F_e is the squared norm of the projection of the final state in (6) onto the subspace associated with the initial entangled state $|\psi_0^{RQ}\rangle$. It depends only on $\rho := \Sigma_i p_i|i^Q\rangle\langle i^Q|$, and is given by $\Sigma_i|\mathrm{tr}\, A_i\rho|^2$. When $\rho = |\psi\rangle\langle\psi|$, it is equal to the input–output fidelity $\langle\psi|\mathcal{A}(|\psi\rangle\langle\psi|)|\psi\rangle$, that is, the fidelity of the final state of Q to its inital state.

As in the classical case for correlation, so in the quantum case we argue that this approach does not reflect a perverse fixation on entanglement, but also provides an appropriate fidelity criterion even when it is preservation of pure states on the system Q that we are concerned with, and no entangled system R in fact exists. For the entanglement fidelity $F_e(\rho^Q,\mathcal{A})$ is a lower bound on the average input–output fidelity $\Sigma_i q_i\langle\psi_i|\mathcal{A}(|\psi_i\rangle\langle\psi_i|)|\psi\rangle$ for *any* pure-state ensemble on Q having density operator ρ^Q.

While this is a good lower bound to the input–output fidelities of pure-state ensembles, there is not a tight lower bound on the input–output fidelity in terms of the entanglement fidelity. Thus if one is really interested only in the effect of a quantum channel on a particular ensemble, one might get fidelities much higher than the entanglement fidelity suggests. We will be interested in one such case, the input–output fidelity for an orthonormal set of states, related to the ability to preserve essentially *classical* information coded in a quantum channel. In order to treat this case simultaneously with entanglement fidelity, we introduce a notion which generalizes both: average entanglement fidelity.

For an ensemble $E = \{p_i, \rho_i\}$ (where state ρ_i occurs with probability p_i), we define the *average entanglement fidelity* by $\overline{F_e}(E,\mathcal{A}) := \Sigma_i p_i F_e(\rho_i,\mathcal{A})$. A special case is

$$F_{\mathrm{cl}}(\rho,\mathcal{A}) := \sum_i p_i\langle i|\mathcal{A}(|i\rangle\langle i|)|i\rangle = \overline{F_e}(\{p_i, |i\rangle\langle i|\},\mathcal{A}), \tag{7}$$

where the $|i\rangle$ form an eigenbasis of ρ and $\rho = \Sigma_i p_i|i\rangle\langle i|$. This is the *classical fidelity* for the classical information [quantified by $S(\rho)$] of the ensemble of orthogonal eigenstates of the input density operator ρ. Another special case is an ensemble consisting of a single density operator ρ. In this case $\overline{F_e}$ is just $F_e(\rho,\mathcal{A})$ and may be viewed as the fidelity for transmission of the amount $S(\rho)$ of *quantum* information.

The average entanglement fidelity can equivalently be defined as the norm squared of the projection of the overall final state onto the subspace in which entangled states $|\psi_i^{RQ}\rangle$ representing the initial ensemble are correctly correlated with orthogonal states of an additional reference system S:

$$\begin{aligned}\overline{F_e} &= ||P_c \otimes I^E|\Psi_f\rangle||^2 \\ &= \mathrm{tr}\, P_c(\mathcal{I}^{RS} \otimes \mathcal{A})|\psi_0^{RQS}\rangle\langle\psi_0^{RQS}|,\end{aligned} \tag{8}$$

where $P_c := \Sigma_i |i^S\rangle\langle i^S| \otimes |\psi_i^{RQ}\rangle\langle\psi_i^{RQ}|$. The initial state of RQS may be $|\psi_0^{RQS}\rangle := \Sigma_i \sqrt{p_i}|i^S\rangle|\psi_i^{RQ}\rangle$, with the ensemble of entangled states in RQ produced by entanglement with S. Alternatively, the initial state of RQS may be mixed, with perfect classical correlation rather than entanglement, between the states of a basis of S and the different entangled states of RQ. In this case $|\psi_0^{RQS}\rangle\langle\psi_0^{RQS}|$ is given by $\Sigma_i p_i |i^S\rangle\langle i^S| \otimes |\psi_i^{RQ}\rangle\langle\psi_i^{RQ}|$. The average entanglement measure (8) is insensitive to whether entanglement, or merely classical correlation, exists between S and RQ.

For example, consider the special case of F_{cl}. Here the reference system R plays no role as the ρ_i are pure. After suppressing R, $P_c = \Sigma_i |i^S\rangle|i^Q\rangle\langle i^Q|\langle i^S|$. S contains a record of the classical information sent. S and Q may be supposed to be either entangled or classically correlated, with $\rho_0^{SQ} = \Sigma_{i,j}\sqrt{p_i p_j}|i^S\rangle\langle j^S| \otimes |i^Q\rangle\langle j^Q|$ or $\rho_0^{SQ} = \Sigma_i p_i |i^S\rangle\langle i^S| \otimes |i^Q\rangle\langle i^Q|$, for orthonormal system and reference bases $|i\rangle$, where the system basis is the eigenbasis of ρ. In either case, computing the probability $\mathrm{tr}(P_c \rho_f^{SQ})$ that the final system-reference state falls into the subspace in which system and reference exhibit perfect classical correlation in the desired bases, gives the classical fidelity $F_{\mathrm{cl}}(\rho, \mathcal{A})$.

IV. THE REVERSAL OPERATION

We motivate the definition of the near-optimal reversal operation $\mathcal{R}_{\mathcal{A},\rho}$ by considering operations $\mathcal{A}$ that are perfectly reversible on a "code" subspace C. Let P_C be the projector onto C. Perfectly reversible operations have a decomposition A_i for which $A_i P_C = \sqrt{p_i} W_i$, where the W_i are isometries from C into orthogonal subspaces, which means that $W_i^\dagger W_j = \delta_{ij} P_C$.[3,4] (Intuitively, this means that as far as its action on the code subspace is concerned, the operation just maps the state isometrically ("unitarily") into one of a set of mutually orthogonal subspaces.) Without loss of generality, assume that the ranges of the W_i span the state space. The reversal operation has a decomposition consisting of the operators $W_i^\dagger = P_C A_i^\dagger / \sqrt{p_i}$. (Intuitively, it may be thought of as measurement of which of the subspaces the state was mapped isometrically to, followed by the inverse of that isometry to put it correctly back into the code space.) This resembles the adjoint [defined using the Hilbert–Schmidt inner product $(A,B) := \mathrm{tr}\, A^\dagger B$ on operators] $\mathcal{A}_C^\dagger$ of the restriction $\mathcal{A}_C$ of $\mathcal{A}$ to C, which is given by $\mathcal{A}_C^\dagger \sim \{P_C A_i^\dagger\} = \{\sqrt{p_i} W_i^\dagger\}$. To get the reversal operation, the $\sqrt{p_i}$ need to be removed, which also makes the operation trace preserving. The general definition of $\mathcal{R}_{\mathcal{A},\rho}$ is also based on the adjoint, suitably corrected to ensure that it is trace preserving [and continuous in the density operator when, as we assume, $\mathcal{A}(\rho)$'s support is the entire Hilbert space]:

$$\mathcal{R}_{\mathcal{A},\rho} \sim \{\rho^{1/2} A_i^\dagger \mathcal{A}(\rho)^{-1/2}\}. \tag{9}$$

If we apply this definition to an operation $\mathcal{A}$ perfectly reversible on a code, using as our input ρ any state supported precisely on the code, it is a simple but useful exercise to verify that we get the reversal operation for codes described previously.

The notation $\mathcal{R}_{\mathcal{A},\rho}$ is justified by:

Lemma 1: The definition of the reversal operation $\mathcal{R}_{\mathcal{A},\rho}$ is independent of the decomposition $\{A_i\}$ of $\mathcal{A}$.

Proof: Let $\mathcal{A} \sim \{B_i\}$ be another decomposition. By adding null operators to one of the two decompositions, we can ensure that both have the same number of operators. Note that adding null operators to $\{A_i\}$ does not change the action of $\mathcal{R}_{\mathcal{A},\rho}$. Then there exist u_{ij} such that $B_i = \Sigma_j u_{ij} A_j$, where the matrix u defined by u_{ij} is unitary. The decomposition of $\mathcal{R}_{\mathcal{A},\rho}$ given in (9) transforms via the coefficients of $u^\dagger$ into a decomposition given in terms of the $B_i^\dagger$. As $u^\dagger$ is also unitary, the result is another decomposition of the same operation. ■

A simple but important property of $\mathcal{R}_{\mathcal{A},\rho}$ is easily verified directly from the definition:

Proposition 1: $\mathcal{R}_{\mathcal{A},\rho}(\rho) = \rho$.

The operation $\mathcal{R}_{\mathcal{A},\rho}$ is near-optimal in the sense given by the following theorem.

Theorem 2: Let $E=\{p_i,\rho_i\}$ be an ensemble of commuting density matrices, and let $\rho := \Sigma_i p_i\rho_i$. Then for any trace-preserving completely positive map $\mathcal{R}$, $\overline{F}_e(E,\mathcal{R}_{\mathcal{A},\rho}\mathcal{A}) \geqslant \overline{F}_e(E,\mathcal{R}\mathcal{A})^2$.

As a corollary, if $\overline{F}_e(E,\mathcal{R}\mathcal{A})=1-\eta$, then $\overline{F}_e(E,\mathcal{R}_{\mathcal{A},\rho}\mathcal{A})\geqslant(1-\eta)^2\geqslant 1-2\eta$. That is, $\mathcal{R}_{\mathcal{A},\rho}$'s error (defined as one minus the entanglement fidelity) is never greater than twice that of the best reversal operation.

Proof: Without loss of generality, assume that $\mathcal{R}\sim\{R_i\}$'s domain is the algebra of operators on $\mathrm{supp}(\mathcal{A}(\rho))$ and its range is $\mathrm{supp}(\rho)$. Allowing more general reversal operations cannot increase entanglement fidelity. Then there exist operators B_i such that

$$R_i=\rho^{1/2}B_i^\dagger\mathcal{A}(\rho)^{-1/2}, \tag{10}$$

namely those defined by $B_i^\dagger := \rho^{-1/2}R_i\mathcal{A}(\rho)^{1/2}$. (Generalized inverses are to be understood here.) Let $\mathcal{B}\sim\{B_i\}$. We have

$$\overline{F}_e(E,\mathcal{R}\mathcal{A})=\sum_l p_l\sum_{ij}|\mathrm{tr}\,\rho^{1/2}B_i^\dagger\mathcal{A}(\rho)^{-1/2}A_j\rho_l|^2. \tag{11}$$

Define $X^l_{ij} := \mathrm{tr}\,\rho^{1/2}B_i^\dagger\mathcal{A}(\rho)^{-1/2}A_j^\dagger\rho_l$. By proper ($l$-dependent) choice of operator decompositions $\mathcal{B}\sim\{B_i^l\}$ and $\mathcal{A}\sim\{A_i^l\}$ (corresponding to singular value decompositions—cf. Ref. 5, Sec. 7.3—of the matrices X^l), we may obtain the same expression, but with the inner sum having just one index. Then applying the cyclicity of the trace, the fact that $[\rho,\rho_l]=0$, and defining $X_{li} := p_l^{1/4}\mathcal{A}(\rho)^{-1/4}A_i^l\rho^{1/4}\rho_l^{1/2}$, $Y_{li} := p_l^{1/4}\mathcal{A}(\rho)^{-1/4}B_i^l\rho^{1/4}\rho_l^{1/2}$, gives

$$\begin{aligned}
\overline{F}_e(E,\mathcal{R}\mathcal{A})&=\sum_l p_l\sum_i|\mathrm{tr}\,\rho^{1/2}B_i^{l\dagger}\mathcal{A}(\rho)^{-1/2}A_i^l\rho_l|^2\\
&=\sum_{il}|\mathrm{tr}\,Y_{li}^\dagger X_{li}|^2\leqslant\sum_{il}\mathrm{tr}\,X_{li}^\dagger X_{li}\mathrm{tr}\,Y_{li}^\dagger Y_{li}\\
&\leqslant\left(\sum_{il}|\mathrm{tr}\,X_{li}^\dagger X_{li}|^2\sum_{i'l'}|\mathrm{tr}\,Y_{l'i'}^\dagger Y_{l'i'}|^2\right)^{1/2}\\
&\leqslant\left(\sum_{il}|\mathrm{tr}\,X_{li}^\dagger X_{li}|^2\right)^{1/2}\leqslant\left(\sum_{ijl}|\mathrm{tr}\,X_{li}^\dagger X_{lj}|^2\right)^{1/2}\\
&=\left(\sum_l p_l\sum_{ij}|\mathrm{tr}\,\rho^{1/2}A_i^{l\dagger}\mathcal{A}(\rho)^{-1/2}A_j^l\rho_l|^2\right)^{1/2}\\
&=\overline{F}_e(E,\mathcal{R}_{\mathcal{A},\rho}\mathcal{A})^{1/2}.
\end{aligned} \tag{12}$$

Here the first two inequalities are Schwarz inequalities, the third uses the fact that

$$\sum_i|\mathrm{tr}\,\rho^{1/2}B_i^\dagger\mathcal{A}(\rho)^{-1/2}B_i\rho_l|^2\leqslant F_e(\rho,\mathcal{R}\mathcal{B})\leqslant 1, \tag{13}$$

the fourth just adds positive terms inside the square root. The last identity depends on Lemma 1. Since $\mathcal{B}$ is not necessarily trace-preserving, (13) is not immediate, but from (11) and the trace-preserving condition on $\mathcal{R}$,

$$\sum_i R_i^\dagger R_i=\sum_i\mathcal{A}(\rho)^{-1/2}B_i\rho B_i^\dagger\mathcal{A}(\rho)^{-1/2}=I. \tag{14}$$

It follows that $\mathcal{B}(\rho)=\mathcal{A}(\rho)$, a normalized density operator. Let $|\psi_0^{RQ}\rangle$ be a purification of ρ. Then the states $(\mathcal{I}^R\otimes\mathcal{B}^Q)(|\psi_0^{RQ}\rangle\langle\psi_0^{RQ}|)$ and $(\mathcal{I}^R\otimes\mathcal{R}^Q\mathcal{B}^Q)(|\psi_0^{RQ}\rangle\langle\psi_0^{RQ}|)$ are also normalized density matrices, whence $F_e(\rho,\mathcal{RB})=\mathrm{tr}\,P_0(\mathcal{I}^R\otimes\mathcal{R}^Q\mathcal{B}^Q)(|\psi_0^{RQ}\rangle\langle\psi_0^{RQ}|)\leqslant 1$. ■

Important special cases of Theorem 2 are noted in:

Corollary 2: For any trace-preserving completely positive $\mathcal{R}$, $F_{\mathrm{cl}}(\rho,\mathcal{RA})\leqslant\sqrt{F_{\mathrm{cl}}(\rho,\mathcal{R}_{\mathcal{A},\rho}\mathcal{A})}$ and $F_e(\rho,\mathcal{RA})\leqslant\sqrt{F_e(\rho,\mathcal{R}_{\mathcal{A},\rho}\mathcal{A})}$.

When the members of the input ensemble ρ_i do not commute, we do not know whether $\mathcal{R}_{\mathcal{A},\rho}$, for $\rho:=\Sigma_i p_i\rho_i$, is still near-optimal.

V. RELATIONSHIP TO THE "PRETTY GOOD MEASUREMENT"

The above-presented analysis of the fidelity of reversal makes it clear that $\mathcal{R}_{\mathcal{A},\rho}$ provides a method for distinguishing, with close to optimal average error, density matrices from the ensemble $\{p_j,\hat{\rho}_j\}$, where $\hat{\rho}_j:=\mathcal{A}(|j\rangle\langle j|)$, and $\rho=\Sigma_j p_j|j\rangle\langle j|$. This provides a near-optimal method for distinguishing density matrices in an arbitrary ensemble, for any ensemble $\{p_j,\hat{\rho}_j\}$ may be constructed by an operation

$$\mathcal{A}\sim\{\sqrt{\lambda_{ij}}|v_{ij}\rangle\langle j|\},\tag{15}$$

where $\hat{\rho}_j=\Sigma_i\lambda_{ij}|v_{ij}\rangle\langle v_{ij}|$ are the spectral decompositions of the density matrices to be distinguished. The operation $\mathcal{A}$ may be thought of as measuring in the orthogonal basis $|j\rangle$, and then producing the corresponding $\hat{\rho}_j$, for example by randomly applying, with probabilities λ_{ij}, unitary rotations taking $|j\rangle$ to $|v_{ij}\rangle$. With $\mathcal{A}$ as defined previously,

$$\mathcal{R}_{\mathcal{A},\rho}\sim\{R_{ij}\}=\{\sqrt{p_j}\sqrt{\lambda_{ij}}|j\rangle\langle v_{ij}|\rho_{\mathrm{out}}^{-1/2}\}.\tag{16}$$

The "pretty good measurement" (PGM) was introduced by Holevo[6] (the term "pretty good measurement" is from Ref. 7) for the case of linearly independent pure states, in which case the PGM is a measurement of orthogonal projectors, and as Holevo showed, the optimal such measurement. For an ensemble of unnormalized density matrices $\rho_j:=p_j\hat{\rho}_j$, where $\rho_{\mathrm{out}}:=\Sigma_j\rho_j$ is a normalized density operator, the PGM is defined by the set of operators consisting of the

$$X_j:=\rho_{\mathrm{out}}^{-1/2}\rho_j\rho_{\mathrm{out}}^{-1/2}.\tag{17}$$

For pure $\rho_j\propto|j\rangle\langle j|$, these are just the operators corresponding to the "ρ-distorted"[8] states $\rho_{\mathrm{out}}^{-1/2}|j\rangle$. Note that for a doubly indexed ensemble of unnormalized states ρ_{ij}, $\Sigma_i X_{ij}=X_j$, where the X_j are the PGM for the $\rho_j:=\Sigma_i\rho_{ij}$. The operation (16) may be viewed, via the given representation, as performing the PGM for the ensemble of unnormalized states $\sqrt{p_j}\sqrt{\lambda_{ij}}|v_{ij}\rangle$, and returning $|j\rangle$ when the measurement result ij is obtained. Indeed, for that ensemble $R_{ij}^\dagger R_{ij}=X_{ij}$, and therefore $\Sigma_i R_{ij}^\dagger R_{ij}=X_j$. Thus the operation may also be viewed as doing the PGM for the ρ_j, and returning $|j\rangle\langle j|$ when the measurement result is j. (Since $|j\rangle$ are orthogonal, this is "classical information:" the value of j is viewed as the estimate of which j was input.) However, a given ensemble ρ_j may in general arise from orthogonal states $|j\rangle$ by actions of channels different from the "classicizing" one (15), which completely decoheres the orthogonal states $|j\rangle$ before producing $\hat{\rho}_j$. For example, if the $\hat{\rho}_j$ are orthogonal and pure they may be produced either by measurement in the basis $|j\rangle$ followed by an appropriate unitary operator U, or by applying U without prior measurement. In the first case quantum coherence is completely destroyed, while in the second case it is perfectly preserved. When the channel producing the $\hat{\rho}_j$ is not of the form (15), the reversal operation $\mathcal{R}_{\mathcal{A},\rho}$ will be different from (16). Although (16) still gives near-optimal classical fidelity, it will not necessarily give good entanglement fidelity, since in some sense it decoheres the states $\hat{\rho}_j$. $\mathcal{R}_{\mathcal{A},\rho}$, however, will have near-optimal entanglement fidelity while retaining near-optimal classical fidelity. $\mathcal{R}_{\mathcal{A},\rho}$ thus takes advantage of whatever coherence remains between the $\hat{\rho}_j$; it avoids decohering the $\hat{\rho}_j$ if the channel has not decohered them already.

VI. A BOUND ON THE CLASSICAL FIDELITY OF REVERSAL

To bound a fidelity of reversal it is sufficient to bound the fidelity for the near optimal reversal operation and apply Theorem 2. Here we have a look at such bounds for classical fidelities of reversal for $\mathcal{A}$ of the form (15). In this case, the classical fidelities are average probabilities of success for measurements that attempt to infer which of the eigenprojectors $|j\rangle\langle j|$ of the input state $\rho=\Sigma_j p_j|j\rangle\langle j|$ was actually transmitted. The expression for the PGM gives the following bound on the optimal probability of success F_{cl} (with the definitions of Sec. V):

$$\begin{aligned} F_{\mathrm{cl}}^2 &\geqslant F_{\mathrm{cl}}(\rho,\mathcal{R}_{\mathcal{A},\rho}\mathcal{A}) \\ &= \sum_j \mathrm{tr}\,(\rho_{\mathrm{out}}^{-1/2}\rho_j\rho_{\mathrm{out}}^{-1/2}\rho_j) \\ &= 1-\sum_{i,j:i\neq j} \mathrm{tr}(\rho_{\mathrm{out}}^{-1/2}\rho_i\rho_{\mathrm{out}}^{-1/2}\rho_j), \end{aligned} \tag{18}$$

where we used the identity $\Sigma_{i,j}\,\mathrm{tr}(\rho_{\mathrm{out}}^{-1/2}\rho_i\rho_{\mathrm{out}}^{-1/2}\rho_j)=1$. Thus the probability of error E_{cl} is bounded above by $2\Sigma_{i,j:i\neq j}\,\mathrm{tr}(\rho_{\mathrm{out}}^{-1/2}\rho_i\rho_{\mathrm{out}}^{-1/2}\rho_j)$, which is a multiple of the sum of the Hilbert–Schmidt inner products of the different $\rho_{\mathrm{out}}^{-1/4}\rho_j\rho_{\mathrm{out}}^{-1/4}$. When ρ_{out} is uniform (proportional to a projection), this sum can be easy to estimate. An often used measure of overlap between density matrices is the Bures–Uhlmann fidelity.[9,10] This measure depends only on the pair of density matrices, and is defined by $F_{\mathrm{BU}}(\sigma_1,\sigma_2):=\mathrm{tr}\sqrt{\sigma_1^{1/2}\sigma_2\sigma_1^{1/2}}$. The expression for the optimal reversal given in (16) can be used to derive a bound on the probability of error in terms of the Bures–Uhlmann fidelities.

Theorem 3:

$$F_{\mathrm{cl}}^2 \geqslant 1-\sum_{i,j:i\neq j}\sqrt{p_ip_j}F_{\mathrm{BU}}(\hat{\rho}_i,\hat{\rho}_j). \tag{19}$$

Proof: Let A_j be the matrix whose ith column is $\sqrt{p_j}\sqrt{\lambda_{ij}}|v_{ij}\rangle$, and A the matrix obtained by placing the A_j in a row. Then $AA^\dagger=\rho_{\mathrm{out}}$. Let R_j be the matrix whose ith row is $\sqrt{p_j}\sqrt{\lambda_{ij}}\langle v_{ij}|\rho_{\mathrm{out}}^{-1/2}$ and R the matrix obtained by placing the R_j in a column. R is simply an explicit matrix form of $\mathcal{R}_{\mathcal{A},\rho}$. Since $R=A^\dagger(AA^\dagger)^{-1/2}$, R is a matrix with the property that RA is positive semidefinite. (In fact, this gives an alternative approach to defining $\mathcal{R}_{\mathcal{A},\rho}$). The matrix RA has a natural block structure that mirrors that used to define R and A. It is readily verified that F_{cl} for $\mathcal{R}_{\mathcal{A},\rho}$ is given by the sum of the squared Frobenius norms $|(RA)_{jj}|_2^2:=\mathrm{tr}(RA)_{jj}^\dagger(RA)_{jj}$ of the diagonal blocks. Since $|RA|_2^2$ is one, it suffices to estimate the sum of the squared Frobenius norms of the off-diagonal blocks to bound the optimal F_{cl}. To do so, observe that $(RA)^2=A^\dagger A$. The block at block position l,k in $B:=A^\dagger A$ is given by $B_{lk}=A_l{}^\dagger A_k$. Since $A_lA_l{}^\dagger=\rho_l$,

$$\begin{aligned} B_{lk}{}^\dagger B_{lk} &= A_k{}^\dagger\rho_lA_k \\ &= U\rho_k^{1/2}\rho_l\rho_k^{1/2}U^\dagger \end{aligned}$$

(by polar decomposition of A_k) for some unitary operator U. Consequently, the L_1-norm of B_{lk}, defined by $|B_{lk}|_1:=\mathrm{tr}\sqrt{B_{lk}{}^\dagger B_{lk}}$ is given by $\sqrt{p_lp_k}F_{\mathrm{BU}}(\hat{\rho}_l,\hat{\rho}_k)$. It therefore suffices to relate the Frobenius norms of the off-diagonal blocks of a positive semidefinite matrix to the L_1 norms of the off-diagonal blocks of its square, via the following lemma.

Lemma 4: Let

$$M=\begin{pmatrix} a & b^\dagger \\ b & c \end{pmatrix}$$

be positive semidefinite, with a,b,c matrices. Write

$$M^{1/2}=\begin{pmatrix} x & y^{\dagger} \\ y & z \end{pmatrix}$$

with the same block structure. Then $|y|_2^2 \leq |b|_1$.

Proof of Lemma 4: Without loss of generality, assume that y is non-negative diagonal. Otherwise, with a block-diagonal unitary

$$U=\begin{pmatrix} u & 0 \\ 0 & v \end{pmatrix}$$

with u and v chosen to implement the singular value decomposition of y, we may transform M and $M^{1/2}$ so that y is a diagonal matrix with non-negative diagonal entries (for rectangular y, the upper or left-hand square portion is diagonalized). This does not affect the norms, since U transforms blocks independently and the L_1 and Frobenius norms are both unitarily invariant. Let y_i be the diagonal entries of y. Note that $b=yx+zy$ and $|b|_1 \geq \mathrm{tr}\, b$ (cf. Ref. 5, p. 432). Now tr $(yx+zy)=\Sigma_i y_i(x_{ii}+z_{ii})$. By the positivity of $M^{1/2}$, $y_i^2 \leq x_{ii}z_{ii}$, so y_i is less than at least one of x_{ii}, z_{ii}. Thus $|y|_2^2=\Sigma_i y_i^2 \leq \mathrm{tr} b \leq |b|_1$, as desired. ■

To complete the proof of Theorem 3, consider first the block decomposition of RA and B determined by B_{11}. By Lemma 4, the squared Frobenius norm of the first block row and column excluding $(RA)_{11}$ is bounded by the sum of the L_1 norms of the corresponding block row and column in B_{11}. By subadditivity of the norm, this is at most $\Sigma_{i>1}(|B_{1i}|_1+|B_{i1}|_1)$. After a suitable permutation, the same argument applies to the row and column determined by B_{ii}, for each i. The proof of the theorem then follows by summing over the resulting inequalities and noting that each off-diagonal block occurs twice on both sides. ■

VII. EXAMPLES AND APPLICATIONS

By a slight extension of an example already given, $\mathcal{R}_{\mathcal{A},\rho}$ is optimal for $\mathcal{A}$ perfectly reversible on some code subspace, when ρ is a state with no support outside the code. Applications to reversing other simple quantum operations may be instructive. For instance, for a depolarizing channel $\mathcal{A} \sim \{(1-p)^{1/2}I, (p/3)^{1/2}\sigma_i\}_{i=1,2,3}$ acting on $\rho=I/d$, $\mathcal{R}_{\mathcal{A},\rho}$ is another application of the depolarizing channel, whereas the optimal reversal is to do nothing. (This case saturates the inequality of Theorem 3.)

Due to its near optimality, the reversal operation $\mathcal{R}_{\mathcal{A},\rho}$ can be used in any situation where classical or quantum information has been corrupted by noise with known behavior. $\mathcal{R}_{\mathcal{A},\rho}$ has a simple definition, but whether it or a good approximation can be implemented efficiently depends on the details of the situation. Whether or not it can be efficiently implemented, because its error is at most twice the optimum, it can be used as a theoretical tool to obtain upper bounds on the achievable fidelities in a given situation. The upper bounds can then be compared to the fidelity achieved by simpler algorithms. An example of this occurs in the use of stabilizer codes for quantum error-correction. When the noise model is independent and depolarizing, classical coding theory immediately suggests a combinatorially straightforward error-correction algorithm based on maximum likelihood error syndrome decoding. Comparing this method to $\mathcal{R}_{\mathcal{A},\rho}$ suggests itself as a fruitful path of investigation with applications to asymptotic bounds in quantum coding theory.[11,12] More generally, for any encoding scheme capable of transmitting quantum information through a given channel at a given rate when appropriate decoding is used, $\mathcal{R}_{\mathcal{A},\rho}$ may be used to provide such a decoding (with $\mathcal{A}$ taken to be the concatenation of encoding and noise).

Another application is to query complexity for quantum oracles. Here we are given a quantum black box implementing an unknown quantum operation from some set. A simple method for attempting to determine which operation we are given is to apply it to copies of some input state and attempt to distinguish the output state. A bound on the probability of success can then be obtained by using bounds such as the one of Theorem 3. This was how the fact that the hidden subgroup problem has low query complexity was first realized.[13]

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Optimal control in laser-induced population transfer for two- and three-level quantum systems

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We apply the techniques of control theory and of sub-Riemannian geometry to laser-induced population transfer in two- and three-level quantum systems. The aim is to induce complete population transfer by one or two laser pulses minimizing the pulse fluences. Sub-Riemannian geometry and singular-Riemannian geometry provide a natural framework for this minimization, where the optimal control is expressed in terms of geodesics. We first show that in two-level systems the well-known technique of "π-pulse transfer" in the rotating wave approximation emerges naturally from this minimization. In three-level systems driven by two resonant fields, we also find the counterpart of the "π-pulse transfer." This geometrical picture also allows one to analyze the population transfer by adiabatic passage. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1465516]

I. INTRODUCTION: PHYSICAL CONTEXT

A. Generalities

Design of external laser fields (amplitudes and frequencies) to reach a selected state of a quantum system is of primary importance for the control of quantum dynamics. The techniques for this state-selectivity that have been developed are essentially based on (i) adiabatic passage (see, e.g., the recent works[1–4]), (ii) multiphoton quasiresonant pumping[5] by "generalized π-pulses,"[6] and (iii) optimal control theory (see, e.g., Refs. 7 and 8).

Adiabatic passage has the advantage of robustness in the sense that significant deviations of the fields do not significantly modify the final result. On the other hand, optimal control is a systematic framework to design the field parameters (or control variables) to reach selectivity in maximizing or minimizing a quantity (the cost) depending functionally on the state and control variables. This design is in general not robust, in contrast with standard adiabatic passage. Since the robustness is difficult to quantify as a cost, we do not expect in general the adiabatic passage to emerge from an optimal control solution. This has been discussed for specific simple systems.[9,10] However optimality for adiabatic passages has been characterized in Ref. 11.

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The success of these coherent laser-induced processes requires, in general, use of as short as possible external pulses, to minimize incoherent effects of relaxation (through spontaneous emission, collisions, etc.). It is essential that the total time of the pulse is shorter than the characteristic times of the incoherent losses. Coherent transfers also need as low as possible pulse intensities in order to (i) minimize incoherent phenomena induced by strong fields such as ionization for atoms or molecules, and (ii) avoid involving other energy levels, that are not included in the models. Otherwise the population is spread among these levels and the transfer becomes inefficient.

Depending on the concrete physical setting there are several possible choices of the cost functional. One choice, which has been studied in Ref. 12, is to minimize the total time of the control process. However, the total time minimization presented in Ref. 12 assumes that arbitrarily large laser intensities can be used. The relations between our results and the results of Ref. 12 will be made clear in Sec. II C.

In this paper we address the two- and three-level problem from the geometric control theory point of view. We consider several functionals to be minimized, which are geometrically very natural, and that physically reflect the practical constraints mentioned previously [fluence, see formula (5) for the two-level case and formula (7) for the three-level case, or transfer time with bounded controls, etc.]. The choice of these costs will be discussed in Sec. II C. We will also use the classical tracking technique, often used in in geometric control theory (see Ref. 13), that will allow in particular achievement of adiabatic transfer.

Remark 1: In the choice of the cost to be minimized, it is useful to consider optimal problems that are independent of time reparametrization. Indeed, in that case, very slowly varying solutions, comparable with the ones used in experiments, can be obtained just by time reparametrization. This point will be taken into account in the following, in particular see Sec. II C. But we will also consider problems that do not have this feature.

B. Content of the paper

In this work we apply geometric control theory in two- and three-level systems, which we briefly describe in the following. Moreover we make the connection with the adiabatic passage.

1. The two-level case

We first study the population transfer in a two-level quantum system (of energies E_1 and E_2) driven by an external field of arbitrary time-dependent shape, starting at t_0 and ending at t_1. The dynamics is governed by the time-dependent Schrödinger equation (in a system of units such that $\hbar=1$):

$$i\frac{\mathrm{d}\psi(t)}{\mathrm{d}t}=H\psi(t), \tag{1}$$

$\psi(.):\mathbb{R}\to\mathbb{C}^n$, $n=2$, where

$$H=\begin{pmatrix} E_1 & \Omega(t) \\ \Omega^*(t) & E_2 \end{pmatrix}. \tag{2}$$

is the Hamiltonian of the system (we have assumed no diagonal coupling). We choose the most general situation where the off-diagonal element is complex: $\Omega(t):\mathbb{R}\to\mathbb{C}$.

In the two-level system (2), complete controllability (on spheres) is obvious (see the following for the precise definition of controllability). We show that the natural optimal control problem of minimizing the integral of the laser amplitude:

$$\mathcal{C}=\int_{t_0}^{t_1}|\Omega|\ \mathrm{d}t \tag{3}$$

has the following features.

(a) After some transformations the problem can be formulated as a problem of Sub-Riemannian geometry (see Remark 3).

(b) The optimal control solution has the expected resonance property, i.e., Ω can be written as

$$\Omega(t)=b(t)e^{i[(E_2-E_1)t+\alpha]}, \tag{4}$$

where α is an arbitrary constant, $b(.):\mathbb{R}\to\mathbb{R}^+$ is a real function with compact support $[t_0,t_1]$.

(c) The optimal amplitude $b(t)$ satisfies

$$\int_{t_0}^{t_1} b(t)=\pi/2.$$

Remark 2: We thus recover the well-known strategy of "π-pulse transfer" of a resonant pulse in the rotating wave approximation,[14] which gives complete transfer with $\Omega(t)=\mu\mathcal{F}(t)e^{i\phi(t)}/2$, $\dot{\phi}(t)=E_2-E_1$, and $\not{\ell}=|\mu|\int_{t_0}^{t_1}\mathcal{F}(t)\mathrm{d}t/2=\pi/2$. Here μ is the intrinsic coupling between the two levels and $\mathcal{F}(t)$ the external pulsed field. This shows in particular that an additional controllable time-dependent frequency ("chirping," see, e.g., Ref. 15) does not improve the minimization with respect to this cost. We thus show that in the model of the rotating wave approximation, the "π-pulse transfer" corresponding to the minimum pulse area to achieve the complete transfer is a consequence of purely geometric considerations.

(d) The solution is independent of time reparametrization, i.e., derivatives of controls can be made as small as required simply by choosing an appropriate time parametrization. Moreover, with an adequate choice of the parametrization it minimizes the *fluence* for fixed transfer time t_1-t_0:

$$\mathcal{E}=\int_{t_0}^{t_1}|\Omega|^2(t)\mathrm{d}t=\int_{t_0}^{t_1}b^2(t)\mathrm{d}t, \tag{5}$$

or equivalently the transfer time, with the constraint on the amplitude $|b(t)|\leqslant 1$. More details about the relations between these costs are given in Sec. II C.

Remark 3: A control problem is called *distributional* if the set of admissible velocities is a *distribution*, i.e., a nonintegrable field of planes. It is called *contact* if the distribution is a *contact distribution*, i.e., if the field of planes is defined as the kernel of the one-form ω, then $\mathrm{d}\omega$ is nondegenerate when restricted to $\mathrm{Ker}(\omega)$. A control problem is said to be *sub-Riemannian* if additionally one gives a Riemannian metric on the distribution, and one minimizes the Riemannian length. For sub-Riemannian geometry we refer to Refs. 16–18.

In fact, as we shall see, the two-level problem reduces to a three-dimensional contact sub-Riemannian problem, with a special feature: it has a symmetry, transverse to the distribution. It is a standard fact that such a sub-Riemannian problem is in fact an isoperimetric problem (in the sense of the calculus of variations) on the quotient by the symmetry. Such isoperimetric contact three-dimensional sub-Riemannian problems have been studied in detail at the local level in Ref. 19, for instance. In fact, the above-given statement is nothing but the (trivial) solution of the classical isoperimetric problem (or Dido problem) on the Riemannian sphere.

The study of this two-level case is described in Sec. III.

2. The three-level case

For three-level systems, labeled 1, 2, and 3, of respective energies E_1, E_2, and E_3, driven by two resonant monochromatic fields of respective envelopes $\mathcal{F}_j(t)$, $j=1,2$ and of frequencies ω_1 and ω_2, the Hamiltonian, in the rotating wave approximation (RWA), reads

$$H=\begin{pmatrix} E_1 & u_1(t)e^{i\omega_1 t} & 0 \\ u_1(t)e^{-i\omega_1 t} & E_2 & u_2(t)e^{i\omega_2 t} \\ 0 & u_2(t)e^{-i\omega_2 t} & E_3 \end{pmatrix}, \tag{6}$$

where

$$\omega_1 := E_2 - E_1, \quad u_1(.):\mathbb{R}\to\mathbb{R},$$

$$\omega_2 := E_3 - E_2, \quad u_2(.):\mathbb{R}\to\mathbb{R}.$$

The controls $u_j(t)$, $j=1,2$ are connected to the physical parameters by $u_j(t)=\mu_j\mathcal{F}_j(t)/2$, with the couplings μ_j, intrinsic to the quantum system, that we have restricted to couple only levels j and $j+1$ by pairs. We allow the control variables, starting at t_0 and ending at t_1, to have any shape.

Controllability. For a control system, the *accessibility set* of a point x_0 in the configuration space is the set of points that can be joined from x_0 by a trajectory of the system. A control system is said to be *controllable* if the accessible set of every x_0 is the whole configuration space. For an analytic distributional system, it is known that the configuration space is foliated by accessible sets, called *orbits* in that case. These orbits are exactly the Hermann–Nagano orbits (see the Hermann–Nagano Theorem in the following and Ref. 22 for details).

In the following we first prove that this three-level system reduces to a distributional problem which is not controllable, since the orbits under consideration are two-dimensional spheres. Then we show that on each of these spheres the control problem reduces to a singular-Riemannian problem. The ''relevant locus,'' which is the union of all the orbits (spheres) passing through state number 1, has an interesting nontrivial geometric description. It is the only nonorientable sphere-bundle over S^1 (see Sec. IV A).

Optimal solutions. In this case we first consider the problem of minimizing the fluence for fixed transfer time t_1-t_0 (which is a parametrization-dependent cost):

$$\mathcal{E}=\int_{t_0}^{t_1}(u_1^2+u_2^2)\mathrm{d}t. \tag{7}$$

Again let us notice that minimization of the functional:

$$\ell=\int_{t_0}^{t_1}\sqrt{u_1^2+u_2^2}\mathrm{d}t, \tag{8}$$

leads to the same motion in the space state, parametrized in any way. Moreover, minimizing the functional $\mathcal{E}$ is equivalent to minimizing the transfer-time for controls bounded in the following way:

$$u_1^2+u_2^2\leqslant 1. \tag{9}$$

This will be explained in detail in Sec. II C.

For the three-level system (6), the main known ways to completely populate state 3 from the initial condition in state 1 are the following:

(i) application of two successive π-pulses (without overlap), giving $\ell=\pi$ in the system (6);
(ii) interaction with two completely overlapping control variables: $u_1(t)=u_2(t)$ (with two different pulses assuming that the couplings between 1 and 2 and between 2 and 3 are different), giving also $\ell=\pi$;[20]
(iii) adiabatic passage by delayed pulses (of the same shape) such that $u_2(t)$ starts before $u_1(t)$ (known as ''counterintuitive'' pulse sequence).[1] This way of transferring the population is energetically expensive since it requires $\ell\gg\pi$.

For this three-level system, we show that the cost ℓ can be significantly reduced, finding its minimum value

$$\ell = \frac{\sqrt{3}}{2}\pi \approx 0.866\pi,$$

corresponding to the singular-Riemannian geodesic. This is also the minimum transfer time under the constraint (9).

The minimum value for the functional $\mathcal{E}$ is

$$\mathcal{E} = \frac{3}{4}\pi^2 \frac{1}{t_1 - t_0}$$

[where $(t_1 - t_0)$ is the fixed interaction time]. These results are described by Theorem 4 of Sec. IV.

We show that the associated pulse sequence is such that $u_1(t)$ starts before $u_2(t)$ (''intuitive'' sequence) and we construct symmetric smooth pulses of the same shape giving this minimum. We compute the geodesic joining the initial state to the final state, and we give some examples of time reparametrized optimal controls. The results thus show very natural control strategies that do not look like the standard strategy in this type of problem. This study is the content of Sec. IV.

Tracking. In Sec. V we construct for the three-level problem a geometric representation of adiabatic passage and compare it with the strategies of optimal control. This allows one to reformulate the adiabatic passage as explicitly fixing the trajectory leading from state 1 to state 3 and in controlling the rate of transient population in the intermediate state 2. This procedure improves on the standard adiabatic passage in that it exactly reaches the target state. This tracking technique is standard in control theory. A solution of this type is generated by a counterintuitive sequence of controls, in the adiabatic approximation.[1]

II. PRELIMINARIES, ELIMINATION OF THE DRIFT, AND CHOICE OF THE COST

A. Preliminaries

We start with a quantum system with finite number of (distinct) levels in interaction with a time-dependent external field such that the Hamiltonian reads:

$$\begin{aligned} H &= \begin{pmatrix} E_1 & \Omega_1(t) & 0 & \cdots & 0 \\ \Omega_1^*(t) & E_2 & \Omega_2(t) & \ddots & \vdots \\ 0 & \Omega_2^*(t) & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & E_{n-1} & \Omega_{n-1}(t) \\ 0 & \cdots & 0 & \Omega_{n-1}^*(t) & E_n \end{pmatrix} \\ &= D + \begin{pmatrix} 0 & \Omega_1(t) & 0 & \cdots & 0 \\ \Omega_1^*(t) & 0 & \Omega_2(t) & \ddots & \vdots \\ 0 & \Omega_2^*(t) & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & \Omega_{n-1}(t) \\ 0 & \cdots & 0 & \Omega_{n-1}^*(t) & 0 \end{pmatrix}, \end{aligned} \tag{10}$$

with $D := \mathrm{diag}(E_1, \ldots, E_n)$ and the energies of the system states appearing on the diagonal. Time-dependent elements $\Omega_j(.): \mathbb{R} \to \mathbb{C}$, $j = 1, \ldots, n-1$ are different from zero only between times t_0 and t_1. They couple the states by pairs. The term D is called *drift*. Section II B is devoted to the elimination of D via a unitary transformation.

The state-vector $\psi(t)$, solution of the time-dependent Schrödinger equation (1), can be expanded in the canonical basis of $\mathbb{C}^n$, formed by elements $\varphi_1=(1,0,\ldots,0)$, $\varphi_2=(0,1,\ldots,0),\ldots\ \varphi_n=(0,,0,\ldots,1)$: $\psi(t)=c_1(t)\varphi_1+c_2(t)\varphi_2+\cdots+c_n(t)\varphi_n$, with $|c_1(t)|^2+|c_2(t)|^2+\cdots+|c_n(t)|^2=1$. For $t<t_0$ and $t>t_1$, $|c_i(t)|^2$ is the probability of measuring energy E_i. Notice that

$$\frac{\mathrm{d}}{\mathrm{d}t}|c_i(t)|^2=0 \quad \text{for } t<t_0 \text{ and } t>t_1.$$

Our problem can be stated in the following way: Assuming $|c_1(t)|^2=1$ for $t<t_0$, we want to determine suitable interaction functions $\Omega_i(.)$, $i=1,\ldots,n-1$, such that $|c_j(t)|^2=1$ for time $t>t_1$ and some chosen $j\in\{2,\ldots,n\}$, requiring that they minimize the cost (8).

Remark 4: This problem is a control problem on the real $2n$-1 dimensional sphere in $\mathbb{R}^{2n}$ (or on the complex sphere in $\mathbb{C}^n$). Standard considerations from control theory allow one to conclude on the controllability on the sphere [even with arbitrarily small bounds on the controls $\Omega_i(.)$], i.e., it is possible to drive the system from any initial condition to any terminal condition on the sphere. Also, control problems of this type have finite dimensional Lie-algebra: the reductive Lie algebra $su(n)\times\mathbb{R}$. They can be lifted to left-invariant control problems on the compact Lie group $\mathrm{SU}(n)\times S^1$ (S^1, the circle), and the controllability of the lifted control system also holds.

We will also consider the "real resonant case" in which the controls Ω_i correspond to lasers that are in resonance:

$$\Omega_i(t)=u_i(t)e^{i\omega_i t}, \quad \omega_i=E_{i+1}-E_i,$$

$$i=1,\ldots,n-1, \quad u_i(.):\mathbb{R}\to\mathbb{R}. \tag{11}$$

Notice that in this case we consider real controls which always leads to lack of controllability.

In the following we treat the $n=2$ and $n=3$ cases. The $n=2$ case is treated in the most general setting, in the sense that we control both the amplitude and the phase of the laser pulses. We obtain that the optimal strategy is realized with an external pulse in resonance in the rotating wave form. The $n=3$ case is treated directly with pulses in resonance in the rotating wave approximation.

In the $n=3$ case, it is an open question if it is possible to reduce the value of the cost (8), when controlling both amplitude and phase of the lasers.

In the following, to compute the orbits of the control systems under consideration, we will make use of the standard Hermann–Nagano theorem. Moreover to compute optimal trajectories we will use the well-known Pontryagin Maximum Principle.[21] For convenience we recall these two theorems in the following. Proofs can be found for instance in Ref. 22.

Theorem (Hermann–Nagano): *Let M be an analytic manifold and $\mathcal{F}$ a family of analytic vector fields on M. Then:*

(1) each orbit of $\mathcal{F}$ is an analytic submanifold of M,
(2) if $\mathcal{O}(\mathbf{x}_0)$ is an orbit containing the point $\mathbf{x}_0$, then the tangent space of $\mathcal{O}(\mathbf{x}_0)$ at $\mathbf{x}$ is given by $\mathrm{Lie}_{\mathbf{x}}(\mathcal{F})$. In particular the dimension of $\mathrm{Lie}_{\mathbf{x}}(\mathcal{F})$ is constant as $\mathbf{x}$ varies over $\mathcal{O}(\mathbf{x}_0)$.

Theorem (Pontryagin Maximum Principle): *Consider a control system of the form $\dot{x}=f(x,u)$ with a cost of the form $\int_0^T f^0(x,u)\mathrm{d}t$, where x belongs to a manifold M and $u\in U\subset\mathbb{R}^m$. Assume moreover that M,f,f^0 are smooth. If the couple $(u(.),x(.)):[0,T]\subset\mathbb{R}\to U\times M$ is optimal, then there exists a never vanishing field of covectors along $x(.)$, that is an absolutely continuous function $(p(.),p^0):t\in[0,T]\mapsto p(t)\in T^*_{x(t)}M\times\mathbb{R}$ (where $p_0\leqslant 0$ is a constant) such that:*

(i) $\dot{x}(t)=\partial\mathcal{H}/\partial p\,(x(t),p(t),u(t))$,
(ii) $\dot{p}(t)=-\partial\mathcal{H}/\partial x\,(x(t),p(t),u(t))$,

where by definition

$$\mathcal{H}(x,p,u) := <p, f(x,u)> + p_0 f^0(x,u). \tag{12}$$

Moreover:

(iii) $\mathcal{H}(x(t),p(t),u(t)) = \mathcal{H}_M(x(t),p(t))$, *for a.e.* $t \in [0,T]$,

where $\mathcal{H}_M(x(t),p(t)) := \max_{v \in U} \mathcal{H}(x(t),p(t),v)$.

The real-valued map on $T^*M \times U$, defined in (12), is called Hamiltonian. The couples $(u(.),x(.))$ satisfying conditions (i)–(iii) with $p_0 = 0$ are called *abnormal extremals*.

B. Elimination of the drift term

In both cases (2) and (6) we show how to eliminate the drift term [i.e., diag(E_1,E_2) and diag(E_1,E_2,E_3) respectively] from the Hamiltonian. In case (6) this elimination will be made just by a unitary change of coordinates that at the same time eliminates the explicit dependence on the time. In case (2) it will moreover require a unitary change of controls. This difference is simply a consequence of the fact that in the three-level case we start with ''real controls in resonance,'' while in the two-level case we use general complex controls.

Assume that $\psi(t)$ satisfies the Schrödinger equation (1). Let $U(t)$ be a unitary time-dependent matrix and set $\psi(t) = U(t)\psi'(t)$ (interaction representation). Then $\psi'(t)$ satisfies the Schrödinger equation:

$$i\frac{d\psi'(t)}{dt} = H'(t)\psi'(t),$$

with the new Hamiltonian:

$$H' = U^{-1}HU - iU^{-1}\frac{dU}{dt}. \tag{13}$$

Here we consider the Hamiltonian (10), and we choose

$$U = \mathrm{diag}(e^{-iE_1 t}, e^{-iE_2 t}, \ldots, e^{-iE_n t}).$$

We get:

$$H' = \begin{pmatrix} 0 & \Omega_1(t)e^{-i(E_2-E_1)t} & 0 & \cdots & 0 \\ \Omega_1^*(t)e^{i(E_2-E_1)t} & 0 & \Omega_2(t)e^{-i(E_3-E_2)t} & \ddots & \vdots \\ 0 & \Omega_2^*(t)e^{i(E_3-E_2)t} & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & \Omega_{n-1}(t)e^{-i(E_n-E_{n-1})t} \\ 0 & \cdots & 0 & \Omega_{n-1}^*(t)e^{i(E_n-E_{n-1})t} & 0 \end{pmatrix}. \tag{14}$$

As a consequence, if we write $\psi(t) = c_1(t)\varphi_1 + c_2(t)\varphi_2 + \cdots + c_n(t)\varphi_n$, and $\psi'(t) = c_1'(t)\varphi_1 + c_2'(t)\varphi_2 + \cdots + c_n'(t)\varphi_n$, then $|c_i(t)|^2 = |c_i'(t)|^2$, $i = 1,2,\ldots,n$, that is H and H' have the same population distribution.

For the three-level system (6), this leads to (dropping the prime)

$$H = \begin{pmatrix} 0 & u_1(t) & 0 \\ u_1(t) & 0 & u_2(t) \\ 0 & u_2(t) & 0 \end{pmatrix}. \tag{15}$$

For the two-level system (2), redefining

$$u(t) := e^{-i(E_2-E_1)t}\ \Omega(t), \tag{16}$$

we get (dropping the prime)

$$H=\begin{pmatrix} 0 & u(t) \\ u^*(t) & 0 \end{pmatrix}, \tag{17}$$

In the following we set $u(t)=u_1(t)+iu_2(t)$, where $u_1(.)$ and $u_2(.)$ are two real functions.

Remark 5: Notice that the unitary transformations on the states and on the controls preserve the cost and the probabilities. As a consequence they preserve the initial and final conditions $|c_1(t_0)|^2=1$, $|c_j(t_1)|^2=1$.

Remark 6: This reduction procedure can be easily extended to the case where the drift term in (10) is time-dependent:

$$D=\mathrm{diag}(E_1(t),\ldots,E_n(t)). \tag{18}$$

The key point is that the couplings have to be only between successive levels. For the two-level case, this requirement is obviously met. The elimination of the drift (18) in (10) requires the matrix

$$U=\mathrm{diag}\left(\exp\left(-i\int_{t_0}^{t}E_1(s)\mathrm{d}s\right),\exp\left(-i\int_{t_0}^{t}E_2(s)\mathrm{d}s\right),\ldots,\exp\left(-i\int_{t_0}^{t}E_n(s)\mathrm{d}s\right)\right).$$

In this case the new Hamiltonian has the form (14) with $i(E_{i+1}-E_i)t$ replaced by $i\int_{t_0}^{t}(E_{i+1}(s)-E_i(s))\mathrm{d}s$ and the resonance condition (11) becomes

$$\Omega_i(t)=u_i(t)\exp\left(i\int_{t_0}^{t}(E_{i+1}(s)-E_i(s))\mathrm{d}s\right),\quad i=1,\ldots,n-1,\quad u_i(.):\mathbb{R}\to\mathbb{R}.$$

C. Choice of different costs and relation between them

1. Minimizing length and energy

As we will show, both the $n=2$ and $n=3$ problems can be stated as control problems that are linear with respect to the controls (i.e., ''distributional control problems''):

$$\dot{\mathbf{x}}=u_1F_1+u_2F_2, \tag{19}$$

where $\mathbf{x}\in S^3$ for $n=2$ and $\mathbf{x}\in S^5$ for $n=3$, with F_1 and F_2 two vector fields on the d-dimensional sphere S^d. It is thus natural to treat this problem as a sub-Riemannian problem (in the three-level case it is in fact singular-Riemannian problem on S^2, see Sec. IV), to which is associated the length

$$\ell=\int_{t_0}^{t_1}\sqrt{u_1^2+u_2^2}\mathrm{d}t. \tag{20}$$

This length represents the cost, i.e., the quantity that has to be minimized in our problem. This cost is time-reparametrization invariant. Thus, with such a cost one can always reparametrize the time of the optimal solution in order to obtain controls with slow variation (i.e., with $\dot{u}_1$ and $\dot{u}_2$ small), that are closer to realistic pulses in practice.

Standard considerations show that it is equivalent to minimize the fluence for fixed transfer time t_1-t_0:

$$\mathcal{E}=\int_{t_0}^{t_1}(u_1^2+u_2^2)dt, \tag{21}$$

instead of the length ℓ (20). Indeed a curve minimizes the cost $\mathcal{E}$ among all curves joining the points q_0 and q_1 in time t_1-t_0 if:

(a) it minimizes the length ℓ among all curves joining q_0 to q_1, and
(b) it is a curve parametrized by a multiple of the arclength.

Once we have a curve minimizing $\mathcal{E}$, we can then change the parametrization to have derivatives of controls as small as required.

Remark 7: Notice that, if we do not fix the time, the minimum of the cost $\mathcal{E}$ is zero and it is not attained.

2. Minimizing the time

Reparametrizing the geodesics of the control system (19), (20) by the arclength, i.e., setting

$$\mathrm{d}s=\sqrt{u_1^2+u_2^2}\mathrm{d}t,$$

we get the control problem:

$$\dot{\mathbf{x}}=u_1F_1+u_2F_2, \quad u_1^2+u_2^2=1, \tag{22}$$

and the question is to minimize the transfer time, from the initial to the terminal condition.

Taking into account the homogeneity of the problem (22), it is clear that it is the same as to minimize the transfer time for the system $\dot{\mathbf{x}}=u_1F_1+u_2F_2$, with the constraint

$$u_1^2+u_2^2\leqslant 1.$$

It follows that, for the control system (19), the problem of minimizing the cost (20), using a parametrization with arclength [that is using the cost (21), with t_1-t_0 equal to the total length], is equivalent to minimizing the time under the constraint on the controls $u_1^2+u_2^2\leqslant 1$.

Remark 8: Notice that the transformation on the controls necessary to eliminate the drift does not affect the conditions $u_1^2+u_2^2\leqslant 1$, $u_1^2+u_2^2=1$.

Remark 9: The problem of minimizing the transfer time for the system (19) under the constraint $u_1^2+u_2^2\leqslant 1$, makes sense by itself. However, notice that if we drop the condition $u_1^2+u_2^2\leqslant 1$, then by the Hermann–Nagano theorem, the minimizing time between any two initial and terminal conditions is zero.

In a recent article[12] some related questions in the control of spin systems were discussed. The problem is, however, distinctly different from the ones considered here. The authors also consider a quantum system with a drift:

$$\dot{\mathbf{x}}=X_0(\mathbf{x})+\sum_{i=1}^{p} u_iX_i(\mathbf{x}),$$

left invariant on some compact group G. But, in their case, all vector fields $X_i(x)$ belong to $\mathbf{k}$, a Lie subalgebra of the Lie algebra $\mathbf{g}$ of G. They consider a Cartan decomposition $\mathbf{g}=\mathbf{k}\oplus\mathbf{p}$, with the standard Cartan's commutation relations, and hence, the Lie algebra generated by the X_i's, $i>1$, is not equal to $\mathbf{g}$ (it is only $\mathbf{k}$). Therefore in their case, to move from a point in a coset $K\cdot x_0$ to another point in a coset $K\cdot x_1$ requires the use of the drift X_0 and hence requires a bounded speed.

This implies that, in their case, even for unbounded controls there is a minimum time, which is strictly larger than zero (and not attained in general). As mentioned previously, if we relax the constraint $u_1^2+u_2^2\leqslant 1$, in our case, the minimum time is zero (also not attained in general).

3. Conclusions on the choice of the costs

There are three costs under consideration:

(a) The length (20). In the two–level case it is the sub-Riemannian length and coincides with the integral of the absolute value of the amplitude. In the three-level case it is a singular-Riemannian length.
(b) The fluence (21), for fixed transfer time t_1-t_0.
(c) The time under the constraint $u_1^2+u_2^2\leqslant 1$.

Only the first of these costs is parametrization invariant, but all cases (a), (b), (c) lead to the same trajectories in the phase space.

III. THE TWO-LEVEL SYSTEM

In this section, we study a two-level quantum system in interaction with a laser for which we control both the amplitude and the phase. The Hamiltonian becomes after elimination of the drift

$$H=\begin{pmatrix} 0 & u(t) \\ u^*(t) & 0 \end{pmatrix}. \tag{23}$$

Our aim is to transfer all the population from level E_1 to level E_2 minimizing (here we set $t_0=0$)

$$\int_0^{t_1}|\Omega(t)|\mathrm{d}t=\int_0^{t_1}|u(t)|\mathrm{d}t. \tag{24}$$

Writing $\psi(t)=c_1(t)\varphi_1+c_2(t)\varphi_2$, where $\varphi_1=(1,0)$, $\varphi_2=(0,1)$, we start from any point satisfying $|c_1(0)|^2=1$, and our target is defined by $|c_2(t_1)|^2=1$.

Remark 10: This new Hamiltonian clearly gives rise to a driftless (or ''distributional'') control system, while the original Hamiltonian (2) had a drift term. Notice that since we have assumed $\Omega\in\mathbb{C}$, this simplification works without any additional hypothesis on Ω. The fact that the optimal strategy has the laser in resonance [i.e., $\Omega(t)=b(t)e^{i[\omega t+\alpha]}$, $\omega=E_2-E_1$, $\alpha\in\mathbb{R}$, $b(.)$ real function] will be obtained as a consequence.

The Schrödinger equation corresponding to the Hamiltonian given by formula (23) is equivalent to the system of ordinary differential equations (ODE) for the c_i's:

$$\begin{cases} \dot{c}_1=-iu(t)c_2, \\ \dot{c}_2=-iu^*(t)c_1. \end{cases} \tag{25}$$

Setting $c_1=x_1+ix_2$, $c_2=x_3+ix_4$, $u=u_1+iu_2$, Eq. (25) becomes

$$\dot{\mathbf{x}}=u_1F_1+u_2F_2,$$

where

$$\mathbf{x}=\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}, \quad F_1=\begin{pmatrix} x_4 \\ -x_3 \\ x_2 \\ -x_1 \end{pmatrix}, \quad F_2=\begin{pmatrix} x_3 \\ x_4 \\ -x_1 \\ -x_2 \end{pmatrix}. \tag{26}$$

and the functional (24) to be minimized is now

$$\int_0^{t_1}\sqrt{u_1^2+u_2^2}\mathrm{d}t. \tag{27}$$

In these new variables the condition $|c_1(t)|^2+|c_2(t)|^2=1$ is $\Sigma_{i=1}^4 x_i^2(t)=1$, so in fact $\mathbf{x}\in S^3$. The initial condition is now one point on the circle $S^1_{in}:=\{\mathbf{x}\in S^3\colon x_1^2+x_2^2=1\}$ and the target is the circle $S^1_{\text{fin}}:=\{\mathbf{x}\in S^3\colon x_3^2+x_4^2=1\}$. These targets are preserved by the transformations eliminating the drift. The problem of minimizing (27) is a classical sub-Riemannian problem on S^3, which is contact, as we shall see immediately.

The Lie algebra of the distribution. Let us compute the Lie algebra of the distribution. By setting $F_3=[F_1,F_2]$, we have

$$F_3=2\begin{pmatrix} x_2\\ -x_1\\ -x_4\\ x_3\end{pmatrix} \quad \text{and} \quad \begin{cases} [F_1,F_2]=F_3,\\ [F_2,F_3]=4F_1,\\ [F_3,F_1]=4F_2,\end{cases} \quad \text{so Lie}(\mathcal{F})=su(2)\sim so(3). \tag{28}$$

A. Controllability and minimizers

Let $\mathcal{F}:=\{F_1,F_2\}$. Since $\mathcal{F}$ is an analytic family of vector fields on an analytic manifold, we can use the Hermann–Nagano theorem (see Sec. I). In this case, $\text{Lie}_{\mathbf{x}_0}(\mathcal{F})$ is the vector space having $F_1(x)$, $F_2(x)$, and $F_3(x)$ as base vectors. The Hermann–Nagano theorem says that the orbit is an analytic submanifold of S^3 of dimension given by $\text{Lie}_{\mathbf{x}}(\mathcal{F})$, where $\mathbf{x}$ is any point of the orbit. Let $n(\mathbf{x}),\mathbf{x}\in S^3$ be the rank of the distribution. We have:

$$n(\mathbf{x}):=\text{rank}_{\mathbf{x}}(F_1,F_2,F_3)=\text{rank}_{\mathbf{x}}\begin{pmatrix} x_4 & x_3 & 2x_2\\ -x_3 & x_4 & -2x_1\\ x_2 & -x_1 & -2x_4\\ -x_1 & -x_2 & 2x_3\end{pmatrix}=3.$$

It follows:

Proposition 1: The control system (26) is completely controllable.

Remark 11: This controllability property, using only the first bracket, is equivalent, in the three-dimensional case, to the fact that the distribution is contact.

Remark 12: The sub-Riemannian problem is not generic at all: first as we shall see, it is isoperimetric (it has a symmetry). Second, even among isoperimetric sub-Riemannian problems, it is non generic in the sense that the main basic sub-Riemannian invariant vanishes (see Refs. 19, 23, and 24).

Remark 13: The control system (26) is invariant under the following transformation:

$$\begin{pmatrix} x_1\\ x_2\\ x_3\\ x_4\end{pmatrix}\to\begin{pmatrix} \cos(\alpha) & \sin(\alpha) & 0 & 0\\ -\sin(\alpha) & \cos(\alpha) & 0 & 0\\ 0 & 0 & \cos(\alpha) & \sin(\alpha)\\ 0 & 0 & -\sin(\alpha) & \cos(\alpha)\end{pmatrix}\begin{pmatrix} x_1\\ x_2\\ x_3\\ x_4\end{pmatrix}. \tag{29}$$

This means that all the initial conditions $\mathbf{x}_0\in S_{\text{in}}$ are equivalent. Notice that transformation (29) is generated by the Lie bracket $[F_1,F_2]=F_3$.

Minimizing geodesics. We will be able to find optimal trajectories joining our boundary conditions without making any computation. In fact F_1 and F_2 are two orthogonal vectors for the standard metric of S^3:

$$F_1\cdot F_2=\sum_{i=1}^4 (F_1)_i(F_2)_i=0.$$

Hence, the length of an admissible curve is just its standard Riemannian length on S^3. Therefore, if we find an admissible trajectory going from state 1 to state 2, which is a minimizing geodesic

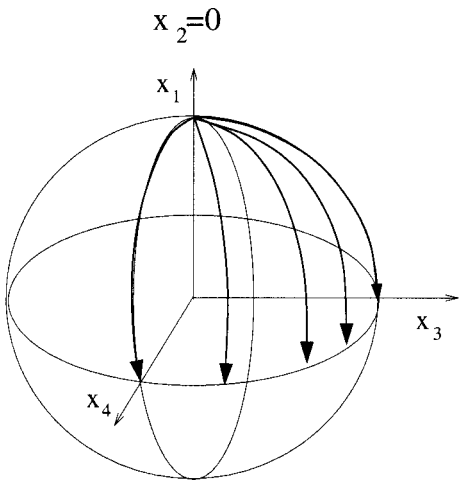

FIG. 1. The sphere S^3 and the geodesics from $x_1=1$ in the space $x_2=0$.

for the Riemannian metric on S^3, then it is also a minimizer for our sub-Riemannian problem. Now, each integral curve of the vector field $b(\cos(\alpha)F_1+\sin(\alpha)F_2)$ $(b\in\mathbb{R},\alpha\in[0,2\pi])$ are such admissible trajectories. It follows that:

Theorem 1: *Every constant control of the form:*

$$\begin{cases} u_1=b\cos(\alpha) \\ u_2=b\sin(\alpha) \end{cases}, \quad b\in\mathbb{R}, \quad \alpha\in[0,2\pi] \tag{30}$$

is optimal and the target is reached at time $t_1=(\pi/2)(1/b)$. *Moreover if* $\mathbf{x}_0\in S_{\text{in}}$ *is defined by* $x_1=\cos(\beta)$, $x_2=\sin(\beta)$, *then the equations of the geodesics corresponding to the controls (30) are:*

$$\begin{cases} x_1=\cos(\beta)\cos(bt), \\ x_2=\sin(\beta)\cos(bt), \\ x_3=-\sin(\alpha-\beta)\sin(bt), \\ x_4=-\cos(\alpha-\beta)\sin(bt). \end{cases} \tag{31}$$

The second part of Theorem 1 is easily checked.

Now since the functional (27) is invariant under time reparametrizations, one can take b to be a function of the time so that every optimal control has the form given by

$$\Omega(t)=b(t)e^{i[(E_2-E_1)t+\alpha]},$$

where α is an arbitrary constant, $b(.):\mathbb{R}\to\mathbb{R}^+$ is a real function with compact support $[0,t_1]$ and satisfying $\int_0^{t_1} b(t)=\pi/2$. In Fig. 1 are shown the geodesics issued from the point $x_1=1$ in the space $x_2=0$.

B. Another interpretation: The Hopf fibration and the Isoarea problem

The Hopf fibration (see, e.g., Ref. 18), $\pi:S^3\to S^2$ is defined by the following map. Let S^3 be described by the variables (x_1,x_2,x_3,x_4), $\Sigma x_i^2=1$ and S^2 by the variables (z_1,z_2,z_3), $\Sigma z_i^2=1/4$. We have:

$$(z_1,z_2,z_3)=\pi(x_1,x_2,x_3,x_4):=(\tfrac{1}{2}(x_1^2+x_2^2-x_3^2-x_4^2),x_1x_3-x_2x_4,x_2x_3+x_1x_4). \tag{32}$$

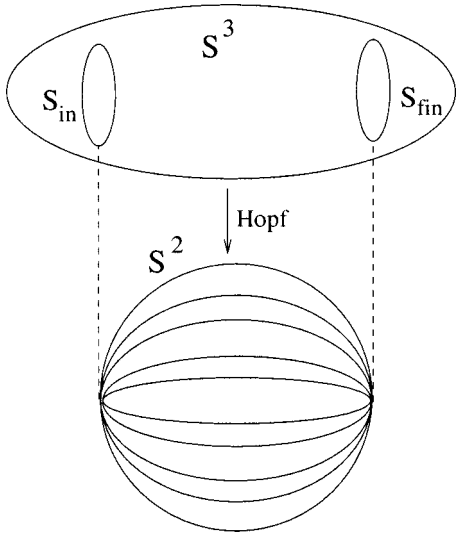

FIG. 2. Schematic representation of the Hopf fibration $\pi: S^3 \to S^2$. The geodesics given by Theorem 1 are also drawn.

The Hopf fibration gives to S^3 the structure of a principal bundle with base S^2 and fiber $S^1 \sim U(1)$. The following proposition (that one easily checks) shows why the Hopf fibration is connected to our problem:

Proposition 2: Let $F_3 := [F_1, F_2]$ *[see formula (28)], and* π *the Hopf fibration defined above. Then* $F_3 \in Ker(d\pi)$.

Notice that F_3 is the generator of the symmetry that "transports" along S_{in} and S_{fin} (cf. Remark 13) that means the following. If $\mathbf{x}_0 \in S_{\text{in}}$ (respectively, $\mathbf{x}_0 \in S_{\text{fin}}$) then the orbit $\mathcal{O}(x_0)$ of F_3 coincides with S_{in} (respectively, S_{fin}). From Proposition 2 it follows that S_{in} and S_{fin} shrink into two points through π. In particular these points are, respectively, the opposite points $(z_1, z_2, z_3) = (\pm \frac{1}{2}, 0, 0)$. The situation is illustrated by Fig. 2. Notice that we have a one parameter family of geodesics connecting S_{in} and S_{fin}, since their images under π are opposite points on S^2.

In fact, the sub-Riemannian problem we have, is as follows: The distribution (transversal to the fibers of the Hopf fibration) defines a connection over this (circle) principal bundle. It is easily seen that the curvature form of this connection is just the pull back (by the bundle projection) of the volume form of the Euclidean metric on S^2.

As a consequence (see Ref. 19), our sub-Riemannian problem corresponds to the "isoarea problem" on the Riemannian sphere S^2: given two points (antipodal on S^2 in our case), and any fixed curve $x(.)$ joining these two points, find another curve $y(.)$, joining also the two points, such that the length of $y(.)$ is minimal, and the area encircled by the curves $x(.), y(.)$ has a given value.

Corollary: There is no other minimizing curve [than the circle (31)] joining S_{in} and S_{fin}.

Proof: Assume that $\gamma: [0, t_1] \to S^3$ is such a minimizing curve. Then it has length $\pi/2$, and its projection on S^2 is one of the circles in Fig. 2. Now each of these circles is lifted in a unique way, via the connection, in one of the curves (31), once the initial point is chosen in S_{in}. Hence γ is one of the circles (31). ■

Our (very special) solutions exhibited previously are in fact geodesics of the Euclidean metric on S^2: they correspond to the choice of geodesics for the curve $x(.)$, and to the zero value of the area.

IV. THE THREE-LEVEL RESONANT PROBLEM

Statement of the Problem. In this section, we study a three-level quantum system, with only neighboring levels coupled, controlled by two laser pulses in resonance, i.e., with frequencies $\omega_1 = E_2 - E_1$, $\omega_2 = E_3 - E_2$; E_1, E_2, E_3 being the three energy levels.

The aim is to transfer all the population from the state with energy E_1 to the state with energy E_3 minimizing (again we set $t_0=0$)

$$\int_0^{t_1}\sqrt{u_1^2+u_2^2}\mathrm{d}t. \tag{33}$$

Writing $\psi(t)=c_1(t)\varphi_1+c_2(t)\varphi_2+c_3(t)\varphi_3$, where $\varphi_1=(1,0,0)$, $\varphi_2=(0,1,0)$, $\varphi_3=(0,0,1)$, we start from one point satisfying $|c_1(0)|^2=1$, and our target is defined by $|c_3(t_1)|^2=1$.

Remark 14: As in Sec. III, this new Hamiltonian gives rise to a driftless autonomous control system, while the control system corresponding to the old Hamiltonian (6) was time dependent and with drift. But in this case (i.e., with real controls), to obtain this strong simplification it is essential to use lasers in resonance.

The Control System. The Schrödinger equation corresponding to the Hamiltonian given by formula (15) is equivalent to the system of ODE for the c_i:

$$\begin{cases}\dot c_1=-iu_1(t)c_2,\\ \dot c_2=-i(u_1(t)c_1+u_2(t)c_3),\\ \dot c_3=-iu_2(t)c_2.\end{cases} \tag{34}$$

Setting $c_1=x_1+ix_2$, $c_2=x_4-ix_3$, $c_3=x_5+ix_6$, Eq. (34) becomes

$$\dot{\mathbf{x}}=u_1F_1+u_2F_2$$

where

$$x=\begin{pmatrix}x_1\\x_2\\x_3\\x_4\\x_5\\x_6\end{pmatrix},\quad F_1=\begin{pmatrix}-x_3\\-x_4\\x_1\\x_2\\0\\0\end{pmatrix},\quad F_2=\begin{pmatrix}0\\0\\x_5\\x_6\\-x_3\\-x_4\end{pmatrix}. \tag{35}$$

Here, the notations are such that the real parts (respectively, imaginary parts) of c_1,c_2,c_3 are x_1,x_4,x_5 (respectively $x_2,-x_3,x_6$). This convention will be very convenient later on.

In these new variables the condition $|c_1(t)|^2+|c_2(t)|^2+|c_3(t)|^2=1$ is $\Sigma_{i=1}^6x_i^2(t)=1$, so in fact $\mathbf{x}\in S^5$. The initial condition is now one point on the circle $S^1_{\text{in}}:=\{\mathbf{x}\in S^5: x_1^2+x_2^2=1\}$ and the target is $S^1_{\text{fin}}:=\{\mathbf{x}\in S^5: x_5^2+x_6^2=1\}$. With the choice (33) of the functional to be minimized, our problem looks like a classical sub-Riemannian problem on S^5, but, as we shall see, it is very degenerate.

The Lie algebra of the distribution. Let us compute the Lie algebra of the distribution. By setting $F_3=[F_1,F_2]$, we have

$$F_3=\begin{pmatrix}x_5\\x_6\\0\\0\\-x_1\\-x_2\end{pmatrix},\quad \begin{cases}[F_1,F_2]=F_3,\\ [F_2,F_3]=F_1,\\ [F_3,F_1]=F_2,\end{cases}$$

so $\mathrm{Lie}(\mathcal{F})=su(2)\sim so(3)$.

A. General properties of the orbit

Let $n(\mathbf{x})$, $\mathbf{x}\in S^5$ be the rank of the distribution. We have

$$n(\mathbf{x}):=\mathrm{rank}_{\mathbf{x}}(F_1,F_2,F_3)=\mathrm{rank}_{\mathbf{x}}\begin{pmatrix} -x_3 & 0 & x_5 \\ -x_4 & 0 & x_6 \\ x_1 & x_5 & 0 \\ x_2 & x_6 & 0 \\ 0 & -x_3 & -x_1 \\ 0 & -x_4 & -x_2 \end{pmatrix}=\begin{cases} 2 & \text{if } \mathbf{x}\in Q \\ 3 & \text{if } \mathbf{x}\in S^5\backslash Q, \end{cases} \tag{36}$$

where Q is the subset of S^5 defined by

$$x_3x_6-x_4x_5=0, \tag{37}$$

$$x_1x_6-x_2x_5=0, \tag{38}$$

$$x_3x_2-x_4x_1=0. \tag{39}$$

Notice that if x_1,x_3,x_5 are all different from zero, Eqs. (37), (38), and (39) are equivalent to

$$\frac{x_2}{x_1}=\frac{x_4}{x_3}=\frac{x_6}{x_5}. \tag{40}$$

Now since every initial condition lies in Q (i.e., $S^1_{\mathrm{in}}\in Q$), from the Hermann–Nagano theorem it follows:

Proposition 3: For each $\mathbf{x}_0\in S^1_{\mathrm{in}}$, *the orbit* $\mathcal{O}(\mathbf{x}_0)$ *is an analytic two-dimensional submanifold of* S^5.

More precisely defining $\mathbf{x}_0(\alpha)$ as the initial condition corresponding to

$$\begin{cases} x_1(0)=\cos(\alpha), \\ x_2(0)=\sin(\alpha), \end{cases} \tag{41}$$

where $\alpha\in[0,2\pi[$, we get the following:

Theorem 2: *The orbit* $O(\mathbf{x}_0(\alpha))$, $\alpha\in[0,2\pi[$ *is the two-dimensional sphere of equation* $x'^2_1+x'^2_3+x'^2_5=1$ *where*

$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \\ x_4' \\ x_5' \\ x_6' \end{pmatrix}=\begin{pmatrix} \cos(\alpha) & \sin(\alpha) & 0 & 0 & 0 & 0 \\ -\sin(\alpha) & \cos(\alpha) & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos(\alpha) & \sin(\alpha) & 0 & 0 \\ 0 & 0 & -\sin(\alpha) & \cos(\alpha) & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos(\alpha) & \sin(\alpha) \\ 0 & 0 & 0 & 0 & -\sin(\alpha) & \cos(\alpha) \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix}. \tag{42}$$

Proof: Assume first $\alpha=0$. This means that the initial condition is defined by $x_1(0)=1$ and the variables with the prime coincide with those without the prime.

In Eq. (35) the variables x_1,x_3,x_5 are decoupled from the other (in fact, we have a product system, of two subsystems on $\mathbb{R}^3$). It follows $\mathcal{O}(\mathbf{x}_0(\alpha))\subset\{\mathbf{x}\in S^5: x_1^2+x_3^2+x_5^2=1\}$. But all the points of this sphere belong to the orbit since they can be reached by using a control of the form:

$$(u_1(t),u_2(t))=\begin{cases} (1,0) & \text{for } t\in[0,t_a] \\ (0,1) & \text{for } t\in[t_a,t_b] \end{cases}$$

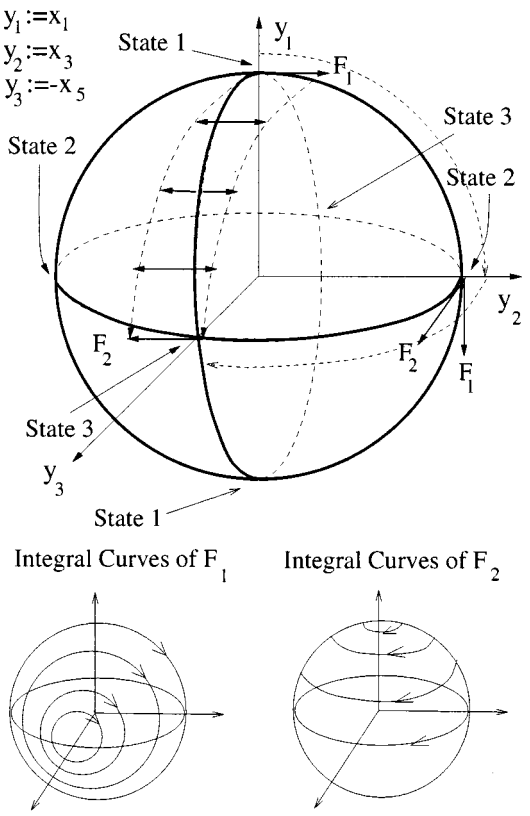

FIG. 3. The vector fields F_1 and F_2 on the sphere.

for some $t_a, t_b > 0$. In fact, in the (x_1, x_3, x_5) space, each integral curve of F_1 (respectively, F_2) is a circle that lies in the plane $x_5 = \text{const}$ (respectively, $x_1 = \text{const}$) and the center of which belongs to the x_5 (respectively, x_1) axis, see Fig. 3. At time t_a one reaches the point:

$$\begin{cases} x_1(t_a) = \cos(t_a), \\ x_3(t_a) = \sin(t_a), . \\ x_5(t_a) = 0. \end{cases}$$

At time t_b one reaches the point:

$$\begin{cases} x_1(t_b) = \cos(t_a), \\ x_3(t_b) = \sin(t_a)\cos(t_b), \\ x_5(t_b) = -\sin(t_b). \end{cases}$$

So all the points of the sphere $x_1^2 + x_3^2 + x_5^2 = 1$ can be reached for suitable t_a and t_b. The Theorem is proved for $\alpha = 0$.

Assume now that we start from the point $\mathbf{x}_0(\alpha)$ for an arbitrary α. Making the change of coordinates given by formula (42), one is back to the situation $\alpha = 0$ for the variables with the prime. This concludes the proof. ■

Notice that, for fixed $\mathbf{x}_0(\alpha)$, one can reach only two points of the final target. For instance if $\alpha = 0$, i.e., $x_1(0) = 1$, we can reach S^1_{fin} only in the two points $x_5 = \pm 1$. The situation is illustrated by Fig. 4.

More precisely as a consequence of the symmetry given by formula (42) we have the following:

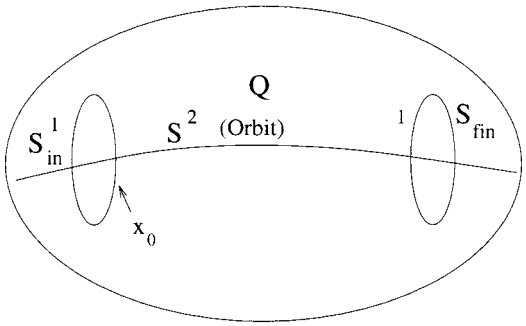

FIG. 4. The foliation of Q.

Corollary of Theorem 2: Fix $\alpha\in[0,2\pi]$, *let* $\mathbf{x}=(x_1,\ldots,x_6)\in\mathcal{O}(\mathbf{x}_0(\alpha))$, *and define* $\alpha_{12}(\mathbf{x})$, $\alpha_{34}(\mathbf{x})$, $\alpha_{56}(\mathbf{x})$ *to be the angles (illustrated in Fig. 5) such that*

$$\begin{cases} x_1=\sqrt{x_1^2+x_2^2}\cos(\alpha_{12}(\mathbf{x})),\\ x_2=\sqrt{x_1^2+x_2^2}\sin(\alpha_{12}(\mathbf{x})),\end{cases}$$

$$\begin{cases} x_3=\sqrt{x_3^2+x_4^2}\cos(\alpha_{34}(\mathbf{x})),\\ x_4=\sqrt{x_3^2+x_4^2}\sin(\alpha_{34}(\mathbf{x})),\end{cases}$$

$$\begin{cases} x_5=\sqrt{x_5^2+x_6^2}\cos(\alpha_{56}(\mathbf{x})),\\ x_6=\sqrt{x_5^2+x_6^2}\sin(\alpha_{56}(\mathbf{x})).\end{cases}$$

Then, for each such $\mathbf{x}$, *there exist* $n_{12}(\mathbf{x}),n_{34}(\mathbf{x}),n_{56}(\mathbf{x})\in\{0,\pm1\}$ *such that*

$$\alpha_{12}(\mathbf{x})=\alpha\pm n_{12}\pi \quad \textit{if} \quad \alpha_{12} \textit{ is defined } (\textit{i.e., } x_1,x_2 \textit{ not both vanishing}), \tag{43}$$

$$\alpha_{34}(\mathbf{x})=\alpha\pm n_{34}\pi \quad \textit{if} \quad \alpha_{34} \textit{ is defined } (\textit{i.e., } x_3,x_4 \textit{ not both vanishing}), \tag{44}$$

$$\alpha_{56}(\mathbf{x})=\alpha\pm n_{56}\pi \quad \textit{if} \quad \alpha_{56} \textit{ is defined } (\textit{i.e., } x_5,x_6 \textit{ not both vanishing}). \tag{45}$$

Moreover at least one of the three angles $\alpha_{12},\alpha_{34},\alpha_{56}$ *is defined.*

The Structure of Q. Let us now study the structure of Q. From the Hermann–Nagano theorem we have

$$Q\supseteq\bigcup_{\mathbf{x}_0\in S^1_{\text{in}}}\mathcal{O}_{\mathbf{x}_0}$$

but in fact this equation holds with equality as a consequence of the fact that relations (37), (38), and (39) defining Q are equivalent to Eqs. (43), (44), (45), that hold on the orbit. More precisely let $\overline{\mathbf{x}}=(\overline{x_1},\ldots,\overline{x_6})$ be a point of Q and $\overline{\alpha}$ the angle between $\overline{x_1}$ and $\overline{x_2}$ measured counterclockwise, if defined. If not $\overline{\alpha}$ will be the angle between the variables $\overline{x_3}$ and $\overline{x_4}$, or between the

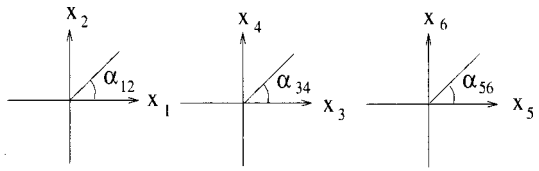

FIG. 5. The definition of the angles $\alpha_{12}(\mathbf{x})$, $\alpha_{34}(\mathbf{x})$, $\alpha_{56}(\mathbf{x})$.

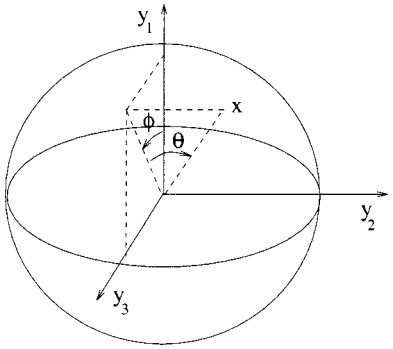

FIG. 6. The angles θ and ϕ.

variables $\overline{x_5}$ and $\overline{x_6}$ (in the spirit of the Corollary of Theorem 2). Because of (40), $\overline{\alpha}$ can be actually defined in this way. One clearly has $\overline{x} \in \mathcal{O}(\mathbf{x}_0(\overline{\alpha}))$. Hence we have proved the following:

Proposition 4: We have $Q = \cup_{\mathbf{x}_0 \in S^1_{\text{in}}} \mathcal{O}_{\mathbf{x}_0}$.

Let σ be the antipodal involution of $S^1 \times S^2$, that is, $\sigma(\alpha, p) = (\alpha + \pi, -p)$. The involution σ has no fixed point, and is orientation reversing. Also, clearly, by Theorem 2, our orbits are σ stable. Hence: $Q = (S^1 \times S^2)/\sim$ where $\mathbf{x} \sim \mathbf{x}'$ if $\sigma(x) = \sigma(\mathbf{x}')$. Therefore, it is not hard to see that:

Theorem 3: *Q is the (only) nonorientable sphere-bundle over* S^1.

B. Geodesic equations on the sphere

Due to the invariance under the transformation (42) all the points of S_{in} can be considered equivalently. In the following we will study the optimal control problem on the orbit $\mathcal{O}(\mathbf{x}_0)$, where $\mathbf{x}_0$ is defined by $x_1 = 1$. Then $\mathcal{O}(\mathbf{x}_0)$ is the sphere of equation $x_1^2 + x_3^2 + x_5^2 = 1$. In what follows, we will keep the notation F_1 and F_2 for the restrictions of F_1 and F_2 to this sphere.

In order to get labels for coordinates corresponding to quantum states, and in order to have F_2 pointing in the positive direction from the point $x_3 = 1$, we define $y_1 = x_1$, $y_2 = x_3$, $y_3 = -x_5$. The control system under consideration is then

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = u_1 F_1 + u_2 F_2,$$

where

$$F_1 = \begin{pmatrix} -y_2 \\ y_1 \\ 0 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 0 \\ -y_3 \\ y_2 \end{pmatrix}.$$

The vector fields are plotted in Fig. 3. The initial condition is the point $y_1 = 1$. The state number 1 (respectively, 2, 3) correspond to the points $y_1 = \pm 1$ (respectively, $y_2 = \pm 1$, $y_3 = \pm 1$). State 2 can be reached from state 1 using only F_1 and state 3 can be reached from state 2 using only F_2 (dotted lines). However, state 3 cannot be reached from state 1 using a trajectory contained in the circle of equation:

$$y_2 = 0 \quad (\text{i.e., } y_1^2 + y_3^2 = 1), \tag{46}$$

since no piece of this circle is an admissible trajectory. This is due to the fact that F_1 is collinear to F_2 on the circle (46), and not tangent to this circle.

A new orthogonal frame. Let us describe the orbit in spherical coordinates (see Fig. 6):

$$\begin{cases} y_1 = \cos(\theta)\cos(\phi), \\ y_2 = \sin(\theta), \\ y_3 = \cos(\theta)\sin(\phi). \end{cases} \tag{47}$$

We have

$$\begin{pmatrix} F_1 \\ F_2 \end{pmatrix} = R \begin{pmatrix} G_1 \\ G_2 \end{pmatrix},$$

where

$$R := \begin{pmatrix} \cos(\phi) & \sin(\phi) \\ -\sin(\phi) & \cos(\phi) \end{pmatrix}, \quad \begin{cases} G_1 = \partial_\theta \\ G_2 = \tan(\theta)\partial_\phi . \end{cases}$$

Since $R \in \mathrm{SO}(2)$, the couple (G_1, G_2) is a new orthonormal frame for the singular-Riemannian length. For this new frame the control system is then

$$\begin{pmatrix} \dot{\theta} \\ \dot{\phi} \end{pmatrix} = v_1 G_1 + v_2 G_2, \tag{48}$$

and the functional to be minimized is $\int_0^{t_1} \sqrt{v_1^2 + v_2^2}\,dt$. The relation between u_1, u_2 and v_1, v_2 is obtained from $u_1 F_1 + u_2 F_2 \equiv v_1 G_1 + v_2 G_2$:

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = R \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}. \tag{49}$$

The metric defined by the frame (G_1, G_2) is a singular metric. Indeed when $\theta = 0$ we have $G_2 = 0$, that is exactly on the circle (46). Notice that the singularity of the metric for $\theta = \pi/2$ is only due to the choice of the coordinates system.

The Hamiltonian. Let us compute the geodesics using the Maximum Principle. Here, for standard reasons, we use as cost the fluence (21). The final time is fixed by requiring the parametrization by arclength that is $v_1^2 + v_2^2 = 1$ (this means to normalize $\mathcal{H}_M = 1/2$, see the Pontryagin Maximum Principle in Sec. I for the definition of $\mathcal{H}_M$). Notice that from formula (49) we have

$$v_1^2 + v_2^2 = u_1^2 + u_2^2.$$

As explained in Sec. II C 2 this corresponds to minimizing the time under the constraint $u_1^2 + u_2^2 \leqslant 1$. Let $P = (P_\theta, P_\phi) \in T^*_{\theta,\phi} M$. By definition the Hamiltonian is

$$\begin{aligned} \mathcal{H}(\theta, \phi, P_\theta, P_\phi, v_1, v_2) &= \langle P, v_1 G_1 + v_2 G_2 \rangle + p_0 (v_1^2 + v_2^2) \\ &= v_1 P_\theta + v_2 P_\phi \tan(\theta) + p_0 (v_1^2 + v_2^2). \end{aligned} \tag{50}$$

It is easily checked that, as for the Riemannian case, we can always assume $p_0 \neq 0$ (there are no abnormal extremals) and we can normalize $p_0 = -\frac{1}{2}$. Extremal controls are computed from the maximum condition:

$$\frac{\partial \mathcal{H}}{\partial v_1} = 0, \quad \frac{\partial \mathcal{H}}{\partial v_2} = 0, \quad \Rightarrow v_1 = P_\theta, \quad v_2 = P_\phi \tan(\theta). \tag{51}$$

Hence, we obtain that the extremals are projections on the (θ, ϕ) space of integral curves of the Hamiltonian vector field corresponding to the following Hamiltonian:

$$\mathcal{H}_M = \tfrac{1}{2} (P_\theta^2 + (\tan(\theta) P_\phi)^2). \tag{52}$$

The Hamiltonian equations are

$$\dot{\theta}=\frac{\partial \mathcal{H}_M}{\partial P_\theta}=P_\theta,$$

$$\dot{\phi}=\frac{\partial \mathcal{H}_M}{\partial P_\phi}=P_\phi \tan^2(\theta),$$

$$\dot{P}_\theta=-\frac{\partial \mathcal{H}_M}{\partial \theta}=-P_\phi^2 \tan(\theta)(1+\tan^2(\theta)),$$

$$\dot{P}_\phi=-\frac{\partial \mathcal{H}_M}{\partial \phi}=0.$$

Setting $a:=P_\phi$ finally we have

$$\dot{\theta}=P_\theta, \quad \dot{\phi}=a\tan^2(\theta), \quad \dot{P}_\theta=-a^2\tan(\theta)(1+\tan^2(\theta)). \tag{53}$$

This Hamiltonian system is Liouville integrable since we have two independent and commuting constants of the motion $\mathcal{H}_M$ and $P_\phi=a$.

1. Minimizing the length

Let us find the geodesic without the parametrization, i.e., a relation between θ and ϕ. We have

$$\frac{d\phi}{d\theta}=\frac{\dot{\phi}}{\dot{\theta}}=\frac{\dot{\phi}}{P_\theta}=\pm\frac{a\tan^2(\theta)}{\sqrt{1-a^2\tan^2(\theta)}}, \tag{54}$$

where we have expressed P_θ using relation (52) and normalized $\mathcal{H}_M=1/2$. So we have the two families of solutions parametrized by the value of a:

$$\begin{aligned}\phi_a^{\pm}(\theta)&=\pm\int_0^\theta \frac{a\tan^2(s)}{\sqrt{1-a^2\tan^2(s)}}ds\\ &=\pm\left[\arctan\left(\frac{a}{\Xi(\theta,a)}\sin(\theta)\right)-\frac{a}{\sqrt{1+a^2}}\arctan\left(\frac{\sqrt{1+a^2}}{\Xi(\theta,a)}\sin(\theta)\right)\right],\end{aligned} \tag{55}$$

where $\Xi(\theta,a):=\sqrt{\frac{1}{2}(1-a^2+(1+a^2)\cos(2\theta))}$.

To fix the ideas, let us consider only the family ϕ_a^+ with $a>0$ and suppose $\theta\geqslant 0$, the other cases being symmetric. Let us call this family $\phi_a(\theta)$. Expression (55) defines $\phi_a(\theta)$ in the interval $[0,\overline{\theta}_a[$ where $\overline{\theta}_a$ is the value of θ at which the denominator of formula (54) vanishes:

$$\overline{\theta}_a:=\arctan\left(\frac{1}{a}\right). \tag{56}$$

Notice that $\lim_{\theta\to\overline{\theta}_a}\Xi[\theta,a]=0$ so

$$\lim_{\theta\to\overline{\theta}_a}\phi_a(\theta)=\frac{\pi}{2}\left(1-\frac{a}{\sqrt{1+a^2}}\right). \tag{57}$$

In the following we consider $\phi_a(\theta)$ defined in $[0,\overline{\theta}_a]$ where by definition $\phi_a(\overline{\theta}_a)$ is the value given by formula (57). Indeed, from the symmetries of the system, we have to consider two branches (illustred in Fig. 7) to describe the whole relation between θ and ϕ:

$$\phi_a^1(\theta)=\phi_a(\theta),$$

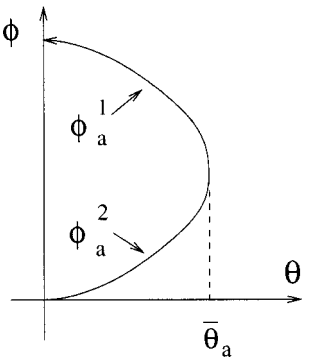

FIG. 7. The geodesic curve as a relation between θ and ϕ.

$$\phi_a^2(\theta)=2\phi_a(\overline{\theta}_a)-\phi_a(\theta).$$

The geodesic reaching the target is the one satisfying $\phi_a(\overline{\theta}_a)=\pi/4$. From Eq. (57) we get $a:=1/\sqrt{3}$.

Remark 15: By considering both signs in formula (55) (or equivalently a positive and negative) and $\theta\in[-\pi,\pi]$ one gets four equivalent optimal trajectories reaching the state 3 (see Fig. 8). Moreover the set of geodesics parametrized by a allows one to easily compute an optimal synthesis for the problem.

A smooth parametrization of the geodesic. To get an explicit expression of the controls (as function of the time) reaching the final point $\theta=0$, $\phi=\pi/2$, one should first fix a parametrization $\theta(t)$ in such a way that:

(1) $\theta(0)=\theta(t_1)=0$,

(2) for some $\overline{t}\in]0,t_1[$ it holds:

$$\begin{cases}\theta(\overline{t})=\overline{\theta}_{1/\sqrt{3}}=\pi/3,\\ \theta(t) \quad \text{is increasing for } t\in[0,\overline{t}],\\ \theta(t) \quad \text{is decreasing for } t\in[\overline{t},t_1].\end{cases}$$

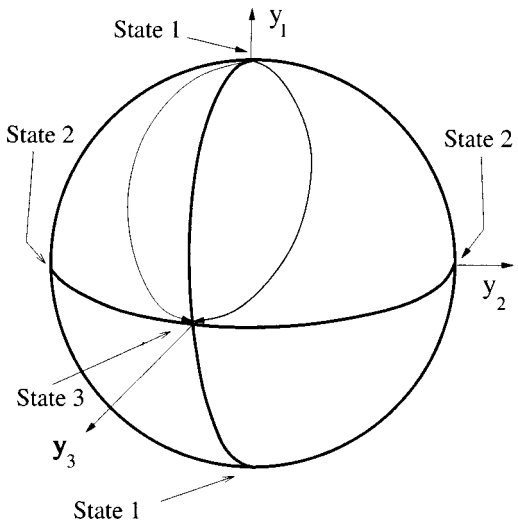

FIG. 8. The four geodesics reaching the state 3. Two are on the other side and reach the point $y_3=-1$.

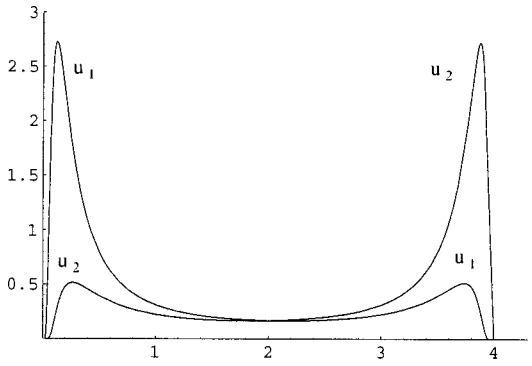

FIG. 9. Example 1: $\mathcal{C}^\infty$ optimal controls.

The best choice is of course a sufficiently regular symmetric function. In this case we have $\bar{t}=t_1/2$ and

$$\phi(t)=\begin{cases}\phi_{1/\sqrt{3}}(\theta(t)) & \text{if } t\in[0,t_1/2[,\\ 2\phi_{1/\sqrt{3}}(\theta(t_1/2))-\phi_{1/\sqrt{3}}(\theta(t_1-t)) & \text{if } t\in[t_1/2,t_1].\end{cases} \tag{58}$$

The controls $v_1(t)$ and $v_2(t)$ can be obtained from the relation $\dot{\theta}(t)\partial_\theta+\dot{\phi}(t)\partial_\phi=v_1(t)\partial_\theta+v_2(t)\tan(\theta(t))\partial_\phi$ from which we have

$$v_1(t)=\dot{\theta}(t),\quad v_2(t)=\frac{\dot{\phi}(t)}{\tan(\theta(t))}. \tag{59}$$

Remark 16: Notice that relations (59) coincide with relations (51) only in the case in which the curve $(\theta(t),\phi(t))$ is parametrized with constant velocity.

Finally the amplitudes of the lasers are obtained with formula (49).

Example 1: Consider the $\mathcal{C}^\infty$ function:

$$\theta(t)=\begin{cases}0 & \text{if } t<0 \text{ or } t>t_1\\ \dfrac{\pi}{3}e^{1/(t_1-t)(-t)} & \text{otherwise.}\end{cases} \tag{60}$$

The corresponding laser amplitudes $u_1(t)$ and $u_2(t)$ (for $t_1=4$) are shown in Fig. 9.

Example 2: Consider the function:

$$\theta(t)=\begin{cases}0 & \text{if } t<0 \text{ or } t>t_1\\ \dfrac{(-1+e^{-36t(t-t_1)/t_1^2})\pi}{3(-1+e^9)} & \text{otherwise.}\end{cases} \tag{61}$$

The corresponding laser amplitudes $u_1(t)$ and $u_2(t)$ (for $t_1=4$) are shown in Fig. 10.

2. Minimizing either the fluence or the time for constrained controls

To minimize the fluence, one should also get the parametrization from the Hamiltonian equations. From the equation (after fixing $a=1/\sqrt{3}$):

$$\dot{\theta}=P_\theta=\sqrt{1-a^2\tan^2(\theta)},$$

we have

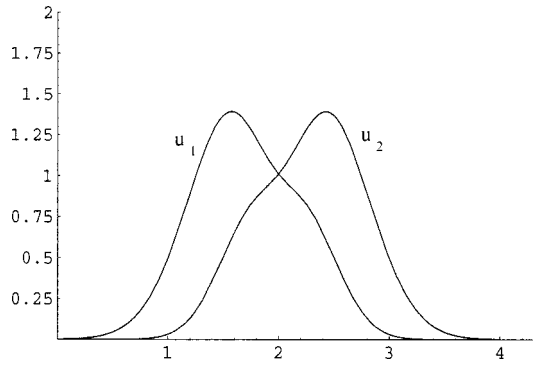

FIG. 10. Example 2: a possible choice of optimal controls.

$$t(\theta)=\frac{\arctan\left(\dfrac{2\sin(\theta)}{\sqrt{1+2\cos(2\theta)}}\right)\sqrt{1+2\cos(2\theta)}\sec(\theta)}{2\sqrt{1-\tan(\theta)^2/3}}.$$

Using the inverse function theorem, this formula permits one to describe $\theta(t)$ in the interval $[0,\bar{t}]$ where

$$\bar{t}:=\lim_{\theta\to\bar{\theta}_a} t(\theta)=\frac{\sqrt{3}}{4}\pi.$$

By symmetry this is exactly half of the final time. Finally $\dot{\phi}(t)$ can be obtained integrating the equation $\dot{\phi}(t)=a\ \tan^2(\theta(t))$. Controls $u_1(t)$ and $u_2(t)$ can be obtained with formulas (59) and (49) and they are shown in Fig. 11.

Remark 17: Notice that these controls are not smooth at $t=0$ and at the final time $2\bar{t}=(\sqrt{3}/2)\ \pi$.

From this analysis we get the values of the costs for the optimal trajectory:

Theorem 4: *For the three costs described in Sec. II C, the following relations hold.*

(a) Length:

$$\mathrm{Min}\left(\int_0^{t_1}\sqrt{u_1^2+u_2^2}\,\mathrm{d}t\right)=\frac{\sqrt{3}}{2}\pi.$$

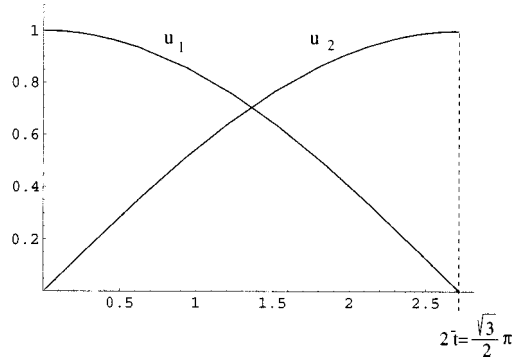

FIG. 11. Optimal controls minimizing fluence or time.

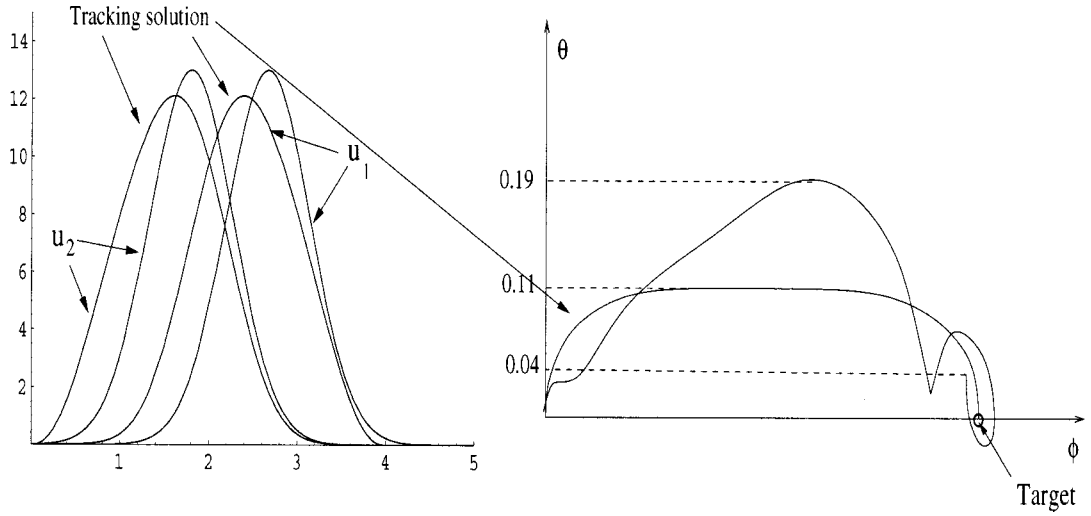

FIG. 12. Usual-adiabatic and tracking solutions.

(b) Fluence, with fixed transfer time T:

$$\mathrm{Min}\left(\int_0^T (u_1^2+u_2^2)\,\mathrm{d}t \right) = \frac{3}{4}\pi^2 \frac{1}{T}. \tag{62}$$

(c) Time under the constraint $u_1^2+u_2^2 \leqslant 1$,

$$T_{\min} = \frac{\sqrt{3}}{2}\pi. \tag{63}$$

V. THE TRACKING COUNTERINTUITIVE SOLUTIONS

For practical applications, trajectories joining state 1 to state 3, that take as small as possible the population of state 2 [i.e., with $\theta(t)$ closed to zero], are also interesting. We recall that the nonadmissible trajectory is contained in the circle (46). In this section we study a trajectory in which $\phi(t)$ is monotonously increasing between 0 and $\pi/2$, and

$$\theta(t) \leqslant \varepsilon, \quad \text{for every } t \in [0,t_1], \tag{64}$$

for some small $\varepsilon>0$ fixed. This means that the population in state 2 $[0,t_1]$ is always small, less or equal than $\sin^2(\varepsilon)=\varepsilon^2+O(\varepsilon^4)$ [see formula (47)].

It is well known[1,25] that the nonadmissible trajectory can be approximated using controls $u_1(t)$ and $u_2(t)$ in the so-called "counterintuitive" sequence: (see Fig. 12 for such a sequence). In the following we show how to build a trajectory satisfying condition (64) and connecting exactly the points P_1 defined by $(\phi,\theta)=(0,0)$ and P_2 defined by $(\phi,\theta)=(\pi/2,0)$.

The idea is to track a trajectory connecting these two points taking care of the constraints that we have on the derivatives at P_1 and P_2. More precisely we should find a function $\theta(\phi)$ such that the following holds. Let $\phi^1(\theta)$ (respectively, $\phi^2(\theta)$) be the inverse function of $\theta(\phi)$ in a neighborhood of P_1 (respectively, P_2). Since F_1 and F_2 vanish, respectively, at points P_1 and P_2, we must have

$$\left.\frac{\mathrm{d}\phi^1}{\mathrm{d}\theta}\right|_{\theta=0} = 0, \tag{65}$$

$$\left.\frac{\mathrm{d}\phi^2}{\mathrm{d}\theta}\right|_{\theta=0}=0. \tag{66}$$

A possible choice is the symmetric function is

$$\theta(\phi)=\varepsilon\frac{4}{\pi}\sqrt{\phi\left(\frac{\pi}{2}-\phi\right)}, \tag{67}$$

which reaches the value ε only at the point $\phi=\pi/4$, as shown in Fig. 12.

Now we have to choose a parametrization $(\theta(t),\phi(t))$. To have continuous controls satisfying $u_1(0)=0$, $u_2(0)=0$, $u_1(t_1)=0$, $u_2(t_1)=0$ we must have

$$\dot{\theta}^1(t)|_0=0,$$

$$\dot{\theta}^2(t)|_{t_1}=0.$$

From Eqs. (65), (66) we get

$$\ddot{\phi}^1(t)|_0=0,$$

$$\ddot{\phi}^2(t)|_{t_1}=0.$$

To get controls having zero derivative at the initial and final points, we can use the following function:

$$\phi(t)=\frac{6006\pi}{t_1^{13}}\left(\frac{t^{13}}{13}-\frac{t^{12}t_1}{2}+\frac{15t^{11}t_1^2}{11}-2\,t^{10}t_1^3+\frac{5t^9t_1^4}{3}-\frac{3t^8t_1^5}{4}+\frac{t^7t_1^6}{7}\right). \tag{68}$$

Notice that this function satisfies $\phi^1(\overline{t})=\phi^2(\overline{t})=\phi^3(\overline{t})=\phi^4(\overline{t})=\phi^5(\overline{t})=\phi^6(\overline{t})=0$ for $\overline{t}=0,t_1$. The corresponding controls are computed with relations (59) and (49).

Remark 18: Let us use a parametrization $\phi(t)$ with $\phi^{(i)}(t)|_{t=0}=0$, $\phi^{(i)}(t)|_{t=t_1}=0)$, $i=1,\ldots,n$, $n\geqslant 2$, then the following holds:

(1) if $n=2$ then $u_1(0)=u_2(0)=0$, $\lim_{t\to t_1}\dot{u}_1(t)=-\infty$, $\lim_{t\to 0}\dot{u}_2(t)=\infty$,

(2) if $n=3$ then $u_1(0)=u_2(0)=0$, $0>\dot{u}_1(t_1)>-\infty$, $0<\dot{u}_2(0)<\infty$,

(3) if $n\geqslant 4$ then $u_1(0)=u_2(0)=0$,
$u_1^{(i)}(0)=u_2^{(i)}=0$ for $i=1,\ldots,n-3$. So if ϕ is $\mathcal{C}^n$, in $]-\delta,t_1+\delta[$ $(\delta>0,\quad \phi(t)=0$ in $]-\delta,0]\cup[t_1,t_1+\delta[)$ then u_1 and u_2 are $\mathcal{C}^{n-3}$ in $]-\delta,t_1+\delta[$.

Notice that for very small values of ε one gets very big values of the controls. We would like to stress the fact that the trajectory obtained with this tracking reaches exactly the final target for any fixed value of ε. While in the ''counterintuitive'' strategies used in literature, if ε_c is the maximum value reached by θ, then the final target is reached with an error smaller than ε_c but different from zero.

In the last picture the tracking solution corresponding to the expression of (68), for $\varepsilon=2/19$, and $t_1=4$ and a typical strategy used in literature:

$$\begin{cases} u_1(t)=\dfrac{-5}{e^{16}}+\dfrac{13}{e^{(-4+1.5\,t)^2}}, \\ u_2(t)=\dfrac{-5}{e^{9}}+\dfrac{13}{e^{(-2.7+1.5\,t)^2}} \end{cases} \tag{69}$$

are compared. Notice that the pulses have similar area. Moreover, notice that the trajectory corresponding to the controls (69) (obtained integrating numerically the Schrödinger equation) reaches negative values of θ.

VI. CONCLUSION

In summary, we have shown how optimal controls for two- and three-level models can be constructed on the basis of geometric arguments. For the two-level modes we recover the well-known ''π-pulse'' strategy, and obtain the corresponding generalization for the resonant three-level model. The optimal trajectories appear as geodesics (Riemannian or singular-Riemannian) on two-dimensional spheres. Furthermore, besides the optimal control strategies, the standard tracking technique from geometric control theory allows us to analyze a method of adiabatic control used in recent experiments. It leads to an improvement that allows one to reach the target state precisely. The extension of these results to the treatment of more general N-level systems will be presented in forthcoming work.

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Two families of superintegrable and isospectral potentials in two dimensions

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As an extension of the intertwining operator idea, an algebraic method which provides a link between supersymmetric quantum mechanics and quantum (super)integrability is introduced. By realization of the method in two dimensions, two infinite families of superintegrable and isospectral stationary potentials are generated. The method makes it possible to perform Darboux transformations in such a way that, in addition to the isospectral property, they acquire the superintegrability preserving property. Symmetry generators are second and fourth order in derivatives and all potentials are isospectral with one of the Smorodinsky–Winternitz potentials. Explicit expressions of the potentials, their dynamical symmetry generators, and the algebra they obey as well as their degenerate spectra and corresponding normalizable states are presented. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1463217]

I. INTRODUCTION

A Hamiltonian system of N degrees of freedom is said to be completely integrable, in the Liouville–Arnold sense, if it possesses functionally independent globally defined and single-valued N integrals of motion in involution.[1,2] It is called superintegrable if it admits more than N integrals of motion. Not all the integrals of the superintegrable system can be in involution, but they must be functionally independent otherwise the extra invariants are trivial. In analogy to the classical mechanics, a quantum mechanical system described in N-dimensional (ND) Euclidean space by a stationary Hamiltonian operator H is called completely integrable if there exists a set of $N-1$ (together with H,N) algebraically independent linear operators $X_i, i=1,2,\ldots,N-1$ commuting with H and among each other.[3–11] If there exist k additional operators $Y_j, j=1,2,\ldots,k$ where $0<k\leqslant N-1$, commuting with H it is said to be superintegrable. The superintegrability is said to be minimal if $k=1$ and maximal if $k=N-1$.

Classical and quantum mechanical examples of the maximally superintegrable systems for any finite N are the Kepler-Coulomb problem, the harmonic oscillator with rational frequency ratio, the Calogero–Moser system in a harmonic well, and the Winternitz (or, Smorodinsky–Winternitz) system. The first two are known, for $N=3$, since the time of Laplace and the superintegrability of the last two systems were established for the first time, respectively, by Wojciechowski[5] and by Evans.[6] The first systematic search for other possible superintegrable

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systems was begun by Winternitz and co-workers. They first found four independent two-dimensional (2D) potentials that are separable in more than one coordinate system,[3] and then they extended this to $N=3$.[4] This approach is based on two assumptions; (1) Hamiltonians are of potential form; (2) integrals of motion are at most quadratic in momenta (or, in derivatives). The Winternitz program has been completed in Ref. 7 where a complete list consisting of, up to the equivalence of linear transformations, thirteen different three-dimensional potentials with four or five independent integrals of motion is given. Winternitz potentials have also been considered by different formulations such as path integral formulation,[8] Lagrangian formalism,[9] and evolutionary vector fields formalism.[10]

In this paper we report an infinite family of 2D potentials which are not only superintegrable, but at the same time isospectral. We shall give explicit expressions of the potentials, their dynamical symmetry generators and the algebra they obey, as well as their degenerate spectrum and corresponding normalizable states. We achieve this goal by following an algebraic method which is based on and, in fact, is an extension of intertwining operator idea. This is closely connected with the supersymmetric (SUSY) methods such as the Darboux transformation, and Schrödinger factorization which deal with pairs of Hamiltonians having the same energy spectra but different eigenstates.[12–15] It turns out that each member of this infinite family is a triplet of potentials one of which is the same for entire family and the other two change from member to member. Hence, we have, in fact, two different infinite families of superintegrable and isospectral potentials. The fixed potential turns out to be one of 2D Winternitz potentials and determines the spectra of both families and the other two are intertwined to it by Darboux-type transformations. The generators of these transformations depend on eigenfunctions of two associated solvable one-dimensional problems that result from the separation of the Winternitz potential in different coordinates. We should emphasize that our approach makes it possible to apply Darboux transformations simultaneously to potential and to its symmetry generators in such a way that superintegrability property is preserved.

Formal aspects of our method together with a brief review of the main points of the intertwining operator idea will be given in Sec. II. Sections III–V are devoted to explicit realization of our method. In Sec. IV we present the most general form of 2D integrable and isospectral potentials in the plane polar coordinates. Two subfamilies of superintegrable and isospectral potentials and then their general forms are presented in Secs. VI and VII. Section VIII contains a review of bound states of the associated one-dimensional (1D) problems and the above-mentioned Winternitz potential. After investigating the symmetry generators and their algebra in Sec. IX, the normalizable states of the generated superintegrable and isospectral potentials are given in Sec. X.

II. MULTIPLE INTERTWINING METHOD

The object of the intertwining method is to construct a linear differential operator $\mathcal{L}$ which intertwines two Hamiltonian operators H_0 and H_1 such that $\mathcal{L}H_0=H_1\mathcal{L}$. Two important facts that immediately follow from this relation are as follows. (i) If ψ^0 is an eigenfunction of H_0 with eigenvalue of E^0 then $\psi^1=\mathcal{L}\psi^0$ is an (unnormalized) eigenfunction of H_1 with the same eigenvalue E^0. (ii) When H_0 and H_1 are self-adjoint (on some common function space) $\mathcal{L}^\dagger$ intertwines in the other direction $H_0\mathcal{L}^\dagger=\mathcal{L}^\dagger H_1$ and this in turn implies that $[H_0,\mathcal{L}^\dagger\mathcal{L}]=0=[\mathcal{L}\mathcal{L}^\dagger,H_1]$, where the dagger (†) and $[,]$ stand for Hermitian conjugation and commutator. The first property shows that $\mathcal{L}$ transforms one solvable problem into another, and the second one means that two hidden dynamical symmetries of H_0 and H_1 are immediately constructed in terms of $\mathcal{L}$. These are dimension and form independent general properties of this method.[16,17] In the context of 1D systems where $\mathcal{L}$ is taken to be the first-order differential operator and Hamiltonians are of the potential forms two additional properties arise: (i) every eigenfunction of H_0 (without regard to boundary conditions or normalizability) can be used to generate a transformation to a new solvable problem; (ii) a direct connection to a SUSY algebra can be established.[18] The first property is a manifestation of the celebrated Darboux transformation and its generalization (Crum transformation). The second property enables us to express in a compact algebraic form of the spectral equivalence of the intertwined systems.

Now suppose that there are three self-adjoint Hamiltonian operators H_0, H_1, H_2 which are intertwined as

$$\mathcal{L}_{10}H_0 = H_1\mathcal{L}_{10}, \quad \mathcal{L}_{21}H_1 = H_2\mathcal{L}_{21}. \tag{1}$$

The subscripts of the intertwining operators are used to distinguish them and to denote the intertwined Hamiltonians. Equation (1) immediately implies that $\mathcal{L}_{20} \equiv \mathcal{L}_{21}\mathcal{L}_{10}$ will intertwine H_0 and H_2 as follows:

$$\mathcal{L}_{20}H_0 = H_2\mathcal{L}_{20}. \tag{2}$$

Equations (1) and (2) can be unified into the following diagram:

$$\begin{array}{ccc} H_0 & \rightarrow & H_1 \\ & \searrow\downarrow & \\ & H_2 & \end{array}, \tag{3}$$

which must be understood in the sense described by (1) and (2).

Adjoints of (1) and (2) yield

$$\mathcal{L}_{21}^{\dagger}H_2 = H_1\mathcal{L}_{21}^{\dagger}, \quad \mathcal{L}_{10}^{\dagger}H_1 = H_0\mathcal{L}_{10}^{\dagger}, \quad \mathcal{L}_{20}^{\dagger}H_2 = H_0\mathcal{L}_{20}^{\dagger}. \tag{4}$$

That is, the adjoints of the intertwining operators will intertwine in the reverse directions and this can be represented by a diagram the same as (3) with reversed directions of arrows. Making use of (1)–(4) it is easy to show that each of H_0, H_1, H_2 has two dynamical symmetry generators respectively given by

$$\begin{aligned} X_0 &= \mathcal{L}_{10}^{\dagger}\mathcal{L}_{10}, \quad Y_0 = \mathcal{L}_{20}^{\dagger}\mathcal{L}_{20}, \\ X_1 &= \mathcal{L}_{10}\mathcal{L}_{10}^{\dagger}, \quad Y_1 = \mathcal{L}_{21}^{\dagger}\mathcal{L}_{21}, \\ X_2 &= \mathcal{L}_{21}\mathcal{L}_{21}^{\dagger}, \quad Y_2 = \mathcal{L}_{20}\mathcal{L}_{20}^{\dagger}. \end{aligned} \tag{5}$$

The subscripts of X_j, Y_j indicate the Hamiltonians they belong to. Throughout this paper we assume that the domains of definition of Hamiltonians and intertwining operators are some linear subspaces of a common Hilbert space $\mathcal{H} = L^2(\Omega)$ with the standard sesquilinear inner product. $L^2(\Omega)$ is the space of all square-integrable functions (and distributions) defined on a subspace Ω of ND Euclidean space R^N.[19–21]

For all $N \geqslant 2$, diagram (3) implies a triplet of isospectral Hamiltonians such that each has two dynamical symmetries. By construction, all the symmetry operators obtained in this manner will be factorized, and have even orders depending on the order of intertwining operators. They will be of the same order only for H_1. According to the von Neumann theorem (see Ref. 19, p. 141 and Ref. 20, p. 275) $\mathcal{L}_{ij}\mathcal{L}_{ij}^{\dagger}$ (and $\mathcal{L}_{ij}^{\dagger}\mathcal{L}_{ij}$) are self-adjoint and non-negative if $\mathcal{L}_{ij}$ are closed with dense domains of definition. Otherwise there may exist states in which they have negative expectation values (see Sec. X). If $\mathcal{L}_{10}$ and $\mathcal{L}_{21}$ are taken to be algebraically independent, the independence of X_i, Y_i pairs will be guaranteed from the outset. Extensions of these ideas to higher dimensions will be, generically, called multiple intertwining method. A simple observation that this work initiated from is that, in the particular case of $N = 2$, diagram (3) guarantees the superintegrability of the three Hamiltonians. In the case of $N = 3$ such a diagram will imply, provided that symmetry generators are commutative, the integrability of the potentials.

The rest of the paper is devoted to explicit realization of these formal observations for 2D systems. First we will determine the most general form of the potentials and the first-order intertwining operator for two Hamiltonians. We then construct the intertwinings $H_0 \rightarrow H_1$ and $H_1 \rightarrow H_2$ by special forms of the intertwining operator. We end this section by explaining our use

of the adjective ''isospectral.'' Two Hamiltonians are said to be isospectral if they have the same eigenvalue spectrum.[18,22,23] In this sense two linearly intertwined Hamiltonians are always formally isospectral except for the eigenvalues corresponding to the kernel of the intertwining operator. Even for these exceptional cases one can construct eigenfunctions corresponding to these eigenvalues at least for 1D and 2D systems by appealing to the Liouville formula and its 2D version.[14] However, due to physical requirements, in the case of the bound states mainly due to normalizability conditions, some eigenvalues of one of the partner potentials are to be discarded. For higher dimensional systems also the degree of degeneracy of a common eigenvalue may be different (see Sec. X). These will just mean that a finite number of eigenvalues are to be disregarded for they are not physically admissible.

III. INTERTWINING IN TWO DIMENSIONS

We start by considering a pair of 2D one-particle systems characterized by the Hamiltonian operators of potential form

$$H_i=-\nabla^2+V_i, \quad H_f=-\nabla^2+V_f, \tag{6}$$

where the potentials V_i, V_f (and eigenvalues of H_i, H_f) are expressed in terms of $2m/\hbar^2$ and

$$\nabla^2=\partial_r^2+\frac{1}{r}\partial_r+\frac{1}{r^2}\partial_\theta^2$$

is the Laplace operator in the plane polar coordinates (r,θ). m is the mass of the particle and $\hbar$ denotes the Planck constant. Here and in the following we use the notation ∂_x for partial derivative $\partial/\partial x$ and the subindexes ''i,'' ''f'' as the shorthands for the ''initial'' and ''final.'' We suppose that the Hamiltonians are intertwined by

$$\mathcal{L}_{fi}H_i=H_f\mathcal{L}_{fi} \tag{7}$$

and propose the ansatz that $\mathcal{L}_{fi}$ is the most general first-order linear operator

$$\mathcal{L}_{fi}=L_0+L_d=L_0+L_1\partial_r+L_2\partial_\theta, \tag{8}$$

where $L_d=L_1\partial_r+L_2\partial_\theta$ will be referred to as the differential part of $\mathcal{L}_{fi}$. The potentials and L_0, L_1, L_2 are some real functions of (r,θ) which are to be determined from consistency equations of the intertwining relation (7).

In view of (6) and (8) the relation (7) explicitly reads as

$$[\nabla^2,L_d]=-[\nabla^2,L_0]+[V_i,L_d]+P\mathcal{L}_{fi}, \tag{9}$$

where $P=V_f-V_i$. The second-order derivatives come, together with some first-order derivatives, only from

$$\begin{aligned}[\nabla^2,L_d]=&\left(\nabla^2L_1+\frac{1}{r^2}L_1\right)\partial_r+(\nabla^2L_2)\partial_\theta\\&+2\left(\frac{1}{r^2}\partial_\theta L_1+\partial_r L_2\right)\partial_\theta\partial_r+2(\partial_r L_1)\partial_r^2+\frac{2}{r^3}(L_1+r\partial_\theta L_2)\partial_\theta^2,\end{aligned} \tag{10}$$

and by setting their coefficients to zero we obtain

$$\partial_\theta L_1+r^2\partial_r L_2=0, \quad \partial_r L_1=0, \quad L_1+r\partial_\theta L_2=0.$$

It is straightforward to show that the general solutions of these equations are

$$L_1 = A\sin(\theta+\phi), \quad L_2 = B + \frac{A}{r}\cos(\theta+\phi), \tag{11}$$

where A,B, and ϕ are integration constants. Since $\nabla^2 L_1 = -L_1/r^2$, and $\nabla^2 L_2 = 0$, we have from (10) $[\nabla^2, L_d] = 0$. As a result of this the relation (9) simplifies to

$$[\nabla^2, L_0] = -L_1\partial_r V_i - L_2\partial_\theta V_i + P(L_0 + L_d). \tag{12}$$

By substituting

$$[\nabla^2, L_0] = \nabla^2 L_0 + 2(\partial_r L_0)\partial_r + \frac{2}{r^2}(\partial_\theta L_0)\partial_\theta,$$

into (12), and then by equating the coefficients of the first and zeroth powers of derivatives we obtain

$$2\partial_r L_0 = PL_1, \tag{13}$$

$$2\partial_\theta L_0 = r^2 PL_2, \tag{14}$$

$$(-\nabla^2 + P)L_0 = L_1\partial_r V_i + L_2\partial_\theta V_i. \tag{15}$$

These three partial differential equations, the first two of which are linear and the third is nonlinear, constitute a reduced form of the consistency conditions for three unknown functions L_0, V_i, and V_f.

IV. GENERAL FORM OF 2D INTEGRABLE ISOSPECTRAL POTENTIALS IN POLAR COORDINATES

Equations (11), (13), and (14) and the compatibility condition $\partial_r\partial_\theta L_0 = \partial_\theta\partial_r L_0$ imply that

$$2\nabla^2 L_0 = L_d P, \quad ZL_0 = 0, \quad ZP = 2BrP,$$

where $Z = L_1\partial_\theta - r^2 L_2\partial_r$. From the second and third of these equations [or, from (13) and (14)] we have $L_0 = f(w)$, and $P = -2A^2 f'(w)/r^2 L_1^2$, where f is an arbitrary function of

$$w = B\cot(\theta+\phi) + \frac{A}{r\sin(\theta+\phi)}.$$

Prime stands for derivative with respect to the argument and when there is no risk of confusion the argument will be suppressed. By combining $2\nabla^2 L_0 = L_d P$ with (15) and using the found L_0 and P we obtain an inhomogeneous equation from the general solution of which the general form of potentials are found to be

$$V_i = h(\kappa) + \frac{\mathcal{V}_-(w)}{\kappa^2}, \quad V_f = h(\kappa) + \frac{\mathcal{V}_+(w)}{\kappa^2}. \tag{16}$$

Here h is an arbitrary function of $\kappa = [A^2 + B^2 r^2 + 2ABr\cos(\theta+\phi)]^{1/2}$ such that $L_d h = 0$ and

$$\mathcal{V}_\pm(w) = f^2(w) \mp (w^2 + B^2) f'(w). \tag{17}$$

Equation (16) represents the most general form of the 2D integrable and isospectral potentials in polar coordinates.

Let us define the operators

$$T_1=\cos\theta\partial_r-\frac{1}{r}\sin\theta\partial_\theta,\quad T_2=\sin\theta\partial_r+\frac{1}{r}\cos\theta\partial_\theta,\quad J=\partial_\theta, \tag{18}$$

which close in the defining relations of the Euclidean Lie algebra $e(2)$ in two dimensions

$$[J,T_1]=-T_2,\quad [J,T_2]=T_1,\quad [T_1,T_2]=0. \tag{19}$$

Now L_d can be rewritten as

$$L_d=A\sin\phi T_1+A\cos\phi T_2+BJ, \tag{20}$$

which shows that the differential part of $\mathcal{L}_{fi}$ is an element of $e(2)$. In terms of the Cartesian coordinates $x=r\cos\theta, y=r\sin\theta$ we have $T_1=\partial_x, T_2=\partial_y, J=x\partial_y-y\partial_x$, and $T_i^\dagger=-T_i, J^\dagger=-J$. These relations can also be verified from (18) by noting that $(\partial_r)^\dagger=-(r^{-1}+\partial_r), (\partial_\theta)^\dagger=-\partial_\theta$. Now from (5) and (17) the symmetry generators of H_i and H_f are

$$\mathcal{L}_{fi}^\dagger\mathcal{L}_{fi}=\mathcal{V}_--L_d^2,\quad \mathcal{L}_{fi}\mathcal{L}_{fi}^\dagger=\mathcal{V}_+-L_d^2,$$

where L_d^2 is at most quadratic operator in generators of $e(2)$.

V. CONSTRUCTION OF THE INTERTWINING OPERATORS

We shall construct the legs of the diagram (3) by adopting particular forms of (20) as the differential parts of $\mathcal{L}_{10}$ and $\mathcal{L}_{21}$. In doing that we shall make use of the orbit structure of $e(2)$ under the adjoint action of the Euclidean group $E(2)$ in two dimensions.[24]

Under a unitary similarity transformation, generated by

$$U=e^{a_0J}e^{a_1T_1+a_2T_2},\quad U^\dagger=U^{-1}=e^{-(a_1T_1+a_2T_2)}e^{-a_0J}, \tag{21}$$

where a_i's are real parameters and U^{-1} stands for the inverse of $U\in E(2)$, relation (7) transforms into $\overline{\mathcal{L}}_{fi}\overline{H}_i=\overline{H}_f\overline{\mathcal{L}}_{fi}$, where $\overline{X}=UXU^\dagger$. Since $\nabla^2=T_1^2+T_2^2$ is the Casimir invariant of $e(2)$, only V_i, V_f, and $\mathcal{L}_{fi}$ will change under this $E(2)$ action. Now suppose that L_d is of the form (20). Making use of the well-known operator identity

$$e^{bK}Me^{-bK}=M+b[K,M]+\frac{b^2}{2!}[K,[K,M]]+\cdots,$$

where b is a constant and K,M are two arbitrary operators, one can easily show that

$$\overline{L}_d=BJ+e^{a_0J}[T_1(A\sin\phi-a_2B)+T_2(A\cos\phi+a_1B)]e^{-a_0J}.$$

Hence, if $B\neq0$ we can take $\overline{L}_d=BJ$ by choosing $a_1=-A\cos\phi/B, a_2=A\sin\phi/B$. On the other hand, if $B=0, A\neq0$ we get $\overline{L}_d=AT_1$ (or, $\overline{L}_d=AT_2$) for the choice $a_0=\phi$ (or, $a_0=-\phi$). Therefore, under the adjoint action of $E(2)$, $e(2)$ has two orbits represented by J and T_2. Since L_d and cL_d belong to the same orbit for $c\neq0$, we can choose $L_d=J$ for $\mathcal{L}_{10}$ and $L_d=T_2$ for $\mathcal{L}_{21}$. In such a case the potentials and L_0 will be specified up to the adjoint action of $E(2)$.

For the first leg $H_0\rightarrow H_1$ of (3) we take $A=0, B=1$ in Eq. (11) and redefine the Hamiltonians as $H_i=H_0$ and $H_f=H_1$. Hence $L_1=0, L_2=1$ and Eqs. (13) and (14) imply that $L_0=f(\theta)$ and

$$\mathcal{L}_{10}=f(\theta)+\partial_\theta,\quad P=V_1-V_0=\frac{2}{r^2}f'(\theta), \tag{22}$$

where f is an arbitrary differentiable function of θ. Noting that $\nabla^2L_0=f''(\theta)/r^2$ we obtain from (15) and (22)

$$V_0 = h(r) + \frac{V_-(\theta)}{r^2}, \quad V_1 = h(r) + \frac{V_+(\theta)}{r^2}, \tag{23}$$

where h is an arbitrary differentiable function of r and

$$V_\pm(\theta) = f^2(\theta) \pm f'(\theta). \tag{24}$$

As a result the first $H_0 \to H_1$ leg of the diagram (3) has been constructed.

For the second leg we take $B=0, A=1$, fix the form of H_1 and denote it as $H_i = H_1$. We then look for $H_f = H_2$ such that $\mathcal{L}_{21} H_1 = H_2 \mathcal{L}_{21}$ and $\mathcal{L}_{21} = L_0 + \sin\phi T_1 + \cos\phi T_2$. In that case from Eqs. (13) to (14) we get $L_0 = g(u)$ and

$$\mathcal{L}_{21} = g(u) + \sin(\theta+\phi)\partial_r + \frac{1}{r}\cos(\theta+\phi)\partial_\theta, \tag{25}$$

$$P = V_2 - V_1 = 2g'(u), \tag{26}$$

where g is an arbitrary differentiable function of $u = r\sin(\theta+\phi)$. It only remains to solve the nonlinear equation (15) which now takes the form

$$\partial_u[g^2(u) - g'(u)] = \sin(\theta+\phi)h'(r) + \frac{1}{r^3}[\cos(\theta+\phi)V'_+(\theta) - 2\sin(\theta+\phi)V_+(\theta)], \tag{27}$$

where we have made use of $\nabla^2 L_0 = g''(u)$ and of the second equation of (23). Note that we could have chosen $\phi = 0$, but since it costs almost nothing we keep ϕ in our formulas in order to see that action of $E(2)$.

Since it further restricts the three arbitrary functions specifying the potentials, Eq. (27) is the main equation which determines the final form of the potentials. As a consistency condition the right-hand side of Eq. (27) must be only a function of u. Nevertheless this requirement provides us with many possibilities for f, g, and h, which are investigated in Secs. VI and VII. Note that for any solutions of Eq. (27) the potentials will be connected to each other as follows:

$$V_0 = V_1 - \frac{2}{r^2}f'(\theta), \quad V_2 = V_1 + 2g'(u), \quad V_0 = V_2 - 2\left[g'(u) + \frac{f'(\theta)}{r^2}\right]. \tag{28}$$

VI. TWO SUBFAMILIES OF POTENTIALS

We construct the simplest family of potentials by taking, in (24) and (27), $h = (\lambda_1/r^2) + a, V_+ = -\lambda_1$. These lead us to

$$f^2 + f' = -\lambda_1, \quad g^2 - g' = -\lambda_2, \tag{29}$$

where a, λ_1, λ_2 are some arbitrary constants. Then, by Eqs. (23) and (24) and (26), we obtain

$$V_0 = \frac{2}{r^2}(f^2 + \lambda_1) + a, \quad V_1 = a, \quad V_2 = 2(g^2 + \lambda_2) + a. \tag{30}$$

The general solution of $g^2 - g' = -\lambda_2$ is

$$g = \begin{cases} \lambda_2^{1/2}\tan(\lambda_2^{1/2}u + a_1) & \text{for } \lambda_2 > 0, \\ -\dfrac{1}{u + a_1} & \text{for } \lambda_2 = 0, \\ (-\lambda_2)^{1/2}\tanh[(-\lambda_2)^{1/2}u + a_1] & \text{for } \lambda_2 < 0, \end{cases}$$

where a_1 is a constant. The solution of $f^2+f'=-\lambda_1$ can be directly read from the above-given relation after the replacement $(g,u,\lambda_2)\to(f,-\theta,\lambda_1)$.

An important point is that, by the usual linearization of the Riccati equation, if we substitute

$$f(\theta)=\frac{\psi'(\theta)}{\psi(\theta)}, \quad g(u)=-\frac{\Psi'(u)}{\Psi(u)}, \tag{31}$$

into (29) we arrive at two 1D Schrödinger equations,

$$-\psi''(\theta)=\lambda_1\psi(\theta), \quad -\Psi''(u)=\lambda_2\Psi(u). \tag{32}$$

While the second one can be considered as a free motion, this is not the case for the first since $0\leqslant\theta<2\pi$. An appealing case is to consider one or both of them as infinite square-well problem. Normalized eigenfunctions subjected to boundary conditions, say, $\psi(0)=0=\psi(2\pi)$ and corresponding eigenvalues are

$$\psi_k(\theta)=\pi^{-1/2}\sin\left(\frac{1}{2}k\theta\right), \quad \lambda_{1,k}=\frac{k^2}{4}, \quad k=1,2,\ldots. \tag{33}$$

Hence $f_k=(k/2)\cot(k\theta/2)$ and by virtue of Eqs. (22) and (24) we have

$$V_0^{(k)}=\frac{k^2}{2r^2\sin^2\frac{1}{2}k\theta}+a, \quad \mathcal{L}_{10}^{(k)}=\frac{k}{2}\cot\left(\frac{1}{2}k\theta\right)+\partial_\theta. \tag{34}$$

To distinguish the resulting potentials, corresponding intertwining operators and the parameter λ_1 we have labeled them by the quantum number k. The u-problem can be treated in a similar way. In any case, the potentials and transformations among them are generated by solutions of these two auxiliary 1D problems. The existence of $V_1=a$ explicitly shows that the member potentials are isospectral to a 2D free motion. As a result we have found a five-parameter $(a,a_1,\lambda_1,\lambda_2,\phi)$ family of 2D potentials that are generated, in a nontrivial way, by two 1D problems.

We specify a second subfamily of potentials by taking, in (23)–(24) and (27),

$$h=\frac{\lambda_1}{r^2}+\frac{1}{2}\alpha r^2+a, \tag{35}$$

and $V_+=-\lambda_1$. These lead us to the same equation as in (29) for f and to the Riccati's equation

$$g^2-g'-\tfrac{1}{2}\alpha u^2+\lambda_2=0 \tag{36}$$

for g. By Eqs. (23)–(24) and (26) the member potentials are found to be

$$V_0=\frac{1}{2}\alpha r^2+\frac{2(f^2+\lambda_1)}{r^2}+a,$$

$$V_1=\tfrac{1}{2}\alpha r^2+a, \tag{37}$$

$$V_2=\tfrac{1}{2}\alpha r^2\cos 2(\theta+\phi)+2g^2(u)+(a+2\lambda_2),$$

where g is any solution of (36) and f is any solution of $f^2+f'=-\lambda_1$.

Now the ansatz (31) for g transforms (36) into

$$-\Psi''(u)+\tfrac{1}{2}\alpha u^2\Psi(u)=\lambda_2\Psi(u), \tag{38}$$

which is the well-known Schrödinger equation for the 1D harmonic oscillator. In that case the entire family will have 2D isotropic harmonic oscillator spectrum given by the eigenvalues

$$E_{\ell}^{(1)}=\hbar\omega(\ell+1), \quad \ell=0,1,2,\ldots, \tag{39}$$

which are $\ell+1$ times degenerate for a given ℓ. For concrete examples we recall the normalized eigenfunctions and corresponding eigenvalues of the 1D harmonic oscillator:

$$\Psi_n(u)=N_n e^{-\beta^2u^2/2}H_n(\beta u), \quad E_n=\frac{\hbar^2}{2m}\lambda_{2,n}=\hbar\omega\left(n+\frac{1}{2}\right), \quad n=0,1,2,\ldots, \tag{40}$$

where N_n is the normalization constant, H_n denote the Hermite polynomials, and

$$\beta=\left(\frac{m\omega}{\hbar}\right)^{1/2}=\left(\frac{\alpha}{2}\right)^{1/4}, \quad N_n=\left(\frac{\beta}{\pi^{1/2}2^n n!}\right)^{1/2}. \tag{41}$$

In writing Eqs. (39)–(41) we have restored $2m/\hbar^2$ in our notation in which the dimension of β is $(\text{length})^{-1}$. Like λ_2, also $V_2, \mathcal{L}_{21}$ and the function g must be labeled by the quantum number n:

$$g_n(u)=-\frac{\Psi_n'(u)}{\Psi_n(u)}=\beta^2u-\partial_u\ln[H_n(\beta u)],$$

$$V_2^{(n)}=\beta^4r^2\cos 2(\theta+\phi)+2g_n^2(u)+a+4\beta^2(n+\tfrac{1}{2}), \tag{42}$$

$$\mathcal{L}_{21}^{(n)}=g_n(u)+\sin(\theta+\phi)\partial_r+\frac{1}{r}\cos(\theta+\phi)\partial_\theta.$$

For the first three Hermite polynomials $H_0(x)=1, H_1(x)=2x, H_2(x)=4x^2-2$, we have

$$g_0=\beta^2u, \quad g_1=\beta^2u-\frac{1}{u}, \quad g_2=\beta^2\frac{2\beta^2u^2-5}{2\beta^2u^2-1}u.$$

Considering the f-problem as noted previously, $\mathcal{L}_{10}^{(k)}$ is given by (34) and V_0 is

$$V_0^{(k)}=\frac{1}{2}\alpha r^2+\frac{k^2}{2r^2\sin^2(\frac{1}{2}k\theta)}+a. \tag{43}$$

VII. GENERAL FORM OF THE POTENTIALS

Returning the general discussion of Sec. V, the most general potentials are obtained by choosing, in Eq. (27), h as in (35) and by postulating the equation

$$\cos(\theta+\phi)V_+'(\theta)-2\sin(\theta+\phi)V_+(\theta)=2\lambda_1\sin(\theta+\phi)-\frac{2c}{\sin^3(\theta+\phi)} \tag{44}$$

for V_+. It is not hard to check that (35) and (44) are the most general relations which make the right-hand side of Eq. (27) only a function of the u variable. The general solution of Eq. (44) is

$$V_+=f^2(\theta)+f'(\theta)=\frac{b}{\cos^2(\theta+\phi)}+\frac{c}{\sin^2(\theta+\phi)}-\lambda_1, \tag{45}$$

where λ_1, b, and c are some constants. When (35) and (44) are inserted into (27) we obtain a new Riccati's equation for $g(u)$,

$$g^2-g'=\frac{1}{2}\alpha u^2+\frac{c}{u^2}-\lambda_2. \tag{46}$$

By virtue of (23), (28), (35), (45), and (46) the corresponding potentials can be written as

$$V_0=\frac{1}{2}\alpha r^2-\frac{1}{r^2}\left[\frac{b}{\cos^2(\theta+\phi)}+\frac{c}{\sin^2(\theta+\phi)}\right]+\frac{2(f^2+\lambda_1)}{r^2}+a,$$

$$V_1=\frac{1}{2}\alpha r^2+\frac{1}{r^2}\left[\frac{b}{\cos^2(\theta+\phi)}+\frac{c}{\sin^2(\theta+\phi)}\right]+a, \tag{47}$$

$$V_2=\frac{1}{2}\alpha r^2\cos 2(\theta+\phi)+\frac{1}{r^2}\left[\frac{b}{\cos^2(\theta+\phi)}-\frac{c}{\sin^2(\theta+\phi)}\right]+2\left(g^2+\lambda_2+\frac{a}{2}\right).$$

V_1 is immediately recognized as one of 2D Smorodinsky–Winternitz potentials which accepts separation of variables in the Cartesian, polar, and elliptic coordinates. Being fixed in the whole family it determines the structure of spectrum of all potentials. While V_0 is separable in the plane polar coordinates V_2 is separable only in the Cartesian coordinates. V_0 and V_2 represent two families of the superintegrable and isospectral potentials generated by the functions f and g which are subjected to Eqs. (45) and (46). The normalized eigenfunctions, corresponding eigenvalues, and the symmetry generators will be the subject of Secs. VII, IX, and X.

Having specified the most general forms of the potentials we now show how to develop a hierarchy of the potentials.

On substituting (31) into (45) and (46) we arrive at the following two 1D problems:

$$H_{\mathrm{PT}}\psi_k(\theta)=\lambda_{1,k}\psi_k(\theta),\quad H_{\mathrm{SO}}\Psi_n(u)=\lambda_{2,n}\Psi_n(u), \tag{48}$$

where k and n are possible quantum numbers and

$$H_{\mathrm{PT}}=-\frac{\mathrm{d}^2}{\mathrm{d}\theta^2}+V_{\mathrm{PT}},\quad V_{\mathrm{PT}}=\frac{b}{\cos^2(\theta+\phi)}+\frac{c}{\sin^2(\theta+\phi)}, \tag{49}$$

$$H_{\mathrm{SO}}=-\frac{\mathrm{d}^2}{\mathrm{d}u^2}+V_{\mathrm{SO}},\quad V_{\mathrm{SO}}=\frac{1}{2}\alpha u^2+\frac{c}{u^2}. \tag{50}$$

These are the well-known generalized Pöschl–Teller (PT) and singular oscillator (hence the subscript SO), or the radial oscillator potentials. By virtue of (28) and (31) the potentials can be rewritten as

$$V_0^{(k)}=V_1-\frac{2}{r^2}\partial_\theta^2\ln\psi_k(\theta),\quad V_2^{(n)}=V_1-2\partial_u^2\ln\Psi_n(u). \tag{51}$$

Here and in the following we label the potentials by the quantum numbers of the associated 1D problems that generate them. Equation (51) explicitly shows that $V_0^{(k)}$ and $V_2^{(n)}$ are generated from V_1 by the Darboux-type transformations. The functions that generate these transformations are the eigenfunctions of the associated 1D problems. This constitutes an extension of Darboux transformations for 2D problems. Another point worth emphasizing is that any solution of these 1D problems can be used in generating the potentials. But, as easily accessible results from the literature, only normalizable solutions of these problems will be presented in the following. From now on we take $\phi=0$ and in Secs. VIII and X we include $2m/\hbar^2$ into our notation.

VIII. BOUND STATES OF THE ASSOCIATED PROBLEMS AND V_1

Provided that $c \geqslant -1/4$, the bound states of H_{SO} belonging to the Hilbert space $L^2(0,\infty)$ are given as follows:[3,25–27]

$$\Psi_n^{\varepsilon}(u) = N_n^{\mathrm{SO}} u^{1/2+\varepsilon\nu} e^{-\beta^2 u^2/2} L_n^{\varepsilon\nu}(\beta^2 u^2),$$

$$E_n^{\varepsilon} = \frac{\hbar^2}{2m}\lambda_{2,n}^{\varepsilon} = \hbar\omega(2n+\varepsilon\nu+1), \quad n=0,1,2,\ldots, \tag{52}$$

$$N_n^{\mathrm{SO}} = \left[\frac{n!\,2\beta^{2(1+\varepsilon\nu)}}{\Gamma(n+\varepsilon\nu+1)}\right]^{1/2}, \quad \nu = \frac{1}{2}(1+4c)^{1/2},$$

where N_n^{SO} is the normalization constant, $L_n^{\varepsilon\nu}(z)$ are the generalized Laguerre polynomials, β is defined by Eq. (41), Γ stands for the gamma function, and $\varepsilon = \pm$. $\Psi_n^{\varepsilon}(u)$'s satisfy the orthogonality relation[28]

$$\int_0^{\infty} \Psi_n^{\varepsilon}(u)\Psi_{n'}^{\varepsilon}(u)\,\mathrm{d}u = \delta_{nn'}, \tag{53}$$

which is valid for $\varepsilon\nu > -1$. This implies that for $c \in I = [-1/4, 3/4)$ (that is for $-1/4 \leqslant c < 3/4$) both values of $\varepsilon = \pm$, and for $c \geqslant 3/4$ only $\varepsilon = +$ can be used for each n. Although the generated potentials do not depend on the normalization constants of the associated 1D problems we write them for completeness.

From the most general point of view and in accordance with the fact that H_{SO} is parity invariant, defined parity states of H_{SO} belonging to the Hilbert space $L^2(-\infty,\infty)$ can be given as follows:[26]

$$\Psi_n^{\varepsilon}(u) = \frac{1}{2^{1/2}} N_n^{\mathrm{SO}} \begin{cases} |u|^{1/2+\varepsilon\nu} e^{-\beta^2 u^2/2} L_n^{\varepsilon\nu}(\beta^2 u^2) & \text{for } u \geqslant 0, \\ -\varepsilon |u|^{1/2+\varepsilon\nu} e^{-\beta^2 u^2/2} L_n^{\varepsilon\nu}(\beta^2 u^2) & \text{for } u < 0. \end{cases} \tag{54}$$

These obey the following orthogonality relation:

$$\int_{-\infty}^{\infty} \Psi_n^{\varepsilon}(u)\Psi_{n'}^{\bar{\varepsilon}}(u)\,\mathrm{d}u = \delta_{nn'}\delta_{\varepsilon\bar{\varepsilon}}, \tag{55}$$

where $\varepsilon, \bar{\varepsilon}$ may equal $\pm$. For $\varepsilon = \bar{\varepsilon}$ (55) follows from the orthogonality of the generalized Laguerre polynomials[28] and for $\varepsilon \neq \bar{\varepsilon}$ from the parity reasons as can be verified directly from (54). The corresponding energy eigenvalues are given by (52). For $c < -1/4$ the energy spectrum is not bounded from below which implies "falling of the particle to the center" and physical interpretation is lost.[26,27] As $c \to 0$, $\nu \to 1/2$, and $\Psi_n^{\varepsilon}(u)$'s go over, for $\varepsilon = +$ to odd parity and for $\varepsilon = -$ to even parity harmonic oscillator wave functions. This follows from the relations between the Hermite and Laguerre polynomials.[26,28] The corresponding limits of the energy eigenvalues are obvious from (52).

The normalized eigenfunctions and corresponding eigenvalues of V_1 can now be written as

$$\Psi_{\ell}^{(1)\bar{\varepsilon}\varepsilon}(x,y) = \Psi_{n_1}^{\bar{\varepsilon}}(x)\Psi_{n_2}^{\varepsilon}(y),$$

$$E_{\ell}^{\bar{\varepsilon}\varepsilon} = E_{n_1}^{\bar{\varepsilon}} + E_{n_2}^{\varepsilon} = \hbar\omega(2\ell + \overline{\varepsilon\nu} + \varepsilon\nu + 1), \tag{56}$$

$$\ell = n_1 + n_2, \quad \ell, n_1, n_2 = 0,1,2,\ldots,$$

where $\overline{\nu}=(1+4b)^{1/2}/2$. $\Psi^{\overline{\varepsilon}}_{n_1}(x)$, $\Psi^{\varepsilon}_{n_2}(y)$, and $E^{\overline{\varepsilon}}_{n_1}$, $E^{\varepsilon}_{n_2}$ are given by (52) [or (54)] with suitable replacements of the parameters and variables. It follows that bound states of V_1 exist for $b,c \geqslant -1/4$. For $b,c\in I$ there are four different states for each value of ℓ. In the case of $b\in I, c \geqslant 3/4$, or $c\in I, b\geqslant 3/4$ there are two different states for each value of ℓ, and one state in the case of $b,c\geqslant 3/4$. In each case, for a given value of ℓ the state with energy $E^{\overline{\varepsilon}\varepsilon}_{\ell}$ is $(\ell+1)$-fold degenerate. We should also note that if we require the wave functions to be separately continuous at the origin the interval $I=[-1/4,3/4)$ and the conditions $b,c\geqslant 3/4$ must be replaced as $I=[-1/4,0]$ and as $b,c\geqslant 0$.

The singular oscillator problem has the spectrum generating algebra $su(1,1)=\{J_0,J_\pm:[J_0,J_\pm]=\pm J_\pm,[J_+,J_-]=-2J_0\}$ realized as[25,29]

$$J_0=\frac{H_{\mathrm{SO}}}{4\beta^2},\quad J_\pm=-\frac{1}{4}\left[\beta^2(u\mp\beta^{-2}\partial_u)^2-\frac{c}{\beta^2u^2}\right], \tag{57}$$

with the Casimir invariant $C^2=-J_+J_-+J_0^2-J_0=(4c-3)/16$. Therefore, as will be shown in Sec IX, the symmetry algebra of the H_1-problem is closely connected with this kind two commuting copies of $su(1,1)$ algebra.

For later use it will be convenient to consider the H_{PT}-problem in relation with the solution of the H_1-problem in the polar coordinates. In this case the eigenvalue equation of H_1 separates, by taking $\Psi^{(1)}(r,\theta)=R_{k_1}(r)\psi_k(\theta)$, into the Pöschl–Teller problem given by (48) and into the radial equation

$$\left[-\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}+\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)+\rho^2+\frac{\lambda_{1,k}}{\rho^2}\right]R_{k_1}(\rho)=\lambda R_{k_1}(\rho), \tag{58}$$

where $\rho=\beta r$ and $\lambda=E/\beta^2$. In terms of $v=\sin^2\theta$, and $\psi_k(\theta)=v^{(1/2)(1/2+\varepsilon\nu)}(1-v)^{(1/2)(1/2+\varepsilon\overline{\nu})}F(v)$, the eigenvalue equation of H_{PT} leads us to the hypergeometric equation for $F(v)$:

$$v(1-v)\frac{\mathrm{d}^2F}{\mathrm{d}v^2}+[\zeta-v(\gamma+\eta+1)]\frac{\mathrm{d}F}{\mathrm{d}v}-\gamma\eta F=0.$$

The general solution of this equation is

$$F(v)=A\,{}_2F_1(\gamma,\eta;\zeta;v)+Bv^{1-\zeta}\,{}_2F_1(\gamma-\zeta+1,\eta-\zeta+1;2-\zeta;v),$$

where A and B are arbitrary constants, ${}_2F_1$ denotes the hypergeometric function and

$$\gamma=\tfrac{1}{2}(1+\varepsilon\nu+\overline{\varepsilon\nu}+\sqrt{\lambda_{1,k}}),\quad \eta=\tfrac{1}{2}(1+\varepsilon\nu+\overline{\varepsilon\nu}-\sqrt{\lambda_{1,k}}),\quad \zeta=1+\varepsilon\nu.$$

For normalizable solutions B must be zero and γ (or η) must be a negative integer, say, $-k$. In that case the hypergeometric function goes over to Jacobi polynomials $P_k^{(\varepsilon\nu,\overline{\varepsilon\nu})}(1-2v)$ and the resulting eigenfunctions and eigenvalues can be written as follows:[7,30]

$$\psi_k(\theta)=N_k^{PT}\sin^{1/2+\varepsilon\nu}\theta\cos^{1/2+\overline{\varepsilon\nu}}\theta P_k^{(\varepsilon\nu,\overline{\varepsilon\nu})}(\cos 2\theta),$$

$$E_k=\frac{\hbar^2}{2m}\lambda_{1,k}=\frac{\hbar^2}{2m}(2k+\varepsilon\nu+\overline{\varepsilon\nu}+1)^2,\quad k=0,1,2,\ldots, \tag{59}$$

$$N_k^{\mathrm{PT}}=\left[\frac{2(2k+\varepsilon\nu+\overline{\varepsilon\nu}+1)\Gamma(k+1)\Gamma(k+\varepsilon\nu+\overline{\varepsilon\nu}+1)}{\Gamma(k+\varepsilon\nu+1)\Gamma(k+\overline{\varepsilon\nu}+1)}\right]^{1/2}.$$

Substituting $\lambda_{1,k}=(2k+\varepsilon\nu+\overline{\varepsilon\nu}+1)^2$ into Eq. (58) and trying the solution $R_{k_1}(\rho)=\rho^{\mu}e^{-\rho^2/2}G_{k_1}(\rho)$ we end up, for $\mu=\sqrt{\lambda_{1,k}}=(2k+\varepsilon\nu+\overline{\varepsilon\nu}+1)$, with

$$z\frac{d^2G_{k_1}}{dz^2}+(\mu+1-z)\frac{dG_{k_1}}{dz}-\frac{1}{4}[2(\mu+1)-\lambda]G_{k_1}=0, \tag{60}$$

where $z=\rho^2$. Provided that $-[2(\mu+1)-\lambda]/4$ is an integer, say $k_1=0,1,2,\ldots$, the solutions of (60) are the generalized Laguerre polynomials. Hence, the radial solutions are

$$R_{k_1}(\rho)=N_{k_1}\rho^{\mu}e^{-\rho^2/2}L_{k_1}^{\mu}(\rho^2),\quad N_{k_1}=\left[\frac{2\Gamma(k_1+1)}{\Gamma(k_1+\mu+1)}\right]^{1/2}. \tag{61}$$

One can easily verify that $\psi_k(\theta)$'s and $R_{k_1}(\rho)$'s obey the following orthogonality relations:

$$\int_0^{\infty}R_{k_1}(\rho)R_{k_1'}(\rho)r\,dr=\delta_{k_1k_1'},\quad \int_0^{\pi/2}\psi_k(\theta)\psi_{k'}(\theta)d\theta=\delta_{kk'}. \tag{62}$$

As a result the eigenfunctions of H_1 can be written in polar coordinates as follows:

$$\Psi_{\ell}^{(1)\overline{\varepsilon\varepsilon}}(r,\theta)=N_{k_1}N_{k_2}^{\mathrm{PT}}(\beta r)^{\mu}e^{-\beta^2r^2/2}\sin^{1/2+\varepsilon\nu}\theta\cos^{1/2+\overline{\varepsilon\nu}}\theta L_{k_1}^{\mu}(\beta^2r^2)P_{k_2}^{(\varepsilon\nu,\overline{\varepsilon\nu})}(\cos 2\theta), \tag{63}$$

with $\ell=k_1+k_2;\ell,k_1,k_2=0,1,2,\ldots$, and $\mu=(2k_2+\varepsilon\nu+\overline{\varepsilon\nu}+1)$. Since $\psi_k(\theta)$ given by (59) will be used in generating $V_0^{(k)}$ potentials, in writing (63) we have changed the quantum number k as k_2. Observe that a similar change $(n\to n_2)$ has been made in writing (56). Note also that the condition $-[2(\mu+1)-\lambda]/4=k_1$ gives the eigenvalue (56) for the V_1-problem, with $\ell=k_1+k_2$. We should also note that, as has been done in Eq. (54), the solutions (63) may be extended to all xy plane such that they have definite parity under 2D parity transformation: $(r,\theta)\to(r,\theta+\pi)$.

Inserting ψ_k and Ψ_n into (51) explicit expressions of the potentials labeled by the quantum numbers k and n become available. Besides that presented in Sec. VI several more special subfamilies can be identified. In doing that one should take care of the range of the parameters and the domain of definition for potentials. The bound states of $V_0^{(k)}$ and $V_2^{(n)}$ will be taken up in Sec. X after considering the symmetry generators in Sec. IX.

IX. SYMMETRY GENERATORS AND THEIR ALGEBRAS

As is apparent from Secs. VII and VIII, the intertwining operators, symmetry generators, and the Hamiltonians H_0, H_2 must be labeled by the quantum numbers (k,n) of the associated potentials. In terms of $e(2)$ generators the labeled intertwining operators are

$$\begin{aligned}\mathcal{L}_{10}^{(k)}&=f_k(\theta)+J,\quad \mathcal{L}_{10}^{(k)\dagger}=f_k(\theta)-J,\\ \mathcal{L}_{21}^{(n)}&=g_n(u)+T_2,\quad \mathcal{L}_{21}^{(n)\dagger}=g_n(u)-T_2.\end{aligned} \tag{64}$$

It is easy to verify that they obey the following commutators:

$$\begin{aligned}&[\mathcal{L}_{10}^{(k)},\mathcal{L}_{10}^{(k)\dagger}]=2f_k'(\theta),\quad [\mathcal{L}_{21}^{(n)},\mathcal{L}_{21}^{(n)\dagger}]=2g_n'(u),\\ &[\mathcal{L}_{10}^{(k)},\mathcal{L}_{21}^{(n)}]=K_{-}^{(k,n)}+T_1,\quad [\mathcal{L}_{10}^{(k)\dagger},\mathcal{L}_{21}^{(n)\dagger}]=-K_{-}^{(k,n)}+T_1,\\ &[\mathcal{L}_{10}^{(k)},\mathcal{L}_{21}^{(n)\dagger}]=K_{+}^{(k,n)}-T_1,\quad [\mathcal{L}_{10}^{(k)\dagger},\mathcal{L}_{21}^{(n)}]=-K_{+}^{(k,n)}-T_1,\end{aligned} \tag{65}$$

where

$$K_{\pm}^{(k,n)}=r\cos\theta\left[g_n'(u)\pm\frac{1}{r^2}f_k'(\theta)\right].$$

By virtue of (28) we have

$$K_{+}^{(k,n)}=\tfrac{1}{2}r\cos\theta[H_2^{(k)}-H_0^{(n)}],\quad K_{-}^{(k,n)}=\tfrac{1}{2}r\cos\theta[H_0^{(k)}+H_2^{(n)}-2H_1]. \tag{66}$$

It will be convenient to start with the symmetry generators of H_1,

$$X_1^{(k)}=\mathcal{L}_{10}^{(k)}\mathcal{L}_{10}^{(k)\dagger}=H_{\mathrm{PT}}-\lambda_{1,k}, \tag{67}$$

$$Y_1^{(n)}=\mathcal{L}_{21}^{(n)\dagger}\mathcal{L}_{21}^{(n)}=H_{\mathrm{SO}}-\lambda_{2,n}, \tag{68}$$

where we have made use of $T_2 g_n(u)=g_n'(u)$. H_{PT} and H_{SO} are defined by (49) and (50). Second-order symmetry generators of $H_0^{(k)}$ and $H_2^{(n)}$ can also be written as follows:

$$X_0^{(k)}=\mathcal{L}_{10}^{(k)\dagger}\mathcal{L}_{10}^{(k)}=V_{-}^{(k)}-J^2=\overline{H}_{\mathrm{PT}}^{(k)}-\lambda_{1,k}, \tag{69}$$

$$X_2^{(n)}=\mathcal{L}_{21}^{(n)}\mathcal{L}_{21}^{(n)\dagger}=g_n^2+g_n'-T_2^2=\overline{H}_{\mathrm{SO}}^{(n)}-\lambda_{2,n}, \tag{70}$$

where

$$\overline{H}_{\mathrm{PT}}^{(k)}=-\frac{\mathrm{d}^2}{\mathrm{d}\theta^2}+V_{\mathrm{PT}}-2\partial_\theta^2\ln\psi_k(\theta), \tag{71}$$

$$\overline{H}_{\mathrm{SO}}^{(n)}=-\frac{\mathrm{d}^2}{\mathrm{d}u^2}+V_{\mathrm{SO}}-2\partial_u^2\ln\Psi_n(u). \tag{72}$$

These are the so-called super partners of H_{PT} and H_{SO}. As a result, the Hamiltonians of 1D auxiliary problems are, up to some constants, the second-order symmetry generators of H_1 and their super partners are the second-order symmetry generators of $H_0^{(k)}$ and $H_2^{(n)}$.

The simplest forms of remaining fourth-order generators seem to be their factorized forms given by (5). Making use of (65) and (67)–(70) these can be expressed in a variety of ways, some of which are as follows:

$$\begin{aligned}Y_0^{(k,n)}&=\mathcal{L}_{10}^{(k)\dagger}Y_1^{(n)}\mathcal{L}_{10}^{(k)}=\mathcal{L}_{10}^{(k)\dagger}H_{\mathrm{SO}}\mathcal{L}_{10}^{(k)}-\lambda_{2,n}X_0^{(k)}\\&=Y_1^{(n)}X_0^{(k)}-[(K_{-}^{(k,n)}-T_1)\mathcal{L}_{21}^{(n)}+\mathcal{L}_{21}^{(n)\dagger}(K_{+}^{(k,n)}+T_1)]\mathcal{L}_{10}^{(k)}\\&=X_0^{(k)}Y_1^{(n)}-\mathcal{L}_{10}^{(k)\dagger}[(K_{+}^{(k,n)}-T_1)\mathcal{L}_{21}^{(n)}+\mathcal{L}_{21}^{(n)\dagger}(K_{-}^{(k,n)}+T_1)],\end{aligned} \tag{73}$$

$$\begin{aligned}Y_2^{(k,n)}&=\mathcal{L}_{21}^{(n)}X_1^{(k)}\mathcal{L}_{21}^{(n)\dagger}=\mathcal{L}_{21}^{(n)}H_{PT}\mathcal{L}_{21}^{(n)\dagger}-\lambda_{1,k}X_2^{(n)}\\&=X_1^{(k)}X_2^{(n)}-[(K_{-}^{(k,n)}+T_1)\mathcal{L}_{10}^{(k)\dagger}-\mathcal{L}_{10}^{(k)}(K_{+}^{(k,n)}+T_1)]\mathcal{L}_{21}^{(n)\dagger}\\&=X_2^{(n)}X_1^{(k)}-\mathcal{L}_{21}^{(n)}[\mathcal{L}_{10}^{(k)}(K_{-}^{(k,n)}-T_1)-(K_{+}^{(k,n)}-T_1)\mathcal{L}_{10}^{(k)\dagger}].\end{aligned} \tag{74}$$

At this point we have to emphasize the following. The existence of $\lambda_{1,k}$ and $\lambda_{2,n}$ as additive constants in $X_1^{(k)}$, $Y_1^{(n)}$ and $X_0^{(k)}$, $X_2^{(n)}$ seems to be redundant in regard of superintegrability of H_1. In particular, our labeling of the fourth-order generators with two indices may seem as if we have more symmetries than is needed for superintegrability. But an inspection of the first lines of Eqs. (73) and (74) immediately shows that, for a given, say, k and all n the set $\{Y_0^{(k,n)},X_0^{(k)}\}$ spans only a 2D vector space. As fourth-order symmetries labeled with one index one may take

$$\overline{Y}_0^{(k)}\equiv Y_0^{(k,n)}+\lambda_{2,n}X_0^{(k)}=\mathcal{L}_{10}^{(k)\dagger}H_{\mathrm{SO}}\mathcal{L}_{10}^{(k)},$$

$$\overline{Y_2^{(n)}} \equiv Y_2^{(k,n)} + \lambda_{1,k} X_2^{(n)} = \mathcal{L}_{21}^{(n)} H_{\rm PT} \mathcal{L}_{21}^{(n)\dagger} - \lambda_{1,k} X_2^{(n)}.$$

However, for overall consistency of the hierarchy such as intertwining of H_1 with $H_0^{(k)}$, $H_2^{(n)}$ and, as we will show in Sec. V, in determining the spectra of $H_0^{(k)}$ and $H_2^{(n)}$ these seemingly redundant constants and labels play an essential role.

One of the virtues of our approach is that the commutativity of the symmetry generators with the corresponding Hamiltonian is guaranteed by construction from the outset. For justification we first note that the relations

$$[H_1, X_1^{(k)}] = 0 = [H_1, Y_1^{(k)}], \quad k = 0,1,\ldots, \tag{75}$$

immediately follow from the fact that $X_1^{(k)}$ and $Y_1^{(k)}$ emerge from the separation of H_1 in different coordinate systems. Second at a glimpse of Eqs. (67)–(72) we observe that

$$X_0^{(k)} = X_1^{(k)} - 2\partial_\theta^2 \ln \psi_k(\theta), \quad X_2^{(n)} = Y_1^{(n)} - 2\partial_u^2 \ln \Psi_n(u).$$

That is, the second-order symmetry generators of $H_0^{(k)}$ and $H_2^{(n)}$ are Darboux transforms of symmetry generators of H_1 as are, apart from the factor r^{-2}, $H_0^{(k)}$ and $H_2^{(n)}$ Darboux transforms of H_1 along different legs of diagram (3). In view of this fact the relations

$$[H_0^{(k)}, X_0^{(k)}] = 0 = [H_2^{(n)}, X_2^{(n)}], \quad n,k = 0,1,\ldots, \tag{76}$$

follow from, or, in a sense, are Darboux transforms of (75). Only the explicit check of

$$[H_0^{(k)}, Y_0^{(k,n)}] = 0 = [H_2^{(n)}, Y_2^{(k,n)}], \quad n,k = 0,1,\ldots, \tag{77}$$

tediously takes a lot of time. This shows an advantage of our method compared with the conventional approach in which much effort is devoted to verify the commutativity for specified forms of generators. There it is known that for symmetries higher than second order, equations resulting from commutativity are almost intractable.

It is not so hard to check that $[X_j^{(\,)}, Y_j^{(\,)}] \neq 0$, $j = 0,1,2$, since the highest order derivatives with constant coefficients will appear on the right-hand side. For example,

$$[X_0^{(k)}, Y_0^{(k,n)}]_{\rm hot} = [J^2, JT_2^2 J] = 4T_1T_2J^3 + 2(2T_1^2 - 2T_2^2 + T_1T_2)J^2 - 8T_1T_2J,$$

$$[X_2^{(n)}, Y_2^{(k,n)}]_{\rm hot} = [T_2^2, T_2J^2T_2] = 2T_2^4 - 6T_1^2T_2^2 - 4T_1T_2^3J,$$

where $[X_0^{(k,n)}, Y_0^{(k,n)}]_{\rm hot}$ represents only the highest order terms resulting from $[X_0^{(k)}, Y_0^{(k,n)}]$. Therefore, the symmetry generators of each potential do not close in a finite dimensional Lie algebra structure. Note that by the Jacobi identity $Z_j = [X_j, Y_j]$, $j = 0,1,2$, is also a symmetry generator, but it is algebraically dependent to X_j and Y_j.

There is an elegant way of expressing the symmetry algebra of H_1. For this purpose we introduce the generators

$$X_\pm = \frac{1}{4\beta^2}\left(-\partial_x^2 \pm \frac{1}{2}\alpha x^2 + \frac{b}{x^2}\right), \quad D_1 = \frac{1}{4}(1 + 2x\partial_x), \tag{78}$$

$$Y_\pm = \frac{1}{4\beta^2}\left(-\partial_y^2 \pm \frac{1}{2}\alpha y^2 + \frac{c}{y^2}\right), \quad D_2 = \frac{1}{4}(1 + 2y\partial_y), \tag{79}$$

which obey the Lie algebras

$$[X_\pm, D_1] = X_\mp, \quad [X_+, X_-] = D_1, \tag{80}$$

$$[Y_\pm, D_2] = Y_\mp, \quad [Y_+, Y_-] = D_2, \tag{81}$$

with the Casimir invariants

$$X_+^2 - X_-^2 + D_1^2 = \frac{4b-3}{16}, \quad Y_+^2 - Y_-^2 + D_2^2 = \frac{4c-3}{16}. \tag{82}$$

It is straightforward to show that in terms of (78) and (79) we have

$$\begin{aligned} H_1 &= 4\beta^2(X_+ + Y_+), \\ X_1^{(k)} &= 8(X_+Y_+ - X_-Y_- + D_1D_2) + K, \\ Y_1^{(n)} &= 4\beta^2 Y_+ - \lambda_{2,n}, \end{aligned} \tag{83}$$

where $K = b + c - \lambda_{1,k} - (1/2)$. Equations (80)–(82) are defining relations of two commuting copies of a $su(1,1)$ algebra which can be written as a direct sum $su(1,1) \oplus su(1,1)$. The basis given by (78) and (79) is connected with that mentioned in Sec. VIII by linear transformations, for instance, by comparing (57) and (79) we have $Y_+ = J_0$, $Y_- \pm D_2 = J_\pm$. Equation (83) shows that the symmetries of H_1 are quadratic in the generators of centrally extended (because of the constant K) $su(1,1) \oplus su(1,1)$ algebra.

By defining

$$W^{(k,n)} \equiv \tfrac{1}{8}[X_1^{(k)}, Y_1^{(n)}] = 4\beta^2(X_-D_2 - Y_-D_1), \tag{84}$$

one can easily show that

$$\begin{aligned} [X_1^{(k)}, W^{(k,n)}] = \{X_1^{(k)}, Y_1^{(n)}\} + X_1^{(k)}(2\lambda_{2,n} - H_1) + (2Y_1^{(n)} \\ + 2\lambda_{2,n} - H_1)(\lambda_{1,k} - 1) + H_1(b-c), \end{aligned} \tag{85}$$

$$[Y_1^{(n)}, W^{(k,n)}] = (Y_1^{(n)} + \lambda_{2,n})(H_1 - Y_1^{(n)} - \lambda_{2,n}) - 2\beta^4(X_1^{(k)} - K), \tag{86}$$

where $\{,\}$ represents the anticommutator. These explicitly show that the extended symmetry algebra of H_1 spanned by $\{H_1, X_1^{(k)}, Y_1^{(n)}, W^{(k,n)}\}$, with the inclusion of $W^{(k,n)}$, closes in a quadratic associative algebra for all values of k,n. We also observe that this algebra is a cubic associative algebra in the enveloping algebra of the centrally extended $su(1,1) \oplus su(1,1)$. Recently such finitely generated associative algebras have attracted a great deal of interest. The structure we have obtained coincides, up to some additive constants, with that presented in Ref. 31 for the Winternitz potential V_1. In Ref. 29 this structure is constructed as a cubic associative algebra in which counterparts of X_1, Y_1 are taken to be purely quadratic in the generators of $su(1,1) \oplus su(1,1)$. We end this section by emphasizing that exploring similar algebraic structures for $H_0^{(k)}$ and $H_2^{(n)}$ and connection between them seems to be an important problem which deserves to be taken up in another study.

X. BOUND STATES OF $H_0^{(k)}$, $H_2^{(n)}$ AND THEIR DEGENERACIES

Representing $\Psi_{n_1}^{\bar{\varepsilon}}$, $\Psi_{n_2}^{\varepsilon}$, and $\Psi_{\ell}^{(1)\bar{\varepsilon}\varepsilon}$ given by (52) and (56), in the Dirac notation, respectively, by the kets $|n_1\bar{\varepsilon}\rangle$, $|n_2\varepsilon\rangle$, and $|1;\ell\bar{\varepsilon}\varepsilon\rangle$, we write (56) as follows:

$$|1;\ell\bar{\varepsilon}\varepsilon\rangle = |n_1\bar{\varepsilon}\rangle|n_2\varepsilon\rangle, \quad \ell = n_1 + n_2. \tag{87}$$

In this notation, the corresponding isospectral states of $H_2^{(n)}$ are

$$|2n;\ell\bar{\varepsilon}\varepsilon\rangle = \mathcal{L}_{21}^{(n)}|1;\ell\bar{\varepsilon}\varepsilon\rangle. \tag{88}$$

From (53) [or, (55)], (56), (68), and (87) one can easily show that

$$\langle 2n;\ell\overline{\varepsilon\varepsilon}|2n;\ell\overline{\varepsilon\varepsilon}\rangle=\langle 1;\ell\overline{\varepsilon\varepsilon}|Y_1^{(n)}|1;\ell\overline{\varepsilon\varepsilon}\rangle=\langle n_2\varepsilon|H_{\rm SO}|n_2\varepsilon\rangle-\lambda_{2,n}=2\hbar\omega(n_2-n), \quad (89)$$

where $\langle\cdot|\cdot\rangle$ represents the usual inner product of $\mathcal{H}=L^2(R^2)$ and in the third line we have included $2m/\hbar^2$ into the notation. Since $\ell=n_1+n_2$, this implies that as physically acceptable states only those with $\ell>n$ will survive in the spectrum of $H_2^{(n)}$. Moreover, the degeneracies of the survived states will be shifted to $\ell-n$ since the states corresponding to $n_2\leqslant n$ cannot be normalized. As a result, the normalized states of $H_2^{(n)}$ are as follows:

$$|2n;\ell\overline{\varepsilon\varepsilon}\rangle=[2\hbar\omega(n_2-n)]^{-1/2}\mathcal{L}_{21}^{(n)}|1;\ell\overline{\varepsilon\varepsilon}\rangle, \quad (90)$$

provided that $\ell=n_1+n_2$ and $n_2>n$.

In a similar way, if we represent ψ_{k_2} and R_{k_1}'s given by (59) and (61), respectively, by the kets $|k_2\overline{\varepsilon\varepsilon}\rangle$ and $|k_1\overline{\varepsilon\varepsilon}\rangle$, the states given by (63) can be expressed as

$$|1;\ell\overline{\varepsilon\varepsilon}\rangle=|k_1\overline{\varepsilon\varepsilon}\rangle|k_2\overline{\varepsilon\varepsilon}\rangle, \quad \ell=k_1+k_2. \quad (91)$$

In that case the corresponding isospectral states of $H_0^{(k)}$ are $|0k;\ell\overline{\varepsilon\varepsilon}\rangle=\mathcal{L}_{10}^{(k)\dagger}|1;\ell\overline{\varepsilon\varepsilon}\rangle$ and by virtue of (62), (67), and (91) we have

$$\langle 0k;\ell\overline{\varepsilon\varepsilon}|0k;\ell\overline{\varepsilon\varepsilon}\rangle=\langle 1;\ell\overline{\varepsilon\varepsilon}|X_1^{(k)}|1;\ell\overline{\varepsilon\varepsilon}\rangle=\langle k_2\overline{\varepsilon\varepsilon}|H_{\rm PT}|k_2\overline{\varepsilon\varepsilon}\rangle-\lambda_{1,k}$$
$$=\frac{2\hbar^2}{m}(k_2-k)(k+k_2+\overline{\varepsilon\nu}+\varepsilon\nu+1). \quad (92)$$

Hence, the normalized states of $H_0^{(k)}$ are

$$|0k;\ell\overline{\varepsilon\varepsilon}\rangle=\left[\frac{2\hbar^2}{m}(k_2-k)(k+k_2+\overline{\varepsilon\nu}+\varepsilon\nu+1)\right]^{-1/2}\mathcal{L}_{10}^{(k)\dagger}|1;\ell\overline{\varepsilon\varepsilon}\rangle, \quad (93)$$

provided that $\ell=k_1+k_2$ and $k_2>k$. In this case the degeneracy of the state $|0k;\ell\overline{\varepsilon\varepsilon}\rangle$ is $\ell-k$. Explicit functional realizations of the states (91) and (93) can easily be obtained by applying $\mathcal{L}_{21}^{(n)}$, $\mathcal{L}_{10}^{(k)\dagger}$ to the wave functions given by (56) and (63).

XI. CONCLUDING REMARKS

The method of intertwining is a unified approach widely used in various fields of physics and mathematics such as in investigating particle propagation on a curved space,[16,24,32] in constructing matrix-Hamiltonian to realize higher dimensional superalgebras,[17,33] in solving both ordinary and partial differential equations,[16] in generating exact solutions of nonstationary Schrödinger equation,[17,34] and in constructing isospectral potentials in an arbitrary space dimension.[35] The method we have introduced increases the power and enlarges the range of applicability of the intertwining operator idea. It allows us to perform Darboux transformations in higher dimensions in such a manner that, in addition to their isospectral deformation property, they acquire integrability and superintegrability preserving property. In particular, as we have shown the realization of this method for 2D systems generates two infinite families of isospectral and superintegrable quantum systems intertwined to a 2D Winternitz system. Work on 3D realization of the method is in progress.

The space of purely second-order operators quadratic in the generators of $e(2)$ has, under the adjoint action of $E(2)$, only four orbits whose representatives can be taken to be; T_1^2, J^2, $J^2+a_0T_1^2$ and T_1J+JT_1, where a_0 is a constant. Existence of only four types Winternitz potentials is closely connected with this orbit structure since each corresponds to a different 2D orthogonal coordinate system.[3,24] T_1^2, J^2 constitute the differential parts of the symmetry generators of V_1 and account for its separation in the Cartesian and polar (hence in elliptic) coordinates. Therefore, the appearance of the Winternitz potential V_1 as the common member of two families is of no surprise; it is a direct result of our orbit prescription in constructing the intertwinings in Sec. V. We

also observe that since only T_1^2 and J^2 can be factorized as $\mathcal{L}\mathcal{L}^\dagger$ (or, as $\mathcal{L}^\dagger\mathcal{L}$) the other three Winternitz potentials cannot be utilized as V_1 in the context of this paper. In this regard, a combination of our method and the conventional approach may be used for similar purposes. Finally we point out that what made it possible to implement Darboux transformations in our approach is that when the eigenvalue equation of V_1 is separated in the Cartesian and polar coordinates, at least one of the separated equation is of the Schrödinger type.

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Generalized boundary conditions for the Aharonov–Bohm effect combined with a homogeneous magnetic field

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The most general admissible boundary conditions are derived for an idealized Aharonov–Bohm flux intersecting the plane at the origin on the background of a homogeneous magnetic field. A standard technique based on self-adjoint extensions yields a four-parameter family of boundary conditions; the other two parameters of the model are the Aharonov–Bohm flux and the homogeneous magnetic field. The generalized boundary conditions may be regarded as a combination of the Aharonov–Bohm effect with a point interaction. Spectral properties of the derived Hamtonians are studied in detail. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1463712]

I. INTRODUCTION

The purpose of this paper is to determine the most general admissible boundary conditions for the Aharonov–Bohm (AB) effect in the plane on the background of a homogeneous magnetic field, and also to investigate the basic properties of Hamiltonians obtained this way. The history of the effect goes four decades back and starts from the observation of Aharonov and Bohm[1] that the behavior of a charged quantum particle is influenced by a magnetic flux even if the field is zero in the region where the particle is localized. A particularly elegant treatment is possible in case of an idealized setup in which the AB flux is concentrated along a line perpendicularly intersecting the plane, conventionally at the origin.[2]

The boundary conditions of the previously mentioned paper are not the most general ones; the full family of such conditions giving the AB effect in the plane was derived in Ref. 3, and simultaneously also in Ref. 4. These generalized boundary conditions may be interpreted as a combination of the AB effect with a point interaction supported, too, at the origin, although this is just one possible point of view. In any case they can be described and investigated by the technique of self-adjoint extensions, which is in principle the same one as that used in Ref. 5 in which two-dimensional point interactions were introduced.

A natural question is what happens if such a system is placed into a background homogeneous magnetic field. This problem attracted some attention recently, even with a controversy: Refs. 6–8 consider the ''pure'' AB effect in this setting for the Pauli operator, i.e., a spin 1/2 particle. The last named property leads to specific behavior related to the Aharonov–Casher effect, which we will not discuss here.

Our aim here is different: we are going to consider a spinless particle with a point flux and a homogeneous background, and ask about the most general class of boundary conditions analogous to those of Refs. 3 and 4. The basic difference between the situations without and with a homogeneous magnetic field is that in the former case the spectrum is absolutely continuous and equal

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to the positive half-line possibly augmented with at most two negative eigenvalues (depending on the choice of boundary conditions), while in the latter case the spectrum is pure point and the point flux and interaction gives rise to eigenvalues in each gap between neighboring Landau levels. Our goal is to discuss these spectral properties in detail.

II. FORMULATION OF THE PROBLEM: PRELIMINARIES

We consider the symmetric operator

$$L=-(\nabla-A(\nabla))^2, \quad \mathrm{Dom}(L)=C_0^\infty(\mathbb{R}^2\backslash\{0\}),$$

where the vector potential A is a sum of two parts, $A=A_{\mathrm{hmf}}+A_{\mathrm{AB}}$, with the part A_{hmf} corresponding to the homogeneous magnetic field in the circular gauge,

$$A_{\mathrm{hmf}}=-\frac{\iota B}{2}(-x_2\,\mathrm{d}x_1+x_1\,\mathrm{d}x_2),$$

and with the part A_{AB} corresponding to the idealized AB effect,

$$A_{\mathrm{AB}}=\frac{\iota\Phi}{2\pi r^2}(-x_2\,\mathrm{d}x_1+x_1\,\mathrm{d}x_2), \quad r^2=x_1^2+x_2^2.$$

Without loss of generality we may assume that $B>0$. Further, we rescale the Aharonov–Bohm flux,

$$\alpha=-\frac{\Phi}{2\pi},$$

to have a variable which expresses the number of flux quanta and, as usual, we make use of the gauge symmetry allowing us to assume that $\alpha\in]0,1[$. Hence the case $\Phi\in 2\pi\mathbb{Z}$ is excluded since it is gauge equivalent to the vanishing AB flux. Our goal is to describe all the self-adjoint extensions of L as well as to investigate their basic properties.

It is straightforward to determine the adjoint operator L^*,

$$\psi\in\mathrm{Dom}(L^*)\Leftrightarrow\psi\in L^2(\mathbb{R}^2,\mathrm{d}^2x)\cap H^{2,2}_{\mathrm{loc}}(\mathbb{R}^2\backslash\{0\}) \ \text{ and } \ (\nabla-A(\nabla))^2\psi\in L^2(\mathbb{R}^2,\mathrm{d}^2x).$$

Next we can employ the rotational symmetry when using the polar coordinates (r,θ) and decomposing the Hilbert space into the orthogonal sum of the eigenspaces of the angular momentum,

$$L^2(\mathbb{R}^2,\mathrm{d}^2x)=\sum_{m\in\mathbb{Z}}^{\oplus}L^2(\mathbb{R}_+,r\,\mathrm{d}r)\otimes\mathbb{C}e^{\iota m\theta}. \tag{1}$$

In the polar coordinates the operator L (and correspondingly L^*) takes the form

$$L=-\frac{1}{r}\partial_r r\partial_r+\frac{1}{r^2}\left(-\iota\partial_\theta+\alpha+\frac{Br^2}{2}\right)^2.$$

The operator L^* commutes on $\mathrm{Dom}(L^*)$ with the projectors P_m onto the eigenspaces of the angular momentum,

$$P_m\psi(r,\theta)=\frac{1}{2\pi}\int_0^{2\pi}\psi(r,\theta')e^{\iota m(\theta-\theta')}\,\mathrm{d}\theta',$$

and therefore L^* decomposes in correspondence with the orthogonal sum (1),

$$L^* = \sum_{m \in \mathbb{Z}}^{\oplus} (L^*)_m . \tag{2}$$

Thus we can reduce the problem and work in the sectors $\mathrm{Ran}\, P_m$, $m \in \mathbb{Z}$. For a given spectral parameter $\lambda \in \mathbb{C}$ we choose two independent solutions (except of particular values of λ) of the differential equation

$$\left(-\frac{1}{r}\partial_r r \partial_r + \frac{1}{r^2}\left(m + \alpha + \frac{Br^2}{2} \right)^2 \right) g(r) = \lambda\, g(r), \tag{3}$$

namely

$$\begin{aligned} g_m^1(\lambda; r) &= r^{|m+\alpha|} F\left(\beta(m,\lambda), \gamma(m), \frac{Br^2}{2} \right) \exp\left(-\frac{Br^2}{4} \right), \\ g_m^2(\lambda; r) &= r^{|m+\alpha|} G\left(\beta(m,\lambda), \gamma(m), \frac{Br^2}{2} \right) \exp\left(-\frac{Br^2}{4} \right), \end{aligned} \tag{4}$$

where

$$\begin{aligned} \beta(m,\lambda) &= \frac{1}{2}\left(1 + m + \alpha + |m+\alpha| - \frac{\lambda}{B} \right), \\ \gamma(m) &= 1 + |m+\alpha|. \end{aligned} \tag{5}$$

Here F and G are confluent hypergeometric functions (Ref. 9, Chap. 13),

$$F(\beta,\gamma,z) = \sum_{n=0}^{\infty} \frac{(\beta)_n z^n}{(\gamma)_n n!},$$

and

$$G(\beta,\gamma,z) = \frac{\Gamma(1-\gamma)}{\Gamma(\beta-\gamma+1)} F(\beta,\gamma,z) + \frac{\Gamma(\gamma-1)}{\Gamma(\beta)} z^{1-\gamma} F(\beta-\gamma+1, 2-\gamma, z). \tag{6}$$

Notice that $F(\beta,\gamma,z)$ and $G(\beta,\gamma,z)$ are linearly dependent if and only if $\beta \in -\mathbb{Z}_+$. Moreover, $F(\beta,\gamma,z)$ is an entire function, particularly, it is regular at the origin while $G(\beta,\gamma,z)$ has a singularity there provided $\gamma > 1$ and $\beta \notin -\mathbb{Z}_+$, and in that case it holds true that

$$\lim_{z \to 0_+} z^{\gamma-1} G(\beta,\gamma,z) = \frac{\Gamma(\gamma-1)}{\Gamma(\beta)}.$$

Thus in the case when $1 < \gamma < 2$ we have the asymptotic behavior, as $z \to 0_+$,

$$G(\beta,\gamma,z) = \frac{\Gamma(\gamma-1)}{\Gamma(\beta)} z^{1-\gamma} + \frac{\Gamma(1-\gamma)}{\Gamma(\beta-\gamma+1)} + O(z^{2-\gamma}). \tag{7}$$

We shall also need some information about the asymptotic behavior at infinity. If $\beta \in -\mathbb{Z}_+$ then $F(\beta,\gamma,z)$ is a polynomial with the leading term $(\Gamma(\gamma)/\Gamma(\gamma-\beta))(-z)^{-\beta}$, and if $\beta \notin -\mathbb{Z}_+$ then it holds true that

$$F(\beta,\gamma,z) = \frac{\Gamma(\gamma)}{\Gamma(\beta)} e^z z^{\beta-\gamma} (1 + O(z^{-1})) \quad \text{for } z \to +\infty. \tag{8}$$

Further,

$$G(\beta,\gamma,z)=z^{-\beta}(1+O(z^{-1})) \quad \text{for } z\to+\infty.$$

III. THE STANDARD AHARONOV–BOHM HAMILTONIAN

With the above-mentioned preliminaries it is straightforward to solve the spectral problem for the standard AB Hamiltonian as we mentioned in Sec. I. This means to solve the eigenvalue problem

$$L^*\psi=\lambda\psi$$

with the boundary condition

$$\lim_{r\to 0_+}\psi(r,\theta)=0. \tag{9}$$

By virtue of the decomposition (2) the problem is reduced to the countable set of equations

$$(L^*)_m f=\lambda f, \quad m\in\mathbb{Z},$$

and hence to the differential equations (3).

The solution $g_m^2(\lambda;r)$ of (3) is ruled out because it contradicts the condition (9) and the solution $g_m^1(\lambda;r)$ belongs to $L^2(\mathbb{R}_+,r\,\mathrm{d}r)$ if and only if $\beta(m,\lambda)=-n$, with $n\in\mathbb{Z}_+$. Since it holds

$$F(-n,1+\sigma,z)=\frac{n!\,\Gamma(\sigma+1)}{\Gamma(n+\sigma+1)}L_n^\sigma(z), \quad n\in\mathbb{Z}_+,$$

we get a countable set of eigenvalues,

$$\lambda_{m,n}=B\,(m+\alpha+|m+\alpha|+2n+1), \quad m\in\mathbb{Z},n\in\mathbb{Z}_+,$$

with the corresponding eigenfunctions

$$f_{m,n}(r,\theta)=C_{m,n}\,r^{|m+\alpha|}\,L_n^{|m+\alpha|}\left(\frac{Br^2}{2}\right)\exp\left(-\frac{Br^2}{4}\right)e^{\imath m\theta},$$

where $L_n^\sigma(z)$ is a Laguerre polynomial and

$$C_{m,n}=\left(\frac{B}{2}\right)^{(1/2)(|m+\alpha|+1)}\left(\frac{n!}{\pi\,\Gamma(n+|m+\alpha|+1)}\right)^{1/2}$$

are the normalization constants.

As it is well known if we fix $m\in\mathbb{Z}$ then the functions $\{f_{m,n}(r,\theta)\}_{n=0}^\infty$ form an orthonormal basis in $L^2(\mathbb{R}_+,r\,\mathrm{d}r)\otimes\mathbb{C}\,e^{\imath m\theta}$ and so the complete set of eigenfunctions $\{f_{m,n}(r,\theta)\}_{m\in\mathbb{Z},n\in\mathbb{Z}_+}$ is an orthonormal basis in $L^2(\mathbb{R}_+,r\,\mathrm{d}r)\otimes L^2([0,2\pi],\mathrm{d}\,\theta)$. Since all the eigenvalues $\lambda_{m,n}$ are real we get in this way a well-defined self-adjoint operator which is an extension of L. We conventionally call it the standard AB Hamiltonian and denote it by H^{AB}. Thus the spectrum of H^{AB} is pure point and can be written as a union of two parts,

$$\sigma(H^{\mathrm{AB}})=\sigma_{pp}(H^{\mathrm{AB}})=\{B(2k+1);k\in\mathbb{Z}_+\}\cup\{B(2\alpha+2k+1);k\in\mathbb{Z}_+\}.$$

Notice that the eigenvalues belonging to the first part are nothing but the Landau levels. All the eigenvalues $B(2k+1)$ have infinite multiplicities while the multiplicity of the eigenvalue $B(2\alpha+2k+1)$ is finite and equals $k+1$.

A final short remark concerning the Hamiltonian H^{AB} is devoted to the Green function. Naturally, the Green function is expressible as an infinite series

$$G^{\mathrm{AB}}(z;r_1,\theta_1,r_2,\theta_2)=\frac{1}{2\pi}\sum_{m=-\infty}^{\infty} G_m^{\mathrm{AB}}(z;r_1,r_2)\,e^{\imath m(\theta_1-\theta_2)},$$

where

$$G_m^{\mathrm{AB}}(z;r_1,r_2)=2\left(\frac{B}{2}\right)^{|m+\alpha|+1}(r_1r_2)^{|m+\alpha|}\exp\left(-\frac{1}{4}B({r_1}^2+{r_2}^2)\right)\times\sum_{n=0}^{\infty}\frac{n!}{\Gamma(n+|m+\alpha|+1)}$$
$$\times\frac{L_n^{|m+\alpha|}(\frac{1}{2}B{r_1}^2)\,L_n^{|m+\alpha|}(\frac{1}{2}B{r_2}^2)}{B(m+\alpha+|m+\alpha|+2n+1)-z}.$$

The radial parts can be rewritten with the aid of the standard construction of the Green function for ordinary differential operators of second order,

$$G_m^{\mathrm{AB}}(z;r_1,r_2)=\left(\frac{B}{2}\right)^{|m+\alpha|+1}(r_1r_2)^{|m+\alpha|}\exp\left(-\frac{1}{4}B({r_1}^2+{r_2}^2)\right)\frac{\Gamma(-w(m,z))}{\Gamma(|m+\alpha|+1)}F(-w(m,z),|m$$
$$+\alpha|+1,r_<)\times G(-w(m,z),|m+\alpha|+1,r_>),$$

where

$$w(m,z)=\frac{z}{2B}-\frac{1}{2}(m+\alpha+|m+\alpha|+1)$$

and $r_<=\min(r_1,r_2)$, $r_>=\max(r_1,r_2)$. This amounts to the identity

$$\sum_{n=0}^{\infty}\frac{n!}{\Gamma(n+\sigma+1)}\frac{L_n^{\sigma}(y_1)\,L_n^{\sigma}(y_2)}{n-w}=\frac{\Gamma(-w)}{\Gamma(\sigma+1)}F(-w,\sigma+1,y_<)G(-w,\sigma+1,y_>).$$

We do not expect that a simpler form for the Green function could be derived since the Hamiltonian H^{AB} enjoys only the rotational symmetry.

IV. SELF-ADJOINT EXTENSIONS OF *L*

Recalling what has been summarized in Sec. II. it is easy to determine the deficiency indices. The solution $g_m^1(\pm\imath;r)$ diverges exponentially at infinity [cf. (8)] while $g_m^2(\pm\imath;r)$ behaves well at infinity but has a singularity at the origin of the order $r^{-|m+\alpha|}$. Thus $g_m^2(\pm\imath;r)\in L^2(\mathbb{R}_+,r\,\mathrm{d}r)$ if and only if $m=-1$ or $m=0$. This means that the deficiency indices are (2,2). For a basis in the deficiency subspaces $\mathcal{N}_{\pm\imath}$ we can choose

$$\left\{f_{m,\pm}(r,\theta)=\frac{1}{\sqrt{2\pi}}N_m\,g_m^2(\pm\imath;r)\,e^{\imath m\theta};m=-1,0\right\}.$$

Thus

$$f_{-1,\pm}(r,\theta)=\frac{1}{\sqrt{2\pi}}N_{-1}\,r^{1-\alpha}\,G\left(\frac{1}{2}\mp\frac{\imath}{2B},2-\alpha,\frac{Br^2}{2}\right)\exp\left(-\frac{Br^2}{4}\right)e^{-\imath\theta},$$

$$f_{0,\pm}(r,\theta)=\frac{1}{\sqrt{2\pi}}N_0\,r^{\alpha}\,G\left(\frac{1}{2}+\alpha\mp\frac{\imath}{2B},1+\alpha,\frac{Br^2}{2}\right)\exp\left(-\frac{Br^2}{4}\right),$$

where N_{-1} and N_0 are normalization constants making the basis orthonormal.

We shall need the explicit values of N_{-1} and N_0. Using the relation

$$W_{v,\tau}(z)=z^{\tau+1/2}e^{-z/2}\,G(\tfrac{1}{2}-v+\tau,2\tau+1,z),$$

where W is the Whittaker function we get

$$N_m^{-2}=\int_0^\infty |g_m^2(\pm\iota;r)|^2\,r\,\mathrm{d}r=\frac{1}{2}\left(\frac{2}{B}\right)^{|m+\alpha|+1}\int_0^\infty x^{-1}W_{\varrho,\sigma}(x)\,W_{\bar{\varrho},\sigma}(x)\mathrm{d}x,$$

where

$$\varrho=\frac{1}{2}\left(-m-\alpha+\frac{\iota}{B}\right),\quad \sigma=\frac{1}{2}|m+\alpha|.$$

Combining the identities (Ref. 10, 2.19.24.6)

$$\int_0^\infty x^{-1}W_{\varrho,\sigma}(x)\,W_{\mu,\sigma}(x)\mathrm{d}x=\frac{\pi}{\sin(2\pi\sigma)}\times\left(-\frac{1}{\Gamma(\frac{1}{2}-\sigma-\mu)\Gamma(\frac{3}{2}+\sigma-\varrho)}\right.$$
$$\left.{}_2F_1\left(\frac{1}{2}+\sigma-\mu,1;\frac{3}{2}+\sigma-\varrho;1\right)+\frac{1}{\Gamma(\frac{1}{2}+\sigma-\mu)\,\Gamma(\frac{3}{2}-\sigma-\varrho)}\right.$$
$$\left.{}_2F_1\left(\frac{1}{2}-\sigma-\mu,1;\frac{3}{2}-\sigma-\varrho;1\right)\right)$$

and

$${}_2F_1(a,b;c;z)=\frac{\Gamma(c)\,\Gamma(c-a-b)}{\Gamma(c-a)\,\Gamma(c-b)}\,{}_2F_1(a,b;a+b-c+1;1-z)$$
$$+\frac{\Gamma(c)\,\Gamma(a+b-c)}{\Gamma(a)\,\Gamma(b)}(1-z)^{c-a-b}\,{}_2F_1(c-a,c-b;c-a-b+1;1-z)$$

we arrive at the relation

$$\int_0^\infty x^{-1}W_{\varrho,\sigma}(x)\,W_{\mu,\sigma}(x)\mathrm{d}x=\frac{\pi}{\sin(2\pi\sigma)(\mu-\varrho)}$$
$$\times\left(-\frac{1}{\Gamma(\frac{1}{2}-\mu-\sigma)\Gamma(\frac{1}{2}-\varrho+\sigma)}+\frac{1}{\Gamma(\frac{1}{2}-\mu+\sigma)\,\Gamma(\frac{1}{2}-\varrho-\sigma)}\right).$$

Finally we get

$$N_{-1}=\left(\frac{B}{2}\right)^{(1/2)(1-\alpha)}\sqrt{\frac{\sin(\pi\alpha)}{2\pi}}\left(\mathrm{Im}\,\frac{1}{\Gamma\left(-\frac{1}{2}+\alpha+\frac{\iota}{2B}\right)\Gamma\left(\frac{1}{2}-\frac{\iota}{2B}\right)}\right)^{-1/2},$$

$$N_0=\left(\frac{B}{2}\right)^{(1/2)\,\alpha}\sqrt{\frac{\sin(\pi\alpha)}{2\pi}}\left(\mathrm{Im}\,\frac{1}{\Gamma\left(\frac{1}{2}+\frac{\iota}{2B}\right)\Gamma\left(\frac{1}{2}+\alpha-\frac{\iota}{2B}\right)}\right)^{-1/2}.$$

Let us have a look at the asymptotic behavior at the origin of the basis functions in the deficiency subspaces $\mathcal{N}_{\pm\iota}$. By (4) and (7) we have

$$\begin{aligned} g^2_{-1}(\pm\iota;r) &= a_{-1,\pm}\, r^{-1+\alpha} + b_{-1,\pm}\, r^{1-\alpha} + O(r^{1+\alpha}), \\ g^2_0(\pm\iota;r) &= a_{0,\pm}\, r^{-\alpha} + b_{0,\pm}\, r^{\alpha} + O(r^{2-\alpha}), \end{aligned} \tag{10}$$

where

$$a_{-1,\pm} = \frac{\Gamma(1-\alpha)}{\Gamma\left(\frac{1}{2} \mp \frac{\iota}{2B}\right)} \left(\frac{B}{2}\right)^{-1+\alpha}, \quad b_{-1,\pm} = \frac{\Gamma(-1+\alpha)}{\Gamma\left(-\frac{1}{2} + \alpha \mp \frac{\iota}{2B}\right)},$$

$$a_{0,\pm} = \frac{\Gamma(\alpha)}{\Gamma\left(\frac{1}{2} + \alpha \mp \frac{\iota}{2B}\right)} \left(\frac{B}{2}\right)^{-\alpha}, \quad b_{0,\pm} = \frac{\Gamma(-\alpha)}{\Gamma\left(\frac{1}{2} \mp \frac{\iota}{2B}\right)}.$$

The coefficients $a_{m,\pm}$, $b_{m,\pm}$ are related to the normalization constants N_m for it holds true that

$$\det M_{-1} = -\frac{\iota}{1-\alpha}(N_{-1})^{-2}, \quad \det M_0 = -\frac{\iota}{\alpha}(N_0)^{-2}. \tag{11}$$

where

$$M_m = \begin{pmatrix} a_{m,+} & b_{m,+} \\ a_{m,-} & b_{m,-} \end{pmatrix}.$$

Particularly, we shall need the fact that the matrices M_{-1} and M_0 are regular.

Let us now describe the closure of the operator L. In virtue of the decomposition (2) we have

$$\overline{L} = \sum_{m\in\mathbb{Z}}^{\oplus} \overline{L_m},$$

where $\overline{L_m} = (L^*)^*_m$. As is well known, $\psi \in \mathrm{Dom}(L^*)$ belongs to $\mathrm{Dom}(\overline{L})$ if and only if $\langle \psi, L^*\varphi\rangle = \langle L^*\psi, \varphi\rangle$ for all $\varphi \in \mathcal{N}_\iota + \mathcal{N}_{-\iota}$. Thus $(L^*)_m = \overline{L_m}$ for $m \notin \{-1,0\}$, and if $m \notin \{-1,0\}$ then $\varphi(r)\, e^{\iota m\theta} \in \mathrm{Dom}((L^*)_m)$ belongs to $\mathrm{Dom}(\overline{L_m})$ if and only if

$$\lim_{r\to 0_+} r\, W(\overline{\varphi(r)}, g^2_m(\pm\iota, r)) = 0,$$

where $W(f,g) = (\partial_r f)g - f\,\partial_r g$ is the Wronskian. Using the asymptotic behavior (10) and the regularity of the matrix M_m we arrive at two conditions

$$\lim_{r\to 0_+} \left(-|m+\alpha|\, r^{-|m+\alpha|}\varphi(r) - r^{-|m+\alpha|+1}\partial_r\varphi(r)\right) = 0,$$

$$\lim_{r\to 0_+} \left(|m+\alpha|\, r^{|m+\alpha|}\varphi(r) - r^{|m+\alpha|+1}\partial_r\varphi(r)\right) = 0,$$

which can be rewritten in the equivalent form,

$$\lim_{r\to 0_+} r^{-2|m+\alpha|+1}\partial_r(r^{|m+\alpha|}\varphi(r)) = 0, \quad \lim_{r\to 0_+} r^{|m+\alpha|}\varphi(r) = 0.$$

But since

$$r^{-|m+\alpha|}|\varphi(r)| \leqslant \frac{1}{2|m+\alpha|} \sup_{x\in\,]0,r[} |x^{-2|m+\alpha|+1}\partial_x(x^{|m+\alpha|}\varphi(x))|$$

we finally get a sufficient and necessary condition for $\varphi(r)e^{\imath m\theta}\in \mathrm{Dom}((L^*)_m)$ to belong to $\mathrm{Dom}(\overline{L})$, namely

$$\begin{aligned} &\lim_{r\to 0_+} r^{-1+\alpha}\varphi(r)=0 \ \text{ and } \lim_{r\to 0_+} r^{\alpha}\varphi'(r)=0 \quad \text{if } \ m=-1, \\ &\lim_{r\to 0_+} r^{-\alpha}\varphi(r)=0 \ \text{ and } \lim_{r\to 0_+} r^{-\alpha+1}\varphi'(r)=0 \ \text{ if } \ m=0. \end{aligned} \tag{12}$$

This shows that if $\psi\in \mathrm{Dom}(L^*)=\mathrm{Dom}(\overline{L})+\mathcal{N}_\imath+\mathcal{N}_{-\imath}$ then

$$\psi(r,\theta)=(\Phi_1^1(\psi)r^{-1+\alpha}+\Phi_2^1(\psi)r^{1-\alpha})e^{-\imath\theta}+\Phi_1^2(\psi)r^{-\alpha}+\Phi_2^2(\psi)r^{\alpha}+\text{a regular part.}$$

Let us formally introduce the functionals Φ_j^k on $\mathrm{Dom}(L^*)$,

$$\Phi_1^{-1}(\psi)=\lim_{r\to 0_+} r^{1-\alpha}\frac{1}{2\pi}\int_0^{2\pi}\psi(r,\theta)\,e^{\imath\theta}\,\mathrm{d}\theta,$$

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

$$\Phi_1^0(\psi)=\lim_{r\to 0_+} r^{\alpha}\frac{1}{2\pi}\int_0^{2\pi}\psi(r,\theta)\mathrm{d}\theta,$$

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

Notice that the upper index refers to the sector of angular momentum while the lower index refers to the order of the singularity. If $\psi\in\mathrm{Dom}(\overline{L})$ then according to (12) it actually holds $\Phi_j^k(\psi)=0$ for $j=1,2$, $k=-1,0$. On the other hand, if $\psi\in\mathcal{N}_\imath+\mathcal{N}_{-\imath}$ and $\Phi_j^k(\psi)=0$ for all indices $j=1,2$, $k=-1,0$, then $\psi=0$ (this is again guaranteed by the regularity of the matrices M_{-1} and M_0).

Let us introduce some more notation. It is convenient to arrange the functionals Φ_j^k into column vectors as follows:

$$\Phi_j(\psi)=\begin{pmatrix}\Phi_j^{-1}(\psi)\\ \Phi_j^0(\psi)\end{pmatrix},\quad j=1,2.$$

Further, applying the functionals to the basis functions in $\mathcal{N}_\imath+\mathcal{N}_{-\imath}$ we obtain four 2×2 diagonal matrices. More precisely, set

$$(\Phi_{j,\pm})_{k\ell}=\sqrt{2\pi}\,\Phi_j^{k-2}(f_{\ell-2,\pm}),\quad j,k,\ell=1,2.$$

Then

$$\Phi_{1,\pm}=\begin{pmatrix}N_{-1}a_{-1,\pm} & 0\\ 0 & N_0\,a_{0,\pm}\end{pmatrix},\quad \Phi_{2,\pm}=\begin{pmatrix}N_{-1}b_{-1,\pm} & 0\\ 0 & N_0\,b_{0,\pm}\end{pmatrix}.$$

Now it is straightforward to give a formal definition of a self-adjoint extension H^U of the symmetric operator L determined by a unitary operator $U:\mathcal{N}_\imath\to\mathcal{N}_{-\imath}$. We identify U with a

unitary 2×2 matrix via the choice of the orthonormal bases $\{f_{-1,\pm}, f_{0,\pm}\}$ in $\mathcal{N}_{\pm\imath}$. The self-adjoint operator H^U is unambiguously defined by the condition: $H^U \subset L^*$ and $\psi \in \mathrm{Dom}(L^*)$ belongs to $\mathrm{Dom}(H^U)$ if and only if

$$\begin{pmatrix} \Phi_1(\psi) \\ \Phi_2(\psi) \end{pmatrix} \in \mathrm{Ran}\begin{pmatrix} \Phi_{1,+} + \Phi_{1,-}U \\ \Phi_{2,+} + \Phi_{2,-}U \end{pmatrix}. \tag{13}$$

However condition (13) is rather inconvenient and we shall replace it in Sec. V by another one which is more suitable for practical purposes.

V. BOUNDARY CONDITIONS

To turn (13) into a convenient requirement which would involve boundary conditions we shall need the following proposition. Set

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

There is a one-to-one correspondence between unitary matrices $U \in U(2)$ and couples of matrices $X_1, X_2 \in \mathrm{Mat}(2,\mathbb{C})$ obeying

$$\mathrm{rank}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = 2 \tag{14}$$

and

$$X_1^* D X_2 = X_2^* D X_1 \tag{15}$$

modulo the right action of the group of regular matrices $GL(2,\mathbb{C})$. The one-to-one correspondence is given by the equality

$$\mathrm{Ran}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \mathrm{Ran}\begin{pmatrix} \Phi_{1,+} + \Phi_{1,-}U \\ \Phi_{2,+} + \Phi_{2,-}U \end{pmatrix}.$$

Let us note that the equivalence class of a couple (X_1, X_2) modulo $GL(2,\mathbb{C})$ corresponds to a two-dimensional subspace in $\mathbb{C}^4$ and hence to a point in the Grassmann manifold $\mathbb{G}_2(\mathbb{C}^4)$. The complex dimension of $\mathbb{G}_2(\mathbb{C}^4)$ equals 4, i.e., $\dim_{\mathbb{R}} \mathbb{G}_2(\mathbb{C}^4) = 8$. The points of $\mathbb{G}_2(\mathbb{C}^4)$ obeying the (''real'') condition (15) form a real four-dimensional submanifold which is diffeomorphic, according to the proposition, to the unitary group $\mathrm{U}(2)$.

To verify the proposition we first show that to any couple (X_1, X_2) with the properties (14), (15) there are related unique $Y \in GL(2,\mathbb{C})$ and $U \in \mathrm{U}(2)$ such that

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} Y = \mathbf{J}\begin{pmatrix} I \\ U \end{pmatrix}, \tag{16}$$

where we have set

$$\mathbf{J} = \begin{pmatrix} \Phi_{1,+} & \Phi_{1,-} \\ \Phi_{2,+} & \Phi_{2,-} \end{pmatrix} = \begin{pmatrix} N_{-1}a_{-1,+} & 0 & N_{-1}a_{-1,-} & 0 \\ 0 & N_0 a_{0,+} & 0 & N_0 a_{0,-} \\ N_{-1}b_{-1,+} & 0 & N_{-1}b_{-1,-} & 0 \\ 0 & N_0 b_{0,+} & 0 & N_0 b_{0,-} \end{pmatrix}.$$

Using (11) one easily finds that $\mathbf{J}$ is regular and

$$\mathbf{J}^{-1}=\iota\begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}\begin{pmatrix} \Phi_{2,-} & -\Phi_{1,-} \\ -\Phi_{2,+} & \Phi_{1,+} \end{pmatrix}.$$

Let us introduce another couple of matrices, $V_+, V_- \in \mathrm{Mat}(2,\mathbb{C})$, by the relation

$$\begin{pmatrix} V_- \\ V_+ \end{pmatrix}=\mathbf{J}^{-1}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix},$$

thus $V_\pm = \mp\,\iota D(\Phi_{2,\pm}X_1-\Phi_{1,\pm}X_2)$. It follows that

$$V_\pm^* V_\pm=(X_1^* X_2^*)\begin{pmatrix} \Phi_{2,\pm}^* D^2\Phi_{2,\pm} & -\Phi_{2,\pm}^* D^2\Phi_{1,\pm} \\ -\Phi_{1,\pm}^* D^2\Phi_{2,\pm} & \Phi_{1,\pm}^* D^2\Phi_{1,\pm} \end{pmatrix}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$$

and, consequently,

$$V_-^* V_- - V_+^* V_+=(X_1^* X_2^*)\begin{pmatrix} 0 & -\iota D \\ \iota D & 0 \end{pmatrix}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix}=\iota(X_2^* D X_1 - X_1^* D X_2)$$

for $\Phi_{j,\pm}$ and D commute (all of them are diagonal), $\Phi_{j,\pm}^*=\Phi_{j,\mp}$ and

$$-\Phi_{1,+}\Phi_{2,-}+\Phi_{1,-}\Phi_{2,+}=\iota D^{-1}$$

[cf. (11)]. Owing to the property (15) we have

$$V_-^* V_- = V_+^* V_+, \tag{17}$$

which jointly with the property (14) implies that

$$\mathrm{Ker}\, V_- = \mathrm{Ker}\, V_+ = \mathrm{Ker}\begin{pmatrix} V_- \\ V_+ \end{pmatrix}=\mathrm{Ker}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix}=0.$$

The only possible choice of the matrices Y and U satisfying (16) is

$$Y=V_-^{-1}, \quad U=V_+ V_-^{-1}.$$

The matrix U is actually unitary because of (17).

Conversely, we have to show that any couple of matrices X_1, X_2 related to a unitary matrix U according to the rule

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix}=\mathbf{J}\begin{pmatrix} I \\ U \end{pmatrix}$$

obeys (14) and (15). Condition (14) is obvious since $\mathbf{J}$ is regular and condition (15) is again a matter of a direct computation. In more detail, since it holds

$$X_1^* D X_2 - X_2^* D X_1=(IU^*)\mathbf{J}^*\begin{pmatrix} 0 & D \\ -D & 0 \end{pmatrix}\mathbf{J}\begin{pmatrix} I \\ U \end{pmatrix}$$

it suffices to verify that

$$\mathbf{J}^*\begin{pmatrix} 0 & D \\ -D & 0 \end{pmatrix}\mathbf{J}=\iota\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.$$

This concludes the proof of the above proposition.

Using this correspondence one can relate to a couple X_1, $X_2 \in \mathrm{Mat}(2,\mathbb{C})$ obeying (14) and (15) a self-adjoint extension H determined by the condition

$$\psi \in \mathrm{Dom}(H) \Leftrightarrow \begin{pmatrix} \Phi_1(\psi) \\ \Phi_2(\psi) \end{pmatrix} \in \mathrm{Ran} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}. \tag{18}$$

Two couples (X_1, X_2) and (X_1', X_2') determine the same self-adjoint extension if and only if there exists a regular matrix Y such that $(X_1', X_2') = (X_1 Y, X_2 Y)$. Moreover, all the self-adjoint extensions can be obtained in this way.

We shall restrict ourselves to an open dense subset in the space of all self-adjoint extensions by requiring the matrix X_2 to be regular. In that case we can set directly $X_2 = I$ and rename $X_1 = \Lambda$. Thus Λ is a 2×2 complex matrix satisfying

$$D\Lambda = \Lambda^* D. \tag{19}$$

The corresponding self-adjoint extension will be denoted H^Λ. The condition (18) simplifies in an obvious way. We conclude that $H^\Lambda \subset L^*$ and $\psi \in \mathrm{Dom}(L^*)$ belongs to $\mathrm{Dom}(H^\Lambda)$ if and only if

$$\Phi_1(\psi) = \Lambda \Phi_2(\psi), \tag{20}$$

and this is in fact the sought boundary condition.

Matrices Λ obeying (19) can be parametrized by four real parameters (or two real and one complex). We choose the parametrization

$$\Lambda = \begin{pmatrix} u & \alpha \overline{w} \\ (1-\alpha) w & v \end{pmatrix}, \quad u, v \in \mathbb{R}, w \in \mathbb{C}.$$

The relation between Λ and U reads

$$\Lambda = (\Phi_{1,+} + \Phi_{1,-} U)(\Phi_{2,+} + \Phi_{2,-} U)^{-1} \tag{21}$$

(provided the right-hand side makes sense).

The "most regular" among the boundary conditions is $\Phi_1(\psi) = 0$, i.e., the one determined by $\Lambda = 0$, and the corresponding self-adjoint extension is nothing but the standard Aharonov–Bohm Hamiltonian H^{AB} discussed in Sec. III. According to (21) H^{AB} corresponds to the unitary matrix

$$U = -\Phi_{1,-}^{-1} \Phi_{1,+} = \mathrm{diag} \left\{ -\frac{\Gamma\left(\frac{1}{2} + \frac{\iota}{2B}\right)}{\Gamma\left(\frac{1}{2} - \frac{\iota}{2B}\right)}, -\frac{\Gamma\left(\frac{1}{2} + \alpha + \frac{\iota}{2B}\right)}{\Gamma\left(\frac{1}{2} + \alpha - \frac{\iota}{2B}\right)} \right\}.$$

VI. THE SPECTRUM

Let us now proceed to the discussion of spectral properties of the described self-adjoint extensions. It is clear from what has been explained up to now that everything interesting is happening in the two critical sectors of the angular momentum labeled by $m = -1$ and $m = 0$. To state it more formally we decompose the Hilbert space into an orthogonal sum of the "stable" and "critical" parts,

$$\mathcal{H} = \mathcal{H}_s \oplus \mathcal{H}_c,$$

where

$$\mathcal{H}_s = \sum_{m \in \mathbb{Z} \setminus \{-1,0\}}^{\oplus} L^2(\mathbb{R}_+, r\,\mathrm{d}r) \otimes \mathbb{C} e^{\iota m \theta}, \quad \mathcal{H}_c = L^2(\mathbb{R}_+, r\,\mathrm{d}r) \otimes (\mathbb{C} e^{-\iota\theta} \oplus \mathbb{C}1).$$

A self-adjoint extension H^Λ decomposes correspondingly,

$$H^\Lambda = H^\Lambda|_{\mathcal{H}_s} \oplus H^\Lambda|_{\mathcal{H}_c},$$

and we know that on $\mathcal{H}_s$ the operator H^Λ coincides with the standard AB Hamiltonian,

$$H^\Lambda|_{\mathcal{H}_s} = H^{\mathrm{AB}}|_{\mathcal{H}_s}.$$

Thus

$$\sigma(H^\Lambda) = \sigma(H^{\mathrm{AB}}|_{\mathcal{H}_s}) \cup \sigma(H^\Lambda|_{\mathcal{H}_c})$$

and, as explained in Sec. III,

$$\sigma(H^{\mathrm{AB}}|_{\mathcal{H}_s}) = \{B(2k+1); k \in \mathbb{Z}_+\} \cup \{B(2k+2\alpha+1); k \in \mathbb{N}\},$$

where the multiplicity of the eigenvalue $B(2k+1)$ is infinite while the multiplicity of the eigenvalue $B(2k+2\alpha+1)$ equals k. On the other hand,

$$\sigma(H^{\mathrm{AB}}|_{\mathcal{H}_c}) = \{B(2k+1); k \in \mathbb{Z}_+\} \cup \{B(2k+2\alpha+1); k \in \mathbb{Z}_+\},$$

where all the eigenvalues are simple (the first set is a contribution of the sector $m=-1$ while the second one comes from the sector $m=0$). Since the deficiency indices are finite the Krein's formula[11] jointly with Weyl's theorem (Ref. 12, Theorem XIII.14) tells us that the essential spectrum $\sigma_{\mathrm{ess}}(H^\Lambda|_{\mathcal{H}_c})$ is empty for any Λ. Thus the spectrum of $H^\Lambda|_{\mathcal{H}_c}$ is formed by eigenvalues which are at most finitely degenerated and have no finite accumulation points.

Let us derive the equation on eigenvalues for the restriction $H^\Lambda|_{\mathcal{H}_c}$. Let $\lambda \in \mathbb{R}$. In each of the sectors $m=-1,0$ there exists exactly one (up to a multiplicative constant) solution of the equation $(L^*)_m f = \lambda f$ which is L^2-integrable at infinity (with respect to the measure $r\,\mathrm{d}r$) and we may take for it the function $g^2_m(\lambda;r)\,e^{\imath m\theta}$ [cf. (4)]. For a second linearly independent solution one may take $g^1_m(\lambda;r)\,e^{\imath m\theta}$ provided $\beta(m,\lambda) \notin -\mathbb{Z}_+$ [cf. (5)]. If $\beta(m,\lambda) \in -\mathbb{Z}_+$ then a possible choice of a second linearly independent solution is

$$r^{|m+\alpha|}\, H\left(\beta(m,\lambda), \gamma(m), \frac{Br^2}{2}\right) \exp\left(-\frac{Br^2}{4}\right),$$

where

$$H(\beta,\gamma,z) = z^{1-\gamma} F(\beta-\gamma+1, 2-\gamma, z)$$

[cf. (6)].

Thus λ is an eigenvalue of $H^\Lambda|_{\mathcal{H}_c}$ if and only if there exists a vector $(\mu,\nu) \in \mathbb{C}^2 \setminus \{0\}$ such that the function

$$\psi_\lambda(r,\theta) = \mu\, g^2_{-1}(\lambda;r)\, e^{-\imath\theta} + \nu\, g^2_0(\lambda;r)$$

satisfies the boundary condition (20). Using again (4) and (7) one finds that

$$\Phi_1(\psi_\lambda) = \begin{pmatrix} a_{-1} & 0 \\ 0 & a_0 \end{pmatrix} \begin{pmatrix} \mu \\ \nu \end{pmatrix}, \quad \Phi_2(\psi_\lambda) = \begin{pmatrix} b_{-1} & 0 \\ 0 & b_0 \end{pmatrix} \begin{pmatrix} \mu \\ \nu \end{pmatrix},$$

where

$$a_{-1}=\frac{\Gamma(1-\alpha)}{\Gamma\left(\frac{1}{2}-\frac{\lambda}{2B}\right)}\left(\frac{B}{2}\right)^{-1+\alpha},\quad b_{-1}=\frac{\Gamma(-1+\alpha)}{\Gamma\left(-\frac{1}{2}+\alpha-\frac{\lambda}{2B}\right)},$$

$$a_0=\frac{\Gamma(\alpha)}{\Gamma\left(\frac{1}{2}+\alpha-\frac{\lambda}{2B}\right)}\left(\frac{B}{2}\right)^{-\alpha},\quad b_0=\frac{\Gamma(-\alpha)}{\Gamma\left(\frac{1}{2}-\frac{\lambda}{2B}\right)}.$$

This immediately leads to the desired equation on eigenvalues which takes the form $\det\mathbf{A}=0$ where

$$\mathbf{A}=\begin{pmatrix} a_{-1} & 0 \\ 0 & a_0 \end{pmatrix}-\Lambda\begin{pmatrix} b_{-1} & 0 \\ 0 & b_0 \end{pmatrix}.$$

After the substitution

$$z=\frac{1}{2}-\frac{\lambda}{2B},$$

$$\text{i.e.,}\quad \lambda=B(1-2z),$$

we get

$$\frac{\Gamma(1-\alpha)\Gamma(\alpha)}{\Gamma(z)\Gamma(z+\alpha)}\frac{2}{B}-\frac{\Gamma(\alpha)\Gamma(\alpha-1)}{\Gamma(z+\alpha-1)\Gamma(z+\alpha)}\left(\frac{2}{B}\right)^{\alpha}u-\frac{\Gamma(1-\alpha)\Gamma(-\alpha)}{\Gamma(z)^2}\left(\frac{2}{B}\right)^{1-\alpha}v$$
$$+\frac{\Gamma(\alpha-1)\Gamma(-\alpha)}{\Gamma(z)\Gamma(z+\alpha-1)}(uv-\alpha(1-\alpha)|w|^2)=0.$$

To simplify somewhat the form of the equation it is convenient to rescale the parameters as follows:

$$\xi=\left(\frac{B}{2}\right)^{1-\alpha}\frac{\Gamma(\alpha)}{\Gamma(2-\alpha)}u,\quad \eta=\left(\frac{B}{2}\right)^{\alpha}\frac{\Gamma(1-\alpha)}{\Gamma(1+\alpha)}v,\quad \zeta=\sqrt{\frac{B}{2}}|w|. \tag{22}$$

Finally we arrive at an equation depending on three real parameters ξ,η,ζ, namely

$$\frac{1}{\Gamma(z)\,\Gamma(z+\alpha)}+\frac{\xi}{\Gamma(z+\alpha-1)\,\Gamma(z+\alpha)}+\frac{\eta}{\Gamma(z)^2}+\frac{\xi\,\eta-\zeta^2}{\Gamma(z)\,\Gamma(z+\alpha-1)}=0. \tag{23}$$

There is no chance to solve Eq. (23) explicitly apart from some particular cases. One of them, of course, corresponds to the standard AB Hamiltonian. This case is determined by the values of parameters $\xi=\eta=\zeta=0$ and the roots of (23) form the set $-\mathbb{Z}_+\cup(-\alpha-\mathbb{Z}_+)$. Consider also the case when $\xi=\eta=0$ and $\zeta\neq0$ with the set of roots equal to $-\mathbb{Z}_+\cup(-\alpha-\mathbb{Z}_+)\cup\{1-\alpha+\zeta^{-2}\}$. Comparing the latter case to the former one we see that there is one additional root, namely $1-\alpha+\zeta^{-2}$, which escapes to infinity when $\zeta\to0$.

In the last particular case one can also consider the limit $\zeta\to\infty$. More generally, suppose that $\det\Lambda\neq0$, i.e., $\xi\eta-\zeta^2\neq0$, replace Λ with $t\,\Lambda$ in (20) and take the limit $t\to\infty$. The limiting boundary condition reads

$$\Phi_2(\psi)=0$$

and the corresponding self-adjoint extension which we shall call H^∞ is one of those omitted when we restricted ourselves to an open dense subset in the space of all self-adjoint extensions (regarded as a a four-dimensional real manifold). Equation (23) reduces in this limit to

$$\frac{1}{\Gamma(z)\,\Gamma(z+\alpha-1)}=0 \tag{24}$$

with the set of roots $-\mathbb{Z}_+\cup(1-\alpha-\mathbb{Z}_+)$.

Another case when Eq. (23) simplifies though it is not solvable explicitly is $\zeta=0$. This is easy to understand since if $\zeta=0$ then the matrix Λ is diagonal and the two critical sectors of angular momentum do not interfere. This is reflected in the fact that Eq. (23) splits into two independent equations,

$$\frac{1}{\Gamma(z)}+\frac{\xi}{\Gamma(z+\alpha-1)}=0, \quad \frac{1}{\Gamma(z+\alpha)}+\frac{\eta}{\Gamma(z)}=0.$$

Let us briefly discuss the dependence of roots of Eq. (23) on the parameters ξ,η,ζ. Since the derivative of the left-hand side of (23) with respect to z and with the values of parameters $(\xi,\eta,\zeta)=(0,0,0)$ equals

$$\frac{(-1)^m m!}{\Gamma(-m+\alpha)}\neq 0 \quad \text{for } z=-m, \quad \text{and} \frac{(-1)^m m!}{\Gamma(-m-\alpha)}\neq 0 \quad \text{for } z=-m-\alpha,$$

where $m\in\mathbb{Z}_+$, the standard implicit function theorem (analytic case) is sufficient to conclude that the roots are analytic functions in ξ,η,ζ at least in some neighborhood of the origin (depending in general on the root). Let us denote by $z_{1,m}(\xi,\eta,\zeta)$ and $z_{2,m}(\xi,\eta,\zeta)$ the roots of (23) regarded as analytic functions in ξ,η,ζ and such that $z_{1,m}(0,0,0)=-m$ and $z_{2,m}(0,0,0)=-\alpha-m$, with $m\in\mathbb{Z}_+$. A straightforward computation results in the following power series truncated at degree 4.

Set

$$h^0_m(z)=\sum_{j=1}^{m}\frac{1}{j}-\gamma-\psi(z),$$

$$h^1_m(z)=\frac{\pi^2}{6}+\sum_{j=1}^{m}\frac{1}{j^2}-\psi'(z),$$

$$h^2_m(z)=-2\,\boldsymbol{\zeta}(3)+2\sum_{j=1}^{m}\frac{1}{j^3}-\psi''(z),$$

where γ is the Euler constant, $\psi(z)=\Gamma'(z)/\Gamma(z)$ is the digamma function, and $\boldsymbol{\zeta}$ is the zeta function. Then

$$\begin{aligned} z_{1,m}(\xi,\eta,\zeta)=&-m+\frac{(-1)^{m+1}}{m!\,\Gamma(-1-m+\alpha)}\xi+\frac{h^0_m(-1-m+\alpha)}{(m!)^2\,\Gamma(-1-m+\alpha)^2}\xi^2\\ &+\frac{(-1)^{m+1}(3\,h^0_m(-1-m+\alpha)^2+h^1_m(-1-m+\alpha))}{2\,(m!)^3\,\Gamma(-1-m+\alpha)^3}\xi^3+\frac{(-1)^m(1+m-\alpha)}{m!\,\Gamma(-1-m+\alpha)}\xi\,\zeta^2\\ &+\frac{1}{6\,(m!)^4\,\Gamma(-1-m+\alpha)^4}(4\,h^0_m(-1-m+\alpha)(4\,h^0_m(-1-m+\alpha)^2+3\,h^2_m(-1 \end{aligned}$$

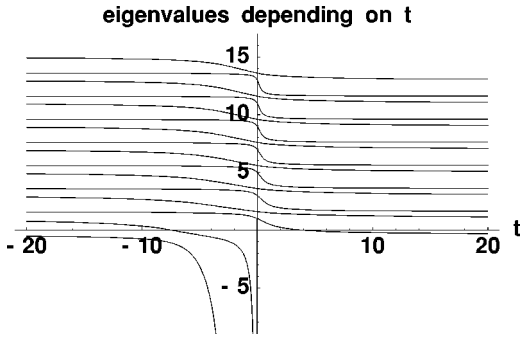

FIG. 1. The Hamiltonian is determined by the boundary conditions corresponding to the parameters $(\xi,\eta,\zeta)=(0.95\,t,0.25\,t,0.25\,t)$, $\alpha=0.3$, $B=1$.

$$-m+\alpha))+h_m^2(-1-m+\alpha))\,\xi^4+\frac{3-2\,(1+m-\alpha)\,h_m^0(-m+\alpha)}{(m!)^2\,\Gamma(-1-m+\alpha)^2}\,\xi^2\zeta^2+\cdots, \tag{25}$$

$$\begin{aligned} z_{2,m}(\xi,\eta,\zeta)=&-\alpha-m+\frac{(-1)^{m+1}}{m!\,\Gamma(-m-\alpha)}\,\eta+\frac{h_m^0(-m-\alpha)}{(m!)^2\,\Gamma(-m-\alpha)^2}\,\eta^2\\ &+\frac{(-1)^{m+1}(3\,h_m^0(-m-\alpha)^2+h_m^1(-m-\alpha))}{2\,(m!)^3\,\Gamma(-m-\alpha)^3}\,\eta^3+\frac{(-1)^m\,(m+1)}{m!\,\Gamma(-m-\alpha)}\,\eta\,\zeta^2\\ &+\frac{1}{6\,(m!)^4\,\Gamma(-m-\alpha)^4}(4\,h_m^0(-m-\alpha)(4\,h_m^0(-m-\alpha)^2+3\,h_m^2(-m-\alpha))\\ &+h_m^2(-m-\alpha))\,\eta^4+\frac{1-2\,(m+1)\,h_m^0(-m-\alpha)}{(m!)^2\,\Gamma(-m-\alpha)^2}\,\eta^2\zeta^2+\cdots. \end{aligned} \tag{26}$$

A similar analysis can be carried out to get the asymptotic behavior of roots for ξ,η,ζ large. To this end assume that $\xi\eta-\zeta^2\neq 0$ and set

$$\xi'=\frac{\xi}{\xi\eta-\zeta^2},\quad \eta'=\frac{\eta}{\xi\eta-\zeta^2},\quad \zeta'=\frac{\zeta}{\xi\eta-\zeta^2}.$$

Notice that $\xi'\,\eta'-\zeta'^2=(\xi\eta-\zeta^2)^{-1}$. Equation (23) becomes

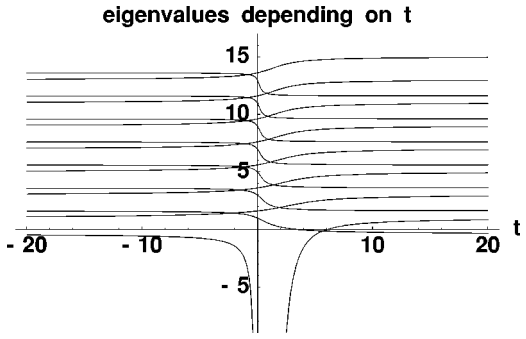

FIG. 2. The Hamiltonian is determined by the boundary conditions corresponding to the parameters $(\xi,\eta,\zeta)=(0.95\,t,-0.25\,t,0)$, $\alpha=0.3$, $B=1$.

TABLE I. Roots in the interval $]1-\alpha,+\infty[$.

Interval $]1-\alpha,+\infty[$			
Conditions			Number of roots
$\xi\geqslant 0$	$\eta\geqslant 0$	$\zeta^2>\xi\eta$	1
$\xi\geqslant 0$	$\eta\geqslant 0$	$\zeta^2\leqslant\xi\eta$	0
$\xi\geqslant 0$	$-\Gamma(1-\alpha)<\eta<0$	no condition	1
$\xi\geqslant 0$	$\eta\leqslant-\Gamma(1-\alpha)$	no condition	0
$\xi<0$	$\eta\geqslant 0$	no condition	1
$\xi<0$	$-\Gamma(1-\alpha)<\eta<0$	$\zeta^2\geqslant\xi\eta$	1
$\xi<0$	$-\Gamma(1-\alpha)<\eta<0$	$\zeta^2<\xi\eta$	2
$\xi<0$	$\eta\leqslant-\Gamma(1-\alpha)$	$\zeta^2\geqslant\xi\eta$	0
$\xi<0$	$\eta\leqslant-\Gamma(1-\alpha)$	$\zeta^2<\xi\eta$	1

$$\frac{\xi'\eta'-\zeta'^2}{\Gamma(z)\,\Gamma(z+\alpha)}+\frac{\xi'}{\Gamma(z+\alpha-1)\,\Gamma(z+\alpha)}+\frac{\eta'}{\Gamma(z)^2}+\frac{1}{\Gamma(z)\,\Gamma(z+\alpha-1)}=0. \tag{27}$$

Roots of (27) are analytic functions in ξ',η',ζ' at least in some neighborhood of the origin. Again, it would be possible to compute the beginning of the corresponding power series and to derive formulas similar to those of (25) and (26) but we avoid doing it here explicitly.

Instead we prefer to plot two graphs (Figs. 1 and 2) in order to give the reader some impression about how the eigenvalues may depend on the parameters, i.e., on the boundary conditions. In each graph we choose a line in the parameter space, $\{(\xi t,\eta t,\zeta t)\in\mathbb{R}^3; t\in\mathbb{R}\}$, and we depict the dependence on t of several first eigenvalues for the corresponding self-adjoint extension restricted to $\mathcal{H}_c$ [see (22) for the substitution]. In both graphs we have set $\alpha=0.3$ and $B=1$.

Probably the most complete general information which is available about solutions of Eq. (23) might be a localization of roots of this equation with respect to a suitable splitting of the real line into intervals. Let us choose the splitting into intervals with boundary points coinciding with the roots of Eq. (24). To get the localization let us rewrite Eq. (23), equivalently provided $z\neq -\mathbb{Z}_+\cup(1-\alpha-\mathbb{Z}_+)$, as follows:

$$\left(\frac{\Gamma(z-1+\alpha)}{\Gamma(z)}+\xi\right)\left(\frac{\Gamma(z)}{\Gamma(z+\alpha)}+\eta\right)=\zeta^2. \tag{28}$$

Put

$$F_\alpha(z)=\frac{\Gamma(z-1+\alpha)}{\Gamma(z)}$$

so that Eq. (28) can be rewritten as

$$(F_\alpha(z)+\xi)(F_{1-\alpha}(z+\alpha)+\eta)=\zeta^2. \tag{29}$$

It is easy to carry out some basic analysis of the function $F_\alpha(z)$. We have $F_\alpha'(z)=F_\alpha(z)\,(\psi(z-1+\alpha)-\psi(z))$. One observes that $F_\alpha(z)>0$ for $z\in\,]1-\alpha,+\infty[\,\cup(\cup_{m\in\mathbb{Z}_+}]-\alpha$

TABLE II. Roots in the interval $]0,1-\alpha[$.

Interval $]0,1-\alpha[$		
Conditions		Number of roots
$\xi\leqslant 0$	$\eta\geqslant-\Gamma(1-\alpha)$	0
$\xi\leqslant 0$	$\eta<-\Gamma(1-\alpha)$	1
$\xi>0$	$\eta\geqslant-\Gamma(1-\alpha)$	1
$\xi>0$	$\eta<-\Gamma(1-\alpha)$	2

TABLE III. Roots in the intervals $]-\alpha-m,-m[, m\in\mathbb{Z}_+$.

Conditions		Intervals $]-\alpha-m,-m[, m\in\mathbb{Z}_+$ Number of roots
$\xi\geqslant 0$	$\eta\leqslant 0$	0
$\xi\geqslant 0$	$\eta>0$	1
$\xi<0$	$\eta\leqslant 0$	1
$\xi<0$	$\eta>0$	2

$-m,-m[)$, and $F_\alpha(z)<0$ for $z\in\cup_{m\in\mathbb{Z}_+}]-m,1-\alpha-m[$, and in any case $F_\alpha{}'(z)<0$. In the former case this follows from the fact that $\psi(z)$ is strictly increasing on each of the intervals $]0,+\infty[$ and $]-m-1,-m[$, with $m\in\mathbb{Z}_+$. In the latter case this is a consequence of the identity

$$\psi(z-1+\alpha)-\psi(z)=\frac{\pi\sin(\pi\alpha)}{\sin(\pi z)\sin(\pi(z+\alpha))}+\int_0^\infty \frac{e^{-(1-z)t}(1-e^{-(1-\alpha)t})}{1-e^{-t}}\,\mathrm{d}t.$$

Moreover,

$$\lim_{z\to+\infty} F_\alpha(z)=0,\qquad \lim_{z\to(1-\alpha-m)\pm} F_\alpha(z)=\pm\infty,\quad F_\alpha(-m)=0\quad \text{for } m\in\mathbb{Z}_+.$$

This also implies that $F_{1-\alpha}(z+\alpha)>0$ for $z\in]0,+\infty[\cup(\cup_{m\in\mathbb{Z}_+}]-1-m,-\alpha-m[)$ and $F_{1-\alpha}(z)<0$ for $z\in\cup_{m\in\mathbb{Z}_+}]-\alpha-m,-m[$, in any case $F_{1-\alpha}{}'(z+\alpha)<0$, and

$$\lim_{z\to+\infty} F_{1-\alpha}(z+\alpha)=0,\qquad \lim_{z\to-m\pm} F_{1-\alpha}(z+\alpha)=\pm\infty,$$

$$\text{and } F_{1-\alpha}(-\alpha-m)=0 \text{ for } m\in\mathbb{Z}_+.$$

With the knowledge of these basic properties of the function $F_\alpha(z)$ it is a matter of an elementary analysis to determine the number of roots of Eq. (29) in each of the intervals $]1-\alpha,+\infty[$, $]-m,1-\alpha-m[$ and $]-\alpha-m,-m[$, with $m\in\mathbb{Z}_+$. The result is summarized in Tables I–IV.

This is to be completed with the simple observation that $1-\alpha$ is a root of (23) if and only if $\eta=-\Gamma(1-\alpha)$, and $-m$, with $m\in\mathbb{Z}_+$, is a root if and only if $\xi=0$, and finally $-\alpha-m$, with $m\in\mathbb{Z}_+$, is a root if and only if $\eta=0$.

Let us note that this localization is in agreement with a general result according to which if A and B are two self-adjoint extensions of the same symmetric operator with finite deficiency indices (d,d) then any interval $J\subset\mathbb{R}$ not intersecting the spectrum of A contains at most d eigenvalues of the operator B (including multiplicities) and no other part of the spectrum of B (Ref. 13, Sec. 8.3). Thus in our example if J is an open interval whose boundary points are either two subsequent eigenvalues of H^∞ or the lowest eigenvalue of H^∞ and $-\infty$ then any self-adjoint extension H^Λ has at most two eigenvalues in J.

TABLE IV. Roots in the intervals $]-1-m,-\alpha-m[, m\in\mathbb{Z}_+$.

Conditions		Intervals $]-1-m,-\alpha-m[, m\in\mathbb{Z}_+$ Number of roots
$\xi\leqslant 0$	$\eta\geqslant 0$	0
$\xi\leqslant 0$	$\eta<0$	1
$\xi>0$	$\eta\geqslant 0$	1
$\xi>0$	$\eta<0$	2

VII. CONCLUDING REMARKS

The above-presented discussion does not exhaust all questions related to the system under consideration. One may ask, for instance, how the state of such a particle evolves under an adiabatic change of parameters. In particular, since the model exhibits eigenvalue crossings, one may expect that there are parameter loops exhibiting a nontrivial Berry phase. Another question concerns the physical meaning of our idealized model. More specifically, one is interested in which sense the model Hamiltonian can be approximated by those with smeared flux and a regular interaction. We leave these problems to a future publication.

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Phase-amplitude method for numerically exact solution of the differential equations of the two-center Coulomb problem

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A numerically exact phase-amplitude method that has been presented earlier by P. O. Fröman, Larsson, and Hökback [J. Math. Phys. **40**, 1764–1779 (1999)] is particularized and modified in order to make it adapted to the solution of the differential equations of the two-center Coulomb problem. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1465098]

I. INTRODUCTION

We start by quoting some well-known results.

The time-independent Schrödinger equation for the motion of an electron of mass μ and charge $-e(e>0)$ in the field of two fixed Coulomb centers with charges Z_1e and Z_2e takes the following form:

$$\left(-\frac{\hbar^2}{2\mu}\Delta_{\mathbf{r}}-\frac{Z_1e}{r_1}-\frac{Z_2e}{r_2}\right)\psi(\mathbf{r})=E\psi(\mathbf{r}), \tag{1.1}$$

where r_1 and r_2 are the distances of the electron from the two centers, $\mathbf{r}$ is the position vector of the electron, and E is the electronic energy. To obtain the total energy one must add the potential energy of the two fixed charges, getting

$$E_{\text{total}}=Z_1Z_2e^2/r_{12}+E, \tag{1.2}$$

where r_{12} is the distance between the two centers. The differential equation (1.1) is separable in elliptic coordinates. If one introduces the variables

$$\xi=\frac{r_1+r_2}{r_{12}}, \quad 1\leqslant\xi<+\infty, \tag{1.3a}$$

$$\eta=\frac{r_1-r_2}{r_{12}}, \quad -1\leqslant\eta\leqslant+1, \tag{1.3b}$$

and puts

$$\psi(\mathbf{r})=X(\xi)Y(\eta)e^{im\varphi}, \tag{1.4}$$

where m is the magnetic quantum number (integer or zero), and φ is the corresponding angle, the separation yields, in *atomic units* ($\hbar=e=\mu=1$), the two differential equations

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left((\xi^2-1)\frac{\mathrm{d}X}{\mathrm{d}\xi}\right)+\left(-p^2\xi^2+b'\xi+A-\frac{m^2}{\xi^2-1}\right)X=0, \tag{1.5a}$$

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\left((1-\eta^2)\frac{\mathrm{d}Y}{\mathrm{d}\eta}\right)+\left(p^2\eta^2+b\eta-A-\frac{m^2}{1-\eta^2}\right)Y=0, \tag{1.5b}$$

where A is the separation constant and

$$p^2=-\tfrac{1}{2}r_{12}^2E, \tag{1.6a}$$

$$b'=r_{12}(Z_2+Z_1), \tag{1.6b}$$

$$b=r_{12}(Z_2-Z_1). \tag{1.6c}$$

The differential equations (1.5a) and (1.5b) are to be solved under the boundary conditions that the functions $X(\xi)$ and $Y(\eta)$ are regular, and hence finite, for $\xi=+1$, $\xi=+\infty$ and $\eta=-1$, $\eta=+1$.

The differential equations (1.5a) and (1.5b) or the corresponding differential equations in Rydberg units have been solved in various ways by several authors. In Rydberg units, results have been given by Bates, Ledsham, and Stewart,[1] Bates and Carson,[2] Bates and Reid,[3] Rosenthal and Wilson,[4] and Murai and Takatsu.[5] In atomic units, results have been given by Wallis and Hulburt,[6] Wind,[7] Peek,[8,9] Ponomarev and Puzynina,[10] Rothstein,[11] Murai,[12] Murai and Takatsu,[13] and Bhattacharje *et al.*[14] Due to the difficulty of the numerical problem these results are not in complete agreement with each other. In the present paper we shall treat the two-center Coulomb problem in a new way by means of a numerically exact method that has been fruitful in connection with other problems.

Putting

$$X(\xi)=\frac{f(\xi)}{(\xi^2-1)^{1/2}}, \tag{1.7a}$$

$$Y(\eta)=\frac{g(\eta)}{(1-\eta^2)^{1/2}}, \tag{1.7b}$$

we can transform the differential equations (1.5a) and (1.5b) into

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}+\tilde{R}(\xi)\right)f(\xi)=0, \tag{1.8a}$$

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}+R(\eta)\right)g(\eta)=0, \tag{1.8b}$$

where

$$\tilde{R}(\xi)=-p^2+\frac{b'\xi+A'}{\xi^2-1}-\frac{m^2-1}{(\xi^2-1)^2}, \tag{1.9a}$$

$$R(\eta)=-p^2+\frac{b\eta-A'}{1-\eta^2}-\frac{m^2-1}{(1-\eta^2)^2}, \tag{1.9b}$$

with

$$A'=A-p^2. \tag{1.10}$$

The differential equations (1.8a) and (1.8b) are to be solved under the boundary conditions that the functions $f(\xi)$ and $g(\eta)$ are regular and equal to zero for $\xi=+1$, $\xi=+\infty$ and $\eta=-1$, $\eta=+1$. The effective potential corresponding to the function $-\tilde{R}(\xi)$ always has the form of a single-well

potential on the interval $1 \leqslant \xi < +\infty$, while the effective potential corresponding to the function $-R(\eta)$ has the character of either a single-well potential or a double-well potential on the interval $-1 \leqslant \eta \leqslant +1$. To solve the differential equations (1.8a) and (1.8b) we shall particularize and modify the numerically exact phase-amplitude method described in Appendix B of P. O. Fröman, Larsson, and Hökback.[15] For the general background and for the notations we refer to the brief summary of that appendix that is presented in our appendix. To start the integrations of the q-equations corresponding to the differential equations (1.8a) and (1.8b) we approximate $\hat{\tilde{q}}(\xi)$ and $\hat{q}(\eta)$ in the middle of the classically allowed regions by the base functions (see Chap. 1 in Fröman and Fröman[16])

$$\tilde{Q}(\xi) = \left(-p^2 + \frac{b'\xi + A' - \tilde{C}}{\xi^2 - 1} - \frac{m^2}{(\xi^2-1)^2} \right)^{1/2}, \tag{1.11a}$$

$$Q(\eta) = \left(-p^2 + \frac{b\eta - A' + C}{1-\eta^2} - \frac{m^2}{(1-\eta^2)^2} \right)^{1/2}, \tag{1.11b}$$

where $\tilde{C}$ and C are so far unspecified constants, which are to be chosen conveniently. By solving the q-equations simultaneously one can obtain the energy eigenvalue E and the redefined separation constant A' as functions of the distance r_{12} and the quantum numbers.

II. TREATMENT OF THE ξ-EQUATION

For the differential equation (1.8a) we have $N=1$ in our appendix, and the q-equation is

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\hat{\tilde{q}}_1^{-1/2} + \tilde{R}(\xi)\hat{\tilde{q}}_1^{-1/2} = \hat{\tilde{q}}_1^{3/2}, \quad 1 \leqslant \xi < +\infty. \tag{2.1}$$

We satisfy the boundary condition at $\xi = +1$ by writing

$$f(\xi) = \tilde{F}_1 \hat{\tilde{q}}_1^{-1/2}(\xi) \sin\left(\int_1^{\xi} \hat{\tilde{q}}_1(\xi)\mathrm{d}\xi \right), \quad 1 \leqslant \xi < +\infty, \tag{2.2}$$

and then we satisfy the boundary condition at $\xi = +\infty$ by requiring that

$$\int_1^{+\infty} \hat{\tilde{q}}_1(\xi)\mathrm{d}\xi = (\hat{\tilde{s}}+1)\pi, \quad \hat{\tilde{s}} = 0,1,2,\ldots . \tag{2.3}$$

The numerical calculation of the integral in (2.3) is rather easily performed except when $m=0$, in which case $\hat{\tilde{q}}_1(\xi)$ approaches zero so slowly as $\xi \to +1$ that the integral in (2.3) cannot be calculated numerically with sufficient accuracy by conventional methods. P. O. Fröman, Hökback, and N. Fröman[17] have overcome this difficulty with the use of the comparison equation technique. Recalling their approximate formula (8.3.16′), we can replace (2.3) by

$$\arctan \frac{2(\xi-1)\hat{\tilde{q}}_1(\xi)}{1 + \dfrac{\xi-1}{\hat{\tilde{q}}_1(\xi)} \dfrac{\mathrm{d}\hat{\tilde{q}}_1(\xi)}{\mathrm{d}\xi}} + \int_{\xi}^{+\infty} \hat{\tilde{q}}_1(\xi)\mathrm{d}\xi = (\hat{\tilde{s}}+1)\pi, \quad \hat{\tilde{s}} = 0,1,2,\ldots, \tag{2.3′}$$

where we choose ξ to lie so close to $+1$ that the expression on the left-hand side of (2.3′) remains constant (within the prescribed degree of numerical accuracy) when ξ decreases further toward $+1$. One thus evaluates the expression on the left-hand side of (2.3′) for various values of ξ that decrease toward $+1$, and one continues until the expression in question remains constant within the prescribed degree of numerical accuracy.

III. TREATMENT OF THE η-EQUATION

The η-equation has the character of a Schrödinger equation associated with either a single-well potential or a double-well potential. For our purpose it is natural to consider the case of a single-well potential for superbarrier energies and the case of a double-well potential for subbarrier energies.

A. The case of a single-well potential

For the differential equation (1.8b) we have in this case $N=1$ in our appendix, and the q-equation is

$$\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}\hat{q}_1^{-1/2}+R(\eta)\hat{q}_1^{-1/2}=\hat{q}_1^{3/2}\ , \quad -1\leqslant\eta\leqslant+1. \tag{3.1}$$

We satisfy the boundary condition at $\eta=-1$ by writing

$$g(\eta)=F_1\hat{q}_1^{-1/2}(\eta)\sin\left(\int_{-1}^{\eta}\hat{q}_1(\eta)\mathrm{d}\eta\right), \quad -1\leqslant\eta\leqslant+1, \tag{3.2}$$

and then we satisfy the boundary condition at $\eta=+1$ by requiring that

$$\int_{-1}^{+1}\hat{q}_1(\eta)\mathrm{d}\eta=(\hat{s}+1)\pi, \quad \hat{s}=0,1,2,\ldots. \tag{3.3}$$

When $m=0$ one encounters the same difficulty with (3.3) as with (2.3), and thus one replaces (3.3) by

$$\arctan\frac{2(1+\eta')\hat{q}_1(\eta')}{1+\dfrac{1+\eta'}{\hat{q}_1(\eta')}\dfrac{\mathrm{d}\hat{q}_1(\eta')}{\mathrm{d}\eta'}}+\int_{\eta'}^{\eta''}\hat{q}_1(\eta)\mathrm{d}\eta+\arctan\frac{2(1-\eta'')\hat{q}_1(\eta'')}{1-\dfrac{1-\eta''}{\hat{q}_1(\eta'')}\dfrac{\mathrm{d}\hat{q}_1(\eta'')}{\mathrm{d}\eta''}}=(\hat{s}+1)\pi,$$

$$\hat{s}=0,1,2,\ldots, \tag{3.3$'$}$$

where one chooses η' and η'' $(>\eta')$ to lie so close to -1 and $+1$, respectively, that the expression on the left-hand side of (3.3$'$) remains constant (within the prescribed degree of numerical accuracy) when η' and η'' further approach -1 and $+1$, respectively. One thus evaluates the expression on the left-hand side of (3.3$'$) for various values of η' that decrease toward -1 and various values of η'' that increase toward $+1$, and one continues until the expression in question remains constant within the prescribed degree of numerical accuracy.

The case when the single-well potential is symmetric $(b=0)$. In this case the wave function $g(\eta)$ is either symmetric or antisymmetric. When it is symmetric, it has an even number of nodes, and the quantum number $\hat{s}$ is an even number which we write as $\hat{s}=2\hat{s}'$. When it is antisymmetric, it has an odd number of nodes, and the quantum number $\hat{s}$ is an odd number which we write as $\hat{s}=2\hat{s}'+1$. One starts the integration of (3.1) at $\eta=0$ by approximating there $\hat{q}_1(\eta)$ by the symmetric (with respect to the origin) base function $Q(\eta)$, i.e., with initial conditions such that $\hat{q}_1(\eta)$ becomes symmetric with respect to the origin. From (3.3) one then obtains

$$\int_{-1}^{0}\hat{q}_1(\eta)\mathrm{d}\eta=(\hat{s}'+\Delta)\pi, \quad \hat{s}'=0,1,2,\ldots, \tag{3.3$''$}$$

with $\Delta=1/2$ for the symmetric wave functions $g(\eta)$ and $\Delta=1$ for the antisymmetric wave functions $g(\eta)$. When $m=0$ the function $\hat{q}_1(\eta)$ approaches zero so slowly as $\eta\to-1$ that there appear difficulties in the accurate numerical calculation of the integral in (3.3$''$), and one therefore replaces this equation by

$$\arctan\frac{2(1+\eta')\hat{q}_1(\eta')}{1+\dfrac{1+\eta'}{\hat{q}_1(\eta')}\dfrac{\mathrm{d}\hat{q}_1(\eta')}{\mathrm{d}\eta'}}+\int_{\eta'}^{0}\hat{q}_1(\eta)\,\mathrm{d}\eta=(\hat{s}'+\Delta)\pi,\quad \hat{s}'=0,1,2,\ldots, \tag{3.3'''}$$

and proceeds similarly as described below (2.3′).

B. The case of a double-well potential

For the differential equation (1.8b) we have in this case $N=2$ in our appendix, and the q-equations are

$$\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}\hat{q}_n^{-1/2}+R(\eta)\hat{q}_n^{-1/2}=\hat{q}_n^{3/2},\quad n=1,2, \tag{3.4}$$

where $-1\leqslant\eta\leqslant\eta_1$ for $n=1$ and $\eta_1\leqslant\eta\leqslant+1$ for $n=2$, η_1 being a point in the potential barrier. We satisfy the boundary condition at $\eta=-1$ by writing

$$g(\eta)=F_1\hat{q}_1^{-1/2}(\eta)\sin\left(\int_{-1}^{\eta}\hat{q}_1(\eta)\,\mathrm{d}\eta\right),\quad -1\leqslant\eta\leqslant\eta_1. \tag{3.5}$$

Writing

$$g(\eta)=F_2\hat{q}_2^{-1/2}(\eta)\sin\left(\int_{\eta_1}^{\eta}\hat{q}_2(\eta)\,\mathrm{d}\eta\right)+G_2\hat{q}_2^{-1/2}(\eta)\cos\left(\int_{\eta_1}^{\eta}\hat{q}_2(\eta)\,\mathrm{d}\eta\right),\quad \eta_1\leqslant\eta\leqslant+1, \tag{3.6}$$

and matching the two expressions (3.5) and (3.6) for $g(\eta)$ at $\eta=\eta_1$, we obtain from (A5a) and (A5b) with $N=2$, $n=1$, and $G_1=0$,

$$\frac{F_2}{F_1}=\hat{q}_1^{-1/2}(\eta_1)\hat{q}_2^{-1/2}(\eta_1)\left(\frac{\hat{q}_2'(\eta_1)}{2\hat{q}_2(\eta_1)}-\frac{\hat{q}_1'(\eta_1)}{2\hat{q}_1(\eta_1)}\right)\sin\left(\int_{-1}^{\eta_1}\hat{q}_1(\eta)\,\mathrm{d}\eta\right)+\frac{\hat{q}_1^{1/2}(\eta_1)}{\hat{q}_2^{1/2}(\eta_1)}\cos\left(\int_{-1}^{\eta_1}\hat{q}_1(\eta)\,\mathrm{d}\eta\right), \tag{3.7a}$$

$$\frac{G_2}{F_1}=\frac{\hat{q}_2^{1/2}(\eta_1)}{\hat{q}_1^{1/2}(\eta_1)}\sin\left(\int_{-1}^{\eta_1}\hat{q}_1(\eta)\,\mathrm{d}\eta\right). \tag{3.7b}$$

According to (3.6) the boundary condition at $\eta=+1$ gives

$$F_2\sin\left(\int_{\eta_1}^{+1}\hat{q}_2(\eta)\,\mathrm{d}\eta\right)+G_2\cos\left(\int_{\eta_1}^{+1}\hat{q}_2(\eta)\,\mathrm{d}\eta\right)=0. \tag{3.8}$$

Inserting (3.7a) and (3.7b) into (3.8), we obtain

$$\frac{\hat{q}_2'(\eta_1)/\hat{q}_2(\eta_1)-\hat{q}_1'(\eta_1)/\hat{q}_1(\eta_1)}{2\hat{q}_1(\eta_1)\hat{q}_2(\eta_1)}\tan\left(\int_{-1}^{\eta_1}\hat{q}_1(\eta)\,\mathrm{d}\eta\right)\tan\left(\int_{\eta_1}^{+1}\hat{q}_2(\eta)\,\mathrm{d}\eta\right)+\frac{1}{\hat{q}_1(\eta_1)}\tan\left(\int_{-1}^{\eta_1}\hat{q}_1(\eta)\,\mathrm{d}\eta\right)+\frac{1}{\hat{q}_2(\eta_1)}\tan\left(\int_{\eta_1}^{+1}\hat{q}_2(\eta)\,\mathrm{d}\eta\right)=0. \tag{3.9}$$

When $m=0$ one encounters the same difficulty with (3.9) as with (3.3), and one masters this difficulty analogously as described below (3.3), i.e., by replacing in (3.9)

$$\int_{-1}^{\eta_1}\hat{q}_1(\eta)\mathrm{d}\eta$$

by

$$\arctan\frac{2(1+\eta')\hat{q}_1(\eta')}{1+\dfrac{1+\eta'}{\hat{q}_1(\eta')}\dfrac{\mathrm{d}\hat{q}_1(\eta')}{\mathrm{d}\eta'}}+\int_{\eta'}^{\eta_1}\hat{q}_1(\eta)\mathrm{d}\eta$$

and

$$\int_{\eta_1}^{+1}\hat{q}_2(\eta)\mathrm{d}\eta$$

by

$$\int_{\eta_1}^{\eta''}\hat{q}_2(\eta)\mathrm{d}\eta+\arctan\frac{2(1-\eta'')\hat{q}_2(\eta'')}{1-\dfrac{1-\eta''}{\hat{q}_2(\eta'')}\dfrac{\mathrm{d}\hat{q}_2(\eta'')}{\mathrm{d}\eta''}}.$$

After having modified (3.9) as described previously, one thus evaluates the expression on the left-hand side for various values of η' that decrease toward -1 and various values of η'' that increase toward $+1$, and one continues until the expression in question remains constant within the prescribed degree of numerical accuracy.

The case when the double-well potential is symmetric ($b=0$). When the double-well potential is symmetric, η_1 is chosen to be equal to zero and hence to lie at the symmetry point of the potential. To determine $\hat{q}_1(\eta)$ and $\hat{q}_2(\eta)$ we start the integrations of (3.4) by approximating $\hat{q}_1(\eta)$ and $\hat{q}_2(\eta)$ in the middle of the classically allowed regions by the symmetric (with respect to the origin) base function $Q(\eta)$, i.e., with such initial conditions that $\hat{q}_1(\eta)$ and $\hat{q}_2(\eta)$ become mirror symmetric with respect to the origin. Then we have

$$\hat{q}_1(0)=\hat{q}_2(0)>0, \tag{3.10a}$$

$$\hat{q}_1'(0)=-\hat{q}_2'(0)<0, \tag{3.10b}$$

$$\hat{q}_1(-\eta)=\hat{q}_2(\eta), \tag{3.10c}$$

$$\int_{-1}^{0}\hat{q}_1(\eta)\mathrm{d}\eta=\int_{0}^{+1}\hat{q}_2(\eta)\mathrm{d}\eta>0. \tag{3.10d}$$

Using (3.10a), (3.10b), and (3.10d), we can write (3.7a), (3.7b), and (3.9) with $\eta_1=0$ as

$$\frac{F_2}{F_1}=\frac{\hat{q}_2'(0)}{\hat{q}_2^2(0)}\sin\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right)+\cos\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right), \tag{3.11a}$$

$$\frac{G_2}{F_1}=\sin\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right), \tag{3.11b}$$

and

$$\tan\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right)\left[\tan\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right)+\frac{2\hat{q}_2^2(0)}{\hat{q}_2'(0)}\right]=0. \tag{3.12}$$

From (3.12) we obtain the two quantization conditions

$$\int_0^{+1} \hat{q}_2(\eta)\mathrm{d}\eta=(\hat{s}+1)\pi, \tag{3.13a}$$

$$\int_0^{+1} \hat{q}_2(\eta)\mathrm{d}\eta=(\hat{s}+1)\pi-\arctan\frac{2\hat{q}_2^2(0)}{\hat{q}_2'(0)}, \tag{3.13b}$$

where $\hat{s}$ is an integer. When $m=0$ one encounters the same difficulty with (3.13a) and (3.13b) as with (3.9), and one masters this difficulty in a similar way as is described below (3.3).

In the following we shall show that (3.13a) and (3.13b) are the quantization conditions for the states with antisymmetric and symmetric wave functions $g(\eta)$, respectively.

The *antisymmetric* wave function $g(\eta)$ must be equal to zero for $\eta=0$, and therefore we obtain from (3.5) with $\eta_1=0$ and (3.10d) the quantization condition

$$\int_0^{+1} \hat{q}_2(\eta)\mathrm{d}\eta=(\hat{s}+1)\pi, \quad \hat{s}=0,1,2,\ldots, \tag{3.14}$$

which is in agreement with (3.13a). Recalling (3.5) with $\eta_1=0$ and (3.10c), we realize that for $0\leqslant\eta\leqslant+1$ the antisymmetric wave function is

$$\begin{aligned} g(\eta)&=F_1\hat{q}_2^{-1/2}(\eta)\sin\left(\int_{+1}^{\eta}\hat{q}_2(\eta)\mathrm{d}\eta\right)\\ &=F_1\hat{q}_2^{-1/2}(\eta)\sin\left(\int_0^{\eta}\hat{q}_2(\eta)\mathrm{d}\eta-\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right)\\ &=F_1\cos\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right)\hat{q}_2^{-1/2}(\eta)\sin\left(\int_0^{\eta}\hat{q}_2(\eta)\mathrm{d}\eta\right)\\ &\quad -F_1\sin\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right)\hat{q}_2^{-1/2}(\eta)\cos\left(\int_0^{\eta}\hat{q}_2(\eta)\mathrm{d}\eta\right), \quad 0\leqslant\eta\leqslant+1. \end{aligned} \tag{3.15}$$

Comparing (3.6) for $\eta_1=0$ with (3.15), we see that

$$F_2=F_1\cos\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right), \tag{3.16a}$$

$$G_2=-F_1\sin\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right). \tag{3.16b}$$

With the use of (3.14) one can obtain (3.16a) and (3.16b) from (3.11a) and (3.11b) Recalling (3.14), we obtain from (3.16a) and (3.16b)

$$F_2=(-1)^{\hat{s}+1}F_1, \tag{3.17a}$$

$$G_2=0. \tag{3.17b}$$

The *symmetric* wave function $g(\eta)$ fulfills the condition $g'(0)=0$ which, with the aid of (3.5) with $\eta_1=0$, (3.10a), (3.10b), and (3.10d), can be written as

$$\tan\left(\int_0^{+1}\hat{q}_2(\eta)\mathrm{d}\eta\right)=-\frac{2\hat{q}_2^2(0)}{\hat{q}_2'(0)}. \tag{3.18}$$

It is seen that this quantization condition is in agreement with (3.13b). Recalling (3.5) with $\eta_1 = 0$ and (3.10c), we realize that for $0 \leqslant \eta \leqslant +1$ the symmetric wave function is

$$\begin{aligned} g(\eta) &= -F_1 \hat{q}_2^{-1/2}(\eta) \sin\left(\int_{+1}^{\eta} \hat{q}_2(\eta) \mathrm{d}\eta \right) \\ &= -F_1 \hat{q}_2^{-1/2}(\eta) \sin\left(\int_0^{\eta} \hat{q}_2(\eta) \mathrm{d}\eta - \int_0^{+1} \hat{q}_2(\eta) \mathrm{d}\eta \right) \\ &= -F_1 \cos\left(\int_0^{+1} \hat{q}_2(\eta) \mathrm{d}\eta \right) \hat{q}_2^{-1/2}(\eta) \sin\left(\int_0^{\eta} \hat{q}_2(\eta) \mathrm{d}\eta \right) \\ &\quad + F_1 \sin\left(\int_0^{+1} \hat{q}_2(\eta) \mathrm{d}\eta \right) \hat{q}_2^{-1/2}(\eta) \cos\left(\int_0^{\eta} \hat{q}_2(\eta) \mathrm{d}\eta \right), \quad 0 \leqslant \eta \leqslant +1. \end{aligned} \tag{3.19}$$

Comparing (3.6) for $\eta_1 = 0$ with (3.19), we see that

$$F_2 = -F_1 \cos\left(\int_0^{+1} \hat{q}_2(\eta) \mathrm{d}\eta \right), \tag{3.20a}$$

$$G_2 = F_1 \sin\left(\int_0^{+1} \hat{q}_2(\eta) \mathrm{d}\eta \right). \tag{3.20b}$$

It is seen that (3.20b) agrees with (3.11b), and with the aid of (3.18) we can obtain (3.20a) from (3.11a).

IV. NUMERICAL RESULTS

Before presenting our numerical results, we shall give a brief description of the formulas that are to be used in calculations of the energy levels and the separation constants of the two-center Coulomb system.

When $-Q^2(\eta)$ has the character of a single-well potential, which is the case when r_{12} is sufficiently small, the functions $\hat{\tilde{q}}_1(\xi)$ and $\hat{q}_1(\eta)$ are obtained by means of the differential equations (2.1) and (3.1). For given values of the quantum numbers, the quantities p^2 and A', which according to (1.6a) and (1.10) are closely related to the energy E and the separation constant A, are obtained from the appropriate ones of the quantization conditions (2.3), (2.3′), (3.3), (3.3′), (3.3″), and (3.3‴).

When $-Q^2(\eta)$ has the character of a double-well potential, which is the case when r_{12} is sufficiently large, the functions $\hat{\tilde{q}}_1(\xi)$ and $\hat{q}_1(\eta)$, $\hat{q}_2(\eta)$ are obtained by means of the differential equations (2.1) and (3.4). For given values of the quantum numbers, the quantities p^2 and A', which according to (1.6a) and (1.10) are closely related to the energy E and the separation constant A, are obtained from the appropriate ones of the quantization conditions (2.3), (2.3′), (3.9), (3.13a), and (3.13b), of which (3.9), (3.13a), and (3.13b) are to be modified when $m = 0$ as described below (3.9).

We have calculated the energy eigenvalues and the separation constants for some states of the hydrogen molecule ion with different values of the internuclear distance. We shall explain how we have performed these calculations by describing briefly our calculations for the state $1s\sigma$ with the internuclear distance equal to 10 a.u. To start the integration of the q-equations one must in some way or another have obtained fairly accurate approximate initial values of p^2 and A'. We used the initial values $p^2 = 30$ and $A' = -10$, which we obtained by approximating the numerically exact values obtained by Murai and Takatsu[13] and quoted later in this section. Using the approximate initial values $p^2 = 30$ and $A' = -10$, we thus started the numerical integration of the q-equations by approximating $\hat{\tilde{q}}(\xi)$ and $\hat{q}_1(\eta)$, $\hat{q}_2(\eta)$ by the base functions $\tilde{Q}(\xi)$ and $Q(\eta)$, respectively, in

TABLE I. The numerically exact values quoted have been obtained by Murai and Takatsu (Ref. 13). The number of digits in our results is chosen such that the error is at most five units in the last decimal.

State	r_{12} (a.u.)	Initial values p^2	Initial values $-A'$	Values obtained by the first use of the program p^2	Values obtained by the first use of the program $-A'$	Values obtained by the second use of the program p^2	Values obtained by the second use of the program $-A'$	Numerically exact values p^2	Numerically exact values $-A'$
	0.5	0.2	0.13	0.216 873 502	0.143 880 78	0.216 873 500 2	0.143 880 78	0.216 873 500 0	0.143 880 765 5
$1s\sigma$	10	30	10	30.028 936 2	9.895 643 5	30.028 936 3	9.895 643 7	30.028 936 446 8	9.895 643 268 8
	25	168	25	168.751 812 2	24.959 984 8	168.751 812 9	24.959 983	168.751 812 751 1	24.959 984 433 8
	0.5	0.06	2.02	0.064 610 682 8	2.025 815 68	0.064 610 683 1	2.025 815 667	0.064 610 683 1	2.025 815 664 3
$2p\sigma$	10	30	10	29.995 06	9.902 955 4	29.995 053 47	9.902 954 5	29.995 053 430 6	9.902 954 530 1
	25	169	25	168.751 80	24.959 983	168.751 812 8	24.959 984	168.751 812 590 0	24.959 984 447 2
	0.5	0.03	6.03	0.027 821 268 8	6.015 895	0.027 821 268 5	6.015 894 858 7	0.027 821 268 5	6.015 894 858 6
$3d\pi$	10	10	11	10.495 848	11.560 302	10.495 843 8	11.560 299 5	10.495 843 726 5	11.560 299 387 8
	25	51	25	51.489 792 2	26.529 466 28	51.489 791 91	26.529 466 30	51.489 791 921 1	26.529 466 292 0
	0.5	0.01	12.01	0.010 004 764	12.005 335	0.010 004 763 7	12.005 336 00	0.010 004 763 7	12.005 336 010 7
$5f\pi$	10	4.3	14.3	4.319 564 07	14.339 446 4	4.319 564 019 6	14.339 446 548	4.319 564 019 4	14.339 446 548 9
	25	22	25.5	22.343 044 52	25.820 881 2	22.343 044 471	25.820 881 259 9	22.343 044 470 6	25.820 881 259 9

the middle of the classically allowed regions for the ξ- and η-equations. A computer iteration program yielded the values $p^2=30.028\,936\,2$ and $A'=-9.895\,643\,5$, but could not produce more accurate values. With these values of p^2 and A' as initial values we used the computer iteration program again and obtained the values $p^2=30.028\,936\,3$ and $A'=-9.895\,643\,7$. When we again used the program with these values of p^2 and A' as initial values, the program was not able to improve the accuracy, and this was the case also for the other states for which we performed calculations. The numerically exact values for the state $1s\sigma$ with $r_{12}=10$ are $p^2=30.028\,936\,446\,8$ and $A'=-9.895\,643\,268\,8$. Our results for some states and different internuclear distances r_{12} of the hydrogen molecule ion, obtained as described previously, are presented in Table I together with numerically exact results obtained by Murai and Takatsu.[13]

APPENDIX: EXTENSION OF THE PHASE-AMPLITUDE METHOD FOR ACCURATE NUMERICAL SOLUTION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

The phase-amplitude method developed by Milne,[18] Wilson,[19] Young,[20,21] and Wheeler[22] is an efficient method for numerically exact solution of the one-dimensional Schrödinger equation that describes the motion of a quantal particle in a single-well potential. It has been extended by P. O. Fröman, Larsson, and Hökback[15] to apply to the Schrödinger equation describing a quantal particle confined in a potential with N wells separated by $N-1$ superdense barriers. This extension is, like the original phase-amplitude method, in principle numerically exact but may meet with numerical difficulties that limit the accuracy obtainable. It will be described briefly in this appendix.

Consider the differential equation

$$\frac{\mathrm{d}^2\psi}{\mathrm{dz}^2}+R(z)\psi=0, \tag{A1}$$

where, for real z-values, $R(z)$ is positive in N regions that are separated by $N-1$ regions in which $R(z)$ is negative. The boundary conditions are imposed at the points z_0 and $z_N(>z_0)$ which lie in regions where $R(z)$ is negative and are separated by N regions where $R(z)$ is positive and $N-1$ regions where $R(z)$ is negative. We introduce in the $N-1$ regions where $R(z)$ is negative further points $z_1,\ldots,z_{N-1}$ such that $z_0<z_1<\cdots<z_{N-1}<z_N$.

To solve the differential equation (A1) numerically we put

$$\psi = F_n \hat{q}_n^{-1/2}(z)\sin\left(\int_{z_{n-1}}^{z}\hat{q}_n(z)\,dz\right) + G_n \hat{q}_n^{-1/2}(z)\cos\left(\int_{z_{n-1}}^{z}\hat{q}_n(z)\,dz\right),$$
$$z_{n-1} \leqslant z \leqslant z_n, \quad n = 1,...,N, \tag{A2}$$

where F_n and G_n are constants, and $\hat{q}_n(z)$ is to be determined numerically as a nonoscillating solution of the q-equation

$$\frac{d^2}{dz^2}\hat{q}_n^{-1/2} + R(z)\hat{q}_n^{-1/2} = \hat{q}_n^{+3/2}, \tag{A3}$$

which one obtains by inserting (A2) into (A1) and requiring that the resulting equation be satisfied for arbitrary constant values of F_n and G_n. In passing we remark that the q-equation appears not only in the phase-amplitude method[15,18–22] but also in connection with the Ermakov–Lewis invariant,[23,24] which is discussed in Chap. 1 of Ref. 16; see also Ref. 25. This invariant is, however, not needed in the present paper. To determine the functions $\hat{q}_n(z)$ one starts the integration of the differential equation (A3) in the middle of the actual potential well by using for $\hat{q}_n(z)$ a phase-integral expression of convenient order. The boundary condition imposed at z_0 determines the ratio G_1/F_1. If $N=1$ the boundary condition imposed at z_1 gives rise to a quantization condition. If $N>1$ the continuity of $\psi(z)$ and $\psi'(z)$ at $z=z_n$, where $1\leqslant n\leqslant N-1$, implies the conditions

$$F_n\left[\hat{q}_n^{-1/2}(z)\sin\left(\int_{z_{n-1}}^{z}\hat{q}_n(z)\,dz\right)\right]_{z=z_n} + G_n\left[\hat{q}_n^{-1/2}(z)\cos\left(\int_{z_{n-1}}^{z}\hat{q}_n(z)\,dz\right)\right]_{z=z_n}$$
$$= F_{n+1}\left[\hat{q}_{n+1}^{-1/2}(z)\sin\left(\int_{z_n}^{z}\hat{q}_{n+1}(z)\,dz\right)\right]_{z=z_n} + G_{n+1}\left[\hat{q}_{n+1}^{-1/2}(z)\cos\left(\int_{z_n}^{z}\hat{q}_{n+1}(z)\,dz\right)\right]_{z=z_n} \tag{A4a}$$

and

$$F_n\left\{\frac{d}{dz}\left[\hat{q}_n^{-1/2}(z)\sin\left(\int_{z_{n-1}}^{z}\hat{q}_n(z)\,dz\right)\right]\right\}_{z=z_n} + G_n\left\{\frac{d}{dz}\left[\hat{q}_n^{-1/2}(z)\cos\left(\int_{z_{n-1}}^{z}\hat{q}_n(z)\,dz\right)\right]\right\}_{z=z_n}$$
$$= F_{n+1}\left\{\frac{d}{dz}\left[\hat{q}_{n+1}^{-1/2}(z)\sin\left(\int_{z_n}^{z}\hat{q}_{n+1}(z)\,dz\right)\right]\right\}_{z=z_n}$$
$$+ G_{n+1}\left\{\frac{d}{dz}\left[\hat{q}_{n+1}^{-1/2}(z)\cos\left(\int_{z_n}^{z}\hat{q}_{n+1}(z)\,dz\right)\right]\right\}_{z=z_n}, \tag{A4b}$$

from which we obtain

$$F_{n+1} = \frac{\hat{q}'_{n+1}(z_n)/\hat{q}_{n+1}(z_n) - \hat{q}'_n(z_n)/\hat{q}_n(z_n)}{2\hat{q}_{n+1}^{1/2}(z_n)\hat{q}_n^{1/2}(z_n)}\left[F_n\sin\left(\int_{z_{n-1}}^{z_n}\hat{q}_n(z)\,dz\right) + G_n\cos\left(\int_{z_{n-1}}^{z_n}\hat{q}_n(z)\,dz\right)\right]$$
$$+ \frac{\hat{q}_n^{1/2}(z_n)}{\hat{q}_{n+1}^{1/2}(z_n)}\left[F_n\cos\left(\int_{z_{n-1}}^{z_n}\hat{q}_n(z)\,dz\right) - G_n\sin\left(\int_{z_{n-1}}^{z_n}\hat{q}_n(z)\,dz\right)\right], \quad n = 1,...,\ N-1, \tag{A5a}$$

and

$$G_{n+1}=\frac{\hat{q}_{n+1}^{1/2}(z_n)}{\hat{q}_n^{1/2}(z_n)}\left[F_n\sin\left(\int_{z_{n-1}}^{z_n}\hat{q}_n(z)\mathrm{d}z\right)+G_n\cos\left(\int_{z_{n-1}}^{z_n}\hat{q}_n(z)\mathrm{d}z\right)\right],\quad n=1,...,\ N-1. \tag{A5b}$$

Formula (A5a) is a corrected version of Eq. (B6a) in Ref. 15. The numerator of the factor in front of the first bracket on the right-hand side of Eq. (B6a) in Ref. 15 is in fact to be replaced by $\hat{q}'_{n+1}(z_n)/\hat{q}_{n+1}(z_n)-\hat{q}'_n(z_n)/\hat{q}_n(z_n)$. The error appeared in a rather late version of the manuscript of Ref. 15. All calculations of the results presented there had then been performed with the use of the correct formula. Starting from the value of G_1/F_1 one can with the aid of (A5a) and (A5b) succesively obtain the values of G_n/F_n up to $n=N$. With the use of the last one of these values and the boundary condition imposed at z_N one obtains a quantization condition.

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On gauge transformations of Bäcklund type and higher order nonlinear Schrödinger equations

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We introduce a new, more general type of nonlinear gauge transformation in nonrelativistic quantum mechanics that involves derivatives of the wave function and belongs to the class of Bäcklund transformations. These transformations satisfy certain reasonable, previously proposed requirements for gauge transformations. Their application to the Schrödinger equation results in higher order partial differential equations. As an example, we derive a general family of sixth-order nonlinear Schrödinger equations, closed under our nonlinear gauge group. We also introduce a new gauge invariant current $\sigma=\rho\nabla\Delta\ln\rho$, where $\rho=\bar{\psi}\psi$. We derive gauge invariant quantities, and characterize the subclass of the sixth-order equations that is gauge equivalent to the free Schrödinger equation. We relate our development to nonlinear equations studied by Doebner and Goldin, and by Puszkarz. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1465514]

I. INTRODUCTION

The notion of nonlinear gauge transformation, introduced in quantum mechanics by Doebner and Goldin, extends the usual group of unitary gauge transformations.[1–3] The resulting nonlinear transformations act on a parametrized family of nonlinear Schrödinger equations (NLSEs) that includes the linear Schrödinger equation as a special case. They are called gauge transformations because they leave invariant the outcomes of all physical measurements. In this paper we extend the notion of gauge transformation further to include transformations that depend explicitly on derivatives of the wave function. The result is a group of transformations of Bäcklund type.[4]

As described in earlier work,[3] a (nonlinear) gauge transformation is implemented by a transformation $\psi'=\mathcal{N}[\psi]$, assumed to satisfy the following conditions.

(1) The *principle of gauge-independence of positional measurements:* Invariance is required of all quantities describing outcomes of positional measurements, including *sequences* of measurements performed successively at different times. In particular, $\rho(\mathbf{x},t)=|\psi(\mathbf{x},t)|^2$ should be invariant under $\mathcal{N}$ for the single-particle wave function ψ.

(2) *Strict locality:* If ψ is a single-particle function, the value of ψ' at $(\mathbf{x},t)$ is assumed to depend only on the value of $\mathbf{x}$, the value of t, and the value of ψ at $(\mathbf{x},t)$.

(3) A *separation condition:* If $\psi^{(N)}$ is a wave function describing a set of N noninteracting particles (i.e., a product state), then $\psi^{(N)'}$ is well defined as the product of gauge transformed single-particle wave functions. This condition ensures that gauge transformations extend to the whole N-particle hierarchy of wave functions in a way that subsystems that are uncorrelated remain so in the gauge-transformed theory.

Here we modify the condition of strict locality, allowing $\psi'(\mathbf{x},t)$ to depend not only on the

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values of $\psi(\mathbf{x},t)$, $\mathbf{x}$, and t, but also on finitely many spatial derivatives of ψ evaluated at $(\mathbf{x},t)$. Thus our transformations are local, in that $\psi'(\mathbf{x},t)$ does not depend on space-time points any distance from $(\mathbf{x},t)$, but they are no longer "strictly" local, since derivative terms are allowed. We shall call this property *weak locality*. One motivation for introducing this generalization is to explore the relation between the resulting nonlinear gauge generalization of the Schrödinger equation and the equations proposed by Puszkarz.[5]

The condition that our set of transformations forms a group (i.e., that it is closed under composition and includes all inverse transformations) while the number of derivatives of ψ remains bounded, imposes an additional restriction. This *group property* is automatically satisfied in the strictly local theory, but here it requires explicit discussion. Thus, we shall add it to the conditions already mentioned. We then call the transformations that obey the following four conditions *weakly local gauge transformations:* (1) the principle of gauge-independence of positional measurements; $(2')$ weak locality; (3) the separation condition; and (4) the group property.

In Sec. II of this paper, we first consider a general class of nonlinear, single-particle Schrödinger equations that are equivalent to the free Schrödinger equation under the assumption that condition (1) is satisfied. Using the other three conditions, we obtain a particularly simple form for weakly local gauge transformations. Following the method of "gauge generalization," [3] we then derive a general family of sixth-order nonlinear Schrödinger equations, closed under our nonlinear gauge group, which are not all equivalent to the free second-order Schrödinger equation. In Sec. III we construct a complete set of gauge invariant quantities. As particular cases, we use these to characterize the subclass of the sixth-order equations that are gauge equivalent to the Schrödinger equation, and those equivalent to the wider class of nonlinear equations studied by Doebner and Goldin. We further relate our development to the nonlinear equations proposed by Puszkarz based on additional quantum currents that involve higher derivatives of ψ.

II. GAUGE TRANSFORMATIONS AND NLSEs

Consider the transformation

$$\psi'(\mathbf{x},t)=e^{i\varphi}\psi(\mathbf{x},t), \tag{2.1}$$

where φ is a real-valued functional that depends on $\psi,\mathbf{x}$, and t. By this we mean that φ can depend explicitly on ψ, $\overline{\psi}$, derivatives of ψ and $\overline{\psi}$ of arbitrary order, integrals or integral transforms of ψ and $\overline{\psi}$, etc., as well as directly on $\mathbf{x}$ and t. Equation (2.1) preserves the probability density $\rho(\mathbf{x},t)=\overline{\psi}(\mathbf{x},t)\psi(\mathbf{x},t)$, as required by the first condition in Sec. I, but if nonlocal it does not generally respect sequences of positional measurements. The following then describes the general class of NLSEs that are equivalent via (2.1) to the free Schrödinger equation: if ψ' satisfies

$$i\frac{\partial\psi'}{\partial t}+\frac{\hbar}{2m}\Delta\psi'=i\frac{\partial\psi'}{\partial t}-\nu_1'\Delta\psi'=0, \tag{2.2}$$

then ψ satisfies the NLSE

$$i\frac{\partial\psi}{\partial t}-\nu_1'\Delta\psi+iI[\psi,\mathbf{x},t]\psi+R[\psi,\mathbf{x},t]\psi=0, \tag{2.3}$$

where

$$R[\psi,\mathbf{x},t]=\frac{\partial\varphi}{\partial t}-2\nu_1'\left(\frac{\nabla\varphi\cdot\hat{\mathbf{j}}}{\rho}+\frac{1}{2}(\nabla\varphi)^2\right) \tag{2.4}$$

and

$$I[\psi,\mathbf{x},t]=\nu_1'\left(\Delta\varphi+\frac{\nabla\varphi\cdot\nabla\rho}{\rho}\right)=\nu_1'\left[\frac{1}{\rho}\nabla\cdot(\rho\nabla\varphi)\right], \tag{2.5}$$

with

$$\hat{\mathbf{j}}=\frac{m}{\hbar}\mathbf{j}=\frac{1}{2i}[\bar{\psi}\nabla\psi-(\nabla\bar{\psi})\psi]. \tag{2.6}$$

The verification is by direct substitution of (2.1) into (2.2).

As was shown by Doebner and Goldin,[1] a general form for strictly local gauge transformations (that satisfy all the initial requirements discussed in Sec. I) corresponds to the choice

$$\varphi=\tfrac{1}{2}\gamma(t)\ln\rho+[\Lambda(t)-1]S+\theta(\mathbf{x},t),\quad \Lambda\neq 0, \tag{2.7}$$

where $\psi=\sqrt{\rho}\,e^{iS}$. For simplicity, we consider γ and Λ independent of t, and $\theta(\mathbf{x},t)\equiv 0$. The family of NLSEs with arbitrary coefficients that directly generalizes (2.3) and is invariant (as a family) under gauge transformations (2.1) with φ as in (2.7), then has the form[1]

$$i\frac{\partial\psi}{\partial t}=\left\{i\sum_{j=1}^{2}\nu_jR_j+\sum_{j=1}^{5}\mu_jR_j\right\}\psi, \tag{2.8}$$

where, the ν_j and μ_j are real, and

$$R_1=\frac{\nabla\cdot\hat{\mathbf{j}}}{\rho},\quad R_2=\frac{\Delta\rho}{\rho},\quad R_3=\frac{\hat{\mathbf{j}}^2}{\rho^2},\quad R_4=\frac{\hat{\mathbf{j}}\cdot\nabla\rho}{\rho^2},\quad R_5=\frac{(\nabla\rho)^2}{\rho^2}. \tag{2.9}$$

In obtaining (2.8), one uses the identity $\Delta\psi/\psi=iR_1+\frac{1}{2}R_2-R_3-\frac{1}{4}R_5$. Invariance of the family (2.8) under (2.1) and (2.7) means that if ψ satisfies an equation in this family with coefficients ν_j and μ_j, then ψ' satisfies another equation in the family with coefficients ν_j' and μ_j'; thus our choice of the primed coefficient ν_1' in writing Eq. (2.2).

Now the class of nonlinear gauge transformations in quantum mechanics can be essentially extended if we replace strict locality by weak locality, thus allowing the gauge functional φ to depend on derivatives of ψ. Under this assumption the gauge transformation is no longer simply a point transformation; it is a *Bäcklund transformation*.[4] Here we consider gauge transformations of Bäcklund type that form a group, satisfying the physically motivated requirements discussed in Sec. I, with strict locality replaced by weak locality.

We observe that if φ is permitted to depend on derivatives of S as well as derivatives of ρ, then the set of gauge transformations in general does not respect the group property. However, if the derivatives of S are excluded from φ, then the transformations do respect this property. One way to see this is to write nonlinear gauge transformations as they act on logarithmic coordinates T and S, with $\ln\psi=T+iS$ (so that $T=\frac{1}{2}\ln\rho$), omitting for simplicity the explicit $\mathbf{x}$ and t dependence:

$$\begin{pmatrix}S'\\T'\end{pmatrix}=\begin{pmatrix}L & G\\0 & 1\end{pmatrix}\begin{pmatrix}S\\T\end{pmatrix}, \tag{2.10}$$

where L is a linear or nonlinear functional of S and its derivatives, and G is a linear or nonlinear functional of T and its derivatives. In the strictly local case, we have $L[S]=\Lambda S$ and $G[T]=\gamma T$. If we perform two transformations (2.10) successively, $T''=T'=T$ and $S''=L_2[L_1[S]+G_1[T]\,]+G_2[T]$. Then derivatives present in the form of G never act successively, so that their order does not increase; but derivatives in the form of L do act successively. Thus the group property, with the condition that the number of derivatives of ψ remains bounded, rules out derivative terms in L—but not in G.

Now a simple gauge transformation that is no longer strictly local, but satisfies the four requirements discussed in Sec. I, has the form (2.1) with

$$\varphi=\tfrac{1}{2}\gamma\ln\rho+(\Lambda-1)S+\eta\Delta\ln\rho=\tfrac{1}{2}\gamma\ln\rho+(\Lambda-1)S+\eta(R_2-R_5), \tag{2.11}$$

where η is a real parameter that, like γ and Λ, can in principle depend on t. This corresponds to the choice $G[T]=\gamma T+\eta\Delta T$ in (2.10). Thus we have a group of nonlinear gauge transformations modeled on three (in general time-dependent) parameters, obeying the group law

$$\mathcal{N}_{(\gamma_2,\Lambda_2,\eta_2)}\circ\mathcal{N}_{(\gamma_1,\Lambda_1,\eta_1)}=\mathcal{N}_{(\gamma_2+\Lambda_2\gamma_1,\Lambda_2\Lambda_1,\eta_2+\Lambda_2\eta_1)}. \tag{2.12}$$

But we note further that $G[T]$ need not be linear in T. Indeed, while the linear term $\Delta\ln\rho=R_2-R_5$ satisfies the separation condition, its nonlinear parts R_2 and R_5 do so separately! Considering a two-particle product wave function $\psi^{(2)}(\mathbf{x}_1,\mathbf{x}_2,t)=\psi_1(\mathbf{x}_1,t)\psi_2(\mathbf{x}_2,t)$, and defining $\rho^{(2)}=\overline{\psi^{(2)}}\psi^{(2)}$, $\rho_1=\overline{\psi}_1\psi_1$, and $\rho_2=\overline{\psi}_2\psi_2$, we have

$$R_2^{(2)}[\psi^{(2)}]=\frac{\Delta^{(2)}\rho^{(2)}}{\rho^{(2)}}=\frac{\Delta^{(2)}(\rho_1\rho_2)}{\rho_1\rho_2}=\frac{\Delta_1\rho_1}{\rho_1}+\frac{\Delta_2\rho_2}{\rho_2}=R_2[\psi_1]+R_2[\psi_2],$$

where $\Delta^{(2)}=\Delta_1+\Delta_2$. Similarly for R_5:

$$R_5^{(2)}[\psi^{(2)}]=\frac{[\nabla^{(2)}\rho^{(2)}]^2}{(\rho^{(2)})^2}=\frac{[(\nabla_1,\nabla_2)\rho_1\rho_2]^2}{(\rho_1\rho_2)^2}=R_5[\psi_1]+R_5[\psi_2].$$

Thus a further generalization of (2.11) that gives weakly local nonlinear gauge transformations is to allow the derivative terms to enter with different coefficients:

$$\varphi=\tfrac{1}{2}\gamma\ln\rho+(\Lambda-1)S+\eta_1R_2+\eta_2R_5. \tag{2.13}$$

Let us next write the gauge generalized family of NLSEs derived from (2.11). Beginning with the standard, free Schrödinger equation in the form

$$i\frac{\partial\psi'}{\partial t}=-\frac{\hbar}{2m}\left[iR_1'+\left(\frac{1}{2}R_2'-R_3'-\frac{1}{4}R_5'\right)\right]\psi', \tag{2.14}$$

where R_j' means $R_j[\psi']$, we transform by (2.1) with φ as in (2.11), and from (2.3) to (2.5) we find the form of the resulting NLSEs for ψ. We generalize, following Ref. 3, by allowing arbitrary coefficients for the nonlinear functionals, maintaining the invariance of the family of NLSEs under the nonlinear gauge group. In this fashion, we obtain

$$i\frac{\partial\psi}{\partial t}=\left\{i\sum_{j=1,2,6}\nu_jR_j+\sum_{j=1}^{12}\mu_jR_j\right\}\psi=\{i\hat{I}+\hat{R}\}\psi, \tag{2.15}$$

where $R_1,\ldots,R_5$ are as in (2.9), and where the new functionals $R_6,\ldots,R_{12}$ are given by

$$R_6=\frac{\nabla\cdot\sigma}{\rho},\quad R_7=\frac{\hat{\mathbf{j}}\cdot\sigma}{\rho^2},\quad R_8=\frac{\sigma\cdot\nabla\rho}{\rho^2}, \tag{2.16}$$

$$R_9=\frac{\sigma^2}{\rho^2},\quad R_{10}=\Delta R_1,\quad R_{11}=\Delta R_2,\quad R_{12}=\Delta R_6,$$

with

$$\sigma=\rho\nabla\Delta\ln\rho=\rho\nabla(R_2-R_5). \tag{2.17}$$

Note that the functionals $R_6,\ldots,R_{11}$ involve no higher than fourth derivatives of ψ, but the presence of the term R_{12} in (2.15) makes it in general of sixth order. If we use (2.13) in place of (2.11), we shall need separately the new currents $\rho\nabla R_2$ and $\rho\nabla R_5$. These give rise to additional nonlinear functionals in ψ.

Equation (2.15) still conserves the quantum probability $\bar{\psi}\psi$. It gives rise to the gauge invariant current

$$\mathbf{J}^{\mathrm{gi}}=-2(\nu_1\hat{\mathbf{J}}+\nu_2\nabla\rho+\nu_6\sigma) \tag{2.18}$$

that enters the continuity equation

$$\frac{\partial\rho}{\partial t}=-\nabla\cdot\mathbf{J}^{\mathrm{gi}}=2\hat{I}\rho. \tag{2.19}$$

III. GAUGE TRANSFORMATIONS AND INVARIANTS FOR THE FAMILY OF SIXTH-ORDER NLSEs

Under the gauge transformations (2.1), with φ given by (2.11), the coefficients ν_j, μ_j of (2.15) transform as follows:

$$\nu_1'=\frac{\nu_1}{\Lambda},\quad \nu_2'=\nu_2-\frac{1}{2}\gamma\frac{\nu_1}{\Lambda},\quad \nu_6'=\nu_6-\frac{\eta\nu_1}{\Lambda}, \tag{3.1}$$

$$\mu_1'=\mu_1-\frac{\gamma\nu_1}{\Lambda},\quad \mu_2'=\Lambda\mu_2-\frac{1}{2}\gamma\mu_1+\frac{\gamma^2}{2\Lambda}\nu_1-\gamma\nu_2,\quad \mu_3'=\frac{\mu_3}{\Lambda},$$

$$\mu_4'=\mu_4-\frac{\gamma\mu_3}{\Lambda},\quad \mu_5'=\Lambda\mu_5-\frac{1}{2}\gamma\mu_4+\frac{\gamma^2}{4\Lambda}\mu_3,$$

$$\mu_6'=\Lambda\mu_6-\gamma\nu_6-\eta\mu_1+\frac{\eta\gamma}{\Lambda}\nu_1,\quad \mu_7'=\mu_7-\frac{2\eta\mu_3}{\Lambda}, \tag{3.2}$$

$$\mu_8'=\Lambda\mu_8-\eta\mu_4-\frac{1}{2}\gamma\mu_7+\frac{\gamma\eta\mu_3}{\Lambda},\quad \mu_9'=\Lambda\mu_9-\eta\mu_7+\frac{\eta^2\mu_3}{\Lambda},\quad \mu_{10}'=\mu_{10}-\frac{2\eta\nu_1}{\Lambda},$$

$$\mu_{11}'=\Lambda\mu_{11}-2\eta\nu_2-\frac{1}{2}\gamma\mu_{10}+\frac{\gamma\eta\nu_1}{\Lambda},\quad \mu_{12}'=\Lambda\mu_{12}-2\eta\nu_6-\eta\mu_{10}+\frac{2\eta^2\nu_1}{\Lambda}.$$

Note that as expected, η does not enter the transformation laws for ν_1, ν_2, or $\mu_1,\ldots,\mu_5$, which are the same as in Refs. 1–3. Note also that if we begin with $\mu_{12}=0$, then $\eta\neq0$ leads to $\mu_{12}'\neq0$; thus we cannot have an invariant family of fourth-order partial differential equations for these transformations.

We now write functionally independent gauge invariants $\tau_j(j=1,2,\ldots,12)$ as follows:

$$\tau_1=\nu_2-\frac{\mu_1}{2},\quad \tau_2=\nu_1\mu_2-\mu_1\nu_2,\quad \tau_3=\frac{\mu_3}{\nu_1},\quad \tau_4=\mu_4-\mu_1\frac{\mu_3}{\nu_1},\quad \hat{\tau}_5=\mu_5\mu_3-(1/4)\mu_4^2,$$

$$\tau_6=\mu_6\nu_1-\mu_1\nu_6,\quad \tau_7=\mu_7-2\nu_6\frac{\mu_3}{\nu_1},\quad \tau_8=\mu_8\nu_1-\mu_4\nu_6+\mu_6\mu_3-(1/2)\mu_7\mu_1, \tag{3.3}$$

$$\tau_9=\mu_9\mu_3-(1/4)\mu_7^2,\quad \tau_{10}=\mu_{10}-2\nu_6,\quad \tau_{11}=\mu_{11}\nu_1-\mu_{10}\nu_2,\quad \tau_{12}=\mu_{12}\nu_1-\nu_6^2-(1/4)\mu_{10}^2.$$

In this list of gauge invariants, we have included a new quantity $\hat{\tau}_5$ instead of the original $\tau_5=\nu_1\mu_5-\nu_2\mu_4+\nu_2^2(\mu_3/\nu_1)$ that was used in Refs. 1–3, since the expression for $\hat{\tau}_5$ is simpler. The relation between these two gauge invariants is, of course, wholly gauge invariant: $\hat{\tau}_5=\tau_3\tau_5+\tau_1\tau_3(\tau_4-\tau_1\tau_3)-(1/4)\tau_4^2=\tau_3\tau_5-(\tau_1\tau_3-\frac{1}{2}\tau_4)^2$.

It should be noted that (2.15) is invariant under Galilean transformations

$$\tilde{\mathbf{x}}=\mathbf{x}-\mathbf{v}t,\quad \tilde{t}=t,\quad \tilde{\psi}(\tilde{\mathbf{x}},\tilde{t})=\psi(\mathbf{x},t)\exp\left(\frac{i}{2\nu_1}\left(\mathbf{x}\cdot\mathbf{v}+\frac{1}{2}v^2t\right)\right) \tag{3.4}$$

when

$$\frac{\mu_3}{\nu_1}=-1,\quad \mu_1+\mu_4=0,\quad \mu_7+\mu_{10}=0, \tag{3.5}$$

and consequently, the gauge invariants $\tau_1,\ldots,\tau_{12}$ must satisfy the conditions

$$\tau_3=-1,\quad \tau_4=0,\quad \tau_7+\tau_{10}=0. \tag{3.6}$$

Under time reversal, all the coefficients ν_j, μ_j change sign. Thus time reversal invariance requires

$$\tau_1=0,\quad \tau_4=0,\quad \tau_7=0,\quad \tau_{10}=0. \tag{3.7}$$

In particular, when (2.15) is the Schrödinger equation, we have

$$\nu_1=-\frac{\hbar}{2m},\quad \mu_2=-\frac{\hbar}{4m},\quad \mu_3=\frac{\hbar}{2m},\quad \mu_5=\frac{\hbar}{8m}, \tag{3.8}$$

and all other coefficients are zero. Equations (3.7) then give

$$\tau_2=\frac{\hbar^2}{8m^2},\quad \tau_3=-1,\quad \tau_5=\frac{\hbar^2}{16m^2}, \tag{3.9}$$

with all other τ's equal to zero. For the equations studied by Doebner and Goldin, $\tau_1,\ldots,\tau_5$ are arbitrary, but $\tau_6,\ldots,\tau_{12}$ are zero.

Some of the equations discussed by Puszkarz,[5] belong to the class (2.15), when $\mu_{12}=0$. Puszkarz's modification of the Schrödinger equation is the formal extension of the equations of Doebner and Goldin obtained by modifying the current (2.6), adding to it any or all of the following terms with higher derivatives:

$$\rho\Delta\left(\frac{\mathbf{j}}{\rho}\right),\quad \rho\nabla\left(\frac{\mathbf{j}\cdot\nabla\rho}{\rho^2}\right),\quad \rho\nabla\left(\frac{\mathbf{j}^2}{\rho^2}\right),\quad \rho\nabla R_2,\quad \rho\nabla R_5.$$

Since Puszkarz's modification directly affects only the imaginary part of the nonlinear functional for $i(\partial\psi/\partial t)/\psi$, namely $(-1/2\rho)\nabla\cdot\mathbf{J}$ where $\mathbf{J}$ is the current that appears in the equation of continuity, and does not change the real part, the resulting equation is fouth-order. Our equations are in general sixth-order because of the term with R_{12}, which is needed in order to maintain invariance under the nonlinear gauge group. The equations of Puszkarz with the first three currents do not belong to any family that is closed under a group of weakly local nonlinear gauge transformations, since the transformations giving rise to those currents involve derivatives of the phase S. His equations with the latter two currents belong to the family obtained from (2.15) through gauge generalization.

In short, we have obtained a natural family of sixth-order partial differential equations invariant (as a family) under nonlinear gauge transformations of Bäcklund type, that includes a subclass gauge equivalent to the linear Schrödinger equation, a wider subclass gauge equivalent to the equations that Doebner and Goldin studied, and another subclass that intersects the family of

equations proposed by Puszkarz. Given a particular equation in our family, we can calculate the 12 gauge-invariant parameters, and from these immediately determine whether the equation is physically equivalent to the free Schrödinger equation or an equation of Doebner–Goldin type, and whether it is Galilean and/or time-reversal invariant.

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Quantum information geometry and standard purification

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We investigate relations between Uhlmann's parallelism, monotone Riemannian metrics and dual affine connections on the space of density matrices. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1467966]

I. INTRODUCTION

On the space of density operators, several differential geometrical structures were defined. In finite dimensional case, the class of monotone Riemannian metrics was specified by Petz in Ref. 1, using the set of real symmetric operator monotone functions. These metrics are the quantum generalizations of the classical Fisher metric, which is, together with the class of dual α-connections, the basic structure of the classical information geometry.

The quantum counterpart of the classical exponential and mixture connections was defined by Nagaoka in Ref. 2 and this definition was generalized to α-connections for $\alpha \in [-3,3]$ in Ref. 3.

In Ref. 4, the geometric phase of curves of pure states was extended to mixed states, using purifying lifts of curves of density matrices. Among such lifts, the one with the least Hilbert space length is used to define the phase. As it turns out, this defines a connection form a^{geo} in the space $\mathcal{W}$ of Hilbert–Schmidt operators, which is the $U(n)$–principal bundle over the space of non-normalized density operators $\mathcal{M}$, here n is the dimension of the underlying Hilbert space $\mathcal{H}$. Later, in Ref. 5 a class of such connection forms was introduced, containing the above form a^{geo}.

It is natural to ask what the relations between the above structures are. In Ref. 6 it was shown that the connection forms are naturally linked with some Riemannian or Hermitian metrics on the purifying space $\mathcal{W}$. Such metrics can be projected onto $\mathcal{M}$ and all the monotone metrics are obtained in this way. Further, in Ref. 7, a parallel transport, respecting the connection form a^{geo} was defined on $\mathcal{W}$, such that, if projected onto $\mathcal{M}$, it coincides with Nagaoka's (e)-connection. The aim of the present paper is to obtain all the affine α-connections and their duals in a similar way. For the sake of simplicity, we will assume that the underlying Hilbert space is finite dimensional and the density operators are invertible.

Section II below gives a brief description of purification and some formulas to be used later. In Sec. III, we define the class of connection forms and Riemannian metrics on $\mathcal{W}$ and relate them to the class of monotone metrics on $\mathcal{M}$ as in Ref. 6. In Secs. IV and V, we use the duality of two real subspaces in the tangent space to $\mathcal{W}$ to define two dual parallel transports, induced from the trivial affine connection on $\mathcal{B}=\mathcal{B}(\mathcal{H})$. We show that the projections of such parallel transports onto $\mathcal{M}$ coincide with the α-connection and its dual. Finally, we define a natural notion of duality of Riemannian metrics on $\mathcal{M}$.

II. THE PURIFICATION PROCEDURE

Let $\mathcal{H}$ be Hilbert space (not necessarily of finite dimension) and let $\mathcal{B}=\mathcal{B}(\mathcal{H})$ be the algebra of bounded operators acting on $\mathcal{H}$. Let $\mathcal{K}$ be another Hilbert space, with $\dim(\mathcal{H}) \leqslant \dim(\mathcal{K})$ and let

$$\mathcal{A}=\mathcal{B}(\mathcal{H}\otimes\mathcal{K}).$$

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Let us consider the *-representation $\phi:\mathcal{B}\to\mathcal{A}$, given by $b\mapsto b\otimes 1_{\mathcal{K}}$. Let ρ be a positive linear functional on $\mathcal{B}$. The vector $\xi\in\mathcal{H}\otimes\mathcal{K}$ is said to be a purification of ρ if for each $b\in\mathcal{B}$

$$\rho(b)=\mathrm{Tr}\rho b=\langle\xi,\phi(b)\xi\rangle=\mathrm{Tr}b\otimes 1P_{\xi},$$

here the density operator was also denoted by ρ and P_{ξ} is the orthogonal projector onto the subspace spanned by ξ. It is clear that ξ is a purification of ρ if

$$\rho=\mathrm{Tr}_2P_{\xi},$$

where Tr_2 is the partial trace over $\mathcal{K}$.

In the sequel, we will use the choice $\mathcal{K}=\mathcal{H}^*$. The Hilbert space $\mathcal{H}\otimes\mathcal{H}^*$ can be identified with the space of Hilbert–Schmidt operators over $\mathcal{H}$, with the Hilbert–Schmidt inner product

$$\langle w_1,w_2\rangle=\mathrm{Tr}w_1^*w_2.$$

This identification is easily seen if we use Dirac's notations, then the product vectors are identified with

$$\varphi\otimes\psi^*\mapsto|\varphi\rangle\langle\psi|,$$

where $\psi^*(\varphi)=\langle\psi,\varphi\rangle$. The operation $w\mapsto w^*$ on $\mathcal{W}$ corresponds to the anti-unitary operator J on $\mathcal{H}\otimes\mathcal{H}^*$, given by

$$J(\varphi\otimes\psi^*)=\psi\otimes\varphi^*.$$

The representation ϕ is equivalent to $b\mapsto L_b$, where $L_b(w)=bw$ is the left multiplication operator on $\mathcal{W}$. Then $w\in\mathcal{W}$ is a purification of ρ if

$$\rho(b)=\mathrm{Tr}b\rho=\langle w,L_bw\rangle=\mathrm{Tr}w^*bw=\mathrm{Tr}b\,\pi(w),$$

for each $b\in\mathcal{B}$, where $\pi(w)=ww^*$.

In a similar way, we may represent the algebra $\mathcal{B}^*=\mathcal{B}(\mathcal{H}^*)$ in $\mathcal{A}$ by

$$\phi':b\mapsto 1\otimes b\mapsto R_{b^*}.$$

Here, $b\in\mathcal{B}^*$ is the linear operator given by $b\varphi^*=(b\varphi)^*$ and $R_b(w)=wb$ is the right multiplication operator on $\mathcal{W}$. Then $\phi'(\mathcal{B}^*)$ is the commutant of $\phi(\mathcal{B})$. If σ is a positive linear functional on $\mathcal{B}^*$, the vector ξ purifies σ if

$$\sigma=\mathrm{Tr}_1P_{\xi}=\mathrm{Tr}_2P_{J\xi},$$

where Tr_1 is the partial trace over $\mathcal{H}$. This is equivalent to

$$\sigma=\pi'(w),\quad \pi'(w)=w^*w$$

where w is the Hilbert–Schmidt operator corresponding to the vector ξ.

Let $w\in\mathcal{W}$ be invertible, $\pi(w)=\rho$, $\pi'(w)=\sigma$ and let $w=\rho^{1/2}u=u\sigma^{1/2}$ be the polar decomposition of w. Then

$$\rho=\sum_i\lambda_i|\varphi_i\rangle\langle\varphi_i|,\quad \sigma=\sum_i\lambda_i|\psi_i\rangle\langle\psi_i|,$$

$\lambda_i>0$ for all i are the spectral decompositions of ρ and σ and $w=\Sigma_i\lambda_i^{1/2}|\varphi_i\rangle\langle\psi_i|$, where $u\psi_i=\varphi_i$.

Following Ref. 6, we will use a certain class of operators from $\mathcal{B}(\mathcal{W})$ to introduce a Riemannian structure in $\mathcal{W}$. Let us denote $L=L_\rho$, $R=R_\rho$, $\tilde{L}=L_\sigma$ and $\tilde{R}=R_\sigma$ and let Δ be the modular operator $\Delta=L\tilde{R}^{-1}$. Then the spectral decomposition of Δ is

$$\Delta=\sum_i \frac{\lambda_i}{\lambda_j}(P_{\varphi_i}\otimes P_{\psi_j^*}),$$

so that if f is a smooth function and $x\in\mathcal{W}$, we have

$$f(\Delta)(x)=\sum_i f\left(\frac{\lambda_i}{\lambda_j}\right)|\varphi_i\rangle\langle\varphi_i|x\psi_j\rangle\langle\psi_j|.$$

Similar expressions are obtained for $f(LR^{-1})$, $f(\tilde{L}\tilde{R}^{-1})$, etc.

III. CONNECTION FORMS AND MONOTONE METRICS

Let $\dim(\mathcal{H})=n$. Let $\mathcal{W}_0\subset\mathcal{W}$ be the open subset of invertible operators, then it can be viewed as a real $2n^2$-dimensional differentiable manifold. Let T_w denote the tangent space at w, then T_w can be identified with $\mathcal{W}$ with the structure of a real linear space. Throughout the text, the capital letters X, Y, etc. denote the elements of T_w as differential operators, whereas small letters refer to their representations $x=X(w)$.

Let $\mathcal{M}\subset\mathcal{W}_0$ be the submanifold of (non-normalized) density matrices, i.e., the positive complex matrices. Then $\mathcal{W}_0$ can be realized as the principal bundle with base space $\mathcal{M}$ and structure group $U(n)$. The projection $\pi:\mathcal{W}_0\to\mathcal{M},\pi(w)=ww^*$ is the canonical projection. Let $T_\rho(\mathcal{M})$ be the tangent space of $\mathcal{M}$ at ρ. The canonical projection induces a linear map $T_w\to T_{\pi(w)}(\mathcal{M})$ (also denoted by π)

$$\pi(x)=xw^*+wx^*.$$

The vertical subspace $V_w\subset T_w$ is given by the condition

$$x\in V_w\Leftrightarrow\pi(x)=0.$$

It is easy to see that

$$V_w=\{wa:a+a^*=0\}.$$

We will describe the class of connections defined in Refs. 5 and 6. If a connection is defined in $\mathcal{W}_0$, the tangent space T_w is decomposed as the direct sum of V_w and a horizontal subspace H_w. For each vector $x\in T_w$ there is a unique decomposition $x=x^h+x^v$ into its horizontal and vertical part. We introduce a Riemannian structure in $\mathcal{W}_0$ as follows. Let $(\cdot,\cdot)$ denote the real part of the Hilbert–Schmidt inner product, i.e.,

$$(x,y)=\Re\langle x,y\rangle=\tfrac{1}{2}\mathrm{Tr}(x^*y+y^*x).$$

Let $k:\mathbb{R}^+\to\mathbb{R}^+$ be a smooth function such that $k(1)=1$ and let Δ be the modular operator. Let us define

$$(x,y)_w=(x,k(\Delta)^{-1}(y)),\quad x,y\in T_w.$$

The horizontal subspace H_w is defined as the orthogonal complement of V_w with respect to $(\cdot,\cdot)_w$. A tangent vector x is then horizontal iff it has the form

$$x=k(\Delta)(gw)=k(L/R)(g)w,\quad g=g^*.$$

The corresponding connection form is given by

$$\omega = r(\tilde{L}/\tilde{R})(w^{-1}dw) - r(\tilde{R}/\tilde{L})(w^{-1}dw)^* \tag{1}$$

$$= w^{-1}dw - (w^{-1}dw)^* + w^{-1}(F(L/R)d\rho)(w^{-1})^*, \tag{2}$$

where r is a smooth positive function with $r(t)+r(t^{-1})=1$ and $F(t)=r(t)-r(t^{-1})$. The functions r and k are connected by

$$r(t) = \frac{tk(t^{-1})}{k(t)+tk(t^{-1})}.$$

The above Riemannian structure can be projected onto the base space $\mathcal{M}$ via the projection π: Let $\pi(w)=\rho$ and let $h \in T_\rho(\mathcal{M})$. Then there exists a unique vector $\hat{h} \in T_w$ such that $\hat{h}$ is horizontal and $\pi(\hat{h})=h$, it is called the horizontal lift of h to w. We have

$$\hat{h} = \tfrac{1}{2}R^{-1}(1-F(L/R))(h)w = r(R/L)(h)(w^*)^{-1}.$$

Let us define

$$\langle h,k\rangle_\rho = 4(\hat{h},\hat{k})_w \quad h,k \in T_\rho(\mathcal{M}). \tag{3}$$

It is easy to see that the right-hand side depends only on $ww^*=\rho$, so that this defines a Riemannian structure on $\mathcal{M}$. We are particularly interested in Riemannian metrics that are monotone with respect to completely positive, trace preserving maps. It was proved by Petz in Ref. 1, that such metrics are of the form

$$\langle h,k\rangle_\rho = \mathrm{Tr} h J_\rho(k) \quad J_\rho = R^{-1}f(L/R)^{-1}, \tag{4}$$

where f is an operator monotone function which is symmetric, i.e., it satisfies $f(t)=tf(t^{-1})$. If we require that this metric coincides with the Fisher information metric on commutative submanifolds, we need an additional condition $f(1)=1$. The last requirement also gives rise to the multiplication factor 4 in (3).

If the induced Riemannian metric on $\mathcal{M}$ is of the form (4) for some smooth positive function f, then we have

$$k(t) = f(t)(1-F(t)), \quad f(t) = \tfrac{1}{2}(k(t)+tk(t^{-1})). \tag{5}$$

It is easy to see that given a monotone Riemannian metric, the connection that induces it is not unique. On the other hand, as the connection depends only from $k(t)/k(t^{-1})$, the induced Riemannian metric is again not unique. To get uniqueness, one more condition is needed. A natural requirement is that the inner product $(\cdot,\cdot)_w$ in T_w coincides with the real part of the Hilbert–Schmidt inner product, if restricted to horizontal vectors. It was proved in Ref. 6 that for each operator monotone function f there is a unique positive function k such that the above condition is satisfied. Let us put

$$p(t) = \frac{k(t)}{k(t^{-1})},$$

then $k(t)=\sqrt{p(t)}q(t)$, where the function $q(t)=q(t^{-1})$ is uniquely given by the condition $(x,k(\Delta)^{-1}y)=(x,y)$ for $x,y \in H_w$. Thus we have

Theorem 3.1: *For each monotone metric $\langle\cdot,\cdot\rangle_\rho$ on $\mathcal{M}$, there exists a unique smooth function $p:\mathbb{R}^+\to\mathbb{R}^+$ satisfying $p(t^{-1})=(p(t))^{-1}$, such that*

(i) *if*

$$r(t)=\frac{t}{p(t)+t},$$

then the corresponding connection form induces the given monotone metric;

(ii) *if*

$$k(t)=p(t)\frac{p(t)+t}{p(t)^2+t}, \tag{6}$$

then $p(t)=k(t)/k(t^{-1})$ *and the corresponding connection is the same as in* (i). *Moreover,* $(x,y)_w=(x,y)$ *for all horizontal vectors* x, y;

(iii) *the corresponding operator monotone function is of the form*

$$2f(t)=\frac{(p(t)+t)^2}{p(t)^2+t}.$$

In the sequel, we will always suppose that k and p are smooth functions related by Eq. (6).

Example 3.1: Let $p(t)=1$. Then $f(t)=(1+t)/2$ is the largest symmetric operator monotone function. It is related to the Bures metric, J_ρ is the symmetric logarithmic derivative (SLD). Here, $k(t)=1$ and $r(t)=t/(1+t)$. The horizontal subspace H_w consists of vectors of form $x=gw$, $g=g^*$. See Refs. 8 and 9.

Example 3.2: For the smallest symmetric operator monotone function $f(t)=2t/(1+t)$, we have $p(t)=t$, $k(t)=2t/(1+t)$ and $r(t)=\frac{1}{2}$. The vector $x\in H_w$ if and only if $x=2L/(L+R)(g)w$ for $g=g^*$. This is equivalent to $x=wh$ for some $h=h^*$. In this case, $J_\rho(h)=\frac{1}{2}(h\rho^{-1}+\rho^{-1}h)$ and the monotone metric is called the metric of the right logarithmic derivative (RLD). The connection form given by r is the canonical connection form on the bundle $GL(n)/U(n)$.[10]

Example 3.3: For $p(t)=\sqrt{t}$, we obtain the operator monotone function $f(t)=(1+\sqrt{t})^2/4$. The corresponding monotone metric is the smallest in a special class of monotone metrics, defined in Refs. 11 and 12. This class is important in the context of quantum information geometry, see Ref. 13. It contains also the monotone metric from the previous example. Here, $k(t)=(1+\sqrt{t})/2$ and $r(t)=\sqrt{t}/(1+\sqrt{t})$. The horizontal vectors for $w=\sqrt{ww^*}u$ are of the form $x=gu$, $g=g^*$.

IV. DUAL AFFINE CONNECTIONS

For the Riemannian manifold $\mathcal{M}$ with a monotone metric, Nagaoka in Ref. 2 defined the quantum version of the exponential and mixture connections of the classical information geometry. There, the mixture connection ((m)-connection) coincides with the trivial affine structure on $\mathcal{M}$ and the exponential (e)-connection is its dual with respect to the given Riemannian structure. The corresponding parallel transports of a vector $h\in T_{\rho_0}(\mathcal{M})$ along a curve $\rho\in\mathcal{M}$, with $\rho(0)=\rho_0$, $\rho(1)=\rho_1$, are given by

$$\Pi_\rho^{(m)}(h)=h,$$

$$J_{\rho_1}(\Pi_\rho^{(e)}(h))=J_{\rho_0}(h).$$

The aim of this section is to show that this structure on $\mathcal{M}$ appears naturally in the context of Sec. III.

Let us fix a monotone metric on $\mathcal{M}$ and let k be as in theorem 3.1. To define the two dual connections, it is convenient to use a different characterization of the horizontal subspace, given in Ref. 6. Let us consider the space

$$T_w=\{gw\ :\ g\in\mathcal{B}\}=\{wg\ :\ g\in\mathcal{B}\},$$

with the complex Hilbert space structure, $\langle x,y\rangle_w=\langle x,k(\Delta)^{-1}(y)\rangle$, ($\langle\cdot,\cdot\rangle$ is the Hilbert–Schmidt inner product.) Let S and F be the conjugate linear operators of the Tomita–Takesaki theory, given by $S(gw)=g^*w$, $F(wg)=wg^*$, $S=J\Delta^{1/2}=\Delta^{-1/2}J$ and $F=\Delta^{1/2}J=J\Delta^{-1/2}$, where J is the modular conjugation. Let S^k be the modification of S given by

$$S^k(k(\Delta)(gw))=k(\Delta)(g^*w).$$

Then H_w is the fix point set of S^k.

Lemma 4.1:

(i) $S^k=Sp(\Delta)^{-1}=p(\Delta)S$;
(ii) *The adjoint of* S^k *with respect to* $\langle\cdot,\cdot\rangle_w$ *is* F;
(iii) *The polar decomposition of* S^k *is* $S^k=J^k(\Delta^k)^{1/2}$, *where*

$$J^k=Jp(\Delta)^{-1/2}=p(\Delta)^{1/2}J \quad \Delta^k=p(\Delta)^{-1}\Delta,$$

(iv) *let* H_w^* *be the fix point set of the operator* F. *Then for* $x\in H_w$, $y\in H_w^*$ *we have* $\langle x,y\rangle_w\in\mathbb{R}$.

Proof: (i) Observe first, that $k(\Delta)(gw)=\sqrt{p(\Delta)}(q(L/R)(g)w)$ with $q(t)=q(t^{-1})$, so that $S^k=S^{\sqrt{p}}$. Obviously

$$S^{\sqrt{p}}=p(\Delta)^{1/2}Sp(\Delta)^{-1/2}=p(\Delta)S=Sp(\Delta)^{-1}.$$

The statements (ii) and (iii) are easy to prove. To prove (iv), let $x\in H_w$ and $y\in H_w^*$. Then

$$\begin{aligned}\langle x,y\rangle_w&=\langle S^k(x),y\rangle_w\\&=\langle F(y),x\rangle_w=\langle y,x\rangle_w=\langle x,y\rangle_w^-\in\mathbb{R}.\end{aligned}$$

□

Let us introduce a linear operator $\mathcal{J}:H_w\to H_w^*$, such that for $x\in\mathcal{H}_w$, $\pi(x)=\pi(\mathcal{J}(x))$. Then $\mathcal{J}$ is well defined and invertible. Indeed, note that the real vector subspace $H_w^*=\{wg,g=g^*\}$ coincides with the horizontal subspace H_w from Example 3.2, so that both $\pi|_{H_w}$ and $\pi|_{H_w^*}$ are isomorphisms.

Further, let $\mathcal{L}_w^k$, $\mathcal{K}_w$ be two linear maps $T_w\to\mathcal{B}$, given by

$$\mathcal{L}_w^k(x)w=k(\Delta)^{-1}(x),\quad \mathcal{K}_w(x)=xw^*.$$

The operators $\mathcal{L}_w^k$ and $\mathcal{K}_w$ are invertible and $\mathcal{L}_w^k(H_w)=\mathcal{B}_h$, $\mathcal{K}_w(H_w^*)=\mathcal{B}_h$, where $\mathcal{B}_h$ is the subset of hermitian operators in $\mathcal{B}$. For $x,y\in T_w$, we have

$$\langle x,y\rangle_w=\langle\mathcal{L}_w^k(x),\mathcal{K}_w(y)\rangle. \tag{7}$$

Let $h\in T_\rho(\mathcal{M})$. The horizontal lift of h to w satisfies

$$\mathcal{L}_w^k(\hat{h})=\tfrac{1}{2}J_\rho(h), \tag{8}$$

$$y=\mathcal{J}(\hat{h})\Leftrightarrow\mathcal{K}_w(y)=\tfrac{1}{2}h. \tag{9}$$

Proposition 4.1: Let us define the bilinear form $(\cdot,\cdot)_w^\sim$ *on* H_w *by*

$$(x,y)_w^\sim=\langle x,\mathcal{J}(y)\rangle_w,$$

then we have $(x,y)_w^\sim=(x,y)_w$. *Moreover, the operator* $\mathcal{J}$ *coincides with the restriction of*

$$\tfrac{1}{2}(1+\Delta^k)=\tfrac{1}{2}(1+p(\Delta)^{-1}\Delta),$$

to H_w.

Proof: Let $x,y \in H_w$ and let $\pi(x)=h,\ \pi(y)=k$. Then $\mathcal{K}_w(\mathcal{J}(y))=\frac{1}{2}k$ and $\mathcal{L}_w^k(x)=\frac{1}{2}J_\rho(h)$. It follows from (7) that

$$(x,y)_w^{\sim}=\langle x,\mathcal{J}(y)\rangle_w=\tfrac{1}{4}\langle J_\rho(h),k\rangle$$
$$=\tfrac{1}{4}\langle h,k\rangle_\rho=(x,y)_w.$$

Let now $x \in H_w$, then

$$F(1+\Delta^k)(x)=F(1+F)(x)=(1+\Delta^k)(x),$$

so that $\frac{1}{2}(1+\Delta^k)(x) \in H_w^*$. From

$$\langle x,\Delta^k(y)\rangle_w=\langle x,FS^k(y)\rangle_w=\langle S^k(y),S^k(x)\rangle_w=\langle y,x\rangle_w$$

we have that

$$\langle x,\tfrac{1}{2}(1+\Delta^k)(y)\rangle_w=(x,y)_w=(x,y)_w^{\sim}.$$

□

From the above Proposition, we see that we may extend $\mathcal{J}$ to a positive operator on T_w. The inner product $(\cdot,\cdot)_w^{\sim}$ on T_w, given by

$$(x,y)_w^{\sim}=\langle x,\mathcal{J}(y)\rangle_w,$$

corresponds to the complexification of the real Hilbert space H_w with the inner product $(\cdot,\cdot)_w$.

Example 4.1: Let $k=1$. Let $\rho(\theta),\ \theta \in \Theta \subseteq \mathbb{R}^N$ be a smooth parametrization of the manifold $\mathcal{M}$. Let us denote

$$h_i(\theta)=\frac{\partial}{\partial\theta_i}\rho(\theta).$$

For simplicity, we will omit the indication of the point θ in the sequel.

In Ref. 14, Holevo introduced the symmetric logarithmic derivative L_i^S by

$$h_i=\tfrac{1}{2}(L_i^S\rho+\rho L_i^S),$$

and the right and left logarithmic derivatives

$$h_i=\rho L_i^R,\quad L_i^L=(L_i^R)^*.$$

It is easy to see that in our setting, the horizontal subspace H_w is spanned by the vectors

$$l_i^S=L_i^S w=2\hat{h}_i,\quad i=1,\ldots,N$$

and

$$\mathcal{J}(l_i^S)=l_i^L=L_i^L w,$$

so that H_w^* is the real linear span of $\{l_i^L,\ i=1,\ldots,N\}$, note that this is true for all k. We also have

$$l_i^R=L_i^R w=\Delta^{-1}(l_i^L).$$

Further, Holevo defined the sesquilinear forms in $a,b \in \mathcal{B}$

$$\langle a,b\rangle_\rho=\tfrac{1}{2}\mathrm{Tr}\,(a^*\rho b+a^*b\rho)=(aw,bw)^{\sim},$$

$$\langle a,b\rangle_\rho^+ = \mathrm{Tr}\, a^*b\rho = \langle aw, bw\rangle,$$

$$[a,b]_\rho = i\mathrm{Tr}\,(\rho a^*b - \rho ba^*) = \langle aw, i(1-\Delta)(bw)\rangle.$$

Another important notion is the commutation operator $\mathcal{D}_\rho$, given by

$$\langle a, \mathcal{D}_\rho(b)\rangle_\rho = [a,b]_\rho.$$

It is easy to see that the operator $aw \mapsto \mathcal{D}_\rho(a)w$ is equal to

$$i\mathcal{J}^{-1}(1-\Delta) = 2i\frac{1-\Delta}{1+\Delta} = -2iF(\Delta).$$

Example 4.2: Let $k(t) = 2t/(1+t)$, then $p(t) = t$, so that $\Delta^k = 1$. The horizontal subspace H_w coincides with H_w^* and the operator $\mathcal{J}$ is the identity. Clearly, $\hat{h}_i = \frac{1}{2}l_i^L$, $i = 1,\ldots,N$. Let us denote by $\mathcal{J}^S$ the operator $\frac{1}{2}(1+\Delta)$ from the previous example, then $k(\Delta) = (\mathcal{J}^S)^{-1}\Delta$ and we get

$$(l_i^L, l_j^L)_w = \langle l_i^L, l_j^L\rangle_w = \langle l_i^L, \mathcal{J}^S(l_j^R)\rangle = (l_i^L, l_j^R)^\sim,$$

where $(x,y)^\sim = \langle x, \mathcal{J}^S(y)\rangle$.

We can also describe the horizontal and vertical part of a vector in T_w, using the operators F, S^k, and $\mathcal{J}$ as follows. Let P be the orthogonal projector from T_w onto H_w with respect to $(\cdot,\cdot)_w$, then

$$P = \tfrac{1}{2}\mathcal{J}^{-1}(1+F).$$

Indeed, for each $x \in T_w$, we have $\frac{1}{2}(1+F)(x) \in H_w^*$ and $\pi(\frac{1}{2}(1+F)(x)) = \pi(x) = \pi(x^h)$. It follows that:

$$\tfrac{1}{2}\mathcal{J}^{-1}(1+F)(x) = x^h = Px.$$

From this, we have

$$x^v = x - x^h = \tfrac{1}{2}\mathcal{J}^{-1}(\Delta^k - F)(x) = \tfrac{1}{2}\mathcal{J}^{-1}F(S^k - 1)(x).$$

We will now define dual affine connections in $\mathcal{W}_0$. The space $\mathcal{B}$ is a differentiable manifold and $\mathcal{W}_0$ is an open submanifold in $\mathcal{B}$. Let us consider the trivial affine connection in $\mathcal{B}$. The maps $\mathcal{L}_w^k : T_w \to T_w(\mathcal{B})$ and $\mathcal{K}_w : T_w \to T_w(\mathcal{B})$ induce affine connections in $\mathcal{W}_0$. Let Π^* and Π be the corresponding parallel transports and let γ be a smooth curve in $\mathcal{W}_0$, $\gamma(0) = w_0$, $\gamma(1) = w_1$. Then for $X \in T_w$,

$$\mathcal{K}_{w_1}(\Pi_\gamma(X)) = \mathcal{K}_{w_0}(X),$$

$$\mathcal{L}_{w_1}^k(\Pi_\gamma^*(X)) = \mathcal{L}_{w_0}^k(X).$$

The corresponding covariant derivatives ∇ and ∇^* are given by

$$\mathcal{K}_w(\nabla_X Y) = X\mathcal{K}_w(Y) = \mathcal{K}_w(XY) + yx^*,$$

$$\mathcal{L}_w^k(\nabla_X^* Y) = X\mathcal{L}_w^k(Y),$$

where X, Y are smooth vector fields on $\mathcal{W}_0$.

It is clear from (7) that $\langle X, Y\rangle_{w_0} = \langle \Pi_\gamma(X), \Pi_\gamma^*(Y)\rangle_{w_1}$ so that the connections ∇ and ∇^* are dual with respect to $\langle\cdot,\cdot\rangle_w$.

As we are interested in the projections onto $\mathcal{M}$, we restrict the parallel transports to horizontal vectors. From $\mathcal{L}_w^k(H_w)=\mathcal{B}_h$, we see that the restriction of Π^* to the bundle $\cup\{(w,H_w),\ w\in\mathcal{W}_0\}$ is induced from the trivial parallel transport restricted to $\cup\{(b,\mathcal{B}_h),\ b\in\mathcal{B}\}$. It means that the parallel transport of a horizontal vector stays horizontal. This is not necessarily true for Π. On the other hand, the above restriction of the trivial connection on $\mathcal{B}$ induces the restriction of Π to the bundle $\cup\{(w,H_w^*),\ w\in\mathcal{W}_0\}$. We may therefore define the parallel transport Π^h for $x\in H_w$ by

$$\Pi^h(x)=\mathcal{J}^{-1}(\Pi(\mathcal{J}(x))).$$

Then the parallel transports Π^* and Π^h are dual with respect to $(\cdot,\cdot)_w$. Indeed, if $x,y\in H_w$,

$$\begin{aligned}(\Pi_\gamma^*(x),\Pi_\gamma^h(y))_{w_1}&=\langle\Pi_\gamma^*(x),\Pi_\gamma(\mathcal{J}(y))\rangle_{w_1}\\&=\langle x,\mathcal{J}(y)\rangle_{w_0}=(x,y)_{w_0}.\end{aligned}$$

Note also that Π^h coincides with the horizontal part of Π.

Proposition 4.2: Let γ be a smooth curve in $\mathcal{W}_0$, $\gamma(0)=w_0$, $\gamma(1)=w_1$, where w_0 and w_1 are any elements of $\mathcal{W}_0$, satisfying $\pi(w_0)=\rho_0$ and $\pi(w_1)=\rho_1$. Let $h\in T_{\rho_0}(\mathcal{M})$ and let $\hat{h}$ be the horizontal lift to w_0. Then

$$\Pi_{\pi(\gamma)}^{(m)}(h)=\pi(\Pi_\gamma(\hat{h}))=\pi(\Pi_\gamma^h(\hat{h})),$$

$$\Pi_{\pi(\gamma)}^{(e)}(h)=\pi(\Pi_\gamma^*(\hat{h})).$$

Proof: Follows easily from (8) and (9). □

Let H,K be vector fields on $\mathcal{M}$ and let $\hat{H},\hat{K}$ be horizontal lifts. From the above Proposition, it also follows that $\pi(\nabla_{\hat{H}}^*\hat{K})=\nabla_H^{(e)}K$, so that $\nabla_{\hat{H}}^*\hat{K}$ is a horizontal lift of $\nabla_H^{(e)}K$. Similarly, $\nabla_{\hat{H}}^h\hat{K}$ is the horizontal lift of $\nabla_H^{(m)}K$.

V. THE α-CONNECTIONS

In Ref. 3, the α-connections on $\mathcal{M}$ were defined as generalizations of the (e) and (m)-connections for $\alpha\in[-3,3]$. There, the α-connection was given by the trivial affine structure on $g_\alpha(\mathcal{M})$, where

$$g_\alpha(t)=\begin{cases}\dfrac{2}{1-\alpha}t^{(1-\alpha)/2} & \alpha\neq 1\\ \log t & \alpha=1\end{cases}.$$

The connection was determined using the differentiation operators $L_\alpha[\rho]:T_\rho(\mathcal{M})\to T_{g_\alpha(\rho)}(\mathcal{M})$, given by

$$L_\alpha[\rho](H)=\frac{d}{dt}g_\alpha(\rho+tH)|_{t=0}.$$

The corresponding α-parallel transport from ρ_0 to ρ_1 along a curve ρ is

$$L_\alpha[\rho_1](\Pi_\rho^{(\alpha)}(X))=L_\alpha[\rho_0](X),\quad X\in T_{\rho_0}(\mathcal{M}).$$

The parallel transport $\Pi_\rho^{(\alpha)*}$, dual with respect to the given monotone metric is given by

$$L_\alpha^{-1}[\rho_1]J_{\rho_1}(\Pi_\rho^{(\alpha)*}(X))=L_\alpha^{-1}[\rho_0]J_{\rho_0}(X).$$

Again, we will show that the above affine connections are closely related to the class of connection forms from Sec. III. To this end, we define the projection π^α from $\mathcal{W}_0$ to $\mathcal{M}$ by

$$\pi^\alpha(w)=g_\alpha(ww^*).$$

Let $\rho=ww^*$. The induced linear map $\pi^\alpha: T_w\to T_{\pi^\alpha(w)}(\mathcal{M})$ is

$$\pi^\alpha(x)=L_\alpha[\rho](xw^*+wx^*).$$

The operator $L_\alpha[\rho]$ is invertible, therefore,

$$\pi^\alpha(x)=0\Leftrightarrow\pi(x)=0,$$

so that we have the same vertical subspace V_w. Hence we have the horizontal subspace H_w and the dual space H_w^* as in the previous section. Let $k\in T_{g_\alpha(\rho)}(\mathcal{M})$ and let us denote $\hat{k}^\alpha$ the horizontal lift of k with respect to π^α, i.e. a horizontal vector such that $\pi^\alpha(\hat{k}^\alpha)=k$. Let $h\in T_\rho(\mathcal{M})$. The horizontal lifts with respect to π and π^α are connected by

$$\hat{h}=\hat{k}^\alpha\Leftrightarrow k=L_\alpha[\rho](h). \tag{10}$$

In the sequel, we extend the differential operator $L_\alpha[\rho]$ to all of $\mathcal{B}$. We define the two maps $\mathcal{L}_w^\alpha,\mathcal{K}_w^\alpha: T_w\to\mathcal{B}$ by

$$\mathcal{L}_w^\alpha(X)=L_\alpha^{-1}[\rho](\mathcal{L}_w(X)),$$

$$\mathcal{K}_w^\alpha(X)=L_\alpha[\rho](\mathcal{K}_w(X)).$$

The operators $\mathcal{K}_w^\alpha$ and $\mathcal{L}_w^\alpha$ have similar properties as $\mathcal{K}_w$ and $\mathcal{L}_w$. We also have

$$\langle x,y\rangle_w=\langle\mathcal{L}_w(X),\mathcal{K}_w(Y)\rangle=\langle\mathcal{L}_w^\alpha(X),\mathcal{K}_w^\alpha(Y)\rangle. \tag{11}$$

The horizontal lift $\hat{h}^\alpha$ of a vector $h\in T_{\pi^\alpha(w)}(\mathcal{M})$ satisfies the conditions

$$\mathcal{L}_w^\alpha(\hat{h}^\alpha)=\tfrac{1}{2}L_\alpha^{-1}[\rho]J_\rho L_\alpha^{-1}[\rho](h)=:\tfrac{1}{2}K_\alpha(h), \tag{12}$$

$$y=\mathcal{J}(\hat{h}^\alpha)\Leftrightarrow\mathcal{K}_w^\alpha(y)=\tfrac{1}{2}h. \tag{13}$$

The induced inner product in $T_{\pi^\alpha(w)}(\mathcal{M})$ is then

$$\begin{aligned}4(\hat{h}^\alpha,\hat{k}^\alpha)_w&=4\langle\hat{h}^\alpha,\mathcal{J}(\hat{k}^\alpha)\rangle_w\\&=4\langle\mathcal{L}_w^\alpha(\hat{h}^\alpha),\mathcal{K}_w^\alpha(\mathcal{J}(\hat{k}^\alpha))\rangle=\langle K_\alpha(h),k\rangle.\end{aligned}$$

This coincides with the inner product, induced from $\langle\cdot,\cdot\rangle_\rho$ in the α-representation of the cotangent space, see Ref. 3.

As in the previous section, we use the trivial affine connection on $\mathcal{B}$ and the maps $\mathcal{K}_w^\alpha$ and $\mathcal{L}_w^\alpha$ to obtain the parallel transports Π^α and $\Pi^{\alpha*}$ on $\mathcal{W}_0$. From Eq. (11) it follows that the parallel transports are dual. The parallel transports Π^α and $\Pi^{\alpha*}$ can again be restricted to the bundles $\cup\{(w,H_w^*),\ w\in\mathcal{W}_0\}$ and $\cup\{(w,H_w),\ w\in\mathcal{W}_0\}$, respectively. We put

$$\Pi^{\alpha h}(x)=\mathcal{J}^{-1}\Pi^\alpha(\mathcal{J}(x)),$$

for $x\in H_w$. As before, this corresponds to the horizontal part of Π^α and the parallel transports $\Pi^{\alpha*}$ and $\Pi^{\alpha h}$ are dual with respect to $(\cdot,\cdot)_w$.

In the next Proposition, we show how these connections are projected onto $\mathcal{M}$.

Proposition 5.1: Let γ be a smooth curve in $\mathcal{W}_0$, $\gamma(0)=w_0$, $\gamma(1)=w_1$, where w_0 and w_1 are any elements of $\mathcal{W}_0$, satisfying $\pi(w_0)=\rho_0$ and $\pi(w_1)=\rho_1$. Let $h\in T_{\rho_0}(\mathcal{M})$. Then

$$\Pi^{(\alpha)}_{\pi(\gamma)}(h)=\pi(\Pi^{\alpha}_{\gamma}(\hat{h}))=\pi(\Pi^{\alpha h}_{\gamma}(\hat{h})),$$

$$\Pi^{(\alpha*)}_{\pi(\gamma)}(h)=\pi(\Pi^{\alpha*}_{\gamma}(\hat{h})).$$

Proof: The proof follows from (10), (12), (13) and the definition of the (α)- and (α^*)-parallel transports. □

From the above Proposition, it also follows that $\nabla^{\alpha h}_{\hat{H}}\hat{K}$ and $\nabla^{\alpha*}_{\hat{H}}\hat{K}$ are the π-horizontal lifts of $\nabla^{(\alpha)}_{H}K$ and $\nabla^{(\alpha*)}_{H}K$, respectively.

Let us now compute the Riemannian curvature of the α-connections.

Proposition 5.2: Let R^{α} and $R^{\alpha}*$ be the Riemannian curvature tensor of ∇^{α} and $\nabla^{\alpha}*$. Then

$$R^{\alpha}=R^{\alpha}*=0.$$

Proof: We have for smooth vector fields X,Y,Z on $\mathcal{W}$

$$\begin{aligned}\mathcal{L}^{\alpha}(R^{\alpha}*(X,Y)Z)&=\mathcal{L}^{\alpha}(\nabla^{\alpha}_{X}\nabla^{\alpha}_{Y}Z-\nabla^{\alpha}_{Y}\nabla^{\alpha}_{X}Z-\nabla^{\alpha}_{[X,Y]}Z)\\&=X\mathcal{L}^{\alpha}(\nabla^{\alpha}_{Y}Z)-Y\mathcal{L}^{\alpha}(\nabla^{\alpha}_{X}Z)-[X,Y]\mathcal{L}^{\alpha}(Z)\\&=(XY-YX-[X,Y])\mathcal{L}^{\alpha}(Z)=0.\end{aligned}$$

The statement for R^{α} can be proved similarly. It follows also from duality of the corresponding parallel transports.

□

VI. THE CURVATURE FORM

In this section, we compute the curvature form of the connection ω and show the relation between the curvature form and the torsion of the α-connections.

Let us choose a connection form ω from Sec. III 1. We will compute its curvature form. From the structure equation

$$d\omega=-\tfrac{1}{2}[\omega,\omega]+\Omega,$$

it follows that:

$$\omega[X,Y]=-2\Omega(X,Y), \tag{14}$$

for horizontal vector fields X,Y, see Ref. 10, pp. 81.

Let $w\in\mathcal{W}_0$ and let $\pi(w)=\rho$. Let us define the operator $C_{\rho}:\mathcal{B}\to\mathcal{B}$, given by

$$C_{\rho}(a)=R^{-1}r(R/L)(a)$$

Proposition 6.1: Let H,K be smooth vector fields on $\mathcal{M}$, such that $[H,K]=0$. Then

$$\begin{aligned}\Omega_{w}(\hat{H},\hat{K})=-\tfrac{1}{2}w^{-1}(&HC_{\rho}(k)\\&-KC_{\rho}(h)-[C_{\rho}(h),C_{\rho}(k)]_{\mathcal{B}})w,\end{aligned}$$

where $[a,b]_{\mathcal{B}}=ab-ba$ is the usual commutator on matrices.

Proof: From $\pi([\hat{H},\hat{K}])=[H,K]=0$ and Eq. (14), it follows that:

$$[\hat{H},\hat{K}]=[\hat{H},\hat{K}]^{v}=w\omega([\hat{H},\hat{K}])=-2w\Omega(\hat{H},\hat{K}).$$

Further, the horizontal lift of H is given by the condition

$$\hat{H}(w)=r(R/L)(H(\rho))(w^*)^{-1}=C_\rho(H(\rho))w,$$

so that

$$\hat{H}\hat{K}(w)=\hat{H}[C_\rho(k)]w+C_\rho(k)\hat{H}(w)=(HC_\rho(k)+C_\rho(k)C_\rho(h))w$$

It is now easy to finish the proof.

□

Example 6.1: Let $k=1$. Then $r(t)=t/(1+t)$ and $C_\rho=\frac{1}{2}J_\rho$. Let H,K be vector fields on $\mathcal{M}$, such that $[H,K]=0$. Let us denote $L_H^S=J_\rho(h)$. Then

$$-2w\Omega(\hat{H},\hat{K})w^{-1}=\tfrac{1}{2}(HL_K^S-KL_H^S)-\tfrac{1}{4}[L_H^S,L_K^S]_{\mathcal{B}}.$$

Let T^* be the torsion of the (e)-connection on $\mathcal{M}$, then

$$T^*(H,K)=J_\rho^{-1}(HL_K^S-KL_H^S)=\tfrac{1}{4}[[L_H^S,L_K^S]_{\mathcal{B}},\rho]_{\mathcal{B}},$$

see Refs. 2 and 6. We compute

$$\Omega(\hat{H},\hat{K})=\tfrac{1}{8}w^*J_\rho([L_H^S,L_K^S]_{\mathcal{B}})w.$$

We see that the curvature form $\Omega(H,K)=0$ if and only if the symmetric logarithmic derivatives commute. In this case also the torsion $T^*(H,K)$ vanishes.

Example 6.2: Let $\omega=\omega^{\mathrm{can}}$ be the connection form of the canonical connection (Example 3.2). Then $r=\frac{1}{2}$ and $C_\rho=\frac{1}{2}R^{-1}$. Let us denote $L_H^L=h\rho^{-1}=2C_\rho$. The curvature form is

$$\begin{aligned}\Omega^{\mathrm{can}}(H,K)&=\tfrac{1}{8}w^{-1}[L_K^L,L_H^L]_{\mathcal{B}}w\\&=\tfrac{1}{8}[w^{-1}k(w^*)^{-1},w^{-1}h(w^*)^{-1}]_{\mathcal{B}}.\end{aligned}$$

Again, the curvature form is zero iff the left (or, equivalently, the right) logarithmic derivatives commute. We have $T^*(H,K)=\Re[L_H^L,L_K^L]_{\mathcal{B}}$, so that the torsion also vanishes.

We see that in both examples, there is a close relation between the curvature form of ω and the exponential connection on $\mathcal{M}$: Vanishing of the curvature form implies vanishing of the torsion of the (e)-connection. As we shall see next, this is not always true.

Example 6.3: Let ω be the connection form from Example 3.3. Let $u\in U(n)$ and let us define $\sigma:\mathcal{M}\to\mathcal{W}_0$ by $\sigma(\rho)=\rho^{\frac{1}{2}}u$. Then σ is a global horizontal section. It follows that the curvature form of Ω vanishes. On the other hand, the torsion of the (e)-connection is not always zero, see Ref. 13.

Let now T^α and $T^{\alpha*}$ be the torsion of the connection $\nabla^{\alpha h}$ and $\nabla^{\alpha *}$ on $\mathcal{W}_0$.

Proposition 6.2: Let H,K be vector fields on $\mathcal{M}$ and let $T^{(\alpha*)}$ be the torsion of the connection $\nabla^{(\alpha*)}$ on $\mathcal{M}$. Then the horizontal part of $T^{\alpha*}(\hat{H},\hat{K})$ is the horizontal lift of $T^{(\alpha*)}(H,K)$ and

$$\omega(T^{\alpha*}(\hat{H},\hat{K}))=2\Omega(\hat{H},\hat{K}),$$

where Ω is the curvature form of ω.

Proof: The vector fields $\nabla_{\hat{H}}^{\alpha*}\hat{K}$ and $\nabla_{\hat{K}}^{\alpha*}\hat{H}$ are horizontal lifts of $\nabla_H^{(\alpha*)}K$ and $\nabla_K^{(\alpha*)}H$, so that

$$(T^{\alpha*}(\hat{H},\hat{K}))^h=\nabla_{\hat{H}}^{\alpha*}\hat{K}-\nabla_{\hat{H}}^{\alpha*}\hat{K}-[\hat{H},\hat{K}]^h.$$

But $[\hat{H},\hat{K}]^h$ is the horizontal lift of $[H,K]$, so that

$$\pi(T^{\alpha *}(\hat{H},\hat{K}))=T^{(\alpha *)}(H,K).$$

It also follows that

$$\omega(T^{\alpha *}(\hat{H},\hat{K}))=-\omega([\hat{H},\hat{K}])=2\Omega(\hat{H},\hat{K}).$$

□

Proposition 6.3: Let H, K be as above and let $T^{(\alpha)}$ be the torsion of the connection $\nabla^{(\alpha)}$ on $\mathcal{M}$. Then $T^{\alpha}(\hat{H},\hat{K})$ is vertical, with

$$\omega(T^{\alpha}(\hat{H},\hat{K}))=2\Omega(\hat{H},\hat{K}).$$

Proof: The proof is analogical to the previous proof, using the fact that the connection $\nabla^{(\alpha)}$ on $\mathcal{M}$ is torsion-free.

□

Proposition 6.4: *Let $x,y\in H_w^*$ and let $\overline{T^{\alpha}}$ be the torsion of the connection ∇^{α}. Then $\overline{T^{\alpha}}(X,Y)$ is vertical and*

$$\overline{T^{\alpha}}(X,Y)=2w\Omega^{\mathrm{can}}(X,Y)$$

Proof: Let the horizontal subspace be given by the cannonical connection, then $H_w=H_w^*$ and $\mathcal{J}$ is the identity map. It follows that $\nabla^{\alpha}=\nabla^{\alpha h}$. The vectors $X,Y\in H_w^*$ can be extended to vector fields on $\mathcal{W}_0$, such that $\pi(X)$ and $\pi(Y)$ are smooth vector fields on $\mathcal{M}$. The statement now follows from the previous Proposition.

□

Remark 6.1: If $\alpha=-1$, i.e., $\nabla^{\alpha}=\nabla$, it is easy to compute that

$$\mathcal{K}_w(\overline{T}(X,Y))=yx^*-xy^*,$$

and $\overline{T}(X,Y)$ is, therefore, vertical for all smooth vector fields X,Y.

VII. DUAL RIEMANNIAN METRICS

It follows from symmetry of the representation $\mathcal{B}\otimes 1$ and its commutant $1\otimes\mathcal{B}$ that we may equally well use the projection $\pi':\mathcal{W}_0\to\mathcal{M}$,

$$\pi':w\mapsto w^*w,$$

instead of π. In this case, the induced linear map $T_w\to T_{w^*w}(\mathcal{M})$ is

$$\pi'(x)=x^*w+w^*x.$$

It is easy to show that $\pi'(x)=0$ if xw^{-1} is anti-Hermitian, so that the vertical subspace is given by

$$V'_w=\{aw:a+a^*=0\}.$$

Let the horizontal subspace H'_w be the orthogonal complement of V'_w with respect to

$$(x,y)'_w=(x,k(\Delta^{-1})^{-1}(y)),$$

for a positive function k. It is quite clear that given a function k, we obtain the same Riemannian structure on $\mathcal{M}$ from $(\cdot,\cdot)'_w$ and π' as from $(\cdot,\cdot)_w$ and π. Moreover, $(\cdot,\cdot)_w$ coincides with $(\cdot,\cdot)$ on H_w if and only if the same is true for $(\cdot,\cdot)'_w$ and H'_w.

Let F^k be the modification of the Tomita–Takesaki operator F, given by

$$F^k(k(\Delta^{-1})(wg))=k(\Delta^{-1})(wg^*).$$

Lemma 7.1:

(i) $F^k=Fp(\Delta)=p(\Delta)^{-1}F$;
(ii) *The horizontal subspace* H'_w *is the fix point space of* F^k;
(iii) F^k *is the adjoint operator of* S^k *with respect to* $\langle\cdot,\cdot\rangle$;
(iv) *The polar decomposition of* S^k *with respect to* $\langle\cdot,\cdot\rangle$ *is* $S^k=J\Delta^{\sim k1/2}$, *where*

$$\Delta^{\sim k}=\Delta p(\Delta)^{-2}=\frac{\tilde{p}(\Delta)}{p(\Delta)}=\tilde{p}(\Delta)p(\Delta^{-1}),$$

(v) $F^{\sqrt{p}}=S^{\sqrt{\tilde{p}}}$, *where* $\tilde{p}=tp(t^{-1})=t/p(t)$

Proof: (i) is proved similarly as Lemma 4.1 (i), the statements (ii)–(iv) are easy to prove. To get (v), write

$$F^{\sqrt{p}}=Fp(\Delta)=J\Delta^{-1/2}p(\Delta)=J\Delta^{1/2}\tilde{p}(\Delta)^{-1}=S^{\sqrt{\tilde{p}}}.$$

□

Let the functions f and $\tilde{f}$ be obtained from p and $\tilde{p}$ as in Theorem 3.1 (iii). Then we will say that the corresponding Riemannian metrics on $\mathcal{M}$ are dual.

From the above Lemma, we see that the horizontal subspace H'_w, given by the function p, coincides with the subspace H_w, obtained from $\tilde{p}$. It means that a pair of dual Riemannian structures on $\mathcal{M}$ is obtained from the real part of Hilbert–Schmidt inner product on a horizontal subspace (H_w or H'_w), using the projections π and π'. Another way to do it is to use the same projection (π or π') on two dual subspaces H_w and H'_w.

Example 7.1: It is easy to see that if $k=1$, the dual subspace H'_w coincides with H^*_w from Sec. IV. Moreover, H_w and H^*_w are the SLD and RLD subspaces from Examples 3.1 and 3.2. It follows that SLD and RLD are dual Riemannian metrics. The metric from Example 3.3 is the unique self-dual Riemannian metric.

Let H_w and H'_w be two dual horizontal subspaces given by the function k, i.e., H_w and H'_w are the fix point space of S^k and F^k, respectively. Let $\mathcal{J}^k$ be the operator $H_w\to H'_w$, satisfying

$$\langle x,\mathcal{J}^k(y)\rangle=(x,y)_w,\quad x,y\in H_w.$$

Then

$$\mathcal{J}^k=\tfrac{1}{2}(1+\Delta^{\sim k})|_{H_w}.$$

Indeed, let $x,y\in H_w$, then

$$(1+\Delta^{\sim k})(x)=x+F^k(x)\in H'_w$$

and

$$\tfrac{1}{2}\langle x,(1+\Delta^{\sim k})(y)\rangle=\tfrac{1}{2}(\langle x,y\rangle+\langle x,F^kS^k(y)\rangle)=(x,y)=(x,y)_w.$$

Let now $h_1,h_2\in T_\rho(\mathcal{M})$ and let $\langle\cdot,\cdot\rangle_\rho$ be the inner product, given by the function $f=\frac{1}{2}(k(t)+tk(t^{-1}))$. Then it can be realized on H^*_w as

$$\begin{aligned}\langle h_1,h_2\rangle_\rho&=\langle l_1^L,\mathcal{J}^{-1}\mathcal{J}^k\mathcal{J}^{-1}(l_2^L)\rangle\\&=\langle l_1^L,2(1+\tilde{p}(\Delta))^{-1}[1+\tilde{p}(\Delta)p(\Delta^{-1})]\\&\quad\times(1+\tilde{p}(\Delta))^{-1}(L_2^L)\rangle,\end{aligned}$$

where $l_i^L = h_i(w^*)^{-1}$, $i=1,2$. Note that this corresponds to the decomposition of the function f

$$f(t) = \frac{1}{2}\frac{(1+\tilde{p}(t))^2}{1+\tilde{p}(t)p(t^{-1})},$$

from Theorem 3.1 (iii).

We conclude with two natural questions:

(1) From Theorem 3.1, we see that there is a one-to-one correspondence between the set of all operator monotone functions and a subset of
$$\{p:\mathbb{R}^+\to\mathbb{R}^+,\ p \text{ is smooth},\ p(t^{-1})=p(t)^{-1}\}.$$
How is this subset characterized?

(2) Let the Riemannian metric $\langle\cdot,\cdot\rangle_\rho$ be monotone. Does it follow that the dual Riemannian metric is monotone?

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Exact evolution equations for SU(2) quasidistribution functions

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We derive an exact (differential) evolution equation for a class of SU(2) quasiprobability distribution functions. Linear and quadratic cases are considered as well as the quasiclassical limit of the large dimension of representation, $S \gg 1$. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1463711]

I. INTRODUCTION

Phase-space representation provides a very useful insight into nonrelativistic quantum mechanics and allows us to treat it as a statistical theory in a classical phase space. Since the famous paper of Wigner[1] the phase-space methods have been successfully applied in different branches of quantum mechanics (see, e.g., Ref. 2). Special attention has been paid to Heisenberg–Weyl quasidistribution functions[3] describing a quantum system dynamics in the flat q-p $(\alpha-\alpha^*)$ space. The dynamics of quasiprobability distributions in phase space is governed by quantum Liouville-like equations, which in the limit $\hbar \to 0$ turn to the classical Liouville equation,[4–6] providing the most suitable approach to the quasiclassical limit in quantum mechanics.

The phase-space description of spin systems was initiated by Stratonovich,[7] Beresin,[8] and Agarwal[9] (see also Refs. 10–15), where different types of the quasiprobability distribution function on the sphere $(\theta,\phi) \in \mathcal{S}_2$ have been introduced. These functions, naturally related to the SU(2) dynamical group, are useful to visualize nonclassical properties of a collection of two-level atoms.[16,17] In the present article we find the exact differential form of the evolution equations for some special types of SU(2) quasidistribution functions and discuss quasiclassical limit of the large dimension of representation. In particular we will be interested in P- and Q-Beresin symbols and the Stratonovich–Weyl function W (see Ref. 12 for review). These SU(2) quasidistribution functions can be unified introducing an s-parametrized family of phase-space functions[15,18] defined as follows:

$$W_\rho^{(s)}(\theta,\phi) = \mathrm{Tr}(\rho \hat{w}_s(\theta,\phi)), \tag{1}$$

where ρ is the system density matrix and $\hat{w}_s(\theta,\phi)$ is the operator

$$\hat{w}_s(\theta,\phi) = \frac{2\sqrt{\pi}}{\sqrt{2S+1}} \sum_{L=0}^{2S} \sum_{M=-L}^{L} (C_{SS,L0}^{SS})^{-s} Y_{LM}^*(\theta,\phi) \hat{T}_{LM}^{(S)}, \tag{2}$$

where $Y_{LM}(\theta,\phi)$ are the spherical harmonics, $\hat{T}_{LM}^{(S)}$ are the irreducible tensor operators[19] which form an orthogonal operator basis in the space of $(2S+1)\times(2S+1)$ matrices and are defined as

$$\hat{T}_{LM}^{(S)} = \sqrt{\frac{2L+1}{2S+1}} \sum_{m,m'=-S}^{S} C_{Sm,LM}^{Sm'} |S,m'\rangle \langle S,m|. \tag{3}$$

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Here $C^{Sm'}_{Sm,LM}$ are the Clebsch–Gordan coefficients which couple two representations of spin S and L $(0\leqslant L\leqslant 2S)$ to a total spin S. The value $s=0$ corresponds to the Stratonovich–Weyl function, meanwhile $s=\pm 1$ leads to contravariant P-symbol and covariant Q-symbol correspondingly. Both self-dual $\hat{w}_{s=0}(\theta,\phi)$ and dual $\hat{w}_{s=\pm 1}(\theta,\phi)$ kernels are normalized according to

$$\mathrm{Tr}\,\hat{w}_s(\theta,\phi)=1, \quad \frac{2S+1}{4\pi}\int_{\mathcal{S}_2} \mathrm{d}\Omega\, \hat{w}_s(\theta,\phi)=I. \tag{4}$$

The quasidistribution functions $W^{(s)}_\rho(\theta,\phi)$ are covariant under rotations and provide the overlap relation

$$\frac{2S+1}{4\pi}\int_{\mathcal{S}_2} \mathrm{d}\Omega\, W^{(s)}_\rho(\theta,\phi) W^{(-s)}_A(\theta,\phi)=\mathrm{Tr}(\rho A), \tag{5}$$

where $\mathrm{d}\Omega=\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$ is the invariant measure on the sphere and $W^{(s)}_A(\theta,\phi)$ is the (s-ordered) Weyl symbol of the operator $\hat{A}$,

$$W^{(s)}_A(\theta,\phi)=\mathrm{Tr}(\hat{A}\hat{w}_s(\theta,\phi)). \tag{6}$$

The density matrix can be reconstructed from any quasidistribution function (1) through the following relation:

$$\rho=\frac{2S+1}{4\pi}\int_{\mathcal{S}_2} \mathrm{d}\Omega\, \hat{w}_{-s}(\theta,\phi) W^{(s)}_\rho(\theta,\phi). \tag{7}$$

In what follows we will consider only *integer* spin S, which corresponds to the SO(3) rather than the SU(2) group.

II. EVOLUTION EQUATIONS

A. General systems

Let us consider the dynamics of quasidistribution functions $W^{(s)}_\rho(\theta,\phi)$ under the action of a Hamiltonian from $2S+1$ dimensional representation of the universal enveloping algebra of $su(2)$. We represent the Hamiltonian as a series on the irreducible tensor operators $\hat{T}^{(S)}_{lk}$ (3),

$$H=\sum_{l=0}^{2S}\sum_{k=-l}^{l}\alpha_{lk}\hat{T}^{(S)}_{lk}. \tag{8}$$

The degree of nonlinearity [on the generators of the $su(2)$ algebra] of the Hamiltonian (8), $\deg H$, is defined by the maximum value of l, such that $\alpha_{lk}\neq 0$. Substituting the density matrix in terms of the quasidistribution function $W^{(s)}_\rho(\theta,\phi)$ (7) to the equation of motion,

$$i\partial_t\rho=[H,\rho], \tag{9}$$

we obtain

$$i\int_{\mathcal{S}_2}\mathrm{d}\Omega\,\hat{w}_{-s}(\theta,\phi)\partial_t W^{(s)}_\rho(\theta,\phi)=\int_{\mathcal{S}_2}\mathrm{d}\Omega[H,\hat{w}_{-s}(\theta,\phi)]W^{(s)}_\rho(\theta,\phi). \tag{10}$$

The commutator of two irreducible tensor operators can be represented as a linear form on irreducible tensor operators,[19]

$$[\hat{T}^{(S)}_{lk},\hat{T}^{(S)}_{LM}]=\sqrt{(2l+1)(2L+1)}\sum_{L',M'}[(-1)^{L'}-(-1)^{L+l}]C^{L'M'}_{lk,LM}\begin{Bmatrix} l & L & L' \\ S & S & S \end{Bmatrix}\hat{T}^{(S)}_{L'M'}, \quad (11)$$

where $\{\begin{smallmatrix} l & L & L' \\ S & S & S \end{smallmatrix}\}$ are $6j$-symbols. We will use the following representation [which can be obtained by comparing Eqs. 9.2.1 (5) and 8.2.1 (4) from Ref. 19] of $6j$-symbols in terms of expansion on the Clebsch–Gordan coefficients,

$$\begin{Bmatrix} l & L & L' \\ S & S & S \end{Bmatrix}=\frac{(-1)^l}{\sqrt{(2l+1)}}\left(\frac{F(L)F(l)}{F(L')}\right)^{1/2}\sum_j a_j b^L_{jl}C^{lj}_{Lj,L'0}, \quad (12)$$

where

$$a_j=\frac{(-1)^j}{j!(2S+j+1)!}, \quad b^L_{jl}=\left[\frac{(L+j)!(l+j)!}{(L-j)!(l-j)!}\right]^{1/2}, \quad (13)$$

and

$$F(L)=\sqrt{(2S+L+1)!(2S-L)!}. \quad (14)$$

Making use of (11) and (12) we get

$$[H,\hat{w}_{-s}(\theta,\phi)]=\frac{2\sqrt{\pi}}{\sqrt{2S+1}}\sum_{l,k}\alpha_{lk}\sum_{L,M}(C^{SS}_{SS,L0})^s Y^*_{LM}(\theta,\phi)$$
$$\times\sum_{L',M'}[1-(-1)^{L+l+L'}]\hat{T}^{(S)}_{L'M'}C^{LM}_{L'M',l-k}g(L,L',l), \quad (15)$$

$$g(L,L',l)=\sqrt{\frac{(2L'+1)(2l+1)}{2L+1}}\,\frac{F(L)F(l)}{F(L')}\sum_j a_j b^L_{jl}C^{Lj}_{L'0,lj}, \quad (16)$$

where we have used the following transformation properties of the Clebsch-Gordan coefficients:

$$C^{L'M'}_{lk,LM}=(-1)^{l-k}\sqrt{\frac{2L'+1}{2L+1}}C^{LM}_{L'M',l-k}, \quad C^{lj}_{Lj,L'0}=(-1)^{L'}\sqrt{\frac{2l+1}{2L+1}}C^{Lj}_{L'0,lj}. \quad (17)$$

Using the integral representation[19] for a product of two Clebsch–Gordan coefficients in terms of the Wigner D-function,

$$C^{Lj}_{L'0,lj}C^{LM}_{L'M',l-k}=\frac{2L+1}{8\pi^2}\int \mathrm{d}V D^{L'}_{M'0}(\phi,\theta,\psi)D^{l}_{-kj}(\phi,\theta,\psi)D^{L*}_{Mj}(\phi,\theta,\psi), \quad (18)$$

where $\mathrm{d}V=\mathrm{d}\phi\,\mathrm{d}\Omega$, and relations

$$D^{L'}_{M'0}(\phi,\theta,\psi)=\sqrt{\frac{4\pi}{2L'+1}}Y^*_{L'M'}(\theta,\phi),$$

$$D^{l}_{-kj}(\phi,\theta,\psi)=(-1)^k\sqrt{\frac{4\pi}{2l+1}}\sqrt{\frac{(l-j)!}{(l+j)!}}S^{+j}Y_{lk}(\theta,\phi), \quad (19)$$

$$D^{L*}_{Mj}(\phi,\theta,\psi)=\sqrt{\frac{4\pi}{2L+1}}\sqrt{\frac{(L-j)!}{(L+j)!}}S^{-j}Y_{LM}(\theta,\phi),$$

where

$$S^{\pm}=ie^{\mp i\psi}\left(\pm\cot\theta\frac{\partial}{\partial\psi}+i\frac{\partial}{\partial\theta}\mp\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right), \tag{20}$$

$$S^{\pm}D^{L}_{mm'}(\phi,\theta,\psi)=-\sqrt{L(L+1)}C^{Lm'\pm1}_{Lm,1\pm1}D^{L}_{mm'\pm1}(\phi,\theta,\psi) \tag{21}$$

are contravariant components of angular momentum operator in the rotating frame,[19] we obtain from (15)

$$[H,\hat{w}_{-s}(\theta,\phi)]=\frac{2}{\sqrt{2S+1}}\sum_{l,k}\alpha_{lk}\sum_{L,M}(C^{SS}_{SS,L0})^{s}Y^{*}_{LM}(\theta,\phi)\sum_{L',M'}\hat{T}^{(S)}_{L'M'}\sum_{j}a_j f_j(L,L',l), \tag{22}$$

$$f_j(L,L',l)=\frac{F(L)F(l)}{F(L')}\int dV Y^{*}_{L'M'}(\theta,\phi)[S^{+j}Y_{lk}(\theta,\phi)S^{-j}Y_{LM}(\theta,\phi) -S^{-j}Y_{lk}(\theta,\phi)S^{+j}Y_{LM}(\theta,\phi)]. \tag{23}$$

Now we note that the function $F(L)$ (14) depends on the combination $L(L+1)$ rather than on L itself and, thus, we can write

$$F(L)Y_{LM}(\theta,\phi)=\tilde{F}(\mathcal{L}^2)Y_{LM}(\theta,\phi), \tag{24}$$

where $\tilde{F}(\mathcal{L}^2)$ is some function (whose explicit form is not needed for concrete calculations) of the Casimir operator on the sphere $\mathcal{L}^2$,

$$\mathcal{L}^2=-\left[\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right], \tag{25}$$

such that $\mathcal{L}^2Y_{L,M}(\theta,\phi)=L(L+1)Y_{L,M}(\theta,\phi)$. Taking into account that

$$C^{SS}_{SS,L0}=\frac{\sqrt{(2S+1)!(2S)!}}{F(L)}, \tag{26}$$

we obtain after integrating by parts Eq. (23)

$$(C^{SS}_{SS,L0})^{s}f_j(L,L',l)=(-1)^{j}\int \mathrm{d}V\, Y_{LM}(\theta,\phi)\tilde{F}^{1-s}(\mathcal{L}^2) \times[S^{-j}(\tilde{F}^{-1}(\mathcal{L}^2)Y^{*}_{L'M'}(\theta,\phi)S^{+j}\tilde{F}(\mathcal{L}^2)Y_{lk}(\theta,\phi)) -S^{+j}(\tilde{F}^{-1}(\mathcal{L}^2)Y^{*}_{L'M'}(\theta,\phi)S^{-j}\tilde{F}(\mathcal{L}^2)Y_{lk}(\theta,\phi))][(2S+1)!(2S)!]^{s/2}. \tag{27}$$

Due to the sum

$$\sum_{L,M}Y^{*}_{LM}(\theta,\phi)Y_{LM}(\theta',\phi')=K(\Omega,\Omega') \tag{28}$$

is a reproductive kernel on the sphere,[12] i.e.,

$$\int \mathrm{d}\Omega\, Z(\Omega)K(\Omega,\Omega')=Z(\Omega') \tag{29}$$

for any function $Z(\Omega)$ defined on the sphere. We get from (22) and (27)

$$[H,\hat{w}_{-s}(\theta,\phi)]=\frac{\sqrt{2S+1}}{2\pi}\sum_j (-1)^j a_j \int \mathrm{d}\psi\, \tilde{F}^{1-s}(\mathcal{L}^2)$$
$$\times[S^{-j}(\tilde{F}^{s-1}(\mathcal{L}^2)\hat{w}_{-s}(\theta,\phi)S^{+j}\tilde{F}(\mathcal{L}^2)W_H^{(0)}(\theta,\phi))$$
$$-S^{+j}(\tilde{F}^{s-1}(\mathcal{L}^2)\hat{w}_{-s}(\theta,\phi)S^{-j}\tilde{F}(\mathcal{L}^2)W_H^{(0)}(\theta,\phi))], \tag{30}$$

where

$$W_H^{(0)}(\theta,\phi)=\frac{2\sqrt{\pi}}{\sqrt{2S+1}}\sum_{l,k}\ \alpha_{lk}Y_{lk}(\theta,\phi) \tag{31}$$

is a symmetrized, $s=0$ (Stratonovich–Weyl) symbol of the Hamiltonian (8). Substituting (30) into (10) and integrating by parts we obtain (after integrating over the angle ψ)

$$i\partial_t W_\rho^{(s)}(\theta,\phi)=\sqrt{2S+1}\tilde{F}^{s-1}(\mathcal{L}^2)\sum_j\ a_j[S^{-(j)}(\tilde{F}^{1-s}(\mathcal{L}^2)W_\rho^{(s)}(\theta,\phi))S^{+(j)}(\tilde{F}(\mathcal{L}^2)W_H^{(0)}(\theta,\phi))$$
$$-S^{+(j)}(\tilde{F}^{1-s}(\mathcal{L}^2)W_\rho^{(s)}(\theta,\phi))S^{-(j)}(\tilde{F}(\mathcal{L}^2)W_H^{(0)}(\theta,\phi))], \tag{32}$$

where symbolic power $S^{\pm(j)}$ has been introduced according to

$$S^{\pm j}=e^{\mp ij\psi}S^{\pm(j)}, \tag{33}$$

such that

$$S^{\pm(j)}=\Pi_{k=0}^{j-1}\left(k\cot\theta-\frac{\partial}{\partial\theta}\mp\frac{i}{\sin\theta}\frac{\partial}{\partial\phi}\right). \tag{34}$$

It follows from (21) and (33) that

$$S^{\pm(j)}W_H^{(0)}(\theta,\phi)=0,\quad j>\deg H. \tag{35}$$

Equation (32) can be rewritten in the following suitable form:

$$i\partial_t W_\rho^{(s)}(\theta,\phi)=(\hat{\mu}-\hat{\mu}^*)(W_\rho^{(s)}(\theta,\phi)W_H^{(0)}(\theta,\phi)), \tag{36}$$

where

$$\hat{\mu}=\sqrt{2S+1}\tilde{F}^{s-1}(\mathcal{L}^2)\sum_j\ a_j(S^{-(j)}\tilde{F}^{1-s}(\mathcal{L}^2))_\rho\otimes(S^{+(j)}\tilde{F}(\mathcal{L}^2))_H, \tag{37}$$

$$\hat{\mu}^*=\sqrt{2S+1}\tilde{F}^{s-1}(\mathcal{L}^2)\sum_j\ a_j(S^{+(j)}\tilde{F}^{1-s}(\mathcal{L}^2))_\rho\otimes(S^{-(j)}\tilde{F}(\mathcal{L}^2))_H, \tag{38}$$

and the operator with subindex "ρ" acts on $W_\rho^{(s)}(\theta,\phi)$, the operator with subindex "H" acts on $W_H^{(s)}(\theta,\phi)$, whereas the external operator $\tilde{F}^{s-1}(\mathcal{L}^2)$ acts on both terms. The number of terms in the sums (37) and (38) is defined by the degree of nonlinearity of the Hamiltonian (8), i.e., $j=0,1,\ldots,j_{\max}$, $j_{\max}=\deg H$, although formally, because of (35), these sums can be extended to infinity. Equations (36)–(38) is the main result of this paper. It is worth noting that although the operator function $\tilde{F}(\mathcal{L}^2)$ has explicitly entered into (37) and (38), the property (24) is sufficient to obtain the evolution equation for any particular Hamiltonian of the form (8).

Note that as a consequence of (33) the symbolic powers $S^{\pm(j)}$in Eqs. (37) and (38) can be substituted by normal powers of the operators (20). This allows us formally to rewrite (37) and (38) in the following form:

$$\hat{\mu}=\sqrt{2S+1}\tilde{F}^{s-1}(\mathcal{L}^2)\sigma(S_\rho^-\otimes S_H^+)\tilde{F}^{1-s}(\mathcal{L}^2)_\rho\otimes\tilde{F}(\mathcal{L}^2)_H,$$
$$\hat{\mu}^*=\sqrt{2S+1}\tilde{F}^{s-1}(\mathcal{L}^2)\sigma(S_\rho^+\otimes S_H^-)\tilde{F}^{1-s}(\mathcal{L}^2)_\rho\otimes\tilde{F}(\mathcal{L}^2)_H, \tag{39}$$

where the function $\sigma(z)$ is defined as

$$\sigma(z)=\sum_j \frac{(-1)^j}{j!(2S+j+1)!}z^j=\frac{1}{z^{S+1/2}}J_{2S+1}(2\sqrt{z}), \tag{40}$$

and $J_n(x)$ is the Bessel function.

Let us consider the first nontrivial term $(j=1)$ in (37) and (38) in $\hat{\mu}-\hat{\mu}^*$,

$$\frac{\sqrt{2S+1}}{(2S+2)!}\tilde{F}^{s-1}(\mathcal{L}^2)[(S^{+(1)})_\rho\otimes(S^{-(1)})_H-(S^{-(1)})_\rho\otimes(S^{+(1)})_H]\tilde{F}^{1-s}(\mathcal{L}^2)_\rho\otimes\tilde{F}(\mathcal{L}^2)_H. \tag{41}$$

One can observe that

$$(S^{+(1)})_\rho\otimes(S^{-(1)})_H-(S^{-(1)})_\rho\otimes(S^{+(1)})_H=\frac{2i}{\sin\theta}\left(\frac{\partial}{\partial\phi_\rho}\otimes\frac{\partial}{\partial\theta_H}-\frac{\partial}{\partial\theta_\rho}\otimes\frac{\partial}{\partial\phi_H}\right)=2i\{,\}_P, \tag{42}$$

where $\{,\}_P$ means the Poisson brackets on the sphere. Thus, the first term on the right-hand side of (36) acquires the form of the Poisson brackets:

$$2i\frac{\sqrt{2S+1}}{(2S+2)!}\tilde{F}^{s-1}(\mathcal{L}^2)\{\tilde{F}^{1-s}(\mathcal{L}^2)W_\rho^{(s)}(\theta,\phi),\tilde{F}(\mathcal{L}^2)W_H^{(0)}(\theta,\phi)\}_P. \tag{43}$$

B. Linear Hamiltonians

In the particular case of linear Hamiltonians, $l=1$ in (8) [when only the term with $j=1$ contributes to (37) and (38)],

$$H=\omega_0 S_z+gS_++g^*S_-, \tag{44}$$

the Weyl symbol of the Hamiltonian takes the form

$$W_H^{(0)}(\theta,\phi)=\frac{2\sqrt{\pi}}{\sqrt{2S+1}}\sum_{k=-1}^{1}\alpha_{1k}Y_{1k}(\theta,\phi),$$
$$\alpha_{10}=\sqrt{2}A_S\omega_0,\quad \alpha_{11}=-2A_Sg,\quad \alpha_{1-1}=2A_Sg^*, \tag{45}$$
$$A_S=\sqrt{\frac{S(S+1)(2S+1)}{6}}.$$

The above expressions can be represented in a more familiar form[12]

$$W_H^{(0)}(\theta,\phi)=\omega_0W_{S_z}^{(0)}(\theta,\phi)+gW_{S_+}^{(0)}(\theta,\phi)+g^*W_{S_-}^{(0)}(\theta,\phi), \tag{46}$$

where

$$W_{S_z}^{(0)}(\theta,\phi)=\sqrt{S(S+1)}\cos\theta,\quad W_{S_\pm}^{(0)}(\theta,\phi)=\sqrt{S(S+1)}\sin\theta e^{\pm i\phi}. \tag{47}$$

In this case due to

$$\{Y^*_{LM}(\theta,\phi),Y_{1k}(\theta,\phi)\}_P \sim Y^*_{LM-k}(\theta,\phi), \quad k=0,\pm 1, \tag{48}$$

we obtain

$$(\hat{\mu}-\hat{\mu}^*)(W^{(s)}_\rho(\theta,\phi)W^{(0)}_H(\theta,\phi))=\frac{2i\sqrt{2S+1}F(1)}{(2S+2)!}\{W^{(s)}_\rho(\theta,\phi),W^{(0)}_H(\theta,\phi)\}_P,$$
$$F(1)=\sqrt{(2S+2)!(2S-1)!}, \tag{49}$$

which leads to the following evolution equation

$$\partial_t W^{(s)}_\rho(\theta,\phi)=\frac{1}{\sqrt{S(S+1)}}\{W^{(s)}_\rho(\theta,\phi),W^{(0)}_H(\theta,\phi)\}_P. \tag{50}$$

Thus, in the case of the linear Hamiltonian the evolution equation for s-ordered quasidistribution functions (1) coincides with the classical Liouville equation.[12]

C. Quadratic Hamiltonians

In the nonlinear case quantum corrections to classical evolution equation come from two different sides. First of all, more terms in the sums (37) and (38) appear. On the other hand, the relation (48) is not true for higher spherical harmonics (with $L\geqslant 2$), which means that expression (43) is not reduced to simple Poisson brackets of $W^{(s)}_\rho(\theta,\phi)$ and $W^{(0)}_H(\theta,\phi)$. Let us write the evolution equation (36) for the case of quadratic Hamiltonians, $\deg H=2$. We have

$$\begin{aligned} i\partial_t W^{(s)}_\rho(\theta,\phi)&=2i\frac{\sqrt{2S+1}}{(2S+2)!}\tilde{F}^{s-1}(\mathcal{L}^2)\{\tilde{F}^{1-s}(\mathcal{L}^2)W^{(s)}_\rho(\theta,\phi),\tilde{F}(\mathcal{L}^2)W^{(0)}_H(\theta,\phi)\}_P \\ &+\frac{\sqrt{2S+1}}{2(2S+3)!}\tilde{F}^{s-1}(\mathcal{L}^2)((S^{-(2)})_\rho\otimes(S^{+(2)})_H-(S^{+(2)})_\rho\otimes(S^{-(2)})_H) \\ &\times(\tilde{F}^{1-s}(\mathcal{L}^2)W^{(s)}_\rho(\theta,\phi)\tilde{F}(\mathcal{L}^2)W^{(0)}_H(\theta,\phi)). \end{aligned} \tag{51}$$

We note that the second term in the above equation is not equal to zero only for the part of the symbol $W^{(0)}_H(\theta,\phi)$ which corresponds to quadratic [on the $su(2)$ algebra generators] terms of the Hamiltonian (8) (the linear part of $W^{(0)}_H(\theta,\phi)$ disappears under the action of the operators $S^{\pm(2)}$). After some algebra the second term on the right-hand side of (51) can be rewritten in the following form

$$-\frac{i}{\sqrt{(2S+3)(S+1)S(2S-1)}}\tilde{F}^{s-1}(\mathcal{L}^2)(\hat{Q}_\rho\otimes\hat{P}_H-\hat{P}_\rho\otimes\hat{Q}_H)(\tilde{F}^{1-s}(\mathcal{L}^2)W^{(s)}_\rho(\theta,\phi)W^{(0)}_H(\theta,\phi)), \tag{52}$$

where we have introduced

$$\hat{Q}=\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\left(\frac{\partial}{\partial\theta}-\cot\theta\right),$$
$$\hat{P}=\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}-\left(\frac{\partial}{\partial\theta}-\cot\theta\right)\frac{\partial}{\partial\theta}. \tag{53}$$

Here we took into account that $\tilde{F}(\mathcal{L}^2)Y_{2k}(\theta,\phi)=F(2)Y_{2k}(\theta,\phi)$ and, from (14), $F(2)=\sqrt{(2S-2)!(2S+3)!}$. Finally, the evolution equation acquires the form

$$\partial_t W_\rho^{(s)}(\theta,\phi)=2\frac{\sqrt{2S+1}}{(2S+2)!}\tilde{F}^{s-1}(\mathcal{L}^2)\{\tilde{F}^{1-s}(\mathcal{L}^2)W_\rho^{(s)}(\theta,\phi),\tilde{F}(\mathcal{L}^2)W_H^{(0)}(\theta,\phi)\}_P$$

$$+\frac{1}{2\alpha}\tilde{F}^{s-1}(\mathcal{L}^2)\{\tilde{F}^{1-s}(\mathcal{L}^2)W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_{P_1}. \tag{54}$$

where

$$\alpha=1/2\sqrt{(2S+3)(2S-1)S(S+1)} \tag{55}$$

and we defined

$$\{,\}_{P_1}=\hat{P}_\rho\otimes\hat{Q}_H-\hat{Q}_\rho\otimes\hat{P}_H. \tag{56}$$

Obviously, the brackets $\{,\}_{P_1}$ conserve the area on the sphere, i.e.,

$$\int d\Omega\{f,g\}_{P_1}=0, \tag{57}$$

for any two functions defined on the sphere. Separating the Hamiltonian into linear H_1, and quadratic H_2 parts, $H=H_1+H_2$, we get

$$W_H^{(0)}(\theta,\phi)=W_{H_1}^{(0)}(\theta,\phi)+W_{H_2}^{(0)}(\theta,\phi), \tag{58}$$

and Eq. (54) takes the form

$$\partial_t W_\rho^{(s)}(\theta,\phi)=\frac{1}{\sqrt{S(S+1)}}\{W_\rho^{(s)}(\theta,\phi),W_{H_1}^{(0)}(\theta,\phi)\}_P+\frac{1}{2\alpha}\tilde{F}^{s-1}(\mathcal{L}^2)[(2S+3)$$

$$\times\{\tilde{F}^{1-s}(\mathcal{L}^2)W_\rho^{(s)}(\theta,\phi),W_{H_2}^{(0)}(\theta,\phi)\}_P+\{\tilde{F}^{1-s}(\mathcal{L}^2)W_\rho^{(s)}(\theta,\phi),W_{H_2}^{(0)}(\theta,\phi)\}_{P_1}]. \tag{59}$$

D. Example

Let us consider, for example, the simplest nonlinear Hamiltonian (for physical applications see, e.g., Refs. 20–22)

$$H=\chi S_z^2. \tag{60}$$

The corresponding $W_H^{(0)}(\theta,\phi)$ symbol has the form

$$W_H^{(0)}(\theta,\phi)=\alpha\frac{4}{3}\sqrt{\frac{\pi}{5}}Y_{20}(\theta,\phi)+\frac{S(S+1)}{3}=\alpha\left(\cos^2\theta-\frac{1}{3}\right)+\frac{S(S+1)}{3}, \tag{61}$$

where α is defined in (55). Taking into account that

$$\{W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_P=-2\alpha\cos\theta\partial_\phi W_\rho^{(s)}(\theta,\phi),$$

$$\{\tilde{F}^{1-s}(\mathcal{L}^2)W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_P=-2\alpha\cos\theta\tilde{F}^{1-s}(\mathcal{L}^2)\partial_\phi W_\rho^{(s)}(\theta,\phi), \tag{62}$$

and

$$\hat{Q}W_H^{(0)}(\theta,\phi)=0, \quad \hat{P}W_H^{(0)}(\theta,\phi)=2\alpha\sin^2\theta, \tag{63}$$

we obtain from (54)

$$\partial_t W_\rho^{(s)}(\theta,\phi)=-\chi[2(S+1)\tilde{F}^{s-1}(\mathcal{L}^2)\cos\theta\tilde{F}^{1-s}(\mathcal{L}^2) + \tilde{F}^{s-1}(\mathcal{L}^2)\sin\theta\partial_\theta\tilde{F}^{1-s}(\mathcal{L}^2)]\partial_\phi W_\rho^{(s)}(\theta,\phi). \tag{64}$$

One can show (see the Appendix) that Eq. (64) acquires the following forms according to the value of the parameter s:

$$\partial_t W_\rho^{(1)}(\theta,\phi)=-\chi[2(S+1)\cos\theta+\sin\theta\partial_\theta]\partial_\phi W_\rho^{(1)}(\theta,\phi), \tag{65}$$

$$\partial_t W_\rho^{(0)}(\theta,\phi)=-\chi\left[\left(S+\frac{1}{2}\right)\Phi(\mathcal{L}^2)\cos\theta+\varepsilon\Phi^{-1}(\mathcal{L}^2)\left(\frac{3}{2}\cos\theta+\sin\theta\partial_\theta\right)\right]\partial_\phi W_\rho^{(0)}(\theta,\phi), \tag{66}$$

$$\partial_t W_\rho^{(-1)}(\theta,\phi)=-\chi[2S\cos\theta-\sin\theta\partial_\theta]\partial_\phi W_\rho^{(-1)}(\theta,\phi), \tag{67}$$

where the function $\Phi(\mathcal{L}^2)$ is defined as

$$\Phi(\mathcal{L}^2)=[2-\varepsilon^2(2\mathcal{L}^2+1)+2\sqrt{1-\varepsilon^2(2\mathcal{L}^2+1)+\varepsilon^4\mathcal{L}^4}]^{1/2}, \tag{68}$$

and

$$\varepsilon=\frac{1}{2S+1}. \tag{69}$$

One can observe that Eq. (65) is just an equation for the P-function [which can be easily obtained by using the $su(2)$ coherent states method].

E. Large dimensions of representation

Now let us consider the limit of the large dimension of representation, $S\gg 1$ (in this case $\varepsilon \ll 1$). In this limit it is useful to represent the function $\tilde{F}(\mathcal{L}^2)$ in the following form

$$\tilde{F}(\mathcal{L}^2)=\frac{(2S+1)!}{\sqrt{2S+1}}\left(1+\frac{\varepsilon}{2}\mathcal{L}^2+O(\varepsilon^2)\right). \tag{70}$$

Taking into account that

$$\sum_{j=0}^{\infty}\frac{(-x)^j}{j!(2S+j+1)!}=f\left(x\frac{\partial}{\partial x}\right)\exp(-\varepsilon x), \tag{71}$$

where the function $f(z)$ in the above equation is a series on ε,

$$f(z)=1-\frac{\varepsilon}{2}(z^2+z)+O(\varepsilon^2), \tag{72}$$

we can approximate the evolution equation (36) as follows:

$$\partial_t W_\rho^{(s)}(\theta,\phi)\approx 2\varepsilon\{W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_P+2\varepsilon^2\Bigg[\frac{1-s}{2}\{\mathcal{L}^2W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_P$$
$$+\frac{1}{2}\{W_\rho^{(s)}(\theta,\phi),\mathcal{L}^2W_H^{(0)}(\theta,\phi)\}_P+\left(\frac{s-1}{2}\mathcal{L}^2-1\right)\{W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_P$$
$$+\{W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_{P_1}\Bigg]. \tag{73}$$

Taking into account the following relation between $\{,\}_P$ and $\{,\}_{P_1}$:

$$\{f,g\}_{P_1}=(\tfrac{1}{2}\mathcal{L}^2+1)\{f,g\}_P-\tfrac{1}{2}\{\mathcal{L}^2f,g\}_P-\tfrac{1}{2}\{f,\mathcal{L}^2g\}_P, \tag{74}$$

where $f(\theta,\phi)$ and $g(\theta,\phi)$ are functions on the sphere, Equation (73) is rewritten in the form

$$\partial_t W_\rho^{(s)}(\theta,\phi)=2\varepsilon\{W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_P+\varepsilon^2 s[\mathcal{L}^2\{W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_P$$
$$-\{\mathcal{L}^2W_\rho^{(s)}(\theta,\phi),W_H^{(0)}(\theta,\phi)\}_P]+O(\varepsilon^3). \tag{75}$$

The first term on the right-hand side of Eq. (75) is, as expected, a classical evolution equation [Poisson brackets of the s-ordered quasidistribution function $W_\rho^{(s)}(\theta,\phi)$ and symmetrized Stratonovich–Weyl symbol of the system Hamiltonian]. The second term represents a first correction to the classical evolution equation. One can observe that this correction vanishes when $s=0$, i.e., the first correction to the classical evolution of motion is absent for the Stratonovich–Weyl quasidistribution function.

For example, in the case of the Hamiltonian (60) we get for the symmetrized Stratonovich–Weyl symbol the following approximate equation of motion [corresponding to expansion of the function $\Phi(\mathcal{L}^2)$ in (66) in series on ε]

$$\partial_t W_\rho^{(0)}(\theta,\phi)=-\chi[(2S+1)\cos\theta\partial_\phi+\varepsilon\,\hat{\Xi}]W_\rho^{(0)}(\theta,\phi), \tag{76}$$

where $\hat{\Xi}$ is a diffusion-like operator

$$\hat{\Xi}=-\tfrac{1}{2}[(\cos\theta+1)\mathcal{L}^2+\sin\theta\partial_\theta]\partial_\phi, \tag{77}$$

which describes quantum corrections to the quasiclassical motion in analogy to the quasiclassical expansion in the Moyal equation for the Heisenberg–Weyl group. It is worth noting that in general only the evolution equation for the Stratonovich–Weyl quasidistribution function $W_\rho^{(0)}(\theta,\phi)$ (not for Q- or for P-Beresin symbols) reduces to the classical equation of motion in the limit $\varepsilon\to 0$ [compare, for example, (62) with (65) and (67)].

III. CONCLUSIONS

In summary, we have found exact evolution equations for the s-parametrized family SU(2) quasiprobability distribution functions on the sphere. It was shown that for polynomial [on the generators of the $su(2)$ algebra] Hamiltonians the equation of motion contains a finite number of terms, defined by the degree of nonlinearity of the Hamiltonian. For linear systems the evolution equation reduces to the Liouville equation. We also have given an explicit form of the equation of motion for quadratic systems, which are the most usual in quantum-optical applications (see, e.g., Ref. 23 and references therein). In the limit of the large value of spin ($S\gg 1$) the first term of the quasiclassical expansion is just the Poisson brackets (on the sphere) of the s-ordered quasidistribution function with the symmetrized (Stratonovich–Weyl) symbol of the Hamiltonian.

Connection with the star-product of generalized Weyl symbols on the SU(2) group[11] and its contraction to the Heisenberg-Weyl group will be considered elsewhere.

APPENDIX: DERIVATION OF EQS. (65)–(67)

In this Appendix we obtain Eqs. (65)–(67) starting from Eq. (64).

To transform Eq. (64) to a more simple form we use the following algebraic relations

$$\tilde{F}^{s-1}(\mathcal{L}^2)\cos\theta\tilde{F}^{1-s}(\mathcal{L}^2)Y_{LM}(\theta,\phi)=[\tfrac{1}{2}(f_L+3g_L)\cos\theta+g_L\sin\theta\partial_\theta]Y_{LM}(\theta,\phi), \tag{A1}$$

$$\begin{aligned}&\tilde{F}^{s-1}(\mathcal{L}^2)\sin\theta\partial_\theta\tilde{F}^{1-s}(\mathcal{L}^2)Y_{LM}(\theta,\phi)\\&\quad=[(L+2)(L-1)g_L\cos\theta+\tfrac{1}{2}(f_L-3g_L)\sin\theta\partial_\theta]Y_{LM}(\theta,\phi),\end{aligned} \tag{A2}$$

where

$$f_L=a_L+a_{L+1}^{-1},\quad g_L=\frac{a_L-a_{L+1}^{-1}}{2L+1}, \tag{A3}$$

$$a_L=F^{s-1}(L)F^{1-s}(L-1)=\left(\frac{2S+1-L}{2S+1+L}\right)^{\frac{1-s}{2}}, \tag{A4}$$

and the relation between $F(L)$ and $\tilde{F}(\mathcal{L}^2)$ is given by (24).

One can observe that Eqs. (65) and (67) are obtained directly by substituting (A3) and (A4) and (A1) and (A2) into (64) for values $s=\pm1$. In the following we deduce Eq. (66), when the parameter takes value $s=0$. To this end we rewrite Eq. (A4) as follows:

$$a_L=\frac{\varphi_L}{1+\varepsilon L},\quad a_{L+1}^{-1}=\frac{\varphi_{L+1}}{1-\varepsilon(L+1)}, \tag{A5}$$

where

$$\varphi_L=\sqrt{1+\varepsilon^2L^2}. \tag{A6}$$

Then we obtain from (A1) and (A2)

$$\begin{aligned}&\tilde{F}^{s-1}(\mathcal{L}^2)[2(S+1)\cos\theta+\sin\theta\partial_\theta]\tilde{F}^{1-s}(\mathcal{L}^2)Y_{LM}(\theta,\phi)\\&\quad=\frac{1}{\varepsilon}\left[\frac{\varphi_L+\varphi_{L+1}}{2}\cos\theta+\frac{\varphi_L-\varphi_{L+1}}{2L+1}\left(\frac{3}{2}\cos\theta+\sin\theta\partial_\theta\right)\right]Y_{LM}(\theta,\phi).\end{aligned} \tag{A7}$$

Now we take into account

$$\frac{\varphi_L-\varphi_{L+1}}{2L+1}=\frac{\varepsilon^2}{\varphi_L+\varphi_{L+1}}, \tag{A8}$$

and observe that

$$(\varphi_L+\varphi_{L+1})Y_{LM}(\theta,\phi)=\Phi(\mathcal{L}^2)Y_{LM}(\theta,\phi), \tag{A9}$$

where the operator function $\Phi(\mathcal{L}^2)$ is defined in (68). Equations (A7) and (A9) immediately lead to (66).

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Det-Det correlations for quantum maps: Dual pair and saddle-point analyses

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An attempt is made to clarify the ballistic nonlinear sigma model formalism recently proposed for quantum chaotic systems, by looking at the spectral determinant $Z(s)=\mathrm{Det}(1-sU)$ for quantized maps $U\in \mathrm{U}(N)$, and studying the correlator $\omega_U(s)=\int d\theta |Z(e^{i\theta}s)|^2$. By identifying $\mathrm{U}(N)$ as one member of a dual pair acting in the spinor representation of $\mathrm{Spin}(4N)$, the expansion of $\omega_U(s)$ in powers of s^2 is shown to be a decomposition into irreducible characters of $\mathrm{U}(N)$. In close analogy with the ballistic nonlinear sigma model, a coherent-state integral representation of $\omega_U(s)$ is developed. For generic U this integral has $\binom{2N}{N}$ saddle points and the leading-order saddle-point approximation turns out to reproduce $\omega_U(s)$ *exactly*, up to a constant factor. This miracle is explained by interpreting $\omega_U(s)$ as a character of $\mathrm{U}(2N)$, and arguing that the leading-order saddle-point result corresponds to the *Weyl character formula*. Unfortunately, the Weyl decomposition behaves nonsmoothly in the semiclassical limit $N\to\infty$, and to make further progress some additional averaging needs to be introduced. Several schemes are investigated, including averaging over basis states and an ''isotropic'' average. The saddle-point approximation applied in conjunction with these schemes is demonstrated to give incorrect results in general, one notable exception being a semiclassical averaging scheme, for which all loop corrections vanish identically. As a side product of the dual pair decomposition with isotropic averaging, the crossover between the Poisson and CUE limits is obtained. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1462417]

I. INTRODUCTION

One of the striking characteristics of a quantized chaotic Hamiltonian system is found in the correlations inherent in its spectrum at small energy differences. Extensive numerical work has shown that various quantities (such as the nearest-neighbor spacing distribution and the two-level correlation function) of a quantum chaotic system are *universal*: their behavior coincides with that of a Wigner–Dyson random matrix ensemble of the appropriate symmetry class.[1] This property, first noticed in billiards, was found to apply to many chaotic systems, including symplectic *maps*. In contrast, if the dynamics is integrable (in the sense that the $2f$-dimensional phase space foliates into f-dimensional submanifolds invariant under the Hamiltonian flow), the generic behavior of the eigenvalues is expected[2] to be that of independent random variables, so that their correlations are in the Poisson universality class.

The present article will be concerned with quantum maps, i.e., with quantizations of some canonical transformation $\phi: M\to M$ of a compact symplectic manifold M. We assume that the problem of quantization itself has been tackled, so the phase space has been prequantized into a Hilbert space $\mathcal{H}_N$ of dimension $N\sim\hbar^{-1}$, and the quantum map acts on it as a unitary operator.[3,4] With respect to a basis of $\mathcal{H}_N$ this operator is represented by an $N\times N$ unitary matrix $U_{\phi,N}$. The latter has a semiclassical limit, in the sense that traces of its powers can be estimated in terms of

classical periodic points.[4] For a system with one degree of freedom, the Gutzwiller-Tabor trace formula reads

$$\mathrm{Tr}(U_{\phi,N}^n) \overset{N\to\infty}{\sim} \sum_{p\subset \mathrm{Fix}(\phi^n)} N^{\dim(p)/2} A_p \mathrm{e}^{\mathrm{i}N\Phi p}, \tag{1}$$

where p is one component of the set of n-periodic points; for an Anosov system, it is an isolated point $[\dim(p)=0]$, whereas if the dynamics conserves energy, p is one-dimensional. Φ_p and A_p are purely classical quantities related to the dynamics around the set p.

The quantum spectrum consists of the N eigenvalues (pseudo-energies) $\{\mathrm{e}^{\mathrm{i}\theta_j}\}_{j=1,\ldots,N}$ of $U_{\phi,N}$. The first analytical estimates of the two-level correlation function [which is the Fourier transform of the *form factor* $F(n)=|\mathrm{Tr}(U_{\phi,N}^n)|^2$] for such spectra were based on the above trace formula, combined with some known ergodic properties of long periodic orbits.[5] In the present article we focus attention on another statistic, namely the autocorrelation function of the spectral determinant:

$$\Omega_U(\gamma) \overset{\mathrm{def}}{=} \gamma^{-N/2} \int_0^{2\pi} \frac{d\phi}{2\pi} \mathrm{Det}(1-\gamma \mathrm{e}^{\mathrm{i}\phi} U)\mathrm{Det}(1-\mathrm{e}^{-\mathrm{i}\phi} U^\dagger). \tag{2}$$

(The parameter γ will be a complex number close to unity, with the scaling $|\gamma-1|\sim 1/N$.) This correlation function has already been considered[6,7] for chaotic versus integrable quantum maps, and the same universality was observed as for the form factor or the nearest-neighbor distribution. A semiclassical analysis of this correlation function was performed using the Gutzwiller trace formula in Ref. 7.

The computation of correlation functions from the trace formula (1) always requires some sort of averaging. In the semiclassical theory of the form factor $F(n)$ one wants to use the so-called diagonal approximation, neglecting the off-diagonal terms in the double-sum over periodic orbits.[5] To justify this step one must average over energy or some family of systems: one needs slight variations in the classical actions Φ_p to make the phase interferences $\sim \mathrm{e}^{\mathrm{i}N(\Phi_p-\Phi_{p'})}$ average to zero. The need for averaging was emphasized in Refs. 6 and 8, where it was pointed out that the spectrum of an individual quantum system is too noisy to allow universality to be seen in its bare form factor. In addition to the noise problem, there exist some quantum chaotic systems with arithmetic symmetries, which lead to periodic orbit degeneracies and nonuniversal spectral correlations.[9,10] (Such systems are nongeneric, however, in any decent space of smooth maps.)

Thus universal behavior is expected only in the generic case, and to make a correct mathematical statement about universality of the spectral correlations of a general system one ought to define the precise meaning of the word "generic." (In the case of integrable systems, the spectral correlations could sometimes be studied directly, by utilizing the explicit expressions for the eigenvalues; two-point correlations were shown to be Poisson for a rather subtle set of parameters.)[11] We can avoid the issue of genericity by averaging the correlation function over some set of quantum maps. That is, we specify a measure $\mathrm{d}\mathcal{P}_N(U)$ on the unitary group $\mathrm{U}(N)$, and the function to be studied then reads

$$\langle \Omega_U(\gamma)\rangle = \int_{\mathrm{U}(N)} \mathrm{d}\mathcal{P}_N(U)\Omega_U(\gamma).$$

We want this measure to be very concentrated (or "local") around the quantum map $U_{\phi,N}$ (see Secs. IV C and VI). In the course of this article, we will also consider cases for which this measure has a broader support (Sec. V), including the case where the measure is the Haar measure on $\mathrm{U}(N)$. We are then dealing with the circular unitary ensemble (CUE), for which the determinant correlation function has been thoroughly investigated.[6,12]

The Gutzwiller trace formula has the attractive feature of relating quantum to classical properties, but its use for estimating the spectral correlation functions still raises questions. The prob-

lem is that the formula is rigorous in general only for times shorter than the Ehrenfest time: $n \leqslant \log N$ (and $N \to \infty$). Yet, long-time traces ($n \sim N$) are needed to obtain spectral correlation functions at the scale of the mean level spacing where universality emerges. The diagonal approximation, which assumes statistical independence of the different periodic orbits, is unsatisfactory at large times where the exponential proliferation of periodic orbits clashes with the finite (N) number of eigenvalues: the classical information is then overcomplete, which implies some sort of hidden correlation between the contributions from classical orbits. A recipe to overcome this difficulty has been devised by Bogomolny and Keating,[13] but so far lacks rigorous justification.

To bypass these problems, a second approach to estimate spectral correlations has recently emerged, inspired by the study of disordered metals. It consists in expressing the correlation function as a quantum field theory (or functional integral) of the type of a nonlinear sigma model (NLσM). One then tries to analyze the functional integral by standard field-theoretic methods such as perturbation expansion, saddle-point analysis and the renormalization group. This approach was first applied successfully to systems with disorder, where the dynamics is governed by a diffusion operator.[14] The formalism was later extended to the ''ballistic case,'' [15,16] and quantum correlation functions were put in relation with the spectrum of the Frobenius–Perron operator (i.e., the evolution operator for classical densities). Although quite elegant, this approach suffered from several drawbacks. Among these are the appearance of unwanted zero modes around the main saddle point, and the problem of ''mode locking.'' [17] Besides, the results do not exactly agree with the correlations calculated numerically for the Riemann zeta function (the prototype of a quantum chaotic spectral determinant);[13] nor do they explain the nongeneric spectral correlations featured by systems with arithmetic symmetries. More recent treatments of the ballistic NLσM have also stressed the need for averaging over a smooth disorder if one wants to avoid the above problems.[18,19]

In an attempt to resolve these uncertainties, we have adapted the latter approach, which had originally been conceived for Hamiltonian systems, to the case of quantum maps $U_{\phi,N}$. Our objective was to prove the universality of the determinant correlation function $\Omega_U(\gamma)$ (Sec. II B) upon averaging wrt a suitable measure on U(N). This correlation function is easier to treat than the two-level correlation function, as it does not require the use of a supersymmetric representation[15,16] but can be expressed as an ordinary c-number integral over a finite-dimensional manifold $\mathcal{M}_N$ (Sec. II D). We write this integral in the form

$$\Omega_U(\gamma) = \int_{\mathcal{M}_N} dQ \mathrm{e}^{-S(\gamma,U,Q)}, \tag{3}$$

where $S(\gamma,U,\cdot)$ is called the *effective action*.

For the reasons stated, we will consider averages of Ω_U with respect to certain probability measures $\mathrm{d}\mathcal{P}_N(U)$. The averaged correlation function, denoted by $\langle \Omega_U(\gamma) \rangle$, can still be obtained by integrating the Boltzmann weight given by an effective action:

$$\langle \Omega_U(\gamma) \rangle = \int_{\mathcal{M}_N} dQ \mathrm{e}^{-S_{\mathrm{av}}(\gamma,Q)}.$$

To estimate these integrals, we apply the same technique that was used in Ref. 15: we expand $S_{\mathrm{av}}(\gamma,Q)$ up to quadratic order around its saddle-points Q_{crit}, and perform the Gaussian integrals. The result obtained in this way,

$$\langle \Omega_U(\gamma) \rangle_{|\text{s.p. exp.}} = \sum_{Q_{\mathrm{crit}}} \{\mathrm{Det}\delta^2 S_{\mathrm{av}}(\gamma,Q_{\mathrm{crit}})\}^{-1/2} \mathrm{e}^{-S_{\mathrm{av}}(\gamma,Q_{\mathrm{crit}})}, \tag{4}$$

is called the leading-order saddle-point expansion of the integral.

Owing to the absence of a large parameter in front of the action S_{av}, the expansion is *a priori* not justified mathematically. A more careful treatment should in principle include perturbative corrections around each critical point (we actually compute the expansion up to two loops in a particular case, see Sec. IV D).

We have succeeded in computing the leading-order term for a few averaging schemes. For an individual matrix U_N we can actually reproduce the exact value of the correlation function (3) in this way (Sec. III). In Sec. IV C we define a ''semiclassical'' averaging scheme, which we think is a good candidate to obtain universality of correlations;[20] unfortunately, in that case we can only compute the contributions from the two standard saddle points.

In order to test the leading-order saddle-point approximation, we selected a sequence of statistical ensembles [i.e., a sequence of measures $\mathrm{d}\mathcal{P}_N(U)$] for which the averaged correlation function can be computed exactly, and compared the exact result with the saddle-point approximation for the corresponding effective action. All these ensembles are U(N)-rotation invariant, that is, we first average over all bases of $\mathcal{H}_N$ (Sec. V), then possibly over the spectrum of U_N (Secs. V C and VI A). In most cases, the saddle-point expansion of these ensembles yields erroneous results. We still hope that the expansion is better behaved in the case of local averages, like the semiclassical one.

These disappointing results seem to challenge the use of NLσM methods for the study of quantum ballistic systems, unless our understanding and control of these methods significantly improves. In Sec. VI, we introduce a U(N)-isotropic local averaging scheme which we treat by an alternative method; unfortunately, this scheme does not discriminate between the different universal behaviors that are expected for chaotic versus integrable maps. Nevertheless, we use it in Sec. VI A to compute the correlations along a crossover between the Poisson and CUE universality classes.

II. ALGEBRAIC MANIPULATION OF Ω_U

A. Fourier decomposition of Ω_U

We first remind the reader of some known results concerning the correlation function Ω_U.[6,7] The spectral determinant of $U \in \mathrm{U}(N)$ may be expanded as

$$\mathrm{Det}(1-sU)=\sum_{k=0}^{N} s^k a_k(U). \tag{5}$$

The unitarity of U implies a ''self-inversive'' property for the secular coefficients:[21]

$$a_{N-k}(U)=\mathrm{Det}(-U)a_k(\overline{U}).$$

Each coefficient a_k may be obtained from the traces $\{t_l=\mathrm{Tr}U^l\}$ by

$$a_k=-\frac{1}{k}\left(t_k+\sum_{l=1}^{k-1} a_l t_{k-l}\right)=\frac{(-1)^k}{k!}\begin{vmatrix} t_1 & t_2 & t_3 & \dots & t_k \\ 1 & t_1 & t_2 & \dots & t_{k-1} \\ 0 & 2 & t_1 & \ddots & t_{k-2} \\ 0 & 0 & 3 & & \vdots \\ \vdots & \ddots & & & \vdots \\ 0 & \dots & \dots & k-1 & t_1 \end{vmatrix}.$$

Because this dependence is highly nonlinear, the secular coefficients inherit non-Gaussian distributions in the RMT ensembles.[6] However, to compute the ensemble averages of $\Omega_U(\gamma)$ one only needs to know their variances, since

$$\Omega_U(\gamma)=\sum_{k=0}^{N}\ \gamma^{k-N/2}\ |a_k|^2=\sum_{k=0}^{N/2}\ (\gamma^{k-N/2}+\gamma^{N/2-k})|a_k|^2. \tag{6}$$

For the Poisson and the CUE ensemble of random matrices, these variances were computed in Ref. 6, and have the following large-N asymptotics:

$$\langle|a_k|^2\rangle_{\text{Poisson}}=\binom{N}{k},\quad \langle|a_k|^2\rangle_{\text{CUE}}=1, \tag{7}$$

$$\langle\Omega_U(e^{ix/N})\rangle_{\text{Poisson}}\sim 2^N,\quad \langle\Omega_U(e^{ix/N})\rangle_{\text{CUE}}\sim N\frac{\sin(x/2)}{x/2}. \tag{8}$$

In Ref. 7, a semiclassical estimation of the $|a_k|^2$ was given for integrable and chaotic quantum maps. The authors used the explicit expression in terms of the traces t_l, and estimated the latter by the Gutzwiller trace formula (1). They made a generalized diagonal approximation treating the traces t_l as statistically independent variables. To obtain the correlation function, one has to estimate the $|a_k|^2$ (and hence the t_k) up to times $k\lesssim N/2$, where the Gutzwiller formula is nonrigorous.

B. Representation-theoretic content of Ω_U

We now introduce a more group-theoretic expression for the correlation function. Instead of performing the expansion (5), we will express $\Omega_U(\gamma)$ as a *character* in a certain irreducible representation of U($2N$), which is best described using the physical language of fermions.

Let $\mathcal{F}_N$ be the Fock space for N types of fermions f_i, $f_i^\dagger$. In mathematics $\mathcal{F}_N$ is known as the spinor representation space of the group Spin($2N$). Then, for any $N\times N$ unitary matrix U,

$$\mathrm{Det}(1-U)=\mathrm{Tr}_{\mathcal{F}_N}(-1)^{\sum_i f_i^\dagger f_i}\exp\sum_{i,j=1}^{N} f_i^\dagger(\log U)_{ij}f_j.$$

The exponential on the right-hand side can be shown to be well defined in spite of the multivaluedness of $\log U$. To account for both determinants, we use $2N$ fermions, whose creation operators are denoted by $f_{+j}^\dagger$ and $f_{-j}^\dagger$, $j=1,\ldots,N$. The integration over ϕ in the integral (2) projects on the subspace $\mathcal{F}\underset{\text{def}}{=}\mathrm{Ker}(F_+-F_-)$, where $F_\pm=\Sigma_i f_{\pm i}^\dagger f_{\pm i}$ are the number operators for the two types of fermions. The correlation function reads

$$\Omega_U(\gamma)=\mathrm{Tr}_{\mathcal{F}}\gamma^{(F_++F_--N)/2}\exp\sum_{i,j=1}^{N}(\log U)_{ij}(f_{+i}^\dagger f_{+j}-f_{-j}^\dagger f_{-i}). \tag{9}$$

The operator under the trace belongs to an irreducible representation R of the group U($2N$), realized on the space $\mathcal{F}$, which has dimension $\binom{2N}{N}$. This representation may be defined through its Lie algebra version: any skew-Hermitian $2N\times 2N$ matrix $\mathbf{X}=\left(\begin{smallmatrix}a & b\\ c & d\end{smallmatrix}\right)$ is represented by the operator

$$R(\mathbf{X})=\sum_{i,j=1}^{N} a_{ij}f_{+i}^\dagger f_{+j}+b_{ij}f_{+i}^\dagger f_{-j}^\dagger+c_{ij}f_{-i}f_{+j}+d_{ij}f_{-i}f_{-j}^\dagger. \tag{10}$$

By exponentiating, $R(\exp\mathbf{X})=\exp R(\mathbf{X})$, we obtain a U($2N$)-representation, which we still denote by R. The correlation function $\Omega_U(\gamma)$ for any $N\times N$ unitary matrix U may be recast as a character in this representation:

$$\Omega_U(\gamma)=\gamma^{-N/2}\mathrm{Det}(U)^{-1}\ \mathrm{Tr}\,R(\Gamma\mathbf{U}) \tag{11}$$

where

$$\mathbf{U} \overset{\text{def}}{=} \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}, \quad \Gamma \overset{\text{def}}{=} \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix} \in \mathrm{U}(2N).$$

As it stands, the construction assumes $\gamma = e^{i\theta} \in \mathrm{U}(1)$. It can also be used for other values of γ, since R naturally extends to a representation of $\mathrm{GL}(2N, \mathbb{C})$. In the following, matrices in bold print will always be of size $2N \times 2N$.

The assignment $U \mapsto \mathbf{U}$ embeds $\mathrm{U}(N)$ into $\mathrm{U}(2N)$. By this embedding, R restricts to a *reducible* representation of $\mathrm{U}(N)$ on $\mathcal{F}$, which we simply denote by $R(U)$. To express the correlation function, we may also consider the $\mathrm{U}(N)$-representation $R_{-1}(U) \overset{\text{def}}{=} \det(U)^{-1} R(U)$.

In the next section, we decompose $R(U)$ [or equivalently $R_{-1}(U)$] into irreducible representations (irreps) of $\mathrm{U}(N)$, thus expressing the correlation function $\Omega_U(\gamma)$ as a sum of $\mathrm{U}(N)$-characters.

C. Ω_U as a sum of U(N)-characters

The crucial mathematical tool to use is the *dual pair* structure.[22] The subalgebra $\{X_N \otimes \mathbb{I}_2 \,|\, X_N \in \mathfrak{u}(N)\}$ of $\mathfrak{u}(2N)$ commutes with the subalgebra $\{\mathbb{I}_N \otimes x_2 \,|\, x_2 \in \mathfrak{u}(2)\}$, and each is the commutant of the other inside $\mathfrak{u}(2N)$: they are said to form a dual pair. This means that for all $U \in \mathrm{U}(N)$, the operator $R(U)$ commutes with the set

$$J_\uparrow = \sum_i f_{+i}^\dagger f_{-i}^\dagger,$$

$$J_\downarrow = \sum_i f_{-i} f_{+i},$$

$$J_0 = F_+ + F_- - N.$$

The operators J_0, $J^\uparrow$ and $J^\downarrow$ generate an $\mathfrak{su}(2)$ algebra. The equation $J_0 R(U) = R(U) J_0$ implies that $R(U)$ conserves the total number of particles and hence acts inside the subspaces $\mathcal{F}^p = \mathcal{F} \cap \mathrm{Ker}(F_+ + F_- - 2p)$.

The dual pair structure provides us with a prescription[22] to decompose $R(U)$. Inside the reduced Fock space $\mathcal{F}$, we consider the subspace of lowest SU(2) weights, ${}^0\mathcal{F} = \mathcal{F} \cap \mathrm{Ker} J_\downarrow$, and expand it according to its particle content: ${}^0\mathcal{F}^p \overset{\text{def}}{=} {}^0\mathcal{F} \cap \mathcal{F}^p$. Classical results of invariant theory, due mostly to H. Weyl[23] and succinctly summarized by R. Howe,[22] amount to the following statements:

(i) The operator $R(U)$ acts inside each space ${}^0\mathcal{F}^p$, through a certain irrep $\tilde{\rho}_p(U)$ of $\mathrm{U}(N)$. Equivalently, $R_{-1}(U)$ acts on this space through $\rho_p(U) = \mathrm{Det}(U)^{-1} \tilde{\rho}_p(U)$. Furthermore, two irreps ρ_p and $\rho_{p'}$ are inequivalent if $p \neq p'$.

(ii) The image of ${}^0\mathcal{F}^p$ under $(J_\uparrow)^k$ is the space ${}^k\mathcal{F}^{p+k} \subset \mathcal{F}^{p+k}$ which is either trivial (if $k > N - 2p$) or carries the irrep ρ_p (if $k \leqslant N - 2p$). The operators $J_\uparrow$, $J_\downarrow$, J_0 act on this tower of spaces according to the $\mathfrak{su}(2)$-irrep of dimension $N - 2p + 1$.

(iii) The direct sum of these towers exhausts $\mathcal{F}$.

We summarize these statements in the following diagram. All entries in a given row are subspaces containing the same number of fermions; all entries in a given column (or tower) carry the same $\mathrm{U}(N)$-irrep. We only show the case where N is an even integer (the odd-N case being very similar):

$$
\begin{array}{lcccccccc}
\mathcal{F}^N & = & {}^N\mathcal{F}^N & & & & & & \\
 & & \uparrow J_\uparrow & & & & & & \\
\mathcal{F}^{N-1} & = & {}^{N-1}\mathcal{F}^{N-1} & \oplus & {}^{N-2}\mathcal{F}^{N-1} & & & & \\
\vdots & & \uparrow J_\uparrow & & \uparrow J_\uparrow & & \ddots & & \\
\vdots & & \vdots & & \vdots & & & & {}^0\mathcal{F}^{N/2} \\
\vdots & & \uparrow J_\uparrow & & \uparrow J_\uparrow & & \uparrow J_\uparrow & & \\
\mathcal{F}^2 & = & {}^2\mathcal{F}^2 & \oplus & {}^1\mathcal{F}^2 & \oplus & {}^0\mathcal{F}^2 & & \\
 & & \uparrow J_\uparrow & & \uparrow J_\uparrow & & & & \\
\mathcal{F}^1 & = & {}^1\mathcal{F}^1 & \oplus & {}^0\mathcal{F}^1 & & & & \\
 & & \uparrow J_\uparrow & & & & & & \\
\mathcal{F}^0 & = & {}^0\mathcal{F}^0 & & & & & & \\
U(N)-\text{irreps:} & & \rho_0 & & \rho_1 & & \rho_2 & \cdots & \rho_{N/2}
\end{array}
\tag{12}
$$

The leftmost tower on the right-hand side carries the trivial $\mathfrak{u}(N)$-irrep, so all spaces ${}^p\mathcal{F}^p = (J_\uparrow)^p\,{}^0\mathcal{F}^0$ are one-dimensional.

Each irrep ρ_p (or $\tilde{\rho}_p$) may be described by a Young diagram. ρ_p mixes the action of U on p fermions f_+ with the action of $\overline{U}$ on p fermions f_-. Owing to antisymmetrization, it corresponds to the diagram with p rows of length 2 followed by $N-2p$ rows of length one:

$$\tilde{\rho}_p(U_N) = \mathrm{Det}(U_N)\rho_p(U_N) = U_N^{[2^p\,1^{N-2p}]}.$$

In view of the above diagram, the dimensions of the representation spaces ${}^k\mathcal{F}^{k+p}$ follow immediately from those of the spaces $\mathcal{F}^p$:

$$\dim({}^k\mathcal{F}^{k+p}) = \dim(\mathcal{F}^p) - \dim(\mathcal{F}^{p-1}) = \binom{N}{p}^2 - \binom{N}{p-1}^2. \tag{13}$$

By doing the sum over each $\mathfrak{su}(2)$-multiplet we can now express the correlation function (11) in terms of the irreps ρ_p:

$$\Omega_U(\gamma) = \sum_{p=0}^{N/2} \mathrm{Tr}\rho_p(U)\,\frac{\gamma^{p-N/2} - \gamma^{N/2+1-p}}{1-\gamma}, \tag{14}$$

or, making the substitution $\gamma = \mathrm{e}^{\mathrm{i}x/N}$,

$$\Omega_U(\mathrm{e}^{\mathrm{i}x/N}) = \sum_{p=0}^{N/2} \mathrm{Tr}\rho_p(U)\,\frac{\sin\{(x/2)\,[1-(2p-1)/N]\}}{\sin(x/2N)}.$$

For large values of N we may replace the denominator $\sin(x/2N)$ by $x/2N$. A quick comparison shows that this decomposition is actually equivalent to the pedestrian expansion (6) written down in Sec. II A. The squared coefficients $|a_k|^2$ now acquire a representation-theoretic meaning:

$$\forall p \leqslant N/2: \quad |a_p(U)|^2 = \mathrm{Tr}_{\mathcal{F}^p} R_{-1}(U) = \sum_{k=0}^{p} \mathrm{Tr}\rho_k(U), \tag{15}$$

or, equivalently,

$$\mathrm{Tr}\rho_p(U) = |a_p(U)|^2 - |a_{p-1}(U)|^2.$$

As it stands, the decomposition into irreducibles (14) is not very informative if one takes for U the matrix of a quantum map. We have no way *a priori* to estimate the character $\mathrm{Tr}\rho_p(U_N)$ from semiclassical information, except by using the relationship, via the $|a_k|^2$, to the original traces $\mathrm{Tr}(U_N^k)$, as was done in Ref. 7. This decomposition will, however, allow us to obtain rigorous results when adopting a $\mathrm{U}(N)$-isotropic averaging centered around U_N (see Sec. VI).

D. Ω_U as a coherent-state integral

Instead of decomposing the character $\mathrm{Tr}R_{-1}(U)$ into irreducibles, we can rewrite it as an integral over the symmetric space $\mathcal{M}_N=\mathrm{U}(2N)/\mathrm{U}(N)\times\mathrm{U}(N)$. This integral can be interpreted as a variant of the nonlinear sigma model used in Ref. 15 to study the spectral statistics of quantum chaotic Hamiltonians on infinite-dimensional Hilbert spaces. In our case the integral representation is exact, and is well defined mathematically.

To write the character $\Omega_U(\gamma)$ as an integral, one uses the coherent states $R(\mathbf{g})|0\rangle$, where $|0\rangle$ is the vacuum of $\mathcal{F}$ and $\mathbf{g}$ is any matrix in $\mathrm{U}(2N)$.[24] These coherent states provide a resolution of unity on $\mathcal{F}$, i.e., they can be combined to build the orthogonal projector on $\mathcal{F}$, as

$$P_{\mathcal{F}}\overset{\text{def}}{=}\int_{\mathrm{U}(2N)} d\mathbf{g}\quad R(\mathbf{g})|0\rangle\langle 0|R(\mathbf{g})^{-1},$$

where the Haar measure $d\mathbf{g}$ has to be suitably normalized. Let H_N be the block-diagonal subgroup $\mathrm{U}(N)\times\mathrm{U}(N)$ of $\mathrm{U}(2N)$. Then for all $\mathbf{h}\in H_N$, the states $R(\mathbf{g})|0\rangle$ and $R(\mathbf{gh})|0\rangle$ only differ by a phase factor. Therefore, it suffices to integrate over the equivalence classes in $\mathrm{U}(2N)$ modulo H_N:

$$P_{\mathcal{F}}=\int_{\mathrm{U}(2N)/H_N} d[\mathbf{g}]_H R(\mathbf{g})|0\rangle\langle 0|R(\mathbf{g})^{-1}.$$

It is convenient to represent the H_N-equivalence classes (i.e., the points on $\mathcal{M}_N$) by $2N\times 2N$ matrices. To each $\mathbf{g}\in\mathrm{U}(2N)$ one associates $Q_{\mathbf{g}}=\mathbf{g}\Sigma_3\mathbf{g}^{-1}$, where $\Sigma_3=\mathbb{I}_N\otimes\sigma_3$. The set of all these matrices Q is isomorphic to $\mathcal{M}_N$. It is the set of all Hermitian matrices with two eigenvalues, $+1$ and -1, each with multiplicity N. This nonlinear set of matrices is naturally equipped with $\mathrm{U}(2N)$-invariant symplectic structure and metric (and therefore an invariant measure dQ).

The matrix elements Q_{ij} are not all independent, and for practical calculations we need to introduce a bona fide coordinate system on $\mathcal{M}_N$. If we denote by $Q_{\mathbf{12}}$, $Q_{\mathbf{22}}$ the two $N\times N$ blocks in the right half of the matrix Q, the entries of the complex matrix $Z=Q_{\mathbf{12}}(Q_{\mathbf{22}}-1)^{-1}$ are good coordinates on the open subset of $\mathcal{M}_N$ where $(Q_{\mathbf{22}}-1)$ is invertible. Geometrically, these $N\times N$ complex coordinates represent a certain stereographic mapping of $\mathcal{M}_N$ onto $\mathbb{C}^{N\times N}$. The matrix Z corresponding to a point $Q_{\mathbf{g}}$ can be extracted from the Gaussian decomposition of $\mathbf{g}$:

$$\mathbf{g}=\begin{pmatrix}1 & Z\\ 0 & 1\end{pmatrix}\begin{pmatrix}A & 0\\ C & D\end{pmatrix}. \tag{16}$$

These complex coordinates also provide a simple definition of the coherent states. Indeed, $R(\mathbf{g})|0\rangle$ is co-linear with

$$|Z\rangle\overset{\text{def}}{=}\exp\left\{\sum_{i,j=1}^{N} f_{+i}^{\dagger}Z_{ij}f_{-j}^{\dagger}\right\}|0\rangle=\exp\left\{R\begin{pmatrix}0 & Z\\ 0 & 0\end{pmatrix}\right\}|0\rangle=R\begin{pmatrix}1 & Z\\ 0 & 1\end{pmatrix}|0\rangle. \tag{17}$$

As it stands, $|Z\rangle$ is not normalized, but has the following properties:

(i) The overlap between two coherent states reads $\langle Z|Z'\rangle=\mathrm{Det}(1+Z^{\dagger}Z')$. In particular, the norm of $|Z\rangle$ is $\mathrm{Det}(1+Z^{\dagger}Z)^{1/2}$.

(ii) The resolution of unity takes the form

$$P_{\mathcal{F}}=\int_{\mathbb{C}^{N\times N}} d\mu_N(Z,Z^\dagger)\frac{|Z\rangle\langle Z|}{\mathrm{Det}(1+Z^\dagger Z)}, \tag{18}$$

where the measure $d\mu_N(Z,Z^\dagger)=C_N\times\mathrm{Det}(1+Z^\dagger Z)^{-2N}\Pi_{i,j=1}^N d^2Z_{ij}/\pi$ is the expression for dQ in the coordinates Z_{ij}. The value of the normalization factor C_N is given at the end of Appendix B.

(iii) The group $\mathrm{U}(2N)$ acts on these coherent states as follows:

$$R\begin{pmatrix} A & B \\ C & D \end{pmatrix}|Z\rangle=\mathrm{Det}(CZ+D)\,|(AZ+B)(CZ+D)^{-1}\rangle. \tag{19}$$

The resolution of unity allows us to write the character (11) as

$$\begin{aligned}\Omega_U(\gamma)&=\gamma^{-N/2}\mathrm{Det}(U)^{-1}\int_{\mathcal{M}_N} d[\mathbf{g}]_H\ \langle 0|R(\mathbf{g})^{-1}R\begin{pmatrix}\gamma U & 0\\ 0 & U\end{pmatrix}R(\mathbf{g})|0\rangle\\ &=\gamma^{-N/2}\int_{\mathbb{C}^{N\times N}} d\mu_N(Z,Z^\dagger)\ \frac{\mathrm{Det}(1+\gamma Z^\dagger UZU^{-1})}{\mathrm{Det}(1+Z^\dagger Z)}\\ &=\int_{\mathcal{M}_N} dQ\ \ \mathrm{e}^{-S(\gamma,U,Q)}.\end{aligned} \tag{20}$$

This expression is the central result of the current section. It is an exact formula, which parallels the ''ballistic'' nonlinear sigma model derived in Ref. 15 for Hamiltonian systems with an infinite-dimensional Hilbert space. In our finite-dimensional framework, the non local field $Q(q',q)$ of 4×4 supermatrices on configuration space is replaced by a ''lattice field'' $Q_{i\alpha,j\beta}$ of 2×2 matrices (with elements indexed by α,β) depending on two discrete positions i,j. The ''effective action'' of the present model,

$$S(\gamma,U,Q)=-\mathrm{Tr}\{\log(1+\gamma Z^\dagger UZU^{-1})-\log(1+ZZ^\dagger)\}+\frac{N}{2}\log\gamma, \tag{21}$$

can be presented[17] in the form

$$S(\mathrm{e}^{\mathrm{i}x/N},U,Q)=-\mathrm{Tr}\log[\cosh(H_{x,U})-\sinh(H_{x,U})Q],$$

with

$$H_{x,U}\overset{\mathrm{def}}{=}\frac{\mathrm{i}x}{4N}\Sigma_3+\frac{1}{2}\log\mathbf{U}.$$

In Ref. 17, this action was further transformed, using the Wigner representation of wave functions, to obtain the same ballistic non-linear sigma model as in Ref. 15. We will not perform these steps, which require some further approximations, but rather try to estimate the integral with the above (purely quantum) effective action.

III. SADDLE-POINT ANALYSIS OF THE ACTION $S(\gamma,U,Q)$

To estimate the field integral of their nonlinear sigma model, the authors in Ref. 15 expand the effective action around two critical points (usually referred to as saddle points in this context). Since there is no large parameter in front of this action, a leading-order saddle-point expansion—see Eq. (4)—is not justified mathematically *a priori*. In the present section we explicitly compute this expansion for the action (21) and compare it to the results of Ref. 15 and the exact correlation function.

The saddle points are determined by requiring the variation of the action to be zero. In the absence of a large parameter, one first needs to understand exactly which action to vary. This point is not entirely obvious: one might be tempted to lift (part of) the denominator $\mathrm{Det}(1+ZZ^\dagger)^{-2N}$ of the measure $d\mu_N(Z,Z^\dagger)$ into the exponent; this modification of the effective action would yield a different saddle-point expansion. However, the requirement of coordinate invariance tells us to keep the U($2N$)-invariant measure dQ as it is, forbidding such manipulations. With this convention the saddle-point expansion of $S(\gamma,U,Q)$ will turn out to yield *the exact* γ*-dependence* for $\Omega_U(\gamma)$. In particular, the problem of "unphysical zero modes" occurring in Refs. 15 and 17 is resolved.

We now describe the saddle-point analysis of $S(\gamma,U,Q)$ in some detail. We first use the fact that the action is invariant under simultaneous rotations of both U and Q:

$$S(\gamma,U,Q)=S(\gamma,VUV^{-1},\mathbf{V}Q\mathbf{V^{-1}}), \tag{22}$$

where we used the shorthand notation $\mathbf{V}=V\otimes\mathbb{I}_2$, for $V\in\mathrm{U}(N)$. Such a V-rotation of Q is an isometry of the Riemannian manifold $\mathcal{M}_N$ and leaves the measure dQ invariant. It therefore suffices to study the simpler situation where U is *diagonal*: $U\equiv D=\mathrm{diag}(e^{i\theta_j})$.

One sees from formula (21) that the point $Z=0$ (or equivalently, $Q=\Sigma_3$) is a saddle point, and the quadratic approximation to S for small Z reads

$$S(\gamma,D,Z)\approx\frac{1}{2}N\log\gamma-\mathrm{Tr}(\gamma Z^\dagger DZD^{-1}-Z^\dagger Z)\approx\frac{1}{2}N\log\gamma+\sum_{i,j=1}^{N}|Z_{ij}|^2(1-\gamma e^{i(\theta_i-\theta_j)}).$$

This saddle point is the only one on $\mathcal{M}_N$ which is located at a finite Z. It is sometimes called the "perturbative" saddle point in the physics literature. For a generic matrix U, there are N directions Z_{jj} that have a coefficient $(1-\gamma)\sim-ix/N$; these directions are called "zero modes,"[15] because their coefficient vanishes as $x\to0$. Doing the integral in this quadratic approximation around $Z=0$ yields

$$\Omega_U(\gamma)_{|\Sigma_3}=C_N\frac{\gamma^{-N/2}}{(1-\gamma)^N\Pi_{i\neq j}(1-\gamma e^{i(\theta_i-\theta_j)})}. \tag{23}$$

We chose to separate the zero mode contributions from the others.

The existence of a second saddle point was pointed out (in the context of the diffusive nonlinear sigma model) in Ref. 25. It may be exhibited through the change of variable $Z'=1/Z$, which amounts to switching to the stereographic projection of $\mathcal{M}_N$ from the antipodal point. In terms of the new variable Z', the integrand reads

$$\gamma^{N/2}\frac{\mathrm{Det}(1+\gamma^{-1}Z'^\dagger UZ'U^{-1})}{\mathrm{Det}(1+Z'^\dagger Z')},$$

so it has the same structure as the original integrand, but for the replacement $\gamma\to\gamma^{-1}$. Quadratic expansion around $Z'=0$ (or, equivalently, around $Q=-\Sigma_3$) yields

$$\Omega_U(\gamma)_{|-\Sigma_3}=C_N\frac{\gamma^{N/2}}{(1-\gamma^{-1})^N\Pi_{i\neq j}(1-\gamma^{-1}e^{i(\theta_i-\theta_j)})}. \tag{24}$$

These two saddle points $Q=\pm\Sigma_3$ (we call them "standard") are the only ones taken into account in the treatment of the ballistic nonlinear sigma model in Refs. 15 and 17. The problem with this approximation is that, in the limit $\gamma\to1$, the sum of the two contributions Eq. (23) and (24) diverges at least as strongly as $1/(1-\gamma)^{N-1}$, whereas the exact correlation function is bounded. This phenomenon was attributed to the $N-1$ "unphysical" zero modes appearing at each saddle

point (as opposed to the single ''ergodic'' zero mode $\Sigma_j Z_{jj}$). More generally, these contributions become singular each time U and γU happen to have common eigenvalues.

We will argue below that this problem with zero modes is actually resolved by taking into account *further* saddle points of the effective action.

A. Weyl character formula

To identify all saddle points, we return to the expression (20) of the integrand. We still study the case where $U=D$ is diagonal, and we write $\Gamma\mathbf{D}\equiv\mathrm{diag}(\gamma D,D)$.

Let ζ be a complex $N\times N$ matrix. The point $Q_{\mathbf{g}}$ of $\mathcal{M}_N$ is a saddle point of the integrand iff the Taylor expansion of $\langle\zeta|R(\mathbf{g}^{-1}\Gamma\mathbf{D}\mathbf{g})|\zeta\rangle$ around $\zeta=0$ contains no term linear in ζ and $\zeta^\dagger$. (Note that this statement is independent of the choice of representative $\mathbf{g}$ for $Q_{\mathbf{g}}$.) Moreover, we do not want the integrand to vanish at $\zeta=0$. If we decompose the unitary matrix as $\mathbf{g}^{-1}\Gamma\mathbf{D}\mathbf{g}=\left(\begin{smallmatrix}a & b\\ c & d\end{smallmatrix}\right)$, these conditions read

$$b=c=0, \quad \mathrm{Det}(d)\neq 0. \tag{25}$$

This means that the matrix $\mathbf{g}^{-1}\Gamma\mathbf{D}\mathbf{g}$ [for $\gamma=\mathrm{e}^{\mathrm{i}x/N}\in\mathrm{U}(1)$] belongs to the subgroup H_N of $\mathrm{U}(2N)$, which in turn allows $\mathbf{g}$ to be written as the product of a *permutation matrix* $\mathbf{g}_\sigma$ with some element $\mathbf{h}\in H_N$. By $\mathbf{g}_\sigma$ we mean the unitary matrix $(\mathbf{g}_\sigma)_{ij}=\delta_{i,\sigma(j)}$, where σ is a permutation of $\{1,\ldots,2N\}$. To each permutation σ there corresponds a single point $Q_\sigma=\mathbf{g}_\sigma\Sigma_3\mathbf{g}_\sigma{}^{-1}$. Moreover, two permutations σ, σ' lead to the same point if $\sigma=\sigma'\tau$ where τ permutes indices separately inside $\{1,\ldots,N\}$ and $\{N+1,...,2N\}$; this property defines a partition of the symmetric group $\mathfrak{S}_{2N}$ into $\binom{2N}{N}$ equivalence classes, each one corresponding to a saddle point of the integrand.

These classes are in one-to-one correspondence with the sets $S=\sigma(\{1,\ldots,N\})$, so we can write $Q_\sigma=Q_S$. Q_S is then the diagonal matrix with entries $+1$ at the positions $j\in S$, and -1 at the positions $j\in\overline{S}$ (the complement of S in $\{1,\ldots,2N\}$). We partition the set S into $S_1=S\cap\{1,\ldots,N\}$ and $\widetilde{S}_2=S\cap\{N+1,\ldots,2N\}$. In the following we will also use the set $S_2=\{j-N|j\in\widetilde{S}_2\}$, and the sets $\overline{S_1}$ and $\overline{S_2}$ which are the complements in $\{1,\ldots,N\}$ of S_1, resp. S_2. The point Q_S corresponds to the following (coherent) state in $\mathcal{F}$:

$$|S\rangle\overset{\mathrm{def}}{=}R(\mathbf{g}_\sigma)|0\rangle=\pm\prod_{i\in\overline{S_1}} f^\dagger_{+i}\prod_{j\in S_2} f^\dagger_{-j}|0\rangle. \tag{26}$$

The matrix $\mathbf{g}_\sigma$ admits a Gaussian decomposition (16) iff σ is in the trivial class, i.e., $S=\{1,\ldots,N\}$, which explains why only the perturbative saddle point $Q=\Sigma_3$ could be exhibited from the Z-coordinates.

We now compute the leading-order contribution from each saddle point Q_S. In the vicinity of Q_S the integrand in (20) takes the values

$$\langle\zeta|R(\mathbf{g}_\sigma^{-1}\Gamma\mathbf{D}\mathbf{g}_\sigma)|\zeta\rangle/\langle\zeta|\zeta\rangle,$$

where the entries of the matrix ζ are ''small'' (ζ defines a local coordinate system near Q_S). We partition the diagonal matrix $\mathbf{g}_\sigma^{-1}\Gamma\mathbf{D}\mathbf{g}_\sigma$ into two halves: $\mathbf{g}_\sigma^{-1}\Gamma\mathbf{D}\mathbf{g}_\sigma=\mathrm{diag}(\Delta_1,\Delta_2)$. The above integrand then reads

$$\mathrm{Det}(D)\times\frac{\mathrm{Det}(1+\zeta^\dagger\Delta_1\zeta\Delta_2^{-1})}{\mathrm{Det}(1+\zeta^\dagger\zeta)}.$$

Expanding to quadratic order and integrating over $\zeta,\zeta^\dagger$, we obtain from the saddle point Q_S a contribution similar to (23):

$$\Omega_D(\gamma)_{|Q_S}=C_N\gamma^{-N/2}\prod_{\substack{i\in S_1\\ j\in S_2}}\gamma e^{i(\theta_i-\theta_j)}\prod_{\substack{i\in S_1\\ j\in \overline{S_2}}}(1-\gamma e^{i(\theta_i-\theta_j)})^{-1}\prod_{\substack{i\in S_1\\ j\in S_2}}(1-\gamma^{-1}e^{-i(\theta_i-\theta_j)})^{-1}$$

$$\times\prod_{\substack{i\in \overline{S_1}\\ j\in S_1}}(1-e^{i(\theta_i-\theta_j)})^{-1}\prod_{\substack{i\in S_2\\ j\in S_2}}(1-e^{-i(\theta_i-\theta_j)})^{-1}. \tag{27}$$

Note that the product contains a factor, $(1-\gamma)^{-N+2r}$, with $r=\sharp(S_1\cap S_2)$. The most singular case $r=0$ arises for $S_2=\overline{S_1}$, i.e., saddle points of the type $\Pi_{i\in\overline{S_1}}f^\dagger_{+i}f^\dagger_{-i}|0\rangle$.

In the general case $U=VDV^{-1}$, the saddle points are the points $Q_{V,S}=\mathbf{V}Q_S\mathbf{V^{-1}}$, and they lead to the same contributions (cf. the covariance of the action and the measure dQ). The two standard saddle points $Q=\pm\Sigma_3$ are the only ones unaffected by these V-rotations.

It is illuminating to present the result of the approximation (27) in an alternative fashion. For that purpose, we denote the nonzero elements of the diagonal matrix $\Gamma\mathbf{D}$ by $e^{i\phi_\nu}$ ($\nu=1,\ldots,2N$). The sum of contributions (27) can then be rewritten in the form

$$\Omega_D(\gamma)=C_N\gamma^{-N/2}\sum_S\frac{\Pi_{\mu\in\overline{S}_1}\Pi_{\nu\in\tilde{S}_2}e^{i(\phi_\mu-\phi_\nu)}}{\Pi_{\mu\in S}\Pi_{\nu\in\overline{S}}(1-e^{i(\phi_\mu-\phi_\nu)})}. \tag{28}$$

Save for the prefactor C_N, the expression (28) agrees with the result that follows from the *Weyl character formula*[26] for the trace of $R(\Gamma\mathbf{D})$ over $\mathcal{F}$. In general, this formula expresses the character of an element of U($2N$) [more generally, GL($2N,\mathbb{C}$)] in some representation R as a sum over all permutations $\sigma\in\mathfrak{S}_{2N}$ [this being the so-called Weyl group of U($2N$)]. In our case, the terms from the $(2N)!$ elements of $\mathfrak{S}_{2N}$ may be grouped into $\binom{2N}{N}$ classes, according to the equivalence relation described above. Since Weyl's formula is an exact result, the expression (28) remains finite in the limit $\gamma\to1$, which means that the singularities $1/(1-\gamma)^{N-2r}$ of the various terms cancel each other. The complete sum over saddle-point contributions thus solves the problem of "unphysical zero modes," i.e., the divergence problem of the two standard saddle points.

The mathematical reason behind the "almost exactness" of the leading-order saddle-point expansion is as follows. The action of $R(\mathbf{g})$ on coherent states $|Z\rangle$ may be interpreted as the equivariant action of $\mathbf{g}$ on the space of holomorphic sections of a certain complex line bundle $\mathcal{L}_R$ over $\mathcal{M}_N$.[27] This equivariant action can be extended to the (infinite-dimensional) space of square-integrable differential forms of degree $(0,p)$ on the bundle. On the enlarged space, the character becomes a (super)trace, which can still be written as an integral over $\mathcal{M}_N$. Owing to an $N=2$ supersymmetry, the integrand may be continuously deformed without changing the value of the integral. In one limit of the deformation, one gets $\mathrm{Tr}R(\mathbf{g})$; in the other, the integrand *localizes* at the fixed points of $\mathbf{g}$ on $\mathcal{M}_N$, yielding Gaussian integrals around these points.

It turns out that these fixed points coincide with our $Q_{V,S}$, and their (Gaussian) contributions are equal to (27), save for the prefactor C_N. As a result, the leading-order saddle-point approximation (for our nonlocalized integrand) delivers the correct answer (omitting the prefactor). In Sec. IV D, we investigate the higher-order terms of the expansion at $Q=\Sigma_3$ up to two loops: we find that these terms only renormalize the prefactor C_N, without affecting the U- or γ-dependence. We speculate that the (adequately resummed) full series yields the exact answer, including the correct normalization.

To achieve agreement with the Weyl character formula, it was crucial to regard the denominator $\mathrm{Det}(1+Z^\dagger Z)^{-2N}$ as part of the measure (as opposed to lifting it into the action). Indeed, in order for the mechanism of equivariant localization to take effect, the integration measure must be U($2N$)-invariant—a property not enjoyed by the flat measure $\Pi_{i,j}d^2Z_{ij}$ without the factor $\mathrm{Det}(1+Z^\dagger Z)^{-2N}$.

IV. WHY DO WE NEED AVERAGING?

While the Weyl character formula for $\Omega_U(\gamma)$ constitutes an exact result, it is of no use—at least not as it stands—towards our goal of proving universality of the correlation function. This formula relies on the knowledge of the eigenphases $e^{i\theta_i}$ of U, which are not given *a priori*. It does not exhibit the semiclassical features of the quantum map at all. On the contrary, it is a "purely quantum" decomposition of the correlation function, a complicated reordering of the Fourier decomposition (6).

As was explained in the Introduction, it is not conceivable in general that a universal result for Ω_U can be obtained without doing some kind of averaging over the matrix U. Given the results of the previous section, one might try to perform the averaging term by term in the Weyl decomposition, hoping that most of the terms might average to zero. Such a hope is quickly discouraged by a look at the expression (23): aside from having an Nth-order singularity at $\gamma=1$, whose degree increases each time some $\gamma e^{i(\theta_i-\theta_j)}$ crosses unity, this contribution to $\Omega_U(\gamma)$ is *strictly positive* for real $\gamma<1$. We know that the singularities are artifacts of the Weyl decomposition, as the correlation function $\Omega_U(\gamma)$ itself is uniformly bounded wrt U and γ. Unfortunately, because of the positivity of (23) the singularities can only be removed by reorganizing the entire sum of contributions, not by averaging individual terms.

For this reason, we will adopt a different strategy: we first perform the $d\mathcal{P}_N(U)$ average on the *integrand* of the coherent-state integral, obtaining a new effective action

$$e^{-S_{\rm av}(\gamma,Q)} \overset{\rm def}{=} \langle e^{-S(\gamma,U,Q)} \rangle_{\mathcal{P}_N}. \tag{29}$$

We then estimate the resulting Q-integral by performing a saddle-point approximation on the action $S_{\rm av}(Q)$.[20]

A priori, this approximation is no more justified than the one in the previous section, as $S_{\rm av}$ is preceded by no large parameter either. The absence of a large parameter also implies that averaging and making the saddle-point approximation are noncommuting operations. Therefore, the saddle-point expansion of $S_{\rm av}$ will yield qualitatively different results from the direct expansion for $S(\gamma,U,Q)$. We explained above that averaging the Weyl character formula is hopeless for our aims. The other way around (i.e., performing the expansion after averaging the action) will prove more interesting.

A. Where are the critical points of $S_{\rm av}$?

For any averaging measure $d\mathcal{P}_N$, the two points $Q=\pm\Sigma_3$ remain saddle points of $S_{\rm av}(\gamma,Q)$. In the vicinity of Σ_3, the integrand expands as

$$\left\langle \frac{\mathrm{Det}(1+\gamma Z^\dagger U Z U^{-1})}{\mathrm{Det}(1+Z^\dagger Z)} \right\rangle \approx \exp \mathrm{Tr}(\langle \gamma Z^\dagger \mathrm{Ad}U\cdot Z\rangle - Z^\dagger Z) = e^{-\mathrm{Tr}\, Z^\dagger(\mathbb{I}-\gamma\langle \mathrm{Ad}U\rangle)Z},$$

where $\mathrm{Ad}U\cdot Z \overset{\rm def}{=} UZU^{-1}$ is the adjoint action of U on Z. The approximation is valid for Z small. For larger values of Z, one should add higher cumulants to the right-hand side. However, for the time being we stick to the purely quadratic approximation, and carry out the Gaussian integral to obtain

$$\langle \Omega_U(\gamma)\rangle_{|\Sigma_3} = C_N \gamma^{-N/2} \mathrm{Det}(\mathbb{I}-\gamma\langle \mathrm{Ad}U\rangle)^{-1}. \tag{30}$$

When the averaging is absent (that is, $d\mathcal{P}_N$ is a Dirac δ-measure at U), we recover the contribution (23). The saddle point $Q=-\Sigma_3$ yields the same result, with $\gamma\to\gamma^{-1}$. On setting $\gamma=e^{ix/N}$, the sum of contributions becomes

$$\langle \Omega_U(e^{ix/N})\rangle_{|\Sigma_3\cup-\Sigma_3} = 2C_N \Re\left(\frac{e^{-ix/2}}{\mathrm{Det}(\mathbb{I}-e^{ix/N}\langle \mathrm{Ad}U\rangle)} \right). \tag{31}$$

In the next section, we examine the possible occurrence of further saddle points of $S_{\rm av}$.

1. Searching for other saddle points

In Sec. III A we located the saddle points of the function $Q \mapsto \langle Z(Q)|R(\Gamma\mathbf{U})|Z(Q)\rangle$, using the action of the group $\mathrm{U}(2N)$ on the coherent states $|Z\rangle$. This function may be interpreted as the *Husimi function* (or Q-symbol) of the operator $R(\Gamma\mathbf{U})$ acting on $\mathcal{F}$, and we denote it by $H_{R(\Gamma\mathbf{U})}(Q)$. By the same procedure we can obtain the saddle points of $H_{R(\mathbf{g})}(Q)$ for any nondegenerate matrix $\mathbf{g}\in\mathrm{U}(2N)$; in that case, the saddle points $Q_{\rm crit}$ are given in general by finite matrices $Z_{\rm crit}$ and $Z_{\rm crit}^\dagger$, which are solutions of the saddle-point equations

$$\frac{\partial}{\partial Z_{ij}} H_{R(\mathbf{g})}(Z,Z^\dagger)=0=\frac{\partial}{\partial \overline{Z}_{ij}} H_{R(\mathbf{g})}(Z,Z^\dagger) \qquad (i,j=1,\ldots,N). \tag{32}$$

It is useful to extend $H_{R(\mathbf{g})}$ to a function of two independent complex matrices Z,Z^* (that makes $2N^2$ complex variables). The saddle-point equations pose $2N^2$ constraints on the degrees of freedom Z and Z^*, which yields isolated solutions (Z_i,Z_i^*), provided that the constraints are independent of each other.

The *reality* of these solutions (i.e., $Z_i^*=(Z_i)^\dagger$) is due to a symmetry of the operator $R(\mathbf{g})$, which is not conserved if we replace $R(\mathbf{g})$ by any operator $\mathcal{R}$ on $\mathcal{F}$. For instance, if the representation R is extended to matrices $\mathbf{G}\in\mathrm{GL}(2N,\mathbb{C})$, one can show that the saddle points of $H_{R(\mathbf{G})}(Z,Z^*)$ are real iff $\mathbf{G}$ is a normal matrix (i.e., $\mathbf{G}\mathbf{G}^\dagger=\mathbf{G}^\dagger\mathbf{G}$). We are presently unable to determine the conditions for the saddle points to be real for the most general $\mathcal{R}$. In any case, the saddle points will be real if $\mathcal{R}$ is a Hermitian operator. The Husimi function is then real, and Morse theory applies to it. By Morse's theorem,[28] the number of saddle points (which we assume to be isolated) is at least the sum of all Betti numbers of $\mathcal{M}_N$, which is $\binom{2N}{N}$.[29] This is exactly the number of saddle points we found for $H_{R(\mathbf{X})}(Q)$ when $\mathbf{X}$ is a $2N\times 2N$ Hermitian matrix, so this function is called a *perfect Morse function* for $\mathcal{M}_N$. $\mathbf{X}$ can be joined to $\mathbf{g}\in\mathrm{U}(2N)$ by a continuous path inside the set of nondegenerate normal matrices: this explains why $H_{R(\Gamma\mathbf{U})}$, although a complex function, still has $\binom{2N}{N}$ real saddle points.

Unlike reality, the property that the solutions of (32) are isolated points is robust; (Z_i,Z_i^*) are the common zeros of $2N^2$ polynomials in Z and Z^*, so they are *stable* wrt perturbations of the coefficients, as long as the equations do not become degenerate. In Sec. III A the saddle points of $H_{R(\Gamma\mathbf{U})}(Q)$ were called $Q_{V,S}$. We now switch to such complex coordinates ζ that a saddle point $Q_{V,S}$ is situated at $\zeta=0=\zeta^\dagger$, and perturb $R(\Gamma\mathbf{U})$ in $\mathrm{GL}(\mathcal{F})$ to $\mathcal{R}=R(\Gamma\mathbf{U})+\epsilon\,\delta\mathcal{R}$. Then for ϵ small, $H_{\mathcal{R}}(\zeta,\zeta^\dagger)$ will have an isolated saddle point at $(\zeta_\epsilon,\zeta_\epsilon^*)$, where both ζ_ϵ and ζ_ϵ^* are of order ϵ. Even if it is not real, this saddle point will contribute to the integral over $\mathcal{M}_N$: starting from real coordinates $\Re\zeta_{ij},\Im\zeta_{ij}$, we can locally deform the contour so as to reach the point

$$(\Re\zeta_{ij})^{\rm crit}=(\zeta_{\epsilon,ij}+\zeta_{\epsilon,ji}^*)/2, \qquad (\Im\zeta_{ij})^{\rm crit}=(\zeta_{\epsilon,ij}-\zeta_{\epsilon,ji}^*)/2\mathrm{i},$$

and we can compute the saddle-point expansion of $\int H_{\mathcal{R}}(\Re\zeta,\Im\zeta)$ around it.

The averaged integrands we want to consider are all of the type $H_{\mathcal{R}}(Q)$, where

$$\mathcal{R}=\int_{\mathrm{U}(N)} \mathrm{d}\mathcal{P}_N(V)\ \frac{1}{\mathrm{Det}V} R(\Gamma\mathbf{V}),$$

and $\mathrm{d}\mathcal{P}_N(V)$ is a normalized measure on $\mathrm{U}(N)$. If this measure is very strongly peaked near a matrix U_N, the resulting operator will be a perturbation of $R(\Gamma\mathbf{U}_N)/\mathrm{Det}U_N$, so the above stability arguments apply: the saddle points are then isolated points near the unperturbed ones, and they are "almost real" and hence will lie on the integration contour after a slight contour deformation.

For less concentrated measures $\mathrm{d}\mathcal{P}_N(V)$, the structure of the saddle points can change. In Sec. V we exhibit an averaging scheme for which the saddle points are real but not isolated: they form submanifolds of $\mathcal{M}_N$; this is also the case for $H_{R(\mathbf{g})}$ if $\mathbf{g}$ is degenerate. We do not have a good

estimate of the typical ''width'' of the measure $d\mathcal{P}_N(V)$ above which saddle points can coalesce, spread over higher-dimensional sets, or cease to contribute to the integral (for instance, when they depart too far away from reality).

In general, we are unable to explicitly locate these extra saddle points, even for the relatively narrow averages described in Secs. IV C and IV F; consequently, we cannot do better than stick to the approximation (31) to describe the correlation function. The remaining task then is to investigate the spectrum of the operator $\langle \mathrm{Ad}U\rangle$, which depends on U and on $d\mathcal{P}_N$.

B. Common spectral features of $\langle \mathrm{Ad}U\rangle$

The spectrum of $\langle \mathrm{Ad}U\rangle$ has a few features that are independent of the averaging scheme. Before averaging, the eigenvalue unity occurs in $\mathrm{Ad}U$ with multiplicity N, corresponding to the N-dimensional space spanned by the U-eigenstate projectors $|\psi_j\rangle\langle\psi_j|$ $(j=1,\ldots,N)$, and the remaining N^2-N eigenvalues lie on the unit circle. After averaging, only the uniform mode $\mathbb{I}_N = \Sigma_j |\psi_j\rangle\langle\psi_j|$ is left with eigenvalue at unity, while all other eigenvalues have moved inside the unit disk. As a result, the sum of the contributions (31) stays finite in the limit $\gamma\to 1$. Averaging thus removes the ''unphysical zero mode'' problem associated with the two standard saddle points in Sec. III.

More precisely, the large-N behavior of $\langle \Omega_U(e^{ix/N})\rangle_{|\pm\Sigma_3}$ for finite x mostly depends on the positions of the eigenvalues of $\langle \mathrm{Ad}U\rangle$ *closest to unity*. Within the approximation (31), these eigenvalues are *the relevant dynamical data* of the correlation function.

C. Semiclassical averaging

In Ref. 20, a semiclassical averaging scheme around a quantized map $U_{\phi,N}$ was proposed as a promising candidate to obtain universal spectral statistics, differentiating between integrability versus chaotic behavior of the classical map ϕ. One chooses a finite set of Hamiltonian functions H_j, corresponding to Hamiltonian vector fields Ξ_{H_j} $(j=1,\ldots,r)$, on the classical phase space. These Hamiltonians are quantized on each of the quantum Hilbert spaces $\mathcal{H}_N$, yielding operators $\{\hat{H}_j\}$, which are represented by Hermitian $N\times N$ matrices wrt an orthonormal basis of $\mathcal{H}_N$. An ensemble average is then introduced by

(1) composing $U_{\phi,N}$ with the operator $\exp(-i\Sigma_j t_j \hat{H}_j/\hbar)$, where the ''times'' t_j are real numbers;
(2) averaging over the parameters t_j in a window around the origin of width ϵ using, for instance, the Gaussian weight $(\epsilon^2\pi)^{-r/2} e^{-\Sigma_j t_j^2/\epsilon^2}$.

The width ϵ is taken to be $\hbar$-dependent: $\epsilon\sim\hbar^\alpha\sim N^{-\alpha}$ for some $1>\alpha>0$, so that the probability measure for the classical maps $\exp(\Sigma_j t_j \Xi_{H_j})\circ\phi$ shrinks to a single point, ϕ, in the classical limit $N\to\infty$. The set of Hamiltonians $\{H_j\}$ is chosen once and for all, and is independent of N and the map ϕ. The only constraint on this set is that the second-order differential operator $-\Delta = \Sigma_j \Xi_{H_j}^2$ must be *elliptic*.[20]

As explained in the Introduction, this averaging procedure is introduced in order to suppress the nongeneric spectral statistics of quantum chaotic systems with arithmetic symmetries. In this respect we must mention the results obtained in Ref. 10, where the authors show how nonlinear perturbations of quantum cat maps exhibit generic spectral statistics, as long as one perturbs in both directions of the two-dimensional phase space; in contradistinction, perturbation in a single direction may leave one arithmetic symmetry intact, leading to nongeneric quantum spectral statistics. This need for ''phase-space-isotropy'' of the perturbations is very similar to our ellipticity requirement: Δ is elliptic only if the vector fields Ξ_{H_j} span the whole tangent space at every point of phase space.

Some recent articles[30,31] have dealt with the spectral analysis of the operator $\langle \mathrm{Ad}U\rangle_{\mathrm{semiclas}}$, and obtained interesting results concerning its largest eigenvalues. For a classically chaotic map, these were shown to converge (as $N\to\infty$) to the *Ruelle–Pollicott resonances* of the corresponding

Frobenius-Perron operator.[32] These resonances are inside the unit circle, which means that $\langle \mathrm{Ad}U_N\rangle_{\mathrm{semiclas}}$ has a *finite gap* between unity and the rest of the spectrum, for $N\to\infty$. The huge majority of eigenvalues tend to accumulate on the origin (see the discussion at the end of Sec. V A).

These properties allow us to estimate the contribution from the two standard saddle points for the case of a quantum chaotic map. To lowest order in $1/N$,

$$\langle \Omega_{U_N}(\gamma=\mathrm{e}^{\mathrm{i}x/N})\rangle_{\mathrm{semiclas}|\pm\Sigma_3} \overset{N\to\infty}{\approx} \frac{NC_N}{\mathrm{Det}_\perp(\mathbb{I}-\langle \mathrm{Ad}U\rangle_{\mathrm{semiclas}})}\,\frac{\sin(x/2)}{x/2}, \tag{33}$$

where $\mathrm{Det}_\perp$ means that the determinant is computed after restriction to the traceless matrices, i.e., to the subspace orthogonal to the uniform mode $\mathbb{I}_N$. Apart from the non-universal prefactor, the x-dependence agrees with the CUE result (8) in the limit of large matrices.

In the case of an integrable map, the eigenvalues of $\langle \mathrm{Ad}U_N\rangle_{\mathrm{semiclas}}$ behave differently: some of them populate more and more densely a few curves which connect the origin to some point on the unit circle (including unity). For this reason, one cannot separate unity in $\mathrm{Det}(\mathbb{I}-\mathrm{e}^{\mathrm{i}x/N}\langle \mathrm{Ad}U\rangle_{\mathrm{semiclas}})$ from the rest of the spectrum. All we can say is that the approximation (31) does not yield the CUE formula in that case (in general it does not yield the Poisson answer either).

1. Warning

One might be tempted to present formula (33) as a ''physicist's proof'' of a weak universality conjecture for quantum chaotic maps. The reason why it is not a proof is clear:

(i) As was explained in Sec. IV A 1, there certainly exist other saddle points of (29). The calculation of their contributions is a difficult task, which we have not yet performed. It is far from obvious why these saddle points should be less important than $Q=\pm\Sigma_3$ in the semiclassical averaging scheme.

(ii) As was emphasized before, there is no large parameter in front of the effective action. Without such a parameter, the correction terms of the asymptotic expansion around each saddle point are not small, and their neglect in the formula (33) seems to be unjustified.

The second worry is addressed in the next subsection.

D. Loop expansion

We are now going to investigate those corrections to the formula (33) that result from systematically expanding around the saddle point $Q=\Sigma_3$. The computations will be done up to what is called two-loop order in field-theoretic language.

As a first step, we approximate the integrand by taking the ensemble average inside the determinant:

$$\langle \mathrm{Det}(1+\gamma Z^\dagger \mathrm{Ad}U\cdot Z)\rangle_{\mathrm{semiclas}} \approx \mathrm{Det}(1+\gamma Z^\dagger \langle \mathrm{Ad}U\rangle_{\mathrm{semiclas}}\cdot Z). \tag{34}$$

Although ϵ, the ''width'' of the perturbation, decreases like $\hbar^\alpha$, its effect is strong enough to completely modify the spectrum of $\mathrm{Ad}U$, even in the semiclassical limit. This shows that the above approximation is not necessarily valid if we just suppose that the matrices Z are bounded (uniformly wrt N) in the operator norm on $\mathcal{H}_N$. Using the expansion

$$\mathrm{Det}(1+A)=1+\mathrm{Tr}A+\sum_{j=2}^{N}\mathrm{Tr}(\wedge^j A),$$

Eq. (34) will hold as long as the terms for $j \geqslant 2$ are small compared to $\mathrm{Tr}A$. A sufficient condition for that is $\mathrm{Tr}(|A|) \ll 1$, where $|A| \stackrel{\text{def}}{=} \sqrt{A^\dagger A}$. Upon the replacement $A = \gamma Z^\dagger \mathrm{Ad}U \cdot Z$, this condition will be met if

$$\mathrm{Tr}(Z^\dagger Z) = \sum_{i,j=1}^{N} |Z_{ij}|^2 \ll 1, \tag{35}$$

uniformly wrt N. It would be desirable to better control the error in (34) for the larger set of matrices Z satisfying (N-uniformly) $\|Z\|_{\mathcal{L}(\mathcal{H}_N)} \leqslant \mathrm{const}$.

Taking (34) for granted, we proceed to the computation of higher loops. To simplify the notation we abbreviate $T \stackrel{\text{def}}{=} \gamma \langle \mathrm{Ad}U \rangle_{\mathrm{semiclas}}$. Next we formally introduce a parameter M (which will be reset to unity at the end of the calculation) by making in the integrand the replacement

$$\frac{\mathrm{Det}(1+Z^\dagger T Z)}{\mathrm{Det}(1+Z^\dagger Z)} \to \left(\frac{\mathrm{Det}(1+Z^\dagger T Z)}{\mathrm{Det}(1+Z^\dagger Z)} \right)^M .$$

A contribution to the perturbative saddle-point expansion is said to be of n-loop order if it varies as M^{-n} relative to the leading-order term. On rescaling the integration variables to $\zeta = Z\sqrt{M}$ and $\zeta^\dagger = Z^\dagger \sqrt{M}$, the $1/M$ expansion of the integrand looks as follows:

$$d\mu_N(Z,Z^\dagger) \frac{\mathrm{Det}^M(1+Z^\dagger T Z)}{\mathrm{Det}^M(1+Z^\dagger Z)} = C_N \prod_{i,j=1}^{N} \frac{d^2\zeta_{ij}}{\pi M} \mathrm{e}^{-\mathrm{Tr}\zeta^\dagger(1-T)\zeta} (1 + M^{-1} f_1 + M^{-2} f_2 + \cdots)$$

where f_1 and f_2 are the one- and two-loop terms, respectively, and are given by

$$f_1 = \frac{1}{2}\mathrm{Tr}(\zeta^\dagger\zeta)^2 - \frac{1}{2}\mathrm{Tr}(\zeta^\dagger T \zeta)^2 - 2N\mathrm{Tr}\zeta^\dagger\zeta,$$

$$\begin{aligned} f_2 = &-\frac{1}{3}\mathrm{Tr}(\zeta^\dagger\zeta)^3 + \frac{1}{3}\mathrm{Tr}(\zeta^\dagger T\zeta)^3 + \frac{1}{8}[\mathrm{Tr}(\zeta^\dagger\zeta)^2 - \mathrm{Tr}(\zeta^\dagger T\zeta)^2]^2 \\ &+ 2N^2(\mathrm{Tr}\zeta^\dagger\zeta)^2 + N\mathrm{Tr}(\zeta^\dagger\zeta)^2 - N\mathrm{Tr}(\zeta^\dagger\zeta)(\mathrm{Tr}(\zeta^\dagger\zeta)^2 - \mathrm{Tr}(\zeta^\dagger T\zeta)^2). \end{aligned}$$

The Gaussian integral at leading order just yields the result (30). Using standard diagrammatic techniques to do the one-loop integral we find the following expression:

$$\begin{aligned} \frac{1}{2} C_N M^{-N\times N} \mathrm{Det}(1-T)^{-1} \Bigg\{ &-4N \sum_{ij} \left(\frac{1}{1-T} \right)_{ij,ij} + \sum_{ijkl} \left(\frac{1}{1-T} \right)_{ij,kj} \left(\frac{1}{1-T} \right)_{kl,il} \\ &- \sum_{ijkl} \left(\frac{T}{1-T} \right)_{ij,kj} \left(\frac{T}{1-T} \right)_{kl,il} + \sum_{ijkl} \left(\frac{1}{1-T} \right)_{ij,il} \left(\frac{1}{1-T} \right)_{kl,kj} - \sum_{ijkl} \left(\frac{T}{1-T} \right)_{ij,il} \left(\frac{T}{1-T} \right)_{kl,kj} \Bigg\}. \end{aligned}$$

By the relation $(1-T)^{-1} = 1 + T(1-T)^{-1}$ these terms combine to yield the simple answer

$$C_N \int_{\mathbb{C}^{N\times N}} \prod_{i,j=1}^{N} \frac{d^2\zeta_{ij}}{\pi M} \mathrm{e}^{-\mathrm{Tr}\zeta^\dagger(1-T)\zeta} f_1(\zeta,\zeta^\dagger) = C_N M^{-N\times N} \mathrm{Det}(1-T)^{-1}(-N^3).$$

We see that the dependence of the one-loop contribution on T cancels completely, leaving only a constant, $-N^3$. This cancellation is not accidental but continues to higher loop order. By a lengthy but straightforward calculation, the complete perturbative result up to two-loop order can be shown to be

$$\int_{\mathbb{C}^{N\times N}} d\mu_N(Z,Z^\dagger)\,\frac{\mathrm{Det}^M(1+Z^\dagger TZ)}{\mathrm{Det}^M(1+Z^\dagger Z)}$$
$$= C_N M^{-N\times N}\mathrm{Det}(1-T)^{-1}\left(1-M^{-1}N^3+M^{-2}\left(\frac{1}{2}N^6+\frac{7}{12}N^4-\frac{1}{12}N^2\right)+\mathcal{O}(M^{-3})\right).$$

Again, all the T-dependence has disappeared from the loop correction terms. This is true for all M including the case of interest, $M=1$.

The cancellation does not come as a total surprise. The above perturbation expansion, whose low-order terms we have computed, is formally identical to the same expansion *before* averaging. The latter is obtained from the former by simply substituting $\gamma\mathrm{Ad}U$ for $T=\gamma\langle\mathrm{Ad}U\rangle_{\mathrm{semiclas}}$. In the case before averaging we know from Ref. 27 that an index-theoretic mechanism (sometime called *localization*) causes the perturbation expansion to be deformable (by an underlying $N=2$ supersymmetry) to a harmonic oscillator problem (or, equivalently, a Gaussian integral) at $Z=0$. The process of deformation to the Gaussian limit explains why the dependence on $\gamma\mathrm{Ad}U$ is exhausted by the leading-order term. It leads to the Weyl character formula, which implies that the contribution to the character from $Z=0$ (or $Q=\Sigma_3$) is *exactly* given by

$$\int_{\mathbb{C}^{N\times N}} d\mu_N(Z,Z^\dagger)\,\frac{\mathrm{Det}(1+Z^\dagger\gamma\mathrm{Ad}U\cdot Z)}{\mathrm{Det}(1+Z^\dagger Z)}\Big|_{Z=0,\text{all orders}}=\mathrm{Det}(\mathbb{I}-\gamma\mathrm{Ad}U)^{-1},$$

where the normalization constant C_N has now been replaced by unity. The last fact provides the raison d'ĉtre for the N-dependent terms produced by the loop expansion: their role is to cancel, after proper resummation, the prefactor C_N. This property does not depend on the unitarity of $\gamma\mathrm{Ad}U$, so it holds as well after replacing it by its average. Thus, after summing all orders of the perturbation expansion, we expect that the saddle point $Z=0$ contributes to the correlation function as

$$\langle\Omega_U(\gamma)\rangle_{|\Sigma_3,\text{all orders}}=\gamma^{-N/2}\,\mathrm{Det}(\mathbb{I}-\gamma\langle\mathrm{Ad}U\rangle)^{-1}.$$

This perturbative result should be used with some care. Although the function $f(Z,Z^\dagger;T)=\mathrm{Det}(1+Z^\dagger TZ)/\mathrm{Det}(1+Z^\dagger Z)$ is locally well defined, it does not extend to a global smooth function on the manifold $\mathcal{M}_N$ (in particular, this function is NOT the Husimi function of an operator on $\mathcal{F}$). Indeed, setting $Z=zG$ with any invertible matrix G and sending $z\to\infty$ always leads to the same point $Q=-\Sigma_3$ on $\mathcal{M}_N$, regardless of which matrix G we choose, whereas the limit of $f(zG,\overline{z}\overline{G}^\dagger;T)$ as $z\to\infty$ does depend on the choice of G. Thus, the function $f(Z,Z^\dagger;T)$ is not smooth at $Q=-\Sigma_3$.

This singularity reflects the fact that the cumulants neglected by our basic approximation (34) are small (compared to the terms kept) only for small matrices Z [cf. the discussion following Eq. (34)]. If $Z,Z^\dagger$ (or some matrix elements thereof) are allowed to go to infinity, the approximation clearly loses its validity. To control the error incurred near the saddle point $Q=-\Sigma_3$, one needs to switch to another scheme, by first changing coordinates $Z\to 1/Z$ and $Z^\dagger\to 1/Z^\dagger$ and only afterwards repeating the above steps. The contribution from $Q=-\Sigma_3$ can then be calculated in the same way as the one for $Q=\Sigma_3$. The treatment of further saddle points remains an open problem.

What makes this procedure unsatisfactory is that we are simultaneously working with several approximation schemes, each of which is only locally controlled. To localize the integral at the saddle points in a mathematically rigorous manner, we would need an approximation that is *globally well defined* and well controlled. It is not clear whether such an approximation exists, given the stringent requirement that the integrand should also have the index-theoretic features that allow localization techniques to be used.

V. AVERAGING *U* OVER EIGENBASES

By its definition (2) as a correlation function of spectral determinants, $\Omega_U(\gamma)$ is invariant under any change of basis $U \mapsto VUV^{-1}$, with V an arbitary unitary matrix. In the Q-matrix formulation, this invariance is reflected by the relation $S(\gamma,U,Q)=S(\gamma,VUV^{-1},\mathbf{V}Q\mathbf{V}^{-1})$. Since the transformation $Q \mapsto \mathbf{V}Q\mathbf{V}^{-1}$ has unit Jacobian, we may absorb $\mathbf{V}$ into the integration variable Q and compute $\Omega_U(\gamma)$ by first averaging $\mathrm{e}^{-S(\gamma,U,Q)}$ over all rotations $U \mapsto VUV^{-1}$:

$$\mathrm{e}^{-S_{V\mathrm{av}}(\gamma,U,Q)} \overset{\text{def}}{=} \frac{1}{\mathrm{Vol\ U}(N)} \int_{\mathrm{U}(N)} dV \exp\{-S(\gamma,VUV^{-1},Q)\}, \tag{36}$$

and then integrating $\mathrm{e}^{-S_{V\mathrm{av}}}$ over Q. We saw in Sec. III A that if the matrix $D=V^{-1}UV$ is diagonal, then the saddle points of $S(\gamma,U,Q)$ are situated on the points $Q_{V,S}=\mathbf{V}Q_S\mathbf{V}^{-1}$. Because the locations of these points explicitly *depend* on V, we expect that a smoothing mechanism takes place and the divergences of the individual terms in the Weyl character formula disappear on averaging over V. In fact, as we will see, the expansion obtained by saddle-point analysis of the effective action $S_{V\mathrm{av}}(\gamma,U,Q)$ is qualitatively quite different from Weyl's formula.

A. Analysis around $\pm\Sigma_3$

We first describe $S_{V\mathrm{av}}(\gamma,U,Q)$ near the two saddle points $Q=\pm\Sigma_3$ (cf. Sec. IV A). The V-averaged adjoint operator $\langle \mathrm{Ad}\rangle_V$ has a rather simple spectrum: unity is a simple eigenvalue (associated with $\mathbb{I}_N$), and on the remaining (N^2-1)-dimensional space the operator is proportional to the identity:

$$\langle \mathrm{Ad}U\rangle_V = P_{\mathbb{I}} + (1-P_{\mathbb{I}})\frac{|\mathrm{Tr}U|^2-1}{N^2-1}. \tag{37}$$

($P_{\mathbb{I}}$ is the orthogonal projector on $\mathbb{I}_N$.) We see that $\langle \mathrm{Ad}U\rangle_V$ has a large gap between unity and the second eigenvalue, and this gap has the maximal degeneracy. Assuming that this degenerate eigenvalue is small ($|\mathrm{Tr}U| \ll N$), we get the following leading-order contribution:

$$\langle \Omega_U(\mathrm{e}^{\mathrm{i}x/N})\rangle_{V|\Sigma_3 \cup -\Sigma_3} \sim \frac{2NC_N}{(1-\alpha/N)^{N^2}} \frac{\sin\{x(1/2-\alpha)\}}{x}, \tag{38}$$

$$\text{with} \qquad \alpha \overset{\text{def}}{=} (|\mathrm{Tr}U|^2-1)/N. \tag{39}$$

Within this approximation, the correlation function depends on $U=U_{\phi,N}$ only through the simple quantity $|\mathrm{Tr}U|^2$, which can be estimated semiclassically by the Gutzwiller–Tabor trace formula (1): typically, α is of order $\mathcal{O}(1/N)$ for a chaotic map, and of order $\mathcal{O}(1)$ for an integrable one.

Notice that, due to the high degeneracy of the second eigenvalue, we do not get in general the CUE result (8), although this eigenvalue is far inside the unit circle. This shows that, to obtain the CUE result (33), we not only need a finite gap in the spectrum of $\langle \mathrm{Ad}U\rangle$, but also a fast accumulation of the eigenvalues to the origin. The precise condition on the eigenvalues is $\Sigma_{j=2}^{N^2}[\lambda_j/(1-\lambda_j)] \ll N$. In the present averaging scheme, this means $\alpha \ll 1$.

B. Critical submanifolds

We need to investigate the possible influence of other saddle points of $S_{V\mathrm{av}}(\gamma,U,Q)$; for the present averaging scheme, we will explicitly describe a critical set, which we believe to be exhaustive. The effective action possesses the symmetry $S_{V\mathrm{av}}(Q)=S_{V\mathrm{av}}(\mathbf{W}Q\mathbf{W}^{-1})$ for all $W \in \mathrm{U}(N)$. Therefore, the saddle points are grouped into stationary *submanifolds*, each of them invariant under $\mathrm{U}(N)$.

1. Description of the manifolds

In Appendix A we prove the following statement: for any initial matrix U and any γ, the action (36) is stationary at the points $Q=\mathbf{W}Q_\sigma\mathbf{W}^{-1}$, for all rotations $W\in \mathrm{U}(N)$ and any permutation σ (see Sec. III A for the notations σ, $S=S_1\cup S_2$, etc). Since $\mathrm{U}(N)$ is connected, the points $\mathcal{M}_S \overset{\text{def}}{=} \{\mathbf{W}Q_S\mathbf{W}^{-1} \,|\, W\in \mathrm{U}(N)\}$ form a connected submanifold of $\mathcal{M}_N$.

Let τ be any permutation among N indices. The set $S'=(\tau(S_1),\tau(S_2))$ is in general different from S, and we have $Q_S\neq Q_{S'}$; however, $Q_{S'}\in\mathcal{M}_S$, or equivalently $\mathcal{M}_S=\mathcal{M}_{S'}$. Putting $p=\sharp S_2$ and $r=\sharp(S_1\cap S_2)$, we find that $\mathcal{M}_S$ contains $\binom{N}{p}\binom{p}{r}\binom{N-p}{r}$ different points $Q_{S'}$. The manifolds $\mathcal{M}_S$ are in one-to-one correspondence with the integers (p,r), and their total number is $(N/2+1)^2$ for N even, and $(N+1)(N+3)/4$ for N odd (including the isolated points $\pm\Sigma_3$ in the count).

For generic U and $\gamma\neq 1$ [genericity means here that the matrix $\mathrm{diag}(\gamma U,U)$ is not degenerate], we conjecture that the submanifolds $\mathcal{M}_{(p,r)}$ exhaust all the critical points of the action $S_{V\mathrm{av}}(\gamma,U,Q)$.

2. Contributions of the manifolds

The leading-order contribution of each submanifold $\mathcal{M}_S$ to the Q-integral is calculated by separating the tangent space at Q_S into two parts, one parallel and one transverse to $\mathcal{M}_S$. The integrand in the vicinity of Q_S then reads (to quadratic order)

$$\mathrm{e}^{-S_{V\mathrm{av}}(Q_S)}\mathrm{e}^{-\mathrm{Hess}_T(X_T)+\mathcal{O}(|X_T|^3)},$$

where Hess_T is the Hessian of $S_{V\mathrm{av}}$ around $\mathcal{M}_S$, viewed as a nondegenerate quadratic form on the transverse part of tangent space (coordinatized by X_T). The exact integral over $\mathcal{M}_S$ and the Gaussian integral over the transverse directions yield the contribution

$$\langle\Omega_U(\gamma)\rangle_{|\mathcal{M}_S}=C_N\gamma^{-N/2+p}\frac{\mathrm{Vol}\mathcal{M}_S}{\sqrt{\mathrm{Det}(\mathrm{Hess}_T)}}\mathrm{e}^{-S_{V\mathrm{av}}(\gamma,Q_S)}. \tag{40}$$

In Appendix B, we explicitly compute the volumes of the submanifolds $\mathcal{M}_S=\mathcal{M}_{(p,r)}$:

$$\mathrm{Vol}\mathcal{M}_{(p,r)}=\frac{(\Gamma(1)\cdots\Gamma(r))^2\Gamma(1)\cdots\Gamma(p-r)\Gamma(1)\cdots\Gamma(N-p-r)}{\Gamma(1)\cdots\Gamma(N)}.$$

For all submanifolds $\mathcal{M}_S\neq\{\pm\Sigma_3\}$ (i.e., $0<p<N$), these volumes are N-exponentially small. The quantities Hess_T and $S_{V\mathrm{av}}(Q_S)$ depend on U and γ; we are unable to compute them in general. What we know for sure is that $|\mathrm{e}^{-S_{V\mathrm{av}}}|\leqslant 1$, since $\mathrm{e}^{-S(\gamma,U,Q)}$ has this property.

For a nondegenerate U and $\gamma=\mathrm{e}^{\mathrm{i}x/N}$, the Hessian around $\mathcal{M}_S$ will possess a single eigenvalue that vanishes with x, while all other eigenvalues stay at least of order $\mathcal{O}(1)$. This means that the contribution from $\mathcal{M}_S$ goes like $1/x$ as $x\to 0$. However, the "particle-hole duality" between the submanifolds $\mathcal{M}_{(p,r)}$ and $\mathcal{M}_{(N-p,r)}$ cancels this divergence in the sum of their two contributions (as it does for $\pm\Sigma_3$).

As a result, we conjecture that each contribution $\langle\Omega_U(\gamma)\rangle_{|\mathcal{M}_S\cup\mathcal{M}_S^-}$ is x-uniformly, N-exponentially small compared to that from $\pm\Sigma_3$ for large N, owing to the small volumes of $\mathcal{M}_{(p,r)}$. Since the number of critical submanifolds grows like N^2, we deduce that the leading-order saddle-point expansion for the action $S_{V\mathrm{av}}(U,\gamma,Q)$ can be truncated to (38) for large N.

C. Averaging over random matrix ensembles

We may go further and average e^{-S} not only over the conjugates of a fixed matrix U, but also over the spectrum $\{\mathrm{e}^{\mathrm{i}\theta_j}\}$. For instance, we can average U over all matrices in $\mathrm{U}(N)$, with a weight corresponding to one of the standard random matrix ensembles (Poisson, CUE). The averaged

action will be U(N)-rotation invariant, and its saddle points will still lie on the submanifolds $\mathcal{M}_S$. As a result, the leading-order saddle-point (l.o.s.p.) expansion for such ensemble-averaged actions can again be truncated to the contribution (38), upon replacing the coefficient α by its average $\langle\alpha\rangle_{\text{ensemble}}$ over the ensemble considered.

D. Conclusion: No l.o.s.p. expansion for the *V*-averaged actions

The contribution (38) depends in a very simple manner on the matrix U, namely only on its first trace. This is in contradiction with the fact that *a priori*, all traces up to $\mathrm{Tr}(U^{N/2})$ enter into $\Omega_U(\gamma)$ [cf. Eq. (14)]. By selecting some particular cases, it becomes obvious that the l.o.s.p. expansion (38) deviates strongly from the exact correlation function. The most immediate counterexample is the Poisson ensemble, whose correlation function is given in Eq. (8). For this ensemble, $\langle\alpha\rangle_{\text{Poisson}}=1$, which yields the CUE result (!) when inserted into the formula (38). We are hence forced to abandon the l.o.s.p. expansion for the V-averaged actions.

Nevertheless, we hope that this expansion is still meaningful when the averaging over U is *local* in U(N), which is the case for the semiclassical average in Sec. IV C (but not for the V-average). Hopefully, a local average will still conserve some memory of the "localization" property, which entailed the "almost exactness" of the l.o.s.p. expansion for $S(\gamma,U,Q)$.

In the next section, we will consider a local averaging scheme different from the semiclassical one. It possesses group-theoretic properties, which will allow us to analyze it from the character decomposition (14) instead of the coherent-state integral.

VI. ISOTROPIC AVERAGING

Starting from a fixed matrix U, one may define an *isotropic* averaging around U, by composing U with the $N\times N$ unitary matrices $\mathrm{e}^{-\mathrm{i}H}$, weighted by $\exp(-\mathrm{Tr}H^2/4\epsilon)dH$ with small ϵ (so that the weight is concentrated at the identity). Isotropy here means that the measure dH is U(N)-invariant. Note that this in sharp contrast with the semiclassical averaging of Sec. IV C, where H was a linear combination of r matrices $\hat{H}_j$, with r independent of N. In the semiclassical case, the perturbation spanned only a r-dimensional submanifold, whereas in the present case the perturbation completely fills the N^2-dimensional ϵ-ball centered at $H=0$.

One can replace the Gaussian weight by any positive normalized U(N)-invariant function of H. For our purposes, it is convenient to use the *heat kernel* on U(N), i.e., the kernel of the regularizing operator $\exp(-\epsilon\Delta)$, where Δ is the (positive) Laplace–Beltrami operator on U(N). The heat kernel centered on U is defined as follows:

$$\forall\,\epsilon>0:\ -\Delta_V K_\epsilon(V,U)=\frac{\partial}{\partial\epsilon}K_\epsilon(V,U)$$

$$\lim_{\epsilon\to+0} K_\epsilon(V,U)=\delta_U(V).$$

Owing to the compactness of U(N), the density $K_\epsilon(\cdot,U)$ for any matrix U converges to the uniform density on U(N) as $\epsilon\to\infty$. Switching ϵ from 0 to ∞ therefore realizes a crossover from the Dirac delta measure $\delta_U(\cdot)$ to the Haar (or CUE) measure. For small values of ϵ, the kernel $K_\epsilon(V,U)=k_\epsilon(VU^{-1})$ is concentrated around $\mathrm{e}^{-\mathrm{i}H}=VU^{-1}\approx 1$ and is approximately given by the Gaussian weight introduced above: $k_\epsilon(\mathrm{e}^{-\mathrm{i}H})\sim\exp(-\mathrm{Tr}H^2/4\epsilon)$.

Schur's lemma ensures that Δ is proportional to the identity on each U(N)-irreducible subspace of $L^2(\mathrm{U}(N))$. As a consequence, its action on each representation matrix $\rho_p(U)$ of Eq. (14) is simply a multiplication by a positive factor, called the quadratic Casimir invariant, which we denote by $\rho_p(\Delta)$. In formulas,

$$\int_{\mathrm{U}(N)} dV\rho_p(V)K_\epsilon(V,U)\overset{\text{def}}{=}\mathrm{e}^{-\epsilon\Delta_U}\rho_p(U)=\mathrm{e}^{-\epsilon\rho_p(\Delta)}\rho_p(U).$$

The factor $\rho_p(\Delta)$ may be computed from the Young diagram of ρ_p; a more direct way is to express Δ in terms of fermionic operators acting on the Fock space $\mathcal{F}$:

$$\Delta|_{\mathcal{F}}=\sum_{i,j=1}^{N}(f_{+i}^{\dagger}f_{+j}-f_{-j}^{\dagger}f_{-i})(f_{+j}^{\dagger}f_{+i}-f_{-i}^{\dagger}f_{-j})=(N+1)(F_{+}+F_{-})-(F_{+}^{2}+F_{-}^{2})-2J_{\uparrow}J_{\downarrow}.$$

Applying this to any element of the subspace ${}^{0}\mathcal{F}^{p}$ (which carries ρ_p) we find

$$\rho_p(\Delta)=2p(N+1-p). \tag{41}$$

On employing the decomposition (14), the heat-kernel averaged correlation function for $\gamma=e^{ix/N}$ takes the form

$$\langle\Omega_U(\gamma)\rangle_{\epsilon}\overset{\text{def}}{=}e^{-\epsilon\Delta_U}\Omega_U(\gamma)=\sum_{p=0}^{N/2}e^{-2\epsilon p(N+1-p)}\mathrm{Tr}\rho_p(U)\,\frac{\sin[x/2\,(1-(2p-1)/N)]}{\sin(x/2N)}. \tag{42}$$

The effect of the averaging procedure is to damp the large-p traces, which are difficult to estimate from the Gutzwiller trace formula. In the above equation the $\epsilon\to\infty$ behavior is obvious: all traces except the trivial one $\mathrm{Tr}\rho_0(U)=1$ are killed by the exponential, no matter what the matrix U is. It is actually not necessary to set ϵ to ∞ to get the CUE correlation. Since the irreps ρ_p are unitary, their traces are bounded by

$$|\mathrm{Tr}\rho_p(U)|\leqslant\dim\rho_p=\mathrm{Tr}\rho_p(\mathbb{I}).$$

The dimensions of the ρ_p's are given in Eq. (13); for finite p, they are bounded by $\dim\rho_p\leqslant N^{2p}$. In the limit $N,p\to\infty$ with $y=p/N$ fixed, Stirling's formula yields

$$\dim(\rho_{p=Ny})\sim(\pi N)^{-1}\frac{f'(y)}{y(1-y)}e^{2Nf(y)},$$

where the function $f(y)=-y\log y-(1-y)\log(1-y)$ increases monotonically from $f(0)=0$ to $f(1/2)=\log 2$.

For any sequence $\{U_N\}_{N\in\mathbb{N}}$, if we tune ϵ (possibly varying with N) such that

$$\varepsilon\overset{\text{def}}{=}N\epsilon\gg 1,$$

all the terms making a significant contribution to (42) satisfy $p\ll N$. The x-dependence of all these terms is the same [being given by the CUE correlation $x^{-1}\sin(x/2)$], so the averaged correlation will also have this dependence. Only the prefactor will depend on the matrices U_N explicitly. If ϵ is increased further to $\varepsilon\gg\log N$, the prefactor itself becomes universal.

These statements hold even in the most general case, when the sequence $\{U_N\}$ is completely arbitrary. Therefore, to be able to differentiate between integrable and chaotic quantum maps, one must tune the "disorder strength" ε to smaller values, so that contributions from the "high" traces $\mathrm{Tr}\rho_p(U_N)$ start to contribute. To recover the Poisson behavior for integrable maps, one actually needs contributions to (42) coming from the whole region $p\lesssim N/2$.

This puts us in a no-win situation. On the one hand, we should tune ε to small enough values so that the high traces $p\sim Ny$ $(y>0)$ survive and Poisson behavior stands a chance to emerge. On the other hand, for a chaotic map we have no control over these high traces (we don't for an integrable map either).

For our purposes, the present averaging scheme is probably "too algebraic," as opposed to the semiclassical average presented in Sec. IV C. To motivate this statement in the spirit of Sec. IV C, let us compare the spectra of the operators $\langle\mathrm{Ad}U\rangle$ for the two schemes:

(i) The spectrum of $\langle \mathrm{Ad}U\rangle_{\mathrm{semiclas}}$ *qualitatively* depends on the nature of the classical dynamics (see Sec. IV C). It has a finite gap for a chaotic map, whereas eigenvalues accumulate near the unit circle for an integrable one.

(ii) In the isotropic scheme, $\langle \mathrm{Ad}U\rangle_{\epsilon}$ is decomposed into the irreps $\rho_0(U)\oplus\rho_1(U)$. Therefore, apart from the single eigenvalue unity, $\langle \mathrm{Ad}U\rangle_{\varepsilon}$ has the eigenvalues $\{e^{-2\varepsilon}e^{i(\theta_i-\theta_j)}\}$, where $\{e^{i\theta_j}\}$ are the eigenvalues of U; the eigenvalue $e^{-2\varepsilon}$ is $(N-1)$-fold degenerate. This spectrum is qualitatively the same for chaotic versus integrable systems.

A. Crossover Poisson-CUE

We now present an application of the above scheme in the area of random matrices. More precisely, we use the isotropic averaging to build a crossover between the Poisson and CUE ensembles, and we derive the transitional determinant correlation function that interpolates between the formulas (8). This crossover, as well as the method used to compute $\langle\Omega_U\rangle$, can be compared to the GOE→GUE crossover studied in Ref. 7.

Our crossover is defined as follows. We start from the Poisson ensemble, then convolute it with the isotropic (heat kernel) measure of width ϵ:

$$\langle\Omega_U(\gamma)\rangle_{\mathrm{Poisson},\epsilon}\overset{\mathrm{def}}{=}\int_{\mathrm{U}(N)}\mathrm{d}\mathcal{P}_{\mathrm{Poisson}}(U)\int_{\mathrm{U}(N)}dV\,K_{\epsilon}(V,U)\Omega_V(\gamma).$$

For $\epsilon=0$, this is the Poisson ensemble. In the large-ϵ limit, the second integral converges U-uniformly to the CUE correlation function, so the output $\langle\Omega_U(\gamma)\rangle_{\mathrm{Poisson},\epsilon}$ does, too.

To calculate the correlation function along the crossover, we will use the decomposition (42) as in the previous section: averaging being a linear operation, we only need to replace the characters $\mathrm{Tr}\rho_p(U)$ by their Poisson averages [see Eqs. (7) and (15)]:

$$\langle\mathrm{Tr}\rho_p(U)\rangle_{\mathrm{Poisson}}=\binom{N}{p}-\binom{N}{p-1}.$$

The asymptotics of these traces in the regime $p,N\to\infty$ with $y=p/N$ fixed, again follows easily from Stirling's formula:

$$\langle\mathrm{Tr}\rho_p(U)\rangle_{\mathrm{Poisson}}\sim(2\pi N)^{-1/2}\frac{f'(y)}{\sqrt{y(1-y)}}e^{Nf(y)}. \tag{43}$$

The sum over characters therefore approaches the following integral (as $N\to\infty$):

$$\langle\Omega_U(e^{ix/N})\rangle_{\mathrm{Poisson},\epsilon}\sim\frac{2N^2}{\sqrt{2\pi N}}\int_0^{1/2}dy\,\frac{f'(y)}{\sqrt{y(1-y)}}\frac{\sin(\frac{1}{2}x-yx)}{x}e^{N(f(y)-2\varepsilon y(1-y))}. \tag{44}$$

In the limit $N\to\infty$, this integral is determined by the saddle points (rather, the maximum) of $f_{\varepsilon}(y)\overset{\mathrm{def}}{=}f(y)-2\varepsilon y(1-y)$ on $[0,\frac{1}{2}]$. Three cases have to be distinguished:

(i)If $\varepsilon<1$, the boundary point $y=\frac{1}{2}$ is a maximum of f_{ε} and is the only critical point on $[0,\frac{1}{2}]$. Because of the vanishing of the integrand at $y=\frac{1}{2}$, the saddle-point analysis requires some care. For x of order $\mathcal{O}(N^0)$ the result turns out to be independent of x:

$$\langle\Omega_U(e^{ix/N})\rangle_{\mathrm{Poisson},\varepsilon}\sim 2^N e^{-N\varepsilon/2}(1-\varepsilon)^{-3/2},$$

which shows that the Poisson result 2^N is retrieved in the limit $\varepsilon\to0$. The correlation functions starts depending on x on scales of order $x\sim\mathcal{O}(N^{1/2})$.

(ii) If $\varepsilon>1$, the maximum of f_ε is situated at the point $y_\varepsilon \in (0,\frac{1}{2})$ which solves the transcendental equation $f'_\varepsilon(y)=0$. The correlation function depends on $x\sim\mathcal{O}(N^0)$ as

$$\langle \Omega_U(\mathrm{e}^{\mathrm{i}x/N})\rangle_{\mathrm{Poisson},\varepsilon} \propto \frac{\sin[x(\frac{1}{2}-y_\varepsilon)]}{x}. \tag{45}$$

The flat correlation function has been replaced by an oscillatory function, with the period of oscillation being controlled by the ''frequency shift'' y_ε. When ε becomes large, the shift vanishes as $y_\varepsilon\sim \mathrm{e}^{-2\varepsilon}$, so the CUE correlation function is retrieved.

(iii) If $\varepsilon=1$, the correlation function is ''critical'' (in the sense of a phase transition), as the two points $y=\frac{1}{2}$ and y_ε coalesce for $\varepsilon\to 1$ to form a degenerate critical point. In this case the correlation function varies on scales $x\sim\mathcal{O}(N^{1/4})$.

VII. CONCLUSIONS

In this article we have adapted the NLσM approach introduced in Refs. 15 and 16 to the framework of quantized maps on a Hilbert space of dimension $N\sim\hbar^{-1}$. We focused on the spectral determinant correlation function $\Omega_U(\gamma)$ instead of the pair correlation function, thereby obviating the need to introduce supersymmetry; we obtained an *exact* expression for the correlation function as an ordinary integral over a N^2-dimensional complex manifold. Because the manifold is compact and the integrand uniformly bounded, no regularization needs to be introduced (unlike in Ref. 15).

To estimate this integral we expand the integrand around its saddle points, first restricting ourselves to the leading-order perturbative expansion around each point. Owing to the absence of a large parameter in front of the effective action, this approximation is uncontrolled, and the connection between its output and the exact value of the integral seems fortuitous at best.

Yet, for any matrix $U\in \mathrm{U}(N)$, we find that the result from lowest-order saddle-point expansion of the effective action $S(\gamma,U,Q)$ coincides with the exact correlation function, up to a global prefactor:

$$\Omega_U(\gamma)_{|\mathrm{l.o.s.p.\ exp.}} = C_N\ \ \Omega_U(\gamma)_{\mathrm{exact}}. \tag{46}$$

This remarkable coincidence is linked to a cancellation property of the higher-order terms of the perturbation expansion, which modify only the prefactor, and is explained by the group-theoretic structure of the integrand and the Weyl character formula. Unfortunately, the expansion is of no use for estimating the correlation function of quantized maps in the semiclassical limit.

We argue that a decent semiclassical estimate of the correlation function $\Omega_U(\gamma)$ can only be reached if one takes an average over a set of unitary matrices in the vicinity of U. To estimate this averaged correlation, we first average the integrand $\mathrm{e}^{-S(\gamma,U,Q)}$ over U, and then perform the saddle-point expansion of the output. Because averaging and saddle-point expansion are operations that do not commute, this procedure yields an expansion different from that of the ''individual'' action. At the same time, averaging *a priori* breaks the group-theoretic structure, and with it the exactness (modulo prefactor) of the leading-order saddle-point expansion. Moreover, the explicit computation of saddle points and their contributions is, in general, a nontrivial task for a general averaging scheme.

We have been able to locate the complete set of critical points only for a certain type of average, namely averaging over all bases of Hilbert space. This produces a U(N)-invariant effective action, the critical points of which are grouped into submanifolds, and are independent of the matrix U we started from (as long as its spectrum is nondegenerate). Two of these submanifolds are isolated points; we conjectured that the contributions from these two ''standard'' saddle points, which can be computed explicitly, always dominate the leading-order saddle-point expansion.

The contributions from these two points are unfortunately ''too simple'' to constitute a good approximation of the correlation function, except in some exceptional cases, which we do not truly

understand. If we average over $U \in \mathrm{U}(N)$ with the Poisson measure, the saddle-point result strongly differs from the exact one. We are thus led to conclude that the leading-order saddle-point expansion of rotation-averaged effective actions does not yield a good estimate of the full integral.

What happens in the case of a *local* average, i.e., when the weight of the probability measure is concentrated near the quantized map U_N, is unclear. For one thing, we are only able to exhibit the two standard saddle points of the averaged action, but there surely exist many more.

In the case of the ''semiclassical'' averaging scheme, expansion around these saddle points yields results similar to those obtained in Ref. 15, except that the ''resonances'' we identify are eigenvalues of a quantum operator. Yet, these resonances for large N seem related to the (classical) Ruelle–Pollicott resonances,[30,31] in particular they indicate whether the classical dynamics is chaotic or integrable.

To connect these resonances with the determinant correlation function on a rigorous footing, we need two nontrivial assumptions to be fulfilled. First, we must assume that the leading-order saddle-point expansion of the (local average) $S_{\mathrm{semiclas}}(\gamma, U_N, Q)$ makes sense, i.e., gives a good approximation of the exact result; the two-loop calculation around $\pm\Sigma_3$ in Sec. IV D seems to support this assumption. Second, hindered by our inability to compute the contributions from further saddle points, we are forced to assume that the full expansion can be truncated to the two standard saddle points, or at least that this truncation provides a reasonable approximation. We presently see no way to prove these assumptions.

APPENDIX A: PROOF OF CRITICALITY OF THE SUBMANIFOLDS $\mathcal{M}_S$

To prove that the V-averaged integrand $\mathrm{e}^{-S_{V\mathrm{av}}(\gamma,U,Q)}$ is stationary on the submanifolds $\mathcal{M}_S \subset \mathcal{M}_N$, we employ the coherent-state formulation of the Q-integral. The point Q_S corresponds to the state $|S\rangle = R(\mathbf{g}_\sigma)|0\rangle$, and the points in a neighborhood of Q_S may be parametrized as $R(\mathbf{g}_\sigma)|\zeta\rangle$, where ζ runs through the $N\times N$ matrices (with small coefficients) and $|\zeta\rangle$ is the corresponding coherent state. The permutation $\sigma \in \mathfrak{S}_{2N}$ is chosen in such a way as to interchange the sets $\overline{S_1}$ and $\widetilde{S}_2 = S_2 + N$, and to keep S_1 and $\widetilde{\overline{S_2}} = \overline{S_2} + N$ fixed.

We write the $2N\times 2N$ matrix $\mathbf{g}_\sigma^{-1}\mathbf{\Gamma}\mathbf{U}\mathbf{g}_\sigma$ in the block form $\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$, and first compute the value of the integrand in the vicinity of Q_S *before averaging*:

$$\frac{\langle\zeta|R(\mathbf{g}_\sigma^{-1}\mathbf{\Gamma}\mathbf{U}\mathbf{g}_\sigma)|\zeta\rangle}{\langle\zeta|\zeta\rangle} = \mathrm{Det}(D)\left(1+\mathrm{Tr}(D^{-1}C\zeta + BD^{-1}\zeta^\dagger) + \mathcal{O}(|\zeta|^2)\right).$$

Then we perform the V-average on U (recall that $V \in \mathrm{U}(N)$ acts on $U \in \mathrm{U}(N)$ by conjugation: $U \mapsto VUV^{-1}$), and study its output on the right-hand side of the above equation. To first order in ζ and $\zeta^\dagger$, we need the averages $\langle \mathrm{Det}(D)\rangle_V$, $\langle D^{-1}C\ \mathrm{Det}(D)\rangle_V$ and $\langle BD^{-1}\mathrm{Det}(D)\rangle_V$. By decomposing the sets $\{1,\ldots,N\} = S_1 \cup \overline{S_1}$ and $\{N+1,\ldots,2N\} = \widetilde{S}_2 \cup \widetilde{\overline{S_2}}$, the $N\times N$ matrices B,C,D may be written in block form:

$$B = \begin{pmatrix} \gamma U_{S_1\overline{S_1}} & 0 \\ 0 & U_{S_2\overline{S_2}} \end{pmatrix}, \quad C = \begin{pmatrix} \gamma U_{\overline{S_1}S_1} & 0 \\ 0 & U_{\overline{S_2}S_2} \end{pmatrix}, \quad D = \begin{pmatrix} \gamma U_{\overline{S_1}\overline{S_1}} & 0 \\ 0 & U_{\overline{S_2}\overline{S_2}} \end{pmatrix},$$

where each entry $U_{ss'}$ is a matrix of size $\sharp s \times \sharp s'$, whose indices take values in the sets s, s'. Thus the V-averaged coefficients of the term linear in ζ are the following matrix elements:

$$\langle \mathrm{Det}(U_{\overline{S_1}\overline{S_1}})\mathrm{Det}(U_{\overline{S_2}\overline{S_2}})(U^{-1}_{\overline{S_1}\overline{S_1}}U_{\overline{S_1}S_1})_{ik}\rangle_V, \quad \langle \mathrm{Det}(U_{\overline{S_1}\overline{S_1}})\mathrm{Det}(U_{\overline{S_2}\overline{S_2}})(U^{-1}_{\overline{S_2}\overline{S_2}}U_{\overline{S_2}S_2})_{lm}\rangle_V,$$

where we have displayed only the dependence on U (and omitted the γ-dependence). We now use the invariance of the Haar measure dV under (left) multiplication by any unitary matrix and any diagonal unitary matrix $\delta = \mathrm{diag}(\delta_1,\ldots,\delta_N)$ in particular. Under such a left translation, the above matrix elements acquire extra factors δ_i/δ_k (resp. δ_l/δ_m). Hence

$$\langle \mathrm{Det}(D)(D^{-1}C)_{ik}\rangle_V = \langle \mathrm{Det}(D)(D^{-1}C)_{ik}\rangle_V \delta_i/\delta_k \quad \text{for any} \quad \delta_i, \delta_k .$$

Since $i \in \overline{S_1}$ and $k \in S_1$ (resp. $l \in \overline{S_2}$ and $m \in S_2$) are never equal and the ratio δ_i/δ_k may take any value in U(1), we conclude

$$\langle \mathrm{Det}(D)(D^{-1}C)_{ik}\rangle_V = 0.$$

By the same reasoning, the terms linear in $\zeta^\dagger$ vanish after V-averaging.

We have thus shown that the point Q_S on $\mathcal{M}_N$ is a critical point of the V-averaged action $S_{V\mathrm{av}}$, Eq. (36). By the U(N)-invariance of $S_{V\mathrm{av}}$, it follows that the whole submanifold $\mathcal{M}_S$ is critical for the V-averaged action, no matter what U is.

APPENDIX B: VOLUMES OF THE CRITICAL SUBMANIFOLDS

We treat the general case with $\sharp S_1 = \sharp \overline{S_2} = N-p$, $\sharp \overline{S_1} = \sharp S_2 = p$, $\sharp(S_1 \cap S_2) = \sharp(\overline{S_1} \cap \overline{S_2}) = r$, and to build Q_S we use the same permutation σ as in the previous appendix.

The manifold $\mathcal{M}_S$ is given by the set of states $\{R(\mathbf{V}\mathbf{g}_\sigma)|0\rangle | V \in \mathrm{U}(N)\}$. These states may be written (up to normalization) in the form $R(\mathbf{g}_\sigma)|\zeta_V\rangle$ where the coherent state $|\zeta_V\rangle$ is determined by the matrix

$$\zeta_V = \begin{pmatrix} V_{S_1\overline{S_1}} V_{\overline{S_1}\overline{S_1}}^{-1} & 0 \\ 0 & V_{S_2\overline{S_2}} V_{\overline{S_2}\overline{S_2}}^{-1} \end{pmatrix} \overset{\mathrm{def}}{=} \begin{pmatrix} \zeta^{(1)} & 0 \\ 0 & \zeta^{(2)} \end{pmatrix} \tag{B1}$$

according to Eqs. (16) and (17). The block structure of this matrix derives from the sets (S_1, S_2) vertically, and $(\overline{S_1}, \overline{S_2})$ horizontally.

When V runs through U(N), the upper-left matrix $\zeta^{(1)}$ takes all possible values in $\mathbb{C}^{(N-p)\times p}$. The matrix $\zeta^{(2)}$ is not independent of $\zeta^{(1)}$. For a fixed $\zeta^{(1)}$, we need to identify the remaining degrees of freedom in $\zeta^{(2)}$, which is quite easy to do if $\zeta^{(1)}=0$, i.e., if V has the structure $V = \mathrm{diag}(V_{S_1S_1}, V_{\overline{S_1}\overline{S_1}})$. The matrices $V_{S_2\overline{S_2}}$ and $V_{\overline{S_2}\overline{S_2}}$ in this case block decompose as

$$V_{S_2\overline{S_2}} = \begin{pmatrix} V_{12,\overline{12}} & 0 \\ 0 & V_{\overline{12},\overline{12}} \end{pmatrix}, \quad V_{\overline{S_2}\overline{S_2}} = \begin{pmatrix} V_{\overline{12},\overline{12}} & 0 \\ 0 & V_{\overline{12},12} \end{pmatrix}$$

where the index 12 refers to the set $S_1 \cap S_2$, etc. The degrees of freedom of the lower-right part of ζ_V are thus two matrices, $\zeta^{(11)} \overset{\mathrm{def}}{=} V_{12,\overline{12}} V_{\overline{12},\overline{12}}^{-1} \in \mathbb{C}^{r\times(N-p-r)}$, and $\zeta^{(\overline{11})} \overset{\mathrm{def}}{=} V_{\overline{12},12} V_{\overline{12},\overline{12}}^{-1} \in \mathbb{C}^{(p-r)\times r}$. They are independent of each other, and take all possible values in their respective vector spaces. Since the subgroup U($N-p$)$\times$U(p) of U(N) acts transitively on the submanifold $\zeta^{(1)}=0$ of $\mathcal{M}_S$, there exists a natural choice of invariant measure on that submanifold. It has the factorized form

$$\mathrm{Det}(1+\zeta^{(11)\dagger}\zeta^{(11)})^{N-p} \prod_{i,j} d^2\zeta_{ij}^{(11)}/\pi \times \mathrm{Det}(1+\zeta^{(\overline{11})\dagger}\zeta^{(\overline{11})})^{p} \prod_{i,j} d^2\zeta_{ij}^{(\overline{11})}/\pi .$$

The matrix $\zeta^{(1)}$ parametrizes a coset space U(N)/U($N-p$)$\times$U(p), with the corresponding invariant measure being $\mathrm{Det}(1+\zeta^{(1)\dagger}\zeta^{(1)})^N \Pi_{i,j} d^2\zeta_{ij}^{(1)}/\pi$. By group invariance arguments, the volume element of $\mathcal{M}_S$ (normalized so that it agrees with the Riemannian measure inherited from the Riemannian manifold $\mathcal{M}_N$) is the product of the measures for $\zeta^{(1)}$, $\zeta^{(11)}$, and $\zeta^{(\overline{11})}$ above. Using this fact and the result[33]

$$I(m,n) \overset{\mathrm{def}}{=} \int_{\mathbb{C}^{m\times n}} \prod_{i=1}^{m} \prod_{j=1}^{n} \frac{d^2Z_{ij}}{\pi} \mathrm{Det}(1+Z^\dagger Z)^{-n-m} = \frac{\Gamma(1)\cdots\Gamma(n)\ \ \Gamma(1)\cdots\Gamma(m)}{\Gamma(1)\cdots\Gamma(n+m)},$$

we obtain the volume of $\mathcal{M}_S$:

$$\mathrm{Vol}\mathcal{M}_S = I(p,N-p)I(r,p-r)I(r,N-p-r).$$

A similar integral yields the normalization factor C_N of the measure $d\mu_N(Z,Z^\dagger)$ on the full manifold $\mathcal{M}_N$:

$$\frac{1}{C_N} = \int_{\mathbb{C}^{N\times N}} \prod_{i,j=1}^{N} \frac{d^2 Z_{ij}}{\pi} \mathrm{Det}(1+Z^\dagger Z)^{-2N-1} = \frac{\Gamma(2)\cdots\Gamma(N+1)}{\Gamma(N+2)\cdots\Gamma(2N+1)}.$$

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Coherent states and annihilation–creation operators associated with the irreducible unitary representations of $\mathfrak{su}(1,1)$

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We construct a kind of annihilation–creation operators related to the affine coherent states. Next, we re-interpret them as annihilation–creation operators associated with the irreducible unitary representation of the algebra $\mathfrak{su}(1,1)$, by adding another generator to the two generators of the unitary representation of the one-dimensional affine group. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1470707]

I. INTRODUCTION

In quantum mechanical systems, the canonical commutation relation

$$[X,Y]=-iI \tag{1}$$

is important, and the annihilation and creation operators, coherent states, number states, and the number operator are derived from this commutation relation. Here, we will treat the commutation relation

$$[X,Y]=-iX \tag{2}$$

similar to (1). The Lie group associated with this algebra is called the (one-dimensional) affine group ($ax+b$ group), and it is well known that it has only two irreducible unitary representations in the sense of unitary equivalence (see Gel'fand and Naimark,[1] or Aslaksen and Klauder[2]). For the commutation relation (2), in a similar manner to the case of the canonical commutation relation (1), the corresponding coherent states (affine coherent states) have been known.[3,4] The affine coherent states are the minimum uncertainty states between an operator and the inverse of the other operator of the canonical commutation pair. In signal processing, the wave packets corresponding to the affine coherent states are called Cauchy wavelets and they are important in the theory of the continuous wavelet transformation.[5]

In this paper, in this context, we will derive not only the coherent states but also the analogs of the annihilation and creation operators, the number operator, and the number states which are associated to the commutation relation (2). Moreover, we will interpret them more naturally by starting from the irreducible unitary representation of the algebra $\mathfrak{su}(1,1)$, because the irreducible unitary representation of the affine group is closely related to the irreducible unitary representation of the algebra $\mathfrak{su}(1,1)$ associated with the Lie group SU(1,1).

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II. ANNIHILATION–CREATION RELATION RELATED TO IRREDUCIBLE UNITARY REPRESENTATION OF AFFINE GROUP: A HEURISTIC APPROACH

It has been known[2] that the irreducible unitary representation of the affine group can be reduced to

$$Y=\frac{PQ+QP}{2}, \quad X=Q \ \text{ on } \ L^2(\mathbb{R}^+),$$

$$Y=\frac{PQ+QP}{2}, \quad X=Q \ \text{ on } \ L^2(\mathbb{R}^-),$$

where Q denotes the position coordinate operator and P denotes the momentum operator. In the following discussions, we will treat only the former representation, because the latter representation can be discussed in almost the same way only with minor changes of the signs.

It has been known that the wave function of the coherent state $|\eta\rangle^k$ associated with the affine group is

$${}_Q\langle x|\eta\rangle^k := \sqrt{\frac{(2\ \mathrm{Im}\ \eta)^{2k+1}}{\Gamma(2k+1)}}\, x^k \ \ e^{i\eta x}, \quad \eta\in H,$$

where H denotes the upper half plane and k is a real parameter ($k>-\frac{1}{2}$). In particular, in the cases of the representations with $k>0$, the system of the coherent states constitutes the resolution of identity

$$\frac{1}{2k}\int_H |\eta\rangle^k \ \ {}^k\langle\eta| \frac{d^2\eta}{4\pi(\mathrm{Im}\ \eta)^2}=I,$$

while this does not exist in the cases of the representations with $-1/2<k<0$ because of the divergence of the integration.

Next, we will introduce the operator which has $|\eta\rangle^k$ as its eigenvector associated with the eigenvalue η for $\forall\,\eta\in H$. Define

$$A_k := P+ikQ^{-1},$$

formally. Since this operator is unbounded, precisely, we should give its precise definition taking its domain into consideration. The precise definition and its justification will be done from a viewpoint of group representation in Sec. IV. For this operator defined formally and the above-mentioned coherent states, it is easily shown that

$$A_k|\eta\rangle^k=\eta|\eta\rangle^k, \quad \forall\,\eta\in H.$$

The operator A_k has a similar property to the boson annihilation operator in the sense that it has the coherent states as its eigenvectors. However, the operator A_k does not have the property of the annihilation operator which decreases the number of states.

We can find heuristically an operator having both of the above-mentioned properties, as a function of A_k, as follows. Define

$$a_k := (A_k-iI)(A_k+iI)^{-1}. \tag{3}$$

Then

$$a_k|\eta\rangle^k=\frac{\eta-i}{\eta+i}|\eta\rangle^k, \quad \forall\,\eta\in H.$$

By letting $\zeta := (\eta - i)/(\eta + i)$ and $|\zeta\rangle_a^k := |\eta\rangle^k$, we have

$$a_k|\zeta\rangle_a^k = \zeta|\zeta\rangle_a^k, \quad \forall \zeta \in D,$$

where D denotes the inside of the unit disk. Moreover, by regarding $|0\rangle_a^k$ as the vacuum, define

$$|n\rangle_N^k := \frac{1}{||(a_k^*)^n|0\rangle_a^k||}(a_k^*)^n|0\rangle_a^k.$$

Then we have a kind of annihilation–creation relations

$$a_k|n\rangle_N^k = \sqrt{\frac{n}{n+2k}}\,|n-1\rangle_N^k,$$

$$a_k^*|n\rangle_N^k = \sqrt{\frac{n+1}{n+2k+1}}\,|n+1\rangle_N^k.$$

Moreover, by defining

$$N_k := \tfrac{1}{2}(PQP + k^2Q^{-1} + Q - (2k+1)I),$$

we have

$$N_k|n\rangle_N^k = n|n\rangle_N^k,$$

where N_k can be regarded as the number operator. The wave function of the number state is

$${}_Q\langle x|n\rangle_N^k = \sqrt{\frac{2^{2k+1}n!}{\Gamma(n+2k+1)}}\,e^{-x}x^k S_n^{2k}(2x),$$

where $S_n^l(x)$ is the Sonine polynomial (or the associated Laguerre polynomial) defined by

$$S_n^l(x) := \sum_{m=0}^{n} \frac{(-1)^m}{(n-m)!}\frac{\Gamma(n+l+1)x^m}{\Gamma(m+l+1)m!}.$$

(Sometimes another definition with $n+l$ instead of l is used.)

Among the operators a_k, a_k^*, and N_k, the following relations hold;

$$a_k^* a_k = (N_k + 2kI)^{-1}N_k,$$

$$a_k a_k^* = (N_k + (2k+1)I)^{-1}(N_k + I),$$

$$[a_k, a_k^*] = 2k(N_k + 2kI)^{-1}(N_k + (2k+1)I)^{-1},$$

$$[a_k, N_k] = a_k, \tag{4}$$

$$[N_k, a_k^*] = a_k^*, \tag{5}$$

where relations (4) and (5) have the same forms as usual boson cases.

III. INTERPRETATION OF ANNIHILATION–CREATION RELATIONS RELATED TO AFFINE GROUP IN TERMS OF ALGEBRA $\mathfrak{su}(1,1)$

The linear fractional transform (Möbius transform) used in (3) was found only heuristically. However, in this section, we will give a natural derivation of this structure from the context of the

irreducible unitary representation of the algebra $\mathfrak{su}(1,1)$ which satisfies some conditions. In this context, we will re-interpret the annihilation–creation relations introduced in Sec. II more clearly in this section and Sec. IV.

The irreducible unitary representation of the algebra $\mathfrak{su}(1,1)$ is given by the triple of skew-adjoint operators (E_0,E_+,E_-) satisfying the commutation relations

$$[E_0,E_\pm]=\pm 2E_\pm, \quad [E_+,E_-]=E_0. \tag{6}$$

(Note that the unitary representation of the affine group is given here if we pay attention only to $-iE_0$ and $-iE_+$.) Here, be careful about the fact that the representation of the Lie group SU(1,1) cannot always be constructed from the representation of the algebra $\mathfrak{su}(1,1)$, because SU(1,1) is not a universal covering group. Since the operators E_0, E_+, and E_- have continuous spectra usually under each unitary representation, it is difficult to analyze the forms of the representation. In order to avoid this difficulty, instead of the triple (E_0,E_+,E_-), we will use the triple (L_0,L_+,L_-) defined by

$$L_0 := i(E_- - E_+),$$

$$L_\pm := (E_0 \pm i(E_+ + E_-))/2,$$

where the triple (L_0,L_+,L_-) satisfies the same commutation relations

$$[L_0,L_\pm]=\pm 2L_\pm, \quad [L_+,L_-]=L_0. \tag{7}$$

The operators L_0, L_+, and L_- are not skew-adjoint, but they satisfy

$$L_0^*=L_0, \quad L_+^*=L_-. \tag{8}$$

It has been known that giving the triple of skew-adjoint operators which satisfy (6) is equivalent to giving the triple which satisfies (7) and (8).[6] The commutation relation $[L_0,L_\pm]=\pm 2L_\pm$ shows that the operator $L_\pm$ is a kind of up/down-ladder of the eigenvector system of L_0. From this fact, and from the irreducibility and the unitarity, it is shown that only the following three cases are possible;

$$\text{Case 1:} \quad \dim \mathrm{Ker}\, L_+ = 0, \quad \dim \mathrm{Ker}\, L_- = 1,$$

$$\text{Case 2:} \quad \dim \mathrm{Ker}\, L_+ = 1, \quad \dim \mathrm{Ker}\, L_- = 0,$$

$$\text{Case 3:} \quad \dim \mathrm{Ker}\, L_+ = 0, \quad \dim \mathrm{Ker}\, L_- = 0.$$

Case 2 can be reduced to case 1 by some changes of the signs. In this paper, we will not treat case 3, and we will discuss only case 1 in the following. In this case, the minimum eigenvalue of L_0 exists.

Let λ be the minimum eigenvalue of L_0. From the unitarity of the representation, λ should be positive.[6] Let v_0 be the eigenvector of L_0 associated with the eigenvalue λ. Then, we have

$$L_0 v_n=(\lambda+2n)v_n (n\geqslant 0), \quad L_+ v_n = v_{n+1} (n\geqslant 0),$$

$$L_- v_n = -n(\lambda+n-1)v_{n-1} (n\geqslant 1), \quad L_- v_0 = 0$$

for

$$v_n := (L_+)^n v_0.$$

Here, from the irreducibility of the representation, we can show that $\{v_n | n=0,1,2,3,\ldots\}$ constitutes a CONS.

These facts show that the minimum eigenvalue λ of L_0 specifies the irreducible unitary representation uniquely in case 1. Especially, in case 1, the irreducible unitary representation of the Lie group SU(1,1), which is not a universal covering group, can be constructed if and only if λ is a positive integer.

For the normalization of v_n, we define

$$|n\rangle_N := \sqrt{\frac{\Gamma(\lambda)}{n!\Gamma(\lambda+n)}}v_n, \quad N := \frac{1}{2}(L_0-\lambda).$$

Then we have

$$N|n\rangle_N = n|n\rangle_N,$$

hence N and $|n\rangle_N$ are regarded as the number operator and the number state, respectively.

Next, we define $a := L_+^{-1}N = \frac{1}{2}L_+^{-1}(L_0-\lambda)$, where the well-definedness is guaranteed because $\mathrm{Ran}\,L_+$ is included in $\mathrm{Ran}\,N$. Then, we have

$$a|n\rangle_N = \sqrt{\frac{n}{n+\lambda-1}}|n-1\rangle_N,$$

and similarly we have

$$a^*|n\rangle_N = \sqrt{\frac{n+1}{n+\lambda}}|n+1\rangle_N.$$

Moreover, we have the following relations;

$$a^*a = (N+(\lambda-1)I)^{-1}N,$$

$$aa^* = (N+\lambda I)^{-1}(N+I),$$

$$[a,a^*] = (\lambda-1)(N+(\lambda-1)I)^{-1}(N+\lambda I)^{-1},$$

$$[a,N] = a,$$

$$[N,a^*] = a^*.$$

Thus, with the correspondence $\lambda = 2k+1$, we have made a systematic derivation of the same type of the relations as the relations introduced at the end of Sec. II, in terms of the irreducible unitary representation of the algebra $\mathfrak{su}(1,1)$.

Next we will introduce the coherent states. According to Perelomov,[7] define the coherent state associated with SU(1,1) by

$$\begin{aligned}|\zeta\rangle_a &:= U\left(\frac{1}{2}e^{i\arg\zeta}\ln\frac{1+|\zeta|}{1-|\zeta|}\right)|0\rangle_N \\ &= \exp(\zeta L_+)\exp\left(\frac{1}{2}\ln(1-|\zeta|^2)L_0\right)\exp(\zeta^* L_-)|0\rangle_N \\ &= (1-|\zeta|^2)^{\lambda/2}\exp(\zeta L_+)|0\rangle_N\end{aligned}$$

with

$$U(\xi) := \exp(\xi L_+ - \xi^* L_+^*).$$

Then, from the commutation relation $[a,\exp(\zeta L_+)]=\zeta\exp(\zeta L_+)$ which is derived from $[a,L_+]=I$, and by using the relation $\exp(\frac{1}{2}\ln(1-|\zeta|^2)L_0)\exp(\zeta^* L_-)|0\rangle_N=(1-|\zeta|^2)^{\lambda/2}|0\rangle_N$, we have

$$a|\zeta\rangle_a=\exp(\zeta L_+)a|0\rangle_N+\zeta\exp(\zeta L_+)|0\rangle_N=\zeta|\zeta\rangle_a.$$

This shows that the operator a has the other property of the annihilation operator—the property that it has the coherent states as its eigenvectors.

Thus, the annihilation–creation relations and their relation to the coherent states have been defined naturally from the context of the irreducible unitary representation of the algebra $\mathfrak{su}(1,1)$. In our framework, we have not used L_- as the annihilation operator but we have used $a=L_+^{-1}N$, because L_- does not have the coherent states as the eigenvectors.

Note that the above-mentioned operator a approaches the boson annihilation operator as λ tends to infinity, in the following sense. Let $U_\lambda:\mathcal{H}\to L^2(\mathbb{R})$ be the unitary map such that $U_\lambda(|n\rangle_N)=|n\rangle_{\text{boson}}$. Then, we can show that $U_\lambda a U_\lambda^*$ converges to the boson annihilation operator in the sense of the weak convergence as λ tends to infinity.

IV. CONCRETE REPRESENTATION OF $\mathfrak{su}(1,1)$ CORRESPONDING TO DISCUSSIONS FOR AFFINE GROUP GIVEN IN SEC. II

In this section, we will discuss what concrete representation explains the correspondence between the framework given in Sec. III in terms of the irreducible unitary representation and the heuristic discussions for the affine group given in Sec. III.

On $L^2(\mathbb{R}^+)$, we choose two generators of $\mathfrak{su}(1,1)$ from two generators of affine group as:

$$E_0=i(PQ+QP),\quad E_+=iQ.$$

Adding the other generator,

$$E_-:=-i(PQP+k^2Q^{-1})$$

formally, we construct a representation of $\mathfrak{su}(1,1)$ from a representation of affine group. [Conversely, choosing two generators E_0 and E_+, we can construct a representation of affine group from a representation of $\mathfrak{su}(1,1)$.]

In the following, the discussion for the affine group given in Sec. II is directly derived from the general framework given in Sec. III. However, especially in the cases where $-1/2<k<1/2$, we should be careful about the domain of the operator E_-, as will be shown.

First, define the operator

$$\tilde{E}_{-,k}:=-i(PQP+k^2Q^{-1})\quad(k>-1/2)$$

on the dense subspace $\mathcal{D}_0(\tilde{E}_{-,k})$ of $L^2(\mathbb{R}^+)$ defined by

$$\mathcal{D}_0(\tilde{E}_{-,k}):=\left\{\begin{array}{c|c} f(x)=x^k f_0(x) & (2k+1)x^k f_0'(x)+x^{k+1}f_0''(x)\in L^2(\mathbb{R}^+), \\ \in L^2(\mathbb{R}^+)\cap C^1(\mathbb{R}^+) & \limsup_{s\to 0} f_0(s)<\infty, \\ & x^k f_0(x)\to 0 \ \text{ as } \ x\to\infty \end{array}\right\}.$$

Then, it is confirmed that the operator $i\tilde{E}_{-,k}=PQP+k^2Q^{-1}$ is a symmetric operator on $\mathcal{D}_0(\tilde{E}_{-,k})$ from the fact that the difference

$$\int_s^t ((PQP+k^2Q^{-1})f)^*(x)g(x)\,dx-\int_s^t (f(x))^*((PQP+k^2Q^{-1})g)(x)\,dx$$
$$=[x(f'(x))^*g(x)-xg'(x)(f(x))^*]_s^t$$
$$=t(f'(t))^*g(t)-tg'(t)(f(t))^*-\left(sg(s)\left((f'(s))^*-\frac{k}{s}(f(s))^*\right)\right.$$
$$\left.-s(f(s))^*\left(g'(s)-\frac{k}{s}g(s)\right)\right)$$
$$=t(f'(t))^*g(t)-tg'(t)(f(t))^*-(sg(s)s^k(f_0'(s))^*-s(f(s))^*s^kg_0'(s))$$

tends to zero as $s\to 0, t\to\infty$. Moreover, we can show that $\mathcal{D}_0(\tilde{E}_{-,k}^*)\cap C^2(\mathbb{R}^+)=\mathcal{D}_0(\tilde{E}_{-,k})$. Therefore, $\tilde{E}_{-,k}$ is a closable operator and $iE_{-,k}:=i\overline{\tilde{E}_{-,k}}$ is a self-adjoint operator. Hence, we can show that $\tilde{E}_{-,k}$ is a closable operator and the operator $iE_{-,k}:=i\overline{\tilde{E}_{-,k}}$ is a self-adjoint operator. Note that the operator $E_{-,k}$ is quite different from $E_{-,-k}$.

By letting $L_{+,k}, L_{-,k}, L_{0,k}, \tilde{A}_k, N_k$ be $L_+, L_-, L_0, \tilde{A}, N$, $|n\rangle_N$, respectively, with $\tilde{A}:=-i(a+I)(a-I)^{-1}$ defined on the vector space whose elements are finite linear sums of $\{|n\rangle_N\}_{n=0}^{\infty}$, we have

$$L_{+,k}=\tfrac{1}{2}(i(PQ+QP)-Q+PQP+k^2Q^{-1}),$$
$$L_{-,k}=\tfrac{1}{2}(i(PQ+QP)+Q-PQP-k^2Q^{-1}),$$
$$L_{0,k}=(PQP+k^2Q^{-1}+Q),\quad A_k=P+ikQ^{-1},$$
$$N_k=\tfrac{1}{2}(PQP+k^2Q^{-1}+Q-1-2k).$$

In this representation, the minimum eigenvalue of $L_{0,k}$ is $\lambda=2k+1$. Moreover, the number state $|n\rangle_N^k$ is shown to be the $\mathfrak{su}(1,1)$-number state $|n\rangle_N$.

The domain of the adjoint operator $\tilde{A}_k$ is given by

$$\mathcal{D}_0(\tilde{A}_k^*)\cap C^1(\mathbb{R}^+)=\left\{x^{-k}f(x)\in L^2(\mathbb{R}^+)\cap C^1(\mathbb{R}^+)\,\middle|\,\begin{matrix}x^{-k}f'(x)\in L^2(\mathbb{R}^+)\\ f(s)\to 0\ \text{ as }\ s\to 0,\end{matrix}\right\},\tag{9}$$

which implies that $\mathcal{D}_0(\tilde{A}_k^*)$ is dense in $L^2(\mathbb{R}^+)$. Thus $\tilde{A}_k$ is shown to be a closable operator. Since $A_k=\overline{\tilde{A}_k}$, the relation

$$\mathcal{D}_0(A_k)\cap C^1(\mathbb{R}^+)=\left\{x^kf(x)\in L^2(\mathbb{R}^+)\cap C^1(\mathbb{R}^+)\,\middle|\,\begin{matrix}x^kf'(x)\in L^2(\mathbb{R}^+),\\ \limsup_{s\to 0} f(s)<\infty\end{matrix}\right\}.\tag{10}$$

is confirmed. Note that $\overline{X}=X^{**}$ and $X^*=\overline{X}^*$ hold for a densely defined linear operator X, and that $\limsup_{x\to\infty} f_0(x)=0$ for $k>-\frac{1}{2}$ when $x^kf_0(x)\in L^2(\mathbb{R}^+)$. From (10), we can show that $|\zeta\rangle^k$ belongs to $\mathcal{D}_0(A_k)$ and coincides with the $\mathfrak{su}(1,1)$-coherent state $|-i(\zeta+1)/(\zeta-1)\rangle_a$. Thus, the whole discussion given in Sec. II has been justified and reinterpreted in terms of the irreducible unitary representations of the algebra $\mathfrak{su}(1,1)$.

In the following, we discuss the properties of A_k and A_k^*, more deeply. The subspaces $\mathcal{D}_0(A_k^*)\cap C^1(\mathbb{R}^+)$ and $\mathcal{D}_0(A_k)\cap C^1(\mathbb{R}^+)$ are the cores of A_k^* and A_k.[8] When $-\frac{1}{2}<k<\frac{1}{2}$, the domain of A_k is larger than the domain of A_{-k}^*, though A_k and A_{-k}^* are the same formally, i.e., $A_{-k}^*\subset_{\neq}A_k$. In the special case where $\lambda=1$ (i.e., where $k=0$), A_0^* is symmetric. Since $A_0=A_0^{**}$ has no spectrum in the lower half plane, A_0^*'s deficiency indices are (1,0). (For the definition of deficiency indices, see p. 138 of Reed and Simon[9] or p. 360 of Rudin.[10]) Therefore,

the operator A_0^* is a maximal symmetric operator. These relations $\mathcal{D}_0(A_k^*)\subset\mathcal{D}_0(A_k)$ and $\mathcal{D}_0(A_k^*)\subset\mathcal{D}_0(E_+^{-1})$ are shown in the cases where $\lambda<1(k>0)$, only the relation $\mathcal{D}_0(A_k^*)\subset\mathcal{D}_0(A_k)$ is shown when $\lambda=1(k=0)$, and these relations $\mathcal{D}_0(A_k)\subset\mathcal{D}_0(A_k^*)$ and $\mathcal{D}_0(A_k)\subset\mathcal{D}_0(E_+^{-1})$ are shown when $0<\lambda<1(-\frac{1}{2}<k<0)$.

As another representation of $\mathfrak{su}(1,1)$ on $L^2(\mathbb{R})$, the Holstein–Primakoff representation is known as[11,12]

$$L_0 := Q^2+P^2+2k-2,$$

$$L_+ := \frac{1}{\sqrt{2}}(Q-iP)\sqrt{\frac{1}{2}(Q^2+P^2)+2k-\frac{3}{2}},$$

$$L_+ := \frac{1}{\sqrt{2}}\sqrt{\frac{1}{2}(Q^2+P^2)+2k-\frac{3}{2}}(Q+iP).$$

This representation is algebraicly equivalent with our representation. However, it has a completely different form from our representation.

V. CONCLUSION

We have derived a kind of annihilation/creation relation similar to the boson annihilation/creation relation, from the irreducible unitary representation of the algebra $\mathfrak{su}(1,1)$. The proposed framework contains an annihilation/creation relation related to the affine coherent states as a special case. In signal processing, in a similar manner to the boson-annihilation/creation relation which is applied to the operator method in Wiener–Hermite expansion of Gaussian stochastic processes, our results may be applied to an analogous operator method for the stochastic processes related to the χ^2-distribution and the wavelets, because the affine coherent states are closely related to them. This discussion can be treated from another viewpoint[13,14]

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The Bargmann transform and canonical transformations[a)]

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This paper concerns a relationship between the kernel of the Bargmann transform and the corresponding canonical transformation. We study this fact for a Bargmann transform introduced by Thomas and Wassell [J. Math. Phys. **36**, 5480–5505 (1995)]—when the configuration space is the two-sphere S^2 and for a Bargmann transform that we introduce for the three-sphere S^3. It is shown that the kernel of the Bargmann transform is a power series in a function which is a generating function of the corresponding canonical transformation (a classical analog of the Bargmann transform). We show in each case that our canonical transformation is a composition of two other canonical transformations involving the complex null quadric in $\mathbf{C}^3$ or $\mathbf{C}^4$. We also describe quantizations of those two other canonical transformations by dealing with spaces of holomorphic functions on the aforementioned null quadrics. Some of these quantizations have been studied by Bargmann and Todorov [J. Math. Phys. **18**, 1141–1148 (1977)] and the other quantizations are related to the work of Guillemin [Integ. Eq. Operator Theory **7**, 145–205 (1984)]. Since suitable infinite linear combinations of powers of the generating functions are coherent states for $L^2(S^2)$ or $L^2(S^3)$, we show finally that the studied Bargmann transforms are actually coherent states transforms. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1468254]

I. INTRODUCTION

Bargmann[1] introduced the so-called Bargmann transform as a unitary transformation from $L^2(\mathbf{R}^n)$ onto a space $\mathcal{B}_n$ of analytic functions (of n complex variables) which are square integrable with respect to a Gaussian measure. The Bargmann transform is defined as the integral operator

$$\mathbf{B}_{\mathbf{R}^n}\Psi(\mathbf{z}) \equiv \frac{1}{\pi^{n/4}} \int_{\mathbf{R}^n} \exp\left(-\frac{1}{2}(\mathbf{z}^2+\mathbf{x}^2) + \sqrt{2}\mathbf{z}\cdot\mathbf{x} \right) \Psi(\mathbf{x}) d\mathbf{x} \tag{1.1}$$

(see Sec. I for notation). The Bargmann transform is also called the ''Segal–Bargmann transform.'' (See Ref. 2 for a historical remark about Bargmann and Segal's work on this transform. Segal[3] studied the infinite dimensional case $n=\infty$.)

The Bargmann space $\mathcal{B}_n$ provides a very adequate framework to represent and study the n-dimensional quantum harmonic oscillator (i.e., the addition of n one-dimensional harmonic oscillators with the same frequency). It is known[4] that the Hamiltonian of such an oscillator can be written as

$$\hat{H} = \sum_{j=1}^{n} a_j^\dagger a_j, \tag{1.2}$$

where $a_j^\dagger$ and a_j, $j=1,2,\ldots,n$ are creation and annihilation operators given by

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$$a_j^\dagger = \frac{1}{\sqrt{2}}(\hat{q}_j - \imath\hat{p}_j) = \frac{1}{\sqrt{2}}\left(q_j - \frac{\partial}{\partial q_j}\right),$$
$$a_j = \frac{1}{\sqrt{2}}(\hat{q}_j + \imath\hat{p}_j) = \frac{1}{\sqrt{2}}\left(q_j + \frac{\partial}{\partial q_j}\right), \tag{1.3}$$

with $\widehat{q_j}$ the operator of multiplication by the coordinate q_j and $\hat{p}_j = -\imath(\partial/\partial q_j)$.

The operators corresponding to $a_j^\dagger$, a_j, and $\hat{H}$ in the Bargmann space $\mathcal{B}_n$ are multiplication by the complex variable z_j, partial derivative with respect to z_j and $\Sigma_{j=1}^n z_j(\partial/\partial z_j)$, respectively. In particular, the spectrum of the n-dimensional quantum harmonic oscillator is easy to compute because in the Bargmann representation the monomials $z_1^{a_1}z_2^{a_2}\cdots z_n^{a_n}$ (with a_j, $j=1,2,\ldots,n$, nonnegative integers) are the eigenfunctions of the operator $\Sigma_{j=1}^n z_j\,\partial/\partial z_j)$.

From the viewpoint of classical mechanics, the problem of an n-dimensional harmonic oscillator can be studied in the phase space $\mathbf{R}^{2n}=\{(\mathbf{q},\mathbf{p})|\mathbf{q},\mathbf{p}\in\mathbf{R}^n\}$ with symplectic form $\omega_n = \Sigma_{j=1}^n \mathrm{d}q_j\wedge\mathrm{d}p_j$ and Hamiltonian

$$H = \frac{1}{2}\sum_{j=1}^n p_j^2 + q_j^2. \tag{1.4}$$

It is known[4] that this problem can also be described by introducing complex variables $z_j = (1/\sqrt{2})(q_j - \imath p_j)$, $j=1,2,\ldots,n$. In these complex variables, the Hamiltonian H is given by $\Sigma_{j=1}^n z_j\overline{z_j}$. This is the classical analog of Eq. (1.2).

A remarkable and fundamental idea for this paper is the following: as in Ref. 5, let us consider the exponent of the kernel of the Bargmann transform in Eq. (1.1),

$$\Phi_n(\mathbf{q},\mathbf{z}) \equiv -\imath(-\tfrac{1}{2}(\mathbf{z}^2+\mathbf{q}^2) + \sqrt{2}\mathbf{z}\cdot\mathbf{q}). \tag{1.5}$$

It turns out that the function $\Phi_n(\mathbf{q},\mathbf{z})$ *is a generating function of a canonical transformation (symplectomorphism) from the phase space* $(\mathbf{R}^{2n},\omega_n)$ *onto the phase space* $(\mathbf{C}^n,\mu_n)$, *where* μ_n *is the symplectic form* $\mu_n = -\imath\Sigma_{j=1}^n \mathrm{d}z_j\wedge\mathrm{d}\overline{z_j}$ (see Sec. III for details). Thus we shall say that $\mathcal{C}_n$ is the classical analog of the Bargmann transform (or that $\mathbf{B}_{\mathbf{R}^n}$ is the quantization of $\mathcal{C}_n$) in the sense that $\mathbf{B}_{\mathbf{R}^n}$ is a unitary transformation between the Hilbert spaces $L^2(\mathbf{R}^n)$ and $\mathcal{B}_n$, and $\mathcal{C}_n$ is a diffeomorphism between the phase spaces $(\mathbf{R}^{2n},\omega_n)$ and $(\mathbf{C}^n,\mu_n)$.

This paper concerns the same relationship between the Bargmann transform and a corresponding canonical transformation when the configuration space $\mathbf{R}^n$ is replaced by the two-sphere S^2 or the three sphere S^3 (here we mean by S^n the set of unit vectors in $\mathbf{R}^{n+1}$). For the S^2 case, Thomas and Wassell[6] introduced a Bargmann transform from $L^2(S^2)$ onto a proper subspace of $\mathcal{B}_2$. For the S^3 case, a Bargmann transform was introduced by Villegas-Blas.[7] This last transform goes from $L^2(S^3)$ onto a proper subspace of $\mathcal{B}_4$ determined by the kernel of an operator which carries the restriction in quantum mechanics of the classical fact that the angular momentum and Runge–Lenz vectors should be orthogonal for the Kepler problem. We show in both cases—S^2 and S^3—that the kernel of the Bargmann transform is a power series in a function which plays the role of a generating function of a canonical transformation which in turn is the classical analog of the Bargmann transform.

In Sec. II, we describe the Bargmann transform for the three cases $\mathbf{R}^n$, S^2, and S^3. The mentioned relationship between the Bargmann transform and corresponding canonical transformations is established in Sec. III. For the S^2 and S^3 cases we do this by using spherical coordinates (a local chart). In order to define and extend our canonical transformations to the whole spaces $T^*S^2-\{0\}$ and $T^*S^3-\{0\}$ (we need to remove the zero section in both cases to avoid singularities) we use a key property of the generating functions, namely that these functions can be written as the inner product of the position vector $\mathbf{x}$ (in S^2 or S^3) and a complex vector in the null quadric

$\mathbf{Q}^2$ (for the S^2 case) and $\mathbf{Q}^3$ (for the S^3 case). Here, for n a positive integer, the null quadric $\mathbf{Q}^n$ is the set of vectors in $\mathbf{C}^{n+1}$ such that the addition of the square of their components is zero. Note that a vector in $\mathbf{C}^{n+1}$ belongs to $\mathbf{Q}^n$ if and only if the norm of its real and imaginary parts is the same and these two vectors are orthogonal to one another. Thus $\mathbf{Q}^2-\{0\}$ and $\mathbf{Q}^3-\{0\}$ can be identified with $T^*S^2-\{0\}$ and $T^*S^3-\{0\}$, respectively.

Thus we are able to extend our canonical transformation as the inverse of a composition of two maps. For the S^2 case, one map $\rho_2(\mathbf{z})$ goes from $\tilde{\mathbf{C}}^2-\{0\}$ [that is $\mathbf{C}^2$ minus the origin and (z_1,z_2) identified with $(-z_1,-z_2)$] onto $\mathbf{Q}^2-\{0\}$ and the other one, σ_2, goes from $\mathbf{Q}^2-\{0\}$ onto $T^*S^2-\{0\}$. These maps are symplectomorphisms with T^*S^2 endowed with the restriction of the canonical symplectic form of the ambient $T^*\mathbf{R}^3$, and $\mathbf{Q}^2-\{0\}$ endowed with the symplectic form given by the pull-back of the symplectic form on T^*S^2 under the map σ_2. We remark here that the symplectic form on $\mathbf{Q}^2-\{0\}$ is not the restriction of the canonical symplectic form for the ambient $\mathbf{C}^3$. For the S^3 case, we have a similar extension, but instead of $\tilde{\mathbf{C}}^2-\{0\}$, we have a six real-dimensional phase space $\tilde{\mathbf{C}}^4-\{0\}$ which is a quotient of a submanifold of $\mathbf{C}^4$ and determined by reduction. Thus in this second case we extend our canonical transformation by considering the inverse of the composition of two maps ρ_3 (from $\tilde{\mathbf{C}}^4-\{0\}$ onto $\mathbf{Q}^3-\{0\}$) and σ_3 (from $\mathbf{Q}^3-\{0\}$ onto $T^*S^3-\{0\}$).

Once we have, for each case S^2 or S^3, the symplectomorphisms between the three phase spaces, a natural question is to ask for a description of their corresponding quantizations. This is the goal of Section IV. Bargmann and Todorov[8] have already considered the quantizations of ρ_2 and ρ_3 by introducing Hilbert spaces of holomorphic functions on the null quadrics $\mathbf{Q}^2$ and $\mathbf{Q}^3$, respectively. However, we include a brief description of such quantizations for completeness and to introduce some notation. Our procedure differs from the one followed by Bargmann and Todorov in the way the measure on the null quadric is introduced. We also include in Sec. IV a discussion on the relation between our quantizations of σ_2 and σ_3 and work of Guillemin.[9]

The fact that our generating functions for the S^2 and S^3 cases are inner products of position vectors and vectors in the null quadric has another important implication. The Bargmann transforms described in Sec. II for S^2 and S^3 are *coherent states transforms*. That is, they can be written as inner products with coherent states. This is in analogy with the Bargmann transform $\mathbf{B}_{\mathbf{R}^n}$, which acting on a function is the inner product of the function and a coherent state of the n-dimensional harmonic oscillator. The coherent states appearing here are infinite linear combinations of integer powers of our generating functions. The latter functions are known in the literature (see Ref. 10) and sometimes they are called coherent states as well. We prefer to call them great-circle states because they concentrate on great circles of S^2 or S^3 in the semiclassical regime. The great-circle states give a resolution of the identity for each eigenspace of the spherical Laplacian on S^2 or S^3, respectively [these eigenspaces are irreducible representations of the groups SO(3) or SO(4)]. As a consequence, we also obtain a resolution of the identity for $L^2(S^2)$ and $L^2(S^3)$ through our coherent states.

Section V is devoted to the describing the Bargmann transforms as coherent states transforms. In this Section we also show how the great-circle states help us to obtain reproducing kernels for the range of our Bargmann transforms for both the $\mathcal{S}^2$ and $\mathcal{S}^3$ cases. We also show reproducing kernels for spaces of holomorphic functions on the null quadrics $\mathbf{Q}^2$ and $\mathbf{Q}^3$ related with the range and domain of the quantizations described in Sec. IV.

There are other Bargmann-type transforms introduced by Rawnsley[11] (for the n-sphere), Ii[12] and Wada[13] (for the n-sphere), Hall[2,14,15] (for compact Lie groups), Stenzel[16] (for symmetric spaces of compact type), Kowalski and Rembieliński[17,18] (for the two-sphere), and Hall and Mitchell[19] (for the n-sphere); but they are different from the transformations introduced in this paper. We devote Sec. VI to briefly describe these Bargmann-type transformations.

We also include two appendices to prove that the kernel of the Bargmann transforms for both spheres $\mathcal{S}^2$ and $\mathcal{S}^3$ is a power series in a certain function.

We finally remark that the case of the three-sphere is physically relevant in both quantum and classical mechanics. The symmetries of the bound states of the hydrogen atom are given by the

Lie algebra of the group SO(4) (see Refs. 7 and 20). In this way we can explain the degeneracy of the negative energies for the hydrogen atom. In classical mechanics, Moser[21] showed that the Hamiltonian flow for the Kepler problem (with negative energy) is equivalent, after a time reparametrization, to the geodesic flow on S^3. In this way, Moser is able to regularize the motion of the Kepler problem.

II. BARGMANN TRANSFORM FOR $L^2(S^2)$ AND $L^2(S^3)$

The purpose of this section is to describe both the Bargmann transform for $L^2(S^2)$ (introduced by Thomas and Wassell[6]) and $L^2(S^3)$ (introduced by Villegas-Blas[7]). In both cases we need the usual Bargmann spaces introduced by Bargmann[1] in his transform for $L^2(\mathbf{R}^n)$. To that end, and as a reference for the following sections, we begin by reviewing these spaces and their Bargmann transforms.

A. Bargmann transform for $L^2(\mathbf{R}^n)$

In this section we review important properties of the Bargmann transform that are needed for later sections of this paper. For a detailed explanation and proofs see Refs. 1 and 2.

The Bargmann space $\mathcal{B}_n$ is the space of analytic functions of n complex variables $\mathbf{z}=(z_1,z_2,\ldots,z_n)$ which are square integrable with respect to the Gaussian measure

$$d\nu_n(\mathbf{z})=\frac{1}{\pi^n}\exp(-|\mathbf{z}|^2)\prod_{j=1}^{n} dx_j\,dy_j, \tag{2.1}$$

where $|\mathbf{z}|^2=|z_1|^2+|z_2|^2+\cdots+|z_n|^2$ and $z_j=x_j+\imath y_j$, x_j, $y_j\in\mathbf{R}$, with $j=1,2,\ldots,n$.

The space $\mathcal{B}_n$ is a Hilbert space with inner product

$$\langle F,G\rangle_{\mathcal{B}_n}=\int_{\mathbf{C}^n} F(\mathbf{z})\overline{G}(\mathbf{z})d\nu_n(\mathbf{z}). \tag{2.2}$$

The set of all monomials $(z_1^{a_1}z_2^{a_2}\cdots z_n^{a_n})/(\sqrt{a_1!a_2!\cdots a_n!})$, with $a_1,a_2,\ldots,a_n$ non-negative integers, is an orthonormal basis of $\mathcal{B}_n$.

The coherent states in $\mathcal{B}_n$,

$$\Psi_{\mathbf{a}}(\mathbf{z})=\exp(\overline{\mathbf{a}}\mathbf{z}) \quad \text{with} \quad \mathbf{a}\in\mathbf{C}^n, \tag{2.3}$$

provide a reproducing kernel for the space $\mathcal{B}_n$. That is, for $\Phi\in\mathcal{B}_n$,

$$\Phi(\mathbf{z})=\langle\Phi,\Psi_{\mathbf{z}}\rangle_{\mathcal{B}_n}=\int_{\mathbf{C}^n}\exp(\mathbf{z}\overline{\mathbf{w}})\Phi(\mathbf{w})d\nu_n(\mathbf{w}). \tag{2.4}$$

The Bargmann transform for $L^2(\mathbf{R}^n)$ is defined as the operator $\mathbf{B}_{\mathbf{R}^n}:L^2(\mathbf{R}^n)\mapsto\mathcal{B}_n$ given by

$$\mathbf{B}_{\mathbf{R}^n}\Psi(\mathbf{z})=\frac{1}{\pi^{n/4}}\int_{\mathbf{R}^n}A(\mathbf{x},\mathbf{z})\Psi(\mathbf{x})d\mathbf{x}, \quad \Psi\in L^2(\mathbf{R}^n), \tag{2.5}$$

where $d\mathbf{x}$ is the usual Lebesgue measure on $\mathbf{R}^n$ and

$$A(\mathbf{x},\mathbf{z})=\exp(-\tfrac{1}{2}(\mathbf{z}^2+\mathbf{x}^2)+\sqrt{2}\mathbf{z}\cdot\mathbf{x}), \tag{2.6}$$

with $\mathbf{z}^2=z_1^2+z_2^2+\cdots+z_n^2$, $\mathbf{x}=(x_1,x_2,\ldots,x_n)$, $\mathbf{x}^2=x_1^2+x_2^2+\cdots+x_n^2$, and $\mathbf{z}\cdot\mathbf{x}=z_1x_1+z_2x_2+\cdots+z_nx_n$. The Bargmann transform $\mathbf{B}_{\mathbf{R}^n}$ is a unitary operator [with $L^2(\mathbf{R}^n)$ endowed with the usual inner product].

The inverse $\mathbf{B}_{\mathbf{R}^n}^{-1}$ is given by

$$\mathbf{B}_{\mathbf{R}^n}^{-1} f(\mathbf{x}) = \lim_{M \mapsto \infty} \int_{|\mathbf{z}| \leqslant M} \overline{A(\mathbf{x},\mathbf{z})} f(\mathbf{z}) \mathrm{d}\nu_n(\mathbf{z}). \tag{2.7}$$

Here we need to take the limit because the integral over all the space $\mathbf{C}^n$ might not exist [note that, for fixed $\mathbf{x}$, $A(\mathbf{x},\mathbf{z}) \notin \mathcal{B}_n$].

B. Bargmann transform for $L^2(S^2)$

Let us first define the space $L^2(S^n)$ for a given integer n. Let $\mathrm{d}\sigma_n$ be the usual normalized Lebesgue surface measure on S^n. Let us define $L^2(S^n)$ as the space of Lebesgue measurable functions on S^n which are square integrable with respect to the measure $\mathrm{d}\sigma_n$.

The space $L^2(S^n)$ is a Hilbert space with inner product

$$\langle F,G \rangle_{S^n} = \int_{S^n} F(\mathbf{x}) \overline{G}(\mathbf{x}) \mathrm{d}\sigma_n(\mathbf{x}). \tag{2.8}$$

In order to define the Bargmann transform for $L^2(S^2)$, we first remind the reader of some well-known facts about two different representations of the SO(3) group of rotations of the space $\mathbf{R}^3$.

Let us consider the Laplacian operator on the two-sphere S^2 denoted by Δ_{S^2}. We will actually consider the normalized Laplacian operator with spectrum the set $\{(\ell+1/2)^2 | \ell = 0,1,2...\}$.

Let $0 < \theta < \pi$, $0 \leqslant \phi \leqslant 2\pi$ be spherical coordinates on S^2:

$$x_1 = \sin(\theta)\cos(\phi), \quad x_2 = \sin(\theta)\sin(\phi), \quad x_3 = \cos(\theta). \tag{2.9}$$

The expression for the Laplacian on S^2 in spherical coordinates is

$$\Delta_{S^2} = -\frac{1}{\sin(\theta)} \frac{\partial}{\partial\theta} \sin(\theta) \frac{\partial}{\partial\theta} - \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial\phi^2} + \frac{1}{4}. \tag{2.10}$$

The Laplacian Δ_{S^2} is in turn related to the addition of the square of the generators L_j of rotations in $\mathbf{R}^3$ around the plane perpendicular to the axis x_j for $j = 1,2,3$:

$$\Delta_{S^2} = L_1^2 + L_2^2 + L_3^2 + 1/4, \tag{2.11}$$

where

$$L_1 = \iota \sin(\phi) \frac{\partial}{\partial\theta} + \iota \cot(\theta)\cos(\phi) \frac{\partial}{\partial\phi},$$

$$L_2 = -\iota \cos(\phi) \frac{\partial}{\partial\theta} + \iota \cot(\theta)\sin(\phi) \frac{\partial}{\partial\phi}, \tag{2.12}$$

$$L_3 = -\iota \frac{\partial}{\partial\phi}.$$

The operators L_j act on a dense subspace of $L^2(S^2)$ and provide a representation for the Lie algebra $so(3)$ of SO(3). They also satisfy the commutation relations

$$[L_i, L_j] = \iota \epsilon_{ijk} L_k, \quad i,j,k = 1,2,3, \tag{2.13}$$

where $\{i,j,k\}$ is a permutation of $\{1,2,3\}$. If this permutation is even (odd) then $\epsilon_{ijk} = 1$ ($\epsilon_{ijk} = -1$).

It is known that the eigenfunctions of the Laplacian Δ_{S^2} provide a basis for $L^2(S^2)$. Moreover, $L^2(S^2)$ is the direct sum of the eigenspaces of the Laplacian. For each $\ell=0,1,2...$, we shall denote by V_ℓ the eigenspace of the Laplacian Δ_{S^2} associated with the eigenvalue $(\ell+1/2)^2$.

The group SO(3) acts on $L^2(S^2)$ as follows. Given $R\in \mathrm{SO}(3)$, we define $T_R: L^2(S^2)\mapsto L^2(S^2)$ by

$$T_R\Psi(\mathbf{x})=\Psi(R^{-1}\mathbf{x}), \quad \mathbf{x}\in S^2. \tag{2.14}$$

A particular and important basis of $L^2(S^2)$ is obtained by taking common normalized eigenfunctions of both operators Δ_{S^2} and L_3 (these two operators commute). These functions are known as ''spherical harmonics'' and we shall denote them by

$$Y_{\ell m} \quad \text{with } \ell=0,1,2... \text{ and } m=-\ell,-\ell+1,\ldots,\ell. \tag{2.15}$$

Moreover, if, for each $\ell=0,1,2,\ldots$, we let the group $\{T_R|R\in \mathrm{SO}(3)\}$ act on the space

$$V_\ell=\mathrm{span}\{Y_{\ell m}|m=-\ell,-\ell+1,\ldots,\ell\}, \tag{2.16}$$

then we obtain all the irreducible representations of SO(3).

On the other hand, we can obtain irreducible representations for SO(3) on the basis of the knowledge of irreducible representations of SU(2) (the group of two by two unitary matrices with complex entries and determinant one). An important representation of the SU(2) group is obtained by letting this group act on the Bargmann space $\mathcal{B}_2$ of analytic functions in two complex variables $\mathbf{z}=(z_1,z_2)$ in a similar way as we made the SO(3) group act on $L^2(S^2)$.

Let us denote by $\mathbf{S}$ the set of all numbers of the form $p/2$ with p a non-negative integer. For $s\in\mathbf{S}$, let us also denote by $\mathcal{W}_s$ the subspace of $\mathcal{B}_2$ of homogeneous polynomials in two complex variables (z_1,z_2) of degree $2s$. An orthonormal basis for $\mathcal{W}_s$ is given by the monomials

$$y_{sm}=\frac{z_1^{s+m}z_2^{s-m}}{\sqrt{(s+m)!(s-m)!}} \tag{2.17}$$

with $m=-s,-s+1,\ldots,s-1,s$.

When we restrict the action of SU(2) to the spaces $\mathcal{W}_s$, we get all of the irreducible representations of SU(2). In particular, when we take $s=\ell$ a non-negative integer, we obtain all of the irreducible representations of SO(3).

In order to define a Bargmann transform for $L^2(S^2)$, the above-given description of two types of irreducible representations of SO(3) suggests defining the following assignment:

$$Y_{\ell m}\mapsto y_{\ell m} \quad \text{for all } \ell=0,1,2,\ldots \text{ and } m=-\ell,-\ell+1,\ldots,\ell. \tag{2.18}$$

Thus we define the Bargmann transform $\mathbf{B}_{S^2}$ for $L^2(S^2)$ as the linear extension of this assignment. Notice that $\mathbf{B}_{S^2}$ is a unitary operator from $L^2(S^2)$ onto the closed subspace $\mathcal{B}_{S^2}$ of $\mathcal{B}_2$ generated by the monomials with even degree, that is $\mathcal{B}_{S^2}=\oplus\mathcal{W}_\ell$ (where the direct sum is taken over all non-negative integers).

The Bargmann transform $\mathbf{B}_{S^2}$ can be written as an integral operator

$$\mathbf{B}_{S^2}\Psi(\mathbf{z})=\int_{\mathbf{x}\in S^2}K_{S^2}(\mathbf{x},\mathbf{z})\Psi(\mathbf{x})\mathrm{d}\sigma_2(\mathbf{x}), \tag{2.19}$$

with kernel

$$K_{S^2}(\mathbf{x},\mathbf{z})=\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{m=\ell}\overline{Y}_{\ell m}(\mathbf{x})y_{\ell m}(\mathbf{z}). \tag{2.20}$$

This kernel has the property of being a power series in the function

$$\Phi_{S^2}(\mathbf{x},\mathbf{z})=\sum_{m=-1}^{m=1}\overline{Y}_{1m}(\mathbf{x})y_{1m}(\mathbf{z}) \tag{2.21}$$

in the following way:

$$K_{S^2}(\mathbf{x},\mathbf{z})=\sum_{\ell=0}^{\infty}\frac{\sqrt{2\ell+1}}{\ell!}\left(\frac{1}{\sqrt{3}}\right)^{\ell}(\Phi_{S^2}(\mathbf{x},\mathbf{z}))^{\ell}, \tag{2.22}$$

with the following explicit expression for $\Phi_{S^2}(\mathbf{x},\mathbf{z})$:

$$\Phi_{S^2}(\mathbf{x},\mathbf{z})=(\sqrt{3}/2)\,(-\sin(\theta)\exp(-\imath\phi)z_1^2+2\cos(\theta)z_1z_2+\sin(\theta)\exp(\imath\phi)z_2^2). \tag{2.23}$$

We give a proof of this fact in Appendix A.

The Bargmann transform $\mathbf{B}_{S^2}$ intertwines L_1,L_2,L_3,Δ_S^2 with the following operators:

$$\begin{aligned}
L_1'&=\frac{1}{2}\left(z_1\frac{\partial}{\partial z_2}+z_2\frac{\partial}{\partial z_1}\right),\\
L_2'&=\frac{1}{2\imath}\left(z_1\frac{\partial}{\partial z_2}-z_2\frac{\partial}{\partial z_1}\right),\\
L_3'&=\frac{1}{2}\left(z_1\frac{\partial}{\partial z_1}-z_2\frac{\partial}{\partial z_2}\right),\\
\Delta_{S^2}'&=\left(\frac{1}{2}\left(z_1\frac{\partial}{\partial z_1}+z_2\frac{\partial}{\partial z_2}\right)+\frac{1}{2}\right)^2,
\end{aligned} \tag{2.24}$$

respectively.

Notice that the operator $L_0=z_1(\partial/\partial z_1)+z_2(\partial/\partial z_2)$ is the sum of Hamiltonians of two independent harmonic oscillators $z_j(\partial/\partial z_j)$, $j=1,2$, with the same frequency.

C. Bargmann transform for $L^2(S^3)$

In analogy with the case $L^2(S^2)$, let us consider the spherical normalized Laplacian on S^3. In spherical coordinates:

$$\begin{aligned}
x_1&=\sin(\lambda)\sin(\theta)\cos(\phi),\quad x_2=\sin(\lambda)\sin(\theta)\sin(\phi),\\
x_3&=\sin(\lambda)\cos(\theta),\quad x_4=\cos(\lambda),
\end{aligned} \tag{2.25}$$

where $0<\theta,\lambda<\pi$ and $0\leqslant\phi\leqslant 2\pi$.

The expression for Δ_{S^3} is

$$\Delta_{S^3}=-\frac{\partial^2}{\partial\lambda^2}-2\cot(\lambda)\frac{\partial}{\partial\lambda}+\frac{\Delta_2}{\sin^2(\lambda)}+1, \tag{2.26}$$

where

$$\Delta_2=\frac{-1}{\sin(\theta)}\frac{\partial}{\partial\theta}\sin(\theta)\frac{\partial}{\partial\theta}+\frac{-1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}. \tag{2.27}$$

Note that we are taking Δ_{S^3} such that its spectrum is the set $\{n^2|n$ is a positive integer$\}$.

Let us also consider generators for rotations on the (μ,ν) plane with $\mu,\nu=1,2,3,4$, given by restrictions to S^3 of the following operators:

$$E_{\mu\nu}=\frac{1}{\iota}\left(x_\mu\frac{\partial}{\partial x_\nu}-x_\nu\frac{\partial}{\partial x_\mu}\right),\quad \mu,\nu=1,2,3,4. \tag{2.28}$$

There are six linearly independent operators among the operators $E_{\mu\nu}$. These operators provide a representation of the Lie algebra $so(4)$. It is well known that this Lie algebra describes the symmetries of the hydrogen atom problem[7,20] for a fixed negative energy. This can be shown by considering restrictions of the angular momentum operator $\mathbf{L}=(L_1,L_2,L_3)$ and the Runge–Lenz $\mathbf{A}=(A_1,A_2,A_3)$ operator to eigenspaces of the Hamiltonian of the hydrogen atom problem. In order to keep track of this fact, we rename the operators $L_1=E_{23}$, $L_2=E_{31}$, $L_3=E_{12}$, $A_j=E_{4j}$ $j=1,2,3$.

The expressions for the operators $\mathbf{L}$ and $\mathbf{A}$ in spherical coordinates are

$$\begin{aligned}
L_1&=\iota\left(\sin(\phi)\frac{\partial}{\partial\theta}+\cot(\theta)\cos(\phi)\frac{\partial}{\partial\phi}\right),\\
L_2&=-\iota\left(\cos(\phi)\frac{\partial}{\partial\theta}-\cot(\theta)\sin(\phi)\frac{\partial}{\partial\phi}\right),\\
L_3&=-\iota\frac{\partial}{\partial\phi},\\
A_1&=-\iota\cot(\lambda)\left(\cos(\theta)\cos(\phi)\frac{\partial}{\partial\theta}-\frac{\sin(\phi)}{\sin(\theta)}\frac{\partial}{\partial\phi}\right)-\iota\sin(\theta)\cos(\phi)\frac{\partial}{\partial\lambda},\\
A_2&=-\iota\cot(\lambda)\left(\cos(\theta)\sin(\phi)\frac{\partial}{\partial\theta}+\frac{\cos(\phi)}{\sin(\theta)}\frac{\partial}{\partial\phi}\right)-\iota\sin(\theta)\sin(\phi)\frac{\partial}{\partial\lambda},\\
A_3&=-\iota\left(\cos(\theta)\frac{\partial}{\partial\lambda}-\sin(\theta)\cot(\lambda)\frac{\partial}{\partial\theta}\right).
\end{aligned} \tag{2.29}$$

Note that if we denote $L^2=L_1^2+L_2^2+L_3^2$ and $A^2=A_1^2+A_2^2+A_3^2$, then we have

$$\Delta_{S^3}=L^2+A^2+1. \tag{2.30}$$

Since Δ_{S^3}, L^2, and L_3 commute, we can find common normalized eigenfunctions of these operators. We shall call these functions hyperspherical harmonics[22] and denote them by $Y_{n\ell m}$ with $n=1,2,3...$, $\ell=0,1,\ldots,n-1$, $m=-\ell,-\ell+1,\ldots,\ell$. For each n, we have n^2 linearly independent hyperspherical harmonics, which is exactly the multiplicity of the corresponding eigenvalues of Δ_{S^3} and the Hamiltonian of the hydrogen atom[7,20]. The n^2-dimensional vector spaces generated by $Y_{n\ell m}$ (one space for each n) provide irreducible representations of the group SO(4).

In order to find a Hilbert space of analytic functions related to $L^2(S^3)$, we notice that the commutation relations satisfied by $\mathbf{L}$ and $\mathbf{A}$ are

$$\begin{aligned}
[L_i,L_j]&=\iota\epsilon_{ijk}L_k,\\
[L_i,A_j]&=\iota\epsilon_{ijk}A_k,\\
[A_i,A_j]&=\iota\epsilon_{ijk}L_k.
\end{aligned} \tag{2.31}$$

Now let us define the operators

$$\mathbf{C}=\frac{\mathbf{L}+\mathbf{A}}{2},\quad \mathbf{D}=\frac{\mathbf{L}-\mathbf{A}}{2}. \tag{2.32}$$

The commutation relation for these operators are

$$[C_i,C_j]=\imath\epsilon_{ijk}C_k,$$
$$[D_i,D_j]=\imath\epsilon_{ijk}D_k, \tag{2.33}$$
$$[C_i,D_j]=0.$$

Thus we obtain $so(4)=su(2)\times su(2)$.

Notice that the operators **L** and **A** satisfy the relation

$$\mathbf{L}\cdot\mathbf{A}\Psi=(L_1A_1+L_2A_2+L_3A_3)\Psi=0. \tag{2.34}$$

This relation implies

$$C^2\Psi=D^2\Psi=\left(\frac{L^2+A^2}{4}\right)\Psi. \tag{2.35}$$

Since the eigenvalues of the operators C^2 and D^2 are of the form $u(u+1)$ and $v(v+1)$ (with $u,v\in\mathbf{S}$), respectively, then we must have $u(u+1)=v(v+1)$. This equation implies $u=v$.

Since $\Delta_{S^3}=L^2+A^2+1$ and the eigenvalues of Δ_{S^3} are n^2, then we have $n^2=4u(u+1)+1$, which in turn implies $u=v=(n-1)/2$. Since n is a positive integer, **S** is the set of permitted values of u and v (including $\frac{1}{2}$, $\frac{3}{2}$, ...).

From the previous discussion, we want to consider two copies of the representation of su(2) on the Bargmann space $\mathcal{B}_2$ of analytical functions of two complex variables described previously.

Let us consider the Bargmann space $\mathcal{B}_4=\mathcal{B}_2\otimes\mathcal{B}_2$ of analytical functions of four complex variables (z_1,z_2,z_3,z_4). For each positive integer n, let us also consider the n^2-dimensional subspaces $\mathcal{M}_n$ of $\mathcal{B}_4$ given by

$$\mathcal{M}_n=\mathcal{W}_{(n-1)/2}\otimes\mathcal{W}_{(n-1)/2}, \tag{2.36}$$

with $\mathcal{W}_{(n-1)/2}$ the vector space of homogeneous polynomials of degree $n-1$ in two complex variables.

The functions

$$y_{nm_1m_2}=\frac{z_1^{(n-1)/2+m_1}z_2^{(n-1)/2-m_1}z_3^{(n-1)/2+m_2}z_4^{(n-1)/2-m_2}}{\sqrt{\left(\frac{n-1}{2}+m_1\right)!\left(\frac{n-1}{2}-m_1\right)!\left(\frac{n-1}{2}+m_2\right)!\left(\frac{n-1}{2}-m_2\right)!}}, \tag{2.37}$$

with $-(n-1)/2\leqslant m_1,m_2\leqslant(n-1)/2$ provide a basis for the space $\mathcal{M}_n$.

Since we want to assign an analytic function (of four complex variables) to the hyperspherical harmonics $Y_{n\ell m}$ and these functions are in turn common eigenfunctions of Δ_{S^3}, L^2, and L_3, we must assign to each $Y_{n\ell m}$ a function which is an eigenfunction of the representations of the operators Δ_{S^3}, L^2, and L_3 in the Bargmann space $\mathcal{B}_4$. Since $\mathbf{L}=\mathbf{C}+\mathbf{D}$ and by the theory of addition of angular momenta,[23] the function to be assigned to each $Y_{n\ell m}$ is

$$y_{n\ell m}(z_1,z_2,z_3,z_4)=\sum_{m_1+m_2=m}C\left(\frac{n-1}{2},m_1,\frac{n-1}{2},m_2;\ell,m\right)y_{nm_1m_2}, \tag{2.38}$$

where $C((n-1)/2,m_1,(n-1)/2,m_2;\ell,m)$ are Clebsh–Gordon coefficients.[23]

Let us define the Bargmann transform for $L^2(S^3)$ as the linear extension of the previous assignment. Thus

$$\mathbf{B}_{S^3}:L^2(S^3)\mapsto\mathcal{F}_4, \tag{2.39}$$

where $\mathcal{F}_4$ is the closed subspace of $\mathcal{B}_4$ generated by the spaces $\mathcal{M}_n$: that is $\mathcal{F}_4=\oplus_{n=1}^{\infty}\mathcal{M}_n$.

The Bargmann transform $\mathbf{B}_{S^3}$ is a unitary operator and intertwines the operators L_1, L_2, L_3, A_1, A_2, A_3 with the following operators:

$$\begin{aligned}
L_1'&=\frac{1}{2}\left(z_1\frac{\partial}{\partial z_2}+z_3\frac{\partial}{\partial z_4}+z_2\frac{\partial}{\partial z_1}+z_4\frac{\partial}{\partial z_3}\right),\\
L_2'&=\frac{1}{2\iota}\left(z_1\frac{\partial}{\partial z_2}+z_3\frac{\partial}{\partial z_4}-z_2\frac{\partial}{\partial z_1}-z_4\frac{\partial}{\partial z_3}\right),\\
L_3'&=\frac{1}{2}\left(z_1\frac{\partial}{\partial z_1}+z_3\frac{\partial}{\partial z_3}-z_2\frac{\partial}{\partial z_2}-z_4\frac{\partial}{\partial z_4}\right),\\
A_1'&=\frac{1}{2}\left(z_1\frac{\partial}{\partial z_2}+z_2\frac{\partial}{\partial z_1}-z_3\frac{\partial}{\partial z_4}-z_4\frac{\partial}{\partial z_3}\right),\\
A_2'&=\frac{1}{2\iota}\left(z_1\frac{\partial}{\partial z_2}+z_4\frac{\partial}{\partial z_3}-z_2\frac{\partial}{\partial z_1}-z_3\frac{\partial}{\partial z_4}\right),\\
A_3'&=\frac{1}{2}\left(z_1\frac{\partial}{\partial z_1}+z_4\frac{\partial}{\partial z_4}-z_2\frac{\partial}{\partial z_2}-z_3\frac{\partial}{\partial z_3}\right),
\end{aligned}\tag{2.40}$$

respectively.

The Laplacian on S^3 is intertwined with the operator

$$\Delta_{S^3}'=\left(\frac{1}{2}\left(z_1\frac{\partial}{\partial z_1}+z_2\frac{\partial}{\partial z_2}+z_3\frac{\partial}{\partial z_3}+z_4\frac{\partial}{\partial z_4}\right)+1\right)^2.\tag{2.41}$$

Thus the Laplacian Δ_{S^3}' is essentially the square of the sum of four harmonic oscillators having the same frequency.

The expression for $\mathbf{L}\cdot\mathbf{A}$ in the space $\mathcal{F}_4$ is given by the following operator:

$$\mathcal{L}\equiv z_1\frac{\partial}{\partial z_1}+z_2\frac{\partial}{\partial z_2}-z_3\frac{\partial}{\partial z_3}-z_4\frac{\partial}{\partial z_4}.\tag{2.42}$$

The restriction $(\mathbf{L}\cdot\mathbf{A})\Psi=0$ is already included in the space $\mathcal{F}_4$, as the following proposition establishes it:

Proposition 2.1: The range of the Bargmann transform $\mathbf{B}_{S^3}$ is equal to the kernel of the operator $\mathcal{L}$, that is

$$\mathcal{F}_4=\{f\in\mathcal{B}_4\,|\,\mathcal{L}f=0\}\equiv\mathrm{Ker}\,\mathcal{L}.\tag{2.43}$$

Proof: Let f in $\mathcal{F}_4$. Then

$$f=\sum_{n=0}^{\infty}\sum_{m_1,m_2}A_{nm_1m_2}\frac{z_1^{(n-1)/2+m_1}z_2^{(n-1)/2-m_1}z_3^{(n-1)/2+m_2}z_4^{(n-1)/2-m_2}}{\sqrt{\left(\frac{n-1}{2}+m_1\right)!\left(\frac{n-1}{2}-m_1\right)!\left(\frac{n-1}{2}+m_2\right)!\left(\frac{n-1}{2}-m_2\right)!}}\tag{2.44}$$

where the convergence is with respect to the norm of $\mathcal{B}_4$.

Since norm-convergence in $\mathcal{B}_4$ implies pointwise convergence (this is because $\mathcal{B}_4$ has a reproducing kernel and the Schwartz inequality) then f is an analytic function which can be differentiated termwise.

Since

$$\mathcal{L}(z_1^{(n-1)/2+m_1}z_2^{(n-1)/2-m_1}z_3^{(n-1)/2+m_2}z_4^{(n-1)/2-m_2})=0$$

for all permitted values of n,m_1,m_2, we conclude $f\in\mathrm{Ker}\,\mathcal{L}$.

Conversely, suppose $f\in\mathrm{Ker}\,\mathcal{L}$. Since

$$\left\{\left.\frac{z_1^{a_1}z_2^{a_2}z_3^{a_3}z_4^{a_4}}{\sqrt{a_1!a_2!a_3!a_4!}}\right| a_j \text{ is a non-negative integer } j=1,2,3,4\right\}$$

is an orthonormal basis of $\mathcal{B}_4$, f can be written as

$$f=\sum_{\mathbf{a}} A_{\mathbf{a}}\frac{z_1^{a_1}z_2^{a_2}z_3^{a_3}z_4^{a_4}}{\sqrt{a_1!a_2!a_3!a_4!}} \tag{2.45}$$

with $\mathbf{a}=(a_1,a_2,a_3,a_4)$. Thus we have

$$0=\mathcal{L}f=\sum_{\mathbf{a}} A_{\mathbf{a}}(a_1+a_2-a_3-a_4)\frac{z_1^{a_1}z_2^{a_2}z_3^{a_3}z_4^{a_4}}{\sqrt{a_1!a_2!a_3!a_4!}}. \tag{2.46}$$

Now consider the case when $\mathbf{b}=(b_1,b_2,b_3,b_4)$ is such that $b_1+b_2-b_3-b_4\neq 0$. By taking the inner product of $\mathcal{L}f$ with $z_1^{b_1}z_2^{b_2}z_3^{b_3}z_4^{b_4}$ we obtain $A_{\mathbf{b}}=0$. Thus f must be a linear combination of monomials $z_1^{b_1}z_2^{b_2}z_3^{b_3}z_4^{b_4}$ where $b_1+b_2-b_3-b_4=0$. But each one of these monomials belongs to some space $\mathcal{M}_n$, therefore $f\in\mathcal{F}_4$. □

The Bargmann transform $\mathbf{B}_{S^3}$ is an integral operator

$$\mathbf{B}_{S^3}\Psi(\mathbf{z})=\int_{x\in S^3}K_{S^3}(\mathbf{x},\mathbf{z})\Psi(\mathbf{x})\mathrm{d}\sigma_3(\mathbf{x}) \tag{2.47}$$

with kernel

$$K_{S^3}(\mathbf{x},\mathbf{z})=\sum_{n=1}^{\infty}\sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{\ell}\overline{Y}_{n\ell m}(\mathbf{x})y_{n\ell m}(\mathbf{z}). \tag{2.48}$$

As in the case of the two-sphere, K_{S^3} can be written as a power series in the function

$$\Phi_{S^3}=\sum_{\ell=0}^{1}\sum_{m=-\ell}^{m=\ell}\overline{Y}_{2\ell m}(\mathbf{x})y_{2\ell m}(\mathbf{z}) \tag{2.49}$$

in the following way:

$$K_{S^3}=\sum_{n=1}^{\infty}\frac{\sqrt{2n}}{(n-1)!}\frac{1}{2^{n/2}}(\Phi_{S^3})^{n-1} \tag{2.50}$$

with the following explicit expression for $\Phi_{S^3}(\mathbf{x},\mathbf{z})$:

$$\begin{aligned}\Phi_{S^3}(\mathbf{x},\mathbf{z})=\sqrt{2}[&z_1z_4(\cos(\lambda)-\iota\cos(\theta)\sin(\lambda))-z_2z_3(\cos(\lambda)+\iota\cos(\theta)\sin(\lambda))\\&+\iota z_1z_3\sin(\theta)\sin(\lambda)\exp(-\iota\phi)-\iota z_2z_4\sin(\theta)\sin(\lambda)\exp(\iota\phi)].\end{aligned} \tag{2.51}$$

The proof of this last fact is given in Appendix B.

III. THE KERNEL OF THE BARGMANN TRANSFORM AND CANONICAL TRANSFORMATIONS

In this section we describe a beautiful relationship between the Bargmann transform and a corresponding canonical transformation which plays the role of its classical analog. This fact occurs in the three cases described in Sec. II. Namely, we have shown that the kernel of the Bargmann transform is a power series in a certain function. This function is in turn a generating function of the above mentioned canonical transformation. This will give us symplectomorphisms mapping the phase space of a particle moving in $\mathbf{R}^n$, S^2, or S^3 onto a phase space described by complex variables.

We start by describing this relationship in the case of the Bargmann transform for $L^2(\mathbf{R}^n)$ and then for the cases $L^2(S^2)$ and $L^2(S^3)$.

A. Canonical transformation for a particle moving in $\mathbf{R}^n$

In this case the relationship between the kernel of the Bargmann transform and a corresponding canonical transformation is well known (see Refs. 5 and 24).

Following Graffi and Parmeggiani,[5] let us consider the function

$$\Phi_n(\mathbf{q},\mathbf{z}) = -\iota(-\tfrac{1}{2}(\mathbf{z}^2+\mathbf{q}^2)+\sqrt{2}\mathbf{z}\cdot\mathbf{q}), \tag{3.1}$$

which appears in the argument of the exponential function giving the kernel $A(\mathbf{q},\mathbf{z})$ of $\mathbf{B}_{\mathbf{R}^n}$.

Let us consider now a particle moving in $\mathbf{R}^n$. The phase space in this case is $T^*\mathbf{R}^n$ with coordinates $(\mathbf{q},\mathbf{p})$ and symplectic form $\omega_n = \sum_{j=1}^n \mathrm{d}q_j \wedge \mathrm{d}p_j$.

Now consider the function Φ_n as a generating function of a canonical transformation mapping the variables $(\mathbf{q},\mathbf{p})$ to the variables $(\mathbf{z},\mathbf{w}) \in T^*(\mathbf{C}^n)$ via the following:

$$\begin{aligned} p_j &= -\frac{\partial \Phi_n}{\partial q_j}, \quad j=1,2,\ldots,n, \\ w_j &= \iota \frac{\partial \Phi_n}{\partial z_j}, \quad j=1,2,\ldots,n. \end{aligned} \tag{3.2}$$

Note that by considering these equations we guarantee that

$$\sum_{j=1}^n \mathrm{d}q_j \wedge \mathrm{d}p_j = -\iota \sum_{j=1}^n \mathrm{d}z_j \wedge \mathrm{d}w_j. \tag{3.3}$$

The expressions for $(\mathbf{z},\mathbf{w})$ in terms of $(\mathbf{q},\mathbf{p})$ are

$$\begin{aligned} z_j &= \frac{1}{\sqrt{2}}(q_j - \iota p_j), \\ w_j &= \frac{1}{\sqrt{2}}(q_j + \iota p_j). \end{aligned} \tag{3.4}$$

In this way we see that w_j must be the complex conjugate of z_j. This fact suggests that we define the following submanifold of $T^*(\mathbf{C}^n)$:

$$\mathcal{D}_n = \{(\mathbf{z},\mathbf{w}) \in \mathbf{C}^{2n} \mid w = \overline{\mathbf{z}}\}. \tag{3.5}$$

Since the space $T^*(\mathbf{C}^n)$ is a symplectic manifold with symplectic form $\kappa_n = -\iota \sum_{j=1}^n \mathrm{d}z_j \wedge \mathrm{d}w_j$, we may consider $\mathcal{D}_n$ as a symplectic manifold with symplectic form τ_n given by the restriction of

κ_n to $\mathcal{D}_n$. Notice that we may regard the symplectic manifold $(\mathcal{D}_n,\tau_n)$ as the symplectic manifold $(\mathbf{C}_n,\mu_n)$, where $\mu_n=-\iota\Sigma_{j=1}^n dz_j\wedge d\overline{z_j}$ and $(\mathbf{z},\overline{\mathbf{z}})\mapsto(\mathbf{z})$ being the symplectomorphism between $(\mathcal{D}_n,\tau_n)$ and $(\mathbf{C}_n,\mu_n)$.

Thus we obtain the following

Theorem 3.1: *The function Φ_n is a generating function of a linear canonical transformation, which is a symplectomorphism $\mathcal{C}_n$ from $(T^*\mathbf{R}^n,\omega_n)$ onto $(\mathbf{C}_n,\mu_n)$ given by the equations $z_j=(1/\sqrt{2})(q_j-\iota p_j)$, $j=1,2,\ldots,n$. The transformation $\mathcal{C}_n$ maps the Hamiltonian $H=\frac{1}{2}\Sigma_{j=1}^n q_j^2+p_j^2$ to the Hamiltonian $H'=\Sigma_{j=1}^n z_j\overline{z_j}$.*

This theorem gives the classical analog of the Bargmann transform $\mathbf{B}_{\mathbf{R}^n}$ in the sense that $\mathbf{B}_{\mathbf{R}^n}$ is a unitary operator from $L^2(\mathbf{R}^n)$ onto the Bargmann space $\mathcal{B}_n$ and intertwines the quantum Hamiltonian of the harmonic oscillator $\hat{H}=\frac{1}{2}\Sigma_{j=1}^n(-\partial^2/\partial q_j^2+q_j^2)-n/2$ with the operator $\hat{H}'=\Sigma_{j=1}^n z_j(\partial/\partial z_j)$.

B. Canonical transformation for a particle moving on S^2

The above-noted description for a particle moving in $\mathbf{R}^n$ suggests considering the function $(-\iota/\sqrt{3})\Phi_{S^2}(\mathbf{x},\mathbf{z})$ (the factor $1/\sqrt{3}$ is just to scale variables in a convenient way) as a generating function of a canonical transformation $\mathcal{C}_{S^2}$ which maps the phase space $T^*S^2-\{0\}$ (i.e., T^*S^2 minus the zero section) onto a submanifold of $T^*\mathbf{C}^2$.

Thus let us consider

$$p_\theta=-\frac{\partial}{\partial\theta}\frac{-\iota}{\sqrt{3}}\Phi_{S^2},\quad p_\phi=-\frac{\partial}{\partial\phi}\frac{-\iota}{\sqrt{3}}\Phi_{S^2}$$

$$w_j=\iota\frac{\partial}{\partial z_j}\frac{-\iota}{\sqrt{3}}\Phi_{S^2},\quad j=1,2. \tag{3.6}$$

From Eq. (2.23), the equations above take the following explicit form:

$$\begin{aligned}
p_\theta&=-\frac{\iota}{2}(\cos(\theta)\exp(-\iota\phi)z_1^2+2\sin(\theta)z_1z_2-\cos(\theta)\exp(\iota\phi)z_2^2),\\
p_\phi&=\frac{-1}{2}(\sin(\theta)\exp(-\iota\phi)z_1^2+\sin(\theta)\exp(\iota\phi)z_2^2),\\
w_1&=-\sin(\theta)\exp(-\iota\phi)z_1+\cos(\theta)z_2,\\
w_2&=\cos(\theta)z_1+\sin(\theta)\exp(\iota\phi)z_2.
\end{aligned} \tag{3.7}$$

Note that by working with spherical coordinates for S^2, we are dealing with a specific local chart of S^2 and hence with a local chart for $T^*S^2-\{0\}$. Later on we shall define the canonical transformation $\mathcal{C}_{S^2}$ by extending the relationship between $(\theta,\phi,p_\theta,p_\phi)$ and (z_1,z_2,w_1,w_2) [determined by Eq. (3.7)] to the whole space $T^*S^2-\{0\}$.

In order to identify the submanifold of $T^*\mathbf{C}^2$ which is the image of $T^*S^2-\{0\}$, we need to find how the variables (w_1,w_2) are related to (z_1,z_2). To do this, we shall make use of the fact that the variables $\theta,\phi,p_\theta,p_\phi$ are real variables. Thus from the first two equations of (3.7) and the reality condition $\theta=\overline{\theta}$, $\phi=\overline{\phi}$, $p_\theta=\overline{p_\theta}$, $p_\phi=\overline{p_\phi}$, we obtain

$$\sin(\theta)=\frac{|\overline{z_1}z_2-z_2^2|}{|z_1|^2+|z_2|^2},$$

$$\cos(\theta)=\pm\frac{\overline{z_1}\overline{z_2}+z_1z_2}{|z_1|^2+|z_2|^2},$$
$$\exp(\iota\phi)=\pm\frac{\overline{z}_2^2-z_1^2}{|\overline{z}_2^2-z_1^2|}. \tag{3.8}$$

If we substitute Eq. (3.8) into the last two equations of (3.7), we obtain

$$w_1=\pm\overline{z_1},\quad w_2=\pm\overline{z_2}. \tag{3.9}$$

We shall restrict ourselves to considering the plus sign in Eqs. (3.8) and (3.9) in such a way that $(w_1,w_2)=(\overline{z_1},\overline{z_2})$. It can be shown, by expressing (z_1,z_2) in terms of $(\theta,\phi,p_\theta,p_\phi)$, that given $(\theta,\phi,p_\theta,p_\phi)$, there are four solutions for (z_1,z_2) [note that, if (z_1,z_2) is a solution then $(-z_1,-z_2)$, $(\overline{z_2},-\overline{z_1})$ and $(-\overline{z_2},\overline{z_1})$ are solutions too]. Two of these solutions correspond to considering the plus sign in Eqs. (3.8) and (3.9) and the other two correspond to the minus sign. The two solutions corresponding to the plus sign are related to each other by a minus sign [i.e., if (z_1,z_2) is a solution of Eq. (3.7), with $(\theta,\phi,p_\theta,p_\phi)$ given, then $(-z_1,-z_2)$ is a solution too]. Thus we need to identify (z_1,z_2) with $-(z_1,z_2)$ in order to make our canonical transformation $\mathcal{C}_{S^2}$ a function. In this way, we see that $\mathcal{C}_{S^2}$ takes values in the following submanifold of $T^*\mathbf{C}^2$:

$$\mathcal{D}_2=\{(z_1,z_2,w_1,w_2)\in\mathbf{C}^4|w_1=\overline{z_1},\ \ w_2=\overline{z_2}\}/\{1,-1\}. \tag{3.10}$$

Note that the symplectic manifold $(\mathcal{D}_2,\tau_2)$ can be regarded as $\mathbf{C}^2/\{1,-1\}$ with symplectic form $\mu_2=-\iota(dz_1\wedge d\overline{z_1}+dz_2\wedge d\overline{z_2})$.

Once we have chosen the plus sign in Eqs. (3.8) and (3.9), we find the following expressions for p_θ,p_ϕ in terms of $(z_1,z_2,\overline{z_1},\overline{z_2})$:

$$p_\theta=\left(\frac{z_1z_2-\overline{z_1}\overline{z_2}}{2\iota}\right)\left(\frac{|z_1|^2+|z_2|^2}{z_1^2-\overline{z}_2^2}\right),\quad p_\phi=\frac{1}{2}(|z_1|^2-|z_2|^2),$$
$$H=p_\theta^2+\frac{1}{\sin^2(\theta)}p_\phi^2=\left(\frac{|z_1|^2+|z_2|^2}{2}\right)^2. \tag{3.11}$$

Note that we have a singularity in Eq. (3.8) when the energy H is zero. Thus we need to remove the zero section of T^*S^2 (which we shall denote by $\{0\}$) and the origin of the manifold $\mathbf{C}_2/\{1,-1\}$. (denoted by $\{0\}$, too). The other singularity in the expression for p_θ corresponds to the point $z_1^2=\overline{z}_2^2$, which in turn is equivalent to the equation $\sin(\theta)=0$ (north and south poles). We actually do not have such a singularity since we are taking $0<\theta<\pi$, and (as we shall see later on) it will not appear in the extension of our canonical transformation.

Canonical transformation for S^2 and the null quadric $\mathbf{Q}^2$. In the following we identify the equations giving $(\theta,\phi,p_\theta,p_\phi)$ as functions of $(z_1,z_2,\overline{z_1},\overline{z_2})$ with the composition of two maps involving the null quadric in $\mathbf{C}^3$, defined by

$$\mathbf{Q}^2\equiv\{(\alpha_1,\alpha_2,\alpha_3)\in\mathbf{C}^3/\alpha_1^2+\alpha_2^2+\alpha_3^2=0\}. \tag{3.12}$$

One of the maps takes $\mathbf{C}^2/\{1,-1\}-\{0\}$ onto $\mathbf{Q}^2-\{0\}$ and the other one takes $\mathbf{Q}^2-\{0\}$ onto $T^*S^2-\{0\}$. In this manner, we shall extend our canonical transformation $\mathcal{C}_{S^2}$ to be the inverse of such a composition. The map that goes from $\mathbf{C}^2/\{1,-1\}-\{0\}$ onto $\mathbf{Q}^2-\{0\}$ has also been considered by Bargmann and Todorov.[8] We will refer to their work in Sec. IV when we describe the quantization of the above mentioned maps.

The generating function $(-\iota/\sqrt{3})\,\Phi_{S^2}$ of our canonical transformation $\mathcal{C}_{S^2}$ can be written as an inner product:

$$\frac{-\iota}{\sqrt{3}}\Phi_{S^2}=-\iota(\alpha(\mathbf{z})\cdot\mathbf{x}), \tag{3.13}$$

where

$$\begin{gathered}\mathbf{x}=(\sin(\theta)\cos(\phi),\sin(\theta)\sin(\phi),\cos(\theta)),\\ \alpha(\mathbf{z})=\tfrac{1}{2}(-z_1^2+z_2^2,\iota z_1^2+\iota z_2^2,2z_1z_2).\end{gathered} \tag{3.14}$$

Here we are taking the usual inner product of two vectors $\alpha=(\alpha_1,\alpha_2,\alpha_3)$ and $\beta=(\beta_1,\beta_2,\beta_3)$ in $\mathbf{C}^3$:

$$\alpha\cdot\beta\equiv\alpha_1\overline{\beta_1}+\alpha_2\overline{\beta_2}+\alpha_3\overline{\beta_3}. \tag{3.15}$$

Notice the relevant fact that $\alpha(\mathbf{z})$ is in the null quadric $\mathbf{Q}^2$. This suggests that $\mathbf{Q}^2$ might have an important role to play related to our canonical transformation $\mathcal{C}_{S^2}$. Thus let us define the following map:

$$\begin{gathered}\rho_2:\tilde{\mathbf{C}}^2\mapsto\mathbf{Q}^2,\\ \rho_2(z_1,z_2)=\tfrac{1}{2}(-z_1^2+z_2^2,\iota z_1^2+\iota z_2^2,2z_1z_2),\end{gathered} \tag{3.16}$$

where we define $\tilde{\mathbf{C}}^2$ as the set of equivalence classes of $\mathbf{C}^2$ identifying (z_1,z_2) with $(-z_1,-z_2)$.

Now being in the null quadric $\mathbf{Q}^2-\{0\}$, we can go to $T^*S^2-\{0\}$ through the following map:

$$\begin{gathered}\sigma_2:\mathbf{Q}^2-\{0\}\mapsto T^*S^2-\{0\},\\ \sigma_2(\alpha_1,\alpha_2,\alpha_3)=\left(\frac{\Re(\alpha)}{|\Re(\alpha)|},-\Im(\alpha)\right).\end{gathered} \tag{3.17}$$

Here $\Re(\alpha)$ and $\Im(\alpha)$ are the real and imaginary parts of $\alpha=(\alpha_1,\alpha_2,\alpha_3)$, respectively.

Thus the composition map is

$$\begin{aligned}&\sigma_2\circ\rho_2:\tilde{\mathbf{C}}^2-\{0\}\mapsto T^*S^2-\{0\},\\ &\sigma_2\circ\rho_2(z_1,z_2)=\left(\frac{\Re(-z_1^2+z_2^2)}{|z_1|^2+|z_2|^2},\frac{\Re(\iota z_1^2+\iota z_2^2)}{|z_1|^2+|z_2|^2},\frac{\Re(2z_1z_2)}{|z_1|^2+|z_2|^2},\right.\\ &\qquad\left.-\frac{1}{2}\Im(z_2^2-z_1^2),-\frac{1}{2}\Im(\iota z_1^2+\iota z_2^2),-\frac{1}{2}\Im(2z_1z_2)\right).\end{aligned} \tag{3.18}$$

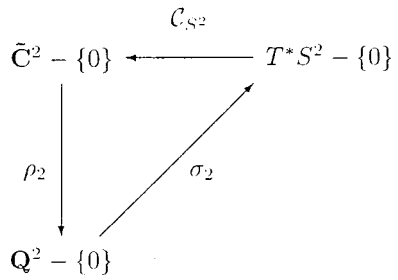
On the other hand, since a point in T^*S^2 can be described in spherical coordinates by

$$\begin{aligned}&\left(\sin(\theta)\cos(\phi),\sin(\theta)\sin(\phi),\cos(\theta),\cos(\theta)\cos(\phi)p_\theta-\frac{\sin(\phi)}{\sin(\theta)}p_\phi,\cos(\theta)\sin(\phi)p_\theta\right.\\ &\qquad\left.+\frac{\cos(\phi)}{\sin(\theta)}p_\phi,-\sin(\theta)p_\theta\right)\end{aligned} \tag{3.19}$$

then, we find after some computation [by using Eqs. (3.7) and (3.8)] that this point in T^*S^2 expressed in terms of $(z_1,z_2,\overline{z_1},\overline{z_2})$ is exactly the same point that the composition $\sigma_2\circ\rho_2$ assigns

to $(z_1,\ z_2,\ \overline{z_1},\ \overline{z_2})$. This conclusion allows us to extend our canonical transformation $\mathcal{C}_{S^2}$ (without referring to spherical coordinates) as the map $(\sigma_2\circ\rho_2)^{-1}$. Let us state our conclusions in the following theorem:

Theorem 3.2: *The function* $(-\iota/\sqrt{3})\,\Phi_{S^2}$ *is a generating function of a transformation that can be extended as a canonical transformation* $\mathcal{C}_{S^2}$ *which makes the following triangle of canonical transformations commute:*



where (a) the symplectic form ν_2 *on* T^*S^2 *is given by the restriction to* T^*S^2 *of the canonical symplectic form* ω_3 *on* $T^*\mathbf{R}^3$,
(b) the symplectic form μ_2 *on* $\tilde{\mathbf{C}}^2-\{0\}$ *is given by*

$$\mu_2=-\iota(\mathrm{d}z_1\wedge\mathrm{d}\overline{z_1}+\mathrm{d}z_2\wedge\mathrm{d}\overline{z_2}), \tag{3.20}$$

(c) the symplectic form q_3 *on* $\mathbf{Q}^2-\{0\}$ *is given by*

$$q_3=\frac{1}{2\iota|\Re\alpha|}\sum_{j=1}^{3}\mathrm{d}\alpha_j\wedge d\overline{\alpha}_j-\frac{1}{8\iota|\Re\alpha|^3}\sum_{j,k=1}^{3}(\alpha_j+\overline{\alpha}_j)(\alpha_k+\overline{\alpha}_k)\mathrm{d}\alpha_j\wedge\mathrm{d}\overline{\alpha}_k, \tag{3.21}$$

which is not the restriction to $\mathbf{Q}^2-\{0\}$ *of the symplectic form* $\Sigma_{j=1}^{3}\mathrm{d}\alpha_j\wedge\mathrm{d}\overline{\alpha}_j$ *defined on the ambient* $\mathbf{C}^3$.

The transformation $\mathcal{C}_{S^2}$ *maps the components* (L_1,L_2,L_3) *of the angular momentum and the energy* H *as follows:*

$$\begin{aligned}
L_1&=-\sin(\phi)p_\theta-\frac{\cos(\theta)\cos(\phi)}{\sin(\theta)}p_\phi=\frac{1}{2}(z_1\overline{z_2}+\overline{z_1}z_2),\\
L_2&=\cos(\phi)p_\theta-\frac{\cos(\theta)\sin(\phi)}{\sin(\theta)}p_\phi=\frac{-\iota}{2}(z_1\overline{z_2}-\overline{z_1}z_2),\\
L_3&=p_\phi=\tfrac{1}{2}(|z_1|^2-|z_2|^2),\\
H&=\frac{1}{2}\left(p_\theta^2+\frac{1}{\sin^2(\theta)}p_\phi^2\right)=\frac{1}{2}\left(\frac{|z_1|^2+|z_2|^2}{2}\right)^2,
\end{aligned} \tag{3.22}$$

which is the classical analog of what the Bargmann transform $\mathbf{B}_{S^2}$ *does in quantum mechanics [see eq. (2.24)].*

C. Canonical transformation for a particle moving on S^3

In analogy with the cases where the configuration space is $\mathbf{R}^n$ or S^2, we want to consider the function $(-\iota/\sqrt{2})\,\Phi_{S^3}$ as a generating function of a canonical transformation $\mathcal{C}_{S^3}$ which maps $T^*S^3-\{0\}$ onto a space involving four complex variables and their conjugates [we used four complex variables when we defined the Bargmann transform for $L^2(S^3)$]. Notice that $T^*S^3-\{0\}$ is a six (real) dimensional manifold, whereas to determine four complex variables we need

eight real parameters. Thus we expect to have some restrictions among the four complex variables. The first restriction we expect is the following [in analogy with Eq. (2.34) in quantum mechanics]:

$$|z_1|^2+|z_2|^2=|z_3|^2+|z_4|^2. \tag{3.23}$$

This equation is actually contained in the equations determined by the generating function $(-\iota/\sqrt{2})\,\Phi_{S^3}$ as we show it in the following. The second restriction comes from an S^1 invariance of those equations.

Thus let us consider the canonical transformation generated by $(-\iota/\sqrt{2})\,\Phi_{S^3}$ through the following equations:

$$\begin{gathered} p_\theta=-\frac{\partial}{\partial\theta}\frac{-\iota}{\sqrt{2}}\Phi_{S^3},\quad p_\phi=-\frac{\partial}{\partial\phi}\frac{-\iota}{\sqrt{2}}\Phi_{S^3},\quad p_\lambda=-\frac{\partial}{\partial\lambda}\frac{-\iota}{\sqrt{2}}\Phi_{S^3},\\ w_j=\iota\frac{\partial}{\partial z_j}\frac{-\iota}{\sqrt{2}}\Phi_{S^3},\quad j=1,2,3,4. \end{gathered} \tag{3.24}$$

From Eq. (2.51) we obtain

$$\begin{aligned} p_\theta&=-z_1z_4\sin(\theta)\sin(\lambda)-z_2z_3\sin(\theta)\sin(\lambda)-z_1z_3\cos(\theta)\sin(\lambda)\exp(-\iota\phi)\\ &\quad+z_2z_4\cos(\theta)\sin(\lambda)\exp(\iota\phi),\\ p_\phi&=\iota\sin(\theta)\sin(\lambda)[z_1z_3\exp(-\iota\phi)+z_2z_4\exp(\iota\phi)],\\ p_\lambda&=-\iota z_1z_4(\sin(\lambda)+\iota\cos(\theta)\cos(\lambda))-\iota z_2z_3(-\sin(\lambda)+\iota\cos(\theta)\cos(\lambda))\\ &\quad-z_1z_3\sin(\theta)\cos(\lambda)\exp(-\iota\phi)+z_2z_4\sin(\theta)\cos(\lambda)\exp(\iota\phi),\\ w_1&=z_4(\cos(\lambda)-\iota\cos(\theta)\sin(\lambda))+\iota z_3\sin(\theta)\sin(\lambda)\exp(-\iota\phi),\\ w_2&=-z_3(\cos(\lambda)+\iota\cos(\theta)\sin(\lambda))-\iota z_4\sin(\theta)\sin(\lambda)\exp(\iota\phi),\\ w_3&=-z_2(\cos(\lambda)+\iota\cos(\theta)\sin(\lambda))+\iota z_1\sin(\theta)\sin(\lambda)\exp(-\iota\phi),\\ w_4&=z_1(\cos(\lambda)-\iota\cos(\theta)\sin(\lambda))-\iota z_2\sin(\theta)\sin(\lambda)\exp(\iota\phi). \end{aligned} \tag{3.25}$$

As in the case for S^2, let us state the reality condition:

$$\begin{gathered} \theta=\overline{\theta},\quad \phi=\overline{\phi},\quad \lambda=\overline{\lambda},\\ p_\theta=\overline{p_\theta},\quad p_\phi=\overline{p_\phi},\quad p_\lambda=\overline{p_\lambda}. \end{gathered} \tag{3.26}$$

This condition implies

$$\sin(\theta)=\frac{|z_1z_3+\overline{z_2}\,\overline{z_4}|}{\sqrt{(|z_1|^2+|z_2|^2)(|z_3|^2+|z_4|^2)-(\Re(z_1z_4-z_2z_3))^2}},$$

$$\cos(\theta)=\frac{\pm\Im(z_1z_4+z_3z_2)}{\sqrt{(|z_1|^2+|z_2|^2)(|z_3|^2+|z_4|^2)-(\Re(z_1z_4-z_2z_3))^2}},$$

$$\exp(\iota\phi)=\pm\frac{\iota|z_2z_4+\overline{z_1}\,\overline{z_3}|}{z_2z_4+\overline{z_1}\,\overline{z_3}},$$

$$\sin(\lambda)=\frac{\sqrt{(|z_1|^2+|z_2|^2)(|z_3|^2+|z_4|^2)-(\Re(z_1z_4-z_2z_3))^2}}{\sqrt{(|z_1|^2+|z_2|^2)(|z_3|^2+|z_4|^2)}},\tag{3.27}$$

$$\cos(\lambda)=\pm\frac{\Re(z_1z_4-z_2z_3)}{\sqrt{(|z_1|^2+|z_2|^2)(|z_3|^2+|z_4|^2)}}.$$

These equations in turn imply

$$(w_1,w_2,w_3,w_4)=\pm(\overline{z_1},\overline{z_2},\overline{z_3},\overline{z_4}).\tag{3.28}$$

We shall choose the plus sign wherever we have a choice of either a plus or minus sign in the above-given equations. Thus we have the relation $(w_1,w_2,w_3,w_4)=(\overline{z_1},\overline{z_2},\overline{z_3},\overline{z_4})$. Using this relation in the last four equations we obtain the expected restriction

$$|z_1|^2+|z_2|^2=|z_3|^2+|z_4|^2.\tag{3.29}$$

This restriction will appear as part of the definition of the manifold where our canonical transformation $\mathcal{C}_{S^3}$ should take values in.

On the other hand, the expressions for p_θ, p_ϕ, p_λ in terms of (z_1,z_2,z_3,z_4) are

$$p_\theta=-\frac{\Re(z_1z_4)(|z_3|^2+|z_2|^2)+\Re(z_2z_3)(|z_1|^2+|z_4|^2)}{|z_1z_3+\overline{z_2}\overline{z_4}|},$$

$$p_\phi=\tfrac{1}{2}(|z_1|^2-|z_2|^2+|z_3|^2-|z_4|^2),\tag{3.30}$$

$$p_\lambda=\frac{(|z_3|^2+|z_4|^2)\Im(z_1z_4+\overline{z_2}\overline{z_3})}{\sqrt{(|z_3|^2+|z_4|^2)^2-(\Re(z_1z_4-z_2z_3))^2}}.$$

Now notice the following relevant property of Eq. (3.25): Suppose $(\theta,\phi,\lambda,p_\theta,p_\phi,p_\lambda)$ is given. If (z_1,z_2,z_3,z_4) is a solution of Eq. (3.25), then, for any real number ψ, $(z_1\exp(\imath\psi),z_2\exp(\imath\psi),z_3\exp(-\imath\psi),z_4\exp(-\imath\psi))$ is a solution, as well. Thus we define the following equivalence relation $\sim$ in $\mathbf{C}^4$ in order to consider the invariance of Eq. (3.25):

$$(z_1,z_2,z_3,z_4)\sim(z_1',z_2',z_3',z_4') \text{ iff } \exists\psi\in\mathbf{R} \text{ such that}$$

$$(z_1',z_2',z_3',z_4')=(z_1\exp(\imath\psi),z_2\exp(\imath\psi),z_3\exp(-\imath\psi),z_4\exp(-\imath\psi)).\tag{3.31}$$

We shall denote by $[(z_1,z_2,z_3,z_4)]$ the equivalence class of (z_1,z_2,z_3,z_4).

Thus our canonical transformation $\mathcal{C}_{S^3}$ should take values in the following six (real) dimensional set:

$$\tilde{\mathbf{C}}^4\equiv\{(z_1,z_2,z_3,z_4)\in\mathbf{C}^4\,|\,|z_1|^2+|z_2|^2=|z_3|^2+|z_4|^2\}/\sim.\tag{3.32}$$

We shall regard the manifold $\tilde{\mathbf{C}}^4-\{0\}$ as a symplectic manifold endowed with the following symplectic form:

$$\mu_3=-\imath(dz_1\wedge d\overline{z_1}+dz_2\wedge d\overline{z_2}+dz_3\wedge d\overline{z_3}+dz_4\wedge d\overline{z_4}).\tag{3.33}$$

Canonical transformation for S^3 and the null quadric $\mathbf{Q}^3$. Now we want to extend the assignment $(\theta,\phi,\lambda,p_\theta,p_\phi)\mapsto[(z_1,z_2,z_3,z_4)]$ given by Eq. (3.25) to the whole space $T^*S^3-\{0\}$ in a similar way as we did for the case of S^2. Here again the null quadric

$$\mathbf{Q}^3=\{(\alpha_1,\alpha_2,\alpha_3,\alpha_4)\in\mathbf{C}^4/\alpha_1^2+\alpha_2^2+\alpha_3^2+\alpha_4^2=0\}\tag{3.34}$$

will play an important role and we will extend the mentioned assignment as the inverse of a composition of two maps, one going from $\tilde{\mathbf{C}}^4-\{0\}$ onto $\mathbf{Q}^3-\{0\}$ and the other one from $\mathbf{Q}^3-\{0\}$ onto $T^*S^3-\{0\}$. A similar map to the first one appears in the work of Bargmann and Todorov,[8] we will be back to this point in Sec. IV.

Let us write the generating function $(-\iota/\sqrt{2})\Phi_{S^3}$ as an inner product:

$$\frac{-\iota}{\sqrt{2}}\Phi_{S^3}=-\iota(\alpha(\mathbf{z})\cdot\mathbf{x}), \tag{3.35}$$

where

$$\begin{gathered}\alpha(\mathbf{z})=(\iota z_1z_3-\iota z_2z_4,z_1z_3+z_2z_4,-\iota z_1z_4-\iota z_2z_3,z_1z_4-z_2z_3),\\ \mathbf{x}=(\sin(\lambda)\sin(\theta)\cos(\phi),\sin(\lambda)\sin(\theta)\sin(\phi),\sin(\lambda)\cos(\theta),\cos(\lambda)).\end{gathered} \tag{3.36}$$

Now notice that for all $(z_1,z_2,z_3,z_4)\in\mathbf{C}^4$, the vector $\alpha(\mathbf{z})$ belongs to the null quadric $\mathbf{Q}^3$. This suggests defining the following map:

$$\begin{gathered}\rho_3:\tilde{\mathbf{C}}^4\mapsto\mathbf{Q}^3,\\ \rho_3([\mathbf{z}])=(\iota z_1z_3-\iota z_2z_4,z_1z_3+z_2z_4,-\iota z_1z_4-\iota z_2z_3,z_1z_4-z_2z_3)\end{gathered} \tag{3.37}$$

with (z_1,z_2,z_3,z_4) a representative of the equivalent class $[z_1,z_2,z_3,z_4]$. From now on we shall denote $\rho_3([z_1,z_2,z_3,z_4])$ just by $\rho_3(z_1,z_2,z_3,z_4)$.

Let us also define the map

$$\begin{gathered}\sigma_3:\mathbf{Q}^3-\{0\}\mapsto T^*S^3-\{0\},\\ \sigma_3(\alpha)=\left(\frac{\Re\alpha}{|\Re\alpha|},-\Im\alpha\right).\end{gathered} \tag{3.38}$$

As in the case for S^2, we shall extend our assignment $(\theta,\phi,\lambda,p_\theta,p_\phi)\mapsto[(z_1,z_2,z_3,z_4)]$ determined by Eq. (3.25) to the whole space $T^*S^3-\{0\}$. For this purpose, we first check that if we consider a point in $T^*S^3-\{0\}$ given in spherical coordinates by

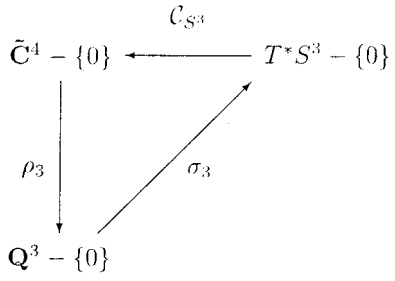
$$\begin{gathered}(\sin(\lambda)\sin(\theta)\cos(\phi),\sin(\lambda)\sin(\theta)\sin(\phi),\sin(\lambda)\cos(\theta),\cos(\lambda),\\ \cos(\lambda)\sin(\theta)\cos(\phi)p_\lambda+\cos(\theta)\cos(\phi)p_\theta/\sin(\lambda)-\frac{\sin(\phi)p_\phi}{\sin(\lambda)\sin(\theta)},\\ \cos(\lambda)\sin(\theta)\sin(\phi)p_\lambda+\cos(\theta)\sin(\phi)p_\theta/\sin(\lambda)-\frac{\cos(\phi)p_\phi}{\sin(\lambda)\sin(\theta)},\\ \cos(\lambda)\cos(\theta)p_\lambda-\sin(\theta)p_\theta/\sin(\lambda),-\sin(\lambda)p_\lambda)\end{gathered} \tag{3.39}$$

and we use Eq. (3.27), then we obtain a map which assigns to the point (z_1,z_2,z_3,z_4) the same element in T^*S^3 as the evaluation of the function $\sigma_3\circ\rho_3$ in (z_1,z_2,z_3,z_4). This allows us to extend our canonical transformation $\mathcal{C}_{S^3}$ as the map $(\sigma_3\circ\rho_3)^{-1}$.

Let us state our conclusions in the following

Theorem 3.3: *The function* $(-\iota/\sqrt{2})\Phi_{S^3}$ *generates a transformation which can be extended as a canonical transformation* $\mathcal{C}_{S^3}$ *that makes the following triangle of canonical transformations*

commute:



where (a) the symplectic form ν_3 on T^*S^3 is given by the restriction to T^*S^3 of the canonical symplectic form ω_4 on $T^*\mathbf{R}^4$,

(b) the symplectic form μ_3 on $\tilde{\mathbf{C}}^4-\{0\}$ is given by

$$\mu_3=-\iota(\mathrm{d}z_1\wedge\mathrm{d}\overline{z_1}+\mathrm{d}z_2\wedge\mathrm{d}\overline{z_2}+\mathrm{d}z_3\wedge\mathrm{d}\overline{z_3}+\mathrm{d}z_4\wedge\mathrm{d}\overline{z_4}), \tag{3.40}$$

(c) the symplectic form q_4 on $\mathbf{Q}^3-\{0\}$ is given by

$$q_4=\frac{1}{2\iota|\Re\alpha|}\sum_{j=1}^{4}\mathrm{d}\alpha_j\wedge\mathrm{d}\overline{\alpha}_j-\frac{1}{8\iota|\Re\alpha|^3}\sum_{j,k=1}^{4}(\alpha_j+\overline{\alpha}_j)(\alpha_k+\overline{\alpha}_k)\mathrm{d}\alpha_j\wedge\mathrm{d}\overline{\alpha}_k, \tag{3.41}$$

which is not the restriction to $\mathbf{Q}^3-\{0\}$ of the symplectic form $\Sigma_{j=1}^4\,\mathrm{d}\alpha_j\wedge\mathrm{d}\overline{\alpha}_j$ defined on the ambient $\mathbf{C}^4$. The components of the angular momentum and Runge–Lenz vectors are

$$\begin{aligned}
L_1&=\tfrac{1}{2}(z_1\overline{z_2}+z_3\overline{z_4}+z_2\overline{z_1}+z_4\overline{z_3}),\\
L_2&=\frac{1}{2\iota}(z_1\overline{z_2}+z_3\overline{z_4}-z_2\overline{z_1}-z_4\overline{z_3}),\\
L_3&=\tfrac{1}{2}(z_1\overline{z_1}+z_3\overline{z_3}-z_2\overline{z_2}-z_4\overline{z_4}),\\
A_1&=\tfrac{1}{2}(z_1\overline{z_2}+z_2\overline{z_1}-z_3\overline{z_4}-z_4\overline{z_3}),\\
A_2&=\frac{1}{2\iota}(z_1\overline{z_2}+z_4\overline{z_3}-z_2\overline{z_1}+z_3\overline{z_4}),\\
A_3&=\tfrac{1}{2}(z_1\overline{z_1}+z_4\overline{z_4}-z_2\overline{z_2}+z_3\overline{z_3}).
\end{aligned} \tag{3.42}$$

The expressions for $L^2=L_1^2+L_2^2+L_3^2$, $A^2=A_1^2+A_2^2+A_3^2$ and the energy H are

$$\begin{aligned}
L^2&=\tfrac{1}{4}(z_1\overline{z_1}+z_2\overline{z_2})^2+\tfrac{1}{4}(z_3\overline{z_3}+z_4\overline{z_4})^2+\tfrac{1}{2}(4\Re(z_1z_4\overline{z_2}\overline{z_3})+(|z_2|^2-|z_1|^2)(|z_4|^2-|z_3|^2)),\\
A^2&=\tfrac{1}{4}(z_1\overline{z_1}+z_2\overline{z_2})^2+\tfrac{1}{4}(z_3\overline{z_3}+z_4\overline{z_4})^2-\tfrac{1}{2}(4\Re(z_1z_4\overline{z_2}\overline{z_3})+(|z_2|^2-|z_1|^2)(|z_4|^2-|z_3|^2)),
\end{aligned} \tag{3.43}$$

$$H=\frac{1}{2}\left(p_\lambda^2+\frac{p_0^2}{\sin^2(\lambda)}+\frac{p_\phi^2}{\sin^2(\lambda)\sin^2(\theta)}\right)=\frac{1}{2}\left(\frac{\Sigma_{j=1}^4 z_j\overline{z_j}}{2}\right)^2.$$

IV. QUANTIZATIONS OF THE MAPS ρ_2,σ_2 AND ρ_3,σ_3

Once we have the commuting triangles of canonical transformations of Theorems (3.2) and (3.3), and the analogy between $\mathbf{B}_{S^2}$, $\mathbf{B}_{S^3}$ and their corresponding canonical transformations $\mathcal{C}_{S^2}$, $\mathcal{C}_{S^3}$, a natural question to ask is about the description of unitary transformations which play the

role of quantizations of the maps ρ_2, σ_2 and ρ_3, σ_3 (for the case of S^2 and S^3, respectively). Such a description is the goal of this section. The unitary transformations corresponding to σ_2, and σ_3 are related to work of Guillemin.[9] The unitary transformations corresponding to ρ_2, and ρ_3 have been studied by Bargmann and Todorov.[8] For completeness of this paper, we will describe these last unitary transformations, too.

A. Quantizations of ρ_2 and σ_2

Let $d\mu_2(\alpha)$ be the measure on $\mathbf{Q}^2$ obtained from the Gaussian measure

$$d\nu_2(\mathbf{z}) = \frac{1}{\pi^2} \exp(-|\mathbf{z}|^2) \prod_{j=1}^{2} dx_j\, dy_j \tag{4.1}$$

through the map ρ_2 (here we are actually regarding the map ρ_2 as a function from $\mathbf{C}^2$ onto $\mathbf{Q}^2$).

Given $\ell \geqslant 0$ an integer, let $\mathcal{X}_\ell$ be the complex vector space of homogeneous polynomials of order ℓ in three complex variables $(\alpha_1, \alpha_2, \alpha_3)$ with the restriction $\alpha_1^2 + \alpha_2^2 + \alpha_3^2 = 0$. The space $\mathcal{X}_\ell$ has dimension $2\ell + 1$ and a particular basis for it can be obtained by considering the monomials

$$y_{\ell m} = \frac{z_1^{\ell+m} z_2^{\ell-m}}{\sqrt{(\ell+m)!(\ell-m)!}}$$

and the map ρ_2^{-1}. That is, we shall consider the following functions as a basis for $\mathcal{X}_\ell$:

$$\Upsilon_{\ell m}(\alpha) = y_{\ell m}(\mathbf{z}(\alpha)), \quad m = -\ell, -\ell+1 \ldots \ell, \quad \alpha = (\alpha_1, \alpha_2, \alpha_3), \tag{4.2}$$

with $\mathbf{z}(\alpha)$ determined by

$$z_1^2 = -\alpha_1 - \iota\alpha_2, \quad z_2^2 = \alpha_1 - \iota\alpha_2, \quad z_1 z_2 = \alpha_3. \tag{4.3}$$

Note that the functions $y_{\ell m}$ depend on $\mathbf{z} = (z_1, z_2)$ through integer powers of z_1^2, z_2^2 and $z_1 z_2$, so Eq. (4.3) is enough in order to express $y_{\ell m}$ in terms of α_1, α_2, and α_3.

Let $\mathcal{E}_2$ be the Hilbert space generated by all of the spaces $\mathcal{X}_\ell$ endowed with the inner product:

$$\langle F, G \rangle = \int_{\alpha \in \mathbf{Q}^2} F(\alpha) \overline{G(\alpha)}\, d\mu_2(\alpha). \tag{4.4}$$

Thus the quantization of the map ρ_2 is the unitary transformation $\mathbf{U}_{\rho_2}: \mathcal{B}_{S^2} \mapsto \mathcal{E}_2$ given by

$$\mathbf{U}_{\rho_2} \Psi(\alpha) = \Psi(\mathbf{z}(\alpha)), \quad \Psi \in \mathcal{B}_{S^2}. \tag{4.5}$$

where $\mathbf{z}(\alpha)$ is determined by Eq. (4.3).

Bargmann and Todorov[8] have considered the space $\mathcal{E}_2$ [with the same inner product and a measure very similar to $d\mu_2(\alpha)$] and actually the inverse of $\mathbf{U}_{\rho_2}$. They introduce the measure $d\mu_2(\alpha)$ in a different way than we do. They require that the adjoint of the multiplication operators by coordinates in the null quadric $\mathbf{Q}^2 - \{0\}$ must have a given expression. Their expression for the map ρ_2 is very similar to ours. In terms of the Pauli matrices

$$\beta_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \beta_2 = \begin{pmatrix} 0 & -\iota \\ \iota & 0 \end{pmatrix}, \quad \beta_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.6}$$

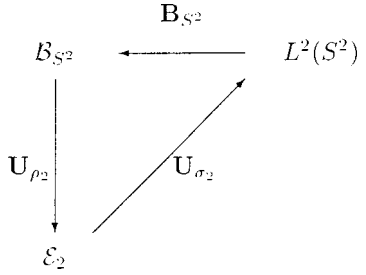
the expression they consider for the map $\rho_2(z_1, z_2)$ is $(1/2\sqrt{2})\,(z_1, z_2)\epsilon\beta_j(z_1, z_2)^t$ where j $= 1,2,3$; $(z_1, z_2)^t$ is the transpose of the vector (z_1, z_2) and the matrix $\epsilon = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$. Our expression for $\rho_2(z_1, z_2)$ in the same notation is $\frac{1}{2}(-1)^j (z_1, z_2)\epsilon\beta_j(z_1, z_2)^t$.

The quantization of σ_2, $\mathbf{U}_{\sigma_2}:\mathcal{E}_2\mapsto L^2(S^2)$, can be found by considering the orthonormal basis $\{Y_{\ell m}\}$ and $\{Y_{\ell m}\}$ of the Hilbert spaces $\mathcal{E}_3$ and $L^2(S^2)$, respectively:

$$\mathbf{U}_{\sigma_2}\Psi(\mathbf{x})=\lim_{M\mapsto\infty}\left(\int_{|\alpha|\leq M}\sum_{\ell=0}^{\infty}\frac{\sqrt{2\ell+1}}{\ell!}(\mathbf{x}\cdot\alpha)^{\ell}\right)\Psi(\alpha)\mathrm{d}\mu_2(\alpha),\quad \Psi\in\mathcal{E}_2. \tag{4.7}$$

Let us summarize the conclusions of this section in the following

Theorem 4.1: *The following triangle of unitary transformations commutes*:



This triangle is the quantum version of the commuting triangle of canonical transformations in Theorem (3.2).

Remark 1: Guillemin[9] has introduced a transformation p_* which is related to our unitary transformation $\mathbf{U}_{\sigma_2}:\mathcal{E}_2\mapsto L^2(S^2)$. The transformation p_* can be described in our terms as follows. The unit cotangent bundle $S^*(S^2)$ of S^2 can be identified with the following subset of the null quadric $\mathbf{Q}^2$:

$$X\equiv\{\mathbf{x}+\imath\mathbf{y}|\|\mathbf{x}\|=\|\mathbf{y}\|=1,\ \mathbf{x}\cdot\mathbf{y}=0\}. \tag{4.8}$$

Let V_ℓ be the subspace of $L^2(S^2)$ generated by the spherical harmonics of order ℓ as previously. Let $f\in V_\ell$. Let us denote by $F_\ell(x_1,x_2,x_3)$ the unique polynomial in three real variables $(x_1,x_2,x_3)\in\mathbf{R}^3$ which is homogeneous of degree ℓ, harmonic ($\Delta_{\mathbf{R}^3}F_\ell\equiv\Sigma_{k=1}^3(\partial^2/\partial x_k^2)F_\ell=0$) and whose restriction to S^2 is equal to f. Let $\tilde{F}_\ell(w_1,w_2,w_3)$ be the polynomial in three complex variables $(w_1,w_2,w_3)\in\mathbf{C}^3$ obtained from F_ℓ by replacing (x_1,x_2,x_3) by (w_1,w_2,w_3). Let us denote by $\mathbf{S}_1$ the assignment $f\mapsto\tilde{F}_\ell$. Now let $\mathbf{S}_2$ be the operator which assigns to $\tilde{F}_\ell$ its restriction $\tilde{F}_\ell|_X$ to the space X. Then finally let us introduce the transformation p_* which applied to $\tilde{F}_\ell|_X$ gives us a function in the space V_ℓ:

$$p_*\tilde{F}_\ell|_X(\mathbf{x})\equiv\int_{\mathbf{y}\in\mathcal{C}_\mathbf{x}}\tilde{F}_\ell|_X(\mathbf{x},\mathbf{y})\mathrm{d}\mu(\mathbf{y}), \tag{4.9}$$

where, for fixed $\mathbf{x}$, the integration is on the unit circle $\mathcal{C}_\mathbf{x}$ in the cotangent space of $\mathbf{x}\in S^2$ and $\mathrm{d}\mu$ is the usual normalized measure on that circle.

It can be shown that the operator $p_*\mathbf{S}_2\mathbf{S}_1$ commutes with all the rotation operators in the representation of SO(3) acting on the space $L^2(S^2)$. Thus, by Schur's lemma, there exist a constant λ_ℓ such that

$$p_*\mathbf{S}_2\mathbf{S}_1f=\lambda_\ell f,\quad f\in V_\ell. \tag{4.10}$$

The constant λ_ℓ can be evaluated by considering the polynomial $(x_1+\imath x_2)^\ell$ and the point $\mathbf{x}=(1,0,0)$ (see Ref. 9). In this way we have $\lambda_\ell=(2\ell-1)!!/\ell!$.

Since the elements of $\mathcal{X}_\ell$ are homogeneous polynomials of degree ℓ in the null quadric $\mathbf{Q}^2$, the exposition above for the operator $p_*\mathbf{S}_2\mathbf{S}_1$ suggests considering the following operator.

Let $f \in V_\ell$ and consider the function $\mathbf{U}_{\sigma_2}^{-1} f$ defined on $\mathbf{Q}^2$. Let G_ℓ be the unique homogeneous polynomial of order ℓ in three complex variables (z_1, z_2, z_3) which is harmonic ($\Delta_{\mathbf{C}^3} F_\ell \equiv \Sigma_{k=1}^{3} (\partial^2/\partial z_k^2) F_\ell = 0$) and whose restriction to $\mathbf{Q}^2$ is equal to $\mathbf{U}_{\sigma_2}^{-1} f$ (denote the assignment $\mathbf{U}_{\sigma_2}^{-1} f \mapsto G_\ell$ by $\mathbf{T}$). Let us now consider the operator $p_* \mathbf{S}_2 \mathbf{T} \mathbf{U}_{\sigma_2}^{-1}$. It can be shown that the operator $p_* \mathbf{S}_2 \mathbf{T} \mathbf{U}_{\sigma_2}^{-1}$ also commutes with all the rotation operators in the representation of SO(3) acting on $L^2(S^2)$. Thus, by Schur's lemma, there exist a constant μ_ℓ such that

$$p_* \mathbf{S}_2 \mathbf{T} \mathbf{U}_{\sigma_2}^{-1} f = \mu_\ell f, \quad f \in V_\ell. \tag{4.11}$$

To evaluate the constant μ_ℓ, we also consider the polynomial $(x_1 + \iota x_2)^\ell$ in V_ℓ and the point $\mathbf{x} = (1,0,0)$, to obtain $\mu_\ell = 1/\ell! \sqrt{2\ell + 1}$.

Thus we finally have, for $F \in \mathcal{X}_\ell$:

$$p_* \mathbf{S}_2 \mathbf{T} F = \frac{1}{\ell! \sqrt{2\ell + 1}} \mathbf{U}_{\sigma_2} F. \tag{4.12}$$

Therefore, we can think of the operator $\mathbf{U}_{\sigma_2}$ as the unitarization of the operator $p_* \mathbf{S}_2 \mathbf{T}$.

B. Quantizations of ρ_3 and σ_3

As in Sec. IV A, let $d\mu_3(\alpha)$ be the measure on $\mathbf{Q}^3$ obtained from the measure $d\nu_4(\mathbf{z}) = (1/\pi^4) \exp(-|\mathbf{z}|^2) \Pi_{j=1}^{4} dx_j\, dy_j$ by push forward along the map ρ_3 (again, here we are regarding the map ρ_3 as a function from $\mathbf{C}^4$ onto $\mathbf{Q}^3$).

Now, given $n \geqslant 1$, let $\mathcal{Z}_n$ be the space of homogeneous polynomials of degree $n-1$ in four complex variables $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ with the restriction $\alpha_1^2 + \alpha_2^2 + \alpha_3^2 + \alpha_4^2 = 0$. We shall consider the following inner product in $\mathcal{Z}_n$,

$$\langle F, G \rangle = \int_{\alpha \in \mathbf{Q}^3} F(\alpha) \overline{G(\alpha)} d\mu_3(\alpha). \tag{4.13}$$

The space $\mathcal{Z}_n$ has dimension n^2 and the following particular orthonormal basis:

$$\Upsilon_{n\ell m} = y_{n\ell m}(\mathbf{z}(\alpha)), \tag{4.14}$$

where since $y_{n\ell m}$ depend on $\mathbf{z}$ through the variables $z_1 z_3$, $z_1 z_4$, $z_2 z_3$, $z_2 z_4$, we mean by $\mathbf{z}(\alpha)$,

$$z_1 z_3 = \frac{-\iota \alpha_1 + \alpha_2}{2}, \quad z_1 z_4 = \frac{\iota \alpha_3 + \alpha_4}{2}, \quad z_2 z_3 = \frac{\iota \alpha_3 - \alpha_4}{2}, \quad z_2 z_4 = \frac{\iota \alpha_1 + \alpha_2}{2}. \tag{4.15}$$

Let $\mathcal{E}_3$ be the Hilbert space generated by the spaces $\mathcal{Z}_n$ with the inner product (4.13).

The quantization of ρ_3 is the unitary operator $\mathbf{U}_{\rho_3} : \mathcal{F}_4 \mapsto \mathcal{E}_3$ given by

$$\mathbf{U}_{\rho_3} \Psi((\alpha)) = \Psi(\mathbf{z}(\alpha)). \tag{4.16}$$

Bargmann and Todorov[8] have studied the inverse of $\mathbf{U}_{\rho_3}$ and considered the space $\mathcal{E}_3$ of holomorphic functions on the null quadric $\mathbf{Q}^3$. As in Sec. IV A, they find the measure $d\mu_3(\alpha)$ by requiring that certain given operators are adjoints of the multiplicative operators by the coordinates in $\mathbf{Q}^3$. The expression they consider for the map ρ_3 has components $(1/\sqrt{2})(\overline{w}_1, \overline{w}_2) q_j(z_1, z_2)^t$ where $j = 1,2,3,4$, $(\overline{w}_1, \overline{w}_2) \in \mathbf{C}^2$ and the 2×2 matrices $q_j = \iota \beta_j$ for $j = 1,2,3$ and q_4 is the 2×2 identity matrix. The expression that we consider in the above-given notation is $(-1)^{j+1}(z_3, z_4) \epsilon q_j (z_1, z_2)^t$.

From Bargmann and Todorov's work we have that the space $\mathcal{F}_4$ is the same subspace of $\mathcal{B}_4$ given by $\{f \in \mathcal{B}_4 | Mf = f\}$, where Mf is the mean value of f:

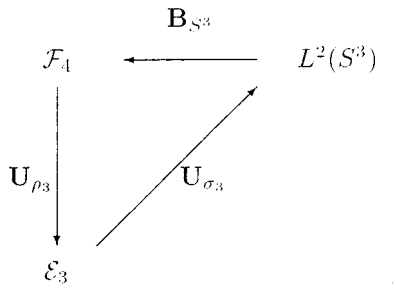
$$Mf(\mathbf{z}) \equiv \int_0^{\pi} f(z_1 \exp(\imath\psi), z_2 \exp(\imath\psi), z_3 \exp(-\imath\psi), z_4 \exp(-\imath\psi)) \frac{d\psi}{2\pi}. \tag{4.17}$$

One can prove this fact by following the proof of proposition (2.1).

The quantization of σ_3 is the unitary map $\mathbf{U}_{\sigma_3}: \mathcal{E}_3 \mapsto L^2(S^3)$ given by the linear extension of the assignment $\Upsilon_{n\ell m} \mapsto Y_{n\ell m}$:

$$\mathbf{U}_{\sigma_3}\Psi(\mathbf{x}) = \lim_{M\mapsto\infty} \int_{|\alpha|\leq M} \left(\sum_{n=1}^{\infty} \frac{\sqrt{n}}{(n-1)!} (\mathbf{x}\cdot\alpha)^{n-1} \right) \Psi(\alpha) d\mu_3(\alpha), \quad \Psi \in \mathcal{E}_3. \tag{4.18}$$

Theorem 4.2: *The following triangle of unitary transformations commutes:*



This triangle is the quantum version of the commuting triangle of canonical transformations in Theorem (3.3).

Remark 2: We can also relate our transformation $\mathbf{U}_{\sigma_3}: \mathcal{E}_4 \mapsto L^{(2)}(S^3)$ with the transformation p_* of Guillemin:[9] For $F \in \mathcal{Z}_n$,

$$p_* \mathbf{S}_2 \mathbf{T} F = \frac{1}{n!\sqrt{n}} \mathbf{U}_{\sigma_3} F, \tag{4.19}$$

where the operators $\mathbf{S}_2$ and $\mathbf{T}$ are defined in a similar way as previously. The proof of this last equation follows the same steps as the one to prove Eq. (4.12). Thus we can think of the operator $\mathbf{U}_{\sigma_3}$ as the unitarization of $p_* \mathbf{S}_2 \mathbf{T}$.

V. THE BARGMANN TRANSFORM AS A COHERENT STATE TRANSFORM

It is known that the Bargmann transform $\mathbf{B}_{\mathbf{R}^n}$ can be identified as a coherent state transform. That is, for any $F \in L^2(\mathbf{R}^n)$, the function $\mathbf{B}_{\mathbf{R}^n} F(\mathbf{z})$ can be expressed as the inner product of F with a canonical coherent state, labeled by $\mathbf{z} \in \mathbf{C}^n$, of the n-dimensional harmonic oscillator.

In this section we show that both Bargmann transforms $\mathbf{B}_{S^2}$ and $\mathbf{B}_{S^3}$ can also be written as coherent states transforms. Here sets of coherent states in $L^2(S^2)$ $[L^2(S^3)]$ appear as linear combinations of states (which we will call great-circle states) for each irreducible representation of SO(3) [SO(4)] that we considered when we defined the Bargmann transform $\mathbf{B}_{S^2}$ $[\mathbf{B}_{S^3}]$.

A. $\mathbf{B}_{\mathbf{R}^n}$ as a coherent state transform

Let us note that the kernel of $\mathbf{B}_{\mathbf{R}^n}$ can be expressed in the following way: let us take $\mathbf{z} = (\mathbf{q} - \imath\mathbf{p})/\sqrt{2}$ with $\mathbf{q}, \mathbf{p} \in \mathbf{R}^n$, then

$$A(\mathbf{x}, \mathbf{z}) = \exp\left(-\frac{(\mathbf{x}-\mathbf{q})^2}{2} + \frac{\imath\mathbf{p}\cdot\mathbf{q}}{2} - \imath\mathbf{p}\cdot\mathbf{x} + \frac{\mathbf{q}^2+\mathbf{p}^2}{4} \right). \tag{5.1}$$

Now let us denote

$$\Phi^{(\mathbf{z})}(\mathbf{x}) = \frac{1}{\pi^{n/4}} \overline{A(\mathbf{x},\mathbf{z})}. \tag{5.2}$$

The functions $\Phi^{(\mathbf{z})} \in L^2(\mathbf{R}^n)$, labeled by $\mathbf{z} \in \mathbf{C}^n$, are the canonical coherent states of the n-dimensional harmonic oscillator.

Since

$$\frac{1}{\pi^{n/2}} \int_{\mathbf{x}\in\mathbf{R}^n} A(\mathbf{x},\mathbf{w})\overline{A(\mathbf{x},\mathbf{z})}\,\mathrm{d}\mathbf{x} = \exp(\overline{\mathbf{z}}\mathbf{w}), \quad \mathbf{z},\mathbf{w} \in \mathbf{C}^n, \tag{5.3}$$

then we have that the Bargmann transform sends the coherent states of the n-dimensional harmonic oscillator into the coherent states defined in Sec. II:

$$\mathbf{B}_{\mathbf{R}^n}\Phi^{(\mathbf{z})}(\mathbf{w}) = \Psi_{\mathbf{z}}(\mathbf{w}), \tag{5.4}$$

thus the Bargmann transform $\mathbf{B}_{\mathbf{R}^n}$ acting on a function $F \in L^2(\mathbf{R}^n)$ can be expressed as a coherent state transform:

$$\mathbf{B}_{\mathbf{R}^n}F(\mathbf{z}) = \langle F, \Phi^{(\mathbf{z})}\rangle = \int_{\mathbf{x}\in\mathbf{R}^n} F(\mathbf{x})\overline{\Phi^{(\mathbf{z})}(\mathbf{x})}\,\mathrm{d}\mathbf{x}. \tag{5.5}$$

It is also known that the set of coherent states $\Phi^{(\mathbf{z})}$ gives a resolution of the identity in the sense that every function $F \in L^2(\mathbf{R}^n)$ can be written as

$$F(\mathbf{x}) = \lim_{M\mapsto\infty} \int_{|\mathbf{z}|\le M} \langle F, \Phi^{(\mathbf{z})}\rangle_{\mathbf{R}^n}\Phi^{(\mathbf{z})}(\mathbf{x})\,\mathrm{d}\nu_n(\mathbf{z}), \tag{5.6}$$

where $\mathrm{d}\nu_n(\mathbf{z})$ is the measure given in Eq. (2.1).

B. $\mathbf{B}_{S^2}$ as a coherent state transform

In Sec. III we showed that the generating function Φ_{S^2} can be written as the inner product of the vectors $\rho_2(\mathbf{z}) \in \mathbf{Q}^2$ and $\mathbf{x} \in S^2$ [see Eq. (3.13)]. Thus we are able to establish the following

Theorem 5.1: *The Bargmann transform* $\mathbf{B}_{S^2}$ *is a coherent state transform in the sense that* $\mathbf{B}_{S^2}$ *acting on a function* $\Psi \in L^2(S^2)$ *can be written in the following way:*

$$\mathbf{B}_{S^2}\Psi(\mathbf{z}) = \langle \Psi, \Phi_{\rho_2(\mathbf{z})}\rangle_{S^2} \tag{5.7}$$

where, for each $\alpha \in \mathbf{Q}^2$, *we define the coherent states*

$$\Phi_\alpha(\mathbf{x}) = \sum_{\ell=0}^{\infty} \frac{\sqrt{2\ell+1}}{\ell!}\Phi_{\alpha,\ell}(\mathbf{x}) \tag{5.8}$$

with the states $\Phi_{\alpha,\ell}$ *given by*

$$\Phi_{\alpha,\ell}(\mathbf{x}) = (\mathbf{x}\cdot\alpha)^{\ell}. \tag{5.9}$$

The states $\Phi_{\alpha,\ell}$ have the following properties.

(a) For each integer $\ell \ge 1$, the states $\Phi_{\alpha,\ell}$, belong to the eigenspace V_ℓ of the Laplacian Δ_{S^2} (see Ref. 10).

(b) For large ℓ, and $\alpha \neq 0$, the state $\Phi_{\alpha,\ell}$ is concentrated around the great circle in S^2 (classical orbit) generated by the vectors $\Re(\alpha)/\|\Re(\alpha)\|$ in S^2 and $-\Im(\alpha)$ in T^*S^2 at the point $\Re(\alpha)/\|\Re(\alpha)\|$. The concentration is in the sense that most of the $L^2(S^2)$-norm of $\Phi_{\alpha,\ell}$ comes from a small neighborhood of the great circle (see Ref. 7). This is the reason why we call the states $\{\Phi_{\alpha,\ell}\}$ great-circle states.

(c) The states $\{\Phi_{\alpha,\ell}\}$ give a resolution of the identity in the space V_ℓ. Namely, for each function $\Psi \in V_\ell$, the following equation holds

$$\Psi(\mathbf{x}) = r(\ell)\int_{\mathbf{Q}^2}\langle \Psi, \Phi_{\alpha,\ell}\rangle_{S^2}\Phi_{\alpha,\ell}(\mathbf{x})\,\mathrm{d}\mu_2(\alpha) \tag{5.10}$$

for some constant $r(\ell)$ which will be evaluated in the following.

This equation is a consequence of the following three facts: (i) the operator on the right-hand side of Eq. (5.10) commutes with all the rotations in SO(3) acting as operators on V_ℓ, (ii) the irreducibility of the representation of SO(3) acting on V_ℓ, and (iii) the invariance of the measure $\mathrm{d}\mu_2(\alpha)$ under rotations in SO(3), which we state as follows:

Proposition 5.2: Let $R \in \mathrm{SO}(3)$, then for any $\mathrm{d}\mu_2$-integrable function $f(\alpha)$ we have

$$\int_{\mathbf{Q}^2} f(R\alpha)\,\mathrm{d}\mu_2(\alpha) = \int_{\mathbf{Q}^2} f(\alpha)\,\mathrm{d}\mu_2(\alpha). \tag{5.11}$$

Here, $R\alpha$ means $R\Re(\alpha) + \imath R\Im(\alpha)$.

We are calling the states Φ_α coherent states because, for $\alpha \neq 0$, they are labeled by elements of $T^*(S^2) - \{0\}$ (through the map σ_2) and they give a resolution of the identity for the space $L^2(S^2)$:

$$\Psi(\mathbf{x}) = \int_{\mathbf{Q}^2}\langle \Psi, \Phi_\alpha\rangle_{S^2}\Phi_\alpha(\mathbf{x})\,\mathrm{d}\mu_2(\alpha), \qquad \Psi \in L^2(S^2). \tag{5.12}$$

This last equation is a consequence of Eq. (5.10) and the fact that homogeneous polynomials in $\mathcal{E}_2$ of different order are orthogonal.

For each ℓ, the images of the great-circle states $\Phi_{\alpha,\ell}$ under the transformation $\mathbf{U}_{\sigma_2}^{-1} = \mathbf{B}_{S^2} \circ \mathbf{U}_{\rho_2}$ provides a reproducing kernel for the space $\mathcal{X}_\ell$. The proof of this fact is based on the following two propositions:

Proposition 5.3: The inner product of two great-circle states $\Phi_{\beta,\ell}$ and $\Phi_{\alpha,k}$ in $L^2(S^2)$ $(\alpha, \beta \in \mathbf{Q}^2)$ is

$$\langle \Phi_{\beta,\ell}, \Phi_{\alpha,k}\rangle_{S^2} = \frac{\gamma_\ell}{2^{\ell+1}}(\alpha\cdot\beta)^\ell \delta_{\ell,k}, \tag{5.13}$$

with $\gamma_\ell \equiv \int_0^\pi \sin^{2\ell+1}(\theta)\,\mathrm{d}\theta = 2[(2\ell)!!/(2\ell+1)!!]$ [here the notation $(2\ell)!!$ means the product of all positive even integers less than or equal to 2ℓ, the notation for $(2\ell+1)!!$ is similar].

Proof: Given $\beta \in \mathbf{Q}^2 - 0$, there exists $\lambda > 0$ and a rotation $R \in \mathrm{SO}(3)$ such that $\beta = \lambda R(\mathbf{e}_1 - \imath\mathbf{e}_2)$ (with $\{\mathbf{e}_j, j = 1,2,3\}$ the canonical orthonormal basis of $\mathbf{R}^3$). Thus

$$\langle \Phi_{\beta,\ell}, \Phi_{\alpha,\ell}\rangle_{S^2} = \lambda^\ell \int_{\mathbf{x}\in S^2} (\mathbf{x}\cdot R(\mathbf{e}_1 - \imath\mathbf{e}_2))^\ell \overline{(\mathbf{x}\cdot\alpha)^\ell}\,\mathrm{d}\sigma_2(\mathbf{x}). \tag{5.14}$$

By making the change of variable $\mathbf{y} = R^{-1}\mathbf{x}$, using spherical coordinates for the variable $\mathbf{y}$ and the orthogonality of the matrix R, the result follows by a straightforward computation. □

Proposition 5.4: The Bargmann transform $\mathbf{B}_{S^2}$ of the great-circle state $\Phi_{\beta,\ell}$ $(\beta \in \mathbf{Q}^2)$ is

$$\mathbf{B}_{S^2}\Phi_{\beta,\ell}(\mathbf{z}) = \frac{\sqrt{2\ell+1}}{\ell!}\,\frac{\gamma_\ell}{2^{\ell+1}}(\rho_2(\mathbf{z})\cdot\beta)^\ell. \tag{5.15}$$

Thus the image of the coherent state $\Phi_{\beta,\ell}$ under the transformation $\mathbf{U}_{\sigma_2}^{-1}$ is

$$\mathbf{U}_{\sigma_2}^{-1}\Phi_{\beta,\ell}(\alpha) = \frac{\sqrt{2\ell+1}}{\ell!}\,\frac{\gamma_\ell}{2^{\ell+1}}(\alpha\cdot\beta)^\ell. \tag{5.16}$$

The factor $(\alpha\cdot\beta)^{\ell}$ appearing in Eq. (5.16) provides us with a reproducing kernel for the space $\mathcal{X}_{\ell}$, as the following theorem establishes it:

Theorem 5.5: *For each integer* $\ell \geqslant 1$, *the function* $K_{\mathbf{Q}^2,\ell}:\mathbf{Q}^2\times\mathbf{Q}^2\mapsto\mathbf{C}$ *given by*

$$K_{\mathbf{Q}^2,\ell}(\alpha,\beta)=\frac{2^{\ell}}{(2\ell)!}(\beta\cdot\alpha)^{\ell} \tag{5.17}$$

is a reproducing kernel for the space $\mathcal{X}_{\ell}$, *that is,*

$$\int_{\mathbf{Q}^2} f(\alpha)K_{\mathbf{Q}^2,\ell}(\alpha,\beta)\mathrm{d}\mu_2(\alpha)=f(\beta), \qquad f\in\mathcal{X}_{\ell}. \tag{5.18}$$

Proof: It is enough to prove Eq. (5.18) when $f=\Upsilon_{\ell,m}$. From the definition of $\mathrm{d}\mu_2$ we have

$$\int_{\mathbf{Q}^2}\Upsilon_{\ell,m}(\alpha)K(\alpha,\beta)\mathrm{d}\mu_2(\alpha)=\int_{\mathbf{z}\in\mathbf{C}^2} y_{\ell,m}(\mathbf{z})\frac{2^{\ell}}{(2\ell)!}\overline{(\rho_2(\mathbf{z})\cdot\boldsymbol{\beta})^{\ell}}\mathrm{d}\nu_2(\mathbf{z}). \tag{5.19}$$

Now let us define the function

$$\Phi_{\rho_2}(\mathbf{z},\alpha)\equiv\overline{y_{1,1}(\mathbf{z})}\Upsilon_{1,1}(\alpha)+\overline{y_{1,0}(\mathbf{z})}\Upsilon_{1,0}(\alpha)+\overline{y_{1,-1}(\mathbf{z})}\Upsilon_{1,-1}(\alpha)=\alpha\cdot\rho_2(\mathbf{z}). \tag{5.20}$$

Since

$$(\Phi_{\rho_2}(\mathbf{z},\beta))^{\ell}=\frac{(2\ell)!}{2^{\ell}}\sum_{m=-\ell}^{\ell}\overline{y_{\ell,m}}(\mathbf{z})\Upsilon_{\ell,m}(\beta), \tag{5.21}$$

the result follows. □

We can use this theorem, in particular, to evaluate the constant $r(\ell)$ appearing in Eq. (5.10) in the following manner: Let us apply Eq. (5.10) to the state $\Phi_{\beta,\ell}$:

$$\begin{aligned}\Phi_{\beta,\ell}(\mathbf{x})&=r(\ell)\int_{\alpha\in\mathbf{Q}^2}\langle\Phi_{\beta,\ell}\Phi_{\alpha,\ell}\rangle_{S^2}\Phi_{\alpha,\ell}(\mathbf{x})\mathrm{d}\mu_2(\alpha)\\&=r(\ell)\frac{\gamma_{\ell}}{2^{\ell+1}}\int_{\alpha\in\mathbf{Q}^2}(\alpha\cdot\beta)^{\ell}\Phi_{\alpha,\ell}(\mathbf{x})d\mu_2(\alpha)\\&=r(\ell)\frac{\gamma_{\ell}(2\ell)!}{2^{2\ell+1}}\overline{\int_{\alpha\in\mathbf{Q}^2}(\alpha\cdot\mathbf{x})^{\ell}K_{\mathbf{Q}^2,\ell}(\alpha,\beta)\mathrm{d}\mu_2(\alpha)}.\end{aligned} \tag{5.22}$$

Thus from Eq. (5.18) we must have

$$r(\ell)=\frac{2^{2\ell+1}}{\gamma_{\ell}(2\ell)!}. \tag{5.23}$$

From Theorem (5.5) we also obtain a reproducing kernel for the space $\mathcal{E}_3$:

Theorem 5.6: *The function*

$$K_{\mathbf{Q}^2}(\alpha,\beta)\equiv\sum_{\ell=0}^{\infty}\frac{2^{\ell}}{(2\ell)!}(\beta\cdot\alpha)^{\ell}=\frac{1}{2}(\exp(\sqrt{2\beta\cdot\alpha})+\exp(-\sqrt{2\beta\cdot\alpha})) \tag{5.24}$$

is an analytic function in the space $\mathcal{E}_3$ *(for* α *fixed) and provides a reproducing kernel for this space:*

$$\int_{\mathbf{Q}^2} f(\alpha) K_{\mathbf{Q}^2}(\alpha,\beta)\mathrm{d}\mu_2(\alpha) = f(\beta), \qquad f \in \mathcal{E}_3. \tag{5.25}$$

Note that Eq. (5.24) is independent of the branch of the square root function we have chosen.

Proof: The series $\Sigma_{\ell=0}^{\infty}[2^{\ell}/(2\ell)!]z^{\ell}$ is absolutely convergent for all values of $z \in \mathbf{C}$, so $K_{\mathbf{Q}^2}(\alpha,\beta)$ is an analytic function in the variable β (α fixed).

Moreover, each function $2^{\ell}(\beta\cdot\alpha)^{\ell}/(2\ell)!$ belongs to the space $\mathcal{X}_{\ell}$ and its norm $a_{\ell}^2 \equiv \|2^{\ell}(\beta\cdot\alpha)^{\ell}/(2\ell)!\|^2$ is equal to $2^{3\ell+1}/(2\ell+1)\gamma_{\ell}(\ell!/(2\ell)!)^2|\alpha|^{2\ell}$. Since $\Sigma_{\ell=0}^{\infty} a_{\ell}^2$ is finite, we conclude that the kernel $K_{\mathbf{Q}^2}$ is in $\mathcal{E}_3$ (α fixed). The equality in Eq. (5.24) can be checked directly by using the Taylor series of the exponential function. □

The kernel $K_{\mathbf{Q}^2}$ and the function ρ_2 give an expected reproducing kernel for the space $\mathcal{B}_{S^2}$:

Theorem 5.7: *The following function* $\frac{1}{2}(\exp(\mathbf{z}\cdot\mathbf{w}) + \exp(-\mathbf{z}\cdot\mathbf{w}))$ *is a reproducing kernel of the space* $\mathcal{B}_{S^2}$. *This function is in the space* $\mathcal{B}_{S^2}$ *for* $\mathbf{w}$ *fixed.*

C. B_{S^3} as a coherent state transform

This section is the analog of Sec. IV B concerning the Bargmann Transform $\mathbf{B}_{S^3}$. Namely, we will show that this transform can also be written as a coherent state transform (with the coherent states defined in a similar way as before), and we also have a reproducing kernel for the spaces $\mathcal{Z}_n$, $\mathcal{E}_4$, and $\mathcal{F}_4$.

From the definition of $\mathbf{B}_{S^3}$, Eq. (2.47), we obtain:

Theorem 5.8:

$$\mathbf{B}_{S^3}\Psi(\mathbf{z}) = \langle \Psi, \Phi_{\rho_3(\mathbf{z})}\rangle_{S^3}, \quad \Psi \in L^2(S^3), \tag{5.26}$$

where the coherent states in $L^2(S^3)$ *are defined by*

$$\Phi_{\alpha}(\mathbf{x}) = \sum_{n=1}^{\infty} \frac{\sqrt{n}}{(n-1)!}\Phi_{\alpha,n-1}(x), \qquad \alpha \in \mathbf{Q}^3 \tag{5.27}$$

and the great-circle states $\Phi_{\alpha,n-1}$ *are defined by*

$$\Phi_{\alpha,n-1}(\mathbf{x}) = (\mathbf{x}\cdot\alpha)^{n-1}, \qquad \alpha \in \mathbf{Q}^3, \qquad n \geqslant 1. \tag{5.28}$$

The great-circle states $\Phi_{\alpha,n-1}$ have properties analogous to those of the states defined in Sec. IV B and in particular they provide a resolution of the identity:

For $\Psi \in \mathcal{M}_n$, the following equation holds:

$$\Psi(\mathbf{x}) = \frac{n}{((n-1)!)^2}\int_{\mathbf{Q}^3-\{0\}} \langle \Psi, \Phi_{\alpha,n-1}\rangle_{S^3}\Phi_{\alpha,n-1}(\mathbf{x})\mathrm{d}\mu_4(\alpha), \tag{5.29}$$

and therefore the coherent states Φ_{α}, $\alpha \in \mathbf{Q}^3$, give a resolution of the identity for $L^2(S^3)$:

$$\Psi(\mathbf{x}) = \int_{\mathbf{Q}^3-\{0\}} \langle \Psi, \Phi_{\alpha}\rangle_{S^3}\Phi_{\alpha}(\mathbf{x})\mathrm{d}\mu_4(\alpha), \qquad \Psi \in L^2(S^3). \tag{5.30}$$

Note that the coherent states Φ_{α} are labeled by elements of $T^*S^3 - \{0\}$ through the map σ_3.

Equation (5.29) is a consequence of the following four facts:

Proposition 5.9: The inner product of two coherent states in $L^2(S^3)$ *is*

$$\langle \Phi_{\beta,k}, \Phi_{\alpha,\ell}\rangle_{S^3} = \frac{1}{(k+1)2^k}(\alpha\cdot\beta)^k\delta_{\ell,k}, \qquad k \geqslant 0. \tag{5.31}$$

The invariance of the measure $\mathrm{d}\mu_4$ under rotations $R \in \mathrm{SO}(4)$:

Proposition 5.10: Let $R \in \mathrm{SO}(4)$. *for any* $\mathrm{d}\mu_4$*-integrable function* $f(\alpha)$ *the following equation holds:*

$$\int_{\mathbf{Q}^3} f(R\alpha)\mathrm{d}\mu_4(\alpha) = \int_{\mathbf{Q}^3} f(\alpha)\mathrm{d}\mu_4(\alpha). \tag{5.32}$$

Proposition 5.11: The Bargmann transform $\mathbf{B}_{S^3}$ *maps the great-circle states* $\Phi_{\beta,k}$ *as follows:*

$$\mathbf{B}_{S^3}\Phi_{\beta,k}(\mathbf{z}) = \frac{\sqrt{k+1}}{(k+1)!\,2^k}(\rho_3(\mathbf{z})\cdot\beta)^k, \qquad k \geqslant 0 \tag{5.33}$$

and then the image of the coherent states $\Phi_{\beta,k}$ *under the unitary transformation* $\mathbf{U}_{\sigma_3}^{-1}$ *is*

$$\mathbf{U}_{\sigma_3}^{-1}\Phi_{\beta,k}(\alpha) = \frac{\sqrt{k+1}}{(k+1)!\,2^k}(\alpha\cdot\beta)^k, \qquad k \geqslant 0. \tag{5.34}$$

Theorem 5.12: *For each integer* $n \geqslant 1$, *the function* $K_{\mathbf{Q}^3,n}: \mathbf{Q}^3 \times \mathbf{Q}^3 \mapsto \mathbf{C}$ *given by*

$$K_{\mathbf{Q}^3,n-1}(\alpha,\beta) \equiv \frac{1}{((n-1)!)^2 2^{n-1}}(\beta\cdot\alpha)^{n-1} \tag{5.35}$$

is a reproducing kernel for the space $\mathcal{Z}_n$.

The proofs of these facts are similar to those given in Sec. IV B.

Theorem 5.12 provides us with a reproducing kernel for the space $\mathcal{E}_4$:

Theorem 5.12: *The function*

$$K_{\mathbf{Q}^3}(\alpha,\beta) \equiv \sum_{n=1}^{\infty} \frac{1}{((n-1)!)^2 2^{n-1}}(\beta\cdot\alpha)^{n-1} \tag{5.36}$$

belongs to the space $\mathcal{E}_4$ *(for* α *fixed) and it is a reproducing kernel of this space.*

From this last theorem and the map ρ_3 we obtain the following

Theorem 5.13: *The function*

$$\tilde{K}_{\mathbf{Q}^3}(\mathbf{z},\mathbf{w}) \equiv \sum_{n=1}^{\infty} \frac{1}{((n-1)!)^2}((\overline{w}_1 z_1 + \overline{w}_2 z_2)(\overline{w}_3 z_3 + \overline{w}_4 z_4))^{n-1} \tag{5.37}$$

belongs to the space $\mathcal{F}_4$ *(for* $\mathbf{w}$ *fixed) and it is a reproducing kernel of this space.*

As noted by Bargmann and Todorov,[8] the function $\tilde{K}_{\mathbf{Q}^3}$ can be expressed in terms of the modified Bessel function of the first kind $I_0(z) \equiv \Sigma_{m=0}^{\infty}[1/(m!)^2](z/2)^{2m}$:

$$\tilde{K}_{\mathbf{Q}^3}(\mathbf{z},\mathbf{w}) = I_0(2\sqrt{(\overline{w}_1 z_1 + \overline{w}_2 z_2)(\overline{w}_3 z_3 + \overline{w}_4 z_4)}). \tag{5.38}$$

VI. DISCUSSION

The transformations $\mathbf{U}_{\sigma_2}$ and $\mathbf{U}_{\sigma_3}$ can be generalized to a unitary transformation $\mathbf{U}_{\sigma_n}$ for the case of the n-sphere S^n (with $n \geqslant 2$) on the basis of the work of Bargmann and Todorov.[8] Namely, these two authors describe a Hilbert space $\mathcal{E}_n$ of holomorphic functions on the null quadric $\mathbf{Q}^n$ endowed with an inner product which in turn is determined by an $\mathrm{SO}(n+1)$ invariant measure on $\mathbf{Q}^n$. Thus, by taking the hyperspherical harmonics as a basis of $L^2(S^n)$ and assigning to them corresponding elements of a basis of $\mathcal{E}_n$, we can define $\mathbf{U}_{\sigma_n}$ as the linear extension of such assignment. The detailed description of this transform will appear in a further work.

There are other Bargmann-type transforms like $\mathbf{U}_{\sigma_2}$, $\mathbf{U}_{\sigma_3}$, and $\mathbf{U}_{\sigma_n}$ that have been introduced by several authors. They all are different from our transforms. Here we briefly discuss these transforms and compare them with ours.

Rawnsley,[11] in analogy with the case of the Bargmann transform for $L^2(\mathbf{R}^n)$, considered real and complex polarizations of the phase space $T^*S^n-\{0\}$ and the half-form pairing between them (which turns out to be nonunitary).

Ii[12] considered an integral operator between $L^2(S^n)$, with $n\geqslant 2$ even, and a Hilbert space of holomorphic functions on the null quadric $\mathbf{Q}^n$. This operator is defined through an integral kernel given by the exponential of $\alpha\cdot\mathbf{x}$ ($\alpha\in\mathbf{Q}^n$, and $\mathbf{x}\in S^n$), whereas we consider a different power series in this function. Ii makes his integral operator unitary by endowing $\mathbf{Q}^n$ with a different measure than the one considered by ourselves and Bargmann and Todorov. Note that our transform $\mathbf{U}_{\sigma_n}$ is defined first by setting the measure on $\mathbf{Q}^n$ and then by adjusting the coefficients of the power series in $\alpha\cdot\mathbf{x}$ in order to make $\mathbf{U}_{\sigma_n}$ unitary. Wada[13] was able to remove the condition that n must be even and then she obtained a unitary transformation for all $n\geqslant 2$ that coincides with the transformation of Ii for n even.

Hall[14,15] and Stenzel[16] have considered a Bargmann-type transform when the configuration space is either a compact Lie group or a symmetric space of compact type. They base their approach on the heat kernel for the corresponding manifold. Thus they define their Bargmann transform and coherent states. One of the main differences with our approach is that they consider the quadric $\{\alpha\in\mathbf{C}^{(n+1)}|\,\alpha_1^2+\cdots\alpha_{n+1}^2=1\}$ whereas we consider the null quadric $\mathbf{Q}^n$.

Kowalski and Rembieliński[17] have considered coherent states for the two-sphere as eigenvectors of suitable operators. On the basis of a suggestion by Hall, the states of Kowalski and Rembieliński can be related with the coherent states appearing in the work of Hall[14,15] and Stenzel.[16] This suggestion allowed Kowalski and Rembieliński[18] to solve an equation through a heat kernel and then to be able to set up a Bargmann-type transform for $L^2(S^2)$. They also deal with the quadric $\{\alpha\in\mathbf{C}^{(n+1)}|\,\alpha_1^2+\cdots\alpha_{n+1}^2=1\}$.

Inspired in part by the work of Kowalski and Rembieliński,[18] Hall and Mitchell[19] have written a recent paper describing in detail coherent states and a Bargmann-type transform for $L^2(S^n)$ related to the work of Hall[14,15] and Stenzel.[16]

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APPENDIX A: THE KERNEL OF THE BARGMANN TRANSFORM FOR S^2

The purpose of this appendix is to prove Eqs. (2.22) and (2.23). We want to do this by showing that the following equation holds for all $k\geqslant 0$:

$$\mathcal{K}_k(\mathbf{x},\mathbf{z})=\frac{\sqrt{2k+1}}{k!}\left(\frac{1}{\sqrt{3}}\right)^k(\Phi_{S^2})^k(\mathbf{x},\mathbf{z}),$$

with $\mathcal{K}_k(\mathbf{x},\mathbf{z})=\Sigma_{m=-k}^{k}Y_{km}^*(\mathbf{x})y_{km}(\mathbf{z})$.

The main idea of the proof is based on the fact that the following function $G_k(\mathbf{x},\mathbf{z})\equiv\mathcal{K}_k(\mathbf{x},\mathbf{z})/c(k)(\Phi_{S^2}(\mathbf{x},\mathbf{z}))^k$ [with $c(k)$ some constant] satisfies an homogeneous system of first-

order differential equations with initial condition $G_k(\mathbf{x}_0,\mathbf{z}_0)=1$. Then we show that the gradient of G_k must be zero, which implies that the solution of the system must be $G_k(\mathbf{x},\mathbf{z})\equiv 1$, i.e., $\mathcal{K}_k(\mathbf{x},\mathbf{z})=c(k)(\Phi_{S^2}(\mathbf{x},\mathbf{z}))^k$. Next, we evaluate the constant $c(k)$.

We know that the Bargmann transform $\mathbf{B}_{S^2}$ intertwines the operators L_i and L_i', $i=1,2,3$. Thus for any smooth function $\Psi(\mathbf{x})$,

$$L_i'\mathbf{B}_{S^2}\Psi=\mathbf{B}_{S^2}L_i\Psi.$$

Now we want to show that for any $k\geqslant 0$,

$$(L_i+L_i')\mathcal{K}_k(\mathbf{x},\mathbf{z})=0, \qquad i=1,2,3.$$

Let P_k be the projector on the span of $\{y_{km}(\mathbf{z})/m=-k,\ldots,k\}$. P_k acts on the Bargmann space $\mathcal{B}_2$. Thus we have for any smooth function $\Psi(\mathbf{x})$,

$$P_k\mathbf{B}_{S^2}\Psi(\mathbf{z})=\int_{\mathbf{x}\in S^2}\mathcal{K}_k(\mathbf{x},\mathbf{z})\Psi(\mathbf{x})\mathrm{d}\Omega(\mathbf{x}),$$

which implies

$$P_k\mathbf{B}_{S^2}L_i\Psi(\mathbf{z})=-\int_{\mathbf{x}\in S^2}(L_i\mathcal{K}_k(\mathbf{x},\mathbf{z}))\Psi(\mathbf{x})\mathrm{d}\Omega(\mathbf{x}),$$

where we have used the self-adjointness of L_i.

On the other hand, if we apply P_k to both sides of the equation $L_i'\mathbf{B}_{S^2}\Psi=\mathbf{B}_{S^2}L_i\Psi$ and use the fact that P_k commutes with L_i', $i=1,2,3$, we get

$$P_k\mathbf{B}_{S^2}L_i\Psi(\mathbf{z})=\int_{\mathbf{x}\in S^2}L_i'\mathcal{K}_k(\mathbf{x},\mathbf{z})\Psi(\mathbf{x})\mathrm{d}\Omega(\mathbf{x}).$$

Since the last two equations hold for a dense set in $L^2(S^2)$, we conclude that $(L_i+L_i')\mathcal{K}_k(\mathbf{x},\mathbf{z})=0$, $i=1,2,3$.

The function $\mathcal{K}_k$ satisfies another differential equation which is a consequence that $\mathcal{K}_k$ is an homogeneous polynomial of degree $2k$ in the variables (z_1,z_2). Thus we must have for all $k\geqslant 0$:

$$(H_0-2k)\mathcal{K}_k=0 \quad \text{with} \quad H_0=z_1\partial_1+z_2\partial_2.$$

The above-given analysis must hold, in particular, for $k=1$. Thus we have

$$(L_i+L_i')\Phi_{S^2}(\mathbf{x},\mathbf{z})=0, \quad i=1,2,3 \quad \text{and} \quad (H_0-2)\Phi_{S^2}=0.$$

Since L_i, L_i', and H_0 are first-order linear differential operators, we have for all $k\geqslant 0$,

$$(L_i'+L_i)\Phi_{S^2}^k=0, \quad (H_0-2k)\Phi_{S^2}^k=0.$$

Now consider a particular point $(\mathbf{x}_0,\mathbf{z}_0)$ where $\Phi_{S^2}(\mathbf{x}_0,\mathbf{z}_0)\neq 0$. Let

$$c(k)=\mathcal{K}_k(\mathbf{x}_0,\mathbf{z}_0)/\Phi_{S^2}^k(\mathbf{x}_0,\mathbf{z}_0).$$

Define the function

$$G_k(\mathbf{x},\mathbf{z})=\frac{\mathcal{K}_k(\mathbf{x},\mathbf{z})}{c(k)\Phi_{S^2}^k(\mathbf{x},\mathbf{z})}.$$

This function satisfies the following system of homogeneous first-order differential equations:

$$(L_i' + L_i)G_k(\mathbf{x},\mathbf{z}) = 0, \quad i = 1,2,3 \quad \text{and} \quad H_0 G_k(\mathbf{x},\mathbf{z}) = 0$$

with initial condition $G_k(\mathbf{x}_0,\mathbf{z}_0) = 1$.

The system of equations can also be written as

$$\mathbf{M}\nabla G_k = 0$$

with $\nabla = (\partial/\partial\theta, \partial/\partial\phi, \partial/\partial z_1, \partial/\partial z_2)$ and $\mathbf{M}$ a 4×4 matrix given by

$$\mathbf{M} = \begin{bmatrix} \imath \sin(\phi) & \imath \cot(\theta)\cos(\phi) & \frac{1}{2}z_2 & \frac{1}{2}z_1 \\ -\imath \cos(\phi) & \imath \cot(\theta)\sin(\phi) & -\frac{1}{2\imath}z_2 & \frac{1}{2\imath}z_1 \\ 0 & -\imath & \frac{1}{2}z_1 & \frac{-1}{2}z_2 \\ 0 & 0 & z_1 & z_2 \end{bmatrix}.$$

The determinant of the matrix $\mathbf{M}$ is

$$\det \mathbf{M} = \frac{-1}{\sqrt{3}\sin(\theta)}\Phi_{S^2}(\mathbf{x},\mathbf{z}).$$

Since $\Phi_{S^2}(\mathbf{x}_0,\mathbf{z}_0) \neq 0$, $\mathbf{M}$ is then invertible on a neighborhood $\mathcal{V}$ of the point $(\mathbf{x}_0,\mathbf{z}_0)$. Therefore, we must have

$$G_k(\mathbf{x},\mathbf{z}) = 1 \quad \text{for all} \quad (\mathbf{x},\mathbf{z}) \in \mathcal{V}$$

and then

$$\mathcal{K}_k = c(k)\Phi_{S^2}^k(\mathbf{x},\mathbf{z}) \quad \text{for all} \quad (\mathbf{x},\mathbf{z}) \in \mathcal{V}.$$

Since $\mathcal{K}_k$ and $\Phi_{S^2}^k$ are analytic functions of $(\mathbf{x}, \mathbf{z})$, the last equation must actually hold for all $(\mathbf{x}, \mathbf{z})$.

Finally, we want to evaluate the constant $c(k)$ appearing in the last equation. By using

$$Y_{11}(\mathbf{x}) = -\sqrt{\frac{3}{2}}\sin(\theta)\exp(\imath\phi), \quad Y_{1-1}(\mathbf{x}) = \sqrt{\frac{3}{2}}\sin(\theta)\exp(-\imath\phi),$$

$$Y_{10}(\mathbf{x}) = \sqrt{3}\cos(\theta), \quad y_{11}(\mathbf{z}) = \frac{z_1^2}{\sqrt{2}}, \quad y_{10}(\mathbf{z}) = z_1 z_2, \quad y_{1-1}(\mathbf{z}) = \frac{z_2^2}{\sqrt{2}},$$

we obtain Eq. (2.23).

Now consider the relation

$$Y_{km}(\mathbf{x}) = \sqrt{\frac{(2k+1)(k-m)!}{(k+m)!}}P_k^m(\cos(\theta))\exp(\imath m\phi),$$

with P_k^m the associated Legendre polynomials. By taking $\theta = 0$ and since $P_k^m(1) = 1\,\delta_{m0}$,

$$\sqrt{(2k+1)}\frac{z_1^k z_2^k}{k!}=c(k)(\sqrt{3}z_1z_2)^k,$$

which in turn implies $c(k)=[\sqrt{2k+1}/k!](1/\sqrt{3})^k$, and then Eq. (2.22).

APPENDIX B: THE KERNEL OF THE BARGMANN TRANSFORM FOR S^3

The purpose of this appendix is to demonstrate Eqs. (2.50) and (2.51).

We want to do it by showing that for all $n\geqslant 1$:

$$\tilde{\mathcal{K}}_n(\mathbf{x},\mathbf{z})=\frac{\sqrt{2n}}{(n-1)!}\frac{1}{2^{n/2}}(\Phi_{S^3})^{n-1}(\mathbf{x},\mathbf{z})$$

with

$$\tilde{\mathcal{K}}_n(\mathbf{x},\mathbf{z})=\sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{m=\ell}Y^*_{n\ell m}(\mathbf{x})y_{n\ell m}(\mathbf{z}).$$

The idea of the proof is exactly the same as the one we used in Appendix A. Thus for each $n\geqslant 1$, let us define the function

$$F_n(\mathbf{x},\mathbf{z})=\tilde{\mathcal{K}}_n(\mathbf{x},\mathbf{z})/(c(n)(\Phi_{S^3})^{n-1}(\mathbf{x},\mathbf{z}))$$

[in a neighborhood $\mathcal{V}$ of a point $(\mathbf{x}_0,\mathbf{z}_0)$ where $(\Phi_{S^3})(\mathbf{x}_0,\mathbf{z}_0)\neq 0$] such that F_n is a solution of the system of differential equations:

$$\mathbf{M}\nabla F_n=0$$

with $\nabla=(\partial/\partial\theta,\partial/\partial\phi,\partial/\partial\lambda,\partial/\partial z_1,\partial/\partial z_2,\partial/\partial z_3,\partial/\partial z_4)$ and $\mathbf{M}$ the 7×7 matrix

$$\begin{bmatrix}
\imath\sin(\phi) & \imath\cot(\theta)\cos(\phi) & 0 & \frac{z_2}{2} & \frac{z_1}{2} & \frac{z_4}{2} & \frac{z_3}{2}\\
-\imath\cos(\phi) & \imath\cot(\theta)\sin(\phi) & 0 & -\frac{z_2}{2\imath} & \frac{z_1}{2\imath} & -\frac{z_4}{2\imath} & \frac{z_3}{2\imath}\\
0 & -\imath & 0 & \frac{z_1}{2} & -\frac{z_2}{2} & \frac{z_3}{2} & -\frac{z_4}{2}\\
f(\phi,\lambda) & \frac{-\cot(\lambda)\sin(\phi)}{\imath\sin(\theta)} & -\imath\sin(\theta)\cos(\phi) & \frac{z_2}{2} & \frac{z_1}{2} & -\frac{z_4}{2} & -\frac{z_3}{2}\\
g(\phi,\lambda) & \frac{\cot(\lambda)\cos(\phi)}{\imath\sin(\theta)} & -\imath\sin(\theta)\sin(\phi) & -\frac{z_2}{2\imath} & \frac{z_1}{2\imath} & \frac{z_4}{2\imath} & -\frac{z_3}{2\imath}\\
\frac{\sin(\theta)\cot(\lambda)}{-\imath} & 0 & -\imath\cos(\theta) & \frac{z_1}{2} & -\frac{z_2}{2} & -\frac{z_3}{2} & \frac{z_4}{2}\\
0 & 0 & 0 & z_1 & z_2 & z_3 & z_4
\end{bmatrix}$$

with $f(\phi,\lambda)=-\imath\cot(\lambda)\cos(\theta)\cos(\phi)$ and $g(\phi,\lambda)=-\imath\cot(\lambda)\cos(\theta)\sin(\phi)$. The function F_n also satisfies the initial condition $F_n(\mathbf{x}_0,\mathbf{z}_0)=1$.

The determinant of $\mathbf{M}$ is

$$\det\mathbf{M}=\frac{-1}{4\sin^2(\lambda)\sin(\theta)}(\Phi_{S^3}(\mathbf{x},\mathbf{z}))^2.$$

Since $\Phi_{S^3}(\mathbf{x}_0,\mathbf{z}_0)\neq 0$, we proceed as in Appendix A to conclude that

$$\tilde{\mathcal{K}}_n(\mathbf{x},\mathbf{z})=c(n)(\Phi_{S^3})^{n-1}(\mathbf{x},\mathbf{z}).$$

It is just left to evaluate the constant $c(n)$. Since,

$$Y_{100}=1,\quad Y_{200}=2\cos(\lambda),\quad Y_{211}=-\imath\sqrt{2}\sin(\theta)\sin(\lambda)e^{\imath\phi},$$

$$Y_{210}=2\imath\cos(\theta)\sin(\lambda),\quad Y_{21-1}=\imath\sqrt{2}\sin(\theta)\sin(\lambda)e^{-\imath\phi},$$

$$y_{100}=1,\quad y_{200}=\frac{1}{\sqrt{2}}[z_1z_4-z_2z_3],\quad y_{211}=z_1z_3,$$

$$y_{210}=\frac{1}{\sqrt{2}}[z_1z_4+z_2z_3],\quad y_{21-1}=z_2z_4$$

we obtain Eq. (2.51)

Now consider $\lambda=0$. Since $Y_{n\diagup m}(\theta,\phi,\lambda=0)=n\delta_{\diagup 0}$ we get

$$ny_{n00}(\mathbf{z})=c(n)(\sqrt{2}(z_1z_4-z_2z_3))^{n-1}.$$

By taking the norm in both sides of the last equation, we have

$$n=c(n)2^{(n-1)/2}\sqrt{n}(n-1)!,$$

where we used $\|(z_1z_4-z_2z_3)^{n-1}\|=\sqrt{n}(n-1)!$.

Thus we conclude $c(n)=[\sqrt{2n}/(n-1)!](1/2^{n/2})$ and prove Eq. (2.50).

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New solutions of relativistic wave equations in magnetic fields and longitudinal fields

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We demonstrate how one can describe explicitly the present arbitrariness in solutions of relativistic wave equations in external electromagnetic fields of special form. This arbitrariness is connected to the existence of a transformation, which effectively reduces the number of variables in the initial equations. Then we use the corresponding representations to construct new sets of exact solutions, which may have a physical interest. Namely, we present new sets of stationary and nonstationary solutions in magnetic field and in some superpositions of electric and magnetic fields. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1461428]

I. INTRODUCTION

Relativistic wave equations (Dirac and Klein–Gordon) provide a basis for relativistic quantum mechanics and quantum electrodynamics of spinor and scalar particles.[1] In relativistic quantum mechanics, solutions of relativistic wave equations are referred to as one-particle wave functions of fermions and bosons in external electromagnetic fields. In quantum electrodynamics, such solutions allow the development of the perturbation expansion known as the Furry picture, which incorporates the interaction with the external field exactly, while treating the interaction with the quantized electromagnetic field perturbatively.[2] The physically most important exact solutions of the Klein–Gordon and the Dirac equations are: an electron in a Coulomb field, a uniform magnetic field, the field of a plane wave, the field of a magnetic monopole, the field of a plane wave combined with a uniform magnetic and electric fields parallel to the direction of wave propagation, crossed fields, and some simple one-dimensional electric fields (for a complete review of solutions of relativistic wave equations see Ref. 3).

Considering, for example, stationary solutions of relativistic wave equations, we can see that in the general case, there exist different sets of stationary solutions for one and the same Hamiltonian. The possibility to get different sets of stationary states reflects the existence of an arbitrariness in the solutions of the eigenvalue problem for a Hamiltonian. Considering nonstationary solutions, we also encounter the possibility of constructing different complete sets of such solutions. There is no regular method of describing such an arbitrariness explicitly. Especially in the presence of an external field the problem appears to be nontrivial.

In the present article we demonstrate how one can describe explicitly the present arbitrariness in solutions of the relativistic wave equations for some types of external electromagnetic fields, namely, for uniform magnetic fields and combination of these fields with some electric fields. This arbitrariness is connected to the existence of a transformation, which effectively reduces the number of variables in the initial equations. Then we use the corresponding representations to construct new sets of exact solutions, which may have a physical interest. In Sec. II we consider relativistic wave equations in pure uniform magnetic fields. Here we derive a representation for the exact solutions, in which the above-mentioned arbitrariness is described explicitly by an

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arbitrary function. From a suitable choice of this function, we get both the well-known set of solutions and new ones. Section II contains the most complete (at present) description of the problem of a uniform magnetic field in relativistic quantum mechanics. Among new sets of solutions there are both stationary, generalized coherent solutions and nonstationary solutions. Then, in Sec. III, we consider more complicated configurations of external electromagnetic fields, namely, longitudinal electromagnetic fields. Here we describe all the arbitrariness in the solutions, and on this basis present various sets of new exact solutions. In Sec. IV we interpret the above-mentioned results from the point of view of the general theory of differential equations.

II. UNIFORM MAGNETIC FIELD

A. Arbitrariness in solutions of relativistic wave equations

Consider a uniform magnetic field $\mathbf{H}=(0,0,H)$ directed along the x^3 axis $(H>0)$. The electromagnetic potentials are chosen in the symmetric gauge

$$A_0=A_3=0,\ A_1=\tfrac{1}{2}Hx^2,\quad A_2=-\tfrac{1}{2}Hx^1. \tag{2.1}$$

We write the Klein–Gordon and the Dirac equations in the form

$$\begin{gathered}\mathcal{K}\Psi=0,\quad \hbar^2\mathcal{K}=\mathcal{P}^2-m_0^2c^2,\quad \mathcal{P}_\mu=i\hbar\partial_\mu-\frac{e}{c}A_\mu,\\ \mathcal{D}\Theta=0,\quad \hbar\mathcal{D}=\gamma^\mu\mathcal{P}_\mu-m_0c.\end{gathered} \tag{2.2}$$

Here $e=-|e|$ and γ-matrices are chosen in the standard representation.[3]

In the field under consideration, the operators $\mathcal{P}_0$ and $\mathcal{P}_3$ are mutually commuting integrals of motion, $[\mathcal{K},\mathcal{P}_0]=[\mathcal{K},\mathcal{P}_3]=[\mathcal{D},\mathcal{P}_0]=[\mathcal{D},\mathcal{P}_3]=[\mathcal{P}_0,\mathcal{P}_3]=0$.

In the case of the Klein–Gordon equation, the operator L_z,

$$L_z=i\hbar(x^2\partial_1-x^1\partial_2),\quad [L_z,\mathcal{P}_0]=[L_z,\mathcal{P}_3]=[\mathcal{K},L_z]=0, \tag{2.3}$$

can be included (together with $\mathcal{P}_0$ and $\mathcal{P}_3$) in the complete set of integrals of motion, whereas for the Dirac equation case, the operator J_z,

$$J_z=L_z+\frac{\hbar}{2}\Sigma_3,\quad [J_z,\mathcal{P}_0]=[J_z,\mathcal{P}_3]=[\mathcal{D},J_z]=0, \tag{2.4}$$

can be included (together with $\mathcal{P}_0$ and $\mathcal{P}_3$) in the complete set of integrals of motion. Here $\Sigma_3=\mathrm{diag}(\sigma_3,\sigma_3)$.

We are going to use dimensionless coordinates $-\infty<x<\infty$, $-\infty<y<\infty$ or $0\leqslant\rho<\infty$, $0\leqslant\varphi<2\pi$ defined by

$$\begin{gathered}\sqrt{\frac{\gamma}{2}}x^1=x=\sqrt{\rho}\cos\varphi,\quad \sqrt{\frac{\gamma}{2}}x^2=y=\sqrt{\rho}\sin\varphi,\quad \gamma=\frac{|e|H}{c\hbar}>0,\\ \mathrm{d}x^1\,\mathrm{d}x^2=\frac{2}{\gamma}\mathrm{d}x\,\mathrm{d}y=\frac{1}{\gamma}\mathrm{d}\rho\,\mathrm{d}\varphi,\quad x+iy=\sqrt{\rho}\exp i\varphi.\end{gathered} \tag{2.5}$$

It is useful to introduce the operators a_1, a_2, $a_1^\dagger$, $a_2^\dagger$,

$$a_2=\frac{1}{\sqrt{2\gamma\hbar}}[\mathcal{P}_2-i\mathcal{P}_1+\hbar\gamma(x^1+ix^2)]=\frac{1}{2}(x+iy+\partial_x+i\partial_y)=\frac{e^{i\varphi}}{2\sqrt{\rho}}(\rho+i\partial_\varphi+2\rho\partial_\rho),$$

$$a_2^\dagger=\frac{1}{\sqrt{2\gamma\hbar}}[\mathcal{P}_2+i\mathcal{P}_1+\hbar\gamma(x^1-ix^2)]=\frac{1}{2}(x-iy-\partial_x+i\partial_y)=\frac{e^{-i\varphi}}{2\sqrt{\rho}}(\rho+i\partial_\varphi-2\rho\partial_\rho).$$

$$a_1=-\frac{1}{\sqrt{2\gamma\hbar}}(i\mathcal{P}_1+\mathcal{P}_2)=\frac{1}{2}(x-iy+\partial_x-i\partial_y)=\frac{e^{-i\varphi}}{2\sqrt{\rho}}(\rho-i\partial_\varphi+2\rho\partial_\rho), \tag{2.6}$$

$$a_1^\dagger=\frac{1}{\sqrt{2\gamma\hbar}}(i\mathcal{P}_1-\mathcal{P}_2)=\frac{1}{2}(x+iy-\partial_x-i\partial_y)=\frac{e^{i\varphi}}{2\sqrt{\rho}}(\rho-i\partial_\varphi-2\rho\partial_\rho).$$

They obey the commutation relations

$$[a_k,a_s^\dagger]=\delta_{k,s},\quad [a_k,a_s]=[a_k^\dagger,a_s^\dagger]=0,\quad k,s=1,2. \tag{2.7}$$

Thus, we can interpret these operators as creation and annihilation ones. One can also find the following relations:

$$\mathcal{P}_1^2+\mathcal{P}_2^2=\hbar^2\gamma(a_1a_1^\dagger+a_1^\dagger a_1)=2\hbar^2\gamma\mathcal{N}+\hbar^2\gamma,$$
$$L_z=\hbar(\mathcal{N}-a_2^\dagger a_2),\quad \mathcal{N}=a_1^\dagger a_1. \tag{2.8}$$

Then the Klein–Gordon and the Dirac operators can be written as

$$\mathcal{K}=\hbar^{-2}(\mathcal{P}_0^2-\mathcal{P}_3^2)-2\gamma\mathcal{N}-\gamma-m^2,\quad m=\frac{m_0c}{\hbar},$$
$$\mathcal{D}=\hbar^{-1}(\gamma^0\mathcal{P}_0+\gamma^3\mathcal{P}_3)-\sqrt{\frac{\gamma}{2}}[(\gamma^2-i\gamma^1)a_1+(\gamma^2+i\gamma^1)a_1^\dagger]-m. \tag{2.9}$$

The operator $\mathcal{N}$ commutes with $\mathcal{P}_0,\mathcal{P}_3,\ L_z$, plus it is an integral of motion in the case of the Klein–Gordon equation. Its generalization for the Dirac equation has the form $\mathcal{N}_D=\mathcal{N}+\frac{1}{2}\Sigma_3$.

One ought to remark that the operators $\mathcal{K}$ and $\mathcal{D}$ do not contain the operators $a_2^\dagger$, a_2. Thus, the latter operators are integrals of motion, which commute with $\mathcal{N}$, $\mathcal{N}_D$, $\mathcal{P}_0$, $\mathcal{P}_3$, but do not commute with L_z and J_z.

The operators of creation and annihilation with different numbers commute. One can find a representation in which these operators are acting on different variables. To this end, we present the wave functions from (2.2) in the following form (we make a Fourier transform in the variable y only, and call such a representation the semi-momentum representation):

$$\Psi(x,y)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{iky}\tilde{\Psi}(x,k)\mathrm{d}k. \tag{2.10}$$

Of course the functions Ψ and $\tilde{\Psi}$ depend on the variables x^2 and x^3 as well, but we do not indicate this dependence explicitly. In terms of $\tilde{\Psi}$ the multiplication and differentiation have the form $y\to i\partial_k,\quad i\partial_y\to -k$. Then, the expressions for the creation and annihilation operators in the semi-momentum representation take the form

$$2a_1 = x + k + \partial_x + \partial_k, \quad 2a_1^\dagger = x + k - \partial_x - \partial_k,$$
$$2a_2 = x - k + \partial_x - \partial_k, \quad 2a_2^\dagger = x - k - \partial_x + \partial_k. \tag{2.11}$$

Now we pass from x, k to new variables ξ, η,

$$\sqrt{2}\xi = x + k, \quad \sqrt{2}\eta = x - k, \quad \sqrt{2}x = \xi + \eta, \quad \sqrt{2}k = \xi - \eta. \tag{2.12}$$

Then the creation and annihilation operators can be written as

$$\sqrt{2}a_1 = \xi + \partial_\xi, \quad \sqrt{2}a_1^\dagger = \xi - \partial_\xi, \quad \sqrt{2}a_2 = \eta + \partial_\eta, \quad \sqrt{2}a_2^\dagger = \eta - \partial_\eta. \tag{2.13}$$

In the new variables,

$$2\mathcal{N} = \xi^2 - \partial_\xi^2 - 1, \tag{2.14}$$

and the Klein–Gordon and the Dirac operators read

$$\mathcal{K} = \hbar^{-2}(\mathcal{P}_0^2 - \mathcal{P}_3^2) + \gamma(\partial_\xi^2 - \xi^2) - m^2,$$
$$\mathcal{D} = \hbar^{-1}(\gamma^0\mathcal{P}_0 + \gamma^3\mathcal{P}_3) - \sqrt{\gamma}(\gamma^2\xi - i\gamma^1\partial_\xi) - m. \tag{2.15}$$

One can see that the latter operators do not contain the variable η. Notice that both operators L_z and J_z contain variables ξ, η. For example,

$$2L_z = \xi^2 - \partial_\xi^2 - \eta^2 + \partial_\eta^2. \tag{2.16}$$

The integration over k in (2.10) can be replaced by an integration over η,

$$\Psi(x,y) = \frac{e^{ixy}}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-i\sqrt{2}y\eta}\tilde{\Psi}(\xi,\eta)\mathrm{d}\eta, \quad \xi = \sqrt{2}x - \eta. \tag{2.17}$$

Besides, one can write

$$(\Psi,\Phi) = \int_{-\infty}^{\infty}\mathrm{d}x \quad \int_{-\infty}^{\infty}\mathrm{d}y\ \Psi^*(x,y)\Phi(x,y) = (\tilde{\Psi},\tilde{\Phi}) = \int_{-\infty}^{\infty}\mathrm{d}\xi\int_{-\infty}^{\infty}\mathrm{d}\eta\ \tilde{\Psi}^*(\xi,\eta)\tilde{\Phi}(\xi,\eta). \tag{2.18}$$

The independence of the operators (2.15) on the variable η will allow us to separate explicitly the functional arbitrariness in the solutions (2.17), as will be seen in the following.

B. Stationary states

1. Arbitrariness in stationary states

Known sets of stationary solutions in a uniform magnetic field (that were found in the first works[4–8]) are eigenfunctions of the operators $\mathcal{P}_0, \mathcal{P}_3, \mathcal{N}$ in the scalar case and of the operators $\mathcal{P}_0$, $\mathcal{P}_3$, $\mathcal{N}_D$ in the spinor case. Thus for scalar wave functions Ψ we have the conditions

$$\mathcal{P}_0\Psi = \hbar k_0\Psi, \quad \mathcal{P}_3\Psi = \hbar k_3\Psi, \quad \mathcal{N}\Psi = n\Psi, \quad n = 0,1,2,\ldots, \tag{2.19}$$

and for Dirac wave functions $\mathbf{\Theta}$ the conditions

$$\mathcal{P}_0\mathbf{\Theta} = \hbar k_0\mathbf{\Theta}, \quad \mathcal{P}_3\mathbf{\Theta} = \hbar k_3\mathbf{\Theta}, \quad \mathcal{N}_D\mathbf{\Theta} = (n - \tfrac{1}{2})\mathbf{\Theta}, \quad n = 0,1,2,\ldots. \tag{2.20}$$

Consider first the scalar case. It follows from (2.15) that

$$k_0^2=m^2+\gamma+k_3^2+2\gamma n=m^{*2}+k_3^2+2\gamma n, \quad m^{*2}=m^2+\gamma, \tag{2.21}$$

and

$$\Psi_{n,k_3}(x^\mu)=N\exp(-ik_0x^0-ik_3x^3)\Psi_n(x,y). \tag{2.22}$$

Here N is a normalization factor. In the semi-momentum representation (2.10) the function $\Psi_n(x,y)$ has the following image:

$$\tilde{\Psi}_n(\xi,\eta)=U_n(\xi)\Phi(\eta), \quad \xi=\sqrt{2}x-\eta. \tag{2.23}$$

Here Eqs. (2.19) and (2.14) were used. $U_n(\xi)$ are Hermite functions; they are related to the corresponding polynomials $H_n(\xi)$ as $U_n(x)=(2^n n!\sqrt{\pi})^{-\frac{1}{2}}\exp(-x^2/2)H_n(x)$.[9] The function $\Phi(\eta)$ is arbitrary. The functions $\Psi_n(x,y)$ from (2.22) obey the relations

$$a_1\Psi_n=\sqrt{n}\Psi_{n-1}, \quad a_1^\dagger\Psi_n=\sqrt{n+1}\Psi_{n+1}, \quad \Psi_n(x,y)=\frac{(a_1^\dagger)^n}{\sqrt{\Gamma(n+1)}}\Psi_0(x,y), \tag{2.24}$$

$$\Psi_0(x,y)=\pi^{-3/4}\exp(-x^2+ixy)\int_{-\infty}^{\infty}d\eta\exp\left[-\frac{\eta^2}{2}+\sqrt{2}\eta(x-iy)\right]\Phi(\eta). \tag{2.25}$$

Dirac wave functions are of the form $\mathbf{\Theta}_{n,k_3}(x^\mu)=N\exp(-ik_0x^0-ik_3x^3)\mathbf{\Theta}_{k_3,n}(x,y)$ with bispinors $\mathbf{\Theta}_{k_3,n}(x,y)$ having the structure

$$\mathbf{\Theta}^T_{n,k_3}(x,y)=(c_1\Psi_{n-1}(x,y), \quad ic_2\Psi_n(x,y), \quad c_3\Psi_{n-1}(x,y), \quad ic_4\Psi_n(x,y)). \tag{2.26}$$

The functions $\Psi_n(x,y)$ are defined by relations (2.17), (2.23), whereas the constant bispinor C (with the elements c_k) obeys an algebraic system of equations

$$AC=0, \quad A=\gamma^0k_0+\gamma^3k_3-\sqrt{2\gamma n}\gamma^1-m. \tag{2.27}$$

The condition $\det A=(k_0^2-k_3^2-2\gamma n-m^2)^2=0$ results in an equation which is an analog of (2.21),

$$k_0^2=k_3^2+2\gamma n+m^2. \tag{2.28}$$

Since the rank of the matrix A is equal to 2, a general solution of (2.27) has the form

$$C=\begin{pmatrix}(k_0+m)v\\(\sqrt{2\gamma n}\sigma_1-k_3\sigma_3)v\end{pmatrix}, \quad C^+C=2k_0(k_0+m)v^+v, \tag{2.29}$$

where v is an arbitrary constant bispinor and σ are Pauli matrices. We can specify v selecting a spin integral of motion (see Ref. 3). The state $n=0$ is a special case. Here we must set $c_1=c_3=0$, which corresponds to the choice $v^T=(0, \quad c_2)$, $c_2\neq 0$. The latter means that $\Sigma_3\Theta_D=-\Theta_D$. Thus, for $n=0$, the electron spin can only point to the direction opposite to the magnetic field.

Expressions for $\Psi_n(x,y)$ in the semi-momentum representation explicitly contain a functional arbitrariness, which means that every energy level is infinitely degenerated. Let us demand that the scalar and spinor wave functions be eigenvectors of the operators L_z and J_z, respectively. According to (2.4) and (2.8) that means that the functions $\Psi_n(x,y)$ have to obey an additional condition

$$a_2^\dagger a_2 \Psi_n(x,y) = s\Psi_n(x,y), \quad s=0,1,2,\ldots,$$
$$L_z = \hbar(n-s) = \hbar l, \quad l = n-s, \quad n \geqslant l > -\infty, \quad J_z = \hbar(l-\tfrac{1}{2}). \tag{2.30}$$

This condition defines the function $\Phi(\eta)$ according to (2.13), $a_2^\dagger a_2 \Phi_s(\eta) = s\Phi_s(\eta)$, therefore $\Phi_s(\eta) = U_s(\eta)$. Substituting this result into (2.23) and into (2.17), and doing the integral over η, we find in the coordinate representation,

$$\Psi_{n,s}(x,y) = \frac{(-1)^n}{\sqrt{2\pi}} e^{il\varphi} I_{s,n}(\rho) = \frac{(-1)^n}{\sqrt{2\pi}} \left(\frac{x+iy}{x-iy}\right)^{(n-s)/2} I_{s,n}(x^2+y^2). \tag{2.31}$$

Here $I_{m,n}(x)$ are Laguerre functions, which are connected to the corresponding polynomials $L_n^\alpha(x)$ by the relations (see Ref. 9) $I_{m,n}(x) = (\Gamma(n+1)/\Gamma(m+1))^{1/2} e^{-x/2} x^{\alpha/2} L_n^\alpha(x)$, $\alpha = m-n$. The states (2.31) were first obtained in Refs. 4–8. Besides (2.24) and (2.25), the functions (2.31) obey the following relations as well:

$$a_2 \Psi_{n,s} = \sqrt{s}\,\Psi_{n,s-1}, \quad a_2^\dagger \Psi_{n,s} = \sqrt{s+1}\,\Psi_{n,s+1},$$
$$\Psi_{n,s} = \frac{(a_1^\dagger)^n (a_2^\dagger)^s}{\sqrt{\Gamma(n+1)\Gamma(s+1)}} \Psi_{0,0}, \quad \Psi_{0,0}(x,y) = \frac{1}{\sqrt{\pi}} \exp\left[-\frac{1}{2}(x^2+y^2)\right] = \frac{e^{-\rho/2}}{\sqrt{\pi}}. \tag{2.32}$$

In the following we are going to find new sets of solutions imposing complementary conditions different from (2.30). This results in a different form for the function $\Phi(\eta)$.

2. Generalized squeezed coherent states

Taking into account that the operators $a_2^\dagger$, a_2 are integrals of motion, we may construct stationary states, which are eigenvectors of a linear combination $A_2^{\alpha,\beta}$ of these operators,

$$A_2^{\alpha,\beta} = \alpha a_2 + \beta a_2^\dagger. \tag{2.33}$$

Here α, β are arbitrary complex numbers. Here one has to distinguish three nonequivalent cases.

(1) If $|\alpha|^2 < |\beta|^2$, then there do not exist any normalizable eigenvectors of the operator (2.33). We are not going to consider such case.

(2) If $|\alpha|^2 = |\beta|^2$, then $A_2^{\alpha,\beta}$ is, in fact, reduced to a Hermitian operator

$$A_2^\mu = \mu a_2 + \mu^* a_2^\dagger, \quad A_2^{+\mu} = A_2^\mu, \quad \mu \neq 0, \tag{2.34}$$

where μ is an arbitrary complex number.

(3) If $|\alpha|^2 > |\beta|^2$, then without loss of generality we can assume that operators $A_2^{\alpha,\beta}$ have the form

$$A_2^{\alpha,\beta} = \alpha a_2 + \beta a_2^\dagger, \quad |\alpha|^2 - |\beta|^2 = 1, \quad [A_2^{\alpha,\beta}, A_2^{+\alpha,\beta}] = 1. \tag{2.35}$$

Then $A_2^{+\alpha,\beta}$, $A_2^{\alpha,\beta}$ are creation and annihilation operators, which are related to $a_2^\dagger$, a_2 by a canonical transformation,

$$a_2 = \alpha^* A_2^{\alpha,\beta} - \beta A_2^{+\alpha,\beta}, \quad a_2^\dagger = \alpha A_2^{+\alpha,\beta} - \beta^* A_2^{\alpha,\beta}. \tag{2.36}$$

Consider eigenvectors of the operator (2.34), i.e., $A_2^\mu \Psi_{n,z}^\mu(x,y) = z\Psi_{n,z}^\mu(x,y)$, $z = z^*$. This equation results in the equation $A_2^\mu \Phi_z^\mu(\eta) = z\Phi_z^\mu(\eta)$ for the function $\Phi(\eta)$. Taking into account (2.13), one can find that solutions of the latter equation are

$$\Phi_z^{\mu}(\eta)=\left[\frac{\mu}{\sqrt{2}\pi|\mu|(\mu-\mu^*)}\right]^{1/2}\exp Q_1,$$

$$4(\mu-\mu^*)Q_1=-2(\mu+\mu^*)\eta^2+4\sqrt{2}z\eta-z^2(\mu+\mu^*)|\mu|^{-2}. \tag{2.37}$$

These solutions obey the orthonormality and completeness relations,

$$\int_{-\infty}^{\infty}\Phi_{z'}^{*\,\mu}(\eta)\Phi_z^{\mu}(\eta)\mathrm{d}\eta=\delta(z-z'),\quad \int_{-\infty}^{\infty}\Phi_z^{*\,\mu}(\eta')\Phi_z^{\mu}(\eta)\mathrm{d}z=\delta(\eta-\eta'). \tag{2.38}$$

Their overlapping has the form

$$R^{\mu',\mu}(z',z)=\int_{-\infty}^{\infty}\Phi_{z'}^{*\,\mu'}(\eta)\Phi_z^{*\,\mu}(\eta)\mathrm{d}\eta=N_1\exp\left[\frac{Q_2}{4(\mu'\mu^*-\mu\mu'^*)}\right],$$

$$N_1^2=\frac{\mu'^*\mu}{2\pi^2|\mu'||\mu|(\mu\mu'^*-\mu'\mu^*)}, \tag{2.39}$$

$$Q_2=\left(z\sqrt{\frac{\mu'}{\mu}}-z'\sqrt{\frac{\mu}{\mu'}}\right)^2+\left(z\sqrt{\frac{\mu'^*}{\mu^*}}-z'\sqrt{\frac{\mu^*}{\mu'^*}}\right)^2.$$

It defines the mutual decomposition

$$\Phi_z^{\mu}(\eta)=\int_{-\infty}^{\infty}\Phi_{z'}^{\mu'}(\eta)R^{\mu',\mu}(z',z)\mathrm{d}z'. \tag{2.40}$$

The coordinate representation (2.17) for the solutions under consideration has the form

$$\Psi_{n,z}^{\mu}(x,y)=(\sqrt{2}\pi|\mu|)^{-1/2}\left(\frac{\mu^*}{\mu}\right)^{n/2}U_n(p_1)\exp iQ_3,$$

$$4|\mu|^2Q_3=[i(\mu^*-\mu)x+(\mu+\mu^*)y][(\mu+\mu^*)x+i(\mu-\mu^*)y-2z], \tag{2.41}$$

$$\sqrt{2}|\mu|p_1=(\mu+\mu^*)x+i(\mu-\mu^*)y-z.$$

Their scalar product (2.18) reads $(\Psi_{n',z'}^{\mu},\Psi_{n,z}^{\mu})=\delta_{n,n'}\delta(z-z')$. Relation (2.40) results in the following decomposition in the coordinate representation:

$$\Psi_{n,z}^{\mu}(x,y)=\int_{-\infty}^{\infty}\Psi_{n,z'}^{\mu'}(x,y)R^{\mu',\mu}(z',z)\mathrm{d}z'. \tag{2.42}$$

In particular, in the cases of real or pure imaginary μ, such wave functions were known before.[3]

Consider eigenvectors of the operator (2.35), i.e., $A_2^{\alpha,\beta}\Psi_{n,z}^{\alpha,\beta}(x,y)=z\Psi_{n,z}^{\alpha,\beta}(x,y)$, where z is a complex number. In fact, we get coherent (squeezed) stationary states. They are labeled by z and by two complex parameters α, β, which are related by the condition (2.35). In the semi-momentum representation the above-given equation is reduced to

$$A_2^{\alpha,\beta}\Phi_z^{\alpha,\beta}(\eta)=z\Phi_z^{\alpha,\beta}(\eta). \tag{2.43}$$

It is well known that such solutions form a complete (overcomplete) set at any fixed α, β. Solutions within each set are not orthogonal. One can use these functions to construct an orthogonal set of solutions.

Since the operators $A_2^{+\alpha,\beta}$, $A_2^{\alpha,\beta}$ are integrals of motion (both for the Klein–Gordon equation and for the Dirac equation), they are symmetry operators for the equations. The action of these operators on a solution again provides a solution. For example, applying the operators $(\Gamma(1+s))^{-1/2}(A_2^{+\alpha,\beta}-z^*)^s$, $s=0,1,2,\ldots$ to normalized solutions of Eq. (2.43), we get normalized solutions labeled by the index s. These new solutions are orthogonal with respect to s,

$$\Phi_{s,z}^{\alpha,\beta}(\eta)=\frac{(A_2^{+\alpha,\beta}-z^*)^s}{\sqrt{\Gamma(1+s)}}\Phi_z^{\alpha,\beta}(\eta),\quad \Phi_{0,z}^{\alpha,\beta}(\eta)=\Phi_z^{\alpha,\beta}(\eta),$$
$$\int_{-\infty}^{\infty}\Phi_{s',z}^{*\,\alpha,\beta}(\eta)\Phi_{s,z}^{\alpha,\beta}(\eta)d\eta=\delta_{s,s'}\int_{-\infty}^{\infty}|\Phi_z^{\alpha,\beta}(\eta)|^2\,\mathrm{d}\eta. \tag{2.44}$$

We call such states generalized squeezed coherent states. It is possible to get an explicit form for these states,

$$\begin{aligned}\Phi_{s,z}^{\alpha,\beta}(\eta)&=\left[\frac{\alpha}{|\alpha|(\alpha-\beta)}\right]^{1/2}\left(\frac{\alpha^*-\beta^*}{\alpha-\beta}\right)^{s/2}e^{Q_4}U_s(p_2),4|\alpha-\beta|^2Q_4\\&=2(\alpha\beta^*-\alpha^*\beta)\eta^2+2\sqrt{2}\,\eta[z(\alpha^*-\beta^*)-z^*(\alpha-\beta)]+z^{*2}(\alpha-\beta)^2\\&\quad-z^2(\alpha^*-\beta^*)^2,2|\alpha-\beta|p_2=2\eta-\sqrt{2}z(\alpha^*-\beta^*)-\sqrt{2}z^*(\alpha-\beta).\end{aligned} \tag{2.45}$$

The functions (2.45) form a complete set for each fixed z,

$$\sum_{s=0}^{\infty}\Phi_{s,z}^{*\,\alpha,\beta}(\eta')\Phi_{s,z}^{\alpha,\beta}(\eta)=\delta(\eta'-\eta), \tag{2.46}$$

and for each fixed s,

$$\int\frac{\mathrm{d}^2z}{\pi}\Phi_{s,z}^{*\,\alpha,\beta}(\eta')\Phi_{s,z}^{\alpha,\beta}(\eta)=\delta(\eta-\eta'),\quad \mathrm{d}^2z=\mathrm{d}\,\mathrm{Re}\,z\,\mathrm{d}\,\mathrm{Im}\,z. \tag{2.47}$$

The overlapping

$$R_{s',s}^{\alpha',\beta';\alpha,\beta}(z',z)=\int_{-\infty}^{\infty}\Phi_{s',z'}^{*\,\alpha',\beta'}(\eta)\Phi_{s,z}^{\alpha,\beta}(\eta)\mathrm{d}\eta, \tag{2.48}$$

allows us to find mutual decompositions

$$\Phi_{s,z}^{\alpha,\beta}(\eta)=\sum_{s'=0}^{\infty}R_{s',s}^{\alpha',\beta';\alpha,\beta}(z',z)\Phi_{s',z'}^{\alpha',\beta'}(\eta),\quad \Phi_{s,z}^{\alpha,\beta}(\eta)=\int\mathrm{d}^2z'R_{s',s}^{\alpha',\beta';\alpha,\beta}(z',z)\Phi_{s',z'}^{\alpha',\beta'}(\eta). \tag{2.49}$$

Unfortunately, the overlapping (2.48) has a complicated form via a finite sum of Hermite functions. In some particular cases this sum can be simplified. For example, if $\alpha'=\alpha$, $\beta'=\beta$, then the overlapping does not depend on α,β and has the form

$$R_{s',s}^{\alpha,\beta;\alpha,\beta}(z',z)=R_{s',s}(z',z)=\left(\frac{z-z'}{z^*-z'^*}\right)^{(s'-s)/2}\exp\left[\frac{1}{2}(zz'^*-z^*z')\right]I_{s',s}(|z-z'|^2). \tag{2.50}$$

For $s=s'=0$ we get

$$R_{0,0}^{\alpha',\beta';\alpha,\beta}(z',z)=\sqrt{\frac{\alpha\alpha'^*}{|\alpha\alpha'|}}(\alpha\alpha'^*-\beta\beta'^*)^{-1/2}\exp Q_5,$$
$$2Q_5=\frac{z^2(\alpha'^*\beta^*-\alpha^*\beta'^*)+(z'^*)^2(\alpha\beta'-\alpha'\beta)+2zz'^*}{\alpha\alpha'^*-\beta\beta'^*}-z'z^*-zz'^*-|z-z'^*|^2. \tag{2.51}$$

The wave function $\Psi_{n,s,z}^{\alpha,\beta}(x,y)$ also has a very complicated form in the general case. However, in some particular cases it can be simplified. For example,

$$\Psi_{n,s,z}^{1,0}(x,y)=\frac{(-1)^n}{\sqrt{\pi}}\left(\frac{x+iy-z}{x-iy-z^*}\right)^{(n-s)/2}e^M I_{s,n}(|x+iy-z|^2),$$
$$M=z(x-iy)-z^*(x+iy). \tag{2.52}$$

For $z=0$ we arrive at the set (2.31).

For $s=0$ we get a compact form for a set of stationary squeezed coherent states,

$$\Psi_{n,0,z}^{\alpha,\beta}(x,y)=\Psi_{n,z}^{\alpha,\beta}(x,y)=(-1)^n\frac{\pi^{1/4}}{\sqrt{|\alpha|}}\left(\frac{\beta}{\alpha}\right)^{n/2}U_n\left(\frac{p_3}{\sqrt{2\alpha\beta}}\right)\exp Q_6,$$
$$p_3=z-\alpha(x+iy)-\beta(x-iy), \tag{2.53}$$
$$4\alpha\beta Q_6=(1+2|\beta|^2)z^2-2\alpha\beta|z|^2+(z+p_3)[\beta(x-iy)-\alpha(x+iy)].$$

Additional simplifications are available for $\alpha=1,\beta=0$,

$$\Psi_{n,z}^{1,0}(x,y)=\Psi_{n,z}(x,y)=\varphi_{n,z}(x,y)\exp(-\tfrac{1}{2}|z|^2),$$
$$\varphi_{n,z}(x,y)=\frac{(x+iy-z)^n}{\sqrt{\pi\Gamma(n+1)}}\exp\left[z(x-iy)-\frac{1}{2}(x^2+y^2)\right]. \tag{2.54}$$

Namely, these states were found in Ref. 10. However, the meaning of the parameter z was not clarified.

For arbitrary α, β, the functions $\Psi_{n,s,z}^{\alpha,\beta}(x,y)$ obey, besides (2.24), the following:

$$A_2^{\alpha,\beta}\Psi_{n,s,z}^{\alpha,\beta}=z\Psi_{n,s,z}^{\alpha,\beta}+\sqrt{s}\Psi_{n,s-1,z}^{\alpha,\beta},\quad A_2^{+\alpha,\beta}\Psi_{n,s,z}^{\alpha,\beta}=z^*\Psi_{n,s,z}^{\alpha,\beta}+\sqrt{s+1}\Psi_{n,s+1,z}^{\alpha,\beta}. \tag{2.55}$$

Taking into account that $a_2^\dagger\varphi_{n,z}=\partial\varphi_{n,z}/\partial z$, we can construct a new set of stationary states by successive differentiations,

$$\overline{\Psi}_{n,s,z}(x,y)=\frac{(-1)^nN}{\sqrt{\pi}}\exp\left[i(n-s)\varphi+\frac{\rho-q}{2}\right]\left(\frac{q}{\rho}\right)^{(n-s)/2}I_{s,n}(q)$$
$$=\frac{(-1)^nN}{\sqrt{\pi}}\exp\left[\frac{z}{2}(x+iy)\right]\left(\frac{x+iy-z}{x-iy}\right)^{(n-s)/2}I_{s,n}(q),$$
$$q=\rho-z\sqrt{\rho}e^{-i\varphi}=(x-iy)(x+iy-z). \tag{2.56}$$

For $N=1$ the above-mentioned set obeys [besides (2.24)]

$$a_2\overline{\Psi}_{n,s,z}=z\overline{\Psi}_{n,s,z}+\sqrt{s}\overline{\Psi}_{n,s-1,z},\quad a_2^\dagger\overline{\Psi}_{n,s,z}=\frac{\partial}{\partial z}\overline{\Psi}_{n,s,z}=\sqrt{s+1}\overline{\Psi}_{n,s+1,z}. \tag{2.57}$$

The set (2.31) is a particular case of (2.56), it corresponds to $z=0$. The set (2.56) is not orthogonal,

$$(\overline{\Psi}_{n',s',z'},\overline{\Psi}_{n,s,z})=N'^{*}N\delta_{n,n'}\mathcal{J}_{s,s'}(z,z'),$$

$$\mathcal{J}_{s,s'}(z,z')=\sqrt{\frac{\Gamma(s+1)}{\Gamma(s'+1)}}z^{s'-s}e^{zz'^{*}}L_{s}^{s'-s}(-zz'^{*}),\quad s\leqslant s', \tag{2.58}$$

$$\mathcal{J}_{s,s'}(z,z')=\sqrt{\frac{\Gamma(s'+1)}{\Gamma(s+1)}}(z'^{*})^{s-s'}e^{zz'^{*}}L_{s'}^{s-s'}(-zz'^{*}),\quad s'\leqslant s.$$

The functions from the set (2.56) are normalized to unity for $N=N_s(z)=\exp(-|z|^2/2)[L_s(-|z|^2)]^{-1/2}$. For $N=1$, the following mutual decompositions take place:

$$\overline{\Psi}_{n,s+k,z'}(x,y)=\sqrt{\frac{\Gamma(k+1)}{\Gamma(s+k+1)}}\int\frac{\mathrm{d}^2z}{\pi}z^{*\,s}e^{(z'z^{*}-|z|^2)}\overline{\Psi}_{n,k,z}(x,y),$$

$$\overline{\Psi}_{n,s,z'}(x,y)=\sum_{k=0}^{\infty}\sqrt{\frac{\Gamma(k+s+1)}{\Gamma(s+1)}}\frac{(z'-z)^k}{k!}\overline{\Psi}_{n,s+k,z}(x,y). \tag{2.59}$$

That means, in particular, that (2.56) is a complete set since the set (2.31) is complete.

Selecting different forms for the function $\Phi(\eta)$, we can get other sets of stationary states for a charge in a uniform magnetic field.

C. Nonstationary states

1. Generalized coherent states

The most interesting nonstationary solutions of relativistic wave equations for a charge in a uniform magnetic field are coherent states; such solutions were presented for the first time in Refs. 11–14, see also Ref. 3. In the following we present a new family of nonstationary solutions, which includes the above-mentioned coherent states as a particular case.

Here we are going to use light-cone variables $u^0=x^0-x^3$, $u^3=x^0+x^3$, and the corresponding momentum operators

$$\widetilde{\mathcal{P}}_0=i\hbar\widetilde{\partial}_0=\tfrac{1}{2}(\mathcal{P}_0-\mathcal{P}_3),\quad \widetilde{\mathcal{P}}_3=i\hbar\widetilde{\partial}_3=\tfrac{1}{2}(\mathcal{P}_0+\mathcal{P}_3), \tag{2.60}$$

where $\widetilde{\partial}_0=\partial/\partial u^0$, $\widetilde{\partial}_3=\partial/\partial u^3$. Then the Klein–Gordon operator can be presented in the form

$$\mathcal{K}=4\hbar^{-2}\widetilde{\mathcal{P}}_3\widetilde{\mathcal{P}}_0-2\gamma\mathcal{N}-m^{*2}, \tag{2.61}$$

whereas the Dirac equation reads ($\boldsymbol{\Theta}$ is a Dirac bispinor)

$$4\hbar^{-2}\widetilde{\mathcal{P}}_3\widetilde{\mathcal{P}}_0\Theta_{(-)}=(2\gamma\mathcal{N}_D+m^{*2})\Theta_{(-)},\quad 2\widetilde{\mathcal{P}}_3\Theta_{(+)}=[(\alpha\mathcal{P}_\perp)+\hbar\rho_3 m]\Theta_{(-)},$$
$$\mathcal{P}_\perp=-(\mathcal{P}_1,\mathcal{P}_2,0),\quad \boldsymbol{\Theta}=\Theta_{(+)}+\Theta_{(-)},\quad \Theta_{(\pm)}=p_\pm\boldsymbol{\Theta},\quad 2p_\pm=1\pm\alpha_3. \tag{2.62}$$

Here α and ρ_3 are Dirac matrices,[3] and $p_\pm$ projection operators.

In the case of the uniform magnetic field under consideration, the operators $\widetilde{\mathcal{P}}_3$, $\widetilde{\mathcal{P}}_0$ are integrals of motion. Thus, we will consider solutions that are eigenvectors of $\widetilde{\mathcal{P}}_3$,

$$\widetilde{\mathcal{P}}_3\Psi=\hbar\frac{\lambda}{2}\Psi. \tag{2.63}$$

The scalar wave function obeys (2.63) and can be written as

$$\Psi(x^\mu)=N\exp\left(-i\frac{\lambda}{2}u^3-i\frac{m^{*2}}{2\lambda}u^0\right)\psi(u^0,x,y). \tag{2.64}$$

It is easy to see that $\psi(u^0,x,y)$ obeys a first-order equation, which can be treated as a Schrödinger equation,

$$i\partial_0\psi(u^0,x,y)=\omega a_1^\dagger a_1\psi(u^0,x,y),\quad \omega=\frac{\gamma}{\lambda}. \tag{2.65}$$

Suppose Eq. (2.63) holds, then $\Theta_{(-)}$ can be presented in the form:

$$\Theta_{(-)}(x^\mu)=N\exp\left(-i\frac{\lambda}{2}u^3-i\frac{m^{*2}}{2\lambda}u^0\right)W(1-\alpha_3)C\psi(u^0,x,y). \tag{2.66}$$

Here C is an arbitrary constant bispinor, and W is a unitary matrix (φ_0 is a constant phase),

$$W=\cos\kappa-i\Sigma_3\sin\kappa,\quad 2\kappa=\omega u^0+\varphi_0,\quad W^+W=I, \tag{2.67}$$

and $\psi(u^0,x,y)$ is a scalar function. The latter function obeys Eq. (2.65). Then, the $\Theta_{(+)}$ projection can be found from (2.62), $\Theta_{(+)}=(\hbar\lambda)^{-1}[(\alpha\mathcal{P}_\perp)+\hbar m\rho_3]\Theta_{(-)}$.

Thus, both in the scalar and spinor cases we have to solve the same Eq. (2.65).

In the semi-momentum representation, the corresponding function $\tilde{\psi}(u^0,\xi,\eta)$ obeys the same Eq. (2.65), where, however, one has to use expression (2.14) for the operator $\mathcal{N}=a_1^\dagger a_1$. The relation between the functions $\tilde{\psi}(u^0,\xi,\eta)$ and $\psi(u^0,x,y)$ still has the form (2.17).

Let us introduce the operators

$$A_1^{f,g}=fa_1+ga_1^\dagger,\quad A_1^{+f,g}=f^*a_1^\dagger+g^*a_1, \tag{2.68}$$

where the complex quantities f and g can depend on u^0. These operators are integrals of motion whenever f, g obey (derivatives with respect to u^0 are denoted by dots)

$$i\dot{f}+\omega f=0,\quad i\dot{g}-\omega g=0. \tag{2.69}$$

It is easy to find

$$f=f_0\exp(i\omega u^0),\quad g=g_0\exp(-i\omega u^0), \tag{2.70}$$

where f_0, g_0 are some complex constants. Bearing in mind considerations related to operators (2.33), we are going to consider two nonequivalent cases only. The first one corresponds to $|f|^2=|g|^2$ or equivalently to $|f_0|^2=|g_0|^2$. In this case we can, in fact, only consider the Hermitian operator

$$A_1^\nu=\nu a_1+\nu^*a_1^\dagger,\quad \nu=\nu_0e^{i\omega u^0},\quad \nu_0=\text{const}. \tag{2.71}$$

The second case corresponds to $|f|^2>|g|^2$, and here we can suppose that

$$|f|^2-|g|^2=|f_0|^2-|g_0|^2=1, \tag{2.72}$$

without the loss of generality. In both cases the operators (2.68) are, within constant complex factors, creation and annihilation operators.

Let us include operators (2.71) and (2.34) (they are integrals of motion) into the complete set of operators. Then

$$A_1^{\nu}\psi^{\nu,\mu}_{z_1,z_2}=z_1\psi^{\nu,\mu}_{z_1,z_2},\quad A_2^{\mu}\psi^{\nu,\mu}_{z_1,z_2}=z_2\psi^{\nu,\mu}_{z_1,z_2},\quad z_k^*=z_k,\quad k=1,2. \tag{2.73}$$

In the semi-momentum representation we find

$$\tilde{\psi}(u^0,\xi,\eta)=\Phi^{\nu}_{z_1}(\xi)\Phi^{\mu}_{z_2}(\eta), \tag{2.74}$$

where functions $\Phi^{\nu}_{z_1}$ are defined in (2.37). The corresponding coordinate representation reads

$$\begin{aligned}\psi^{\nu,\mu}_{z_1,z_2}(u^0,x,y)&=\left[\frac{\mu\nu}{2\pi^2|\mu||\nu|(\mu\nu-\mu^*\nu^*)}\right]^{1/2}\exp\left[\frac{Q_6}{4(\mu^*\nu^*-\mu\nu)}\right],\\ Q_6&=2(\mu+\mu^*)(\nu+\nu^*)x^2+2(\mu-\mu^*)(\nu-\nu^*)y^2+4i(\mu\nu^*-\mu^*\nu)xy\\ &\quad-4x[z_1(\mu+\mu^*)+z_2(\nu+\nu^*)]-4iy[z_1(\mu-\mu^*)-z_2(\nu-\nu^*)]\\ &\quad+\left(z_1\sqrt{\frac{\mu^*}{\nu}}+z_2\sqrt{\frac{\nu}{\mu^*}}\right)^2+\left(z_1\sqrt{\frac{\mu}{\nu^*}}+z_2\sqrt{\frac{\nu^*}{\mu}}\right)^2.\end{aligned} \tag{2.75}$$

These solutions are orthogonal at any fixed u^0, $(\psi^{\nu,\mu}_{z_1',z_2'},\psi^{\nu,\mu}_{z_1,z_2})=\delta(z_1-z_1')\,\delta(z_2-z_2')$, and obey the completeness relation

$$\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}\mathrm{d}z_2\,\psi^{*\nu,\mu}_{z_1,z_2}(u^0,x',y')\,\psi^{\nu,\mu}_{z_1,z_2}(u^0,x,y)=\delta(x-x')\,\delta(y-y'). \tag{2.76}$$

Consider now generalized squeezed coherent states, which can be constructed by analogy with (2.44) in the semi-momentum representation. Here we use the operators (2.68) supposing that relations (2.69), (2.70), (2.72), and (2.35) hold,

$$\tilde{\psi}^{f,g;\alpha,\beta}_{n,s;z_1,z_2}(u^0,\xi,\eta)=\Phi^{f,g}_{n,z_1}(\xi)\Phi^{\alpha,\beta}_{s,z_2}(\eta). \tag{2.77}$$

The functions $\Phi^{a,b}_{n,z}(x)$ are defined in (2.45). Thus,

$$\psi^{f,g;\alpha,\beta}_{n,s;z_1,z_2}(u^0,x,y)=\frac{(A_1^{+f,g}-z_1^*)^n(A_2^{+\alpha,\beta}-z_2^*)^s}{\sqrt{\Gamma(n+1)\Gamma(s+1)}}\psi^{f,g;\alpha,\beta}_{z_1,z_2}(u^0,x,y),\psi^{f,g;\alpha,\beta}_{z_1,z_2}=\psi^{f,g;\alpha,\beta}_{0,0;z_1,z_2}. \tag{2.78}$$

The solutions (2.78) obey the relations

$$\begin{aligned}&(A_1^{f,g}-z_1)\,\psi^{f,g;\alpha,\beta}_{n,s;z_1,z_2}=\sqrt{n}\,\psi^{f,g;\alpha,\beta}_{n-1,s;z_1,z_2},(A_1^{+f,g}-z_1^*)\,\psi^{f,g;\alpha,\beta}_{n,s;z_1,z_2}=\sqrt{n+1}\,\psi^{f,g;\alpha,\beta}_{n+1,s;z_1,z_2},\\ &(A_2^{\alpha,\beta}-z_2)\,\psi^{f,g;\alpha,\beta}_{n,s;z_1,z_2}=\sqrt{s}\,\psi^{f,g;\alpha,\beta}_{n,s-1;z_1,z_2},(A_2^{+\alpha,\beta}-z_2^*)\,\psi^{f,g;\alpha,\beta}_{n,s;z_1,z_2}=\sqrt{s+1}\,\psi^{f,g;\alpha,\beta}_{n,s+1;z_1,z_2}.\end{aligned} \tag{2.79}$$

Equation (2.78) describes the most general form of relativistic wave equation solutions in a constant uniform magnetic field. All the formerly known solutions can be obtained from this equation by a particular choice of parameters. For instance, by selecting $f_0=\alpha=1$, $g=\beta=0$, $z_1=0$, $z_2=z$ with $z=0$ we get the states (2.31), on the other hand, if one puts $s=0$, $z\neq 0$, then one gets the states (2.54). For $n=s=0$, $f_0=\alpha=1$, $g=\beta=0$, we get coherent states.[11–14]

In the general case, an explicit coordinate representation for solutions (2.78) looks complicated enough. However, some particular cases admit essential simplifications. For example, suppose $f_0=\alpha=1$, $g=\beta=0$, then

$$\Psi^{1,0;1,0}_{n,s;z_1,z_2}(u^0,x,y)=\frac{(-1)^n}{\sqrt{\pi}}\left(\frac{x+iy-\overline{z_1}^*-z_2}{x-iy-\overline{z_1}-z_2^*}\right)^{(n-s)/2}e^{M_1}I_{s,n}(p_4),$$

$$2M_1=(\overline{z_1}-z_2^*)(x+iy)-(\overline{z_1}^*-z_2)(x-iy)+\overline{z_1}^*z_2-\overline{z_1}z_2^*-2in\omega u^0, \tag{2.80}$$

$$p_4=|x+iy-\overline{z_1}^*-z_2|^2,\quad \overline{z_1}=z_1\exp(-i\omega u^0).$$

For $n=s=0$, we get the coordinate representation for the squeezed coherent states in the form

$$\Psi^{f;g;\alpha,\beta}_{z_1,z_2}(u^0,x,y)=\left[\frac{\alpha f}{(\alpha f-\beta g)\pi|\alpha||f|}\right]^{1/2}\exp Q_7,$$

$$Q_7=-\frac{1}{2}(|z_1|^2+|z_2|^2)+\frac{q}{2(\alpha f-\beta g)}, \tag{2.81}$$

$$q=-(\alpha+\beta)(f+g)x^2-(\alpha-\beta)(f-g)y^2+2i(\beta f-\alpha g)xy+2x[(\alpha+\beta)z_1+(f+g)z_2]$$
$$+2iy[(\alpha-\beta)z_1-(f-g)z_2]+(\alpha g^*-\beta f^*)z_1^2+(\beta^* f-\alpha^* g)z_2^2-2z_1z_2.$$

Solutions from Refs. 11 to 14 are particular cases of (2.81) for $f_0=\alpha=1$, $g=\beta=0$.

Calculating mean values in the states (2.78), we get (one can obtain the same results using spinor wave functions for the calculations)

$$\overline{\mathcal{P}_1}=i\hbar\sqrt{\frac{\gamma}{2}}[(f^*+g^*)z_1-(f+g)z_1^*],\quad \overline{\mathcal{P}_2}=-\hbar\sqrt{\frac{\gamma}{2}}[(f^*-g^*)z_1+(f-g)z_1^*]. \tag{2.82}$$

Here we have taken into account the relations (2.6), (2.36), (2.79), and the orthogonality of the states with respect to the indices n,s. Remember now that in classical theory the corresponding momenta $\mathcal{P}_1^{\rm cl}$, $\mathcal{P}_2^{\rm cl}$ have the following parametric representation [with u^0 being the evolution parameter, R radius of the classical orbit, and κ is given by (2.67)]:

$$\mathcal{P}_1^{\rm cl}=\hbar\gamma R\sin 2\kappa,\quad \mathcal{P}_2^{\rm cl}=-\hbar\gamma R\cos 2\kappa. \tag{2.83}$$

It is easy to see that (2.82) coincides with (2.83) for $z_1=(\gamma/2)^{1/2}R(f_0e^{-i\varphi_0}+g_0e^{i\varphi_0})$. Calculating mean values of the coordinates $\overline{x^1}$, $\overline{x^2}$, we find that they evolve as the corresponding classical quantities $x^{1\rm cl}$, $x^{2\rm cl}$ ($x^1_{(0)}$, $x^2_{(0)}$ are coordinates of the orbit center),

$$x^{1\rm cl}=R\cos\kappa+x^1_{(0)},\quad x^{2\rm cl}=R\sin\kappa+x^2_{(0)}, \tag{2.84}$$

for $z_2=(\gamma/2)^{1/2}[(\alpha+\beta)x^1_{(0)}+i(\alpha-\beta)x^2_{(0)}]$.

Thus, mean-value trajectories in the plane x^1, x^2 do not depend on quantum numbers n,s. These trajectories have classical forms under a proper choice of z_1, z_2.

Calculating quadratic fluctuations in the states (2.78), we get

$$2\overline{(\Delta\mathcal{P}_1)^2}=\hbar^2\gamma|f+g|^2(2n+1),\quad 2\overline{(\Delta\mathcal{P}_2)^2}=\hbar^2\gamma|f-g|^2(2n+1),$$

$$2\gamma\overline{(\Delta x^1)^2}=|f-g|^2(2n+1)+|\alpha-\beta|^2(2s+1),$$

$$2\gamma\overline{(\Delta x^2)^2}=|f+g|^2(2n+1)+|\alpha+\beta|^2(2s+1), \tag{2.85}$$

$$\sigma_1=-\sigma_2=i(fg^*-gf^*)(2n+1),$$

$$\sigma_k=\overline{(\Delta x^k)(\Delta P_k)+(\Delta P_k)(\Delta x^k)},\quad k=1,2.$$

They do not depend on z_1, z_2, but do depend on quantum numbers n,s and on parameters f_0, g_0, α, β. The relations (2.85) imply the generalized Heisenberg inequalities

$$4\mathcal{J}_1=\hbar^2(2n+1)[(2n+1)+(2s+1)|(\alpha-\beta)(f+g)|^2]\geqslant\hbar^2,$$

$$4\mathcal{J}_2=\hbar^2(2n+1)[(2n+1)+(2s+1)|(\alpha+\beta)(f-g)|^2]\geqslant\hbar^2, \tag{2.86}$$

$$\mathcal{J}_k=\overline{(\Delta x^k)^2(\Delta\mathcal{P}_k)^2}-\frac{1}{4}\sigma_k^2, \quad k=1,2.$$

One can fix any given $\overline{(\Delta x^k)^2}$ or $\overline{(\Delta\mathcal{P}_k)^2}$ in a given "instant" u^0 by means of a choice of parameters f_0, g_0, α, β. Then they evolve with "time" u^0 according Eq. (2.85).

2. Eigenfunctions of the L_z operator

In the following we present another type of nonstationary states, which are quite different from the above-mentioned generalized coherent states. Recall that the problem was reduced to solving Eq. (2.65) under the condition (2.63). All the integrals of motion for such an equation can be constructed as functional combination of the operators

$$fa_1, \quad ga_1^\dagger, \quad a_2, \quad a_2^\dagger, \tag{2.87}$$

whenever f, g obey relations (2.69) and (2.70). Constructing integrals of motion that are linear combinations of these operators, we get coherent states. Any linear combinations of the operators (2.87) do not commute with the operator L_z (2.8) or J_z (2.4). Thus, coherent states with definite values of these quantities cannot be constructed. The generalized squeezed coherent states (2.44) and (2.77) are eigenvectors of the operators $\mathcal{N}_1$, $\mathcal{N}_2$ [that follows from (2.79)]. The latter operators are integrals of motion and are quadratic in creation and annihilation operators,

$$\mathcal{N}_1=(A_1^{+f,g}-z_1^*)(A_1^{f,g}-z_1), \quad \mathcal{N}_2=(A_2^{+\alpha,\beta}-z_2^*)(A_2^{\alpha,\beta}-z_2). \tag{2.88}$$

The operators $A_1^{f,g}$ are defined in (2.68), and $A_2^{\alpha,\beta}$ are defined in (2.35). The operators (2.88) do not commute with L_z, J_z as well.

One can see that besides the operators a_1a_2, $a_1^\dagger a_2^\dagger$, the only one quadratic combination that commutes with L_z, J_z is

$$\overline{A}=fa_1a_2+ga_1^\dagger a_2^\dagger. \tag{2.89}$$

It is known[15] that eigenvectors for such an operator can be normalized only for $|f|>|g|$, or for $|f|=|g|$. In the first case the eigenvectors have a finite norm, and in the second case they can be normalized to a δ function. Let us consider the case $|f|\geqslant|g|$ only. Here the operator (2.89) differs from

$$A^p=e^{i\kappa}(a_1a_2-\overline{p}^2a_1^\dagger a_2^\dagger), \quad \overline{p}=pe^{-i\kappa}, \quad -1\leqslant p\leqslant 1, \quad \kappa=\omega u^0+\kappa_0, \quad \kappa_0=\text{const} \tag{2.90}$$

by a complex factor only. Thus, it is enough to consider the latter operator only. Let us demand that functions $\psi(u^0,\rho,\varphi)$ be solutions of Eq. (2.65), and, at the same time, eigenvectors of the operators A^p, L_z,

$$A^p\psi_{q,l}^p=-q\psi_{q,l}^p, \quad L_z\psi_{q,l}^p=\hbar l\psi_{q,l}^p, \quad l=0,\pm1,\pm2,\ldots. \tag{2.91}$$

Such solutions can be constructed in terms of the Laguerre functions $I_{n,m}(x)$ with noninteger indices,

$$\psi^p_{q,l}(u^0,\rho,\varphi)=N\exp(il\varphi-\Gamma)(1+\overline{p})^{-\alpha}(1-\overline{p})^{-\beta}I_{|l|+s,s}(x),$$

$$\Gamma=i\frac{l\omega u^0}{2}+\frac{1+\overline{p^2}}{2(1-\overline{p^2})}\rho,\quad \alpha=\frac{p-q}{2p},\quad \beta=\frac{p+q}{2p},\tag{2.92}$$

$$s=\frac{q}{2p}-\frac{|l|+1}{2},\quad x=\frac{2\overline{p}\rho}{1-\overline{p^2}},$$

$$I_{n,m}(x)=\sqrt{\frac{\Gamma(1+n)}{\Gamma(1+m)}}\frac{\exp\left(-\frac{x}{2}\right)}{\Gamma(1+n-m)}x^{(n-m)/2}\Phi(-m,n-m+1;x).$$

Here $\Phi(\alpha,\beta;x)$ is the degenerate hypergeometric function (see Ref. 9, 9.210). For $p^2=1$, the operator (2.90) is anti-Hermitian and q is imaginary, $\mathrm{Re}\,q=0$. For $p=0$, solutions have a very simple form

$$\psi^0_{q,l}(u^0,\rho,\varphi)=N_0\exp(il\varphi+\overline{q}-\Gamma_0)J_{|l|}(2\sqrt{\overline{q}\rho}),\quad \Gamma_0=\frac{i}{2}l\omega u^0+\frac{\rho}{2},\quad \overline{q}e^{-ik},\tag{2.93}$$

where $J_\nu(x)$ is the Bessel function (see Ref. 9, 8.402). The functions (2.93) can be obtained from (2.92) as a limit $p\to 0$, as can be seen with the help of the property

$$\lim_{r\to\infty} I_{r+\alpha,r+\beta}\left(\frac{x^2}{4r}\right)=J_{\alpha-\beta}(x).\tag{2.94}$$

The functions (2.92) and (2.93) are orthogonal only with respect to quantum numbers l,

$$(\psi^p_{q',l'},\psi^p_{q,l})=\delta_{l,l'}QF(-s,-s'^*;1+|l|;y),\quad y=\left(\frac{2p}{1+p^2}\right)^2,$$

$$Q=\left[\frac{\Gamma(1+|l|+s)\Gamma(1+|l|+s'^*)}{p^2\Gamma(1+s)\Gamma(1+s'^*)}\right]^{1/2}\frac{\pi NN'^*}{\Gamma(1+|l|)}y^{(1+|l|)/2}(1-y)^{-(q+q^*)/4p},$$

$$(\psi^0_{q',l'},\psi^0_{q,l})=\delta_{l,l'}2\pi N_0N_0'^*I_{|l|}(2\sqrt{qq'^*}).\tag{2.95}$$

Here $F(\alpha,\beta;\gamma;x)$ is the hypergeometric function (see Ref. 9, 9.100), and $I_\alpha(x)$ is the Bessel function of imaginary argument (see Ref. 9, 8.404). Calculating (2.95), we have used the integral table (see Ref. 9, 6.633.2; 7.622.1).

The states (2.92) are not coherent states, however, they are, in a sense, close to such states. Indeed, let us consider the equations (2.6) on classical trajectories. Then we get a classical relation

$$\rho=\rho(u^0)=\sqrt{L_z^2\hbar^{-2}+4|a_1a_2|^2}-a_1a_2-a_1^\dagger a_2^\dagger.\tag{2.96}$$

For $p=0$, it follows from (2.91) that $a_1a_2=-\overline{q}$, $L_z=\hbar l$. Thus, we can rewrite (2.96) in the form

$$\rho(u^0)=\rho_0^{\mathrm{cl}}+\overline{q}+\overline{q}^*,\quad \rho_0^{\mathrm{cl}}=\sqrt{l^2+4|q|^2}.\tag{2.97}$$

Calculating the mean value $\overline{\rho}$ by means of the functions (2.93), we find

$$\overline{\rho}=\rho_0+\overline{q}+\overline{q}^*,\quad \rho_0=|l|-1-2|q|\frac{I_{|l|-1}(2|q|)}{I_{|l|}(2|q|)}.\tag{2.98}$$

Thus, the time dependence of $\overline{\rho}$ is classical. The only constant which can differ from its classical value is ρ_0.

III. EXACT SOLUTIONS OF RELATIVISTIC WAVE EQUATIONS IN LONGITUDINAL FIELDS

A. Definition of fields

Consider here longitudinal electromagnetic fields, which have the form

$$\mathbf{E}=\mathbf{n}E, \quad \mathbf{H}=\mathbf{n}H. \tag{3.1}$$

Here $\mathbf{n}$ is a unit vector, $\mathbf{n}^2=1$. Suppose $\mathbf{n}$ is directed along x^3 axis. Then, the fields (3.1) obey the free Maxwell equations whenever

$$E=E(x^0,x^3), \quad H=H(x^1,x^2),$$

where $E(x^0,x^3)$, $H(x^1,x^2)$ are arbitrary functions of the indicated arguments. Thus, the fields under consideration can be represented by potentials of the form

$$\begin{gathered} A_0=A_0(x^0,x^3), \quad A_1=A_1(x^1,x^2), \quad A_3=A_3(x^0,x^3), \quad A_2=A_2(x^1,x^2), \\ E=\partial_0 A_3-\partial_3 A_0, \quad H=\partial_2 A_1-\partial_1 A_2. \end{gathered} \tag{3.2}$$

Thus, the operators (2.6) do not depend on the electric field (on A_0, A_3). Therefore, imposing restrictions only on the magnetic field, we can maintain relations (2.6)–(2.11). For a uniform magnetic field (2.1), the commutation relations (2.7) are still valid and we use the semi-momentum representation, where these operators act on different variables [see (2.10)–(2.12), (2.17)].

Lorentz equations have the following form

$$\begin{gathered} m\ddot{x}^0+E\dot{x}^3=0, \quad m\ddot{x}^3+E\dot{x}^0=0, \\ m\ddot{x}^1+H\dot{x}^2=0, \quad m\ddot{x}^2+H\dot{x}^1=0, \quad \dot{x}^\mu\dot{x}_\mu=1, \end{gathered} \tag{3.3}$$

which implies the following first integrals of motion:

$$m^2((\dot{x}_1)^2+(\dot{x}_2)^2)=k_1^2, \quad m^2((\dot{x}_0)^2-(\dot{x}_3)^2)=m^2+(k_1)^2, \tag{3.4}$$

where k_1 is an integration constant.

B. Klein–Gordon equation

Consider the Klein–Gordon equation in the fields under consideration. Representing the wave function as

$$\Psi=\varphi(x^0,x^3)\,\psi(x^1,x^2), \tag{3.5}$$

we find

$$(\mathcal{P}_1^2+\mathcal{P}_2^2-k_1^2)\,\psi(x^1,x^2)=0, \quad (\mathcal{P}_0^2-\mathcal{P}_3^2-m^2-k_1^2)\,\varphi(x^0,x^3)=0. \tag{3.6}$$

Using the variables x, y, η, ξ defined in (2.5) and (2.12), we can rewrite the equation for $\psi(x^1,x^2)$ in the following form:

$$(\xi^2-\partial_\xi^2-k_1'^2)\,\psi(x^1,x^2)=0, \quad k_1'^2=\frac{k_1^2}{\hbar^2\gamma}. \tag{3.7}$$

The operator $(\xi^2-\partial_\xi^2-k_1'^2)$ does not depend on η. Thus, it is convenient to go over to the semi-momentum representation,

$$\psi(x,y)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{iky}\tilde{\psi}(x,k)\mathrm{d}k.$$

Substituting the integration over k by an integration over η, we obtain

$$\psi(x,y)=\frac{e^{ixy}}{\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-i\sqrt{2y}\,\eta}\tilde{\psi}(\xi,\eta)\mathrm{d}\eta,\quad \xi=\sqrt{2}x-\eta. \tag{3.8}$$

The function ψ is an eigenvector of the operator $\mathcal{N}$ (2.14). The latter operator commutes with the operators from Eq. (3.6). In the semi-momentum representation we can write

$$\mathcal{N}\tilde{\psi}_n=n\tilde{\psi}_n\Rightarrow\tilde{\psi}_n(\xi,\eta)=U_n(\xi)\Phi(\eta), \tag{3.9}$$

where $\Phi(\eta)$ is an arbitrary function of η. It follows from (2.8) and the first equation in (3.6) that

$$\mathcal{P}_1^2+\mathcal{P}_2^2=2\hbar^2\gamma\mathcal{N}+\hbar^2\gamma,\quad k_1^2=2\hbar^2\gamma n+\hbar^2\gamma.$$

Solution of the last equation in (3.6) can be found for fields that admit separation of the variables x^0, x^3. For example, let us choose the potentials in the form: $|e|A_0=A(x^3)$, $A_3=0$, $|e|E=-\partial_3 A$. In this case, stationary solutions of Eq. (3.6) read

$$\varphi(x^0,x^3)=e^{-ik_0x^0}\chi(x^3),\quad \chi''+R\chi=0,\quad R(x^3)=(k_0+A)^2-m^2-k_1^2. \tag{3.10}$$

Thus, the functions (3.5) being written in the semi-momentum representation take the form

$$\Psi_n=e^{-ik_0x^0}\chi(x^3)U_n(\xi)\Phi(\eta). \tag{3.11}$$

Equation (3.10) for χ can be solved exactly for the following choices of the function $A(x^3)$:

$$A(x^3)=\alpha x,\quad A(x^3)=\alpha\exp(\beta x^3),\quad A(x^3)=\frac{\alpha}{x^3},$$

$$A(x^3)=\alpha\tanh(\beta x^3),\quad A(x^3)=\alpha\tan(\beta x^3),\quad A(x^3)=\beta\coth(\beta x^3).$$

The corresponding exact solutions are presented in Ref. 3. Demanding that the Klein–Gordon function be an eigenvector of the operator L_z (2.16), we get an equation for the function $\Phi(\eta)$ from (3.11),

$$a_2^\dagger a_2\Phi(\eta)=s\Phi(\eta). \tag{3.12}$$

Thus, $\Phi(\eta)=U_s(\eta)$, and $L_Z\Psi_{ns}=\hbar(n-s)\Psi_{ns}$. Keeping this in mind and doing the integral (3.8), we obtain

$$\Psi_{n,s}=e^{-ik_0x^0}\chi(x^3)\frac{(-1)^n}{\sqrt{2\pi}}\left(\frac{x+iy}{x-iy}\right)^{(n-s)/2}I_{n,s}(x^2+y^2),$$

where $I_{n,s}$ are the Laguerre functions. Solutions of Eq. (3.12) have been analyzed above.

C. Dirac equation

Let us present the Dirac wave function in the form

$$\mathbf{\Theta}=\mathbf{M}\begin{pmatrix}\psi_1\\ \psi_{-1}\end{pmatrix}\varphi(x^0,x^3)v,$$

$$\mathbf{M}=\begin{pmatrix}k_1(m+\mathcal{P}_0+\mathcal{P}_3-ik_1\sigma_2) & (\mathcal{P}_1-i\mathcal{P}_2)(m+\mathcal{P}_0+\mathcal{P}_3-ik_1\sigma_2)\\ (\mathcal{P}_1+i\mathcal{P}_2)[(m-\mathcal{P}_0-\mathcal{P}_3)\sigma_3-k_1\sigma_1] & k_1[(m-\mathcal{P}_0-\mathcal{P}_3)\sigma_3-k_1\sigma_1]\end{pmatrix},$$

where ν is an arbitrary spinor, which can be fixed by supplementary conditions. Then the following equations take place:

$$(\mathcal{P}_0^2-\mathcal{P}_3^2-m^2-k')\varphi(x^0,x^3)=0,\quad k'=k_1^2+ieE, \tag{3.13}$$

$$(\mathcal{P}_1+i\mathcal{P}_2)\psi_1(x^1,x^2)=\hbar k_1\psi_{-1}(x^1,x^2), \tag{3.14}$$

$$(\mathcal{P}_1-i\mathcal{P}_2)\psi_{-1}(x^1,x^2)=\hbar k_1\psi_1(x^1,x^2). \tag{3.15}$$

As a consequence of Eqs. (3.14) and (3.15), we get

$$a_1\psi_{-1}=-i\sqrt{n}\psi_1,\quad a_1^\dagger\psi_1=i\sqrt{n}\psi_{-1},\quad k_1^2=2\gamma n.$$

Thus, we see that $\psi_1=\psi_{n-1}$, $\psi_{-1}=-i\psi_n$, and the problem is reduced to solving Eq. (3.13). The latter coincides with the second equation in (3.6).

Considering, for example, the constant and uniform magnetic field (2.1) together with the electric field described by potentials $|e|A_0=A(x^3)$, $A_3=0\Rightarrow|e|E=-\partial_3 A$, we get

$$\varphi(x^0,x^3)=\exp(-ik_0x^0)\chi(x^3),\quad \chi''+(i\partial_3+k_0+A)\chi=0.$$

All possible solutions of the latter equation for the function χ are presented in Ref. 3.

IV. PECULIARITIES OF INTEGRATION OF LINEAR DIFFERENTIAL EQUATIONS WITH NONCOMMUTATIVE SYMMETRIES

Here we are going to return to the above-mentioned results from a point of view of general theory of differential equation. Recall that we succeeded to explicitly find the transformation (2.10)–(2.13) which has effectively reduced the number of the variables in the initial equations. In fact, that was the main starting point for all further constructions. However, one can see that this ''reduction'' of variables is a particular example of a general situation, which is described briefly in the following.

Consider first the case of an integrable classical $2N$-dimensional Hamiltonian system with the Hamiltonian H. Suppose this system has N independent integrals of motion that are in involution. It is well known that in such a case the variables of the type action-angle $(J,\ \varphi)$ are available, and the Hamiltonian depends on the action variables only, $H=H(J)$. Let us suppose that for such a system exists one more independent integral of motion Y. Since Y is independent, it cannot commute with the former integrals, and, therefore, Y must depend on the angle variables. One can demonstrate that in such a case the Hamiltonian system is degenerate, $\det\|\partial H(J)/\partial J_i\partial J_j\|=0$, and, therefore, the Hamiltonian does not depend on some combinations of the action variables. For example, suppose the integral Y does not commute with the integral J_N only. Then the Hamiltonian can depend on the variables $J_1,\ldots,J_{N-1}$ only, otherwise H cannot commute with Y. Thus, we see that the noncommutative algebra of integrals of motion allows one to find canonical variables such that part of the corresponding action variables disappears from the Hamiltonian. This phenomenon is closely related to the topological properties of orbits for the Hamiltonian system. Namely, trajectories of the integrable Hamiltonian system with N-dimensional commuta-

tive set of integrals of motion form (in the compact case) a winding of N-torus in $2N$-dimensional phase space. If the set of the integrals is noncommutative then the dimension of the corresponding torus is $r<N$ (see Ref. 16).

The phenomenon of variable ''reduction'' takes place in the quantum integrable Hamiltonian system as well. As will be demonstrated in the following, by constructing a special isomorphism of linear functional spaces, we can transform the initial differential operator of an equation into another one with a reduced number of variables. The method which we are going to use for such a demonstration, is, in fact, the harmonic analysis on the noncommutative functional algebras.

Consider a differential equation

$$H(x,\partial_x)\psi(x)=0, \tag{4.1}$$

for functions $\psi(x)\in\mathcal{L}$ of N independent variables $x\in R^N$. The space $\mathcal{L}\subset C^\infty(R^N)$ and depends on the problem under consideration. Some suppositions about $\mathcal{L}$ will be introduced below. Suppose that Eq. (4.1) admits a noncommutative algebra of functionally independent symmetry operators $\mathcal{F}=\{X_a(x,\partial_x)\}$. The corresponding commutation relations are in the general case nonlinear,

$$\frac{i}{\hbar}[X_a,X_b]=\Omega_{ab}(X), \quad a,b=1,\ldots,n\equiv\dim\mathcal{F}. \tag{4.2}$$

Here $\Omega_{ab}(X)$ are symmetric operator functions. The linear case, when $\Omega_{ab}(X)=C_{ab}^cX_c$, corresponds to a Lie algebra, the quadratic symmetric functions $\Omega_{ab}(X)$ correspond to a quadratic algebra, and so on. The algebra $\mathcal{F}$ corresponds to the algebra $\mathcal{F}'=\{Y_\alpha(x,\partial_x)\}$ of the invariant operators on $\mathcal{L}$:

$$[X_a,Y_\alpha]=0, \quad \frac{i}{\hbar}[Y_\alpha,Y_\beta]=\omega_{\alpha\beta}(Y), \quad \alpha,\beta=1,\ldots,n'\equiv\dim\mathcal{F}'. \tag{4.3}$$

We denote via $E(\mathcal{F})$ and $E(\mathcal{F}')$ enveloping fields for the algebras $\mathcal{F}$ and $\mathcal{F}'$, respectively. Elements of $E(\mathcal{F})$ and $E(\mathcal{F}')$ are symmetrized operator functions of the generating operators X_a Y_α. It is clear that the centers of the enveloping fields coincide, i.e., $Z(E(\mathcal{F}))=Z(E(\mathcal{F}'))$. The elements of the center $Z=Z(E(\mathcal{F}))$ are called Casimir operators. The number of the independent Casimir operators, which generate the center Z, is called the index of the algebra $\mathcal{F}$: $r\equiv\operatorname{ind}\mathcal{F}$ $=\operatorname{ind}\mathcal{F}'$. If we replace the operators X and Y in the operator functions $\omega_{\alpha\beta}(Y)$ and $\Omega_{ab}(X)$ by arbitrary complex numbers ξ and f, then the index of the algebras $\mathcal{F}$ and $\mathcal{F}'$ can be calculated according to

$$r=\sup_{\xi\in C}\operatorname{corank}\,\Omega_{ab}(\xi)=\sup_{f\in C}\operatorname{corank}\,\omega_{\alpha\beta}(f). \tag{4.4}$$

One can show that the following relation takes place:

$$n+n'=2N. \tag{4.5}$$

Let us introduce the notion of the λ-representation of the algebra $\mathcal{F}$.[17] In fact, the λ-representation is the result of the quantization of the classical Poisson bracket and can be understood as a realization of the algebra $\mathcal{F}$ by an irreducible set of differential operators $\tilde{X}$ $=\tilde{X}(q,\partial_q,j)$, dependent on r parameters $j=(j_1,\ldots,j_r)$, and acting in a space of functions of $[q]=(n-r)/2$ independent variables (via $[q]$ we denote the number of the variables q, similar notations are used in the following) $q\in Q$,

$$\frac{i}{\hbar}[\tilde{X}_a,\tilde{X}_b]=-\Omega_{ab}(\tilde{X}), \quad K_\mu(\tilde{X}(q,\partial_q,j))=\kappa_\mu(j), \quad \det\left\|\frac{\partial\kappa_\mu(j)}{\partial j_\nu}\right\|\neq 0. \tag{4.6}$$

Here K_μ are all the independent Casimir operators of $\mathcal{F}$. In a similar manner, we construct the λ-representation $\{\tilde{Y}\}$ of $\mathcal{F}'$ in a space of functions of $[q']=(n'-r)/2$ independent variables q' $\in Q'$,

$$\frac{i}{\hbar}[\tilde{Y}_\alpha,\tilde{Y}_\beta]=\omega_{\alpha\beta}(\tilde{Y}),\quad K'_\mu(\tilde{Y}(q',\partial_{q'},j))=K_\mu(\tilde{X}(q,\partial_q,j))=\kappa_\mu(j). \tag{4.7}$$

Suppose that in the spaces of functions of x, of q, and of q' are defined scalar products

$$(\varphi,\psi)=\int_{R^N}\overline{\varphi(x)}\psi(x)\mathrm{d}\mu(x),\quad (\tilde{\varphi},\tilde{\psi})=\int_Q\overline{\tilde{\varphi}(q)}\tilde{\psi}(q)\mathrm{d}\mu(q),$$
$$(\tilde{\varphi},\tilde{\psi})'=\int_{Q'}\overline{\tilde{\varphi}(q')}\tilde{\psi}(q')\mathrm{d}\mu(q'), \tag{4.8}$$

where $\mathrm{d}\mu(x)$, $\mathrm{d}\mu(q)$, and $\mathrm{d}\mu(q')$ are some measures on R^N, Q, and Q', respectively. And suppose that the operators $X_a(x,\partial_x)$, $Y_\alpha(x,\partial_x)$ and the operators $\tilde{X}_a(q,\partial_q,j),\tilde{Y}(q',\partial_{q'},j)$ are self-conjugate with respect to the corresponding scalar products (this supposition is not necessary and is introduced to simplify the consideration). Now we define the set of distributions $D^j_{qq'}(x)$ as a solution of the overdetermined system of the equations:

$$[X_a(x,\partial_x)-\tilde{X}_a(q,\partial_q,j)]D^j_{qq'}(x)=0;\quad [Y_\alpha(x,\partial_x)-\tilde{Y}_a(q',\partial_{q'},j)]D^j_{qq'}(x)=0. \tag{4.9}$$

The distributions $D^j_{qq'}(x)$ obey the completeness and orthogonality relations:

$$\int\overline{D^j_{qq'}(x)}D^{\tilde{j}}_{\tilde{q}\tilde{q}'}(x)\,\mathrm{d}\mu(x)=\delta(j,\tilde{j})\,\delta(q,\tilde{q})\,\delta(q',\tilde{q}'), \tag{4.10}$$

$$\int\overline{D^j_{qq'}(x)}D^j_{qq'}(\tilde{x})\mathrm{d}\mu(j)\mathrm{d}\mu(q)\mathrm{d}\mu(q')=\delta(x,\tilde{x}). \tag{4.11}$$

Here $\mathrm{d}\mu(j)$ is the spectral measure of the Casimir operators $K(X)(=K'(Y))$. Due to Eqs. (4.6), (4.7) and (4.9) the distributions $D^j_{qq'}(x)$ are eigenfunctions of all the Casimir operators,

$$K_\mu(X(x,\partial_x))D^j_{qq'}(x)=\kappa_\mu(j)D^j_{qq'}(x),\quad \mu=1,\ldots,r. \tag{4.12}$$

Usually one can find $D^j_{qq'}(x)$ by an integration, at least in the case when $\mathcal{F}$ is a Lie algebra. As a consequence of (4.11) and (4.10) we can define the direct and the inverse Fourier transforms:

$$\tilde{\psi}(q,q',j)=\int D^j_{qq'}(x)\overline{\psi(x)}\,\mathrm{d}\mu(x), \tag{4.13}$$

$$\psi(x)=\int D^j_{qq'}(x)\overline{\tilde{\psi}(q,q',j)}\mathrm{d}\mu(j)\mathrm{d}\mu(q)\mathrm{d}\mu(q'). \tag{4.14}$$

Equations (4.13) and (4.14) establish an isomorphism of the spaces $\mathcal{L}$ and $\tilde{\mathcal{L}}=\{\tilde{\psi}\}$. It is important to stress that under such an isomorphism the operators X, Y are transformed into the differential operators $\tilde{X},\tilde{Y}$ that act in the spaces of functions, which depend on a smaller number of variables,

$$X(x,\partial_x)\psi(x)\leftrightarrow\tilde{X}(q,\partial_q,j)\tilde{\psi}(q,q',j),\quad Y(x,\partial_x)\psi(x)\leftrightarrow\tilde{Y}(q',\partial_{q'},j)\tilde{\psi}(q,q',j). \tag{4.15}$$

Let us return to Eq. (4.1). Here we can conclude that $H\in E(\mathcal{F}')$ since the operator H commutes with all the operators of the algebra $\mathcal{F}=\{X_a\}$. In turn, that means that there exists an operator function $H(Y)$ such that $H(x,\partial_x)=H(Y(x,\partial_x))$. Let us look for solutions of Eq. (4.1) in the form (4.14). Using the isomorphism (4.15), we get

$$H(\tilde{Y}(q',\partial_{q'},j))\tilde{\psi}(q,q',j)=0. \tag{4.16}$$

Thus, departing from Eq. (4.1) without loss of any information, we have arrived at a differential equation with $\tilde{N}=[q']=(n'-r)/2$ independent variables. Taking into account (4.5), one can obtain

$$\tilde{N}=N-\tfrac{1}{2}(\dim\mathcal{F}+\operatorname{ind}\mathcal{F}). \tag{4.17}$$

Thus, the existence of a noncommutative symmetry algebra results in the phenomenon of variable reduction. Indeed, we started with $N=[q']+[q]+r$ variables. $[q]$ variables have disappeared completely, and $r=[j]$ variables remain in the equations as some parameters. The solution of Eq. (4.16) contains as a factor an arbitrary function of the variables q,j. The number of variables q is equal to $[q]=(n-r)/2=(\dim\mathcal{F}-\operatorname{ind}\mathcal{F})/2$. In the commutative case: $\operatorname{ind}\mathcal{F}=\dim\mathcal{F}$, and $[q]=0$. In the noncommutative case: $\dim\mathcal{F}>\operatorname{ind}\mathcal{F}$, and $[q]>0$. Thus, the reduction of variables always takes place when there exists a noncommutative algebra of the integrals of motion.

Let us apply the above-mentioned consideration to the Klein–Gordon equation (2.2) in a uniform magnetic field. In this case we have four ($N=4$) variables and five ($n=5$) independent symmetry operators: $\mathcal{F}=\{P_0,P_3,a_2,a_2^\dagger,L_z=\hbar L\}$,

$$P_0=i\hbar\partial_0,\quad P_3=i\hbar\partial_3,\quad L=u\partial_u-\bar{u}\partial_{\bar{u}},\quad a_2=\partial_{\bar{u}}+u/2,\quad a_2^\dagger=-\partial_u+\bar{u}/2,\quad u\equiv x+iy.$$

The nonzero commutation relations are $[a_2,a_2^\dagger]=1$, $[L,a_2]=a_2$, $[L,a_2^\dagger]=-a_2^\dagger$. It follows from (4.4) that $r=\operatorname{ind}\mathcal{F}=3$. $\tilde{N}=[q']=0$ $\mathcal{K}\in Z$ according to (4.17). Thus, Eq. (4.16) presents algebraic relations on the parameters j (and on the parameters of the equation itself). Besides, $\dim\mathcal{F}'=3=r$, due to (4.5). Thus, the algebra of the invariant operators is placed completely in the center. Or more simply, there are no operators $Y,\tilde{Y}$ and variables q' in the case under consideration. The center Z is generated by three Casimir operators, those are $K_1=P_0$, $K_2=P_3$, $K_3=\mathcal{N}=L+a_2^\dagger a_2=L+\frac{1}{2}(a_2^\dagger a_2+a_2a_2^\dagger-1)$.

Let us construct the λ-representation of the algebra $\mathcal{F}$:

$$\tilde{P}_0=j_1=\hbar k_0,\quad \tilde{P}_3=j_2=\hbar k_3,\quad \tilde{a}_2=q,\quad \tilde{a}_2^+=\partial_q,\quad \tilde{L}=-q\partial_q+n,\quad n=j_3=0,1,\ldots.$$

The operators $\tilde{a}_2$ and $\tilde{a}_2^+$ are mutually conjugate with respect to the scalar product (4.8) with the measure $\mathrm{d}\mu(q)=\exp(-q\bar{q})\mathrm{d}^2q/\pi,(\mathrm{d}^2q\equiv\mathrm{d}q_1\mathrm{d}q_2,\quad q=q_1+iq_2)$. The operator $\tilde{L}$ is self-conjugate, and the space $\tilde{\mathcal{L}}$ is built up from analytic functions dependent on the variable q and on the parameters $j=(k_0,k_3,n)$. Here the Casimir operator $\tilde{\mathcal{N}}$ has the following form $\tilde{\mathcal{N}}=\tilde{L}+\frac{1}{2}(\tilde{a}_2^+\tilde{a}_2+\tilde{a}_2\tilde{a}_2^+-1)=n$.

From Eq. (4.9) we can find the set $D_q^j(x)$ that obeys the completeness and orthogonality relations. Such a set has the form

$$D_q^j(x)=e^{i(k_0x^0+k_3x^3)}e^{q\bar{u}-u\bar{u}/2}(u-q)^n/(2\pi\sqrt{\pi n!}), \tag{4.18}$$

$$\int\overline{D_q^j(x)}\tilde{D_{\tilde{q}}^j}(x)\mathrm{d}x=\delta(k_0-\tilde{k}_0)\,\delta(k_3-\tilde{k}_3)\,\delta(\tilde{q},q)\,\delta_{n\tilde{n}}, \tag{4.19}$$

$$\sum_{n=0}^{\infty}\int\overline{D_q^j(x)}D_q^j(\tilde{x})\,\mathrm{d}k_0\mathrm{d}k_3\mathrm{d}\mu(q)=\delta(x^0-\tilde{x}^0)\,\delta(x^3-\tilde{x}^3)\,\delta(x-\tilde{x})\,\delta(y-\tilde{y}). \tag{4.20}$$

In Eq. (4.19) $\delta(\tilde{q},q)=\exp(\bar{q}\tilde{q})$ is a δ-function with respect to the measure $\mathrm{d}\mu(q)$. To justify the validity of (4.19) and (4.20) one can use the following relations.[18]

$$\int\overline{v_n(q)}v_m(q)\,d\mu(q)=\delta_{nm},\quad \sum_{n=0}^{\infty}\overline{v_n(q)}v_n(\tilde{q})=\delta(\tilde{q},q)=\exp(\bar{q}\tilde{q}),\quad v_n(q)\equiv q^n/\sqrt{n!}.$$

As was previously mentioned, the Klein–Gordon operator $\mathcal{K}$ belongs to the center Z, and, therefore, can be presented in a polynomial form of the Casimir operators $P_0, P_3, \mathcal{N}$, which generate this center. Such a representation is given by Eq. (2.9). The Klein–Gordon equation in the space $\tilde{\mathcal{L}}$, i.e., Eq. (4.16), is, in fact, relation (2.21) for the parameters $j=(k_0, k_3, n)$. Thus, the functions (4.18) form a basis of the Klein–Gordon equation (2.2) [with allowance made for (2.21)].

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Finite dimensional Hamiltonian formalism for gauge and quantum field theories

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We discuss in this article the canonical structure of classical field theory in finite dimensions within the *pataplectic* Hamiltonian formulation, where we put forward the role of Legendre correspondence. We define the generalized Poisson $\mathfrak{p}$-brackets which are the analogs of the Poisson bracket on forms. We formulate the equations of motion of forms in terms of $\mathfrak{p}$-brackets. As illustration of our formalism we present three examples: the interacting scalar fields, conformal string theory and the electromagnetic field. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In the standard Hamiltonian formulation of classical point particle mechanics, the phase space of a system with N degrees of freedom is a $2N$ dimensional manifold, which represents the space of possible positions and momenta of the system. In field theories the dynamical objects typically have an infinite number of degrees of freedom. Thus we need to employ infinite dimensional manifolds to model their evolution. This requires a generalization of the familiar theory of finite dimensional manifolds, and so we are motivated to stipulate that an infinite dimensional manifold is a manifold modeled for example on an infinite dimensional Banach space.

Infinite dimensional manifolds do, of course, differ in many significant ways from their finite dimensional counterparts. No infinite dimensional manifold is locally compact, for instance, although every finite dimensional one is. Furthermore, the fact that the tangent spaces are infinite dimensional leads to some complications which are not present in the finite dimensional case. Two are worth mentioning here:

(1) In the finite dimensional case, a linear map $T:V\to V$ is one to one iff it is onto; in the infinite dimensional case a linear operator on V can be one to one but not onto.
(2) Similarly, in the finite dimensional case, all linear operators are continuous maps from V to V; in the infinite dimensional case, the continuous linear operators, i.e., the bounded operators, often have as their domain of definition a dense (proper) subset of V.

A crucial step in the formulation of Hamiltonian mechanics is the construction of the Poisson bracket of a pair of physical observables. This is obtained from the natural symplectic structure on $T^\star M$ (where M is the configuration space of the physical system). In this phase space approach to classical mechanics, the dynamical evolution from an initial point $x_O \in T^\star M$ is the solution to Hamilton's first order differential equations. Geometrically, dynamical trajectories in phase space can be identified with the flow lines of a special vector field ξ_H on $T^\star M$ associated with the Hamiltonian function H. Those dynamical equations imply the time rate of change of any physical observable $f \in C^\infty(T^\star M, \mathbb{R})$, precisely through the Poisson bracket of f with H which is defined

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thanks to Hamiltonian vector fields ξ_f on $T^\star M$ associated to each f. There are a couple of potential difficulties here. If $T^\star M$ is infinite dimensional, then some perfectly good functions may not have a Hamiltonian vector field (this problem does not arise in the finite dimensional case). Even when ξ_f exists, its integral curves may be incomplete (i.e., the vector field is only locally defined).

Further, in this viewpoint space and time are treated asymmetrically, therefore we do not have a covariant scheme.

In order to avoid these difficulties, an alternative approach is to construct covariant canonical formulations of (finite dimensional) field theories which treat the space and time on equal footing (symmetrically). Remark that there is a whole variety of such theories and interestingly enough they offer a generalization of the Hamilton canonical equations of motion to field theory (see, for instance Refs. 1–4, 11, 12, and 24). Further details can be found in Refs. 5–15, 19, 22, and 23. One point there is that the observable quantities are not represented by (generalized) functions on a phase space, but rather by $(n-1)$-forms, whose integrals on Cauchy hypersurfaces give back the usual observables. But many of those approaches share a characteristic, which is an obstacle to the development of a field quantization: the lack of an appropriate generalization of the Poisson bracket. And even if a Poisson bracket was proposed, the related construction was too restrictive and not appropriate for representing the generalized Hamiltonian field equations in Poisson bracket formulation.

More recently, a definition of the Poisson brackets on a subclass of forms and the equations of motion of forms from De Donder–Weyl point of view was given (see Refs. 16, 17, 20, and 21). [In this approach we associate to the generalized coordinates (the field variables) u^i a set of n momentumlike variables (which are defined from the Lagrangian as the conjugate momenta associated with each space–time—here $\alpha=1,\ldots,n$ is the space–time index—derivative of the field), $p_i^\alpha := \partial L/\partial(\partial_\alpha u^i)$, and we have the Legendre transform: $\partial_\alpha u^i \to p_i^\alpha$, $L(u^i,\partial_\alpha u^i,x^\alpha) \to H(u^i,p_i^\alpha,x^\alpha) := p_i^\alpha \partial_\alpha u^i - L$. So, the phase space is replaced by a finite dimensional space.] The main point is to derive the Hamiltonian fields equations from the Poincaré–Cartan n-form and its differential, called there *polysymplectic form* using ''vertical multivector fields'' (which generalize the Hamiltonian vector fields in mechanics). Constructions of brackets can be done using also the polysymplectic form, but a correct expression of the dynamics of these forms requires a decomposition of forms and multivectors along ''vertical'' and ''horizontal'' components. This decomposition, however, essentially implies a triviality of the ''extended polymomentum phase space'' as a bundle over the space–time manifold. Moreover, we notice that in those works although a natural link between Poisson brackets and dynamics exists for $n-1$-forms, in the case of forms of arbitrary degrees the link is not clear. [This generalization of the Poisson bracket formulation of the equations of motion to forms of arbitrary degree requires a certain extension, namely by adding horizontal forms of degree n and the vertical-vector valued horizontal one-forms (objects of formal degree zero) associated with n-forms. This extension calls for a generalization of Lie, Schouten–Nijenhuis and Frölicher–Nijenhuis brackets.] This affect the possibility of a precise formulation, for example (of the dynamics), of Maxwell's electrodynamics. In addition, we do not have a representation of the energy-momentum tensor.

In this article we exhibit a general construction of a *universal* Hamiltonian formalism (which contains all previously known formalisms, which explains the appelation *universal*) and define the generalized Poisson $\mathfrak{p}$-brackets, the analogs of the Poisson bracket on forms, as defined in Refs. 16 and 17. We formulate the equations of motion of forms in terms of those $\mathfrak{p}$-brackets. The main focus in this construction is on the role of Legendre correspondence and the hypothesis concerning the generalized Legendre condition. We want to emphasize here that in our formalism there is no need of the decomposition into ''vertical'' and ''horizontal'' parts thanks to the use of Eq. (17), which is much more enlightened than Eq. (15). This implies Theorems 2 and 3. On the other hand, the energy-momentum tensor is clearly represented and the Hamiltonian formulation of Maxwell's electrodynamics, for instance, is properly given.

In Sec. II we establish the Hamiltonian formalism: the Euler–Lagrange equations, Legendre's correspondence (and the generalized Legendre condition) and Hamilton's equations. In fact, we

recover the Hamilton's equations using three different approaches: (a) as necessary and sufficient conditions for the existence of a critical point $u:\mathcal{X}\to\mathcal{Y}$, (b) by contracting the *pataplectic* form Ω with any n-vector $X\in\Lambda^n T_{(q,p)}\mathcal{M}$ where $\mathcal{M}=\Lambda^n T^\star(\mathcal{X}\times\mathcal{Y})$ and for any $(q,p)\in\mathcal{M}$ and, finally, (c) by variational formulation, i.e., as the Euler–Lagrange equations of some simple functional. In Sec. III we review the usual approach to quantum field theory from the standard canonical viewpoint and *pataplectic* geometry point of view where we express the various brackets using an analog of the Poisson brackets, the Poisson $\mathfrak{p}$-brackets, defined on $(n-1)$-forms. In Sec. III D we give a dynamical formulation for the $(n-1)$-forms in terms of $\mathfrak{p}$-brackets with the n-form $\mathcal{H}\omega$.

In Sec. IV, and after introducing the internal and external $\mathfrak{p}$-brackets, we generalize the definition of $\mathfrak{p}$-bracket on $(n-1)$-forms to a class of forms of an arbitrary degrees $0\leqslant p\leqslant n$ using anticommuting (Grassmann) variables $\tau_1,\ldots,\tau_n$, which behave under change of coordinates like $\partial/\partial x^1,\ldots,\partial/\partial x^n$. Notice also that the generalized Poisson bracket obtained here differs from the one proposed in Refs. 16 and 17 for forms of degree lower than $n-1$. In particular, one of our results is that these p-forms are composed basically of "position" observables unless we have some gauge symmetry and constraints. Then we can represent some "momentum" observable by a p-form with $p\leqslant n$ (in Sec. V C we study the electromagnetic field which is an instance of such a situation). Finally, in Sec. V we present three examples: the interacting scalar fields, conformal string theory and the electromagnetic field.

II. CONSTRUCTION OF THE HAMILTONIAN FORMALISM

In this section we show how to build a universal Hamiltonian formalism for variational problems involving a Lagrangian functional depending on first derivatives, and that for the case of maps between two manifolds. We derive it through a universal Legendre correspondence.

A. Notations

Let $\mathcal{X}$ and $\mathcal{Y}$ be two differentiable manifolds. $\mathcal{X}$ plays the role of the space–time manifold and $\mathcal{Y}$ is the target manifold. We fix some volume form ω on $\mathcal{X}$. This volume form may be chosen according to the variational problem that we want to study (for instance, if we look at the Klein–Gordon functional on some pseudo-Riemannian manifold, we choose ω to be the Riemannian volume), but in more general situation with less symmetries we just choose some arbitrary volume form. We set $n=\dim\mathcal{X}$ and $k=\dim\mathcal{Y}$. We denote $\{x^1,\ldots,x^n\}$ local coordinates on $\mathcal{X}$ and $\{y^1,\ldots,y^k\}$ local coordinates on $\mathcal{Y}$. For simplicity we shall assume that the coordinates x^α are always chosen such that $dx^1\wedge\cdots\wedge dx^n=\omega$, though it is not essential. Then on the product $\mathcal{X}\times\mathcal{Y}$ we denote $\{q^1,\ldots,q^{n+k}\}$ local coordinates in such a way that

$$q^\mu=x^\alpha \quad \text{if } 1\leqslant\mu=\alpha\leqslant n,$$

$$q^\mu=y^i \quad \text{if } n+1\leqslant\mu\leqslant n+k \text{ and } i=\mu-n.$$

Generally we shall denote the indices running from 1 to n by $\alpha,\beta,\ldots$, the indices between 1 and k by $i,j,\ldots$, and the indices between 1 and $n+k$ by $\mu,\nu,\ldots$. To any map $u:\mathcal{X}\to\mathcal{Y}$ we may associate the map

$$U:\mathcal{X}\to\mathcal{X}\times\mathcal{Y},$$

$$x\mapsto(x,u(x)),$$

whose image is the graph of u, $\{(x,u(x))/x\in\mathcal{X}\}$. We also associate to u the bundle $u^\star T\mathcal{Y}\otimes_{\mathcal{X}}T^\star\mathcal{X}$ over $\mathcal{X}$. This bundle is naturally equipped with the coordinates $(x^\alpha)_{1\leqslant\alpha\leqslant n}$ (for $\mathcal{X}$) and $(v^i_\alpha)_{1\leqslant i\leqslant k;1\leqslant\alpha\leqslant n}$, such that a point $(x,v)\in u^\star T\mathcal{Y}\otimes_{\mathcal{X}}T^\star\mathcal{X}$ is represented by

$$v=\sum_{\alpha=1}^{n}\sum_{i=1}^{k}v^i_\alpha\frac{\partial}{\partial y^i}\otimes dx^\alpha.$$

We can think $u^\star T\mathcal{Y}\otimes_{\mathcal{X}} T^\star\mathcal{X}$ as a subset of $T\mathcal{Y}\otimes_{\mathcal{X}\times\mathcal{Y}} T^\star\mathcal{X}:=\{(x,y,v)/(x,y)\in\mathcal{X}\times\mathcal{Y}, v\in T_y\mathcal{Y}\otimes T_x^\star\mathcal{X}\}$ by the inclusion map $(x,v)\mapsto(x,u(x),v)$.

The differential of u, du is a section of the bundle $u^\star T\mathcal{Y}\otimes_{\mathcal{X}} T^\star\mathcal{X}$ over $\mathcal{X}$. Hence the coordinates for du are simply $v_\alpha^i=\partial u^i/\partial x^\alpha$. Notice that $u^\star T\mathcal{Y}\otimes_{\mathcal{X}} T^\star\mathcal{X}$ is an analog of the tangent bundle $T\mathcal{Y}$ to a configuration space $\mathcal{Y}$ in classical particle mechanics.

It turns out to be more convenient to consider $\Lambda^n T(\mathcal{X}\times\mathcal{Y})$ the analog of $T(\mathbb{R}\times\mathcal{Y})$, the tangent bundle to a space–time, or rather $S\Lambda^n T(\mathcal{X}\times\mathcal{Y})$, the submanifold of $\Lambda^n T(\mathcal{X}\times\mathcal{Y})$, as the analog of the subset $ST(\mathbb{R}\times\mathcal{Y}):=\{(t,x;\xi^0,\vec{\xi})\in T(\mathbb{R}\times\mathcal{Y})/dt(\xi^0,\vec{\xi})=1\}$, which is diffeomorphic to $\mathbb{R}\times T\mathcal{Y}$ by the map $(t,x,\xi)\mapsto(t,x,\vec{\xi})$, and where

$$S\Lambda^n T(\mathcal{X}\times\mathcal{Y}):=\{(q,z)\in\Lambda^n T(\mathcal{X}\times\mathcal{Y})/z=z_1\wedge\cdots\wedge z_n, z_1,\ldots,z_n\in T_q(\mathcal{X}\times\mathcal{Y}), \omega(z_1,\ldots,z_n)=1\}.$$

For any $(x,y)\in\mathcal{X}\times\mathcal{Y}$, the fiber $S\Lambda^n T_{(x,y)}(\mathcal{X}\times\mathcal{Y})$ can be identified with $T_y\mathcal{Y}\otimes T_x^\star\mathcal{X}$ by the diffeomorphism

$$\begin{aligned} &T_y\mathcal{Y}\otimes T_x^\star\mathcal{X}\to S\Lambda^n T_{(x,y)}(\mathcal{X}\times\mathcal{Y}),\\ &v=\sum_{\alpha=1}^{n}\sum_{i=1}^{k} v_\alpha^i\frac{\partial}{\partial y^i}\otimes dx^\alpha\mapsto z=z_1\wedge\cdots\wedge z_n, \end{aligned} \tag{1}$$

where for all $1\leqslant\beta\leqslant n$, $z_\beta=\partial/\partial x^\alpha+\Sigma_{i=1}^k v_\alpha^i\,\partial/\partial y^i$. We denote by $(z_\alpha^\mu)_{1\leqslant\mu\leqslant n+k;1\leqslant\alpha\leqslant n}$ the coordinates of z_α, so that $z_\beta=\Sigma_{\mu=1}^{n+k} z_\alpha^\mu\,\partial/\partial q^\mu$ (or $z_\alpha^\beta=\delta_\alpha^\beta$ for $1\leqslant\beta\leqslant n$ and $z_\alpha^{n+i}=v_\alpha^i$ for $1\leqslant i\leqslant k$). This induces an identification $T\mathcal{Y}\otimes_{\mathcal{X}\times\mathcal{Y}} T^\star\mathcal{X}\simeq S\Lambda^n T(\mathcal{X}\times\mathcal{Y})$.

Thus coordinates $(x^\alpha,y^i,v_\alpha^i)$ [or equivalentely $(x^\alpha,y^i,z_\alpha^\mu)$] can be thought as coordinate on $T\mathcal{Y}\otimes_{\mathcal{X}\times\mathcal{Y}} T^\star\mathcal{X}$ or $S\Lambda^n T(\mathcal{X}\times\mathcal{Y})$.

Given a Lagrangian function $L: T\mathcal{Y}\otimes_{\mathcal{X}\times\mathcal{Y}} T^\star\mathcal{X}\mapsto\mathbb{R}$, we define the functional

$$\mathcal{L}[u]:=\int_{\mathcal{X}} L(x,u(x),du(x))dx.$$

B. The Euler–Lagrange equations

The critical points of the action are the maps $u:\mathcal{X}\to\mathcal{Y}$ which are solutions of the system of Euler–Lagrange equations

$$\frac{\partial}{\partial x^\alpha}\left(\frac{\partial L}{\partial v_\alpha^i}(x,u(x),du(x))\right)=\frac{\partial L}{\partial y^i}(x,u(x),du(x)). \tag{2}$$

This equation implies also other equations involving the *stress-energy* tensor associated to $u:\mathcal{X}\to\mathcal{Y}$:

$$S_\beta^\alpha(x):=\delta_\beta^\alpha L(x,u(x),du(x))-\frac{\partial L}{\partial v_\alpha^i}(x,u(x),du(x))\,\frac{\partial u^i}{\partial x^\beta}(x).$$

Indeed, for any u,

$$\frac{\partial S^\alpha_\beta}{\partial x^\alpha}(x)=\delta^\alpha_\beta\left(\frac{\partial L}{\partial x^\alpha}(x,u,du)+\frac{\partial L}{\partial y^i}(x,u,du)\,\frac{\partial u^i}{\partial x^\alpha}(x)+\frac{\partial L}{\partial v^i_\gamma}(x,u,du)\,\frac{\partial^2 u^i}{\partial x^\alpha\partial x^\gamma}(x)\right)$$
$$-\frac{\partial}{\partial x^\alpha}\left(\frac{\partial L}{\partial v^i_\alpha}(x,u,du)\right)\frac{\partial u^i}{\partial x^\beta}(x)-\frac{\partial L}{\partial v^i_\alpha}(x,u,du)\,\frac{\partial^2 u^i}{\partial x^\alpha\partial x^\beta}(x)$$
$$=\frac{\partial L}{\partial x^\beta}(x,u,du)-\left[\frac{\partial}{\partial x^\alpha}\left(\frac{\partial L}{\partial v^i_\alpha}(x,u(x),du(x))\right)-\frac{\partial L}{\partial y^i}(x,u(x),du(x))\right]\frac{\partial u^i}{\partial x^\beta}(x).$$

Thus we conclude that if u is a solution of (2), then

$$\frac{\partial S^\alpha_\beta}{\partial x^\alpha}(x)=\frac{\partial L}{\partial x^\beta}(x,u,du). \tag{3}$$

It follows that if L does not depend on x, then S^α_β is divergence-free for all solutions of (2), a property which can be predicted by Noether's theorem.

C. The Legendre correspondence

Let $\mathcal{M}:=\Lambda^n T^\star(\mathcal{X}\times\mathcal{Y})$. Every point $(q,p)\in\mathcal{M}$ has coordinates q^μ and $p_{\mu_1\dots\mu_n}$ such that $p_{\mu_1\dots\mu_n}$ is completely antisymmetric in $(\mu_1,\dots,\mu_n)$ and

$$p=\sum_{\mu_1<\dots<\mu_n} p_{\mu_1\dots\mu_n}dq^{\mu_1}\wedge\cdots\wedge dq^{\mu_n}.$$

We shall define a Legendre correspondence

$$S\Lambda^n T(\mathcal{X}\times\mathcal{Y})\times\mathbb{R}\leftrightarrow\mathcal{M}=\Lambda^n T^\star(\mathcal{X}\times\mathcal{Y}),$$

$$(q,v,w)\leftrightarrow(q,p),$$

where $w\in\mathbb{R}$ is some extra parameter (its significance is not clear for the moment, w is related to the possibility of fixing arbitrarily the value of some Hamiltonian). Notice that we do not name it a transform, like in the classical theory, but a correspondence, since generally there will be many possible values of (q,p) corresponding to a single value of (q,v,w). But we expect that, in generic situations, there corresponds a unique (q,v,w) to some (q,p). This correspondence is generated by the function

$$W:S\Lambda^n T(\mathcal{X}\times\mathcal{Y})\times\mathcal{M}\to\mathbb{R},\quad (q,v,p)\mapsto\langle p,v\rangle-L(q,v),$$

where

$$\langle p,v\rangle\simeq\langle p,z\rangle:=\langle p,z_1\wedge\cdots\wedge z_n\rangle=\sum_{\mu_1,\dots,\mu_n} p_{\mu_1\dots\mu_n}z_1^{\mu_1}\cdots z_n^{\mu_n}.$$

Definition 1: We *write that* $(q,v,w)\leftrightarrow(q,p)$ *if and only if*

$$L(q,v)+w=\langle p,v\rangle\quad\text{or}\quad W(q,v,p)=w \tag{4}$$

and

$$\frac{\partial L}{\partial v^i_\alpha}(q,v)=\frac{\partial\langle p,v\rangle}{\partial v^i_\alpha}=\left\langle p,z_1\wedge\cdots\wedge z_{\alpha-1}\wedge\frac{\partial}{\partial y^i}\wedge z_{\alpha+1}\wedge\cdots\wedge z_n\right\rangle\quad\text{or}\frac{\partial W}{\partial v^i_\alpha}(q,v,p)=0. \tag{5}$$

Notice that for any $(q,v,w)\in S\Lambda^n T(\mathcal{X}\times\mathcal{Y})\times\mathbb{R}$ there exist $(q,p)\in\mathcal{M}$ such that $(q,v,w)\leftrightarrow(q,p)$. This will be proven in Sec. II F. But (q,p) is not unique in general. In the following we shall need to suppose that the inverse correspondence is well-defined.

Hypothesis: Generalized Legendre condition: *There exists an open subset $\mathcal{O}\subset\mathcal{M}$ which is nonempty such that for any $(q,p)\in\mathcal{O}$ there exists a unique $v\in T_x\mathcal{Y}\otimes T_y^\star\mathcal{X}$ [or equivalentely a unique $z\in S\Lambda^n T_q(\mathcal{X}\times\mathcal{Y})$] which is a critical point of $v\mapsto W(q,v,p)$. We denote $v=\mathcal{V}(q,p)$ this unique solution (or $z=\mathcal{Z}(q,p)$). We assume further that $\mathcal{V}$ is a smooth function on $\mathcal{O}$ (or the same for $\mathcal{Z}$).*

We now suppose that this hypothesis is true. Then we can define on $\mathcal{O}$ the following Hamiltonian function:

$$\mathcal{H}:\mathcal{O}\to\mathbb{R},$$

$$(q,p)\mapsto\langle p,\mathcal{V}(q,p)\rangle-L(q,\mathcal{V}(q,p))=W(q,\mathcal{V}(q,p),p).$$

We then remark that (4) is equivalent to $w=\mathcal{H}(q,p)$.

We now compute the differential of $\mathcal{H}$. The main point is to exploit the condition

$$\frac{\partial W}{\partial v_\alpha^i}(q,\mathcal{V}(q,p),p)=0 \tag{6}$$

(which defines $\mathcal{V}$):

$$\begin{aligned}d\mathcal{H}=&\sum_\mu\frac{\partial W}{\partial q^\mu}(q,\mathcal{V}(q,p),p)dq^\mu+\sum_{\mu,\nu}\sum_\alpha\frac{\partial W}{\partial v_\alpha^\nu}(q,\mathcal{V}(q,p),p)\frac{\partial\mathcal{V}_\alpha^\nu}{\partial q^\mu}dq^\mu\\&+\sum_{\nu,\alpha}\sum_{\mu_1<\cdots<\mu_n}\frac{\partial W}{\partial v_\alpha^\nu}(q,\mathcal{V}(q,p),p)\frac{\partial\mathcal{V}_\alpha^\nu}{\partial p_{\mu_1\cdots\mu_n}}dp_{\mu_1\cdots\mu_n}\\&+\sum_{\mu_1<\cdots<\mu_n}\frac{\partial W}{\partial p_{\mu_1\cdots\mu_n}}(q,\mathcal{V}(q,p),p)dp_{\mu_1\cdots\mu_n}\\=&\sum_\mu\frac{\partial W}{\partial q^\mu}(q,\mathcal{V}(q,p),p)dq^\mu+\sum_{\mu_1<\cdots<\mu_n}\frac{\partial W}{\partial p_{\mu_1\cdots\mu_n}}(q,\mathcal{V}(q,p),p)dp_{\mu_1\cdots\mu_n}.\end{aligned}$$

Now since

$$\frac{\partial W}{\partial q^\mu}(q,v,p)=-\frac{\partial L}{\partial q^\mu}(q,v)$$

and

$$\frac{\partial W}{\partial p_{\mu_1\cdots\mu_n}}(q,v,p)=\begin{vmatrix}z_1^{\mu_1}&\cdots&z_n^{\mu_1}\\\vdots&&\vdots\\z_1^{\mu_n}&\cdots&z_n^{\mu_n}\end{vmatrix},$$

we get

$$d\mathcal{H}=-\sum_\mu\frac{\partial L}{\partial q^\mu}(q,\mathcal{V}(q,p))dq^\mu+\sum_{\mu_1<\cdots<\mu_n}\mathcal{Z}_{1\cdots n}^{\mu_1\cdots\mu_n}(q,p)dp_{\mu_1\cdots\mu_n}, \tag{7}$$

where

$$\mathcal{Z}_{1\ldots n}^{\mu_1\cdots\mu_n}(q,p) := \begin{vmatrix} \mathcal{Z}_1^{\mu_1}(q,p) & \ldots & \mathcal{Z}_n^{\mu_1}(q,p) \\ \vdots & & \vdots \\ \mathcal{Z}_1^{\mu_n}(q,p) & \ldots & \mathcal{Z}_n^{\mu_n}(q,p) \end{vmatrix}$$

are the components of the n-vector

$$\mathcal{Z}_1(q,p)\wedge\cdots\wedge\mathcal{Z}_n(q,p) = \sum_{\mu_1<\cdots<\mu_n} \mathcal{Z}_{1\ldots n}^{\mu_1\cdots\mu_n}(q,p)\,\frac{\partial}{\partial q^{\mu_1}}\wedge\cdots\wedge\frac{\partial}{\partial q^{\mu_n}}.$$

To conclude let us see how the stress-energy tensor appears in this Hamiltonian setting. We define the Hamiltonian tensor on $\mathcal{C}$ to be $H(q,p)=\Sigma_{\alpha,\beta}H_\beta^\alpha(q,p)\,\partial/\partial x^\alpha\otimes dx^\beta$, with

$$H_\beta^\alpha(q,p) := \frac{\partial L}{\partial v_\alpha^i}(q,\mathcal{V}(q,p))\mathcal{V}_\beta^i(q,p) - \delta_\beta^\alpha L(q,\mathcal{V}(q,p)).$$

It is clear that if $(x,u(x),du(x),w)\leftrightarrow(q,p)$, then

$$H_\beta^\alpha(q,p) = -S_\beta^\alpha(x).$$

Let us now compute $H_\beta^\alpha(q,p)$. We first use (5):

$$\begin{aligned}
&\sum_i \frac{\partial L}{\partial v_\alpha^i}(q,\mathcal{V}(q,p))\mathcal{V}_\beta^i(q,p) \\
&\quad= \sum_i \frac{\partial\langle p,v\rangle}{\partial v_\alpha^i}_{|v=\mathcal{V}(q,p)}\mathcal{V}_\beta^i(q,p) \\
&\quad= \sum_i \left\langle p,\mathcal{Z}_1(q,p)\wedge\cdots\wedge\mathcal{Z}_{\alpha-1}(q,p)\wedge\frac{\partial}{\partial y^i}\wedge\mathcal{Z}_{\alpha+1}(q,p)\wedge\cdots\wedge\mathcal{Z}_n(q,p)\right\rangle\mathcal{V}_\beta^i(q,p) \\
&\quad= \sum_\mu \left\langle p,\mathcal{Z}_1(q,p)\wedge\cdots\wedge\mathcal{Z}_{\alpha-1}(q,p)\wedge\frac{\partial}{\partial q^\mu}\wedge\mathcal{Z}_{\alpha+1}(q,p)\wedge\cdots\wedge\mathcal{Z}_n(q,p)\right\rangle\mathcal{Z}_\beta^\mu(q,p) \\
&\qquad- \left\langle p,\mathcal{Z}_1(q,p)\wedge\cdots\wedge\mathcal{Z}_{\alpha-1}(q,p)\wedge\frac{\partial}{\partial x^\beta}\wedge\mathcal{Z}_{\alpha+1}(q,p)\wedge\cdots\wedge\mathcal{Z}_n(q,p)\right\rangle \\
&\quad= \langle p,\mathcal{Z}_1(q,p)\wedge\cdots\wedge\mathcal{Z}_{\alpha-1}(q,p)\wedge\mathcal{Z}_\beta(q,p)\wedge\mathcal{Z}_{\alpha+1}(q,p)\wedge\cdots\wedge\mathcal{Z}_n(q,p)\rangle \\
&\qquad- \left\langle p,\mathcal{Z}_1(q,p)\wedge\cdots\wedge\mathcal{Z}_{\alpha-1}(q,p)\wedge\frac{\partial}{\partial x^\beta}\wedge\mathcal{Z}_{\alpha+1}(q,p)\wedge\cdots\wedge\mathcal{Z}_n(q,p)\right\rangle \\
&\quad= \delta_\beta^\alpha\langle p,\mathcal{Z}_1(q,p)\wedge\cdots\wedge\mathcal{Z}_n(q,p)\rangle \\
&\qquad\times\left\langle p,\mathcal{Z}_1(q,p)\wedge\cdots\wedge\mathcal{Z}_{\alpha-1}(q,p)\wedge\frac{\partial}{\partial x^\beta}\wedge\mathcal{Z}_{\alpha+1}(q,p)\wedge\cdots\wedge\mathcal{Z}_n(q,p)\right\rangle.
\end{aligned}$$

Hence since

$$\langle p, \mathcal{Z}_1(q,p) \wedge \ldots \wedge \mathcal{Z}_n(q,p) \rangle = \mathcal{H}(q,p) + L(q, \mathcal{V}(q,p)),$$

$$H^\alpha_\beta(q,p) = \delta^\alpha_\beta \mathcal{H}(q,p) - \left\langle p, \mathcal{Z}_1(q,p) \wedge \cdots \ \mathcal{Z}_{\alpha-1}(q,p) \wedge \frac{\partial}{\partial x^\beta} \wedge \mathcal{Z}_{\alpha+1}(q,p) \cdots \ \wedge \mathcal{Z}_n(q,p) \right\rangle$$

$$= \delta^\alpha_\beta \mathcal{H}(q,p) - \frac{\partial \langle p,z \rangle}{\partial z^\beta_\alpha}_{|z=\mathcal{Z}(q,p)}. \tag{8}$$

D. Hamilton equations

Let $x \mapsto (q(x),p(x))$ be some map from $\mathcal{X}$ to $\mathcal{O}$. To insure that this map is related to a critical point $u: \mathcal{X} \to \mathcal{Y}$, we find that the necessary and sufficient conditions split in two parts:

(1) *What are the conditions on* $x \mapsto (q(x),p(x))$ *for the existence of a map* $x \mapsto u(x)$ *such that* $(x,u(x),du(x)) \leftrightarrow (q(x),p(x))$?

The first obvious condition is $q(x) = (x,u(x)) = U(x)$. The second condition is that in $T\mathcal{Y} \otimes T^\star\mathcal{X}$, $(x,y,v^i_\alpha) = (x,y,\partial u^i/\partial x^\alpha)$ coincides with $(q(x), \mathcal{V}^i_\alpha(q(x),p(x)))$. If we translate that using (1), we obtain that in $S\Lambda^n T(\mathcal{X} \times \mathcal{Y})$,

$$\frac{\partial q}{\partial x^1} \wedge \ \cdots \wedge \frac{\partial q}{\partial x^n} = \frac{\partial U}{\partial x^1} \wedge \ \cdots \wedge \frac{\partial U}{\partial x^n} = \mathcal{Z}_1(q(x),p(x)) \wedge \ \cdots \wedge \mathcal{Z}_n(q(x),p(x)).$$

But we found in (7) that the components in the basis $(\partial/\partial q^{\mu_1} \wedge \cdots \wedge \partial/\partial q^{\mu_n})$ of the right-hand side are $\mathcal{Z}^{\mu_1 \ldots \mu_n}_{1 \ldots n}(q(x),p(x)) = \partial \mathcal{H}/\partial p_{\mu_1 \ldots \mu_n}(q(x),p(x))$. Hence denoting

$$\frac{\partial(q^{\mu_1}, \ldots, q^{\mu_n})}{\partial(x^1, \ldots, x^n)} := \begin{vmatrix} \dfrac{\partial q^{\mu_1}}{\partial x^1} & \cdots & \dfrac{\partial q^{\mu_1}}{\partial x^n} \\ \vdots & & \vdots \\ \dfrac{\partial q^{\mu_n}}{\partial x^1} & \cdots & \dfrac{\partial q^{\mu_n}}{\partial x^n} \end{vmatrix},$$

so that

$$\frac{\partial q}{\partial x^1} \wedge \cdots \wedge \frac{\partial q}{\partial x^n} = \sum_{\mu_1 < \ldots < \mu_n} \frac{\partial(q^{\mu_1}, \ldots, q^{\mu_n})}{\partial(x^1, \ldots, x^n)} \frac{\partial}{\partial q^{\mu_1}} \wedge \cdots \wedge \frac{\partial}{\partial q^{\mu_n}},$$

we obtain the condition

$$\frac{\partial(q^{\mu_1}, \ldots, q^{\mu_n})}{\partial(x^1, \ldots, x^n)}(x) = \frac{\partial \mathcal{H}}{\partial p_{\mu_1 \ldots \mu_n}}(q(x),p(x)). \tag{9}$$

(2) *Now what are the conditions on* $x \mapsto (q(x),p(x))$ *for* u *to be a solution of the Euler–Lagrange equations*?

It amounts to eliminating u in (2) in function of (q,p). For that purpose we use (5) to derive

$$\begin{aligned}
&\sum_\alpha \frac{\partial}{\partial x^\alpha}\left\langle \frac{\partial L}{\partial v^i_\alpha}(x,u(x),du(x))\right\rangle\\
&\quad=\sum_\alpha \frac{\partial}{\partial x^\alpha}\left\langle p,\frac{\partial U}{\partial x^1}\wedge\cdots\wedge\frac{\partial U}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial y^i}\wedge\frac{\partial U}{\partial x^{\alpha+1}}\wedge\cdots\wedge\frac{\partial U}{\partial x^n}\right\rangle\\
&\quad=\sum_\alpha \left\langle \frac{\partial p}{\partial x^\alpha},\frac{\partial U}{\partial x^1}\wedge\cdots\wedge\frac{\partial U}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial y^i}\wedge\frac{\partial U}{\partial x^{\alpha+1}}\wedge\cdots\wedge\frac{\partial U}{\partial x^n}\right\rangle\\
&\qquad+\sum_{\alpha\neq\beta}\left\langle p,\frac{\partial U}{\partial x^1}\wedge\cdots\wedge\frac{\partial^2 U}{\partial x^\alpha\partial x^\beta}\wedge\cdots\wedge\frac{\partial U}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial y^i}\wedge\frac{\partial U}{\partial x^{\alpha+1}}\wedge\cdots\wedge\frac{\partial U}{\partial x^n}\right\rangle\\
&\quad=\sum_\alpha \left\langle \frac{\partial p}{\partial x^\alpha},\frac{\partial U}{\partial x^1}\wedge\cdots\wedge\frac{\partial U}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial y^i}\wedge\frac{\partial U}{\partial x^{\alpha+1}}\wedge\cdots\wedge\frac{\partial U}{\partial x^n}\right\rangle.
\end{aligned}$$

On the other hand, we know from (7) that $(\partial\mathcal{H}/\partial q^i)(q,p)=-(\partial L/\partial q^i)(q,\mathcal{V}(q,p))$. Thus we obtain

$$\sum_\alpha \left\langle \frac{\partial p}{\partial x^\alpha},\frac{\partial q}{\partial x^1}\wedge\cdots\wedge\frac{\partial q}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial y^i}\wedge\frac{\partial q}{\partial x^{\alpha+1}}\wedge\cdots\wedge\frac{\partial q}{\partial x^n}\right\rangle=-\frac{\partial\mathcal{H}}{\partial q^i}(q(x),p(x)). \tag{10}$$

The latter equation may be transformed using the relation

$$\begin{aligned}
&\sum_\alpha \left\langle \frac{\partial p}{\partial x^\alpha},\frac{\partial q}{\partial x^1}\wedge\cdots\wedge\frac{\partial q}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial y^i}\wedge\frac{\partial q}{\partial x^{\alpha+1}}\wedge\cdots\wedge\frac{\partial q}{\partial x^n}\right\rangle\\
&\quad=\sum_\alpha \sum_{\substack{\mu_1<\cdots<\mu_n\\ \mu_\alpha=n+i}}\begin{vmatrix}
\frac{\partial q^{\mu_1}}{\partial x^1} & \cdots & \frac{\partial q^{\mu_1}}{\partial x^n}\\
\vdots & & \vdots\\
\frac{\partial q^{\mu_{\alpha-1}}}{\partial x^1} & \cdots & \frac{\partial q^{\mu_{\alpha-1}}}{\partial x^n}\\
\frac{\partial p_{\mu_1\cdots\mu_n}}{\partial x^1} & \cdots & \frac{\partial p_{\mu_1\cdots\mu_n}}{\partial x^n}\\
\frac{\partial q^{\mu_{\alpha+1}}}{\partial x^1} & \cdots & \frac{\partial q^{\mu_{\alpha+1}}}{\partial x^n}\\
\vdots & & \vdots\\
\frac{\partial q^{\mu_n}}{\partial x^1} & \cdots & \frac{\partial q^{\mu_n}}{\partial x^n}
\end{vmatrix}\\
&\quad=\sum_\alpha \sum_{\substack{\mu_1<\cdots<\mu_n\\ \mu_\alpha=n+i}}\frac{\partial(q^{\mu_1},\ldots,q^{\mu_{\alpha-1}},p_{\mu_1\cdots\mu_n},q^{\mu_{\alpha+1}},\ldots,q^{\mu_n})}{\partial(x^1,\ldots,x^n)}.
\end{aligned}$$

We summarize: the necessary and sufficient conditions we were looking for are

$$\frac{\partial(q^{\mu_1},\ldots,q^{\mu_n})}{\partial(x^1,\ldots,x^n)}=\frac{\partial\mathcal{H}}{\partial p_{\mu_1\ldots\mu_n}}(q,p),$$
$$\sum_\alpha \sum_{\substack{\mu_1<\cdots<\mu_n\\ \mu_\alpha=n+i}} \frac{\partial(q^{\mu_1},\ldots,q^{\mu_{\alpha-1}},p_{\mu_1\ldots\mu_n},q^{\mu_{\alpha+1}},\ldots,q^{\mu_n})}{\partial(x^1,\ldots,x^n)}=-\frac{\partial\mathcal{H}}{\partial y^i}(q,p). \tag{11}$$

Some further relations: Besides these equations, we have to remark also that Eq. (3) on the stress-energy tensor has a counterpart in this formalism. For that purpose we use Eq. (8). Assuming that $(x,u(x),du(x))\leftrightarrow(q(x),p(x))$, we have

$$\begin{aligned}-\frac{\partial S^\alpha_\beta}{\partial x^\alpha}(x)&=\frac{\partial H^\alpha_\beta(q(x),p(x))}{\partial x^\alpha}\\ &=\frac{\partial\mathcal{H}(q(x),p(x))}{\partial x^\beta}-\frac{\partial}{\partial x^\alpha}\left\langle p(x),\frac{\partial q(x)}{\partial x^1}\wedge\cdots\wedge\frac{\partial q(x)}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial x^\beta}\wedge\frac{\partial q(x)}{\partial x^{\alpha+1}}\wedge\cdots\wedge\frac{\partial q(x)}{\partial x^n}\right\rangle\\ &=\frac{\partial\mathcal{H}(q(x),p(x))}{\partial x^\beta}-\left\langle\frac{\partial p(x)}{\partial x^\alpha},\frac{\partial q(x)}{\partial x^1}\wedge\cdots\wedge\frac{\partial q(x)}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial x^\beta}\wedge\frac{\partial q(x)}{\partial x^{\alpha+1}}\wedge\cdots\wedge\frac{\partial q(x)}{\partial x^n}\right\rangle.\end{aligned}$$

Now assume that u is a critical point. Then, because of (3) and (7),

$$\frac{\partial S^\alpha_\beta}{\partial x^\alpha}(x)=\frac{\partial L}{\partial x^\beta}(x,u(x),du(x))=-\frac{\partial\mathcal{H}}{\partial x^\beta}(q(x),p(x)),$$

and we obtain

$$\left\langle\frac{\partial p}{\partial x^\alpha},\frac{\partial q}{\partial x^1}\wedge\cdots\wedge\frac{\partial q}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial x^\beta}\wedge\frac{\partial q}{\partial x^{\alpha+1}}\wedge\cdots\wedge\frac{\partial q}{\partial x^n}\right\rangle-\frac{\partial}{\partial x^\beta}(\mathcal{H}(q,p))=-\frac{\partial\mathcal{H}}{\partial x^\beta}(q,p)$$

or equivalently

$$\sum_\alpha\sum_{\substack{\mu_1<\ldots<\mu_n\\ \mu_\alpha=\beta}}\frac{\partial(q^{\mu_1},\ldots,q^{\mu_{\alpha-1}},p_{\mu_1\ldots\mu_n},q^{\mu_{\alpha+1}},\ldots,q^{\mu_n})}{\partial(x^1,\ldots,x^n)}-\frac{\partial}{\partial x^\beta}(\mathcal{H}(q,p))=-\frac{\partial\mathcal{H}}{\partial x^\beta}(q,p). \tag{12}$$

Conclusion: The Hamilton equations (11) can be completed by adding (12) [which are actually a consequence of (11)]. We thus obtain

$$\frac{\partial(q^{\mu_1},\ldots,q^{\mu_n})}{\partial(x^1,\ldots,x^n)}=\frac{\partial\mathcal{H}}{\partial p_{\mu_1\ldots\mu_n}}(q,p),$$
$$\sum_\alpha\sum_{\substack{\mu_1<\cdots<\mu_n\\ \mu_\alpha=\nu}}\frac{\partial(q^{\mu_1},\ldots,q^{\mu_{\alpha-1}},p_{\mu_1\ldots\mu_n},q^{\mu_{\alpha+1}},\ldots,q^{\mu_n})}{\partial(x^1,\ldots,x^n)}-\sum_\alpha\delta^\alpha_\nu\frac{\partial}{\partial x^\alpha}(\mathcal{H}(q,p))$$
$$=-\frac{\partial\mathcal{H}}{\partial q^\nu}(q,p). \tag{13}$$

E. The Cartan–Poincaré and pataplectic forms on $\mathcal{M}=\Lambda^nT^*(\mathcal{X}\times\mathcal{Y})$

Motivated by the previous contruction, we define the Cartan–Poincaré form on $\Lambda^nT^*(\mathcal{X}\times\mathcal{Y})$ to be

$$\theta := \sum_{\mu_1 < \ldots < \mu_n} p_{\mu_1 \ldots \mu_n} dq^{\mu_1} \wedge \ldots \wedge dq^{\mu_n}.$$

Its differential is

$$\Omega := \sum_{\mu_1 < \ldots < \mu_n} dp_{\mu_1 \ldots \mu_n} \wedge dq^{\mu_1} \wedge \ldots \wedge dq^{\mu_n},$$

which we will call the *pataplectic form*, a straightforward generalization of the symplectic form.

A first property is that we can express the system of Hamilton's equations (13) in an elegant way using Ω. For any $(q,p) \in \mathcal{M}$ and any n-vector $X \in \Lambda^n T_{(q,p)}\mathcal{M}$ we define $X \rfloor \Omega \in T^\star_{(q,p)}\mathcal{M}$ as follows. If X is decomposable, i.e., if there exist n vectors $X_1, \ldots, X_n \in T_{(q,p)}\mathcal{M}$ such that $X = X_1 \wedge \ldots \wedge X_n$, we let

$$X \rfloor \Omega(V) := \Omega(X_1, \ldots, X_n, V), \quad \forall V \in T_{(q,p)}\mathcal{M}.$$

We extend this definition to non-decomposable X by linearity. Let us analyze $X \rfloor \Omega$ using coordinates. Writing X as

$$\sum_{\mu_1 < \ldots < \mu_n} X^{\mu_1 \ldots \mu_n} \partial_{\mu_1} \wedge \ldots \wedge \partial_{\mu_n}$$

$$+ \sum_{\substack{\mu_1 < \ldots < \mu_{\alpha-1} < \mu_{\alpha+1} < \ldots < \mu_n \\ \nu_1 < \ldots < \nu_n}} X^{\mu_1 \ldots \mu_{\alpha-1} \{\nu_1 \ldots \nu_n\} \mu_{\alpha+1} \ldots \mu_n} \partial_{\mu_1}$$

$$\wedge \cdots \wedge \partial_{\mu_{\alpha-1}} \wedge \partial^{\nu_1 \ldots \nu_n} \wedge \partial_{\mu_{\alpha+1}} \wedge \cdots \wedge \partial_{\mu_n} + \quad \text{etc.},$$

with the notations $\partial_\mu := \partial/\partial q^\mu$, $\partial^{\nu_1 \ldots \nu_n} := \partial/\partial p_{\nu_1 \ldots \nu_n}$, we have

$$X \rfloor \Omega = (-1)^n \left[\sum_{\mu_1 < \ldots < \mu_n} X^{\mu_1 \ldots \mu_n} dp_{\mu_1 \ldots \mu_n} \right.$$

$$\left. - \sum_\nu \sum_\alpha \sum_{\substack{\mu_1 < \ldots < \mu_n \\ \mu_\alpha = \nu}} X^{\mu_1 \ldots \mu_{\alpha-1} \{\mu_1 \ldots \mu_n\} \mu_{\alpha+1} \ldots \mu_n} dq^\nu \right].$$

Algebraic similarities with (13) are evident if we replace X by $\partial(q,p)/\partial(x^1, \ldots, x^n) := \partial(q,p)/\partial x^1 \wedge \cdots \wedge \partial(q,p)/\partial x^n$. In particular we can see easily that the coefficients of dy^i and $dp_{\mu_1 \ldots \mu_n}$ in $(-1)^n \partial(q,p)/\partial(x^1, \ldots, x^n) \rfloor \Omega$ and $d\mathcal{H}$ coincide if and only if the Hamilton system (11) holds. Thus we are led to define $\mathcal{I}$ to be the algebraic ideal in $\Lambda^\star \mathcal{M}$ spanned by $\{dx^1, \ldots, dx^n\}$ and hence (11) is equivalent to

$$(-1)^n \frac{\partial(q,p)}{\partial(x^1, \ldots, x^n)} \rfloor \Omega = d\mathcal{H} \mod \mathcal{I}. \tag{14}$$

Definition 2: An n-vector $X \in \Lambda^n T_{(q,p)}\mathcal{M}$ is $\mathcal{H}$-Hamiltonian if and only if

$$(-1)^n X \rfloor \Omega = d\mathcal{H} \mod \mathcal{I}. \tag{15}$$

For such an X, it is possible to precise the relation between the left- and right-hand sides of (15) in the case where X is decomposable, i.e., $X = X_1 \wedge \cdots \wedge X_n$. Notice that (15) implies in

particular $X^{1\cdots n}=\partial\mathcal{H}/\partial\epsilon=1$ [where $\epsilon:=p_{1\cdots n}$, see (13)], which is equivalent to $\omega(X_1,\ldots,X_n)=1$. Hence we may always assume without loss of generality that the X_α are chosen so that $dx^\beta(X_\alpha)=\delta^\beta_\alpha$. Such vectors are unique.

Lemma 1: Let $X=X_1\wedge\cdots\wedge X_n\in\Lambda^n T_{(q,p)}\mathcal{M}$ *such that* $dx^\beta(X_\alpha)=\delta^\beta_\alpha$. *Then* X *is* $\mathcal{H}$*-Hamiltonian if and only if one of the two following relations is satisfied:*

$$(-1)^n X\rfloor\Omega=d\mathcal{H}-\sum_\alpha d\mathcal{H}(X_\alpha)dx^\alpha \tag{16}$$

or

$$X\rfloor(\Omega-d(\mathcal{H}\omega))=0. \tag{17}$$

Proof: Let us prove first that (15) implies (16). Since for any α, β, $dx^\beta(X_\alpha-\partial/\partial x^\alpha)=0$, Eq. (15) implies that for all α,

$$\begin{aligned}(-1)^n X\rfloor\Omega\left(X_\alpha-\frac{\partial}{\partial x^\alpha}\right)=d\mathcal{H}\left(X_\alpha-\frac{\partial}{\partial x^\alpha}\right)&\Leftrightarrow(-1)^n\Omega\left(X_1,\ldots,X_n,X_\alpha-\frac{\partial}{\partial x^\alpha}\right)\\&=d\mathcal{H}(X_\alpha)-\frac{\partial\mathcal{H}}{\partial x^\alpha}\Leftrightarrow(-1)^n X\rfloor\Omega\left(\frac{\partial}{\partial x^\alpha}\right)=\frac{\partial\mathcal{H}}{\partial x^\alpha}-d\mathcal{H}(X_\alpha).\end{aligned}$$

This implies

$$(-1)^n\sum_\alpha X\rfloor\Omega\left(\frac{\partial}{\partial x^\alpha}\right)dx^\alpha=\sum_\alpha\frac{\partial\mathcal{H}}{\partial x^\alpha}dx^\alpha-\sum_\alpha d\mathcal{H}(X_\alpha)dx^\alpha. \tag{18}$$

Now if we rewrite (15) as

$$\begin{aligned}&(-1)^n\left(\sum_i X\rfloor\Omega\left(\frac{\partial}{\partial y^i}\right)dy^i+\sum_{\mu_1<\cdots<\mu_n}X\rfloor\Omega\left(\frac{\partial}{\partial p_{\mu_1\cdots\mu_n}}\right)dp_{\mu_1\cdots\mu_n}\right)\\&=\sum_i\frac{\partial\mathcal{H}}{\partial y^i}dy^i+\sum_{\mu_1<\cdots<\mu_n}\frac{\partial\mathcal{H}}{\partial p_{\mu_1\cdots\mu_n}}dp_{\mu_1\cdots\mu_n},\end{aligned}$$

and sum with (18), we obtain exactly (16).

Now relation (17) is equivalent to (16) because of the following calculation. For all vector V and for any decomposable n-vector $X=X_1\wedge\cdots\wedge X_n\in\Lambda^n T_{(q,p)}\mathcal{M}$ such that $dx^\beta(X_\alpha)=\delta^\beta_\alpha$ (not necessarily $\mathcal{H}$-Hamiltonian), we have

$$\begin{aligned}X\rfloor d(\mathcal{H}\omega)(V)&=d\mathcal{H}\wedge\omega(X_1,\ldots,X_n,V)\\&=\sum_\alpha(-1)^{\alpha-1}d\mathcal{H}(X_\alpha)\omega(X_1,\ldots,X_{\alpha-1},X_{\alpha+1},\ldots,X_n,V)\\&\quad+(-1)^n d\mathcal{H}(V)\omega(X_1,\ldots,X_n,V)\\&=\sum_\alpha(-1)^{n-1}d\mathcal{H}(X_\alpha)dx^\alpha(V)+(-1)^n d\mathcal{H}(V),\end{aligned}$$

thus

$$X\rfloor d(\mathcal{H}\omega)=(-1)^n\left(d\mathcal{H}-\sum_\alpha d\mathcal{H}(X_\alpha)dx^\alpha\right)$$

and (16) $\Leftrightarrow$ (17). Conversely, it is obvious that (16) and (17) implies (15). ■

As a Corollary of this result we deduce that a reformulation of (14) is

$$\frac{\partial(q,p)}{\partial(x^1,\ldots,x^n)}\rfloor\Omega=\frac{\partial(q,p)}{\partial(x^1,\ldots,x^n)}\rfloor(d\mathcal{H}\wedge\omega). \tag{19}$$

It is an exercise to check that actually this relation is a direct translation of (13).

F. A variational formulation of (13)

We shall now prove that Eqs. (13) are the Euler–Lagrange equations of some simple functional. For that purpose, let Γ be an oriented submanifold of dimension n in $\Lambda^n T^\star(\mathcal{X}\times\mathcal{Y})$ such that $\omega_{|\Gamma}>0$ everywhere. Then we define the functional

$$\mathcal{A}[\Gamma]:=\int_\Gamma \theta-\lambda\mathcal{H}(q,p)\omega.$$

Here λ is a (real) scalar function defined over Γ which plays the role of a Lagrange multiplier. We now characterize submanifolds Γ which are critical points of $\mathcal{A}$.

1. Variations with respect to p

Let δp be some infinitesimal variation of Γ with compact support. We compute

$$\delta\mathcal{A}_\Gamma(\delta p)=\int_\Gamma \delta p_{\mu_1\ldots\mu_n}\left(dq^{\mu_1}\wedge\cdots\wedge dq^{\mu_n}-\lambda\frac{\partial\mathcal{H}}{\partial p_{\mu_1\ldots\mu_n}}\omega\right).$$

Assuming that this vanishes for all δp, we obtain

$$(dq^{\mu_1}\wedge\cdots\wedge dq^{\mu_n})_{|\Gamma}=\lambda\frac{\partial\mathcal{H}}{\partial p_{\mu_1\ldots\mu_n}}\omega_{|\Gamma}.$$

This relation means that for any orientation preserving parametrization $(t^1,\ldots,t^n)\mapsto(q,p)\times(t^1,\ldots,t^n)$ of Γ,

$$\frac{\partial(q^{\mu_1},\ldots,q^{\mu_n})}{\partial(t^1,\ldots,t^n)}=\lambda\frac{\partial\mathcal{H}}{\partial p_{\mu_1\ldots\mu_n}}\omega\left(\frac{\partial q^{\mu_1}}{\partial t^1},\ldots,\frac{\partial q^{\mu_n}}{\partial t^n}\right).$$

But we remark that because $\partial\mathcal{H}/\partial p_{1\ldots n}=1$, the above relation for $(\mu_1,\ldots,\mu_n)=(1,\ldots,n)$ forces $\lambda=1$. Hence

$$\mathcal{A}[\Gamma]=\int_\Gamma \theta-\mathcal{H}(q,p)\omega.$$

Moreover, the equation obtained here can be written using the natural parametrization $(x^1,\ldots,x^n)\mapsto(x,u(x),p(x))$ [for which $\omega(\partial/\partial x^1,\ldots,\partial/\partial x^n)=1$] and then we obtain

$$\frac{\partial q}{\partial x^1}\wedge\cdots\wedge\frac{\partial q}{\partial x^n}=\frac{\partial\mathcal{H}}{\partial p}(q,p),$$

i.e., exactly Eq. (9). [Note that this relation actually implies $\mathcal{A}[\Gamma]=\int_\mathcal{X} L(x,q,dq)\omega$. Hence, as in the one-dimensional Hamilton formalism, $\theta-\mathcal{H}\omega$ plays the role of the Lagrangian density.]

2. Variations with respect to q

Now δq is some infinitesimal variation of Γ with compact support. And we have

$$\delta\mathcal{A}_\Gamma(\delta q)=\int_\Gamma \sum_{\mu_1<\ldots<\mu_n}\sum_\alpha p_{\mu_1\ldots\mu_n} dq^{\mu_1}\wedge\cdots\wedge d(\delta q^{\mu_\alpha})\wedge\cdots\wedge dq^{\mu_n} - \sum_\mu \frac{\partial\mathcal{H}}{\partial q^\mu}\delta q^\mu\omega-\mathcal{H}(q,p)\,\delta\omega.$$

We pay special attention to $\delta\omega$:

$$\delta\omega=d(\delta x^1)\wedge\cdots\wedge dx^n+\cdots+dx^1\wedge\cdots\wedge d(\delta x^n).$$

Hence

$$\int_\Gamma \mathcal{H}(q,p)\,\delta\omega=-\int_\Gamma \delta x^1(d(\mathcal{H}(q,p))\wedge\cdots\wedge dx^n)+\cdots+\delta x^n(dx^1\wedge\cdots\wedge d(\mathcal{H}(q,p)))$$

$$=-\sum_\alpha \delta x^\alpha\frac{\partial}{\partial x^\alpha}(\mathcal{H}(q,p))\omega.$$

Thus after integrations by parts, we obtain

$$\delta\mathcal{A}_\Gamma(\delta q)=\int_\Gamma -\sum_{\mu_1<\ldots<\mu_n}\sum_\alpha \delta q^{\mu_\alpha} dq^{\mu_1}\wedge\cdots\wedge dq^{\mu_{\alpha-1}}\wedge dp_{\mu_1\ldots\mu_n}\wedge dq^{\mu_{\alpha+1}}\wedge\cdots\wedge dq^{\mu_n} - \sum_\mu\frac{\partial\mathcal{H}}{\partial q^\mu}\delta q^\mu\omega+\sum_\alpha \delta x^\alpha\frac{\partial}{\partial x^\alpha}(\mathcal{H}(q,p))\omega.$$

And this vanishes if and only if

$$\sum_\alpha \sum_{\substack{\mu_1<\cdots<\mu_n\\ \mu_\alpha=\nu}} dq^{\mu_1}\wedge\cdots\wedge dq^{\mu_{\alpha-1}}\wedge dp_{\mu_1\ldots\mu_n}\wedge dq^{\mu_{\alpha+1}}\wedge\cdots\wedge dq^{\mu_n}-\sum_\alpha \delta^\alpha_\nu\frac{\partial}{\partial x^\alpha}(\mathcal{H}(q,p))\omega$$

$$=-\frac{\partial\mathcal{H}}{\partial q^\nu}\omega.$$

Again by choosing the parametrization $(x^1,\ldots,x^n)\mapsto(x,u(x),p(x))$, this relation is easily seen to be equivalent to (10) and (12).

By the same token we have proven that if we look to critical points of the functional $\int_\Gamma\theta$ with the constraint $\mathcal{H}(q,p)=h$, for some constant h, then the Lagrange multiplier is 1 and they satisfy the same equations.

Theorem 1: *Let Γ be an oriented submanifold of dimension n in $\Lambda^n T^\star(\mathcal{X}\times\mathcal{Y})$ such that $\Omega_{|\Gamma}>0$ everywhere. Then the three following assertions are equivalent*

(i) Γ *is the graph of a solution of the generalized Hamilton equations (13).*
(ii) Γ *is a critical point of the functional* $\int_\Gamma\theta-\mathcal{H}(q,p)\omega$.
(iii) Γ *is a critical point of the functional* $\int_\Gamma\theta$ *under the constraint that* $\mathcal{H}(q,p)$ *is constant.*

G. Some particular cases

By restricting the variables (q,p) to lie in some submanifold of $\mathcal{M}=\Lambda^n T^\star(\mathcal{X}\times\mathcal{Y})$, the Legendre correspondence becomes in some situations a true map.

(a) We assume that all components $p_{\mu_1,\ldots\mu_n}$ vanished except for

$$p_{1\ldots n}=:\epsilon \quad \text{and} \quad p_{1\ldots(\alpha-1)(n+i)(\alpha+1)\ldots n}=:p_i^\alpha$$

and all obvious permutations in the indices. This defines a submanifold $\mathcal{M}_{\text{Weyl}}$ of $\mathcal{M}$. It means that

$$\theta_{|\mathcal{M}_{\text{Weyl}}}=\epsilon dx^1\wedge\cdots\wedge dx^n+\sum_\alpha\sum_i p_i^\alpha dx^1\wedge\cdots\wedge dx^{\alpha-1}\wedge dy^i\wedge dx^{\alpha+1}\wedge\cdots\wedge dx^n.$$

Then for any $(q,p)\in\mathcal{M}_{\text{Weyl}}$, $\langle p,z_1\wedge\cdots\wedge z_n\rangle=\epsilon+\Sigma_\alpha\Sigma_i p_i^\alpha v^i_\alpha$, $W(q,v,p)=\epsilon+\Sigma_\alpha\Sigma_i p_i^\alpha v^i_\alpha - L(q,v)$. Hence the relation (5) $(\partial W/\partial v^i_\alpha)(q,v)=0$ is equivalent to

$$p_i^\alpha=\frac{\partial L}{\partial v^i_\alpha}(q,v)\Leftrightarrow v^i_\alpha=\mathcal{V}^i_\alpha(q,p).$$

The relation (4) $W(q,v,p)=w$ gives

$$\epsilon=w+L(q,v)-\sum_\alpha\sum_i\frac{\partial L}{\partial v^i_\alpha}(q,v)v^i_\alpha.$$

Last we have that $\mathcal{H}(q,p)=\epsilon+\Sigma_\alpha\Sigma_i p_i^\alpha\mathcal{V}^i_\alpha(q,p)-L(q,\mathcal{V}(q,p))$.

This example shows that for any $(q,v,w)\in S\Lambda^nT(\mathcal{X}\times\mathcal{Y})\times\mathbb{R}$, there exist $(q,p)\in\mathcal{M}$ such that $(q,v,w)\leftrightarrow(q,p)$ and this (q,p) is unique if it is chosen in $\mathcal{M}_{\text{Weyl}}$.

To summarize, we recover the Weyl theory (see Refs. 4 and 10). As an exercise, the reader can check that in this situation, Eqs. (11) are equivalent to

$$\frac{\partial y^i}{\partial x^\alpha}=\frac{\partial\mathcal{H}}{\partial p_i^\alpha},\quad \sum_\alpha\frac{\partial p_i^\alpha}{\partial x^\alpha}=-\frac{\partial\mathcal{H}}{\partial y^i}. \tag{20}$$

(b) We assume that (q,p) are such that there exist coefficients $(\pi^\alpha_\mu)_{\alpha,\mu}$ with

$$p_{\mu_1\ldots\mu_n}=\begin{vmatrix}\pi^1_{\mu_1} & \cdots & \pi^1_{\mu_n}\\ \vdots & & \vdots\\ \pi^n_{\mu_1} & \cdots & \pi^n_{\mu_n}\end{vmatrix}.$$

This constraint defines a submanifold $\mathcal{M}_{\text{Carathéodory}}$ of $\mathcal{M}$. Then

$$\theta_{|\mathcal{M}_{\text{Carathéodory}}}=\left(\sum_{\mu_1}\pi^1_{\mu_1}dq^{\mu_1}\right)\wedge\cdots\wedge\left(\sum_{\mu_n}\pi^1_{\mu_n}dq^{\mu_n}\right).$$

Then it is an exercise to see that, by choosing $w=0$, it leads to the formalism developed in Refs. 4 and 10 associated to the Carathéodory theory of equivalent integrals. However, it is not clear in general whether it is possible to perform the Legendre transform in this setting by being able to fix arbitrarily the value of w. It is so if we do not impose a condition on w (see Ref. 10).

III. COMPARISON WITH THE USUAL HAMILTONIAN FORMALISM FOR QUANTUM FIELDS THEORY

A. Reminder of the usual approach to quantum field theory

Here we compare the preceeding construction with the classical approach to quantum field theory by so-called canonical quantization. We shall first explore it in the case where $\mathcal{X}$ is the Minkowski space $\mathbb{R}\times\mathbb{R}^{n-1}$ and $y=\phi$ is a real scalar field. Hence $\mathcal{Y}=\mathbb{R}$. Our functional is

$$\mathcal{L}[\phi]:=\int_{\mathbb{R}\times\mathbb{R}^{n-1}}L(x,\phi,d\phi)dx.$$

For simplicity, we may keep in mind the following example of a Lagrangian:

$$\int_{\mathbb{R}\times\mathbb{R}^{n-1}} L(x,\phi,d\phi)dx = \int_{\mathbb{R}\times\mathbb{R}^{n-1}} \left(\frac{1}{2}\left(\frac{\partial\phi}{\partial x^0}\right)^2 - \frac{1}{2}\sum_{\alpha=1}^{n-1}\left(\frac{\partial\phi}{\partial x^\alpha}\right)^2 - V(\phi)\right) dx^0 d\vec{x},$$

where we denote $\vec{x}=(x^\alpha)_{1\leqslant\alpha\leqslant n-1}$. We shall also denote $t=x^0$.

The usual approach consists in selecting a global time coordinate t as we already implicitly assumed here. Then for each time the instantaneous state of the field is seen as a point in the infinite dimensional "manifold" $\mathfrak{F}:=\{\Phi:\mathbb{R}^{n-1}\to\mathbb{R}\}$. Hence we view the field ϕ rather as a path:

$$\mathbb{R}\to\mathfrak{F},$$

$$t\mapsto[\vec{x}\mapsto\phi(t,\vec{x})=\Phi^{\vec{x}}(t)].$$

We thus recover the problem of studying the dynamics of a point moving in a configuration space $\mathfrak{F}$. The prices to pay are (1) $\mathfrak{F}$ is infinite dimensional and (2) we lose relativistic invariance.

In this viewpoint, $\mathcal{L}[\phi]=\int_{\mathbb{R}}\mathfrak{L}[t,\Phi(t),(d\Phi/dt)(t)]dt$, where $\Phi(t)=[\vec{x}\mapsto\phi(t,\vec{x})]\in\mathfrak{F}$, $(d\Phi/dt)(t)=[\vec{x}\mapsto\partial\phi/\partial t(t,\vec{x})]\in T_{\Phi(t)}\mathfrak{F}$ and $\mathfrak{L}[t,\Phi(t),(d\Phi/dt)(t)]=\int_{\mathbb{R}^{n-1}}L(x,\phi(x),d\phi(x))d\vec{x}$.

Then we consider the "symplectic" manifold which is formally $T^\star\mathfrak{F}$, i.e., we introduce the dual variable

$$\Pi:=\frac{\partial\mathfrak{L}}{\partial(d\Phi/dt)},$$

or equivalently $\Pi(t)=[\vec{x}\mapsto\pi(t,\vec{x})=\Pi_{\vec{x}}(t)]$ with

$$\Pi_{\vec{x}}(t)=\frac{\partial\mathfrak{L}}{\partial d\Phi^{\vec{x}}/dt}[t,\Phi(t),(d\Phi/dt)(t)]\Leftrightarrow\pi(t,\vec{x})$$

$$=\frac{\delta\mathfrak{L}}{\delta(\partial\phi(t,\vec{x})/\partial t)}[t,\Phi(t),(d\Phi/dt)(t)]=\frac{\partial L}{\partial v_0}(x,\phi(x),d\phi(x)).$$

Here $\delta/\delta\phi(\vec{x})$ is the Fréchet derivative. In our example

$$\Pi_{\vec{x}}(t)=\frac{\partial\phi}{\partial t}(t,\vec{x}).$$

We define the Hamiltonian functional to be

$$\mathfrak{H}[\Phi,\Pi]:=\int_{\mathbb{R}^{n-1}}\Pi_{\vec{x}}\dot{\Phi}^{\vec{x}}d\vec{x}-\mathfrak{L}[t,\Phi,(d\Phi/dt)]=\int_{\mathbb{R}^{n-1}}\left(\frac{1}{2}\pi(\vec{x})^2+\frac{1}{2}|\nabla\phi(\vec{x})|^2+V(\phi(\vec{x}))\right)d\vec{x}.$$

Now we can write the equations of motion as

$$\frac{\partial\pi}{\partial t}(t,\vec{x})=\frac{d\Pi_{\vec{x}}}{dt}=-\frac{\partial\mathfrak{H}}{\partial\Phi^{\vec{x}}}(\Phi,\Pi)=\Delta\phi-V'(\phi),$$

$$\frac{\partial\phi}{\partial t}(t,\vec{x})=\frac{d\Phi^{\vec{x}}}{dt}=\frac{\partial\mathfrak{H}}{\partial\Pi^{\vec{x}}}(\Phi,\Pi)=\pi(t,\vec{x}).$$

A Poisson bracket can be defined on the set of functionals $\{A:T^\star\mathfrak{F}\mapsto\mathbb{R}\}$ by

$$\{A,B\}:=\int_{\mathbb{R}^{n-1}}\left(\frac{\delta A}{\delta\pi(\vec{x})}\frac{\delta B}{\delta\phi(\vec{x})}-\frac{\delta A}{\delta\phi(\vec{x})}\frac{\delta B}{\delta\pi(\vec{x})}\right)d\vec{x},$$

where $\delta A/\delta\phi(\vec{x})$ is the Fréchet derivative with respect to $\phi(\vec{x})$, i.e., the distribution such that for any smooth compactly supported deformation $\delta\phi$ of ϕ,

$$dA_\phi[\,\delta\phi]=\int_{\mathbb{R}^{n-1}}\delta\phi(\vec{x})\frac{\delta A}{\delta\phi(\vec{x})}d\vec{x}.$$

And we may formulate the dynamical equations using the Poisson bracket as

$$\frac{d\Pi_{\vec{x}}}{dt}=\{\mathfrak{H},\Pi_{\vec{x}}\},$$

$$\frac{d\Phi^{\vec{x}}}{dt}=\{\mathfrak{H},\Phi^{\vec{x}}\},$$

with

$$\{\Phi^{\vec{x}},\Phi^{\vec{x}'}\}=\{\Pi_{\vec{x}},\Pi_{\vec{x}'}\}=0,\quad\{\Pi_{\vec{x}},\Phi^{\vec{x}'}\}=\delta_{\vec{x}}^{\vec{x}'}=\delta^{n-1}(\vec{x}-\vec{x}').$$

This singular Poisson bracket means that for any test functions $f,\ g\in\mathcal{C}_c^\infty(\mathbb{R}^{n-1},\mathbb{R})$,

$$\left\{\int_{\mathbb{R}^{n-1}}g(\vec{x})\Pi_{\vec{x}}d\vec{x},\int_{\mathbb{R}^{n-1}}f(\vec{x}')\Phi^{\vec{x}'}d\vec{x}'\right\}=\int_{\mathbb{R}^{n-1}}f(\vec{x})g(\vec{x})d\vec{x}.$$

This implies in particular

$$\left\{\int_{\mathbb{R}^{n-1}}g(\vec{x})\Pi_{\vec{x}}d\vec{x},\int_{\mathbb{R}^{n-1}}f(\vec{x}')V(\Phi^{\vec{x}'})d\vec{x}'\right\}=\int_{\mathbb{R}^{n-1}}V'(\Phi^{\vec{x}})f(\vec{x})g(\vec{x})d\vec{x},$$

because of the derivation property of the Poisson bracket.

B. Translation in pataplectic geometry

We first adapt and modify our notations: the coordinates on $\mathcal{M}=\Lambda^nT^\star(\mathbb{R}\times\mathbb{R}^{n-1}\times\mathbb{R})$ are now written $(q^\mu,p_{\mu_1\ldots\mu_n})=(x^\alpha,y,\epsilon,p^\alpha)$ where $0\leqslant\alpha\leqslant n-1$, $q^0=x^0=t$, $(x^\alpha)_{1\leqslant\alpha\leqslant n-1}=\vec{x}$, $q^n=y$ and

$$\epsilon:=p_{0\ldots(n-1)},\quad p^\alpha:=p_{0\ldots(\alpha-1)n(\alpha+1)\ldots(n-1)}.$$

Hence

$$\theta=\epsilon dx^0\wedge\cdots\wedge dx^{n-1}+\sum_{\alpha=0}^{n-1}p^\alpha dx^0\wedge\cdots\wedge dx^{\alpha-1}\wedge dy\wedge dx^{\alpha+1}\wedge\cdots\wedge dx^{n-1},$$

or letting $\omega:=dx^0\wedge\cdots\wedge dx^{n-1}$ and $\omega_\alpha:=(-1)^\alpha dx^0\wedge\cdots\wedge dx^{\alpha-1}\wedge dx^{\alpha+1}\wedge\cdots\wedge dx^{n-1}=\frac{\partial}{\partial x^\alpha}\rfloor\omega$,

$$\theta=\epsilon\omega+\sum_{\alpha=0}^{n-1}p^\alpha dy\wedge\omega_\alpha\quad\text{and}\quad\Omega=d\epsilon\wedge\omega+\sum_{\alpha=0}^{n-1}dp^\alpha\wedge dy\wedge\omega_\alpha.$$

Thus we see that in the present case the pataplectic formalism reduces essentially to the Weyl formalism, because the fields are one dimensional.

Let us consider some field ϕ and a map $x \mapsto p(x)$ such that $(x,\phi(x),d\phi(x)) \leftrightarrow (x,\phi(x),p(x))$ [meaning that for some w: $\mathbb{R}\times\mathbb{R}^{n-1}\to\mathbb{R}$, we have $(x,\phi(x),d\phi(x),w(x)) \leftrightarrow (x,\phi(x),p(x))$]. This implies the following relations:

$$p^\alpha = \frac{\partial L}{\partial v_\alpha}(x,\phi(x),d\phi(x)) \quad \text{and} \quad \epsilon = w + L(x,\phi(x),d\phi(x)) - \sum_{\alpha=0}^{n-1} p^\alpha \frac{\partial \phi}{\partial x^\alpha}(x).$$

We let $\Gamma := \{(x,\phi(x),p(x))/x \in \mathbb{R}\times\mathbb{R}^{n-1}\} \subset \mathcal{M}$ and we consider the instantaneous slices $S_t := \Gamma \cap \{x^0 = t\}$. These slices are oriented by the condition $\partial/\partial t \rfloor \omega_{|S_t} > 0$. Then we can express the observables

$$\Phi^f(t) := \int_{\mathbb{R}^{n-1}} f(\vec{x})\Phi^{\vec{x}}(t)d\vec{x}, \quad \Pi_g(t) := \int_{\mathbb{R}^{n-1}} g(\vec{x})\Pi_{\vec{x}}(t)d\vec{x}$$

and

$$\mathfrak{H}[\Phi(t),\Pi(t)] = \int_{\mathbb{R}^{n-1}} \left(\pi(t,\vec{x})\frac{\partial \phi}{\partial t}(t,\vec{x}) - L(t,\vec{x},\phi(x),d\phi(x)) \right) d\vec{x} = \int_{\mathbb{R}^{n-1}} H_0^0(t,\vec{x},\phi)\,\omega_0$$

as integrals of $(n-1)$-forms on S_t. First

$$\Phi^f(t) = \int_{S_t} f(\vec{x})\phi(t,\vec{x})dx^1\wedge\cdots\wedge dx^{n-1} = \int_{S_t} Q^f, \quad \text{with } Q^f := f(\vec{x})y\,\omega_0,$$

$$\Pi_g(t) = \int_{S_t} g(\vec{x})\pi(t,\vec{x})dx^1\wedge\cdots\wedge dx^{n-1} = \int_{S_t} P_g, \quad \text{with } P_g := g(\vec{x})\sum_{\alpha=0}^{n-1} p^\alpha \omega_\alpha,$$

because $\pi(t,\vec{x}) = \partial L/\partial v_0(x,\phi(x),d\phi(x)) = p^0$ and $\omega_{\alpha|S_t} = 0$ if $\alpha \geqslant 1$.

And, finally,

$$\mathfrak{H}[\Phi(t),\Pi(t)] = \int_{\mathbb{R}^{n-1}} \mathcal{H}(q,p)\,\omega_0 - \int_{\mathbb{R}^{n-1}} \epsilon\omega_0 + \sum_{\alpha=1}^{n-1} p^\alpha dy \wedge \left(\frac{\partial}{\partial x^\alpha} \rfloor \omega_0 \right) = \int_{S_t} \eta_0,$$

where

$$\eta_0 := \mathcal{H}(q,p)\,\omega_0 - \left(\epsilon\omega_0 + \sum_{\alpha=1}^{n-1} p^\alpha dx^1\wedge\cdots\wedge dx^{\alpha-1}\wedge dy\wedge dx^{\alpha+1}\wedge\cdots\wedge dx^{n-1} \right),$$

because $H_0^0(x,\phi) = \mathcal{H}(q,p) - \langle p, \partial/\partial t \wedge z_1 \wedge\cdots\wedge z_{n-1}\rangle = \mathcal{H}(q,p) - (\epsilon + \Sigma_{\alpha=1}^{n-1} p^\alpha \partial\phi/\partial x^\alpha)$.

We remark that

$$\eta_0 = -\frac{\partial}{\partial t} \rfloor (\theta - \mathcal{H}(q,p)\omega).$$

[We observe also that $P_g = g(\vec{x})\partial/\partial y \rfloor \theta = g(\vec{x})\partial/\partial y \rfloor (\theta - \mathcal{H}(q,p)\omega)$.]

C. Recovering the usual Poisson brackets as a local expression

Our aim is now to express the various Poisson brackets involving the quantities $\Phi^f(t)$ and $\Pi_g(t)$ along Γ using some analog of the Poisson bracket defined on $(n-1)$-forms. We generalize slightly the definition of Q^f to be

$$Q^f = \sum_{\alpha=0}^{n-1} f^\alpha(x) y \omega_\alpha, \tag{21}$$

where $f := \Sigma_{\alpha=0}^{n-1} f^\alpha(x)\, \partial/\partial x^\alpha$ is some vector field. Hence our observables become

$$\Phi^f(t) = \int_{S_t} Q^f \quad \text{and} \quad \Pi_g(t) = \int_{S_t} P_g, \tag{22}$$

where $P_g := g(x) \Sigma_{\alpha=0}^{n-1} p^\alpha \omega_\alpha$ as before. [Notice that actually $\int_{S_t} Q^f = \int_{S_t} f^0(x) y \omega_0$.] We shall see here that we can define a bracket operation $\{.,.\}$ between Q^f, P_g and η_0 such that the usual Poisson bracket of fields actually derives from $\{.,.\}$ by

$$\int_{S_t} \{P_g, Q^f\} = \left\{ \int_{S_t} P_g, \int_{S_t} Q^f \right\}, \text{ etc.} \tag{23}$$

First we remark that

$$dQ^f = \sum_{\alpha=0}^{n-1} f^\alpha dy \wedge \omega_\alpha + \sum_{\alpha=0}^{n-1} y \frac{\partial f^\alpha}{\partial x^\alpha} \omega = \sum_{\alpha=0}^{n-1} f^\alpha \frac{\partial}{\partial p^\alpha} \rfloor \Omega + \sum_{\alpha=0}^{n-1} y \frac{\partial f^\alpha}{\partial x^\alpha} \frac{\partial}{\partial \epsilon} \rfloor \Omega = -\xi_{Qf} \rfloor \Omega$$

and

$$dP_g = \sum_{\alpha=0}^{n-1} p^\alpha \frac{\partial g}{\partial x^\alpha} \omega + \sum_{\alpha=0}^{n-1} g\, dp^\alpha \wedge \omega_\alpha = \sum_{\alpha=0}^{n-1} p^\alpha \frac{\partial g}{\partial x^\alpha} \frac{\partial}{\partial \epsilon} \rfloor \Omega - g \frac{\partial}{\partial y} \rfloor \Omega = -\xi_{P_g} \rfloor \Omega,$$

where

$$\xi_{Qf} := -\sum_{\alpha=0}^{n-1} f^\alpha \frac{\partial}{\partial p^\alpha} - y \sum_{\alpha=0}^{n-1} \frac{\partial f^\alpha}{\partial x^\alpha} \frac{\partial}{\partial \epsilon} \tag{24}$$

and

$$\xi_{P_g} := g \frac{\partial}{\partial y} - \sum_{\alpha=0}^{n-1} p^\alpha \frac{\partial g}{\partial x^\alpha} \frac{\partial}{\partial \epsilon}. \tag{25}$$

Also notice that

$$d\eta_0 = (d\mathcal{H} - d\epsilon) \wedge \omega_0 - \sum_{\alpha=1}^{n-1} dp^\alpha \wedge dy \wedge \left(\frac{\partial}{\partial x^\alpha} \rfloor \omega_0 \right).$$

Definition 3: We define the Poisson $\mathfrak{p}$*-brackets of these* $(n-1)$*-forms to be*

$$\{\eta_0, Q^f\} := -\xi_{Qf} \rfloor d\eta_0, \quad \{\eta_0, P_g\} := -\xi_{P_g} \rfloor d\eta_0,$$

$$\{P_g, Q^f\} := -\xi_{Qf} \rfloor dP_g = \xi_{P_g} \rfloor dQ^f = \xi_{Qf} \rfloor (\xi_{P_g} \rfloor \Omega),$$

and

$$\{Q^f, Q^{f'}\} := \xi_{Qf'} \rfloor (\xi_{Qf} \rfloor \Omega), \quad \{P_g, P_{g'}\} := \xi_{P_{g'}} \rfloor (\xi_{P_g} \rfloor \Omega).$$

Let us now compute these $\mathfrak{p}$-brackets. We use in particular the fact that $\partial\mathcal{H}/\partial\epsilon = 1$:

$$\{\eta_0,Q^f\}=\left(\sum_{\alpha=0}^{n-1} f^\alpha\frac{\partial}{\partial p^\alpha}+y\sum_{\alpha=0}^{n-1}\frac{\partial f^\alpha}{\partial x^\alpha}\frac{\partial}{\partial\epsilon}\right)\rfloor\left((d\mathcal{H}-d\epsilon)\wedge\omega_0-\sum_{\alpha=1}^{n-1} dp^\alpha\wedge dy\wedge\left(\frac{\partial}{\partial x^\alpha}\rfloor\omega_0\right)\right)$$
$$=\sum_{\alpha=0}^{n-1} f^\alpha\frac{\partial\mathcal{H}}{\partial p^\alpha}\omega_0-\sum_{\alpha=1}^{n-1} f^\alpha dy\wedge\left(\frac{\partial}{\partial x^\alpha}\rfloor\omega_0\right),$$

$$\{\eta_0,P_g\}=\left(\sum_{\alpha=0}^{n-1} p^\alpha\frac{\partial g}{\partial x^\alpha}\frac{\partial}{\partial\epsilon}-g\frac{\partial}{\partial y}\right)\rfloor\left((d\mathcal{H}-d\epsilon)\wedge\omega_0-\sum_{\alpha=1}^{n-1} dp^\alpha\wedge dy\wedge\left(\frac{\partial}{\partial x^\alpha}\rfloor\omega_0\right)\right)$$
$$=-g\frac{\partial\mathcal{H}}{\partial y}\omega_0-g\sum_{\alpha=1}^{n-1} dp^\alpha\wedge\left(\frac{\partial}{\partial x^\alpha}\rfloor\omega_0\right),$$

$$\{P_g,Q^f\}=\left(\sum_{\alpha=0}^{n-1} f^\alpha\frac{\partial}{\partial p_\alpha}+y\sum_{\alpha=0}^{n-1}\frac{\partial f^\alpha}{\partial x^\alpha}\frac{\partial}{\partial\epsilon}\right)\rfloor\left(\sum_{\alpha=0}^{n-1} p^\alpha\frac{\partial g}{\partial x^\alpha}\omega-g\frac{\partial}{\partial y}\rfloor\Omega\right)=g\sum_{\alpha=0}^{n-1} f^\alpha\omega_\alpha,$$

and $\{Q^f,Q^{f'}\}=\{P_g,P_{g'}\}=0$. We now integrate the $\mathfrak{p}$-brackets on a constant time slice $S_t\subset\Gamma$. We immediately see that

$$\int_{S_t}\{P_g,Q^f\}=\int_{S_t} g\,f^0\omega_0=\{\pi_g(t),\Phi^f(t)\}=\left\{\int_{S_t}P_g,\int_{S_t}Q^f\right\}$$

and we recover (23). Second,

$$\int_{S_t}\{\eta_0,Q^f\}=\int_{S_t}\sum_{\alpha=0}^{n-1} f^\alpha\frac{\partial\mathcal{H}}{\partial p^\alpha}\omega_0-\sum_{\alpha=1}^{n-1} f^\alpha\frac{\partial\phi}{\partial x^\alpha}\omega_0.$$

Third,

$$\int_{S_t}\{\eta_0,P_g\}=\int_{S_t}-g\frac{\partial\mathcal{H}}{\partial y}\omega_0-\sum_{\alpha=1}^{n-1} g\frac{\partial p^\alpha}{\partial x^\alpha}\omega_0.$$

Now let us assume that Γ is the graph of a solution of the Hamilton equations (11) or (20). Since then $\partial\phi/\partial x^\alpha=\partial\mathcal{H}/\partial p^\alpha$ along Γ,

$$\int_{S_t}\{\eta_0,Q^f\}=\int_{S_t} f^0\frac{\partial\phi}{\partial t}\omega_0,$$

and because of $-\partial\mathcal{H}/\partial y-\Sigma_{\alpha=1}^{n-1}\partial p^\alpha/\partial x^\alpha=\partial p^0/\partial t$,

$$\int_{S_t}\{\eta_0,P_g\}=\int_{S_t} g\frac{\partial p^0}{\partial t}\omega_0.$$

We conclude that

$$\frac{d}{dt}\int_{S_t}Q^f=\frac{d}{dt}\Phi^f(t)=\int_{S_t} f^0\frac{\partial\phi}{\partial t}\omega_0+\frac{\partial f^0}{\partial t}\phi\omega_0=\int_{S_t}\{\eta_0,Q^f\}+\Phi^{\partial f/\partial t}(t)$$

and

$$\frac{d}{dt}\int_{S_t}P_g=\frac{d}{dt}\Pi_g(t)=\int_{S_t} g\frac{\partial p^0}{\partial t}\omega_0+\frac{\partial g}{\partial t}p^0\omega_0=\int_{S_t}\{\eta_0,P_g\}+\Pi_{\partial g/\partial t}(t).$$

This has to be compared with the usual canonical equations for fields:

$$\frac{d}{dt}\int_{S_t} Q^f = \left\{ \int_{S_t} \eta_0, \int_{S_t} Q^f \right\} + \Phi^{\partial f/\partial t}(t) \qquad \text{and} \qquad \frac{d}{dt}\int_{S_t} P_g = \left\{ \int_{S_t} \eta_0, \int_{S_t} P_g \right\} + \Pi_{\partial g/\partial t}(t).$$

D. An alternative dynamical formulation using $\mathfrak{p}$-brackets

We can also define the $\mathfrak{p}$-bracket of an n-form with forms Q^f or P_g as given by (21) and (22). If ψ is such an n-form,

$$\{\psi, Q^f\} := -\xi_{Qf} \rfloor d\psi \qquad \text{and} \qquad \{\psi, P_g\} := -\xi_{P_g} \rfloor d\psi,$$

where (24) and (25) have been used. An important instance is for $\psi = \mathcal{H}\omega$:

$$\{\mathcal{H}\omega, Q^f\} = \sum_{\alpha=0}^{n-1} f^\alpha \frac{\partial \mathcal{H}}{\partial p^\alpha}\omega + \sum_{\alpha=0}^{n-1} y \frac{\partial f^\alpha}{\partial x^\alpha}\omega.$$

We shall integrate this $\mathfrak{p}$-bracket on $\Gamma_{t_1}^{t_2} := \{(q,p) \in \Gamma / t_1 < t < t_2\}$, where we still assume that Γ is the graph of a solution of the Hamilton equations (19). An integration by parts gives

$$\int_{\Gamma_{t_1}^{t_2}} \{\mathcal{H}\omega, Q^f\} = \int_{\partial\Gamma_{t_1}^{t_2}} \phi \sum_{\alpha=0}^{n-1} f^\alpha \omega_\alpha + \int_{\Gamma_{t_1}^{t_2}} \sum_{\alpha=0}^{n-1} f^\alpha \left(\frac{\partial \mathcal{H}}{\partial p^\alpha} - \frac{\partial \phi}{\partial x^\alpha} \right) \omega = \int_{\partial\Gamma_{t_1}^{t_2}} Q^f = \int_{S_{t_2}} Q^f - \int_{S_{t_1}} Q^f.$$

Similarly we find that

$$\{\mathcal{H}\omega, P_g\} = \sum_{\alpha=0}^{n-1} p^\alpha \frac{\partial g}{\partial x^\alpha}\omega - g\frac{\partial \mathcal{H}}{\partial y}\omega,$$

and thus

$$\int_{\Gamma_{t_1}^{t_2}} \{\mathcal{H}\omega, P_g\} = \int_{\partial\Gamma_{t_1}^{t_2}} \sum_{\alpha=0}^{n-1} g p^\alpha \omega_\alpha - \int_{\Gamma_{t_1}^{t_2}} g \left(\frac{\partial \mathcal{H}}{\partial y} + \sum_{\alpha=0}^{n-1} \frac{\partial p^\alpha}{\partial x^\alpha} \right) \omega = \int_{\partial\Gamma_{t_1}^{t_2}} P_g = \int_{S_{t_2}} P_g - \int_{S_{t_1}} P_g.$$

We are tempted to conclude that

$$\mathbf{d}Q^f = \{\mathcal{H}\omega, Q^f\} \quad \text{and} \quad \mathbf{d}P_g = \{\mathcal{H}\omega, P\},$$

where $\mathbf{d}$ is the differential along a graph Γ of a solution of the Hamilton equations (11). This is precisely what will be proven in the next section.

IV. POISSON $\mathfrak{p}$-BRACKETS FOR $(p-1)$-FORMS ON $\mathcal{M}$

We have seen on some examples that the Poisson bracket algebra of the classical field theory can actually be derived from brackets on $(n-1)$-forms which are integrated on constant time slices. Actually these constructions can be generalized in several ways.

A. $\mathfrak{p}$-brackets on $(n-1)$-forms

We turn back to $\mathcal{M} = \Lambda^n T^\star(\mathcal{X}\times\mathcal{Y})$ and to the notation of the previous section. Let $\Gamma(\mathcal{M}, \Lambda^{n-1}T^\star\mathcal{M})$ be the set of smooth $(n-1)$-forms on $\mathcal{M}$. We consider the subset $\mathfrak{P}^{n-1}\mathcal{M}$ of $\Gamma(\mathcal{M}, \Lambda^{n-1}T^\star\mathcal{M})$ of forms a such that there exists a vector field $\xi_a = \Xi(a)$ which satisfies the property

$$da = -\xi_a \rfloor \Omega.$$

Obviously $\Xi(a)$ depends only on a modulo exact forms and the map $a\mapsto\Xi(a)$ from $\mathfrak{P}^{n-1}\mathcal{M}$ to the set of vector fields induces a map on the quotient $\mathfrak{P}^{n-1}\mathcal{M}/C^{n-1}(\mathcal{M})$, where $C^{n-1}(\mathcal{M})$ is the set of closed $(n-1)$-forms. A property of vector fields $\Xi(a)$ is that there are infinitesimal symmetries of Ω, for

$$\mathcal{L}_{\Xi(a)}\Omega = d(\Xi(a)\rfloor\Omega) + \Xi(a)\rfloor d\Omega = -d\circ da = 0.$$

We shall denote $\mathfrak{pp}\mathcal{M}$ the set of pataplectic vector fields, i.e., vector fields X such that $X\rfloor\Omega$ is exact. Clearly $\Xi:\mathfrak{P}^{n-1}\mathcal{M}/C^{n-1}(\mathcal{M})\to\mathfrak{pp}\mathcal{M}$ is a vector space isomorphism.

Then we define the *internal* $\mathfrak{p}$-*bracket* on $\mathfrak{P}^{n-1}\mathcal{M}$ by

$$\{a,b\} := \Xi(b)\rfloor\Xi(a)\rfloor\Omega.$$

Lemma 2: For any $a,b\in\mathfrak{P}^{n-1}\mathcal{M}$,

$$d\{a,b\} = -[\Xi(a),\Xi(b)]\rfloor\Omega. \tag{26}$$

Proof: Let $\xi_a=\Xi(a)$ and $\xi_b=\Xi(b)$. Then denoting $\mathcal{L}_{\xi_a}$ the Lie derivative with respect to ξ_a,

$$\begin{aligned}[\xi_a,\xi_b]\rfloor\Omega &= \mathcal{L}_{\xi_a}(\xi_b)\rfloor\Omega = \mathcal{L}_{\xi_a}(\xi_b\rfloor\Omega) - \xi_b\rfloor\mathcal{L}_{\xi_a}(\Omega)\\ &= d(\xi_a\rfloor\xi_b\rfloor\Omega) + \xi_a\rfloor d(\xi_b\rfloor\Omega) - \xi_b\rfloor(d(\xi_a\rfloor\Omega) + \xi_a\rfloor d\Omega).\end{aligned}$$

But since $d\Omega = d(\xi_a\rfloor\Omega) = d(\xi_b\rfloor\Omega) = 0$, we find that $[\xi_a,\xi_b]\rfloor\Omega = d(\xi_a\rfloor\xi_b\rfloor\Omega) = -d\{a,b\}$. ■

Lemma 3: $\Xi:\mathfrak{P}^{n-1}\mathcal{M}/C^{n-1}(\mathcal{M})\to\mathfrak{pp}\mathcal{M}$ *is a Lie algebra isomorphism. More precisely we have*

$$\Xi(\{a,b\}) = [\Xi(a),\Xi(b)]. \tag{27}$$

This implies the Jacobi identity modulo exact terms in $\mathfrak{P}^{n-1}\mathcal{M}$*:*

$$\{\{a,b\},c\} + \{\{b,c\},a\} + \{\{c,a\},b\} = d(\xi_c\rfloor\xi_b\rfloor\xi_a\rfloor\Omega). \tag{28}$$

Proof: Relation (27) is a direct consequence of (26) in Lemma 2. The Jacobi identity follows from

$$\begin{aligned}\{\{a,b\},c\} = \xi_c\rfloor[\xi_a,\xi_b]\rfloor\Omega &= \xi_c\rfloor d(\xi_a\rfloor\xi_b\rfloor\Omega)\\ &= \mathcal{L}_{\xi_c}(\xi_a\rfloor\xi_b\rfloor\Omega) - d(\xi_c\rfloor\xi_a\rfloor\xi_b\rfloor\Omega)\\ &= [\xi_c,\xi_a]\rfloor\xi_b\rfloor\Omega + \xi_a\rfloor[\xi_c,\xi_b]\rfloor\Omega + \xi_a\rfloor\xi_b\rfloor\mathcal{L}_{\xi_c}(\Omega) + d(\xi_c\rfloor\xi_b\rfloor\xi_a\rfloor\Omega)\\ &= -\{\{c,a\},b\} - \{\{b,c\},a\} + d(\xi_c\rfloor\xi_b\rfloor\xi_a\rfloor\Omega),\end{aligned}$$

where we have used (27). ■

We can extend the definition of the $\mathfrak{p}$-bracket: for any $0\leqslant p\leqslant n$ the *external* $\mathfrak{p}$-bracket of a p-form $a\in\Gamma(\mathcal{M},\Lambda^pT^\star\mathcal{M})$ with a form $b\in\mathfrak{P}^{n-1}\mathcal{M}$ is

$$\{a,b\} = -\{b,a\} := -\Xi(b)\rfloor da.$$

Of course this definition coincides with the previous one when $a\in\mathfrak{P}^{n-1}\mathcal{M}$.

1. Examples of external $\mathfrak{p}$-brackets

For any $a\in\mathfrak{P}^{n-1}\mathcal{M}$,

$$\{\theta,a\} = -\Xi(a)\rfloor d\theta = -\Xi(a)\rfloor\Omega = da.$$

We can add that it is worthwhile to write in the external $\mathfrak{p}$-brackets of observable forms like q^μ, $q^\mu dq^\nu$, etc.:

$$\{P_{i,g},q^\mu\}=\Xi(P_{i,g})\rfloor dq^\mu=g\,\delta_i^\mu,$$

$$\{Q^{i,f},q^\mu\}=\Xi(Q^{i,f})\rfloor dq^\mu=0,$$

$$\{P_{i,g},q^\mu dq^\nu\}=\Xi(P_{i,g})\rfloor dq^\mu\wedge dq^\nu=g(\delta_i^\mu dq^\nu-\delta_i^\nu dq^\mu).$$

Theorem 2: *Let* Γ *be the graph in* $\mathcal{M}$ *of a solution of the Hamilton equations (11) and write* $\mathcal{U}:x\mapsto\mathcal{U}(x)=(x,u(x),p(x))$ *the natural parametrization of* Γ. *Then for any form* $a\in\mathfrak{P}^{n-1}\mathcal{M}$,

$$\mathbf{d}a=\{\mathcal{H}\omega,a\},$$

where **d** *is the differential along* Γ (*meaning that* $da_{|\Gamma}=\{\mathcal{H}\omega,a\}_{|\Gamma}$).

Proof: We choose an arbitrary open subset $D\subset\Gamma$ and, denoting $\xi_a=\Xi(a)$, we compute

$$\begin{aligned}\int_D\{\mathcal{H}\omega,a\}&=-\int_D\xi_a\rfloor(d\mathcal{H}\wedge\omega)\\&=-\int_{\mathcal{U}^{-1}(D)}d\mathcal{H}\wedge\omega\left(\xi_a,\frac{\partial\mathcal{U}}{\partial x^1},\ldots,\frac{\partial\mathcal{U}}{\partial x^n}\right)\omega\\&=-\int_{\mathcal{U}^{-1}(D)}(-1)^n\frac{\partial\mathcal{U}}{\partial x^1\ldots\partial x^n}\rfloor(d\mathcal{H}\wedge\omega)(\xi_a)\omega.\end{aligned}$$

We use Eq. (19) and obtain

$$\begin{aligned}\int_D\{\mathcal{H}\omega,a\}&=-\int_{\mathcal{U}^{-1}(D)}(-1)^n\frac{\partial\mathcal{U}}{\partial x^1\ldots\partial x^n}\rfloor\Omega(\xi_a)\omega\\&=-\int_{\mathcal{U}^{-1}(D)}\Omega\left(\xi_a,\frac{\partial\mathcal{U}}{\partial x^1},\ldots,\frac{\partial\mathcal{U}}{\partial x^n}\right)\omega\\&=-\int_D\xi_a\rfloor\Omega=\int_D da.\end{aligned}$$

And Theorem 2 follows. ■

Another way to state this result is that

$$\int_D\{\mathcal{H}\omega,a\}=\int_{\partial D}a \tag{29}$$

along any solution of (11).

B. Expression of the standard observable $(n-1)$-forms

These quantities are integrals of $(n-1)$-forms on hypersurfaces which are thought of as "constant time slices," the transversal dimension being then considered as a local time. The target coordinates observables are weighted integrals of the value of the field and are induced by the "*position*" $\mathfrak{p}$-*forms*

$$Q^{i,f}:=y^i\sum_\alpha f^\alpha(x)\omega_\alpha=y^i f\rfloor\omega,$$

where $f=\Sigma_\alpha f^\alpha(x)\,\partial/\partial x^\alpha$ is a tangent vector field on $\mathcal{X}$ and $\omega_\alpha=\partial/\partial x^\alpha\rfloor\omega$. (Comparing with the one-dimensional Hamiltonian formalism, we can see these target coordinates as generalizations of the position observables.) The ''momentum'' and ''energy'' observables are obtained from the *momentum form*

$$P^\star_{\mu,g}:=g(x)\frac{\partial}{\partial q^\mu}\rfloor(\theta-\mathcal{H}(q,p)\omega),$$

where g is a smooth function on $\mathcal{X}$. Alternatively we may sometimes prefer to use the $\mathfrak{p}$-forms

$$P_{\mu,g}:=g(x)\frac{\partial}{\partial q^\mu}\rfloor\theta.$$

For $1\leqslant\mu=\alpha\leqslant n$, $P^\star_{\mu,g}=:H_{\alpha,g}$ generates the components of the Hamiltonian tensor but $P_{\alpha,g}$ (which is different from $P^\star_{\alpha,g}$) does not in general. However, the restrictions of $P^\star_{\mu,g}$ and $P_{\mu,g}$ on the hypersurface $\mathcal{H}=0$ coincide so that if we work on this hypersurface both forms can be used. For $n+1\leqslant\mu=n+i\leqslant n+k$, $P^\star_{\mu,g}=P_{\mu,g}=:P_{i,g}$ generates the momentum components. (The advantage of $P_{\mu,g}$ with respect to $P^\star_{\mu,g}$ is that $P_{\mu,g}$ belongs to $\mathfrak{P}^{n-1}\mathcal{M}$ for all values of μ.)

To check that, we consider a parametrization $\mathcal{U}:x\mapsto(x,u(x),p(x))$ of some graph Γ and look at the pull-back of these forms by $\mathcal{U}$. We write $\mathcal{U}^\star P^\star_{\mu,g}=\Sigma_\beta s^\beta\omega_\beta$, which implies $s^\beta\omega=dx^\beta\wedge\mathcal{U}^\star P^\star_{\mu,g}$ and we compute

$$\begin{aligned}s^\beta&=g(x)\left\langle p,\frac{\partial q}{\partial x^1}\wedge\cdots\wedge\frac{\partial q}{\partial x^{\beta-1}}\wedge\frac{\partial}{\partial q^\mu}\wedge\frac{\partial q}{\partial x^{\beta+1}}\wedge\cdots\wedge\frac{\partial q}{\partial x^n}\right\rangle_{|z=\partial U/\partial x}-g(x)\,\delta^\beta_\mu\mathcal{H}\\&=g(x)\frac{\partial\langle p,z\rangle}{\partial z^\mu_\beta}{}_{|z=\partial U/\partial x}-g(x)\,\delta^\beta_\mu\mathcal{H}.\end{aligned}$$

Hence we find that

$$\mathcal{U}^\star H_{\alpha,g}=-g(x)\sum_\beta H^\beta_\alpha(q(x),p(x))\omega_\beta=g(x)\sum_\beta S^\beta_\alpha(x,u(x),du(x))\omega_\beta,$$

$$\mathcal{U}^\star P_{i,g}=g(x)\sum_\beta\frac{\partial\langle p,z\rangle}{\partial z^i_\beta}{}_{|z=\partial U/\partial x}\omega_\beta=g(x)\sum_\beta\frac{\partial L}{\partial v^i_\beta}(x,u(x),du(x))\omega_\beta.$$

We shall prove below that $P_{\mu,g}$ (and hence $P_{i,g}$) and $Q^{i,f}$ belong to $\mathfrak{P}^{n-1}\mathcal{M}$.

1. Larger classes of observables

These forms, which are enough to translate most of the observables studied in the usual field theory, are embedded in two more general classes of observables, the definition of which follows.

(a) Generalized positions. They are forms Q^ζ in $\Lambda^{n-1}T^\star(\mathcal{X}\times\mathcal{Y})$, i.e.,

$$Q^\zeta:=\sum_{\mu_1<\ldots<\mu_{n-1}}\zeta_{\mu_1\ldots\mu_{n-1}}(q)dq^{\mu_1}\wedge\cdots\wedge dq^{\mu_{n-1}}.$$

An example is $Q^{i,f}=y^i f(x)\partial_\alpha\rfloor\omega$. We denote $\mathfrak{P}^{n-1}_Q\mathcal{M}=\Lambda^{n-1}T^\star(\mathcal{X}\times\mathcal{Y})$.

(b) Generalized momenta. For each section of $T(\mathcal{X}\times\mathcal{Y})$, i.e., a vector field

$$\xi:=\sum_\mu\xi^\mu(q)\frac{\partial}{\partial q^\mu},$$

we define the $(n-1)$-form

$$P_\xi := \xi \rfloor \theta = \sum_\mu \xi^\mu \frac{\partial}{\partial q^\mu} \rfloor \theta.$$

An example is that for $\xi = g(x)\,\partial/\partial q^\mu$, then we obtain $P_{g(x)\,\partial/\partial q^\mu} = P_{\mu,g}$. We denote $\mathfrak{P}_P^{n-1}\mathcal{M}$ the set of such $(n-1)$-forms.

Lemma 4: $\mathfrak{P}_Q^{n-1}\mathcal{M}$ *ans* $\mathfrak{P}_P^{n-1}\mathcal{M}$ *are subsets of* $\mathfrak{P}^{n-1}\mathcal{M}$, *precisely*

$$\Xi(Q^\zeta) = \sum_{\mu_1 < \ldots < \mu_n} \sum_\alpha (-1)^\alpha \frac{\partial \zeta_{\mu_1 \ldots \mu_{\alpha-1}\mu_{\alpha+1} \ldots \mu_n}}{\partial q^{\mu_\alpha}} \frac{\partial}{\partial p_{\mu_1 \ldots \mu_n}},$$

$$\Xi(P_\xi) = \xi - \sum_\mu \sum_\nu \frac{\partial \xi^\mu}{\partial q^\nu} \Pi_\mu^\nu,$$

where

$$\Pi_\mu^\nu := \sum_{\mu_1 < \ldots < \mu_n} \sum_\alpha p_{\mu_1 \ldots \mu_{\alpha-1}\mu\mu_{\alpha+1} \ldots \mu_n} \delta^\nu_{\mu_\alpha} \frac{\partial}{\partial p_{\mu_1 \ldots \mu_n}}$$

so that

$$dq^\nu \wedge \frac{\partial}{\partial q^\mu} \rfloor \theta = \Pi_\mu^\nu \rfloor \Omega.$$

Proof: We have

$$\begin{aligned} dQ^\zeta &= \sum_\nu \sum_{\mu_1 < \ldots < \mu_{n-1}} \frac{\partial \zeta_{\mu_1 \ldots \mu_{n-1}}}{\partial q^\nu} dq^\nu \wedge dq^{\mu_1} \wedge \cdots \wedge dq^{\mu_{n-1}} \\ &= \sum_\alpha \sum_{\mu_1 < \ldots < \mu_n} \frac{\partial \zeta_{\mu_1 \ldots \mu_{\alpha-1}\mu_{\alpha+1} \ldots \mu_n}}{\partial q^{\mu_\alpha}} dq^{\mu_\alpha} \wedge dq^{\mu_1} \wedge \cdots \wedge dq^{\mu_{\alpha-1}} \wedge dq^{\mu_{\alpha+1}} \wedge \cdots \wedge dq^{\mu_n} \\ &= \sum_\alpha (-1)^{\alpha-1} \sum_{\mu_1 < \ldots < \mu_n} \frac{\partial \zeta_{\mu_1 \ldots \mu_{\alpha-1}\mu_{\alpha+1} \ldots \mu_n}}{\partial q^{\mu_\alpha}} \frac{\partial}{\partial p_{\mu_1 \ldots \mu_n}} \rfloor \Omega. \end{aligned}$$

And the expression for $\Xi(Q^\zeta)$ follows.

Next we write

$$dP_\xi = \sum_\mu \sum_\nu \frac{\partial \xi^\mu}{\partial q^\nu} dq^\nu \wedge \frac{\partial}{\partial q^\mu} \rfloor \theta - \sum_\mu \xi^\mu \frac{\partial}{\partial q^\mu} \rfloor \Omega$$

and we conclude by computing $dq^\nu \wedge \partial/\partial q^\mu \rfloor \theta$, indeed

$$\begin{aligned} dq^\nu \wedge \frac{\partial}{\partial q^\mu} \rfloor \theta &= \sum_{\mu_1 < \ldots < \mu_n} \sum_\alpha p_{\mu_1 \ldots \mu_n} \delta^{\mu_\alpha}_\mu dq^{\mu_1} \wedge \cdots \wedge dq^{\mu_{\alpha-1}} \wedge dq^\nu \wedge dq^{\mu_{\alpha+1}} \wedge \cdots \wedge dq^{\mu_n} \\ &= \sum_{\mu_1 < \ldots < \mu_n} \sum_\alpha p_{\mu_1 \ldots \mu_{\alpha-1}\mu\mu_{\alpha+1} \ldots \mu_n} \delta^\nu_{\mu_\alpha} dq^{\mu_1} \wedge \cdots \wedge dq^{\mu_n} \\ &= \sum_{\mu_1 < \ldots < \mu_n} \sum_\alpha p_{\mu_1 \ldots \mu_{\alpha-1}\mu\mu_{\alpha+1} \ldots \mu_n} \delta^\nu_{\mu_\alpha} \frac{\partial}{\partial p_{\mu_1 \ldots \mu_n}} \rfloor \Omega. \end{aligned}$$

Hence we deduce the result on P_ξ. ■

(c) Poisson $\mathfrak{p}$*-brackets*. We are now in position to compute the $\mathfrak{p}$-brackets of these forms. The results are summarized in the following proposition.

Proposition 1: The $\mathfrak{p}$*-brackets of forms in* $\mathfrak{P}_Q^{n-1}\mathcal{M}$ *and* $\mathfrak{P}_P^{n-1}\mathcal{M}$ *are the following*:

$$\{Q^\zeta, Q^{\tilde{\zeta}}\}=0,$$

$$\{P_\xi, P_{\tilde{\xi}}\}=P_{[\xi,\tilde{\xi}]}+d(\tilde{\xi}\rfloor\xi\rfloor\theta),$$

$$\{P_\xi, Q^\zeta\}=\sum_{\mu_1<\cdots<\mu_n}\sum_\alpha\sum_\mu(-1)^{\alpha+1}\xi^\mu\frac{\partial\zeta_{\mu_1\cdots\mu_{\alpha-1}\mu_{\alpha-1}\cdots\mu_n}}{\partial q^{\mu_\alpha}}\frac{\partial}{\partial q^\mu}\rfloor dq^{\mu_1}\wedge\cdots\wedge dq^{\mu_n}.$$

Proof: These results are all straighforward except for $\{P_\xi, P_{\tilde{\xi}}\}$. We remark that $\Xi(P_\xi)\rfloor\theta=\xi\rfloor\theta=P_\xi$ and

$$\mathcal{L}_{\Xi(P_\xi)}(\theta)=\Xi(P_\xi)\rfloor d\theta+d(\Xi(P_\xi)\rfloor\theta)=\Xi(P_\xi)\rfloor\Omega+dP_\xi=0, \tag{30}$$

so that $\Xi(P_\xi)$ may be viewed as the extension of ξ to a vector field leaving θ invariant. Now we deduce that

$$\begin{aligned}[\xi,\tilde{\xi}]\rfloor\theta&=[\Xi(P_\xi),\Xi(P_{\tilde{\xi}})]\rfloor\theta=\mathcal{L}_{\Xi(P_\xi)}(\Xi(P_{\tilde{\xi}}))\rfloor\theta=\mathcal{L}_{\Xi(P_\xi)}(\Xi(P_{\tilde{\xi}})\rfloor\theta)-\Xi(P_{\tilde{\xi}})\rfloor\mathcal{L}_{\Xi(P_\xi)}\theta\\&=\Xi(P_\xi)\rfloor d(\Xi(P_{\tilde{\xi}})\rfloor\theta)+d(\Xi(P_\xi)\rfloor\Xi(P_{\tilde{\xi}})\rfloor\theta)-\Xi(P_{\tilde{\xi}})\rfloor 0=\Xi(P_\xi)\rfloor dP_{\tilde{\xi}}+d(\xi\rfloor\tilde{\xi}\rfloor\theta)\\&=-\Xi(P_\xi)\rfloor\Xi(P_{\tilde{\xi}})\rfloor\Omega+d(\xi\rfloor\tilde{\xi}\rfloor\theta)=\{P_\xi,P_{\tilde{\xi}}\}-d(\tilde{\xi}\rfloor\xi\rfloor\theta),\end{aligned}$$

and the result follows. ■

2. Back to the standard observables

As an application of the previous results we can express the pataplectic vector fields associated to $Q^{i,f}$ and $P_{\mu,g}$ and their $\mathfrak{p}$-brackets. For that purpose, it is useful to introduce other notations:

$$\epsilon:=p_{1\ldots n},$$

$$p_i^\alpha:=p_{1\ldots(\alpha-1)(n+i)(\alpha+1)\ldots n},$$

$$p_{i_1i_2}^{\alpha_1\alpha_2}:=p_{1\ldots(\alpha_1-1)(n+i_1)(\alpha_1+1)\ldots(\alpha_2-1)(n+i_2)(\alpha_2+1)\ldots n},\ \text{etc.},$$

and

$$\omega_\alpha^i:=dy^i\wedge\left(\frac{\partial}{\partial x^\alpha}\rfloor\omega\right)=:(dy^i\wedge\partial_\alpha)\rfloor\omega,$$

$$\omega_{\alpha_1\alpha_2}^{i_1i_2}:=(dy^{i_1}\wedge\partial_{\alpha_1})\rfloor(dy^{i_2}\wedge\partial_{\alpha_2})\rfloor\omega,\ \text{etc.},$$

in such a way that

$$\theta=\epsilon\omega+\sum_{p=1}^n\frac{1}{p^{!2}}\sum_{i_1,\ldots,i_p;\alpha_1,\ldots,\alpha_p}p_{i_1\ldots i_p}^{\alpha_1\ldots\alpha_p}\omega_{\alpha_1\ldots\alpha_p}^{i_1\ldots i_p}.$$

(Notice that the Weyl theory corresponds to the assumption that $p^{\alpha_1 \cdots \alpha_p}_{i_1 \cdots 1_p}=0$, $\forall p \geqslant 2$.) We have

$$dQ^{i,f}=\sum_\alpha f^\alpha \frac{\partial}{\partial p^\alpha_i}\rfloor\Omega + y^i \sum_\alpha \frac{\partial f^\alpha}{\partial x^\alpha}\frac{\partial}{\partial \epsilon}\rfloor\Omega,$$

$$dP_{\mu,g}=\sum_\alpha \frac{\partial g}{\partial x^\alpha}\Pi^\alpha_\mu\rfloor\Omega - g\frac{\partial}{\partial q^\mu}\rfloor\Omega,$$

where

$$\Pi^\alpha_\beta=\delta^\alpha_\beta \epsilon \frac{\partial}{\partial \epsilon}+\sum_{p=1}^n \frac{1}{p!^2}\sum_{i_1,\ldots,i_p;\alpha_1,\ldots,\alpha_p}\left(p^{\alpha_1\cdots\alpha_p}_{i_1\cdots i_p}\delta^\alpha_\beta - \sum_{j=1}^p p^{\alpha_1\cdots\alpha_{j-1}\,\alpha\alpha_{j+1}\cdots\alpha_n}_{i_1\cdots i_{j-1}\,i_j i_{j+1}\cdots i_n}\delta^{\alpha_j}_\beta\right)\frac{\partial}{\partial p^{\alpha_1\cdots\alpha_p}_{i_1\cdots i_p}},$$

$$\Pi^\alpha_{n+i}=\sum_{p=0}^{n-1}\frac{1}{p!^2}\sum_{i_1,\ldots,i_p;\alpha_1,\ldots,\alpha_p} p^{\alpha\alpha_1\cdots\alpha_p}_{i i_1\cdots i_p}\frac{\partial}{\partial p^{\alpha_1\cdots\alpha_p}_{i_1\cdots i_p}}.$$

The pataplectic vector fields are

$$\Xi(Q^{i,f})=-\sum_\alpha f^\alpha\frac{\partial}{\partial p^\alpha_i}-y^i\sum_\alpha\frac{\partial f^\alpha}{\partial x^\alpha}\frac{\partial}{\partial\epsilon},$$

$$\Xi(P_{\mu,g})=g\frac{\partial}{\partial q^\mu}-\sum_\alpha\frac{\partial g}{\partial x^\alpha}\Pi^\alpha_\mu.$$

Finally, by using Proposition 1, the Poisson $\mathfrak{p}$-brackets will be

$$\{Q^{i,f},Q^{j,\tilde f}\}=0,$$

$$\{P_{i,g},P_{j,\tilde g}\}=d\left(g\tilde g\frac{\partial}{\partial y^j}\rfloor\frac{\partial}{\partial y^i}\rfloor\theta\right),$$

$$\{P_{i,g},Q^{j,f}\}=\delta^j_i\sum_\alpha f^\alpha g\omega_\alpha.$$

Hence if g and $\tilde g$ have compact support, we obtain that on any submanifold S of dimension $n-1$ without boundary,

$$\int_S\{Q^{i,f},Q^{j,\tilde f}\}=\int_S\{P_{i,g},P_{j,\tilde g}\}=0 \quad \text{and} \quad \int_S\{P_{i,g},Q^{j,f}\}=\delta^j_i\int_S\sum_\alpha f^\alpha g\omega_\alpha.$$

C. Extension of the $\mathfrak{p}$-bracket to forms of degree less than $n-1$

The $\mathfrak{p}$-brackets defined above allow us to express the dynamics of an observable which is in $\mathfrak{P}^{n-1}\mathcal{M}$. We shall extend this bracket to some forms in $\Gamma(\mathcal{M},\Lambda^p T^\star\mathcal{M})$, where $0\leqslant p\leqslant n-1$. Like in the case $p=n-1$, not every p-form is admissible and, as we shall see, the class of such p-forms is quite restricted and is basically composed of ''position'' observables. However, when the Hamiltonian system is degenerate, due to some gauge symmetry and constraints, some ''mo-

mentum'' observable can be represented by p-forms with $p<n-1$. An instance of such a situation is the electromagnetic field studied in Sec. V C. Our aim now is to find a generalization of Theorem 2, using the following construction:

For $1\leqslant p\leqslant n$, we define $\mathfrak{P}^{p-1}\mathcal{M}$ to be the set of sections a of $\Gamma(\mathcal{M},\Lambda^{p-1}T^\star\mathcal{M})$ such that, for all $1\leqslant\alpha_1<\cdots<\alpha_{n-p}\leqslant n$,

$$dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a\in\mathfrak{P}^{n-1}\mathcal{M}.$$

We introduce anticommuting (Grassmann) variables $\tau_1,\ldots,\tau_n$, which behave under a change of coordinates like $\partial/\partial x^1,\ldots,\partial/\partial x^n$. We shall consider functions and forms depending on the variables $(\tau_\alpha,x^\alpha,y^i,p_{\mu_1,\ldots,\mu_n})$. Alternatively they can be seen as functions on the bundle $\Pi T\mathcal{X}\otimes_{\mathcal{X}}\mathcal{M}$, where $\Pi T\mathcal{X}$ is a copy of $T\mathcal{X}$ in which the parity of vectors in the fibers $T_x\mathcal{X}$ has been reversed. We consider ${}^s\Gamma(\mathcal{M},\Lambda^{n-1}T^\star\mathcal{M})$ to be the set of $(n-1)$-forms on $\mathcal{M}$ whose coefficients are in the algebra $\mathbb{R}[\tau_1,\ldots,\tau_n]$. More intrinsically, ${}^s\Gamma(\mathcal{M},\Lambda^{n-1}T^\star\mathcal{M})$ can be identified with $\mathcal{C}^\infty(\Pi T\mathcal{X})\otimes_{\mathcal{C}^\infty(\mathcal{X})}\Gamma(\mathcal{M},\Lambda^{n-1}T^\star\mathcal{M})$, meaning that any form $A\in{}^s\Gamma(\mathcal{M},\Lambda^{n-1}T^\star\mathcal{M})$ is a finite sum of terms of the form $\phi(x,\tau)\theta$, where $\phi\in\mathcal{C}^\infty(\Pi T\mathcal{X})$ and $\theta\in\Gamma(\mathcal{M},\Lambda^{n-1}T^\star\mathcal{M})$. Through this identification we can define ${}^s\mathfrak{P}^{n-1}\mathcal{M}$ to be the subset of ${}^s\Gamma(\mathcal{M},\Lambda^{n-1}T^\star\mathcal{M})$ linearly spanned by $\phi(x,\tau)\theta$, where $\phi\in\mathcal{C}^\infty(\Pi T\mathcal{X})$ and $\theta\in\mathfrak{P}^{n-1}\mathcal{M}$.

Obviously for any $A\in{}^s\mathfrak{P}^{n-1}\mathcal{M}$, there exists some vector field $\Xi(A)$ on $\mathcal{M}$ with coefficients in $\mathbb{R}[\tau_1,\ldots,\tau_n]$ such that $dA=-\Xi(A)\rfloor\Omega$. A more geometrical description of $\Xi(A)$ is that it is a section of the bundle $\Pi T\mathcal{X}\otimes_{\mathcal{X}}T\mathcal{M}$ over $\mathcal{M}$.

We embed each $\mathfrak{P}^{p-1}\mathcal{M}$ in ${}^s\mathfrak{P}^{n-1}\mathcal{M}$ by

$$\mathfrak{P}^{p-1}\mathcal{M}\to{}^s\mathfrak{P}^{n-1}\mathcal{M},$$

$$a\mapsto{}^sa,$$

where the ''s-form'' ${}^sa$ is defined by

$${}^sa:=\sum_{\alpha_1<\ldots<\alpha_{n-p}}\tau_{\alpha_1}\cdots\tau_{\alpha_{n-p}}dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a.$$

Then

$$\Xi({}^sa)=\sum_{\alpha_1<\ldots<\alpha_{n-p}}\tau_{\alpha_1}\cdots\tau_{\alpha_{n-p}}\Xi(dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a).$$

We endow ${}^s\mathfrak{P}^{n-1}\mathcal{M}$ with the Poisson $\mathfrak{p}$-sbracket defined by

$$\{A,B\}_s:=(\Xi(A)\wedge\Xi(B))\rfloor\Omega,$$

where assuming that A and B are homogeneous in τ_α and are given by

$$A=\sum_{\alpha_1<\ldots<\alpha_{n-p}}\tau_{\alpha_1}\cdots\tau_{\alpha_{n-p}}A^{\alpha_1\cdots\alpha_{n-p}},$$

$$B=\sum_{\beta_1<\ldots<\beta_{n-q}}\tau_{\beta_1}\cdots\tau_{\beta_{n-q}}B^{\beta_1\cdots\beta_{n-q}},$$

$$\{A,B\}_s=\sum_{\alpha_1<\ldots<\alpha_{n-p}}\ \sum_{\beta_1<\ldots<\beta_{n-q}}\tau_{\alpha_1}\cdots\tau_{\alpha_{n-p}}\tau_{\beta_1}\cdots\tau_{\beta_{n-q}}\Xi(B^{\beta_1\cdots\beta_{n-q}})\rfloor\Xi(A^{\alpha_1\cdots\alpha_{n-p}})\rfloor\Omega.$$

Lemma 2 implies immediately that

$$d\{A,B\}_s = -[\xi_A,\xi_B]_s \rfloor \Omega,$$

where $\xi_A = \Xi(A)$, $\xi_B = \Xi(B)$ and the s-Lie bracket $[.,.]_s$ is defined for homogeneous forms A and B by $[\xi_A,\xi_B]_s f = \xi_A \rfloor d(\xi_B \rfloor df) + (-1)^{|A||B|+1}\xi_B \rfloor d(\xi_A \rfloor df)$ (here $|A|$ and $|B|$ are the homogeneity degrees in the variables τ_α). Furthermore, one can deduce easily from Lemma 3 the following relations for all homogeneous forms A, B and C in ${}^s\mathfrak{P}^{n-1}\mathcal{M}$:

$$\{A,B\}_s = (-1)^{|A||B|+1}\{B,A\}_s,$$

$$(-1)^{|A||C|}\{\{A,B\}_s,C\}_s + (-1)^{|B||A|}\{\{B,C\}_s,A\}_s + (-1)^{|C||B|}\{\{C,A\}_s,B\}_s$$
$$= (-1)^{|A||C|} d((\xi_A \wedge \xi_B \wedge \xi_C)\rfloor \Omega).$$

Hence ${}^s\mathfrak{P}^{n-1}\mathcal{M}$ has the structure of a graded Lie algebra modulo exact terms.

Now suppose that we can prove that for some forms $a \in \mathfrak{P}^{p-1}\mathcal{M}$ and $b \in \mathfrak{P}^{q-1}\mathcal{M}$, $\{{}^s a, {}^s b\}_s$ is equal to some ${}^s c$ where $c \in \mathfrak{P}^{p+q-n-1}\mathcal{M}$. Then we could define the *internal* $\mathfrak{p}$-bracket between a and b by $\{a,b\} := c$. This turns out actually to be true for a simple reason: all these brackets vanish by Proposition 2 which follows (except of course the case where $p=n$ or $q=n$). However, this fact is no longer true in general in the interesting case where we have constraints as shown in Sec. V C.

Lemma 5: For $1 \leqslant p < n$, $\mathfrak{P}^{p-1}\mathcal{M}$ *coincides with* $\Lambda^{p-1}T^\star(\mathcal{X}\times\mathcal{Y})$.

Proof: First step: let $1 \leqslant p < n$ and $a \in \mathfrak{P}^{p-1}\mathcal{M}$ and choose any $1 \leqslant \alpha_1 < \cdots < \alpha_{n-p} \leqslant n$, so that $dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a \in \mathfrak{P}^{n-1}\mathcal{M}$. Let us denote $\xi := \Xi(dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a)$. Decompose ξ:

$$\xi = \sum_\mu \xi^\mu \frac{\partial}{\partial q^\mu} + \sum_{\mu_1 < \ldots < \mu_n} \xi_{\mu_1 \ldots \mu_n} \frac{\partial}{\partial p_{\mu_1 \ldots \mu_n}}.$$

Then

$$-\xi\rfloor\Omega = -\sum_{\mu_1<\ldots<\mu_n} \xi_{\mu_1\ldots\mu_n} dq^{\mu_1}\wedge\cdots\wedge dq^{\mu_n} - \sum_\nu \xi^\nu$$
$$\times \sum_{\alpha=1}^{n} (-1)^\alpha \sum_{\substack{\mu_1<\cdots<\mu_n \\ \mu_\alpha=\nu}} dp_{\mu_1\ldots\mu_n}\wedge dq^{\mu_1}\wedge\ldots\wedge dq^{\mu_{\alpha-1}}\wedge dq^{\mu_{\alpha+1}}\wedge\ldots\wedge dq^{\mu_n}.$$

This expression should be equal to $(-1)^{n-p-1}dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge da$. Note that for any $1 \leqslant \nu \leqslant n+k$, there exist n integers $\mu_1<\cdots<\mu_n$ such that $\nu \in \{\mu_1,\ldots,\mu_n\}$ but $\alpha_1 \notin \{\mu_1,\ldots,\mu_n\}$. This forces $\xi^\nu = 0$. Hence we are left with

$$(-1)^{n-p-1}dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge da = -\sum_{\mu_1<\ldots<\mu_n} \xi_{\mu_1\ldots\mu_n} dq^{\mu_1}\wedge\cdots\wedge dq^{\mu_n},$$

which implies that a does not depend on the variables $p_{\mu_1\ldots\mu_n}$. Hence $a \in \Lambda^{p-1}T^\star(\mathcal{X}\times\mathcal{Y})$.

Second step: Conversely let $a \in \Lambda^{p-1}T^\star(\mathcal{X}\times\mathcal{Y})$. Then, for each $1 \leqslant \alpha_1 < \cdots < \alpha_{n-p} \leqslant n$, $dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a$ belongs to $\Lambda^{n-1}T^\star(\mathcal{X}\times\mathcal{Y})$, which is a subset of $\in \mathfrak{P}^{n-1}\mathcal{M}$ by Lemma 4. So $a \in \mathfrak{P}^{p-1}\mathcal{M}$. ■

Proposition 2: (a) *For* $1 \leqslant p,q < n$, $a \in \mathfrak{P}^{p-1}\mathcal{M}$ *and* $b \in \mathfrak{P}^{q-1}\mathcal{M}$ *the* $\mathfrak{p}$*-s bracket of* ${}^s a$ *with* ${}^s b$ *vanishes:* $\{{}^s a, {}^s b\}_s = 0$ *and hence the internal* $\mathfrak{p}$*-bracket* $\{a,b\}$ *exists and is equal to 0.*

(b) *For* $1 \leqslant p < n$, $a \in \mathfrak{P}^{n-1}\mathcal{M}$ *and* $b \in \mathfrak{P}^{p-1}\mathcal{M}$,

$$\{{}^s a, {}^s b\}_s = -{}^s(db)\Xi(a)(\tau) + {}^s\{a,b\}, \tag{31}$$

where $\{a,b\} = \Xi(a)\rfloor db$ *is the external* $\mathfrak{p}$*-bracket and*

$$\Xi(a)(\tau) := \sum_{\alpha} dx^{\alpha}(\Xi(a))\tau_{\alpha}.$$

(*It is actually a superfunction on* $\Pi T\mathcal{X}$.) *As a consequence, if* $dx^{\alpha}(\Xi(a))=0$, $\forall\alpha$, *the internal* $\mathfrak{p}$*-bracket* $\{a,b\}$ *exists and coincides with the external* $\mathfrak{p}$*-bracket*.

Remark: We think that the first term on the right-hand side of (31) does not play an essential role in our construction, which may be the case in other contexts. We believe that in a much more elaborate construction this term will not appear.

Proof: Case (a): By Lemma 5 a and b are in $\Lambda^{p-1}T^{\star}(\mathcal{X}\times\mathcal{Y})$ and $\Lambda^{q-1}T^{\star}(\mathcal{X}\times\mathcal{Y})$, respectively, so ${}^{s}a$ and ${}^{s}b$ are in $\mathcal{C}^{\infty}(\Pi T\mathcal{X})\otimes_{\mathcal{C}^{\infty}(\mathcal{X})}\Lambda^{n-1}T^{\star}(\mathcal{X}\times\mathcal{Y})$. Hence their $\mathfrak{p}$-sbracket vanishes by Proposition 1.

Let us consider the case b. Let us denote $\xi_a=\Xi(a)$ and write

$$\xi_a=\sum_{\mu}\xi_a^{\mu}\frac{\partial}{\partial q^{\mu}}+\sum_{\mu_1<\ldots<\mu_n}\xi_{a,\mu_1\ldots\mu_n}\frac{\partial}{\partial p_{\mu_1\ldots\mu_n}},$$

then

$$\begin{aligned}
\{a,{}^{s}b\}_s &= \sum_{\alpha_1<\ldots<\alpha_{n-p}}(-1)^{n-p}\tau_{\alpha_1}\ldots\tau_{\alpha_{n-p}}\xi_a\rfloor(dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge db)\\
&=(-1)^{n-p}\sum_{\alpha}\sum_{\alpha_1<\ldots<\alpha_{n-p}}\sum_{l=1}^{n-p}\delta_{\alpha}^{\alpha_l}\xi_a^{\alpha}\tau_{\alpha_l}\tau_{\alpha_1}\cdots\tau_{\alpha_{l-1}}\tau_{\alpha_{l+1}}\\
&\quad\cdots\tau_{\alpha_{n-p}}dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{l-1}}\wedge dx^{\alpha_{l+1}}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge db\\
&\quad+\sum_{\alpha_1<\ldots<\alpha_{n-p}}\tau_{\alpha_1}\cdots\tau_{\alpha_{n-p}}dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge(\xi_a\rfloor db)\\
&=(-1)^{n-p}\sum_{\alpha}\xi_a^{\alpha}\tau_{\alpha}\sum_{\alpha_1<\ldots<\alpha_{n-p-1}}\tau_{\alpha_1}\ldots\tau_{\alpha_{n-p-1}}dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p-1}}\wedge db+{}^{s}(\xi_a\rfloor db)\\
&=(-1)^{n-p}\sum_{\alpha}\xi_a^{\alpha}\tau_{\alpha}{}^{s}(db)+{}^{s}\{a,b\}.
\end{aligned}$$

And the claim is proved. ■

One simple example is the zero-form y^j. The associated s-form is

$${}^{s}y^j=\sum_{\alpha}y^j(-1)^{\alpha-1}\tau_1\cdots\tau_{\alpha-1}\tau_{\alpha+1}\cdots\tau_n\frac{\partial}{\partial x^{\alpha}}\rfloor\omega.$$

Since

$$d\,{}^{s}y^j=\sum_{\alpha}(-1)^{\alpha-1}\tau_1\cdots\tau_{\alpha-1}\tau_{\alpha+1}\cdots\tau_n\omega_{\alpha}^{j},$$

we have

$$\Xi({}^{s}y^j)=\sum_{\alpha}(-1)^{\alpha}\tau_1\cdots\tau_{\alpha-1}\tau_{\alpha+1}\cdots\tau_n\frac{\partial}{\partial p_j^{\alpha}}.$$

Let us compute the $\mathfrak{p}$-sbracket with $P_i=\partial/\partial y^i\rfloor\theta$:

$$\{P_i, {}^s y^j\}_s = \sum_\alpha (-1)^\alpha \tau_1 \cdots \tau_{\alpha-1}\tau_{\alpha+1}\cdots \tau_n \frac{\partial}{\partial p_j^\alpha} \rfloor \frac{\partial}{\partial y^i} \rfloor \Omega$$

$$= \sum_\alpha (-1)^{\alpha-1} \tau_1 \cdots \tau_{\alpha-1}\tau_{\alpha+1}\cdots \tau_n \delta_i^j \frac{\partial}{\partial x_\alpha} \rfloor \omega = {}^s\delta_i^j .$$

Thus

$$\{P_i, y^j\} = \delta_i^j .$$

D. Integral of an observable in $\mathfrak{P}^{p-1}\mathcal{M}$ and dynamical equations

Let Γ be a submanifold of dimension n on $\mathcal{M}$ and let D be be some oriented submanifold with boundary of dimension p $(1 \leqslant p \leqslant n)$ included in Γ. We consider D_Γ, the fiber bundle over D whose fiber at the point $m \in D$ is the oriented tangent space to Γ at m.

Definition 4: Let $a \in \mathfrak{P}^{p-1}\mathcal{M}$ and $\psi \in \Gamma(\mathcal{M}, \Lambda^n T^\star \mathcal{M})$. We define the $\mathfrak{p}$-bracket

$$\{\psi, {}^s a\}_s := -\Xi({}^s a) \rfloor d\psi = -\sum_{\alpha_1 < \cdots < \alpha_{n-p}} \tau_{\alpha_1} \cdots \tau_{\alpha_{n-p}} \Xi(dx^{\alpha_1} \wedge \ldots \wedge dx^{\alpha_{n-p}} \wedge a) \rfloor d\psi. \quad (32)$$

We define the integral of $\{\psi, {}^s a\}_s$ over D_Γ to be

$$\int_{D_\Gamma} \{\psi, {}^s a\}_s := -\int_D \sum_{\alpha_1 < \ldots < \alpha_{n-p}} (X_{\alpha_1} \wedge \cdots \wedge X_{\alpha_{n-p}} \wedge \Xi(dx^{\alpha_1} \wedge \cdots \wedge dx^{\alpha_{n-p}} \wedge a)) \rfloor d\psi, \quad (33)$$

where $X = X_1 \wedge \cdots \wedge X_n$ is the n-vector tangent to Γ at m such that $dx^\alpha(X_\beta) = \delta_\beta^\alpha$. Notice that this definition does not depend on the parametrization which is used.

Theorem 3: *Assume that Γ is the graph of some solution of the Hamilton equations (19). Then for any $a \in \mathfrak{P}^{p-1}\mathcal{M}$,*

$$\int_D da = \int_{D_\Gamma} \{\mathcal{H}\omega, {}^s a\}_s . \quad (34)$$

Proof: We can always assume that D is the image of some parametrization

$$\Delta \to D,$$

$$t \mapsto \mathcal{U}(x(t)) = (x(t), u(t), p(t)),$$

where Δ is an open subset of $\mathbb{R}^p$. Then

$$\int_{D\Gamma} \{\mathcal{H}\omega, {}^s a\}_s$$

$$= \int_\Delta - \sum_{\alpha_1 < \ldots < \alpha_{n-p}} (X_{\alpha_1} \wedge \cdots \wedge X_{\alpha_{n-p}} \wedge \Xi(dx^{\alpha_1} \wedge \cdots \wedge dx^{\alpha_{n-p}} \wedge a)) \rfloor d\mathcal{H}$$

$$\wedge \omega\left(\frac{\partial \mathcal{U} \circ x}{\partial t^1}, \ldots, \frac{\partial \mathcal{U} \circ x}{\partial t^p}\right) dt^1 \wedge \cdots \wedge dt^p$$

$$= \int_\Delta - \sum_{\alpha_1 < \ldots < \alpha_{n-p}} \sum_{\beta_1 < \ldots < \beta_p} d\mathcal{H} \wedge \omega(X_{\alpha_1}, \ldots, X_{\alpha_{n-p}}, \Xi(dx^{\alpha_1} \wedge \ldots \wedge dx^{\alpha_{n-p}} \wedge a),$$

$$\times X_{\beta_1}, \ldots, X_{\beta_p}) \det\left(\frac{\partial x^{\beta_1}}{\partial t^1}, \ldots, \frac{\partial x^{\beta_p}}{\partial t^p}\right) dt^1 \wedge \cdots \wedge dt^p .$$

Now by using (19),

$$\begin{aligned}
&\int_{D_\Gamma}\{\mathcal{H}\omega,{}^s a\}_s\\
&\quad=\int_\Delta(-1)^{n-p+1}\sum_{\alpha_1<\ldots<\alpha_{n-p}}\sum_{\beta_1<\ldots<\beta_p}\Omega(\Xi(dx^{\alpha_1}\\
&\qquad\wedge\ldots\wedge dx^{\alpha_{n-p}}\wedge a),X_{\alpha_1},\ldots,X_{\alpha_{n-p}},X_{\beta_1},\ldots,X_{\beta_p})\det\left(\frac{\partial x^{\beta_1}}{\partial t^1},\ldots,\frac{\partial x^{\beta_p}}{\partial t^p}\right)dt^1\wedge\cdots\wedge dt^p\\
&\quad=\int_\Delta\sum_{\alpha_1<\ldots<\alpha_{n-p}}\sum_{\beta_1<\ldots<\beta_p}dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge da(X_{\alpha_1},\ldots,X_{\alpha_{n-p}},X_{\beta_1},\ldots,X_{\beta_p})\\
&\qquad\times\det\left(\frac{\partial x^{\beta_1}}{\partial t^1},\ldots,\frac{\partial x^{\beta_p}}{\partial t^p}\right)dt^1\wedge\cdots\wedge dt^p\\
&\quad=\int_\Delta\sum_{\beta_1<\ldots<\beta_p}da(X_{\beta_1},\ldots,X_{\beta_p})\det\left(\frac{\partial x^{\beta_1}}{\partial t^1},\ldots,\frac{\partial x^{\beta_p}}{\partial t^p}\right)dt^1\wedge\cdots\wedge dt^p=\int_D da.
\end{aligned}$$

■

There exists, however, a much simpler concept of a bracket between $\mathcal{H}\omega$ and observables in $\mathfrak{P}^{p-1}\mathcal{M}$ which is also suitable for the dynamical equation in most cases. Namely we call a form a in $\mathfrak{P}^{p-1}\mathcal{M}$ an *admissible* form if $\forall\,\alpha_1<\cdots<\alpha_{n-p}$,

$$\begin{gathered}
dx^\alpha(\Xi(dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a))=0,\quad\forall\,\alpha\\
\text{or equivalently}\quad dx^\alpha(\Xi({}^s a))=0,\quad\forall\,\alpha.
\end{gathered}\tag{35}$$

The reader may wonder about the meaning of this definition since, in view of Lemma 5, all forms in $\mathfrak{P}^{p-1}\mathcal{M}$ are admissible for $p<n$. Again the point is that we may encounter variational problems with gauge symmetry and constraints for which nonadmissible forms exist in $\mathfrak{P}^{p-1}\mathcal{M}$.

Definition 5: Assume that $a\in\mathfrak{P}^{p-1}\mathcal{M}$ satisfies (35) and let $\psi\in\Gamma(\mathcal{M},\Lambda^n T^\star\mathcal{M})$. Then we define the $\mathfrak{p}$*-bracket*

$$\{\psi,a\}:=-\sum_{\alpha_1<\ldots<\alpha_{n-p}}\frac{\partial}{\partial x^{\alpha_1}}\wedge\cdots\wedge\frac{\partial}{\partial x^{\alpha_{n-p}}}\wedge\Xi(dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a)\rfloor d\psi.$$

Lemma 6: Let $a\in\mathfrak{P}^{p-1}\mathcal{M}$ be an admissible form [i.e., such that (35) holds] and let Γ be an n-dimensional submanifold of $\mathcal{M}$ which is a graph over $\mathcal{X}$. Then for any oriented submanifold D of dimension p included in Γ,

$$\int_{D_\Gamma}\{\mathcal{H}\omega,{}^s a\}_s=\int_D\{\mathcal{H}\omega,a\}.\tag{36}$$

Proof: We use the same notations as in the proof of Theorem 3. Because of the condition (35),

$$\sum_{\alpha_1<\ldots<\alpha_{n-p}} d\mathcal{H}\wedge\omega(X_{\alpha_1},\ldots,X_{\alpha_{n-p}},\Xi(dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a),X_{\beta_1},\ldots,X_{\beta_{n-p}})$$

$$=\sum_{\alpha_1<\ldots<\alpha_{n-p}} (-1)^{n-p} d\mathcal{H}(\Xi(dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a))\omega(X_{\alpha_1},\ldots,X_{\alpha_{n-p}},X_{\beta_1},\ldots,X_{\beta_{n-p}})$$

$$=\sum_{\alpha_1<\ldots<\alpha_{n-p}} (-1)^{n-p} d\mathcal{H}(\Xi(dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a))\omega$$

$$\times\left(\frac{\partial}{\partial x^{\alpha_1}},\ldots,\frac{\partial}{\partial x^{\alpha_{n-p}}},X_{\beta_1},\ldots,X_{\beta_{n-p}}\right)$$

$$=\sum_{\alpha_1<\ldots<\alpha_{n-p}} d\mathcal{H}\wedge\omega\left(\frac{\partial}{\partial x^{\alpha_1}},\ldots,\frac{\partial}{\partial x^{\alpha_{n-p}}},\Xi(dx^{\alpha_1}\wedge\cdots\wedge dx^{\alpha_{n-p}}\wedge a),X_{\beta_1},\ldots,X_{\beta_{n-p}}\right)$$

$$=-\sum_{\alpha_1<\ldots<\alpha_{n-p}} \{\mathcal{H}\omega,a\}(X_{\beta_1},\ldots,X_{\beta_{n-p}}).$$

This implies the result by summation over $\beta_1<\cdots<\beta_{n-p}$ and integration over D. ■

Corollary 1: Let $a\in\mathfrak{P}^{p-1}\mathcal{M}$ be an admissible form and let Γ be an n-dimensional submanifold of $\mathcal{M}$ which is a graph over $\mathcal{X}$ of a solution of the Hamilton equations (19). Then for any oriented submanifold D of dimension p included in Γ,

$$\int_D \{\mathcal{H}\omega,a\}=\int_D da. \tag{37}$$

Examples: The zero-form y^i and the one-form $y^i dy^j$ are admissible and

$$\{\mathcal{H}\omega,y^i\}=\sum_\alpha \frac{\partial\mathcal{H}}{\partial p_i^\alpha}\,dx^\alpha,$$

$$\{\mathcal{H}\omega,y^i dy^j\}=\sum_{\alpha<\beta} \frac{\partial\mathcal{H}}{\partial p_{ij}^{\alpha\beta}}\,dx^\alpha\wedge dx^\beta.$$

E. Noether theorem

It is natural to relate the Noether theorem to the pataplectic structure.

Let ξ be a tangent vector field on $\mathcal{X}\times\mathcal{Y}$. The ξ will be an infinitesimal symmetry of the variational problem if

$$\mathcal{L}_{\Xi(P_\xi)}(\theta-\mathcal{H}\omega)=0,$$

since then the integral $\int_\Gamma\theta-\mathcal{H}\omega$ is invariant under the action of the flow of ξ. Then for any solution $x\mapsto(U(x),p(x))$, of the Hamilton equations, the form $P_\xi^\star$ is closed along the graph of this solution. This means that if Γ is the graph of (U,p),

$$dP^\star_{\xi|\Gamma}=d(\xi](\theta-\mathcal{H}\omega))_{|\Gamma}=0.$$

This is a direct consequence of Theorem 2 and of the following calculation.

Lemma 7: For any section ξ of $\Gamma(\mathcal{X}\times\mathcal{Y},T(\mathcal{X}\times\mathcal{Y}))$, we have the relation

$$\{\mathcal{H}\omega,P_\xi\}=\mathcal{L}_{\Xi(P_\xi)}(\theta-\mathcal{H}\omega)+d(\xi]\mathcal{H}\omega). \tag{38}$$

Proof: Using the definition of $\{\mathcal{H}\omega,P_\xi\}$, we have

$$\mathcal{L}_{\Xi(P_\xi)}(\theta-\mathcal{H}\omega)=\Xi(P_\xi)\rfloor(d\theta-d\mathcal{H}\wedge\omega)+d(\Xi(P_\xi)\rfloor(\theta-\mathcal{H}\omega))=\Xi(P_\xi)\rfloor\Omega-\Xi(P_\xi)\rfloor d\mathcal{H}\wedge\omega$$
$$+d(\xi\rfloor\theta-\xi\rfloor\mathcal{H}\omega)=-dP_\xi+\{\mathcal{H}\omega,P_\xi\}+d(P_\xi-\xi\rfloor\mathcal{H}\omega),$$

and the result follows. ■

Remark 1: It appears that it will be interesting to study solutions of the Hamilton equations with the constraint $\mathcal{H}=0$. This is possible, because of the freedom left in the Legendre correspondence, thanks to the parameter ϵ. The advantage is that then the energy-momentum observables are described by $P_{a,g}$ which belongs to $\mathfrak{P}^{n-1}\mathcal{M}$.

Remark 2: As a consequence of these observations it is clear that on the submanifold $\mathcal{H}=0$, the set of Noether currents can be identified with $\mathfrak{P}_P^{n-1}\mathcal{M}$. So we can interpret the results of Proposition 1 concerning $\mathfrak{P}_P^{n-1}\mathcal{M}$ by saying that the set of Noether currents equipped with the $\mathfrak{p}$-bracket is a representation modulo exact terms of the Lie algebra of vector fields on $\mathcal{X}\times\mathcal{Y}$ with the Lie bracket. We recover thus various constructions of brackets on Noether currents (see for instance, Ref. 18).

V. EXAMPLES

We present here some examples from mathematical physics in order to illustrate our formalism. We shall see that, by allowing variants of the above theory, one can find formalisms which are more adapted to some special situations.

A. Interacting scalar fields

As the simplest example, consider a system of interacting scalar fields $\{\phi^1,\ldots,\phi^k\}$ on an oriented (pseudo-)Riemannian manifold $(\mathcal{X},g)$. One should keep in mind that $\mathcal{X}$ is a four-dimensional space–time and $g_{\alpha\beta}$ is a Minkowski metric. These fields can be seen as a map ϕ from $\mathcal{X}$ to $\mathbb{R}^k$ with its standard Euclidian structure. The metric g on $\mathcal{X}$ induces a volume form which reads in local coordinates

$$\omega:=g\,dx^1\wedge\cdots\wedge dx^n,\quad \text{where}\quad g:=\sqrt{|\det g_{\alpha\beta}(x)|}.$$

Let $V:\mathcal{X}\to\mathbb{R}^k$ be the interaction potential of the fields. Then the Lagrangian density is

$$L(x,\phi,d\phi):=\frac{1}{2}g^{\alpha\beta}(x)\frac{\partial\phi^i}{\partial x^\alpha}\frac{\partial\phi_i}{\partial x^\beta}-V(\phi(x)).$$

Here $\phi_i=\phi^i$ and we assume that we sum over all repeated indices. Alternatively one could work with the volume form being $dx^1\wedge\cdots\wedge dx^n$ and the Lagrangian density being gL, in order to apply directly the theory constructed in the previous sections. But we shall not choose this approach here and use a variant which makes clear the covariance of the problem.

We restrict ourselves to the Weyl theory, i.e., we work on the the submanifold $\mathcal{M}_{\text{Weyl}}$, as in Sec. II G. So we introduce the momentum variables ϵ and p_i^α and we start from the Cartan form,

$$\theta=\epsilon\omega+p_i^\alpha d\phi^i\wedge\omega_\alpha,$$

where $\omega_\alpha:=\partial_\alpha\rfloor\omega$. But here ω_α is not closed in general (because g is not constant), so

$$\Omega=d\theta=d\epsilon\wedge\omega+dp_i^\alpha\wedge d\phi^i\wedge\omega_\alpha-p_i^\alpha\frac{1}{g}\frac{\partial g}{\partial x^\alpha}d\phi^i\wedge\omega.$$

The Legendre transform is given by

$$p_i^\alpha=\frac{\partial L}{\partial(\partial_\alpha\phi^i)}=g^{\alpha\beta}\frac{\partial\phi^i}{\partial x^\beta}\Leftrightarrow\frac{\partial\phi^i}{\partial x^\alpha}=g_{\alpha\beta}p_i^\beta,$$

and the Hamiltonian is

$$\mathcal{H}(x,\phi,p)=\epsilon+\tfrac{1}{2}g_{\alpha\beta}p_i^\alpha p_i^\beta+V(\phi).$$

We use as conjugate variables the zero-forms ϕ^j and the $(n-1)$-forms

$$P_{i,f}:=f(x)p_i^\alpha\omega_\alpha=f(x)\frac{\partial}{\partial\phi^i}\rfloor\theta\in\mathfrak{P}^{n-1}\mathcal{M}_{\text{Weyl}}.$$

Taking account of the fact that ω_α is not closed, one finds

$$\Xi(P_{i,f})=f\frac{\partial}{\partial\phi^i}-\frac{\partial f}{\partial x^\alpha}p_i^\alpha\frac{\partial}{\partial\epsilon}$$

and

$$\{P_{i,f},\phi^j\}=\Xi(P_{i,f})\rfloor d\phi^j=f\delta_i^j.$$

Also the observables ϕ^j are admissible: $\Xi({}^s\phi^j)=\Sigma_\alpha(-1)^\alpha/g\ \tau_1\ldots\tau_{\alpha-1}\tau_{\alpha+1}\ldots\tau_n\,\partial/\partial p_j^\alpha$, and, according to Definition 5,

$$\{\mathcal{H}\omega,\phi^j\}=\frac{\partial\mathcal{H}}{\partial p_j^\alpha}dx^\alpha=g_{\alpha\beta}p_j^\beta dx^\alpha.$$

Moreover,

$$\{\mathcal{H}\omega,P_{i,f}\}=-\Xi(P_{i,f})\rfloor d(\mathcal{H}\omega)=\left(-f\frac{\partial V}{\partial\phi^i}+\frac{\partial f}{\partial x^\alpha}p_i^\alpha\right)\omega.$$

The dynamical equations are those along the graph of a solution,

$$\mathbf{d}\phi^i=\{\mathcal{H}\omega,\phi^i\}=g_{\alpha\beta}p_i^\beta dx^\alpha,$$

$$\mathbf{d}(fp_i^\alpha\omega_\alpha)=\{\mathcal{H}\omega,P_{i,f}\}=\left(-f\frac{\partial V}{\partial\phi^i}+\frac{\partial f}{\partial x^\alpha}p_i^\alpha\right)\omega.$$

The second equation gives

$$\frac{f}{g}\left(\frac{\partial g}{\partial x^\alpha}p_i^\alpha+g\frac{\partial p_i^\alpha}{\partial x^\alpha}+g\frac{\partial V}{\partial\phi^i}\right)=0, \tag{39}$$

while the first relation gives $\partial\phi^i/\partial x^\alpha=g_{\alpha\beta}p_i^\beta$. By substitution in (39) we find

$$\frac{1}{g}\frac{\partial}{\partial x^\alpha}\left(g\,g^{\alpha\beta}\frac{\partial\phi^i}{\partial x^\beta}\right)+\frac{\partial V}{\partial\phi^i}=0,$$

the Euler–Lagrange equations of the problem.

B. Conformal string theory

We consider maps u from a two-dimensional (pseudo-)Riemannian manifold $(\mathcal{X},g)$ with values in another (pseudo-)Riemannian manifold $(\mathcal{Y},h)$ of arbitrary dimension. The most general bosonic action for such maps is $\mathcal{L}[u]:=\int_{\mathcal{X}}L(x,u,du)\omega$ with $\omega:=g(x)dx^1\wedge dx^2$ and $g(x):=\sqrt{|\det g_{\alpha\beta}(x)|}$ as before, and

$$L(x,u,du) := \frac{1}{2}\left(h_{ij}(u(x))g^{\alpha\beta}(x) + b_{ij}(u(x))\frac{\epsilon^{\alpha\beta}}{g(x)}\right)\frac{\partial u^i}{\partial x^\alpha}\frac{\partial u^j}{\partial x^\beta},$$

where $b := \Sigma_{i<j} b_{ij}(y)dy^i \wedge dy^j$ is a given two-form on $\mathcal{Y}$ and $\epsilon^{12} = -\epsilon^{21} = 1$, $\epsilon^{11} = \epsilon^{22} = 0$. Hence

$$\mathcal{L}[u] = \int_{\mathcal{X}} \frac{1}{2} h_{ij}(u) g^{\alpha\beta}(x) \frac{\partial u^i}{\partial x^\alpha}\frac{\partial u^j}{\partial x^\beta}\omega + u^\star b.$$

Setting

$$G_{ij}^{\alpha\beta}(x,y) := h_{ij}(y)g^{\alpha\beta}(x) + b_{ij}(y)\frac{\epsilon^{\alpha\beta}}{g(x)} = G_{ji}^{\beta\alpha}(x,y),$$

we see that $L(x,u,du) = 1/2\, G_{ij}^{\alpha\beta}(x,u)(\partial u^i/\partial x^\alpha)(\partial u^j/\partial x^\beta)$ and the Euler–Lagrange equation for this functional is

$$\frac{1}{g}\frac{\partial}{\partial x^\alpha}\left(g\, G_{ij}^{\alpha\beta}(x,u(x))\frac{\partial u^j}{\partial x^\beta}\right) = \frac{\partial G_{jk}^{\beta\gamma}}{\partial y^i}\frac{\partial u^j}{\partial x^\beta}\frac{\partial u^k}{\partial x^\gamma}. \tag{40}$$

More covariant formulations exists for the case $b = 0$, which correspond to the harmonic map equation or when the metric on $\mathcal{X}$ is Riemannian using conformal coordinates and complex variables (see Ref. 10). The Cartan–Poincaré form on $\mathcal{M}$ is

$$\theta := \epsilon\omega + \sum_{\alpha,i} p_i^\alpha \omega_\alpha^i + \sum_{i<j} p_{ij}\omega_{12}^{ij}$$

(where $\omega_1^i = g\, dy^i \wedge dx^2$, $\omega_2^i = g\, dx^1 \wedge dy^i$ and $\omega_{12}^{ij} = g\, dy^i \wedge dy^j$). The pataplectic form is

$$\Omega = d\theta = d\epsilon\wedge\omega + \sum_{\alpha,i} dp_i^\alpha \wedge \omega_\alpha^i + \sum_{i<j} dp_{ij}\wedge\omega_{12}^{ij} - \sum_{\alpha,i}\frac{p_i^\alpha}{g}\frac{\partial g}{\partial x^\alpha}dy^i\wedge\omega$$
$$+ \sum_{i<j}\sum_\alpha p_{ij}\frac{\partial g}{\partial x^\alpha}dx^\alpha\wedge dy^i\wedge dy^j.$$

The Legendre correspondence is generated by the function

$$W(x,u,v,p) := \epsilon + p_i^\alpha v_\alpha^i + p_{ij}v_1^i v_2^j - L(x,u,v) = \epsilon + p_i^\alpha v_\alpha^i - \tfrac{1}{2}M_{ij}^{\alpha\beta}(x,y,p)v_\alpha^i v_\beta^j,$$

where we have denoted

$$M_{ij}^{\alpha\beta}(x,y,p) := h_{ij}(y)g^{\alpha\beta}(x) + \left(\frac{b_{ij}(y)}{g(x)} - p_{ij}\right)\epsilon^{\alpha\beta} = G_{ij}^{\alpha\beta}(x,y) - p_{ij}\epsilon^{\alpha\beta}.$$

This correspondence is given by the relation $\partial W/\partial v_\alpha^i = 0$ which gives

$$M_{ij}^{\alpha\beta}(x,y,p)v_\beta^j = p_i^\alpha. \tag{41}$$

Thus, given (x,y,p), finding (x,y,v,w) such that $(x,u,v,w)\leftrightarrow(x,y,p)$ amounts to solving first the linear system (41) for v and then w is just $W(x,y,v,p)$. This system has a solution in general in the open subset $\mathcal{O}$ of $\mathcal{M}$ on which the matrix

$$M=\begin{pmatrix} h_{ij}(y)g^{11}(x) & h_{ij}(y)g^{12}(x)+\dfrac{b_{ij}(y)}{g(x)}-p_{ij} \\ h_{ij}(y)g^{21}(x)-\dfrac{b_{ij}(y)}{g(x)}+p_{ij} & h_{ij}(y)g^{22}(x) \end{pmatrix}$$

is invertible. We remark that $\mathcal{O}$ contains actually the submanifold $\mathcal{R}:=\{(x,y,p)\in\mathcal{M}/g(x)p_{ij}=b_{ij}(y)\}$, so that the Legendre correspondence induces a diffeomorphism between $T\mathcal{Y}\otimes T^{\star}\mathcal{X}$ and $\mathcal{R}$.

We shall need to define on $\mathcal{O}$ the inverse of M, i.e., $K^{ij}_{\alpha\beta}(x,y,p)$ such that

$$K^{ij}_{\alpha\beta}(x,y,p)M^{\beta\gamma}_{jk}(x,y,p)=\delta^i_k\delta^\gamma_\alpha. \tag{42}$$

Now we can express the solution of (41) by

$$v^i_\alpha=K^{ij}_{\alpha\beta}(x,y,p)p^\beta_j, \tag{43}$$

and the Hamiltonian function is

$$\mathcal{H}(x,y,p):=\epsilon+\tfrac{1}{2}K^{ij}_{\alpha\beta}(x,y,p)p^\alpha_i p^\beta_j.$$

We use as conjugate variables the position functions y^i and the momentum one-forms

$$P_i:=\frac{\partial}{\partial y^i}\rfloor\theta=p^\alpha_i\omega_\alpha+gp_{ij}dy^j.$$

The Poisson brackets are obtained as follows. First, concerning $\{\mathcal{H}\omega,y^i\}$, we compute $\Xi({}^sy^i)=(1/g)(\tau_1\,\partial/\partial p^2_i-\tau_2\,\partial/\partial p^1_i)$. Since $dx^\alpha(\Xi({}^sy^i))=0$, $\forall\alpha$,

$$\{\mathcal{H}\omega,y^i\}=-\frac{1}{g}\left(\frac{\partial}{\partial x^1}\wedge\frac{\partial}{\partial p^2_i}-\frac{\partial}{\partial x^2}\wedge\frac{\partial}{\partial p^1_i}\right)\rfloor d\mathcal{H}\wedge\omega=\frac{\partial\mathcal{H}}{\partial p^\alpha_i}dx^\alpha=K^{ij}_{\alpha\beta}p^\beta_j dx^\alpha.$$

Next we compute dP_i:

$$dP_i=dp^\alpha_i\wedge\omega_\alpha+gdp_{ij}\wedge dy^j+p^\alpha_i\frac{\partial g}{\partial x^\alpha}\frac{\omega}{g}+p_{ij}\frac{\partial g}{\partial x^\alpha}dx^\alpha\wedge dy^j=-\frac{\partial}{\partial y^i}\rfloor\Omega.$$

Hence

$$\Xi(P_i)=\frac{\partial}{\partial y^i}.$$

Because of $dx^\alpha(\Xi(P_i))=0$, $\forall\alpha$, and of Proposition 2 we deduce that

$$\{P_i,y^j\}=\Xi(P_i)\rfloor dy^j=\delta^j_i,$$

$$\{\mathcal{H}\omega,P_i\}=-\Xi(P_i)\rfloor d(\mathcal{H}\omega)=-\frac{\partial K^{jk}_{\alpha\beta}}{\partial y^i}p^\alpha_j p^\beta_k\omega.$$

Notice that, because of (42),

$$\frac{\partial K^{jk}_{\alpha\beta}}{\partial y^i}=-K^{jl}_{\alpha\gamma}\frac{\partial M^{\gamma\delta}_{lm}}{\partial y^i}K^{mk}_{\delta\beta},$$

and thus

$$\{\mathcal{H}\omega, P_i\} = \frac{\partial M_{lm}^{\gamma\delta}}{\partial y^i} K_{\alpha\gamma}^{jl} K_{\delta\beta}^{mk} p_j^\alpha p_k^\beta \omega.$$

The equations of motion are

$$\begin{aligned} \mathbf{d}y^i &= \{\mathcal{H}\omega, y^i\} = K_{\alpha\beta}^{ij} p_j^\beta dx^\alpha, \\ \mathbf{d}P_i &= \{\mathcal{H}\omega, P_i\} = \frac{\partial M_{lm}^{\gamma\delta}}{\partial y^i} K_{\alpha\gamma}^{jl} K_{\delta\beta}^{mk} p_j^\alpha p_k^\beta \omega, \end{aligned} \tag{44}$$

along the graph Γ of any solution of the Hamilton equations. From the first equation we deduce that

$$\frac{\partial y^i}{\partial x^\alpha} = K_{\alpha\beta}^{ij} p_j^\beta \Leftrightarrow p_i^\alpha = M_{ij}^{\alpha\beta} \frac{\partial y^j}{\partial x^\beta}. \tag{45}$$

Now using (45) we see that along Γ,

$$\begin{aligned} P_{i|\Gamma} = (p_i^\alpha \omega_\alpha + g p_{ij} dy^j)_{|\Gamma} &= \left(M_{ij}^{\alpha\beta} \frac{\partial y^j}{\partial x^\beta} + p_{ij} \epsilon^{\alpha\beta} \frac{\partial y^j}{\partial x^\beta} \right) \omega_\alpha \\ &= G_{ij}^{\alpha\beta} \frac{\partial y^j}{\partial x^\beta} \omega_\alpha = \left(h_{ij} g^{\alpha\beta} + \frac{b_{ij}}{g} \epsilon^{\alpha\beta} \right) \frac{\partial y^j}{\partial x^\beta} \omega_\alpha, \end{aligned}$$

and so the left-hand side of the second equation of (44) is

$$dP_{i|\Gamma} = \frac{1}{g} \frac{\partial}{\partial x^\alpha} \left[g G_{ij}^{\alpha\beta} \frac{\partial y^j}{\partial x^\beta} \right] \omega.$$

And still using (45) the right-hand side of the second equation of (44) along Γ is

$$\frac{\partial M_{jk}^{\alpha\beta}}{\partial y^i} \frac{\partial y^j}{\partial x^\alpha} \frac{\partial y^k}{\partial x^\beta} \omega.$$

Hence we recover the Euler–Lagrange equation (40).

C. The electromagnetic field

Here the field is a one-form $A = A_\alpha dx^\alpha$ defined on the (pseudo-)Riemannian manifold $\mathcal{X}$ [which can also be thought of as a connection one-form on a U(1)-bundle]. Its differential $dA := F$ is the electromagnetic field. We still denote $g_{\alpha\beta}$ the metric on $\mathcal{X}$ and $\omega = g dx^1 \wedge \cdots \wedge dx^n$ the volume form. We are given some vector field $\vec{J} = j^\alpha \partial_\alpha$ on $\mathcal{X}$ (the electric current field) and we define the Lagrangian density by

$$L(x, A, dA) := -\tfrac{1}{4} F_{\alpha\beta} F^{\alpha\beta} - j^\alpha A_\alpha,$$

where $F_{\alpha\beta} := \partial_\alpha A_\beta - \partial_\beta A_\alpha$ and $F^{\alpha\beta} := g^{\alpha\gamma} g^{\beta\delta} F_{\gamma\delta}$.

The Euler–Lagrange equation could be written

$$\frac{1}{g} \frac{\partial}{\partial x^\alpha} (g F^{\alpha\beta}) \omega_\beta = j^\beta \omega_\beta, \tag{46}$$

or using the notations

$$\star F := \sum_{\alpha<\beta} F^{\alpha\beta} \frac{\partial}{\partial x^\alpha} \rfloor \frac{\partial}{\partial x^\beta} \rfloor \omega \quad \text{and} \quad j := j^\alpha \omega_\alpha ,$$
$$d(\star F) = j. \tag{47}$$

We remark that in order to have solutions it is necessary to suppose that $dj=0$, which is the electric charge conservation law. [Note also that by writing the electromagnetic functional $\int 1/2 F\wedge\star F - A\wedge j$, one sees immediately that the condition $dj=0$ ensures that this functional is invariant by gauge transformations $A\mapsto A+df$ up to the addition of $\int d(fj)$.]

In our framework the fact that the field is a one-form means that we replace the configuration space $\mathcal{X}\times\mathcal{Y}$ by $T^\star\mathcal{X}$. Thus the pataplectic manifold is $\mathcal{M} := \Lambda^n T^\star(T^\star\mathcal{X})$. We shall here restrict to the "Weyl" submanifold of $\mathcal{M}$ (see Sec. II G) which is described by

$$\mathcal{M}_{\text{Weyl}} := \{(x,A,p)/x\in\mathcal{X}, A\in T^\star_x\mathcal{X}, p\in\Lambda^n T^\star_{(x,A)}(T^\star\mathcal{X}), \partial_{A_\alpha}\wedge\partial_{A_\beta}\rfloor p=0, \forall\,\alpha,\beta\}.$$

The latter condition on p means that in local coordinates, $p=\epsilon\omega+\Sigma_{\alpha,\beta}p^{A_\alpha\beta}dA_\alpha\wedge\omega_\beta$. The Cartan form is

$$\theta := \epsilon\omega + \sum_{\alpha,\beta} p^{A_\alpha\beta} dA_\alpha\wedge\omega_\beta ,$$

with still $\omega_\beta := \partial_\beta\rfloor\omega$, and the pataplectic form is

$$\Omega := d\theta = d\epsilon\wedge\omega + \sum_{\alpha,\beta} dp^{A_\alpha\beta}\wedge dA_\alpha\wedge\omega_\beta - \sum_{\alpha,\beta} p^{A_\alpha\beta}\frac{1}{g}\frac{\partial g}{\partial x^\beta} dA_\alpha\wedge\omega.$$

Computing the Legendre transform in $\mathcal{M}_{\text{Weyl}}$, using $W(x,A,dA,p)=\epsilon+\Sigma_{\alpha,\beta}p^{A_\alpha\beta}\partial_\beta A_\alpha - L(x,A,dA)$, gives the momenta

$$p^{A_\alpha\beta} := \frac{\partial L}{\partial(\partial_\beta A_\alpha)} = F^{\alpha\beta}.$$

We see that the Legendre transform works only provided the compatibility condition

$$p^{A_\alpha\beta} + p^{A_\beta\alpha} = 0 \tag{48}$$

is satisfied. It is an example of a Dirac primary constraint. Henceforth we shall be restricted to the submanifold

$$\mathcal{M}_{\text{Maxwell}} := \{(x,A,p)\in\mathcal{M}_{\text{Weyl}}/p^{A_\alpha\beta}+p^{A_\beta\alpha}=0\},$$

along which we are able to obtain an expression for the Hamiltonian

$$\mathcal{H}(x,A,p) = \epsilon - \tfrac{1}{4} g_{\alpha\gamma} g_{\beta\delta} p^{A_\alpha\beta} p^{A_\gamma\delta} + j^\alpha A_\alpha .$$

A naive use of this Hamiltonian function leads to incorrect dynamical equations. Another possibility, which was already proposed in Ref. 16, is to use the one-form on $\mathcal{M}_{\text{Maxwell}}$ as dynamical variable

$$A := A_\alpha dx^\alpha .$$

Note that here A_α is not a local function of x but fiber coordinate. Then, as it will be proved below, the momentum variable canonically conjugate to A may be chosen to be the $(n-2)$-form

$$\pi := \frac{1}{2}\sum_{\alpha,\beta} p^{A_\alpha\beta}\frac{\partial}{\partial x^\alpha}\rfloor\frac{\partial}{\partial x^\beta}\rfloor\omega.$$

Its associated s-form is

$${}^s\pi = \frac{1}{2}\sum_{\alpha,\beta} p^{A_\alpha\beta}\left(\tau_\alpha\frac{\partial}{\partial x^\beta} - \tau_\beta\frac{\partial}{\partial x^\alpha}\right)\rfloor\omega = \sum_{\alpha,\beta} p^{A_\alpha\beta}\tau_\alpha\frac{\partial}{\partial x^\beta}\rfloor\omega.$$

Hence, using (48),

$$d\,{}^s\pi = \sum_{\alpha,\beta}\tau_\alpha dp^{A_\alpha\beta}\wedge\left(\frac{\partial}{\partial x^\beta}\rfloor\omega\right) + \sum_{\alpha,\beta}\frac{p^{A_\alpha\beta}}{g}\tau_\alpha\frac{\partial g}{\partial x^\beta}\omega = -\sum_\alpha \tau_\alpha\frac{\partial}{\partial A_\alpha}\rfloor\Omega$$

and

$$\Xi({}^s\pi) = \sum_\alpha \tau_\alpha\frac{\partial}{\partial A_\alpha}.$$

We also have (denoting $\omega_\beta := \partial/\partial x^\beta\rfloor\omega$ and $\tau_{1\ldots\ldots n}^{\ldots\alpha\ldots\beta\ldots} := \tau_1\cdots\tau_{\alpha-1}\tau_{\alpha+1}\cdots\tau_{\beta-1}\tau_{\beta+1}\cdots\tau_n$)

$${}^sA = \sum_{\alpha<\beta}(-1)^{n+\alpha+\beta}\frac{A_\alpha}{g}\tau_{1\ldots\ldots n}^{\ldots\alpha\ldots\beta\ldots}\omega_\beta - \sum_{\beta<\alpha}(-1)^{n+\alpha+\beta}\frac{A_\alpha}{g}\tau_{1\ldots\ldots n}^{\ldots\beta\ldots\alpha\ldots}\omega_\beta$$

and

$$\Xi({}^sA) = \sum_{\alpha<\beta}(-1)^{n+\alpha+\beta+1}\frac{A_\alpha}{g}\tau_{1\ldots\ldots n}^{\ldots\alpha\ldots\beta\ldots}\frac{\partial}{\partial p^{A_\alpha\beta}} - \sum_{\beta<\alpha}(-1)^{n+\alpha+\beta+1}\frac{A_\alpha}{g}\tau_{1\ldots\ldots n}^{\ldots\beta\ldots\alpha\ldots}\frac{\partial}{\partial p^{A_\alpha\beta}}.$$

A computation using (48) gives

$$\begin{aligned}\{{}^s\pi, {}^sA\}_s &= \sum_{\alpha,\beta,\gamma}(-1)^{n+\alpha+\beta+1}\tau_\gamma\left(\sum_{\alpha<\beta}\frac{A_\alpha}{g}\tau_{1\ldots\ldots n}^{\ldots\alpha\ldots\beta\ldots} - \sum_{\beta<\alpha}\frac{A_\alpha}{g}\tau_{1\ldots\ldots n}^{\ldots\beta\ldots\alpha\ldots}\right)\frac{\partial}{\partial p^{A_\alpha\beta}}\rfloor\frac{\partial}{\partial A_\gamma}\rfloor\Omega\\ &= 2(-1)^n(n-1)\sum_\alpha \tau_1\cdots\tau_{\alpha-1}\tau_{\alpha+1}\cdots\tau_n\frac{\partial}{\partial x^\alpha}\rfloor dx^1\wedge\cdots\wedge dx^n\\ &= {}^s(2(-1)^n(n-1)).\end{aligned}$$

Thus

$$\{\pi, A\} = 2(-1)^n(n-1).$$

As it may be anticipated by Corollary 1, the dynamical equations are described by the following identities to be true along the graph of a solution of the Hamilton equations:

$$\mathbf{d}A=\{\mathcal{H}\omega,A\}$$

$$=(-1)^{n+\alpha+\beta}\Bigg[\sum_{\alpha<\beta}\frac{1}{g}\frac{\partial}{\partial x^1}\wedge\cdots\frac{\partial}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial x^{\alpha+1}}\wedge\cdots\frac{\partial}{\partial x^{\beta-1}}\wedge\frac{\partial}{\partial x^{\beta+1}}\wedge\cdots\frac{\partial}{\partial x^n}\wedge\frac{\partial}{\partial p^{A_\alpha\beta}}$$

$$-\sum_{\beta<\alpha}\frac{1}{g}\frac{\partial}{\partial x^1}\wedge\cdots\frac{\partial}{\partial x^{\beta-1}}\wedge\frac{\partial}{\partial x^{\beta+1}}\wedge\cdots\frac{\partial}{\partial x^{\alpha-1}}\wedge\frac{\partial}{\partial x^{\alpha+1}}\wedge\cdots\frac{\partial}{\partial x^n}\wedge\frac{\partial}{\partial p^{A_\alpha\beta}}\Bigg]\rfloor d\mathcal{H}\wedge\omega$$

$$=\sum_{\alpha,\beta}\frac{\partial\mathcal{H}}{\partial p^{A_\alpha\beta}}dx^\beta\wedge dx^\alpha=\sum_{\alpha<\beta}g_{\alpha\gamma}g_{\beta\delta}p^{A_\gamma\delta}dx^\alpha\wedge dx^\beta,$$

$$\mathbf{d}\pi=\{\mathcal{H}\omega,\pi\}=-\sum_\alpha\frac{\partial}{\partial x^\alpha}\wedge\frac{\partial}{\partial A_\alpha}\rfloor d\mathcal{H}\wedge\omega=\frac{\partial\mathcal{H}}{\partial A_\alpha}\omega_\alpha=j^\alpha\omega_\alpha=j.$$

The first equation leads to $\partial A_\beta/\partial x^\alpha-\partial A_\alpha/\partial x^\beta=g_{\alpha\gamma}g_{\beta\delta}p^{A_\gamma\delta}$ which implies $F_{\alpha\beta}=g_{\alpha\gamma}g_{\beta\delta}p^{A_\gamma\delta}$ or equivalently $p^{A_\alpha\beta}=F^{\alpha\beta}$. This can be translated into the relation

$$\pi=\star F,\quad \text{along } \Gamma.$$

By substitution in the second equation, $\mathbf{d}\pi=j$, it gives immediately (47).

A last observation is that infinitesimal gauge transformations $\delta A=df$ [for $f\in\mathcal{C}^\infty(\mathcal{X})$] are generated by the Poisson bracket with $df\wedge\pi$. We have indeed

$$d(df\wedge\pi)=-df\wedge d\pi=-\sum_\alpha\frac{\partial f}{\partial x^\alpha}\frac{\partial}{\partial A_\alpha}\rfloor\Omega,$$

so that $df\wedge\pi\in\mathfrak{P}^{n-1}\mathcal{M}$ and $\Xi(df\wedge\pi)=\Sigma_\alpha\partial f/\partial x^\alpha\partial/\partial A_\alpha$. We deduce that

$$\{df\wedge\pi,\pi\}=\Xi(df\wedge\pi)\rfloor d\pi=0,$$

$$\{df\wedge\pi,A\}=\Xi(df\wedge\pi)\rfloor dA=df.$$

Notice that we could replace $df\wedge\pi$ by $-fd\pi$ or $f(j-d\pi)$ without changing the brackets with π and A.

VI. CONCLUSION

We obtained a Hamiltonian formulation for variational problems with an arbitrary number of variables. This could be the starting point for building a covariant quantum field theory without requiring the space–time to be Minkowskian. Notice also that we may enlarge the concept of pataplectic manifolds as manifolds equipped with a closed $(n+1)$-form, and extend to this context notions like the $\mathfrak{p}$-bracket. Some of these questions will be treated in a forthcoming paper.

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Quantizing Yang–Mills theory on a two-point space

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We perform the Batalin–Vilkovisky quantization of Yang–Mills theory on a two-point space, discussing the formulation of Connes–Lott as well as Connes' real spectral triple approach. Despite the model's apparent simplicity the gauge structure reveals infinite reducibility and the gauge fixing is afflicted with the Gribov problem. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1467096]

I. INTRODUCTION

Noncommutative geometry constitutes one of the fascinating new concepts in current theoretical physics research with many promising impacts and applications in a diverse set of fields.[1–5] Specifically we mention the construction of the classical action of the standard model,[6,7] unifying the Einstein–Hilbert action, the Yang–Mills action, the Dirac action, and the Klein–Gordon action with the Higgs potential and spontaneous symmetry breaking.

The basic idea of noncommutative geometry is to replace the notion of differential manifolds and functions by specific noncommutative algebras of functions; the geometric setting of gauge theories as fiber bundles finds a noncommutative generalization in terms of finitely generated projective modules over noncommutative algebras.

It seems, however, that within this noncommutative algebraic framework the concepts of *quantizing* gauge theories, specifically the issues of gauge fixing and the proper definition of a path integral measure for the standard model, are not yet fully understood.[8] Our intention for this paper is not to present new results in these rather fundamental issues. Instead we quantize one of the simplest toy models for noncommutative gauge theories, which is Yang–Mills theory on a two-point space, by applying the standard Batalin–Vilkovisky method.[9–12] Somewhat surprisingly we find that despite the model's original simplicity the gauge structure reveals infinite reducibility and the gauge fixing is afflicted with the Gribov[13] problem.

In Sec. II we work out the formulation of the model following the approach of Connes–Lott.[14] In Sec. III the infinite reducibility of the gauge symmetry is explained; the Batalin–Vilkovisky quantization of the model is performed in Sec. IV. We discuss the Gribov problem in Sec. V and finally, in Sec. VI, recast our results within Connes' real spectral triple approach.[6,15]

II. THE FORMULATION OF CONNES–LOTT

Following Ref. 14 we define the Yang–Mills Theory on a two-point space in terms of the algebra $\mathbf{A}=C\oplus C$, which is represented by diagonal complex valued 2×2 matrices; the Dirac operator D is given by $D=\left(\begin{smallmatrix}0 & \mu\\ \mu & 0\end{smallmatrix}\right)$, where $\mu\in\mathrm{R}$ is an arbitrary parameter. The differential p-forms ω_p are constant, diagonal or off-diagonal 2×2 matrices, depending on whether p is even or odd, respectively. One has a $\mathcal{Z}_2$ grading of matrices (to be diagonal or off-diagonal) and obtains a matrix derivative $\mathbf{d}$. Acting on 2×2 matrices it is a nilpotent graded derivation, $\mathbf{d}a=i\mu\left(\begin{smallmatrix}a_{21}+a_{12} & a_{22}-a_{11}\\ a_{11}-a_{22} & a_{21}+a_{12}\end{smallmatrix}\right)$ where $a=\left(\begin{smallmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{smallmatrix}\right)$, $a_{ij}\in\mathrm{C}$, with respect to the matrix product and the matrix $\mathcal{Z}_2$ grading.

Specifically the one-forms are given by $\omega_1=a\,\mathbf{d}b$, where $a,b\in\mathbf{A}$, which are odd (i.e., off-diagonal) matrices. The subset of anti-Hermitean one-forms $\mathcal{A}$ can be parametrized by

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$$\mathcal{A}=\begin{pmatrix} 0 & i\mu\phi \\ i\mu\overline{\phi} & 0 \end{pmatrix} \tag{2.1}$$

and constitute the gauge fields of the model; here $\phi\in\mathrm{C}$ denotes a (constant) scalar field. The (rigid) gauge transformations of $\mathcal{A}$ are defined by

$$\mathcal{A}^U=U^{-1}\mathcal{A}U+U^{-1}\mathbf{d}U \tag{2.2}$$

with U being a unitary element of the algebra **A**. It is a constant, even and unitary matrix which we define to have only Abelian entries; it can exponentially be parametrized by the even matrix ϵ,

$$U=\begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{i\beta} \end{pmatrix}=e^{i\epsilon},\quad \epsilon=\begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix},\quad \alpha,\beta\in\mathrm{R}. \tag{2.3}$$

We point out that the Yang–Mills theory on the two-point space is an ideal play ground to study quantization techniques: Due to the non-Abelian form of the gauge transformations (2.2) the model shares many interesting features with the standard Yang–Mills theory, yet it has no physical space–time dependence and allows extremely simple calculations. We even restrict ourselves to just Abelian entries along the diagonal of U, thus studying a $U(1)\times U(1)$ gauge model with non-Abelian features.

We define a scalar product for 2×2 matrices a,b by $\langle a|b\rangle=\mathrm{tr}\, a^\dagger b$ where † denotes taking the Hermitian conjugate. The curvature $\mathcal{F}$ is defined as usual by $\mathcal{F}=\mathbf{d}\mathcal{A}+\mathcal{A}\mathcal{A}$ and transforms under gauge transformations as $\mathcal{F}^U=U^{-1}\mathcal{F}U$; for an action which is automatically invariant under the gauge transformations (2.2) one takes

$$S_{\mathrm{inv}}=\tfrac{1}{2}\langle\mathcal{F}|\mathcal{F}\rangle. \tag{2.4}$$

Written out in components the scalars' contribution is given by

$$S_{\mathrm{inv}}=\mu^4((\phi+\overline{\phi})+\phi\overline{\phi})^2. \tag{2.5}$$

It was pointed out in Refs. 16 and 17 that the most general form of the gauge invariant action also allows a term proportional to $\mathrm{tr}\,\mathcal{F}$,

$$\hat{S}_{\mathrm{inv}}=\tfrac{1}{2}(\langle\mathcal{F}|\mathcal{F}\rangle+\gamma\,\mathrm{tr}\,\mathcal{F}) \tag{2.6}$$

where $\gamma\in R$ is an arbitrary parameter. We note, however, that one requires the scalars ϕ to be vanishing at the minimum of the action so that in the case of (2.6) the scalars have to be shifted appropriately. Explicitly we have

$$\hat{S}_{\mathrm{inv}}=\mu^4(2u+u^2+v^2)\left(2u+u^2+v^2-\frac{\gamma}{\mu^2}\right), \tag{2.7}$$

where we introduced $\phi=u+iv$. Whereas the local maximum is at

$$u_{\max}=-1,\quad v_{\max}=0, \tag{2.8}$$

the circle of local minima is given by

$$(u+1)^2+v^2=1+\frac{\gamma}{2\mu^2},\quad \text{where}\quad \gamma\geqslant-2\mu^2. \tag{2.9}$$

We choose

$$u_{\min}=\sqrt{1+\frac{\gamma}{2\mu^2}}-1, \quad v_{\min}=0 \tag{2.10}$$

and define shifted scalars $\tilde{\phi}=\phi-u_{\min}$ which by construction are vanishing at the minimum of the action. From

$$\hat{S}_{\text{inv}}=\mu^4\left((\tilde{\phi}+\bar{\tilde{\phi}})\sqrt{1+\frac{\gamma}{2\mu^2}}+\tilde{\phi}\bar{\tilde{\phi}}\right)^2-\frac{\gamma^2}{2}. \tag{2.11}$$

we omit the irrelevant constant $-\gamma^2/2$, rescale $\tilde{\phi}=\hat{\phi}\sqrt{1+\gamma/2\mu^2}$ and $\mu\sqrt{1+\gamma/2\mu^2}=\hat{\mu}$ so that finally

$$\hat{S}_{\text{inv}}=\hat{\mu}^4((\hat{\phi}+\bar{\hat{\phi}})+\hat{\phi}\bar{\hat{\phi}})^2. \tag{2.12}$$

We see that the inclusion of the action term linear in $\mathcal{F}$ can be compensated by shifting and rescaling of the scalar field ϕ, as well as by rescaling of the parameter μ. As the scalar fields and the parameter are arbitrary from the outset the inclusion of the action term linear in $\mathcal{F}$ appears to be unnecessary. In the following we will set $\mu=1$ for simplicity and stick to the action term (2.4) quadratic in $\mathcal{F}$.

III. GAUGE TRANSFORMATIONS AND INFINITE REDUCIBILITY

The (zero-stage) gauge transformations (2.2) explicitly are given by

$$\mathcal{A}^U=\begin{pmatrix} 0 & ie^{i(\beta-\alpha)}(\phi+1)-i \\ ie^{-i(\beta-\alpha)}(\bar{\phi}+1)-i & 0 \end{pmatrix}, \tag{3.1}$$

so that the usual Abelian gauge transformations are implied for the Higgs fields $H=\phi+1$ and $\bar{H}=\bar{\phi}+1$. To discuss infinitesimal (zero-stage) gauge transformations we introduce an even, infinitesimal (zero-stage) gauge parameter matrix $\boldsymbol{\epsilon}_e^0$ in terms of which $U\simeq\mathbf{1}+\boldsymbol{\epsilon}_e^0$. The infinitesimal (zero-stage) gauge variation of $\mathcal{A}$ derives as

$$\delta_{\boldsymbol{\epsilon}_e^0}\mathcal{A}=i\mathbf{R}^0\,\boldsymbol{\epsilon}_e^0,$$

$$\text{where} \quad \mathbf{R}^0=\mathbf{D}. \tag{3.2}$$

Here the (zero-stage) gauge generator $\mathbf{R}^0$ is defined in terms of the covariant matrix derivative $\mathbf{D}$, which acting on $\boldsymbol{\epsilon}_e^0$ is given by $\mathbf{D}\boldsymbol{\epsilon}_e^0=\mathbf{d}\boldsymbol{\epsilon}_e^0+[\mathcal{A},\boldsymbol{\epsilon}_e^0]$.

A gauge symmetry is called irreducible if the (zero-stage) gauge generator $\mathbf{R}^0$ does not possess any zero mode.[9–12]

It is amusing to note that the Yang–Mills theory on the two-point space reveals an infinitely reducible gauge symmetry: We observe that $\mathbf{D}\,\mathbf{d}$ is vanishing on arbitrary odd matrices. Thus there exists a zero mode $\boldsymbol{\epsilon}_e^1$ for the (zero-stage) gauge generator $\mathbf{R}^0$, such that

$$\mathbf{R}^0\boldsymbol{\epsilon}_e^1=0$$

$$\text{where} \quad \boldsymbol{\epsilon}_e^1=\mathbf{R}^1\boldsymbol{\epsilon}_o^1 \quad \text{with} \quad \mathbf{R}^1=\mathbf{d}. \tag{3.3}$$

Here $\boldsymbol{\epsilon}_o^1$ denotes an odd, infinitesimal (first-stage) gauge parameter matrix and $\mathbf{R}^1$ the corresponding (first-stage) gauge generator. As a matter of fact an infinite tower of (higher-stage) gauge generators $\mathbf{R}^s$, $s=1,2,3,\ldots$ with never ending gauge invariances for gauge invariances is arising: We define $\mathbf{R}^s=\mathbf{d}$ for $s=1,2,3,\ldots$ so that for each gauge generator there exists an additional zero mode

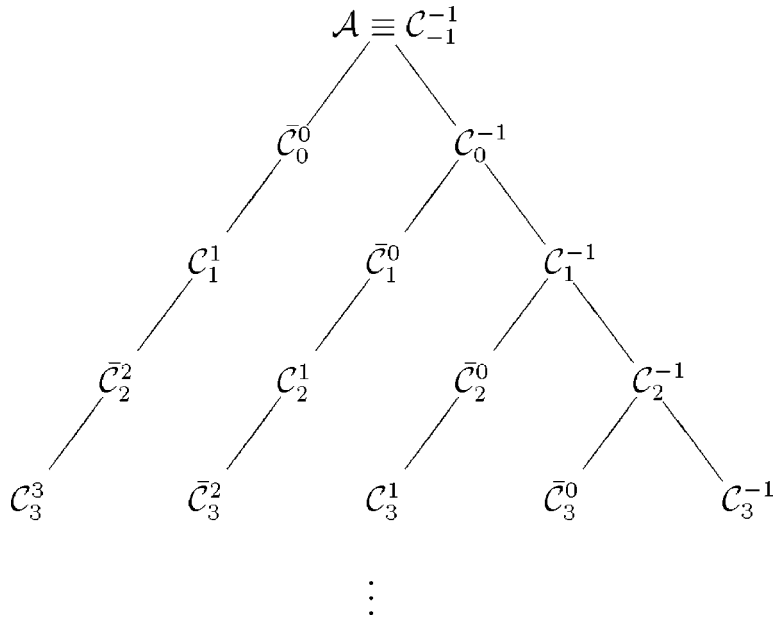

FIG. 1. The infinite tower of ghost fields

$$\begin{aligned} &\mathbf{R}^1\epsilon_o^2=0 \quad (\epsilon_o^2=\mathbf{R}^2\epsilon_e^2),\\ &\mathbf{R}^2\epsilon_e^3=0 \quad (\epsilon_e^3=\mathbf{R}^3\epsilon_o^3),\\ &\cdots \quad \cdots \end{aligned} \tag{3.4}$$

due to the nilpotency $\mathbf{d}^2=0$.

IV. GAUGE FIXING AND *BV*-QUANTIZATION

In this section we straightforwardly apply the usual field theory *BV*-path integral quantization scheme[10–12] to the Connes–Lott two-point model: In addition to the original gauge field $\mathcal{A}$, which for notational convenience we temporarily denote by $\mathcal{A}\equiv\mathcal{C}_{-1}^{-1}$, we introduce ghost fields $\mathcal{C}_s^k$, $\infty\geqslant s\geqslant -1$, $s\geqslant k\geqslant -1$ with k odd, as well as auxiliary ghost fields $\bar{\mathcal{C}}_s^k$, $\infty\geqslant s\geqslant 0$, $s\geqslant k\geqslant 0$ with k even (see Fig. 1).

Furthermore we add Lagrange multiplier fields π_s^k, $\infty\geqslant s\geqslant 1, s\geqslant k\geqslant 1$ with k odd and $\bar{\pi}_s^k$, $\infty\geqslant s\geqslant 0$, $s\geqslant k\geqslant 0$ with k even. Finally we introduce antifields $\mathcal{C}_s^k{}^*$, $\bar{\mathcal{C}}_s^k{}^*$. All the ghosts $\mathcal{C}_s^k$, $\bar{\mathcal{C}}_s^k$, multiplier fields π_s^k, $\bar{\pi}_s^k$, and antifields $\mathcal{C}_s^k{}^*$, $\bar{\mathcal{C}}_s^k{}^*$ are matrices which are even for s even and odd for s odd, respectively. We define all the ghost fields $\mathcal{C}_s^k$, $\bar{\mathcal{C}}_s^k$ to be anti-Hermitean, all the multiplier fields π_s^k, $\bar{\pi}_s^k$ to be Hermitean. When s is taken to be odd the ghosts are bosonic whereas the multiplier fields are fermionic; for s even the ghosts are fermionic and the multiplier fields are bosonic, respectively.

An important quantity for the construction of the *BV*-action is the commutator of (zero-stage) infinitesimal gauge transformations $[\delta_{\epsilon_1},\delta_{\epsilon_2}]\mathcal{A}$, where $\delta_{\epsilon_k}\mathcal{A}=i\mathbf{R}^0\epsilon_k$ with even matrices ϵ_k, $k=1,2$. It is easy to see that this commutator is vanishing. The *BV*-action therefore obtains as

$$S_{BV}=S_{\text{inv}}+S_{\text{aux}}-\langle\mathcal{C}_{-1}^{-1}{}^*|\mathbf{D}\,\mathcal{C}_0^{-1}\rangle-\sum_{s=1,3,5,\ldots}^{\infty}\langle\mathcal{C}_s^{-1}{}^*|\mathbf{d}\,\mathcal{C}_{s+1}^{-1}\rangle-i\sum_{s=0,2,4,\ldots}^{\infty}\langle\mathcal{C}_s^{-1}{}^*|\mathbf{d}\,\mathcal{C}_{s+1}^{-1}\rangle, \tag{4.1}$$

where we denote by S_{aux} the auxiliary field action

$$S_{\text{aux}}=\sum_{k=0,2,4,\ldots}^{\infty}\sum_{s=k}^{\infty}\langle\overline{\pi}_s^k|\overline{\mathcal{C}}_s^k *\rangle+\sum_{k=1,3,5,\ldots}^{\infty}\sum_{s=k}^{\infty}\langle\mathcal{C}_s^k *|\pi_s^k\rangle. \tag{4.2}$$

By $\boldsymbol{\delta}$ we denote a nilpotent matrix coderivative operator, $\boldsymbol{\delta}a=i\left(\begin{smallmatrix}a_{12}-a_{21} & -a_{11}-a_{22}\\ -a_{11}-a_{22} & -a_{12}+a_{21}\end{smallmatrix}\right)$ where $a=\left(\begin{smallmatrix}a_{11}\,a_{12}\\ a_{21}\,a_{22}\end{smallmatrix}\right)$, $a_{ij}\in\mathrm{C}$, which is defined by $\langle\boldsymbol{\delta}a_o|b_e\rangle=\langle a_o|\mathbf{d}b_e\rangle$ and $\langle\boldsymbol{\delta}a_e|b_o\rangle=\langle a_e|\mathbf{d}b_o\rangle$. It allows one to define gauge fixing conditions

$$\begin{aligned}&\boldsymbol{\delta}\mathcal{C}_s^k=0,\quad \infty\geqslant s\geqslant -1,\quad s\geqslant k\geqslant -1\quad \text{with } k \text{ odd},\\ &\boldsymbol{\delta}\overline{\mathcal{C}}_s^k=0,\quad \infty\geqslant s\geqslant 0,\quad s\geqslant k\geqslant 0\quad \text{with } k \text{ even},\end{aligned} \tag{4.3}$$

which are similar to the Feynman gauge in standard Yang–Mills theory. In the BV-approach we implement these gauge fixing conditions by defining the gauge fixing fermion $\Psi=\Psi_\delta+\Psi_\pi$ by

$$\Psi_\delta=\sum_{s=0,2,4,\ldots}^{\infty}\sum_{k=0,2,4,\ldots k\leqslant s}(-\langle\overline{\mathcal{C}}_s^k|\,\boldsymbol{\delta}\mathcal{C}_{s-1}^{k-1}\rangle+\langle\boldsymbol{\delta}\overline{\mathcal{C}}_{s+1}^k|\,\mathcal{C}_{s+2}^{k+1}\rangle+i\langle\overline{\mathcal{C}}_{s+1}^k|\,\boldsymbol{\delta}\mathcal{C}_s^{k-1}\rangle+i\langle\boldsymbol{\delta}\overline{\mathcal{C}}_s^k|\,\mathcal{C}_{s+1}^{k+1}\rangle),$$

$$\begin{aligned}\Psi_\pi=\frac{1}{2}\sum_{s=0,2,4,\ldots}^{\infty}\sum_{k=0,2,4,\ldots k<s}&(\langle\overline{\mathcal{C}}_s^k|\,\pi_s^{k+1}\rangle+\langle\overline{\pi}_s^k|\,\mathcal{C}_s^{k+1}\rangle+i\langle\overline{\mathcal{C}}_{s+1}^k|\,\pi_{s+1}^{k+1}\rangle\\&+i\langle\overline{\pi}_{s+1}^k|\,\mathcal{C}_{s+1}^{k+1}\rangle)+\frac{1}{2}\sum_{k=0,2,4,\ldots}^{\infty}\langle\overline{\mathcal{C}}_k^k|\,\overline{\pi}_k^k\rangle.\end{aligned} \tag{4.4}$$

We eliminate the antifields by using the gauge fixing fermion Ψ via

$$\langle\mathcal{C}_s^k *|=\frac{\partial\Psi}{\partial|\mathcal{C}_s^k\rangle},\quad |\overline{\mathcal{C}}_s^k *\rangle=\frac{\partial\Psi}{\partial\langle\overline{\mathcal{C}}_s^k|}, \tag{4.5}$$

so that the gauge fixed action S_Ψ reads

$$\begin{aligned}S_\Psi=S_{\text{inv}}&-i\langle\overline{\mathcal{C}}_0^0|\,\boldsymbol{\delta}\mathbf{D}\,\mathcal{C}_0^{-1}\rangle-i\sum_{s=1,3,5,\ldots}^{\infty}\langle\overline{\mathcal{C}}_{s+1}^0|\,\boldsymbol{\delta}\mathbf{d}\,\mathcal{C}_{s+1}^{-1}\rangle+\sum_{s=0,2,4,\ldots}^{\infty}\langle\overline{\mathcal{C}}_{s+1}^0|\,\boldsymbol{\delta}\mathbf{d}\,\mathcal{C}_{s+1}^{-1}\rangle\\&+\sum_{k=0,2,4,\ldots}^{\infty}\sum_{s=k+1,\text{ odd}}^{\infty}(i\langle\overline{\pi}_s^k|\,\pi_s^{k+1}\rangle+\langle\overline{\pi}_s^k|\,(i\,\boldsymbol{\delta}\mathcal{C}_{s-1}^{k-1}+\mathbf{d}\mathcal{C}_{s+1}^{k+1})\rangle+\langle(i\,\boldsymbol{\delta}\overline{\mathcal{C}}_{s-1}^k-\mathbf{d}\overline{\mathcal{C}}_{s+1}^{k+2})|\,\pi_s^{k+1}\rangle)\\&+\sum_{k=0,2,4,\ldots}^{\infty}\sum_{s=k+2,\text{ even}}^{\infty}(\langle\overline{\pi}_s^k|\,\pi_s^{k+1}\rangle+\langle\overline{\pi}_s^k|\,(-\boldsymbol{\delta}\mathcal{C}_{s-1}^{k-1}+i\,\mathbf{d}\mathcal{C}_{s+1}^{k+1})\rangle+\langle(\boldsymbol{\delta}\overline{\mathcal{C}}_{s-1}^k\\&+i\,\mathbf{d}\overline{\mathcal{C}}_{s+1}^{k+2})|\,\pi_s^{k+1}\rangle)+\sum_{k=0,2,4,\ldots}^{\infty}\left\langle\overline{\pi}_k^k\middle|\left(-\boldsymbol{\delta}\mathcal{C}_{k-1}^{k-1}+i\,\mathbf{d}\mathcal{C}_{k+1}^{k+1}+\frac{1}{2}\overline{\pi}_k^k\right)\right\rangle.\end{aligned} \tag{4.6}$$

We can now eliminate the Lagrange multiplier fields π_s^k and $\overline{\pi}_s^k$ and arrive at

$$S_\Psi \to S_{\rm inv} + \tfrac{1}{2}\langle \mathcal{A} \,|\, \mathbf{d}\boldsymbol{\delta}\mathcal{A}\rangle - i\langle \overline{\mathcal{C}}_0^0 \,|\, (\boldsymbol{\delta}\mathbf{D} + \mathbf{d}\boldsymbol{\delta})\, \mathcal{C}_0^{-1}\rangle - i \sum_{s=1,3,5,\ldots}^{\infty} \langle \overline{\mathcal{C}}_{s+1}^0 \,|\, (\boldsymbol{\delta}\mathbf{d} + \mathbf{d}\boldsymbol{\delta})\, \mathcal{C}_{s+1}^{-1}\rangle$$
$$+ \sum_{s=0,2,4,\ldots}^{\infty} \langle \overline{\mathcal{C}}_{s+1}^0 \,|\, (\boldsymbol{\delta}\mathbf{d} + \mathbf{d}\boldsymbol{\delta})\, \mathcal{C}_{s+1}^{-1}\rangle - i \sum_{k=0,2,4,\ldots}^{\infty} \sum_{s=k+1,\ \text{odd}}^{\infty} \langle \overline{\mathcal{C}}_{s+1}^{k+2} \,|\, (\boldsymbol{\delta}\mathbf{d} + \mathbf{d}\boldsymbol{\delta})\, \mathcal{C}_{s+1}^{k+1}\rangle$$
$$+ \sum_{k=0,2,4,\ldots}^{\infty} \sum_{s=k+2,\ \text{even}}^{\infty} \langle \overline{\mathcal{C}}_{s+1}^{k+2} \,|\, (\boldsymbol{\delta}\mathbf{d} + \mathbf{d}\boldsymbol{\delta})\, \mathcal{C}_{s+1}^{k+1}\rangle + \frac{1}{2} \sum_{k=0,2,4,\ldots}^{\infty} \langle \mathcal{C}_{k+1}^{k+1} \,|\, (\boldsymbol{\delta}\mathbf{d} + \mathbf{d}\boldsymbol{\delta})\, \mathcal{C}_{k+1}^{k+1}\rangle. \tag{4.7}$$

All the higher-stage ghost contributions can be integrated away without any effect as $\boldsymbol{\delta}\mathbf{d} + \mathbf{d}\boldsymbol{\delta} = 4 \cdot \mathbf{1}$ and we simply obtain

$$S_\Psi \to S_{\rm inv} + \tfrac{1}{2}\langle \mathcal{A} \,|\, \mathbf{d}\boldsymbol{\delta}\mathcal{A}\rangle - i\langle \overline{\mathcal{C}}_0^0 \,|\, (\boldsymbol{\delta}\mathbf{D} + \mathbf{d}\boldsymbol{\delta})\, \mathcal{C}_0^{-1}\rangle \tag{4.8}$$

We see that the gauge fixed action contains the invertible quadratic part $2\langle \mathcal{A} \,|\, \mathcal{A}\rangle$ for the gauge field, as well as $-4i\langle \overline{\mathcal{C}}_0^0 \,|\, \mathcal{C}_0^{-1}\rangle$ for the $\overline{\mathcal{C}}_0^0$, $\mathcal{C}_0^{-1}$ ghost fields.

V. THE GRIBOV PROBLEM

The Yang–Mills theory on the two-point space suffers from a Gribov problem[13] even for the Abelian $U(1)\times U(1)$ case. This can be demonstrated easily by recasting the ghost part of the gauge fixed action (4.8) into the form

$$\langle \overline{\mathcal{C}}_0^0 \,|\, (\boldsymbol{\delta}\mathbf{D} + \mathbf{d}\boldsymbol{\delta})\, \mathcal{C}_0^{-1}\rangle = (\overline{c_1} \quad \overline{c_2}) \begin{pmatrix} 4 + \phi + \overline{\phi} & -\phi - \overline{\phi} \\ -\phi - \overline{\phi} & 4 + \phi + \overline{\phi} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \tag{5.1}$$

where we introduced the component ghosts fields $\overline{c_1}, \overline{c_2}$ and c_1, c_2 which are the diagonal elements of $\overline{\mathcal{C}}_0^0$ and $\mathcal{C}_0^{-1}$, respectively. The Faddeev–Popov matrix $M_{\rm FP}$

$$M_{\rm FP} = \begin{pmatrix} 4 + \phi + \overline{\phi} & -\phi - \overline{\phi} \\ -\phi - \overline{\phi} & 4 + \phi + \overline{\phi} \end{pmatrix} \tag{5.2}$$

has a vanishing determinant for $2 + \phi + \overline{\phi} = 0$ which forces $\phi = u + iv$ to lie on the line $u = -1$. We note the distinguished value $\phi = -1$, which we discussed previously by demanding the action to be maximal, see (2.8). Now this value arises by inserting the gauge fixing condition $\boldsymbol{\delta}\mathcal{A} = 0$ into the Faddeev–Popov determinant $\det M_{\rm FP}$.

We observe that the classical action $S_{\rm inv}$ not only has an invariance under the (rigid) gauge transformations (2.2), but also under the discrete charge conjugation operation (conveniently expressed in terms of the Higgs fields $H, \overline{H}$)

$$H \to -\overline{H}, \quad \overline{H} \to -H. \tag{5.3}$$

After the spontaneous symmetry breakdown this discrete symmetry guarantees that the minima of the action are degenerated. In the quantum case, however, due to the Gribov problem, these discrete jumps no longer are allowed and the quantum corrections to the action will lift the classical degeneracy of the minima.

VI. CONNES' REAL SPECTRAL TRIPLE FORMULATION

The formulation of the Yang–Mills theory model on the two-point space in terms of Connes's real spectral triple approach proceeds by specifying the spectral triple $(\mathbf{A}, \mathcal{H}, D)$ together with the

antilinear isometry $\mathcal{J}$, fulfilling a set of specific properties.[6,15] We represent the elements $a=(a_1,a_2,a_3)$ of the algebra $\mathbf{A}=C\oplus C\oplus C$, as well as D and $\mathcal{J}$, by specific 4×4 matrices; the Hilbert space $\mathcal{H}$ simply is C^4. Specifically we have

$$a=\begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & a_3 \end{pmatrix}, \quad D=\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathcal{J}=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}\circ \text{c.c.}, \tag{6.1}$$

where c.c. denotes complex conjugation. As an example one sees that for $a, b\in\mathbf{A}$ the differential one-form $\omega_1=a[iD,b]$ is given by

$$\omega_1=i\begin{pmatrix} 0 & a_1(b_2-b_1) & 0 & 0 \\ a_2(b_1-b_2) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6.2}$$

We recognize that apart from irrelevant zeros in the upper right, lower left and lower right matrix corners of the differential forms our previous discussion of the gauge symmetries, the gauge fixing and the ghost structure proves right as well.

We conclude that the quantization of the Yang–Mills theory model on the two-point space within the Connes–Lott scheme and within Connes' real spectral triple approach are equivalent; the model reveals infinite reducibility and is afflicted with the Gribov problem.

Note added in proof: After finishing our paper a related article[18] appeared. One of its main purposes is to analyze in depth the counting argument of Feynman diagrams in the presence of spontaneous symmetry breaking. Concerning the gauge fixing procedure and the introduction of ghost fields, however, the investigation appears to be incomplete.

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Self-dual Chern–Simons vortices on Riemann surfaces

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We study self-dual multivortex solutions of Chern–Simons Higgs theory in a background curved space–time. The existence and decaying property of a solution are demonstrated. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1471365]

I. INTRODUCTION

Chern–Simons gauge theories have provided intriguing questions and answers to various subjects of both physics and mathematics. One of the interdisciplinary topics that has attracted attention is the so-called self-dual Chern–Simons solitons.[1–3] A natural extension is to include gravity which can be background[4,5] or dynamical.[6,7] Once the Bogomolnyi-type bound is obtained and detailed mathematical properties of those self-dual vortices are studied in the Chern–Simons Higgs model in the presence of background gravity, it would be helpful to address related physics-wise problems involving condensed matter systems, e.g., quantum Hall effects, supergravity, Lorentz-symmetry breaking due to parity-violating term, existence of time-like closed curve around gravitating spinning strings, cosmological implication of cosmic strings, and even cosmological constant problem.

Because it is applicable to diverse fields, mathematical study of self-dual Chern–Simons solitons is going on. The existence of a topological multivortex solution of relativistic Chern–Simons–Higgs theory in flat R^2 is shown by Wang.[8] In the same setting, rotationally symmetric nontopological solitons and vortices were proven to exist by Spruck and Yang.[9] Yang also proved the existence of a topological self-dual multivortex solution when the gauge symmetry is extended to non-Abelian.[10] When the topological vortices or nontopological solitons are generated in condensed matter systems or in the early universe, they are likely to form a lattice structure or a network. In such sense important works have been done on torus[11–14] or on standard sphere.[4,15] Condensed matter experiments are usually performed by turning on constant external electric or magnetic field. In relation to this, Chae *et al.* demonstrated the existence of soliton solutions of the self-dual Chern–Simons Higgs model coupled to an external background charge density.[16] Another study to have cosmological implications was done by Kurata and Choe with nontopological soliton solutions under decaying metric.[17,18]

Now let us take into account the curved space–time geometry of a straight string in the early universe. Then, an extremely small core region of the string is curved by matter fields, and the intermediate region is slightly curved or locally flat because of no graviton to the transverse directions. However, the asymptote of the global universe is known to be flat. All of such geometry should be dynamically determined by examining Einstein equations in the exact sense, but it is practically too difficult to do with mathematical rigor. A meaningful starting point is to assume a physically allowable set of background metrics and to study possible string configurations. In this paper, we study Chern–Simons Higgs theory on a uniformly Euclidean metric, which is not necessarily radial. A spatial metric $\gamma_{ij}=b(x,y)\delta_{ij}$ is called uniformly Euclidean metric if there

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exist positive constants a_1 and a_2 with $a_1 \leqslant b(x,y) \leqslant a_2$. We show the existence of a self-dual topological multivortex solution and the fast decay property of a solution at infinity. The mathematical conditions we bring up are relevant to the physical situation discussed previously, e.g., the gravity is not far from that of the flat case at the end of universe.

A brief outline of the paper is in order. In Sec. II, under the most general static metric, we shall derive the Bogomolnyi-type bound of the Chern–Simons Higgs theory in background gravity. In Sec. III, we present the existence and asymptotic behavior of a solution of the self-dual Chern–Simons vortices. Conclusions with some discussions about our results are presented in Sec. IV.

II. BOGOMOLNYI BOUND OF CHERN–SIMONS HIGGS THEORY IN BACKGROUND GRAVITY

In this section we recapitulate derivation of the so-called Bogomolnyi bound of the Chern–Simons Higgs theory coupled to background gravity by assuming the general static metric

$$ds^2 = N^2(x^k)dt^2 - \gamma_{ij}(x^k)dx^i\,dx^j \quad (i,j,k,\ldots = 1,2), \tag{2.1}$$

where the metric of the two-dimensional spatial hypersurface can always be diagonalized by a conformal gauge $\gamma_{ij} = \delta_{ij} b(x^k)$. Later we shall show that the Bogomolnyi bound is attained only when the lapse function $N(x^i)$ is constant, i.e., $N(x^k) = 1$ after a rescaling of time coordinate t.

The Chern–Simons Higgs theory is described by the action

$$S = \int d^3x \sqrt{g} \left[\frac{\kappa}{2} \frac{\epsilon^{\mu\nu\rho}}{\sqrt{g}} A_\mu \partial_\nu A_\rho + \frac{1}{2} g^{\mu\nu} \overline{D_\mu \phi} D_\nu \phi - V(|\phi|) \right], \tag{2.2}$$

where $\phi = e^{i\Theta}|\phi|$ is a complex scalar field, A_μ a U(1) gauge field, and $D_\mu = \partial_\mu - ieA_\mu$ is gauge-covariant but not covariant under general coordinate transformation. Since the Bogomolnyi limit is our interest, the form of the scalar potential $V(|\phi|)$ is taken to be

$$V(|\phi|) = \frac{e^4}{8\kappa^2} |\phi|^2 (|\phi|^2 - v^2)^2. \tag{2.3}$$

From here on all the metric components and fields are assumed to be static because the self-dual solitons of our interest are static objects.

Symmetric energy–momentum tensor is

$$T_{\mu\nu} = \tfrac{1}{2}(\overline{D_\mu \phi} D_\nu \phi + \overline{D_\nu \phi} D_\mu \phi) - g_{\mu\nu}[\tfrac{1}{2} g^{\rho\sigma} \overline{D_\rho \phi} D_\sigma \phi - V(|\phi|)]. \tag{2.4}$$

A physically meaningful derivation of the Bogomolnyi bound is to investigate vanishing of stress components of the energy–momentum tensor. Since the lapse function $N(x^i)$ disappears in every stress component by the help of Gauss' law $\kappa NB = e^2 A_0 |\phi|^2$, an appropriate rearrangement of them gives

$$T^{ij} = \frac{1}{2}\gamma^{ij}\left[\frac{\kappa^2}{2e^2} \frac{B^2}{|\phi|^2} - V(|\phi|) \right] - \frac{1}{2}(\gamma^{ij}\gamma^{kl} - \gamma^{ik}\gamma^{jl} - \gamma^{il}\gamma^{jk}) \overline{D_k \phi} D_l \phi \tag{2.5}$$

$$
\begin{aligned}
&= \frac{\kappa^2}{2e^2}\frac{\gamma^{ij}}{|\phi|^2}\left[B-\frac{e^3}{2\kappa^2}\left|\phi\right|^2(|\phi|^2-v^2)\right]\left[B+\frac{e^3}{2\kappa^2}\left|\phi\right|^2(|\phi|^2-v^2)\right] \\
&\quad+\frac{1}{8}\left\{\left[\overline{\left(D^i\phi\mp i\frac{\epsilon^{ik}}{\sqrt{\gamma}}\gamma_{kl}D^l\phi\right)}\left(D^j\phi\pm i\frac{\epsilon^{jm}}{\sqrt{\gamma}}\gamma_{mn}D^n\phi\right)\right.\right. \\
&\quad\left.+\overline{\left(D^j\phi\pm i\frac{\epsilon^{jk}}{\sqrt{\gamma}}\gamma_{kl}D^l\phi\right)}\left(D^i\phi\mp i\frac{\epsilon^{im}}{\sqrt{\gamma}}\gamma_{mn}D^n\phi\right)\right] \\
&\quad+\left[\overline{\left(D^i\phi\pm i\frac{\epsilon^{ik}}{\sqrt{\gamma}}\gamma_{kl}D^l\phi\right)}\left(D^j\phi\mp i\frac{\epsilon^{jm}}{\sqrt{\gamma}}\gamma_{mn}D^n\phi\right)\right. \\
&\quad\left.\left.+\overline{\left(D^j\phi\mp i\frac{\epsilon^{jk}}{\sqrt{\gamma}}\gamma_{kl}D^l\phi\right)}\left(D^i\phi\pm i\frac{\epsilon^{im}}{\sqrt{\gamma}}\gamma_{mn}D^n\phi\right)\right]\right\},
\end{aligned}
\tag{2.6}
$$

where γ^{ij} is inverse of the γ_{ij}, $\sqrt{\gamma}=\sqrt{\det\gamma_{ij}}$, and the magnetic field is defined by $B=-(\epsilon^{ij}/\sqrt{\gamma})\,\partial_i A_j$.

We read the first-order Bogomolnyi equations from Eq. (2.6),

$$
B=\mp\frac{e^3}{2\kappa^2}|\phi|^2(|\phi|^2-v^2), \tag{2.7}
$$

$$
D_i\phi\mp i\sqrt{\gamma}\epsilon_{ij}\gamma^{jk}D_k\phi=0. \tag{2.8}
$$

The second equation (2.8) expresses the spatial components of the gauge field A_i in terms of the scalar field, i.e., $eA_i=\partial_i\Theta\mp\sqrt{\gamma}\epsilon_{ij}\gamma^{jk}\partial_k\ln|\phi|$. Substituting it into the first Bogomolnyi equation (2.7) together with the conformal gauge, we have

$$
\partial^2\ln|\phi|=\frac{e^4}{2\kappa^2}b|\phi|^2(|\phi|^2-v^2)\mp\epsilon^{ij}\partial_i\partial_j\Theta, \tag{2.9}
$$

where the Dirac-delta function like contribution of the scalar phase Θ comes from multivalued function such as $\Theta=\Sigma_{k=1}^{n}\tan^{-1}(x^2-x_k^2)/(x^1-x_k^1)$.

Let us check a consistency condition to determine whether or not the Bogomolnyi equations (2.7) and (2.8) reproduce second-order Euler–Lagrange equations. Since we used Gauss' law, let us consider the scalar field equation

$$
\frac{1}{\sqrt{g}}D_\mu(\sqrt{g}g^{\mu\nu}D_\nu\phi)=-\frac{\phi}{|\phi|}\frac{\mathrm{d}V}{\mathrm{d}|\phi|}. \tag{2.10}
$$

For a static configuration, insertion of the Bogomolnyi equations (2.7), (2.8), and (2.8) into the scalar equation (2.10) leads to

$$
\frac{1}{N}\gamma^{ij}\partial_i N\partial_j|\phi|=0. \tag{2.11}
$$

As is well known, for every configuration of the self-dual solitons, derivative of the scalar amplitude vanishes nowhere, and both derivatives, $\partial_i N$ and $\partial_j|\phi|$, are not perpendicular to each other. Then, the lapse function N should be a constant which we set to be one by a rescaling of time variable, i.e., $\mathrm{d}t\to\mathrm{d}t/N$. Note that the spatial components of the gauge-field equation are automatically reproduced for $N=1$ without giving any additional constraint.

Now that we have the condition $N=1$, the derivation of the Bogomolnyi bound reduces to the original one by Schiff.[4] The energy is exactly proportional to the magnetic flux $\Phi=\int d^2x\sqrt{\gamma}B$ as follows

$$E=\int \mathrm{d}^2x\sqrt{\gamma}\left[\frac{\kappa^2}{2e^2}\frac{B^2}{|\phi|^2}+\frac{1}{2}\gamma^{ij}\overline{D_i\phi}D_j\phi+V(|\phi|)\right]$$

$$=\int \mathrm{d}^2x\sqrt{\gamma}\Bigg\{\frac{\kappa^2}{2e^2}\frac{1}{|\phi|^2}\left[B\pm\frac{e^3}{2\kappa^2}|\phi|^2(|\phi|^2-v^2)\right]^2$$

$$+\frac{1}{4}\gamma^{ij}(\overline{D_i\phi\mp i\sqrt{\gamma}\epsilon_{ik}\gamma^{kl}D_l\phi})(D_j\phi\pm i\sqrt{\gamma}\epsilon_{jm}\gamma^{mn}D_n\phi)$$

$$\pm\frac{ev^2}{2}B\pm\frac{i}{4}\frac{1}{\sqrt{\gamma}}\partial_i[\epsilon^{ij}(\overline{\phi}D_j\phi-\overline{D_j\phi}\phi)]\Bigg\} \tag{2.12}$$

$$\geqslant\left|\frac{ev^2}{2}\Phi\right|. \tag{2.13}$$

The first and second lines of Eq. (2.12) vanish by substituting the Bogomolnyi equations (2.7) and (2.8), and the last total-divergence term in the third line of Eq. (2.12) does not contribute to the energy since U(1) current decays rapidly at spatial asymptote.

We read possible boundary conditions of the scalar amplitude at spatial infinity from the scalar potential (2.3), that is, $\lim_{|x|\to\infty}|\phi|\to 0$ or v. The former is a nontopological soliton or vortex, and the latter a topological vortex. All of them carry the magnetic flux Φ [or equivalently U(1) charge $Q=e\int \mathrm{d}^2x\sqrt{\gamma}A_0|\phi|^2$ related by the Gauss' law], and spin

$$J\equiv\int \mathrm{d}^2x\sqrt{\gamma}\sqrt{\gamma}\epsilon_{ij}x^iT_0^j \tag{2.14}$$

$$=\int \mathrm{d}^2x\sqrt{\gamma}\frac{1}{2}\sqrt{\gamma}\epsilon_{ij}x^i(\overline{D^j\phi}D_0\phi+\overline{D_0\phi}D^j\phi) \tag{2.15}$$

$$=\frac{e^2}{8\kappa}\int \mathrm{d}^2x\sqrt{\gamma}x^i\partial_i(|\phi|^2-v^2)^2, \tag{2.16}$$

which distinguishes the Chern–Simons solitons from the solitons in Abelian Higgs model.

III. EXISTENCE OF A SOLUTION

Throughout this section, we denote that (R^2,γ) is a two-dimensional complete Riemann surface which is diffeomorphic to R^2 with the metric $\gamma_{ij}=b(x,y)\delta_{ij}$. We assume that there exist positive constants a_1 and a_2 with $a_1\leqslant b(x,y)\leqslant a_2$ for all $z=(x,y)\in R^2$ ($x^1=x$ and $x^2=y$ from here on). Let $\Delta=[1/\sqrt{\det(\gamma_{ij})}](\partial^2/\partial x^2+\partial^2/\partial y^2)$ ($\Delta_0=\partial^2/\partial x^2+\partial^2/\partial y^2$), $|\nabla u|(|\nabla u|_E)$ and $\delta(\delta_E)$ is the Laplacian, the norm of the gradient and Dirac-delta function with respect to the metric γ_{ij} (Euclidean metric). We denote $\mathrm{d}z=\mathrm{d}x\,\mathrm{d}y$, $\mathrm{d}V_\gamma=b(x,y)\mathrm{d}z$ and H_1^2 is the Sobolev space, which is the completion of $C_c^\infty(R^2)$ with respect to the norm $||w||=(\int_{R^2}|\nabla w|^2+w^2\,dV_\gamma)^{1/2}$.

In this section, we show the following Theorem.

Theorem 1: There exists a solution for the following self-dual Chern–Simons vortex equation on (R^2,γ);

$$\Delta w=e^w(e^w-1)+4\pi\sum_{k=1}^{n}\delta(z-z_k) \tag{3.1}$$

with the boundary condition $\lim_{|z|\to\infty} w=0$. Moreover, w satisfies $-ae^{-b|x|}\leqslant w(x)<0$ at infinity for some positive constants a and b.

Equation (3.1) comes from Eq. (2.9) by rescaling the scalar field $|\phi|=ve^{w}$ and the spatial coordinates $x^i\to(\kappa/e^2v^2)x^i$.

When there is no vortex, there is no nontrivial H_1^2 solution for

$$\Delta w=e^{w}(e^{w}-1) \tag{3.2}$$

because

$$\int_{\Omega} e^{w}(e^{w}-1)w\,dV_{\gamma}=-\int_{\Omega}|\nabla w|^2\,dV_{\gamma}+\int_{\partial\Omega} w\frac{\partial w}{\partial\eta}dS \tag{3.3}$$

for a sufficiently large smooth bounded domain Ω (see Ref. 4). Note that the second term of (3.3) goes to zero for suitably large Ω because $w\in H_1^2$. Applying the maximum principle for H_1^2 solution (cf. Theorem 8.1 of Ref. 19), we see that any H_1^2 solution w of Eq. (3.1) satisfies $w\leqslant 0$. For this, take $\Omega'=\{p\in R^2|w(p)>0\}$. Note that $z_k\notin\Omega'$. If Ω' is bounded, $w(p)\leqslant 0$ by taking $\Omega=\Omega'$ in Eq. (3.3). When Ω' is not bounded, take a sequence of smooth bounded domains $K(r)$, and $\partial K(r)$, the boundary of $K(r)$, for $r=1,2\ldots$, satisfying $K(r)\subset K(r+1), R^2=\cup K(r)$, and $\int_{\partial K(r)} w(\partial w/\partial\eta)\,dS\to 0$, as $r\to\infty$. Then,

$$\int_{\Omega'\cap K(r)} e^{w}(e^{w}-1)w\,dV_{\gamma}=-\int_{\Omega'\cap K(r)}|\nabla w|^2\,dV_{\gamma}+\int_{\partial\Omega'} w\frac{\partial w}{\partial\eta}dS+\int_{\Omega'\cap\partial K(r)} w\frac{\partial w}{\partial\eta}dS, \tag{3.4}$$

where the second term vanishes and third term goes to zero as $r\to\infty$. Therefore Ω' is the empty set and $w\leqslant 0$ on R^2.

Proof of Theorem 1: To show the existence of a solution, we follow Ref. 8. Take u_0 to be

$$u_0=-\sum_{k=1}^{n}\ln(1+\mu|z-z_k|^{-2}), \tag{3.5}$$

then

$$\Delta_0 u_0=-4\sum_{k=1}^{n}\frac{\mu}{(\mu+|z-z_k|^2)^2}+4\pi\sum_{k=1}^{n}\delta_E(z-z_k). \tag{3.6}$$

Define h_0, h, and B as

$$h_0=4\sum_{k=1}^{n}\frac{\mu}{(\mu+|z-z_k|^2)^2},\quad h=h_0/b,$$

and

$$B=e^{u_0}=\prod_{k=1}^{n}\frac{|z-z_k|^2}{\mu+|z-z_k|^2}. \tag{3.7}$$

Take $w=u_0+u$, then Eq. (3.1) turns out to be

$$\Delta u=Be^{u}(Be^{u}-1)+h. \tag{3.8}$$

A critical point of functional E defined on H_1^2 is a solution of Eq. (3.8) where

$$E(u)=\int_{R^2}|\nabla u|^2+(Be^u-1)^2+2hu\,dV_\gamma. \tag{3.9}$$

By the basic inequality,

$$(e^u-1)^2\geqslant\frac{|u|^2}{(1+|u|)^2}, \tag{3.10}$$

and

$$\int_{R^2}2hu\,dV_\gamma=\int_{R^2}2h_0\,u\,dz\leqslant 2\left(\int_{R^2}h_0^2\,dz\right)^{1/2}\left(\int_{R^2}u^2\,dz\right)^{1/2}. \tag{3.11}$$

Note that there exist constants c_1 and c_2 such that

$$2\left(\int_{R^2}h_0^2\,dz\right)^{1/2}\leqslant\frac{c_1}{\sqrt{\mu}} \tag{3.12}$$

and

$$\int_{R^2}(B-1)^2\,dV_\gamma\leqslant c_2. \tag{3.13}$$

Note that Eq. (3.13) holds when $dV_\gamma<cr^{3-\epsilon}\,dr$ for any positive constant c and any positive small constant ϵ. The second term of Eq. (3.9) can be estimated as

$$\int_{R^2}(Be^u-1)^2\,dV_\gamma\geqslant\frac{1}{2}\int_{R^2}B^2(e^u-1)^2-(B-1)^2\,dV_\gamma. \tag{3.14}$$

Let us define $\Omega_1=\{x\in R^2|B^2(x)\leqslant 1/2\}$ and $|\Omega_1|$ be the area of Ω_1. The finiteness of $|\Omega_1|$ implies

$$\int_{\Omega_1}\left(B^2-\frac{1}{2}\right)\frac{|u|^2}{(1+|u|)^2}dV_\gamma\geqslant\int_{\Omega_1}-\frac{1}{2}\frac{|u|^2}{(1+|u|)^2}dV_\gamma\geqslant-\frac{1}{2}|\Omega_1|. \tag{3.15}$$

From Eqs. (3.10) and (3.15), there is a constant c_3 that

$$\begin{aligned}\int_{R^2}B^2(e^u-1)^2\,dV_\gamma&\geqslant\int_{R^2}\frac{B^2|u|^2}{(1+|u|)^2}dV_\gamma\\&=\int_{R^2-\Omega_1}\frac{B^2|u|^2}{(1+|u|)^2}dV_\gamma+\int_{\Omega_1}\frac{B^2|u|^2}{(1+|u|)^2}dV_\gamma\\&\geqslant\frac{1}{2}\int_{R^2}\frac{|u|^2}{(1+|u|)^2}dV_\gamma-c_3.\end{aligned} \tag{3.16}$$

For $f\in H_1^1(R^2)$, $\int_{R^2}f^2dz\leqslant 1/4(\int_{R^2}|\nabla f|dz)^2$. Set $f=u^2$ and we have

$$\int_{R^2}u^4\,dz\leqslant\left(\int_{R^2}|u\nabla u|\,dV_\gamma\right)^2\leqslant\int_{R^2}u^2\,dz\int_{R^2}|\nabla u|^2\,dz, \tag{3.17}$$

and

$$\left(\int_{R^2} u^2\,dz\right)^2 \leqslant \left[\int_{R^2}\left(\frac{|u|}{1+|u|}\right)(1+|u|)|u|\,dz\right]^2$$
$$\leqslant \int_{R^2}\left(\frac{|u|}{1+|u|}\right)^2 dz \int_{R^2} u^2(1+|u|)^2\,dz$$
$$\leqslant 2\int_{R^2}\left(\frac{|u|}{1+|u|}\right)^2 dz \int_{R^2} u^2+u^4\,dz. \tag{3.18}$$

Using Eqs. (3.17) and (3.18), we obtain

$$\int_{R^2} u^2\,dz \leqslant 2\int_{R^2}\left(\frac{|u|}{1+|u|}\right)^2 dz\left(1+\int_{R^2}|\nabla u|^2\,dz\right). \tag{3.19}$$

By the Hölder inequality and Eq. (3.19), $u\in H_1^2(R^2)$ satisfies

$$\left(\int_{R^2} u^2\,dz\right)^{1/2} \leqslant \int_{R^2}\frac{|u|^2}{(1+|u|)^2}\,dz+2\int_{R^2}|\nabla u|_E^2\,dz+2. \tag{3.20}$$

From the above, there exists a constant c_4 such that

$$E(u)\geqslant \int_{R^2}|\nabla u|^2\,dV_\gamma+\frac{1}{2}\int_{R^2}\frac{|u|^2}{(1+|u|)^2}\,dV_\gamma$$
$$-\frac{c_1}{\sqrt{\mu}}\left[\int_{R^2}\frac{|u|^2}{(1+|u|)^2}\,dz+2\int_{R^2}|\nabla u|_E^2\,dz+2\right]-c_3-c_2 \tag{3.21}$$
$$\geqslant\left(1-\frac{2c_1}{\sqrt{\mu}}\right)\int_{R^2}|\nabla u|^2\,dV_\gamma+\left(\frac{1}{2}-\frac{c_1}{a_1\sqrt{\mu}}\right)\int_{R^2}\frac{|u|^2}{(1+|u|)^2}\,dV_\gamma-c_4, \tag{3.22}$$

where we used $\int_{R^2}|\nabla u|^2\,dV_\gamma=\int_{R^2}|\nabla u|_E^2\,dz$. From Eq. (3.20) and by taking large μ, there exist constants c_5 and c_6 such that

$$E(u)\geqslant c_5\left(\int_{R^2}|\nabla u|^2+u^2\,dV_\gamma\right)^{1/2}-c_6. \tag{3.23}$$

Therefore $E(u)$ is coercive on H_1^2 and $\inf_{u\in H_1^2}E(u)$ is finite. Moreover, $E(u)$ is weakly lower semicontinuous functional on H_1^2. We take a minimizing sequence $\{u_n\}$ for $\inf_{u\in H_1^2}E(u)$. Then $\{u_n\}$ is bounded on H_1^2, which has a subsequence $\{u_{n_k}\}$ converging to $u\in H_1^2$, a minimizer for $\inf_{u\in H_1^2}E(u)$. By the elliptic regularity, u is smooth. Finally, u satisfies Eq. (3.8).

Next we study the behavior of solution of Eq. (3.1). From above u is smooth, therefore $w=u_0+u$ is smooth on $R^2-\{z_1,\ldots,z_n\}$. By the argument below Eq. (3.3), $w\leqslant 0$, which implies $\Delta w=e^w(e^w-1)\leqslant 0$ on $R^2-\{z_1,\ldots,z_n\}$. Following Ref. 8, take $\beta=1-e^w$. On $R^2-\{z_1,\ldots,z_n\}$, β is smooth and satisfies

$$\Delta\beta=-e^w(|\nabla w|^2+e^w(e^w-1))\leqslant(\beta-1)^2\beta. \tag{3.24}$$

Applying the strong maximum principle for β, we have $\beta>0$ on R^2. Therefore $w<0$ on R^2. Since w is superharmonic on the ball $B(x,1)$ whose radius is one and center x lies in the outside of a large compact set, we have $-c||w||_{L^2(B(x,1))}\leqslant w(x)<0$ for some positive constant c (see Ref. 19). Therefore w decays to zero uniformly at infinity because $w\in L_2(R^2)$. For a sufficiently small positive constant δ, $-\delta<w<0$ implies

$$w\Delta_0 w = be^w(e^w-1)w \geqslant \frac{w^2}{2}. \tag{3.25}$$

By Jaffe and Taubes[20] methods (p. 83), $-ae^{-b|x|} \leqslant w(x) < 0$ for some positive constants a and b at infinity.

Remarks: Since a_2 does not appear in Eq. (3.22), we can generalize Theorem 1 if the integral value of Eq. (3.13) is bounded. For example, Theorem 1 holds if $c'\,\mathrm{d}r \leqslant dV_\gamma = b(x,y)dz \leqslant cr^{3-\epsilon}\,\mathrm{d}r$ at infinity for any positive constants c', c and any small positive constant ϵ.

IV. CONCLUDING REMARKS

We extend the existence and decay property of topological multivortex solutions of Chern–Simons Higgs theory in a general background curved space–time, which have been studied on flat space or on special background metric. Finding the borderline of growth or decaying condition of the given metric, which gives Theorem 1, is an interesting question. Related issues, e.g., the existence of nontopological solitons and vortices, self-dual topological vortices in a suitably decaying metric and Chern–Simons solitons under a dynamical gravity, need further study.

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Local existence proofs for the boundary value problem for static spherically symmetric Einstein–Yang–Mills fields with compact gauge groups

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We prove local existence and uniqueness of static spherically symmetric solutions of the Einstein–Yang–Mills (EYM) equations for an arbitrary compact semisimple gauge group in the so-called regular case. By this we mean the equations obtained when the rotation group acts on the principal bundle on which the Yang–Mills connection takes its values in a particularly simple way (the only one ever considered in the literature). The boundary value problem that results for possible asymptotically flat soliton or black hole solutions is very singular and just establishing that local power series solutions exist at the center and asymptotic solutions at infinity amounts to a nontrivial algebraic problem. We discuss the possible field equations obtained for different group actions and solve the algebraic problem on how the local solutions depend on initial data at the center and at infinity. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1463216]

I. INTRODUCTION

Over the last dozen years much has been learned about the classical interaction of Yang–Mills fields with the gravitational field of Einstein's general relativity. Most investigations have concentrated on Yang–Mills fields with the gauge group SU(2) starting with Bartnik and Mckinnon's[1] discovery of globally regular and asymptotically flat numerical solutions. Their global existence was analytically proved[2,3] and many further properties like stability of these particlelike or soliton solutions and the corresponding black hole solutions were investigated numerically as well as analytically. Moreover, many different matter fields can be minimally coupled to the gravitational and Yang–Mills fields, and corresponding spherically symmetric solutions have been, mostly numerically, but sometimes also analytically studied. We refer for the (hundreds of) references to the review article.[4]

Some similar phenomena were found for special models with gauge groups SU(n) for $n>2$,[5–8] and the general static spherically symmetric equations for general compact gauge groups were derived already quite early.[9,10]

For larger gauge groups than SU(2) the notion of spherical symmetry is no longer straight forward enough for a simple ansatz to work. Instead one needs to consider the possible actions of the symmetry group SO(3) or SU(2) by automorphisms of principal bundles over space–times whose structure group G is the gauge group of the Yang–Mills field. A conjugacy class of such automorphisms is characterized by a generator Λ_0 which is an element of a Cartan subalgebra $\mathfrak{h}$ of the complexified Lie algebra $\mathfrak{g}$ of G.[9,10] Mostly one restricts consideration to fields which are regular at the center or, for black hole fields, to those for which the Yang–Mills-curvature falls off sufficiently fast at infinity. In Ref. 11 these are called regular models. They also correspond to the ''no magnetic charge'' case in Ref. 12. For these group actions the element Λ_0 of $\mathfrak{h}$ must be an A_1-*vector* or *defining vector* of an $\mathfrak{sl}(2)$-subalgebra of $\mathfrak{g}$. That there is a remarkable variety of possible actions was shown by Bartnik[11] for the case where G is any group with Lie algebra

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$\mathfrak{su}(n)$. More generally, for arbitrary semisimple Lie algebras these A_1-vectors were classified by Mal'cev[13] and Dynkin[14] and can now also be obtained more conveniently from the theory of nilpotent orbits.[15]

One of these classes of actions of the symmetry group is somewhat distinguished. It corresponds to a principal A_1-vector in Dynkin's terminology and we will call it a *principal action*. To our knowledge almost all work for larger gauge groups has been done for this case.[8,16–18] For a slightly bigger class of actions, the ''generic'' class in Ref. 12 which we will call *regular*, the A_1-vector lies in the interior of a fundamental Weyl chamber. Brodbeck and Straumann[12,19] proved that all regular static asymptotically flat solutions are unstable against time dependent perturbations. They were able to do this without establishing existence or any properties of these solutions.

While it is easy to show that, at least for the regular case, some global solutions exist, namely those which arise by scaling from some imbedded SU(2) solutions, only isolated, mostly numerical, results have been obtained about more general global solutions for the principal SU(n) actions for $n=3, 4, 5$.[8,16–18,20]

The purpose of this paper is to discuss the classification of all the regular actions of SU(2) by automorphisms of G-principal bundles over spherically symmetric static space–times and to analyze the resulting Einstein–Yang–Mills field equations to the extent of establishing that the singular boundary value problem obtained for the globally regular and asymptotically flat solutions is well defined ''at both ends,'' namely at the center or the black hole horizon and at infinity. The local solutions that we obtain near these points are actually analytic. Consequently, there exists convergent powerseries representations for these solutions at least for small distances from the center, the black hole horizon and infinity. Essentially we generalize the results of Ref. 16 from the principal action on SU(n)-bundles to regular actions on bundles with (simply connected) semisimple compact structure groups. Although this represents only a first step in an analysis of possible (nonscaled) global solutions establishing these local existence theorems is already quite complicated. It is worthwhile to note, that if any of the local solutions can be extended to a global one, then the results of Brodbeck and Straumann[19] apply and show that the solution must be unstable.

For all these regular models it turns out that the Yang–Mills potential can be chosen (i.e., suitably gauged) to depend only on ℓ real-valued functions of a radial coordinate r where ℓ is the rank of the Lie algebra of the gauge group. In addition, the metric will be given by two more functions of r. These $(\ell+2)$ functions satisfy a nonlinear system of ordinary differential equations which has singularities at $r=0$, when $r\to\infty$, and at the horizon where $r=r_H$, say. We need to analyze these singularities to determine the ''initial conditions'' for these functions and the number of free parameters that can be chosen when solving the equations numerically, for example, by the method of shooting to a meeting point. In this paper we will only establish what these parameters are, we will not solve the equations numerically.

There are many models for which the A_1-vector Λ_0 is on the boundary of a Weyl chamber. To our knowledge almost no results have been obtained for them, but we have reason to believe that some of our methods may also be useful for these irregular models.

In Sec. II we review the description of the class of static spherically symmetric models and in Sec. III we show, starting from the field equations, that the special class of models we call regular can be reduced to the principal case for imbedded semisimple groups. We discuss the initial value problems somewhat informally in Sec. IV where we derive the relatively complicated way in which a solution depends on parameters chosen at the endpoints of the r-interval. In Sec. V we extend some elementary facts that are well known for SU(2)-solutions to general compact G. Finally, the major part of this paper consists of the proofs, divided into Sec. VI containing algebraic lemmas and the proof of the local existence theorems for the differential equation system in Sec. VII.

II. CLASSES OF SPHERICALLY SYMMETRIC YANG–MILLS CONNECTIONS

Since there is no natural action of the symmetry group on the principal bundle we need to consider all possibilities, i.e., all conjugacy classes of actions of SO(3), or for simplicity, SU(2) by

automorphisms on principal G-bundles P over space–time M which project onto isometries of M with orbits diffeomorphic to two-spheres. We assume throughout that G is a compact semisimple connected and simply connected Lie group.

Then these conjugacy classes are in one-to-one correspondence with integral elements Λ_0 of the closed fundamental Weyl chamber $\overline{W(S)}$ belonging to some basis S of the roots of $\mathfrak{g}$ for some chosen Cartan subalgebra $\mathfrak{h}$.[9–11] Here $\mathfrak{g}=(\mathfrak{g}_0)_{\mathbb{C}}$ stands for the complexification of the Lie algebra $\mathfrak{g}_0$ of the structure group G of P. If $\{\tau_i\}$ is a standard basis of the Lie algebra $\mathfrak{su}(2)$ such that $[\tau_i,\tau_j]=\epsilon_{ij}^k\tau_k$ then Λ_0 may be chosen such that

$$\Lambda_0=2i\lambda(\tau_3),$$

where λ is the (induced Lie algebra) homomorphism from the isotropy group I_{x_0} of the SU(2)-action on M at $x_0\in M$ determined by $k\cdot u_0=u_0\cdot\lambda(k)\forall k\in I_{x_0}$ if $u_0\in\pi^{-1}(x_0)$.

Wang's theorem[21,22] on connections that are invariant under actions transitive on the base manifold has been adapted to spherically symmetric space–time manifolds by Brodbeck and Straumann.[10] They show that in a Schwarzschild type coordinate system (t,r,θ,ϕ) and the metric

$$g=-NS^2dt^2+N^{-1}dr^2+r^2(d\theta^2+\sin^2\theta d\phi^2), \tag{2.1}$$

a gauge can always be chosen such that the Yang–Mills-connection form is locally given by

$$A=\tilde{A}+\hat{A},$$

where $\tilde{A}$ is a one-form on the quotient space parametrized by the r and t coordinates and

$$\hat{A}=\Lambda_1 d\theta+(\Lambda_2\sin\theta+\Lambda_3\cos\theta)d\phi, \tag{2.2}$$

where $\Lambda_3=-(i/2)\Lambda_0$ is the constant isotropy generator and Λ_1 and Λ_2 are functions of r and t that satisfy

$$[\Lambda_2,\Lambda_3]=\Lambda_1 \quad \text{and} \quad [\Lambda_3,\Lambda_1]=\Lambda_2. \tag{2.3}$$

Since we only consider static fields we can assume that Λ_1 and Λ_2 depend only on r. Moreover, we will also concentrate on the ''magnetic'' case and assume that the part $\tilde{A}$ of the gauge potential which contributes ''electric'' or ''Coulomb'' terms vanishes, i.e., we put

$$\tilde{A}=0.$$

This condition is not as restrictive as it seems. For, as proved in Ref. 12, it also follows in the regular case (defined below) if the field is smooth at the center $r=0$ and falls off sufficiently fast at infinity.

So far we still have infinitely many possible actions of SU(2) on the principal bundle, namely one for each element in the intersection $\overline{W(S)}\cap I$ of the fundamental Weyl chamber and the integral lattice $I:=\ker(\exp|_{\mathfrak{h}})$. However, since we want the Yang–Mills-connection to be regular also at a center ($r=0$, defined as a connected set of fixed points of the SU(2)-action on M) and/or the Yang–Mills-field to fall off in an asymptotic region (have no magnetic charge according to Ref. 12) we must have

$$[\Omega_1^0,\Omega_2^0]=\Lambda_3 \quad \text{and/or} \quad [\Omega_1^\infty,\Omega_2^\infty]=\Lambda_3, \tag{2.4}$$

where

$$\Omega_i^{0,\infty}:=\lim_{r\to 0,\infty}\Lambda_i(r), \quad (i=1,2).$$

In other words, in these limits there must exist a Lie algebra homomorphism of $\mathfrak{su}(2)$ into $\mathfrak{g}_0$. This is shown most easily by observing that the Einstein equations would otherwise lead to infinite pressure or density at a center.

Since Λ_3 is constant, however, Eqs. (2.4) represent not only conditions on $\Lambda_1(r)$ and $\Lambda_2(r)$, but also on Λ_3 and hence on Λ_0 which must now be the generating (or defining) vector of an $\mathfrak{sl}(2)$ (i.e., A_1) subalgebra of $\mathfrak{g}$. (If both limits exist it then also follows that there must be an automorphism of $\mathfrak{g}$ taking Ω_i^0 into Ω_i^∞.) The set of these so-called A_1-vectors, however, is finite [and in one-to-one correspondence with conjugacy classes of $\mathfrak{sl}(2)$ subalgebras]. It has been studied and tabulated by Mal'cev[13] and Dynkin[14] and is described by so-called weighted Dynkin diagrams (called *characteristics* in Ref. 14), where to each simple root in the diagram is associated a number from the set $\{0,1,2\}$. (See Ref. 15 for a more recent exposition). These numbers represent the values of the simple roots on the generating vector Λ_0 chosen such that it lies in $\overline{W(S)}$.

Thus these tables serve as a classification of all the spherically symmetric magnetic Einstein–Yang–Mills models which are regular at the center and/or obey the standard fall-off conditions at infinity for any given compact gauge group.

III. FIELD EQUATIONS AND REDUCTION OF THE REGULAR MODELS

The field equations are well known. We state them here in a form following Ref. 10 for the static regular case only, where Λ_0 is an A_1-vector. Let the space–time metric g be given by (2.1) and the Yang–Mills-potential $A=\hat{A}$ by (2.2). Define, in addition to Λ_0

$$\Lambda_\pm := \mp\Lambda_1 - i\Lambda_2,$$

so that the Wang Eqs. (2.3) become

$$[\Lambda_0,\Lambda_\pm] = \pm 2\Lambda_\pm. \tag{3.1}$$

Then $\Lambda_+(r)$ and $\Lambda_-(r)\}$ are $\mathfrak{g}$-valued functions, Λ_0 a (constant) vector in the fundamental Weyl chamber of $\mathfrak{h}$ and $\{\Lambda_0,\Lambda_+,\Lambda_-\}$ is a standard triple in the limit $r\to 0$ or $r\to\infty$ for the Lie algebra $\mathfrak{g}$. Now $\mathfrak{h}$ is the Cartan subalgebra of the complexified Lie algebra $\mathfrak{g}$, i.e., $\mathfrak{h}=\mathfrak{h}_0\oplus i\mathfrak{h}_0$, where $\mathfrak{h}_0$ is the real Cartan subalgebra of a compact real form $\mathfrak{g}_0$ of $\mathfrak{g}$, and we choose conventions such that the conjugation operator $c:\mathfrak{g}\to\mathfrak{g}$ satisfies $c(X+iY)=X-iY\,\forall X,Y\in\mathfrak{g}_0$. Then

$$\Lambda_- = -c(\Lambda_+), \tag{3.2}$$

so that the dependent variables consist only of N, S, and the components of Λ_+.
The field equations now reduce to

$$m' = (NG + r^{-2}P), \tag{3.3}$$

$$S^{-1}S' = 2r^{-1}G, \tag{3.4}$$

$$r^2N\Lambda_+'' + 2(m - r^{-1}P)\Lambda_+' + \mathcal{F} = 0, \tag{3.5}$$

$$[\Lambda_+,\Lambda_-'] - [\Lambda_+',\Lambda_-] = 0, \tag{3.6}$$

where $'=d/dr$ and

$$N =: 1 - \frac{2m}{r}, \quad G := \frac{1}{2}(\Lambda_+',\Lambda_-'), \quad P := -\frac{1}{2}(\hat{F},\hat{F}),$$

$$\hat{F} := \frac{i}{2}(\Lambda_0 - [\Lambda_+,\Lambda_-]), \tag{3.7}$$

$$\mathcal{F} := -i[\hat{F}, \Lambda_+]. \tag{3.8}$$

Here $(,)$ is an invariant inner product on $\mathfrak{g}$. It is determined up to a factor on each simple component of a semisimple $\mathfrak{g}$ and induces a norm $|\cdot|$ on (the Euclidean) $\mathfrak{h}$ and therefore its dual. We choose these factors so that $(,)$ is a positive multiple of the Killing form on each simple component. If they are chosen such that the length of the long simple roots are all 1 then the equations will agree with those in Ref. 16 for the principal SU(n) case.

Note that $G \geqslant 0$ and also $P \geqslant 0$. This follows from (3.2), $c(\hat{F}) = \hat{F}$, and the fact that $\langle X|Y\rangle := -[c(X), Y]$ is a Hermitian inner product on $\mathfrak{g}$ [cf. (6.1)]. Energy density, radial and tangential pressure are then given by

$$4\pi e = r^{-2}(NG + r^{-2}P), \quad 4\pi p_r = r^{-2}(NG - r^{-2}P),$$

$$4\pi p_\theta = r^{-4}P. \tag{3.9}$$

We now choose a Chevalley–Weyl basis of $\mathfrak{g}$ using mostly the notation of Ref. 23. Let R be the set of roots in $\mathfrak{h}^*$, $S = \{\alpha_1, \ldots, \alpha_\ell\}$ a base of R (ℓ being the rank of $\mathfrak{g}$), define

$$\langle \alpha, \beta \rangle := \frac{2(\alpha, \beta)}{|\beta|^2},$$

$$(\mathbf{t}_\alpha, X) := \alpha(X) \forall X \in \mathfrak{h},$$

and

$$\mathbf{h}_\alpha := \frac{2\mathbf{t}_\alpha}{|\alpha|^2}.$$

Then $\{\mathbf{h}_i := \mathbf{h}_{\alpha_i}, \mathbf{e}_\alpha, \mathbf{e}_{-\alpha} | i = 1, \ldots, \ell, \alpha \in R\}$ is a basis of $\mathfrak{g}$ corresponding to the decomposition

$$\mathfrak{g} = \mathfrak{h} \oplus \bigoplus_{\alpha \in R^+} (\mathfrak{g}_\alpha \oplus \mathfrak{g}_{-\alpha}),$$

(R^+ being the set of positive roots with respect to the base S) for which we choose the conventions

$$[\mathbf{e}_\alpha, \mathbf{e}_{-\alpha}] = \mathbf{h}_\alpha, \quad [\mathbf{e}_{-\alpha}, \mathbf{e}_{-\beta}] = -[\mathbf{e}_\alpha, \mathbf{e}_\beta],$$

$$(\mathbf{e}_\alpha, \mathbf{e}_{-\alpha}) = \frac{2}{|\alpha|^2}. \tag{3.10}$$

Now it follows directly[14] from the defining relations

$$[\mathbf{e}_0, \mathbf{e}_\pm] = \pm 2\mathbf{e}_\pm, \quad [\mathbf{e}_+, \mathbf{e}_-] = \mathbf{e}_0,$$

of an $\mathfrak{sl}(2)$-subalgebra span$\{\mathbf{e}_0, \mathbf{e}_\pm\}$ of $\mathfrak{g}$, with the help of

$$[\mathbf{h}, \mathbf{e}_\alpha] = \alpha(\mathbf{h})\mathbf{e}_\alpha,$$

that $\mathbf{e}_0$ can only be an A_1-vector provided

$$\alpha(\mathbf{e}_0) = 2 \quad \text{for some} \quad \alpha \in R.$$

Thus, if we let

$$\Lambda_0 = \sum_{i=1}^{\ell} \lambda_i \mathbf{h}_i \in \mathfrak{h}. \tag{3.11}$$

then Eqs. (3.1) imply that

$$\Lambda_+(r) = \sum_{\alpha \in S_\lambda} w_\alpha(r) \mathbf{e}_\alpha,$$

where

$$S_\lambda := \{\alpha \in R \mid \alpha(\Lambda_0) = 2\}, \tag{3.12}$$

is a set of roots depending only on the homomorphism λ or, equivalently, on the coefficients λ_i in (3.11).

Similarly we have

$$\Lambda_-(r) = \sum_{\alpha \in S_\lambda} v_\alpha(r) \mathbf{e}_{-\alpha}, \tag{3.13}$$

but by (3.2) and the fact that complex conjugation maps

$$c: \mathbf{h}_i \mapsto -\mathbf{h}_i, \quad \mathbf{e}_\alpha \mapsto -\mathbf{e}_{-\alpha},$$

it follows that

$$v_\alpha(r) = \overline{w}_\alpha(r).$$

Our system is thus determined once the two real functions $m(r)$ and $S(r)$ and the complex functions $w_\alpha(r)$ for all $\alpha \in S_\lambda$ are known.

If we now substitute (3.13) into Eqs. (3.3)–(3.8) we need to calculate the Lie brackets between the various $\mathbf{e}_\alpha$ for $\alpha \in S_\lambda$. In general, this may produce many more equations than dependent variables. On the other hand the Yang–Mills-potential $\hat{A}$ determined by Λ_+ still contains some gauge freedom. It is not known, at present, whether there is any systematic method to solve this system of equations.

However, as Brodbeck and Straumann[12] have observed, there are special symmetry actions for which this system of equations is much simpler, in fact, very similar to the principal SU(n) case. This happens when Λ_0 is a vector in the *open* fundamental Weyl chamber of $\mathfrak{h}$. They call these models generic, but since, as we will see, they are really a small minority of all possible ones we will call them *regular*.

In the following Λ_0 is not required to be an A_1-vector.

Theorem 1 (Brodbeck–Straumann[12]): *If Λ_0 is in the open Weyl chamber $W(S)$ then the set S_λ is a* Π*-system, i.e., satisfies*

(*i*) *if $\alpha, \beta \in S_\lambda$ then $\alpha - \beta \notin R$,*

(*ii*) *S_λ is linearly independent,*

and is therefore the base of a root system R_λ which generates a Lie subalgebra $\mathfrak{g}_\lambda$ of $\mathfrak{g}$ spanned by $\{\mathbf{h}_\alpha, \mathbf{e}_\alpha, \mathbf{e}_{-\alpha} | \alpha \in R_\lambda\}$.

Moreover, if $\mathfrak{h}_\lambda := \operatorname{span}\{\mathbf{h}_\alpha | \alpha \in S_\lambda\}$ and $\mathfrak{h}_\lambda^\perp := \cap_{\alpha \in S_\lambda} \ker \alpha$ then

$$\mathfrak{h} = \mathfrak{h}_\lambda'' \oplus \mathfrak{h}_\lambda^\perp \quad \textit{and} \quad \Lambda_0 = \Lambda_0'' + \Lambda_0^\perp \quad \textit{with} \quad \Lambda_0'' = \sum_{\alpha \in R_\lambda^+} \mathbf{h}_\alpha.$$

If Λ_0 is an A_1-vector then $\Lambda_0^\perp = 0$ (but $\mathfrak{h}_\lambda^\perp$ need not be trivial).

In particular, Λ_0'' is twice the lowest weight vector of $\mathfrak{h}_\lambda$ and we have by the definitions of S_λ and $\mathfrak{h}_\lambda^\perp$

$$\alpha(\Lambda_0'')=2 \quad \text{and} \quad \alpha(\Lambda_0^{\perp})=0 \quad \forall \quad \alpha\in S_\lambda\,.$$

We will from now on only consider the regular case.

First, Λ_+ can be treated as a $\mathfrak{g}_\lambda$-valued function

$$\Lambda_+(r)=\sum_{j=1}^{\ell_\lambda} w_j(r)\tilde{\mathbf{e}}_j\,,$$

where now $\{\tilde{\alpha}_1,\ldots,\tilde{\alpha}_{\ell_\lambda}\}$ is the base of S_λ and $\tilde{\mathbf{e}}_j:=\mathbf{e}_{\tilde{\alpha}_j}$. Moreover, $\Lambda_0''=\Sigma_j^{\ell_\lambda}\lambda_j''\tilde{\mathbf{h}}_j$ with $\tilde{\mathbf{h}}_j:=\mathbf{h}_{\tilde{\alpha}_j}$. Then, by (3.7) noting also that $\tilde{\alpha}_j(\Lambda_0^{\perp})=0$,

$$\begin{aligned}\hat{F}&=\frac{i}{2}\left(\sum_{j=1}^{\ell_\lambda}\lambda_j''\tilde{\mathbf{h}}_j+\Lambda_0^{\perp}-\left[\sum_{j=1}^{\ell_\lambda} w_j\tilde{\mathbf{e}}_j,\sum_{k=1}^{\ell_\lambda}\overline{w}_k\tilde{\mathbf{e}}_k\right]\right)\\&=\frac{i}{2}\left(\sum_{j=1}^{\ell_\lambda}(\lambda_j''-|w_j|^2)\tilde{\mathbf{h}}_j+\Lambda_0^{\perp}\right),\end{aligned}\tag{3.14}$$

where (3.10) was used and the fact that differences of two simple roots are not roots which implies that

$$[\mathbf{e}_\alpha,\mathbf{e}_{-\beta}]=0 \quad \forall \quad \alpha,\beta\in S_\lambda\,, \quad \alpha\neq\beta.\tag{3.15}$$

Substituting this expression into (3.8) gives

$$\begin{aligned}\mathcal{F}=&\frac{1}{2}\sum_{j,k=1}^{\ell_\lambda} w_j\langle\tilde{\alpha}_j,\tilde{\alpha}_k\rangle(\lambda_k''-|w_k|^2)\tilde{\mathbf{e}}_j\\&+\frac{1}{2}\sum_{j=1}^{\ell_\lambda} w_j[\Lambda_0^{\perp},\tilde{\mathbf{e}}_j].\end{aligned}\tag{3.16}$$

But since $[\Lambda_0^{\perp},\tilde{\mathbf{e}}_k]=\tilde{\alpha}_k(\Lambda_0^{\perp})\tilde{\mathbf{e}}_k=0$, in view of the definition of $S_\lambda^{\perp}$, the last term vanishes. Equation (3.5), therefore, becomes

$$r^2Nw_j''+2(m-r^{-1}P)w_j'+\frac{1}{2}\sum_{k=1}^{\ell_\lambda} w_jc_{jk}(\lambda_k''-|w_k|^2)=0,$$

where we have introduced

$$c_{jk}:=\langle\tilde{\alpha}_j,\tilde{\alpha}_k\rangle,$$

for the Cartan matrix of $\mathfrak{g}_\lambda$ and where now

$$P=\frac{1}{8}\sum_{j,k=1}^{\ell_\lambda}(\lambda_j''-|w_j|^2)h_{jk}(\lambda_k''-|w_k|^2)+|\Lambda_0^{\perp}|^2$$

$$\text{with} \quad h_{jk}:=\frac{2\langle\tilde{\alpha}_j,\tilde{\alpha}_k\rangle}{|\tilde{\alpha}_j|^2},\tag{3.17}$$

$$G=\sum_{j=1}^{\ell_\lambda}\frac{|w_j'|^2}{|\tilde{\alpha}_j|^2}.\tag{3.18}$$

Finally, (3.6) simply becomes in view of (3.10)

$$\sum_{j,k=1}^{\ell_\lambda} (w_j \overline{w}_k' - w_j' \overline{w}_k)[\mathbf{e}_{\tilde{\alpha}_j}, \mathbf{e}_{-\tilde{\alpha}_k}] = \sum_{j=1}^{\ell_\lambda} (w_j \overline{w}_j' - w_j' \overline{w}j)\tilde{\mathbf{h}}_j = 0, \tag{3.19}$$

so that the phase of w_j is constant and may be chosen to be zero by a gauge transformation. One can thus assume that the $w_j(r)$ are real-valued functions.

It remains to determine the subalgebra $\mathfrak{g}_\lambda$ for a given A_1-vector Λ_0 in the open fundamental Weyl chamber.

First, we note that for a semisimple group for which the Cartan subalgebra $\mathfrak{h}$ splits into an orthogonal sum $\mathfrak{h} = \oplus \mathfrak{h}_k$ the decomposition in Theorem 1 splits into corresponding decompositions of each of the $\mathfrak{h}_k$. So we need only investigate the regular actions of simple Lie groups.

Now the A_1-vector in the Cartan subalgebra $\mathfrak{h}$ of a semisimple Lie algebra $\mathfrak{g}$ is uniquely given by the numbers

$$\boldsymbol{\chi} = (\chi_1, \ldots, \chi_\ell) := (\alpha_1(\Lambda_0), \ldots, \alpha_\ell(\Lambda_0)), \tag{3.20}$$

called the *characteristic* in Ref. 14. It is known[14,15] that if Λ_0 is in the closed fundamental Weyl chamber then $\chi_k \in \{0,1,2\}$, and all possible such characteristic have been found and tabulated. It is clear from the definition of S_λ in (3.12) that $\chi_k = 2\ \forall\ k$ for $\mathfrak{h}_\lambda$. Such A_1-vectors define *principal* A_1-subalgebras and thus *principal actions* of SU(2) on the bundle. We now have

Theorem 2:

(*i*) *The possible regular A_1-subalgebras of simple Lie algebras consist of the principal subalgebras of all Lie algebras A_ℓ, B_ℓ, C_ℓ, D_ℓ, E_ℓ, F_4 and G_2 and of those subalgebras of $A_\ell = \mathfrak{sl}(\ell+1)$ with even ℓ corresponding to partitions $[\ell+1-k,k]$ for any integer $k = 1,\ldots,\ell/2$ or, equivalently, characteristic* (22..211..112..22) (2k '1's *in the middle,* '2's *in all other positions*);

(*ii*) *the Lie algebra $\mathfrak{g}_\lambda$ is equal to $\mathfrak{g}$ in the principal case, and for A_ℓ with even ℓ equal to $A_{\ell-1}$ for $k=1$ and to $A_{\ell-k} \oplus A_{k-1}$ for $k = 2,\ldots,\ell/2$;*

(*iii*) in the principal case $\mathfrak{h}_\lambda'' = \mathfrak{h}$. *For all A_1-subalgebras of A_ℓ with even ℓ the orthogonal space $\mathfrak{h}_\lambda^\perp$ is one-dimensional.*

Proof: Part (i) follows quite easily from the discussion and the tables in Ref. 15 (Secs. 5.3 and 4.4).

For part (ii) that $\mathfrak{h}_\lambda = \mathfrak{h}$ in the principal case is obvious. To compute S_λ for a given $\ell = 2m$ and given $k > 0$ note that all positive roots of A_ℓ are of the form $\Sigma_{p=j}^k \alpha_p$ for $1 \leqslant j \leqslant k \leqslant 2m$ so that using that $\alpha_i(\Lambda_0) = 2$ for $i = 1,\ldots,m-k$ and $i = m+k+1,\ldots,2m$ and $\alpha_i(\Lambda_0) = 1$ otherwise one sees that

$$S_\lambda = \bigcup_{i=1}^{m-k} \alpha_i \cup \bigcup_{j=1}^{2k-1} (\alpha_{m-k+j} + \alpha_{m-k+j+1}) \ \cup \bigcup_{i=m+k+1}^{2m} \alpha_i . \tag{3.21}$$

Recalling that for A_ℓ

$$\langle \alpha_i, \alpha_j \rangle = \begin{cases} 2 & \text{if } i = j \\ -1 & \text{if } |i-j| = 1, \\ 0 & \text{otherwise} \end{cases}$$

it is seen immediately that the Cartan matrix for S_λ is the one for $A_{\ell-1}$ if $k=1$ while it takes a simple reordering of the roots to verify the statement in (ii) for $k = 2,\ldots,\ell/2$.

(iii) That $\mathfrak{h}_\lambda'' = \mathfrak{h}$ in the principal case is obvious from the definition and that $\dim S_\lambda^\perp = 1$ follows from the observation that $\alpha(X) = 0\ \forall\ \alpha \in S_\lambda$ amounts to $2m-1$ linearly independent equations according to (3.21). □

In summary, we have shown that all regular models can be reduced to those with the principal action for semisimple gauge groups. Also the term $\Lambda_0^{\perp}$ occuring in (3.14), (3.16), and (3.17) can now be dropped.

IV. CONSTRUCTING LOCAL SOLUTIONS REGULAR AT THE CENTER, HORIZON OR AT INFINITY

So far we have shown that the static spherically symmetric and magnetic EYM equations for the regular action reduce to those for the principal action for semisimple gauge groups. (We now drop the index λ from $\mathfrak{g}$, $\mathfrak{h}$, etc.) They consist of (3.4), which can be integrated easily once the other equations are solved, and

$$m' = (NG + r^{-2}P), \tag{4.1}$$

$$r^2 N w_j'' + 2(m - r^{-1}P)w_j' + \frac{1}{2}\sum_{k=1}^{\ell} w_j c_{jk}(\lambda_k - w_k^2) = 0, \tag{4.2}$$

where the w_k are real-valued functions of r, $(c_{ij}) := (\langle \alpha_j, \alpha_k \rangle)$ is the Cartan matrix of the reduced structure group, and

$$P = \frac{1}{8}\sum_{j,k=1}^{\ell} (\lambda_j - w_j^2) h_{jk} (\lambda_k - w_k^2), \tag{4.3}$$

$$G = \sum_{j=1}^{\ell} \frac{w_j'^2}{|\alpha_j|^2}, \tag{4.4}$$

$$h_{jk} = \frac{2c_{jk}}{|\alpha_j|^2}, \tag{4.5}$$

$$\lambda_j = 2\sum_{k=1}^{\ell} (c^{-1})_{jk}. \tag{4.6}$$

The expressions for components λ_k of the A_1-vector Λ_0 follow from (3.20) and the fact that for the principal action $\chi_k = 2 \forall k$.

In this section we will discuss the general problem of finding solutions that are regular at the center or at the horizon and have an appropriate fall off as $r \to \infty$. Proofs will be given later in Secs. VI and VII.

Equations (4.1) and (4.2) are very similar to the corresponding ones in the principal SU(n) case analyzed in detail in Ref. 16. So we can expect most of those results to generalize. First of all, when the dependent variables m and w_k are expanded in power series in terms of r at $r = 0$, in terms of $r - r_H$ at $r = r_H$, and in terms of r^{-1} at infinity (under the assumption that all the quantities are finite in these limits) then (4.1) and (4.2) yield a system of algebraic equations. For example, at $r = 0$ with $f(r) = \Sigma_{k=0}^{\infty} f_k r^k$ we find

$$m_{k+1} = \frac{1}{k+1}\left(G_k + P_{k+2} - 2\sum_{h=2}^{k-2} m_{k-h} G_h \right), \tag{4.7}$$

$$\sum_{j=1}^{\ell} (A_{ij} - k(k+1)\delta_{ij}) w_{j,k+1} = b_{i,k}, \tag{4.8}$$

for $k = 0,1,2,\ldots$ where

TABLE I. The eigenvalues of the coefficient matrix $\mathbf{A}$ for the simple Lie algebras are given by the set $\mathrm{spec}(\mathbf{A})=\{k(k+1)|k\in\mathcal{E}\}$. For the classical Lie algebras the table entry gives k_j for $j=1,2,\ldots=\ell=\mathrm{rank}(\mathfrak{g})$. Note that $k=1$ belongs to $\mathcal{E}$ for all Lie algebras.

Lie algebra	$\mathcal{E}$
A_ℓ	j
B_ℓ	$2j-1$
C_ℓ	$2j-1$
D_ℓ	$\begin{cases} 2j-1 & \text{if } j<(\ell+2)/2 \\ \ell-1 & \text{if } j=(\ell+2)/2 \\ 2j-3 & \text{if } j>(\ell+2)/2 \end{cases}$
E_6	1,4,5,7,8,11
E_7	1,5,7,9,11,13,17
E_8	1,7,11,13,17,19,23,29
F_4	1,5,7,11
G_2	1,5

$$A_{ij}:=w_{i,0}c_{ij}w_{j,0}, \tag{4.9}$$

and the $b_{i,k}$ are complicated expressions involving lower order terms. For the lowest order terms we find

$$m_0=m_1=m_2=0, \quad w_{i,0}^2=\lambda_i, \quad w_{i,1}=0. \tag{4.10}$$

That $r=0$ is a singular point for the system (4.1),(4.2) manifests itself in the fact that the initial data at $r=0$ for regular solutions are not simply the values of the functions m, w_i, and w_i' but that some of these values are restricted like in (4.10) and some higher order coefficients in the power series for the w_i remain arbitrary, namely for those orders k for which the matrix $\mathbf{A}=(A_{ij})$ has eigenvalue $k(k+1)$. It now turns out that the eigenvalues of $\mathbf{A}$ are precisely of this form for certain integer values of k. In fact, for the simple Lie algebras we can calculate the spectrum directly from the Cartan matrix and find the values given in Table I. The proof for the classical Lie algebras of arbitrary rank follows from the properties of the root system and results at the end of Sec. 6.

The eigenspaces for the simple Lie algebras are all onedimensional except for D_ℓ where certain "middle" eigenvalues occur twice. For semisimple Lie algebras the matrix $\mathbf{A}$ will be a direct sum of those for the simple components and thus may have multiple eigenvalues.

It is now clear that a formal power series solution of Eqs. (4.1) and (4.2) is well defined and contains ℓ free parameters provided Eq. (4.8) can be solved, i.e., provided the vector $\mathbf{b}_k:=(b_{1,k},\ldots,b_{\ell,k})$ lies in the left kernel of $(\mathbf{A}-k(k+1)\mathbb{I})$. Since $\mathbf{b}_k$ is a very complicated expression this is cumbersome to prove in general. In Ref. 16 the proof for $G=\mathrm{SU}(n)$ was achieved using properties of a class of orthogonal polynomials, an approach that does not easily generalize to other groups. In Secs. VI and VII we present a proof that depends directly on the root structure of the Lie algebra $\mathfrak{g}$ treated as an $\mathfrak{sl}(2,\mathbb{C})$-module.

The structure of the recursion relations for the power series of regular solutions in r^{-1} at infinity is very similar to the one at $r=0$. At the remaining singular point of (4.2), namely at a regular horizon $(N(r_H)=0, N'(r_H)>0)$, however, the only conditions on initial values turn out to be some inequalities.

Calculating the formal power series is indeed necessary to start off numerical integration when searching for global regular solutions. For an existence and uniqueness proof, however, it is more convenient to recast the equations in a form to which the following (slight generalization of a) theorem by Breitenlohner, Forgács, and Maison[3] applies.

Theorem 3: *The system of differential equations*

$$t\frac{du_i}{dt}=t^{\mu_i}f_i(t,u,v),\quad i=1,\ldots,m, \tag{4.11}$$

$$t\frac{dv_j}{dt}=-h_j(u)v_j+t^{\nu_j}g_j(t,u,v),\quad j=1,\ldots,n, \tag{4.12}$$

where μ_i, ν_j *are integers greater than 1,* f_i *and* g_j *analytic functions in a neighborhood of* $(0,c_0,0)\in\mathbb{R}^{1+m+n}$, *and* $h_j:\mathbb{R}^m\to\mathbb{R}$ *functions, positive in a neighborhood of* $c_0\in\mathbb{R}^m$, *has a unique analytic solution* $t\mapsto(u_i(t),v_j(t))$ *such that*

$$u_i(t)=c_i+O(t^{\mu_i})\quad \textit{and}\quad v_j(t)=O(t^{\nu_j}), \tag{4.13}$$

for $|t|<R$ *for some* $R>0$ *if* $|c-c_0|$ *is small enough. Moreover, the solution depends analytically on the parameters* c_i.

Proof: By the standard method solving the differential equation with initial data is replaced by finding a fixed point for the map $T:(u,v)\mapsto(\tilde{u},\tilde{v})$ with

$$\tilde{u}_i(t)=c_i+\int_0^t \tau^{\mu_i-1}f_i[\tau,u(\tau),v(\tau)]\,d\tau, \tag{4.14}$$

$$\tilde{v}_j(t)=t^{-\kappa_j}\int_0^t \tau^{\kappa_j\nu_j-1}\hat{g}_i[\tau,u(\tau),v(\tau)]\,d\tau, \tag{4.15}$$

where $\kappa_j:=h_j(c)$ and $\hat{g}(j)(t,u,v):=g_j(t,u,v)-t^{-\nu_j}[h_j(u)-h_j(c)]v_j$. To show that T is a contracting map on a suitable Banach space one can use a method very similar to the one in Ref. 16.□

To bring systems (4.1) and (4.2) into a form that satisfies the hypotheses of theorem 3 it is necessary to make a suitable transformation of the variables m and w_j. The proofs that this can be done are basically equivalent to showing that the formal power series exist and are given in Sec. VII. We then have

Theorem 4: *Systems* (4.1) *and* (4.2) *has an analytic solution for small* r *of the form*

$$w_i(r)=w_{i,0}+\sum_{j=1}^{\ell} C_{ij}r^{k_j+1}u_j(r),\quad i=1,\ldots,\ell \tag{4.16}$$

where $C=(C_{ij})$ *is a nonsingular matrix whose* j*th column is an eigenvector to eigenvalue* $k_j(k_j+1)$ *of the matrix* **A**. *The solution is uniquely determined by the initial values* $u_j(0)=\beta_j$ *for arbitrary* β_j. *The function* $m(r)$ *is then determined and satisfies* $m(r)=O(r^3)$ *for small* r.

Note that the $w_{i,0}$ are determined up to the sign by (4.10). From (7.18), we see that solutions from theorem 4 satisfy $P=O(r^4)$ and $G=O(r^2)$. It follows that for these solutions all physical quantities such as the pressure and mass density are finite at $r=0$.

The situation is rather similar for solutions analytic in r^{-1} near infinity. We have, with the same matrix C.

Theorem 5: *The systems (4.1) and (4.2) has an analytic solution for small* $z=r^{-1}$ *of the form*

$$w_i(r)=w_{i,\infty}+\sum_{j=1}^{\ell} C_{ij}r^{-k_j}u_j(r^{-1}),\quad i=1,\ldots,\ell, \tag{4.17}$$

$$m(r)=m_\infty+O(r^{-1}). \tag{4.18}$$

The solution is uniquely determined by the initial values $u_j(0)=\alpha_j$ *and* m_∞ *for arbitrary* α_j *and* m_∞.

Again $w_{i,\infty}$ is determined up to the sign by $w_{i,\infty}^2=\lambda_i$. An overall sign in $w_i(r)$ does not affect the Yang–Mills field nor the geometry and physics. But $w_{i,0}$ and $w_{i,\infty}$ may have the same or different signs for global solutions.

Finally we have the corresponding theorem for local solutions near a regular horizon.

Theorem 6: *The systems (4.1) and (4.2) has a solution analytic in $t=r-r_H$ for small t at a regular horizon, i.e., where $N(r_H)=0$ and $N'(rH)>0$. The solution is uniquely determined by the values of $w_j(r_H)$ which must be chosen such that*

$$N'(r_H)=\frac{1}{r_H}-\frac{2}{r_H^3}P(r_H)>0, \tag{4.19}$$

or, equivalently,

$$2P(r_H)=\frac{1}{4}\sum_{i,j=1}^{\ell}(\lambda_i-w_i(r_H))h_{ij}(\lambda_j-w_j(r_H))<r_H^2. \tag{4.20}$$

V. ELEMENTARY PROPERTIES AND SCALED SOLUTIONS

The observation already made in Ref. 1 for SU(2) and generalized to SU(n) that global solutions, if they exist, must be bounded by their values at infinity (or zero) is easily extended to the regular case for arbitrary G.

Theorem 7: *If a solution $(m,w_1,\ldots,w_\ell)$ is defined and C^2 in the connected outer domain $D:=\{r|0\leqslant r_H\leqslant r<\infty\}$ (where $N(r)>0$) and if*

$$m(r)=m_\infty+O(1/r) \quad \text{and} \quad w_j(r)=w_{j,\infty}+O(1/r) \quad \text{as} \quad r\to\infty$$

then

$$w_j(r)^2\leqslant w_{j,\infty}^2=\lambda_j \quad \forall r\in\mathring{D}.$$

Moreover, if G is a simple group and $w_j(r_1)=w_{j,\infty}$ for some j and for some $r_1\in\mathring{D}$ then $w_j(r)=w_{j,\infty}\forall r\in D$, $m=$const, the Yang–Mills field vanishes, and the metric is the Schwarzschild one.

If G is semisimple and $w_j(r_1)=w_{j,\infty}$ for some j and for some $r_1\in\mathring{D}$ then the field equations reduce to those of the subgroup of G obtained by deleting from the Cartan subalgebra $\mathfrak{h}$ of $\mathfrak{g}$ the simple component in which $\mathbf{h}_j$ lies.

Proof: Let $v_j:=w_j^2$. Then $v_j(r)\geqslant 0\forall r$ and (4.2) gives

$$2r^2Nv_jv_j''-r^2Nv_j'^2+4(m-r^{-1}P)v_jv_j'+2v_j^2\sum_{k=1}^{\ell}c_{jk}(\lambda_k-v_k)=0. \tag{5.1}$$

Let $V_j:=\sup_{r\in D}v_j(r)$. Then $V_j>0$ because the asymptotic value of $v_j(r)$ is $\lambda_j>0$. Now assume that $v_j(r_j)=V_j$ for some $r_j\in\mathring{D}$. Then $v_j(r_j)$ is an absolute maximum so that $v_j'(r_j)=0$ and $v_j''(r_j)\leqslant 0$. It follows from (5.1) that $\Sigma_{j=1}^{\ell}c_{ij}(\lambda_j-v_j(r_j))\geqslant 0$ which in view of (4.6) is equivalent to

$$\sum_{j=1}^{\ell}c_{ij}v_j(r_j)\leqslant 2\forall i,$$

or

$$v_i(r_i)\leqslant 1+\frac{1}{2}\sum_{j\neq i}(-c_{ij})v_j(r_i)\leqslant 1+\frac{1}{2}\sum_{j\neq i}(-c_{ij})\sup_{r\in D}v_j(r),$$

whence $V_i \leqslant 1 + \frac{1}{2}\Sigma_{j\neq i}(-c_{ij})V_j$ or

$$\sum_{j=1}^{\ell} c_{ij}V_j \leqslant 2 \forall i.$$

(Note that for all Cartan matrices $c_{ii}=2$ and $c_{ij}\leqslant 0$ if $i\neq j$.)
This last set of inequalities, however, can be multiplied with the inverse Cartan matrix since the latter has only positive entries. Using (4.6) again then gives $0\leqslant V_j \leqslant \lambda_j \forall j$, thus $V_j=\lambda_j$ since λ_j is the asymptotic value.

Suppose now that $v_i(r_*)=\lambda_i$ for some i and some $r_* \in \mathring{D}$. Then we find from (5.1)

$$r_* N(r_*) v_i''(r_*) = \lambda_i \sum_{j\neq i} (-c_{ij})(\lambda_j - v_j(r_*)) \geqslant 0,$$

which contradicts that $v_i(r)$ has a maximum at r_* unless $v_j''(r_*)=0$ and, in the case of a simple Lie algebra, the neighboring v_j also assume their maximal values. (For a simple Lie algebra there is a $c_{ij}<0$ for some $j\neq i$ for any i.) It follows that all $v_j(r_*)=\lambda_j$ for all j for which the root α_j is in the same simple component of $\mathfrak{h}^*$.

However, if all $v_j(r_*)=\lambda_j$ and thus $v_j'(r_*)=0\ \forall j$ then the initial conditions for the differential equations (5.1) are all trivial and since r_* is not a singular point it follows by the uniqueness of the solution that it must by the one for which $v_j(r)\equiv\lambda_j$. It then also follows from (4.1) that $m=$const so that the Yang–Mills field vanishes and the geometry is the one of the Schwarzschild solution. □

Theorem 7 shows among other things that for a given semisimple gauge group G and a given group action (characterized by Λ_0) there may be special solutions that reduce the YM-connection to a subgroup of G that is a product of some of the simple factors of G. Somewhat similarly, since the group SU(2) can be isomorphically imbedded in every compact (simply connected) semisimple or simple Lie group the Bartnik–McKinnon solution[1] can be obtained as a special solution for all the models considered here. The following special BM-solution for arbitrary compact G was already obtained in Ref. 24.

Consider the gauge group G and the symmetry group action (characterized by Λ_0) fixed and such that Λ_0 is regular so that the field equations are given by (3.4), (4.1), and (4.2). Select any Ω_+ such that the set $\{\Lambda_0,\Omega_+,\Omega_-\}$ is a standard triple with $c(\Omega_+)=-\Omega_-$ and let $\Lambda_+(r)=u(r)\Omega_+$ or, equivalently, $w_i(r)=w_{i,\infty}u(r)$. Then the field equations become

$$m' = g_0(Nu'^2 + \tfrac{1}{2}r^{-2}(1-u^2)^2), \tag{5.2}$$

$$r^2 N u'' + (2m - g_0 r^{-1}(1-u^2)^2)u' + u(1-u^2) = 0, \tag{5.3}$$

$$S^{-1}S' = 2g_0 r^{-1} u'^2. \tag{5.4}$$

where $g_0=\frac{1}{4}\Sigma_{i,j}\lambda_i h_{ij}\lambda_j$. By introducing a new radial variable $x:=r g_0^{-1/2}$ one sees easily that (5.2)–(5.4) reduce to the well studied equations for the SU(2)-Einstein–Yang–Mills fields.

Since Λ_0 fixes the conjugacy class of the symmetry group action on the bundle different choices of Ω_+ will lead to isomorphic gauge connections, namely reductions of the G-connection to an SU(2)-connection on the principal bundle for the particular space–time. They are thus physically equivalent.

In view of the existence theorems for the $G=\mathrm{SU}(2)$ case[2,3,25] it now follows that the systems (4.1) and (4.2) always admits some global solutions

Theorem 8: *There exists a countably infinite family of globally regular solutions of the Einstein–Yang–Mills–equations for any simply connected compact semisimple gauge group G on*

a static spherically symmetric asymptotically flat space–time diffeomorphic to $\mathbb{R}^4$. *Similarly, for any* $r_H>0$ *there exists an infinite family of asymptotically flat black hole solutions with black hole radius* r_H.

VI. THE LIE ALGEBRA $\mathfrak{g}$ AS AN $\mathfrak{sl}(2,\mathbb{C})$ SUBMODULE

In this section we collect all of the algebraic results needed to prove theorems 4 and 5. Introduce a nondegenerate Hermitian inner product $\langle\,|\,\rangle:\mathfrak{g}\times\mathfrak{g}\to\mathbb{C}$ by

$$\langle X|Y\rangle := -(c(X),Y) \quad \forall X,Y\in\mathfrak{g}, \tag{6.1}$$

recalling that $c:\mathfrak{g}\to\mathfrak{g}$ is the conjugation operator determined by the compact real form $\mathfrak{g}_0$. Then $\langle\,|\,\rangle$ restricts to a real positive definite inner product on $\mathfrak{g}_0$. From the invariance properties of $(\ ,\ )$ it follows that $\langle\,|\,\rangle$ satisfies

$$\langle X|Y\rangle=\overline{\langle Y|X\rangle},$$

$$\langle c(X)|c(Y)\rangle=\overline{\langle X|Y\rangle},$$

$$\langle [X,c(Y)]|Z\rangle=\langle X|[Y,Z]\rangle$$

for all $X,Y,Z\in\mathfrak{g}$. Treating $\mathfrak{g}$ as a $\mathbb{R}$-linear space by restricting scalar multiplication to multiplication by reals, we can introduce a positive definite inner product $\langle\langle\,|\,\rangle\rangle:\ \mathfrak{g}\times\mathfrak{g}\to\mathbb{R}$ on $\mathfrak{g}$ defined by

$$\langle\langle X|Y\rangle\rangle := \mathrm{Re}\langle X|Y\rangle \quad \forall X,Y\in\mathfrak{g}.$$

Let $\|\ \|$ denote the norm induced on $\mathfrak{g}$ by $\langle\langle\,|\,\rangle\rangle$, i.e.,

$$\|X\|=\sqrt{\langle\langle X|X\rangle\rangle} \quad \forall\ \ X\in\mathfrak{g}. \tag{6.2}$$

From the above properties satisfied by $\langle\,|\,\rangle$, it straighforward to verify that $\langle\langle\,|\,\rangle\rangle$ satisfies

$$\langle\langle X|Y\rangle\rangle=\langle\langle Y|X\rangle\rangle,$$

$$\langle\langle c(X)|c(Y)\rangle\rangle=\langle\langle X|Y\rangle\rangle, \tag{6.3}$$

$$\langle\langle [X,c(Y)]|Z\rangle\rangle=\langle\langle X|[Y,Z]\rangle\rangle$$

for all $X,Y,Z\in\mathfrak{g}$.

Let $\Omega_+,\Omega_-\in\mathfrak{g}$ be two vectors such that

$$[\Lambda_0,\Omega_\pm]=\pm 2\Omega_\pm,\ \ [\Omega_+,\Omega_-]=\Lambda_0,\ \text{ and }\ c(\Omega_+)=-\Omega_-.$$

Then $\mathrm{span}_{\mathbb{C}}\{\Lambda_0,\Omega_+,\Omega_-\}\simeq\mathfrak{sl}(2,\mathbb{C})$. The dot notation will often be used to denote the adjoint action of $\mathrm{span}_{\mathbb{C}}\{\Lambda_0,\Omega_+,\Omega_-\}$ on $\mathfrak{g}$, i.e.,

$$X.Y := \mathrm{ad}(X)(Y) \quad \forall\ \ X\in\mathrm{span}_{\mathbb{C}}\{\Lambda_0,\Omega_+,\Omega_-\},\quad Y\in\mathfrak{g}.$$

Because Λ_0 is a semisimple element, $\mathrm{ad}(\Lambda_0)$ is diagonalizable and it follows from $\mathfrak{sl}(2)$-representation theory[23] that the eigenvalues are integers. Let V_n denote the eigenspaces of $\mathrm{ad}(\Lambda_0)$, i.e.,

$$V_n := \{X\in\mathfrak{g}\,|\,\Lambda_0.X=nX\},\quad n\in\mathbb{Z}.$$

It also follows from $\mathfrak{sl}(2,\mathbb{C})$-representation theory that if $X\in\mathfrak{g}$ is a highest weight vector of the adjoint representation of $\mathrm{span}_{\mathbb{C}}\{\Lambda_0,\Omega_+,\Omega_-\}$ with weight n, and we define $X_{-1}=0$, $X_0=X$ and $X_j=(1/j!)\Omega_-^j.X_0\ (j\geqslant 0)$, then

$$\Lambda_0 . X_j = (n-2j) X_j ,$$

$$\Omega_- . X_j = (j+1) X_{j+1} , \tag{6.4}$$

$$\Omega_+ . X_j = (n-j+1) X_{j-1} \quad (j \geqslant 0).$$

Proposition 1: There exists M highest weight vectors $\xi^1, \xi^2, \ldots, \xi^M$ *for the adjoint representation of* $\mathrm{span}_{\mathbb{C}}\{\Lambda_0, \Omega_+, \Omega_-\}$ *on* $\mathfrak{g}$ *that satisfy*

(*i*) *the* ξ^j *have weights* $2k_j$ *where* $j = 1,2,\ldots,M$ *and* $1 = k_1 \leqslant k_2 \leqslant \cdots \leqslant k_M$,

(*ii*) *if* $V(\xi^j)$ *denotes the irreducible submodule of* $\mathfrak{g}$ *generated by* ξ^j, *then the sum* $\Sigma_{j=1}^{M} V(\xi^j)$ *is direct,*

(*iii*) *if* $\xi_l^j = (1/l!)\Omega_-^l . \xi^j$ *then*

$$c(\xi_l^j) = (-1)^l \xi_{2k_j - l}^j , \tag{6.5}$$

(*iv*) $M = |S_\lambda|$ *and the set* $\{\xi_{k_j - 1}^j | j = 1,2,\ldots M\}$ *forms a basis for* V_2 *over* $\mathbb{C}$.

Proof: (*i*) and (*ii*): The conjugation operator c satisfies

$$c([X,Y]) = [c(X), c(Y)] \quad \forall X, Y \in \mathfrak{g}. \tag{6.6}$$

Because $\Lambda_0 \in i\mathfrak{h}_0$

$$c(\Lambda_0) = -\Lambda_0 . \tag{6.7}$$

Using (3.2), (6.6), and (6.7), it is easy to see that

$$c \circ \mathrm{ad}(\Omega_\pm)^n = (-1)^n \mathrm{ad}(\Omega_\pm)^n \circ c \quad \text{for every } n \in \mathbb{Z}_{\geqslant 0}$$

$$\text{and} \quad c \circ \mathrm{ad}(\Lambda_0) = -\mathrm{ad}(\Lambda_0) \circ c. \tag{6.8}$$

As usual, define the Casimir operator $\mathcal{C}$ by

$$\mathcal{C} = \tfrac{1}{2}\mathrm{ad}(\Lambda_0)^2 + \mathrm{ad}(\Omega_+)\mathrm{ad}(\Omega_-) + \mathrm{ad}(\Omega_-)\mathrm{ad}(\Omega_+).$$

Then $\mathfrak{g}$ can be decomposed as follows:[26]

$$\mathfrak{g} = \bigoplus_p V(s_p, v^p), \tag{6.9}$$

where $V(s_p, v^p)$ is a highest weight module generated by the highest weight vector v^p of weight s_p, and it has the property

$$\mathcal{C}|_{V(s_p, v^p)} = (\tfrac{1}{2}s_p^2 + s_p)\mathrm{id}_{V(s_p, v^p)} \quad \forall \ p. \tag{6.10}$$

From (6.8) it follows that $\mathcal{C} \circ c = c \circ \mathcal{C}$. Using this result and (6.10), we see that

$$c(V(s_p, v^p)) \subset V(s_p, v^p) \quad \forall p. \tag{6.11}$$

Let $\{s_{p_1}, s_{p_2}, \ldots, s_{p_M}\}$ be the set of weights from the decomposition (6.9) that are even and greater than zero. We will assume that they are ordered so that $s_{p_1} \leqslant s_{p_2} \leqslant \cdots \leqslant s_{p_M}$. Define $k_j = s_{p_j}/2$. Then the k_j are positive integers that satisfy $k_1 \leqslant k_2 \leqslant \cdots \leqslant k_M$. Note that $k_1 = 1$ because Ω_+ is a highest weight vector with weight 2. To simplify notation, set $v^j := v^{p_j}$. As before with highest weight vectors [see (6.4)], we let $v_l^j = (1/l!)\Omega_-^l . v^j$. Define

$$\xi^j=\begin{cases} iv^j+c(iv^j_{2k_j}) & \text{if } c(v^j_{2k_j})=-c(v^j) \\ v^j+c(v^j_{2k_j}) & \text{otherwise} \end{cases}, \tag{6.12}$$

for $j=1,2,\ldots M$. Then straightforward calculation using (6.8) and (6.4) shows that $\Lambda_0.\xi^j=2k_j\xi^j$ and $\Omega_+.\xi^j=0$ for $j=1,2,\ldots M$. This implies that the ξ^j are all highest weight vectors of weight $2k_j$. Let $V(\xi^j)$ denote the irreducible submodule generated by ξ^j. From (6.11) and (6.12) it is clear that $\xi^j\subset V(2k_j,v^j)$ and hence $V(\xi^j)=V(2k_j,v^j)$. Thus the decomposition (6.9) shows that the sum $\Sigma_{j=1}^M V(\xi^j)$ is direct.

(iii): The relationship (6.5) follows from (6.8), (6.12), and (6.4).

(iv): Because the numbers $2k_1,2k_2,\ldots,2k_M$ exhaust all the positive even weights and the sum $\Sigma_{j=1}^M V(\xi^j)$ is direct, it follows from $\mathfrak{sl}(2,\mathbb{C})$-representation theory that $\{\xi^j|j=1,2,\ldots M\}$ is a basis over $\mathbb{C}$ for V_2. But $\{\mathbf{e}_\alpha|\alpha\in S_\lambda\}$ is also a basis over $\mathbb{C}$ for V_2. Therefore we must have $M=|S_\lambda|$. □

Define an $\mathbb{R}$-linear operator $A:\mathfrak{g}\to\mathfrak{g}$ by

$$A=\tfrac{1}{2}\mathrm{ad}(\Omega_+)\circ(\mathrm{ad}(\Omega_-)+\mathrm{ad}(\Omega_+)\circ c). \tag{6.13}$$

Proposition 2: The $\mathbb{R}$-linear operator A is symmetric with respect to the inner product $\langle\langle\ |\ \rangle\rangle$, i.e., $\langle\langle A(X)|Y\rangle\rangle=\langle\langle X|A(Y)\rangle\rangle\forall\ \ X,Y\in\mathfrak{g}$.

Proof: From (3.2) and the properties (6.3) of the inner product $\langle\langle\ |\ \rangle\rangle$, it is not hard to show that $\langle\langle[\Omega_+,[\Omega_-,X]]|Y\rangle\rangle=\langle\langle X|[\Omega_+,[\Omega_-,Y]]\rangle\rangle$ and $\langle\langle[\Omega_+,[\Omega_+,c(X)]]|Y\rangle\rangle=\langle\langle X|[\Omega_+,[\Omega_+,c(Y)]]\rangle\rangle$ for every $X,Y\in\mathfrak{g}$. From the definition of A, it is then obvious that $\langle\langle A(X)|Y\rangle\rangle=\langle\langle X|A(Y)\rangle\rangle$ for every $X,Y\in\mathfrak{g}$. □

Lemma 1:

$$A(V_2)\subset V_2. \tag{6.14}$$

Proof: It follows from $\mathfrak{sl}(2,\mathbb{C})$-representation theory that $\Omega_\pm.V_n\subset V_{n\pm2}$. From (6.8) it is clear that $c(V_n)\subset V_n$. Thus $\Omega_+.\Omega_-.V_2\subset V_2$ and $\Omega_+.\Omega_+.c(V_2)\subset V_2$ which implies that $A(V_2)\subset V_2$. □

This proposition shows that A restricts to an operator on V_2. We denote this operator by

$$A_2:=A|_{V_2}. \tag{6.15}$$

Label the integers k_j from proposition 1 as follows

$$1=k_{J_1}=k_{J_1+1}=\cdots=k_{J_1+m_1-1}<k_{J_2}=k_{J_2+1}=\cdots=k_{J_2+m_2-1}$$
$$<\cdots<k_{J_I}=k_{J_I+1}=\cdots=k_{J_I+m_I-1},$$

where $J_1=1$, $J_l+m_l=J_{l+1}$ for $l=1,2,\ldots,I$ and $J_{I+1}=M-1$. Define

$$\mathsf{k}_l:=k_{J_l}\quad l=1,2,\ldots,I. \tag{6.16}$$

The set $\{\xi^j_{k_j-1}|j=1,2,\ldots M\}$ forms a basis over $\mathbb{C}$ of V_2 by proposition 1 (iv). Therefore, the set of vectors $\{X^l_s,Y^l_s|l=1,2,\ldots,I;s=0,1,\ldots,m_l-1\}$ where

$$X^l_s:=\begin{cases} \xi^{J_l+s}_{\mathsf{k}_l-1} & \text{if } \mathsf{k}_l \text{ is odd} \\ i\xi^{J_l+s}_{\mathsf{k}_l-1} & \text{if } \mathsf{k}_l \text{ is even} \end{cases} \text{ and } Y^l_s:=iX^l_s, \tag{6.17}$$

forms a basis of V_2 over $\mathbb{R}$. By proposition 2, we know that A is symmetric and therefore diagonalizable. This forces A_2 to also be diagonalizable. The next lemma shows that $\{X_s^l, Y_s^l | l = 1,2,\ldots, Is = 0,1,\ldots, m_l - 1\}$ is in fact an eigenbasis of A_2.

Lemma 2:

$$A_2(X_s^l) = \mathsf{k}_l(\mathsf{k}_l+1)X_s^l \quad \textit{and} \quad A_2(Y_s^l) = 0 \quad \textit{for} \quad l = 1,2,\ldots,I \tag{6.18}$$

and $s = 0,1,\ldots, m_l - 1$.

Proof: Using the formulas (6.4) and proposition 1 (*iii*) it is easy to show that $A(\xi^j_{k_j-1}) = \frac{1}{2}k_j(k_j+1)(1+(-1)^{k_j-1})\xi^j_{k_j-1}$ and $A(i\xi^j_{k_j-1}) = \frac{1}{2}k_j(k_j+1)(1+(-1)^{k_j})i\xi^j_{k_j-1}$ for $j = 1,2,\ldots M$. The proposition then follows from (6.16) and 6.17. □

An immediate consequence of this lemma is that $\text{spec}(A_2) = \{0\} \cup \{\mathsf{k}_j(\mathsf{k}_j+1) | j = 1,2,\ldots I\}$ and m_j is the dimension of the eigenspace corresponding to the eigenvalue $\mathsf{k}_j(\mathsf{k}_j+1)$. Note that I is the number of distinct positive eigenvalues of A_2.

Define

$$E_0^l = \text{span}_{\mathbb{R}}\{Y_s^l | s = 0,1,\ldots, m_l - 1\},$$

$$E_+^l = \text{span}_{\mathbb{R}}\{X_s^l | s = 0,1,\ldots, m_l - 1\} \tag{6.19}$$

and

$$E_0 = \bigoplus_{l=1}^{I} E_0^l, \quad E_+ = \bigoplus_{l=1}^{I} E_+^l. \tag{6.20}$$

Then $E_0 = \ker(A_2)$ and E_+^l is the eigenspace of A_2 corresponding to the eigenvalue $\mathsf{k}_l(\mathsf{k}_l+1)$. Moreover, using proposition 1 (*iv*), we see that

$$V_2 = E_0 \oplus E_+. \tag{6.21}$$

Lemma 3: Suppose $X \in V_2$. *Then* $X \in \oplus_{q=1}^{l} E_0^q \oplus E_+^q$ *if and only if* $\Omega_+^{\mathsf{k}_l}.X = 0$.

Proof: From the formulas (6.4), we get

$$\Omega_+^{q-1}.\xi^l_{k_l-1} = \begin{cases} 0 & \text{if } q > k_l \\ d(q,k_l)\xi^l_{k_l-q} & \text{if } q \leqslant k_l \end{cases},$$

where $d(q,r) = (q+r)!/(r+1)!$. This implies that

$$\Omega_+^{l-1}.X_p^q = \begin{cases} 0 & \text{if } l > \mathsf{k}_q \\ \beta_q d(l,\mathsf{k}_q)\xi^{J_q+p}_{\mathsf{k}_q-l} & \text{if } l \leqslant \mathsf{k}_q \end{cases} \tag{6.22}$$

and

$$\Omega_+^{l-1}.Y_p^q = \begin{cases} 0 & \text{if } l > \mathsf{k}_q \\ \overline{\beta}_q\, d(l,\mathsf{k}_q) i\xi^{J_q+p}_{\mathsf{k}_q-l} & \text{if } l \leqslant \mathsf{k}_q \end{cases}, \tag{6.23}$$

where

$$\beta_q = \begin{cases} 1 & \text{if } \mathsf{k}_q \text{ is odd} \\ i & \text{if } \mathsf{k}_q \text{ is even} \end{cases}.$$

Suppose $X \in V_2 = \oplus_{q=1}^{I} E_0^q \oplus E_+^q$. Then there exists real constants a_{qp} and b_{qp} such that

$$X=\sum_{q=1}^{I}\sum_{p=0}^{m_q-1}(a_{qp}\,Y_p^q+b_{qp}\,X_p^q). \tag{6.24}$$

Suppose $\Omega_+^{\mathsf{k}_l}.X=0$. Then (6.22)–(6.24) imply that

$$\sum_{q=l+1}^{I}\sum_{p=0}^{m_q-1}(a_{qp}\,\overline{\beta}_q\,d(\mathsf{k}_l+1,\mathsf{k}_q)i\,\xi^{J_q+p}_{\mathsf{k}_q-\mathsf{k}_l-1}+b_{qp}\,\beta_q\,d(\mathsf{k}_l+1,\mathsf{k}_q)\,\xi^{J_q+p}_{\mathsf{k}_q-\mathsf{k}_l-1})=0.$$

But the set of vectors

$$\{\overline{\beta}_q i\,\xi^{J_q+p}_{\mathsf{k}_q-\mathsf{k}_l-1},\beta_q\,\xi^{J_q+p}_{\mathsf{k}_q-\mathsf{k}_l-1}|q=l+1,l+2,\ldots I,p=0,1,\ldots,m_q-1\},$$

is linearly independent over $\mathbb{R}$. Therefore, $X=\Sigma_{q=1}^{l}\Sigma_{p=0}{}^{m_q+1}(a_{qp}Y_p^q+b_{qp}X_p^q)$ which implies that $X\in\oplus_{q=1}^{l}E_0^q\oplus E_+^q$.

Conversely, suppose $X\in\oplus_{q=1}^{l}E_0^q\oplus E_+^q$. The X can be written in the form (6.24) and it is easy using (6.22) and (6.23) to verify that $\Omega_+^{\mathsf{k}_l}.X=0$. □

Lemma 4: Suppose $X\in V_2$. Then $X\in\oplus_{q=1}^{l}E_0^q\oplus E_+^q$ if and only if $\Omega_+^{\mathsf{k}_l+2}.c(X)=0$.

Proof: Proved in a similar fashion as lemma 3. □

Lemma 5: Let $\widetilde{\ }:\mathbb{Z}_{\geqslant -1}\to\{1,2,\ldots,I\}$ be the map defined by

$$\widetilde{-1}=\widetilde{0}=1\quad and\quad \tilde{s}=\max\{l|\mathsf{k}_l\leqslant s\}\quad if\quad s>0.$$

Then

(*i*) $\mathsf{k}_{\tilde{s}}\leqslant s$ *for every* $s\in\mathbb{Z}_{\geqslant 0}$.

(*ii*) $\mathsf{k}_{\tilde{s}}\leqslant s<\mathsf{k}_{\tilde{s}+1}$ *for every* $s\in\{0,1,\ldots\mathsf{k}_I-1\}$.

Proof: (*i*) This is obvious from the definition of $\widetilde{\ }$.

(*ii*) From part (i), $\mathsf{k}_{\tilde{s}}\leqslant s$. So suppose $\mathsf{k}_{\tilde{s}+1}\leqslant s$. Then from the definition of $\widetilde{\ }$ it is clear $\mathsf{k}_{\tilde{s}+1}\leqslant\mathsf{k}_{\tilde{s}}$. But because $\mathsf{k}_1<\mathsf{k}_2<\cdots<\mathsf{k}_I$, it follows that $\tilde{s}+1\leqslant s$ which is a contradiction. Thus $\mathsf{k}_{\tilde{s}+1}>s$ and we are done. □

Lemma 6: If $X\in V_2$, $\mathsf{k}_{\tilde{p}}+s<\mathsf{k}_{\tilde{p}+1}$ $(s\geqslant 0)$, and $\Omega_+^{\mathsf{k}_{\tilde{p}}+s}.X=0$, then $\Omega_+^{\mathsf{k}_{\tilde{p}}}.X=0$.

Proof: Assume $s>0$, otherwise we are done. Because $X\in V_2$, we have $\Omega_+^{\mathsf{k}_{\tilde{p}}+s-1}.X\in V_{2(\mathsf{k}_{\tilde{p}}+s)}$. By assumption $\Omega_+^{\mathsf{k}_{\tilde{p}}+s}.X=0$, so

$$\Omega_+^{\mathsf{k}_{\tilde{p}}+s-1}.X\in V_{2(\mathsf{k}_{\tilde{p}}+s)}\cap\ker(\mathrm{ad}(\Omega_+)).$$

But, if $n\in\mathbb{Z}_{>0}$, then

$$V_{2n}\cap\ker(\mathrm{ad}(\Omega_+))\neq\{0\}\Leftrightarrow n\in\{\mathsf{k}_1,\mathsf{k}_2,\ldots,\mathsf{k}_I\},$$

because otherwise $\mathfrak{g}$ would contain an irreducible $\mathrm{span}_{\mathbb{C}}\{\Lambda_0,\Omega_+,\Omega_-\}$-submodule with weight $2n\in\mathbb{Z}_{>0}\backslash\{2\mathsf{k}_1,2\mathsf{k}_2,\ldots,2\mathsf{k}_I\}$. This is impossible as the set $\{2\mathsf{k}_1,2\mathsf{k}_2,\ldots,2\mathsf{k}_I\}$ exhausts all the positive even weights of the irreducible $\mathrm{span}_{\mathbb{C}}\{\Lambda_0,\Omega_+,\Omega_-\}$-submodules in $\mathfrak{g}$. Therefore $\Omega_+^{\mathsf{k}_{\tilde{p}}+s-1}.X=0$ as $\mathsf{k}_{\tilde{p}}<\mathsf{k}_{\tilde{p}}+s<\mathsf{k}_{\tilde{p}+1}$ implies that $(\mathsf{k}_{\tilde{p}}+s)$ is not in $\{\mathsf{k}_1,\mathsf{k}_2,\ldots,\mathsf{k}_I\}$. Repeat the above argument with $s'=s-1$ to arrive at $\Omega_+^{\mathsf{k}_{\tilde{p}}+s'-1}.X=\Omega_+^{\mathsf{k}_{\tilde{p}}+s-2}.X=0$. Continuing in this manner, we find $\Omega_+^{\mathsf{k}_{\tilde{p}}}.X=0$. □

The next theorem is the key result needed to prove that the EYM equations can be put into a form where theorem 3 applies in a neighborhood of the origin $r=0$.

Theorem 9: *Suppose $p\in\{1,2,\ldots,\mathsf{k}_I-1\}$ and $Z_0,Z_1,\ldots,Z_{p+1}\in V_2$ is a sequence of vectors that satisfy $Z_0\in E_0^1\oplus E_+^1$ and $Z_{n+1}\in\oplus_{q=1}^{\tilde{n}}E_0^q\oplus E_+^q$ for $n=0,1,\ldots p$. Then for every $j\in\{1,2,\ldots,p+1\}$, $s\in\{0,1,2,\ldots,j\}$*

(*i*) $[[c(Z_{j-s}),Z_s],Z_{p+2-j}]\in\oplus_{q=1}^{\tilde{p}}E_0^q\oplus E_+^q$,

(ii) $[[c(Z_{p+2-j}),Z_{j-s}],Z_s]\in\oplus_{q=1}^{\tilde{p}}E_0^q\oplus E_+^q$.

Proof: (i) Suppose $Z_0,Z_1,\ldots,Z_{p+1}\in V_2$ is a sequence satisfying $Z_0\in E_0^1\oplus E_+^1$ and $Z_{n+1}\in\oplus_{q=1}^{\tilde{n}}E_0^q\oplus E_+^q$ for $n=0,1,\ldots p$. Then

$$\Omega_+^{\mathsf{k}_{(n-1)^\sim}}.Z_n=\Omega_+^{\mathsf{k}_{(n-1)^\sim}+2}.c(Z_n)=0, \tag{6.25}$$

for $n=0,1,2,\ldots,p+1$ by lemmas 3 and 4. Now, if $j\in\{1,2,\ldots,p+1\}$ and $s\in\{0,1,\ldots,j\}$, then

$$\Omega_+^p.[[c(Z_{j-s}),Z_s],Z_{p+2-j}]=\sum_{l=0}^{p}\sum_{m=0}^{l}\binom{p}{l}\binom{l}{m}a_{psjlm},$$

where

$$a_{psjlm}=[[\Omega_+^m.c(Z_{j-s}),\Omega_+^{l-m}.Z_s],\Omega_+^{p-l}.Z_{p+2-j}].$$

Applying (6.25) yields $a_{psjlm}=0$ if $m-2\geqslant\mathsf{k}_{(j-s-1)^\sim}$ or $l-m\geqslant\mathsf{k}_{(s-1)^\sim}$ or $p-l\geqslant\mathsf{k}_{(p+1-j)^\sim}$. But because of lemma 5 (i), this implies that $a_{psjlm}=0$ if $m-2\geqslant j-s-1$ or $l-m\geqslant s-1$ or $p-l\geqslant p+1-j$. It follows that $a_{psjlm}=0$ unless l and m satisfy $j-1<l<m+s-1<j$ which is impossible. Therefore, $a_{psjlm}=0$ for all l and m. Thus $\Omega_+^p.[[c(Z_{j-s}),Z_s],Z_{p+2-j}]=0$. But then it follows from lemmas 5 (ii) and 6 that $\Omega_+^{\tilde{p}}.[[c(Z_{j-s}),Z_s],Z_{p+2-j}]=0$ and hence $[[c(Z_{j-s}),Z_s],Z_{p+2-j}]\in\oplus_{q=1}^{\tilde{p}}E_0^q\oplus E_+^q$ by lemma 3.

(ii) It follows from similar arguments that $[[c(Z_{p+2-j}),Z_{j-s}],Z_s]\in\oplus_{q=1}^{\tilde{p}}E_0^q\oplus E_+^q$. □

It is worthwhile to note that all the the above results did not depend on Λ_0 being regular. However, for what follows we will need Λ_0 to be regular.

Proposition 3: Suppose Λ_0 is regular. Then $span_{\mathbb{C}}\{\xi^1,\xi^2,\ldots,\xi^M\}$ is an Abelian subalgebra of $\mathfrak{g}_\lambda$ and hence also an Abelian subalgebra of $\mathfrak{g}$.

Proof: From the definition of $\mathfrak{g}_\lambda$, it follows that $\mathrm{span}_{\mathbb{C}}\{\Lambda_0,\Omega_+,\Omega_-\}\subset\mathfrak{g}_\lambda$ and $V_2\subset\mathfrak{g}_\lambda$. But by proposition 1 $V_2=\mathrm{span}_{\mathbb{C}}\{\xi^1_{k_1-1},\xi^2_{k_2-1},\xi^M_{k_M-1}\}$, and hence

$$\frac{(k_l+1)!}{(2k_l)!}\Omega_+^{k_l-1}.\xi^l_{k_l-1}=\xi^l\in\mathfrak{g}_\lambda,$$

for $i=1,2,\ldots,M$. Therefore $\mathrm{span}_{\mathbb{C}}\{\xi^1,\xi^2,\ldots,\xi^M\}\subset\mathfrak{g}_\lambda$. The ξ^j are highest weight vectors, consequently

$$\mathrm{span}_{\mathbb{C}}\{\xi^1,\xi^2,\ldots,\xi^M\}\subset\mathfrak{g}_\lambda^{\Omega_+} \tag{6.26}$$

where $\mathfrak{g}_\lambda^{\Omega_+}=\{X\in\mathfrak{g}_\lambda|[\Omega_+,X]=0\}$. Define $V_{\lambda,n}:=\{X\in\mathfrak{g}_\lambda|\Lambda_0.X=nX\}$. By theorem 1, S_λ is a base a system of roots of $\mathfrak{g}_\lambda$ and $\alpha(\Lambda_0)=2$ for every $\alpha\in S_\lambda$ and hence it follows that $V_{\lambda,2}=V_2$. Using $\mathfrak{sl}(2,\mathbb{C})$-representation theory, it is not hard to show that $\dim_{\mathbb{C}}\mathfrak{g}_\lambda^{\Omega_+}=\dim_{\mathbb{C}}V_{\lambda,2}$. But $\dim_{\mathbb{C}}V_2=|S_\lambda|$, and therefore $\dim_{\mathbb{C}}\mathfrak{g}_\lambda^{\Omega_+}=|S_\lambda|$. By proposition 1, $|S_\lambda|=M$ and hence we get from (6.26) that

$$\mathrm{span}_{\mathbb{C}}\{\xi^1,\xi^2,\ldots,\xi^M\}=\mathfrak{g}_\lambda^{\Omega_+}. \tag{6.27}$$

Theorem 1 proved that $|S_\lambda|=\dim_{\mathbb{C}}\mathfrak{h}_\lambda$ which in turn gives, via the above result, $\dim_{\mathbb{C}}\mathfrak{g}_\lambda^{\Omega_+}=\dim_{\mathbb{C}}\mathfrak{h}_\lambda$. Applying lemma 2.1.15 of Ref. 15 then shows that

$$\dim_{\mathbb{C}}\mathfrak{g}_\lambda^{\Omega_+}=\min\{\dim_{\mathbb{C}}\mathfrak{g}_\lambda^X|X\in\mathfrak{g}_\lambda\}. \tag{6.28}$$

We can identify $\mathfrak{g}_\lambda$ with the dual $\mathfrak{g}_\lambda^*$ using the form $(\ ,\ )$, i.e.,

$$\iota:\mathfrak{g}_{\lambda,0}\to\mathfrak{g}_{\lambda,0}^*;\quad \iota(X)(\cdot)=(X,\cdot).$$

So if $f\in\mathfrak{g}_\lambda^*$ and we define $\mathfrak{g}_\lambda^f=\{X\in\mathfrak{g}_\lambda|\mathrm{ad}_X^*(f)=0\}$, then it can be shown that

$$\mathfrak{g}_\lambda^{\iota(X)}=\mathfrak{g}_\lambda^X\quad\forall X\in\mathfrak{g}. \tag{6.29}$$

Let G_λ be a connected complex semisimple Lie group with Lie algebra $\mathfrak{g}_\lambda$. Then for $f\in\mathfrak{g}_\lambda^*$, $\mathfrak{g}_\lambda^f$ is the Lie algebra of coadjoint isotropy group $G_{\lambda,f}=\{a\in G_\lambda|\mathrm{Ad}_a^*(f)=f\}$. But then (6.27), (6.28), (6.29) and a straightforward generalization of theorem 9.3.10 in Ref. 27 to complex Lie groups imply that $\mathrm{span}_{\mathbb{C}}\{\xi^1,\xi^2,\ldots,\xi^M\}$ is an Abelian subalgebra. □

The next theorem is the key result needed to prove that the EYM equations can be put into a form where theorem 3 applies in a neighborhood $r=\infty$. Although this theorem looks very similar to theorem 9, it is more difficult to prove. Similar arguments as in theorem 9 are employed, but these only go part of the way. Proposition 3 is needed to complete the proof.

Theorem 10: *Assume that Λ_0 is regular. Suppose $p\in\{0,1,2,\ldots,\mathsf{k}_I\}$ and $Z_0,Z_1,\ldots,Z_p\in V_2$ is a sequence of vectors that satisfy $Z_n\in\oplus_{q=1}^{\tilde{n}}E_0^q\oplus E_+^q$ for $n=0,1,2...p$. Then for every $j\in\{1,2,\ldots,p\}$, $s\in\{0,1,\ldots,j\}$*

(i) $[[c(Z_{j-s}),Z_s],Z_{p+1-j}]\in\oplus_{q=1}^{\tilde{p}}E_0^q\oplus E_+^q$,

(ii) $[[c(Z_{p+1-j}),Z_{j-s}],Z_s]\in\oplus_{q=1}^{\tilde{p}}E_0^q\oplus E_+^q$.

Proof: *(i)* Suppose $Z_0,Z_1,\ldots,Z_p\in V_2$ is a sequence satisfying $Z_n\in\oplus_{q=1}^{\tilde{n}}E_0^q\oplus E_+^q$ for $n=0,1,\ldots p$. Then

$$\Omega_+^{\mathsf{k}_{\tilde{n}}}.Z_n=\Omega_+^{\mathsf{k}_{\tilde{n}}+2}.c(Z_n)=0, \tag{6.30}$$

for $n=0,1,2,\ldots,p$ by lemmas 3 and 4. Suppose $j\in\{1,2,\ldots,p\}$ and $s\in\{0,1,\ldots,j\}$. Then

$$\Omega_+^p.[[c(Z_{j-s}),Z_s],Z_{p+1-j}]=\sum_{l=0}^{p}\sum_{m=0}^{l}\binom{p}{l}\binom{l}{m}a_{psjlm}, \tag{6.31}$$

where

$$a_{psjlm}=[[\Omega_+^m.c(Z_{j-s}),\Omega_+^{l-m}.Z_s],\Omega_+^{p-l}.Z_{p+1-j}].$$

Applying (6.30) yields $a_{psjlm}=0$ if $m-2\geqslant\mathsf{k}_{(j-s)^\sim}$ or $l-m\geqslant\mathsf{k}_{\tilde{s}}$ or $p-l\geqslant\mathsf{k}_{(p+1-j)^\sim}$. But because of lemma 5 (i), this implies that $a_{psjlm}=0$ if $m-2\geqslant j-s$ or $l-m\geqslant s$ or $p-l\geqslant p+1-j$. It follows that $a_{psjlm}=0$ unless l and m satisfy $j-1<l<m+s<j+2$ which implies that $l=j$ and $m+s=j+1$. Thus the sum (6.31) reduces to

$$\Omega_+^p.[[c(Z_{j-s}),Z_s],Z_{p+1-j}]=\binom{p}{j}\binom{j}{j+1-s}[[X_1,X_2],X_3],$$

where $X_1=\Omega_+^{j-s+1}.c(Z_{j-s})$, $X_2=\Omega_+^{s-1}.Z_s$, and $X_3=\Omega_+^{p-j}.Z_{p+1-j}$. Applying (6.30) then shows that $\Omega_+.X_a=0$ for $a=1,2,3$. Because the X_a have even weights,

$$X_1,X_2,X_3\in\mathrm{span}_{\mathbb{C}}\{\xi^1,\xi^2,\ldots,\xi^M\}.$$

But $\mathrm{span}_{\mathbb{C}}\{\xi^1,\xi^2,\ldots,\xi^M\}$ is an Abelian subalgebra by proposition 3, so $[[X_1,X_2],X_3]=0$ which implies that $\Omega_+^p.[[c(Z_{j-s}),Z_s],Z_{p+1-j}]=0$. We then get via lemma 6 that $\Omega_+^{\mathsf{k}_{\tilde{p}}}.[[c(Z_{j-s}),Z_s],Z_{p+1-j}]=0$ and hence $[[c(Z_{j-s}),Z_s],Z_{p+1-j}]\in\oplus_{q=1}^{\tilde{p}}E_0^q\oplus E_+^q$ by lemma 3.
(ii) The proof that $[[c(Z_{p+1-j}),Z_{j-s}],Z_s]\in\oplus_{q=1}^{\tilde{p}}E_0^q\oplus E_+^q$ is similar to part *(i)*. □

Proposition 4: If $\Omega_+\in\Sigma_{\alpha\in S_\lambda}\mathbb{R}\mathbf{e}_\alpha$ and Λ_0 is regular, then $E_+=\Sigma_{\alpha\in S_\lambda}\mathbb{R}\mathbf{e}_\alpha$.

Proof: Introduce a basis $\{Z_j|1\leqslant j\leqslant M\}$ over $\mathbb{R}$ for E_+ by defining

$$Z_j=\begin{cases}\xi^j_{k_j-1} & \text{if } k_j \text{ is odd}\\ i\,\xi^j_{k_j-1} & \text{if } k_j \text{ is even}\end{cases}\qquad 1\leqslant j\leqslant M.$$

Equations (6.4) and proposition 1 (iii) can be used to show that

$$\Omega_+ .c(Z_j)=\Omega_- .Z_j \quad 1\leqslant j\leqslant M. \tag{6.32}$$

By assumption $\Omega_+=\Sigma_{\alpha\in S_\lambda}w_\alpha\mathbf{e}_\alpha$ for some set of constants $w_\alpha\in\mathbb{R}$. Because $c(\Omega_+)=-\Omega_-$ and $c(\mathbf{e}_\alpha)=-\mathbf{e}_{-\alpha}$, $\Omega_-=\Sigma_{\alpha\in S_\lambda}w_\alpha\mathbf{e}_{-\alpha}$. Since $Z_j\in V_2$, $Z_j=\Sigma_{\alpha\in S_\lambda}a_{j\alpha}\mathbf{e}_\alpha$ for some set of constants $a_{j\alpha}\in\mathbb{C}$. So then $c(Z_j)=-\Sigma_{\alpha\in S_\lambda}\overline{a}_{j\alpha}\mathbf{e}_{-\alpha}$. Now, since Λ_0 is regular, Eq. (3.15) holds. Therefore,

$$\Omega_- .Z_j=\sum_{\alpha\in S_\lambda} w_\alpha a_{j\alpha}[\mathbf{e}_{-\alpha},\mathbf{e}_\alpha]=\sum_{\alpha\in S_\lambda} -w_\alpha a_{j\alpha}\mathbf{h}_\alpha, \tag{6.33}$$

while

$$\Omega_+ .c(Z_j)=\sum_{\alpha\in S_\lambda} -w_\alpha\overline{a}_{j\alpha}[\mathbf{e}_\alpha,\mathbf{e}_{-\alpha}]=\sum_{\alpha\in S_\lambda} -w_\alpha\overline{a}_{j\alpha}\mathbf{h}_\alpha. \tag{6.34}$$

The three results (6.32)–(6.34) then yield

$$\sum_{\alpha\in S_\lambda} w_\alpha(a_{j\alpha}-\overline{a}_{j\alpha})\mathbf{h}_\alpha=0.$$

Since Λ_0 is regular, it follows that $w_\alpha\neq 0$ for all $\alpha\in S_\lambda$ and the set $\{\mathbf{h}_\alpha|\alpha\in S_\lambda\}$ is linearly independent.[12] Thus $a_{j\alpha}-\overline{a}_{j\alpha}=0$ for all $\alpha\in S_\lambda$ and $j=1,2,\ldots,M$. So $Z_j\in\Sigma_{\alpha\in S_\lambda}\mathbb{R}\mathbf{e}_\alpha$ for $j=1,2,\ldots,M$ which implies that $E_+\subset\Sigma_{\alpha\in S_\lambda}\mathbb{R}\mathbf{e}_\alpha$. However, $\dim_{\mathbb{R}}E_+=\dim_{\mathbb{R}}(\Sigma_{\alpha\in S_\lambda}\mathbb{R}\mathbf{e}_\alpha)=|S_\lambda|$ and, therefore, $E_+=\Sigma_{\alpha\in S_\lambda}\mathbb{R}\mathbf{e}_\alpha$. □

Suppose Λ_0 is regular and $\Omega_+=\Sigma_{\alpha\in S_\lambda}w_\alpha\mathbf{e}_\alpha$ where $w_\alpha\in\mathbb{R}$ for every $\alpha\in S_\lambda$. Then using (3.10), (3.15), and the fact that $c(\mathbf{e}_\alpha)=-\mathbf{e}_{-\alpha}$, it is not difficult to show that

$$A_2(\mathbf{e}_\alpha)=\sum_{\beta\in S_\lambda} w_\beta\langle\beta,\alpha\rangle w_\alpha\mathbf{e}_\beta.$$

This result along with (6.21) and proposition 4 shows that $\{\mathbf{e}_\alpha|\alpha\in S_\lambda\}$ can be completed to a basis over $\mathbb{R}$ of V_2 so that the matrix of A_2 with respect to this basis takes the form

$$[A_2]=\begin{pmatrix}0 & 0\\ 0 & [A_{\alpha\beta}]\end{pmatrix}, \tag{6.35}$$

with

$$A_{\alpha\beta}=w_\alpha\langle\alpha,\beta\rangle w_\beta. \tag{6.36}$$

VII. LOCAL UNIQUENESS AND EXISTENCE PROOFS

In this section we present the proofs of theorems 4–6. The proof of theorem 6 is the easiest and does not depend on the results of the Sec. 6.
Define

$$\mathcal{E}:=\{\mathsf{k}_j|j=1,2,\ldots I\},$$

with the k_j defined in (6.16) and let

$$\mathrm{pr}_+^q : E_+ \to E_+^q \quad q = 1,2,\ldots I,$$

denote the projection operators between the spaces defined in (6.19) and (6.20). If $a \in \mathbb{R}$, we will use $I_\epsilon(a)$ to denote an interval of radius ϵ about a, i.e.,

$$I_\epsilon(a) = (a-\epsilon, a+\epsilon).$$

From proposition 4 and (3.19), we know that the the solution $\Lambda_+(r)$ to Eq. (3.6) is, up to a gauge transformation, completely characterized by the condition

$$\Lambda_+(r) \in E_+ \quad \forall r. \tag{7.1}$$

As discussed previously, if we can solve the two EYM equations (3.3) and (3.5) for the variables $\{\Lambda_+(r), m(r)\}$ the remaining equation (3.4) can be integrated to yield S. Consequently, we are only interested in Eqs. (3.3) and (3.5).

Proof of theorem 4: The proof of this theorem involves finding a change of variables to put the system of differential equations (3.3) and (3.5) into a form where theorem 3 applies in a neighborhood of $r=0$.

Since Λ_+ satisfies (7.1), we can introduce new variables $\{u_{s+1}(r) | s \in \mathcal{E}\}$ that satisfy

$$\Lambda_+(r) = \Omega_+ + \sum_{s \in \mathcal{E}} u_{s+1}(r) r^{s+1}, \tag{7.2}$$

where $\Omega_+ = \Lambda_+(0)$ and $u_{s+1}(r) \in E_+^{\tilde{s}}$ for all r and $s \in \mathcal{E}$. Because $E_+ = \oplus_{q=1}^I E_+^q$, it is obvious that this transformation is invertible. Define

$$\chi_{s+1} = \begin{cases} 1 & \text{if } s \in \mathcal{E} \\ 0 & \text{otherwise} \end{cases}.$$

Then we can write $\Lambda_+(r) = \Omega_+ + \Sigma_{k=0}^\infty \chi_k u_k(r) r^k$. Substituting this in (3.8) shows that there exists an integer N_1 such that

$$\mathcal{F} = -\sum_{k \in \mathcal{E}} A_2(u_{k+1}) r^{k+1} + \sum_{k=2}^{N_1} f_k r^k,$$

where

$$f_k = \frac{1}{2} \sum_{j=2}^{k-2} \Big\{ [[\Omega_+, c(\chi_j u_j)] + [\Omega_-, \chi_j u_j], \chi_{k-j} u_{k-j}] + [[\chi_j u_j, c(\chi_{k-j} u_{k-j})], \Omega_+] + \sum_{s=2}^{j-2} [[\chi_s u_s, c(\chi_{j-s} u_{j-s})], \chi_{k-j} u_{k-j}] \Big\}.$$

But $A_2(u_{k+1}) = k(k+1) u_{k+1}$ for every $k \in \mathcal{E}$ by lemma 2 and hence

$$\mathcal{F} = -\sum_{k \in \mathcal{E}} k(k+1) u_{k+1} r^{k+1} + \sum_{k=2}^{N_1} f_k r^k. \tag{7.3}$$

Define

$$v_{s+1} = u'_{s+1} \quad \forall s \in \mathcal{E}. \tag{7.4}$$

Using (7.2), (7.3) and (7.4), the EYM equation (3.5) can be written as

$$r\sum_{k\in\mathcal{E}} v'_{k+1}r^{k+1} = -2\sum_{k\in\mathcal{E}}(k+1)v_{k+1}r^{k+1} + \sum_{k\in\mathcal{E}}\frac{k(k+1)}{r}\left(\frac{1}{N}-1\right)u_{k+1}r^{k+1} - \frac{2}{rN}\left(m-\frac{1}{r}P\right)\sum_{k\in\mathcal{E}}(v_{k+1}r^{k+1}+(k+1)u_{k+1}r^k) - \frac{1}{N}\sum_{k=4}^{N_1} f_k r^{k-1}. \quad (7.5)$$

Applying the projections $\mathrm{pr}_+^{\tilde{k}}$ for every $k\in\mathcal{E}$ to Eq. (7.5) yields

$$\begin{aligned} rv'_{k+1} = &-2(k+1)v_{k+1} - \frac{2}{rN}\left(m-\frac{1}{r}P\right)v_{k+1} \\ &+ \frac{k(k+1)}{r}\left(\frac{1}{N}-1\right)u_{k+1} - \frac{2}{r^2N}\left(m-\frac{1}{r}P\right) \\ &\times(k+1)u_{k+1}r^k - \frac{1}{r^{k+1}N}\sum_{s=2}^{N_1-2}\mathrm{pr}_+^{\tilde{k}}(f_{s+2})r^{s+1} \quad \forall k\in\mathcal{E}. \end{aligned} \quad (7.6)$$

The last term in (7.6) is the main obstruction to putting the equation into a form where theorem 3 applies. It seems to contain terms of order $r^{-s}(s>0)$. However, as we shall now see, the results of Sec. VI can be used to show that

$$\frac{1}{r^{k+1}N}\sum_{s=0}^{N_1-2}\mathrm{pr}_+^{\tilde{k}}(f_{s+2})r^{s+1} = \frac{1}{N}\sum_{s=k}^{N_1-2}\mathrm{pr}_+^{\tilde{k}}(f_{s+2})r^{s-k}. \quad (7.7)$$

Namely, by using proposition 4, we can show that $f_k\in E_+$ for all k. From the definition of the u_{s+1} it is clear that $\chi_{s+1}u_{s+1}\in\oplus_{q=1}^{\tilde{s}}E_+^q$ for $0\leqslant s\leqslant \mathsf{k}_I$, and so it follows from theorem 9 by letting $Z_0=\Omega_+$ and $Z_{k+1}=\chi_{k+1}u_{k+1}$ for $k\geqslant 0$ that $f_{s+2}\in\oplus_{q=1}^{\tilde{s}}E_+^q$. Consequently, for every $k\in\mathcal{E}$

$$\mathrm{pr}_+^{\tilde{k}}(f_{s+2}) = 0 \quad \text{if } s<k,$$

because $k\in\mathcal{E}$ implies that $k=\mathsf{k}_{\tilde{k}}$ and hence it follows for $s<k=\mathsf{k}_{\tilde{k}}$ that $\tilde{s}<\tilde{k}$. This proves (7.7). Therefore, we can rewrite (7.6) as

$$\begin{aligned} rv'_{k+1} = &-2(k+1)v_{k+1} - \frac{2}{rN}\left(m-\frac{1}{r}P\right)v_{k+1} + \frac{k(k+1)}{r}\left(\frac{1}{N}-1\right)u_{k+1} - \frac{2}{r^2N}\left(m-\frac{1}{r}P\right) \\ &\times(k+1)u_{k+1} - \frac{r}{N}\sum_{s=k}^{N_1-1}\mathrm{pr}_+^{\tilde{k}}(f_{s+3})r^{s-k} + \left(1-\frac{1}{N}\right)\mathrm{pr}_+^{\tilde{k}}(f_{k+2}) - \mathrm{pr}_+^{\tilde{k}}(f_{k+2}) \quad \forall k\in\mathcal{E}. \end{aligned} \quad (7.8)$$

Using the properties (6.3) of $\langle\langle\ |\ \rangle\rangle$ and the fact that $A_2(u_2)=2u_2$, it can be shown that there exists analytic functions

$$\hat{P}:E_+\times\mathbb{R}\to\mathbb{R} \quad \text{and} \quad \hat{G}:E_+\times E_+\times\mathbb{R}\to\mathbb{R},$$

such that

$$P = r^4\|u_2\|^2 + r^5\hat{P}(u,r) \ \text{ and } \ G = r^2 2\|u_2\|^2 + r^3\hat{G}(u,v,r), \quad (7.9)$$

where $u=\Sigma_{s\in\mathcal{E}}u_{s+1}$, $v=\Sigma_{s\in\mathcal{E}}v_{s+1}$, and $\|\ \|$ is defined by (6.2). Introduce a new "mass" variable μ by

$$\mu = \frac{1}{r^3}(m - r^3\|u_2\|^2). \tag{7.10}$$

Recall that $\mathsf{k}_1 = 1$, so 1 is always in $\mathcal{E}$ and hence u_2 is always defined. We can then write the EYM equation (3.3) as

$$r\mu' = -3\mu + r\{\hat{P}(u,r) + \hat{G}(u,v,r) - 2\langle\langle\, u_2 | v_2 \,\rangle\rangle - 2r(\mu + \|u_2\|^2)(2\|u_2\|^2 + r\hat{G}(u,v,r))\}. \tag{7.11}$$

Introduce one last change of variables via

$$\hat{v}_{k+1} = v_{k+1} + \frac{1}{2(k+1)}\,\mathrm{pr}_+^{\tilde{k}}(f_{k+2}). \tag{7.12}$$

Fix $X \in E_+$ and define $\hat{v} = \Sigma_{s\in\mathcal{E}}\hat{v}_{s+1}$. Then using (7.8), (7.10), and (7.12), it can be shown that there exists a neighborhood of $\mathcal{N}_X$ of X in E_+, an $\epsilon > 0$, and a sequence of analytic maps

$$\mathcal{G}_k : \mathcal{N}_X \times E_+ \times I_\epsilon(0) \times I_\epsilon(0) \to E_0^{\tilde{k}} \forall k \in \mathcal{E},$$

such that

$$r\hat{v}'_{k+1} = -2(k+1)\hat{v}_{k+1} + r\mathcal{G}_k(u,\hat{v},\mu,r) \forall k \in \mathcal{E}. \tag{7.13}$$

Also from (7.4), (7.11), and (7.12), it is not difficult to show that there exists analytic maps

$$\mathcal{H}_k : E_+ \times E_+ \to E_+^{\tilde{k}} \forall k \in \mathcal{E} \text{ and } \mathcal{K} : E_+ \times E_+ \times \mathbb{R} \times \mathbb{R} \to \mathbb{R},$$

such that

$$ru'_{k+1} = r\mathcal{H}_k(u,\hat{v}) \quad \forall k \in \mathcal{E}, \tag{7.14}$$

$$r\mu' = -3\mu + r\mathcal{K}(u,\hat{v},\mu,r). \tag{7.15}$$

The system of differential equations (7.13)–(7.15) are in the form for which theorem 3 applies. Applying this theorem shows that for fixed $X \in E_+$ there exist a unique solution $\{u_{k+1}(r,Y), \hat{v}_{k+1}(r,Y), \mu(r,Y)\}$ to this system of differential equations that is analytic in a neighborhood of $(r,Y) = (0,X)$ and that satisfies

$$u_{s+1}(r,Y) = Y_s + O(r) \quad \forall s \in \mathcal{E}, \tag{7.16}$$

$$\hat{v}_{s+1}(r,Y) = O(r) \quad \forall s \in \mathcal{E}, \tag{7.17}$$

$$\mu(r,Y) = O(r),$$

where $Y_s = \mathrm{pr}_+^{\tilde{s}}(Y)$. From Eq. (7.10), it is then clear that mass m satisfies

$$m(r) = O(r^3).$$

Also from (7.9), (7.12), (7.16), and (7.17) it is not difficult to see that

$$P = O(r^4) \text{ and } G = O(r^2). \tag{7.18}$$

From the results of the previous section there exists an orthonormal basis $\{\mathbf{f}_j | j = 1,2,\ldots M\}$ for E_+ consisting of eigenvectors for A_2, i.e, $A_2(\mathbf{f}_j) = k_j(k_j+1)\mathbf{f}_j$. Thus we can introduce new variables $\{\hat{u}_j(r) | j = 1,2,\ldots M\}$ via

$$\sum_{s\in\mathcal{E}} u_{s+1}(r)r^{s+1}=\sum_{j=1}^{M}\hat{u}_j(r)r^{k_j+1}\mathbf{f}_j. \tag{7.19}$$

From proposition 1 we know that $M=|S_\lambda|$. So we can write $S_\lambda=\{\alpha_j|j=1,2,\ldots M\}$ and we get from proposition 4 that $\{\mathbf{e}_{\alpha_j}|j=1,2,\ldots M\}$ is also a basis for E_+. Therefore there exists a real nonsingular matrix C_{ij} such that

$$\mathbf{f}_j=\sum_{k=1}^{M} C_{kj}\mathbf{e}_{\alpha_k}. \tag{7.20}$$

Expand Ω_+ and Λ_+ in the basis $\{\mathbf{e}_{\alpha_j}|j=1,2,\ldots M\}$ as follows:

$$\Omega_+=\sum_{j=1}^{M} w_{j,0}\mathbf{e}_{\alpha_j} \quad \text{and} \quad \Lambda_+(r)=\sum_{j=1}^{M} w_j(r)\mathbf{e}_{\alpha_j}. \tag{7.21}$$

Then results (7.2), (7.19)–(7.21) imply that

$$w_i(r)=w_{i,0}+\sum_{j=1}^{M} C_{ij}\hat{u}_j(r)r^{k_j+1} \quad i=1,2,\ldots M,$$

while from (7.16) and (7.19) it is clear that

$$\hat{u}_j(r,Y)=\beta_j(Y)+O(r) \quad j=1,2\ldots,M,$$

where $\beta_j(Y)=\langle\langle\mathbf{f}_j|Y\rangle\rangle$. □

Proof of theorem 5: The proof of this theorem involves finding a change of variables to put the system of differential equations (3.3) and (3.5) into a form where theorem 3 applies in a neighborhood of $z=0$ where $z=1/r$. This proof is similar to the proof of theorem 4 with the exception that theorem 10 is needed instead of theorem 9.

Since Λ_+ satisfies (7.1), we can introduce new variables $\{u_s(z)|s\in\mathcal{E}\}$ that satisfy

$$\Lambda_+(z)=\Omega_++\sum_{s\in\mathcal{E}} u_s(z)z^s, \tag{7.22}$$

where $\Omega_+=\Lambda_+|_{z=0}$ and $u_s(z)\in\tilde{E_+^s}$ for all z and $s\in\mathcal{E}$. Because $E_+=\oplus_{q=1}^{I}E_+^q$, it is obvious that this transformation is invertible. Define

$$\chi_s=\begin{cases}1 & \text{if } s\in\mathcal{E}\\ 0 & \text{otherwise}\end{cases}.$$

Then we can write $\Lambda_+(z)=\Omega_++\Sigma_{k=0}^{\infty}\chi_k u_k(z)z^k$. Substituting this in (3.8) shows that there exists an integer N_1 such that

$$\mathcal{F}=-\sum_{k\in\mathcal{E}} A_2(u_k)z^k+\sum_{k=1}^{N_1} f_k z^k,$$

where

$$f_k=\frac{1}{2}\sum_{j=1}^{k-1}\Big\{[[\Omega_+,c(\chi_j u_j)]+[\Omega_-,\chi_j u_j],\chi_{k-j}u_{k-j}]+[[\chi_j u_j,c(\chi_{k-j}u_{k-j})],\Omega_+]$$
$$+\sum_{s=1}^{j-1}[[\chi_s u_s,c(\chi_{j-s}u_{j-s})],\chi_{k-j}u_{k-j}]\Big\}.$$

But $A_2(u_k)=k(k+1)u_k$ for every $k\in\mathcal{E}$ by lemma 2 and hence

$$\mathcal{F}=-\sum_{k\in\mathcal{E}}k(k+1)u_k z^k+\sum_{k=1}^{N_1}f_k z^k. \tag{7.23}$$

Define

$$v_s=\mathring{u}_s \quad \forall s\in\mathcal{E}. \tag{7.24}$$

where $\mathring{(\cdot)}=d/dz(\cdot)$. Using (7.22)–(7.24), the EYM equation (3.5) can be written as

$$\sum_{k\in\mathcal{E}}\mathring{v}_k z^{k+1}=\sum_{k\in\mathcal{E}}-2(k+1)v_k z^k+\sum_{k\in\mathcal{E}}\Big\{\frac{2}{z}\Big(1-\frac{1}{N}\Big)v_k+\frac{1}{z^2}\Big(\frac{1}{N}-1-2mz\Big)k(k-1)u_k$$
$$+\frac{4m}{z}\Big(\frac{1}{N}-1\Big)ku_k+\frac{2}{N}(2m-z^2P)v_k-\frac{zP}{N}ku_k\Big\}z^{k+1}$$
$$+\sum_{k\in\mathcal{E}}2mk(k+1)u_k z^k-\frac{1}{N}\sum_{k=1}^{N_1}f_k z^{k-1}. \tag{7.25}$$

Applying the projections $\mathrm{pr}_+^{\tilde{k}}$ for every $k\in\mathcal{E}$ to Eq. (7.25) yields

$$z\mathring{v}_k=-2(k+1)v_k+z\Big\{\frac{2}{z}\Big(1-\frac{1}{N}\Big)v_k+\frac{1}{z^2}\Big(\frac{1}{N}-1-2mz\Big)k(k-1)u_k$$
$$+\frac{4m}{z}\Big(\frac{1}{N}-1\Big)ku_k+\frac{2}{N}(2m-z^2P)v_k-\frac{zP}{N}ku_k\Big\}$$
$$+2mk(k+1)u_k-\frac{1}{z^kN}\sum_{s=0}^{N_1-1}\mathrm{pr}_+^{\tilde{k}}(f_{s+1})z^s \quad \forall k\in\mathcal{E}. \tag{7.26}$$

The last term in (7.26) is the main obstruction to putting this equation into a form where theorem 3 applies. It seems to contain terms of order $z^{-s}(s>0)$. But this is not the case as the results of Sec. VI can be used to show that

$$\frac{1}{z^kN}\sum_{s=0}^{N_1-1}\mathrm{pr}_+^{\tilde{k}}(f_{s+1})z^s=\frac{1}{N}\sum_{s=k}^{N_1-1}\mathrm{pr}_+^{\tilde{k}}(f_{s+1})z^{s-k}.$$

Namely, using proposition 4, it can be shown that $f_k\in E_+$ for all k. From the definition of the u_s it is obvious that $\chi_s u_s\in\oplus_{q=1}^{\tilde{s}}E_+^q$ for $1\leqslant s\leqslant \mathsf{k}_I$, and therefore, by letting $Z_0=\Omega_+$ and $Z_k=\chi_k u_k$ for $k\geqslant 1$ we get $f_{s+1}\in\oplus_{q=1}^{\tilde{s}}E_+^q$ via theorem 10. Consequently, for every $k\in\mathcal{E}$

$$\mathrm{pr}_+^{\tilde{k}}(f_{s+1})=0 \quad \text{if } s<k,$$

because $k\in\mathcal{E}$ implies that $k=\mathsf{k}_{\tilde{k}}$ and hence it follows for $s<k=\mathsf{k}_{\tilde{k}}$ that $\tilde{s}<\tilde{k}$. Therefore we can rewrite (7.26) as

$$z\mathring{v}_k=-2(k+1)v_k+z\Bigg\{\frac{2}{z}\left(1-\frac{1}{N}\right)v_k+\frac{1}{z^2}\left(\frac{1}{N}-1-3mz\right)k(k-1)u_k$$
$$+\frac{4m}{z}\left(\frac{1}{N}-1\right)ku_k+\frac{2}{N}(2m-z^2P)v_k-\frac{zP}{N}ku_k-\frac{z}{N}\sum_{s=k+1}^{N_1-1}\mathrm{pr}_+^{\tilde{k}}(f_{s+1})z^{s-k-1}$$
$$+\left(1-\frac{1}{N}\right)\mathrm{pr}_+^{\tilde{k}}(f_{k+1})\Bigg\}+2mk(k+1)u_k-\mathrm{pr}_+^{\tilde{k}}(f_{k+1})\quad\forall k\in\mathcal{E}. \tag{7.27}$$

It is clear that there exists analytic functions

$$\hat{P}:E_+\times\mathbb{R}\to\mathbb{R}\ \text{ and }\ \hat{G}:E_+\times E_+\times\mathbb{R}\to\mathbb{R},$$

such that

$$P=\hat{P}(u,z)\ \text{ and }\ G=z^4\hat{G}(u,v,z),$$

where $u=\Sigma_{s\in\mathcal{E}}u_s$ and $v=\Sigma_{s\in\mathcal{E}}v_s$. The EYM equation (3.3) can then be written as

$$z\mathring{m}=z[(2mz-1)z^2\hat{G}(u,v,z)-P(u,z)]. \tag{7.28}$$

Introduce one last change of variables via

$$\hat{v}_k=v_k+\frac{1}{2(k+1)}\mathrm{pr}_+^{\tilde{k}}(f_{k+1})-kmu_k. \tag{7.29}$$

Fix $a>0$ and define $\hat{v}=\Sigma_{s\in\mathcal{E}}\hat{v}_s$. Then using (7.27), and (7.29), it can be shown that there exists and $\epsilon>0$, and a sequence of analytic maps

$$\mathcal{G}_k:E_+\times E_+\times I_\epsilon(a)\times I_\epsilon(0)\to E_0^{\tilde{k}}\quad\forall k\in\mathcal{E},$$

such that

$$z\mathring{\hat{v}}_k=-2(k+1)\hat{v}_k+z\mathcal{G}_k(u,\hat{v},m,z)\quad\forall k\in\mathcal{E}. \tag{7.30}$$

Also from (7.24), (7.28), and (7.29), it is not hard to show that there exists analytic maps

$$\mathcal{H}_k:E_+\times E_+\times\mathbb{R}\to E_+^{\tilde{k}}\quad\forall k\in\mathcal{E}$$
$$\text{and}\quad\mathcal{K}:E_+\times E_+\times\mathbb{R}\times\mathbb{R}\to\mathbb{R}, \tag{7.31}$$

such that

$$z\mathring{u}_k=z\mathcal{H}_k(u,\hat{v},m)\quad\forall k\in\mathcal{E}, \tag{7.32}$$

$$z\mathring{m}=z\mathcal{K}(u,\hat{v},m,z). \tag{7.33}$$

The system of differential equations (7.30), (7.32), and (7.33) are in the form for which theorem 3 applies. Applying this theorem shows that for fixed $(X,a)\in E_+\times(0,\infty)$ there exist a unique solution $\{u_k(z,Y,m_\infty),\hat{v}_k(z,Y,m_\infty),m(z,Y,m_\infty)\}$ to this system of differential equations that is analytic in a neighborhood of $(z,Y,m_\infty)=(0,X,a)$ and satisfies

$$u_s(z,Y,m_\infty)=Y_s+O(z) \quad \forall s\in\mathcal{E},$$

$$\hat{v}_s(z,Y,m_\infty)=O(z) \quad \forall s\in\mathcal{E}, \tag{7.34}$$

$$m(z,Y,m_\infty)=m_\infty+O(z),$$

where $Y_s=\mathrm{pr}_+^{\tilde{s}}(Y)$. Let $\{\mathbf{f}_j|j=1,2,\ldots M\}$ and $\{\mathbf{e}_{\alpha_j}|j=1,2,\ldots M\}$ be the same basis for E_+ as introduced in the proof of theorem 4. Then we can introduce new variables $\{\hat{u}_j(z)|j=1,2,\ldots M\}$ via

$$\sum_{s\in\mathcal{E}} u_s(z)z^s=\sum_{j=1}^{M}\hat{u}_j(z)z^{k_j}\mathbf{f}_j. \tag{7.35}$$

Expand Ω_+ and Λ_+ in the basis $\{\mathbf{e}_{\alpha_j}|j=1,2,\ldots M\}$ as follows:

$$\Omega_+=\sum_{j=1}^{M} w_{j,\infty}\mathbf{e}_{\alpha_j} \quad \text{and} \quad \Lambda_+(z)=\sum_{j=1}^{M} w_j(z)\mathbf{e}_{\alpha_j}. \tag{7.36}$$

Results (7.22), (7.35), (7.20), and (7.36) then imply that

$$w_i(z)=w_{i,\infty}+\sum_{j=1}^{M} C_{ij}\hat{u}_j(z)z^{k_j} \quad i=1,2,\ldots M,$$

while from (7.34) and (7.35) it is clear that

$$\hat{u}_j(z,Y,m_\infty)=\alpha_j(Y)+O(z) \quad j=1,2\ldots,M,$$

where $\alpha_j(Y)=\langle\langle\mathbf{f}_j|Y\rangle\rangle$. □

Proof of theorem 6: The proof of this theorem involves finding a change of variables to put the system of differential equations (3.3) and (3.5) into a form where theorem 3 applies in a neighborhood of $r=r_H$.

Note that although we use the space E_+ which was defined in Sec. VI, this proof does not depend on the results of Sec. VI. Indeed, E_+ can be replaced by $\Sigma_{\alpha\in S_\lambda}\mathbb{R}\mathbf{e}_\alpha$ everywhere in the proof below and one does not have to know that $E_+=\Sigma_{\alpha\in S_\lambda}\mathbb{R}\mathbf{e}_\alpha$, which is the content of proposition 4. The notation E_+ is used for convenience.

Introduce new variables t, μ, and υ via

$$t=r-r_H, \quad N=t(\mu+\nu), \quad \upsilon=(\mu+\nu)\Lambda_+'. \tag{7.37}$$

where ν is a constant. Then

$$t\frac{d\Lambda_+}{dt}=t\left(\frac{\upsilon}{\mu+\nu}\right), \tag{7.38}$$

and it is clear that there exists analytic maps

$$\hat{\mathcal{F}}:E_+\to E_+ \quad \text{and} \quad \hat{P}:E_+\to\mathbb{R},$$

such that

$$\hat{\mathcal{F}}(\Lambda_+)=\mathcal{F} \quad \text{and} \quad \hat{P}(\Lambda_+)=P.$$

Assume $|\nu|>0$. Define a analytic map

$$\hat{G}: E_+ \times I_{|\nu|}(0) \to \mathbb{R},$$

by

$$\hat{G}(X,a) = \frac{1}{2(a+\nu)^2}\|X\|^2.$$

Then

$$G = \hat{G}(v,\mu).$$

Using these new variables, we can write the EYM equations (3.3) and (3.5) as

$$t\frac{d\mu}{dt} = -(\mu+\nu) + \frac{1}{r_H} - \frac{2}{r_H^3}\hat{P}(\Lambda_+) + t\left[\frac{1}{t}\left(\frac{1}{t+r_H} - \frac{1}{r_H}\right) - \frac{2}{t}\left(\frac{1}{(t+r_H)^3} - \frac{1}{r_H^3}\right)\hat{P}(\Lambda_+) + \left(\frac{\mu+\nu}{t+r_H}\right)(1+2\hat{G}(v,\mu))\right] \tag{7.39}$$

and

$$t\frac{dv}{dt} = -v - \frac{1}{(t+r_H)^2}\hat{\mathcal{F}}(\Lambda_+) - t\left(\frac{2\hat{G}(v,\mu)}{t+r_H}\right)v, \tag{7.40}$$

respectively. Introduce two new variables μ and $\hat{v}$ via

$$\hat{\mu} = \mu + \nu - \frac{1}{r_H} + \frac{2}{r_H^3}\hat{P}(\Lambda_+), \tag{7.41}$$

$$\hat{v} = v + \frac{1}{r_H^2}\hat{\mathcal{F}}(\Lambda_+). \tag{7.42}$$

Define an analytic map

$$\gamma: E_+ \times \mathbb{R} \to \mathbb{R},$$

by

$$\gamma(X,a) = a - \nu + \frac{1}{r_H} - \frac{2}{r_H^3}\hat{P}(X).$$

Fix a vector $Z \in E_+$ that satisfies $\| 1/r_H - 2/r_H^3\hat{P}(Z)\| > 0$. Then if we set

$$\nu = \frac{1}{r_H} - \frac{2}{r_H^3}\hat{P}(Z),$$

we get $\gamma(Y,0) = 0$. So we can define an open neighborhood D of $(Z,0) \in E_+ \times \mathbb{R}$ by

$$D = \{(X,a) | \| \gamma(X,a)\| < \|\nu\|\}.$$

Then from (7.38)–(7.42), it is not hard to show that there exists an $\epsilon > 0$ and analytic maps

$$\mathcal{G}: E_+ \times D \to \mathbb{R},$$

$$\mathcal{H}: E_+ \times D \times I_\epsilon(0) \to \mathbb{R},$$

$$\mathcal{K}: E_+ \times D \times I_\epsilon(0) \to \mathbb{R},$$

such that

$$t\frac{d\Lambda_+}{dt} = t\mathcal{G}(\hat{v}, \Lambda_+, \hat{\mu}), \tag{7.43}$$

$$t\frac{d\hat{v}}{dt} = -\hat{v} + t\mathcal{H}(\hat{v}, \Lambda_+, \hat{\mu}, t), \tag{7.44}$$

$$t\frac{d\hat{\mu}}{dt} = -\hat{\mu} + t\mathcal{K}(\hat{v}, \Lambda_+, \hat{\mu}, t\ddot{u}. \tag{7.45}$$

The system of differential equations (7.43)–(7.45) is in the form for which theorem 3 applies. Applying this theorem shows that exists a unique solution $\{\Lambda_+(t,Y), \hat{v}(t,Y), \hat{\mu}(t,Y)\}$ to this system of differential equations that is analytic in a neighborhood of $(t,Y) = (0,Z)$ and that satisfies

$$\Lambda_+(t,Y) = Z + O(t), \tag{7.46}$$

$$\hat{v}(t,Y) = O(t),$$

$$\hat{\mu}(t,Y) = O(t). \tag{7.47}$$

Expand Z and Λ_+ in the basis $\{\mathbf{e}_\alpha | \alpha \in S_\lambda\}$ as follows:

$$Z = \sum_{\alpha \in S_\lambda} w_{\alpha, r_H} \mathbf{e}_\alpha \quad \text{and} \quad \Lambda_+(t) = \sum_{\alpha \in S_\lambda} w_\alpha(t) \mathbf{e}_\alpha .$$

Then Eq. (7.46) shows that

$$w_\alpha(t,Z) = w_{\alpha, r_H} + O(t) \quad \forall \alpha \in S_\lambda .$$

It also not difficult to show that Eqs. (7.37), (7.41), and (7.47) imply that

$$N(t,Z) = \nu t + O(t^2).$$

From this it follows immediately that

$$N(r_H) = 0 \quad \text{and} \quad N'(r_H) = \nu.$$

□

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Lax–Phillips scattering theory of a relativistic quantum field theoretical Lee–Friedrichs model and Lee–Oehme–Yang–Wu phenomenology

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The scattering theory of Lax and Phillips, originally developed for classical wave equations, has recently been extended to the description of the evolution of resonant states in the framework of quantum theory. The resulting evolution law of the unstable system is that of a semigroup, and the resonant state is a well-defined function in the Lax–Phillips Hilbert space. In this paper we apply this theory to a relativistically covariant quantum field theoretical form of the two (or more) channel relativistic quantum field theoretical form of the Lee model. We show that this theory provides a rigorous underlying basis for the Lee–Oehme–Yang–Wu construction. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1461426]

I. INTRODUCTION

The theory of Lax and Phillips (1967),[1] originally developed for the description of resonances in electromagnetic or acoustic scattering phenomena, has been used as a framework for the construction of a description of irreversible resonant phenomena in the quantum theory[2–5] (which we will refer to as the quantum Lax–Phillips theory). This leads to a time evolution of resonant states which is of semigroup type, i.e., essentially exponential decay. Semigroup evolution is necessarily a property of irreversible processes.[6] It appears experimentally that elementary particle decay, to a high degree of accuracy, follows a semigroup law, and hence such processes seem to be irreversible.

The theory of Weisskopf and Wigner,[7] which is based on the definition of the survival amplitude of the initial state ϕ (associated with the unstable system) as the scalar product of that state with the unitarily evolved state,

$$(\phi, e^{-iHt}\phi), \tag{1.1}$$

cannot have exact exponential behavior.[8] One can easily generalize this construction to the problem of more than one resonance.[9,10] If P is the projection operator into the subspace of initial states (N-dimensional for N resonances), the reduced evolution operator is given by

$$Pe^{-iHt}P. \tag{1.1$'$}$$

Since the Laplace transform of this operator has a cut and not just poles, this operator cannot be an element of an exact semigroup.[8]

Experiments on the decay of the neutral K-meson system[11] show clearly that the phenomenological description of Lee, Oehme, and Yang,[12] and Wu and Yang,[13] by means of a 2×2 effective Hamiltonian which corresponds to an exact semigroup evolution of the unstable system, provides a very accurate description of the data. It can be proved that the Wigner–Weisskopf theory cannot provide a semigroup evolution law[8] and, thus, the effective 2×2 Hamiltonian cannot emerge in the framework of this theory. Furthermore, it has been shown, using estimates based on the

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quantum mechanical Lee–Friedrichs model,[14] that the experimental results appear to rule out the application of the Wigner–Weisskopf theory to the decay of the neutral K-meson system. While the exponential decay law can be exhibited explicitly in terms of a Gel'fand triple[15] (rigged Hilbert space), the representation of the resonant state in this framework is in a space which does not coincide with the quantum mechanical Hilbert space, and does not have the properties of a Hilbert space, such as scalar products and the possibility of calculating physical properties associated with expectation values.

The seminal work of Lax and Phillips[1] has provided us with the basic ideas necessary for the construction of a fundamental theoretical description, in the framework of the quantum theory,[2–5] of a resonant system which has exact semigroup evolution, and represents the resonance as a *state in a Hilbert space*. In the following, we briefly describe the structure of this theory, a rather straightforward generalization of standard quantum scattering theory, and give some physical interpretation for the states of the Lax–Phillips Hilbert space.

The Lax–Phillips theory is defined in a Hilbert space $\overline{H}$ of states which contains two distinguished subspaces, $D_{\pm}$, called "outgoing" and "incoming." There is a unitary evolution law which we denote by $U(\tau)$, for which these subspaces are invariant in the following sense:

$$U(\tau)D_{+}\subset D_{+}, \quad \tau\geqslant 0,$$
$$U(\tau)D_{-}\subset D_{-}, \quad \tau\leqslant 0. \tag{1.2}$$

The translates of $D_{\pm}$ under $U(\tau)$ are dense, i.e.,

$$\overline{\bigcup_{\tau} U(\tau)D_{\pm}}=\overline{H} \tag{1.3}$$

and the asymptotic property

$$\bigcap_{\tau} U(\tau)D_{\pm}=\varnothing \tag{1.4}$$

is assumed. It follows from these properties that

$$Z(\tau)=P_{+}U(\tau)P_{-}, \tag{1.5}$$

where $P_{\pm}$ are projections into the subspaces orthogonal to $\mathcal{D}_{\pm}$, is a strongly contractive semigroup,[1] i.e.,

$$Z(\tau_1)Z(\tau_2)=Z(\tau_1+\tau_2) \tag{1.6}$$

for τ_1, τ_2 positive, and $\|Z(\tau)\|\to 0$ for $\tau\to 0$. It follows from (1.2) that $Z(\tau)$ takes the subspace $\mathcal{K}$, the orthogonal complement of $D_{\pm}$ in $\overline{H}$ (associated with the resonances in the Lax–Phillips theory), into itself,[1] i.e.,

$$Z(\tau)=P_{\mathcal{K}}U(\tau)P_{\mathcal{K}}. \tag{1.7}$$

The relation (1.7) is of the same structure as (1.1′); there is, as we shall see in the following, an essential difference in the way that the subspaces associated with resonances are defined. The argument that (1.1') cannot form a semigroup is not valid[3] for (1.7); the generator of $U(\tau)$ restricted to $\mathcal{K}$ is not self-adjoint.

A Hilbert space with the properties that there are distinguished subspaces satisfying, with a given law of evolution $U(\tau)$, the properties (1.2), (1.3), and (1.4) has a foliation[16] into a one-parameter (which we shall denote as s) family of isomorphic Hilbert spaces, which are called *auxiliary* Hilbert spaces, $\{H_s\}$, for which

$$\overline{H}=\int_{\oplus} H_s\,. \tag{1.8}$$

Representing these spaces in terms of square-integrable functions, we define the norm in the direct integral space as

$$\|f\|^2=\int_{-\infty}^{\infty} \mathrm{d}s\|f_s\|_H^2\,, \tag{1.9}$$

where $f\in\overline{H}$ represents a vector in the L^2 function space $\overline{H}=L^2(-\infty,\infty,H)$; f_s is an element of H, the L^2 function space (the *auxiliary space*) corresponding to H_s for any s (we shall not add in what follows a subscript to the norm or scalar product symbols for scalar products of elements of the auxiliary Hilbert space associated with a point s on the foliation axis since these spaces are all isomorphic).

There are representations for which the action of the full evolution group $U(\tau)$ on $L^2(-\infty,\infty;H)$ is translation by τ units. Given $D_{\pm}$ there is such a representation, called the *incoming representation*,[1] for which the set of all functions in D_- have support in $(-\infty,0)$ and constitute the subspace $L^2(-\infty,0;H)$ of $L^2(-\infty,\infty;H)$; there is another representation, called the *outgoing representation*, for which functions in D_+ have support in $(0,\infty)$ and constitute the subspace $L^2(0,\infty;H)$ of $L^2(-\infty,\infty;H)$. The fact that $Z(\tau)$ in Eq. (1.7) is a semigroup is a consequence of the definition of the subspaces $D_{\pm}$ in terms of support properties on intervals along the foliation axis in the *outgoing* and *incoming* translation representations, respectively. The non-self-adjoint character of the generator of the semigroup $Z(\tau)$ is a consequence of this structure.[3]

Lax and Phillips[1] show that there are unitary operators $W_{\pm}$, called wave operators, which map elements in $\overline{H}$ to these representations. They define an S matrix,

$$S=W_+W_-^{-1} \tag{1.10}$$

which connects the incoming to the outgoing representations; it is unitary, commutes with translations, and maps $L^2(-\infty,0;H)$ into itself. Since S commutes with translations, it is diagonal in Fourier (spectral) representation. As pointed out by Lax and Phillips,[1] according to a special case of a theorem of Fourès and Segal,[17] an operator with these properties can be represented as a multiplicative operator-valued function $S(\sigma)$ which maps H into itself, and satisfies the following conditions:

(a) $S(\sigma)$ *is the boundary value of an operator-valued function* $S(z)$ *analytic for* $\mathrm{Im}\,z>0$,
(b) $\|S(z)\|\leqslant 1$ *for all* z *with* $\mathrm{Im}\,z>0$,
(c) $S(\sigma)$ *is unitary for almost all real* σ.

An operator with these properties is known as an inner function;[18] such operators arise in the study of shift invariant subspaces, the essential mathematical content of the Lax–Phillips theory. The singularities of this S matrix, in what is called *spectral representation* (defined in terms of the Fourier transform on the foliation variable s), correspond to the spectrum of the generator of the semigroup characterizing the evolution of the unstable system.

In the framework of quantum theory, one may identify the Hilbert space H with a space of physical states, and the variable τ with the laboratory time (the semigroup evolution is observed in the laboratory according to this time). The representation of this space in terms of the foliated L^2 space $\overline{H}$ provides a natural probabilistic interpretation for the auxiliary spaces associated with each value of the foliation variable s, i.e., the quantity $\|f_s\|^2$ corresponds to the probability density for

the system to be found in the neighborhood of s. For example, consider an operator A defined on $\overline{H}$ which acts pointwise, i.e., contains no shift along the foliation. Such an operator can be represented as a direct integral

$$A=\int_{\oplus} A_s. \tag{1.11}$$

It produces a map of the auxiliary space H into H for each value of s, and thus, if it is self-adjoint, A_s may act as an observable in a quantum theory associated with the point s;[4] The expectation value of A_s in a state in this Hilbert space defined by the vector ψ_s, the component of $\psi\in\overline{H}$ in the auxiliary space at s, is

$$\langle A_s\rangle_s=\frac{(\psi_s,A_s\psi_s)}{\|\psi_s\|^2}. \tag{1.12}$$

Taking into account the *a priori* probability density $\|\psi_s\|^2$ that the system is found at this point on the foliation axis, we see that the expectation value of A in $\overline{H}$ is

$$\langle A\rangle=\int \mathrm{d}s\langle A_s\rangle_s\|\psi_s\|^2=\int \mathrm{d}s(\psi_s,A_s\psi_s), \tag{1.13}$$

the direct integral representation of $(\psi,A\psi)$.

As we have remarked previously, in the translation representations for $U(\tau)$ the foliation variable s is shifted (this shift, for sufficiently large $|\tau|$, induces the transition of the state into the subspaces $D_{\pm}$). It follows that s may be identified as an intrinsic time associated with the evolution of the state; since it is a variable of the measure space of the Hilbert space $\overline{H}$, this quantity itself has the meaning of a quantum variable.

We are presented here with the notion of a virtual history. To understand this idea, suppose that at a given time τ_0, the function which represents the state has some distribution $\|\psi_s^{\tau_0}\|^2$. This distribution provides an *a priori* probability that the system would be found at time s (greater or less than τ_0), if the experiment were to be performed at time s corresponding to $\tau=s$ on the laboratory clock. The state of the system therefore contains information on the structure of the *history* of the system as it is inferred at τ_0.

We shall assume the existence of a unitary evolution on the Hilbert space $\overline{H}$, and that for

$$U(\tau)=e^{-iK\tau}, \tag{1.14}$$

the generator K can be decomposed as

$$K=K_0+V \tag{1.15}$$

in terms of an unperturbed operator K_0 with spectrum $(-\infty,\infty)$ and a perturbation V, under which this spectrum is stable. We shall, furthermore, assume that wave operators exist, defined on some dense set, as

$$\Omega_{\pm}=\lim_{\tau\to\pm\infty} e^{iK\tau}e^{-iK_0\tau}. \tag{1.16}$$

In the soluble model that we shall treat as an example in this paper, the existence of the wave operators is assured.

With the help of the wave operators, we can define translation representations for $U(\tau)$. The translation representation for K_0 is defined by the property

$${}_0\langle s,\alpha|e^{-iK_0\tau}f)={}_0\langle s-\tau,\alpha|f), \tag{1.17}$$

where α corresponds to a label for the basis of the auxiliary space. Noting that

$$K\Omega_{\pm}=\Omega_{\pm}K_0 \tag{1.18}$$

we see that

$${}_{\text{in}}^{\text{out}}\langle s,\alpha|e^{-iK\tau}f\rangle={}_{\text{in}}^{\text{out}}\langle s-\tau,\alpha|f\rangle, \tag{1.19}$$

where

$${}_{\text{in}}^{\text{out}}\langle s,\alpha|f\rangle={}_0\langle s,\alpha|\Omega_{\pm}^{\dagger}f\rangle. \tag{1.20}$$

It will be convenient to work in terms of the Fourier transform of the in and out translation representations; we shall call these the in and out spectral representations, i.e.,

$${}_{\text{in}}^{\text{out}}\langle\sigma,\alpha|f\rangle=\int_{-\infty}^{\infty}e^{-i\sigma s}{}_{\text{in}}^{\text{out}}\langle s,\alpha|f\rangle. \tag{1.21}$$

In these representations, (1.20) is

$${}_{\text{in}}^{\text{out}}\langle\sigma,\alpha|f\rangle={}_0\langle\sigma,\alpha|\Omega_{\pm}^{\dagger}f\rangle \tag{1.22}$$

and (1.19) becomes

$${}_{\text{in}}^{\text{out}}\langle\sigma,\alpha|e^{-iK\tau}|f\rangle=e^{-i\sigma\tau}{}_{\text{in}}^{\text{out}}\langle\sigma,\alpha|f\rangle. \tag{1.23}$$

Equation (1.17) becomes, under Fourier transform,

$${}_0\langle\sigma,\alpha|e^{-iK_0\tau}f\rangle=e^{-i\sigma\tau}{}_0\langle\sigma,\alpha|f\rangle. \tag{1.24}$$

For f in the domain of K_0, (1.24) implies that

$${}_0\langle\sigma,\alpha|K_0f\rangle=\sigma\,{}_0\langle\sigma,\alpha|f\rangle. \tag{1.25}$$

With the solution of (1.25), and the wave operators, the in and out spectral representations of a vector f can be constructed from (1.24).

We are now in a position to construct the subspaces $D_{\pm}$, which are not given *a priori* (as they are in the classical theory[1]) in the Lax–Phillips quantum theory. We shall define D_+ as the set of functions with support in $(0,\infty)$ in the *outgoing* translation representation. Similarly, we shall define D_- as the set of functions with support in $(-\infty,0)$ in the *incoming* translation representation. The corresponding elements of $\overline{H}$ constitute the subspaces $D_{\pm}$. By construction, $D_{\pm}$ have the required invariance properties under the action of $U(\tau)$.

The *outgoing spectral representation* of a vector $g\in\mathcal{H}$ is

$$\begin{aligned}{}_{\text{out}}\langle\sigma\alpha|g\rangle={}_0\langle\sigma\alpha|\Omega_+^{-1}g\rangle&=\int\mathrm{d}\sigma'\sum_{\alpha'}\,{}_0\langle\sigma\alpha|\mathbf{S}|\sigma'\alpha'\rangle_0\,{}_0\langle\sigma'\alpha'|\Omega_-^{-1}g\rangle\\&=\int\mathrm{d}\sigma'\sum_{\alpha'}\,{}_0\langle\sigma\alpha|\mathbf{S}|\sigma'\alpha'\rangle_0\,{}_{\text{in}}\langle\sigma'\alpha'|g\rangle,\end{aligned} \tag{1.26}$$

where we call

$$\mathbf{S}=\Omega_+^{-1}\Omega_- \tag{1.27}$$

the quantum Lax–Phillips S operator. We see that the kernel ${}_0\langle\sigma\alpha|\mathbf{S}|\sigma'\alpha'\rangle_0$ maps the incoming to outgoing spectral representations. Since $\mathbf{S}$ commutes with K_0, it follows that

$$ {}_0\langle\sigma\alpha|\mathbf{S}|\sigma'\alpha'\rangle_0 = \delta(\sigma-\sigma')S^{\alpha\alpha'}\cdot(\sigma). \tag{1.28}$$

It follows from (1.16) and (1.22), in the standard way,[19] that

$$ {}_0\langle\sigma\alpha|\mathbf{S}|\sigma'\alpha'\rangle_0 = \lim_{\epsilon\to 0}\delta(\sigma-\sigma')\{\delta^{\alpha\alpha'}-2\pi i\,{}_0\langle\sigma\alpha|\mathbf{T}(\sigma+i\epsilon)|\sigma'\alpha'\rangle_0\}, \tag{1.29}$$

where

$$ \mathbf{T}(z)=V+VG(z)V=V+VG_0(z)\mathbf{T}(z). \tag{1.30}$$

We remark that, by this construction, $S^{\alpha\alpha'}(\sigma)$ is *analytic in the upper half plane* in σ. The Lax–Phillips S matrix[1] is given by the inverse Fourier transform,

$$ S=\{{}_0\langle s\alpha|\mathbf{S}|s'\alpha'\rangle_0\}; \tag{1.31}$$

this operator clearly commutes with translations.

From (1.29) it follows that the inner function property (a) of $S(\sigma)$ above is true. Property (c), unitarity for real σ, is equivalent to asymptotic completeness, a property which is stronger than the existence of wave operators. For the relativistic Lee model, which we shall treat in this paper, this condition is satisfied. In the model that we shall study here, we shall see that there is a wide class of potentials V for which the operator $S(\sigma)$ satisfies the property (b).

In Sec. II, we briefly review the structure of the relativistic Lee model,[19] and explicitly construct the Lax–Phillips spectral representations and S matrix. Introducing auxiliary space variables, we then characterize the properties of the finite rank Lee model potential which assure that the S matrix is an inner function, i.e., that property (b) listed above is satisfied.

II. THE MULTICHANNEL RELATIVISTIC LEE–FRIEDRICHS MODEL

The multichannel relativistic Lee–Friedrichs model is defined in terms of bosonic quantum fields on space–time. These fields, which emerge from the second quantization of the Stueckelberg covariant quantum theory,[20] evolve with an invariant evolution parameter[5] τ (which we identify here with the evolution parameter of the Lax–Phillips theory discussed previously); at equal τ, they satisfy the commutation relations (with $\psi_i^\dagger$ as the canonical conjugate field to ψ_i; the fields ψ_i, which satisfy first-order evolution equations as for nonrelativistic Schrödinger fields, are just annihilation operators)

$$ [\psi_{i\tau}(x),\psi_{j\tau}^\dagger(x')]=\delta^4(x-x')\,\delta_{ij}. \tag{2.1}$$

Transforming to momentum space, in which we have

$$ \psi_{i\tau}(p)=\frac{1}{(2\pi)^2}\int d^4x\, e^{-ip_\mu x^\mu}\psi_{i\tau}(x), \tag{2.2}$$

relation (2.1) becomes

$$ [\psi_{i\tau}(p),\psi_{j\tau}^\dagger(p')]=\delta^4(p-p')\,\delta_{ij}. \tag{2.3}$$

The manifestly covariant space–time structure of these fields is admissible when $E,\mathbf{p}$ are not *a priori* constrained by a sharp mass–shell relation. In the mass–shell limit (for which the variation in m^2 defined by $E^2-\mathbf{p}^2$ is small), multiplying both sides of (2.3) by $\Delta E=\Delta m^2/2E$, one obtains the usual commutation relations for on shell fields,

$$[\tilde{\psi}_{i\tau}(\mathbf{p}),\tilde{\psi}^{\dagger}_{j\tau}(\mathbf{p})]=2E\,\delta^3(\mathbf{p}-\mathbf{p}')\,\delta_{ij}\,, \tag{2.4}$$

where $\tilde{\psi}_{i\tau}(\mathbf{p})=\sqrt{\Delta m^2}\psi_{i\tau}(\mathbf{p})$. In this limit, t and τ coincide. The generator of evolution

$$K=K_0+V \tag{2.5}$$

for which the Heisenberg picture fields are

$$\psi_{i\tau}(p)=e^{iK\tau}\psi_{i0}(p)e^{-iK\tau} \tag{2.6}$$

is given, in this model, as (we write $p^2=p_\mu p^\mu, k^2=k_\mu k^\mu$ in the following)

$$K_0=\sum_{i=1,2}\left\{\int \mathrm{d}^4p\,\frac{p^2}{2M_{V_i}}b_i^{\dagger}(p)b_i(p)+\int \mathrm{d}^4p\,\frac{p^2}{2M_{N_i}}a_{N_i}^{\dagger}(p)a_{N_i}(p)\right\}$$
$$+\sum_{i=1,2}\int \mathrm{d}^4p\,\frac{p^2}{2M_{\theta_i}}a_{\theta_i}^{\dagger}(p)a_{\theta_i}(p) \tag{2.7}$$

and

$$V=\sum_{i,j=1,2}\int \mathrm{d}^4p\int \mathrm{d}^4k(f_{ij}(k)b_i^{\dagger}(p)a_{N_j}(p-k)a_{\theta_j}(k)+f_{ij}^{*}(k)b_i(p)a_{N_j}^{\dagger}(p-k)a_{\theta_j}^{\dagger}(k)). \tag{2.8}$$

(We remark that Antoniou *et al.*[21] have constructed a relativistic Lee model of a somewhat different type; their field equation is second order in derivative with respect to the variable conjugate to the mass.) This model describes the process $V_i\rightarrow N_j+\theta_j$. We assume that the fields associated with different particles commute. The fields $b_i(p)$, $a_{N_i}(p)$ and a_{θ_i} are annihilation operators for the V_i, N_i, and θ_i particles, respectively. We take M_{V_i}, M_{N_i}, and M_{θ_i} to be the mass parameters for the fields.[19,22] We restrict our development to the two channel case in the following. The generalization to any number of channels is straightforward.

The following operators are conserved:

$$Q_1=\sum_{i=1,2}\int \mathrm{d}^4p(b_i^{\dagger}(p)b_i(p)+a_{N_i}^{\dagger}(p)a_{N_i}(p)),$$

$$Q_2=\int \mathrm{d}^4p\ \ (a_{N_1}^{\dagger}(p)a_{N_1}(p)-a_{\theta_1}^{\dagger}(p)a_{\theta_1}(p)), \tag{2.9}$$

$$Q_3=\int \mathrm{d}^4p(a_{N_2}^{\dagger}(p)a_{N_2}(p)-a_{\theta_2}^{\dagger}(p)a_{\theta_2}(p)).$$

This fact enables us to decompose the Fock space to sectors. We study the sector with $Q_1=1, Q_2=0, Q_3=0$. This is identified as a sector containing either one V_i particle *or* one N_j together with one θ_j particle. It follows from the commutativity of the fields that the states $|V_1\rangle, |V_2\rangle$, as well as $|N_1\theta_1\rangle, |N_2,\theta_2\rangle$, which exist in this sector, are orthogonal. In this sector the generator of evolution K can be rewritten in the form

$$K=\int \mathrm{d}^4pK^p=\int \mathrm{d}^4p(K_0^p+V^p),$$

where

$$K_0^p=\sum_{i=1,2}\left\{\frac{p^2}{2M_{V_i}}b_i^\dagger(p)b_i(p)+\int \mathrm{d}^4k\left(\frac{(p-k)^2}{2M_{N_i}}+\frac{k^2}{2M_{\theta_i}}\right)a_{N_i}^\dagger(p-k)a_{\theta_i}^\dagger(k)a_{\theta_i}(k)a_{N_i}(p-k)\right\}$$

and

$$V^p=\sum_{i,j=1,2}^{n}\int \mathrm{d}^4k(f_{ij}(k)b_i^\dagger(p)a_{N_j}(p-k)a_{\theta_j}(k)+f_{ij}^*(k)b_i(p)a_{N_j}^\dagger(p-k)a_{\theta_j}^\dagger(k)).$$

In this form it is clear that both K and K_0 have a direct integral structure. This implies a similar structure for the wave operator $\Omega_\pm$ and the possibility of defining restricted wave operators $\Omega_\pm^p$ for each value of p. We see from the expression for K_0^p that $|V_i(p)\rangle=b_i^\dagger(p)|0\rangle$ can be regarded as a set of discrete eigenstates of K_0^p (for each p) which span a subspace which is, therefore, annihilated by the restricted wave operators $\Omega_\pm^p$. This implies immediately that $\Omega_\pm|V(p)\rangle=0$ for every p (an explicit demonstration of this fact is given in Appendix A).

In order to construct the Lax–Phillips incoming and outgoing spectral representations for the model presented here it is necessary, according to the discussion following Eq. (1.25), to obtain appropriate expressions for the wave operators $\Omega_\pm^\dagger$ and the spectral representation for the generator K_0 of free evolution, i.e, the solution of Eq. (1.25).

We begin our discussion with a derivation of the appropriate expressions, for the model considered here, of the wave operators $\Omega_\pm$. We first calculate the following matrix elements of Ω_+:

$$\langle V_m(q)|\Omega_+|N_n(p),\theta_n(k)\rangle,\quad \langle N_m(p'),\theta_m(k')|\Omega_+|N_n(p),\theta_n(k)\rangle.$$

Equation (1.16) can be rewritten, following the standard procedure,[23] in the integral form

$$\Omega_+=1+i\lim_{\epsilon\to 0}\int_0^{+\infty}U^\dagger(\tau)VU_0(\tau)e^{-\epsilon\tau}\mathrm{d}\tau, \tag{2.10}$$

where $U(\tau)=e^{-iK\tau}$, $U_0(\tau)=e^{-iK_0\tau}$. Using (2.7), we have

$$\begin{aligned}\Omega_+&|N_n(p_1),\theta_n(p_2)\rangle\\ &=|N_n(p_1),\theta_n(p_2)\rangle+i\lim_{\epsilon\to 0}\int_0^{+\infty}\mathrm{d}\tau\, e^{-\epsilon\tau}U^\dagger(\tau)VU_0(\tau)a_{N_n}^\dagger(p)a_{\theta_n}^\dagger(k)|0\rangle\\ &=|N_n(p_1),\theta_n(p_2)\rangle+i\lim_{\epsilon\to 0}\int_0^{+\infty}\mathrm{d}\tau\, e^{-i(\omega_{N_n}(p_1)+\omega_{\theta_n}(p_2)-i\epsilon)\tau}U^\dagger(\tau)Va_{N_n}^\dagger(p)a_{\theta_n}^\dagger(k)|0\rangle,\end{aligned} \tag{2.11}$$

where $\omega_{N_n}(p)=p^2/2M_{N_n}$, $\omega_{\theta_n}(p)=p^2/2M_{\theta_n}$. Using (2.8) we find

$$Va_{N_n}^\dagger(p_1)a_{\theta_n}^\dagger(p_2)|0\rangle=\sum_{k=1,2}f_{kn}(p_2)b_k^\dagger(p_1+p_2)|0\rangle. \tag{2.12}$$

Inserting (2.12) into (2.11) and changing the integration variable from τ to $-\tau$ it follows that

$$\begin{aligned}\Omega_+&|N_n(p_1),\theta_n(p_2)\rangle\\ &=|N_n(p_1),\theta_n(p_2)\rangle-i\lim_{\epsilon\to 0}\sum_{k=1,2}\int_0^{-\infty}\mathrm{d}\tau\, e^{i(\omega_{N_n}(p_1)+\omega_{\theta_n}(p_2)-i\epsilon)\tau}U(\tau)f_{kn}(p_2)b_k^\dagger(p_1+p_2)|0\rangle.\end{aligned} \tag{2.13}$$

In order to continue with the evaluation of the integral in (2.13) we find the time evolution of some arbitray state χ under the action of $U(\tau)$,

$$\psi(\tau)=U(\tau)\chi=e^{-iK\tau}\chi. \tag{2.14}$$

In the sector of the Fock space that we are considering, the state $\psi(\tau)$ at any time τ can be expanded as

$$\psi(\tau)=\sum_{i=1,2}\int \mathrm{d}^4q A_i(q,\tau)b_i^\dagger(q)|0\rangle+\sum_{i=1,2}\int \mathrm{d}^4p\int \mathrm{d}^4k B_i(p,k,\tau)a_{N_i}^\dagger(p)a_{\theta_i}^\dagger(k)|0\rangle. \tag{2.15}$$

In particular, we see that the initial conditions for the evolution in (2.13), where the state χ is taken to be $\psi_0=\Sigma_k f_{kn}(p_2)b_k^\dagger(p_1+p_2)|0\rangle$, are

$$A_i(q,0)=f_{in}(p_2)\,\delta^4(q-p_1-p_2),\quad B_i(p,k,0)=0. \tag{2.16}$$

The equations of evolution for the coefficients $A(q,\tau)$ and $B(p,k,\tau)$ are then obtained from (2.14) and (2.15), i.e.,

$$\begin{aligned} i\frac{\partial B_i(p-k,k,\tau)}{\partial\tau}&=B_i(p-k,k,\tau)\left(\frac{(p-k)^2}{2M_{N_i}}+\frac{k^2}{2M_{\theta_i}}\right)+\sum_{j=1,2}f_{ji}^*(k)A_j(p,\tau),\\ i\frac{\partial A_i(p,\tau)}{\partial\tau}&=\frac{p^2}{2M_{V_i}}A_i(p,\tau)+\sum_{j=1,2}\int \mathrm{d}^4k f_{ij}(k)B_j(p-k,k,\tau). \end{aligned} \tag{2.17}$$

These equations can be solved algebraically[10,19] by performing Laplace transforms and defining

$$\begin{aligned} \tilde{B}_i(p,k,z)&=\int_{-\infty}^0 \mathrm{d}\tau\, e^{iz\tau}B_i(p,k,\tau),\quad \mathrm{Im}\,z<0,\\ \tilde{A}_i(p,z)&=\int_{-\infty}^0 \mathrm{d}\tau\, e^{iz\tau}A_i(p,\tau),\quad \mathrm{Im}\,z<0. \end{aligned} \tag{2.18}$$

Equation (2.17) is transformed into

$$\begin{aligned} \tilde{B}_i(p-k,k,z)\left(z-\frac{(p-k)^2}{2M_{N_i}}-\frac{k^2}{2M_{\theta_i}}\right)&=iB_i(p-k,k,0)+\sum_{j=1,2}f_{ji}^*(k)\tilde{A}_j(p,z),\\ \tilde{A}_i(p,z)\left(z-\frac{p^2}{2M_{V_i}}\right)&=iA_i(p,0)+\sum_{j=1,2}\int \mathrm{d}^4k f_{ij}(k)\tilde{B}_j(p-k,k,z). \end{aligned} \tag{2.19}$$

Using the initial conditions (2.16) we obtain the following expressions for the Laplace transformed coefficients:

$$\begin{aligned} \tilde{A}_k(p,z)&=i\sum_{i=1}^n W_{ki}^{-1}(z,p)A_i(p,0),\\ \tilde{B}_j(p-k,k,z)&=i\left(\frac{z-(p-k)^2}{2M_{N_j}}-\frac{k^2}{2M_{\theta_j}}\right)^{-1}\left[\sum_{k,i=1,2}^n f_{kj}^*(k)W_{ki}^{-1}(z,p)A_i(p,0)\right], \end{aligned} \tag{2.20}$$

where

$$W_{ik}(z,p)=\delta_{ik}\left(z-\frac{p^2}{2M_{V_i}}\right)-\sum_{j=1,2}^{n}\int \mathrm{d}^4k\,\frac{f_{ij}(k)f_{kj}^*(k)}{z-\frac{(p-k)^2}{2M_{N_j}}-\frac{k^2}{2M_{\theta_j}}}. \tag{2.21}$$

The Laplace transform of $\psi(\tau)$ is then

$$\begin{aligned}\psi(z)=&i\sum_{i,k=1,2}\int \mathrm{d}^4q\,W_{ik}^{-1}(z,q)A_k(q,0)b_i^\dagger(q)|0\rangle\\&+i\sum_{i,j,k=1,2}\int \mathrm{d}^4p\int \mathrm{d}^4k\,\frac{f_{ki}^*(k)W_{kj}^{-1}(z,p+k)A_j(p+k,0)}{\left(z-\frac{p^2}{2M_{N_i}}-\frac{k^2}{2M_{\theta_i}}\right)}a_{N_i}^\dagger(p)a_{\theta_i}^\dagger(k)|0\rangle.\end{aligned} \tag{2.22}$$

From (2.13), (2.22) and the initial conditions—Eq. (2.16)—we get

$$\begin{aligned}&\Omega_+|N_n(p_1),\theta_n(p_2)\rangle\\&\quad=|N_n(p_1),\theta_n(p_2)\rangle+i\sum_{i,k=1,2}W_{ik}^{-1}(\omega_n-i\epsilon,p_1+p_2)f_{kn}(p_2)b_i^\dagger(p_1+p_2)|0\rangle\\&\qquad+i\sum_{i,j,k=1,2}\int \mathrm{d}^4k\,\frac{f_{ki}^*(k)W_{kj}^{-1}(\omega_n-i\epsilon,p_1+p_2)f_{jn}(p_2)}{\omega_n-i\epsilon-\frac{(p_1+p_2-k)^2}{2M_{N_i}}-\frac{k^2}{2M_{\theta_i}}}a_{N_i}^\dagger(p_1+p_2-k)a_{\theta_i}^\dagger(k)|0\rangle,\end{aligned} \tag{2.23}$$

where we denote $\omega_n\equiv\omega_{N_n}(p_1)+\omega_{\theta_n}(p_2)$. We can now evaluate the desired matrix elements of the wave operator Ω_+. From (2.23) one fimds

$$\langle V_m(p)|\Omega_+|N_n(p_1),\theta_n(p_2)\rangle=\sum_{k=1,2}W_{mk}^{-1}(\omega_n-i\epsilon,p_1+p_2)f_{kn}(p_2)\,\delta^4(p-p_1-p_2) \tag{2.24}$$

and

$$\begin{aligned}&\langle N_m(\tilde{p}_1),\theta_m(\tilde{p}_2)|\Omega_+|N_n(p_1),\theta_n(p_2)\rangle\\&\quad=\delta_{mn}\delta^4(\tilde{p}_1-p_1)\,\delta^4(\tilde{p}_2-p_2)\\&\qquad+\sum_{k,j=1,2}\frac{f_{km}^*(\tilde{p}_2)W_{kj}^{-1}(\omega_n-i\epsilon,p_1+p_2)f_{jn}(p_2)}{\omega_n-i\epsilon-\frac{\tilde{p}_1^2}{2M_{N_m}}-\frac{\tilde{p}_2^2}{2M_{\theta_m}}}\,\delta^4(p_1+p_2-\tilde{p}_1-\tilde{p}_2).\end{aligned} \tag{2.25}$$

In a similar fashion one can find the corresponding matrix elements of the wave operator Ω_-:

$$\langle V_m(p)|\Omega_-|N_n(p_1),\theta_n(p_2)\rangle=\sum_{k=1,2}W_{mk}^{-1}(\omega_n+i\epsilon,p_1+p_2)f_{kn}(p_2)\,\delta^4(p-p_1-p_2) \tag{2.26}$$

and

$$\langle N_m(\tilde{p}_1),\theta_m(\tilde{p}_2)|\Omega_-|N_n(p_1),\theta_n(p_2)\rangle$$
$$=\delta_{mn}\delta^4(\tilde{p}_1-p_1)\,\delta^4(\tilde{p}_2-p_2)$$
$$+\sum_{k,j=1,2}\frac{f^*_{km}(\tilde{p}_2)W^{-1}_{kj}(\omega_n+i\epsilon,p_1+p_2)f_{jn}(p_2)}{\omega_n+i\epsilon-\dfrac{\tilde{p}_1^2}{2M_{N_m}}-\dfrac{\tilde{p}_2^2}{2M_{\theta_m}}}\,\delta^4(p_1+p_2-\tilde{p}_1-\tilde{p}_2). \quad (2.27)$$

According to Eqs. (1.22) and (1.25) the complete transformation to the *incoming* or *outgoing* representations requires us to solve for the (improper) eigenvectors with spectrum $\{\sigma\}$ on $(-\infty, +\infty)$ of K_0. The complete set of these states is decomposed into two subsets corresponding to the quantum numbers for states containing N and θ particles and states containing a V particle. These quantum numbers are denoted σ, α (for the $N+\theta$ states)and σ, β (V states), respectively. For the projections into these two subspaces, we have

$$|\sigma,\alpha\rangle_0=\sum_{n=1,2}\int \mathrm{d}^4p\int \mathrm{d}^4k|N_l(p),\theta_l(k)\rangle\langle N_l(p),\theta_l(k)|\sigma,\alpha\rangle_0,$$
$$|\sigma,\beta\rangle_0=\sum_{m=1}\int \mathrm{d}^4p|V_m(p)\rangle\langle V_m(p)|\sigma,\beta\rangle_0. \quad (2.28)$$

It is convenient to define

$$O^{\sigma,\alpha}_{n,p,k}\equiv\langle N_n(p),\Theta_n(k)|\sigma,\alpha\rangle_0,$$
$$O^{\sigma,\beta}_{m,p}\equiv\langle V_m(p)|\sigma,\beta\rangle_0. \quad (2.29)$$

With the help of these definitions we can rewrite (2.28) as

$$|\sigma,\alpha\rangle_0=\sum_{n=1,2}\int \mathrm{d}^4p\int \mathrm{d}^4kO^{\sigma,\alpha}_{n,p,k}|N_l(p),\theta_l(k)\rangle,$$
$$|\sigma,\beta\rangle_0=\sum_{m=1,2}\int \mathrm{d}^4pO^{\sigma,\beta}_{m,p}|V_m(p)\rangle. \quad (2.30)$$

It follows from Eqs. (1.25) and (2.30) that

$$K_0|\sigma,\alpha\rangle_0=\sum_{n=1,2}\int \mathrm{d}^4p\int \mathrm{d}^4k(\omega_{N_n}(p)+\omega_{\theta_n}(k))O^{\sigma,\alpha}_{n,p,k}|N_n(p),\Theta_n(k)\rangle=\sigma|\sigma,\alpha\rangle_0,$$
$$K_0|\sigma,\beta\rangle_0=\sum_{m=1,2}\int \mathrm{d}^4p\,\omega_{V_m}(p)O^{\sigma,\beta}_{m,p}|V_m(p)\rangle=\sigma|\sigma,\beta\rangle_0. \quad (2.31)$$

From the orthogonality of the final state channels, it follows that we must have

$$O^{\sigma,\alpha}_{n,p,k}=\delta(\sigma-\omega_{N_n}(p)-\omega_{\theta_n}(k))\tilde{O}^{\sigma,\alpha}_{n,p,k},$$
$$O^{\sigma,\beta}_{m,p}=\delta(\sigma-\omega_{V_m}(p))\tilde{O}^{\sigma,\beta}_{m,p} \quad (2.32)$$

to satisfy the kinematic conditions imposed by Eq. (2.31). A more detailed analysis of the structure of the matrix elements (2.32) requires further knowledge regarding the nature of the variables α, β. We will postpone the discussion of this point to later and remark here only that orthogonality and completeness requires that

$$\sum_{\alpha} \int \mathrm{d}\sigma (O^{\sigma,\alpha}_{n,p,k})^* O^{\sigma,\alpha}_{n',p',k'} = \delta^4(p-p')\,\delta^4(k-k')\,\delta_{nn'},$$

$$\sum_{n=1,2} \int \mathrm{d}^4p \int \mathrm{d}^4k (O^{\sigma,\alpha}_{n,p,k})^* O^{\sigma',\alpha'}_{n,p,k} = \delta(\sigma-\sigma')\,\delta_{\alpha,\alpha'}, \tag{2.33}$$

$$\sum_{\beta} \int \mathrm{d}\sigma (O^{\sigma,\beta}_{m,p})^* O^{\sigma,\beta}_{m',p'} = \delta^4(p-p')\,\delta_{mm'},$$

$$\sum_{m=1,2} \int \mathrm{d}^4p (O^{\sigma,\beta}_{m,p})^* O^{\sigma',\beta'}_{m,p} = \delta(\sigma-\sigma')\,\delta_{\beta,\beta'}. \tag{2.34}$$

To complete the transformation to the *outgoing* spectral representation we have to calculate, according to Eq. (1.22), the following quantities:

$$\langle V_m(p)|\Omega_+|\sigma,\beta\rangle_0, \quad \langle N_n(p),\theta_n(k)|\Omega_+|\sigma,\beta\rangle_0$$

and

$$\langle V_m(p)|\Omega_+|\sigma,\alpha\rangle_0, \quad \langle N_n(p),\Theta_n(k)|\Omega_+|\sigma,\alpha\rangle_0.$$

From the second equation of (2.31), the discussion following Eq. (2.9) and the results of Appendix A, it is clear that the first two transformation matrix elements are identically zero (since $\Omega_+|V(p)P=0$). We obtain expressions for the second pair with the help of (2.24), (2.25), and (2.32). For the first matrix element in the second pair above we have

$$\begin{aligned}
&\langle V_m(p)|\Omega_+|\sigma,\alpha\rangle_0 \\
&\quad = \sum_{n=1,2} \int \mathrm{d}^4p_1 \int \mathrm{d}^4p_2 \langle V_m(p)|\Omega_+|N_n(p_1),\theta_n(p_2)\rangle \langle N_n(p_1),\theta_n(p_2)|\sigma,\alpha\rangle_0 \\
&\quad = \sum_{n=1,2} \int \mathrm{d}^4p_1 \int \mathrm{d}^4p_2 \sum_{k=1,2} W^{-1}_{mk}(\omega_n - i\epsilon, p_1+p_2) f_{kn}(p_2)\,\delta^4(p-p_1-p_2) O^{\sigma,\alpha}_{n,p_1,p_2} \\
&\quad = \sum_{k=1,2} W^{-1}_{mk}(\sigma - i\epsilon, p) \sum_{n=1,2} \int \mathrm{d}^4p_2 f_{kn}(p_2) O^{\sigma,\alpha}_{n,p-p_2,p_2} \\
&\quad = \sum_{k=1,2} W^{-1}_{mk}(\sigma - i\epsilon, p) F^{\alpha}_{k}(\sigma,p),
\end{aligned} \tag{2.35}$$

where we have used (2.30) and the defininition

$$F^{\alpha}_{k}(\sigma,p) \equiv \sum_{n=1,2} \int \mathrm{d}^4p' f_{kn}(p') O^{\sigma,\alpha}_{n,p-p',p'}. \tag{2.36}$$

For the second matrix element we get in a similar way

$$\langle N_m(p_1),\theta_m(p_2)|\Omega_+|\sigma,\alpha\rangle_0$$
$$=\sum_{n=1,2}\int d^4p_1'\int d^4p_2'\langle N_m(p_1),\theta_m(p_2)|\Omega_+|N_n(p_1'),\theta_n(p_2')\rangle\langle N_n(p_1'),\theta_n(p_2')|\sigma,\alpha\rangle_0$$
$$=O^{\sigma,\alpha}_{m,p_1,\tilde{p}_2}+\sum_{k,j=1,2}\frac{f^*_{km}(\tilde{p}_2)W^{-1}_{kj}(\sigma-i\epsilon,p_1+p_2)F^\alpha_j(\sigma,p_1+p_2)}{\sigma-i\epsilon-\frac{{p_1}^2}{2M_{N_m}}-\frac{{p_2}^2}{2M_{\theta_m}}}. \tag{2.37}$$

Following the same steps we obtain for the matrix elements of the wave operator Ω_-,

$$\langle V_m(p)|\Omega_-|\sigma,\alpha\rangle_0=\sum_{k=1,2}W^{-1}_{mk}(\sigma+i\epsilon,p)F^\alpha_k(\sigma,p) \tag{2.38}$$

and

$$\langle N_m(p_1),\theta_m(p_2)|\Omega_-|\sigma,\alpha\rangle_0=O^{\sigma,\alpha}_{m,p_1,p_2}+\left(\sigma+i\epsilon-\frac{{p_1}^2}{2M_{N_m}}-\frac{{p_2}^2}{2M_{\theta_m}}\right)^{-1}$$
$$\times\sum_{k,j=1,2}f^*_{km}(p_2)W^{-1}_{kj}(\sigma+i\epsilon,p_1+p_2)F^\alpha_j(\sigma,p_1+p_2). \tag{2.39}$$

This completes the calculation of the Lax–Phillips wave operators providing the transformation to the *incoming* and *outgoing* (spectral) representations. Given these transformations it is possible in principle to construct the subspaces $D_\pm$ according to the method described in Sec. I. We can now calculate the Lax–Phillips S matrix mapping the incoming representation into the outgoing representation. If this S matrix satisfies the conditions (a), (b), (c) given in Sec. I then there exist incoming and outgoing subspaces $D_\pm$ orthogonal to each other and the Lax–Phillips structure is complete.

From Eq. (1.26) we see that the Lax–Phillips S matrix is given by ${}_0\langle\sigma',\alpha'|S|\sigma,\alpha\rangle_0$. We can calculate explicitly the Lax–Phillips S matrix for the model presented here with the help of the following useful expression (valid in the sector of the Fock space in which we are working):

$${}_0\langle\sigma',\alpha'|S|\sigma,\alpha\rangle_0=\sum_{m=1,2}\int d^4p\ {}_0\langle\sigma',\alpha'|\Omega_+^\dagger|V_m(p)\rangle\langle V_m(p)|\Omega_-|\sigma,\alpha\rangle_0$$
$$+\sum_{m=1,2}\int d^4\tilde{p}_1\int d^4\tilde{p}_2\ {}_0\langle\sigma',\alpha'|\Omega_+^\dagger|N_m(\tilde{p}_1),\theta_m(\tilde{p}_2)\rangle$$
$$\times\langle N_m(\tilde{p}_1),\theta_m(\tilde{p}_2)|\Omega_-|\sigma,\alpha\rangle_0. \tag{2.40}$$

Using the expressions obtained for the wave operator equations (2.35), (2.37), (2.38), (2.39) and the definition (2.36) we get

$${}_0\langle\sigma',\alpha'|S|\sigma,\alpha\rangle_0=\sum_{m=1,2}\int d^4p\sum_{k,k'=1,2}W^{-1*}_{mk}(\sigma'+i\epsilon,p)F^{\alpha'*}_k(\sigma',p)W^{-1}_{mk'}(\sigma+i\epsilon,p)F^\alpha_{k'}(\sigma,p)$$
$$+\delta(\sigma'-\sigma)\delta_{\alpha\alpha'}+\frac{1}{\sigma-\sigma'+i\epsilon}$$
$$\times\int d^4p_1\sum_{k',j'}F^{\alpha'*}_{k'}(\sigma',p_1)W^{-1}_{k'j'}(\sigma+i\epsilon,p_1)F^\alpha_{j'}(\sigma,p_1)+\frac{1}{\sigma'-\sigma+i\epsilon}$$

$$\times \int \mathrm{d}^4 p_1 \sum_{k,j} F_k^{\alpha}(\sigma,p_1) W_{kj}^{-1\,*}(\sigma'+i\epsilon,p_1) F_j^{\alpha'\,*}(\sigma',p_1)$$

$$+ \sum_{m=1,2} \int \mathrm{d}^4 p_1 \int \mathrm{d}^4 p_2$$

$$\times \Bigg[\sum_{k,j,k',j'=1,2} \frac{f_{km}(p_2) W_{kj}^{-1\,*}(\sigma'+i\epsilon,p_1+p_2) F_j^{\alpha'\,*}(\sigma',p_1+p_2)}{\sigma'+i\epsilon-\frac{p_1^{\,2}}{2M_{N_m}}-\frac{p_2^{\,2}}{2M_{\theta_m}}}$$

$$\times \frac{f_{k'm}^{*}(p_2) W_{k'j'}^{-1}(\sigma+i\epsilon,p_1+p_2) F_{j'}^{\alpha}(\sigma,p_1+p_2)}{\sigma+i\epsilon-\frac{p_1^{\,2}}{2M_{N_m}}-\frac{p_2^{\,2}}{2M_{\theta_m}}} \Bigg]. \tag{2.41}$$

The last term in Eq. (2.41) can be put into a simpler form by the following manipulation:

$$\sum_{m=1,2} \int \mathrm{d}^4 p_1 \int \mathrm{d}^4 p_2 \Bigg[\sum_{k,j,k',j'=1,2} \frac{f_{km}(p_2) W_{kj}^{-1\,*}(\sigma'+i\epsilon,p_1+p_2) F_j^{\alpha'\,*}(\sigma',p_1+p_2)}{\sigma'+i\epsilon-\frac{p_1^{\,2}}{2M_{N_m}}-\frac{p_2^{\,2}}{2M_{\theta_m}}}$$

$$\times \frac{f_{k'm}^{*}(p_2) W_{k'j'}^{-1}(\sigma+i\epsilon,p_1+p_2) F_{j'}^{\alpha}(\sigma,p_1+p_2)}{\sigma+i\epsilon-\frac{p_1^{\,2}}{2M_{N_m}}-\frac{p_2^{\,2}}{2M_{\theta_m}}} \Bigg]$$

$$= \int \mathrm{d}^4 p_1 \sum_{k,j,k',j'=1,2} \frac{1}{\sigma-\sigma'} [\delta_{kk'}(\sigma'-\sigma) - W_{kk'}(\sigma'+i\epsilon,p_1) + W_{kk'}(\sigma+i\epsilon,p_1)]$$

$$\times W_{kj}^{-1\,*}(\sigma'+i\epsilon,p_1) F_j^{\alpha'\,*}(\sigma',p_1) W_{k'j'}^{-1}(\sigma+i\epsilon,p_1) F_{j'}^{\alpha}(\sigma,p_1)$$

$$= -\int \mathrm{d}^4 p_1 \sum_{k,j,j'=1,2} W_{kj}^{-1\,*}(\sigma'+i\epsilon,p_1) F_j^{\alpha'\,*}(\sigma',p_1) W_{kj'}^{-1}(\sigma+i\epsilon,p_1) F_{j'}^{\alpha}(\sigma,p_1)$$

$$+ P\frac{1}{\sigma-\sigma'} \int \mathrm{d}^4 p_1 \sum_{j,j'=1,2} F_{j'}^{\alpha}(\sigma,p_1) W_{j'j}^{-1\,*}(\sigma'+i\epsilon,p_1) F_j^{\alpha'\,*}(\sigma',p_1)$$

$$- P\frac{1}{\sigma-\sigma'} \int \mathrm{d}^4 p_1 \sum_{j,j'=1,2} F_j^{\alpha'\,*}(\sigma',p_1) W_{jj'}^{-1}(\sigma+i\epsilon,p_1) F_{j'}^{\alpha}(\sigma,p_1), \tag{2.42}$$

where P stands for the principle part and we have performed a partial fraction decomposition at the second step in (2.41) and used the definition Eq. (2.21) of $W_{ik}(z,p)$. Combining (2.42) and (2.41) we find for the Lax–Phillips S matrix

$$ {}_0\langle \sigma',\alpha'|S|\sigma,\alpha\rangle_0 = \delta(\sigma-\sigma') \Bigg[\delta_{\alpha\alpha'} - 2\pi i \int \mathrm{d}^4 p \sum_{k,j} F_k^{\alpha}(\sigma,p) W_{kj}^{-1\,*}(\sigma'+i\epsilon,p) F_j^{\alpha'\,*}(\sigma',p_1) \Bigg]$$

$$= \delta(\sigma-\sigma') \Bigg[\delta_{\alpha\alpha'} - 2\pi i \int \mathrm{d}^4 p \sum_{k,j} F_j^{\alpha'\,*}(\sigma,p) W_{jk}^{-1}(\sigma+i\epsilon,p) F_k^{\alpha}(\sigma,p) \Bigg]. \tag{2.43}$$

[In (2.42) we use a partial fraction decomposition of the denominators of the form $(\sigma+i\epsilon_1-A)^{-1}\times(\sigma'+i\epsilon_2-A)^{-1}=(\sigma-\sigma'+i(\epsilon_2-\epsilon_1))^{-1}\times((\sigma'+i\epsilon_1-A)^{-1}-(\sigma+i\epsilon_2-A)^{-1})$

$=(P(\sigma-\sigma')^{-1}\pm i\pi\delta(\sigma-\sigma'))\times((\sigma'+i\epsilon_1-A)^{-1}-(\sigma+i\epsilon_2-A)^{-1})=P(\sigma-\sigma')^{-1}\times((\sigma'+i\epsilon_1-A)^{-1}$
$-(\sigma+i\epsilon_2-A)^{-1})$.] We observe that in Eq. (2.43) the quantity $F_j^{\alpha *}(\sigma,p)$ can be considered, for each fixed value of $\tilde{p}_1'$, as a vector-valued function on the independent variable σ, taking its values in an auxiliary Hilbert space defined by the variables α. We write it as [see Eqs. (2.29) and (2.36)]

$$F_j^{\alpha *}(\sigma,p)\equiv(|n_j\rangle_{\sigma,p})^{\alpha}, \tag{2.44}$$

where (for a fixed value of p) $(|n_j\rangle_{\sigma,p})^{\alpha}$ is the α component of the vector valued function $|n_j\rangle_{\sigma,p}$. With this notation we have (we supress the auxiliary Hilbert space variables α)

$$S(\sigma)=1-2\pi i\int \mathrm{d}^4p\sum_{k,j}\ |n_j\rangle_{\sigma,p}W_{jk}^{-1}(\sigma+i\epsilon,p)_{\sigma,p}\langle n_k|. \tag{2.45}$$

Further simplification of the expression given here for the S matrix can be achieved by identifying the auxiliary Hilbert space variables α. This results in an observation of the direct integral structure of the S matrix on the center of momentum P and the definition of the reduced S matrix $S_P(\sigma)$ for each value of P. Another important result is the fact that the requirement that the Lax–Phillips S matrix is an inner function implies that an analysis of its action involves a consideration of only a two-dimensional subspace of the auxiliary Hilbert space. These simplifications in the structure of the Lax–Phillips S matrix is the subject of Sec III.

III. THE AUXILIARY HILBERT SPACE AND CHARACTERIZATION OF THE LAX–PHILLIPS *S* MATRIX

The auxiliary Hilbert space of the Lax–Phillips representation of the relativistic Lee–Friedrichs model acquires a complete characterization when an exact specification of the variables α in the transformation matrix $O_{n,p.k}^{\sigma,\alpha}$ of Eq. (2.29) is given. To achieve this goal we proceed in two steps. The first one is to define a new set of independent variables $\{n,p,k\}\rightarrow\{n,P,p_{\mathrm{rel}}\}$ by the following linear combination of p and k:

$$a.\quad P=p+k,\quad b.\quad p_{\mathrm{rel}}=\frac{M_{\theta_n}p-M_{N_n}k}{M_{\theta_n}+M_{N_n}}. \tag{3.1}$$

These momentum space variables correspond to the following configuration space variables:

$$a.\quad X_{\mathrm{c.m.}}=\frac{M_{N_n}x_1+M_{\theta_n}x_2}{M_{N_n}+M_{\theta_n}},\quad b.\quad x_{\mathrm{rel}}=x_1-x_2.$$

From Eq. (2.32) we know that

$$O_{n,p,k}^{\sigma,\alpha}=\delta(\sigma-\omega_{N_n}(p)-\omega_{\Theta_n}(k))\tilde{O}_{n,p,k}^{\sigma,\alpha}.$$

This implies that

$$\sigma=\frac{p^2}{2M_{N_n}}+\frac{k^2}{2M_{\theta_n}}=\frac{P^2}{2M_n}+\frac{p_{\mathrm{rel}}^2}{2\mu_n}, \tag{3.2}$$

where $M_n=M_{N_n}+M_{\theta_n}$ and $\mu=M_{N_n}M_{\theta_n}/(M_{N_n}+M_{\theta_n})$. We take σ and P to be independent variables. In this case p_{rel}^2 is a dependent variable with a value given by

$$p_{\mathrm{rel}}^2=2\mu_n\left(\sigma-\frac{P^2}{2M_n}\right).$$

To complete the set of independent quantum numbers we have to find a complete set of commuting operators that commute with $p_{\rm rel}^2$ and P. Since $p_{\rm rel}^2$ is a Casimir of the Poincaré group on the relative coordinates, we may take for the set of commuting operators on the *relative motion*, the second Casimir of the Lorentz group and L^2, L_3. We denote by γ the full set of quantum numbers corresponding to the latter three operators. We then have $\{\sigma,\alpha\}\equiv\{\sigma,n,P,\gamma\}$. It follows from Eqs. (2.32) and (3.1*a*.) that

$$O^{\sigma,\alpha}_{n,p,k}\equiv O^{\sigma,P,\gamma,i}_{n,p,k}=\delta(\sigma-p^2/2M_{N_n}-k^2/2M_{\theta_n})\,\delta_{ni}\,\delta^4(P-p-k)\,\hat{O}^{n,p_{\rm rel}^2,\gamma}_{n,p_{\rm rel}}\Big|_{\substack{p_{\rm rel}^2=2\mu_n(\sigma-P^2/2M_n)\\ p_{\rm rel}=(M_{\theta_n}p-M_{N_n}k)/M_n}} \tag{3.3}$$

Inserting this into the definition of $F_k^{\alpha}(\sigma,p)(\equiv F_k^{P,\gamma,i}(\sigma,p))$, Eq. (2.36) we get

$$\begin{aligned}
&F_k^{P,\gamma,i}(\sigma,p)\\
&\equiv\delta^4(P-p)\sum_{n=1,2}\int {\rm d}^4p'\,f_{kn}(p')\,\delta_{ni}\,\delta\left(\sigma-\frac{(p-p')^2}{2M_{N_n}}-\frac{p'^2}{2M_{\theta_n}}\right)\hat{O}^{n,p_{\rm rel}^2,\gamma}_{n,p_{\rm rel}}\Big|_{\substack{p_{\rm rel}^2=2\mu_n(\sigma-P^2/2M_n)\\ p_{\rm rel}=M_{\theta_n}P/M_n-p'}}\\
&=\delta^4(P-p)\sum_{n=1,2}\int {\rm d}^4p_{\rm rel}f_{kn}(M_{\theta_n}P/M_n-p_{\rm rel})\,\delta_{ni}\,\delta\left(\sigma-\frac{P^2}{2M_n}-\frac{p_{\rm rel}^2}{2\mu_n}\right)\hat{O}^{n,p_{\rm rel}^2,\gamma}_{n,p_{\rm rel}}.
\end{aligned}\tag{3.4}$$

We define the following P-dependent vector valued function:

$$(|n_k\rangle_{\sigma,P})^{\gamma,i}\equiv\sum_{n=1,2}\int {\rm d}^4p_{\rm rel}f^*_{kn}(M_{\theta_n}P/M_n-p_{\rm rel})\,\delta_{ni}\,\delta\left(\sigma-\frac{P^2}{2M_n}-\frac{p_{\rm rel}^2}{2\mu_n}\right)(\hat{O}^{n,p_{\rm rel}^2,\gamma}_{n,p_{\rm rel}})^* \tag{3.5}$$

so that $F_k^{P,\gamma,i}(p,\sigma)^*=\delta^4(P-p)(|n_k\rangle^{\gamma,i}_{\sigma,P}$. When this form of $F_k^{\alpha}(p,\sigma)$ is used in Eq. (2.43) we get

$${}_0\langle\sigma',\alpha'|S|\sigma,\alpha\rangle_0={}_0\langle\sigma',P',\gamma',i'|S|\sigma,P,\gamma,i\rangle_0=\delta(\sigma'-\sigma)\,\delta(P'-P)S_P^{\gamma',i',\gamma,i}(\sigma), \tag{3.6}$$

where we define the reduced S matrix, for a specified value of the center of momentum four-vector P, to be

$$S_P^{\gamma',i',\gamma,i}(\sigma)=\left[1-2\pi i\sum_{k,j=1,2}|n_j\rangle_{\sigma,P}W^{-1}_{jk}(\sigma+i\epsilon,P)_{\sigma,P}\langle n_k|\right]^{\gamma',i',\gamma,i}. \tag{3.7}$$

The form of $S_P(\sigma)$ allows for a further simplification. For each value of σ the two vectors $|n_k\rangle_{\sigma,P}$, $k=1,2$ span a two-dimensional subspace of the auxiliary Hilbert space. These vectors are, in general, not orthogonal. We find the orthogonal projection onto the two-dimensional subspace using these nonorthogonal vectors by finding linear combinations, denoted ${}_{\sigma,P}\langle F_i|$ such that

$${}_{\sigma,P}\langle F_i|n_j\rangle_{\sigma,P}=\delta_{ij}\,. \tag{3.8}$$

Denoting the projection operator on the subspace spanned by $|n_k\rangle_{\sigma,P}$, $k=1,2$ by $P_2(\sigma,P)$ we have

$$P_2(\sigma,P)=\sum_{i=1,2}|n_i\rangle_{\sigma,P}\ {}_{\sigma,P}\langle F_i|. \tag{3.9}$$

With this projection we construct the unit operator $1_{\sigma,P}$ on the auxiliary Hilbert space and write

$$1_{\sigma,P}=(1_{\sigma,P}-P_2(\sigma,P))+P_2(\sigma,P).$$

Multiplying $S_P(\sigma)$ of Eq. (3.7) by this unit operator from the right we obtain (here, and in the sequel, we suppress reference to the auxiliary Hilbert space variables γ', i, γ, i)

$$S_P(\sigma)=1-P_2(\sigma,P)$$
$$+\sum_i \left[|n_i\rangle_{\sigma,P}\ {}_{\sigma,P}\langle F_i| - 2\pi i \sum_{k,j} |n_j\rangle_{\sigma,P} W^{-1}_{jk}(\sigma+i\epsilon,P)_{\sigma,P}\langle n_k|n_i\rangle_{\sigma,P}\ {}_{\sigma,P}\langle F_i| \right]$$
$$=1-P_2(\sigma,P)+\sum_{i,j} |n_j\rangle_{\sigma,P}\left[\delta_{ji} - 2\pi i \sum_k W^{-1}_{jk}(\sigma+i\epsilon,P)_{\sigma,P}\langle n_k|n_i\rangle_{\sigma,P}\right]_{\sigma,P}\langle F_i|. \tag{3.10}$$

We now write the Kronecker delta δ_{ij} in the form $\delta_{ji}=\Sigma_k W^{-1}_{jk}(\sigma+i\epsilon,P)W_{ki}(\sigma+i\epsilon,P)$ and get

$$S_P(\sigma)=1-P_2(\sigma,P)+\sum_{i,j,k} |n_j\rangle_{\sigma,P} W^{-1}_{jk}(\sigma+i\epsilon,P)[W_{ki}(\sigma+i\epsilon,P)-2\pi i_{\sigma,p}\langle n_k|n_i\rangle_{\sigma,P}]_{\sigma,P}\langle F_i|. \tag{3.11}$$

In order to proceed at this point it is necessary to evaluate explicitly the expression ${}_{\sigma,P}\langle n_k|n_i\rangle_{\sigma,P}$. Using the definition (3.5) we obtain

$${}_{\sigma,P}\langle n_k|n_i\rangle_{\sigma,P}=\sum_j \int \mathrm{d}^4 p_{\mathrm{rel}} \int \mathrm{d}^4 p'_{\mathrm{rel}} f^*_{kj}(M_{\theta_j}P/M_j-p_{\mathrm{rel}}) f_{ij}(M_{\theta_j}P/M_j-p'_{\mathrm{rel}})$$
$$\times \delta\left(\sigma-\frac{P^2}{2M_j}-\frac{p^2_{\mathrm{rel}}}{2\mu_j}\right)\delta\left(\frac{p^2_{\mathrm{rel}}}{2\mu_j}-\frac{p'^2_{\mathrm{rel}}}{2\mu_j}\right)\sum_\gamma (\hat{O}^{j,p^2_{\mathrm{rel}},\gamma}_{j,p_{\mathrm{rel}}})^* \hat{O}^{j,p^2_{\mathrm{rel}},\gamma}_{j,p'_{\mathrm{rel}}}$$
$$=\sum_j \int \mathrm{d}^4 p_{\mathrm{rel}} \delta\left(\sigma-\frac{P^2}{2M_j}-\frac{p^2_{\mathrm{rel}}}{2\mu_j}\right) f^*_{kj}(M_{\theta_j}P/M_j-p_{\mathrm{rel}}) f_{ij}(M_{\theta_j}P/M_j-p_{\mathrm{rel}})$$
$$=\sum_j \int \mathrm{d}^4 k \,\delta\left(\sigma-\frac{(P-k)^2}{2M_{N_j}}-\frac{k^2}{2M_{\theta_j}}\right) f^*_{kj}(k) f_{ij}(k). \tag{3.12}$$

We compare this result with the jump across the cut on the real axis of the complex σ plane of $W_{ki}(\sigma,P)$. With the help of the definition (2.21) we find

$$W_{ki}(\sigma+i\epsilon,P)-W_{ki}(\sigma-i\epsilon,P)=2\pi i\sum_j \int \mathrm{d}^4 k\,\delta\left(\sigma-\frac{(P-k)^2}{2M_{N_j}}-\frac{k^2}{2M_{\theta_j}}\right) f^*_{kj}(k) f_{ij}(k). \tag{3.13}$$

Using Eqs. (3.12) and (3.13) we can write Eq. (3.11) as

$$S_P(\sigma)=1-P_2(\sigma,P)+\sum_{i,j,k} |n_j\rangle_{\sigma,P} W^{-1}_{jk}(\sigma+i\epsilon,P) W_{ki}(\sigma-i\epsilon,P)_{\sigma,P}\langle F_i|. \tag{3.14}$$

The operator valued function $P_2(\sigma,P)$ defined in Eq. (3.9) is a projection operator for each value of σ,

$$P_2(\sigma,P)P_2(\sigma,P)=P_2(\sigma,P).$$

It is, therefore, a bounded positive operator on the real σ axis. In order to characterize $P_2(\sigma,P)$ we need several definitions and results from operator theory on positive operator valued functions. We give these in the appendix, where we prove that $P_2(\sigma,P)$ is an *outer function*[18] and that it is actually independent of σ, that is

$$P_2(\sigma,P)=P_{2,P}, \tag{3.15}$$

where $P_{2,P}$ is a projection operator on some fixed two-dimensional subspace of the auxiliary space. This proof rests on the properties of $S_P(\sigma)$ as an *inner function*.[18] We shall assume that the functions $f_{ij}(k)$ are such that the operator valued function defined by Eq. (3.14) has the appropriate analytic properties in the upper half plane.

In Eqs. (3.8) and (3.9) the vectors $|n_i\rangle_{\sigma,P}$ and ${}_{\sigma,P}\langle F_i|$ may depend on σ, but this dependence is such that the projection operator $P_2(\sigma,P)$ projects on a fixed two-dimensional subspace of the auxiliary space for each and every value of σ. Equation (3.14) can then be written in the form

$$S_P(\sigma)=1-P_{2,P}+\sum_{i,j,k}|n_j\rangle_{\sigma,P}W^{-1}_{jk}(\sigma+i\epsilon,P)W_{ki}(\sigma-i\epsilon,P)\,{}_{\sigma,P}\langle F_i| \tag{3.16}$$

and we see that the S matrix $S_P(\sigma)$ acts in a non trivial way only on a two-dimensional subspace of the auxiliary space.

We now complete the characterization of the Lax–Phillips S matrix $S_P(\sigma)$. Equation (3.15) implies that the projection valued function $P_2(\sigma,P)$ projects the Hilbert space $L^2(-\infty,+\infty;H)$ on the subspace $L^2(-\infty,+\infty;H_2)$ of vector valued functions taking their values in some fixed two-dimensional subspace H_2 of the auxiliary Hilbert space. We again use the notation $P_{2,P}$ to denote the projection $P_2(\sigma,P)$ as an operator valued function projecting on $L^2(-\infty,+\infty;H_2)$, that is

$$P_{2,P}:L^2(-\infty,+\infty;H)\to L^2(-\infty,+\infty;H_2). \tag{3.17}$$

We denote by $P_{I-2,P}$ the operator projecting on the subspace of functions with a range in $H\ominus H_2$. We have

$$P_{I-2,P}:L^2(-\infty,+\infty;H)\to L^2(-\infty,+\infty;H\ominus H_2). \tag{3.18}$$

It is obvious from Eqs. (3.17) and (3.18) that

$$L^2(-\infty,+\infty;H)=P_{2,P}L^2(-\infty,+\infty;H)\oplus P_{I-2,P}L^2(-\infty,+\infty;H). \tag{3.19}$$

In particular, if $U(\tau)$ is the operator of right translation by τ units then any left translation invariant subspace $I^-_H\subset H^2_H(\Pi)$ can be written as

$$I^-_H=P_{2,P}I^-_H\oplus P_{I-2,P}I^-_H. \tag{3.20}$$

The translation $U(\tau)$ commutes with the projections $P_{2,P}$, $P_{I-2,P}$ and, since I^-_H is a left translation invariant subspace, we have $U(\tau)I^-_H\subset I^-_H$. Denoting $I^-_{H_2}=P_{2,P}I^-_H$ we find

$$U(\tau)I^-_{H_2}=U(\tau)P_{2,P}I^-_H=P_{2,P}U(\tau)I^-_H\subset P_{2,P}I^-_H=I^-_{H_2}. \tag{3.21}$$

We see that if I^-_H is a left translation invariant subspace then $I^-_{H_2}=P_{2,P}I^-_H$ is a two-dimensional invariant subspace under left translations.

In the Lax–Phillips theory the Lax–Phillips S matrix is an inner function that generates a left translation invariant subspace from the Hardy class $H^2_H(\Pi)$ (this corresponds to the stability property of $\mathcal{D}_-$). In this case we can write

$$I^-_H=S^{\mathrm{LP}}H^2_H(\Pi), \tag{3.22}$$

where S^{LP} is the Lax–Phillips S matrix. From Eq. (3.16) we see that in the case of the two channel relativistic Lee-model we have [$S_P(\sigma)$ is the realization of S^{LP} in terms of an operator valued function]

$$[S^{\mathrm{LP}},P_{2,P}]=0. \tag{3.23}$$

From Eqs. (3.22) and (3.23) and the definition of $I^-_{H_2}$ we find that

$$I^-_{H_2}=P_{2,P}I^-_H=P_{2,P}S^{\mathrm{LP}}H^2_H(\Pi)=S^{\mathrm{LP}}P_{2,P}H^2_H(\Pi)=S^{\mathrm{LP}}H^2_{H_2}(\Pi),$$

where $H^2_{H_2}(\Pi)\equiv P_{2,P}H^2_H(\Pi)$. We can write this result in the form

$$I^-_{H_2}=P_{2,P}S^{\mathrm{LP}}P_{2,P}H^2_{H_2}(\Pi). \tag{3.24}$$

From this we see that $P_{2,P}S^{\mathrm{LP}}P_{2,P}$, when it acts on the Hardy space $H^2_{H_2}(\Pi)$, generates a two-dimensional left translation invariant subspace. From Eq. (3.16) we get [if A is an operator on a Hardy class $H^2_H(\Pi)$ or $H^2_{H_2}(\Pi)$ then $T(A)$ is its realization in terms of an operator valued function]

$$T(P_{2,P}S^{\mathrm{LP}}P_{2,P})=\delta(\sigma-\sigma')\sum_{i,j,k}|n_j\rangle_{\sigma,P}W^{-1}_{jk}(\sigma+i\epsilon,P)W_{ki}(\sigma-i\epsilon,P)\,{}_{\sigma,P}\langle F_i|. \tag{3.25}$$

According to Eq. (3.24) this immediately implies that the right-hand side of Eq. (3.25) is an *inner function* acting on the Hardy space $H^2_{H_2}(\Pi)$ consisting of vector valued functions taking their values in some fixed two-dimensional subspace of the auxiliary Hilbert space. This observation allows for a complete characterization of the Lax–Phillips S matrix, Eq. (3.16). Such an inner function can be represented as a product of a *rational* inner function containing the poles and zeros of $S_P(\sigma)$ and a factor which is an inner function with nonvanishing determinant.[24] If the latter factor is bounded exponentially, it corresponds to a trivial inner factor[1] and does not change the spectrum of the semigroup. In the following, we consider the case of a purely rational S matrix.

IV. THE RESONANT STATES FOR A RATIONAL *S* MATRIX

In this section we shall identify the resonant states of the relativistic two channel Lee model in the Lax–Phillips *outgoing* translation representation for the case of a rational S matrix of the form

$$S(\sigma)=1+\left(\frac{\mathrm{Res}\,S(z_1)}{\sigma-z_1}+\frac{\mathrm{Res}\,S(z_2)}{\sigma-z_2}\right),\qquad \mathrm{Im}\,z_1,\mathrm{Im}\,z_2<0. \tag{4.1}$$

We also have

$$S^\dagger(\sigma)=1+\left(\frac{\mathrm{Res}\,S^\dagger(\overline{z_1})}{\sigma-\overline{z_1}}+\frac{\mathrm{Res}\,S^\dagger(\overline{z_2})}{\sigma-\overline{z_2}}\right),\qquad \mathrm{Im}\,\overline{z_1},\mathrm{Im}\,\overline{z_2}>0. \tag{4.2}$$

A rational S matrix of this form implies the property, as assumed in the remarks following Eq. (3.15), that $S(\sigma)$ is an inner factor. There are simple conditions, which we shall discuss elsewhere, for which the converse is true, i.e., that an inner function is rational.

In order to identify the resonant states we obtain, in the *outgoing* translation representation, an expression for the generator of the Lax–Phillips semigroup. We then find the eigenfunctions of this generator. Lax and Phillips then assert that these are the resonant states associated with the poles of the Lax–Phillips S matrix.

The Lax–Phillips semigroup is defined as $Z(\tau)=P_+U(\tau)P_-,\tau>0$. The generator of the semigroup is given by

$$B=i\lim_{\tau\to 0^+}\frac{Z(\tau)-Z(0)}{\tau}. \tag{4.3}$$

In the outgoing translation representation we have

$$
\begin{aligned}
{}_{\text{out}}\langle s,\beta|B|s',\beta'\rangle_{\text{out}} = i \lim_{\tau\to 0^+}\frac{1}{\tau}\sum_{\gamma,\gamma'}\int \mathrm{d}\eta\int \mathrm{d}\eta' \\
\times[{}_{\text{out}}\langle s,\beta|P_+|\eta,\gamma\rangle_{\text{out out}}\langle \eta,\gamma|U(\tau)|\eta',\gamma'\rangle_{\text{out out}}\langle \eta',\gamma'|P_-|s',\beta'\rangle_{\text{out}} \\
-{}_{\text{out}}\langle s,\beta|P_+|\eta,\gamma\rangle_{\text{out out}}\langle \eta,\gamma|U(0)|\eta',\gamma'\rangle_{\text{out out}}\langle \eta',\gamma'|P_-|s',\beta'\rangle_{\text{out}}].
\end{aligned}
\tag{4.4}
$$

In this representation the subspace D_+ is given by $L^2(-\infty,+\infty;H)$, i.e., it is defined in a simple way by its support properties. Therefore, the operator P_+, the projection into the subspace $K\oplus D_-$ is given simply by

$$
{}_{\text{out}}\langle s,\beta|P_+|\eta,\gamma\rangle_{\text{out}} = \Theta(-s)\,\delta(s-\eta)\,\delta_{\gamma,\gamma'}.
$$

Furthermore, in the outgoing translation representation the evolution is just translation

$$
{}_{\text{out}}\langle \eta,\gamma|U(\tau)|\eta',\gamma'\rangle_{\text{out}} = \delta(\eta-\tau-\eta')\,\delta_{\gamma,\gamma'}.
$$

Then (4.4) becomes

$$
{}_{\text{out}}\langle s,\beta|B|s',\beta'\rangle_{\text{out}} = i\lim_{\tau\to 0^+}\frac{1}{\tau}[\Theta(-s)\,{}_{\text{out}}\langle s-\tau,\beta|P_-|s',\beta'\rangle_{\text{out}} - \Theta(-s)\,{}_{\text{out}}\langle s,\beta|P_-|s',\beta'\rangle_{\text{out}}].
\tag{4.5}
$$

We use the fact that the subspace D_- is given in the incoming translation representation in terms of its support properties. This allows us to write

$$
P_- = \sum_\gamma \int \mathrm{d}\eta\,|\eta,\gamma\rangle_{\text{in}}\Theta(\eta)\langle\eta,\gamma|_{\text{in}} = \sum_\gamma \int \mathrm{d}\eta\,\Omega_-|\eta,\gamma\rangle_f\Theta(\eta)\langle\eta,\gamma|_f\Omega_-^\dagger.
\tag{4.6}
$$

In the outgoing translation representation we have

$$
\begin{aligned}
{}_{\text{out}}\langle s,\beta|P_-|s',\beta'\rangle_{\text{out}} &= \sum_\gamma \int \mathrm{d}\eta\,\text{out}\langle s,\beta|\Omega_-|\eta,\gamma\rangle_f\Theta(\eta)\langle\eta,\gamma|_f\Omega_-^\dagger|s',\beta'\rangle_{\text{out}} \\
&= \sum_\gamma \int \mathrm{d}\eta\, f\langle s,\beta|\Omega_+^\dagger\Omega_-|\eta,\gamma\rangle_f\Theta(\eta)\langle\eta,\gamma|_f\Omega_-^\dagger\Omega_+|s',\beta'\rangle_f \\
&= \sum_\gamma \int \mathrm{d}\eta\, f\langle s,\beta|S|\eta,\gamma\rangle_f\Theta(\eta)\langle\eta,\gamma|_f S^\dagger|s',\beta'\rangle_f.
\end{aligned}
$$

In this expression we would like to represent the scattering operator S and its adjoint $S^\dagger$ in the spectral representation. Performing the appropriate Fourier transforms we get

$$
\begin{aligned}
{}_{\text{out}}\langle s,\beta|P_-|s',\beta'\rangle_{\text{out}} &= \int \mathrm{d}\sigma\int \mathrm{d}\sigma'\sum_\alpha \int \mathrm{d}\eta\, e^{i\sigma s}S^{\beta,\alpha}(\sigma)e^{-i\eta\sigma}\Theta(\eta)e^{i\eta\sigma'}S^\dagger(\sigma')^{\alpha,\beta}e^{-i\sigma' s'} \\
&= \frac{-i}{4\pi^2}\int \mathrm{d}\sigma\int \mathrm{d}\sigma'\sum_\alpha e^{i\sigma s}\frac{S^{\beta,\alpha}(\sigma)S^\dagger(\sigma')^{\alpha,\beta'}}{\sigma-(\sigma'+i\epsilon)}e^{-i\sigma' s'}.
\end{aligned}
\tag{4.7}
$$

The operator valued function $S(\sigma)$ is analytic in the upper half of the complex σ plane. Its adjoint $S^\dagger(\sigma)$ is analytic in the lower half plane. We assume that $S(\sigma)$ has the form (4.1) and has two poles in the lower half plane, located at z_1 and z_2. The poles of $S^\dagger(\sigma)$ are thus at $\overline{z_1}$ and $\overline{z_2}$. The

form of $S(\sigma)$ and of $S^\dagger(\sigma)$ allows the integrals in (4.7) to performed by contour integration, according to the various possible signs of s and s'. The result is (through the rest of this section we suppress in our notation the auxiliary Hilbert space variables)

$$
\begin{aligned}
{}_{\text{out}}\langle s|P_-|s'\rangle_{\text{out}} &= \Theta(s)\,\delta(s-s') + \frac{1}{2\pi}\Theta(-s)\Bigg[e^{iz_1 s}\operatorname{Res} S(z_1)\int \mathrm{d}\sigma' \frac{S^\dagger(\sigma')}{z_1-(\sigma'+i\epsilon)} e^{-i\sigma' s'} \\
&\quad + e^{iz_2 s}\operatorname{Res} S(z_2)\int \mathrm{d}\sigma' \frac{S^\dagger(\sigma')}{z_2-(\sigma'+i\epsilon)} e^{-i\sigma' s'}\Bigg] \\
&= \Theta(s)\,\delta(s-s') - i\Theta(-s)\Theta(s')\big[e^{iz_1 s}\operatorname{Res} S(z_1) S^\dagger(z_1) e^{-iz_1 s'} \\
&\quad + e^{iz_2 s}\operatorname{Res} S(z_2) S^\dagger(z_2) e^{-iz_2 s'}\big] + i\Theta(-s)\Theta(-s') \\
&\quad \times\Bigg[e^{iz_1 s}\operatorname{Res} S(z_1)\left(\frac{\operatorname{Res} S^\dagger(\overline{z_1})}{z_1-\overline{z_1}} e^{-i\overline{z_1} s'} + \frac{\operatorname{Res} S^\dagger(\overline{z_2})}{z_1-\overline{z_2}} e^{-i\overline{z_2} s'}\right) \\
&\quad + e^{iz_2 s}\operatorname{Res} S(z_2)\left(\frac{\operatorname{Res} S^\dagger(\overline{z_1})}{z_2-\overline{z_1}} e^{-i\overline{z_1} s'} + \frac{\operatorname{Res} S^\dagger(\overline{z_2})}{z_2-\overline{z_2}} e^{-i\overline{z_2} s'}\right)\Bigg].
\end{aligned}
\tag{4.8}
$$

The Lax–Phillips S matrix is analytic in the upper half-plane. Its analytic continuation into the lower half-plane is given by $S(\sigma)\equiv(S^\dagger(\overline{\sigma}))^{-1}$, $\operatorname{Im}\sigma<0$. Similarily, $S^\dagger(\sigma)$ is analytic in the lower half-plane and its analytic continuation to the upper half-plane is given by $S^\dagger(\sigma)\equiv(S(\sigma))^{-1}$, $\operatorname{Im}\sigma>0$. At any point in the complex plane we have

$$
S(\sigma)S^\dagger(\sigma) = S^\dagger(\sigma)S(\sigma) = 1. \tag{4.9}
$$

This relation is obtained by analytic continuation and does not imply unitarity of the S matrix off the real axis. From (4.2) and (4.9) we have

$$
S(\sigma)\left[1+\left(\frac{\operatorname{Res} S^\dagger(\overline{z_1})}{\sigma-\overline{z_1}} + \frac{\operatorname{Res} S^\dagger(\overline{z_2})}{\sigma-\overline{z_2}}\right)\right] = 1.
$$

In the limit as σ goes to $\overline{z_1}$ or to $\overline{z_2}$ we then get

$$
\begin{aligned}
&S(\sigma)\operatorname{Res} S^\dagger(\overline{z_1}) \simeq A_1(\sigma-\overline{z_1}), \quad \sigma\to\overline{z_1}, \\
&S(\sigma)\operatorname{Res} S^\dagger(\overline{z_2}) \simeq A_2(\sigma-\overline{z_2}), \quad \sigma\to\overline{z_2}, \\
&\operatorname{Res} S^\dagger(\overline{z_1})S(\sigma) \simeq \hat{A}_1(\sigma-\overline{z_1}), \quad \sigma\to\overline{z_1}, \\
&\operatorname{Res} S^\dagger(\overline{z_2})S(\sigma) \simeq \hat{A}_2(\sigma-\overline{z_2}), \quad \sigma\to\overline{z_2}
\end{aligned}
\tag{4.10}
$$

for some fixed (i.e., independent of σ) operators A_1, A_2, $\hat{A}_1$, $\hat{A}_2$. From (4.1) and (4.9) we have

$$
S^\dagger(\sigma)\left[1-\left(\frac{\operatorname{Res} S(z_1)}{\sigma-z_1} + \frac{\operatorname{Res} S(z_2)}{\sigma-z_2}\right)\right] = 1
$$

and in the limit as σ approaches z_1 or z_2 we get

$$
\begin{aligned}
&S^\dagger(\sigma)\operatorname{Res} S(z_1) \simeq -B_1(\sigma-z_1), \quad \sigma\to z_1, \\
&S^\dagger(\sigma)\operatorname{Res} S(z_2) \simeq -B_2(\sigma-z_2), \quad \sigma\to z_2, \\
&\operatorname{Res} S(z_1)S^\dagger(\sigma) \simeq -\hat{B}_1(\sigma-z_1), \quad \sigma\to z_1,
\end{aligned}
\tag{4.11}
$$

$$\mathrm{Res}\, S(z_2)S^{\dagger}(\sigma)\simeq -\hat{B}_2(\sigma-z_2),\quad \sigma\to z_2.$$

With the help of Eq. (4.11) we find that the second term of Eq. (4.8) vanishes and the representation of P_- in the outgoing translation representation to be

$$\begin{aligned}
{}_{\mathrm{out}}\langle s,\beta|P_-|s',\beta'\rangle_{\mathrm{out}} &= \Theta(s)\,\delta(s-s')-\frac{1}{2\pi}\Theta(-s)\Bigg[e^{iz_1 s}\mathrm{Res}\, S(z_1)\int \mathrm{d}\sigma'\frac{S^{\dagger}(\sigma')}{z_1-(\sigma'+i\epsilon)}e^{-i\sigma' s'}\\
&\quad + e^{iz_2 s}\mathrm{Res}\, S(z_2)\int \mathrm{d}\sigma'\frac{S^{\dagger}(\sigma')}{z_2-(\sigma'+i\epsilon)}e^{-i\sigma' s'}\Bigg]\\
&= \Theta(s)\,\delta(s-s')+i\Theta(-s)\Theta(-s')\\
&\quad\times\Bigg[e^{iz_1 s}\mathrm{Res}\, S(z_1)\left(\frac{\mathrm{Res}\, S^{\dagger}(\overline{z_1})}{z_1-\overline{z_1}}e^{-i\overline{z_1}s'}+\frac{\mathrm{Res}\, S^{\dagger}(\overline{z_2})}{z_1-\overline{z_2}}e^{-i\overline{z_2}s'}\right)\\
&\quad + e^{iz_2 s}\mathrm{Res}\, S(z_2)\left(\frac{\mathrm{Res}\, S^{\dagger}(\overline{z_1})}{z_2-\overline{z_1}}e^{-i\overline{z_1}s'}+\frac{\mathrm{Res}\, S^{\dagger}(\overline{z_2})}{z_2-\overline{z_2}}e^{-i\overline{z_2}s'}\right)\Bigg].
\end{aligned}\tag{4.12}$$

Inserting (4.12) in (4.5) we get for the generator of the semigroup

$$\begin{aligned}
{}_{\mathrm{out}}\langle s,\beta|B|s',\beta'\rangle_{\mathrm{out}} &= i\lim_{\tau\to 0^+}\frac{1}{\tau}[\Theta(-s)_{\mathrm{out}}\langle s-\tau,\beta|P_-|s',\beta'\rangle_{\mathrm{out}}-\Theta(-s)_{\mathrm{out}}\langle s,\beta|P_-|s',\beta'\rangle_{\mathrm{out}}]\\
&= i\lim_{\tau\to 0^+}\frac{1}{\tau}\{\Theta(-s)(\Theta(s-\tau)\,\delta(s-\tau-s')+i\Theta(-s+\tau)\Theta(-s')\\
&\quad\times[e^{iz_1(s-\tau)}\mathrm{Res}\, S(z_1)K_1(s')+e^{iz_2(s-\tau)}\mathrm{Res}\, S(z_2)K_2(s')])-\Theta(-s)\\
&\quad\times(\Theta(s)\,\delta(s-s')+i\Theta(-s)\Theta(-s')[e^{iz_1 s}\mathrm{Res}\, S(z_1)K_1(s')\\
&\quad + e^{iz_2 s}\mathrm{Res}\, S(z_2)K_2(s')])\}\\
&= i\Theta(-s)\Theta(-s')\lim_{\tau\to 0^+}\frac{1}{\tau}[(e^{iz_1(s-\tau)}-e^{iz_1 s})\\
&\quad\times\mathrm{Res}\, S(z_1)K_1(s')+(e^{iz_2(s-\tau)}-e^{iz_2 s})\mathrm{Res}\, S(z_2)K_2(s')]\\
&= \Theta(-s)\Theta(-s')[z_1\,e^{iz_1 s}\mathrm{Res}\, S(z_1)K_1(s')+z_2\,e^{iz_2 s}\mathrm{Res}\, S(z_2)K_2(s')],
\end{aligned}\tag{4.13}$$

where we have denoted

$$\begin{aligned}
K_1(s') &= \frac{\mathrm{Res}\, S^{\dagger}(\overline{z_1})}{z_1-\overline{z_1}}e^{-i\overline{z_1}s'}+\frac{\mathrm{Res}\, S^{\dagger}(\overline{z_2})}{z_1-\overline{z_2}}e^{-i\overline{z_2}s'},\\
K_2(s') &= \frac{\mathrm{Res}\, S^{\dagger}(\overline{z_1})}{z_2-\overline{z_1}}e^{-i\overline{z_1}s'}+\frac{\mathrm{Res}\, S^{\dagger}(\overline{z_2})}{z_2-\overline{z_2}}e^{-i\overline{z_2}s'}.
\end{aligned}\tag{4.14}$$

We show that, in the outgoing translation representation, the eigenvectors of the generator B of the Lax–Phillips semigroup are

$$\psi_1(s)=\Theta(-s)\mathrm{Res}\, S(z_1)e^{iz_1 s},\quad \psi_2(s)=\Theta(-s)\mathrm{Res}\, S(z_2)e^{iz_2 s}\tag{4.15}$$

in the sense that a vector in $\overline{H}$ given by $\psi_\beta(s)=\Theta(-s)e^{iz_1 s}(\mathrm{Res}\,S(z_1))^{\beta\beta'}\phi^{\beta'}$ or by $\psi_\beta(s)=\Theta(-s)e^{iz_2 s}(\mathrm{Res}\,S(z_2))^{\beta\beta'}\phi^{\beta'}$ where $\phi\in H$, is an eigenvector of the generator of the semigroup. This is achieved by demostrating that these vectors satisfy the eigenvalue equation

$$\int \mathrm{d}s'\,{}_{\mathrm{out}}\langle s,\beta|B|s',\beta'\rangle_{\mathrm{out}}\psi_{1,2}^{\beta'}(s')=z_{1,2}\psi_{1,2}^{\beta}(s'). \tag{4.16}$$

We verify Eq. (4.16) for $\psi_1(s)$. Inserting (4.13) into (4.16) and performing the integration we find for the second term, containing the factor z_2,

$$\begin{aligned}
&\mathrm{Res}\,S(z_2)\int_{-\infty}^{0}\left(\frac{\mathrm{Res}\,S^\dagger(\overline{z_1})}{z_2-\overline{z_1}}e^{-i\overline{z_1}s'}+\frac{\mathrm{Res}\,S^\dagger(\overline{z_2})}{z_2-\overline{z_2}}e^{-i\overline{z_2}s'}\right)e^{iz_1s'}\mathrm{Res}\,S(z_1)\\
&\quad=\frac{i}{z_2-z_1}\mathrm{Res}\,S(z_2)\left(\frac{\mathrm{Res}\,S^\dagger(\overline{z_1})}{z_2-\overline{z_1}}+\frac{\mathrm{Res}\,S^\dagger(\overline{z_1})}{\overline{z_1}-z_1}+\frac{\mathrm{Res}\,S^\dagger(\overline{z_2})}{z_2-\overline{z_2}}+\frac{\mathrm{Res}\,S^\dagger(\overline{z_2})}{\overline{z_2}-z_1}\right)\mathrm{Res}\,S(z_1)\\
&\quad=\mathrm{Res}\,S(z_2)(S^\dagger(z_2)-S^\dagger(z_1))\mathrm{Res}\,S(z_1)=0
\end{aligned} \tag{4.17}$$

and for the first term containing the factor z_1,

$$\begin{aligned}
&\mathrm{Res}\,S(z_1)\int_{-\infty}^{0}\left(\frac{\mathrm{Res}\,S^\dagger(\overline{z_1})}{z_1-\overline{z_1}}e^{-i\overline{z_1}s'}+\frac{\mathrm{Res}\,S^\dagger(\overline{z_2})}{z_1-\overline{z_2}}e^{-i\overline{z_2}s'}\right)e^{iz_1s'}\mathrm{Res}\,S(z_1)\\
&\quad=-i\mathrm{Res}\,S(z_1)\left(\frac{\mathrm{Res}\,S^\dagger(\overline{z_1})}{(z_1-\overline{z_1})^2}+\frac{\mathrm{Res}\,S^\dagger(\overline{z_2})}{(z_1-\overline{z_2})^2}\right)\mathrm{Res}\,S(z_1)\\
&\quad=i\mathrm{Res}\,S(z_1)\frac{dS^\dagger(\sigma)}{d\sigma}\bigg|_{\sigma=z_1}\mathrm{Res}\,S(z_1).
\end{aligned} \tag{4.18}$$

In order to simplify this last expression we need two identities, the first of which is obtained by exploiting the unitarity of $S(\sigma)$ for real σ. Taking the derivative $\mathrm{d}/\mathrm{d}\sigma(S^\dagger(\sigma)S(\sigma))$ we can write

$$\frac{\mathrm{d}S^\dagger(\sigma)}{\mathrm{d}\sigma}=-S^\dagger(\sigma)\frac{\mathrm{d}S(\sigma)}{\mathrm{d}\sigma}S^\dagger(\sigma). \tag{4.19}$$

The second identity is obtained with the help of Eq. (4.1)

$$\mathrm{Res}\,S(z_1)=S(\sigma)S^\dagger(\sigma)\mathrm{Res}\,S(z_1)=\left(1-\frac{\mathrm{Res}\,S(z_1)}{\sigma-z_1}-\frac{\mathrm{Res}\,S(z_2)}{\sigma-z_2}\right)S^\dagger(\sigma)\mathrm{Res}\,S(z_1).$$

From this identity and Eq. (4.10) we get, for small values of $|\sigma-z_1|$,

$$\mathrm{Res}\,S(z_1)S^\dagger(\sigma)\mathrm{Res}\,S(z_1)\simeq-\mathrm{Res}\,S(z_1)(\sigma-z_1). \tag{4.20}$$

When Eqs. (4.19) and (4.20) are used in (4.18) we get

$$\begin{aligned}
&i\,\mathrm{Res}\,S(z_1)\frac{\mathrm{d}S^\dagger(\sigma)}{\mathrm{d}\sigma}\bigg|_{\sigma=z_1}\mathrm{Res}\,S(z_1)\\
&\quad=(-i)\lim_{\sigma\to z_1}\mathrm{Res}\,S(z_1)S^\dagger(\sigma)\frac{\mathrm{d}S(\sigma)}{\mathrm{d}\sigma}S^\dagger(\sigma)\mathrm{Res}\,S(z_1)\\
&\quad=-i\lim_{\sigma\to z_1}\mathrm{Res}\,S(z_1)S^\dagger(\sigma)\left(\frac{\mathrm{Res}\,S(z_1)}{(\sigma-z_1)^2}+\frac{\mathrm{Res}\,S(z_2)}{(\sigma-z_2)^2}\right)S^\dagger(\sigma)\mathrm{Res}\,S(z_1)
\end{aligned}$$

$$= -i \lim_{\sigma \to z_1} \frac{1}{(\sigma - z_1)^2} \operatorname{Res} S(z_1) S^\dagger(\sigma) \operatorname{Res} S(z_1) S^\dagger(\sigma) \operatorname{Res} S(z_1) = -i \operatorname{Res} S(z_1). \tag{4.21}$$

Making use of the results (4.21), (4.17) it is easy to verify Eq. (4.16) for $\psi_1(s)$. A similar calculation shows that $\psi_2(s)$ also satisfies Eq. (4.16).

A rational Lax–Phillips S matrix is a rational, operator valued inner function. Such an operator can be written as[25]

$$S(\sigma) = \frac{\sigma - \overline{z}_1 P_1}{\sigma - z_1 P_1} \frac{\sigma - \overline{z}_2 P_2}{\sigma - z_2 P_2}, \tag{4.22}$$

where $P_1 = |n_1\rangle\langle n_1|$ and $P_2 = |n_2\rangle\langle n_2|$ are projectors on one-dimensional subspaces of the auxiliary Hilbert space (we take $|n_1\rangle$ and $|n_2\rangle$ to be normalized and that, in general, $P_1 P_2 \neq 0$). This S matrix can be rewritten in a form corresponding to Eq. (4.1) as

$$S(\sigma) = 1 + \frac{1}{\sigma - z_1}\left[(z_1 - \overline{z}_1) P_1 \frac{z_1 - \overline{z}_2 P_2}{z_1 - z_2 P_2}\right] + \frac{1}{\sigma - z_2}\left[\frac{z_2 - \overline{z}_1 P_1}{z_2 - z_1 P_1}(z_2 - \overline{z}_2) P_2\right]. \tag{4.23}$$

From Eq. (4.23) we identify the two residues

$$\begin{aligned} \operatorname{Res} S(z_1) &= (z_1 - \overline{z}_1) P_1 \left(1 + \frac{z_2 - \overline{z}_2}{z_1 - z_2} P_2\right), \\ \operatorname{Res} S(z_2) &= \left(1 + \frac{z_1 - \overline{z}_1}{z_2 - z_1} P_1\right)(z_2 - \overline{z}_2) P_2. \end{aligned} \tag{4.24}$$

Inserting in (4.24) the expressions for P_1 and P_2 in terms of $|n_1\rangle$ and $|n_2\rangle$ we find

$$\begin{aligned} \operatorname{Res} S(z_1) &= (z_1 - \overline{z}_1)|n_1\rangle\left(\langle n_1| + \frac{z_2 - \overline{z}_2}{z_1 - z_2}\langle n_1|n_2\rangle\langle n_2|\right), \\ \operatorname{Res} S(z_2) &= \left(|n_2\rangle + \frac{z_1 - \overline{z}_1}{z_2 - z_1}|n_1\rangle\langle n_1|n_2\rangle\right)(z_2 - \overline{z}_2)\langle n_2|. \end{aligned} \tag{4.25}$$

The eigenvectors of the generator B of the semigroup, which we denote by $|\chi_1\rangle$ and $|\chi_2\rangle$, can now be immediately identified, in light of the remarks following Eq. (4.15), from Eq. (4.25),

$$\begin{aligned} |\chi_1\rangle &= \Theta(-s)(z_1 - \overline{z}_1)|n_1\rangle e^{iz_1 s}, \\ |\chi_2\rangle &= \Theta(-s)\left(|n_2\rangle + \frac{z_1 - \overline{z}_1}{z_2 - z_1}|n_1\rangle\langle n_1|n_2\rangle\right) e^{iz_2 s}. \end{aligned} \tag{4.26}$$

Once the residues of the S matrix and the eigenvectors $|\chi_1\rangle$, $|\chi_2\rangle$ are given explicitly in Eqs. (4.25) and (4.26) we can insert these expressions into Eq. (4.13) to achieve an explicit expression for the generator B of the semigroup. We find that

$$B = z_1 |\chi_1\rangle\langle\tilde{\chi}_1| + z_2 |\chi_2\rangle\langle\tilde{\chi}_2|, \tag{4.27}$$

where $\langle\chi_i|\chi_j\rangle = \delta_{ij}$ and

$$\langle\tilde{\chi}_1| = a_1\langle\chi_1| + b_1\langle\chi_2|,$$
$$\langle\tilde{\chi}_2| = a_2\langle\chi_1| + b_2\langle\chi_2| \tag{4.28}$$

with the coefficients a_1, b_1, a_2, b_2 given by

$$a_1 = |\langle n_1|n_2\rangle|^2 \frac{(z_1-\overline{z_2})(\overline{z_2}-z_2)}{z_1-z_2} + 1,$$
$$b_1 = \frac{\overline{z_2}-z_2}{z_1-z_2}\langle n_1|n_2\rangle,$$
$$a_2 = \frac{z_2-\overline{z_2}}{\overline{z_2}-\overline{z_1}}\langle n_2|n_1\rangle, \tag{4.29}$$
$$b_2 = \overline{z_2}-z_2.$$

Equation (4.27) has the diagonalized form of the Lee–Oehme–Yang–Wu phenomenological Hamiltonian in the subspace of the two resonance channel containing, in this case, the K^0 and $\overline{K^0}$ (or K_S, K_L) states. One sees from Eqs. (3.12) and (3.13) that the jump function containing the essential parameters of the S matrix in this subspace contain the matrix elements $\{f_{ij}\}$ of the perturbation. These transition matrix elements coincide in form with the quantities calculated in quantum field theoretical models for the vertex for neutral K meson decay. The theory that we have given here explains how the neutral K meson corresponds to a *state* in the quantum mechanical Hilbert space (even though it is relatively short-lived) with an exact semigroup decay law, as seen to high accuracy in experiment.[11]

V. DISCUSSION AND CONCLUSIONS

We have shown that the quantum mechanical formulation of Lax–Phillips theory for the description of resonances and decay[5] can be generalized to a system with a finite discrete set of resonances. If this set of resonances spans the unstable system subspace, the most general form of the S matrix is that of a rational inner function,[25] treated in detail in Sec. IV for the two-dimensional case.

The eigenstates corresponding to the poles of the S matrix are well-defined vectors in the full Hilbert space $\overline{H}$, and the left and right eigenvectors are orthogonal with respect to the scalar product of $\overline{H}$. They span a two-dimensional subspace of $\overline{H}$; the S matrix acts nontrivially on a two-dimensional subspace of the auxiliary space H for each value of the foliation parameter σ (independently of σ). This corresponds to an ideal form of ''resonance dominance.''

The relation between the eigenvectors of the generator of the semigroup in the space $\overline{H}$ and the vectors spanning the two-dimensional subspace of H is very simple [see Eq. (4.15)]. We are therefore able to construct a model completely within the two-dimensional subspace, containing an effective non-Hermitian generator of the semigroup, and a set of vectors in a two-dimensional space with scalar products taking the same value as the corresponding vectors in the full space. This two-dimensional (in general, N-dimensional) space and the generator of the semigroup acting on it coincides with the Lee–Oehme–Yang–Wu model. Moreover, as we have seen in the simple Lee model which we have studied here, the matrix elements of the model Hamiltonian are related to the perturbation formally in the same way as in the framework of the Wigner–Weisskopf model.

APPENDIX A

We show that $\Omega_\pm|V_i(\tilde{p})\rangle = 0$ applying the methods used in Sec. II. The procedure is explicitly performed for $\Omega_+|V_i(\tilde{p})\rangle = 0$. The result for $\Omega_-|V_i(\tilde{p})\rangle = 0$ is obtained in a similar way.

We start with the integral representation of the wave operator [see Eq. (2.10)]

$$\Omega_+ = 1 + i \lim_{\epsilon\to 0} \int_0^{+\infty} U^\dagger(\tau) V U_0(\tau) e^{-\epsilon\tau} \mathrm{d}\tau; \tag{A1}$$

applying this operator to $|V_i(\tilde{p})\rangle$ we get

$$\begin{aligned}\Omega_+ |V_i(\tilde{p})\rangle &= |V(\tilde{p})\rangle + i \lim_{\epsilon\to 0} \int_0^{+\infty} \mathrm{d}\tau\, U^\dagger(\tau) V U_0(\tau) e^{-\epsilon\tau} b_i^\dagger(\tilde{p})|0\rangle \\ &= |V_i(\tilde{p})\rangle - i \lim_{\epsilon\to 0} \int_0^{-\infty} \mathrm{d}\tau\, U(\tau) V e^{i(\omega_{V_i}(\tilde{p}) - i\epsilon)\tau} b_i^\dagger(\tilde{p})|0\rangle,\end{aligned} \tag{A2}$$

where $\omega_{V_i}(p) = p^2/2M_{V_i}$. As in Sec. II, we want to evaluate the time evolution in the integral and perform a Laplace transform. The result of the action of the potential operator, given in Eq. (2.8) to $|V_i(p)\rangle$, is

$$V|V_i(\tilde{p})\rangle = V b_i^\dagger(\tilde{p})|0\rangle = \sum_{j=1,2} \int \mathrm{d}^4k f_{ij}^*(k) a_{N_j}^\dagger(\tilde{p}-k) a_{\theta_j}^\dagger(k)|0\rangle. \tag{A3}$$

A general form of a state in the sector of the Fock space with $Q_1 = 1$, $Q_2 = 0$ is given in Eq. (2.20). From Eq. (A3) we find, at time $\tau = 0$,

$$A_j(q,0) = 0, \quad B_j(p,k,0) = f_{ij}^*(k)\,\delta^4(\tilde{p}-p-k). \tag{A4}$$

Defining the Laplace transformed coefficients $\tilde{A}_j(q,z)$ and $\tilde{B}_j(p,k,z)$ as in Eq. (2.18), we use Eq. (2.19) and the fact that in Eq. (A4) $A_j(q,0) = 0$ to obtain

$$\begin{aligned}\tilde{A}_l(p,z)\left(z - \frac{p^2}{2M_{V_l}}\right) &= \sum_{j=1,2} \int \mathrm{d}^4k f_{lj}(k) \tilde{B}_j(p-k,k,z), \\ \tilde{B}_l(p-k,k,z)\left(z - \frac{(p-k)^2}{2M_{N_l}} - \frac{k^2}{2M_{\theta_l}}\right) &= iB_l(p-k,k,0) + \sum_{j=1,2} f_{jl}^*(k)\tilde{A}_j(p,z).\end{aligned} \tag{A5}$$

Solving for $\tilde{A}_l(p,z)$ we get

$$\begin{aligned}\tilde{A}_l(p,z) &= i \sum_{i=1,2} W_{lk}^{-1}(z,p) \sum_{j=1,2} \int \mathrm{d}^4k \frac{f_{ij} B_j(p-k,k,0)}{z - \dfrac{(p-k)^2}{2M_{N_l}} - \dfrac{k^2}{2M_{\theta_l}}}, \\ \tilde{B}_l(p-k,k,z) &= \left(z - \frac{(p-k)^2}{2M_{N_l}} - \frac{k^2}{2M_{\theta_l}}\right)^{-1} \left[iB_l(p-k,k,0) + \sum_{j=1,2} f_{jl}^*(k)\tilde{A}_j(p,z)\right].\end{aligned} \tag{A6}$$

Inserting the initial condition for $B_l(p-k,k,0)$ from Eq. (A4) in Eq. (A6) we have

$$\begin{aligned}\tilde{A}_l(p,z) &= i\left[W_{li}^{-1}(p,z)\left(z - \frac{p^2}{2M_{V_i}}\right) - \delta_{li}\right]\delta^4(p-\tilde{p}), \\ \tilde{B}_l(p-k,k,z) &= \left(z - \frac{(p-k)^2}{2M_{N_l}} - \frac{k^2}{2M_{\theta_l}}\right)^{-1} \sum_{j=1,2} i f_{jl}^*(k) W_{ji}^{-1}(p,z)\left(z - \frac{p^2}{2M_{V_i}}\right)\delta^4(p-\tilde{p}).\end{aligned} \tag{A7}$$

Performing the Laplace transform of Eq. (2.15) implied by Eq. (A2), we use the coefficients from Eq. (A7) and evaluate the resulting expression at the point $z=\omega_{V_i}(\tilde{p})-i\epsilon=\tilde{p}^2/2M_{V_i}-i\epsilon$. This procedure gives the simple answer

$$\lim_{\epsilon\to 0}\int_0^{-\infty} d\tau\, U(\tau)Ve^{i(\omega_{V_i}(\tilde{p})-i\epsilon)}b_i^\dagger(\tilde{p})|0\rangle=-ib_i^\dagger(\tilde{p})|0\rangle=-i|V_i(\tilde{p})\rangle \tag{A8}$$

and this implies the desired result.

APPENDIX B

We prove here that the value taken by the projection valued function $P_{2,P}(\sigma)$ is actually a projection operator, for all values of σ, on a fixed two-dimensional subspace of the auxiliary Hilbert space of the Lax–Phillips representation of the relativistic Lee–Friedrichs model, this projection operator is denoted $P_{2,P}$, i.e., we prove that

$$P_{2,P}(\sigma)=P_{2,P}.$$

We start with the observation made at the begining of Sec. IV [see Eq. (4.1) and the discussion following it] that the operator valued function $P_{2,P}(\sigma)$, defined in Eq. (3.14) is a projection operator for each value of σ,

$$P_{n,P}(\sigma)P_{n,P}(\sigma)=P_{n,P}(\sigma). \tag{B1}$$

It is, therefore, a bounded positive operator on the real σ axis.

In order to proceed we need several definitions and results from the theory of operator valued functions. We denote the upper half plane of the complex σ plane by Π. If b is some separable Hilbert space, we denote by $\mathcal{B}(b)$ the set of bounded linear operators on b. We define the following sets of $\mathcal{B}(b)$ valued functions.[18]

Definition A:

(i) A holomorphic $\mathcal{B}(b)$ valued function $f(\sigma)$ on Π is of bounded type on Π if $\log^+|f(\sigma)|_{\mathcal{B}(b)}$ has a harmonic majorant on Π. The class of all such functions is denoted $N_{\mathcal{B}(b)}(\Pi)$.

(ii) If ϕ is any strongly convex function, then by $\mathcal{H}_{\phi,\mathcal{B}(b)}(\Pi)$ we mean the class of all holomorphic $\mathcal{B}(b)$ valued functions $f(\sigma)$ on Π such that $\phi(\log^+|f(z)|_{\mathcal{B}(b)})$ has a harmonic majorant on Π.

(iii) We define $N^+_{\mathcal{B}(b)}(\Pi)=\cup\mathcal{H}_{\phi,\mathcal{B}(b)}(\Pi)$, where the union is over all strongly convex functions ϕ.

(iv) By $H^\infty_{\mathcal{B}(b)}(\Pi)$ we mean the set of all bounded holomorphic $\mathcal{B}(b)$ valued functions on Π.

Here $\log^+ t=\max(\log t,0)$ for $t>0$ and $\log 0=-\infty$. The sets $N_{\mathcal{B}(b)}$ and $N^+_{\mathcal{B}(b)}$ are called Nevanlinna classes and $\mathcal{H}_{\phi,\mathcal{B}(b)}(\Pi)$ is a Hardy–Orlicz class.

We will need the following theorems and definitions:

Theorem A: The following

$$H^\infty_{\mathcal{B}(b)}(\Pi)\subseteq\mathcal{H}_{\phi,\mathcal{B}(b)}(\Pi)\subseteq N^+_{\mathcal{B}(b)}(\Pi)\subseteq N_{\mathcal{B}(b)(\Pi)}$$

is a valid sequence.

Definition B: Let u,v be nonzero scalar valued functions in $N^+(R)$ [$N^+(R)$ is the boundary function for a scalar Nevanlinna class function]. A $\mathcal{B}(b)$-valued function F on R is of class $\mathcal{M}(u_i,v_i)$ if $uF,vF^*\in N^+_{\mathcal{B}(b)}(R)$.

Definition C: If $A\in H^\infty_{\mathcal{B}(b)}(\Pi)$ then:

(i) A is an *inner function* if the operator

$$T(A):f\to Af,\quad f\in H^2_b(\Pi)$$

is a *partial isometry* on $H^2_b(\Pi)$;

(ii) A is an *outer function* if

$$\cup\{Af: f \in H_b^2(\Pi)\} = H_M^2(\Pi)$$

for some subspace M of b.

The main theorem which we will apply here is the following:

Theorem B: Let v be any nonzero scalar function in $N^+(R)$. If F is any nonnegative $\mathcal{B}(b)$-valued function of class $\mathcal{M}(v,v)$ on R then

$$F = G^* G$$

on R, where G is an outer function of class $\mathcal{M}(1,v)$ on R. The factorization of F is essentially unique.

As we have remarked previously, we have assumed that the functions $f_{ij}(k)$ of the Lee model are such that $S_P(\sigma)$ is an inner function. Since $P_{n,P}(\sigma)$ is a bounded operator then, from definition A(iv), the relation (3.14), and Theorem A, we see that

$$P_{n,P}(\sigma) \in N^+_{\mathcal{B}(H)}(\Pi),$$

where H is the auxiliary Hilbert space of the Lax–Phillips representation of the relativistic Lee–Friedrichs model, defined by the variables γ in Eq. (3.3) [or eqs. (3.5) and (3.6)]. Furthermore, the projection operator $P_{2,P}(\sigma)$ satisfies $(P_{2,P}(\sigma))^* = P_{2,P}(\sigma)$ and, from definition B we immediately have

$$P_{2,P}(\sigma) \in \mathcal{M}(1,1).$$

We can apply theorem B with the result that there is a unique decomposition of $P_{2,P}(\sigma)$,

$$P_{2,P}(\sigma) = G^* G = (P_{2,P}(\sigma))^* P_{2,P}(\sigma) = P_{2,P}(\sigma) P_{2,P}(\sigma)$$

and that $G = P_{2,P}(\sigma)$ is an *outer function*. We denote by P the operator on $H_H^2(\Pi)$ for which the realization is the operator valued function $P_{2,P}(\sigma)$. From definition C(ii) we therefore have

$$\{\cup Pf: f \in H_H^2(\Pi)\} = H_M^2(\Pi) \tag{B2}$$

where M is a subspace of the auxiliary Hilbert space H.

Now $P_{2,P}(\sigma)$ is a projection operator for each value of σ. We have that the range of $P_{2,P}(\sigma)$ is a two-dimensional subspace of the auxiliary Hilbert space H for each σ. We denote $M(\sigma) = \mathrm{Im}\, P_{2,P}(\sigma)$. Define

$$\hat{M} = \sum_{\sigma} M(\sigma).$$

For each vector valued function $f \in H_H^2(\Pi)$ we have

$$P_{2,P}(\sigma) f(\sigma) \in \hat{M}. \tag{B3}$$

Furthermore, there is no subspace of $\hat{M}$ that has the property (B3). Since $(Pf)(\sigma) = P_{2,P}(\sigma) f(\sigma) \in \hat{M}$ for $f \in H_H^2(\Pi)$ we must have

$$\{\cup Pf: f \in H_H^2(\Pi)\} = H_{\hat{M}}^2(\Pi). \tag{B4}$$

We conclude that $\hat{M}$ must be a two-dimensional subspace of the auxiliary Hilbert space H. If it has a higher dimension we consider two different values of σ, say $\sigma = \sigma_0$ and $\sigma = \sigma_1 \neq \sigma_0$, such that $P_{2,P}(\sigma_1) \neq P_{2,P}(\sigma_0)$. We then take a vector $v_0 \in P_{2,P}(\sigma_0)H, v_0 \in (P_{2,P}(\sigma_1)H)^\perp$, a scalar valued Hardy class function $g(\sigma) \in H^2(\Pi)$ and construct the vector valued function $j(\sigma)$

$=g(\sigma)v_0$. Clearly, $j \in H^2_{\hat{M}}(\Pi)$ [where we denote by j the vector valued function taking the value $j(\sigma)$ at the point σ] but $j \notin \{\cup Pf: f \in H^2_H(\Pi)\}$, since for any $f \in H^2_H(\Pi)$ we have $j(\sigma_1) = g(\sigma_1)v_0 \perp (Pf)(\sigma_1) = P_{2,P}(\sigma_1)f(\sigma_1)$. Therefore we have

$$\{Pf: f \in H^2_H(\Pi)\} \subset H^2_{\hat{M}}(\Pi) \tag{B5}$$

and we have a contradiction with Eq. (B3).

Since $\mathrm{Dim}\,\hat{M} = 2$ we must have $P_{2,P}(\sigma) = P_{2,P}(\sigma')$ for arbitrary σ and σ' and we may write

$$P_{2,P}(\sigma) = P_{2,P},$$

where $P_{2,P}$ is a projection operator on some fixed (independent of σ) two-dimensional subspace of H, which is the desired result.

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On higher-dimensional dynamics

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Technical results are presented on motion in $N(>4)$D manifolds to clarify the physics of brane theory, Kaluza–Klein theory, induced-matter theory, and string theory. The so-called canonical or warp metric in five dimensions (5D) effectively converts the manifold from a coordinate space to a momentum space, resulting in a new force (per unit mass) parallel to the four-dimensional (4D) velocity. The form of this extra force is actually independent of the form of the metric, but for an unbound particle is tiny because it is set by the energy density of the vacuum or cosmological constant. It can be related to a small change in the rest mass of a particle, and can be evaluated in two convenient gauges relevant to gravitational and quantum systems. In the quantum gauge, the extra force leads to Heisenberg's relation between increments in the position and momenta. If the 4D action is quantized then so is the higher-dimensional part, implying that particle mass is quantized, though only at a level of 10^{-65} g or less, which is unobservably small. It is noted that massive particles which move on timeline paths in 4D can move on null paths in 5D. This agrees with the view from inflationary quantum field theory, that particles acquire mass dynamically in 4D but are intrinsically massless. A general prescription for dynamics is outlined, wherein particles move on null paths in an $N(>4)$D manifold which may be flat, but have masses set by an embedded 4D manifold which is curved. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The motion of a test particle in a higher-dimensional manifold is a prime way to investigate extensions of four-dimensional (4D) Einstein theory. In five-dimensional (5D) Kaluza-Klein theory, older studies concentrated on the case where the 4D space-time was independent of the extra coordinate.[1–6] This condition was relaxed in newer work on 5D induced-matter theory, where the 5D field equations for apparent vacuum are broken down into 4D ones with an energy–momentum tensor derived from the extra dimension.[7–15] Dynamical effects in 4D, when the metric is allowed to depend on one or more extra coordinates, have also become the subject of studies in string and membrane theory.[16–19] The main result is the appearance in 4D of extra forces.[16,20,21] These are expected to be small in gravitational problems, but could be significant in particle physics, where a unification of the interactions could be achieved via ten-dimensional superstrings or eleven-dimensional supergravity.[22,23] In view of current interest in the subject, some results will be given aimed at clarifying higher-dimensional dynamics.

II. GEODESICS IN *N* DIMENSIONS AND 4D

Consider an N-dimensional Riemannian manifold with a metric tensor g_{AB} that depends on coordinates x^C, with a line element $dS^2 = g_{AB}dx^A dx^B$, through which a particle moves along a path described by an affine parameter λ. It contains a 4D submanifold with line element $ds^2 = g_{\alpha\beta}dx^\alpha dx^\beta$. Here and in the following it is instructive to concentrate on the 5D case, when Latin indices run from 0 to 4 and Greek indices run from 0 to 3.

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In general relativity, the particle moves along a geodesic which minimizes s via $\delta[\int \mathrm{d}s] = 0$. For a particle with mass m, $\lambda = s$ is normally chosen, the geodesic is non-null, and the four-momentum is defined by $p^\alpha \equiv m u^\alpha$, where the four-velocity is $u^\alpha \equiv \mathrm{d}x^\alpha/\mathrm{d}s$. For a massless particle (photon), λ is often unspecified because the geodesic is null and can be obtained directly from the metric. The four-velocities are conventionally normalized for non-null and null paths via $u^\alpha u_\alpha = 1, 0$, respectively. However, S contains s, and the former defines geodesics via $\delta[\int \mathrm{d}S] = 0$.

A question which arises in the literature is whether the particle should follow a geodesic in ND or in 4D (in brane theory, this is connected with whether the particle is constrained to move on the brane or can wander through the bulk). The answer is that it is most natural to assume that the motion is geodesic in S, provided that the extra terms which then appear in the geodesic in s are compatible with observation (see the following). In this regard, it should be recalled that even in 4D the acceleration of the particle $\mathrm{d}^2x^\alpha/\mathrm{d}s^2$ is *not* a covariantly defined vector. The appropriate quantity is the absolute or covariant derivative, which defines the path via $Du^\alpha/\mathrm{d}s \equiv \mathrm{d}u^\alpha/\mathrm{d}s + \Gamma^\alpha_{\beta\gamma} u^\beta u^\gamma = 0$, where $\Gamma^\alpha_{\beta\gamma}$ are the Christoffel symbols. It is the latter which yield the forces on the particle, which are thereby recognized as being inertial in origin, meaning that they arise from the motion of the reference frame. In ND, the same philosophy should hold. We can use $\delta[\int \mathrm{d}S] = 0$, and the absolute derivative or the Lagrange equations to obtain the dynamics, but the latter will in general contain terms which arise from the motion with respect to the larger reference frame.

The only comment which needs to be added to this concerns the case of null geodesics with $\mathrm{d}S = 0$. This has been considered by several workers.[1,14,24,25] It should be recalled that 4D causility is defined by $\mathrm{d}s^2 \geqslant 0$, and does not constrain $\mathrm{d}S^2$.[5] There is no impediment to assuming that particles with $m \neq 0$ move along paths with $\mathrm{d}S^2 = 0$, when their motions can be described consistently by choosing $\lambda = s$.

There is, however, another issue which relates to geodesics and requires notice. Geodesics in general relativity really describe accelerations, not forces or changes in momentum. The distinction is often unnecessary, because the mass is constant. But even in Newtonian mechanics, a rocket changes mass as its fuel burns, feeling a force along the direction of its motion. And in inflationary quantum field theory, particles are intrinsically massless, gaining mass by a dynamical mechanism involving the Higgs field.[26] As noted occasionally in the literature,[27] the correct dynamics in situations where the mass changes, follows not from $\delta[\int \mathrm{d}s] = 0$ but from $\delta[\int m\,\mathrm{d}s] = 0$. That is, dynamics is a theory not of four-velocities but of four-momenta. In this regard, it should be noted that there is no *contradiction* between the normalization condition used in relativity for the four-velocities $u^\alpha u_\alpha = 1$, and the condition used in particle physics for the four-momenta $p^\alpha p_\alpha = m^2$. (The latter is often written $E^2 - p^2 = m^2$ and effectively uses the energy and three-momentum to define the rest mass of a particle.) It is just that the conventional geodesic does not give any information about the origin or variability of mass, a problem which is of central importance in cosmology.

The subjects of the preceding paragraphs, while perhaps familiar, underlie much of the recent work which has been done on higher-dimensional dynamics.[1–27] While it is not exclusive, we wish to concentrate in the following on an approach which resolves most of the issues raised previously.[7–16] Specifically, we wish to present new results on metrics of the so-called canonical or warp type in 5D (the extension to $N > 5$ is straightforward). This has line element

$$\mathrm{d}S^2 = \frac{\ell^2}{L^2} g_{\alpha\beta}(x^\gamma, \ell)\,\mathrm{d}x^\alpha\,\mathrm{d}x^\beta - \mathrm{d}\ell^2, \tag{2.1}$$

where $x^4 = \ell$ is the extra coordinate and L is a constant length. Certain things are already known about this metric, and certain others may be deduced from the comments made previously. It is convenient to list these here. (a) Mathematically (2.1) is general, insofar as the five available coordinate degrees of freedom have been used to set $g_{4\alpha} = 0$, $g_{44} = -1$. Physically, this removes the potentials of electromagnetic type and flattens the potential of scalar type. (b) The metric (2.1)

has been extensively used in the field equations, which in terms of the Ricci tensor are $R_{AB}=0$, and many solutions are known.[14] These include solutions for the one-body problem[28] and cosmology[29] which have acceptable dynamics, and solutions with the opposite sign for g_{44} which describe waves.[30] (c) When $\partial g_{\alpha\beta}/\partial\ell=0$ in (2.1), the 15 field equations $R_{AB}=0$ contain as a subset the 10 field equations of general relativity, which in terms of the Einstein tensor are $G_{\alpha\beta}=3g_{\alpha\beta}/L^2$. The scale L is thereby identified, in cosmology, in terms of the cosmological constant via $\Lambda=3/L^2$ and in other situations as the characteristic size of the four-space.[12] (d) This kind of local embedding of a 4D Riemann space in a 5D Ricci-flat space can be applied to any N, and is guaranteed by Campbell's theorem.[31–35] (e) The factorization in (2.1) says in effect that the 4D part of the 5D interval is $(\ell/L)\mathrm{d}s$, which defines a *momentum* space rather than a *coordinate* space if ℓ is related to m.[8] This resolves the issue of forces versus accelerations noted previously. (f) Partial confirmation of this comes from a study of the 5D geodesic and a comparison of the constants of the motion in 5D and 4D.[14,36,37] In the Minkowski limit, the energy of a particle moving with velocity v is $E=\ell(1-v^2)^{-1/2}$ in 5D, which agrees with the expression in 4D if $\ell=m$. (g) The five components of the geodesic equation for (2.1) split naturally into four space–time components and an extra component. For $\partial g_{\alpha\beta}/\partial\ell\neq 0$, the former contain terms parallel to the four-velocity u^α as noted previously for the case of a rocket.[12,37] For $\partial g_{\alpha\beta}/\partial\ell=0$, the motion is not only geodesic in 5D but geodesic in 4D.

III. THE NATURE OF THE CANONICAL METRIC

The metric (2.1) is not mathematically unique but is physically rich, which prompts a deeper examination of its nature.

Consider a 4D space with $\mathrm{d}s^2=g_{\alpha\beta}\mathrm{d}x^\alpha\mathrm{d}x^\beta$ embedded in a 5D space with line element

$$\mathrm{d}S^2=\mathrm{d}s^2-\mathrm{d}\ell^2. \tag{3.1}$$

Then the transformation

$$\begin{aligned} s&\to\ell\sinh\ (s/L),\\ \ell&\to\ell\cosh\ (s/L), \end{aligned} \tag{3.2}$$

causes (2.1) to become

$$\mathrm{d}S^2=\frac{\ell^2}{L^2}\mathrm{d}s^2-\mathrm{d}\ell^2. \tag{3.3}$$

This is of the canonical form, which is therefore recognized to be a spherical form of a two-plane (the opposite sign for g_{44} may be obtained by replacing the hyperbolic functions by their trigonometric counterparts). Physically, there is an analogy with the angular momentum (per unit mass) of a particle rv moving with velocity v at distance r from the center of a circle. Recalling from the previous discussion that ℓ plays the role of m in the canonical metric, we see that mu^α is the product of the velocity in 4D with the distance in the orthogonal fifth direction. In other words, p^α is a true 5D moment.

The above suggests that physically significant 4D structure may even be present in a flat 5D manifold. The latter in spherical polars has line element

$$\mathrm{d}S^2=\mathrm{d}t^2-\mathrm{d}r^2-r^2\,\mathrm{d}\Omega^2-\mathrm{d}\ell^2, \tag{3.4}$$

where $\mathrm{d}\Omega^2\equiv(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\phi^2)$. Introducing a dimensionless parameter α, consider the transformation

$$t \to \left(\frac{\alpha}{2}\right) t^{1/\alpha} \ell^{1/(1-\alpha)} \left(1 + \frac{r^2}{\alpha^2}\right) - \frac{\alpha}{2(1-2\alpha)} [t^{-1} \ell^{\alpha/(1-\alpha)}]^{(1-2\alpha)/\alpha},$$

$$r \to r t^{1/\alpha} \ell^{1/(1-\alpha)}, \tag{3.5}$$

$$\ell \to \left(\frac{\alpha}{2}\right) t^{1/\alpha} \ell^{1/(1-\alpha)} \left(1 - \frac{r^2}{\alpha^2}\right) + \frac{\alpha}{2(1-2\alpha)} [t^{-1} \ell^{\alpha/(1-\alpha)}]^{(1-2\alpha)/\alpha}$$

with $\theta \to \theta$, $\phi \to \phi$. Then some algebra shows that (3.4) becomes

$$dS^2 = \ell^2 \, dt^2 - t^{2/\alpha} \ell^{2/(1-\alpha)} (dr^2 + r^2 \, d\Omega^2) - \alpha^2 (1-\alpha)^{-2} t^2 \, d\ell^2. \tag{3.6}$$

This is the metric of a class of cosmological models first found as solutions of the field equations $R_{AB} = 0$ by Ponce de Leon.[38] They are separable in ℓ, t and reduce to the 4D Friedmann–Robertson–Walker models with flat three-dimensional sections on the hypersurfaces ℓ = constant. (The dust or Einstein–de Sitter solution has $\alpha = 3/2$ while the radiation solution has $\alpha = 2$.) For this reason they are often regarded as the standard 5D cosmologies, but (3.5) shows that they are actually canonical forms of 5D Minkowski space.

The same cannot be said of the standard one-body solution of $R_{AB} = 0$.[28] This has the line element

$$dS^2 = \frac{\Lambda \ell^2}{3} \left\{ \left[1 - \frac{2M}{r} - \frac{\Lambda r^2}{3} \right] dt^2 - \left[1 - \frac{2M}{r} - \frac{\Lambda r^2}{3} \right]^{-1} dr^2 - r^2 \, d\Omega^2 \right\} - d\ell^2, \tag{3.7}$$

where M is a constant usually identified with the mass at the center of the three-geometry. Metric (3.7) is pure canonical in the sense that it has the form (2.1) with $\Lambda = 3/L^2$ and $\partial g_{\alpha\beta} / \partial \ell = 0$. However, it is not 5D flat like (3.6), as may be verified by computer. This agrees with the well-known fact that the 4D Schwarzschild–de Sitter solution [given by the part inside the large brackets in Eq. (3.7)] can only be embedded in a flat space with dimension $N \geqslant 6$. However, since any 4D solution can be embedded in $N \geqslant 10$, the use of the canonical form obviously has relevance to superstring theory.

The field equations $R_{AB} = 0$ mentioned previously clearly contain physical information which is relevant to why the canonical metric (2.1) is so effective. These fifteen relations can in general be broken down into one wave equation, four conservation equations, and ten Einstein equations $G_{\alpha\beta} = 8\pi T_{\alpha\beta}$ with an effective or induced energy–momentum tensor.[39] However, only the last quantity contains u^α, and via the 4D covariant derivative $T^{\alpha\beta}{}_{;\beta} = 0$ is usually interpreted as describing the dynamics of a fluid consisting of particles. We will return to the field equations later, but let us here take a look at particle dynamics.

This subject has been studied using both the geodesic equation[7,8] and the Lagrange equations.[12,15] These approaches are compatible, of course, but the latter is the more instructive for investigating the special status of (2.1). Thus consider a Lagrangian which generalizes (2.1) and has the form

$$\mathcal{L} = \left\{ \frac{\ell^2}{L^2} g_{\alpha\beta}(x^\gamma, \ell) \frac{dx^\alpha}{d\lambda} \frac{dx^\beta}{d\lambda} - \Phi^2(x^\gamma, \ell) \left(\frac{d\ell}{d\lambda}\right)^2 \right\}^{1/2}. \tag{3.8}$$

This is dimensionless, and contains a scalar field $g_{44} = -\Phi^2$ which is the classical analog of the Higgs potential that is responsible for particle masses in quantum field theory.[14,26] The Lagrangian (3.8) defines an action $I = \int \mathcal{L}(x^A, \dot{x}^A) \, d\lambda$, where λ is an affine parameter along the path of the particle and $\dot{x}^A \equiv dx^A/d\lambda$ is its five-velocity. The action is an extremum if

$$\frac{d}{d\lambda} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}^A} \right) - \frac{\partial \mathcal{L}}{\partial x^A} = 0. \tag{3.9}$$

The space–time and extra components of this can be worked out explicitly once λ is chosen. A natural choice might appear to be $\lambda = S$,[8] in which case (3.9) is equivalent to

$$\frac{dU^A}{dS} + \Gamma^A_{BC} U^B U^C = 0, \tag{3.10}$$

the 5D geodesic equation in $U^A \equiv dx^A/dS$ with appropriately defined Christoffel symbols (see Sec. II). However, this is undefined for 5D null geodesics, and if another affine parameter λ is used instead then (3.10) acquires an extra term on the right-hand side equivalent to $U^A \mathcal{L}^{-1} d\mathcal{L}/d\lambda$.[40] Also, the object of the exercise is to understand 4D dynamics in $u^\alpha \equiv dx^\alpha/ds$ rather than 5D dynamics in $U^A \equiv dx^A/dS$. For these reasons, we choose $\lambda = s$.[7,12,15] We also choose $u_\alpha u^\alpha = 1$ for a massive particle following a timelike 4D path. Then the substitution of (3.8) into (3.9) results in two rather complicated expressions for the α, four components of the motion, of which the second is the more enlightening:

$$\frac{\ell}{\Phi^2}\left(\frac{\Phi^2 \dot{\ell}}{\ell}\right)^{\cdot} - \frac{L^2 \Phi \dot{\Phi} \dot{\ell}^3}{\ell^2} - \frac{1}{L\Phi}\left(1 - \frac{L^2 \Phi^2 \dot{\ell}^2}{\ell^2}\right)\left(1 + \frac{\ell u^\alpha u^\beta}{2}\frac{\partial g_{\alpha\beta}}{\partial \ell} - \frac{L^2 \Phi \dot{\Phi} \dot{\ell}^2}{\ell}\right) = 0. \tag{3.11}$$

Remarkably, this is satisfied with no constraint on the last parentheses by $(L\Phi\dot{\ell}/\ell)^2 = 1$, which by (3.8) implies $\mathcal{L} = 0$. That is, the particle is traveling along a timelike path in 4D but a null path in 5D.

We end this section by stating explicitly the equations of motion which follow from (3.9) or (3.10). The space–time components can be written as a part which is geodesic in s and an extra part:

$$\frac{du^\mu}{ds} + \Gamma^\mu_{\beta\gamma} u^\beta u^\gamma = F^\mu, \tag{3.12}$$

$$F^\mu \equiv \left(-g^{\mu\alpha} + \frac{u^\mu u^\alpha}{2}\right) u^\beta \frac{\partial g_{\alpha\beta}}{\partial \ell}\frac{d\ell}{ds}. \tag{3.13}$$

Here F^μ is a force per unit (inertial) mass, or acceleration. It can be written as a sum of components normal and parallel to u^μ, so $F^\mu = N^\mu + P^\mu$ where

$$N^\mu = (-g^{\mu\alpha} + u^\mu u^\alpha) u^\beta \frac{\partial g_{\alpha\beta}}{\partial \ell}\frac{d\ell}{ds}, \tag{3.14}$$

$$P^\mu = \frac{-u^\mu}{2}\left(u^\alpha u^\beta \frac{\partial g_{\alpha\beta}}{\partial \ell}\right)\frac{d\ell}{ds}. \tag{3.15}$$

The normal component obeys $N^\mu u_\mu = 0$ (by construction), which is the behavior typical of Einstein gravity and Maxwell electromagnetism.[12,14] The parallel component obeys

$$P^\mu u_\mu = \frac{-u^\alpha u^\beta}{2}\frac{\partial g_{\alpha\beta}}{\partial \ell}\frac{d\ell}{ds} \equiv \beta. \tag{3.16}$$

Here the four-velocities are still normalized via $u^\alpha u_\alpha = 1$ (see above and Sec. IV). But the scalar quantity β is finite if $\partial g_{\alpha\beta}/\partial \ell \neq 0$ in the canonical metric (2.1), and there is motion in the extra dimension as measured with the particle's proper 4D time s. The quantity β is a kind of power per unit (inertial) mass. *It has no analog in standard 4D field theory*. The magnitude of β depends on $d\ell/ds$, which is given by the extra component of the equation of motion:

$$\frac{d^2\ell}{ds^2}-\frac{2}{\ell}\left(\frac{d\ell}{ds}\right)^2+\frac{\ell}{L^2}=-\frac{1}{2}\left[\frac{\ell^2}{L^2}-\left(\frac{d\ell}{ds}\right)^2\right]u^\alpha u^\beta\frac{\partial g_{\alpha\beta}}{\partial\ell}. \tag{3.17}$$

This implies that there is no intrinsic state of rest for the particle in the extra dimension. [Formally, Eq. (3.17) is satisfied with $\ell=\ell_0$, $u^{123}=0$, $u^0=1$, and $g_{\alpha\beta}=L^2/\ell_0^2$, but then $d\ell=0$ and the metric reverts to a 4D one.] This is basically because the 4D proper time has been used as a parameter for the 5D motion. Thus in general, $d\ell/ds\neq 0$ in (3.17), $\partial g_{\alpha\beta}/\partial\ell\neq 0$ in (2.1), and $\beta\neq 0$ in (3.16). The existence of finite scalar quantities like β is expected to be typical of the dynamics of any $N(>4)$-dimensional theory.

IV. EXTRA FORCES IN $N(>4)$D THEORY

In Sec. II, it was noted that the word ''force'' has to be treated with some caution, because theories like general relativity describe accelerations while theories of particle physics describe momenta, and the two concepts can only be consistently joined via a suitable definition of mass. The canonical metric (2.1) opens a route to this, as well as providing a number of other interesting results. In Sec. III, it was seen that the effectiveness of the canonical metric can be traced partly to the fact that it is an algebraically convenient way to parametize a 5D manifold, but mainly to the fact that it is a natural basis for 5D dynamics. In the present section we wish to go beyond the canonical metric and note some general results on forces.

It is straightforward to see that any $N(>4)$D theory will yield extra accelerations as viewed in 4D, which modulo an appropriate definition of mass will be interpreted as extra forces.[16,20,21] Given an ND line element $dS^2=g_{AB}dx^Adx^B$, the N velocities $u^A\equiv dx^A/dS$ are normalized for a non-null path via $U^AU_A=1$, and the path is extremized in terms of an ND covariant derivative via $U^BU^A{}_{;B}=0$. This when contracted gives $U_AF^A=0$, where the F^A are forces per unit (inertial) mass. However, this implies $U_\alpha F^\alpha=-U_{(N-\alpha)}F^{(N-\alpha)}\neq 0$ when viewed from 4D.

To relate this to what was done in Sec. III, consider one extra coordinate and the normalization condition

$$g_{\alpha\beta}(x^\gamma,\ell)u^\alpha u^\beta=1. \tag{4.1}$$

Differentiating this with respect to an affine parameter λ gives

$$g_{\alpha\beta,\gamma}\ u^\gamma u^\alpha u^\beta+\frac{\partial g_{\alpha\beta}}{\partial\ell}\frac{d\ell}{d\lambda}u^\alpha u^\beta+2g_{\alpha\mu}\frac{du^\mu}{d\lambda}u^\alpha=0, \tag{4.2}$$

where $u^\alpha\equiv dx^\alpha/d\lambda$ and $g_{\alpha\beta,\gamma}\equiv\partial g_{\alpha\beta}/\partial\ell$. Introducing the Christoffel symbols and noting symmetries under the exchange of α and β, the first term on the left-hand side of (4.2) can be rewritten using

$$(g_{\alpha\beta,\gamma}+g_{\alpha\gamma,\beta}-g_{\beta\gamma,\alpha})u^\gamma u^\alpha u^\beta=2g_{\alpha\mu}\Gamma^\mu_{\beta\gamma}u^\gamma u^\alpha u^\beta. \tag{4.3}$$

Then (4.2) reads

$$2g_{\alpha\mu}u^\alpha\left(\frac{du^\mu}{d\lambda}+\Gamma^\mu_{\beta\gamma}\ u^\beta u^\gamma\right)+\frac{\partial g_{\alpha\beta}}{\partial\ell}\frac{d\ell}{d\lambda}u^\alpha u^\beta=0. \tag{4.4}$$

With $F^\mu\equiv(du^\mu/d\lambda+\Gamma^\mu_{\beta\gamma}u^\beta u^\gamma)$ as in (3.12) this says

$$u_\mu F^\mu=-\frac{u^\alpha u^\beta}{2}\frac{\partial g_{\alpha\beta}}{\partial\ell}\frac{d\ell}{d\lambda}. \tag{4.5}$$

There is clearly a force per unit (inertial) mass parallel to u^μ given by

$$P^\mu = -\frac{u^\mu}{2}\left(u^\alpha u^\beta \frac{\partial g_{\alpha\beta}}{\partial \ell}\right)\frac{d\ell}{d\lambda}. \tag{4.6}$$

When $\lambda = s$ this is identical to (3.15), which was derived starting from the canonical metric (2.1). But here, we started from the normalization condition (4.1) for a massive particle following a 4D timelike path. This means that the existence of (4.6) does not depend on the form of the metric. It is a consequence of defining and normalizing four-velocities in the conventional way when space–time is part of a bigger manifold.

Given the manner in which 4D dynamics is conventionally set up, it is difficult to conceive of any way in which a force parallel to the four-velocity could be interpreted other than by relating it to the mass of the particle which feels it. For a particle moving under the influence of standard gravity and the extra force, the equation of motion in space–time is

$$\frac{du^\mu}{ds} + \Gamma^\mu_{\alpha\beta}\ u^\alpha u^\beta = P^\mu \tag{4.7}$$

with P^μ given by (4.6) with $\lambda = s$. In the following, we will consider some significant applications of (4.7). Here, as an illustration, we can take a canonical metric with $g_{\alpha\beta} = (\ell^2/L^2)\,\eta_{\alpha\beta}$ where $\eta_{\alpha\beta}$ = diagonal $(1,-1,-1,-1)$. Then $\partial g_{\alpha\beta}/\partial\ell = (2/\ell) g_{\alpha\beta}$ and $u^\alpha u^\beta \partial g_{\alpha\beta}/\partial\ell = 2/\ell$ in (4.6). The equation of motion (4.7) reads

$$\frac{du^\mu}{ds} = -\frac{u^\mu}{\ell}\frac{d\ell}{ds}, \tag{4.8}$$

which yields $\ell u^\mu = \ell_0$ where ℓ_0 is a constant of the (4D) motion. The latter is clearly the momentum mu^μ, confirming that in canonical coordinates the extra coordinate plays the role of particle mass. [See Sec. II and Refs. 8, 12, 14 and 15. Equation (4.8) is the analog of what is sometimes called the rocket equation in Newtonian mechanics, which just says that $d(mv)/dt = 0$ or $dv/dt = -(v/m)dm/dt$.] However, while $p^\mu = mu^\mu$ is a constant of the 4D motion, it should be noted that $m = m(s)$ in general.

This cannot be fixed in the conventional approach to 4D dynamics, except by appeal to some external condition. But in 5D dynamics it can, notably by the extra component of the geodesic (3.17). This in general requires a solution of the field equations, but as noted in Sec. III a natural parametrization of 5D geodesics is via $dS = 0$. Then for the canonical metric (2.1) we have

$$dS^2 = 0 = \frac{\ell^2}{L^2}ds^2 - d\ell^2, \tag{4.9}$$

which yields

$$\ell = \ell_0 e^{\pm s/L}. \tag{4.10}$$

The rate of variation of ℓ depends on the characteristic dimension of the four-space L. As noted in Sec. II, for pure-canonical metrics with $\partial g_{\alpha\beta}/\partial\ell = 0$, $L = (3/\Lambda)^{1/2}$, where Λ is the cosmological constant.[12,14] Thus from (4.10), with the identification $\ell = m$, the rate of variation of the rest mass is given by

$$\frac{1}{m}\left|\frac{dm}{ds}\right| \simeq \frac{1}{m}\left|\frac{dm}{dt}\right| = \left(\frac{\Lambda}{3}\right)^{1/2}. \tag{4.11}$$

The value of Λ is severely constrained by astrophysical data.[41–43] These indicate $|\dot{m}|/m \lesssim 2 \times 10^{-18}\ \mathrm{s}^{-1}$ by (4.11), which is observationally acceptable. There are also other constraints on extra forces like (4.6), but these are relatively weak.[44] However, it should be noted that Λ mea-

sures the energy density of the vacuum in general relativity,[14] and this could be larger on small scales,[26] so in principle mass variation and extra forces could be measured.

To do this in practice, though, requires solutions of the field equations. These in turn require the specification of a system of coordinates or gauge. In this context, it should be noted that the extra force P^μ of (4.6) for the 5D case is a four-vector. As such, it is covariant under the usual group of 4D coordinate transformations $x^\mu \rightarrow x^\mu(x^\nu)$, but will in general change under the group of 5D coordinate transformations $x^A \rightarrow x^A(x^B)$. This is inevitable given that the field equations $R_{AB}=0$ are covariant in 5D, but may represent a problem regarding the interpretation of observations made in 4D. This problem will be greater in the (algebraically straightforward) extension of the results of this section to $N(>5)$D. There is a considerable relevant literature on gauges.[14,22,23,45,46] Fortunately, if attention is restricted to dynamics there are only two natural gauges, to which we now turn our attention.

V. THE EINSTEIN AND PLANCK GAUGES

It has been seen that the pure canonical gauge, namely (2.1) with a factor ℓ^2 attached to an ℓ-independent space–time, is remarkably successful as a basis for conventional 4D dynamics. This is because the use of $\ell=m$ effectively converts the 4D part of the 5D manifold from a coordinate space to a momentum space. However, that success concerns the classical concept of momentum as the product of mass and velocity. In modern quantum field theory the mass of a particle is not defined *a priori*,[26] and even in old quantum theory the momentum is described by a de Broglie wave and derived from a wave function. A superior formulation of dynamics ought to address both the classical and quantum nature of momentum. In this section, we will assume that the differences in description are due to differences in gauge choices for a higher-dimensional metric, and narrow the choices for the gauges using field equations.

The latter are still the subject of discussion in ND field theory, but in 5D there is a consensus that they are given by the Ricci tensor as

$$R_{AB}=0 \quad (A,B=0,1,2,3,4). \tag{5.1}$$

Let us consider these for a generalized form of the pure canonical metric (2.1) with line element

$$dS^2=\left(\frac{L}{\ell}\right)^{2a}\overline{g}_{\alpha\beta}(x^\gamma)dx^\alpha dx^\beta-\left(\frac{L}{\ell}\right)^{4b}d\ell^2. \tag{5.2}$$

Here a, b are constants which it is desired to constrain using (5.1). These fifteen, 5D relations can be decomposed into 4D ones under only the four coordinate conditions $g_{\alpha 4}=0$.[39] For (5.2) it is convenient to take the components in the order $AB=44$, 4α, $\alpha\beta$. The result is

$$a^2-2ab+a=0, \tag{5.3}$$

$$V^\beta_{\alpha;\beta}=0,$$
$$V^\beta_\alpha \equiv \frac{1}{2|g_{44}|^{1/2}}\left(g^{\beta\sigma}\frac{\partial g_{\sigma\alpha}}{\partial\ell}-\delta^\beta_\alpha g^{\mu\nu}\frac{\partial g_{\mu\nu}}{\partial\ell}\right)=\frac{3a\,\delta^\beta_\alpha}{\ell}\left(\frac{\ell}{L}\right)^{2b}, \tag{5.4}$$

$$G_{\alpha\beta}=\frac{(2a^2+2ab-a)}{\ell^2}\left(\frac{L}{\ell}\right)^{2a-4b}\overline{g}_{\alpha\beta}. \tag{5.5}$$

Here a semicolon denotes the usual 4D covariant derivative, $g_{\alpha\beta}=(L/\ell)^{2a}\overline{g}_{\alpha\beta}$, $g_{44}=-(L/\ell)^{4b}$ and indices have been raised and lowered using $g_{\alpha\beta}$ in order to get the 4D Einstein tensor. This in mixed form is $G^\beta_\alpha=(2a^2+2ab-a)\ell^{-2}(\ell/L)^{4b}\delta^\beta_\alpha$, and as usual $G^\beta_\alpha \equiv R^\beta_\alpha - R\delta^\beta_\alpha/2$ in terms of the 4D Ricci tensor and Ricci scalar. The latter may be found by direct calculation, and is

$$R=\frac{-12a^2}{\ell^2}\left(\frac{\ell}{L}\right)^{4b}. \tag{5.6}$$

This determines the curvature of the 4D part of the manifold, which by (5.5) has the form of a vacuum space with an effective cosmological constant $\Lambda=(2a^2+2ab-a)\ell^{-2}(L/\ell)^{2a-4b}$. This is zero for $a=b=0$, in which case (5.2) describes general relativity embedded in a flat and physically innocuous extra dimension. For $a=-1$, $b=0$ we have $\Lambda=3/L^2$, and (5.2) is the pure canonical metric already discussed. Interestingly, the same value of Λ results for $a=+1$, $b=+1$, which implies that (5.5) would give the same 4D physics even though the metric (5.2) does not have the canonical form. We will return to this later. Here we note that the 4D physics is contained in the ten Einstein equations (5.5), while the four conservation equations (5.4) are satisfied, and the one scalar relation (5.3) provides a constraint between the constants a, b. In this regard it should be noted that the relation $G=-R$ (which follows from the definition of the Einstein tensor), when combined with (5.6) reproduces (5.3), which is the only meaningful constraint.

The comments of the preceding paragraph imply that (5.2) as constrained by (5.3) contains interesting physics in (5.5). For example, the fact that the 4D cosmological constant depends in general on 5D parameters opens the way to a resolution of the conflict in its size as inferred from cosmology and particle physics.[47–49] However, it is apparent that for dynamics there are two natural gauges, namely those with $a=-1$, $b=0$ and $a=+1$, $b=+1$. For these (5.2) has the forms

$$dS^2=\frac{\ell^2}{L^2}\overline{g}_{\alpha\beta}(x^\gamma)dx^\alpha dx^\beta-d\ell^2, \tag{5.7}$$

$$dS^2=\frac{L^2}{\ell^2}\overline{g}_{\alpha\beta}(x^\gamma)dx^\alpha dx^\beta-\frac{L^4}{\ell^4}d\ell^2. \tag{5.8}$$

Mathematically, these are equivalent since (5.7)$\rightarrow$(5.8) under the simple coordinate transformation

$$\ell\rightarrow L^2/\ell. \tag{5.9}$$

Physically, this corresponds to changing the way the rest mass of a particle is described. We saw previously that for the pure canonical metric the dynamics implies the identification $\ell=m$. Let us restore physical units for the speed of light c, the gravitational constant G, and Planck's constant h. Then (5.7) corresponds to the shift from gravitational ''units,'' to quantum ''units,'' where the extra coordinate in (5.7), (5.8) is given, respectively, by

$$\ell=\frac{Gm}{c^2},\quad \ell=\frac{h}{mc}. \tag{5.10}$$

There is nothing really fundamental about the presence of the dimensional constants here. Dimensional analysis is an elementary group-theoretic technique based on the Pi theorem.[50–52] The purpose of c, G, and h in (5.10) is merely to transpose the dimensions of mass to length so that it can be geometrized. And since the dimensions of these quantities are LT^{-1}, $M^{-1}L^3T^{-2}$, and ML^2T^{-1} and are not degenerate,[51] they can all be set to unity as is the common practice. This said, it is convenient to rename the pure canonical metric (5.7) the Einstein gauge and its other form (5.8) the Planck gauge.

The dynamics in these gauges can be studied for (5.7) by using (3.12)–(3.17), and for both (5.7) and (5.8) by using (4.6) and (4.7). As an illustration, let us revisit the short calculation which

led to (4.8) but now in both gauges. That is, we take $g_{\alpha\beta}=(L/\ell)^{2a}\eta_{\alpha\beta}$ so $\partial g_{\alpha\beta}/\partial\ell=-(2a/\ell)g_{\alpha\beta}$ and $u^\alpha u^\beta\partial g_{\alpha\beta}/\partial\ell=-2a/\ell$, which causes the 4D equation of motion (4.7) with the parallel force (4.6) to read

$$\frac{du^\mu}{ds}=P^\mu=-\frac{u^\mu}{2}\left(u^\alpha u^\beta\frac{\partial g_{\alpha\beta}}{\partial\ell}\right)\frac{d\ell}{ds}=\frac{au^\mu}{\ell}\frac{d\ell}{ds}. \tag{5.11}$$

This yields $u^\mu=(\ell/\ell_0)^a$, where ℓ_0 is a constant of the 4D motion. Alternatively, Eq. (5.11) can be written as

$$d(\ell^{-a}u^\mu)=0. \tag{5.12}$$

This says that in the Einstein gauge ($a=-1$) ℓu^μ is conserved, while in the Planck gauge ($a=+1$) u^μ/ℓ is conserved. That is, by (5.10), the conserved quantities are the classical momentum $(G/c^2)mu^\mu$ and the quantum momentum or inverse de Broglie wavelength $(c/h)mu^\mu$. These are as expected, but as before in both quantities $m=m(s)$ in general. If as in (4.9) we take a null 5D geodesic, (5.2) gives

$$dS^2=0=\left(\frac{L}{\ell}\right)^{2a}ds^2-\left(\frac{L}{\ell}\right)^{4b}d\ell^2. \tag{5.13}$$

This yields for *both* gauges

$$\ell=\ell_0 e^{\pm s/L}=\ell_0\exp[\pm(\Lambda/3)^{1/2}s], \tag{5.14}$$

which is the same as (4.10) and has similar implications for mass variation.

This process is intrinsic to 5D dynamics and warrants a closer examination, because it opens the way to understanding the Heisenberg uncertainty relation. The latter is not a part of classical 4D dynamics, and neither is the parallel 4D acceleration P^μ derived previously. This was calculated from the canonical metric (2.1) in (3.15) and has an associated scalar power per unit (inertial) mass (3.16), but was also calculated from the normalization condition (4.1) in (4.6) where it was found to be of general form. This agrees with the Hamiltonian approach to Kaluza–Klein theory, where a $(4+1)$ split can always be performed in order to recover Einstein theory.[53–55] In the Einstein and Planck gauges, P^μ has the form (5.11), whose associated scalar is $P^\mu u_\mu=(a/\ell)d\ell/ds$ where $a=\pm1$. This quantity has no analog in conventional classical dynamics, whose forces as noted before obey $F^\mu u_\mu=0$. However, an observer could interpret P^μ as causing an anomalous change in momentum $d\overline{p}^\mu$, such that by (5.11)

$$\frac{1}{m}\frac{d\overline{p}^\mu}{ds}=P^\mu=\frac{au^\mu}{\ell}\frac{d\ell}{ds}. \tag{5.15}$$

This implies the associated scalar quantity

$$dx_\mu d\overline{p}^\mu=\frac{am}{\ell}d\ell\,ds. \tag{5.16}$$

For both the Einstein gauge and the Planck gauge, this reads

$$dx_\mu d\overline{p}^\mu=-dm\,ds. \tag{5.17}$$

That is, there is a Heinsenberg-type relation in 4D which depends on the mass change associated with 5D. The relation (5.17) is general, insofar as no use has been made of (5.14) for $m=m(s)$ which follows from (5.13) for a null 5D geodesic. The generality of (5.17) may also be appreciated by recalling from previous work that the momentum is really conserved along a 5D path, so

$d(mu^\mu)=0$ or $m\,du^\mu+u^\mu\,dm=0$, where the second term represents an anomalous change in momentum $d\bar{p}^\mu=-u^\mu\,dm$, so there is a scalar $dx_\mu d\bar{p}^\mu=-dx_\mu(dx^\mu/ds)dm=-dm\,ds$.

Let us now ask how a 5D null path with $dS^2=0$ relates to the motion of a particle of mass m moving along a 4D timelike path with $ds^2>0$. We work in the Planck gauge with conventional units. Then (5.14) gives $dm=\pm L^{-1}m\,ds$, and (5.17) may be written

$$dx_\mu d\bar{p}^\mu=\frac{(mc\,ds)^2}{h}\left(\frac{\ell}{L}\right). \tag{5.18}$$

The first term in parentheses here is the 4D action, which as usual is defined and quantized for integers n via

$$I\equiv\int mc\,ds,\quad dI=nh. \tag{5.19}$$

The second term in parentheses in (5.18) is the ratio of the Compton wavelength of the particle $l=h/mc$ and the characteristic dimension of the four-space it inhabits $L=(3/\Lambda)^{1/2}$. Now the 5D null condition (5.13) in the Planck gauge ($a=1$, $b=1$) shows that if the 4D action is quantized via (5.19) then so is the extra part of the 5D line element. We therefore put $L/\ell=n$, which says that the Compton wavelength is an excitation of the fundamental mode. The result is that (5.18) reads

$$dx_\mu d\bar{p}^\mu=nh, \tag{5.20}$$

which is Heisenberg's relation. The above-mentioned approach can clearly be generalized to other box sizes. But if free particles have masses set by the energy density of the vacuum,[26] constraints on the cosmological constant[41–43] show that mass is quantized in units of

$$m=\frac{h}{cL}=\frac{h}{c}\left(\frac{\Lambda}{3}\right)^{1/2}\lesssim 10^{-65}g. \tag{5.21}$$

This is too small to detect with current methods, and miniscule compared to the so-called Planck mass $(hc/G)^{1/2}\approx 10^{-5}$ g, which is seen to be an artifact produced by a mixture of the Einstein and Planck gauges discussed in this section.

VI. WAVES IN $N(>4)$D THEORY

Section V showed that Heisenberg's relation follows as a consequence of the extra force which results when a causal 4D manifold is extended to a null 5D one. It is therefore natural to ask if other aspects of particles, including their wave nature, can be understood as manifestations of an $N(>4)$-dimensional space. That quantum field theory and general relativity are in principle compatible has been shown by work on the Hartle-Hawking and Vilenkin wave functions.[56–58] And exact solutions of Einstein's equations are known which can describe nongravitational waves.[30,46,59–64] There is of course the potential problem that the metric may be complex,[65–70] but this can be avoided if the view is taken that only the physically relevant quantities calculated from it need to be real.[30,46,64] In this section we will therefore proceed to see if it is possible to set up a consistent framework for 4D wave mechanics in $N(>4)$D theory, concentrating as before on the 5D case.

The 4D Klein–Gordon equation for a relativistic particle with zero spin and finite mass should be derivable, based on what has been shown previously, from the 5D equation for a null geodesic. However, since the Klein–Gordon equation is a second-order relation in a complex wave function, we take the line element to have signature $(+----)$. Then

$$dS^2=0=\left(\frac{L}{\ell}\right)^{2a}ds^2+\left(\frac{L}{\ell}\right)^{4b}d\ell^2, \tag{6.1}$$

where $g_{\alpha\beta}=(L/\ell)^{2a}\overline{g}_{\alpha\beta}dx^\alpha dx^\beta$ and $a=(-1,+1)$ with $b=(0,+1)$ for the Einstein and Planck gauges as before. The last relation is satisfied by

$$\ell=\ell_0 e^{\pm is/L}, \tag{6.2}$$

which is the complex analog of (4.10). The mass (squared) involves $\ell\ell^*=\ell_0^2$ and is constant and real. Without loss of generality we can take the upper sign in (6.2) and define a dimensionless wave function

$$\psi=e^{is/L}. \tag{6.3}$$

This satisfies a hierachy of wave equations

$$\frac{d^n\psi}{ds^n}=\left(\frac{i}{L}\right)^n\psi, \tag{6.4}$$

where we are interested primarily in the cases $n=1, 2$. [The n in (6.4) should not be confused with that in (5.19).] The first-order equation of (6.4) implies $i\psi/L=dx/ds=(\partial\psi/\partial x^\alpha)(dx^\alpha/ds)=(\partial\psi/\partial x^\alpha)u^\alpha$ or $1=(L/i\psi)(\partial\psi/\partial x^\alpha)u^\alpha$. But $1=u^\alpha u_\alpha$, so

$$u_\alpha=\frac{L}{i\psi}\frac{\partial\psi}{\partial x^\alpha}. \tag{6.5}$$

This for the fundamental mode of the Planck gauge with $L=h/mc$ just says $p_\alpha=(h/ic\psi)\partial\psi/\partial x^\alpha$, which is the usual prescription for obtaining the momenta from the wave function. The second-order equation of (6.4) can be treated similarly, and with (6.5) yields

$$\frac{u^\alpha u^\beta}{\psi}\frac{\partial^2\psi}{\partial x^\alpha\partial x^\beta}+\frac{1}{L^2}+\frac{iu_\alpha}{L}\frac{du^\alpha}{ds}=0. \tag{6.6}$$

The imaginary part of this is $u_\alpha du^\alpha/ds=0$ or the usual orthogonality relation. The parallel acceleration (4.6) or (5.11) which follows from the metric in form (5.2) does not appear, which agrees with the fact that the effective mass is a constant for the metric in form (6.1). In this regard, it is instructive to consider the geodesic equation $dU^\mu/d\lambda+\Gamma^\mu_{\beta\gamma}U^\beta U^\gamma=0$ with $U^\alpha\equiv dx^\alpha/d\lambda$, $d\lambda=e^{\mp is/L}ds$ and $\Gamma^\mu_{\beta\gamma}$ constructed from $g_{\alpha\beta}=(L/\ell)^{\pm1}\overline{g}_{\alpha\beta}$, as implied by (6.1). This geodesic, it may be verified, splits naturally into real and imaginary parts:

$$\frac{du^\mu}{ds}+\overline{\Gamma}^\mu_{\beta\gamma}u^\beta u^\gamma=0, \tag{6.7}$$

$$u^\mu=\overline{g}^{\mu\alpha}\left(\overline{g}_{\alpha\gamma}\frac{\partial s}{\partial x^\beta}+\overline{g}_{\alpha\beta}\frac{\partial s}{\partial x^\gamma}-\overline{g}_{\gamma\beta}\frac{\partial s}{\partial x^\alpha}\right)u^\beta u^\gamma. \tag{6.8}$$

Here $u^\mu\equiv dx^\mu/ds$ and $\overline{\Gamma}^\mu_{\beta\gamma}$ is constructed from $\overline{g}_{\alpha\beta}$. We see from (6.7) that the motion is geodesic in the embedded four-space. And (6.8) is identically satisfied if $s=\int u_\alpha dx^\alpha$ so $\partial s/\partial x^\alpha=u_\alpha$ as usual for the four-interval. In other words, the 4D dynamics is standard. Returning now to (6.6), its real part may be rewritten by noting that $u^\alpha u^\beta\partial^2\psi/\partial x^\alpha\partial x^\beta=\overline{g}^{\alpha\beta}\partial^2\psi/\partial x^\alpha\partial x^\beta$, which can be shown using (6.5) and $u^\alpha u_\alpha=1$. Then for the fundamental mode of the Planck gauge, the real part of (6.6) reads

$$\overline{g}^{\alpha\beta}\frac{\partial^2\psi}{\partial x^\alpha \partial x^\beta}+\frac{m^2c^2\psi}{L^2}=0. \tag{6.9}$$

This is the standard 4D Klein–Gordon equation.

The preceding paragraph started with the complex metric (6.1) and ended with the relativistic wave equation (6.9). Both are statements about dynamics, and neither uses the field equations. Solutions of the latter of relevant type were mentioned previously.[30,46,59–64] It would be inappropriately long to discuss these here; but to show that there is a match between the dynamics and the field equations, let us take the metric (6.1) in the Planck gauge ($a=1$, $b=1$) and consider the 5D field equations $R_{AB}=0(A,B=0,1,2,3,4)$. The latter may be shown to be satisfied, either tardily using algebra[39] or quickly using a computer package,[71] by

$$dS^2=\left(\frac{L}{\ell}\right)^2(dt^2-e^{i(\omega t+k_x x)}dx^2-e^{i(\omega t+k_y y)}dy^2-e^{i(\omega t+k_z z)}dz^2)+\left(\frac{L}{\ell}\right)^4 d\ell^2. \tag{6.10}$$

Here k_{xyz} are arbitrary wave numbers along the Cartesian axes and ω is a frequency fixed by the field equations as $\omega=\pm 2/L$. This solution may be regarded as the canonical one in 5D, since not only does the Ricci tensor R_{AB} vanish but the Riemann tensor R_{ABCD} does also. That is, (6.10) describes a wave propogating in the 4D part of a *flat* 5D manifold. However, the 4D part of (6.10) is *curved*. In the induced-matter picture,[14] it is curved by a cosmological constant $\Lambda=-3\ell^2/L^4$. If the latter is modeled as in general relativity by a classical pressure and density, the wave in 4D is supported by a medium with the equation of state $8\pi p=-8\pi\rho=-\Lambda=3\ell^2/L^4$ typical of the classical vacuum. Another way of appreciating what is involved here is by considering the extra coordinate ℓ, or equivalently the inertial rest mass of the particle m. By (6.2), ℓ oscillates in and out of the 4D space–time hypersurface defined by s. The average value of ℓ is zero, agreeing with the fact that R_{ABCD} describes a flat 5D manifold; but the average value of its square is finite, agreeing with the fact that the 4D manifold is curved. By (6.10) directly, or by (5.6) modulo a sign due to the change in signature from (5.2) to (6.1), the 4D Ricci scalar is

$$R=\frac{12\ell^2}{L^4}=\frac{12m^2c^2}{h^2}. \tag{6.11}$$

Here we have put $\ell=L=h/mc$ for the fundamental mode in the Planck gauge. The last relation just says that the scalar curvature of the 4D space is set by the Compton wavelength or mass of the particle which inhabits it. This agrees with Mach's principle,[14] and with the idea from inflationary quantum field theory that particles are intrinsically massless.[26] There is no contradiction, as long as the view is taken that particles with finite rest mass are 4D objects in a 5D vacuum.

The generalization of the above is expected to be straightforward, both for spin-1/2 particles described by the Dirac equation in 5D[72,73] and spin-0 particles described by scalar wave equations in ND.[14,74] In the latter context, it is clear that the defining equation for classical dynamics in terms of the N velocities should be $U^A U_A=0$. The corresponding quantum wave function can be derived from the metric as fixed by solutions of $R_{AB}=0(A,B=0,1,2,3,\ldots,N)$. Probabilities should be defined from the metric using the element of proper volume $(|g|)^{1/2}dx^N$, so $|g|$ will be a nontrivial factor. [This is already evident in 5D from metrics like (6.10), where the 4D wave function may be augmented by g_{44} to yield a 5D one whose extra component will be related to the spectrum of particle masses.] It is expected that these issues will be reported on in the future.

VII. CONCLUSION

In Sec. II, we noted that the canonical 5D metric (2.1) justifies its name by providing a basis for $N(>4)$D geodesics and leading to many useful results. The utility of the canonical (or warp) metric can be understood as a result of embeddings, which on 4D hypersurfaces reduce to physically acceptable solutions for cosmology (3.6) and the one-body problem (3.7). However, as shown elsewhere in Sec. III, its efficacy is mainly due to the fact that it converts a *coordinate*

space to a *momentum* space, *with the extra coordinate playing the role of rest mass even for null 5D geodesics*. In general, the velocity in the extra dimension results in a new inertial force (per unit mass) given by (3.15). This and its associated power (per unit mass) given by (3.16) have no analog in conventional 4D dynamics. The same is true of any nontrivial ND manifold. In Sec. IV, it was seen that the normalization condition (4.1) results in an extra acceleration parallel to the four-velocity which has the form (4.6) independent of the coordinate system. This can most logically be handled by connecting it to the change in the (inertial) rest mass of the particle which feels it, which means that the 4D motion is technically nongeodesic in the four-velocity (4.7), even though it agrees with the conventional law for the conservation of the four-momentum as applied (say) to the motion of a rocket (4.8). However, the rate of variation of mass in the Minkowski limit is set by the cosmological constant as in (4.11) and is tiny, so for apparently free particles there is no conflict with observed dynamics. In Sec. V, the field equations (5.1) were used to constrain the form of a generalized canonical metric (5.2), leading to the recognition of two natural choices for the extra coordinate in (5.7) and (5.8). These are related by an elementary coordinate transformation (5.9), whose physical meaning is however significant: classical physics uses the gravitational constant of Newton or Einstein to geometrize the mass, while quantum physics uses Planck's constant to geometrize the mass, as in (5.10). That is, classical and quantum dynamics in 4D are descriptions of 5D dynamics in what can be termed the Einstein and Planck gauges. In both gauges, the extra or parallel force (per unit mass) of (5.15) leads to a relation between the increments in the coordinates and momenta (5.17) which is reminiscent of Heisenberg's relation. Further study confirms that the extra force—which is inertial is the Einstein sense of coming from the motion in the (extra part of the) coordinate frame—results in Heisenberg's uncertainty relation (5.20). A corollary of this is that the inertial rest mass of a particle is quantized, though the unit is set by the cosmological constant and is less than 10^{-65} g by (5.21) and so too small to be observed using current methods. These results prompted the brief study in Sec. VI of waves in $N(>4)$D. In 5D, what is in effect a Wick rotation of the extra part of the null metric (6.1) was found to lead to a wave function (6.3) which satisfies a hierachy of wave equations (6.4). The first of these, (6.5), is a restatement of the standard prescription for the derivation of four-momenta from a wave function. The second, (6.6), splits naturally into two parts, of which one is a restatement of the geodesic equation of classical theory (6.7), while the other is equivalent to the Klein–Gordon equation of relativistic quantum theory (6.9). It should be noted that the latter was derived without the use of operators, and of course contains the Schrödinger equation in the nonrelativistic limit. More importantly, it should be noted that solutions of the 5D field equations exist which have complex metrics but which result (because of the structure of the field equations) in measurable quantities which are real. An example is (6.10), which is the canonical solution for a wave in a 5D manifold. It describes an oscillation of the extra coordinate in and out of the hypersurface called space–time. The mass of the particle associated with the wave also oscillates, with a mean value which is zero, in accordance with inflationary quantum field theory and the flatness of the 5D manifold. However, the square of the mass is finite and in fact set by (6.11), which says that the square of the inverse Compton wavelength of the particle is proportional to the Ricci scalar of the embedded and curved 4D manifold. This last property is manifestly Machian, and is expected to be generic to $N(>4)$D manifolds which contain submanifolds that proscribe the 4D ''boxes'' which particles inhabit. The general prescription for dynamics in N-dimensional spaces would appear to be a null product of N-vectors (specifying the coordinate velocities in the classical case or the wave numbers in the quantum case). This means that particles are in causal contact in ND even though they appear to be out of contact in 4D, so there are obvious implications for the Aharanov–Bohm effect and the double-slit experiment. These phenomena, and other consequences for membranes and strings especially, will surely repay further investigation.

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dedicated to the memory of Professor J. Moriaty, whose monograph *The Dynamics of an Asteroid* ''ascends to such rarefied heights of pure mathematics that it is said that there was no man in the scientific press capable of criticizing it.'' [75]

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Global prescribed mean curvature foliations in cosmological space–times. I

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This work investigates some global questions about cosmological space–times with two-dimensional spherical, plane, and hyperbolic symmetry containing ''well-behaved'' matter. The result is that these space–times admit a global foliation by prescribed mean curvature surfaces, which extends at least toward a crushing singularity. The time function of the foliation is geometrically defined and unique up to the choice of an initial Cauchy surface. This work generalizes a similar analysis on constant mean curvature foliations and avoids the topological obstructions arising from the existence problem. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The flavor of General Relativity viewed as an initial value problem for the field equations is based on the geometrical nature of the equations, which implies the diffeomorphism invariance and the absence of a metric background structure. This has consequences for spacelike foliations, in that the time function of a foliation is not canonical, but arbitrary unless it is tied to some geometrical quantity. The latter would turn the analysis of the global structure of space–times into an investigation of the asymptotic behavior of such a foliation.

In space–times with certain symmetries some global foliations, defined by time coordinates tied to the symmetries, are known, e.g., Rein (1996), Andréasson (1999).

A geometrically defined foliation which does not depend on the symmetries are the well-known constant mean curvature (CMC) foliations, where the time coordinate is given by the mean curvature of the leaves, which varies continuously from leaf to leaf, see Rendall (1996) for a survey of this topic and Rendall (1995b), Rendall (1997c) for foliations of space–times with symmetries.

Unfortunately the CMC constructions suffer from the existence problem, which is unsolved in general. To overcome this difficulty, a foliation with leaves of prescribed mean curvature (PMC) has been constructed at least locally in time in (Henkel, 2001b) for cosmological space–times. The prescription is given implicitly, letting the mean curvature vary continuously along the normal vector field of the foliation relative to a given Cauchy surface. The time function of the foliation is geometrically defined and turns out to be intrinsic, in that coupled to Einstein's field equations adapted to the leaves, one obtains Cauchy data for space–times foliated by PMC leaves.

The aim of the present paper is to globalize this result for certain space–times. Motivated by the method in Rendall (1995a), where satisfying results about cosmic censorship have been obtained for spatially homogeneous models, I consider here cosmological space–times with two-dimensional spherical, plane, and hyperbolic symmetry. This choice is the first step of successively lowering the degree of symmetry to obtain more and more general results. I focus on the following questions: How large is the maximal interval for the time function and does this maximal foliation cover the whole space–time?

One guideline taken from Rendall (1995a) is that the foliation may be extendible as long as

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the mean curvature of the leaves remains finite. We will see that this principle stays true with some modifications.

Another important aspect for the construction of global foliations is the choice of an appropriate matter model. The key requirements for the matter fields are their regularity in a regular geometric background as well as some energy conditions. These requirements are not trivially satisfied, since the former rules out matter such as the perfect fluid, which is known to develop singularities (shocks) in a regular geometric background. For dust it has been shown in Rendall (1997b) and Isenberg (1998) that there is no way to construct a global CMC foliation which covers the whole dust-filled cosmological space–time. These counterexamples dramatically emphasize the importance of choosing appropriate matter models. Furthermore demanding energy conditions seems natural and obvious, but we will see, that the non-negative pressures condition plays a special role in the improvements in Sec. III E.

Section II fixes notation and states some basic definitions. We attack the main questions in Sec. III, following closely the treatment in Rendall (1995b). The results will be discussed in Sec. IV.

II. BASIC DEFINITIONS AND FORMULAS

A. Space–times and foliations

A space–time is a pair (M,g), where M denotes a four-dimensional smooth and orientable Lorentz manifold with metric g and signature $(-+++)$. The metric induces the Levi-Civita connection ${}^4\nabla$ on M. If $\{X_\alpha\}$ denotes a local basis of vector fields on M, we define the connection coefficients ${}^4C^\gamma_{\alpha\beta}$ relative to this basis by ${}^4\nabla_{X_\alpha}X_\beta={}^4C^\gamma_{\alpha\beta}X_\gamma$ and we get the Christoffel symbols ${}^4\Gamma$ and Ricci rotation coefficients ${}^4\gamma$ by specializing to a coordinate basis or an orthonormal frame, respectively. The sign convention for the curvature is fixed by the definition ${}^4R(X,Y)Z := {}^4\nabla_X{}^4\nabla_Y Z-{}^4\nabla_Y{}^4\nabla_X Z-{}^4\nabla_{[X,Y]}Z$, where X, Y Z are vector fields. The curvature tensor is then defined as ${}^4R(W,Z,X,Y):=g(W,{}^4R(X,Y)Z)$ with Ricci tensor ${}^4R_{\alpha\beta}={}^4R^\mu_{\alpha\mu\beta}$ and scalar curvature ${}^4R={}^4R^\mu_\mu$, written in abstract index notation of the Ricci calculus.

Then the Einstein tensor reads $G_{\alpha\beta}={}^4R_{\alpha\beta}-\frac{1}{2}{}^4Rg_{\alpha\beta}$ and the field equations are $G_{\alpha\beta}=8\pi T_{\alpha\beta}$ or equivalently ${}^4R_{\alpha\beta}=8\pi(T_{\alpha\beta}-\frac{1}{2}(\mathrm{tr}\,T)g_{\alpha\beta})$, where $T_{\alpha\beta}$ denotes the energy momentum tensor of the matter fields. The matter quantities are the energy density $\rho:=T_{\mu\nu}n^\mu n^\nu$, the momentum density $j_\beta:=-T_{\mu\nu}n^\mu h^\nu_\beta$ and the stress tensor $S_{\alpha\beta}:=T_{\mu\nu}h^\mu_\alpha h^\nu_\beta$ with respect to an observer, represented by a unit timelike vector n, where $h_{\alpha\beta}:=g_{\alpha\beta}+n_\alpha n_\beta$ denotes the orthogonal projector on $\{n\}^\perp$ in covariant notation.

Einstein's field equations in vacuum ($T_{\alpha\beta}=0$) have a well-posed Cauchy problem in harmonic coordinates, thus one obtains space–times as solutions of Einstein's field equations with matter, whenever the equations describing the matter fields and the energy momentum tensor couple to the field equations in harmonic coordinates, such that the Cauchy problem remains well posed. We will see examples in Sec. II B (compare Wald, 1984 and Friedrich and Rendall, 2000) for an introduction/analysis of the Cauchy problem for Einstein's equations.

In this work we confine ourselves to *cosmological* solutions (M,g) of Einstein's field equations. Due to Bartnik (1988) these are globally hyperbolic and spatially compact space–times, where the Ricci tensor contracted twice with any timelike vector is non-negative (timelike convergence condition). This last condition can be reexpressed in terms of the matter variables as $\rho+\mathrm{tr}\,S\geqslant 0$ for any observer, which is the strong energy condition.

Now let us pay attention to an additional structure. A foliation $\{S_t\}$, $t\in I\subset\mathbb{R}$ (I interval containing zero) of (a part of) (M,g) by spacelike hypersurfaces induces on each leaf the unit normal vector field n, the metric $h_{\alpha\beta}=g_{\alpha\beta}+n_\alpha n_\beta$, which also serves as orthogonal projection and the second fundamental form $k_{\alpha\beta}:=-h^\mu_\alpha h^\nu_\beta{}^4\nabla_\mu n_\nu$ (the definition of $k_{\alpha\beta}$ fixes the sign conventions used in this work). The second fundamental form is a symmetric tensor, intrinsic to the leaves of the foliation, and can also be written as the Lie derivative of the three-metric h with respect to the normal vector field, $k_{\alpha\beta}=-\frac{1}{2}\mathcal{L}_n h_{\alpha\beta}$. The three-metric determines further geometri-

cal objects on the leaves, such as the Levi-Civita connection ∇, the Christoffel symbols Γ, the Ricci rotation coefficients γ, and the curvature tensor $R(\cdot)$. Tensors intrinsic to the leaves of the foliation will carry Latin indices in the abstract index notation.

The parameter t of the foliation has timelike gradient and thus can be regarded as (coordinate) time. Given local coordinates (x^i) on S_0, we can Lie-transport them to neighboring leaves along an arbitrary family of transversal curves, parametrized by x. We will express equations containing coordinate components with respect to the adapted coordinates (t,x).

The lapse function N and the shift vector $\nu \perp n$ on the leaves are defined by $\partial_t = Nn + \nu$, thus $N = -g(\partial_t, n)$ and $\nu = \partial_t - Nn$. Then we have $1 = \mathrm{d}t(\partial_t) = N\,\mathrm{d}t(n)$. Further, $\mathrm{d}t$ is (co-)orthogonal to the leaves and if we denote the conormal of the leaves by σ we see that $\mathrm{d}t = -N^{-1}\sigma$ or $\sigma = -N\,\mathrm{d}t$, thus N^{-1} measures the length of $\mathrm{d}t$.

The most common example involving the lapse function is the event horizon in Schwarzschild space–time, where the coordinate time explodes along the worldline of infalling observers n, thus N^{-1} explodes or $N \to 0$. In this work we will be faced with a complementary scenario, where we have to ensure that the lapse function does not explode, corresponding to the phenomena of recollapse, where coordinate time freezes as $\mathrm{d}t \to 0$. If this occurs, one could try to reparametrize the foliation by setting $\tilde{t} = f(t)$ for some monotone function f and one gets $\mathrm{d}\tilde{t} = f'(t)\mathrm{d}t$,

$$\tilde{N} = \frac{1}{f'(t)} N = \frac{\mathrm{d}t}{\mathrm{d}\tilde{t}} N,$$

and the same relation holds for shift.

The $3+1$ split of the space–time geometry by means of lapse and shift ends up in the $3+1$ form of the field equations. The constraint equations are

$$R + H^2 - |K|^2 = 16\pi\rho \quad \text{(Hamiltonian constraint)}, \tag{1a}$$

$$\nabla^j k_{ij} - \nabla_i H = 8\pi j_i \quad \text{(momentum constraint)}, \tag{1b}$$

with $|k|^2 = k_{\alpha\beta}k^{\alpha\beta}$ and $H = \mathrm{tr}\,k$ denotes the mean curvature of the leaves. The Arnowitt–Deser–Misner (ADM) equations read

$$\partial_t h_{ij} = -2Nk_{ij} + \nabla_i \nu_j + \nabla_j \nu_i, \tag{2a}$$

$$\begin{aligned}\partial_t k_{ij} = &-\nabla_i\nabla_j N + N(R_{ij} + Hk_{ij} - 2k_i^r k_{rj} - 8\pi(S_{ij} + \tfrac{1}{2}(\rho - \mathrm{tr}\,S)h_{ij})) \\ &+ \nu^r \nabla_r k_{ij} + k_{rj}\nabla_i \nu^r + k_{ir}\nabla_j \nu^r.\end{aligned} \tag{2b}$$

Taking the trace of the second equation and eliminating the scalar curvature R by the Hamiltonian constraint we obtain the lapse equation

$$\Delta N + N(|k|^2 + 4\pi(\rho + \mathrm{tr}\,S)) = (\partial_t - \nu)H, \tag{3}$$

which serves as a constraint of the foliation. Note that in cosmological space–times the term in brackets is always non-negative. If it turns out to be nonvanishing, then the left-hand side of (3) can be shown to be an isomorphic mapping of N, considered as an element of some Sobolev space H^s into H^{s-2}. This observation motivates the following

Definition 2.1: A *prescribed mean curvature (PMC) foliation* is defined to be a foliation $\{S_t\}$ satisfying (3), with

$$(\partial_t - \nu)H = Nn(H) := 1, \tag{4}$$

thus the mean curvature of the leaves is forced to vary uniformly along the normals of the leaves. In Henkel (2001b) I proved the following local in time result:

Theorem 2.2: *Let (M,g) be a smooth, globally hyperbolic space–time, obeying the strong energy condition, with compact Cauchy surface* Σ *and*

$$\lambda = |k|^2 + 4\pi(\rho + \operatorname{tr} S) \tag{5}$$

does not vanish identically on Σ. *Then there exists a* $T>0$ *and a unique smooth PMC foliation* $\{S_t\}$, $t \in [-T,T]$ *in* (M,g), *with* $\Sigma = S_0$.

Note that the setting here is quite general, no symmetry assumptions have to be made, and essentially the strong energy condition turns out to be sufficient for the local in time existence of a unique PMC foliation up to the choice of an initial Cauchy surface.

The aim of the present paper is to globalize the result. Here are two problems involved: How large is the interval of values taken by the time coordinate and does the global foliation then cover the whole space–time? To answer these questions in general there seem to be no techniques available up to now. One strategy to obtain global results is to study first space–times with some spatial symmetry, taking advantage of the simplifications of the equations. Then the hope is that the techniques developed in these cases give insight into the nature of more general classes of space–times, by successively lowering the degree of symmetry. Here we will focus on space–times with two-dimensional spacelike orbits of symmetry and three (local) Killing vector fields. In the second part of this paper we will consider space–times with two commuting (local) Killing vector fields. These cases are indeed the first steps of this program, since the initial analysis for locally spatially homogeneous space–times has already been done and leads to very strong results (see Rendall, 1995a) for the exact analysis or Henkel (2001a) for an overview about the results in the present context.

B. Matter models

Before getting deeper into the analysis just motivated I introduce some matter models and their coupling to the Einstein equations, with special emphasis on the Cauchy problem. Since energy conditions will play an important role in the estimates we perform later on, I assemble the relevant ones for the present work first.

(1) The dominant energy condition. Its statement is that for all orthonormal frames $\{{}^4e_\alpha\}$ with ${}^4e_0$ timelike

$$T({}^4e_0, {}^4e_0) \geqslant |T({}^4e_\alpha, {}^4e_\beta)|.$$

Another formulation of this condition is, that for any observer, the local energy density ρ is non-negative and the momentum density j is nonspacelike, thus "matter cannot travel faster than light," a statement that can be proved rigorously (see, e.g., Sec. 4.3 of Hawking (1973)), leading to the result that if the energy momentum tensor obeys the dominant energy condition and vanishes on a set S, then it vanishes on the whole Cauchy development $D(S)$ of the set, thus $D(S)$ is a vacuum space–time.

(2) The strong energy condition states that for all timelike vectors v the inequality

$$T(v,v) \geqslant \tfrac{1}{2}(\operatorname{tr} T) g(v,v)$$

holds, or equivalently for any observer $\rho + \operatorname{tr} S \geqslant 0$, thus the stresses do not become too negative. Another formulation is ${}^4R(v,v) \geqslant 0$, also known as the timelike convergence condition, which contributes to the expansion of timelike geodesic congruences a negative term, thus shifting the balance toward contraction to a final singularity of the congruence. Hawking's famous singularity theorems then guarantee geodesic incompleteness in the past provided further the existence of a Cauchy surface with uniform negative mean curvature.

We already used the strong energy condition as an integral part in the definition of cosmological space–times and its meaning for foliations.

(3) The non-negative pressures condition demands the stress tensor S to be positive definite. This condition ensures in some sense that the pressures contribute more to attraction than to

repulsion, leading to a finite lifetime of the space–time under certain circumstances. This somewhat unexpected behavior is a true relativistic effect, which does not have a Newtonian counterpart.

1. The Maxwell equations

The Maxwell field is described by a two-form F, subject to the Maxwell equations

$$dF=0\Leftrightarrow {}^4\nabla_{[k}F_{\mu\nu]}=0, \tag{6a}$$

$$d\star F=4\pi\star J\Leftrightarrow {}^4\nabla_\mu F^{\alpha\mu}=4\pi J^\alpha, \tag{6b}$$

where J denotes the electromagnetic charge current density. Alternatively the covariant derivatives can be replaced by ordinary derivatives.

It is well known that the Maxwell equations admit (locally) a reformulation in terms of the vector potential A, a one-form with $\mathrm{d}A=F$. Then the remaining inhomogeneous equation reads ${}^4\nabla^\mu{}^4\nabla_\alpha A_\mu-{}^4\nabla^\mu{}^4\nabla_\mu A_\alpha=4\pi J_\alpha$. Fixing the gauge invariance of the equation by the Lorentz gauge, we obtain the system

$${}^4\nabla^\mu A_\mu=0 \quad \text{(Lorentz-gauge)}, \tag{7a}$$

$$\Box A_\alpha=4\pi J_\alpha-R_{\alpha\mu}A^\mu, \tag{7b}$$

with $\Box=-{}^4\nabla^\mu{}^4\nabla_\mu$ and the curvature term arises as a consequence of some commutations of derivative operators. In this formulation the second equation is a wave equation, and hence can be brought into first-order symmetric hyperbolic form, if the source term is appropriate. Thus we get local existence and uniqueness for this equation in a given space–time. One can further show then that the Lorentz gauge propagates and we indeed get a unique local solution of the Maxwell equations. Spatially global solution can be obtained by the usual patching argument, arising from localizing the equation with respect to an appropriate partition of unity of the initial data on some Cauchy surface.

Given an electromagnetic field F we can form the associated energy momentum tensor E, defined as

$$E_{\alpha\beta}=\frac{1}{4\pi}\left(F_{\alpha\mu}F_\beta{}^\mu-\tfrac{1}{4}|F|^2 g_{\alpha\beta}\right), \tag{8}$$

where $|F|^2=F^{\mu\nu}F_{\mu\nu}$.

E is trace-free, satisfies the relation ${}^4\nabla_\mu E^{\alpha\mu}=-F^\alpha{}_\mu J^\mu$ and the dominant and strong energy conditions hold.

Since the Maxwell equations turn out to be symmetric hyperbolic at least locally, we can couple them to the Einstein equation to get a symmetric hyperbolic system of equations in harmonic coordinates. Thus we end up with a well-posed Cauchy problem for the Einstein–Maxwell system, as long as the electromagnetic charge current density is in appropriate form.

2. The Vlasov equation

The Vlasov equation is a model for a collisionless gas. It describes the motion of a huge number of structureless particles in space–time. We need only the case where the particles have unit mass, where the equation is composed of a non-negative function f, defined on the mass shell of particles of mass one $P:=\{v\in TM\,|\,g(v,v)=-1,\ \text{future pointing}\}$, representing the particle distribution, and a geodesic spray X on P. The equation reads

$$X(f)=0 \tag{9a}$$

with

$$X = p^\mu \partial_\mu - {}^4\Gamma^k_{\mu\nu} p^\mu p^\nu \frac{\partial}{\partial p^k} = v^\alpha {}^4e_\alpha - {}^4\gamma^k_{\mu\nu} v^\mu v^\nu \frac{\partial}{\partial v^k}, \tag{9b}$$

where p^μ denotes the components of the momentum of the particles with respect to the given coordinates and v^α are the components of the momentum with respect to an orthonormal frame. They are related by $p^\mu = ({}^4e_\alpha)^\mu v^\alpha$ and on the mass shell p^0 is determined by the components p^i and $v^0 = \sqrt{1 + \delta_{ij} v^i v^j}$.

Inserting the definition ${}^4e_\alpha = ({}^4e_\alpha)^\mu \partial_\mu$ and doing a $3+1$ decomposition (with the exception that we do not write down the explicit expression for ${}^4\gamma^k_{0j}$) we can reformulate the Vlasov equation as

$$\begin{aligned} 0 = {} & \partial_t f + \left(N \frac{v^j}{v^0} (e_j)^i - \nu^i \right) \partial_i f \\ & - \left(e_i(N) v^0 + N(-k_{rs}(e_i)^r (e_j)^s + \delta_{ik} {}^4\gamma^k_{0j}) v^j + N \delta_{ik} \gamma^k_{rs} \frac{v^r v^s}{v^0} \right) \frac{\partial}{\partial v^i} f. \end{aligned} \tag{9'}$$

The Cauchy problem for the Vlasov equation in a given space–time is easy, since it is a linear, scalar equation with characteristic vector field (Y,Q) satisfying

$$\dot{Y}^\alpha = Q^\alpha,$$

$$\dot{Q}^\alpha = - {}^4\Gamma^\alpha_{\kappa\lambda} Q^\kappa Q^\lambda,$$

and since $X(f) = 0$, f is constant along the characteristics.

From the particle distribution f one can construct other physically meaningful quantities such as the energy–momentum tensor by integration over the tangent spaces. We denote the part of the mass shell in the fiber over $x \in M$ by $P_x := P \cap T_x M$. Then we define the energy–momentum tensor T by

$$T_{\alpha\beta}(x) := - \int_{P_x} f p_\alpha p_\beta \sqrt{|g|} / p_0 \mathrm{d}p^1 \mathrm{d}p^2 \mathrm{d}p^3. \tag{10}$$

T is divergence free and satisfies the dominant and strong energy condition and the non-negative pressures condition.

To obtain the matter quantities ρ, j, and S one has to calculate the components of the energy–momentum tensor with respect to an orthonormal frame. These components have the following representation:

$$T({}^4e_\alpha, {}^4e_\beta)(x) = \int_{P_x} f v_\alpha v_\beta / v^0 \mathrm{d}v^1 \mathrm{d}v^2 \mathrm{d}v^3. \tag{10'}$$

Now let us consider the Einstein–Vlasov system. The energy–momentum tensor automatically satisfies $\operatorname{div} T = 0$ as mentioned previously, thus there arise no additional equations from the Bianchi identities. But unfortunately the coupled system of equations is not symmetric hyperbolic in any sense, due to the fact that it is a system of integro-differential equations. Nevertheless, the local existence proof applies similar techniques as in the case of quasilinear symmetric hyperbolic systems where the peculiarity in the construction for the Einstein–Vlasov system consists in bounding the support of f in the tangent space: There is no *a priori* bound on the velocities of the particles, and no localization argument available as for the space–time coordinates. In order to estimate the matter quantities appearing in the coupled system, one has to control the maximal velocity uniformly during the construction. This has been done, for example, in Rendall (1997a), establishing a well-posed Cauchy problem for the Einstein–Vlasov system.

With this result at hand, it is easy to extend this result to the Einstein–Vlasov–Maxwell system, since the Einstein–Maxwell equations are symmetric hyperbolic and when coupling the Vlasov equation to them nothing new appears.

C. Further conventions

I adopt the convention of denoting any generic constant by C. For the convenience of the reader I cite the well-known Gronwall estimate, which is central to the analysis of partial differential equations and will be used here in this work.

Proposition 2.3 (Gronwall's inequality): Let $I\subset\mathbb{R}$ *be an interval,* $t_0\in I$ *and* α, β, $u\in C(I,\mathbb{R}_+)$, *with*

$$u(t)\leqslant\alpha(t)+\left|\int_{t_0}^{t}\beta(s)u(s)\mathrm{d}s\right|$$

for all $t\in I$.

Then

$$u(t)\leqslant\alpha(t)+\left|\int_{t_0}^{t}\alpha(s)\beta(s)\exp\int_{s}^{t}\beta(r)\mathrm{d}r|\mathrm{d}s|\right|$$

holds for all $t\in I$.

The proof of Gronwall's inequality in this particular form can be found in Amann (1995).

III. SPACE–TIMES WITH TWO-DIMENSIONAL SPHERICAL, PLANE, AND HYPERBOLIC SYMMETRY

A. The geometry of surface symmetric space–times

Let (M,g) be a smooth, globally hyperbolic space–time which is topologically of the form $\mathbb{R}\times S^1\times F$, with F a compact, orientable surface. The submanifolds $\{\tau\}\times S^1\times F$ are assumed to be Cauchy surfaces of M. The universal covering $\hat{F}$ of F induces a space–time $(\hat{M},\hat{g})$ by $\hat{M}=\mathbb{R}\times S^1\times\hat{F}$ and $\hat{g}=p^*g$, $p:\hat{M}\to M$ the canonical projection. Moreover, there is a group G of isometries acting on $(\hat{M},\hat{g})$.

Then (M,g)

(1) is called *spherically symmetric*, if $F=S^2$ and $G=\mathrm{SO}(3)$ acts isometrically and without fixed points on $S^1\times S^2$,
(2) is *plane symmetric*, if $F=T^2$ and $G=E_2$ (Euclidian group) acts isometrically on $\hat{F}=\mathbb{R}^2$,
(3) has *hyperbolic symmetry*, if F has genus greater than one and the connected component of the symmetry group G of the hyperbolic plane, H^2, acts isometrically on $\hat{F}=H^2$ (thus $F=H^2/\Gamma$, with Γ a discrete group of isometries of H^2)

and the matter quantities remain invariant under the isometries.

To collect these cases, each such space–time is called *surface symmetric*, the diffeomorphic images of F in the product decomposition of M *surfaces of symmetry* and each surface in M diffeomorphic to $S^1\times F$ will be called *symmetric*.

In expressions involving indices, lower case Greek indices range from 0 to 3, lower case Latin indices (preferably taken from the middle of the alphabet) range from 1 to 3, and upper case Latin indices (from the beginning of the alphabet) take the values 2 or 3.

The isometric action forces the curvature of the surfaces of symmetry up to rescaling to be $\epsilon=1,\ 0,\ -1$ in the spherical, plane, and hyperbolic cases, respectively. Therefore they admit coordinates (ϑ,φ) which cast the metric $\tilde{g}$ of the surfaces of symmetry (considered for a moment as abstract manifolds) into the form

$$\tilde{g}=\mathrm{d}\vartheta^2+\epsilon_\vartheta^2\mathrm{d}\varphi^2,\quad \epsilon_\vartheta:=\begin{cases}\sin\vartheta, & \epsilon=1\\ 1, & \epsilon=0\\ \sinh\vartheta, & \epsilon=-1.\end{cases} \tag{11}$$

Define the area radius function r on a surface of symmetry F (embedded in M) to be

$$r=\sqrt{\frac{1}{4\pi}\mathrm{Vol}(F)}, \tag{12}$$

then r is independent of (ϑ,φ) and the metric of F reads

$$\overline{g}=r^2\tilde{g}. \tag{13}$$

With respect to any symmetric Cauchy surface S we have the timelike unit normal vector n of S in M. Regarding n as a normal vector to F in M, we can define a second unit normal m of F by the conditions that m is tangent to S and the system $(n,m,\overline{e_2},\overline{e_3})$ is positively oriented, where we set $\overline{e_A}:=r^{-1}\tilde{e}_A$, $\tilde{e}_2:=\partial_2$, $\tilde{e}_3:=\epsilon_\vartheta^{-1}\partial_3$. We denote the associated second fundamental forms of $(F,\overline{g})$ in (M,g) by κ and λ, with

$$\lambda_{AB}=-\frac{1}{2}m(\overline{g}_{AB})=-\frac{1}{2}m(r^2)\tilde{g}_{AB}=\frac{1}{2}(\mathrm{tr}\,\lambda)\overline{g}_{AB},\quad \mathrm{tr}\,\lambda=-\frac{2}{r}m(r), \tag{14a}$$

$$\kappa_{AB}=-\frac{1}{2}n(\overline{g}_{AB})=-\frac{1}{2}n(r^2)\tilde{g}_{AB}=\frac{1}{2}(\mathrm{tr}\,\kappa)\overline{g}_{AB},\quad \mathrm{tr}\,\kappa=-\frac{2}{r}n(r). \tag{14b}$$

Consider now a Gaussian coordinate neighborhood (x',ϑ,φ) of a surface of symmetry F, covering (a part of) a symmetric Cauchy surface S. The metric h of S then takes the form $h=\mathrm{d}x'^2+\sqrt{|h|}\tilde{g}$. The projection of geodesics starting in $(\hat{M},\hat{g})$ orthogonal at F remain orthogonal to all surfaces of symmetry. Following them until their projection meets F again, the symmetry allows only two possibilities: The point of return is the same as the starting point or an antipodal point, in which case we force the geodesic to turn a second time around the circle. Let L denote the length of the geodesic. Setting $a=2\pi(\int_0^L|h(z)|^{-1/4}\mathrm{d}z)^{-1}$, we define a new coordinate $x(x')$ by $a\int_0^{x'}|h(z)|^{-1/4}\mathrm{d}z$. In the coordinates $(x^i)=(x,\vartheta,\varphi)$ the metric has the representation

$$h=A^2(dx^2+a^2\tilde{g})=A^2\mathrm{d}x^2+\overline{g} \tag{15}$$

with $A(x)=a^{-1}|h(x)|^{1/4}$ defined on S^1. Comparing this with Eq. (13) shows $r=Aa$. The corresponding Laplacian Δ acting on a function ψ on S can now be calculated to

$$\begin{aligned}\Delta\psi&=-h^{ij}\nabla_i\nabla_j\psi=-h^{11}\nabla_1\nabla_1\psi-h^{AB}\nabla_A\nabla_B\psi\\ &=-h^{11}\nabla_1\nabla_1\psi+h^{AB}\Gamma^1_{AB}\psi'+\overline{\Delta}\psi\\ &=-A^{-2}(\psi''+A^{-1}A'\psi')+\overline{\Delta}\psi,\end{aligned}$$

where $\overline{\Delta}$ denotes the Laplacian of $\overline{g}$, and the prime differentiation with respect to x, a convention, which we adopt for the rest of this work.

Furthermore, the symmetry and the given coordinate representations permit the second fundamental form k to have the form

$$k=A^2K\,\mathrm{d}x^2+\tfrac{1}{2}(\mathrm{tr}\,\kappa)\overline{g}, \tag{16}$$

where the coefficients are functions on S^1. Taking the trace yields the mean curvature $H=\mathrm{tr}\,k$ and we get the relation

$$H-K=\operatorname{tr}\kappa. \tag{17}$$

So far we know the intrinsic and extrinsic geometry for a symmetric Cauchy surface Σ in M. Let us turn now to the $3+1$-geometry. Theorem 2.2 states the conditions to guarantee local in time existence for a PMC foliation $\{S_t\}$ of a neighborhood of Σ. We need that λ defined by Eq. (5) is non-negative and does not vanish identically on Σ. Again n is the unit normal on Σ and T the energy–momentum tensor of the space–time. Therefore we get a sufficient condition by the assumption that M satisfies the strong energy condition [hence the matter term in (5) is non-negative] and that there exists at least one point in Σ, with $\lambda>0$. The strictness of the inequality is not a restriction, since one always can perform a slight deformation of Σ, such that the second fundamental form is not identically zero, which does the job. The same reasoning works, of course, if M satisfies the dominant energy condition and the non-negative-pressures condition [then both parts of the matter term in (5) are non-negative]. Thus, in surface symmetric space–times, some energy conditions are sufficient for the existence of a local in time PMC foliation.

Having constructed a local in time PMC foliation, one can ask if the leaves of the foliation are symmetric, when Σ has been chosen to be symmetric [note that due to symmetry $\lambda=\lambda(x)$ is a function on S^1 only]. As described in Henkel (2001b) the PMC foliation is given as a limit (w,N) of functions (w^j,N^j) on Σ in some Sobolev space. Here w^j describes a family of spacelike hypersurfaces in M and N^j converges toward the lapse function of w. (w^j,N^j) are defined as solutions of the sequence of symmetric-hyperbolic elliptic systems

$$\partial_t w^j+A^i(w^{j-1},N^{j-1})\partial_i w^j+B(w^{j-1},N^{j-1},DN^{j-1})=0,$$

$$\Delta(w^{j-1})N^j+\lambda(w^{j-1},Dw^{j-1})N^j=1$$

with w^0 representing Σ and $N^0=1$, hence respecting the symmetries. The underlying metric structure of the system is the sequence of first fundamental forms h_{j-1} of the surfaces w^{j-1}. If all the (w^j,N^j) respect the symmetries, then the PMC foliation also, hence it suffices to show that (w^j,N^j) respects the symmetries, if w^{j-1},N^{j-1} does so. This is clear for w^j, because the symmetric-hyperbolic equation can be localized, and the pullback to $\hat{M}$ is invariant under the action of the isometry group.

Suppressing the index $j-1$ from some quantities determined by the metric h_{j-1}, the Laplacian reads

$$\Delta(w^{j-1})N^j=-A^{-2}((N^j)''+A^{-1}A'(N^j)')+\overline{\Delta}(w^{j-1})N^j.$$

The elliptic equation then becomes

$$-A^{-2}((N^j)''+A^{-1}A(N^j)')+\lambda(w^{j-1},Dw^{j-1})N^j+\overline{\Delta}(w^{j-1})N^j=1.$$

If $\overline{\Omega}=\sqrt{|\overline{g}|}=r^2\epsilon_\vartheta$ denotes the volume form of the surfaces of symmetry F in M, one finds $\mathrm{Vol}(F)=\int_{[0,\pi]\times[0,2\pi]}\overline{\Omega}=4\pi r^2$, as desired. Setting

$$L:=-A^{-2}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}+A^{-1}A'\frac{\mathrm{d}}{\mathrm{d}x}\right)\quad\text{and}\quad\widetilde{N}^j(x):=\frac{1}{\mathrm{Vol}(F)}\int_{[0,\pi]\times[0,2\pi]}N^j\overline{\Omega}=\frac{1}{4\pi}\int_{[0,\pi]\times[0,2\pi]}N^j\epsilon_\vartheta,$$

then integration of the elliptic equation, $\int_{[0,\pi]\times[0,2\pi]}\epsilon_\vartheta(L+\lambda+\overline{\Delta})N^j=\int_{[0,\pi]\times[0,2\pi]}\epsilon_\vartheta=4\pi$, yields

$$(L+\lambda+\overline{\Delta})\widetilde{N}^j=1,$$

since on the one hand $\int_{[0,\pi]\times[0,2\pi]}(L+\lambda)N^j\epsilon_\vartheta = 4\pi(L+\lambda)\tilde{N}^j$ and on the other hand $\int_{[0,\pi]\times[0,2\pi]}(\overline{\Delta}N^j)\epsilon_\vartheta = r^{-2}\int_{[0,\pi]\times[0,2\pi]}(\overline{\Delta}N^j)\overline{\Omega} = r^{-2}\int_F \overline{\Delta}N^j$ vanishes as well as $\overline{\Delta}\tilde{N}^j$. Thus $\tilde{N}^j$ is a solution of the elliptic equation. Uniqueness then gives us $N^j=\tilde{N}^j$, thus $N^j=N^j(x)$, which expresses the symmetry of N^j, as desired.

Thus we have shown, given a symmetric Cauchy surface Σ in M admitting a local in time PMC foliation, that all leaves of the foliation are symmetric, too, and coordinatizing them in the above-described way yields:

Proposition 3.1: Let (M, g) be a surface symmetric space–time obeying the strong energy condition. Then there are coordinates $(x^\mu)=(t,x,\vartheta,\varphi)$ *adapted to a local in time PMC foliation* $\{S_t\}$ *of a neighborhood* $U=]t_1,t_2[\times\Sigma$ *of* $\Sigma=S_0$ *in M, which cast the metric into the form*

$$g=-N^2\mathrm{d}t^2+A^2((\mathrm{d}x+\nu\,\mathrm{d}t)^2+a^2\tilde{g}). \tag{18}$$

All coefficients except a are functions on $]t_1,t_2[\times S^1$, *whereas a depends only on the time function t. A and a are everywhere positive, N denotes the lapse function of the foliation, and* ν *the nonvanishing component of the shift vector, uniquely fixed by the condition* $\nu(t,0)=0$.

Supplementary to the notation already introduced, let an overdot denote differentiation with respect to *t*, while keeping the prime as a marker for differentiation with respect to the coordinate *x*.

Finally we find for the orthonormal frame $\{{}^4e_\mu\}$ and its dual $\{{}^4\sigma^\mu\}$ canonically induced by the $3+1$-split:

$$
\begin{aligned}
{}^4e_0 &= n = N^{-1}(\partial_0-\nu\partial_1), \quad {}^4\sigma^0 = N\,\mathrm{d}t,\\
{}^4e_1 &= m = A^{-1}\partial_1, \quad {}^4\sigma^1 = A(\nu\,\mathrm{d}t+\mathrm{d}x^1),\\
{}^4e_2 &= (Aa)^{-1}\partial_2, \quad {}^4\sigma^2 = Aa\,\mathrm{d}x^2,\\
{}^4e_3 &= (Aa\epsilon_\vartheta)^{-1}\partial_3, \quad {}^4\sigma^3 = Aa\epsilon_\vartheta\,\mathrm{d}x^3.
\end{aligned}
$$

B. The field equations

1. 3+1 decomposition of the filled squared lines

Given the PMC foliation, we can write down the field equations in the $3+1$-representation. The symmetries suggest representing the matter quantities completely with respect to an orthonormal frame, thus we define $j:=-T(n,m)=A^{-1}j_1$ and $S_{ij}=T({}^4e_i,{}^4e_j)$.
Then one calculates the constraint equations (1) to be

$$(A^{1/2})''=\tfrac{1}{8}A^{5/2}(H^2-\tfrac{1}{2}(H-K)^2-K^2-16\pi\rho)+\tfrac{1}{4}A^{1/2}a^{-2}\epsilon, \tag{19}$$

$$K'=-3A^{-1}A'K+A^{-1}A'H+H'+8\pi Aj. \tag{20}$$

The foliation is fixed by the lapse equation (3) and the PMC condition (4)

$$N''=-A^{-1}A'N'+A^2N(\tfrac{1}{2}(H-K)^2+K^2+4\pi(\rho+\mathrm{tr}\,S))-A^2, \tag{21}$$

$$\dot{H}=1+\nu H', \tag{22}$$

and the evolution equations (2) read

$$\dot{A}=-NAK+A\nu'+A'\nu, \tag{23}$$

$$\dot{a}=-\tfrac{1}{2}Na(H-3K)-a\nu', \tag{24}$$

$$\dot{K}=\nu K'-A^{-2}(N''-A^{-1}A'N')+N(-4A^{-5/2}(A^{1/2})''+(A^{-2}A')^2 + HK-8\pi(A^{-2}S_{11}+\tfrac{1}{2}(\rho-\operatorname{tr}S))). \tag{25}$$

Integrating the equation for a over the circle yields $\dot{a}=\mu a$, with $\mu=-1/2\int_{S^1}N(H-3K)$, since $\int_{S^1}\nu'$ vanishes. Inserting this back gives an equation for shift:

$$\nu'=-\frac{1}{2}N(H-3K)+\frac{1}{2}\int_{S^1}N(H-3K). \tag{26}$$

Differentiation of the equation for H with respect to x yields an equation for H':

$$(\partial_t-\nu\partial_x)H'=\nu'H'. \tag{27}$$

In summary we have equations for space and time derivatives of the fundamental forms h and k. Moreover there are equations for the spacelike derivatives of lapse and shift, but unfortunately there is no information about their time derivatives.

So far we started with a given surface symmetric space–time, admitting a local in time PMC foliation, to which we adapted the field equations. This raises the opposite question: Given Eqs. (19)–(27) and appropriate data, does there exist a solution, and how unique is it? To answer this question we first need to state more precisely the term ''appropriate data:''

Definition 3.2: A *symmetric initial data set* is a smooth collection (Σ, h, k) consisting of a three-manifold Σ diffeomorphic to $S^1\times F$ with metric h and a symmetric tensor field k on Σ, where Σ admits coordinates, such that h and k could be written in the form shown in Sec. III A.

If there are matter fields present, then it is assumed that there is also smooth symmetric matter data and equations, leading to a well-posed Cauchy problem of the reduced field equations in harmonic coordinates.

The smoothness of the quantities appearing in the definition is required, since the transformation to harmonic coordinates involves derivatives.

Proposition 3.3: Let (Σ, h, k) *be a symmetric initial data set, with matter obeying the strong energy condition and [compare Eq. (5) for definition]* $\lambda>0$ *somewhere on* Σ. *Further, let* t_0 *denote an arbitrary real number*.

Then there exists a $\delta>0$ *and a PMC foliated surface symmetric space–time* $(\overline{M},\overline{g})$ *diffeomorphic to* $]t_0-\delta,t_0+\delta[\times\Sigma$ *with an embedding* $\iota:\Sigma\to\overline{M}$, *satisfying* $\iota(\Sigma)=S_{t_0}$ *and* ι_*h, ι_*k *are the first and second fundamental form of* S_{t_0} *in* $(\overline{M},\overline{g})$. $(\overline{M},\overline{g})$ *obeys the strong energy condition and* $\overline{g}$ *can be written in the form described in Proposition 3.1. This construction is unique up to the choice of* t_0 *and* δ.

Proof: On the induced manifold $\hat{\Sigma}$ diffeomorphic to $S^1\times\hat{F}$ the induced data are invariant under the group action, hence the Cauchy developments also and we get a surface symmetric Cauchy development of the data, admitting a symmetric local in time PMC foliation near Σ on some time interval $]t_0-\delta,t_0+\delta[$ and allowing a set of coordinates stated in Proposition 3.1. The uniqueness property stated previously follows from the geometric uniqueness of solutions of Einstein's equations associated with the uniqueness of the PMC foliation, once the remaining degree of freedom has been fixed by the requirement $\iota(\Sigma)=S_{t_0}$. Note that lapse is fixed by the ellipticity of the respective PMC equation and shift is fixed by Eq. (26) and the condition $\nu(t,0)=0$. ■

In surface symmetric space–times, there is another way to express the constraint equations (19) and (20) in terms of ''optical scalars,'' see Guven (1995) for an enlightening presentation.

The geodesic null congruences determined by $k_\pm=m\pm n$ give rise to the null expansions

$$\vartheta_\pm:=-(\operatorname{tr}\lambda\pm\operatorname{tr}\kappa)=\frac{2}{r}(m(r)\pm n(r))=\frac{2}{r}k_\pm(r)=2A^{-2}A'\mp(H-K), \tag{28}$$

where (14) with (17) has been used, together with the relation $r=Aa$ for the area radius defined in (12). The formula illustrates the definition of r as a volume measure, whose variation along $k_{\pm}$ is described by the (negative of the) trace of the second fundamental form associated with this direction.

Now we can write the constraint equations for an arbitrary symmetric Cauchy surface S symmetrically as

$$8\pi(\rho+j)=-m(\vartheta_-)-\tfrac{3}{4}\vartheta_-^2+\vartheta_-H+r^{-2}\epsilon,$$

$$8\pi(\rho-j)=-m(\vartheta_+)-\tfrac{3}{4}\vartheta_+^2-\vartheta_+H+r^{-2}\epsilon$$

and taking $\omega_{\pm}:=r\vartheta_{\pm}$ as the fundamental variable we get [compare Guven (1995)]

$$m(\omega_{\pm})=-8\pi r(\rho\mp j)\mp\omega_{\pm}H+\frac{1}{4r}(\omega_+\omega_--2\omega_{\pm}^2+4\epsilon). \tag{29}$$

Furthermore, the area radius serves as a warping function in the warped product $M=B\times_r F$ of the two-dimensional space–time $(B,\underline{g})$ with $(F,\overline{g})$, where $B=\mathbb{R}\times S^1$ is the quotient M/G and $\underline{g}=g_{|B}$. We adopt the convention that lower case Latin letters from the beginning of the alphabet range from 0 to 1, and objects intrinsic or orthogonally projected to $(B,\underline{g})$ will be marked by an underbar. Einsteins equations in this framework can be considered as equations in $(B,\underline{g})$ for the field $r:B\to\mathbb{R}$:

$$\underline{\nabla}_a\underline{\nabla}_b r=\frac{M}{r^2}\underline{g}_{ab}-4\pi r(\underline{T}_{ab}-\mathrm{tr}\ \underline{T}\underline{g}_{ab}), \tag{30}$$

where $\underline{T}$ denotes the projected energy–momentum tensor into the space–time $(B,\underline{g})$ and the mass function M is defined as

$$M:=\tfrac{1}{2}r(\epsilon-\underline{\nabla}^a r\underline{\nabla}_a r)=\tfrac{1}{2}r(\epsilon-{}^4\nabla^\alpha r\,{}^4\nabla_\alpha r)=\tfrac{1}{2}r(\epsilon-\tfrac{1}{4}r\vartheta_+r\vartheta_-), \tag{31}$$

since $\vartheta_+\vartheta_-=4/r^2{}^4\nabla^\alpha r\,{}^4\nabla_\alpha r$. M turns out to be the Hawking mass $m_H(F)$ (up to a factor $-\frac{1}{2}\chi$ for genus $(F)\geqslant 3$):

$$m_H(F):=\frac{\mathrm{Vol}(F)^{1/2}}{(4\pi)^{3/2}}\left(\pi\chi(F)-1/8\int_F\vartheta_+\vartheta_-\right) \tag{32}$$

and differentiation of (31) yields the mass flux equation

$$\underline{\nabla}_a M=4\pi r^2(\underline{T}_{ab}-\mathrm{tr}\,\underline{T}\underline{g}_{ab})\underline{\nabla}^b r. \tag{33}$$

2. Expanding and recollapsing models

Let us first consider the definition of mass in (31). In the spherically symmetric case we see, that grad r is spacelike as long as $2M<r$ holds, a condition we are familiar with in connection with the Schwarzschild space–time.

In the plane and hyperbolic case the picture is quite different, since grad r turns out to be timelike, as long as $2M/r>\epsilon$. In fact, Lemmas 2.3, 2.4, and 2.5 in Rendall (1995b) prove for space–times with hyperbolic symmetry and in nonflat plane symmetric space–times grad r is timelike, provided the dominant energy condition is fulfilled. Thus we cannot think about r as some radial, spacelike coordinate any longer and this fact will play a central role in our further analysis.

We can choose the time orientation in those space–times to find r past pointing, *throughout the whole space–time*. Then we define the time orientation on the cotangent bundle by metric transport from the tangent bundle, such that dr turns out to be future pointing. Therefore r increases with time, which means that the area of the surfaces of symmetry increases with time, and the space–time expands in this sense. Thus we will call these space–times expanding. We get

an equivalent characterization by the relation between grad r and the null expansions: ϑ_+ and ϑ_- have fixed and opposite signs (in particular $\vartheta_+>0$, $\vartheta_-<0$), since $\vartheta_\pm=(2/r)k_\pm(r)=(2/r)dr(k_\pm)$ is the contraction of a timelike with a null vector.

Therefore we can decide, given a symmetric initial data set (Σ,h,k) with nonflat plane or hyperbolic symmetry, with matter obeying the dominant energy condition, which direction is expanding or contracting. This is important, since we expect some singularity toward the contracting direction and therefore we will pay attention to the past development $D^-(\Sigma)$, which represents the contracting direction with respect to our conventions.

Note that we obtained this information without referring to the mean curvature $H=\operatorname{tr} k$. But it turns out that the mean curvature of an arbitrary Cauchy surface S in expanding space–times is also restricted in some way.

First, remember that $H=\operatorname{tr} k=-\operatorname{div} n$ measures the convergence of the geodesic congruence, future pointing and orthogonal to S. Thus, $H<0$ everywhere on S corresponds to the notion of expansion and Hawking's theorem proves the existence of a singularity in the past. In an expanding space–time in our sense, H is not necessarily confined to be negative everywhere. But we will see that it is impossible for H to become non-negative everywhere on S: The explicit formula (28) for $\vartheta_\pm$ shows, in connection with our sign conventions, that $H<K$. If H were non-negative, then $|H|<|K|$, thus $H^2-K^2<0$ and integration of the Hamiltonian constraint (19) over S^1 yields a contradiction.

With the dominant energy condition we can show more. Writing the Hamiltonian constraint as $R+H^2-|k|^2=16\pi\rho$ we get $R+H^2\geqslant 0$. Assuming $H\equiv 0$ on S, we would get $R\geqslant 0$. But symmetric surfaces S in space–times with plane and hyperbolic symmetry obey, respectively, the topological conditions (i) and (ii) of theorem 5.2 in Schoen and Yau (1979), which imply that S cannot have positive scalar curvature and must be flat in the case of non-negative scalar curvature. Thus S must be flat and the scalar curvature vanishes. This in turn forces $\rho=0$ and $k=0$ by the Hamiltonian constraint. In the plane symmetric case then the space–time is flat by $k=0$, $\rho=0$ and the dominant energy condition, contradiction. In the hyperbolic symmetric case integration of Eq. (19) yields a contradiction, too. Putting all this together we conclude without loss of generality, that surface symmetric space–times, obeying the dominant energy condition, which are plane symmetric and not flat or have hyperbolic symmetry, are everywhere expanding, with dr timelike future pointing, $\vartheta_+>0$, $\vartheta_-<0$, and any symmetric Cauchy surface S is not maximal with mean curvature not everywhere positive on S.

Of course, these arguments do not work in the spherically symmetric case, where grad r is spacelike in $\{2M<r\}$ and no fixed sign of the expansions $\vartheta_\pm$ can be expected, fitting into the general belief in the closed universe recollapse conjecture, which precludes expansion of the whole space–time. In particular we expect the existence of a maximal hypersurface in M.

C. *A priori* estimates for the field equations

Our aim now is to get sufficient estimates that allow the construction of a global PMC foliation. The ''size'' of the foliation is measured by the mean curvature H, thus *we are looking for* uniform *estimates of the geometric and matter quantities in terms of H*.

So let (M, g) be a surface symmetric space–time, satisfying the dominant and strong energy condition. Let us assume that there is a Cauchy surface Σ in M with mean curvature $H<0$. In particular we get a local in time PMC foliation $\{S_t\}$, $t\in]t_1,t_2[$ with $\Sigma=S_0$ by Theorem 2.2. If the space–time possesses plane or hyperbolic symmetry, we choose the time orientation in correspondence to the conventions introduced in Sec. III B, thus H decreases with decreasing PMC time. If (M, g) is spherically symmetric we choose the time orientation that H decreases with PMC time, too. Then in either case we expect to find a singularity at least in the past $D^-(\Sigma)$ of Σ.

In $D^-(\Sigma)$ the mean curvature is bounded from above by $H\leqslant\overline{H}<0$ and $H=\overline{H}$ only on Σ. Thus $|H|$ is bounded from below and we find the following estimates for the field equations in $D^-(\Sigma)$ as long as H remains finite:

(1) At first we consider the constraint equation (29) on a fixed leaf. At the critical points of $\omega_\pm$

we find together with the dominant energy condition the important inequality

$$|r\vartheta_{\pm}| \leqslant 2(|Hr| + \sqrt{(Hr)^2 + \epsilon}) \tag{34}$$

as shown in Rendall (1995b).

For plane and hyperbolic symmetry this inequality (34) can be strengthened to

$$|\vartheta_{\pm}| \leqslant 4|H| \leqslant C \Rightarrow |A^{-2}A'| \leqslant C \quad \text{and} \quad |K| \leqslant C$$

by the definition (28) of the null expansions.

In the spherically symmetric case the argument is more complicated: First, the work of Burnett (1991) shows that under the additional assumption of the non-negative-pressures condition we have $r \leqslant C$ and $0 < C \leqslant M$. Using the upper bound for r on the right-hand side of (34) we get with (31)

$$|r\vartheta_{\pm}| \leqslant C \Rightarrow \frac{M}{r} \leqslant C.$$

Thus we get $r^{-1} \leqslant C_{M^{-1}} \leqslant C$; hence r is bounded above and below away from zero. Inserting this in the estimate (34) leads to $|\vartheta_{\pm}| \leqslant Cr^{-1} \leqslant C$ and we are in the same situation as in the plane/hyperbolic case, hence $|A^{-2}A'| \leqslant C$ and $|K| \leqslant C$.

(2) Now consider the lapse equation (21) on a fixed leaf. At the point where N attains its maximum $\overline{N}$, we have

$$\overline{N} \leqslant (\tfrac{1}{2}(H-K)^2 + K^2 + 4\pi(\rho + \operatorname{tr} S))^{-1} \leqslant C/H^2 \leqslant C$$

due to the strong energy condition. Hence we have a bound for $|N|$.

(3) Next, there is a bound for shift. Examination of formula (26) shows that all quantities on the right-hand side are bounded, so we get $|\nu'| \leqslant C$, and therefore, using $\nu(t,0) = 0$: $|\nu(t,x| \leqslant |\nu(t,0)| + \int'_{S^1} |\nu'| \leqslant C$.

(4) By the way, Eq. (27) for H' provides a bound for $|H'|$, since the coefficient on the right-hand side is bounded and applying Gronwall gives the desired estimate.

(5) With the information about ν' examination of (24), $\dot{a} = a(-\frac{1}{2}N(H-3K) - \nu')$ shows that the factor in brackets is already bounded and we get an inequality of the form $|\partial_t \ln|a|| \leqslant C$, which leads to a bound for $|a|$ and $|a^{-1}|$.

(6) The same line of argumentation works for A. Equation (23) can be written as $\dot{A} - \nu A' = A(-NK + \nu')$, with the factor on the right-hand side bounded. So we get bounds for $|A|$ and $|A^{-1}|$, too.

Since we have already bounded the null expansions $\vartheta_{\pm} = 2A^{-2}A' \pm (H-K)$, one sees easily that even $|A'| \leqslant C$.

(7) Integration of Eq. (19) over the circle yields an inequality

$$\frac{1}{8}\int_{S^1} A^{5/2} 16\pi\rho = \frac{1}{8}\int_{S^1} A^{5/2}\left(H^2 - K^2 - \frac{1}{2}(H-K)^2\right) + \frac{1}{4}\int_{S^1} A^{1/2}a^{-2}\epsilon$$

$$\leqslant \frac{1}{8}\int_{S^1} A^{5/2}H^2 + \frac{1}{4}\int_{S^1} A^{1/2}a^{-2}.$$

From this one concludes the boundedness of $\int_{S^1}\rho$, and by the dominant energy condition the boundedness of $\int_{S^1}|j|$ and $\int_{S^1}|S|$. Now integrating Eq. (21) starting at a point where $N' = 0$, we get

$$N' = -\int A^{-1}A'N' + \int A^2 N\left(\frac{1}{2}(H-K)^2 + K^2 + 4\pi(\rho + \operatorname{tr} S)\right) - \int A^2,$$

$$|N'| \leqslant C + \int |A^{-1}A'N'|.$$

The bound for $|N'|$ then follows from Gronwall's inequality.

(8) Furthermore, the bounds for A, A^{-1} together with the basic estimate for ϑ_+ and the boundedness of $\int_{S^1}\rho$ are enough to apply the proof of the lemma in Rendall (1997b), which ends up with $|N^{-1}| \leqslant C$.

Collecting all these estimates we get the

Proposition 3.4: Let (M,g) *be a surface symmetric space–time, obeying the dominant and strong energy condition and in the spherically symmetric case the non-negative-pressures condition, too. Assume the existence of a symmetric Cauchy surface* Σ *with strictly negative mean curvature. In particular we get from Proposition 3.1 a PMC time coordinate* t, *ranging in* $]t_1,t_2[$ *with* $\Sigma=\{t=0\}$ *and* H *decreases with decreasing* t.

Then we have uniformly on $]t_1,0]$,

$$|A|,|A^{-1}|,|A'|,|a|,|a^{-1}|,|H|,|H'|,|K|,|N|,|N^{-1}|,|N'|,|\nu|,|\nu'| \leqslant C.$$

To put this result into some framework, we establish some formalism to have useful abbreviations at hand as well as to make clear the dependence between estimates of geometric quantities and matter variables.

Definition 3.5:

$$\mathcal{F} := (A,a,N,\nu,H,K)$$

collects the quantities describing the geometry of the foliation and

$$\Phi := (\rho,j,S)$$

abbreviates the matter quantities.

We have already estimated the quantities $\mathcal{F}$, A^{-1}, a^{-1}, N^{-1}, as well as A', N', ν', H' and $\dot{A}$, $\dot{a}$, $\dot{H}$ (by inspection of the field equations). The idea is now to bound all quantities $\mathcal{F}$, Φ together with all of their derivatives uniformly on the time interval $]t_1,0]$. Then there exists a smooth extension to the closure of the interval, which serves as a new symmetric initial data set for the field equations in the sense described in Definition 3.2. Note that the bounds for A^{-1}, a^{-1}, N, N^{-1} ensure that the geometry remains regular at the boundary of the time interval and the C^∞-bounds for lapse and shift turn out to be necessary to obtain C^∞-bounds for the fundamental forms.

Proposition 3.3 then sets us in the position to extend the foliation at least in the past direction, where $H<0$ holds: Construct the solution stated in Proposition 3.3 and embed M into the maximal Cauchy development of the data.

To carry out this program, we need some knowledge about the matter quantities. First, the matter has to obey the dominant and strong energy conditions. Second, assume that the regularity of the geometry guarantees the regularity of the matter in a certain way. For all non-negative integers m and n we have

$$\begin{aligned} |\partial_t^m \partial_x^n \mathcal{F}| \leqslant C &\Rightarrow |\partial_t^m \partial_x^n \Phi| \leqslant C \\ |\partial_t^m \partial_x^{n+1} \mathcal{F}| \leqslant C &\Rightarrow |\partial_t^{m+1} \partial_x^n \Phi| \leqslant C, \end{aligned} \tag{35}$$

then the following lemmas hold.

Lemma 3.6: Assume that the matter fulfills (35). Then for arbitrary non-negative integers m, n,

$$\left.\begin{array}{l}\forall_{k<m}\forall_l|\partial_t^k\partial_x^l\mathcal{F}|\leqslant C\\ \forall_{l<n}|\partial_t^m\partial_x^l\mathcal{F}|\leqslant C\end{array}\right\}\Rightarrow|\partial_t^m\partial_x^{n+1}\mathcal{F}|\leqslant C$$

holds.

Lemma 3.7: Assume that the matter fulfills (35). Then for arbitrary non-negative integers m, n,

$$\left.\begin{array}{l}\forall_{k<m}\forall_l|\partial_t^k\partial_x^l\mathcal{F}|\leqslant C\\ \forall_{l<n+1}|\partial_t^m\partial_x^l\mathcal{F}|\leqslant C\end{array}\right\}\Rightarrow|\partial_t^{m+1}\partial_x^n\mathcal{F}|\leqslant C$$

holds.

Together with Proposition 3.4 the lemmas accomplish the task of bounding all necessary derivatives of the geometric quantities, by first bounding all spatial derivatives $\partial_x^n\mathcal{F}$ (Proposition 3.4 and Lemma 3.6) and then successively all derivatives $\partial_t^k\partial_x^l\mathcal{F}$, with $k+l=n$ by alternative applications of the lemmas. Therefore, in view of Proposition 3.4 the validity of property (35) will be enough to extend the foliation. We will prove (35) for some matter models in the next section. But first, of course, we have to prove the lemmas.

Proof of Lemma 3.6:

A: Applying $\partial_t^m\partial_x^n$ on Eq. (19) and integrating along S^1 yields a bound for the difference $|(\partial_t^m\partial_x^nA^{1/2})'(y)-(\partial_t^m\partial_x^nA^{1/2})'(x)|$ and using $\int_{S^1}(\partial_t^m\partial_x^nA^{1/2})'=0$ (hence is bounded) gives a bound for $\partial_t^m\partial_x^{n+1}A^{1/2}$, hence for $\partial_t^m\partial_x^{n+1}A$.

a: Trivial.

ν: Apply $\partial_t^m\partial_x^n$ on (26), then the right-hand side of (26) is bounded by assumption, from which the claim follows immediately.

N: Again applying $\partial_t^m\partial_x^n$ on the lapse equation (21) yields an equation of the form (21) for $\partial_t^m\partial_x^nN''$ plus some already bounded term (by assumption and the already proven bound for $\partial_t^m\partial_x^nA'$). The boundedness of $\partial_t^m\partial_x^nN'$ follows then from Gronwall's estimate after integrating the equation for $\partial_t^m\partial_x^nN''$ along S^1 starting at a point with $\partial_t^m\partial_x^nN'=0$.

H: Differentiation of Eq. (27) gives an expression of the form $(\partial_t-\nu\partial_x)\partial_t^m\partial_x^nH'=B_1\partial_t^m\partial_x^nH'+B_2$, with B_1, B_2 bounded, where the assumptions and the already obtained bound for $\partial_t^m\partial_x^{n+1}\nu$ have been used. Thus applying Gronwall's inequality yields a bound for $\partial_t^k\partial_x^{n+1}H$.

K: Apply $\partial_t^m\partial_x^n$ on Eq. (20), then the right-hand side is bounded by the previous estimates, hence bounding $\partial_t^m\partial_x^{n+1}K$. ■

Proof of Lemma 3.7:

A: Applying $\partial_t^m\partial_x^n$ on (23) yields immediately a bound for $\partial_t^m\partial_x^n\dot{A}$, since the right-hand side is already bounded.

a: The same argument with ∂_t^m instead of $\partial_t^m\partial_x^n$ applied to Eq. (24) works in this case to bound $\partial_t^m\partial_x^n\dot{a}$.

H: And again, $\partial_t^m\partial_x^n$ on Eq. (22) yields an estimate for $\partial_t^m\partial_x^n\dot{H}$.

K: Apply $\partial_t^m\partial_x^n$ on Eq. (25), then the only terms on the right-hand side not already known to be bounded are $\partial_t^m\partial_x^nN''$ and $\partial_t^m\partial_x^nA''$. But inserting Eqs. (21) and (19) for N'' and A'', respectively, one sees easily that $\partial_t^m\partial_x^nN''$ and $\partial_t^m\partial_x^nA''$ indeed are bounded by the right-hand sides of their equations, hence $\partial_t^{m+1}\partial_x^nK$ is bounded.

N: Unfortunately there is no explicit equation for $\dot{N}$. So we have to apply the derivative operator $\partial_t^{m+1}\partial_x^n$ to Eq. (21), therefore producing already estimated terms involving $\partial_t^{m+1}\partial_x^n$ applied on the quantities treated previously, as well as on Φ [bounded by property (35)], but also a term involving $\partial_t^{m+1}\partial_x^{n+1}A$ on the right-hand side. If this term turns out to be bounded, then the equation for $\partial_t^{m+1}\partial_x^nN''$ has the form

$$\partial_t^{m+1}\partial_x^nN''=B-A^{-1}A'\partial_t^{m+1}\partial_x^nN'+A^2\partial_t^{m+1}\partial_x^nN((\tfrac{1}{2}H-K)^2+K^2+4\pi(\rho+\mathrm{tr}\,S))-A^2$$

with $|B|$ bounded. On S^1, $\partial_t^{m+1}\partial_x^nN$ attains its maximum, from which we can infer

$$\partial_t^{m+1}\partial_x^n N \leqslant \{(1-B/A^2)(\tfrac{1}{2}(H-K)^2+K^2+4\pi(\rho+\mathrm{tr}\,S))^{-1}\}_{\max}$$

hence it is bounded from above. Similarly for the minimum,

$$\partial_t^{m+1}\partial_x^n N \geqslant \{(1-B/A^2)(\tfrac{1}{2}(H-K)^2+K^2+4\pi(\rho+\mathrm{tr}\,S))^{-1}\}_{\min},$$

which is bounded from below and we get $|\partial_t^{m+1}\partial_x^n N| \leqslant C$.

It remains to show the boundedness of $\partial_t^{m+1}\partial_x^{n+1}A = \partial_t^m \partial_x^{n+1}\dot{A}$. Inserting Eq. (23) for $\dot{A}$, we see on the right-hand side beside a bounded term the quantities $\partial_t^m\partial_x^n A''$ and $\partial_t^m\partial_x^{n+1}\nu'$. Inserting Eq. (19) for A'' and Eq. (26) for ν', we finally obtain bounds for $\partial_t^m\partial_x^n A''$ and $\partial_t^m\partial_x^{n+1}\nu'$, and hence for $\partial_t^m\partial_x^{n+1}\dot{A}$, as desired.

ν: The final estimate is straightforward: Apply the operator $\partial_t^{m+1}\partial_x^{n-1}$ to Eq. (26), which immediately yields a bound for $\partial_t^{m+1}\partial_x^n\nu$ since the right-hand side of the equation is already bounded by the above-given arguments. ■

D. Higher order estimates

Here we prove the matter regularity condition (35) for Einstein–Vlasov, Einstein–Maxwell, and the Einstein–Vlasov–Maxwell systems, achieving the goal of this work.

1. Collisionless matter

The $3+1$-split of the Vlasov equation (9) with respect to the symmetries reads

$$0 = \partial_t f + \left(NA^{-1}\frac{v^1}{v^0} - \nu\right)\partial_x f + \left(-A^{-1}N'v^0 + NKv^1 + NA^{-2}A'\frac{(v^2)^2+(v^3)^3}{v^0}\right)\frac{\partial}{\partial v^1}f$$
$$-N\left(A^{-2}A'\frac{v^1}{v^0} - \frac{1}{2}(H-K)\right)v^B\frac{\partial}{\partial v^B}f, \tag{36}$$

where $v^0 := \sqrt{1+\delta_{ij}v^iv^j}$ and $0 = \partial_{x^2}f = \partial_{x^3}f = v^3(\partial/\partial v^2)f - v^2(\partial/\partial v^3)f$ (by symmetry) has been used.

The energy–momentum tensor (10) associated with the Vlasov equation leads to the matter quantities

$$\rho = \int f v^0 \,\mathrm{d}v,$$

$$j = \int f v^1 \,\mathrm{d}v,$$

$$S_{ab} = \int f v_a v_b / v^0 \,\mathrm{d}v.$$

Now we investigate the matter regularity property (35). Since f is constant along the characteristics of the Vlasov equation, given an initial particle distribution f_0 on the mass shell over Σ, we get the matter distribution for each time t as a function $f(t,y,w)$ on the mass shell over the leaf S_t by $f(t,y,w) = f_0(Y(t,y,w),V(t,y,w))$, where (Y,V) denotes the characteristic curve of the Vlasov equation through the point $(0,y,w) \in P_{(0,y)}$, $(0,y) \in \Sigma$.

Thus the matter quantities ρ,j,S are bounded, provided the support of f remains bounded. Define now

$$\overline{P}_f(t) := \{\sup|v| \,|\, v \in \mathrm{supp}\, f(t,y,w) \forall_{(0,y,w)\in P_{(0,y)}}\},$$

then the matter quantities are bounded by $C(1+\overline{P}_f(t))^4$, hence it is sufficient to control $\overline{P}_f(t)$ on $]t_1,0]$.

Since the characteristic curves (Y,V) are integral curves of X and all coefficients in the components of X are already bounded by Proposition 3.4, the characteristics themselves are bounded, $\overline{P}_f(t)\leqslant C$ as desired.

Now we need to iterate this procedure. Assume, that all $\partial_t^k\partial_x^l\mathcal{F}$ and $\partial_t^k\partial_x^l\Phi$ for $k+l=m+n$ are bounded. To bound the derivatives of the matter quantities of order $m+n+1$, differentiate the Vlasov equation $m+n+1$ times (with respect to t and x only). This yields linear equations for $\partial_t^{\overline{k}}\partial_x^{\overline{l}}f$, for all non-negative integers $\overline{k}+\overline{l}=m+n+1$ of the form

$$X(\partial_t^{\overline{k}}\partial_x^{\overline{l}}f)=B,$$

where B vanishes outside the support of f, which bounds the support of B. Moreover, B involves derivatives of order $m+n+1$ of the quantities $\mathcal{F}$ and A', N'. For derivatives of order at most m in t, we see the boundedness of $|B|$ by applying similar arguments as used in the proof of Lemma 3.6. Thus in this case $\partial_t^{\overline{k}}\partial_x^{\overline{l}}f$ is bounded and $\overline{P}_{\partial_t^{\overline{k}}\partial_x^{\overline{l}}f}$, since they have the same characteristics. Hence the derivatives of the matter quantities of order $m+n+1$, involving derivatives of order at most m in t, are bounded. Moreover, due to the simple dependence of the characteristics on the frame variables v, all derivatives of f with respect to v are bounded, too.

In view of this fact, we are able to bound all derivatives of order $m+n+1$ of the matter quantities by considering the Vlasov equation as an equation for $\partial_t^{m+1}\partial_x^{n+1}f$, for which the right-hand side is known to be bounded.

Therefore the first part of property (35) holds. For the second part we must show that the spacelike derivatives of $\mathcal{F}$ can be redistributed to timelike derivatives of Φ. But this has already been done in the proof of the first part of (35), and we get the

Theorem 3.8: *Let (M,g,f) be a surface symmetric solution of the Einstein–Vlasov system, which possesses a symmetric Cauchy surface Σ with strictly negative mean curvature $H\leqslant\overline{H}<0$ and $H=\overline{H}$ somewhere on Σ.*

Then all of the past of Σ admits a PMC foliation $\{S_t\}$, where t takes all values in the interval $]-\infty,0]$ and H takes all values in $]-\infty,\overline{H}]$.

2. Maxwell field

Let F denote the electromagnetic field. The symmetry simplifies F: Due to the symmetries F can be written relative to the orthonormal coframe $\{{}^4\sigma^\mu\}$ introduced in Sec. III A as

$$F=-\hat{e}(t,x)\,{}^4\sigma^0\wedge{}^4\sigma^1+\hat{b}(t,x)\,{}^4\sigma^2\wedge{}^4\sigma^3,$$

since all other components are forced to vanish and F and ${}^4\sigma^0\wedge{}^4\sigma^1$, ${}^4\sigma^2\wedge{}^4\sigma^3$ remain invariant under the action of the symmetry group.

To obtain an explicit form of the Maxwell equations, F and $*F$ are represented in the given coordinates by

$$F_{\alpha\beta}\sim\begin{pmatrix}0&-e&0&0\\ e&0&0&0\\ 0&0&0&b\\ 0&0&-b&0\end{pmatrix},\quad \begin{aligned}&e(t,x)=NA\hat{e},\\ &b(t,x,\vartheta)=(Aa)^2\epsilon_\vartheta\hat{b},\end{aligned}$$

$$*F_{\alpha\beta}\sim\begin{pmatrix} 0 & \kappa b & 0 & 0 \\ -\kappa b & 0 & 0 & 0 \\ 0 & 0 & 0 & \kappa^{-1}e \\ 0 & 0 & -\kappa^{-1}e & 0 \end{pmatrix}, \quad \sqrt{|g|}=NA^3a^2|\epsilon_\vartheta|, \quad \kappa:=NA^{-1}a^{-2}|\epsilon_\vartheta^{-1}|.$$

The Maxwell equations (6) in vacuum are given by setting $J^\alpha=0$. We get for the magnetic field

$$F'_{23}=0 \qquad b'=0$$
$$\Leftrightarrow$$
$$\dot{F}_{23}=0 \qquad \dot{b}=0\,.$$

Since ϵ_ϑ does not depend on (t,x), we find $\partial_\alpha((Aa)^2\hat{b})=0$ for $\alpha=0,1$, hence

$$\hat{b}=C(Aa)^{-2},$$

$$b=C\epsilon_\vartheta\,.$$

For the electric field we find

$$*F'_{23}=0 \qquad (\kappa^{-1}e)'=0$$
$$\Leftrightarrow$$
$$*\dot{F}_{23}=0 \qquad (\kappa^{-1}e)^{\cdot}=0\,.$$

(Note, that $*F_{01,2}$ vanishes, since κb contains no ϵ_ϑ.) Again, since ϵ_ϑ does not depend on (t,x), we get $\partial_\alpha((Aa)^2\hat{e})=0$, for $\alpha=0$, 1, hence

$$\hat{e}=C(Aa)^{-2},$$

$$e=CNA^{-1}a^{-2}.$$

Since N, A^{-1}, a^{-1} are already bounded, the same is true for the electromagnetic fields e and b.

The energy–momentum tensor (8) takes the simple form

$$E({}^4e_\alpha,{}^4e_\beta)=\frac{1}{8\pi}(\hat{e}^2+\hat{b}^2)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

and we get the matter quantities as

$$\rho=E({}^4e_0,{}^4e_0)=-S_{11}=\operatorname{tr}S=\frac{1}{8\pi}(\hat{e}^2+\hat{b}^2)=\frac{1}{8\pi}(C(Aa)^{-4}+C(Aa)^{-4}),$$

$$j=0.$$

The property (35) posed in Sec. III C is obviously fulfilled, hence we get

Theorem 3.9: *Let (M,g,F) be a surface symmetric solution of the Einstein–Maxwell system with plane or hyperbolic symmetry, which possesses a symmetric Cauchy surface Σ with strictly negative mean curvature $H\leqslant\overline{H}<0$ and $H=\overline{H}$ somewhere on Σ. Then all of the past of Σ admits a PMC foliation $\{S_t\}$, where t takes all values in the interval $]-\infty,0]$ and H takes all values in $]-\infty,\overline{H}]$.*

Note that the restriction to plane and hyperbolic symmetry is necessary, since the electromagnetic energy–momentum tensor does not obey the non-negative pressures condition, and therefore fails to satisfy the assumptions of Proposition 3.4 in the case of spherical symmetry.

3. Charged particles

Now consider the Vlasov–Maxwell system in (M,g). We obtain the coupled equations by modifying the uncharged Vlasov equation (36) by adding the term

$$e\left(A^{-1}+A^{-2}A'-N^{-1}\nu(1+A^{-1}A')\frac{v^1}{v^0}\right)\frac{\partial f}{\partial v^1}$$

on the right-hand side. The matter current J according to the energy–momentum tensor

$$\Theta=T+E,\quad \begin{matrix}\rho=\Theta({}^4e_0,{}^4e_0)\\ j=-\Theta({}^4e_0,{}^4e_1),\end{matrix}$$

is of the form

$$J=\rho\,{}^4e_0+j\,{}^4e_1=N^{-1}\rho\partial_0+(A^{-1}j-N^{-1}\nu\rho)\partial_1.$$

The homogeneous Maxwell equations remain unchanged, which yields as before

$$\hat{b}=C(Aa)^{-2},$$

$$b=C\epsilon_\vartheta.$$

Since ${}^*J_{\alpha\beta\gamma}=\sqrt{|g|}\epsilon_{\mu\alpha\beta\gamma}J^\mu$, and again for $\alpha=0$, 1, $\partial_\alpha(\kappa^{-1}e)=|\epsilon_\vartheta|\partial_\alpha((Aa)^2\hat{e})$ the inhomogeneous equations read

$$(\kappa^{-1}e)'=4\pi\sqrt{|g|}J^0 \qquad \hat{e}'=-2A^{-1}A'\hat{e}+4\pi A\rho$$

$$\Leftrightarrow$$

$$(\kappa^{-1}e)^{\cdot}=-4\pi\sqrt{|g|}J^1 \qquad \dot{\hat{e}}=-2(Aa)^{-1}(Aa)^{\cdot}\hat{e}+4n(A\nu\rho\text{-}Nj).$$

To get a bound for $\hat{e}$, note that the inhomogeneous Maxwell equations are of the form

$$\partial_\alpha\hat{e}=\varphi_\alpha\hat{e}+\psi_\alpha\cdot\begin{pmatrix}\rho\\ j\end{pmatrix},\quad \alpha=0,1$$

with $\varphi_\alpha,\psi_\alpha$ bounded by Proposition 3.4. Integrating the second equation gives

$$\left|\int_{S^1}\dot{\hat{e}}\right|=\left|\int_{S^1}\varphi_0\hat{e}+\int_{S^1}\psi_0\cdot\begin{pmatrix}\rho\\ j\end{pmatrix}\right|\leqslant C\left|\int_{S^1}\hat{e}\right|+C,$$

since $\int_{S^1}\rho$, $\int_{S^1}|j|\leqslant C$ by integrating Eq. (19), as shown in the proof of Proposition 3.4. Then using the inequality

$$\left|\int_{S^1}\hat{e}\right|(t)\leqslant\left|\int_{S^1}\hat{e}\right|(0)+\int_0^t\left|\int_{S^1}\dot{\hat{e}}\right|$$

and applying Gronwall's inequality on $|\int_{S^1}\hat{e}|$ we obtain

$$\left|\int_{S^1}\hat{e}\right|\leqslant C.$$

Now using the first equation, we get analogously

$$|\hat{e}(t,y)-\hat{e}(t,x)|=\left|\int_x^y \hat{e}'\right|=\left|\int_{S^1}\varphi_1\hat{e}+\int_{S^1}\psi_1\cdot\begin{pmatrix}\rho\\ j\end{pmatrix}\right|\leqslant C\left|\int_{S^1}\hat{e}\right|+C\leqslant C,$$

where $\left|\int_{S^1}\hat{e}\right|\leqslant C$ has been used.
Thus we have

$$\left.\begin{aligned}&|\hat{e}(t,y)-\hat{e}(t,x)|\leqslant C\\ &\left|\int_{S^1}\hat{e}\right|\leqslant C\end{aligned}\right\}\Rightarrow\quad |\hat{e}|\leqslant C$$

as desired.

Now property (35) is obtained by bounding appropriate derivatives of $\hat{e}$: Application of $\partial_t^m\partial_x^{n-1}$ on the equation for $\hat{e}'$ shows the first part of property (35) and application of $\partial_t^m\partial_x^n$ on the equation for $\dot{\hat{e}}$ establishes the second part. This proves:

Theorem 3.10: *Let* (M,g,f,F) *be a surface symmetric solution of the Einstein–Vlasov–Maxwell system with plane or hyperbolic symmetry, which possesses a symmetric Cauchy surface* Σ *with strictly negative mean curvature* $H\leqslant\overline{H}<0$ *and* $H=\overline{H}$ *somewhere on* Σ. *Then all of the past of* Σ *admits a PMC foliation* $\{S_t\}$, *where t takes all values in the interval* $]-\infty,0]$ *and H takes all values in* $]-\infty,\overline{H}]$.

E. Improving the results

The purpose of this section is to get rid of the requirement of strictly negative mean curvature on the Cauchy surfaces, which seems to be a rather technical restriction. Let us instead assume Σ to be a symmetric Cauchy surface in the surface symmetric space–time (M,g) with matter obeying the dominant and strong energy condition as well as the non-negative pressures condition, such as the surface symmetric Einstein–Vlasov system (M,g,f). Note that we assume the non-negative pressures condition not only for the spherically symmetric case. Indeed we will see that this energy condition is necessary for the arguments given in this section, thus we cannot apply them to matter involving electromagnetic fields.

As pointed out in Sec. III B 2 there is an important difference between the possible types of surface symmetry and it turns out to be a good idea to analyze the spherically symmetric case separately.

1. Spherically symmetric space–times

There are some results already obtained elsewhere, so we can exclude some special cases from our analysis. Namely for the Einstein–Vlasov system (as well as for the massless scalar field) it has been proven in Rendall (1995b) and Burnett (1996) that given an arbitrary symmetric constant mean curvature Cauchy surface, there exists a global CMC foliation with the mean curvature taking all real values. So we may assume that the mean curvature H on Σ is not constant, and we immediately get from Theorem 2.2 the existence of a local in time PMC foliation $]t_1,t_2[\times\Sigma$ of a neighborhood of Σ in M.

There are some *a priori* estimates:

(1) It is shown in Burnett (1991) that r and M^{-1} are bounded. Theorem 2.1 in Burnett (1991) then shows that all timelike curves have finite length.

(2) Inserting the bound for r on the right-hand side of the estimate (34), we get from (31) bounds for r^{-1} and M on any finite time interval.

(3) Section III in Burnett (1996) shows that in light of the fact that all timelike curves have finite lengths, the volumes of two arbitrary Cauchy surfaces Σ_1 and Σ_2 are related by

$$\mathrm{Vol}(\Sigma_2) \leqslant \mathrm{Vol}(\Sigma_1)\left(1 + C \sup_{\Sigma_1} |H|\right)^3.$$

This implies that the volumes of all Cauchy surfaces S in M are bounded above by the volume of Σ and, since H is bounded on each finite time interval, interchanging the roles of Σ and S shows that the volumes are bounded from below, too, on each finite time interval.

If we denote the volume form of a PMC leaf S_t by Ω and the volume of S_t by $V(t)$ we have $\Omega = \sqrt{|h|}$ and $V(t) = \int \Omega \, \mathrm{d}x \mathrm{d}\vartheta \mathrm{d}\varphi = 4\pi a^{-1} \int_{S^1} r^3$.

With the bounds of V, V^{-1}, r, r^{-1} we now get a, $a^{-1} \leqslant C$, and again using the bounds for the radius function we get A, $A^{-1} \leqslant C$, thus the first fundamental form of the leaves is bounded from above and below on each finite time interval.

Moreover, as shown in Sec. III C, the estimate (34) bounds $|A^{-2}A'|$ and $|K|$, so that the second fundamental form is also bounded (from above) on each finite time interval as well as $|A'| = |A^2||A^{-2}A'|$.

Consider now the lapse equation (21), written in the form

$$(AN')' = A^3 N(\tfrac{1}{2}(H-K)^2 + K^2 + 4\pi(\rho + \mathrm{tr}\, S)) - A^3,$$

where the term in brackets is non-negative. Therefore, setting this term to zero, we get the estimate $(AN')' \geqslant -C$, hence, for arbitrary $p, q \in S_t$: $(AN')(p) - (AN')(q) \geqslant -C$. Now choosing q to be a critical point of N yields $N'(p) \geqslant -C$, and similarily choosing p as a critical point of N gives $N'(q) \leqslant C$. From this we see that $|N'|$ is bounded, since p, respectively, q is arbitrary on S_t.

The difference from the situation considered in Sec. III C is that we are no longer confined to a mean curvature, having everywhere fixed sign. The difficulty with the estimates done there is that they provide no information about the behavior of the lapse function, when H becomes zero. The estimates done here so far do not rely on this fact and the uniform bound of N' shows that either lapse remains finite or diverges uniformly to infinity.

In order to prove the global existence of a symmetric PMC foliation assume that $]t_1, t_2[$ is the maximal time interval of existence. Without loss of generality let us consider only a possible extension toward the past, where H decreases with decreasing t. Thus, we are looking for regular symmetric initial data for $t = t_1$ in the sense of Definition 3.2.

Then there are two cases: First, $H(t)$ is everywhere positive or everywhere negative near t_1, the arguments in Sec. III C apply (the fixed sign of H is enough to perform the estimates, whether H is positive or negative), extending the foliation and we get a contradiction to the maximality of the time interval, hence $t_1 = -\infty$.

Second, $\lim_{t \to t_1} H(t)$ possesses no unique sign near t_1. Then we have to prove Proposition 3.4 and the two subsequent Lemmas 3.6 and 3.7. The discussion at the beginning of this section has shown that some of these quantities are already bounded. The crucial step is to find a bound for lapse and its derivatives.

The idea is to reparametrize the foliation as has been done for a CMC foliation in Burnett (1996). The effect of the reparametrization on lapse and shift was outlined in Sec. II A. Let us introduce a function τ by

$$\tau := t + \int_{t_1}^{t} N(u, x_0)\, \mathrm{d}u,$$

where $\int_{t_1}^{t}$ means $\lim_{s \to t_1} \int_s^t$. It is well defined, since $\int N(\gamma(u))\mathrm{d}u$ along the integral curves of the normals of the leaves measures the length of γ, which we already know to be finite, and $|N'| \leqslant C$ ensures the integrability of $N(t, x_0) \leqslant N(\gamma(t)) + C$. This construction works in either case, whether N is bounded or diverges uniformly to infinity. The function $t \mapsto \tau(t)$ is monotone since $\mathrm{d}\tau/\mathrm{d}t = 1 + N(t, x_0)$ and turns out to be an orientation preserving diffeomorphism $]t_1, t_2[\to]\tau_1 = t_1, \tau_2[$, thus τ can be used as a new time function for the foliation, which squeezes the time

differences of neighboring leaves compared with the normal vector by adding to t the normal component of the length of the piece of the $x_0=\text{const}$ line connecting (t_1,x_0) with (t,x_0). This produces a new lapse function and a new shift vector:

$$\tilde{N}=\left(\frac{\mathrm{d}\tau}{\mathrm{d}t}\right)^{-1}N=\frac{N}{1+N(t,x_0)},$$

$$\tilde{\nu}=\left(\frac{\mathrm{d}\tau}{\mathrm{d}t}\right)^{-1}\nu=\frac{\nu}{1+N(t,x_0)}.$$

Conversely, t stretches time differences of adjacent leaves, such that we get the inverse transformation by $t=\tau-\int_{\tau_1}^{\tau}\tilde{N}(u,x_0)\mathrm{d}u$, which subtracts from τ the former added "length" of the $x_0=\text{const}$ line now expressed in terms of the new time coordinate. By the inverse transformation, we see that $\mathrm{d}t/\mathrm{d}\tau=1-\tilde{N}(\tau,x_0)$, and therefore get the relation $1-\tilde{N}(\tau,x_0)=(1+N(t,x_0))^{-1}$ in points with spatial coordinate x_0.

The benefit of this reparametrization is, that due to $|N'|\leqslant C$, $\tilde{N}$ and $|\tilde{N}'|$ remain bounded, and we could try to analyze the field equations according to the reparametrized foliation. Inspection of these equations shows that we get the field equations in the new coordinates from Eqs. (19) to (27) by replacing everywhere ∂_t by ∂_τ, N by $\tilde{N}$, ν by $\tilde{\nu}$ (since reformulating of the constraint and evolution equations preserves their form) while the lapse equation (21) and the PMC condition (22) depend on the parametrization, and hence have to be modified: The subtraction of A^2 on the right-hand side stems from the term $A^2Nn(H)$, where the PMC condition sets $Nn(H)$ equal to one. Replacing N by $\tilde{N}$ yields $(Nn(H))(1+N(t,x_0))^{-1}=(1+N(t,x_0))^{-1}=1-\tilde{N}(\tau,x_0)$. The PMC condition (22), which holds in the old parametrization, can be formulated in the new coordinates by expressing ν in terms of $\tilde{\nu}$, which produces an additional summand $1-\tilde{N}(\tau,x_0)$ on the right-hand side, besides the replacement of ν by $\tilde{\nu}$.

Now we start to analyze the new field equations, trying to retain the same line of thought of Sec. III C: The analysis already done here bounds A, A^{-1}, $|A'|$, a, a^{-1}, $|H|$, $|K|$ as well as, of course, $\tilde{N}$ and $|\tilde{N}'|$. The arguments carried out in Sec. III C now bound $|\tilde{\nu}|$, $|\tilde{\nu}'|$ and $|H'|$. Finally we need a bound for $\tilde{N}^{-1}$. Since it is not clear, in the case where N diverges near t_1, whether N grows monotonically or not, we divide the time interval $]t_1,t_2[$ into two subsets. First consider all points, where $N(t,x_0)\geqslant M$, with some suitable chosen real number M, which will be specified later. Then we get the estimate

$$|1-\tilde{N}(\tau,x)|=\left|1-\frac{N(t,x)}{1+N(t,x_0)}\right|=\left|\frac{1+N(t,x_0)-N(t,x)}{1+N(t,x_0)}\right|\leqslant\frac{1+C}{1+M},$$

where C is an upper bound for $|N(t,x_0)-N(t,x)|$, whose existence is guaranteed by the bounds for $|N'|$ and the volume of the leaves of the foliation. Choose now $M=2C$ and we get

$$|1-\tilde{N}|\leqslant\frac{1+C}{1+2C}<1,$$

thus $\tilde{N}$ is bounded away from zero for all points where $N(t,x_0)\geqslant M$. Consider now the points where $N(t,x_0)\leqslant M$. Then we have

$$|1-\tilde{N}(\tau,x_0)|=\left|1-\frac{N(t,x_0)}{1+N(t,x_0)}\right|=\left|\frac{1+N(t,x_0)-N(t,x_0)}{1+N(t,x_0)}\right|\geqslant\frac{1}{1+M}.$$

Now we can apply the arguments in Rendall (1997b) to the modified lapse equation, as has been done in Sec. III C [whereupon the factor $1-\tilde{N}(\tau,x_0)$ causes no trouble, since it is bounded from above and below] and we get a bound for $\tilde{N}^{-1}$ for all points, where $N(t,x_0)\leqslant M$, and we are done.

Therefore we have estimated all quantities appearing in Proposition 3.4. Lemma 3.6 is also true for the new field equations without the need to modify the proof, while the proof of Lemma 3.7 has to be modified, since the argument bounding $|\partial_t^{m+1}\partial_x^n\tilde{N}|$ does not carry over. The lapse equation and the equation for its time derivatives are

$$(A\tilde{N}')' = A^3\tilde{N}(\tfrac{1}{2}(H-K)^2+K^2+4\pi(\rho+\mathrm{tr}\,S))-A^3(1-\tilde{N}(\tau,x_0))$$

$$(A\partial_t^m\tilde{N}')' = A^3\partial_t^m\tilde{N}(\tfrac{1}{2}(H-K)^2+K^2+4\pi(\rho+\mathrm{tr}\,S))-A^3(1-\partial_t^m\tilde{N}(\tau,x_0))+B,$$

where B denotes an already bounded quantity at the corresponding stage in the inductive argument in Lemma 3.7. In this situation Lemma 1 in Burnett (1996) applies literally, bounding the time derivatives of the lapse function, therefore completing the proof of Lemma 3.7.

Putting all arguments together we are able to extend the foliation beyond t_1, contradicting the assumed maximality of the interval of existence, thus arriving at the following:

Theorem 3.11: *Let (M,g,f) be a surface symmetric solution of the Einstein–Vlasov system with spherical symmetry. Then we can foliate the whole space–time by a PMC foliation, where the time function takes on all real values and the mean curvature of the leaves tends uniformly to $\pm\infty$ for $t\to\pm\infty$, thus producing crushing singularities.*

This theorem provides barrier surfaces [see Gerhardt (1983)], establishing now the existence of CMC hypersurfaces for each value of the mean curvature, therefore proving the closed universe recollapse conjecture in this case:

Corollary 3.12: In the situation of Theorem 3.11, the space–time possesses a global CMC foliation and the mean curvature takes on all real values. In particular, the space–time admits a maximal Cauchy surface.

2. Space–times with plane and hyperbolic symmetry

We will see that most of the arguments performed in the spherically symmetric case carry over to the past domain of dependence $D^-(\Sigma)$ in the expanding models (compare Sec. III B 2 for a precise definition of this terminology). Due to this fact we perform the following analysis only on the half-open time interval $]t_1,0[$ and assume further, (M,g) to be nonflat in the plane symmetric case and the mass function (31) to be positive on Σ in the hyperbolic case.

Again we can exclude some cases already investigated (although this does not matter, since the arguments here apply to these cases). It has been proven in Rendall (1995b) and Burnett (1996) that given a symmetric Cauchy surface with negative constant mean curvature H_0 (remember the restrictions on the mean curvature in the expanding models, compare Sec. III B 2), there exists a global CMC foliation with the mean curvature taking all values in the interval $]-\infty,H_0[$. So we can assume without loss of generality that the mean curvature H on Σ is not constant and not everywhere positive. Again, this assumption ensures the existence of a local in time PMC foliation $]t_1,t_2[\times\Sigma$ of a neighborhood of Σ in M.

Now we find similar *a priori* bounds.

(1) In $D^-(\Sigma)$ r is bounded, since dr is future pointing timelike everywhere and Σ is compact. M^{-1} is bounded on Σ by assumption in the hyperbolic case and in the plane symmetric case this follows from Lemma 2.4 in Rendall (1995b). By the mass flux equation (33) together with the non-negative pressures condition, M grows along past pointing timelike curves, thus M^{-1} is bounded in all of $D^-(\Sigma)$. Theorem 2.1 in Burnett (1991) then shows that all timelike curves in $D^-(\Sigma)$ have finite length.

(2) Applying the arguments in the corresponding place of Sec. III E 1 we get bounds for r^{-1} and M for any finite time interval of the form $]t_1,0]$.

(3) Again, the corresponding argument performed in the spherically symmetric case holds, and we get upper and lower bounds for the volumes of arbitrary Cauchy surfaces in M.

Finally, the volume of the leaves S_t is given by $V(t)=Ca^{-1}\int_{S^1} r^3$, establishing bounds for the first fundamental form and its inverse (in $D^-(\Sigma)$) as has been shown in Sec. III E 1, therefore all of the remaining arguments performed there apply and we get the

Theorem 3.13: *Let (M,g,f) be a surface symmetric solution of the Einstein–Vlasov system with plane or hyperbolic symmetry and Σ a symmetric Cauchy surface in M. If (M,g) is nonflat in the plane symmetric case and the mass function is positive on Σ in the hyperbolic case, then we can foliate all of the past of Σ by PMC hypersurfaces, where the time function takes on all values in the interval $]-\infty,0]$ and the mean curvature of the leaves tends uniformly to $-\infty$ for $t\to-\infty$.*

Again using the PMC leaves as barrier surfaces we get the

Corollary 3.14: *In the situation of Theorem 3.13 $D^-(\Sigma)$ possesses a CMC Cauchy surface for each value of the mean curvature in $]-\infty,\min_\Sigma H[$.*

3. Comparing the results

To close Sec. III, there are some remarks concerning Theorems 3.11 and 3.13 and the relation to the work done in the preceding sections.

At first, it is obvious that Theorem 3.11 generalizes Theorem 3.8 in the spherically symmetric case. In the plane and hyperbolic case Theorem 3.13 does not generalize Theorems 3.8, 3.9, and 3.10. The latter ones only establish a global PMC foliation unless the mean curvature of the leaves becomes zero somewhere (and again the leaves provide barrier surfaces for CMC Cauchy surfaces, establishing Corollary 3.14 in the situation of those theorems). Theorem 3.13 is not restricted to this condition, but it needs the extra non-negative pressures condition, which excludes electromagnetic fields.

Apart from the non-negative pressures condition the assumption of positive mass on Σ is a nontrivial constraint in the hyperbolic case, while automatically fulfilled in the nonflat plane symmetric case by Lemma 2.4 in Rendall (1995b). As shown previously, the positivity of mass is needed to obtain a bound for the length of timelike curves in *M*, by applying the arguments in Burnett (1991), and thus necessary to the construction done here.

IV. CONCLUSION AND OUTLOOK

First I list the main results achieved in this work.

(1) For the space–times considered so far the existence of a global PMC foliation has been shown, where several matter models have been taken into account.

(2) For the model, which is not expanding or contracting everywhere, the closed universe recollapse conjecture has been proved. In particular the foliation covers the whole Cauchy development of the initial hypersurface, with a crushing singularity both in the distant past and future. Moreover the space–time possesses a maximal hypersurface.

(3) In the expanding models the foliation covers at least the whole past of the initial hypersurface toward a crushing singularity.

The choice of matter turned out to be important only insofar as some energy conditions are satisfied and the matter fields do not become singular in a regular geometric background.

The necessary energy conditions are the dominant and strong energy conditions. Furthermore to obtain stronger results, which do not rely on a fixed sign condition for the mean curvature, the non-negative pressures condition is required to ensure that the Hawking mass does not tend to zero, contributing enough attraction that the lifetime of timelike curves becomes finite.

The rather strong results about locally spatially homogeneous space–times in Rendall (1995a) likewise rely on this condition, which appears in the slightly relaxed form, that only the sum of the pressures has to be non-negative, due to the high degree of symmetry in those models. This relaxed condition even permits electromagnetic fields, a type of matter which does not satisfy the non-negative pressures condition, thus not leading to the stronger results in the context of space–times with less symmetry.

The close analogy of the proofs for the global existence of CMC and PMC foliations indicates that all results obtained for CMC foliations may also be proved for PMC foliations. If this

conjecture turns out to be true (the second part of this paper will give another positive example for this conjecture), then we are no longer concerned with the topological restrictions imposed on the existence of CMC hypersurfaces, having a much more flexible tool at hand. Moreover, the global results on PMC foliations can be used to provide barrier surfaces, which guarantee the existence of a CMC foliation, where the mean curvature ranges between these barriers (compare Corollaries 3.12 and 3.14).

The results demonstrate that in the cases considered in this work a satisfying answer has been given to the global existence problem for PMC foliations. Then the related question arises—whether the foliation covers the whole space–time. The present work gives only a partial answer to this question. Denoting the initial Cauchy surface by Σ, we saw that we have covered the whole past $D^-(\Sigma)$ in the expanding space–times and the whole Cauchy development $D(\Sigma)$ in the recollapsing models. These positive results have two limits.

(1) In the expanding models there remains an open question about the future of Σ in M. Either the mean curvature becomes zero somewhere or there is no control on the radius function toward the expanding direction. In each case the present techniques do not apply. In addition there are topological obstructions in the expanding direction, preventing the mean curvature from becoming positive, a foliation of the future of Σ must stop before this happens. But this does not imply that the whole of $D^+(\Sigma)$ can be covered by such a foliation, since the leaves of the foliation may become null or noncompact where the general notion of singularity avoidance comes up. Namely, compared with the strong results obtained in Rendall (1995a) in the locally spatially homogeneous models, we require more information about the asymptotic behavior of the foliation to obtain results on geodesic completeness.

(2) In the contracting direction and in the recollapsing models things look different. In the contracting direction the theorems ensure the existence of crushing singularities, and all of the Cauchy development of Σ is covered by the foliation. This is a consequence of Hawking's famous incompleteness theorem for globally hyperbolic space–times, satisfying the timelike convergence condition, where the maximal time of existence is estimated by $3/|H|$ and $H \to -\infty$. But there is no information about the boundary of $D(\Sigma)$, which might be either a curvature singularity or merely a Cauchy horizon.

The work in Rendall (1995a) indicates roughly what remains to be done. Relating the particle current density to the energy density and investigating the asymptotic behavior of the former may give rise to unbounded curvature and produce a curvature singularity.

For the space–times considered here, the work is Rein (1996) is important. He succeeded in finding satisfying answers to the above questions by using a time function intimately tied to the symmetry. Unfortunately it is not clear how to generalize his approach to other space–times. Although the estimates done here also exploit the high symmetry of the models, the construction itself does not depend on it, motivating this work. A generalization to space–times with two commuting local Killing vector fields will be the content of the second part.

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Global prescribed mean curvature foliations in cosmological space–times. II

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This paper is devoted to the investigation of global properties of prescribed mean curvature (PMC) foliations in cosmological space–times with local $U(1)\times U(1)$ symmetry and matter described by the Vlasov equation. It turns out that these space–times admit a global foliation by PMC surfaces as well, but the techniques to achieve this goal are more complex than in the cases considered in Paper I [Henkel (2002)]. © *2002 American Institute of Physics.*
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I. INTRODUCTION

For the main motivation see the introduction in Paper I [Henkel (2002)]. Only some remarks special to the present situation remain.

The structure of this paper (Paper II) is as close as possible to the structure of Paper I. Although the preliminary section (Sec. II) of Paper I has been omitted, the formulas here refer to it as well.

The space–times considered here are cosmological space–times with two commuting local Killing vector fields. This symmetry will be referred to as (local) $U(1)\times U(1)$ symmetry. In comparison with Paper I, there are now only two (local) Killing fields instead of three, generalizing the plane symmetric case of Paper I. The absence of a third Killing field requires a more detailed description of the geometry and a deeper analysis to control the momenta of the Vlasov particles. Thus the estimates in this work rely on the simple structure of the Vlasov equation. Despite this there seems to exist no crucial obstructions for other types of ''well-behaved'' matter.

II. SPACE–TIMES WITH LOCAL $U(1)\times U(1)$ SYMMETRY

A. The geometry of space–times with local $U(1)\times U(1)$ symmetry

Following the analysis in Rendall (1997), we consider now the globally hyperbolic space–time (M,g) with topology $\mathbb{R}\times\Sigma$, where Σ denotes a bundle with base S^1 and compact orientable fiber F. As usual it is assumed that the submanifolds $\{t\}\times\Sigma$ are Cauchy hypersurfaces in M. The coordinates of Σ are denoted by $(x,y^2,y^3)=(x,y^A)$, $A=2,3$, where (y^A) denote coordinates on F. As usual, Greek indices range in the interval 0,...,3, lower case Latin indices from the middle of the alphabet take values in 1,...,3, while those from the beginning of the alphabet take the values 0,1 and upper case ones are confined to the values 2, 3.

The covering map $\mathbb{R}\to S^1$ defines a pullback of the bundle Σ with base $\mathbb{R}$, hence we get a trivial bundle. If $\hat{F}$ denotes the universal covering space of F, we get a natural covering $\hat{\Sigma}=\mathbb{R}\times\hat{F}$ of Σ with canonical projection p. Now we can associate a space–time $(\hat{M},\hat{g})$, where $\hat{M}=\mathbb{R}\times\hat{\Sigma}$ and $\hat{g}$ is the pullback of g under the projection $\mathrm{id}\times p$.

The fibers $\hat{F}$ in the trivial bundle $\hat{M}$ are assumed to be the orbits of a two-dimensional translation group G of isometries of $\hat{g}$. Hence $\hat{F}$ is the Euclidean space form E_2 and $F=E_2/\Gamma$, for a discrete subgroup Γ of G. The compactness and orientability of F then implies $F=T^2$, so Γ can

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be represented by a two-parameter lattice, Σ turns out to be a torus bundle over the circle, and the induced action of G on (M,g) is given by the quotient action $G/\Gamma = U(1)\times U(1)$ with orbits F. As in Paper I we will call the orbits surfaces of symmetry, hypersurfaces in M diffeomorphic to $\{t\}\times\Sigma$, which consist of a union of surfaces of symmetry called symmetric surfaces and we call (M,g) a space–time with local $U(1)\times U(1)$ symmetry.

The induced action of $U(1)\times U(1)$ on (M,g) is local, if the bundle is nontrivial. In that case we have to deal with nontrivial transformations for the transition $x\mapsto x+2\pi$ in S^1 by lattice preserving translations and automorphisms $\mathrm{GL}(2,\mathbb{Z})$ of G. To represent the metric $\overline{g}$ of the orbits in M at first locally for $x\in[0,2\pi[$, define the area radius by $r:=\sqrt{(4\pi)^{-1}\,\mathrm{Vol}(F)}$, and write the metric as

$$\overline{g}=r^2\tilde{g}, \tag{1}$$

with a metric $\tilde{g}$ of unit determinant. Due to symmetry, both quantities (r and $\tilde{g}$) do not depend on the points of F, and one easily verifies that the curvature of $\overline{g}$ vanishes, as required. For $\tilde{g}$ there are two remaining degrees of freedom, V and W, and we can use them to parametrize the metric:

$$\tilde{g}=\begin{pmatrix} e^{W}\cos V & \sin V \\ \sinh V & e^{-W}\cosh V \end{pmatrix}. \tag{2}$$

If the bundle is trivial, then this representation of the metric is global, but if the bundle is not trivial, then the translation of 2π in S^1 induces a transformation of $\overline{g}$ by an element Z of $\mathrm{GL}(2,\mathbb{Z})$,

$$\overline{g}(x+2\pi)=Z^T\overline{g}(x)Z, \tag{3}$$

which fixes the geometry of the space–time.

Given a globally acting symmetry we can specialize to some well known geometries: If $V=W=0$ then we get the plane symmetric case $\epsilon=0$ of Paper I. Setting only $V=0$ we get a symmetry called polarized, corresponding to the reflection symmetries $y^2\mapsto -y^2$ or $y^3\mapsto -y^3$, respectively. If the composition of these reflections is an isometry (regardless whether the individual reflections act isometrically), we call this symmetry *Gowdy-type*, since the Gowdy space–times are defined by this symmetry and the additional requirement that the space–time is vacuum. Thus, in general $V\neq 0$ in a space–time with Gowdy-type symmetry, but if V vanishes also we call the Gowdy-type symmetry polarized.

We construct the coordinate system $\{x^\mu\}$ mentioned in the beginning of this section locally by the following procedure. Consider first an arbitrary symmetric Cauchy surface S in M. Then we extend the coordinates (y^A) of F to a Gaussian neighborhood of F in S. Later on we will do some rescaling along S^1, such that we choose the coordinates, such that the metric h of S takes the general form $h=A^2\,\mathrm{d}x+\overline{g}$. Now we embed this structure into the space–time. In general the time coordinate t defines lapse N and shift $\nu=\nu^i\partial_i$, thus the space–time metric g is not in block diagonal form. The components g_{0A} which prevent g being block diagonal can be represented by $\overline{\nu_A}:=\overline{g}_{AB}\nu^B$.

1. The 2+2-geometry

Now we want to investigate the geometry of $(F,\overline{g})$ in (M,g) more closely. As before let S denote a symmetric Cauchy surface in M, foliated by its symmetric surfaces. The unit normal of F in $S\subset M$ will be denoted by m and n is the unit normal of S in M, as usual. Then there are some canonical geometrical objects induced:

(a) the two second fundamental forms

$$\lambda(v,w)=g({}^4\nabla_v w,m), \tag{4a}$$

$$\kappa(v,w)=g({}^4\nabla_v w,n) \tag{4b}$$

for $v,w\in TF$ with arbitrary extensions to vector fields, in order to make the expressions well defined. In the sequel it turns out to be convenient to deal with the trace free parts $\tilde{\lambda}$ and $\tilde{\kappa}$ instead, defined by $\lambda=\tilde{\lambda}+\frac{1}{2}\mathrm{tr}\,\lambda\bar{g}$ and $\kappa=\tilde{\kappa}+\frac{1}{2}\mathrm{tr}\,\kappa\bar{g}$, respectively.

In the given coordinates we have explicit formulas:

$$\lambda_{AB}=-\tfrac{1}{2}m(\bar{g}_{AB})=-\tfrac{1}{2}A^{-1}(\bar{g}_{AB})',$$

$$\mathrm{tr}\,\lambda=-\tfrac{1}{2}\bar{g}^{AB}m(\bar{g}_{AB})=-\frac{1}{2}\frac{m(\det\bar{g})}{\det\bar{g}}=-\frac{2}{r}m(r)=-2A^{-2}A',$$

$$\kappa_{AB}=-\tfrac{1}{2}n(\bar{g}_{AB})=-\tfrac{1}{2}N^{-1}(\bar{g}_{AB})^{\cdot}-N^{-1}A\nu^{1}\lambda_{AB},$$

$$\mathrm{tr}\,\kappa=-\frac{2}{r}n(r),$$

reflecting the definition of the area radius r as a volume measure and the second fundamental forms as its rate of change. In the above-mentioned formulas $\bar{g}$ is considered as intrinsic to F (and we maintain this from now on) and $\bar{g}^{AB}=r^{-2}\tilde{g}^{AB}$ denotes the inverse of $\bar{g}_{AB}$. Differentiating $\tilde{g}$ directly one gets from its relation to $\bar{g}$ and the above-mentioned formulas the following representations of the trace free parts of the second fundamental forms:

$$\tilde{\lambda}_{AB}=-\tfrac{1}{2}r^{2}m(\tilde{g}_{AB}),\quad \tilde{\lambda}^{AB}=\tfrac{1}{2}r^{-2}m(\tilde{g}^{AB}),$$

$$\tilde{\kappa}_{AB}=-\tfrac{1}{2}r^{2}n(\tilde{g}_{AB}),\quad \tilde{\kappa}^{AB}=\tfrac{1}{2}r^{-2}n(\tilde{g}^{AB}).$$

(b) The connection in the normal bundle $T^{\perp}F$. This can be represented by a single one-form η, defined as

$$\begin{aligned}\eta(v)&=g({}^{4}\nabla_{v}n,m)=-g({}^{4}\nabla_{v}m,n)\\&=-\tfrac{1}{2}g([n,m],v),\quad v\in TF.\end{aligned}\tag{5}$$

From this formula one can see that $\eta=0$ is equivalent to $[n,m]\in T^{\perp}F$, thus $[T^{\perp}F,T^{\perp}F]\subset T^{\perp}F$ and the theorem of Frobenius tells us that $T^{\perp}F$ is an integrable distribution of two planes in TM. If $T^{\perp}F$ is integrable, then we can decompose the space–time into a direct sum $(M,g)=(F^{\perp},\underline{g})+(F,\bar{g})$, with $g=\underline{g}\oplus\bar{g}$. Sufficient for the existence of an integral manifold $F^{\perp}$ of the distribution $T^{\perp}F$ is the Gowdy-type symmetry $y^{A}\mapsto -y^{A}$, $A=2,3$, since then it follows $\eta=0$ immediately, because $v\mapsto\eta(v)$ is an antisymmetric map.

Whether or not $T^{\perp}F$ is integrable, we can orthogonally split the tensor bundle over M, following Kundu (1978). To perform this task we start with the two-dimensional Riemannian manifold $(F,\bar{g})$. With our choice of space–time coordinates we have Killing fields $Y_{A}=\partial_{A}$. Their space–time components define projection operators

$$p_{A}{}^{\mu}:=Y_{A}{}^{\mu},\quad p_{A}=\partial_{A},$$

$$p^{A}{}_{\mu}:=\bar{g}^{AB}g_{\mu\nu}p_{B}{}^{\nu},\quad p^{A}=\bar{\nu}^{A}\mathrm{d}t+\mathrm{d}y^{A},$$

where $\bar{\nu}^{A}:=\bar{g}^{AB}\bar{\nu}_{B}=\nu^{A}$, and the metric components g_{1B} are zero by our definition of the coordinates.

The projection operators into $T^{\perp}F$ can now be defined as follows: Let the unit normal vectors n and m serve as projection operators $q_{a}{}^{\mu}$ and define their duals by the relations $q_{a}{}^{\mu}q^{b}{}_{\mu}=\delta_{a}^{b}$ and $p_{A}{}^{\mu}q^{b}{}_{\mu}=0$. The result is

$$q_{0}=n=N^{-1}(\partial_{t}-\nu^{i}\partial_{i}),\quad q_{1}=m=A^{-1}\partial_{1},$$

$$q^0 = N\,\mathrm{d}t, \quad q^1 = A\,\nu^1 dt + A\,\mathrm{d}x.$$

Now we are ready to define the transversal metric $\underline{g}$ in $T^\perp F$ by

$$\underline{g}_{ab} = g_{\mu\nu} q_a{}^\mu q_b{}^\nu, \tag{6}$$

thus in the given frame $\underline{g}$ and its inverse are represented by the two-dimensional Minkowski metric and from now on we consider $\underline{g}$ as an intrinsic object in the tensor bundle over $T^\perp F$. In summary we have constructed a complete set of projection operators, projecting orthogonally tensors over (TM,g) into $(TF,\overline{g})$ and $(T^\perp F,\underline{g})$, characterized by the relations

$$p_A{}^\mu p^A{}_\nu + q_a{}^\mu q^a{}_\nu = \delta^\mu_\nu \quad \text{(completeness)},$$

$$p_A{}^\mu p^B{}_\mu = \delta^B_A, \quad p_A{}^\mu q^b{}_\mu = 0,$$

$$q_a{}^\mu p^B{}_\mu = 0, \quad q_a{}^\mu q^b{}_\mu = \delta^b_a \quad \text{(orthogonality)},$$

with $p_A = \partial_A$ and $q_0 \perp q_1$ (these two relations fix the component representations shown previously).

Now we define the convention already used in some expressions previously mentioned that wherever confusion might arise, we attach a bar to quantities, which will be considered as intrinsic to the associated bundle, and a tensor index furnished with such a bar denotes projected components, which also can be considered as intrinsic. For example $\underline{T}_{ab}$ denotes a tensor in the bundle $(T^\perp F,\underline{g})$, but $T_{\underline{ab}} = q_a{}^\mu q_b{}^\nu T_{\mu\nu}$, too, although T might be a space–time tensor. The philosophy lying beyond this $\underline{\ }$ notation is that quantities with a bar attached to them or to their indices can be manipulated by the associated metric, while indices without a bar always denote component indices corresponding to the bundle the tensor is intrinsic to. If we apply this notational convention to the metric itself we get the definitions for $\underline{g}$ and $\overline{g}$ back, e.g., we get the identities $g_{\underline{ab}} = q_a{}^\mu q_a{}^\nu g_{\mu\nu} = \underline{g}_{ab}$ and $g_{\overline{AB}} = p_A{}^\mu p_B{}^\nu g_{\mu\nu} = \overline{g}_{AB}$. In particular we have

$$\underline{\nabla}_a = q_a{}^\mu {}^4\nabla_\mu,$$

$$\overline{\nabla}_A = p_A{}^\mu {}^4\nabla_\mu,$$

defining the Levi-Civita connection in the projected bundles, and the algebraic identity

$$T^\mu_\nu = T^{\underline{a}}_{\underline{a}} + T^{\overline{A}}_{\overline{A}}.$$

For later use we need the projected components of the Ricci tensor. First note that the normal connection η on $(F,\overline{g})$ reads in our new notation

$$\overline{\eta}^A = -\tfrac{1}{2}[q_0,q_1]^{\overline{A}} = -\tfrac{1}{2} p^A{}_\mu [q_0,q_1]^\mu = \tfrac{1}{2} dp^A(q_0,q_1),$$

or equivalently $\epsilon_{ab}\overline{\eta}^A = 1/2\mathrm{d}p^A(q_a,q_b)$, making use of the relation $0 = \nabla(p^A{}_\mu q_a{}^\mu)$, which gives $\nabla q_a{}^\mu = -q_a{}^\nu p_B{}^\mu \nabla p^B{}_\nu$. The ϵ_{ab} here has its standard meaning as the totally antisymmetric symbol (independent of the frame used, so it is not necessary here to attach a bar to it). On $T^\perp F$ we find $\mathrm{d}p_A = \mathrm{d}(\overline{g}_{AB}p^B) = \overline{g}_{AB}\,\mathrm{d}p^B$, so that index manipulations with $\overline{g}$ can be applied, as desired.

After some calculations we arrive at formulas for the projected components of the Ricci tensor:

$${}^4R_{\underline{ab}} = \underline{R}_{ab} - 2r^{-1}\underline{\nabla}_a\underline{\nabla}_b r + 2r^{-2}(\underline{\nabla}_a r)(\underline{\nabla}_b r) + \tfrac{1}{4}(\underline{\nabla}_a \overline{g}_{AB})(\underline{\nabla}_b \overline{g}^{AB}) + 2\underline{g}_{ab}|\,\eta|^2, \tag{7a}$$

$${}^4R_{\overline{A}\underline{b}} = r^{-2}\epsilon^c{}_b \underline{\nabla}_c (r^2 \overline{\eta}_A), \tag{7b}$$

$$ {}^4\overline{R}_{AB} = -\tfrac{1}{2}\overline{g}_{AD}\underline{\nabla}^c(\overline{g}^{CD}\underline{\nabla}_c\overline{g}_{BC}) - r^{-1}(\underline{\nabla}^c r)(\underline{\nabla}_c\overline{g}_{AB}) - 2\,\overline{\eta}_A\overline{\eta}_B\,. \tag{7c} $$

Contraction of the last equation yields a formula for the Laplacian of r (note that the Laplacian is really a wave operator in the present situation):

$$ \underline{\Delta} r = \tfrac{1}{2}\,{}^4\overline{R}^{\overline{A}}_{\overline{A}} + r^{-1}(\underline{\nabla}_c r)(\underline{\nabla}^c r) + r\,|\overline{\eta}|^2, \tag{8} $$

Finally we consider other frames of reference and their relation to the frames already in use in the projected spaces. At first we concentrate on $(TF,\overline{g})$, which is canonically endowed with the coordinate vector fields ∂_A. Alternatively we can introduce the orthonormal frame $\{\overline{e}_A\}$, defined by $\overline{e}_A := r^{-1}\tilde{e}_A$, with

$$ \tilde{e}_2 = e^{-W/2}\cosh V/2\,\partial_2 - e^{W/2}\sinh V/2\,\partial_3, $$

$$ \tilde{e}_3 = -e^{-W/2}\sinh V/2\,\partial_2 + e^{W/2}\cosh V/2\,\partial_3\,. $$

The dual frame $\{\overline{\sigma}^A\}$ is defined by $\overline{\sigma}^A := r\tilde{\sigma}^A$, with $(\tilde{\sigma}^A)_\mu(\tilde{e}_B)^\mu = \delta^A_B$, thus

$$ \tilde{\sigma}^2 = e^{W/2}\cosh V/2\,dy^2 + e^{-W/2}\sinh V/2\,dy^3, $$

$$ \tilde{\sigma}^3 = e^{W/2}\sinh V/2\,dy^2 + e^{-W/2}\cosh V/2\,dy^3. $$

Finally we introduce the two-dimensional quotient manifold $B := M/(U(1)\times U(1))$. Then we have isomorphisms $TB \simeq TM/TF \simeq T^\perp F$ and we can consider the metric $\underline{g}$ as acting on TB, so having constructed the two-dimensional (quotient) space–time $(B,\underline{g})$. If we take (t,x) as coordinates of B, then the metric $\underline{g}$ has coordinate components $\underline{g}_{ab} = -(q^0)^2 + (q^1)^2 = (-N^2 + (A\nu^1)^2)\mathrm{d}t^2 + 2A^2\nu^1\mathrm{d}t\,\mathrm{d}x + A^2\mathrm{d}x^2$, giving an alternative way to describe tensor components in $(T^\perp F,\underline{g})$, even if this bundle is not integrable. The dual base $\{\underline{e}_a\}$ to $\{\underline{\sigma}^a = q^a\}$ in $(B,\underline{g})$ has the coordinate components $\underline{e}_0 = N^{-1}(\partial_t - \nu^1\partial_x)$, $\underline{e}_1 = A^{-1}\partial_x$. The component notation just introduced conflicts with the conventions described previously, and in the following sections we are forced to make clear which conventions we will follow.

2. The 3+1-geometry

To describe the three-geometry of an arbitrary symmetric Cauchy surface S, we construct the coordinate system (x',y^A) explicitly. On the surface of symmetry $F \subset S$ we already have coordinates, such that the scaled metric $\tilde{g}$ takes the form (2). In a Gaussian neighborhood of F the metric h of S then has the form $h = \mathrm{d}x'^2 + \sqrt{|h|}\tilde{g}(x')$. Now we introduce a scale factor $a = 2\pi(\int_0^L |h(z)|^{-1/4}\mathrm{d}z)^{-1}$, where L denotes the length of a (projected) geodesic along all of S^1 orthogonal to the orbits F. Define a new coordinate x by $x(x') = a\int_0^{x'}|h(z)|^{-1/4}\mathrm{d}z$, then we get a convenient representation of h as

$$ h(x) = A(x)^2(\mathrm{d}x^2 + a^2\tilde{g}(x)) \tag{9} $$

with $A(x) = a^{-1}|h(x)|^{1/4}$ defined on S^1, and $\tilde{g}$ transforms under some element of $\mathrm{GL}(2,\mathbb{Z})$ like $\overline{g}$ in (3). By the way, from this explicit formula and the definition of $\overline{g}$ in (1) it follows easily that the relation $r = Aa$ holds.

The Laplacian of S acting on functions ψ then has the form

$$ \Delta\psi = -h^{11}\nabla_1\nabla_1\psi + h^{AB}\Gamma^1_{AB}\psi' + \overline{\Delta}\psi $$

$$ = -A^{-2}(\psi'' + A^{-1}A'\psi') + \overline{\Delta}\psi $$

with $\overline{\Delta}\psi = -h^{AB}\partial_A\partial_B\psi$ since $\overline{\Gamma}^C_{AB} = 0$.

Finally we cast the second fundamental form k of S into a convenient form. Set $K := k(m,m) = A^{-2}k_{11}$ and observe $k_{1B} = -{}^4\nabla_B n_1 = -A\,\eta_B$ we get

$$k(x) = A^2 K\,\mathrm{d}x - 2A\,\eta_B\,\mathrm{d}x\,\mathrm{d}y^B + \kappa_{AB}\mathrm{d}y^A\,\mathrm{d}y^B, \tag{10}$$

where all quantities on the right-hand side depend on x. Taking the trace yields the relation

$$H - K = \mathrm{tr}\,\kappa.$$

3. The four-geometry

We will describe the four-geometry (locally) in terms of a PMC foliation by symmetric Cauchy surfaces (Σ, h). It turns out that there is not much left to do. Of course, we need the strong energy condition in M, and we can choose Σ without loss of generality to have nonvanishing second fundamental form. In view of Theorem 2.2 of Paper I this is enough to guarantee the existence of a local in time PMC foliation of a neighborhood of Σ in M. The remaining question is if the leaves of the foliation turn out to be symmetric. But the arguments given in the corresponding place in Paper I do apply to the present situation, since the Laplacian of Σ splits into the Laplacian of F and a part depending only on x, which coincides with the one in the plane symmetric case and we end up with

Proposition 2.1: Let (M,g) be a globally hyperbolic, spatially compact space–time with local $U(1)\times U(1)$ symmetry, obeying the strong energy condition.

Then there exists a local in time PMC foliation $\{S_t\}$ in M, covering a neighborhood $]t_1,t_2[\times\Sigma$ of $\Sigma = S_0$, in M. Moreover, if Σ is symmetric, then all the leaves of the foliation are symmetric, too, and there are coordinates $(x^\mu) = (t,x,y^2,y^3)$ adapted to the foliation, which cast the metric into the form

$$g = \begin{pmatrix} -N^2 + (A\nu^1)^2 + |\overline{\nu}|^2 & A^2\nu^1 & \overline{\nu_2} & \overline{\nu_3} \\ A^2\nu^1 & A^2 & 0 & 0 \\ \overline{\nu_2} & 0 & \overline{g_{22}} & \overline{g_{23}} \\ \overline{\nu_3} & 0 & \overline{g_{32}} & \overline{g_{33}} \end{pmatrix}, \tag{11}$$

where N,A, ν^1, $\nu^A = \overline{\nu^A}$, $\overline{\nu_A} = \overline{g_{AB}}\,\overline{\nu^B}$, $\overline{g} = r^2\tilde{g}$ are functions on $]t_1,t_2[\times S^1$, with $r = Aa$ and $a = a(t)$ only. The quantities with an overbar transform under some representation of $\mathrm{GL}(2,\mathbb{Z})$ after each transition $x \mapsto x + 2\pi$ in S^1. The shift functions are fixed by the conditions $\nu^1(t,0) = \nu^1(t,2\pi) = 0$ and $\nu^A(t,0) = 0$.

The orthonormal frames $\{{}^4e_\mu\}$ and $\{{}^4\sigma^\mu\}$ associated with the $3+1$-split read explicitly

$${}^4e_0 = n = N^{-1}(\partial_t - \nu^i\partial_i),$$

$${}^4e_1 = m = A^{-1}\partial_1,$$

$${}^4e_2 = e_2 = (Aa)^{-1}(+e^{-W/2}\cosh V/2\,\partial_2 - e^{W/2}\sinh V/2\,\partial_3),$$

$${}^4e_3 = e_3 = (Aa)^{-1}(-e^{-W/2}\sinh V/2\,\partial_2 + e^{W/2}\cosh V/2\,\partial_3),$$

$${}^4\sigma^0 = N\,\mathrm{d}t,$$

$${}^4\sigma^1 = A(\nu^1\mathrm{d}t + \mathrm{d}x),$$

$${}^4\sigma^2 = (Aa)(e^{W/2}\cosh V/2(\overline{\nu^2}\,\mathrm{d}t + \mathrm{d}y^2) + e^{-W/2}\sinh V/2(\overline{\nu^3}\mathrm{d}t + \mathrm{d}y^3)),$$

$${}^4\sigma^3 = (Aa)(e^{W/2}\sinh V/2(\overline{\nu^2}\mathrm{d}t + \mathrm{d}y^2) + e^{-W/2}\cosh V/2(\overline{\nu^3}\mathrm{d}t + \mathrm{d}y^3)).$$

Finally, the Ricci rotation coefficients will be calculated. Some expressions are not explicitly given, since they turn out to be too complicated. Instead, the dependence on the geometric quantities involved will be specified in square brackets:

$$
\begin{gathered}
{}^4\gamma^0_{01}={}^4\gamma^1_{00}=A^{-1}N^{-1}N',\\
{}^4\gamma^0_{0B}={}^4\gamma^B_{00}=0,\\
{}^4\gamma^0_{11}={}^4\gamma^1_{01}=-K,\\
{}^4\gamma^0_{1B}={}^4\gamma^B_{10}=(Aa)^{-1}\overline{e}_B{}^C\eta_C,\\
{}^4\gamma^0_{AB}={}^4\gamma^B_{A0}=-\overline{e}_A{}^C\overline{e}_B{}^D\kappa_{CD},\\
{}^4\gamma^1_{01}=0,\\
{}^4\gamma^1_{0B}={}^4\gamma^1_{0B}[N^{-1},\overline{\nu},\overline{\nu}',A,A^{-1},A',a,a^{-1},V,W,V',W',\dot{V},\dot{W}]=-{}^4\gamma^B_{01},\\
{}^4\gamma^C_{0B}={}^4\gamma^C_{0B}[N^{-1},\nu^1,A,A^{-1},A',a,a^{-1},V,W,V',W',\dot{V},\dot{W}],\\
{}^4\gamma^k_{ij}=\gamma^k_{ij}[A^{-1},A',V,W,V',W'].
\end{gathered}
$$

where the dependence on the derivatives of V and W is linear.

B. The field equations

Again we represent the matter quantities by $\rho=T(n,n)$, $j=-T(n,m)=A^{-1}j_1$ and $S_{ij}=T({}^4e_i,{}^4e_j)$.

1. 2+1-decomposition of the constraints

First consider the Hamiltonian constraint

$$R+H^2-|k|^2=16\pi\rho.$$

Decomposing R by the Gauss–Codazzi formula and k by (10) we get

$$m(\mathrm{tr}\lambda)=8\pi\rho-H\,\mathrm{tr}\,\kappa+|\eta|^2+\tfrac{1}{2}(\tfrac{3}{2}(\mathrm{tr}\,\lambda)^2+|\tilde{\lambda}|^2)+\tfrac{1}{2}(\tfrac{3}{2}(\mathrm{tr}\,\kappa)^2+|\tilde{\kappa}|^2). \tag{12}$$

The first component of the momentum constraint

$$\nabla^i k_{i1}-\nabla_1 H=8\pi j_1$$

can be decomposed into

$$m(\mathrm{tr}\,\kappa)=-8\pi j_1-H\,\mathrm{tr}\,\lambda+\tfrac{3}{2}\mathrm{tr}\,\kappa\,\mathrm{tr}\,\lambda+\tilde{\lambda}^{AB}\tilde{\kappa}_{AB} \tag{13}$$

(where the symmetry forced div $\eta=0$). The other components of the momentum constraints are calculated analogously to (again some terms cancel out due to symmetry)

$$m(\eta_B)=-8\pi j_B+(\mathrm{tr}\,\lambda)\,\eta_B. \tag{14}$$

As in Paper I a convenient form of the equation is achieved by introducing the null expansions

$$\vartheta_\pm:=-(\mathrm{tr}\,\lambda\pm\mathrm{tr}\,\kappa)=\frac{2}{r}k_\pm(r) \tag{15}$$

(compare the formulas for λ and κ in Sec. II A 1), which yields an easy formula for the Hawking mass

$$\mathrm{M} := m_H(F) = -\tfrac{1}{8} r(r\vartheta_+)(r\vartheta_-) = -\tfrac{1}{2} r({}^4\nabla^\alpha r)({}^4\nabla_\alpha r), \tag{16}$$

by $\vartheta_+\vartheta_- = 4/r^2({}^4\nabla^\alpha r)({}^4\nabla_\alpha r)$.

Adding and subtracting the constraint equations now yield

$$m(\vartheta_\pm) = -8\pi(\rho \mp j_1) - |\eta|^2 - \tfrac{1}{2}|\tilde{\lambda} \pm \tilde{\kappa}|^2 \mp H\vartheta_\pm - \tfrac{3}{4}\vartheta_\pm^2 \tag{17}$$

and the transition to the variables $\omega_\pm := r\vartheta_\pm$ casts this equation into

$$\begin{aligned} m(\omega_\pm) &= m(r)\vartheta_\pm + r m(\vartheta_\pm) \\ &= -8\pi r(\rho \mp j_1) - r|\eta|^2 - \frac{1}{2} r|\tilde{\lambda} \pm \tilde{\kappa}|^2 \mp H\omega_\pm + \frac{1}{4\pi}(\omega_+\omega_- - 2\omega_\pm^2), \end{aligned} \tag{18}$$

where the identity $m(r)\vartheta_\pm = (1/4\pi)((\omega_+ + \omega_-)\omega_\pm)$ has been used.

2. 2+2-decomposition of the field equations

With the $2+2$-geometry in mind, where we denote tensor components with respect to the frame of projection operators $\{q_a, p_A\}$, we write Eq. (7a) for ${}^4\underline{R}_{ab}$ in terms of $\tilde{g}$,

$${}^4\underline{R}_{ab} = \underline{R}_{ab} - 2r^{-1}\underline{\nabla}_a\underline{\nabla}_b r + \tfrac{1}{4}(\underline{\nabla}_a\tilde{g}_{AB})(\underline{\nabla}_b\tilde{g}^{AB}) + 2\underline{g}_{ab}|\eta|^2,$$

as a field equation in the quotient space–time $(B, \underline{g})$ for the radius function r. We still have to eliminate the unknown $\underline{R}_{ab} = -\underline{K}\underline{g}_{ab}$, where $\underline{K} := \underline{R}_{0101}$ denotes the Gaussian curvature of $(B, \underline{g})$ in (M, g). Contracting the equation for $\underline{R}_{ab}$ and replacing $\underline{\Delta} r$ by (8) yields an equation for $\underline{K}$:

$$\underline{K} = \tfrac{1}{2}(-{}^4\underline{R}^c_{\underline{c}} + {}^4\underline{R}^A_{\underline{A}}) + r^{-2}(\underline{\nabla}^c r)(\nabla_{\underline{c}} r) + \tfrac{1}{8}(\underline{\nabla}^c\tilde{g}_{AB})(\underline{\nabla}_c\tilde{g}^{AB}) + 3|\eta|^2.$$

Inserting this into the equation for ${}^4\underline{R}_{ab}$ results in

$$\begin{aligned} \underline{\nabla}_a\underline{\nabla}_b r = &-\tfrac{1}{2} r^{-1}(\underline{\nabla}^c r)(\underline{\nabla}_c r)\underline{g}_{ab} - \tfrac{1}{2} r({}^4\underline{R}_{ab} - \tfrac{1}{2}({}^4\underline{R}^c_{\underline{c}} - {}^4\underline{R}^{\overline{A}}_{\overline{A}})\underline{g}_{ab}) \\ &+ \tfrac{1}{8} r((\underline{\nabla}_a\tilde{g}_{AB})(\underline{\nabla}_b\tilde{g}^{AB}) - \tfrac{1}{2}(\underline{\nabla}^c\tilde{g}_{AB})(\underline{\nabla}_c\tilde{g}^{AB})\underline{g}_{ab}) - \tfrac{1}{2} r|\eta|^2\underline{g}_{ab}. \end{aligned}$$

Now we are going to interpret the first three terms appearing on the right-hand side of the field equation: Recalling the definition of the mass function M in (16) we can write the first term as $(M/r^2)\underline{g}_{ab}$. The curvature expression in the second term can be rewritten using Einstein's equations in terms of the projected energy momentum tensor $\underline{T}$ in the form $8\pi(\underline{T}_{ab} - \mathrm{tr}\underline{T}\,\underline{g}_{ab})$.

To simplify the third term, there is more structure involved than already presented. The space of two-dimensional metrics Bil(2, $\mathbb{R}$) is a three-dimensional real vector space, whose elements we denote by $\tilde{\phi} = \tilde{\phi}^i E_i$, where the basis $\{E_i\}$ has been chosen as $E_1 = \left(\begin{smallmatrix}1 & 0\\ 0 & 1\end{smallmatrix}\right)$, $E_2 = \left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$, $E_3 = \left(\begin{smallmatrix}0 & 1\\ 1 & 0\end{smallmatrix}\right)$. In this picture the determinant is a quadratic form on Bil(2, $\mathbb{R}$), and the matrix representation with respect to the given basis turns out to be $-\eta_{ij}$, where $\eta_{ij} = \mathrm{diag}(-++)$ denotes the standard Minkowski metric in three-dimensional Minkowski space. The restriction of this space to the hypersurface $\eta(\tilde{\phi}, \tilde{\phi}) = -1 \Leftrightarrow \det\tilde{\phi} = 1$ is the well-known hyperbolic plane H^2, and we have established a correspondence between the two-dimensional unit-determinant metrics $\tilde{g}$ and the elements of the hyperbolic plane. Considering $\tilde{\phi}$ as a function on the quotient manifold B, introduced in Sec. II A 1, we have a map $\tilde{\phi}: (B, \underline{g}) \to (H^2 \subset \mathbb{R}^{2,1}, \eta_{ij})$, $(t,x) \mapsto \tilde{\phi}^i(\tilde{g}(t,x))E_i$. Now let us interpret $\tilde{\phi}$ for a moment as a wave map from B to H^2, then the energy–momentum tensor ${}^\phi\underline{T}$ associated with $\tilde{\phi}$ reads

$$ {}^{\phi}\underline{T}_{ab} = \underline{\nabla}_a \tilde{\phi}^i \underline{\nabla}_b \tilde{\phi}_i - \tfrac{1}{2}(\underline{\nabla}^c \tilde{\phi}^i \underline{\nabla}_c \tilde{\phi}_i)\underline{g}_{ab} \tag{19} $$

and with the correspondences $\tilde{\phi}_i = \eta_{ij}\tilde{\phi}^j = -\tilde{g}^{AB}$ and $\tilde{\phi}_i\tilde{\phi}^i = -\frac{1}{2}\tilde{g}_{AB}\tilde{g}^{AB}$, we see that the third term in the field equation for r can be rewritten as $-\frac{1}{4}r\,{}^{\phi}\underline{T}_{ab}$.

Collecting all these things together we get the field equation for r in a convenient form:

$$ \underline{\nabla}_a\underline{\nabla}_b r = \frac{M}{r^2}\underline{g}_{ab} - 4\pi r(\underline{T}_{ab} - \operatorname{tr}\underline{T}\underline{g}_{ab}) - \frac{1}{4}r\,{}^{\phi}\underline{T}_{ab} - \frac{1}{2}r|\eta|^2\underline{g}_{ab}. \tag{20} $$

Differentiating the mass function we find for the mass flux equation the formula

$$ \underline{\nabla}_a M = (4\pi r^2(\underline{T}_{ab} - \operatorname{tr}\underline{T}\underline{g}_{ab}) + \tfrac{1}{4}r\,{}^{\phi}\underline{T}_{ab})(\underline{\nabla}^b r) + \tfrac{1}{2}r^2|\eta|^2\underline{\nabla}_a r. \tag{21} $$

The contribution of ${}^{\phi}\underline{T}$ to the right-hand sides of these equations is known insofar that ${}^{\phi}\underline{T}$ obeys the dominant and strong energy conditions. Furthermore, we can again rewrite its components using the formulas for the trace free parts of λ and κ in Sec. II A 1 (remember that ∇_0, ∇_1 act as n, respectively, m, on $\tilde{g}$, in the formula for ${}^{\phi}\underline{T}_{ab}$). The result is

$$ {}^{\phi}\rho = {}^{\phi}p = |\tilde{\lambda}|^2 + |\tilde{\kappa}|^2, \tag{22a} $$

$$ {}^{\phi}j_{\underline{1}} = -2\tilde{\lambda}_{AB}\tilde{\kappa}^{AB}. \tag{22b} $$

Now we want to analyze the underlying wave map. To make things more explicit, consider the parameters V, W of $\tilde{g}$ as coordinates of H^2 in view of the correspondence $\tilde{\phi}^i E_i$. The pullback under this parametrization yields a representation $\hat{h}$ of the metric $(\eta_{ij})_{|H^2}$, with the explicit form $\hat{h}_{IJ} = \mathrm{d}V^2 + (\cosh V)^2\mathrm{d}W^2$, leading to $\hat{\Gamma}^3_{23} = \tanh V$ and $\hat{\Gamma}^2_{33} = -\sinh V\cosh V$ as nonvanishing Christoffel symbols. The pullback of the map $\tilde{\phi}$ under this parametrization induces a map $\phi:(B,\underline{g})\to(H^2,\hat{h})$, $\phi(t,x) = (V(t,x),W(t,x))$. The wave map ϕ is then defined to obey

$$ \underline{\nabla}^c\underline{\nabla}_c\phi^K + \hat{\Gamma}^K_{IJ}\underline{\nabla}^c\phi^I\underline{\nabla}\phi^J = 0. \tag{23} $$

Let us turn back to the field equations. Writing Eq. (7c) in the form

$$ {}^4\overline{R_{AB}} + 2\,\overline{\eta}_A\,\overline{\eta}_B = -\tfrac{1}{2}r^{-2}\overline{g}_{AD}\underline{\nabla}^c(r^2\overline{g}^{CD}\underline{\nabla}_c\overline{g}_{BC}) = -\tfrac{1}{2}\tilde{g}_{AD}\underline{\nabla}^c(\tilde{g}^{CD}\underline{\nabla}_c r^2\tilde{g}_{BC}) $$

we arrive after some calculation at

$$ \underline{\nabla}^c(r^2\underline{\nabla}_c\tilde{g}_{AB}) = r^2\tilde{g}^{CD}(\underline{\nabla}^c\tilde{g}_{AD})(\underline{\nabla}_c\tilde{g}_{BC}) - 16\pi(\overline{T}_{AB} - \tfrac{1}{2}\operatorname{tr}\overline{T}\overline{g}_{AB}) - 4(\overline{\eta}_A\,\overline{\eta}_B - \tfrac{1}{2}|\eta|^2\overline{g}_{AB}), $$

where $\overline{T}$ denotes the orthogonal projection of the energy momentum tensor T into $(F,\overline{g})$. More explicitly we get

$$ \begin{aligned} \underline{\nabla}^c(r^2\underline{\nabla}_c V) = {} & r^2\sinh V\cosh V(\underline{\nabla}^c W)(\underline{\nabla}_c W) - 2r^2(\cosh V)^{-1}((T_{23} - \tfrac{1}{2}\tilde{g}^{AB}T_{AB}\tilde{g}_{23}) \\ & - \tfrac{1}{2}(\eta_2\eta_3 - \tfrac{1}{2}\tilde{g}^{AB}\eta_A\eta_B\tilde{g}_{23})), \end{aligned} \tag{24a} $$

$$ \begin{aligned} \underline{\nabla}^c(r^2\underline{\nabla}_c W) = {} & -r^2\tanh V(\underline{\nabla}^c W)(\underline{\nabla}_c V) - r^2(\cosh V)^{-1}((e^{-W}T_{22} - e^{W}T_{33}) \\ & - \tfrac{1}{2}(e^{-W}(\eta_2)^2 - e^{W}(\eta_3)^2)), \end{aligned} \tag{24b} $$

or

$$ \begin{aligned} \underline{\nabla}^c\underline{\nabla}_c V - \sinh V\cosh V(\underline{\nabla}^c W)(\underline{\nabla}_c W) = {} & -2/r(\underline{\nabla}^c r)(\underline{\nabla}_c V) - 2(\cosh V)^{-1}((T_{23} - \tfrac{1}{2}\tilde{g}^{AB}T_{AB}\tilde{g}_{23}) \\ & - \tfrac{1}{2}(\eta_2\eta_3 - \tfrac{1}{2}\tilde{g}^{AB}\eta_A\eta_B\tilde{g}_{23})), \end{aligned} \tag{25a} $$

$$\nabla^c\nabla_c W+\tanh V(\nabla^c W)(\nabla_c V)=-2/r(\nabla^c r)(\nabla_c W)-(\cosh V)^{-1}((e^{-W}T_{22}-e^{W}T_{33}) -\tfrac{1}{2}(e^{-W}(\eta_2)^2-e^{W}(\eta_3)^2)). \tag{25b}$$

The left-hand sides of Eq. (25) coincide with the left-hand side of (23) and we conclude that V and W solve an inhomogeneous wave map.

3. 3+1-decomposition of the field equations

Now we want to calculate the ADM equations and bring them into a form most similar to the equations in the plane symmetric case of Paper I. The formulas concerning the three-geometry in Sec. III A 2 are of particular importance for the calculations here, as well as the definitions of λ, κ, and η in Sec. II A 1. A straightforward calculation then yields the following set of equations.

The constraint equations,

$$(A^{1/2})''=\tfrac{1}{8}A^{5/2}(H^2-\tfrac{1}{2}(H-K)^2-K^2-|\tilde{\kappa}|^2-|\tilde{\lambda}|^2-2|\eta|^2-16\pi\rho), \tag{26}$$

$$K'=-3A^{-1}A'K+A^{-1}A'H+H'-A\tilde{\kappa}_{AB}\tilde{\lambda}^{AB}+8\pi Aj, \tag{27}$$

$$\eta_B'=-2A^{-1}A'\eta_B-8\pi Aj_B. \tag{28}$$

The equations fixing the foliation,

$$N''=-A^{-1}A'N'+A^2N(\tfrac{1}{2}(H-K)^2+K^2+|\tilde{\kappa}|^2+2|\eta|^2+4\pi(\rho+\mathrm{tr}\,S))-A^2, \tag{29}$$

$$\dot{H}=1+\nu^1H', \tag{30}$$

$$(\partial_t-\nu^1\partial_x)H'=\nu^{1'}H'. \tag{31}$$

The evolution equations,

$$\dot{A}=-NAK+A\nu^{1'}+A'\nu^1, \tag{32}$$

$$\dot{a}=-\tfrac{1}{2}Na(H-3K)-a\nu^{1'}, \tag{33}$$

$$\dot{K}=\nu^1K'-A^{-2}(N''-A^{-1}A'N')+N(-4A^{-5/2}(A^{1/2})''+(A^{-2}A')^2 +HK-|\tilde{\lambda}|^2+2|\eta|^2-8\pi(A^{-2}S_{11}+\tfrac{1}{2}(\rho-\mathrm{tr}\,S))), \tag{34}$$

$$\dot{\eta}_B=(\tfrac{1}{2}N(H+K)-2A^{-1}A'\nu^1)\eta_B-2N\tilde{\kappa}_{BC}\eta^C+\tfrac{1}{2}A^{-2}A'(H-K)\nu_B -(\tilde{\kappa}_B^D\tilde{\lambda}_{DC}+\tfrac{1}{2}(H-K)\tilde{\lambda}_{BC}-A^{-2}A'\tilde{\kappa}_{BC})\nu^C-8\pi A\nu^1j_B. \tag{35}$$

As in Paper I integration of (33) over the circle yields the analogous equation for the first component of the shift vector,

$$\nu^{1'}=-\frac{1}{2}N(H-3K)+\frac{1}{2}\int_{S^1}N(H-3K) \tag{36}$$

and the definition of the second fundamental form provides some additional equations, namely

$$\nu^{B'}=-2NA\eta^B \tag{37}$$

and the coordinate representations of λ and κ in Sec. II A 1. The remaining equations for V and W are still missing. To this end we supplement the system (26)–(37) by the field equations (24) or (25), and end up with the full system of equations.

As in the plane symmetric case, we can formulate an existence and uniqueness theorem for solutions of Eqs. (26)–(37), (25). First we define a *symmetric initial data set* for a space–time with local $U(1)\times U(1)$ symmetry by the smooth collection (Σ,h,k), where Σ denotes a (possibly nontrivial) torus bundle over the circle and the fundamental forms h and k are represented in a suitable coordinate system as (9) and (10), respectively. If there are matter fields, then we assume the matter data and equations to be smooth and symmetric, leading to a well-posed Cauchy problem coupled to the reduced field equations in harmonic coordinates.

On the universal cover $\hat{\Sigma}$ of Σ the induced data then is invariant under the action of G, hence G acts isometrically on the whole Cauchy development, which induces a local $U(1)\times U(1)$ symmetry on the Cauchy development of (Σ,h,k). Assuming $\lambda := |k|^2 + 4\pi(\rho + \operatorname{tr} S) > 0$ somewhere on Σ, we get for $t_0 \in \mathbb{R}$ a unique symmetric local in time PMC foliation, defined on some time interval containing t_0, with $\Sigma = S_{t_0}$, and coordinates described in Proposition 2.1 and we just have proved:

Proposition 2.2: Let (Σ,h,k) *be a symmetric initial data set for a space–time with local* $U(1)\times U(1)$ *symmetry, with matter obeying the strong energy condition and* $\lambda > 0$ *somewhere on* Σ. *Further, let* t_0 *denote an arbitrary real number.*

Then there exists a $\delta > 0$ *and a PMC foliated surface symmetric space–time* $(\overline{M},\tilde{g})$ *diffeomorphic to* $]t_0-\delta,t_0+\delta[\times\Sigma$ *with an embedding* $\iota:\Sigma\to\overline{M}$, *satisfying* $\iota(\Sigma) = S_{t_0}$ *and* $\iota_* h$, $\iota_* k$ *are the first and second fundamental form of* S_{t_0} *in* $(\overline{M},\overline{g})$. $(\overline{M},\overline{g})$ *obeys the strong energy condition and* $\overline{g}$ *can be written in the form described in Proposition 2.1. This construction is unique up to the choice of* t_0 *and* δ.

4. The expanding model

Now we can proceed in close analogy to the corresponding analysis in Paper I. Formula (16) for the Hawking mass shows that $\operatorname{grad} r$ is timelike as long as $m > 0$. Indeed, Proposition 3.1 in Rendall (1997) proves this, provided the space–time is not flat and the dominant energy condition holds.

Therefore, under these conditions $\operatorname{grad} r$ is timelike and ϑ_+, ϑ_- have fixed and opposite signs. Without loss of generality we choose the time orientation, such that r is past pointing and $\mathrm{d}r$ is future pointing (by the induced time orientation of the cotangent bundle). Then $\vartheta_+ > 0$ and $\vartheta_- < 0$ which classifies the space–time as expanding in the sense described in Paper I.

Again we expect the singularity in the distant past from our symmetric initial data Cauchy surface Σ and any symmetric Cauchy surface S in M is not maximal with mean curvature not everywhere positive on S.

C. *A priori* estimates for the field equations

Assume the dominant and strong energy condition to be fulfilled in (M,g). Let Σ be a symmetric Cauchy surface in M with strictly negative mean curvature H and denote by $\{S_t\}$, $t \in]t_1,t_2[$ the local in time PMC foliation with $\Sigma = S_0$ and the time orientation chosen in correspondence with Sec. II B D, such that H decreases with decreasing PMC time.

We consider the past $D^-(\Sigma)$ of Σ. In $D^-(\Sigma)$ the mean curvature is bounded from above by some $\overline{H} < 0$, and $H = \overline{H}$ only on Σ. Thus $|H|$ is bounded from below and as long as H remains finite, we find the following estimates.

Consider first the constraint equation in the form (18). The dominant energy condition gives the inequality

$$m(\omega_\pm) \leqslant \mp H\omega_\pm + \frac{1}{4\pi}(\omega_+\omega_- - 2\omega_\pm^2),$$

from which we infer the basic estimate

$$|\vartheta_{\pm}| \leqslant 4|H| \Rightarrow |A^{-2}A'| \leqslant C, \quad |K| \leqslant C. \tag{38}$$

Now we can perform nearly the same estimates, as we have done in the corresponding place in Paper I. The additional terms appearing here in the more general equations (26)–(27), (29)–(33), and (36) do not cause any problems. There is only one additional estimate, which will become important in our further analysis, resulting from the integration of Eq. (26) along S^1, bounding not only $\int_{S^1}\rho$, but also $\int_{S^1}(|\tilde{\lambda}|^2+|\tilde{\kappa}|^2+|\eta|^2)=\int_{S^1}({}^{\phi}\rho+|\eta|^2)$, and we can state the analogous

Proposition 2.3: Let (M,g) *be a globally hyperbolic, spatially compact space–time with local* $U(1)\times U(1)$ *symmetry, obeying the dominant and strong energy condition. Assume the existence of a symmetric Cauchy surface* Σ *with strictly negative mean curvature. In particular we get from proposition 2.1 a PMC time coordinate t, ranging in* $]t_1,t_2[$ *with* $\Sigma=\{t=0\}$ *and H decreases with decreasing t.*

Then we have uniformly on $]t_1,0]$

$$|A|,|A^{-1}|,|A'|,|a|,|a^{-1}|,|H|,|H'|,|K|,|N|,|N^{-1}|,|N'|,|\nu^1|,|\nu^{1\prime}| \leqslant C.$$

Until now the control over the coefficients of the fundamental forms h and k is not complete. We still need bounds for the metric coefficients V, W, the components η and κ of k and the remaining components ν^B of the shift vector. We will get bounds for most of these quantities here in this section, using the bound for $\int_{S^1}(\rho+{}^{\phi}\rho+|\eta|^2)$.

Proposition 2.4: Under the hypotheses of Proposition 2.3 we get uniform bounds for

$$|V|,|W|,|\eta_B|,|\nu^B|,|\nu^{B\prime}|$$

on $]t_1,0]$.

Proof: The bounds for η_B, ν^B and $\nu^{B\prime}$ are simple consequences of the bounds for V and W, since having bounded them, we can conclude as follows: The bounds for V and W allow coordinate components to be bounded in terms of components according to the orthonormal frame vectors $\overline{e_2}$, $\overline{e_3}$ in $(F,\overline{g})$ defined in Sec. II A 1. We adopt the convention, that a caret above indices denotes components with respect to an orthonormal frame. Having this in mind we see, that $\int_{S^1}\rho$ bounds $\int_{S^1}j_B \leqslant C\int_{S^1}j_B$ by the dominant energy condition, so integration of the constraint (28) yields a bound for the difference $A^2\eta_B|_{x_1}^{x_2}$, which is independent of t. Using $\eta_B \leqslant C\hat{\eta_B} \leqslant C(1+|\eta|^2)$ we can bound integral $\int_{S^1}|A^2\eta_B|$ by $C\int_{S^1}(1+|\eta|^2)$, which together with the estimated difference yields the desired estimate for η_B. Now we get immediately a bound for $\nu^{B\prime}$ by inspection of Eq. (37), and the condition $\nu^B(t,0)=0$ bounds ν^B.

Let us now investigate the field equations (24) for V and W, considered as equations on $(B,\underline{g})$ endowed with the coordinates (t,x), as described in the end of Sec. II A 1. Then we calculate explicitly in these coordinates

$$\begin{aligned}|\tilde{\lambda}|^2+|\tilde{\kappa}|^2 &= \tfrac{1}{4}(m(\tilde{g}_{AB})m(\tilde{g}^{AB})+n(\tilde{g}_{AB})n(\tilde{g}^{AB}))\\ &= \tfrac{1}{2}A^{-2}(V'^2+(\cosh V)^2W'^2)+\tfrac{1}{2}N^{-2}((\dot{V}-\nu^1V')^2\\ &\quad +(\cosh V)^2(\dot{W}-\nu^1W')^2),\end{aligned}$$

and we see that the first term on the right-hand side of Eq. (24) can be bounded in terms of this expression.

For the second term on the right-hand side of (24) we exploit the special structure appearing there. The first aim is to express the tensor components with respect to an orthonormal frame. Looking at the definitions of the coframe $\{\overline{\sigma}^B\}$ defined in Sec. II A 1 we recognize the relations

$$e^{W/2}\mathrm{d}y^2 = r^{-1}(+\cosh V/2\overline{\sigma}^2-\sinh V/2\overline{\sigma}^3),$$

$$e^{-W/2}\mathrm{d}y^3 = r^{-1}(-\sinh V/2\,\overline{\sigma}^2 + \cosh V/2\,\overline{\sigma}^3).$$

If we mark tensor components expressed in this basis by a tilde, we see that the terms in brackets in both equations (24) are easily rewritten with respect to this basis, by simply putting a tilde above each tensor component and deleting the factors $e^{\pm W/2}$. But we have schematically $\eta = \eta_B\,\mathrm{d}y^B = \widetilde{\eta}_B e^{\pm W/2}\,\mathrm{d}y^B = f_B(\cosh V/2)\,\widetilde{\eta}_B\,\overline{\sigma}^B$, with $f_B(\cosh V/2)\,\widetilde{\eta}_B = \eta_{\hat{B}}$ is the component according to the orthonormal frame. A similar relation holds for T_{AB}. Since we have $\eta_{\hat{B}} \leqslant 1 + |\eta|^2$ and $T_{\hat{A}\hat{B}} \leqslant \rho$ we conclude that the terms in brackets in (24) are bounded by $C\cosh V(1+\rho+|\eta|^2)$, which leads together with our result about the first term on the right-hand side of (24) to

$$|\underline{\nabla}^c(r^2\underline{\nabla}_c\phi)| \leqslant C(1+\rho+|\widetilde{\lambda}|^2+|\widetilde{\kappa}|^2+|\eta|^2),$$

and since the integration of the right-hand side along S^1 is already bounded we get

$$\int_{S'} |\underline{\nabla}^c(r^2\underline{\nabla}_c\phi)| \leqslant C$$

uniformly for each $t \in]t_1,0]$. Note that we use the wave map $\phi=(V,W)$ defined in Sec. II B 2 in order to abbreviate some formulas only.

On the other hand, we can interpret the integrated quantity as a divergence, a fact we will take advantage of to get rid of the integral sign. To this end consider a point (t,x) in the quotient manifold B, with $t \in]t_1,0[$. We need estimates uniformly in t for t approaching t_1. We define the (upside down) characteristics triangle T in B, by its counterclockwise oriented boundary $\partial T = \gamma_+ + \gamma_0 + \gamma_-$, where $\gamma_\pm$ denote the characteristic curves of (24), with $\dot{\gamma}_\pm = k_\pm = m \pm n$ connecting (t,x) with $(0,x_\pm)$ and γ_0 is the curve in the hypersurface $\{t=0\}$ from $(0,x_+)$, to $(0,x_-)$ with $\dot{\gamma}_0 = -m$. Define $v \in T^\perp F$ by $v^a = r^2\underline{\nabla}^a\phi$, then the corresponding one-form ω reads $\omega = \iota(v)\underline{\Omega}$, where $\underline{\Omega}$ denotes the volume form with respect to $\underline{g}$. Expressing tensor components with respect to the project orthonormal frame $\{\underline{e}_a = q_a\}$ (see Sec. II A 1) we have $v^a = r^2\binom{-\nabla_0\phi}{\nabla_1\phi}$, and $\omega = -r^2(m(\phi)\underline{e}^0 + n(\phi)\underline{e}^1)$. The pullback of ω along ∂T has the three parts $\gamma_\pm^*\omega = \mp r^2 k_\pm(\phi\circ\gamma_\pm(u))du$, $\gamma_0^*\omega = r^2 n(\phi(x))A\,\mathrm{d}x$. Thus, setting $\tau := \sqrt{2}t$,

$$\begin{aligned}
\int_{\partial T}\omega &= \int_\tau^0 -r^2 k_+(\phi(\gamma_+(u)))\mathrm{d}u + \int_{x_+}^{x_-} n(\phi(x))A\,\mathrm{d}x + \int_0^\tau + r^2 k_-(\phi(\gamma_-(u)))\mathrm{d}u \\
&= -\int_\tau^0 r^2 k_+(\phi(\gamma_+(u)))\mathrm{d}u - \int_\tau^0 r^2 k_-(\phi(\gamma_-(u)))\mathrm{d}u + \int_{x_+}^{x_-} n(\phi(x))A\,\mathrm{d}x \\
&= -r^2\phi|_{\gamma_+(r)}^{\gamma_+(0)} - r^2\phi|_{\gamma_-(r)}^{\gamma_-(0)} + \int_\tau^0 k_+(r^2)\phi + \int_\tau^0 k_-(r^2)\phi + \int_{x_+}^{x_-} n(\phi(x))A\,\mathrm{d}x,
\end{aligned}$$

where integration by parts has been carried out in the last step. Note, that the last term is bounded, since that integration takes place on the line $t=0$ in B, where ϕ is smooth. In addition $k_\pm(r^2)$ is bounded everywhere by Proposition 2.3. Further, the first terms can be evaluated to $-r^2\phi|_{\gamma_+(\tau)}^{\gamma_+(0)} - r^2\phi|_{\gamma_-(\tau)}^{\gamma_-(0)} = 2(r^2\phi)(t,x) - (r^2\phi)(0,x_+) - (r^2\phi)(0,x_-)$, where the last two terms live on the line $t=0$, and therefore are bounded.

Stokes' theorem now applies to the present situation, $\int_{\partial T}\omega = \int_T \mathrm{d}w = \int_T (\mathrm{div}\,v)\underline{\Omega}$. Putting all this together we get an estimate

$$\|r^2\phi(t)\|_{L^\infty} \leqslant C\left(1 + \int_t^0 \|r^2\phi(s)\|_{L^\infty}\,\mathrm{d}s + \int_t^0\int_{S'} |\underline{\nabla}^c(r^2\underline{\nabla}_c\phi)|\mathrm{d}s\right),$$

where the last term is already known to be bounded uniformly in t by our previous analysis. Hence we can apply Gronwall's inequality and the bounds for r, r^{-1} obtained in Proposition 2.3 complete our argument, arriving finally at $|V|$, $|W| \leq C$ uniformly on $]t_1,0[$. ■

Unfortunately, there is still a lack of control over the components κ of k [respectively, its traceless part, since $(\mathrm{tr}\,\kappa)\underline{g} = (H-K)\underline{g} \leq C$]. It turns out, that the necessary bounds for the first derivatives of ϕ depend on a bound for the matter quantities and vice versa. The analysis of this dependence will be performed in Sec. II D, where we have to take a specific matter model into account.

D. Higher order estimates

1. First-order estimates

We start with the derivation of first-order estimates for the metric coefficients $\phi = (V,W)$. To keep things simple, we consider collisionless matter, as described by the Einstein–Vlasov system.

The particle density f on the mass shell is governed by the geodesic spray X with $X = v^\alpha\, {}^4e_\alpha - {}^4\gamma^\kappa_{\mu\nu} v^\mu v^\nu (\partial/\partial v^\kappa)$, and the killing vector fields ∂_A define two conserved quantities $g(X,\partial_A)$, which bound v^A. To bound v^1 we consider the characteristics of the Vlasov equation (compare the explicit formulas in Paper I):

$$\frac{\mathrm{d}v^1}{\mathrm{d}s} = -(e_1(N)v^0 + N(-k_{rs}e_1{}^r e_j{}^s + {}^4\gamma^1_{0j})v^j + N\gamma^1_{jk}v^j v^k/v^0) \leq C(1 + Q_1(s) + v^1(s)),$$

where $Q_1 := \|\underline{D}\phi\|_{D^\infty}$, $\underline{D} := (\partial_t, \partial_x)$ and we used the fact, that in view of the boundedness of v^A, the vanishing of ${}^4\gamma^1_{01}$ and the special form of the nonvanishing rotation coefficients no term involving the product $Q_1 v^1$ occurs. Thus we find for the quantity $\overline{P_f}(s) = \{\sup|v| \,|\, v \in \mathrm{supp}\, f\}$ (which measures the matter quantities, compare Paper I the Gronwall-like estimate

$$1 + \overline{P_f}(t) \leq C\left(1 + \overline{P_f}(0) + \int_t^0 (\overline{P_f}(s) + Q_1(s))\mathrm{d}s\right).$$

This inequality shows that we indeed have to estimate the matter quantities together with the second fundamental form κ. The next step consists in finding a complementary inequality for Q_1, which yields in combination with the inequality just obtained a true Gronwall estimate for $1 + \overline{P_f} + Q_1$.

We again need the field equations for V and W, but now it is more convenient to analyze the equations in the "wave map form" (25). First consider the left-hand side of the field equation. We want to express this derivative operator in terms of the characteristic vector fields $k_\pm = m \pm n$ tangent to the characteristic curves $\gamma_\pm$ introduced in the previous section (in the proof of Proposition 2.4). In the quotient manifold $(B,\underline{g})$ one calculates the nonvanishing Ricci rotation coefficients to

$$\gamma^0_{01} = \gamma^1_{00} = (AN)^{-1}N',$$

$$\gamma^0_{11} = \gamma^1_{01} = (AN)^{-1}(\dot{A} - (A\nu^1)'),$$

thus $\underline{\nabla}_{\underline{e}_a}\underline{e}_b$ is bounded. The characteristics $k_\pm$ expressed in the coordinates of B are simple linear combinations of the $\underline{e}_a$, hence $\underline{\nabla}_{k_\pm}k_\pm$ is also bounded in B. We will use this fact to estimate commutators such as $[m,n]$ or $[k_+,k_-]$. Transforming from the orthonormal frame $\{\underline{e}_a\}$ in $(B,\underline{g})$ to the frame $\{k_\pm\}$, we can write the left-hand side of (25) as

$$\underline{\nabla}^c\underline{\nabla}_c\phi^K + \hat{\Gamma}^K_{IJ}\underline{\nabla}^c\phi^I\underline{\nabla}\phi^J = \underline{\nabla}_{k_+}(k_-(\phi^K)) + \hat{\Gamma}^K_{IJ}k_+(\phi^I)k_-(\phi^J) + [k_+,k_-](\phi^K)$$

and there is an analogous equation for k_+ and k_- interchanged.

Let us turn now to the right-hand side of (25). The terms not known to be bounded are of the form $k_{\pm}(\phi)$ and T_{AB}. Fortunately we have control over the matter term, since the bounds on V, W, and v^A justify the inequality $T_{AB} \leqslant C\overline{P}_f$ and we obtain

$$\nabla_{k_+}(k_-(\phi^K)) + \hat{\Gamma}^K_{IJ} k_+(\phi^I) k_-(\phi^J) \leqslant C(1 + k_{\pm}(\phi) + \overline{P}_f).$$

The left-hand side is still nonlinear in the first derivatives of ϕ, so this inequality is not in the appropriate form to apply some kind of Gronwall estimate. But we can overcome this difficulty by adapting an observation of Gu (1980), see also Rendall (1997) for explanation, who considered wave maps defined on two-dimensional Minkowski space. We already performed the first step, consisting of a transformation to characteristic coordinates. Now we define the vector field $\hat{k}_{\pm}$ over the map ϕ,

$$\hat{k}_{\pm} := \phi_*(k_{\pm}) = k_{\pm}(\phi) = k_{\pm}(\phi^K) \frac{\partial}{\partial \phi^K} = k_{\pm}(V) \frac{\partial}{\partial V} + k_{\pm}(W) \frac{\partial}{\partial W},$$

thus bounding the length of $\hat{k}_{\pm}$ accomplishes the estimate of Q_1. The vector field $\hat{k}_{\pm}$ over ϕ is a section in the bundle $\phi^*(TH^2)$ over B and the covariant derivative operator $\phi^*\hat{\nabla}$ over ϕ acts like

$$(\phi^*\hat{\nabla})_v \hat{X} = v(\hat{w}^K) \frac{\partial}{\partial \phi^K} + \hat{w}^K \hat{\nabla}_{\phi^* v} \frac{\partial}{\partial \phi^K}$$

for every vector $v \in TB$ and every $\hat{X} = \hat{w}^K(\partial/d\phi^K)$ with $w^K: B \to H^2$.

Evaluating this expression with $v = k_+$ and $\hat{X} = \hat{k}_-$ gives

$$(\phi^*\hat{\nabla})_{k_+} \hat{k}_- = k_+(k_-(\phi^K)) \frac{\partial}{\partial \phi^K} + \hat{\Gamma}^K_{IJ} k_+(\phi^I) k_-(\phi^J) \frac{\partial}{\partial \phi^K}$$

(and analogously for $k_{\pm}$ interchanged). The components in this equation are similar to the left-hand side of the inequality already obtained for the field equations. The remaining term involves $k_{\pm}(\phi)$ times the connection coefficients in B with respect to the frame $\{k_{\pm}\}$, which we know to be bounded. Thus we get for the field equations the inequality

$$|(\phi^*\hat{\nabla})_{k_+} \hat{k}_-| \leqslant C(1 + k_{\pm}(\phi) + \overline{P}_f),$$

expressing an estimate about the growth of $\hat{k}_{\pm}$ during the transport along the characteristic curve $\gamma_{\mp}$. This inequality is in the appropriate form for a Gronwall-like estimate: Taking the maximum for each fixed t allows us to combine the inequalities for $|\hat{k}_+|$ and $|\hat{k}_-|$, replaced collectively in terms of Q_1. Hence

$$Q_1(t) \leqslant C\left(1 + Q_1(0) + \int_t^0 (\overline{P}_f(s) + Q_1(s))\mathrm{d}s\right),$$

where $\gamma_{\pm}$ has been reparametrized in terms of t. Combining this with the inequality for $\overline{P}_f$ we arrive at

$$1 + \overline{P}_f(t) + Q_1(t) \leqslant C\left(1 + \overline{P}_f(0) + Q_1(0) + \int_t^0 (1 + \overline{P}_f(s) + Q_1(s))\mathrm{d}s\right).$$

Performing a Gronwall argument we have proven

Proposition 2.5: Let (M,g,f) be a globally hyperbolic, spatially compact solution of the Einstein–Vlasov system with local $U(1)\times U(1)$ symmetry, which possesses a symmetric Cauchy surface Σ with strictly negative mean curvature. The PMC time coordinate t ranges in $]t_1,t_2[$ with $\Sigma=\{t=0\}$ and H decreases with decreasing t.

Then we get uniform bounds for

$$|\dot{V}|,|\dot{W}|,|V'|,|W'|,\rho$$

on $]t_1,0]$.

2. Second-order estimates

We still have to do one further step before it will be possible to apply some iteration scheme. We need to establish bounds for the second derivatives of $\phi=(V,W)$ together with bounds for the first derivatives of the matter variables. Again it turns out that it is not possible to get separate estimates for these quantities.

First we differentiate the field equation (25) and obtain an equation of the form

$$k_{\pm}(k_{\mp}(\partial_x\phi^K))+2\hat{\Gamma}^K_{IJ}k_{\pm}(\phi^I)k_{\mp}(\partial_x\phi^J)=[\ldots]\partial_x T_{AB}+\text{lower order terms},$$

where [...] is an abbreviation for some term involving already bounded quantities, in particular we see by a quick look at the 3+1-field equations, whose right-hand sides are now bounded, that for the Ricci rotation coefficients $\partial_x\underline{\gamma}\leqslant C$ holds. Note that the differentiation kills the nonlinearity in the equation, but we have to deal with first-order derivatives of the matter variables instead. These quantities cause serious trouble, because if we differentiate the Vlasov equation, terms involving the second derivatives of ϕ times first derivatives of f come up, thus there is no direct Gronwall argument possible. To attack this difficulty we have to combine the equations, using an idea of Glassey (1990).

First we integrate the equation along the characteristics $\gamma_{\pm}$ to get an integral inequality. In order to apply a Gronwall argument all that remains to do is to bound the term $\int_{\gamma_{\pm}}\partial_x T_{AB}$. Then we express T_{AB} in terms of its components with respect to the orthonormal frame, merely producing some already bounded quantities and the frame components of the energy–momentum tensor for Vlasov-type matter look like $\int_{\gamma_{\pm}}(\int v_A v_B/v^0\partial_x f\,dv)$. Finally we represent ∂_x by a linear combination of $k_{\pm}$ and $\underline{X}:=\partial_t+(NA^{-1}v^1/v^0-\nu^1)\partial_x$, which is the part of the characteristic vector field for the Vlasov equation, lying in B. The transformation to this basis is obviously bounded and we can proceed as follows. The part involving $k_{\pm}$ permits a direct application of the integration by parts rule, which contributes something bounded by Proposition 2.5. The remaining part can be treated in a similar fashion, after inserting the Vlasov equation into $\underline{X}(f)$. This yields terms involving only first-order derivations of ϕ (arising from the ${}^4\gamma$'s) times $\partial f/\partial v$, and again we can perform an integration by parts with respect to the velocity integral. The result consists in terms already bounded and we are through. Now applying Gronwall's inequality we arrive at a bound for $\|\partial_x\underline{D}\phi\|_{L^\infty}$ and inserting this result into the field equation (25) we get $Q_2:=\|D^2\phi\|_{L^\infty}$ bounded.

An immediate consequence is that we also have established a bound for the first derivatives of f. Differentiating the Vlasov equation with respect to x or v yields an equation for $\partial_x f$ or $\partial_v f$, respectively, with bounded characteristics and an inhomogeneous term, consisting of $({}^4e_\mu)^\alpha$, ${}^4\gamma^\kappa_{\mu\nu}$ and their derivatives with respect to x. These terms are either bounded by what has been said previously or by inspection of the field equations (26)–(37). Having bounded the spatial and velocity derivatives of f, the structure of the Vlasov equation bounds immediately $\partial_t f$ and we have proven

Proposition 2.6: Under the hypotheses of Proposition 2.5 we get uniform bounds for

$$|\ddot{V}|,|\dot{V}'|,|V''|,|\ddot{W}|,|\dot{W}'|,|W''|\ \text{ and }\ |\dot{\rho}|,|\rho'|$$

on $]t_1,0]$.

3. The iteration scheme

Following the analysis of Paper I we need some additional framework.

Definition 2.7:

$$\mathcal{F} := (A, a, V, W, N, \nu^1, \nu^B, H, K, \eta_B),$$

$$\Phi := (\rho, {}^{\phi}\rho).$$

It turns out that what we have done in the previous subsections are the first steps toward the matter regularity property of Paper I. Here we will define this property adapted to the present situation with the notational conventions introduced as follows: α denotes a multi-index for derivatives in $(B, \underline{g})$ and $\underline{D} := (\partial_t, \partial_x)$. Then the matter regularity property reads

$$|\underline{D}^{\alpha}\mathcal{F}| \leqslant C \Rightarrow |\underline{D}^{\alpha}\Phi| \leqslant C \tag{39}$$

and we state

Proposition 2.8: Under the hypotheses of Proposition 2.5, (39) *holds for all α uniformly on* $]t_1, 0]$.

Proof: We prove the statement by induction with respect to $|\alpha|$. The induction hypotheses for $\alpha = 0$ are contained in the statements of Propositions 2.5 and 2.6. To proceed further let us assume $|\underline{D}^{\alpha}\mathcal{F}| \leqslant C$ for some α with $|\alpha| := p \geqslant 1$. Then we can assume $|\underline{D}^{p-1}\Phi| \leqslant C$ by induction. We have to show $|\underline{D}^{p}\Phi| \leqslant C$, or extending our previous notation, $P_p := \|\underline{D}^{p} f\|_{L^\infty} \leqslant C$ and $Q_{p+1} := \|\underline{D}^{p+1}\phi\|_{L^\infty} \leqslant C$.

Following the analysis of Sec. II D 2 we set $q := p - 1$ and differentiate the field equations (25) with $\partial_x \underline{D}^q$, which yields schematically

$$k_{\pm}(k_{\mp}(\partial_x \underline{D}^q \phi)) = [\partial_x \underline{D}^q \underline{\gamma}, \partial_x \underline{D}^p r, \partial_x \underline{D}^q \phi](k_{\mp}\partial_x \underline{D}^q \phi) + [\underline{D}^q \phi]\partial_x \underline{D}^q T_{AB}$$
$$+ [\partial_x \underline{D}^q \phi, \partial_x \underline{D}^q \eta, \underline{D}^q T_{AB}],$$

where quantities in square brackets abbreviate some expressions formed by them, whose detailed structure is not important for our analysis here. We want to perform the same kind of argument as we have done in the proof of the second-order estimates. In order to do this we must bound the quantities in the square brackets:

(1) The terms in the second and third set of square brackets are bounded by the induction hypotheses.

(2) For the first square bracket we can proceed as follows. $\partial_x \underline{D}^q \phi$ is already bounded. For $\partial_x \underline{D}^p r$ we have to estimate $\partial_x \underline{D}^p A = \partial_x^2 \underline{D}^q A$. This can be done by applying $\underline{D}^q$ to (26) in a strictly analogous manner as in the first item in the proof of Lemma 3.6 in Paper I, applied to Eq. (26). The definition of $\underline{\gamma}$ in Sec. II D 1 shows that the terms in $\partial_x \underline{D}^q \underline{\gamma}$ not already bounded are $\partial_x^2 \underline{D}^q \nu^1$, $\partial_x^2 \underline{D}^q N$, and $\partial_x \partial_t \underline{D}^q A$. Applying $\underline{D}^p$ to (36) gives a bound for the first quantity. Using $\underline{D}^q$ on (29), then the argument in the fourth step in the proof of Lemma 3.6 in Paper I, applied to (29) bounds the second quantity. Now all quantities appearing on the right-hand side of ($\partial_x \underline{D}^q$ applied to) (32) are bounded, and this bounds $\partial_t \partial_x \underline{D}^q A$.

Turning now to the Vlasov equation and applying $\partial_x \underline{D}^q$ yields an inhomogeneous equation for $\partial_x \underline{D}^q f$ with the same characteristics. Thus we can apply the same trick as in Sec. II D 2, substituting ∂_x by $k_{\pm}$ and $\underline{X}$. Then again we are concerned with integration by parts, which yields only bounded terms, and the inhomogeneous term of the differentiated Vlasov equation, which is also bounded by induction hypotheses. All together we can apply Gronwall's inequality to find $\|\partial_x \underline{D}^p \phi\|_{L^\infty} \leqslant C$, and immediately $Q_{p+1} \leqslant C$ by inserting the spatial bounds into the field equation. The Vlasov equation for $\partial_x \underline{D}^q f$ now bounds $\partial_x \underline{D}^q f$ and analogously for $\partial_v \underline{D}^q f$, which automatically bounds $\partial_t \underline{D}^q f$ by inserting the spatial and velocity bounds into the differentiated Vlasov equation. Thus we have also bounded P_p, which completes the proof of the proposition. ■

To extend the local in time PMC foliation, our aim is to find uniform C^∞ bounds of all geometric and matter quantities, when the PMC time t approaches t_1. Property (39) shows that it is enough to bound the geometric quantities $\underline{D}^\alpha \mathcal{F}$ for all α as long as t or, respectively, the mean curvature remains finite. Therefore all we need is the analog of Lemmas 3.6 and 3.7 in Paper I, starting with Propositions 2.3, 2.4, 2.5, and 2.6.

The first part is straightforward, given an arbitrary multi-index α and $|\underline{D}^\alpha \mathcal{F}| \leqslant C$ we find $|\partial_x \underline{D}^\alpha \mathcal{F}| \leqslant C$ by inspection of the relevant (differentiated) field equations (26)–(37) (compare the arguments given in the proof of Lemma 3.6 in Paper I where necessary), with the terms on the right-hand sides bounded by property (39). Moreover, Proposition 2.8 provides not only bounds for the spatial derivatives, but also for the time derivatives of ϕ by the definition of ${}^{\phi}\rho$. This allows us to proceed as follows: First we bound, starting from $\underline{D}^\alpha \mathcal{F}$ all spatial derivatives $\partial_x^k \underline{D}^\alpha \mathcal{F}$, $k=1,2,\ldots$. Then we bound, starting successively from $\partial_x^k \underline{D}^\alpha \mathcal{F}$, $k=1,2,\ldots$, the quantities $\underline{D}^\beta \mathcal{F}$ for all multi-indices β with $|\beta| = |\alpha| + k$, redistributing the spatial derivatives into time derivatives. This procedure will successively bound all derivatives of $\mathcal{F}$, taking advantage of the fact that in each step all lower order derivatives with the same order of time derivatives have been bounded as well as at least one more spatial order derivative in the step with one order less in time derivatives. In a more compact formulation, we have to show the boundedness of $\partial_t \underline{D}^\alpha \mathcal{F}$, having already bounds for $\partial_x \underline{D}^\alpha \mathcal{F}$ and $\underline{D}^\alpha \mathcal{F}$.

We accomplish this step for each member of $\mathcal{F}$, by again considering some of the (differentiated by $\underline{D}^\alpha$) $3+1$-field equations. We see immediately from (32) and (33) that we have bounds for $\partial_t \underline{D}^\alpha A$, $\partial_t \underline{D}^\alpha a$. The bounds for $\partial_t \underline{D}^\alpha$ applied on H, K, and η are straightforward, too. Of course, $\partial_t \underline{D}^\alpha \phi$ is already bounded by property (39). Moreover we can strengthen the regularity. Since we have already a bound for $\partial_x \underline{D}^\alpha \mathcal{F}$ Proposition 2.8 provides us with bounds for $\partial_x \underline{D}^\alpha$ applied to ρ and $\underline{D}\phi$. Applying $\partial_x \underline{D}^\alpha$ to the field equation (25) we first get a bound for $\partial_x \underline{D}^\alpha \phi$ and then for $\partial_t^2 \underline{D}^\alpha \phi$ by inserting the first result into the field equation. This in turn used together with the bounds for the differentiated matter variable in the differentiated Vlasov equation, bounds $\partial_t \underline{D}^\alpha \rho$.

Now we turn to the analysis of the differentiated lapse equation. First we see that the bound for $\partial_t \underline{D}^\alpha \nu$ follows from the bound of $\partial_t \underline{D}^\alpha N$. For the latter one, we follow the argument given in the corresponding place in the proof of Lemma 3.7 in Paper I, where all that is needed has already been bounded by the arguments just given here and we are done.

Therefore we end up with

Theorem 2.9: *Let (M,g,f) be a globally hyperbolic, spatially compact solution of the Einstein–Vlasov system with local $U(1)\times U(1)$ symmetry, which possesses a symmetric Cauchy surface Σ with strictly negative mean curvature $H \leqslant \overline{H} < 0$ and $H = \overline{H}$ somewhere on Σ. Then all of the past of Σ admits a PMC foliation $\{S_t\}$, where t takes all values in the interval $]-\infty, 0]$ and H takes all values in $]-\infty, \overline{H}]$.*

4. Improving the result

Here we will try to do the same construction as in the corresponding place in Paper I, to get rid of the restriction concerning the fixed sign of the mean curvature H on the Cauchy surfaces. So we assume M to be nonflat and denote by Σ an arbitrary symmetric Cauchy surface in M. In order to follow the steps performed in the plane symmetric case in Paper I, remember first from Sec. II B 4, that the space–time is expanding. Note further that the Einstein–Vlasov system fulfills the dominant and strong energy condition as well as the non-negative pressures condition.

Then we find for the past domain of dependence $D^-(\Sigma)$

(1) Since the space–time is expanding, dr is future pointing, thus r is bounded in $D^-(\Sigma)$. By assumption, μ^{-1} is bounded on the compact surface Σ. Unfortunately, unlike in the plane symmetric case we cannot conclude from the non-negative pressures condition and the fact that dr is future pointing, that dμ is past pointing, since in Eq. (21) for the mass flux the term involving η contributes with the wrong sign [luckily, the contribution of the energy momentum tensor ${}^{\phi}T$ (19)

for the wave map ϕ does not cause any trouble, due to the energy conditions automatically fulfilled by ${}^{\phi}T$].

To overcome this difficulty we impose the Gowdy-type symmetry condition, thus η vanishes identically in the space–time [and by the gauge condition $\nu^B(t,0)=0$ this is also true for $\overline{\nu}$ in view of (37)]. Then we conclude that M^{-1} is bounded in $D^-(\Sigma)$ as desired.

Now we want to apply theorem 2.1 in Burnett (1999) to establish a bound for the length of all timelike curves in $D^-(\Sigma)$. For this we have to adapt the proof a little bit. Inspection of the proof shows that the argument relies on the inequality $\ddot{r}\leqslant -\mathrm{M}/r^2$ satisfied by the area radius along timelike geodesics, where the dot denotes differentiation along the curve. But looking at the field equation (20) for the area radius easily establishes this relation (since η vanishes) and we are through.

(2) The basic estimate (38) together with (16) shows that r^{-1} and M are bounded.

(3) Lemma 2 in Burnett (1996) applies and we get bounds for the volume and its inverse for any Cauchy surface in $D^-(\Sigma)$.

The volume $V(t)$ for the leaf S_t of the PMC foliation is given by $V(t)=(4\pi)^2 a^{-1}\int_{S^1} r^3$ and a closer look at the estimates given in the corresponding place in Paper I shows that the arguments apply literally. This relies on the facts that on the one hand the additional equations (25) are unaffected by the reparametrization of the foliation, thus the estimates for ϕ and its derivatives done in the previous subsections hold. On the other hand the construction in Paper I is based mainly on the structures introduced by the matter regularity property and Lemmas 3.6 and 3.7, a program we adapted successfully to the more general situation here.

So we finally arrive at

Theorem 2.10: *Let (M,g,f) be a globally hyperbolic, spatially compact solution of the Einstein–Vlasov system with Gowdy-type local $U(1)\times U(1)$ symmetry and Σ be a symmetric Cauchy surface. If (M,g) is non-flat then we can foliate all of the past of Σ by PMC hypersurfaces, where the time function takes on all values in the interval $]-\infty, 0]$ and the mean curvature of the leaves tends uniformly to $-\infty$ for $t\to-\infty$.*

Using the PMC leaves as barrier surfaces we get the

Corollary 2.11: In the situation of Theorem 2.10 *$D^-(\Sigma)$ possesses a CMC Cauchy surface for each value of the mean curvature in $]-\infty, \min_\Sigma H[$.*

III. CONCLUSION AND OUTLOOK

We have seen in this paper that the program initiated in Paper I has been successfully extended to the more general case of local $U(1)\times U(1)$ symmetric space–times in close analogy to the plane symmetric space–times. Therefore all that has been mentioned in the corresponding place in Paper I applies.

A corresponding analysis for space–times with local $U(1)\times U(1)$ symmetry has been independently performed in Andréasson (1999). His construction leads to stronger results (as well as [Rein (1996)] in the surface symmetric case of Paper I), but the time functions used are defined in terms of the symmetry. Thus it is not clear how to generalize them. In view of Andréasson's work, the present analysis can be seen as a suggestion pointing in a slightly different direction.

In comparison with the space–times considered in Paper I the control of the momenta of the Vlasov particles turned out to be more complicated, in particular the coupling to gravitational waves required second-order estimates before the iteration procedure could be performed. In this process we took advantage from the wave-map structure of the dynamical part of the geometry driven by the simple form of the Vlasov equation. Nevertheless one can hope that the approach may be generalized to other matter models and geometries, since the obstructions seem to be of technical nature only.

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Ellipsoidal, cylindrical, bipolar and toroidal wormholes in 5D gravity

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In this article we construct and analyze new classes of wormhole and flux tubelike solutions for the 5D vacuum Einstein equations. These 5D solutions possess generic local anisotropy which gives rise to a gravitational running or scaling of the Kaluza–Klein ''electric'' and ''magnetic'' charges of these solutions. It is also shown that it is possible to self-consistently construct these anisotropic solutions with various rotational 3D hypersurface geometries (i.e., ellipsoidal, cylindrical, bipolar and toroidal). The local anisotropy of these solutions is handled using the technique of anholonomic frames with their associated nonlinear connection structures [S. Vacaru, Ann. Phys. (N.Y.) **256**, 39 (1997); Nucl. Phys. B **434**, 590 (1997); J. Math. Phys. **37**, 508 (1996); J. High Energy Phys. **09**: 011 (1998); Phys. Lett. B **498**, 74 (2001)]. Through the use of the anholonomic frames the metrics are diagonalized, in contrast to holonomic coordinate frames where the metrics would have off-diagonal components. In the local isotropic limit these solutions are shown to be equivalent to spherically symmetric 5D wormhole and flux tube solutions. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1467967]

I. INTRODUCTION

The first solutions describing black holes and wormholes in 4D and higher dimensional gravity were spherical symmetric solutions with diagonal metrics.[1] Later Salam, Strathee and Perracci[2] showed that including off-diagonal components in higher dimensional metrics is equivalent to including gauge fields. They concluded that geometrical gauge fields could act as sources of exotic matter necessary for the construction of a wormhole. References 3 and 4 examined locally isotropic solutions with off-diagonal metric components for 5D vacuum Einstein equations. These solutions were similar to spherically symmetric 4D wormhole or flux tube metrics with ''electric'' and/or ''magnetic'' fields running along the throat of the wormhole. These ''electromagnetic'' fields arose as a consequence of the off-diagonal elements of the metric. By varying certain free parameters of the off-diagonal elements of the 5D metrics it was possible to change the relative strengths of the fields in the wormhole's throat, and to change the longitudinal and transverse size of the wormhole's throat. In Ref. 5 we constructed *anisotropic* wormhole and flux tube solutions, which reduced to the solutions of Refs. 3 and 4 in the isotropic limit. The anisotropy of these metrics was handled using the method of anholonomic frames with associated nonlinear connections, which has been developed by one of the authors (SV) in Refs. 6 and 7. It was shown that these anisotropic solutions exhibited a variation or running of the ''electromagnetic'' parameters as a result of the angular anisotropies and/or through variations of the extra spatial dimension.

In this article we extend the investigation of Ref. 5 by applying the anholonomic frames method to construct anisotropic wormhole and flux tube solutions to 5D Kaluza-Klein theory which possess a range of different symmetries (elliptic, cylindrical, bipolar, toroidal). We will discuss the physical consequences of these solutions, in particular the variation of the ''electro-

magnetic'' parameters (e.g., the ''electric'' and ''magnetic'' charges associated with the solutions). This variation of the ''electromagnetic'' charges, which here occurs in the context of a higher dimensional gravity theory, can be likened to the variation or running of electric charge that occurs when a real electric charge is placed into some dielectric medium or in a quantum vacuum where quantum fluctuations produce a scale dependent electric charge. We will sometimes loosely refer to this gravitational variation of the ''electromagnetic'' parameters of the solutions as the gravitational running, scaling or renormalization of the charges of the solutions.

II. ANHOLONOMIC FRAMES AND 5D VACUUM EINSTEIN EQUATIONS

In this section we outline the basic formulas for 5D Einstein gravity, and introduce the method of anholonomic frames. We construct locally anisotropic metrics which are generalizations of those considered in Ref. 5. These 5D metrics have a mixture of holonomic and anholonomic variables, and are most naturally dealt with using anholonomic frames. Finally we analyze the physical and mathematical properties of these 5D, locally anisotropic vacuum solutions.

A. Metric ansatz

Let us consider a 5D pseudo-Riemannian space–time of signature $(+,-,-,-,-)$ and denote the local coordinates $u^{\alpha}=(x^i,y^a)=(x^1,x^2,x^3,y^4=s,y^5=p)$, or more compactly $u=(x,y)$, where the Greek indices are split into two subsets x^i (holonomic coordinates) and y^a (anholonomic coordinates) labeled respectively by Latin indices $i,j,k,\ldots=1,2,3$ and $a,b,\ldots=4,5$. The local coordinate bases, $\partial_{\alpha}=(\partial_i,\partial_a)$, and their duals, $d^{\alpha}=(d^i,d^a)$, are written respectively as

$$\partial_{\alpha}\equiv\frac{\partial}{du^{\alpha}}=\left(\partial_i=\frac{\partial}{dx^i},\partial_a=\frac{\partial}{dy^a}\right) \tag{1}$$

and

$$d^{\alpha}\equiv du^{\alpha}=(d^i=dx^i,d^a=dy^a). \tag{2}$$

We can treat an arbitrary coordinate, x^i or y^a, as spacelike (x,y,z), timelike (t) or as the fifth spatial coordinate (χ). The aim is then to study anisotropies and anholonomic constraints for various coordinates.

With respect to the coordinate frame base (2) the 5D pseudo-Riemannian metric

$$dS^2=g_{\alpha\beta}du^{\alpha}du^{\beta} \tag{3}$$

with its metric coefficients $g_{\alpha\beta}$ parametrized as

$$\begin{bmatrix} g_1+w_1^2h_4+n_1^2h_5 & w_1w_2h_4+n_1n_2h_5 & w_1w_3h_4+n_1n_3h_5 & w_1h_4 & n_1h_5 \\ w_1w_2h_4+n_1n_2h_5 & g_2+w_2^2h_4+n_2^2h_5 & w_2w_3h_4+n_2n_3h_5 & w_2h_4 & n_2h_5 \\ w_1w_3h_4+n_1n_3h_5 & w_3w_2h_4+n_2n_3h_5 & g_3+w_3^2h_4+n_3^2h_5 & w_3h_4 & n_3h_5 \\ w_1h_4 & w_2h_4 & w_3h_4 & h_4 & 0 \\ n_1h_5 & n_2h_5 & n_3h_5 & 0 & h_5 \end{bmatrix}. \tag{4}$$

The ansatz functions of this metric are smooth function of the form

$$g_1=1,\quad g_{2,3}=g_{2,3}(x^2,x^3)=\epsilon_{2,3}\exp[2b_{2,3}(x^2,x^3)], \tag{5}$$

$$h_{4,5}=h_{4,5}(x^2,x^3,s)=\exp[2f_{4,5}(x^2,x^3,s)], \tag{6}$$

$$w_1=w_1(x^2),\quad w_{2,3}=w_{2,3}(x^2,x^3,s),$$

$$n_1=n_1(x^2),\quad n_{2,3}=n_{2,3}(x^2,x^3,s);$$

The ansatz functions of the metric are taken to depend on two isotropic variables (x^2,x^3) and on one anisotropic variable, $y^4=s$.

Metric (3) can be greatly simplified into the form

$$\delta S^2=g_{ij}(x)dx^i dx^i+h_{ab}(x,s)\,\delta y^a\,\delta y^b, \tag{7}$$

with diagonal coefficients

$$g_{ij}=\begin{bmatrix}1 & 0 & 0\\ 0 & g_2 & 0\\ 0 & 0 & g_3\end{bmatrix} \quad \text{and} \quad h_{ab}=\begin{bmatrix}h_4 & 0\\ 0 & h_5\end{bmatrix} \tag{8}$$

if instead of coordinate bases (1) and (2) one used anholonomic frames (anisotropic bases)

$$\delta_\alpha\equiv\frac{\delta}{du^\alpha}=\left(\delta_i=\partial_i-N_i^b(u)\partial_b\,,\partial_a=\frac{\partial}{dy^a}\right) \tag{9}$$

and

$$\delta^\alpha\equiv\delta u^\alpha=(\delta^i=dx^i,\delta^a=dy^a+N_k^a(u)dx^k), \tag{10}$$

where the N-coefficients are parametrized as

$$N_1^4=w_1\,,\quad N_{2,3}^4=w_{2,3} \text{ and } N_1^5=n_1\,,\quad N_{2,3}^5=n_{2,3}.$$

They define an associated nonlinear connection (N-connection) structure (see Refs. 6 and 7). Here, we shall not emphasize the N-connection formalism. The anisotropic frames (9) and (10) are anholonomic because, in general, they satisfy some anholonomic relations,

$$\delta_\alpha\delta_\beta-\delta_\beta\delta_\alpha=W_{\alpha\beta}^\gamma\delta_\gamma,$$

with nontrivial anholonomy coefficients

$$\begin{gathered}W_{ij}^k=0,\quad W_{ai}^k=0,\quad W_{ab}^k=W_{ab}^c=0,\\ W_{ij}^a=-\Omega_{ij}^a\,,\quad W_{bj}^a=-\partial_b N_j^a\,,\quad W_{ia}^b=\partial_a N_j^b\,,\end{gathered} \tag{11}$$

where

$$\Omega_{ij}^a=\delta_j N_i^a-\delta_i N_j^a\,.$$

Conventionally, the N-coefficients decompose space–time objects (e.g., tensors, spinors and connections) into objects with mixed holonomic-anholonomic characteristics. The holonomic parts of an object are indicated with indices of type $i,j,k,\ldots$, while the anholonomic parts have indices of type $a,b,c,\ldots$. Tensors, metrics and linear connections with coefficients defined with respect to anholonomic frames (9) and (10) are distinguished (d) by N-coefficients into holonomic and anholonomic subsets and are called d-tensors, d-metrics and d-connections.

B. Einstein equations in holonomic-anholonomic variables

The main ''trick'' of the anholonomic frames method for integrating Einstein's equations in general relativity and various (super)string and higher/lower dimension gravitational theories is to find the coefficients N_j^a such that the block matrices g_{ij} and h_{ab} are diagonalized.[6,7] This greatly simplifies computations. With respect to such anholonomic frames the partial derivatives are N-elongated (locally anisotropic).

Metric (3) with coefficients (4) [or equivalently, the d-metric (7) with coefficients (8)] is assumed to solve the 5D Einstein equations

$$R_{\alpha\beta}-\tfrac{1}{2}g_{\alpha\beta}R=\kappa\Upsilon_{\alpha\beta}, \tag{12}$$

where κ and $\Upsilon_{\alpha\beta}$ are respectively the coupling constant and the energy-momentum tensor. For most of the article we will consider vacuum solutions, $\Upsilon_{\alpha\beta}=0$. The nontrivial components of the Ricci tensor (details of the computations are given in Refs. 5 and 7), for the ansatz, are

$$R_2^2=R_3^3=-\frac{1}{2g_2g_3}\left[\ddot{g_3}-\frac{\dot{g_2}\dot{g_3}}{2g_2}-\frac{(\dot{g_3})^2}{2g_3}+g_2''-\frac{g_2'g_3'}{2g_3}-\frac{(g_2')^2}{2g_2}\right], \tag{13}$$

$$R_4^4=R_5^5=-\frac{\beta}{2h_4h_5}, \tag{14}$$

$$R_{42}=-w_2\frac{\beta}{2h_5}-\frac{\alpha_2}{2h_5},\qquad R_{43}=-w_3\frac{\beta}{2h_5}-\frac{\alpha_3}{2h_5}, \tag{15}$$

$$R_{52}=-\frac{h_5}{2h_4}[n_2^{**}+\gamma n_2^*],\qquad R_{53}=-\frac{h_5}{2h_4}[n_3^{**}+\gamma n_3^*], \tag{16}$$

where

$$\alpha_2=h_5^{*\bullet}-\frac{h_5^*}{2}\left(\frac{\dot{h_4}}{h_4}+\frac{\dot{h_5}}{h_5}\right)=h_5^*(\ln|f_5^*|+f_5-f_4)^{\bullet},\quad h_5^*\neq 0; \tag{17}$$

$$\alpha_3=h_5^{*\prime}-\frac{h_5^*}{2}\left(\frac{h_4'}{h_4}+\frac{h_5'}{h_5}\right)=h_5^*(\ln|f_5^*|+f_5-f_4)',\quad h_5^*\neq 0; \tag{18}$$

$$\beta=h_5^{**}-\frac{h_5^*}{2}\left(\frac{h_5^*}{h_5}+\frac{h_4^*}{h_4}\right)=h_5^*(\ln|f_5^*|+f_5-f_4)^*,\quad h_5^*\neq 0; \tag{19}$$

$$\gamma=\frac{3}{2}\frac{h_5^*}{h_5}-\frac{h_4^*}{h_4}=[3f_5-2f_4]^*. \tag{20}$$

The partial derivatives are denoted as $h^{\bullet}=\partial h/\partial x^2, f'=\partial f/\partial x^3$ and $f^*=\partial f/\partial s$. We have given the formulas both in terms of $h_{4,5}$ and $f_{4,5}$ since we will need this later.

Formulas (13)–(16) were obtained with respect to anholonomic frames for a fixed linear connection adapted to the N-connection structure, called the canonical distinguished connection.[8] [Miron and Anastasiei introduced this connection on vector bundles, but it can be used in a similar fashion on (pseudo) Riemannian spaces if the N-connection is considered.] The coefficients of a distinguished connection $\Gamma^{\alpha}_{\beta\gamma}=(L^i_{jk},L^a_{bk},C^i_{jc},C^a_{bc})$ are computed from the formulas

$$L^i_{jk}=\tfrac{1}{2}g^{in}(\delta_k g_{nj}+\delta_j g_{nk}-\delta_n g_{jk}),$$

$$L^a_{bk}=\partial_b N^a_k+\tfrac{1}{2}h^{ac}(\delta_k h_{bc}-h_{dc}\partial_b N^d_k-h_{db}\partial_c N^d_k), \tag{21}$$

$$C^i_{jc}=\tfrac{1}{2}g^{ik}\partial_c g_{jk},\quad C^a_{bc}=\tfrac{1}{2}h^{ad}(\partial_c h_{db}+\partial_b h_{dc}-\partial_d h_{bc}).$$

The coefficients in (21) reduce to the Christoffel symbols if the metric components g_{ij} depend only on x-variables, the h_{ab} depend only on y-variables, and the N-connection vanishes. We emphasize that if the anholonomic frames are introduced into consideration, there is a certain class

of linear connections which satisfy the metricity condition for a given metric, or inversely, there is a certain class of metrics which satisfy the metricity conditions for a given linear connection. (This result was originally obtained by A. Kawaguchi[9] in 1937. Details can be found in Ref. 8; see Theorems 5.4 and 5.5 in Chapter. III.) So, we need to state explicitly what type of linear connection is used for the definition of the curvature and Ricci tensor if the space-time is provided with an anholonomic frame structure. In this work and in Refs. 5 and 7 the linear connection is considered to be of the form (21). The off-diagonal metrics studied in this article will be compatible with the canonical linear connection, but may not have a trivial limit to a diagonal holonomic metric.

The scalar curvature is

$$R=2(R_2^2+R_4^4).$$

Using this along with the components of the Ricci tensor in Eqs. (13)–(16) one can show that for the metric ansatz (4) the coefficients of the energy-momentum d-tensor satisfy

$$\Upsilon_1^1=\Upsilon_2^2+\Upsilon_4^4, \quad \Upsilon_2^2=\Upsilon_3^3=\Upsilon_2, \quad \Upsilon_4^4=\Upsilon_5^5=\Upsilon_4,$$

with respect to anholonomic bases (9) and (10). Thus the Einstein equations can be written as

$$R_2^2=-\kappa\Upsilon_4, \quad R_4^4=-\kappa\Upsilon_2, \quad R_{4\hat{i}}=\kappa\Upsilon_{4\hat{i}}, \quad R_{5\hat{i}}=\kappa\Upsilon_{5\hat{i}}, \tag{22}$$

where $\hat{i}=2,3$.

With this setup it is possible to construct very general classes of solutions to these equations[5,7] which describe locally anisotropic solitons, black holes, black tori and wormhole solutions.

C. General properties of the anisotropic vacuum solutions

In the vacuum case Eqs. (22) reduce to

$$g_3^{\cdot\cdot}-\frac{g_2^{\cdot}g_3^{\cdot}}{2g_2}-\frac{(g_3^{\cdot})^2}{2g_3}+g_2''-\frac{g_2'g_3'}{2g_3}-\frac{(g_2')^2}{2g_2}=0, \tag{23}$$

$$h_5^{**}-\frac{h_5^*}{2}\left(\frac{h_5^*}{h_5}+\frac{h_4^*}{h_4}\right)=0, \tag{24}$$

$$\beta w_{2,3}+\alpha_{2,3}=0, \tag{25}$$

$$n_{2,3}^{**}+\gamma n_{2,3}^*=0. \tag{26}$$

We now discuss general features for the d-metric coefficients, $(g_2,g_3),(h_4,h_5)$, and the N-connection coefficients $w_{2,3}$ and $n_{2,3}$ which solve this system of equations:

(1) Equation (23) relates two functions $g_2(x^2,x^3)$ and $g_3(x^2,x^3)$ and their partial derivatives in the isotropic coordinates x^2 and x^3. If one of the functions is fixed, by some symmetry and boundary conditions the second function is found by solving a second order partial differential equation. For example, by redefinition of the coordinates or a conformal transformation one can transform g_3, (or conversely, g_2) into a constant. Using this technique one of the authors (SV) was able to construct various 2D soliton-dilaton and black-hole-like configurations[7]

(2) Equation (24) contains partial derivatives of only the anisotropic coordinate s, and relates the two functions $h_4(x^2,x^3,s)$ and $h_5(x^2,x^3,s)$. By fixing one of these functions the second one is found by solving a second or first order differential equation in s (the x-variables being treated as parameters). These equations reduce to the Bernoulli equations,[10] and are satisfied by two arbitrary functions $h_{4,5}(x^2,x^3)$ for which $h_{4,5}^*=0$. Thus there are three classes of solutions:

(a) class A, for which $h_4^*=0,\ h_5^*\neq 0$;
(b) class B, for which $h_5^*=0,\ h_4^*\neq 0$; and

(c) class C, both $h^*_{4,5}\neq 0$.

If the condition $h^*_5\neq 0$ is satisfied, we can write (24), in f-variables [see (19)], as

$$(\ln|f^*_5|+f_5-f_4)^*=0,$$

which is solved by arbitrary functions $f_5(x^2,x^3,s)$ and

$$f_4(x^1,x^2,s)=f_{4[0]}(x^1,x^2)+\ln|f^*_5|+f_5. \tag{27}$$

Bracketed subscripts indicate ''constants'' of integration with respect to the s variable. The general solution of (24) expressing h_5 via h_4 is

$$\begin{aligned} h_5(x^2,x^3,s)&=\left[h_{5[1]}(x^2,x^3)+h_{5[2]}(x^2,x^3)\int\sqrt{h_4(x^2,x^3,s)}ds,\right]^2\\ &=h_{5[0]}(x^2,x^3)[1+\varpi(x^2,x^3)s]^2,\quad h^*_4=0. \end{aligned} \tag{28}$$

The integration ''constants,'' $f_{5[0,1,2]}(x^2,x^3)$ and $\varpi(x^2,x^3)$, are determined by boundary conditions and locally anisotropic limits as well as from the requirement that Eqs. (25) and (26) are compatible. Conversely, for a given h_5, the general solution of (24) is (27) which can be rewritten with respect to variables $h_{4,5}$, as

$$h_4(x^2,x^3,s)=h_{4[0]}(x^2,x^3)[(\sqrt{|h_5(x^2,x^3,s)|})^*]^2. \tag{29}$$

(3) If the functions $h_4(x^2,x^3,s)$ and $h_5(x^2,x^3,s)$ are known, then Eqs. (25) become linearly independent algebraic equations for $w_{2,3}$:

$$w_{2,3}\beta+\alpha_{2,3}=0.$$

If in the case of vacuum Einstein equations $h^*_5=0$; we have $\alpha_{\hat{i}}=\beta=0$ and, as a consequence, Eq. (25) becomes trivial, allowing arbitrary values of the functions $w_{2,3}(x^2,x^3,s)$. For $h^*_5\neq 0$ we must impose the condition $\alpha_{2,3}=0$, or identify these values with the corresponding nondiagonal components of the energy-momentum tensor. We also note that ansatz (4) admits an arbitrary function $w_1(x^2)$ which is not contained in the vacuum Einstein equations. This function can be fixed by requiring that it be compatible with some locally isotropic solutions.

(4) Equations (26) can be solved in general form if the functions $h_4(x^2,x^3,s)$ and $h_5(x^2,x^3,s)$ [and therefore the coefficient γ from (20)] are known:

$$\begin{aligned} n_{2,3}(x^2,x^3,s)&=n_{2,3[0]}(x^2,x^3)+n_{2,3[1]}(x^2,x^3)\int\frac{h_4(x^2,x^3,s)}{h_5^{3/2}(x^2,x^3,s)}ds,\quad \gamma\neq 0;\\ n_{2,3}(x^2,x^3,s)&=n_{2,3[0]}(x^2,x^3)+n_{2,3[1]}(x^2,x^3)s,\quad \gamma=0, \end{aligned} \tag{30}$$

where the functions $n_{2,3[0]}(x^2,x^3)$ and $n_{2,3[1]}(x^2,x^3)$ are defined from some boundary conditions. Again the ansatz (4) admits another arbitrary function $n_1(x^2)$ which is not contained in the vacuum Einstein equations. This function can be fixed by requiring compatibility with some locally isotropic solutions.

If the metric coefficients h_4 and h_5 are solutions to Eq. (24), then one can define two new $[\hat{h}_4=\eta_4 h_4,\ \hat{h}_5=\eta_5 h_5]$ solutions. We call the functions $\eta_{4,5}=\eta_{4,5}(x^2,x^3,s)$ gravitational polarizations since they modify the behavior of the metric coefficients h_4 and h_5 in a manner similar to how a material modifies the behavior of electric and magnetic fields in media.

The ''renormalization'' of $h_{4,5}$ into $\hat{h}_{4,5}$ results in the ''renormalization'' of $n_{2,3}: n_{2,3}\to\hat{n}_{2,3}$ from formula (30) with $h_{4,5}\to\hat{h}_{4,5}$ and $\gamma\to\hat{\gamma}$.

III. LOCALLY ISOTROPIC WORMHOLES, FLUX TUBES, AND ANISOTROPIC RUNNING OF CONSTANTS

We give a brief review of the locally isotropic wormhole and flux tube solutions (DS-solutions) constructed in Refs. 4 and 11, and their anisotropic generalization proposed in Ref. 5. The isotropic DS-solutions represent 5D gravitational field configurations which carry ''electric'' and/or ''magnetic'' charges. Various authors have studied related 5D solutions: Liu and Wesson investigated 5D solitonic solutions;[12] they also considered 5D charged black holes;[13] 5D wormhole configurations with electromagnetic charges were studied in Ref. 14; Ref. 15 looks at 5D solutions with magnetic charge; and a general reference for 5D Kaluza-Klein theory and solutions is Ref. 16. The anisotropic constructions considered in this article are slightly different from Ref. 5. Here we use a fixed conformal factor, in order to construct anisotropic solutions with background geometries more general than spherical. The study of these more general background geometries will be carried out in Sec. V.

A. 5D locally isotropic wormholes and flux tubes

Reference 11 considered the following spherically symmetric 5D metric, with off-diagonal terms

$$ds^2_{(DS)}=e^{2\nu(r)}dt^2-dr^2-a(r)(d\theta^2+\sin^2\theta d\varphi^2) - r_0^2 e^{2\psi(r)-2\nu(r)}[d\chi_{(DS)}+\omega(r)dt+n\cos\theta d\varphi]^2, \tag{31}$$

where $\chi_{(DS)}$ is the fifth coordinate; r, θ,φ are $3D$ spherical coordinates; n is an integer; $r\in\{-R_0,+R_0\}$ ($R_0\leqslant\infty$) and r_0 is a constant. All functions $\nu(r),\psi(r)$ and $a(r)$ were considered to be even functions of r satisfying $\nu'(0)=\psi'(0)=a'(0)=0$. Here we shall study a particular class of this metric, with $\nu(r)=0$. We also introduce a new fifth coordinate

$$\chi=\chi_{(DS)}-\mu(\theta,\varphi)^{-1}\int d\xi(\theta,\varphi)$$

for which

$$d\chi_{(DS)}+n\cos\theta d\varphi=d\chi+n\cos\theta d\theta$$

and

$$\frac{\partial\xi}{\partial\varphi}=\mu n\cos\theta,\quad \frac{\partial\xi}{\partial\theta}=-\mu n\cos\theta,$$

if the factor $\mu(\theta,\varphi)$ is taken, for instance,

$$\mu(\theta,\varphi)=\exp(\theta-\varphi)|\cos\theta|^{-1}.$$

This redefinition of the fifth coordinate $\chi_{(DS)}\to\chi$, with $d\chi$ elongated by N-coefficients proportional to t,r,θ (isotropic coordinates), allows us to consider anisotropies on coordinates (φ,χ). The metric (31), in coordinates $(t,r,\theta,\varphi,\chi)$ and for $\nu(r)=0$, is equivalently rewritten as

$$ds^2_{(DS)}=dt^2-dr^2-a(r)(d\theta^2+\sin^2\theta d\varphi^2)-r_0^2e^{2\psi(r)}[d\chi+\omega(r)dt+n\cos\theta d\theta]^2. \tag{32}$$

This form of the metric will be used to find new, anisotropic solutions of Einstein's equations. The coefficient $\omega(r)$ in (32) is treated as the t-component of the electromagnetic potential and $n\cos\theta$ as the θ-component. These electromagnetic potentials lead to the metric having radial Kaluza–Klein ''electrical'' and ''magnetic'' fields. The 5D Kaluza–Klein ''electric'' field is

$$E_{KK}=r_0\omega' e^{3\psi}=q_0/a(r). \tag{33}$$

The "electric" charge $q_0=r_0\omega'(0)$ can be parametrized as

$$q_0=2\sqrt{a(0)}\sin\alpha_0.$$

The corresponding dual, "magnetic" field is

$$H_{KK}=Q_0/a(r) \tag{34}$$

with "magnetic" charge $Q_0=nr_0$ parametrized as

$$Q_0=2\sqrt{a(0)}\cos\alpha_0.$$

The following "circle" relation,

$$\frac{(q_0^2+Q_0^2)}{4a(0)}=1, \tag{35}$$

relates the "electric" and "magnetic" charges. As the free parameters of the metric are varied there are five classes of solutions with the properties:

(1) $Q_0=0$ or $H_{KK}=0$, a wormholelike "electric" object;
(2) $q_0=0$ or $E_{KK}=0$, a finite "magnetic" flux tube;
(3) $q_0=Q_0$ or $H_{KK}=E_{KK}$, an infinite "electromagnetic" flux tube;
(4) $Q_0<q_0$ or $H_{KK}<E_{KK}$, a wormholelike "electromagnetic" object; and
(5) $Q_0>q_0$ or $H_{KK}>E_{KK}$, a finite, "magnetic-electric" flux tube.

Metric (32) is a particular example of a d-metric of type (7), with the ansatz functions given by (4), or equivalently (8). For the coordinates $x^1=t,x^2=r,x^3=\theta,y^4=s=\chi,y^5=p=\varphi$ the set of ansatz functions

$$\begin{gathered} g_1=1,\quad g_2=-1,\quad g_3=-a(r),\\ h_4=-a(r)\sin^2\theta,\quad h_5=-r_0^2e^{2\psi(r)},\\ w_i=0,\quad n_1=\omega(r),\quad n_2=0,\quad n_3=n\cos\theta \end{gathered} \tag{36}$$

define a trivial, locally isotropic solution of the vacuum Einstein equations (23)–(26) which satisfies the conditions $h^*_{4,5}=0$. We next deal with anisotropic deformations of this solution.

B. Anisotropic generalizations of DS-solution

The simplest way to obtain anisotropic wormhole/flux tube solutions[5] is to take r_0^2 from (32) or (36)) not as a constant, but as "renormalized" via $r_0^2\to\hat{r}_0^2=\hat{r}_0^2(r,\theta,s)$.

1. DS-solutions with anisotropy via $s=\chi$

From the isotropic solution (36) we generate an anisotropic solution of class A by taking

$$\hat{h}_4(r,\theta)=h_4(r,\theta)=-a(r)\sin^2\theta,$$

with $\eta_4=1$ so that $\hat{h}^*_4=h^*_4=0$, but $\hat{h}^*_5=\eta^*_5(r,\theta,\chi)h_5(r)\neq 0$. Using Eq. (28) we parametrize

$$\hat{r}_0^2(\chi)\simeq r^2_{0(0)}[1+\varpi(r,\theta)\chi]^2 \tag{37}$$

so that

$$h_5(r,\theta,\chi)=\eta_5(r,\theta,\chi)h_5(r),$$

$$h_{5[0]}(r,\theta)=h_5(r)=-r_0^2e^{2\psi(r)},\quad \eta_5(r,\theta,\chi)=[1+\varpi(r,\theta)\chi]^2.$$

Under the conditions in this subsection β and $\alpha_{2,3}$ from Eqs. (17)–(19) (and therefore $w_{2,3}$) can be arbitrary functions. Here we will require $w_{2,3}\to 0$ in the locally isotropic limit, $\varpi\chi\to 0$. From Eq. (30) $n_{2,3}$ depends on the anisotropic variable $s=\chi$ in the following way:

$$n_3(r,\theta,\chi)=n_{3[0]}(r,\theta)+n_{3[1]}(r,\theta)[1+\varpi_0\chi]^{-2}$$

with $\varpi(r,\theta)=\varpi_0=\text{const}$. We obtain the locally isotropic limit of (36), for $\varpi\chi\to 0$, if we fix the boundary conditions with $n_{2[0,1]}=0, n_{3[0]}=0$, $n_{3[1]}(r,\theta)=n\cos\theta$ and $n_1=\omega(r)$.

The 5D gravitational vacuum polarization induced by variation of "constant" $\hat{r}_0(\chi)$ renormalizes the electromagnetic charge as $q(\chi)=\hat{r}_0(\chi)\omega'(r=0)$. In terms of the angular parametrization the "electric" charge becomes

$$q(\chi)=2\sqrt{a(0)}\sin\alpha(\chi).$$

The "electric" field from (33) becomes

$$E_{KK}=\frac{q(\chi)}{a(r)}.$$

The renormalization of the magnetic charge, $Q_0\to Q(\chi)$, can be obtained using the renormalized "electric" charge in relationship (35) and solving for $Q(\chi)$. The form of (35) implies that the running of $Q(\chi)$ will be the opposite that of $q(\chi)$. For example, if $q(\chi)$ increases with χ, then $Q(\chi)$ will decrease. The locally anisotropic polarizations $\alpha(\chi)$ are either defined from experimental data or computed from a quantum model of 5D gravity. With the coordinates taken as $x^1=t, x^2=r, x^3=\theta, y^4=s=\chi, y^5=p=\varphi$, one can construct a locally anisotropic solution of the vacuum Einstein equations (23)-(26) by making the following identifications for the ansatz functions from (32):

$$\begin{gathered}g_1=1,\quad g_2=-1,\quad g_3=-a(r),\\ \hat{h}_4=h_4=-a(r)\sin^2\theta,\quad \eta_4=1,\\ \hat{h}_5=\eta_5h_5,\quad h_5(r)=-r_0^2e^{2\psi(r)},\quad \eta_5=[1+\varpi_0\chi]^2,\\ w_i=0,\quad n_1=\omega(r),\quad n_2=0,\quad n_3=n\cos\theta[1+\varpi_0\chi]^{-2}.\end{gathered}\tag{38}$$

This generalizes the DS-solution (32) by allowing the Kaluza-Klein electric and magnetic charges to be dependent on (i.e., scale with) the fifth coordinate $s=\chi$. We will call these the χ-solutions).

2. DS-solutions with anisotropy via φ

In a similar fashion we can consider anisotropic dependencies with respect to $s=\varphi$. These will be called φ-solutions. The simplest option is to take $h_5^*=0$ but $h_4^*\neq 0$, i.e., to define a solution with

$$\hat{h}_4(r,\theta,\varphi)=\eta_4h_4(r),\quad h_4(r)=-r_0^2e^{2\psi(r)},$$

$$\hat{h}_5(r,\theta)=h_5(r,\theta)=-a(r)\sin^2\theta,$$

$$\eta_4=\exp[\varpi(r,\theta,\varphi)],\quad \eta_5=1.$$

This allows $w_{2,3}$ to take arbitrary values since β and $\alpha_{2,3}$ from Eqs. (25) vanish. For small polarizations we can approximate

$$\hat{h}_4(r,\theta,\varphi)=h_{4[0]}(r,\theta)[1+\varpi\varphi].$$

The general solution of (26) for $\hat{\gamma}=-(\ln|\hat{h}_4|)^*$ is

$$n_{2,3}(r,\theta,\varphi)=n_{2,3[0]}(r,\theta)+n_{2,3[1]}(r,\theta)\int \exp\,\varpi(r,\theta,\varphi)d\varphi;$$

we take $w_1=\omega(r), w_2=0, w_3=n\cos\theta$, $n_{2[0]}(r,\theta)=0$ and $n_{3[0]}(r,\theta)=n\cos\theta$, $n_{,3[1]}(r,\theta)=1$ which are compatible with the local isotropic limit [i.e. $\varpi(r,\theta,\varphi)\to 0$ and $\int\varpi(r,\theta,\varphi)d\varphi\to 0$]. Taking the coordinates as $x^1=t, x^2=r, x^3=\theta, y^4=s=\varphi, y^5=p=\chi$ the following form for the ansatz functions,

$$\begin{gathered}
g_1=1,\quad g_2=-1,\quad g_3=-a(r),\\
\hat{h}_4=\eta_4 h_4,\quad h_4=-r_0^2e^{2\psi(r)},\quad \eta_4=\exp[\varpi(r,\theta,\varphi)],\\
\hat{h}_5=h_5,\quad h_5=-a(r)\sin^2\theta,\quad \eta_5=1,\\
w_1=\omega(r),\quad w_2=0,\quad w_3=n\cos\theta,\\
n_1=0,\quad n_{2,3}=n_{2,3[1]}(r,\theta)\int \exp\varpi(r,\theta,\varphi)d\varphi,
\end{gathered}\tag{39}$$

gives a locally anisotropic generalization of the DS-metric (32) for anisotropic dependencies on the angle φ.

We have constructed two classes of locally anisotropic generalizations of the DS-solution: $s=\varphi$ (i.e., anisotropic angular polarizations) or $s=\chi$ (i.e., dependence of the Kaluza-Klein charges on the fifth coordinate). If the metric (32), describing these two classes of solutions, were given with respect to a coordinate frame (1) nondiagonal terms would occur, and the study of these solutions would be more difficult.

IV. GRAVITATIONAL θ-POLARIZATION OF KALUZA–KLEIN CHARGES

We can further generalize the forms (38) and (39) to generate new solutions of the 5D vacuum Einstein equations with deformations of the constants r_0^2 and n with respect to the θ variable. These θ deformations take the form of the equation for an ellipsoid in polar coordinates. This again leads to varying electric, q, and magnetic, Q, charges.

A. Gravitational renormalization of Kaluza–Klein charges via variable r_0

In this subsection we give a solution for which the Kaluza–Klein charges are gravitationally renormalized by the radius becoming dependent on θ [i.e., in Eq. (35) $a(0)\to a(\theta)$].

1. θ-renormalization of charges for χ-solutions

The easiest way to obtain such θ-polarizations for the χ-solutions of (28) and (37) is to consider the coordinates as $x^1=t, x^2=r, x^3=\theta, y^4=s=\chi, y^5=p=\varphi$, and let the ansatz functions take the form

$$\begin{gathered}
g_1=1,\quad g_2=-1,\quad g_3=-a(r),\\
\hat{h}_4=h_4=-a(r)\sin^2\theta,\quad \eta_4=1,\\
\hat{h}_5=\eta_5 h_5(r),\quad h_5(r)=-r_0^2e^{2\psi(r)},\quad \eta_5=[1+\varepsilon_r\cos\theta]^{-2}[1+\varpi_0\chi]^2,\\
w_i=0,\quad n_1=\omega(r),\quad n_2=0,\quad n_3=n\cos\theta[1+\varpi_0\chi]^{-2},
\end{gathered}\tag{40}$$

where η_5 is the polarizaton and

$$\hat{r}_0^2(r,\theta,\chi)\simeq r_{0(0)}^2[1+\varepsilon_r\cos\theta]^{-2}[1+\varpi_0\chi]^2,$$

where ε_r is the eccentricity. The "constant," $\hat{r}_0$, has both an elliptic variation in θ (i.e., $r_{0(0)}[1+\varepsilon_r\cos\theta]^{-1}$) and a linear variation on the fifth coordinate (i.e., $[1+\varpi(r,\theta)\chi]$).

For these χ-solutions with elliptic variations as given above the 5D Kaluza–Klein charges get renormalized through the elliptic variation of $\hat{r}_0(r,\theta,\varepsilon_r,\chi)$. This renormalizes the "electric" charge as

$$q(\theta,\chi)=r_0\sqrt{\eta_5(\theta,\varepsilon_r,\chi)}\omega'(0)=\sqrt{\eta_5(\theta,\varepsilon_r,\chi)}q_0$$

or in terms of the angular parametrization

$$q(\theta,\chi)=2\sqrt{a(0)}\sqrt{\eta_5(\theta,\varepsilon_r,\chi)}\sin\alpha_0.$$

The "electric" field (33) transforms into

$$E_{KK}=\frac{q(\theta,\chi)}{a(r)}=\frac{q_0}{(\sqrt{\eta_5})^{-1}a(r)}.$$

Here $(\sqrt{\eta_5})^{-1}$ can be treated as an anisotropic, gravitationally induced permittivity. The renormalization of the magnetic charge, $Q_0\to Q(\theta,\chi)$, can be obtained from Eq. (35) using $q(\theta,\chi)$ from above. In this case the corresponding dual "magnetic" field is $H_{KK}=Q(\theta,\chi)/a(r)$ with the "magnetic" charge $Q_0=nr_0$ given by

$$Q=2\sqrt{a(0)}\sqrt{\eta_5(\theta,\varepsilon_r,\chi)}\cos\alpha_0.$$

These gravitationally polarized charges satisfy the circumference equation (35) with variable radius $2\sqrt{a(0)}\sqrt{\eta_5(\theta,\varepsilon_r,\chi)}$:

$$\frac{(q_0^2+Q_0^2)}{4a(0)\,\eta_5(\theta,\varepsilon_r,\chi)}=1. \tag{41}$$

2. Elliptic renormalization of charges for φ-solutions

The φ-solutions can also be modified to have an elliptic variation with respect to θ. As in the case of the χ-solutions this gives an effective gravitational renormalization of the charges. With the coordinates defined as $x^1=t,x^2=r,x^3=\theta,y^4=s=\varphi,y^5=p=\chi$ the form of this variation of the φ-solutions is

$$g_1=1,\quad g_2=-1,\quad g_3=-a(r),$$

$$\hat{h}_4=\eta_4 h_4,\quad h_4=-r_0^2e^{2\psi(r)},\quad \eta_4=[1+\varepsilon_r\cos\theta]^{-2}\exp[\varpi(r,\theta,\varphi)],$$

$$\hat{h}_5=h_5=-a(r)\sin^2\theta,\quad \eta_5=1,\quad \hat{h}_5^*=h_5^*=0, \tag{42}$$

$$w_1=\omega(r),\quad w_2=0,\quad w_3=n\cos\theta,$$

$$n_1=0,\quad n_{2,3}=n_{2,3[1]}(r,\theta)\int\exp\varpi(r,\theta,\varphi)d\varphi.$$

The renormalized charges arise as in the previous example via $r_0^2\to\hat{r}_0^2(r,\theta,\varphi)$. The "electric" charge becomes

$$q(\theta,\varphi)=r_0\sqrt{\eta_4(\theta,\varepsilon_r,\varphi)}\,\omega'(0)=\sqrt{\eta_4(\theta,\varepsilon_r,\varphi)}\,q_0.$$

In terms of the angular parametrization this becomes

$$q(\theta,\varphi)=2\sqrt{a(0)}\sqrt{\eta_4(\theta,\varepsilon_r,\varphi)}\sin\alpha.$$

The "electric" field (33) transforms into

$$E_{KK}=\frac{q(\theta,\varphi)}{a(r)}=\frac{q_0}{(\sqrt{\eta_4})^{-1}a(r)}.$$

Here $(\sqrt{\eta_4})^{-1}$ can be treated as an anisotropic gravitationally induced permittivity depending on the angular variables. The renormalized magnetic charge, $Q_0\to Q(\theta,\varphi)$, can be determined using Eq. (35) and $q(\theta,\varphi)$ giving

$$Q(\theta,\varphi)=2\sqrt{a(0)}\sqrt{\eta_4(\theta,\varepsilon_r,\varphi)}\cos\alpha_0.$$

The "magnetic" field is then $H_{KK}=Q(\theta,\varphi)/a(r)$. The gravitationally polarized charges satisfies Eq. (35) with a variable radius of $2\sqrt{a(0)}\sqrt{\eta_4(\theta,\varepsilon_r,4)}$:

$$\frac{(q_0^2+Q_0^2)}{4a(0)\,\eta_4(\theta,\varepsilon_r,\varphi)}=1. \tag{43}$$

There is again an elliptical variation in θ, and also an anisotropic dependence in φ.

Comparing formulas (41) and (43) we find that there are two types of anisotropic gravitational polarizations of the charges: in the first case the running with respect to the fifth coordinate is emphasized; in the second case the anisotropy comes just from the angular variables. In both cases there is an elliptical dependence on θ.

B. Gravitational renormalization of Kaluza–Klein charges via r_0 and n

A different class of solutions from those given in Eqs. (38), (39), (40), and (42) can be constructed if, in addition to r_0, we allow the n in the $n\cos\theta$ term in Eq. (32) to vary. For the χ-solutions this variable n will affect n_3, while for the φ-solutions it will affect w_3. The variability of r_0 and n is parametrized using the gravitational vacuum polarizations $\kappa_r(r,\theta,s)$ and $\kappa_n(r,\theta,s)$ as

$$r_0\to\hat{r}_0=r_0/\kappa_r(r,\theta,s)\qquad\text{and}\qquad n\to\hat{n}=n/\kappa_n(r,\theta,s),$$

where $\kappa_r(r,\theta,s)=[\sqrt{\eta_4(r,\theta,s)}]^{-1}$ or $=[\sqrt{\eta_5(r,\theta,s)}]^{-1}$. The polarized charges are

$$q=q_0/\kappa_r=2\sqrt{a(0)}\sin\alpha_0/\kappa_r$$

and

$$Q=Q_0/\kappa_n=2\sqrt{a(0)}\,\cos\alpha_0/\kappa_n.$$

Using these charges in Eq. (35) gives the formula for an ellipse in the charge space coordinates (q_0,Q_0),

$$\frac{q_0^2}{4a(0)\kappa_r^2}+\frac{Q_0^2}{4a(0)\kappa_n^2}=1, \tag{44}$$

where the axes of the ellipse are $2\sqrt{a(0)}\kappa_r$ and $2\sqrt{a(0)}\kappa_n$. Formula (44) contains formulas (41) and (43) as special cases.

The form of the χ- and φ-solutions from the previous two subsections gets modified by this "elliptic" renormalization of the Kaluza–Klein charges.

(a) With the coordinates defined as $x^1=t,x^2=r,x^3=\theta,y^4=s=\chi,y^5=p=\varphi$ the χ-solutions with $\kappa_r=[\sqrt{\eta_5(r,\theta,\chi)}]^{-1}$ take the form

$$\begin{gathered} g_1=1, \quad g_2=-1, \quad g_3=-a(r), \\ \hat{h}_4=h_4=-a(r)\sin^2\theta, \quad \hat{h}_4^*=0, \quad h_4^*=0, \quad \eta_4=1, \\ \hat{h}_5=\eta_5 h_5, \quad h_5=-r_0^2 e^{2\psi(r)}, \quad \eta_5=1/\kappa_r^2(r,\theta,\chi), \\ w_i=0, \quad n_1=\omega(r), \quad n_2=0, \quad n_3=n\cos\theta/\kappa_n(r,\theta,\chi). \end{gathered} \tag{45}$$

(b) With the coordinates defined as $x^1=t,x^2=r,x^3=\theta,y^4=s=\varphi,y^5=p=\chi$ the φ-solutions with $\kappa_r=[\sqrt{\eta_4(r,\theta,\chi)}]^{-1}$ take the form

$$\begin{gathered} g_1=1, \quad g_2=-1, \quad g_3=-a(r), \\ \hat{h}_4=\eta_4 h_4, \quad h_4=-r_0^2 e^{2\psi(r)}, \quad \eta_4=1/\kappa_r^2(r,\theta,\varphi), \\ \hat{h}_5=h_5=-a(r)\sin^2\theta, \quad \eta_5=1, \quad h_5^*=0, \\ w_1=\omega(r), \quad w_2=0, \quad w_3=n\cos\theta/\kappa_n(r,\theta,\varphi), \\ n_1=0, \quad n_{2,3}=n_{2,3[1]}(r,\theta)\int \ln|\kappa_r(r,\theta,\varphi)|d\varphi. \end{gathered} \tag{46}$$

V. WORMHOLES IN ELLIPSOIDAL, CYLINDRICAL, BIPOLAR AND TOROIDAL BACKGROUNDS

The locally anisotropic wormhole/flux tube solutions presented in the previous sections are anisotropic deformations from a spherical 3D hypersurface background. These solutions can be generalized to other rotational hypersurface geometry backgrounds. In this section we will give the explicit forms for these generalized solutions and analyze their basic properties. The notations and metric relations for the 3D Euclidean rotational hypersurfaces that we use will be those of Ref. 17.

A. Elongated rotation ellipsoid hypersurfaces

An elongated rotation ellipsoid hypersurface (a 3D e-ellipsoid) is given by the formula

$$\frac{x^2+y^2}{\sigma^2-1}+\frac{z^2}{\sigma^2}=\tilde{a}^2(r), \tag{47}$$

where $\sigma\geqslant 1$, and x,y,z here are the usual Cartesian coordinates. $\tilde{a}(r)$ is similar to the radius in the spherical symmetric case. The 3D, ellipsoidal coordinate system is defined

$$x=\tilde{a}\sinh u\sin v\cos s, \quad y=\tilde{a}\sinh u\sin v\sin s, \quad z=\tilde{a}\cosh u\cos v, \tag{48}$$

where $\sigma=\cosh u$ and $0\leqslant u<\infty$, $0\leqslant v\leqslant\pi$, $0\leqslant s<2\pi$. The hypersurface metric is

$$g_{uu}=g_{vv}=\tilde{a}^2(\sinh^2 u+\sin^2 v), \quad g_{ss}=\tilde{a}^2\sinh^2 u\sin^2 v. \tag{49}$$

It will be more useful to consider a conformally transformed metric, where the components in Eq. (49) are multiplied by the conformal factor $\tilde{a}^{-2}(\sinh^2 u+\sin^2 v)^{-1}$, giving

$$ds^2_{(3e)} = du^2 + dv^2 + g_{ss}(u,v)ds^2,$$
$$g_{ss}(u,v) = \sinh^2 u \sin^2 v/(\sinh^2 u + \sin^2 v). \tag{50}$$

B. Flattened rotation ellipsoid hypersurfaces

In a similar fashion we consider the hypersurface equation for a flattened rotation ellipsoid (a 3D f-ellipsoid),

$$\frac{x^2+y^2}{1+\sigma^2} + \frac{z^2}{\sigma^2} = \tilde{a}^2(r), \tag{51}$$

Here $\sigma \geqslant 0$ and $\sigma = \sinh u$. In this case the 3D coordinate system is defined as

$$x = \tilde{a}\cosh u \sin v \cos s, \quad y = \tilde{a}\cosh u \sin v \sin s, \quad z = \tilde{a}\sinh u \cos v, \tag{52}$$

where $0 \leqslant u < \infty$, $0 \leqslant v \leqslant \pi$, $0 \leqslant s < 2\pi$. The hypersurface metric is

$$g_{uu} = g_{vv} = \tilde{a}^2(\sinh^2 u + \cos^2 v), \quad g_{\varphi\varphi} = \tilde{a}^2 \sinh^2 u \cos^2 v. \tag{53}$$

Again for later convenience we consider a conformally transformed version of this metric:

$$ds^3_{(3f)} = du^2 + dv^2 + g_{ss}(u,v)ds^2,$$
$$g_{ss}(u,v) = \sinh^2 u \cos^2 v/(\sinh^2 u + \cos^2 v). \tag{54}$$

C. Ellipsoidal cylindrical hypersurfaces

The formula for an ellipsoidal cylindrical hypersurface is

$$\frac{x^2}{\sigma^2} + \frac{y^2}{\sigma^2 - 1} = \rho^2, \quad z = s, \tag{55}$$

where $\sigma \geqslant 1$. The 3D radial coordinate is given as $\tilde{a}^2 = \rho^2 + s^2$. The 3D coordinate system is defined

$$x = \rho \cosh u \cos v, \quad y = \rho \sinh u \sin v, \quad z = s,$$

where $\sigma = \cosh u$ and $0 \leqslant u < \infty$, $0 \leqslant v \leqslant \pi$. Using the expressions for x,y and Eq. (55) we can make the change $\rho(x,y) \to \rho(u,v)$. The hypersurface metric is

$$g_{uu} = g_{vv} = \rho^2(u,v)(\sinh^2 u + \sin^2 v), \quad g_{ss} = 1;$$

we will again consider a conformally transformed version of this metric:

$$ds^2_{(3c)} = du^2 + dv^2 + g_{ss}(u,v,\rho(u,v))ds^2,$$
$$g_{ss}(u,v) = 1/\rho^2(u,v)(\sinh^2 u + \sin^2 v). \tag{56}$$

D. Bipolar coordinates

Now we consider a bipolar hypersurface given by the formula

$$\left(\sqrt{x^2+y^2} - \frac{\tilde{a}(r)}{\tan\xi}\right)^2 + z^2 = \frac{\tilde{a}^2(r)}{\sin^2\xi}, \tag{57}$$

which describes a hypersurface obtained by rotating the circles

$$\left(y-\frac{\tilde{a}(r)}{\tan\xi}\right)^2+z^2=\frac{\tilde{a}^2(r)}{\sin^2\xi}$$

around the z axis; because $|\tan\xi|^{-1}<|\sin\xi|^{-1}$, the circles intersect the z axis. The relationship between the Cartesian coordinates and the bipolar coordinates is

$$x=\frac{\tilde{a}(r)\sin\xi\cos s}{\cosh\tau-\cos\xi},\quad y=\frac{\tilde{a}(r)\sin\xi\sin s}{\cosh\tau-\cos\xi},\quad z=\frac{\tilde{a}(r)\sinh\tau}{\cosh\tau-\cos\xi},$$

where $-\infty<\tau<\infty,0\leqslant\xi<\pi,0\leqslant s<2\pi$. The hypersurface metric is

$$g_{\tau\tau}=g_{\xi\xi}=\frac{\tilde{a}^2(r)}{(\cosh\tau-\cos\xi)^2},\quad g_{ss}=\frac{\tilde{a}^2(r)\sin^2\xi}{(\cosh\tau-\cos\xi)^2},$$

which, after multiplication by the conformal factor $(\cosh\tau-\cos\sigma)^2/\rho^2$, becomes

$$ds^2_{(3b)}=d\tau^2+d\xi^2+g_{ss}(\xi)ds^2,\quad g_{ss}(\xi)=\sin^2\xi. \tag{58}$$

E. Toroidal coordinates

Now we consider a toroidal hypersurface with nontrivial topology given by the formula

$$(\sqrt{x^2+y^2}-\tilde{a}(r)(\coth\xi))^2+z^2=\frac{\tilde{a}^2(r)}{\sinh^2\xi}. \tag{59}$$

The relationship to the Cartesian coordinates is given by

$$x=\frac{\tilde{a}(r)\sinh\tau\cos s}{\cosh\tau-\cos\xi},\quad y=\frac{\tilde{a}(r)\sin\xi\sin s}{\cosh\tau-\cos\xi},\quad z=\frac{\tilde{a}(r)\sinh\xi}{\cosh\tau-\cos\xi},$$

where $-\pi<\xi<\pi,0\leqslant\tau<\infty,0\leqslant s<2\pi$. The hypersurface metric is

$$g_{\sigma\sigma}=g_{\tau\tau}=\frac{\tilde{a}^2(r)}{(\cosh\tau-\cos\xi)^2},\quad g_{ss}=\frac{\tilde{a}^2(r)\sin^2\xi}{(\cosh\tau-\cos\xi)^2}.$$

After multiplication by the conformal factor $(\cosh\tau-\cos\sigma)^2/\tilde{a}^2(r)$ this takes the same form as (58)

$$ds^3_{(3t)}=d\tau^2+d\xi^2+g_{ss}(\xi)ds^2,\quad g_{ss}(\xi)=\sin^2\xi. \tag{60}$$

Although this looks identical to the metric in (58), the coordinates (τ,ξ,s) have different meanings in each case. This can be seen by the different ranges for the two cases.

F. Anisotropic wormholes in rotation deformed hypersurface backgrounds

In order to construct wormholes which exhibit the various 3D geometries cataloged above, we will associate one of the ansatz functions of the wormhole solutions with $g_{ss}(x^2,x^3)$. For the χ-solutions this is accomplished by letting $h_4=g_{ss}(x^2,x^3)$; for the φ-solutions this is accomplished letting by $h_5=g_{ss}(x^2,x^3)$.

The construction of such solutions is based on the assumption that $g_{ss}(x^2,x^3)$ for the five nonspherical geometries listed above is to be taken as $h_4=g_{ss}(x^2,x^3)$ (for χ-solutions), or as $h_5=g_{ss}(x^2,x^3)$ [for $\varphi(z)$-solutions]. In each case $h_{4,5}$ is multiplied by corresponding gravitational polarizations, $\eta_{4,5}$, so as to give wormhole/flux tube configurations of the form (38), (40), and (45) (for χ-solutions) or configurations of the form (39), (42), and (46) [for $\varphi(z)$-solutions].

1. The χ-solutions

For the five 3D geometries given above, the d-metrics (8) for the χ-solutions from Eqs. (38), (40), and (45) have the coordinates defined as

$$x^k=\begin{cases}(t,u,v),0\leqslant u<\infty,0\leqslant v\leqslant\pi,\cosh u\geqslant 1,\ \text{ellipsoid}\ (47);\\ (t,u,v),0\leqslant u<\infty,0\leqslant v\leqslant\pi,\sinh u\geqslant 0,\ \text{ellipsoid}\ (51);\\ (t,u,v),0\leqslant u<\infty,0\leqslant v\leqslant\pi,\cosh u\geqslant 1,\ \text{cylinder}\ (55);\\ (t,\tau,\xi),-\infty<\tau<\infty,0\leqslant\xi<\pi,\ \text{bipolar}\ (57);\\ (t,\tau,\xi),0\leqslant\tau<\infty,-\pi<\xi<\pi,\ \text{torus}\ (59);\end{cases}$$

$$y^4=s=\chi,\quad y^5=p=\begin{cases}\varphi\in[0,2\pi),\ \text{ellipsoids; bipolar; torus;}\\ z\in(-\infty,\infty),\ \text{cylinder;}\end{cases}$$

and the ansatz functions given as

$$g_1=1,\quad g_2=-1,\quad g_3=-1, \tag{61}$$

$$\hat{h}_4=\eta_4 h_4,\quad h_4=g_{ss}(x^2,x^3)=\begin{cases}\dfrac{\sinh^2 u\sin^2 v}{\sinh^2 u+\sin^2 v},\ \text{ellipsoid}\ (50);\\ \dfrac{\sinh^2 u\cos^2 v}{\sinh^2 u+\cos^2 v},\ \text{ellipsoid}\ (54);\\ \dfrac{\rho^{-2}(u,v)}{\sinh^2 u+\sin^2 v},\ \text{cylinder}\ (55);\\ \sin^2\xi,\ \text{bipolar}\ (57);\ \text{torus}\ (59);\end{cases}$$

$$\eta_4=[(\sqrt{\hat{h}_5(x^2,x^3,\chi)})^*]^2,\ \text{see}\ (27); \tag{62}$$

$$\eta_5=\begin{cases}[1+\varpi_0\chi]^2,\ \text{see}\ (38);\\ [1+\varepsilon_r\cos x^3]^{-2}[1+\varpi_0\chi]^2,\ \text{see}\ (40);\\ 1/\kappa_r^2(x^2,x^3,\chi),\ \text{see}\ (45);\end{cases}$$

$$\hat{h}_5=\eta_5 h_5,\quad h_5(x^2,x^3,\chi)=-r_0^2\exp\{2\psi[r(x^2,x^3,\chi)]\};\quad w_i=0;$$

$$r=\tilde{a}^{(\text{invers})}(x^2,x^3,\chi)\ \ \text{from}\ (47),(51),(55),(57),(59);$$

$$n_1=\omega(x^2),\quad n_2=0,\quad n_3=n\cos x^2\times\begin{cases}[1+\varpi_0\chi]^{-2},\ \text{see}\ (38);\\ [1+\varpi_0\chi]^{-2},\ \text{see}\ (40);\\ 1/\kappa_n(x^2,x^3,\chi),\ \text{see}\ (45)\ .\end{cases}$$

The formulas (61) describe wormhole/flux tube configurations which are defined self-consistently in the various rotational hypersurface backgrounds listed above. As in the case of the spherical background, these solutions have an anisotropic deformation with respect to the given hypersurface backgrounds.

2. The φ-solutions

Now we give the form of the d-metric (8) for the φ-solutions embedded in the five 3D rotational hypersurfaces. The coordinates are taken as

$$x^k=\begin{cases}(t,u,v),0\leqslant u<\infty,\ 0\leqslant v\leqslant\pi,\cosh u\geqslant 1,\ \text{ellipsoid (47)};\\ (t,u,v),0\leqslant u<\infty,\ 0\leqslant v\leqslant\pi,\sinh u\geqslant 0,\ \text{ellipsoid (51)};\\ (t,u,v),0\leqslant u<\infty,\ 0\leqslant v\leqslant\pi,\cosh u\geqslant 1,\ \text{cylinder (55)};\\ (t,\tau,\xi),-\infty<\tau<\infty,\ 0\leqslant\xi<\pi,\ \text{bipolar (57)};\\ (t,\tau,\xi),0\leqslant\tau<\infty,-\pi<\xi<\pi,\ \text{torus (59)};\end{cases}$$

$$y^4=s=\begin{cases}\varphi\in[0,2\pi),\ \text{ellipsoid; bipolar; torus;}\\ z\in(-\infty,\infty),\ \text{cylinder;}\end{cases}\qquad y^5=p=\chi,$$

and the ansatz functions given as

$$g_1=1,\quad g_2=-1,\quad g_3=-1, \tag{63}$$

$$\hat{h}_4=\eta_4 h_4,\quad h_4=g_{ss}(x^2,x^3)=\begin{cases}\dfrac{\sinh^2 u\sin^2 v}{\sinh^2 u+\sin^2 v},\ \text{ellipsoid (50)};\\ \dfrac{\sinh^2 u\cos^2 v}{\sinh^2 u+\cos^2 v},\ \text{ellipsoid (54)};\\ \dfrac{\rho^{-2}(u,v)}{\sinh^2 u+\sin^2 v},\ \text{cylinder (55)};\\ \sin^2\xi,\ \text{bipolar (57); torus (59)};\end{cases}$$

$$\eta_4=\begin{cases}\exp[\varpi(x^2,x^3,s],\ \text{see (39)};\\ [1+\varepsilon_r\cos x^3]^{-2}\exp[\varpi(x^2,x^3,s)],\ \text{see (42)};\\ 1/\kappa_r^2(x^2,x^3,s),\ \text{see (46)};\end{cases} \tag{64}$$

$$\eta_5=\begin{cases}\eta_{5[0]}(x^2,x^3)+\eta_{5[1]}(x^2,x^3)\displaystyle\int\eta_4(x^2,x^3,s)ds,\ \text{for } \hat{h}_4^*\neq 0,\\ \eta_{5[0]}(x^2,x^3)+\eta_{5[1]}(x^2,x^3)s;\ \text{for } \hat{h}_4^*=0;\end{cases}$$

$$\hat{h}_5=\eta_5 h_5,\quad h_5(x^2,x^3,s)=-r_0^2\exp\{2\psi[r(x^2,x^3,s)]\};$$

$$r=\tilde{a}^{(invers)}(x^2,x^3,s)\ \text{ from (47),(51),(55),(57),(59);}$$

$$w_1=\omega(x^2),\quad w_2=0,\quad w_3=n\cos x^2\times\begin{cases}1,\ \text{see (39)};\\ 1,\ \text{see (42)};\\ 1/\kappa_n(x^2,x^3,s),\ \text{see (46)};\end{cases}$$

$$n_1=0,\quad n_{2,3}=n_{2,3[0]}(x^2,x^3)\times\begin{cases}\displaystyle\int\exp\varpi_0(x^2,x^3,s)ds,\ \text{see (39)};\\ \displaystyle\int\exp\varpi_0(x^2,x^3,s)ds,\ \text{see (42)};\\ \displaystyle\int|\ln\kappa_n(x^2,x^3,s)|ds,\ \text{see (46)}.\end{cases}$$

Formulas (63) describe a large class of wormhole/flux tube configurations which are defined self-consistently in the various 3D rotation hypersurface backgrounds. The deformations in this case come from the angular coordinate $s=\varphi$ (for the ellipsoid, bipolar and toroidal cases) or from the axial coordinate $s=z$ (for the cylindrical case). These ''deformation'' or anisotropic coordinates, φ or z, are also third coordinates about which the rotation of the hypersurfaces occurs.

VI. CONCLUSIONS

The construction of wormhole and/or flux tube solutions in modern string theory, extra dimensional gravity and quantum chromodynamics is of fundamental importance in understanding these theories (especially their nonperturbative aspects). Such solutions are difficult to find, and the solutions which are known usually have a high degree of symmetry. In this article we have applied the method of anholonomic frames to construct the general form of wormholes and flux tubes in 5D Kaluza–Klein theory. These solutions have local anisotropy which would make their study using holonomic frames difficult. This helps to demonstrate the usefulness of the anholonomic frames method in studying anisotropic solutions. Most physical situations do not possess a high degree of symmetry, and so the anholonomic frame method provides a useful mathematical framework for studying these less symmetric configurations.

The key result of this article is the demonstration that off-diagonal metrics in 5D Kaluza–Klein theory can be parametrized into forms that define new, interesting classes of solutions of Einstein's vacuum equations. These solutions represent wormhole and flux tube configurations which are locally anisotropic. These anisotropic solutions reduce to previously known spherically symmetric wormhole metrics[3,4,11] in the local isotropic limit. These anisotropic solutions also extend the idea of Salam, Strathee and Perracci[3] that including off-diagonal components in higher dimensional metrics gives rise to gauge fields and charges. Not only do we find ''electric'' and ''magnetic'' charges for our solutions, but the anisotropies in the fifth coordinate (χ) and/or in the angular coordinate (φ) give a gravitational scaling or running of these Kaluza-Klein charges. Such a gravitational scaling of charges could provide an experimental signature for the presence of extra dimensions (i.e., if some charge were observed to exhibit a running which was not in agreement with that given by 4D quantum field theory, this could be evidence for a gravitational running of the charge).

In the first part of this article these anisotropic solutions were constructed as deformations from a spherical background. In the final section of this article we showed that it is possible to construct a large variety of such anisotropic solutions as deformations from various background geometries: elliptic (elongated and flattened), cylindrical, toroidal and bipolar.

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Bi-quasi-Hamiltonian systems

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A general notion of bi-quasi-Hamiltonian systems is introduced and is related to previous work on various special cases of such systems. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1462856]

I. INTRODUCTION

In a previous paper [Crampin and Sarlet (2001)], we have generalized work by Lundmark (2001a,b) on a class of integrable systems, from Euclidean spaces to (pseudo) Riemannian manifolds. In doing so, we came across an interesting class of conformal Killing tensors, called ''special conformal Killing tensors,'' and the integrable systems of interest live on spaces whose metric allows the coexistence of two such tensors. Physically speaking, the integrable systems in question represent Lagrangian systems with nonconservative forces, but whose force form has a kind of double ''generalized potential'' representation. Whereas most classical (finite dimensional) integrable systems are known to have a bi-Hamiltonian formulation, the ones referred to here have a double quasi-Hamiltonian representation and thus could be called bi-quasi-Hamiltonian systems. But they do lead to a bi-Hamiltonian system on an extended space.

In the present paper, we will introduce a general concept of bi-quasi-Hamiltonian systems and explore under what circumstances they can have the property of complete integrability. Bi-quasi-Hamiltonian systems should not be confused with quasi-bi-Hamiltonian systems, as introduced by Brouzet *et al.* (1996) and developed by Morosi and Tondo (1997, 1998). The similarity of the two terms is unfortunate, but the name ''bi-quasi-Hamiltonian system'' describes what we have in mind so well that after some reflection we decided to use it even so. The two concepts are in fact related, but the relation is not entirely straightforward: we discuss it in Sec. VII.

Following the description of the general concept in Secs. II and III, we specialize in Sec. IV to the case where the two Poisson structures involved in the bi-quasi-Hamiltonian representation each come from a Poisson–Nijenhuis structure. Most of the discussion in such a case is transferred from the Poisson structures involved to the type (1,1) tensor fields which generate them. We then make a further specialization, to the case where the manifold is a cotangent bundle and the (1,1) tensors are the complete lifts of tensor fields on the base manifold. This brings us back to the kind of system studied in Crampin and Sarlet (2001), and we take this opportunity to complement our previous work with some results about the possible generation of families of such bi-quasi-Hamiltonian systems. The final section contains an explicit example which illustrates the theory.

We carry out coordinate calculations at various points in the paper; where we do so, we use the Einstein summation convention.

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II. QUASI-HAMILTONIAN SYSTEMS

We begin by recalling some generalities about Poisson structures.

A Poisson structure on a manifold M is a bivector field Π which satisfies $[\Pi,\Pi]=0$, where $[\cdot,\cdot]$ is the Schouten bracket. The associated Poisson bracket of functions f, g is given by $\{f,g\}=\Pi(df,dg)$; the vanishing of the Schouten bracket entails the Jacobi identity for the Poisson bracket. Also associated with such a bivector field is a map P of one-forms to vector fields on M, given by $\langle P(\alpha),\beta\rangle=\Pi(\alpha,\beta)$ for any pair of one-forms α, β. The Poisson bracket can be extended to one-forms with the aid of P, as follows (Magri, 1985): for any one-forms α, β,

$$\{\alpha,\beta\}=\mathcal{L}_{P(\alpha)}\beta-\mathcal{L}_{P(\beta)}\alpha-d(\Pi(\alpha,\beta));$$

then $\{df,dg\}=d\{f,g\}$. The Schouten bracket condition on Π can be stated equivalently in terms of the Poisson map and the bracket of one-forms:

$$[P(\alpha),P(\beta)]=P(\{\alpha,\beta\}).$$

The Poisson structure is nonsingular if its Poisson map is.

The vector field $P(dH)$ is the Hamiltonian vector field corresponding to the Hamiltonian function H. If Z is a Hamiltonian vector field then $\mathcal{L}_Z\Pi=0$, or equivalently $\mathcal{L}_ZP=0$. Conversely, when Π is nonsingular, if $\mathcal{L}_Z\Pi=0$ then Z is locally Hamiltonian, in the sense that in a neighborhood of any point one can find a function H such that $Z=P(dH)$ on that neighborhood. In fact the condition $\mathcal{L}_Z\Pi=0$ states that Z is a cocycle in the Lichnerowicz–Poisson complex corresponding to Π, and Z is Hamiltonian if and only if it is a coboundary. The Poisson map P, when it is nonsingular, induces an isomorphism of the Lichnerowicz–Poisson and the de Rham cohomology groups [Vaisman (1994)], and so the vanishing of the first de Rham cohomology group of M is a sufficient condition for a vector field which satisfies $\mathcal{L}_Z\Pi=0$ to be Hamiltonian. We shall deal mostly with nonsingular Poisson structures, and we shall generally assume that $\mathcal{L}_Z\Pi=0$ is sufficient as well as necessary for Z to be Hamiltonian.

A vector field Z on a Poisson manifold is said to be quasi-Hamiltonian if there is a nowhere-vanishing function F such that FZ is Hamiltonian. Thus $FZ=P(dH)$ for some function H. Note that if M is connected F must be everywhere positive or everywhere negative; we can assume the former without loss of generality by absorbing a negative sign in H if necessary. We assume henceforth that M is connected and F is positive. Now let $V=F^{-1}P(dF)=P(d\log F)$; then $\mathcal{L}_Z\Pi=Z\wedge V$, and of course $\mathcal{L}_V\Pi=0$. Conversely, if $\mathcal{L}_Z\Pi=Z\wedge V$ and $V=P(d\Phi)$ say then

$$\mathcal{L}_{e^{\Phi}Z}\Pi=e^{\Phi}\mathcal{L}_Z\Pi-Z\wedge P(d(e^{\Phi}))=0.$$

Thus if $\mathcal{L}_Z\Pi=Z\wedge V$ where $\mathcal{L}_V\Pi=0$, and Π is nonsingular, then Z is quasi-Hamiltonian, at least locally.

The function H is a first integral of Z.

Let Z be a vector field on a manifold M which is quasi-Hamiltonian with respect to a Poisson bivector Π, so that $FZ=P(dH)$. Then, as shown in Crampin and Sarlet (2001), the bivector $\hat{\Pi}$ on $M\times\mathbb{R}$ given by

$$\hat{\Pi}=\Pi+(Z+zV)\wedge\frac{\partial}{\partial z},$$

where z is the coordinate on $\mathbb{R}$ and $V=F^{-1}P(dF)$, is a Poisson bivector which projects onto Π. Here Π is extended to $M\times\mathbb{R}$ simply by ignoring z. The Hamiltonian vector field with respect to $\hat{\Pi}$ corresponding to $-z$ is $Z+zV$; its restriction to the zero section is Z. Furthermore, $H+zF$ is a Casimir of $\hat{\Pi}$. In fact the conditions for $\hat{\Pi}$ to be Poisson are again

$$\mathcal{L}_Z\Pi=Z\wedge V,\quad \mathcal{L}_V\Pi=0,$$

given that Π is Poisson.

III. BI-QUASI-HAMILTONIAN SYSTEMS

We now set up a general framework for the study of systems with a dual quasi-Hamiltonian representation, within which a notion of complete integrability occurs naturally, and which covers as a special case the class of cofactor pair systems studied in Lundmark (2001a, b) and Crampin and Sarlet (2001).

Definition: A vector field Z on M is said to be bi-quasi- Hamiltonian if

(i) M is equipped with two compatible Poisson structures Π_a, $a=1,2$;
(ii) Z is quasi-Hamiltonian with respect to both Poisson structures, i.e., $F_a Z = P_a(dH_a)$ for some functions H_a and (nowhere vanishing) F_a;
(iii) $\mathcal{L}_{V_1}\Pi_2 + \mathcal{L}_{V_2}\Pi_1 = 0$, where $V_a = (F_a)^{-1} P_a(dF_a)$.

Condition (iii), which is a form of compatibility condition (and will be referred to as such in the following), can be motivated as follows.

Suppose that Z is quasi-Hamiltonian with respect to two Poisson structures Π_1 and Π_2, with $F_a Z = P_a(dH_a)$, $a=1,2$. Then we can form the two extended Poisson structures

$$\hat{\Pi}_a = \Pi_a + (Z + zV_a) \wedge \frac{\partial}{\partial z}.$$

We now ask for the conditions for these Poisson structures to be compatible, that is, for $[\hat{\Pi}_1, \hat{\Pi}_2] = 0$. Now

$$\begin{aligned}
&\left[\Pi_1 + (Z+zV_1)\wedge\frac{\partial}{\partial z}, \Pi_2 + (Z+zV_2)\wedge\frac{\partial}{\partial z}\right] \\
&\quad = [\Pi_1,\Pi_2] + (\mathcal{L}_Z\Pi_1 + z\mathcal{L}_{V_2}\Pi_1)\wedge\frac{\partial}{\partial z} + (\mathcal{L}_Z\Pi_2 + z\mathcal{L}_{V_1}\Pi_2)\wedge\frac{\partial}{\partial z} + (V_1+V_2)\wedge Z\wedge\frac{\partial}{\partial z} \\
&\quad = [\Pi_1,\Pi_2] + z(\mathcal{L}_{V_1}\Pi_2 + \mathcal{L}_{V_2}\Pi_1)\wedge\frac{\partial}{\partial z}
\end{aligned}$$

since $\mathcal{L}_Z\Pi_a = Z\wedge V_a$ by assumption. Thus $\mathcal{L}_{V_1}\Pi_2 + \mathcal{L}_{V_2}\Pi_1 = 0$ is the necessary and sufficient condition for the Poisson structures $\hat{\Pi}_1$ and $\hat{\Pi}_2$ to be compatible, assuming that Π_1 and Π_2 are compatible.

We now establish the existence of involutive first integrals of a bi-quasi-Hamiltonian system.

It follows from the compatibility condition $\mathcal{L}_{V_1}\Pi_2 + \mathcal{L}_{V_2}\Pi_1 = 0$, together with the conditions $\mathcal{L}_{V_a}\Pi_a = 0$, that $\mathcal{L}_{V_1 - tV_2}(\Pi_1 - t\Pi_2) = 0$ for all t. Now if Π_1 is nonsingular so is $\Pi_1 - t\Pi_2$ for t sufficiently close to zero. Thus there is some function $\Phi(t)$ such that $V_1 - tV_2 = (P_1 - tP_2)(d\Phi(t))$. Since further $\mathcal{L}_Z(\Pi_1 - t\Pi_2) = Z\wedge(V_1 - tV_2)$, there is some function $H(t)$ such that $F(t)Z = (P_1 - tP_2)(dH(t))$, where $F(t) = e^{\Phi(t)}$; moreover $H(t)$ is a first integral of Z for all t. On setting $t=0$ we see that $F(0)Z = P_1(dH(0))$.

Now for $k = 0,1,2,\ldots$ set

$$H_{(k)} = \frac{1}{k!}\frac{\partial^k H}{\partial t^k}\Big|_{t=0},$$

and define $F_{(k)}$ similarly. Then each $H_{(k)}$ is a first integral of Z, and

$$F_{(k+1)}Z = P_1(dH_{(k+1)}) - P_2(dH_{(k)}).$$

It follows that for every $j = 0,1,2,\ldots$,

$$\{H_{(j)},H_{(k+1)}\}_1=\{H_{(j)},H_{(k)}\}_2,$$

where $\{\cdot,\cdot\}_a$ is the Poisson bracket of functions defined by Π_a. Thus

$$\{H_{(j)},H_{(k+1)}\}_1=\{H_{(j+1)},H_{(k)}\}_1.$$

It follows that if l and m differ by an even integer then $\{H_{(l)},H_{(m)}\}_1=0$, since

$$\{H_{(l)},H_{(l+2n)}\}_1=\{H_{(l+n)},H_{(l+n)}\}_1.$$

If l and m differ by an odd integer, on the other hand,

$$\{H_{(l)},H_{(m)}\}_1=\{H_{(l)},H_{(m-1)}\}_2;$$

since l and $m-1$ differ by an even integer, $\{H_{(l)},H_{(m-1)}\}_2=0$ by the same argument. Thus $\{H_{(l)},H_{(m)}\}_1=0$ for all l, m, and $\{H_{(l)},H_{(m)}\}_2=0$ likewise. We summarize the results in the following statement.

Theorem: Let Z be bi-quasi-Hamiltonian. Then there exist functions $H_{(k)}$ $(k=0,1,2,\ldots)$, such that

$$F_{(0)}Z=P_1(dH_{(0)}),$$

$$F_{(k+1)}Z=P_1(dH_{(k+1)})-P_2(dH_{(k)}),\quad k=0,1,2,\ldots$$

for some functions $F_{(k)}$. The $H_{(k)}$ are in involution with respect to both Poisson brackets. In particular, if the manifold M is $2n$-dimensional and the functions $H_{(k)}$, $k=0,1,\ldots,n-1$, are functionally independent then Z is completely integrable in the sense of Liouville.

IV. POISSON-NIJENHUIS PENCILS

We now specialize the results of Sec. III to the case where each of the two Poisson structures giving rise to a bi-quasi-Hamiltonian system actually comes from a Poisson–Nijenhuis structure.

A Poisson–Nijenhuis structure (Π,J) on a manifold M consists of a Poisson structure Π and a type (1,1) tensor field J such that $PJ^*=JP$, the Magri–Morosi concomitant $\mu_{P,J}$ of P and J is zero, and the torsion, or Nijenhuis tensor, N_J of J is zero. (Here J^* denotes the adjoint of J.)

The Magri–Morosi concomitant is defined as follows [Magri and Movosi (1984); Nunes da Costa and Marle (1996)]: for any one-form α and vector field X on M,

$$\mu_{P,J}(\alpha,X)=(\mathcal{L}_{P(\alpha)}J)(X)-P(\mathcal{L}_X(J^*\alpha))+P(\mathcal{L}_{J(X)}\alpha).$$

When $PJ^*=JP$, $\mu_{J,P}$ is a type (1,2) tensor field on M.

These conditions are sufficient for JP to define a second Poisson structure on M [Magri and co-workers (1984, 1985); Kosmann–Schwarzbach and Magri (1990)]. We denote the Poisson bivector by Π_J and the associated Poisson map by $P_J=JP=PJ^*$.

Note that when $N_J=0$ we have available the differential d_J of Frölicher–Nijenhuis theory [Frölicher and Nijenhuis (1956)], which satisfies $dd_J+d_Jd=0$, ${d_J}^2=0$; it is determined essentially by these properties and by its action on functions, which is given by $d_Jf=J^*(df)$.

We shall be interested in vector fields Z that are quasi-Hamiltonian with respect to Π_J, with $FZ=P_J(dH)$. Of particular interest are those for which $d_Jd\Phi=0$, where $F=e^{\Phi}$. Alternatively, we then have $dd_J\Phi=0$, so $d_J\Phi=d\phi$ for some function ϕ (at least locally), whence $d_JF=Fd\phi$. One important case covered by this occurs when $\Phi=\log\det J$, so that $F=\det J$ (assuming, without essential loss of generality, that $\det J>0$).

Proposition: For any J such that $N_J=0$, we have $d_J(\det J)=(\det J)d(\operatorname{tr}J)$.

Proof: This follows from the formula

$$d(\det J)=J^i_{j|k}C^j_i dx^k,$$

where C is the cofactor tensor of J, and the calculation is carried out using any symmetric connection (or indeed partial differentiation). Thus

$$\begin{aligned} d_J(\det J) &= J^i_{j|k} J^k_l C^j_i dx^l \\ &= (J^i_{l|k} J^k_j + J^k_{j|l} J^i_k - J^k_{l|j} J^i_k) C^j_i dx^l \\ &= (J^i_{l|k} \delta^k_i + J^k_{j|l} \delta^j_k - J^k_{l|j} \delta^j_k)(\det J) dx^l \\ &= J^k_{k|l} (\det J) dx^l \end{aligned}$$

as asserted. □

It follows that $d_J\Phi = d(\operatorname{tr} J)$, and so $d_J d\Phi = 0$. Slightly more generally, if $F = (\det J)^r$ for some power r then $d_J\Phi = d(r \operatorname{tr} J)$ and $d_J d\Phi = 0$ also.

Definition: A quasi-Hamiltonian vector field Z such that $(\det J)^r Z = P_J(dH)$ will be called a Pfaffian quasi-Hamiltonian vector field.

This is a slight extension of the terminology used in Morosi and Tondo (1997). All of our examples of bi-quasi-Hamiltonian systems, later in the paper, will actually be of the Pfaffian type.

Now suppose that we have two Poisson–Nijenhuis structures with the same initial Poisson bivector Π, and type (1,1) tensors J and K, which both commute with P, have zero Magri–Morosi concomitants with respect to P, and satisfy $N_J = N_K = 0$. Let the corresponding bivectors be Π_J, Π_K.

Definition: The Poisson–Nijenhuis structures (Π, J) and (Π, K) are said to be compatible if the Poisson bivectors Π_J and Π_K are compatible with each other (each is compatible with Π by construction).

Proposition: For Π_J and Π_K to be compatible, it is sufficient that the Nijenhuis bracket $[J,K] = 0$. If P, J, and K are invertible, the condition is also necessary.

Proof: When $[J,K] = 0$, we have $N_{(J+K)} = 0$. Obviously, $J+K$ commutes with P and $\mu_{P,J+K} = \mu_{P,J} + \mu_{P,K} = 0$. Hence,

$$[\Pi_{(J+K)}, \Pi_{(J+K)}] = [\Pi_J + \Pi_K, \Pi_J + \Pi_K] = 2[\Pi_J, \Pi_K] = 0.$$

Conversely, if P, J, and K are invertible, the compatibility of Π_J and Π_K implies that $[J,K] = 0$. Indeed, the condition for the compatibility of two Poisson structures, expressed in terms of their Poisson maps Q, R, say, is

$$[Q(\alpha), R(\beta)] + [R(\alpha), Q(\beta)] = Q(\{\alpha,\beta\}_R) + R(\{\alpha,\beta\}_Q).$$

If we take $Q = P_J$, $R = P_K$, and set $\alpha = P^{-1}(X)$, $\beta = P^{-1}(Y)$ for vector fields X, Y, we obtain

$$[J(X), K(Y)] + [K(X), J(Y)] = JK^{-1}([K(X), K(Y)]) + KJ^{-1}([J(X), J(Y)]).$$

When the facts that $N_J = N_K = 0$ are used to substitute for the terms on the right-hand side, this becomes $[J,K](X,Y) = 0$. □

We consider, therefore, two Poisson–Nijenhuis structures (Π, J), (Π, K) such that $[J,K] = 0$. Then $(\Pi, J - tK)$ is a Poisson–Nijenhuis structure for every constant t. We then have a pencil of Poisson bivectors $\Pi_{J-tK} = \Pi_J - t\Pi_K$, so we call $(\Pi, J - tK)$ a Poisson–Nijenhuis pencil. We shall be mostly interested in the case in which P, J, and K are all invertible.

We next discuss the compatibility condition for a system to be bi-quasi-Hamiltonian with respect to a Poisson–Nijenhuis pencil.

Suppose given a Poisson–Nijenhuis pencil, and a vector field Z such that

$$\mathcal{L}_Z \Pi_J = Z \wedge V, \quad \mathcal{L}_V \Pi_J = 0,$$

$$\mathcal{L}_Z \Pi_K = Z \wedge W, \quad \mathcal{L}_W \Pi_K = 0;$$

thus (still assuming that Π_J and Π_K are nonsingular) Z is quasi-Hamiltonian with respect to both Π_J and Π_K and we can put $V=P_J(d\Phi)=P(d_J\Phi)$, $W=P_K(d\Psi)=P(d_K\Psi)$ for some Φ,Ψ. In order for Z to be bi-quasi-Hamiltonian the compatibility condition

$$\mathcal{L}_W\Pi_J+\mathcal{L}_V\Pi_K=0,$$

or equivalently

$$\mathcal{L}_WP_J+\mathcal{L}_VP_K=0,$$

must hold. When we express P_J and P_K in terms of P we find that

$$\mathcal{L}_WP_J+\mathcal{L}_VP_K=(\mathcal{L}_WJ+\mathcal{L}_VK)P+J\mathcal{L}_WP+K\mathcal{L}_VP.$$

So a particular case of interest occurs when $\mathcal{L}_WP=\mathcal{L}_VP=0$, that is, when V and W are Hamiltonian with respect to the standard Poisson structure P as well as the derived ones P_J, P_K. In such a case there will be functions ϕ, ψ such that

$$V=P(d\phi)\quad\Rightarrow\quad d\phi=d_J\Phi\quad\Rightarrow\quad dd_J\phi=-d_Jd\phi=0;$$

$$W=P(d\psi)\quad\Rightarrow\quad d\psi=d_K\Psi\quad\Rightarrow\quad dd_K\psi=-d_Kd\psi=0.$$

Note that these conditions hold in the Pfaffian case, with $\phi=r\,\mathrm{tr}\,J$, $\Phi=r\log\det J$, etc.

Under these assumptions, the compatibility condition reduces to

$$\mathcal{L}_WJ+\mathcal{L}_VK=0.$$

Now from the vanishing of the Magri–Morosi concomitant,

$$(\mathcal{L}_WJ)(X)=(\mathcal{L}_{P(d\psi)}J)(X)=P(\mathcal{L}_X(d_J\psi)-\mathcal{L}_{JX}d\psi)$$

for all X, whence the compatibility condition becomes

$$\mathcal{L}_X(d_J\psi+d_K\phi)-\mathcal{L}_{JX}d\psi-\mathcal{L}_{KX}d\phi=0.$$

When the homotopy formula is used to express the Lie derivatives, this reduces simply to

$$X]\,(dd_J\psi+dd_K\phi)=0.$$

Thus the compatibility condition can be written

$$d_J\beta+d_K\alpha=0,\quad \alpha=d\phi,\quad \beta=d\psi,$$

where $d_J\alpha=d_Jd\phi=0$, $d_K\beta=d_Kd\psi=0$.

In particular, it follows easily from the coordinate representation of the Nijenhuis bracket that if $[J,K]=0$ then $d_J(\mathrm{tr}\,K)+d_K(\mathrm{tr}\,J)=d(\mathrm{tr}\,JK)$; so the requisite conditions are satisfied in the Pfaffian case, and we have the following result.

Proposition: Suppose that Z is Pfaffian quasi-Hamiltonian with respect to both Π_J and Π_K, so that $(\det J)^rZ=P_J(dG)$ and $(\det K)^rZ=P_K(dH)$ (same power): then the necessary and sufficient condition for Z to be bi-quasi-Hamiltonian is that $[J,K]=0$.

When this condition holds, or more generally for any system that is bi-quasi-Hamiltonian with respect to a Poisson–Nijenhuis pencil, the results of Sec. III concerning the existence of first integrals in involution apply.

V. BI-DIFFERENTIAL CALCULI

We now investigate the conditions for a bi-quasi-Hamiltonian system whose Poisson structures form a Poisson–Nijenhuis pencil, to give rise to a scalar gauged bi-differential calculus, according to the definition given by Dimakis and Müller-Hoissen (2000a), and discussed further in Crampin *et al.* (2000).

We consider two Poisson–Nijenhuis structures (Π,J), (Π,K) such that $[J,K]=0$. Then the operators d_J, d_K satisfy

$$d_J{}^2=d_K{}^2=d_Jd_K+d_Kd_J=0,$$

and therefore form a simple bi-differential calculus [Dimakis and Müller-Hoissen (2000a)] or bicomplex [Dimakis and Müller-Hoissen (2000b)].

Let α be a one-form, and denote by D_J the operator on forms given by

$$D_J\theta=d_J\theta+\alpha\wedge\theta,$$

or $D_J=d_J+\alpha$ for short. Two such operators $D_J=d_J+\alpha$, $D_K=d_K+\beta$ form a scalar gauged bi-differential calculus if

$$D_J{}^2=D_K{}^2=D_JD_K+D_KD_J=0;$$

these conditions hold if and only if

$$d_J\alpha=d_K\beta=d_J\beta+d_K\alpha=0.$$

But as we showed in Sec. IV, the compatibility condition for a system which is quasi-Hamiltonian with respect to a Poisson–Nijenhuis pencil and is such that $\mathcal{L}_VP=\mathcal{L}_WP=0$ is that $d_J\beta+d_K\alpha=0$, where the one-forms α and β satisfy $d_J\alpha=d_K\beta=0$. Thus any bi-quasi-Hamiltonian system of this type, and in particular any Pfaffian bi-quasi-Hamiltonian system, has associated with it a scalar gauged bi-differential calculus.

Furthermore, there are functions ϕ and Φ such that $\alpha=d\phi=d_J\Phi$, and functions ψ and Ψ such that $\beta=d\psi=d_K\Psi$. We can express D_J in the form

$$D_J\theta=d_J\theta+d\phi\wedge\theta=e^{-\Phi}d_J(e^{\Phi}\theta),$$

and similarly for D_K.

Now consider the dynamics Z. We can write

$$\begin{aligned}Z&=e^{-\Phi}P_J(dG)=P(e^{-\Phi}d_JG)=P(D_J(e^{-\Phi}G))\\&=e^{-\Psi}P_K(dH)=P(e^{-\Psi}d_KH)=P(D_K(e^{-\Psi}H))\end{aligned}$$

for Hamiltonian functions G, H. These Hamiltonians are related by $D_J(e^{-\Phi}G)=D_K(e^{-\Psi}H)$; thus the functions $U=e^{-\Phi}G$ and $U=e^{-\Psi}H$ both satisfy the equation $D_JD_KU=0$, a generalization of what was called the fundamental equation in Rauch-Wojciechowski *et al.* (1999) and Lundmark (2001b). If we take the view that the vector fields V and W, or the functions Φ and Ψ, are the givens, then this equation provides a way of generating dynamical vector fields Z which fit the corresponding bi-quasi-Hamiltonian structure; in particular, we can take the Pfaffian set-up with $\Phi=r\log\det J$, $\Psi=r\log\det K$.

In the Poisson–Nijenhuis case the recurrence relation

$$P_J(dH_{(k+1)})-P_K(dH_{(k)})=F_{(k+1)}Z=\frac{F_{(k+1)}}{F_{(0)}}P_J(dH_{(0)})$$

can be expressed in terms of differential operators as follows:

$$d_J H_{(k+1)} = d_K H_{(k)} + \frac{F_{(k+1)}}{F_{(0)}} d_J H_{(0)}.$$

Furthermore, the general formula $V_1 - tV_2 = (P_1 - tP_2)(d\Phi(t))$ from Sec. III here becomes $V - tW = P_{J-tK}(d\Phi(t))$, from which it follows that $d_J\Phi - td_K\Psi = d_{J-tK}\Phi(t)$. For $F(t) = e^{\Phi(t)}$, there results: $d_{J-tK}F(t) = F(t)(d_J\Phi - td_K\Psi) = F(t)(d\phi - td\psi)$. Hence, the $F_{(k)}$ satisfy the recurrence relation

$$d_J F_{(k+1)} - d_K F_{(k)} = F_{(k+1)} d\phi - F_{(k)} d\psi.$$

That is to say, we have

$$d_J F_{(k+1)} - (d\phi) F_{(k+1)} = d_K F_{(k)} - (d\psi) F_{(k)},$$

$$d_J H_{(k+1)} - \vartheta F_{(k+1)} = d_K H_{(k)},$$

where

$$\vartheta = \frac{1}{F_{(0)}} d_J H_{(0)}.$$

Note that $P(\vartheta) = Z$, whence $\vartheta = e^{-\Phi} d_J G = e^{-\Psi} d_K H$; it follows that $d_J\vartheta = \vartheta \wedge d\phi$ and $d_K\vartheta = \vartheta \wedge d\psi$.

Define the 2×2 matrix differential operators

$$\Delta_J = d_J + \begin{bmatrix} -d\phi & 0 \\ -\vartheta & 0 \end{bmatrix}, \quad \Delta_K = d_K + \begin{bmatrix} -d\psi & 0 \\ 0 & 0 \end{bmatrix}.$$

It follows from the formulas for $d_J\vartheta$ and $d_K\vartheta$ just obtained that $\Delta_J{}^2 = \Delta_K{}^2 = 0$ and $\Delta_J\Delta_K + \Delta_K\Delta_J = 0$. Thus Δ_J and Δ_K are the differential operators of a gauged bi-differential calculus operating on two-component column vectors, and

$$\Delta_J \begin{bmatrix} F_{(k+1)} \\ H_{(k+1)} \end{bmatrix} = \Delta_K \begin{bmatrix} F_{(k)} \\ H_{(k)} \end{bmatrix}.$$

A special case of this construction was discussed in Crampin *et al.* (2000).

VI. COFACTOR AND COFACTOR PAIR SYSTEMS

In Secs. IV and V, the discussion centered on a general Poisson manifold (M,P), with additional structure coming from some type (1,1) tensor fields on M. An interesting particular case occurs when M is a cotangent bundle T^*Q say, equipped with its standard Poisson structure Π, and the type (1,1) tensors on M are complete lifts of torsionless tensors L on the base manifold Q. For the complete lift $\tilde{L}$ of L, we have $\det\tilde{L} = (\det L)^2$. Moreover, for any two such tensors L_1, L_2,

$$[\tilde{L}_1, \tilde{L}_2] = \widetilde{[L_1, L_2]};$$

so a vector field Z on T^*Q which is Pfaffian quasi-Hamiltonian with respect to $\tilde{L}_1$ and $\tilde{L}_2$ will be bi-quasi-Hamiltonian if and only if $[L_1, L_2] = 0$. This result, which we have deduced from the more general analysis of Sec. IV, can also be proved easily by an explicit computation.

The following class of quasi-Hamiltonian systems has been studied in Marciniak and Rauch-Wojciechowski (1998), Rauch-Wojciechowski *et al.* (1999), Lundmark (2001a, b), and Crampin and Sarlet (2001). Let g be a (pseudo) Riemannian metric on Q and L a symmetric type (0,2) tensor field such that

$$(\nabla_X L)(Y,Z)=\tfrac{1}{2}(g(X,Y)\langle Z,\alpha\rangle+g(X,Z)\langle Y,\alpha\rangle).$$

Such a tensor is a conformal Killing tensor of g, and the type (1,1) tensor obtained by raising an index on L with g automatically has vanishing torsion. The one-form α is given by $d(\operatorname{tr} L)$. Such a tensor L is called a special conformal Killing tensor. We shall generally be concerned with special conformal Killing tensors which are nonsingular. We shall denote such a tensor by the same letter whatever the position of its indices. Let A be the cofactor tensor of a special conformal Killing tensor, so that $AL=(\det L)I$, and let μ be a one-form on Q which satisfies $D_L\mu=d_L\mu+d(\operatorname{tr} L)\wedge\mu=0$. Let H be the function on T^*Q given by

$$H(q^i,p_i)=\tfrac{1}{2}A^{ij}p_ip_j+V(q),$$

where V is a function such that $D_L((\det L)^{-1}V)=\mu$. Then the quasi-Hamiltonian vector field Z where $(\det L)Z=P_{\tilde{L}}(dH)$ is called a cofactor system. Since $\det\tilde{L}=(\det L)^2$ it is Pfaffian, with $r=\frac{1}{2}$. The vector field Γ on TQ obtained via the diffeomorphism $(q^i,p_i)\mapsto(q^i,g^{ij}p_j)$ takes the form

$$\Gamma=\Gamma_0-M^V,$$

where Γ_0 is the geodesic field of the metric and M is the vector field obtained by raising the index on μ. It is an example of a nonconservative Lagrangian system, and μ represents a generalized force.

If L_1 and L_2 are two special conformal Killing tensors then clearly L_1+L_2 is also a special conformal Killing tensor. The torsion of L_1+L_2 therefore vanishes; it follows that $[L_1,L_2]=0$, and so the corresponding Poisson–Nijenhuis structures are compatible. If Z is a cofactor system with respect to both special conformal Killing tensors then it is Pfaffian quasi-Hamiltonian with respect to each Poisson–Nijenhuis structure and is therefore bi-quasi-Hamiltonian. The force form μ must satisfy $D_{L_1}\mu=D_{L_2}\mu=0$.

The functions $H(t)$ and $F(t)$ in this case are polynomials in t, and the system is completely integrable; $H(t)$ takes the form

$$H(t)=\tfrac{1}{2}A(t)^{ij}p_ip_j+V(t),$$

where $A(t)$ is the cofactor tensor of L_1-tL_2, and $V(t)$ is a polynomial of degree $n-1$ such that

$$D_{(L_1-tL_2)}(\det(L_1-tL_2)^{-1}V(t))=\mu.$$

For given g, μ there are functions V_1, V_2 such that

$$D_{L_1}((\det L_1)^{-1}V_1)=D_{L_2}((\det L_2)^{-1}V_2)=\mu;$$

these are the ''generalized potentials'' of μ with respect to L_1 and L_2 referred to in Sec. I.

Now consider $\nu=D_{L_2}((\det L_1)^{-1}V_1)$. We have

$$D_{L_1}\nu=-D_{L_2}D_{L_1}((\det L_1)^{-1}V_1)=-D_{L_2}\mu=0,$$

and of course $D_{L_2}\nu=0$: so ν defines a new bi-cofactor system, with the same metric but a different force form. The quadratic part of the new first integral function is unchanged; the ''potential'' part $W(t)$ satisfies

$$D_{(L_1-tL_2)}(\det(L_1-tL_2)^{-1}W(t))=\nu.$$

In fact $W(t)$ is given in terms of $V(t)$ by

$$tW(t)=V(t)-\frac{\det(L_1-tL_2)}{\det L_1}V(0).$$

Note that $V(0)=V_1$. The right-hand side is a polynomial of degree n in t, which takes the value 0 when $t=0$; so $W(t)$ is a polynomial of degree $n-1$. Moreover

$$D_{(L_1-tL_2)}\left(\det(L_1-tL_2)^{-1}\left(V(t)-\frac{\det(L_1-tL_2)}{\det L_1}V(0)\right)\right)$$
$$=\mu-D_{L_1}(\det(L_1)^{-1}V_1)+tD_{L_2}((\det L_1)^{-1}V_1)=t\nu$$

as required. With these considerations, we have supplemented the analysis in Crampin and Sarlet (2001) with the appropriate generalization of Lundmark's construction (Lundmark, 2001b) of a hierarchy of cofactor pair systems.

VII. QUASI-BI-HAMILTONIAN SYSTEMS

The theory we have described previously covers, of course, the special case in which the vector field Z is Hamiltonian, not just quasi-Hamiltonian, with respect to one of the two Poisson structures, so that (say) $F_1=1$ in the notation of Sec. III. This case corresponds roughly to that of a quasi-bi-Hamiltonian system as defined and discussed in Brouzet *et al.* (1996), Morosi and Tondo (1997, 1998); however, the compatibility condition for a bi-quasi-Hamiltonian system, which reduces to $\mathcal{L}_{V_2}\Pi_1=0$, is not required to hold in the definition of a quasi-bi-Hamiltonian system given in those papers. But to the best of our knowledge, all of the examples of quasi-bi-Hamiltonian systems in the literature do fall within our framework: in fact they all appear to be cases of cofactor systems, for which the compatibility condition holds automatically anyway. We therefore feel justified in discussing briefly some of the results in the literature on quasi-bi-Hamiltonian systems in the light of our approach.

We wish first to compare our main integrability result with the following proposition, due to Tondo [Tondo (1995); Morosi and Tondo (1997)]. (The statement of the proposition has been edited to fit in with the notation and terminology of the present paper.)

Proposition: Let M be a $2n$-dimensional manifold equipped with an invertible Poisson tensor P_1, and let Z be a Hamiltonian vector field with Hamiltonian H: $Z=P_1(dH)$. Let a tensor $J:TM\to TM$ exist such that the tensor $P_2:T^*M\to TM$ defined by $P_2=JP_1$ is skew-symmetric. Denote by $\alpha_{(k)}=(J^*)^k dH$ $(k=0,1,2,\dots)$ the one-forms obtained by the iterated action of J^*. If there exist $n-1$ independent functions $H_{(l)}$ $(l=1,2,\dots,n)$ and $\frac{1}{2}n(n+1)$ functions $\rho_{(kl)}$ $(k=0,1,\dots,n-1;\ 0\leqslant l\leqslant k)$ with $\rho_{(00)}=1$ and $\rho_{(kk)}\neq 0$ $(k\neq 0)$, such that the one-forms $\alpha_{(k)}$ can be written as $\alpha_{(k)}=\sum_{l=0}^{k}\rho_{(kl)}dH_{(l)}$ $(k=0,1,\dots,n-1)$, then the functions $H_{(k)}$ are in involution with respect to the Poisson bracket defined by P_1 and are first integrals of Z. The Hamiltonian system is Liouville integrable. Moreover, if P_2 is a Poisson tensor then the functions $H_{(k)}$ are in involution also with respect to the Poisson bracket defined by P_2.

In our analysis, we have assumed the existence of two nonsingular Poisson tensors from the first; we may define J as $P_2P_1^{-1}$. On the other hand, we assume only that Z is quasi-Hamiltonian. To relate our results to Tondo's proposition we must show that the functions $H_{(k)}$ defined in Sec. III are related to the one-forms $\alpha_{(k)}=(J^*)^k dH_{(0)}$ in the manner specified in the proposition. Now we can write

$$F_{(k+1)}Z=P_1(dH_{(k+1)})-P_1(J^*dH_{(k)}),$$

and $F_{(0)}Z=P_1(dH_{(0)})$. Thus

$$dH_{(k+1)}=J^*dH_{(k)}+\hat{F}_{(k+1)}dH_{(0)},$$

where $\hat{F}_{(k)}=F_{(k)}/F_{(0)}$, from which it follows that

$$dH_{(k)}=\sum_{l=0}^{k}\hat{F}_{(k-l)}\alpha_{(l)}.$$

Note that the matrix of coefficients on the right-hand side is lower triangular with 1*s* on the diagonal. When this system of equations is solved for the $\alpha_{(k)}$ we obtain a relation of the required form. In fact we have $\rho_{(kk)}=1$ for all k, not just for $k=0$; and moreover $\rho_{(kl)}=\rho_{(ij)}$ when $k-l=i-j$. In Morosi and Tondo (1997), Tondo's proposition is applied to a couple of examples of quasi-bi-Hamiltonian systems. It is a feature of these examples, not remarked on let alone explained in this paper, that the $\rho_{(ij)}$ follow the pattern identified previously. While Tondo's proposition is rather more general than our result, so far as we know it has been applied only to quasi-bi-Hamiltonian systems, and indeed only to systems of cofactor type (as we have already remarked); so this greater generality is in practice somewhat illusory.

When one considers the examples in Morosi and Tondo (1997) more carefully, one realizes that it is not at all clear what role the fact that the systems in question are quasi-bi-Hamiltonian plays, since the expressions for the $H_{(k)}$ and $\rho_{(kl)}$ are merely quoted and no indication is given as to how they were derived. To clarify what is going on, we shall consider one of these examples, and analyze it using our techniques. We have chosen the first example from the paper for this purpose. It is the Hamiltonian system $Z=P_0(dH)$ where P_0 is the standard Poisson structure on $T^*\mathbb{R}^3$ and

$$H=\tfrac{1}{2}(2p_1p_2+p_3^2)-\tfrac{5}{8}q_1^4+\tfrac{5}{2}q_1^2q_2+\tfrac{1}{2}q_1q_3^2-\tfrac{1}{2}q_2^2.$$

It is stated that Z is also quasi-Hamiltonian with respect to the Poisson tensor P_1 given by

$$P_1=\begin{bmatrix}0 & A\\ -A^T & B\end{bmatrix},\quad \text{where } A=-\begin{bmatrix}q_1 & -1 & 0\\ 2q_2 & q_1 & q_3\\ q_3 & 0 & 0\end{bmatrix},\quad B=-\begin{bmatrix}0 & -p_2 & -p_3\\ p_2 & p_3 & 0\\ 0 & 0 & 0\end{bmatrix};$$

in fact $q_3^2Z=P_1(dH_{(2)})$ where

$$H_{(2)}=\tfrac{1}{2}q_3^2p_2^2+(\tfrac{1}{2}q_1^2+q_2)p_3^2-q_3p_1p_3-q_1q_3p_2p_3+\tfrac{1}{2}q_1^3q_3^2-q_1q_2q_3^2-\tfrac{1}{8}q_3^4.$$

Note first that the terms quadratic in momenta in H are derived from the flat metric whose matrix representation is

$$\begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{bmatrix},$$

which is of normal hyperbolic type. When this metric is used to lower an index on A we obtain the symmetric matrix

$$-\begin{bmatrix}-1 & q_1 & 0\\ q_1 & 2q_2 & q_3\\ 0 & q_3 & 0\end{bmatrix},$$

which is easily seen to be a special conformal Killing tensor. The tensor P_1 is, apart from sign, the Poisson–Nijenhuis tensor associated with the complete lift of the type (1,1) tensor A. The determinant of A is $-q_3^2$, and its cofactor tensor, in type (2,0) form, is

$$-\begin{bmatrix} 0 & 0 & -q_3 \\ 0 & q_3^2 & -q_1q_3 \\ -q_3 & -q_1q_3 & q_1^2+2q_2 \end{bmatrix};$$

it is clear that this determines the terms in $H_{(2)}$ quadratic in momenta. Moreover, it is easy to check that if V represents the potential of $H=H_{(0)}$ and W the potential of $H_{(2)}$ then $d_AW=(\det A)dV$. This is therefore an example of a cofactor system, and the preceding theory applies, explaining for example why the relevant functions $\rho_{(ij)}$ satisfy $\rho_{(11)}=\rho_{(22)}=1$, $\rho_{(21)}=\rho_{(32)}$.

VIII. AN EXAMPLE

We finish with an example of a true bi-quasi-Hamiltonian system. It is a cofactor pair system on the sphere and as such illustrates our generalization [Crampin and Sarlet (2001)] of the work on Euclidean spaces of Lundmark [Lundmark (2001a, b)]. Starting from a known example of a kinetic energy Lagrangian with two further quadratic integrals, we will use a constructive approach to find all force forms which determine a nonconservative system of cofactor pair type.

Take the kinetic energy to be

$$T=\tfrac{1}{2}g_{ij}(q)\dot{q}_i\dot{q}_j=\tfrac{1}{2}(\dot{q}_1^2+\sin^2 q_1\dot{q}_2^2).$$

It is straightforward to verify that the symmetric type (0,2) tensors with matrix representation

$$L_1=\begin{bmatrix} \sin 2q_1\cos q_2 & -\sin^2 q_1\sin q_2 \\ -\sin^2 q_1\sin q_2 & 0 \end{bmatrix},\quad L_2=\begin{bmatrix} \sin 2q_1\sin q_2 & \sin^2 q_1\cos q_2 \\ \sin^2 q_1\cos q_2 & 0 \end{bmatrix},$$

are special conformal Killing tensors with respect to the given metric. The corresponding type (1,1) tensors which one needs to set up the differential operators $D_{L_a}=d_{L_a}+\alpha_a$ read

$$L_1=\sin 2q_1\cos q_2\frac{\partial}{\partial q_1}\otimes dq_1-\sin q_2\left(\frac{\partial}{\partial q_1}\otimes dq_2+\sin^2 q_1\frac{\partial}{\partial q_2}\otimes dq_1\right),$$

$$L_2=\sin 2q_1\sin q_2\frac{\partial}{\partial q_1}\otimes dq_1+\cos q_2\left(\frac{\partial}{\partial q_1}\otimes dq_2+\sin^2 q_1\frac{\partial}{\partial q_2}\otimes dq_1\right).$$

We further have $\alpha_a=d(\operatorname{tr}L_a)$, where $\operatorname{tr}L_1=\sin 2q_1\cos q_2$, $\operatorname{tr}L_2=\sin 2q_1\sin q_2$. All we need now to identify a dynamical system which has a bi-quasi-Hamiltonian representation with respect to the two compatible Poisson–Nijenhuis structures $P_{\tilde{L}_a}$, obtained from the standard Poisson structure P on the cotangent bundle of the sphere, is an admissible force form $\mu=M_1dq_1+M_2dq_2$, that is to say, a solution of the simultaneous equations $D_{L_a}\mu=0$. In coordinates, each of these conditions gives rise to a single, linear first-order partial differential equation for the M_a. Taking suitable linear combinations with $\sin q_2$ and $\cos q_2$, the set of conditions is equivalent to

$$\frac{\partial M_1}{\partial q_1}=\sin^2 q_1\frac{\partial M_2}{\partial q_2},$$

$$\frac{\partial M_2}{\partial q_1}=\left(\frac{3}{2}\tan q_1-\cot q_1\right)M_2.$$

These equations are readily solved and give

$$\mu=\frac{2\rho'(q_2)}{\cos^{1/2}q_1}dq_1+\frac{\rho(q_2)}{\cos^{3/2}q_1\sin q_1}dq_2,$$

where ρ is an arbitrary function of q_2. The ''potentials'' V_a for which $\mu = D_{L_a}((\det L_a)^{-1} V_a)$ are most easily obtained by computing $dV_a = A_a \mu$, where A_a is the cofactor matrix of L_a. We find

$$V_1 = \frac{2\rho(q_2)\sin q_2}{\cos^{1/2} q_1}, V_2 = -\frac{2\rho(q_2)\cos q_2}{\cos^{1/2} q_1}.$$

Since we have actually obtained the most general form of μ, we should not expect here to find new cofactor pair systems by applying the procedure explained in Sec. VI. In fact, we have

$$\nu = D_{L_2}((\det L_1)^{-1} V_1) = (\det L_2)^{-1} d_{L_2}\left(\frac{\det L_2}{\det L_1} V_1\right),$$

and since the ratio of the two determinants depends on q_2 only, it can be absorbed into the arbitrary function ρ; thus ν is indistinguishable from μ.

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Maximum entropy approximation for Lyapunov exponents of chaotic maps

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Let $S:[0,1]\to[0,1]$ be a nonsingular chaotic map that preserves an integrable density f^* that describes the statistics of the orbits. In this article we use the maximum entropy approach to approximate the density f^* and the corresponding Lyapunov exponent. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1465100]

I. INTRODUCTION

In physical sciences, such as statistical physics, mathematical biology, and fluid dynamics, exploration of statistical properties of an underlying dynamical system S defined on $[0,1]$ is the only effective and practical means for understanding the asymptotic behavior of the orbits in phase space.[1] Such an investigation often leads to a study of the existence and computation of the integrable fixed density of the dynamics.[2] Since such fixed densities describe the chaotic dynamics for almost all initial points, they are usually referred to as physical measures. For the determination of these physical measures, one must calculate a fixed density, f^*, of the so-called Frobenius–Perron operator associated with S. In addition, the Lyapunov exponent λ, closely related to the sensitivity of the orbits on the initial conditions, can also be determined in terms of the fixed density as[1]

$$\lambda = \int_0^1 f^*(x)\ln|S'(x)|dx. \tag{1}$$

The exponent describes the average expansion rate: a positive Lyapunov exponent means that small uncertainties in the initial conditions expand on average, while a negative Lyapunov exponent means that the interval of uncertainty shrinks on average. The important issues, therefore, in physical applications of chaotic dynamics are how to numerically determine the density of a physical measure and the associated Lyapunov exponent.

To numerically predict the densities and the associated exponents, we will use the maximum entropy method (maxent). Maxent is widely used in the context of the moment problem which appears naturally in many branches of physics and engineering; it is used to numerically recover the density with ''least bias'' from finitely many known moments.[3] High precision numerical integration techniques permit the sought after density to be determined with up to 20 moments as input. Averages over the approximate distribution are known to be rapidly convergent in many cases of interest.[4,5] The idea of solving operator equations using maxent was first proposed by Mead[6] and has been used by Ding in forming a new numerical method for solving the fixed density problem for the Frobenius–Perron operator.[7] Even with only $N=4$ moments the maxent algorithm performs better than the usual Ulam method.[8,9] In this article, we will sufficiently extend

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the numerical accuracy of the algorithm used by Ding to allow the numerical maxent prediction of the Lyapunov exponent associated with the distribution (physical measure).

The article continues as follows. In the next section, we present some background mathematical preliminaries on which the work is based. In Sec. III, we present the results of numerical calculations for the fixed densities and the exponents. We conclude briefly in Sec. IV.

II. PRELIMINARIES

Let $S:[0,1]\to[0,1]$ be a nonlinear map such that the Lebesgue measure $m(A)=0$ implies $m(S^{-1}(A))=0$ for every measurable set $A\subset[0,1]$. The operator $P:L^1(0,1)\to L^1(0,1)$ defined by

$$Pf(x)=\frac{d}{dx}\int_{S^{-1}([0,x])}f(t)dt \tag{2}$$

is called the *Frobenius–Perron operator* associated with S.

A *density* f is any function $f\geqslant 0$ such that its L^1-norm $\int_0^1 f(t)\,dt=1$. It is obvious that the Frobenius–Perron operator P is a Markov operator which by definition is any linear operator that maps densities to densities. For any density f, the absolutely continuous probability measure

$$\mu(A)=\int_A f dm \quad \forall \text{ measurable sets } A\subset[0,1]$$

is invariant under S: that is, $\mu(S^{-1}(A))=\mu(A)$ for all measurable sets $A\subset[0,1]$, if and only if f is a fixed point of P.

A basis of the maximum entropy method for computing a fixed density of the Frobenius–Perron operator $P:L^1(0,1)\to L^1(0,1)$ associated with $S:[0,1]\to[0,1]$ is the following result which has been proved in Ref. 7. Let D be the set of all densities.

Proposition 2.1: $f^*\in D$ is a fixed point of P if and only if

$$\int_0^1 [x^n-S(x)^n]f^*(x)\,dx=0, \quad =1,2,\ldots. \tag{3}$$

The Boltzmann (information) entropy of $f\in L^1(0,1)$ is defined as

$$H(f)=-\int_0^1 f(x)\log f(x)dx. \tag{4}$$

Then the maximum entropy method for solving the homogeneous system (3) with infinitely many equations is the following:

Algorithm: Choose N and solve the maximum entropy problem

$$\max\left\{H(f):f\in D,\ \int_0^1 [x^n-S(x)^n]f(x)\,dx=0,\ i=1,\ldots,N\right\} \tag{5}$$

to obtain an approximate solution f_N of the operator equation $Pf=f$.

It was shown in Ref. 7 that the above algorithm is well-posed under the mild assumption that the set of N functions

$$x-S(x),\ x^2-S(x)^2,\ldots,x^N-S(x)^N$$

are linearly independent. The optimization problem (5) will then have a unique solution f_N given by

$$f_N(x)=\frac{\exp\Sigma_{n=1}^{N}a_n[x^n-S(x)^n]}{\int_0^1\exp\Sigma_{n=1}^{N}a_n[x^n-S(x)^n]dx}, \tag{6}$$

where $a_1,\ldots,a_N$ satisfy the N constraints

$$\int_0^1[x^i-S(x)^i]\exp\sum_{n=1}^{N}a_n[x^n-S(x)^n]\,dx=0,\quad i=1,\ldots,N. \tag{7}$$

Lastly, the Lyapunov exponent associated with the map can be calculated approximately from Eq. (1) where f^* is replaced by the maxent approximation f_N.

III. NUMERICAL EXPERIMENTS

In this section we present some numerical results from our maximum entropy algorithm using a high precision Gaussian quadrature. The test maps are

$$S_1(x)=\begin{cases}\dfrac{2x}{1-x^2}, & 0\leqslant x\leqslant\sqrt{2}-1\\[2ex] \dfrac{1-x^2}{2x}, & \sqrt{2}-1\leqslant x\leqslant 1\end{cases},$$

$$S_2(x)=\begin{cases}\dfrac{2x}{1-x}, & 0\leqslant x\leqslant\dfrac{1}{3},\\[2ex] \dfrac{1-x}{2x}, & \dfrac{1}{3}\leqslant x\leqslant 1\end{cases},$$

$$S_3(x)=4x(1-x)\quad(\text{logistic map}),$$

$$S_4(x)=\sqrt{2}x-\operatorname{sgn}(x)\quad(\text{sigma-delta modulator}).$$

In the last entry, sgn(x) denotes the sign of x. The third of these maps, $S_3(x)$, is the well-known logistic map. This map played a historical role in the development of the theory of chaos,[1] and appears in ecological population dynamics. The last example, $S_4(x)$, describes chaos in various electronic signal analyzers,[10] and is a direct example taken from practical physics.

The unique fixed densities of S_i are known exactly:

$$f_1^*(x)=\frac{4}{\pi(1+x^2)},$$

$$f_2^*(x)=\frac{2}{(1+x)^2},$$

$$f_3^*(x)=\frac{1}{\pi\sqrt{x(1-x)}},$$

$$f_4^*(x)=\begin{cases}\dfrac{1+\sqrt{2}}{2\sqrt{2}}, & \sqrt{2}-1<|2x-1|<1,\\[2ex] 0, & |2x-1|=\sqrt{2}-1,\\[2ex] \dfrac{1+\sqrt{2}}{2}, & |2x-1|<\sqrt{2}-1.\end{cases}$$

TABLE I. Averages of the computed fixed densities.

N	S_1	S_2	S_3
2	0.314 926	0.298 290	0.358 972
3	0.314 709	0.296 827	0.358 821
4	0.314 178	0.295 487	0.353 476
5	0.314 022	0.294 904	0.353 752
6	0.314 016	0.293 889	0.353 705
7	0.314 018	0.293 881	0.353 391
8	0.314 018	0.293 999	0.348 839
9	0.313 765		0.348 915
10	0.311 964		0.348 916
α^*	0.310 349	0.285 398	0.318 310

The numerical computations were performed on the Cray C90 supercomputer at the Mississippi Center for Super-computing Research. Double precision was used throughout all calculations. In the maxent algorithm, Newton's method is used to solve the nonlinear system of equations (7) to a high precision (up to 15 significant digits). To evaluate the derivative matrix required in the algorithm, we used the 50-node Gaussian quadrature for the numerical integrations. For the first three of these, we compared the quantity

$$\alpha_N \equiv \int_0^1 f_N(x) \frac{\sqrt{x}}{2} dx$$

with the exact average

$$\alpha^* \equiv \int_0^1 f^*(x) \frac{\sqrt{x}}{2} dx$$

to estimate the error. In problems not involving chaos, averages such as α_N are known to be rapidly convergent as the number of input moments increases.[3]

In Table I, we list the quantities α_N versus N for the first three examples with the exact averages α^* for f_1^*, f_2^*, f_3^* listed in the last row. For each of these maps, we have computed the Lyapunov exponent according to Eq. (1). The results are shown in Table II.

IV. CONCLUSIONS

In this article, we are able to compute fixed densities of the Frobenius–Perron operator equation for various chaotic maps with the help of the maximum entropy approach. In addition, we calculated the associated Lyapunov exponents. The exponent was calculated from Eq. (1) which is an average over the fixed density. Normally, one expects such averages to converge rapidly with increasing numbers of input moments; for example, achieving several decimal places of accuracy with from 5 to 10 moments, even if the point-wise convergence of the distribution is poor. Looking at Table I for the three test averages, α, we see that for even as many as ten

TABLE II. Computed Lyapunov exponents and exact values.

Map	N	λ_{exact}	λ_{maxent}
S_1	10	0.664 24	0.692 90
S_2	8	$\ln 2 = 0.693\,147\,0$	0.689 70
S_3	10	$\ln 2 = 0.693\,147\,0$	0.684 25
S_4	12	$\frac{1}{2}\ln 2 = 0.346\,573$	0.346 573

moments of input we obtain averages only at the few percent level, that for S_1 being the most accurate at only about 0.3%. This level of accuracy is also reflected in Table II for the corresponding exponents where the level of accuracy is likewise just a few percent. However, for the modulator map, S_4, the exponent turned out to be accurate to a remarkable nine digits of accuracy (only six are given in the table) with 12 moments of input.

In some cases, therefore, our method may be able to generate Lyapunov exponents of chaotic maps to good accuracy. In others, accuracy may be achieved only at the 1% level with the same number of input moments. Clearly, the moment problem Eqs. (3)–(5) for chaotic maps is an especially challenging numerical problem.[11] In general, it is unclear how much the accuracy of λ may be improved with higher numbers of input moments.

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Solitons in parametrically driven discrete nonlinear Schrödinger systems with the exploding range of intersite interactions

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We present the sequence of parametrically driven discrete nonlinear Schrödinger systems with the progressively extending range of intersite couplings. In the case of time-independent coupling parameters the sequence is reduced to the Ablowitz–Ladik hierarchy, which is known to be integrable by the inverse scattering transform. However the models with the time-dependent intersite interactions are shown to be integrable too irrespective of a particular form of time dependencies of coupling parameters. Any of such parametrically driven systems might exhibit rather complex soliton dynamics and is described by the unconserved Hamiltonian function. We reveal an important subclass of parametrically driven systems demonstrating the parametrical localization of soliton dynamics on a confined domain of space. Meanwhile an appropriate choice of time dependencies in intersite interactions allow us to transform the original parametrically driven system into another one but subjected to the linear external potential. As a result the latter system can be readily integrated as well. In particular the peculiarities of Bloch oscillations in the systems with time-independent long range intersite interactions and linear external potential of constant strength are analyzed. In general, regulating the range of intersite couplings, the strengths and time dependencies of coupling parameters, we are able to model a number of physically important quasi-one-dimensional systems. We develop an alternative approach to solve the Marchenko equations permitting one to obtain the multisoliton solutions in the most simple and natural way. Finally, we point out how to reformulate any model in row in terms of corrected amplitudes with the standard Poisson brackets. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Inspecting recent publications dealing with the integrable nonlinear evolution models on one-dimensional or quasi-one-dimensional lattices, one could readily see that, apart from a few exceptions,[1,2] they treat the couplings between the molecules in longitudinal direction to be of nearest-neighboring type.[3–10] Meanwhile the intermolecular interactions in real physical systems are either the long-range[11,12] or at least moderate-range[13] ones. For example, in unharmonic chains the impact of long-range intermolecular interactions was shown to be so crucial that it is able to affect the whole structure of soliton-like modes.[11,12] In this respect developing physically motivated integrable nonlinear models with moderate-range and long-range intermolecular couplings appear to be reasonable.

In the present paper we will try to fill this gap by extending the range of intersite couplings in discrete nonlinear Schrödinger systems and to inspire, at least indirectly, interest in the effects of moderate-range and long-range couplings feasible, e.g., in arrays of tunnel-coupled nonlinear

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optical fibers[14] or nonlinear transmission lines[15] as well as in discrete geophysical media.[16]

Starting from the Ablowitz–Ladik auxiliary spectral problem[17–19] but relaxing the basic constraint on the form of the auxiliary evolution operator, it is possible both to extend the range of intersite interactions and to postulate an arbitrary time dependence of coupling parameters. The latter fact generates a substantially richer class of dynamical systems as compared with that adopted by the usual definition of integrable hierarchy where the coupling parameters are supposed to be time independent.[20,21] Here we may observe a direct analogy with the dynamics of parametrically driven oscillators (e.g., the Mathieu oscillator[22] or Kapytsya pendulum,[23,24]) which are now developed into a special theory.[25,26]

II. THE SEQUENCE OF INTEGRABLE MODELS

One way to obtain an integrable nonlinear model on the one-dimensional[3–5,17–19] or quasi-one-dimensional[7,10] lattice consists in starting with the set of auxiliary linear problems

$$\mathbf{u}(n+1|z)=L(n|z)\mathbf{u}(n|z), \tag{1}$$

$$\dot{\mathbf{u}}(n|z)=A(n|z)\mathbf{u}(n|z), \tag{2}$$

restricted by the compatibility condition (Lax equation)

$$\dot{L}(n|z)=A(n+1|z)L(n|z)-L(n|z)A(n|z). \tag{3}$$

Here $L(n|z)$ and $A(n|z)$ are the spectral and evolution matrix operators, respectively, while the overdot stands for the derivative with respect to dimensionless time τ. The numerical longitudinal coordinate n is supposed to run from minus to plus infinity whereas the spectral parameter z is supposed to be time independent. According to the general rule[17–19] the Lax equation (3) is nothing but a direct consequence of the so-called cross-differentiation condition

$$[\mathrm{d}\mathbf{u}(m|z)/\mathrm{d}\tau]_{m=n+1}=\mathrm{d}\mathbf{u}(n+1|z)/\mathrm{d}\tau \tag{4}$$

imposed on the column vector $\mathbf{u}(n|z)$ as the most natural demand.

The next step is to postulate the form of the spectral operator and to specify the general form of evolution operator by some reasonable constraint. Then with good luck the Lax equation (3) becomes sufficient both to restore the explicit form of evolution operator and to isolate some nontrivial integrable nonlinear evolution equation by collecting the terms proportional to the same powers in z. The phrase ''good luck'' implies that in practice it is more common to gain either the mathematical contradiction or rather trivial result of minor physical interest.

Nevertheless, there always exists a safe opportunity to use the well-recommended spectral operator but in combination with the evolution operator specified by a new constraint. We will follow this opportunity and take $L(n|z)$ in the form[17–19]

$$L(n|z)=\begin{pmatrix} z & iq(n) \\ ir(n) & 1/z \end{pmatrix}, \tag{5}$$

where the quantities $q(n)$ and $r(n)$ are pretending to become the on-site amplitudes of any model under future consideration.

In this paper we will be interested in the sequence of integrable models built-up under the constraint that the evolution operator of the Mth model in order must contain the spectral parameter z in the same powers as the multiplicative operator $L^{2M}(n|z)$, with $L(n|z)$ given by expression (5). Here M is an arbitrary positive integer.

Relying upon the above-described guiding scheme it may be concluded that any Mth model in row can be written as

$$+i\dot{q}(n)=[1+q(n)r(n)]\partial H/\partial r(n), \tag{6}$$

$$-i\dot{r}(n)=[1+q(n)r(n)]\partial H/\partial q(n) \tag{7}$$

with H given by

$$H=-2\omega_0 I_0-\sum_{\alpha=1}^{M}[\bar{\omega}_\alpha \bar{I}_\alpha+\overset{+}{\omega}_\alpha \overset{+}{I}_\alpha]. \tag{8}$$

Here $\bar{I}_\alpha$, $\overset{+}{I}_\alpha$, and I_0 are, respectively, $-\alpha$th, $+\alpha$th, and zeroth conserved quantities generated by the spectral operator (5), while $\bar{\omega}_\alpha$, $\overset{+}{\omega}_\alpha$ and ω_0 are arbitrary coordinate independent parameters. The first seven conserved quantities are

$$\begin{aligned}\bar{I}_3=&\sum_{m=-\infty}^{\infty} q(m)r(m-3)[1+q(m-2)r(m-2)][1+q(m-1)r(m-1)]\\&+\sum_{m=-\infty}^{\infty} q(m)q(m-1)r^2(m-2)[1+q(m-1)r(m-1)]\\&+\sum_{m=-\infty}^{\infty} q^2(m)r(m-1)r(m-2)[1+q(m-1)r(m-1)]\\&+\sum_{m=-\infty}^{\infty}\frac{1}{3}q^3(m)r^3(m-1),\end{aligned} \tag{9}$$

$$\bar{I}_2=\sum_{m=-\infty}^{\infty} q(m)r(m-2)[1+q(m-1)r(m-1)]+\sum_{m=-\infty}^{\infty}\frac{1}{2}q^2(m)r^2(m-1), \tag{10}$$

$$\bar{I}_1=\sum_{m=-\infty}^{\infty} q(m)r(m-1), \tag{11}$$

$$I_0=\sum_{m=-\infty}^{\infty}\ln[1+q(m)r(m)], \tag{12}$$

$$\overset{+}{I}_1=\sum_{m=-\infty}^{\infty} q(m)r(m+1), \tag{13}$$

$$\overset{+}{I}_2=\sum_{m=-\infty}^{\infty} q(m)r(m+2)[1+q(m+1)r(m+1)]+\sum_{m=-\infty}^{\infty}\frac{1}{2}q^2(m)r^2(m+1), \tag{14}$$

$$\begin{aligned}\overset{+}{I}_3=&\sum_{m=-\infty}^{\infty} q(m)r(m+3)[1+q(m+2)r(m+2)][1+q(m+1)r(m+1)]\\&+\sum_{m=-\infty}^{\infty} q(m)q(m+1)r^2(m+2)[1+q(m+1)r(m+1)]\\&+\sum_{m=-\infty}^{\infty} q^2(m)r(m+1)r(m+2)[1+q(m+1)r(m+1)]\end{aligned}$$

$$+\sum_{m=-\infty}^{\infty}\frac{1}{3}q^3(m)r^3(m+1). \tag{15}$$

The higher ones are obtainable within the framework of the recurrence method proposed by Wadati's team.[3]

In general the parameters $\overset{-}{\omega}_\alpha$, $\overset{+}{\omega}_\alpha$, and ω_0 are proved to be arbitrary functions of time, which is usually either overlooked or deliberately neglected in standard theories of integrable hierarchies.[20,21] As a consequence the Hamiltonian function H (8) is not bound to be conserved and can describe some parametrically driven system with sophisticated dynamics.

For physical applications and in particular for the understanding of low amplitude spectrum it is convenient to write down the linear part of the nonlinear model (6)–(8) explicitly. To do so we observe that up to the bilinear terms the recurrence technique[3] yields

$$\overset{-}{I}_\alpha \sim \sum_{m=-\infty}^{\infty} q(m)r(m-\alpha), \tag{16}$$

$$\overset{+}{I}_\alpha \sim \sum_{m=-\infty}^{\infty} q(m)r(m+\alpha). \tag{17}$$

Hence for the linear part of the Mth model (6)–(8) we obtain

$$+i\dot{q}(n) \sim -2\omega_0 q(n) - \sum_{\alpha=1}^{M} [\overset{-}{\omega}_\alpha q(n+\alpha) + \overset{+}{\omega}_\alpha q(n-\alpha)], \tag{18}$$

$$-i\dot{r}(n) \sim -2\omega_0 r(n) - \sum_{\alpha=1}^{M} [\overset{+}{\omega}_\alpha r(n+\alpha) + \overset{-}{\omega}_\alpha r(n-\alpha)]. \tag{19}$$

Thus the parameters $\overset{-}{\omega}_\alpha$ and $\overset{+}{\omega}_\alpha$ are seen to characterize the coupling strength between two αth-neighboring sites. The terms proportional to ω_0 correspond to the regular energy shift and can be easily eliminated by the standard gauge transformation.

Regulating the strength of coupling parameters $\overset{-}{\omega}_\alpha$ and $\overset{+}{\omega}_\alpha$ and the range of intersite interaction M we gain a remarkable opportunity to model a variety of different physical situations. For example, assuming all $\overset{-}{\omega}_\alpha$ and $\overset{+}{\omega}_\alpha$ except $\overset{-}{\omega}_1$, $\overset{-}{\omega}_M$ and $\overset{+}{\omega}_1$, $\overset{+}{\omega}_M$ are equal to zero, we are in a position to describe the dynamics of some nonlinear intramolecular excitations on a spiral-like chain with M molecules per one wind. Moreover, provided the excitations are charged, it is possible to take into account in this case even an impact of longitudinal spatially homogeneous magnetic field via the complex phases of coupling parameters $\overset{-}{\omega}_1$ and $\overset{+}{\omega}_1$ in a way similar to that used in Ref. 10. At last, the freedom in choosing particular time modulations of coupling parameters $\overset{-}{\omega}_\alpha$, $\overset{+}{\omega}_\alpha$ appears to provide a practically inexhaustible source of parametrically driven physical systems integrable by the inverse scattering transform.

We complete this section by presenting the asymptotic part

$$A(z) \equiv \lim_{|n|\to\infty} A(n|z) \tag{20}$$

of the evolution operator $A(n|z)$ in assumption of rapidly decreasing boundary conditions $q(n)\to 0$ and $r(n)\to 0$ as $|n|\to\infty$, since its full expression already for the third model in row ($M=3$) occupies a lot of place. Specifically for the matrix elements $A_{jk}(z)$ of $A(z)$ we have

$$A_{11}(z) = +i\omega_0 + i\sum_{\alpha=1}^{M} \bar{\omega}_\alpha z^{2\alpha}, \tag{21}$$

$$A_{12}(z) = A_{21}(z) = 0, \tag{22}$$

$$A_{22}(z) = -i\omega_0 - i\sum_{\alpha=1}^{M} \overset{+}{\omega}_\alpha z^{-2\alpha}. \tag{23}$$

Fortunately it is precisely the operator $A(z)$ which is of true practical value.

III. SCATTERING PROBLEM AND MARCHENKO EQUATIONS

Although the basic results on the scattering problem and Marchenko equations related to the spectral operator (5) are already well known,[17–19] here we give a brief sketch of them in terminology more convenient for the compact analytical presentation of any multisoliton solution of the nonlinear model under study (6)–(8).

Thus, restricting ourselves to the case of amplitudes $q(n)$ and $r(n)$ rapidly decreasing at both infinities we define the left $\{\boldsymbol{\varphi}_j(n|z)\}$ and the right $\{\boldsymbol{\psi}_j(n|z)\}$ Jost bases ($j=1,2$) as the two component vector sets satisfying the auxiliary spectral problem (1), (5) and fixed by the asymptotic conditions

$$\boldsymbol{\varphi}_j(n|z) \sim \mathbf{J}_1 \delta_{1j} z^n + \mathbf{J}_2 \delta_{2j} z^{-n} \quad \text{as} \quad n \to -\infty \tag{24}$$

and

$$\boldsymbol{\psi}_j(n|z) \sim \mathbf{J}_1 \delta_{1j} z^n + \mathbf{J}_2 \delta_{2j} z^{-n} \quad \text{as} \quad n \to +\infty, \tag{25}$$

respectively. Here $\mathbf{J}_k$ is the two-component column vector with the ith component J_{ik} equal to δ_{ik}.

The transition matrix $a(z) \equiv [a_{jk}(z)]$ is that transforming one Jost basis into another,

$$\boldsymbol{\varphi}_k(n|z) = \sum_{j=1}^{2} \boldsymbol{\psi}_j(n|z) a_{jk}(z) \quad (k=1,2). \tag{26}$$

Formally resolving this equation with respect to matrix elements $a_{ij}(z)$ we have

$$a_{ij}(z) = \frac{\overset{2}{W}_{k=1}\{(1-\delta_{ik})\boldsymbol{\psi}_k(n|z) + \delta_{ik}\boldsymbol{\varphi}_j(n|z)\}}{\overset{2}{W}_{k=1}\{\boldsymbol{\psi}_k(n|z)\}}. \tag{27}$$

Here

$$\overset{2}{W}_{k=1}\{\mathbf{v}_k(n|z)\} \equiv \det[v_{ik}(n|z)] \tag{28}$$

stands for the Wronskian of any two solutions $\mathbf{v}_1(n|z)$ and $\mathbf{v}_2(n|z)$ of the spectral problem (1), (5) with $v_{ik}(n|z)$ denoting the ith component of vector $\mathbf{v}_k(n|z)$. Further, taking the Wronskian from both parts of (26) we come to the normalizing condition

$$\det[a_{ij}(z)] = \frac{\overset{2}{W}_{k=1}\{\boldsymbol{\varphi}_k(n|z)\}}{\overset{2}{W}_{k=1}\{\boldsymbol{\psi}_k(n|z)\}} = \prod_{m=-\infty}^{\infty} [1+q(m)r(m)], \tag{29}$$

where the following readily checked relations,

$$\overset{2}{W}_{k=1}\{\varphi_k(n|z)\}=\prod_{m=-\infty}^{n-1}[1+q(m)r(m)], \tag{30}$$

$$\overset{2}{W}_{k=1}\{\psi_k(n|z)\}=\prod_{m=n}^{\infty}[1+q(m)r(m)]^{-1}, \tag{31}$$

have been used.

Another important statement says that two sets of vectors $\{\varphi_1(n|z)z^{-n},\psi_2(n|z)z^n\}$ and $\{\psi_1(n|z)z^{-n},\varphi_2(n|z)z^n\}$ must be analytic outside $|z|>1$ and inside $|z|<1$ the unit circle, respectively. On the one hand, it enables us to conclude that the diagonal elements $a_{11}(z)$ and $a_{22}(z)$ of the transition matrix are analytic outside $|z|>1$ and inside $|z|<1$ the unit circle, respectively [see (27)]. On the other hand, we might seek the vectors of right Jost basis in the form

$$\psi_j(n|z)=\sum_{l=n}^{\infty}\mathbf{K}_j(n|l)[\delta_{j1}z^l+\delta_{j2}z^{-l}] \quad (j=1,2). \tag{32}$$

Direct substitution of these expansions into the spectral equation (1) with $L(n|z)$ given by (5) yields

$$q(n)=iK_{12}(n|n+1)/K_{22}(n|n), \tag{33}$$

$$r(n)=iK_{21}(n|n+1)/K_{11}(n|n), \tag{34}$$

where $K_{ij}(n|m)$ is the ith component of $\mathbf{K}_j(n|m)$. These relations resolve the nonlinear problem (6)–(8) provided the quantities $K_{12}(n|n+1)$, $K_{22}(n|n)$ and $K_{21}(n|n+1)$, $K_{11}(n|n)$ are found.

In contrast to the original nonlinear evolution model (6)–(8) the vectors $\mathbf{K}_j(n|m)$ obey the linear summation equations (Marchenko equations) with the time τ inserted parametrically through the evolution of scattering data. To derive the Marchenko equations one must rely only on the auxiliary spectral problem (1), (5) (more precisely, on the analytical properties of transition matrix $[a_{jk}(z)]$ and Jost bases $\{\varphi_j(n|z)\}$, $\{\psi_j(n|z)\}$). In so doing we may follow the main arguments of Ablowitz and Ladik[17–19] or simply adapt formulas derived for the multicomponent auxiliary linear problem[10] for the needs of the two-component one—(1), (5). The result is

$$\mathbf{K}_k(n|m)+\sum_{l=n}^{\infty}\sum_{j=1}^{2}\mathbf{K}_j(n|l)F_{jk}(l+m)=\mathbf{J}_k\delta_{nm} \quad (m\geqslant n; \quad k=1,2). \tag{35}$$

Here the matrix elements $F_{jk}(n)$ of the kernel operator are given by

$$F_{11}(n)=F_{22}(n)=0, \tag{36}$$

$$F_{21}(n)=\frac{1}{2\pi i}\oint_{|z|=1}\mathrm{d}z\,z^{-n-1}\frac{a_{21}(z)}{a_{11}(z)}+\sum_{r=1}^{N_{\mathrm{ext}}}[z_{11}(r)]^{-n-1}\frac{a_{21}(z_{11}(r))}{a'_{11}(z_{11}(r))}, \tag{37}$$

$$F_{12}(n)=\frac{1}{2\pi i}\oint_{|z|=1}\mathrm{d}z\,z^{n-1}\frac{a_{12}(z)}{a_{22}(z)}-\sum_{r=1}^{N_{\mathrm{int}}}[z_{22}(r)]^{n-1}\frac{a_{12}(z_{22}(r))}{a'_{22}(z_{22}(r))}, \tag{38}$$

where $z_{kk}(r)$ stands for the rth root of equation $a_{kk}(z)=0$, $a'_{kk}(z_{kk}(r))$ refers to the derivative $[\mathrm{d}a_{kk}(z)/\mathrm{d}z]_{z=z_{kk}(r)}$, while N_{ext} and N_{int} mark the total number of roots of equations $a_{11}(z)=0$ and $a_{22}(z)=0$, respectively. The equalities (37) and (38) have been found with the understanding of simple roots $z_{kk}(r)$. The case of multiple roots can be covered by obtaining limiting expressions in the final results.

IV. TIME EVOLUTION OF SCATTERING DATA

According to expressions (36)–(38) the time evolution of a kernel operator is determined by that of scattering data $a_{21}(z)/a_{11}(z)$, $z_{11}(r)$, $a_{21}(z_{11}(r))/a'_{11}(z_{11}(r))$ and $a_{12}(z)/a_{22}(z)$, $z_{22}(r)$, $a_{12}(z_{22}(r))/a'_{22}(z_{22}(r))$. The time evolution of scattering data in turn follows from

$$\dot{a}_{jk}(z)=\sum_{i=1}^{2}\,[A_{ji}(z)a_{ik}(z)-a_{ji}(z)A_{ik}(z)]\quad (j=1,2;\quad k=1,2). \tag{39}$$

These equations can be derived thanks to the standard observation[20] that at every $j=1,2$ the combination $\dot{\boldsymbol{\varphi}}_j(n|z)-A(n|z)\boldsymbol{\varphi}_j(n|z)$ satisfies the spectral problem (1), (5) and consequently is presentable by some linear superposition of the left Jost vectors $\Sigma_{i=1}^{2}\,\boldsymbol{\varphi}_i(n|z)d_{ij}(z)$. The key steps of such derivation are based upon the direct use of limiting expressions $\lim_{n\to-\infty}\dot{\boldsymbol{\varphi}}_j(n|z)=\mathrm{col}(0,0)$ and $\lim_{n\to+\infty}\dot{\boldsymbol{\psi}}_j(n|z)=\mathrm{col}(0,0)$ evident from the asymptotic conditions (24) and (25), respectively.

Substituting formulas (21)–(23) for $A_{jk}(z)$ into the evolution equation (39) and using (where necessary) the time independence of roots $\dot{z}_{kk}(r)=0$ [the latter statement is nothing but a direct consequence of $a_{kk}(z_{kk}(r))\equiv 0$, $a'_{kk}(z_{kk}(r))\neq 0$ and $\dot{a}_{kk}(z)=0$] we formally integrate to obtain

$$a_{21}(z|\tau)=a_{21}(z|0)\exp\left\{-2i\,\eta_0(\tau)-i\sum_{\alpha=1}^{M}\,[\overset{-}{\eta}_{\alpha}(\tau)z^{2\alpha}+\overset{+}{\eta}_{\alpha}(\tau)z^{-2\alpha}]\right\}, \tag{40}$$

$$a_{12}(z|\tau)=a_{12}(z|0)\exp\left\{+2i\,\eta_0(\tau)+i\sum_{\alpha=1}^{M}\,[\overset{-}{\eta}_{\alpha}(\tau)z^{2\alpha}+\overset{+}{\eta}_{\alpha}(\tau)z^{-2\alpha}]\right\}, \tag{41}$$

$$a_{kk}(z|\tau)=a_{kk}(z|0)\quad (k=1,2), \tag{42}$$

$$a_{jk}(z_{kk}(r)|\tau)=[a_{jk}(z|\tau)]_{z=z_{kk}(r)}\quad (j\neq k), \tag{43}$$

$$a'_{kk}(z_{kk}(r)|\tau)=a'_{kk}(z_{kk}(r)|0)\quad (k=1,2). \tag{44}$$

Here

$$\eta_0(\tau)=\int_0^{\tau}\mathrm{d}t\;\omega_0(t), \tag{45}$$

$$\overset{-}{\eta}_{\alpha}(\tau)=\int_0^{\tau}\mathrm{d}t\;\overset{-}{\omega}_{\alpha}(t), \tag{46}$$

$$\overset{+}{\eta}_{\alpha}(\tau)=\int_0^{\tau}\mathrm{d}t\;\overset{+}{\omega}_{\alpha}(t), \tag{47}$$

and an explicit indication on time variable τ has been restored: $a_{jk}(z)\equiv a_{jk}(z|\tau)$, $a_{jk}(z_{kk}(r))\equiv a_{jk}(z_{kk}(r)|\tau)$, $\omega_0\equiv\omega_0(\tau)$, $\overset{-}{\omega}_{\alpha}\equiv\overset{-}{\omega}_{\alpha}(\tau)$, $\overset{+}{\omega}_{\alpha}\equiv\overset{+}{\omega}_{\alpha}(\tau)$.

Only in the simplest case, when the coupling parameters ω_0, $\overset{-}{\omega}_{\alpha}$, $\overset{+}{\omega}_{\alpha}$ are assumed to be time independent, does the scattering data come to evolve in a way typical for systems from the standard Ablowitz–Ladik hierarchy.

V. MULTISOLITON SOLUTIONS: AN ALTERNATIVE APPROACH

We begin this section with the standard reshaping of the Marchenko equations (35) into the form where the equations for $\mathbf{K}_1(n|m)$ and $\mathbf{K}_2(n|m)$ are completely splitted

$$\mathbf{K}_1(n|m)-\sum_{l=n}^{\infty}\sum_{p=n}^{\infty}\mathbf{K}_1(n|l)F_{12}(l+p)F_{21}(p+m)=\mathbf{J}_1\delta_{nm}-\mathbf{J}_2F_{21}(n+m)\quad(m\geqslant n),\tag{48}$$

$$\mathbf{K}_2(n|m)-\sum_{l=n}^{\infty}\sum_{p=n}^{\infty}\mathbf{K}_2(n|l)F_{21}(l+p)F_{12}(p+m)=\mathbf{J}_2\delta_{nm}-\mathbf{J}_1F_{12}(n+m)\quad(m\geqslant n).\tag{49}$$

However unlike in the usually adopted scheme,[4,17–19] we will treat Eqs. (48) and (49) in an absolutely different way, omitting the parts for the components $K_{21}(n|m)$ and $K_{12}(n|m)$ as quite unnecessary. Instead we will consider the equations for the components $K_{11}(n|m)$ and $K_{22}(n|m)$,

$$K_{11}(n|m)-\sum_{l=n}^{\infty}\sum_{p=n}^{\infty}K_{11}(n|l)F_{12}(l+p)F_{21}(p+m)=\delta_{nm}\quad(m\geqslant n),\tag{50}$$

$$K_{22}(n|m)-\sum_{l=n}^{\infty}\sum_{p=n}^{\infty}K_{22}(n|l)F_{21}(l+p)F_{12}(p+m)=\delta_{nm}\quad(m\geqslant n),\tag{51}$$

to be the basic ones.

Indeed, knowing the solutions $K_{11}(n|m)$ and $K_{22}(n|m)$ reduces two of the four components of the original Marchenko equations (35) taken at $m=n+1$ to the sheer definitions of $K_{21}(n|n+1)$ and $K_{12}(n|n+1)$. Namely, we have

$$K_{21}(n|n+1)=-\sum_{l=n}^{\infty}K_{22}(n|l)F_{21}(l+n+1),\tag{52}$$

$$K_{12}(n|n+1)=-\sum_{l=n}^{\infty}K_{11}(n|l)F_{12}(l+n+1),\tag{53}$$

which in combination with $K_{11}(n|m)$, $K_{22}(n|m)$ and (33), and (34) formally resolves the nonlinear problem of interest—(6)–(8).

Now let us analyze Eqs. (50) and (51) and expressions (52) and (53) using the parity properties of transition matrix $[a_{jk}(z)]$. These properties are as follows: $a_{11}(-z)=a_{11}(z)$, $a_{22}(-z)=a_{22}(z)$, $a_{12}(-z)=-a_{12}(z)$, $a_{21}(-z)=-a_{12}(z)$, and can easily be proved for rapidly abating amplitudes $q(n)$ and $r(n)$ close to those on the compact support. When applied to the matrix elements (37) and (38) of the kernel operator they allow us to conclude that $F_{21}(n)$ and $F_{12}(n)$ must be equal to zero identically at every even n. As a result the equations for $K_{11}(n|n+2m)$ become separated from those for $K_{11}(n|n+2m+1)$ while the equations for $K_{22}(n|n+2m)$ become separated from those for $K_{22}(n|n+2m+1)$ [see (50) and (51)]. Moreover the right-hand sides of expressions (52) and (53) must contain only the terms with $K_{22}(n|n+2m)$ and $K_{11}(n|n+2m)$, respectively.

Hence all information of interest can be obtained from

$$K_{11}(n|n+2m)-\sum_{l=0}^{\infty}\sum_{p=0}^{\infty}K_{11}(n|n+2l)F_{12}(2l+2n+1+2p)F_{21}(2p+1+2n+2m)$$
$$=\delta_{0m}\quad(m\geqslant 0),\tag{54}$$

$$K_{22}(n|n+2m)-\sum_{l=0}^{\infty}\sum_{p=0}^{\infty}K_{22}(n|n+2l)F_{21}(2l+2n+1+2p)F_{12}(2p+1+2n+2m)$$
$$=\delta_{0m}\quad(m\geqslant 0),\tag{55}$$

supplemented by the relations

$$K_{21}(n|n+1)=-\sum_{m=0}^{\infty} K_{22}(n|n+2m)F_{21}(2m+1+2n), \tag{56}$$

$$K_{12}(n|n+1)=-\sum_{m=0}^{\infty} K_{11}(n|n+2m)F_{12}(2m+1+2n). \tag{57}$$

In order to proceed with the multisolitonic solutions we must equalize the scattering data of continuous spectrum $a_{21}(z)/a_{11}(z)$ and $a_{12}(z)/a_{22}(z)$ to zero at $|z|=1$. Then, on the one hand, the matrix elements of the kernel operator appeared in Eqs. (54) and (55) become degenerate [see (37) and (38)] and, on the other, the form of the diagonal matrix elements $a_{kk}(z)$ can be reconstructed explicitly

$$a_{11}(z)=\prod_{s=1}^{N}\frac{z^2-\exp[\mu_{11}(s)+ik_{11}(s)]}{z^2-\exp[-\mu_{22}(s)+ik_{22}(s)]} \quad (|z|\geqslant 1), \tag{58}$$

$$a_{22}(z)=\prod_{s=1}^{N}\frac{z^{-2}-\exp[\mu_{22}(s)-ik_{22}(s)]}{z^{-2}-\exp[-\mu_{11}(s)-ik_{11}(s)]} \quad (|z|\leqslant 1). \tag{59}$$

Here $k_{11}(s)$ and $k_{22}(s)$ are real constants, whereas $\mu_{11}(s)$ and $\mu_{22}(s)$ are positive real constants. Except for the restrictions imposed by the assumed simplicity of roots $z_{kk}(r)$, the constants $\mu_{11}(s)$, $k_{11}(s)$ and $\mu_{22}(s)$, $k_{22}(s)$ are supposed to be arbitrary in all other respects. Finally, N represents an arbitrary but fixed positive integer, being the number of solitons in a particular multisoliton solution. Evidently $N_{\text{ext}}=N_{\text{int}}=2N$.

Despite being valid only for the reflectionless case, expressions (58) and (59) are consistent with the analyticity conditions [$a_{11}(z)$ is analytical at $|z|>1$ and $a_{22}(z)$ is analytical at $|z|<1$] and parity conditions $a_{kk}(-z)=a_{kk}(z)$ as well as with the normalizing condition (29) and limiting conditions $\lim_{|z|\to\infty} a_{11}(z)=1$ and $\lim_{|z|\to 0} a_{22}(z)=1$. Although not mentioned earlier, the limiting conditions for $a_{kk}(z)$ are a direct consequence of those for the scattering vectors $\mathbf{S}_{kk}(n|z)$, defined by $\mathbf{S}_{kk}(n|z)a_{kk}(z)\equiv\varphi_k(n|z)$.

Adopting the roots $z_{kk}(r)$ in (37) and (38) to be enumerated in accordance with

$$z_{kk}(2s)=-z_{kk}(2s-1) \quad (s=1,2,3,\ldots,N) \tag{60}$$

and using (58) and (59) to find them, we can write $F_{21}(2n+1)$ and $F_{12}(2n+1)$ for the reflectionless case as follows:

$$F_{21}(2n+1)=\sum_{s=1}^{N} b_{21}(s)\exp[-\sigma_{11}(s)n], \tag{61}$$

$$F_{12}(2n+1)=\sum_{s=1}^{N} b_{12}(s)\exp[-\sigma_{22}(s)n]. \tag{62}$$

Here

$$b_{21}(s)\equiv\frac{2a_{21}(z_{11}(2s))}{[z_{11}(2s)]^2 a'_{11}(z_{11}(2s))}, \tag{63}$$

$$b_{12}(s)\equiv-\frac{2a_{12}(z_{22}(2s))}{a'_{22}(z_{22}(2s))}, \tag{64}$$

$$\sigma_{11}(s)\equiv\mu_{11}(s)+ik_{11}(s), \tag{65}$$

$$\sigma_{22}(s) \equiv \mu_{22}(s) - ik_{22}(s). \tag{66}$$

Combining the reduced Marchenko equations (54) and (55) with the explicit expressions for matrix elements of kernel operator (61) and (62) we introduce two auxiliary functions,

$$X_{11}(n|s) \equiv \sum_{m=0}^{\infty} K_{11}(n|n+2m)\exp[-\sigma_{22}(s)m], \tag{67}$$

$$X_{22}(n|s) \equiv \sum_{m=0}^{\infty} K_{22}(n|n+2m)\exp[-\sigma_{11}(s)m], \tag{68}$$

which are proved to be governed by two sets of linear algebraic equations,

$$X_{11}(n|s) - \sum_{s'=1}^{N} X_{11}(n|s')\langle s'|\hat{B}_{12}(n)\hat{B}_{21}(n)|s\rangle = 1 \quad (s=1,2,3,\ldots,N), \tag{69}$$

$$X_{22}(n|s) - \sum_{s'=1}^{N} X_{22}(n|s')\langle s'|\hat{B}_{21}(n)\hat{B}_{12}(n)|s\rangle = 1 \quad (s=1,2,3,\ldots,N). \tag{70}$$

Here

$$\langle s'|\hat{B}_{12}(n)\hat{B}_{21}(n)|s\rangle \equiv \sum_{s''=1}^{N} \langle s'|\hat{B}_{12}(n)|s''\rangle\langle s''|\hat{B}_{21}(n)|s\rangle, \tag{71}$$

$$\langle s'|\hat{B}_{21}(n)\hat{B}_{12}(n)|s\rangle \equiv \sum_{s''=1}^{N} \langle s'|\hat{B}_{21}(n)|s''\rangle\langle s''|\hat{B}_{12}(n)|s\rangle \tag{72}$$

with $\langle s'|\hat{B}_{12}(n)|s''\rangle$ and $\langle s''|\hat{B}_{21}(n)|s'\rangle$ defined by

$$\langle s'|\hat{B}_{12}(n)|s''\rangle = \frac{b_{12}(s')\exp[-\sigma_{22}(s')n]}{1-\exp[-\sigma_{22}(s')-\sigma_{11}(s'')]}, \tag{73}$$

$$\langle s''|\hat{B}_{21}(n)|s'\rangle = \frac{b_{21}(s'')\exp[-\sigma_{11}(s'')n]}{1-\exp[-\sigma_{11}(s'')-\sigma_{22}(s')]}. \tag{74}$$

Then all quantities of interest are seen to be presented in terms of $X_{11}(n|s)$ and $X_{22}(n|s)$ exclusively. Indeed, the direct use of definitions (67) and (68) in formulas (54)–(57) gives rise to

$$K_{11}(n|n) = 1 + \sum_{s'=1}^{N}\sum_{s''=1}^{N} X_{11}(n|s')\langle s'|\hat{B}_{12}(n)|s''\rangle b_{21}(s'')\exp[-\sigma_{11}(s'')n], \tag{75}$$

$$K_{22}(n|n) = 1 + \sum_{s'=1}^{N}\sum_{s''=1}^{N} X_{22}(n|s')\langle s'|\hat{B}_{21}(n)|s''\rangle b_{12}(s'')\exp[-\sigma_{22}(s'')n], \tag{76}$$

$$K_{21}(n|n+1) = -\sum_{s=1}^{N} X_{22}(n|s)b_{21}(s)\exp[-\sigma_{11}(s)n], \tag{77}$$

$$K_{12}(n|n+1) = -\sum_{s=1}^{N} X_{11}(n|s)b_{12}(s)\exp[-\sigma_{22}(s)n]. \tag{78}$$

Thus the only question yet to be handled is to write down the solutions of (69) and (70) explicitly. To do so we define $N\times N$ matrixes $\hat{C}_{11}(n)\equiv[\langle s'|\hat{C}_{11}(n)|s''\rangle]$ and $\hat{C}_{22}(n)\equiv[\langle s'|\hat{C}_{22}(n)|s''\rangle]$ by their matrix elements

$$\langle s'|\hat{C}_{11}(n)|s''\rangle=\delta_{s's''}-\langle s'|\hat{B}_{12}(n)\hat{B}_{21}(n)|s''\rangle \tag{79}$$

and

$$\langle s'|\hat{C}_{22}(n)|s''\rangle=\delta_{s's''}-\langle s'|\hat{B}_{21}(n)\hat{B}_{12}(n)|s''\rangle, \tag{80}$$

respectively, and obtain

$$X_{11}(n|s)=\sum_{s'=1}^{N}\frac{\partial \ln\det \hat{C}_{11}(n)}{\partial\langle s|\hat{C}_{11}(n)|s'\rangle}, \tag{81}$$

$$X_{22}(n|s)=\sum_{s'=1}^{N}\frac{\partial \ln\det \hat{C}_{22}(n)}{\partial\langle s|\hat{C}_{22}(n)|s'\rangle}. \tag{82}$$

Hence according to formulas (33), (34) and (75)–(78) any multisoliton solution of the nonlinear problem (6)–(8) looks as follows:

$$\begin{aligned} q(n)&=iK_{12}(n|n+1)/K_{22}(n|n)\\ &=\frac{-i\sum_{s=1}^{N}X_{11}(n|s)b_{12}(s)\exp[-\sigma_{22}(s)n]}{1+\sum_{s'=1}^{N}\sum_{s''=1}^{N}X_{22}(n|s')\langle s'|\hat{B}_{21}(n)|s''\rangle b_{12}(s'')\exp[-\sigma_{22}(s'')n]}, \end{aligned} \tag{83}$$

$$\begin{aligned} r(n)&=iK_{21}(n|n+1)/K_{11}(n|n)\\ &=\frac{-i\sum_{s=1}^{N}X_{22}(n|s)b_{21}(s)\exp[-\sigma_{11}(s)n]}{1+\sum_{s'=1}^{N}\sum_{s''=1}^{N}X_{11}(n|s')\langle s'|\hat{B}_{12}(n)|s''\rangle b_{21}(s'')\exp[-\sigma_{11}(s'')n]}, \end{aligned} \tag{84}$$

where $X_{11}(n|s)$ and $X_{22}(n|s)$ are given by (81) and (82), respectively. Here, of course, we should understand the scattering data $b_{12}(s)$ and $b_{21}(s)$ to be the time dependent ones:

$$\begin{aligned} b_{12}(s)&\equiv b_{12}(s|\tau)\\ &=b_{12}(s|0)\exp\left\{+2i\eta_0(\tau)+i\sum_{\alpha=1}^{M}[\overset{-}{\eta}_{\alpha}(\tau)\exp(-\alpha\sigma_{22}(s))+\overset{+}{\eta}_{\alpha}(\tau)\exp(+\alpha\sigma_{22}(s))]\right\} \end{aligned} \tag{85}$$

$$\begin{aligned} b_{21}(s)&\equiv b_{21}(s|\tau)\\ &=b_{21}(s|0)\exp\left\{-2i\eta_0(\tau)-i\sum_{\alpha=1}^{M}[\overset{-}{\eta}_{\alpha}(\tau)\exp(+\alpha\sigma_{11}(s))+\overset{+}{\eta}_{\alpha}(\tau)\exp(-\alpha\sigma_{11}(s))]\right\}. \end{aligned} \tag{86}$$

We complete this section by adapting the obtained time dependencies (85) and (86) for the needs of reduction $r(n)=q^*(n)$.

Then the dynamical equations (6) and (7) will be mutually consistent under the constraint $H^*=H$. As a consequence the parameter ω_0 must be purely real, while $\overset{-}{\omega}_\alpha$ and $\overset{+}{\omega}_\alpha$ can be parametrized by two real parameters, ω_α and φ_α. In particular,

$$\overset{-}{\omega}_\alpha=\omega_\alpha\exp(-i\varphi_\alpha), \tag{87}$$

$$\overset{+}{\omega}_\alpha=\omega_\alpha\exp(+i\varphi_\alpha), \tag{88}$$

where in general $\omega_\alpha\equiv\omega_\alpha(\tau)$ and $\varphi_\alpha\equiv\varphi_\alpha(\tau)$ are supposed to be time dependent.

Moreover, calculating the matrix elements of $a^+(1/z^*)a(z)$ and combining them with the normalizing condition (29) we can obtain

$$a_{11}^*(1/z^*)=a_{22}(z), \tag{89}$$

$$a_{21}^*(1/z^*)=-a_{12}(z). \tag{90}$$

These relations yield

$$z_{11}(r)=1/z_{22}^*(r), \tag{91}$$

$$\left[\frac{a_{12}(z_{22}(r))}{a_{22}'(z_{22}(r))}\right]^*=\frac{a_{21}(z_{11}(r))}{[z_{11}(r)]^2a_{11}'(z_{11}(r))}. \tag{92}$$

Hence seeking the multisoliton solutions we have to set

$$\mu_{11}(s)=\mu_{22}(s)\equiv\mu(s), \tag{93}$$

$$k_{11}(s)=k_{22}(s)\equiv k(s), \tag{94}$$

$$b_{12}^*(s)=-b_{21}(s). \tag{95}$$

As a result the expressions (85) and (86) for $b_{12}(s|\tau)$ and $b_{21}(s|\tau)$ can be reduced to

$$b_{12}(s|\tau)=2i\,\mathrm{sh}\mu(s)\exp[\mu(s)x(s)+i\theta(s)]\cdot\exp\left\{+2i\int_0^\tau \mathrm{d}t\;\omega_0(t)+2i\sum_{\alpha=1}^{M}\int_0^\tau \mathrm{d}t\;\omega_\alpha(t)\,\mathrm{ch}[\alpha\mu(s)-i\alpha k(s)+i\varphi_\alpha(t)]\right\}, \tag{96}$$

$$b_{21}(s|\tau)=2i\,\mathrm{sh}\mu(s)\exp[\mu(s)x(s)-i\theta(s)]\cdot\exp\left\{-2i\int_0^\tau \mathrm{d}t\;\omega_0(t)-2i\sum_{\alpha=1}^{M}\int_0^\tau \mathrm{d}t\;\omega_\alpha(t)\,\mathrm{ch}[\alpha\mu(s)+i\alpha k(s)-i\varphi_\alpha(t)]\right\}, \tag{97}$$

where the parametrization

$$b_{12}(s|0)=2i\,\mathrm{sh}\mu(s)\exp[\mu(s)x(s)+i\theta(s)], \tag{98}$$

$$b_{21}(s|0)=2i\,\mathrm{sh}\mu(s)\exp[\mu(s)x(s)-i\theta(s)] \tag{99}$$

has been adopted.

Depending on a particularly chosen swing in amplitudes $\omega_\alpha(\tau)$ and phases $\varphi_\alpha(\tau)$ of coupling parameters the nonlinear dynamical system (6)–(8) might exhibit a variety of absolutely different

regimes of soliton dynamics from the uniform infinite motion to the dynamical localization. We will consider some such regimes in Sec. VII although, in principle, their number appears to be inexhaustible. Of course a variety of effects in soliton dynamics may be caused also by the interplay between the different coupling parameters, which as we know couple the molecules on different spatial distances.

VI. TRANSFORMATION TO THE PHYSICALLY CORRECTED AMPLITUDES

Although the Poisson brackets related to models (6)–(8) are proved to be nonstandard they are unable to cause any discrepancy in physical applications. Indeed, introducing the corrected amplitudes[27]

$$Q(n)=\sqrt{[q(n)/r(n)]\ln[1+q(n)r(n)]}, \tag{100}$$

$$R(n)=\sqrt{[r(n)/q(n)]\ln[1+q(n)r(n)]}, \tag{101}$$

we might always transform any original model (6)–(8) into the standard form

$$+i\dot{Q}(n)=\partial H/\partial R(n)\equiv+i\{H,Q(n)\}, \tag{102}$$

$$-i\dot{R}(n)=\partial H/\partial Q(n)\equiv-i\{H,R(n)\} \tag{103}$$

with the Poisson brackets given by

$$\{Q(n),R(m)\}=+i\delta_{nm}, \quad \{R(n),Q(m)\}=-i\delta_{nm}, \tag{104}$$

$$\{Q(n),Q(m)\}=0, \quad \{R(n),R(m)\}=0. \tag{105}$$

Here, in order to write H in terms of $Q(n)$ and $R(n)$ we simply must substitute

$$q(n)=\sqrt{[\exp(Q(n)R(n))-1]Q(n)/R(n)}, \tag{106}$$

$$r(n)=\sqrt{[\exp(Q(n)R(n))-1]R(n)/Q(n)} \tag{107}$$

into formula (8).

Remarkably, the corrected model (102), (103) possesses the same linear part (18) and (19) as the original one (6)–(8) and hence exhibits the same low amplitude spectrum.

The precise meaning of amplitudes $Q(n)$ and $R(n)$ depends on a particular adopted reduction. For example, in the case when $r(n)=q^*(n)$ [and hence $R(n)=Q^*(n)$] the amplitudes $Q(n)$ and $R(n)$ are nothing but the probability amplitudes since according to expression (12) the total number of excitations,

$$I_0=\sum_{m=-\infty}^{\infty} Q(m)R(m), \tag{108}$$

has to be conserved.

The use of probability amplitudes allows us to calculate the mean value $\langle\Phi(n)\rangle$ of any physical quantity $\Phi(n)$ in the most natural way

$$\langle\Phi(n)\rangle=\frac{\Sigma_{m=-\infty}^{\infty}\Phi(m)Q(m)R(m)}{\Sigma_{m=-\infty}^{\infty}Q(m)R(m)}. \tag{109}$$

In Sec. VII we apply this definition to the analysis of one soliton dynamics.

VII. ONE SOLITON DYNAMICS: PARAMETRICAL LOCALIZATION

Assuming the reduction $r(n)=q^*(n)$ let us discuss the dynamics of the model (6)–(8) in one soliton case $N=1$.

According to general expressions (83), (84) and (96), (97) the one soliton solution itself looks as follows:

$$q(n|\tau)=\frac{\mathrm{sh}\mu\,\exp[+ikn+i\theta-i\int_0^\tau \mathrm{d}t\,\Omega(k|t|\mu)]}{\mathrm{ch}\{\mu[n-x-\int_0^\tau \mathrm{d}t\,v(k|t|\mu)]\}}, \tag{110}$$

$$r(n|\tau)=\frac{\mathrm{sh}\mu\,\exp[-ikn-i\theta+i\int_0^\tau \mathrm{d}t\,\Omega(k|t|\mu)]}{\mathrm{ch}\{\mu[n-x-\int_0^\tau \mathrm{d}t\,v(k|t|\mu)]\}}, \tag{111}$$

where

$$\Omega(k|\tau|\mu)=-2\omega_0(\tau)-2\sum_{\alpha=1}^{M}\omega_\alpha(\tau)\mathrm{ch}(\alpha\mu)\cos[\alpha k-\varphi_\alpha(\tau)], \tag{112}$$

$$v(k|\tau|\mu)=\frac{2}{\mu}\sum_{\alpha=1}^{M}\omega_\alpha(\tau)\mathrm{sh}(\alpha\mu)\sin[\alpha k-\varphi_\alpha(\tau)] \tag{113}$$

and we have denoted $\mu(1)\equiv\mu$, $k(1)\equiv k$, $x(1)\equiv x$, $\theta(1)\equiv\theta$.

To analyze this solution we rely on the explicit formula for the coordinate of soliton center

$$x(k|\tau|\mu)\equiv\langle n\rangle_s=x+\int_0^\tau \mathrm{d}t\,v(k|t|\mu)\,. \tag{114}$$

We also estimate the typical soliton width $d(\langle n\rangle_s)$ defined by

$$d(\langle n\rangle_s)=2\sqrt{\langle(n-\langle n\rangle_s)^2\rangle_s}. \tag{115}$$

Here the brackets $\langle\ \rangle_s$ stand for the average operation (109) taken on the corrected [according to (100) and (101)] one-soliton amplitudes (110) and (111). The result written on the right-hand side of expression (114) is an exact one and has been calculated via the well-known Poisson summation formula [see, e.g., formula (A2) in the Appendix].

From expression (114) we clearly see that x marks the coordinate of soliton center in an initial moment $\tau=0$ whereas $v(k|\tau|\mu)$ describe the velocity of the soliton center in an arbitrary moment. According to formula (113) this velocity consists of superposition of partial velocities emanated from the different coupling parameters. The αth partial velocity is determined by the amplitude $\omega_\alpha(\tau)$ and phase $\varphi_\alpha(\tau)$ modulations of the αth coupling parameter as well as by the product αk. The amplitude of the αth partial velocity in turn is enhanced by the factor $(2/\mu)\mathrm{sh}(\alpha\mu)$.

In a particular case of uniform motion, when the nonlinear system (6)–(8) is parametrically undriven $\omega_\alpha(\tau)\equiv\omega_\alpha(0)$ and $\varphi_\alpha(\tau)\equiv\varphi_\alpha(0)$, the parameter k may be identified with the momentum of a soliton as a whole. However in general this meaning may be completely devaluated.

Indeed assuming that $\omega_\alpha(\tau)\equiv\omega_\alpha(0)$ and $\varphi_\alpha(\tau)\equiv\varphi_\alpha(0)-\mathcal{E}_\alpha(0)\tau$ we come to the case of parametrically localized soliton dynamics with the coordinate of soliton center oscillating by the law

$$x(k|\tau|\mu)=x-\frac{2}{\mu}\sum_{\alpha=1}^{M}\frac{\omega_\alpha(0)}{\mathcal{E}_\alpha(0)}\mathrm{sh}(\alpha\mu)\{\cos[\mathcal{E}_\alpha(0)\tau+\alpha k-\varphi_\alpha(0)]-\cos[\alpha k-\varphi_\alpha(0)]\} \tag{116}$$

on a confined domain of space. Thus we have obtained the superposition of incommensurate oscillations where the product αk simply merges with the initial phase $\varphi_\alpha(0)$ of the respective coupling parameter. When the partial frequencies $|\mathcal{E}_\alpha(0)|/2\pi$ are decreased the amplitudes of oscillations are increased so that in the limit of zero frequencies $|\mathcal{E}_\alpha(0)|/2\pi \to 0$ we come back to the case of uniform soliton motion on an unconfined spatial domain,

$$x(k|\tau|\mu) = x + \frac{2\tau}{\mu} \sum_{\alpha=1}^{M} \omega_\alpha(0)\,\mathrm{sh}(\alpha\mu)\sin[\alpha k - \varphi_\alpha(0)]. \tag{117}$$

Of course in the general case of an arbitrary parametrical swing the soliton center might exhibit rather complex dynamics, e.g., the regular drift and oscillations combined.

Calculating the soliton width $d(\langle n\rangle_s)$ (see the Appendix for some details) we have observed that it has to breathe between its two extreme values $d_{\min} \equiv d(0)$ and $d_{\max} \equiv d(\pm 1/2)$, although the peculiarities of such oscillations should undoubtedly be governed by a particular dynamics of soliton center. At $\mu \ll 1$ the amplitude of this breathing mode is exponentially suppressed and both extreme soliton widths $d(0)$ and $d(\pm 1/2)$ become practically indistinguishible: $d(0) \simeq d(\pm 1/2) \simeq \pi/\mu\sqrt{3}$. However at $\mu > 1$ the breathing effect is strictly pronounced and the soliton width is determined not only by the parameter $1/\mu$ but also by the position of soliton center-of-mass $\langle n\rangle_s$ with the easily checked properties $d(y) = d(y - [y])$ and $d(-y) = d(y)$ bearing in mind. Specifically for $d(0)$ and $d(\pm 1/2)$ at large μ (i.e., at $\mu \gg 1$) we have $d(0) \simeq \sqrt{(4/\mu)\ln 2}$ and $d(\pm 1/2) \simeq 1$. These results have nothing to do with those for continuous integrable models where the soliton width d could not breathe and is determined by the single parameter $1/\mu$ via unique formula $d = \pi/\mu\sqrt{3}$ at all positive μ.

It is interesting to note that the one soliton solution (110), (111) is also characterized by the time-dependent cyclic frequency $\Omega(k|\tau|\mu)$ (112) which is formally analogous to the energy spectrum of the low amplitude mode with k playing the role of wave number. This analogy becomes especially clear in the limit of wide solitons $\mu \to 0$ when the identity

$$v(k|\tau|0) = \partial\Omega(k|\tau|0)/\partial k, \tag{118}$$

similar to the definition of group velocity of planar wave holds. The frequency $\Omega(k|\tau|\mu)$ (112) consists of partial frequencies and might exhibit the nonmonotonic dependence on parameter k. The latter facts extend the general rule established for the low amplitude excitations in spatially regular structures with the long-range interaction[28] to the case of soliton-like excitations.

VIII. DISCRETE NONLINEAR SCHRÖDINGER SYSTEMS IN LINEAR POTENTIAL: BLOCH OSCILLATIONS

Let us consider the dynamical system

$$+i\dot{q}(n) = [1 + q(n)r(n)]\partial\mathcal{H}/\partial r(n), \tag{119}$$

$$-i\dot{r}(n) = [1 + q(n)r(n)]\partial\mathcal{H}/\partial q(n) \tag{120}$$

with the Hamiltonian

$$\mathcal{H} = -2\omega_0 I_0 - \sum_{m=-\infty}^{\infty} \mathcal{E}m \ln[1 + q(m)r(m)] - \sum_{\alpha=1}^{M} \omega_\alpha[\exp(-i\psi_\alpha)\bar{I}_\alpha + \exp(+i\psi_\alpha)\overset{+}{I}_\alpha], \tag{121}$$

where $\omega_0 \equiv \omega_0(\tau)$, $\omega_\alpha \equiv \omega_\alpha(\tau)$, $\psi_\alpha \equiv \psi_\alpha(\tau)$, and $\mathcal{E} \equiv \mathcal{E}(\tau)$ are supposed to be time-dependent real parameters, whereas $r(n) \equiv q^*(n)$. At $\mathcal{E} = 0$ and $\psi_\alpha = \varphi_\alpha$ this system coincides literally with that given by (6)–(8) provided the reduction $r(n) = q^*(n)$ is adopted and the parametrization (87) and (88) is used. At $\mathcal{E} \neq 0$ the system (119)–(121) can be treated as the parametrically driven system of

nonlinear Schrödinger type subjected to linear potential with strength $\mathcal{E}$. The latter statement becomes especially clear when we reformulate the model (119)–(121) in terms of corrected amplitudes (100) and (101).

The question arises whether it is possible to convert the system (119)–(121) into the form

$$+i\dot{q}(n)=[1+q(n)r(n)]\partial H/\partial r(n), \tag{122}$$

$$-i\dot{r}(n)=[1+q(n)r(n)]\partial H/\partial q(n), \tag{123}$$

$$H=-2\omega_0 I_0-\sum_{\alpha=1}^{M}\omega_\alpha[\exp(-i\varphi_\alpha)\bar{I}_\alpha+\exp(+i\varphi_\alpha)\overset{+}{I}_\alpha], \tag{124}$$

and hence to integrate it by the inverse scattering transform.

In a particular case of nearest-neighboring coupling $M=1$ with $\omega_1(\tau)=1$ and $\psi_1(\tau)=0$ the answer is known to be positive,[29] which actually had been preordained earlier in Refs. 30 and 31.

In the general case of a parametrically driven system with the exploding range of intersite couplings in the presence of linear potential (119)–(121), the reply happens to be positive too. Indeed, replacing $q(n)$ and $r(n)$ in (119)–(121) by the rule

$$q(n)\to q(n)\exp\left[+in\int_0^\tau \mathrm{d}t\,\mathcal{E}(t)\right], \tag{125}$$

$$r(n)\to r(n)\exp\left[-in\int_0^\tau \mathrm{d}t\,\mathcal{E}(t)\right], \tag{126}$$

we readily come to the system (122)–(124) with $\varphi_\alpha(\tau)$ given by

$$\varphi_\alpha(\tau)=\psi_\alpha(\tau)-\alpha\int_0^\tau \mathrm{d}t\,\mathcal{E}(t). \tag{127}$$

Thus in order to obtain the solutions $q(n)$ and $r(n)$ of the system in linear potential (119)–(121) we have to multiply the solutions of the system without linear potential (122)–(124) on $\exp[+in\int_0^\tau \mathrm{d}t\,\mathcal{E}(t)]$ and $\exp[-in\int_0^\tau \mathrm{d}t\,\mathcal{E}(t)]$, respectively, substituting simultaneously expression (127) for $\varphi_\alpha(\tau)$.

We demonstrate this recipe for system (119)–(121) with the constant parameters $\omega_0\equiv\omega_0(0)$, $\omega_\alpha=\omega_\alpha(0)$, $\psi_\alpha\equiv\psi_\alpha(0)$, and $\mathcal{E}\equiv\mathcal{E}(0)$ on an example of one soliton solution and obtain

$$q(n|\tau)=\frac{\mathrm{sh}\mu\,\exp[+i(k+\mathcal{E}(0)\tau)n+i\theta-i\int_0^\tau \mathrm{d}t\,\Omega(k|t|\mu)]}{\mathrm{ch}\{\mu[n-x(k|\tau|\mu)]\}}, \tag{128}$$

$$r(n|\tau)=\frac{\mathrm{sh}\mu\,\exp[-i(k+\mathcal{E}(0)\tau)n-i\theta+i\int_0^\tau \mathrm{d}t\,\Omega(k|t|\mu)]}{\mathrm{ch}\{\mu[n-x(k|\tau|\mu)]\}}. \tag{129}$$

Here

$$\int_0^\tau \mathrm{d}t\,\Omega(k|t|\mu)=-2\omega_0(0)\tau - 2\sum_{\alpha=1}^{M}\frac{\omega_\alpha(0)}{\alpha\mathcal{E}(0)}\mathrm{ch}(\alpha\mu)\{\sin[\alpha\mathcal{E}(0)\tau+\alpha k-\psi_\alpha(0)]-\sin[\alpha k-\psi_\alpha(0)]\}, \tag{130}$$

$$x(k|\tau|\mu)=x-\frac{2}{\mu}\sum_{\alpha=1}^{M}\frac{\omega_\alpha(0)}{\alpha\mathcal{E}(0)}\mathrm{sh}(\alpha\mu)\{\cos[\alpha\mathcal{E}(0)\tau+\alpha k-\psi_\alpha(0)]-\cos[\alpha k-\psi_\alpha(0)]\}. \tag{131}$$

Thus the linear potential of constant strength $\mathcal{E}(0)$ gives rise to the dynamically localized soliton motion in a parametrically undriven system resembling the parametrically localized soliton dynamics described in Sec. VII. However here the frequencies of oscillations $\alpha|\mathcal{E}(0)|/2\pi$ are bound to be commensurate and are determined by the single parameter $\mathcal{E}(0)$, i.e., by the strength of external field.

In condensed matter physics the oscillations caused by the interplay between the linear potential and the spatial discreteness of the lattice are known as the Bloch oscillations.[32,33] Such effects are experimentally observable only in spatially discrete systems (e.g., on semiconductor superlattices[34]) and are principally forbidden in continuous ones. When related to the bent arrays of optical waveguides, the effects, generally analogous to those of Bloch oscillations and dynamical localization, have also recently been described.[35]

IX. CONCLUSION

Summarizing, we have shown how to extend step by step the range of intersite interactions in discrete nonlinear Schrödinger systems generated by the Ablowitz–Ladik auxiliary spectral problem. As a result it is possible to obtain the sequence of nonlinear models with the Hamiltonians given by some special type of linear superpositions of conserved quantities. However unlike in the standard Ablowitz–Ladik hierarchy, where the superposing coefficients are assumed to be constant, we have observed that they may be either constants or arbitrary functions of time. These superposing coefficients play the role of intersite coupling parameters and hence in general can beget the parametrically driven systems with rather rich soliton dynamics. The Hamiltonian of any such parametrically driven system is not bound to be conserved, however the system itself still remains to be integrable by the inverse scattering transform.

We have revealed an important subclass of parametrically driven systems demonstrating the effects of parametric localization of solitons on a confined domain of space and have analyzed the corresponding one soliton dynamics.

In some particular cases it is possible to establish the formal equivalence between the original parametrically driven system and another parametrically driven system but subjected to the additional linear potential. When the strength of the potential field is constant the total Hamiltonian of the new dynamical system becomes conserved, provided its coupling parameters are time independent. Nevertheless the infinite soliton trajectories in the latter system are forbidden due to the so-called dynamical localization accompanied by the Bloch–Zener oscillations of soliton center of mass.

We point out once again that the alternative method of solving the Marchenko equations developed here appears to be more straightforward than the early known ones.[4,17–19] The final formulas for the multisoliton solutions (83) and (84) are also the original ones. Moreover, unlike in the usual approaches, they were derived for the most general case relinquishing any particular reduction for the amplitudes $q(n)$ and $r(n)$. The detailed analysis of such unreduced solutions goes beyond the scope of present report, however, the interested reader could look through their one soliton prototype recently obtained for the undriven nonlinear Schrödinger system on a ladder lattice with nearest-neighboring intermolecular couplings [see formulas (86) and (87) in Ref. 7].

Finally we have reformulated the models of interest in terms of corrected amplitudes with the standard Poisson brackets, which sometimes seems to be a necessary step useful for physical applications. So we have presented the explicit formulas of respective transformations.

We believe that the wide possibilities in extending the range of intersite interactions as well as in appropriate choice of coupling parameters (i.e., their strengths and time dependencies) could stimulate the described class of parametrically driven integrable models to be applied to the needs of different physically motivated discrete quasi-one-dimensional systems.[14–16,34,35]

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APPENDIX: CALCULATIONS OF SQUARED SOLITON WIDTH

According to definition (115) the squared typical soliton width $d^2(y)$ as a function of mean coordinate of soliton pattern $x(k|\tau|\mu)\equiv y$ can be presented in the form

$$d^2(y)=\frac{4\Sigma_{m=-\infty}^{\infty}(m-y)^2\ln[1+\mathrm{sh}^2\mu\,\mathrm{sech}^2\,\mu(m-y)]}{\Sigma_{m=-\infty}^{\infty}\ln[1+\mathrm{sh}^2\mu\,\mathrm{sech}^2\mu(m-y)]}. \tag{A1}$$

Applying the Poisson summation formula[36]

$$\sum_{m=-\infty}^{\infty}V(m)=\sum_{f=-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}\eta\exp(2\pi i f\eta)V(\eta) \tag{A2}$$

to the denominator of (A1) we obtain

$$\sum_{m=-\infty}^{\infty}\ln[1+\mathrm{sh}^2\mu\,\mathrm{sech}^2\,\mu(m-y)]=2\mu \tag{A3}$$

and hence

$$d^2(y)=\frac{2}{\mu}\sum_{m=-\infty}^{\infty}(m-y)^2\ln[1+\mathrm{sh}^2\mu\,\mathrm{sech}^2\,\mu(m-y)]. \tag{A4}$$

From this expression we see clearly that both $d^2(-y)$ and $d^2(y\pm1)$ coincide with $d^2(y)$, i.e., $d^2(y)$ is an even periodic function of its argument with the period equal to unity or the same to the lattice constant. Another confirmation of this statement follows from an alternative expression

$$d^2(y)=\frac{2}{3}\left[1+\frac{1}{2}(\pi/\mu)^2\right]-\frac{4}{\mu}\sum_{f=1}^{\infty}\frac{\cos(2\pi fy)}{f\,\mathrm{sh}(\pi^2 f/\mu)} \tag{A5}$$

obtainable within the framework of Poisson summation formula (A2).

Formula (A5) allows us to detect at least two sets of extremums, namely at $y=\ldots,-2,-1,0,+1,+2,\ldots$ and at $y=\ldots,-3/2,-1/2,+1/2,+3/2,\ldots$ corresponding to the location of the soliton center on a lattice site and precisely between two neighboring lattice sites, respectively. All of the extremums in a particular set are physically equivalent due to periodicity of $d^2(y)$. Hence we can restrict ourselves to the interval $-1/2\leqslant y\leqslant+1/2$. Evidently $d^2(0)<d^2(\pm1/2)$ and moreover $d^2(0)$ is seen to be the smallest possible value of $d^2(y)$. As to the value $d^2(\pm1/2)$ we claim it to be an absolute maximum of $d^2(y)$ relying on the direct computer simulations with the formula (A4) as well as on the analytical estimations by formula (A4) at $\mu\gg1$ and by formula (A5) at $\mu\ll1$.

For the sake of convenience we will write down here one more result of summation

$$\sum_{m=-\infty}^{\infty}m\ln[1+\mathrm{sh}^2\mu\,\mathrm{sech}^2\,\mu(m-y)]=2\mu y, \tag{A6}$$

which along with formula (A3) becomes useful in calculating the mean coordinate of soliton pattern (114).

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Piezoelectricity and Piezomagnetism: Duality in two-dimensional checkerboards

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The duality approach in two-dimensional two-component regular checkerboards is extended to piezoelectricity and piezomagnetism. The relation between the effective piezoelectric and piezomagnetic moduli is found for a checkerboard with the $p6'mm'$-plane symmetry group (*dichromatic triangle*). © *2002 American Institute of Physics.* [DOI: 10.1063/1.1466881]

I. INTRODUCTION

A duality transformation for two-dimensional (2D) heterogeneous composites was discovered by Keller[1] and Dykhne.[2] It is based upon the simple observation that any 2D divergence-free vector field, when rotated locally at each point by 90° becomes curl free and vice versa. This leads to duality relations for the effective physical properties of 2D two-component composites, like electrical conductivity $\hat{\sigma}_{\mathsf{ef}}$, thermal conductivity $\hat{\kappa}_{\mathsf{ef}}$, and other second rank symmetric tensors $\hat{\upsilon}_{\mathsf{ef}}$. All these physical problems can be described by the same set of equations

$$\mathbf{Y}=\hat{\upsilon}\cdot\mathbf{X}, \quad \nabla\cdot\mathbf{Y}=\nabla\times\mathbf{X}=0, \quad \hat{\upsilon}_{ij}=\hat{\upsilon}_{ji}. \tag{1}$$

The duality relations are universal[3] and do not depend on composite's microstructure. For nonisotropic structures they become[2,4]

$$\det\hat{\upsilon}_{\mathsf{ef}}=\sqrt{\det\hat{\upsilon}_{\mathsf{a}}\cdot\det\hat{\upsilon}_{\mathsf{b}}}, \tag{2}$$

where subscripts ''a'' and ''b'' correspond to the a and b components of composite, respectively, while ''ef'' denotes an effective medium.

The further attempts[5] to extend the dual symmetry onto 2D elasticity

$$\mathbf{u}^{ij}=\hat{\mathcal{K}}^{ij}_{kl}\cdot\tau_{kl}, \quad \sum_j \partial_j\tau_{ij}=0, \tag{3}$$

$$\partial^2_{yy}u^{xx}+\partial^2_{xx}u^{yy}=2\ \partial^2_{xy}u^{xy} \tag{4}$$

had shown no duality transformation for the strain $\mathbf{u}^{ij}$ and the stress $\hat{\tau}_{kl}$ tensor fields. Therefore, one cannot write a duality relation for the fourth rank compliance tensor $\hat{\mathcal{K}}^{ij}_{kl}$.

In this paper we consider physical phenomena which one can describe using the third rank tensors when a high symmetry of 2D two-component checkerboard makes it possible to exploit the duality transformation. The best known phenomena are the piezoelectricity and the piezomagnetism.

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II. DUALITY RELATIONS

Let us consider a homogeneous 2D medium under mechanical stress $\hat{\tau}$, which produces a dielectric displacement **D** and a magnetic induction **B**,

$$D^i=\hat{e}^i_{jk}\cdot\tau_{jk},\quad B^i=\hat{m}^i_{jk}\cdot\tau_{jk},\quad \tau_{jk}=\tau_{kj},$$
$$\nabla\cdot\mathbf{D}=\nabla\cdot\mathbf{B}=0,\quad \sum_j \partial_j\tau_{ij}=0. \tag{5}$$

The piezoelectric $\hat{e}^i_{jk}$ and the piezomagnetic $\hat{m}^i_{jk}$ coefficients are polar and axial tensors of the rank three, respectively,

$$\hat{e}^i_{jk}=\hat{e}^i_{kj},\quad \hat{m}^i_{jk}=\hat{m}^i_{kj}.$$

In order to represent this problem in a form similar to (1) we define the following vectors:

$$\mathbf{t}_1=(\tau_{xx},\tau_{xy}),\quad \mathbf{t}_2=(\tau_{yx},\tau_{yy}),\quad \nabla\cdot\mathbf{t}_k=0, \tag{6}$$

that simplifies (5)

$$\mathbf{D}=\hat{g}_{11}\cdot\mathbf{t}_1+\hat{g}_{12}\cdot\mathbf{t}_2,\quad \mathbf{B}=\hat{g}_{21}\cdot\mathbf{t}_1+\hat{g}_{22}\cdot\mathbf{t}_2. \tag{7}$$

It is convenient to represent each of the tensors $\hat{e}^i_{jk}$, $\hat{m}^i_{jk}$ by two nonsymmetric tensors of the second rank

$$\hat{g}_{11}=\begin{pmatrix} e^x_{xx} & e^x_{xy}\\ e^y_{xx} & e^y_{xy}\end{pmatrix},\quad \hat{g}_{12}=\begin{pmatrix} e^x_{yx} & e^x_{yy}\\ e^y_{yx} & e^y_{yy}\end{pmatrix},$$
$$\hat{g}_{21}=\begin{pmatrix} m^x_{xx} & m^x_{xy}\\ m^y_{xx} & m^y_{xy}\end{pmatrix},\quad \hat{g}_{22}=\begin{pmatrix} m^x_{xy} & m^x_{yy}\\ m^y_{xy} & m^y_{yy}\end{pmatrix}. \tag{8}$$

The general case of the inner symmetry allows only six independent piezomoduli of each tensor $\hat{e}^i_{jk}$ and $\hat{m}^i_{jk}$.

Our approach is based on the validity of the matrix identities for a special kind of inner symmetry group G of the transport tensors $\hat{g}_{kl}(G)$:

$$\hat{g}_{11}(G)=\hat{M}\cdot\hat{g}_{21}(G),\quad \hat{g}_{12}(G)=\hat{M}\cdot\hat{g}_{22}(G), \tag{9}$$

where $\hat{M}$ is a nondegenerated 2×2 transform matrix. This point symmetry group G will be specified later.

The relation

$$\mathbf{D}=\hat{M}\cdot\hat{g}_{21}(G)\cdot\mathbf{t}_1+\hat{M}\cdot\hat{g}_{22}(G)\cdot\mathbf{t}_2=\hat{M}\cdot\mathbf{B} \tag{10}$$

makes our problem similar to (1) if we link a divergence-free field **D** and a curl-free field $\hat{\mathcal{R}}\mathbf{B}$,

$$\mathbf{D}=\hat{L}\cdot\hat{\mathcal{R}}\mathbf{B},\quad \hat{L}=\hat{M}\cdot\hat{\mathcal{R}}^{-1},$$
$$\nabla\cdot\mathbf{D}=\nabla\times\hat{\mathcal{R}}\mathbf{B}=0,\quad \hat{\mathcal{R}}=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}. \tag{11}$$

Here $\hat{\mathcal{R}}$ is a 90° rotation operator. Applying the duality transformation to (11) and making use of the relation (2) results in

$$\det \hat{M}_{\mathrm{ef}} = \sqrt{\det \hat{M}_{\mathrm{a}} \cdot \det \hat{M}_{\mathrm{b}}}. \tag{12}$$

III. SYMMETRY CONSIDERATIONS

Let us look for such symmetry group G that makes valid two relations (9), which can be reduced

$$\hat{g}_{11} = \hat{g}_{12} \cdot \hat{g}_{22}^{-1} \cdot \hat{g}_{21}. \tag{13}$$

This should be satisfied not accidentally.

Following Ref. 6 we recall some basic facts about a coexistence of piezoelectric and piezomagnetic properties in anisotropic media. In three-dimensional media there exist 45 Shubnikov point groups permitting both piezoelectricity and piezomagnetism. In general case the forms of $\hat{e}^i_{jk}$ and $\hat{m}^i_{jk}$ coincide[6] only in 20 point groups (9 ferromagnetic and 11 antiferromagnetic). In 2D media these numbers diminish: there are only 4 ferromagnetic point groups 1, m', 3, $3m'$. Let us consider the point group $G=3$ which leaves only two independent piezomoduli of each tensor $\hat{e}^i_{jk}$ and $\hat{m}^i_{jk}$,[7]

$$\begin{aligned} \hat{g}_{11}(3) &= \begin{pmatrix} e_1 & e_2 \\ e_2 & -e_1 \end{pmatrix}, \quad \hat{g}_{12}(3) = \begin{pmatrix} e_2 & -e_1 \\ -e_1 & -e_2 \end{pmatrix}, \\ \hat{g}_{21}(3) &= \begin{pmatrix} m_1 & m_2 \\ m_2 & -m_1 \end{pmatrix}, \quad \hat{g}_{22}(3) = \begin{pmatrix} m_2 & -m_1 \\ -m_1 & -m_2 \end{pmatrix}, \end{aligned} \tag{14}$$

where e_k, m_k are real numbers. It is easy to see that matrices (14) satisfy the requirement (13) and $\hat{M}$ is an antisymmetric positive definite matrix

$$\hat{M} = \frac{1}{m_1^2 + m_2^2} \begin{pmatrix} m_1 e_1 + m_2 e_2 & m_2 e_1 - m_1 e_2 \\ m_1 e_2 - m_2 e_1 & m_1 e_1 + m_2 e_2 \end{pmatrix}. \tag{15}$$

Up to this moment we have not specified a crystallographic type of two-component tessellation of the plane since according to Ref. 3 a duality relation is universal there. Due to Curie principle[8] the point symmetry group G_{ef} of a physical phenomenon in composed medium is a maximal common subgroup of the microstructure group G_{st} and inner symmetry groups G_{a}, G_{b} of this phenomenon in both components "a," "b"

$$G_{\mathrm{ef}} = G_{\mathrm{st}} \cap G_{\mathrm{a}} \cap G_{\mathrm{b}}. \tag{16}$$

We will look for 2D checkerboards with regular *dichromatic* tessellation by polygons that are compatible with point symmetry group $G=3$. From 46 *dichromatic plane mosaics*[9] the only compatible is *dichromatic triangle* which possesses a $p6'mm'$-plane group (Fig. 1). The choice of the three-symmetry is not accidental but is concerned with the special properties of the transport tensors $\hat{g}_{kl}$ in (14), namely,

$$3 = 6'mm' \cap 3 \cap 3.$$

Making use of (12) and (15) after simple algebra we obtain finally

$$\frac{e_{1\mathrm{ef}}^2 + e_{2\mathrm{ef}}^2}{m_{1\mathrm{ef}}^2 + m_{2\mathrm{e}}^2} = \sqrt{\frac{e_{1\mathrm{a}}^2 + e_{2\mathrm{a}}^2}{m_{1\mathrm{a}}^2 + m_{2\mathrm{a}}^2} \cdot \frac{e_{1\mathrm{b}}^2 + e_{2\mathrm{b}}^2}{m_{1\mathrm{b}}^2 + m_{2\mathrm{b}}^2}}. \tag{17}$$

If the inner symmetry G_{a}, G_{b} will be upgraded up to $G=3m'$ we have in (14): $e_2 = m_2 = 0$, and the duality relation (17) looks more simple

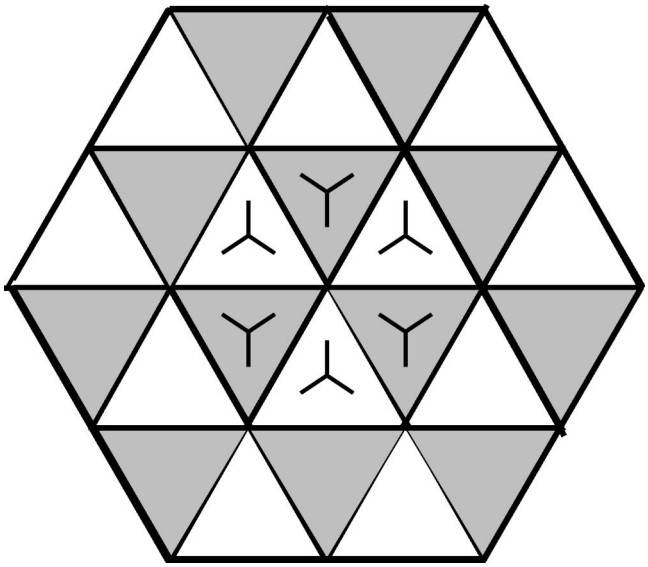

FIG. 1. Dichromatic plane mosaic $G_{\mathrm{st}}p6'mm'$. The principal axes of inner medium symmetry $G_{\mathrm{a}}=G_{\mathrm{b}}=3$ are pointed out within the triangles.

$$\frac{e_{1\mathrm{ef}}^2}{m_{1\mathrm{ef}}^2}=\left|\frac{e_{1\mathrm{a}}}{m_{1\mathrm{a}}}\cdot\frac{e_{1\mathrm{b}}}{m_{1\mathrm{b}}}\right|. \tag{18}$$

Note that Eq. (7) does not permit one to write the duality relations for the piezoelectric $\hat{e}_{jk}^{i}$ and piezomagnetic $\hat{m}_{jk}^{i}$ tensors separately.

IV. CONCLUSION

In the present paper we have considered the coexistence of the piezoelectric and the piezomagnetic phenomena in 2D two-component composites with triangular tessellation of the plane ($p6'mm'$-plane symmetry group). The duality approach for 2D two-component regular composites was extended onto physical problem dealt with third rank tensors.

In the conclusion we will mention some compounds which have a trigonal symmetry and the piezoelectricity and the piezomagnetism coexist.[10] These are the rare-earth maganites having the overall formula $RMnO_3$, where R=Y, Ho, Er, Tm, Yb, Lu, or Sc. The Mn atoms lie inside the bipyramidial bonds, while the rare-earth atoms lie inside the bipyramids.

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A new approach to static force-free electromagnetic fields

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In the early 1950s, Lundquist showed the significance of electromagnetic fields with a vanishing Lorentz force density to magnetohydrostatic fluids. Today, these fields are known as force-free electromagnetic fields. Later that decade, Lüst and Schlüter demonstrated that cosmic magnetic fields are force-free and Chandrasekhar and Kendall then constructed a large class of force-free fields whose electric charge density field is also vanishing. In this article, we constructed force-free fields without assuming that the electric charge density vanishes, and in some cases we established a connection between force-free fields and nonlinear Schrödinger equations. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In his study of magnetohydrostatic fluids in the early 1950s, Lundquist[1] showed the significance of electromagnetic fields with a vanishing Lorentz force density. Such fields are now known as force-free fields. Later, in the mid-1950s Lüst and Schlüter[2] noted that cosmic magnetic fields are force-free. A few years later, Chandrasekhar and Kendall,[3,4] working from the assumption that the electric charge density vanishes, characterized a large class of force-free fields by resolving the magnetic field into its poloidal and toroidal components, and they called these fields *force-free magnetic* fields. In this case, the electric and magnetic terms in the force density are separately equal to zero. For recent work on such fields, the reader should consult Marsh,[5,6] Neukirch and Rastätter,[7] Démoulin, Cuperman, and Semel,[8] and Cuperman, Li, and Semel.[9] Additionally, recent work by MacLeod[10] has characterized force-free magnetic fields by making use of the work of Moses[11] on the eigenfunctions of the curl.

Force-free magnetic fields have many applications to cosmic magnetic fields, magnetic clouds, and magnetohydrodynamics in general.[12–14] Two recent review articles[15,16] discuss the astrophysical significance of force-free magnetic fields; additionally, there is an older review article by Michel.[17] In comparison to force-free magnetic fields, the more general concept of a force-free field has received less attention. Some work on general force-free fields has been done by Chu and Ohkawa,[18,19] who have investigated fields with **E** and **B** parallel. The investigations most closely related to this article are the articles by Osherovich[20,21] and Osherovich and Gliner.[22] The first two of these articles investigates oscillations of cylindrically symmetric force-free fields; the third presents an example of a force-free electromagnetic wave in one space and one time dimension. Central to these three papers is the use of the Poisson bracket to demonstrate a functional dependence. We make extensive use of functional dependency between fields and potentials as well.

The theory of force-free magnetic fields is well developed, but a theory of more general force-free fields is lacking. In this article, we partially fill this gap by introducing techniques for constructing force-free fields with nonvanishing electric charge density and with planar and rotational symmetry. Assuming Gaussian units, the static Maxwell equations are

$$\nabla\cdot\mathbf{B}=0, \quad \nabla\cdot\mathbf{E}=4\pi\rho,$$

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$$\nabla\times\mathbf{B}=\frac{4\pi}{c}\mathbf{J},\quad \nabla\times\mathbf{E}=\mathbf{0}.$$

Specifically, we construct fields for which

$$0=\mathbf{J}\cdot\mathbf{E},\quad \mathbf{0}=\rho\mathbf{E}+\frac{1}{c}\mathbf{J}\times\mathbf{B}.$$

We begin with the observations that when the charge density ρ is nonzero, the second condition implies the first, and further, again when ρ is nonzero, these conditions also imply that $\mathbf{E}$ and $\mathbf{B}$ are perpendicular.

We cover planar symmetry in Sec. II and rotational symmetry in Sec. III. Finally, in Sec. IV, a general result on force-free null fields is given.

II. PLANAR SYMMETRY

In this section, we construct two types of force-free fields with planar symmetry. For the first field, we assume that the magnetic field is parallel to the z axis, and for the second we assume that the electric and magnetic fields are coplanar.

For the first case, we set $\mathbf{E}=-\nabla\Phi$ and $\mathbf{B}=g\mathbf{k}$, where the functions Φ and g are z independent and $\mathbf{k}$ is the standard Cartesian unit vector. The Maxwell equations $\operatorname{div}\mathbf{B}=0$ and $\operatorname{curl}\mathbf{E}=\mathbf{0}$ are satisfied while $\mathbf{J}\cdot\mathbf{E}=0$ implies

$$0=g_y\Phi_x-g_x\Phi_y,$$

where the subscripts indicate partial derivatives. From this we conclude that $\nabla\Phi$ and ∇g are parallel; therefore, Φ and g are functionally dependent. Thus we introduce a function $U:\mathbf{R}^1\rightarrow\mathbf{R}^1$ for which $g=U(\Phi)$. [Here, and throughout this paper, by $U(\Phi)$ we mean the composition of U with Φ.] Using this relation to eliminate g in the expression for the Lorentz force density, we obtain a nonlinear Schrödinger equation for the potential

$$-\Delta\Phi+(UU')(\Phi)=0. \tag{1}$$

The function U is arbitrary; however, if $U(x)=k\sqrt{x^2+c^2}$, where k and c are real constants, Eq. (1) reduces to a Helmholtz equation. In this case, the charge density is proportional to the electric potential.

Assuming Φ is a function of the cylindrical coordinate r only, the solutions to Eq. (1) have a simple representation. Provided $\mathbf{E}$ vanishes toward infinity, the fields are given by

$$\mathbf{E}(r)=\pm\left(g^2(r)+(2/r^2)\int_r^\infty sg^2(s)\mathrm{d}s\right)^{1/2}\mathbf{e}_r,$$

$$\mathbf{B}(r)=g(r)\mathbf{e}_z,$$

where g is any integrable function that vanishes sufficiently rapidly toward infinity and $\mathbf{e}_r$ and $\mathbf{e}_z$ are the usual cylindrical coordinate unit vectors. The electric field diverges like $1/r$ toward the origin. As an example, let

$$g(r)=-\frac{\sigma\exp(-r/\mu)}{\sqrt{2}\pi\mu},$$

where μ and σ are real positive constants. Then

$$\mathbf{E}(r)=\pm\frac{\sigma\sqrt{2\,r^2+2\,\mu r+\mu^2}\,\exp(-r/\mu)}{2\,\pi\mu r}\mathbf{e}_r,$$

$$\mathbf{B}(r)=-\frac{\sigma\exp(-r/\mu)}{\sqrt{2}\,\pi\mu}\mathbf{e}_z.$$

The charge per unit length is $\mp\sigma$.

For the second case, we assume that **E** and **B** are coplanar. To proceed, we introduce an analytic function $u+iv$ and we set **E** and **B** equal to

$$\mathbf{E}=\nabla H(u)=H'(u)\nabla u,\quad \mathbf{B}=g(u,v)\nabla v,$$

where $H:\mathbf{R}^1\to\mathbf{R}^1$. Since $u+iv$ is analytic, $\nabla u\cdot\nabla v=0$; consequently, $\mathbf{E}\cdot\mathbf{B}=0$. Using the fact that the Laplacian of v vanishes, the Maxwell equation $\operatorname{div}\mathbf{B}=0$ implies that the function g depends on u only. Substituting $g(u,v)=U(u)$, where U is an arbitrary function, in the force-free condition yields

$$\rho H'(u)\nabla u+U(u)U'(u)(\nabla u\times\nabla v)\times\nabla v=0. \tag{2}$$

After expanding the vector products and verifying that $\rho=H''(u)\|\nabla u\|^2$, we find that Eq. (2) reduces to a scalar differential equation

$$H'H''-UU'=0.$$

Thus U and H are related by $U^2=H'^2+k$, where k is an integration constant. To generate radially symmetric fields, let $u+iv=\log(x+iy)$. Then

$$\mathbf{E}(r)=h(r)\mathbf{e}_r,\quad \mathbf{B}(r)=\pm\sqrt{h^2(r)+k/r^2}\,\mathbf{e}_\theta,$$

where h is an arbitrary smooth function and k is a constant. Finally, if $k=0$ and assuming integrability, the field satisfies $\mathbf{E}\cdot\mathbf{B}=0$ and $E^2=B^2$; in the terminology of Barut,[23] such a field is known as a null field or a pure radiation field. For additional background on the significance of null fields, the reader may also consult Parrott.[24]

Section III examines rotational symmetry.

III. ROTATIONAL SYMMETRY

We now construct two types of force-free fields that have rotational symmetry. First, we assume the magnetic field is purely azimuthal; and second, we assume that the azimuthal components of the electric and magnetic fields vanish.

For the first case we use circular cylindrical coordinates and we set

$$\mathbf{E}=-\nabla\Phi=-\Phi_r\mathbf{e}_r-\Phi_z\mathbf{e}_z,\quad \mathbf{B}=g\mathbf{e}_\theta,$$

where Φ and g are θ independent. The Maxwell equations $\operatorname{curl}\mathbf{E}=\mathbf{0}$ and $\operatorname{div}\mathbf{B}=0$ are satisfied while the Lorentz force density is zero provided that

$$\Phi_r((r\Phi_r)_r+r\Phi_{zz})=g(rg)_r, \tag{3}$$

$$\Phi_z((r\Phi_r)_r+r\Phi_{zz})=g(rg)_z. \tag{4}$$

Eliminating Φ_{zz} from these equations, we find that

$$(rg)_z\Phi_r=(rg)_r\Phi_z.$$

Thus there is a function $U:\mathbf{R}^1\to\mathbf{R}^1$ for which $rg=U(\Phi)$. Eliminating g from (3) and (4), we derive a single equation for the potential

$$-\Delta\Phi+(U'U)(\Phi)/r^2=0. \tag{5}$$

In general, this is a nonlinear Schrödinger equation with potential $1/r^2$; however, assuming that $U(x)=kx$, where k is a real constant, Eq. (5) reduces to the linear equation

$$\Phi_{rr}+\Phi_r/r+\Phi_{zz}=k^2\Phi/r^2.$$

A general solution of this equation is

$$\Phi(r,z)=r^k\int_{-1}^{1}(1-s^2)^{k-1/2}(A(iz+rs)+B(-iz+rs))\mathrm{d}s,$$

where A and B are arbitrary functions and i is the imaginary unit. Choosing $k=1/2$, $A(x)=i/x^3$, and $B(x)=0$, we find

$$\Phi(r,z)=-\frac{2\sqrt{r}z}{(z^2+r^2)^2}.$$

For the second case, we assume that the azimuthal components of the electric and magnetic fields vanish. In spherical coordinates the fields are given by

$$\mathbf{E}=-\nabla\Phi=-\Phi_r\mathbf{e}_r-\Phi_\theta\mathbf{e}_\theta/r,$$

$$\mathbf{B}=g(\Phi_\theta\mathbf{e}_r/r-\Phi_r\mathbf{e}_\theta)/r\sin\theta,$$

where Φ and g depend only on r and θ and are independent of the azimuthal variable φ. The Maxwell equation $\nabla\cdot\mathbf{B}=0$ implies Φ and g are functionally dependent; thus we define g by $g=U(\Phi)$. We can show that the field is force-free provided that

$$0=\nabla\cdot\left(\frac{U^2-r^2\sin^2\theta}{r^2\sin^2\theta}\nabla\Phi\right)-UU'\|\nabla\Phi\|^2/2\,r^2\sin^2\theta. \tag{6}$$

Given the singularities in Eq. (6), it is not clear that there are solutions that have a well-behaved charge density. Using numerical integration, we will give evidence that suggests that such solutions do exist. A Lagrangian density $\mathcal{L}$ for this equation is

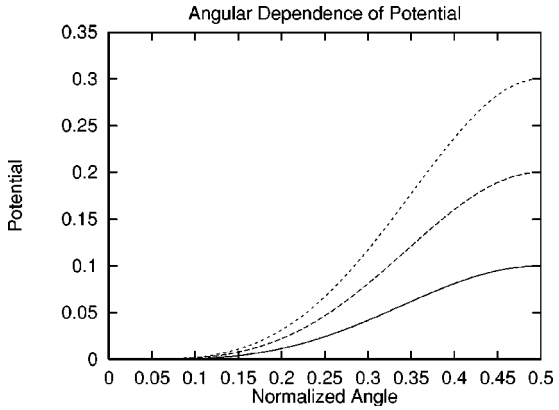

FIG. 1. Angular dependence of the potential ($n=2$) as a function of normalized angle (θ/π) for three initial values of $Q(\pi/2)$.

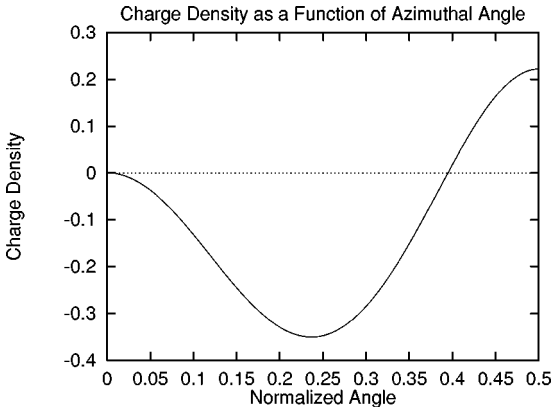

FIG. 2. Charge density ($n=2$) as a function of normalized angle (θ/π) for $Q(\pi/2)=0.1$.

$$\mathcal{L}(\Phi,\nabla\Phi,r)=(U^2-r^2\sin^2\theta)\|\nabla\Phi\|^2/2\,r^2\sin^2\theta.$$

If U is a power function $U(x)=\alpha x^{-1/n}$, where n and α are nonzero real constants, then Eq. (6) has separated variable solutions of the form $\Phi(r,\theta)=Q(\theta)/r^n$. For $n=1$, a solution is

$$\Phi=\sqrt{2}\,\alpha/r\sin\theta.$$

For $n=2$, a series expansion reveals there is a solution that behaves like

$$Q=\theta^4\,(q_0-2q_0\theta^2/3+q_0\,\theta^4/5+\cdots),\quad \theta\to 0,$$

where $q_0\in\mathbf{R}$ is arbitrary. Using numerical integration and initial conditions $Q(\pi/2)=0.1, 0.2$, and 0.3 and $Q'(0)=0$, we get the results shown in Fig. 1. As the series solution suggests, each solution approaches zero toward the poles sufficiently rapidly to make the charge density well behaved there. A graph of the charge density for the case $Q(0)=0.1$ is shown in Fig. 2.

IV. NULL FIELDS

In this section, we give a rule for transforming one force-free null field into another field with the same properties.

Let $\mathbf{E}=-\nabla\Phi$ and $\mathbf{B}$ be force-free and null. Thus $\mathbf{E}\cdot\mathbf{B}=0$ and $\|\mathbf{E}\|=\|\mathbf{B}\|$. Define a new field (the field with a caret) by $\widehat{\mathbf{E}}=\sigma(\Phi)\mathbf{E}$ and $\widehat{\mathbf{B}}=\mu(\Phi)\mathbf{B}$. The field with a caret satisfies $\operatorname{curl}\mathbf{E}=\mathbf{0}$ and $\operatorname{div}\mathbf{B}=0$; further, its Lorentz force density is

$$\hat{\rho}\,\widehat{\mathbf{E}}+\widehat{\mathbf{J}}\times\widehat{\mathbf{B}}=((\mu^2-\sigma^2)\nabla\cdot\mathbf{E}+(\mu\mu'-\sigma\sigma')\|\mathbf{E}\|^2)\mathbf{E}.$$

If $\mu=\pm\sigma$, the field with a caret is force-free and null.

V. CONCLUSION

We have introduced techniques for constructing force-free electromagnetic fields. In a few cases, we established a relation between force-free fields and nonlinear Schrödinger equations.

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Enstrophy dynamics of stochastically forced large-scale geophysical flows

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Enstrophy is an averaged measure of fluid vorticity. This quantity is particularly important in *rotating* geophysical flows. We investigate the dynamical evolution of enstrophy for large-scale quasi-geostrophic flows under random wind forcing. We obtain upper bounds on the enstrophy, as well as results establishing its Hölder continuity and describing the small-time asymptotics. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1459755]

I. INTRODUCTION

Randomness is ubiquitous in fluid systems. Macroscopic partial differential equation models for fluid flows contain such randomness as stochastic forcing, uncertain parameters, random sources, and random boundary conditions.

There has been active recent research on stochastic approaches to geophysical flows[1–5] and numerical simulations of stochastically forced geophysical flows.[6–10] It is generally understood that random fluctuations can have delicate impact on geophysical fluid dynamics.[1,3,6,7,11]

A class of large-scale geophysical flows under random forcing are modeled by the quasi-geostrophic equation:[1]

$$\Delta\psi_t + J(\psi,\Delta\psi) + \beta\psi_x = \nu\Delta^2\psi - r\Delta\psi + \dot{W}, \tag{1}$$

where $\psi(x,y,t)$ is the stream function ($\psi_x := \partial_x\psi$), $\beta \geqslant 0$ is the meridional gradient of the Coriolis parameter, $\nu > 0$ is the viscous dissipation constant, $r > 0$ is the Ekman dissipation constant, and $W(x,y,t)$ is a space–time Wiener process to be defined below on a probability space $(\Omega,\mathcal{A},\mathbb{P})$. Moreover, $J(f,g) = f_x g_y - f_y g_x$ denotes the Jacobian operator. The generalized time derivative $\dot{W}$ models the noisy wind forcing.

Introducing $\omega(x,y,t) = \Delta\psi(x,y,t)$, Eq. (1) can be rewritten in the form

$$\omega_t + J(\psi,\omega) + \beta\psi_x = \nu\Delta\omega - r\omega + \dot{W}, \tag{2}$$

where $(x,y) \in D$ and $D \subset \mathbb{R}^2$ denotes a bounded domain with sufficiently smooth boundary. The boundary conditions are no normal flow ($\psi = 0$ on ∂D) and free-slip ($\omega = 0$ on ∂D) as in Pedlosky (Ref. 12, p. 34) or in Dymnikov and Kazantsev:[13]

$$\psi = \omega = 0 \text{ on } \partial D. \tag{3}$$

An appropriate initial condition $\omega(0)$ is also imposed.

The mean enstrophy for a fluid flow is half the squared mean-square norm of the vorticity,[14,15] i.e., we have

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$$\mathrm{Ens}(t)=\frac{1}{2}\cdot\mathbb{E}\int_D|\omega(x,y,t)|^2d(x,y).$$

The enstrophy $\mathrm{Ens}(t)$ is an averaged measure of fluid vorticity $\omega(t)$. In this article, we discuss the time evolution of the enstrophy. We present results which establish upper bounds on the enstrophy, as well as results on Hölder continuity and small-time asymptotics for $\mathrm{Ens}(t)$. These results are contained in Secs. III, IV, and V, respectively. The mathematical framework for our discussion is described in Sec. II.

II. MATHEMATICAL FRAMEWORK

As it stands, the stochastic quasi-geostrophic equation (2) still has to be given a mathematically precise meaning. This can be accomplished using the framework of stochastic partial differential equations, as described, for example, in Ref. 16. In our situation, we formally rewrite (2) in the Ito formulation

$$d\omega=(\nu\Delta\omega-r\omega-\beta\psi_x-J(\psi,\omega))dt+dW. \tag{4}$$

In the following we use the abbreviations $L^2=L^2(D)$, $L^\infty=L^\infty(D)$, $H_0^k=H_0^k(D)$, $H^k=H^k(D)$, $0<k<\infty$, for the standard Sobolev spaces. Let $\langle\cdot,\cdot\rangle$ and $\|\cdot\|$ denote the standard scalar product and norm in L^2, respectively. Moreover, the norms for H_0^k and L^∞ are denoted by $\|\cdot\|_{H^k}$ and $\|\cdot\|_\infty$, respectively. Due to the Poincaré inequality (Ref. 17 p. 164), the expression $\|\Delta\cdot\|$ is an equivalent norm for H_0^2. It is well-known that the operator $A=\nu\Delta:L^2\to L^2$ with domain $D(A)=H^2\cap H_0^1$ is self-adjoint. Note that A generates an analytic semigroup $S(t)$ on L^2.[18] The spectrum of A consists of eigenvalues $0>\lambda_1>\lambda_2\geqslant\lambda_3\geqslant\cdots$ with corresponding normalized eigenfunctions φ_1, $\varphi_2,\ldots$. The set of these eigenfunctions is complete in L^2. For example, for the square domain $D=(0,1)\times(0,1)$ the eigenvalues are given by $-\nu(m^2+n^2)\pi^2$ for $m,n\in\mathbb{N}$, and the associated eigenfunctions are suitable multiples of $\sin(m\pi x)\sin(n\pi y)$.

Now we can define an appropriate class of Wiener processes W. Let β_k, $k\in\mathbb{N}$, denote a family of independent real-valued standard Brownian motions. Furthermore, choose positive constants μ_k, $k\in\mathbb{N}$, such that

$$\sum_{k=1}^{\infty}\frac{\mu_k^2}{|\lambda_k|^{1-\theta}}<\infty \tag{5}$$

for some $0<\theta<1$. Then we consider the Wiener process W defined by

$$W(t):=\sum_{k=1}^{\infty}\mu_k\cdot\beta_k(t)\cdot\varphi_k,\quad t\geqslant 0. \tag{6}$$

Note that we explicitly allow Wiener processes W whose covariance operator is not of trace class, i.e., for which $\Sigma_{k=1}^{\infty}\mu_k^2=\infty$.

For the domain D we basically assume that the eigenfunctions φ_k of A satisfy

$$\begin{gathered}\varphi_k\in C_0(\overline{D}),\quad |\varphi_k(x,y)|\leqslant C,\\ |\nabla\varphi_k(x,y)|\leqslant C\sqrt{|\lambda_k|},\end{gathered} \tag{7}$$

for all $(x,y)\in D$ and $k\in\mathbb{N}$, where $C>0$ denotes a constant which depends only on D. Domains D which satisfy these conditions include rectangular domains, as well as equilateral triangles. Unfortunately, there are many domains for which they are violated. See, for example, Ref. 19. However, in this paper it is conjectured that in (7) one generally should expect an upper bound which is logarithmic in $|\lambda_k|$. Even though our results remain valid in this situation, we will assume the above stronger condition.

Under the above assumptions, Theorem 5.2.9 in Ref. 20 guarantees that the stochastic convolution

$$W_A(t)=\int_0^t S(t-s)dW(s), \quad t>0, \tag{8}$$

has a continuous version with values in $C_0(D)$, the Banach space of continuous functions satisfying zero Dirichlet boundary conditions on D. To be more precise, W_A has a version which is even Hölder continuous with some small exponent, which depends on the asymptotic behavior of the coefficients μ_k.

If we define the nonlinear operator F by $F(\omega)=-r\omega-\beta\psi_x-J(\psi,\omega)$, then (4) can be rewritten as the abstract evolution equation together with initial condition

$$\begin{aligned} d\omega&=(A\omega+F(\omega))dt+dW,\\ \omega(0)&=\omega_0. \end{aligned} \tag{9}$$

For technical reasons we translate the operator A by a suitable multiple of the identity. Consider a constant $\alpha\geqslant 0$ which will be chosen later on, usually sufficiently large. Defining $A_\alpha := A-\alpha I$, we get the initial value problem

$$\begin{aligned} d\omega&=(A_\alpha\omega+F(\omega)+\alpha\omega)dt+dW,\\ \omega(0)&=\omega_0 \end{aligned}$$

or in mild (integral) form

$$\omega(t)=S_\alpha(t)\omega_0+\int_0^t S_\alpha(t-s)(F(\omega(s))+\alpha\omega(s))ds+W_{A_\alpha}(t), \tag{10}$$

where the analytic semigroup S_α is given by $S_\alpha(t)=e^{-t\alpha}\cdot S(t)$ for $t>0$ and the stochastic convolution $W_{A_\alpha}(t)$ is defined as in (8) with the semigroup S replaced by S_α. Finally, let $U:=\omega-W_{A_\alpha}$. Then U is the weak solution of

$$\begin{aligned} \partial_t U&=AU+F(U+V)+\alpha V,\\ U(0)&=\omega_0, \end{aligned}$$

where we use the abbreviation $V:=W_{A_\alpha}$. Notice that both U and V depend on α.

III. ENSTROPHY ESTIMATE: UPPER BOUNDS

We begin by establishing upper bounds on the time evolution of the enstrophy $\mathrm{Ens}(t)=\mathbb{E}\|\omega(t)\|^2/2$. Improving the *a priori* estimate of Ref. 5 Sec. 3, we obtain

$$\begin{aligned} \frac{1}{2}\cdot\frac{d}{dt}\|U(t)\|^2 \leqslant{}& \|\nabla U(t)\|^2\cdot(\varepsilon-\nu)\\ &+\|U(t)\|^2\cdot((\varepsilon-r+c_1\beta)+C\cdot\|V\|_\infty\cdot(1+C_\varepsilon\cdot\|V\|_\infty))\\ &+C_\varepsilon\cdot(r+\beta+\alpha^2)\cdot\|V\|_\infty^2+C\cdot\|V\|_\infty^3+C_\varepsilon\cdot\|V\|_\infty^4, \end{aligned} \tag{11}$$

where C denotes a generic constant which depends only on D, and whose specific value may change from line to line. Similarly, C_ε denotes a generic constant which depends only on D and

ε, where $\varepsilon>0$ is some arbitrarily small number. The constant c_1 denotes the optimal constant in the Poincare inequality $\|U\|\leqslant c_1\|\nabla U\|$ for mean zero functions U. For $\varepsilon<\nu$ the improved *a priori* estimate immediately yields the following lemma.

Lemma 1: For any $\gamma>-\nu\cdot c_1^{-2}-r+c_1\cdot\beta$ there exist constants depending only on γ, D, β, and r which are all denoted by C such that

$$\frac{d}{dt}\|U(t)\|^2\leqslant A(t)\|U(t)\|^2+B(t),\quad t\geqslant 0, \tag{12}$$

with

$$\begin{aligned} A(t)&=2\gamma+C\cdot(\|V\|_\infty+\|V\|_\infty^2),\\ B(t)&=C\cdot((1+\alpha^2)\cdot\|V\|_\infty^2+\|V\|_\infty^4)>0. \end{aligned} \tag{13}$$

Together with Theorem I.6.1 in Ref. 21 this yields

$$\|U(t)\|^2\leqslant\|\omega_0\|^2\cdot e^{\int_0^t A(s)ds}+\int_0^t B(s)e^{\int_s^t A(\tau)d\tau}ds,\quad t\geqslant 0. \tag{14}$$

Suppose for simplicity that ω_0 and W are stochastically independent. It is possible to drop this assumption in this section, but in this case we additionally need $\mathbb{E}\|\omega_0\|^{2+\delta}<\infty$ for some small $\delta>0$.

The critical term for taking the expectation in (14) is the squared L^∞-norm of $V=W_{A_\alpha}$ in the exponent, which is in general not finite. To complicate matters further, the L^∞-norm in the exponent cannot easily be dealt with, since we do not have a Hilbert space structure.

For our situation we will improve on some ideas of Ref. 22. Using Fernique's Theorem (Ref. 16, Theorem 2.6) we get that $\mathbb{P}(t\|V(\tau)\|_\infty^2>r^2)\leqslant 1/(1+e^{1+32\lambda r^2})$ implies $\mathbb{E}(e^{\lambda t\|V(\tau)\|_\infty^2})\leqslant e^{16\lambda r^2}+e^2/(e^2-1)$ for any $t,\tau,r,\lambda>0$. Hence, by Jensen's inequality

$$\mathbb{E}(e^{\lambda\int_0^t\|V(\tau)\|_\infty^2 d\tau})\leqslant\frac{1}{t}\cdot\int_0^t\mathbb{E}(e^{\lambda t\|V(\tau)\|_\infty^2})d\tau\leqslant C_\lambda,$$

provided $\mathbb{P}(t\|V(\tau)\|_\infty^2>1)\leqslant 1/(1+e^{1+32\lambda})$ for any $\tau\leqslant t$. The latter inequality follows immediately from Chebychev's inequality, provided we have

$$t\cdot\mathbb{E}\|V(\tau)\|_\infty^2\leqslant\frac{1}{1+e^{1+32\lambda}} \tag{15}$$

for any $\tau\leqslant t$. The following lemma is proven similarly as Ref. 16, Theorem 5.20.

Lemma 2: For any $p\geqslant 1$ and any sufficiently small $\theta>0$ there exists a constant C which depends only on p, θ, and D such that for any $\tau\geqslant 0$

$$\mathbb{E}\|V(\tau)\|_\infty^{2p}\leqslant C\cdot\underbrace{\left(\sum_{k=1}^\infty\frac{\mu_k^2}{\alpha-\lambda_k}\cdot|\lambda_k|^\theta\right)^p}_{=:\varphi(\alpha)^p}. \tag{16}$$

We remark that the assumption (7) on the eigenfunctions is essential for the proof of this lemma. Notice also that the series in (16) is finite according to (5). Lemma 2 implies that (15) is satisfied for any $t\leqslant C/\varphi(\alpha)$. It is now straightforward to verify that

$$\mathbb{E}e^{m\int_s^t A(\tau)d\tau}\leqslant C\cdot e^{m(t-s)2\gamma}$$

for any $s \leqslant t \leqslant C/\varphi(\alpha)$ and $m=1,2$, where γ and $A(t)$ were defined in Lemma 1. Moreover, Lemma 2 implies for $B(t)$ in (13)

$$(\mathbb{E}B(t)^2)^{1/2} \leqslant C \cdot ((1+\alpha^2)\cdot\varphi(\alpha)+\varphi(\alpha)^2)$$

for any $t>0$. We finally obtain from (14) that

$$\begin{aligned}\mathbb{E}\|U(t)\|^2 &\leqslant \mathbb{E}\left(\|\omega_0\|^2 \cdot e^{\int_0^t A(s)ds} + \int_0^t B(s) e^{\int_s^t A(\tau)d\tau} ds \right) \\ &\leqslant \mathbb{E}\|\omega_0\|^2 \cdot \mathbb{E}e^{\int_0^t A(s)ds} + \int_0^t (\mathbb{E}B(s)^2)^{1/2} (\mathbb{E}e^{2\int_s^t A(\tau)d\tau})^{1/2} ds \\ &\leqslant C \cdot \mathbb{E}\|\omega_0\|^2 \cdot e^{2\gamma t} + C\cdot((1+\alpha^2)\cdot\varphi(\alpha)+\varphi(\alpha)^2)\cdot \int_0^t e^{2\gamma\tau} d\tau \end{aligned} \tag{17}$$

for any $t \leqslant C/\varphi(\alpha)$. Using $\mathbb{E}\|\omega\|^2 \leqslant 2\mathbb{E}\|U\|^2 + 2\mathbb{E}\|V\|^2$, this immediately implies the following theorem on upper bounds for the enstrophy.

Theorem 1 (upper bound): *Suppose that ω_0 and W are stochastically independent and that $\mathbb{E}\|\omega_0\|^2 < \infty$. Moreover, let $\gamma > -\nu \cdot c_1^{-2} - r + c_1 \cdot \beta$. Then* $\mathrm{Ens} \in L^\infty([0,T])$ *for any $T>0$. More precisely,*

$$\begin{aligned}\mathrm{Ens}(t) &\leqslant C \cdot \mathbb{E}\|\omega_0\|^2 \cdot e^{2\gamma t} + C\cdot\varphi(\alpha) \\ &\quad + C\cdot((1+\alpha^2)\cdot\varphi(\alpha)+\varphi(\alpha)^2)\cdot\int_0^t e^{2\gamma\tau} d\tau\end{aligned}$$

for any $t \leqslant C/\varphi(\alpha)$, with constants C independent of t, α, and ω_0.

Remark 1: It can be shown that for any choice of $p \geqslant 1$ similar bounds hold for $\mathbb{E}\sup_{\tau\in[0,t]}\|U(\tau)\|^{2p}$, provided both $\mathbb{E}\|\omega_0\|^{2p} < \infty$ and $t \leqslant C/\varphi(\alpha)$.

Moreover, all bounds on $\mathbb{E}\|U(t)\|^{2p}$ or $\mathbb{E}\sup_{\tau\in[0,t]}\|U(\tau)\|^{2p}$ immediately imply analogous bounds on $\mathrm{Ens}(t)$ *or $\mathbb{E}\sup_{\tau\in[0,t]}\|\omega(\tau)\|^{2p}$. For this one has to employ estimates for $\mathbb{E}\sup_{\tau\in[0,t]}\|W_{A_\alpha}(\tau)\|^{2p}$ which can be obtained for example as in Ref. 23, Corollary 2.3.*

In order to obtain a bound for $t\to\infty$, we note that for $\alpha\to\infty$ one obviously has $\varphi(\alpha)\to 0$. However, the rate of convergence is essential. To this end, we distinguish two cases. If we suppose that $\Sigma_{k=1}^\infty \mu_k^2 \cdot |\lambda_k|^\theta < \infty$ for some $\theta > 0$, then the estimate $\varphi(\alpha) \leqslant \Sigma_{k=1}^\infty \mu_k^2 \cdot |\lambda_k|^\theta/\alpha$ is immediate—and choosing α proportional to t in Theorem 1 furnishes

$$\mathrm{Ens}\,(t) \leqslant C\cdot\left(\mathbb{E}\|\omega_0\|^2 \cdot e^{2\gamma t} + t\cdot\int_0^t e^{2\gamma\tau} d\tau + 1 \right) \quad \text{for all } \ t \geqslant 0.$$

If, on the other hand, $\Sigma_{k=1}^\infty \mu_k^2 \cdot |\lambda_k|^\theta = \infty$, we additionally assume $\mu_k^2 \leqslant C k^{-\mu}$ for some $\mu \in (\theta, 1]$, with arbitrarily small θ defined in Lemma 2. (For $\mu > 1$ we can always find some small θ such that the first case applies.) Using the fact that $|\lambda_k| \sim Ck$ for $k\to\infty$ (cf. Ref. 24) we obtain

$$\begin{aligned}\varphi(\alpha) &\leqslant C\cdot\sum_{k=1}^\infty \frac{k^{-\mu}}{ck+\alpha}\cdot k^\theta \leqslant C\cdot\int_0^\infty \frac{k^{\theta-\mu}}{ck+\alpha} dk \\ &= C\cdot\alpha^{\theta-\mu}\cdot\int_0^\infty \frac{\tau^{\theta-\mu}}{c\tau+1} d\tau.\end{aligned}$$

Choosing $\alpha^{\mu-\theta}$ proportional to t in Theorem 1, we derive

$$\mathrm{Ens}(t) \leqslant C\cdot\left(\mathbb{E}\|\omega_0\|^2 \cdot e^{2\gamma t} + t^{2/(\mu-\theta)-1}\cdot\int_0^t e^{2\gamma\tau} d\tau + 1 \right) \quad \text{for all} \quad t \geqslant 0.$$

Notice that $2/(\mu-\theta)-1>1$. We have proved the following result.

Theorem 2 (global upper bound): *Assume again that ω_0 and W are stochastically independent, that $\mathbb{E}\|\omega_0\|^2<\infty$, and let $\gamma>-\nu\cdot c_1^{-2}-r+c_1\cdot\beta$. Then the following holds.*

(a) If $\mu_k^2\leqslant Ck^{-\mu}$ for some $\mu\in(0,1]$, we can find a $\tilde{\mu}\in(0,\mu)$ such that

$$\mathrm{Ens}(t)\leqslant C\cdot\left(\mathbb{E}\|\omega_0\|^2\cdot e^{2\gamma t}+t^{(2-\tilde{\mu})/\tilde{\mu}}\cdot\int_0^t e^{2\gamma\tau}d\tau+1\right)\quad \text{for all } t\geqslant 0.$$

(b) If $\Sigma_{k=1}^{\infty}\mu_k^2\cdot|\lambda_k|^{\theta}<\infty$ for some $\theta>0$, then

$$\mathrm{Ens}(t)\leqslant C\cdot\left(\mathbb{E}\|\omega_0\|^2\cdot e^{2\gamma t}+t\cdot\int_0^t e^{2\gamma\tau}d\tau+1\right)\quad \text{for all } t\geqslant 0.$$

The constants C are independent of t and ω_0, but they can depend on θ, γ, μ, $\tilde{\mu}$, the domain D, or the coefficients in (1).

Remark 2: If $-\nu\cdot c_1^{-2}-r+c_1\cdot\beta\geqslant 0$, then necessarily $\gamma>0$. In this case we obtain an exponentially growing upper bound for $\mathrm{Ens}(t)$ *with growth rate slightly larger than $-\nu\cdot c_1^{-2}-r+c_1\cdot\beta$.*

If, on the other hand, $-\nu\cdot c_1^{-2}-r+c_1\cdot\beta<0$, then we can choose $\gamma<0$. This furnishes a polynomial upper bound which grows at least linearly in time. The precise growth exponent is determined by the regularity of the noise.

Remark 3: As we already stated in the beginning of this section, one can remove the condition of stochastic independence of ω_0 and W in the previous theorem, if one additionally assumes $\mathbb{E}\|\omega_0\|^{2+\delta}<\infty$ for some small δ.

Our above results hold for a large class of noise processes, in particular also for more irregular Wiener processes W whose covariance operator is not of trace class. If, however, one assumes that the Wiener process is of trace class, i.e., if $\mathrm{Tr}(Q)=\Sigma_{k=1}^{\infty}\mu_k^2<\infty$, then the results can be improved significantly by employing Ito's formula. One advantage of this approach is that it avoids the conditions on the eigenfunction in (7). Therefore, we will briefly outline the main ideas.

By applying Ito's formula (Ref. 16, Sec. 4.5) to the squared L^2-norm of the vorticity $\omega(t)$, it can easily be verified that

$$\mathbb{E}\|\omega(t)\|^2=2\,\mathbb{E}\int_0^t\langle A\omega(\tau)+F(\omega(\tau)),\omega(\tau)\rangle d\tau+\mathrm{Tr}(Q)\cdot t,$$

where $\mathrm{Tr}(Q)=\Sigma_{k=1}^{\infty}\mu_k^2$ denotes the trace of the covariance operator Q of W. Using calculations analogous to the ones leading to the *a priori* estimate in Lemma 1, we formally obtain

$$\begin{aligned}\partial_t\mathbb{E}\|\omega(t)\|^2&=2\,\mathbb{E}\langle A\omega(\tau)+F(\omega(\tau)),\omega(\tau)\rangle+\mathrm{Tr}(Q)\\&\leqslant 2\gamma\cdot\mathbb{E}\|\omega(t)\|^2+\mathrm{Tr}(Q),\end{aligned}$$

where $\gamma>-\nu\cdot c_1^{-2}-r+c_1\cdot\beta$ as in Lemma 1. Hence, for any $t\geqslant 0$ we have

$$\mathrm{Ens}(t)\leqslant\mathrm{Ens}(0)\cdot e^{2\gamma\cdot t}+\mathrm{Tr}(Q)\cdot\frac{e^{2\gamma\cdot t}-1}{4\gamma}.\tag{18}$$

Especially if one can choose a growth exponent $\gamma<0$, this significantly improves the estimates of Theorem 2, since in this case the right-hand side of (18) approaches $-\mathrm{Tr}(Q)/(4\gamma)$ for $t\to\infty$.

IV. ENSTROPHY ESTIMATE: HÖLDER CONTINUITY

In this section we establish regularity properties of the enstrophy as a function of time. More precisely, we will prove that $\mathrm{Ens}(t)=\mathbb{E}\|\omega(t)\|^2/2$ is Hölder continuous. To this end, we need the following lemma from Ref. 5

Lemma 3: Define a nonlinear mapping $\mathcal{F}: C([0,T];H_0^1) \to C([0,T];L^2)$ *by*

$$(\mathcal{F}(\omega))(t) := \int_0^t S(t-s)F(\omega(s))ds, \quad \text{for} \quad t \in [0,T],$$

where $\omega \in C([0,T];H_0^1)$, *and* A *and* F *are as in* (9). *Then* $\mathcal{F}$ *is continuous, and it can be extended to a continuous mapping from the space* $C([0,T];L^2)$ *to* $C([0,T];L^2)$. *Furthermore, the image of the extended mapping* $\mathcal{F}$ *is contained in* $C([0,T],H^a(D))$ *for* $0 \leqslant a < \frac{1}{2}$.

In fact, it is shown in Ref. 5 that for arbitrary positive constants $a \in [0,\frac{1}{4})$ and $\rho \in (0,\frac{1}{4})$ satisfying $0 < \rho + a < \frac{1}{4}$ the estimate

$$\begin{aligned}\left\| (-A)^a \int_0^t S(t-s)F(\omega(s))ds \right\| &\leqslant \frac{rc+\beta c}{1-a} \cdot t^{1-a} \cdot \sup_{0\leqslant s\leqslant t} \|\omega(s)\| \\ &\quad + \left(\frac{8c}{1-4\rho-4a} \cdot t^{1/4-\rho-a} + \frac{4c}{1-2\rho-2a} \cdot t^{1/2-\rho-a} \right) \cdot \sup_{0\leqslant s\leqslant t} \|\omega(s)\|^2\end{aligned}$$

holds. Especially for $a = 0$ we obtain

$$\begin{aligned}\|\mathcal{F}(\omega)(t)\| = \left\| \int_0^t S(t-s)F(\omega(s))ds \right\| &\leqslant (rc+\beta c) \cdot t \cdot \sup_{0\leqslant s\leqslant t} \|\omega(s)\| \\ &\quad + \left(\frac{8c}{1-4\rho} \cdot t^{1/4-\rho} + \frac{4c}{1-2\rho} \cdot t^{1/2-\rho} \right) \cdot \sup_{0\leqslant s\leqslant t} \|\omega(s)\|^2,\end{aligned}$$

for every $0 < \rho < \frac{1}{4}$. Together with Theorem 1 and Remark 1 these bounds immediately furnish the following result.

Lemma 4: Suppose that ω_0 *and* W *are stochastically independent and that for some* $p \geqslant 1$ *we have* $\mathbb{E}\|\omega_0\|^{2p} < \infty$. *Moreover, let* $T > 0$ *be arbitrary, and let* $a \in [0,\frac{1}{4})$ *and* $\rho \in (0,\frac{1}{4})$ *be such that* $0 < \rho + a < \frac{1}{4}$. *Then there exists a constant* C *such that*

$$\mathbb{E}\|(-A)^a \mathcal{F}(\omega)(t)\|^p \leqslant C \cdot t^{p\cdot(1/4-\rho-a)} \quad \textit{for all} \quad t \in [0,T].$$

The following theorem states our main result on the regularity of the enstrophy. It will be proved in the remainder of this section.

Theorem 3 (Hölder continuity): *Suppose that* ω_0 *and* W *are stochastically independent and that* $\mathbb{E}\|\omega_0\|^4 < \infty$. *Then the enstrophy* $\mathrm{Ens}(\cdot)$ *defined by* $\mathrm{Ens}(t) = \mathbb{E}\|\omega(t)\|^2/2$ *is Hölder continuous with arbitrary exponent less than* $\frac{1}{4}$ *on every compact interval in* $(0,\infty)$.

Remark 4: Note that in general we cannot expect the solution ω *to be Hölder continuous with arbitrary exponent less than* $\frac{1}{4}$, *since* W_A *is in general less regular. As one can see from (10) with* $\alpha = 0$, *one cannot expect* ω *to be more regular than* W_A.

To prove the above theorem establishing the Hölder continuity of the enstrophy, we first define

$$\mathcal{G}(\omega)(t) := S(t)\omega_0 + \mathcal{F}(\omega)(t). \tag{19}$$

According to (10) for $\alpha = 0$, we therefore have $\omega(t) = \mathcal{G}(\omega)(t) + W_A(t)$. Consider a fixed interval $J = [\varepsilon, T] \subset (0,\infty)$. For $t \in J$ and h with $t + h \in J$ the identity (10) then implies

$$\begin{aligned}\mathbb{E}\|\omega(t+h)\|^2-\mathbb{E}\|\omega(t)\|^2&=\mathbb{E}\|\mathcal{G}(\omega)(t+h)+W_A(t+h)\|^2-\mathbb{E}\|\mathcal{G}(\omega)(t)+W_A(t)\|^2\\&=\mathbb{E}\|\mathcal{G}(\omega)(t+h)\|^2-\mathbb{E}\|\mathcal{G}(\omega)(t)\|^2+2\mathbb{E}\langle\mathcal{G}(\omega)(t+h),W_A(t+h)\rangle\\&\quad-2\mathbb{E}\langle\mathcal{G}(\omega)(t),W_A(t)\rangle+\mathbb{E}\|W_A(t+h)\|^2-\mathbb{E}\|W_A(t)\|^2\\&=:D_1+2D_2+D_3.\end{aligned}$$

For simplicity we assume $h>0$ in the following. The case $h<0$ can be treated analogously.

We begin by estimating D_3. Due to Ref. 25 one has $\mathbb{E}\|W_A(\cdot)\|^2\in C^\infty(0,\infty)$. Hence, $|D_3|\leqslant C\cdot h$ for some constant $C>0$.

In order to estimate D_2, we define the shift-operator τ_t by $\tau_t\omega=\omega(t+\cdot)$ for $t>0$. Then the definitions of $\mathcal{G}$ and $\mathcal{F}$ in (19) and Lemma 3, respectively, furnish

$$\mathcal{G}(\omega)(t+h)=S(h)\mathcal{G}(\omega)(t)+\mathcal{F}(\tau_t\omega)(h). \tag{20}$$

Since $\{\omega(s)\}_{s\in[0,t]}$ is stochastically independent of $\{W(s)\}_{s\in[t,t+h]}$ we get

$$\begin{aligned}\mathbb{E}\langle\mathcal{G}(\omega)(t+h),W_A(t+h)\rangle&=\mathbb{E}\left\langle S(h)\mathcal{G}(\omega)(t),\int_0^t S(t+h-s)dW(s)\right\rangle+\mathbb{E}\langle\mathcal{F}(\tau_t\omega)(h),W_A(t+h)\rangle\\&=\mathbb{E}\langle S(h)\mathcal{G}(\omega)(t),S(h)W_A(t)\rangle+\mathbb{E}\langle\mathcal{F}(\tau_t\omega)(h),W_A(t+h)\rangle\end{aligned}$$

and together with the self-adjointness of $S(h)$ we finally arrive at

$$D_2=\mathbb{E}\langle(S(2h)-I)\mathcal{G}(\omega)(t),W_A(t)\rangle+\mathbb{E}\langle\mathcal{F}(\tau_t\omega)(h),W_A(t+h)\rangle. \tag{21}$$

The boundedness of $\mathbb{E}\|W_A(t)\|^2$ on J and Lemma 4 now yield

$$|\mathbb{E}\langle\mathcal{F}(\tau_t\omega)(h),W_A(t+h)\rangle|\leqslant(\mathbb{E}\|\mathcal{F}(\tau_t\omega)(h)\|^2)^{1/2}\cdot(\mathbb{E}\|W_A(t+h)\|^2)^{1/2}\leqslant C\cdot h^{1/4-\rho}.$$

As for the first term in (21), notice that

$$\|(S(h)-I)v\|\leqslant\int_0^h\|(-A)S(s)v\|ds\leqslant C\cdot h^a\cdot\|(-A)^a v\| \tag{22}$$

for any $v\in D((-A)^a)$, with a constant C which depends on $a\in[0,1)$. Thus,

$$\begin{aligned}&|\mathbb{E}\langle(S(2h)-I)\mathcal{G}(\omega)(t),W_A(t)\rangle|\\&\quad\leqslant C\cdot h^{1/4-\rho}\cdot(\mathbb{E}\|(-A)^{1/4-\rho}\mathcal{F}(\omega)(t)\|^2+\mathbb{E}\|(-A)^{1/4-\rho}S(t)\omega_0\|^2)^{1/2}\end{aligned}$$

for any $\rho\in(0,\frac{1}{4})$. Together with $\|(-A)^{1/4-\rho}S(t)\omega_0\|\leqslant C\cdot\varepsilon^{\rho-1/4}\cdot\|\omega_0\|$ and Lemma 4 we eventually obtain

$$|D_2|\leqslant C\cdot h^{1/4-\rho}. \tag{23}$$

Finally we turn our attention to D_1. Its definition and (20) imply

$$\begin{aligned}D_1&=\mathbb{E}\|\mathcal{G}(\omega)(t+h)\|^2-\mathbb{E}\|\mathcal{G}(\omega)(t)\|^2\\&=\mathbb{E}\langle\mathcal{G}(\omega)(t+h)-\mathcal{G}(\omega)(t),\underbrace{\mathcal{G}(\omega)(t+h)+\mathcal{G}(\omega)(t)}_{=:D_{\mathcal{G}}}\rangle\\&=\mathbb{E}\langle(S(h)-I)\mathcal{G}(\omega)(t),D_{\mathcal{G}}\rangle+\mathbb{E}\langle\mathcal{F}(\tau_t\omega)(h),D_{\mathcal{G}}\rangle.\end{aligned}$$

As in the discussion leading to (23), we obtain for any $\tilde{a}\in[0,\frac{1}{4})$

$$|\mathbb{E}\langle (S(h)-I)\mathcal{G}(\omega)(t), D_{\mathcal{G}}\rangle| \leq C\cdot h^{2\tilde{a}}\cdot \mathbb{E}(\|(-A)^{\tilde{a}}\mathcal{G}(\omega)(t)\|\cdot\|(-A)^{\tilde{a}}D_{\mathcal{G}}\|) \leq C\cdot h^{2\tilde{a}}. \tag{24}$$

Using again Lemma 4 we further derive

$$|\mathbb{E}\langle \mathcal{F}(\tau_t\omega)(h), D_{\mathcal{G}}\rangle| \leq C\cdot(\mathbb{E}\|\mathcal{F}(\tau_t\omega)(h)\|^2)^{1/2}\cdot(\mathbb{E}\|\|D_{\mathcal{G}}\|^2)^{1/2} \leq C\cdot h^{1/4-\rho}. \tag{25}$$

Combining (24) for fixed $\tilde{a}$ near $\frac{1}{4}$ with (25) furnishes $|D_1| \leq C\cdot h^{1/4-\rho}$, and we finally obtain

$$|\mathrm{Ens}(t+h)-\mathrm{Ens}(t)| \leq C\cdot h^{1/4-\rho}$$

for arbitrary $\rho\in(0,\frac{1}{4})$. This completes the proof of Theorem 3.

V. ENSTROPHY ESTIMATE: ASYMPTOTICS

In Sec. III we established upper bounds on the growth of the enstrophy $\mathrm{Ens}(t) = \mathbb{E}\|\omega(t)\|^2/2$. Unfortunately, these bounds fail to accurately describe the dynamics of $\mathrm{Ens}(t)$ as $t\to 0$. For example, the bound derived in Theorem 1 will generally not even converge to $\mathrm{Ens}(0)$ as $t\to 0$. Therefore, this section is devoted to investigating the small-time asymptotics of the enstrophy. Similar to Ref. 25 and 26 this will be accomplished by relating $\mathrm{Ens}(t)$ to the stochastic convolution.

In order to bound the growth of $\mathbb{E}\|W_A(t)\|^2$, we assume that the coefficients μ_k in (6) are bounded by $\mu_k^2 \leq c_\mu\cdot k^{-\delta}$ for some $\delta\in(0,1)$ and some positive constant $c_\mu>0$. In this situation we obtain similar to Ref. 25, Theorem 5.4, the estimate

$$\mathbb{E}\|W_A(t)\|^2 \leq C_0\cdot t^{\delta} \tag{26}$$

for arbitrary $t\in[0,T]$, where C_0 denotes a positive constant which depends on T. Using the mild integral form (10) we further get

$$\|\omega(t)-\omega_0-W_A(t)\| \leq \|(S(t)-I)\omega_0\| + \|\mathcal{F}(\omega)(t)\|.$$

If we now assume that $\mathbb{E}\|\omega_0\|^4<\infty$, then an application of Lemma 4 furnishes

$$\begin{aligned}\mathbb{E}\|\omega(t)-\omega_0-W_A(t)\|^2 &\leq 2\mathbb{E}\|(S(t)-I)\omega_0\|^2 + 2\mathbb{E}\|\mathcal{F}(\omega)(t)\|^2\\ &\leq 2\mathbb{E}\|(S(t)-I)\omega_0\|^2 + C\cdot t^{1/2-2\rho}\\ &\leq C\cdot t^{2\gamma}\cdot\mathbb{E}\|(-A)^{\gamma}\omega_0\|^2 + C\cdot t^{1/2-2\rho}\end{aligned} \tag{27}$$

for fixed $\rho\in(0,\frac{1}{4})$ and $\gamma\in[0,1)$. Thus, the additional assumption $\mathbb{E}\|(-A)^{\gamma}\omega_0\|^2<\infty$ for some small $\gamma\in[0,1)$ implies

$$\mathbb{E}\|\omega(t)-\omega_0-W_A(t)\|^2 \leq C\cdot t^{2\gamma}.$$

Hence,

$$\begin{aligned}(\mathbb{E}\|\omega(t)\|^2)^{1/2} &\leq (\mathbb{E}\|\omega_0\|^2)^{1/2} + (\mathbb{E}\|W_A(t)\|^2)^{1/2} + (\mathbb{E}\|\omega(t)-\omega_0-W_A(t)\|^2)^{1/2}\\ &= (\mathbb{E}\|\omega_0\|^2)^{1/2} + \mathcal{O}(t^{\gamma}+t^{\delta/2}).\end{aligned}$$

Similarly one obtains

$$\begin{aligned}(\mathbb{E}\|\omega(t)\|^2)^{1/2} &\geq (\mathbb{E}\|\omega_0\|^2)^{1/2} - (\mathbb{E}\|W_A(t)\|^2)^{1/2} - (\mathbb{E}\|\omega(t)-\omega_0-W_A(t)\|^2)^{1/2}\\ &= (\mathbb{E}\|\omega_0\|^2)^{1/2} + \mathcal{O}(t^{\gamma}+t^{\delta/2}),\end{aligned}$$

and together these estimates show that $\mathbb{E}\|\omega(t)\|^2 = \mathbb{E}\|\omega_0\|^2 + \mathcal{O}(t^{\gamma}+t^{\delta/2})$. If, on the other hand, we have $\omega_0=0$, then (27) implies

$$\mathbb{E}\|\omega(t)-W_A(t)\|^2 \leqslant t^{1/2-2\rho},$$

which analogously results in $\mathbb{E}\|\omega(t)\|^2=\mathbb{E}\|W_A(t)\|^2+\mathcal{O}(t^{\frac{1}{4}-\rho+\delta/2})$. Using the definition of Ens, this furnishes the following result on the small-time asymptotics of the enstrophy.

Theorem 4(asymptotics): *Assume that* $\mathbb{E}\|(-A)^{\gamma}\omega_0\|^2<\infty$ *for some small constant* $\gamma>0$ *and that* $\mathbb{E}\|\omega_0\|^4<\infty$. *Furthermore, suppose that (26) holds for some small* $\delta>0$. *Then*

$$\mathrm{Ens}(t)=\tfrac{1}{2}\cdot\mathbb{E}\|\omega_0\|^2+\mathcal{O}(t^{\gamma}+t^{\delta/2}).$$

If in addition we have $\omega_0=0$ *and let* $\rho\in(0,\frac{1}{4})$ *be arbitrary, then*

$$\mathrm{Ens}(t)=\tfrac{1}{2}\cdot\mathbb{E}\|W_A(t)\|^2+\mathcal{O}(t^{(1+2\delta)/4-\rho}).$$

Notice that in the case $\omega_0=0$ the second term on the right-hand side is of higher order than $\mathbb{E}\|W_A(t)\|^2/2$ only under additional assumptions. For this we need $\delta<\frac{1}{2}-2\rho$, as well as a suitable lower bound on the growth of the first term $\mathbb{E}\|W_A(t)\|^2/2$ for small values of t. The latter can be achieved by imposing a lower bound on the growth of the coefficients μ_k. For details we refer the reader to Refs. 25 and 27.

VI. SUMMARY

The enstrophy $\mathrm{Ens}(t)=\mathbb{E}\|\omega(t)\|^2/2$ is an averaged measure of fluid vorticity $\omega(t)$. We have investigated the enstrophy evolution of large-scale quasi-geostrophic flows under random wind forcing. Thereby we have obtained results on upper bounds (Theorems 1 and 2), Hölder continuity (Theorem 3), as well as small-time asymptotics (Theorem 4) for the enstrophy.

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Annihilation-diffusion processes: An exactly solvable model

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A family of diffusion-annihilation processes is introduced, which is exactly solvable. This family contains parameters that control the diffusion and annihilation rates. The solution is based on the Bethe ansatz and using special boundary conditions to represent the reaction. The processes are investigated, both on the lattice and on the continuum. Special cases of this family of processes are the simple exclusion process and the drop-push model. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1466532]

I. INTRODUCTION

In recent years, the asymmetric exclusion process and the problems related to it, including, for example, the biopolymerization,[1] dynamical models of interface growth,[2] traffic models,[3] the noisy Burgers equation,[4] and the study of shocks,[5,6] have been extensively studied. The dynamical properties of this model have been studied in Refs. 6–8. As the results obtained by approaches like mean field are not reliable in one dimension, it is useful to introduce solvable models and analytic methods to extract exact physical results. Among these methods is the coordinate Bethe ansatz, which was used in Ref. 9 to solve the asymmetric simple exclusion process on a one-dimensional lattice. In Ref. 10, a similar technique was used to solve the drop-push model,[11] and a generalized one-parameter model interpolating between the asymmetric simple exclusion model and the drop-push model. In Ref. 12, this family was further generalized to a family of processes with arbitrary left- and right-diffusion rates. All of these models were lattice models. Finally, the behavior of the latter model on continuum was investigated in Ref. 13. The continuum models of this kind are also investigated in Refs. 14 and 15.

In the generalized model interpolating between the asymmetric simple exclusion model and the drop-push model,[10,12,13] there are two parameters λ and μ, which control the pushing rate. Normalizing the diffusion rate to one, it is seen that the sum of these two parameters should be one to ensure the conservation of probability. These two parameters appear in the boundary condition used instead of the reaction. The question arises of what happens if this conservation of probability is violated. This is what is investigated in the present paper. The main point of the paper is that the Bethe-ansatz approach, which is normally used for exactly solvable systems with constant number of particles, can also be used for some exactly solvable systems in them the number of particles decreases.

The scheme of the paper is the following. In Sec. II, the allowed boundary conditions are investigated. It is shown that if $\lambda+\mu<1$, then the number of the particles will be decreasing, that is, there is an annihilation process as well. It is shown that one can in fact write a two-particle to one-particle annihilation process which results in such a boundary condition.

In Sec. III, the Bethe-ansatz solution for the N-particle probability of this process is obtained, and its large-time behavior is investigated. This is done for the process on the lattice as well as on the continuum. Finally, in Sec. IV the special case of the two-particle initial condition is fully

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investigated, and it is explicitly shown that at large times, there remains only one particle. For a special value of the annihilation rate, an explicit form for the one-particle density is also obtained.

II. BOUNDARY CONDITIONS

Consider the following master equation for an asymmetric exclusion process:

$$\frac{\partial}{\partial t}P(x_1,x_2,\ldots,x_N;t)=P(x_1-1,x_2,\ldots,x_N;t)+P(x_1,x_2-1,\ldots,x_N;t)+\cdots$$
$$+P(x_1,x_2,\ldots,x_N-1;t)-NP(x_1,x_2,\ldots,x_N;t). \tag{1}$$

This equation describes a collection of N particles drifting to the right with unit rate. If the particles are to exclude each other, that is if no two particles are to occupy the same site, then (1) is valid only for

$$x_i<x_{i+1}-1. \tag{2}$$

One can, however, assume that (1) is correct for all of the physical region $x_i<x_{i+1}$, and impose certain boundary conditions for $x_i=x_{i+1}$. Note that if $x_i=x_{i+1}-1$ for some i, then on the right-hand side of (1) there will be terms with $x_i=x_{i+1}$, which is out of the physical region. The boundary condition determines the nature of the interaction between particles. But what are the allowed boundary conditions? Let us rewrite (1) for the case of two particles and use the conservation of probability. We arrive at

$$\frac{\partial}{\partial t}\sum_{x_2}\sum_{x_1<x_2}P(x_1,x_2;t)=\sum_{x_2}\sum_{x_1<x_2}P(x_1,x_2;t)-\sum_{x}P(x,x+1;t)$$
$$+\sum_{x_2}\sum_{x_1<x_2}P(x_1,x_2;t)+\sum_{x}P(x,x;t)-2\sum_{x_2}\sum_{x_1<x_2}P(x_1,x_2;t),$$
$$=-\sum_{x}P(x,x+1;t)+\sum_{x}P(x,x;t). \tag{3}$$

If the right-hand side of (3) is to be identical to zero, then $P(x,x)$ should be a linear combination of $P(x-1+i,x+i)$'s. This may work for the two-particle process, but in many-particle processes it may introduce terms with $x_i>x_{i+1}$, which need additional boundary conditions. The only exception is when $P(x,x)$ is a linear combination of only $P(x,x+1)$ and $P(x-1,x)$. So one can write

$$P(x,x)=\lambda P(x,x+1)+\mu P(x-1,x). \tag{4}$$

Inserting this in (3), one arrives at

$$\frac{\partial}{\partial t}\sum_{x_2}\sum_{x_1<x_2}P(x_1,x_2;t)=(\lambda+\mu-1)\sum_{x}P(x,x+1;t). \tag{5}$$

In order that the right-hand side of (5) be zero, one must impose

$$\lambda+\mu=1. \tag{6}$$

This is the boundary condition used in Refs. 10, 12, and 13.

This kind of boundary condition ensures the conservation of particle number. But in a process where annihilation exists as well, the number of the particles is not conserved; it is decreasing. It is seen that if

$$\lambda+\mu<1, \tag{7}$$

then the probability of finding two particles is decreasing. Suppose one begins with two particles. They drift to right with unit rate. If they meet each other, either the left particle is stopped, or one of them is annihilated. That is, we have the following processes:

$$\begin{aligned} &A\varnothing\rightarrow\varnothing A, \quad \text{with rate } 1,\\ &AA\rightarrow\varnothing A, \quad \text{with rate } \alpha,\\ &AA\rightarrow A\varnothing, \quad \text{with rate } \beta. \end{aligned} \tag{8}$$

In this case, still the more-than-two particle densities are zero, since no particles are generated during the process. But the two-particle density does not determine the one-particle density. And the summation of the former need not be a constant (one). It is seen that the master equation for the two-particle probability is

$$\frac{\partial}{\partial t}P(x_1,x_2;t)=P(x_1-1,x_2;t)+P(x_1,x_2-1;t)-2P(x_1,x_2;t), \quad x_1<x_2-1, \tag{9}$$

and

$$\frac{\partial}{\partial t}P(x,x+1;t)=P(x-1,x+1;t)-(1+\alpha+\beta)P(x,x+1;t). \tag{10}$$

But (10) is the same as (9), provided one uses the boundary condition

$$P(x,x)=\lambda P(x,x+1), \tag{11}$$

with

$$\lambda=1-(\alpha+\beta). \tag{12}$$

So the difference $1-\lambda$ is in fact related to the annihilation rate, as expected. There is one other thing to be noted. As the number of particles is not conserved, one cannot calculate the one-particle probability by a simple summation of the two-particle probability. That is,

$$P(x)\neq\sum_{y>x}P(x,y)+\sum_{y<x}P(y,x). \tag{13}$$

In fact, for the process described, the particles interact and annihilate each other, until there remains only one particle. This means that at $t\rightarrow\infty$, there will be only one particle. So the more-than-one-particle probabilities will tend to zero, whereas the summation of the one-particle probability tends to one. However, if the initial condition is that there are N particles, one can write differential equations for n-particle probabilities in which n-particle probabilities and $n+1$-particle probabilities occur (if $n<N$). For $n>N$, the n-particle probability is identically zero, and the equation for the N-particle probability is closed. So, in principle, one can find the N-particle probability first and use this to find less-than-N-particle probabilities. To be specific, the evolution equation for the one-particle probability is

$$\begin{aligned} \frac{\partial}{\partial t}P(x;t)=&[P(x-1;t)-P(x-1,x;t)]-[P(x;t)-P(x,x+1;t)]\\ &-\alpha P(x,x+1;t)-\beta P(x-1,x;t). \end{aligned} \tag{14}$$

III. BETHE-ANSATZ SOLUTION FOR THE *N*-PARTICLE PROBABILITY

Consider the master equation (1), with the boundary condition

$$P(\ldots,x,x,\ldots)=\lambda P(\ldots,x,x+1,\ldots), \tag{15}$$

where $\lambda<1$. Following Refs. 9, 10, 12, and 13, one can obtain the conditional probability using the Bethe ansatz. Writing

$$P(\mathbf{x};t)=e^{Et}\Psi(\mathbf{x}), \tag{16}$$

and

$$\Psi(\mathbf{x})=\sum_{\sigma} A_{\sigma}e^{i\sigma(\mathbf{p})\cdot\mathbf{x}}, \tag{17}$$

where the summation runs over the elements of the permutation group, one arrives at

$$E=-N+\sum_{j} e^{-ip_j}, \tag{18}$$

and

$$A_{\sigma\sigma_i}=S[\sigma(p_i),\sigma(p_{i+1})]A_{\sigma}, \tag{19}$$

where σ is that permutation which only interchanges p_i and p_{i+1}. One also finds that

$$S_{jk}:=S(p_j,p_k)=-\frac{1-\lambda e^{ip_k}}{1-\lambda e^{ip_j}}. \tag{20}$$

This is the same as what found in Refs. 10 and 12 with $\mu=0$, and if one puts $\lambda=1$, the result of Ref. 9 is obtained. The conditional probability is thus written as

$$P(\mathbf{x};t|\mathbf{y};0)=\int \frac{\mathrm{d}^N p}{(2\pi)^N}\Psi_{\mathbf{p}}(\mathbf{x})e^{E(\mathbf{p})t-i\mathbf{p}\cdot\mathbf{y}}, \tag{21}$$

where Ψ is defined as (17) with $A_{\text{identity}}=1$. This looks like similar to what obtained in Refs. 9, 10, and 12. There is, however, a difference. As $\lambda<1$, there is no pole in S, and hence in A. So for large times, when the probability distribution becomes smooth and its Fourier transform for large frequencies tends to vanish, one can put $p_j=0$ in S as an approximation to arrive at

$$S\approx -1, \tag{22}$$

and

$$A_{\sigma}\approx(-1)^{\sigma}. \tag{23}$$

One can also approximate $E(\mathbf{p})$ as

$$E(\mathbf{p})\approx\sum_{j}\left(-ip_j-\frac{p_j^2}{2}\right). \tag{24}$$

So, for large times,

$$P(\mathbf{x};t|\mathbf{y};0)\approx\frac{1}{(2\pi t)^{N/2}}\sum_{\sigma}(-1)^{\sigma}\exp\left(-\sum_{j}[x_j-\sigma(y_j)-t]^2/(2t)\right). \tag{25}$$

It is clearly seen that the integral of this distribution over the physical region tends to zero as $t\to\infty$. This should be the case, since the number of the particles does not remain constant and decreases.

Using the boundary condition (4) with (7), does not change the results drastically. In fact, E does not change at all, while S is changed to

$$S_{jk}=-\frac{1-\lambda e^{ip_k}-\mu e^{-ip_j}}{1-\lambda e^{ip_j}-\mu e^{-ip_k}}. \tag{26}$$

The approximate result for large times does not depend on λ or μ, so long as their sum is less than 1.

One can also investigate the continuous-space form of the evolution. Following Ref. 13, the master equation is changed to

$$\frac{\partial}{\partial t}P(\mathbf{x};t)=-\sum_j \partial_j P(\mathbf{x};t)+\frac{1}{2}\sum_j \partial_j^2 P(\mathbf{x};t), \tag{27}$$

and the boundary condition to

$$(1-\lambda-\mu-\lambda\partial_{j+1}+\mu\partial_j)P|_{x_{j+1}=x_j}=0. \tag{28}$$

Using the Galilean transformation $x_i\to x_i+vt$ and $t\to t$, the master equation (27) is simplified to

$$\frac{\partial}{\partial t}P(\mathbf{x};t)=\frac{1}{2}\nabla^2 P(\mathbf{x};t). \tag{29}$$

Using a Bethe-ansatz solution like (16) and (17), one arrives at

$$E=-\frac{1}{2}\sum_j p_j^2, \tag{30}$$

and

$$S_{jk}=-\frac{1-\lambda-\mu-i\lambda p_k+i\mu p_j}{1-\lambda-\mu-i\lambda p_j+i\mu p_k}. \tag{31}$$

For large times, one can approximate S to -1, and arrive at a result similar to (25). The difference is that in the exponent the term $x_j-t-\sigma(y_j)$ is replaced by $x_j-\sigma(y_j)$, as the Galilean transformation used has canceled the drift from the master equation.

IV. TWO-PARTICLE SYSTEMS AND THE EXACT SOLUTION

As was seen in Sec. III, the conditional probability for the two-particle system described by (9) and (11) is

$$P(\mathbf{x};t|\mathbf{y};0)=\int \frac{\mathrm{d}^2p}{4\pi^2}e^{Et-i\mathbf{p}\cdot\mathbf{y}}\times\left[e^{i(p_1x_1+p_2x_2)}-\frac{1-\lambda e^{ip_2}}{1-\lambda e^{ip_1}}e^{i(p_1x_2+p_2x_1)}\right], \tag{32}$$

where E is obtained from (18). This integration is easily done and the result is

$$P(\mathbf{x};t|\mathbf{y};0)=e^{-2t}\frac{t^{x_1-y_1}}{(x_1-y_1)!}\frac{t^{x_2-y_2}}{(x_2-y_2)!}$$
$$+e^{-2t}\sum_{l=0}^{\infty}\frac{t^{l+x_2-y_1}}{(l+x_2-y_1)!}\frac{t^{x_1-y_2}}{(x_1-y_2)!}\lambda^l\left(-1+\frac{\lambda t}{x_1-y_2+1}\right). \tag{33}$$

Another interesting quantity is the average number of the particles. This is equal to the summation of the one-particle probability:

$$N(t):=\sum_x P(x;t). \tag{34}$$

Using (14), one arrives at

$$\dot{N}=-(\alpha+\beta)\sum_x P(x-1,x;t)$$
$$=-\frac{1-\lambda}{\lambda}\sum_x P(x,x;t). \tag{35}$$

The right-hand side can be calculated using the Bethe-ansatz solution directly. Using (32), one has

$$\sum_x P(x,x;t)=\int\frac{\mathrm{d}^2p}{2\pi}\delta(p_1+p_2)[1+S(p_1,p_2)]e^{Et-i(p_1y_1+p_2y_2)}$$
$$=\lambda\int\frac{\mathrm{d}p}{2\pi}e^{2t(\cos p-1)+ip(y_2-y_1)}\frac{e^{-ip}-e^{ip}}{1-\lambda e^{ip}}$$
$$=\lambda\int\frac{\mathrm{d}p}{2\pi}e^{2t(\cos p-1)+ip(y_2-y_1)}\times\sum_{m=0}^{\infty}\lambda^m[e^{i(m-1)p}-e^{i(m+1)p}]$$
$$=\lambda\sum_{m=0}^{\infty}e^{-2t}\lambda^m[\mathrm{I}_{y_2-y_1+m-1}(2t)-\mathrm{I}_{y_2-y_1+m+1}(2t)]$$
$$=\lambda\sum_{m=0}^{\infty}e^{-2t}\lambda^m\frac{y_2-y_1+m}{t}\mathrm{I}_{y_2-y_1+m}(2t), \tag{36}$$

where I denotes the modified Bessel function. This can be inserted in (35) to obtain

$$N(t)=N(0)-\frac{1-\lambda}{\lambda}\int_0^t\mathrm{d}t'\sum_x P(x,x;t')$$
$$=N(0)-(1-\lambda)\sum_{m=0}^{\infty}\int_0^t\mathrm{d}t'\ e^{-2t'}\lambda^m\frac{y_2-y_1+m}{t'}\mathrm{I}_{y_2-y_1+m}(2t'). \tag{37}$$

This is simplified for $t\to\infty$. Using

$$\int_0^\infty\mathrm{d}s\frac{e^{-s}}{s}\mathrm{I}_n(s)=\frac{1}{n}, \tag{38}$$

one arrives at

$$N(\infty)=N(0)-(1-\lambda)\sum_{m=0}^{\infty}\lambda^m=N(0)-1. \tag{39}$$

But note that

$$N(0)=2, \tag{40}$$

since at the beginning there were two particles at y_1 and y_2. That is,

$$P(x;0)=\delta(x-y_1)+\delta(x-y_2). \tag{41}$$

So, at $t\to\infty$, there remains only one particle, as one of the two particles has been annihilated.

The continuous-space analog of this model can also be solved easily. Using (29) as the master equation, and (30) and (31) (with $\mu=0$), one is led to

$$P(\mathbf{x};t|\mathbf{y};0)=\int \frac{\mathrm{d}^2p}{4\pi^2}e^{Et-i\mathbf{p}\cdot\mathbf{y}} \times\left[e^{i(p_1x_1+p_2x_2)}-\frac{1-\lambda-i\lambda p_2}{1-\lambda-i\lambda p_1}e^{i(p_1x_2+p_2x_1)}\right]. \tag{42}$$

Using the change of variable $p:=p_1+i(1-\lambda)/\lambda$ in the second integral, (42) is written as

$$P(\mathbf{x};t|\mathbf{y};0)=\frac{1}{2\pi t}e^{-[(x_1-y_1)^2+(x_2-y_2)^2]/(2t)}+\frac{1}{\sqrt{8\pi t}} \times\left[A+\frac{x_1-y_2}{t}\right]e^{-(x_1-y_2)^2/(2t)}e^{[2A(x_2-y_1)+tA^2]/2}\times\left\{-1+\mathrm{erf}\left[\frac{1}{\sqrt{2t}}(x_2-y_1+tA)\right]\right\}, \tag{43}$$

where

$$A:=\frac{1-\lambda}{\lambda}. \tag{44}$$

One notes that at $t\to\infty$, the conditional probability is simplified. We have

$$1-\mathrm{erf}(x)\approx\frac{e^{-x^2}}{x\sqrt{\pi}}, \quad \text{for large } x. \tag{45}$$

From this, it is seen that at $t\to\infty$,

$$P(\mathbf{x};t|\mathbf{y};0)\approx\frac{1}{2\pi t}\{e^{-[(x_1-y_1)^2+(x_2-y_2)^2]/(2t)}-e^{-[(x_1-y_2)^2+(x_2-y_1)^2]/(2t)}\}. \tag{46}$$

This is a special case of what was obtained in Sec. III.

Another quantity to be considered is the one-point probability. In the continuum limit, and after performing the Galilean transformation, (14) becomes

$$\frac{\partial}{\partial t}P(x;t)=\frac{1}{2}\frac{\partial^2}{\partial x^2}P(x;t)+(\partial_1+\partial_2)P(x,x;t)-[\alpha(1+\partial_2)+\beta(1-\partial_1)]P(x,x;t). \tag{47}$$

From this, using the boundary condition (28), with $\mu=0$, one arrives at

$$\dot{N}(t)=-\frac{1-\lambda}{\lambda}\int \mathrm{d}x\ P(x,x;t), \tag{48}$$

where

$$N(t)\coloneqq\int \mathrm{d}x\ P(x;t). \tag{49}$$

Using (42), the integral at the right-hand side is calculated to be

$$\int \mathrm{d}x\ P(x,x;t)=\int \frac{\mathrm{d}p}{2\pi}\frac{-2i\lambda p}{1-\lambda-i\lambda p}e^{-tp^2+ip(y_2-y_1)}. \tag{50}$$

To obtain $N(\infty)$, one integrates (50) from 0 to ∞. This results in

$$\int_0^\infty \mathrm{d}t\int \mathrm{d}x\ P(x,x;t)=\frac{\lambda}{\pi}\,\mathrm{P}\int \frac{\mathrm{d}p}{ip}\frac{e^{ip(y_2-y_1)}}{1-\lambda-i\lambda p}=\frac{\lambda}{1-\lambda}. \tag{51}$$

The symbol P denotes the Cauchy's principle value, and use has been made of the fact that $y_2>y_1$. From this, it is found that

$$N(\infty)=N(0)-1=1. \tag{52}$$

This is the same result obtained for the lattice, as expected.

The special case $\lambda=0$. $\lambda=0$, or $\alpha+\beta=1$, means that the diffusion rate is equal to the annihilation rate. This criterion simplifies the boundary condition to

$$P(x,x;t)=0. \tag{53}$$

Using this, it is easily seen that the two-point function on the continuum is

$$P(\mathbf{x};t|\mathbf{y};0)=\frac{1}{2\pi t}\{e^{-[(x_1-y_1)^2+(x_2-y_2)^2]/(2t)}-e^{-[(x_1-y_2)^2+(x_2-y_1)^2]/(2t)}\}. \tag{54}$$

One notes that this means that the approximate result (46) for large times is here an exact result for all times.

For the one-point function on the continuum, using (47) and (53), one arrives at

$$\dot{P}(x;t)=\frac{1}{2}\frac{\partial^2}{\partial x^2}P(x;t)-\partial_2 P(x,x;t). \tag{55}$$

This is a diffusion equation with a sink term. The solution to it is

$$\begin{aligned}P(x;t)=&\frac{1}{\sqrt{2\pi t}}\int \mathrm{d}x'\ e^{-(x-x')^2/(2t)}P(x';0)\\&+\int_0^t \mathrm{d}t'\int \mathrm{d}x'\ \frac{1}{\sqrt{2\pi(t-t')}}e^{-(x-x')^2/[2(t-t')]}\times[-\partial_2 P(x',x';t')],\end{aligned} \tag{56}$$

which can be simplified as

$$P(x;t)=\frac{1}{\sqrt{2\pi t}}[e^{-(x-y_1)^2/(2t)}+e^{-(x-y_2)^2/(2t)}]$$

$$-\int_0^t dt'\ \frac{y_2-y_1}{\sqrt{4\pi^2 t'^3(2t-t')}}e^{-(y_2-y_1)^2/(4t')}e^{-(x-Y)^2/(2t-t')}, \tag{57}$$

where use has been made of the initial condition

$$P(x;0)=\delta(x-y_1)+\delta(x-y_2), \tag{58}$$

with $y_2>y_1$, and we have defined

$$Y:=\frac{y_1+y_2}{2}. \tag{59}$$

From (57), one can also obtain the explicit time dependence of N, the particle number. This is the integral of the one-point function, and we have

$$N(t)=2-\int_0^t dt'\ \frac{y_2-y_1}{2\sqrt{\pi t'^3}}\,e^{-(y_2-y_1)/(4t')}, \tag{60}$$

which can be simplified as

$$N(t)=1+\mathrm{erf}\left(\frac{y_2-y_1}{2\sqrt{t}}\right). \tag{61}$$

It is clearly seen that this quantity tends to 1 as $t\to\infty$, as is expected. One also notes that the time scale for annihilation is the square of the initial distance between the particles. This is also expected, as after a time of this order the particles reach each other.

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The dilute A_4 model, the E_7 mass spectrum and the tricritical Ising model[a)]

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The exact perturbation approach is used to derive the (seven) elementary correlation lengths and related mass gaps of the two-dimensional dilute A_4 lattice model in regime 2^- from the Bethe Ansatz solution. This model provides a realization of the integrable $\phi_{(1,2)}$ perturbation of the $c=\frac{7}{10}$ conformal field theory, which is known to describe the off-critical thermal behavior of the tricritical Ising model. The E_7 masses predicted from purely elastic scattering theory follow in the approach to criticality. Universal amplitudes for the tricritical Ising model are calculated. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1465515]

I. INTRODUCTION

The deep relationship between conformal field theory and criticality has provided a wealth of detailed information on phase transitions and critical phenomena. Moreover, *perturbed* conformal field theory provides a description of the *approach* to criticality in certain models.[1] One of the most striking examples is the $\phi_{(1,2)}$ perturbation of the minimal unitary conformal field theory $\mathcal{M}_{3,4}$ which is known to describe the scaling limit of the two-dimensional Ising model at $T=T_c$ in a magnetic field. In particular, Zamolodchikov's construction of nontrivial local integrals of motion and thus an integrable quantum field theory led to the remarkable prediction of eight fundamental mass ratios for the magnetic Ising model.[2] The masses coincide with the components of the Perron–Frobenius vector of the Cartan matrix of the Lie algebra E_8.

In another development, the exactly solvable dilute A_3 lattice model was discovered[3] and (in regime 2 of its four regimes) seen to be in the same universality class as the magnetic Ising model. Most importantly the dilute A_L model[3,4] admits an off-critical extension in which the Boltzmann weights are parametrized in terms of elliptic theta functions.[3] In the dilute A_3 model the elliptic nome plays the role of magnetic field. Its hidden E_8 structure has been revealed by a number of studies.[5–13] The masses, obtained from the eigenspectrum, may be summarized by the formula[11,13]

$$m_j \sim \sum_a \sin\left(\frac{a\pi}{g}\right), \tag{1}$$

where index j labels the eight particles, $g=30$ is the Coxeter number for E_8 and the set of allowed a values is given in Table I.

In addition to the correspondence between the dilute A_3 model and E_8, there are similar correspondences between the dilute A_4 model and E_7, and the dilute A_6 model and E_6. In regime 2 these models are lattice realizations of the $\phi_{(1,2)}$ perturbation of the $\mathcal{M}_{4,5}$ and $\mathcal{M}_{6,7}$ minimal

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TABLE I. The integers appearing in (1) and (3) for $L=3$.

j	a
1	1, 11
2	7, 13
3	2, 10, 12
4	6, 10, 14
5	3, 9, 11, 13
6	6, 8, 12, 14
7	4, 8, 10, 12, 14
8	5, 7, 9, 11, 13, 15

unitary conformal field theories, respectively, known to have connection to the other exceptional Lie algebras.[14] Some E-type structures have been observed for these dilute A models.[15,16]

Based on the results for the eigenspectrum of the dilute A_3 model[13] and general inversion relations, we proposed[17,18] that, in the thermodynamic limit and in the appropriate regime, the row transfer matrix eigenvalue excitations

$$r_j(w)=\lim_{N\to\infty}\frac{\Lambda_j(w)}{\Lambda_0(w)} \tag{2}$$

of the dilute A_3, A_4 and A_6 models are given by the following general expression.

Proposition: The excitation spectrum of the dilute A_3, A_4 and A_6 models in regime 2 is given by

$$r_j(w)=\prod_a w\,\frac{E(-x^{6sa/g}/w,x^{12s})E(-x^{6s(g-a)/g}/w,x^{12s})}{E(-x^{6sa/g}w,x^{12s})E(-x^{6s(g-a)/g}w,x^{12s})}. \tag{3}$$

Here the elliptic nome is $p=e^{-\epsilon}$, $w=e^{-2\pi u/\epsilon}$, and $x=e^{-\pi^2/r\epsilon}$. Regime 2 is specified by the range of the spectral parameter: $0<u<3\lambda$, and the value of the crossing parameter: $\lambda=\pi s/r$ where $s=L+2$ and $r=4(L+1)$. For the dilute A_4 model the E_7 Coxeter number is $g=18$, while for the A_6 model the E_6 Coxeter number is $g=12$. The standard (conjugate modulus) elliptic function is defined by

$$E(z,q)=\prod_{n=1}^{\infty}(1-q^{n-1}z)(1-q^n/z)(1-q^n).$$

The numbers a appearing in (3) are given in Tables I–III. The integers in these tables have appeared in other contexts in relation to the E-algebras.[19,20]

In this article we explicitly derive the elementary excitation spectrum of the dilute A_4 model, thereby confirming our Proposition in this case. The result (3) leads to the inverse correlation lengths and mass gaps. Our input to these calculations are the string solutions to the Bethe equations found by Grimm and Nienhuis.[9,10,21] As discussed later in Sec. IV, our results are

TABLE II. The integers appearing in (3) for $L=4$.

j	a
1	6
2	1, 7
3	4, 8
4	5, 7
5	2, 6, 8
6	4, 6, 8
7	3, 5, 7, 9

TABLE III. The integers appearing in (3) for $L=6$.

j	a
$1, \overline{1}$	4
2	1, 5
$3, \overline{3}$	3, 5
4	2, 4, 6

applicable to the tricritical Ising model which is in the same universality class. In particular, the elliptic nome appearing in the dilute A_4 weights in regime 2 corresponds to the leading thermal off-critical perturbation in the tricritical Ising model. This perturbation is identified with $\phi_{(1,2)}$[22] and has been shown to exhibit E_7 structures.[14,23] We are able to obtain exact results for some universal amplitudes of the tricritical Ising model. These results are in agreement with those found recently by other means.[24,25]

The outline of the article is as follows. The dilute A_L lattice model is defined along with the corresponding Bethe equations in Sec. II. The bulk free energy and the eigenvalue expressions in regime 2 for $L=4$ associated with the seven E_7 masses are derived via the exact perturbation approach in Sec. III (continued in the Appendix). The article concludes in Sec. IV with a discussion of the results and their relevance to universal behavior in the tricritical Ising model.

II. THE DILUTE A_4 MODEL

We here give a short summary of facts about the dilute A_L models[26,13] which are pertinent to our calculations.

The dilute A_L model is an exactly solvable, L-state restricted solid-on-solid model defined on the square lattice. Its adjacency diagram is the Dynkin diagram of A_L with the additional possibility that a state may be adjacent to itself on the lattice. The model is solvable in four off-critical regimes, with the elliptic nome p of its Boltzmann weights taking the model off-critical. At criticality, the dilute A_L model can be constructed[3,4] from the dilute O(n) loop model.[27,28] In regime 2 of the model the central charge is

$$c=1-\frac{6}{L(L+1)}.$$

In the majority of exactly solved models the elliptic nome plays the role of temperature.[29] In the dilute A_L model the interpretation of the elliptic nome differs according to whether L is even or odd. For L odd the elliptic nome plays the role of a magnetic field,[3] and $p>0$ and $p<0$ are related by simple label reversal of the heights. For L even the nome plays a thermal role, and the behavior of the model depends on whether $p>0$ (regime 2^+) or $p<0$ (regime 2^-). More specifically, it was shown[26] that in regime 2 the nome corresponds to perturbation of the $\mathcal{M}_{L,L+1}$ minimal unitary conformal field theories by the operator $\phi_{(1,2)}$.

Using the conjugate variables introduced after (3), and setting $w_j=e^{-2\pi u_j/\epsilon}$, the eigenvalues of the row transfer matrix of the dilute A models (for a periodic strip of width N where for convenience N has been taken as even) can be written[5]

$$\begin{aligned}\Lambda(w)=\omega&\left[\frac{E(x^{4s}/w,x^{2r})E(x^{6s}/w,x^{2r})}{E(x^{4s},x^{2r})E(x^{6s},x^{2r})}\right]^N\prod_{j=1}^{N} w_j^{1-2s/r}\frac{E(x^{2s}w/w_j,x^{2r})}{E(x^{2s}w_j/w,x^{2r})}\\
&+\left[\frac{x^{2s}}{w}\frac{E(w,x^{2r})E(x^{6s}/w,x^{2r})}{E(x^{4s},x^{2r})E(x^{6s},x^{2r})}\right]^N\prod_{j=1}^{N} w_j\frac{E(w/w_j,x^{2r})E(x^{6s}w_j/w,x^{2r})}{E(x^{2s}w_j/w,x^{2r})E(x^{4s}w_j/w,x^{2r})}\\
&+\omega^{-1}\left[x^{2s}\frac{E(w,x^{2r})E(x^{2s}/w,x^{2r})}{E(x^{4s},x^{2r})E(x^{6s},x^{2r})}\right]^N\prod_{j=1}^{N} w_j^{2s/r}\frac{E(x^{8s}w_j/w,x^{2r})}{E(x^{4s}w_j/w,x^{2r})},\end{aligned}\tag{4}$$

TABLE IV. String positions u_j and corresponding eigenvalue bands for the seven elementary mass excitations m_i of the dilute A_4 model in regime 2^-.[21] The strings are in units of $\pi/20$.

i	String positions	Band
1	$\pm 2,10$	w
2	± 7	w^2
3	$\pm 6,10$	w^2
4	$\pm 3,\pm 9$	w^2
5	$\pm 6,\pm 8$	w^3
6	$\pm 4,\pm 8,10$	w^3
7	$\pm 5,\pm 7,\pm 9$	w^4

where $\omega=\exp(i\pi\ell/(L+1))$ for $\ell=1,\ldots,L$, and $s=L+2$ and $r=4(L+1)$ in regime 2. The Bethe equations which give the N roots u_j have the form

$$\omega\left[w_j\frac{E(x^{2s}/w_j,x^{2r})}{E(x^{2s}w_j,x^{2r})}\right]^N=-\prod_{k=1}^{N} w_k^{2s/r}\frac{E(x^{2s}w_j/w_k,x^{2r})E(x^{4s}w_k/w_j,x^{2r})}{E(x^{2s}w_k/w_j,x^{2r})E(x^{4s}w_j/w_k,x^{2r})}. \tag{5}$$

In the limit $|p|\to 1$ with u/ϵ fixed, or equivalently $x\to 0$, the excitations in the eigenspectrum $r_j(w)$, defined in (2), break up into a number of distinct bands labeled by integer powers of w. Numerical investigations of the eigenspectrum[5,9,10,21,17] have revealed eight and seven thermodynamically significant excitations for $L=3$ and $L=4$, respectively, and provided the data in Table IV.

We previously[12,13] applied the exact perturbation approach initiated by Baxter[30] to calculate the excitations in the eigenspectrum for $L=3$. This involved perturbing away from the strong magnetic field limit at $p\to 1$; for $L=4$ this limit corresponds to moving far away from the critical temperature. The calculations follow.

III. MASS SPECTRUM

A. Preliminaries

To apply the perturbation technique[30] to find the form of the excitations (4), the string structure of the Bethe ansatz roots (5) is required input. The groundstate roots all have u_j pure imaginary, so that $w_j=e^{-2\pi u_j/\epsilon}=a_j$ for $j=1,\ldots,N$ with $|a_j|=1$; in this sense they all live on a unit circle. For each excitation i, certain roots acquire a real part $m\pi/20$, as shown in Table IV. (If there are n_i such roots, one says there is an n_i-string associated with the excitation.) For these roots $w_j=b_jx^{2m}$, so that the string entries can be thought of as living on circles of radius x^{2m} with phase b_j, while the other $N-n_i$ roots again lie on the unit circle.

The process of finding the excitations involves using the Bethe equations (5) to set up recurrence relations for auxiliary functions of the unknown roots a_j. As the roots only enter the eigenvalue expression (4) through the auxiliary functions, it just remains to solve the recurrence relations by iteration and to simplify the resulting expressions. The largest eigenvalue Λ_0, relative to which excitations are measured, was calculated previously in this way[13] for all L.

The relationship between the excitations (2), the correlation lengths ξ_j and the mass spectrum m_j of the associated field theory is

$$\xi_j^{-1}=-\log r_j=m_j, \tag{6}$$

where we take the isotropic value $u=3\lambda/2$.

It is convenient to use the notation for products:

$$(z;p_1,\ldots,p_k)_\infty=\prod_{n_1,\ldots n_k=0}^{\infty}(1-p_1^{n_1}\cdots p_k^{n_k}z),$$

$$(z_1,\ldots z_m;p_1,\ldots,p_k)_\infty=\prod_{j=1}^{m}(z_j;p_1,\ldots,p_k)_\infty,$$

which satisfy many identities, the ones used repeatedly in what follows being

$$\frac{(z;p)_\infty}{(zp;p)_\infty}=(1-z),$$

$$\frac{(z;p,q)_\infty}{(zp;p,q)_\infty}=(z;q)_\infty,$$

$$\frac{(zq/p;p,q)_\infty}{(z;p,q)_\infty}=\frac{(zq/p;q)_\infty}{(z;p)_\infty}.$$

The standard elliptic function is thus rewritten as

$$E(z,q)=\prod_{n=1}^{\infty}(1-q^{n-1}z)(1-q^n/z)(1-q^n)=(z,q/z,q;q)_\infty. \tag{7}$$

It also proves convenient to use the shorthand notation $\Pi_{j=1}^{m}a_j=A_m$.

For each m_i, if the associated string of excited roots has length n_i, we define the required auxiliary functions of the as-yet-unknown roots to be

$$F_i(w)=\prod_{j=1}^{N-n_i}(w/a_j;x^{2r})_\infty,$$

$$G_i(1/w)=\prod_{j=1}^{N-n_i}(x^{2r}a_j/w;x^{2r})_\infty. \tag{8}$$

In fact, we actually solve for combinations of these:

$$\mathcal{F}_i(w)=F_i(w)/F_i(x^{16}w)=F_i(w)/F_i(x^{2r-4s}w),$$

$$\mathcal{G}_i(1/w)=G_i(1/w)/G_i(1/x^{16}w)=G_i(1/w)/G_i(1/x^{2r-4s}w), \tag{9}$$

for $i=2,4,5,6,7$ (but for $i=1,3$ slightly different definitions are convenient and are given as required).

So far as possible, we write factors and powers which are common to all eigenvalues (or indeed to all the eigenvalues for other A_L models) in terms of the generic r and s to distinguish them from the particular integers which arise from the input strings. Of course, $r=20$ and $s=6$ throughout. Once the particular string form for the roots has been applied, the calculations are straightforward for all masses except m_1 and m_3. For this reason, we sketch below the details for the first three masses. The other cases follow similar paths to m_2 or indeed to most of the masses for the dilute A_3 model,[13] so we relegate them to the appendix. We make some comments concerning m_1, m_3 and m_6 later on.

B. Mass m_1

We begin the perturbation argument with the structure $w_j=a_j$ for $j=1,\ldots,N-3$ with $w_{N-1}=b_1x^{-4}$, $w_{N-2}=b_2x^4$ and $w_N=b_3x^{20}$, so that the string length is $n_1=3$. From the Bethe equations (5) for $j=N-2$, $j=N-1$ and $j=N$ in the limit $x\to 0$ we can show that $b_1=b_2=b_3=b$. The Bethe equation for the other roots $a_k=a$ is then

$$-\omega\left[a\frac{E(x^{2s}/a)}{E(x^{2s}a)}\right]^N=(A_{N-3}b^3)^{3/5}\frac{a^2}{b^2}\times\frac{E(x^4b/a)E(x^{24}b/a)E(x^{28}b/a)}{E(x^4a/b)E(x^{24}a/b)E(x^{28}a/b)}\prod_{j=1}^{N-3}\frac{E(x^{2s}a/a_j)E(x^{4s}a_j/a)}{E(x^{2s}a_j/a)E(x^{4s}a/a_j)}. \quad (10)$$

In the $x\to 0$ limit this gives the equation

$$a^{N-2}+\frac{1}{\omega}(A_{N-3}b^3)^{3/5}/b^2=0, \quad (11)$$

which is an equation of order $(N-2)$, so that there is a missing root on the unit circle, a ''hole'' which we call a_{N-2}. Since this is an equation for the roots, its left hand side must be equivalent to $\Pi_{j=1}^{N-2}(a-a_j)$, and equating the constant terms from these two expressions we obtain

$$\frac{1}{\omega}(A_{N-3}b^3)^{3/5}=A_{N-2}b^2=A_{N-3}a_{N-2}b^2 \quad (12)$$

(which we later apply to prefactors in Λ_1). The Bethe equations for b, taken together in this limit and combined with (12), give

$$\left[\frac{1}{\omega}(A_{N-3}b^3)^{3/5}\right]^3=-b^6(A_{N-3})^2\Rightarrow A_{N-3}(a_{N-2})^3=-1.$$

We use this, together with the fact that each root a_j, including the hole, must satisfy (11), to show

$$(a_{N-2})^{N-2}=-A_{N-3}a_{N-2}\Rightarrow(a_{N-2})^N=1. \quad (13)$$

We define the following auxiliary functions of the roots [see (8)]:

$$\mathcal{F}_1(w)=\frac{F_1(w)}{F_1(x^{16}w)}\frac{(x^4w/b;x^{2r})_\infty}{(x^{12}w/b;x^{2r})_\infty},$$

$$\mathcal{G}_1(1/w)=\frac{G_1(1/w)}{G_1(1/x^{16}w)}\frac{(x^{36}b/w;x^{2r})_\infty}{(x^{24}b/w;x^{2r})_\infty}.$$

They must satisfy recurrence relations arising from (10):

$$\mathcal{F}_1(a)=\left[\frac{(x^{2s}a;x^{2r})_\infty}{(x^{2r-2s}a;x^{2r})_\infty}\right]^N\frac{(x^{24}a/a_{N-2},x^{28}a/a_{N-2};x^{2r})_\infty}{(x^{12}a/a_{N-2},x^{16}a/a_{N-2};x^{2r})_\infty}\frac{\mathcal{F}_1(x^{2s}a)}{\mathcal{F}_1(x^{4s}a)},$$

$$\mathcal{G}_1(1/a)=\left[\frac{(x^{2r+2s}/a;x^{2r})_\infty}{(x^{6s}/a;x^{2r})_\infty}\right]^N\frac{(x^{36}a_{N-2}/a,x^{40}a_{N-2}/a;x^{2r})_\infty}{(x^{48}a_{N-2}/a,x^{52}a_{N-2}/a;x^{2r})_\infty}\frac{\mathcal{G}_1(x^{2s}/a)}{\mathcal{G}_1(x^{4s}/a)}. \quad (14)$$

Solving these we obtain

$$\mathcal{F}_1(a)=\mathcal{F}_0(a)\,\frac{(x^{40}a/a_{N-2};x^{2r})_\infty}{(x^{16}a/a_{N-2};x^{2r})_\infty}\,\frac{(x^{36}a/a_{N-2},x^{48}a/a_{N-2};x^{12s})_\infty}{(x^{12}a/a_{N-2},x^{72}a/a_{N-2};x^{12s})_\infty},$$
$$\mathcal{G}_1(1/a)=\mathcal{G}_0(1/a)\,\frac{(x^{40}a_{N-2}/a;x^{2r})_\infty}{(x^{64}a_{N-2}/a;x^{2r})_\infty}\,\frac{(x^{36}a_{N-2}/a,x^{96}a_{N-2}/a;x^{12s})_\infty}{(x^{60}a_{N-2}/a,x^{72}a_{N-2}/a;x^{12s})_\infty}. \tag{15}$$

Here $\mathcal{F}_0$ and $\mathcal{G}_0$ arise from the square bracketed factors in (14) and give rise to the square bracketed factor in (16). They are related to the groundstate eigenvalue Λ_0, they are common to the calculation of each mass and we will suppress these factors for $m_2,\ldots,m_7$. We now write the eigenvalue expression in terms of the auxiliary functions, the first term being

$$\frac{\Lambda_1}{3}=-\frac{w}{a_{N-2}}\left[\frac{(x^{2r-6s}w,x^{2r-4s}w,x^{4s}/w,x^{6s}/w;x^{2r})_\infty}{(x^{2r-6s},x^{2r-4s},x^{4s},x^{6s};x^{2r})_\infty}\right]^N$$
$$\times\frac{(x^{28}w/a_{N-2},x^{12}a_{N-2}/w;x^{2r})_\infty}{(x^{12}w/a_{N-2},x^{28}a_{N-2}/w;x^{2r})_\infty}\mathcal{F}_1(x^{2s}w)\mathcal{G}_1(1/x^{2s}w). \tag{16}$$

Substituting the solutions (15) gives an expression for the excitation $r_1(w)$ which may be written in elliptic functions (7) as

$$\frac{\Lambda_1}{\Lambda_0}=w\,\frac{E(-x^{12}/w,x^{12s})E(-x^{48}w,x^{12s})}{E(-x^{12}w,x^{12s})E(-x^{48}/w,x^{12s})}, \tag{17}$$

where we have set $a_{N-2}=-1$. (The other two terms in the eigenvalue always give identical elliptic function expressions to the first, upon simplification.)

The Bethe equations involving b and the ''hole'' equation, which is (10) with $a=a_{N-2}$, can also be expressed in terms of the auxiliary functions. Application of identities and simplification gives

$$E(x^{12}b/a_{N-2},x^{2r-4s})=E(x^{12}a_{N-2}/b,x^{2r-4s}),$$
$$\left[\frac{E(x^{12}a_{N-2},x^{12s})E(x^{48}/a_{N-2},x^{12s})}{E(x^{12}/a_{N-2},x^{12s})E(x^{48}a_{N-2},x^{12s})}\right]^N=(a_{N-2})^N.$$

Clearly $a_{N-2}=b=-1$ (identified initially from numerical studies) satisfy these conditions; the second reduces to (13) in the $x\to 0$ limit, and note the similarities with (17).

C. Mass m_2

We begin the perturbation argument with the structure $w_j=a_j$ for $j=1,\ldots,N-2$ with $w_{N-1}=b_1x^{-14}$ and $w_N=b_2x^{14}$, so that $n_2=2$. From the Bethe equations for $j=N-1$ and $j=N$ we can show that $b_1=b_2=b$. The Bethe equation for the other roots $a_k=a$ is then

$$-\omega\left[a\,\frac{E(x^{2s}/a)}{E(x^{2s}a)}\right]^N=(A_{N-2}b^2)^{3/5}\frac{a^2}{b^2}\,\frac{E(x^{10}b/a)E(x^{14}b/a)}{E(x^{10}a/b)E(x^{14}a/b)}\prod_{j=1}^{N-2}\frac{E(x^{2s}a/a_j)E(x^{4s}a_j/a)}{E(x^{2s}a_j/a)E(x^{4s}a/a_j)}. \tag{18}$$

In the $x\to 0$ limit this gives the equation

$$a^{N-2}+\frac{1}{\omega}(A_{N-2}b^2)^{3/5}/b^2=0,$$

which has the same order as the number of unknown roots $(N-2)$ so that there is no hole. Equating this with $\Pi_{j=1}^{N-2}(a-a_j)$ we obtain

$$\frac{1}{\omega}(A_{N-2}b^2)^{3/5}=A_{N-2}b^2$$

(which we later apply to prefactors in Λ_2). From the other Bethe equations in this limit,

$$\left[\frac{1}{\omega}(A_{N-2}b^2)^{3/5}\right]^2=\frac{(A_{N-2}b^2)^2}{b^{2N}}\Rightarrow b^{2N}=1. \tag{19}$$

Treating the Bethe equation (18) as before gives, in terms of the functions defined in (8) and (9), the recurrences

$$\mathcal{F}_2(a)=\frac{(x^{26}a/b,x^{30}a/b;x^{2r})_\infty}{(x^{10}a/b,x^{14}a/b;x^{2r})_\infty}\frac{\mathcal{F}_2(x^{2s}a)}{\mathcal{F}_2(x^{4s}a)},$$

$$\mathcal{G}_2(1/a)=\frac{(x^{38}b/a,x^{34}b/a;x^{2r})_\infty}{(x^{50}b/a,x^{54}b/a;x^{2r})_\infty}\frac{\mathcal{G}_2(x^{2s}/a)}{\mathcal{G}_2(x^{4s}/a)}.$$

Solving these we obtain

$$\mathcal{F}_2(a)=\frac{(x^{30}a/b,x^{42}a/b;x^{2r})_\infty}{(x^{14}a/b,x^{26}a/b;x^{2r})_\infty}\frac{(x^{26}a/b,x^{38}a/b,x^{46}a/b,x^{58}a/b;x^{12s})_\infty}{(x^{10}a/b,x^{22}a/b,x^{62}a/b,x^{74}a/b;x^{12s})_\infty},$$

$$\mathcal{G}_2(1/a)=\frac{(x^{38}b/a,x^{50}b/a;x^{2r})_\infty}{(x^{54}b/a,x^{66}b/a;x^{2r})_\infty}\frac{(x^{34}b/a,x^{46}b/a,x^{86}b/a,x^{98}b/a;x^{12s})_\infty}{(x^{50}b/a,x^{62}b/a,x^{70}b/a,x^{82}b/a;x^{12s})_\infty}.$$

We now substitute these into the eigenvalue expression, the first term of which is

$$\frac{\Lambda_2}{3}=\frac{w^2}{b^2}\frac{(x^{26}w/b,x^{38}w/b,x^2b/w,x^{14}b/w;x^{2r})_\infty}{(x^2w/b,x^{14}w/b,x^{26}b/w,x^{38}b/w;x^{2r})_\infty}\mathcal{F}_2(x^{2s}w)\mathcal{G}_2(1/x^{2s}w).$$

This gives an expression for the excitation in elliptic functions (setting $b=-1$):

$$\frac{\Lambda_2}{\Lambda_0}=w^2\frac{E(-x^2/w,x^{12s})E(-x^{14}/w,x^{12s})E(-x^{38}w,x^{12s})E(-x^{50}w,x^{12s})}{E(-x^2w,x^{12s})E(-x^{14}w,x^{12s})E(-x^{38}/w,x^{12s})E(-x^{50}/w,x^{12s})}. \tag{20}$$

If the product of the six Bethe equations involving b is expressed in terms of the auxiliary functions, the equation for b [generalizing $b^{2N}=1$ seen in the $x\to 0$ limit in (19)] is clearly satisfied by $b=-1$:

$$\left[\frac{E(x^2b,x^{12s})E(x^{14}b,x^{12s})E(x^{38}/b,x^{12s})E(x^{50}/b,x^{12s})}{E(x^2/b,x^{12s})E(x^{14}/b,x^{12s})E(x^{38}b,x^{12s})E(x^{50}b,x^{12s})}\right]^N=b^{2N}.$$

Compare the pattern of powers of x in this equation with those in (20); this equation has a precise analog for each mass $m_4,\ldots,m_7$, which will not be given.

D. Mass m_3

We begin the perturbation argument with the string structure $w_j=a_j$ for $j=1,\ldots,N-3$ with $w_{N-2}=b_1x^{-12}$, $w_{N-1}=b_2x^{12}$ and $w_N=b_3x^{20}$. From the Bethe equations for $j=N-2$ and $j=N-1$ we can show that $b_1=b_2=\alpha$, but the Bethe equation for $j=N$ does not link $b_3=b$ to α in the $x\to 0$ limit. (This feature was observed also in the $L=3$ case, for a string of odd length.[13]) The Bethe equation for the other roots $a_k=a$ is then

$$-\omega\left[a\frac{E(x^{2s}/a)}{E(x^{2s}a)}\right]^N=(A_{N-3}\alpha^2 b)^{3/5}\frac{a^3}{\alpha b^2}\frac{E(x^4b/a)E(x^8b/a)}{E(x^4a/b)E(x^8a/b)}$$
$$\times\frac{E(x^{12}\alpha/a)E(x^{16}\alpha/a)E(x^{36}\alpha/a)}{E(x^{12}a/\alpha)E(x^{16}a/\alpha)E(x^{36}a/\alpha)}\prod_{j=1}^{N-3}\frac{E(x^{2s}a/a_j)E(x^{4s}a_j/a)}{E(x^{2s}a_j/a)E(x^{4s}a/a_j)}. \quad (21)$$

In the $x\to 0$ limit this gives the equation

$$a^{N-3}-\frac{1}{\omega}(A_{N-3}\alpha^2 b)^{3/5}/\alpha b^2=0.$$

Equating this as usual with $\Pi_{j=1}^{N-3}(a-a_j)$, we obtain

$$\frac{1}{\omega}(A_{N-3}\alpha^2 b)^{3/5}=A_{N-3}\alpha b^2$$

(which we later apply to prefactors in Λ_3). From the other Bethe equations in this limit,

$$\left[\frac{1}{\omega}(A_{N-3}\alpha^2 b)^{3/5}\right]^3=\frac{(A_{N-3}\alpha b^2)^3}{b^{2N}}\Rightarrow b^{2N}=1.$$

In this case it is convenient to define

$$\mathcal{F}_3(w)=\frac{F_3(w)}{F_3(x^{16}w)}\frac{(x^{12}w/\alpha;x^{2r})}{(x^4w/\alpha;x^{2r})},$$
$$\mathcal{G}_3(1/w)=\frac{G_3(1/w)}{G_3(1/x^{16}w)}\frac{(x^{28}\alpha/w;x^{2r})}{(x^{36}\alpha/w;x^{2r})}, \quad (22)$$

because this choice will make it clear that α is a spectator in the solution to the recurrence relation; it does not appear in the eigenvalue expression.

Treating the Bethe equation (21) as before gives the recurrences

$$\mathcal{F}_3(a)=\frac{(x^{32}a/b,x^{36}a/b;x^{2r})_\infty}{(x^4a/b,x^8a/b;x^{2r})_\infty}\frac{\mathcal{F}_3(x^{2s}a)}{\mathcal{F}_3(x^{4s}a)},$$
$$\mathcal{G}_3(1/a)=\frac{(x^{56}b/a,x^{60}b/a;x^{2r})_\infty}{(x^{28}b/a,x^{32}b/a;x^{2r})_\infty}\frac{\mathcal{G}_3(x^{2s}/a)}{\mathcal{G}_3(x^{4s}/a)}.$$

Solving these we obtain

$$\mathcal{F}_3(a)=\frac{(x^{36}a/b;x^{2r})_\infty}{(x^{20}a/b;x^{2r})_\infty}\frac{(x^{32}a/b,x^{40}a/b,x^{44}a/b,x^{52}a/b;x^{12s})_\infty}{(x^4a/b,x^8a/b,x^{16}a/b,x^{68}a/b;x^{12s})_\infty},$$
$$\mathcal{G}_3(1/a)=\frac{(x^{44}b/a;x^{2r})_\infty}{(x^{60}b/a;x^{2r})_\infty}\frac{(x^{28}b/a,x^{32}b/a,x^{40}b/a,x^{92}b/a;x^{12s})_\infty}{(x^{56}b/a,x^{64}b/a,x^{68}b/a,x^{76}b/a;x^{12s})_\infty}.$$

We now substitute these into the eigenvalue expression, the first term of which is, in terms of the functions (22),

$$\frac{\Lambda_3}{3}=\frac{w^2}{b^2}\frac{(x^{32}w/b,x^8b/w;x^{2r})_\infty}{(x^8w/b,x^{32}b/w;x^{2r})_\infty}\mathcal{F}_3(x^{2s}w)\mathcal{G}_3(1/x^{2s}w).$$

With $b=-1$ this gives the expression in elliptic functions

$$\frac{\Lambda_3}{\Lambda_0}=w^2\frac{E(-x^8/w,x^{12s})E(-x^{16}/w,x^{12s})E(-x^{44}w,x^{12s})E(-x^{52},w,x^{12s})}{E(-x^8w,x^{12s})E(-x^{16}w,x^{12s})E(-x^{44}/w,x^{12s})E(-x^{52}/w,x^{12s})}. \tag{23}$$

The Bethe equations involving α and b, also expressed in terms of the auxiliary functions, give

$$E(x^{12}b/\alpha,x^{2r-4s})=E(x^{12}\alpha/b,x^{2r-4s}),$$

$$\left[\frac{E(x^8b,x^{12s})E(x^{16}b,x^{12s})E(x^{44}/b,x^{12s})E(x^{52}/b,x^{12s})}{E(x^8/b,x^{12s})E(x^{16}/b,x^{12s})E(x^{44}b,x^{12s})E(x^{52}b,x^{12s})}\right]^N=b^{2N}.$$

Notice that $b=-1$ satisfies this second equation, and the (so far missing) link between α and b is provided by the first.

E. Comments on the "odd" strings

To close this rather technical section of the article, we wish to briefly comment on the strings of odd length (see Table IV).

For this model strings of odd length appear for the first, third and sixth masses. In the first case, the odd string of excited roots is accompanied by a "hole" among the roots on the unit circle; it is only this hole a_{N-2} which appears in the eigenvalue expression. In the case of the third mass, the phase b of the string entry $m=10$ appears alone in the eigenvalue expression, and the other entries of the string seem to have a spectator role. (For the sixth mass, there was nothing special about the calculation.) In the calculations for dilute A_3 (Ref. 13) odd strings were involved for masses 4 and 6, where again the calculation of the associated excitation was less straightforward than for even strings. In one case, both the coefficient of the "odd" entry *and* a hole appeared in the eigenvalue, while the other calculation resembles that of m_3 in this article. In general the string entries come in pairs $\pm m$, except for $m=r/2$, which stands alone if it occurs, due to the period of the original elliptic functions in u_j. This is the only source of strings of odd length; we can only conclude that when such an entry occurs, it in some sense dominates calculations following the exact perturbation technique. For strings of even length, all the excited roots seem to contribute in a more equal fashion to the calculation and to the resulting eigenvalue expression.

IV. DISCUSSION

In this article we have made use of the Bethe Ansatz string solutions found by Grimm and Nienhuis to derive the excitation spectrum of the dilute A_4 model via the exact perturbation approach. Our expressions for the seven thermodynamically significant excitations for the dilute A_4 eigenspectrum in regime 2^- are given in (17), (20), (23), (A2), (A4), (A6) and (A7). In this way we have verified for a second case the Proposition given by (3).

It is perhaps unsatisfying that an elegant closed form expression such as (3) has been confirmed in the A_4 case by relying on numerical data for the strings (Table IV). Indeed, as described for the A_3 case in Ref. 13, and in the detailed study of Ref. 10, tracing the strings from $p=0$ (criticality) to the position they take in the scaling (massive) limit reveals complicated structure (reported with one difference by two groups of authors[5,10]). Fortunately, (3) was conjectured[17,18] on the basis of general properties of the dilute A models and of the E-type algebras, known to be linked by their common connection to the $\phi_{(1,2)}$ perturbation of the minimal unitary series; the (scaling limit) string data used here has not contradicted it, and (admittedly limited) numerical studies agreed with the lower eigenvalues.[17] A forthcoming paper[31] should shed some new light, from the perspective of Coxeter geometry, on the excitations (3) and, hence, among other things, on the string conjectures to which they are related as demonstrated here in the $L=4$ case.

Recall that the central charge for dilute A_4 in regime 2 is $c=\frac{7}{10}$. There are several other known manifestations of the $c=\frac{7}{10}$ theory. The Blume–Capel model[32] is related to the Blume–Emery–Griffiths model,[33] a classical spin-1 Ising model with lattice Hamiltonian

TABLE V. The four perturbations of the tricritical Ising model, and the objects from statistical mechanics to which they are related in the scaling limit.

Perturbation	Field	Weight	IRF model	$\mathcal{H}_{\mathrm{BEG}}$
Leading magnetic	$\phi_{(2,2)}$	$\frac{3}{80}$	Not integrable	H
Leading thermal	$\phi_{(1,2)}$	$\frac{1}{10}$	Dilute A_4, regime 2	$1/J$
Subleading magnetic	$\phi_{(2,1)}$	$\frac{7}{16}$	Dilute A_3, regime 1	H_3
Subleading thermal	$\phi_{(1,3)}$	$\frac{3}{5}$	ABF A_4, regime III	D

$$\mathcal{H}_{\mathrm{BEG}}=-J\sum_{\langle i,j\rangle} S_iS_j-D\sum_i (1-S_i^2)-H\sum_i S_i-H_3\sum_{\langle i,j\rangle} S_iS_j(S_i+S_j), \tag{24}$$

where J is the nearest-neighbor interaction, D is a crystal field, H a magnetic field term, and H_3 is a staggered magnetic field. The phase diagrams of these models exhibit a tricritical point, as had been observed in physical systems.[34] The critical exponents, known from renormalization group studies, are related to the Kac table of the $c=\frac{7}{10}$ conformal field theory.[1]

After the Ising critical point, the universality class of the tricritical Ising model corresponds to the second simplest unitary conformal field theory in two dimensions. It is also the first of the super-conformal minimal models. It can be perturbed by its four relevant scaling fields, shown in Table V ordered according to the associated conformal weight. The leading magnetic perturbation is believed to be nonintegrable,[22] and each of the other three perturbations give integrable quantum field theories. In the scaling limit these can each be associated with a solvable interaction round a face (IRF) model [or to the terms in (24)]. The ABF A_4 model in regime III[35,36] realizes the subleading thermal perturbation. A lattice realization of the subleading magnetic perturbation is given by the dilute A_3 model in regime 1,[37] and the scaling limit of the leading thermal perturbation corresponds to the dilute A_4 model as considered in this article.

The leading thermal perturbation is known to be integrable and massive, the masses being described by E_7 Toda field theory.[14,23] Numerical results from a finite-size analysis in the spin-chain formulation,[38] and from field theory via the truncated conformal space approach[22] demonstrated the first few masses.

These are

$$\begin{aligned}
m_1&=1 && \text{odd},\\
m_2&=2\cos\frac{5\pi}{18}=1.285\,575\ldots && \text{even},\\
m_3&=2\cos\frac{\pi}{9}=1.879\,385\ldots && \text{odd},\\
m_4&=2\cos\frac{\pi}{18}=1.969\,615\ldots && \text{even},\\
m_5&=4\cos\frac{\pi}{18}\cos\frac{5\pi}{18}=2.532\,088\ldots && \text{even},\\
m_6&=4\cos\frac{\pi}{9}\cos\frac{2\pi}{9}=2.879\,385\ldots && \text{odd},\\
m_7&=4\cos\frac{\pi}{18}\cos\frac{\pi}{9}=3.701\,666\ldots && \text{even}.
\end{aligned} \tag{25}$$

The mass spectrum can be classified[22] into even and odd states [as indicated in (25)] corresponding to the $\mathbb{Z}_2$ symmetry of the affine E_7 Dynkin diagram. Each of the above seven masses appears in the high-temperature phase of the tricritical Ising model. However, only the even subset appears in the low-temperature phase. This is consistent with the numerical observations on the eigenspectrum of the dilute A_4 model.[21,17] For regime 2^+, in a study of the low-lying excitations, the first and third were absent. As we have demonstrated, all seven excitations are present in regime 2^- which (through a quirk in labelling) corresponds to $T>T_c$.

Our expression (3) gives the correlation lengths and related masses (6), expressed in terms of standard elliptic functions and the original nome p, as

$$m_j=\xi_j^{-1}=2\sum_a \log\frac{\vartheta_4(a\pi/36+\pi/4,p^{5/9})}{\vartheta_4(a\pi/36-\pi/4,p^{5/9})}. \tag{26}$$

In the critical limit $p\to 0$ the leading order behavior is

$$m_j\sim 8p^{5/9}\sum_a \sin\frac{a\pi}{18}. \tag{27}$$

Substituting the integers of Table II, applying trigonometric identities and taking mass ratios it was demonstrated[17] that the E_7 mass spectrum (25) is recovered.

The ground states of the tricritical Ising model (in zero magnetic field) have been identified.[32,22] For $T<T_c$, the system is in a two-phase region of spontaneously broken spin reversal symmetry, with two degenerate ground states in the thermodynamic limit. For $T>T_c$ there is one ground state. This ground state picture is also consistent with that of the dilute A_4 model[39] as $|p|\to 1$. In regime 2^+ there are two possible ferromagnetic ground states, while in regime 2^- there is a single disordered ground state. (It is the presence of such disordered states for L even which complicates the calculation of order parameters for this half of the dilute A_L hierarchy.)

Very recently, an array of universal ratios for the critical amplitudes of the tricritical Ising model have been calculated[24,25] by field theoretic methods. Not all of these quantities appear to be accessible via the dilute A_4 model. However, one such ratio involves the correlation length prefactors $\xi_0^{\pm}$, above and below the critical temperature. Our results and observations on the eigenspectrum of dilute A_4 give this same value:

$$\frac{\xi_0^+}{\xi_0^-}=\frac{\xi_1}{\xi_2}=2\cos\frac{5\pi}{18}.$$

We previously[17] derived the amplitude

$$f_s\xi_1^2=\frac{1}{8\sqrt{3}\cos(2\pi/9)}=0.094\,20\ldots, \tag{28}$$

where f_s is the singular part of the free energy. This agrees with the determination of this quantity for the $\phi_{(1,2)}$ perturbation of the $c=\frac{7}{10}$ field theory.[40] A related universal quantity is the amplitude ratio associated with the correlation length[41]

$$R_\xi^{\pm}=A^{1/2}\xi_0^{\pm},$$

where A/α is the amplitude of the specific heat and α is the related critical exponent. Our expressions for these quantities are

$$R_\xi^+=\left[\frac{10}{9^3\sqrt{3}\cos(2\pi/9)}\right]^{1/2}=0.101\,678\ldots,$$

$$R_\xi^- = \left[\frac{5}{2^3 9^2 \sqrt{3} \cos(5\pi/18)\sin(5\pi/9)} \right]^{1/2} = 0.083\,889\ldots,$$

which agree with the numerical values of Ref. 25 (allowing for a difference in definition by a factor $\alpha^{1/2}$). As remarked,[24,25] such values may be observed in experimental systems within the tricritical Ising universality class.

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APPENDIX: FURTHER MASS CALCULATIONS

1. Mass m_4

We begin the perturbation argument with the structure $w_j = a_j$ for $j = 1,\ldots,N-4$ with $w_{N-3} = b_1 x^{-18}$, $w_{N-2} = b_2 x^{18}$, $w_{N-1} = b_3 x^{-6}$ and $w_N = b_4 x^6$. From the Bethe equations for $j = N-3,\ldots,N$ we can show that $b_1 = b_2 = b_3 = b_4 = b$. The Bethe equation for the other roots is

$$-\omega \left[a \frac{E(x^{2s}/a)}{E(x^{2s}a)} \right]^N = (A_{N-4} b^4)^{3/5} \frac{a^4}{b^4} \frac{E(x^2 b/a)E(x^6 b/a)}{E(x^2 a/b)E(x^6 a/b)} \prod_{j=1}^{N-4} \frac{E(x^{2s}a/a_j)E(x^{4s}a_j/a)}{E(x^{2s}a_j/a)E(x^{4s}a/a_j)}. \tag{A1}$$

In the $x \to 0$ limit this gives the equation

$$a^{N-4} + \frac{1}{\omega}(A_{N-4} b^4)^{3/5}/b^4 = 0,$$

so that as usual we find an expression involving the prefactors

$$\frac{1}{\omega}(A_{N-4} b^4)^{3/5} = A_{N-4} b^4.$$

Using this with the other Bethe equations in the $x \to 0$ limit we obtain

$$\left[\frac{1}{\omega}(A_{N-4} b^4)^{3/5} \right]^4 = \frac{(A_{N-4} b^4)^4}{b^{4N}} \Rightarrow b^{4N} = 1.$$

From (A1) come the recurrences

$$\mathcal{F}_4(a) = \frac{(x^{34}a/b, x^{38}a/b; x^{2r})_\infty}{(x^2 a/b, x^6 a/b; x^{2r})_\infty} \frac{\mathcal{F}_4(x^{2s}a)}{\mathcal{F}_4(x^{4s}a)},$$

$$\mathcal{G}_4(1/a) = \frac{(x^{30}b/a, x^{26}b/a; x^{2r})_\infty}{(x^{58}b/a, x^{62}b/a; x^{2r})_\infty} \frac{\mathcal{G}_4(x^{2s}/a)}{\mathcal{G}_4(x^{4s}/a)}.$$

The solutions are

$$\mathcal{F}_4(a) = \frac{(x^{38}a/b, x^{42}a/b, x^{50}a/b, x^{54}a/b; x^{2r})_\infty}{(x^2 a/b, x^6 a/b, x^{14}a/b, x^{18}a/b; x^{2r})_\infty} \frac{(x^{34}a/b, x^{38}a/b, x^{46}a/b, x^{50}a/b; x^{12s})_\infty}{(x^{70}a/b, x^{74}a/b, x^{82}a/b, x^{86}a/b; x^{12s})_\infty},$$

$$\mathcal{G}_4(1/a)=\frac{(x^{26}b/a,x^{30}b/a,x^{38}b/a,x^{42}b/a;x^{2r})_\infty}{(x^{62}b/a,x^{66}b/a,x^{74}b/a,x^{78}b/a;x^{2r})_\infty}\frac{(x^{94}b/a,x^{98}b/a,x^{106}b/a,x^{110}b/a;x^{12s})_\infty}{(x^{58}b/a,x^{62}b/a,x^{70}b/a,x^{74}b/a;x^{12s})_\infty}.$$

In terms of these functions the eigenvalue may be represented as

$$\frac{\Lambda_4}{3}=\frac{w^2}{b^2}\frac{(x^{18}w/b,x^{30}w/b,x^{10}b/w,x^{22}b/w;x^{2r})_\infty}{(x^{10}w/b,x^{22}w/b,x^{30}b/w,x^{18}b/w;x^{2r})_\infty}\mathcal{F}_4(x^{2s}w)\mathcal{G}_4(1/x^{2s}w).$$

Thus, application of the perturbation argument yields the excitation to be

$$\frac{\Lambda_4}{\Lambda_0}=w^2\frac{E(-x^{10}/w,x^{12s})E(-x^{14}/w,x^{12s})E(-x^{46}w,x^{12s})E(-x^{50}w,x^{12s})}{E(-x^{10}w,x^{12s})E(-x^{14}w,x^{12s})E(-x^{46}/w,x^{12s})E(-x^{50}/w,x^{12s})},\tag{A2}$$

where we have put $b=-1$.

2. Mass m_5

We begin the perturbation argument with $w_j=a_j$ for $j=1,\ldots,N-4$ and $w_{N-3}=b_1x^{-16}$, $w_{N-2}=b_2x^{16}$, $w_{N-1}=b_3x^{-12}$, $w_N=b_4x^{12}$. We can show that the b_i are equal, and we call them b. The Bethe equation for the other roots is

$$-\omega\left[a\frac{E(x^{2s}/a)}{E(x^{2s}a)}\right]^N=(A_{N-4}b^4)^{3/5}\frac{a^4}{b^4}\frac{E(x^8b/a)E^2(x^{12}b/a)}{E(x^8a/b)E^2(x^{12}a/b)}\times\frac{E(x^{16}b/a)}{E(x^{16}a/b)}\prod_{j=1}^{N-4}\frac{E(x^{2s}a/a_j)E(x^{4s}a_j/a)}{E(x^{2s}a_j/a)E(x^{4s}a/a_j)}.\tag{A3}$$

In the $x\to 0$ limit this gives the equation

$$a^{N-4}+\frac{1}{\omega}(A_{N-4}b^4)^{3/5}/b^4=0,$$

which leads in the usual way to a prefactor expression

$$\frac{1}{\omega}(A_{N-4}b^4)^{3/5}=A_{N-4}b^4.$$

From this and the other Bethe equations

$$\left[\frac{1}{\omega}(A_{N-4}b^4)^{3/5}\right]^4=\frac{(A_{N-4}b^4)^4}{b^{5N}}\Rightarrow b^{5N}=1.$$

Rearranging (A3), the auxiliary functions obey the recurrences

$$\mathcal{F}_5(a)=\frac{(x^{24}a/b,x^{28}a/b,x^{28}a/b,x^{32}a/b;x^{2r})_\infty}{(x^8a/b,x^{12}a/b,x^{12}a/b,x^{16}a/b;x^{2r})_\infty}\frac{\mathcal{F}_5(x^{2s}a)}{\mathcal{F}_5(x^{4s}a)},$$

$$\mathcal{G}_5(1/a)=\frac{(x^{32}b/a,x^{36}b/a,x^{36}b/a,x^{40}b/a;x^{2r})_\infty}{(x^{48}b/a,x^{52}b/a,x^{52}b/a,x^{56}b/a;x^{2r})_\infty}\frac{\mathcal{G}_5(x^{2s}/a)}{\mathcal{G}_5(x^{4s}/a)}.$$

The solutions are

$$\mathcal{F}_5(a)=\frac{(x^{32}a/b,x^{40}a/b,x^{44}a/b;x^{2r})_\infty}{(x^{12}a/b,x^{16}a/b,x^{24}a/b;x^{2r})_\infty}\frac{(x^{28}a/b,x^{36}a/b,x^{40}a/b,x^{44}a/b,x^{48}a/b,x^{56}a/b;x^{12s})_\infty}{(x^8a/b,x^{12}a/b,x^{20}a/b,x^{64}a/b,x^{72}a/b,x^{76}a/b;x^{12s})_\infty},$$

$$\mathcal{G}_5(1/a)=\frac{(x^{40}b/a,x^{36}b/a,x^{48}b/a;x^{2r})_\infty}{(x^{56}b/a,x^{64}b/a,x^{68}b/a;x^{2r})_\infty}\frac{(x^{32}b/a,x^{36}b/a,x^{44}b/a,x^{88}b/a,x^{96}b/a,x^{100}b/a;x^{12s})_\infty}{(x^{52}b/a,x^{60}b/a,x^{64}b/a,x^{68}b/a,x^{72}b/a,x^{80}b/a;x^{12s})_\infty},$$

which we next substitute into the eigenvalue expression

$$\frac{\Lambda_5}{3}=-\frac{w^3}{b^3}\frac{(x^{24}w/b,x^{28}w/b,x^{36}w/b,x^4b/w,x^{12}b/w,x^{16}b/w;x^{2r})_\infty}{(x^4w/b,x^{12}w/b,x^{16}w/b,x^{24}b/w,x^{28}b/w,x^{36}b/w;x^{2r})_\infty}\mathcal{F}_5(x^{2s}w)\mathcal{G}_5(1/x^{2s}w),$$

to obtain (with $b=-1$) an expression in elliptic functions of nome x^{12s},

$$\frac{\Lambda_5}{\Lambda_0}=w^3\frac{E(-x^4/w)E(-x^{12}/w)E(-x^{16}/w)E(-x^{40}w)E(-x^{48}w)E(-x^{52}w)}{E(-x^4w)E(-x^{12}w)E(-x^{16}w)E(-x^{40}/w)E(-x^{48}/w)E(-x^{52}/w)}. \tag{A4}$$

3. Mass m_6

We begin the perturbation argument with $w_j=a_j$ for $j=1,\ldots,N-5$ and $w_{N-4}=b_1x^{20}$, $w_{N-3}=b_2x^{-16}$, $w_{N-2}=b_3x^{16}$, $w_{N-1}=b_4x^{-8}$, $w_N=b_5x^8$. We can show that the b_i are equal, and we call them b. The Bethe equation for the other roots is

$$\omega\left[a\frac{E(x^{2s}/a)}{E(x^{2s}a)}\right]^N=(A_{N-5}b^5)^{3/5}\frac{a^5}{b^5}\frac{E(x^4b/a)E(x^8b/a)}{E(x^4a/b)E^2(x^8a/b)}\times\frac{E(x^{12}b/a)E(x^{16}b/a)}{E(x^{12}a/b)E(x^{16}a/b)}\prod_{j=1}^{N-5}\frac{E(x^{2s}a/a_j)E(x^{4s}a_j/a)}{E(x^{2s}a_j/a)E(x^{4s}a/a_j)}. \tag{A5}$$

In the $x\to 0$ limit this gives the equation

$$a^{N-5}-\frac{1}{\omega}(A_{N-5}b^5)^{3/5}/b^5=0,$$

which leads in the usual way to the expression

$$\frac{1}{\omega}(A_{N-5}b^5)^{3/5}=A_{N-5}b^5.$$

From this and the other Bethe equations

$$\left[\frac{1}{\omega}(A_{N-5}b^5)^{3/5}\right]^5=\frac{(A_{N-5}b^5)^5}{b^{5N}}\Rightarrow b^{5N}=1.$$

After rearranging (A5), the auxiliary functions obey the recurrences

$$\mathcal{F}_6(a)=\frac{(x^{24}a/b,x^{28}a/b,x^{32}a/b,x^{36}a/b;x^{2r})_\infty}{(x^4a/b,x^8a/b,x^{12}a/b,x^{16}a/b;x^{2r})_\infty}\frac{\mathcal{F}_6(x^{2s}a)}{\mathcal{F}_6(x^{4s}a)},$$

$$\mathcal{G}_6(1/a)=\frac{(x^{28}b/a,x^{32}b/a,x^{36}b/a,x^{40}b/a;x^{2r})_\infty}{(x^{48}b/a,x^{52}b/a,x^{56}b/a,x^{60}b/a;x^{2r})_\infty}\frac{\mathcal{G}_6(x^{2s}/a)}{\mathcal{G}_6(x^{4s}/a)}.$$

The solutions are

$$\mathcal{F}_6(a)=\frac{(x^{36}a/b,x^{40}a/b;x^{2r})_\infty}{(x^{16}a/b,x^{20}a/b;x^{2r})_\infty}\frac{(x^{32}a/b,x^{36}a/b,x^{40}a/b,x^{44}a/b,x^{48}a/b,x^{52}a/b;x^{12s})_\infty}{(x^4a/b,x^8a/b,x^{12}a/b,x^{16}a/b,x^{68}a/b,x^{72}b/a;x^{12s})_\infty},$$

$$\mathcal{G}_6(1/a)=\frac{(x^{40}b/a,x^{44}b/a;x^{2r})_\infty}{(x^{60}b/a,x^{64}b/a;x^{2r})_\infty}\frac{(x^{28}b/a,x^{32}b/a,x^{36}b/a,x^{40}b/a,x^{92}b/a,x^{96}b/a;x^{12s})_\infty}{(x^{56}b/a,x^{60}b/a,x^{64}b/a,x^{68}b/a,x^{72}b/a,x^{76}b/a;x^{12s})_\infty},$$

which we next substitute into the eigenvalue expression

$$\frac{\Lambda_6}{3}=-\frac{w^3}{b^3}\frac{(x^{28}w/b,x^{32}w/b,x^8b/w,x^{12}b/w;x^{2r})_\infty}{(x^8w/b,x^{12}w/b,x^{28}b/w,x^{32}b/w;x^{2r})_\infty}\mathcal{F}_6(x^{2s}w)\mathcal{G}_6(1/x^{2s}w),$$

to obtain (with $b=-1$) an expression in elliptic functions of nome x^{12s},

$$\frac{\Lambda_6}{\Lambda_0}=w^3\frac{E(-x^8/w)E(-x^{12}/w)E(-x^{16}/w)E(-x^{44}w)E(-x^{48}w)E(-x^{52}w)}{E(-x^8w)E(-x^{12}w)E(-x^{16}w)E(-x^{44}/w)E(-x^{48}/w)E(-x^{52}/w)}. \tag{A6}$$

4. Mass m_7

We begin with $w_j=a_j$ for $j=1,\ldots,N-6$ and $w_{N-5}=b_1x^{-18}$, $w_{N-4}=b_2x^{18}$, $w_{N-3}=b_3x^{-14}$, $w_{N-2}=b_4x^{14}$, $w_{N-1}=b_5x^{-10}$, $w_N=b_6x^{10}$. Once again the $b_i(=b)$ are all equal. The Bethe equation for the other roots is

$$-\omega\left[a\frac{E(x^{2s}/a)}{E(x^{2s}a)}\right]^N=(A_{N-6}b^6)^{3/5}\frac{a^6}{b^6}\frac{E(x^6b/a)E^2(x^{10}b/a)}{E(x^6a/b)E^2(x^{10}a/b)}$$
$$\times\frac{E^2(x^{14}b/a)E(x^{18}b/a)}{E^2(x^{14}a/b)E(x^{18}a/b)}\prod_{j=1}^{N-6}\frac{E(x^{2s}a/a_j)E(x^{4s}a_j/a)}{E(x^{2s}a_j/a)E(x^{4s}a/a_j)}.$$

In the $x\to 0$ limit this gives

$$a^{N-6}+\frac{1}{\omega}(A_{N-6}b^6)^{3/5}/b^6=0,$$

which leads to the expression in the various coefficients

$$\frac{1}{\omega}(A_{N-6}b^6)^{3/5}=A_{N-6}b^6,$$

and from the six Bethe equations involving b,

$$\left[\frac{1}{\omega}(A_{N-6}b^6)^{3/5}\right]^6=\frac{(A_{N-6}b^6)^6}{b^{4N}}\Rightarrow b^{4N}=1.$$

The recurrences to be solved for the auxiliary functions are

$$\mathcal{F}_7(a)=\frac{(x^{22}a/b,x^{26}a/b,x^{26}a/b,x^{30}a/b,x^{30}a/b,x^{34}a/b;x^{2r})_\infty}{(x^6a/b,x^{10}a/b,x^{10}a/b,x^{14}a/b,x^{14}a/b,x^{18}a/b;x^{2r})_\infty}\frac{\mathcal{F}_7(x^{2s}a)}{\mathcal{F}_7(x^{4s}a)},$$

$$\mathcal{G}_7(1/a)=\frac{(x^{30}b/a,x^{34}b/a,x^{34}b/a,x^{38}b/a,x^{38}b/a,x^{42}b/a;x^{2r})_\infty}{(x^{46}b/a,x^{50}b/a,x^{50}b/a,x^{54}b/a,x^{54}b/a,x^{58}b/a;x^{2r})_\infty}\frac{\mathcal{G}_7(x^{2s}/a)}{\mathcal{G}_7(x^{4s}/a)},$$

which have solution

$$\mathcal{F}_7(a)=\frac{(x^{34}a/b\,,x^{38}a/b\,,x^{42}a/b\,,x^{46}a/b\,;x^{2r})_\infty}{(x^{10}a/b\,,x^{14}a/b\,,x^{18}a/b\,,x^{22}a/b\,;x^{2r})_\infty}$$
$$\times\frac{(x^{30}a/b\,,x^{34}a/b\,,x^{38}a/b\,,x^{42}a/b\,,x^{42}a/b\,,x^{46}a/b\,,x^{50}a/b\,,x^{54}a/b\,;x^{12s})_\infty}{(x^{6}a/b\,,x^{10}a/b\,,x^{14}a/b\,,x^{18}a/b\,,x^{66}a/b\,,x^{70}a/b\,,x^{74}a/b\,,x^{78}a/b\,;x^{12s})_\infty},$$

$$\mathcal{G}_7(1/a)=\frac{(x^{34}b/a\,,x^{38}b/a\,,x^{42}b/a\,,x^{46}b/a\,;x^{2r})_\infty}{(x^{58}b/a\,,x^{62}b/a\,,x^{66}b/a\,,x^{70}b/a\,;x^{2r})_\infty}$$
$$\times\frac{(x^{30}b/a\,,x^{34}b/a\,,x^{38}b/a\,,x^{42}b/a\,,x^{90}b/a\,,x^{94}b/a\,,x^{98}b/a\,,x^{102}b/a\,;x^{12s})_\infty}{(x^{54}b/a\,,x^{58}b/a\,,x^{62}b/a\,,x^{66}b/a\,,x^{66}b/a\,,x^{70}b/a\,,x^{74}b/a\,,x^{78}b/a\,;x^{12s})_\infty}.$$

Substitution into

$$\frac{\Lambda_7}{3}=\frac{w^4}{b^4}\,\frac{(x^{22}w/b,x^{26}w/b,x^{30}w/b,x^{34}w/b,x^{6}b/w,x^{10}b/w,x^{14}b/w,x^{18}b/w;x^{2r})_\infty}{(x^{6}w/b,x^{10}w/b,x^{14}w/b,x^{18}w/b,x^{22}b/w,x^{26}b/w,x^{30}b/w,x^{34}b/w;x^{2r})_\infty}$$
$$\times\mathcal{F}_7(x^{2s}w)\mathcal{G}_7(1/x^{2s}w)$$

yields the result (with $b=-1$ and elliptic nome x^{12s})

$$\frac{\Lambda_7}{\Lambda_0}=w^4\frac{E(-x^6/w)E(-x^{10}/w)E(-x^{14}/w)E(-x^{18}/w)}{E(-x^6w)E(-x^{10}w)E(-x^{14}w)E(-x^{18}w)}$$
$$\times\frac{E(-x^{42}w)E(-x^{46}w)E(-x^{50}w)E(-x^{54}w)}{E(-x^{42}/w)E(-x^{46}/w)E(-x^{50}/w)E(-x^{54}/w)}. \tag{A7}$$

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Nonlinear Fokker–Planck equation exhibiting bifurcation phenomena and generalized thermostatistics

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A nonlinear Fokker–Planck equation exhibiting bifurcation phenomena is proposed within the framework of generalized thermostatistics. The nonlinearity responsible for the occurrence of bifurcation of solutions is assumed to be of the form appearing in the standard mean field model. A Liapunov function is defined that takes the form of free energy involving generalized entropies of Tsallis and an H-theorem is proved to show that the free energy, which is bounded below, continues to decrease until the system approaches one of the equilibrium distributions. The H-theorem ensures, instead of uniqueness of the equilibrium distribution, global stability of the system in that either one of multisolutions must be approached for large times. Local stability analysis is conducted and the second-order variation of the Liapunov function is computed to find its relevant part whose sign governs stability of the equilibrium distribution of the system. The case with a bistable potential is investigated, as an example of confirming the theory, to give the bifurcation diagram displaying the order parameter as a function of the coefficient of the nonlinear diffusion term. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Tsallis developed generalized thermostatistics[1–3] using generalized nonextensive entropies[4–10] which are obtained by extending the well-known Boltzmann entropy. Equilibrium properties of the novel thermostatistics have extensively been studied by a number of researchers to understand similarity as well as dissimilarity between the standard Boltzmann statistics and the generalized one.[11] A characteristic feature of the generalized thermostatistics is a power-law type equilibrium probability distribution that is derived from the maximum entropy principle with a certain constraint of internal energy.[1–3]

One may, however, expect that an equilibrium distribution should be derived, as a fixed point type solution, from a certain dynamical evolution equation of a time-dependent probability distribution such as a master equation of a Markovian dynamics. Several authors have studied nonlinear Fokker–Planck equations that are related to generalized thermostatistics.[12–20] Plastino and Plastino[12] proposed a nonlinear Fokker–Planck equation with a nonlinear diffusion term characterized by a real parameter q,

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\left(-\frac{\partial \phi}{\partial x}p\right) + D\frac{\partial^2}{\partial x^2}p^q \tag{1}$$

and showed that it exhibits an equilibrium solution taking the form of Tsallis equilibrium distribution of the so-called first choice[1]

$$P_{\mathrm{eq}}(x) = [(Dq\beta)^{-1}(1-\beta(q-1)\phi(x))]^{1/(q-1)}, \tag{2}$$

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where β is determined by the normalization condition. In the absence of the drift term in Eq. (1) with $\phi(x)=\text{const}$ there exists no equilibrium distribution and one has nonlinear diffusion, which was studied by several authors in connection with diffusion in porous media.[21–25]

In the case where the potential $\phi(x)$ is quadratic, the nonlinear Fokker–Planck equation (NFPE) was shown to be solved for its temporal solution in a rigorous way.[12,15,16] A phenomenological derivation of the NFPE itself was given in Refs. 13 and 14, where the author considered a stochastic differential equation with a self-reference type feedback representing the nonlinear diffusion term.

While the Tsallis equilibrium distribution was shown to satisfy the NFPE, its stability and uniqueness has been another problem. The relationship between the NFPE and the generalized entropy is also of interest and worth studying.

In the case of linear Fokker–Planck equations, which appear as master equations for stochastic systems with Markovian dynamics, stability and uniqueness of their equilibrium solutions is known to be ensured by the so-called H-theorems.[26–30] Liapunov functions as the H-functions can be chosen as closely related to the free energy of a system[31] and also to the conventional Kullback–Leibler divergence[26–30,32] or generalized Kullback–Leibler divergences.[31,33–39]

Recently I have tackled the above-mentioned kind of problems with the NFPE to provide a dynamics-level linkage of the generalized entropy to the NFPE together with knowledge of the asymptotic approach of temporal solutions of the NFPE to its equilibrium solution.[18] Constructing a Lyapunov functional that takes the form of a free energy based on the generalized entropy,[18]

$$F=\int_{-\infty}^{\infty}\phi p\,\mathrm{d}x-\frac{D}{q-1}\left[1-\int_{-\infty}^{\infty}p^{q}\,\mathrm{d}x\right], \tag{3}$$

I showed that an H-theorem holds for the NFPE (1):[18]

$$\frac{\mathrm{d}F}{\mathrm{d}t}\leqslant 0, \tag{4}$$

which ensures stability and uniqueness of its equilibrium solution. Such convergence property with an H-theorem is not specific to the system described by the above-mentioned NFPE (1). A NFPE with a nonlocal time-dependent nonlinear diffusion coefficient,[18]

$$\frac{\partial p}{\partial t}=-\frac{\partial}{\partial x}(A(x)p)+\frac{1}{\beta}\left(\int_{-\infty}^{\infty}p^{Q}\,\mathrm{d}x\right)^{-(Q+1)/Q}\frac{\partial^{2}}{\partial x^{2}}p^{Q}, \tag{5}$$

which allows for an equilibrium solution corresponding to another type of equilibrium distribution of Tsallis thermostatistics (the escort probability distribution of the so-called third version[3]),

$$P_{\mathrm{eq}}(x)=\tilde{C}_{0}(Q)^{-Q/(Q-1)}\left[1-\frac{\beta(Q-1)}{\tilde{C}_{0}(Q)Q}(\phi(x)-\langle\phi\rangle)\right]^{1/(Q-1)}, \tag{6}$$

also exhibits similar convergence properties based on an H-theorem, when the modified generalized entropy

$$\tilde{S}\equiv\frac{1}{\frac{1}{Q}-1}\left[1-\left(\int_{-\infty}^{\infty}p^{Q}\,\mathrm{d}x\right)^{-1/Q}\right] \tag{7}$$

is considered.[18] The above-mentioned entropy is a special case of the Sharma and Mittal entropy.[6] H-theorems for a little more general types of NFPEs related to generalized thermostatistics including Eq. (1) have recently been studied by Frank and Daffertshofer.[19]

The above-mentioned results indicate that although the time evolution equations (1) and (5) are nonlinear, there occurs no bifurcation of solutions with change in parameters characterizing the system. This situation is in sharp contrast to the case of NFPE for a mean field model, where one deals with another type of NFPE that is derived, in the thermodynamic limit, for a coupled Langevin equation system.[40–42] The simplest NFPE exhibiting bifurcation phenomena reads[40–42]

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\left[\left(x - x^3 + \varepsilon \int_{-\infty}^{\infty} xp\, \mathrm{d}x\right)p\right] + D\frac{\partial^2}{\partial x^2}p \tag{8}$$

Such mean field type of NFPE has attracted much attention from researchers in a number of areas of physical science, since it is quite convenient to observe the effect of noise on a variety of cooperative phenomena of coupled systems and to systematically study equilibrium as well as nonequilibrium phase transitions. The NFPE (8) with a double well potential $\phi(x) = -(x^2/2) + (x^4/4)$ can describe ferro–para magnetic phase transitions of mean field type.[40–43] NFPEs corresponding to mean field coupled limit cycle[44] or phase oscillator systems[45–48] have been studied by several authors from the viewpoint of synchronization–desynchronization transitions due to noise and of neural network theory. An NFPE for chaotic systems has been recently studied in the light of control of chaos with noise.[49]

The problem of phase transitions within the framework of Tsallis thermostatistics will be of interest, but it has been far less studied.[50]

The purpose of this paper is to study the occurrence of bifurcations for NFPEs that are related to Tsallis thermostatistics. To this end I propose a double nonlinear Fokker–Planck equation that is obtained by introducing such a mean field type nonlinear term as considered in Eq. (8) into the NFPE (1) and investigate the issue of convergence to equilibrium solutions together with their global and local stability.

After describing the model in Sec. II, I show in Sec. III that a Liapunov function for our double NFPE can be defined so that it takes the form of free energy involving generalized entropies of Tsallis. I prove an H-theorem to show that the free energy, which is bounded below, continues to decrease until the system approaches one of the equilibrium distributions. The H-theorem ensures, instead of uniqueness of the equilibrium distribution, global stability of the system in that either one of multisolutions must be approached for large times. In Sec. IV local stability analysis is conducted and the second-order variation of the Liapunov function is computed to find its relevant part whose sign governs stability of the equilibrium distribution of the system. As an example of confirming the theory, I investigate the case with a bistable potential to give the bifurcation diagram displaying the order parameter as a function of the coefficient of the nonlinear diffusion term. In Sec. V I present a summary and discussion.

II. MODEL

We consider a double nonlinear Fokker–Planck equation of the following form:

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\left[\left(A(x) + \varepsilon \int_I xp\, \mathrm{d}x\right)p\right] + D\frac{\partial^2}{\partial x^2}p^q, \tag{9}$$

which is obtained by introducing, into the drift coefficient of the NFPE (1), a term representing nonlocal feedback from the entire system in terms of the average of the state variable x. Here ε (a real number) controls the magnitude of the feedback, and q is a real number, D a positive constant, and $A(x)$ in the drift coefficient an arbitrary function with potential $\phi(x)$:

$$\phi(x) = -\int^x A(x)\mathrm{d}x. \tag{10}$$

The symbol I in the integral denotes the region where non-negative valued $p(t,x)$ is defined. Since the equation with $\varepsilon=0$ itself is already a nonlinear one, we will refer to the above-mentioned nonlinear Fokker Planck equation as double nonlinear Fokker–Planck equation (DNFPE).

Since introducing the probability current j,

$$j=\left(A(x)+\varepsilon\int_I xp\,\mathrm{d}x\right)p-D\frac{\partial}{\partial x}p^q, \tag{11}$$

one can rewrite our DNFPE in the form of the continuity equation. The conservation law of probability holds:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_I p\,\mathrm{d}x=0$$

under the boundary condition that the probability current j vanishes at the boundary of I. For the sake of simplicity, in this article we consider the case of $I=R^1\equiv(-\infty,\infty)$ to choose the natural boundary condition:

$$p(t,\pm\infty)=0,\quad \frac{\partial p^q}{\partial x}(t,\pm\infty)=0. \tag{12}$$

Since $\partial p/\partial t=0$ implies $j=0$, one has

$$P_{\mathrm{eq}}^{q-1}=\frac{-(q-1)\tilde{\phi}(x)}{Dq}+(Dq\beta)^{-1}, \tag{13}$$

where

$$\tilde{\phi}(x)=\phi(x)-\varepsilon x\int_I xP_{\mathrm{eq}}\,\mathrm{d}x$$

and the integration constant is set to be $(Dq\beta)^{-1}$.

Accordingly, the equilibrium distribution for the DNFPE (9) can be formally obtained as

$$P_{\mathrm{eq}}(x)=[(Dq\beta)^{-1}(1-\beta(q-1)\tilde{\phi}(x))]^{1/(q-1)}, \tag{14}$$

where β will be determined by normalization of $P_{\mathrm{eq}}(x)$.

For the purpose of studying phenomena of spontaneous symmetry breaking, it will suffice to suppose the potential ϕ to take the form of double well type such as $\phi=ax^2+bx^4$ $(a<0,b>0)$. When $\phi(x)\to\infty$ as $|x|\to\infty$, Eq. (14) implies $0<q<1$ and hence $P_{\mathrm{eq}}\to 0(|x|\to\infty)$. Assuming that $0<q<1$ and $\phi(x)\approx|x|^m$ with $m>0$ $(|x|\to\infty)$, one also has

$$\frac{\partial {P_{\mathrm{eq}}}^q}{\partial x}\approx|x|^{mq/(q-1)-1}\to 0(|x|\to\infty).$$

In what follows we deal with the case with $0<q<1$, where the natural boundary condition (12) makes sense, and assume the existence of the integrals $\int\phi p\,\mathrm{d}x$ and $\int p^q\,\mathrm{d}x$, where the integrals are meant to be performed over the real line $I=R^1\equiv(-\infty,\infty)$ and hereafter the I will be omitted. For $p=P_{\mathrm{eq}}$ and $\phi(x)\approx|x|^m$ (for large $|x|$), the condition of such integrability becomes $1/(m+1)<q<1$.

Since the expression for the equilibrium distribution P_{eq} contains P_{eq} itself, the problem of approach to the equilibrium distribution is not trivial. This issue can be more clearly seen in the study of nonlinear stability analysis of the solutions.

III. H-THEOREM

We define a Liapunov functional taking the form of a free energy based on Tsallis entropy as

$$F(p(\cdot))=\int\left(\phi-\varepsilon x\int_R xp\,\mathrm{d}x\right)p\,\mathrm{d}x+\frac{\varepsilon}{2}\left(\int_R xp\,\mathrm{d}x\right)^2-\frac{D}{q-1}\left[1-\int p^q\,\mathrm{d}x\right]=U-DS, \quad (15)$$

where the energy U represents the first two terms on the right-hand side of the first line:

$$U=\int\left(\phi-\varepsilon x\int_R xp\,\mathrm{d}x\right)p\,\mathrm{d}x+\frac{\varepsilon}{2}\left(\int_R xp\,\mathrm{d}x\right)^2=\int\phi p\,\mathrm{d}x-\frac{\varepsilon}{2}\left(\int_R xp\,\mathrm{d}x\right)^2 \quad (16)$$

and the entropy S is the nonextensive one given within Tsallis thermostatistics:[1–3]

$$S\equiv\frac{1}{q-1}\left[1-\int p^q\,\mathrm{d}x\right]. \quad (17)$$

With this Liapunov functional taken as the H-functional we can show an H-theorem for the DNFPE (9).

H-theorem: Let $0<q<1$. Let $p(t,x)$ satisfy the DNFPE (9). Then we have
(1) the free energy $F(p(t,\cdot))$ is bounded from below:

$$F(p(t,\cdot))>C_F(\text{const}); \quad (18)$$

(2) $F(p(t,\cdot))$ is decreasing with time:

$$\frac{\mathrm{d}F(p(t,\cdot))}{\mathrm{d}t}\leqslant 0. \quad (19)$$

Proof of (1): In the case with $\varepsilon\leqslant 0$, it immediately follows from Eqs. (15) and (16) that

$$F(p(\cdot))\geqslant\int\phi p\,\mathrm{d}x-\frac{D}{q-1}\left(1-\int p^q\,\mathrm{d}x\right)\equiv F^{(\varepsilon=0)}(p(\cdot)). \quad (20)$$

Note that as was studied in Ref. 18 the free energy $F^{(\varepsilon=0)}(p(\cdot))$ with $0<q<1$ is bounded from below:

$$F^{(\varepsilon=0)}(p(\cdot))\geqslant F^{(\varepsilon=0)}(P_{\mathrm{eq}}(\cdot;\varepsilon=0))=-D\int {P_{\mathrm{eq}}}^q(\cdot;\varepsilon=0)\mathrm{d}x+\frac{1}{q-1}\left(\frac{1}{\beta}-D\right), \quad (21)$$

where $P_{\mathrm{eq}}(\cdot;\varepsilon=0)$ is given by the equilibrium distribution (2).
Accordingly one has

$$F(p(\cdot))\geqslant F^{(\varepsilon=0)}(P_{\mathrm{eq}}(\cdot;\varepsilon=0)) \quad (22)$$

to confirm Eq. (18).

To deal with the case with $\varepsilon>0$ putting

$$\langle x\rangle_p\equiv\int_R xp\,\mathrm{d}x \quad (23)$$

we first note that one can define the normalized positive-valued function $R_p(t,x)$ as

$$\phi-\varepsilon x\langle x\rangle_p=\frac{Dq\beta_0{R_p}^{q-1}-1}{(1-q)\beta_0}, \quad (24)$$

$$\int R_p(t,x)\mathrm{d}x=1$$

with β_0 denoting a constant determined uniquely as a function of D and $\varepsilon\langle x\rangle_p$. The existence of such β_0 can easily be confirmed by noting that the integral of the solution R_p to the first equation of Eq. (24) as a function of β_0 would monotonically increase from 0 to ∞ as β_0 varies from

$$\beta_0=+0 \quad \text{to} \quad \beta_0=\frac{-1}{(1-q)\mathrm{Min}_{-\infty<x<\infty}(\phi(x)-\varepsilon x\langle x\rangle_p)}>0$$

where we have assumed, for simplicity, that the minimum of $\phi(x)$ is negative to make β_0 of the latter positive. Note that in general β_0 in Eq. (24) may be determined to take a negative value.

The R_p turns out to satisfy

$$-\frac{\partial}{\partial x}\{(-\phi_x(x)+\varepsilon\langle x\rangle_p)R_p\}+D\frac{\partial^2}{\partial x^2}R_p^q=0. \tag{25}$$

To prove inequality (18) with $\varepsilon>0$, using (24) we rewrite $F(p(t,\cdot))$ as

$$F(p(\cdot))=\frac{D}{q-1}\int (p^q-qpR_p^{q-1}+(q-1)R_p^q)\mathrm{d}x+\frac{1}{q-1}\left(\frac{1}{\beta_0}-D\right)+\frac{\varepsilon}{2}[\langle x\rangle_p]^2-D\int R_p^q\,\mathrm{d}x. \tag{26}$$

Since for $0<q<1$,

$$p^q-qpR_p^{q-1}+(q-1)R_p^q=R_p^q(y^q-qy+q-1)\leqslant 0 \tag{27}$$

with $y\equiv p/R_p$ and equality being given only by $y=1$, we have

$$\frac{D}{q-1}\int (p^q-qpR_p^{q-1}+(q-1)R_p^q)\mathrm{d}x\geqslant 0 \tag{28}$$

and hence

$$F(p(\cdot))\geqslant L(\varepsilon\langle x\rangle_p), \tag{29}$$

where we have defined L as a function of $\varepsilon\langle x\rangle_p$ as

$$L(\varepsilon\langle x\rangle_p)=\frac{1}{2\varepsilon}(\varepsilon\langle x\rangle_p)^2+\frac{1}{q-1}\left(\frac{1}{\beta_0}-D\right)-D\int R_p^q\,\mathrm{d}x. \tag{30}$$

We will show that L is bounded from below. To this end, we differentiate L with respect to $\varepsilon\langle x\rangle_p$:

$$\frac{\mathrm{d}L(h)}{\mathrm{d}h}=\frac{h}{\varepsilon}+\frac{\partial\tilde{F}(D,h)}{\partial h}, \tag{31}$$

where we have defined

$$\tilde{F}(D,h)=\frac{1}{q-1}\left(\frac{1}{\beta_0}-D\right)-D\int R_p^q\,\mathrm{d}x \tag{32}$$

with $h=\varepsilon\langle x\rangle_p$.

Here we note that the above-defined $\tilde{F}(D,h)$ turns out to be the free energy function[18] corresponding to the equilibrium distribution (2) with $\phi(x)$ being replaced by $\phi(x)-hx$ and $\beta=\beta_0$, which the R_p (24) with $h=\varepsilon\langle x\rangle_p$ coincides with.

Then it follows that

$$\frac{\partial\tilde{F}(D,h)}{\partial h}=-\langle x\rangle_{R_{D,h}}\equiv-\int xR_{D,h}(x)\mathrm{d}x \tag{33}$$

together with

$$\frac{\partial\tilde{F}(D,h)}{\partial D}=-S, \tag{34}$$

which exhibit the Legendre transform structure of the Tsallis thermostatistics of the first choice, and can be confirmed by straightforward calculations. In Eq. (33) we have written $R_{D,h}$ instead of R_p to emphasize the h-dependence of R in Eq. (24) with $h=\varepsilon\langle x\rangle_p$.

Furthermore, $\partial\tilde{F}/\partial h$ has the following properties:

(A)

$$-\frac{\partial^2\tilde{F}}{\partial h^2}>0. \tag{35}$$

(B) If $\phi(x)$ increases faster than $\phi(x)\propto x^2$ when $|x|\to\infty$, then

$$-\frac{1}{h}\frac{\partial\tilde{F}}{\partial h}\to 0 \quad (h\to\pm\infty). \tag{36}$$

The proof is given in the appendices.

Applying Eq. (36) to Eq. (31) one has $\mathrm{d}L(h)/\mathrm{d}h>0$ (for large h) and $\mathrm{d}L(h)/\mathrm{d}h<0$ (for large $-h$) when $\varepsilon>0$.

This implies that $L(h)$ can exhibit its minimum at a certain $\bar{h}$ satisfying $\mathrm{d}L(\bar{h})/\mathrm{d}h=0$ to have a lower bound: $L(h)\geqslant L(\bar{h})$, which together with Eq. (29) shows that $F(p(\cdot))$ is bounded from below.

Proof of (2): To prove the second inequality (19) we differentiate $F(p(t,\cdot))$ with respect to t. Using Eq. (9) one obtains

$$\begin{aligned}\frac{\mathrm{d}F(p(t,\cdot))}{\mathrm{d}t}&=\int(\phi-\varepsilon x\langle x\rangle_p)\frac{\partial p}{\partial t}\mathrm{d}x-\frac{\mathrm{d}}{\mathrm{d}t}\frac{D}{q-1}\left[1-\int p^q\,\mathrm{d}x\right]\\&=\int\left(\phi-\varepsilon x\langle x\rangle_p+\frac{Dq}{q-1}p^{q-1}\right)\left[-\frac{\partial}{\partial x}\{(-\phi_x(x)+\varepsilon\langle x\rangle_p)p\}+D\frac{\partial^2}{\partial x^2}p^q\right]\mathrm{d}x\\&=\int\left[\frac{\partial}{\partial x}\left(\phi-\varepsilon x\langle x\rangle_p+\frac{Dq}{q-1}p^{q-1}\right)\right]\left[(-\phi_x(x)+\varepsilon\langle x\rangle_p)p-D\frac{\partial}{\partial x}p^q\right]\mathrm{d}x,\end{aligned} \tag{37}$$

where integration by parts has been used in the last line.

Substituting (24) into (37), we further rewrite $\mathrm{d}F/\mathrm{d}t$ as

$$\frac{\mathrm{d}F(p(t,\cdot))}{\mathrm{d}t}=\int\left[B_1\left(\frac{\partial p}{\partial x}\right)^2+B_2\frac{\partial p}{\partial x}\frac{\partial R_p}{\partial x}+B_3\left(\frac{\partial R_p}{\partial x}\right)^2\right]\mathrm{d}x, \tag{38}$$

where

$$B_1 = -D^2 q^2 p^{2q-3},$$
$$B_2 = 2D^2 q^2 p^{q-1} {R_p}^{q-2}, \tag{39}$$
$$B_3 = -D^2 q^2 p {R_p}^{2q-4}$$

and we have assumed

$$\int p^{2q-3} \left(\frac{\partial p}{\partial x} \right)^2 \mathrm{d}x < \infty,$$
$$\int p {R_p}^{2q-4} \left(\frac{\partial R_p}{\partial x} \right)^2 \mathrm{d}x < \infty.$$

Then it follows that

$$\begin{aligned} \frac{\mathrm{d}F(p(t,\cdot))}{\mathrm{d}t} &= -D^2 q^2 \int p \left(p^{q-2} \frac{\partial p}{\partial x} - {R_p}^{q-2} \frac{\partial R_p}{\partial x} \right)^2 \mathrm{d}x \\ &= -\frac{D^2 q^2}{(q-1)^2} \int p \left[\frac{\partial}{\partial x} (p^{q-1} - {R_p}^{q-1}) \right]^2 \mathrm{d}x \\ &\leqslant 0. \end{aligned} \tag{40}$$

This concludes the proof.

We see that equality is implied by

$$p^{q-1} - {R_p}^{q-1} = c(\text{const}). \tag{41}$$

Since $F(p(t,\cdot))$ is decreasing with time and is bounded from below, $\mathrm{d}F/\mathrm{d}t = 0$ is attained when $t \to \infty$, and then p must satisfy Eq. (41):

$$p = R_p, \tag{42}$$

where we have set $c = 0$, because the R_p is already normalized [see Eq. (24)].

This means that the distribution p_∞ that is approached for large times takes the form of the equilibrium distribution (14) of the DNFPE (9):

$$p_\infty = [(Dq\beta)^{-1}(1 - \beta(q-1)(\phi - \varepsilon x \langle x \rangle_{p_\infty}))]^{1/(q-1)}, \tag{43}$$

where the value of β and the order parameter $\langle x \rangle_{p_\infty}$ should be determined simultaneously by the normalization condition and the self-consistent equation

$$\langle x \rangle_{p_\infty} = \int x p_\infty \mathrm{d}x. \tag{44}$$

We note that since conservation of probability holds for the DNFPE (9), the $p_\infty(x)$ in (43) should be normalizable. Although our system allows for the H-theorem, unlike the case with $\varepsilon = 0$ we can no longer expect uniqueness of the equilibrium distribution $p_\infty(x)$ in the case with $\varepsilon > 0$, where the self-consistent equations, in general, admit multisolutions (m,β) with $m = \langle x \rangle_{p_\infty}$. This arises from the fact that $R_p(x)$ appearing in Eq. (40) is not a fixed function such as an equilibrium distribution, but does depend on the time-dependent probability distribution $p(t,x)$ [see Eq. (24)]. Which of those multisolutions are relevant has to be determined by the stability condition. In other words, there may occur bifurcation phenomena involving stability switches, as the control parameter D varies. This situation is reminiscent of the mean field model of phase

transitions that is described by the NFPE (8).[40–42] It is noted that owing to the expression of the free energy (15) together with the thermodynamic relation (34) the parameter D can be viewed as playing the role of temperature of Boltzmann–Gibbs statistics.

IV. LOCAL STABILITY ANALYSIS

To conduct local stability analysis we follow the procedure developed previously by the author[40] for the NFPE (8) of mean field models and calculate the second-order variation of the Liapunov functional (15). Differentiating F with respect to p one obtains

$$\delta F=\delta U-\delta DS=\int\left(\phi-\varepsilon x\int xp\,\mathrm{d}x\right)\delta p\,\mathrm{d}x+\frac{D}{q-1}\int qp^{q-1}\delta p\,\mathrm{d}x. \tag{45}$$

Substituting Eq. (24) and noting

$$\int\delta p\,\mathrm{d}x=0, \tag{46}$$

one obtains

$$\delta F=\frac{Dq}{q-1}\int(p^{q-1}-{R_p}^{q-1})\,\delta p\,\mathrm{d}x. \tag{47}$$

Let P_{eq} be one of the probability distributions satisfying Eq. (43) for p_∞. The first-order variation $\delta F^{(1)}|_{\mathrm{eq}}$ evaluated at $p=P_{\mathrm{eq}}$ turns out to vanish because of Eqs. (42) and (46). Differentiating δF again with respect to p one has

$$2\,\delta F^{(2)}=Dq\int[p^{q-2}(\delta p)^2-{R_p}^{q-2}\delta p\,\delta R_p]\mathrm{d}x. \tag{48}$$

Using

$$\varepsilon x\int x\delta p\,\mathrm{d}x=Dq{R_p}^{q-2}\delta R_p+\frac{1}{1-q}\frac{\partial\left(\frac{1}{\beta_0}\right)}{\partial\varepsilon\langle x\rangle_p}\varepsilon\int x\delta p\,\mathrm{d}x, \tag{49}$$

which follows from Eq. (24), one obtains

$$2\,\delta F^{(2)}=Dq\int p^{q-2}(\delta p)^2\mathrm{d}x-\varepsilon\left(\int x\delta p\,\mathrm{d}x\right)^2. \tag{50}$$

Putting $p=P_{\mathrm{eq}}$ leads to the second-order variation $\delta F^{(2)}|_{\mathrm{eq}}$ evaluated at the equilibrium point:

$$2\,\delta F^{(2)}|_{\mathrm{eq}}=Dq\int {P_{\mathrm{eq}}}^{q-2}(\delta p)^2\mathrm{d}x-\varepsilon\left(\int x\delta p\,\mathrm{d}x\right)^2, \tag{51}$$

which will be used to determine stability of the equilibrium point.

Assuming $\varphi(x)\in L^2$ (class of square integrable functions) we put

$$\delta p={P_{\mathrm{eq}}}^{(2-q)/2}\varphi(x). \tag{52}$$

We further assume that

$$\int x^2{P_{\mathrm{eq}}}^{2-q}\,\mathrm{d}x<\infty. \tag{53}$$

Decomposing $\varphi(x)$ as

$$\varphi(x)=\alpha P_{\mathrm{eq}}^{(2-q)/2}+\gamma x P_{\mathrm{eq}}^{(2-q)/2}+\varphi_{\perp}, \tag{54}$$

where $\varphi_{\perp}$ is the subspace of L^2 perpendicular to the subspace spanned by

$$P_{\mathrm{eq}}^{(2-q)/2} \text{ and } xP_{\mathrm{eq}}^{(2-q)/2},$$

we compute the second-order variation $\delta F^{(2)}|_{\mathrm{eq}}$.

Substituting Eq. (52) into Eq. (51) yields

$$2\,\delta F^{(2)}|_{\mathrm{eq}}=Dq\int[(\alpha P_{\mathrm{eq}}^{(2-q)/2}+\gamma x P_{\mathrm{eq}}^{(2-q)/2})^2+\varphi_{\perp}{}^2]\mathrm{d}x$$
$$-\varepsilon\left[\int xP_{\mathrm{eq}}^{(2-q)/2}(\alpha P_{\mathrm{eq}}^{(2-q)/2}+\gamma x P_{\mathrm{eq}}^{(2-q)/2}+\varphi_{\perp})\mathrm{d}x\right]^2. \tag{55}$$

Put

$$I_0=\int P_{\mathrm{eq}}{}^{2-q}\,\mathrm{d}x,\quad I_1=\int xP_{\mathrm{eq}}{}^{2-q}\,\mathrm{d}x,\quad I_2=\int x^2P_{\mathrm{eq}}{}^{2-q}\,\mathrm{d}x. \tag{56}$$

Noting that Eq. (46) gives

$$0=\int \delta p\,\mathrm{d}x=\alpha I_0+\gamma I_1, \tag{57}$$

one has from Eq. (55)

$$2\,\delta F^{(2)}|_{\mathrm{eq}}=Dq\left[\int \varphi_{\perp}{}^2\,\mathrm{d}x+\alpha^2I_0+\gamma^2I_2+2\alpha\gamma I_1-\frac{\varepsilon}{Dq}(\alpha I_1+\gamma I_2)^2\right]$$
$$=Dq\int \varphi_{\perp}{}^2\,\mathrm{d}x+Dq\,\gamma^2\left(I_2-\frac{I_1{}^2}{I_0}\right)\left[1-\frac{\varepsilon}{Dq}\left(I_2-\frac{I_1{}^2}{I_0}\right)\right]. \tag{58}$$

It follows from Schwartz's inequality that

$$I_2-\frac{I_1{}^2}{I_0}\geqslant 0. \tag{59}$$

Accordingly the stability condition $\delta F^{(2)}|_{\mathrm{eq}}>0$ can be reduced to

$$1-\frac{\varepsilon}{Dq}\left(I_2-\frac{I_1{}^2}{I_0}\right)>0 \tag{60}$$

and the stability switch occurs at a certain critical value D_c satisfying

$$1-\frac{\varepsilon}{D_cq}\left(I_2-\frac{I_1{}^2}{I_0}\right)=0. \tag{61}$$

This condition can also be derived from another kind of analysis based on the graphical representation[40] of the equation determining the order parameter of the system [see Eq. (44)]:

$$m=\int x[(Dq\beta)^{-1}(1-\beta(q-1)(\phi-\varepsilon x m))]^{1/(q-1)}\mathrm{d}x, \tag{62}$$

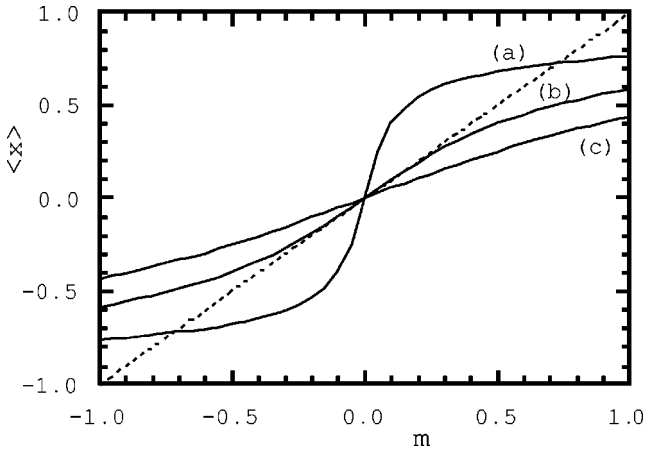

FIG. 1. Graphical representation of solving Eqs. (62) and (63) for determining the order parameter of a bistable system with $\phi(x)=-x^2+x^4$. $q=0.4$ and $\varepsilon=0.5$ are assumed. Plots as a function of m are shown of the order parameter $\langle x\rangle_{p_\infty}$ given by the right-hand side of Eq. (62) with $\beta=\beta(m)$ from Eq. (63) being substituted, for three typical values of D: (a) $D<D_c$ ($D=0.1$), (b) $D=D_c$ ($\approx 0.346\,54$), and (c) $D>D_c$ ($D=0.6$). At the bifurcation point $D=D_c$ the $\langle x\rangle_{p_\infty}$ curve (b) touches the straight line (dashed) representing the left-hand side of Eq. (62) at $m=0$.

$$1=\int [(Dq\beta)^{-1}(1-\beta(q-1)(\phi-\varepsilon xm))]^{1/(q-1)}\mathrm{d}x, \tag{63}$$

where we put $m\equiv\langle x\rangle_{p_\infty}$.

If the potential $\phi(x)$ is symmetric, i.e., $\phi(x)=\phi(-x)$, $m=0$ turns out to be a solution of the above-mentioned equations. The onset of instability of the $m=0$ solution is given by the tangency condition at $m=0$ for the curve representing the right-hand side of Eq. (62) as a function of m. In general, the tangency condition at arbitrary m reads

$$1=\frac{\mathrm{d}}{\mathrm{d}m}\int x[(Dq\beta(m))^{-1}(1-\beta(m)(q-1)(\phi-\varepsilon xm))]^{1/(q-1)}\mathrm{d}x, \tag{64}$$

which is obtained by differentiating Eq. (62) with respect to m.
Differentiating Eq. (63) with respect to m yields

$$\frac{\mathrm{d}\beta}{\mathrm{d}m}=\frac{\varepsilon(q-1)\beta^2\int x p_{\infty\,m}^{2-q}\mathrm{d}x}{\int p_{\infty\,m}^{2-q}\mathrm{d}x}, \tag{65}$$

where the m dependence of p_∞ is expressed as $p_{\infty\,m}$. Substituting this into Eq. (64) one immediately obtains

$$1=\frac{\varepsilon}{Dq}\left[\int x^2 p_{\infty\,m}^{2-q}\mathrm{d}x-\frac{(\int x p_{\infty\,m}^{2-q}\mathrm{d}x)^2}{\int p_{\infty\,m}^{2-q}\mathrm{d}x}\right]. \tag{66}$$

This is exactly the same as Eq. (61) with $P_{\mathrm{eq}}=p_{\infty\,m}$ and $D=D_c$.

We show an example of the occurrence of bifurcations for a bistable system having the potential $\phi(x)=-x^2+x^4$. Figure 1 displays the behavior of the right-hand side of Eq. (62) with $\beta=\beta(m)$, that is, the order parameter $\langle x\rangle_{p_\infty}$, plotted as a function of m for three typical values of D and how those $\langle x\rangle_{p_\infty}$ curves intersect the straight line representing the left-hand side of Eq. (62). Since the potential has symmetry, one always has the intersection at the origin that gives rise to the

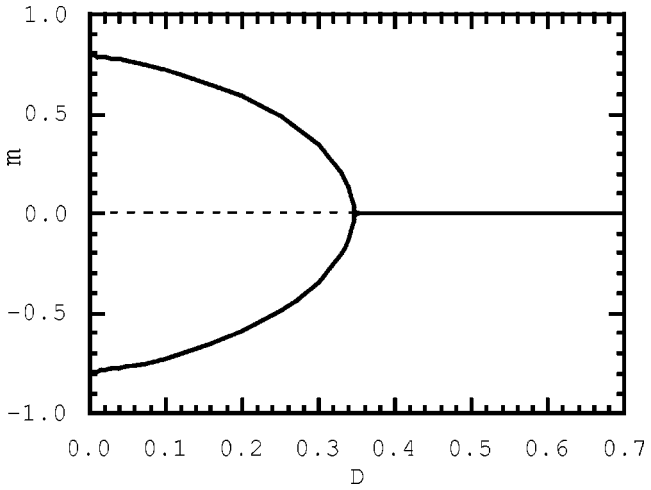

FIG. 2. Bifurcation diagram of pitch-fork type for the bistable system of Fig. 1 showing the dependence of the order parameter of the stable branch on the control parameter D together with stability switches at $D=D_c$ between stable (solid line) and unstable (dashed line) branches.

trivial solution $m=0$. We see the $\langle x\rangle_{p_\infty}$ curve for the critical value D_c touches the straight line at the origin to satisfy the criticality condition given by Eq. (66). While for $D>D_c$ the symmetric probability distribution with the order parameter $m=0$ is stable with

$$1>\frac{\mathrm{d}}{\mathrm{d}m}\int x[(Dq\beta(m))^{-1}(1-\beta(m)(q-1)(\phi-\varepsilon xm))]^{1/(q-1)}\mathrm{d}x, \tag{67}$$

it becomes unstable for $D<D_c$ and two symmetrically generated intersection points having $m\neq 0$ gain stability, because the stability condition (60) is broken. Note that in this example the symmetric probability distribution with $m=0$ for $D=D_c$ is stable because of the global stability of the system implied by the H-theorem [Eqs. (18) and (19)].

We depict in Fig. 2 the bifurcation diagram showing the dependence of the order parameter of the stable branch on the control parameter D together with stability switches between stable and unstable branches. We see as D is decreased from high values passing through the critical value D_c a symmetry breaking phenomenon occurs. When the diffusion constant D is viewed as temperature, such behavior is reminiscent of the ferromagnetic phase transition.

V. SUMMARY AND DISCUSSION

We have proposed a double nonlinear Fokker–Planck equation (DNFPE) (9) exhibiting bifurcation phenomena within the framework of generalized thermostatistics based on nonextensive-type generalized entropies. The nonlinearity responsible for the occurrence of bifurcations, which is added to the drift term of the previously known nonlinear Fokker–Planck equation of Plastino type, takes the form appearing in the standard mean field model. Our DNFPE exhibits, in general, multisolutions unlike the original NFPE (1) and then criteria for choosing relevant solutions are required.

To tackle this problem we have proven an H-theorem by constructing a Liapunov function that takes the form of free energy involving generalized entropies of Tsallis. Our H-theorem shows that the free energy, which is bounded below, continues to decrease until the system approaches one of the equilibrium distributions. More precisely, it ensures, instead of uniqueness of the equilibrium distribution, global stability of the system in that either one of the multisolutions must be approached for large times.

Stability of each ergodic component is determined by the local stability analysis in which the second-order variation of the Liapunov function takes positive values. We have computed the

second-order variation of the Liapunov function to find its relevant part whose sign governs stability of the equilibrium distribution of the system, and found that the latter can be amenable to graphical analysis used in graphically solving the order parameters.

We have given an example of the systems exhibiting bifurcation phenomena to confirm our theory. We have dealt with the case with a bistable potential and shown the bifurcation diagram displaying the order parameter as a function of the coefficient of the nonlinear diffusion term. The resultant bifurcation is similar to the behavior of the standard mean field model of ferromagnetic phase transitions.

As far as the thermodynamic equilibrium is concerned, the problem of phase transitions for infinite-range Ising ferromagnet was studied in Ref. 50 within generalized thermostatistics. Their treatment allows for energy-constant-dependent physical quantities in the thermodynamic limit, which may come from the use of the so-called second choice[2,3] of Tsallis thermostatistics, where average of unity is not unity. In our approach the constant term in the potential energy $\phi(x)$ does not matter in the equilibrium distribution (35) [see Eq. (33)] to give a standard result.

In this paper we have studied the DNFPE obtained based on the NFPE (1) exhibiting the equilibrium distribution of the first choice rather than on the NFPE of Eq. (5) that was recently proposed for the dynamics associated with the third choice of Tsallis thermostatistics. Since both choices of thermostatistics are quite similar to each other if viewed from the NFPEs,[18] we consider that it will suffice to deal with the simplest case as given by the present model to explore the crux of bifurcation phenomena exhibited by the DNFPEs within the framework of generalized thermostatistics.

Although our DNFPE is, to date, not known to have appropriate corresponding N-body Langevin equations or equivalently N-body linear Fokker–Planck equation as considered in the case of the NFPE (8), this work might help search for possible candidates for models explaining dynamic aspects of mean-field type phase transitions within the framework of Tsallis or generalized thermostatistics.

APPENDIX A

Proof of Eq. (35): $-(\partial^2\tilde{F}/\partial h^2)>0$.

Noting

$$\phi - hx = \frac{DqR_{D,h}^{q-1}}{1-q} - \frac{1}{(1-q)\beta_0}, \tag{A1}$$

we differentiate it with respect to h to have

$$-x = -DqR_{D,h}^{q-2}\frac{\partial R_{D,h}}{\partial h} - \frac{1}{1-q}\frac{\partial}{\partial h}\left(\frac{1}{\beta_0}\right). \tag{A2}$$

Then using Eq. (33) one has

$$\begin{aligned} -\frac{\partial^2\tilde{F}}{\partial h^2} = \frac{\partial}{\partial h}\int xR_{D,h}\mathrm{d}x &= \int x\frac{\partial}{\partial h}R_{D,h}\mathrm{d}x \\ &= Dq\int {R_{D,h}}^{q-2}\left(\frac{\partial R_{D,h}}{\partial h}\right)^2\mathrm{d}x + \frac{1}{1-q}\frac{\partial}{\partial h}\left(\frac{1}{\beta_0}\right)\frac{\partial}{\partial h}\int R_{D,h}\mathrm{d}x \\ &= Dq\int {R_{D,h}}^{q-2}\left(\frac{\partial R_{D,h}}{\partial h}\right)^2\mathrm{d}x > 0. \end{aligned} \tag{A3}$$

APPENDIX B

Proof of Eq. (36): $-(1/h)(\partial\tilde{F}/\partial h)\to 0$ $(h\to\pm\infty)$.

Taking the probability distribution $R_{D,h}(x)$ in the form

$$R_{D,h}(x)=[(Dq\beta_0)^{-1}\{1-\beta_0(q-1)(\phi(x)-hx)\}]^{1/(q-1)} \quad (0<q<1) \tag{B1}$$

with

$$\phi(x)=\sum_{k=0}^{n-1} a_k x^{n-k} \quad (a_0>0,\ n(:\text{even})\geqslant 4) \tag{B2}$$

and noting Eq. (33), we will show that

$$\lim_{h\to\infty} h^{-1/(n-1)}\int xR_{D,h}\mathrm{d}x=\omega \ \ (\text{const}). \tag{B3}$$

Note that when D is a given constant, β_0 is determined as a function of D and h and that the partition function Z defined below remains constant as h is varied:

$$Z=\int\left[\frac{1}{q\beta_0(D,h)}+\frac{(1-q)}{q}(\phi(x)-hx)\right]^{-1/(1-q)}\mathrm{d}x=D^{1/(q-1)}. \tag{B4}$$

Introducing a change of variable as

$$x=h^{1/(n-1)}y \tag{B5}$$

one has

$$\langle x\rangle=\int xR_{D,h}\mathrm{d}x=h^{1/(n-1)}\int y\tilde{R}(y,h)\mathrm{d}y, \tag{B6}$$

where

$$\tilde{R}(y,h)=\frac{1}{Z}h^{\alpha}g(y,h)^{-1/(1-q)} \tag{B7}$$

with

$$g(y,h)=\frac{1-q}{q}\psi(y,h)+\frac{1}{q\beta_0}h^{-n/(n-1)}>0 \quad (\forall y,h),$$

$$\psi(y,h)=a_0y^n-y+\sum_{k=1}^{n-1} a_k h^{-k/(n-1)}y^{n-k}$$

$$\alpha=\frac{n+q-1}{(n-1)(q-1)}<0. \tag{B8}$$

We note that

$$\lim_{h\to\infty}\mathrm{Min}_{-\infty<y<\infty}\psi(y,h)=\mathrm{Min}_{-\infty<y<\infty}(a_0y^n-y)=\frac{1-n}{n}\left(\frac{1}{na_0}\right)^{1/(n-1)}\equiv\omega<0 \tag{B9}$$

and the minimum of the right-hand side of Eq. (B9) is attained at

$$y=y^*=\left(\frac{1}{na_0}\right)^{1/(n-1)}. \tag{B10}$$

Since $\int \tilde{R}(y,h)\mathrm{d}y=1$, $\alpha<0$, and Z remains constant, it follows

$$\int g(y,h)^{-1/(1-q)}\mathrm{d}y\to\infty \quad (h\to\infty), \tag{B11}$$

and hence the minimum of $g(y,h)$ over $-\infty<y<\infty$, $\Omega(h)$,

$$\Omega(h)\equiv\frac{1-q}{q}\mathrm{Min}_{-\infty<y<\infty}\psi(y,h)+\frac{1}{q\beta_0}h^{-n/(n-1)}, \tag{B12}$$

which must be positive, tends to 0 as $h\to\infty$. Accordingly one has

$$\lim_{h\to\infty}\frac{1}{q\beta_0}h^{-n/(n-1)}=\frac{-(1-q)\omega}{q}>0. \tag{B13}$$

Letting $\varepsilon>0$ be an arbitrary number, we evaluate the integral

$$\begin{aligned} I(h)\equiv\int y\tilde{R}(y,h)\mathrm{d}y-y^*&=\int (y-y^*)\tilde{R}(y,h)\mathrm{d}y \\ &=\int_{|y-y^*|<\varepsilon}(y-y^*)\tilde{R}(y,h)\mathrm{d}y+\int_{|y-y^*|\geqslant\varepsilon}(y-y^*)\tilde{R}(y,h)\mathrm{d}y. \end{aligned} \tag{B14}$$

One then has

$$\left|\int_{|y-y^*|<\varepsilon}(y-y^*)\tilde{R}(y,h)\mathrm{d}y\right|\leqslant\varepsilon. \tag{B15}$$

Since, using the dominated convergence theorem, one has

$$\begin{aligned} &\lim_{h\to\infty}\int_{|y-y^*|\geqslant\varepsilon}|y-y^*|g(y,h)^{-1/(1-q)}\mathrm{d}y \\ &\quad=\int_{|y-y^*|\geqslant\varepsilon}|y-y^*|\left[\frac{(1-q)}{q}(-\omega+a_0y^n-y)\right]^{-1/(1-q)}\mathrm{d}y, \end{aligned} \tag{B16}$$

it follows that for sufficiently large h,

$$\frac{h^\alpha}{Z}\int_{|y-y^*|\geqslant\varepsilon}|y-y^*|g(y,h)^{-1(1-q)}\mathrm{d}y<\varepsilon. \tag{B17}$$

Accordingly, from Eqs. (B14), (B15), and (B17) we obtain

$$\lim_{h\to\infty}I(h)=0 \tag{B18}$$

to have

$$\lim_{h\to\infty}\int y\tilde{R}(y,h)\mathrm{d}y=y^*, \tag{B19}$$

which together with Eq. (B6) yields Eq. (B3) with $\omega=y^*$.

Since the case with $h\to-\infty$ can be dealt with in the same way, we have Eq. (36) to conclude the proof.

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Lévy flights: Exact results and asymptotics beyond all orders

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A comprehensive study of the symmetric Lévy stable probability density function is presented. This is performed for orders both less than 2, and greater than 2. The latter class of functions are traditionally neglected because of a failure to satisfy non-negativity. The complete asymptotic expansions of the symmetric Lévy stable densities of order greater than 2 are constructed, and shown to exhibit intricate series of transcendentally small terms—asymptotics beyond all orders. It is demonstrated that the symmetric Lévy stable densities of any arbitrary rational order can be written in terms of generalized hypergeometric functions, and a number of new special cases are given representations in terms of *special functions*. A link is shown between the symmetric Lévy stable density of order 4, and Pearcey's integral, which is used widely in problems of optical diffraction and wave propagation. This suggests the existence of applications for the symmetric Lévy stable densities of order greater than 2, despite their failure to define a probability density function. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1467095]

I. INTRODUCTION

It is widely recognized that the Lévy stable densities have enormously varied applicability to stochastic phenomena in the physical sciences. The characteristic feature of these densities is the divergence of their low order moments. Random walks in which the steps are of random length and distributed according to a Lévy stable density are referred to as Lévy flights,[1] and are much discussed in the literature.[2] Continuous time random walks (CTRWs) in which the pausing time distributions follow a Lévy stable law are also widely studied.[2–4]

The Gaussian density is an important case of the Lévy stable densities, as is the Cauchy density which is known to physicists in the context of atomic line shapes. Another early physical application of the Lévy stable densities is the Holtsmark distribution of the random fluctuations of the gravitational field of stars.[5] Apart from these cases however, physical applications of the Lévy stable densities were scarce prior to the ''fractal revolution,'' and their chief applications were traditionally to probability theory itself; notably to limit theorems, and random processes such as branching processes and random determinants.[6] A flood of physical applications of Lévy flights have arisen in recent years, notable amongst these are models of turbulence, polymer transport, and Hamiltonian chaos. A remarkable feature of turbulent flows is enhanced diffusion which requires a probability distribution with infinite moments, and recently work has been done in applying Lévy flights and their generalizations to this phenomenon.[7,8] A review of the application of Lévy stable densities to anomalous diffusion can be found in Ref. 9. CTRWs distributed according to Lévy stable laws prove important in studies of charge transport in amorphous materials.[3,4] Articles discussing these and many more topics appear in Ref. 2.

Biological applications of Lévy stable densities have become plentiful, and Lévy flights have been harnessed in modeling wide ranging phenomena, from the structure of DNA[2] to the flight paths of the wandering albatross.[10] Such is the great utility of the stable densities, they even pervade less piquant disciplines such as economics. Lévy stable densities are asymptotically of the form $1/x^{\alpha+1}$.[11] The economic sociologist Pareto[12] first noted that empirical data of the income

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distributions for various countries followed an inverse power law distribution, and it is now believed[13] that many economic quantities display this behavior. In the economics literature densities with such asymptotic behavior are referred to as Pareto densities. Mandelbrot[13,14] has attempted to explain this asymptotic behavior by arguing that quantities such as price change are ruled by Lévy stable distributions. For a more recent discussion on the use of stochastic processes in finance see Ref. 15.

The Lévy stable densities are stable in the sense that if independent random variables X and Y are distributed according to the same type of Lévy stable density, then $X+Y$ will again be distributed according to this density. More precisely, let X_1 and X_2 be independent random variables with the same probability density function (pdf) $p_\alpha(x)$. $p_\alpha(x)$ is defined to be Lévy stable if it is a solution to the following,[4,16–19] for all positive c_1 and c_2,

$$c_1X_1+c_2X_2=cX, \tag{1.1}$$

where X has the same pdf as X_1 and X_2.

The constant c is determined via

$$c_1^\alpha+c_2^\alpha=c^\alpha. \tag{1.2}$$

We refer to α as the order of the stable density.

The question, ''when is the sum of independent and identically distributed random variables again distributed in the same way,'' expressed in modern terminology translates into that paradigm of fractals, self-similarity: ''when does the whole look like its parts?'' It is known that the trajectory of a Lévy flight is self-similar and that the order of the corresponding stable density, α, is equal to the Hausdorff–Besicovitch dimension of this trajectory.[4,13] This self-similarity manifests itself as a hierarchy of clusters in the trajectory of a Lévy flight, see, e.g., Refs. 3 and 13. The origin of this self-similar scaling behavior lies in the divergence of the moments of the Lévy stable density. This divergence of the moments of Lévy stable pdfs can be understood quite simply from their $1/x^{\alpha+1}$ leading order asymptotic behavior, which implies that all moments $\langle x^m\rangle$ for $m\geqslant\alpha$ diverge.[20]

The divergence of the moments is also obvious from the structure of the Fourier transform, $\tilde{p}_\alpha(k)$, of the symmetric Lévy stable density

$$\tilde{p}_\alpha(k)=\exp(-|k|^\alpha), \tag{1.3}$$

which clearly displays leading order nonanalytic behavior. It is well known (e.g., Ref. 16) that the moments of a pdf, if they exist, are proportional to the coefficients of the power series expansion of the corresponding characteristic function. Thus we see that the moments of the symmetric Lévy stable pdfs will not exist in general, and hence there exists no characteristic scale. It is this divergence of moments and the consequent nonexistence of characteristic scales that endows the Lévy stable densities with their great utility, and intrinsic interest.

Taking the inverse Fourier transform of (1.3), it follows that the symmetric Lévy stable density, $p_\alpha(x)$, has the following form:

$$p_\alpha(x)=\frac{1}{\pi}\int_0^\infty \cos(kx)\exp(-k^\alpha)\mathrm{d}k. \tag{1.4}$$

We note here that the most general form of $\tilde{p}_\alpha(k)$ is actually $\tilde{p}_\alpha(k)=\exp(-a|k|^\alpha)$ for some non-negative a, where a has the dimension of (length)$^\alpha$. However we can clearly scale a out of the integral defining $p_\alpha(x)$ with no loss of generality, and thus we neglect a in all future discussions. This implies that x is being scaled by $a^{1/\alpha}$ and is therefore dimensionless.

It will be the analytic and asymptotic behavior of the integral (1.4) that will be the focus of this work. Equation (1.4) only defines a pdf when $0<\alpha\leqslant 2$, because for $\alpha>2$ it fails the nonnegativity requirement,[21,22] although it is interesting to note that it is still both stable and normal-

izable. We shall not be dissuaded from investigating the interesting properties of (1.4) for $\alpha>2$ however, and in fact this is one of the principle aims of this work. We shall refer to the integral in (1.4) as $p_\alpha(x)$, even when it does not define a pdf. We show that the asymptotic forms of $p_\alpha(x)$ for $\alpha>2$ possess highly intricate transcendentally small terms lying beyond all orders of the asymptotic power series. We study these structures in detail and discuss why these results will likely find interesting physical applications despite the inability of using $p_\alpha(x)$ as a pdf in this region. This work further demonstrates our continuing interest in the newly emerging field of asymptotics beyond all orders.[23–25]

It is easily shown that $p_4(x)$ is related to a special case of Pearcey's integral, $P(y,z)$,[26,27]

$$P(y,z)=2e^{i(\pi/8)}\int_0^\infty \mathrm{d}k\,\exp(-k^4-yk^2)\cos(zk) \tag{1.5}$$

via

$$P(0,z)=2\pi e^{(i\pi/8)}p_4(z). \tag{1.6}$$

The dominant exponential asymptotics displayed by $P(0,z)$, discussed in Ref. 26, is a perfect example of the behavior displayed by $p_\alpha(x)$ when α is an even integer. As we shall show, in these cases the asymptotic power series generated by the standard Mellin transform technique vanishes. Pearcey's integral is important in the theoretical treatment of short wavelength problems, e.g., wave propagation and optical diffraction.[26] It is the oscillatory nature of the exponential asymptotics that endows $p_4(x)$ with its utility in such problems, and it is behavior that is displayed by all other $p_\alpha(x)$ when $\alpha>2$. We thus feel it perfectly natural to anticipate that similar applications will exist for $p_\alpha(x)$ for other values of α.

There exists a wealth of knowledge of the analytic properties of the function $p_\alpha(x)$, e.g., Refs. 3 and 6. However, finding an expression for $p_\alpha(x)$ for general α in terms of known functions is traditionally considered impossible, e.g., Ref. 17. We demonstrate that for all rational α, $p_\alpha(x)$ can in fact be expressed as a finite sum of generalized hypergeometric functions, ${}_pF_q$.[28] It is also known,[29] albeit perhaps not widely, that the Lévy stable pdfs can be expressed in terms of the Fox H-function.[30] The Fox H-function is a generalization of the Meijer G-function, which in turn is a generalization of the less complicated generalized hypergeometric functions ${}_pF_q$.[31] The hypergeometric representation of $p_\alpha(x)$ is more practical since the analytic and asymptotic properties of the ${}_pF_q$, which we employ extensively, have been well studied.[31,32]

Zolotarev[33] provides a small list of values of α for which $p_\alpha(x)$ can be expressed in terms of *special functions*, and one of these results is recovered in Ref. 29. We not only recover Zolotarev's results but add a number of new cases, and display for the first time a detailed exposition of the compelling asymptotics beyond all orders for $\alpha>2$.

II. SERIES REPRESENTATIONS FOR $p_\alpha(x)$

Here we demonstrate a convenient method of deriving the known[2–4,16,17] convergent series, and asymptotic power series representations of $p_\alpha(x)$, since we shall have need to employ these expansions in later discussions. One can easily construct the Mellin–Barnes integral representation of $p_\alpha(x)$ by simply calculating its Mellin transform and then using the inverse Mellin transform formula.

$$p_\alpha(x)=\frac{1}{\pi}\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\mathrm{d}s\,\frac{\cos\left(\frac{\pi s}{2}\right)\Gamma(s)\Gamma\left(\frac{1-s}{\alpha}\right)}{\alpha}x^{-s},\quad 0<\sigma<1. \tag{2.1}$$

Obtaining series expansions of $p_\alpha(x)$ is then merely a case of closing the contour to either the left or the right and calculating the residues. If we close to the left we obtain the small x expansion,

$$p_\alpha(x)=\frac{1}{\alpha\pi x}\sum_{m=0}^{\infty}(-1)^m x^{2m+1}\frac{\Gamma\left[\dfrac{2m+1}{\alpha}\right]}{\Gamma[2m+1]},\quad \forall\, x,\quad \alpha>1,$$
$$p_\alpha(x)\sim\frac{1}{\alpha\pi x}\sum_{m=0}^{\infty}(-1)^m x^{2m+1}\frac{\Gamma\left[\dfrac{2m+1}{\alpha}\right]}{\Gamma[2m+1]},x\to 0,\quad \alpha<1. \tag{2.2}$$

Via application of the ratio test we determine that (2.2) provides a convergent series representation of $p_\alpha(x)$ for all real x when $\alpha>1$, and an asymptotic expansion as $x\to 0$ for $\alpha<1$.

Closing the contour to the right we obtain the large x expansion of $p_\alpha(x)$,

$$p_\alpha(x)=\frac{\alpha}{\pi x}\sum_{m=0}^{\infty}\sin\left[\frac{(m+1)\pi\alpha}{2}\right](-1)^m(x^{-\alpha})^{m+1}\frac{\Gamma[(m+1)\alpha]}{\Gamma[m+1]},\quad x>0,\quad 0<\alpha<1,$$
$$p_\alpha(x)\sim\frac{\alpha}{\pi x}\sum_{m=0}^{\infty}\sin\left[\frac{(m+1)\pi\alpha}{2}\right](-1)^m(x^{-\alpha})^{m+1}\frac{\Gamma[(m+1)\alpha]}{\Gamma[m+1]},\quad x\to\infty,\quad \alpha>1. \tag{2.3}$$

Thus we have a convergent large x expansion of $p_\alpha(x)$ when $\alpha<1$. When $\alpha>1$ (2.3) provides an asymptotic expansion, but as we shall discuss later there are certain interesting cases in which this expansion is not *complete*.[34,35] In particular when α is integral and greater than 2, we find that (2.3) provides only the asymptotic power series component of the complete asymptotic expansion, i.e., there are a series of exponentially small terms that (2.3) neglects. If α is an even integer (2.3) vanishes identically, which for $\alpha=2$ expresses the fact that in the limit of large argument the Gaussian is smaller than any power. For even integral α, with $\alpha>2$, we see that the exponentially small terms lying beyond all orders of (2.3) become dominant, and the complete asymptotic expansion of $p_\alpha(x)$ consists solely of these transcendentally small series. We shall return to the delicate problem of calculating the terms that lie beyond all orders of (2.3) when $\alpha>2$. We devote an extensive section to the detailed construction of the exponential asymptotics for $p_\alpha(x)$ for the cases $\alpha=3,4,5,6,7$, which will demonstrate the increasing intricacy of the exponentially small asymptotic series as α increases.

III. $p_{p/q}(x)$ EXPRESSED IN TERMS OF HYPERGEOMETRIC FUNCTIONS

If we let $\alpha=p/q$, i.e., let α be rational, then $p_{p/q}(x)$ can be expressed as a finite sum of generalized hypergeometric functions. The serendipitous process by which we discovered this fact originated in the investigation of the exponential asymptotics of a number theoretic series which we refer to as the generalized Euler–Jacobi series, and denote by $S_{p/q}(a)$.[24] After a suitable transformation of the summand of $S_{p/q}(a)$, it becomes apparent that this summand is very simply related to $p_{p/q}(x)$. Thus the detailed asymptotic and analytic of investigation $S_{p/q}(a)$ that was undertaken in Ref. 24 can be applied to the investigation of $p_{p/q}(x)$. It is for this reason that we now discuss the relationship between $S_{p/q}(a)$ and $p_{p/q}(x)$.

We define the generalized Euler–Jacobi series as

$$S_{p/q}(a)\equiv\sum_{m=0}^{\infty}e^{-am^{p/q}} \tag{3.1}$$

and upon application of the Euler–Maclaurin summation formula this becomes

$$S_{p/q}(a)=\frac{q\Gamma\left(\dfrac{q}{p}\right)}{pa^{q/p}}+\frac{1}{2}+\sum_{n=1}^{\infty}\frac{a}{n\pi}\int_0^{\infty}\mathrm{d}t\,\sin(2n\pi t^{q/p})\exp(-at). \tag{3.2}$$

We refer to (3.2) as the inversion formula for $S_{p/q}(a)$. In order to simplify (3.2) a systematic study of integrals of the form

$$I_{p/q}(a,\beta)=\int_0^\infty \mathrm{d}t\,\exp(-at)\sin(\beta t^{q/p}) \tag{3.3}$$

was carried out in Ref. 24.

To see the relationship between $p_{p/q}(x)$ and $I_{p/q}(\alpha,\beta)$ we take $p_{p/q}(x)$ and integrate by parts

$$\begin{aligned} p_{p/q}(x)&=\frac{1}{\pi}\int_0^\infty \mathrm{d}k\,\cos(kx)\exp(-k^{p/q}),\\ p_{p/q}(x)&=\frac{1}{\pi x}\int_0^\infty \mathrm{d}(k^{p/q})\,\exp(-k^{p/q})\sin(kx), \end{aligned} \tag{3.4}$$

$$p_{p/q}(x)=\frac{1}{\pi x^{p/q+1}}\int_0^\infty \mathrm{d}t\,\exp\left(\frac{-t}{x^{p/q}}\right)\sin(t^{q/p}), \tag{3.5}$$

$$p_{p/q}(x)=\frac{1}{\pi x^{p/q+1}}I_{p/q}(x^{-p/q},1). \tag{3.6}$$

Hence we identify the summand in the generalized Euler–Jacobi inversion formula with $p_{p/q}(x)$. Specifically we see that

$$S_{p/q}(a)=\frac{q\Gamma\left(\frac{q}{p}\right)}{pa^{q/p}}+\frac{1}{2}+\frac{2\pi}{a^{q/p}}\sum_{n=1}^{\infty} p_{p/q}\left(\frac{2n\pi}{a^{q/p}}\right). \tag{3.7}$$

Thus the number theoretic series $S_{p/q}(a)$ can be interpreted as a sum over Lévy flights of different arguments.

All analytic and asymptotic results in Ref. 24 for $I_{p/q}(\alpha,\beta)$ or $S_{p/q}(a)$ can now be translated into results for $p_{p/q}(x)$ by application of this simple algorithm. We shall utilize this fact in the following sections to list a number of significant examples of the analytic behavior of $p_{p/q}(x)$ for various values of p/q, and also to discuss the delicate exponential asymptotic behavior of $p_{p/q}(x)$ for $p/q>2$.

One fundamental result of the analysis of $I_{p/q}(\alpha,\beta)$ in Ref. 24 is the representation of $I_{p/q}(\alpha,\beta)$ in terms of a sum of hypergeometric functions, which forms the foundation of the asymptotic results discussed therein. The method of construction of such a representation for $I_{p/q}(\alpha,\beta)$ suggests an obvious method for constructing a corresponding representation of $p_\alpha(x)$ in terms of hypergeometric functions, which we shall now delineate.

We begin our analysis with (2.2), letting $\alpha=p/q$. This series could also be obtained by simply expanding $\sin(t^{q/p})$ in (3.5) into its Maclaurin series and integrating term by term. As noted in Sec. II, (2.2) is convergent $\forall x$ when $p/q>1$, but is divergent when $p/q<1$. Despite this we will still identify (2.2) with $p_{p/q}(x)$ even for $p/q<1$, and when necessary the technique of Borel summation[36] can be utilized to recast the original series, for specific p/q, into convergent integrals which can then be evaluated. This process is discussed in detail in Ref. 24 in the treatment of $I_{p/q}(a,\beta)$.

The series representation for the generalized hypergeometric equation is

$${}_jF_k\left(\begin{matrix}\alpha_1,\alpha_2,\ldots,\alpha_j\\ \beta_1,\beta_2,\ldots,\beta_k\end{matrix}\middle| z\right)=\sum_{m=0}^{\infty}\frac{z^m\,\Pi_{h=1}^{j}(\alpha_h)_m}{m!\,\Pi_{h=1}^{k}(\beta_h)_m}, \tag{3.8}$$

where $(a)_m$ is Pochhammer's symbol

$$(a)_m=\frac{\Gamma(a+m)}{\Gamma(a)}. \tag{3.9}$$

We can see from (3.8) and (3.9) that (2.2) clearly displays hypergeometric behavior, in that its coefficients are a ratio of gamma functions. To make this identification manifest we need to massage the gamma functions into the form $\Gamma(m+\text{stuff})$. We begin by using the change of index $m=np+l$,

$$p_{p/q}(x)=\frac{q}{\pi px}\sum_{n=0}^{\infty}\sum_{l=0}^{p-1}e^{i\pi(np+l)}x^{2np+2l+1}\frac{\Gamma\left[2nq+\dfrac{(2l+1)q}{p}\right]}{\Gamma(2np+2l+1)} \tag{3.10}$$

then we follow this with $s=2n$,

$$p_{p/q}(x)=\frac{q}{\pi px}\sum_{s=0}^{\infty}\left[\frac{1+(-1)^s}{2}\right]\sum_{l=0}^{p-1}e^{i\pi(sp/2+l)}x^{sp+2l+1}\frac{\Gamma\left[sq+\dfrac{(2l+1)q}{p}\right]}{\Gamma(sp+2l+1)}. \tag{3.11}$$

Finally we can now transform the ratio of gamma functions into the required form by utilizing Gauss' multiplication formula[31] and (3.9), which results in

$$\begin{aligned}&\frac{\Gamma\left[sq+\dfrac{(2l+1)q}{p}\right]}{\Gamma(sp+2l+1)}\\&\quad=\frac{(2\pi)^{(p-q)/2}q^{sq+(2l+1)q/p-1/2}}{p^{sp+2l+1/2}}\frac{\displaystyle\prod_{h=1}^{(q-1)}\Gamma\left[\frac{(2l+1)}{p}+\frac{h}{q}\right]}{\displaystyle\prod_{h=1}^{(p-1)}\Gamma\left[\frac{(2l+1)}{p}+\frac{h}{p}\right]}\frac{\left(\dfrac{2l+1}{p}+\dfrac{h}{q}\right)_s}{\left(\dfrac{2l+1}{p}+\dfrac{h}{p}\right)_s}.\end{aligned} \tag{3.12}$$

Inserting (3.12) into (3.11)

$$\begin{aligned}p_{p/q}(x)=&\frac{q^{q/p+1/2}}{p^{3/2}}(2\pi)^{(p-q-2)/2}\sum_{l=0}^{p-1}(-1)^l\left(\frac{q^qx^p}{p^p}\right)^{2l/p}\frac{\displaystyle\prod_{h=1}^{(q-1)}\Gamma\left[\frac{(2l+1)}{p}+\frac{h}{q}\right]}{\displaystyle\prod_{h=1}^{(p-1)}\Gamma\left[\frac{(2l+1)}{p}+\frac{h}{p}\right]}\\&\times\sum_{t=0}^{1}\sum_{s=0}^{\infty}\left((-1)^te^{p\pi i/2}\frac{q^qx^p}{p^p}\right)^s\frac{1}{s!}\frac{(1)_s\displaystyle\prod_{h=1}^{(q-1)}\left(\dfrac{2l+1}{p}+\dfrac{h}{q}\right)_s}{\displaystyle\prod_{h=2}^{p}\left(\dfrac{2l+h}{p}\right)_s}.\end{aligned} \tag{3.13}$$

The following useful notation, $f(\pm z)^{\pm}\equiv f(z)\pm f(-z)$ for some function f, will be used throughout this work. Using (3.13) and (3.8) then, we finally obtain

$$p_{p/q}(x)=\frac{q^{q/p+1/2}}{p^{3/2}}(2\pi)^{(p-q-2)/2}\sum_{l=0}^{p-1}(-1)^l\left(\frac{q^q x^p}{p^p}\right)^{2l/p}\times\frac{\prod_{h=1}^{(q-1)}\Gamma\left[\frac{(2l+1)}{p}+\frac{h}{q}\right]}{\prod_{h=1}^{(p-1)}\Gamma\left[\frac{(2l+1)}{p}+\frac{h}{p}\right]}\times{}_qF_{p-1}\left(\left.\begin{matrix}1,\frac{2l+1}{p}+\frac{1}{q},\frac{2l+1}{p}+\frac{2}{q},\ldots,\frac{2l+1}{p}+\frac{q-1}{q}\\ \frac{2l+2}{p},\frac{2l+3}{p},\ldots,\frac{2l+p}{p}\end{matrix}\right|\pm i^p\frac{q^q x^p}{p^p}\right)^+. \quad (3.14)$$

In order to simply the appearance of this further, we can use the known relationship between the Meijer G-function and the generalized hypergeometric function[31] to obtain

$$p_{p/q}(x)=\frac{q^{q/p+1/2}}{p^{3/2}}(2\pi)^{(p-q-2)/2}\sum_{l=0}^{p-1}(-1)^l\left(\frac{q^q x^p}{p^p}\right)^{2l/p}\times G_{q,p}^{1,q}\left(\left.\pm i^p\frac{q^q x^p}{p^p}\right|\begin{matrix}0,\frac{1}{q}-\frac{2l+1}{p},\frac{2}{q}-\frac{2l+1}{p},\ldots,\frac{q-1}{q}-\frac{2l+1}{p}\\ 0,\frac{-2l}{p},\frac{1}{p}-\frac{2l}{p},\ldots,\frac{p-2l-2}{p}\end{matrix}\right)^+. \quad (3.15)$$

IV. SPECIAL FUNCTION REPRESENTATIONS OF $p_{p/q}(x)$

In this section we list a number of new cases of special function representations of $p_{p/q}(x)$, in which (3.15) decomposes into simpler forms. We also recover, and in one instance correct, some results obtained by Zolotarev. We begin by deriving the familiar forms of the the Cauchy and Gaussian densities from (3.15) in order to illustrate how the general expression simplifies in these more transparent cases. We show that the Holtsmark density can be expressed as a sum of Bessel functions. For details of the derivation of these results the reader should consult Ref. 24, applying (3.7).

A. The Cauchy and Gaussian densities

It is easily shown that for $\alpha=1$, (3.14) decomposes as follows:

$$p_1(x)=\frac{1}{2\pi}{}_1F_0(1;\pm ix)^+,$$
$$p_1(x)=\frac{1}{\pi(1+x^2)}. \quad (4.1)$$

This second expression will be recognized as the well-known Cauchy pdf.

Recovering the Gaussian pdf from (3.14) when $\alpha=2$ is equally straightforward,

$$p_2(x)=\frac{1}{2\sqrt{4\pi}}\sum_{l=0}^{1}(-1)^l\left(\frac{x^2}{4}\right)^l {}_1F_1\left(1;l+1;\pm\frac{x^2}{4}\right)^+,$$
$$p_2(x)=\frac{e^{-x^2/4}}{\sqrt{4\pi}}. \tag{4.2}$$

Thus our general result (3.14) easily reproduces the standard forms of these two principal special cases of $p_{p/q}(x)$.

B. $\alpha=3/2$: The Holtsmark density

With the exception of the Gaussian and Cauchy densities, the Holtsmark density was the first recognized application of the Lévy stable densities to the physical sciences. Chandrasekhar[5] gives an elegant derivation of the pdf for the force per unit mass acting on a given star due to the gravitational attraction of the neighboring stars, which shows this pdf to be $p_{3/2}(x)$. He did not give the closed form expression for the pdf however, but instead tabulated various numerically obtained values for it. We now present the special functions representation for the Holtsmark density, in which $J_\mu(x)$ is the Bessel function of the first kind of order μ,

$$p_{3/2}(x)=\frac{2^{2/3}}{3^{3/2}\sqrt{\pi}}\sum_{l=0}^{2}\left(\frac{4x^3}{27}\right)^{2l/3}(-1)^l G_{2,3}^{1,2}\left(\pm i\frac{4x^3}{27}\,\middle|\,\begin{matrix}0,\frac{1}{2}-\frac{2l+1}{3}\\ 0,\frac{-2l}{3},\frac{1}{3}-\frac{2l}{3}\end{matrix}\right)^+, \tag{4.3}$$

$$p_{3/2}(x)=\frac{4x^2}{27\sqrt{3}}\cos\left(\frac{2x^3}{27}\right)J_{-2/3}\left(\frac{2x^3}{27}\right)-\frac{4x^2}{27\sqrt{3}}\cos\left(\frac{2x^3}{27}\right)J_{2/3}\left(\frac{2x^3}{27}\right)-\frac{4x^2}{27\sqrt{3}}\sin\left(\frac{2x^3}{27}\right)J_{-1/3}\left(\frac{2x^3}{27}\right)$$
$$-\frac{4x^2}{27\sqrt{3}}\sin\left(\frac{2x^3}{27}\right)J_{1/3}\left(\frac{2x^3}{27}\right)+\frac{x^2}{6\pi}{}_2F_2\left(1,\frac{3}{2};\frac{4}{3},\frac{5}{3};\pm\frac{i4x^3}{27}\right)^+.$$

C. Zolotarev's results: Correcting $p_{2/3}(x)$ and recovering $p_{1/2}(x)$

Zolotarev[33] states a representation of $p_{2/3}(x)$ in terms of a Whittaker function, but this result, which is much quoted, e.g. Ref. 3, is incorrect. That the result in Ref. 33 cannot be correct can be simply deduced by observing its large x behavior and comparing it to (2.3). We now list the correct result in terms of a Tricomi confluent hypergeometric function $\Psi(\beta,\gamma,z)$. We also state the result less elegantly in terms of a Whittaker function, $W_{a,b}(z)$, which is similar in form to the incorrect result stated in Ref. 33,

$$p_{2/3}(x)=\frac{3}{4\sqrt{\pi}}{}_2F_0\left(\frac{5}{6},\frac{7}{6};-\frac{27x^2}{4}\right),$$
$$p_{2/3}(x)=\frac{x^{-5/3}}{2^{1/3}3^{3/2}\sqrt{\pi}}\Psi\left(\frac{5}{6},\frac{2}{3};\frac{4}{27x^2}\right), \tag{4.4}$$
$$p_{2/3}(x)=\frac{1}{6x}\sqrt{\frac{3}{\pi}}\exp\left(\frac{2}{27x^2}\right)W_{-1/2,1/6}\left(\frac{4}{27x^2}\right).$$

In Ref. 33 Zolotarev derives $p_{1/2}(x)$ by a rather complicated procedure. By massaging (3.14) appropriately we obtain

$$p_{1/2}(x)=\frac{1}{\pi}{}_2F_0\left(1,\frac{3}{2};\pm i4x\right)^+,$$

$$p_{1/2}(x)=\frac{1}{8x^2}\left[J_{1/2}\left(\frac{1}{4x}\right)+J_{-1/2}\left(\frac{1}{4x}\right)\right]-\frac{1}{2\pi\sqrt{2}x^2}\left[\mathbf{J}_{1/2}\left(\frac{1}{4x}\right)+\mathbf{E}_{1/2}\left(\frac{1}{4x}\right)\right], \tag{4.5}$$

$$p_{1/2}(x)=\frac{1}{\sqrt{2\pi}x^{3/2}}\left[\frac{1}{2}-C\left(\frac{1}{\sqrt{2\pi x}}\right)\right]\cos\left(\frac{1}{4x}\right)+\frac{1}{\sqrt{2\pi}x^{3/2}}\left[\frac{1}{2}-S\left(\frac{1}{\sqrt{2\pi x}}\right)\right]\sin\left(\frac{1}{4x}\right),$$

where $\mathbf{J}_\nu(\mathbf{z})$ and $\mathbf{E}_\nu(\mathbf{z})$ are the Anger and Weber functions, respectively, and $C(z)$, $S(z)$ are the Fresnel integrals. The last form listed in (4.5) in terms of the Fresnel integrals is in agreement with that stated by Zolotarev.

D. A miscellany of other new results: $\alpha=1/3,3,4/3$

By an examination of the integral[24] corresponding to $p_{1/3}(x)$, it was found that the case of $p_{1/3}(x)$ has an especially simple representation in terms of a complex conjugate pair of Lommel functions. This is a new and rather attractive result,

$$\begin{aligned}p_{1/3}(x)&=\frac{27\sqrt{3}}{(2\pi)^2}\Gamma\left(\frac{4}{3}\right)\Gamma\left(\frac{5}{3}\right){}_3F_0\left(1,\frac{4}{3},\frac{5}{3};\pm i27x\right)^+,\\ p_{1/3}(x)&=\frac{1}{3\sqrt{3}\pi x^{3/2}}e^{-i\pi/4}S_{0,1/3}\left(\frac{2e^{i\pi/4}}{3\sqrt{3x}}\right)+\frac{1}{3\sqrt{3}\pi x^{3/2}}e^{i\pi/4}S_{0,1/3}\left(\frac{2e^{-i\pi/4}}{3\sqrt{3x}}\right).\end{aligned} \tag{4.6}$$

The case of $\alpha=3$ is especially interesting and we discuss in detail its asymptotic properties in Sec. V. Here we observe that the integral for $p_3(x)$ is exactly solvable and is again given by a complex conjugate pair of Lommel functions,

$$\begin{aligned}p_3(x)&=\frac{1}{3\sqrt{3}}\sum_{l=0}^{2}(-1)^l\left(\frac{x^2}{9}\right)^l G^{1,1}_{1,3}\left(\pm i\frac{x^3}{27}\middle|{}^{0}_{0,-2l/3,(1-2l)/3}\right)^+,\\ p_3(x)&=\frac{1}{3\pi}\sqrt{\frac{x}{3}}e^{i\pi/4}S_{0,1/3}\left[2e^{3i\pi/4}\left(\frac{x}{3}\right)^{3/2}\right]+\frac{1}{3\pi}\sqrt{\frac{x}{3}}e^{-i\pi/4}S_{0,1/3}\left[2e^{-3i\pi/4}\left(\frac{x}{3}\right)^{3/2}\right].\end{aligned} \tag{4.7}$$

Due to the appearance of the Cauchy density, $\alpha=1$, Gaussian density, $\alpha=2$, and Pearcey integral, $\alpha=4$, in physical applications, and also the elegance of the closed form representation of $p_3(x)$, it seems unlikely that nature would choose not to also utilize $p_3(x)$ in her description.

It will be noticed that the Lommel function representation of $p_3(x)$, (4.7), is very similar in form to that of the Lommel function representation of $p_{1/3}(x)$ (4.6). There is no direct relationship between $p_3(x)$ and $p_{1/3}(x)$ in the sense of a duality transform[17,33,6] however, since such a transform sends symmetric Lévy stable densities to asymmetric Lévy stable densities in general, and both our $p_3(x)$ and $p_{1/3}(x)$ are symmetric. To see the reason for the similarity in structure and also to illuminate the absence of a direct map between $p_3(x)$ and $p_{1/3}(x)$, we compare the series representations discussed in Sec. II for the case of $\alpha>1$ and $1/\alpha$. Using the simple identity

$$\sum_{n=0}^{\infty}(-1)^n a_n=\sum_{m=0}^{\infty}(-1)^m\sin\left[\frac{(m+1)\pi}{2}\right]a_{m/2} \tag{4.8}$$

we can transform (2.2) into a form very similar to (2.3). Using (2.3) with order $1/\alpha$ we arrive at

$$p_\alpha(x)=\frac{1}{\alpha\pi x}\sum_{m=0}^{\infty}\sin\left[\frac{(m+1)\pi}{2}\right](-1)^m x^{m+1}\frac{\Gamma\left(\frac{m+1}{\alpha}\right)}{\Gamma(m+1)}, \tag{4.9}$$

$$p_{1/\alpha}(x)=\frac{1}{\alpha\pi x}\sum_{m=0}^{\infty}\sin\left[\frac{(m+1)\pi}{2\alpha}\right](-1)^m (x^{-1/\alpha})^{m+1}\frac{\Gamma\left(\frac{m+1}{\alpha}\right)}{\Gamma(m+1)}. \tag{4.10}$$

The only difference in the structure of (4.9) versus (4.10), apart from $x\to x^{-1/\alpha}$, is the factor of $1/\alpha$ in the argument of the sine. This difference however prohibits us from producing $p_\alpha(x)$ via any transform of the argument of $p_{1/\alpha}(x)$, since it is impossible to express

$$\sin\left[\frac{(m+1)\pi}{2}\right]$$

as a multiple of

$$\sin\left[\frac{(m+1)\pi}{2\alpha}\right].$$

Thus we see that there is good reason for the similar structure of (4.7) and (4.6), but there exists no rule whereby we can construct one by knowing the other.

We list for completeness another useful form of $p_3(x)$ in terms of Anger functions, and the Kelvin functions $ber_\nu(z)$ and $bei_\nu(z)$,

$$\begin{aligned}p_3(x)=&\frac{\sqrt{2x}}{9}[ber_{-1/3}(2\sqrt{x^3/27})-bei_{-1/3}(2\sqrt{x^3/27})]+\frac{\sqrt{2x}}{9}[bei_{1/3}(2\sqrt{x^3/27})\\&-ber_{1/3}(2\sqrt{x^3/27})]-\frac{\sqrt{ix}}{9}[\mathbf{J}_{1/3}(2e^{-i\pi/4}\sqrt{x^3/27})-\mathbf{J}_{-1/3}(2e^{-i\pi/4}\sqrt{x^3/27})]\\&-\frac{1}{9}\sqrt{\frac{x}{i}}\,[\mathbf{J}_{1/3}(2e^{i\pi/4}\sqrt{x^3/27})-\mathbf{J}_{-1/3}(2e^{i\pi/4}\sqrt{x^3/27})].\end{aligned} \tag{4.11}$$

We finally list the case of $p/q=4/3$, in which the sum over the eight G functions decomposes into two ${}_2F_2$ functions. It would be expected that similar simplifications should exist for other cases such as $p/q=5/3$ should they be sought,

$$p_{4/3}(x)=\frac{3^{5/4}}{8\sqrt{2\pi}}\sum_{l=0}^{3}(-1)^l\left(\frac{3^{3/2}x^2}{16}\right)^l G^{1,3}_{3,4}\left(\pm\frac{3^3x^4}{4^4}\,\middle|\,\begin{matrix}0,\frac{1}{3}-\frac{2l+1}{4},\frac{2}{3}-\frac{2l+1}{4}\\0,\frac{-l}{2},\frac{1-2l}{4},\frac{1-l}{2}\end{matrix}\right)^+, \tag{4.12}$$

$$\begin{aligned}p_{4/3}(x)=&\frac{3^{5/4}}{4\sqrt{2\pi}}\frac{\Gamma(\frac{7}{12})\Gamma(\frac{11}{12})}{\Gamma(\frac{1}{2})\Gamma(\frac{3}{4})}{}_2F_2\left(\frac{7}{12},\frac{11}{12};\frac{1}{2},\frac{3}{4};\frac{3^3x^4}{4^4}\right)\\&-\frac{3^{11/4}x^2}{4^3\sqrt{2\pi}}\frac{\Gamma(\frac{13}{12})\Gamma(\frac{17}{12})}{\Gamma(\frac{3}{2})\Gamma(\frac{5}{4})}{}_2F_2\left(\frac{13}{12},\frac{17}{12};\frac{3}{2},\frac{5}{4};\frac{3^3x^4}{4^4}\right).\end{aligned}$$

V. COMPLETE ASYMPTOTIC EXPANSIONS AS $x\to\infty$

It has been shown previously that $p_{p/q}(x)$ can be represented as a sum of hypergeometric functions, which is convergent when $p/q>1$. Hence, when $p/q>1$, the complete asymptotic expansions of $p_{p/q}(x)$ for large x can be deduced in a straightforward way by making use of the known complete asymptotic expansions of the hypergeometric function ${}_qF_{p-1}$.

For the cases of $p/q<1$ no such asymptotic large x expansion is required since the convergent expansion, (2.3), is already a large x expansion. Consequently, since all $p_{p/q}(x)$ with $p/q<1$ possess a convergent large x power series, their asymptotic behavior in this limit must be purely algebraic. This fact manifests itself in the special functions representations discussed in Sec. IV since $p_{1/2}(x)$, $p_{2/3}(x)$ and $p_{1/3}(x)$ all have special functions representations in which the arguments of these special functions contain negative powers of x. Thus the convergent, small argument series expansions of these special functions provide the large x behavior of these $p_{p/q}(x)$. This observation explains why the large x asymptotic expansion of $p_{1/3}(x)$ is totally algebraic whereas that of $p_3(x)$ contains both algebraic and transcendental terms, as we shall show, despite the fact that these two functions have very similar representations in terms of the same Lommel function, $S_{0,1/3}$. That is, because $p_3(x)$ is expressed in terms of Lommel functions whose argument contains positive powers of x, whereas $p_{1/3}(x)$ is expressed in terms of Lommel functions whose arguments contain negative powers.

Luke (Ref. 31, Chap. 5), gives a detailed discussion of the complete asymptotic expansions of the Meijer G function and the generalized hypergeometric function, and the particular nuances of the complete expansions of ${}_jF_{k-1}$ are discussed fully in Ref. 24. The complete asymptotic expansion of ${}_jF_{k-1}$, for $j\leqslant k-2$, is given by

$$\begin{aligned}&\frac{\Pi_{h=1}^{j}\Gamma(\alpha_h)}{\Pi_{h=1}^{k-1}\Gamma(\rho_h)}{}_jF_{k-1}\left(\begin{matrix}\alpha_1,\alpha_2,\ldots,\alpha_j\\ \rho_1,\rho_2,\ldots,\rho_{k-1}\end{matrix}\middle|-z\right)\\ &\quad\sim\sum_{m=0}^{r-1}\Gamma_k^{1,j}(m)K_{j,k-1}(ze^{-i\pi(2m+1)})\\ &\qquad+\sum_{m=0}^{k-j-r-1}\overline{\Gamma}_k^{1,j}(m)K_{j,k-1}(ze^{i\pi(2m+1)})+L_{j,k-1}(z),\end{aligned}\tag{5.1}$$

$$K_{j,k-1}(z)=\frac{(2\pi)^{(j+1-k)/2}}{(k-j)^{1/2}}e^{(k-j)z^{1/(k-j)}}z^{\gamma}\sum_{m=0}^{\infty}N_m z^{-m/(k-j)},\tag{5.2}$$

$$L_{j,k-1}=\sum_{t=1}^{j}z^{-\alpha_t}\frac{\Pi_{t=1}^{j}\Gamma(\alpha_t)\Gamma(\alpha_j-\alpha_t)^*}{\Pi_{t=1}^{k-1}\Gamma(\rho_{k-1}-\alpha_t)}{}_kF_{j-1}\left(\begin{matrix}\alpha_t,1+\alpha_t-\rho_{j-1}\\ 1+\alpha_t-\alpha_j^*\end{matrix}\middle|\frac{(-)^{k-j-1}}{z}\right),\tag{5.3}$$

where the asterisk signifies that $\Gamma(\alpha_j-\alpha_j)$ is excluded, and r is an arbitrary integer such that $0\leqslant r\leqslant k-j$. The values of the $\Gamma_k^{1,j}(m)$ and $\overline{\Gamma}_k^{1,j}(m)$ are given in Ref. 31. The argument of z is subject to the two constraints $|\arg(z)|\leqslant 2\pi-\delta$ with $\delta<0$, and $\delta_1+(4r-3k+3j-2)\pi/2\leqslant\arg(z)\leqslant\delta_2+(4r-k+j+2)\pi/2$ where δ_1 and δ_2 are arbitrarily small. The N_m are found recursively, and the details of the recursion relation in the general case, as well as the specific recursion relations for the cases $\alpha=3,4,5,6,7$ and there construction, can be found in Ref. 24. We shall not discuss the construction of the N_m here, since the procedure is straightforward but unenlightening. We note, however, that the N_m are dependent on the parameters of the given hypergeometric function.

We refer in this work, following the above-given notation used in the complete asymptotic expansions of the generalized hypergeometric functions, to the component asymptotic power series of a given hypergeometric function or $p_\alpha(x)$ as the L asymptotics of that function, and to the series of exponentially small terms as the K asymptotics of that function.

The L asymptotics of the sum of hypergeometric functions composing a given $p_{p/q}(x)$ must conspire to reproduce (2.3), since the K asymptotics contain no algebraic terms. This is verified to occur for the asymptotic expansions of the equivalent $I_{p/q}(\alpha,\beta)$ in Ref. 24, for all the special cases of $p_{p/q}(x)$ considered in Sec. IV. There is also a formal demonstration in Ref. 24 of how the L asymptotics of the $I_{2n+1}(\alpha,\beta)$ corresponding to $p_{2n+1}(x)$ coalesce into (2.3). When p/q is an even integer the L asymptotics of the complete asymptotic expansion of $p_{p/q}(x)$ vanish, as discussed previously. The L asymptotics for $p/q=3,4,5,6,7$ are thus easily found and require little discussion. We list the nonvanishing series here for completeness,

$$p_3(x)\sim\frac{3}{\pi x}\sum_{m=0}^{\infty}\frac{(-1)^{m+1}}{(2m)!}\frac{\Gamma(6m+3)}{(x^3)^{2m+1}}, \tag{5.4}$$

$$p_5(x)\sim\frac{5}{\pi x}\sum_{m=0}^{\infty}\frac{(-1)^{m}}{(2m)!}\frac{\Gamma(10m+5)}{(x^5)^{2m+1}}, \tag{5.5}$$

$$p_7(x)\sim\frac{7}{\pi x}\sum_{m=0}^{\infty}\frac{(-1)^{m+1}}{(2m)!}\frac{\Gamma(14m+7)}{(x^7)^{2m+1}}. \tag{5.6}$$

Upon investigation of the special cases $p_{4/3}(x)$ and $p_{3/2}(x)$ discussed in Sec. IV, it is found that the K asymptotic series exactly cancel in both of these cases, thus producing purely algebraic complete asymptotic expansions. The derivations of these results can be deduced from Ref. 24.

It is found however that the asymptotics of the $p_n(x)$ for integral n possess intricate series of exponentially small terms when $n>2$, i.e., nonvanishing K asymptotics. In order to determine the contribution of the K asymptotics to the complete asymptotic expansion of $p_n(x)$, which we denote by $p_n^K(x)$, we simply use our expression for $p_n(x)$ in terms of hypergeometric functions and then substitute the K asymptotic series from (5.2). We sketch the procedure for the case of $p_3(x)$, and then simply state the results for the other cases. Details of the construction of all the cases listed may be deduced from Ref. 24 using (3.7).

For convenience we introduce the notation $z=q^q x^p/p^p$ so that (4.7) reduce to

$$3\sqrt{3}p_3(x)=G_{1,3}^{1,1}(\pm iz|_{0,0,1/3}^{0})^{+}-z^{2/3}G_{1,3}^{1,1}(\pm iz|_{0,-2/3,-1/3}^{0})^{+}+z^{4/3}G_{1,3}^{1,1}(\pm iz|_{0,-4/3,-1}^{0})^{+}. \tag{5.7}$$

By massaging this expression we find that the G functions reduce to

$$G_{1,3}^{1,1}(\pm iz|_{0,0,1/3}^{0})^{+}=\Gamma\left(\frac{2}{3}\right)^{-1}{}_0F_1\left(\frac{2}{3};\pm iz\right)^{+}, \tag{5.8}$$

$$G_{1,3}^{1,1}(\pm iz|_{0,-2/3,-1/3}^{0})^{+}=\left[\Gamma\left(\frac{4}{3}\right)\Gamma\left(\frac{5}{3}\right)\right]^{-1}{}_1F_2\left(1;4/3,\frac{5}{3};\pm iz\right)^{+}, \tag{5.9}$$

$$G_{1,3}^{1,1}(\pm iz|_{0,-4/3,-1}^{0})^{+}=\frac{1}{iz}\Gamma\left(\frac{4}{3}\right)^{-1}{}_0F_1\left(4/3;\pm iz\right)^{-}. \tag{5.10}$$

We note that the asymptotic expansions of (5.8) and (5.10) contain only K asymptotic expansions since the sum in (5.3) is void in these cases. Thus (5.4) is constructed purely from the L asymptotics of (5.9).

The complete asymptotic expansion of (5.8) is constructed using (5.1) and (5.2). We obtain

$$\Gamma(\tfrac{2}{3})^{-1}{}_0F_1(\tfrac{2}{3};\pm iz)^{+}\sim K_{0,1}(e^{\pm\pi i/2}z)^{+}+K_{0,1}(e^{\pm 3\pi i/2}z)^{+}, \tag{5.11}$$

where

$$K_{0,1}(e^{\pm\pi i/2}z)^+ = \frac{z^{-1/12}}{\sqrt{\pi}} e^{\sqrt{2z}} \sum_{m=0}^{\infty} N_m z^{-m/2} \cos\left(\sqrt{2z} - \frac{\pi}{24} - \frac{m\pi}{4} \right), \tag{5.12}$$

$$K_{0,1}(e^{\pm 3\pi i/2}z)^+ = \frac{z^{-1/12}}{\sqrt{\pi}} e^{-\sqrt{2z}} \sum_{m=0}^{\infty} N_m z^{-m/2} \cos\left(\sqrt{2z} - \frac{3\pi}{24} - \frac{3m\pi}{4} \right). \tag{5.13}$$

The K asymptotics of (5.9) and (5.10) are found in a similar way and yield

$$\begin{aligned} \frac{{}_1F_2(1;\frac{4}{3},\frac{5}{3};\pm iz)^+}{[\Gamma(\frac{4}{3})\Gamma(\frac{5}{3})]} \sim{}& \frac{z^{-3/4}}{\sqrt{\pi}} e^{\sqrt{2z}} \sum_{m=0}^{\infty} N_m z^{-m/2} \cos\left(\sqrt{2z} - \frac{3\pi}{8} - \frac{m\pi}{4} \right) \\ &+ \frac{z^{-3/4}}{\sqrt{\pi}} e^{-\sqrt{2z}} \sum_{m=0}^{\infty} N_m z^{-m/2} \cos\left(\sqrt{2z} - \frac{9\pi}{8} - \frac{3m\pi}{4} \right) + L \text{ asymptotics}, \end{aligned} \tag{5.14}$$

$$\begin{aligned} \Gamma\left(\frac{4}{3}\right)^{-1} {}_0F_1\left(\frac{4}{3};\pm iz\right)^- \sim{}& \frac{z^{-5/12}}{\sqrt{\pi}} e^{\sqrt{2z}} \sum_{m=0}^{\infty} N_m z^{-m/2} \sin\left(\sqrt{2z} - \frac{5\pi}{24} - \frac{m\pi}{4} \right) \\ &- \frac{z^{-5/12}}{\sqrt{\pi}} e^{-\sqrt{2z}} \sum_{m=0}^{\infty} N_m z^{-m/2} \sin\left(\sqrt{2z} - \frac{5\pi}{8} - \frac{3m\pi}{4} \right). \end{aligned} \tag{5.15}$$

An interesting thing to note is the presence in the K asymptotics of all three hypergeometric contributions, of terms which grow exponentially with z. Since the integral representation of $p_\alpha(x)$ does not display such drastic behavior, it must be the case that the N_m are the same for all three contributions so that the exponentially growing terms can cancel. When the recurrence relation for the N_m, which is dependent on the parameters in the given G function, is calculated[24] it is in fact found to be the same in all three cases. This coincidence of the N_m and consequent cancellation of exponentially growing terms is in fact a general trend in the K asymptotics of $p_n(x)$, and occurs for all of the cases we display in the following.

Investigation of the recurrence relation for the N_m of $p_3(x)$ results in[24]

$$N_m = \frac{\Gamma(m+1/6)\Gamma(m+5/6)}{2^{2m} m! \Gamma(1/6)\Gamma(5/6)}. \tag{5.16}$$

Adding the three separate contributions (5.11), (5.14), and (5.15) we obtain the K asymptotic contribution to the asymptotic expansion of $p_3(x)$. We note that the exponentially growing terms do in fact cancel as expected. The complete asymptotic expansion is obtained by adding (5.4),

$$p_3^K(x) \sim \frac{1}{\sqrt{\pi}(3x)^{1/4}} \exp\left(-\sqrt{\frac{2x^3}{27}} \right) \sum_{m=0}^{\infty} N_m \left(\sqrt{\frac{27}{x^3}} \right)^m \cos\left(\sqrt{\frac{2x^3}{27}} - \frac{\pi}{8} - \frac{3m\pi}{4} \right). \tag{5.17}$$

Since $p_3(x)$ has such an elegant representation in terms of Lommel functions, (4.7), one might be tempted to construct the asymptotic expansion of $p_3(x)$ from the tabulated asymptotic expansions of the Lommel functions. We note however that the asymptotic expansions for the Lommel functions that are listed in books, e.g., Refs. 31 and 37, contain only a power series, whereas we find using the general theory of the asymptotics of G functions that $p_3(x)$ contains both a power series and series of exponentially small terms that lie beyond all orders of this power series. Hence the commonly quoted asymptotic expansions of the Lommel functions must be incomplete, and it

seems that the complete asymptotic expansions of the Lommel functions are unknown. The complete asymptotic expansions of the Lommel functions will form the subject of a future publication.

The complete asymptotic expansions of $p_n(x)$ for larger values of n can be found from the asymptotic expansions of the hypergeometric function in a similar manner to that used for $p_3(x)$. We list below the expansion for $n=4,5,6,7$. The details of the derivations can be deciphered from the discussion in Ref. 24. We see that as n increases the complexity of the K asymptotic expansions increases. We list here the first four N_m for each case, but avoid details of the recursion relation, the details of which can be found in Ref. 24,

$$p_4^K(x)\sim \frac{2^{1/6}}{\sqrt{3\pi}x^{1/3}}\exp\left(\frac{-3x^{4/3}}{2^{11/3}}\right)\sum_{m=0}^{\infty} N_m\left(\frac{4}{x}\right)^{4m/3}\cos\left(\frac{3\sqrt{3}}{2^{11/3}}x^{4/3}-\frac{\pi}{6}-\frac{2m\pi}{3}\right). \tag{5.18}$$

Due to the intimate relationship between $p_4(x)$ and Pearcey's integral we include the values of N_m for $0\leqslant m\leqslant 20$ in Table I. The N_m for $m>20$ may be obtained from the following recursion relation, with $N_m=3^{-m}c_m$:

$$c_m=(7/48m-1+m)c_{m-1}+(7/48m-13/16+m-m^2/3)c_{m-2}, \tag{5.19}$$

$$p_5^K(x)\sim \frac{1}{\sqrt{2\pi}5^{1/8}x^{3/8}}\sum_{m=0}^{\infty} N_m\left(\frac{5}{x}\right)^{5m/4}\exp\left[4\cos\left(\frac{5\pi}{8}\right)\left(\frac{x}{5}\right)^{5/4}\right]\cos\left[4\sin\left(\frac{5\pi}{8}\right)\left(\frac{x}{5}\right)^{5/4}-\frac{3\pi}{16}-\frac{5m\pi}{8}\right], \tag{5.20}$$

where $N_0=1$, $N_1=\frac{9}{160}$, $N_2=\frac{441}{51\,200}$, $N_3=\frac{202\,509}{81\,920\,000}$,

$$p_6^K(x)\sim \frac{1}{2\sqrt{15\pi}}\sum_{m=0}^{\infty} N_m\left(\frac{6}{x}\right)^{(6/5)(m+1/3)}(-1)^m\exp\left[-5\left(\frac{x}{6}\right)^{6/5}\right]+\frac{1}{\sqrt{15\pi}}\sum_{m=0}^{\infty} N_m\left(\frac{6}{x}\right)^{(6/5)(m+1/3)}$$
$$\times\exp\left[5\cos\left(\frac{3\pi}{5}\right)\left(\frac{x}{6}\right)^{6/5}\right]\cos\left[5\sin\left(\frac{3\pi}{5}\right)\left(\frac{x}{6}\right)^{6/5}-\frac{\pi}{5}-\frac{3m\pi}{5}\right], \tag{5.21}$$

where $N_0=1$, $N_1=\frac{11}{180}$, $N_2=\frac{517}{64\,800}$, $N_3=\frac{-22\,253}{174\,960\,000}$,

$$p_7^K(x)\sim \frac{1}{7^{1/12}\sqrt{3\pi}x^{5/12}}\sum_{m=0}^{\infty} N_m\left(\frac{7}{x}\right)^{(7/6)m}\exp\left[6\cos\left(\frac{7\pi}{12}\right)\left(\frac{x}{7}\right)^{7/6}\right]\cos\left[6\sin\left(\frac{7\pi}{12}\right)\left(\frac{x}{7}\right)^{7/6}-\frac{5\pi}{24}\right.$$
$$\left.-\frac{7m\pi}{12}\right]+\frac{1}{7^{1/12}\sqrt{3\pi}x^{5/12}}\sum_{m=0}^{\infty} N_m\left(\frac{7}{x}\right)^{(7/6)m}\exp\left[6\cos\left(\frac{11\pi}{12}\right)\left(\frac{x}{7}\right)^{7/6}\right]$$
$$\times\cos\left[6\sin\left(\frac{11\pi}{12}\right)\left(\frac{x}{7}\right)^{7/6}-\frac{\pi}{24}-\frac{11m\pi}{12}\right], \tag{5.22}$$

where $N_0=1$, $N_1=\frac{65}{1008}$, $N_2=\frac{219\,307}{33\,592\,320}$, $N_3=\frac{8\,304\,286\,951}{995\,515\,121\,664}$.

Note that for $p_6(x)$ and $p_7(x)$ there are two exponentially small series not just one. We should therefore expect that the K asymptotic expansions of $p_n(x)$ will contain ever more decaying exponentials as n increases.

VI. MOMENTS

The divergence of the moments of $p_\alpha(x)$ was explained in Sec. I to be a consequence of the $1/x^{\alpha+1}$ asymptotic power law behavior. We have shown in Sec. V however that the large x asymptotic behavior of $p_{2n}(x)$ is purely exponential and contains no algebraic terms, which leads one to expect that their moments might exist. One also reaches this conclusion by observing that

TABLE I. Values of N_m for $p_4(x)$.

m	N_m(exact)	N_m(decimal)
0	1	$1.000\,000\,0000\times10^{0}$
1	$\frac{7}{144}$	$4.861\,111\,111\times10^{-2}$
2	$\frac{385}{41\,472}$	$9.283\,371\,913\times10^{-3}$
3	$\frac{39\,655}{17\,915\,904}$	$2.213\,396\,544\times10^{-3}$
4	$\frac{665\,665}{10\,319\,560\,704}$	$6.450\,516\,830\times10^{-5}$
5	$-\frac{1\,375\,739\,365}{1\,486\,016\,741\,376}$	$-9.257\,899\,50\times10^{-4}$
6	$-\frac{2\,053\,160\,864\,755}{1\,283\,918\,464\,548\,864}$	$-1.599\,136\,48\times10^{-3}$
7	$-\frac{400\,804\,002\,473\,875}{184\,884\,258\,895\,036\,416}$	$-2.167\,864\,39\times10^{-3}$
8	$-\frac{545\,523\,697\,484\,891\,125}{212\,986\,666\,247\,081\,951\,232}$	$-2.561\,304\,45\times10^{-3}$
9	$-\frac{639\,409\,620\,356\,437\,805\,875}{276\,030\,719\,456\,218\,208\,796\,672}$	$2.316\,443\,69\times10^{-3}$
10	$-\frac{7\,400\,680\,096\,069\,804\,168\,625}{79\,496\,847\,203\,390\,844\,133\,441\,536}$	$-9.309\,400\,75\times10^{-5}$
11	$\frac{85\,225\,571\,098\,153\,435\,685\,610\,875}{11\,447\,545\,997\,288\,281\,555\,215\,581\,184}$	$7.444\,876\,929\times10^{-3}$
12	$\frac{548\,115\,663\,843\,414\,041\,224\,022\,298\,125}{19\,781\,359\,483\,314\,150\,527\,412\,524\,285\,952}$	$2.770\,869\,536\times10^{-2}$
13	$\frac{212\,014\,635\,165\,656\,643\,273\,521\,106\,914\,375}{2\,848\,515\,765\,597\,237\,675\,947\,403\,497\,177\,088}$	$7.442\,986\,193\times10^{-2}$
14	$\frac{133\,126\,972\,240\,163\,358\,184\,968\,745\,634\,504\,375}{820\,372\,540\,492\,004\,450\,672\,852\,207\,187\,001\,344}$	$1.622\,762\,411\times10^{-1}$
15	$\frac{90\,364\,081\,190\,288\,921\,441\,174\,372\,687\,896\,958\,125}{354\,400\,937\,492\,545\,922\,690\,672\,153\,504\,784\,580\,608}$	$2.549\,769\,812\times10^{-1}$
16	$\frac{9\,019\,416\,081\,298\,899\,889\,215\,820\,334\,616\,981\,356\,875}{816\,539\,759\,982\,825\,805\,879\,308\,641\,675\,023\,673\,720\,832}$	$1.104\,589\,944\times10^{-2}$
17	$-\frac{260\,021\,114\,680\,943\,473\,566\,117\,212\,676\,037\,766\,397\,671\,875}{117\,581\,725\,437\,526\,916\,046\,620\,444\,401\,203\,409\,015\,799\,808}$	$-2.211\,407\,544\times10^{0}$
18	$-\frac{3\,854\,975\,958\,092\,062\,993\,212\,896\,945\,123\,288\,990\,286\,762\,353\,125}{304\,771\,832\,334\,069\,766\,392\,840\,191\,887\,919\,236\,168\,953\,102\,336}$	$-1.264\,872\,783\times10^{1}$
19	$-\frac{2\,230\,702\,885\,075\,796\,330\,282\,978\,287\,686\,945\,999\,335\,191\,018\,440\,625}{43\,887\,143\,856\,106\,046\,360\,568\,987\,631\,860\,370\,008\,329\,246\,736\,384}$	$-5.082\,816\,262\times10^{1}$
20	$-\frac{4\,085\,674\,814\,497\,803\,591\,523\,660\,096\,191\,996\,942\,460\,008\,554\,035\,146\,875}{25\,278\,994\,861\,117\,082\,703\,687\,736\,875\,951\,573\,124\,797\,646\,120\,157\,184}$	$-1.616\,233\,096\times10^{2}$

in general the nonanalytic behavior of the Fourier transform, $\tilde{p}_\alpha(k)=\exp(-|k|^\alpha)$, is intimately involved in the divergence of sufficiently late moments of $p_\alpha(x)$, because if $\tilde{p}_\alpha(k)$ were analytic it would possess an expansion of the following form:

$$\tilde{p}_\alpha(k)=\sum_{m=0}^{\infty}\frac{(ik)^m}{m!}\langle x^m\rangle, \tag{6.1}$$

where we define $\langle x^m \rangle$ in the usual way as

$$\langle x^m \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, x^m p_\alpha(x). \tag{6.2}$$

When $0<\alpha<2$, so that $p_\alpha(x)$ defines a pdf, $\langle x^m \rangle$ is therefore the mth moment. Regardless of whether $p_\alpha(x)$ defines a pdf or not (6.2) is still perfectly well defined, we therefore shall refer to $\langle x^m \rangle$ as the mth moment in both cases.

When $\alpha=2n$, $\tilde{p}_\alpha(k)$ is analytic and hence according to (6.1) the moments of $p_{2n}(x)$ must exist. This implies that $p_{2n}(x)$ will not display the self-similar Lévy behavior discussed in Sec. I, but is a rather different type of mathematical animal.

Since $p_\alpha(x)$ is an even function the $(2m+1)$th moment vanishes by symmetry for all $m \geqslant 0$, regardless of the value of α. The calculation of the $2m$th moment is somewhat subtle and is facilitated by considering not (6.2), but instead the following integral, $\langle x^{2m} \rangle_\lambda$, which is tempered by the factor $e^{-\lambda x}$.

$$\langle x^{2m} \rangle_\lambda = \frac{2}{\pi} \int_0^\infty \int_0^\infty \mathrm{d}k\, \mathrm{d}x\, e^{-\lambda x} x^{2m} \cos(kx) \exp(-k^\alpha). \tag{6.3}$$

By observing the small λ behavior of this well-behaved integral we can determine whether the $2m$th moment diverges for a given α, and if this moment is finite we can calculate its numerical value by taking $\lambda \to 0$. To ascertain the small λ behavior of $\langle x^{2m} \rangle_\lambda$ we wish to construct a Mellin–Barnes contour integral representation of $\langle x^{2m} \rangle_\lambda$ from which we shall be able to derive a small λ expansion by simply closing the contour. To this end we insert into (6.3) the contour integral representation of e^{-k^α} obtained by expressing it as the inverse Mellin transform of its Mellin transform.

$$\langle x^{2m} \rangle_\lambda = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \mathrm{d}s \left(\frac{2}{\pi\alpha} \right) \Gamma\left(\frac{s}{\alpha} \right) \int_0^\infty \mathrm{d}x\, x^{2m} e^{-\lambda x} \int_0^\infty \mathrm{d}k\, k^{-s} \cos(xk), \quad c>0. \tag{6.4}$$

The integral over k is well known and can be identified with $x^{s-1}\Gamma(1-s)\sin(s\pi/2)$. The integral over x is then simply a gamma function,

$$\begin{aligned} \langle x^{2m} \rangle_\lambda &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \mathrm{d}s \left(\frac{2}{\pi\alpha} \right) \Gamma(1-s) \lambda^{-s-2m} \Gamma\left(\frac{s}{\alpha} \right) \Gamma(2m+s) \sin\left(\frac{s\pi}{2} \right), \quad 0<c<1, \\ \langle x^{2m} \rangle_\lambda &= \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} \mathrm{d}s \left(\frac{-2}{\pi\alpha} \right) \Gamma(1+s) \lambda^{s-2m} \Gamma\left(\frac{-s}{\alpha} \right) \Gamma(2m-s) \sin\left(\frac{s\pi}{2} \right), \quad -1<\sigma<0. \end{aligned} \tag{6.5}$$

In the last step we have chosen to let $s \to -s$ so that all the relevant poles needed to construct the expansion in ascending powers of λ by closing the contour will lie on the positive real axis.

To obtain the small λ expansion of $\langle x^{2m} \rangle_\lambda$ from (6.5) we close the contour to the right. If we denote the integrand by $R(s)$, the terms of this small λ expansion then arise from the residues of $R(s)$ at the poles of $\Gamma(-s/\alpha)\Gamma(2m-s)\sin(s\pi/2)$. We denote the set of all poles of $R(s)$ for $\Re(s)>-1$ by $\mathcal{P}$. When this series in ascending powers of λ is constructed for a given choice of α and $2m$ the leading term will behave like $\lambda^{\Delta-2m}$ where $\Delta=\min(\mathcal{P})$, i.e., Δ is the pole closest to the origin on the positive real line. Hence we see that it is Δ alone that determines the existence or nonexistence of the $2m$th moment of $p_\alpha(x)$. If $\Delta<2m$ the limit as $\lambda \to 0$ will not exist and the corresponding moment diverges. The sign of the residue at this pole determines if the divergence is to positive or negative infinity. For a class of values of $\alpha>2$ the moments in fact diverge to $-\infty$ as we will show, which is a consequence of the fact that $p_\alpha(x)$ is then not a pdf. If $\Delta>2m$ the limit as $\lambda \to 0$ vanishes, and the corresponding moment exists but is zero. The interesting case is when $\Delta=2m$ in which case the limit $\lambda \to 0$ exists and is nonzero.

The set $\mathcal{P}$ is the difference of the set of zeros of the sine function, with the union of the poles of the gamma functions.

$$\begin{aligned}\mathcal{P}&=\{\alpha,2\alpha,3\alpha,\dots\}\cup\{2m,2m+1,2m+2,\dots\}\backslash\{2,4,6,\dots\},\\ \mathcal{P}&=\{2m+1,2m+3,2m+5,\dots\}\cup\{\alpha,2\alpha,3\alpha,\dots\}\backslash\{2,4,6,\dots,2(m-1)\}.\end{aligned}\tag{6.6}$$

Note that the even poles of $\Gamma(2m-s)$ have all been cancelled by the zeros of $\sin(s\pi/2)$. The pole of $\Gamma(-s/\alpha)$ and the zero of $\sin(s\pi/2)$ at the origin have been neglected since they cancel and there is then no pole at the origin provided $m>0$, which we shall assume. The case $m=0$ merely corresponds to the normalization requirement for $p_\alpha(x)$, which is easily shown to result in $\langle x^0\rangle=1$.

If α is not an even integer there can be no further cancellation of poles with zeros and $\mathcal{P}=\{2m+1,2m+3,2m+5,\dots\}\cup\{\alpha,2\alpha,3\alpha,\dots\}\Rightarrow\Delta=\min\{2m+1,\alpha\}$. We thus deduce for non-even integral α that if $\alpha>2m$ then $\langle x^{2m}\rangle$ will exist and vanish, and that if $\alpha<2m$ then $\langle x^{2m}\rangle$ will diverge. Thus if α is not an even integer we can never obtain a finite nonzero moment of any order for $p_\alpha(x)$. To ascertain whether $\langle x_{2m}\rangle$ diverges to positive or negative infinity when $\Delta=\alpha<2m$ and α is not an even integer we calculate the residue at $s=\alpha$, which we denote by $\mathrm{Res}(R(s)|s=\alpha)$. This is straightforward and yields

$$\mathrm{Res}(R(s)|s=\alpha)=-\left[\frac{2}{\pi}\Gamma(1+\alpha)\Gamma(2m-\alpha)\right]\sin\left(\frac{\alpha\pi}{2}\right)\frac{1}{\lambda^{2m-\alpha}}.\tag{6.7}$$

Closing the contour to the right results in an additional minus sign and hence $\langle x^{2m}\rangle_\lambda$ behaves like

$$\langle x^{2m}\rangle_\lambda=\left[\frac{2}{\pi}\Gamma(1+\alpha)\Gamma(2m-\alpha)\right]\sin\left(\frac{\alpha\pi}{2}\right)\frac{1}{\lambda^{2m-\alpha}}+o(\lambda^{\alpha-2m}),\quad \lambda\to 0.\tag{6.8}$$

When $\alpha<2m$ we note that $[(2/\pi)\,\Gamma(1+\alpha)\Gamma(2m-\alpha)]>0$ and thus the sign of the divergence of $\langle x^{2m}\rangle$ depends only on the sign of $\sin(\alpha\pi/2)$. We conclude then that for $\alpha\notin\{2,4,6,\dots\}$ and $\alpha<2m$,

$$\langle x^{2m}\rangle\to+\infty,\quad \alpha\in\cup_{k=0}^{\infty}(4k,4k+2),\tag{6.9}$$

$$\langle x^{2m}\rangle\to-\infty,\quad \alpha\in\cup_{k=0}^{\infty}(4k+2,4k+4).\tag{6.10}$$

Note that $\langle x^{2m}\rangle\to+\infty$ when $0<\alpha<2$ and $\alpha<2m$ as one would expect since in this region $p_\alpha(x)$ is the symmetric Lévy stable pdf.

If α is an even integer we definitely cannot obtain a diverging moment since in order to do this we would require $\Delta=2k\in\{\alpha,2\alpha,3\alpha,\dots\}$ and $2k<2m$, but $2k<2m\Rightarrow 2k\leqslant 2(m-1)\Rightarrow 2k\in\{2,4,6,\dots 2(m-1)\}$ in which case this pole at $s=2k$ would cancel with the zero at $s=2k$, which contradicts the assumption that $\Delta=2k$. Thus all moments are finite when α is an even integer. When $2m=\min(\mathcal{P})$ the $2m$th moment will be nonzero, which implies that we obtain nonzero moments only when $2m=j\alpha$ and $m/j\in\{1,2,3,..\}$, where $j\in\{1,2,3,\dots\}$. In other words, for a given even integral value of α only the moments $\langle x^{j\alpha}\rangle$, $\forall j\in\{1,2,3,\dots\}$, will be nonzero. We now calculate these nonzero moments for $m\in\{1,2,3,\dots\}$ and $\alpha\in\{2,4,6,\dots\}$.

$\Gamma(2m-s)\sin(s\pi/2)$ is analytic around $s=2m$ since the simple zero cancels the simple pole. Hence the pole of $R(s)$ at $s=2m$ is due to $\Gamma(-s/\alpha)$. Multiplying the Laurent expansion of $\Gamma(2m-s)$ with the Taylor expansion of $\sin(s\pi/2)$ around $s=2m$ we obtain

$$\Gamma(2m-s)\sin\left(\frac{s\pi}{2}\right)=\frac{(-1)^{m+1}\pi}{2}+O(s-2m).\tag{6.11}$$

The residue of $R(s)$ at the pole $s=2m$ is then given by

$$\mathrm{Res}(R(s)|s=2m)=\frac{(-1)^m}{\alpha}(2m)!\lim_{s\to 2m}(s-2m)\Gamma\left(\frac{-s}{\alpha}\right),$$
$$\mathrm{Res}(R(s)|s=2m)=\frac{(-1)^{m+1+j}}{j!}(2m)!. \tag{6.12}$$

Since we closed the contour to the right $\langle x^{j\alpha}\rangle=-\mathrm{Res}(R(s)|s=2m)$. All the other terms in the small λ expansion vanish upon taking $\lambda\to 0$ because $\Delta=2m$ by assumption. Thus the only finite nonzero moments of $p_\alpha(x)$ are

$$\langle x^{j\alpha}\rangle=\frac{(-1)^{j\alpha+j}(j\alpha)!}{j!},\quad \forall j\in\{1,2,3,\ldots\}, \tag{6.13}$$

where $\alpha\in\{2,4,6,\ldots\}$.

It is easily seen that by inserting this result into (6.1) that the correct analytic power series expansion of $\tilde{p}_{2n}(k)$ is recovered.

We can summarize the moments of $p_\alpha(x)$ quite simply then as

$$\langle x^{2m}\rangle=\begin{cases}\dfrac{(-1)^{m+j}(2m)!}{j!}, & \alpha=2\dfrac{m}{j}\in\{2,4,6,\ldots\}\\ +\infty, & \alpha<2m \text{ and } \alpha\in\cup_{k=0}^{\infty}(4k,4k+2)\\ -\infty, & \alpha<2m \text{ and } \alpha\in\cup_{k=0}^{\infty}(4k+2,4k+4)\\ 0, & \text{otherwise}\end{cases}. \tag{6.14}$$

VII. DISCUSSION

Various properties of $p_\alpha(x)$ have been expounded in the preceding sections, and in this section we seek to briefly discuss their utility. The utility of the representations of $p_\alpha(x)$ in terms of hypergeometric functions and special functions when $0<\alpha<2$ is obvious, so we shall constrain the discussion to the cases of $\alpha>2$.

The intricate exponential asymptotic behavior of $p_\alpha(x)$ as $x\to\infty$ when $\alpha>2$ provides another powerful case study into the exciting new field of asymptotics beyond all orders, and is a principal reason why we carried out this study. The increasing complexity of the K-asymptotics of $p_n(x)$ as n increases is an example of the level of information that can be contained in these components of a complete asymptotic expansion which traditionally have been neglected.

The discussion of the moments has demonstrated to us that $\{p_\alpha(x):0<\alpha<\infty\}$ is composed of two classes of functions whose behavior is in one sense quite different. The functions $p_{2n}(x)$ have finite moments of all orders and hence do not display the type of scale invariant behavior that makes the Lévy stable pdfs so ubiquitous in applications. This is a direct consequence of the fact that the complete asymptotic expansion of $p_{2n}(x)$ contains no algebraic terms and is purely exponential. Despite, or perhaps because of this fact, we know already that the two lowest order members of this class, $p_2(x)$ and $p_4(x)$, have important applications in the physical sciences, even though $p_4(x)$ does not define a pdf. It is quite reasonable to expect then that other members of this class, e.g., $p_6(x),p_8(x),\ldots,$ should also find similar applications. Looking at things in the opposite light however, the functions in the complement of this class, i.e., all the $p_\alpha(x)$ with α not an even integer, do display the self-similar behavior that makes the Lévy stable pdfs so utile and thus for this reason we might expect that they also will find applications in the fullness of time. With such a diversity of interesting and useful properties it would seem quite uncharacteristic of nature not to harness some of the functions in $\{p_\alpha(x):2<\alpha<\infty\}$.

Standing firmly on the platform of concrete mathematical results that we have delineated herein, we would now like to ascend into a Lévy flight of fancy. The situation with $p_\alpha(x)$ for $\alpha>2$ is reminiscent of the role played by the Wigner function in quantum theory. The Wigner

function is in some sense a measure of probability and is highly useful in applications, but does not satisfy the non-negativity axiom required to define a pdf. In the same way we find applications of $p_4(x)$ to wave phenomena appearing, despite the fact that it does not define a pdf. Perhaps though it may be fruitful to extend the notion of probability to include negative numbers, and hence to consider $p_\alpha(x)$ as a pdf for all $\alpha>0$. There has been a steady flow of articles on *negative probabilities* ever since the advent of quantum mechanics, including notable articles by Feynman.[38,39] For a reasonably up-to-date review article with a large list of references we direct the reader to Ref. 40. In the literature negative probabilities are investigated in order to solve a plethora of problems from the inherent divergences in quantum field theories to issues of interpretation in quantum theory itself such as the Einstein–Podolsky–Rosen paradox. One interesting idea that we would like to mention is the possible connection between classical mechanics and a theory of quantum mechanics with negative probabilities discussed by Feynman.[38] To quote Feynman,

"...a closer study of the relation of classical and quantum theory might involve us in negative probabilities." We find it interesting to table the idea that since the Lévy stable densities are so fundamentally useful in classical stochastic processes, that perhaps $\{p_\alpha(x):\alpha>2\}$ might play a similar role in a stochastic formulation of quantum theory in which negative probabilities are allowed. In general, if it should emerge that extended theories of probability do bear fruit, then $\{p_\alpha(x):\alpha>2\}$ must surely play as fundamental a role in it as the Lévy stable densities play in classical probability theory.

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APPENDIX A: ERRATA GENERALIZED EULER–JACOBI INVERSION FORMULA AND ASYMPTOTICS BEYOND ALL ORDERS

We present here a list of typographical errors that appear in Ref. 24, and which were detected during the preparation of this work. The errors and their corrections are emphasized via boldface.

In (5.13), $\Sigma_{n=1}^{\infty}\mathbf{4}/z^{3/2}$ should read $\Sigma_{n=1}^{\infty}\mathbf{8}/z^{3/2}$.

In (6.29), $\cos((\sqrt{3}/2)y-k\pi/3-\pi/6)$ should read $\cos((\sqrt{3}/2)y-\mathbf{2}(k\pi/3)-\pi/6)$.

In (6.52), the correct argument of the Lommel functions is $(\mathbf{2}/\sqrt{a})(2n\pi/3)^{3/2}e^{\pm 3\pi i/4}$ not $\sqrt{\mathbf{2}/\mathbf{a}}(2n\pi/3)^{3/2}e^{\pm 3\pi i/4}$ as stated.

In (6.58), ${}_0F_1(4/3;\pm iz)^{+}$ should read ${}_0F_1(4/3;\pm iz)^{-}$.

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Phases for dyadic orthonormal wavelets

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We consider real-valued functions $\alpha(s)$ and wavelets $\psi \in L^2(\mathbb{R})$ such that $e^{i\alpha(s)}|\hat{\psi}(s)|$ is the Fourier transform of a wavelet. Such a function $\alpha(s)$ is called an attainable phase for the wavelet ψ. It is known that for all multiresolution analysis (MRA) wavelets, the phase function $\alpha(s)=\frac{1}{2}s$ is attainable, and any real function $\alpha(s)$ is attainable by any minimally-supported-frequency (MSF) wavelet. Besides this, very little is known in the literature about attainable phases for wavelets. We study the problem of determining functions which are attainable phases for some (non-MSF) wavelets. We prove that there exists a non-MSF wavelet for which there is no attainable ''set-wise'' linear phase. This answers a basic question about wavelet phases. Although we do not know whether for any irrational number a, as is attainable by some non-MSF wavelets, we show that there exist certain rational numbers a such that as is not attainable by any non-MSF wavelet. We also prove that there exists a large class of rational numbers a such that as is attainable by some non-MSF wavelets. We examine the relationship between different classes of wavelets admitting linear phases. In particular we present an example of a non-MSF wavelet which is not an MRA wavelet but admits linear phase $\frac{1}{2}s$. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1462416]

I. INTRODUCTION

Wavelet analysis arises from many branches of science and provides means of representing functions in a way similar to Fourier series. Recall that a *dyadic orthonormal (or orthogonal) wavelet* is a function $\psi \in \mathcal{L}^2(\mathbb{R})$ (the Hilbert space of square-integrable functions on $\mathbb{R}$) with the property that the set

$$\{2^{n/2}\psi(2^n t-l): n,l \in \mathbb{Z}\}$$

is an orthonormal basis for $\mathcal{L}^2(\mathbb{R})$, where $\mathbb{Z}$ is the set of all the integers. Let $\mathcal{F}$ be the Fourier–Plancherel transformation on $\mathcal{L}^2(\mathbb{R})$, normalized so that it is unitary. Thus for $f,g \in \mathcal{L}^1(\mathbb{R}) \cap \mathcal{L}^2(\mathbb{R})$,

$$\mathcal{F}(f)(s) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ist} f(t)\,dt$$

and

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$$\mathcal{F}^{-1}(f)(s) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ist} f(t)\, dt.$$

We will write $\mathcal{F}(h)$ as $\hat{h}$ throughout this article. Recall from Ref. 1 that a wavelet ψ is called an *MSF (minimally-supported-frequency) wavelet* if $\operatorname{supp}\hat{\psi}$ has measure 2π. It is also called an *s-elementary wavelets* in Refs. 2 and 3. A wavelet which is not an MSF wavelet will be referred to as a *non-MSF wavelet*. It is well known that a wavelet ψ is an MSF wavelet if and only if for almost any $s \in \mathbb{R}$ with $\hat{\psi}(s) \neq 0$, we have $\hat{\psi}(s + 2l\pi) = 0$ whenever $l \in \mathbb{Z}\setminus\{0\}$. In this article, we will use this fact to determine whether any given wavelet ψ is an MSF wavelet. More importantly, the following characterization of wavelets quoted from Ref. 1 will play a central role in this article. If $\psi \in \mathcal{L}^2(\mathbb{R})$, then ψ is a wavelet iff the norm of ψ is 1 and

$$\sum_{\ell \in \mathbb{Z}} |\hat{\psi}(2^{\ell} s)|^2 = \frac{1}{2\pi}, \quad \text{a.e. } s \in \mathbb{R}, \tag{1.1}$$

$$\sum_{\ell=0}^{\infty} \hat{\psi}(2^{\ell} s)\, \overline{\hat{\psi}(2^{\ell}(s + 2k\pi))} = 0. \quad \text{a.e. } s \in \mathbb{R}, \quad \text{for each } k \in 2\mathbb{Z}+1. \tag{1.2}$$

In wavelet analysis, one of the most important concepts is *multiresolution analysis*, which was introduced and developed by Mallat[4] and Meyer[5] as an important tool in constructing orthogonal wavelets. Wavelets obtained through multiresolution analysis are called *MRA wavelets*. We refer to standard books (cf. Refs. 1 and 5–7) for the definition of multiresolution (MRA) wavelets. For the purpose of this article, we will use the fact (Ref. 1) that a wavelet ψ is an MRA wavelet if and only if its *dimension function* $D_{\psi}(s) = (2\pi)\Sigma_{n=1}^{\infty}\Sigma_{k\in\mathbb{Z}} |\hat{\psi}(2^n(s + 2k\pi))|^2 = 1$, a.e. $s \in \mathbb{R}$.

For any function $h \in \mathcal{L}^2(\mathbb{R})$, the *phase* of h is the real-valued function $\alpha(s)$ defined on the support of $\hat{h}$ determined uniquely a.e. modulo 2π by the equation $\hat{h}(s) = e^{i\alpha(s)}|\hat{h}(s)|$. Phases carry useful information contained in signals. For instance, an electrocardiogram or a video image can be represented in terms of magnitude and phase information. Since wavelets provide building blocks in reconstructing signals, we are interested in knowing more about phases of wavelets.

The phase of a given wavelet could be quite complicated, even when the wavelet is an MRA wavelet. However, it was established in Refs. 8 and 9 that for any MRA wavelet ψ, $e^{i(1/2)s}|\hat{\psi}(s)|$ is always the Fourier transform of some MRA wavelet. This fact was used to study wavelet multipliers and the connectivity properties of MRA wavelet (cf. Refs. 8 and 9). Naturally, it leads one to the consideration of the case when ψ is a wavelet in general. We say that a function $\alpha(s)$ is an *attainable* phase (or simply attainable) for wavelet ψ, or that wavelet ψ admits phase function $\alpha(s)$, if $e^{i\alpha(s)}|\hat{\psi}(s)|$ is the Fourier transform of a wavelet. Using this terminology, the above mentioned result says that function $\frac{1}{2}s$ is attainable for any MRA wavelet.

When ψ is an MSF wavelet, we see that for almost any $s \in \mathbb{R}$, each $k \in 2\mathbb{Z}+1$, and $\ell \in \mathbb{N}\cup\{0\}$, the term $\hat{\psi}(2^{\ell} s)\,\overline{\hat{\psi}(2^{\ell}(s + 2k\pi))}$ to the left of equation (1.2) in the characterization of wavelets is 0, therefore $e^{i\alpha(s)}|\hat{\psi}|$ also satisfies all the equations in the characterization of wavelets for any real function $\alpha(s)$. Hence any real function is an attainable phase for any fixed MSF wavelet. Therefore, when we talk about attainable phases, we are only interested in those that are attainable by non-MSF wavelets.

It is known (cf. Ref. 6) that admitting linear phase $\alpha(s) = as + b$ can be a useful property for a wavelet to have, and it was expected that all the wavelets admit the phase $\frac{1}{2}s$. Therefore, one would expect that at least every wavelet admits a linear phase. Unfortunately this is not true, as a counterexample constructed in Ref. 8 shows. However, the wavelet in that example admits a piece-wise linear phase. Therefore, it is natural to ask the following question.

Question 1: Does every wavelet admit at least a piece-wise linear phase?

The answer to this question is also negative. In Sec. IV, we construct an example of a wavelet such that it even does not admit any ''set-wise'' linear phase function (Example 4.2). The main

part of this article is devoted to linear phase functions. First, let us note that the following can be easily checked by using the two equations in the characterization of wavelets.

Lemma 1.1: If function $\alpha(s)$ is attainable for a wavelet ψ, then $-\alpha(s)$ and $\alpha(s)+ks+r$ are also attainable for the same wavelet ψ where k is any integer and r is any real number.

Because of the above lemma, we only need to consider linear phase functions of the form $\alpha(s)=as$ for $a\in[0,\frac{1}{2}]$. Hence we are interested in the following question:

Question 2: For which $a\in[0,\frac{1}{2}]$ is there a non-MSF wavelet that admits the phase function $\alpha(s)=as$?

Although we are not able to completely answer this question, we obtain the following theorems.

Theorem 1.2: *Let a be a real number such that either*

(i) $a=m/2^j n$ *with* $m, n\in 2\mathbb{Z}+1$ *and* $j\in\mathbb{N}$, *or*

(ii) $a=m/9n$ *with* $n\in 2\mathbb{Z}+1$ *and* $m\in\mathbb{Z}\backslash\{0\}$ *such that* m *is not divisible by* 3. *Then there exists a non-MSF wavelet ψ which admits the phase function $\alpha(s)=as$.*

We also prove (Proposition 2.1) that 0, $\frac{1}{3}s$, $\frac{1}{7}s$, $\frac{2}{7}s$, $\frac{3}{7}s$ are not attainable for any non-MSF wavelets. We do not know whether there exists an irrational a such that as is a phase for a non-MSF wavelet. This illustrates the complexity of the problem.

In Sec. III, we will concentrate on the class of wavelets which admits linear phase $\frac{1}{2}s$. If we denote by $\mathcal{W}_a$ the set of all the wavelets that admit phase function as, then, as we mentioned in the abstract, $\mathcal{W}_{1/2}$ contains all the MRA wavelets. Example 4.1 in this article shows that there exists a non-MSF wavelet which is not an MRA wavelet and admits phase $\frac{1}{2}s$. In other words, $\mathcal{W}_{1/2}$ is larger than the set of all MRA wavelets (modulo the MSF wavelets). We also study the relationship between $\mathcal{W}_{1/2}$ and $\mathcal{W}_a$ with various $a\in[0,\frac{1}{2}]$. In particular, we give characterizations for wavelets in $\mathcal{W}_{1/2}$ and $\mathcal{W}_{1/4}$, and prove the following:

Theorem 1.3: *Let a be a real number. Then there exists a non-MSF wavelet admitting both phases as and $\frac{1}{2}s$ if and only if $a=m/2n$ for some $m, n\in 2\mathbb{Z}+1$. In particular, $\mathcal{W}_{1/2}\cap\mathcal{W}_a$ does not contain any non-MSF wavelets if a is irrational.*

II. LINEAR PHASES OF WAVELETS

Before giving proof of Theorem 1.2, we first prove that there exist rational numbers $a\in[0,1/2]$ such that $\alpha(s)=as$ is not attainable by any non-MSF wavelet. Note that to determine whether or not any choice of $a\in[0,1/2]$ yields an attainable phase $\alpha(s)=as$ for a wavelet ψ, we only need to look at Eq. (1.2) in the characterization of wavelets, since the choices of function $\alpha(s)$ do not affect any other conditions.

Proposition 2.1: If $a\in\{m/3,m/7:m\in\mathbb{Z}\}$, then phase function $\alpha(s)=as$ is attainable only by MSF wavelets.

Proof: Let m be an arbitrary fixed number in $\mathbb{Z}$. First we consider the case when $\alpha(s)=(m/3)s$ is attainable for a wavelet ψ. Applying Eq. (1.2) to the wavelet whose Fourier transform is $e^{i\alpha(s)}|\hat{\psi}(s)|$, after taking complex conjugates to both sides of the resulting equation, we have that

$$\sum_{j=0}^{\infty} e^{i(2^j 2km\pi/3)}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|=0 \tag{2.1}$$

holds for a.e. $s\in\mathbb{R}$ and for each $k\in 2\mathbb{Z}+1$.

Equation (2.1) implies that

$$\sum_{j=0}^{\infty} |\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|=0 \tag{2.2}$$

holds for a.e. $s\in\mathbb{R}$ and for each $k\in 2\mathbb{Z}+1$ with $km\in 3\mathbb{Z}$.

Note that for each $j=2\ell\in 2(\mathbb{N}\cup\{0\})$, we can write $2^{j+1}=2^{2\ell+1}=2(4^{\ell}-1)+2$. Likewise, for each $j=2\ell+1\in 2(\mathbb{N}\cup\{0\})+1$, we can write $2^{j+1}=2^{2\ell+2}=4(4^{\ell}-1)+4$. Hence Eq. (2.1) also implies that

$$\sum_{j\in 2(\mathbb{N}\cup\{0\})} e^{i2\pi/3}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|+\sum_{j\in 2(\mathbb{N}\cup\{0\})+1} e^{i4\pi/3}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|=0 \tag{2.3}$$

holds for a.e. $s\in\mathbb{R}$ and for each $k\in 2\mathbb{Z}+1$ with $mk\in 3\mathbb{Z}+1$.

Similarly, Eq. (2.1) implies that

$$\sum_{j\in 2(\mathbb{N}\cup\{0\})} e^{i4\pi/3}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|+\sum_{j\in 2(\mathbb{N}\cup\{0\})+1} e^{i2\pi/3}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|=0 \tag{2.4}$$

holds for a.e. $s\in\mathbb{R}$ and for each $k\in 2\mathbb{Z}+1$ with $mk\in 3\mathbb{Z}+2$.

Note that for non-negative real numbers a and b, $ae^{i2\pi/3}+be^{i4\pi/3}=0$ implies $a=0$ and $b=0$. It follows then from Eqs. (2.2)–(2.4) that for almost all $s\in\mathbb{R}$, and each $k\in 2\mathbb{Z}+1$ and each $j\in\mathbb{N}\cup\{0\}$, $|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|=0$.

When $j=0$, the above says that for any $s\in\mathbb{R}$ such that $|\hat{\psi}(s)|\neq 0$, we have $|\hat{\psi}(s+2k\pi)|=0$ for each $k\in 2\mathbb{Z}+1$. When $j\in\mathbb{N}$, by using a substitution, we see from above that for any $s\in\mathbb{R}$ such that $|\hat{\psi}(s)|\neq 0$, we must have $|\hat{\psi}(s+2^j 2k\pi)|=0$ for each $k\in 2\mathbb{Z}+1$. Thus we conclude that for any $s\in\mathbb{R}$ such that $|\hat{\psi}(s)|\neq 0$, we must have $|\hat{\psi}(s+2\ell\pi)|=0$ for each $l\ell\in\mathbb{Z}$. This implies that ψ is an MSF wavelet.

Next, we consider the case when $\alpha(s)=(m/7)s$ is attainable for a wavelet ψ. Similarly, from Eq. (1.2) we have that

$$\sum_{j=0}^{\infty} e^{i(2^j 2km\pi/7)}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|=0 \tag{2.5}$$

holds for a.e. $s\in\mathbb{R}$ and for each $k\in 2\mathbb{Z}+1$.

Just as before, we discuss how Eq. (2.5) turns out for different $k\in 2\mathbb{Z}+1$. To avoid repetition, we point out first that Eq. (2.5) implies that for almost all $s\in\mathbb{R}$ and each $k\in 2\mathbb{Z}+1$ with $mk\in 7\mathbb{Z}+1$,

$$\sum_{j\in 3(\mathbb{N}\cup\{0\})} e^{i2\pi/7}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|+\sum_{j\in 3(\mathbb{N}\cup\{0\})+1} e^{i4\pi/7}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|$$
$$+\sum_{j\in 3(\mathbb{N}\cup\{0\})+2} e^{i8\pi/7}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|=0.$$

Other cases (seven cases altogether) turn out to be similar. Equation (2.5) implies that for almost all $s\in\mathbb{R}$ and each $k\in 2\mathbb{Z}+1$ with $mk\in 7\mathbb{Z}+2$ (respectively, $mk\in 7\mathbb{Z}+3$, or $mk\in 7\mathbb{Z}+4$, or $mk\in 7\mathbb{Z}+5$, or $mk\in 7\mathbb{Z}+6$), an equation similar to the above holds with only the numbers $2\pi/7$, $4\pi/7$, $8\pi/7$ replaced by $4\pi/7$, $8\pi/7$, $2\pi/7$ (respectively, $6\pi/7$, $12\pi/7$, $10\pi/7$, or $8\pi/7$, $2\pi/7$, $4\pi/7$, or $10\pi/7$, $6\pi/7$, $12\pi/7$, or $12\pi/7$, $10\pi/7$, $6\pi/7$) in that order.

Lastly, Eq. (2.5) implies that for almost all $s\in\mathbb{R}$ and each $k\in 2\mathbb{Z}+1$ with $mk\in 7\mathbb{Z}$, $\Sigma_{j=0}^{\infty}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|=0$.

Note that for non-negative real numbers a, b and c, $ae^{i2\pi/7}+be^{i4\pi/7}+ce^{i8\pi/7}=0$ implies that a, b and c are necessarily 0. Likewise, $ae^{i6\pi/7}+be^{i10\pi/7}+ce^{i12\pi/7}=0$ also implies that a, b and c are necessarily 0. Thus we conclude that for almost all $s\in\mathbb{R}$, for each $k\in 2\mathbb{Z}+1$, and each j

$\in \mathbb{N}\cup\{0\}$, $|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|=0$. Applying the same argument as in the case when $\alpha(s)=m/3s$ is attainable, we conclude also that ψ is an MSF wavelet. □

From the above proposition we have that for $a\in\{0,1/3,1/7,2/7,3/7\}\subset[0,1/2]$, phase function $\alpha(s)=as$ is attainable only by MSF wavelets. However, Theorem 1.2 tells us that there exist "many" rationals a such that as is attainable by non-MSF wavelets.

To prove Theorem 1.2, we need a result of Speegle in Ref. 10 concerning path-connectedness of the s-elementary wavelets. Let $\tilde{\tau}:\mathbb{R}\to[-2\pi,-\pi)\cup[\pi,2\pi)$ and $\tilde{d}:\mathbb{R}_0=(\mathbb{R}\backslash\{0\})\to[-2\pi,-\pi)\cup[\pi,2\pi)$ be the measurable maps defined by $\tilde{\tau}(x)=x+2\pi m(x)$, $\tilde{d}(x)=2^{n(x)}x$, where m and n are the unique integers which map x into $[-2\pi,-\pi)\cup[\pi,2\pi)$ under translation by $2\pi m$ and dilation by 2^n, respectively. Then a measurable subset W of $\mathbb{R}$ is called a *subwavelet set* if both $\tilde{d}|_W$ and $\tilde{\tau}|_W$ are injections modulo null sets. Moreover, W is a *wavelet set* if and only if $\tilde{d}|_W$ and $\tilde{\tau}|_W$ are bijections (modulo null sets). Equivalently, W is a wavelet set if and only if both $\{W+2km\pi:m\in\mathbb{Z}\}$ and $\{2^nW:n\in\mathbb{Z}\}$ are partitions (modulo null sets) for $\mathbb{R}$. We point out in passing that wavelet sets are exactly the support set of MSF wavelets. For a subwavelet set A we define two subsets of $[-2\pi,-\pi)\cup[\pi,2\pi)$ by $A^d=\tilde{d}(A)$ and $A^\tau=\tilde{\tau}(A)$.

Lemma 2.2:[10] *Let A be a subwavelet set. Suppose*

(1) there is an $\epsilon>0$ such that $A^\tau\subset[-2\pi+\epsilon,-\pi)\cup[\pi,2\pi-\epsilon)$ and

(2) $S:=([-2\pi,-\pi)\cup[\pi,2\pi))\backslash A^d$ has a nonempty interior.

Then there is a wavelet set $W\supset A$.

Proof of Theorem 1.2:

Case (i): $a=m/2^jn$, $m,n\in 2\mathbb{Z}+1$, $j\in\mathbb{N}$:

Without loss of generality, we may only consider the case when $n\in 2(\mathbb{N}\cup\{0\})+1$. For fixed $n\in 2(\mathbb{N}\cup\{0\})+1$ and $j\in\mathbb{N}$, let $A_1=[-\pi,-\pi/2)$ and $A_2=2^jn\pi+[-\pi/2,-\pi/4)$. Let us first show that $A=A_1\cup A_2$ is a subwavelet set, namely that both $\tilde{\tau}|_A$ and $\tilde{d}|_A$ are injective.

To this end, it suffices to show that for some k_1, $k_2\in\mathbb{Z}$, $A_1+2k_1\pi$ and $A_2+2k_2\pi$ are disjoint subsets of $[-2\pi,-\pi)\cup[\pi,2\pi)$, and also that for some j_1, $j_2\in\mathbb{Z}$, $2^{j_1}A_1$ and $2^{j_2}A_2$ are disjoint subsets of $[-2\pi,-\pi)\cup[\pi,2\pi)$.

Indeed, $A_1+2\pi=[\pi,\frac{3}{2}\pi)$, $A_2-2^jn\pi+2\pi=[\frac{3}{2}\pi,\frac{7}{4}\pi)$.

Observe that when $n=1$, $A_2=2^j\pi+[-\pi/2,-\pi/4)=2^{j-1}[2\pi-(\pi/2^j),2\pi-(\pi/2^{j+1}))$. Clearly $[2\pi-(\pi/2^j),2\pi-(\pi/2^{j+1}))\subset[\pi,2\pi)$. When $n\in 2\mathbb{N}+1$, there exists $k\in\mathbb{N}$ such that $2^k<n<2^{k+1}$. Thus $2^k<(n-(1/2^{j+1}))$. Since $A_2=2^jn\pi+[-\pi/2,-\pi/4)=2^{j+k}[(n/2^k)\pi-(\pi/2^{j+k+1}),(n/2^k)\pi-(\pi/2^{j+k+2}))$. It follows that A_2 is contained in $2^{j+k}[\pi,2\pi)$. On the other hand, we always have $2A_1=[-2\pi,-\pi)$. Thus both $\tilde{\tau}|_A$ and $\tilde{d}|_A$ are injective, so A is a subwavelet set.

Now let us check that conditions in Lemma 2.2 are satisfied. From the last paragraph, we see that the ϵ in the first condition can be taken as large as $\pi/4$ and that the interior of set S in the second condition contains the open interval $(2\pi-(\pi/2^{j+1}),2\pi)$ when $n=1$ and the open interval $((n/2^k)\pi-(\pi/2^{j+k+2}),2\pi)$ when $n\in 2\mathbb{N}+1$ (where $k\in\mathbb{N}$ and $2^k<n<2^{k+1}$). According to Lemma 2.2, there is a wavelet set $W\supset A$.

Now let $B_1=[-\pi/2,-\pi/4)$ and $B_2=2^{j+1}n\pi+[-\pi,-\pi/2)$. We see that $2B_1=A_1$, $2A_2=B_2$. Also $A_1+2^{j+1}n\pi=B_2$ and $B_1+2^jn\pi=A_2$. Thus $B=B_1\cup B_2$ is also a subwavelet set. Note that sets A and B are disjoint from each other. Also, because the disjoint union of sets $W\backslash A$ and A is a wavelet set, so for any $j\in\mathbb{Z}$, $2^j(W\backslash A)$ is disjoint from A; for any $k\in\mathbb{Z}$, $W\backslash A+2k\pi$ is also disjoint from A. Thus from the relations between A_1, A_2 and B_1, B_2, we see that $W\backslash A$ is disjoint from B and the disjoint union of $W\backslash A$ and B also forms a wavelet set. Now we can construct a non-MSF wavelet which admits phase $(m/2^jn)s$.

We first define a measurable function g on $A\cup B$ in the following way: Let g be any measurable function on A_1. By using the relations between sets A_1, A_2 and B_1, B_2, we define g so that $g(s)=g(s-2^{j+1}n\pi)$ when $s\in B_2$, $g(s)=g(2s-2^{j+1}n\pi)$ when $s\in A_2$ and $g(s)=g(2s)$ when $s\in B_1$. Let

$$|f(s)|=\begin{cases}\dfrac{|\sin(g(s))|}{\sqrt{2\pi}}, & s\in A,\\ \dfrac{|\cos(g(s))|}{\sqrt{2\pi}}, & s\in B,\\ \dfrac{1}{\sqrt{2\pi}}, & s\in W\backslash A,\\ 0, & \text{otherwise.}\end{cases}$$

First we compute the norm of $|f|$. By definition of g and relations between sets A and B, through change of variables in integration, we see that $\int_A|\cos(g(s))|^2\,ds=\int_B|\cos(g(s))|^2\,ds$. Also note that since W is a wavelet set, we have $\mu(W)=2\pi$, where μ is the Lebesgue measure on $\mathbb{R}$. Thus

$$\|f\|^2=\int_{\mathbb{R}}|f(s)|^2ds=\frac{1}{2\pi}\left(\int_A|\sin(g(s))|^2ds+\int_B|\cos(g(s))|^2ds+\mu(W\backslash A)\right)$$
$$=\frac{1}{2\pi}(\mu(A)+\mu(W\backslash A))=\frac{\mu(W)}{2\pi}=1.$$

Second, we check whether Eq. (1.1) is satisfied by the function whose Fourier transform has modulus $|f|$. Since W is a wavelet set, it follows that $\{2^\ell W:\ell\in\mathbb{Z}\}$ forms a partition of $\mathbb{R}$ (modulo a measure zero set). So it suffices to check (1.1) for $s\in W$. If $s\in A_1$, then $2^{-1}s\in B_1$ and $g(2^{-1}s)=g(s)$ by definition of g. Also, for any $\ell\neq 0,\ -1$, since $2^\ell s\in\mathbb{R}\backslash(W\cup B)$, we have $f(2^\ell)=0$. Thus,

$$\sum_{\ell\in\mathbb{Z}}|f(2^\ell s)|^2=|f(s)|^2+|f(2^{-1}s)|^2$$
$$=\frac{1}{2\pi}(|\sin g(s)|^2+|\cos g(2^{-1}s)|^2)$$
$$=\frac{1}{2\pi}(|\sin g(s)|^2+|\cos g(s)|^2)=\frac{1}{2\pi}.$$

Hence (1.1) holds when $s\in A_1$. Similarly, it holds when $s\in A_2$. When $s\in W\backslash A$, all the terms in (1.1) are zero except for $|f(s)|^2$ which is $1/2\pi$. Therefore we conclude that (1.1) holds for all $s\in W$.

For any fixed $m\in 2\mathbb{Z}+1$, we claim that $\hat{\psi}(s)=e^{ims/n2^j}|f(s)|$ is Fourier transform of a wavelet, and hence ψ is a wavelet admitting the phase $(m/2^jn)s$. (Obviously we can choose g such that ψ is not an MSF wavelet.) Taking all the properties enjoyed by $|f|$ into consideration, we see that we only need to check that $\hat{\psi}$ satisfies Eq. (1.2). By definition of g and relations between sets A_1, A_2, and B_1, B_2, we see that every term to the left of Eq. (1.2) is 0 unless when $s\in 2^{-j+1}B_1$, $k=n$ or when $s\in 2^{-j+1}A_2$, $k=-n$. In the first case, we have $2^{j-1}s\in B_1$, $2^{j-1}(s+2n\pi\in A_2)$, $2^js\in A_1$ and $2^j(s+2n\pi)\in B_2$. Thus

$$\sum_{\ell=0}^{\infty} \hat{\psi}(2^{\ell}s)\overline{\hat{\psi}(2^{\ell}(s+2n\pi))} = \hat{\psi}(2^{j-1}s)\overline{\hat{\psi}(2^{j-1}(s+2n\pi))} + \hat{\psi}(2^{j}s)\overline{\hat{\psi}(2^{j}(s+2n\pi))}$$

$$= \frac{1}{2\pi}(-|\cos g(2^{j-1}s)\|\sin g(2^{j-1}s+2^{j}n\pi)|$$

$$+|\sin g(2^{j}s)\|\cos g(2^{j}s+2^{j+1}n\pi)|)$$

$$= \frac{1}{2\pi}(-|\cos g(2^{j-1}s)\|\sin g(2^{j-1}s)|$$

$$+|\sin g(2^{j-1}s)\|\cos g(2^{j-1}s)|) = 0.$$

We use both translation and dilation periodicity properties of g on $A\cup B$ in the above calculation. The second case can be treated similarly.

Case (ii): $a=m/9n$, $n\in 2\mathbb{Z}+1$, $m\in\mathbb{Z}\backslash\{0\}$, $m\notin 3\mathbb{Z}$:

The proof of case (*ii*) is similar to that of case (*i*). So we will be brief at certain places. Again, as in case (*i*), it suffices to consider the case when n is a positive odd integer. Fix an $n\in 2(\mathbb{N}\cup\{0\})+1$, let $A_1=[-\pi,-\pi/2)$, $A_2=8n\pi+[-\pi/4,-\pi/8)$ and $A_3=4n\pi+[-\pi/16,-\pi/32)$. We first show that the set $A=A_1\cup A_2\cup A_3$ is a subwavelet set.

First note that $A_1+2\pi=[\pi,\frac{3}{2}\pi)$, $A_2-8n\pi+2\pi=[2\pi-(\pi/4),2\pi-(\pi/8))$, $A_3-4n\pi+2\pi=[2\pi-(\pi/16),2\pi-(\pi/32))$. Therefore $\tilde{\tau}|_A$ is injective.

Observe also that when $n=1$, $A_2=8\pi+[-\pi/4,-\pi/8)=4[\frac{31}{16}\pi,\frac{63}{32}\pi)$, and $A_3=4\pi+[-\pi/16,-\pi/32)=2[\frac{63}{32}\pi,\frac{127}{64}\pi)$. When $n\in 2\mathbb{N}+1$, there exists $k\in\mathbb{N}$ such that $2^k<n<2^{k+1}$, thus $2^k<(n-\frac{1}{32})$. Note that $2A_3$ and A_2 are disjoint and $2A_3\cup A_2=8n\pi+[-\pi/4,-\pi/16)=2^{k+3}[(n/2^k)\pi-(1/2^{k+5})\pi,(n/2^k)\pi-(1/2^{k+7})\pi)$. Hence, $2A_3\cup A_2$ is contained in $2^{k+3}[\pi,2\pi)$. On the other hand, $2A_1=[-2\pi,-\pi)$. Thus $\tilde{d}|_A$ is injective. So A is a subwavelet set.

To check that the conditions in Lemma 2.2 are satisfied, we observe that from the last paragraph the ϵ in the first condition can be taken as large as $\pi/32$ and that the interior of set S in the second condition contains the open interval $(\frac{127}{64}\pi,2\pi)$ in the case $n=1$ and the open interval $((n/2^k)\pi-(1/2^{k+7})\pi,2\pi)$ in the case $n\in 2\mathbb{N}+1$ (where $k\in\mathbb{N}$ such that $2^k<n<2^{k+1}$). According to Lemma 2.2, there is a wavelet set $W\supset A$.

Now let $B_1=[-\pi/4,-\pi/8)$, $B_2=2n\pi+[-\pi/16,-\pi/32)$ and $B_3=64n\pi+[-\pi,-\pi/2)$. Also let $C_1=[-\pi/16,-\pi/32)$, $C_2=32n\pi+[-\pi,-\pi/2)$ and $C_3=16n\pi+[-\pi/4,-\pi/8)$. Note that $A_1=4B_1=16C_1$, $C_2=4A_2=16B_2$, and $B_3=4C_3=16A_3$. Also $A_1=C_2-32n\pi=B_3-64n\pi$, $B_1=A_2-8n\pi=C_3-16n\pi$, and $C_1=B_2-2n\pi=A_3-4n\pi$. Thus $B=B_1\cup B_2\cup B_3$, $C=C_1\cup C_2\cup C_3$ are also subwavelet sets. Observe that sets A, B and C are mutually disjoint from each other. Moreover, $W\backslash A$ is disjoint from B and C, and the union of $W\backslash A$ and B also forms a wavelet set. So does the disjoint union of $W\backslash A$ and C.

Let us define function f so that

$$|f(s)| = \begin{cases} \dfrac{1}{\sqrt{6\pi}}, & s\in A\cup B\cup C, \\ \dfrac{1}{\sqrt{2\pi}}, & s\in W\backslash A, \\ 0, & \text{otherwise.} \end{cases}$$

As in case (*i*), one can easily check that $\|f\|=1$ and Eq. (1.1) is satisfied by $|f|$. To see that for each $m\in\mathbb{Z}\backslash\{0\}$ such that m is not divisible by 3, $e^{i(m/9n)s}|f|$ is a Fourier transform of a wavelet, it is left to check whether Eq. (1.2) is satisfied by the function whose Fourier transform is $e^{i(m/9n)s}|f|$. By definition of f and relations between sets A_1,A_2,A_3, B_1,B_2,B_3 and C_1,C_2,C_3,

we see that each term to the left of Eq. (1.2) is 0 unless one of the following is true: (1) $s \in C_1$, $k=n$; (2) $s \in \frac{1}{2}C_1$, $k=n$; (3) $s \in B_2$, $k=n$; (4) $s \in B_2$, $k=-n$; (5) $s \in A_3$, $k=-n$; and (6) $s \in \frac{1}{2}A_3$, $k=-n$. In case (1), when $s \in C_1$, we have that $4s \in B_1$, $16s \in A_1$ and that $s+2n\pi \in B_2$, $4(s+2n\pi) \in A_2$, $16(s+2n\pi) \in C_2$. Thus when $m=9m_1+1$ with some $m_1 \in \mathbb{Z}$, we have

$$\sum_{\ell=0}^{\infty} \hat{\psi}(2^{\ell}s)\overline{\hat{\psi}(2^{\ell}(s+2n\pi))} = \hat{\psi}(s)\overline{\hat{\psi}(s+2n\pi)} + \hat{\psi}(4s)\overline{\hat{\psi}(4(s+2n\pi))} + \hat{\psi}(16s)\overline{\hat{\psi}(16(s+2n\pi))}$$
$$= \frac{1}{6\pi}(e^{-i(2/9)\pi} + e^{-i(8/9)\pi} + e^{-i(32/9)\pi}) = 0,$$

Similarly, when $m=9m_1+2$ (resp. $m=9m_1+4$) with some $m_1 \in \mathbb{Z}$, we see that $\Sigma_{\ell=0}^{\infty}\hat{\psi}(2^{\ell}s)\overline{\hat{\psi}(2^{\ell}(s+2n\pi))}$ is $(1/6\pi)(e^{-i(4/9)\pi}+e^{-i(16/9)\pi}+e^{-i(64/9)\pi})=0$ [resp. $(1/6\pi)\times(e^{-i(8/9)\pi}+e^{-i(32/9)\pi}+e^{-i(128/9)\pi})=0$]. Finally, when $m=9m_1-1$ (resp. $m=9m_1-2$, or $m=9m_1-4$) with some $m_1 \in \mathbb{Z}$, the left-hand side of Eq. (2.1) becomes the complex conjugate of what one gets when $m=9m_1+1$ (resp. $m=9m_1+2$, or $m=9m_1+4$). Thus we are done for $s \in C_1$, $k=n$.

The other five cases are treated similarly. Therefore $\hat{\psi}=e^{i(m/9n)s}|f(s)|$ defines a non-MSF wavelet ψ which admits the phase function $\alpha(s)=(m/9n)s$. □

We end this section with the following comments:

Proposition 2.1 is based on a simple fact that vectors with certain specific angles between them never add up to zero unless each vector is zero in the first place. We can generalize Proposition 2.1 to all applicable linear phase functions and get the following Proposition 2.3.

First, for any real number a, let us define $res(a)$ such that $a-res(a) \in \mathbb{Z}$ and $0 \leqslant res(a) < 1$.

Proposition 2.3: Let a be any real number. The phase function as is not attainable for any non-MSF wavelet, if for any $k \in 2\mathbb{Z}+1$, the difference between the supremum and infimum the set $\{res(2^j ka): j \in \mathbb{N}\cup\{0\}\}$ is less than $\frac{1}{2}$.

The proof of Proposition 2.3 is essentially the same as that of Proposition 2.1 and so we omit it. Theorem 1.2 suggests the following conjecture.

Conjecture 1: Let $a=p/qr$ be a rational number where $p, q \in \mathbb{Z}\setminus\{0\}$, $r \in 2\mathbb{Z}+1$ and p, q are relatively prime. If there is a non-MSF wavelet which admits phase function $(1/q)s$, then there is a (possibly different) non-MSF wavelet which admits phase function $\alpha(s)=as$.

III. WAVELETS WHICH ADMIT PHASE FUNCTION $\frac{1}{2}s$

In this section we study the class of wavelets which admit phase function $\frac{1}{2}s$. We know that all MRA wavelets admit phase function $\frac{1}{2}s$. In a sense, this class holds more attraction than other classes of wavelets. First of all, let us introduce some notation.

For any $a \in [0,1/2]$, we denote by $\mathcal{W}_a$ the set of all wavelets which admit phase function as. As pointed out earlier, such $\mathcal{W}_a$ is never empty since it contains the set of all MSF wavelets. Note that from the proof of Theorem 1.2 above, we see that $\mathcal{W}_a \cap \mathcal{W}_b$ contains also non-MSF wavelets for certain a, b. In fact, for fixed $n \in 2(\mathbb{N}\cup\{0\})+1$ and $j \in \mathbb{N}$, in the proof of Theorem 1.2 we constructed a wavelet which admits phase function $(m/2^j n)s$ for any $m \in 2\mathbb{Z}+1$. In general, the relationship between different $\mathcal{W}_a$ can be very complicated. Here we concentrate on $\mathcal{W}_{1/2}$, to explore its relationship with various $\mathcal{W}_a$. As a byproduct, we also obtain similar results concerning $\mathcal{W}_{1/4}$.

First we give a characterization of wavelets in $\mathcal{W}_{1/2}$.

Proposition 3.1: If $a=1/2$, then phase function $\alpha(s)=as$ is attainable for a wavelet ψ if and only if the wavelet ψ satisfies the condition that for almost all $s \in \mathbb{R}$ and each $k \in 2\mathbb{Z}+1$,

$$|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)| = \sum_{j=1}^{\infty} |\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))|. \tag{3.1}$$

Proof: Assume that ψ is a wavelet. Observe that $e^{i(1/2)s}|\hat{\psi}(s)|$ is a Fourier transform of a wavelet if and only if for almost all $s \in \mathbb{R}$ and for each $k \in 2\mathbb{Z}+1$,

$$\sum_{j=0}^{\infty} e^{i2^j k\pi}|\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))| = 0,$$

due to the fact that for each fixed $k \in 2\mathbb{Z}+1$, $e^{i2^j k\pi} = 1$ for any $j \in \mathbb{N}$ and $e^{i2^0 k\pi} = -1$. The condition above is equivalent to the condition that for almost all $s \in \mathbb{R}$ and each $k \in 2\mathbb{Z}+1$,

$$|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)| = \sum_{j=1}^{\infty} |\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))|.$$

□

Observe that with the same argument employed in the proof of Proposition 2.1, we see that if phase function $\frac{1}{2}s$ is attainable for a wavelet ψ, and if for almost all $s \in \mathbb{R}$ and each $k \in 2\mathbb{Z}+1$, $|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)| = 0$, then it follows that ψ is an MSF wavelet. So, in particular, Proposition 3.1 says that if a non-MSF wavelet ψ admits phase $\frac{1}{2}s$, then there exists a set A of positive measure and some $k \in 2\mathbb{Z}+1$ such that $|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)| \neq 0$ for all $s \in A$.

Proposition 3.2: Let a be any real number. If both phase functions $s/2$ and $\alpha(s) = as$ are attainable for a non-MSF wavelet ψ, then a must be of the form $m/2n$ for some m, $n \in 2\mathbb{Z}+1$.

Proof: Since ψ is a non-MSF wavelet and admits phase function $\frac{1}{2}s$, according to Proposition 3.1 and the comments after its proof, there exists a set A of positive measure and some $k \in 2\mathbb{Z}+1$ such that $|\hat{\psi}(s)||\hat{\psi}(s+2k\pi)| \neq 0$ for all $s \in A$ and

$$|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)| = \sum_{j=1}^{\infty} |\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))|$$

holds in particular for the same $k \in 2\mathbb{Z}+1$ and all $s \in A$.

Thus for each fixed $s \in A$, there must be at least one nonzero term to the right of the above equation. By passing to a subset of A, we can assume that the Jth term is nonzero for all $s \in A$ and some $J \in \mathbb{N}$. Since ψ also admits phase function $\alpha(s) = as$, Eq. (1.2) implies in particular that for that same $k \in 2\mathbb{Z}+1$ and all $s \in A$,

$$|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)| = (-1)\sum_{j=1}^{\infty} e^{i2k(1-2^j)a\pi}|\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))|.$$

This implies that $(-1)e^{i2k(1-2^J)a\pi} = 1$. Therefore, $2k(1-2^J)a\pi = (2\ell+1)\pi$ for some $\ell \in \mathbb{Z}$. Hence a must be of the form $m/2n$ for some m, $n \in 2\mathbb{Z}+1$. □

Proof of Theorem 1.3: One direction is precisely Proposition 3.2. For the other direction, note that we only need to consider the case when $n \in 2(\mathbb{N}\cup\{0\})+1$ and $m \in \mathbb{Z}+1$. Recall that in the proof of Theorem 1.2, for each fixed $n \in 2(\mathbb{N}\cup\{0\})+1$, we actually constructed a non-MSF wavelet which is contained in $\mathcal{W}_{m/2n}$ for any $m \in \mathbb{Z}+1$. In particular, this wavelet is in $\mathcal{W}_{1/2}$. Hence $\mathcal{W}_{1/2} \cap \mathcal{W}_{m/2n}$ contains a non-MSF wavelet for any $n \in 2(\mathbb{N}\cup\{0\})+1$ and $m \in \mathbb{Z}+1$. □

For the rest of this section, we consider possibly containment between $\mathcal{W}_{1/2}$ and various $\mathcal{W}_a$. The main result is the following Theorem, which shows the complexity of the situation.

Theorem 3.3:

(i) $\mathcal{W}_{1/2}$ *is not contained in any* $\mathcal{W}_a$ *with* $a \in [0,\frac{1}{2})$.
(ii) $\mathcal{W}_{1/6}$ *is contained in* $\mathcal{W}_{1/2}$.
(iii) $\mathcal{W}_{1/10}$ *is not contained in* $\mathcal{W}_{1/2}$.

Proof: (i) The Fourier transform of a wavelet which is in $\mathcal{W}_{1/2}$ but not in $\mathcal{W}_a$ for any $a \in [0,1/2)$ is found by letting $n=1$ and $j=1$ in the construction presented in the proof of Theorem 1.2. Indeed, for $n=j=1$, the wavelet ψ constructed in the proof of Theorem 1.2 is in $\mathcal{W}_{m/2}$ for any $m \in 2\mathbb{Z}+1$. According to Lemma 1.1, $\mathcal{W}_{m/2}=\mathcal{W}_{1/2}$ for each $m \in 2\mathbb{Z}+1$.

Now we prove that the above mentioned wavelet ψ is not in $\mathcal{W}_a$ for $a \in [0,1/2)$. In fact, assume that ψ admits $\alpha(s)=as$ as a phase function. Equation (1.2), when applied to the wavelet whose Fourier transform is $\epsilon^{i\alpha(s)}|\hat{\psi}|$, says that, in particular, for $s \in B_1$ and $k=1$, we have

$$\sum_{\ell \in \mathbb{Z}} \hat{\psi}(2^{\ell}s)\overline{\hat{\psi}(2^{\ell}(s+2k\pi))} = \frac{1}{2\pi}(e^{-i2a\pi}|\cos g(s)||\sin g(s)| + e^{-i4a\pi}|\cos g(s)||\sin g(s)|) = 0.$$

It follows that $2a$ must be $2\ell+1$ for some $\ell \in \mathbb{Z}$. Thus $a=(2l+1)/2$, which is impossible since a is assumed to be in $[0, 1/2)$. Hence $\psi \notin \mathcal{W}_a$ for $a \in [0,\frac{1}{2})$.

(ii) Let ψ be a wavelet admitting phase function $\frac{1}{6}s$. We need to show that $\hat{\psi}$ satisfies the condition (3.1) in Proposition 3.1. According to Eq. (1.2), for almost all $s \in \mathbb{R}$ and for each $k \in 2\mathbb{Z}+1$, we must have

$$\sum_{j=0}^{\infty} e^{i(2^j 2k\pi/6)}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))| = 0. \tag{3.2}$$

When $k \in 6\mathbb{Z}+3$, from (3.2) we have that for almost all $s \in \mathbb{R}$,

$$|\hat{\psi}(s)||\hat{\psi}(s+2k\pi)| = \sum_{j=1}^{\infty} |\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|.$$

When $k \in 6\mathbb{Z}+1$, from (3.2), we have that for almost all $s \in \mathbb{R}$,

$$e^{i(1/3)\pi}|\hat{\psi}(s)||\hat{\psi}(s+2k\pi)| + e^{i(2/3)\pi} \sum_{j \in 2(\mathbb{N}\cup\{0\})+1} |\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))|$$

$$+ e^{i(4/3)\pi} \sum_{j \in 2\mathbb{N}} |\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))| = 0.$$

It then follows that the second term to the left side of the above equality must be zero, i.e.,

$$\sum_{n \in 2(\mathbb{N}\cup\{0\})+1} |\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))| = 0.$$

Consequently, for almost all $s \in \mathbb{R}$,

$$e^{i(1/3)\pi}|\hat{\psi}(s)||\hat{\psi}(s+2k\pi)| + \sum_{j \in 2\mathbb{N}} e^{i(4/3)\pi}|\hat{\psi}(2^j s)||\hat{\psi}(2^j(s+2k\pi))| = 0.$$

Hence,

$$
\begin{aligned}
|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)| &= \sum_{j\in 2\mathbb{N}} |\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))| \\
&= \sum_{j\in 2\mathbb{N}} |\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))| + \sum_{j\in 2(\mathbb{N}\cup\{0\})+1} |\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))| \\
&= \sum_{j=1}^{\infty} |\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))|,
\end{aligned}
$$

i.e., (3.1) holds when $k\in 6\mathbb{Z}+1$.

Similar discussion yields that (3.1) holds when $k\in 6\mathbb{Z}+5$. Hence, by Proposition 3.1, $\psi \in \mathcal{W}_{1/2}$ as claimed.

(iii) We construct a non-MSF wavelet $\psi\in\mathcal{W}_{1/10}$ such that ψ does not admit phase $\frac{1}{2}s$.

We use similar sets as defined in the proof of Theorem 1.2 (*ii*). Let $A_1=[-\pi,-\pi/2)$, $A_2=8\pi+[-\pi/2,-\pi/4)$ and $A_3=4\pi+[-\pi/8,-\pi/16)$. Let us first show that $A=A_1\cup A_2\cup A_3$ is a subwavelet set. In fact, since $A_1+2\pi=[\pi,\frac{3}{2}\pi)$, $A_2-8\pi+2\pi=[2\pi-\pi/2,2\pi-\pi/4)$, and $A_3-4\pi+2\pi=[2\pi-\pi/8,2\pi-\pi/16)$, it follows that $\tilde{\tau}|_A$ is injective. Similarly, since $2A_1=[-2\pi,-\pi)$, $A_2=4[\frac{15}{8}\pi,\frac{31}{16}\pi)$, and $A_3=2[\frac{31}{16}\pi,\frac{63}{32}\pi)$, we have that $\tilde{d}|_A$ is injective. Therefore A is a subwavelet set.

Now to see that conditions in Lemma 2.2 are satisfied, we observe that the ϵ in the first condition can be taken as large as $\pi/16$ and that the interior of set S in the second condition contains the open interval $(\frac{63}{32}\pi,2\pi)$. According to Lemma 2.2, there is a wavelet set $W\supset A$.

Now let $B_1=[-\pi/2,-\pi/4)$, $B_2=2\pi+[-\pi/8,-\pi/16)$ and $B_3=32\pi+[-\pi,-\pi/2)$. Also let $C_1=[-\pi/8,-\pi/16)$, $C_2=16\pi+[-\pi,-\pi/2)$ and $C_3=16\pi+[-\pi/2,-\pi/4)$. Note that $A_1=2B_1=8C_1$, $C_2=2A_2=8B_2$, and $B_3=2C_3=8A_3$. Also $A_1=C_2-16\pi=B_3-32\pi$, $B_1=A_2-8\pi=C_3-16\pi$, and $C_1=B_2-2\pi=A_3-4\pi$. Thus $B=B_1\cup B_2\cup B_3$ and $C=C_1\cup C_2\cup C_3$ are also subwavelet sets. It can be checked that sets A_1, A_2, A_3, B_1, B_2, B_3 and C_1, C_2, C_3 are mutually disjoint from each other. Moreover, $W\backslash A$ is disjoint from B and C, and the union of sets $W\backslash A$ and B also forms a wavelet set. So does the union of $W\backslash A$ and C.

We define a function f in such a way that:

$$
|f(s)| = \begin{cases}
\dfrac{1}{\sqrt{2\pi}}, & s\in W\backslash A, \\
\dfrac{1}{\sqrt{2+2\cos(\pi/5)}\sqrt{2\pi}}, & s\in A_1\cup B_1\cup B_3\cup C_3, \\
\dfrac{\sqrt{2\cos(\pi/5)}}{\sqrt{2+2\cos(\pi/5)}\sqrt{2\pi}}, & s\in A_2\cup A_3\cup C_1\cup C_2, \\
\dfrac{1}{2\cos(\pi/5)\sqrt{2+2\cos(\pi/5)}\sqrt{2\pi}}, & s\in B_2, \\
0, \quad \text{otherwise.}
\end{cases}
$$

First we check that $\|f\|^2=1$. By definition of $|f|$ and relations between sets A_i, B_i, C_i for $i\in\{1,2,3\}$, through a change of variables in integration, we see that

$$
\int_{A_1}|f(s)|^2ds+\int_{C_2}|f(s)|^2ds+\int_{B_3}|f(s)|^2ds=\frac{1}{2\pi}\int_{A_1}\frac{1+2\cos(\pi/5)+1}{2+2\cos(\pi/5)}ds=\frac{1}{2\pi}\int_{A_1}ds.
$$

Likewise, we have

$$\int_{B_1}|f(s)|^2ds+\int_{A_2}|f(s)|^2ds+\int_{C_3}|f(s)|^2ds=\frac{1}{2\pi}\int_{A_2}\frac{1+2\cos(\pi/5)+1}{2+2\cos(\pi/5)}ds=\int_{A_2}ds$$

and

$$\int_{C_1}|f(s)|^2ds+\int_{B_2}|f(s)|^2ds+\int_{A_3}|f(s)|^2ds$$
$$=\frac{1}{2\pi}\int_{A_3}\frac{2\cos(\pi/5)+\{1/[4\cos^2(\pi/5)]\}+2\cos(\pi/5)}{2+2\cos(\pi/5)}ds=\int_{A_3}ds.$$

The last equality follows from the identity $8\cos^3(\pi/5)+1=8\cos^2\pi/5$.

Hence,

$$\|f\|^2=\int_{\mathbb{R}}|f(s)|^2ds=\frac{1}{2\pi}\left(\int_A|f(s)|^2ds+\int_B|f(s)|^2ds+\int_C|f(s)|^2ds+\mu(W\backslash A)\right)$$
$$=\frac{1}{2\pi}(\mu(A)+\mu(W\backslash A))=\frac{\mu(W)}{2\pi}=1.$$

Next we check that Eq. (1.1) holds by the function whose Fourier transform has modulus $|f|$. As we reasoned before, it suffices to check (1.1) for $s\in W$. If $s\in A_1$, then $2^{-1}s\in B_1$ and $2^{-3}s\in C_1$. For any $\ell\neq 0,-1,-3$, since $2^{\ell}s\in\mathbb{R}\backslash(W\cup B\cup C)$, we have $|f(2^{\ell}s)|=0$.

Thus

$$\sum_{\ell\in\mathbb{Z}}|f(2^{\ell}s)|^2=|f(s)|^2+|f(2^{-1}s)|^2+|f(2^{-3}s)|^2=\frac{1}{2\pi}\left(\frac{1+2\cos(\pi/5)+1}{2+2\cos(\pi/5)}\right)=\frac{1}{2\pi}.$$

Hence (1.1) holds when $s\in A_1$. Similarly, we can check that (1.1) holds when $s\in A_3$. We point out that to verify that (1.1) holds for $s\in A_2$, the identity $8\cos^3(\pi/5)+1=8\cos^2(\pi/5)$ may be useful.

Now let $\hat{\psi}(s)=e^{i(1/10)s}|f(s)|$. To prove that ψ is a wavelet, the only thing left is to check that Eq. (1.2) is satisfied by ψ. By definition of $|f|$ and relations between sets A_i, B_i, C_i for $i\in\{1,2,3\}$, every term to the left of Eq. (1.2) is 0 unless one of the following is true: (1) $s\in C_1$, $k=1$, (2) $s\in\frac{1}{2}C_1$, $k=1$, (3) $s\in B_2$, $k=1$, (4) $s\in B_2$, $k=-1$, (5) $s\in A_3$, $k=-1$, or (6) $s\in\frac{1}{2}A_3$, $k=-1$.

In case (1), when $s\in C_1$, we have that $4s\in B_1$ and $8s\in A_1$ and that $s+2\pi\in B_2$, $4(s+2\pi)\in A_2$, and $8(s+2\pi)\in C_2$. Thus we have

$$\sum_{\ell=0}^{\infty}\hat{\psi}(2^{\ell}s)\overline{\hat{\psi}(2^{\ell}(s+2\pi))}=\hat{\psi}(s)\overline{\hat{\psi}(s+2\pi)}+\hat{\psi}(4s)\overline{\hat{\psi}(4(s+2\pi))}+\hat{\psi}(8s)\overline{\hat{\psi}(8(s+2\pi))}$$
$$=\frac{1}{2\pi}\frac{1}{2+2\cos\pi/5}\left(e^{-i(2/10)\pi}\frac{1}{\sqrt{2\cos\pi/5}}+e^{-i(8/10)\pi}\sqrt{2\cos\frac{\pi}{5}}\right.$$
$$\left.+e^{-i(16/10)\pi}\sqrt{2\cos\frac{\pi}{5}}\right)=0.$$

The last equality can be verified in many different ways. (The quickest way probably is to view it as a representation of three vectors which sum to zero and use geometry.) We omit the details.

Thus we checked the first case. The cases (3)–(5) turn out to be similar. In cases (2) and (4), the final equality looks quite different. For instance, in case (2), we are required to verify the following equality:

$$\frac{1}{2\pi}\frac{1}{2+2\cos(\pi/5)}\left(e^{-i(4/10)\pi}2\cos\frac{\pi}{5}+e^{-i(16/10)\pi}+e^{-i(32/10)\pi}\right)=0.$$

We omit the calculation.

To show that $\psi\notin\mathcal{W}_{1/2}$, we use characterization of $\mathcal{W}_{1/2}$ in Proposition 3.1. Again, take $s\in C_1$ and $k=1$. Through similar computation we see that for the function whose Fourier transform is $e^{i(1/2)s}|f|$, satisfying Eq. (3.1) would imply $1=4\cos(\pi/5)$, which is untrue. (In fact, $1=4\cos(\pi/5)\cos(2\pi/5)$.) The proof is completed. □

As a byproduct of the proof of (*ii*), we obtain a characterization of $\mathcal{W}_{1/6}$.

Proposition 3.4: Wavelet ψ is in $\mathcal{W}_{1/6}$ if and only if for almost all $s\in\mathbb{R}$ and each $k\in 6\mathbb{Z}+3$,

$$|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)|=\sum_{j=1}^{\infty}|\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))|;$$

and for almost all $s\in\mathbb{R}$, each $k\in 6\mathbb{Z}+1$ or $k\in 6\mathbb{Z}+5$, each $j\in 2(\mathbb{N}\cup\{0\})+1$, $|\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))|=0$ and

$$|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)|=\sum_{j\in 2\mathbb{N}}|\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+2k\pi))|=0.$$

We point out that parallel investigation of $\mathcal{W}_{1/4}$ yields some results similar to that of $\mathcal{W}_{1/2}$. We only list results with a few comments. The proofs are omitted since technically they are quite the same as their counterpart.

Lemma 3.5: If $a=1/4$, then phase function $\alpha(s)=as$ is attainable for a wavelet ψ if and only if ψ satisfies the condition that for almost all $s\in\mathbb{R}$ and for each $k\in 2\mathbb{Z}+1$, $|\hat{\psi}(s)\|\hat{\psi}(s+2k\pi)|=0$ and

$$|\hat{\psi}(s)\|\hat{\psi}(s+4k\pi)|=\sum_{j=1}^{\infty}|\hat{\psi}(2^j s)\|\hat{\psi}(2^j(s+4k\pi))|.$$

The only thing new in the proof of Lemma 3.5 is the observation that for real numbers $\{a_k\}$ with $k\in N$ such that $a_1 e^{i(1/2)\pi}+\Sigma_{k=2}^{\infty}a_k=0$, a_1 must be 0.

We point out some consequences of Lemma 3.5. First, we note that by the same argument employed in the proof of Proposition 2.3, it follows from Lemma 3.5 that if phase function $\frac{1}{4}s$ is attainable for a wavelet ψ, and if for almost all $s\in\mathbb{R}$ and each $k\in 2\mathbb{Z}+1$, $|\hat{\psi}(s)\|\hat{\psi}(s+4k\pi)|=0$, then ψ is a MSF wavelet. In other words, if a non-MSF wavelet ψ admits phase $\frac{1}{4}s$, then there exists a set A of positive measure and some $k\in 2\mathbb{Z}+1$ such that $|\hat{\psi}(s)\|\hat{\psi}(s+4k\pi)|\neq 0$ for all $s\in A$.

Second, by using Eq. (1.2), it follows from Lemma 3.5 that for any wavelet ψ admitting phase $(\frac{1}{4})s$, for almost every $s\in\mathbb{R}$ and each $k\in 2\mathbb{Z}+1$, we have

$$\sum_{\ell=0}^{\infty}\hat{\psi}(2^{\ell}s)\overline{\hat{\psi}(2^{\ell}(s+4k\pi))}=0.$$

Using these consequences of Lemma 3.5, we obtain a proof of Proposition 3.6 similar to the proof of Proposition 3.2. Now a proof of Theorem 3.7 is not much different from that of Theorem 1.3.

Proposition 3.6: Let a be any real number. If both phase functions $s/4$ and $\alpha(s)=as$ are attainable for a non-MSF wavelet ψ, then a must be of the form $m/4n$ for some m, $n\in 2\mathbb{Z}+1$.

Theorem 3.7: *Let a be a real number. Then there exists a non-MSF wavelet admitting both phases as and $\frac{1}{4}s$ if and only if $a=m/4n$ for some m, $n\in 2\mathbb{Z}+1$. In particular, $\mathcal{W}_{1/4}\cap\mathcal{W}_a$ does not contain any non-MSF wavelets if a is irrational.*

Fourier transform of a wavelet in $\mathcal{W}_{1/4}$ is found by letting $n=1$ and $j=2$ in the construction presented in the proof of Theorem 1.2 (*i*). The assumption that such a wavelet admits also $\alpha(s)=as$ as a phase function leads to the conclusion that $4a$ must be $2\ell+1$ for some $\ell\in\mathbb{Z}$. Thus the wavelet is only in $\mathcal{W}_{(2\ell+1)/4}$ which, according to Lemma 1.1, is exactly the same as $\mathcal{W}_{1/4}$. Therefore we have the following.

Proposition 3.8: $\mathcal{W}_{1/4}$ is not contained in $\mathcal{W}_a$ for any $a\in[0,1/2]\backslash\{\frac{1}{4}\}$.

To finish this section, we point out that a similar method does not produce a characterization of wavelets in $\mathcal{W}_{m/8}$ for $m\in\{1,3\}$, nor some counterpart to (*ii*) and (*iii*) in Theorem 3.3. Things apparently get harder as one progresses from $\mathcal{W}_{1/2}$ to other $\mathcal{W}_a$'s.

IV. TWO EXAMPLES

In this section we provide the two important examples mentioned in the Introduction. The first one shows that $\mathcal{W}_{1/2}$ is larger (modulo the MSF wavelets) than the set of all MRA wavelets. We refer to standard books (cf. Refs. 1, 6, and 7) for the definition of multiresolution (MRA) wavelets. We will use the fact (cf. Ref. 1) that a wavelet ψ is an MRA wavelet if and only if its *dimension function* $D_\psi(s)=(2\pi)\Sigma_{n=1}^{\infty}\Sigma_{k\in\mathbb{Z}}|\hat{\psi}(2^n(s+2k\pi))|^2=1$, a.e. $s\in\mathbb{R}$.

The second example shows that there exists a non-MSF wavelet which does not even admit any piece-wise linear phase function. A function $\alpha(s)$ on $(-\infty,\infty)$ is called *set-wise linear* if $(-\infty,\infty)$ can be decomposed into countable disjoint (modulo null sets) union of measurable subsets such that $\alpha(s)$ is linear on each subset.

Example 4.1: There exists a non-MSF wavelet ψ such that ψ is not an MRA wavelet and ψ admits phase $\frac{1}{2}s$.

Proof: Let $A_1=[-\frac{8}{15}\pi,-\frac{2}{5}\pi)$ and $A_2=[\frac{176}{15}\pi,\frac{64}{5}\pi)$. Then $A_1\cup A_2$ is a subwavelet set contained in wavelet set $A_1\cup A_2\cup C$ where $C=[-\frac{2}{5}\pi,-\frac{4}{15}\pi)\cup[\frac{4}{5}\pi,\frac{22}{15}\pi)$. Also define $B_1=[\frac{22}{15}\pi,\frac{8}{5}\pi)=A_1+2\pi=1/8A_2$ and $B_2=[-\frac{64}{15}\pi,-\frac{16}{5}\pi)=A_2-16\pi=8A_1$.

Let us define function f to be such that

$$|f(s)|=\begin{cases}\dfrac{1}{\sqrt{2\pi}}, & s\in C,\\[2ex] \dfrac{1}{2\sqrt{\pi}}, & s\in A_1\cup A_1\cup B_1\cup B_2,\\[2ex] 0, & \text{otherwise.}\end{cases}$$

Then $\|f\|^2=(1/2\pi)\mu(C)+(1/4\pi)\mu(A_1\cup A_1\cup B_1\cup B_2)=\frac{6}{15}+\frac{9}{15}=1$. To check that Eq. (1.1) is satisfied by any function whose Fourier transform has modulus $|f|$, we note that it suffices to check (1.1) for s in the wavelet set $A_1\cup A_2\cup C$. When $s\in C$, $|f(s)|$ is the only nonzero term to the left of Eq. (1.1). So $\Sigma_{\ell\in\mathbb{Z}}|f(2^\ell s)|^2=|f(s)|^2=1/2\pi$. If $s\in A_1$, then $\Sigma_{\ell\in\mathbb{Z}}|f(2^\ell s)|^2=|f(s)|^2+|f(2^3s)|^2=1/2\pi$. Similarly, when $s\in A_2$, we have $\Sigma_{\ell\in\mathbb{Z}}|f(2^\ell s)|^2=|f(s)|^2+|f(2^{-3}s)|^2=1/2\pi$.

To prove that $\hat{\psi}(s)=e^{i(1/2)s}|f(s)|$ is Fourier transform of a wavelet, it is left to check that Eq. (1.2) is satisfied by ψ. We see that each term to the left of Eq. (1.2) is 0 unless when $s\in A_1$, $k=1$, or when $s\in B_1$, $k=-1$. In the first case, the only nonzero terms in (1.2) involve $s\in A_1$, $s+2\pi\in B_1$, $2^3s\in A_2$ and $2^3(s+2\pi)\in B_2$. Hence

$$\sum_{\ell=0}^{\infty} \overline{\hat{\psi}}(2^{\ell}s)\overline{\hat{\psi}(2^{\ell}(s+2\pi))} = \hat{\psi}(s)\overline{\hat{\psi}((s+2\pi))} + \hat{\psi}(2^3 s)\overline{\hat{\psi}(2^3(s+2\pi))} = \frac{1}{4\pi}(e^{-\pi i}+e^{-8\pi i}) = 0.$$

The second case is similar.

Finally we show that ψ is not an MRA wavelet. For this, we need to note that $\frac{1}{4}A_1+6\pi = [-\frac{2}{15}\pi,-\frac{1}{10}\pi)+6\pi = [\frac{88}{15}\pi,\frac{59}{10}\pi)\subset[\frac{88}{15}\pi,\frac{32}{5}\pi) = \frac{1}{2}A_2$, and $\frac{1}{4}A_1-2\pi\subset\frac{1}{2}B_2$. Let $s\in\frac{1}{4}A_1 = [-\frac{2}{15}\pi,-\frac{1}{10}\pi)$. Direct calculation shows then that $2^2 s\in A_1$, $2^5 s\in B_2$, $2(s+6\pi)\in A_2$ and $2(s-2\pi)\in B_2$. Thus

$$D_{\psi}(s)\geqslant(2\pi)(|\hat{\psi}(2^2 s)|^2+|\hat{\psi}(2^5 s)|^2+|\hat{\psi}(2(s+6\pi))|^2+|\hat{\psi}(2(s-2\pi))|^2) = 2.$$

Therefore ψ is not an MRA wavelet. □

Example 4.2: There exists a non-MSF wavelet ψ such that ψ does not admit any set-wise linear phase $\alpha(s)=as$.

Proof: Let A_1, A_2, A_3, B_1, B_2, B_3, C_1, C_2, C_3 and A, B, C be defined as in the proof of Theorem 3.3 (*iii*), and W be the wavelet set containing A. Also recall that $A_1=[-\pi,-\pi/2)$ and all these subsets satisfy the following conditions: $A_1=2B_1=8C_1$, $C_2=2A_2=8B_2$, $B_3=2C_3=8A_3$, $A_1=C_2-16\pi=B_3-32\pi$, $B_1=A_2-8\pi=C_3-16\pi$ and $C_2=B_2-2\pi=A_3-4\pi$.

Let $g(x)$ be defined on $C_1=[-\pi/8,-\pi/16)$ such that $g(-\pi/8)=0$, $g(-\pi/16)=1/\sqrt{3}$ and that $g(x)$ is linear. Then we extend the definition of $g(x)$ to the union of $A\cup B\cup C$ in such a way that $g(s)=g(s+2\pi)$ and $g(s)=g(2s)$ holds whenever s, $s+2\pi$ or s, $2s$ are in the union of $A\cup B\cup C$. Using the relations among sets A_i, B_i, C_i with $i\in\{1,2,3\}$, we can verify that g is well defined.

Now we define function f as follows:

$$f(s)=\begin{cases} \dfrac{1}{\sqrt{2\pi}}, & s\in W\backslash A,\\[2ex] \dfrac{1}{\sqrt{2\pi}}g(s), & s\in B\cup C,\\[2ex] \dfrac{1}{\sqrt{2\pi}}\sqrt{1-2g^2(s)}, & s\in A,\\[2ex] 0, & \text{otherwise.}\end{cases}$$

Note that f is well defined and $f\geqslant 0$ since $g^2(s)\leqslant\frac{1}{3}$. Similar to all the other examples, it can be checked that $\|f\|^2=1$ and $\Sigma_{\ell\in\mathbb{Z}}|f(2^{\ell}s)|^2=1/2\pi$, a. e. $s\in\mathbb{R}$.

Let $\alpha(s)$ be zero on $B\cup C$ and $\frac{1}{2}\pi+\arcsin g(s)/2\sqrt{1-2g^2(s)}$ on A and 0 everywhere else. We claim that $\hat{\psi}(s)=e^{i\alpha(s)}f(s)$ is the Fourier transform of a wavelet. By the above paragraph we only need to check Eq. (1.2). Similarly, we only need to check the following six cases: (1) $s\in C_1$, $k=1$; (2) $s\in\frac{1}{2}C_1$, $k=1$; (3) $s\in B_2$, $k=1$; (4) $s\in B_2$, $k=-1$; (5) $s\in A_3$, $k=-1$; and (6) $s\in\frac{1}{2}A_3$, $k=-1$. We treat only the first case, and the other five cases can be dealt similarly. In case (1), we have $s\in C_1$, $2^2 s\in B_1$, $2^3 s\in A_1$, $s+2\pi\in B_2$, $2^2(s+2\pi)\in A_2$, and $2^3(s+2\pi)\in C_2$. Thus

$$\sum_{j=0}^{\infty} |\hat{\psi}(2^j s)\overline{\hat{\psi}(2^j(s+2\pi))} = \hat{\psi}(s)\overline{\hat{\psi}(s+2\pi)} + \hat{\psi}(2^2 s)\overline{\hat{\psi}(2^2(s+2\pi))} + \hat{\psi}(2^3 s)\overline{\hat{\psi}(2^3(s+2\pi))}$$

$$= \frac{1}{2\pi} g^2(s) + \frac{1}{2\pi} g(s)\sqrt{1-2g^2(s)}\left[\exp\left(-\frac{\pi}{2} - \arcsin\frac{g(s)}{2\sqrt{1-2g^2(s)}}\right)\right.$$

$$\left. + \exp\left(\frac{\pi}{2} + \arcsin\frac{g(s)}{2\sqrt{1-2g^2(s)}}\right)\right]$$

$$= \frac{1}{2\pi} g^2(s) - \frac{1}{2\pi} g(s)\sqrt{1-2g^2(s)}\frac{g(s)}{\sqrt{1-2g^2(s)}} = 0.$$

Now, suppose that the wavelet also admits set-wise linear phase $\beta(s)$. It follows that there exists subset E of C_1 such that E has positive measure and $\beta(s)$ is linear on E. By passing to a subset of E, we can also assume that $\beta(s)$ is linear on each set 2^2E, 2^3E, $E+2\pi$, $2^2(E+2\pi)$, $2^3(E+2\pi)$. Considering (1.2), we see that when $s \in E$ there are only three nonzero terms which involve the above six sets. Hence, by the definition of f, it follows from Eq. (1.2) that

$$e^{i(a_1 s+b_1)} g(s) + (e^{i(a_2 s+b_2)} + e^{i(a_3 s+b_3)})\sqrt{1-2g^2(s)} = 0$$

holds for all $s \in E$, where a_1, a_2, a_3, b_1, b_2, b_3 are real constants. After multiplying $e^{-i(a_1 s+b_1)}$ on both sides, we see that

$$g(s) + (e^{i(as+b)} + e^{i(cs+d)})\sqrt{1-2g^2(s)} = 0$$

holds for all $s \in E$, where a, b, c, d are real constants. By considering the real and imaginary parts, we obtain

$$(\sin(as+b) + \sin(cs+d))\sqrt{1-2g^2(s)} = 0 \tag{4.1}$$

and

$$g(s) + (\cos(as+b) + \cos(cs+d))\sqrt{1-2g^2(s)} = 0 \tag{4.2}$$

for $s \in E$. Since $0 < g(s) < 1\sqrt{3}$ on E, it follows from (4.1) and (4.2) that $\sin(as+b)+\sin(cs+d) = 0$ and $\cos(as+b)+\cos(cs+d) \neq 0$ for $s \in E$, which implies from (4.2) that

$$\cos(as+b) = -\frac{g(s)}{2\sqrt{1-2g^2(s)}}$$

and hence

$$\cos^2(as+b) = \frac{g^2(s)}{4(1-2g^2(s))} \tag{4.3}$$

holds for $s \in E$.

Note that $g(s) = (16/\pi\sqrt{3})s + (2/\sqrt{3})$ on E and hence

$$h(z) := \frac{((16/\pi\sqrt{3})z + 2/\sqrt{3})^2}{4(1-2((16/\pi\sqrt{3})z + 2/\sqrt{3})^2)}$$

is a nonconstant rational function. By (4.3) and a standard complex analysis argument we will have $\cos(az+b)=h(z)$ for all $z\in\mathbb{C}$ such that $1-2((16/\pi\sqrt{3})z+2/\sqrt{3})^2\neq 0$, which is obviously impossible. Therefore ψ does not admit any set-wise linear phase. □

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Recursive construction for a class of radial functions. I. Ordinary space

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A class of spherical functions is studied which can be viewed as the matrix generalization of Bessel functions. We derive a recursive structure for these functions. We show that they are only special cases of more general radial functions which also have a properly generalized, recursive structure. Some explicit results are worked out. For the first time, we identify a subclass of such radial functions which consist of a finite number of terms only. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1463709]

I. INTRODUCTION

In 1957, Harish-Chandra[1] derived a famous formula for a certain class of group integrals. Let $\mathcal{G}$ be a compact semisimple Lie group and let a and b be elements of its Cartan subalgebra $\mathcal{H}$, then

$$\int_{U\in\mathcal{G}} \mathrm{d}\mu(U)\exp(\mathrm{tr}\,U^{-1}aUb)=\frac{1}{|\mathcal{W}|}\sum_{w\in\mathcal{W}}\frac{\exp(\mathrm{tr}\,w(a)b)}{\Pi(a)\Pi(w(b))}. \tag{1.1}$$

Here, $\mathrm{d}\mu(U)$ is the invariant measure, $\Pi(a)$ is the product of all positive roots of $\mathcal{H}$, and $\mathcal{W}$ is the Weyl reflection group of $\mathcal{G}$ with $|\mathcal{W}|$ elements w.

This result depends crucially on the condition that a and b are in the Cartan subalgebra $\mathcal{H}$. In other words, $U^{-1}aUb$ has to be in the algebra of the group. If one replaces a and b in the integral on the left-hand side with more general matrices x and k which are not in $\mathcal{H}$, formula (1.1) is *not valid anymore*. The *spherical functions* introduced by Gelfand[2,3] form an important class of such integrals which are, in general, not covered by Harish-Chandra's result (1.1). In another work, Harish-Chandra[4] studies in great detail the harmonic analysis involving these spherical functions. In a more physics oriented contribution, Olshanetsky and Perelomov[5] discussed them in the framework of quantum integrable systems.

Here, we wish to address spherical functions of the following kind: we take x and k as diagonal matrices containing the eigenvalues of a Hamiltonian in a matrix representation. The Hamiltonian is diagonalized by the integration matrix U. In particular, we assume that the Hamiltonian $U^{-1}xU$ or, equivalently, UkU^{-1} is real-symmetric, Hermitian, or Hermitian self-dual. Thus, $\mathcal{G}$ is the orthogonal, the unitary or the unitary-symplectic group. We will refer to these spherical functions as *matrix Bessel functions*. We notice that the unitary case is special: since it so happens that the eigenvalues x and k do lie in the Cartan subalgebra $\mathcal{H}$, the result (1.1) applies and coincides with the Itzykson–Zuber formula.[6] In the orthogonal and the unitary-symplectic cases, however, formula (1.1) is not valid.

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We choose the term matrix Bessel function for the spherical functions to be discussed here, because they can be viewed as a natural extension of the ordinary vector Bessel functions. However, due to the rich features of the spherical functions, other extensions relating to ordinary Bessel functions are equally natural. Related functions have been discussed and terms similar to matrix Bessel functions have already been used by Hertz,[7] by Gross and Kunze,[8,9] by Holman,[10] and by Okounkov and Olshanski.[11] Kontsevich[12] introduced the matrix Airy functions.

Duistermaat and Heckman[13] developed a stationary phase approach involving localization for a class of spherical functions, see also the treatise by Szabo.[14]

Remarkably, our matrix Bessel functions are only special cases of more general objects which we call *radial functions*. Moreover, there is an important connection to the Calogero–Sutherland models which we will discuss separately, see the following.

The matrix Bessel functions are of considerable interest for applications in physics. They appear in random matrix theory,[15–17] which models spectral fluctuations of complex systems, such as quantum chaotic ones. In particular, they are the kernels of Dyson's Brownian motion[18,19] describing crossover transitions between different symmetry or invariance classes. Unfortunately, only the case of broken time-reversal invariance can be treated explicitly with the help of the Itzykson–Zuber formula. In the physically important cases of conserved time-reversal invariance, the kernels are not known analytically, as argued previously. Muirhead[20] discusses spherical functions in the framework of multivariate statistical theory. In his book, an expansion in terms of Jack polynomials for the orthogonal case can be found. Such an expansion for arbitrary Dyson index was recently worked out by Okounkov and Olshanski.[11]

The goal of the present paper is to explore the structure of the radial functions which contain the matrix Bessel functions as special cases. In particular, we show how explicit results can be obtained. The paper is organized as follows. In Sec. II, we briefly review some properties of the vector Bessel functions. In doing so we wish to help the reader in developing an intuition for the matrix Bessel functions which we introduce in Sec. III. In Sec. IV, we state and derive a fundamental recursive structure for matrix Bessel functions. We show in Sec. V that this recursion is an iterative solution of general radial functions which contain group integrals defining the matrix Bessel functions as special case. Sections IV and V are our main results. In Sec. VI we illustrate how the recursion can lead to closed and explicit formulas. Because of its special importance, we discuss the connection to Calogero–Sutherland models separately in Sec. VII. In Sec. VIII, we summarize and conclude. Various aspects and calculations are collected in the appendices.

II. VECTOR BESSEL FUNCTIONS REVISITED

Before turning to the matrix case, we compile, for the convenience of the reader, some well-known results for the vector case.

In a real, d dimensional space with $d=2,3,4,\ldots$, we consider a position vector $\vec{r}=(x_1,\ldots,x_d)$ and a wave vector $\vec{k}=(k_1,\ldots,k_d)$. The plane wave $\exp(i\vec{k}\cdot\vec{r})$ satisfies the wave equation

$$\Delta \exp(i\vec{k}\cdot\vec{r}) = -\vec{k}^2 \exp(i\vec{k}\cdot\vec{r}), \tag{2.1}$$

where we define the Laplacian as in the physics literature,

$$\Delta = \frac{\partial^2}{\partial \vec{r}^2} = \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}. \tag{2.2}$$

The zeroth-order Bessel function in this space is the angular average of the plane wave,

$$\chi^{(d)}(kr) = \int \mathrm{d}\Omega \exp(i\vec{k}\cdot\vec{r}), \tag{2.3}$$

over the solid angle Ω, defining the orientation of either $\vec{r}$ or $\vec{k}$. In our context, it is advantageous to take Ω as the solid angle of $\vec{k}$. Obviously, only the relative angle between $\vec{r}$ and $\vec{k}$ matters and $\chi^{(d)}(kr)$ can only depend on the product of the lengths $r=|\vec{r}|$ and $k=|\vec{k}|$ of the two vectors. We normalize the measure $d\Omega$ with the volume $2\pi^{d/2}/\Gamma(d/2)$ of the unit sphere, i.e., we have

$$\int d\Omega = 1. \tag{2.4}$$

Thus, by construction, we also have

$$\chi^{(d)}(0) = 1. \tag{2.5}$$

It is convenient to view $\vec{r}$ as the azimuthal direction of the coordinate system in which we measure Ω. Thus, in these spherical coordinates, one finds $\vec{k}\cdot\vec{r} = kr\cos\vartheta$ where ϑ is the azimuthal angle. The measure $d\Omega$ contains $\sin^{d-2}\vartheta$ and one has

$$\chi^{(d)}(kr) = \frac{\Gamma(d/2)}{\sqrt{\pi}\Gamma((d-1)/2)} \int_0^\pi \exp(ikr\cos\vartheta)\sin^{d-2}\vartheta\, d\vartheta = 2^{(d-2)/2}\Gamma(d/2)\,\frac{J_{(d-2)/2}(kr)}{(kr)^{(d-2)/2}}, \tag{2.6}$$

where $J_\nu(z)$ is the standard Bessel function[21] of order ν. The functions (2.6) are often referred to as zonal functions.

There is a remarkable difference for the functions $\chi^{(d)}(kr)$ if one compares even and odd dimensions. For example, one has in $d=2$ dimensions $\chi^{(2)}(kr) = J_0(kr)$ and in $d=3$ dimensions $\chi^{(3)}(kr) = (\pi/2)^{1/2}J_{1/2}(kr)/(kr)^{1/2} = j_0(kr)$ with the spherical Bessel function $j_0(z)$ of zeroth order.[21] In $d=2$ dimensions, $J_0(z)$ is a complicated infinite series in the argument z, in $d=3$ dimensions, however, $j_0(z)$ is the simple ratio $j_0(z) = \sin z/z$. One easily sees how this generalizes. Upon introducing $\xi = \cos\vartheta$ as integration variable in Eq. (2.6), one finds the representation

$$\chi^{(d)}(kr) = \frac{\Gamma(d/2)}{\sqrt{\pi}\Gamma((d-1)/2)} \int_{-1}^{+1} \exp(ikr\xi)(1-\xi^2)^{(d-3)/2}\, d\xi. \tag{2.7}$$

In dimensions $d \geqslant 3$, this can be cast into the form

$$\chi^{(d)}(kr) = \frac{2\Gamma(d/2)}{\sqrt{\pi}\Gamma((d-1)/2)} \sum_{\mu=0}^{\infty} \binom{(d-3)/2}{\mu} \frac{\partial^{2\mu}}{\partial(kr)^{2\mu}} \frac{\sin kr}{kr}. \tag{2.8}$$

For even d, the exponent $(d-3)/2$ is a fraction $-1/2, +1/2, +3/2, \ldots$, and the function $(1-\xi^2)^{(d-3)/2}$ in the integrand in Eq. (2.7) is an *infinite* power series. This yields, for $d=4,6,8,\ldots$, the complicated power series (2.8) involving an infinite number of inverse powers of kr. However, if d is odd, the exponent $(d-3)/2$ is an integer $0,1,2,\ldots$, and the function $(1-\xi^2)^{(d-3)/2}$ is a *finite* polynomial of order $(d-3)/2$ in ξ^2. Thus, $\chi^{(d)}(kr)$ acquires a comparatively simple structure, because it only contains a finite number of inverse powers of kr. Formally, this means that for odd d all binomial coefficients for $\mu > (d-3)/2$ are zero.

The differential equation for the functions $\chi^{(d)}(kr)$ is easily obtained by averaging Eq. (2.1) over the solid angle Ω of $\vec{k}$, i.e., by integrating both sides,

$$\Delta \int d\Omega \exp(i\vec{k}\cdot\vec{r}) = -\vec{k}^2 \int d\Omega \exp(i\vec{k}\cdot\vec{r}). \tag{2.9}$$

We notice that the Laplacian Δ commutes with the integral, because the former is in the space of the position vector, the latter in the space of the wave vector. Moreover, the integral trivially commutes with $\vec{k}^2 = k^2$. Hence, one arrives at

$$\Delta_r \chi^{(d)}(kr) = -k^2 \chi^{(d)}(kr). \tag{2.10}$$

Since $\chi^{(d)}(kr)$ depends exclusively on radial variables, we replaced the full Laplacian Δ with its radial part

$$\Delta_r = \frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} = \frac{\partial^2}{\partial r^2} + \frac{d-1}{r} \frac{\partial}{\partial r}. \tag{2.11}$$

In general, there are two fundamental solutions $\chi_+^{(d)}(kr)$ and $\chi_-^{(d)}(kr)$ of the differential equation (2.10) which behave as $\exp(\pm ikr)/(kr)^{(d-1)/2}$ for large arguments kr. Thus, to obtain the full solutions, one can make the Hankel ansatz

$$\chi_\pm^{(d)}(kr) = \frac{\exp(\pm ikr)}{(kr)^{(d-1)/2}} w_\pm^{(d)}(kr). \tag{2.12}$$

Here, $w_\pm^{(d)}(kr)$ is a function with the property $w_\pm^{(d)}(kr) \to 1$ for $kr \to \infty$. The differential equation follows easily from Eq. (2.11) and is given by

$$\left(\frac{\partial^2}{\partial r^2} \pm i2k \frac{\partial}{\partial r} - \frac{d-1}{2} \left(\frac{d-1}{2} - 1 \right) \frac{1}{r^2} \right) w_\pm^{(d)}(kr) = 0. \tag{2.13}$$

For $d \geqslant 3$, one uses the ansatz as an asymptotic power series

$$w_\pm^{(d)}(kr) = \sum_{\mu=0}^{\infty} \frac{a_\mu}{(\pm kr)^\mu}, \tag{2.14}$$

which yields a recursion for the coefficients

$$a_{\mu+1} = \frac{1}{i2(\mu+1)} \left(\mu(\mu+1) - \frac{d-1}{2} \left(\frac{d-1}{2} - 1 \right) \right) a_\mu, \tag{2.15}$$

with the starting value $a_0 = 1$. A special situation occurs when the integer running index μ reaches the critical value $\mu_c = (d-3)/2$. If d is odd, μ_c is integer and the recursion terminates at $\mu = \mu_c$, i.e., one has $a_\mu = 0$, $\mu > \mu_c$. Thus, the asymptotic series becomes a *finite* polynomial in inverse powers of kr. However, if d is even, μ_c is half-odd integer and the series cannot terminate, it is always *infinite*. This explains the different structure of the Bessel functions in even and odd dimensional spaces from the viewpoint of the differential equation.

In Appendix A we discuss an alternative integral representation which has an interesting analog in the matrix space.

III. MATRIX BESSEL FUNCTIONS

We compile the basics features of the matrix spaces we want to work with in Sec. III A before we define the matrix Bessel functions as group integrals in Sec. III B.

Two general aspects are shifted into the appendices. First, we present an interesting alternative integral representation in Appendix B. Second, the matrix Bessel functions play a crucial role in harmonic analysis or, equivalently, in Fourier–Bessel analysis in matrix spaces. For the general theory, we refer the reader to Harish-Chandra's treatise in Ref. 4 and to Helgason's book.[3] However, to achieve our goal of being explicit, we collect, for the convenience of the reader, some results for the Fourier–Bessel analysis of invariant functions in matrix spaces in Appendix C.

A. Basics and notation

We introduce $N \times N$ matrices H whose elements H_{nm}, $n,m = 1,\ldots,N$ are real, complex, or quaternion variables. In other words, each element H_{nm} has β real components $H_{nm}^{(\alpha)}$, $\alpha = 0,\ldots,(\beta-1)$ with $\beta = 1,2,4$, respectively,

$$H_{nm}=\sum_{\alpha=0}^{\beta-1} H_{nm}^{(\alpha)}\tau^{(\alpha)}. \tag{3.1}$$

Here, we use the basis $\tau^{(\alpha)}$, $\alpha=0,\ldots,(\beta-1)$. We have $\tau^{(0)}=1$ for the real case with $\beta=1$. For the complex case with $\beta=2$, we have $\tau^{(0)}=1$ and $\tau^{(1)}=i$. Finally, we have

$$\tau^{(0)}=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},\quad \tau^{(1)}=\begin{bmatrix}0 & +1\\ -1 & 0\end{bmatrix},$$
$$\tau^{(2)}=\begin{bmatrix}0 & -i\\ -i & 0\end{bmatrix},\quad \tau^{(3)}=\begin{bmatrix}+i & 0\\ 0 & -i\end{bmatrix} \tag{3.2}$$

in the quaternion case for $\beta=4$ where the $\tau^{(\alpha)}$, $\alpha=1,2,3$ are the Pauli matrices. We notice that the total H is a $2N\times 2N$ matrix for $\beta=4$. However, here and in the following, the dimensions that we use always refer to the number of matrix elements such as H_{nm}. These are scalar for $\beta=1,2$ and quaternion for $\beta=4$. The label β is often referred to as Dyson index.

We assume that the matrix H is real symmetric, Hermitian, or Hermitian self-dual in the three cases $\beta=1,2,4$. We always write $H^{\dagger}=H$ to indicate this symmetry. There are N independent real variables $H_{nn}=H_{nn}^{(0)}$, $n=1,\ldots,N$ on the diagonal and $\beta N(N-1)/2$ independent real variables $H_{nm}^{(\alpha)}$, $\alpha=0,\ldots,(\beta-1),1\leqslant n<m\leqslant N$ outside the diagonal. We write the volume element of H in the form

$$\mathrm{d}[H]=\prod_{n=1}^{N}\mathrm{d}H_{nn}^{(0)}\prod_{n<m}\prod_{\alpha=0}^{\beta-1}\mathrm{d}H_{nm}^{(\alpha)}. \tag{3.3}$$

The matrix H is diagonalized by the matrix U, with columns U_n, $n=1,\ldots,N$. Depending on the value of β, the matrix U is either orthogonal, unitary, or unitary-symplectic. Following Gilmore's notation,[22] we write $U\in \mathrm{U}(N;\beta)$ with $\mathrm{U}(N;1)=\mathrm{SO}(N)$, $\mathrm{U}(N;2)=\mathrm{U}(N)$ and $\mathrm{U}(N;4)=\mathrm{USp}(2N)$. The volume of these groups is given by

$$\mathrm{vol}\,\mathrm{U}(N;\beta)=\prod_{n=1}^{N}\frac{2\pi^{\beta n/2}}{\Gamma(\beta n/2)}=\frac{2^N\pi^{\beta N(N+1)/4}}{\Pi_{n=1}^{N}\Gamma(\beta n/2)}. \tag{3.4}$$

We use it to normalize the invariant measure $\mathrm{d}\mu(U)$ of $U\in\mathrm{U}(N;\beta)$ to unity,

$$\int \mathrm{d}\mu(U)=1. \tag{3.5}$$

The N real eigenvalues x_n, $n=1,\ldots,N$ of H are ordered in the diagonal matrix x. We have $x=\mathrm{diag}(x_1,\ldots,x_N)$ for $\beta=1$ and $\beta=2$. For $\beta=4$, the eigenvalues are doubly degenerate and we have $x=\mathrm{diag}(x_1,x_1,\ldots,x_N,x_N)$. Physically, this doubling of the eigenvalues is due to Kramer's degeneracies. Thus, the diagonalization reads

$$H=U^{\dagger}xU,\quad \text{with}\quad H_{nm}=U_n^{\dagger}xU_m. \tag{3.6}$$

The diagonalizing matrix U has the property $U^{-1}=U^{\dagger}$. The volume element in eigenvalue–angle coordinates is given by[15,23]

$$\mathrm{d}[H]=C_N^{(\beta)}|\Delta_N(x)|^{\beta}\mathrm{d}[x]\mathrm{d}\mu(U) \tag{3.7}$$

where $\mathrm{d}[x]$ denotes the product of all differentials dx_n. We have introduced the Vandermonde determinant

$$\Delta_N(x) = \prod_{n<m} (x_n - x_m). \tag{3.8}$$

The normalization constant

$$C_N^{(\beta)} = \frac{\pi^{\beta N(N-1)/4}}{N!} \frac{\Gamma^N(\beta/2)}{\Pi_{n=1}^N \Gamma(\beta n/2)} \tag{3.9}$$

obtains from the constants given in Mehta's book[15] and from Eq. (3.4).

To avoid inconveniences and to ensure a compact notation, we define the trace Tr and the determinant Det with Tr=tr and Det=det for $\beta=1,2$ and with

$$\mathrm{Tr}\, K = \tfrac{1}{2}\mathrm{tr} K, \quad \mathrm{Det}\, K = \sqrt{\det K} \tag{3.10}$$

in the case $\beta=4$ for a matrix K with quaternion entries. If k denotes the diagonal matrix of the eigenvalues of a real-symmetric, Hermitian or Hermitean self-dual matrix, it is also useful to define the associate matrix $\hat{k}$. In all three cases β, it is the $N\times N$ matrix $\hat{k} = \mathrm{diag}(k_1, k_2, ..., k_N)$, i.e., we have $\hat{k}=k$ for $\beta=1,2$ and no degeneracies for $\beta=4$.

B. Integral definition and differential equation

As in the case of vector Bessel functions, we start in the matrix case with the plane wave. For two matrices H and K with the same symmetries $H^\dagger = H$ and $K^\dagger = K$, we introduce the matrix plane wave as $\exp(i\,\mathrm{Tr}\, HK)$ where the trace is the proper scalar product in the matrix space. The matrix plane wave has the property

$$\frac{1}{(2\pi)^N \pi^{\beta N(N-1)/2}} \int \mathrm{d}[H] \exp(i\mathrm{Tr}\, HK) = \delta(K), \tag{3.11}$$

where $\delta(K)$ is the product of the δ distributions of all independent variables. We define the matrix gradient $\partial/\partial H$ and the Laplacian operator

$$\Delta = \mathrm{Tr} \frac{\partial^2}{\partial H^2} = \sum_{n=1}^{N} \frac{\partial^2}{\partial H_{nn}^{(0)2}} + \frac{1}{2} \sum_{n<m} \sum_{\alpha=0}^{\beta-1} \frac{\partial^2}{\partial H_{nm}^{(\alpha)2}}, \tag{3.12}$$

which acts on the matrix plane wave as

$$\Delta \exp(i\,\mathrm{Tr}\, HK) = -\,\mathrm{Tr}\, K^2 \exp(i\mathrm{Tr}\, HK). \tag{3.13}$$

We notice that, for $\beta=4$, inconvenient factors of 2 would occur if we used tr instead of Tr.

Analogously to vector Bessel functions, we define the matrix Bessel functions as the angular average

$$\Phi_N^{(\beta)}(x,k) = \int \mathrm{d}\mu(U) \exp(i\,\mathrm{Tr}\, HK). \tag{3.14}$$

The diagonal matrix k contains the eigenvalues of K, which is diagonalized by a matrix V such that $K = V^\dagger k V$. Due to the invariance of the measure $\mathrm{d}\mu(U)$, the matrix V is absorbed and the functions $\Phi_N^{(\beta)}(x,k)$ depend on the eigenvalues x and k only,

$$\Phi_N^{(\beta)}(x,k) = \int \mathrm{d}\mu(U) \exp(i\,\mathrm{Tr}\, U^\dagger x U k). \tag{3.15}$$

Thus, in the scalar product $\mathrm{Tr}\, HK$, solely the relative angles between H and K matter. The matrix Bessel functions are symmetric in the arguments,

$$\Phi_N^{(\beta)}(x,k)=\Phi_N^{(\beta)}(k,x) \tag{3.16}$$

and normalized to unity,

$$\Phi_N^{(\beta)}(x,0)=1, \quad \Phi_N^{(\beta)}(0,k)=1 \tag{3.17}$$

due to Eq. (3.5). These are spherical functions in the sense of Ref. 2.

As in the vector case, the differential equation is obtained by averaging Eq. (3.13) over the relative angles,

$$\Delta \int \mathrm{d}\mu(V)\exp(i\,\mathrm{Tr}\,HK)=-\mathrm{Tr}\,K^2 \int \mathrm{d}\mu(V)\exp(i\,\mathrm{Tr}\,HK). \tag{3.18}$$

Again, the Laplacian Δ commutes with the integral, because the former is in the space of the matrix H, the latter over the diagonalizing matrix V of K. The integral also commutes with $\mathrm{Tr}\,K^2=\mathrm{Tr}\,k^2$. Due to the symmetry between H and K, the integral is obviously identical to the definition (3.15) and we find

$$\Delta_x \Phi_N^{(\beta)}(x,k)=-\mathrm{Tr}\,k^2\,\Phi_N^{(\beta)}(x,k). \tag{3.19}$$

Since the matrix Bessel function $\Phi_N^{(\beta)}(x,k)$ depends only on the radial variables, i.e., on the eigenvalues, we replaced the full Laplacian with its radial part Δ_x. Because of the transformation rule (3.7), it reads

$$\begin{aligned}\Delta_x &= \sum_{n=1}^{N} \frac{1}{|\Delta_N(x)|^\beta}\frac{\partial}{\partial x_n}|\Delta_N(x)|^\beta \frac{\partial}{\partial x_n} \\ &= \sum_{n=1}^{N}\frac{\partial^2}{\partial x_n^2}+\sum_{n<m}\frac{\beta}{x_n-x_m}\left(\frac{\partial}{\partial x_n}-\frac{\partial}{\partial x_m}\right).\end{aligned} \tag{3.20}$$

We notice that these steps are fully parallel to the corresponding discussion in Sec. II. Importantly, due to the symmetry (3.16), the functions $\Phi_N^{(\beta)}(x,k)$ must also solve the differential equation in the k_n, $n=1,\ldots,N$, which results from Eq. (3.19) by exchanging x and k. Obviously, this a very restrictive requirement.

Comparing the radial operator (2.10) in the vector case and the radial operator (3.20), we see that it is the β that corresponds to the *spatial* dimension d or, more precisely, to $d-1$. The role played by the *matrix* dimension N is a different one. To illustrate this, we study the two simplest cases. First, we can formally set $N=1$ and find from the definition (3.14) that $\Phi_1^{(\beta)}(x,k)=\exp(ix_1k_1)$, where $H_{11}=x_1$ and $K_{11}=k_1$. In this case, the matrix U has dropped out trivially. This reflects simply that the scalar product $\vec{k}\cdot\vec{r}$ is linear in the relative solid angle Ω between the vectors whereas the scalar product $\mathrm{Tr}\,HK$ is quadratic in the relative diagonalizing matrix U. The corresponding radial Laplacian Δ_x for $N=1$ is identical to the Cartesian Δ. Therefore, the case $N=1$ is too trivial to give any further insight. Second, we set $N=2$ and find straightforwardly from the differential equation (3.19)

$$\Phi_2^{(\beta)}(x,k)=\exp\left(i\frac{(x_1+x_2)(k_1+k_2)}{2}\right)\chi^{(\beta+1)}\left(\frac{(x_1-x_2)(k_1-k_2)}{2}\right), \tag{3.21}$$

where $\chi^{(d)}$ is the vector Bessel function in d dimensions as defined in Eq. (2.3). This functions appears in the solution, because the differences x_1-x_2 and k_1-k_2 directly correspond to the lengths $|\vec{r}|$ and $|\vec{k}|$. In higher matrix dimensions N, this simple correspondence is lost. However, we will see in great detail that the features of the functions $\Phi_N^{(\beta)}(x,k)$, in particular whether or not explicit solutions can be constructed, are more strongly influenced by β than by N.

Another point in this context deserves to be underlined. In the vector case, the differential equation (2.10) and the solution (2.6) were constructed for integer dimensions d. However, both equations are also well defined for any real and positive d. Similarly, we observe in the matrix case that the differential equation (3.19) was derived for the cases $\beta=1,2,4$. However, neither itself nor its solution (3.21) for $N=2$ are confined to these cases $\beta=1,2,4$, they are valid for any real and positive β. Thus, the cases $\beta=1,2,4$ which correspond to a matrix model, i.e., to the defining integral (3.14) of the matrix Bessel functions, are only special cases of a much more general problem, namely finding the solutions of the differential equation (3.19) for every integer N and for *arbitrary* real values of β. We will return to this in Sec. V.

IV. RECURSION FORMULA

The matrix Bessel functions show a recursive structure which we construct by introducing radial Gelfand–Tzetlin coordinates. The result is stated in Sec. IV A and derived in Sec. IV B. The corresponding invariant measure is calculated in Sec. IV C.

A. Statement of the result

The matrix Bessel functions, defined in Eq. (3.15),

$$\Phi_N^{(\beta)}(x,k)=\int \mathrm{d}\mu(U)\exp(i\,\mathrm{Tr}\,U^{\dagger}xUk) \tag{4.1}$$

depend on the radial space of the eigenvalues x and k. As before, we write $x=\mathrm{diag}(x_1,...,x_N)$ and $k=\mathrm{diag}(k_1,...,k_N)$ for $\beta=1,2$ and, for $\beta=4$, we write $x=\mathrm{diag}(x_1,x_1,...,x_N,x_N)$ and $k=\mathrm{diag}(k_1,k_1,...,k_N,k_N)$. We emphasize that the radial spaces do not lie in the manifolds covered by the groups $\mathrm{U}(N;\beta)$. However, we will show that the group integral (4.1) can be exactly mapped onto a recursive structure which acts exclusively in the radial space. This remarkable feature is the main result of this section.

Under rather general circumstances, the matrix Bessel functions $\Phi_N^{(\beta)}(x,k)$ can be calculated iteratively by the explicit *recursion formula*

$$\Phi_N^{(\beta)}(x,k)=\int \mathrm{d}\mu(x',x)\exp(i\,(\mathrm{Tr}\,x-\mathrm{Tr}\,x')k_N)\Phi_{N-1}^{(\beta)}(x',\tilde{k}), \tag{4.2}$$

where $\Phi_{N-1}^{(\beta)}(x',\tilde{k})$ is the group integral (4.1) over $\mathrm{U}(N-1;\beta)$. We have introduced the diagonal matrix $\tilde{k}=\mathrm{diag}(k_1,...,k_{N-1})$ for $\beta=1,2$ and $\tilde{k}=\mathrm{diag}(k_1,k_1,...,k_{N-1},k_{N-1})$ for $\beta=4$ such that $k=\mathrm{diag}(\tilde{k},k_N)$ for $\beta=1,2$ and $k=\mathrm{diag}(\tilde{k},k_N,k_N)$ for $\beta=4$. Importantly, the $N-1$ integration variables x_n', $n=1,\ldots,N-1$, ordered in the diagonal matrix $x'=\mathrm{diag}(x_1',...,x_{N-1}')$ for $\beta=1,2$ and $x'=\mathrm{diag}(x_1',x_1',...,x_{N-1}',x_{N-1}')$ for $\beta=4$ are arguments of $\Phi_{N-1}^{(\beta)}(x',\tilde{k})$. Moreover, we notice that their further appearance in the exponential is a simple one due to the trace.

The coordinates x' are constructed in the spirit of, but they are different from, the Gelfand–Tzetlin coordinates of Refs. 24 and 25. To clearly distinguish these two sets of coordinates from each other, we refer to the latter as *angular* Gelfand–Tzetlin coordinates and to the variables x' as *radial* Gelfand–Tzetlin coordinates. The difference is at first sight minor, but of crucial importance. In the angular case, x is in the Cartan subalgebra belonging to $\mathrm{U}(N;\beta)$. In the radial case, however, x is in the *radial* space of the eigenvalues of the real-symmetric, Hermitian, or Hermitian self-dual matrix H, which are the arguments of the functions (4.1). While the angular Gelfand–Tzetlin coordinates never leave the group space, the radial ones establish an exact and unique relation between the group and the radial space. The radial Gelfand–Tzetlin coordinates reparametrize the sphere that is described by the Nth column U_N of the matrix $U\in\mathrm{U}(N;\beta)$. The recursion formula (4.2) can only be constructed in the radial coordinates x', but not in the angular ones. The radial and the angular Gelfand–Tzetlin coordinates are, in general, different. They happen to coincide for $\beta=2$, i.e., for the unitary group $\mathrm{U}(N)$. This illustrates, in the framework of our recursion formula, the special role played by the unitary group.

The invariant measure $d\mu(x',x)$ is, apart from phase angles, the invariant measure $d\mu(U_N)$ on the sphere in question, expressed in the radial coordinates x'. It only contains algebraic functions and reads explicitly

$$d\mu(x',x)=\frac{2^{N-1}\Gamma(N\beta/2)}{\pi^{N(\beta-2)(\beta-4)/6}}\frac{\Delta_{N-1}(x')}{\Delta_N^{\beta-1}(x)}\left(-\prod_{n,m}(x_n-x'_m)\right)^{(\beta-2)/2}d[x']. \tag{4.3}$$

The normalization constant obtains from results in Gilmore's book.[22] It ensures normalization to unity according to Eq. (3.5). The domain of integration is compact and given by

$$x_n\leqslant x'_n\leqslant x_{n+1},\quad n=1,\ldots,(N-1), \tag{4.4}$$

reflecting a ''betweenness condition'' for the radial Gelfand–Tzetlin coordinates. This is why no absolute value signs appear in the measure (4.3).

The general recursion formula (4.2) states an iterative way for constructing the matrix Bessel function $\Phi_N^{(\beta)}(x,k)$ for arbitrary N from the matrix Bessel function $\Phi_2^{(\beta)}(x,k)$ for $N=2$ which can usually be obtained trivially. We remark that the recursion formula allows one to express the matrix Bessel functions in the form

$$\begin{aligned}\Phi_N^{(\beta)}(x,k)=&\int\prod_{n=1}^{N-1}d\mu(x^{(n)},x^{(n-1)})\\&\times\exp(i(\mathrm{Tr}\,x^{(n-1)}-\mathrm{Tr}\,x^{(n)})k_{N-n+1})\exp(ix_1^{(N-1)}k_1),\end{aligned} \tag{4.5}$$

where we have introduced the radial Gelfand–Tzetlin coordinates $x_m^{(n)}$, $m=1,\ldots,N-n$ on $N-1$ levels $n=1,\ldots,(N-1)$. We define $x^{(0)}=x$ and $x^{(1)}=x'$.

B. Derivation

We introduce a matrix $V=\mathrm{diag}(\tilde{V},V_0)$ with $\tilde{V}\in\mathrm{U}(N-1;\beta)$ and $V_0\in\mathrm{U}(1;\beta)$ such that $V\in\mathrm{U}(N-1;\beta)\otimes\mathrm{U}(1;\beta)\subset\mathrm{U}(N;\beta)$ and multiply the right-hand side of the definition (4.1) with

$$1=\int d\mu(V)=\int d\mu(V_0)\int d\mu(\tilde{V}). \tag{4.6}$$

The invariance of the Haar measure $d\mu(U)$ allows us to replace U with $UV^\dagger$ and to write

$$\Phi_N^{(\beta)}(x,k)=\int d\mu(V_0)\int d\mu(\tilde{V})\int d\mu(U)\exp(i\,\mathrm{Tr}\,U^\dagger xUV^\dagger kV). \tag{4.7}$$

We collect the first $N-1$ columns U_n of U in the $N\times(N-1)$ rectangular matrix B such that $B=[U_1\,U_2\cdots U_{N-1}]$ and $U=[B\,U_N]$. We notice that

$$\begin{aligned}B^\dagger B&=1_{N-1},\\BB^\dagger&=\sum_{n=1}^{N-1}U_nU_n^\dagger=1_N-U_NU_N^\dagger.\end{aligned} \tag{4.8}$$

As already stated in Sec. III A, the elements of a vector or a matrix are scalar for $\beta=1,2$ and quaternion for $\beta=4$. In this sense, we also write 1_N as the unit matrix for $\beta=4$ because its elements are $\tau^{(0)}$. By defining the $(N-1)\times(N-1)$ square matrices $\tilde{H}=B^\dagger xB$ and $\tilde{K}=\tilde{V}^\dagger\tilde{k}\tilde{V}$ we may rewrite the trace in Eq. (4.7) as

$$\mathrm{Tr}\,U^\dagger xUV^\dagger kV=\mathrm{Tr}\,\tilde{H}\tilde{K}+H_{NN}k_N \tag{4.9}$$

with $H_{NN}=U_N^\dagger x U_N$ according to Eq. (3.6). We notice that V_0 has dropped out. Since the first term of the right-hand side of Eq. (4.9) depends only on the first $N-1$ columns U_n collected in B and the second term depends only on U_N, we use the decomposition

$$\mathrm{d}\mu(U)=\mathrm{d}\mu(B)\mathrm{d}\mu(U_N) \tag{4.10}$$

of the measure to cast Eq. (4.7) into the form

$$\Phi_N^{(\beta)}(x,k)=\int \mathrm{d}\mu(U_N)\exp(iH_{NN}k_N)\int \mathrm{d}\mu(\tilde{V})\int \mathrm{d}\mu(B)\exp(i\,\mathrm{Tr}\,\tilde{H}\tilde{K}), \tag{4.11}$$

where we have already done the trivial integration over V_0.

The difficulty to overcome lies in the decomposition (4.10). While $\mathrm{d}\mu(U_N)$ is simply the invariant measure on the sphere described by U_N, the measure $\mathrm{d}\mu(B)$ is rather complicated. Pictorially speaking, the degrees of freedom in $\mathrm{d}\mu(B)$ have always to know that they are locally orthogonal to U_N. Thus, $\mathrm{d}\mu(B)$ depends on U_N. Luckily, there is one distinct set of coordinates that is perfectly suited to this situation. It is the system of the radial Gelfand–Tzetlin coordinates. We construct it by transferring the methods of Ref. 26 for the angular case to the radial case.

The $N\times N$ matrix $(1_N-U_NU_N^\dagger)$ is a projector onto the $(N-1)\times(N-1)$ space obtained from the original $N\times N$ space by slicing off the vector U_N. We project the radial coordinates x onto this space and study its spectrum. The defining equation reads

$$(1_N-U_NU_N^\dagger)\,x\,(1_N-U_NU_N^\dagger)\,E_n'=x_n'\,E_n',\quad n=1,\ldots,N-1. \tag{4.12}$$

Equation (4.12) determines the $N-1$ radial Gelfand–Tzetlin coordinates x_n' and the corresponding vectors E_n' as eigenvalues and eigenvectors of the matrix $(1_N-U_NU_N^\dagger)\,x\,(1_N-U_NU_N^\dagger)$ which has the rank $N-1$. Since we have by construction $U_N^\dagger E_n'=0$, we may as well write

$$(1_N-U_NU_N^\dagger)\,x\,E_n'=x_n'\,E_n',\quad n=1,\ldots,N-1. \tag{4.13}$$

The eigenvalues $x_n', n=1,\ldots,N$ are obtained from the characteristic equation

$$\begin{aligned}0&=\mathrm{Det}((1_N-U_NU_N^\dagger)x-x_n')\\&=\mathrm{Det}(x-x_n')\det(1_N-(x-x_n')^{-1}U_NU_N^\dagger x)\\&=\mathrm{Det}(x-x_n')\left(1-U_N^\dagger\frac{x}{x-x_n'}U_N\right)\\&=-x_n'\,\mathrm{Det}(x-x_n')\,\mathrm{Tr}U_N^\dagger\frac{1_N}{x-x_n'}U_N.\end{aligned} \tag{4.14}$$

Together with the normalization $\mathrm{Tr}\,U_N^\dagger U_N=1$, this yields the N equations

$$\begin{aligned}1&=\mathrm{Tr}\,U_N^\dagger U_N=\sum_{n=1}^{N}\sum_{\alpha=0}^{\beta-1}U_{nN}^{(\alpha)2},\\0&=\mathrm{Tr}\,U_N^\dagger\frac{1_N}{x-x_n'}U_N=\sum_{m=1}^{N}\sum_{\alpha=0}^{\beta-1}\frac{U_{mN}^{(\alpha)2}}{x_m-x_n'},\quad n=1,\ldots,N-1.\end{aligned} \tag{4.15}$$

In these formulas, the trace Tr is only needed in the symplectic case. We notice that the equations for the variables x' depend on the variables x as parameters. We emphasize once more that x in these equations is in the radial space and, in general, not in the Cartan subalgebra of $\mathrm{U}(N;\beta)$.

At this point, it is not clear yet why the introduction of the radial Gelfand–Tzetlin coordinates is at all helpful. The great advantage will reveal itself when we express the matrix $\tilde{H}$ and the matrix element H_{NN} in the trace (4.11) in these coordinates. To this end, we first multiply Eq. (4.12) from the right with $E_n'^{\dagger}$ and sum over n,

$$(1_N - U_N U_N^{\dagger})\, x\, (1_N - U_N U_N^{\dagger}) = \sum_{n=1}^{N-1} x_n' E_n' E_n'^{\dagger}, \tag{4.16}$$

where we used the completeness relation

$$\sum_{n=1}^{N-1} E_n' E_n'^{\dagger} + U_N U_N^{\dagger} = 1_N. \tag{4.17}$$

Taking the trace of the spectral expansion (4.16) we find immediately

$$\mathrm{Tr}\, x - \mathrm{Tr}\, x' = \mathrm{Tr}\, U_N^{\dagger} x U_N = H_{NN}. \tag{4.18}$$

This is a remarkably simple result. An analogous expression exists for the NN matrix element of the unitary group in the theory of angular Gelfand–Tzetlin coordinates for the unitary group.[24,25] Here we have shown that Eq. (4.18) is a general feature in every radial space.

We now turn to the $(N-1)\times(N-1)$ matrix $\tilde{H}$. Its $N-1$ eigenvalues y_n, $n=1,\ldots,N-1$ are determined by the characteristic equation

$$\begin{aligned} 0 &= \mathrm{Det}(\tilde{H} - y_n) = \mathrm{Det}(B^{\dagger} x B - y_n) \\ &= -\frac{1}{y_n} \mathrm{Det}(B B^{\dagger} x - y_n) \\ &= -\frac{1}{y_n} \mathrm{Det}((1_N - U_N U_N^{\dagger}) x - y_n), \end{aligned} \tag{4.19}$$

where we used Eq. (4.8) and reexpressed an $(N-1)\times(N-1)$ determinant as an $N\times N$ determinant. The comparison of Eq. (4.19) with Eq. (4.14) shows that, most advantageously, we have $y_n \equiv x_n'$, $n=1,\ldots,N-1$. Thus we may write

$$\tilde{H} = B^{\dagger} x B = \tilde{U}^{\dagger} x' \tilde{U} \tag{4.20}$$

by introducing the $(N-1)\times(N-1)$ *square* matrix $\tilde{U}$ which diagonalizes $\tilde{H}$. Obviously, $\tilde{U}$ must be a complicated function of the $N\times(N-1)$ *rectangular* matrix B, i.e., of the columns U_n, $n=1,\ldots,N-1$. However, all we need to know is that $\tilde{U}$ must be in the group $\mathrm{U}(N-1;\beta)$ because, by construction, $\tilde{H}$ has the symmetry $\tilde{H}^{\dagger} = \tilde{H}$.

Collecting everything, we cast Eq. (4.11) into the form

$$\begin{aligned} \Phi_N^{(\beta)}(x,k) = &\int \mathrm{d}\mu(x',x) \exp(i(\mathrm{Tr}\, x - \mathrm{Tr} x')k_N) \\ &\times \int \mathrm{d}\mu(\tilde{V}) \int \mathrm{d}\mu(B) \exp(i\, \mathrm{Tr}\, \tilde{U}^{\dagger} x' \tilde{U} \tilde{V}^{\dagger} \tilde{k} \tilde{V}). \end{aligned} \tag{4.21}$$

We may now use the invariance of the Haar measure $\mathrm{d}\mu(\tilde{V})$ to absorb $\tilde{U}$ such that

$$\Phi_N^{(\beta)}(x,k)=\int \mathrm{d}\mu(x',x)\exp(i(\mathrm{Tr}\,x-\mathrm{Tr}\,x')k_N)$$
$$\times\int \mathrm{d}\mu(\widetilde{V})\exp(i\,\mathrm{Tr}\,x'\widetilde{V}^{\dagger}\widetilde{k}\widetilde{V})\int \mathrm{d}\mu(B). \tag{4.22}$$

Thus, the integration over B is trivial and yields unity due to our normalization. The remaining integration over $\widetilde{V}$ gives precisely the matrix Bessel function $\Phi_{N-1}^{(\beta)}(x',\widetilde{k})$. This completes the derivation of the recursion formula in Sec. IV A. The reader experienced with group integration has realized that the introduction of the matrix $V=\mathrm{diag}(\widetilde{V},V_0)$ was not strictly necessary. Alternatively, one could have shown that the measure $\mathrm{d}\mu(B)$ can be identified with $\mathrm{d}\mu(\widetilde{U})$ and have done the corresponding integral. However, we believe that the introduction of V makes this part of the derivation more transparent.

C. Invariant measure

The invariant measure $\mathrm{d}\mu(U_N)$ has to be expressed in terms of the radial coordinates x'. To this end, we first have to solve Eq. (4.15) for the moduli squared of the vector U_N as a function of the new coordinates x'. Since Eq. (4.15) for the total moduli square for all β coincides with the equation for the *angular* Gelfand–Tzetlin coordinates of the unitary group, we can use the results as derived in Refs. 24 and 25. We have in the three cases

$$|U_{nN}|^2=\sum_{\alpha=0}^{\beta-1}(U_{nN}^{(\alpha)})^2=\frac{\Pi_{m=1}^{N-1}(x_n-x'_m)}{\Pi_{m\neq n}(x_n-x_m)}. \tag{4.23}$$

The betweenness condition (4.4) follows from the positive definiteness of this expression. We parametrize the remaining degrees of freedom of U_{nN} in the cases $\beta=2,4$. We set $U_{nN}^{(0)}=\cos\gamma_n^{(1)}$ and $U_{nN}^{(1)}=\sin\gamma_n^{(1)}$ in the case $\beta=2$ and

$$U_{nN}=\begin{bmatrix}\cos\psi_n\exp(i\gamma_n^{(1)}) & \sin\psi_n\exp(i\gamma_n^{(2)})\\ -\sin\psi_n\exp(-i\gamma_n^{(2)}) & \cos\psi_n\exp(-i\gamma_n^{(1)})\end{bmatrix} \tag{4.24}$$

for $\beta=4$ in the basis (3.2). The invariant length element reads

$$\mathrm{Tr}\,\mathrm{d}U_N^{\dagger}\,\mathrm{d}U_N=\sum_{n=1}^{N}\sum_{\alpha=0}^{\beta-1}(\mathrm{d}U_{nN}^{(\alpha)})^2$$
$$=\sum_{n=1}^{N}\left(\frac{1}{4|U_{nN}|^2}(\mathrm{d}|U_{nN}|^2)^2\right.$$
$$\left.+\sum_{i=1}^{\beta/2}|U_{nN}|^2(\mathrm{d}\gamma_n^{(i)})^2+\delta_{\beta 4}|U_{nN}|^2(\mathrm{d}\cos\psi_n)^2\right). \tag{4.25}$$

To express the differential $\mathrm{d}|U_{nN}|^2$ in terms of the $\mathrm{d}x'_n$, we again take advantage of the results in Refs. 24 and 25,

$$\sum_{n=1}^{N}\frac{1}{4|U_{nN}|^2}(\mathrm{d}|U_{nN}|^2)^2=\sum_{n=1}^{N-1}\frac{\Pi_{m=1}^{N-1}(x'_m-x'_n)}{4\Pi_{m=1}^{N}(x_m-x'_n)}(\mathrm{d}x'_n)^2. \tag{4.26}$$

From these equations, we can read off the metric g in the basis of the coordinates x'_n, $\gamma_n^{(i)}$ and ψ_n. Conveniently, it is diagonal. The determinant of g is given by

$$\det g = \frac{\Delta_{N-1}^2(x')}{\Delta_N^{2\beta-2}(x)} \prod_{n,m} (x_n - x'_m)^{(\beta-2)}, \tag{4.27}$$

which yields the invariant measure $d\mu(U_N)$ in terms of the x'_n and of the additional coordinates $\gamma_n^{(j)}$ and ψ_n. These angles can be integrated out trivially. This yields Eq. (4.3).

V. RADIAL FUNCTIONS FOR ARBITRARY β

Remarkably, the recursion introduced in Sec. IV, is the iterative solution of the radial equation for arbitrary values of β. Thus, the matrix Bessel functions are special cases of more general functions which we want to refer to as radial functions. We give the precise formulation of the problem in Sec. V A and show in Sec. V B that the recursion is the general iterative solution. In Sec. V C, we discuss a Hankel ansatz for the radial functions.

A. Definition by the differential equation

In Sec. III B, we defined the matrix Bessel function through the group integral (3.14) or, equivalently, the group integral (3.15). This definition confines the dimension β to the values $\beta = 1,2,4$, corresponding to the groups $U(N;\beta)$. However, discussing the simplest case $N=2$, we already saw in Sec. III B that $\Phi_2^{(\beta)}$ is well defined for *arbitrary* values of β. This was a simple consequence of the explicit form (3.21) which expresses $\Phi_2^{(\beta)}$ in terms of the Bessel function $\chi^{(\beta+1)}$. The latter is known to be well defined for arbitrary β. Hence, we conclude that the cases $\beta=1,2,4$ which relate to matrices and groups are embedded into a space of far more general functions.

It seems natural that this phenomenon also extends to $N>2$. The problem has to be posed as follows: We seek the solutions $\Phi_N^{(\beta)}$ of the differential equation

$$\Delta_x \Phi_N^{(\beta)}(x,k) = -\sum_{n=1}^{N} k_n^2 \Phi_N^{(\beta)}(x,k), \tag{5.1}$$

where the operator is given by

$$\Delta_x = \sum_{n=1}^{N} \frac{\partial^2}{\partial x_n^2} + \sum_{n<m} \frac{\beta}{x_n - x_m} \left(\frac{\partial}{\partial x_n} - \frac{\partial}{\partial x_m} \right). \tag{5.2}$$

Here, β is arbitrary. For technical reasons, however, we restrict ourselves for the time being to real and positive values of β. We make no reference whatsoever to matrices, eigenvalues, and groups. To emphasize this, we view x and k as sets of N variables x_n, $n=1,\ldots,N$ and k_n, $n=1,\ldots,N$ for every positive β. We do not use traces.

We require that the solutions are symmetric in the argument

$$\Phi_N^{(\beta)}(x,k) = \Phi_N^{(\beta)}(k,x) \tag{5.3}$$

and normalized

$$\Phi_N^{(\beta)}(0,k) = 1 \quad \text{or} \quad \Phi_N^{(\beta)}(x,0) = 1 \tag{5.4}$$

at the origin $x=0$ and $k=0$. Due to the symmetry, one of the two normalization conditions suffices.

In the sequel, we want to refer to the functions $\Phi_N^{(\beta)}(x,k)$ for arbitrary β as *radial functions* while we reserve the term *matrix Bessel functions* to the cases $\beta=1,2,4$ where the direct connection to matrices and Lie groups exists.

B. Recursive solution

We claim that the solutions are, for arbitrary β, given as an iteration in N by the recursion formula

$$\Phi_N^{(\beta)}(x,k)=\int \mathrm{d}\mu(x',x)\exp\left(i\left(\sum_{n=1}^{N} x-\sum_{n=1}^{N-1} x' \right) k_N \right) \Phi_{N-1}^{(\beta)}(x',\tilde{k}), \tag{5.5}$$

where $\Phi_{N-1}^{(\beta)}(x',\tilde{k})$ is the solution of the differential equation (5.2) for $N-1$. Here, $\tilde{k}$ denotes the set of variables k_n, $n=1,\ldots,(N-1)$ and x' the set of integration variables x_n', $n=1,\ldots,(N-1)$. The integration measure

$$\mathrm{d}\mu(x',x)=G_N^{(\beta)}\frac{\Delta_{N-1}(x')}{\Delta_N^{\beta-1}(x)}\left(-\prod_{n,m}(x_n-x_m') \right)^{(\beta-2)/2} \mathrm{d}[x'] \tag{5.6}$$

is the continuation of Eq. (4.3) to arbitrary positive β. The normalization constant

$$G_N^{(\beta)}=2^{N-1}\frac{\Gamma(N\beta/2)}{\Gamma^N(\beta/2)} \tag{5.7}$$

is also the continuation of the constant in Eq. (4.3). We calculate it in Appendix F. As in the cases $\beta=1,2,4$, the inequalities

$$x_n\leqslant x_n'\leqslant x_{n+1}, \quad n=1,\ldots,(N-1) \tag{5.8}$$

define the domain of integration.

We stress that we derived the recursion formula (5.5) in Sec. IV for the cases $\beta=1,2,4$. To prove that it is the iterative solution for arbitrary positive β, we show that it solves the differential equation (5.1). The keystone for the proof is the identity

$$\Delta_x\Phi_N^{(\beta)}(x,k)=-k_N^2\Phi_N^{(\beta)}(x,k)+\int \mathrm{d}\mu(x',x)\exp\left(i\left(\sum_{n=1}^{N} x_n-\sum_{n=1}^{N-1} x_n' \right) k_N \right) \Delta_{x'}\Phi_{N-1}^{(\beta)}(x',\tilde{k}), \tag{5.9}$$

which is derived in Appendix D. Equation (5.9) establishes a not immediately obvious, but nevertheless natural connection between, on the one hand, the action of the Laplacian Δ_x in the N variables x_n on the radial function in N dimensions, i.e., on the recursion integral (5.5), and, on the other hand, the recursion integral over the Laplacian $\Delta_{x'}$ in the $N-1$ variables x_n' acting on the radial function in $N-1$ dimensions. There is a compensation term which is just $-k_N^2\Phi_N^{(\beta)}(x,k)$. Thus, we can prove the eigenvalue equation (5.1) by induction: assuming that it is correct for $N-1$, identity (5.9) implies Eq. (5.1) for N. The induction starts with $N=2$ where the eigenvalue equation (5.1) is clearly valid for arbitrary β as shown in Sec. III B by deriving the explicit solution (3.21).

The symmetry relation (5.3) is nontrivial. In the matrix cases $\beta=1,2,4$, it is obvious from the integral definitions (3.14) and (3.15). For arbitrary β, we cannot use this argument, we only have the recursion (5.5). In Appendix E, we prove the symmetry relation (5.3) by an explicit change of variables.

The normalization $\Phi_N^{(\beta)}(x,0)=1$ in Eq. (5.4) follows directly from the normalization of the measure (5.6). The symmetry relation (5.3) then also yields $\Phi_N^{(\beta)}(0,k)=1$.

Regarding the domain of β, a comment is in order. We have seen in Sec. III B that for $N=2$ the matrix Bessel function is well defined for arbitrary complex β. This should also be true for our recursion formula (5.5). However, for $\beta\leqslant 0$ nonintegrable singularities arise at the boundaries in the integral in Eq. (5.5). At the same time the normalization constant becomes zero for $\beta=0$,

$-2,-4,\ldots$, compensating the singularities of the integral. This makes the recursion formula for $\beta \leqslant 0$ not ill-defined but it gets more difficult to treat. Therefore, we have restricted ourselves to positive values of β.

In the work of Okounkov and Olshanski[11] an expansion of the radial functions for arbitrary β in Jack polynomials is derived. The series run over sets of partitions $\{\lambda\}$. These authors also derive a recursion formula for the Jack polynomials depending on one set of continuous variables x, say, and belonging to such partitions $\{\lambda\}$. It is related to, but different from ours, which involves two sets of continuous varables x and k. The crucial difference rests in the exponential function which is present in our formula (5.5), but not in the formula of Ref. 11. Importantly, it is this exponential term which makes sure that the symmetry condition (5.3) is fulfilled on all levels of the recursion. Since the Jack polynomials themselves do not obey such a symmetry condition, there is no exponential term in the recursion formula of Ref. 11. However, it must be possible to derive the recursion formula for the radial functions from the one for the Jack polynomials. An interesting, although probably not very elegant approach would be the following: If one inserted the recursion formula for the Jack polynomials into the expansion[11] of the radial functions in terms of these Jack polynomials, one ought to see that the series over the partitions can, at least partly, be *resummed* to yield the exponential function present in the recursion formula (5.5). This is remarkable and could be very helpful for the application of Jack polynomials, because, in general, resummations over partitions are known to be difficult and involved. For the connection to Calogero–Sutherland models, we refer the reader to Sec. VII.

C. Hankel ansatz

In the spirit of Eq. (2.12) for the vector case, we make a Hankel ansatz for our radial functions for arbitrary positive β. We also do this in view of the applications in Sec. VI. Since the sum over the k_n^2 on the right-hand side of the eigenvalue equation (5.1) is invariant under all permutations of the k_n or, equivalently, their indices n, we can label a set of solutions $\Phi^{(\beta)}_{N,\omega}(x,k)$ by an element ω of the permutation group S_N of N objects. For these solutions, we make the ansatz

$$\Phi^{(\beta)}_{N,\omega}(x,k)=\frac{\exp(i\Sigma_{n=1}^{N}x_n k_{\omega(n)})}{|\Delta_N(x)\Delta_N(k)|^{\beta/2}}\,W^{(\beta)}_{N,\omega}(x,k), \tag{5.10}$$

where $\omega(k)$ is the diagonal matrix constructed from k by permuting the k_n, or the indices n. The full solution $\Phi^{(\beta)}_N(x,k)$, satisfying the constraints (5.3) and (5.4), is then, apart from possible normalization constants, given as the linear combination

$$\Phi^{(\beta)}_N(x,k)=\frac{1}{N!}\sum_{\omega\in S_N}(-1)^{\pi(\omega)}\Phi^{(\beta)}_{N,\omega}(x,k) \tag{5.11}$$

of the functions (5.10). Here, $\pi(\omega)$ is the parity of the permutation.

We find for the function $W^{(\beta)}_{N,\omega}(x,k)$ the differential equation

$$L_{x,\omega(k)}\,W^{(\beta)}_{N,\omega}(x,k)=0, \tag{5.12}$$

where the operator is given by

$$L_{x,\omega(k)}=\sum_{n=1}^{N}\frac{\partial^2}{\partial x_n^2}+i2\sum_{n=1}^{N}k_{\omega(n)}\frac{\partial}{\partial x_n}-\beta\left(\frac{\beta}{2}-1\right)\sum_{n<m}\frac{1}{(x_n-x_m)^2}. \tag{5.13}$$

This differential equation generalizes Eq. (2.13) to the matrix case for $\beta=1,2,4$ and, furthermore, the latter to general radial functions for arbitrary β. Due to the symmetry (5.3), the differential equation (5.12) must also hold if x and $\omega(k)$ are interchanged.

The functions $W^{(\beta)}_{N,\omega}(x,k)$ are translation invariant, i.e., they depend only on the differences (x_n-x_m). We show this in Appendix G. Again, because of the symmetry, this argument carries

over to k, and $W_{N,\omega}^{(\beta)}(x,k)$ depends only on the differences (k_n-k_m) as well. Moreover, the symmetry implies that it depends only on the products $(k_{\omega(n)}-k_{\omega(m)})(x_n-x_m)$.

It is the last term of the operator $L_{x,\omega(k)}$ that makes the differential equation (5.12) so difficult. In the sequel, we are only interested in solutions $W_{N,\omega}^{(\beta)}(x,k)$ which are translation invariant. Moreover, in the case $\beta=2$, when the last term of the operator $L_{x,\omega(k)}$ vanishes, oscillatory solutions can be possible. We exclude them because, first, they are, in general, not translation invariant and, second, they can be absorbed in the oscillatory part of the ansatz (5.10). Thus, we simply have $W_{N,\omega}^{(2)}(x,k)=1$. This is the Itzykson–Zuber case[6] corresponding to unitary matrices $U\in \mathrm{U}(N)$. For arbitrary β, it is obvious from the differential operator that $W_{N,\omega}^{(\beta)}(x,k)\to 1$ if $|x_n-x_m|\to\infty$ for all pairs $n<m$. Once more, this must also be true if $|k_n-k_m|\to\infty$. Thus, we expect that $W_{N,\omega}^{(\beta)}(x,k)$ is some kind of asymptotic series, generalizing Eq. (2.14) in the vector case.

Hence, we rederive a known result by concluding that the leading contribution in an asymptotic expansion of the functions (5.10) is given by

$$\Phi_{N,\omega}^{(\beta)}(x,k)\sim \frac{\exp(i\Sigma_{n=1}^{N}x_nk_{\omega(n)})}{|\Delta_N(x)\Delta_N(k)|^{\beta/2}}. \tag{5.14}$$

According to Eq. (5.11), this means that

$$\Phi_{N}^{(\beta)}(x,k)\sim \frac{\det[\exp(ix_nk_m)]_{n,m=1,\ldots,N}}{|\Delta_N(x)\Delta_N(k)|^{\beta/2}} \tag{5.15}$$

is the asymptotic behavior of the radial functions $\Phi_N^{(\beta)}(x,k)$ if the differences $|x_n-x_m|$ and $|k_n-k_m|$ are large for all pairs $n<m$.

Collecting all pieces of information, we make the ansatz

$$W_{N,\omega}^{(\beta)}(x,k)=\sum_{\{\mu\}}\frac{a_{\mu_{12}\mu_{13}\cdots\mu_{(N-1)N}}}{\Pi_{n<m}((k_{\omega(n)}-k_{\omega(m)})(x_n-x_m))^{\mu_{nm}}} \tag{5.16}$$

with coefficients $a_{\mu_{12}\mu_{13}\cdots\mu_{(N-1)N}}$ that depend on $N(N-1)/2$ integer indices μ_{nm}, as many as there are differences. The summation is over the set of these indices. The presence of the k_n makes it very difficult to solve Eq. (5.12) with the ansatz (5.16). In the vector case, one easily sees that the differential equation (2.13) in r can be transformed into an equation in the dimensionless variables kr such that k does not appear anymore. This leads to the simple recursion (2.15) for the coefficients. Here, in the matrix case, the k_n cannot easily be absorbed and the recursion formulas for the coefficients will depend on the k_n in a nontrivial way. However, in some simple cases, it is possible to solve them. These difficulties were an important motivation for us to develop the methods which we introduced in Sec. IV.

VI. APPLICATIONS

Can we obtain an explicit formula for the radial functions by using the recursion formula (5.5)?—At least in some cases, this ought to be possible. Here, we present some results.

For the sake of completeness, we comment once more on the special case $\beta=2$, i.e., the unitary case. Obviously, the measure (5.6) simplifies enormously. This is so because the radial Gelfand–Tzetlin coordinates coincide with the angular ones. Thus, the case $\beta=2$ is identical to the rederivation of the Itzykson–Zuber integral by Shatashvili.[25]

We now consider the orthogonal case $\beta=1$. The recursion formula reads

$$\Phi_N^{(1)}(x,k)=G_N^{(1)}\int\frac{\Delta_{N-1}(x')}{\sqrt{-\Pi_{n,m}(x_n-x'_m)}}\exp\left(i\left(\sum_{n=1}^{N}x_n-\sum_{n=1}^{N-1}x'\right)k_N\right)\Phi_{N-1}^{(1)}(x',\tilde{k})\mathrm{d}[x']. \tag{6.1}$$

The square roots appearing in the measure make a further evaluation very difficult. As is obvious from the trivial case $N=2$, given in Eq. (3.21), the function $\Phi_N^{(1)}(x,k)$ will be an *infinite* series for all values of N. However, we expect that, due to the different construction, this series is different from the expansion in *zonal functions* which was obtained by Muirhead.[20]

Obviously, there is a pattern emerging. The integration measure (5.6) is purely *rational* for all even and positive values of β. This is reminiscent of the situation for vector Bessel functions in *odd* dimensions d, which consist of a *finite* number of terms, as discussed in Sec. II. Hence, we conjecture that the radial functions $\Phi_N^{(\beta)}(x,k)$ can also be written as a *finite* sum, exclusively containing exponential and rational functions.

For all other values of β, the measure (5.6) is algebraic, but not rational, and the radial functions $\Phi_N^{(\beta)}(x,k)$ must be *infinite* series. Nevertheless, these infinite series contain exponential and rational functions. Thus, they are different from expansions in terms of zonal polynomials.

To furnish our conjecture about the form of the radial functions for even and positive values of β with an illustrative example, we turn to the unitary-symplectic case $\beta=4$. The results given here in the sequel were first derived by the present authors in Ref. 27. Later, they were also given by Brézin and Hikami in Ref. 28.

To simplify the notation we avoid the imaginary unit by writing

$$\Phi_N^{(4)}(-ix,k)=\int_{U\in \mathrm{USp}(2N)} \exp(\mathrm{Tr}\, u^{-1}xuk)\mathrm{d}\mu(U), \tag{6.2}$$

where $x=\mathrm{diag}(x_1,x_1,\ldots,x_N,x_N)$ and $k=\mathrm{diag}(k_1,k_1,\ldots,k_N,k_N)$ are diagonal matrices with Kramers degeneracies. The starting point of the recursion is the smallest nontrivial case $N=2$, i.e., the group USp(4). We obtain after an elementary calculation

$$\Phi_2^{(4)}(-ix,k)=G_2^{(4)}\sum_{\omega\in S_2}\left(\frac{1}{\Delta_2^2(x)\Delta_2^2(\omega(k))}-\frac{2}{\Delta_2^3(x)\Delta_2^3(\omega(k))}\right)\exp(\mathrm{Tr}\, x\omega(k)). \tag{6.3}$$

The sum runs over the elements of the permutation group S_N for $N=2$. Inserting Eq. (6.3) into the recursion formula, we find for USp(6), the next step in the recursion,

$$\Phi_3^{(4)}(-ix,k)=G_3^{(4)}G_2^{(4)}\sum_{\omega\in S_2}\int_{x_1}^{x_2}\mathrm{d}x_1'\int_{x_2}^{x_3}\mathrm{d}x_2'\frac{\Pi_{i=1}^3\Pi_{j=1}^2(x_i-x_j')}{\Delta_3^3(x)\Delta_2^2(\omega(\tilde{k}))}\exp((\mathrm{Tr}\, x-\mathrm{Tr}\, x')k_3+\mathrm{Tr}\, x\omega(\tilde{k}))$$
$$\times\left(\frac{1}{\Delta_2(x')}-\frac{2}{\Delta_2^2(x')\Delta_2(\omega(\tilde{k}))}\right). \tag{6.4}$$

Although the integrand is finite everywhere, in particular at $x_1'=x_2'=x_2$, the denominators $\Delta_2(x')$ and $\Delta_2^2(x')$ raise a technical difficulty. The key to remove them is to use the identity

$$\frac{2}{\Delta_2^2(x')}=-\left(\frac{\partial}{\partial x_1'}-\frac{\partial}{\partial x_2'}\right)\frac{1}{\Delta_2(x')} \tag{6.5}$$

and to observe that the product $\Pi_{i=1}^3\Pi_{j=1}^2(x_i-x_j')$ annihilates all boundary terms. Hence, we can integrate by parts and arrive at

$$\Phi_3^{(4)}(-ix,k)=G_3^{(4)}G_2^{(4)}\sum_{\omega\in S_2}\frac{1}{\Delta_3^3(x)\Delta_2^3(\omega(\tilde{k}))}\int_{x_1}^{x_2}\mathrm{d}x_1'\int_{x_2}^{x_3}\mathrm{d}x_2'\sum_{i=1}^3\prod_{\substack{j=1\\ j\neq i}}^3(x_j-x_1')(x_j-x_2')$$
$$\times\exp((\mathrm{Tr}\, x-\mathrm{Tr}\, x')k_3+\mathrm{Tr}\, x\omega(\tilde{k})), \tag{6.6}$$

where no denominator is left. Due to the permutation symmetry of the original integral, we can restrict ourselves to the unity element e of the permutation group in the further evaluation of Eq. (6.6). Thus we need only to consider the limits $x_i' \to x_i$, $i=1,2$ while integrating by parts. After collecting orders in k we find

$$\Phi_{3,e}^{(4)}(-ix,k) = G_3^{(4)} G_2^{(4)} \frac{1}{\Delta_3^3(x)\Delta_3^3(k)} \left(-\Delta_3(x)\Delta_3(k) + 2\sum_{i<j}^{3} \left(\frac{\Delta_3(x)\Delta_3(k)}{(x_i-x_j)(k_i-k_j)} \right) \right.$$
$$\left. -4\sum_{i<j}^{3} (x_i-x_j)(k_i-k_j) + 12 \right) \exp(\mathrm{Tr}\, xk). \tag{6.7}$$

By introducing the composite variables

$$z_{\omega(ij)} = (x_i - x_j)(k_{\omega(i)} - k_{\omega(j)}), \quad i,j = 1,\ldots,3, \quad \omega \in S_3, \tag{6.8}$$

we can express $\Phi_3^{(4)}(-ix,k)$ in a compact form as

$$\Phi_3^{(4)}(-ix,k) = G_3^{(4)} G_2^{(4)} \sum_{\omega \in S_3} \frac{1}{\Delta_3^3(x)\Delta_3^3(\omega(k))} \left(4 + \prod_{i<j}^{3} (2 - z_{\omega(ij)}) \right) \exp(\mathrm{Tr}\, x\omega(k)). \tag{6.9}$$

So far, we have not been able to extend this procedure to all values of N.

However, we succeeded in calculating $\Phi_4^{(4)}(-ix,k)$, i.e., the case of the group USp(8), by an hybrid method which combines information obtained from the recursion with a Hankel ansatz as described previously. We extend the right hand side of Eq. (6.9) for $N=3$ to $N=4$ and use this expression as an ansatz for the function $W_{N,\omega}^{(4)}(x,k)$. As it turns out, a correction term is needed and, furthermore a correction to the correction. Fortunately, there is a structure to this. We give the details in Appendix H. We emphasize that the knowledge of $\Phi_3^{(4)}(-ix,k)$ is essential for this hybrid procedure, in particular the fact that $\Phi_3^{(4)}(-ix,k)$ contains only linear terms in every composite variable $z_{\omega(ij)}$. Up to a normalization, $\Phi_4^{(4)}(-ix,k)$ is given by

$$\Phi_4^{(4)}(-ix,k) = \sum_{\omega \in S_4} \frac{1}{\Delta_4^3(x)\Delta_4^3(\omega(k))} \left(\prod_{i<j} (2 - z_{\omega(ij)}) + 2^2 \sum_{l<m<n} \prod_{\substack{i<j \\ \neq lm \\ \neq ln \\ \neq mn}} (2 - z_{\omega(ij)}) \right.$$
$$\left. + 2^3 \sum_{\substack{l<m \\ k<n}} \prod_{\substack{i<j, \neq lk, \neq ln \\ \neq mk, \neq mn, \neq kn}} (2 - z_{\omega(ij)}) \right) \exp(\mathrm{Tr}\, x\omega(k)). \tag{6.10}$$

Comparing this result with Eq. (6.9) we notice that, once more, the composite variables $z_{\omega(ij)}$ enter only linearly in the polynomial part of $\Phi_4^{(4)}(-ix,k)$. Similarly, the spherical Bessel function $j_1(z)$, which is the counterpart of $\Phi_N^{(4)}(x,k)$ in the vector case given in Eqs. (2.6) and (3.21), has a polynomial part linear in z. We expect that such analogies are also present for higher values of β and the dimension d.

Formula (6.10) indicates a general structure for $\Phi_N^{(4)}(x,k)$. The leading term is always the generating function of the elementary symmetric functions in z. To this term combinations of other symmetric functions are added, where certain combinations of indices are cut out. In the supersymmetric case, we could apply the present method in even more complicated cases and also find explicit results.[40]

VII. CONNECTION TO CALOGERO–SUTHERLAND MODELS

The radial functions are related to, but different from, the eigenfunctions which are usually employed in models of the Calogero–Sutherland type. Since this issue is so important for applications and so often raised in discussions, we briefly collect the main points.

The radial Laplace operator defined in Eq. (5.2) is closely related to the Calogero–Sutherland Hamiltonians. In general one can always cast a Fokker–Planck operator in a Hamilton operator by adjunction[29] with the square root of the stationary probability distribution defined through $\Delta_x P_{\mathrm{eq}}(x)=0$. Choosing $P_{\mathrm{eq}}(x)=|\Delta_N(x)|^{-\beta/2}$, the operator (5.2) can be associated with the Hamiltonian

$$H_D=-\sum_{n=1}^{N}\frac{\partial^2}{\partial x_n^2}+\frac{\beta(\beta-2)}{2}\sum_{n<m}^{N}\frac{1}{(x_n-x_m)^2}. \tag{7.1}$$

It describes a scattering system with a continuous spectrum, the large time behavior is determined by the states near the ground state. Apart from a sign, this operator H_D coincides with the operator $L_{x,0}$ in Eq. (5.13) for $k=0$. We also notice that the interaction vanishes for $\beta=2$.

To have a well-defined thermodynamic limit one often confines the motion of the particles to a circle. This yields the Calogero–Sutherland Hamiltonian

$$H_{\mathrm{CS}}=-\sum_{n=1}^{N}\frac{\partial^2}{\partial x_n^2}+\frac{\beta(\beta-2)}{2}\sum_{n<m}^{N}\frac{(\pi/N)^2}{\sin^2(\pi(x_n-x_m)/N)}, \tag{7.2}$$

which can also be derived directly from Dyson's circular ensembles.[15] Another way of confining the particles is by a harmonic potential. This leads to the Calogero Hamiltonian[30]

$$H_C=-\sum_{n=1}^{N}\frac{\partial^2}{\partial x_n^2}+\frac{\beta(\beta-2)}{2}\sum_{n<m}^{N}\frac{1}{(x_m-x_m)^2}+\frac{1}{16}\sum_{n=1}^{N}x_n^2. \tag{7.3}$$

In the thermodynamic limit the particle density $R_1(x)$ of the ground state is described by Wigner's semicircle law. The mean particle level spacing $D=1/R_1(0)$ scales as $D\propto 1/\sqrt{N}$. Therefore in the thermodynamic limit the harmonic confining term in Eq. (7.3) vanishes on the scale of the mean level spacing. On this *unfolded scale* the correlation functions become independent of the confinement mechanism. The three Hamiltonians H_C, H_D, and H_{CS} are known to be integrable systems for arbitrary β.[31] However, the three values $\beta=1,2,4$ are distinguished, since they establish a connection to the random matrix ensembles. Indeed, for these values of β they belong to a much wider class of integrable systems, which can be constructed by means of the root space of a simple Lie algebra or—still more generally—of a Kac–Moody algebra.[5] This class comprises Hamiltonians which can be derived by an adjunction procedure from a Laplace–Beltrami operator of a group acting in a symmetric space. This space has positive curvature for H_{CS} and zero curvature for H_D, H_C. In Refs. 32 and 33 it was pointed out that the Dorokhov–Mello–Pereyra–Kumar equation for scattering matrices with broken time reversal symmetry corresponds to a Laplace–Beltrami operator in a symmetric space of negative curvature.

Eigenfunctions $\psi_{N,E}^{(\beta)}(x)$ of the Hamiltonians $H_C, H_D, H_{\mathrm{CS}}$ with eigenenergy E for arbitrary β are known. Essentially, these solutions are products of the ground state wave function and symmetric polynomials in the coordinates x of the N particles. In case of the Calogero–Sutherland Hamiltonian H_{CS}, these polynomials are the Jack polynomials.[34–36] In this approach, the energy eigenvalues E are labeled by a partition of length N. The crucial difference to the matrix Bessel functions is that the Jack polynomials are symmetric polynomials in one set of variables x only whereas the matrix Bessel functions $\Phi_N^{(\beta)}(x,k)$ are symmetric in two sets of variables x and k. Importantly, they are, in addition, symmetric under interchange of the two sets of variables, $\Phi_N^{(\beta)}(x,k)=\Phi_N^{(\beta)}(k,x)$. This is reflected in the fact that the operator $L_{x,\omega(k)}$ emerging in the Hankel ansatz depends on k while H_D does not. Due to their symmetry, the matrix Bessel func-

tions $\Phi_N^{(\beta)}(x,k)$ are, at least for H_D, the more natural eigenfunctions. This is so, because, to obtain orthogonality conditions, one has to sum the $\psi_{N,E}^{(\beta)}(x)$ over an infinite number of partitions. On the other hand, orthogonality relations are an inherent feature of the $\Phi_N^{(\beta)}(x,k)$ due to their meaning in the Fourier–Bessel analysis, as discussed in Appendix C.

In other words, the functions $\psi_{N,E}^{(\beta)}(x)$ can be viewed as a basis in an expansion of the $\Phi_N^{(\beta)}(x,k)$. We can consider the variables k as a set of real numbers corresponding to the energies E labeling the eigenstates of H_D. The matrix Bessel functions (3.15) are solutions of the Schrödinger equation with Hamiltonian H_D for the coupling parameters $\beta=1,2,4$. The recursion formula (5.5) represents an analytic continuation of these integral solutions to arbitrary positive β. All these functions $\Phi_N^{(\beta)}(x,k)$ have for arbitrary β additional features: the symmetry in x and k, which has no analog in the functions $\psi_{N,E}^{(\beta)}(x)$. The merit of our recursion formula lies in the fact that, *a priori*, no infinite resummation is required to obtain functions of the type $\Phi_N^{(\beta)}(x,k)$. Nevertheless Forrester[35] and Forrester and Nagao[37] showed that such resummed expressions can successfully be used in certain cases. They treated the case of Poissonian initial conditions[37] for the Calogero–Sutherland Hamiltonian H_{CS} and derived exact expressions for the correlation functions for arbitrary β for one or two particles. This is also related to the works of Muirhead[20] and Pandey.[38]

VIII. SUMMARY AND CONCLUSION

We presented a recursive construction for certain spherical functions. We referred to them as matrix Bessel functions because, first, they are a natural extension of vector Bessel functions in the sense that the integration over a group corresponds to the integration over a solid angle and, second, they satisfy a partial differential equation generalizing the Bessel ordinary differential equation. For matrices, the index β labeling the groups appears analogous to the dimension d in the case of vectors. The introduction of radial Gelfand–Tzetlin coordinates, which are related to but different from the ordinary angular ones, was crucial for the recursion. The Cayley transformation ought to provide a connection between the angular and the radial Gelfand–Tzetlin coordinates.[39] As evident from its construction, the recursion maps an integral over a group fully onto an iteration which exclusively takes place in the radial space.

Remarkably, the recursion turned out to be far more general than was to be expected, at first sight, from the proof which involved Lie groups. We showed that our recursion is also the iterative solution of the corresponding partial differential equation for arbitrary values of β. We introduced the term radial functions for this generalization of matrix Bessel functions. We expect that one has to employ the theory of quantum groups to give a group theoretical derivation of the recursion formula for arbitrary values of β.

Using the recursion formula, we discussed the structure of radial Bessel functions. We conjectured that, for even β, they can be written as finite sums involving only exponential and rational functions. We illustrated that by working out, for $\beta=4$, the cases of $N=3$ and $N=4$ distinct eigenvalues. Further evaluation of explicit formulas for arbitrary N and, maybe, for all even β does not seem impossible. Work is in progress. The extension of the stationary phase approach by Duistermaat and Heckman[13] to higher orders could, for even β, be an alternative to derive such explicit results, because the expansion terminates. In this context, we mention that the radial functions for higher values of β are, to some extent, but not fully, the higher order radial functions for lower values of β. This also generalizes the situation for ordinary Bessel functions. However, there are many more higher order radial functions; they are not at all exhausted by this mapping between values of β.

In the present contribution, we only focused on ordinary spaces, i.e., spaces which are built upon commuting numbers. In a second study[40] we also address superspaces which involve commuting and anticommuting variables.

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APPENDIX A: ALTERNATIVE INTEGRAL REPRESENTATION FOR VECTOR BESSEL FUNCTIONS

The Bessel functions $\chi^{(d)}(kr)$ are defined as an integral over angles in Eq. (2.1), but they can also be written as integrals over the entire or half real axis.[21] To make possible an instructive comparison with the matrix case, we quote and rederive the representation

$$\chi^{(d)}(kr)=\frac{\Gamma(d/2)}{i2\pi}\left(\frac{2}{ikr}\right)^{(d-2)/2}\int_{-\infty}^{+\infty}\exp\left(-i\frac{kr}{2}\left(t+\frac{1}{t}\right)\right)\frac{\mathrm{d}t}{t^{d/2}}. \tag{A1}$$

The singularities have to be treated properly.

The position vector in the d dimensional space is $\vec{r}=r\vec{e}_r$, where the vector $\vec{e}_r$ parametrizes the unit sphere. To integrate over its orientation, i.e., over the solid angle Ω, one can reexpress the measure as

$$\mathrm{d}\Omega=\frac{\Gamma(d/2)}{\pi^{d/2}}\,\delta(\vec{e}_r^{\,2}-1)\mathrm{d}^d e_r\,. \tag{A2}$$

Here, the vector $\vec{e}_r$ is reinterpreted: its components live on the entire real axis and the domain of integration is the full d dimensional space with the Cartesian measure $\mathrm{d}^d e_r$. The δ distribution confines the vector to the unit sphere. Writing this distribution as a Fourier transform, we obtain from Eq. (2.1)

$$\begin{aligned}\chi^{(d)}(kr)&=\frac{\Gamma(d/2)}{\pi^{d/2}}\,\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}t\int\mathrm{d}^d e_r\exp(it(\vec{e}_r^{\,2}-1))\exp(i\vec{k}\cdot r\vec{e}_r)\\&=\frac{\Gamma(d/2)}{2\pi}\int_{-\infty}^{+\infty}\frac{\exp(-it)}{(it)^{d/2}}\exp\left(-i\frac{(kr)^2}{4t}\right)\mathrm{d}t,\end{aligned} \tag{A3}$$

where the integral over $\vec{e}_r$ gave a Gaussian in d dimensions. The contour for the integration over t has to be chosen appropriately. Upon a trivial change of variables, this result yields Eq. (A1).

APPENDIX B: ALTERNATIVE INTEGRAL REPRESENTATION FOR MATRIX BESSEL FUNCTIONS

The matrix Bessel functions $\Phi_N^{(\beta)}(x,k)$ for $\beta=1,2,4$ can be be written in an alternative way. Although we can hardly believe that this representation is completely new, we could not find it in the literature. Similar to Eq. (A1) in the vector case, we can write

$$\Phi_N^{(\beta)}(x,k)=A_N^{(\beta)}\int\mathrm{d}[T]\exp(i\,\mathrm{Tr}\,T)\,\mathrm{Det}^{-\beta/2}(x\otimes\hat{k}-T\otimes 1_N), \tag{B1}$$

where 1_N is the $N\times N$ unit matrix. The normalization constant is given by

$$A_N^{(\beta)}=\frac{i^{\beta N^2/2}\pi^{\beta N(N-1)/4}}{\beta^{N+\beta N(N-1)/2}}\prod_{n=1}^{N}\Gamma(\beta n/2). \tag{B2}$$

The matrix T in Eq. (B1) is real symmetric, Hermitian, or Hermitian self-dual, respectively, for $\beta=1,2,4$. The measure $\mathrm{d}[T]$ is Cartesian and given by Eq. (3.3). All independent variables in T are integrated over the entire real axis. To ensure convergence, the diagonal elements of T have to be given a proper imaginary increment. We notice that x and T are $N\times N$ matrices for $\beta=1,2$ and $2N\times 2N$ for $\beta=4$ with doubly degenerated eigenvalues. The matrix $\hat{k}$ is, in all three cases β, just the $N\times N$ matrix $\hat{k}=\mathrm{diag}(k_1,k_2,...,k_N)$, as defined following Eq. (3.10).

The integral representation (B1) leads to an interesting integral equation for the matrix Bessel functions,

$$\Phi_N^{(\beta)}(x,k)=B_N^{(\beta)}\,\mathrm{Det}^{1-\beta/2}x\int \mathrm{d}[t]\,|\Delta_N(t)|^{\beta}\frac{\Phi_N^{(\beta)}(x,t)}{\Pi_{n,m}(k_m-t_n)^{\beta/2}}, \tag{B3}$$

where the normalization constant reads

$$B_N^{(\beta)}=\frac{i^{\beta N^2/2}\Gamma^N(\beta/2)}{(2\pi)^N N!}. \tag{B4}$$

The t_n in Eq. (B3) have a proper imaginary increment and their domain of integration is the real axis. Due to the symmetry relation (3.16), the variables x and k can be interchanged in Eqs. (B1) and (B3).

It is not difficult to see from the integral equation (B3) that the product in the denominator of its right-hand side can, in the case $\beta=2$, be written as

$$\frac{B_N^{(2)}}{\Pi_{n,m}(k_m-t_n)}=\frac{\det[\,\delta(x_n-t_m)]_{n,m=1,\ldots,N}}{|\Delta_N(k)\Delta_N(t)|^{1/2}}. \tag{B5}$$

For $\beta\neq 2$, the term $\mathrm{Det}^{1-\beta/2}x$ contributes. Nevertheless, the product still shares features with a δ distribution.

To derive this alternative integral representation, we proceed analogously to Eq. (A2) by rewriting the invariant measure of $U\in \mathrm{U}(N;\beta)$ using δ distributions. The invariance simply means that all columns U_n, $n=1,\ldots,N$ are orthonormal, $\mathrm{Tr}\,U_n^{\dagger}U_m=\delta_{nm}$. The trace Tr is only needed for $\beta=4$, because the entries of U are quaternions in this case. Thus, we may write

$$\mathrm{d}\mu(U)=M_N^{(\beta)}\,\mathrm{d}[U]\prod_{n=1}^{N}\delta(\mathrm{Tr}\,U_n^{\dagger}U_n-1)\prod_{n<m}\delta(\mathrm{Tr}\,U_n^{\dagger}U_m), \tag{B6}$$

where $\mathrm{d}[U]$ is the Cartesian measure of all entries of U and the integration is for all variables over the entire real axis. The constant $M_N^{(\beta)}$ will be determined later. Ullah[41,42] used such forms for the measure to work out certain probability density functions. The bilinear forms in the δ distributions have β components for $n\neq m$,

$$U_n^{\dagger}U_m=\sum_{\alpha=0}^{\beta-1}[U_n^{\dagger}U_m]^{(\alpha)}\tau^{(\alpha)}. \tag{B7}$$

We notice that $[U_n^{\dagger}U_n]^{(\alpha)}=0$ for $\alpha>0$ in the case $n=m$, because the length of every vector is real. Thus, because of Eq. (B7), the δ distributions in the measure (B6) have to be products of δ distributions for every nonzero component $[U_n^{\dagger}U_m]^{(\alpha)}$. We now introduce Fourier representations

$$\delta([U_n^{\dagger}U_m]^{(\alpha)})=\frac{1}{\pi}\int_{-\infty}^{+\infty}\mathrm{d}T_{nm}^{(\alpha)}\exp(-i2[U_n^{\dagger}U_m]^{(\alpha)}T_{nm}^{(\alpha)}), \tag{B8}$$

$$\delta([U_n^\dagger U_n]^{(0)}-1)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dT_{nn}^{(0)}\exp(-i([U_n^\dagger U_n]^{(0)}-1)T_{nm}^{(0)})$$

for $n\neq m$ and $n=m$, respectively. The Fourier variables form the elements

$$T_{nm}=\sum_{\alpha=0}^{\beta-1} T_{nm}^{(\alpha)}\,\tau^{(\alpha)} \tag{B9}$$

of a matrix T which is real-symmetric, Hermitian or Hermitian self-dual according to $\beta=1,2,4$. We notice that the diagonal elements $T_{nn}=T_{nn}^{(0)}$ are always real,

$$\delta(\mathrm{Tr}\,U_n^\dagger U_m)=\frac{1}{\pi^\beta}\int d^\beta T_{nm}\exp(-i\,\mathrm{Tr}\,U_n^\dagger(T_{nm}\otimes 1_N)U_m-i\,\mathrm{Tr}\,U_m^\dagger(T_{nm}^*\otimes 1_N)U_n),$$
$$\delta(\mathrm{Tr}\,U_n^\dagger U_n-1)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dT_{nn}\exp(i\,\mathrm{Tr}\,T_{nn}-i\,\mathrm{Tr}\,U_n^\dagger(T_{nn}\otimes 1_N)U_n) \tag{B10}$$

for $n\neq m$ and $n=m$, as previously. Just as for the trace Tr, the direct product is only needed in the case $\beta=4$.

We order the columns U_n, $n=1,\ldots,N$ of the matrix U in a vector $\vec{U}=(U_1,U_2,\ldots,U_N)^T$ with N^2 elements. For $\beta=1,2$, the elements are scalars; for $\beta=4$, they are quaternions. Collecting everything, we can rewrite the measure (B6) in the form

$$d\mu(U)=\frac{M_N^{(\beta)}d[U]}{(2\pi)^N\pi^{\beta N(N-1)/2}}\int d[T]\exp(i\,\mathrm{Tr}\,T-i\,\mathrm{Tr}\,\vec{U}^\dagger(T\otimes 1_N)\vec{U}). \tag{B11}$$

For the unitary case, a related Fourier integral form for integration measures was used by Fyodorov and Khoruzhenko[43] in the context of quantum chaotic scattering. To use the measure (B11) in the integral (3.15) for the matrix Bessel functions $\Phi_N^{(\beta)}(x,k)$, we also take advantage of the relation

$$\mathrm{Tr}\,U^{-1}xUk=\mathrm{Tr}\,\vec{U}^\dagger(x\otimes\hat{k})\vec{U}, \tag{B12}$$

which allows us to write

$$\Phi_N^{(\beta)}(x,k)=\frac{M_N^{(\beta)}}{(2\pi)^N\pi^{\beta N(N-1)/2}}\int d[U]\int d[T]\exp(i\,\mathrm{Tr}\,T)\exp(i\,\mathrm{Tr}\,\vec{U}^\dagger(x\otimes\hat{k}-T\otimes 1_N)\vec{U})$$
$$=\frac{M_N^{(\beta)}i^{\beta N^2}\pi^{\beta N/2}}{(2\pi)^N}\int d[T]\exp(i\,\mathrm{Tr}\,T)\,\mathrm{Det}^{-\beta/2}(x\otimes\hat{k}-T\otimes 1_N). \tag{B13}$$

Thus, the integration over U could be done as a Gaussian one and gave the result (B1). Obviously, the Gaussian integrals over $\vec{U}$ only converge, if the diagonal elements of T have a proper imaginary increment.

Formula (B13) yields immediately the integral equation (B3). Upon making the change of variables

$$T=x^{1/2}T'x^{1/2},$$
$$\text{implying}\quad d[T]=\mathrm{Det}^{1+\beta(N-1)/2}x\,d[T'], \tag{B14}$$

we bring x into the exponential function and remove it from the determinant. We diagonalize $T'=V'^{-1}t'V'$ and find

$$\mathrm{Det}^{-\beta/2}(x\otimes\hat{k}-T\otimes 1_N)=\mathrm{Det}^{-\beta N/2}x\prod_{n,m}(k_m-t'_n)^{-\beta/2}. \tag{B15}$$

The integral over V' is then just the integral definition (3.15) of the matrix Bessel function $\Phi_N^{(\beta)}(x,t')$ and we arrive at Eq. (B3).

The normalization constants remain to be derived. Conveniently, they nicely relate to a special form of Selberg's integral which is given in Eq. (17.5.2) of Mehta's book,[15]

$$\begin{aligned}J_N&=\int \mathrm{d}[t]|\Delta_N(t)|^{2\gamma}\prod_{n=1}^{N}(a_1+it_n)^{-b_1}(a_2-it_n)^{-b_2}\\&=\frac{(2\pi)^N}{(a_1+a_2)^{(b_1+b_2)N-\gamma N(N-1)-N}}\\&\quad\times\prod_{n=0}^{N-1}\frac{\Gamma(1+(n+1)\gamma)\Gamma(b_1+b_2-(N+n-1)\gamma-1)}{\Gamma(1+\gamma)\Gamma(b_1-n\gamma)\Gamma(b_2-n\gamma)}.\end{aligned} \tag{B16}$$

We now put $x=0$ or $k=0$ and have $\Phi_N^{(\beta)}(0,k)=1$ or $\Phi_N^{(\beta)}(x,0)=1$ on the left-hand side of Eq. (B13). We diagonalize $T=V^{-1}tV$ and use the invariance of the integral. Employing the measure (3.7) and the constant $C_N^{(\beta)}$ given in Eq. (3.9), we find the condition

$$1=\frac{M_N^{(\beta)}C_N^{(\beta)}\pi^{\beta N/2}}{(2\pi)^N}\int \mathrm{d}[t]|\Delta_N(t)|^{\beta}\prod_{n=1}^{N}\frac{\exp(it_n)}{(it_n)^{\beta N/2}}. \tag{B17}$$

We map this onto Selberg's integral (B16) by setting $\gamma=\beta/2$, $b_1=\beta N/2$, and $a_2=b_2$, by using

$$\lim_{a_2\to\infty}\frac{a_2^{a_2}}{(a_2-it_n)^{a_2}}=\exp(it_n) \tag{B18}$$

and by considering $a_2^{Na_2}J_N$ in the limits $a_1\to 0$ and $a_2\to\infty$. With the help of some standard asymptotic formulas for the Γ function, we obtain $M_N^{(\beta)}$ and, eventually, the constants $A_N^{(\beta)}$ and $B_N^{(\beta)}$ in Eqs. (B2) and (B4).

APPENDIX C: FOURIER–BESSEL ANALYSIS

The Fourier–Bessel analysis involving matrix Bessel functions was discussed by Harish-Chandra[4] in a general and formal way. To show the connection to our results, we summarize here some essential features of the Fourier–Bessel analysis on an explicit level.

We write the Fourier transform of a function $f(H)$ as

$$F(K)=D_N^{(\beta)}\int \mathrm{d}[H]\exp(i\,\mathrm{Tr}\,HK)f(H), \tag{C1}$$

where the matrices H and K have the same symmetries. If we choose a symmetric normalization,

$$D_N^{(\beta)}=\frac{1}{(2\pi)^{N/2}\pi^{\beta N(N-1)/4}}, \tag{C2}$$

we can write the inverse transform as

$$f(H)=D_N^{(\beta)}\int \mathrm{d}[K]\exp(-i\mathrm{Tr}KH)F(K). \tag{C3}$$

We notice that, according to Eq. (3.11), the Fourier transform of the constant $D_N^{(\beta)}$ is the δ distribution $\delta(K)$ and vice versa.

If f is an invariant function such that $f(H)=f(x)$, its Fourier transform turns out to be invariant as well, $F(K)=F(k)$. Introducing eigenvalue-angle coordinates, we easily find

$$F(k)=D_N^{(\beta)}C_N^{(\beta)}\int \mathrm{d}[x]|\Delta_N(x)|^{\beta}\Phi_N^{(\beta)}(x,k)f(x) \tag{C4}$$

for the Fourier transform and

$$f(x)=D_N^{(\beta)}C_N^{(\beta)}\int \mathrm{d}[k]\,|\Delta_N(k)|^{\beta}\Phi_N^{(\beta)*}(k,x)F(k) \tag{C5}$$

for its inverse. We now insert the transform (C4) into the inverse (C5) and conclude that

$$(D_N^{(\beta)}C_N^{(\beta)})^2\int \mathrm{d}[k]|\Delta_N(k)|^{\beta}\,\Phi_N^{(\beta)}(x,k)\,\Phi_N^{(\beta)*}(k,y)=\frac{\det[\,\delta(x_n-y_m)\,]_{n,m=1,\ldots,N}}{|\Delta_N(x)\Delta_N(y)|^{\beta/2}}. \tag{C6}$$

This is the analog of Hankel's expansion of the δ distribution. From Eq. (C6), the formula

$$\int \mathrm{d}\mu(U)\,\delta(U^{\dagger}xU-y)=\frac{1}{C_N^{(\beta)}}\,\frac{\det[\,\delta(x_n-y_m)\,]_{n,m=1,\ldots,N}}{|\Delta_N(x)\Delta_N(y)|^{\beta/2}} \tag{C7}$$

obtains. To see this, we introduce a matrix G having the same symmetries as H and write

$$\delta(H-G)=(D_N^{(\beta)})^2\int \mathrm{d}[K]\exp(-i\,\mathrm{Tr}\,K(H-G)). \tag{C8}$$

Averaging over the diagonalizing matrix U of H yields

$$\int \mathrm{d}\mu(U)\,\delta(H-G)=(D_N^{(\beta)})^2\int \mathrm{d}[K]\,\Phi_N^{(\beta)*}(x,k)\exp(i\,\mathrm{Tr}\,KG), \tag{C9}$$

by using the invariance of the measure. We now introduce eigenvalue-angle coordinates for K and do the integral over V, the diagonalizing matrix of K,

$$\int \mathrm{d}\mu(U)\,\delta(H-G)=(D_N^{(\beta)})^2C_N^{(\beta)}\int \mathrm{d}[k]|\Delta_N(k)|^{\beta}\,\Phi_N^{(\beta)*}(x,k)\Phi_N^{(\beta)}(k,y), \tag{C10}$$

where we have, once more, employed the invariance of the measure. Since the right-hand side of this equation does only depend on the eigenvalues y of G, we may replace G on the left-hand side with y. Together with Eq. (C6), this gives formula (C7).

For the convolution in matrix space of two functions $f_1(H)$ and $f_2(H)$, we straightforwardly find the generalization of the standard convolution theorem,

$$f(H)=\int \mathrm{d}[G]f_1(G)f_2(H-G)=\int \mathrm{d}[K]\exp(-i\,\mathrm{Tr}\,HK)F_1(K)F_2(K), \tag{C11}$$

where G has the same symmetries as H. The functions $F_1(K)$ and $F_2(K)$ are the Fourier transforms of $f_1(H)$ and $f_2(H)$, respectively. If the functions are invariant, the second equation of (C11) acquires the form

$$f(x)=C_N^{(\beta)}\int \mathrm{d}[k]|\Delta_N(k)|^{\beta}\,\Phi_N^{(\beta)*}(x,k)F_1(k)F_2(k). \tag{C12}$$

On the other hand, we find from the first equation of (C11)

$$f(x)=C_N^{(\beta)}\int \mathrm{d}[y]|\Delta_N(y)|^\beta f_1(y)\hat{f}_2(x,y), \tag{C13}$$

where y are the eigenvalues of G. This formula is a convolution in the curved space of the eigenvalues. The second function is given by

$$\hat{f}_2(x,y)=\int \mathrm{d}\mu(U) f_2(x-U^\dagger y U). \tag{C14}$$

We insert the Fourier integral for $F_1(k)$ according to Eq. (C4) into Eq. (C12), compare with Eq. (C13) and obtain the Fourier decomposition

$$\hat{f}_2(x,y)=D_N^{(\beta)}C_N^{(\beta)}\int \mathrm{d}[k]|\Delta_N(k)|^\beta \Phi_N^{(\beta)*}(x,k)F_2(k)\Phi_N^{(\beta)}(k,y). \tag{C15}$$

Formulas (C6) and (C7) can be viewed as special cases of these results.

APPENDIX D: ACTION OF THE LAPLACIAN ON THE RADIAL FUNCTIONS FOR ARBITRARY β

We make the notation more compact by defining

$$\tilde{\mu}(x',x)\mathrm{d}[x']=\mathrm{d}\mu(x',x)\exp\left(i\left(\sum_{n=1}^{N}x_n-\sum_{n=1}^{N-1}x_n'\right)k_N\right), \tag{D1}$$

where the measure is given in Eq. (5.6). To prove the identity (5.9), we write the integral using Θ functions. The left hand side of Eq. (5.9) reads

$$\Delta_x\int \tilde{\mu}(x',x)\Phi_{N-1}^{(\beta)}(x',\tilde{k})\prod_{i>j}\Theta(x_i-x_j')\prod_{j\geqslant l}\Theta(x_j'-x_l)\mathrm{d}[x'], \tag{D2}$$

where now the integration domain is the real axis for all variables. Thus, we can directly calculate the action of the operator Δ_x onto the integral. We find

$$\begin{aligned}
&\Delta_x\int \tilde{\mu}(x',x)\Phi_{N-1}^{(\beta)}(x',\tilde{k})\prod_{i>j}\Theta(x_i-x_j')\prod_{j\geqslant l}\Theta(x_j'-x_l)\mathrm{d}[x']\\
&\quad=\int \Phi_{N-1}^{(\beta)}(x',\tilde{k})\prod_{i>j}\Theta(x_i-x_j')\prod_{j\geqslant l}\Theta(x_j'-x_l)\\
&\qquad\times\left(\Delta_{x'}^{(-)}+\beta\sum_{n\neq m}\frac{1}{(x_n'-x_m')^2}-k_N^2\right)\tilde{\mu}(x',x)\mathrm{d}[x']\\
&\qquad+\int \Phi_{N-1}^{(\beta)}(x',\tilde{k})\tilde{\mu}(x',x)\Delta_x\prod_{i>j}\Theta(x_i-x_j')\prod_{j\geqslant l}\Theta(x_j'-x)\mathrm{d}[x']\\
&\qquad+2\int \Phi(x',\tilde{k})\sum_{n=1}^{N}\frac{\partial}{\partial x_n}\tilde{\mu}(x',x)\frac{\partial}{\partial x_n}\prod_{i>j}\Theta(x_i-x_j')\prod_{j\geqslant l}\Theta(x_j'-x_l)\mathrm{d}[x'],
\end{aligned} \tag{D3}$$

where we define the operator

$$\Delta_{x'}^{(-)}=\sum_{n=1}^{N}\frac{\partial^2}{\partial x_n^2}-\sum_{n<m}\frac{\beta}{x_n-x_m}\left(\frac{\partial}{\partial x_n}-\frac{\partial}{\partial x_m}\right). \tag{D4}$$

By a series of integrations by parts, the operator $\Delta_{x'}^{(-)}$ acting on $\tilde{\mu}(x',x)$ is transformed to $\Delta_{x'}$ acting only on $\Phi(x',\tilde{k})$. At taking the derivative of the Θ functions, we notice that only adjacent levels contribute, because otherwise terms like $\Theta(x_i-x_j)$ with $i<j$ arise which annihilate the integral due to the chosen ordering. Therefore, we can write

$$\frac{\partial}{\partial x_n}\prod_{i>j}\Theta(x_i-x_j')\prod_{j\geqslant l}\Theta(x_j'-x_l)=\prod(\Theta_{\neq nn'},\Theta_{\neq(n-1)'n})(\delta(x_n-x_n')\Theta(x_{n-1}'-x_n) - \delta(x_{n-1}'-x_n)\Theta(x_n-x_n')), \tag{D5}$$

where $\Pi(\Theta_{\neq nn'},\Theta_{\neq(n-1)'n})$ is short-hand for the product on the left-hand side of Eq. (D5) without the two factors $\Theta(x_{n-1}'-x_n)\Theta(x_n-x_n')$. Importantly, this product is symmetric in x_{n-1}' and x_n'. The second derivatives yield

$$\frac{\partial}{\partial x_n}\prod_{i>j}\Theta(x_i-x_j')\prod_{j\geqslant l}\Theta(x_j'-x_l)=\prod(\Theta_{\neq nn'},\Theta_{\neq(n-1)'n})(\delta'(x_n-x_n')\Theta(x_{n-1}'-x_n) + \delta'(x_{n-1}'-x_n)\Theta(x_n-x_n')+\delta(x_{n-1}'-x_n)\delta(x_n-x_n')). \tag{D6}$$

The last term vanishes upon integration, since it is symmetric in x_{n-1}' and x_n', whereas the rest of the integrand is antisymmetric due to the Vandermonde determinant $\Delta_{N-1}(x')$ in the measure (5.6). Differentiation with respect to x_n' gives

$$\frac{\partial}{\partial x_n'}\prod_{i>j}\Theta(x_i-x_j')\prod_{j\geqslant l}\Theta(x_j'-x_l)=\prod(\Theta_{\neq n'(n+1)},\Theta_{\neq nn'})(\delta(x_n'-x_{n+1})\Theta(x_n-x_n') - \delta(x_n-x_n')\Theta(x_n'-x_{n+1})). \tag{D7}$$

Integration by parts of the first term of the right hand side of Eq. (D3) yields

$$\begin{aligned}\Delta_x\int\tilde{\mu}(x',x)\Phi_{N-1}^{(\beta)}(x',\tilde{k})\prod_{i>j}\Theta(x_i-x_j')\prod_{j\geqslant l}\Theta(x_j'-x_l)\mathrm{d}[x'] \\ =\int\tilde{\mu}(x',x)\Delta_{x'}\Phi_{N-1}^{(\beta)}(x',\tilde{k})\mathrm{d}[x']-k_N^2\int\tilde{\mu}(x',x)\Phi_{N-1}^{(\beta)}(x',\tilde{k})\mathrm{d}[x'] \\ +2\int\Phi_{N-1}^{(\beta)}(x',\tilde{k})\sum_{n=1}^{N-1}\Bigg(\prod(\Theta_{\neq n'(n+1)},\Theta_{\neq nn'}) \\ \times(\delta(x_n-x_n')\Theta(x_n'-x_{n+1})+\delta(x_n'-x_{n+1})\Theta(x_n-x_n')) \\ \times\left(\frac{\partial}{\partial x_n}+\frac{\partial}{\partial x_n'}+\frac{1}{2}\sum_{m\neq n}\frac{\beta}{x_n-x_m}+-\frac{1}{2}\sum_{m\neq n}\frac{\beta}{x_n'-x_m'}\right)\Bigg)\tilde{\mu}(x',x)\mathrm{d}[x'].\end{aligned} \tag{D8}$$

Inserting in Eq. (D8) the function $\tilde{\mu}(x',x)$ as given in Eq. (D1) and (5.6) we find after a straightforward calculation

$$\Delta_x \int \tilde{\mu}(x',x)\Phi_{N-1}^{(\beta)}(x',\tilde{k})\mathrm{d}[x']$$

$$= \int \tilde{\mu}(x',x)\Delta_{x'}\Phi_{N-1}^{(\beta)}(x',\tilde{k})\mathrm{d}[x'] - k_N^2 \int \tilde{\mu}(x',x)\Phi_{N-1}^{(\beta)}(x',\tilde{k})\mathrm{d}[x']$$

$$+2\int \Phi_{N-1}^{(\beta)}(x',\tilde{k})\sum_{n=1}^{N-1}\Bigg(\prod\,(\Theta_{\neq n'(n+1)},\Theta_{\neq nn'})(g(x_n';y_n;x,x')-g(x_n';x_n;x,x'))$$

$$\times(\delta(x_n-x_n')\Theta(x_n'-x_{n+1})+\delta(x_n'-x_{n+1})\Theta(x_n-x_n'))\Bigg)\tilde{\mu}(x',x)\mathrm{d}[x'], \tag{D9}$$

with

$$g(x_n;x_n';x,x') = (\beta/2-1)\left(\sum_{m=1}^{N-1}\frac{1}{x_n-x_m'}-\sum_{m\neq n}\frac{1}{x_n-x_m}\right),$$
$$g(x_n';x_n;x,x') = (\beta/2-1)\left(\sum_{m\neq n}\frac{1}{x_n'-x_m'}-\sum_{m=1}^{N}\frac{1}{x_n'-x_m}\right). \tag{D10}$$

We now can perform the integration of the δ distributions in Eq. (D9). We notice that the difference $(g(x_n';x_n;x,x')-g(x_n';x_n;x,x'))$ vanishes linearly, whenever x_n' approaches one of the boundaries of its integration domain. Thus the second integral in Eq. (D9) yields zero as long as the measure diverges less than $(x_n-x_n')^{-1}$ when x_n' approaches x_n. This is always the case for $\beta>0$. Collecting everything, we arrive at the identity (5.9).

APPENDIX E: SYMMETRY OF THE RADIAL FUNCTIONS FOR ARBITRARY β

Applying the recursion formula (5.5) to all $N-1$ levels, we can extend Eq. (4.5) to arbitrary β and write

$$\Phi_N^{(\beta)}(x,k) = \int \prod_{n=1}^{N-1}\mathrm{d}\mu(x^{(n)},x^{(n-1)})\exp\left(i\left(\sum_{m=1}^{N-n+1}x_m^{(n-1)}-\sum_{m=1}^{N-n}x_m^{(n)}\right)k_{N-n+1}\right)\exp(ix_1^{(N-1)}k_1), \tag{E1}$$

where $x^{(0)}=x$. Analogously, we also find

$$\Phi_N^{(\beta)}(k,x) = \int \prod_{n=1}^{N-1}\mathrm{d}\mu(k^{(n)},k^{(n-1)})\exp\left(i\left(\sum_{m=1}^{N-n+1}k_m^{(n-1)}-\sum_{m=1}^{N-n}k_m^{(n)}\right)x_{N-n+1}\right)\exp(ik_1^{(N-1)}x_1) \tag{E2}$$

with $k^{(0)}=k$ for the solution of the differential equation which results from Eq. (5.1) by interchanging x and k. We have to show that these two radial functions (E1) and (E2) are identical. To this end, we change in Eq. (E1) on the nth level the variables $x_m^{(n)}, m=1,\ldots,(N-n)$ to $k_m^{(n)}, m=1,\ldots,(N-n)$ by setting

$$\frac{\Pi_{l=1}^{N-n-1}(x_m^{(n-1)}-x_l^{(n)})}{\Pi_{l\neq m}(x_m^{(n-1)}-x_l^{(n-1)})} = r_m^{(n)} = \frac{\Pi_{l=1}^{N-n-1}(k_m^{(n-1)}-k_l^{(n)})}{\Pi_{l\neq m}(k_m^{(n-1)}-k_l^{(n-1)})} \tag{E3}$$

for $n=1,\ldots,(N-1)$. These are, on the nth level, $N-n+1$ equations for making a change of $N-n$ variables. However, one has

$$\sum_{m=1}^{N-n+1} r_m^{(n)} = 1 \tag{E4}$$

on all levels which eliminates one of the $N-n+1$ equations.

Of course, the substitution (E3) is motivated by the radial Gelfand–Tzetlin coordinates which we introduced to construct the recursion formula for $\beta=1,2,4$. In this case, the $r_m^{(n)}$ are the moduli squared of a column of a matrix $U\in \mathrm{U}(N-n;\beta)$. Here, we do not use this connection to matrices and groups. We simply view Eq. (E3) as a standard change of variables in an integral. We underline that Eq. (E3) does not involve β at all. Equation (E4) is just the normalization of a column of U for $\beta=1,2,4$. Since it is independent of β, it also holds for arbitrary β. One can also verify Eq. (E4) by a direct calculation.

The original domains of integration are $x_m^{(n-1)}\leqslant x_m^{(n)}\leqslant x_{m+1}^{(n-1)}$. In these boundaries, the $r_m^{(n)}$ are positive definite. Hence, to satisfy this when changing the variables, we must have $k_m^{(n-1)}\leqslant k_m^{(n)}\leqslant k_{m+1}^{(n-1)}$ for the new domains of integration.

To work out the measure in the new variables $k_m^{(n)}$, we interpret Eq. (E3) as a change to the integration variables $r_m^{(n)}$, too. This yields immediately

$$\frac{\Delta_{N-n}(x^{(n)})}{\Delta_{N-n+1}(x^{(n-1)})}\,\mathrm{d}[x^{(n)}]=\mathrm{d}\mu(r^{(n)})=\frac{\Delta_{N-n}(k^{(n)})}{\Delta_{N-n+1}(k^{(n-1)})}\,\mathrm{d}[k^{(n)}]. \tag{E5}$$

The first equality sign goes back to the radial Gelfand–Tzetlin coordinates. We may use this piece of information, because it is independent of β. The second equality sign is simply due to Eq. (E3). Using this result, we find for the full and β dependent measure

$$\begin{aligned}\mathrm{d}\mu(x^{(n)},x^{(n-1)})&=G_{N-n+1}^{(\beta)}\left(\frac{\Pi_{l,m}(x_m^{(n-1)}-x_l^{(n)})}{\Delta_{N-n+1}^2(x^{(n-1)})}\right)^{(\beta-2)/2}\frac{\Delta_{N-n}(x^{(n)})}{\Delta_{N-n+1}(x^{(n-1)})}\,\mathrm{d}[x^{(n)}]\\&=G_{N-n+1}^{(\beta)}\left(\prod_{m=1}^{N-n+1}r_m^{(n)}\right)^{(\beta-2)/2}\frac{\Delta_{N-n}(x^{(n)})}{\Delta_{N-n+1}(x^{(n-1)})}\,\mathrm{d}[x^{(n)}]\\&=G_{N-n+1}^{(\beta)}\left(\frac{\Pi_{l,m}(k_m^{(n-1)}-k_l^{(n)})}{\Delta_{N-n+1}^2(k^{(n-1)})}\right)^{(\beta-2)/2}\\&\quad\times\frac{\Delta_{N-n}(k^{(n)})}{\Delta_{N-n+1}(k^{(n-1)})}\,\mathrm{d}[k^{(n)}]=\mathrm{d}\mu(k^{(n)},k^{(n-1)}).\end{aligned} \tag{E6}$$

For $\beta=1,2,4$, this result is a direct consequence of the invariance of the group measure $\mathrm{d}\mu(U)$. Here, we have derived it for arbitrary β. This, in turn, implies that the invariance of the group measure $\mathrm{d}\mu(U)$ is embedded into and reflects much more general features.

We now collect all these intermediate results and plug them into Eq. (E1). Apart from the expressions in the exponential functions, we have full agreement with the right-hand side of Eq. (E2). Hence, it remains to be shown that the change of variables (E3) leads to the identity

$$\begin{aligned}&\sum_{n=1}^{N-1}\left(\sum_{m=1}^{N-n+1}x_m^{(n-1)}-\sum_{m=1}^{N-n}x_m^{(n)}\right)k_{N-n+1}+x_1^{(N-1)}k_1\\&\quad=\sum_{n=1}^{N-1}\left(\sum_{m=1}^{N-n+1}k_m^{(n-1)}-\sum_{m=1}^{N-n}k_m^{(n)}\right)x_{N-n+1}+k_1^{(N-1)}x_1.\end{aligned} \tag{E7}$$

Since the symmetry relation (5.3) holds for $\beta=1,2,4$, we know that Eq. (E7) must be true in these cases. However, as Eq. (E7) does not involve β at all, it must also be valid for arbitrary β. Inserting this into the right-hand side of Eq. (E1), we recover Eq. (E2), as desired. We notice that this line of arguing cannot be spoiled by any other contribution to the argument of the exponential functions, because all other terms in the integrand are purely algebraic. This completes the proof of the symmetry relation (5.3) for arbitrary β.

APPENDIX F: CALCULATION OF THE NORMALIZATION CONSTANT $G_N^{(\beta)}$

In Appendix E, we introduced the coordinates $r_n'=r_n^{(1)}, n=1,\ldots,N$ on the first level of the recursion. They are the moduli squared of the coordinates on the unit sphere in the complex N dimensional space. Thus, it is natural to use the following type of hyper spherical coordinates

$$\begin{aligned}\sqrt{r_n'}&=\cos\vartheta_n\prod_{\nu=1}^{n-1}\sin\vartheta_\nu,\quad n=1,\ldots,(N-1),\\ \sqrt{r_N'}&=\sin\vartheta_{N-1}\prod_{\nu=1}^{N-2}\sin\vartheta_\nu,\end{aligned}\tag{F1}$$

where the positive semidefiniteness of the r_n' restricts the domain of integration to $0\leqslant\vartheta_n<\pi/2$, $n=1,\ldots,(N-1)$. Thus, we integrate over a (2^N)th segment of the unit sphere. The measure

$$\mathrm{d}\mu(r')=\prod_{n=1}^{N-1}\sin^{2(N-n)-1}\vartheta_n\cos\vartheta_n\,\mathrm{d}\vartheta_n\tag{F2}$$

is, apart from the phase angles, the measure on the unit sphere. Collecting everything, we have

$$\begin{aligned}1=\int\mathrm{d}\mu(x',x)&=G_N^{(\beta)}\int\left(\prod_{n=1}^{N}\sqrt{r_n'}\right)^{\beta-2}\mathrm{d}\mu(r')\\&=G_N^{(\beta)}\prod_{n=1}^{N-1}\int_0^{\pi/2}\sin^{(N-n)\beta-1}\vartheta_n\cos^{\beta-1}\vartheta_n\,\mathrm{d}\vartheta_n\\&=G_N^{(\beta)}\prod_{n=1}^{N-1}\frac{\Gamma((N-n)\beta/2)\Gamma(\beta/2)}{2\Gamma((N-n+1)\beta/2)}=G_N^{(\beta)}\frac{\Gamma^N(\beta/2)}{2^{N-1}\Gamma(N\beta/2)},\end{aligned}\tag{F3}$$

where the integral over ϑ_n is just Euler's integral of the first kind.

APPENDIX G: TRANSLATION INVARIANCE OF $W_{N,\omega}^{(\beta)}(x,k)$

We shift every x_n in the the recursion formula (5.5) for arbitrary β by a constant $\overline{x}$ and obtain

$$\Phi_N^{(\beta)}(x+\overline{x},k)=\int\mathrm{d}\mu(x',x+\overline{x})\exp\left(i\left(\sum_{n=1}^{N}x+N\overline{x}-\sum_{n=1}^{N-1}x'\right)k_N\right)\Phi_{N-1}^{(\beta)}(x',\tilde{k})\tag{G1}$$

with $x_n+\overline{x}\leqslant x_n'\leqslant x_{n+1}+\overline{x}$ as the domains of integration. The change of variables $x_n'\to x_n'+\overline{x}$ removes $\overline{x}$ from the measure given in Eq. (5.6) and the domains of integration, we find

$$\Phi_N^{(\beta)}(x+\overline{x},k)=\exp(i\overline{x}k_N)\int\mathrm{d}\mu(x',x)\exp\left(i\left(\sum_{n=1}^{N}x-\sum_{n=1}^{N-1}x'\right)k_N\right)\Phi_{N-1}^{(\beta)}(x'+\overline{x},\tilde{k}).\tag{G2}$$

We want to employ an induction. We assume that the radial functions for arbitrary β have the property

$$\Phi_N^{(\beta)}(x+\overline{x},k)=\exp\left(i\overline{x}\sum_{n=1}^{N}k_n\right)\Phi_N^{(\beta)}(x,k).\tag{G3}$$

If this is correct for $N-1$, formula (G2) implies that it is also true for N. The induction starts with $N=2$ where the correctness of Eq. (G3) is immediately obvious from the explicit solution (3.21) for arbitrary β. Thus, Eq. (G3) is valid for all N.

Since the k_n are arbitrary and since the sum over all k_n is invariant under the permutations $\omega(k)$, the property (G3) must also be true for every function $\Phi^{(\beta)}_{N,\omega}(x,k)$ with $\omega \in S_N$. We compare this with

$$\Phi^{(\beta)}_{N,\omega}(x+\overline{x},k)=\exp\left(i\overline{x}\sum_{n=1}^{N} k_n \right)\frac{\exp(i\Sigma_{n=1}^{N}x_n k_{\omega(n)})}{|\Delta_N(x)\Delta_N(k)|^{\beta/2}}\, W^{(\beta)}_{N,\omega}(x+\overline{x},k), \tag{G4}$$

which results from the Hankel ansatz (5.10). Hence, we conclude that we necessarily have

$$W^{(\beta)}_{N,\omega}(x+\overline{x},k)=W^{(\beta)}_{N,\omega}(x,k). \tag{G5}$$

This is the translation invariance.

APPENDIX H: CALCULATION OF $\Phi^{(4)}_4(x,k)$

We perform the calculation for $\Phi^{(4)}_4(-ix,k)$ to avoid inconvenient factors of i. The operator $L_{x,\omega(k)}$ defined in Eq. (5.13) splits into two parts. The first part

$$\tilde{\Delta}_{x,\omega(k)}=\sum_{n=1}^{N}\frac{\partial^2}{\partial x_n^2}-4\sum_{n<m}\frac{1}{(x_n-x_m)^2} \tag{H1}$$

does not change the order in k, while the second one,

$$\Lambda_{x,\omega(k)}=2\sum_{n=1}^{N} k_{\omega(n)}\frac{\partial}{\partial x_n}, \tag{H2}$$

raises the order in k by one. Since we can restrict ourselves to one element of the permutation group, we discuss only the identity permutation in the sequel. The symmetry of x and k together with the result for $\Phi^{(4)}_3(x,k)$ suggests that one try an expansion in the composite variable z_{ij} as defined in Eq. (6.8). To this end we define the elementary symmetric functions

$$e_\nu(z)=\sum_{i_1j_1<i_2j_2<\cdots<i_\nu j_\nu}\prod_{l=1}^{\nu} z_{i_lj_l}. \tag{H3}$$

Here, we assume the following ordering of the composite index $\{i_lj_l\}$, $i_l<j_l$. We say $\{i_lj_l\}<\{i_mj_m\}$ if $i_l<i_m$ or $i_l=i_m$ and $j_l<j_m$. All indices run to N. The highest order elementary symmetric function is of order $N(N-1)/2$ and is given by $\Delta_N(x)\Delta_N(k)$. The asymptotic formula (5.14) yields the leading term for large arguments. It is the starting point for a recursion in powers of z^{-1},

$$W^{(4)}_N(z)=\sum_{\nu=0}^{N(N-1)/2} p_\nu(z^{-1}), \tag{H4}$$

where $p_\nu(z)$ is a symmetric function of order ν in x_i and k_i. We investigate the action of the two operators defined in Eqs. (H1) and (H2) and find

$$\Lambda_{x,k}e_\nu(z^{-1})=-2\sum_{n<m}^{N}\frac{1}{(x_n-x_m)^2}e_{\nu-1}(z^{-1}_{\neq nm}), \tag{H5}$$

$$\tilde{\Delta}_{x,k} e_\nu(z^{-1}) = -4 \sum_{n<m}^{N} \frac{1}{(x_n - x_m)^2} e_\nu(z^{-1}_{\neq nm}) - 2 \sum_{\substack{n<m \\ k\neq n \\ k\neq m}}^{N} \frac{1}{(x_n - x_m)^2} z_{nk}^{-1} z_{mk}^{-1} e_{\nu-2}(z^{-1}_{\substack{\neq nm \\ \neq nk \\ \neq mk}}). \quad \text{(H6)}$$

The function $e_\nu(z_{\neq nm})$ is the elementary symmetric function $e_\nu(z)$ with all terms containing z_{nm} omitted. For $\nu = 0,1,2$ we simply have $p_\nu(z^{-1}) = (-2)^\nu e_\nu(z^{-1})$. For $\nu \geqslant 3$ the last term in Eq. (H5) causes corrections to the elementary symmetric functions. This arises due to the mixed derivatives which have to be taken into account in the action of $\tilde{\Delta}_{x,k}$ onto $e_\nu(z^{-1})$ for $\nu \geqslant 3$. Because of this term the Hankel ansatz becomes increasingly cumbersome as higher values of N are considered. More and more correction terms have to be constructed. So far, the construction was only possible for $N=4$. To construct the correction terms explicitly for the case $N=4$, we define a new set of symmetric functions as follows:

$$f_\nu(z^{-1}) = \sum_{k<l<m}^{N} z_{kl}^{-1} z_{km}^{-1} z_{lm}^{-1} e_{\nu-3}(z^{-1}_{\substack{\neq kl \\ \neq km \\ \neq lm}}). \quad \text{(H7)}$$

Again we have to investigate the action of $\Lambda_{x,k}$ and $\tilde{\Delta}_{x,k}$ on $f_\nu(z^{-1})$. We find

$$\tilde{\Delta}_{x,k} f_3(z^{-1}) = -4 \sum_{n<m}^{N} \frac{1}{(x_n - x_m)^2} f_3(z^{-1}_{\neq nm}) \quad \text{(H8)}$$

and

$$\Lambda_{x,k} f_3(z^{-1}) = -2 \sum_{\substack{n<m \\ k\neq n \\ k\neq m}}^{N} \frac{1}{(x_n - x_m)^2} z_{nk}^{-1} z_{mk}^{-1}, \quad \text{(H9)}$$

thus $f_3(z^{-1})$ is the desired correction term. We have

$$p_3(z^{-1}) = -2^3 (e_3(z^{-1}) + \tfrac{1}{2} f_3(z^{-1})). \quad \text{(H10)}$$

Fortunately, due to Eq. (H8) in the next step the correction term itself does not have to be corrected and we find

$$p_4(z^{-1}) = 2^4 (e_4(z^{-1}) + \tfrac{1}{2} f_4(z^{-1})). \quad \text{(H11)}$$

Up to now these results are valid for arbitrary N. The action of $\tilde{\Delta}_{x,k}$ onto the symmetric function $f_4(z^{-1})$ is not as simple as Eq. (H8). After a series of manipulations we arrive at

$$\tilde{\Delta}_{x,k} f_4(z^{-1}) = -4 \sum_{n<m}^{N} \frac{1}{(x_n - x_m)^2} f_4(z^{-1}_{\neq nm}) \quad \text{(H12)}$$

$$-2 \sum_{\substack{n<m \\ k\neq n \\ k\neq m}}^{N} \frac{1}{(x_n - x_m)^2} z_{nk}^{-1} z_{mk}^{-1} f_2(z^{-1}_{\substack{\neq nm \\ \neq nk \\ \neq mk}}). \quad \text{(H13)}$$

The contribution (H6) has to be added to this expression stemming from the action of $\tilde{\Delta}_{x,k}$ onto $e_4(z^{-1})$. On the other hand we calculate

$$\Lambda_{x,k} f_5(z^{-1}) = -2 \sum_{n<m}^{N} \frac{1}{(x_n - x_m)^2} f_4(z^{-1}_{\neq nm}) \tag{H14}$$

$$-2 \sum_{\substack{n<m \\ k\neq n \\ k\neq m}}^{N} \frac{1}{(x_n - x_m)^2} z_{nk}^{-1} z_{mk}^{-1} e_2(z^{-1}_{\substack{\neq nm \\ \neq nk \\ \neq mk}}). \tag{H15}$$

Thus, we have to find yet another correction term to compensate the second term in Eq. (H13). We define

$$f_5'(z^{-1}) = \sum_{i_1<i_2<i_3<i_4} \prod_{r<j} z^{-1}_{i_r i_j} \sum_{r<j} z_{i_r i_j} = \sum_{\substack{j<k \\ l<m}} z_{jl}^{-1} z_{jm}^{-1} z_{kl}^{-1} z_{km}^{-1} z_{lm}^{-1} \tag{H16}$$

and see that $\Lambda_{x,k} f_5'(z^{-1})$ yields exactly the desired second term of Eq. (H13). Pushing forward this procedure becomes more complicated step by step. There seems to be no obvious way of constructing the additional terms. Apparently for higher orders the correction terms also involve an increasing amount of indices. Nevertheless for $N=4$ we are already at the end of the procedure. Then the general expression

$$p_5(z^{-1}) = -2^5 (e_5(z^{-1}) + \tfrac{1}{2} f_5(z^{-1}) + \tfrac{1}{4} f_5'(z^{-1})) \tag{H17}$$

reduces to

$$p_5(z^{-1}) = -72 e_5(z^{-1}). \tag{H18}$$

The last step can readily be done, since the action of $\tilde{\Delta}_{x,k}$ onto $e_5(z^{-1})$ is already known by Eq. (H6). Thus we arrive at

$$p_6(z^{-1}) = 288 e_6(z^{-1}). \tag{H19}$$

Importantly, we have

$$\tilde{\Delta}_{x,k} e_6(z^{-1}) = \tilde{\Delta}_{x,k} \frac{1}{\Delta_4(x)\Delta_4(k)} = 0. \tag{H20}$$

That means, the sequence finishes after the sixth step. Collecting everything and observing that, for $N=4$, $f_5(z) = 2e_5(z)$ and $f_6(z) = 4e_6(z)$, we obtain

$$W_4^{(4)}(x,k) = \sum_{\nu=1}^{6} (-2)^{\nu} e_\nu(z^{-1}) + \sum_{\nu=3}^{6} (-2)^{\nu-1} f_\nu(z^{-1}) - 8e_5(z^{-1}) + 96 e_6(z^{-1}). \tag{H21}$$

This can be rewritten in a more compact way as

$$W_4^{(4)}(x,k) = \frac{1}{\Delta_4(x)\Delta_4(k)} \times \left(\prod_{i<j} (2 - z_{ij}) + 2^2 \sum_{l<m<n} \prod_{\substack{i<j \\ \neq lm \\ \neq ln \\ \neq mn}} (2 - z_{ij}) + 2^3 \sum_{\substack{l<m \\ k<n}} \prod_{\substack{i<j \\ \neq mk}} \prod_{\substack{\neq lk \\ \neq mn}} \prod_{\substack{\neq ln \\ \neq kn}} (2 - z_{ij}) \right), \tag{H22}$$

which yields Eq. (6.10).

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Recursive construction for a class of radial functions. II. Superspace

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We extend the recursion formula for matrix Bessel functions, which we obtained previously, to superspace. It is sufficient to do this for the unitary orthosymplectic supergroup. By direct computations, we show that fairly explicit results can be obtained, at least up to dimension 8×8 for the supermatrices. Since we introduce a new technique, we discuss various of its aspects in some detail. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1463218]

I. INTRODUCTION

In a previous work, we studied properties of matrix Bessel functions in ordinary space.[1] Here, we generalize these investigations to superspace. For the introductory remarks and the mathematical and physical background relevant for the ordinary space, and also relevant as the basis for the present study, we refer the reader to Ref. 1.

In mathematics, supersymmetry was pioneered by Berezin[2] and, in particular group theoretical aspects, by Kac.[3,4] The theory of nonlinear σ models in spaces of supermatrix fields was developed in physics of disordered systems by Efetov.[5,6] Verbaarschot, Weidenmüller, and Zirnbauer[7,8] used his approach to study models in random matrix theory. In Ref. 9, the first supersymmetric generalization of the Itzykson–Zuber integral[10] was given. In Ref. 11, Gelfand–Tzetlin coordinates[12] were constructed for the unitary supergroup. Extending Shatashvili's[13] method, the supersymmetric Itzykson–Zuber integral was also rederived in Ref. 11 in its most general form. Using the techniques of Ref. 9, such a calculation was also performed in Ref. 14.

From a mathematical viewpoint, Efetov's work[5] is the basis for a harmonic analysis in certain supersymmetric coset spaces, the Efetov spaces, which are relevant for the nonlinear σ models. In the full superspaces, a technique involving convolution integrals and ingredients of the corresponding harmonic analysis was introduced in Ref. 15. In the Efetov spaces, the theory of harmonic analysis, in both its mathematical and physical aspects, was developed by Zirnbauer[16] and was applied to disordered systems in Refs. 17 and 18. In the present contribution, we do not focus on the Efetov spaces, rather we address the full supergroup spaces. The supersymmetric Itzykson–Zuber integral[9] and its application in Ref. 15 is the simplest example of a supermatrix Bessel function appearing in this kind of harmonic analysis.

The matrix Bessel functions in superspace find direct application in random matrix theory. For general reviews, see Refs. 19–21. In Ref. 22 it was shown that they are the kernels for the supersymmetric analog of Dyson's Brownian motion.

The paper is organized as follows: In Sec. II, we introduce the supermatrix Bessel functions and collect basic definitions and notations. In Sec. III, we extend the recursion formula of Ref. 1 to superspaces. Since it is one of our goals to demonstrate that explicit results for supermatrix

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Bessel functions can indeed be obtained, we present, in some detail, such calculations for certain supermatrix Bessel functions in Secs. IV and V, respectively. The asymptotics and the normalization are discussed in Sec. VI. We briefly comment on applications in Sec. VII and we summarize and conclude in Sec. VIII. Various calculations are shifted to the appendices.

II. SUPERMATRIX BESSEL FUNCTIONS

Similar to ordinary spaces,[1] the superunitary case, i.e., integration over the supergroup $\mathrm{U}(k_1/k_2)$, is the simplest one. Since this was already discussed in detail in Refs. 9, 11, and 22, we refrain from reconsidering it here. Thus, it turns out that we may restrict ourselves to the supermatrix Bessel function of the unitary orthosymplectic group $\mathrm{UOSp}(k_1/2k_2)$. As discussed by Kac,[3,4] the supergroups $\mathrm{U}(k_1/k_2)$ and $\mathrm{UOSp}(k_1/2k_2)$ exhaust almost all classical compact supergroups, apart from some exotic exceptions which are of little relevance for applications. Hence, the integral we have to deal with is given by

$$\Phi_{k_1 2k_2}(s,r)=\int_{u\in \mathrm{UOSp}(k_1/2k_2)} \exp(i\,\mathrm{trg}\,u^{-1}sur)\mathrm{d}\mu(u), \tag{2.1}$$

where $\mathrm{d}\mu(u)$ is the invariant measure. The arguments of the function (2.1) are the diagonal matrices $s=\mathrm{diag}(\sqrt{c}s_1,\sqrt{-c}s_2)$ and $r=\mathrm{diag}(\sqrt{c}r_1,\sqrt{-c}r_2)$. Here, we use Wegner's notation[23] and introduce the label $c=\pm 1$ to distinguish the two possible forms. We will return to this issue. The matrices s_1, s_2 and r_1, r_2 are given by

$$\begin{aligned} s_1&=\mathrm{diag}(s_{11},s_{21},\ldots,s_{k_1 1}), \quad s_2=\mathrm{diag}(s_{12}1_2,\ldots,s_{k_2 2}1_2),\\ r_1&=\mathrm{diag}(r_{11},r_{21},\ldots,r_{k_1 1}), \quad r_2=\mathrm{diag}(r_{12}1_2,\ldots,r_{k_2 2}1_2). \end{aligned} \tag{2.2}$$

There is a twofold degeneracy in s_2 and r_2, because the matrix $u^{-1}su$ or, equivalently, uru^{-1} has to be a *real Hermitian* supermatrix[23] of the form

$$\sigma=\begin{bmatrix} \sqrt{c}\sigma^{(R)} & \sigma^{(A)\dagger} \\ \sigma^{(A)} & \sqrt{-c}\sigma^{(HSd)} \end{bmatrix}, \quad c=\pm 1. \tag{2.3}$$

The matrices $\sigma^{(R)}$ and $\sigma^{(HSd)}$ have ordinary commuting entries, i.e., bosons, they are real symmetric and Hermitian self-dual, respectively. The matrix $\sigma^{(A)}$ has anticommuting or Grassmann entries, i.e., fermions, and is of the form

$$\sigma^{(A)}=[\sigma_1^{(A)},\ldots,\sigma_{k_1}^{(A)}], \quad \sigma_i^{(A)}=\begin{bmatrix} \sigma_{1i}^{(A)} \\ \sigma_{1i}^{(A)*} \\ \vdots \\ \sigma_{k_2 i}^{(A)} \\ \sigma_{k_2 i}^{(A)*} \end{bmatrix}. \tag{2.4}$$

We can now appreciate the meaning of the parameter c which enters the definition (2.3) of the real Hermitian matrices. For $c=1$, it yields the real symmetric and for $c=-1$ the Hermitian self-dual matrix as boson–boson block, and vice versa for the fermion–fermion block. In the framework of random matrix theory, we find the supermatrices corresponding to the Gaussian orthogonal ensemble (GOE) for $c=+1$ and those for the Gaussian symplectic ensemble (GSE) for $c=-1$.

The infinitesimal volume element is given by

$$\mathrm{d}[\sigma]=\prod_{i=1}^{k_1}\prod_{j=1}^{k_2}\mathrm{d}\sigma_{ij}^{(A)*}\mathrm{d}\sigma_{ij}^{(A)}\prod_{i<j}\mathrm{d}\sigma_{ij}^{(R)}\prod_{i=1}^{k_1}\mathrm{d}\sigma_{ii}^{(R)}\prod_{i<j}\mathrm{d}[\sigma_{ij}^{(HSd)}]\prod_{i=1}^{k_2}\mathrm{d}\sigma_{ii}^{(HSd)}, \tag{2.5}$$

where $d[\sigma_{ij}^{(HSd)}]$ is the product of the differentials of all independent elements of the quaternion $\sigma_{ij}^{(HSd)}$.

The supermatrix Bessel functions (2.1) are eigenfunctions of a wave equation in the curved space of the eigenvalues s or r. As in the ordinary case, a supermatrix gradient $\partial/\partial\sigma$ is introduced and the Laplace operator is defined by

$$\Delta = \mathrm{trg}\left(\frac{\partial}{\partial\sigma}\right)^2. \tag{2.6}$$

The plane waves $\exp(i\,\mathrm{trg}\,\sigma\rho)$ are the eigenfunctions, i.e., we have

$$\Delta\,\exp(i\,\mathrm{trg}\,\sigma\rho) = -\,\mathrm{trg}\,\rho^2\exp(i\,\mathrm{trg}\,\sigma\rho). \tag{2.7}$$

Here, both σ and ρ are real Hermitian. As in ordinary space, the supermatrix Bessel functions are obtained by averaging over the angular coordinates, i.e., over the diagonalizing group. The Laplacian commutes with the average and we arrive at the differential equation

$$\Delta_s\Phi_{k_1 2k_2}(s,r) = -\,\mathrm{trg}\,r^2\Phi_{k_1 2k_2}(s,r), \tag{2.8}$$

where the radial part of of the Laplacian (2.6) reads

$$\Delta_s = \frac{1}{\tilde{B}^{(c)}_{k_1k_2}(s)}\left(\sum_{p=1}^{k_1}\frac{\partial}{\partial s_{p1}}\tilde{B}^{(c)}_{k_1k_2}(s)\frac{\partial}{\partial s_{p1}} + \frac{1}{2}\sum_{p=1}^{k_2}\frac{\partial}{\partial s_{p2}}\tilde{B}^{(c)}_{k_1k_2}(s)\frac{\partial}{\partial s_{p2}}\right). \tag{2.9}$$

The Jacobian or Berezinian is given by[22]

$$\tilde{B}^{(1)}_{k_1k_2}(s) = \frac{|\Delta_{k_1}(s_1)|\Delta^4_{k_2}(is_2)}{\Pi_{p=1}^{k_1}\Pi_{q=1}^{k_2}(s_{p1}-is_{q2})^2}, \quad \tilde{B}^{(-1)}_{k_1k_2}(s) = \frac{|\Delta_{k_1}(is_1)|\Delta^4_{k_2}(s_2)}{\Pi_{p=1}^{k_1}\Pi_{q=1}^{k_2}(is_{p1}-s_{q2})^2}. \tag{2.10}$$

One easily convinces oneself that Δ_s depends on c only through a factor $\sqrt{c}$. Thus, without loss of generality, we set $c=1$ and omit the index c.

At this point, an important comment is in order. The normalization in ordinary space according to Eq. (3.17) in Ref. 1, $\Phi_N^{(\beta)}(x,0)=1$ and $\Phi_N^{(\beta)}(0,k)=1$, does not carry over to the supersymmetric case. This is due to the fact that the volume of some supergroups is zero[2] resulting in the vanishing of $\Phi_{k_1 2k_2}(0,s)$ for certain values of k_1 and k_2. This collides with the normalization of the plane waves (2.7) to unity at the origin. The reason for this contradiction is a well-known phenomenon in superanalysis. In going from Cartesian to angle eigenvalue coordinates, one has to add additional terms to the measure to preserve the symmetries of the original integral. These are called Efetov–Wegner–Parisi–Sourlas terms in the physics literature. A full-fledged mathematical theory of these boundary terms was given by Rothstein.[24]

To solve this normalization problem, we use the following strategy. First, we evaluate the supermatrix Bessel functions without taking care of the normalization. We just multiply the integrals with a normalization constant $\hat{G}_{k_1 2k_2}$. Having done the integrals, we determine the normalization by comparing the asymptotics of the supermatrix Bessel function for large arguments with the Gaussian integral.

III. SUPERSYMMETRIC RECURSION FORMULA

We extend the recursion formula in ordinary space[1] to superspace. After stating the result in Sec. III A, we present the derivation and the calculation of the invariant measure in Secs. III B and III C, respectively.

A. Statement of the result

Let $\Phi_{k_1 2 k_2}(s,r)$ be defined through the group integral in Eq. (2.1). It has two diagonal matrices defined as in Eq. (2.2) as arguments. It can be calculated iteratively by the *recursion formula*

$$\Phi_{k_1 2 k_2}(s,r) = \hat{G}_{k_1 2 k_2} \int \mathrm{d}\mu(s',s)\, \exp(i(\mathrm{trg}\, s - \mathrm{trg}\, s')r_{11}) \Phi_{(k_1-1)2k_2}(s',\tilde{r}), \tag{3.1}$$

where $\Phi_{(k_1-1)2k_2}(s',\tilde{r})$ is the group integral (2.1) over $\mathrm{UOSp}((k_1-1)/2k_2))$ and $\hat{G}_{k_1 2 k_2}$ is a normalization constant, see Secs. II and VI. As in the ordinary case,[1] the coordinates s' are *radial* Gelfand–Tzetlin coordinates. Again, they are different from the *angular* Gelfand–Tzetlin coordinates, which will be discussed elsewhere.[25] We also introduced the diagonal matrix

$$\tilde{r} = \mathrm{diag}(r_{21},\ldots,r_{k_1 1}, i r_2) = \mathrm{diag}(\tilde{r}_1, i\tilde{r}_2) \tag{3.2}$$

such that $r = \mathrm{diag}(r_{11},\tilde{r})$ and the diagonal matrix

$$s' = \mathrm{diag}(s'_{11},\ldots,s'_{(k_1-1)1}, i s'_2) = \mathrm{diag}(s'_1, i s'_2). \tag{3.3}$$

The invariant measure reads

$$\begin{aligned}
\mathrm{d}\mu(s',s) &= 2^{k_2+1} \mu_B(s'_1,s_1)\mu_F(s'_2,s_2)\mu_{BF}(s',s)\mathrm{d}[\xi']\mathrm{d}[s'_1], \\
\mu_B(s'_1,s_1) &= \frac{\Delta_{k_1}(s'_1)}{\sqrt{-\prod_{p=1}^{k_1}\prod_{q=1}^{k_1-1}(s_{p1}-s'_{q1})}}, \\
\mu_F(s'_2,s_2) &= \frac{\Delta^4_{k_2}(i s'_2)}{\prod_{p=1}^{k_2}\prod_{q=1}^{k_2}(i s_{p2} - i s'_{q2})^2}, \\
\mu_{BF}(s',s) &= \frac{\prod_{p=1}^{k_1}\prod_{l=1}^{k_2}\prod_{q=1}^{k_1-1}(i s'_{l2}-s_{p1})(i s_{l2}-s'_{q1})}{\prod_{p=1}^{k_1-1}\prod_{l=1}^{k_2}(i s'_{l2}-s'_{p1})^2}.
\end{aligned} \tag{3.4}$$

Here, we have introduced

$$\mathrm{d}[\xi'] = \prod_{p=1}^{k_2} \mathrm{d}\xi'^*_p\, \mathrm{d}\xi'_p, \quad \mathrm{d}[s'_1] = \prod_{p=1}^{k_1-1} \mathrm{d}s'_{p1}. \tag{3.5}$$

The domain of integration for the bosonic variables is compact and given by

$$s_{p1} \leqslant s'_{p1} \leqslant s_{(p+1)1}, \quad p = 1,\ldots,(k_1-1). \tag{3.6}$$

The fermionic eigenvalues $i s'_{p2}$ are related to Grassmann variables ξ'_p and ξ'^*_p through

$$|\xi'_p|^2 = i s'_{p2} - i s_{p2}. \tag{3.7}$$

The Jacobian or Berezinian consists of three parts. One of them, $\mu_B(s'_1,s_1)$, depends only on bosonic eigenvalues and one, $\mu_F(s'_1,s_1)$, only on fermionic eigenvalues, i.e., only on Grassmann variables. The third part mixes commuting and anticommuting integration variables. To underline once more the difference between radial and angular Gelfand–Tzetlin coordinates which is also present in superspace, we mention that the radial measure (3.4) is quite different from the angular one.[25]

As in ordinary space, the recursion formula is an exact map of the group integration onto an iteration exclusively in the radial space. Having done the iteration on the first k_1 levels, we have treated all Grassmann variables. Thus, in the integrand, we are left with the matrix Bessel function $\Phi_{k_2}^{(4)}(-i2s_2^{(k_1-1)},r_2)$ for USp$(2k_2)$ in ordinary space.[1] We notice the occurrence of the factor $-i2$ in the argument of $\Phi_{k_2}^{(4)}(-i2s_2^{(k_1-1)},r_2)$. Collecting everything, we arrive at

$$\Phi_{k_1 2k_2}(s,r)=\int \prod_{n=1}^{k_1-1} \mathrm{d}\mu(s^{(n)},s^{(n-1)})\exp(i(\mathrm{trg}\, s^{(n-1)}-\mathrm{trg}\, s^{(n)})r_{n1}) \times \exp(is_{11}^{(k_1-1)}r_{k_1 1})\Phi_{k_2}^{(4)}(-i2s_2^{(k_1-1)},r_2). \tag{3.8}$$

We have set $s=s^{(0)}$ and $s'=s^{(1)}$. It is worthwhile to notice that the radial Gelfand–Tzetlin coordinates have a highly appreciated and valuable property: The Grassmann variables only appear as moduli squared in the integrand. Thus, the number of integrals over anticommuting variables is only *half* the number of the independent Grassmann variables. Moreover, advantageously, the exponential is a simple function of the integration variables. Thus, we may conclude that the radial Gelfand–Tzetlin coordinates are the natural coordinates of the matrix and the supermatrix Bessel functions, because their intrinsic features are reflected.

B. Derivation

All crucial steps needed for the derivation of the supersymmetric recursion formula (3.1) carry over from the ordinary recursion formula in Ref. 1. We order the columns of the matrix $u \in \mathrm{UOSp}(k_1/2k_2)$ in the form $u=[u_1 u_2 \cdots u_{k_1} u_{k_1+1}\cdots u_{k_1+k_2}]$. We also introduce a rectangular matrix $b=[u_2\cdots u_{k_1} u_{k_1+1}\cdots u_{k_1+k_2}]$ such that $u=[u_1 b]$. Analogous to the ordinary case, we have

$$\begin{aligned} b^\dagger b &= 1_{(k_1-1)2k_2}, \\ bb^\dagger &= \sum_{p=2}^{k_1} u_p u_p^\dagger + \sum_{p=k_1+1}^{k_1+k_2} u_p u_p^\dagger = 1_{k_1 2k_2} - u_1 u_1^\dagger . \end{aligned} \tag{3.9}$$

We define the square matrix $\tilde{\sigma}=b^\dagger s b$ and rewrite the trace in the exponent as

$$\mathrm{trg}\, u^\dagger s u r = \mathrm{trg}\, \tilde{\sigma}\tilde{r} + \sigma_{11} r_{11}, \tag{3.10}$$

with $\sigma_{11}=u_1^\dagger s u_1$. Similar to the ordinary case, the first term on the right-hand side of Eq. (3.10) depends on the last k_1-1+k_2 columns u_p collected in b and the second term depends only on u_1. Thus, it is useful to decompose the invariant measure,

$$\mathrm{d}\mu(u)=\mathrm{d}\mu(b)\mathrm{d}\mu(u_1), \tag{3.11}$$

and to write Eq. (2.1) in the form

$$\Phi_{k_1 2k_2}(s,r)=\int \mathrm{d}\mu(u_1)\exp(i\sigma_{11}r_{11})\int \mathrm{d}\mu(b)\exp(i\,\mathrm{trg}\,\tilde{\sigma}\tilde{r}). \tag{3.12}$$

Since the coordinates b are locally orthogonal to u_1, the measure $\mathrm{d}\mu(b)$ also depends on u_1.

We now generalize the radial Gelfand–Tzetlin coordinates introduced in Ref. 1 for the ordinary spaces to the superspace. Naturally, the projector reads $(1_{k_1 2k_2}-u_1 u_1^\dagger)$ and we have the defining equation

$$(1_{k_1 2k_2}-u_1 u_1^\dagger)s(1_{k_1 2k_2}-u_1 u_1^\dagger)e_p'=s_p' e_p', \quad p=1,\ldots,k_1-1,k_1+1,\ldots,k_1+k_2 \tag{3.13}$$

for the (k_1-1+k_2) radial Gelfand–Tzetlin coordinates s'_p and the corresponding vectors e'_p as eigenvalues and eigenvectors of the matrix $(1_{k_1 2k_2}-u_1u_1^\dagger)s(1_{k_1 2k_2}-u_1u_1^\dagger)$ which has the generalized rank k_1-1+k_2. Due to $u_1^\dagger e'_p=0$, we find

$$(1_{k_1 2k_2}-u_1u_1^\dagger)se'_p=s'_pe'_p, \quad p=1,\ldots,k_1-1,k_1+1,\ldots,k_2. \tag{3.14}$$

As in Ref. 11, the eigenvalues s'_p are calculated from the characteristic function

$$z(s'_p)=\mathrm{detg}((1_{k_1 2k_2}-u_1u_1^\dagger)s-s'_p)=-s'_p\,\mathrm{detg}(s-s'_p)u_1^\dagger\frac{1_{k_1 2k_2}}{s-s'_p}u_1, \tag{3.15}$$

which has to be discussed in the limits

$$z(s'_p)\to\begin{cases}0 & \text{for } p=1,\ldots,k_1-1\\ \infty & \text{for } p=k_1+1,\ldots,k_1+k_2.\end{cases} \tag{3.16}$$

Thus, together with the normalization $u_1^\dagger u_1=1$, these are k_1+k_2 equations for the elements of u_1.

The two parts of the integral (3.12) have to be expressed in terms of the radial Gelfand–Tzetlin coordinates s'_p. In a calculation fully analogous to the ordinary case, we find

$$\sigma_{11}=\mathrm{trg}\,s-\mathrm{trg}\,s'. \tag{3.17}$$

The eigenvalues t_p, $p=1,\ldots,k_1-1,k_1+1,\ldots,k_1+k_2$ of $\tilde{\sigma}$ obtain from the characteristic function

$$w(t_p)=\mathrm{detg}(\tilde{\sigma}-t_p)=-\frac{1}{t_p}\mathrm{detg}((1_{k_1 2k_2}-u_1u_1^\dagger)s-t_p). \tag{3.18}$$

Comparison with Eq. (3.15) shows that the characteristic functions $w(t_p)$ and $z(s'_p)$ are, apart from the nonzero factor $-t_p$, identical. This implies $t_p\equiv s'_p$, $p=1,\ldots,k_1-1,k_1+1,\ldots,k_1+k_2$. Thus, by introducing the square matrix $\tilde{u}$ which diagonalizes $\tilde{\sigma}$, we may write

$$\tilde{\sigma}=b^\dagger sb=\tilde{u}^\dagger s'\tilde{u}. \tag{3.19}$$

By construction, $\tilde{u}$ must be in the group $\mathrm{UOSp}(k_1-1/2k_2)$, because σ and $\tilde{\sigma}$ share the same symmetries.

These intermediate results allow us to transform Eq. (3.12) into

$$\Phi_{k_1 2k_2}(s,r)=\int \mathrm{d}\mu(s',s)\exp(i(\mathrm{trg}\,s-\mathrm{trg}\,s')r_{11})\int \mathrm{d}\mu(b)\exp(i\,\mathrm{trg}\,\tilde{u}^\dagger s'\tilde{u}\tilde{r}), \tag{3.20}$$

where $\mathrm{d}\mu(s',s)$ is, apart from phase angles, the invariant measure $\mathrm{d}\mu(u_1)$, expressed in the radial Gelfand–Tzetlin coordinates s'. To do the integration over b, we view, for the moment, the vector u_1 as fixed and observe that the measure $\mathrm{d}\mu(b)$ is the invariant measure of the group $\mathrm{UOSp}(k_1-1/2k_2)$ under the constraint that b is locally orthogonal to u_1. The matrix $\tilde{u}\in\mathrm{UOSp}(k_1-1/2k_2)$ is constructed from b under the same constraint. Thus, since b and $\tilde{u}$ cover the same manifold, the integral over b in Eq. (3.20) must yield the supermatrix Bessel function $\Phi_{(k_1-1)2k_2}(s',\tilde{r})$ and we arrive at the supersymmetric recursion formula (3.1). In the last step, we used a line of arguing slightly different from the derivation in ordinary space. In this way we avoided a discussion related to the ill-defined supergroup volume. The invariance of the measure is the crucial property we need for the proof and this holds both in superspace and in ordinary space.

C. Invariant measure

In order to evaluate the invariant measure, we have to solve the system of equations (3.15) for $|v_p^{(1)}|^2=|u_{p1}|^2$, $p=1,\ldots,k_1$ and $|\alpha_p^{(1)}|^2=|u_{(k_1+2p)1}|^2+|u_{(k_1+2p-1)1}|^2$, $p=1,\ldots,k_2$ in terms of the bosonic eigenvalues $s_p'=s_{p1}'$, $p=1,\ldots,k_1-1$ and the fermionic eigenvalues $s_{k_1+2p}'=s_{k_1+2p-1}'=is_{p2}'$, $p=1,\ldots,k_2$,

$$1=\sum_{p=1}^{k_1}|v_p^{(1)}|^2+\sum_{p=1}^{k_2}|\alpha_p^{(1)}|^2, \tag{3.21}$$

$$0=\sum_{q=1}^{k_1}\frac{|v_q^{(1)}|^2}{s_{q1}-s_{p1}'}+\sum_{q=1}^{k_2}\frac{|\alpha_q^{(1)}|^2}{is_{q2}-s_{p1}'},\quad p=1,\ldots,k_1-1, \tag{3.22}$$

$$z_p=is_{p2}'\frac{\Pi_{q=1}^{k_1}(s_{q1}-is_{p2}')}{\Pi_{q=1}^{k_2}(is_{q2}-is_{p2}')^2}\left(\sum_{q=1}^{k_1}\frac{|v_q^{(1)}|^2}{s_{q1}-is_{p2}'}+\sum_{q=1}^{k_2}\frac{|\alpha_q^{(1)}|^2}{is_{q2}-is_{p2}'}\right),\quad z_p\to\infty,\quad p=1,\ldots,k_2. \tag{3.23}$$

In Appendix A, we sketch the solution of this system for small dimensions. Inspired by these solutions one can conjecture the general solutions and verify them by plugging them directly into Eqs. (3.21)–(3.23); one finds

$$\begin{aligned}|v_p^{(1)}|^2&=\frac{\Pi_{q=1}^{k_1-1}(s_{p1}-s_{q1}')\Pi_{q=1}^{k_2}(s_{p1}-is_{q2})^2}{\Pi_{q=1}^{k_2}(s_{p1}-is_{q2}')^2\Pi_{q=1,q\neq p}^{k_1}(s_{p1}-s_{q1})},\quad p=1,\ldots,k_1,\\ |\alpha_p^{(1)}|^2&=2(is_{p2}'-is_{p2})\frac{\Pi_{q=1}^{k_1-1}(is_{p2}-s_{q1}')\Pi_{q=1,q\neq p}^{k_2}(is_{p2}-is_{q2})^2}{\Pi_{q=1,q\neq p}^{k_2}(is_{p2}-is_{q2}')^2\Pi_{q=1}^{k_1}(is_{p2}-s_{q1})},\quad p=1,\ldots,k_2.\end{aligned} \tag{3.24}$$

These expressions are reminiscent of the ones derived in Ref. 11 for unitary matrices. However, importantly, all products in (3.24) involving fermionic eigenvalues are squared. This reflects the degeneracy of s in the fermion–fermion block. We have introduced new anticommuting variables $\xi_p',\xi_p'^*$ with $|\xi_p'|^2=is_{p2}'-is_{p2}$ according to definition (3.7).

From this point on, the invariant measure can be calculated in the same way as for the angular Gelfand–Tzetlin coordinates, see Ref. 11 for details. The result is summarized in Eq. (3.4).

IV. THE FUNCTION $\Phi_{22}(s,r)$

We use the recursion formula (3.1) to calculate the supermatrix Bessel function for UOSp(2/2). To avoid the imaginary unit in the exponent, we study $\Phi_{22}(-is,r)$. The recursion formula reads

$$\Phi_{22}(-is,r)=\hat{G}_{22}\int \mathrm{d}\mu(s',s)\exp((\mathrm{trg}\,s-\mathrm{trg}\,s')r_{11})\Phi_{12}(-is',\tilde{r}). \tag{4.1}$$

The function $\Phi_{12}(-is',\tilde{r})$ is easily found to be

$$\Phi_{12}(-is',\tilde{r})=\hat{G}_{12}(1-2(r_{21}-ir_{12})(s_{11}'-is_{12}'))\exp(2r_{12}s_{12}). \tag{4.2}$$

The measure of the coset UOSp(2/2)/UOSp(1/2) is according to formula (3.4) given by

$$\mathrm{d}\mu(s',s)=\frac{(is_{12}-s_{11}')\Pi_{n=1}^{2}(is_{12}'-s_{n1})}{\sqrt{-\Pi_{n=1}^{2}(s_{11}'-s_{n1})}(is_{12}'-s_{11}')^2}\mathrm{d}s_{11}'\,\mathrm{d}\xi_1'^*\,\mathrm{d}\xi_1'. \tag{4.3}$$

We do the Grassmann integration and find

$$\Phi_{22}(-is,r)=\hat{G}_{22}\exp(r_{11}(s_{11}+s_{21})-2is_{12}ir_{12})$$
$$\times\int_{s_{11}}^{s_{21}}\mu_B(s',s)\prod_{q=1}^{2}(is_{12}-s_{q1})\Bigg(4\prod_{j=1}^{2}(ir_{12}-r_{j1})-2(ir_{12}-r_{11})$$
$$\times\sum_{q=1}^{2}\frac{1}{is_{12}-s_{q1}}+2M_{11}(s_1',s_1)\Bigg)\exp(s_{11}'(r_{21}-r_{11}))\mathrm{d}s_{11}', \tag{4.4}$$

where we have introduced the operator

$$M_{mj}(s_1',s_1)=\frac{1}{(is_{m2}-s_{j1}')}\left(\frac{1}{2}\sum_{n=1}^{k_1}\frac{1}{is_{m2}-s_{n1}}-\frac{1}{is_{m2}-s_{j1}'}-\sum_{\substack{n=1\\n\neq j}}^{k_1}\frac{1}{s_{j1}'-s_{n1}'}-\frac{\partial}{\partial s_{j1}'}\right). \tag{4.5}$$

For later purposes, we introduced general indices m and j. Obviously, the Grassmann integration yielded eigenvalues in the denominator. This is somewhat surprising because of the following observation: we can always parametrize the group element $u\in\mathrm{UOSp}(2/2)$ in a noncanonical coset parametrization in the spirit of an Euler parametrization in ordinary space. Inserting this parametrization into the defining equation of the supermatrix Bessel function (2.1) one can expand the trace in all Grassmann variables. The expansion coefficients are polynomials in the commuting integration variables and—more important—in the matrix elements of s and r. The invariant measure can be expanded in the Grassmann variables as well. It does not depend on r and s. Although this procedure gets rapidly out of hand even for small groups, it is clear that the outcome of this expansion will be polynomial in the eigenvalues of s and r. In other words: eigenvalues can only appear in the denominator by an integration over commuting variables and never by a Grassmann integration. Therefore, before performing any integral over commuting variables, there must exist a form of $\Phi_{22}(-is,r)$, which is polynomial in the eigenvalues of s and r.

To remove the denominators and to obtain such a polynomial expression, we use the following result. Let $f(s_1')$ be an analytic, symmetric function in s_{1i}', $i=1,\ldots,k_1$. Furthermore, define the operator

$$L_m(s)=\sum_{j=1}^{k_1}\frac{1}{is_{m2}-s_{j1}}\frac{\partial}{\partial s_{j1}}. \tag{4.6}$$

Then the action of the operator on the integral over the bosonic part of the measure is given by

$$L_m(s)\int_{s_{11}}^{s_{21}}\cdots\int_{s_{(k_1-1)1}}^{s_{k_11}}\mu_B(s',s)f(s_1')\mathrm{d}[s_1']$$
$$=-\int_{s_{11}}^{s_{21}}\cdots\int_{s_{(k_1-1)1}}^{s_{k_11}}\mu_B(s',s)\sum_{j=1}^{k_1-1}M_{mj}(s_1',s_1)f(s_1')\mathrm{d}[s_1']. \tag{4.7}$$

This formula is derived in Appendix B.

We now set $f(s_1')=\exp(-s_{11}'(r_{21}-r_{11}))$ and insert Eq. (4.7) into Eq. (4.4), we arrive at

$$\Phi_{22}(-is,r)=\hat{G}_{22}\exp(-2is_{12}ir_{12})\Bigg(4\prod_{j=1}^{2}(ir_{12}-r_{j1})(is_{12}-s_{j1})$$
$$-2\sum_{q=1}^{2}(is_{12}-s_{q1})\left(ir_{12}-r_{21}-r_{11}-\frac{\partial}{\partial s_{q1}}\right)\Bigg)\Phi_2^{(1)}(-is_1,r_1), \tag{4.8}$$

where $\Phi_2^{(1)}(s_1,r_1)$ is the matrix Bessel function of the orthogonal group O(2) in ordinary space as defined in Ref. 1. Although this can already be taken as the result, we underline the symmetry between s and r by using the explicit form (3.21) of Ref. 1 for $\Phi_2(s_1,r_1)$,

$$\Phi_{22}(-is,r)=\hat{G}_{22}\exp\left(\mathrm{trg}\,rs-\frac{z}{2}\right)$$
$$\times\left(4\prod_{j=1}^{2}(ir_{12}-r_{j1})(is_{12}-s_{j1})-\sum_{q=1}^{2}(is_{12}-s_{q1})\sum_{p=1}^{2}(ir_{12}-r_{p1})-z\frac{\mathrm{d}}{\mathrm{d}z}\right)2\pi I_0(z/2), \tag{4.9}$$

where we have introduced $z=(s_{11}-s_{21})(r_{11}-r_{21})$ and the modified Bessel function I_0 as defined in Ref. 26.

The result (4.7) was crucial in the derivation of $\Phi_{22}(-is,r)$. By means of this formula, the denominator problem was overcome in one step. Because of its importance, we want to gain more insight into this problem: In Appendix C, we rederive $\Phi_{22}(-is,r)$ in two other ways. It is clear that the methods of Appendix C cannot be used for higher dimensions k_1 and $2k_2$, but it will help to understand the mechanisms needed when working with radial Gelfand–Tzetlin coordinates.

V. THE SERIES OF FUNCTIONS $\Phi_{k_14}(s,r)$

We calculate iteratively the four supermatrix Bessel functions $\Phi_{k_14}(s,r)$ for $k_1=1,2,3,4$. We do this in Secs. V A–V D, respectively.

A. First level $k_1=1$

According to the recursion formulas (3.1) and (3.8), the starting point is the matrix Bessel function for the unitary symplectic group $\Phi_2^{(4)}(s_2,r_2)$, which was already calculated in Ref. 1. Up to a normalization, we have

$$\Phi_2^{(4)}(i2s_2,r_2)=\sum_{\omega\in S_2}\left(\frac{1}{\Delta_2^2(is_2)\Delta_2^2(\omega(ir_2))}-\frac{1}{\Delta_2^3(is_2)\Delta_2^3(\omega(ir_2))}\right)\exp(-\mathrm{tr}is_2\omega(ir_2)). \tag{5.1}$$

Since the subgroup O(1) of UOSp(1/4) is trivial, no commuting integral has to be performed to derive $\Phi_{14}(-is,r)$. Inserting the measure (3.4) into the recursion formula and performing the Grassmann integrations yields straightforwardly

$$\Phi_{14}(-is,r)=\hat{G}_{14}\exp(\mathrm{trg}\,rs)\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)(2(is_{21}-s_{11})(ir_{21}-r_{11})-1)$$
$$\times(2(is_{22}-s_{11})(ir_{22}-r_{11})-1)-\hat{G}_{14}\frac{\exp(\mathrm{trg}(rs))}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}+(ir_{12}\leftrightarrow ir_{22}). \tag{5.2}$$

The exchange term $(ir_{12}\leftrightarrow ir_{22})$ accounts for the permutation group S_2 in Eq. (5.1). Anticipating that the structure of $\Phi_{14}(-is,r)$ will, remarkably, survive on all levels up to $\Phi_{44}(-is,r)$, we state that $\Phi_{14}(-is,r)$ essentially consists of two parts. A comparison with Eqs. (4.2), and (5.1) shows that the first part of $\Phi_{14}(-is,r)$ is a product of an exponential with three other terms. The first one,

$$\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right), \tag{5.3}$$

stems from the integral over the USp(4) subgroup. The other two terms can be identified with the supermatrix Bessel functions

$$\Phi_{12}(-is,r) \quad \text{with} \quad s=\mathrm{diag}(s_{11},is_{12},is_{12}), \quad r=\mathrm{diag}(r_{11},ir_{12},ir_{12}) \tag{5.4}$$

and

$$\Phi_{12}(-is,r) \quad \text{with} \quad s=\mathrm{diag}(s_{11},is_{22},is_{22}), \quad r=\mathrm{diag}(r_{11},ir_{22},ir_{22}). \tag{5.5}$$

The second part can be considered as a correction term, which destroys the product structure of $\Phi_{14}(-is,r)$. We may identify the different parts of the product with the integrations over the corresponding subsets of the group. Thus, $\Phi_2^{(4)}(-is_2,r_2)$ arises from the integration over the USp(4) subgroup, the O(1) integration yields unity, and the other two factors come from the integration over the coset $\mathrm{UOSp}(1/4)/(\mathrm{USp}(4)\otimes\mathrm{O}(1))$.

B. Second level $k_1=2$

We now have to do one integration over a commuting variable. After the Grassmann integration, we are left with a considerable amount of terms. To arrange them in a convenient way, we introduce the following notation for the product of two operators $D_1(s)D_2(s)$ acting on a function $f(s)$, we define

$$[D_1^{\rightarrow}(s)D_2(s)]f(s)=D_1(s)D_2(s)f(s)-(D_1(s)D_2(s))f(s). \tag{5.6}$$

This means, an operator with an arrow only acts on the terms outside the squared bracket. With this notation we can write

$$\begin{aligned}
\Phi_{24}(-is,r)=\hat{G}_{24}\exp(\mathrm{tr}(r_2s_2)+r_{21}(s_{11}+s_{21}))\int_{s_{11}}^{s_{21}}\mathrm{d}\mu_B(s_1',s_1)\Bigg[&\prod_{i=1}^{2}\prod_{j=1}^{2}(is_{i2}-s_{j1})\\
&\times\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)\\
&\times\left(4\prod_{i=1}^{2}(ir_{12}-r_{i1})+2\sum_{k=1}^{2}\frac{r_{21}-ir_{12}}{is_{12}-s_{k1}}+2M_{11}(s_1',s_1)\right)\\
&\times\left(4\prod_{i=1}^{2}(ir_{22}-r_{i1})+2\sum_{k=1}^{2}\frac{r_{21}-ir_{22}}{is_{22}-s_{k1}}+2M_{21}(s_1',s_1)\right)\\
&+\left(\frac{1}{\Delta_2^2(ir_2)\Delta_3^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\right)\\
&\times\left(\frac{4}{is_{12}-s_{11}'}M_{21}(s_1',s_1)-\frac{2}{is_{22}-s_{11}'}M_{11}(s_1',s_1)\right)\\
&+\frac{2}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\left(2\,\mathrm{tr}\,r_1-\mathrm{tr}\,ir_2+\sum_{i=1}^{2}\frac{1}{is_{22}-s_{i1}}\right)M_{11}(s_1',s_1)\\
&-\frac{2}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\left(2\,\mathrm{tr}\,r_1-\mathrm{tr}\,ir_2+\sum_{i=1}^{2}\frac{1}{is_{12}-s_{i1}}\right)M_{21}(s_1',s_1)\\
&-\frac{4}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\sum_{k=1}^{2}\prod_{j=1}^{2}\frac{r_{21}-ir_{j2}}{s_{k1}-is_{j2}}\Bigg]\exp(s_{11}'(r_{11}-r_{21}))+(ir_{12}\leftrightarrow ir_{22}).
\end{aligned} \tag{5.7}$$

As in Sec. IV, a denominator problem occurs. It becomes obvious in the product $M_{11}^{\rightarrow}(s_1',s_1)M_{21}(s_1',s_1)$. Thus, we expect an identity similar to formula (4.7). This identity should map a product of operators $L_1(s)L_2(s)$ acting on the integral onto a product of operators

$M_{11}(s_1',s_1)M_{21}(s_1',s_1)$ acting under the integral. Neither the outer operators, $L_m(s)$, nor the inner ones, $M_{mj}(s)$, commute. Hence, the desired identity must be a nontrivial one. It is given by the following result.

We have the same conditions as in formula (4.7), furthermore we define

$$[L_m^{\rightarrow}(s)L_l(s)]=\sum_{n=1}^{k_1}\sum_{q=1}^{k_1}\frac{1}{(is_{m2}-s_{n1})(is_{l2}-s_{q1})}\frac{\partial^2}{\partial s_{n1}\partial s_{q1}}. \tag{5.8}$$

Then the following formula holds

$$\begin{aligned}
&[L_m^{\rightarrow}(s)L_l(s)]\int_{s_{11}}^{s_{21}}\cdots\int_{s_{(k_1-1)1}}^{s_{k_1 1}}\mu_B(s',s)\,\mathrm{d}[s_1']\,f(s_1')\\
&\quad=\int_{s_{11}}^{s_{21}}\cdots\int_{s_{(k_1-1)1}}^{s_{k_1 1}}\mu_B(s',s)\Bigg[\sum_{j=1}^{k_1-1}\sum_{k=1}^{k_1-1}M_{mj}(s_1',s_1)M_{lk}(s_1',s_1)\\
&\qquad-\frac{1}{is_{l2}-is_{m2}}\sum_{j=1}^{k_1-1}\left(\frac{1}{is_{m2}-s_{j1}'}M_{lj}(s_1',s_1)-\frac{1}{is_{l2}-s_{j1}'}M_{mj}(s_1',s_1)\right)\\
&\qquad-\frac{1}{2}\sum_{k\neq j}^{k_1-1}\frac{1}{(is_{m2}-s_{k1}')(is_{m2}-s_{j1}')(is_{l2}-s_{k1}')(is_{l2}-s_{j1}')}\Bigg]f(s_1')\,\mathrm{d}[s_1'].
\end{aligned}\tag{5.9}$$

The derivation is along the same lines as the one for formula (4.7), it also involves formula (4.7). With the identities (5.9) and (4.7) the denominator problem is again solved in one step. After some further manipulations we arrive at

$$\begin{aligned}
\Phi_{24}(-is,r)&=2\pi\hat{G}_{24}\exp\left(\mathrm{trg}\,rs-\frac{z}{2}\right)\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)\\
&\quad\times\Bigg[\left(4\prod_{i=1}^{2}(r_{i1}-ir_{12})(s_{i1}-is_{12})-\sum_{\substack{i=1\\j=1}}^{2}(s_{j1}-is_{12})(r_{i1}-ir_{12})-z\frac{\partial^{\rightarrow}}{\partial z}\right)\\
&\quad\times\left(4\prod_{i=1}^{2}(r_{i1}-ir_{22})(s_{i1}-is_{22})-\sum_{\substack{i=1\\j=1}}^{2}(s_{j1}-is_{22})(r_{i1}-ir_{22})-z\frac{\partial}{\partial z}\right)\Bigg]I_0(z/2)\\
&\quad-2\pi\hat{G}_{24}\exp\left(\mathrm{trg}\,rs-\frac{z}{2}\right)\frac{2}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\\
&\quad\times\sum_{\substack{i=1\\k=1}}^{2}\prod_{j=1}^{2}(s_{i1}-is_{j2})(r_{k1}-ir_{j2})I_0(z/2)-2\pi\hat{G}_{24}\exp\left(\mathrm{trg}\,rs-\frac{z}{2}\right)\\
&\quad\times\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}((\mathrm{trg}\,s)(\mathrm{trg}\,r)-1)z\frac{\partial}{\partial z}I_0(z/2)+(ir_{12}\leftrightarrow ir_{22}).
\end{aligned}\tag{5.10}$$

As in Sec. IV, we used the composite variable $z=(s_{11}-s_{12})(r_{11}-r_{12})$. A comparison with Eqs. (4.8) and (5.2) shows the similarity in the structures of $\Phi_{24}(-is,r)$ and $\Phi_{14}(-is,r)$. The former also decomposes into two parts. The first part is a product, whose factors can be assigned to the integrations over the different submanifolds of the group in the same way as in the case of $\Phi_{14}(-is,r)$. The other one can be interpreted as a correction term due to the noncommutativity of the operators L_m in formula (5.9).

C. Third level $k_1=3$

This structure of $\Phi_{k_14}(-is,r)$ emerging in the previous calculations is likely to also be present for arbitrary k_1. However, for $k_1>2$, we have so far not been able to treat the general case. Fortunately, in important physics applications, one matrix argument of the supermatrix Bessel function has an additional twofold degeneracy in the boson–boson block. In this case, it is possible to carry on the recursion up to $\Phi_{44}(-is,r)$ by extending the techniques developed for $k_1=1$ and $k_2=2$. Thus, from now on, we restrict ourselves to this case.

At first sight, one might hope to achieve some simplification by applying the projection procedure onto the degenerate matrix, because this results in a considerable simplification of the invariant measure. However, it turned out that the integrations are easier if one does the recursion with the nondegenerate coordinates. Hence, we use the measure as it stands in Eq. (3.4). We consider $\Phi_{34}(-is,r)$ in the case that

$$r_1=\mathrm{diag}(r_{11},r_{21},r_{21}). \tag{5.11}$$

Having performed the Grassmann integral, one can arrange the terms in a way similar to Eq. (5.7). The complete expression and further details are given in Appendix D. We then can use formula (5.9) and find after some further algebra

$$\begin{aligned}
\Phi_{34}(-is,r)=4\ \hat{G}_{34}\exp(\mathrm{tr}\, r_2s_2)(r_{21}-ir_{12})(r_{21}-ir_{22})\Bigg[&\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)\\
&\times\Bigg(4\prod_{k=1}^{2}(r_{k1}-ir_{12})\prod_{k=1}^{3}(s_{k1}-is_{12})+2\sum_{k=1}^{3}\prod_{j\neq k}^{3}(s_{j1}-is_{12})\\
&\times\left(r_{11}+r_{21}-ir_{12}-\frac{\partial^{\rightarrow}}{\partial s_{k1}}\right)\Bigg)\\
&\times\Bigg(4\prod_{k=1}^{2}(r_{k1}-ir_{22})\prod_{k=1}^{3}(s_{k1}-is_{22})+2\sum_{k=1}^{3}\prod_{j\neq k}^{3}(s_{j1}-is_{22})\\
&\times\left(r_{11}+r_{21}-ir_{22}-\frac{\partial}{\partial s_{k1}}\right)\Bigg)-\frac{4}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\sum_{i=1}^{3}\prod_{\substack{j=1\\j\neq i}}^{3}(s_{j1}-is_{12})(s_{j1}-is_{22})\\
&\times\Bigg(r_{11}^2+r_{21}^2+r_{11}r_{21}-(r_{11}+r_{21})(ir_{12}+ir_{22})+ir_{12}ir_{22}\\
&-(r_{11}+r_{21}-ir_{12}-ir_{22})\frac{\partial}{\partial s_{i1}}\Bigg)-\frac{2}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\\
&\times\sum_{i,k}^{3}\prod_{\substack{j=1\\j\neq i}}^{3}\prod_{\substack{l=1\\l\neq k}}^{3}(s_{j1}-is_{12})(s_{l1}-is_{22})\left(\frac{\partial}{\partial s_{i1}}-\frac{\partial}{\partial s_{k1}}\right)\Bigg]\\
&\times\Phi_3^{(1)}(-is_1,r_1),\quad +(ir_{12}\leftrightarrow ir_{22}),
\end{aligned}\tag{5.12}$$

where $\Phi_3^{(1)}(s_1,r_1)$ is the matrix Bessel function of the orthogonal group O(3). We notice that the structure of $\Phi_{14}(-is,r)$ and $\Phi_{24}(-is,r)$ reappears in $\Phi_{34}(-is,r)$.

D. Fourth level $k_1=4$

In the calculation of $\Phi_{44}(-is,r)$, we again consider the case that the matrix r is degenerate,

$$r_1=\mathrm{diag}(r_{11},r_{11},r_{21},r_{21}). \tag{5.13}$$

The main problem is to find a convenient representation for the matrix Bessel function $\Phi_3^{(1)}(-is_1',\tilde{r}_1)$ appearing on the third level in Eq. (5.12). It turns out that the representation derived in Appendix B of Ref. 1 is very well suited to our purpose. Due to the degeneracy in $\tilde{r}_1$, the original threefold integral can be reduced to an integral over just one single variable

$$\Phi_3^{(1)}(-is_1',\tilde{r}_1)=\frac{\exp(r_{21}\,\mathrm{tr}\,s_1')}{\sqrt{|r_{11}-r_{21}|}}\int_{-\infty}^{+\infty}\mathrm{d}t\,\frac{\exp(i(r_{11}-r_{21})t)}{\Pi_{i=1}^3\sqrt{s_{i1}'-it}}. \tag{5.14}$$

Here, we again neglected the normalization because we want to fix it afterwards as explained previously. Similarly, $\Phi_4^{(1)}(-is_1,r_1)$ can be written as a double integral,

$$\Phi_4^{(1)}(-is_1,r_1)=\frac{\exp(r_{21}\,\mathrm{tr}\,s_1)}{|r_{11}-r_{21}|}\int_{-\infty}^{+\infty}\mathrm{d}t_1\int_{-\infty}^{+\infty}\mathrm{d}t_2|t_1-t_2|\,\frac{\exp(i(r_{11}-r_{21})(t_1+t_2))}{\Pi_{i=1}^4\Pi_{n=1}^2\sqrt{s_{i1}-it_n}}. \tag{5.15}$$

Singularities have to be taken care of appropriately. After inserting Eq. (5.10) into the recursion formula and performing the Grassmann integration, one can arrange the terms in a similar way as in the case of $\Phi_{34}(-is,r)$. At this point, we notice that formulas (4.7) and (5.9) need to be supplemented by further identities. We state the most important one in the following.

The same conditions as for formula (4.7) apply. Moreover, we define the operator

$$\tilde{L}_m(s)=\sum_{q=1}^{k_1}\frac{1}{is_{m2}-s_{q1}}\frac{\partial^2}{\partial s_{q1}^2}+\frac{1}{2}\sum_{q\neq n}\frac{1}{(is_{m2}-s_{q1})(s_{q1}-s_{n1})}\left(\frac{\partial}{\partial s_{q1}}-\frac{\partial}{\partial s_{n1}}\right). \tag{5.16}$$

Then we have

$$\begin{aligned}&\tilde{L}_m(s)\int_{s_{11}}^{s_{11}}\cdots\int_{s_{(k_1-1)1}}^{s_{k_1 1}}\mu_B(s',s)\mathrm{d}[s_1']f(s_1')\\&\quad=-\int_{s_{11}}^{s_{21}}\cdots\int_{s_{(k_1-1)1}}^{s_{k_1 1}}\mu_B(s',s)\left[\sum_{j=1}\overrightarrow{M_{mj}}(s_1',s_1)\frac{\partial}{\partial s_{j1}'}\right]f(s_1')\,\mathrm{d}[s_1'].\end{aligned} \tag{5.17}$$

Again, the proof is along the same lines as the proof of formula (4.7) and the proof of formula (5.9) in Ref. 1.

Thus, there is a family of rules to transform operators symmetric in s_{i1} $L_m(s),\tilde{L}_m(s)$ acting onto an integral into an operator acting under the integral. We need one more such transformation rule which tells us how the product $[L_m(s)\tilde{L}_l(s)]$ transforms into operators acting under the integral. This formula and further details are given in Appendix E. Collecting everything, we finally arrive at

$$\begin{aligned}\Phi_{44}(-is,r)=4\hat{G}_{44}\exp(-\mathrm{tr}\,(r_2s_2))\prod_{i,j}(r_{i1}-ir_{j2})\Bigg[&\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)\\&\times\left(8\prod_{i=1}^2(r_{i1}-ir_{12})\prod_{j=1}^4(s_{j1}-is_{12})+4\sum_{i=1}^4\prod_{j\neq i}^4(s_{j1}-is_{12})\left(r_{11}+r_{21}-ir_{12}-\frac{\partial^{\rightarrow}}{\partial s_{i1}}\right)\right)\\&\times\left(8\prod_{i=1}^2(r_{i1}-ir_{22})\prod_{j=1}^4(s_{j1}-is_{22})+4\sum_{i=1}^4\prod_{j\neq i}^4(s_{j1}-is_{22})\left(r_{11}+r_{21}-ir_{22}-\frac{\partial}{\partial s_{i1}}\right)\right)\\&-\frac{16}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\sum_{i=1}^4\prod_{j\neq i}^4(s_{j1}-is_{12})(s_{j1}-is_{22})\Big(r_{11}^2+r_{21}^2+r_{11}r_{21}-(ir_{12}+ir_{22})\end{aligned}$$

$$\times(r_{11}+r_{21})+ir_{12}ir_{22}-\frac{1}{2}\mathrm{trg}\,r\frac{\partial}{\partial s_{i1}}\Bigg)-\frac{8}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\sum_{\substack{i=1\\j=1}}^{4}\prod_{l\neq i}^{4}(s_{l1}-is_{12})$$

$$\times\prod_{l\neq j}^{4}(s_{l1}-is_{22})\left(\frac{\partial}{\partial s_{i1}}-\frac{\partial}{\partial s_{j1}}\right)\Bigg]\Phi_4^{(1)}(-is_1,r_1)+(ir_{12}\leftrightarrow ir_{22}). \tag{5.18}$$

We mention that in the derivation of this result we frequently used properties of the matrix Bessel functions $\Phi_3^{(1)}(s_1,r_1)$ and $\Phi_4^{(1)}(s_1,r_1)$ that only hold for the case that one matrix has an additional degeneracy.

VI. ASYMPTOTICS AND NORMALIZATION

The asymptotic behavior of the supermatrix Bessel functions calculated in the previous sections is a useful check which also allows us to fix the normalization constants. We find from the expressions in Eqs. (4.1), (4.8) and in Eqs. (5.2), (5.10), (5.12), and (5.18),

$$\lim_{\substack{s\to\infty\\r\to\infty}}\Phi_{k_1 2k_2}(-is,r)=2^{k_1k_2}\hat{G}_{k_1 2k_2}\frac{\Pi_{l=1}^{k_1}\Pi_{m=1}^{k_2}(s_{l1}-is_{m2})(r_{l1}-ir_{m2})}{\Delta_{k_2}^2(is_2)\Delta_{k_2}^2(ir_2)}$$

$$\times\det[\exp(2s_{i2}r_{j2})]_{i,j=1\cdots k_2}\lim_{\substack{s_1\to\infty\\r_1\to\infty}}\Phi_{k_1}^{(1)}(-is_1,r_1). \tag{6.1}$$

In the degenerate case, each degenerate eigenvalue contributes according to its multiplicity. The asymptotics of the matrix Bessel functions of the orthogonal group is given by[27,28]

$$\lim_{t\to 0}\Phi_{k_1}^{(1)}(-is_1/t,r_1)=\hat{C}^{(k_1)}t^{(k_1-1)k_1/4}\frac{\det[\exp(s_{n1}r_{m1}/t)]_{n,m=1,\ldots,k_1}}{|\Delta_{k_1}(s_1)\Delta_{k_1}(r_1)|^{1/2}}, \tag{6.2}$$

where the constant can be found in Muirhead's book,[28]

$$\hat{C}^{(k_1)}=\frac{\Gamma(k_1/2)}{k_1!}\pi^{k_1^2/2-k_1/4}. \tag{6.3}$$

Thus we find

$$\lim_{t\to 0}\Phi_{k_1 2k_2}(-is/t,r)=2^{k_1k_2}t^{((k_1-2k_2)^2+(k_1-2k_2))/4}\hat{C}^{(k_1)}\hat{G}_{k_1 2k_2}$$

$$\times\frac{\det[\exp(s_{n1}r_{m1}/t)]_{n,m=1,\ldots,k_1}\det[\exp(2s_{i2}r_{j2}/t)]_{i,j=1\cdots k_2}}{\sqrt{\tilde{B}_{k_1k_2}(s)\tilde{B}_{k_1k_2}(r)}} \tag{6.4}$$

for the asymptotic behavior.

On the other hand, the supermatrix Bessel function relates to the kernel of Dyson's Brownian motion in superspace.[22] Due to the normalization of the Gaussian integral,

$$\left(\frac{\pi}{2t}\right)^{-((k_1-2k_2)^2+(k_1-2k_2))/4}2^{k_2^2-k_2-k_1/2}\int\mathrm{d}[\sigma]\exp\left(-\frac{1}{t}(\sigma-\rho)\right)=1, \tag{6.5}$$

the kernel

$$\Gamma_{k_1k_2}(s,r,t)=\left(\frac{\pi}{2t}\right)^{-((k_1-2k_2)^2+(k_1-2k_2))/4}2^{k_2^2-k_2-k_1/2}\int_{u\in \mathrm{UOSp}(k_1/2k_2)}\mathrm{d}\mu(u)\exp\left(-\frac{1}{t}(\sigma-\rho)\right) \tag{6.6}$$

is also normalized. Since it is obviously connected with to the supermatrix Bessel function by

$$\Gamma_{k_1k_2}(s,r,t)=\left(\frac{\pi}{2t}\right)^{-((k_1-2k_2)^2+(k_1-2k_2))/4}2^{k_2^2-k_2-k_1/2}\exp\left(-\frac{1}{t}(\mathrm{trg}\,s^2+\mathrm{trg}\,r^2)\right)\Phi_{k_1 2k_2}(-is/t,r) \tag{6.7}$$

we can fix the normalization by using the asymptotic behavior

$$\lim_{t\to 0}\Gamma_{k_1k_2}(s,r,t)=\left(\frac{\pi}{2}\right)^{-((k_1-2k_2)^2+(k_1-2k_2))/4}\frac{2^{k_2^2-k_2-k_1/2}}{k_1!\,k_2!}\times\frac{\det[\,\delta(s_{i1}-r_{j1})]_{i,j=1\cdots k_1}\det[\,\delta(s_{i2}-r_{j2})]_{i,j=1\cdots k_2}}{\sqrt{\tilde{B}_{k_1k_2}(s)\tilde{B}_{k_1k_2}(r)}} \tag{6.8}$$

of the kernel. Comparing Eq. (6.4) with Eq. (6.8), we find

$$\hat{G}_{k_1 2k_2}=\frac{2^{3k_2(k_2-k_1)+k_1^2/4-5k_2/2-k_1/2}}{\pi^{((k_1-2k_2)^2+2k_1^2-2k_2)/4}k_2!\,\Gamma(k_1/2)}. \tag{6.9}$$

We mention that this calculation also shows that the diffusion kernels of the one-point function and of the two-point function of Dyson's Brownian motion,[22] i.e., the function $\Gamma_{(2k)k}(s,r,t)$ which was denoted by $\Gamma_k(s,r,t)$ in Ref. 22, indeed satisfy the proper initial condition.

VII. APPLICATIONS

Although we focus in this contribution on the mathematical aspects, we now briefly comment on a particular kind of application. As the reader will realize, our results derived in Sec. VI are, in some sense, more general than what we need in those applications on which we focus here. We take this as an indication that explicit results for even more complex supermatrix Bessel functions can also be obtained. The results of the previous sections yield the kernels of the supersymmetric analog of Dyson's Brownian Motion for the GOE and the GSE in the cases $k=1$ and $k=2$. We do not present the physics background here. The reader interested in these applications is asked to consult Refs. 19–21 for generalities and Ref. 22, in particular Sec. 4.2, for the issue discussed here. In the present contribution, we use the same notations and conventions. We restrict ourselves to the transition toward the GOE and suppress the index c. The corresponding formulas for the transition toward the GSE are derived accordingly. We treat the one- and two-point functions in Secs. VII A and VII B, respectively.

Forrester and Nagao[29] derived expressions for generalized one-point functions of Dyson's Brownian motion model with Poissonian initial conditions. They used an expansion of the Green function in terms of Jack polynomials. Datta and Kunz[30] employed a supersymmetric technique to address the two-level correlation function of the Poisson GOE transition. They arrive at a finite number of ordinary and Grassmannian integrals which are still to be performed. In our approach, we also arrive at a representation of the correlation function in terms of a finite number of integrals. However, since we managed to integrate over almost all angular integrals in the previous sections, our result contains considerably less integrals, in particular, no Grassmannian ones. It has a clear structure due to the fact that, apart from two integrals, all others are eigenvalue integrals, i.e., live in the curved eigenvalue space of Dyson's Brownian motion. Moreover, since our formulas for the kernel are valid on all scales, our result is also exact for finite level number.

A. Level density

We use the result (4.9), derived in Sec. IV, for the supermatrix Bessel function $\Phi_{22}(-is,r)$. Using the replacement $r\to(x+J)$ and $s\to s/t$ and the relation (6.7), we obtain the diffusion kernel for the level density

$$\Gamma_1(s,x+J,t)=(2\pi)^{-1/2}\frac{J_1}{2t}\exp\left(-\frac{1}{t}(s_{11}-x_1-J_1)^2-\frac{1}{t}(s_{21}-x_1-J_1)^2+\frac{2}{t}(is_{12}-x_1+J_1)^2\right)$$
$$\times\left(-2\frac{J_1}{t}\prod_{j=1}^{2}(is_{12}-s_{j1})+\sum_{q=1}^{2}(is_{12}-s_{q1})\right). \tag{7.1}$$

We take the derivative with respect to the source variable J_1 and arrive at the level density

$$\hat{R}_1(x_1,t)=\frac{1}{(2\pi)^{3/2}t}\int\exp\left(-\frac{1}{t}(s_{11}-x_1)^2-\frac{1}{t}(s_{21}-x_1)^2+\frac{2}{t}(is_{12}-x_1)^2\right)$$
$$\times((is_{12}-s_{11})+(is_{12}-s_{21}))\tilde{B}_{21}(s)\,Z_1^{(0)}(s)\,d[s], \tag{7.2}$$

where the Berezinian is given by Eq. (2.10) for $k_1=2$ and $k_2=1$. This result is exact for an arbitrary initial condition and for arbitrary N. In the case of a diagonal matrix $H^{(0)}$ as the initial condition, we have for arbitrary k,

$$Z_k^{(0)}(s)=\int \mathrm{d}[H^{(0)}]P(H^{(0)})\prod_{n=1}^{N}\frac{\Pi_{j=1}^{k}(is_{j2}-H_{nn}^{(0)})}{\Pi_{j=1}^{2k}(s_{j1}+i\varepsilon-H_{nn}^{(0)})^{1/2}} \tag{7.3}$$

and analogously for the GSE. This has to be used in Eq. (7.2) for $k=1$.

In the limit $t\to\infty$ the stationary distribution of classical Gaussian random matrix theory is recovered. This can be seen by rewriting Eq. (7.1) for the rescaled energy $\tilde{x}_1=x_1/t$ and the rescaled source variable $\tilde{J}_1=J_1/t$, see also Ref. 22. In this limit the initial condition yields unity and we arrive at an integral representation of the one-point correlation function of the pure GOE,

$$R_1(x_1)=\frac{1}{(2\pi)^{3/2}}\Im\int\exp(-(s_{11}-x_1)^2-(s_{21}-x_1)^2+(is_{12}-x_1)^2)$$
$$\times\frac{|s_{11}-s_{21}|}{(is_{12}-s_{11})(is_{12}-s_{21})}\left(\frac{1}{is_{12}-s_{11}}+\frac{1}{is_{12}-s_{21}}\right)\frac{(is_{12})^N}{(s_{11}+i\varepsilon)^{N/2}(s_{21}+i\varepsilon)^{N/2}}\mathrm{d}[s] \tag{7.4}$$

where the symbol $\Im$ denotes the imaginary part. Equation. (7.4) is equivalent to the classical expressions for the one-point functions as in Mehta's book.[19]

Finally, we state an integral expression for the one-point function for the case of Poissonian initial conditions, see Eq. (5.1) of Ref. 22. We have

$$Z_k^{(0)}(s)=\left(\int \mathrm{d}z\,p(z)\frac{\Pi_{j=1}^{k}(is_{j2}-z)}{\Pi_{j=1}^{2k}(s_{j1}+i\varepsilon-z)^{1/2}}\right)^N. \tag{7.5}$$

Inserting this initial condition for $k=1$ into Eq. (7.2) yields the level density of a transition ensemble between Poisson regularity and GOE in terms of a fourfold integral. A further analysis will be published elsewhere.

B. Two-point function

The result (5.18), derived in Sec. V, for the supermatrix Bessel function $\Phi_{44}(-is,r)$ gives, with the replacement $r\to(x+J)$ and $s\to s/t$ and according to Eq. (6.7), the diffusion kernel for the two-point function

$$\Gamma_k(s,x+J,t)=\exp\left(-\frac{1}{t}(\mathrm{trg}\,s^2+\mathrm{trg}\,(x+J)^2)\right)\Phi_{44}(-2is/t,x+J). \tag{7.6}$$

The derivative with respect to the source terms leaves us with the two-point correlation function

$$\begin{aligned}\hat{R}_2(x_1,x_2,t)=\frac{2^6\hat{G}_{44}}{t^2\pi^2}\Im\int\Bigg(&\sqrt{\tilde{B}_{42}(s)}\sqrt{|\Delta_4(s_1)|}Z_2^{(0)}(s)\exp\Bigg(-\frac{1}{t}(\mathrm{trs}_1^2+2x_1^2+2x_2^2-2(is_{12}-x_1)^2\\&-2(is_{22}-x_2)^2)\Bigg)\sum_{k,j}\Bigg[\frac{1}{(is_{12}-s_{k1})(is_{22}-s_{j1})}\left(\frac{2x_1}{t}-\frac{\partial}{\partial s_{j1}}\right)\left(\frac{2x_2}{t}-\frac{\partial}{\partial s_{k1}}\right)\\&+\frac{t}{2(x_1-x_2)(is_{12}-is_{22})(is_{12}-s_{k1})(is_{22}-s_{j1})}\left(\frac{2x_1}{t}-\frac{\partial}{\partial s_{j1}}\right)\left(\frac{2x_2}{t}-\frac{\partial}{\partial s_{k1}}\right)\\&\times-\frac{1}{4}\frac{t}{(x_1-x_2)(is_{12}-s_{k1})(is_{22}-s_{j1})(is_{12}-is_{22})^2}\left(\frac{\partial}{\partial s_{j1}}-\frac{\partial}{\partial s_{k1}}\right)\Bigg]\\&\times\Phi_4^{(1)}(-2is_1/t,x)\Bigg)\,\mathrm{d}[s]+(x_1\leftrightarrow x_2).\end{aligned} \tag{7.7}$$

The last line indicates that the integral with x_1 and x_2 interchanged has to be added. Since the terms antisymmetric in x_1 and x_2 are antisymmetric in s_{i2} and s_{22} as well this yields just a factor 2 in Eq. (7.7). The symbol $\Im$ denotes a certain linear combination of $\hat{R}_2(x_1,x_2,t)$ as explained in Ref. 22. The normalization constant obtains from Eq. (6.9) and is given by $\hat{G}_{44}=2(2\pi)^{-4}$. This result is an exact expression for the two-point function of Dyson's Brownian motion for every initial condition. Plugging in the initial condition of Eq. (7.5) for $k=2$, we find an integral representation of the two-point function for the transition toward the GOE. We notice that $\Phi_4^{(1)}(-2is_1/t,x)$ is, according to Eq. (5.15), given as a double integral.

In the previous discussion, we referred to properties of the kernels which can be seen from the explicit formulas. In Ref. 22, only the explicit form of the kernel for $\beta=2$ was available. However, some of the general properties of the kernels for $\beta=1$ and $\beta=4$ could be anticipated in Ref. 22 from scaling relations of the supersymmetric version of Dyson's Brownian motion. The explicit formulas derived in the present contribution allow one to derive the integral representations (7.2) and (7.7) for the one-point and for the two-point function. Moreover, we emphasize that the kernels for the supersymmetric version of Dyson's Brownian motion are the same on all energy scales.[22] Thus, the integral representation derived here for the two-level correlation function is, apart from the initial condition, the same on the so-called unfolded scale which is relevant for physics applications. The initial condition on the unfolded scale is found along the lines given in Ref. 22.

VIII. SUMMARY AND CONCLUSION

We extended the recursion formula of Ref. 1 to superspace. Due to the group structures in superspace, we could restrict ourselves to the unitary orthosymplectic supergroup. As in the ordinary case, the recursion formula is an exact map of a group integration onto an iteration in the radial space. We used it to calculate explicit expression for certain supermatrix Bessel functions.

In ordinary space, we saw that the matrix Bessel functions are only special cases of the radial functions.[1] We have not yet studied this further, but in our opinion a similar generalization is likely to also exist in superspace.

It is a major advantage of the radial Gelfand–Tzetlin coordinates in superspace that the Grassmann variables appear only as moduli squared. Thus, the number of Grassmann integrals is *a priori* reduced by half. As we showed in detail, this is a highly welcome feature for explicit calculations. As a remarkable consequence of this recursive way to proceed, the structure of the supermatrix Bessel functions is only very little influenced by the matrix dimension. We also saw that the basic structures of the supermatrix Bessel function for smaller matrix dimensions survive during the iteration to higher ones. The matrix Bessel functions in ordinary space show similar features. There, the structure of the matrix Bessel functions is much more influenced by the group parameter β than by the matrix dimension. However, as in ordinary space, it remains a challenge to find the structure of these functions for arbitrary matrix dimension.

An interesting feature occurred which sheds light on the general properties of the recursion. Total derivatives showed up in the integral over the commuting variables after having done the Grassmann integration. Since similar terms already occurred in ordinary space, they are likely to be an intrinsic property of the recursion formula. Here, we succeeded in constructing a series of operator identities to remove them. This was a crucial step for the application of the recursion formula. A deeper understanding of these identities is highly desired.

It should be emphasized that the total derivatives are no boundary terms in the sense of Rothstein. We showed in detail that such terms cannot occur because we always work in a compact space. Thus, according to a theorem due to Berezin,[2] the transformation of the invariant measure to our radial Gelfand–Tzetlin coordinates cannot yield Rothstein boundary terms. However, if further integration over the eigenvalues is required, such terms can emerge.

As an application, we worked out some kernels for the supersymmetric analog of Dyson's Brownian motion.

The radial Gelfand–Tzetlin coordinates are the natural coordinate system for the matrix Bessel functions in superspace. This parametrization represents the appropriate tool for the recursive integration of Grassmann variables. Once the particular features of this parametrization are better understood, they may allow for the evaluation of higher dimensional group integrals.

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APPENDIX A: RADIAL GELFAND–TZETLIN COORDINATES FOR THE UNITARY ORTHOSYMPLECTIC GROUP UOSp($k_1/2k_2$)

We wish to express the moduli squared of the elements of an orthogonal $(k_1/2k_2)$ dimensional unit supervector in radial Gelfand–Tzetlin coordinates. To illustrate the mechanism, we start with the smallest nontrivial case, the group UOSp(2/4). We notice that there are at first sight minor, yet crucial, differences to the calculation in Ref. 11 where we also started with the smallest nontrivial case. The set of solutions of the Gelfand–Tzetlin equations (3.23) involves one bosonic and two fermionic eigenvalues. The eigenvalue equations read

$$1=\sum_{p=1}^{2}\left(|v_p^{(1)}|^2+|\alpha_p^{(1)}|^2\right), \tag{A1}$$

$$0=\sum_{q=1}^{2}\left(\frac{|v_q^{(1)}|^2}{s_{q1}-s_1^{(1)}}+\frac{|\alpha_q^{(1)}|^2}{is_{q2}-s_1^{(1)}}\right), \tag{A2}$$

$$z_1 = is_2^{(1)} \prod_{q=1}^{2} \frac{(s_{q1} - is_2^{(1)})}{(is_{q2} - is_2^{(1)})^2} \sum_{q=1}^{2} \left(\frac{|v_q^{(1)}|^2}{s_{q1} - is_2^{(1)}} + \frac{|\alpha_q^{(1)}|^2}{is_{q2} - is_2^{(1)}} \right), \tag{A3}$$

where the last equation has to be solved in the limit $z_1 \to \infty$. The bosonic equation (A2) has a unique solution $s_1^{(1)} = s'_{11}$. Taking s'_{11} as new parameter, Eqs. (A1) and (A2) can be solved,

$$|v_p^{(1)}|^2 = \frac{s_{p1} - s'_{11}}{s_{p1} - s_{q1}} \left(1 - \sum_{k=1}^{2} \frac{is_{k2} - s_{q1}}{is_{k2} - s'_{11}} |\alpha_k^{(1)}|^2 \right), \quad p = 1,2. \tag{A4}$$

We insert these relations in Eq. (A3) and obtain

$$z_1 = is_2^{(1)}(s'_{11} - is_2^{(1)}) \prod_{q=1}^{2} \frac{(s_{q1} - is_2^{(1)})}{(is_{q2} - is_2^{(1)})^2} \left(1 + \sum_{k=1}^{2} \frac{c_k}{is_{k2} - is_2^{(1)}} |\alpha_k^{(1)}|^2 \right) \tag{A5}$$

with $z_1 \to \infty$. Here, we have defined the commuting variables

$$c_k = \frac{\Pi_{q=1}^{2}(is_{k2} - s_{q1})}{is_{k2} - s'_{11}}, \quad k = 1,2. \tag{A6}$$

It remains to determine the set of solutions of the fermionic eigenvalue equation (A5). To this end, both sides are inverted

$$0 = \prod_{q=1}^{2} (is_{q2} - is_2^{(1)})^2 \left(1 - \sum_{k=1}^{2} \frac{c_k}{is_{k2} - is_2^{(1)}} |\alpha_k^{(1)}|^2 + 2 \prod_{k=1}^{2} \frac{c_k}{is_{k2} - is_2^{(1)}} |\alpha_k^{(1)}|^2 \right). \tag{A7}$$

We can now take the square root on both sides

$$0 = \prod_{q=1}^{2} (is_{q2} - is_2^{(1)}) \left(1 - \frac{1}{2} \sum_{k=1}^{2} \frac{c_k}{is_{k2} - is_2^{(1)}} |\alpha_k^{(1)}|^2 + \frac{3}{4} \prod_{k=1}^{2} \frac{c_k}{is_{k2} - is_2^{(1)}} |\alpha_k^{(1)}|^2 \right). \tag{A8}$$

The most general form of the fermionic eigenvalue is

$$is_2^{(1)} = a_0 + \sum_{k=1}^{2} a_k |\alpha_k^{(1)}|^2 + a_{12} \prod_{k=1}^{2} |\alpha_k^{(1)}|^2. \tag{A9}$$

After inserting this ansatz in Eq. (A8), we obtain two sets of solutions for the coefficients a_{i0}, a_{i12} and a_{ij} with $i = 1,2, j = 1,2$

$$\begin{aligned} is'_{12} &= is_{12} + \left(c_1 + \frac{c_1 c_2}{is_{12} - is_{22}} |\alpha_2^{(1)}|^2 \right) \frac{|\alpha_1^{(1)}|^2}{2}, \\ is'_{22} &= is_{22} + \left(c_2 + \frac{c_1 c_2}{is_{22} - is_{12}} |\alpha_1^{(1)}|^2 \right) \frac{|\alpha_2^{(1)}|^2}{2}. \end{aligned} \tag{A10}$$

Remarkably, we have $a_{12} = a_{21} = 0$. This allows us to write the nilpotent part of is'_{k2} as the modulus squared of a new anticommuting coordinate,

$$is'_{k2} = is_{k2} + |\xi'_k|^2. \tag{A11}$$

We solve Eq. (A10) for $|\alpha_p^{(1)}|^2$, insert the results in Eq. (A4) and arrive at

$$|v_p^{(1)}|^2=\frac{(s_{p1}-s'_{11})\Pi_{n=1}^{2}(s_{p1}-is_{n2})^2}{(s_{p1}-s_{q1})\Pi_{n=1}^{2}(s_{p1}-is'_{n2})^2},$$
$$|\alpha_p^{(1)}|^2=2(is'_{p2}-is_{p2})\frac{(is_{p2}-s'_{11})(is_{p2}-is_{q2})^2}{(is_{p2}-is'_{q2})^2\Pi_{n=1}^{2}(is_{p2}-s_{n1})},\quad p,q=1,2\ ,\quad q\neq p. \tag{A12}$$

The structure of Eq. (A12) indicates the form of the solutions for groups of higher order as they were stated in Eq. (3.24). They are checked by inserting them directly into the Gelfand–Tzetlin equations (3.23). The algebra needed is, although tedious, straightforward and similar to the one here.

APPENDIX B: DERIVATION OF FORMULA (4.7)

The technique we use is an extension of the one developed in Appendix D of Ref. 1. First, we rewrite the integral in terms of Θ functions. The left hand side reads

$$L_m(s)\int \mu_B(s',s)f(s'_1)\mathrm{d}[s'_1]\prod_{k\leqslant l}\Theta(s_{k1}-s'_{l1})\prod_{l<n}\Theta(s'_{l1}-s_{n1}). \tag{B1}$$

The integration domain is now the real axis for all variables. The action of $L_m(s)$ on the integral yields:

$$\int\left(\mu_B(s',s)\sum_{i=1}^{k_1}\sum_{j=1}^{k_1-1}\frac{1}{2}\frac{-1}{(is_{12}-s_{i1})(s_{i1}-s'_{j1})}f(s'_1)\prod_{k\leqslant l}\Theta(s_{k1}-s'_{l1})\prod_{l<n}\Theta(s'_{l1}-s_{n1})\right)\mathrm{d}[s'_1]$$
$$+\int\mu_B(s',s)\sum_{i=1}^{k_1}\frac{1}{is_{m2}-s_{i1}}\frac{\partial}{\partial s_{i1}}\prod_{k\leqslant l}\Theta(s_{k1}-s'_{l1})\prod_{l<n}\Theta(s'_{l1}-s_{n1})\mathrm{d}[s'_1]. \tag{B2}$$

We decompose the first term in partial fractions and find

$$\int\left(\mu_B(s',s)\sum_{i=1}^{k_1}\sum_{j=1}^{k_1-1}\frac{1}{2}\frac{-1}{(is_{12}-s_{i1})(is_{12}-s'_{j1})}\ f(s'_1)-\Delta_{k_1}(s'_1)\ f(s'_1)\right.$$
$$\times\sum_{j=1}^{k_1-1}\frac{1}{is_{12}-s'_{j1}}\frac{\partial}{\partial s'_{j1}}\frac{1}{\sqrt{-\Pi_{i=1}^{k_1}(s_{i1}-s'_{j1})}}\prod_{k\leqslant l}\Theta(s_{k1}-s'_{l1})\prod_{l<n}\Theta(s'_{l1}-s_{n1})\mathrm{d}[s'_1]$$
$$+\int\mu_B(s',s)\ f(s')\sum_{i=1}^{k_1}\frac{1}{is_{m2}-s_{i1}}\frac{\partial}{\partial s_{i1}}\prod_{k\leqslant l}\Theta(s_{k1}-s'_{l1})\prod_{l<n}\Theta(s'_{l1}-s_{n1})\mathrm{d}[s'_1]. \tag{B3}$$

An integration by parts yields

$$\int\mu_B(s',s)\sum_{j=1}^{k_1-1}(-M_{mj}(s'_1,s_1))\prod_{k\leqslant l}\Theta(s_{k1}-s'_{l1})\prod_{l<n}\Theta(s'_{l1}-s_{n1})\mathrm{d}[s'_1]+\int\mu_B(s',s)\,f(s')$$
$$\times\left(\sum_{i=1}^{k_1}\frac{1}{is_{m2}-s_{i1}}\frac{\partial}{\partial s_{i1}}+\sum_{j=1}^{k_1-1}\frac{1}{is_{m2}-s'_{j1}}\frac{\partial}{\partial s'_{j1}}\right)\prod_{k\leqslant l}\Theta(s_{k1}-s'_{l1})\prod_{l<n}\Theta(s'_{l1}-s_{n1})\mathrm{d}[s'_1]. \tag{B4}$$

The derivatives of the Θ functions yield δ distributions. Upon integration of the δ distribution the two terms in the last integral cancel each other. Hence the last term vanishes identically. This completes the proof.

APPENDIX C: ALTERNATIVE DERIVATIONS OF $\Phi_{22}(s,r)$

We present two different alternative derivations. We do this in some detail, because the calculations give helpful informations on the rôle played by the radial Gelfand–Tzetlin coordinates.

First, we use an angular parametrization of the coset UOSp(2/2)/UOSp(1/2) by writing the first column of $u \in \mathrm{UOSp}(2/2)$ as

$$u_1 = \begin{bmatrix} \sqrt{1-|\alpha|^2}\cos\vartheta \\ \sqrt{1-|\alpha|^2}\sin\vartheta \\ \frac{1}{\sqrt{2}}\alpha \\ \frac{1}{\sqrt{2}}\alpha^* \end{bmatrix}. \tag{C1}$$

This is a canonical way to parametrize the supersphere $S^{1|2}$ that is isomorphic to the coset UOSp(2/2)/UOSp(1/2), see Ref. 31. It coincides with a special choice of the *angular* Gelfand–Tzetlin coordinates. The invariant measure is in these coordinates simply $\mathrm{d}\mu(u_1)=\mathrm{d}\alpha^*\,\mathrm{d}\alpha\mathrm{d}\vartheta$. Thus, one directly obtains the the volume $V(S^{1|2})=0$, see Ref. 31. In the parametrization of the measure by *radial* Gelfand–Tzetlin coordinates (4.3), one has to perform the Grassmann integration and to apply formula (4.7) to achieve this result.

Although we use a different coordinate system, we still take advantage of the recursion formula (3.1). To use it in the parametrization (C1), one has to solve the Gelfand–Tzetlin equations (3.21)–(3.23) for the eigenvalues. The unique solution of the bosonic equation (3.22) is

$$s'_{11}=a_0+\frac{\Pi_{i=1}^2(s_{i1}-a_0)}{is_{12}-a_0}|\alpha|^2, \quad a_0=\frac{s_{11}+s_{21}}{2}-\frac{s_{11}-s_{12}}{2}\cos 2\vartheta. \tag{C2}$$

The fermionic equation yields

$$is'_{12}=is_{12}+\frac{\Pi_{i=1}^2(s_{i1}-is_{12})}{is_{12}-a_0}|\alpha|^2. \tag{C3}$$

After inserting Eqs. (C2) and (C3) and the measure $\mathrm{d}\mu(u_1)$ into the recursion formula (3.1), the Grassmann integration can be performed. Remarkably, we arrive at the denominator–free expression

$$\begin{aligned}\Phi_{22}(s,r)=\hat{G}_{22}\int_0^{2\pi}\mathrm{d}\vartheta\exp\left(\mathrm{trg}\,rs-\frac{z}{2}+\frac{z}{2}\cos 2\vartheta\right)\\ \times\Bigg[\left(\prod_{i=1}^{2}(r_{i1}-ir_{12})(s_{i1}-is_{12})+\frac{1}{2}\sum_{\substack{i=1\\ j=1}}^{2}(s_{j1}-is_{12})(r_{i1}-ir_{12})\right)\\ -\frac{1}{2}\left(ir_{12}-\frac{1}{2}(r_{11}+r_{21})\right)(s_{11}-s_{21})\cos 2\vartheta-\frac{z}{8}(ir_{12}-r_{21})(s_{11}-s_{21})\sin^2 2\vartheta\Bigg].\end{aligned} \tag{C4}$$

To make contact with Eq. (4.9) one has to realize that in Eq. (C4) an additional total derivative appears in the integrand. This becomes obvious if one adds and subtracts $z/4\cos 2\vartheta$ in the square bracket of Eq. (C4),

$$\Phi_{22}(s,r)=\hat{G}_{22}\int_0^{2\pi}\mathrm{d}\vartheta\,\exp\left(\mathrm{trg}\,rs-\frac{z}{2}+\frac{z}{2}\cos 2\vartheta\right)$$
$$\times\left(\prod_{i=1}^{2}(r_{i1}-ir_{12})(s_{i1}-is_{12})+\frac{1}{2}\sum_{\substack{i=1\\j=1}}^{2}(s_{j1}-is_{12})(r_{i1}-ir_{12})-\frac{z}{4}\cos 2\vartheta\right)$$
$$+\frac{ir_{12}-r_{21}}{r_{21}-r_{11}}\int_0^{2\pi}\mathrm{d}\vartheta\,\frac{\partial^2}{\partial(2\vartheta)^2}\exp\left(\mathrm{trg}\,rs-\frac{z}{2}(1-\cos 2\vartheta)\right). \tag{C5}$$

While the first integral reproduces Eq. (4.9), the second one vanishes identically. In general, in performing Grassmann integrations, one has to take care of boundary contributions.[2,24] These contributions can appear whenever even coordinates are shifted by nilpotents and the function one integrates does not have compact support.[2] However, in our case the basis space is always given by an n dimensional sphere, i.e., by a compact manifold *without boundary*. Thus in a properly chosen coordinate system, no boundary terms should appear. With regard to Eq. (C5) this means: the fact that the last term vanishes is a direct consequence of the compactness of the circle and of the analyticity of the function, that we integrate. However, in the radial Gelfand–Tzetlin coordinates, only the moduli squared of the vector u_1 are determined. Therefore, not the whole sphere, but only a (2^{n+1})th segment of it is covered by Eq. (3.24). In our case, not the circle but only a quarter of it is parametrized. This is allowed since the supermatrix Bessel functions depend only on the moduli squared $|u_{i1}|^2$. Nevertheless, one has to ensure that the introduction of these artificial boundaries does not alter the result. To this end we use the following integration formula.

Let $s_{11}<s'_{11}<s_{21}$ be real and let ξ',ξ'^* be anticommuting. Furthermore, define

$$f(s'_{11},\xi,\xi^*)=f_0(s'_{11})+f_1(s'_{11})|\xi|^2, \tag{C6}$$

with two analytic functions $f_0(s'_{11}),f_1(s'_{11})$. Then the integral

$$I=\int_{s_{11}}^{s_{21}}\mathrm{d}s'_{11}\,\mathrm{d}\xi^*\,\mathrm{d}\xi f(s'_{11},\xi,\xi^*) \tag{C7}$$

transforms under a shift of s'_{11} by nilpotents

$$s'_{11}=y+g(y)|\xi|^2 \tag{C8}$$

in the following way:

$$I=\int_{s_{11}}^{s_{21}}\mathrm{d}y\,\mathrm{d}\xi^*\mathrm{d}\xi\frac{\partial s'_{11}}{\partial y}f(y(s'_{11}),\xi,\xi^*)-[f_0(s_{21})g(s_{21})-f_0(s_{11})g(s_{11})]. \tag{C9}$$

The proof is by direct calculation. The second term in Eq. (C9) is often referred to as boundary term. It can be viewed as the integral of a total derivative, i.e., an exact one-form, that has to be added to the integration measure for functions with noncompact support.[24] For functions of an arbitrary number of commuting and anticommuting arguments, a similar integral formula holds with additional boundary terms.[2] In going from the canonical coordinates $(\vartheta,\alpha,\alpha^*)$ to the radial ones $(s'_{11},\xi'_1,\xi'^*_1)$, in principle boundary terms can arise, since the bosonic Gelfand–Tzetlin eigenvalue (C2) contains nilpotents. However, the crucial quantity is $g(y)$ in formula (C9) which, in our case, is given by

$$g(s'_{11})=\frac{\Pi_{i=1}^{2}(s_{i1}-s'_{11})}{is_{12}-s'_{11}}. \tag{C10}$$

Thus, $g(s'_{11})$ causes the boundary term to vanish at s_{11} and s_{21}. It is the product structure of the left-hand side of Eq. (3.24) which always guarantees the vanishing of the boundary terms, when one goes from the Cartesian set of coordinates to the radial Gelfand–Tzetlin coordinates.

Therefore, one may think of the denominators, arising in Eqs. (4.4) and (4.5), as belonging to total derivatives of functions, which vanish at the boundaries. Keeping this in mind we derive Eq. (4.9) in yet another way. We expand the product

$$\prod_{q=1}^{k_1}(is_{m2}-s_{q1})=\sum_{n=0}^{k_1}\frac{1}{n!}(is_{m2}-s'_{j1})^n\frac{\partial^n}{\partial(s'_{j1})^n}\prod_{q=1}^{k_1}(s'_{j1}-s_{q1}), \tag{C11}$$

and insert it into the integral

$$\begin{aligned}&\int_{s_{11}}^{s_{21}}\cdots\int_{s_{(k_1-1)1}}^{s_{k_1 1}}\mu_B(s'_1,s_1)K_{mj}(s'_1,s_1)f(s'_1)\mathrm{d}[s'_1]\\&\quad=\int_{s_{11}}^{s_{21}}\cdots\int_{s_{(k_1-1)1}}^{s_{k_1 1}}\mu_B(s'_1,s_1)\prod_{n=1}^{k_1}(is_{m2}-s_{n1})M_{mj}(s'_1,s_1)\,f(s'_1)\,\mathrm{d}[s'_1].\end{aligned} \tag{C12}$$

We can remove the term proportional to $(is_{m2}-s'_{j1})^{-2}$ in the integrand by an integration by parts. Through the expansion (C11), the vanishing of the boundary terms is assured. We arrive at

$$\begin{aligned}K_{mj}(s'_1,s_1)=&-\sum_{n=2}^{k_1}\frac{1}{n!}(is_{m2}-s'_{j1})^{n-2}\frac{\partial^n}{\partial(s'_{j1})^n}\prod_{q=1}^{k_1}(s'_{j1}-s_{q1})\\&+\frac{\Pi_{q=1}^{k_1}(is_{m2}-s_{q1})-\Pi_{q=1}^{k_1}(s'_{j1}-s_{q1})}{is_{m2}-s'_{j1}}\\&\times\left(\frac{1}{2}\sum_{q=1}^{k_1}\frac{1}{is_{m2}-s_{q1}}-\frac{1}{2}\sum_{q=1}^{k_1}\frac{1}{s'_{j1}-s_{q1}}-\sum_{\substack{q=1\\q\neq j}}^{k_1}\frac{1}{s'_{j1}-s'_{q1}}-\frac{\partial}{\partial s'_{j1}}\right).\end{aligned} \tag{C13}$$

We notice that in the new operator $K_{mj}(s'_1,s_1)$ all denominators of the type $(is_{m2}-s'_{j1})^{-1}$ have disappeared. For $k_1=2$, we calculate

$$K_{11}=-(is_{12}+s'_{11}-s_{11}-s_{21})\frac{\partial}{\partial s'_{q1}}, \tag{C14}$$

which can be inserted into Eq. (4.4) by using the definition (C12). Finally, the result (4.9) is reproduced by the substitution

$$s'_{11}=\frac{s_{11}+s_{21}}{2}-\frac{s_{11}-s_{12}}{2}\cos 2\vartheta, \tag{C15}$$

see Eq. (C2). In other words, we have seen that the result of this procedure is summarized in formula (4.7).

Finally, some remarks are in order: First, from this discussion, one might conclude that the radial Gelfand–Tzetlin coordinates are less adapted to the problem than the canonical parametrization (C1), because, in the latter, no denominators appear. We stress that this is not true. Certainly, the denominators appear due to the shift of the bosonic variable by nilpotents in Eq. (C2). However, the difficulty in deriving Eq. (4.9) is the identification of the different parts of the integrand after the Grassmann integration. Some of them belong to total derivatives and this problem exists in both parametrizations. Second, we emphasize that the appearance of total derivatives in the integrand is not a peculiarity of supersymmetry. Already in Ref. 1 where the matrix

Bessel functions in ordinary space were treated we had to solve a similar problem. The appearance of these total derivatives is an intrinsic property of the recursion formula. A geometrical interpretation of this phenomenon is highly desired.

APPENDIX D: DETAILS FOR THE DERIVATION OF $\Phi_{34}(-is,r)$

We always consider the case that one matrix has an additional degeneracy according to Eqs. (5.11) and (5.13). We introduce the notation

$$S_{ij}=(s_{i1}-is_{j2}),\quad R_{ij}=(r_{i1}-ir_{j2}). \tag{D1}$$

Due to the degeneracy, $\Phi_{24}(-is,\tilde{r})$ simplifies enormously as compared to the general result (5.10). We insert it into the recursion formula (3.1) and do the trivial integral over the O(2) subgroup. After performing the Grassmann integrals we arrive at an expression similar to Eq. (5.7),

$$\begin{aligned}
\Phi_{34}(-is,r)=4\hat{G}_{34}\exp(\mathrm{tr}\, r_2 s_2+r_{11}(s_{11}+s_{21}))\int \mathrm{d}\mu_B(s_1',s_1)\prod_{i=1}^{2} R_{1i}\prod_{j=1}^{3} S_{ji}\\
\times\Bigg[\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)\left(4\prod_{i=1}^{2} R_{i1}-2\sum_{k=1}^{3} R_{21}S_{k1}^{-1}\right.\\
\left.+2\sum_{j=1}^{2} M_{1j}(s_1',s_1)\right)\left(4\prod_{i=1}^{2} R_{i2}-2\sum_{k=1}^{3} R_{22}S_{k2}^{-1}+2\sum_{j=1}^{2} M_{2j}(s_1',s_1)\right)\\
+\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^3(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\right)\\
\times\sum_{j=1}^{2}\left(\frac{4}{is_{12}-s_{j1}'}M_{2j}(s_1',s_1)-\frac{4}{is_{22}-s_{j1}'}M_{1j}(s_1',s_1)\right)\\
-\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^3(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)\prod_{\substack{k=1\\ j=1}}^{2}\frac{2}{is_{k2}-s_{j1}'}+\frac{2}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\\
\times\left(\mathrm{trg}\, r+r_{11}-\sum_{i=1}^{2} S_{i2}^{-1}\right)\sum_{j=1}^{2} M_{1j}(s_1',s_1)-\frac{2}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\\
\times\left(\mathrm{trg}\, r+r_{11}-\sum_{i=1}^{2} S_{i1}^{-1}\right)\sum_{j=1}^{2} M_{2j}(s_1',s_1)\\
-\frac{4}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\sum_{k=1}^{3}\prod_{j=1}^{2} R_{2j}S_{kj}^{-1}\Bigg]\exp((s_{21}'+s_{11}')(r_{21}-r_{11}))+(ir_{12}\leftrightarrow ir_{22}).
\end{aligned} \tag{D2}$$

Formulas (5.9) and (4.7) are needed to remove the denominators, in a way similar as for $\Phi_{24}(s,r)$. A single sum $\Sigma_{j=1}^{2} M_{1j}(s_1',s_1)$ transforms according to formula (4.7). Moreover, we observe that parts of Eq. (D2) together with the product $\Sigma_{j=1}^{2} M_{1j}(s_1',s_1)\Sigma_{k=1}^{2} M_{2k}(s_1',s_1)$ yield exactly the integrand of formula (5.9). Thus, it can be transformed accordingly. After rearranging terms, we arrive at the result (5.12).

APPENDIX E: DETAILS FOR THE DERIVATION OF $\Phi_{44}(-is,r)$

For the recursion, we need $\Phi_{34}(s,r)$ with degenerate $\tilde{r}=\mathrm{diag}(r_{11},r_{21},r_{21})$ according to Eq. (5.11). Using the integral representation (5.14) for $\Phi_3^{(1)}(-is_1',\tilde{r}_1)$ we find the helpful identity

$$\frac{\partial}{\partial s_{i1}'}\frac{\partial}{\partial s_{j1}'}\exp(-r_{21}\,\mathrm{tr}\,s_1')\Phi_3^{(1)}(-is_1',\tilde{r}_1)=\frac{1}{2}\frac{1}{s_{i1}'-s_{j1}'}\left(\frac{\partial}{\partial s_{i1}'}-\frac{\partial}{\partial s_{j1}'}\right)\exp(-r_{21}\mathrm{trs}_1')\Phi_3^{(1)}(-is_1',\tilde{r}_1). \tag{E1}$$

We stress that this relation, which is crucial in the derivation, only holds, because of the degeneracy in the matrix $\tilde{r}_1$. Employing Eq. (5.14) and another identity,

$$\sum_{i=1}^{3}\frac{\partial}{\partial s_{i1}'}\exp(-r_{21}\mathrm{tr}\,s_1')\Phi_3^{(1)}(-is_1',\tilde{r}_1)=(r_{11}-r_{21})\exp(-r_{21}\,\mathrm{tr}\,s_1')\Phi_3^{(1)}(-is_1',\tilde{r}_1). \tag{E2}$$

We insert $\Phi_{34}(s',\tilde{r})$ into the recursion formula (3.1). We then can arrange the terms emerging from the Grassmann integration in a way similar to the former cases. We obtain

$$\begin{aligned}
\Phi_{44}(-is,r)=4\hat{G}_{44}\exp(\mathrm{tr}\,r_2s_2+r_{11}\,\mathrm{tr}\,s_1)\int \mathrm{d}\mu_B(s_1',s_1)\prod_{i=1}^{2}R_{2i}\prod_{j=1}^{4}S_{ji}\\
\times\Bigg[\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)\\
\times\left(8R_{21}R_{11}^2-4R_{11}R_{21}\sum_{k=1}^{4}S_{k1}^{-1}+4\sum_{j=1}^{3}\left(R_{21}-\frac{\partial^{\rightarrow}}{\partial s_{j1}'}\right)M_{1j}^{\rightarrow}(s_1',s_1)\right)\\
\times\left(8R_{22}R_{12}^2-4R_{12}R_{22}\sum_{k=1}^{4}S_{k2}^{-1}+4\sum_{j=1}^{3}\left(R_{22}-\frac{\partial^{\rightarrow}}{\partial s_{j1}'}\right)M_{2j}(s_1',s_1)\right)\\
+\frac{16}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\sum_{j=1}^{3}M_{1j}^{\rightarrow}(s_1',s_1)\Bigg(\frac{1}{2}R_{11}R_{12}\left(\mathrm{trg}\,r-\sum_{i=1}^{4}S_{i1}^{-1}\right)\\
+\left(r_{21}-r_{11}-\frac{\partial}{\partial s_{j1}'}\right)\left(R_{22}R_{12}+R_{11}R_{12}+R_{11}R_{21}+\frac{1}{2}(R_{12}+R_{22})\sum_{i=1}^{4}S_{i1}^{-1}\right)\Bigg)\\
-\frac{16}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\sum_{j=1}^{3}M_{2j}^{\rightarrow}(s_1',s_1)\Bigg(\frac{1}{2}R_{11}R_{12}\left(\mathrm{trg}\,r-\sum_{i=1}^{4}S_{i2}^{-1}\right)\\
+\left(r_{21}-r_{11}-\frac{\partial}{\partial s_{j1}'}\right)\left(R_{11}R_{21}+R_{11}R_{12}+R_{12}R_{22}+\frac{1}{2}(R_{12}+R_{22})\sum_{i=1}^{4}S_{i2}^{-1}\right)\Bigg)\\
-\frac{16}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\sum_{k=1}^{4}\prod_{i,j}^{2}R_{ij}S_{kj}^{-1}\exp(-r_{11}\,\mathrm{tr}\,s_1')\Phi_3^{(1)}(-is_1',\tilde{r}_1)+C(s,r)\\
+(ir_{12}\leftrightarrow ir_{22}).
\end{aligned} \tag{E3}$$

Again, all operators with an arrow are understood to act only onto the term outside the squared bracket, i.e., onto $\exp(-r_{11}\,\mathrm{tr}\,s_1')\Phi_3^{(1)}(-is_1',\tilde{r}_1)$. In the function $C(s,r)$, we summarized the terms that are expected to arise due to noncommutativity of some operators acting on the integral and some operators acting under the integral. The last two lines in formula (5.9) are examples of such terms

$$
\begin{aligned}
C(s,r) = 4\hat{G}_{44} \exp(\mathrm{tr}\, r_2 s_2 + r_{11}\mathrm{tr} s_1) \int \mathrm{d}\mu_B(s_1', s_1) \prod_{i=1}^{2} R_{2i} \prod_{j=1}^{4} S_{ji} \Bigg[\Bigg(& \frac{1}{\Delta_2^2(ir_2)\Delta_2^3(is_2)} \\
& + \frac{1}{\Delta_2^3(ir_2)\Delta_2^4(is_2)} \Bigg) \sum_{j=1}^{3} \left(R_{11}R_{12} + (R_{11}+R_{12})(r_{21}-r_{11}) - (R_{11}+R_{12}) \frac{\partial^{\rightarrow}}{\partial s_{j1}'} \right) \\
& \times \left(\frac{16}{is_{12}-s_{j1}'} M_{2j}(s_1', s_1) - \frac{16}{is_{22}-s_{j1}'} M_{1j}(s_1', s_1) \right) \\
& - \left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)} + \frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)} \right) \\
& \times \prod_{k=1}^{2} \prod_{j=1}^{3} \left(R_{11}R_{12} + (R_{11}+R_{12})(r_{21}-r_{11}) - (R_{11}+R_{12}) \frac{\partial^{\rightarrow}}{\partial s_{j1}'} \right) \\
& \times \frac{8}{is_{k2}-s_{j1}'} - \left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)} + \frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)} \right) \\
& \times \sum_{j,k}^{3} \left((r_{21}-r_{11}) - \frac{\partial^{\rightarrow}}{\partial s_{j1}'} \right) \left((r_{21}-r_{11}) - \frac{\partial^{\rightarrow}}{\partial s_{k1}'} \right) M_{1j}^{\rightarrow} M_{2k} - \frac{8}{\Delta_2^2(ir_2)\Delta_2^3(is_2)} \\
& \times \sum_{j=1}^{3} \left((r_{21}-r_{11}) - \frac{\partial^{\rightarrow}}{\partial s_{j1}'} \right) \left(\sum_{k=1}^{4} S_{k2}^{-1} M_{j1}^{\rightarrow} - \sum_{k=1}^{4} S_{k1}^{-1} M_{j2} \right) \\
& + \frac{8}{\Delta_2^2(ir_2)\Delta_2^3(is_2)} \left(\sum_{i \neq j} M_{j1} M_{j2}^{\rightarrow} \left(\frac{\partial^{\rightarrow}}{\partial s_{i1}'} - \frac{\partial^{\rightarrow}}{\partial s_{j1}'} \right) \right) \Bigg] \exp(-r_{11}\mathrm{tr} s_1') \Phi_3^{(1)}(-is_1', \tilde{r}_1).
\end{aligned}
\tag{E4}
$$

In order to evaluate Eqs. (E3) and (E4) we need some more properties of the matrix Bessel function $\Phi_4^{(1)}(-is_1, r_1)$. We investigate the action of $\tilde{L}_k$ on $\Phi_4^{(1)}(-is_1, r_1)$ using the integral representation (5.15).

After a straightforward calculation involving an integration by parts we find

$$
\begin{aligned}
& \tilde{L}_k \exp(-r_{11}\mathrm{tr}\, s_1) \Phi_4^{(1)}(-is_1, r_1) \\
& \quad = \sum_{i=1}^{4} \frac{1}{is_{k2}-s_{i1}} \left((r_{21}-r_{11})^2 + (r_{21}-r_{11}) \frac{\partial}{\partial s_{i1}} \right) \exp(-r_{11}\,\mathrm{tr}\, s_1) \Phi_4^{(1)}(-is_1, r_1).
\end{aligned}
\tag{E5}
$$

Now Eqs. (E3) and (E4) can be enormously simplified by the observation that

$$
((r_{21}-r_{11})L_k - \tilde{L}_k) \exp(-r_{11}\mathrm{tr} s_1) \Phi_4^{(1)}(-is_1, r_1) = 0, \tag{E6}
$$

which follows directly from Eq. (E5). We find for Eq. (E3)

$$\Phi_{44}(-is,r)=4\hat{G}_{44}\exp(\mathrm{tr}\, r_2 s_2+r_{11}\mathrm{tr} s_1)\int \mathrm{d}\mu_B(s_1',s_1)\prod_{i=1}^{2} R_{1i}\prod_{k=1}^{4} S_{ki}$$
$$\times\Bigg[\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)\left(R_{12}R_{11}\left(8R_{12}R_{22}-4R_{22}\sum_{k=1}^{4} S_{k2}^{-1}\right)\right.$$
$$\times\left(8R_{11}R_{21}-4R_{21}\sum_{k=1}^{4} S_{k1}^{-1}+4\sum_{j=1}^{3} M_{1j}^{\rightarrow}(s_1',s_1)\right)$$
$$+R_{12}R_{11}\left(8R_{11}R_{21}-4R_{21}\sum_{k=1}^{4} S_{k1}^{-1}\right)$$
$$\times\left(8R_{22}R_{12}-4R_{22}\sum_{k=1}^{4} S_{k2}^{-1}+4\sum_{j=1}^{3} M_{2j}(s_1',s_1)\right)$$
$$+\sum_{j,i} R_{11}\left(r_{21}-r_{11}-\frac{\partial^{\rightarrow}}{\partial s_{j1}'}\right)M_{1i}^{\rightarrow}(s_1',s_1)M_{2j}(s_1',s_1)$$
$$+\sum_{j,i} R_{12}\left(r_{21}-r_{11}-\frac{\partial^{\rightarrow}}{\partial s_{i1}'}\right)M_{1i}^{\rightarrow}(s_1',s_1)M_{2j}(s_1',s_1)$$
$$+\sum_{j,i} R_{21}R_{22}M_{1j}^{\rightarrow}(s_1',s_1)M_{2i}(s_1',s_1)+\frac{8}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}R_{11}R_{12}$$
$$\times\left(\mathrm{tr} g\, r-\sum_{i=1}^{4} S_{i1}^{-1}\right)\sum_{j=1}^{3}\left(M_{1j}(s_1',s_1)-M_{2j}(s_1',s_1)\right)$$
$$\left.-\frac{16}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\sum_{k=1}^{4}\prod_{i,j}^{2} R_{ij}S_{kj}^{-1}\right]$$
$$\times\exp(-r_{11}\mathrm{tr}\, s_1')\Phi_3^{(1)}(-is_1',\tilde{r}_1)+C(s,r)+(ir_{12}\leftrightarrow ir_{22}). \tag{E7}$$

The terms contained in Eq. (E4) simplify, too. We arrive at

$$C(s,r)=4\hat{G}_{44}\exp(\mathrm{tr}\, r_2 s_2+r_{11}\,\mathrm{tr}\, s_1)\int \mathrm{d}\mu_B(s_1',s_1)\prod_{i=1}^{2} R_{1i}\prod_{j=1}^{4} S_{ji}$$
$$\times\Bigg[\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^3(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\right)$$
$$\times\sum_{j=1}^{3}\left(R_{11}R_{12}+(R_{11}+R_{12})(r_{21}-r_{11})-(R_{11}+R_{12})\frac{\partial^{\rightarrow}}{\partial s_{j1}'}\right)$$
$$\times\left(\frac{16}{is_{12}-s_{j1}'}M_{2j}(s_1',s_1)-\frac{16}{is_{22}-s_{j1}'}M_{1j}(s_1',s_1)\right)$$
$$-\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)$$
$$\times\prod_{\substack{k=1\\ j=1}}^{2}\left(R_{11}R_{12}+(R_{11}+R_{12})(r_{21}-r_{11})-(R_{11}+R_{12})\frac{\partial^{\rightarrow}}{\partial s_{j1}'}\right)$$
$$\left.\times\frac{8}{is_{k2}-s_{j1}'}+\frac{8}{\Delta_2^2(ir_2)\Delta_2^3(is_2)}\left(\sum_{i\neq j} M_{j1}^{\rightarrow}(s_1',s_1)M_{j2}(s_1',s_1)\left(\frac{\partial^{\rightarrow}}{\partial s_{i1}'}-\frac{\partial^{\rightarrow}}{\partial s_{j1}'}\right)\right)\right]$$
$$\times\exp(-r_{11}\mathrm{tr}\, s_1')\Phi_3^{(1)}(-is_1',\tilde{r}_1). \tag{E8}$$

To further evaluate the expressions, we can now invoke a symmetry argument between the eigenvalues r_{11} and r_{21}, respectively. Since the product $R_{11}R_{12}$ appears as a prefactor in front of the integral (E7), $R_{21}R_{22}$ must also appear as a prefactor in the final result. Thus, all terms in Eqs. (E7) and (E8) which do not contain $R_{21}R_{22}$ as a factor must yield zero. The remaining terms which are proportional to $R_{21}R_{22}$ can again be treated using formulas (4.7) and (5.9). However, we want to show explicitly that this line of arguing is correct and that the other terms indeed vanish. To this end, we need an additional identity to treat the operator product

$$\sum_{j=1}^{2} \frac{\partial^{\rightarrow}}{\partial s'_{j1}} M_{1j}(s'_1,s_1) \sum_{k=1}^{2} M_{2k}(s'_1,s_1). \tag{E9}$$

The required identity is given by the following formula: The same conditions as for formula (4.7) apply, furthermore we define

$$L_m^{\rightarrow}(s)\tilde{L}_n(s) = \sum_{i,j} \frac{1}{(is_{m2}-s_{i1})(is_{n2}-s_{j1})} \frac{\partial^3}{\partial s_{i1}\partial s_{j1}^2} + \frac{1}{2}\sum_{i,j} \frac{1}{(is_{m2}-s_{i1})(is_{n2}-s_{j1})} \times \frac{\partial}{\partial s_{i1}} \sum_{k\neq j}^{k_1} \frac{1}{s_{j1}-s_{k1}} \left(\frac{\partial}{\partial s_{j1}} - \frac{\partial}{\partial s_{k1}} \right). \tag{E10}$$

Then we have

$$\begin{aligned} & L_m^{\rightarrow}(s)\tilde{L}_n(s) \int_{s_{11}}^{s_{21}} \cdots \int_{s_{(k_1-1)1}}^{s_{k_1 1}} \mu_B(s',s)\mathrm{d}[s'_1] f(s'_1) \\ &= \int_{s_{11}}^{s_{21}} \cdots \int_{s_{(k_1-1)1}}^{s_{k_1 1}} \Bigg[\sum_{j=1}^{k_1-1} \sum_{i=1}^{k_1-1} M_{mi}^{\rightarrow}(s'_1,s_1) \frac{\partial^{\rightarrow}}{\partial s'_{j1}} M_{nj}(s'_1,s_1) f(s'_1) - \frac{1}{is_{n2}-is_{m2}} \\ &\times \sum_{i=1}^{k_1-1} \left(\frac{1}{is_{m2}-s'_{i1}} \frac{\partial^{\rightarrow}}{\partial s'_{i1}} M_{ni}(s'_1,s_1) - \frac{1}{is_{n2}-s'_{i1}} \frac{\partial^{\rightarrow}}{\partial s'_{i1}} M_{mi}(s'_1,s_1) \right) \\ &- \frac{1}{2}\sum_{k\neq l} \frac{1}{(is_{m2}-s'_{k1})(is_{n2}-s'_{k1})(s'_{k1}-s'_{l1})^2} \frac{\partial^{\rightarrow}}{\partial s_{k1}} \\ &+ \frac{1}{2}\sum_{k\neq l} \frac{1}{(is_{m2}-s'_{k1})(is_{n2}-s'_{l1})(s'_{k1}-s'_{l1})^2} \frac{\partial^{\rightarrow}}{\partial s_{k1}} \Bigg] f(s'_1)\mu_B(s',s)\mathrm{d}[s'_1]. \end{aligned} \tag{E11}$$

The proof is similar to the one of formula (4.7). We notice that the arrow in Eq. (E10) is used slightly differently than previously. The operator $L_m^{\rightarrow}(s)$ acts also on a part of $\tilde{L}_n(s)$. This is not consistent with the definition in Eq. (5.6). However, since this is obvious where it occurs, we still use the same arrow. We can now translate the left-hand side of Eq. (E8) into an expression in terms of $\Phi_4^{(1)}(-is,r)$. After some further manipulations involving the identities in Eqs. (E6), (E1), and (E2) we arrive at

$$\Phi_{44}(-is,r)=\hat{G}_{44}\exp(\mathrm{tr}\, r_2 s_2+r_{11}\,\mathrm{tr}\, s_1)\prod_{i,j}^{2} R_{ji}\prod_{k=1}^{4} S_{ki}\Bigg[\left(\frac{1}{\Delta_2^2(ir_2)\Delta_2^2(is_2)}+\frac{1}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\right)$$
$$\times\left(8R_{12}R_{22}-4R_{22}\sum_{k=1}^{4} S_{k2}^{-1}-4L_2(s)\right)\left(8R_{11}R_{21}-4R_{21}\sum_{k=1}^{4} S_{k1}^{-1}-4L_1(s)\right)$$
$$-\frac{8}{\Delta_2^3(ir_2)\Delta_2^4(is_2)}\left(\mathrm{trg}\, r-\sum_{i=1}^{4} S_{i1}^{-1}\right)(L_1(s)-L_2(s))$$
$$-\frac{16}{\Delta_2^3(ir_2)\Delta_2^3(is_2)}\sum_{k=1}^{4}\prod_{j=1}^{2} R_{2j}S_{kj}^{-1}\Bigg]\exp(-r_{11}\mathrm{tr}\, s_1')\Phi_4^{(1)}(s_1',\tilde{r}_1)(ir_{12}\leftrightarrow ir_{22}). \tag{E12}$$

After rearranging terms this yields the result (5.18) for $\Phi_{44}(-is,r)$.

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A second look at $U_q(Sl2)$ at third root of unity[a)]

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We revisit the 27-dimensional quotient of $\mathbf{U}_q(Sl2)$ at third roots of unity within a presentation adapted to a Hopf bar-operation. We describe in detail the regular representation and display the Hopf automorphisms and the Hopf bar-operations.
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I. INTRODUCTION

This paper offers a detailed description (regular representation, Hopf automorphisms, and Hopf bar-operations) of the 27-dimensional quotient (called $\mathbf{H}_1$ for brevity) of the archetypical quantum group $\mathbf{U}_q(Sl2)$.[1] Our interest in this object stems from the hope that it governs the basic structure of fermions as suggested by Alain Connes[2]—a fascinating proposal opening crucial perspectives in basic physics: first-principles construction of the Lagrangian of the standard model, computation of the fermion masses, improved supersymmetry—see Ref. 3 for a detailed comment, and Ref. 4 [**IIh**] for a possible scenario. In this perspective one wishes to gather detailed information on $\mathbf{H}_1$ (in the first place on its regular representation—which we computed amongst other features in Ref. 4 independently of Ref. 5. In Ref. 6 we displayed a ''Hopf bar-operation'' Γ making $\mathbf{H}_1$ the complexification of the real Hopf fixpoint-algebra $\mathbf{H}_1^\Gamma$ (or real dimension 27). This feature is congenial to the fact that the inner space real spectral triple of the standard model works with algebras over the reals. In the traditional presentation of $\mathbf{H}_1$—by generators $E,F,K=\exp G$ (E,F,G the quantum coordinates, E and F playing asymmetric roles)—Γ has the somewhat strange expression $\Gamma k=k$, $\Gamma E=-qKF$, $\Gamma F=-qK^{-1}E$ (perhaps responsible for its absence in the literature (see Ref. 7 where other examples are mentioned). However there is a presentation (Ref. 8) of $\mathbf{U}_q(Sl2)$ (or rather of its double-cover) which uses more symmetrical generators x, y, k (specifically $x=-ik^{-1}F$, $y=-iEk$, $k=k^{-2}=K=\exp\frac{1}{2}G$) making Γ the mere exchange of x and y. Our $\mathbf{H}_1$ is obtained by ''halving'' the object of Ref. 8 at sixth root of unity by taking instead the third root (whilst the whole object would give $\mathbf{H}_2$ of Ref. 4)—we also multiplied the two first coordinates by i to get the simple form of Γ. The present more symmetrical description was already signaled in Ref. 6 but not exploited there.

In Sec. II we rewrite the whole theory from scratch in this more limpid langage, displaying the underlying real Hopf algebra $\mathbf{H}_1^\Gamma$ and a still smaller (real 15-dimensional) bialgebra $\mathbf{H}_1^\Gamma\cap\mathbf{H}_1^\Omega$ obtained from a ''pseudo-Hopf bar-operation'' Ω stemming from the fact that the coproduct involves only real numbers in the ''**MNF** basis.''

In Sec. III we display the (scarce) Hopf automorphisms and Hopf bar-operations (unique up to scale), a rigidity result showing that the prospective role of $\mathbf{H}_1$ in physics is largely ''frozen.'' We bypass in the proofs a considerable amount of routine computations expounded in detail in the Marseille preprints[9] available on request.

II. THE 27-DIMENSIONAL HOPF ALGEBRA H_1. REGULAR REPRESENTATION. NILRADICAL AND SEMI-SIMPLE QUOTIENT. HOPF BAR-OPERATION

1. Definition—proposition: (the Hopf algebra $\mathbf{H}_1$ with generators x,y,k).

(i) The complex algebra $\mathbf{H}_1$, coherently defined by generators and relations

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$$\begin{cases} kk^{-1}=k^{-1}k=\mathbb{1}, \\ kx=vxk, \text{ i.e., } kxk^{-1}=vx, \\ ky=v^{-1}yk, \text{ i.e., } kyk^{-1}=v^{-1}y, \\ xy-yx=-\dfrac{k^2-k^{-2}}{v-v^{-1}}, \end{cases} \tag{1a}$$

$$\begin{cases} x^3=0, \\ y^3=0, \\ k^3=\mathbb{1}, \end{cases} \tag{1b}$$

where $v=e^{2\pi i/3}$ (whence $v^3=1$, $v^{-1}=v^2$, and $1+v+v^2=0$) becomes a Hopf algebra with coproduct Δ, antipode S, and counit ϵ such that

$$\begin{cases} \Delta k=k\otimes k, \\ \Delta k^{-1}=k^{-1}\otimes k^{-1}, \\ \Delta x=x\otimes k+k^{-1}\otimes x, \\ \Delta y=y\otimes k+k^{-1}\otimes v \end{cases} \tag{2a}$$

$$\begin{cases} Sk=k^{-1} \\ Sk^{-1}=k, \\ Sx=-vx, \\ Sy=-v^{-1}y, \end{cases} \tag{2b}$$

$$\begin{cases} \epsilon(k)=1, \\ \epsilon(x)=0, \\ \epsilon(y)=0, \end{cases} \tag{2c}$$

and with central Casimir operator.

$$C=-xy+\frac{vk^{-2}+v^{-1}k^2}{(v-v^{-1})^2}=-yx+\frac{v^{-1}k^{-2}+vk^2}{(q-q^{-1})^2}, \tag{3}$$

(ii) The ternary Hopf automorphism

$$S^{-2}=adk \tag{4}$$

yields a $\mathbb{Z}/3$-grading of $\mathbf{H}_1$:

$$\mathbf{H}_1=\mathbf{H}_1^{(0)}\oplus\mathbf{H}_1^{(1)}\oplus\mathbf{H}_1^{(2)},$$

where

$$\mathbf{H}_1^{(i)}=\{a\in\mathbf{H}_1;kak^{-1}=v^ia,\ \ i\in\mathbb{Z}/3\} \tag{5}$$

for which $\mathbf{H}_1$ is a $\mathbb{Z}/3$-graded Hopf algebra: one has $\mathbf{H}_1^{(i)}\cdot\mathbf{H}_1^{j}c\mathbf{H}_1^{(i+j)}, i,j\in\mathbb{Z}/3$.

Proof: The coherence of definitions (1a) and (1b) and (2a)–(2c) is classical. For the Casimir operator we refer to *3* below. The fact that S^{-2} is a $\mathbb{Z}/3$-grading of $\mathbf{H}_1$ follows from (2b) implying $S^{-2}k=k$, $S^{-2}k^{-1}=k^{-1}$, $S^{-2}x=vx$, $S^{-2}y=v^{-1}y$ implying (4) by (1a). Commutation with the coproduct is readily checked on generators.

2. Definitions-lemma: (*-operations, Hopf bar-, and pseudo-Hopf bar-operations.)

(i) Setting

$$\begin{cases} k^{*}=k^{-1}, \\ x^{*}=-y, \\ y^{*}=-x, \end{cases} \tag{6a}$$

$$\begin{cases} k^{\underline{*}}=k^{-1}, \\ x^{\underline{*}}=y, \\ y^{\underline{*}}=x \end{cases} \tag{6b}$$

specifies respective*-operations$^{*},^{\underline{*}}$ fulfilling

$$\begin{cases} \Delta\circ *=(*\otimes *)\circ\tau\circ\Delta, \\ S\circ *=*\circ S, \\ \epsilon\circ *=\bar{}\circ\epsilon, \end{cases} \tag{7a}$$

$$\begin{cases} \Delta\circ \underline{*}=(\underline{*}\otimes \underline{*})\circ\tau\circ\Delta, \\ S\circ \underline{*}=\underline{*}\circ S, \\ \epsilon\circ \underline{*}=\bar{}\circ\epsilon. \end{cases} \tag{7b}$$

One has $\underline{*}=*\circ\xi=\xi\circ *$ with $\xi\in \mathrm{Aut}\mathbf{H}_1$ specified by

$$\begin{cases} \xi k=k, \\ \xi x=-x, \\ \xi y=-y. \end{cases} \tag{8}$$

(ii) Setting

$$\begin{cases} \Gamma k=k, \\ \Gamma k^{-1}=k^{-1}, \\ \Gamma x=y, \\ \Gamma y=x, \end{cases} \tag{9a}$$

$$\begin{cases} \Omega k=k^{-1}, \\ \Omega k^{-1}=k, \\ \Omega x=x, \\ \Omega y=y \end{cases} \tag{9b}$$

specifies respective bar-operations (antilinear, multiplicative, involutory) Γ, Ω, Hopf and pseudo-Hopf in the sense

$$\begin{cases} \Delta\circ\Gamma=(\Gamma\otimes\Gamma)\circ\Delta, \\ S\circ\Gamma=\Gamma\circ S, \\ \epsilon\circ\Gamma=\bar{}\circ\epsilon, \end{cases} \tag{10a}$$

$$\begin{cases} \Delta\circ\Omega=(\Omega\otimes\Omega)\circ\Delta, \\ S\circ\Omega=\Omega\circ S^{-1}, \\ \epsilon\circ\Omega=\bar{}\circ\epsilon. \end{cases} \tag{10b}$$

(iii) The maps $*,^{\underline{*}}$, Γ, Ω, ξ all commute.

(iv) Let $\mathbf{H}_1^{\Gamma}$, respectively, $\mathbf{H}_1^{\Omega}$, be the sets of fix points of $\mathbf{H}_1$ under Γ, respectively Ω, and consider $\mathbf{H}_1$ as an algebra over the reals. Then $\mathbf{H}_1^{\Gamma}$ and $\mathbf{H}_1^{\Omega}$ (and thus $\mathbf{H}_1^{\Gamma}\cap\mathbf{H}_1^{\Omega}$) are real subalgebras of $\mathbf{H}_1$, all three mapped by Δ into their tensor squares. Furthermore one has the inclusion $S\mathbf{H}_1^{\Gamma}\subset\mathbf{H}_1^{\Gamma}$ (however $S\mathbf{H}_1^{\Omega}\not\subset\mathbf{H}_1^{\Omega}$, $S\mathbf{H}_1^{\Gamma}\cap\mathbf{H}_1^{\Omega}\not\subset\mathbf{H}_1^{\Gamma}\cap\mathbf{H}_1^{\Omega}$). Consequently $\mathbf{H}_1^{\Gamma}$ is a real Hopf algebra under Δ, ϵ, and S, and $\mathbf{H}_1^{\Omega}$ and $\mathbf{H}_1^{\Gamma}\cap\mathbf{H}_1^{\Omega}$ are real bialgebras under Δ and ϵ.

The real Hopf nature of $\mathbf{H}_1^{\Gamma}$ stemming from the existence of the Hopf bar-operation Γ is a basic feature of $\mathbf{H}_1$, thus obtained (as a complex Hopf algebra) by ''complexifying'' a real Hopf algebra of the same (now real) dimension. This fact has important consequences, amongst others a tendency of purely algebraically defined representations to become *-representations on appropriate Hilbert spaces. The bialgebra nature of both $\mathbf{H}_1^{\Omega}$ and $\mathbf{H}_1^{\Gamma}\cap\mathbf{H}_1^{\Omega}$ sheds light on the nature of the coproduct.

Proof: Straightforward verifications.

3 Proposition (generators x, y, e_0, e_1, e_2)*:* $\mathbf{H}_1$ has the alternative generators x, y, e_0, e_1, e_2 such that

$$\begin{cases} 3e_0=\mathbb{1}+k+k^2, \\ 3e_1=\mathbb{1}+vk+v^2k^2, \\ 3e_2=\mathbb{1}+v^2k+vk^2, \end{cases}$$

$$\text{i.e.,}\quad e_i=\Sigma_{m\in\mathbb{Z}/3}v^{im}k^m,\quad i\in\mathbb{Z}/3, \tag{11}$$

$$\begin{cases} \mathbb{1}=e_0+e_1+e_2, \\ k=e_0+v^2e_1+ve_2, \\ k^2=k^{-1}=e_0+ve_1+v^2e_2 \end{cases}$$

$$\text{i.e.,}\quad k^j=\Sigma_{n\in\mathbb{Z}/3}v^{-nj}e_n,\quad j\in\mathbb{Z}/3 \tag{12}$$

with the relations:

$$\begin{cases} e_ie_k=\delta_{ik}e_i, \\ \Sigma_{i=0,1,2}e_i=\mathbb{1}, \end{cases} \tag{13a}$$

$$\begin{cases} xe_i=e_{i-1}x, \\ ye_i=e_{i+1}y, \\ xy-yx=e_2-e_1, \end{cases} \tag{13b}$$

$$\begin{cases} x^3=0, \\ y^3=0, \end{cases} \tag{13c}$$

implying

$$\begin{cases} yx=xy+e_1-e_2, \\ yx^2=x^2y+(e_0-e_2)x, \\ y^2x=xy^2+(e_1-e_0)y, \\ y^2x^2=x^2y^2+(e_1-e_2)xy+e_1, \end{cases} \tag{14a}$$

$$\begin{cases} e_0k=ke_0=e_0, \\ e_1k=ke_1=v^2e_1 \\ e_2k=ke_2=ve_2. \end{cases} \tag{14b}$$

The Casimir operator reads

$$C=C^*=C^{\bar{*}}=\tfrac{1}{3}\mathbb{1}-xy-e_1=\tfrac{1}{3}\mathbb{1}-yx-e_2. \tag{15}$$

Δ, ϵ, S,*, $\bar{*}$, Γ are specified as follows on e_0, e_1, e_2:

$$\begin{cases} \Delta e_0=e_0\otimes e_0+e_1\otimes e_2+e_2\otimes e_1, \\ \Delta e_1=e_1\otimes e_0+e_0\otimes e_1+e_2\otimes e_2, \\ \Delta e_2=e_2\otimes e_0+e_0\otimes e_2+e_1\otimes e_1, \end{cases} \tag{16a}$$

$$\begin{cases} \epsilon e_0 = 1, \\ \epsilon e_1 = 0, \\ \epsilon e_2 = 0, \end{cases} \tag{16b}$$

$$\begin{cases} S e_0 = 0, \\ S e_1 = e_2, \\ S e_2 = e_1, \end{cases} \tag{16c}$$

$$e_i{}^* = e_i, \quad i = 0,1,2, \tag{17a}$$

$$e_i{}^{\underline{*}} = e_i, \quad i = 0,1,2, \tag{17b}$$

$$\begin{cases} \Gamma e_0 = e_0, \\ \Gamma e_1 = e_2, \\ \Gamma e_2 = e_1, \end{cases} \tag{18a}$$

$$\begin{cases} \Omega e_0 = e_0, \\ \Omega e_1 = e_1, \\ \Omega e_2 = e_2. \end{cases} \tag{18b}$$

We now turn to the decomposition of the regular representation of $\mathbf{H}_1$. The technique is based on the remark that projectors on different eigenspaces λ, μ of the central Casimir operator generate principal ideals $\mathbf{I}_\lambda$, $\mathbf{I}_\mu$ such that $\mathbf{I}_\lambda \mathbf{I}_\mu = \mathbf{I}_\mu \mathbf{I}_\lambda = 0$. The eigenvalues $-\frac{2}{3}$ and $\frac{1}{3}$ then generate, respectively, the principal ideal $\mathbf{M} \cong \mathbf{M}_3(\mathbb{C})$ and the radical $\mathbf{N}$ of respective dimensions 9 and 13. Since these eigenvalues of C do not exhaust the 27 dimensions of $\mathbf{H}_1$, there is a five-dimensional "residual space" $\mathbf{F} \cong \mathbf{M}_1(\mathbb{C}) \oplus \mathbf{M}_2(\mathbb{C})$. As a consequence the semisimple quotient $\mathbf{H}_1$ is $\mathbf{H}_1/\mathbf{N} \cong \mathbf{M}_1(\mathbb{C}) \oplus \mathbf{M}_2(\mathbb{C}) \oplus \mathbf{M}_3(\mathbb{C})$.

4 Proposition (ideal $\mathbf{M}$ eigenspace of C to the eigenvalue $-\frac{2}{3}$)*:*

(i) The elements of the eigenspace $\mathbf{M}$ of C to the eigenvalue $-\frac{2}{3}$ are related to each other as shown in the following diagram:

$$\begin{array}{ccccc}
0 & & 0 & & 0 \\
\uparrow y\cdot & & \uparrow y\cdot & & \uparrow y\cdot \\
0 \underset{\cdot x}{\leftarrow} m_{11} = e_1(\mathbb{1} + xy + x^2y^2)e_1 & \underset{\cdot x}{\overset{\cdot y}{\rightleftarrows}} & m_{10} = e_1(\mathbb{1} + xy)ye_0 & \underset{\cdot x}{\overset{\cdot y}{\rightleftarrows}} & m_{12} = e_1y^2e_2 \overset{\cdot y}{\rightarrow} 0 \\
x\cdot \downarrow \uparrow y\cdot & & x\cdot \downarrow \uparrow y\cdot & & x\cdot \downarrow \uparrow y\cdot \\
0 \underset{\cdot x}{\leftarrow} m_{01} = e_0x(\mathbb{1} + xy)e_1 & \underset{\cdot x}{\overset{\cdot y}{\rightleftarrows}} & m_{00} = e_0x(\mathbb{1} + xy)ye_0 & \underset{\cdot y}{\overset{\cdot x}{\rightleftarrows}} & m_{02} = e_0xy^2e_2 \overset{\cdot y}{\rightarrow} 0 \\
x\cdot \downarrow \uparrow y\cdot & & x\cdot \downarrow \uparrow y\cdot & & x\cdot \downarrow \uparrow y\cdot \\
0 \underset{\cdot x}{\leftarrow} m_{21} = e_2x^2e_1 & \underset{\cdot x}{\overset{\cdot y}{\rightleftarrows}} & m_{20} = e_2x^2ye_0 & \underset{\cdot x}{\overset{\cdot y}{\rightleftarrows}} & m_{22} = e_2x^2y^2e_2 \overset{\cdot y}{\rightarrow} 0 \\
x\cdot \downarrow & & x\cdot \downarrow & & x\cdot \downarrow \\
0 & & 0 & & 0
\end{array} \tag{19}$$

$\underline{*}$-symmetric with respect to its first diagonal (elements and arrows):

$$m_{mn}{}^{\underline{*}} = m_{nm}, \quad m,n = 0,1,2. \tag{20}$$

(ii) One has in $\mathbf{M}$ the matrix unit-relations:

$$m_{mn}m_{pq}=\delta_{np}m_{mq}, \quad m,n,p,q=0,1,2. \tag{21}$$

(iii) $\mathbf{M}$ is a principal ideal with central projection

$$e_{\mathbf{M}}=m_{00}+m_{11}+m_{22}, \tag{22}$$

thus with supplementary ideal $\mathbf{M}^{\perp}$.

Proof: Construction of the diagram (19) of the ideal $\mathbf{M}$: starting from the upper right element: $m_{12}=e_1{y^2}_2$, $y^3=0$, and ${e_1}^2=e_1$ implying $Cm_{12}=-\frac{2}{3}m_{12}$, deduce the other elements by means of the arrows.

Matrix units relations (21): $m_{ik}m_{jl}=0$ for $j\neq k$ follows from the orthogonality of the projections e_i. The other relations follow by applying x and y.

We notice the following consequence of the relations (21): the m_{ik}, $i,k=1,0,2$, are either all zero or linearly independent: indeed from (21) it follows $m_{ii}=0\Rightarrow m_{ik}=m_{ki}=0$ for all $k\Rightarrow m_{kk}=0$ for all $k\Rightarrow m_{ij}=0$ for all i and j, with in turn $m_{ik}=0\Rightarrow m_{ii}=0$ with the above vanishing. This remark goes along toward a direct proof of the PBW-theorem which could be accomplished for $\mathbf{H}_1$ in an explicit way without the Diamond Lemma.

5 Proposition (ideal $\mathbf{N}$ eigenspace of C to the eigenvalue $\frac{1}{3}$)*:*

(i) The elements of the eigenspace $\mathbf{N}$ of C to the eigenvalue $\frac{1}{3}$ are mutually related as shown in the following diagram:

$$\begin{array}{ccccccccc}
 & & \begin{matrix}0\\ \uparrow -y\cdot\end{matrix} & & \begin{matrix}0\\ \uparrow -y\cdot\end{matrix} & & & & \\
x_{00}=e_0x^2y^2e_0 & \overset{\cdot y}{\#\rightleftarrows 0}_{\cdot -x} & r_{02}=e_0(1-xy)ye_2 & \overset{\cdot y}{\rightleftarrows}_{\cdot -x} & r_{01}=e_0y^2e_1 & \overset{\cdot y}{\rightarrow}0 & & & \\
\begin{matrix}*\\ -x\cdot\downarrow\uparrow y\cdot\\ 0\end{matrix} & & \begin{matrix}0\\ -x\cdot\downarrow\uparrow y\cdot\end{matrix} & & \begin{matrix}0\\ -x\cdot\downarrow\uparrow y\cdot\end{matrix} & & \begin{matrix}0\\ \uparrow y\cdot\end{matrix} & & \\
0\underset{\cdot -x}{\leftarrow}r_{20}=-e_2x(1+xy)e_0 & \overset{\cdot y}{0\rightleftarrows}_{\cdot -x} & x_{22}=e_2x(1-xy)ye_2 & \overset{\cdot y}{\rightleftarrows}_{\cdot -x} & x_{21}=e_2xy^2e_1 & \overset{\cdot y}{\rightleftarrows 0}_{\cdot -x} & s_{20}=e_2y^2e_0 & \overset{\cdot y}{\rightarrow}0 & \\
-x\cdot\downarrow\uparrow y\cdot & & -x\cdot\downarrow\uparrow y\cdot & & -x\cdot\downarrow\uparrow y\cdot & & -x\cdot\downarrow\uparrow y\cdot & & \\
0\underset{\cdot -x}{\leftarrow}r_{10}=e_1x^2e_0 & \overset{\cdot y}{0\rightleftarrows}_{\cdot -x} & x_{12}=e_1x^2ye_2 & \overset{\cdot y}{\rightleftarrows}_{\cdot -x} & x_{11}=e_1x^2y^2e_1 & \overset{\cdot y}{\rightleftarrows 0}_{\cdot -x} & s_{10}=e_1xy^2e_0 & \overset{\cdot y}{\rightarrow}0 & \\
\begin{matrix}-x\cdot\downarrow\\ 0\end{matrix} & & \begin{matrix}-x\cdot\downarrow\uparrow y\cdot\\ 0\end{matrix} & & \begin{matrix}-x\cdot\downarrow\uparrow y\cdot\\ 0\end{matrix} & & \begin{matrix}0\\ -x\cdot\downarrow\uparrow y\cdot\end{matrix} & & \\
 & 0\underset{\cdot -x}{\leftarrow} & s_{02}=e_0x^2e_2 & \overset{\cdot y}{\rightleftarrows}_{\cdot -x} & s_{01}=e_0x^2ye_1 & \overset{\cdot y}{0\rightleftarrows}_{\cdot -x} & x_{00}=e_0x^2y^2e_0 & \overset{\cdot y}{\#\rightleftarrows 0}_{\cdot -x} & \\
 & & \begin{matrix}x\cdot\downarrow\\ 0\end{matrix} & & \begin{matrix}x\cdot\downarrow\\ 0\end{matrix} & & \begin{matrix}-x\cdot\downarrow\uparrow y\cdot\\ 0\end{matrix} & &
\end{array} \tag{23}$$

This diagram is *-symmetric with respect to its first diagonal (elements and arrows).
(Note that this diagram lies on a cylinder rather than a plane, x_{00},*, and # in the left upper and in the right lower corners being the same).

(ii) The nonvanishing products in $\mathbf{N}$ are

$$\begin{cases} r_{0i}r_{i0}=s_{0i}s_{i0}=x_{00}, \\ r_{i0}r_{0k}=s_{i0}s_{0k}=x_{ik}, \end{cases} \quad i,k=1,2. \tag{24}$$

(iii) $\mathbf{N}$ is an ideal of $\mathbf{H}_1$ consisting of nilpotent elements (of vanishing square). Since $\mathbf{H}_1/\mathbf{N}$ is semisimple (see the following) $\mathbf{N}$ is the radical of $\mathbf{H}_1$.

Proof: (i) Construction of the diagram (23) of the ideal $\mathbf{N}$. Element s_{20}: (15) yields $y^2e_0C=\frac{1}{3}y^2e_0$. Element r_{01}: (15) yields $Ce_0y^2=\frac{1}{3}e_0y^2$. One then use the arrows.

(ii) Nonvanishing products (24) in **N**: Since all arrows starting from x_{00} point to 0 one has $x_{00}h=hx_{00}=0$ for any polynomial in x and y. The relations $r_{10}r_{02}=e_1x^2y=x_{12}$, $s_{20}r_{01}=0$, $s_{02}r_{20}=0$, $s_{02}x_{22}=0$, $s_{02}x_{21}=0$, $s_{02}s_{20}=x_{00}$, $r_{01}x_{12}=0$, $r_{10}s_{02}=0$, $r_{10}s_{01}=0$ are obvious. The others are then obtained using the arrows.

6 Proposition (residual five-dimensional subspace $\mathbf{F}\subset\mathbf{M}^{\perp}$. Modified **PWB** and **MNF** basis)*:* (i) $\mathbf{H}_1$ is linearly spanned by the elements in the diagrams (19) and (23), plus the elements: (diagram *-symmetric with respect to first diagonal) spanning the subspace **F** and yielding the central projection $e_{\mathbf{M}^{\perp}}=\phi_{00}+\phi_{11}+\phi_{22}$,

$$\begin{aligned}&\phi_{00}=e_0(\mathbb{1}-xy-x^2y^2)e_0, \quad \phi_{22}=e_2(\mathbb{1}-x^2y^2)e_2, \quad \phi_{21}=e_2(\mathbb{1}+\tfrac{1}{2}xy)ye_1,\\ &\qquad\qquad \phi_{12}=-e_1x(\mathbb{1}+\tfrac{1}{2}xy)e_2, \quad \phi_{11}=-e_1x(\mathbb{1}+xy)ye_1,\end{aligned} \tag{25}$$

Table displaying the system $\{m_{ik},\phi_{00},\phi_{mn},r_{0m},r_{m0},s_{0m},s_{m0},x_{mn}\}_{i,k=0,1,2;m,n=1,2}$ spanning $\mathbf{H}_1$ [in fact a basis, called the MNF-basis (see the following)]:

$$\begin{aligned}&m_{11}=e_1(\mathbb{1}+xy+x^2y^2)e_1, \quad m_{10}=e_1(y+xy^2)e_0, \quad m_{12}=e_1y^2e_2,\\ &x_{11}=e_1x^2y^2e_1, \quad s_{10}=-e_1xy^2e_0, \quad x_{12}=e_1x^2ye_2,\end{aligned}$$

$$\phi_{11}=-e_1(xy+x^2y^2)e_1, \quad r_{10}=e_1x^2e_0, \quad \phi_{12}=-e_1x(\mathbb{1}+\tfrac{1}{2}xy)e_2.$$

$$\begin{aligned}&m_{01}=e_0(x+x^2y)e_1, && m_{00}=e_0(xy+x^2y^2)e_0, && m_{02}=e_0xy^2e_2,\\ &s_{01}=e_0x^2ye_1, && x_{00}=e_0x^2y^2e_0, && s_{02}=-e_0x^2e_2,\\ &r_{01}=e_0y^2e_1, && \phi_{00}=e_0(\mathbb{1}-xy-x^2y^2), && r_{02}=e_0(y-xy^2)e_2,\\ &m_{21}=e_2x^2e_1, && m_{20}=e_2x^2ye_0, && m_{22}=e_2x^2y^2e_2,\\ &x_{21}=-e_2xy^2e_1, && s_{20}=e_2y^2e_0, && x_{22}=-e_2(xy-x^2y^2)e_2,\\ &\phi_{21}=e_2(\mathbb{1}+\tfrac{1}{2}xy)ye_1, && r_{20}=-e_2(x-x^2y)e_0, && \phi_{22}=e_2(\mathbb{1}-x^2y^2)e_2.\end{aligned} \tag{26}$$

The system $\{e_ix^py^q\}_{i,p,q=0,1,2}$ is given as follows in terms of the system (26):

$$\begin{cases}e_0=m_{00}+\phi_{00},\\ e_1=m_{11}+\phi_{11},\\ e_2=m_{22}+\phi_{22},\end{cases}$$

$$\begin{cases}e_0x=m_{01}-s_{01},\\ e_1x=-\phi_{12}-\tfrac{1}{2}x_{12},\\ e_2x=m_{20}-r_{20},\end{cases} \quad \begin{cases}e_0y=m_{02}+r_{02},\\ e_1y=m_{10}+s_{10},\\ e_2y=\phi_{21}+\tfrac{1}{2}x_{21},\end{cases}$$

$$\begin{cases}e_0x^2=s_{02},\\ e_1x^2=r_{10},\\ e_2x^2=m_{21},\end{cases} \quad \begin{cases}e_0xy=m_{00}-x_{00},\\ e_1xy=-\phi_{11}-x_{11},\\ e_2xy=m_{22}-x_{22},\end{cases} \quad \begin{cases}e_0y^2=r_{01},\\ e_1y^2=m_{12},\\ e_2y^2=s_{20},\end{cases} \tag{27}$$

$$\begin{cases}e_0x^2y=-s_{01},\\ e_1x^2y=x_{12},\\ e_2x^2y=m_{20},\end{cases} \quad \begin{cases}e_0xy^2=m_{02},\\ e_1xy^2=-s_{01},\\ e_2xy^2=-x_{21},\end{cases}$$

$$\begin{cases}e_0x^2y^2=x_{00},\\ e_1x^2y^2=x_{11},\\ e_2x^2y^2=m_{22}.\end{cases}$$

The tabulation (26) is arranged according to polynomial order: here is an alternative version arranged according to indices which reveals the splitting of the coordinate change:

$$\begin{array}{lll}
e_1\mathbb{1}=m_{11}+\phi_{11}, & e_1y=m_{10}+s_{10}, & e_1x=-\phi_{12}-\tfrac{1}{2}x_{12},\\
e_1xy=\phi_{11}-x_{11}, & e_1x^2=r_{10}, & e_1y^2=m_{12},\\
e_1x^2y^2=x_{11}, & e_1xy^2=-s_{10}, & e_1x^2y=x_{12},\\
e_0x=m_{01}-s_{01}, & e_0\mathbb{1}=m_{00}+\phi_{00}, & e_0y=m_{02}+r_{02},\\
e_0y^2=r_{01}, & e_0xy=m_{00}-x_{00}, & e_0x^2=s_{02},\\
e_0x^2y=s_{01}, & e_0x^2y^2=x_{00}, & e_0xy^2=m_{02},\\
e_2y=\phi_{21}+\tfrac{1}{2}x_{21}, & e_2x=m_{20}-r_{20}, & e_2\mathbb{1}=m_{22}+\phi_{22},\\
e_2x^2=m_{21}, & e_2y^2=s_{20}, & e_2xy=m_{22}-x_{22},\\
e_2xy^2=-x_{21}, & e_2x^2y=m_{20}, & e_2x^2y^2=m_{22}.
\end{array} \tag{28}$$

(ii) The nonvanishing products in **F** are as follows:

$$\begin{cases} \phi_{00}\phi_{00}=\phi_{00},\\ \phi_{mn}\phi_{nj}=\phi_{mj}, \end{cases} \quad m,\ j=1,2. \tag{29}$$

(iii) Additional nonvanishing products in $\mathbf{M}^{\perp}$ (products **MN** and **NM**):

$$\begin{cases} \phi_{ij}r_{jk}=r_{ik}\\ \phi_{ij}s_{jk}=s_{ik}\\ \phi_{ij}x_{jk}=x_{ik} \end{cases} \quad \begin{cases} r_{ij}\phi_{jk}=r_{ik}\\ s_{ij}\phi_{jk}=s_{ik}, \\ x_{ij}\phi_{jk}=x_{ik} \end{cases} \quad i,j,k=1,2,0, \text{ whenever these make sense.} \tag{30}$$

In particular ϕ_{00}, ϕ_{11}, and ϕ_{22} acting on the right (left) are the respective projections on $e_0\mathbf{M}^{\perp}$, $e_1\mathbf{M}^{\perp}$, and $e_2\mathbf{M}^{\perp}$ (on $\mathbf{M}^{\perp}e_0$, $\mathbf{M}^{\perp}e_1$, and $\mathbf{M}^{\perp}e_2$); we have

$$m_{22}+m_{00}+m_{11}+\phi_{22}+\phi_{00}+\phi_{11}=e_{\mathbf{M}}+e_{\mathbf{M}^{\perp}}=\mathbb{1}. \tag{31}$$

(iv) In fact both generating systems (25) and (26) are linearly independent: they thus yield basis of $\mathbf{H}_1$, the respective *MNF-basis* and *modified PBW-basis* (the *PBW-basis* is the system $\{k^px^my^n\}_{p,m,n=0,1,2}$). $\mathbf{H}_1$ is thus 27-dimensional.

Proofs (i) and (ii): Construction of the residual five-dimensional subspace **F**): we need additional $5=27-9-13$ elements (expected to span $\mathbf{M}_1\oplus\mathbf{M}_2$) to get a basis of $\mathbf{H}_1$ together with the above elements of **M** and **N**. The inventory of the latter is given by (26). Computation of the additional elements ϕ_{00}, ϕ_{22}, ϕ_{21}, ϕ_{12}, ϕ_{11}:

Diagonal $\phi_{ii}=\alpha e_i+\beta m_{ii}+\gamma x_{ii}$.

We want $0=e_{\mathbf{M}}\phi_{ii}=\alpha m_{ii}+\beta m_{ii}$, whence $\alpha+\beta=0$: we have $\phi_{ii}=\alpha(e_i-m_{ii})+\gamma x_{ii}$.

We want $0=\phi_{ii}{}^2-\phi_{ii}=\alpha^2(e_i-m_{ii})+2\alpha\gamma x_{ii}-\alpha(e_i-m_{ii})-\gamma x_{ii}=\alpha(\alpha-1)(e_i-m_{ii})+(2\alpha-1)\gamma x_{ii}$. Multiplying by x_{ii} shows that $\alpha(\alpha-1)=0$, $\alpha=0$ is excluded, thus $\alpha=1$, implying vanishing of $(2\alpha-1)\gamma=\gamma$: we end up with $\phi_{ii}=e_i-m_{ii}$: we find

$$\phi_{11}=e_1-m_{11}=-e_1(xy+x^2y^2)e_1,$$

$$\phi_{00}=e_0-m_{00}=e_0(\mathbb{1}-xy-x^2y^2)e_0,$$

$$\phi_{22}=e_2-m_{22}=e_2(\mathbb{1}-x^2y^2)e_2.$$

Off-diagonal $\phi_{12}=\lambda e_1x+\mu m_{12}+\nu x_{12}$, and $\phi_{21}=\lambda' e_2y+\mu' m_{21}+\nu' x_{21}$.

We want $0=e_{\mathbf{M}}\phi_{12}=\lambda m_{11}x+\mu m_{12}=0+\mu m_{12}$: this reads $\mu=0$,

$$0=e_{\mathbf{M}}\phi_{21}=\lambda' m_{22}y+\mu' m_{21}=0+\mu' m_{21}:\ \text{this reads}\ \ \mu'=0$$

where we used $m_{11}x=m_{22}y=0$ [cf. diagram (19)].

We have then on the one hand $\phi_{11}\phi_{12}=\phi_{12}\phi_{22}=\phi_{12}$, since, by (19):

$$m_{11}\phi_{12}=m_{11}(\lambda e_1 x+\nu x_{12})=\lambda m_{11}x=0,\ \text{and}\ \ \phi_{12}m_{22}=(\lambda e_1 x+\nu x_{12})m_{22}=\lambda x m_{22}=0$$

and on the other hand $\phi_{22}\phi_{21}=\phi_{21}\phi_{11}=\phi_{21}$, since by (18):

$$m_{22}\phi_{21}=m_{22}(\lambda' e_2 y+\nu' x_{21})=\lambda' m_{22}y=0,\ \text{and}\ \ \phi_{21}m_{11}=(\lambda' e_2 y+\nu' x_{21})m_{11}=\lambda' y m_{11}=0.$$

We want in addition $\phi_{12}\phi_{21}=\phi_{11}$, and $\phi_{12}\phi_{21}=\phi_{11}$: now, since, using (13b) and (23),

$$\begin{aligned}\phi_{12}\phi_{21}&=(\lambda e_1 x+\nu x_{12})(\lambda' e_2 y+\nu' x_{21})=\lambda\lambda' e_1 xy+\lambda\nu' e_1 x x_{21}+\lambda'\nu e_1 x_{12}y\\&=\lambda\lambda' e_1 xy-\lambda\nu' x_{11}+\lambda'\nu x_{11}=e_1[\lambda\lambda' xy-(\lambda\nu'-\lambda'\nu)x^2y^2].\end{aligned}$$

The first requirement leads to $\lambda\lambda'=-1$ and $\lambda\nu'-\lambda'\nu=1$; and since, using (14),

$$\begin{aligned}\phi_{21}\phi_{12}&=(\lambda' e_2 y+\nu' x_{21})(\lambda e_1 x+\nu x_{12})=\lambda\lambda' e_2 yx+\lambda'\nu e_2 y x_{12}+\lambda\nu' e_2 x_{21}x\\&=\lambda\lambda' e_2(xy+e_1-e_2)e_2+(\lambda'\nu-\lambda\nu')x_{22}=\lambda\lambda' e_2(xy-\mathbb{1})e_2-(\lambda'\nu-\lambda\nu')x_{22}\\&=\lambda\lambda' e_2(xy-\mathbb{1})e_2-(\lambda'\nu-\lambda\nu')e_2(x^2y^2-xy)e_2,\end{aligned}$$

the second leads to to the same relations $\lambda\lambda'=-1$, $\lambda\overline{\lambda'}=\lambda'\nu-\lambda\nu'$ and $\lambda\nu'-\lambda'\nu=1$. The symmetry $\phi_{21}{}^*=\phi_{12}$ is impossible [would require $\lambda\overline{\lambda}=-1$, cf. (17a) and (17b)]. We require *-symmetry, $\lambda'=1$, $\lambda=-1$ then yields (25), whence (26)–(28). (iii): ϕ_{ii} bilaterally acts on $\mathbf{M}^\perp$ e_i as follows from $\phi_{ii}=e_i-m_{ii}$. Further ϕ_{21}, respectively, ϕ_{12} act bilaterally on $\mathbf{M}$ like $e_2 y e_1$, respectively, $e_1 x e_2$, cf. (26), since by (22) $x_{21}\mathbf{N}=\mathbf{N}x_{21}=0$, and $x_{12}\mathbf{N}=\mathbf{N}x_{12}=0$: (28) for $i\neq j$ then proceeds from the arrows $\overset{y}{\rightarrow}$ and $\underset{-x}{\leftarrow}$.

(iv) By the PWB-theorem ordered monomials (we chose the order *kxy*) build the PWB-basis, the relations (11) and (12) yielding the *modified PWB*-basis. The mutual correspondence (26) and (27) then yield the MNF basis.

7 Additional features of $\mathbf{H}_1$. We state for completeness miscellaneous results which are established as in Ref. 4 [**IIb**] to which the reader is referred for proofs.

(i) (Center of $\mathbf{H}_1$). The center $\mathbf{Z}_1$ of $\mathbf{H}_1$ is

$$\mathbf{Z}_1=\mathbb{C}e_{\mathbf{M}}\oplus\mathbb{C}e_{\mathbf{M}^\perp}\oplus\mathbb{C}x_{00}\oplus\mathbb{C}W\quad(W=x_{22}+x_{11}).\tag{32}$$

In this context the Casimir operator C is written as

$$C=-\tfrac{2}{3}e_{\mathbf{M}}+\tfrac{1}{3}e_{\mathbf{M}^\perp}+x_{00}+x_{22}+x_{11}.\tag{33}$$

The cental idempotents of $\mathbf{H}_1$ are 0, $e_{\mathbf{M}}$, $e_{\mathbf{M}^\perp}$, and $e_{\mathbf{M}}+e_{\mathbf{M}^\perp}=\mathbb{1}$. Consequently the ideals $\mathbf{M}$ and $\mathbf{M}^\perp$ are left stable by all automorphisms of $\mathbf{H}_1$.

(ii) (The linear form Tr_λ and the semipositive scalar product $(\cdot,\cdot)$.) The trace Tr_λ of the left regular representation λ of $\mathbf{H}_1$ on itself: vanishes on $\mathbf{N}$, and passes to the semisimple quotient $\mathbf{H}_1/\mathbf{N}\cong\mathbf{M}_1(\mathbb{C})\oplus\mathbf{M}_2(\mathbb{C})\oplus\mathbf{M}_3(\mathbb{C})$ (or restricts to the isomorphic sub-algebra $\mathbf{A}=\mathbf{M}\oplus\mathbf{F}$) as $6\mathrm{tr}_{\mathbf{M}_1}\oplus 6\mathrm{tr}_{\mathbf{M}_2}\oplus 3\mathrm{tr}_{\mathbf{M}_3}$, where $\mathrm{tr}_{\mathbf{M}_n}$ denotes the usual trace of $n\times n$ matrices yielding the semi-positive scalar product $\langle\cdot,\cdot,\rangle$ in conjunction with the *-operation $\times$:

$$\langle a,b\rangle=\mathrm{Tr}_\lambda(a\times b),\quad a,b\in H_1,\tag{34}$$

$$\begin{cases} \times = \overset{*}{-} & \text{in restriction to } \mathbf{M}, \\ \times = * & \text{in restriction to } \mathbf{M}^{\perp}. \end{cases} \tag{35}$$

This scalar product has the nilradical **N** as his space of null-vectors and is positive-definite in restriction to $\mathbf{A}=\mathbf{M}\oplus\mathbf{F}$ which thereby acquires a Hilbert space structure. Here the trace of matrices is the sum of their diagonal elements with the traces of endomorphisms of finite-dimensional vector spaces the trace of their matrices. In spite of the apparently ad hoc definition (35) the Hilbert space topology of **M** is canonical: this topology indeed also stems from the adjoint representation of $\mathbf{H}_1$, cf. Ref. 4 [**IId**].

Note the fact that the nilradical consists of the nullvectors of a semipositive scalar product—a phenomenon which we also observed at fourth root of the unit[11] and which also shows up with the longitudinal photons of Lorentz-gauge electrodynamics. We propose this ''synonimy of positivity and semisimplicity as an axiom of the ''medusae'' (=generalized supermanifolds, which it would be interesting to define precisely and axiomatize as Alain Connes did for the spin manifolds.[2]

8 Proposition (antipode in *MNF*-basis) (i) (Antipode in *M*)*:* One has

$$\begin{gathered} Sm_{11}=m_{22}, \quad Sm_{10}=-v^{-1}m_{02}, \quad Sm_{12}=vm_{12}, \\ Sm_{01}=-vm_{20}, \quad Sm_{00}=m_{00}, \quad Sm_{02}=-v^{-1}m_{10}, \\ Sm_{21}=-v^{-1}m_{21}, \quad Sm_{20}=-vm_{01}, \quad Sm_{22}=m_{11}. \end{gathered} \tag{36}$$

(ii) (antipode in **N**). One has

$$\begin{array}{llll} Sx_{00}=x_{00}, & Sr_{02}=-v^{-1}s_{10}, & Sr_{01}=vs_{20}, & \\ Sr_{20}=-vs_{01}, & Sx_{22}=x_{11}, & Sx_{21}=v^{-1}x_{21}, & Ss_{20}=vr_{01}, \\ Sr_{10}=v^{-1}s_{02}, & Sx_{12}=-vx_{12}, & Sx_{11}=x_{22}, & Ss_{10}=v^{-1}r_{02}, \\ & Ss_{02}=v^{-1}r_{10}, & Ss_{01}=-vr_{20}, & Sx_{00}=x_{00}. \end{array} \tag{37}$$

(iii) (antipode in **F**). One has
$S\phi_{00}=\phi_{00}$

$$\begin{gathered} S\phi_{22}=\phi_{11}, \quad S\phi_{21}=-v^{-1}\phi_{21}, \\ S\phi_{12}=-v\phi_{12}, \quad S\phi_{11}=\phi_{22} \end{gathered} \tag{38}$$

(note that *S* maps $\mathbf{H}_1^{(0)}$ into itself and exchanges $\mathbf{H}_1^{(1)}$ and $\mathbf{H}_1^{(2)}$).

Proof: Straightforward verifications. Notice that one has $S\mathbf{H}_1^{\Gamma}\subset\mathbf{H}_1^{\Gamma}$.

9 Proposition (Hopf bar-operation in **MNF**-basis)*:* The Hopf bar-operation Γ leaves **M**, **N**, and **F** stable, acting there as follows:

(i) in (18) Γ is symmetry with respect to the diagram centrum:

$$\begin{gathered} \Gamma m_{11}=m_{22}, \quad \Gamma m_{10}=m_{20}, \quad \Gamma m_{12}=m_{21}, \\ \Gamma m_{01}=m_{02}, \quad \Gamma m_{00}=m_{00}, \quad \Gamma m_{02}=m_{01}, \\ \Gamma m_{21}=m_{12}, \quad \Gamma m_{20}=m_{10}, \quad \Gamma m_{22}=m_{11}. \end{gathered} \tag{39}$$

(ii) In (22) Γ is symmetry with respect to diagram centrum with a sign-change for the pairs (r_{02},s_{01}), (r_{20},s_{10}) *and* (x_{21},x_{12}):

$$\begin{array}{llll} \Gamma x_{00}=x_{00}, & \Gamma r_{02}=-s_{01}, & \Gamma r_{01}=s_{02}, & \\ \Gamma r_{20}=-s_{10}, & \Gamma x_{22}=x_{11}, & \Gamma x_{21}=-x_{12}, & \Gamma s_{20}=r_{10}, \\ \Gamma r_{10}=s_{20}, & \Gamma x_{12}=-x_{21}, & \Gamma x_{11}=x_{22}, & \Gamma s_{10}=-r_{20}, \\ & \Gamma s_{02}=r_{01}, & \Gamma s_{01}=-r_{02}, & \Gamma x_{00}=x_{00}. \end{array} \tag{40}$$

(iii) In (25) Γ is given by
$\Gamma\phi_{00}=\phi_{00}$,

$$\begin{array}{ll} \Gamma\phi_{22}=\phi_{11}, & \Gamma\phi_{21}=-\phi_{12}, \\ \Gamma\phi_{12}=-\phi_{21}, & \Gamma\phi_{11}=\phi_{22}. \end{array} \tag{41}$$

Proof: Straightforward verifications.

10 Remark (pseudo-Hopf bar-operation in the **MNF**-basis)*:* The pseudo-Hopf bar-operation Ω leaves unchanged each of the elements of the **MNF** basis because these are products of the e_i by polynomials in x and y with real coefficients, the multiplicative antilinear Ω leaving all these invariant, cf. (9) and (18b).

11 Proposition (the real Hopf algebra $\mathbf{H}_1^\Gamma$)*:* As an algebra over $\mathbb{R}$ $\mathbf{H}_1^\Gamma$ is the direct sum $\mathbf{F}^\Gamma \oplus \mathbf{M}^\Gamma \oplus \mathbf{N}^\Gamma$, where, as real algebras:

(i) $\mathbf{M}^\Gamma \cong \mathbf{M}_3(\mathbb{R})$ with the matrix units:

$$\begin{array}{lll} \mu_{11}=\frac{1}{2}(m_{11}+m_{22}-m_{12}-m_{21}), & \mu_{10}=\frac{1}{i\sqrt{2}}(m_{10}-m_{20}), & \mu_{12}=\frac{1}{2i}(m_{11}-m_{22}+m_{12}-m_{21}), \\ \mu_{01}=\frac{i}{\sqrt{2}}(m_{01}-m_{02}), & \mu_{00}=m_{00}, & \mu_{02}=\frac{1}{\sqrt{2}}(m_{01}+m_{02}), \\ \mu_{21}=\frac{i}{2}(m_{11}-m_{22}-m_{12}+m_{21}), & \mu_{20}=\frac{1}{\sqrt{2}}(m_{10}+m_{20}), & \mu_{22}=\frac{1}{2}(m_{11}+m_{22}+m_{12}+m_{21}), \end{array} \tag{42}$$

such that $\mu_{im}\mu_{nj}=\delta_{mn}\mu_{ij}$.

(ia) $\mathbf{M}^\Gamma \cap \mathbf{H}_1^\Omega$ is spanned by μ_{11}, μ_{00}, μ_{02}, μ_{20}, and μ_{22} [thus isomorphic to $\mathbb{R}\oplus\mathbf{M}_3(\mathbb{R})$ as a real algebra].

(ii) $\mathbf{F}^\Gamma \cong \mathbb{R}\oplus\mathbb{H}$, with $\mathbb{R}$ spanned by ϕ_{00} and $\mathbb{H}$ spanned by the

$$1_{\mathrm{H}}=\phi_{22}+\phi_{11}, \quad I=\frac{1}{i}(\phi_{21}+\phi_{12}), \quad J=\phi_{21}-\phi_{12}, \quad K=\frac{1}{i}(\phi_{22}-\phi_{11}) \tag{43}$$

fulfilling the quaternionic relations:

$$1_{\mathrm{H}}1_{\mathrm{H}}=1_{\mathrm{H}}, \tag{44a}$$

$$\begin{cases} 1_{\mathrm{H}}I=I1_{\mathrm{H}}=I, \\ 1_{\mathrm{H}}J=J1_{\mathrm{H}}=J, \\ 1_{\mathrm{H}}K=K1_{\mathrm{H}}=K, \end{cases} \tag{44b}$$

$$\begin{cases} IJ=-JI=-K, \\ JK=-KJ=-I, \\ KI=-IK=-J, \end{cases} \tag{44c}$$

$$\begin{cases} I^2=-1_{\mathrm{H}}, \\ J^2=-1_{\mathrm{H}}, \\ K^2=-1_{\mathrm{H}}. \end{cases} \tag{44d}$$

(iia) $\mathbf{F}^{\Gamma}\cap\mathbf{H}_1^{\Omega}$ is spanned by ϕ_{00}, 1_{H}, and J (thus isomorphic to $\mathbb{R}\oplus\mathbb{C}$ as a real algebra).
(iii) $\mathbf{N}^{\Gamma}$ is spanned by the

$$\begin{cases} x_{00}, \\ x'=x_{11}+x_{22}, \quad x''=\dfrac{1}{i}(x_{11}-x_{22}), \\ y'=x_{21}-x_{12}, \quad y''=\dfrac{1}{i}(x_{21}+x_{12}) \end{cases} \tag{45a}$$

$$\begin{cases} q'=r_{01}+s_{02}, \quad q''=\dfrac{1}{i}(r_{01}-s_{02}), \\ r'=r_{02}-s_{01}, \quad r''=\dfrac{1}{i}(r_{02}+s_{01}), \\ s'=s_{10}-r_{20}, \quad s''=\dfrac{1}{i}(s_{10}+r_{20}), \\ t'=s_{20}+r_{10}, \quad t''=\dfrac{1}{i}(s_{20}-r_{10}) \end{cases} \tag{45b}$$

with nonvanishing products:

$$r's'=-q''t''=r''s''=-2x_{00}, \tag{46a}$$

$$\begin{cases} t'q'=s'r'=t''q''=-s''r''=x', \\ t''q'=-s''r'=-t'q''=-s'r=-x'', \\ s'q'=t'r'=s''q''=t''r''=-y', \\ s''q'=t''r'=-s'q''=t'q''=y''. \end{cases} \tag{46b}$$

(iiia) $\mathbf{N}^{\Gamma}\cap\mathbf{H}_1^{\Omega}$ is spanned by x_{00}, x', y', q', r', s', t'.
(iv) The nonvanishing products between elements of $\mathbf{F}$ and $\mathbf{N}$ are

$$\begin{cases} \phi_{00}x_{00}=x_{00}, \\ \phi_{00}q'=q', \quad \phi_{00}q''=q'', \\ \phi_{00}r'=r', \quad \phi_{00}r''=r'', \end{cases} \tag{47a}$$

$$\begin{cases} x_{00}\phi_{00}=x_{00}, \\ s'\phi_{00}=s', \quad s''\phi_{00}=s'', \\ t'\phi_{00}=t', \quad t''\phi_{00}=t'', \end{cases} \tag{47b}$$

$$\begin{cases} 1_{\mathrm{H}}x'=x', \\ 1_{\mathrm{H}}x''=x'', \\ 1_{\mathrm{H}}y'=y', \\ 1_{\mathrm{H}}y''=y'', \end{cases} \tag{47c}$$

$$\begin{cases} 1_{\mathbb{H}}s' = s', \\ 1_{\mathbb{H}}s'' = s'', \\ 1_{\mathbb{H}}t' = t', \\ 1_{\mathbb{H}}t'' = t'', \end{cases} \tag{47d}$$

$$\begin{cases} x'1_{\mathbb{H}} = x', \\ x''1_{\mathbb{H}} = x'', \\ y'1_{\mathbb{H}} = y', \\ y''1_{\mathbb{H}} = y'', \end{cases} \tag{37e}$$

$$\begin{cases} q'1_{\mathbb{H}} = q', \\ q''1_{\mathbb{H}} = q'', \\ r'1_{\mathbb{H}} = r', \\ r''1_{\mathbb{H}} = r'', \end{cases} \tag{47f}$$

$$\begin{cases} Ix' = y'', & Iy'' = -x', \\ Ix'' = -y', & Iy' = x'', \\ Is' = t'', & It'' = -s', \\ Is'' = -t', & It' = s'', \end{cases} \tag{47g}$$

$$\begin{cases} x'I = y'', & y''I = -x', \\ x''I = -y', & y'I = x'', \\ q'I = r'', & r''I = -q', \\ r'I = q'', & q''I = -r', \end{cases} \tag{47h}$$

$$\begin{cases} Jx' = y', & Jy' = -x', \\ Jx'' = y'', & Jy'' = -x'', \\ Js' = t', & Jt' = -s', \\ Js'' = t'', & Jt'' = -s'', \end{cases} \tag{47i}$$

$$\begin{cases} x'J = y', & y'J = -x', \\ x''J = -y'', & y''J = x'', \\ q'J = -r', & r'J = q', \\ q''J = -r'', & r''J = q'', \end{cases} \tag{47j}$$

$$\begin{cases} Kx' = -x'', & Kx'' = x', \\ Ky' = y'', & Ky'' = -y', \\ Ks' = -s'', & Ks'' = s', \\ Kt' = t'', & Kt'' = -t', \end{cases} \tag{47k}$$

$$\begin{cases} x'K = x'', & x''K = -x', \\ y'K = -y'', & y''K = y', \\ q'K = -q'', & q''K = q', \\ r'K = r'', & r''K = -r'. \end{cases} \tag{47l}$$

Proof: Straightforward verifications.

III. HOPF AUTOMORPHISMS, AND HOPF BAR-OPERATIONS

We now investigate the Hopf automorphisms and the Hopf bar-operations. The Hopf automorphism-group is shown to be a complex one-parameter group—in fact the group of a (truncated) $\mathbb{Z}$-grading with degree the excess of powers of x over those of y in ordered PBW-monomials (with quotient through $3\mathbb{Z}$ the $\mathbb{Z}/3$-group of powers of the antipode). The Hopf bar-operation is unique up to scale. These (relative rigidity) results indicate the kind of freedom one expects in the prospective use of $\mathbf{H}_1$ for describing the basic structure of fermions.

The main technical problem is the classification of the Hopf automorphisms. Our method consists in first exploiting the commutation with the antipode, much simpler than commutation with the coproduct which we use only for passing from the commutant of S in Aut$\mathbf{H}_1$. Section 12 exhibits the (truncated) Hopf $\mathbb{Z}$-grading. Section 13 computes the commutant of S in Aut$\mathbf{H}_1$. Section 14 describes the passage from there to Aut$\mathbf{H}_1$ which turns out to be the group of the truncated $\mathbb{Z}$-grading of Sec. 12. This yields the description of the Hopf bar-operations in 15, found unique up to scale

12 Proposition (the truncated $\mathbb{Z}$-grading $\mathbf{H}_1=\oplus_{n\in\mathbb{Z}}\mathbf{H}_1^{[n]}$ of $\mathbf{H}_1$)*:*

(i) Let $a\in\mathbb{C}$, $a\neq 0$: setting

$$\begin{cases} \alpha_a k=k, \\ \alpha_a k^{-1}=k^{-1}, \\ \alpha_a x=ax, \\ \alpha_a y=a^{-1}y, \end{cases} \tag{48}$$

specifies on generators a Hopf automorphism α_a of $\mathbf{H}_1$ in such a way that $a\to\alpha_a$ is a complex one-parameter group $\mathcal{G}$ of automorphisms of $\mathbf{H}_1$. One has

$$\alpha_a(hh')=(\alpha_a h)(\alpha_a h'), \quad h,h'\in\mathbf{H}_1, \tag{49}$$

$$\alpha_a\alpha_b=\alpha_{ab}, \quad a,b\in\mathbb{C}, \quad ab\neq 0, \tag{50}$$

$$\alpha_1=id_{\mathbf{H}_1}. \tag{51}$$

(ii) Defining

$$\mathbf{H}_1^{[i]}=\{h\in\mathbf{H}_1;\ \ \alpha_a h=a^i h\}, \tag{52}$$

$\mathcal{G}$ is in fact the grading group of a Hopf $\mathbb{Z}$-grading $\mathbf{H}_1=\oplus_{n\in\mathbb{Z}}\mathbf{H}_1^{[n]}$ of $\mathbf{H}_1$ where the degree n measures the excess of powers of x over those of y in ordered polynomials (x written before y). For $h\in\mathbf{H}_1^{[i]}$: we write $\partial_{\mathbb{Z}}=i$ and call i the $\mathbb{Z}$*-degree of* h.

(iii) Division of the Hopf $\mathbb{Z}$-grading through $3\mathbb{Z}$ yields the $\mathbb{Z}/3$-grading $H_1=\oplus_{n\in\mathbb{Z}}H_1^{(n)}$ of H_1 described in *I* (cf. (8) in 1—observe the distinction in notation).

(iv) The Hopf $\mathbb{Z}$-grading of $\mathbf{H}_1$ induces on the subalgebras, $\mathbf{M}$, $\mathbf{F}$, $\mathbf{N}$, and $\mathbf{M}^{\perp}$ respective $\mathbb{Z}$-gradings $\mathbf{M}=\oplus_{n\in\mathbb{Z}}\mathbf{M}^{[n]}$, $\mathbf{F}=\oplus_{n\in\mathbb{Z}}\mathbf{F}^{[n]}$, $\mathbf{N}=\oplus_{n\in\mathbb{Z}}\mathbf{N}^{[n]}$ and $\mathbf{M}^{\perp}=\oplus_{n\in\mathbb{Z}}\mathbf{M}^{\perp[n]}$: one has $\mathbf{H}_1^{[n]}=\mathbf{M}^{[n]}\oplus\mathbf{F}^{[n]}\oplus\mathbf{N}^{[n]}$, $\mathbf{n}\in\mathbb{Z}$, where

$$\begin{cases} \mathbf{M}^{[2]}=\mathbb{C}m_{21}, \\ \mathbf{M}^{[1]}=\mathbb{C}m_{01}+\mathbb{C}m_{20}, \\ \mathbf{M}^{[0]}=\mathbb{C}m_{11}+\mathbb{C}m_{00}+\mathbb{C}m_{22}, \quad \mathbf{M}^{[i]}=\{0\} \ \text{ if } \ i>2 \ \text{ or } \ i<-2, \\ \mathbf{M}^{[-1]}=\mathbb{C}m_{10}+\mathbb{C}m_{02}, \\ \mathbf{M}^{[-2]}=\mathbb{C}m_{12}, \end{cases} \tag{53}$$

$$\begin{cases} \mathbf{F}^{[1]}=\mathbb{C}\phi_{21}, \\ \mathbf{F}^{[0]}=\mathbb{C}\phi_{00}+\mathbb{C}\phi_{22}+\mathbb{C}\phi_{11}, \quad \mathbf{F}^{[i]}=\{0\} \text{ if } i>1 \text{ or } i<-1, \\ \mathbf{F}^{[-1]}=\mathbb{C}\phi_{12}, \end{cases} \tag{54}$$

$$\begin{cases} \mathbf{N}^{[2]}=\mathbb{C}r_{10}+\mathbb{C}s_{02}, \\ \mathbf{N}^{[1]}=\mathbb{C}r_{20}+\mathbb{C}x_{12}+\mathbb{C}s_{01}, \\ \mathbf{N}^{[0]}=\mathbb{C}x_{00}+\mathbb{C}x_{22}+\mathbb{C}x_{11}, \quad \mathbf{N}^{[i]}=\{0\} \text{ if } i>2 \text{ or } i<-2. \\ \mathbf{M}^{[-1]}=\mathbb{C}r_{02}+\mathbb{C}x_{21}+\mathbb{C}s_{10}, \\ \mathbf{M}^{[-2]}=\mathbb{C}r_{01}+\mathbb{C}s_{20}. \end{cases} \tag{55}$$

Remarks: (i) For simplicity the $\mathbb{Z}$-graded algebra $\oplus_{n\in\mathbb{Z}}\mathbf{H}_1^{[n]}$ is denoted by $\mathbf{H}_1$ instead of $\mathbf{H}_1\oplus\{0\}$, and analogously for $\mathbf{M}$, $\mathbf{F}$, $\mathbf{N}$, and $\mathbf{M}^{\perp}$ (the $\mathbb{Z}$-grading is "truncated" in that all but a finite number of $\mathbf{H}_1^{[n]}$ vanish).

(ii) Looked at on the diagrams of $\mathbf{M}$, $\mathbf{N}$, and $\mathbf{F}$ in Sec. I (cf. 1, 2, 3) the $\mathbb{Z}$-grading exhibits the following features: the elements of the same degree are located on lines parallel to the first diagonal, with decreasing grading (from 2 to -2 for $\mathbf{M}$ and $\mathbf{N}$, from 1 to -1 for $\mathbf{F}$) on the second diagonal oriented SW–NE (see the following).

(iii) Replacing in diagrams $\mathbf{M}$ and $\mathbf{F}$ the index 2 by $-1=2\,\mathrm{mod}\,\mathbb{Z}/3$ the degree becomes $\partial_{\mathbb{Z}}m_{ij}=j-i$.

We reproduce those diagrams for the convenience of the reader, and indicate the nonvanishing products.

Diagram **M**			Diagram **N**				Diagram **F**			
			x_{00}	r_{02}	r_{01}					
m_{11}	m_{10}	m_{12}	r_{20}	x_{22}	x_{21}	s_{20}	ϕ_{00}			
m_{01}	m_{00}	m_{02}	r_{10}	x_{12}	x_{11}	s_{10}		ϕ_{11}	ϕ_{12}	
m_{21}	m_{20}	m_{22}		s_{02}	s_{01}	x_{00}		ϕ_{21}		ϕ_{22}

Products in $\mathbf{M}$: $m_{ij}m_{pq}=\delta_{jp}m_{iq}$, $i,j,p,q=1,0,-1$.
Products in $\mathbf{F}$: $\phi_{00}\phi_{00}=\phi_{00}$, $\phi_{00}\phi_{ij}=\phi_{ij}\phi_{00}=0$, $\phi_{pq}=\delta_{jp}\phi_{iq}$, $i,j,p,q=1,-1$.
Other nonvanishing products in: $\mathbf{M}^{\perp}$:

$$\begin{array}{llll} \phi_{00}r_{01}=r_{01}, & \phi_{00}r_{02}=r_{02}, & \phi_{00}s_{01}=s_{01}, & \phi_{00}s_{02}=s_{02}, \\ \phi_{11}r_{10}=r_{10}, & \phi_{11}x_{12}=x_{12}, & \phi_{11}x_{11}=x_{11}, & \phi_{11}s_{10}=s_{10}, \\ \phi_{22}r_{20}=r_{20}, & \phi_{22}x_{22}=x_{22}, & \phi_{22}x_{21}=x_{21}, & \phi_{22}s_{20}=s_{20}, \\ \phi_{12}r_{20}=r_{10}, & \phi_{12}x_{22}=x_{12}, & \phi_{12}x_{21}=x_{11}, & \phi_{12}s_{20}=s_{10}, \\ \phi_{21}r_{10}=r_{20}, & \phi_{21}x_{12}=x_{22}, & \phi_{21}x_{11}=x_{21}, & \phi_{21}s_{10}=s_{20}. \end{array}$$

Proof of 12: (i) The relations (48) obviously comply with the definition of $\mathbf{H}_1$ by symbols and relations (cf. *1*). Linearity and multiplicativity of α_a hold by definition. Properties (49)–(51) need only be checked on generators where they are obvious.

(ii) Definition (52) obviously defines a $\mathbb{Z}$-grading for which the degree is as indicated. Claims (iii) and (iv) are obvious. Check of the Hopf property: It suffices to show commutation of the α_a with Δ, which it is enough to check on generators owing to multiplicativity of Δ. Now:

$$\Delta(\alpha_a k)=\Delta k=k\otimes k \quad \text{whilst} \quad (\alpha_a\otimes\alpha_a)\Delta k=(\alpha_a\otimes\alpha_a)k\otimes k=k\otimes k,$$

$$\Delta(\alpha_a x)=\Delta(ax)=a\Delta x \quad \text{whilst} \quad (\alpha_a\otimes\alpha_a)\Delta x=(\alpha_a\otimes\alpha_a)(x\otimes k+k^{-1}\otimes x)=(ax\otimes k+k^{-1}\otimes ax),$$

$$\Delta(\alpha_a y)=\Delta(a^{-1}y)=a^{-1}\Delta y$$

$$\text{whilst } (\alpha_a\otimes\alpha_a)\Delta y=(\alpha_a\otimes\alpha_a)(y\otimes k+k^{-1}\otimes y)=(a^{-1}y\otimes k+k^{-1}\otimes a^{-1}y).$$

It is instructive to check the $\mathbb{Z}$-grading properties on the elements of the **MNF**-basis along the lines of (iv). for this we want to check that for homogeneous h, $h'\in\mathbf{H}_1$ one has $\delta_{\mathbb{Z}}h+\delta_{\mathbb{Z}}h'=\delta_{\mathbb{Z}}hh'$. For $hh'=0$ this is trivial because $0\in\mathbf{H}_1^{[n]}$ for all $n\in\mathbb{Z}$. Hence we need only look at the nonvanishing products listed previously. For the products in **M**, by the above remark (iii) we have $\partial_{\mathbb{Z}}(m_{ij}m_{jq})=\partial_{\mathbb{Z}}m_{iq}=q-i$ whilst $\partial_{\mathbb{Z}}m_{ij}+\partial_{\mathbb{Z}}m_{jq}=j-i+q-j=q-i$. The same reasoning settles the nonvanishing products between ϕ_{ij}, $i, j=1, -1$. Remain the other products for which one checks individually by inspection of the diagrams **N** and **F** that, for h in line i and h' in line j, hh' lies in line $i+j$.

We now embark upon the characterization of Hopf automorphisms. An $\alpha\in\mathrm{Aut}_{\mathrm{Hopf}}\mathbf{H}_1$ maps the ideals **M** and **N** into ideals of the same dimension, and thus preserves **M** and **N**. Hence $\alpha e_{\mathbf{M}}=e_{\mathbf{M}}$, and α thus preserves also $\mathbf{M}^{\perp}$. Moreover α commuting with S also commutes with $S^2=adh$, and thus leaves stable the subsets $\mathbf{H}_1^{(i)}$, $i=0,1,2$, hence the intersections $\mathbf{M}^{(i)}=\mathbf{M}\cap\mathbf{H}_1^{(i)}$, $\mathbf{N}^{(i)}=\mathbf{N}\cap\mathbf{H}_1^{(i)}$, $\mathbf{M}^{\perp(i)}=\mathbf{M}^{\perp}\cap\mathbf{H}_1^{(i)}$, which are also stable under S. By exploiting the multiplicativity of α and its commutativity with S, we first obtain Proposition 13. By the (less easily exploitable) commutativity of α with Δ we pass from 13 to the characterization 14 of the Hopf automorphisms. This then allows the description 15 of the Hopf bar-operations. We first state those results, and then sketch the proofs (the details of which are contained in the preprints[9]).

13 Proposition: (The group $\mathcal{A}$ of automorphisms of the complex algebra $\mathbf{H}_1$ commuting with S) With $a, \beta, \gamma, A, K, L, M, N$ complex constants such that

$$\begin{cases} a\beta AKN\neq 0 \\ \beta(KN-LM)=A, \end{cases} \tag{56}$$

we specify the $\mathbb{C}$-linear operator $\alpha=\alpha_{a\beta AKN}$ of $\mathbf{H}_1$ by requiring:
(1) on **M**:

$$\begin{cases} \alpha m_{11}=m_{11}, \\ \alpha m_{00}=m_{00}, \\ \alpha m_{22}=m_{22}, \end{cases} \quad \begin{cases} \alpha m_{01}=a m_{01}, \\ \alpha m_{12}=a^{-2}m_{12}, \\ \alpha m_{20}=a m_{20}, \end{cases} \quad \begin{cases} \alpha m_{10}=a^{-1}m_{10}, \\ \alpha m_{21}=a^{2}m_{21}, \\ \alpha m_{02}=a^{-1}m_{02}, \end{cases} \tag{57}$$

(2) on **F**:

$$\begin{cases} \alpha\phi_{11}=\phi_{11}, \\ \alpha\phi_{00}=\phi_{00}, \\ \alpha\phi_{22}=\phi_{22}, \end{cases} \quad \begin{cases} \alpha\phi_{12}=\beta\phi_{12}+\gamma x_{12}, \\ \alpha\phi_{21}=\beta^{-1}\phi_{21}-\beta^{-2}\gamma x_{21}, \end{cases} \tag{58}$$

(3)on **N**:

$$\begin{cases} \alpha x_{11}=A x_{11}, \\ \alpha x_{00}=A x_{00}, \\ \alpha x_{22}=A x_{22}, \end{cases} \quad \begin{cases} \alpha x_{12}=A\beta x_{12}, \\ \alpha x_{21}=A\beta^{-1}x_{21}, \end{cases} \tag{59}$$

$$\begin{cases} \alpha r_{01}=Kr_{01}+Ls_{01}, \\ \alpha s_{01}=Mr_{01}+Ns_{01}, \end{cases} \quad \begin{cases} \alpha r_{20}=Nr_{20}-Ms_{20}, \\ \alpha s_{20}=-Lr_{20}+Ks_{20}, \end{cases} \tag{60}$$

$$\begin{cases} \alpha r_{10}=\beta Nr_{10}-\beta Ms_{10}, \\ \alpha s_{10}=-\beta Lr_{10}+\beta Ks_{10}, \end{cases} \quad \begin{cases} \alpha r_{02}=\beta Kr_{02}+\beta Ls_{02}, \\ \alpha s_{02}=\beta Mr_{02}+\beta Ns_{02}. \end{cases}$$

The set of $\alpha_{a\beta AKN}$ is a subgroup of the automorphism group Aut$\mathbf{H}_1$ of the complex algebra $\mathbf{H}_1$, namely the subgroup of elements of Aut$\mathbf{H}_1$ commuting with S. One has
(1) *the product* $\alpha_{a\beta AKN}\alpha_{a'\beta'A'K'N'}=\alpha_{a''\beta''A''K''N''}$ with

$$\begin{cases} a''=aa', \\ \beta''=\beta\beta', \\ A''=AA', \\ K''=KK'+LM', \quad L''=KL'+LN', \\ M''=MK'+NM', \quad N''=ML'+NN', \end{cases}$$

(2) *the inverse* $(\alpha_{\beta AKN})^{-1}=\alpha_{\beta''' A''' K''' N'''}$ with

$$\begin{cases} a'''=a^{-1}, \\ \beta'''=\beta^{-1}, \\ A'''=A^{-1}, \\ K'''=\beta A^{-1}N, \quad L'''=-\beta A^{-1}L, \\ M'''=-\beta A^{-1}M, \quad N'''=\beta A^{-1}K. \end{cases}$$

Proof: Let $C_S\mathbf{X}$ be the requirement that α commute with S in restriction to $\mathbf{X}\subset\mathbf{H}_1$. The proof evolves in six steps (a) through (f):
(a) $C_S\mathbf{M}^{(0)}\Rightarrow\alpha$ acts on $\mathbf{M}^{(0)}$ either as the identity or as the exchange of m_{11} and m_{22}.
(b) $C_S\mathbf{M}^{(1)}$ (b)$\Rightarrow$(i): α acts on $\mathbf{M}^{(0)}$ as the identity
(ii) α acts on $\mathbf{M}^{(1)}$ as

$$\begin{cases} \alpha m_{01}=am_{01}, \\ \alpha m_{12}=a^{-2}m_{12}, \\ \alpha m_{20}=am_{20}, \end{cases}$$

respectively on $\mathbf{M}^{(2)}$ as

$$\begin{cases} \alpha m_{10}=a^{-1}m_{10}, \\ \alpha m_{21}=a^{2}m_{21}, \\ \alpha m_{02}=a^{-1}m_{02}. \end{cases}$$

(c) $C_S\mathbf{F}^{(0)}\Rightarrow\mathbf{F}^{(0)}$ is stable under α which acts on it as the identity.
(d) $C_S\mathbf{F}^{(1)}$ and $C_S\mathbf{F}^{(1)}\Rightarrow$one has

$$\begin{cases} \alpha\phi_{12}=\beta\phi_{12}+\gamma x_{12}, \\ \alpha\phi_{21}=\beta^{-1}\phi_{21}-\beta^{-1}\gamma\beta^{-1}x_{21}. \end{cases}$$

(e) $C_S\mathbf{N}^{(0)}\Rightarrow$(i): one has

$$\begin{cases} \alpha x_{11}=Ax_{11}, \\ \alpha x_{00}=Ex_{00}, \\ \alpha x_{22}=Ax_{22}. \end{cases}$$

(ii) One has anticipating on the next paragraph

$$\begin{cases} \alpha x_{12}=A\beta x_{12}, \\ \alpha x_{21}=A\beta' x_{21}. \end{cases}$$

(f) $C_S\mathbf{N}^{(1)}\Rightarrow$(i): one has

$$\begin{cases} \alpha r_{01}=Kr_{01}+Ls_{01}, \\ \alpha s_{01}=Mr_{01}+Ns_{01}, \end{cases} \quad \begin{cases} \alpha r_{20}=Nr_{20}-Ms_{20}, \\ \alpha s_{20}=-Lr_{20}+Ks_{20}, \end{cases}$$

$$\begin{cases} \alpha r_{10}=\beta Nr_{10}-\beta Ms_{10}, \\ \alpha s_{10}=-\beta Lr_{10}+\beta Ks_{10}, \end{cases} \quad \begin{cases} \alpha r_{02}=\beta Kr_{02}+\beta Ls_{02}, \\ \alpha s_{02}=\beta Mr_{02}+\beta Ns_{02}. \end{cases}$$

(ii) One has

$$\beta(KN-LM)=A=E.$$

14 Theorem: Let α be a Hopf automorphism of $\mathbf{H}_1$. We have the following action of α on the elements of the **MNF**-basis:

(1) in **M**: $\alpha m_{11}=m_{11}$, $\alpha m_{10}=a^{-1}m_{10}$, $\alpha m_{12}=a^{-2}m_{12}$,
$\alpha m_{01}=am_{01}$, $\alpha m_{00}=m_{00}$, $\alpha m_{02}=a^{-1}m_{02}$,
$\alpha m_{21}=a^2m_{21}$, $\alpha m_{20}=am_{20}$, $\alpha m_{22}=m_{22}$,

(2) in **F**: $\alpha\phi_{00}=\phi_{00}$,
$\alpha\phi_{22}=\phi_{22}$, $\alpha\phi_{21}=a^{-1}\phi_{21}$,
$\alpha\phi_{12}=a\phi_{12}$, $\alpha\phi_{11}=\phi_{11}$,

(3) in **N**: $\alpha x_{00}=x_{00}$, $\alpha r_{02}=a^{-1}r_{02}$, $\alpha r_{01}=a^{-2}r_{01}$,
$\alpha r_{20}=ar_{20}$, $\alpha x_{22}=x_{22}$, $\alpha x_{21}=a^{-1}x_{21}$, $\alpha s_{20}=a^{-2}s_{20}$,
$\alpha r_{10}=a^2r_{10}$, $\alpha x_{12}=ax_{12}$, $\alpha x_{11}=x_{11}$, $\alpha s_{10}=a^{-1}s_{10}$,
$\alpha s_{02}=a^2s_{02}$, $\alpha s_{01}=as_{01}$, $\alpha x_{00}=x_{00}$.

Conferring this with 12 Remarks (iii) this amounts to saying that α coincides with the automorphism α_a defined in (52). Hence $\mathrm{Aut}_{\mathrm{Hopf}}\mathbf{H}_1$ is the same as the group $\mathcal{G}$ of automorphisms of $\mathbf{H}_1$ furnished by the $\mathbb{Z}$-grading of $\mathbf{H}_1$.

Proof: We shall now exploit the rule $\Delta\circ\alpha=(\alpha\otimes\alpha)\circ\Delta$ (commutativity of α with the coproduct). Writing that the automorphism α commutes with Δ is trivial. What is not obvious is which elements one should adress to obtain the properties of α in 14.

Our proof relies on the tabulation[10] [4a] of the coproduct of $\mathbf{H}_1$. Although the latter was computed using the traditional version of $\mathbf{H}_1$, it works for our present purposes: indeed, as we shall see, we need only to know which elements of the **MNF**-basis figure in their coproduct: the precise knowledge of the numerical coefficients is immaterial for the coming proof.

Showing that $\beta=a$.

We read off p. 433 of Ref. 10 [4a] that the $\mathbf{F}\otimes\mathbf{N}$-component of Δm_{11} is of the form:

$$\Delta m_{11}=\lambda\phi_{22}\otimes x_{22}+\mu\phi_{21}\otimes r_{20}+\nu\phi_{12}\otimes r_{02}+\rho\phi_{11}\otimes x_{00} \tag{61}$$

with the constants λ, μ, ν, ρ all nonvanishing. Writing $(\alpha\otimes\alpha)\Delta m_{11}=\Delta(\alpha m_{11})$ and using relations (58)–(60) this equals

$$\begin{aligned}(\alpha\otimes\alpha)\Delta m_{11}=&\lambda\phi_{22}\otimes Ax_{22}+\mu(\beta^{-1}\phi_{21}-\beta^{-2}\gamma x_{21})\otimes(Nr_{20}-Ms_{20})\\&+\nu(\beta\phi_{12}+\gamma x_{12})\otimes(\beta Kr_{02}+\beta Ls_{02})+\rho\phi_{11}\otimes Ax_{00}.\end{aligned} \tag{62}$$

Equating coefficients yields after division through nonzero constants:
$1=A$, $1=\beta^{-1}N$, $1=\beta^2K$ whence $\beta=N$ $\beta^{-2}=K$,

$\beta^{-1}M=\beta^{-2}\gamma N=\beta^{-2}\gamma M=\gamma\beta K=\beta^2L=\gamma\beta L=0$ whence $M=L=\gamma=0$.
Corroboration of (56): we have $A=1=\beta KN=\beta\beta^{-2}\beta$.

We read off p. 440 of Ref. 4 [4a] that the $\mathbf{M}\otimes\mathbf{M}$-component of $\Delta\phi_{12}$ is of the form:

$$\Delta\phi_{12}=\lambda' m_{11}\otimes m_{01}+\mu' m_{01}\otimes m_{11}+\nu' m_{20}\otimes m_{22}+\rho' m_{22}\otimes m_{20} \tag{63}$$

with the constants γ',μ',ν',ρ' all nonvanishing. Writing $\beta\Delta(\phi_{12})=(\alpha\otimes\alpha)\Delta\phi_{12}$ (observe that $\alpha\phi_{12}=\beta\phi_{12}$ since we showed that $\gamma=0$) and furthermore using (57) we get

$$\begin{aligned}&\beta[\lambda' m_{11}\otimes m_{01}+\mu' m_{01}\otimes m_{11}+\nu' m_{20}\otimes m_{22}+\rho' m_{22}\otimes m_{20}]\\&\quad=\lambda' m_{11}\otimes am_{01}+\mu' am_{01}\otimes m_{11}+\nu' am_{20}\otimes m_{22}+\rho' m_{22}+\rho' m_{22}\otimes am_{20}.\end{aligned}$$

Equating coefficients yields after division through nonzero constants yields $\beta=a$. Collecting results yields our claim: $A=1$, $a=\beta=\mathrm{N}$, $a^2=K$, $M=L=\gamma=0$.

15 Theorem: The Hopf bar-operations of $\mathbf{H}_1$ are of the type $\Gamma_r=\alpha_r\Gamma$, $r\in\mathbb{R}^+$, thus specified as follows on generators:

$$\Gamma k=k,\quad \Gamma x=rx,\quad \Gamma y=r^{-1}x. \tag{64}$$

In other terms the Hopf bar-operation is unique up to a scaling factor.

Proof: We know (cf. Appendix B) that all Hopf bar-operations are of the type $w\Gamma=\Gamma w^{-1}$, w a Hopf automorphism of the type α_a, $0\neq a\in\mathbb{C}$. Now $\alpha_a\Gamma=\Gamma\alpha_a{}^{-1}$ iff Γ is real: indeed $\alpha_a\Gamma k=\Gamma\alpha_a{}^{-1}k=k$, $\alpha_a\Gamma x=\alpha_a y=a^{-1}y$ whilst $\Gamma\alpha_a{}^{-1}x=\Gamma a^{-1}x=\overline{a^{-1}}y$, and $\alpha_a\Gamma y=\alpha_a x=ax$ whilst, $\Gamma\alpha_a{}^{-1}y=\Gamma ay=\overline{a}x$.

APPENDIX A: BAR-OPERATIONS OF COMPLEX ALGEBRAS

[A1] Definitions: With $\mathbf{A}$ an algebra over $\mathbb{C}$ a *bar-operation of* $\mathbf{A}$ is a map $\Gamma:\mathbf{A}\to\mathbf{A}$ which is: (a) antilinear, (b) involutive, (c) multiplicative (in other terms the bar-operations of the complex algebra $\mathbf{A}$ are the $\mathbb{Z}/2$ gradings of the real algebra $\mathbf{A}$ which anticommute with i).

We denote by Bar $\mathbf{A}$ the set of bar-operations of $\mathbf{A}$. The elements of Bar $\mathbf{A}$ are so to speak the "mirror symmetries" of $\mathbf{A}$. They leave invariant the unit of $\mathbf{A}$ if $\mathbf{A}$ is unital.

[A2] Proposition (the groupoïd Bar $\mathbf{A}\times$Bar $\mathbf{A}$): With $\mathbf{A}$ and Bar $\mathbf{A}$ as in *[A1]*, the Cartesian product Bar $\mathbf{A}\times$Bar $\mathbf{A}$ is a bipoint-groupoïd (transitive and unicursal)*:*

(i) *Given* Γ_1, $\Gamma_2\in$Bar $\mathbf{A}$ there is a unique $w_{12}\in$Aut $\mathbf{A}$ s.t.$\Gamma_2=\Gamma_1 w_{12}$, namely $w_{12}=\Gamma_1\Gamma_2$ Γ_1, Γ_2 are groupoïd units and w_{12} is the only morphism: $\Gamma_1\to\Gamma_2$.

(ii) Given Γ_1, $\Gamma_2\in$Bar $\mathbf{A}$ there is a unique $w_{21}\in$Aut $\mathbf{A}$ s.t. $\Gamma_2=w_{21}\Gamma_1$, namely $w_{21}=\Gamma_2\Gamma_1$. Γ_1, Γ_2 are groupoïd units and w_{21} is the only morphism: $\Gamma_2\to\Gamma_1$.

(iii) w_{12} and w_{21} are inverse of each other. Given $\Gamma\in$Bar $\mathbf{A}$ and $w\in$Aut $\mathbf{A}$ one has $\Gamma w\in$Bar $\mathbf{A}$ iff $\Gamma w=w^{-1}\Gamma$ (respectively, $w\Gamma\in$Bar $\mathbf{A}$ iff $w\Gamma=\Gamma w^{-1}$).

(iv) One has the equivalences: $w_{21}=w_{12}\Leftrightarrow(w_{12})^2=\mathrm{id}\Leftrightarrow(w_{21})^2=\mathrm{id}\Leftrightarrow\Gamma_1$ and Γ_2 commute.

[A3] Proposition (the real fix-point algebra $\mathbf{A}^\Gamma$)*:* Let $\mathbf{A}$ be an algebra over $\mathbb{C}$ and let $\Gamma\in$Bar $\mathbf{A}$. Then:

(i) the set $\mathbf{A}^\Gamma=\{a\in\mathbf{A};\Gamma a=a\}$ is an algebra over $\mathbb{R}$.

(ii) $\frac{1}{2}(\mathrm{id}+\Gamma)$ and $\frac{1}{2}(\mathrm{id}-\Gamma)$ are complementary projections of $\mathbf{A}$. We have

$$\mathbf{A}^\Gamma=\mathrm{Ker}\,\tfrac{1}{2}(\mathrm{id}-\Gamma)=\mathrm{Im}\,\tfrac{1}{2}(\mathrm{id}+\Gamma), \tag{A1}$$

and

$$i\mathbf{A}^\Gamma=\mathrm{Ker}\,\tfrac{1}{2}(\mathrm{id}+\Gamma)=\mathrm{Im}\,\tfrac{1}{2}(\mathrm{id}-\Gamma), \tag{A2}$$

hence

$$\mathbf{A}=\mathbf{A}^\Gamma\oplus i\mathbf{A}^\Gamma. \tag{A3}$$

(iii) If $\mathbf{A}$ has a finite complex dimension n, $\mathbf{A}^\Gamma$ has the real dimension n.
Note that a general $\mathbb{Z}/2$ grading Γ of the algebra $\mathbf{A}$ over $\mathbb{R}$ does not need to have $\dim_{\mathbb{R}}\mathbf{A}^+ = \dim_{\mathbb{R}}\mathbf{A}^-$—but this is the case if Γ anticommutes with i, due to $\mathbf{A}^- = i\mathbf{A}^+$.

[A4] Proposition: With $\mathbf{A}$ an algebra over $\mathbb{C}$, the following objects are one-to-one:
(i) the *bar operations* of $\mathbf{A}$.
(ii) the subalgebras $\mathbf{A}^\Gamma$ of the real algebra $\mathbf{A}$ such moreover that $\mathbf{A}=\mathbf{A}^\Gamma\oplus i\mathbf{A}^\Gamma$ as complex algebras: we call those the *real spines of* $\mathbf{A}$.

The bijection is as follows:
(i) $\rightarrow$ (ii):

$$\mathbf{A}^\Gamma=\{a\in\mathbf{A};\Gamma a=a\} \tag{A4}$$

(ii) $\rightarrow$ (i):

$$\Gamma(a'+ia'')=a'-ia'',\quad a',a''\in\mathbf{A}^\Gamma. \tag{A5}$$

[A5] Remarks: (i) If $\mathbf{A}$ is n-dimensional each basis $\{a_i\}_{i=1,\ldots,n}$ of $\mathbf{A}$ giving rise to a real multiplication table yields a real spine of $\mathbf{A}$ $(\{ua_iu^{-1}\}_{i=1,\ldots,n}$, $u\in\mathbf{A}$ invertible, another.
(ii): Given a fixed real spine Γ_0 of $\mathbf{A}$ the real spines of $\mathbf{A}$ are one-to-one with the $\phi\Gamma_0$ for the $\phi\in\mathrm{Aut}\,\mathbf{A}$ such that $\phi\Gamma_0\phi\Gamma_0=\mathrm{id}$, or alternatively such that $\phi\Gamma_0\phi=\Gamma_0$.

APPENDIX B: HOPF BAR-OPERATIONS AND MODULAR *-OPERATIONS OF HOPF ALGEBRAS

In what follows $\mathbf{H}(m,\Delta,e,\epsilon,S)$ is a Hopf algebra over $\mathbb{C}$.

[B1] Definitions: (i) A Hopf bar-operation of $\mathbf{H}$ is a $\Gamma\in\mathrm{Bar}\,\mathbf{H}$ which is Hopf in the sense:

$$\begin{cases}\epsilon(\Gamma a)=\epsilon(\overline{a}),\\ \Delta\Gamma a=(\Gamma\otimes\Gamma)\Delta a,\quad a\in\mathbf{H}.\\ \Gamma S=S\Gamma.\end{cases} \tag{B1}$$

We denote by Hopf bar $\mathbf{H}$ the set of Hopf bar-operations of $\mathbf{H}$.
(ii) A modular *-operation of $\mathbf{H}$ is a map $\Sigma:\mathbf{H}\rightarrow\mathbf{H}$, which is
(a) antilinear,
(b) of square S^2,
(c) antimultiplicative,
(d) Hopf in the sense:

$$\begin{cases}\epsilon(\Sigma a)=\epsilon(\overline{a}),\\ \Delta\Sigma a=(\Sigma\otimes\Sigma)\Delta P_{12}a,\quad a\in\mathbf{H}.\\ \Sigma S=S\Sigma.\end{cases} \tag{B2}$$

[B2] Proposition: Let $\mathbf{H}$ be a Hopf algebra with invertible antipode. The following objects are one-to-one:
(i) the Hopf bar operations Γ of $\mathbf{H}$,
(ii) the modular*-operations Σ of $\mathbf{H}$,
with the bijection given by $\Sigma=\Gamma S=S\Gamma$, $\Gamma=S^{-1}\Sigma=\Sigma S^{-1}$.

[B3] Proposition: Let $\Gamma_1,\Gamma_2\in\mathrm{Hopf\ bar}\,\mathbf{H}$: $w_{12}=\Gamma_1\Gamma_2$ is a Hopf automorphism of $\mathbf{H}$.

[B4] Proposition: Assume the Hopf algebra $\mathbf{H}$ of finite complex dimension n.
(i): Let $\Gamma\in\mathrm{Hopf\ bar}\,\mathbf{H}$. The algebra $\mathbf{H}^\Gamma=\{a\in\mathbf{H};\Gamma a=a\}$ of fixpoints of Γ (cf. *[A3]*) is a real Hopf algebra of real dimension n. In particular one has
(a) $\Delta\mathbf{H}^\Gamma\in\mathbf{H}^\Gamma\otimes\mathbf{H}^\Gamma$
(a) $S\mathbf{H}^\Gamma\in\mathbf{H}^\Gamma$.

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On quasicrystal Lie algebras

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We realize the aperiodic Witt and Virasoro algebras as well as other quasicrystal Lie algebras as factor algebras of some subalgebras of the higher rank Virasoro algebras. This realization allows us to generalize the notion of quasicrystal Lie algebras. In the case when the constructed algebra admits a conjugation, we compute the Kac determinant for the Shapovalov form on the corresponding Verma modules. In the case of the aperiodic Virasoro algebra this proves the conjecture of R. Twarock. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1468255]

I. INTRODUCTION

This article has grown from my attempt to understand the recently introduced notion of quasicrystal Lie algebras and the aperiodic Witt and Virasoro algebras (Patera *et al.*, 1998; Twarock, 2000a). These algebras form a new family of infinite-dimensional Lie algebras, whose generators are indexed by points of an aperiodic set (which is in fact a one-dimensional cut-and-project quasicrystal, an object, intensively studied by many authors) (see, e.g., Katz, 1998; Kramer, 1999; Radin, 1999, and references therein).

Quasicrystal Lie algebras and their representations were studied by several authors, (see, for example, Patera and Twarock, 1999; Patera *et al.*, 1998; Twarock, 2000a), and in Twarock (2000b, c) some applications of these algebras to the construction of some integrable models in quantum mechanics were given. However, there are many important questions about quasicrystal Lie algebras, which are still open. For example, in Twarock (2000a) the author constructs a triangular decomposition for the aperiodic Virasoro algebra, hence constructing Verma modules, and conjectures a formula for the Kac determinant of the Shapovalov form on these modules. This formula is important both for the description of simple highest weight modules and for picking up those of them which can be unitarizable, which is the question of primary interest in physical applications.

It was clear from the very first definition of quasicrystal Lie algebras that this notion should be closely connected with the notion of the higher rank Virasoro algebras, defined in Patera and Zassenhaus (1991). The major difference between these algebras is that the indexing set for quasicrystal Lie algebras is a discrete subset of $\mathbb{R}$ while for the higher rank Virasoro algebras the corresponding set is everywhere dense. In the present article we establish this connection by realizing quasicrystal Lie algebras as factor algebras of some subalgebras of the higher rank Virasoro algebras. This realization allows us to generalize quasicrystal Lie algebras in several directions, preserving the property to have a discrete indexing set. Moreover, the notion and construction of a triangular decomposition for these algebras appears naturally in this framework. Further, we discuss the existence of conjugation on the constructed algebras, which pairs the components of the positive and negative parts. In the case when such pairing exists, the definition of the Shapovalov form on Verma modules (see Shapovalov, 1972; Moody and Pianzola, 1995) is straightforward and we compute the Kac determinant (see Shapovalov, 1972; Kac and Kazhdan, 1979); Moody and Pianzola, 1995; Kac and Raina, 1987 of this form. In the case of the aperiodic Virasoro algebras this proves Twarock, 2000a, Conjecture V.7.

The article is organized as follows: in Secs. II and III we recall the definitions of quasicrystal Lie algebras and higher rank Virasoro algebras. We give a realization of quasicrystal Lie algebras

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as factor algebras of certain subalgebras of the higher rank Virasoro algebras in Sec. IV and use it to construct parabolic and triangular decompositions of our algebras in Sec. V. In Sec. VI we study the Verma modules and, in particular, calculate the determinant of the Shapovalov form on them. We finish with discussing several generalizations of our construction in Secs. VII and VIII.

II. QUASICRYSTAL LIE ALGEBRAS

Denote by $(\cdot)^{\#}$ the unique nontrivial automorphism of the field $\mathbb{Q}(\sqrt{5})$ and let $\mathbb{F}$ be a field of characteristic 0, containing $\sqrt{5}$. Let Ω be a nonempty, connected and bounded real set, whose set of inner points does not contain 0. Set $\tau=\frac{1}{2}(1+\sqrt{5})$. Then the *cut-and-project quasicrystal* $\Sigma(\Omega)$ associated with Ω is the set of all $x\in\mathbb{Z}[\tau]$, such that $x^{\#}\in\Omega$ (see Duneau and Katz, 1985). The *quasicrystal Lie algebra* $L(\Omega)$, associated with Ω, is defined as follows (see Patera *et al.*, 1998): it is generated over $\mathbb{F}$ by L_x, $x\in\Sigma(\Omega)$, with the Lie bracket defined via

$$[L_x,L_y]=\begin{cases}(y-x)L_{x+y}, & x+y\in\Sigma(\Omega),\\ 0, & \text{otherwise.}\end{cases}$$

To define the aperiodic Witt and Virasoro algebras as it is done in Twarock (2000a), we introduce the map $\varphi:\mathbb{Z}[\tau]\to\mathbb{Z}$, which sends $x=a+b\tau$ to $\varphi(x)=b$. Then *the aperiodic Witt algebra* $AW([0,1],\mathbb{F})$ is generated over $\mathbb{F}$ by L_x, $x\in\Sigma([0,1])$, with the Lie bracket defined via

$$[L_x,L_y]=\begin{cases}(\varphi(y)-\varphi(x))L_{x+y}, & x+y\in\Sigma([0,1]),\\ 0, & \text{otherwise.}\end{cases}$$

By Twarock (2000a), Theorem III.4, the algebra $AW([0,1],\mathbb{F})$ admits the unique central extension $AV([0,1],\mathbb{F})$, called *the aperiodic Virasoro algebra*, which is generated over $\mathbb{F}$ by L_x, $x\in\Sigma([0,1])$, and $\mathfrak{c}$, with the Lie bracket defined via

$$[L_x,L_y]=\begin{cases}(\varphi(y)-\varphi(x))L_{x+y}+\delta_{\varphi(x),-\varphi(y)}\dfrac{\varphi(x)^3-\varphi(x)}{12}\mathfrak{c}, & x+y\in\Sigma([0,1]),\\ 0, & \text{otherwise.}\end{cases}$$

III. THE HIGHER RANK VIRASORO ALGEBRAS

Let P denote the free Abelian group $\mathbb{Z}^k$ of finite rank k and $\psi:P\to(\mathbb{F},+)$ a group monomorphism. The *rank k Virasoro* algebra $V(\psi,\mathbb{F})$, associated with ψ, is generated over $\mathbb{F}$ by elements e_x, $x\in P$, and central term $\mathfrak{c}$, with the Lie bracket defined via

$$[e_x,e_y]=(\psi(y)-\psi(x))e_{x+y}+\delta_{x,-y}\frac{\psi(x)^3-\psi(x)}{12}\mathfrak{c}.$$

The *rank k Witt* algebra $W(\psi,\mathbb{F})$ is the quotient of $V(\psi,\mathbb{F})$ modulo the central ideal $\mathbb{F}c$.

We will need the notion of a triangular decomposition for $V(\psi,\mathbb{F})$ and $W(\psi,\mathbb{F})$, introduced and studied in Mazorchuk (1999). The *standard triangular decomposition* of $\mathfrak{G}=W(\psi,\mathbb{F})$ [or $\mathfrak{G}=V(\psi,\mathbb{F})$] is associated with a linear order, $<$, on the Abelian group P, satisfying the Archimed law: for any $0<a<b\in T$ there exists $k\in\mathbb{N}$ such that $b<ka$. After fixing such $<$ we define $\mathfrak{G}_+$ (resp. $\mathfrak{G}_-$) as generated by e_x, $x>0$ (resp. $x<0$), and $\mathfrak{G}_0$ as the span of e_0 [and c in case of $V(\psi,\mathbb{F})$]. We get $\mathfrak{G}=\mathfrak{G}_-\oplus\mathfrak{G}_0\oplus\mathfrak{G}_+$. The disadvantage of this construction is that the Verma modules $U(\mathfrak{G})\otimes_{U(\mathfrak{G}_0\oplus\mathfrak{G}_+)}\mathbb{F}_\lambda$, $\lambda:\mathfrak{G}_0\to\mathbb{F}$, associated with this decomposition, have infinite-dimensional weight spaces. The reason why this is the case is explained by the fact that any injective additive real one-dimensional projection of the set, indexing $\mathfrak{G}_-$, is not discrete. The linear orders on P, satisfying the Archimed law, will be called *admissible*. For an admissible order, $<$, on P, we denote by P_+ the set $\{x\in P:0<x\}$ and by P_- the set $\{x\in P:x<0\}$. We also set $P_+^0=P_+\cup\{0\}$ and $P_-^0=P_-\cup\{0\}$.

The notions of the rank k Virasoro and Witt algebras have an immediate generalization if one forgets about the requirement on ψ to be a monomorphism. From now on we will not require this, but, however, will assume that ψ is nonzero. We will then understand the notions of the rank k Virasoro and Witt algebras in this more general sense.

IV. REALIZATION OF QUASICRYSTAL LIE ALGEBRAS

In this section we realize the quasicrystal Lie algebras as quotients of the positive part of a higher rank Virasoro algebra. Since the quasicrystal Lie algebras are defined in terms of $\mathbb{Z}[\tau]$, which is a free Abelian group of rank 2, we naturally reduce our consideration to the case of rank 2 Virasoro algebras. So, we assume that $P \simeq \mathbb{Z}^2$. If $<$ is an admissible order on P and I is a *non-negative ideal* of P, i.e., $I \subset P_+^0$ and $x \in I$, $x < y$, implies $y \in I$, then we denote by $L(\mathfrak{G}, <, I)$ the Lie subalgebra of $\mathfrak{G}$, generated by all e_x, $x \in I$. Our main statement about the realization of quasicrystal algebras is the following.

Theorem 1: *Let L be a quasicrystal Lie algebra. Then there exist a rank 2 Witt algebra, $\mathfrak{G} = W(\psi, \mathbb{F})$, an admissible order, $<$, on P, and two non-negative ideals $I \supset J$ of $\mathfrak{G}$, such that L is isomorphic to the quotient algebra $L(\mathfrak{G}, <, I)/L(\mathfrak{G}, <, J)$.*

Proof: Let $\psi: P \to \mathbb{F}$ be the monomorphism sending a fixed basis, $\{a, b\}$, of P to $\{1, \tau\}$. For a, $b \in P$ we define $a < b$ provided $0 < (\psi(b) - \psi(a))^{\#}$ and claim that this is an admissible order on P. Indeed, $<$ is obviously antisymmetric, antireflexive and transitive. So, it is a partial order. But from the definition it also follows immediately that $<$ is linear. Further, for any $a < b$ in P and $c \in P$ we have $(\psi(a+c) - \psi(b+c))^{\#} = (\psi(a+c-b-c))^{\#} = (\psi(a-b))^{\#} = (\psi(a) - \psi(b))^{\#} < 0$ and hence $a + c < b + c$, thus $<$ is compatible with the addition in P. Finally, if $0 < a < b$, then $0 < (\psi(a))^{\#}$ and hence there always exists $k \in \mathbb{N}$ such that $(\psi(b) - \psi(ka))^{\#} = (\psi(b))^{\#} - k(\psi(a))^{\#} < 0$, which shows that the order is admissible.

Consider the rank 2 Witt algebra $\mathfrak{G} = W(\psi, \mathbb{F})$. Without loss of generality we can assume that $\Omega \subset \mathbb{R}_{\geqslant 0}$, as otherwise we can work with the order opposite to $<$. As Ω is a connected bounded subset of $\mathbb{R}$, it has one of the following four forms: $[a,b]$, $(a,b]$, $[a,b)$, (a,b) for some non-negative real numbers a, b. We define I and J as follows: I is generated by all e_x such that $\psi(x)^{\#} > a$ [resp. $\psi(x)^{\#} \geqslant a$] if $a \notin \Omega$ (resp. $a \in \Omega$); and J is generated by all e_x such that $\psi(x)^{\#} > b$ [resp. $\psi(x)^{\#} \geqslant b$] if $b \in \Omega$ (resp. $b \notin \Omega$). From the definition it follows immediately that both I and J are non-negative ideals of P with respect to $<$. Hence, the algebras $L(\mathfrak{G}, <, I)$ and $L(\mathfrak{G}, <, J)$ are well-defined subalgebras of $\mathfrak{G}$ and $L(\mathfrak{G}, <, J) \subset L(\mathfrak{G}, <, I)$ by definition.

Now we show that $L(\mathfrak{G}, <, J)$ is actually an ideal of $L(\mathfrak{G}, <, I)$. Indeed, if $x \in I$ and $y \in J$, we get that $x + y \in J$ as J is an ideal of P and $x \in P_+^0$. Hence $[e_x, e_y] \in L(\mathfrak{G}, <, J)$ for any $e_x \in L(\mathfrak{G}, <, I)$ and $e_y \in L(\mathfrak{G}, <, J)$.

Finally, we consider the map $f: L(\mathfrak{G}, <, I) \to L(\Omega)$ defined by

$$f(e_x) = \begin{cases} L_x, & x^{\#} \in \Omega, \\ 0, & \text{otherwise.} \end{cases}$$

From the definition of the Lie brackets in $L(\Omega)$ (Sec. II) and in $\mathfrak{G}$ (Sec. III) we immediately get that f is a Lie algebra homomorphism. Moreover, it is also clear that its kernel coincides with $L(\mathfrak{G}, <, J)$. This completes the proof. □

Theorem 1 motivates the following definition: let $\mathfrak{G} = W(P, \psi)$ be a higher rank Witt algebra (it is important here that $k > 1$, i.e., that $\mathfrak{G}$ is not the classical Witt algebra), $<$ be an admissible order on P, and $I \supset J$ be two non-negative ideals of P with respect to the order $<$. Then we define the *Lie algebra $\mathfrak{A}(P, \psi, <, I, J)$ of quasicrystal type* as the quotient algebra $L(\mathfrak{G}, <, I)/L(\mathfrak{G}, <, J)$. In particular, all quasicrystal Lie algebras are Lie algebra of quasicrystal type. Now we can formulate some basic properties of Lie algebras of quasicrystal type and we see that these algebras share a lot of properties of classical quasicrystal Lie algebras. We start with the following easy observations.

Lemma 1: Let $<$ be an admissible order on $\mathbb{Z}^k$. Then there exists a homomorphism, $\sigma: P \to \mathbb{R}$, such that $\sigma(P_{\pm}) \subset \mathbb{R}_{\pm}$.

Proof: Identify P with $\mathbb{Z}^k \subset \mathbb{R}^k$. Using the description of admissible orders on an Abelian group from Zaytseva (1953), we find a hyperplane, H, of $\mathbb{R}^k$, such that P_+ coincides with the set of points from $\mathbb{Z}^k$, which are settled on the same side with respect to H. Then σ can be taken, e.g., as the projection onto $H^\perp$ with respect to H (here $\mathbb{R}^k$ is considered as an Euclidean space in a natural way).

For given $\mathfrak{G}=W(P,\psi)$ and $<$ we fix some σ, which exists by Lemma 1. We define $a=\inf_{x\in I}(\sigma(x))$ and $b=\inf_{x\in J}(\sigma(x))$ and will use this notation in the following statement.

Proposition 1: Let $\mathfrak{A}(P,\psi,<,I,J)$ be a Lie algebra of quasicrystal type.

(1) $\mathfrak{A}(P,\psi,<,I,J)$ is Abelian if and only if $2a\geqslant b$.
(2) $\mathfrak{A}(P,\psi,<,I,J)$ has a nontrivial center if and only if $a\neq 0$.
(3) $\mathfrak{A}(P,\psi,<,I,J)$ is nilpotent if and only if $a>0$ and $J\neq\varnothing$.
(4) The algebra *$\mathfrak{A}(P,\psi,<,I,J)$ is perfect if and only if $a=0$ and $0\notin I$.*
(5) If $J\neq\varnothing$, then the algebra $\mathfrak{A}(P,\psi,<,I,J)$ is locally finite, that is, any finite set of elements from $\mathfrak{A}(P,\psi,<,I,J)$ generates a finite-dimensional Lie subalgebra of $\mathfrak{A}(P,\psi,<,I,J)$. In particular, $\mathfrak{A}(P,\psi,<,I,J)$ has finite-dimensional subalgebras of arbitrary non-negative dimension.

Proof: All statements are easy corollaries of the fact that the indices of the generating elements are added under the Lie bracket. Indeed, with this remark the first statement reduces to the fact that $x\geqslant a$ and $y\geqslant a$ implies $x+y\geqslant 2a\geqslant b$; the second one reduces to the fact that for any $x\geqslant a$ and $y>b-a$ one has $x+y>b$; and the third one reduces to the fact that for $ka>b$ we have $kx>b$ for any $x\geqslant a$. If $a\neq 0$, the algebra $\mathfrak{A}(P,\psi,<,I,J)$ is nilpotent by statement 3 and hence not perfect. It is also clear that it is impossible to get 0 in the derived algebra. But if $a=0$ and $0\notin I$, then $L(\mathfrak{G},<,I)=\mathfrak{G}_+$, $\sigma(P_+)$ is dense in $\mathbb{R}_+$ and hence for any $x>0$ there exist y, $z\in P_+$ such that $y+z=x$. This implies that $\mathfrak{A}(P,\psi,<,I,J)$ is perfect in this case and hence property 4 holds.

The first part of the last statement is equivalent to the trivial statement that a finite subset of $\mathbb{R}_+$ generates an additive semigroup, whose intersection with any bounded set is finite. To prove the second part it is sufficient to consider the span of e_{ix}, $i=1,\ldots,n$, such that $nx<b$ and $(n+1)x>b$. This completes the proof. □

For example, to realize the aperiodic Witt algebra $AW([0,1])$, defined in Twarock (2000a), as a Lie algebra of quasicrystal type, one should take $P=\mathbb{Z}^2$, ψ being the projection onto the second coordinate; $<$ defined by $x<y$ if and only if the inner product of $y-x$ with $(1,\frac{1}{2}(1-\sqrt{5}))=(1,\tau^{\#})$ is greater than zero; $I=P_+^0$; $J=\{x\in P:(1,0)<x\}$.

V. STANDARD AND NONSTANDARD TRIANGULAR DECOMPOSITIONS

The realization of Lie algebras of quasicrystal type, obtained in the previous section, allows us to adopt the technique from Mazorchuk (1999) to construct various triangular and parabolic decompositions of these algebras. The general procedure will look as follows.

Let $\mathfrak{A}=\mathfrak{A}(P,\psi,<,I,J)$ be a Lie algebra of quasicrystal type. Abusing notation we will denote by e_x, $x\in I\backslash J$, the generators of $\mathfrak{A}$. Choose any linear pre-order, $\preccurlyeq$, on the Abelian group P, which is different from $<$ and its opposite. Define $\mathfrak{A}_\pm$ as the Lie subalgebras of $\mathfrak{A}$, generated by all e_x, $0\preccurlyeq\pm x$, and set $\mathfrak{A}_0$ to be the Lie subalgebra of $\mathfrak{A}$, generated by all e_x, $0\preccurlyeq x$ and $x\preccurlyeq 0$. We get the following obvious fact.

Lemma 2: $\mathfrak{A}=\mathfrak{A}_-\oplus\mathfrak{A}_0\oplus\mathfrak{A}_+$.

Proof: Clearly, $\mathfrak{A}=\mathfrak{A}_-+\mathfrak{A}_0+\mathfrak{A}_+$. The fact that this is actually a direct sum decomposition follows easily from the property $x\preccurlyeq y$ implies $x+z\preccurlyeq y+z$. □

It is natural to call the decomposition $\mathfrak{A}=\mathfrak{A}_-\oplus\mathfrak{A}_0\oplus\mathfrak{A}_+$ the *parabolic decomposition* of $\mathfrak{A}$ associated with $\preccurlyeq$. Given a parabolic decomposition and a simple $\mathfrak{A}_0$-module, V, one can extend V to a $\mathfrak{A}_0\oplus\mathfrak{A}_+$-module with the trivial action of $\mathfrak{A}_+$ and construct the associated *generalized Verma module* $M(V)$ as follows: $M(V)=U(\mathfrak{A})\otimes_{U(\mathfrak{A}_0\oplus\mathfrak{A}_+)}V$.

If $\mathfrak{A}_0$ happens to be rather special, it is natural to rename the corresponding parabolic decomposition into it *triangular decomposition*. However, this is a subtle question and the terminology

I give here represents only my point of view and is inspired by the corresponding notions for the higher rank Witt algebras (Mazorchuk, 1999).

We will say that the decomposition $\mathfrak{A}=\mathfrak{A}_-\oplus\mathfrak{A}_0\oplus\mathfrak{A}_+$ is a *standard triangular decomposition* provided that $\mathfrak{A}_0=\mathbb{F}e_x$ for some $x\in P$, which is not maximal in $I\backslash J$. We call $\mathfrak{A}=\mathfrak{A}_-\oplus\mathfrak{A}_0\oplus\mathfrak{A}_+$ a *nonstandard triangular decomposition* provided that $\mathfrak{A}_0$ is a commutative Lie algebra and the parabolic decomposition fails to be standard triangular. In the case of a triangular decomposition, generalized Verma modules become classical *Verma modules* as in this case $\dim(V)=1$.

The first case is natural and corresponds to triangular decompositions of the higher rank Witt algebras (Mazorchuk, 1999). Actually, here one has to be careful because, depending on whether $\preccurlyeq$ satisfies the Archimed law or not, one can further distinguish two cases of standard triangular decompositions. We will not do this, as we will not study the difference between the corresponding situations. But the second case has a striking difference from the first one and comes from the definition of triangular decompositions for the aperiodic Virasoro algebra in Twarock (2000a). This means that the triangular decomposition for the aperiodic Virasoro algebra, constructed in Twarock (2000a), is an example of a nonstandard triangular decomposition. We now will study analogous situations in more detail.

We retain the notation for σ, a,b from the previous section and further assume that $a=0$ and that there is an element, $e_u\in\mathfrak{A}$, such that $\sigma(u)=b$ and $\psi(u)=0$. Since $<$ is an admissible order, such an element is unique and we retain the notation e_u for it.

Lemma 3: Under the above assumptions we consider the vector space $\mathfrak{A}'=\mathfrak{A}\oplus\mathbb{F}\mathfrak{c}$. *Then the formula*

$$[e_x+a\mathfrak{c},e_y+b\mathfrak{c}]=[e_x,e_y]+\frac{\psi(x)^3-\psi(x)}{12}\delta_{x,u-y}\mathfrak{c}$$

defines on $\mathfrak{A}'$ *the structure of a Lie algebra, which is a central extension of* $\mathfrak{A}$. *Furthermore, if* $e_0\in\mathfrak{A}$, *the algebra* $\mathfrak{A}'$ *is the unique nontrivial central extension of* $\mathfrak{A}$.

Proof: Up to an automorphism we can assume that $u=(1,0)$. Let a now denote the unique element of $I\backslash J$, which can be written $a=(a_1,1)$. Then it is obvious that for any element $y\in I\backslash J$ either $y+a+in I\backslash J$ or $y+a-(1,0)\in I\backslash J$. Using this description of the minimal distances in $I\backslash J$, one can repeat the proof of Twarock (2000a, Theorem III.4) word by word. □

The algebra $\mathfrak{A}$, constructed in Lemma 3, is a natural generalization of the aperiodic Virasoro algebra from Twarock (2000a). In particular, the aperiodic Virasoro algebra coincides with $\mathfrak{A}'$ for those $\mathfrak{A}$ constructed at the end of the previous section. However, if, e.g., the rank of P is bigger than 2, we get an example of $\mathfrak{A}'$, which differs from the aperiodic Virasoro algebra. We will call such algebras $\mathfrak{A}'$ *Virasoro-like algebras of quasicrystal type*.

By assigning to the element $\mathfrak{c}$ the index u we easily transfer the notions of parabolic and both standard and nonstandard triangular decompositions to the algebra $\mathfrak{A}'$. If P has rank 2, then, up to taking the opposite order, the nonstandard triangular decomposition of $\mathfrak{A}$, for which $\mathfrak{A}_0'$ contains e_u, is unique, and in the case of the aperiodic Virasoro algebra this coincides with the triangular decomposition, constructed in Twarock (2000a Sec. V). For the rank 2 case one can easily construct an example of $\mathfrak{A}'$ such that with respect to the unique natural nonstandard triangular decomposition mentioned above, $\dim(\mathfrak{A}_0')$ is an arbitrary positive integer. Hence even in the rank 2 case one gets a lot of examples of $\mathfrak{A}'$, which are different from the aperiodic Virasoro algebras. All these algebras will have discrete aperiodic root systems, and, if considered as graded by the action of e_0, all roots will be multiples with multiplicity $\dim(\mathfrak{A}_0')-2$. In the case of the aperiodic Virasoro algebra we have $\dim(\mathfrak{A}_0')=3$ and hence all roots (with nonzero action of e_0) are multiplicity free. We will discuss this situation in more detail in the next section, when we will define the Shapovalov form on the Verma modules and compute its determinant.

VI. SHAPOVALOV FORM AND KAC DETERMINANT

In this section we present several results on the structure of Verma modules over Lie and Virasoro-like algebras of quasicrystal type. As in the case of the Witt and the Virasoro algebras,

their representation theory is more complicated, which, in particular, gives a bigger variety of simple highest weight modules. Our main tool in the case of the Virasoro-like algebras of quasicrystal type and the corresponding Lie algebras of quasicrystal type will be the Shapovalov form on Verma modules, first defined in Shapovalov (1972) for simple finite-dimensional Lie algebras. However, we start with the more elementary general case of Lie algebras of quasicrystal type, which happens to be really trivial. Before starting we just note that in this section we always assume that $\mathbb{F}$ is an algebraically closed field of characteristic zero.

We recall that, given a triangular decomposition, $\mathfrak{A}=\mathfrak{A}_-\oplus\mathfrak{A}_0\oplus\mathfrak{A}_+$, a $\mathfrak{A}$-module, M, is called a *highest weight module*, if there exists a generator, $v\in M$, such that $\mathfrak{A}_+v=0$.

Proposition 2: All simple highest weight modules over Lie algebras of quasicrystal type, which correspond to a standard triangular decompositions with $\mathfrak{A}_0=\mathbb{F}e_x\mathfrak{C}[\mathfrak{A},\mathfrak{A}]$, *are one-dimensional. In particular, the corresponding Verma modules are always reducible*.

Proof: This is a direct consequence of $\mathfrak{A}_0=\mathbb{F}e_x$ and $e_x\notin[\mathfrak{A},\mathfrak{A}]$. □

Proposition 3: All Verma modules over a Lie algebra of quasicrystal type, which correspond to a standard triangular decompositions with $\mathfrak{A}_0=\mathbb{F}e_x\subset[\mathfrak{A},\mathfrak{A}]$, *are reducible. The corresponding unique simple quotients are one-dimensional if and only if the eigenvalue of* e_x *on the primitive generator of the module is zero. Otherwise they are infinite-dimensional*.

Proof: Let v be the canonical generator of the Verma module in question. The reducibility follows from the fact that x is not maximal in $I\backslash J$, and hence there are infinitely many elements $y\in P_-$ satisfying $e_x\notin[e_y,\mathfrak{A}]$, which implies that $U(\mathfrak{A})e_yv$ is a proper submodule of the Verma module.

The second statement follows considering the set of elements e_y, $y\in P_-$, satisfying $e_x\in[e_y,\mathfrak{A}]$, which is obviously infinite. □

So, we can now move on to the case of nonstandard triangular decompositions. First, we reduce our consideration to the natural case of weight modules with finite-dimensional weight spaces, which corresponds to the situation when the root system of $\mathfrak{A}$ is discrete. This is only possible in the case when $P\simeq\mathbb{Z}^2$. Here our main tool will be the Shapovalov form and to be able to work with it we will also need the following assumptions from the previous section: $e_0\in\mathfrak{A}$; and there is $e_u\in\mathfrak{A}$, such that $\sigma(u)=b$ and $\psi(u)=0$. As it was mentioned above, this situation covers, for example, the case of the aperiodic Witt algebra. Since in the case of the algebra $\mathfrak{A}'$ the arguments will be absolutely the same, we consider both cases simultaneously with all the notation for the algebra $\mathfrak{A}'$. The case of $\mathfrak{A}$ is then easily obtained by factoring $\mathfrak{c}=0$ out.

We define conjugation on P via $\omega(x)=u-x$ and it follows immediately from our assumptions that $e_x\in\mathfrak{A}'$ implies $e_{\omega(x)}\in\mathfrak{A}'$. However, it is easy to see that ω does not extend to an (anti)involution on $\mathfrak{A}'$. We note that $\sigma(\omega(x))=b-\sigma(x)$.

We recall that the algebra $\mathfrak{A}'$ is graded by the adjoint action of e_0 (or, more generally, $\mathfrak{A}_0'$) and for $\mathbb{C}\ni\alpha\neq0$ the dimension of $\mathfrak{A}_\alpha'$ is either 0 or $\dim(\mathfrak{A}_0')-2$ [$(\dim(\mathfrak{A}_0)-1$ in the case of the algebra $\mathfrak{A}$]. We denote by Δ the set of all (nonzero) roots of $\mathfrak{A}'$ with respect to this action and by $\Delta_\pm$ the sets of all positive and negative roots corresponding to our triangular decomposition. Obviously, ω extends to a linear bijection $\mathfrak{A}_\alpha'\to\mathfrak{A}_{-\alpha}'$ for any $\alpha\in\Delta\cup\{0\}$.

As $\mathfrak{A}_0'$ is commutative, simple $\mathfrak{A}_0'$-modules are one-dimensional and have the form V^λ, where λ is an element from the dual space $(\mathfrak{A}_0')^*$, and the action is defined via $g(v)=\lambda(g)v$ for $v\in V^\lambda$ and $g\in\mathfrak{A}_0'$. Let v_λ denote a canonical generator of $M(V^\lambda)$.

Let Δ' (resp. $\Delta_\pm'$) denote the semigroup, generated by Δ (resp. $\Delta_\pm$). Then the module $M(V^\lambda)$ is a weight module with respect to $\mathfrak{A}_0'$ with the support $\lambda\cup\lambda-\Delta_+'$. All weight spaces of $M(V^\lambda)$ are finite dimensional. Moreover, $M(V^\lambda)$ is isomorphic to $U(\mathfrak{A}_-')v_\lambda$ as a vector space.

The $\Delta_\pm$-gradation of $\mathfrak{A}_\pm'$ extends to the $\Delta_\pm'$-gradation of $U(\mathfrak{A}_\pm')$ and, in the antinvolutive way, ω extends to a linear componentwise isomorphism from $U(\mathfrak{A}_+')$ to $U(\mathfrak{A}_-')$ and back, which matches $U(\mathfrak{A}_+')_\alpha$ with $U(\mathfrak{A}_-')_{-\alpha}$.

For $\mu\in\mathrm{supp}(M(V^\lambda))$, $\mu=\lambda-\nu$, $\nu\in\Delta_+'$, we define the it *Shapovalov form* $F_{\lambda,\nu}$ on $M(V^\lambda)_\mu$ by setting that $F_{\lambda,\nu}(fv_\lambda,gv_\lambda)$, $f,g\in U(\mathfrak{A}_-')_{-\nu}$, equals the coefficient of $\omega(f)gv_\lambda\in M(V^\lambda)_\lambda$, written in the basis $\{v_\lambda\}$. The following properties of $F_\lambda=\oplus_{\nu\in\Delta'}F_{\lambda,\nu}$ are standard and the reader can consult Kac and Kazhdan (1979) and Moody and Pianzola (1995) for the arguments.

Lemma 4: (1.) $M(V^\lambda)$ *is simple if and only if* F_λ is nondegenerate. *(2.) The kernel of* F_λ *coincides with the unique maximal submodule of* $M(V^\lambda)$.

Hence in order to study the reducibility of $M(V^\lambda)$ it is sufficient to compute the determinant of $F_{\lambda,\nu}$ for all λ and ν. To be able to do this we consider the following monomial generators of $U(\mathfrak{A}'_-)_{-\nu}$: $\mathcal{G}=\mathcal{G}(\nu)=\{g(x_1,\ldots,x_k)=e_{x_1}\ldots e_{x_k}: x_i\in\Delta_-;\ \Sigma_i x_i=-\nu;\sigma(x_i)\leqslant\sigma(x_{i+1})\}$. We define the linear order $\preccurlyeq$ on this set of generators as the lexicographical order with respect to the values of $\sigma(x_i)$. The key property of this construction is the following.

Lemma 5: If $g(x_1,\ldots,x_k)\in\mathcal{G}$ *and* $g(y_1,\ldots,y_m)\in\mathcal{G}$ *are such that* $g(x_1,\ldots,x_k)\preccurlyeq g(y_1,\ldots,y_m)$, *then* $F_{\lambda,\nu}(g(x_1,\ldots,x_k)v_\lambda, g(y_1,\ldots,y_m)v_\lambda)=0$.

Proof: Consider the smallest index i such that $\sigma(x_i)<\sigma(y_i)$. Then $\sigma(\omega(x_i))>b-\sigma(y_i)$ and hence $e_{\omega(x_i)}$ commutes with e_{y_i} and thus with all e_{y_j}, $j\geqslant i$, since for such j we have $\sigma(y_j)\geqslant\sigma(y_i)$ from the definition of $\mathcal{G}$. For $j<i$ we have $x_j=u_j$ and thus $[e_{\omega(x_j)},e_{y_j}]\in\mathfrak{A}'_0$. We can write

$$e_{\omega(x_i)}(\omega(e_{x_1}\cdots e_{x_{i-1}})e_{y_1}\cdots e_{y_{i-1}})e_{y_i}\cdots e_{y_m}v_\lambda=\varepsilon(\omega(e_{x_1}\cdots e_{x_{i-1}})e_{y_1}\cdots e_{y_{i-1}})e_{\omega(x_i)}e_{y_i}\cdots e_{y_m}v_\lambda + \text{further terms}$$

for some $\varepsilon\in\mathbb{F}$, where in the further terms of the expansion some $e_{\omega(x_j)}$, $j<i$, occur already after the corresponding e_{y_j}. As $e_{\omega(x_i)}$ commutes with all e_{y_j}, $j\geqslant i$, we get that the first summand equals zero.

Now consider one of the *other terms* and let $e_{\omega(x_j)}$ be the factor occurring most to the right in the monomial. This means, in particular, that for $s<j$ this monomial contains $[e_{\omega(x_s)},e_{y_s}]$, which are the elements of $\mathfrak{A}'_0$ and thus, up to a scalar factor, can be moved to the left. In particular, $\sigma(\omega(x_s))$ is the biggest value among all others occurring in this monomial. If the element e_y, standing next to $e_{\omega(x_j)}$ satisfies $y\neq x_j$, this means that $e_{\omega(x_j)}$ commutes with e_y and hence the monomial contributes 0 to the global sum. Otherwise the number of factors, standing to the right from $e_{\omega(x_j)}$, which equal x_j, is less than the same number before the last commutation. Hence induction in this number reduces the problem to the case $y\neq x_j$, thus proving that all monomials occurring in *other terms* contribute 0 to the global sum.

From this it follows directly that $F_{\lambda,\nu}(g(x_1,\ldots,x_k)v_\lambda, g(y_1,\ldots,y_m)v_\lambda)=0$, which completes the proof. □

From Lemma 5 we immediately get the following statement, which, in particular, proves Twarock (2000a, Conjecture V.7).

Corollary 1: The determinant of $F_{\lambda,\nu}$ *coincides with the product of diagonal elements* $F_{\lambda,\nu}(g(x_1,\ldots,x_k)v_\lambda, g(x_1,\ldots,x_k)v_\lambda)$.

Now we can formulate explicit results for the determinant of the Shapovalov form and the corresponding corollaries for the structure of $M(V^\lambda)$. Denote by P' the set of all nonzero $x\in P$ such that $e_x\in\mathfrak{A}'$ is nonzero. Then the decomposition $\Delta=\Delta_-\cup\Delta_+$ induces a decomposition $P'=P'_-\cup P'_+$. For $\nu\in\Delta'_+$ and $x\in P'_-$ we denote by $p_\nu(x)$ the number of occurrences of e_x as factors in the canonical decomposition of all monomials in $\mathcal{G}(\nu)$.

Theorem 2: *Up to a nonzero constant the determinant of* $F_{\lambda,\nu}$ *equals*

$$\prod_{x\in P'_-}\left(\lambda(e_u)-\frac{\psi(x)^2-1}{24}\lambda(\mathfrak{c})\right)^{p_\nu(x)}.$$

Proof: According to Lemma 4, the corresponding determinant is the product of

$$F_{\lambda,\mu}(g(x_1,\ldots,x_k)v_\lambda, g(x_1,\ldots,x_k)v_\lambda)$$

over all $g(x_1,\dots,x_k)\in\mathcal{G}(\nu)$. First, for $x\in P'_-$ we observe that $[e_{u-x},e_u]=\psi(2x)e_u-[\psi(x)^3-\psi(x)/12]\mathfrak{c}$, as $\psi(u)=0$. Moreover, $[e_{u-x},e_u]$ is in fact central in $\mathfrak{A}'$. Hence, we can move the nonzero factor $2\psi(x)$ out and get that, up to a nonzero constant factor, we have

$$F_{\lambda,\mu}(g(x_1,\dots,x_k)v_\lambda,g(x_1,\dots,x_k)v_\lambda)=\prod_{i=1}^{k}\left(\lambda(e_u)-\frac{\psi(x_i)^2-1}{24}\lambda(\mathfrak{c})\right).$$

The general formula is now obtained by multiplying these expressions for all $g(x_1,\dots,x_k)\in\mathcal{G}(\nu)$. □

This theorem immediately implies the following structural result for $M(V^\lambda)$.

Corollary 2: $M(V^\lambda)$ is irreducible if and only if $24\lambda(e_u)\neq(\alpha^2-1)\lambda(\mathfrak{c})$ for all $\alpha\in\Delta'_-$.

Proof: Follows from Theorem 2 and the fact that we have $\psi(x)=\alpha$ provided that $x\in\mathfrak{A}'_\alpha$. □

In particular, we see that the reducibility of $M(V^\lambda)$ depends only on $\lambda(e_u)$ and $\lambda(\mathfrak{c})$ and does not depend on the values of λ on other generators of $\mathfrak{A}'_0$.

Let $\mathbb{F}=\mathbb{C}$. Call a $\mathfrak{A}'$-module, M, *ω-unitarizable* provided that there exists an inner product, $(\cdot,\cdot)$, on M such that $(e_xv,w)=(v,e_{\omega(x)}w)$ [resp. $(\mathfrak{c}v,w)=(v,\mathfrak{c}w)$] for all $v,w\in M$. For the unique simple quotient of the Verma module $M(V^\lambda)$ this is equivalent to the fact that the Shapovalov form on $M(V^\lambda)$ is non-negative (Of course, the Shapovalov form, being symmetric, cannot be considered as an inner product; however, one can consider it on the real part and extend to the complexification in the Hermitian way.) Here our determinant formula immediately implies the following unitarizability result.

Corollary 3: Assume that $\psi(P)\subset\mathbb{R}$ and $\psi(x)\leqslant-1$ for all $x\in P'_-$, $\lambda(e_u)\leqslant0$, $\lambda(c)\geqslant0$. Then the unique simple quotient of $M(V^\lambda)$ is ω-unitarizable.

Proof: Under these conditions all factors of the diagonal elements of the matrix of the Shapovalov form are non-negative and hence all leading minors are non-negative as well. This implies the statement. □

Using these results we also get some information about highest weight modules, associated with standard triangular decompositions.

Corollary 4: The dimensions of the weight spaces of infinite-dimensional highest weight modules over Lie algebras of quasicrystal type, associated with standard triangular decompositions, are not uniformly bounded.

Proof: Let $\mathfrak{A}_0=\mathbb{F}e_x$ be the zero component of the given standard triangular decomposition. Then we can factor our an ideal of $\mathfrak{A}$ such that the factor algebra is still of quasicrystal type, but the element x is maximal in the corresponding $I\backslash J$, and hence the induced triangular decomposition is nonstandard. Now we have $\lambda(e_x)\neq0$ and hence the corresponding Verma module over this algebra is simple and the dimensions of its weight spaces are obviously unbounded. But this module naturally embeds (as a vector subspace) into the simple highest weight module which we started with. □

VII. FURTHER GENERALIZATIONS OF QUASICRYSTAL LIE ALGEBRAS

Geometrical realization of the algebra $\mathfrak{A}$, obtained in Sec. IV, motivates the following generalization of the class of Lie algebras of quasicrystal type.

We consider an arbitrary rank n Witt algebra $\mathfrak{G}=\mathfrak{G}(P,\psi)$ with $P\simeq\mathbb{Z}^n$ being realized in $\mathbb{R}^n$ in a natural way. Let Ω be a convex subset of $\mathbb{R}^n$, containing at least one nonzero point of P, and satisfying the following it 0-*star* condition: $v\in\Omega$ implies $\lambda v\in\Omega$ for all $\lambda>1$. In this case we will call Ω a 0-*star set*. Denote by $L(\Omega)$ the vector subspace in $\mathfrak{G}$, spanned by e_x, $x\in\Omega$.

Lemma 6: $L(\Omega)$ is a Lie subalgebra of $\mathfrak{G}$.

Proof: If $x,y\in P\cap\Omega$, then $x+y=2(\frac{1}{2}x+\frac{1}{2}y)$. $\frac{1}{2}x+\frac{1}{2}y$ belongs to Ω because of convexity and thus $x+y\in\Omega$ by the 0-star condition. □

Lemma 7: Let Ω be a 0-star set, $v\in\Omega$ and $\lambda>0$. Then, if the set $\Omega_{\lambda,v}=\lambda v+\Omega$ contains at least one nonzero point of P, it is a 0-star set. Moreover, $\Omega_{\lambda,v}\subset\Omega$.

Proof: Clearly, $\Omega_{\lambda,v}$ is convex. Further, if $w\in\Omega$ and $\gamma>1$, then $\gamma(w+\lambda v)=\gamma(\lambda+1)\times([1/(\lambda+1)]w+[\lambda/(\lambda+1)]v)$ belongs to Ω by the same arguments as in Lemma 6. This completes the proof. □

Lemma 8: Let Ω be a 0-star set, $v\in\Omega$ and $\lambda>0$. Then $L(\Omega_{\lambda,v})$ is an ideal of $L(\Omega)$.

Proof: If $w\in\Omega$ and $w'=w''+v\in\Omega_{\lambda,v}$ for some $w''\in\Omega$, then $w+w'=w+w''+v\in\Omega_{\lambda,v}$. This implies the statement. □

Hence, for arbitrary $\mathfrak{G}$, Ω and v as above we can form the algebra $\mathfrak{A}(P,\psi,\Omega,\lambda,v)=L(\Omega)/L(\Omega_{\lambda,v})$, which we will call a *Lie algebra of convex quasicrystal type*. To obtain the usual Lie algebra of quasicrystal type, one should take Ω to be a half-space (open or closed), which does not contain 0 as an inner point. The basic properties of Lie algebras of convex quasicrystal type are similar to those of Lie algebra of quasicrystal type, however, their formulation is more complicated because it usually depends on the structure of Ω. Here we list only some most straightforward ones.

Proposition 4: Let $\mathfrak{A}=\mathfrak{A}(P,\psi,\Omega,\lambda,v)$ be a Lie algebra of convex quasicrystal type and let a denote the infimum over the distances of the points in $\Omega\cap P$ to 0. Assume that $\dim(\mathfrak{A})>1$ *and that for any $x\in\Omega$ some neighborhood (in $\mathbb{R}^n$) of $2x$ belongs to Ω. Then*

(1) if $a>0$, then any element of $\mathfrak{A}$ is nilpotent.
(2) $\mathfrak{A}$ is locally finite.

Proof: If $x\in S=\Omega\backslash\Omega_{\lambda,v}$, then there always exists y such that $|x-y|\leqslant|v|$ and such that $y\notin\Omega$. Let $w\in\Omega$. If some ball of radius r about $2w$ belongs to Ω, then for $\lambda>1$ the point $2\lambda w$ belongs to Ω together with the ball of radius λr around it. Making $\lambda r>|v|$ we get that $2\lambda w\in\Omega_{\lambda,v}$. This implies the first statement.

If the set $\{w_1,\ldots,w_k\}\subset\Omega$ is finite, then we find some r such that $2w_i$ belongs to Ω together with its ball of radius r about $2w_i$. Then the same is true for all linear combinations of these elements with non-negative integer coefficients. By the same arguments as in the previous paragraph, there exists $N\in\mathbb{N}$ such that any linear combination of $\{Nw_1,\ldots,Nw_k\}$ with non-negative integer coefficients belongs to $\Omega_{\lambda,v}$. This implies the second statement. □

Let us study an example of such an algebra, which, as we will show, has some interesting properties. Take $P=\mathbb{Z}^2$, ψ the projection onto the second component, $\Omega=\{w\in\mathbb{R}^2:(w,(1,1))\geqslant 0$ and $(w,(1,-1))\geqslant 0\}$, $v=(n+\epsilon,0)$, $n\in\mathbb{N}$, $\epsilon\in(0,1)$. The corresponding algebra $\mathfrak{A}=\mathfrak{A}(P,\psi,\Omega,\lambda,v)$ is graded with respect to the e_0 action with graded components corresponding to all integers and having dimension n. In particular, one can define and study triangular (parabolic) decompositions of this algebra and corresponding (generalized) Verma modules. The set $P'=P\cap(\Omega\backslash\Omega_{\lambda,v})$ coincides with $\{(a,b):0\leqslant a-|b|\leqslant n\}$. Define the conjugation ω on this set via $\omega(a,b)=(2|b|+n-a,-b)$. Then we have the natural notions of Verma modules and the Shapovalov form on them. In our situation we have $\Delta_+=\mathbb{N}$.

Lemma 9: The Verma module $M(V^\lambda)$ is always reducible. However, the unique simple quotient of $M(V^\lambda)$ is infinite dimensional if and only if at least one of the numbers $\lambda(e_{(2,0)}),\ldots,\lambda(e_{(n,0)})$ is nonzero. Otherwise it is one-dimensional.

Proof: We note that the intersection of $[\mathfrak{A},\mathfrak{A}]$ with $\mathfrak{A}_0$ coincides with the linear span $\tilde{\mathfrak{A}}_0$ of elements $\{e_{(2,0)},\ldots,e_{(n,0)}\}$. Hence, if the restriction of λ to $\tilde{\mathfrak{A}}_0$ is zero, the Shapovalov form is identically zero on all $M(V^\lambda)_{\lambda-k}$, $k\in\mathbb{N}$.

Otherwise, assume that $\lambda(e_{(i,o)})\neq 0$ and take $e_x\in\mathfrak{A}_1$ and $e_y\in\mathfrak{A}_{-1}$ such that $[e_x,e_y]=e_{(i,0)}$. We get $F_{\lambda,k}(e^k_{\omega(y)},e^k_x)\neq 0$ and the statement is proved. □

From Lemma 9 it follows that there exists a large family of infinite-dimensional highest weight modules over $\mathfrak{A}$ with respect to this triangular decomposition. The study of the properties of these modules, e.g., their characters, multiplicities and unitarizability seems to be an interesting problem.

VIII. APPLICATION TO THE *q*-ANALOG OF THE VIRASORO ALGEBRAS

All constructions described above work perfectly also in the case of different quantum analogs of the Virasoro algebra [and, actually, in the case of arbitrary $\mathbb{Z}^n$-graded Lie algebra, in particular,

everything works smoothly for generalized Witt algebras in the sense of Kaplansky (see Ree, 1956)]. As we saw that the most interesting case is that of rank 2, we would like to finish this article with outlining some results related to the q-analog of the Virasoro algebra, defined in Kirkman *et al.* (1994). Let $\mathbb{F}=\mathbb{C}$ and $q\in\mathbb{C}$ be such that $q\neq 0$ and q is not a root of unity. We set $P=\mathbb{Z}^2$ and will write an element, $x\in P$, as $x=(x_1,x_2)$. Then the algebra $\mathcal{V}_q$ is generated by e_x, $x\in P\backslash\{(0,0)\}$, with the Lie brackets defined via $[e_x,e_y]=(q^{x_2y_1}-q^{x_1y_2})e_{x+y}$. For $<$, I and J as in Sec. IV, we define the algebra $\mathfrak{A}(\mathcal{V}_q,<,I,J)$ in the same way as for $\mathfrak{A}(P,<,I,J)$ but using the algebra $\mathcal{V}_q$ instead of the rank 2 Virasoro algebra. We extend the algebra $\mathfrak{A}(P,<,I,J)$ by a derivation, d, satisfying $[d,e_x]=x_1e_x$, and will denote the extended algebra also by $\mathfrak{A}(P,<,I,J)$. The element d will always belong to $\mathfrak{A}_0$ in any parabolic decomposition and the notions of standard triangular and triangular decompositions are transfered modulo d. We will also assume that $I=P_+$ and that $I\backslash J$ has the maximal element u.

Theorem 3:

(1) Any parabolic decomposition of $\mathfrak{A}(\mathcal{V}_q,\leqslant,I,J)$ is in fact a triangular decomposition.
(2) All Verma modules over $\mathfrak{A}(\mathcal{V}_q,\leqslant,I,J)$ associated with a triangular decomposition satisfying $e_u\notin\mathfrak{A}_0$ are reducible.
(3) The unique simple quotient of a Verma module, $M(V^\lambda)$, is one-dimensional if and only if $\lambda(e_x)=0$ for all $e_x\in\mathfrak{A}_0$. Otherwise it is infinite-dimensional.
(4) The Verma module $M(V^\lambda)$ associated with a triangular decomposition satisfying $e_u\in\mathfrak{A}_0$ is simple if and only if $\lambda(e_u)\neq 0$.
(5) If q is real and the dimension of the unique simple quotient of $M(V^\lambda)$ is greater that one, this module is not ω-unitarizable and the dimensions of its weight spaces are not bounded.

Proof: The first statement follows from the fact that $[e_x,e_y]=0$ in $\mathcal{V}_q$ provided that $x=\lambda y$. The second and the third ones are analogous to Proposition 3. For the fourth statement we can use the arguments of Lemma 5 and derive that the determinant of the Shapovalov form on $M(V^\lambda)_\mu$ is the product of factors of the form $q^{-x_2x_1}(q^{u_2x_1}-q^{u_1x_2})\lambda(e_u)$. Since $x\in P'_-$ and u cannot be proportional, we derive that this factor is nonzero if and only if $\lambda(e_u)\neq 0$, which implies the fourth statement. The first part of the last statement follows from the observation that for any real q we can always find $x\in P'$, arbitrary small with respect to $<$, such that $q^{u_2x_1}-q^{u_1x_2}$ is positive (resp. negative) and the second part is analogous to Corollary 4. □

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Static Bloch sums for the square array

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We consider sums arising in doubly quasiperiodic Green's functions for the Laplace equation, over the square array. The sums are represented as Fourier series, and it is shown that the coefficients in the series can be obtained as polynomials. We give expressions from which the first six array sums can be evaluated efficiently, and accurate to better than one part in 10^7, over most of the Brillouin zone. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1467968]

I. INTRODUCTION

Lattice sums for Laplace's equation have a long history, as discussed by Glasser and Zucker.[1] They were introduced into physics by Appell,[2] and important contributions to sums for arrays and lattices were made by Rayleigh in 1892.[3] Glasser and Zucker discuss the many investigations relating to Madelung sums in solid state physics, and numerical methods of summation related to Ewald's method.[4] They also stress the value of sums which can be evaluated in closed form.

Here, we wish to consider a class of sums for the square array, which can be developed in the form of rapidly convergent Fourier series, with coefficients which are polynomials in form. The sums in question appear not to have been considered in two dimensions before, but they are close in form to lattice sums studied by Born and Bradburn.[5] They differ from the multipole sums of Rayleigh and subsequent authors by the insertion of a Bloch factor, depending on a wave vector or crystal momentum $\mathbf{k}_0$. Such a factor would arise in a study of electrostatic problems, in the quasistatic limit, involving arrays of inclusions with dielectric constant modulated by a plane wave optical beam, for example. We analyze the sums in Fourier series according to the angle θ_0 specifying the direction of $\mathbf{k}_0$. The Fourier coefficients depend on the magnitude k_0 in a way we show is given by array sums calculated in closed form by Nicorovici *et al.*[6]

We show that these Fourier series converge rapidly, and exhibit formulas for the first seven, most slowly convergent of the sums. These formulas can be used to calculate the sums over most of the Brillouin zone to an accuracy better than one part in 10^7.

II. BLOCH SUMS AND FOURIER SERIES

We consider the following two-dimensional lattice sums:

$$\sigma_l(\mathbf{k}_0)=\sum_{p\neq 0}\frac{\exp(il\varphi_p)}{R_p^l}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}. \tag{1}$$

Here we sum over a two-dimensional array specified by points $\mathbf{R}_p=(R_p,\varphi_p)$, the latter being the polar representation. The exponential term containing $\mathbf{k}_0$ will be recognized as a Bloch factor, with $\mathbf{k}_0$ being the crystal momentum. We specify in polar form $\mathbf{k}_0=(k_0,\theta_0)$. We will be interested primarily in sums of order l in the range zero to six. The sums for orders $l>6$ can be easily evaluated by direct summation.

We relate the static sums (1) to corresponding dynamic forms arising for the Helmholtz equation:

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$$S_l^Y(k,\mathbf{k}_0)=\sum_{p\neq 0} Y_l(kR_p)\, e^{il\varphi_p}\, e^{i\mathbf{k}_0\cdot\mathbf{R}_p}, \tag{2}$$

for which we know that[7]

$$S_l^Y(k,\mathbf{k}_0)J_l(k\xi)=-Y_0(k\xi)\,\delta_{l,0}-\frac{4i^l}{A}\sum_h \frac{J_l(Q_h\xi)}{Q_h^2-k^2}e^{il\theta_h}. \tag{3}$$

Here the sum is carried out over the reciprocal array of vectors $\mathbf{K}_h$, and $\mathbf{Q}_h=\mathbf{K}_h+\mathbf{k}_0=(Q_h,\theta_h)$. Also, A denotes the area of the unit cell in the direct lattice.

If we take the limit as $k\to 0$ in (2), we find for $l\neq 0$,

$$\lim_{k\to 0}\left[\frac{-\pi}{(l-1)!}\left(\frac{k}{2}\right)^l S_l^Y(k,\mathbf{k}_0)\right]=\sum_{p\neq 0}\frac{\exp(il\varphi_p)}{R_p^l}e^{i\mathbf{k}_0\cdot\mathbf{R}_p}=\sigma_l(\mathbf{k}_0). \tag{4}$$

Then, by substituting (3) in (4), we obtain

$$\sigma_l(\mathbf{k}_0)=\frac{4\pi l i^l}{A\xi^l}\sum_h \frac{J_l(Q_h\xi)}{Q_h^2}e^{il\theta_h}, \tag{5}$$

where ξ is an arbitrary length, no longer than the distance from the origin to the nearest point on the unit cell boundary in direct space. This expression can be accelerated by successive integration,[7] and forms one method for evaluating the static Bloch sums.

We write the definition (1) in the form

$$\sigma_l(\mathbf{k}_0)=\sum_{p\neq 0}\frac{\exp(il\varphi_p)}{R_p^l}e^{ik_0R_p\cos(\theta_0-\varphi_p)}, \tag{6}$$

and expand the second exponential factor to give

$$\sigma_l(\mathbf{k}_0)=\sum_{p\neq 0}\frac{\exp(il\varphi_p)}{R_p^l}\sum_q i^q J_q(k_0R_p)e^{iq(\theta_0-\varphi_p)}. \tag{7}$$

Hence, if we write $\sigma_l(\mathbf{k}_0)$ in the form of an angular Fourier series

$$\sigma_l(\mathbf{k}_0)=\sum_q c_q^l(k_0)e^{iq\theta_0}, \tag{8}$$

we can identify the coefficients as

$$c_q^l(k_0)=i^q\sum_{p\neq 0}\frac{J_q(k_0R_p)}{R_p^l}\exp^{i(l-q)\varphi_p}. \tag{9}$$

We now specialize to the case of a square array of period d. Then the array sums in (9) are nonzero only if the integer $l-q$ is divisible by four. This is a direct consequence of the C_{4v} symmetry of the array: the sums (9) remain unchanged under rotations of $\pi/2$.

We compare the array sums with the dimensionless sums studied by Nicorovici *et al.*:[6]

$$\mathcal{S}_{l,4m,n}(\xi/D)=\frac{1}{D^n}\sum_{h\neq 0}\frac{J_l(K_h\xi)}{K_h^n}e^{i4m\psi_h}, \tag{10}$$

where $K_h=(2\pi/D)(h_1,h_2)$ runs over the reciprocal array (itself a square array) to a square array of period D. Given that $R_p=d(p_1,p_2)$, we see that

$$c_q^l(k_0) = i^q \left(\frac{2\pi}{d}\right)^l \mathcal{S}_{q,l-q,l}\left(\frac{k_0 d}{2\pi}\right), \tag{11}$$

where $l-q$ must be divisible by four for the sum to be nonzero.

Using (11) in (8), we obtain

$$\sigma_l(\mathbf{k}_0) = \left(\frac{2\pi i}{d}\right)^l \sum_{m=-\infty}^{\infty} \mathcal{S}_{l-4m,4m,l}\left(\frac{k_0 d}{2\pi}\right) e^{i(l-4m)\theta_0}. \tag{12}$$

III. THE LOWEST SUM AND ITS CONSEQUENCES

$$\sigma_0(\mathbf{k}_0) = \sum_{p\neq 0} e^{i\mathbf{k}_0\cdot\mathbf{R}_p} = \sum_m \mathcal{S}_{4m,4m,0}\left(\frac{k_0 d}{2\pi}\right) e^{-4im\theta_0}, \tag{13}$$

for the square array. Now,

$$\sum_{p\neq 0} e^{i\mathbf{k}_0\cdot\mathbf{R}_p} = \frac{4\pi^2}{A}\sum_h \delta(\mathbf{k}_0 - K_h) - 1 = \frac{4\pi^2}{A}\delta(\mathbf{k}_0) - 1, \tag{14}$$

for $\mathbf{k}_0$ in the Brillouin zone. Evaluating the Fourier coefficients of the delta function, we find

$$\mathcal{S}_{4m,4m,0}(\xi/D) = \left[\frac{1}{2\pi}\frac{\delta(\xi/D)}{\xi/D} - 1\right]\delta_{m,0}. \tag{15}$$

Hence, the Fourier series for σ_0 reduces to a single, distributive term:

$$\sigma_0(\mathbf{k}_0) = \frac{2\pi}{k_0 d^2}\delta(k_0) - 1, \tag{16}$$

for $\mathbf{k}_0$ in the first Brillouin zone.

We can use the result (15) to build up analytic formulas for those lattice sums $\mathcal{S}_{l,m,n}$ for which the index sum $l+m+n$ is even. We can increase the indices l and n using the following formula:[6]

$$\int_0^{\xi} \eta^{l+1}\mathcal{S}_{l,m,n}(\eta)\,\mathrm{d}\eta = \xi^{l+1}\mathcal{S}_{l+1,m,n+1}(\xi), \tag{17}$$

working in dimensionless variables (i.e., replacing ξ/D by ξ in working). This gives, used once,

$$\mathcal{S}_{4m+1,4m,1}(\xi/D) = \left[\frac{D}{2\pi\xi} - \frac{\xi}{2D}\right]\delta_{m,0}. \tag{18}$$

Continuing this process, for $l \geqslant 1$, we obtain

$$\mathcal{S}_{4m+l,4m,l}(\xi/D) = \frac{1}{(2l)!!}\left[\frac{l}{\pi}\left(\frac{\xi}{D}\right)^{l-2} - \left(\frac{\xi}{D}\right)^l\right]\delta_{m,0}, \tag{19}$$

where $(2l)!! = 2l(2l-2)(2l-4)\ldots 2$.

The result (19) is very useful. It guarantees that all negative m terms in the expansion (12) are zero, and also gives the term $m=0$:

$$\sigma_l(\mathbf{k}_0) = \left(\frac{2\pi i}{d}\right)^l \left\{\frac{1}{(2l)!!}\left[\frac{l}{\pi}\left(\frac{k_0 d}{2\pi}\right)^{l-2} - \left(\frac{k_0 d}{2\pi}\right)^l\right] + \sum_{m\geqslant 1}^{\infty} \mathcal{S}_{l-4m,4m,l}\left(\frac{k_0 d}{2\pi}\right) e^{-4im\theta_0}\right\} e^{il\theta_0}. \tag{20}$$

We can extend these results, using[6]

$$\mathcal{S}_{l+1,m,n-1}(\xi) = -\xi^l[\xi^{-l}\mathcal{S}_{l,m,n}(\xi)]', \tag{21}$$

with the prime denoting differentiation. Using this once with (19), we obtain for $l \geqslant 1$,

$$\mathcal{S}_{4m+l+1,4m,l-1}(\xi/D) = \frac{2}{2\pi(2l-2)!!}\left(\frac{\xi}{D}\right)^{l-3}\delta_{m,0}. \tag{22}$$

Thus, the sum for $m=0$ is singular at $\xi=0$ for $l=1,2$, and regular for $l>3$. Using (21) a second time, we have for $l \geqslant 2$

$$\mathcal{S}_{4m+l+2,4m,l-2}(\xi/D) = \frac{2\times 4}{2\pi(2l-2)!!}\left(\frac{\xi}{D}\right)^{l-4}\delta_{m,0}. \tag{23}$$

Generalizing, we find for an arbitrary positive integer p

$$\mathcal{S}_{4m+l+p,4m,l-p}(\xi/D) = \frac{(2p)!!}{2\pi(2l-2)!!}\left(\frac{\xi}{D}\right)^{l-p-2}\delta_{m,0}. \tag{24}$$

Three simple double sums which are particular cases of the above-given results are

$$\sum_h J_0(K_h\xi) = \sum_{h_1,h_2=-\infty}^{\infty} J_0[2\pi(\xi/D)\sqrt{h_1^2+h_2^2}] = \frac{\delta(\xi/D)}{2\pi\xi/D}, \tag{25}$$

$$\sum_h J_2(K_h\xi) = \frac{1}{\pi}\left(\frac{D}{\xi}\right)^2, \tag{26}$$

and

$$\sum_h J_4(K_h\xi) = \frac{2}{\pi}\left(\frac{D}{\xi}\right)^2. \tag{27}$$

The general form is

$$\sum_h J_{2l}(K_h\xi) = \frac{l}{\pi}\left(\frac{D}{\xi}\right)^2. \tag{28}$$

We give numerical confirmation of the results (26) and (27) in Fig. 1. Note that the averages of the numerical sums over the ranges shown are 1.2737 and 2.5483; the analytic values are $4/\pi \simeq 1.2732$ and $8/\pi \simeq 2.5465$, respectively. Thus, even though the raw sums in Fig. 1 oscillate rapidly, their average over a large ensemble of regions of summation can be used as a good indicator of the correct value.

IV. ANALYTIC FORMS FOR THE FOURIER SERIES

We will now assemble the series for the σ_l, with $l>0$. Note that, in this section, we will use the notations $\tau=\xi/D$ and $\kappa=k_0d/2\pi$ to simplify the formulas.

We first consider the case $l=1$. The sums we require are then of the form $\mathcal{S}_{1-4m,4m,1} = -\mathcal{S}_{4m-1,4m,1}$, and can be evaluated using the following general expression:[6]

$$\mathcal{S}_{l-4m,4m,l}(\tau) = \frac{(-1)^l(4m-l)!}{\pi 2^l(l-1)!}\sum_{s=0}^{l-1}\frac{(4m+1-l)_s(1-l)_s}{s!(s+4m-l)!}\sigma^{(4m)}_{2s+4m-2l+2}\,\tau^{2s+4m-l} - \frac{1}{l!}\left(\frac{\tau}{2}\right)^l\delta_{l,2m}. \tag{29}$$

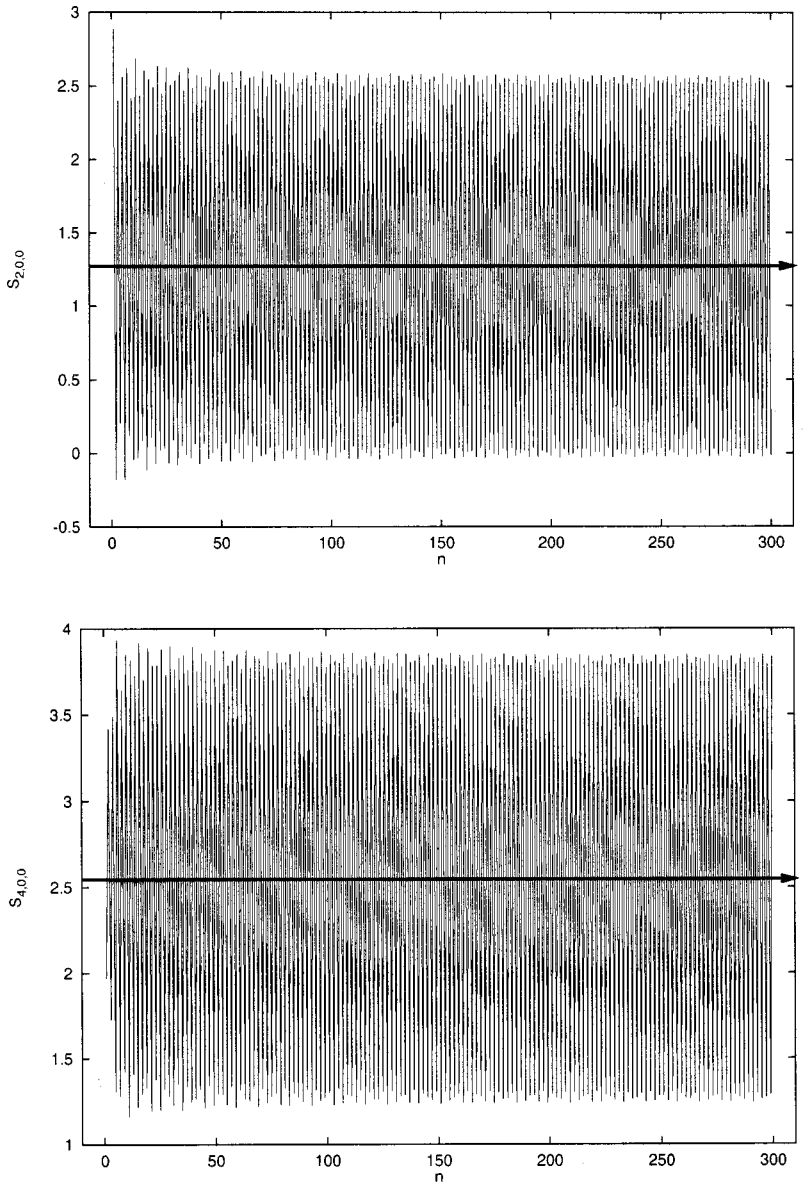

FIG. 1. The sums (26) (above) and (27) (below) as a function of the size of the square summation region. The analytic results are indicated by the arrows.

Here we have used the Pochhammer symbol: $(a)_0=1$, $(a)_s=a(a+1)\cdots(a+s-1)$, and the quantities $\sigma_n^{(m)}$ are lattice sums with no Bloch factor:

$$\sigma_n^{(m)}-\frac{2\pi}{m}\delta_{n,2}=\sum_{p\neq 0}\frac{\exp(im\varphi_p)}{R_p^n}. \tag{30}$$

They are nonzero unless m is a multiple of four, except for $n=2$, when they are conditionally convergent. If $n=2$, we denote the left-hand side of (30) by $\tilde{\sigma}_n^{(m)}$, which has the effect of combining together the Kronecker delta term in (29) with the term $s=0$ from the sum. The necessary sums for $l=1$ require only one term in (29):

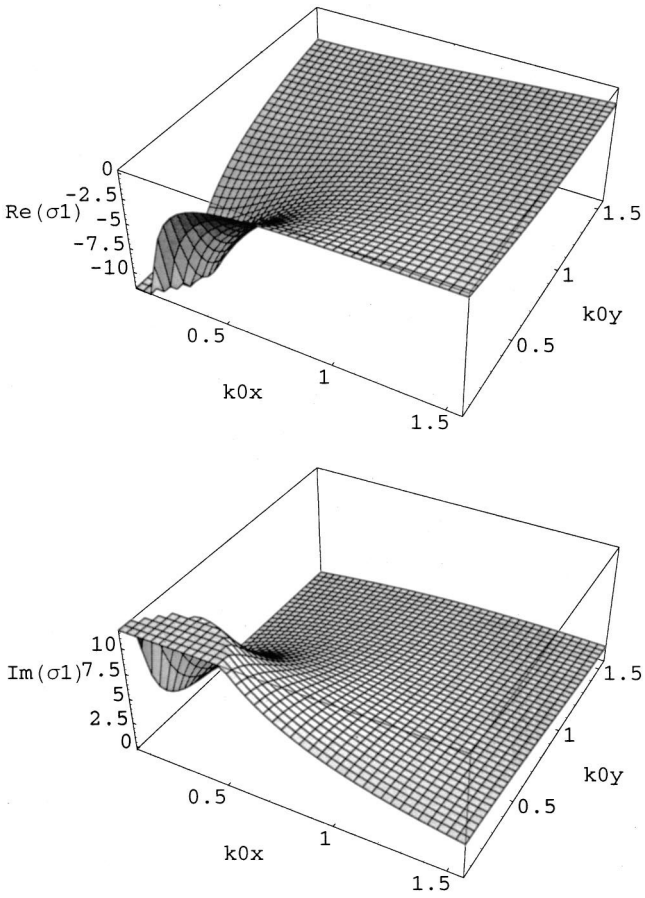

FIG. 2. Real part (above) and imaginary part (below) of σ_1 in the Brillouin zone.

$$\mathcal{S}_{1-4m,4m,1}(\tau)=-\frac{\sigma_{4m}^{(4m)}}{2\pi}\tau^{4m-1}. \tag{31}$$

The result (31) enables us to derive the desired series for σ_1:

$$\sigma_1(\mathbf{k}_0)=\frac{i}{d}\left(\frac{1}{\kappa}-\pi\kappa-\sum_{m=1}^{\infty}\sigma_{4m}^{(4m)}\kappa^{4m-1}e^{-4im\theta_0}\right)e^{i\theta_0}. \tag{32}$$

We have derived this expression in another way, using a result given by Glasser,[8] expressing

$$\Phi=\sum_{k\neq 0}\frac{\exp(i\mathbf{k}\cdot\mathbf{S})}{k^2}, \tag{33}$$

a two-dimensional sum over a square or rectangular array, in terms of the logarithm of the Jacobi theta function θ_1. From Glasser's result, we may obtain σ_1 by application of the complex gradient operator $\partial/\partial k_{0x}+i\partial/\partial k_{0y}$. Figure 2 shows the variation of σ_1 in the first quadrant of the Brillouin zone, with the singularity at the origin or Γ point the most prominent feature.

We next consider $l=2$. Here,

$$\mathcal{S}_{2-4m,4m,2}(\tau)=S_{4m-2,4m,2}(\tau), \tag{34}$$

and, using (29),

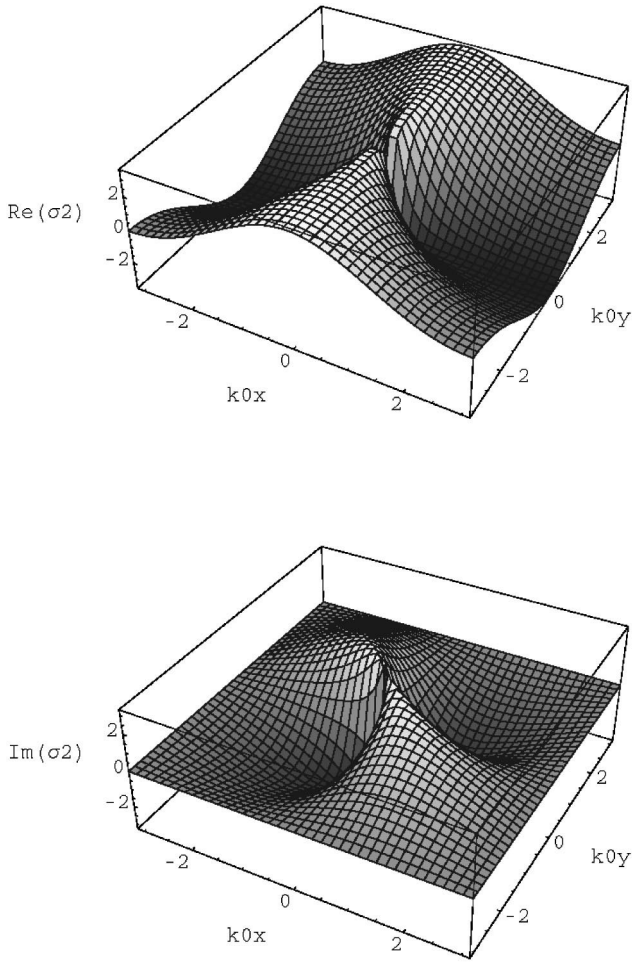

FIG. 3. Real part (above) and imaginary part (below) of σ_2 in the Brillouin zone.

$$\mathcal{S}_{2-4m,4m,2}(\tau)=\frac{1}{4\pi}(\sigma_{4m-2}^{(4m)}\tau^{4m-2}-\sigma_{4m}^{(4m)}\tau^{4m})-\frac{1}{2}\left(\frac{\tau}{2}\right)^2\delta_{m,1}. \tag{35}$$

Using (35) in (20), we obtain

$$\sigma_2(\mathbf{k}_0)=\frac{-\pi}{d^2}\left\{1-\frac{\pi}{2}\kappa^2+\sum_{m=1}^{\infty}\left[\left(\sigma_{4m-2}^{(4m)}-\frac{\pi}{2}\delta_{m,1}\right)\kappa^{4m-2}-\sigma_{4m}^{(4m)}\kappa^{4m}\right]e^{-4im\theta_0}\right\}e^{2i\theta_0}. \tag{36}$$

We have attempted to derive this expression from Glasser's results, but the algebra involved is considerably more involved than in the case $l=1$. Figure 3 shows the variation of σ_2 across the Brillouin zone; note the nonanalytic nature of the behavior near Γ, evident from the form of (36).

If $l\geqslant 3$, special sums occur in (20) which cannot be evaluated using the general form (29). For $l=3$, the only special sum is

$$\mathcal{S}_{-1,4,3}(\tau)=-\mathcal{S}_{1,4,3}(\tau)=-\left[\frac{1}{(2\pi)^2}\tilde{\sigma}_2^{(4)}\frac{\tau}{2}-\frac{1}{\pi}\tilde{\sigma}_2^{(4)}\left(\frac{\tau}{2}\right)^3+\frac{2}{\pi}\sigma_4^{(4)}\left(\frac{\tau}{2}\right)^5\right], \tag{37}$$

where $\tilde{\sigma}_2^{(4)}=\sigma_2^{(4)}-\pi/2$. The third order sum is

$$\sigma_3(\mathbf{k}_0)=\left(\frac{2\pi i}{d}\right)^3\left[\frac{1}{16\pi}\kappa-\frac{1}{48}\kappa^3-\mathcal{S}_{1,4,3}(\kappa)\,e^{-4i\theta_0}-\sum_{m=2}^{\infty}\mathcal{S}_{4m-3,4m,3}(\kappa)\,e^{-4im\theta_0}\right]e^{3i\theta_0}. \tag{38}$$

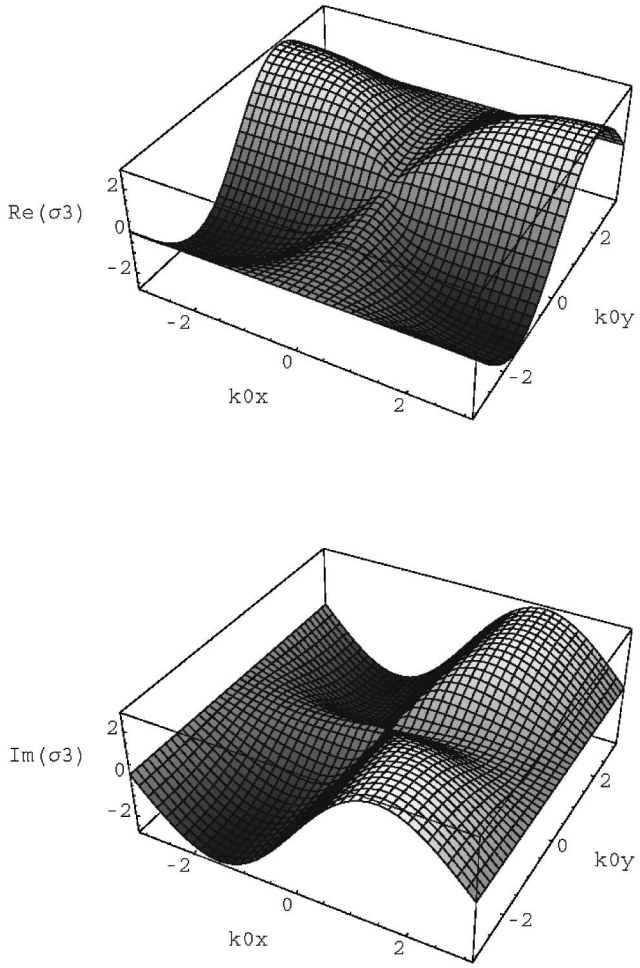

FIG. 4. Real part (above) and imaginary part (below) of σ_3 in the Brillouin zone.

We show the variation of σ_3 across the Brillouin zone in Fig. 4. The sum is now continuous at Γ.

For $l=4$, we require

$$\mathcal{S}_{0,4,4}(\tau)=\frac{1}{(2\pi)^4}\sigma_4^{(4)}-\frac{1}{(2\pi)^2}\tilde{\sigma}_2^{(4)}\left(\frac{\tau}{2}\right)^2+\frac{1}{2\pi}\tilde{\sigma}_2^{(4)}\left(\frac{\tau}{2}\right)^4-\frac{2}{3\pi}\sigma_4^{(4)}\left(\frac{\tau}{2}\right)^6. \tag{39}$$

The fourth-order sum consequently is

$$\sigma_4(\mathbf{k}_0)=\left(\frac{2\pi i}{d}\right)^4\left[\frac{1}{384}\left(\frac{4}{\pi}\kappa^3+\kappa^4\right)+\mathcal{S}_{0,4,4}(\kappa)\,e^{-4i\theta_0}+\sum_{m=2}^{\infty}\mathcal{S}_{4m-4,4m,4}(\kappa)\,e^{-4im\theta_0}\right]e^{4i\theta_0}. \tag{40}$$

We show the variation of σ_4 across the Brillouin zone in Fig. 5.

For $l=5$, the special sums are

$$\mathcal{S}_{1,4,5}(\tau)=\frac{1}{(2\pi)^4}\sigma_4^{(4)}\frac{\tau}{2}-\frac{1}{8\pi^2}\tilde{\sigma}_2^{(4)}\left(\frac{\tau}{2}\right)^3+\frac{1}{6\pi}\tilde{\sigma}_2^{(4)}\left(\frac{\tau}{2}\right)^5-\frac{1}{6\pi}\sigma_4^{(4)}\left(\frac{\tau}{2}\right)^7, \tag{41}$$

and

$$\mathcal{S}_{3,8,5}(\tau)=\frac{\tau^3}{768\,\pi^2}[\,\pi^2\,\tau^2+\pi\,\tau^2\,(-4\,\sigma_2^{(8)}+6\,\tau^2\,\sigma_4^{(8)}-4\,\tau^4\,\sigma_6^{(8)}+\tau^6\,\sigma_8^{(8)})+4\,\tilde{\sigma}_2^{(8)}], \tag{42}$$

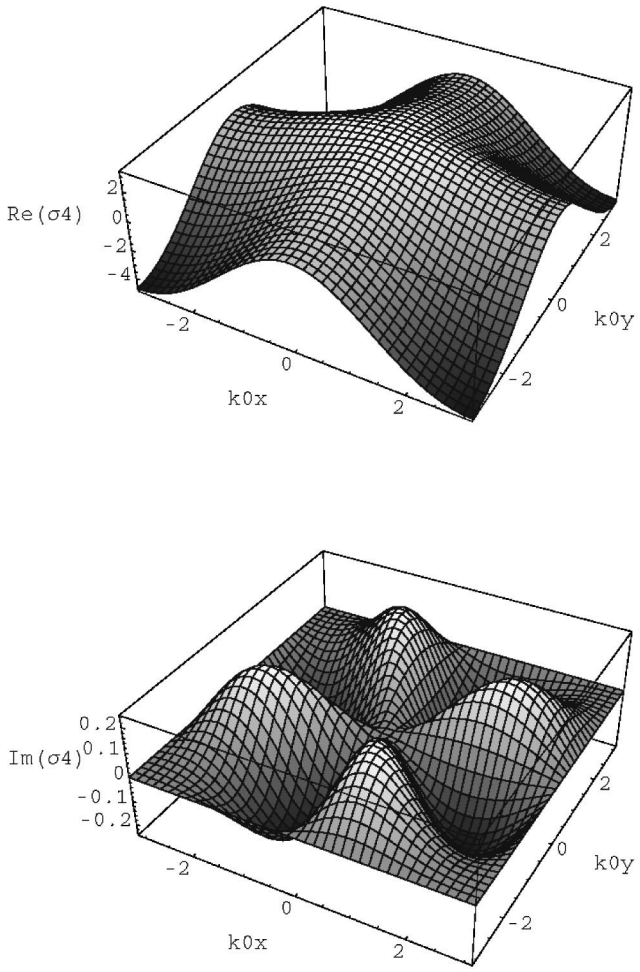

FIG. 5. Real part (above) and imaginary part (below) of σ_4 in the Brillouin zone.

where $\tilde{\sigma}_2^{(8)}=\sigma_2^{(8)}-\pi/4$. So, the fifth-order sum is

$$\sigma_5(\mathbf{k}_0)=\left(\frac{2\pi i}{d}\right)^5\left[\frac{1}{3840}\left(\frac{5}{\pi}\kappa^3-\kappa^5\right)+\mathcal{S}_{1,4,5}(\kappa)\,e^{-4i\theta_0}-\sum_{m=2}^{\infty}\mathcal{S}_{4m-5,4m,5}(\kappa)\,e^{-4im\theta_0}\right]e^{5i\theta_0}. \tag{43}$$

We show the variation of σ_5 across the Brillouin zone in Fig. 6.

Lastly, for $l=6$, we need

$$\mathcal{S}_{2,4,6}(\tau)=\frac{\tau^2}{7680\,\pi^4}[(60-\pi^3\,\tau^6)\,\sigma_4^{(4)}+5\,\pi^2\,\tau^2\,(-4+\pi\,\tau^2)\,\tilde{\sigma}_2^{(4)}], \tag{44}$$

and

$$\mathcal{S}_{2,8,6}(\tau)=\frac{-\tau^2}{15\,360\,\pi^4}[5\,\pi^4\,\tau^4-120\,\sigma_4^{(8)}+2\,\pi^3\,\tau^4\,(-10\,\sigma_2^{(8)}+10\,\tau^2\,\sigma_4^{(8)}-5\,\tau^4\,\sigma_6^{(8)}+\tau^6\,\sigma_8^{(8)})$$
$$+40\,\pi^2\,\tau^2\,\tilde{\sigma}_2^{(8)}]. \tag{45}$$

So, the sixth-order sum is

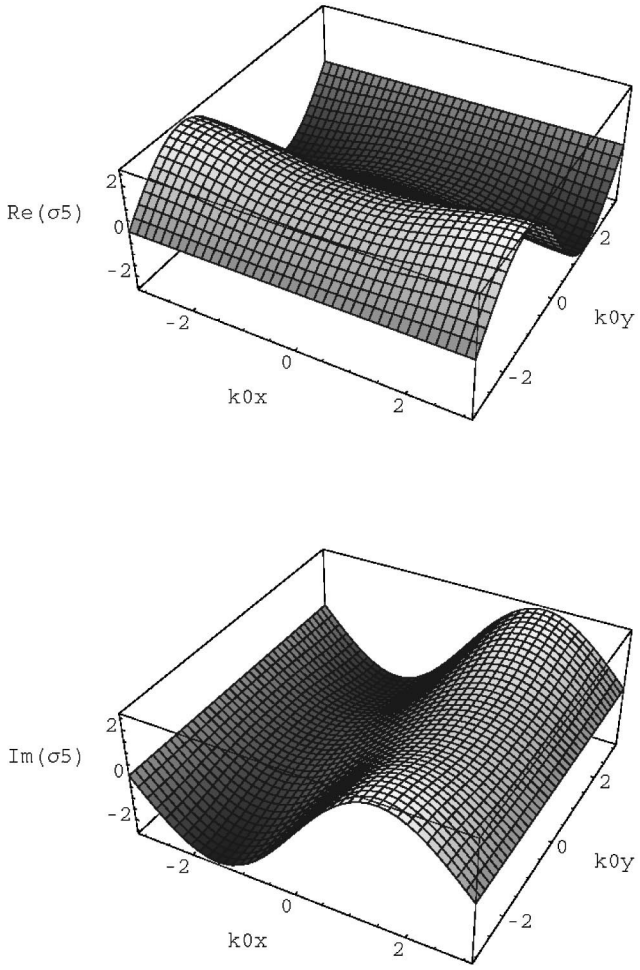

FIG. 6. Real part (above) and imaginary part (below) of σ_5 in the Brillouin zone.

$$\sigma_6(\mathbf{k}_0)=\left(\frac{2\pi i}{d}\right)^6\left[\frac{1}{46\,080}\left(\frac{6}{\pi}\kappa^4+\kappa^6\right)+\mathcal{S}_{2,8,6}(\kappa)e^{-4i\theta_0}+\sum_{m=2}^{\infty}\mathcal{S}_{4m-6,4m,6}(\kappa)e^{-4im\theta_0}\right]e^{6i\theta_0}. \tag{46}$$

We show the variation of σ_6 across the Brillouin zone in Fig. 7.

One interesting trend evident in Figs. 1–6 is that σ_l tends to become increasingly smooth in its angular variation with increasing l. The prefactor $\exp(il\theta_0)$ might suggest the contrary, but in fact the dominant contribution comes from $m=1$, not $m=0$, i.e., the angular variation goes as $\exp[i(l-4)\theta_0]$ for moderate l.

The figures in this section were calculated with expansions running up to $m=6$. The necessary static lattice sums $\sigma_n^{(m)}$ are given to ten figures accuracy in Table I; some of these have previously been tabulated by Movchan *et al.*,[9] Helsing,[10] and Berman and Greengard.[11] For $n\geqslant 4$, they can be evaluated readily by direct summation. For $n=2$, they are evaluated by the method described by Nicorovici *et al.*:[6] a rapidly convergent sum $\mathcal{S}$ is found in which the relevant σ occurs, and the former is evaluated, being used in an equation for the desired σ. Of course, direct summation is not possible for sums σ_2^{4m}, since the result obtained depends on the shape chosen for the summation region. Table II shows that $m=6$ gives relative precision of better than one part in 10^7 at a point halfway across the Brillouin zone; accuracy better than this can be expected at points further inside the Brillouin zone.

For general l, we exhibit the form:

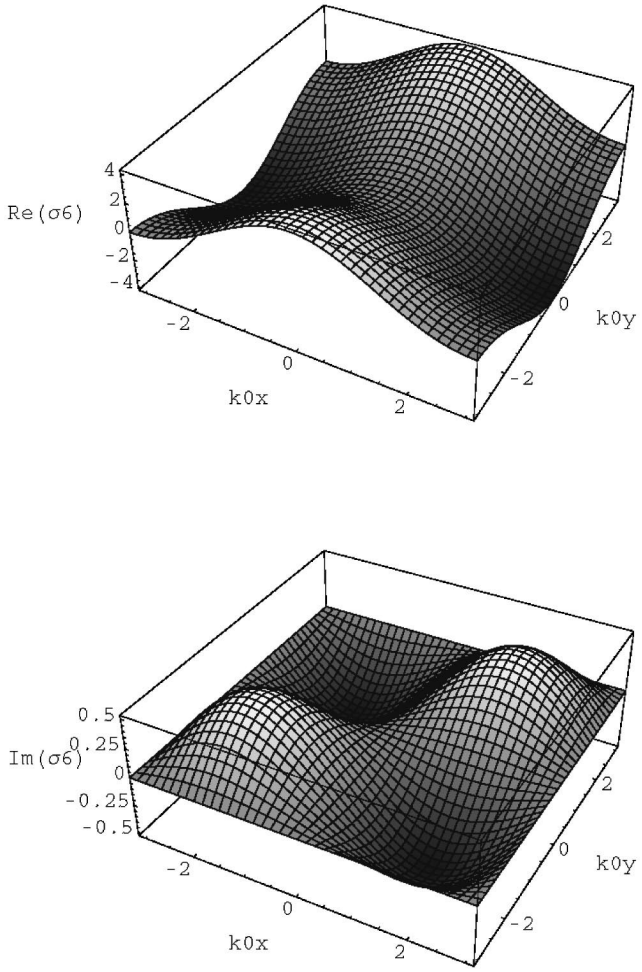

FIG. 7. Real part (above) and imaginary part (below) of σ_6 in the Brillouin zone.

$$\sigma_l(\mathbf{k}_0)=\left(\frac{2\pi i}{d}\right)^l\left[\frac{1}{(2l)!!}\left(\frac{l}{\pi}\kappa^{l-2}-\kappa^l\right)+\sum_{m\geqslant 1,l-4m>0}\mathcal{S}_{l-4m,4m,l}(\kappa)\,e^{-4im\theta_0}\right.$$
$$\left.+\sum_{4m\geqslant l}^{\infty}(-1)^l\mathcal{S}_{4m-l,4m,l}(\kappa)\,e^{-4im\theta_0}\right]e^{il\theta_0}. \tag{47}$$

Here, exceptional sums have $l<2m$; all other sums may be evaluated using (29). This expression

TABLE I. The lattice sums $\sigma_n^{(4m)}$ $(n=4m,4m-2,...)$ for the square array.

	n					
m	$4m$	$4m-2$	$4m-4$	$4m-6$	$4m-8$	$4m-10$
1	3.151 212 002 2	4.078 451 161 2				
2	4.255 773 035 4	4.515 515 435 4	5.030 666 214 7	6.790 313 626 7		
3	3.938 849 012 8	3.880 730 845 9	3.774 451 370 1	3.604 335 558 1	3.441 886 923 8	4.358 151 998 0
4	4.015 695 033 0	4.031 540 313 8	4.063 717 271 7	4.130 191 080 2	4.272 712 121 1	4.603 234 338 0
5	3.996 096 753 2	3.992 198 698 9	3.984 415 731 6	3.968 892 733 6	3.937 971 863 3	3.876 416 335 0
6	4.000 976 805 3	4.001 954 100 8	4.003 910 177 5	4.007 828 339 1	4.015 689 074 5	4.031 510 506 5

TABLE II. Convergence of σ_l at the point $(k_{0x},k_{0y})=(\pi/2,\pi/2)$. The value of σ shown is calculated with terms up to $m=6$; Δ gives the relative difference between sums (29) with terms up to $m=5$ and $m=6$ included.

l	σ_l	Δ
1	$1.311\,028\,777\times(-1+i)$	-8.88×10^{-11}
2	$-1.718\,796\,455\times i$	7.45×10^{-10}
3	$2.253\,391\,614\times(1+i)$	-1.56×10^{-9}
4	$-0.295\,426\,125$	4.38×10^{-8}
5	$1.936\,560\,760\times(-1+i)$	9.00×10^{-9}
6	$0.507\,777\,377\times i$	7.76×10^{-8}

may be regarded as complementary to expressions (1) and (5). As we have $\kappa=k_0d/2\pi\leqslant1/\sqrt{2}$ in the Brillouin zone of the square array, the series involved in (47) converge rapidly, but as l increases they become more and more cumbersome. On the other hand, as l increases, direct summation of (1) becomes more and more computationally viable. The expressions (5) can be used for all l, but the occurrence of Bessel functions in the summand means they can be slow to compute. Thus, we recommend use of (47) for small l, and (1) for l moderate to large.

ACKNOWLEDGMENT

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Pseudo-Hermiticity versus *PT*-symmetry. II. A complete characterization of non-Hermitian Hamiltonians with a real spectrum

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We give a necessary and sufficient condition for the reality of the spectrum of a non-Hermitian Hamiltonian admitting a complete set of biorthonormal eigenvectors. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1461427]

Recently, we have explored in Ref. 1 the basic mathematical structure underlying the spectral properties of PT-symmetric Hamiltonians.[2] In particular, we have shown that these properties are associated with a class of more general (not necessarily Hermitian) Hamiltonians H satisfying

$$H^\dagger = \eta H \eta^{-1}, \tag{1}$$

where a dagger denotes the adjoint of the corresponding operator and η is a Hermitian invertible linear operator. We have termed such a Hamiltonian "*η-pseudo-Hermitian.*" Hermitian and the PT-symmetric Hamiltonians that admit a complete set of biorthonormal eigenvectors constitute subsets of the set of pseudo-Hermitian Hamiltonians. For a PT-symmetric Hamiltonian, the exactness of PT-symmetry ensures the reality of the energy spectrum. The purpose of this article is to provide a complete characterization of the Hamiltonians that have a real spectrum assuming that they are endowed with a complete set of biorthonormal eigenvectors.

By definition, a PT-symmetric Hamiltonian has a symmetry given by an antilinear operator, namely PT. It is well-known that if a Hamiltonian satisfies

$$[H,A] = 0, \tag{2}$$

for an anti-linear operator A, then

(★) either the eigenvalues of H are real or they come in complex conjugate pairs.

Furthermore, an eigenvalue of H is real provided that a corresponding eigenvector is invariant under the action of A, i.e., Eq. (2), together with

$$H|E\rangle = E|E\rangle, \tag{3}$$

and

$$A|E\rangle = |E\rangle \tag{4}$$

imply $E \in \mathbb{R}$. Therefore, a Hamiltonian with an antilinear symmetry has a real spectrum if the symmetry is exact.

In Ref. 1, we have shown that every pseudo-Hermitian Hamiltonian has the property (★).

Furthermore, for Hamiltonians with a complete set of biorthonormal eigenvectors this property is the necessary and sufficient condition for pseudo-Hermiticity. This, in particular, means that pseudo-Hermiticity is a necessary condition for having a real spectrum, but it is not sufficient. In the following we give the necessary and sufficient condition for the reality of the spectrum of any

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Hamiltonian that admits a complete set of biorthonormal eigenvectors. We shall only consider the case of discrete spectra. The generalization to continuous spectra does not seem to involve major difficulties.

We first recall the defining properties of a Hamiltonian admitting a complete set of biorthonormal eigenvectors.[3] If a Hamiltonian H has a complete set of biorthonormal eigenvectors $\{|\psi_n\rangle,|\phi_n\rangle\}$, then

$$H|\psi_n\rangle=E_n|\psi_n\rangle, \quad H^\dagger|\phi_n\rangle=E_n^*|\phi_n\rangle, \tag{5}$$

$$\langle\phi_m|\psi_n\rangle=\delta_{mn}, \tag{6}$$

$$\sum_n |\psi_n\rangle\langle\phi_n|=1, \tag{7}$$

where n is the spectral label, δ_{mn} denotes the Kronecker delta function, and 1 is the identity operator.

Theorem: Let $H:\mathcal{H}\to\mathcal{H}$ be a Hamiltonian that acts in a Hilbert space $\mathcal{H}$, has a discrete spectrum, and admits a complete set of biorthonormal eigenvectors $\{|\psi_n\rangle,|\phi_n\rangle\}$. Then the spectrum of H is real if and only if there is an invertible linear operator $O:\mathcal{H}\to\mathcal{H}$ such that H is $OO^\dagger$-pseudo-Hermitian.

Proof: Let $\{|n\rangle\}$ be a complete orthonormal basis of $\mathcal{H}$, i.e.,

$$\langle m|n\rangle=\delta_{mn}, \quad \sum_n |n\rangle\langle n|=1, \tag{8}$$

and $O:\mathcal{H}\to\mathcal{H}$ and $H_0:\mathcal{H}\to\mathcal{H}$ be defined by

$$O:=\sum_n |\psi_n\rangle\langle n|, \quad H_0:=\sum_n E_n|n\rangle\langle n|. \tag{9}$$

Then, in view of (5)–(9), O is invertible with the inverse given by

$$O^{-1}=\sum_n |n\rangle\langle\phi_n|, \tag{10}$$

and

$$O^{-1}HO=H_0. \tag{11}$$

Now suppose that the spectrum of H is real. Then, H_0 is Hermitian, and taking the adjoint of both sides (11), we have

$$O^{-1}HO=O^\dagger H^\dagger O^{-1\dagger} \tag{12}$$

or alternatively

$$H=(OO^\dagger)H^\dagger(OO^\dagger)^{-1}. \tag{13}$$

This equation shows that H is $OO^\dagger$-pseudo-Hermitian. This completes the proof of necessity. Next we suppose that H is $OO^\dagger$-pseudo-Hermitian. Then (13) and consequently (12) hold. On the other hand, in view of (6) and (9), we have

$$H_0=O^{-1}HO, \quad H_0^\dagger=O^\dagger H^\dagger O^{-1\dagger}.$$

Therefore, (12) implies that H_0 is Hermitian, and the eigenvalues E_n are all real. □

It should be emphasized that the characterization of the non-Hermitian Hamiltonians with a real spectrum given by the preceding theorem applies to the Hamiltonians that admit a complete biorthonormal system of eigenvectors. A generalization of this result to the case of arbitrary Hamiltonians is not known.

The basic idea of the present work was originated from a comment made by Z. Ahmed about his checking the results the author had reported in Ref. 1 for a specific example of a non-Hermitian Hamiltonian with a real spectrum. This project was supported by the Young Researcher Award Program (GEBIP) of the Turkish Academy of Sciences.

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Compatibility and decompositions of effects

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Compatibility relations in effect algebras and their connections with refinements of the orthogonal partitions of unity are studied. Properties of blocks as maximal sets of compatible elements are discussed. Some special kinds of effect algebras are characterized using properties of compatibility. Using refinements, an additional structure on the effect test spaces is introduced and used to a characterization of different types of effect algebras. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Effect algebras (Foulis and Bennett, 1994), alternatively D-posets (Kôpka and Chovanec, 1994), have been introduced as an algebraic generalization of the set of Hilbert space effects, i.e., self-adjoint operators between 0 and I on a Hilbert space. These effects play an important role in the theory of unsharp quantum measurements and positive operator valued (POV) measures (Bush *et al.*, 1991).

Besides the Hilbert space effects, effect algebras include the most important structures used in quantum and classical logic: orthomodular lattices, orthomodular posets, Boolean algebras, and also MV-algebras, an algebraic base of multivalued logic (Chang, 1958). For basic properties of effect algebras and D-posets, see Dvurečenskij and Pulmannová (2000).

In the present article we study compatibility relations on effect algebras and their connections with refinements of the orthogonal partitions of unity. We use properties of compatibility to a characterization of some types of effect algebras and their blocks.

Using refinements, we introduce additional structures to effect test spaces and characterize test spaces of different types of effect algebras.

II. BASIC DEFINITIONS AND PROPERTIES OF EFFECT ALGEBRAS

An *effect algebra* is a partial algebra $(E;\oplus,0,1)$ with a binary partial operation $\oplus$ and two nullary operations 0, 1 satisfying the following conditions.

(E1) If $a\oplus b$ is defined, then $b\oplus a$ is defined and $a\oplus b=b\oplus a$.

(E2) If $a\oplus b$ and $(a\oplus b)\oplus c$ are defined, then $b\oplus c$ and $a\oplus(b\oplus c)$ are defined and $a\oplus(b\oplus c)=(a\oplus b)\oplus c$.

(E3) For every $a\in E$ there is a unique $a'\in E$ such that $a\oplus a'=1$.

(E4) If $a\oplus 1$ is defined, then $a=0$.

Effect algebras in this setting have been introduced in Foulis and Bennett (1994). Essentially equivalent structures, called D-posets, were introduced in Kôpka and Chovanec (1994). Another equivalent structure, called weak orthoalgebra, was introduced in Giuntini and Greuling (1989), and so-called quasilogics were introduced in Belavkin (1987).

For brevity we denote the effect algebra $(E;\oplus,0,1)$ by E. We write $a\leqslant b$ if there is a $c\in E$ with $a\oplus c=b$. It is easy to check that each effect algebra is cancellative, i.e., $a\oplus b=a\oplus c$ implies $b=c$, and positive, i.e., $a\oplus b=0$ implies $a=b=0$. We can derive from this that $\leqslant$ is a partial order with 0 as the least and 1 as the greatest element. Moreover, it is possible to introduce a new

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partial operation $\ominus$ such that $b\ominus a$ is defined iff $a\leqslant b$ and then $a\oplus(b\ominus a)=b$. We can also prove that $a\oplus b$ is defined iff $a\leqslant b'$, equivalently, iff $b\leqslant a'$. For convenience, we will write $a\perp b$ if $a\oplus b$ is defined, and say that a and b are *orthogonal*.

Let E_0 be a subset of E such that $a\in E_0$ implies $a'\in E_0$ and $a,b\in E_0$, $a\perp b$ implies $a\oplus b\in E_0$. Let $a,b\in E_0$ such that $a\leqslant b$. Then $b'\in E_0$ and $a\perp b'$ implies that $b\ominus a=(b'\oplus a)'\in E_0$, so that E_0 is closed under $\ominus$. Then E_0 is called the *subeffect algebra* of E. Another possibility to construct a substructure of E is to consider an element $a\in E$ and the interval $[0,a]$ of E, and to restrict the $\oplus$ operation letting a act as the unit element. We denote such effect algebra by $[0,a]_E$. Observe that for x, y in $[0,a]_E$, $x\perp_a y$ iff $x\oplus y$ exists in E and $x\oplus y\leqslant a$.

An effect algebra satisfying $a\perp a\Rightarrow a=0$ is called an *orthoalgebra*. An effect algebra E is an *orthomodular poset* (OMP, for short) if for a, b, $c\in E$, $a\perp b$, $b\perp c$, $c\perp a$ implies that $a\oplus b\oplus c$ exists (Foulis and Bennett, 1994). An orthoalgebra is an *orthomodular lattice* (OML, for short) if it is lattice ordered. An effect algebra E is said to have the *Riesz decomposition property* (RDP) (Ravindran, 1996) if for any a_1, a_2, b_1, $b_2\in E$ with $a_1\oplus a_2=b_1\oplus b_2$ there are elements $(w_{ij})_{i,j=1}^2$ such that $w_{11}\oplus w_{12}\oplus w_{21}\oplus w_{22}$ is defined and $a_i=\oplus_{j=1}^2 w_{ij}$, $b_j=\oplus_{i=1}^2 w_{ij}$. Alternatively, E has the Riesz decomposition property if $a\leqslant b\oplus c$ implies $a=b_1\oplus c_1$, $b_1\leqslant b$, $c_1\leqslant c$. If E is lattice ordered and has the RDP, then E can be organized into an MV-algebra (cf., e.g., Dvurečenskij and Pulmannová, 2000). An interesting weakening of the RDP was recently introduced in Jenča (2001): an effect algebra E is called *homogeneous* if $a\leqslant b\oplus c$, and $a\leqslant(b\oplus c)'$ implies $a=b_1\oplus c_1$, $b_1\leqslant b$, $c_1\leqslant c$. Finally, an MV-algebra which is an orthoalgebra is a Boolean algebra.

III. COMPATIBILITY IN EFFECT ALGEBRAS

Let E be an effect algebra. Let $C=(c_1,\ldots,c_n)$ be a finite sequence of elements of E. We say that C is *jointly orthogonal* (or simply *orthogonal*) if the sum $c_1\oplus\cdots\oplus c_n$ is defined. We then write $\oplus C=c_1\oplus\cdots\oplus c_n$. For $n=0$ we define $\oplus C=0$.

Let $\sigma:=(P_1,\ldots,P_k)$ be an ordered partition of the set $\{1,\ldots,n\}$. We put $\|\sigma\|:=k$. Then $\sigma(C)=(\oplus_{i\in P_1}c_i,\ldots,\oplus_{i\in P_k}c_i)$ is an orthogonal sequence and $\oplus\sigma(C)=\oplus_{l=1}^k\oplus_{i\in P_l}c_i=\oplus C$. We will say that C is a *refinement* of $\sigma(C)$. To every ordered partition σ of $\{1,\ldots,n\}$ we can define a function $f_\sigma:\{1,\ldots,n\}\to\{1,\ldots,k\}$ by $f_\sigma(i)=j$ iff $i\in P_j$. Conversely, every such surjection f defines a partition of $\{1,\ldots,n\}$. We will call f_σ the *refinement mapping*.

Observe that if $C=(c_1,\ldots,c_n)$ is an orthogonal sequence, then there may exist different partitions of $\{1,\ldots,n\}$ with different refinement mappings leading to the same orthogonal sequence $D=\{d_1,\ldots,d_k\}$ of which C is a refinement. This may happen only if there is $c\in C$ such that $c\perp c$.

Let E be an effect algebra. A finite family M of elements of E is said to be *jointly compatible* (or simply *compatible*) if there is an orthogonal sequence $C=(c_1,\ldots,c_n)$ such that for every $a\in M$ there is a set $I_a\subset\{1,\ldots,n\}$ such that $a=\oplus_{i\in I_a}c_i$. We say that C *covers* M, and call C a *cover* of M. If M is any subset of E, we say that M is compatible if every finite subset of M is compatible.

An ordered pair (a,b) of elements of M is said to be *Mackey compatible* if there is an orthogonal sequence (a_1,b_1,c) such that $a=a_1\oplus c$, $b=b_1\oplus c$. The sequence (a_1,b_1,c) is called a *Mackey decomposition* of (a,b). Clearly, if (a,b) is Mackey compatible, then (b,a) is Mackey compatible with the decomposition (b_1,a_1,c). We will write $a\leftrightarrow b$ if (a,b) are Mackey compatible.

Let F be a subset of E. We say that events $A=(a_1,\ldots,a_n)$ are *compatible in* F if A is compatible with a cover $C\subset F$. A subset M of E is called *compatible in* F if any finite subset of M is compatible with covers in F. We say that M is *internally compatible* if M is compatible in M. We say that elements (a,b) are *Mackey compatible in* F if there is a Mackey decomposition (a_1,b_1,c) of (a,b) with a_1, b_1, $c\in F$, and we write $a\leftrightarrow^F b$

In the following propositions we collect some basic properties of compatibility (Kôpka, 1995; Dvurečenskij and Pulmannová, 2000).

Proposition 1: Let a, b be elements of an effect algebra E.

(i) $a \leftrightarrow a,\ 0 \leftrightarrow a,\ 1 \leftrightarrow a,\ \forall a \in E.$
(ii) $a \leqslant b \Rightarrow a \leftrightarrow b,\ a \perp b \Rightarrow a \leftrightarrow b.$
(iii) $a \leftrightarrow b \Rightarrow a' \leftrightarrow b.$
(iv) *If elements* $a_1,\ldots,a_n$ *are jointly compatible, they are pairwise Mackey compatible. If* $n \geqslant 3$, *the converse need not hold even in OMP* (Pták and Pulmannová, 1991).

Proof of the above statement is straightforward.

Proposition 2: Let (a,b) *be an ordered pair of elements in* E. *The following statements are equivalent.*

(C1) $a \leftrightarrow b$.

(C2) a,b *are jointly compatible.*

(C3) $a = x \oplus y$ *with* $x \leqslant b,\ y \leqslant b'$.

(C4) *There are elements* u,v such that $u \leqslant a,\ b \leqslant v$ and $a \ominus u = v \ominus b$.

Proof: (C1)$\Rightarrow$(C2). Let (a_1,b_1,c) be a Mackey decomposition of (a,b). The orthogonal sequence (a_1,b_1,c) covers (a,b), so $a,\ b$ are jointly compatible.

(C2)$\Rightarrow$(C3): Let $(c_1,\ldots,c_n)$ be a cover of a,b. Then $a = \oplus_{i \in I_a} c_i,\ b = \oplus_{i \in I_b} c_i$, where $I_a,\ I_b$ are subsets of $\{1,\ldots,n\}$. Putting $P_1 = I_a \cap I_b,\ P_2 = I_a \cap I_b^c,\ P_3 = I_a^c \cap I_b,\ P_4 = I_a^c \cap I_b^c$, where $I_a^c,\ I_b^c$ are complements of $I_a,\ I_b$ in $\{1,\ldots,n\}$, respectively, we obtain a partition of $\{1,\ldots,n\}$. Clearly, $I_a = P_1 \cup P_2$, and $I_b = P_1 \cup P_3$. Then $a_1 = \oplus_{i \in P_2} c_i,\ b_1 = \oplus_{i \in P_3} c_i,\ c = \oplus_{i \in P_1} c_i$ is a Mackey decomposition of (a,b). Put $d = (c_1 \oplus \cdots \oplus c_n)'$. Then $b \oplus b' = \oplus_{i=1}^n c_i \oplus d = 1$, and by cancellativity, $b' = \oplus_{i \in I_b^c} c_i \oplus d$. Therefore $a_1 = \oplus_{i \in I_a \cap I_b^c} c_i \leqslant b'$, and $c \leqslant b$. Putting $x = c,\ y = a_1$ concludes the proof.

(C3)$\Rightarrow$(C4). Let $a = x \oplus y,\ x \leqslant b,\ y \leqslant b'$. Then $x \leqslant a,\ x \leqslant b$ and $a \leqslant b \oplus y,\ b \leqslant b \oplus y$. In addition, $a \ominus x = y = (b \oplus y) \ominus b$. Putting $u = x,\ v = b \oplus y$ yields the desired statement.

(C4)$\Rightarrow$(C1). Let $u \leqslant a,\ b \leqslant v$ and $a \ominus u = v \ominus b$. Then $a = u \oplus (a \ominus u),\ b = u \oplus (b \ominus u),\ v = b \oplus (v \ominus b) = u \oplus (b \ominus u) \oplus (a \ominus u)$, which shows that $(a \ominus u, b \ominus u, u)$ is a Mackey decomposition of (a,b). □

We will say that elements a,b in E are *strongly compatible* if there is a Mackey decomposition (a_1,b_1,c) of the ordered pair (a,b) such that $a_1 \wedge b_1 = 0$ (in the sense that $x \leqslant a_1,\ x \leqslant b_1$ implies $x = 0$). We will write $a \leftrightarrow^c b$. More generally, we say that a finite set $A = (a_1,\ldots,a_n)$ of elements are *jointly strongly compatible* if there is a cover $C = (c_1,\ldots,c_m)$ of A such that for every a_i,a_j in A,

$$\oplus_{k \in I_{a_i} \cap I_{a_j^c}} c_k \wedge \oplus_{k \in I_{a_i^c} \cap I_{a_j}} c_k = 0.$$

We then say that C *strongly covers* A (or that C is a strong cover of A).

Lemma 1: Let (a_1,b_1,c) *be a Mackey decomposition of* (a,b). *Let* $c \leqslant \overline{c} \leqslant a,b$. *Then* $(a \ominus \overline{c}, b \ominus \overline{c}, \overline{c})$ *is a Mackey decomposition of* (a,b).

Proof: We can write $a = \overline{c} \oplus (a \ominus \overline{c}),\ b = \overline{c} \oplus (b \ominus \overline{c})$. Then $a \oplus (b \ominus \overline{c}) \leqslant a \oplus (b \ominus c) = a_1 \oplus b_1 \oplus c$. It follows that $(a \ominus \overline{c}, b \ominus \overline{c}, \overline{c})$ is a Mackey decomposition of (a,b). □

Proposition 3: Let a,b *be elements of an effect algebra* E. *Let* (a_1,b_1,c) *be a Mackey decomposition of* (a,b). *The following statements are equivalent.*

(i) (a_1,b_1,c) *is a strong Mackey decomposition of* (a,b);
(ii) c *is a maximal lower bound of* a,b;
(iii) $d := a_1 \oplus b_1 \oplus c$ *is a minimal upper bound of* a,b.

Proof: $(i) \Rightarrow (ii)$: Let (a_1,b_1,c) be a strong Mackey decomposition of (a,b). Let $\overline{c} \in E$ be such that $c \leqslant \overline{c} \leqslant a,b$. There is an $x \in E$ such that $\overline{c} = c \oplus x$. We have

$$a = \overline{c} \oplus (a \ominus \overline{c}) = c \oplus x \oplus (a \ominus \overline{c}) = c \oplus a_1,$$

hence $a_1 = x \oplus (a \ominus c)$, and

$$b=\overline{c}\oplus(b\ominus\overline{c})=c\oplus x\oplus(b\ominus\overline{c})=c\oplus b_1,$$

hence $b_1=x\oplus(b\ominus\overline{c})$. It follows that $x\leqslant a_1,b_1$, so $x=0$. Therefore c is a maximal lower bound of a,b.

$(ii)\Rightarrow(i)$: Let c be a maximal lower bound of a,b and let (a_1,b_1,c) be a Mackey decomposition of (a,b). Assume that $x\leqslant a_1,b_1$. Then $a_1=x\oplus\overline{a_1}$, $b_1=x\oplus\overline{b_1}$, so that $a=x\oplus c\oplus\overline{a_1}$, $b=x\oplus c\oplus\overline{b_1}$. Hence $c\leqslant x\oplus c\leqslant a,b$. As c is a maximal lower bound of a,b then $x=0$, and (a_1,b_1,c) is a strong Mackey decomposition of (a,b).

$(ii)\Leftrightarrow(iii)$: Assume that (a_1,b_1,c) is a Mackey decomposition of (a,b). Put $d:=a_1\oplus b_1\oplus c$. Then $a\ominus c=d\ominus b$. Let there be a $\overline{d}$ with $a,b\leqslant\overline{d}\leqslant d$. There is $y\in E$ such that $d=\overline{d}\oplus y$. So we obtain $a\ominus c=(\overline{d}\oplus y)\ominus b=(\overline{d}\ominus b)\oplus y$, and hence $(a\ominus c)\ominus y=\overline{d}\ominus b$, which implies that $a\ominus(c\oplus y)=\overline{d}\ominus b$. Hence $c\oplus y\leqslant a$, and similarly we prove that $c\oplus y\leqslant b$. So if d is not a minimal upper bound of a,b, then c is not a maximal lower bound of a,b. By reversing the implications we obtain the converse. It follows that c is a maximal lower bound of a,b iff d is a minimal upper bound of a,b. □

Remark 1: Let E be an effect algebra.

(a) E is an orthoalgebra iff every Mackey decomposition is strong. Indeed, $(a,a',0)$ is a Mackey decomposition of (a,a') for every $a\in E$. If it is strong, then $a\wedge a'=0$. The converse is clear.

(b) E is an OMP iff for every Mackey decomposition (a_1,b_1,c) of (a,b), $a_1\oplus b_1\oplus c=a\vee b$. That is, every Mackey decomposition is strong and unique. The converse need not hold, there are orthoalgebras with unique Mackey decompositions which are not OMPs.

(c) E is an MV-algebra iff E is lattice ordered and $a\leftrightarrow b$ for every a,b in E (Chovanec and Kôpka, 1995; Pulmannová, 1997a; Dvurečenskij and Pulmannová, 2000). Indeed, according to Chovanec and Kôpka (1995), a lattice ordered effect algebra can be organized into an MV-algebra iff $a\ominus(a\wedge b)=(a\vee b)\ominus b$ holds for every $a,b\in E$. It is easy to see that $(a\ominus(a\wedge b),b\ominus(a\wedge b),a\wedge b)$ is a Mackey decomposition of (a,b). If E is a lattice and $a\leftrightarrow b$, then it can be derived from Lemma 1 and Proposition 3 that $(a\ominus(a\wedge b),b\ominus(a\wedge b),a\wedge b)$ is a strong Mackey decomposition of (a,b). It follows that $((a\ominus(a\wedge b))\oplus b$ is a minimal upper bound of a,b, which is $a\vee b$.

Recall that a partially ordered set P satisfies the *Riesz interpolation property* (RIP) if whenever $x,y\leqslant a,b$ there is an element c in P such that $x,y\leqslant c\leqslant a,b$. In partially ordered Abelian groups the Riesz interpolation property and the Riesz decomposition property are equivalent. In an effect algebra, the Riesz decomposition property implies the Riesz interpolation property, but the converse need not hold (Ravindran, 1996).

Proposition 4: Let E be an effect algebra with RIP. If the elements a,b in E are strongly compatible, there is a unique strong Mackey decomposition (a_1,b_1,c) of (a,b) and $c=a\wedge b$, $d=a_1\oplus b_1\oplus c=a\vee b$.

Proof: Let (a_1,b_1,c) be a strong Mackey decomposition of (a,b). Then $c\leqslant a,b$ and let $x\in E$ be any lower bound of a,b. By RIP, there is $y\in E$ such that $x,c\leqslant y\leqslant a,b$. Since c is maximal, we have $y=c$. Therefore $c=a\wedge b$. Similarly we prove that $d=a\vee b$. □

Corollary 1: An effect algebra E with RIP is an MV-algebra iff any two elements are strongly compatible.

Proof: If any two elements are strongly compatible, it follows by Proposition 4 that E is a lattice. Since any two elements are compatible, E is an MV-algebra. The converse statement is well known (see, e.g., Pulmannová, 1997a). □

Recall that for $u\in E$, $[0,u]_E$ denotes the interval $0\leqslant x\leqslant u$ in E with the operation $\oplus$ defined with respect u as the unit element. Two elements $a,b\in[0,u]_E$ are said to be compatible in $[0,u]_E$ if there is a Mackey decomposition (a_1,b_1,c) of (a,b) such that $a_1\oplus b_1\oplus c\in[0,u]_E$. In Cattaneo *et al.* (2000), the following characterization of different types of effect algebras has been given.

Theorem 1: *Let E be an effect algebra.*

(1) *E satisfies RDP if and only if every pair* (a,b) *of elements of* E *is compatible in every interval* $[0,x]_E$ *which contains* a,b.
(2) *E is an MV-algebra if and only if for every elements* (a,b) *there is a Mackey decomposition* (a_1,b_1,c) *such that* $a_1\oplus b_1\oplus c\in[0,x]_E$ *whenever* $a,b\leqslant x$.

The following characterization of effect algebras with the RDP has been proved in Jenča (2001), Theorem 3.5. It shows what we need to add to the joint compatibility of all finite subfamilies of elements of E to obtain the RDP.

Proposition 5: Let E be an effect algebra. The following statements are equivalent.

(a) *E satisfies the RDP.*
(b) *Every finite family of elements in E is jointly compatible and the following weakening of the RDP holds for any* $x,a,b\in E$: (*) *If* $x\leqslant a\oplus b$, *and* $x\leqslant(a\oplus b)'$, *then there are* $a_1\leqslant a$, $b_1\leqslant b$ *such that* $x=a_1\oplus b_1$.

Proof: (a)⇒(b): Let $a_1,\ldots,a_n$ be elements of E. We will proceed by induction on n. If $n=1$, there is nothing to prove. Now assume that an orthogonal cover exists for $n-1$, and consider elements $(a_1,\ldots,a_n)$. By induction hypothesis, there is an orthogonal cover of $(a_1,\ldots,a_{n-1})$, say $(c_1,\ldots,c_k)$. Put $c=\oplus_{i=1}^k c_i$. Then (c,a_n) have an orthogonal cover-Mackey decomposition (y_1,y_2,z). So $a_n=z\oplus y_2$, where $z\leqslant c$, $y_2\leqslant c'$. Since $z\leqslant c=\oplus_{i=1}^k c_i$, there are elements $d_i\leqslant c_i$, $i=1,\ldots,k$, such that $z=\oplus_{i=1}^k d_i$, and then $(d_1,\ldots,d_k,c_1\ominus d_1,\ldots,c_k\ominus d_k,y_2)$ is an orthogonal cover of $(a_1,\ldots,a_n)$. It is immediate that (*) is satisfied.

(b)⇒(a): Let a,b,x be elements of E such that $a,b\leqslant x$. We wish to prove that a,b are compatible in the interval $[0,x]_E$. First we prove that for any cover C of (a,x) with $a\leqslant x$ there exists a refinement D such that a cover of a in D is contained in a cover of x in D (see Jenča, 2001, Proposition 3.2). So let $C=(c_1,\ldots,c_n)$ be an orthogonal cover of (a,x). Then there are subsets $A\subset\{1,\ldots,n\}$, $X\subset\{1,\ldots,n\}$ such that $a=\oplus_A c_i$, $x=\oplus_X c_i$. Without any loss of generality, we may assume that $A\setminus X=\{1,\ldots,r\}$, $A\cap X=\{r+1,\ldots,s\}$, and $X\setminus A=\{s+1,\ldots,n\}$ with $r<s<n$. Define $a_1=\oplus_{i=1}^r c_i$, $d=\oplus_{i=r+1}^s c_i$, $x_1=\oplus_{i=s+1}^n c_i$. Then $a=a_1\oplus d$, $x=x_1\oplus d$. From $a\leqslant x$ and cancellativity we get $a_1\leqslant x_1$, and since C is an orthogonal family, we also have $a_1\leqslant x_1'$. Now for any c_i, $i=1,\ldots,r$, we have $c_i\leqslant x_1$ and $c_i\leqslant x_1'$. Using (*) we obtain that $c_i=\oplus_{j=s+1}^t d_j^i$, where $d_j^i\leqslant c_j$, $j=s+1,\ldots,n$. It is then easy to check that $(d_j^i)_{i=1,\ldots,r;j=s+1,\ldots,n}\cup(c_i)_{i=r+1,\ldots,s}\cup(c_i\ominus\oplus_{j=1}^r d_j^i)_{i=s+1,\ldots,n})$ is a refinement of C with the desired property.

Now we can find a cover $W=(w_1,\ldots,w_n)$ of a,b,x and subsets A,B,X of $\{1,\ldots,n\}$ with $A\subset X$, $B\subset X$ with $a=\oplus_A w_i$, $B=\oplus_B w_i$, $X=\oplus_X w_i$. Putting $a_1=\oplus_{A\setminus B}w_i$, $b_1=\oplus_{B\setminus A}w_i$, $c=\oplus_{A\cap B}w_i$ we obtain a Mackey decomposition of a,b in $[0,x]_E$. □

The following proposition collects some characterizations of MV-algebras among effect algebras with the RDP.

Proposition 6: Let E be an effect algebra with the RDP. The following statements are equivalent.

(i) *E is an MV-algebra.*
(ii) *Every two elements in E are strongly compatible.*
(iii) *E is lattice ordered.*
(iv) *The partial operation* $\oplus$ *can be extended uniquely to a total operation* $+$ *which is commutative, associative, monotone and such that* $a'=\wedge\{x:a+x=1\}$.

Proof: (*i*)⇒(*ii*): See Corollary 1.
(*ii*)⇒(*iii*): Follows by Proposition 4.
(*iii*)⇒(*iv*): Recall that the RDP implies that for any elements a,b,

$$b\leqslant a\oplus a'\Rightarrow b=c\oplus b_1,\ c\leqslant a \text{ and } b_1\leqslant a'.$$

Therefore any two elements a,b have a Mackey decomposition. Since E is lattice ordered, by Lemma 1, (a,b) have also a strong Mackey decomposition (a_1,b_1,c) with $c=a\wedge b$, $a_1\oplus b_1\oplus c=a\vee b$. It follows that $a\ominus(a\wedge b)=(a\vee b)\ominus b$.

Define $a+b:=a\oplus(a'\wedge b)$. Clearly, $+$ coincides with $\oplus$ if $a\perp b$, and is monotone in b. By the interplay between $\oplus$ and $\ominus$, we obtain

$$(a+b)'=a'\ominus(a'\wedge b)=(a'\vee b)\ominus b=(a\wedge b'\oplus b)'=(b+a)'.$$

Therefore $+$ is commutative. Further, using $a\ominus(a\wedge b)=(a\vee b)\ominus b$, and the fact that $a\oplus(b\wedge c)=(a\oplus b)\wedge(a\oplus c)$ if $a\perp b,a\perp c$, we have

$$\begin{aligned}(a+b)+c&=(a\oplus a'\wedge b)\oplus((a\oplus a'\wedge b))'\wedge c=(a\oplus a'\wedge b)\oplus(a'\ominus a'\wedge b)\wedge a'\wedge c\\&=(a\oplus(a'\ominus a'\wedge b)\wedge a'\wedge c)\oplus a'\wedge b=(a\oplus(a'\ominus a'\wedge b)\wedge(a\oplus a'\wedge c))\oplus a'\wedge b\\&=(a'\ominus(a'\ominus a'\wedge b)\vee(a'\ominus a'\wedge c))'\oplus a'\wedge b=(a'\wedge b\vee(a'\ominus a'\wedge c))'\oplus a'\wedge b\\&=((a'\wedge b\vee(a'\ominus a'\wedge c))\ominus a'\wedge b)'=((a'\ominus a'\wedge c)\ominus(a'\ominus a'\wedge c)\wedge a'\wedge b)'\\&=(a\oplus a'\wedge c)\oplus(a\oplus a'\wedge c)'\wedge b=(a+c)+b.\end{aligned}$$

This proves associativity of $+$.

If $a+x=1$, then $0=(a+x)'=(a\oplus a'\wedge x)'=a'\ominus a'\wedge x$, hence $a'=a'\wedge x$, so that $a'\leqslant x$. Since $a+a'=a\oplus a'=1$, the operation $+$ has the desired property.

$(iv)\Rightarrow(i)$: Let there exist an operation $+$ with the desired properties. First we prove that $(p'+q)'+q$ is an upper bound of both p and q in E. We have $1=(p'+q)+(p'+q)'=p'+(q+(p'+q)')$ assuming commutativity and associativity of $+$. Hence $p\leqslant(p'+q)'+q$ by the last property of $+$. By monotony of $+$, $q\leqslant(p'+q)'+q$. Put $s=(p'+q)'+q$. We have just proved that s is an upper bound of p,q. Suppose that there is x in E with $x\geqslant p$, $x\geqslant q$. We want to prove that $x\geqslant s$. We may write

$$x=(x\ominus q)\oplus q \tag{1}$$

$$=(x'\oplus q)'\oplus q=(x'+q)'+q, \tag{2}$$

since $+$ is an extension of $\oplus$. From $x\geqslant p$ we obtain $x'\leqslant p'$, and by monotony of $+$, we get $x'+q\leqslant p'+q$. Since $'$ is order reversing, by repeated application of the monotony of $+$ we obtain

$$(p'+q)'+q\leqslant(x'+q)'+q,$$

and so

$$x'=((x'+q)'+q)'\leqslant((p'+q)'+q)'=s';$$

i.e., $s\leqslant x$, as required. This proves that $p\vee q=(p'+q)'+q$.

It remains to prove the uniqueness of $+$. Let E be an effect algebra with the RDP. Assume that there are two total extensions of $\oplus$ with the desired properties and denote them by $+_1$ and $+_2$. We want to prove that $+_1=+_2$. Assume that there are $q,r\in E$ such that $q+_1r\neq q+_2r$. Putting $p=r'$, we get $q+_1p'\neq q+_2p'$ and hence $(p'+_1q)'\neq(p+_2q)'$. Put $z:=(p'+_1q)'$. Then $q\leqslant q+_1p'=z'$. Hence $q\perp z$, so $q\oplus z=q+_1z$. By the last part of the above proof, we have $p\vee q=(p+_1q)'+_1q=z+_1q=z\oplus q$. Similarly, letting $y:=(p'+_2q)'$, we prove that $y\perp q$, and we obtain $p\vee q=y\oplus q=y+_2q$. We conclude $y=z$, in contradiction with our suppositions. □

Remark 2: The equivalence $(i)\Leftrightarrow(iv)$ was proved in Mundici and Panti (1993) in relation with the K_0 theory for AF C^*-algebras. Our proof was based purely on the algebraic properties of E. Combining it with the result of Effross *et al.* (1980), which proves that Elliott's invariant is an interval in a partially ordered group with the RDP and so it has a RDP itself, the result of Mundici and Panti (1993) follows.

Remark 3: Let (a_1,b_1,c) be a strong Mackey decomposition of (a,b). Then (b_1,a_1,d') where $d=a_1\oplus b_1\oplus c$ is a strong Mackey decomposition of (a',b'). Indeed, by Proposition 3 c is a maximal lower bound of a,b and d is a minimal upper bound of a,b. Then d' is a maximal lower bound of a',b', and (b_1,a_1,d') is a Mackey decomposition of (a',b'). By Proposition 3 (ii), (b_1,a_1,d') is a strong Mackey decomposition of (a',b'). Strong compatibility of (a,b'), resp. (a',b), can be derived iff a_1 is a maximal lower bound of a,b', resp. b_1 is a maximal lower bound of a',b. In particular, if c is any lower bound of a,a', then $(a\ominus c,a'\ominus c,c)$ is a Mackey decomposition of a,a', but a,a' are strongly compatible iff they have a maximal lower bound.

Evidently, strong Mackey decompositions need not exist even for compatible elements, and if they exist, they may be not unique. In the following theorem we show that in any Hilbert space effect algebra $\mathcal{E}(H)$, there exist strong Mackey decompositions (not necessarily unique) for any two compatible elements. This follows from the existence of maximal lower bounds (Moreland and Gudder, 1999, Theorem 4.5).

Theorem 2: *In $\mathcal{E}(H)$, any two Mackey compatible effects have also a strong Mackey decomposition.*

Proof: If $a,b\in\mathcal{E}(H)$ are Mackey compatible, there are $c,d\in\mathcal{E}(H)$ such that $c\leqslant a$, $b\leqslant d$ and $a\ominus c=d\ominus b$. Put $S:=\{x\in\mathcal{E}(H):c\leqslant x\leqslant a,b\}$. Let $K\subset S$ be a chain. S is partially ordered and nonempty, since $c\in S$. K can be considered as an increasing net in $\mathcal{E}(H)$ and by Topping (1971), Lemma 1, $\lim_K\langle x\phi,\phi\rangle=\langle x_0\phi,\phi\rangle$ for some $x_0\in\mathcal{E}(H)$ and every $\phi\in H$. It follows that $x_0\in S$ and $c\leqslant x\leqslant x_0$ for every $x\in K$. By Zorn's lemma, S has a maximal element c_1, say, such that $c\leqslant c_1$. By Lemma 1, $(a\ominus c_1,b\ominus c_1,c_1)$ is a Mackey decomposition of (a,b), and by Proposition 3, it is a strong Mackey decomposition. □

IV. BLOCKS IN EFFECT ALGEBRAS

Recall than an *observable* on an effect algebra E is a morphism $\alpha:B\to E$ from a Boolean algebra B to E. Let $\mathrm{ran}(\alpha)=\{\alpha(b):b\in B\}$ denote the range of α. An observable α is finite if there is a finite set $\{a_1,\ldots,a_n\}$ of elements in B such that $(\alpha(a_1),\ldots,\alpha(a_n))$ is a finite partition of unity in E, and $\mathrm{ran}(\alpha)$ consists of all $\oplus$-sums of $(\alpha(a_1),\ldots,\alpha(a_n))$. Conversely, to every finite partition of unity in E, there corresponds a finite observable.

We say that two observables α and β are *coexistent* if there is an observable γ such that $\mathrm{ran}(\alpha)\cup\mathrm{ran}(\beta)\subseteq\mathrm{ran}(\gamma)$. Clearly, $\mathrm{ran}(\alpha)$ is a compatible set. A system $A=(\alpha_i)_{i\in I}$ will be called *coexistent* (in A) if every two observables α,β in A are coexistent with $\gamma\in A$, where $\mathrm{ran}(\alpha)\cup\mathrm{ran}(\beta)\subseteq\mathrm{ran}(\gamma)$. Clearly, the system A is coexistent iff $\cup_{i\in I}\mathrm{ran}(\alpha_i)$ is compatible with covers in itself.

By a *block* of E we mean a maximal subsystem A of E such that every finite subset of elements of A is compatible in A. Alternatively, a block is union of the ranges of a maximal coexistent system of finite observables on E. Using Zorn lemma, we can prove that every effect algebra E can be expressed as the union of its blocks. The structure of blocks in effect algebras is not known, in general. In fact, we can only say that the blocks bear a structure of a compatible quasi-effect algebra (see Cattaneo *et al.*, 2000). A *quasi-effect algebra* is a structure $(A;\leqslant,\oplus,',1,0)$ where $(A;\leqslant,',1,0)$ is a bounded involutive poset, and $\oplus$ is a partially defined binary operation such that

(1) $\exists(a\oplus b)$ implies $\exists(b\oplus a)$ and $a\oplus b=b\oplus a$.
(2) $a\oplus a'=1$.
(3) $\exists(a\oplus 1)$ implies $a=0$.
(4) $a\leqslant b$ and $\exists(a\oplus c)$ and $\exists(b\oplus c)$ implies $a\oplus c\leqslant b\oplus c$.

Let α be an observable on E. Then $A=\mathrm{ran}(\alpha)$ can be organized into a quasi-effect algebra $(A;\leqslant_A,\oplus_A,'_A,1_A,0_A)$ where $\leqslant_A$ is the restriction of $\leqslant$ in E to A, $'_A='$, $1_A=1$, $0_A=0$, and $\exists(a\oplus_A b)$ iff $\exists(a\oplus b)$ and $a\oplus b\in A$, and then $a\oplus_A b=a\oplus b$ (Cattaneo *et al.*, 2000, Lemma 1).

We say that a system $(\alpha_i)_{i\in I}$ of observables is directed if to every $i,j\in I$ there is $k\in I$ such that $\mathrm{ran}(\alpha_i)\cup\mathrm{ran}(\alpha_j)\subseteq\mathrm{ran}(\alpha_k)$. Let $(\alpha_i)_{i\in I}$ be a directed system of observables. Put A

$=\cup_{i\in I}\mathrm{ran}(\alpha_i)$. With partial order $\leqslant$ and orthosupplementation $'$ and 0,1 inherited from E, A is an involutive, bounded poset. Define $\oplus_A$ as follows: $a\oplus_A b$ is defined if there is $i\in I$ with $a,b,a\oplus b\in\mathrm{ran}(\alpha_i)$ and then put $a\oplus_A b=a\oplus b$. Clearly, $(A;\leqslant_A,\oplus_A,{}'_A,1,0)$ is a quasi-effect algebra. We may conclude that, in general, a block of an effect algebra is a compatible quasi effect algebra.

Theorem 3: *A block A of an effect algebra E is a subeffect algebra of E if and only if the following condition is satisfied: $\{a_1,a_2\ldots,a_n\}$ is a compatible set and $a_1\perp a_2$ implies that $\{a_1,a_2,\ldots,a_n,a_1\oplus a_2\}$ is a compatible set.*

Proof: If a block A is a subeffect algebra of E, then $a_1,a_2\in A$ and $a_1\perp a_2$ implies $a_1\oplus a_2\in A$. Since every finite subset of A is compatible, we have, for any finite set $\{b_1,\ldots,b_n\}$ in A that $\{a_1,a_2,b_1,\ldots,b_n,a_1\oplus a_2\}$ is a compatible set.

Conversely, if $a_1,a_2\in A$, $a_1\perp a_2$ and for any $b_1,\ldots,b_n$ in A the set $a_1,a_2,b_1,\ldots,b_n,a_1\oplus a_2$ is compatible, then the maximality of A implies that $a_1\oplus a_2\in A$. □

Observe that in the above theorem, the condition $a_1,a_2,\ldots,a_n$ compatible and $a_1\perp a_2$ implies $a_1,a_2,\ldots,a_n,a_1\oplus a_2$ compatible can be replaced by the condition $a_1,a_2,\ldots,a_n$ compatible and $a_1\leqslant a_2$ implies $a_1,a_2,\ldots,a_n,a_2\ominus a_1$ compatible.

In analogy with orthomodular posets, we say that an effect algebra E is *regular* if any pairwise compatible finite set is jointly compatible. In a regular effect algebra, a block is a maximal system of pairwise compatible elements.

The following special cases are known.

Case 1: Let E be an orthoalgebra. It is well known that the range of every observable α is a subeffect algebra of E which, endowed with ''local'' lattice operations $\vee_\alpha,\wedge_\alpha$ taken with respect to $\mathrm{ran}(\alpha)$, is a Boolean algebra. Moreover, the mapping $\alpha:B\to\mathrm{ran}(\alpha)$ is a Boolean algebra homomorphism. The corresponding ''global'' suprema and infima in E need not exist, and even if they exist, they need not belong to $\mathrm{ran}(\alpha)$.

Let $(\alpha_i)_{i\in I}$ be a maximal coexistent system of finite observables, so that $\cup_{i\in I}\mathrm{ran}(\alpha_i)$ is a block. Then $(\mathrm{ran}(\alpha_i))_{i\in I}$ form a directed system of Boolean algebras. Indeed, if $\mathrm{ran}(\alpha_i)\subseteq\mathrm{ran}(\alpha_j)$, then by well known theorems by Sikorski and Varadarajan (Varadarajan, 1985), there is a function $f:\Omega_j\to\Omega_i$ where Ω_i,Ω_j are finite sets such that $\alpha_i(\Omega_i)=1$, $\alpha_j(\Omega_j)=1$, such that for every $X\in 2^{\Omega_i}$, $\alpha_i(X)=\alpha_j(f^{-1}(X))$. Let $a,b\in\mathrm{ran}(\alpha_i)$, $a=\alpha_i(X)$, $b=\alpha_i(Y)$. Then

$$a\wedge_i b=\alpha_i(X\cap Y)=\alpha_j(f^{-1}(X\cap Y))=\alpha_j(f^{-1}(X)\cap f^{-1}(Y))=\alpha_j(f^{-1}(X))\wedge_j\alpha(f^{-1}(Y))=a\wedge_j b.$$

Let $A=\cup_{i\in I}\mathrm{ran}(\alpha_i)$ be a block. It is clear that A is a bounded orthocomplemented poset. For every $a,b,c\in A$ there is a $k\in I$ such that $a,b,c\in\mathrm{ran}(\alpha_k)$. It follows that A is a subeffect algebra of E and, with suprema and infima taken in A, it is a distributive lattice, hence a Boolean algebra. The lattice operations in a block coincide with those in E iff E is an orthomodular poset.

Case 2: Let E be a lattice ordered effect algebra. It has been proved in Riečanová (2000) that the maximal pairwise compatible subsets are subeffect algebras of E which are closed under the lattice operations and form MV-algebras. It follows that lattice ordered effect algebras are regular and blocks are MV-algebras with the lattice operations inherited from E.

Case 3: Homogeneous effect algebras introduced in Jenča (2001) have blocks that form subeffect algebras of E satisfying the Riesz decomposition property. Homogeneous effect algebras include orthoalgebras and lattice ordered effect algebras as special cases. In both these subcases, blocks form distributive lattices, but the nature of lattice operations may be different.

Case 4: According to Dvurečenskij (2002), if an effect algebra satisfies the Riesz interpolation property (RIP) and so-called difference meet property (DMP), that is, if $a,b,c\in E$, $a\leqslant b$, are such that $a\wedge c,b\wedge c$ exist in E, then $(b\ominus a)\wedge c$ exists in E, then E can be covered by MV-algebras, which are maximal sets of pairwise strongly compatible subsets of E. The lattice operations in the MV-algebras coincide with the lattice operations in E. Since every lattice ordered effect algebra satisfies RIP and DMP, and in a lattice ordered effect algebra any two compatible elements are also strongly compatible, this case generalizes the case of lattice ordered effect algebras. It is not known whether the maximal strongly compatible sets coincide with the maximal compatible sets.

Case 5: Let H be a Hilbert space (complex, separable). Consider a maximal subset A of the effect algebra $\mathcal{E}(H)$ consisting of pairwise commuting elements. Using well-known results of von Neumann (1955) and Varadarajan (1985), there is an observable (self-adjoint operator) u and Borel functions $f_a:\mathbb{R}\to[0,1]$ such that every $a\in A$ is a function of u, $a=f_a(u)$. Since A is maximal, the set $\{f_a:a\in A\}$ consists of all measurable functions. The functions $f_a:\mathbb{R}\to[0,1]$ can be endowed with a structure of an MV-algebra, if we define (Cattaneo *et al.*, 2000) $(f\oplus g)(x)=\min(1,f(x)+g(x)),x\in\mathbb{R}$.

Using the functional calculus, we can transfer the MV-algebra structure to the operators in A. In this way, $\mathcal{E}(H)$ can be covered by MV-algebras.

By the functional calculus, we have

$$\begin{aligned} a\wedge_A b&=\int_0^1 \min(f_a(\lambda),f_b(\lambda))u(d\lambda)\\ &=\int_a^b \frac{1}{2}(f_a+f_b-|f_a-f_b|)u(d\lambda)\\ &=\tfrac{1}{2}(a+b-|a-b|)=a\sqcap b. \end{aligned}$$

According to Gudder (1996), $a\sqcap b\geqslant 0$ and it is a maximal lower bound of a,b. Since, again by the functional calculus, $a+(b-a\sqcap b)=\frac{1}{2}(a+b+|a-b|)=a\sqcup b\leqslant 1$, a,b are strongly compatible. The infimum of a,b in A is then equal to $a\sqcap b$, which is equal to $a\wedge b$ iff $a\wedge b$ exists in $\mathcal{E}(H)$. We note that $a\wedge b$ need not exist in $\mathcal{E}(H)$ even if a and b commute. Let $a\in\mathcal{E}(H)$ be a regular effect such that 0,1 do not belong to the point spectrum of a (recall that a is regular if a and a' are incomparable). By Ando (1999), the infimum $a\wedge a'$ in $\mathcal{E}(H)$ exists iff

$$\int_{0+}^{1-}\lambda\,du(\lambda)\quad\text{and}\quad\int_{0+}^{1-}(1-\lambda)du(\lambda),$$

where $\lambda\to u(\lambda)$ is the spectral measure of a, are comparable, and then the infimum is the smaller of both. But if the point spectrum of a does not contain 0,1, then the above integrals coincide with a and $a'=1-a$, respectively, which are regular, hence incomparable. Therefore, $a\wedge a'$ does not exist.

We conclude that in the MV-algebras A corresponding to maximal sets of commuting effects, the lattice operations in A need not coincide with the lattice operations in $\mathcal{E}(H)$.

It can be shown that there are noncommuting effects a,b in $\mathcal{E}(H)$ such that (a,b) have a Mackey decomposition $(a\ominus a\sqcap b,b\ominus a\sqcap b,a\sqcap b)$. Let ϕ and ψ be different unit vectors in H. Put $a=\lambda\phi$, $b=\mu\psi$, $0<\lambda$, $\mu<1$. We can choose λ and μ such that $a+b\leqslant I$. Then $a\wedge b=0=a\sqcap b$ in $\mathcal{E}(H)$, and $(a,b,0)$ is a strong Mackey decomposition of (a,b).

We conclude that the above MV-algebras do not correspond to maximal compatible sets in $\mathcal{E}(H)$.

V. EFFECT TEST SPACES

In Dvurečenskij and Pulmannová (1994, 2000), Gudder (1997), and Foulis *et al.* (1996) close relations between effect algebras and so-called D-test spaces, resp. effect test spaces, were shown. D-test spaces and effect test spaces are essentially equivalent and they are a generalized form of test spaces introduced by Foulis and Randall (1972) and Randall and Foulis (1973). Let us recall some basic facts about effect test spaces.

Let X be a nonempty set; elements of X are called *outcomes*. Let I be a nonempty set. A function $F:I\to X$ is said to be of *finite multiplicity* if for every $x\in X$, $F^{-1}(x)$ is of finite cardinality. Observe that if $I=\emptyset$, then $X^I=\{\emptyset\}$. For arbitrary sets I,J and functions $F\in X^I$, $G\in X^J$ define $F\subset G$ if there is an injection $\sigma:I\to J$ such that $F=G\circ\sigma$, i.e., $F(i)=G(\sigma(i))$ for all $i\in I$. If $F\subset G$ and $\sigma:I\to J$ is a bijection, we say that F and G are *equivalent*, in symbols $F\sim G$.

Sometimes we will identify equivalent functions, and write $F=G$. Let $F\in X^I$, $G\in X^J$. We can now define unambiguously a function $F\dot\cup G$ as follows: Let $K=I'\cup J'$, $I'\cap J'=\emptyset$, and $\phi:I\to I'$, $\psi:J\to J'$ be bijections. Then $F\dot\cup G\in X^K$, and $F\dot\cup G(k)=F(i)$ if $k=\phi(i), i\in I$, and $F\dot\cup G(k)=G(j)$ if $k=\psi(j), j\in J$. Evidently, $\dot\cup$ is commutative and associative.

For $F\in X^I$, let $\mathcal{R}(F):=\{x\in X: x=F(i) \text{ for some } i\in I\}$, denote the range of F.

Definition 1: Let $\mathcal{J}$ be a nonvoid family of index sets, $X\neq\emptyset$, and let $\mathcal{T}\subseteq\{T\in X^I: I\in\mathcal{J}\}$. We say that $(X,\mathcal{T})$ is an **effect test space** *if the following conditions are satisfied*:

(i) *any $T\in\mathcal{T}$ is of finite multiplicity,*
(ii) *for every $x\in X$ there is a $T\in\mathcal{T}$ such that $x\in\mathcal{R}(T)$,*
(iii) *if $S,T\in\mathcal{T}$ and $S\subset T$, then $S\sim T$.*

An element $T\in\mathcal{T}$ is said to be a **test**.

Notice that if $T\in\mathcal{T}$ and $T\in X^I$, then $I\neq\emptyset$. For otherwise by (*iii*), $\emptyset\subset T\Rightarrow\emptyset=T$ for all tests T, contradicting (*ii*). A function $G\in X^J$ is called an *event* if there is a $T\in\mathcal{T}$ such that $G\subset T$. Denote the set of all events by $\mathcal{E}=\mathcal{E}(X,\mathcal{T})$.

Definition 2: Let F,G be events. We say that F and G are

(i) **orthogonal** (*written $F\perp G$*) *if there is a $T\in\mathcal{T}$ such that $F\dot\cup G\subset T$,*
(ii) **local complements** *of each other* (Floc$G$) *if there is a $T\in\mathcal{T}$ with $F\dot\cup G=T$,* or
(iii) **perspective with axis** H ($F\approx_H G$, *or simply $F\approx G$*) *if they share a common complement H.*

Observe that if $\emptyset\approx G$, then $G\sim\emptyset$. Moreover, two arbitrary tests R,S are perspective with axis $\emptyset$.

Definition 3: An effect test space $(X,\mathcal{T})$ is **algebraic** *if for $F,G,H\in\mathcal{E}$, $F\approx G$ and $F\perp H$ implies $G\perp H$.*

Equivalently, $(X,\mathcal{T})$ is algebraic iff $F,G,H\in\mathcal{E}$, F loc H and $F\approx G$ implies G loc H. If $(X,\mathcal{T})$ is algebraic, then the relation $\approx$ becomes an equivalence relation. Denote by $\Pi=\Pi(X,\mathcal{T})$ the set of all equivalence classes of events. For $F\in\mathcal{E}$, define $\Pi(F)'=\Pi(G)$, where G is any local complement of F. Then $\Pi(F)'$ is well defined. For $F,G\in\mathcal{E}$ define $\Pi(F)\oplus\Pi(G):=\Pi(H)$ iff $F\perp G$ and $H=F\dot\cup G$. Putting $0:=\Pi(\emptyset)$ and $1:=\Pi(T)$, for any $T\in\mathcal{T}$, it can be proved that $\Pi(X,\mathcal{T})$ becomes an effect algebra.

Conversely, let $(E,\oplus,0,1)$ be an effect algebra. Recall that a finite sequence $(a_1,a_2,\ldots,a_n)$ of nonzero elements of E is a finite partition of unity if $a_1\oplus a_2\cdots\oplus a_n$ is defined in $\mathcal{E}$ and equals 1. Put $X:=E\setminus\{0\}$ and let $\mathcal{F}$ be the family of all finite partitions of unity in E. Then $(X,\mathcal{F})$ is an algebraic effect test space, where two events $A=(a_i)_{i\leqslant n}$, $B=(b_j)_{j\leqslant m}$ are perspective iff $\oplus_{i\leqslant n}a_i=\oplus_{j\leqslant m}b_j$. The logic $\Pi(X,\mathcal{F})$ is isomorphic with E. Such a test space is called the *standard test space* for the effect algebra E.

In what follows, we consider an algebraic effect test space $(X,\mathcal{T})$. Let $T\in\mathcal{T}$ be a test. We may assume that $T\in X^{I_T}$, where I_T denotes the index set of T. Let $\sigma(I_T)$ be an ordered partition of I_T. Then there is a mapping $f_\sigma: I_T\to\sigma(I_T)$, such that $f_\sigma(i)=j$ iff $i\in P_j$ where $P_j\in\sigma(I_T)$. Let $\|\sigma\|$ denote the cardinality of $\sigma(I_T)$. We may consider $\{j: P_j\in\sigma(I_T)\}$ as a new index set and assume that there exists a test $\sigma(T)$ in $\mathcal{T}$ such that

$$\sigma(T)(j)\approx\dot\cup_{i\in f_\sigma^{-1}(j)}T(i)=\dot\cup_{i\in P_j}T(i).$$

We will say that $\sigma(T)$ is a *coarsening* of T, or that T is a *refinement* of $\sigma(T)$.

Consider the index set $I_{\sigma(T)}$ of $\sigma(T)$. Let τ be any ordered partition of $I_{\sigma(T)}$. We can build a function $\tau(\sigma(T))$ putting

$$\tau(\sigma(T))(j)\approx\dot\cup_{k\in f_\tau^{-1}(j)}\dot\cup_{i\in f_\sigma^{-1}(k)}T(i)=\dot\cup_{k\in Q_j}(\dot\cup_{i\in P_k}T(i)),$$

where $Q_j\in\tau(\sigma(T))$.

Using the refinement mappings $f_\sigma, f_\tau, f_\kappa$ we can show associativity of compositions. If σ is an ordered partition of I_T, τ is an ordered partition of $I_{\sigma(T)}$ and κ is an ordered partition of $I_{\tau(\sigma(T))}$, then we have

$$\kappa\cdot(\tau\cdot\sigma)(T)=(\kappa\cdot\tau)\cdot\sigma(T).$$

For every $n\in\mathbb{N}$ let σ_n denote the n-ary partition of I_T, so $\|\sigma_n\|=n$. Then $I_{\sigma_n(T)}=\{1,\ldots,n\}$, and we obtain an n-ary test

$$\sigma_n(T)=(\sigma_n(T)(1),\ldots,\sigma_n(T)(n)).$$

In what follows, we show examples of test spaces, where coarsenings and refinements make sense.

Example 1: Let $X=2^Y\setminus\{\varnothing\}$ be the set of all nonempty subsets of nonempty set Y, and consider a classical test space $(X,\mathcal{T})$, i.e., for every test $T\in\mathcal{T}$ the cardinality of $T^{-1}(x)$, $x\in X$, is at most 1. For any test $T\in X^{I_T}$ and any ordered partition $\sigma=\{P_j:j\in J\}$ of I_T, the sets $\cup\{T(i):i\in P_j\}$, $j\in J$ belong to X. Therefore it makes sense to define a function $F:J\to X$ putting $F(j)=\cup\{T(i):i\in P_j\}$. Instead of 2^Y we can consider a subfamily of it, e.g., a σ field of sets, and consider partitions with members in that family.

Example 2: Let $(X,+,0)$ be a positive cone. Let U be a subset of X such that $v\in X$, $u\leqslant v$ for some $u\in U$ implies $v\notin U$. Put $I_n=\{1,\ldots,n\}$ $n\in\mathbb{N}$, and define a function $f:I_n\to X$ to be a test if $\Sigma_{i=1}^n f(i)$ belongs to U. Let $\mathcal{T}$ denote the set of all tests. Then $(X\setminus\{0\},\mathcal{T})$ is an effect test space, and the structure of X enables us to take into account partitions of index sets and the corresponding coarsenings, resp. refinements.. If f is an event, we denote it by $\Sigma f:=\Sigma_{i\in I_f}f(i)$, where I_f is the index set of f. An event h is a local complement of f if $\Sigma_i f(i)+\Sigma_j h(j)\in U$. Events f and g are perspective if they share a common complement. The test space is algebraic iff whenever two events share one local complement, they share all local complements. In this case, the quotient with respect to the perspectivity relation is an effect algebra. For example, if $U=\{u\}$ is a one-element set, then by cancellativity of the positive cone, the test space is algebraic, and we obtain an interval effect algebra. More generally, a positive cone may be replaced by a partial Abelian monoid (cf. Wilce, 1998; Pulmannová and Wilce, 1995, Pulmannová, 1997b).

Example 3: Let $(E\setminus\{0\},\mathcal{T})$ be a standard effect test space of an effect algebra E. Tests in $\mathcal{T}$ are orthogonal subsets $(a_1,\ldots,a_n)$ of nonzero elements such that $\oplus_{i=1}^n a_i=1$. If $(P_1,\ldots,P_s)$ is any partition of the set $\{1,\ldots,n\}$, then $(b_1,\ldots,b_s)$, where $b_i=\oplus_{\{j\in P_i\}}a_j$, is also a test. This example is a special case of Example 2.

Example 4: Let $(X,\mathcal{T})$ be an effect test space, and $\mathcal{E}$ be the set of its events. Put $Z:=\mathcal{E}\setminus\{\varnothing\}$. Consider the set $\mathcal{F}$ of functions $\tilde{F}:I_n\to Z$, where I_n denotes the set $\{1,\ldots,n\}$, $n\in\mathbb{N}$, such that $\dot\cup_{i=1}^n\tilde{F}(i)\in\mathcal{T}$. We prove that $(Z,\mathcal{F})$ is an effect test space. Let $E\in\mathcal{E}-\{\varnothing\}$. Then for any local complement E' of E, the function $\tilde{F}:\{1\}\to Z$, $\tilde{F}(1)=E$ if E is a test, $\tilde{F}:\{1,2\}\to Z$, $\tilde{F}(1)=E$, $\tilde{F}(2)=E'$ otherwise, belongs to $\mathcal{F}$. Hence the union of ranges of functions in $\mathcal{F}$ covers Z. Assume that $\tilde{F}:I_m\to Z$, $\tilde{G}:I_n\to Z$ belong to $\mathcal{F}$, and $\tilde{F}\subset\tilde{G}$. Then there must be an injection $\sigma:I_m\to I_n$ such that $\tilde{F}(\sigma(i))=\tilde{G}(j)$ whenever $\sigma(i)=j$. Then

$$\dot\cup_{\{j\in I_n:j=\sigma(i)\}}\tilde{G}(j)=\dot\cup_{\{i\in I_m\}}\tilde{F}(i)\in\mathcal{T}$$

and hence $\tilde{G}(k)=0$ for $k\in I_n\setminus\sigma(I_m)$, so that $\tilde{F}=\tilde{G}$. This proves that $(Z,\mathcal{F})$ is an effect test space. Denote by $\tilde{\mathcal{E}}$ the set of events of $(Z,\mathcal{F})$. For every $\tilde{E}:I_n\to Z$ in $\tilde{\mathcal{E}}$, define $w(\tilde{E}):=\dot\cup_{i\in I_n}\tilde{E}(i)$. Clearly $w(\tilde{E})$ belongs to $\mathcal{E}$ and $w:\tilde{\mathcal{E}}\to\mathcal{E}$ is a surjective mapping. In addition, if $\tilde{E}\perp\tilde{F}$, then $w(E)\perp w(F)$ and $w(\tilde{E}\dot\cup\tilde{F})=w(\tilde{E})\dot\cup w(\tilde{F})$, and also $w(\tilde{E})\perp w(\tilde{F})$ implies $\tilde{E}\perp\tilde{F}$.

Assume that $(X,\mathcal{T})$ is an algebraic effect test space. We show that $(Z,\mathcal{F})$ is also an algebraic effect test space. Moreover, the corresponding effect algebras $\Pi(X)$ and $\Pi(Z)$ are isomorphic. To prove it, assume that $\tilde{E},\tilde{F},\tilde{G}\in\tilde{\mathcal{E}}$, and $\tilde{E}\approx_{\tilde{G}}\tilde{F}$. Then $w(\tilde{E})\dot{\cup}w(\tilde{G})\in\mathcal{T}$, $w(\tilde{F})\dot{\cup}w(\tilde{G})\in\mathcal{T}$, and hence $w((\tilde{E})\approx_{w(\tilde{G})}w(\tilde{F})$.

Conversely, let $w(\tilde{E})\approx_{w(\tilde{G})}w(\tilde{F})$. Then $w(\tilde{E})\dot{\cup}w(\tilde{G})\in\mathcal{T}$, $w(\tilde{F})\dot{\cup}w(\tilde{G})\in\mathcal{T}$, so that $\tilde{E}\dot{\cup}\tilde{G}\in\mathcal{F}$, $\tilde{F}\dot{\cup}\tilde{G}\in\mathcal{F}$, and hence $\tilde{E}\approx_{\tilde{G}}\tilde{F}$.

Define $\nu:\Pi(Z)\to\Pi(X)$ by $\nu(\Pi(\tilde{E}))=\Pi(w(\tilde{E}))$. If $\tilde{E}\perp\tilde{F}$, then

$$\begin{aligned}\nu(\Pi(\tilde{E})\oplus\Pi(\tilde{F}))&=\nu(\Pi(\tilde{E}\dot{\cup}\tilde{F}))\\&=\Pi(w(\tilde{E}\dot{\cup}\tilde{F}))\\&=\Pi(w(\tilde{E})\dot{\cup}w(\tilde{F}))=\Pi(w(\tilde{E}))\oplus\Pi(w(\tilde{F}))=\nu(\Pi(\tilde{E}))\oplus\nu(\Pi(\tilde{F})).\end{aligned}$$

Clearly, $\nu(\Pi(0))=0$, and $\nu(\Pi(\tilde{T}))=\Pi(w(\tilde{T})=1$ whenever $\tilde{T}\in\mathcal{F}$. Hence ν is a surjective morphism of effect algebras. Since

$$\nu(\Pi(\tilde{E})\perp\nu(\Pi(\tilde{F}))\Rightarrow\Pi(w(\tilde{E}))\perp\Pi(w(\tilde{F}))\Rightarrow w(\tilde{E})\perp w(\tilde{F})\Rightarrow\tilde{E}\perp\tilde{F},$$

ν is an isomorphism.

It is easy to see that if $\tilde{E}$ is any event in $(Z,\mathcal{F})$, $\tilde{E}:I_n\to Z$, and $\kappa(I_n)=(P_1,\ldots,P_{\|\kappa\|})$ is any partition of I_n, then $\tilde{F}:I_{\|\kappa\|}\to Z$, $\tilde{F}(i)=\dot{\cup}(\tilde{E}(j):j\in P_i)\}$ is an event in $(Z,\mathcal{F})$.

VI. TEST SPACES WITH REFINEMENTS

The following definition is inspired by Harding (2001).

Definition 4: Let $(X,\mathcal{T})$ be an effect test space. We will say that $(X,\mathcal{T})$ is a **leveled effect test space** *if for every test $T:I_T\to X$ in $\mathcal{T}$ and every finite partition $\sigma(I_T)=(P_1,\ldots,P_n)$, $\|\sigma\|=n$, $n\in\mathbb{N}$, of the set I_T, there is a test $\sigma(T):\{1,\ldots,n\}\to X$ such that $\sigma(T)(i)=\dot{\cup}_{j\in P_i}T(j)$.*

Let $(X,\mathcal{T})$ be a leveled algebraic effect test space and $\mathcal{E}$ be its set of events. We say that an event F is a *refinement* of an event E if there is a mapping $\kappa:I_F\to I_E$ such that for every $i\in I_E$, $E(i)\approx\dot{\cup}\{F(j):j\in\kappa^{-1}(i)\}$. Clearly, if F is a refinement of E, then $F\approx E$. We say that two events E and G have a *common refinement*, if there is an event F which is a refinement of both E and G. Clearly, if E and G have a common refinement, then $E\approx G$.

We say that events $E_1,\ldots,E_k$ *can be built* from an event F if there are subevents $F_1,\ldots,F_k$ of F which are refinements of $E_1,\ldots,E_k$, respectively.

Let $A,B:\{1,2\}\to X$ be binary events, and let $C:I_C\to X$ be their common refinement. Then there are partitions (I_1,I_2) and (J_1,J_2) of the set I_C such that $A(1)=\dot{\cup}_{i\in I_1}C(i)$, $A(2)=\dot{\cup}_{i\in I_2}C(i)$, $B(1)=\dot{\cup}_{j\in J_1}C(j)$, $B(2)=\dot{\cup}_{j\in J_2}C(j)$. We can construct a partition of I_C consisting of sets $I_1\cap J_1,I_1\cap J_2,I_2\cap J_1,I_2\cap J_2$ and define the events $W_{ij}=\dot{\cup}_{k\in I_i\cap J_j}C(k)$, $i,j=1,2$. The four-element event $(W_{ij})_{i,j=1}^2$ is a common refinement of A and B. Any two binary events A,B which have a common refinement also have a common refinement of the latter type. We say that the events A, B admit a *strong common refinement* if they have a common refinement $(W_{ij})_{i,j=1}^2$ such that $W_{12}\cap W_{21}=\varnothing$, that is, there is no nonempty event V under W_{12} and W_{21}.

Theorem 4: *Let $(X,\mathcal{T})$ be an algebraic leveled effect test space. Let $\mathbb{E}=\Pi(\mathcal{E})$ be the corresponding effect algebra. The following statements are equivalent.*

(i) *Elements $a_1,\ldots,a_n$ in $\mathbb{E}$ are compatible.*
(ii) *There are events $A_1,\ldots,A_n$ in $\mathcal{E}$, $\Pi(A_i)=a_i$, that can be built from a test T in $\mathcal{T}$.*
(iii) *There are binary tests B_i with $\Pi((B_i)(1))=a_i$, $i=1,\ldots,n$, which have a common refinement.*

Moreover, elements a,b in E are strongly compatible if and only if there are binary events A,B, such that $\Pi(A)=a,\Pi(B)=b$ and A,B admit a strong common refinement.

Proof: $(i)\Rightarrow(ii)$. By (i), there is an orthogonal set $(c_1,\ldots,c_k)$ such that $a_i=\oplus_{j\in I_i}c_j$, $I_i\subset\{1,\ldots,k\}$, $i=1,\ldots,n$. Hence there are orthogonal events $C_1,\ldots,C_k$ with $\Pi(C_i)=c_i$, $i=1,\ldots,k$, and a test $T\in\mathcal{T}$ to which $C_1,\ldots,C_k$ belong. We then have $a_i=\Pi(\dot{\cup}_{j\in I_i}C_j)$, $i=1,\ldots,n$, and $A_i=\dot{\cup}_{j\in I_i}C_j$, $i=1,\ldots,n$, can be built from T.

$(ii)\Rightarrow(iii)$. Let $a_i=\Pi(A_i)$, $i=1,\ldots,n$, and $A_1,\ldots,A_n$ can be built from a test T. We may assume, with no loss of generality, that $A_1,\ldots,A_n$ are subevents of T. Then there are subsets $I_1,\ldots,I_n$ of the index set I_T of T such that $A_k=\dot{\cup}_{j\in I_k}T(j)$, $k=1,\ldots,n$. Taking partitions $(I_k,I_T\setminus I_k)$ of I_T, we obtain binary tests B_k, $k=1,\ldots,n$, with $B_k(1)\approx A_k=\dot{\cup}_{i\in I_k}T(j)$, which can be built from T.

$(iii)\Rightarrow(i)$. Let B_i, $i=1,\ldots,n$, be binary tests with $\Pi(B_i(1))=a_i$ which can be built from a test T. Then there are subsets I_i of I_T with $B_i(1)\approx\dot{\cup}_{j\in I_i}T(i)$. Taking a suitable coarsening if necessary, we may assume that I_T is finite, $I_T=\{1,\ldots,k\}$. Then $c_j=\pi(T(j))$, $j=1,\ldots,k$, is an orthogonal sequence, and $a_i=\Pi(\dot{\cup}_{j\in I_i}T(j))=\oplus_{j\in I_i}c_j$.

To prove the remaining part, assume that (a,b) in E have a strong Mackey decomposition (a_1,b_1,c) and put $d=a_1\oplus b_1\oplus c$. Let A,B be any events such that $\Pi(A)=a$, $\Pi(B)=b$. Then there are orthogonal events A_1,B_1,C,D' belonging to a test T, such that $\Pi(A_1)=a_1,\Pi(B_1)=b_1,\Pi(C)=c$ and $\Pi(D')=d'$. We have $\Pi(A_1\dot{\cup}C)=a$, $\Pi(B_1\dot{\cup}C)=b$, hence $A\approx A_1\dot{\cup}C$, $B\approx B_1\dot{\cup}C$, and (A_1,B_1,C,D') is a common refinement of the binary tests (A,A') and (B,B'). From $a_1\wedge b_1=0$, we obtain that there is no event $V\neq\varnothing$ lying under A_1 and B_1.

The proof of the opposite statement is analogous. □

In the following theorem, we give a characterization of the most important types of effect algebras by properties of leveled effect test spaces. Notice that statements similar to (ii) and (iii) in terms of ordinary effect test spaces have been proved in Di Nola and Dvurečenskij (2001).

Theorem 5: *Let $(X,\mathcal{T})$ be a leveled algebraic effect test space, $\mathcal{E}$ its set of events and $\mathbb{E}=\Pi(\mathcal{E})$ the corresponding effect algebra. The following statements hold.*

(i) *$\mathbb{E}$ is an orthoalgebra if and only if every test is an injective function.*
(ii) *$\mathbb{E}$ is an OMP if and only if every pairwise orthogonal event E,F,G can be built from one test T.*
(iii) *$\mathbb{E}$ has the RDP if and only if every two perspective binary events have a common refinement.*
(iv) *$\mathbb{E}$ is an MV-algebra if and only if every two perspective binary events have a strong common refinement.*

Proof: (i) is well-known. (ii) easily follows from the fact that an effect algebra E is an OMP iff for any a,b,c in $\mathbb{E}$ which are pairwise orthogonal $a\oplus b\oplus c$ exists.

(iii) Let $\mathbb{E}$ have the RDP. Let $A:\{1,2\}\to X$, $B:\{1,2\}\to X$ be perspective binary events. Put $\pi(A(1))=a_1$, $\pi(A(2))=a_2$, $\pi(B(1))=b_1$, $\pi(B(2))=b_2$. By assumption $A\approx B$, which implies $A(1)\dot{\cup}A(2)\approx B(1)\dot{\cup}B(2)$, and this in turn implies $a_1\oplus a_2=b_1\oplus b_2$. By RDP, there are elements $w_{11},w_{12},w_{21},w_{22}$, jointly orthogonal and such that $a_1=w_{11}\oplus w_{12}$, $a_2=w_{21}\oplus w_{22}$, $b_1=w_{11}\oplus w_{21}$, $b_2=w_{12}\oplus w_{22}$. Then there are events W_{ij}, $i,j\in\{1,2\}$, such that $w_{ij}=\Pi(W_{ij})$, which all belong to one test. The event $W=(W_{11},W_{12},W_{21},W_{22})$ is a common refinement of A and B.

Conversely, assume that every two perspective binary events have a common refinement. Let $a_1\oplus a_2=b_1\oplus b_2$, where a_1,a_2,b_1,b_2 are elements in E. Then there are perspective binary events A,B such that $A(i)=a_i$, $i=1,2$, and $B(j)=b_j$, $j=1,2$. By supposition, they have a common refinement $W=(W_{11},W_{12},W_{21},W_{22})$, $A_i\approx\dot{\cup}_{j=1}^{2}W_{1j}$, $i=1,2$, $B_j=\dot{\cup}_{i=1}^{2}W_{ij}$, $j=1,2$. It follows that $a_1=\oplus_{j=1}^{2}\Pi(W_{ij})$, $i=1,2$, $b_j=\oplus_{i=1}^{2}\Pi(W_{ij})$, $j=1,2$, which yields the RDP.

(iv) Let $\mathbb{E}$ be an MV-algebra and let A, B be perspective binary events. Put $\Pi(A_i)=a_i$ and $\Pi(B_j)=b_j$, $i,j=1,2$. Then we have $a_1\oplus a_2=b_1\oplus b_2$, and since E is an MV-algebra, there are

jointly orthogonal elements $w_{ij}, i,j=1,2$, such that $a_i=\oplus_{j=1}^{2} w_{ij}$, $b_j=\oplus_{i=1}^{2} w_{ij}$ and $w_{12}\wedge w_{21}=0$ (Fuchs, 1963). Then there are orthogonal events W_{ij}, $i,j=1,2$, such that $\Pi(W_{ij})=w_{ij}$, so that $W_{12}\cap W_{21}=\varnothing$. It follows that A and B have a strong common refinement. By reversing the arguments, the converse statement is proved. □

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On the complete solution of the Sturm–Liouville problem $(d^2X/dx^2)+\lambda^2X=0$ over a closed interval

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We discuss the sets of orthogonal functions that form solutions to the Sturm–Liouville problem for the equation $d^2X/dx^2+\lambda^2X=0$ and for the general unmixed boundary conditions over a closed interval of the variable x. The conditions for the presence of the solutions with $\lambda^2\leqslant 0$ are specifically considered and their necessity for completeness of a set of eigenfunctions. Their implications are discussed for three examples from mathematical physics, showing that although for some problems the solutions, corresponding to the negative values of λ^2, may reflect physically unusual boundary conditions, their presence is necessary in the general solution for the drift diffusion equation where they may represent stationary or growing in time solutions. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Second-order partial differential equations are commonly solved in different domains of physics. In our case we need to solve the continuity equation of a fluid with specific boundary conditions, as part of our simulation of gaseous discharges in plasmas. In treating such systems we found that a careful study of the ''separation-of-variables'' constant parameters must be made to assure that we include all the correct physical solutions, analytic or numerical. We have found that the relevant literature does not always provide complete solutions and the choices of solutions are not carefully justified. In the following we make a careful analysis of the Sturm–Liouville problem, point out where problems with the identification of the solutions arise, and provide some characteristic examples.

II. THE STURM–LIOUVILLE PROBLEM

The method of separation-of-variables, when used in second-order partial differential equations with constant coefficients often lead to ordinary differential equations of the form

$$\frac{d^2X}{dx^2}+\lambda^2X=0 \tag{1}$$

for the space part, in an interval with general unmixed boundary conditions

$$\frac{dX}{dx}+h_1X=0 \quad \text{for } x=0, \tag{2a}$$

$$\frac{dX}{dx}+h_2X=0 \quad \text{for } x=1. \tag{2b}$$

Without loss of generality, x will be assumed to take values on the interval [0,1].

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Usually the partial solutions representing different values of parameter λ are then written in the form

$$X_\lambda = A_\lambda \sin(\lambda x) + B_\lambda \cos(\lambda x), \quad \lambda^2 > 0, \tag{3a}$$

$$X_\lambda = A_\lambda x + B_\lambda, \quad \lambda^2 = 0, \tag{3b}$$

$$X_\lambda = A_\lambda \sinh(\lambda x) + B_\lambda \cosh(\lambda x), \quad \lambda^2 < 0, \tag{3c}$$

and the three different cases of the ranges of the values of λ^2 are considered together with the boundary conditions.

The consistency requirement for the system of the two equations obtained after the substitution of (3) into (2) gives the different ranges of the values for λ^2, the eigenvalues, which determine the different types of functions that should be present in the set of solutions. The same equation determines the interdependence of A_λ and B_λ for a given λ.

A differential equation defined on the interval $a \leqslant x \leqslant b$ having the form of

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[k(x)\frac{\mathrm{d}X}{\mathrm{d}x}\right] + [\lambda^2 r(x) - q(x)]X = 0$$

with the boundary conditions

$$a_1 X(a) + a_2 \frac{\mathrm{d}X}{\mathrm{d}x}(a) = 0,$$

$$b_1 X(b) + b_2 \frac{\mathrm{d}X}{\mathrm{d}x}(b) = 0$$

is called the *Sturm–Liouville boundary value problem*. In our case, $k(x)=1$, $q(x)=0$, $r(x)=1$, and $h_1 = a_1/a_2$, $h_2 = b_1/b_2$, limited to the real values of h_1 and h_2.

The set of eigenfunctions X_λ obtained as nontrivial solutions of the Sturm–Liouville boundary value problem corresponding to the eigenvalues λ, is used to construct a general solution

$$X = \sum_\lambda X_\lambda \tag{4}$$

as well as to decompose some given function (that represents the initial conditions) to determine the values of A_λ and B_λ, or to build the Green's function for a differential equation. In this case completeness of the set of functions in the set is critical. Orthogonality of the functions X_λ in the set of solutions for Eq. (1) with the boundary conditions (2) and ${\lambda^2}_1 \neq ({\lambda^2}_2)^*$, assuming that h_1 and h_2 are real, can be easily verified:

$$\begin{aligned}
({\lambda^2}_1 - {\lambda^2}_2{}^*) \int_0^1 X_{\lambda_1} X^*_{\lambda_2}\,\mathrm{d}x &= \int_0^1 [({\lambda^2}_1 X_{\lambda_1}) X^*_{\lambda_2} - ({\lambda^2}_2{}^* X^*_{\lambda_2}) X_{\lambda_1}]\mathrm{d}x \\
&= \int_0^1 \left[\frac{\mathrm{d}^2 X_{\lambda_1}}{\mathrm{d}x^2} X^*_{\lambda_2} - \frac{\mathrm{d}^2 X^*_{\lambda_2}}{\mathrm{d}x^2} X_{\lambda_1}\right]\mathrm{d}x \\
&= \left(X_{\lambda_1} \frac{\mathrm{d}X^*_{\lambda_2}}{\mathrm{d}x} - \frac{\mathrm{d}X_{\lambda_1}}{\mathrm{d}x} X^*_{\lambda_2} \right)\Bigg|_0^1 \\
&= X_{\lambda_1}(0) X^*_{\lambda_2}(0)(h_1 - h_1^*) - X_{\lambda_1}(1) X^*_{\lambda_2}(1)(h_2 - h_2{}^*) = 0.
\end{aligned} \tag{5}$$

These solutions are not orthogonal if h_1 and/or h_2 are complex. It should be noted that in the procedure of building the general solution, *all* possible values of λ^2 corresponding to an eigenfunction X_λ should be taken into account. The failure to include even one of the former will lead to an incomplete set of eigenfunctions unable to decompose the function representing the initial conditions in the general case. The question of completeness is further considered in the Appendix.

Solutions in the form (4) are routinely used today in computational applications. Examples are the computational procedures used to solve partial differential equations with constant coefficients. As can be seen from commonly used textbooks for mathematical physics,[1–4] the long-term teaching practice for treating the method of separation-of-variables is to give the solution of Sturm–Liouville problem for Eq. (1) in an interval for zero boundary conditions, namely $X=0$ for $x=0$ and for $x=1$. This leads only to the positive values of the separation parameter λ^2.[1–4] It may be due to this widespread practice that we can often find examples where only eigenfunctions corresponding to $\lambda^2>0$ are taken into account, whereas those for $\lambda^2\leqslant 0$ are omitted.[1,3] For example, Arfken and Weber[5] state in a footnote that λ^2 depends on the boundary conditions but make no further use of that fact. Whether representing physically existing cases (see example IV A in the following) or physically rare or unusual boundary conditions (see Example IV B in the following), the solutions representing negative values of λ^2 should be carefully taken into account. Furthermore, in the construction of a complete solution or in building a Green's function (see example IV C in the following) completeness is absolutely required. The goal of the present paper is to carefully consider the implications of the cases of the solutions for zero and negative values of λ^2.

III. EFFECT OF THE BOUNDARY CONDITIONS

It is useful then to address the question whether it is possible for certain values of h_1 and h_2, involved in the boundary conditions (2), to find an eigenfunction that corresponds to a certain value of the parameter λ^2. In order to answer this question, we will consider the Sturm–Liouville problem for Eq. (1) satisfying the general unmixed boundary conditions (2). It is convenient to write solutions of (1) in the form

$$X_\lambda(x)=\frac{A_\lambda}{\lambda}\sin(\lambda x)+B_\lambda\cos(\lambda x) \tag{6}$$

that can represent all possible values of the separation constant $\lambda^2\in R$. For $\lambda^2=0$ it is assumed that

$$X_0(x)=\lim_{\lambda\to 0}[X_\lambda(x)]=A_0x+B_0.$$

We should also remark that $X_\lambda(x)=X_{-\lambda}(x)$, so that, in this paper, whenever $\lambda^2\geqslant 0$ then $\lambda=+\sqrt{\lambda^2}$, and if $\lambda^2<0$ then $\lambda=+i\sqrt{|\lambda^2|}$.

When the solution (6) is substituted into the boundary conditions (2) it gives a homogeneous system of linear equations for A and B,

$$A_\lambda+B_\lambda h_1=0, \tag{7a}$$

$$A_\lambda\left(\frac{h_2}{\lambda}\sin\lambda+\cos\lambda\right)+B_\lambda(h_2\cos\lambda-\lambda\sin\lambda)=0, \tag{7b}$$

which must have a zero determinant to be consistent. This condition results in the following transcendental equation for the eigenvalues λ:

$$\frac{\sin\lambda}{\lambda}(\lambda^2+h_2h_1)=(h_2-h_1)\cos\lambda, \tag{8}$$

which should be carefully considered for the different values of h_1 and h_2.

(A) $h_1=h_2=0$. This condition represents the case when $dX/dx=0$ for both $x=0$ and $x=1$. It gives $\lambda\in\{0,\pi,2\pi,3\pi,\ldots\}$, $A_\lambda=0$, and the solution

$$X_\lambda(x)=B_\lambda\cos(\lambda x).$$

(B) $h_1\to\infty$, $h_2\to\infty$. This condition represents the situation when $X=0$ for both $x=0$ and $x=1$, giving $\lambda\in\{\pi,2\pi,3\pi,\ldots\}$, $B_\lambda=0$, and

$$X_\lambda(x)=\frac{A_\lambda}{\lambda}\sin(\lambda x)=A'_\lambda\sin(\lambda x).$$

(C) $h_1=h_2=h\neq 0$. Then $\lambda=\{ih\}\cup\{\pi,2\pi,3\pi,\ldots\}$, i.e., λ^2 has one negative root, $B_\lambda=-A_\lambda/h$, and

$$X_\lambda(x)=\frac{A_\lambda}{h}[\sinh(hx)-\cosh(hx)]=A_\lambda e^{-hx}\quad\text{for }\lambda\in\{ih\},$$

and

$$X_\lambda(x)=A_\lambda\left[\frac{\sin(\lambda x)}{\lambda}-\frac{\cos(\lambda x)}{h}\right]=A_\lambda\sin(\lambda x+\delta_\lambda),\quad \delta_\lambda=-\tan^{-1}(\lambda/h)$$

for $\lambda\in\{\pi,2\pi,3\pi,\ldots\}$. It is worth pointing out that the complete set of eigenfunctions in this case will contain not only sine's and cosine's but also an exponent.

(D) $h_1\neq h_2$. Then Eq. (8) can be rewritten for convenience as

$$\lambda\cot\lambda=\frac{\lambda^2+h_2h_1}{h_2-h_1}. \tag{9}$$

To further demonstrate the influence of the parameters h_1 and h_2 on the type of solution (6), we rewrite Eq. (9) as

$$\lambda\cot\lambda=a\lambda^2+b \tag{10a}$$

for $h_1\neq h_2$, with

$$a=\frac{1}{h_2-h_1},\quad b=\frac{h_2h_1}{h_2-h_1}. \tag{10b}$$

For $\lambda\to 0$, Eq. (10a) should be understood as its limit $1=a\lambda^2+b$. Form (10a) becomes amenable to a graphical illustration of finding its solutions by drawing its left- and right-hand sides separately, as seen in Fig. 1.

The general solution (4) of the Sturm–Liouville problem can be split into two parts, one for $\lambda^2>0$ and one for $\lambda^2\leqslant 0$:

$$X=\sum_\lambda X_\lambda=\sum_\lambda\left[\frac{A_\lambda}{\lambda}\sin(\lambda x)+B_\lambda\cos(\lambda x)\right]=\sum_{\lambda^2\leqslant 0}X_\lambda+\sum_{\lambda^2>0}X_\lambda \tag{11}$$

with the values of A_λ and B_λ restricted by either (7a) or (7b). As can be concluded now from Fig. 1, and depending on the values of h_1, h_2, a, and b [cf. Eq. (10)], the sum $\Sigma_{\lambda^2\leqslant 0}X_\lambda$ can contain two, one, or zero terms, corresponding to lines III, II, and I respectively, in contrast to the case of $\lambda^2>0$ when the sum has an infinite number of terms.

To investigate the possibility of appearance zero and negative eigenvalues we look into the values of function $\lambda\cot(\lambda)$ for $\lambda^2<\pi^2$, represented by curve C in Fig. 1. The slope of this curve

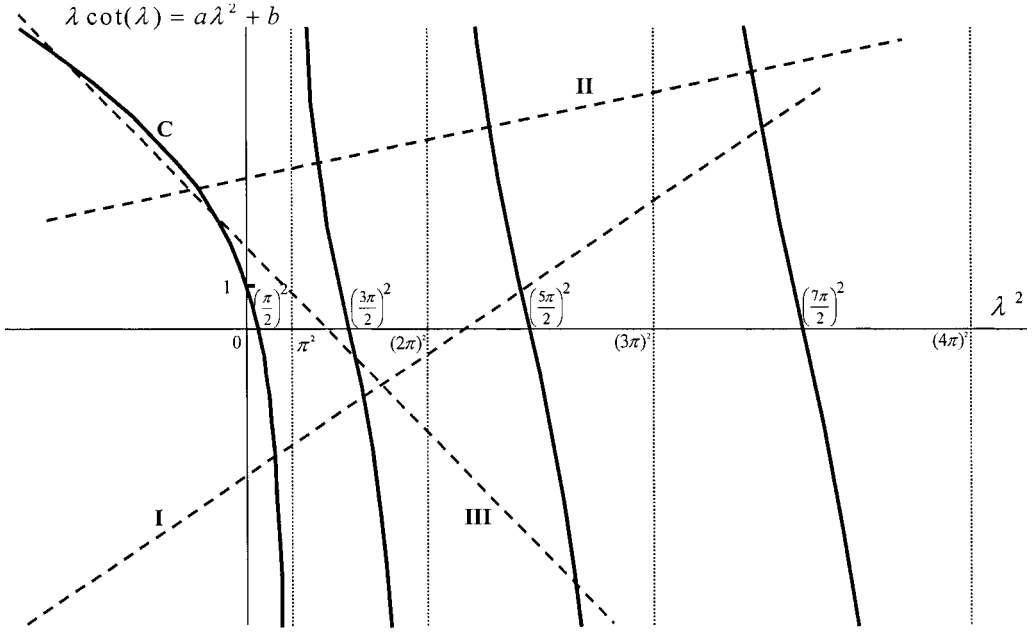

FIG. 1. Graphical solution of the transcendental equation $\lambda \cot\lambda = a\lambda^2 + b$. The numbers above the horizontal axis give the points of intersection of this axis with the displayed graph of the function.

varies from zero, when $\lambda^2 \to -\infty$, to $-\infty$, when $\lambda^2 \to \pi^2$. When $\lambda^2 \to 0$, it equals $-1/3$. Therefore, for any $a<0$ in (10a) it is possible to find the appropriate value $b_0>0$ so that the line $a\lambda^2+b_0$ becomes tangential to curve C. Let T be the point of contact.

(D1) For $\lambda^2<0$, the tangent of curve C (Fig. 2) has a slope varying from $-1/3$ to 0. Let us consider the lines $a\lambda^2+b$ with $-1/3<a<0$ and the following values of b:

(1) $b>b_0$, the region above $a\lambda^2+b_0$ (dashed line I in Fig. 3), gives no negative or zero roots for λ^2 in (10a),
(2) $b=b_0$, coincides with line I and renders one negative root,
(3) $1<b<b_0$, region in between line I and $a\lambda^2+1$ (dashed line II in Fig. 3), two negative roots,
(4) $b=1$, line II, one negative and one zero root,
(5) $b<1$, region below line II, one negative root.

(D2) For $0\leqslant\lambda^2<\pi^2$ the tangent of curve C (Fig. 3) has a slope varying from $-\infty$ to $-1/3$. Following the same geometrical construction as noted previously, for $a\leqslant -1/3$ and different values of b we obtain

(1) $1<b$, region to the right of line II, no negative or zero roots,
(2) $b=1$, line II, one negative and one zero root,
(3) $b<1$, region below line II, one negative root.

(D3) For $0\leqslant a$ line $a\lambda^2+b$ can have only one intersection with curve C. So for:

(1) $1<b$, the region below the dashed line in Fig. 4, the equation has one negative root,
(2) $b=1$, the dashed line, one negative and one zero root,
(3) $b<1$, the region above the dashed line, no negative or zero roots.

Using the parametric dependence of a and b_0 on λ, i.e.,

$$a=\frac{\cot\lambda-\lambda\csc^2\lambda}{2\lambda}, \quad b_0=\frac{\lambda}{2}(\lambda\csc^2\lambda+\cot\lambda), \tag{12}$$

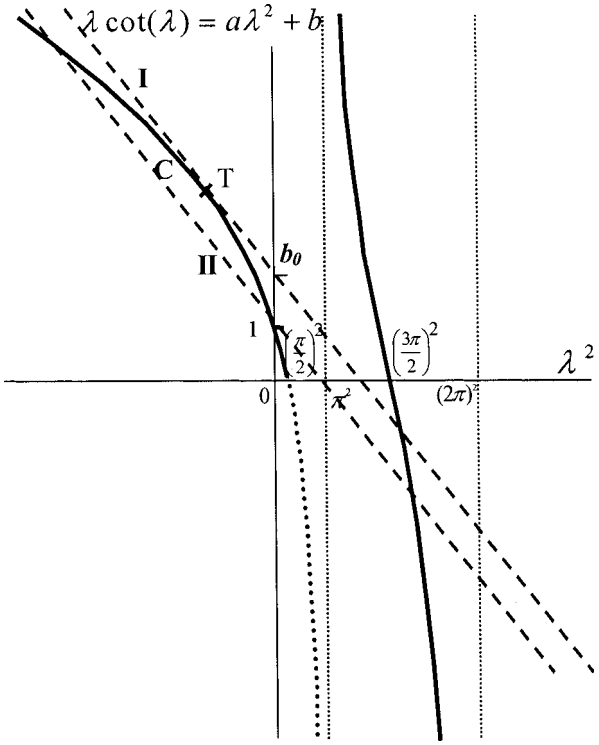

FIG. 2. Same as Fig. 1, highlighting the case of $-1/3 \leqslant a \leqslant 0$.

two useful formulas are easily derivable:

$$ab_0 = -\frac{1}{4}(\lambda^2 \csc^4 \lambda - \cot^2 \lambda), \quad \frac{db_0}{da} = -\lambda^2.$$

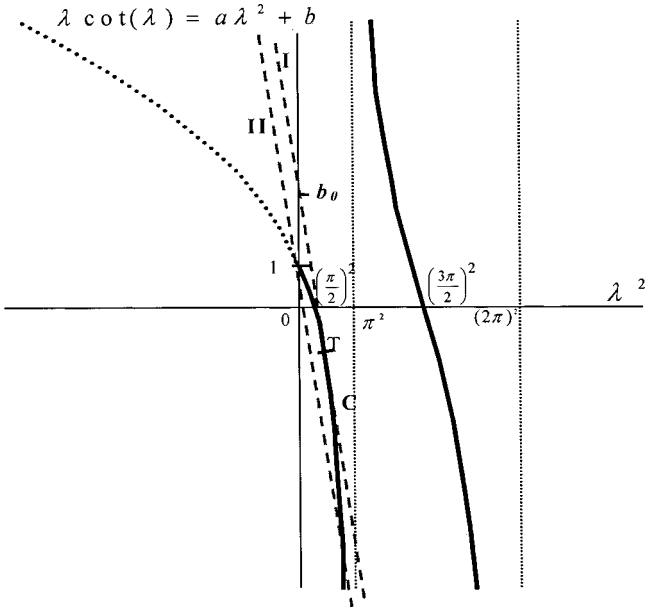

FIG. 3. Same as Fig. 2, highlighting the case of $a \leqslant -1/3$.

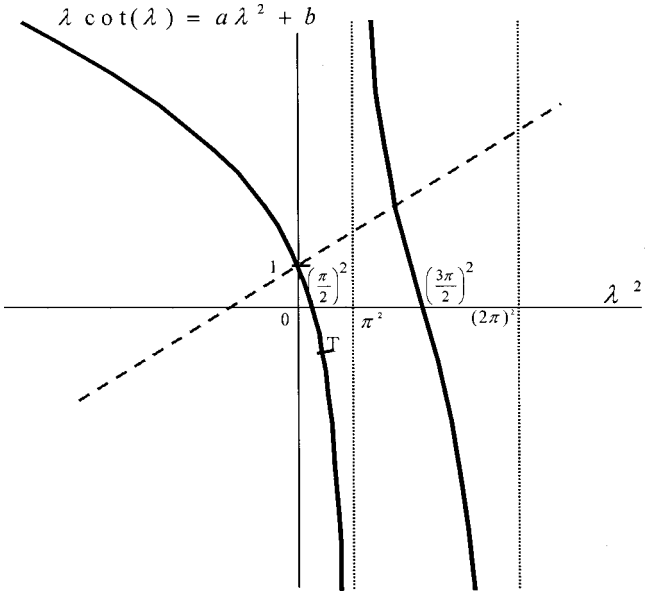

FIG. 4. Same as Fig. 2, highlighting the case of $0 \leqslant a$.

Some other useful expressions are $\lambda^2 \csc^4\lambda - \cot^2\lambda > 1$ for any value of λ^2 and $\lim_{\lambda^2 \to -\infty}(\lambda^2 \csc^4\lambda - \cot^2\lambda) = 1$. These allow us to plot $b_0(a)$ for $a \in (-\frac{1}{3}, 0)$.

Finally, Fig. 5 summarizes cases D1–D3 mentioned previously. Here the two dashed curves correspond to $ab_0 = -\frac{1}{4}$. The solid gray curve illustrates the graph for $b_0(a)$. The line $b = 1$ corresponds to one zero root. The regions $1 < b, 0 \leqslant a$ and $b < 1, 0 < a$, together with the curve $b_0(a)$ give the area where there is one negative root. Finally, the open region bordered by curves $b_0(a)$, $b = 1$, and $a = 0$, renders two negative roots. The arrows at the ends of corresponding curves denote that the end points are excluded. It is worth mentioning that a pair of a and b corresponds to two possible values of h,

$$h_1 = \frac{-1 \mp \sqrt{1+4ab}}{2a}, \quad h_2 = \frac{1 \mp \sqrt{1+4ab}}{2a},$$

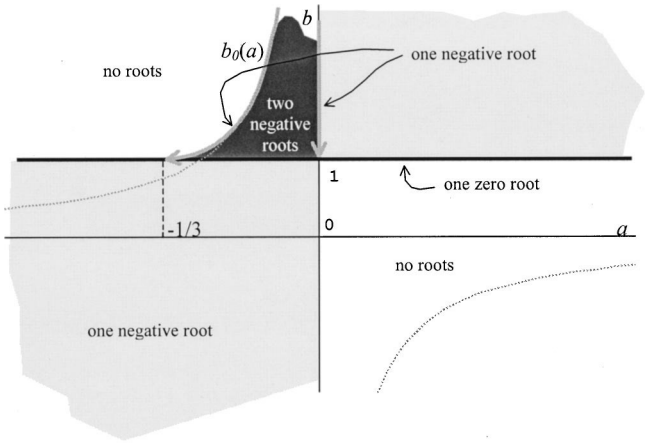

FIG. 5. Summary of the mapping of the zero and negative λ^2 roots as a function of the parameters a and b. Branches of the $ab = -\frac{1}{4}$ graph are shown as dotted lines. The values of the parameters a and b between the branches correspond to real vlaues of h_1 and h_2.

and only the values of a and b between two branches of $ab_0=-\frac{1}{4}$ correspond to the real values of h_1 and h_2.

Some specific examples are presented in the following that demonstrate the above-mentioned analysis for different cases of the values of λ^2.

IV. EXAMPLES

A. Drift-diffusion equation

In our study of gas discharges in plasma displays we use the drift-diffusion equation

$$\frac{\partial n}{\partial t}=\alpha^2\frac{\partial^2 n}{\partial x^2}+\beta\frac{\partial n}{\partial x}+\gamma n, \quad x\in[0,1], \tag{13}$$

to check the behavior of a finite-difference numerical scheme solution against the exact solution derived in the following. This equation can be interpreted as a system of two equations, the continuity equation with *a source*

$$\frac{\partial n}{\partial t}+\frac{\partial J}{\partial x}=\gamma n$$

and the equation determining the density flux

$$J=-\alpha^2\frac{\partial n}{\partial x}-\beta n.$$

By making the substitution

$$n=u\exp(\kappa x+\eta t) \quad \text{with} \quad \kappa=-\beta/2a^2, \quad \eta=\gamma-\beta^2/4a^2,$$

Eq. (13) takes the familiar form of the heat-flow equation

$$\frac{\partial u}{\partial t}=a^2\frac{\partial^2 u}{\partial x^2},$$

which can be solved by the separation of variables method. Assuming that $u(x,t)=\Sigma_i T_i X_i$, we obtain the equations for T_i and X_i: $\mathrm{d}T_\lambda/\mathrm{d}t=-a^2\lambda^2 T_\lambda$, with the solution $T_\lambda=\exp(-a^2\lambda^2 t)$, and $\mathrm{d}^2X/\mathrm{d}x^2+\lambda^2 X=0$.

We are interested in the case when both fluxes are zero at the boundaries. Recalculation of the flux at the boundaries

$$J=-e^{\kappa x+\eta t}\left[a^2\frac{\partial u}{\partial x}+(a^2\kappa+\beta)u\right]=0$$

in terms of u, gives values of constants with the boundary conditions $h_1=h_2=h=\kappa+\beta/\alpha^2=\beta/2\alpha^2$. This represents the previously mentioned case (C), so that $X_\lambda(x)=A_\lambda e^{-hx}$ for $\lambda\in\{ih\}$, and

$$u_\lambda(x)=A_\lambda\sin(\lambda x+\delta_\lambda), \quad \delta_\lambda=-\tan^{-1}(\lambda/h), \quad \lambda\in\{\pi,2\pi,3\pi,\ldots\}.$$

The general solution is then

$$n(x,t)=e^{\kappa x+\eta t}\sum_\lambda T_\lambda X_\lambda=\sum_\lambda \exp\left[\left(\gamma-\frac{\beta^2}{4a^2}-a^2\lambda^2\right)t\right]\exp\left(-\frac{\beta}{2a^2}x\right)X_\lambda.$$

After substitution of X_λ and splitting the sum in parts for $\lambda^2\geqslant 0$ and $\lambda^2<0$ it becomes

$$n(x,t)=A_{ih}e^{\gamma t}\exp\left(-\frac{\beta}{a^2}x\right)+\sum_{\lambda^2\geqslant 0}A_\lambda\exp\left[\left(\gamma-\frac{\beta^2}{4a^2}+a^2\lambda^2\right)t\right]\exp\left(-\frac{\beta}{2a^2}x\right)\sin(\lambda x+\delta_\lambda).$$

It is interesting to remark that in the case of $\gamma=0$, i.e., zero sources and $\int_0^1 n(x,t)\mathrm{d}x=\text{const}$, the term $A_\lambda\exp[-(\beta/a^2+h)x]$ represents the stationary solution which can also be found from a physical reasoning that the stationary solution makes the flux $J=-\alpha^2(\partial n/\partial x)-\beta n$ zero. A physical realization of this case would be the diffusion of particles suspended in the air under the influence of the gravitation field.

B. Oscillations of a fixed rod

To give an example where the eigenfunctions with $\lambda^2<0$ represent a physically impossible situation, let us consider the problem of finding the longitudinal oscillations of the elastically fixed rod over a space interval. This leads to[3]

$$\frac{\mathrm{d}^2u}{\mathrm{d}t^2}=a^2\frac{\mathrm{d}^2u}{\mathrm{d}x^2}$$

with the boundary conditions

$$\frac{\mathrm{d}u}{\mathrm{d}x}-hu=0 \quad \text{for } x=0,$$

$$\frac{\mathrm{d}u}{\mathrm{d}x}+hu=0 \quad \text{for } x=1$$

for all times t. Here h represents the coefficient of elasticity and should be positive to represent a physically meaningful case. Further separation of variables gives $u(x,t)=\Sigma_i T_iX_i$ as the general solution. Equation $\mathrm{d}^2X/\mathrm{d}x^2+\lambda^2X=0$ for the space part X is solved with the boundary conditions $\mathrm{d}X/\mathrm{d}x-hX=0$ for $x=0$ and $\mathrm{d}X/\mathrm{d}x+hX=0$ for $x=1$. This gives $h_1=-h$, $h_2=h$, so that $a=1/(2h)$ and $b=-h/2$ [cf. case (D)]. The possible values of a and b are represented by $ab=-1/4$, the dashed curve in Fig. 5. X_λ with negative and zero values of λ^2 are possible for $a\leqslant 0$ or $h<0$; however, they represent a physically unusual boundary condition since the negative value of h implies a negative sign of Hook's constant, i.e., stretching grows continuously with time.

C. Construction of Green's functions

Smirnov's *Course of Higher Mathematics*[1] considers the equation $\mathrm{d}^2X/\mathrm{d}x^2+\lambda^2X=0$ with boundary conditions $X=0$ for $x=0$ and $\mathrm{d}X/\mathrm{d}x+hX=0$ for $x=1$ in order to find a complete set of eigenfunctions. We should point out that a similar problem would appear in Sec. IV B assuming the rigid fixing of the rod's end at $x=0$ in the previous example, when constructing the general solution in the form (4) or when obtaining the Green's function in the form[1] (see Appendix)

$$G(x,\xi)=\sum_{\lambda_i}\frac{X_{\lambda_i}(x)X_{\lambda_i}(\xi)}{\lambda^2-\lambda^2{}_i}.$$

Obviously, an incomplete basis will not project the correct solution out of the inhomogeneous term.

Although Titchmarsh[6] in a similar case gives the example of negative λ^2, Smirnov[1] mentions the possibility but does not implement such values. For example, Smirnov[1] mentions that the complete set of solutions is (in our notation here) $X_\lambda(x)=A_\lambda\sin(\lambda x)$, where λ is to be found from equation $\tan\lambda+h\lambda=0$ giving all λ^2 to be positive. Since he uses this example several times throughout his multivolume work, but only mentions once (and that only in the Russian edition[7]) that he will limit his consideration to $h>0$, it makes it hard for the reader to consider that

limitation. Following the previously mentioned case (D), with $h_1=\infty$ and $h_2=h$, it is possible to see that here $a=0$ and $b=-h$, so that one zero or negative root of λ^2 is possible for $b\geqslant 1$ or $h\leqslant -1$, giving an additional eigenfunction

$$X_{i|\lambda|}(x)=\frac{B_{i|\lambda|}}{i|\lambda|}\sin[i|\lambda|x]=\frac{B_{i|\lambda|}}{|\lambda|}\sinh[|\lambda|x]$$

for $\lambda^2\leqslant 0$.

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APPENDIX: OUTLINE OF THE COMPLETENESS PROOF

Here we want to briefly illustrate the necessity for taking into account all eigenfunctions corresponding to solutions of (1) with (2) when building a general solution. The argument takes its root in the proof of the expansion theorem. The most straightforward and useful way, for our purpose, is to use the method of contour integration. The application of this method to the boundary value problem of the ordinary linear differential equations of the nth order has been discussed in Ref. 8, and specifically to differential equations of the second order with boundary conditions (2) in Refs. 6 and 9 and we will follow their approach.

The resolvent for

$$\frac{d^2\Phi}{dx^2}+\lambda^2\Phi=f(x) \tag{A1}$$

is the function

$$\Phi(x,\lambda^2)=\frac{\chi(x,\lambda)}{\omega(\lambda)}\int_0^x\phi(y,\lambda)f(y)\mathrm{d}y+\frac{\phi(x,\lambda)}{\omega(\lambda)}\int_x^1\chi(y,\lambda)f(y)\mathrm{d}y, \tag{A2}$$

satisfying the boundary conditions (2). Here ϕ and χ are solutions of homogeneous equation (1) with ϕ satisfying (2a) and χ satisfying (2b), and $\omega(\lambda)=\phi(\mathrm{d}\chi/\mathrm{d}x)-\chi(\mathrm{d}\phi/\mathrm{d}x)$ is the Wronskian of the functions ϕ and χ. The zeroes of the Wronskian coincide with the roots of (9) confirming linear dependence of ϕ and χ at λ_i where $\omega(\lambda_i)=0$ so that $\chi(x,\lambda_i)=k(\lambda_i)\phi(x,\lambda_i)$.

Denoting $\lambda=\sigma+it$ and considering two segments $\sigma=R, -R\leqslant t\leqslant R$ and $t=R, -R\leqslant\sigma\leqslant R$, it is possible to see that they form the closed contour $C(R)$ on the λ^2 plane. Using the explicit form for

$$\phi(x,\lambda)=\frac{\cos(\lambda x)}{h_1}-\frac{\sin(\lambda x)}{\lambda},$$

$$\chi(x,\lambda)=\frac{\cos[\lambda(x-1)]}{h_2}+\frac{\sin[\lambda(x-1)]}{\lambda},$$

and

$$\omega(\lambda)=\frac{\sin(\lambda)(h_1h_2+\lambda^2)-\lambda\cos(\lambda)(h_2-h_1)}{h_1h_2\lambda},$$

the integration can be done over $C(R)$ on the λ^2 plane. Then if $f(x)\in L_1$ it is possible to show[6,9] that for $0<x<1$ and $R\to\infty$:

$$\frac{1}{2\pi i}\int_{C(R)}\Phi(x,\lambda^2)\mathrm{d}\lambda^2\to\frac{1}{2\pi i}\int_{C(R)}\frac{\mathrm{d}\lambda^2}{\lambda\sin(\lambda)}\Bigg\{\cos[\lambda(1-x)]\int_0^x f(y)\cos(\lambda y)\mathrm{d}y + \cos(\lambda x)\Bigg]\int_x^1 f(y)\cos[\lambda(1-y)]\mathrm{d}y\to\frac{1}{2}(f(x+0)+f(x-0)). \tag{A3}$$

On the other hand, $\Phi(x,\lambda^2)$ has residues at $\lambda=\lambda_i$ resulting in

$$\frac{1}{2\pi i}\int_{C(R)}\Phi(x,\lambda^2)d\lambda^2=\sum_{\lambda_i\text{being inside }C(R)}\frac{k(\lambda_i)}{\mathrm{d}\omega(\lambda)/d(\lambda^2)|_{\lambda=\lambda_i}}\phi(x,\lambda_i)\int_0^1\phi(y,\lambda_i)f(y)\mathrm{d}y, \tag{A4}$$

assuming that λ_i are the roots of $\omega(\lambda_i)=0$ with multiplicity one. When $R\to\infty$, this sum includes all of the λ_i.

We should mention that for any $\lambda^2{}_i$ such that $\omega(\lambda_i)=0$ it is possible to find a and b so that also

$$\left.\frac{\mathrm{d}\omega(\lambda)}{\mathrm{d}(\lambda^2)}\right|_{\lambda^2=\lambda^2{}_i}=0,$$

i.e., $\lambda^2{}_i$ is a root of multiplicity two for $\omega(\lambda^2{}_i)$. Line $a\lambda^2+b=0$ then becomes tangential to $\lambda\cot\lambda$ at $\lambda^2{}_i$, so that the values of a and b in this case will be given parametrically by (12). For some $\lambda^2{}_i$ it is possible to satisfy the additional condition

$$\left.\frac{\mathrm{d}^2\omega(\lambda)}{(\mathrm{d}(\lambda^2))^2}\right|_{\lambda^2=\lambda^2{}_i}=0,$$

so that $\lambda^2{}_i$ becomes a root of multiplicity three for $\omega(\lambda^2{}_i)$. As seen from Fig. 6, there are no roots of multiplicity higher than 3 and all of them lie in the region on the outside of the two branches of $ab=-\frac{1}{4}$ corresponding to the imaginary values of h_1 and h_2.

Comparing these two results (A4) and (A5) we see that

$$\frac{1}{2}(f(x+0)+f(x-0))=\lim_{R\to\infty}\frac{1}{2\pi i}\int_{C(R)}\Phi(x,\lambda^2)\mathrm{d}\lambda^2 = \sum_{\lambda_i:\omega(\lambda_i)=0}\frac{k(\lambda_i)}{\left.\frac{\mathrm{d}\omega(\lambda)}{\mathrm{d}(\lambda^2)}\right|_{\lambda=\lambda_i}}\phi(x,\lambda_i)\int_0^1\phi(x,\lambda_i)f(y)\mathrm{d}y \tag{A5}$$

completing the proof. We can see that each root of equation $\omega(\lambda_i)=0$ corresponds to a function used in the expansion (A5). Removing any function, e.g., $\phi(x,\lambda_r)$, from the set will result in the deficient set of functions on the interval $0<x<1$, so that setting $f(y)=\phi(x,\lambda_r)$ and using the expansion (A5) *always* gives $\frac{1}{2}[\phi(x+0,\lambda_r)+\phi(x-0,\lambda_r)]=0$ for $0<x<1$, due to orthogonality (5). This contradiction proves the deficiency.

Using the explicit form for

$$k(\lambda)=\frac{h_1}{h_1\cos(\lambda)+\lambda\sin(\lambda)},$$

$$\frac{\mathrm{d}\omega(\lambda)}{\mathrm{d}(\lambda^2)}=\frac{\lambda\cos(\lambda)-h_1\sin(\lambda)}{2\lambda^3h_1}+\frac{h_1(h_1-1)+\lambda^2}{2\lambda^2h_1[h_1\cos(\lambda)+\lambda\sin(\lambda)]},$$

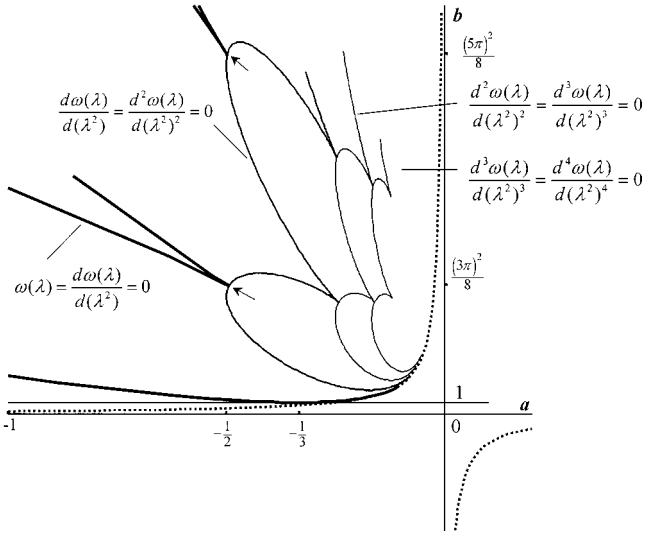

FIG. 6. Higher-multiplicity roots of the Wronskian. $ab=-\frac{1}{4}$ are shown as dotted lines. Solid curves show parameters a and b for which $\omega(\lambda)=0$ has roots of multiplicity two. Arrows indicate roots of multiplicity three.

and (A5) for $f(x)=\phi(x,\lambda_i)$, we can find the normalization constant

$$N_i=\int_0^1 \phi^2(x,\lambda_i)\mathrm{d}y$$

$$=\frac{k(\lambda_i)}{\left.\frac{\mathrm{d}\omega(\lambda)}{\mathrm{d}(\lambda^2)}\right|_{\lambda=\lambda_i}}=\frac{[\lambda\cos(\lambda)-h_1\sin(\lambda)][h_1\cos(\lambda)+\lambda\sin(\lambda)]+\lambda[h_1(h_1-1)+\lambda^2]}{2\lambda^3 {h_1}^2}.$$

Now (A5) takes a well-known form of orthogonal function expansion

$$f(x)=\sum_i c_i\psi_i(x) \tag{A6}$$

with

$$\psi_i=\phi(x,\lambda_i)/\sqrt{N_i}$$

and

$$c_i=\int_0^1 \psi_i(y)f(y)\mathrm{d}y.$$

For the boundary value problem (1) with (2) the resolvent (A2) can be rewritten in the form of the Green's function

$$\Phi(x,\lambda^2)=\int_0^1 G(x,y,\lambda)f(y)\mathrm{d}y$$

with

$$G(x,y,\lambda)=\frac{1}{\omega(\lambda)}\begin{cases}\chi(x,\lambda)\phi(y,\lambda), & y\leqslant x\\ \phi(x,\lambda)\chi(y,\lambda), & y\geqslant x.\end{cases}$$

Assuming that the resolvent itself can be expanded in the form

$$\Phi(x,\lambda^2)=\sum_i a_i(\lambda^2)\psi_i(x),$$

substituting it, together with (A6), into (A1), and using the orthogonality expression (5), it follows that

$$a_i(\lambda^2)=\frac{c_i}{\lambda^2-\lambda_i{}^2}.$$

This yields another form for the Green's function,

$$G(x,y,\lambda)=\sum_i \frac{\psi_i(x)\psi_i(y)}{\lambda^2-\lambda_i{}^2}.$$

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Phase space Feynman path integrals

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A rigorous mathematical formulation of the ''phase space Feynman path integral'' is given in a general setting. This is then applied to yield a representation of solutions of the Schrödinger equation with potential depending both on the position and momentum variables. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Let us consider the Schrödinger equation for the time evolution of a d-dimensional quantum particle:

$$\begin{cases} \dot{\psi} = -\dfrac{i}{\hbar} H\psi, \\ \psi(0, x) = \psi_0(x), \end{cases} \tag{1}$$

where $H = p^2/2m + V$ is the Hamiltonian of the system, $m > 0$ is the mass of the particle, $\hbar$ is the (reduced) Planck' constant, and p is the quantum mechanical momentum operator. Under suitable conditions on the potential V, in the position representation H is realized as the self-adjoint operator in the Hilbert space $\mathcal{H} = \mathcal{L}_2(\mathbb{R}^d)$, obtained by closure of the operator

$$H\psi(x) = -\frac{\hbar^2}{2m}\Delta\psi(x) + V(x)\psi(x), \quad \psi \in D(-\Delta) \cap D(V),$$

$$\psi \in \mathcal{H}, \quad \int_{\mathbb{R}^d} |\psi(x)|^2 \, \mathrm{d}x < +\infty,$$

where $D(A)$ denotes the domain of the operator A in $\mathcal{H}$ (see, e.g. Ref. 1). Let $G(t,x,y)$ be the Green function or propagator, namely the kernel of the unitary group $e^{-itH/\hbar}$,

$$\psi(t,x) = \int_{\mathbb{R}^d} G(t,x,y)\psi_0(y)\mathrm{d}y$$

(see, e.g., Ref. 1 for a discussion on sufficient conditions for the existence of G and for the properties of it). In 1942 Feynman gave a suggestive representation of the propagator and showed the connection between the classical Lagrangian description of the physical world and the quantum one. In fact the kernel of the unitary group can be heuristically computed by means of an infinite dimensional path integral of the following form:

$$G(t,x,y) = \text{const} \int e^{(i/\hbar)\, S(\gamma)} \mathrm{d}\gamma, \tag{2}$$

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where the integration is on the set of paths starting in y at time 0 and ending in x at time t and $S(\gamma)$ is the classical action of the system, evaluated on the path γ:

$$S(\gamma)=\int_0^t (\dot{\gamma}(s)^2/2m - V(\gamma(s))\mathrm{d}s.$$

Expression (2) lacks rigor, e.g., neither the constant in front of the integral nor the ''infinite dimensional Lebesgue measure'' $\mathrm{d}\gamma$ are well defined. Nevertheless a rigorous mathematical formulation of the *Feynman functional* can be given (see Refs. 2 and 3, and references therein; for other approches see also Refs. 4 and 5). Feynman himself (see Ref. 6) gave other heuristic representations of the integral, e.g., the heuristic integration over paths in phase space. For physical discussions of this concept see also Ref. 7.

The aim of the present paper is to give a mathematical definition of a ''phase space path integral:'' a Hamiltonian instead of a Lagrangian representation of the propagator. We want to give mathematical meaning to the Hamiltonian version of formula (2), namely to

$$G(t,x,y)=\text{const}\int e^{(i/\hbar)\,S(q,p)}\mathrm{d}q\,\mathrm{d}p, \tag{3}$$

where $q(s),p(s)$, $s\in[0,t]$ are paths in the phase space and S is the action in the Hamiltonian fomulation: $S(q,p)=\int_0^t(\dot{q}(s)p(s)-H(q(s),p(s)))ds$.

The Hamiltonian formulation is more convenient for two reasons:

(1) for many classical systems it is better than the Lagrangian one;
(2) the discussion of the approach from quantum mechanics to classical mechanics, i.e., the study of the behavior of physical quantities taking into account that $\hbar$ is small, is more natural in a Hamiltonian setting (see, e.g., Refs. 8 and 9 for a discussion of this behavior).

We note that an approach of phase space Feynman path integrals via analytic continuation of ''phase space Wiener integrals'' has been presented by Daubechies and Klauder.[10] Analytic continuation was also used in other ''path space'' approaches, see Refs. 11 and 4, and references therein. Our approach is more direct in the spirit of Ref. 2.

II. LIE–TROTTER PRODUCT FORMULA

We first recall an abstract version of the Lie–Trotter product formula.

Lemma 1: Let A and B be self-adjoint operators in a Hilbert space $\mathcal{H}$ and let $A+B$ be essentially self-adjoint on $D(A)\cap D(B)$. Then

$$s-\lim_{n\to\infty}(e^{ita/n}e^{itB/n})^n=e^{i(A+B)t},\quad t\in\mathbb{R}. \tag{4}$$

Here $s-\lim$ is the strong operator limit. For a proof and a discussion of this lemma see e.g., Refs. 12 and 1.

Let $\mathcal{H}=L^2(\mathbb{R}^d)$ and let us consider a potential V depending both on the position and on the momentum in the following way: $V=V_1(x)+V_2(p)$. V_1 is defined as a self-adjoint operator in $\mathcal{H}$, with its natural domain as a multiplication operator. V_2 is the operator in $\mathcal{H}$ with domain

$$D(V_2(p))=\{\psi\in\mathcal{H}\,|\,\alpha\to V_2(\alpha)\hat{\psi}(\alpha)\in\mathcal{H}\},$$

where $\hat{\psi}$ is the Fourier transform of ψ. It coincides with the operator defined by functional calculus as $V_2(p)$, with p the self-adjoint operator $-i\hbar\nabla$ in $\mathcal{H}$. V is then the sum, as a self-adjoint operator in $\mathcal{H}$, of the self-adjoint operators V_1 and V_2. We assume that the functions V_1 and V_2 are such that the corresponding operators have a common dense domain of essentially self-adjointness D. This is the case, e.g., when $V_1\in L^2(\mathbb{R}^d)+L^\infty(\mathbb{R}^d)$, V_2 is bounded measurable, and $D=C_0^\infty(\mathbb{R}^d)$ or $D=\mathcal{S}(\mathbb{R}^d)$. We assume, in order to apply lemma 1, that V_1, V_2 are such that $-(\hbar^2/2m)\,\Delta+V_2$ and $-(\hbar^2/2m)\,\Delta+V_1+V_2$ are essentially self-adjoint on D. We denote by H the closure of the

latter operator. H (which we also write simply as $-(\hbar^2/2m)\,\Delta+V_1+V_2$) is then the quantum Hamiltonian.

By lemma 1 we have then

$$\exp\left(-\frac{it(p^2/2m+V}{\hbar}\right)=s-\lim_{n\to\infty}\left(\exp\left(-\frac{i\epsilon(p^2/2m+V_2)}{\hbar}\right)\exp\left(-\frac{i\epsilon(V_1)}{\hbar}\right)\right)^n,\quad \epsilon\equiv\frac{t}{n},$$

$$\psi(t)=\exp\left(-\frac{it(p^2/2m+V}{\hbar}\right)\psi_0=\lim_{n\to\infty}\left(\exp\left(-\frac{i\epsilon(p^2/2m+V_2)}{\hbar}\right)\exp\left(-\frac{i\epsilon V_1}{\hbar}\right)\right)^n\psi_0,$$

$$\psi_0\in\mathbb{C}_0^\infty(\mathbb{R}^d),$$

(see, e.g., Refs. 12 and 13 for related uses of the Lie–Trotter formula).

By shifting from the position representation to the momentum representation and vice versa and assuming that V_1 and V_2 are continuous, we can write in the strong $L^2(\mathbb{R}^d)$-sense, for all $t>0$:

$$\begin{aligned}\psi(t,x)&=\lim_{n\to\infty}\int_{\mathbb{R}^d}\exp\left(-\frac{i\epsilon(p_{n-1}^2/2m+V_2(p_{n-1}))}{\hbar}\right)\cdot\left(\exp\left(-\frac{i\epsilon V_1}{\hbar}\right)\right.\\&\quad\left.\times\left(\exp\left(-\frac{i\epsilon(p^2/2m+V_2)}{\hbar}\right)\exp\left(-\frac{i\epsilon(V_1)}{\hbar}\right)\right)^{n-1}\psi_0\right)(p_1)\,\frac{\exp\left(i\,\frac{xp_{n-1}}{\hbar}\right)}{(2\pi\hbar)^{d/2}}\,\mathrm{d}p_{n-1}\\&=\lim_{n\to\infty}\int_{\mathbb{R}^{2d}}\exp\left(-\frac{i\epsilon(p_{n-1}^2/2m+V_2(p_{n-1}))}{\hbar}\right)\exp\left(-\frac{i\epsilon V_1(x_{n-1}}{\hbar}\right)\\&\quad\cdot\left(\left(\exp\left(-\frac{i\epsilon(p^2/2m+V_2)}{\hbar}\right)\exp\left(-\frac{i\epsilon(V_1)}{\hbar}\right)\right)^{n-1}\psi_0\right)(x_{n-1})\,\frac{\exp\left(i\,\frac{xp_{n-1}}{\hbar}\right)}{(2\pi\hbar)^{d/2}}\\&\quad\times\frac{\exp\left(-i\,\frac{x_{n-1}p_{n-1}}{\hbar}\right)}{(2\pi\hbar)^{d/2}}\,\mathrm{d}p_{n-1}\mathrm{d}x_{n-1}\\&=\lim_{n\to\infty}\left(\frac{1}{\sqrt{2\pi\hbar}}\right)^{2nd}\cdot\int_{\mathbb{R}^{2nd}}\exp\left(-\frac{i\epsilon}{\hbar}\sum_{j=0}^{n-1}\left(\frac{p_j^2}{2m}+V_1(x_j)+V_2(p_j)\right.\right.\\&\quad\left.\left.-p_j\,\frac{(x_{j+1}-x_j)}{\epsilon}\right)\right)\psi_0(x_0)\prod_{j=0}^{n-1}\mathrm{d}p_j\mathrm{d}x_j,\end{aligned}\tag{5}$$

where $x_n\equiv x$.

Remark: The integrals above are to be understood as limits as $\Lambda\uparrow\mathbb{R}^d$, $n\to\infty$ in the $L^2(\mathbb{R}^{2nd})$ sense of the corresponding integrals over Λ^{2nd}, with Λ bounded (see Ref. 11). Formula (5) holds first as a strong L^2-limit, but then (possibly by subsequences) also for Lebesgue a.e.x. It also follows from this that (5) gives the solution to the Cauchy problem (1).

The latter expression suggests the following formula for the limit:

$$\begin{aligned}\psi(t,x)&=\mathrm{const}\int_{q(t)=x}e^{(i/\hbar)\,S(q,p)}\psi(0,q(0))\mathrm{d}q\,\mathrm{d}p,\\S(q,p)&=\int_0^t p(s)\dot{q}(s)-H(q(s),p(s))\mathrm{d}s,\end{aligned}\tag{6}$$

which does not yet have a mathematical meaning. It will be rigorously defined in Secs. III and IV.

III. OSCILLATORY INTEGRALS AND THE CAMERON MARTIN FORMULA

In this section we recall for later use some known results, for more details we refer to Refs. 2, 3, and 8.

A. Finite dimensional oscillatory integrals

Let us consider the finite dimensional real Hilbert space $\mathbb{R}^n$, whose elements are denoted by $x,y\in\mathbb{R}^n$ and the scalar product with $\langle x,y\rangle$. Let $T:\mathbb{R}^n\to\mathbb{R}^n$ be a nondegenerate symmetric operator.

Definition 1: A function $f:\mathbb{R}^n\to\mathbb{C}$ is Fresnel integrable with respect to T if and only if for each $\phi\in\mathcal{S}(\mathbb{R}^n)$ such that $\phi(0)=1$ the limit

$$\lim_{\epsilon\to 0}\int e^{i\langle x,Tx\rangle}f(x)\phi(\epsilon x)\mathrm{d}x \tag{7}$$

exists and is independent of ϕ. In this case the limit is called the Fresnel integral of f with respect to T and denoted by

$$\int e^{i\langle x,Tx\rangle}f(x)\mathrm{d}x.$$

There is an important class $\mathcal{F}(\mathbb{R}^n)$ of Fresnel integrable functions: those which are Fourier transforms of complex bounded variation measures on $\mathbb{R}^n$, $\mathcal{M}(\mathbb{R}^n)$:

$$f\in\mathcal{F}(\mathbb{R}^n)\Leftrightarrow f(x)=\int e^{i\langle x,\alpha\rangle}\mu_f(d\alpha),\quad \mu_f\in\mathcal{M}(\mathbb{R}^n),\quad x\in\mathbb{R}^n.$$

$\mathcal{F}(\mathbb{R}^n)$ contains in particular $\mathcal{S}(\mathbb{R}^n)$, hence it is also dense in $L^2(\mathbb{R}^n)$. In this case the Parseval equality gives us the following expression for the limit (7):

$$(2\pi i)^{-n/2}\int e^{(i/2)\langle x,Tx\rangle}f(x)\mathrm{d}x=(\det T)^{-1/2}\int e^{(-i/2)\langle x,T^{-1}x\rangle}\mu_f(\mathrm{d}x).$$

Analogously one can define the normalized Fresnel integral by means of the following expression:

$$\widetilde{\int}\int e^{(i/2)\langle x,Tx\rangle}f(x)\mathrm{d}x:=(\det T)^{1/2}(2\pi)^{-n/2}\int e^{(i/2)\langle x,Tx\rangle}f(x)\mathrm{d}x=\int e^{(-i/2)\langle x,T^{-1}x\rangle}\mu_f(\mathrm{d}x).$$

Note that if we substitute into the latter definition the function $f=1$ we have $\tilde{\int}e^{(i/2)\langle x,Tx\rangle}f(x)\mathrm{d}x=1$.

B. Infinite dimensional oscillatory integrals

Let us consider an infinite dimensional real Hilbert space of paths $\mathcal{H}$ whose elements are denoted by $\gamma,\eta\in\mathcal{H}$ and the scalar product by $\langle\gamma,\eta\rangle$. Let P_n be a sequence of projectors on n-dimensional subspaces of $\mathcal{H}$ such that $P_n\leqslant P_{n+1}$ [i.e., $P_{n+1}=I$ on $P_n(\mathcal{H})$] and $P_n\to I$ strongly as $n\to\infty$; let $f:\mathcal{H}\to\mathbb{C}$ be a function on $\mathcal{H}$ and let $T:D(T)\subseteq\mathcal{H}\to\mathcal{H}$ be a self-adjoint invertible operator.

Definition 2: A function $f:\mathcal{H}\to\mathbb{C}$ is Fresnel integrable with respect to T if and only if for each n the following finite dimensional integral

$$\widetilde{\int}_{P_n\mathcal{H}}e^{i\langle P_n\gamma,TP_n\gamma\rangle}f(P_n\gamma)\mathrm{d}P_n\gamma \tag{8}$$

is well defined and the limit

$$\lim_{n\to\infty} \widetilde{\int}_{P_n\mathcal{H}} e^{i\langle P_n\gamma, TP_n\gamma\rangle} f(P_n\gamma)\mathrm{d}P_n\gamma \tag{9}$$

exists and is independent of the sequence $\{P_n\}$.

In this case the limit is called the Fresnel integral of f *with respect to* T *and is denoted by*

$$\widetilde{\int} e^{i\langle \gamma, T\gamma\rangle} f(\gamma)\mathrm{d}\gamma.$$

Equation (8) is called the normalized finite dimensional approximation of this Fresnel integral.

One can prove that if $f\in\mathcal{F}(\mathcal{H})$ then $f\circ P_n\in\mathcal{F}(P_n(\mathcal{H}))$. Moreover f is Fresnel integrable and the Cameron–Martin-type formula holds:

$$\widetilde{\int} e^{(i/2)\langle \gamma, T\gamma\rangle} f(\gamma)\mathrm{d}\gamma = \int_{\mathcal{H}} e^{-(i/2)\langle \gamma, T^{-1}\gamma\rangle}\mu_f(\mathrm{d}\gamma), \tag{10}$$

see Refs. 8 and 3.

IV. PHASE SPACE FEYNMAN FUNCTIONAL

Let us consider again the expression (6) in the particular case of the free particle, namely when the Hamiltonian is just the kinetic energy: $H=p^2/2m$. In this case we have heuristically

$$\psi(t,x) = \text{const} \int_{q(t)=x} \exp\left(\frac{i}{\hbar}\int_0^t (p(s)\dot{q}(s) - p(s)^2/2m)\mathrm{d}s\right)\psi(0,q(0))\mathrm{d}q\,\mathrm{d}p. \tag{11}$$

We can give a precise meaning to this expression: under suitable hypothesis on the initial wave function ψ_0, it is an infinite dimensional oscillatory integral.[14] In fact, following Ref. 15, let us introduce the Hilbert space $\mathcal{H}_t\times\mathcal{L}_t$, namely the space of paths in the d-dimensional phase space $(q(s),p(s))_{s\in[0,t]}$, such that the path $(q(s))_{s\in[0,t]}$ belongs to the Cameron–Martin space $\mathcal{H}_t$, namely to the space of the absolutely continuous functions q from $[0,t]$ to $\mathbb{R}^d$ such that $q(t)=0$ and $\dot{q}\in\mathcal{L}_2([0,t],\mathbb{R}^d)$, with inner product $\langle q_1,q_2\rangle = \int_0^t \dot{q}_1(s)\dot{q}_2(s)\mathrm{d}s$, while the path in the momentum space $(p(s))_{s\in[0,t]}$ belongs to $\mathcal{L}_t=\mathcal{L}_2([0,t],\mathbb{R}^d)$. $\mathcal{H}_t\times\mathcal{L}_t$ is an Hilbert space with the natural inner product

$$\langle q,p;Q,P\rangle = \int_0^t \dot{q}(s)\dot{Q}(s)\mathrm{d}s + \int_0^t p(s)P(s)\mathrm{d}s.$$

Let us introduce the following bilinear form:

$$[q,p;Q,P] = \int_0^t \dot{q}(s)P(s)\mathrm{d}s + \int_0^t p(s)\dot{Q}(s)\mathrm{d}s - \int_0^t p(s)P(s)\mathrm{d}s = \langle q,p;A(Q,P)\rangle,$$

where A is the following operator in $\mathcal{H}_t\times\mathcal{L}_t$:

$$A(Q,P)(s) = \left(\int_t^s P(u)\mathrm{d}u, \dot{Q}(s) - P(s)\right). \tag{12}$$

$A(Q,P)$ is densely defined, e.g., on $C^1([0,t];\mathbb{R}^d)\times C^1([0,t];\mathbb{R}^d)$. Moreover $A(Q,P)$ is invertible with inverse given by

$$A^{-1}(Q,P)(s) = \left(\int_t^s P(u)\mathrm{d}u + Q(s), \dot{Q}(s)\right) \tag{13}$$

(on the range of A).

Now expression (6) can be realized rigorously as

$$\widetilde{\int}_{\mathcal{H}_t\times\mathcal{L}_t} e^{(i/2\hbar)\langle q,p;A(q,p)\rangle}\psi(0,q(0)+x)\mathrm{d}q\,\mathrm{d}p,$$

where $q+x$ denotes the traslated path $q(s)\to q(s)+x$, and the normalized integral is defined by (10).

In this case the heuristic expression (6) is well defined through Lie–Trotter product formula, namely as the limit of a sequence of finite dimensional integrals, as we saw in Sec. II. We are now going to show that it is also the limit of a sequence of finite dimensional oscillatory integrals in the sense of definition 2.

Let us consider a sequence of partitions π_n of the interval $[0,t]$ into n subintervals of amplitude $\epsilon\equiv t/n$:

$$t_0=0,t_1=\epsilon,\ldots,t_i=i\epsilon,\ldots,t_n=n\epsilon=t.$$

To each π_n we associate a projector $P_n:\mathcal{H}_t\times L_t\to:\mathcal{H}_t\times L_t$ onto a finite dimensional subspace of $\mathcal{H}_t\times L_t$, namely the subspace of polygonal paths. In other words each projector P_n acts on a phase space path $(q,p)\in\mathcal{H}_t\times\mathcal{L}_t$ in the following way:

$$P_n(q,p)(s)=\left(\sum_{i=1}^{n}\chi_{[t_{i-1},t_i]}(s)\left(q(t_{i-1})+\frac{(q(t_i)-q(t_{i-1})}{t_i-t_{i-1}}(s-t_{i-1})\right),\sum_{i=1}^{n}\chi_{[t_{i-1},t_i]}(s)p_i\right),$$

where

$$p_i=\frac{\int_{t_{i-1}}^{t_i}p(s)\mathrm{d}s}{t_i-t_{i-1}}=\frac{1}{\epsilon}\int_{t_{i-1}}^{t_i}p(s)\mathrm{d}s.$$

Theorem 1: *For each $n\in\mathbb{N}$, P_n is a projector in $\mathcal{H}_t\times\mathcal{L}_t$. Moreover for $n\to\infty$ $P_n\to I$ as a bounded operator.*

Proof: P_n is symmetric, indeed for all $(Q,P)\in\mathcal{H}_t\times\mathcal{L}_t$ and all $(q,p)\in\mathcal{H}_t\times\mathcal{L}_t$,

$$\begin{aligned}\langle Q,P;P_n(q,p)\rangle&=\int_0^t\dot{Q}(s)\sum_{i=1}^{n}\chi_{[t_{i-1},t_i]}(s)\frac{(q(t_i)-q(t_{i-1})}{t_i-t_{i-1}}\mathrm{d}s+\int_0^t P(s)\sum_{i=1}^{n}\chi_{[t_{i-1},t_i]}(s)p_i\mathrm{d}s\\&=\sum_{i=1}^{n}\frac{(q(t_i)-q(t_{i-1})(Q(t_i)-Q(t_{i-1})}{t_i-t_{i-1}}+\sum_{i=1}^{n}\frac{\int_{t_{i-1}}^{t_i}p(s)\mathrm{d}s\int_{t_{i-1}}^{t_i}P(s)\mathrm{d}s}{t_i-t_{i-1}}\\&=\langle P_n(Q,P);q,p\rangle.\end{aligned}$$

$P_n^2=P_n$, indeed

$$\begin{aligned}P_n^2(q,p)(s)&=\left(\sum_{i=1}^{n}\chi_{[t_{i-1},t_i]}(s)\left(q(t_{i-1})+\frac{\big(q(t_i)-q(t_{i-1})}{t_i-t_{i-1}}(s-t_{i-1})\right),\sum_{i=1}^{n}\chi_{[t_{i-1},t_i]}(s)p_i\right)\\&=P_n(q,p)(s)\end{aligned}$$

$\forall(q,p)\in\mathcal{H}_t\times\mathcal{L}_t$, $\|P_n(q,p)-(q,p)\|\to 0$ as $n\to\infty$:

Let us consider the subset $\mathcal{K}\subseteq\mathcal{H}_t\times\mathcal{L}_t$, $\mathcal{K}=\{(q,p)\in\mathcal{H}_t\times\mathcal{L}_t:\|P_n(q,p)-(q,p)\|\to 0,n\to\infty\}$. It is enough to prove that the closure of $\mathcal{K}$ is $\mathcal{H}_t\times\mathcal{L}_t$. To prove this it is sufficient to show that $\mathcal{K}$

is a closed subspace of $\mathcal{H}_t \times \mathcal{L}_t$ and contains a dense subset of $\mathcal{H}_t \times \mathcal{L}_t$. This follows from the density of the piecewise linear paths in $\mathcal{H}_t$ and the density of the piecewise constant paths in $\mathcal{L}_t$ (see, e.g., Ref. 14).

Theorem 2: *Let the function* $(q,p) \to \psi_0(x+q(0))$, $\psi_0 \in \mathcal{S}(\mathbb{R}^d)$, *be Fresnel integrable with respect to A [with A defined by (12)]. Then the phase space Feynman path integral, namely the limit*

$$\lim_{n\to\infty} \widetilde{\int}_{P_n(\mathcal{H}_t \times \mathcal{L}_t)} e^{(i/2\hbar)\langle P_n(q,p), AP_n(q,p)\rangle} \psi_0(x+q(0)) \mathrm{d}P_n(q,p) \tag{14}$$

coincides with the limit (5), namely with the solution of the Schrödinger equation with a free Hamiltonian.

Proof: The result follows by direct computation, indeed:

$$\widetilde{\int}_{P_n(\mathcal{H}_t \times \mathcal{L}_t)} e^{(i/2\hbar)\langle P_n(q,p), AP_n(q,p)\rangle} \psi_0(x+q(0)) \mathrm{d}P_n(q,p)$$
$$= \left(\frac{1}{\sqrt{2\pi\hbar}} \right)^{2nd} \int_{\mathbb{R}^{2nd}} \exp\left(-\frac{i\epsilon}{\hbar} \sum_{j=0}^{n-1} \left(\frac{p_j^2}{2m} - p_j \frac{(x_{j+1}-x_j)}{\epsilon} \right) \right) \psi_0(x_0) \prod_{j=0}^{n-1} \mathrm{d}p_j \, \mathrm{d}x_j ,$$

and the two limits (5) and (14) coincide. Indeed (14) is a pointwise limit by hypothesis. On the other hand (5) is a limit in L_2 sense, hence, passing if necessary to a subsequence, it is also a pointwise limit.

Remark 1: The latter result is equivalent to the ''traditional'' formulation of the Feynman path integral in the configuration space. Indeed it can be obtained by means of Fubini theorem[2] and an integration with respect to the momentum variables:

$$\lim_{n\to\infty} \left(\frac{1}{\sqrt{2\pi\hbar}} \right)^{2nd} \int_{\mathbb{R}^{2nd}} \exp\left(-\frac{i\epsilon}{\hbar} \sum_{j=0}^{n-1} \left(\frac{p_j^2}{2m} - p_j \frac{(x_{j+1}-x_j)}{\epsilon} \right) \right) \psi_0(x_0) \prod_{j=0}^{n-1} \mathrm{d}p_j \, \mathrm{d}x_j$$
$$= \lim_{n\to\infty} \left(\frac{1}{\sqrt{2\pi i\hbar}} \right)^{nd} \int_{\mathbb{R}^{nd}} \exp\left(-\frac{i\epsilon}{\hbar} \sum_{j=0}^{n-1} m \frac{(x_{j+1}-x_j)^2}{2\epsilon^2} \right) \psi_0(x_0) \prod_{j=0}^{n-1} \mathrm{d}x_j .$$

The latter expression yields the Feynman functional on the configuration space, i.e., heuristically const $\int \exp(\int_0^t \mathcal{L}(q(s),\dot{q}(s))\mathrm{d}s)\mathrm{d}q$ ($\mathcal{L}$ being the classical Lagrangian density).

Remark 2: The integration with respect to the momentum variables might seem to be superfluous, but it is very useful when we introduce a potential depending on the momentum.

Theorem 3: *Let us consider a semibounded potential V depending explicitly on the momentum:* $V=V(p)$ *and the corresponding quantum mechanical Hamiltonian* $H=-(\hbar^2/2)\Delta+V(p)$. *Let us suppose H is an essentially self-adjoint operator on* $\mathcal{L}_2(\mathbb{R}^d)$. *Let the function* $(q,p) \to \exp(-(\mathrm{i}/\hbar)\int_0^t V(P_n(p(s)))\mathrm{d}s)\,\psi_0(x+q(0))$ *be Fresnel integrable with respect to the operator A, with A defined by* (12). *Then the solution to the Schrödinger equation*

$$\begin{cases} \dot{\psi} = -\dfrac{i}{\hbar} H\psi, \\ \psi(0,x) = \psi_0(x), \quad \psi_0 \in \mathcal{S}(\mathbb{R}^d) \end{cases} \tag{15}$$

is given by the phase space path integral

$$\lim_{n\to\infty}\widetilde{\int}_{P_n(\mathcal{H}_t\times\mathcal{L}_t)}\exp\left(\frac{i}{2\hbar}\langle P_n(q,p),AP_n(q,p)\rangle\right)\exp\left(-\frac{i}{\hbar}\int_0^t V(P_n(p(s)))\mathrm{d}s\right)$$
$$\times\psi_0(x+q(0))\mathrm{d}P_n(q,p).$$

Proof: We can proceed in a completely analogous way as in the proof of Theorem 2, therefore we shall omit the details. □

V. THE PHASE SPACE FEYNMAN–KAC FORMULA

Let us consider a classical potential V depending both on the position $Q\in\mathbb{R}^d$ and on the momentum $P\in\mathbb{R}^d$, but of the special form: $V=V(Q,P)=V_1(Q)+V_2(P)$ (The general case presents problems due to the noncommutativity of the quantized expression of Q and P), for a different approach with more general Hamiltonians see Ref. 16. Moreover let us suppose the function $f:\mathcal{H}_t\times\mathcal{L}_t\to\mathbb{C}$,

$$f(q,p)=\psi_0(x+q(0))\exp\left(-\frac{i}{\hbar}\int_0^t V(q(s)+x,p(s))\mathrm{d}s\right),\quad \psi_0\in\mathcal{S}(\mathbb{R}^d)$$

is the Fourier transform of a complex bounded variation measure μ_f on $\mathcal{H}_t\times\mathcal{L}_t$:[17]

$$f(q,p)=\int_{\mathcal{H}_t\times\mathcal{L}_t}e^{i\langle q,p;Q,P\rangle}\mathrm{d}\mu_f(Q,P).$$

Under additional assumptions on V_1 and V_2 we shall see that the phase space Feynman path integral of the function f can be computed and is given by

$$\widetilde{\int}_{\mathcal{H}_t\times\mathcal{L}_t}\exp\left(\frac{i}{2\hbar}\langle q,p;A(q,p)\rangle\right)\exp\left(-\frac{i}{\hbar}\int_0^t V(q(s)+x,p(s))\mathrm{d}s\right)\psi(0,q(0)+x)\mathrm{d}q\,\mathrm{d}p$$
$$=\int_{\mathcal{H}_t\times\mathcal{L}_t}\exp\left(\frac{-i\hbar}{2}\langle q,p;A^{-1}(q,p)\rangle\right)\mathrm{d}\mu_f(q,p).\tag{16}$$

This follows from Sec. III together with the following.

Lemma 2: Let us consider a potential $V(Q,P)=V_1(Q)+V_2(P)$ and an initial wave function ψ_0 such that V_1, $\psi_0\in\mathcal{F}(\mathbb{R}^d)$ and the function $p(s)_{s\in[0,t]}\to\int_0^t V_2(p(s))\mathrm{d}s\in\mathcal{F}(\mathcal{L}_t)$. Then the functional

$$f(q,p)=\psi_0(x+q(0))\exp\left(-\frac{i}{\hbar}\int_0^t V(q(s)+x,p(s))\mathrm{d}s\right)$$

belongs to $\mathcal{F}(\mathcal{H}_t\times\mathcal{L}_t)$.

Proof: $f(q,p)$ is the product of two functions: the first, say f_1, depends only on the first variable q, while the second f_2 depends only on the variable p, more precisely

$$f_1(q)=\psi_0(x+q(0))\exp\left(-\frac{i}{\hbar}\int_0^t V_1(q(s)+x)\mathrm{d}s\right),\quad f_2(p)=\exp\left(-\frac{i}{\hbar}\int_0^t V_2(p(s))\mathrm{d}s\right).$$

Under the given hypothesis on V_1 and ψ_0, f_1 belongs to $\mathcal{F}(\mathcal{H}_t)$. The proof is given for instance in Ref. 2. For f_2 one must pay more attention: indeed the same proof given for f_1 does not work, as f_2 is defined on a different Hilbert space and we have to require explicitly that $\int_0^t V_2(p(s))\mathrm{d}s\in\mathcal{F}(\mathcal{L}_t)$. Under this hypothesis one can easily prove that (see Ref. 2) $f_2\in\mathcal{F}(\mathcal{L}_t)$.

Now if $f_1=\hat{\mu}_{f_1}\in\mathcal{F}(\mathcal{H}_t)$, f_1 can be extended to a function, denoted again by f_1, in $\mathcal{F}(\mathcal{H}_t\times\mathcal{L}_t)$: it is the Fourier transform of the product measure on $\mathcal{H}_t\times\mathcal{L}_t$ of $\mu_{f_1}(\mathrm{d}q)$ and $\delta_0(\mathrm{d}p)$. The same holds for $f_2=\hat{\mu}_{f_2}$: $f_2=(\delta_0(\mathrm{d}q)\mu_{f_2}(\mathrm{d}p))$.

Finally, as $\mathcal{F}(\mathcal{H}_t\times\mathcal{L}_t)$ is a Banach algebra,[2] the product of two elements f_1f_2 is again an element of $\mathcal{F}(\mathcal{H}_t\times\mathcal{L}_t)$: more precisely it is the Fourier transform of the convolution of the two measures in $\mathcal{M}(\mathcal{H}_t\times\mathcal{L}_t)$ corresponding to f_1 and f_2, respectively., and the conclusion follows. The next theorem shows that the above oscillatory integral (16) gives the solution to the Schrödinger equation.

Theorem 4: *Let us consider the following Hamiltonian*

$$H(Q;P)=\frac{P^2}{2}+V_1(Q)+V_2(P)$$

in $L^2(\mathbb{R}^d)$ *and the corresponding Schrödinger equation*

$$\begin{cases}\dot{\psi}=-\dfrac{i}{\hbar}H\psi,\\ \psi(0,x)=\psi_0(x),\quad x\in\mathbb{R}^d.\end{cases}\tag{17}$$

Let us suppose that V_1, $\psi_0\in\mathcal{F}(\mathbb{R}^d)$ *and* $\int_0^t V_2(p(s))\mathrm{d}s\in\mathcal{F}(\mathcal{L}_t)$. *Then the solution to the Cauchy problem (17) is given by the phase space Feynman path integral:*

$$\widetilde{\int}_{\mathcal{H}_t\times\mathcal{L}_t}\exp\left(\frac{i}{2\hbar}\langle q,p;A(q,p)\rangle\right)\exp\left(-\frac{i}{\hbar}\int_0^t(V_1(q(s)+x)+V_2(p(s)))\mathrm{d}s\right)\psi(0,q(0)+x)\mathrm{d}q\,\mathrm{d}p.$$

Proof: We follow the proof given by Elworthy and Truman in Ref. 3.

For $0\leqslant u\leqslant t$ let $\mu_u(V_1,x)\equiv\mu_u$, $\nu_u^t(V_1,x)\equiv\nu_u^t$, $\eta_u^t(V_2)\equiv\eta_u^t$, and $\mu_0(\psi)$ be the measures on $\mathcal{H}_t\times\mathcal{L}_t$ whose Fourier transforms when evaluated at $(q,p)\in\mathcal{H}_t\times\mathcal{L}_t$ are

$$V_1(x+q(u)),\quad \exp\left(-i\int_u^t V_1(x+q(s))\mathrm{d}s\right),\quad \exp\left(-i\int_u^t V_2(p(s))\mathrm{d}s\right),\quad \psi_0(q(0)+x).$$

We set

$$U(t)\psi_0(x)=\widetilde{\int}_{\mathcal{H}_t\times\mathcal{L}_t}\exp\left(\frac{i}{2\hbar}\langle q,p;A(q,p)\rangle\right)\times\exp\left(-\frac{i}{\hbar}\int_0^t(V_1(q(s)+x)+V_2(p(s)))\mathrm{d}s\right)\psi(0,q(0)+x)\mathrm{d}q\,\mathrm{d}p$$

and

$$U_0(t)\psi_0(x)=\widetilde{\int}_{\mathcal{H}_t\times\mathcal{L}_t}\exp\left(\frac{i}{2\hbar}\langle q,p;A(q,p)\rangle\right)\times\exp\left(-\frac{i}{\hbar}\int_0^t V_2(p(s))\right)\mathrm{d}s\,\psi(0,q(0)+x)\mathrm{d}q\,\mathrm{d}p.$$

By Sec. III we have

$$U(t)\psi_0(x)=\int_{\mathcal{H}_t\times\mathcal{L}_t}e^{(-i\hbar/2)\langle q,p;A^{-1}(q,p)\rangle}(\eta_0^t*\nu_0^t*\mu_0(\psi))(\mathrm{d}q\,\mathrm{d}p).\tag{18}$$

Now, if $\{\mu_u:a\leqslant u\leqslant t\}$ is a family in $\mathcal{M}(\mathcal{H}_t\times\mathcal{L}_t)$, we shall let $\int_a^b\mu_u\,\mathrm{d}u$ denote the measure on $\mathcal{H}_t\times\mathcal{L}_t$ given by

$$f \to \int_a^b \int_{\mathcal{H}_t \times \mathcal{L}_t} f(q,p)\,\mathrm{d}\mu_u(q,p)\,\mathrm{d}u$$

whenever it exists.

Since for any continuous path q,

$$\exp\left(-i\int_0^t V_1(q(s))\mathrm{d}s\right) = 1 - i\int_0^t V_1(q(u))\exp\left(-i\int_u^t V_1(q(s))\mathrm{d}s\right)\mathrm{d}u,$$

the following relation holds:

$$\nu_0^t = \delta_0 - i\int_0^t (\mu_u * \nu_u^t)\mathrm{d}u, \tag{19}$$

where δ_0 is the Dirac measure at $0 \in \mathcal{H}_t$.

Applying this relation to (18) we obtain

$$\begin{aligned} U(t)\psi_0(x) &= \int_{\mathcal{H}_t \times \mathcal{L}_t} \exp\left(\frac{-i\hbar}{2}\langle q,p;A^{-1}(q,p)\rangle\right)(\eta_0^t * \mu_0(\psi))(\mathrm{d}q\,\mathrm{d}p) \\ &\quad - i\int_0^t \int_{\mathcal{H}_t \times \mathcal{L}_t} \exp\left(\frac{-i\hbar}{2}\langle q,p;A^{-1}(q,p)\rangle\right)(\eta_0^t * \mu_u(V_1,x) * \nu_u^t * \mu_0(\psi))(\mathrm{d}q\,\mathrm{d}p)\mathrm{d}u \\ &= U_0(t)\psi_0(x) - i\int_0^t \widetilde{\int}_{\mathcal{H}_t \times \mathcal{L}_t} \exp\left(\frac{i}{2\hbar}\langle q,p;A(q,p)\rangle\right)\exp\left(-\frac{i}{\hbar}\int_u^t V_1(q(s)+x)\mathrm{d}s\right) \\ &\quad \times \exp\left(-\frac{i}{\hbar}\int_0^t V_2(p(s))\right)\mathrm{d}s V_1(q(u)+x)\psi_0(q(0)+x)\mathrm{d}q\,\mathrm{d}p\,\mathrm{d}u. \end{aligned}$$

Now we have, by Fubini theorem for Fresnel integrals,[2]

$$\widetilde{\int}_{\mathcal{H}_t \times \mathcal{L}_t} \exp\left(\frac{i}{2\hbar}\langle q,p;A(q,p)\rangle\right)\exp\left(-\frac{i}{\hbar}\int_u^t V_1(q(s)+x)\mathrm{d}s\right)\exp\left(-\frac{i}{\hbar}\int_0^t V_2(p(s))\right)\mathrm{d}s.$$

$$\begin{aligned} &V_1(q(u)+x)\psi_0(q(0)+x)\mathrm{d}q\,\mathrm{d}p \\ &\quad = \widetilde{\int}_{\mathcal{H}_{t-u} \times \mathcal{L}_{t-u}} \exp\left(\frac{i}{2\hbar}\langle q,p;A(q,p)\rangle_{\mathcal{H}_{t-u} \times \mathcal{L}_{t-u}}\right) \\ &\qquad \times \exp\left(-\frac{i}{\hbar}\int_0^{t-u} V_1(q(s)+x)\mathrm{d}s\right)\left(\exp -\frac{i}{\hbar}\int_0^{t-u} V_2(p(s))\right) \\ &\qquad \times \mathrm{d}s V_1(q(0)+x)\widetilde{\int}_{\mathcal{H}_u \times \mathcal{L}_u} \exp\left(\frac{i}{2\hbar}\langle q_1,p_1;A(q_1,p_1)\rangle_{\mathcal{H}_u \times \mathcal{L}_u}\right) \\ &\qquad \times \exp\left(-\frac{i}{\hbar}\int_0^u V_2(p_1(s))\right)\mathrm{d}s\,\psi_0(q_1(0))\mathrm{d}q_1\mathrm{d}p_1\mathrm{d}q\,\mathrm{d}p p. \end{aligned}$$

Here $q \in \mathcal{H}_{t-u}$ and $q_1 \in \mathcal{H}_u$ are the integration variables, and $\mathcal{H}_s$ denotes the Cameron–Martin space of paths $\gamma:[0,s] \to \mathbb{R}^d$.

We have

$$U(t)\psi_0(x) = U_0(t)\psi_0(x) - i\int_0^t U(t-u)(V_1 U_0(u)\psi_0)(x)\mathrm{d}u$$

$$= U_0(t)\psi_0(x) - i\int_0^t U(u)(V_1 U_0(-u)U_0(t)\psi_0)(x)\mathrm{d}u.$$

The iterative solution of the latter integral equation is the convergent Dyson perturbation series for $U(t)$ with respect to $U_0(t)$, which proves the theorem. □

Remark: We have stated our results for $\psi_0 \in \mathcal{F}(\mathbb{R}^d)$. They can be extended by density to $L^2(\mathbb{R}^d)$.

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Multidimensional Schrödinger equations with Abelian potentials

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We consider two- and three-dimensional complex Schrödinger equations with Abelian potentials and a fixed energy level. The potential, wave function, and the spectral Bloch variety are calculated in terms of the Kleinian hyperelliptic functions associated with a genus two hyperelliptic curve. In the special case in two dimensions when the curve covers two elliptic curves, exactly solvable Schrödinger equations are constructed in terms of the elliptic functions of these curves. The solutions obtained are illustrated by a number of plots. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1470708]

I. INTRODUCTION

Modern physical technologies have led to the manufacture of new materials—films, superlattices, two-dimensional (2D) quantum dots arrays, etc., whose mathematical models are based on the 2D and 3D (three-dimensional) Schrödinger equation with periodic and quasiperiodic potentials. The recent discoveries of soliton theory, which involve the theory of Abelian functions, make it possible to construct exactly solvable Schrödinger equations with Abelian potentials. Progress in this area has been made by Novikov and co-workers since the middle of the 1970s (see, e.g., Ref. 1). In Ref. 2, the multidimensional spectral problem for the Schrödinger equation under the action of an external magnetic field was considered, and the corresponding Bloch solutions were constructed at specific values of the energy. The case of a real *pure potential* was solved in Refs. 3 and 4 for some special hyperelliptic curves which permit involution with two stable points, leading to Prym varieties.

The complex theory of the 2D Schrödinger equation with an Abelian potential was developed by Buchstaber and Enolskii[5] by differentiating the addition theorem for the Baker function of genus two; in this approach, the 2D Schrödinger equation appeared as a compatibility condition for the ansatz introduced in Ref. 5. The key ingredient of this technique is the use of the Weierstrass–Klein realization of the hyperelliptic functions, which is treated in the classical literature[6,7] and more recently developed in Ref. 8.

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The aim of the present paper is to develop the theory for 2D and 3D Schrödinger equations with an Abelian potential using, as the basic ingredient, the Baker function $\Phi(\mathbf{x};\boldsymbol{\alpha})$ of the hyperelliptic curve V of genus g,

$$\Phi_B(\mathbf{x};\boldsymbol{\alpha})=\frac{\sigma(\boldsymbol{\alpha}-\mathbf{x})}{\sigma(\boldsymbol{\alpha})\sigma(\mathbf{x})}\exp(\boldsymbol{\zeta}(\boldsymbol{\alpha})^T\mathbf{x}),$$

where the variable $\mathbf{x}$ and spectral variable $\boldsymbol{\alpha}$ belong to the Jacobi varieties of the underlying hyperelliptic curve, the σ-function is a generalization of the Weierstrass σ-function to higher genera, and $\zeta_i=\partial/\partial x_i \ln\sigma(\mathbf{x})$, $i=1,\ldots,g$ are hyperelliptic ζ-functions. We emphasize that the Baker function is defined on the product of Jacobians $\mathrm{Jac}(V)\times\mathrm{Jac}(V)$ in contrast to the Baker–Akhiezer function, which is defined on the product $V\times\mathrm{Jac}(V)$.

To explain the results, we first consider the n-dimensional Schrödinger equation

$$\left\{\sum_{k=1}^{n}\frac{\partial^2}{\partial x_k^2}-\mathcal{U}(\mathbf{x})\right\}\Psi(\mathbf{x};\boldsymbol{\alpha})=\lambda(\boldsymbol{\alpha})\Psi(\mathbf{x};\boldsymbol{\alpha}),\tag{1.1}$$

where *the potential* $\mathcal{U}(\mathbf{x})$ depends on the column vector $\mathbf{x}$ belonging to the n-dimensional complex space $\mathbb{C}^n$, $\Psi(\mathbf{x};\boldsymbol{\alpha})$ is *the wave function* depending both on $\mathbf{x}$ and *the spectral parameter*, which is a column vector $\boldsymbol{\alpha}\in\mathbb{C}^n$, and $\lambda(\boldsymbol{\alpha})$ is the *spectral function*. We assume that the functions introduced have the following periodicity properties with respect to the $2n$ n-dimensional vectors, which are columns of the $n\times 2n$ matrix $(2\omega,2\omega')$, where ω,ω' are $n\times n$-matrices given by

$$\mathcal{U}(\mathbf{x}+2\omega\mathbf{n}+2\omega'\mathbf{m})=\mathcal{U}(\mathbf{x}),\tag{1.2}$$

$$\Psi(\mathbf{x}+2\omega\mathbf{n}+2\omega'\mathbf{m};\boldsymbol{\alpha})=\xi_{\mathbf{n},\mathbf{m}}(\boldsymbol{\alpha})\Psi(\mathbf{x};\boldsymbol{\alpha}),\tag{1.3}$$

$$\Psi(\mathbf{x};\boldsymbol{\alpha}+2\omega\mathbf{n}+2\omega'\mathbf{m})=\Psi(\mathbf{x};\boldsymbol{\alpha}),\tag{1.4}$$

where $\mathbf{n}$, $\mathbf{m}$ are arbitrary integer column vectors, and the function $\xi_{\mathbf{n},\mathbf{m}}(\boldsymbol{\alpha})$ is *the Bloch factor*. The Bloch factor is assumed to be of the form

$$\xi_{\mathbf{n},\mathbf{m}}(\boldsymbol{\alpha})=\exp\{2\mathbf{k}^T(\boldsymbol{\alpha})(\omega\mathbf{n}+\omega'\mathbf{m})\},\tag{1.5}$$

and the *quasimomentum* $\mathbf{k}(\boldsymbol{\alpha})$ is identified with the eigenvalue of the translation operator on the lattice.

Equations (1.3) and (1.5) represent a natural generalization of the usual Bloch theorem to the case of Abelian potentials. Indeed, after expressing the spectral parameter in terms of the quasimomentum and considering translations in the crystal lattice by a vector of the form $2\omega\mathbf{n}$, with $2\omega=(2\omega_{i,j})_{i,j=1,\ldots,n}$ being the $n\times n$ period matrix, we have from (1.3)

$$\Psi(\mathbf{x}+2\omega\mathbf{n};\mathbf{k})=\mathrm{e}^{2\mathbf{k}^T\omega\mathbf{n}}\Psi(\mathbf{x};\mathbf{k}).\tag{1.6}$$

Similarly, with respect to points of the reciprocal lattice, (1.4) gives

$$\Psi(\mathbf{x};\mathbf{k}+2\tilde{\omega}\mathbf{n})=\Psi(\mathbf{x};\mathbf{k}),\tag{1.7}$$

where $2\tilde{\omega}\mathbf{n}$ is a *reciprocal period*, which is represented as a column of the $n\times n$ *reciprocal period matrix* $2\tilde{\omega}$, which will be shown later to be equal to $i\pi(\omega)^{-1}$.

These properties mean that the Schrödinger equation is considered on the product of tori $T\times T$, $T=\mathbb{C}^n/2\omega\oplus 2\omega'$, which we assume to be generated by a hyperelliptic curve V and therefore T is the Jacobian $\mathrm{Jac}(V)$ of the curve. Since the potential has the periodicity property (1.2), it is an *Abelian function*, as is the corresponding spectral function.

In this case, the periods 2ω and $2\omega'$ are generated by the holomorphic integrals over cycles of the curve V, and it is always possible to fix the parameters of the curve in such a way that the period matrix 2ω is real and the period matrix $2\omega'$ is pure imaginary.

From the physical viewpoint, it is natural to consider the potential and the wave functions as functions of the argument $\imath\mathbf{x}+\mathbf{\Omega}$, where $\mathbf{\Omega}$ is a real half period. Then the potential $\mathcal{U}(\imath\mathbf{x}+\mathbf{\Omega})$ is periodic with respect to the period lattice $2\imath\omega'$ and is smooth and real at real $\mathbf{x}$, and the wave function $\Psi(\imath\mathbf{x}+\mathbf{\Omega};\boldsymbol{\alpha}+\mathbf{\Omega}')$, where $\mathbf{\Omega}'$ is a pure imaginary period, satisfy the periodicity property (1.6)

$$\Psi(\imath\mathbf{x}+\mathbf{\Omega}+2\omega'\mathbf{n};\mathbf{k}(\boldsymbol{\alpha}))=\mathrm{e}^{2\imath\mathbf{k}^T(\boldsymbol{\alpha})\mathrm{Im}(\omega')\mathbf{n}}\Psi(\imath\mathbf{x}+\mathbf{\Omega};\mathbf{k}(\boldsymbol{\alpha})), \tag{1.8}$$

with real quasimomentum $\mathbf{k}(\boldsymbol{\alpha})$.

In this context, we shall call this periodicity property of the wave function the *Bloch property*. The subvariety $\mathcal{B}\subset\mathrm{Jac}(V)$ for which the spectral problem (1.1) can be solved is called the *Bloch variety*.

The Bloch variety, when parametrized in terms of the quasimomentum $\mathbf{k}$, and restricted to a fixed value of the *energy* $\mathcal{E}=\lambda(\boldsymbol{\alpha})=\mathrm{const}$, is called a *Fermi variety*, denoted by $\mathcal{F}$. If the Schrödinger equation permits solutions *only* at a fixed energy level, which is independent of the spectral parameter $\boldsymbol{\alpha}$, then the Bloch variety and the Fermi variety are isomorphic, but generally speaking $\dim\mathcal{B}\geqslant\dim\mathcal{F}$. The Fermi variety is a *Fermi surface* in the case $\dim\mathcal{F}=2$ (this situation is usually realized at $n=3$) and a *Fermi curve* in the case when $\dim\mathcal{F}=1$. In the theory of the electronic structure of metals, most interest lies in those exactly solvable Schrödinger equations which admit nontrivial Fermi varieties.

In what follows we shall interpret all these quantities for the case of 2D and three-dimensional (3D) Schrödinger equations in terms of Abelian functions of genus two and genus three hyperelliptic curves.

We would like to emphasize that the known methods of derivation of exact solutions of multidimensional Schrödinger equations suppose the separability of the potential, i.e., in 2D, $\mathcal{U}(\mathbf{x})=\alpha\wp(x_1)\wp(x_2)$, where the $\wp(x_i)$ are the Weierstrass elliptic functions, and $\alpha=$ const. In this case the lattice structure is necessarily rectangular(cubic) in 2D(3D). The nonseparable potentials which we are considering enable us to investigate more general lattice symmetries, with a greater range of physical applications.

The paper is organized as follows. In Sec. II we consider the well-known case of the one-dimensional (1D) Schrödinger equation with elliptic Lamé potentials. In Sec. III we introduce a suitable generalization of the Kleinian function to higher genera and present a natural extension of the theory of the one-gap Lamé potential to higher dimensions. The results of this section will not be restricted to two dimensions but will be valid also in the 3D case. In Sec. IV we apply the general results of Sec. III to the 2D case, by deriving the explicit form of a certain family of Abelian potentials for which the 2D Schrödinger equation is exactly solvable. A set of figures for the potential profiles, showing that they are periodic, real and nonsingular, and therefore suitable for physical applications, is also given. The corresponding eigenvalues and eigenfunctions are also explicitly displayed. Section V is devoted to the case of reduction of the 2D Abelian potential and associated eigenfunction to elliptic functions. To do this we use the general results of Sec. III together with the explicit formulas for the deformation of the two-gap Lamé potential under the action of the Korteweg–de Vries (KdV) flow and the three-particle dynamics over the locus, to derive exactly solvable 2D Schrödinger equations with elliptic potentials. Finally, in Sec. VI we will consider the extension of the theory to the 3D case.

II. THE 1D SCHRÖDINGER EQUATION WITH ELLIPTIC POTENTIALS

One of the main problems in condensed matter physics is the construction of solutions of the Schrödinger equation with real and nonsingular periodic or quasiperiodic potentials. Except in very few cases, this problem is in general not solvable without resorting to approximations.

One of the few cases for which exact solutions are known is provided by the remarkable example of the one-dimensional *Lamé equation* with an elliptic potential (here and in the following we follow the standard notation of the theory of elliptic functions fixed in Ref. 9),

$$\left\{\frac{d^2}{dx^2}-\mathcal{U}(x)\right\}\Psi(x;\alpha)=\wp(\alpha)\Psi(x;\alpha), \tag{2.1}$$

$$\mathcal{U}(x)=2\wp(x), \quad \Psi(x;\alpha)=\Phi_W(x;\alpha)=\frac{\sigma(\alpha-x)}{\sigma(\alpha)\sigma(x)}\exp\{\zeta(\alpha)x\}. \tag{2.2}$$

Since in the following sections we will consider the generalization of this classical case to higher dimensions, we shall briefly review it here.

We recall that the Weierstrass functions $\wp,\zeta$ are given as logarithmic derivatives of the σ-function,

$$\wp(x)=-\frac{d^2}{dx^2}\ln\sigma(x), \quad \zeta(x)=\frac{d}{dx}\ln\sigma(x).$$

The σ-function, which is the generating function for the whole theory, is constructed from the elliptic curve

$$w^2=4z^3-g_2z-g_3\equiv 4(z-e_1)(z-e_2)(z-e_3) \tag{2.3}$$

equipped with a canonical basis of cycles $\mathfrak{a}$, $\mathfrak{b}$ as follows. The holomorphic differential and the associated meromorphic differential of the second kind are given, respectively, by dz/w and $z\,dz/w$. Their $\mathfrak{a}$ and $\mathfrak{b}$ periods

$$2\omega=\oint_{\mathfrak{a}}\frac{dz}{w}, \quad 2\omega'=\oint_{\mathfrak{b}}\frac{dz}{w}, \tag{2.4}$$

$$2\eta=-\oint_{\mathfrak{a}}\frac{z\,dz}{w}, \quad 2\eta'=-\oint_{\mathfrak{b}}\frac{z\,dz}{w} \tag{2.5}$$

satisfy the *Legendre relation*

$$\eta\omega'-\omega\eta'=\frac{\imath\pi}{2}. \tag{2.6}$$

The Weierstrass σ-function has the form

$$\sigma(x)=\sqrt{\frac{\pi}{\omega}}\frac{1}{\sqrt[8]{\Delta}}\exp\left(\frac{\eta x^2}{2\omega}\right)\vartheta_1\left(\frac{x}{2\omega}\middle|\tau\right), \tag{2.7}$$

where ϑ_1 is the Jacobian θ-function, $\tau=\omega'/\omega$, and $\Delta=16(e_2-e_3)^2(e_3-e_1)^2(e_1-e_2)^2$. This σ-function can be also be represented as the power series

$$\sigma(x)=x-\frac{g_2x^5}{2^4\cdot 3\cdot 5}+\frac{g_3x^7}{2^3\cdot 3\cdot 5\cdot 7}+\cdots$$

with coefficients connected by a recursion relation first found by Weierstrass[10] and documented in Ref. 11 (see also Ref. 12). The Weierstrass σ-function has the periodicity property

$$\sigma(x+2n\omega+2m\omega)=(-1)^{n+m+mn}\exp\{2(n\eta+m\eta')(x+n\omega+m\omega')\}\sigma(x), \tag{2.8}$$

which leads to the following expression for the Bloch factor:

$$\xi_i(\alpha)=\exp(2\omega_i\zeta(\alpha)-2\alpha\eta_i),\quad i=1,2,3. \tag{2.9}$$

The functions $\xi_i(\alpha)$ are elliptic functions with periods $2\omega,2\omega'$, because of the Legendre relation.

To give the physical interpretation of the above-mentioned formulas we shall fix the potential and the wave function as follows:

$$\mathcal{U}(x)=2\wp(\imath x+\omega),\quad \Psi(x;\alpha)=\Phi_W(\imath x+\omega;\alpha+\omega'),\quad x,\alpha\in\mathbb{R}. \tag{2.10}$$

The potential has the real period $-2\imath\omega'$. The associated quasimomentum is given by

$$k(\alpha)=\zeta(\alpha+\omega')-\frac{\eta'}{\omega'}(\alpha+\omega'),\quad \alpha\in\mathbb{R}. \tag{2.11}$$

The wave function, considered as a function of k instead of α, has the periodicity property (1.7) with the reciprocal period

$$2\tilde{\omega}=\frac{\imath\pi}{\omega'}.$$

The Bloch variety $\mathcal{B}$ is the Jacobian of the elliptic curve, which is isomorphic in this case to the elliptic curve itself.

We remark here that the one-dimensional finite-gap potentials appear to be important in applications. For example, Belokolos proved in 1980[13] that the exact solution of the famous Peierls problem is a finite-gap potential.

The simplest generalization of (2.1) to the n-dimensional case can be obtained if we consider the separable potential

$$\mathcal{U}(\mathbf{x})=2\sum_{k=1}^{n}\wp(\imath x_k+\omega^{(k)};2\omega^{(k)},2\omega^{(k)'}),$$

where $\wp(\cdot;2\omega^{(k)},2\omega^{(k)'})$ are Weierstrass elliptic functions with periods $2\omega^{(k)}$ and $2\omega^{(k)'}$. The energy $\mathcal{E}$ and components of the quasimomenta $\mathbf{k}$ are then

$$\mathcal{E}=\sum_{k=1}^{n}\wp(\alpha_k+\omega^{(k)'};2\omega^{(k)},2\omega^{(k)'}),$$

$$k_j(\alpha_j)=\zeta(\alpha_j)-\frac{\eta^{(j)'}}{\omega^{(j)'}}\alpha_j,\quad j=1,\ldots,n.$$

The wave function is given in this case as a product of the functions Φ_W.

In the case $n=3$ such potentials lead to nontrivial and sometimes very interesting Fermi surfaces. For example, Baryakhtar *et al.*[14] have used separable potentials to successfully calculate the electron energy of metals and high-temperature superconductors, and Belokolos and Korostil[15] have studied the electron–phonon interaction function.

Moreover, a general theory for the Schrödinger equations with separable multidimensional Lamé potentials with an arbitrary number of gaps in the spectrum was recently developed in Ref. 16. This approach was shown to be effective for the exact computation of the energy bands and Fermi surfaces of 2D lattices with square or rectangular symmetry. The extension of these results, however, to lattices with more general spatial symmetries seems problematic in the context of separable multidimensional Lamé potentials.

We shall develop in the following another generalization, which leads to a nonseparable potential. Namely we shall show that the Lamé equation (2.1) can be generalized to higher dimensions within the Weierstrass–Klein generalization of Weierstrass elliptic function theory to higher genera, following Refs. 6 and 7 and also Refs. 17 and 8. This generalization enables us to treat more general symmetries than the separable case.

III. MULTIDIMENSIONAL SCHRÖDINGER EQUATIONS AS GENERALIZED LAMÉ EQUATIONS OF HIGHER GENERA

To develop the theory of the multidimensional Schrödinger equation we need a suitable generalization of the *fundamental σ-function* of the hyperelliptic curve $V=V(w,z)$ of genus g,

$$w^2=4\prod_{i=1}^{2g+1}(z-e_i)\equiv 4z^{2g+1}+\sum_{i=0}^{2g}\lambda_i z^i \tag{3.1}$$

by the following formula, which is analogous to that in the elliptic case

$$\sigma(\mathbf{x})=\sqrt{\frac{\pi^g}{\det 2\omega}}\frac{1}{\sqrt[4]{\Pi_{i\neq j}(e_i-e_j)}}\exp\{\mathbf{x}^T\varkappa\mathbf{x}\}\,\theta[\varepsilon]((2\omega)^{-1}\mathbf{x}|\tau). \tag{3.2}$$

The entries to (3.2) are as follows $\theta[\varepsilon](\mathbf{v}|\tau)$ is the standard multidimensional theta function with characteristic

$$\theta[\varepsilon](\mathbf{v}|\tau)=\sum_{\mathbf{m}\in\mathbb{Z}^g}\exp\{\pi\imath(\mathbf{m}+\boldsymbol{\varepsilon}')^T\tau(\mathbf{m}+\boldsymbol{\varepsilon}')+2\pi\imath(\mathbf{m}+\boldsymbol{\varepsilon}')^T(\mathbf{v}+\boldsymbol{\varepsilon})\}; \tag{3.3}$$

$$[\varepsilon]=\begin{bmatrix}\boldsymbol{\varepsilon}'^T\\ \boldsymbol{\varepsilon}^T\end{bmatrix}=\begin{bmatrix}\varepsilon_1' & \dots & \varepsilon_g'\\ \varepsilon_1 & \dots & \varepsilon_g\end{bmatrix}$$

is the necessarily half integer characteristic of the vector of Riemann constants whose base point is chosen as (∞,∞). The matrix

$$\varkappa=\eta(2\omega)^{-1} \tag{3.4}$$

is the symmetric matrix which generalizes the factor $\eta/2\omega$ in the exponential (2.7) to the higher genera. The $2g\times 2g$ period matrix, $\left(\begin{smallmatrix}\omega & \omega'\\ \eta & \eta'\end{smallmatrix}\right)$ satisfies the generalized Legendre relation

$$\begin{pmatrix}\omega & \omega'\\ \eta & \eta'\end{pmatrix}\begin{pmatrix}0 & -1_g\\ 1_g & 0\end{pmatrix}\begin{pmatrix}\omega & \omega'\\ \eta & \eta'\end{pmatrix}^T\begin{pmatrix}0 & -1_g\\ 1_g & 0\end{pmatrix}=-\frac{\imath\pi}{2}, \tag{3.5}$$

where the $g\times g$ period matrices $2\omega,2\omega',2\eta,2\eta'$ are

$$2\omega=\left(\oint_{\mathfrak{a}_i}\mathrm{d}u_j\right)_{i,j=1,\dots,g},\quad 2\omega'=\left(\oint_{\mathfrak{b}_i}\mathrm{d}u_j\right)_{i,j=1,\dots,g},$$

$$2\eta=\left(-\oint_{\mathfrak{a}_i}\mathrm{d}r_j\right)_{i,j=1,\dots,g},\quad 2\eta'=\left(-\oint_{\mathfrak{b}_i}\mathrm{d}r_j\right)_{i,j=1,\dots,g}.$$

Here the $\mathrm{d}u_i$ are the holomorphic differentials

$$\mathrm{d}\mathbf{u}^T=(\mathrm{d}u_1,\dots,\mathrm{d}u_g),\quad \mathrm{d}u_k=\frac{z^{k-1}\mathrm{d}z}{w}, \tag{3.6}$$

and the dr_i are the differentials of the second kind with a pole at infinity

$$\begin{gathered} d\mathbf{r}^T=(dr_1,\ldots,dr_g),\\ dr_j=\sum_{k=j}^{2g+1-j}(k+1-j)\lambda_{k+1+j}\frac{z^k dz}{4w},\quad j=1,\ldots,g. \end{gathered} \tag{3.7}$$

The Kleinian σ-function has the following periodicity property:

$$\sigma(\mathbf{x}+2\boldsymbol{\Omega}(\mathbf{n},\mathbf{m}))=\exp\{2\mathbf{E}^T(\mathbf{n},\mathbf{m})(\mathbf{x}+\boldsymbol{\Omega}(\mathbf{n},\mathbf{m}))\}\exp\{-\imath\pi\mathbf{n}^T\mathbf{m}-2\imath\pi\boldsymbol{\varepsilon}^T\mathbf{m}\}\sigma(\mathbf{x}), \tag{3.8}$$

where $\mathbf{E}(\mathbf{n},\mathbf{m})=\eta\mathbf{n}+\eta'\mathbf{m}$, $\boldsymbol{\Omega}(\mathbf{n},\mathbf{m})=\omega\mathbf{n}+\omega'\mathbf{m}$, $\mathbf{n},\mathbf{m}\in\mathbb{Z}^g$ and $\boldsymbol{\varepsilon}^T$ is the lower line of the characteristic of the vector of the Riemann constant. The Kleinian ζ- and $\wp$-functions are introduced through logarithmic derivatives of the Kleinian σ-function,

$$\zeta_i(\mathbf{x})=\frac{\partial\ln\sigma(\mathbf{x})}{\partial x_i},\quad \wp_{i,j}(\mathbf{x})=-\frac{\partial^2\ln\sigma(\mathbf{x})}{\partial x_i\partial x_j},$$

$$\wp_{i,j,k}(\mathbf{x})=-\frac{\partial^3\ln\sigma(\mathbf{x})}{\partial x_i\partial x_j\partial x_k},\quad i,j,k=1,\ldots,g,\ \text{etc.}$$

We will omit commas between indices when the resulting formula is unambiguous.

The Abel map $\mathfrak{A}:(V)^g\to\mathrm{Jac}(V)$ of the symmetrized product $V\times\cdots\times V$ to the Jacobi variety $\mathrm{Jac}(V)=\mathbb{C}^g/2\omega\oplus 2\omega'$ of the curve V is defined by

$$\sum_{k=1}^{g}\int_{(\infty,\infty)}^{(w_k,z_k)}d\mathbf{u}=\mathbf{x}. \tag{3.9}$$

The Kummer variety is defined as the factor $\mathrm{Kum}(V)=\mathrm{Jac}(V)/\mathbf{x}\to-\mathbf{x}$ by the involution $\mathbf{x}\to-\mathbf{x}$.

The principal results of the theory of the hyperelliptic Kleinian can be formulated using the $(g+2)\times(g+2)$-matrix

$$\begin{aligned} H=\{h_{i,k}\}_{i,k=1,\ldots,g+2},\quad h_{ik}&=4\wp_{i-1,k-1}-2\wp_{k,i-2}-2\wp_{i,k-2}+\tfrac{1}{2}(\delta_{i,k}(\lambda_{2i-2}+\lambda_{2k-2})\\ &+\delta_{k,i+1}\lambda_{2i-1}+\delta_{i,k+1}\lambda_{2k-1}). \end{aligned} \tag{3.10}$$

We denote the minors of the matrix H as follows:

$$H\left[\begin{smallmatrix}k_1&\cdots&k_n\\ j_1&\cdots&j_m\end{smallmatrix}\right]\{h_{i_k,j_l}\}_{k=1,\ldots,m;l=1,\ldots,n}.$$

Theorem 3.1 (Ref. 7): *The matrix H has the following properties*

(1) Let $(w_1,z_1),\ldots,(w_g,z_g)$ be a divisor and $\mathbf{Z}=(1,z,\ldots,z^{g+1})^T$, then for arbitrary vectors

$$w_r w_s=\mathbf{Z}_r^T H\mathbf{Z}_s,$$

and in particular

$$\mathbf{Z}^T H\mathbf{Z}=\sum_{i=0}^{2g+2}\lambda_i z^i.$$

(2) Let $(w_1,z_1),\ldots,(w_g,z_g)$ be the divisor, then the vectors $\mathbf{Z}=(1,z_r,\ldots,z_r^{g+1})^T$, $r=1,\ldots,g$ are orthogonal to the last column of the matrix H or equivalently the z_r are the roots of

$$z^g-\wp_{gg}(\mathbf{x})z^{g-1}-\ldots-\wp_{1g}(\mathbf{x})=0, \tag{3.11}$$

which yields the solution of the Jacobi inversion problem, where the second coordinate of the divisor is defined as follows:

$$w_k = -\sum_{j=1}^{g} \wp_{jgg}(\mathbf{x}) z_k^{g-j}. \tag{3.12}$$

(3) Rank $H=3$ *at generic points and*

$$-\frac{1}{4}\wp_{igg}\wp_{kgg} = \det H\begin{bmatrix} k & g+1 & g+2 \\ i & g+1 & g+2 \end{bmatrix}, \quad \forall i,k=1,\ldots,g. \tag{3.13}$$

The intersection of the $g(g+1)/2$ *cubics defines the Jacobi variety as an algebraic variety in* $\mathbb{C}^{g+(1/2)g(g+1)}$.

(4) The intersection of the $g(g-1)/2$ *quartics*

$$\det H\begin{bmatrix} k & l & g+1 & g+2 \\ i & j & g+1 & g+2 \end{bmatrix} = 0, \quad \forall i \neq j, k \neq l = 1,\ldots,g \tag{3.14}$$

defines the Kummer variety as an algebraic variety in $\mathbb{C}^{(1/2)g(g+1)}$.

(5) The following equality holds:

$$\mathbf{R}^T \boldsymbol{\pi}_{jl} \boldsymbol{\pi}_{ik}^T \mathbf{S} = \frac{1}{4}\det\begin{pmatrix} H\begin{bmatrix} i & k & g+1 & g+2 \\ j & l & g+1 & g+2 \end{bmatrix} & \mathbf{S} \\ \mathbf{R}^T & 0 \end{pmatrix}, \tag{3.15}$$

where $\mathbf{R}$, $\mathbf{S} \in \mathbb{C}^4$ *are arbitrary vectors and*

$$\boldsymbol{\pi}_{ik} = \begin{pmatrix} -\wp_{ggk} \\ \wp_{ggi} \\ \wp_{g,i,k-1} - \wp_{g,i-1,k} \\ \wp_{g-1,i,k-1} - \wp_{g-1,k,i-1} + \wp_{g,k,i-2} - \wp_{g,i,k-2} \end{pmatrix}.$$

On the basis of the above-mentioned relations, we shall construct the linear differential operators for which the spectral variety will be defined in $\mathrm{Jac}(V)$. Following Baker (see Ref. 6, p. 421) we define a function on $\mathrm{Jac}(V)\times\mathrm{Jac}(V)$.

Definition 3.1: The standard Baker function Φ_B of the curve V is the function on the product $\mathrm{Jac}(V)\times\mathrm{Jac}(V)$, and is defined as follows:

$$\Phi_B : \mathrm{Jac}(V)\times \mathrm{Jac}V \to \mathbb{C},$$

$$\Phi_B(\mathbf{x};\boldsymbol{\alpha}) = \frac{\sigma(\boldsymbol{\alpha}-\mathbf{x})}{\sigma(\boldsymbol{\alpha})\sigma(\mathbf{x})}\exp(\boldsymbol{\zeta}^T(\boldsymbol{\alpha})\mathbf{x}),$$

where $\boldsymbol{\zeta}^T(\boldsymbol{\alpha}) = (\zeta_1(\boldsymbol{\alpha}),\ldots,\zeta_g(\boldsymbol{\alpha}))$, and

$$\mathbf{x} = \sum_{k=1}^{g} \int_{(\infty,\infty)}^{(w_k,z_k)} \mathrm{d}\mathbf{u}, \quad \boldsymbol{\alpha} = \sum_{k=1}^{g} \int_{(\infty,\infty)}^{(\nu_k,\mu_k)} \mathrm{d}\mathbf{u} \in \mathrm{Jac}(V),$$

where $((w_1,z_1),\ldots,(w_g,z_g))$ and $((\nu_1,\mu_1),\ldots,(\nu_g,\mu_g))$ are nonspecial divisors on V. The Φ_B-function is meromorphic in $\mathbf{x}$ and has the periodicity property (1.3) with the Bloch factor

$$\xi_{\mathbf{n},\mathbf{m}}(\alpha) = \exp\{2\boldsymbol{\zeta}^T(\boldsymbol{\alpha})\boldsymbol{\Omega}(\mathbf{n},\mathbf{m}) - 2\mathbf{E}^T(\mathbf{n},\mathbf{m})\boldsymbol{\alpha}\}, \quad i=1,\ldots,g, \tag{3.16}$$

where $\mathbf{\Omega}(\mathbf{n},\mathbf{m})=\omega\mathbf{n}+\omega'\mathbf{m}$, $\mathbf{E}(\mathbf{n},\mathbf{m})=\eta\mathbf{n}+\eta'\mathbf{m}$, $\mathbf{n},\mathbf{m}\in\mathbb{Z}^g$ are arbitrary integer vectors. We shall call the Baker function any function which is meromorphic on $\mathrm{Jac}(V)\times\mathrm{Jac}(V)$ and has the periodicity property (1.3) with the Bloch factors (3.16). Evidently in the case of genus one $\Phi_W \equiv \Phi_B$.

We remark that the spectral variety of the standard Baker function is the Jacobi variety of the curve, in contrast with the *Baker–Akhiezer function*, whose spectral parameter is evaluated on the curve. In our notation, the Baker–Akhiezer function is $\Phi_{\mathrm{BA}}(\mathbf{u};(\mu,\nu))$, which is given by (see Ref. 18)

$$\Phi_{\mathrm{BA}}(\mathbf{x};(\mu,\nu))=\frac{\sigma(\int_{(\nu_0,\mu_0)}^{(\nu,\mu)}\mathrm{d}\mathbf{u}-\mathbf{x})}{\sigma(\mathbf{x})}\exp\left(\int_{(\nu_0,\mu_0)}^{(\nu,\mu)}\mathrm{d}\mathbf{r}^T\mathbf{x}\right),$$

where $(\nu,\mu)\in V$, and $\mathbf{x}\in\mathrm{Jac}(V)$. The function Φ_{BA} solves the one-dimensional Schrödinger equation with the potential $2\wp_{gg}$,

$$(\partial_g^2-2\wp_{gg})\Phi_{\mathrm{BA}}=\left(z+\frac{\lambda_{2g}}{4}\right)\Phi_{\mathrm{BA}}, \tag{3.17}$$

with respect to u_g for all $(\nu,\mu)\in V$.

Let us fix as the period lattice the matrix of real periods 2ω. In analogy with the case of genus one, the Bloch factor (3.16) of the standard Baker function can be written as

$$\begin{gathered}\xi_{\mathbf{n}}(\boldsymbol{\alpha})=\exp\{2\mathbf{k}^T(\boldsymbol{\alpha})\omega\mathbf{n}\},\\ \mathbf{k}(\boldsymbol{\alpha})=\boldsymbol{\zeta}(\boldsymbol{\alpha}+\mathbf{\Omega}')-2\varkappa(\boldsymbol{\alpha}+\mathbf{\Omega}'),\end{gathered} \tag{3.18}$$

where $\mathbf{\Omega}'$ is an imaginary half period.

To prove the last formula we take into account the definition and the symmetry property of the matrix $\varkappa$. We have

$$(\eta\mathbf{n})^T\boldsymbol{\beta}=(\varkappa(2\omega)\mathbf{n})^T\boldsymbol{\beta}=2\boldsymbol{\beta}^T\varkappa\omega\mathbf{n}.$$

The Bloch factor is an Abelian function, whose periodicity properties are provided by the periodicity property of the ζ-function and the generalized Legendre relation (3.5).

We shall prove the following

Proposition 3.2: Let V be a hyperelliptic curve of genus $g<4$. Then the $g+1+\frac{1}{2}g(g+1)$ Baker functions on $\mathrm{Jac(V)}\times\mathrm{Jac}(V)$ are

$$\begin{gathered}F_0(\mathbf{x};\boldsymbol{\alpha})=\Phi_B(\mathbf{x};\boldsymbol{\alpha}),\\ F_i(\mathbf{x};\boldsymbol{\alpha})=\frac{\partial}{\partial x_i}\Phi_B(\mathbf{x};\boldsymbol{\alpha}),\quad i=1,\ldots,g,\\ F_{ij}(\mathbf{x};\boldsymbol{\alpha})=\left\{\frac{\partial^2}{\partial x_i\partial x_j}-2\wp_{ij}(\mathbf{x})\right\}\Phi_B(\mathbf{x};\boldsymbol{\alpha}),\quad i\leqslant j=1,\ldots,g,\end{gathered} \tag{3.19}$$

where $\Phi_B(\mathbf{x};\boldsymbol{\alpha})$ is the standard Baker function of the curve. These functions, regarded as functions of $\mathbf{x}$, are linearly dependent, i.e., there exists at least one relation between them of the form

$$c_0(\boldsymbol{\alpha})F_0(\mathbf{x};\boldsymbol{\alpha})+\sum_{i=1}^{g}c_i(\boldsymbol{\alpha})F_i(\mathbf{x};\boldsymbol{\alpha})+\sum_{i\leqslant j=1,\ldots,g}c_{ij}(\boldsymbol{\alpha})F_{ij}(\mathbf{x};\boldsymbol{\alpha})=0, \tag{3.20}$$

where not all functions in $\boldsymbol{\alpha}$: $c_0(\boldsymbol{\alpha}),c_i(\boldsymbol{\alpha}),c_{ij}(\boldsymbol{\alpha})$ are equal to zero.

Proof: We shall prove the statement for $g=2$ and $g=3$. Let us write the standard addition theorem of the second-order θ-functions,

$$\theta\begin{bmatrix}\boldsymbol{\varepsilon}'^T\\ \boldsymbol{\varepsilon}^T+\boldsymbol{\gamma}^T\end{bmatrix}(\mathbf{v}+\mathbf{u}|\tau)\,\theta\begin{bmatrix}\boldsymbol{\varepsilon}'^T\\ \boldsymbol{\varepsilon}^T\end{bmatrix}(\mathbf{v}-\mathbf{u}|\tau)=\sum_{2\boldsymbol{\delta}\in(\mathbb{Z}/2\mathbb{Z})^g}(-1)^{4\boldsymbol{\varepsilon}^T\boldsymbol{\delta}}\theta\begin{bmatrix}\boldsymbol{\delta}^T\\ \boldsymbol{\gamma}^T\end{bmatrix}(2\mathbf{v}|2\tau)\,\theta\begin{bmatrix}\boldsymbol{\varepsilon}'^T+\boldsymbol{\delta}^T\\ \boldsymbol{\gamma}^T\end{bmatrix}(2\mathbf{u}|2\tau).$$

Now set $\mathbf{u}=0$ and $\boldsymbol{\gamma}=\mathbf{0}$,

$$\theta^2\begin{bmatrix}\boldsymbol{\varepsilon}'^T\\ \boldsymbol{\varepsilon}^T\end{bmatrix}(\mathbf{v}|\tau)=\sum_{2\boldsymbol{\delta}\in(\mathbb{Z}/2\mathbb{Z})^g}(-1)^{4\boldsymbol{\varepsilon}^T\boldsymbol{\delta}^T}\theta\begin{bmatrix}\boldsymbol{\delta}^T\\ \mathbf{0}^T\end{bmatrix}(2\mathbf{v}|2\tau)\,\theta\begin{bmatrix}\boldsymbol{\varepsilon}'^T+\boldsymbol{\delta}^T\\ \mathbf{0}^T\end{bmatrix}(\mathbf{0}|2\tau),\tag{3.21}$$

where $\boldsymbol{\delta}^T=(\delta_1,\ldots,\delta_g)$ with $2\delta_i=1$ or 0, $i=1,\ldots,g$. We multiply both sides of (3.21) by the factor $\exp\{2\mathbf{u}^T\varkappa\mathbf{u}\}$, where $\mathbf{v}=(2\omega)^{-1}\mathbf{u}$ and the matrix $\varkappa$ is given in the definition of the fundamental σ-function. One can see that the entire functions

$$\begin{aligned}\psi\begin{bmatrix}\boldsymbol{\varepsilon}'^T\\ \boldsymbol{\varepsilon}^T\end{bmatrix}(\mathbf{v}|\tau)&=\exp\{2\mathbf{u}^T\varkappa\mathbf{u}\}\,\theta^2\begin{bmatrix}\boldsymbol{\varepsilon}'^T\\ \boldsymbol{\varepsilon}^T\end{bmatrix}(\mathbf{v}|\tau),\\ \widetilde{\psi}\begin{bmatrix}\boldsymbol{\delta}^T\\ \mathbf{0}^T\end{bmatrix}(2\mathbf{v}|2\tau)&=\exp\{2\mathbf{u}^T\varkappa\mathbf{u}\}\,\theta\begin{bmatrix}\boldsymbol{\delta}^T\\ \mathbf{0}^T\end{bmatrix}(2\mathbf{v}|2\tau)\end{aligned}\tag{3.22}$$

have the same periodicity property

$$\psi\begin{bmatrix}\boldsymbol{\delta}^T\\ \mathbf{0}^T\end{bmatrix}(2\mathbf{v}+2\boldsymbol{\Omega}(\mathbf{m},\mathbf{m}')|\tau)=\exp\{2\mathbf{E}^T(\mathbf{m},\mathbf{m}')(\mathbf{x}+\boldsymbol{\Omega}(\mathbf{m},\mathbf{m}'))\}\psi\begin{bmatrix}\boldsymbol{\delta}^T\\ \mathbf{0}^T\end{bmatrix}(2\mathbf{v}|\tau),\tag{3.23}$$

with $\mathbf{E}(\mathbf{m},\mathbf{m}')=\eta\mathbf{m}+\eta'\mathbf{m}'$ as defined previously. Therefore any 2^g+1 entire functions which possess the periodicity property (3.23) are linearly dependent. Moreover this statement can be extended to the case of entire functions which have the periodicity property

$$\psi(\mathbf{v}+2\boldsymbol{\Omega}(\mathbf{m},\mathbf{m}'))=\exp\{2\mathbf{E}^T(\mathbf{m},\mathbf{m}')(\mathbf{x}+\boldsymbol{\Omega}(\mathbf{m},\mathbf{m}'))+\gamma(\mathbf{m},\mathbf{m}')\}\psi(\mathbf{v}),\tag{3.24}$$

where $\gamma(\mathbf{m},\mathbf{m}')$ is some constant. The proof given is valid for genera satisfying the inequality

$$2^g<g+\frac{g(g+1)}{2}.$$

These are the cases $g=2$ and $g=3$. □

We remark that in the case of $g=2$ the statement of Proposition 3.2 was derived in Ref. 5, see also Ref. 17, as the condition of the validity of the addition theorem for the Baker function

$$\boldsymbol{\Phi}_B(\mathbf{u}+\mathbf{v};\boldsymbol{\alpha})=\frac{\mathbf{Y}^T(\mathbf{u};\boldsymbol{\alpha})A\mathbf{Y}(\mathbf{v};\boldsymbol{\alpha})}{\mathbf{X}^T(\mathbf{u})A\mathbf{X}(\mathbf{v})}\tag{3.25}$$

with the integer 4×4-matrix A, where $\mathbf{X}(\mathbf{u})$ is a four-component meromorphic vector function and the four-component vector function $\mathbf{Y}(\mathbf{u};\boldsymbol{\alpha})$ has the periodicity properties (1.3) and (1.4).

The origin of the ansatz (3.25) is explained as follows. In the case $g=1$, (3.25) follows from the Weierstrass addition formula for the σ-functions,

$$\frac{\sigma(u+v)\sigma(u-v)}{\sigma^2(u)\sigma^2(v)}=\wp(v)-\wp(u),\tag{3.26}$$

which can be written in the equivalent form

$$\Phi_W(u+v;\alpha)=\frac{\Phi_W(u;\alpha)\Phi'_W(v;\alpha)-\Phi_W(v;\alpha)\Phi'_W(u;\alpha)}{\wp(u)-\wp(v)}. \tag{3.27}$$

This last equality can be rewritten in the form (3.25) with the vectors

$$\mathbf{Y}(u;\alpha)=\begin{pmatrix}\Phi(u;\alpha)\\ \Phi'(u;\alpha)\end{pmatrix},\quad \mathbf{X}(u)=\begin{pmatrix}\wp(u)\\ 1\end{pmatrix}, \tag{3.28}$$

and the 2×2-matrix

$$A=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}. \tag{3.29}$$

In the case of genus $g=2$, a solution of (3.25) was found in Ref. 5 with

$$\mathbf{X}^T(\mathbf{u})=(\wp_{22}(\mathbf{u}),\wp_{12}(\mathbf{u}),\wp_{11}(\mathbf{u}),1),$$

$$\mathbf{Y}^T(\mathbf{u};\boldsymbol{\alpha})=C(F_0(\mathbf{u};\boldsymbol{\alpha}),F_1(\mathbf{u};\boldsymbol{\alpha}),F_2(\mathbf{u};\boldsymbol{\alpha}),F_{12}(\mathbf{u};\boldsymbol{\alpha})),$$

where the functions F_0, F_1, F_2, and F_{12} are defined in (3.19) and the 4×4-matrices A and C are given as follows:

$$A=\begin{pmatrix}0 & -1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & -1 & 0\end{pmatrix},\quad C=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1/\wp_{22}(\boldsymbol{\alpha})\end{pmatrix},$$

The Schrödinger equation (4.11) and the hyperbolic equation (4.16) in this approach are the compatibility condition of the validity of the ansatz (3.25).

We shall show in the following how Proposition 3.2 is used to derive 2D and 3D Schrödinger equations with a potential expressible in terms of Kleinian $\wp$-functions.

IV. THE TWO-DIMENSIONAL SCHRÖDINGER EQUATION WITH AN ABELIAN POTENTIAL

Consider the Riemann surface of a curve $V(x,y)$ of genus 2, in the form

$$w^2=4z^5+\lambda_4z^4+\lambda_3z^3+\lambda_2z^2+\lambda_1z+\lambda_0=4\Pi_{k=1}^5(z-e_k) \tag{4.1}$$

equipped with a homology basis $(\mathfrak{a}_1,\mathfrak{a}_2;\mathfrak{b}_1,\mathfrak{b}_2)\in H_1(V,\mathbb{Z})$. The canonical holomorphic differentials and the associated meromorphic differentials of the second kind have the form

$$\mathrm{d}u_1=\frac{\mathrm{d}z}{w},\quad \mathrm{d}u_2=\frac{z\,\mathrm{d}z}{w},$$

$$\mathrm{d}r_1=\frac{\lambda_3z+2\lambda_4z^2+12z^3}{4w}dz,\quad \mathrm{d}r_2=\frac{z^2}{w}dz.$$

The fundamental Kleinian σ-function is expanded near $\mathbf{x}=0$ as follows

$$\sigma(x_1,x_2)=x_1-\tfrac{1}{3}x_2^3+\tfrac{1}{24}\lambda_2x_1^3+o(\mathbf{x}^3). \tag{4.2}$$

Denote

$$\zeta_i(\mathbf{x})=\frac{\partial}{\partial x_i}\ln\sigma(\mathbf{x}),\quad i=1,2,$$

$$\wp_{ij}(\mathbf{x})=-\frac{\partial^2}{\partial x_i\partial x_j}\ln\sigma(\mathbf{x}),\quad i,j=1,2.$$

The equations of the Jacobi inversion problem

$$x_i=\int_{(\infty,\infty)}^{(w_1,z_1)}\mathrm{d}u_i+\int_{(\infty,\infty)}^{(w_2,z_2)}\mathrm{d}u_i,\quad i=1,2$$

are equivalent to an algebraic equation

$$\mathcal{P}(z,\mathbf{x})=z^2-\wp_{22}(\mathbf{x})z-\wp_{12}(\mathbf{x})=0, \tag{4.3}$$

i.e., the pair (z_1,z_2) is the pair of roots of (4.3). So we have

$$\wp_{22}(\mathbf{x})=z_1+z_2,\ \ \wp_{12}(\mathbf{x})=-z_1z_2. \tag{4.4}$$

The corresponding w_i is expressed as

$$w_i=\wp_{222}(\mathbf{x})z_i+\wp_{122}(\mathbf{x}),\quad i=1,2. \tag{4.5}$$

The function $\wp_{11}(\mathbf{x})$ is expressed in terms of symmetric functions of the divisor as

$$\wp_{11}(\mathbf{x})=\frac{\mathcal{F}(z_1,z_2)-2w_1w_2}{4(z_1-z_2)^2}, \tag{4.6}$$

where the polynomial $\mathcal{F}$ is the *Kleinian polar*

$$\mathcal{F}(z_1,z_2)=\sum_{k=0}^{2}z_1^kz_2^k(2\lambda_{2k}+\lambda_{2k+1}(z_1+z_2)).$$

The three functions $\wp_{11},\wp_{12},\wp_{22}$ are known to be algebraically dependent, being the coordinates of the quartic Kummer surface, which is given by

$$\det\begin{pmatrix}\lambda_0 & \frac{1}{2}\lambda_1 & -2\wp_{11} & -2\wp_{12}\\ \frac{1}{2}\lambda_1 & \lambda_2+4\wp_{11} & \frac{1}{2}\lambda_3+2\wp_{12} & -2\wp_{22}\\ -2\wp_{11} & \frac{1}{2}\lambda_3+2\wp_{12} & \lambda_4+4\wp_{22} & 2\\ -2\wp_{12} & -2\wp_{22} & 2 & 0\end{pmatrix}=0,$$

where the variables $\wp_{22}=X,\wp_{12}=Y,\wp_{11}=Z$ are regarded as coordinates of the surface in $\mathbb{C}^3$.

We are now in a position to formulate the following theorem.

Theorem 4.1: *The following equality is valid for the six Baker functions* $F_0(\mathbf{x};\alpha)$, $F_1(\mathbf{x};\boldsymbol{\alpha})$, $F_2(\mathbf{x};\boldsymbol{\alpha})$, $F_{11}(\mathbf{x};\boldsymbol{\alpha})$, $F_{12}(\mathbf{x};\boldsymbol{\alpha})$, *and* $F_{22}(\mathbf{x};\boldsymbol{\alpha})$ *in the case of genus two*

$$\begin{aligned}&[aF_{11}+bF_{12}+a\wp_{12}(\boldsymbol{\alpha})F_{22}+\tfrac{1}{2}b\wp_{22}(\boldsymbol{\alpha})F_{22}+(a\wp_{122}+\tfrac{1}{2}b\wp_{222}(\boldsymbol{\alpha}))F_2]\\ &\quad=[a(\wp_{11}(\boldsymbol{\alpha})-\wp_{12}(\boldsymbol{\alpha})\wp_{22}(\boldsymbol{\alpha})+\tfrac{1}{4}\lambda_2)-\tfrac{1}{2}b\wp_{22}^2(\boldsymbol{\alpha})]F_0,\end{aligned} \tag{4.7}$$

where a,b are arbitrary and the λ_i parameters of the curve (4.1).

Proof: Consider the six functions,

$$\sigma(\mathbf{x})^2 F(\mathbf{x};\boldsymbol{\alpha}), \quad \sigma(\mathbf{x})^2 F_i(\mathbf{x};\boldsymbol{\alpha}), \quad \sigma(\mathbf{x})^2 F_{ij}(\mathbf{x};\boldsymbol{\alpha}), \quad i,j=1,2. \tag{4.8}$$

These are linearly dependent second-order entire functions, satisfying (3.24) with $\gamma(\mathbf{m},\mathbf{m}') = \boldsymbol{\zeta}^T(\boldsymbol{\alpha})\boldsymbol{\Omega}(\mathbf{m},\mathbf{m}') - \mathbf{E}^T(\mathbf{m},\mathbf{m}')\boldsymbol{\alpha} \equiv \mathbf{k}(\boldsymbol{\alpha})$. Therefore there exist constants $c_0, c_1, c_2, c_{11}, c_{12}, c_{22} \neq 0$, such that

$$c_0 F_0(\mathbf{x};\boldsymbol{\alpha}) + \sum_{k=1,2} c_k F_k(\mathbf{x};\boldsymbol{\alpha}) + \sum_{i,j=1,2} c_{ij} F_{ij}(\mathbf{x};\boldsymbol{\alpha}) = 0. \tag{4.9}$$

Using the expansion (4.2) and the identity $\wp_{112} = \wp_{222}\wp_{12} - \wp_{122}\wp_{22}$, we arrive at

$$\begin{aligned}
c_1 &= 0,\\
c_0 + c_{11}\wp_{11}(\boldsymbol{\alpha}) + \tfrac{1}{4}c_{11}\lambda_2 - c_{22}\wp_{22}(\boldsymbol{\alpha}) &= 0,\\
2c_{11}\wp_{12}(\boldsymbol{\alpha}) + c_{12}\wp_{22}(\boldsymbol{\alpha}) - 2c_{22} &= 0,\\
-2c_2\wp_{12}(\boldsymbol{\alpha}) + c_{12}\wp_{122}(\boldsymbol{\alpha}) + 2c_{22}\wp_{122}(\boldsymbol{\alpha}) &= 0,\\
-c_2\wp_{22}(\boldsymbol{\alpha}) - c_{11}\wp_{112}(\boldsymbol{\alpha}) + c_{22}\wp_{222}(\boldsymbol{\alpha}) &= 0,\\
2c_2 - 2c_{11}\wp_{122}(\boldsymbol{\alpha}) - c_{12}\wp_{222}(\boldsymbol{\alpha}) &= 0,
\end{aligned}$$

whose solution reads

$$\begin{aligned}
c_{11} &= a, \quad c_{12} = b,\\
c_0 &= a(\wp_{11}(\boldsymbol{\alpha}) - \wp_{12}(\boldsymbol{\alpha})\wp_{22}(\boldsymbol{\alpha}) + \tfrac{1}{4}\lambda_2) - \tfrac{1}{2}b\wp_{22}^2(\boldsymbol{\alpha}),\\
c_{22} &= a\wp_{12}(\boldsymbol{\alpha}) + \tfrac{1}{2}b\wp_{22}(\boldsymbol{\alpha}),\\
c_2 &= a\wp_{122}(\boldsymbol{\alpha}) + \tfrac{1}{2}b\wp_{222}(\boldsymbol{\alpha}),
\end{aligned} \tag{4.10}$$

where a and b are arbitrary. The equality (4.7) then follows immediately. □

By choosing the parameters $a=1$, $b=0$ and then $a=0$, $b=1$ we get from the equality (4.7) the following equations on $\mathrm{Jac}(V)\times\mathrm{Jac}(V)$:

$$\begin{aligned}
&\left\{\left[\frac{\partial^2}{\partial x_1^2} - 2\wp_{11}(\mathbf{x})\right] + \wp_{12}(\boldsymbol{\alpha})\left[\frac{\partial^2}{\partial x_2^2} - 2\wp_{22}(\mathbf{x})\right]\right\}\Psi_1(\mathbf{x};\boldsymbol{\alpha})\\
&\quad = \frac{1}{4\wp_{12}(\boldsymbol{\alpha})}(\lambda_0 + \lambda_2\wp_{12}(\boldsymbol{\alpha}) + \lambda_4\wp_{12}^2(\boldsymbol{\alpha}))\Psi_1(\mathbf{x};\boldsymbol{\alpha}),
\end{aligned}$$

where

$$\Psi_1(\mathbf{x};\boldsymbol{\alpha}) = \Phi(\mathbf{x};\boldsymbol{\alpha})\exp\left\{\frac{1}{2}\frac{\wp_{122}(\boldsymbol{\alpha})}{\wp_{12}(\boldsymbol{\alpha})}x_2\right\},$$

and

$$\wp_{22}(\boldsymbol{\alpha})\left\{\left[\frac{\partial^2}{\partial x_1^2}-2\wp_{11}(\mathbf{x})\right]+2\wp_{12}(\boldsymbol{\alpha})\left[\frac{\partial^2}{\partial x_1\partial x_2}-2\wp_{12}(\mathbf{x})\right]\right\}\Psi_2(\mathbf{x};\boldsymbol{\alpha})=-\wp_{22}^2(\boldsymbol{\alpha})\Psi_2(\mathbf{x};\boldsymbol{\alpha}),$$

where

$$\Psi_2(\mathbf{x};\boldsymbol{\alpha})=\Phi(\mathbf{x};\boldsymbol{\alpha})\exp\{-\tfrac{1}{2}\wp_{122}(\boldsymbol{\alpha})x_1\}.$$

Therefore the following theorems are valid for the case of genus two:

Theorem 4.2: *Let V be nonsingular hyperelliptic curve of genus 2 given by Eq. (4.1). Let $\Phi_B(\mathbf{x};\boldsymbol{\alpha})$ be the standard Baker function on $\mathrm{Jac}(V)\times\mathrm{Jac}(V)$. Let $\boldsymbol{\Omega}=(\omega_{11},\omega_{21})^T$, $\boldsymbol{\Omega}'=(\omega_{11},\omega_{21})^T$ be the real and imaginary half periods.*

Then the following 2D Schrödinger equation at a fixed energy level is valid:

$$\left\{\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}-\mathcal{U}_1(\mathbf{x})\right\}\Psi_1(\mathbf{x};\boldsymbol{\alpha})=\tfrac{1}{4}(\lambda_0+\lambda_2+\lambda_4)\Psi_1(\mathbf{x};\boldsymbol{\alpha}), \tag{4.11}$$

where the smooth and real potential $\mathcal{U}_1(\mathbf{x})$ and wave function $\Psi_1(\mathbf{x};\boldsymbol{\alpha})$ have the form

$$\mathcal{U}_1(\mathbf{x})=2\wp_{11}(\imath\mathbf{x}+\boldsymbol{\Omega})+2\wp_{22}(\imath\mathbf{x}+\boldsymbol{\Omega}),\quad \mathbf{x}\in\mathbb{R}^2, \tag{4.12}$$

$$\Psi_1(\mathbf{x};\boldsymbol{\alpha})=\Phi_B(\imath\mathbf{x}+\boldsymbol{\Omega};\boldsymbol{\alpha}+\boldsymbol{\Omega}')\exp\{\tfrac{1}{2}\wp_{122}(\boldsymbol{\alpha}+\boldsymbol{\Omega}')(\imath x_2+\omega_{12}')\},\quad \mathbf{x},\boldsymbol{\alpha}\in\mathbb{R}^2, \tag{4.13}$$

and are restricted to the complex one-dimensional Bloch variety $\mathcal{B}_1$ given by

$$\mathcal{B}_1=\{(\boldsymbol{\alpha})\,|\,\wp_{12}(\boldsymbol{\alpha}+\boldsymbol{\Omega}')=1\}. \tag{4.14}$$

The vector of quasimomentum is real and is given by

$$\mathbf{k}(\boldsymbol{\alpha})=\boldsymbol{\zeta}(\boldsymbol{\alpha}+\boldsymbol{\Omega}')-2\varkappa(\boldsymbol{\alpha}+\boldsymbol{\Omega}')+\tfrac{1}{2}\wp_{122}(\boldsymbol{\alpha}+\boldsymbol{\Omega}')\begin{pmatrix}0\\1\end{pmatrix}. \tag{4.15}$$

Theorem 4.3: *For the conditions of Theorem 4.2, the following hyperbolic equation at the zero energy level is valid:*

$$\left\{\frac{\partial^2}{\partial x_1\partial x_2}-\mathcal{U}_2(\mathbf{x})\right\}\Psi_2(\mathbf{x};\boldsymbol{\alpha})=0, \tag{4.16}$$

where the smooth and real potential $\mathcal{U}_2(\mathbf{x})$ and the wave function have the form

$$\mathcal{U}_2(\mathbf{x})=2\wp_{12}(\imath\mathbf{x}+\boldsymbol{\Omega}),\quad \mathbf{x}\in\mathbb{R}^2, \tag{4.17}$$

$$\Psi_2(\mathbf{x};\boldsymbol{\alpha})=\Phi_B(\imath\mathbf{x}+\boldsymbol{\Omega};\boldsymbol{\alpha}+\boldsymbol{\Omega}')\times\exp\{\tfrac{1}{2}\wp_{122}(\boldsymbol{\alpha})(\imath x_1+\omega_{21}')\},\quad \mathbf{x},\boldsymbol{\alpha}\in\mathbb{R}^2, \tag{4.18}$$

and is restricted to the complex one-dimensional Bloch variety $\mathcal{B}_2$ given by

$$\mathcal{B}_2:\ \{(\boldsymbol{\alpha})\,|\,\wp_{22}(\boldsymbol{\alpha}+\boldsymbol{\Omega}')=0\}. \tag{4.19}$$

The vector of quasimomentum is real and given by

$$\mathbf{k}(\boldsymbol{\alpha})=\boldsymbol{\zeta}(\boldsymbol{\alpha}+\boldsymbol{\Omega}')-2\varkappa(\boldsymbol{\alpha}+\boldsymbol{\Omega}')+\frac{1}{2}\wp_{222}(\boldsymbol{\alpha}+\boldsymbol{\Omega}')\begin{pmatrix}1\\0\end{pmatrix}. \tag{4.20}$$

The Bloch varieties $\mathcal{B}_k\subset\mathrm{Jac}(V)$, $k=1,2$ are pull-backs of the varieties $\tilde{\mathcal{B}}_k\subset\mathrm{Kum}(V)$, $k=1,2$ under the projection $\mathrm{Jac}(V)\to\mathrm{Kum}(V)$, where the $\tilde{\mathcal{B}}_k$ are given by

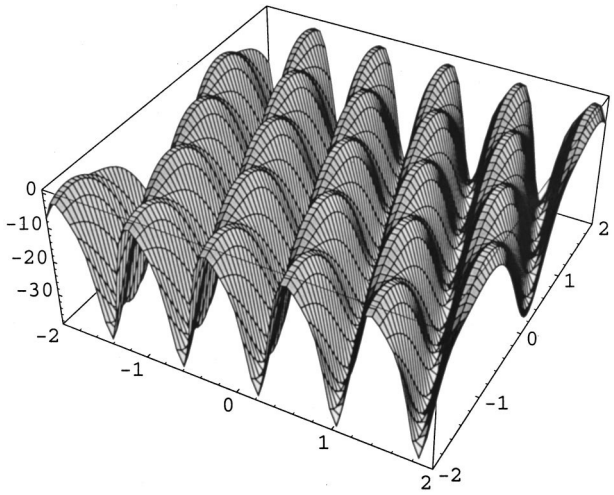

FIG. 1. Potential profile as function of x,y for the branching points $e_1=2\sqrt{3}$, $e_2=3$, $e_3=0$, $e_4=-e_2$, $e_5=-e_1$.

$$\mathcal{B}_1=(X,Z):\det\begin{pmatrix} \lambda_0 & \frac{1}{2}\lambda_1 & -2Z & -2 \\ \frac{1}{2}\lambda_1 & \lambda_2+4Z & \frac{1}{2}\lambda_3+2 & -2X \\ -2Z & \frac{1}{2}\lambda_3+2 & \lambda_4+4X & 2 \\ -2 & -2X & 2 & 0 \end{pmatrix}=0$$

in the case of the 2D Schrödinger equation, and

$$\mathcal{B}_2=(Y,Z):\det\begin{pmatrix} \lambda_0 & \frac{1}{2}\lambda_1 & -2Z & -2Y \\ \frac{1}{2}\lambda_1 & \lambda_2+4Z & \frac{1}{2}\lambda_3+2Y & 0 \\ -2Z & \frac{1}{2}\lambda_3+2Y & \lambda_4 & 2 \\ -2Y & 0 & 2 & 0 \end{pmatrix}=0$$

in the case of the hyperbolic equation.

The Bloch varieties $\mathcal{B}_{1,2}$ are algebraic curves, and it is straightforward to show that these curves are genus two hyperelliptic curves with a branching point at infinity. But in contrast with the case of genus one, these curves are not equivalent to the initial curve at generic $\lambda_0,\ldots,\lambda_4$.

We remark that the explicit description of the varieties $\mathcal{B}_k$, $k=1,2$, which can be realized as algebraic curve of genus 4 with involution, and its link with the results of Veselov and Novikov,[4,3] is given in Ref. 19.

As an application of the above-given theory we show in Figs. 1 and 2, the potential profiles as derived from (4.12), for two different sets of the parameter values (in Figs. 3 and 4 the corresponding level sets of these potentials are also shown). We see from these figures that the potentials are both real and smooth and have a spatial symmetry which is more general than the square or rectangular one considered in Ref. 16. The full choice of more general crystal symmetries which can be found by properly appropriate choices of the parameters $\{e_i\}$, one can arrange is still

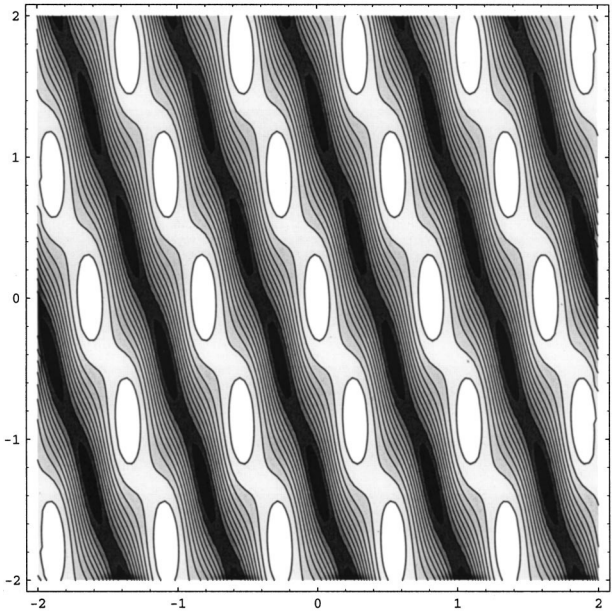

FIG. 2. The same as in Fig. 1 for $e_1=2$, $e_2=1$, $e_3=0$, $e_4=-1$, $e_5=-2$.

under investigation. These properties make the above-mentioned potentials suitable for physical applications. Similar results can be obtained for the potential (4.17) (for simplicity details are omitted).

V. THE TWO DIMENSIONAL SCHRÖDINGER EQUATION WITH AN ELLIPTIC POTENTIAL

In this section we shall construct an elliptic 2D Schrödinger equation with a potential which can be expressed in terms of an elliptic function by using the concept of elliptic solitons for the KdV equation. We shall show that the real and nonsingular potential in the (x,y) plane is provided

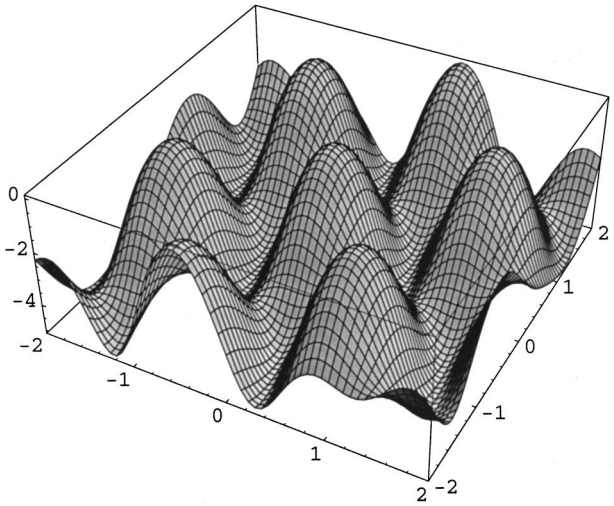

FIG. 3. Topographic map of the potential in the case: $e_1=2\sqrt{3}$, $e_2=3$, $e_3=0$, $e_4=-e_2$, $e_5=-e_1$. The regions between contours are shaded in such a way that the ones with higher values are lighter.

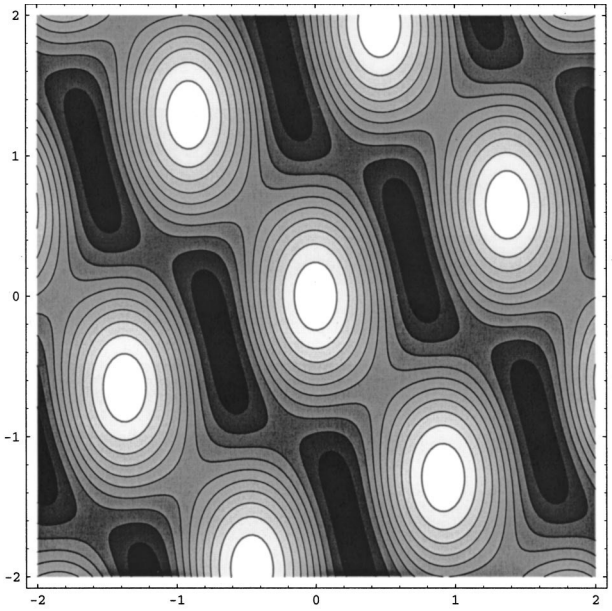

FIG. 4. The same as in Fig. 2 for $e_1=2$, $e_2=1$, $e_3=0$, $e_4=-1$, $e_5=-2$.

by the dynamics over the locus of the Calogero–Moser system. The particle dynamics of the system over locus is essentially complex and was traditionally considered as nonphysical. The equations for the Kleinian $\wp$-functions

$$\wp_{2222}=6\wp_{22}^2+4\wp_{12}+\lambda_4\wp_{22}+\tfrac{1}{2}\lambda_3, \tag{5.1}$$

$$\wp_{1222}=6\wp_{22}\wp_{12}-2\wp_{11}+\lambda_4\wp_{12}, \tag{5.2}$$

represent the KdV hierarchy for genus two curves with respect to the function

$$\mathcal{U}=2\wp_{22}(\mathbf{x})+\tfrac{1}{6}\lambda_4. \tag{5.3}$$

Equation (5.1) becomes, after differentiation by $u_2\equiv x$, the KdV equation,

$$\mathcal{U}_{x_1}=\tfrac{1}{2}(\mathcal{U}_{x_2x_2x_2}-6\mathcal{U}_{x_2}\mathcal{U}), \tag{5.4}$$

while the second equation (5.2) represents the second KdV flow which is stationary for the two-gap potential (5.3).

We further interpret the coordinates (x_1,x_2) as space coordinates $(\mathbf{x})$ and set $(x_1,x_2)=(y,x)$. Consider the elliptic solution of the KdV equation

$$\mathcal{U}(x,y)=2\wp(x-f_1(y))+2\wp(x-f_2(y))+2\wp(x-f_3(y)), \tag{5.5}$$

where $\wp(x)$ is the standard Weierstrass elliptic function, which represents the isospectral deformation of the two-gap Lamé potential $6\wp(x)$ under the action of the KdV flow. The solution of the form (5.5) was introduced for the first time by Dubrovin and Novikov;[20] the general case was investigated by Airault *et al.*[21] We use this elliptic KdV solution in the following to construct a special solution of the 2D problem.

The ansatz (5.5) implies the following structure of the hyperelliptic, genus two, σ-function in the reduction case:

$$\sigma(x,y)=\prod_{i=1}^{3}\sigma(x-f_i(y)), \tag{5.6}$$

where σ is the standard σ-function from the Weierstrass theory of elliptic functions. The associated algebraic curve is known to be of the form

$$w^2=4(z^2-3g_2)(z+3e_1)(z+3e_2)(z+3e_3). \tag{5.7}$$

The remaining Kleinian $\wp$-functions, $\wp_{12}(\mathbf{x})$ and $\wp_{11}(\mathbf{x})$, are expressible from (5.1) and (5.2) as differential polynomials of $\wp_{22}$, and have the form

$$\wp_{12}=-3\sum_{i<j=1,2,3}\wp(x-f_i(y))\wp(x-f_j(y))+\frac{9}{4}g_2, \tag{5.8}$$

$$\begin{aligned}\wp_{11}=&-27\wp(x-f_1(y))\wp(x-f_2(y))\wp(x-f_3(y))\\&+3\sum_{i<j=1,2,3}\wp'(x-f_i(y))\wp'(x-f_j(y))+\frac{21}{4}\sum_{i}^{3}\wp(x-f_i(y)),\end{aligned} \tag{5.9}$$

where $\wp$ is the standard Weierstrass $\wp$-function. This implies that the Abelian elliptic potential for the two-dimensional Schrödinger equation has the form

$$\begin{aligned}\mathcal{U}(x,y)=&-54\wp(x-f_1(y))\wp(x-f_2(y))\wp(x-f_3(y))\\&+6\sum_{i<j=1,2,3}\wp'(x-f_i(y))\wp'(x-f_j(y))+\frac{25}{4}\sum_{i}^{3}\wp(x-f_i(y)).\end{aligned} \tag{5.10}$$

For the proof we remark that the compatibility of the ansatz (5.5) with the KdV equation leads to

$$\frac{df_1}{dy}=-6\mathfrak{B}_{12}-6\mathfrak{B}_{13},$$

$$\frac{df_2}{dy}=-6\mathfrak{B}_{21}-6\mathfrak{B}_{23},$$

$$\frac{df_3}{dy}=-6\mathfrak{B}_{31}-6\mathfrak{B}_{33},$$

with

$$\mathfrak{B}'_{12}+\mathfrak{B}'_{13}=0,\quad \mathfrak{B}'_{21}+\mathfrak{B}'_{23}=0,\quad \mathfrak{B}'_{31}+\mathfrak{B}'_{33}=0. \tag{5.11}$$

Here we denote $\mathfrak{B}_{ij}=\wp(f_i(y)-f_j(y))$. These equations represent the well-known dynamics of the third flow of the integrable Calogero–Moser system, restricted to the stable points of the second flow. We remark that the addition theorem for the Weierstrass $\wp$-function and the equations of the *locus* (5.11) allow us to rewrite the first group of the equations for f_i in the form

$$\frac{df_1}{dy}=6\mathfrak{B}_{23},\quad \frac{df_2}{dy}=6\mathfrak{B}_{13},\quad \frac{df_3}{dy}=6\mathfrak{B}_{12} \tag{5.12}$$

and therefore the elliptic KdV solution is given in the form

$$\mathcal{U}(x,y)=2\sum_{i<j=1,2,3}\wp\left(ix+\omega-6\int_0^y\wp(f_i(y)-f_j(y))dy\right) \tag{5.13}$$

with ω being a constant of integration. We shall find in the following the explicit expressions for the functions $\wp(f_i(y)-f_j(y))$ and show that (5.13) represents an elliptic soliton, i.e., a real and smooth function which is doubly periodic in both x and y. With this aim we consider the equations of the Jacobi inversion problem associated with the curve (5.7):

$$\int_{(\infty,\infty)}^{(w_1,z_1)} \frac{dz}{w} + \int_{(\infty,\infty)}^{(w_2,z_2)} \frac{dz}{w} = x_1 \equiv y, \tag{5.14}$$

$$\int_{(\infty,\infty)}^{(w_1,z_1)} \frac{z\,dz}{w} + \int_{(\infty,\infty)}^{(w_2,z_2)} \frac{z\,dz}{w} = x_2 \equiv x. \tag{5.15}$$

The solution of the problem has the form

$$z_1+z_2=2\sum_{i=1}^{3} \wp(x-f_i(y)), \tag{5.16}$$

$$z_1 z_2 = 3 \sum_{i<j=1,2,3} \wp(x-f_i(y))\wp(x-f_j(y)) - \frac{9}{4} g_2, \tag{5.17}$$

where we use (5.1), (5.2) and (5.5) to derive (5.16) and (5.17). Let us take the limit $x \to f_1(y)$. Then it follows from (5.16) and (5.17)

$$z_2 \to \infty, \quad z_1 \to 3(\mathfrak{P}_{12}+\mathfrak{P}_{13}) \equiv -3\mathfrak{P}_{23},$$

and the equations of the Jacobi inversion problem will take the form

$$\int_{\infty}^{-3\mathfrak{B}_{23}} \frac{dz}{2\sqrt{(z^2-3g_2)(z-3e_1)(z-3e_2)(z-3e_3)}} = y, \tag{5.18}$$

$$\int_{\infty}^{-3\mathfrak{B}_{23}} \frac{z\,dz}{2\sqrt{(z^2-3g_2)(z-3e_1)(z-3e_2)(z-3e_3)}} = x. \tag{5.19}$$

Two other pairs of equations of the form (5.18) and (5.19) appear as the result of cyclic permutations of the indices 1,2,3. To proceed we shall use the reduction formulas of Hermite, under which the hyperelliptic integrals on the left-hand side of (5.14) and (5.15) are reduced to elliptic integrals associated with the elliptic curves:

$$\nu^2 = 4\mu^3 - g_2\mu - g_3, \quad \tilde{\nu}^2 = 4\tilde{\mu}^3 - \tilde{g}_2\tilde{\mu} - \tilde{g}_3, \tag{5.20}$$

whose moduli are linked by the relation

$$\tilde{g}_2 = \frac{4}{g_2^2}(3g_2^3+27g_3), \quad \tilde{g}_3 = \frac{72}{g_2^3}(g_3 g_2^3 - 3g_3^3). \tag{5.21}$$

The equations for the cover are

$$(\mu,\nu) = \left(\frac{w}{27} \frac{z^3-9g_2-54g_3}{z^2-3g_2}, \frac{z^3+27g_3}{9(z^2-3g_2)} \right), \tag{5.22}$$

$$(\tilde{\nu},\tilde{\mu}) = \left(\sqrt{\frac{2}{27g_2^3}} w(4z^2-3g_2), \frac{1}{3g_2}(4z^3-9g_2z+9g_3) \right). \tag{5.23}$$

The reduction of the holomorphic differentials has the form

$$\frac{dz}{w}=\frac{2}{3\sqrt{3g_2}}\frac{d\tilde{\mu}}{\tilde{\nu}},\quad \frac{zdz}{w}=\frac{1}{3}\frac{d\mu}{\nu}. \tag{5.24}$$

The application of the reduction formulas to Eq. (5.18) results in the following cubic equation with respect to $\mathfrak{P}_{23}$:

$$4\mathfrak{P}_{23}^3-g_2\mathfrak{P}_{23}-\tfrac{1}{3}g_3+\tfrac{1}{9}g_2\tilde{\wp}(\tfrac{3}{2}\sqrt{3g_2}y)=0. \tag{5.25}$$

Evidently the remaining two roots are exactly $\mathfrak{P}_{12}$ and $\mathfrak{P}_{13}$. Note that Eq. (5.25) displays the following properties of the functions $\mathfrak{P}_{ij}$ on the locus:

$$\mathfrak{P}_{12}+\mathfrak{P}_{13}+\mathfrak{P}_{23}=0, \tag{5.26}$$

$$\mathfrak{P}_{12}\mathfrak{P}_{13}+\mathfrak{P}_{23}\mathfrak{P}_{13}+\mathfrak{P}_{13}\mathfrak{P}_{23}=-\tfrac{1}{4}g_2. \tag{5.27}$$

Let us show that the application of the reduction formulas to Eq. (5.19) leads to the equivalence. Indeed the substitution of the reduction formula (5.22) into (5.18) implies

$$\wp(3f_1)=\frac{\mathfrak{P}_{23}^3-g_3}{g_2-3\mathfrak{P}_{23}^2}. \tag{5.28}$$

We transform the left-hand side:

$$\begin{aligned}\wp(3f_1)&=\wp(\{f_1-f_2\}+\{f_1-f_3\})\quad(\text{because of the equality}\quad f_1+f_2+f_3=0)\\&=-\mathfrak{P}_{12}-\mathfrak{P}_{13}+\frac{1}{4}\left[\frac{\mathfrak{P}'_{12}-\mathfrak{P}'_{13}}{\mathfrak{P}_{12}-\mathfrak{P}_{13}}\right]^2\\&\quad(\text{because of the addition theorem for the Weierstrass elliptic function})\\&=\mathfrak{P}_{23}+\frac{\mathfrak{P}'^{\,2}_{23}}{(2\mathfrak{P}_{12}+\mathfrak{P}_{23})^2}\\&\quad[\text{because(5.26)and locus equations, which imply}\\&\quad\mathfrak{P}'^{\,2}_{23}-\mathfrak{P}'^{\,2}_{12}=(\mathfrak{P}'_{23}+\mathfrak{P}'_{21})(\mathfrak{P}'_{23}+\mathfrak{P}'_{12})=0].\end{aligned}$$

Further, Eq. (5.27) leads to the relation

$$(2\mathfrak{P}_{12}+\mathfrak{P}_{23})^2=g_2-3\mathfrak{P}_{23}^2.$$

Collecting all these equalities together we transform (5.28) to the equality

$$\mathfrak{P}_{23}+\frac{\mathfrak{P}'^{\,2}_{23}}{g_2-3\mathfrak{P}_{23}^2}\equiv\frac{\mathfrak{P}_{23}^3-g_3}{g_2-3\mathfrak{P}_{23}^2},$$

whose validity can be checked directly.

Therefore we have proved the following proposition (a proof in compressed form was given in Ref. 22, see also Ref. 21, p. 144).

Proposition 5.1: Let (μ,ν) and $(\tilde{\nu},\tilde{\mu})$ be two elliptic curves in the Weierstrass form with the moduli g_2,g_3 and $\tilde{g}_2,\tilde{g}_3$ given in (5.12). Denote by $\wp$ and $\tilde{\wp}$ the corresponding Weierstrass elliptic functions. Then the formula (5.13) describes the elliptic solution of the KdV equation with the integrands

$$\wp(f_i(y)-f_j(y))=\mathfrak{P}_{i,j},\quad (i,j)=(1,2),(1,3),(2,3)$$

being the roots of the cubic equation with coefficients depending on the moduli of the elliptic curve g_2, g_3 and the Weierstrass function $\tilde{\wp}$,

$$4X^3 - g_2 X - \tfrac{1}{3} g_3 + \tfrac{1}{9} g_2 \tilde{\wp}(\tfrac{3}{2}\sqrt{3g_2}\, y) = 0. \tag{5.29}$$

We shall summarize the results as follows:

Theorem 5.2: *Let V be the Lamé curve*

$$w^2 = 4(z^2 - 3g_2)(z + 3e_1)(z + 3e_2)(z + 3e_3),$$

which covers three-sheetedly the two elliptic curves

$$\wp'^2 = 4\wp^3 - g_2\wp - g_3, \quad \tilde{\wp}'^2 = 4\tilde{\wp}^3 - \tilde{g}_2\tilde{\wp} - \tilde{g}_3, \tag{5.30}$$

whose moduli are linked by the relation

$$\tilde{g}_2 = \frac{4}{g_2^2}(3g_2^3 + 27g_3), \quad \tilde{g}_3 = \frac{72}{g_2^3}(g_3 g_2^3 - 3g_3^3). \tag{5.31}$$

Then the wave function

$$\Psi_E(\mathbf{x}; \alpha, \beta) = \prod_{i=1}^{3} \Phi_W(ix + \omega - f_i(y); \alpha - f_i(\beta)), \tag{5.32}$$

where the three functions f_i are given by

$$f_i(y) = -6 \int_0^y X_i(y)\mathrm{d}y,$$

and X_i are the three roots of the cubic equation

$$4X^3 - g_2 X - \tfrac{1}{3} g_3 + \tfrac{1}{9} g_2 \tilde{\wp}(\tfrac{3}{2}\sqrt{3g_2}\, y) = 0, \tag{5.33}$$

satisfy the 2D Schrödinger equation

$$\left\{ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - \mathcal{U}(x,y) \right\} \Psi_E = \Lambda \Psi_E,$$

with the elliptic smooth and nonseparable potential given by

$$\begin{aligned} \mathcal{U}(x,y) = &-54\wp(x - f_1(y))\wp(x - f_2(y))\wp(x - f_3(y)) \\ &+ 6 \sum_{i<j=1}^{3} \wp'(x - f_i(y))\wp'(x - f_j(y)) + \frac{25}{4} \sum_{i}^{3} \wp(x - f_i(y)), \end{aligned} \tag{5.34}$$

on the fixed energy level $\Lambda = -36 g_2 g_3 + 36 g_3$. The spectral variety is a one-dimensional variety given by

$$3 \sum_{i<j=1,2,3} \wp(\alpha - f_i(\beta))\wp(\alpha - f_j(\beta)) - \frac{9}{4} g_2 = 1. \tag{5.35}$$

We remark that the Bloch variety (5.35), which is given as a hyperelliptic curve, is uniformizable in this case by elliptic functions with moduli (5.31).

We note that we could consider other two-gap elliptic potentials in an analogous fashion.

VI. THE 3D SCHRÖDINGER EQUATION

We consider the case of the curve defined by

$$y^2=4x^7+\sum_0^6 \lambda_j x^j.$$

The principal matrix H is given by (3.10) and is a 5×5 matrix of the form

$$H=\begin{pmatrix} \lambda_0 & \frac{1}{2}\lambda_1 & -2\wp_{11} & -2\wp_{12} & -2\wp_{13} \\ \frac{1}{2}\lambda_1 & 4\wp_{11}+\lambda_2 & 2\wp_{12}+\frac{1}{2}\lambda_3 & 4\wp_{13}-2\wp_{22} & -2\wp_{23} \\ -2\wp_{11} & 2\wp_{12}+\frac{1}{2}\lambda_3 & 4\wp_{22}-4\wp_{13}+\lambda_4 & 2\wp_{23}+\frac{1}{2}\lambda_5 & -2\wp_{33} \\ -2\wp_{12} & 4\wp_{13}-2\wp_{22} & 2\wp_{23}+\frac{1}{2}\lambda_5 & 4\wp_{33}+\lambda_6 & 2 \\ -2\wp_{13} & -2\wp_{23} & -2\wp_{33} & 2 & 0 \end{pmatrix}.$$

The expansion of the σ-function of genus 3 in the vicinity of $\mathbf{u}=0$ (found for the first time in Ref. 8) has the form

$$\sigma(u_1,u_2,u_3)=u_1u_3-u_2^2-\tfrac{1}{24}(2\lambda_0u_1^4+2\lambda_1u_1^3u_2+\lambda_2u_1^2(3u_2^2-u_1u_3)+8u_2u_3^3+2\lambda_3u_1u_2^3+2\lambda_4u_2^4 +2\lambda_5u_2^3u_3+\lambda_6u_3^2(3u_2^2-u_1u_3))+\text{higher order terms}. \tag{6.1}$$

We are in position now to prove the following theorem.

Theorem 6.1: *Let $F_{i,j}(\mathbf{x};\boldsymbol{\alpha})$ be the functions (3.19). Then the following equalities are valid for all $\mathbf{x};\boldsymbol{\alpha}\in\mathbb{C}^3$,*

$$4(\wp_{113}(\boldsymbol{\alpha})-\wp_{122}(\boldsymbol{\alpha}))F_{33}(\mathbf{x};\boldsymbol{\alpha})-4(2F_{13}(\mathbf{x};\boldsymbol{\alpha})+F_{22}(\mathbf{x};\boldsymbol{\alpha}))\wp_{133}(\boldsymbol{\alpha})+8F_{23}(\mathbf{x};\boldsymbol{\alpha})\wp_{123}(\boldsymbol{\alpha}) +4F_{11}(\mathbf{x};\boldsymbol{\alpha})\wp_{333}(\boldsymbol{\alpha})=\Lambda F_0(\mathbf{x};\boldsymbol{\alpha}), \tag{6.2}$$

where

$$\Lambda=4(2\wp_{13}(\boldsymbol{\alpha})-\wp_{22}(\boldsymbol{\alpha}))\wp_{133}(\boldsymbol{\alpha})+\lambda_6\wp_{122}(\boldsymbol{\alpha})-4\wp_{33}(\boldsymbol{\alpha})\wp_{113}(\boldsymbol{\alpha})-\lambda_2\wp_{333}(\boldsymbol{\alpha}) +4\wp_{33}(\boldsymbol{\alpha})\wp_{122}(\boldsymbol{\alpha})-4\wp_{11}(\boldsymbol{\alpha})\wp_{333}(\boldsymbol{\alpha})-\lambda_6\wp_{113}(\boldsymbol{\alpha}),$$

and

$$4(2\wp_{123}(\boldsymbol{\alpha})-\wp_{222}(\boldsymbol{\alpha}))F_{33}(\mathbf{x};\boldsymbol{\alpha})+8(\wp_{223}(\boldsymbol{\alpha})-\wp_{133}(\boldsymbol{\alpha}))F_{23}(\mathbf{x};\boldsymbol{\alpha})-4(2F_{13}(\mathbf{x};\boldsymbol{\alpha}) +F_{22}(\mathbf{x};\boldsymbol{\alpha}))\wp_{233}(\boldsymbol{\alpha})+8F_{12}(\mathbf{x};\boldsymbol{\alpha})\wp_{3,3,3}(\boldsymbol{\alpha})=\Lambda F_0(\mathbf{x};\boldsymbol{\alpha}),$$

where

$$\Lambda=4(2\wp_{13}-\wp_{22})\wp_{233}-2\lambda_6\wp_{123}+\lambda_6\wp_{222}-8\wp_{33}\wp_{123}+4\wp_{33}\wp_{222}.$$

Proof: Let us take (3.20) in the case $g=3$ and assume $c_{13}=2c_{22}$. Then we have

$$c_0F_0+\sum_{i=1}^3 c_iF_i+\sum_{i\le j=1,\dots,3} C_{i+j}F_{i,j}=0, \tag{6.3}$$

where we denote $c_{ij}=C_{i+j}$. Let us multiply (6.3) by $\sigma^2(\boldsymbol{\alpha})$ and expand the resulting equality in a power series in u_1,u_2,u_3 by using (6.1). We find

$$c_1=c_2=c_3=0, \tag{6.4}$$

and six equations to define C_0,C_2,C_3,C_4,C_5,C_6:

$$-2C_5+2C_4\wp_{33}+2C_2\wp_{13}+2C_3\wp_{23}=0,$$

$$-4C_2\wp_{12}+(-4\wp_{22}+8\wp_{13})\,C_3+(\lambda_5+4\wp_{23})\,C_4+(8\wp_{33}+2\lambda_6)\,C_5+4C_6=0,$$

$$(\lambda_2-4\wp_{11})\,C_2+(2\lambda_3+8\wp_{12})C_3+(4\lambda_4+12\wp_{22}-8\wp_{13})\,C_4+(2\lambda_5+8\wp_{23})\,C_5+(\lambda_6-4\wp_{33})\,C_6+4C_0=0,$$

$$(\lambda_2+4\wp_{11})\,C_2+(8\wp_{13}-4\wp_{22})\,C_4+(\lambda_6+4\wp_{33})\,C_6+4C_0=0,$$

$$\lambda_1C_2+(8\wp_{11}+2\lambda_2)\,C_3+(\lambda_3+4\wp_{12})\,C_4+(8\wp_{13}-4\wp_{22})\,C_5-4C_6\wp_{23}=0,$$

$$4\lambda_0C_2+2\lambda_1C_3-8C_5\wp_{12}-8C_6\wp_{13}-8C_4\wp_{11}=0.$$

We find from the third equation

$$C_0=-(\wp_{11}-\tfrac{1}{4}\lambda_2)C_2+(\wp_{22}-2\wp_{13})C_4-(\wp_{33}+\tfrac{1}{4}\lambda-6)C_6. \tag{6.5}$$

To define the remaining parameters, add the third equation to the fourth and consider the remaining five equations. They are homogeneous equations with respect to the five variables C_2,C_3,C_4,C_5,C_6, whose matrix is exactly the matrix H. Because the matrix H has rank three, the general solution depends on two arbitrary variables $a=C_2$ and $b=C_3$. The remaining variables are computed by applying formula (3.15).

The matrix of the first equation (6.2) is

$$M_1=\begin{bmatrix} \wp_{333} & 0 & -\wp_{133} \\ 0 & -\wp_{133} & \wp_{123} \\ -\wp_{133} & \wp_{123} & \wp_{113}-\wp_{122} \end{bmatrix}$$

and the matrix of the second equation (6.3) is

$$M_2=\begin{bmatrix} 0 & \wp_{333} & -\wp_{233} \\ \wp_{333} & -\wp_{233} & -\wp_{133}+\wp_{223} \\ -\wp_{233} & -\wp_{133}+\wp_{223} & 2\,\wp_{123}-\wp_{222} \end{bmatrix}.$$

It can be checked by direct substitution that in the rational limit

$$\sigma(\alpha_1,\alpha_2,\alpha_3)=-\alpha_2^2+\alpha_1\alpha_3-\tfrac{1}{3}\alpha_2\alpha_3^3+\tfrac{1}{45}\alpha_3^6$$

there are regions in $(\alpha_1,\alpha_2,\alpha_3)$ space where the principal minors are all nonpositive. □

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Geometric quantization of mechanical systems with time-dependent parameters

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Quantum systems with adiabatic classical parameters are widely studied, e.g., in the modern holonomic quantum computation. We here provide complete geometric quantization of a Hamiltonian system with time-dependent parameters, without the adiabatic assumption. A Hamiltonian of such a system is affine in the temporal derivative of parameter functions. This leads to the geometric Berry factor phenomena. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1477262]

I. INTRODUCTION

At present, quantum systems with classical parameters attract special attention in connection with holonomic quantum computation.[1–3] This approach to quantum computing is based on the generalization of Berry's adiabatic phase to the non-Abelian case corresponding to adiabatically driving an n-fold degenerate eigenstate of a Hamiltonian over the parameter manifold.[4] In the framework of the holonomic quantum computation scheme, information is encoded in this degenerate state, while the parameter manifold plays the role of a control parameter space. The key point of this scheme is that the parallel transport along the curves in the parameter space is assumed to be adiabatic with respect to a dynamic Hamiltonian.

At the same time, the adiabatic condition of Berry's phase phenomena can be removed.[5,6] Moreover, one observes that the Berry factor is a standard ingredient in evolution of quantum systems with classical time-dependent parameters.[7,8] Here, we provide complete geometric quantization of a mechanical system depending on parameters, without adiabatic assumption.

The configuration space of such a system is a composite fiber bundle

$$Q \to \Sigma \to \mathbf{R}, \tag{1}$$

where $\mathbf{R}$ is the time axis and $\Sigma \to \mathbf{R}$ is a fiber bundle whose sections are parameter functions.[7–9] The configuration space (1) is coordinated by (t, σ^λ, q^k), where (t, σ^λ) are bundle coordinates on $\Sigma \to \mathbf{R}$ and t is a fixed Cartesian coordinate on $\mathbf{R}$. The corresponding momentum phase space is the vertical cotangent bundle V^*Q of $Q \to \Sigma$ equipped with holonomic coordinates $(t, \sigma^\lambda, q^k, p_k)$. It is provided with the following canonical Poisson structure. Let T^*Q be the cotangent bundle of Q endowed with the canonical Poisson bracket $\{,\}_T$. Given the canonical fibration

$$\zeta: T^*Q \to V^*Q, \tag{2}$$

the Poisson bracket $\{,\}_V$ on the space $C^\infty(V^*Q)$ of smooth real functions on V^*Q is defined by the relation

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$$\zeta^*\{f,f'\}_V=\{\zeta^*f,\zeta^*f'\}_T, \tag{3}$$

$$\{f,f'\}_V=\partial^k f\partial_k f'-\partial_k f\partial^k f', \quad f,f'\in C^\infty(V^*Q). \tag{4}$$

Its characteristic symplectic foliation coincides with the fibration $V^*Q\to\Sigma$.

It seems natural to quantize the Poisson manifold V^*Q in accordance with the well-known geometric quantization procedure.[10,11] However, one faces the problem that the mean values of quantum operators are defined via integration over the momentum phase space V^*Q, including integration over classical parameters. At the same time, quantization of a system with classical parameters should necessarily imply its quantization under fixed values of parameters. Its generic carrier space is a Hilbert module of sections of a smooth Hilbert bundle over the parameter space Σ,[7,8] i.e., a locally trivial smooth field of Hilbert spaces on Σ in the terminology of Ref. 12. In particular, the instantwise quantization of time-dependent mechanics (where $\Sigma=\mathbf{R}$) is of this type.[13,14] However, geometric quantization of a Poisson manifold need not yield quantization of its symplectic leaves.[15]

To dispose of these problems, we will apply to $V^*Q\to\Sigma$ the technique of leafwise geometric quantization of symplectic foliations.[16] There is one-to-one correspondence between Poisson structures on a smooth manifold and its symplectic foliations. The quantum algebra of a symplectic foliation is a particular quantum algebra of the associated Poisson manifold such that its restriction to each symplectic leaf is defined and quantized. We choose the canonical real polarization of $V^*Q\to\Sigma$ which is the vertical tangent bundle VV^*Q of the fiber bundle $V^*Q\to Q$. The corresponding quantum algebra $\mathcal{A}_\mathcal{F}$ consists of functions on V^*Q which are affine in momenta p_k. It is represented by Schrödinger operators in the pre-Hilbert $C^\infty(\Sigma)$-module E_Q of fiberwise complex half-forms on the fiber bundle $Q\to\Sigma$ whose restriction to each fiber is of compact support.

We show that a Hamiltonian of a quantum system with classical parameters is affine in the temporal derivative of parameter functions χ^λ, namely,

$$\hat{\mathcal{H}}=-i(\Lambda^k_\lambda\partial_k+\tfrac{1}{2}\partial_k\Lambda^k_\lambda)\partial_t\chi^\lambda+\hat{\mathcal{H}}'(\chi), \tag{5}$$

where Λ^k_λ are components of a connection on the fiber bundle $Q\to\Sigma$. The key point is that integration of the first term of this Hamiltonian over time through a parameter function $\chi(t)$ depends only on a trajectory of this function in a parameters space, but not on parametrization of this trajectory by time (i.e., the adiabatic assumption is not necessary). As a consequence, this term is responsible for the geometric Berry factor phenomena. It plays the role of a control operator in holonomic quantum computation.

II. THE LEAFWISE DIFFERENTIAL CALCULUS

Geometric quantization of symplectic foliations is phrased in terms of the leafwise differential calculus on a foliated manifold. Manifolds throughout are assumed to be smooth, Hausdorff, second-countable (i.e., paracompact), and connected.

Recall that a (regular) foliation $\mathcal{F}$ of a manifold Z consists of (maximal) integral manifolds of an involutive distribution $i_\mathcal{F}:T\mathcal{F}\to TZ$ on Z. A foliated manifold $(Z,\mathcal{F})$ admits an adapted coordinate atlas

$$\{(U_\xi;z^\lambda;z^i)\}, \quad \lambda=1,\ldots,\text{codim }\mathcal{F}, \quad i=\text{codim }\mathcal{F}+1,\ldots,\dim Z, \tag{6}$$

such that transition functions of coordinates z^λ are independent of the remaining coordinates z^i and, for each leaf $F\in\mathcal{F}$, the connected components of $F\cap U_\xi$ are given by the equations $z^\lambda=\text{const}$. These connected components coordinated by (z^i) make up a coordinate atlas of a leaf F.

Let $S_\mathcal{F}(Z)$ denote the subring of the ring $C^\infty(Z)$ of smooth real functions on Z which consists of functions constant on leaves of $\mathcal{F}$. Global sections of the distribution $T\mathcal{F}$ constitute the Lie

algebra $\mathcal{T}(\mathcal{F})$ of derivations of the ring $C^\infty(Z)$ regarded as a $S_{\mathcal{F}}(Z)$-ring. Therefore, one can introduce the leafwise differential calculus[17] as the Chevalley–Eilenberg differential calculus over the $S_{\mathcal{F}}(Z)$-ring $C^\infty(Z)$. It is the cochain complex

$$0\to S_{\mathcal{F}}(Z)\to C^\infty(Z)\stackrel{\tilde d}{\to}\mathfrak{F}^1(Z)\cdots\stackrel{\tilde d}{\to}\mathfrak{F}^{\dim\ \mathcal{F}}(Z)\to 0 \tag{7}$$

of global sections of exterior products $\wedge^r T\mathcal{F}^*$ of the dual $T\mathcal{F}^*\to Z$ of $T\mathcal{F}\to Z$.[8] These sections are called the leafwise forms on a foliated manifold $(Z,\mathcal{F})$, and read

$$\phi=\frac{1}{r!}\phi_{i_1\cdots i_r}\tilde{\mathrm{d}}z^{i_1}\wedge\cdots\wedge\tilde{\mathrm{d}}z^{i_r},$$

where $\{\tilde{\mathrm{d}}z^i\}$ are the duals of the holonomic fiber bases $\{\partial_i\}$ for $T\mathcal{F}$. Accordingly, the Chevalley–Eilenberg coboundary operator

$$\tilde{\mathrm{d}}\phi=\frac{1}{r!}\partial_j\phi_{i_1\cdots i_r}\tilde{\mathrm{d}}z^j\wedge\tilde{\mathrm{d}}z^{i_1}\wedge\cdots\wedge\tilde{\mathrm{d}}z^{i_r}$$

is the leafwise exterior differential. The complex (7) is said to be the leafwise de Rham complex (or the tangential de Rham complex in the terminology of Ref. 17). This is the complex $(\mathcal{A}^{0,*},d_f)$ in Ref. 18.

Let us consider the exact sequence

$$0\to\mathrm{Ann}\ \ T\mathcal{F}\to T^*Z\stackrel{i_{\mathcal{F}}^*}{\to}T\mathcal{F}^*\to 0 \tag{8}$$

of vector bundles over Z. The epimorphism $i_{\mathcal{F}}^*$ yields an epimorphism of the graded algebra $\mathcal{O}^*(Z)$ of exterior forms on Z to the algebra $\mathfrak{F}^*(Z)$ of leafwise forms. The relation $i_{\mathcal{F}}^*\circ d=\tilde d\circ i_{\mathcal{F}}^*$ holds and, thereby, we have the cochain morphism

$$i_{\mathcal{F}}^*:(\mathbf{R},\mathcal{O}^*(Z),d)\to(S_{\mathcal{F}}(Z),\mathfrak{F}^*(Z),\tilde d),\quad \mathrm{d}z^\lambda\mapsto 0,\quad \mathrm{d}z^i\mapsto\tilde{\mathrm{d}}z^i \tag{9}$$

of the de Rham complex of Z to the leafwise de Rham complex (7) and the corresponding homomorphism

$$[i_{\mathcal{F}}^*]^*:H^*(Z)\to H^*_{\mathcal{F}}(Z) \tag{10}$$

of the de Rham cohomology of Z to the leafwise de Rham cohomology $H^*_{\mathcal{F}}(Z)$ of the complex (7).

Given a leaf $i_F:F\to Z$ of a foliation $\mathcal{F}$, there is the pull-back homomorphism

$$(\mathbf{R},\mathcal{O}^*(Z),d)\to(\mathbf{R},\mathcal{O}^*(F),d) \tag{11}$$

of the de Rham complex of Z to that of F and the corresponding homomorphism of their cohomology groups

$$H^*(Z)\to H^*(F). \tag{12}$$

Proposition 1: The cohomology morphism (12) factorizes through the leafwise cohomology

$$H^*(Z)\stackrel{[i_{\mathcal{F}}^*]}{\to}H^*_{\mathcal{F}}(Z)\stackrel{[i_F^*]}{\to}H^*(F). \tag{13}$$

Proof: It is readily observed that the pull-back bundles $i_F^*T\mathcal{F}$ and $i_F^*T\mathcal{F}^*$ over F are isomorphic to the tangent and the cotangent bundles of F, respectively. Furthermore, a direct computation shows that $i_F^*(\tilde{d}\phi)=d(i_F^*\phi)$ for any leafwise form ϕ. It follows that the cochain morphism (11) factorizes through the cochain morphism (9) and the cochain morphism

$$i_F^*:(S_{\mathcal{F}}(Z),\mathfrak{F}^*(Z),\tilde{d})\to(\mathbf{R},\mathcal{O}^*(F),d),\quad \tilde{\mathrm{d}}z^i\mapsto \mathrm{d}z^i$$

of the leafwise de Rham complex of $(Z,\mathcal{F})$ to the de Rham complex of F. Then the cohomology sequence (13) takes place.

Turn now to (even) symplectic foliations $\mathcal{F}$. A $\tilde{d}$-closed nondegenerate leafwise two-form $\Omega_{\mathcal{F}}$ on a foliated manifold $(Z,\mathcal{F})$ is called symplectic. Its pull-back $i_F^*\Omega_{\mathcal{F}}$ onto each leaf F of $\mathcal{F}$ is a symplectic form on F. A leafwise symplectic form $\Omega_{\mathcal{F}}$ yields the bundle isomorphism

$$\Omega_{\mathcal{F}}^\flat:T\mathcal{F}\to T\mathcal{F}^*,\quad \Omega_{\mathcal{F}}^\flat:v\mapsto -v\rfloor\Omega_{\mathcal{F}}(z),\quad v\in T_z\mathcal{F}.$$

The inverse isomorphism $\Omega_{\mathcal{F}}^\sharp$ determines the Poisson bivector field

$$w_\Omega(\alpha,\beta)=\Omega_{\mathcal{F}}(\Omega_{\mathcal{F}}^\sharp(i_{\mathcal{F}}^*\alpha),\Omega_{\mathcal{F}}^\sharp(i_{\mathcal{F}}^*\beta)),\quad \forall\alpha,\beta\in T_z^*Z,\quad z\in Z, \tag{14}$$

on Z subordinate to $\overset{2}{\wedge}T\mathcal{F}$. The corresponding Poisson bracket reads

$$\{f,f'\}_{\mathcal{F}}=\vartheta_f\rfloor\tilde{\mathrm{d}}f',\quad \vartheta_f\rfloor\Omega_{\mathcal{F}}=-\tilde{\mathrm{d}}f,\quad f,f'\in C^\infty(Z). \tag{15}$$

Its kernel is $S_{\mathcal{F}}(Z)$. Conversely, let (Z,w) be a (regular) Poisson manifold and $\mathcal{F}$ its characteristic foliation. Since $\mathrm{Ann}\,T\mathcal{F}$ is the kernel of the Poisson bivector field w, the bundle homomorphism $w^\sharp:T^*Z\to TZ$ factorizes in a unique fashion

$$w^\sharp:T^*Z\xrightarrow{i_{\mathcal{F}}^*}T\mathcal{F}^*\xrightarrow{w_{\mathcal{F}}^\sharp}T\mathcal{F}\xrightarrow{i_{\mathcal{F}}}TZ$$

through the bundle isomorphism

$$w_{\mathcal{F}}^\sharp:T\mathcal{F}^*\to T\mathcal{F},\quad w_{\mathcal{F}}^\sharp:\alpha\mapsto -w(z)\rfloor\alpha,\quad \alpha\in T_z\mathcal{F}^*.$$

The inverse isomorphism $w_{\mathcal{F}}^\flat$ yields the symplectic leafwise form

$$\Omega_{\mathcal{F}}(v,v')=w(w_{\mathcal{F}}^\flat(v),w_{\mathcal{F}}^\flat(v')),\quad \forall v,v'\in T_z\mathcal{F},\quad z\in Z. \tag{16}$$

Formulas (14) and (16) establish the above-mentioned correspondence between the Poisson structures on a manifold Z and its symplectic foliations.

III. PREQUANTIZATION OF SYMPLECTIC FOLIATIONS

Prequantization of a symplectic foliation $(\mathcal{F},\Omega_{\mathcal{F}})$ of a manifold Z provides a representation

$$f\mapsto i\hat{f},\quad [\hat{f},\hat{f}']=-i\widehat{\{f,f'\}_{\mathcal{F}}} \tag{17}$$

of the Poisson algebra $(C^\infty(Z),\{f,f'\}_{\mathcal{F}})$ by first-order differential operators on the space $C(Z)$ of sections of the complex line bundle $\pi:C\to Z$. These operators are given by the Kostant–Souriau formula

$$\hat{f}=-i\nabla^{\mathcal{F}}_{\vartheta_f}+f, \tag{18}$$

where ϑ_f is the Hamiltonian vector field (15) and $\nabla^{\mathcal{F}}$ is the covariant differential with respect to a leafwise connection on $C\to Z$ whose curvature form obeys the prequantization condition

$$\widetilde{R}=i\Omega_{\mathcal{F}}. \tag{19}$$

In this section, we provide the cohomology analysis of this condition, and show that prequantization of a symplectic foliation yields prequantization of its symplectic leaves.

The inverse images $\pi^{-1}(F)$ of leaves F of the foliation $\mathcal{F}$ of Z make up a (regular) foliation $C_{\mathcal{F}}$ of the complex line bundle C. Given the tangent bundle $TC_{\mathcal{F}}$ of this foliation, we have the exact sequence of vector bundles

$$0\to VC\underset{C}{\to}TC_{\mathcal{F}}\underset{C}{\to}C\underset{Z}{\times}T\mathcal{F}\to 0, \tag{20}$$

where VC is the vertical tangent bundle of $C\to Z$. A linear leafwise connection on the complex line bundle $C\to Z$ is defined as a splitting of the exact sequence (20) which is linear over C.

One can choose an adapted coordinate atlas $\{(U_\xi;z^\lambda;z^i)\}$ (6) of a foliated manifold $(Z,\mathcal{F})$ such that U_ξ are trivialization domains of the complex line bundle $C\to Z$. Let $(z^\lambda;z^i;c)$, $c\in\mathbf{C}$ be the corresponding bundle coordinates on $C\to Z$. They are also adapted coordinates on the foliated manifold $(C,C_{\mathcal{F}})$. With respect to these coordinates, a leafwise connection is represented by a $TC_{\mathcal{F}}$-valued leafwise one-form

$$A_{\mathcal{F}}=\widetilde{\mathrm{d}}z^i\otimes(\partial_i+A_i c\partial_c), \tag{21}$$

where A_i are local complex functions on C. The covariant differential of sections of the line bundle $C\to Z$ with respect to the leafwise connection (21) reads

$$\nabla^{\mathcal{F}}s=\widetilde{\mathrm{d}}s-A_i s\ \ \widetilde{\mathrm{d}}z^i.\quad s\in C(Z).$$

The exact sequence (20) is obviously a subsequence of the exact sequence

$$0\to VC\underset{C}{\to}TC\underset{C}{\to}C\underset{Z}{\times}TZ\to 0.$$

Consequently, any connection

$$\Gamma=\mathrm{d}z^\lambda\otimes(\partial_\lambda+\Gamma_\lambda c\partial_c)+\mathrm{d}z^i\otimes(\partial_i+\Gamma_i c\partial_c) \tag{22}$$

on the complex line bundle $C\to Z$ yields a leafwise connection

$$\Gamma_{\mathcal{F}}=\widetilde{\mathrm{d}}z^i\otimes(\partial_i+\Gamma_i c\partial_c). \tag{23}$$

Conversely, one can show that any leafwise connection on the complex line bundle $C\to Z$ comes from a connection on it.[16]

The curvature form of the leafwise connection $A_{\mathcal{F}}$ (21) is

$$\widetilde{R}=\tfrac{1}{2}R_{ij}\widetilde{\mathrm{d}}z^i\wedge\widetilde{\mathrm{d}}z^j,\quad R_{ij}=\partial_i A_j-\partial_j A_i. \tag{24}$$

If a leafwise connection $A_{\mathcal{F}}$ comes from a connection A, its curvature form $\widetilde{R}$ (24) is the image $\widetilde{R}=i_{\mathcal{F}}^*R$ of the curvature form R of A with respect to the morphism $i_{\mathcal{F}}^*$ (9).

Let us return to the prequantization condition (19).

Lemma 2: Let us assume that there is a leafwise connection $\Gamma_{\mathcal{F}}$ on the complex line bundle $C\to Z$ which fulfills the prequantization condition (19). Then, for any Hermitian metric g on $C\to Z$, there exists a leafwise connection $A_{\mathcal{F}}^g$ on $C\to Z$ which (i) satisfies the condition (19), (ii) preserves g, and (iii) comes from a $U(1)$-principal connection on $C\to Z$.

Proof: For any Hermitian metric g on $C\to Z$, there exists an associated bundle atlas $\Psi^g=\{(z^\lambda;z^i,c)\}$ of C with $U(1)$-valued transition functions such that

$$g(c,c')=c\overline{c'}. \tag{25}$$

Let the leafwise connection $\Gamma_{\mathcal{F}}$ come from a linear connection Γ (22) on $C\to Z$ written with respect to the atlas Ψ^g. The connection $\Gamma_{\mathcal{F}}$ is split into the sum $A^g+\gamma$ where

$$A^g=dz^\lambda\otimes(\partial_\lambda+\mathrm{Im}(\Gamma_\lambda)c\partial_c)+dz^i\otimes(\partial_i+\mathrm{Im}(\Gamma_i)c\partial_c) \tag{26}$$

is a $U(1)$-principal connection, preserving the Hermitian metric g. The curvature forms R of Γ and R^g of A^g obey the relation $R^g=\mathrm{Im}(R)$. The connection A^g (26) defines the leafwise connection

$$A^g_{\mathcal{F}}=i^*_{\mathcal{F}}A^g=\tilde{d}z^i\otimes(\partial_i+iA^g_ic\partial_c), \quad iA^g_i=\mathrm{Im}(\Gamma_i), \tag{27}$$

preserving the Hermitian metric g (25). Its curvature fulfills the desired relation

$$\tilde{R}^g=i^*_{\mathcal{F}}R^g=\mathrm{Im}(i^*_{\mathcal{F}}R)=i\Omega_{\mathcal{F}}. \tag{28}$$

Since A^g (26) is a $U(1)$-principal connection, we have $R_g=-2\pi ic_1$ where c_1 is the first Chern form of integer de Rham cohomology class. If the prequantization condition (19) holds, the relation (28) shows that the leafwise cohomology class of the leafwise form $(2\pi)^{-1}\Omega_{\mathcal{F}}$ is the image of an integer de Rham cohomology class with respect to the cohomology morphism $[i^*_{\mathcal{F}}]$ (10). Conversely, if a leafwise symplectic form $\Omega_{\mathcal{F}}$ on a foliated manifold $(Z,\mathcal{F})$ is of this type, there exists a complex line bundle $C\to Z$ and a $U(1)$-principal connection A on $C\to Z$ such that the leafwise connection $i^*_{\mathcal{F}}A$ fulfils the relation (19). Thus, we have stated the following.

Proposition 3: A symplectic foliation $(\mathcal{F},\Omega_{\mathcal{F}})$ of a manifold Z admits prequantization (18) iff the leafwise cohomology class of $(2\pi)^{-1}\Omega_{\mathcal{F}}$ is the image of an integer de Rham cohomology class of Z.

Note that the leafwise connection $A^g_{\mathcal{F}}$ in Lemma 2 by no means is unique. Any connection $A^g+ic\phi\otimes\partial_c$ where ϕ is a closed leafwise one-form obeys the prequantization condition (24) and preserves the Hermitian metric (25).

Let F be a leaf of the symplectic foliation $(\mathcal{F},\Omega_{\mathcal{F}})$ provided with the symplectic form $\Omega_F=i^*_F\Omega_{\mathcal{F}}$. In accordance with Proposition 1, the symplectic form $(2\pi)^{-1}\Omega_F$ belongs to an integer de Rham cohomology class if the leafwise symplectic form $\Omega_{\mathcal{F}}$ fulfills the condition of Proposition 3. Thus, if a symplectic foliation admits prequantization, its symplectic leaves do as well. The corresponding prequantization bundle for F is the pull-back complex line bundle i^*_FC, coordinated by (z^i,c). Furthermore, let $A^g_{\mathcal{F}}$ (27) be a leafwise connection on the prequantization bundle $C\to Z$ which obeys Lemma 2, i.e., comes from a $U(1)$-principal connection A^g on $C\to Z$. Then the pull-back

$$A_F=i^*_FA^g=dz^i\otimes(\partial_i+ii^*_F(A^g_i)c\partial_c) \tag{29}$$

of the connection A^g onto $i^*_FC\to F$ satisfies the prequantization condition $R_F=i^*_FR=i\Omega_F$, and preserves the pull-back Hermitian metric i^*_Fg on $i^*_{\mathcal{F}}C\to F$.

IV. QUANTIZATION OF SYMPLECTIC FOLIATIONS

The next step is polarization of the symplectic foliation $(\mathcal{F},\Omega_{\mathcal{F}})$ of a manifold Z. It is defined as a maximal involutive distribution $\mathbf{T}\subset T\mathcal{F}$ on Z such that

$$\Omega_{\mathcal{F}}(u,v)=0, \quad \forall u,v\in\mathbf{T}_z, \quad z\in Z.$$

Given the Lie algebra $\mathbf{T}(Z)$ of vector fields on Z subordinate to $\mathbf{T}$, the quantum algebra of $(\mathcal{F},\Omega_{\mathcal{F}})$ is defined as the complexified subalgebra $\mathcal{A}_{\mathcal{F}}\subset C^\infty(Z)$ of functions f whose Hamiltonian vector fields ϑ_f (15) fulfill the condition $[\vartheta_f,\mathbf{T}(Z)]\subset\mathbf{T}(Z)$. This algebra obviously contains the ring $S_{\mathcal{F}}(Z)$, and is a Lie $S_{\mathcal{F}}(Z)$-algebra.

Let (F,Ω_F) be a symplectic leaf of the symplectic foliation $(\mathcal{F},\Omega_\mathcal{F})$. Given a polarization $\mathbf{T}\to Z$ of $(\mathcal{F},\Omega_\mathcal{F})$, its restriction $\mathbf{T}_F=i_F^*\mathbf{T}\subset i_F^*T\mathcal{F}=TF$ to F is an involutive distribution on F. It obeys the condition

$$i_F^*\Omega_\mathcal{F}(u,v)=0, \quad \forall u,v\in\mathbf{T}_{Fz}, \quad z\in F,$$

i.e., it is a polarization of the symplectic manifold (F,Ω_F). Thus, polarization of a symplectic foliation induces polarization of each symplectic leaf. Clearly, the quantum algebra $\mathcal{A}_F$ of a symplectic leaf F with respect to the polarization $\mathbf{T}_F$ contains all functions i_F^*f of the quantum algebra $\mathcal{A}_\mathcal{F}$ restricted to F.

Every polarization $\mathbf{T}$ of a symplectic foliation $(\mathcal{F},\Omega_\mathcal{F})$ yields polarization of the associated Poisson manifold. Indeed, let Φ be the sheaf of germs of local functions f on Z whose Hamiltonian vector fields ϑ_f (15) are subordinate to $\mathbf{T}$. The Poisson bracket of elements of Φ vanishes. Consequently, Φ is polarization the Poisson manifold $(Z,\{,\}_\mathcal{F})$. Furthermore, one can show that polarization $\mathbf{T}$ of a symplectic foliation $(\mathcal{F},\Omega_\mathcal{F})$ and the corresponding polarization Φ of the Poisson manifold $(Z,\{,\}_\mathcal{F})$ define the same quantum algebra $\mathcal{A}_\mathcal{F}$.[16] However, in order to provide the leafwise quantization of $\mathcal{A}_\mathcal{F}$, we modify the standard metaplectic correction technique[19,20] as follows.

Let us consider the exterior bundle $\overset{m}{\wedge}T\mathcal{F}^*$, $m=\dim\mathcal{F}$. Its structure group is $GL^+(m,\mathbf{R})$ since a symplectic foliation is oriented. One can regard this fiber bundle as being associated to a $GL(m,\mathbf{C})$-principal bundle $P\to Z$. Let us assume that $H^2(Z;\mathbf{Z}_2)=0$. Then the principal bundle P admits a twofold covering principal bundle with the structure metalinear group $ML(m,\mathbf{C})$.[20] As a consequence, there exists a complex line bundle $\mathcal{D}_\mathcal{F}\to Z$ characterized by an atlas $\Psi_\mathcal{F}=\{(U_\xi;z^\lambda;z^i;c)\}$ with the transition functions $c'=S_\mathcal{F}c$ such that $S_\mathcal{F}\overline{S_\mathcal{F}}=J^{-1}$ where J is the Jacobian of the transition functions of coordinates z^i. One can think of its sections as being leafwise half-forms on Z. The metalinear bundle $\mathcal{D}_\mathcal{F}\to Z$ admits the canonical lift of a vector field τ on Z. The corresponding Lie derivative of its sections reads

$$\mathbf{L}_\tau=\tau^i\partial_i+\tfrac{1}{2}\partial_i\tau^i. \tag{30}$$

We define the quantization bundle as the tensor product $Y=C\otimes\mathcal{D}_\mathcal{F}$. Given a leafwise connection $A_\mathcal{F}^q$ (27) and the Lie derivative $\mathbf{L}$ (30), let us associate the first-order differential operator

$$\hat{f}=-i[(\nabla^\mathcal{F}_{\vartheta_f}+if)\otimes\mathrm{Id}+\mathrm{Id}\otimes\mathbf{L}_{\vartheta_f}]=-i[\nabla^\mathcal{F}_{\vartheta_f}+if+\tfrac{1}{2}\partial_i\vartheta_f^i] \tag{31}$$

on sections ρ of Y to each element f of the quantum algebra $\mathcal{A}_\mathcal{F}$. A direct computation shows that the operators (31) obey the Dirac condition (17) and that, if a section ρ fulfills the relation

$$(\nabla^\mathcal{F}_\vartheta\otimes\mathrm{Id}+\mathrm{Id}\otimes\mathbf{L}_\vartheta)\rho=(\nabla^\mathcal{F}_\vartheta+\tfrac{1}{2}\partial_i\vartheta^i)\rho=0 \tag{32}$$

for all Hamiltonian vector field ϑ subordinate to $\mathbf{T}$, then $\hat{f}\rho$ possesses the same property for any $f\in\mathcal{A}_\mathcal{F}$.

Let us restrict the representation of the quantum algebra $\mathcal{A}_\mathcal{F}$ by the operators (31) to the subspace $E\subset Y(Z)$ of sections ρ which obey the condition (32) and whose restriction to each leaf of $\mathcal{F}$ is of compact support. The last condition is motivated by the following.

Since $i_F^*T\mathcal{F}^*=T^*F$, the pull-back $i_F^*\mathcal{D}_\mathcal{F}$ of $\mathcal{D}_\mathcal{F}$ onto a leaf F is a metalinear bundle of half-forms on F. Therefore, the pull-back i_F^*Y of the quantization bundle $Y\to Z$ onto F is a quantization bundle for the symplectic manifold $(F,i_F^*\Omega_\mathcal{F})$. Given the pull-back connection A_F (29) and the polarization $\mathbf{T}_F=i_F^*\mathbf{T}$, this symplectic manifold is subject to the standard geometric quantization by the first-order differential operators

$$\hat{f}=-i(i_F^*\nabla^\mathcal{F}_{\vartheta_f}+if+\tfrac{1}{2}\partial_i\vartheta_f^i), \quad f\in\mathcal{A}_F, \tag{33}$$

on sections ρ_F of $i_F^*Y \to F$ of compact support which obey the condition

$$(i_F^*\nabla_\vartheta^{\mathcal{F}} + \tfrac{1}{2}\partial_i\vartheta^i)\rho_F = 0$$

for all Hamiltonian vector fields ϑ on F subordinate to $\mathbf{T}_F$. These sections constitute a pre-Hilbert space E_F with respect to the Hermitian form

$$\langle \rho_F | \rho_F' \rangle = \left(\frac{1}{2\pi}\right)^{m/2} \int_F \rho_F \overline{\rho_F'}$$

so that $\hat{f}$ (33) are Hermitian operators in E_F. It is readily observed that $i_F^*E \subset E_F$. Moreover, the relation

$$i_F^*(\hat{f}\rho) = (\widehat{i_F^*f})(i_F^*\rho)$$

holds for all elements $f \in \mathcal{A}_{\mathcal{F}}$ and $\rho \in E$. This relation enables one to think of the operators $\hat{f}$ (31) in E as being the leafwise quantization of the $S_{\mathcal{F}}(Z)$-algebra $\mathcal{A}_{\mathcal{F}}$ by Hermitian operators in a pre-Hilbert $S_{\mathcal{F}}(Z)$-module E.

V. QUANTIZATION OF A MECHANICAL SYSTEM WITH PARAMETERS

Let Q (1) be the configuration space of a mechanical system with parameters such that $H^2(Q;\mathbf{Z}_2) = H^2(V^*Q;\mathbf{Z}_2) = 0$. The characteristic symplectic foliation $\mathcal{F}$ of the Poisson structure (4) on the momentum phase space V^*Q is the fibration $V^*Q \to \Sigma$ endowed with the leafwise symplectic form

$$\Omega_{\mathcal{F}} = \tilde{\mathrm{d}}p_k \wedge \tilde{\mathrm{d}}q^k.$$

Since this form is $\tilde{\mathrm{d}}$-exact, its leafwise de Rham cohomology class equals zero, and it is the image of the zero de Rham cohomology class with respect to the morphism $[i_{\mathcal{F}}^*]$ (10). Then, in accordance with Proposition 3, the symplectic foliation $(V^*Q \to \Sigma, \Omega_{\mathcal{F}})$ admits prequantization.

The prequantization bundle $C \to V^*Q$, associated to the zero Chern class, is trivial. Let its trivialization $C = V^*Q \times \mathbf{C}$ hold fixed, and let $(t, \sigma^\lambda, q^k, p_k, c)$ be the corresponding bundle coordinates. Unless Q is specified, we choose the leafwise connection

$$A_{\mathcal{F}} = \tilde{\mathrm{d}}p_k \otimes \partial^k + \tilde{\mathrm{d}}q^k \otimes (\partial_k + ip_k c\partial_c)$$

on $C \to V^*Q$. This connection preserves the Hermitian metric g (25) on C, and its curvature fulfills the prequantization condition $\tilde{R} = i\Omega_{\mathcal{F}}$. The corresponding prequantization operators (18) read

$$\hat{f} = -i\vartheta_f + (f - p_k\partial^k f), \quad \vartheta_f = \partial^k f \partial_k - \partial_k f \partial^k, \quad f \in C^\infty(V^*Q).$$

Let us choose the canonical vertical polarization of the symplectic foliation $(V^*Q \to \Sigma, \Omega_{\mathcal{F}})$ which is the vertical tangent bundle $\mathbf{T} = VV^*Q$ of the fiber bundle $\pi_{VQ}: V^*Q \to Q$. It is readily observed that the corresponding quantum algebra $\mathcal{A}_{\mathcal{F}}$ consists of functions which are affine in momenta p_k.

Following the quantization procedure in Sec. IV, one should define a representation of $\mathcal{A}_{\mathcal{F}}$ in the space E of sections ρ of the quantization bundle $C \otimes \mathcal{D}_{\mathcal{F}}$ which obey the condition (32) and whose restriction to each fiber of $V^*Q \to \Sigma$ is of compact support. The condition (32) reads

$$\partial_k f \partial^k \rho = 0, \quad \forall f \in C^\infty(Q),$$

i.e., elements of E are constant on fibers of $V^*Q \to Q$ and E reduces to $\{0\}$.

Therefore, we modify the quantization procedure as follows. Given a fibration $Q\to\Sigma$, let us consider the corresponding metalinear bundle $\mathcal{D}_Q\to Q$ and the tensor product $Y_Q=C_Q\otimes\mathcal{D}_Q$, where $C_Q=Q\times\mathbf{C}$ is the trivial complex line bundle over Q. It is readily observed that the Hamiltonian vector fields

$$\vartheta_f=a^k\partial_k-(p_r\partial_k a^r+\partial_k b)\partial^k,\quad f=a^k(t,\sigma^\lambda,q^r)p_k+b(t,\sigma^\lambda,q^r),$$

of elements $f\in\mathcal{A}_\mathcal{F}$ are projectable onto Q. Then one can associate to each element f of the quantum algebra $\mathcal{A}_\mathcal{F}$ the first-order differential operator

$$\hat{f}=(-i\nabla_{\pi_{VQ}(\vartheta_f)}+f)\otimes\mathrm{Id}+\mathrm{Id}\otimes\mathbf{L}_{\pi_{VQ}(\vartheta_f)}=-ia^k\partial_k-\frac{i}{2}\partial_k a^k+b \tag{34}$$

in the space E_Q of sections of the fiber bundle $Y_Q\to Q$ whose restriction to each fiber of $Q\to\Sigma$ is of compact support. Since the pull-back of $\mathcal{D}_Q$ onto each fiber Q_σ of $Q\to\Sigma$ is the metalinear bundle of half-forms on Q_σ, the restrictions ρ_σ of elements of $\rho_Q\in E_Q$ to Q_σ constitute a pre-Hilbert space with respect to the nondegenerate Hermitian form

$$\langle\rho_\sigma|\rho'_\sigma\rangle_\sigma=\int_{Q_\sigma}\rho_\sigma\overline{\rho'_\sigma}.$$

The Schrödinger operators (34) are Hermitian operators in the pre-Hilbert $C^\infty(\Sigma)$-module E_Q, and provide the desired geometric quantization of the symplectic foliation $(V^*Q\to\Sigma,\Omega_\mathcal{F})$.

VI. THE CLASSICAL EVOLUTION EQUATION

In order to quantize the evolution equation of a time-dependent mechanical system on the configuration space Q (1), one should bear in mind that this equation is not reduced to the Poisson bracket $\{,\}_V$ on V^*Q, but is expressed into the Poisson bracket $\{,\}_T$ on the cotangent bundle T^*Q.[14,21] Therefore, let us start from the classical evolution equation.

It is convenient to assume for a time that parameters are dynamic variables. The momentum phase space of such a system is the vertical cotangent bundle V^*_RQ of the configuration bundle $Q\to\mathbf{R}$ provided with holonomic coordinates $(t,\sigma^\lambda,q^k,p_\lambda,p_k)$.[8,9] A Hamiltonian on this momentum phase space is defined as a global section

$$h:V^*_RQ\to T^*Q,\quad p\circ h=-\mathcal{H}(t,\sigma^\lambda,q^k,p_\lambda,p_k), \tag{35}$$

of the affine bundle

$$\zeta_R:T^*Q\to V^*_RQ\quad(t,\sigma^\lambda,q^k,p,p_\lambda,p_k)\mapsto(t,\sigma^\lambda,q^k,p_\lambda,p_k).$$

Given the canonical Liouville form Ξ on T^*Q, every Hamiltonian h (35) yields the pull-back Hamiltonian form

$$H=h^*\Xi=p_\lambda\mathrm{d}\sigma^\lambda+p_k\mathrm{d}q^k-\mathcal{H}\,\mathrm{d}t \tag{36}$$

on V^*_RQ. For any Hamiltonian form H (36), there exists a unique vector field γ_H on V^*_RQ such that

$$\gamma_H\rfloor\mathrm{d}t=1,\quad \gamma_H\rfloor\mathrm{d}H=0.$$

This vector field defines the first-order Hamilton equations on V^*_RQ.[7–9,14,21,22] Accordingly,

$$\gamma_H\rfloor\mathrm{d}f=0,\quad f\in C^\infty(V^*_RQ) \tag{37}$$

is the evolution equation. In order to express it into a Poisson bracket, let us consider the pull-back $\zeta_R^* H$ of the Hamiltonian form H (36) onto T^*Q. It is readily observed that the difference $\Xi - \zeta_R^* h^* \Xi$ is a horizontal one-form on $T^*Q \to \mathbf{R}$ and that

$$\mathcal{H}^* = \partial_t \rfloor (\Xi - \zeta^* h^* \Xi)) = p + \mathcal{H} \tag{38}$$

is a function on T^*Q. Then the evolution equation (37) is brought into the form $\{\mathcal{H}^*, \zeta_R^* f\}_T = 0$ adapted for quantization.[14,21]

Let us return to a system where σ^λ are parameters. Its Hamiltonian $\mathcal{H}$ is affine in momenta p_λ, namely,

$$\mathcal{H} = p_\lambda \Gamma^\lambda + p_k(\Lambda^k + \Gamma^\lambda \Lambda_\lambda^k) + \mathcal{H}_\Lambda(t, \sigma^\lambda, q^r, p_r), \tag{39}$$

where $\mathcal{H}_\Lambda \in \zeta^* C^\infty(V^*Q)$ is the pull-back of a function on V^*Q and

$$\Lambda \circ \Gamma = dt \otimes (\partial_t + \Gamma^\lambda \partial_\lambda + (\Lambda^k + \Gamma^\lambda \Lambda_\lambda^k) \partial_k)$$

is a connection on $Q \to \mathbf{R}$ which is the composition of a connection

$$\Gamma = dt \otimes (\partial_t + \Gamma^\lambda \partial_\lambda) \tag{40}$$

on the parameter bundle $\Sigma \to \mathbf{R}$ and a connection

$$\Lambda = dt \otimes (\partial_t + \Lambda^k \partial_k) + d\sigma^\lambda \otimes (\partial_\lambda + \Lambda_\lambda^k \partial_k) \tag{41}$$

on $Q \to \Sigma$.[7–9] Note that the second term of the connection (41) provides the lift

$$\tau^\lambda \partial_\lambda \mapsto \tau^\lambda (\partial_\lambda + \Lambda_\lambda^k \partial_k)$$

onto Q of vertical vector fields on the parameter bundle $\Sigma \to \mathbf{R}$. It plays the role of a control operator in holonomic quantum computation. If a parameter function $\chi: \mathbf{R} \to \Sigma$ is given, the connection Γ (40) on $\Sigma \to \mathbf{R}$ is determined in such a way that

$$\nabla^\Gamma \chi = 0, \quad \Gamma^\lambda(t, \chi^\mu(t)) = \partial_t \chi^\lambda. \tag{42}$$

It is readily observed that, if a Hamiltonian $\mathcal{H}$ is affine in momenta p_λ and if f is a function on V^*Q, then the bracket $\{\mathcal{H}^*, \zeta^* f\}_T$ where ζ is the fibration (2) is the pull-back of a function on V^*Q. It provides a derivation of the $\mathbf{R}$-ring $C^\infty(V^*Q)$. Therefore, one can think of the equality

$$\{\mathcal{H}^*, \zeta^* f\}_T = 0, \quad f \in C^\infty(V^*Q), \tag{43}$$

as being a classical evolution equation on $C^\infty(V^*Q)$.

VII. THE QUANTUM EVOLUTION EQUATION

In order to quantize the evolution equation (43), one should quantize the Poisson manifold $(T^*Q, \{,\}_T)$ so that its quantum algebra $\mathcal{A}_T$ contains $\zeta^* \mathcal{A}_\mathcal{F}$. Let Φ be polarization of the Poisson manifold $(V^*Q, \{,\}_V)$ which determines $\mathcal{A}_\mathcal{F}$. Then, by virtue of the relation (3), $\zeta^* \Phi$ is a polarization of $(T^*Q, \{,\}_T)$. Clearly, $\mathcal{A}_\mathcal{F}$ is a subalgebra of the quantum algebra $\mathcal{A}_T$ of T^*Q determined by this polarization. The quantum algebra $\mathcal{A}_T$ consists of functions on T^*Q which are affine in momenta p, p_λ, p_k. Let us restrict our consideration to its subalgebra $\mathcal{A}_T'$ of functions

$$f = a(t, \sigma^\mu) p + a^\lambda(t, \sigma^\mu) p_\lambda + a^k(t, \sigma^\mu, q^r) p_k + b(t, \sigma^\mu, q^r),$$

where a and a^λ are the pull-back onto T^*Q of functions on the parameter space Σ. Of course, $\mathcal{A}_\mathcal{F} \subset \mathcal{A}_T'$. Moreover, $\mathcal{A}_T'$ admits a representation by the Hermitian operators

$$\hat{f}=-i(a\partial_t+a^\lambda\partial_\lambda+a^k\partial_k)-\frac{i}{2}\partial_k a^k+b$$

in the carrier space E_Q of the representation (34) of $\mathcal{A}_\mathcal{F}$. Then, if $\mathcal{H}^*\in\mathcal{A}'_T$, the evolution equation (43) is quantized as the Heisenberg equation

$$i[\hat{\mathcal{H}}^*,\hat{f}]=0, \quad f\in\mathcal{A}_\mathcal{F}. \tag{44}$$

The problem is that the function $\mathcal{H}^*$ (38) fails to belong to the algebra $\mathcal{A}'_T$, unless the Hamiltonian function $\mathcal{H}_\Lambda$ (39) is affine in momenta p_k. Let us assume that $\mathcal{H}_\Lambda$ is polynomial in momenta. This is the case of almost all physically relevant models.

Lemma 4: Any smooth function f on V^*Q which is a polynomial of momenta p_k is decomposed in a finite sum of products of elements of the algebra $\mathcal{A}_\mathcal{F}$.

The proof follows that of the similar statement in Sec. V of Ref. 14.

By virtue of Lemma 4, one can associate to a polynomial Hamiltonian function $\mathcal{H}_\Lambda$ an element of the enveloping algebra $\overline{\mathcal{A}}_\mathcal{F}$ of the Lie algebra $\mathcal{A}_\mathcal{F}$ (though it by no means is unique). Accordingly, $\mathcal{H}^*$ is represented by an element of the enveloping algebra $\overline{\mathcal{A}}'_T$ of the Lie algebra $\mathcal{A}'_T$. Then the Schrödinger representation of $\mathcal{A}'_T$ and $\mathcal{A}_\mathcal{F}$ is naturally extended to their enveloping algebras $\overline{\mathcal{A}}'_T$ and $\overline{\mathcal{A}}_\mathcal{F}$ that provides quantization $\hat{\mathcal{H}}^*$ of $\mathcal{H}^*$.

Given the operator $\hat{\mathcal{H}}^*$, the bracket

$$\nabla\hat{f}=i[\hat{\mathcal{H}}^*,\hat{f}] \tag{45}$$

defines a derivation of the quantum algebra $\overline{\mathcal{A}}_\mathcal{F}$. Since $\hat{p}=-i\partial_t$, the derivation (45) obeys the Leibniz rule

$$\nabla(r\hat{f})=\partial_t r\hat{f}+r\nabla\hat{f}, \quad r\in C^\infty(\mathbf{R}).$$

Therefore, it is a connection on the $C^\infty(\mathbf{R})$-algebra $\overline{\mathcal{A}}_\mathcal{F}$, which enables one to treat quantum evolution of $\overline{\mathcal{A}}_\mathcal{F}$ as a parallel transport along time.[7,8,14] In particular, $\hat{f}$ is parallel with respect to the connection (45) if it obeys the Heisenberg equation (44). Given a trivialization $Q\cong\mathbf{R}\times M$ and the corresponding (global) decomposition $\hat{\mathcal{H}}^*=-i\partial_t+\hat{\mathcal{H}}$, we can introduce the evolution operator U which obeys the equation

$$\hat{\mathcal{H}}^*\circ U=-iU\circ\partial_t,$$

and can be written as the formal time-ordered exponent

$$U=T\exp\left[-i\int_0^t\hat{\mathcal{H}}\,dt'\right].$$

Now let us consider a mechanical system depending on a given parameter function $\chi:\mathbf{R}\to\Sigma$. Its configuration space is the pull-back bundle $Q_\chi=\chi^*Q$ which is a subbundle $i_\chi:Q_\chi\to Q$ of the fiber bundle $Q\to\mathbf{R}$. The corresponding momentum phase space is the vertical cotangent bundle $V^*Q_\chi=i_\chi^*V^*Q$ of $Q_\chi\to\mathbf{R}$. The pull-back of the Hamiltonian form H (36) onto V^*Q_χ, where the connection Γ obeys the relation (42), reads

$$H_\chi=p_k\,dq^k-\mathcal{H}_\chi\,dt,$$

$$\mathcal{H}_\chi=p_k(\Lambda^k(t,\chi^\mu(t),q^r)+\Lambda^k_\lambda(t,\chi^\mu(t),q^r)\partial_t\chi^\lambda)+\mathcal{H}_\Lambda(t,\chi^\mu(t),q^r,p_r).$$

It characterizes the dynamics of a mechanical system with a given parameter function χ.[7–9]

In order to quantize this system, let us consider the pull-back bundle $\mathcal{D}_\chi = i_\chi^* \mathcal{D}_Q$ over Q_χ and its pull-back sections $\rho_\chi = i_\chi^* \rho_Q$, $\rho_Q \in E_Q$. It is easily justified that these are leafwise half-forms on the fiber bundle $Q_\chi \to \mathbf{R}$ whose restrictions to each fiber $i_t : Q_t \to Q_\chi$ are of compact support. These sections constitute a pre-Hilbert $C^\infty(\mathbf{R})$-module E_χ with respect to the Hermitian forms

$$\langle i_t^* \rho_\chi | i_t^* \rho'_\chi \rangle_t = \int_{Q_t} i_t^* \rho_\chi \overline{i_t^* \rho'_\chi}.$$

Then the pull-back operators

$$(\chi^* \hat{f}) \rho_\chi = (\hat{f} \rho)_\chi, \quad \chi^* \hat{f} = -ia^k(t, \chi^\lambda(t), q^r) \partial_k - \frac{i}{2} \partial_k a^k(t, \chi^\mu(t), q^r) + b(t, \chi^\mu(t), q^r),$$

in E_χ provide the representation of the pull-back functions

$$i_\chi^* f = a^k(t, \chi^\lambda(t), q^r) p_k + b(t, \chi^\lambda(t), q^r), \quad f \in \mathcal{A}_\mathcal{F}$$

on $V^* Q_\chi$. Accordingly, the quantum operator $\hat{\mathcal{H}}_\chi^* = \hat{p} + \hat{\mathcal{H}}_\chi$ coincides with pull-back operator $\chi^* \hat{\mathcal{H}}^*$. Then the Heisenberg equation of a quantum system with a parameter function χ takes the form

$$i[\hat{\mathcal{H}}_\chi^*, \chi^* \hat{f}] = 0,$$

and the corresponding evolution operator reads

$$U = T \exp\left[-i \int_0^t \hat{\mathcal{H}}_\chi \mathrm{d}t' \right]. \tag{46}$$

The Hamiltonian $\hat{\mathcal{H}}_\chi$ in the evolution operator U (46) takes the form (5). Its second term $\hat{\mathcal{H}}'$ can be regarded as a dynamic Hamiltonian of a quantum system, while the first term is responsible for the geometric Berry factor phenomena as follows.

Bearing in mind possible applications to holonomic quantum computations, let us simplify the quantum system in question. The above trivialization $Q \cong \mathbf{R} \times M$ implies a trivialization of the parameter bundle $\Sigma = \mathbf{R} \times S$ such that the fibration $Q \to \Sigma$ reads

$$\begin{array}{ccc} & {\scriptstyle \mathrm{Id} \times \pi_M} & \\ \mathbf{R} \times M & \to & \mathbf{R} \times S, \end{array}$$

where $\pi_M : M \to S$ is a fiber bundle. Let us suppose that the components Λ_λ^k of the connection Λ (41) are independent of time. Then one can regard the second term in this connection as a connection on the fiber bundle $M \to S$. It also follows that the first term in the Hamiltonian (5) depends on time only through parameter functions $\chi^\lambda(t)$. Furthermore, let the two terms in the Hamiltonian (5) mutually commute on $[0,t]$. Then the evolution operator U (46) takes the form

$$U = T \exp\left[-\int_{\chi([0,t])} \left(\Lambda_\lambda^k \partial_k + \frac{1}{2} \partial_k \Lambda_\lambda^k \right) \mathrm{d}\sigma^\lambda \right] \circ T \exp\left[-i \int_0^t \hat{\mathcal{H}}' \mathrm{d}t' \right].$$

One can think of the first factor in this evolution operator as being the parallel displacement operator along the curve $\chi([0,t]) \subset S$ with respect to the connection

$$\nabla^\Lambda \rho_Q = (\partial_\lambda + \Lambda_\lambda^k \partial_k + \tfrac{1}{2} \partial_k \Lambda_\lambda^k) \rho_Q \, \mathrm{d}\sigma^\lambda, \quad \rho_Q \in E_Q$$

on the $C^\infty(S)$-module E_Q. Its peculiarity in comparison with the remaining one lies in the fact that integration over time through a parameter function $\chi(t)$ depends only on a trajectory of this function in a parameter space, but not on parametrization of this trajectory by time. Therefore, one can think of it as being a geometric factor.

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Quantum three-body system in *D* dimensions

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The independent eigenstates of the total orbital angular momentum operators for a three-body system in an arbitrary D-dimensional space are presented by the method of group theory. The Schrödinger equation is reduced to the generalized radial equations satisfied by the generalized radial functions with a given total orbital angular momentum denoted by a Young diagram $[\mu, \nu, 0,..., 0]$ for the SO(D) group. Only three internal variables are involved in the functions and equations. The number of both the functions and the equations for the given angular momentum is finite and equal to $(\mu-\nu+1)$. © *2002 American Institute of Physics.*
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I. INTRODUCTION

From the very early stage of the progress in quantum mechanics in the real three-dimensional world, it has been pointed out that the essence of these theories would be easily understandable if their mathematics were constructed in the nonrelativistic hyperspace worlds.[1,2] The mathematical tools for generalization of the orbital angular momentum in an arbitrary D-dimensional space have been presented.[3–7] Recently, the D-dimensional Coulombic and the harmonic oscillator problems in a two-body system have been studied in some detail by many authors.[8–22]

Exact solutions played very important roles in the development of physics. The exact solutions of the Schrödinger equation in the real three-dimensional space for a hydrogen atom and for a harmonic oscillator were important technical achievements in quantum mechanics,[23] which provided strong evidence in favor of the theory being correct, at least as far as atomic physics is concerned. The next simplest atom is the helium atom, for which the Schrödinger equation cannot be solved analytically, but only numerically.[24–28] In the numerical calculation, one of the main difficulties is how to separate the global rotational degrees of freedom.

In our previous paper[29] we separated completely the global rotational degrees of freedom in the Schrödinger equation for an N-body system in the real three-dimensional space from the internal ones. We have determined a complete set of $(2l+1)$ independent base functions for a given total orbital angular momentum l, which are the homogeneous polynomials in the components of coordinate vectors and do not contain the Euler angles explicitly. Any function with the given angular momentum l in the system can be expanded with respect to the base functions, where the coefficients are the functions of the internal variables, called the generalized radial

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functions. The generalized radial equations satisfied by the functions are established explicitly.[29] For the typical three-body system in the real three-dimensional space,[30,31] such as a helium atom[32,33] and a positronium negative ion,[34] the generalized radial equations[35] have been solved numerically with high precision.

With the recent interest in higher dimensional field theory, we attempt to generalize the study of the D-dimensional two-body system to the D-dimensional three-body system. The purpose of this paper is, for a three-body system in an arbitrary D-dimensional space, to find a complete set of independent base functions with any given total orbital angular momentum and to reduce the Schrödinger equation with a spherically symmetric potential V to the generalized radial equations, where only three internal variables are involved. Any function with the given angular momentum in the system can be expanded with respect to the base functions. It provides a possibility to calculate numerically the energy levels of the three-body system in D-dimensions with high precision.

From the viewpoint of mathematics, the separation of the global rotational degrees of freedom from the internal ones is a typical application of group theory to physics. The properties of the independent base functions for a given total orbital angular momentum would be clearer if they were constructed in arbitrary D-dimensional space rather than in the real three-dimensional space. The total orbital angular momentum for a three-body system in a D-dimensional space is described by an irreducible representation denoted by a Young diagram with one or two rows. For the real three-dimensional space, the rotational symmetry group is SO(3) group, and its only irreducible representations denoted by the Young diagrams with two rows are $[l,1]$, which are equivalent to the representations denoted by the one-row Young diagrams $[l,0]$, respectively. This is the reason why the angular momentum can be described by only one quantum number l for the real three-dimensional space.

This paper is organized as follows. After separating the motion of the center of mass by the Jacobi coordinate vectors in Sec. II, we review in Sec. III the generalization of the orbital angular momentum operators and the properties of the spherical harmonics[4,6] and the harmonic polynomials[7] for a two-body system in D dimensions. In Sec. IV we will define the generalized harmonic polynomials for a three-body system in D dimensions and prove that they constitute a complete set of independent base functions for a given total orbital angular momentum in the system. The generalized radial functions are defined and the generalized radial equations are derived in Sec. V. Some conclusions will be given in Sec. VI.

II. SCHRÖDINGER EQUATION IN D DIMENSIONS

For a quantum N-body system in an arbitrary D-dimensional space, we denote the position vectors and the masses of N particles by $\mathbf{r}_k$ and by m_k, $k=1,2,\ldots,N$, respectively. $M=\Sigma_k m_k$ is the total mass. The Schrödinger equation for the N-body system with a pair potential V, depending upon the distance of each pair of particles, $|\mathbf{r}_j-\mathbf{r}_k|$, is

$$-\frac{1}{2}\sum_{k=1}^{N} m_k^{-1}\nabla_{\mathbf{r}_k}^2\Psi+V\Psi=E\Psi, \tag{1}$$

where $\nabla_{\mathbf{r}_k}^2$ is the Laplace operator with respect to the position vector $\mathbf{r}_k$. For simplicity, the natural units $\hbar=c=1$ are employed throughout this paper. The total orbital angular momentum operators L_{ab} in D dimensions are defined as[4,6]

$$L_{ab}=-L_{ba}=-i\sum_{k=1}^{N}\left\{r_{ka}\frac{\partial}{\partial r_{kb}}-r_{kb}\frac{\partial}{\partial r_{ka}}\right\}, \quad a,b=1,2,\ldots,D, \tag{2}$$

where r_{ka} denotes the ath component of the position vector $\mathbf{r}_k$.

Now, we replace the position vectors $\mathbf{r}_k$ by the Jacobi coordinate vectors $\mathbf{R}_j$:

$$\mathbf{R}_0 = M^{-1/2}\sum_{k=1}^{N} m_k \mathbf{r}_k, \quad \mathbf{R}_j = \left(\frac{m_{j+1}M_j}{M_{j+1}}\right)^{1/2}\left(\mathbf{r}_{j+1} - \sum_{k=1}^{j}\frac{m_k \mathbf{r}_k}{M_j}\right),$$
$$1 \leqslant j \leqslant (N-1), \quad M_j = \sum_{k=1}^{j} m_k, \quad M_N = M, \tag{3}$$

where $\mathbf{R}_0$ describes the position of the center of mass, $\mathbf{R}_1$ describes the mass-weighted separation from the second particle to the first particle. $\mathbf{R}_2$ describes the mass-weighted separation from the third particle to the center of mass of the first two particles, and so on. An additional factor $\sqrt{M}$ is included in $\mathbf{R}_j$ for convenience. The mass-weighted factors in front of the formulas for $\mathbf{R}_j$ are determined by the condition

$$\sum_{k=1}^{N} m_k \mathbf{r}_k^2 = \sum_{j=0}^{N-1} \mathbf{R}_j^2,$$

One may determine the factors one by one from the following schemes. In the center-of-mass frame, if the first j particles coincide with each other and the last $(N-j-1)$ particles are located at the origin, the factor in front of $\mathbf{R}_j$ is determined by

$$\mathbf{r}_1 = \mathbf{r}_2 = \cdots = \mathbf{r}_j = -m_{j+1}\mathbf{r}_{j+1}/M_j, \quad \sum_{k=1}^{j+1} m_k \mathbf{r}_k^2 = \mathbf{R}_j^2. \tag{4}$$

A straightforward calculation by replacement of variables shows that the Laplace operator in Eq. (1) and the total orbital angular momentum operator L_{ab} in Eq. (2) are directly expressed in $\mathbf{R}_j$:

$$\nabla^2 = \sum_{k=1}^{N} m_k^{-1}\nabla_{\mathbf{r}_k}^2 = \sum_{j=0}^{N-1} \nabla_{\mathbf{R}_j}^2,$$
$$L_{ab} = -i\sum_{j=0}^{N-1}\left\{R_{ja}\frac{\partial}{\partial R_{jb}} - R_{jb}\frac{\partial}{\partial R_{ja}}\right\}. \tag{5}$$

In the center-of-mass frame, $\mathbf{R}_0 = 0$. The Laplace operator (5) obviously has the symmetry of the $\mathrm{O}(ND-D)$ group with respect to $(N-1)D$ components of $(N-1)$ Jacobi coordinate vectors. The $\mathrm{O}(ND-D)$ group contains a subgroup $\mathrm{SO}(D)\times\mathrm{O}(N-1)$, where $\mathrm{SO}(D)$ is the rotation group in the D-dimensional space. The space inversion and the different definitions for the Jacobi coordinate vectors in the so-called Jacobi tree[24] can be obtained by $\mathrm{O}(N-1)$ transformations. For the system of identical particles, the permutation group among particles is also a subgroup of the $\mathrm{O}(N-1)$ group.[29]

It is easy to obtain the inverse transformation of Eq. (3):

$$\mathbf{r}_j = \left[\frac{M_{j-1}}{m_j M_j}\right]^{1/2}\mathbf{R}_{j-1} - \sum_{k=j}^{N-1}\left[\frac{m_{k+1}}{M_k M_{k+1}}\right]^{1/2}\mathbf{R}_k + M^{-1/2}\mathbf{R}_0,$$
$$\mathbf{r}_j - \mathbf{r}_k = \left[\frac{M_j}{m_j M_{j-1}}\right]^{1/2}\mathbf{R}_{j-1} + \sum_{i=k}^{j-2}\left[\frac{m_{i+1}}{M_i M_{i+1}}\right]^{1/2}\mathbf{R}_i - \left[\frac{M_{k-1}}{m_k M_k}\right]^{1/2}\mathbf{R}_{k-1}. \tag{6}$$

Thus, the potential V is a function of $\mathbf{R}_j\cdot\mathbf{R}_k$ and is rotationally invariant.

III. HARMONIC POLYNOMIALS IN *D* DIMENSIONS

In the center-of-mass frame, $\mathbf{R}_0=0$. Hence, for a two-body system there is only one Jacobi coordinate vector $\mathbf{R}_1$, which will be denoted by $\mathbf{x}$ for simplicity:

$$\mathbf{x}=\left(\frac{m_1m_2}{m_1+m_2}\right)^{1/2}\{\mathbf{r}_2-\mathbf{r}_1\},$$
$$\nabla^2=\nabla_{\mathbf{x}}^2,\quad L_{ab}=-i\left\{x_a\frac{\partial}{\partial x_b}-x_b\frac{\partial}{\partial x_a}\right\}. \tag{7}$$

Louck[4,6] introduced the hyperspherical coordinates

$$\begin{aligned}
x_1&=r\cos\theta_1\sin\theta_2\cdots\sin\theta_{D-1},\\
x_2&=r\sin\theta_1\sin\theta_2\cdots\sin\theta_{D-1},\\
x_k&=r\cos\theta_{k-1}\sin\theta_k\cdots\sin\theta_{D-1},\quad 3\leqslant k\leqslant D-1,\\
x_D&=r\cos\theta_{D-1}.
\end{aligned} \tag{8}$$

The spherical harmonics $Y^l_{l_{D-2},\ldots,l_1}$ in D dimensions[4,6] are the simultaneous eigenfunctions of the commutant operators $\mathbf{L}_k^2$:

$$\mathbf{L}_1^2=-\frac{\partial^2}{\partial\theta_1^2},\quad \mathbf{L}_k^2=-\left\{\frac{1}{\sin^{k-1}\theta_k}\frac{\partial}{\partial\theta_k}\sin^{k-1}\theta_k\frac{\partial}{\partial\theta_k}-\frac{\mathbf{L}_{k-1}^2}{\sin^2\theta_k}\right\}, \tag{9}$$

$$\mathbf{L}_1^2Y^l_{l_{D-2},\ldots,l_1}(\theta_1\cdots\theta_{D-1})=l_1^2Y^l_{l_{D-2},\ldots,l_1}(\theta_1\cdots\theta_{D-1}),$$
$$\mathbf{L}_k^2Y^l_{l_{D-2},\ldots,l_1}(\theta_1\cdots\theta_{D-1})=l_k(l_k+k-1)Y^l_{l_{D-2},\ldots,l_1}(\theta_1\cdots\theta_{D-1}), \tag{10}$$
$$l\equiv l_{D-1}=0,1,\ldots,\quad l_k=0,1,\ldots,l_{k+1},\quad l_1=-l_2,-l_2+1,\ldots,l_2-1,l_2,$$

where $\mathbf{L}^2\equiv\mathbf{L}_{D-1}^2$, $0\leqslant r<\infty$, $-\pi\leqslant\theta_1\leqslant\pi$, $0\leqslant\theta_k\leqslant\pi$, and $2\leqslant k\leqslant D-1$. The volume element of the configuration space is[4,14]

$$\prod_{j=1}^{D}\mathrm{d}x_j=r^{D-1}\mathrm{d}r\prod_{j=1}^{D-1}(\sin\theta_j)^{j-1}\mathrm{d}\theta_j. \tag{11}$$

Through a direct calculation by replacement of variables, one obtains[4,6]

$$\nabla_{\mathbf{x}}^2=\frac{1}{r^{D-1}}\frac{\partial}{\partial r}r^{D-1}\frac{\partial}{\partial r}-\frac{\mathbf{L}^2}{r^2}, \tag{12}$$

Due to the spherical symmetry, the wave function can be expressed as

$$\psi^l_{l_{D-2},\ldots,l_1}(\mathbf{x})=\phi_l(r)Y^l_{l_{D-2},\ldots,l_1}(\theta_1\cdots\theta_{D-1}), \tag{13}$$

and the D-dimensional Schrödinger equation (1) for a two-body system in the center-of-mass frame reduces to the radial equation

$$\frac{1}{r^{D-1}}\frac{\partial}{\partial r}r^{D-1}\frac{\partial}{\partial r}\phi_l(r)-\frac{l(l+D-2)}{r^2}\phi_l(r)=-2[E-V(r)]\phi_l(r). \tag{14}$$

Bander and Itzykson[7] introduced the harmonic polynomials in D dimensions

$$\mathcal{Y}^l_{l_{D-2},\ldots,l_1}(\mathbf{x}) = r^l Y^l_{l_{D-2},\ldots,l_1}(\theta_1\cdots\theta_{D-1}) \equiv r^l Y^l_{l_{D-2},\ldots,l_1}(\hat{\mathbf{x}}), \tag{15}$$

to avoid the angular functions $Y^l_{l_{D-2},\ldots,l_1}(\theta_1\cdots\theta_{D-1})$. $\mathcal{Y}^l_{l_{D-2},\ldots,l_1}(\mathbf{x})$ is a homogeneous polynomial of degree l in the components of $\mathbf{x}$ and satisfies the Laplace equation

$$\nabla^2_{\mathbf{x}} \mathcal{Y}^l_{l_{D-2},\ldots,l_1}(\mathbf{x}) = 0. \tag{16}$$

The number of linearly independent homogeneous polynomials of degree l in D components of $\mathbf{x}$ is $N(l) = (l+D-1)!/l!(D-1)!$. The Laplace equation (16) gives $N(l-2) = (l+D-3)!/(l-2)!(D-1)!$ constraints. Hence, the number of the harmonic polynomials $\mathcal{Y}^l_{l_{D-2},\ldots,l_1}(\mathbf{x})$ of degree l as well as the number of the spherical harmonics $Y^l_{l_{D-2},\ldots,l_1}(\hat{\mathbf{x}})$ in D dimensions is

$$N(l) - N(l-2) = \frac{(2l+D-2)(l+D-3)!}{l!(D-2)!} = d_D([l,0,\ldots,0]). \tag{17}$$

$d_D([l,0,\ldots,0])$ is the dimension of the irreducible representation of SO(D) denoted by the one-row Young diagram $[l,0,\ldots,0]$. $[l,0,\ldots,0]$ describes the symmetric traceless tensor representation. In fact, any polynomial in the components of one vector $\mathbf{x}$ has to belong to a symmetric representation.

Due to the spherical symmetry, one only needs to write the explicit form of the highest weight state[7]

$$\mathcal{Y}^l_{l,\ldots,l}(\mathbf{x}) = N_l (x_1 + i x_2)^l, \tag{18}$$

where N_l denotes the normalization factor. The partners of $\mathcal{Y}^l_{l,\ldots,l}(\mathbf{x})$ can be simply generated by rotation. Now, the solution to the Schrödinger equation in the center-of-mass frame can be reexpressed as

$$\psi^l_{l,\ldots,l}(\mathbf{x}) = R_l(r)\mathcal{Y}^l_{l,\ldots,l}(\mathbf{x}), \tag{19}$$

and the radial equation is easy to derive:

$$\frac{1}{r^{D-1}}\frac{\partial}{\partial r} r^{D-1}\frac{\partial}{\partial r} R_l(r) + \frac{2l}{r}\frac{\partial}{\partial r} R_l(r) = -2[E - V(r)]R_l(r). \tag{20}$$

Recall $R_l(r) = r^{-l}\phi_l(r)$. Equation (20) coincides with Eq. (14) but the angle variables do not appear explicitly in calculation.

The number (17) of the harmonic polynomials $\mathcal{Y}^l_{l_{D-2},\ldots,l_1}(\mathbf{x})$ of degree l can be understood from another viewpoint. After removing those homogeneous polynomials in the form $r^2 f(\mathbf{x})$, where $f(\mathbf{x})$ is a homogeneous polynomial of degree $(l-2)$, Eq. (17) shows the number of the remaining linearly independent homogeneous polynomials of degree l in the components of $\mathbf{x}$. Therefore, the harmonic polynomials $\mathcal{Y}^l_{l_{D-2},\ldots,l_1}(\mathbf{x})$ construct a complete set of linearly independent base functions for the homogeneous polynomials of degree l in the components of $\mathbf{x}$, excluding those in the form of $r^2 f(\mathbf{x})$.

IV. THREE-BODY SYSTEM IN D-DIMENSIONS

For a three-body system, in the center-of-mass frame there are two Jacobi coordinate vectors $\mathbf{R}_1$ and $\mathbf{R}_2$, which will be denoted by $\mathbf{x}$ and $\mathbf{y}$, respectively:

$$\mathbf{x}=\left[\frac{m_1m_2}{m_1+m_2}\right]^{1/2}\{\mathbf{r}_2-\mathbf{r}_1\},\quad \mathbf{y}=\left[\frac{(m_1+m_2)m_3}{m_1+m_2+m_3}\right]^{1/2}\left\{\mathbf{r}_3-\frac{m_1\mathbf{r}_1+m_2\mathbf{r}_2}{m_1+m_2}\right\},$$

$$\nabla^2=\nabla_{\mathbf{x}}^2+\nabla_{\mathbf{y}}^2, \tag{21}$$

$$L_{ab}=L_{ab}^{(x)}+L_{ab}^{(y)}=-i\left\{x_a\frac{\partial}{\partial x_b}-x_b\frac{\partial}{\partial x_a}\right\}-i\left\{y_a\frac{\partial}{\partial y_b}-y_b\frac{\partial}{\partial y_a}\right\},$$

The Schrödinger equation (1) reduces to

$$\{\nabla_{\mathbf{x}}^2+\nabla_{\mathbf{y}}^2\}\Psi(\mathbf{x},\mathbf{y})=-2\{E-V(\xi_1,\xi_2,\xi_3)\}\Psi(\mathbf{x},\mathbf{y}),$$
$$\xi_1=\mathbf{x}\cdot\mathbf{x},\quad \xi_2=\mathbf{y}\cdot\mathbf{y},\quad \xi_3=\mathbf{x}\cdot\mathbf{y}, \tag{22}$$

where ξ_j are the internal variables. Since Eq. (22) is rotational invariant, the total orbital angular momentum is conserved. The wave function $\Psi(\mathbf{x},\mathbf{y})$ with the given total angular momentum has to belong to an irreducible representation of SO(D). In the traditional method, one calculates the wave function by the Clebsch–Gordan coefficients:

$$\sum_{l_{D-2},\ldots,l_1 l'_{D-2},\ldots,l'_1}\mathcal{Y}^{l}_{l_{D-2},\ldots,l_1}(\mathbf{x})\mathcal{Y}^{l'}_{l'_{D-2},\ldots,l'_1}(\mathbf{y})\langle l,l_{D-2},\ldots,l_1;l',l'_{D-2},\ldots,l'_1|L,M\rangle. \tag{23}$$

As usual, $\mathcal{Y}^{l}_{l_{D-2},\ldots,l_1}(\mathbf{x})$ and $\mathcal{Y}^{l'}_{l'_{D-2},\ldots,l'_1}(\mathbf{y})$ are called the partial angular momentum states, and their combination is called the total angular momentum state, which is a homogeneous polynomial of degrees l and l' in the components of $\mathbf{x}$ and $\mathbf{y}$, respectively.

There are three problems. First, what kinds of representations (or total angular momentum L) appear in the Clebsch–Gordan series for decomposition of the direct product of two representations denoted by one-row Young diagrams $[l,0,\ldots,0]$ and $[l',0,\ldots,0]$? This problem has been solved in group theory by the Littlewood–Richardson rule and traceless conditions. A new character is that the representations denoted by two-row Young diagrams appear in the Clebsch–Gordan series for a three-body system when $D>3$. Those representations denoted by the Young diagrams with more than two rows could not appear because there are only two Jacobi coordinate vectors. For simplicity we denote a one-row or two-row Young diagram by $[\mu,\nu]\equiv[\mu,\nu,0,\ldots,0]$. Hence, we have the Clebsch–Gordan series:

$$[l,0]\otimes[l',0]\simeq\bigoplus_{s=0}^{n}\bigoplus_{t=0}^{n-s}[l+l'-s-2t,s], \tag{24}$$

where n is the minimum between l and l'. The representations with $t=0$ are calculated by the Littlewood–Richardson rule, and the remaining are calculated by the traceless conditions. The dimension of a representation denoted by a two-row Young diagram is

$$d_D([\mu,\nu])=(D+2\mu-2)(D+\mu+\nu-3)(D+2\nu-4)(\mu-\nu+1)$$
$$\times\frac{(D+\mu-4)!(D+\nu-5)!}{(\mu+1)!\,\nu!(D-2)!(D-4)!}. \tag{25}$$

When $D=4$, the representation denoted by a two-row Young diagram reduces to a direct sum of a self-dual representation $[(S)\mu,\nu]$ and an anti-self-dual one $[(A)\mu,\nu]$. Their dimensions are equal to half of $d_4([\mu,\nu])$ given in Eq. (25). When $D=3$, due to the traceless condition, the only representations with the two-row Young diagrams are representations $[\mu,1]$, which are equivalent to that with the one-row Young diagrams $[\mu,0]$, respectively. Equation (25) still holds for $D=3$. The second problem is how to calculate the Clebsch–Gordan coefficients. The calculation must be

very complicated. We will avoid the difficulty by the method of determining the highest weight states directly. The third problem is determining how many base functions are independent for a given total orbital angular momentum such that any wave function with the same angular momentum can be expanded with respect to the base functions where the coefficients are the functions of the internal variables. We are going to solve the last two problems by group theory.

Let us sketch some necessary knowledge of group theory. From the representation theory of Lie groups,[36–38] the Lie algebras of the SO$(2n+1)$ group and the SO$(2n)$ group are B_n and D_n, respectively. Their Chevalley bases with the subscript j, $1\leqslant j\leqslant n-1$, are the same:

$$H_j=L_{(2j-1)(2j)}-L_{(2j+1)(2j+2)},$$

$$E_j=(L_{(2j)(2j+1)}-iL_{(2j-1)(2j+1)}-iL_{(2j)(2j+2)}-L_{(2j-1)(2j+2)})/2, \tag{26a}$$

$$F_j=(L_{(2j)(2j+1)}+iL_{(2j-1)(2j+1)}+iL_{(2j)(2j+2)}-L_{(2j-1)(2j+2)})/2.$$

But, the bases with the subscript n are different:

$$H_n=2L_{(2n-1)(2n)},$$

$$E_n=L_{(2n)(2n+1)}-iL_{(2n-1)(2n+1)}, \tag{26b}$$

$$F_n=L_{(2n)(2n+1)}+iL_{(2n-1)(2n+1)}$$

for SO$(2n+1)$, and

$$H_n=L_{(2n-3)(2n-2)}+L_{(2n-1)(2n)},$$

$$E_n=(L_{(2n-2)(2n-1)}-iL_{(2n-3)(2n-1)}+iL_{(2n-2)(2n)}+L_{(2n-3)(2n)})/2, \tag{26c}$$

$$F_n=(L_{(2n-2)(2n-1)}+iL_{(2n-3)(2n-1)}-iL_{(2n-2)(2n)}+L_{(2n-3)(2n)})/2$$

for SO$(2n)$. H_k span the Cartan subalgebra, and their eigenvalues are the components of a weight vector $\mathbf{m}=(m_1,\ldots,m_n)$:

$$H_k|\mathbf{m}\rangle=m_k|\mathbf{m}\rangle, \quad 1\leqslant k\leqslant n. \tag{27}$$

If the eigenstates for a given weight $\mathbf{m}$ are degeneracy, this weight is called a multiple weight, otherwise a simple one. E_k are called the raising operators and F_k the lowering ones. For an irreducible representation denoted by a Young diagram $[\mu_1,\mu_2,\ldots]$ of SO(D), $\mu_j\geqslant\mu_{j+1}$, there is a highest weight $\mathbf{M}=(M_1,M_2,\ldots)$, which must be simple:

$$M_j=\mu_j-\mu_{j+1}, \quad 1\leqslant j\leqslant n-2,$$

$$M_{n-1}=\mu_{n-1}-\mu_n, \quad M_n=2\mu_n, \text{ for SO}(2n+1),$$

$$M_{n-1}=\mu_{n-1}-\mu_n, \quad M_n=\mu_{n-1}+\mu_n, \quad \text{for self-dual representation in SO}(2n),$$

$$M_{n-1}=\mu_{n-1}+\mu_n, \quad M_n=\mu_{n-1}-\mu_n, \quad \text{for anti-self-dual representation in SO}(2n). \tag{28}$$

Here we are not interested in the spinor representations where M_n is odd for SO$(2n+1)$ and $M_{n-1}+M_n$ is odd for SO$(2n)$. For a given irreducible representation $[\mu_1,\mu_2,\ldots]$ of SO(D), we only need to consider the highest weight state $|\mathbf{M}\rangle$, which satisfies

$$H_k|\mathbf{M}\rangle = M_k|\mathbf{M}\rangle, \quad E_k|\mathbf{M}\rangle = 0, \quad 1 \leqslant k \leqslant n, \tag{29}$$

because its partners can be calculated by the lowering operators F_k. In this paper the highest weight state will simply be called the wave functions with the given angular momentum $[\mu,\nu]$ for simplicity.

Now, we return to our problems. Recalling the Clebsch–Gordan series in Eq. (24), we can rewrite Eq. (23) for the highest weight state $\mathbf{M}$:

$$\mathcal{Y}^{l,l',s,t}_{\mathbf{M}}(\mathbf{x},\mathbf{y}) = \sum_{\mathbf{m}} \mathcal{Y}^{l}_{\mathbf{m}}(\mathbf{x})\mathcal{Y}^{l'}_{\mathbf{M}-\mathbf{m}}(\mathbf{y})\langle l,\mathbf{m},l',(\mathbf{M}-\mathbf{m})|[(l+l'-s-2t),s],\mathbf{M}\rangle, \tag{30}$$

where the subscripts of the harmonic polynomials are changed to the weights for simplicity. $\mathcal{Y}^{l,l',s,t}_{\mathbf{M}}(\mathbf{x},\mathbf{y})$ is the highest weight state of the representation $[(l+l'-s-2t),s]$. It is a homogeneous polynomial of degrees l and l' in the components of $\mathbf{x}$ and $\mathbf{y}$, respectively. Generally speaking, some $\mathcal{Y}^{l,l',s,t}_{\mathbf{M}}(\mathbf{x},\mathbf{y})$ may be expressed as a sum where each term is a product of an internal variable ξ_j and a homogeneous polynomial $f(\mathbf{x},\mathbf{y})$ of lower degree (see p. 042108-5 in Ref. 29). Since $\mathcal{Y}^{l,l',s,t}_{\mathbf{M}}(\mathbf{x},\mathbf{y})$ will be used as a base function for the wave function with a given angular momentum and the combinative coefficient is the function of the internal variables, in this meaning, the base function in the form of $\xi_j f(\mathbf{x},\mathbf{y})$ is not independent, and we should find out the independent and complete base functions for any given angular momentum $[\mu,\nu]$. In the following we are going to prove $\mathcal{Y}^{q,(\mu+\nu-q),\nu,0}_{\mathbf{M}}(\mathbf{x},\mathbf{y})$ and their partners, where $l=q$, $l'=\mu+\nu-q$, $s=\nu$, $t=0$, and $\nu \leqslant q \leqslant \mu$, constitute a complete set of independent base functions for the total orbital angular momentum $[\mu,\nu]$. In other words, those total angular momentum states $\mathcal{Y}^{l,l',s,t}_{\mathbf{M}}(\mathbf{x},\mathbf{y})$ with $t>0$ are not independent, where the sum of the partial angular momentum quantum number l and l' is larger than $\mu+\nu$ for the total angular momentum $[\mu,\nu]$.

The highest weight for the representation $[\mu,\nu]$ is $\mathbf{M}=(\mu-\nu,\nu,0,\ldots,0)$. Removing the normalization factor in $\mathcal{Y}^{q,(\mu+\nu-q),\nu,0}_{\mathbf{M}}(\mathbf{x},\mathbf{y})$, which is irrelevant here, we can determine the explicit form for $\mathcal{Y}^{q,(\mu+\nu-q),\nu,0}_{\mathbf{M}}(\mathbf{x},\mathbf{y})$ according to its orders in the components of $\mathbf{x}$ and $\mathbf{y}$ and the property of the highest weight state (29), and denote it by the generalized harmonic polynomial $Q^{\mu\nu}_q(\mathbf{x},\mathbf{y})$:

$$Q^{\mu\nu}_q(\mathbf{x},\mathbf{y}) = \frac{X_{12}^{q-\nu}Y_{12}^{\mu-q}}{(q-\nu)!(\mu-q)!}(X_{12}Y_{34}-Y_{12}X_{34})^{\nu} \sim \mathcal{Y}^{q,(\mu+\nu-q),\nu,0}_{\mathbf{M}}(\mathbf{x},\mathbf{y}), \quad 0 \leqslant \nu \leqslant q \leqslant \mu,$$
$$X_{12}=x_1+ix_2, \quad X_{34}=x_3+ix_4, \quad Y_{12}=y_1+iy_2, \quad Y_{34}=y_3+iy_4. \tag{31}$$

The formula for $Q^{\mu\nu}_q(\mathbf{x},\mathbf{y})$ holds for $D=3$ ($x_4=y_4=0$, $\nu=0$ or 1)[35,29] and $D>4$. When $D=4$ we denote the highest weight states by $Q^{(S)\mu\nu}_q(\mathbf{x},\mathbf{y})$ and $Q^{(A)\mu\nu}_q(\mathbf{x},\mathbf{y})$ for the self-dual representations and the anti-self-dual representations, respectively:

$$Q^{(S)\mu\nu}_q(\mathbf{x},\mathbf{y}) = \frac{X_{12}^{q-\nu}Y_{12}^{\mu-q}}{(q-\nu)!(\mu-q)!}(X_{12}Y_{34}-Y_{12}X_{34})^{\nu},$$

$$Q^{(A)\mu\nu}_q(\mathbf{x},\mathbf{y}) = \frac{X_{12}^{q-\nu}Y_{12}^{\mu-q}}{(q-\nu)!(\mu-q)!}(X_{12}Y'_{34}-Y_{12}X'_{34})^{\nu}, \tag{32}$$

$$X'_{34}=x_3-ix_4, \quad Y'_{34}=y_3-iy_4.$$

The generalized harmonic polynomial $Q^{\mu\nu}_q(\mathbf{x},\mathbf{y})$ is a homogeneous polynomial of degrees q and $(\mu+\nu-q)$ in the components of $\mathbf{x}$ and $\mathbf{y}$, respectively. It is a simultaneous eigenfunction of $\nabla^2_{\mathbf{x}}$, $\nabla^2_{\mathbf{y}}$, $\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}$, and the total angular momentum operator $\mathbf{L}^2$ [see Eq. (9)],

$$\nabla_{\mathbf{x}}^2 Q_q^{\mu\nu}(\mathbf{x},\mathbf{y}) = \nabla_{\mathbf{y}}^2 Q_q^{\mu\nu}(\mathbf{x},\mathbf{y}) = \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} Q_q^{\mu\nu}(\mathbf{x},\mathbf{y}) = 0,$$

$$\mathbf{L}^2 Q_q^{\mu\nu}(\mathbf{x},\mathbf{y}) = C_2([\mu,\nu]) Q_q^{\mu\nu}(\mathbf{x},\mathbf{y}), \tag{33}$$

$$C_2([\mu,\nu]) = \mu(\mu+D-2) + \nu(\nu+D-4),$$

where $C_2([\mu,\nu])$ is the Casimir calculated by a general formula [see (1.131) in Ref. 38]. The parity of $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ is obviously $(-1)^{\mu+\nu}$.

It is evident that $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ do not contain a function of the internal variables as a factor, nor do their partners due to the rotational symmetry. Therefore, $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ are independent base functions for the given angular momentum described by $[\mu,\nu]$. Now, we are going to prove that $(\mu-\nu+1)$ base functions $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ where $\nu \leqslant q \leqslant \mu$ are complete for the angular momentum $[\mu,\nu]$. That is, $Q_q^{\mu(l-\mu)}(\mathbf{x},\mathbf{y})$ with $0 \leqslant l-\mu \leqslant q \leqslant \mu$ and their partners construct a complete set of linearly independent base functions for the homogeneous polynomials of degree l in the components of $\mathbf{x}$ and $\mathbf{y}$, excluding those in the forms of $\xi_j f(\mathbf{x},\mathbf{y})$, where $f(\mathbf{x},\mathbf{y})$ is a homogeneous polynomial of degree $(l-2)$.

The number of linearly independent homogeneous polynomials of degree l in the components of $\mathbf{x}$ and $\mathbf{y}$ is

$$M_D(l) = \begin{pmatrix} l+2D-1 \\ 2D-1 \end{pmatrix}.$$

After removing those polynomials in the form $\xi_j f(\mathbf{x},\mathbf{y})$, the number $M(l)$ reduces to $K(l)$:

$$\begin{aligned} K_D(l) &= M_D(l) - 3M_D(l-2) + 3M_D(l-4) - M_D(l-6) \\ &= 4(l+D-3)[2l(l+2D-6) + (D-2)(2D-5)] \frac{(l+2D-7)!}{l!(2D-4)!}, \end{aligned} \tag{34}$$

when $l+2D \geqslant 7$, which only excludes one case of $l=0$ and $D=3$, where $K_3(0)=1$.

On the other hand, the number of $Q_q^{\mu(l-\mu)}(\mathbf{x},\mathbf{y})$ with $0 \leqslant l-\mu \leqslant q \leqslant \mu$ and their partners can be calculated directly from Eq. (25):

$$\sum_{l/2 \leqslant \mu \leqslant l} (2\mu - l + 1) d_D([\mu,(l-\mu)]) = K_D(l). \tag{35}$$

Equations (34) and (35) are checked by MATHEMATICA. Thus, we have proved that $(\mu-\nu+1)$ base functions $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ where $0 \leqslant \nu \leqslant q \leqslant \mu$ are independent and complete for the angular momentum $[\mu,\nu]$. Any function with the angular momentum $[\mu,\nu]$ in the system can be expanded with respect to the base functions $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$, where the coefficients are functions of internal variables.

From Eq. (30), for a given total orbital angular momentum $[\mu,\nu]$ there are infinite number of wave functions $\mathcal{Y}_{\mathbf{M}}^{(q+t),(\mu+\nu+t-q),\nu,t}(\mathbf{x},\mathbf{y})$ combined from different partial angular momentum states. Now, what we have proved is that only a finite number of partial angular momentum states $(t=0)$ are involved in the complete set of independent base functions $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ for a given total orbital angular momentum $[\mu,\nu]$.

V. GENERALIZED RADIAL EQUATIONS

In Sec. IV we proved that any function with angular momentum $[\mu,\nu]$ in the quantum three-body system of D dimensions can be expanded with respect to the base functions $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$,

$$\Psi_{\mathbf{M}}^{[\mu,\nu]}(\mathbf{x},\mathbf{y}) = \sum_{q=\nu}^{\mu} \psi_q^{\mu\nu}(\xi_1,\xi_2,\xi_3) Q_q^{\mu\nu}(\mathbf{x},\mathbf{y}), \tag{36}$$

where the coefficients $\psi_q^{\mu\nu}(\xi_1,\xi_2,\xi_3)$ are called the generalized radial functions. When substituting Eq. (36) into the Schrödinger equation (22), the main calculation in the derivation is to apply the Laplace operator (21) to the function $\Psi_{\mathbf{M}}^{[\mu,\nu]}(\mathbf{x},\mathbf{y})$. The calculation consists of three parts. The first is to apply the Laplace operator to the generalized radial functions $\psi_q^{\mu\nu}(\xi_1,\xi_2,\xi_3)$, which can be calculated by replacement of variables:

$$\nabla^2\psi_q^{\mu\nu}(\xi_1,\xi_2,\xi_3)=\{4\xi_1\partial_{\xi_1}^2+4\xi_2\partial_{\xi_2}^2+2D(\partial_{\xi_1}+\partial_{\xi_2})+(\xi_1+\xi_2)\partial_{\xi_3}^2 +4\xi_3(\partial_{\xi_1}+\partial_{\xi_2})\partial_{\xi_3}\}\psi_q^{\mu\nu}(\xi_1,\xi_2,\xi_3), \tag{37}$$

where ∂_ξ denotes $\partial/\partial\xi$ and so on. The second is to apply it to the generalized harmonic polynomials $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$. This part is vanishing because $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ satisfies the Laplace equation. The last part is the mixed application

$$2\{(\partial_{\xi_1}\psi_q^{\mu\nu})2\mathbf{x}+(\partial_{\xi_3}\psi_q^{\mu\nu})\mathbf{y}\}\cdot\nabla_{\mathbf{x}}Q_q^{\mu\nu}+2\{(\partial_{\xi_2}\psi_q^{\mu\nu})2\mathbf{y}+(\partial_{\xi_3}\psi_q^{\mu\nu})\mathbf{x}\}\cdot\nabla_{\mathbf{y}}Q_q^{\mu\nu}. \tag{38}$$

From the definition (31) for $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ we have

$$\begin{gathered}\mathbf{x}\cdot\nabla_{\mathbf{x}}Q_q^{\mu\nu}=qQ_q^{\mu\nu},\quad \mathbf{y}\cdot\nabla_{\mathbf{y}}Q_q^{\mu\nu}=(\mu+\nu-q)Q_q^{\mu\nu}\\ \mathbf{y}\cdot\nabla_{\mathbf{x}}Q_q^{\mu\nu}=(\mu-q+1)Q_{q-1}^{\mu\nu},\quad \mathbf{x}\cdot\nabla_{\mathbf{y}}Q_q^{\mu\nu}=(q-\nu+1)Q_{q+1}^{\mu\nu}.\end{gathered} \tag{39}$$

Hence, we obtain the generalized radial equation, satisfied by the $(\mu-\nu+1)$ functions $\psi_q^{\mu\nu}(\xi_1,\xi_2,\xi_3)$:

$$\begin{aligned}&\nabla^2\psi_q^{\mu\nu}+4q\partial_{\xi_1}\psi_q^{\mu\nu}+4(\mu+\nu-q)\partial_{\xi_2}\psi_q^{\mu\nu}+2(\mu-q)\partial_{\xi_3}\psi_{q+1}^{\mu\nu}+2(q-\nu)\partial_{\xi_3}\psi_{q-1}^{\mu\nu}\\ &\quad=-2(E-V)\psi_q^{\mu\nu},\end{aligned} \tag{40}$$

where $\nabla^2\psi_q^{\mu\nu}$ is given in Eq. (37). Only three invariant variables ξ_1, ξ_2, and ξ_3 are involved both in the equations and in the functions. When $D=4$, Eq. (40) holds for the generalized radial functions either in $[(S)\mu,\nu]$ or in $[(A)\mu,\nu]$, because two representations incorporate to one irreducible representation of the O(4) group when the space inversion is considered. When $D=3$, the equations for the functions in $[\mu,0]$ and in $[\mu,1]$ are different although two representations $[\mu,0]$ and $[\mu,1]$ are equivalent, because the functions have different parity.

At last, we discuss rotational variables and the volume element of the configuration space. We fix the body-fixed frame such that $\mathbf{x}$ is parallel with its Dth axis, and $\mathbf{y}$ is located in its $(D-1)D$ hyperplane with a non-negative $(D-1)$th component. That is, in the body-fixed frame, the nonvanishing components of two Jacobi coordinate vectors $\mathbf{x}'$ and $\mathbf{y}'$ are

$$x_D'=\xi_1^{1/2},\quad y_{D-1}'=(\xi_2-\xi_3^2/\xi_1)^{1/2},\quad y_D'=\xi_3\xi_1^{-1/2}. \tag{41}$$

Let $R=R^{(1)}R^{(2)}\in\mathrm{SO}(D)$ rotate the center-of-mass frame to the body-fixed frame:

$$\begin{gathered}R^{(1)}=R_{12}(\theta_1)R_{31}(\theta_2)R_{43}(\theta_3)R_{54}(\theta_4)\cdots R_{D(D-1)}(\theta_{D-1}),\\ R^{(2)}=R_{12}(\varphi_1)R_{31}(\varphi_2)R_{43}(\varphi_3)R_{54}(\varphi_4)\cdots R_{(D-1)(D-2)}(\varphi_{D-2}),\\ R\mathbf{x}'=\mathbf{x},\quad R\mathbf{y}'=\mathbf{y},\end{gathered} \tag{42}$$

where, for example, $R_{12}(\theta)$ is a rotation on the hyperplane with the first and the second axes through θ angle:

$$R_{12}(\theta)=\begin{pmatrix}\cos\theta & -\sin\theta & 0\\ \sin\theta & \cos\theta & 0\\ 0 & 0 & \mathbf{1}_{D-2}\end{pmatrix}.$$

$(D-1)\,\theta_j$ and $(D-2)\,\varphi_k$ are the rotational variables, called the generalized Euler angles. Through a straightforward calculation, we obtain

$$x_1+ix_2=\xi_1^{1/2}e^{i\theta_1}\prod_{a=2}^{D-1}\sin\theta_a,\quad x_3+ix_4=\xi_1^{1/2}(\cos\theta_2\sin\theta_3+i\cos\theta_3)\prod_{a=4}^{D-1}\sin\theta_a,$$

$$y_1+iy_2=\xi_3\xi_1^{-1/2}e^{i\theta_1}\prod_{a=2}^{D-1}\sin\theta_a+(\xi_2-\xi_3^2/\xi_1)^{1/2}e^{i\theta_1}\Bigg\{i\prod_{a=1}^{D-2}\sin\varphi_a+\sum_{a=1}^{D-2}\cos\theta_{a+1}\cos\varphi_a\Bigg(\prod_{b=2}^{a}\sin\theta_b\Bigg)\Bigg(\prod_{c=a+1}^{D-2}\sin\varphi_c\Bigg)\Bigg\},\tag{43}$$

$$y_3+iy_4=\xi_3\xi_1^{-1/2}(\cos\theta_2\sin\theta_3+i\cos\theta_3)\prod_{a=4}^{D-1}\sin\theta_a+(\xi_2-\xi_3^2/\xi_1)^{1/2}$$
$$\times\Bigg\{-\cos\varphi_1\sin\theta_2\prod_{a=2}^{D-2}\sin\varphi_a+(\cos\theta_2\cos\theta_3-i\sin\theta_3)\cos\varphi_2\prod_{a=3}^{D-2}\sin\varphi_a$$
$$+(\cos\theta_2\sin\theta_3+i\cos\theta_3)\sum_{a=3}^{D-2}\cos\theta_{a+1}\cos\varphi_a\Bigg(\prod_{b=4}^{a}\sin\theta_b\Bigg)\Bigg(\prod_{c=a+1}^{D-2}\sin\varphi_c\Bigg)\Bigg\},$$

where $\Pi_{a=b+1}^{b}F_a=1$. The volume element of the configuration space is

$$\prod_{j=1}^{D}\mathrm{d}x_j\mathrm{d}y_j=\frac{1}{4}(\xi_1\xi_2-\xi_3^2)^{(D-3)/2}\mathrm{d}\xi_1\mathrm{d}\xi_2\mathrm{d}\xi_3\prod_{j=1}^{D-1}(\sin\theta_j)^{j-1}\mathrm{d}\theta_j\prod_{k=1}^{D-2}(\sin\varphi_k)^{k-1}\mathrm{d}\varphi_k.\tag{44}$$

VI. CONCLUSIONS

After separating the motion of center of mass, we have defined the homogeneous polynomial $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ of degree q and $(\mu+\nu-q)$ in the components of the Jacobi coordinate vectors $\mathbf{x}$ and $\mathbf{y}$, respectively. $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ is a solution of the Laplace equation. We have proved that $(\mu-\nu+1)$ generalized harmonic polynomials $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$ constitute a complete set of independent base functions for the total orbital angular momentum $[\mu,\nu]$. Any wave function with the given angular momentum in the system can be expanded with respect to the base functions, where the coefficients are the functions of the internal variables, called the generalized radial functions. The three-body Schrödinger equation with a spherically symmetric potential V in D dimensions reduces to the generalized radial equations satisfied by the generalized radial functions. Only three internal variables are involved in the functions and equations. The number of both the functions and the equations for the given angular momentum $[\mu,\nu]$ is finite and equal to $(\mu-\nu+1)$. Only a finite number of partial angular momentum states are involved in constructing the generalized harmonic polynomials $Q_q^{\mu\nu}(\mathbf{x},\mathbf{y})$, and the contributions from the remaining partial angular momentum states have been incorporated into those from the generalized radial functions.

The generalization of this method to a quantum N-body system in D-dimensions is straightforward. The difficulty is how to obtain the unified forms for the generalized harmonic polynomials, because it needs $D-1$ vectors to determine the body-fixed frame and there are $N-1$ Jacobi coordinate vectors. The cases with $N<D$ are very different from the cases with $N\geqslant D$. We will study this problem elsewhere.

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The reduction of a quantum system of three identical particles on a plane

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Quantum systems of three identical particles on a plane are analyzed from the viewpoint of symmetry. Upon reduction by rotation, such systems are described in the space of sections of a line bundle over a three-dimensional shape space whose origin represents triple collision. It is shown that if the total angular momentum is nonzero, then the wave section must vanish at the origin, while if it is zero, then the wave section can be finite at the origin. Since the particles are assumed to be identical, the quantum system admits the action of the symmetric group S_3 as well, which stands for the group of particle exchanges and is commutative with rotation. Hence the reduced system still admits the S_3 action, so that Bose and Fermi states can be discussed in the space of sections of the line bundle. A detailed analysis of a system of three free particles on a plane is presented in the latter part of the article. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1473872]

I. INTRODUCTION

This article deals with quantum mechanics on the center-of-mass system of three identical particles on a plane, which has manifestly two kinds of symmetries: They are rotation of all particles about the origin and particle exchanges. As is well recognized, symmetry is closely associated with the reduction of dynamical systems. One of the authors (T.I.) has already studied the reduction of quantum planar three-body systems by the use of rotational symmetry.[1] As for the reduction of multiparticle systems with rotational symmetry, a point to make is the fact that the center-of-mass system is made into a principal fiber bundle with the rotation group as structure group, if the center-of-mass system is restricted to a subspace on which the rotation group acts freely. This fact was first proved by Guichardet.[2] On the basis of this bundle picture, a gauge theoretical treatment becomes feasible for multiparticle systems. After Ref. 2, a number of articles[3–8] were published by T.I. for analyzing multiparticle systems in a gauge theoretical manner. The reduction method for multiparticle systems with rotational symmetry has been extended in a rather abstract way by the use of the Peter–Weyl theorem on unitary irreducible representations of compact Lie groups.[9] From a physical point of view, an original article[10] and a review article[11] are of great help for the gauge theoretical treatment of multiparticle systems. The gauge theoretical treatment has been given to deformable bodies as well.[12–14]

As is already known,[1] if the triple collision of particles is excluded, the center-of-mass system for planar three bodies is diffeomorphic with $\dot{\mathrm{R}}^4$ and made into a principal fiber bundle $\dot{\mathrm{R}}^4 \to \dot{\mathrm{R}}^3$ with structure group SO(2), where SO(2) stands for the rotational symmetry whose action is to the left, and the dot symbol indicates that the origin is removed from the space in question. Further, if all the particles are identical, it will be found that the symmetric group S_3, which stands for the symmetry of three-particle exchanges, also acts on the center-of-mass system. This action is to the right and will be shown to be expressed in terms of matrices representing the group S_3. Since the right and left actions commute, the action of S_3 will project to the factor space $\dot{\mathrm{R}}^3 \cong \dot{\mathrm{R}}^4/\mathrm{SO}(2)$. In

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what follows, when the whole center-of-mass system is considered, the triple collision is taken into account.

On the basis of the symmetry of rotation and particle exchanges, the space of wave functions on R^4 is broken up into a series of subspaces that are interpreted as eigenspaces associated with both SO(2) and S_3, and the time evolution of the original quantum system on R^4 induces respective time evolutions in the subspaces, accordingly. The reduction to subsystems is thus accomplished. These subsystems will be identified with reduced systems to be defined on $\dot{\mathrm{R}}^3 \cong \dot{\mathrm{R}}^4/\mathrm{SO}(2)$ along with boundary conditions at the origin. While the theory should apply to a system containing any number of particles, and of course can do in three dimensions, too, we have chosen $n=3$ for the number of particles to present the idea in a simple form.

The organization of this paper is as follows: Section II contains a review of the center-of-mass system and of Jacobi vectors. Section III is a review of the principal bundle $\dot{\mathrm{R}}^4 \to \dot{\mathrm{R}}^3$ with structure group SO(2). A connection form defined on $\dot{\mathrm{R}}^4$ and a metric defined on $\dot{\mathrm{R}}^3$ will also be reviewed, and thereby the distance function with respect to that metric on $\dot{\mathrm{R}}^3$ will be discussed. In Sec. IV, the action of the symmetric group S_3 on the center-of-mass system is represented explicitly in terms of matrices. Since the action of SO(2) and of S_3 commute, the action of S_3 on the center-of-mass system $\dot{\mathrm{R}}^4$ projects to $\dot{\mathrm{R}}^3$, which is given explicitly in Sec. V. In Sec. VI, the L^2 space of wave functions on the center-of-mass system R^4 is decomposed into the sum of spaces of ''equivariant'' functions with respect to the SO(2) action on R^4. If a quantum system is SO(2) invariant, the time evolution in the L^2 space is reduced to that in the space of equivariant functions, accordingly. In Sec. VII, interest will center on what will actually happen at the origin, the boundary of $\dot{\mathrm{R}}^4$, if the triple collision is taken into account. Boundary conditions for wave functions at the origin of R^4 are to be considered by the use of the equivariance condition. It will be shown that according to whether the total angular momentum is nonzero or zero, the wave function vanishes at the origin or takes a finite value there. In Sec. VIII, the symmetry of particle exchanges are discussed in the space of wave functions on the center-of-mass system. The Bose and Fermi states are characterized by the respective representations of the permutation group S_3 acting on the center-of-mass system. Since the action of SO(2) and of S_3 commute, both the Bose and Fermi states can be constructed in the space of equivariant functions. Thus the reduction to subsystems is accomplished by the use of the symmetry of rotation and particle exchanges. Section IX deals with complex line bundles associated with the principal bundle $\dot{\mathrm{R}}^4 \to \dot{\mathrm{R}}^3$. It is shown that the spaces of equivariant functions described in Sec. VI are in one-to-one correspondence with the spaces of ''sections'' in those complex line bundles with boundary conditions at the origin of R^3. Since the action of SO(2) and of S_3 commute, it further turns out that the subsystems studied in Sec. VIII are indeed equivalent to quantum systems defined in the space of sections with the boundary condition at the origin along with the restriction to the Bose or Fermi state. In Sec. X, the reduction procedure is applied to a system of free identical particles on a plane. The time evolution of the system reduces to the time evolution in the space of equivariant functions, which is expressed in the form of integral transform, and further Bose and Fermi states are formed according to the procedure developed in Sec. VIII. Section XI contains a local expression of the boundary conditions studied in Sec. VII, and also deals with a local expression of the integral transform obtained in Sec. X, to show explicitly how the reduction is accomplished indeed. Section XII contains remarks on applications to electrons on a plane.

II. THE CONFIGURATION SPACE

Suppose there are three particles on a plane, each with position vectors $\mathbf{x}_j$, $j=1,2,3$, and masses m_j, $j=1,2,3$, respectively. The set of all possible particle positions, X, is identified with $\mathrm{R}^{2\times 3}$, which consists of ordered triples of position vectors $(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)$.

Given the space X, one can consider two fundamental motions traced by the particles, one of which is translation and the other rotation. The space X is endowed with the inner product $K:X \times X \to \mathrm{R}$ which is defined by

$$K(x,y)=\sum_{j=1}^{3} m_j(\mathbf{x}_j,\mathbf{y}_j), \quad x=(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3), \quad y=(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3)\in X, \tag{1}$$

where $(\mathbf{x},\mathbf{y})$ denotes the standard inner product on R^2.

Getting rid of translational degrees of freedom, we shall focus on the center-of-mass system, which is defined by

$$X_0=\left\{(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\in X\left|\sum_{j=1}^{3} m_j\mathbf{x}_j=0\right.\right\}. \tag{2}$$

From Ref. 1, we find that X_0 has the following orthonormal basis with respect to the metric K:

$$\begin{aligned} f_1&=N_1(-m_2\mathbf{e}_1,m_1\mathbf{e}_1,0),\\ f_2&=N_1(-m_2\mathbf{e}_2,m_1\mathbf{e}_2,0),\\ f_3&=N_2(-m_3\mathbf{e}_1,-m_3\mathbf{e}_1,(m_1+m_2)\mathbf{e}_1),\\ f_4&=N_2(-m_3\mathbf{e}_2,-m_3\mathbf{e}_2,(m_1+m_2)\mathbf{e}_2), \end{aligned} \tag{3}$$

where N_j are the normalizing factors explicitly given by

$$\begin{aligned} N_1&=(m_1m_2(m_1+m_2))^{-1/2},\\ N_2&=(m_3(m_1+m_2)(m_1+m_2+m_3))^{-1/2}. \end{aligned} \tag{4}$$

With respect to $f_j, j=1,\ldots,4$, any $x\in X_0$ is represented as

$$x=\sum_{j=1}^{4} q_jf_j, \quad q_j=K(x,f_j). \tag{5}$$

These coefficients q_j serve as the Cartesian coordinates in X_0.

The space X_0 is isomorphic to R^4 and also to $\mathrm{R}^2\times\mathrm{R}^2$, the set of pair of vectors in R^2. We define the pair of two vectors as follows:

$$\begin{aligned} \mathbf{r}_1&=q_1\mathbf{e}_1+q_2\mathbf{e}_2=\sqrt{\frac{m_1m_2}{m_1+m_2}}(\mathbf{x}_2-\mathbf{x}_1),\\ \mathbf{r}_2&=q_3\mathbf{e}_1+q_4\mathbf{e}_2=\sqrt{\frac{m_3(m_1+m_2)}{m_1+m_2+m_3}}\left(\mathbf{x}_3-\frac{m_1\mathbf{x}_1+m_2\mathbf{x}_2}{m_1+m_2}\right). \end{aligned} \tag{6}$$

The vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ are called the Jacobi vectors, which will be effectively used in dealing with particle exchanges. Figure 1 illustrates the visual view of the Jacobi vectors, but the arrow lengths are not drawn to scale.

Both the orthonormal basis $\{f_j\}_{j=1,\ldots,4}$ and the Jacobi vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ are easily generalized for a planar n-body system,[5] and for a spatial n-body system[3,9] as well.

III. THE INTERNAL SPACE

Having removed the translational degrees of freedom in Sec. II, we now consider in this section the symmetry due to the rotation,

$$x=(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\mapsto gx=(g\mathbf{x}_1,g\mathbf{x}_2,g\mathbf{x}_3), \quad g\in \mathrm{SO}(2), \quad x\in X_0. \tag{7}$$

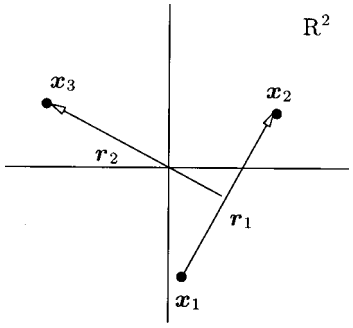

FIG. 1. Illustrating the Jacobi vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ as seen in Eq. (6). $\mathbf{r}_1$ points along the line joining particles 1 and 2, while $\mathbf{r}_2$ points along the line joining particles 3 and the center-of-mass of particles 1 and 2. Note that the arrow lengths are *not* drawn to scale.

For a while, we forget the case where all particles collide at the origin, and consider the configuration space $\dot{X}_0 := X_0 - \{0\}$. Then the SO(2) action becomes free. Further, the SO(2) action defines an equivalence relation on $\dot{X}_0$, and gives rise to a quotient space $\dot{X}/\mathrm{SO}(2)$. We denote by π the natural projection from $\dot{X}_0$ to the quotient space,

$$\pi: \dot{X}_0 \to M := \dot{X}_0/\mathrm{SO}(2), \quad \pi(x) = [x], \quad x \in \dot{X}_0, \tag{8}$$

where $[x]$ denotes the equivalence class of x. The space M turns out to be a manifold which we shall call the internal or the shape space. Thus $\dot{X}_0$ is made into a fiber bundle with structure group SO(2).[1]

To elaborate the discussion, we give the explicit form of the projection (8). Let $q = (q_1, q_2, q_3, q_4)$ denote points of space $\dot{X}_0$, just as was defined in (5). We notice that $X_0 \cong \mathrm{R}^4$ is identified with C^2 by introducing the complex variables z_1, z_2 through

$$z_1 = q_1 + iq_2, \quad z_2 = q_3 + iq_4, \quad i = \sqrt{-1}. \tag{9}$$

On account of $g = \left(\begin{smallmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{smallmatrix}\right)$, the SO(2) action on C^2 turns out to be expressed as

$$z = (z_1, z_2) \mapsto (e^{it} z_1, e^{it} z_2) = e^{it} z. \tag{10}$$

With the identification $X_0 \cong \mathrm{C}^2$, the natural projection π is realized as

$$\pi: (z_1, z_2) \mapsto (\xi_1, \xi_2, \xi_3), \tag{11}$$

where

$$\xi_1 + i\xi_2 = 2z_1\overline{z_2}, \quad \xi_3 = |z_1|^2 - |z_2|^2. \tag{12}$$

Note here that

$$\sqrt{\sum_{k=1}^{3} \xi_k^2} = \sum_{j=1}^{4} q_j^2 . \tag{13}$$

It can be verified that the shape space M is diffeomorphic with $\dot{\mathrm{R}}^3 := \mathrm{R}^3 - \{0\}$;[1]

$$M := \dot{X}_0/\mathrm{SO}(2) \cong \dot{\mathrm{R}}^3. \tag{14}$$

Thus the rotational degree of freedom is removed to provide the shape space M.

In the remainder of this section, we make a review of the connection defined on the SO(2) bundle $\dot{X}_0 \to M$ and of the metric defined on M. A one-form ω defined to be

$$\omega = \frac{1}{\Sigma_{j=1}^{4} q_j^2}(-q_2 dq_1 + q_1 dq_2 - q_4 dq_3 + q_3 dq_4) \tag{15}$$

is called a connection form on the SO(2) bundle $\dot{X}_0 \to M$. The connection form gives rise to a direct sum decomposition of the tangent space $T_x(\dot{X}_0)$ at each point x of $\dot{X}_0$,

$$T_x(\dot{X}_0) = V_x \oplus H_x, \quad H_x := \ker \omega_x, \quad V_x := T_x(\mathcal{O}_x), \tag{16}$$

where ω_x is considered as a linear map from the tangent space $T_x(\dot{X}_0)$ to the Lie algebra $so(2) \cong \mathrm{R}$ of SO(2), and $T_x(\mathcal{O}_x)$ denotes the tangent space at x to the SO(2)-orbit $\mathcal{O}_x$ through $x \in \dot{X}_0$. Note here that the subspaces H_x and V_x are orthogonal to each other with respect to the Euclidean metric K_x on $\dot{X}_0$. Since the subspace H_x is isomorphic, as a vector space, to the tangent space $T_{\pi(x)}(M)$ to M at $\pi(x) = \xi$ through the differential π_* of the projection map π, and since the metric on the center-of-mass system $\dot{X}_0$ is invariant under the SO(2) action, a metric $\tilde{K}$ on M is defined through

$$K_x(U_1, U_2) = \tilde{K}_{\pi(x)}(\pi_* U_1, \pi_* U_2), \quad U_1, U_2 \in H_x. \tag{17}$$

A straightforward calculation shows that $\tilde{K}$ is expressed as

$$\tilde{K} = \frac{1}{4r} \sum_{k=1}^{3} d\xi_k^2, \quad r = \sqrt{\sum_{k=1}^{3} \xi_k^2}. \tag{18}$$

By using the metric $\tilde{K}$, we are to evaluate the distance $d_M(\xi, \xi')$ of two points ξ, ξ' of M, which will be used in Sec. XI. Since $d_M(\xi, \xi')$ is equal to the length of the geodesic joining ξ to ξ', we have to find that geodesic. To this end, we first consider horizontal geodesics in $\dot{X}_0$ with respect to the Euclidean metric, where a curve $c(t)$ in $\dot{X}_0$ is, in general, called horizontal if its tangent vector $\dot{c}(t)$ is horizontal, $\dot{c}(t) \in H_{c(t)}$. We now take $z \in \pi^{-1}(\xi)$ and $w \in \pi^{-1}(\xi')$. The horizontal geodesic in $\dot{X}_0$ which projects to the geodesic in M joining ξ to ξ' should be a horizontal straight line joining $e^{is}z$ to w for a certain real number s,

$$u(t) = w + t(e^{is}z - w), \quad 0 \leqslant t \leqslant 1, \tag{19}$$

where the parameter s is to be determined so that $u(t)$ may be horizontal. By definition, the curve $u(t)$ is horizontal if and only if $\omega(\dot{u}(t)) = 0$. A straightforward calculation along with (15) shows that $\omega(\dot{u}(t)) = 0$ is equivalent to

$$\sum_{k=1}^{2} \left(u_k \frac{d\overline{u_k}}{dt} - \overline{u_k} \frac{du_k}{dt} \right) = -2i \left| \sum_{k=1}^{2} z_k \overline{w_k} \right| \sin(s + \theta) = 0, \tag{20}$$

where θ is the argument of $\Sigma_{k=1}^{2} z_k \overline{w_k}$. Thus, $u(t)$ is horizontal if and only if s is determined so as to satisfy $\sin(s+\theta) = 0$ or $\cos(s+\theta) = \pm 1$. For s thus determined, the horizontal straight line $u(t)$ projects to the geodesic $\pi(u(t))$ joining ξ and ξ'. From the definition of the metric $\tilde{K}$, the length of $u(t)$, $0 \leqslant t \leqslant 1$, with respect to K, is equal to that of $\pi(u(t))$, $0 \leqslant t \leqslant 1$, with respect to $\tilde{K}$. The squared length of the $u(t)$, $0 \leqslant t \leqslant 1$ is now calculated as

$$\sum_{k=1}^{2}|e^{is}z_k-w_k|^2=\sum_{k=1}^{2}|z_k|^2+\sum_{k=1}^{2}|w_k|^2\pm 2\left|\sum_{k=1}^{2}z_k\overline{w_k}\right|. \tag{21}$$

On account of the minimum property of the distance, we must choose the minus sign in Eq. (21). The right-hand side of (21) can be expressed in terms of ξ and ξ', and then provides the squared distance between ξ and ξ',

$$d_M(\xi,\xi')^2=r+r'-\sqrt{2}\sqrt{rr'+\sum_{k=1}^{3}\xi_k\xi'_k}, \tag{22}$$

where

$$r=\sqrt{\sum_{k=1}^{3}\xi_k^2},\quad r'=\sqrt{\sum_{k=1}^{3}\xi_k'^2}. \tag{23}$$

IV. EXCHANGES OF PARTICLES

In Sec. III, we made use of the rotational symmetry to obtain the shape space M. We now turn to another symmetry, the symmetry of configurations arising from exchanges of identical particles. Thus, in this section, we assume that all particles are identical, and without loss of generality put $m_j=1$, $j=1,2,3$. Then the Jacobi vectors defined in Eq. (6) become

$$\begin{aligned}\mathbf{r}_1&=\frac{1}{\sqrt{2}}(\mathbf{x}_2-\mathbf{x}_1),\\ \mathbf{r}_2&=\sqrt{\frac{2}{3}}\left(\mathbf{x}_3-\frac{\mathbf{x}_1+\mathbf{x}_2}{2}\right).\end{aligned} \tag{24}$$

Let S_3 be a symmetric group, the group of permutations of three symbols. If a configuration undergoes the change

$$(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\mapsto(\mathbf{x}_{\sigma(1)},\mathbf{x}_{\sigma(2)},\mathbf{x}_{\sigma(3)}),\quad \sigma\in S_3, \tag{25}$$

the Jacobi vectors associated with the new configuration are given by

$$\begin{aligned}\mathbf{r}_1^{\sigma}&=\frac{1}{\sqrt{2}}(\mathbf{x}_{\sigma(2)}-\mathbf{x}_{\sigma(1)}),\\ \mathbf{r}_2^{\sigma}&=\sqrt{\frac{2}{3}}\left(\mathbf{x}_{\sigma(3)}-\frac{\mathbf{x}_{\sigma(1)}+\mathbf{x}_{\sigma(2)}}{2}\right).\end{aligned} \tag{26}$$

The graphical representation of particle exchanges is given in Fig. 2, indicating which transformation takes the reference Jacobi vectors to which pair of new Jacobi vectors. From (26), one soon realizes that any particle exchanges can be represented by a linear transformation of Jacobi vectors $\mathbf{r}_1$ and $\mathbf{r}_2$. This will imply that the center-of-mass system of three identical particles admits the action of S_3 to the right.

We have to note here that since we are dealing with the right action of matrices, the representation of S_3, $\rho:S_3\to GL(2,\mathrm{R})$, must act on X_0 in the following manner:

$$(\mathbf{r}_1,\mathbf{r}_2)\mapsto(\mathbf{r}_1^h,\mathbf{r}_2^h)=(\mathbf{r}_1,\mathbf{r}_2)\rho(h)^{-1},\quad h\in S_3. \tag{27}$$

A straightforward calculation then provides

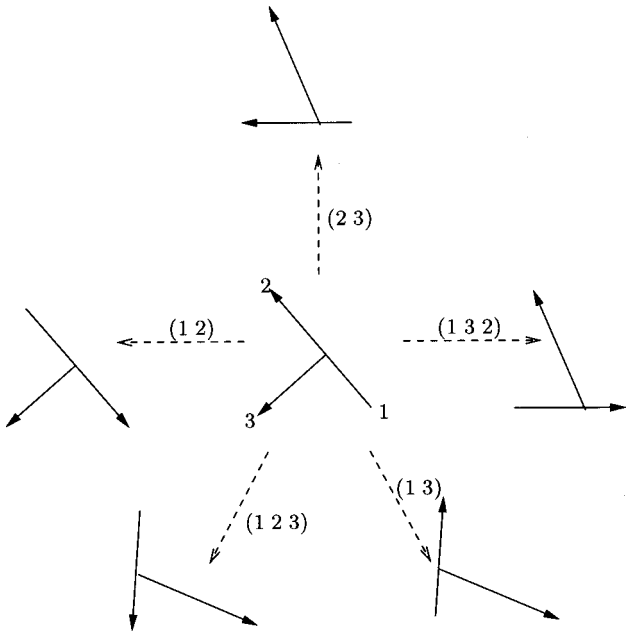

FIG. 2. This diagram represents the graphical view of all possible particle exchanges. Numbers in brackets are the elements of permutations from S_3. By the action of $\sigma \in S_3$, the site occupied by the particle k in the reference configuration gets occupied in turn by the particle $\sigma(k)$.

$$\rho(e)=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},\quad \rho(1\ 2)=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix},$$

$$\rho(1\ 2\ 3)=\begin{pmatrix}-1/2 & \sqrt{3}/2\\ -\sqrt{3}/2 & -1/2\end{pmatrix},\quad \rho(1\ 3\ 2)=\begin{pmatrix}-1/2 & -\sqrt{3}/2\\ \sqrt{3}/2 & -1/2\end{pmatrix}, \tag{28}$$

$$\rho(2\ 3)=\begin{pmatrix}1/2 & \sqrt{3}/2\\ \sqrt{3}/2 & -1/2\end{pmatrix},\quad \rho(1\ 3)=\begin{pmatrix}1/2 & -\sqrt{3}/2\\ -\sqrt{3}/2 & -1/2\end{pmatrix}.$$

It is an easy matter to verify that the matrices in (28) form a discrete subgroup of O(2) which is isomorphic to the symmetric group S_3. It is also well known that the set of the matrices given in (28) forms a unitary irreducible representation of S_3.[15]

So far we have not touched upon collision of particles, or excluded collision configurations from the center-of-mass system X_0. A remarkable point to make on the S_3 action on X_0 is that S_3 acts on the whole space X_0. This means that even if two or three particles collide, where the rank of the 2×2 matrix $(\mathbf{r}_1,\mathbf{r}_2)$ is less than two, Eq. (27) is applicable together with (28).

V. THE ACTION OF S_3 ON M

In Sec. IV, we have observed that the exchanges of identical particles give rise to the action of S_3 on X_0. With the identification $\dot{X}_0 \cong \dot{\mathrm{C}}^2$, the action of S_3 on $\dot{X}_0$ is expressed, like (27), as

$$(z_1,z_2)\mapsto(z_1,z_2)\rho(h)^{-1},\quad h\in S_3. \tag{29}$$

Since the action of SO(2) and of S_3 on X_0 commute, the action of S_3 on M can be defined through

$$[x]\tau(h)^{-1}:=[x\rho(h)^{-1}],\quad x\in\dot{X}_0\cong\dot{\mathrm{C}}^2,\quad h\in S_3, \tag{30}$$

where τ is a homomorphism: $S_3\to\mathrm{GL}(3,\mathrm{R})$, and represented as

$$(\xi_1,\xi_2,\xi_3)\mapsto(\xi_1,\xi_2,\xi_3)\tau(h)^{-1},\quad (\xi_1,\xi_2,\xi_3)\in M,\quad h\in S_3. \tag{31}$$

Note here that the definition (30) is independent of the choice of representatives. A straightforward calculation along with (12), (28), and (30) shows that $\tau(S_3)$ forms a discrete subgroup of SO(3), which is expressed as

$$\tau(e)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\quad \tau(1\ 2)=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix},$$

$$\tau(1\ 2\ 3)=\begin{pmatrix}-1/2&0&-\sqrt{3}/2\\0&1&0\\\sqrt{3}/2&0&-1/2\end{pmatrix},\quad \tau(1\ 3\ 2)=\begin{pmatrix}-1/2&0&\sqrt{3}/2\\0&1&0\\-\sqrt{3}/2&0&-1/2\end{pmatrix}, \tag{32}$$

$$\tau(2\ 3)=\begin{pmatrix}1/2&0&\sqrt{3}/2\\0&-1&0\\\sqrt{3}/2&0&-1/2\end{pmatrix},\quad \tau(1\ 3)=\begin{pmatrix}1/2&0&-\sqrt{3}/2\\0&-1&0\\-\sqrt{3}/2&0&-1/2\end{pmatrix}.$$

At first sight, the dimension of matrices presented in (32) is 3×3, which is larger than those presented in (28), resulting in an increase in the number of dimension by one. This seems not to fit the fact that the dimension of M is less than that of $\dot{X}_0$. However, this is not a contradiction. While we have identified X_0 with $\mathrm{R}^{2\times2}$, the set of Jacobi vectors, we are allowed alternatively to identify X_0 with R^4, the set of row vectors of length 4, so that we would have seen a discrete subgroup of GL(4,R) acting on R^4, and would have been able to see an immediate reduction in the size of matrices. In fact, the O(2) action given in (27) proves to take the form

$$(q_1,q_2,q_3,q_4)\mapsto(q_1,q_2,q_3,q_4)\begin{pmatrix}aI_2&bI_2\\cI_2&dI_2\end{pmatrix}^{-1}\qquad\text{for}\quad\rho(h)=\begin{pmatrix}a&b\\c&d\end{pmatrix}, \tag{33}$$

where $h\in S_3$ and I_2 denotes the 2×2 unit matrix. We also see that the determinant of the 4×4 matrix $\left(\begin{smallmatrix}aI_2&bI_2\\cI_2&dI_2\end{smallmatrix}\right)$ is equal to the square of the determinant of the 2×2 matrix $\left(\begin{smallmatrix}a&b\\c&d\end{smallmatrix}\right)$, so that the S_3 action (33) is represented as a discrete subgroup of SO(4).

VI. REDUCTION BY ROTATIONAL SYMMETRY

In this section, we present the reduction of a quantum system on the center-of-mass system X_0 by rotational symmetry. The reduction procedure runs irrespectively of whether all particles are identical or not. We first need a decomposition of $L^2(\mathrm{C}^2)$ with respect to the SO(2) action. For $f\in L^2(\mathrm{C}^2)$ given, we consider a function $f(e^{is}z)$ with a parameter s, which can be expanded into the Fourier series

$$f(e^{is}z)=\sum_{m=-\infty}^{\infty}f_m(z)e^{ims},\quad f_m(z)=\frac{1}{2\pi}\int_{-\pi}^{\pi}f(e^{is}z)e^{-ims}\,\mathrm{d}s. \tag{34}$$

In particular, for $s=0$, one has

$$f(z)=\sum_{m=-\infty}^{\infty}f_m(z). \tag{35}$$

Note here that the function f_m defined in (34) satisfies $f_m(e^{is}z)=e^{ims}f_m(z)$. In general, a function F on C^2 satisfying the condition

$$F(e^{is}z)=e^{ims}F(z) \tag{36}$$

is called ρ_m-equivariant, where ρ_m denotes a unitary irreducible representation of SO(2) $\cong$U(1); $\rho_m(e^{is})=e^{ims}$ with $m\in\mathrm{Z}$. As is easily seen, the decomposition (35) has remarkable properties,

$$\|f\|^2=\sum_{m=-\infty}^{\infty}\|f_m\|^2, \quad \langle f_n,f_m\rangle=0 \qquad \text{if} \quad n\neq m. \tag{37}$$

Thus $L^2(\mathrm{C}^2)$ is decomposed into the orthogonal direct sum,

$$L^2(\mathrm{C}^2)=\bigoplus_{m=-\infty}^{\infty}L^2_m(\mathrm{C}^2), \tag{38}$$

where each $L^2_m(\mathrm{C}^2)$ is the space of equivariant functions,

$$L^2_m(\mathrm{C}^2)=\{f\in L^2(\mathrm{C}^2)\,|\,f(e^{is}z)=e^{ims}f(z)\}. \tag{39}$$

Suppose we are given a quantum dynamical system on $L^2(\mathrm{C}^2)$, of which the time evolution is expressed as a unitary transformation,

$$\psi_t(z)=\int_{\mathrm{C}^2}G_t(z,w)\psi_{t_0}(w)\mathrm{d}w, \tag{40}$$

where $G_t(z,w)$ is a Green's function. Moreover, we assume that this quantum system is U(1) invariant, so that $G_t(z,w)$ is required to be U(1) invariant,

$$G_t(e^{is}z,e^{is}w)=G_t(z,w). \tag{41}$$

Our task in the following is to decompose the time evolution (40) in $L^2(\mathrm{C}^2)$ into a series of those in respective subspaces $L^2_m(\mathrm{C}^2)$. This process will be called the reduction of the quantum system for simplicity. We will see later how the time evolution in $L^2_m(\mathrm{C}^2)$ is looked upon as the time evolution of a state on the internal space M. Since the Lebesgue measure $\mathrm{d}w$ on C^2 is invariant under the U(1) action, and since $\psi_{t_0}(e^{is}w)$ can be expanded into a Fourier series $\Sigma\psi^m_{t_0}(w)e^{ims}$, the time evolution (40) can be decomposed into the following series:

$$\begin{aligned}\psi_t(z)&=\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}s\int_{\mathrm{C}^2}G_t(z,w)\psi_{t_0}(w)\mathrm{d}w\\&=\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}s\int_{\mathrm{C}^2}G_t(z,e^{-is}w)\psi_{t_0}(e^{-is}w)\mathrm{d}w\\&=\sum_{m=-\infty}^{\infty}\int_{\mathrm{C}^2}G^m_t(z,w)\psi^m_{t_0}(w)\mathrm{d}w,\end{aligned} \tag{42}$$

where

$$G^m_t(z,w):=\frac{1}{2\pi}\int_{-\pi}^{\pi}G_t(e^{is}z,w)e^{-ims}\,\mathrm{d}s, \tag{43}$$

and we have assumed that the order of integration and summation can be interchanged safely, which is the case for $\psi_{t_0}\in\mathcal{S}(\mathrm{C}^2)$, rapidly decreasing C^∞ functions. At a glance of the definition of $G^m_t(z,w)$, we can observe that

$$G_t^m(e^{is}z,w)=e^{ims}G_t^m(z,w), \tag{44}$$

$$G_t^m(z,e^{is}w)=G_t^m(z,w)e^{-ims}. \tag{45}$$

On account of (44), the integral transform

$$\psi_t^m(z)=\int_{\mathrm{C}^2}G_t^m(z,w)\psi_{t_0}^m(w)\mathrm{d}w \tag{46}$$

proves to be in $L_m^2(\mathrm{C}^2)$, so that the map $\psi_{t_0}^m\mapsto\psi_t^m$ becomes also unitary. Thus we have decomposed the time evolution ψ_t of the original system in $L^2(\mathrm{C}^2)$ into a series of those ψ_t^m in $L_m^2(\mathrm{C}^2)$,

$$\psi_t(z)=\sum_{m=-\infty}^{\infty}\psi_t^m(z),\quad \psi_t^m\in L_m^2(\mathrm{C}^2). \tag{47}$$

VII. BOUNDARY CONDITIONS

In treating the shape space in Sec. III, we have started with the restricted center-of-mass system $\dot{X}_0$. In this section, we wish to take the whole space X_0 into account to consider what will happen when the three particles collide at a point. First we note that the quotient space of the whole space X_0 by the SO(2) action becomes homeomorphic to R^3,

$$X_0/\mathrm{SO}(2)\cong\dot{\mathrm{R}}^3\cup\{0\}=\mathrm{R}^3. \tag{48}$$

Let us be reminded of the fact that $M=\dot{X}_0/\mathrm{SO}(2)\cong\dot{\mathrm{R}}^3$ is made into a Riemannian manifold with metric $\tilde{K}$. Since the motion of the three free particles is associated with a geodesic in $\dot{X}_0$, and since the three particles may collide at a point simultaneously, we may expect that the geodesics in $\dot{X}_0$ that correspond to collision motion may project to geodesics in M which may get out of M within a finite time. This suggests that the Riemannian manifold $(M,\tilde{K})$ is not geodesically complete. To prove this, it suffices to show that there is a geodesics which gets to the origin of R^3, a point out of $M=\dot{\mathrm{R}}^3$, within a finite time. One can indeed find such a geodesic as follows: Let w, $z\in\dot{\mathrm{C}}^2=\dot{X}_0$ such that $w=\lambda z$ with $\lambda\neq1$ a real constant. Then the straight line $u(t)=w+t(z-w)$, a geodesic in $\dot{X}_0$, proves to be horizontal, since Eq. (20) is satisfied by this $u(t)$. Now, it is clear that $u(t)$ projects to a geodesic $\pi(u(t))$ approaching the origin of R^3. In fact, one has

$$2u_1(t)\overline{u_2(t)}=(\lambda+t(1-\lambda))^2(\xi_1+i\xi_2),\quad |u_1(t)|^2-|u_2(t)|^2=(\lambda+t(1-\lambda))^2\xi_3, \tag{49}$$

where $2z_1\overline{z_2}=\xi_1+i\xi_2$, $|z_1|^2-|z_2|^2=\xi_3$, so that $\pi(u(t))\to0$ as $t\to\lambda/(\lambda-1)$. We have to point out in addition that Eq. (49) allows of the interpretation that the geodesic $\pi(u(t))$ remains to exist after getting out of M for an instant. In fact, we may interpret that it traces backward the path it has printed before having reached the origin. This interpretation of the continuation of the geodesic comes from the mechanical fact that three particles on a plane may collide at a point, but they may continue to move after the collision.

We are to prove that if three particles collide at a point, the total angular momentum of them must vanish. Let $u(t)=w+tv$ be a geodesic in C^2, which stands for a motion of free particles. We assume here that $w\neq0$, $v\neq0$. We are to consider whether or not $u(t)$ passes through the origin of C^2. A necessary and sufficient condition for $|u(t)|^2=0$ for some real number t is given by $(\mathrm{Re}\langle v,w\rangle)^2=|v|^2|w|^2$. But, in general, one has $|\langle v,w\rangle|\leqslant|v||w|$, so that

$$\mathrm{Im}\langle v,w\rangle=0,\quad\text{and}\quad\lambda v+\mu w=0\quad\text{for}\quad(\lambda,\mu)\neq0,\lambda,\mu\in\mathrm{C}. \tag{50}$$

Since $v\neq 0$, $w\neq 0$ by assumption, Eq. (50) implies that v and w are related by $v=kw$ with k a nonzero real constant. Thus we have verified that if $|u(t)|=0$ for some t, v and w are related by $v=kw$, $k\in \mathrm{R}-\{0\}$. Moreover, the condition $\mathrm{Im}\langle v,w\rangle=0$ implies that

$$\mathrm{Im}\left\langle u(t),\frac{du}{dt}\right\rangle=\mathrm{Im}\langle u(t),v\rangle=\mathrm{Im}\langle w,v\rangle=0, \tag{51}$$

which means that the angular momentum of the orbit $u(t)$ must vanish [see (20)]. Thus we conclude that if three free particles collide at a point simultaneously, the total angular momentum of them must vanish. By contraposition, three free particles with nonvanishing total angular momentum do not collide simultaneously at a point.

This observation suggests that we consider what happens in wave functions at $z=0$ according to whether the total angular momentum vanishes or not. We have to note here that the $L^2_m(\mathrm{C}^2)$ is the space of wave functions with the total angular momentum m. In fact, the ρ_m-equivariance condition (36) for a smooth function F is differentiated with respect to s at $s=0$ to provide

$$\frac{1}{i}\left(-q_2\frac{\partial}{\partial q_1}+q_1\frac{\partial}{\partial q_2}-q_4\frac{\partial}{\partial q_3}+q_3\frac{\partial}{\partial q_4}\right)F(z)=mF(z), \tag{52}$$

where the operator on the left-hand side stands for the total angular momentum operator. Moreover, condition (36) implies that $F(0)=e^{ims}F(0)$ for $z=0$, and hence

$$F(0)=0 \quad \text{for} \quad m\neq 0, \tag{53}$$

which means that if the total angular momentum does not vanish ($m\neq 0$), the three particles do not collide at the origin. If $m=0$, then $F(0)$ should be a finite value.

If some of the wave functions are analytic at $z=0$, we can describe more of the behavior of them at $z=0$. Let $f(z)$ be a function analytic at $z=0$. Then it may be expanded into a power series such as $f(z)=\Sigma c_{j_1j_2k_1k_2}z_1^{j_1}z_2^{j_2}\bar{z}_1^{k_1}\bar{z}_2^{k_2}$. We can rewrite this series in the form

$$f(z)=\sum_{m=0}^{\infty}\sum_{n=m}^{\infty}\sum_{\substack{j_1+j_2-k_1-k_2=m\\ j_1+j_2+k_1+k_2=n}}c_{j_1j_2k_1k_2}z_1^{j_1}z_2^{j_2}\bar{z}_1^{k_1}\bar{z}_2^{k_2}+\sum_{m=-1}^{-\infty}\sum_{n=|m|}^{\infty}\sum_{\substack{j_1+j_2-k_1-k_2=m\\ j_1+j_2+k_1+k_2=n}}{}^{*}. \tag{54}$$

This expansion shows that $f(z)$ is broken up into a series of ρ_m-equivariant functions, each of which takes the form of power series starting with a term of order $|m|$ irrespective of whether m is non-negative or negative. Further, since $n=m+2(k_1+k_2)$, the power series starting with a term of order $|m|$ contains only terms of every other higher order. This fact was pointed out for planar two-body systems,[16] while Ref. 16 mainly studies the behavior of wave functions at the collinear configurations of spatial three-body systems.

In the rest of this section, we describe analytic ρ_m-equivariant functions in terms of the local coordinate system (R,θ,ϕ,ψ) introduced through

$$z_1=\mathrm{R}e^{i(\psi+\phi)/2}\cos\frac{\theta}{2},\quad z_2=\mathrm{R}e^{i(\psi-\phi)/2}\sin\frac{\theta}{2}, \tag{55}$$

$$R\geqslant 0,\quad 0\leqslant\theta\leqslant\pi,\quad 0\leqslant\psi\leqslant 4\pi,\quad 0\leqslant\phi\leqslant 2\pi. \tag{56}$$

A ρ_m-equivariant function F which is assumed to be analytic at $z=0$ is then expanded, on account of (54), into a power series of the form

$$F(z)=e^{im\psi/2}\sum_{\ell=0}^{\infty}R^{|m|+2\ell}\Phi_{m\ell}(\theta,\phi), \tag{57}$$

where

$$\Phi_{m\ell}(\theta,\phi)=\sum_{\substack{j_1+j_2=1/2(|m|+m)+\ell\\ k_1+k_2=1/2(|m|-m)+\ell}} c_{j_1j_2k_1k_2}e^{i\phi(j_1-j_2-k_1+k_2)/2}\left(\cos\frac{\theta}{2}\right)^{j_1+k_1}\left(\sin\frac{\theta}{2}\right)^{j_2+k_2}. \quad (58)$$

From this, we observe that the ρ_m-equivariant function F is expressed as $e^{im\psi/2}$ times a power series in R which starts with a term of the lowest order $|m|$ and contains only terms of every other order. Since R is a measure to describe how configurations of particles are distant from the triple collision, Eq. (57) implies that the more the total angular momentum $|m|$ grows, the less closely the particles get together.

VIII. REDUCTION BY PARTICLE EXCHANGES

This section deals with reduction due to exchanges of identical particles. According to whether particles are all bosons or fermions, the wave function must be symmetric or antisymmetric with respect to particle exchanges. From a wave function ψ on the center-of-mass system $X_0\cong\mathrm{C}^2$, we can construct such wave functions $\psi^{(s)}$ and $\psi^{(a)}$ by the following procedure;

$$\psi^{(s)}(x):=\sum_{h\in S_3}\psi(x\rho(h)^{-1}), \quad (59)$$

$$\psi^{(a)}(x):=\sum_{h\in S_3}\mathrm{sgn}(h)\psi(x\rho(h)^{-1}), \quad (60)$$

where ρ is the representation of S_3 in $\mathrm{O}(2)$, which is given in (28), and $\mathrm{sgn}(g)$ denotes the signum of g; $\mathrm{sgn}(g)$ equals 1 or -1, depending on whether $g\in S_3$ is an even or odd permutation. It is easy to see that the $\psi^{(s)}$ and $\psi^{(a)}$ are symmetric and antisymmetric, respectively, with respect to the S_3 action,

$$\psi^{(s)}(x\rho(g)^{-1})=\psi^{(s)}(x), \quad \psi^{(a)}(x\rho(g)^{-1})=\mathrm{sgn}(g)\psi^{(a)}(x). \quad (61)$$

In comparison with the ρ_m-equivariance with respect to the $\mathrm{SO}(2)\cong\mathrm{U}(1)$ action, Eq. (61) shows that bosonic and fermionic states are equivariant with respect to the trivial representation $\sigma\mapsto 1$ and to the signum representation $\sigma\mapsto\mathrm{sgn}(\sigma)$, respectively.

We assume here that our quantum system $(L^2(\mathrm{C}^2),\psi_t)$ is invariant under the particle exchanges, so that $G_t(z,w)$ is assumed to be invariant under the action of S_3,

$$G_t(z\rho(h)^{-1},w\rho(h)^{-1})=G_t(z,w), \quad h\in S_3. \quad (62)$$

We note further that the Lebesgue measure $\mathrm{d}w$ on $X_0\cong\mathrm{R}^4$ is also invariant under the action of S_3. This is because the S_3 action on X_0 is represented as a discrete subgroup of $\mathrm{SO}(4)$, as is seen from (33). The invariance of the Green's kernel and of the measure $\mathrm{d}w$ under the S_3 action are put together to imply that the time evolution preserves the statistics to which the particles are subject, that is, bosonic or fermionic state remains unchanged during the time evolution. This can be seen from the change that the time evolution (40) undergoes by the S_3 action,

$$\psi_t(z\rho(h)^{-1})=\int_{\mathrm{C}^2}G_t(z,w)\psi_{t_0}(w\rho(h)^{-1})\mathrm{d}w. \quad (63)$$

Since the action of $\mathrm{U}(1)$ and of S_3 commute, the time evolution (63) is decomposed into

$$\psi_t(z\rho(h)^{-1})=\sum_{m=-\infty}^{\infty}\psi_t^m(z\rho(h)^{-1})=\sum_{m=-\infty}^{\infty}\int_{\mathrm{C}^2}G_t^m(z,w)\psi_{t_0}^m(w\rho(h)^{-1})\mathrm{d}w, \quad (64)$$

where the Green's functions are invariant under the S_3 action,

$$G_t^m(z\rho(h)^{-1},w\rho(h)^{-1})=G_t^m(z,w),\quad h\in S_3. \tag{65}$$

Putting (64) together with (59) and (60), we obtain the time evolution of wave functions for Bose or Fermi particles, which are decomposed into

$$\psi_t^{(s)}(z)=\sum_{m=-\infty}^{\infty}\psi_t^{(s)m}(z),\quad \psi_t^{(s)m}(z):=\sum_{h\in S_3}\psi_t^m(z\rho(h)^{-1}), \tag{66}$$

$$\psi_t^{(a)}(z)=\sum_{m=-\infty}^{\infty}\psi_t^{(a)m}(z),\quad \psi_t^{(a)m}(z):=\sum_{h\in S_3}\mathrm{sgn}(h)\psi_t^m(z\rho(h)^{-1}), \tag{67}$$

respectively.

Proposition 1: A planar three-particle quantum system $(L^2(\mathrm{C}^2),\psi_t)$ with symmetry of rotation and particle exchanges is reduced to subsystems $(L_m^2(\mathrm{C}^2),\psi_t^{(s)m})$ or $(L_m^2(\mathrm{C}^2),\psi_t^{(a)m})$ according to whether the particles are bosons or fermions, where $\psi_t^{(s)m}$ and $\psi_t^{(a)m}$ are given by (66) and (67), respectively, along with (46).

IX. COMPLEX LINE BUNDLES

So far we have discussed the reduction to subsystems (see Proposition 1). In this section, we show that these subsystems indeed give rise to reduced quantum systems on the shape space, by introducing complex line bundles associated with the U(1) bundle $\dot{\mathrm{C}}^2\cong\dot{X}_0\to M$. To this end, we first recall that the time evolution ψ_t in $L^2(\mathrm{C}^2)$ was decomposed into the series of those in $L_m^2(\mathrm{C}^2)$,

$$\psi_t^m(z):=\int_{\mathrm{C}^2}G_t^m(z,w)\psi_{t_0}^m(w)\mathrm{d}w,\quad \psi_{t_0}^m\in L_m^2(\mathrm{C}^2). \tag{68}$$

Since the integrand in (68) is invariant under the U(1) action, the integration with respect to w over C^2 will reduce to that over the shape space M, if C^2 is restricted to $\dot{\mathrm{C}}^2$. Hence the time evolution $\psi_t^m(z)$ may define the time evolution of a quantum state on the shape space M. In what follows, we make a brief review of complex line bundles associated with $\dot{\mathrm{C}}^2\cong\dot{X}_0\to M=\dot{\mathrm{R}}^3$ along with boundary conditions at the origin of R^3.

For a unitary irreducible representation ρ_m, the complex line bundle E_m associated with the U(1) bundle $\dot{X}_0\cong\dot{\mathrm{C}}^2\to M$ is defined to be the quotient of the product space $\dot{X}_0\times\mathrm{C}$ by the equivalence relation defined through $(z,\zeta)\sim(e^{is}z,e^{ims}\zeta)$ for $(z,\zeta)\in\dot{\mathrm{C}}^2\times\mathrm{C}$. By $[(z,\zeta)]$ and by π_m we denote the equivalence class in $\dot{X}_0\times\mathrm{C}$ and the projection $E_m\to M$, respectively, so that one has $\pi_m([(z,\zeta)])=\pi(z)$. A section σ in E_m is a map $M\to E_m$ such that $\pi_m\circ\sigma=\mathrm{id}_M$, where id_M is the identity map of M. Then any ρ_m-equivariant function F on $\dot{X}_0$ determines a section σ in E_m by

$$\sigma(\pi(z))=[(z,F(z))]. \tag{69}$$

Sections in E_m and ρ_m-equivariant functions are in one-to-one correspondence. Furthermore, from (53), ρ_m-equivariant functions should be subject to the boundary condition that $F(z)\to 0$ as $z\to 0$ if $m\neq 0$ and that $F(z)$ is bounded as $z\to 0$ if $m=0$, so that the corresponding section $\sigma(\xi)$ should satisfy the corresponding boundary condition as $\xi\to 0$ in M.

For sections σ_1 and σ_2 corresponding to ρ_m-equivariant functions F_1 and F_2, respectively, the inner product $\langle\sigma_1,\sigma_2\rangle$ is defined to be

$$\langle\sigma_1,\sigma_2\rangle=\int_M(\sigma_1,\sigma_2)\mathrm{d}\mu_M=\int_{\mathrm{C}^2}\overline{F_1(z)}F_2(z)\mathrm{d}z, \tag{70}$$

where (σ_1,σ_2) denotes the inner product in each fiber $\pi_m^{-1}(\pi(z))\cong\mathrm{C}$, and $\mathrm{d}\mu_M$ is the measure on M defined for any function χ on M through

$$\int_M \chi(p)\mathrm{d}\mu_M=\int_{\mathrm{C}^2}\chi(\pi(z))\mathrm{d}z \quad \text{with} \quad \pi(z)=p\in M. \tag{71}$$

To put the measure $\mathrm{d}\mu_M$ in an explicit form, it is of great help to use the connection form ω given in (15). A straightforward calculation then shows that the standard volume form on X_0 is put in the form

$$dq_1\wedge dq_2\wedge dq_3\wedge dq_4=\frac{1}{8r}\omega\wedge d\xi_1\wedge d\xi_2\wedge d\xi_3, \quad r=\sqrt{\xi_1^2+\xi_2^2+\xi_3^2}, \tag{72}$$

where $\xi_k, k=1,2,3$, are defined in (12). To be precise, $d\xi_k$ on the right-hand side of (72) should be replaced by $\pi^* d\xi_k$, the pull-back of $d\xi_k$ through π, but we have used $d\xi_k$ for simplicity. From (71) and (72), we conclude after the integration over the fiber $S^1\cong\mathrm{U}(1)$ that

$$\mathrm{d}\mu_M=\frac{\pi}{4r}d\xi_1\wedge d\xi_2\wedge d\xi_3. \tag{73}$$

From (69) and (70), we see that any function $F\in L_m^2(\dot{\mathrm{C}}^2)$ determines a square integrable section in E_m. Taking into account the above-mentioned boundary condition for ρ_m-equivariant functions, we may regard $L_m^2(\mathrm{C}^2)$ as being in one-to-one correspondence to the space of square integrable sections in E_m together with the boundary condition.

For the ρ_m-equivariant function $\psi_t^m(z)$ given in (68), one has the time evolution of the corresponding section σ_t^m in E_m together with the boundary condition,

$$\sigma_t^m(\pi(z))=[(z,\psi_t^m(z))]. \tag{74}$$

Since the time evolution ψ_t^m is unitary, that is, $\|\psi_t^m\|=\|\psi_{t_0}^m\|$, the time evolution of the corresponding section σ_t^m is also unitary, that is, $\|\sigma_t^m\|=\|\sigma_{t_0}^m\|$ for all time t.

The S_3 action on $L_m^2(\mathrm{C}^2)$ can be transferred to that on the space of square integrable sections in E_m. From (66) and (67), we obtain corresponding time evolutions of sections in E_m, respectively,

$$\sigma_t^{(s)m}(\pi(z)):=\sum_{h\in S_3}\sigma_t^m(\pi(z)\tau(h)^{-1}), \tag{75}$$

$$\sigma_t^{(a)m}(\pi(z)):=\sum_{h\in S_3}\mathrm{sgn}(h)\sigma_t^m(\pi(z)\tau(h)^{-1}). \tag{76}$$

The reduction is thus completed for the time evolution of a $\mathrm{U}(1)\cong\mathrm{SO}(2)$ invariant quantum system of three identical particles on a plane.

Theorem 2: If a quantum system for three identical particles on a plane admits the symmetry of rotation and particle exchanges, the time evolution of the quantum system, which is defined in the L^2 space of wave functions on the center-of-mass system, is reduced to that on the L^2 space of sections in the complex line bundle E_m over the internal space M, where sections σ must satisfy the boundary condition that $\sigma(\xi)\to 0$ as $\xi\to 0$ if $m\neq 0$ or that $\sigma(\xi)$ is bounded as $\xi\mapsto 0$ if $m=0$. According to whether the quantum system is bosonic or fermionic, the time evolution is put in the form of (75) or (76).

X. APPLICATION TO FREE PARTICLES

Having set up the reduction method, we are to apply it to a system of free particles. The Schrödinger equation for three free particles on a plane is expressed, in terms of (q_i), as

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2}\nabla^2\psi \quad \text{with} \quad \nabla^2=\sum_{j=1}^{4}\frac{\partial^2}{\partial q_j^2}. \tag{77}$$

In fact, since the operator $\Sigma_{k=1}^{3}(1/m_k)(\partial/\partial\mathbf{x}_k)^2$, a constant multiple of the kinetic energy operator, is the Laplacian ∇^2 with respect to the metric (1) on X, and since this metric is expressed as $\Sigma_{j=1}^{4}dq_j^2$ if restricted to the linear subspace X_0 of X, the Laplacian takes the form $\nabla^2=\Sigma_{j=1}^{4}\partial^2/\partial q_j^2$. As is well known, Eq. (77) can be solved by Fourier transform with little difficulty, to give a solution of the form

$$\psi_t(z)=\int_{\mathrm{C}^2}F_t(z,w)\psi_{t_0}(w)\mathrm{d}w, \tag{78}$$

where F_t is the Green's function given by

$$F_t(z,w)=\left[\frac{1}{2\pi i\hbar(t-t_0)}\right]^2\exp\left(\frac{i|z-w|^2}{2\hbar(t-t_0)}\right). \tag{79}$$

Since the Schrödinger equation (77) is invariant under the U(1) action (10), the free particle system can be reduced after the procedure in Sec. VI. As is easily seen from (79), the Green's kernel $F_t(z,w)$ satisfies the condition (41), so that we can compute explicitly Eq. (43) with F_t replaced for G_t to obtain

$$F_t^m(z,w)=\frac{e^{im(\theta(z,w)-\pi/2)}}{(2\pi i\hbar(t-t_0))^2}\exp\left(\frac{iB(z,w)}{2\hbar(t-t_0)}\right)J_m\left(\frac{A(z,w)}{\hbar(t-t_0)}\right), \tag{80}$$

where J_m is the Bessel function defined as

$$J_m(x)=\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{ix\sin s}e^{-ims}\mathrm{d}s, \quad x\in\mathrm{C}, \tag{81}$$

and

$$B(z,w)=\sum_{j=1}^{2}(|z_j|^2+|w_j|^2), \tag{82}$$

$$A(z,w)=\left|\sum_{j=1}^{2}z_j\overline{w}_j\right|, \tag{83}$$

$$\theta(z,w)=\arg\sum_{j=1}^{2}z_j\overline{w}_j. \tag{84}$$

It is of great interest to observe that $A(z,w)$ and $B(z,w)$ are invariant under the U(1) action, $z\mapsto e^{is}z$ and/or $w\mapsto e^{is}w$, and hence can be expressed in the coordinates of the shape space M. In fact, we can verify that

$$B(z,w)=\tilde{B}(\xi,\xi')\coloneqq\sqrt{\sum_{k=1}^{3}\xi_k^2}+\sqrt{\sum_{k=1}^{3}\xi_k'^2}, \tag{85}$$

$$A(z,w)=\tilde{A}(\xi,\xi'):=\left[\frac{1}{2}\sqrt{\sum_{k=1}^{3}\xi_k^2}\sqrt{\sum_{k=1}^{3}\xi_k'^2}+\frac{1}{2}\sum_{k=1}^{3}\xi_k\xi_k'\right]^{1/2}, \tag{86}$$

where ξ_k' are given by the formula similar to (12). We notice further that under the U(1) action the factor $e^{im\theta(z,w)}$ is subject to the transformation

$$\begin{aligned}\exp(im\theta(e^{is}z,w))&=e^{ims}\exp(im\theta(z,w)),\\ \exp(im\theta(z,e^{is}w))&=\exp(im\theta(z,w))e^{-ims}.\end{aligned} \tag{87}$$

Properties (85)–(87) show that F_t^m is subject to the transformations (44) and (45). Thus the time evolution (78) is reduced to (46) with G_t^m replaced by F_t^m.

Furthermore, since F_t is invariant under the S_3 action, as is seen from (79), so is F_t^m. Thus the free particle system reduces to subsystems according to Proposition 1. Finally, application of Theorem 2 provides reduced systems defined on the complex line bundles E_m.

In conclusion, we note that the reduced Hamiltonian operator, which acts on sections of E_m and is denoted by $\hat{H}_m$, is given by

$$\hat{H}_m=-\frac{\hbar^2}{2}4r\sum_{k=1}^{3}\nabla_k^2+\frac{m^2}{2r}, \tag{88}$$

where ∇_k's are the covariant differential operators with respect to the vector fields $\partial/\partial\xi_k$. See Ref. 1 for details, in which the reduced Hamiltonian operator was studied for a generic Hamiltonian system of planar three particles.

XI. LOCAL EXPRESSION

The purpose of this section is to look into the boundary conditions and the Green's function discussed in previous sections, in terms of local coordinates.

We first consider the boundary condition at $z=0$ for ρ_m-equivariant functions in the coordinates (R,θ,ϕ,ψ) introduced in (55). As is easily seen from (12) and (55), one has

$$\xi_1+i\xi_2=re^{i\phi}\sin\theta,\quad \xi_3=r\cos\theta,\quad r=R^2, \tag{89}$$

which means that (r,θ,ϕ) serve as spherical polar coordinates in the shape space $M\cong\dot{\mathrm{R}}^3$. We take a local section, $s=(s_1,s_2)$, in the bundle $\dot{X}_0\cong\dot{\mathrm{C}}^2\to M$ as follows:

$$s_1(r,\theta,\phi)=\sqrt{r}e^{i\phi/2}\cos\frac{\theta}{2},\quad s_2(r,\theta,\phi)=\sqrt{r}e^{-i\phi/2}\sin\frac{\theta}{2}, \tag{90}$$

where

$$r>0,\quad 0<\theta<\pi,\quad 0<\phi<2\pi. \tag{91}$$

Then one has $z=e^{i\psi/2}s(r,\theta,\phi)$, so that the local section corresponding to a ρ_m-equivariant function F is expressed as $[(z,F(z))]=[s(r,\theta,\phi),F\circ s(r,\theta,\phi)]$. This implies that $F\circ s$ may be identified with a local section in E_m. If F is given by (57), we obtain

$$F\circ s(r,\theta,\phi)=r^{|m|/2}\sum_{\ell=0}^{\infty}r^{\ell}\Phi_{m\ell}(\theta,\phi). \tag{92}$$

This shows that if a ρ_m-equivariant function $F(z)$ is analytic in R at $R=0$, then the corresponding local section is expressed as $r^{|m|/2}$ times an analytic function in r. In particular, the local section associated with the kernel function F_t^m, as a function of z, given in (80) can be expanded in this form.

We turn to expressing the integral transform (68) with G_t^m replaced by F_t^m as the integral of a function on the shape space M explicitly. To this end, we use local sections σ_+ and σ_- in the bundle $\dot{X}_0 \to M$, which are defined to be

$$\sigma_+(\xi)=\left(\frac{\sqrt{r+\xi_3}}{\sqrt{2}},\frac{\xi_1-i\xi_2}{\sqrt{2(r+\xi_3)}}\right) \quad \text{for } \xi\in D_+, \tag{93}$$

$$\sigma_-(\xi)=\left(\frac{\xi_1+i\xi_2}{\sqrt{2(r-\xi_3)}},\frac{\sqrt{r-\xi_3}}{\sqrt{2}}\right) \quad \text{for } \xi\in D_-, \tag{94}$$

where $D_\pm$ are domains in M defined, respectively, to be

$$D_+=\{\xi\in \dot{\mathrm{R}}^3 | \xi_3+r\neq 0\}, \tag{95}$$

$$D_-=\{\xi\in \dot{\mathrm{R}}^3 | \xi_3-r\neq 0\}. \tag{96}$$

The sections σ_+ and σ_- are subject to the transformation in the intersection $D_+\cap D_-$,

$$\sigma_-(\xi)=\frac{\xi_1+i\xi_2}{\sqrt{\xi_1^2+\xi_2^2}}\sigma_+(\xi), \quad \xi\in D_+\cap D_-. \tag{97}$$

By using the section σ_+, points of $\pi^{-1}(D_+)$ are expressed as $z=e^{i\varphi}\sigma_+(\xi)$ with $\xi=\pi(z)$ and φ an angle variable. Thus local coordinates (ξ,φ) are introduced in $\pi^{-1}(D_+)$. Local coordinates are defined in $\pi^{-1}(D_-)$ as well. Then, a ρ_m-equivariant function F restricted on $\pi^{-1}(D_+)$ is put in the form $F(z)=e^{im\varphi}F(\sigma_+(\xi))$. A similar expression of F is available on $\pi^{-1}(D_+)$.

We first divide M into a union $M=M_+\cup M_-$, where $M_\pm$ are the upper and the lower half spaces of $M\cong \dot{\mathrm{R}}^3$; $M_+=\{\xi\in M|\xi_3\geqslant 0\}$, $M_-=\{\xi\in M|\xi_3\leqslant 0\}$, and hence we have the division of $\dot{\mathrm{C}}^2$ in the form $\dot{\mathrm{C}}^2=\pi^{-1}(M_+)\cup\pi^{-1}(M_-)$. Accordingly, the integral transform (68) with F_t^m replaced for G_t^m is broken up into

$$\psi_t^m(z)=\int_{\pi^{-1}(M_+)} F_t^m(z,w)\psi_{t_0}^m(w)\mathrm{d}w+\int_{\pi^{-1}(M_-)} *. \tag{98}$$

We now use the local sections σ_+ and σ_- restricted on M_+ and M_-, respectively, to rewrite the integrals (98) in terms of the variable $w=e^{i\varphi'}\sigma_+(\xi')\in\pi^{-1}(M_+)$, etc. In particular, for $z\in\pi^{-1}(D_+)$, Eq. (98) is put in the form

$$\begin{aligned}\psi_t^m(\sigma_+(\xi))=&\int_{M_+}\tilde{F}_t^m(\xi,\xi')e_{++}^m(\xi,\xi')\psi_{t_0}^m(\sigma_+(\xi'))\mathrm{d}\mu_M(\xi')\\&+\int_{M_-}\tilde{F}_t^m(\xi,\xi')e_{+-}^m(\xi,\xi')\psi_{t_0}^m(\sigma_-(\xi'))\mathrm{d}\mu_M(\xi'),\end{aligned} \tag{99}$$

where the angle variables φ has been canceled out from the both sides, and the definition (71) of $\mathrm{d}\mu_M$ has been used along with

$$\tilde{F}_t^m(\xi,\xi') := \frac{e^{-im\pi/2}}{(2\pi i\hbar(t-t_0))^2}\exp\left(\frac{\tilde{B}(\xi,\xi')}{2\hbar(t-t_0)}\right)J_m\left(\frac{\tilde{A}(\xi,\xi')}{\hbar(t-t_0)}\right), \tag{100}$$

$$e_{++}^m(\xi,\xi') := e^{im\theta(\sigma_+(\xi),\sigma_+(\xi'))}, \tag{101}$$

$$e_{+-}^m(\xi,\xi') := e^{im\theta(\sigma_+(\xi),\sigma_-(\xi'))}. \tag{102}$$

A similar expression for $\psi_t^m(\sigma_-(\xi)), \xi \in D_-$, can be obtained as well with due definition of $e_{-+}^m(\xi,\xi')$ and of $e_{--}^m(\xi,\xi')$. The functions $\psi_t^m(\sigma_-(\xi))$ and $\psi_t^m(\sigma_+(\xi))$ are related on $D_+ \cap D_-$ by

$$\psi_t^m(\sigma_-(\xi)) = \left(\frac{\xi_1 + i\xi_2}{\sqrt{\xi_1^2+\xi_2^2}}\right)^m \psi_t^m(\sigma_+(\xi)), \quad \xi \in D_+ \cup D_-, \tag{103}$$

which is observed from (97) and from the fact that ψ_t^m is ρ_m-equivariant.

In the rest of this section, we are to look into the function $\tilde{F}_t^m(\xi,\xi')$ in detail by using asymptotic expansion of Bessel functions. As is well known, a simple form of the asymptotic expansion of $J_n(x)$ for $|x| \gg 1$ is given by

$$\begin{aligned} J_m(x) &\sim \sqrt{\frac{2}{\pi x}}\cos\left(x - \frac{1}{2}m\pi - \frac{1}{4}\pi\right) \\ &= \frac{1}{2}\sqrt{\frac{2}{\pi x}}\left(\exp\left(i\left(x - \frac{1}{2}m\pi - \frac{1}{4}\pi\right)\right) + \exp\left(-i\left(x - \frac{1}{2}m\pi - \frac{1}{4}\pi\right)\right)\right). \end{aligned} \tag{104}$$

Then one has, for $0 < |t-t_0|\hbar \ll \tilde{A}(\xi,\xi')$,

$$\begin{aligned} J_m\left(\frac{\tilde{A}(\xi,\xi')}{(t-t_0)\hbar}\right) \sim \sqrt{\frac{(t-t_0)\hbar}{2\pi\tilde{A}(\xi,\xi')}}\Bigg(& e^{-\pi i/4}e^{-im\pi/2}\exp\left(i\frac{\tilde{A}(\xi,\xi')}{(t-t_0)\hbar}\right) + e^{\pi i/4}e^{im\pi/2} \\ &\times\exp\left(-i\frac{\tilde{A}(\xi,\xi')}{(t-t_0)\hbar}\right)\Bigg), \end{aligned} \tag{105}$$

where we have assumed that $\tilde{A}(\xi,\xi') \neq 0$. We note in addition that $\tilde{A}(\xi,\xi') = 0$ with $\xi \neq 0, \xi' \neq 0$, if and only if there exists a positive constant $\lambda > 0$ such that $\xi_k' = -\lambda\xi_k, k = 1,2,3$, as observed from (86). Inserting the asymptotic expansion (105) of $J_m(\tilde{A}(\xi,\xi')/(t-t_0)\hbar)$ in the right-hand side of (100), one obtains, for $0 < |t-t_0|\hbar \ll \tilde{A}(\xi,\xi')$,

$$\tilde{F}_t^m(\xi,\xi') \sim -\frac{(-1)^m e^{-\pi i/4}}{\tilde{A}(\xi,\xi')^{1/2}}\frac{1}{(2\pi(t-t_0)\hbar)^{3/2}}\exp\left(\frac{i}{2(t-t_0)\hbar}(r+r'+2\tilde{A}(\xi,\xi'))\right) \tag{106}$$

$$+\frac{1}{\tilde{A}(\xi,\xi')^{1/2}}\frac{1}{(2\pi i(t-t_0)\hbar)^{3/2}}\exp\left(\frac{i}{2(t-t_0)\hbar}(r+r'-2\tilde{A}(\xi,\xi'))\right). \tag{107}$$

We now consider the quantity appearing in the argument of the exponential function in (106). To this end, let

$$\alpha(\xi,\xi') := r + r' + 2\tilde{A}(\xi,\xi'). \tag{108}$$

Then, differentiation of α with respect to ξ' implies that for nonvanishing ξ', $\partial\alpha/\partial\xi'=0$ if and only if

$$\sqrt{2}\sqrt{rr'+\sum_{k=1}^{3}\xi_k\xi_k'}+r+r'\frac{\xi_k}{\xi_k'}=0, \quad k=1,2,3, \tag{109}$$

so that $\partial\alpha/\partial\xi_k'=0$ if and only if $\xi_k=-\nu\xi_k'$, $k=1,2,3$ for a positive constant $\nu>0$. Incidentally, for ξ and ξ' with $\xi=-\nu\xi'$, one obtains $\tilde{A}(\xi,\xi')=0$, which contradicts the assumption that $\tilde{A}(\xi,\xi')\neq 0$. From this it follows that if $\tilde{A}(\xi,\xi')\neq 0$ then $\alpha(\xi,\xi')$ does not attain its stationary values, i.e., $\partial\alpha/\partial\xi_k'\neq 0$, $k=1,2,3$, so that the function

$$\exp\left(\frac{i}{2(t-t_0)\hbar}\alpha(\xi,\xi')\right)$$

rapidly oscillates throughout the ξ'-space with $\xi\neq-\nu\xi'$. Hence, the first term (106) of the right-hand side of the asymptotic expansion (106) and (107) would make no contribution in the integral transform. As for the argument of the exponential function in the second term (107), we find that $r+r'-2\tilde{A}(\xi,\xi')$ is equal to $d_M(\xi,\xi')^2$, the squared distance defined in (22). The distance function takes a minimum if and only if $\xi=\xi'$, so that

$$\exp\left(\frac{i}{2(t-t_0)\hbar}d_M(\xi,\xi')^2\right)$$

makes a definite contribution as part of an integral kernel. Thus, for small $t-t_0$, one may conclude that the function $\tilde{F}_t^m(\xi,\xi')$ has an asymptotic expansion of the form

$$\tilde{F}_t^m(\xi,\xi')\sim\frac{1}{\tilde{A}(\xi,\xi')^{1/2}}\frac{1}{(2\pi i(t-t_0)\hbar)^{3/2}}\exp\left(\frac{i}{2(t-t_0)\hbar}d_M(\xi,\xi')^2\right). \tag{110}$$

XII. REMARKS ON ELECTRONS ON A PLANE

A system of electrons on a plane is of fundamental interest from the viewpoint of the quantum Hall effect. In his lecture[17] on the quantum Hall effect, Laughlin gives a trial wave function for planar three electrons on a plane, which is expressed as

$$\psi_{n,m}(z_1,z_2)=((z_2+iz_1)^{3m}-(z_2-iz_1)^{3m})(z_1^2+z_2^2)^n e^{-(1/4)(|z_1|^2+|z_2|^2)}, \tag{111}$$

up to a constant factor, where z_1 and z_2 are variables given in (9). It is easy to see that this function is equivariant under the U(1) action. We can also verify that the function $\psi_{n,m}$ satisfies the Pauli principle. To show this, we have only to see how z_2+iz_1 and z_2-iz_2 transform under the S_3 action. Writing out the transformation (29) for every element $h\in S_3$ results in the following transformation except for the identity:

$$\begin{gathered}
(z_2+iz_1)\rho(12)^{-1}=z_2-iz_1, \quad (z_2-iz_1)\rho(12)^{-1}=z_2+iz_1,\\
(z_2+iz_1)\rho(13)^{-1}=(z_2-iz_1)e^{-(2\pi/3)i}, \quad (z_2-iz_1)\rho(13)^{-1}=(z_2+iz_1)e^{(2\pi/3)i},\\
(z_2+iz_1)\rho(23)^{-1}=(z_2-iz_1)e^{(2\pi/3)i}, \quad (z_2-iz_1)\rho(23)^{-1}=(z_2+iz_1)e^{-(2\pi/3)i},\\
(z_2+iz_1)\rho(123)^{-1}=(z_2+iz_1)e^{(2\pi/3)i}, \quad (z_2-iz_1)\rho(123)^{-1}=(z_2-iz_1)e^{-(2\pi/3)i},\\
(z_2+iz_1)\rho(132)^{-1}=(z_2+iz_1)e^{-(2\pi/3)i}, \quad (z_2-iz_1)\rho(132)^{-1}=(z_2-iz_1)e^{(2\pi/3)i}.
\end{gathered} \tag{112}$$

From these transformations, it follows that $\psi_{m,n}$ indeed satisfies the Pauli principle under the S_3 action.

According to our procedure (60), we can form another function which satisfies the Pauli principle. For example, taking an equivariant function $(z_2+iz_1)^m$ as a seed, we can form a function

$$(z_2+iz_1)^m+(z_2+iz_1)^m e^{(2m\pi/3)\,i}+(z_2+iz_1)^m e^{-(2m\pi/3)\,i}-(z_2-iz_1)^m$$
$$-(z_2-iz_1)^m e^{(2m\pi/3)\,i}-(z_2-iz_1)^m e^{-(2m\pi/3)\,i}, \tag{113}$$

which is subject to the Pauli principle. We can multiply the function (113) by the factor $e^{-(1/4)(|z_1|^2+|z_2|^2)}$ to form a plausible wave function.

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Reduction of quantum systems with symmetry, continuous and discrete

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Reduction of dynamical systems is closely related with symmetry. The purpose of this article is to show that Fourier analysis both on compact Lie groups and on finite groups serves as a reduction procedure for quantum systems with symmetry on an equal footing. The reduction procedure is applied to systems of many identical particles lying in $\mathbf{R}^3$ which admit the action of a rotation group SO(3) and of a symmetric or permutation group. © *2002 American Institute of Physics.*
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I. INTRODUCTION

As is widely recognized, reduction of dynamical systems is closely related with symmetry. A well-known example of reduction in ordinary quantum mechanics in $\mathbf{R}^3$ comes from rotational symmetry.[1] It gives rise to the conservation of the angular momentum, and thereby the quantum state of the system can be restricted to that with a fixed angular momentum eigenvalue. The restricted state is described by one of the spherical harmonics multiplied by a function of the radial variable. The original Schrödinger equation then reduces to provide a Schrödinger equation for the radial function. In this manner, the original quantum system reduces to a quantum system of lower degree(s) of freedom. This reduction procedure proves to be based upon Fourier analysis on the rotation group SO(3). The reason why Fourier analysis on SO(3) is referred to, instead of that on S^2 with spherical harmonics, is that Fourier analysis on SO(3) reduces to that on S^2 through the bundle structure $\mathrm{SO}(3)\to S^2$, when SO(3) acts on $\mathbf{R}^3$.

As for discrete symmetry, systems of many identical particles admit symmetry by the action of symmetric (or permutation) groups, that is, symmetry of particle exchanges. A point to make here is that the particles are not assumed to be placed at vertices of regular polyhedrons, but free to spread in the space. The center-of-mass system for N identical particles is actually shown to admit the action of the symmetric group S_N. Fourier analysis on finite groups will work well in reducing the quantum system of identical particles. However, the reduction by a finite group does not mean that of degrees of freedom, but a reduction to ''eigenstates'' for the symmetric group.

A key idea to reduction procedure is the Peter–Weyl theorem[2,3] on unitary irreducible representations of compact Lie groups and of finite groups, both of which are stated in the same manner. The Peter–Weyl theorem says that matrix elements of all the inequivalent irreducible unitary representations provide a basis of Fourier analysis on the group in question. The purpose of this article is to show that Fourier analysis both on compact Lie groups and on finite groups serves as a reduction procedure for quantum systems with symmetry, continuous and discrete, on an equal footing.

The fact that the Peter–Weyl theorem on compact Lie groups serves as a reduction procedure for quantum systems has been already stated and applied, in a previous paper,[4] to many-particle systems. To understand how the Peter–Weyl theorem comes to be associated with reduction procedure for many-particle systems, one has to review geometric method for many-particle systems. For a long period before a bundle picture was introduced in the study of many-particle

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systems, a vain effort had been made to separate rotational and vibrational motions. However, the separation of them was shown to be impossible by A. Guichardet[5] by the use of the connection theory or gauge theory applied to the center-of-mass system which is viewed as a principal fiber bundle with structure group SO(3), if collinear configurations of particles are gotten rid of. With this constraint taken into account, reduction procedure was described in the bundle picture.[6] Since then, classical and quantum mechanics for many-particle systems have been studied in the bundle picture.[7–14]

A question has been kept unsettled as to how the collinear configurations should be treated in the study of reduction procedure. An answer to this question is brought about when the problem is put in a generic setting.[4] Since the center-of-mass system admits an SO(3) action, a geometric setting to start with is simply that a manifold M is given on which a compact Lie group G acts. The action of G is not assumed to be free, so that M is not made into a fiber bundle in general. Though the bundle picture fails to work, the theory of unitary representations of compact Lie groups works well on the space, $L^2(M)$, of square integrable functions on M. By an effective use of the Peter–Weyl theorem, $L^2(M)$ is decomposed into a series of subspaces, each of which is isomorphic with the space of equivariant functions taking values in a representation space, and may be viewed as the space of eigenstates assigned by the parameter, like an angular momentum eigenvalue, characterizing the representation chosen. If a given Hamiltonian is G-invariant, the original quantum system reduces to a system on the space of equivariant functions, which may be called a reduced system actually. The question mentioned above is now solved. In fact, the reduction procedure in this sense can be applied to many-particle systems without excluding collinear configurations. In this stage of reduction, we have not taken up a bundle picture, yet. If the action of G is free furthermore, the reduction procedure can be described in the bundle picture. In fact, M is then made into a principal bundle, $M \to M/G$, and the reduced system is brought into one-to-one correspondence with a quantum system defined on a complex vector bundle associated with the principal bundle $M \to M/G$.[10]

A review article by Littlejohn and Reinsch[15] is of great help in studying quantum mechanics of many-particle systems in the bundle picture. A lecture note by Ezra[16] is a unifying survey of rotation, reflection and identical particle symmetry in molecules before the introduction of the bundle theory in many-particle systems.

This article is organized as follows: Section II contains a brief review of the reduction of quantum systems by a compact Lie group on the basis of the study in Ref. 4. Section III is devoted to the study of the reduction by a finite group. The reduction procedure will run in parallel with that by a compact Lie group. Section IV contains examples. To a better comprehension, the reduction procedure is performed for quantum systems on $L^2(\mathbf{R}^3)$ with SO(3) symmetry. As is stated in the beginning of this section, Fourier analysis on SO(3) reduces to that on S^2 according to the bundle structure $\mathrm{SO}(3) \to S^2$, and thereby the quantum system on $L^2(\mathbf{R}^3)$ will reduce to a series of systems defined on the closed half line $\{r \in \mathbf{R} | r \geqslant 0\}$ with r the radial variable. Boundary conditions for wave functions at $r=0$ are also analyzed by the use of the group theory. Section V centers on the application of the reduction procedure to systems of N identical particles. The reduction procedures with both a compact Lie group SO(3) and a symmetric group S_N, a discrete finite group, are performed simultaneously. Matrix representations of S_3 and S_4 will be given explicitly, which act on the center-of-mass systems for three and four particles, respectively.

II. REDUCTION BY A COMPACT LIE GROUP

We put the problem of reduction of quantum systems with symmetry in a general setting. This section is a review from Ref. 4. Let M be a manifold on which a compact Lie group G acts. Let μ_M be a G-invariant measure on M. The space $L^2(M)$ of square integrable functions on M is the Hilbert space that we take as the space of wave functions. The inner product of functions on M is denoted, as usual, by

$$\langle f_1, f_2 \rangle_{L^2(M)} = \int_M \overline{f_1(x)} f_2(x) d\mu_M(x). \tag{1}$$

The group G is represented unitarily in $L^2(M)$ through

$$(U(g)f)(x) = f(g^{-1}x), \quad g \in G, x \in M. \tag{2}$$

By the use of the representation $g \mapsto U(g)$, one can decompose $L^2(M)$ into a direct sum of subspaces. Before describing the decomposition, we have to make a brief review of the Peter–Weyl theorem on unitary representations of compact Lie groups.

Let μ_G and $L^2(G)$ denote the normalized invariant measure on G and the space of square integrable functions on G with respect to μ_G, respectively. Let $(\mathcal{H}^\chi, \rho^\chi)$ be unitary irreducible representations of G, where χ ranges over all the inequivalent unitary irreducible representations. We denote by ρ^χ_{ij} the matrix elements of the representation ρ^χ with respect to some orthonormal basis of the representation space $\mathcal{H}^\chi$, where $i,j = 1,\ldots,d_\chi$, and $d_\chi = \dim \mathcal{H}^\chi$. The Peter–Weyl theorem[2] states that the set of all the matrix elements $\{\sqrt{d_\chi}\rho^\chi_{ij}\}_{\chi,i,j}$ form a complete orthonormal system in $L^2(G)$. Then any function φ in $L^2(G)$ is expanded into a Fourier series:

$$\varphi(h) = \sum_\chi d_\chi \sum_{i,j} \rho^\chi_{ij}(h) \int_G \overline{\rho^\chi_{ij}(g)} \varphi(g) d\mu_G(g) = \sum_\chi d_\chi \sum_i \int_G \rho^\chi_{ii}(g) \varphi(g^{-1}h) d\mu_G(g). \tag{3}$$

This theorem can be used to find a Fourier series expansion of a function on M. Given a function $f \in L^2(M)$, we may view $f(hx)$ as a function of $h \in G$, if $x \in M$ is fixed arbitrarily. We may write this function as f_x, so that $f_x(h) := f(hx)$ for $h \in G$. For $\varphi = f_x$, Eq. (3) provides

$$f(hx) = \sum_\chi d_\chi \sum_i \int_G \rho^\chi_{ii}(g) f(g^{-1}hx) d\mu_G(g). \tag{4}$$

In particular, for $h = e$, this formula gives a Fourier series expansion of f:

$$f(x) = \sum_\chi d_\chi \sum_i \int_G \rho^\chi_{ii}(g) f(g^{-1}x) d\mu_G(g). \tag{5}$$

This expansion suggests we define operators P^χ_i on $L^2(M)$ to be

$$P^\chi_i := d_\chi \int_G \rho^\chi_{ii}(g) U(g) d\mu_G(g). \tag{6}$$

Then, a straightforward calculation shows that

$$(P^\chi_i)^\dagger = P^\chi_i, \quad P^\chi_i P^{\chi'}_j = \delta^{\chi\chi'} \delta_{ij} P^\chi_i. \tag{7}$$

Further, the Fourier series expansion (5) means that

$$\sum_\chi \sum_i P^\chi_i = \mathrm{id}_{L^2(M)}, \tag{8}$$

where $\mathrm{id}_{L^2(M)}$ denotes the identity map of $L^2(M)$. Equations (7) and (8) implies that the set $\{P^\chi_i\}_{\chi,i}$ forms a family of orthogonal projection operators and provides a resolution of unity. Hence one has the orthogonal decomposition of $L^2(M)$,

$$L^2(M) = \bigoplus_\chi \bigoplus_{i=1}^{d_\chi} \mathrm{Im}\, P^\chi_i. \tag{9}$$

Moreover, we define the operators

$$P^{\chi}_{ij} := d_{\chi} \int_G \rho^{\chi}_{ij}(g) U(g) d\mu_G(g), \tag{10}$$

which prove to satisfy that

$$(P^{\chi}_{ij})^{\dagger} = P^{\chi}_{ji}, \quad P^{\chi}_{ij} P^{\chi'}_{k\ell} = \delta^{\chi\chi'} \delta_{jk} P^{\chi}_{i\ell}. \tag{11}$$

In particular, from $P^{\chi}_{ii} = P^{\chi}_{i}$ along with (11), one has

$$P^{\chi}_{ij} P^{\chi}_{j} = P^{\chi}_{i} P^{\chi}_{ij}, \quad (P^{\chi}_{ij})^{\dagger} P^{\chi}_{i} = P^{\chi}_{j} (P^{\chi}_{ij})^{\dagger}, \tag{12}$$

and further

$$(P^{\chi}_{ij})^{\dagger} P^{\chi}_{ij} = P^{\chi}_{j}, \quad P^{\chi}_{ij} (P^{\chi}_{ij})^{\dagger} = P^{\chi}_{i}. \tag{13}$$

From (12) and (13), it follows that when restricted to $\mathrm{Im}\, P^{\chi}_{j}$ the operator P^{χ}_{ij} provides a unitary isomorphism

$$P^{\chi}_{ij} : \ \mathrm{Im}\, P^{\chi}_{j} \tilde{\to} \mathrm{Im}\, P^{\chi}_{i}, \quad i,j = 1,\ldots,d_{\chi}. \tag{14}$$

Furthermore, we can show that the operators P^{χ}_{ij} and $U(g)$ are composed to give

$$P^{\chi}_{ij} U(g) = \sum_k \overline{\rho^{\chi}_{jk}(g)} P^{\chi}_{ik}, \quad U(g) P^{\chi}_{ij} = \sum_k \overline{\rho^{\chi}_{ki}(g)} P^{\chi}_{kj}. \tag{15}$$

We now denote by $\mathcal{H}^{\chi} \otimes L^2(M)$ the space of $\mathcal{H}^{\chi}$-valued square integrable functions on M. The inner product in $\mathcal{H}^{\chi} \otimes L^2(M)$ is defined by

$$\langle \psi, \phi \rangle_{\mathcal{H}^{\chi} \otimes L^2(M)} = \int_M (\psi(x), \phi(x)) d\mu_M(x), \quad \psi, \phi \in \mathcal{H}^{\chi} \otimes L^2(M), \tag{16}$$

where $(\psi(x), \phi(x))$ denotes the inner product of $\psi(x)$ and $\phi(x)$ in $\mathcal{H}^{\chi}$. The second equation of (15) then implies that the map $E^{\chi}_{j} : L^2(M) \to \mathcal{H}^{\chi} \otimes L^2(M)$ defined by

$$E^{\chi}_{j} = \frac{1}{\sqrt{d_{\chi}}} (P^{\chi}_{1j}, P^{\chi}_{2j}, \ldots, P^{\chi}_{d_{\chi} j})^{T}, \tag{17}$$

the superscript T denoting the transpose, satisfies

$$U(g^{-1}) E^{\chi}_{j} = \rho^{\chi}(g) E^{\chi}_{j}, \quad g \in G, \tag{18}$$

which implies that $\mathcal{H}^{\chi}$-valued functions $E^{\chi}_{j} f$ with $f \in L^2(M)$ are subject to the transformation

$$(E^{\chi}_{j} f)(gx) = \rho^{\chi}(g) (E^{\chi}_{j} f)(x), \quad g \in G. \tag{19}$$

Put another way, the $\mathcal{H}^{\chi}$-valued functions $E^{\chi}_{j} f$ are ρ^{χ}-equivariant functions. We here define the space of $\mathcal{H}^{\chi}$-valued ρ^{χ}-equivariant square integrable functions to be

$$L^2(M; \mathcal{H}^{\chi})^{G} = \{ \psi \in \mathcal{H}^{\chi} \otimes L^2(M) \,|\, \psi(gx) = \rho^{\chi}(g) \psi(x), \ g \in G, x \in M \}. \tag{20}$$

We then observe from (19) that the operator E^{χ}_{j} is a map $L^2(M) \to L^2(M; \mathcal{H}^{\chi})^{G}$. The adjoint operator $(E^{\chi}_{j})^{\dagger} : L^2(M; \mathcal{H}^{\chi})^{G} \to L^2(M)$ is defined, of course, through

$$\langle \psi, E_j^\chi f\rangle_{\mathcal{H}^\chi\otimes L^2(M)} = \langle (E_j^\chi)^\dagger \psi, f\rangle_{L^2(M)}, \quad \psi \in L^2(M;\mathcal{H}^\chi)^G, \quad f \in L^2(M). \tag{21}$$

We note here that components of ρ^χ-equivariant functions satisfy

$$P_{ij}^\chi \psi_j = \psi_i \quad \text{for} \quad \psi = (\psi_i) \in L^2(M;\mathcal{H}^\chi)^G. \tag{22}$$

Then, from the definition of $(E_j^\chi)^\dagger$, it follows that

$$(E_j^\chi)^\dagger \psi = \sqrt{d_\chi}\,\psi_j \quad \text{for} \quad \psi = (\psi_i) \in L^2(M;\mathcal{H}^\chi)^G. \tag{23}$$

Further, from (22) and (23), one can easily show that

$$(E_j^\chi)^\dagger E_j^\chi = P_j^\chi, \quad E_j^\chi (E_j^\chi)^\dagger = \mathrm{id}_{L^2(M;\mathcal{H}^\chi)^G}, \tag{24}$$

which implies that when restricted to $\mathrm{Im}\, P_j^\chi$ the map E_j^χ provides a unitary isomorphism

$$E_j^\chi : \ \mathrm{Im}\, P_j^\chi \xrightarrow{\sim} L^2(M;\mathcal{H}^\chi)^G, \quad j = 1,\ldots,d_\chi, \tag{25}$$

so that all $\mathrm{Im}\, P_j^\chi$, $j=1,\ldots,d_\chi$, are unitarily isomorphic to one another.

Forming the direct sum of d_χ copies of $L^2(M;\mathcal{H}^\chi)^G$, we obtain

$$\bigoplus_{j=1}^{d_\chi} \mathrm{Im}\, P_j^\chi \cong (\mathcal{H}^\chi)^* \otimes L^2(M;\mathcal{H}^\chi)^G. \tag{26}$$

From (9) and (26), $L^2(M)$ is decomposed, in conclusion, into

$$L^2(M) \cong \bigoplus_\chi ((\mathcal{H}^\chi)^* \otimes L^2(M;\mathcal{H}^\chi)^G). \tag{27}$$

We are now in a position to describe a method for reducing quantum systems with symmetry. Let $\hat{H}$ be a Hamiltonian operator acting on a dense domain in $L^2(M)$. We assume that $\hat{H}$ and $U(g)$ commute for any $g \in G$. Then $\hat{H}$ and P_i^χ also commute, so that the subspace $\mathrm{Im}\, P_i^\chi$ is invariant under $\hat{H}$. This implies that the quantum system $(L^2(M),\hat{H})$ reduces to a series of subsystems $(\mathrm{Im}\, P_i^\chi,\hat{H})$ or equivalently to $(L^2(M;\mathcal{H}^\chi)^G, \mathrm{id}_{\mathcal{H}^\chi}\otimes\hat{H})$, where $\mathrm{id}_{\mathcal{H}^\chi}\otimes\hat{H}$ means that $\mathcal{H}^\chi$-valued functions are operated componentwise with $\hat{H}$. The assumption we have used so far is that M carries the G-invariant measure μ_M. To give an example of $\hat{H}$ explicitly, we now assume that M is endowed with a Riemannian metric and that G acts on M by isometry. We take $d\mu_M$ as the volume element formed from the metric. As usual, we take $\hat{H} = -\frac{1}{2}\Delta_M + v$, where Δ_M is the Laplacian on M and v is a G-invariant function on M. Since this Hamiltonian is G-invariant, the quantum system $(L^2(M),\hat{H})$ reduces to $(L^2(M;\mathcal{H}^\chi)^G, \mathrm{id}_{\mathcal{H}^\chi}\otimes\hat{H})$.

If the action of the compact Lie group G is free furthermore, M is made into a fiber bundle $M \to M/G$ with structure group G. Then, as is well known, the space of the $\mathcal{H}^\chi$-valued ρ^χ-equivariant functions is in one-to-one correspondence with the space of sections in the complex vector bundle associated with the principal bundle $M \to M/G$. According to this, the Hamiltonian operator $\mathrm{id}_{\mathcal{H}^\chi}\otimes\hat{H}$ gives rise to a Hamiltonian operator $\hat{H}^\chi$ acting on the space of sections. Let $\Gamma_\chi^2(M/G)$ denote the space of square integrable sections in the complex vector bundle. The reduced quantum system $(L^2(M;\mathcal{H}^\chi)^G, \mathrm{id}_{\mathcal{H}^\chi}\otimes\hat{H})$ now determines a quantum system $(\Gamma_\chi^2(M/G),\hat{H}^\chi)$. To find $\hat{H}^\chi$ in an explicit manner, we need a further study, which we do not touch upon here (see Ref. 4 for details).

If the action of G is not free, the orbit space M/G is not a manifold, and hence the bundle picture of reduction procedure stated above fails to work. However, the reduction to

$(L^2(M;\mathcal{H}^\chi)^G, \mathrm{id}_{\mathcal{H}^\chi}\otimes\hat{H})$ remains to be the case. In some cases, orbit spaces become manifolds with boundary. For example, for $M=\mathbf{R}^3$ and $G=\mathrm{SO}(3)$, the orbit space M/G is a closed half line $\{r\in\mathbf{R}|r\geqslant 0\}$. This will be treated in Sec. IV.

III. REDUCTION BY A FINITE GROUP

We wish to show that the reduction procedure will work as well if we take finite groups in place of compact Lie groups. We start with a review of the Peter–Weyl theorem for finite groups. Let H be a finite group. Let π^χ_{ij} denote the matrix elements of the representation $(\mathcal{K}^\chi,\pi^\chi)$ of H, where $i,j=1,\ldots,d^\chi$ with $d^\chi=\dim\mathcal{K}^\chi$, and χ ranges all the inequivalent unitary irreducible representations. The Peter–Weyl theorem for finite groups[3] says that all the matrix elements $\{\pi^\chi_{ij}\}_{\chi,i,j}$ form a complete orthogonal set in $L^2(H)$. The inner product for $\varphi,\psi\in L^2(H)$ is defined, as usual, to be

$$\langle\varphi,\psi\rangle_{L^2(H)}=\sum_{g\in H}\overline{\varphi(g)}\psi(g). \tag{28}$$

The orthogonality of the matrix elements is expressed as

$$\frac{d^\chi}{|H|}\sum_{g\in H}\overline{\pi^\chi_{ij}(g)}\pi^{\chi'}_{i'j'}(g)=\delta_{\chi\chi'}\delta_{ii'}\delta_{jj'}, \tag{29}$$

where $|H|=\#H$, the order of H. The Fourier inversion formula then holds to provide

$$\varphi(g)=\frac{1}{|H|}\sum_\chi d^\chi\sum_{1\leqslant i,j\leqslant d^\chi}\pi^\chi_{ij}(g)\langle\pi^\chi_{ij},\varphi\rangle_{L^2(H)}=\frac{1}{|H|}\sum_\chi d^\chi\sum_{j=1}^{d^\chi}\sum_{k\in H}\overline{\pi^\chi_{jj}(k)}\varphi(gk). \tag{30}$$

Let M be a manifold which admits a right action of H, where the right action means that $x(gh)=(xg)h$ for $x\in M$ and $g,h\in H$. Let $L^2(M)$ denote the space of square integrable functions on M, where the measure μ_M on M is assumed to be invariant under H. The H is unitarily represented in $L^2(M)$ through

$$(V(g)f)(x)=f(xg),\quad x\in M,\ g\in H. \tag{31}$$

Applying the Peter–Weyl formula for $f(xg)$ with $x\in M$ arbitrarily fixed, one obtains

$$f(xg)=\frac{1}{|H|}\sum_\chi d^\chi\sum_{1\leqslant i,j\leqslant d^\chi}\pi^\chi_{ij}(g)\sum_{h\in H}\overline{\pi^\chi_{ij}(h)}f(xh)=\sum_\chi\sum_{j=1}^{d^\chi}\frac{d^\chi}{|H|}\sum_{k\in H}\overline{\pi^\chi_{jj}(k)}f(xgk). \tag{32}$$

In particular, for $g=e$, this formula gives a Fourier series expansion of f,

$$f(x)=\sum_\chi\sum_{j=1}^{d^\chi}\frac{d^\chi}{|H|}\sum_{k\in H}\overline{\pi^\chi_{jj}(k)}f(xk). \tag{33}$$

This suggests we define operators Q^χ_j on $L^2(M)$ by

$$Q^\chi_j=\frac{d^\chi}{|H|}\sum_{k\in H}\overline{\pi^\chi_{jj}(k)}V(k). \tag{34}$$

A straightforward calculation shows that

$$(Q^\chi_i)^\dagger=Q^\chi_i,\quad Q^\chi_iQ^{\chi'}_{i'}=\delta^{\chi\chi'}\delta_{ii'}Q^\chi_i, \tag{35}$$

which means that Q_j^χ's form a family of mutually orthogonal projection operators. The Fourier series expansion (33) is now put in the form

$$f(x)=\sum_\chi \sum_{j=1}^{d^\chi} (Q_j^\chi f)(x), \tag{36}$$

which implies that $L^2(M)$ is decomposed into

$$L^2(M)=\bigoplus_\chi \bigoplus_{j=1}^{d^\chi} \mathrm{Im}\, Q_j^\chi. \tag{37}$$

We now define operators Q_{ij}^χ on $L^2(M)$ to be

$$Q_{ij}^\chi=\frac{d^\chi}{|H|}\sum_{k\in H}\overline{\pi_{ij}^\chi(k)}V(k). \tag{38}$$

A straightforward calculation shows that these operators have the properties

$$(Q_{ij}^\chi)^\dagger=Q_{ji}^\chi, \quad Q_{ij}^\chi Q_{i'j'}^{\chi'}=\delta^{\chi\chi'}\delta_{ji'}Q_{ij'}^\chi. \tag{39}$$

In particular, from $Q_{ii}^\chi=Q_i^\chi$ together with (39), one verifies that

$$Q_{ij}^\chi Q_j^\chi=Q_i^\chi Q_{ij}^\chi=Q_{ij}^\chi, \tag{40}$$

and further that

$$(Q_{ij}^\chi)^\dagger Q_{ij}^\chi=Q_j^\chi, \quad Q_{ij}^\chi(Q_{ij}^\chi)^\dagger=Q_i^\chi. \tag{41}$$

From (40) and (41), it turns out that when restricted to $\mathrm{Im}\, Q_j^\chi$ the map Q_{ij}^χ provides a unitary isomorphism,

$$Q_{ij}^\chi:\ \mathrm{Im}\, Q_j^\chi \xrightarrow{\sim} \mathrm{Im}\, Q_i^\chi, \quad i,j=1,\ldots,d^\chi. \tag{42}$$

We can also verify that Q_{ij}^χ and $V(g)$ are composed to give

$$Q_{ij}^\chi V(g)=\sum_\ell \pi_{j\ell}^\chi(g)Q_{i\ell}^\chi, \quad V(g)Q_{ij}^\chi=\sum_\ell \pi_{\ell i}^\chi(g)Q_{\ell j}^\chi. \tag{43}$$

We here denote by $\mathcal{K}^\chi\otimes L^2(M)$ the space of $\mathcal{K}^\chi$-valued square integrable functions on M. Then the second equation of (43) implies that the operators $F_j^\chi: L^2(M)\to\mathcal{K}^\chi\otimes L^2(M)$ defined to be

$$F_j^\chi:=\frac{1}{\sqrt{d^\chi}}(Q_{1j}^\chi,\ldots,Q_{d^\chi j}^\chi)^T \tag{44}$$

have the property

$$V(g)F_j^\chi=\pi^\chi(g)^T F_j^\chi, \quad g\in H. \tag{45}$$

This implies that for $f\in L^2(M)$ the $\mathcal{K}^\chi$-valued function $F_j^\chi f$ is subject to the transformation

$$(F_j^\chi f)(xg)=\pi^\chi(g)^T(F_j^\chi f)(x), \quad g\in H. \tag{46}$$

We may say that the $\mathcal{K}^\chi$-valued function $F_j^\chi f$ is π^χ-equivariant. We here define the space of $\mathcal{K}^\chi$-valued square integrable π^χ-equivariant functions to be

$$L^2(M;\mathcal{K}^\chi)^H=\{\psi\in\mathcal{K}^\chi\otimes L^2(M)\,|\,\psi(xg)=\pi^\chi(g)^T\psi(x),\ \ g\in H, x\in M\}. \tag{47}$$

Then Eq. (46) shows that the operator F_j^χ is a map $L^2(M)\to L^2(M;\mathcal{K}^\chi)^H$. The adjoint operator $(F_j^\chi)^\dagger: L^2(M;\mathcal{K}^\chi)^H\to L^2(M)$ is defined through

$$\langle\psi,F_j^\chi f\rangle_{\mathcal{K}^\chi\otimes L^2(M)}=\langle(F_j^\chi)^\dagger\psi,f\rangle_{L^2(M)},\quad \psi\in L^2(M;\mathcal{K}^\chi)^H,\ \ f\in L^2(M). \tag{48}$$

We notice here that components ψ_i of $\psi\in L^2(M;\mathcal{K}^\chi)^H$ are related by Q_{ij}^χ:

$$Q_{ij}^\chi\psi_j=\psi_i,\quad i,j=1,\ldots,d^\chi. \tag{49}$$

Then, writing out the defining equation of $(F_j^\chi)^\dagger$, one obtains

$$(F_j^\chi)^\dagger\psi=\sqrt{d^\chi}\psi_j\quad\text{for}\quad\psi=(\psi_i)\in L^2(M;\mathcal{K}^\chi)^H. \tag{50}$$

Now it is easy to verify that

$$(F_j^\chi)^\dagger F_j^\chi=Q_j^\chi,\quad F_j^\chi(F_j^\chi)^\dagger=\mathrm{id}_{L^2(M;\mathcal{K}^\chi)^H}. \tag{51}$$

This implies that when restricted to $\mathrm{Im}\,Q_j^\chi$ the operator F_j^χ provides a unitary isomorphism

$$F_j^\chi:\ \mathrm{Im}\,Q_j^\chi\tilde{\to}L^2(M;\mathcal{K}^\chi)^H,\quad j=1,\ldots,d^\chi, \tag{52}$$

so that all $\mathrm{Im}\,Q_j^\chi, j=1,\ldots,d^\chi$, are unitarily isomorphic to one another.

Forming the direct sum of d^χ copies of $L^2(M;\mathcal{K}^\chi)^H$, we obtain the isomorphism

$$\bigoplus_j\ \mathrm{Im}\,Q_j^\chi\cong(\mathcal{K}^\chi)^*\otimes L^2(M;\mathcal{K}^\chi)^H, \tag{53}$$

and further, from (37),

$$L^2(M)\cong\bigoplus_\chi\ ((\mathcal{K}^\chi)^*\otimes L^2(M;\mathcal{K}^\chi)^H). \tag{54}$$

Reduction procedure for quantum systems with discrete symmetry is quite the same as that for those with compact Lie group symmetry. If the Hamiltonian $\hat{H}$ is invariant under the H action, the original system $(L^2(M),\hat{H})$ reduces to a series of subsystems $(\mathrm{Im}\,Q_j^\chi,\hat{H})$ and then equivalently to $(L^2(M;\mathcal{K}^\chi)^H,\mathrm{id}_{\mathcal{K}^\chi}\otimes\hat{H})$.

IV. EXAMPLES

In this section, we give examples of the reduction procedure discussed in Secs. II and III. As the group SO(3) is the most frequently used compact Lie group in ordinary quantum mechanics, we first perform the reduction procedure with $G=\mathrm{SO}(3)$ and $M=\mathbf{R}^3$. In this case, one has matrix elements $D_{mm'}^\ell$ for ρ_{ij}^χ, where $\ell=0,1,2,\ldots$, $|m|,|m'|\leqslant\ell$, and $d_\chi=2\ell+1$. Then the Fourier series expansion (5) is put in the form

$$f(\mathbf{x})=\sum_{\ell=0}^\infty\ \sum_{|m|\leqslant\ell}\ (2\ell+1)\int_{\mathrm{SO}(3)}\overline{D_{mm}^\ell(h)}f(h\mathbf{x})d\mu(h),\quad \mathbf{x}\in\mathbf{R}^3, \tag{55}$$

where $d\mu(h)$ is the invariant measure on SO(3) and expressed in terms of the Euler angles $h=e^{\phi\hat{\mathbf{e}}_3}e^{\theta\hat{\mathbf{e}}_2}e^{\psi\hat{\mathbf{e}}_3}$ as

$$d\mu(h)=\frac{1}{2\pi^2}\sin\theta\, d\theta d\phi d\psi \quad \text{with} \quad \int_{\mathrm{SO}(3)} d\mu(h)=1, \tag{56}$$

where $\mathbf{e}_k$, $k=1,2,3$, are the standard basis of $\mathbf{R}^3$ and $\hat{\mathbf{e}}_k$ denote the 3×3 matrices defined by $\hat{\mathbf{e}}_k\mathbf{a}=\mathbf{e}_k\times\mathbf{a}$ for $\mathbf{a}\in\mathbf{R}^3$. We wish to show that Eq. (55) provides actually a Fourier series expansion in terms of the spherical harmonics. To this end, we are to write out the integrals on the right-hand side of (55). Let $|\mathbf{x}|=r$ and set $\mathbf{x}=rg\mathbf{e}_3$, $g\in\mathrm{SO}(3)$. Then, introducing new variable $k=hg\in\mathrm{SO}(3)$, one obtains

$$\int_{\mathrm{SO}(3)}\overline{D^{\ell}_{mm}(h)}f(h\mathbf{x})d\mu(h)=\sum_{|n|\leqslant\ell}\int_{\mathrm{SO}(3)}\overline{D^{\ell}_{mn}(k)D^{\ell}_{nm}(g^{-1})}f(rk\mathbf{e}_3)d\mu(k). \tag{57}$$

We now set $k=e^{\phi'\hat{\mathbf{e}}_3}e^{\theta'\hat{\mathbf{e}}_2}e^{\psi'\hat{\mathbf{e}}_3}$, and use the fact that the D-functions[17] are expressed as

$$D^{\ell}_{mn}(k)=e^{-im\phi'}d^{\ell}_{mn}(\theta')e^{-in\psi'}, \tag{58}$$

where we do not need to give the explicit expression of $d^{\ell}_{mn}(\theta')$, but need only to note that the D-functions are factorized in accordance with the Euler variables. Then the integration with respect to $d\mu(k)$ in (57) is put in the form

$$\int_{\mathrm{SO}(3)}\overline{D^{\ell}_{mn}(k)}f(rk\mathbf{e}_3)d\mu(k)=\frac{1}{8\pi^2}\int_0^{2\pi}d\psi' e^{in\psi'}\int_{S^2}d^{\ell}_{mn}(\theta')e^{im\phi'}f(rk\mathbf{e}_3)\sin\theta'\,d\theta'\,d\phi'. \tag{59}$$

Since the right-hand side of (59) vanishes if $n\neq 0$, the Fourier series expansion (55) turns out to take the form

$$\begin{aligned} f(\mathbf{x})&=\sum_{\ell=0}^{\infty}\sum_{|m|\leqslant\ell}(2\ell+1)\int_{\mathrm{SO}(3)}\overline{D^{\ell}_{m0}(k)D^{\ell}_{0m}(g^{-1})}f(rk\mathbf{e}_3)d\mu(k)\\ &=\sum_{\ell=0}^{\infty}\sum_{|m|\leqslant\ell}\overline{Y}_{\ell m}(\theta,\phi)\int_{S^2}Y_{\ell m}(\theta',\phi')f(rk\mathbf{e}_3)\sin\theta'\,d\theta'\,d\phi', \end{aligned} \tag{60}$$

where we have also set $g=e^{\phi\hat{\mathbf{e}}_3}e^{\theta\hat{\mathbf{e}}_2}e^{\psi\hat{\mathbf{e}}_3}$ and used the formulas that relate D-functions to spherical harmonics:[16]

$$\overline{D^{\ell}_{m0}(k)}=\sqrt{\frac{4\pi}{2\ell+1}}Y_{\ell m}(\theta',\phi'),\quad \overline{D^{\ell}_{0m}(g^{-1})}=D^{\ell}_{m0}(g)=\sqrt{\frac{4\pi}{2\ell+1}}\overline{Y}_{\ell m}(\theta,\phi), \tag{61}$$

and $Y_{\ell m}(\theta,\phi)$ are given explicitly by

$$Y_{\ell m}(\theta,\phi)=(-1)^m\sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell-m)!}}P^m_{\ell}(\cos\theta)e^{im\phi}, \tag{62}$$

where P^m_{ℓ} are associated Legendre functions.[16] We notice here that $\overline{Y}_{\ell m}(\theta,\phi)=\overline{Y}_{\ell m}(g\mathbf{e}_3)$ may be considered as functions on S^2. If we introduce the notation

$$\langle\overline{Y}_{\ell m},f\rangle_{S^2}=:\int_{S^2}Y_{\ell m}(\theta',\phi')f(rk\mathbf{e}_3)\sin\theta'\,d\theta'\,d\phi', \tag{63}$$

which is a function of r, the Fourier series expansion (60) is put in the form

$$f(\mathbf{x})=\sum_{\ell=0}^{\infty}\sum_{|m|\leqslant\ell}\overline{Y}_{\ell m}(\theta,\phi)\langle\overline{Y}_{\ell m},f\rangle_{S^2},\quad \mathbf{x}=re^{\phi\hat{\mathbf{e}}_3}e^{\theta\hat{\mathbf{e}}_2}\mathbf{e}_3. \tag{64}$$

Thus we have obtained a Fourier series expansion in terms of spherical harmonics. It is of great interest to view the function $f(rk\mathbf{e}_3)$ in (63) as a function on $\mathbf{R}_+\times S^2$ which is reduced from a function on $\mathbf{R}_+\times\mathrm{SO}(3)$ through the bundle projection $\mathrm{SO}(3)\to S^2$ realized as $k\mapsto k\mathbf{e}_3$.

We proceed to the projection and "transition" operators, which are defined by (6) and (10) and denoted by P^{ℓ}_{m} and P^{ℓ}_{nm}, respectively, in the case of $G=\mathrm{SO}(3)$. Applied to a function $f(\mathbf{x})$ with $|\mathbf{x}|=r$ and $\mathbf{x}=rg\mathbf{e}_3$, the definition (10) gives rise to the function

$$(P^{\ell}_{nm}f)(\mathbf{x})=(2\ell+1)\int_{\mathrm{SO}(3)}D^{\ell}_{nm}(h)f(h^{-1}\mathbf{x})d\mu(h)=\overline{Y}_{\ell n}(\theta,\phi)\langle\overline{Y}_{\ell m},f\rangle_{S^2}, \tag{65}$$

which can be proved in a similar manner to that for bringing (55) into (60). Setting $m=n$ in the above equation results in

$$(P^{\ell}_{m}f)(\mathbf{x})=\overline{Y}_{\ell m}(\theta,\phi)\langle\overline{Y}_{\ell m},f\rangle_{S^2}, \tag{66}$$

which means that $\mathrm{Im}\,P^{\ell}_{m}$ is the space of functions which are expressed as $\overline{Y}_{\ell m}$ times functions of r. In particular, operating $\overline{Y}_{\ell m}$ with P^{ℓ}_{nm}, one obtains

$$(P^{\ell}_{nm}\overline{Y}_{\ell m})(\theta,\phi)=\overline{Y}_{\ell n}(\theta,\phi). \tag{67}$$

Then the unitary isomorphism $P^{\ell}_{nm}:\mathrm{Im}\,P^{\ell}_{m}\to\mathrm{Im}\,P^{\ell}_{n}$ [see (14)] implies that the spaces $\mathrm{Im}\,P^{\ell}_{n}$, $|n|\leqslant\ell$, are isomorphic to one another as spaces of functions of r. In the Dirac notation, we may describe P^{ℓ}_{nm} and P^{ℓ}_{m} as

$$P^{\ell}_{nm}=|\overline{Y}_{\ell n}\rangle\langle\overline{Y}_{\ell m}|,\quad P^{\ell}_{m}=|\overline{Y}_{\ell m}\rangle\langle\overline{Y}_{\ell m}|, \tag{68}$$

respectively. Here, integration must be performed not over $\mathbf{R}^3$ but over S^2, if one wishes to evaluate $P^{\ell}_{m}f$, for example.

We now proceed to the map E^{χ}_{j} defined by (17). From the definition along with (68), we see that $E^{\ell}_{m}:L^2(\mathbf{R}^3)\to\mathcal{H}^{\ell}\otimes L^2(\mathbf{R}^3)$ is given by

$$E^{\ell}_{m}f=\frac{1}{\sqrt{2\ell+1}}\begin{pmatrix}P^{\ell}_{\ell m}f\\ P^{\ell}_{\ell-1\,m}f\\ \vdots\\ P^{\ell}_{-\ell\,m}f\end{pmatrix}=\begin{pmatrix}\overline{Y}_{\ell\ell}\\ \overline{Y}_{\ell\,\ell-1}\\ \vdots\\ \overline{Y}_{\ell\,-\ell}\end{pmatrix}\frac{\langle\overline{Y}_{\ell m},f\rangle_{S^2}}{\sqrt{2\ell+1}}. \tag{69}$$

According to (19), $E^{\ell}_{m}f$ must be a D^{ℓ}-equivariant function, that is, it must satisfy the condition

$$(E^{\ell}_{m}f)(h\mathbf{x})=D^{\ell}(h)(E^{\ell}_{m}f)(\mathbf{x}),\quad h\in\mathrm{SO}(3). \tag{70}$$

However, this can also be shown to hold from the transformation rule for the spherical harmonics,

$$\overline{Y}_{\ell m}(hg\mathbf{e}_3)=\sum_{|n|\leqslant\ell}D^{\ell}_{mn}(h)\overline{Y}_{\ell n}(g\mathbf{e}_3),\quad h\in\mathrm{SO}(3), \tag{71}$$

and from the SO(3) invariance of $\langle\overline{Y}_{\ell m},f\rangle_{S^2}$.

We have to note here that if h is in $G_{\mathbf{x}}$, the isotropy subgroup of SO(3) at $\mathbf{x}=rg\mathbf{e}_3$, Eq. (70) reduces to

$$(E^{\ell}_{m}f)(\mathbf{x})=D^{\ell}(h)(E^{\ell}_{m}f)(\mathbf{x}),\quad h\in G_{\mathbf{x}}. \tag{72}$$

Since the left-hand side of the above equation is independent of h, so is the right-hand side which looks dependent on h. However, this is not a contradiction, but rather accounts for the fact that $P^{\ell}_{nm}f(=\overline{Y}_{\ell n}\langle\overline{Y}_{\ell m},f\rangle_{S^2})$ is expressed as $\overline{Y}_{\ell n}$ times a function of r. The proof runs as follows: Let $h\in G_{\mathbf{x}}$ with $\mathbf{x}\neq 0$. Then h must be a rotation about the $\mathbf{x}$-axis, and is expressed as

$$h=e^{t\hat{\mathbf{x}}/r}=ge^{t\hat{\mathbf{e}}_3}g^{-1},\quad \mathbf{x}=rg\mathbf{e}_3,\quad t\in\mathbf{R}. \tag{73}$$

Put together, Eqs. (72) and (73) give rise to

$$(E^{\ell}_m f)(r\mathbf{e}_3)=D^{\ell}(e^{t\hat{\mathbf{e}}_3})(E^{\ell}_m f)(r\mathbf{e}_3). \tag{74}$$

Since $D^{\ell}_{nm}(e^{t\hat{\mathbf{e}}_3})=e^{-int}\delta_{nm}$, the above equation implies that 2ℓ components of $(E^{\ell}_m f)(r\mathbf{e}_3)$ vanish:

$$(P^{\ell}_{nm}f)(r\mathbf{e}_3)=0\quad \text{if}\quad n\neq 0. \tag{75}$$

From (15) and (75), it follows that

$$(P^{\ell}_{nm}f)(\mathbf{x})=\sum_{|k|\leqslant\ell}D^{\ell}_{nk}(g)(P^{\ell}_{km}f)(r\mathbf{e}_3)=D^{\ell}_{n0}(g)(P^{\ell}_{0m}f)(r\mathbf{e}_3). \tag{76}$$

We observe from (61) and (76) that $(P^{\ell}_{nm}f)(\mathbf{x})$ takes the form of $\overline{Y}_{\ell n}(g\mathbf{e}_3)$ times a function of r, $\sqrt{4\pi/(2\ell+1)}(P^{\ell}_{0m}f)(r\mathbf{e}_3)$.

With $P^{\ell}_m f=\overline{Y}_{\ell m}\langle\overline{Y}_{\ell m},f\rangle_{S^2}$ instead of f, the right-hand side of (69) is unchanged:

$$E^{\ell}_m P^{\ell}_m f=\begin{pmatrix}\overline{Y}_{\ell\ell}\\ \overline{Y}_{\ell\,\ell-1}\\ \vdots\\ \overline{Y}_{\ell\,-\ell}\end{pmatrix}\frac{\langle\overline{Y}_{\ell m},f\rangle_{S^2}}{\sqrt{2\ell+1}}. \tag{77}$$

This equation must be a realization of the unitary isomorphism (25), which is denoted by E^{ℓ}_m: $\mathrm{Im}\,P^{\ell}_m\to L^2(\mathbf{R}^3;\mathcal{H}^{\ell})^{\mathrm{SO}(3)}$ in the present case, where $\mathcal{H}^{\ell}\cong\mathbf{C}^{2\ell+1}$. From (66) and (77), both $\mathrm{Im}\,P^{\ell}_m$ and $L^2(\mathbf{R}^3;\mathcal{H}^{\ell})^{\mathrm{SO}(3)}$ may be identified with the space of functions of the form $\langle\overline{Y}_{\ell m},f\rangle_{S^2}$. This space can be endowed with a suitable norm. We set $\varphi_{\ell m}(r)=\langle\overline{Y}_{\ell m},f\rangle_{S^2}$ for simplicity. Then, the squared norm of $P^{\ell}_m f=\overline{Y}_{\ell m}\varphi_{\ell m}$ is calculated as

$$\int_0^{\infty}dr\int_{S^2}\overline{\varphi_{\ell m}(r)}\varphi_{\ell m}(r)\overline{Y}_{\ell m}Y_{\ell m}\,r^2\sin\theta\,d\theta d\phi=\int_0^{\infty}|\varphi_{\ell m}(r)|^2r^2dr. \tag{78}$$

Thus $L^2(\mathbf{R}^3;\mathcal{H}^{\ell})^{\mathrm{SO}(3)}$ can be identified with the space of functions of r which are subject to the condition

$$\int_0^{\infty}|\varphi(r)|^2r^2dr<+\infty. \tag{79}$$

To consider boundary conditions for $\varphi(r)$ at $r=0$, we now take into account the D^{ℓ}-equivariance condition (70) at the origin. Since the isotropy subgroup at the origin is SO(3) itself, the D^{ℓ}-equivariance condition (70) at the origin is expressed as

$$\overline{Y}_{\ell n}(g\mathbf{e}_3)\varphi_{\ell m}(0)=\sum_{|m'|\leqslant\ell}D^{\ell}_{nm'}(h)\overline{Y}_{\ell m'}(g\mathbf{e}_3)\varphi_{\ell}(0)\quad\text{for}\quad\forall\,h\in\mathrm{SO}(3). \tag{80}$$

This implies that the vector $(\overline{Y}_{\ell n}\varphi_{\ell m}(0))_{|n|\leqslant\ell}\in\mathcal{H}^{\ell}$ is invariant under the action of all the matrices $D^{\ell}(h)$, $h\in\mathrm{SO}(3)$. Since the representation D^{ℓ} is irreducible, $\varphi_{\ell m}(0)$ must vanish if $\dim\mathcal{H}^{\ell}\geqslant 2$, i.e., $\ell\geqslant 1$. If $\ell=0$, then $\dim\mathcal{H}^{0}=1$, so that $\varphi_{\ell m}(0)$ does not need to vanish. It should be a finite value. Thus the space of square integrable functions on the closed half line $\{r\in\mathbf{R}|\ r\geqslant 0\}$, as a reduced space of quantum states, should be given by

$$\left\{\varphi\left|\int_0^{\infty}|\varphi(r)|^2r^2dr<+\infty,\quad \varphi(0)=0\right.\right\}\quad\text{for}\quad \ell\geqslant 1, \tag{81}$$

and

$$\left\{\varphi\left|\int_0^{\infty}|\varphi(r)|^2r^2dr<+\infty,\ \ \varphi(r)\text{is bounded as } r\to 0\right.\right\}\quad\text{for}\quad \ell=0. \tag{82}$$

The reduction procedure for quantum systems with symmetry proceeds as follows: Let $(L^2(\mathbf{R}^3),\hat{H})$ be a quantum system with a Hamiltonian operator $\hat{H}$. Assume that $\hat{H}$ is invariant under the action of SO(3). According to the procedure stated in Sec. II, one obtains a reduced quantum system $(\mathrm{Im}\,P_m^{\ell},\hat{H})$ or $(L^2(\mathbf{R}^3;\mathcal{H}^{\ell})^{\mathrm{SO}(3)},\mathrm{id}_{\mathcal{H}}^{\ell}\otimes\hat{H})$. The space $L^2(\mathbf{R}^3;\mathcal{H}^{\ell})^{\mathrm{SO}(3)}$ may be identified with the L^2-space on the half line which is defined by (81) for $\ell\geqslant 1$ and by (82) for $\ell=0$.

We show that the reduced quantum system $(\mathrm{Im}\,P_m^{\ell},\hat{H})$ gives rise to a quantum system to be defined on the closed half line $\{r\in\mathbf{R}|r\geqslant 0\}$. For simplicity, we assume that the Hamiltonian operator has the form

$$\hat{H}=-\tfrac{1}{2}\Delta+v(r), \tag{83}$$

where Δ and $v(r)$ are the standard Laplacian on $\mathbf{R}^3$ and a potential function depending on $r=|\mathbf{x}|$, respectively. The Δ is expressed, in terms of the spherical polar coordinates, as

$$\Delta=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\Lambda, \tag{84}$$

where Λ is the spherical Laplacian on S^2,

$$\Lambda=\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{85}$$

Operating $P_m^{\ell}f=\overline{Y}_{\ell m}\varphi_{\ell m}$ with $\hat{H}$, one obtains

$$\hat{H}P_m^{\ell}f=\overline{Y}_{\ell m}\left(-\frac{1}{2}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{\ell(\ell+1)}{2r^2}+v(r)\right)\varphi_{\ell m}, \tag{86}$$

where we have used the fact that

$$\Lambda\overline{Y}_{\ell m}=-\ell(\ell+1)\overline{Y}_{\ell m}. \tag{87}$$

Equation (86) shows that the Hamitonian $\hat{H}$ restricted to $\mathrm{Im}\,P_m^{\ell}$ gives rise to the operator

$$\hat{H}^{\ell}:=-\frac{1}{2}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{\ell(\ell+1)}{2r^2}+v(r), \tag{88}$$

which acts on functions of r. Here we have denoted the restricted operator by $\hat{H}^{\ell}$ without referring to m, since it is independent of m, actually. Thus we have obtained reduced quantum systems which are defined on the space given by (81) or (82) together with the reduced Hamiltonian operator $\hat{H}^{\ell}$ given by (88).

In conclusion of this example, we consider what boundary conditions come out on wave functions if those wave functions are assumed to be analytic at the origin. Let f be analytic at the origin. Then f is expressed as

$$f(\mathbf{x})=\sum_{n=0}^{\infty}\sum_{\substack{i+j+k=n\\ i\geqslant 0,j\geqslant 0,k\geqslant 0}} c_{ijk}x_1^i x_2^j x_3^k=\sum_{n=0}^{\infty} r^n\left(Y_n^{(n)}+Y_{n-2}^{(n)}+\cdots+\begin{Bmatrix} Y_0^{(n)} & (\text{if } n \text{ is even})\\ Y_1^{(n)} & (\text{if } n \text{ is odd})\end{Bmatrix}\right), \tag{89}$$

where $Y_k^{(n)}$ are spherical harmonics of degree k, $k=0,2,\ldots,n$ or $k=1,3,\ldots,n$, depending on whether n is even or odd. Here, use has been made of the fact that the space, $P^n(\mathbf{R}^3)$, of homogeneous polynomials of degree n is decomposed into the direct sum[18]

$$P^n(\mathbf{R}^3)=H^n(\mathbf{R}^3)\oplus r^2H^{n-2}(\mathbf{R}^3)\oplus\cdots\oplus\begin{cases} r^nH^0(\mathbf{R}^3) & (\text{if } n \text{ is even}),\\ r^{n-1}H^1(\mathbf{R}^3) & (\text{if } n \text{ is odd}),\end{cases} \tag{90}$$

where $H^k(\mathbf{R}^3)$ denotes the space of solid harmonics of degree k, and each spherical harmonic $Y_k^{(n)}$ in (89) is expressed as a linear combination of the basis of spherical harmonics, Y_{km}, $|m|\leqslant k$, of degree k:

$$Y_k^{(n)}=\sum_{|m|\leqslant k} c_m^{(n)}Y_{km}. \tag{91}$$

If we rewrite the Taylor series (89) as a Fourier series with respect to spherical harmonics $Y_{\ell m}$, and put together the terms containing spherical harmonics of degree ℓ, then we obtain

$$r^{\ell}Y_{\ell}^{(\ell)}+r^{\ell+2}Y_{\ell}^{(\ell+2)}+\cdots=\sum_{|m|\leqslant \ell}(r^{\ell}c_m^{(\ell)}+r^{\ell+2}c_m^{(\ell+2)}+\cdots)Y_{\ell m}. \tag{92}$$

This implies that if a quantum state with the angular momentum eigenvalues $\mathbf{J}^2=\ell(\ell+1)$ and $J_3=m$ is analytic at the origin, it is $Y_{\ell m}$ times an analytic function of r which has the term of the lowest order ℓ and those of every other higher order. This fact was pointed out in Ref. 1 with the assumption that $v(r)$ is analytic at $r=0$. Our conclusion holds true if $v(r)$ is not analytic at $r=0$, as long as a wave function analytic at the origin is admitted as a quantum state.

We turn to an example of the reduction by a finite group. Since we shall deal with a nontrivial application of it in the next section, we give here a quite simple example. Let $M=\mathbf{R}^n$ and $H=\mathbf{Z}_2=\{\pm 1\}$. The group $\mathbf{Z}_2$ acts on $\mathbf{R}^n$ in the manner

$$x\mapsto\varepsilon x,\quad x\in\mathbf{R}^n,\quad \varepsilon\in\mathbf{Z}_2. \tag{93}$$

All the inequivalent unitary irreducible representations are the trivial representation, $\varepsilon\mapsto 1$, and the tautological representation, $\varepsilon\mapsto\varepsilon$. Then the Fourier series expansion (36) becomes simply

$$f(x)=\tfrac{1}{2}(f(x)+f(-x))+\tfrac{1}{2}(f(x)-f(-x)). \tag{94}$$

V. APPLICATION TO MANY-PARTICLE SYSTEMS

We consider a system of many particles lying in $\mathbf{R}^3$. Let $\mathbf{x}_1,\ldots,\mathbf{x}_N$ be position vectors of particles and $m_1,\ldots,m_N$ their masses. Let M be the center-of-mass system, which is defined to be

$$M=\left\{ x=(\mathbf{x}_1,\ldots,\mathbf{x}_N)\left|\sum_{i=1}^{N} m_i\mathbf{x}_i=0\right.\right\}, \tag{95}$$

and isomorphic to $\mathbf{R}^{3(N-1)}$ as a vector space. The rotation group SO(3) acts on M in such a manner that

$$(\mathbf{x}_1,\ldots,\mathbf{x}_N)\mapsto(g\mathbf{x}_1,\ldots,g\mathbf{x}_N),\quad g\in \mathrm{SO}(3). \tag{96}$$

The configurations of particles are characterized by the linear subspaces

$$F_x:=\mathrm{span}\{\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N\},\quad x\in M. \tag{97}$$

According to $\dim F_x=0,1,2,3$, the configurations x are pointlike, collinear, planar, and spatial, respectively. Let M_k, $k=0,1,2,3$, denote the space of respective configurations of particles. Then M is broken up into

$$M=\bigcup_{k=0}^{3} M_k,\quad M_k:=\{x\in M\,|\,\dim F_x=k\}. \tag{98}$$

One can show that SO(3) acts on $\dot{M}:=M_2\cup M_3$ freely, that is, if $gx=x$ for some $x\in M_2\cup M_3$, then $g=I$ (the 3×3 identity matrix). This means that the isotropy subgroup is trivial at every point of $\dot{M}$, that is, $G_x=\{e\}$ for $x\in\dot{M}$. However, the isotropy subgroups G_x at $x\in M_1$ and at $x\in M_0$ are isomorphic with SO(2) and with SO(3), respectively. On restricting M to $\dot{M}$, we can make $\dot{M}$ into a principal fiber bundle $\dot{M}\to\dot{M}/\mathrm{SO}(3)$. However, the total space M cannot be made into a fiber bundle. This is because one has ''singular'' orbits of SO(3) through points outside of $\dot{M}$; the orbits through each point of M_1 and of M_0 are diffeomorphic with $S^2=\mathrm{SO}(3)/\mathrm{SO}(2)$ and with a point, respectively, while generic orbits through $x\in\dot{M}$ are diffeomorphic with SO(3).

Since a Hamiltonian $\hat{H}$ for many-particle systems with internal interaction only is SO(3) invariant, the reduction procedure with compact Lie groups is applied to provide a reduced system $(L^2(M;\mathcal{H}^\ell)^G,\mathrm{id}_{\mathcal{H}^\ell}\otimes\hat{H})$ with $G=\mathrm{SO}(3)$ and $\ell=0,1,2,\ldots$. Note that at this level of reduction, M does not need to be restricted to $\dot{M}$. Equation (19) then takes the form

$$(E_m^\ell f)(gx)=D^\ell(g)(E_m^\ell f)(x),\quad g\in\mathrm{SO}(3),\ x\in M, \tag{99}$$

which implies that the $\mathcal{H}^\ell$-valued function $E_m^\ell f$ describes an eigenstate associated with the eigenvalue $\ell(\ell+1)$ of the total angular momentum operator.

Restricting M to $\dot{M}$, we obtain a principal bundle $\dot{M}\to\dot{M}/\mathrm{SO}(3)$ and can make up the vector bundle associated with $\dot{M}\to\dot{M}/\mathrm{SO}(3)$ by using a representation space $\mathcal{H}^\ell$. The reduced system $(L^2(\dot{M};\mathcal{H}^\ell)^{\mathrm{SO}(3)},\mathrm{id}_{\mathcal{H}^\ell}\otimes\hat{H})$ is then in one-to-one correspondence with $(\Gamma_\ell^2(\dot{M}/\mathrm{SO}(3)),\hat{H}^\ell)$. If we want to treat the whole of M, we must impose boundary conditions on wave functions at the boundary $\partial\dot{M}=M_0\cup M_1$.[4] Since the collinear configurations are in M_1, we have to consider boundary conditions on wave functions at collinear configurations. For a three-body system, Mitchell and Littlejohn[19] studied the behavior of wave functions at collinear configurations from the viewpoint of bundle theory. By a coordinate-based method, Watson[20] studied small vibrations in the neighborhood of collinear configurations.

We turn to the reduction of quantum systems with discrete symmetry. The center-of-mass system M is looked upon as the set of configurations of the Jacobi vectors $(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})$, where $\mathbf{r}_j$'s are defined to be

$$\mathbf{r}_j=\left(\frac{1}{\mu_j}+\frac{1}{m_{j+1}}\right)^{-1/2}\left(\mathbf{x}_{j+1}-\frac{1}{\mu_j}\sum_{i=1}^{j} m_i\mathbf{x}_i\right),\quad \mu_j=\sum_{i=1}^{j} m_i\,. \tag{100}$$

We here assume that all particles are identical and set the masses all equal to one. Then Eq. (100) becomes

$$\mathbf{r}_j=\sqrt{\frac{j}{j+1}}\left(\mathbf{x}_{j+1}-\frac{1}{j}\sum_{i=1}^{j}\mathbf{x}_i\right). \tag{101}$$

Since all particles are identical, the system is unchanged if particles are exchanged mutually. Put another way, the configurations of particles admits symmetry by the action of the symmetric group S_N;

$$(\mathbf{x}_1,\ldots,\mathbf{x}_N)\mapsto(\mathbf{x}_{\sigma(1)},\ldots,\mathbf{x}_{\sigma(N)}),\quad \sigma\in S_N\,. \tag{102}$$

Since new Jacobi vectors associated with a new configuration $(\mathbf{x}_{\sigma(1)},\ldots,\mathbf{x}_{\sigma(N)})$,

$$\mathbf{r}_j^{\sigma}=\sqrt{\frac{j}{j+1}}\left(\mathbf{x}_{\sigma(j+1)}-\frac{1}{j}\sum_{i=1}^{j}\mathbf{x}_{\sigma(i)}\right),\quad j=1,\ldots,N-1, \tag{103}$$

are linearly related with the old Jacobi vectors $\mathbf{r}_j$, there exists an $N\times N$ matrix A depending on $\sigma\in S_N$ such that $(\mathbf{r}_1^{\sigma},\ldots,\mathbf{r}_{N-1}^{\sigma})=(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})A$. Thus one can find a matrix representation π: $S_N\to GL(N-1,\mathbf{R})$ through $\pi(\sigma^{-1})=A$. Thus, S_N acts on M in the manner

$$(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})\mapsto(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})\pi(\sigma^{-1}),\quad \sigma\in S_N\,. \tag{104}$$

We have to note here that since we deal with S_N as acting on M to the right, the product $\sigma\tau$ of σ, $\tau\in S_N$ is interpreted as this: σ comes first and then τ follows, so that one has $(1\,2)(1\,2\,3)=(1\,3)$, for example. If we choose the left action of S_N, we shall obtain $(1\,2)(1\,2\,3)=(2\,3)$, of course.

For example, if $N=3$, one obtains the two-dimensional representation π^2 which has the matrix expression as follows:

$$\begin{gathered}\pi^2(\sigma_1)=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \pi^2(\sigma_4)=\begin{pmatrix}-1&0\\0&1\end{pmatrix},\\ \pi^2(\sigma_2)=\begin{pmatrix}-1/2&\sqrt{3}/2\\-\sqrt{3}/2&-1/2\end{pmatrix},\quad \pi^2(\sigma_5)=\begin{pmatrix}1/2&\sqrt{3}/2\\\sqrt{3}/2&-1/2\end{pmatrix},\\ \pi^2(\sigma_3)=\begin{pmatrix}-1/2&-\sqrt{3}/2\\\sqrt{3}/2&-1/2\end{pmatrix},\quad \pi^2(\sigma_6)=\begin{pmatrix}1/2&-\sqrt{3}/2\\-\sqrt{3}/2&-1/2\end{pmatrix},\end{gathered} \tag{105}$$

where

$$\begin{gathered}\sigma_1=(1),\quad \sigma_2=(1\ 2\ 3),\quad \sigma_3=(1\ 3\ 2),\\ \sigma_4=(1\ 2),\quad \sigma_5=(2\ 3),\quad \sigma_6=(1\ 3).\end{gathered} \tag{106}$$

Incidentally, it is well known that there are three inequivalent unitary irreducible representations of S_3. The π^2 is one of them, and the other two are the trivial representation: $\pi^0(\sigma)=1$, and the signum representation; $\pi^1(\sigma)=\mathrm{sgn}(\sigma)$, both of which are one-dimensional representations. According to the Fourier series expansion formula (36), $f\in L^2(M)$ is decomposed into

$$f(x)=(Q_1^0 f)(x)+(Q_1^1 f)(x)+\sum_{j=1}^{2}(Q_j^2 f)(x), \tag{107}$$

where $Q_j^\ell := Q_j^{\pi^\ell}$, $\ell=0,1,2$, $j=1,...,d^{\pi^\ell}$, are the projection operators defined by (34). Denoting $(\mathbf{r}_1,\mathbf{r}_2)\pi^2(\sigma_\alpha^{-1})$, $\alpha=1,\ldots,6$, simply by $x\sigma_\alpha$, we can show that

$$(Q_1^0 f)(x)=\tfrac{1}{6}(f(x\sigma_1)+f(x\sigma_2)+f(x\sigma_3)+f(x\sigma_4)+f(x\sigma_5)+f(x\sigma_6)), \tag{108}$$

$$(Q_1^1 f)(x)=\tfrac{1}{6}(f(x\sigma_1)+f(x\sigma_2)+f(x\sigma_3)-f(x\sigma_4)-f(x\sigma_5)-f(x\sigma_6)), \tag{109}$$

$$\begin{aligned}(Q_1^2 f)(x)&=\tfrac{1}{3}(f(x\sigma_1)-\tfrac{1}{2}f(x\sigma_2)-\tfrac{1}{2}f(x\sigma_3)-f(x\sigma_4)+\tfrac{1}{2}f(x\sigma_5)+\tfrac{1}{2}f(x\sigma_6)),\\ (Q_2^2 f)(x)&=\tfrac{1}{3}f(x\sigma_1)-\tfrac{1}{2}f(x\sigma_2)-\tfrac{1}{2}f(x\sigma_3)+f(x\sigma_4)-\tfrac{1}{2}f(x\sigma_5)-\tfrac{1}{2}f(x\sigma_6)).\end{aligned} \tag{110}$$

We proceed to the reduction of quantum systems of many identical particles by S_N. Since the Hamiltonian $\hat{H}$ should be permutation invariant, we can apply the reduction procedure with finite groups to obtain $(L^2(M;\mathcal{K}^\chi)^H, \mathrm{id}_{\mathcal{K}^\chi}\otimes\hat{H})$ with $H=S_N$. As for S_N, we have two representations frequently used in many-identical particle systems, one of which is a trivial representation, π^0: $g\mapsto 1$, and the other the signum representation, π^1: $g\mapsto \mathrm{sgn}(g)$, where $\mathrm{sgn}(\sigma)$ is equal to 1 or -1 according to whether σ is an even or odd permutation. For π^0 and π^1, the projection operators defined in (34) take the form

$$Q^0=\frac{1}{N!}\sum_{\sigma\in S_N}V(\sigma) \quad \text{and} \quad Q^1=\frac{1}{N!}\sum_{\sigma\in S_N}\mathrm{sgn}(\sigma)V(\sigma), \tag{111}$$

respectively, where we have denoted Q_1^0 and Q_1^1 simply by Q^0 and Q^1, respectively, as π^0 and π^1 are one-dimensional representations. The operators Q^0 and Q^1 provide a method for forming wave functions obeying Bose and Fermi statistics, respectively. In fact, from (46) with $H=S_N$, one obtains

$$(Q^0 f)(xg)=(Q^0 f)(x), \quad (Q^1 f)(xg)=\mathrm{sgn}(g)(Q^1 f)(x), \quad g\in S_N. \tag{112}$$

Note here that one has $F_1^0=Q^0$ and $F_1^1=Q^0$, since π^0 and π^1 are one-dimensional representations. Thus Bose and Fermi statistics are viewed as π^0-equivariant and π^1-equivariant states, respectively, so that they are considered as reduced states with respect to S_N.

To give another reduced state, we consider the system of three identical particles and the representation π^2 given by (105). Then we can form $\mathbf{C}^2$-valued π^2-equivariant functions $F_j^2 f$ which obey the transformation rule coming from (46):

$$(F_j^2 f)(xg)=\pi^2(g)^T(F_j^2 f)(x), \quad j=1,2, \quad x\in M. \tag{113}$$

Since (113) is a generalization of (112) with $N=3$, we may consider that $F_j^2 f$ obeys some kind of statistics, like Bose or Fermi statistics. The $\mathbf{C}^2$-valued equivariant functions are described explicitly as follows:

$$(F_1^2 f)(x)=\frac{1}{\sqrt{2}}\begin{pmatrix}(Q_{11}^2 f)(x)\\ (Q_{21}^2 f)(x)\end{pmatrix}, \quad (F_2^2 f)(x)=\frac{1}{\sqrt{2}}\begin{pmatrix}(Q_{12}^2 f)(x)\\ (Q_{22}^2 f)(x)\end{pmatrix}, \tag{114}$$

where

$$(Q_{21}^2 f)(x)=\frac{1}{3}\left(-\frac{\sqrt{3}}{2}f(x\sigma_2)+\frac{\sqrt{3}}{2}f(x\sigma_3)+\frac{\sqrt{3}}{2}f(x\sigma_5)-\frac{\sqrt{3}}{2}f(x\sigma_6)\right),$$
$$(Q_{12}^2 f)(x)=\frac{1}{3}\left(\frac{\sqrt{3}}{2}f(x\sigma_2)-\frac{\sqrt{3}}{2}f(x\sigma_3)+\frac{\sqrt{3}}{2}f(x\sigma_5)-\frac{\sqrt{3}}{2}f(x\sigma_6)\right), \tag{115}$$

and $Q_{11}^2=Q_1^2$ and $Q_{22}^2=Q_1^2$ are given in (110). We notice in addition that terms containing $f(x\sigma_1)$ and $f(x\sigma_4)$ disappear on the right-hand sides of (115) on account of vanishing coefficients $\pi_{21}^2(\sigma_1)=\pi_{21}^2(\sigma_4)=0$, etc.

In conclusion, we have to point out that the action (104) of S_N on the center-of-mass system M determines an $(N-1)$-dimensional unitary representation of S_N. For example, for $N=4$, we can show, by the help of computer algebra, that the representation determined by (104) has the matrix expression as follows:

$$\pi(1)^{-1}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}, \tag{116}$$

$$\pi(123)^{-1}=\begin{pmatrix}-\frac{1}{2}&-\frac{1}{2}\sqrt{3}&0\\\frac{1}{2}\sqrt{3}&-\frac{1}{2}&0\\0&0&1\end{pmatrix}, \tag{117}$$

$$\pi(124)^{-1}=\begin{pmatrix}-\frac{1}{2}&-\frac{1}{6}\sqrt{3}&-\frac{1}{3}\sqrt{6}\\\frac{1}{6}\sqrt{3}&\frac{5}{6}&-\frac{1}{3}\sqrt{2}\\\frac{1}{3}\sqrt{6}&-\frac{1}{3}\sqrt{2}&-\frac{1}{3}\end{pmatrix}, \tag{118}$$

$$\pi(132)^{-1}=\begin{pmatrix}-\frac{1}{2}&\frac{1}{2}\sqrt{3}&0\\-\frac{1}{2}\sqrt{3}&-\frac{1}{2}&0\\0&0&1\end{pmatrix}, \tag{119}$$

$$\pi(134)^{-1}=\begin{pmatrix}\frac{1}{2}&-\frac{1}{6}\sqrt{3}&-\frac{1}{3}\sqrt{6}\\-\frac{1}{2}\sqrt{3}&-\frac{1}{6}&-\frac{1}{3}\sqrt{2}\\0&\frac{2}{3}\sqrt{2}&-\frac{1}{3}\end{pmatrix}, \tag{120}$$

$$\pi(142)^{-1}=\begin{pmatrix} -\frac{1}{2} & \frac{1}{6}\sqrt{3} & \frac{1}{3}\sqrt{6} \\ -\frac{1}{6}\sqrt{3} & \frac{5}{6} & -\frac{1}{3}\sqrt{2} \\ -\frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{121}$$

$$\pi(143)^{-1}=\begin{pmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{6}\sqrt{3} & -\frac{1}{6} & \frac{2}{3}\sqrt{2} \\ -\frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{122}$$

$$\pi(234)^{-1}=\begin{pmatrix} \frac{1}{2} & \frac{1}{6}\sqrt{3} & \frac{1}{3}\sqrt{6} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{6} & -\frac{1}{3}\sqrt{2} \\ 0 & \frac{2}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{123}$$

$$\pi(243)^{-1}=\begin{pmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{6}\sqrt{3} & -\frac{1}{6} & \frac{2}{3}\sqrt{2} \\ \frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{124}$$

$$\pi((12)(34))^{-1}=\begin{pmatrix} -1 & 0 & 0 \\ 0 & \frac{1}{3} & \frac{2}{3}\sqrt{2} \\ 0 & \frac{2}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{125}$$

$$\pi((13)(24))^{-1}=\begin{pmatrix} 0 & -\frac{1}{3}\sqrt{3} & \frac{1}{3}\sqrt{6} \\ -\frac{1}{3}\sqrt{3} & -\frac{2}{3} & -\frac{1}{3}\sqrt{2} \\ \frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{126}$$

$$\pi((14)(23))^{-1}=\begin{pmatrix} 0 & \frac{1}{3}\sqrt{3} & -\frac{1}{3}\sqrt{6} \\ \frac{1}{3}\sqrt{3} & -\frac{2}{3} & -\frac{1}{3}\sqrt{2} \\ -\frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{127}$$

$$\pi(12)^{-1}=\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{128}$$

$$\pi(13)^{-1}=\begin{pmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{129}$$

$$\pi(14)^{-1}=\begin{pmatrix} \frac{1}{2} & -\frac{1}{6}\sqrt{3} & -\frac{1}{3}\sqrt{6} \\ -\frac{1}{6}\sqrt{3} & \frac{5}{6} & -\frac{1}{3}\sqrt{2} \\ -\frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{130}$$

$$\pi(23)^{-1}=\begin{pmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{131}$$

$$\pi(24)^{-1}=\begin{pmatrix} \frac{1}{2} & \frac{1}{6}\sqrt{3} & \frac{1}{3}\sqrt{6} \\ \frac{1}{6}\sqrt{3} & \frac{5}{6} & -\frac{1}{3}\sqrt{2} \\ \frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{132}$$

$$\pi(34)^{-1}=\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{3} & \frac{2}{3}\sqrt{2} \\ 0 & \frac{2}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{133}$$

$$\pi(1234)^{-1}=\begin{pmatrix} -\frac{1}{2} & -\frac{1}{6}\sqrt{3} & -\frac{1}{3}\sqrt{6} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{6} & -\frac{1}{3}\sqrt{2} \\ 0 & \frac{2}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{134}$$

$$\pi(1243)^{-1}=\begin{pmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} & 0 \\ \frac{1}{6}\sqrt{3} & -\frac{1}{6} & \frac{2}{3}\sqrt{2} \\ \frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{135}$$

$$\pi(1324)^{-1}=\begin{pmatrix} 0 & \frac{1}{3}\sqrt{3} & -\frac{1}{3}\sqrt{6} \\ -\frac{1}{3}\sqrt{3} & -\frac{2}{3} & -\frac{1}{3}\sqrt{2} \\ \frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{136}$$

$$\pi(1342)^{-1}=\begin{pmatrix} -\frac{1}{2} & \frac{1}{6}\sqrt{3} & \frac{1}{3}\sqrt{6} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{6} & -\frac{1}{3}\sqrt{2} \\ 0 & \frac{2}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{137}$$

$$\pi(1423)^{-1}=\begin{pmatrix} 0 & -\frac{1}{3}\sqrt{3} & \frac{1}{3}\sqrt{6} \\ \frac{1}{3}\sqrt{3} & -\frac{2}{3} & -\frac{1}{3}\sqrt{2} \\ -\frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}, \tag{138}$$

$$\pi(1432)^{-1}=\begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} & 0 \\ -\frac{1}{6}\sqrt{3} & -\frac{1}{6} & \frac{2}{3}\sqrt{2} \\ -\frac{1}{3}\sqrt{6} & -\frac{1}{3}\sqrt{2} & -\frac{1}{3} \end{pmatrix}. \tag{139}$$

It is known that there are two three-dimensional inequivalent unitary representations of S_4, one of which is isomorphic with the group of symmetries of the tetrahedron, and the other with the group

of symmetries of the cube.[18] The former is a discrete subgroup of O(3) and the latter a discrete subgroup of SO(3). Since the group $\pi(S_4)$ given above includes matrices of determinant -1, it must be isomorphic with the group of symmetries of the tetrahedron.

In conclusion, we note that since the actions of SO(3) and S_N commute, one can perform the reduction procedure with SO(3) and further with S_N, so that one can talk about Bose and Fermi statistics for the reduced states in $(\Gamma^2_\ell(\dot{M}/\mathrm{SO}(3);\mathcal{H}^\ell)$.

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Internal Lifshitz tails for Schrödinger operators with random potentials

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In this short note, we prove that, for periodic Schrödinger operators perturbed by an Anderson-type random potential with long-range single site potential, the density of states always show a Lifshitz tail at a band edge. Thus, we correct a mistake made in an earlier paper [F. Klopp, Duke Math. J. **98**, 335–396 (1999)]. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1470706]

I. INTRODUCTION

The present note is devoted to the study of Lifshitz tails for periodic Schrödinger operators perturbed by a random potential of Anderson-type (or alloy-type) with long-range single site potentials. The existence of Lifshitz tails at any band edge is proven.

Lifshitz tails are a special behavior of the density of states at the edges of the spectrum; this behavior is typical for random operators. We refer to Ref. 1 for a more detailed presentation of Lifshitz tails.

Let us describe the model we study. Pick Γ a nondegenerate lattice in $\mathbb{R}^d$. $C(0,0)$ denotes the fundamental cell of the lattice Γ, i.e., if $\Gamma=f(\mathbb{Z}^d)$ where f is linear and invertible, then, we set $C(x,n)=f(\tilde{C}(x,n))$, where $\tilde{C}(x,n)=\{y\in\mathbb{R}^d;\ \text{for } j=1,\dots,d,\ -n-1/2<y_j-x_j\leqslant n+1/2\}$.

Let the potential W be real valued, Γ-periodic, and in $L^p_{\mathrm{loc}}(\mathbb{R}^d)$ (here, $p=2$ if $d\leqslant 3$, $p>2$ if $d=4$, and $p>d/2$ if $d\geqslant 5$) and, let $H=-\Delta+W$ be a periodic Schrödinger operator acting on $L^2(\mathbb{R}^d)$. Then, by Ref. 2, H is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^d)$ with domain $H^2(\mathbb{R}^d)$. Its unique self-adjoint extension is also denoted by H.

It is well known that the spectrum of H is made of bands of purely absolutely continuous spectrum separated by gaps (see, e.g., Refs. 1, 2, 3). We assume that one of the gaps is open (that is nonempty) and that the band above this gap starts at energy 0 (this is not a restriction as W may be shifted by a constant); that is, we assume that $\sigma(H)$, the spectrum of H, has a gap below energy 0 of length at least δ that is:

(H.1) For some $a>0$ and $\delta>0$, $\sigma\cap[0,a]=[0,a]$ and $\sigma\cap[-\delta,0)=\varnothing$.

We now consider the random Schrödinger operator

$$H_\omega=H+V_\omega=H+\sum_{\gamma\in\Gamma}\omega_\gamma V(\cdot-\gamma), \tag{1.1}$$

where V is a real valued function on $\mathbb{R}^d$ satisfying:

(H.2) There exists $\nu\in(d,d+2]$ and $0\leqslant g_-\leqslant g_+$, $g_+\in L^p(C(0,0))$; here, $p=2$ if $d\leqslant 3$, $p>2$ if $d=4$, and $p>d/2$ if $d\geqslant 5$ (see Refs. 2 and 4) and $0<g_-$ on some open set, such that, for any $\gamma\in\Gamma$ and almost every $x\in C(0,0)$, one has

$$g_-(x)\leqslant V(x+\gamma)\cdot(1+|\gamma|)^\nu\leqslant g_+(x), \tag{1.2}$$

and the random variables $(\omega_\gamma)_{\gamma\in\Gamma}$ satisfy

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(H.3)

(1) They are independent, identically distributed, nontrivial and bounded.

(2) They are nonnegative and 0 is in their essential support.

(3) $\limsup_{\epsilon\to 0^+} \log|\log \mathbb{P}(\{\omega_0 \leqslant \epsilon\})|/|\log \epsilon| = 0$.

Remark 1.1: Assumption (H.2) is the correct *long-range condition* for the single site potentials.

The positivity assumption on the $(\omega_\gamma)_{\gamma\in\Gamma}$ is not necessary as using the boundedness of the random variables, we may always shift them to be positive. The price to pay for that is a change in the periodic background potential W.

The second point of the previous assumption ensures that the common probability measure of the i.i.d random variables $(\omega_\gamma)_{\gamma\in\Gamma}$ does not vanish too fast (actually exponentially fast) at 0.

Assumption (H.2) and the boundedness of the random variables guarantee that, for all $\omega = (\omega_\gamma)_{\gamma\in\Gamma}$, V_ω is locally uniformly L^p, i.e., there exists $M>0$ such that, for any $\gamma\in\Gamma$, $\int_{C(\gamma,0)} |V_\omega(x)|^p dx \leqslant M$ (see Refs. 2 and 4).

We define the main object of our study, the integrated density of states. For H_ω defined as above and $n>0$, we define $H^D_{\omega,n}$ to be the Dirichlet restriction of H_ω to the cube $C(0,n)$. $H^D_{\omega,n}$ has only discrete spectrum (Ref. 2). For $E\in\mathbb{R}$, we define

$$N^n_\omega(E) = \frac{\sharp\{\text{eigenvalues of } H^D_{\omega,n} \leqslant E\}}{\mathrm{Vol}(C(0,n))}, \tag{1.3}$$

where $\sharp\mathcal{E}$ denotes the number of points of the set $\mathcal{E}$ and $\mathrm{Vol}(C(0,n))$, the volume of $C(0,n)$.

Under assumptions (H.1)–(H.3), one shows that, ω-almost surely, $N^n_\omega(E)$ has a limit when $n\to+\infty$ (Refs. 4 and 5.) This limit is independent of the realization of ω. It is the *integrated density of states* of H_ω. We denote it by $N(E)$.

Assumptions (H.1)–(H.3) guarantee that Σ, the almost sure spectrum of H_ω, contains some interval of the form $[0,a)$ $(a>0)$ (see Ref. 6). We want to study Lifshitz tails near 0. Therefore, we need to know that 0 is the edge of a gap for Σ. More precisely, for $t\in[0,1]$, we define the random Schrödinger operator $H_\omega(t) = H + tV_\omega$ and its almost sure spectrum, $\Sigma(t)$; we assume that

(H.4) For some $\delta'>0$, for any $t\in[0,1]$, $\Sigma(t)\cap[-\delta',0) = \varnothing$.

Note that, if the random variables or the potential V are sufficiently small, then assumption (H.4) holds by standard perturbation theory.

Our main result is

Theorem 1.1: *Let H and H_ω be constructed as previously, and assume that (H.1), (H.2), (H.3), and (H.4) hold. Then,*

$$\lim_{E\to 0^+} \frac{\log|\log(N(E)-N(0))|}{\log E} = -\frac{d}{\nu-d}. \tag{1.4}$$

Let us comment on this result. First, it corrects a result given in Ref. 1 where it was stated that (1.4) holds if and only if the density of states of H is nondegenerate at 0. Here, we prove that (1.4) is obtained without any condition on the behavior of the integrated density of states of the underlying periodic operator.

The behavior (1.4) was already known at the bottom of the spectrum (see, e.g., Refs. 4, 5, and 7). Note that we stated Theorem 1.1 for lower band edges; under symmetric assumptions, the corresponding result is valid for upper band edge.

We note that Theorem 1.1 also explains the necessity of single sites potentials that decay sufficiently fast at infinity in the study done in Ref. 8.

II. PERIODIC APPROXIMATIONS

Though working in the framework of Ref. 1, we use a method different from the one developed in that paper; it is related to the method used in Refs. 9 and 10. The proof goes roughly as follows. First we prove that the periodic approximations introduced in Sec. 5.1 of Ref. 1 are

exponentially close to the true density of states. Then, for a given small energy, we pick a large enough cube so that the density of states of the periodic approximation is close enough to the density of states of the random operator, and we study the density of states of that approximation.

Let us first recall some facts from the Floquet theory for periodic Schrödinger operators. Basic references where this material may be found are Refs. 2, 11, and 3. Pick $\theta\in\mathbb{R}^d$. As H is Γ-periodic, we consider H_θ the operator defined by the differential expression $-\Delta+W$ acting on L^2_θ, the space of locally square integrable functions satisfying the quasiperiodic boundary conditions $u(\cdot+\gamma)=e^{i\gamma\theta}u(\cdot)$ for all $\gamma\in\Gamma$. As H is essentially self-adjoint with domain $H^2(\mathbb{R}^d)$, H_θ is essentially self-adjoint with domain H^2_θ (i.e., the functions in L^2_θ that are locally in H^2). Moreover, as H is elliptic, the spectrum of H_θ is discrete. Let $E_0(\theta)\leqslant E_1(\theta)\leqslant\cdots\leqslant E_k(\theta)\leqslant\cdots$ be its eigenvalues; they are called *Floquet eigenvalues* of H. It is well known that H admits the Floquet decomposition

$$H=\int_{\mathbb{T}^*}^{\oplus} H_\theta\,\mathrm{d}\theta, \tag{2.1}$$

where $\mathbb{T}^*:=\mathbb{R}^d/\Gamma^*$ where $\Gamma^*=\{\gamma^*\in\mathbb{R}^d;\ \forall\,\gamma\in\Gamma,\ \langle\gamma^*\gamma\rangle\in 2\pi\mathbb{Z}\}$.

Let $n\in\mathbb{N}\backslash\{0\}$ and define the following periodic Schrödinger operator:

$$H_{\omega,n}=H+\sum_{\gamma\in C(0,n)\cap\Gamma}\omega_\gamma\sum_{\beta\in(2n+1)\Gamma}V(x-\gamma-\beta)=H+V_{\omega,n}. \tag{2.2}$$

Then, for any $\omega\in\Omega$ and $n\in\mathbb{N}^*$, $H_{\omega,n}$ is a $(2n+1)$ Γ-periodic, essentially self-adjoint Schrödinger operator. It is an H-bounded perturbation of H with relative bound 0. We notice that the boundedness assumption on the (ω_γ) implies that the family $(H_{\omega,n})_{\omega,n}$ is uniformly H-bounded (see Remark 1.1). $H_{\omega,n}$ also denotes its self-adjoint extension.

The operator $H_{\omega,n}$ admits an integrated density of states denoted by $N_{\omega,n}$ and given by

$$N_{\omega,n}(E)=\frac{1}{\mathrm{Vol}(\mathbb{T}^*_n)}\sum_{k\in\mathbb{N}}\int_{\{\theta\in\mathbb{T}^*_n;\ E_{k,n}(\theta,\omega)\leqslant E\}}\mathrm{d}\theta,$$

where $\mathbb{T}^*_n:=\mathbb{R}^d/((2n+1)\Gamma)^*$ and $(E_{k,n}(\theta,\omega))_{k\geqslant 0}$ are the Floquet eigenvalues of $H_{\omega,n}$. In Ref. 1, we proved

Theorem 2.1 (Ref. 1): *For any $\varphi\in\mathcal{C}^\infty_0(\mathbb{R})$, we have*

$$\lim_{n\to+\infty}\mathbb{E}\left(\int_{\mathbb{R}}\varphi(\lambda)\mathrm{d}N_{\omega,n}\right)=\int_{\mathbb{R}}\varphi(\lambda)\mathrm{d}N. \tag{2.3}$$

Moreover, for $\lambda\in\mathbb{R}$, a continuity point of $N(\lambda)$, one has

$$\lim_{n\to+\infty}\mathbb{E}(N_{\omega,n}(\lambda))=N(\lambda). \tag{2.4}$$

We now give an estimate on the rate of convergence in (2.3) and (2.4). Let $H_{\omega,n}$ be the periodic approximation (2.2) and $N_{\omega,n}$ be its integrated density of state. Then, we prove

Theorem 2.2: *Assume (H.1), (H.2), and (H.3). Pick $\eta_0>0$ and $I\subset\mathbb{R}$, a compact interval. Then, there exists $\nu_0>0$ and $\epsilon_0>0$ such that, for $0<\epsilon<\epsilon_0$, $E\in I$, and $n\geqslant\epsilon^{-\nu_0}$, we have*

$$\begin{aligned}\mathbb{E}(N_{\omega,n}(E+\epsilon/2)-N_{\omega,n}(E-\epsilon/2))-e^{-\epsilon^{-\eta_0}}&\leqslant N(E+\epsilon)-N(E)\\&\leqslant\mathbb{E}(N_{\omega,n}(E+2\epsilon)-N_{\omega,n}(E-2\epsilon))+e^{-\epsilon^{-\eta_0}}.\end{aligned} \tag{2.5}$$

Theorem 2.2 states that the density of states of the random Hamiltonian H_ω is exponentially well approximated by the expectation of the densities of states of the periodic Hamiltonians $H_{\omega,n}$ even for n not very large (i.e., for n of size roughly a negative power of the approximation parameter ϵ).

Proof: Theorem 2.2 is a consequence of a similar result for random operators with compactly supported single site potentials. More precisely, define $V_\epsilon(x)=V(x)\mathbf{1}_{\epsilon\cdot|x|\leqslant 1}$ and the random operator

$$H_{\epsilon,\omega}=H+V_{\epsilon,\omega}=H+\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma V_\epsilon(\cdot-\gamma).$$

Let N_ϵ be the integrated density of states of $H_{\epsilon,\omega}$. We define $H_{\epsilon,\omega,n}$, the periodic approximations of $H_{\epsilon,\omega}$ in the same way as for H_ω [just replace V by V_ϵ in (2.2)]. Let $N_{\epsilon,\omega,n}$ be their integrated density of states.

We first notice that, using the decay assumption (H.2) and the fact that the random variables $(\omega_\gamma)_\gamma$ are bounded, uniformly in n and ω, we have

$$\|(1-\Delta)^{-1}(H_{\epsilon,\omega}-H_\omega)\|+\|(1-\Delta)^{-1}(H_{\epsilon,\omega,n}-H_{\omega,n})\|\leqslant C\epsilon^{\nu-d}.$$

This implies that, uniformly in n and ω, and locally uniformly in E, one has

$$\begin{aligned}N_\epsilon(E-C\epsilon^{\nu-d})\leqslant N(E)\leqslant N_\epsilon(E+C\epsilon^{\nu-d}),\\ N_{\epsilon,\omega,n}(E-C\epsilon^{\nu-d})\leqslant N_{\omega,n}(E)\leqslant N_{\epsilon,\omega,n}(E+C\epsilon^{\nu-d}).\end{aligned}\tag{2.6}$$

So to prove Theorem 2.2, we only need to prove it for $H_{\epsilon,\omega}$ and replace ϵ by $\epsilon^{1/(\nu-d)}$. The gain is that, for the new operators, the single site potential is compactly supported. The proof of Theorem 2.2 in this case relies upon the

Lemma 2.1: Assume that the single site potential V is compactly supported in a ball of radius R centered at 0. Pick I, a relatively compact open interval in $\mathbb{R}$. *For any* $\beta\in(0,1)$, *there exists* $C>1$ *and* $\rho>0$ [*depending only on d, the bound on* $(\omega_\gamma)_\gamma$ *and on* $\|V\|_{\ell^1(L^p)}:=\Sigma_{\gamma\in\Gamma}\|V\|_{L^p(C(\gamma,0))}$] *such that, for any* $\varphi\in\mathcal{C}_0^\infty(I)$, *for* $k\in\mathbb{N}^*$ *and* $n\in\mathbb{N}^*$, $n>R$, *we have*

$$|\mathbb{E}((\varphi,\mathrm{d}N_{\omega,n}))-(\varphi,\mathrm{d}N)|\leqslant C|n-R|^{-(1-\beta)k}\cdot k^k\cdot\sup_{\substack{x\in\mathbb{R}\\0\leqslant j\leqslant k+\rho}}\left|(|x|+C)^{\rho+k}\frac{d^j\varphi}{d^jx}(x)\right|.\tag{2.7}$$

Proof: This lemma was proved in Refs. 9, 10, and 12 in different settings but essentially the same arguments apply in the present case too. The proof relies upon two facts.

(1) For $\varphi\in\mathcal{C}_0^\infty(\mathbb{R})$, one has

$$\mathbb{E}((\varphi,\mathrm{d}N_{\omega,n}))=\frac{1}{\mathrm{Vol}(C(0,0))}\mathbb{E}(\mathrm{tr}(\mathbf{1}_{C(0,0)}\varphi(H_{\omega,n})\mathbf{1}_{C(0,0)})).\tag{2.8}$$

(2) The following estimate on the difference between the resolvents of $H_{\omega,n}$ and H_ω at an energy $z\in\mathbb{C}\backslash\mathbb{R}$:

$$\begin{aligned}\|\mathbf{1}_{C(0,0)}((z-H_{\omega,n})^{-1}-(z-H_\omega)^{-1})\mathbf{1}_{C(0,0)}\|&=\|\mathbf{1}_{C(0,0)}((z-H_{\omega,n})^{-1}(V_{\omega,n}-V_\omega)(z-H_\omega)^{-1})\mathbf{1}_{C(0,0)}\|\\&\leqslant C\exp\left(-\frac{|\mathrm{Im}\,z|}{C\cdot(1+|z|)}|n-R|\right).\end{aligned}\tag{2.9}$$

Equality (2.8) is proved in Ref. 1 [formula (5.7) on p. 357]. Estimate (2.9) is a consequence of the computation done to prove Theorem 5.1 in Ref. 1 (pp. 358–360) of the fact that, by construction, $(V_{\omega,n}-V_\omega)$ vanishes in the cube centered at 0 of side length $2(n-R)+1$ (as V is supported in a

ball of size R), and of the exponential decay of the resolvent kernels $(z-H_\omega)^{-1}$ and $(z-H_{\omega,n})^{-1}$ [this is a consequence of the Combes–Thomas estimates, see, e.g., (Refs. 13 and 14)]. To obtain Lemma 2.1 from (2.9), one then uses the representation formula (5.9) in Ref. 1 for $\varphi(H)$ in terms of almost analytic extensions of φ, and the standard estimates for almost analytic extension (5.8) in Ref. 1. □

Let us now derive Theorem 2.2 from Lemma 2.1. Let φ be a Gevrey class function of Gevrey exponent $\alpha>1$ (see Ref. 15); assume, moreover, that φ has compact support in $(-2,2)$, that $0\leqslant\varphi\leqslant 1$, and that $\varphi\equiv 1$ on $[-1,1]$. Let $E\in\mathbb{R}$ and set

$$\varphi_{E,\epsilon}(\cdot)=\varphi\left(\frac{\cdot-E}{\epsilon}\right).$$

Fix $I\subset\mathbb{R}$ compact. Then, by Lemma 2.1 and the Gevrey estimates on the derivatives of φ, we get that, there exist $C>1$ such that, for $E\in I$, $n>R$, $k\geqslant 1$ and $0<\epsilon<1$, we have

$$\left|\mathbb{E}((\varphi_{E,\epsilon},\mathrm{d}N_{\omega,n}))-(\varphi_{E,\epsilon},\mathrm{d}N)\right|\leqslant\epsilon^{-k-\rho}(k+\rho)^{2\alpha(k+\rho)}(n-R)^{-(1-\beta)k}.$$

We pick $k+\rho=(n-R)^{(1-\beta)/(4\alpha)}$ for $n-R$ large, and get that, there exist $C>1$ such that, for $E\in I$, $n>R+2$, $k\geqslant\rho$ and $0<\epsilon<1$, we have

$$\left|\mathbb{E}((\varphi_{E,\epsilon},\mathrm{d}N_{\omega,n}))-(\varphi_{E,\epsilon},\mathrm{d}N)\right|\leqslant((n-R)^{-(1-\beta)/4}\epsilon^{-\alpha})^{(n-R)^{(1-\beta)/(4\alpha)}}.$$

Now, in the case we are interested in, we have set $R=R_\epsilon\sim\epsilon^{1/(d-\nu)}$. Hence, we choose $\eta>1$, $n\geqslant\epsilon^{-\eta(4\alpha)/(1-\beta)}+R_\epsilon$; so, there exist $\epsilon_0>0$ such that, for $0<\epsilon<\epsilon_0$, we have

$$\left|\mathbb{E}((\varphi_{E,\epsilon},\mathrm{d}N_{\omega,n}))-(\varphi_{E,\epsilon},\mathrm{d}N)\right|\leqslant e^{-\epsilon^{-\eta}}. \tag{2.10}$$

By the definition of φ, as $dN_{\epsilon,\omega,n}$ and dN_ϵ are positive measures, we have

$$\mathbb{E}(N_{\epsilon,\omega,n}(E+\epsilon)-N_{\epsilon,\omega,n}(E-\epsilon))\leqslant\mathbb{E}((\varphi_{E,\epsilon},\mathrm{d}N_{\epsilon,\omega,n}))\leqslant\mathbb{E}(N_{\epsilon,\omega,n}(E+2\epsilon)-N_{\epsilon,\omega,n}(E-2\epsilon)),$$

$$N_\epsilon(E+\epsilon)-N_\epsilon(E-\epsilon)\leqslant(\varphi_{E,\epsilon},\mathrm{d}N)\leqslant N_\epsilon(E+2\epsilon)-N_\epsilon(E-2\epsilon).$$

This, Eqs. (2.6) and (2.10) complete the proof of Theorem 2.2 for $H_{\epsilon,\omega}$ and hence for H_ω. □

III. THE PROOF OF THE LOWER BOUND

We now turn to the proof of

$$\liminf_{\substack{\epsilon\to 0\\ \epsilon>0}}\frac{\log|\log(N(\epsilon)-N(0^-))|}{\log\epsilon}\geqslant-\frac{d}{\nu-d}. \tag{3.1}$$

In Sec. 6 of Ref. 1, it is proved that if 0 is a band edge of the spectrum of H and $\theta_0\in\mathbb{T}^*$ is a Floquet parameter such that, for some $n\geqslant 0$, one has $E_n(\theta_0)=0$, then, there exists V, a neighborhood of θ_0 in $\mathbb{T}^*$, and $f:\theta\in V\mapsto f(\cdot,\theta)$ a real analytic, H^2_θ-valued function such that, for some $C>0$, one has

$$\forall\,\theta\in V,\quad \|H_\theta f(\cdot,\theta)\|_{L^2(C(0,0))}\leqslant C|\theta|^2 \text{ and } \|f(\cdot,\theta)\|_{L^2(C(0,0))}=1. \tag{3.2}$$

Let $\alpha>0$ be a small constant. Pick $\epsilon>0$. Let $\chi\in\mathcal{C}_0^\infty(\{|\theta|<1\})$ be positive, and such that $\int_{\{|\theta|<1\}}\chi^2\,\mathrm{d}\theta=2$. Then, we define

$$w_\epsilon(\theta)=\epsilon^{-d(1+\alpha)/4}\chi(\epsilon^{-(1+\alpha)/2}(\theta-\theta_0))\in L^2(\mathbb{T}^*).$$

We also define

$$w_\epsilon^f(\cdot)=\int_{\mathbb{T}^*} w_\epsilon(\theta)\cdot f(\cdot,\theta)\mathrm{d}\theta.$$

Using (3.2), for ϵ sufficiently small, one checks that

$$\|w_\epsilon^f\|^2=\int_{\mathbb{T}^*}\|f(\cdot,\theta)\|^2_{L^2(C(0,0))}|w_\epsilon(\theta)|^2\mathrm{d}\theta=2 \tag{3.3}$$

and that, for some $C>0$, one has

$$\|Hw_\epsilon^f\|^2\leqslant C\epsilon^{2(1+\alpha)}. \tag{3.4}$$

Using the fact that $f(\cdot,\theta)$ satisfies quasiperiodic boundary conditions, the smoothness of the function $\theta\mapsto f(x,\theta)$ and the nonstationary phase, one proves that, for any $k\in\mathbb{N}$, there exists $C_k>0$ such that, for any $\gamma\in\Gamma$,

$$\begin{aligned}\int_{C(\gamma,0)}|w_\epsilon^f(x)|^2\mathrm{d}x&=\int_{C(0,0)}\left|\int_{\mathbb{T}^*}e^{-i\gamma\theta}w_\epsilon(\theta)f(x,\theta)\mathrm{d}\theta\right|^2\mathrm{d}x\\&=\int_{C(0,0)}\left|\epsilon^{d(1+\alpha)/4}\int_{\{|\theta|<1\}}e^{-i\epsilon^{1+\alpha/2}\gamma\theta}\chi(\theta)f(x,\theta_0+\epsilon^{(1+\alpha)/2}\theta)\mathrm{d}\theta\right|^2\mathrm{d}x\\&\leqslant C_k(1+|\epsilon^{(1+\alpha)/2}\gamma|^2)^{-k/2}.\end{aligned} \tag{3.5}$$

Similar estimates hold for $\int_{C(\gamma,0)}|\nabla w_\epsilon^f(x)|^2\mathrm{d}x$ and for $\int_{C(\gamma,0)}|Hw_\epsilon^f(x)|^2\mathrm{d}x$.

Pick $\tilde{\chi}$, a $\mathcal{C}_0^\infty$-function supported in $|x|\leqslant 2$ such that $\tilde{\chi}\equiv 1$ for $|x|\leqslant 1$; and set $\tilde{\chi}_\epsilon(x)=\tilde{\chi}(\epsilon^{(1+2\alpha)/2}x)$. Then, for ϵ sufficiently small, the function $w_\epsilon=\tilde{\chi}_\epsilon w_\epsilon^f$ satisfies

(1) w_ϵ is supported in a ball of center 0 and radius $2\epsilon^{-(1+2\alpha)/2}$,
(2) $1\leqslant\|w_\epsilon\|^2_{L^2}\leqslant 2$,
(3) $\|Hw_\epsilon\|^2_{L^2}\leqslant C\epsilon^{2(1+\alpha)}$ for some $C>0$.

Point (1) is obvious. Point (2) follows from (3.3) and (3.5). And point (3) follows from (3.4), (3.5) and its analog for ∇w_ϵ^f and Hw_ϵ^f as $\|\nabla\tilde{\chi}_\epsilon\|_\infty\leqslant C\epsilon^{(1+2\alpha)/2}$ and $\|\Delta\tilde{\chi}_\epsilon\|_\infty\leqslant C\epsilon^{1+2\alpha}$.

Pick $n\in\mathbb{N}^*$ such that $n\sim\epsilon^{-\eta}$ for $\eta>\max(\nu_0,1/(\nu-d)+\alpha)$; here, ν_0 is given in Theorem 2.2 for $\eta_0>d/(\nu-d)+\mathrm{d}\alpha$. As w_ϵ has compact support in the interior of $C(0,n)$, it can be "periodized" to satisfy quasiperiodic boundary conditions; for $\theta\in\mathbb{R}^d$, we set

$$w_{\epsilon,\theta}(\cdot)=\sum_{\beta\in(2n+1)\Gamma}e^{-i\beta\theta}w_\epsilon(\cdot+\beta).$$

Then, $w_{\epsilon,\theta}$ satisfies $w_{\epsilon,\theta}(x+\beta)=e^{i\beta\theta}w_{\epsilon,\theta}(x)$ for $x\in\mathbb{R}^d$ and $\beta\in(2n+1)\Gamma$. And, one has

$$\|w_{\epsilon,\theta}\|^2_{L^2(C(0,n))}\geqslant 1. \tag{3.6}$$

We define

$$\Lambda_\alpha(\epsilon)=\{\gamma\in\Gamma;\quad\text{for } 1\leqslant j\leqslant d,\ |\gamma_j|\leqslant\epsilon^{-(1+3\alpha)/(\nu-d)}\}.$$

Using assumption (H.1), one computes

$$V_{\omega,n}(x)=\sum_{\gamma\in\Gamma}\omega_{[\gamma]}V(x-\gamma)\text{where }[\gamma]=\gamma \bmod (2n+1)\Gamma$$

$$\leqslant\sum_{\gamma\in\Gamma}\omega_{[\gamma]}\sum_{\alpha\in\Gamma}g_+(x-\gamma-\alpha)\cdot(1+|\alpha|)^{-\nu}$$

$$=\sum_{\alpha\in\Gamma}A_\alpha(\omega)g_+(x-\alpha)\text{where }A_\alpha(\omega)=\sum_{\gamma\in\Gamma}\omega_{[\gamma]}(1+|\alpha-\gamma|)^{-\nu}. \tag{3.7}$$

If we assume that, for $\gamma\in\Lambda_\alpha(\epsilon)$, one has $\omega_\gamma\leqslant\epsilon^{1+\alpha}$, then (3.7) implies

$$\|V_{\omega,n}w_{\epsilon,\theta}\|\leqslant C\epsilon^{1+\alpha}\|w_{\epsilon,\theta}\|. \tag{3.8}$$

This, (3.6), and point (3) imply that, for some $C>0$ and ϵ sufficiently small, one has

$$\|H_{\omega,n,\theta}w_{\epsilon,\theta}\|\leqslant C\epsilon^{1+\alpha}\|w_{\epsilon,\theta}\|.$$

This proves that, for ϵ sufficiently small, if, for $\gamma\in\Lambda_\alpha(\epsilon)$, one has $\omega_\gamma\leqslant\epsilon^{1+\alpha}$, then for all $\theta\in\mathbb{T}_n^*$, $H_{\omega,n,\theta}$ has an eigenvalue in $[-\epsilon/2,\epsilon/2]$. Hence, we get that

$$\mathbb{E}(N_{\omega,n}(E+\epsilon/2)-N_{\omega,n}(E-\epsilon/2))\geqslant P(\epsilon,\alpha), \tag{3.9}$$

where $P(\epsilon,\alpha)$ is the probability of the event $\{\omega;\ \forall\gamma\in\Lambda_\alpha(\epsilon),\ \omega_\gamma\leqslant\epsilon^{1+\alpha}\}$. By assumption (H.3), one has

$$\liminf_{\substack{\epsilon\to0\\\epsilon>0}}\frac{\log|\log(P(\epsilon,\alpha))|}{\log\epsilon}\geqslant-\frac{d}{\nu-d}(1+3\alpha).$$

Combining this estimate with (3.9) and (2.5) [recall that we picked $\eta_0>d/(\nu-d)+d\alpha$], we obtain

$$\liminf_{\substack{\epsilon\to0\\\epsilon>0}}\frac{\log|\log(N(\epsilon)-N(0^-))|}{\log\epsilon}\geqslant-\frac{d}{\nu-d}(1+3\alpha).$$

As α is an arbitrary positive number, we get (3.1).

IV. THE PROOF OF THE UPPER BOUND

We pick $\eta_0>d/(\nu-d)$ in Theorem 2.2 and $n\sim\epsilon^{-\eta}$ for $\eta>\nu_0$ (ν_0 is given in Theorem 2.2). To complete the proof of (1.4), in view of (2.5), we only need to prove that

$$\limsup_{\epsilon\to0^+}\frac{\log|\log(\mathbb{E}(N_{\omega,n}(\epsilon)-N_{\omega,n}(0)))|}{\log\epsilon}\leqslant-\frac{d}{\nu-d}. \tag{4.1}$$

Indeed, by assumption (H.4), we know that, for ϵ sufficiently small, for all ω and n, one has $N_{\omega,n}(0)=N_{\omega,n}(-\epsilon)$ (see also Sec. 5.2 in Ref. 1).
We prove

Lemma 4.1: Define the potential G by $G(\cdot)=\Sigma_{\gamma\in\Gamma}g_-(\cdot-\gamma)$. Then, if $n\sim\epsilon^{-\rho}$ with $\rho>1/(\nu-d)$, the event $\{\omega;\ V_{\omega,n}\geqslant\epsilon G\}$ has probability at least $1-P_\epsilon$ where P_ϵ satisfies

$$\limsup_{\epsilon\to0^+}\frac{\log|\log(P_\epsilon)|}{\log\epsilon}\leqslant-\frac{d}{\nu-d}. \tag{4.2}$$

Lemma 4.2: There exists $C>0$ *and* $\epsilon_0>0$ *(independent of* n *and* ω*) such that, if* $0<\epsilon<\epsilon_0$ *and* ω *satisfies* $V_{\omega,n}\geqslant C\epsilon G$*, then for* $n\in\mathbb{N}$*, one has* $N_{\omega,n}(0)=N_{\omega,n}(\epsilon)$.

Lemma 4.2 just says that if $V_{\omega,n}\geqslant C\epsilon G$, then $H_{\omega,n}$ has no spectrum in the interval $(0,\epsilon)$.

Estimate (4.1) is now an immediate consequence of Lemmas 4.1 and 4.2. Indeed, picking C as in Lemma 4.2, one computes

$$\begin{aligned}\mathbb{E}(N_{\omega,n}(\epsilon)-N_{\omega,n}(0)) &= \mathbb{E}([N_{\omega,n}(\epsilon)-N_{\omega,n}(0)]\mathbf{1}_{\{\omega;\ V_{\omega,n}\geqslant C\epsilon G\}})\\ &\quad+\mathbb{E}([N_{\omega,n}(\epsilon)-N_{\omega,n}(0)]\mathbf{1}_{\{\omega;\ V_{\omega,n}\not\geqslant C\epsilon G\}})\\ &= \mathbb{E}([N_{\omega,n}(\epsilon)-N_{\omega,n}(0)]\mathbf{1}_{\{\omega;\ V_{\omega,n}\not\geqslant C\epsilon G\}})\leqslant C_0\mathbb{P}(\{\omega;\ V_{\omega,n}\not\geqslant C\epsilon G\})\\ &= C_0(1-\mathbb{P}(\{\omega;\ V_{\omega,n}\geqslant C\epsilon G\}))=C_0P_{C\epsilon}\end{aligned}$$

and we conclude using (4.2) as $(\nu-d)\eta_0>1$. Here, we have used the fact that the integrated density of states of $H_{\omega,n}$ is bounded locally uniformly in energy, uniformly in ω and n.

A. Proof of Lemma 4.2

The operator $H+\epsilon G$ is Γ-periodic. Hence, it is also $(2n+1)\Gamma$-periodic. When doing the Floquet reduction using this period, we call it $(H+\epsilon G)_n$, and $(H+\epsilon G)_{n,\theta}$ denotes this operator considered with quasiperiodic boundary conditions given by θ, i.e., as acting on $\{u\in L^2_{\mathrm{loc}};\ u(\cdot+\gamma)=e^{i\gamma\theta}u(\cdot),\ \forall\gamma\in(2n+1)\Gamma\}$.

Let $\vartheta((H+\epsilon G)_{n,\theta},E)$ denote the number of eigenvalues of $(H+\epsilon G)_{n,\theta}$ below energy E. Standard perturbation theory and the results of Sec. 5.2 in Ref. 1 [see in particular (5.24)] tell us that, for $\epsilon>0$ sufficiently small, one has

$$\vartheta((H+\epsilon G)_{n,\theta},0)=\vartheta((H)_{n,\theta},0)=\vartheta(H_{\omega,n,\theta},0^-). \tag{4.3}$$

Hence, if $V_{\omega,n}\geqslant\epsilon G$, this immediately implies that, for $E\geqslant 0$, one has

$$0\leqslant N_{\omega,n}(E)-N_{\omega,n}(0)\leqslant N_\epsilon(E)-N_\epsilon(0),$$

where N_ϵ is the density of states of the Γ-periodic operator $H+\epsilon G$. So Lemma 4.1 is proved if we prove that there exists $C>0$ (independent of ϵ) such that, for ϵ sufficiently small, one has $N_\epsilon(\epsilon/C)-N_\epsilon(0)=0$. This is a consequence of

Lemma 3.3: Let H *be a* Γ*-periodic Schrödinger operator, and* G *be a non-negative* Γ*-periodic potential in* $L^p_{\mathrm{loc}}(\mathbb{R}^d)$ *[where* p *is chosen as in assumption (H.2)] and such that* $G>0$ *on some open set. Assume that, for some* $\delta>0$, $(-\delta,0)$ *does not intersect the spectrum of* H.

Then, there exists $C>0$ *and* $\epsilon_0>0$ *such that, for* $0\leqslant\epsilon\leqslant\epsilon_0$, $(-\delta/2,\epsilon/C)$ *does not intersect the spectrum of* $H+\epsilon G$.

Proof: Let us first assume that 0 is not in the spectrum of H; then, there exists $\delta'>0$ such that $(-\delta,\delta')$ does not intersect the spectrum of H, and regular perturbation theory tells us that, for ϵ sufficiently small, $(-\delta/2,\delta'/2)$ does not intersect the spectrum of $H+\epsilon G$. This completes the proof of Lemma 4.3 in this case.

We now assume that 0 belongs to the spectrum of H. Let $(E_n(\epsilon,\theta))_{1\leqslant n}$ be the Floquet eigenvalues of $(H+\epsilon G)_\theta$ ordered increasingly; they are continuous in ϵ and θ. Hence, there exists $\epsilon_0>0$ and $n_0\geqslant 1$ such that, for $0\leqslant\epsilon\leqslant 0$, one has that $E_n(\epsilon,\theta)<0$ if and only if $n<n_0$. Then, to prove Lemma 4.3, we need to prove that there exists $C>0$ and $\epsilon_0>0$ such that, for $0\leqslant\epsilon\leqslant\epsilon_0$, one has

$$E_{n_0}(\epsilon,\theta)\geqslant\epsilon/C. \tag{4.4}$$

Define $\mathcal{S}=\{\theta\in\mathbb{T}^*;\ E_{n_0}(0,\theta)=0\}$; $\mathcal{S}$ is compact. Outside of a neighborhood of $\mathcal{S}$, (4.4) is certainly satisfied as, there, one has $E_{n_0}(\epsilon,\theta)\geqslant E_{n_0}(0,\theta)\geqslant\delta'$ (for some $\delta'>0$). So we need only to prove (4.4) in a neighborhood of $\mathcal{S}$.

Therefore, pick $\theta_0\in\mathcal{S}$. Let $p(\theta_0)$ be the multiplicity of 0 as an eigenvalue of $H_\theta=(H+\epsilon G)_{\theta|\epsilon=0}$; it is finite. For θ close to θ_0 and ϵ small, define the Riesz projector

$$\Pi_{\epsilon,\theta}=\frac{1}{2i\pi}\oint_{\mathcal{C}_0}((H+\epsilon G)_\theta-z)^{-1}\mathrm{d}z, \tag{4.5}$$

where $\mathcal{C}_0=\{|z|=\delta'\}$ is a small loop in the complex plane. $\Pi_{\epsilon,\theta}$ is the projector onto the spectral space associated with the interval $(-\delta',\delta')$ and the operator $(H+\epsilon G)_\theta$. It is real analytic in θ and ϵ, hence, of constant rank. Moreover, for some $C>0$, for any ϵ, ϵ' sufficiently small and θ, θ' sufficiently close to θ_0, one has

$$\|\Pi_{\epsilon,\theta}-\Pi_{\epsilon',\theta'}\|\leqslant C(|\epsilon-\epsilon'|+|\theta-\theta|). \tag{4.6}$$

This implies that, for any ϵ, ϵ' sufficiently small and θ, θ' sufficiently close to θ_0, one has

$$\Pi_{\epsilon,\theta}\Pi_{\epsilon',\theta'}\Pi_{\epsilon,\theta}\geqslant\tfrac{1}{2}\,\Pi_{\epsilon,\theta}. \tag{4.7}$$

$E_{n_0}(\epsilon,\theta)$ is the smallest eigenvalue of the finite rank operator $O_{\epsilon,\theta}=\Pi_{\epsilon,\theta}(H+\epsilon G)_\theta\Pi_{\epsilon,\theta}$ [acting on $\Pi_{\epsilon,\theta}L^2_\theta(\mathbb{R}^d)$]. The operator $O_{\epsilon,\theta}$ is real analytic in ϵ and θ. Consider the operator $\tilde{O}_{\epsilon,\theta}=\Pi_{\epsilon,\theta}\Pi_{0,\theta}(H+\epsilon G)_\theta\Pi_{0,\theta}\Pi_{\epsilon,\theta}$. Using $\Pi_{0,\theta}H=H$, one computes

$$\begin{aligned}
O_{\epsilon,\theta}-\tilde{O}_{\epsilon,\theta}&=\Pi_{\epsilon,\theta}(1-\Pi_{0,\theta})(H+\epsilon G)_\theta(1-\Pi_{0,\theta})\Pi_{\epsilon,\theta}+\epsilon\Pi_{\epsilon,\theta}(1-\Pi_{0,\theta})G\Pi_{0,\theta}\Pi_{\epsilon,\theta}\\
&\quad+\epsilon\Pi_{\epsilon,\theta}\Pi_{0,\theta}G(1-\Pi_{0,\theta})\Pi_{\epsilon,\theta}\\
&=\Pi_{\epsilon,\theta}(\Pi_{\epsilon,\theta}-\Pi_{0,\theta})(H+\epsilon G)_\theta(\Pi_{\epsilon,\theta}-\Pi_{0,\theta})\Pi_{\epsilon,\theta}+\epsilon\Pi_{\epsilon,\theta}(\Pi_{\epsilon,\theta}-\Pi_{0,\theta})G\Pi_{0,\theta}\Pi_{\epsilon,\theta}\\
&\quad+\epsilon\Pi_{\epsilon,\theta}\Pi_{0,\theta}G(\Pi_{\epsilon,\theta}-\Pi_{0,\theta})\Pi_{\epsilon,\theta}.
\end{aligned}$$

This implies that, for some $C>0$, for ϵ sufficiently small and θ close to θ_0, one has

$$\|O_{\epsilon,\theta}-\tilde{O}_{\epsilon,\theta}\|\leqslant C\epsilon^2.$$

So, for ϵ sufficiently small positive and θ close to θ_0, one has

$$O_{\epsilon,\theta}\geqslant\tilde{O}_{\epsilon,\theta}-C\epsilon^2\geqslant\epsilon\Pi_{\epsilon,\theta}\Pi_{0,\theta}G\Pi_{0,\theta}\Pi_{\epsilon,\theta}-C\epsilon^2. \tag{4.8}$$

One proves

Lemma 4.4: For some $C>0$ and θ close to θ_0, one has

$$\Pi_{0,\theta}G\Pi_{0,\theta}\geqslant 1/C\Pi_{0,\theta}. \tag{4.9}$$

This, (4.8) and (4.7) imply that, for ϵ positive, sufficiently small, one has

$$O_{\epsilon,\theta}\geqslant\frac{\epsilon}{2C}\,\Pi_{\epsilon,\theta}. \tag{4.10}$$

Equation (4.10) then immediately implies (4.4) for ϵ sufficiently small and θ sufficiently close to θ_0. We then obtain (4.4) for a neighborhood of $\mathcal{S}$ as $\mathcal{S}$ is compact. This completes the proof of Lemma 4.3. □

Proof of Lemma 4.4: First, we note that

$$\Pi_{0,\theta}G\Pi_{0,\theta}=\Pi_{0,\theta}\Pi_{0,\theta_0}G\Pi_{0,\theta_0}\Pi_{0,\theta}-\Pi_{0,\theta}(\Pi_{0,\theta_0}G\Pi_{0,\theta_0}-\Pi_{0,\theta}G\Pi_{0,\theta})\Pi_{0,\theta}.$$

Hence, as $\theta\mapsto\Pi_{0,\theta}G\Pi_{0,\theta}$ is continuous, by (4.7), we just need to prove (4.9) for $\theta=\theta_0$. Let $(\psi_j)_{1\leqslant j\leqslant p(\theta_0)}$ be a basis of eigenvector in the kernel of H_{θ_0}. Then $\Pi_{0,\theta_0}=\Sigma_{1\leqslant j\leqslant p(\theta_0)}\psi_j\otimes\psi_j$. Hence, (4.9) is satisfied if and only if the matrix $((\langle G\psi_i,\psi_j\rangle))_{i,j}$ is positive definite. It is nonnegative. If 0 were an eigenvalue of this matrix, there would exist $\psi\in\mathrm{Span}((\psi_j)_{1\leqslant j\leqslant p(\theta_0)})$ such that $\int_{C(0,0)}G(x)|\psi(x)|^2\mathrm{d}x=0$. Hence, as $G>0$ on some open set, ψ would vanish on this open set: this is not possible by the unique continuation principle as ψ satisfies $H\psi=0$ (see, e.g., Refs. 16 and 17). □

B. Proof of Lemma 3.1

Let us write out $V_{\omega,n}$ and use assumption (H.2). One computes

$$V_{\omega,n}(x)=\sum_{\gamma\in\Gamma}\omega_{[\gamma]}V(x-\gamma)\geqslant\sum_{\gamma\in\Gamma}\omega_{[\gamma]}\sum_{\alpha\in\Gamma}g_-(x-\gamma-\alpha)\cdot(1+|\alpha|)^{-\nu}$$

$$=\sum_{\alpha\in\Gamma}A_\alpha(\omega)g_-(x-\alpha)\text{where }A_\alpha(\omega)=\sum_{\gamma\in\Gamma}\omega_{[\gamma]}(1+|\alpha-\gamma|)^{-\nu}.$$

As $\omega_{[\gamma]}$ is $(2n+1)\Gamma$-periodic, so is $A_\alpha(\omega)$. Define $\Gamma_{2n+1}=\Gamma/(2n+1)\Gamma=\{\gamma\in\Gamma;|\gamma|\leqslant n\}$. Then, we have

$$\mathbb{P}(\{V_{\omega,n}\geqslant\epsilon G\})\geqslant\mathbb{P}(\{\forall\gamma\in\Gamma_{2n+1};\ A_\gamma(\omega)\geqslant\epsilon\})\geqslant1-\sum_{\gamma\in\Gamma_{2n+1}}\mathbb{P}(\{A_\gamma(\omega)\leqslant\epsilon\}).$$

Note that, as the $(\omega_\gamma)_\gamma$ are stationary, the distribution of the random variable $A_\gamma(\omega)$ is independent of γ. Hence

$$\mathbb{P}(\{V_{\omega,n}\geqslant\epsilon G\})\geqslant1-(2n+1)^d\mathbb{P}(\{A_0(\omega)\leqslant\epsilon\}). \tag{4.11}$$

So we only need to estimate $\mathbb{P}(\{A_0(\omega)\leqslant\epsilon\})$. Therefore, we compute

$$A_0(\omega)=\sum_{\beta\in(2n+1)\Gamma}\sum_{\gamma\in\Gamma_{2n+1}}\omega_\gamma(1+|\beta+\gamma|)^{-\nu}$$

$$=\sum_{\gamma\in\Gamma_{2n+1}}\omega_\gamma u_\gamma\text{ where }u_\gamma=\sum_{\beta\in(2n+1)\Gamma}(1+|\beta+\gamma|)^{-\nu}.$$

Using Markov's inequality, for any $\lambda>0$, one obtains

$$\mathbb{P}(A_0(\omega)\leqslant\epsilon)\leqslant\mathbb{E}\left(\exp\left(\lambda\left(\epsilon-\sum_{\gamma\in\Gamma_{2n+1}}\omega_\gamma u_\gamma\right)\right)\right)\leqslant e^{\lambda\epsilon}\prod_{\gamma\in\Gamma_{2n+1}}\mathbb{E}(e^{-\lambda\omega_\gamma u_\gamma}). \tag{4.12}$$

Using the Taylor expansion of $x\mapsto e^{-x}$ at 0, as the random variables $(\omega_\gamma)_\gamma$ are bounded, for $\lambda u_\gamma<\eta$, η sufficiently small, one obtains

$$\mathbb{E}(e^{-\lambda\omega_\gamma u_\gamma})\leqslant1-\mathbb{E}(\omega_\gamma)\lambda u_\gamma+C(\lambda u_\gamma)^2\leqslant1-\mathbb{E}(\omega_\gamma)\lambda u_\gamma(1-C\eta).$$

Hence, we have proved that, there exists $\eta>0$ such that, if $\lambda u_\gamma<\eta$, then

$$\mathbb{E}(e^{-\lambda\omega_\gamma u_\gamma})\leqslant e^{-\overline{\omega_0}\lambda u_\gamma/2}, \tag{4.13}$$

where $\overline{\omega_0}=\mathbb{E}(\omega_0)>0$ by assumption (H.3).
Plugging (4.13) into (4.12), we compute

$$\log(\mathbb{P}(A_0(\omega)\leqslant\epsilon))\leqslant\lambda\epsilon-\frac{\lambda\overline{\omega_0}}{2}\cdot\sum_{\substack{\gamma\in\Gamma_{2n+1}\\ \lambda u_\gamma<\eta}}u_\gamma. \tag{4.14}$$

Assume that $n\geqslant\lambda^{1/\nu}$; then, the definition of u_γ implies that, for some $C>0$, one has

$$\sum_{\substack{\gamma\in\Gamma_{2n+1}\\ \lambda u_\gamma<\eta}}u_\gamma\geqslant\sum_{\substack{\gamma\in\Gamma\\ C\lambda^{1/\nu}\leqslant|\gamma|\leqslant n-\lambda^{1/\nu}}}(1+|\gamma|)^{-\nu}\geqslant\frac{1}{C}\lambda^{(d-\nu)/\nu}.$$

Plugging this back into (4.14) and picking $\lambda=\rho\epsilon^{\nu/(d-\nu)}$, we obtain

$$\log(\mathbb{P}(A_0(\omega)\leqslant\epsilon))\leqslant-\rho(\overline{\omega_0}\rho^{d/\nu}/C-1)\epsilon^{-d/(\nu-d)}\leqslant-\frac{1}{C}\epsilon^{-d/(\nu-d)} \tag{4.15}$$

for ρ sufficiently large.

So that, if we pick, e.g., $n\sim\epsilon^{-p}$ with $p>1/(\nu-d)$, and, we exponentiate estimate (4.15) and plug into (4.11), we complete the proof of Lemma 4.1. □

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Noncommutative tori and universal sets of nonbinary quantum gates

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We address the problem of universality in simulation of evolution of quantum system and in theory of quantum computations related with the possibility of expression or approximation of arbitrary unitary transformation by composition of specific unitary transformations (quantum gates) from given set. In an earlier paper application of Clifford algebras to constructions of universal sets of binary quantum gates $U_k \in U(2^n)$ was shown. For application of a similar approach to nonbinary quantum gates $U_k \in U(l^n)$, in present work we used rational noncommutative torus $\mathbb{T}^{2n}_{1/l}$. A set of universal nonbinary two-gates is presented here as one example. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1476391]

I. INTRODUCTION

Let $\mathcal{H}_l$ be a Hilbert space of quantum systems with l states and $\mathcal{H}_l^n \equiv \mathcal{H}_l^{\otimes n}$ is an l^n-dimensional Hilbert space of n systems expressed as the nth tensor power. For $l=2$ an element of $\mathcal{H}_2$ ($\mathcal{H}_2^n$) is usually called a qubit(s). An algebra $\mathbb{C}(l^n \times l^n)$ of all complex $l^n \times l^n$ matrices corresponds to general linear transformations of $\mathcal{H}_l^n$ and a group of unitary matrices $U(l^n)$ corresponds to physically possible evolution. Because of the natural structure of tensor power it is possible to consider groups of transformations of subsystems $U(l^k) \cong U(l^n) \cap (\mathbb{C}(l^k \times l^k) \otimes \mathbb{1}_l^{\otimes n-k})$. Such transformations correspond to *quantum gates*. For $l=2$ they are usually called k-qubits gates.

The problem of universality in quantum simulation and computation is related to approximation with necessary precision (in some appropriate norm) of arbitrary unitary transformation $U \in U(l^n)$ of $\mathcal{H}_l^n$ as a product of matrices U_k from some fixed set called here the *universal set of quantum gates*. One origin of the task was the idea of generalization of the Church–Turing principle from computer science to physical systems in works by David Deutsch,[1,2] where it was suggested there be some universal set of matrices for "*binary*" quantum gates with $l=2$.

It was found also that it is possible to express necessary conditions of universality by using elegant framework with Lie algebra $\mathfrak{u}(2^n)$ of Lie group $\mathrm{U}(2^n)$.[3–5] In the approach it is necessary to find a set of elements $A_k \in \mathfrak{u}(2^n)$, $A_k^\dagger = -A_k$, which generate full algebra $\mathfrak{u}(2^n)$. It is possible to use $U_k^\tau = \exp(\tau A_k)$ with infinitesimal parameter $\tau \in \mathbb{R}$ as a universal set of quantum gates. In a more physical picture, $A_k \triangleq iH_k$, where H_k are Hamiltonians and Lie brackets also contain multipliers with imaginary unit.

Previous work[6] suggested construction of the universal set by inclusion $\mathfrak{u}(2^n)$ in Clifford algebra $\mathfrak{Cl}(2n,\mathbb{C}) \cong \mathbb{C}(2^n \times 2^n)$ with Lie algebra structure due to bracket operation $[a,b] \equiv ab - ba$ (cf. Ref. 7). Because commutation laws for basis elements of Clifford algebra are simple enough due to canonical relations between generators,

$$\Gamma_j \Gamma_k + \Gamma_k \Gamma_j = 2\delta_{kj}\mathbb{1}, \tag{1.1}$$

it was possible to represent useful constructions of universal sets with $2n+1$ elements (see Ref. 6).

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For generalization of the method for "nonbinary" quantum gates $U(l^n)$, $l>2$, it is useful to find some algebra with simple commutation rules, like Eq. (1.1), and use it to express elements of $\mathfrak{u}(l^n)$. In this article as such, generalization of $\mathfrak{Cl}(2n,\mathbb{C})\cong\mathbb{C}(2^n\times 2^n)$ used a *noncommutative torus* $\mathbb{T}^{2n}_{1/l}\cong\mathbb{C}(l^n\times l^n)$ with $2n$ generators:

$$(T_k)^l=\mathbb{1}, \tag{1.2a}$$

$$T_jT_k=\zeta T_kT_j \quad (j<k), \tag{1.2b}$$

$$\zeta=\exp(2\pi i/l). \tag{1.2c}$$

For $l=2$ Eq. (1.2) coincides with Eq. (1.1). For $l>2$, elements $T_k\notin\mathfrak{u}(l^n)$ for most or all k, but it is possible to use representation $\mathfrak{u}(N)\subset\mathfrak{R}(\mathfrak{gl}(N,\mathbb{C}))$. More concretely, it is enough to find a set of elements $M_k\in\mathfrak{gl}(N,\mathbb{C})$, which generate full algebra $\mathfrak{gl}(N,\mathbb{C})$. It is possible to use $G_k^\tau=\exp(i\tau(M_k+M_k^\dagger))$, $F_k^\tau=\exp(\tau(M_k-M_k^\dagger))$ with infinitesimal parameter $\tau\in\mathbb{R}$ as a universal set of quantum gates.

II. NONCOMMUTATIVE TORUS $\mathbb{T}^2_\theta$ AND QUANTUM ONE-GATES

Let us consider one-particle transformations. For two-dimensional case, $\mathcal{H}_2$, any two Pauli matrices, for example σ_x and σ_z, generate full four-dimensional basis of $\mathbb{C}(2\times 2)$, i.e., $\{\sigma_x^2=\sigma_y^2=\mathbb{1}_2,\sigma_x,\sigma_z,\sigma_y=i\sigma_x\sigma_z\}$.

Analogously, two generators U,V of noncommutative torus $\mathbb{T}^2_\theta$ defined as[8]

$$UV=\exp(2\pi i\theta)VU, \quad VV^\dagger=UU^\dagger=\mathbb{1}, \tag{2.1}$$

produce for rational $\theta=1/l$ an algebra isomorphic to $\mathbb{C}(l\times l)$. The bases of the algebra are l^2 elements U^mV^n, $m,n=0,\ldots,l-1$.

Let us use the Weyl representation of U and V as the right cyclic shift operator and its Fourier transform:

$$U_{kj}=\delta_{k+1(\mathrm{mod}\ l),j}, \quad V_{kj}=\exp(2\pi ik/l)\,\delta_{kj}. \tag{2.2}$$

The representation and U^mV^n basis are well known in quantum information science after application to the theory of quantum error correction.[9]

To find transformation between basis U^mV^n and canonical basis E^{ab} of $\mathbb{C}(l\times l)$, there $(E^{ab})_{jk}=\delta_{aj}\delta_{bk}$, it is enough to use $E^{00}=(1/l)\,\Sigma_{k=0}^{l-1}V^k$ together with $E^{ab}=U^{l-a}E^{00}U^b$.

Let us show that any U^mV^n (except $\mathbb{1}_l$ for $m=n=0$) can be generated from U and V using only commutators $[A,B]\equiv(\mathrm{ad}\ A)\,B\equiv AB-BA$. For U and V commutator is simply $[U,V]=(1-\zeta)\,UV\propto UV$, where $\zeta=\exp(2\pi i/l)$. It is convenient to use "ad" for consecutive commutators, for example, $(\mathrm{ad}\ A)^2B\equiv[A,[A,B]]$, and symbol "proportional," $A\propto B\Rightarrow A=\alpha B$, to avoid unessential nonzero complex multipliers α.

Direct expressions for l^2-1 elements U^mV^n are

$$U^mV^n\propto(\mathrm{ad}\ U)^{m-1(\mathrm{mod}\ l)}((\mathrm{ad}\ V)^{n-1(\mathrm{mod}\ l)}[U,V]), \tag{2.3}$$

where $0\leqslant m,n<l$ for any pair of numbers except $m=n=0$, $(\mathrm{ad}\ U)^0$ or $(\mathrm{ad}\ V)^0$ corresponds to the absence of the term, and $-1(\mathrm{mod}\ l)=l-1$.

Of course it is possible to suggest simpler expression for particular values of m and n, but Eq. (2.3) shows also application of a third element $W\propto UV$:

$$UW=\zeta WU, \quad WV=\zeta VW. \tag{2.4}$$

It is convenient to define

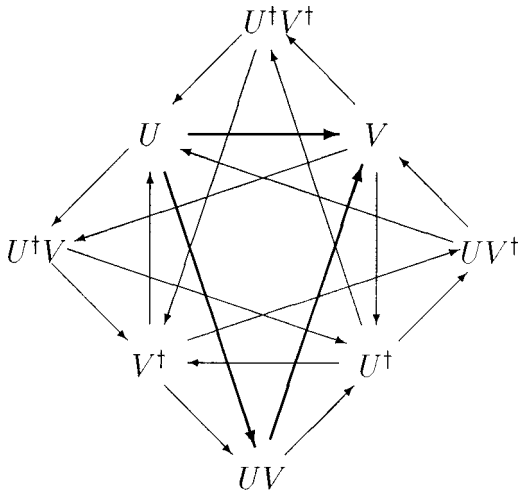
$$W=\zeta^{(l-1)/2}UV, \quad W^l=\mathbb{1}_l. \tag{2.5}$$

Similar with case $l=2$ with $(\sigma_x,\sigma_y,\sigma_z)$, any pair between (U,V,W) may be used for generation of a full algebra due to Eq. (2.3) and due to possibility to express initial pair (U,V) from (U,W) or (V,W):

$$V\propto(\text{ad } U)^{l-1}W, \quad U\propto(\text{ad } V)^{l-1}W, \tag{2.6}$$

but for $l\geqslant 3$ there is a special property that should be taken into account. Let us use notation $A\rightarrow_\zeta B$ for $AB=\zeta BA$. The definition of relation "$\rightarrow_\zeta$" is asymmetric for $l\geqslant 3$.

It is clear from the diagram:



For different sets with three operators the relation may be transitive or not.

For example, $U\rightarrow_\zeta V$ from Eq. (2.1), $U\rightarrow_\zeta W$ and $W\rightarrow_\zeta V$ from Eq. (2.4) and so we have transitive relation $U\rightarrow_\zeta W\rightarrow_\zeta V$, i.e., *ordering*. Let us call it *ζ-order* for certainty. On the other hand, it is simply to check $W^\dagger\rightarrow_\zeta U$ and $V\rightarrow_\zeta W^\dagger$ and here is some cyclic graph. The cyclic case is more symmetric, because all pairs are equivalent.

For the ordered case it is not so, because ζ-order produces a canonical map to a set of natural numbers, i.e., indexes, and it is convenient for construction of noncommutative torus $\mathbb{T}^{2n}_{1/l}$, ζ-ordered by definition: $\mathbb{T}_k\rightarrow_\zeta\mathbb{T}_j$ for $k<j$ [see Eq. (1.2)].

Because of the principle we use the following definition for generators of $\mathbb{T}^2_{1/l}$:

$$T_0\equiv U, \quad T_1\equiv W. \tag{2.7}$$

where U is defined in Eq. (2.2) and W in Eq. (2.5).

III. REPRESENTATIONS OF NONCOMMUTATIVE TORI $\mathbb{T}^{2n}_{1/l}$

Let us use notation $T_x\equiv U$, $T_y\equiv W$, $T_z=V$, where U, V, W are defined in Eqs. (2.2) and (2.5). There is ζ-order $T_x\rightarrow_\zeta T_y\rightarrow_\zeta T_z$, i.e.,

$$T_xT_y=\zeta T_yT_x, \quad T_yT_z=\zeta T_zT_y, \quad T_xT_z=\zeta T_zT_x. \tag{3.1}$$

It is possible to introduce $2n$ generators of $\mathbb{T}^{2n}_{1/l}$ as

$$T_{2k}=\underbrace{\mathbb{1}_l\otimes\cdots\otimes\mathbb{1}_l}_{n-k-1}\otimes T_x\otimes\underbrace{T_z\otimes\cdots\otimes T_z}_{k}, \tag{3.2a}$$

$$T_{2k+1}=\underbrace{\mathbb{1}_l\otimes\cdots\otimes\mathbb{1}_l}_{n-k-1}\otimes T_y\otimes\underbrace{T_z\otimes\cdots\otimes T_z}_{k}, \tag{3.2b}$$

in direct analogy with construction of Clifford algebras.[6,7]

It is clear that different products of T_k generate full matrix algebra $\mathbb{C}(l^n\times l^n)$, because T_x and T_y generate $\mathbb{C}(l\times l)$. Let us prove that generators Eq. (3.2) satisfy definition (1.2) of noncommutative torus $\mathbb{T}^{2n}_{1/l}$:

$T^l_k=\mathbb{1}$ because $T^l_x=T^l_y=T^l_y=\mathbb{1}_l$.

To prove that $T_k\rightarrow_\zeta T_j$ for any $k<j$, it is enough to consider a few cases (here "T" means "any element" and "$\downarrow_\zeta$" marks ζ-order of only a pair of noncommutative terms in the tensor products):

Case 1: $T_{2k}\rightarrow_\zeta T_{2k+1}$, $k\geqslant 0$

$$T_{2k}=\underbrace{\mathbb{1}_l\otimes\cdots\otimes\mathbb{1}_l}_{n-k-1}\otimes T_x\otimes\underbrace{T_z\otimes\cdots\otimes T_z}_{k}$$

$$\downarrow_\zeta$$

$$T_{2k+1}=\mathbb{1}_l\otimes\cdots\otimes\mathbb{1}_l\otimes T_y\otimes T_z\otimes\cdots\otimes T_z$$

Case 2: $T_{2k}\rightarrow_\zeta T_{2k+j+1}$, $k\geqslant 0$, $j>0$

$$T_{2k}=\underbrace{\mathbb{1}_l\otimes\cdots\otimes\mathbb{1}_l}_{n-k-1}\otimes T_x\otimes\underbrace{T_z\otimes\cdots\otimes T_z}_{k}$$

$$\downarrow_\zeta$$

$$T_{2k+1+j}=\mathbb{1}_l\otimes\cdots\otimes T\otimes T_z\otimes T_z\otimes\cdots\otimes T_z$$

Case 3: $T_{2k+1}\rightarrow_\zeta T_{2k+1+j}$, $k\geqslant 0$, $j>0$

$$T_{2k+1}=\underbrace{\mathbb{1}_l\otimes\cdots\otimes\mathbb{1}_l}_{n-k-1}\otimes T_y\otimes\underbrace{T_z\otimes\cdots\otimes T_z}_{k}$$

$$\downarrow_\zeta$$

$$T_{2k+1+j}=\mathbb{1}_l\otimes\cdots\otimes T\otimes T_z\otimes T_z\otimes\cdots\otimes T_z$$

IV. GENERATION OF $\mathbb{T}^{2n}_{1/l}$ BY COMMUTATORS

Let us prove that for $l>2$ it is possible to generate $\mathbb{T}^{2n}_{1/l}$ using only commutators of $2n$ elements T_k. The case with $l=2$, $\mathfrak{CL}(2n,\mathbb{C})\cong\mathbb{T}^{2n}_{1/2}$ was considered in earlier work,[6] and it was shown that $2n$ generators are not enough and it is necessary to add any element of third or fourth order.

We present proof that for $l>2$ $2n$ generators are enough. Let us instead of $T^{n_i}_i T^{n_j}_j\cdots T^{n_k}_k$ write simply $T(n_i,n_j,\ldots,n_k)$ if it is possible without lost of clarity. Sequences of indexes are always chosen ordered $0\leqslant i<j<\cdots<k<2n$. Let us use # for the number of different indexes in product $\#(n_0,\ldots,n_{k-1})\equiv k$ and Σ for total number of terms $\Sigma(n_0,\ldots,n_{k-1})\equiv\Sigma^{k-1}_{j=0}n_j$.

It is possible to prove proposition using recursion. The case with $\#=2$ may be expressed by generalization of Eq. (2.3):

$$T(n_i,n_j)\propto(\mathrm{ad}\ T_i)^{n_i-1(\mathrm{mod}\ l)}((\mathrm{ad}\ T_j)^{n_j-1(\mathrm{mod}\ l)}[T_i,T_j]). \tag{4.1}$$

Let all cases with $T(n_{i_1},\ldots,n_{i_k})$, $2\leqslant k<2n$, $i_1<i_2<\cdots<i_k$, be proved and it is necessary to generate all $T(n_{i_1},\ldots,n_{i_k},n_j)$ with $i_k<j\leqslant 2n$.

There are a few different cases:

Case 1: $\Sigma(n_{i_1},\ldots,n_{i_k})\ \mathrm{mod}\ l\neq 0$:

$$T(n_{i_1},\ldots,n_{i_k},n_j)\propto(\mathrm{ad}\ T_j)^{n_j}T(n_{i_1},\ldots,n_{i_k}). \tag{4.2}$$

Case 2: $\Sigma(n_{i_1},\ldots,n_{i_k})\ \mathrm{mod}\ l=0$ and Eq. (4.2) vanishes:

Case 2.1: $\exists n_i\in(n_{i_1},\ldots,n_i,\ldots,n_{i_k}),n_i\neq n_j$:

$$T(n_{i_1},\ldots,n_{i_k},n_j)\propto[T_i,(\mathrm{ad}\ T_j)^{n_j}T(n_{i_1},\ldots,n_i-1,\ldots,n_{i_k})]. \tag{4.3}$$

Case 2.2: $\nexists n_i\in(n_{i_1},\ldots,n_i,\ldots,n_{i_k}),n_i\neq n_j$, i.e., $n_{i_1}=\ldots=n_{i_k}=n_j$.

Case 2.2.1: $2n_j\neq l$:

$$T(n_{i_1},\ldots,n_{i_k},n_j)\propto[T(n_{i_1},\ldots,n_{i_{k-1}}),T(n_{i_k},n_j)]. \tag{4.4}$$

Case 2.2.2: $2n_j=l$; let $n_{k_i}=n'_{k_i}+n''_{k_i}$:

$$T(n_{i_1},\ldots,n_{i_k},n_j)\propto[T(n_{i_1},\ldots,n'_{k_i}),T(n''_{i_k},n_j)]. \tag{4.5}$$

The cases include all possible variants and so the suggestion is proved by recursion and all l^n-1 possible products of generators except of $\mathbb{1}$ can be represented using commutators.

V. UNIVERSAL SET OF QUANTUM TWO-GATES

Elements T_k have up to n non-unit terms in tensor product Eq. (3.2). Here is described construction with no more than two terms. It is used for description of a universal set of quantum two-gates and also has direct analog with two-qubit gates.[6]

Let us consider $B_0=T_0$, $B_j=T_jT_{j-1}^{\dagger}$, $1\leqslant j<2n$. It is possible to generate full $\mathbb{T}_{1/l}^{2n}$ using the $2n$ elements: $T_1\propto[T_0,B_1]$, $T_i\propto[B_i,T_{i-1}]$, $\forall i>1$, and so it is possible to generate recursively all T_i and use construction of $\mathbb{T}_{1/l}^{2n}$ described above.

With using Eq. (3.2) it is possible to write expressions for B_j:

$$B_0=T_0=\mathbb{1}^{\otimes(n-1)}\otimes T_x, \tag{5.1a}$$

$$B_{2k+1}=T_{2k+1}T_{2k}^{\dagger}\propto\mathbb{1}^{\otimes(n-k-1)}\otimes T_z\otimes\mathbb{1}^{\otimes k}, \tag{5.1b}$$

$$B_{2k+2}=T_{2k+2}T_{2k+1}^{\dagger}\propto\mathbb{1}^{\otimes(n-k-2)}\otimes T_x\otimes T_x^{\dagger}\otimes\mathbb{1}^{\otimes k}, \tag{5.1c}$$

with $k=0,\ldots,n-1$ (or $n-2$).

To produce a universal set of quantum one- and two-gates it is enough to use constructions of unitary matrices mentioned in the Introduction:

$$G_k^{\tau}=e^{i\tau(B_k+B_k^{\dagger})},\quad F_k^{\tau}=e^{\tau(B_k-B_k^{\dagger})}. \tag{5.2}$$

It is possible to choose τ to express an arbitrary matrix with given precision as product of matrices (5.2).

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A note on the improvement ambiguity of the stress tensor and the critical limits of correlation functions

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I study various properties of the critical limits of correlators containing insertions of conserved and anomalous currents. In particular, I show that the improvement term of the stress tensor can be fixed unambiguously, studying the RG interpolation between the UV and IR limits. The removal of the improvement ambiguity is encoded in a variational principle, which makes use of sum rules for the trace anomalies a and a'. Compatible results follow from the analysis of the RG equations. I perform a number of self-consistency checks and discuss the issues in a large set of theories. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In a large set of models, the renormalization-group (RG) flow interpolates between well-defined ultraviolet (UV) and infrared (IR) fixed points, the zeros of the beta function. The RG interpolation can be studied comparing the UV and IR limits of a certain class of correlators. Finite operators play a special role in this context, since they define central charges in the conformal limits.

Among the finite operators, noticeable are the conserved currents, in particular the stress tensor $T_{\mu\nu}$. When the theory contains scalar fields φ, there exists an improvement operator

$$\Delta T_{\mu\nu}=(\partial_\mu\partial_\nu-\Box\delta_{\mu\nu})\varphi^2,$$

which mixes with $T_{\mu\nu}$ under renormalization. It is possible to diagonalize this mixing,[1,2] and this makes the improvement term finite as well. There exists a one-parameter family of finite, conserved, spin-2, dimension-4 operators $T_{\mu\nu}(\eta)=T_{\mu\nu}+\eta\Delta T_{\mu\nu}$. At the level of the Lorentz commutator algebra, the operators $T_{\mu\nu}(\eta)$ are equivalent. At the level of the correlation functions and operator-product expansions, they are not. For example, in a conformal field theory, the embedding in external gravity is fixed unambiguously by conformal invariance. This means that there is no improvement arbitrariness in the UV and IR limits. In most models, the RG equations for η extend the removal of the improvement arbitrariness from the critical points to the intermediate energies.

A universal principle for the removal of the improvement ambiguity can be formulated using the sum rules for the trace anomalies a and a'.[3] This is a sort of variational principle,[4] which fixes a privileged value $\overline{\eta}$ for η. We can distinguish two cases.

(i) When the improvement term survives in a critical limit (typically, the UV), the value $\overline{\eta}$ determined by the variational principle coincides with the value fixed by conformal invariance at criticality and the RG equations. Matching the stress tensor at intermediate energies with its UV limit removes the η-arbitrariness at all energies.

(ii) When the improvement term vanishes at the critical points, all operators $T_{\mu\nu}(\eta)$ are in principle equally acceptable, but the value $\overline{\eta}$ is still privileged. Specifically, the minimum of $\Delta a'(\overline{\eta})$ over the flow trajectories connecting the same pair of fixed points is equal to Δc

in a class of models. (This relation is empirically known to hold in massive Gaussian models, unitary and not unitary. Nevertheless, a satisfactory theoretical understanding of this relation is still lacking.)

There is a universal way to remove the η-arbitrariness and select a unique stress tensor, in accord with all present knowledge.

In this paper I study this issue and other properties of the critical limits of correlators. In Sec. II I discuss the properties of the improvement term and list the criteria for the removal of the η-ambiguity. In Sec. III I illustrate the statements in a set of Gaussian models where calculations can be carried over to the end. Then, I analyze the RG equations in IR-free and UV-free theories. In all cases the parameter η is fixed uniquely with the rules of Sec. II. In the appendix I discuss other aspects of the critical limits of correlators containing insertions of finite and nonfinite operators. In particular, I show that anomalous currents and the topological charge density are finite in various models.

II. REMOVAL OF THE η-AMBIGUITY

The UV and IR limits of correlators containing insertions of the trace of the stress-tensor have been studied systematically in Ref. 3. General sum rules for the central charges a and a' have been written. Particularly meaningful is the notion of flow invariant, that is to say, a flow integral, or combination of flow integrals, whose value depends only on the extrema of the flow.

I briefly summarize the derivation of the sum rules. The theory is embedded in external gravity. The central charges a and a' (and c) are defined by the trace anomaly at criticality, which reads

$$\Theta_* = \frac{1}{(4\pi)^2}\left[c\, W^2 - \frac{a}{4}\mathrm{G} + \frac{2}{3}a'\,\Box R\right], \tag{2.1}$$

where W is the Weyl tensor and $\mathrm{G} = 4R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma} - 16R_{\mu\nu}R^{\mu\nu} + 4R^2$ is the Euler density. The induced action for the background metric is denoted with $\Gamma[g_{\mu\nu}]$. The Θ-correlators are related to the derivatives of $\Gamma[g_{\mu\nu}\mathrm{e}^{2\phi}]$ with respect to the conformal factor ϕ of the metric. In particular,

$$\Theta = -\left.\frac{\delta\Gamma[g_{\mu\nu}\mathrm{e}^{2\phi}]}{\delta\phi}\right|_{\phi=0}.$$

In general, the Θ-correlators have involved expressions, at intermediate energies, but their critical limits are universal and simple: they contain just two local structures, multiplied by a and a', which can be read from (2.1). The sum rules for $\Delta a = a_{\mathrm{UV}} - a_{\mathrm{IR}}$ and $\Delta a' = a'_{\mathrm{UV}} - a'_{\mathrm{IR}}$ are direct consequences of the property that the Θ-correlators tend to the universal critical limits parametrized by a and a'.

The derivation of the sum rules for Δa and $\Delta a'$ simplifies considerably if the metric is conformally flat, $g_{\mu\nu} = \delta_{\mu\nu}\mathrm{e}^{2\phi}$. More general metrics are necessary to derive sum rules for Δc, because Θ_* is insensitive to c on conformally flat spaces. In that case, it is not sufficient to study the critical limits of the correlators of Θ. Correlators with one insertion of Θ and at least two insertions of the full stress tensor $T_{\mu\nu}$ have to be considered.

From now on, I assume that the background metric is conformally flat.

Concretely, I study two sum rules for Δa, taken from Sec. 7 of Ref. 3. The first formula involves integrals of the two- and three-point functions:

$$\Delta a_1=\frac{\pi^2}{48}\int \mathrm{d}^4x\,|x|^4\,\langle\tilde\Theta(x)\,\tilde\Theta(0)\rangle+\frac{\pi^2}{48}\int \mathrm{d}^4x\,\mathrm{d}^4y\;x^2\,y^2\left\{\langle\tilde\Theta(x)\,\tilde\Theta(y)\,\tilde\Theta(0)\rangle\right.$$
$$\left.+\left\langle\frac{\tilde\delta\tilde\Theta(x)}{\tilde\delta\phi(y)}\tilde\Theta(0)\right\rangle+2\left\langle\frac{\tilde\delta\tilde\Theta(x)}{\tilde\delta\phi(0)}\tilde\Theta(y)\right\rangle\right\}. \tag{2.2}$$

The second formula involves integrals of the two-, three- and four-point functions:

$$\Delta a_2=\frac{\pi^2}{48}\int \mathrm{d}^4x\,|x|^4\,\langle\tilde\Theta(x)\,\tilde\Theta(0)\rangle+\frac{\pi^2}{48}\int \mathrm{d}^4x\,\mathrm{d}^4y\,\mathrm{d}^4z\,(x\cdot y)(x\cdot z)\left\langle\tilde\Theta(x)\,\tilde\Theta(y)\,\tilde\Theta(z)\,\tilde\Theta(0)\right.$$
$$+2\,\frac{\tilde\delta\tilde\Theta(x)}{\tilde\delta\phi(y)}\tilde\Theta(z)\,\tilde\Theta(0)+\frac{\tilde\delta\tilde\Theta(x)}{\tilde\delta\phi(0)}\tilde\Theta(y)\,\tilde\Theta(z)+\frac{\tilde\delta\tilde\Theta(y)}{\tilde\delta\phi(z)}\tilde\Theta(x)\,\tilde\Theta(0)+2\,\frac{\tilde\delta\tilde\Theta(y)}{\tilde\delta\phi(0)}\tilde\Theta(x)\,\tilde\Theta(z)$$
$$+\frac{\tilde\delta^2\tilde\Theta(x)}{\tilde\delta\phi(y)\,\tilde\delta\phi(z)}\tilde\Theta(0)+2\,\frac{\tilde\delta^2\tilde\Theta(x)}{\tilde\delta\phi(y)\,\tilde\delta\phi(0)}\tilde\Theta(z)+\frac{\tilde\delta^2\tilde\Theta(y)}{\tilde\delta\phi(z)\,\tilde\delta\phi(0)}\tilde\Theta(x)+2\,\frac{\tilde\delta\tilde\Theta(x)}{\tilde\delta\phi(y)}\,\frac{\tilde\delta\tilde\Theta(z)}{\tilde\delta\phi(0)}$$
$$\left.+\frac{\tilde\delta\tilde\Theta(x)}{\tilde\delta\phi(0)}\,\frac{\tilde\delta\tilde\Theta(y)}{\tilde\delta\phi(z)}\right\rangle. \tag{2.3}$$

The notation is as follows. If ϕ is the conformal factor of the metric and φ denotes generically the dynamical fields of the theory, with conformal weight h, then the $\tilde\delta/\tilde\delta\phi$-derivatives are the derivatives with respect to ϕ at constant $\tilde\varphi\equiv\varphi\,\mathrm{e}^{h\phi}$. We have $\tilde\Theta=-\tilde\delta S/\tilde\delta\phi$, where S denotes the action. It is understood that, after taking the ϕ-derivatives of $\tilde\Theta$, ϕ is set to zero.

I also study the $\Delta a'$-sum rule

$$\Delta a'=\frac{\pi^2}{48}\int \mathrm{d}^4x\,|x|^4\,\langle\tilde\Theta(x)\,\tilde\Theta(0)\rangle. \tag{2.4}$$

The central charge a is unambiguous at criticality, but a' is ambiguous. This ambiguity disappears in the difference $\Delta a'$, which is a physical quantity. These facts have important implications in the context of flow invariance and the dependence on the improvement ambiguity.

We can evaluate the above flow integrals using the one-parameter family of stress tensors $T_{\mu\nu}(\eta)$. Two situations can occur.

If the improvement term of the stress tensor does not vanish at both critical points, some nontrivial functions of η are generated, which depend also on the sum rule. This dependence is emphasized by the subscript i in the labels $\Delta_i a$. Formulas (2.2) and (2.3) define the functions $\Delta_1 a(\eta)$ and $\Delta_2 a(\eta)$, respectively. Formula (2.4) defines $\Delta a'(\eta)$. Since, however, a is unambiguous at criticality, there must be a privileged value of η which resolves the ambiguity and reproduces the correct Δa. This value can be found studying the RG equations for the parameter η, imposing conformal invariance at the critical points.

If the improvement term vanishes at both critical points, all values of η are in principle acceptable. The functions $\Delta_i a(\eta)$ do not depend on i and η and are identically equal to Δa. Instead, since a' has no unambiguous definition at criticality, the function $\Delta a'(\eta)$ can depend on η. We know from Ref. 4 that the value $\overline{\eta}$ at which $\Delta a'(\eta)$ is minimum has particularly interesting properties. Using this, we can remove the improvement ambiguity also in this case.

Both situations are resolved by a universal criterion for the removal of the improvement ambiguity, encoded in a variational principle studied in Ref. 4, which expresses the independence of the flat-space theory from the embedding in external gravity. When both this principle and the analysis of the RG equations fix η, the results agree.

A. Criterion for the removal of the improvement ambiguity

Determine the (unique) $\overline{\eta}$ which satisfies

$$\left.\frac{\mathrm{d}\Delta a'(\eta)}{\mathrm{d}\eta}\right|_{\eta=\overline{\eta}}=0, \quad \left.\frac{\mathrm{d}\Delta_i a(\eta)}{\mathrm{d}\eta}\right|_{\eta=\overline{\eta}}=0. \tag{2.5}$$

The functions $\Delta_i a(\eta)$ and $\Delta a'(\eta)$ are at most quadratic in η (this will be shown explicitly in the next section), so the condition (2.5) has one solution for every sum rule. (In even dimension greater than four, the η-polynomials can have a higher degree. I am grateful to G. Festuccia for this remark.) The solution $\overline{\eta}$ does not depend on the sum rule. The correct stress tensor is $T_{\mu\nu}(\overline{\eta})$ and the correct value of Δa is $\Delta_i a(\overline{\eta})$, independently of i. This criterion fixes also $\Delta a'$ unambiguously.

The integrals of (2.2) and (2.3) are assured to converge, when there is no improvement ambiguity. When the stress tensor admits improvement terms, instead, there can be a divergence in $\Delta a'(\eta)$. This divergence provides alternative criteria for the removal of the η-ambiguity (see Sec. II B). If, on the other hand, the Θ-correlators are expanded perturbatively, the convergence of the term-by-term integration is not assured. Observe that the resolution of the η-ambiguity is intrinsically nonperturbative. A useful perturbative expansion can be defined, although computations are not simple.

B. Shortcuts and other criteria to remove the η-ambiguity

The value $\overline{\eta}$ does not depend on the sum rule and so it can be determined from the simplest of those, i.e., $\Delta a'(\eta)$. The Δa-sum rules involve more complicated flow integrals. In various cases, $\overline{\eta}$ can be fixed by conformal invariance at the critical points. In the next sections I study the criteria for the removal of the improvement ambiguity in a variety of models. These cover essentially all cases. We can have the following behaviors:

(i) The RG equations imply that the improvement term of $T_{\mu\nu}(\eta)$ survives at one of the critical points, where, however, the stress tensor is uniquely fixed by conformal invariance.
(ii) The RG equations imply that the improvement term of $T_{\mu\nu}(\eta)$ diverges at one of the critical points and the divergence disappears if η is chosen appropriately.
(iii) The improvement term vanishes at the critical points, but not sufficiently quickly. The quantity $\Delta a'$ should be finite because it is physically meaningful (although it is not a flow invariant[4]). The finiteness of $\Delta a'(\eta)$ can fix η. This can also be seen as a consequence of (2.5).

In all cases, the $\overline{\eta}$ fixed with the criteria (i), (ii), and (iii) coincides with the $\overline{\eta}$ of (2.5). In the next section I present checks of this.

The fourth situation is when the improvement term disappears quickly enough at both critical points. When this happens, we have $\Delta_i a(\eta)=\Delta a$ for every i and η. The variational principle (2.5) applies also to this case, in the sense that it outlines a noticeable value $\overline{\eta}$, such that $\Delta a'(\overline{\eta})$ has the properties studied in Ref. 4. This behavior is studied in a higher-derivative model.

C. Modified, η-independent sum rules

Following Ref. 4, the criterion (2.5) is equivalent to the η-independence of more complicated sum rules. This illustrates that the removal of the $\overline{\eta}$-ambiguity fixed by (2.5) is compatible with the fact that the quantum field theory in flat space is independent of the nonminimal couplings to external gravity.

We proceed as follows. Using the fact that $\Delta_i a(\eta)$ is at most quadratic in η, we write

$$\Delta_i a(\eta)=\Delta_i a(\tilde{\eta})+(\eta-\tilde{\eta})\frac{\mathrm{d}\Delta_i a(\eta)}{\mathrm{d}\eta}\bigg|_{\tilde{\eta}}+\frac{1}{2}(\eta-\tilde{\eta})^2\frac{\mathrm{d}^2\Delta_i a(\eta)}{\mathrm{d}\eta^2}\bigg|_{\tilde{\eta}}. \tag{2.6}$$

The right-hand side is clearly independent of $\tilde{\eta}$.

Finding $\overline{\eta}$ according to (2.5), inserting it in (2.6) and renaming $\tilde{\eta}\to\eta$, we get

$$\Delta a=\Delta_i a(\overline{\eta})=\Delta_i a(\eta)-\frac{1}{2}\frac{(\mathrm{d}\Delta_i a(\eta)/\mathrm{d}\eta)^2}{\mathrm{d}^2\Delta_i a(\eta)/\mathrm{d}\eta^2}. \tag{2.7}$$

The final expression is an involved combination of flow integrals. It can be seen as a generalized sum rule for Δa, in the spirit of the formulas of Ref. 4. The result is clearly independent of η and gives the correct value of Δa. In the generalized sum rule, we can choose for $\Delta_i a(\eta)$ any equivalent Δa-formula from Ref. 3; for example, (2.2) and (2.3) of the present article. The i-independence of the result can be rephrased in terms of equivalence relations among the flow integrals. These involve correlators of Θ and the improvement operator.

III. CHECKS AND ILLUSTRATIVE EXAMPLES

In this section I study various examples, starting from simplest case, namely the massive free scalar. A richer structure is exhibited by Gaussian nonunitary theories, where the issue of flow invariance is more apparent. This model describes some qualitative features of physical theories with several independent masses or dimensioned parameters. Then, I consider the φ^4-theory and asymptotically free theories, supersymmetric and non-supersymmetric. Finally, I comment on the most general case.

A. Massive scalar field

The action in external gravity is

$$S=\frac{1}{2}\int \mathrm{d}^4x\,\sqrt{g}\,\{g^{\mu\nu}\partial_\mu\varphi\,\partial_\nu\varphi+\eta R\varphi^2+m^2\varphi^2\}.$$

Focusing on the conformal factor ϕ and eliminating a total derivative, we can simplify the action and write

$$S=\frac{1}{2}\int \mathrm{d}^4x\{(\partial_\mu\tilde{\varphi})^2+m^2\tilde{\varphi}^2\mathrm{e}^{2\phi}+(1-6\eta)\tilde{\varphi}^2(\Box\phi+(\partial_\mu\phi)^2)\}, \tag{3.1}$$

where $\tilde{\varphi}=\varphi\,\mathrm{e}^{\phi}$. We need

$$\tilde{\Theta}=-\frac{\tilde{\delta}S}{\tilde{\delta}\phi}=-m^2\tilde{\varphi}^2\mathrm{e}^{2\phi}+\frac{1}{2}(1-6\eta)[\Box(\tilde{\varphi}^2)-2\partial_\mu(\tilde{\varphi}^2\partial_\mu\phi)], \tag{3.2}$$

where $\tilde{\delta}$ is the ϕ-derivative at fixed $\tilde{\varphi}$ (check Ref. 3 for definitions), and the first two derivatives of $\tilde{\Theta}$ with respect to ϕ.

The calculations give

$$\Delta_1 a(\eta) = -\tfrac{89}{360} + 3\eta - 9\eta^2, \quad \Delta_2 a(\eta) = -\tfrac{37}{180} + \tfrac{5}{2}\eta - \tfrac{15}{2}\eta^2.$$

The condition (2.5) gives the (expected) value $\overline{\eta} = \frac{1}{6}$ in both cases and $\Delta_1 a(\overline{\eta}) = \Delta_2 a(\overline{\eta}) = \frac{1}{360} = \Delta a$. It is well-known that the value $\overline{\eta} = \frac{1}{6}$ is such that the action (3.1) is conformal at $m = 0$. The correct stress tensor can be fixed, more simply, by requiring that $\widetilde{\Theta}$ be zero in the UV limit. This is a check that the criterion (2.5) gives the same result as conformal invariance at the critical points, expressed by shortcut (i). On the other hand, $\Delta_1 a(\eta)$ and $\Delta_2 a(\eta)$ do not coincide for $\eta \neq \overline{\eta}$.

The coincidences of the values of $\overline{\eta}$ determined by $\Delta_{1,2} a(\eta)$ and the equality of $\Delta_{1,2} a(\overline{\eta})$ are nontrivial. They are due to identities among the flow integrals. An illustrative example is

$$m^2 \int \mathrm{d}^4x\, \mathrm{d}^4y\; x^2 \langle \varphi^2(x)\, \varphi^2(y)\, \varphi^2(0) \rangle = 2 \int \mathrm{d}^4x\; x^2 \langle \varphi^2(x)\, \varphi^2(0) \rangle,$$

which is relevant for the calculation of $\Delta_1 a(\eta)$. This identity can be verified directly or seen as a consequence of dimensional counting (each integral has the form const/m^2), combined with the property that an insertion of $\int \mathrm{d}^4x\, m^2 \varphi^2(x)$ is equivalent to the derivative $-m\partial/\partial m$. A similar cancellation takes place in $\Delta_2 a(\eta)$. The variational principle (2.5) ''knows'' about such relations.

Let us now study $\Delta a'$. The explicit calculation shows that a coefficient is infinite. Precisely,

$$\Delta a'(\eta) = -\tfrac{3}{40} + \tfrac{1}{2}\eta + (1 - 6\eta)^2 \infty.$$

In the Δa-sum rule (2.2), the infinite term is compensated by a contribution coming from the flow integral of $\langle \widetilde{\delta}\widetilde{\Theta}/\widetilde{\delta}\phi\, \Theta \rangle$ and the sum is finite for each value of η. An analogous compensation occurs in (2.3). Observe that (2.5), applied to $\Delta a'$, still fixes $\overline{\eta}$ to $\frac{1}{6}$, so that, correctly, $\Delta a'(\overline{\eta}) = \frac{1}{120}$.[5,4]

The quantity $\Delta a'$ is much less restricted than Δa. For example, it can depend on the flow connecting the two fixed points.[4] Still, it is a physically meaningful quantity and characterizes the flow. The infinity of $\Delta a'(\eta)$ is not a ''divergence'' to be removed. The correct value of $\Delta a'$ must be finite. In the theory at hand (but also in the φ^4-theory and other models discussed below), finiteness of $\Delta a'$ fixes $\overline{\eta}$. We have a check that the $\overline{\eta}$'s fixed with shortcut (iii) and any of the (2.5) coincide.

B. Flow invariance

Examples of flows interpolating between the same fixed points are easy to construct. As an illustration, take non-Abelian Yang–Mills theory with group $G = \mathrm{SU}(N_c)$, N_f massless quarks and M_f massive quarks in the fundamental representation. In the large N_c limit, with $N_f/N_c \lesssim \frac{11}{2}$ fixed, the theory is UV-free and has an interacting IR fixed point. Indeed, at low energies, the massive fermions decouple and the beta function

$$\beta = -\frac{1}{6\pi}(11N_c - 2N_f)\,\alpha^2 + \frac{25}{(4\pi)^2} N_c^2\, \alpha^3 + \mathcal{O}(\alpha^4)$$

has a second zero. The higher-loop terms can be neglected in the given large-N_c limit.

The UV and IR fixed points do not depend on the values of the masses of the M_f massive quarks. For each set of values of the masses we have a different flow interpolating between the same conformal field theories.

At the computational level, it is not easy to study the sum rules (2.2) and (2.3) in this model. A treatable perturbative expansion of the flow integrals of (2.2) and (2.3) has still to be developed. Gaussian higher-derivative theories, on the other hand, provide an interesting laboratory of flows interpolating between the same fixed points. Calculations are still lengthy, but doable.

C. Higher-derivative scalar field

The Lagrangian of the theory is

$$\mathcal{L}=\tfrac{1}{2}[(\Box\varphi)^2+\beta m^2(\partial_\mu\varphi)^2+m^4\varphi^2]. \tag{3.3}$$

The embedding in external gravity gives

$$\mathcal{L}=\tfrac{1}{2}\sqrt{g}(\varphi\Delta_4\varphi+\beta m^2(\partial_\mu\varphi)(\partial_\nu\varphi)g^{\mu\nu}+\eta R m^2\varphi^2+m^4\varphi^2), \tag{3.4}$$

where the differential operator

$$\Delta_4=\nabla^2\nabla^2+2\nabla_\mu[R^{\mu\nu}-\tfrac{1}{3}g^{\mu\nu}R]\nabla_\nu \tag{3.5}$$

is such that $\sqrt{g}\Delta_4$ is conformally invariant (see, for example, Ref. 6).

I do not consider nonminimal couplings of the form $R^2\varphi^2$. Their coefficients can be set to zero imposing $\Theta=0$ at criticality, as in the previous example. The nonminimal coupling $m^2R\varphi^2$, instead, disappears both in the UV limit ($m\to0$) and IR limit ($m\to\infty$ and $\varphi\to0$, keeping the mass term $m^4\varphi^2$ bounded).

I perform two calculations, with (2.2) and (2.3). The relevant operator is

$$\overline{\Theta}=-\frac{\delta S}{\delta\phi}=-\beta m^2(\partial_\mu\varphi)^2\mathrm{e}^{2\phi}-2m^4\varphi^2\mathrm{e}^{4\phi}+3\eta m^2[\mathrm{e}^{\phi}\Box(\varphi^2\mathrm{e}^{\phi})+\mathrm{e}^{\phi}\varphi^2\Box\mathrm{e}^{\phi}].$$

Tilded quantities are equal to untilded quantities in this model, since the canonical weight of the higher-derivative scalar field is zero.

Cubic and quartic terms in η do not contribute to (2.2) and (2.3). The improvement term (in $\widetilde{\Theta}$ and its ϕ-derivatives) carries a $\Box$. Using integrations by parts, the boxes can be moved and act on the degree-4 polynomials x^2y^2 or $(x\cdot y)(x\cdot z)$. Three boxes kill the polynomials and therefore the integral. This observation implies that the condition (2.5) always has a unique solution.

The sum rules (2.2) and (2.3) give

$$\Delta_1a(\eta)=\Delta_2a(\eta)=-\tfrac{7}{90}=\Delta a,$$

independently of η. I recall that in this model, $a_{\mathrm{UV}}=-7/90$ (Ref. 7) and $a_{\mathrm{IR}}=0$.

The calculations, lengthy and cumbersome, have been done with Mathematica. I do not report here intermediate results, because they do not seem to be particularly instructive.

The flow invariance of $\Delta_ia(\eta)$ and the cancellation of the $\mathcal{O}(\eta)$-terms and $\mathcal{O}(\eta^2)$-terms in (2.2) and (2.3) are consequences of nontrivial identities among flow integrals. Each term of (2.2) and (2.3) separately violates these properties. As for the quantity $\Delta a'$, we have

$$\Delta a'(\eta)=\frac{1+17r^2-17r^4-r^6+10(1+r^2+r^4+r^6)\ln r}{40(r^2-1)^3}+\eta U(r)+\eta^2V(r),$$

$$U(r)=-3r\frac{1-r^4+2(1+r^4)\ln r}{2(r^2-1)^3},\quad V(r)=9r^2\frac{1-r^2+(1+r^2)\ln r}{(r^2-1)^3},$$

where r is defined by $\beta=r+1/r$. r is the unique dimensionless parameter of the theory, besides the improvement coefficient η. Since $\Delta a'(\eta)$ is finite for every η, none of the shortcuts of the previous section applies. All values of η are in principle acceptable, but the value of η which minimizes $\Delta a'(\eta)$ is privileged, in the sense that it has various interesting properties, outlined in Ref. 4. We have

$$\overline{\eta}(r)=-\frac{U(r)}{2V(r)}=\frac{1-r^4+2(1+r^4)\ln r}{12r(1-r^2+(1+r^2)\ln r)}$$

and[4]

$$\Delta a'(\overline{\eta})=-\frac{(r^2-1)^2(3r^4-26r^2+3)+(r^8+18r^6-18r^2-1)\ln r^2-10r^2(r^4+1)\ln^2 r^2}{40(r^2-1)^3(r^2\ln r^2+\ln r^2-2r^2+2)}.$$

The value $\Delta a'(\overline{\eta})$ depends on r, which means that it not a flow invariant. Its minimum coincides with $\Delta c=-1/15$.[4]

In conclusion, the "good" stress tensor of the theory (3.3) is

$$\begin{aligned}T_{\mu\nu}=&-\partial_\nu\Box\varphi\,\partial_\mu\varphi-\partial_\mu\Box\varphi\,\partial_\nu\varphi+2\Box\varphi\,\partial_\mu\partial_\nu\varphi+\frac{2}{3}\partial_\mu\partial_\nu\partial_\alpha\varphi\,\partial_\alpha\varphi-\frac{4}{3}\partial_\mu\partial_\alpha\varphi\,\partial_\nu\partial_\alpha\varphi\\&+\delta_{\mu\nu}\left[\frac{1}{3}\partial_\alpha\Box\varphi\,\partial_\alpha\varphi+\frac{1}{3}(\partial_\alpha\partial_\beta\varphi)^2-\frac{1}{2}(\Box\varphi)^2-\frac{m^4}{2}\varphi^2\right]+\beta m^2\left(\partial_\mu\varphi\,\partial_\nu\varphi-\frac{\delta_{\mu\nu}}{2}(\partial_\alpha\varphi)^2\right)\\&-\overline{\eta}(r)m^2(\partial_\mu\partial_\nu-\Box\delta_{\mu\nu})\varphi^2,\end{aligned}$$

and does not contain more parameters than the flat-space action (3.3).

D. The φ^4-theory

The renormalization mixing between the stress tensor and its improvement term in the φ^4-theory has been studied in detail by Brown and Collins[1] and Hathrell.[2] In the formulas below, the dimensional regularization technique and the minimal subtraction scheme are understood.

The parameter η satisfies the inhomogeneous RG equation[2]

$$\mu\frac{\mathrm{d}\eta}{\mathrm{d}\mu}-\delta(\lambda)\,\eta=\beta_\eta(\lambda)\equiv-\delta(\lambda)d(\lambda). \tag{3.6}$$

Here $\delta(\lambda)$ is the anomalous dimension of the composite operator φ^2, while $d(\lambda)$ is determined by the simple pole in the φ^4-$\Box\varphi^2$ renormalization mixing. Precisely,

$$\frac{\mu^{4-n}[\varphi^4]}{4!}=\frac{(n-4)}{\hat{\beta}}\left\{\frac{\lambda_0\varphi_0^4}{4!}-\frac{\gamma}{n-4}[\mathrm{E}]-\frac{d+L_d}{n-4}\Box[\varphi^2]\right\},$$

where n is the space–time dimension, $[\mathrm{E}]$ is the φ-field equation, γ is the φ-anomalous dimension, $\hat{\beta}=(n-4)\lambda+\beta(\lambda)$, $\beta(\lambda)$ is the beta function, and L_d denotes the poles higher that the simple one. The subscript 0 denotes bare quantities, and the square brackets denote renormalized operators. The trace of the stress tensor reads in four dimensions

$$\widetilde{\Theta}=-\beta\frac{[\varphi^4]}{4!}-\gamma[\mathrm{E}]+(\eta-d)\Box[\varphi^2].$$

The equation (3.6) can be decomposed in the following way:

$$\eta=\widetilde{\eta}(\lambda)+\eta' v(\lambda),$$

where η' is finite ($\mu\mathrm{d}\eta'/\mathrm{d}\mu=0$), $\widetilde{\eta}$ is a particular solution of (3.6), fixed conventionally so that $\widetilde{\eta}(0)=0$, and v satisfies the homogeneous equation:

$$v(\lambda)=\exp\left(\int^\lambda\frac{\delta(\lambda')}{\beta(\lambda')}\mathrm{d}\lambda'\right). \tag{3.7}$$

It is not necessary to specify the second extremum of integration, which can be absorbed in the factor η'. The function $v(\lambda)$ is related to the renormalization constant of the operator φ^2.

The surviving finite constant η' parametrizes the stress-tensor ambiguity, which reads

$$T_{\mu\nu}(\eta') = T_{\mu\nu}(0) - \tfrac{1}{3}\eta' v(\lambda)(\partial_\mu\partial_\nu - \delta_{\mu\nu}\Box)[\varphi^2]. \tag{3.8}$$

It follows immediately from (3.7) that if $T_{\mu\nu}(0)$ is finite ($\mu\, dT_{\mu\nu}(0)/d\mu = 0$), then $T_{\mu\nu}(\eta')$ is also finite.

In Ref. 1 it was observed that η' can be consistently set to zero. In Ref. 2 it was remarked that η' should be fixed "by experiment," since it is the coefficient of the nonminimal coupling to external gravity. Here we want to see if there is a reason why η' should be set *a priori* to a particular value.

There is strong evidence that the φ^4-theory is nonperturbatively trivial. Even if we cannot view this theory as an RG interpolation between a UV and a IR fixed point, we can make a couple of general observations, which apply also to more general cases studied below.

To the lowest order, we have[2]

$$\delta(\lambda) = \frac{\lambda}{(4\pi)^2} + \mathcal{O}(\lambda^2), \quad \beta(\lambda) = 3\frac{\lambda^2}{(4\pi)^2} + \mathcal{O}(\lambda^3), \quad \beta_\eta(\lambda) = -\frac{1}{36}\frac{\lambda^4}{(4\pi)^8},$$

so that

$$\eta = -\frac{1}{288}\frac{\lambda^3}{(4\pi)^6} + \mathcal{O}(\lambda^4) + \eta'\lambda^{1/3}(1 + \mathcal{O}(\lambda)).$$

Let us consider the flow integral (2.4), which defines $\Delta a'(\eta)$. In the absence of information about the UV, we can study the convergence of this integral around the IR limit. Using the perturbative values given above and the Callan–Symanzik equations for the pair of operators $(\varphi^4, \Box\varphi^2)$, the behavior of the integral around the IR is

$$\Delta a'(\eta) \sim \int^\infty dt \left(\frac{a_1}{t^4} + \eta' \frac{a_2}{t^{10/3}} + \eta'^2 \frac{a_3}{t^{2/3}} \right),$$

where the a_i are numerical factors. We see that the $\mathcal{O}(\eta'^2)$-contribution diverges in the IR extremum of integration. Since the integrand is non-negative, this divergence cannot be cured by contributions from intermediate energies or by a hypothetical second fixed point (which exists in the models studied below, to which similar considerations apply). Therefore, the only value compatible with a finite $\Delta a'$ is $\eta' = 0$.

This case is different from the case of a free-massive scalar field. Here the improvement term of (3.8) does disappear at criticality [at a velocity $\lambda(t)^{1/3}$, where $\lambda(t) \sim 1/t$, $t = \ln|x|\mu$], but it does not disappear sufficiently quickly for the sum rule to converge. This forces η' to be zero, by shortcut (iii).

The φ^4-interaction can be nontrivial in several models, which may admit conformal windows. In particular, interesting cases are the supersymmetric models, with or without superpotential. Supersymmetry is not necessary to the logic of the arguments below, but it simplifies the examples.

E. $N=1$ supersymmetric QCD

I consider now $N=1$ supersymmetric QCD with gauge group $G = \mathrm{SU}(N_c)$ and N_f quark and antiquark superfields in the fundamental representation. The theory has no superpotential and a unique coupling constant g. For $N_f < 3N_c$ the theory is asymptotically free. The mass operator $\bar{\varphi}\varphi$, which is essential for the improvement term, is the lowest component of the Konishi

superfield.[8] Since the axial currents have no anomalous dimension at the one-loop order (see the appendix), this is true also of $\overline{\varphi}\varphi$. The two-loop contribution to the anomalous dimension δ can be found in Ref. 9:

$$\delta(g)=4(N_c^2-1)N_f\left(\frac{g^2}{16\pi^2}\right)^2+\mathcal{O}(g^6).$$

The structure of the RG equation for η and the η'-ambiguity of the stress tensor are the same as in (3.6) and (3.8). In particular, the function v is given by the analog of (3.7). The one-loop beta function is $\beta=-g^3(3N_c-N_f)/(16\pi^2)+\mathcal{O}(g^5)$, so that the function

$$v(g)=\exp\left(-\frac{g^2}{8\pi^2}\frac{N_f(N_c^2-1)}{(3N_c-N_f)}+\mathcal{O}(g^4)\right) \tag{3.9}$$

tends to unity at $g\to 0$. Instead, $\beta_\eta(g)$ goes to zero at least as fast as g^8. We conclude that $\eta\to\eta'$ in the UV limit, so that the improvement term of (3.8) survives at criticality. As in the case of the free massive scalar field, this forces η' to be set to zero, by shortcut (i).

F. Supersymmetric theories with a superpotential

The superpotential gives a one-loop contribution to the anomalous dimension of the Konishi operator. An example of UV-free supersymmetric theory with superpotential and a well-defined IR fixed point is the theory obtained adding mesonic fields M_i^j to the $N=1$ supersymmetric QCD. The meson superfields interact with the quarks q_i and $\overline{q}^j$ by means of a superpotential $fM_j^i q_i\overline{q}^j$.[10,11] In complete generality, denoting the superpotential couplings by Y_{ijk}, the one-loop anomalous dimension of the mass operator $\overline{\varphi}\varphi$ is

$$\delta(Y)=\frac{3}{16\pi^2}|Y|^2, \tag{3.10}$$

$|Y|$ being defined by $Y_{ijk}Y^{ijl}=|Y|^2\delta_k^l$. Solving the RG equations around the UV fixed point[10] and applying (3.7), we have

$$v\sim|t|^c, \tag{3.11}$$

for $t\to-\infty$, with c positive numerical constant. The situation is even worse than in the previous model, where the superpotential was absent: the improvement term of the stress tensor diverges in the free-field limit. This forces us again to set $\eta'=0$, by shortcut (ii).

G. Asymptotically free theories and flows with interacting UV fixed points

The arguments of the previous two cases apply to the most general asymptotically free theory with scalar fields, supersymmetric or not. The anomalous dimension of the improvement term can have a vanishing one-loop contribution or a nonvanishing one-loop contribution. In either case, its first radiative correction is positive. On the other hand, the first term of the beta function is negative. Then, $v(t)$ behaves as in (3.9) or (3.11). In the free-field limit, the improvement term of the stress tensor is finite and nonvanishing or divergent. This fixes η'.

The same can be said of flows with interacting UV fixed points, where $\delta_{\rm UV}$ can be nonvanishing. We can conclude, in full generality, that in unitary models the UV behavior of $T_{\mu\nu}(\eta')$ is unacceptable, unless the η'-term of (3.8) is suitably fixed, according to the rules of Sec. II.

IV. CONCLUSIONS

A proper RG interpolation between the UV and IR fixed points removes the improvement ambiguity of the stress tensor. The general criterion for this removal is encoded in the variational principle (2.5). In various cases suitable shortcuts can be more efficient. I have analyzed concrete

examples, one for each relevant situation. In particular, in asymptotically free theories, the RG equations imply that the improvement term survives at one critical point or diverges there, unless the improvement parameter is suitably fixed. In IR free theories, the improvement term does disappear at criticality, but not sufficiently quickly. The behavior of Gaussian higher-derivative theories shows that there are cases in which all improved stress tensors are in principle acceptable. Nevertheless, the criterion (2.5) outlines a privileged stress tensor also in this case. In conclusion, we can always consistently remove the improvement ambiguity with the rules of Sec. II.

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APPENDIX: OTHER REMARKS ABOUT THE CRITICAL LIMITS OF CORRELATORS

In this appendix I consider other ambiguities in the critical limits of correlators. Let us assume that two observers study the same model using different renormalization schemes. We want to know what amount of information the observers can objectively compare and how many quantities they need to normalize before the comparison. I consider correlators of composite operators and distinguish the cases of finite and nonfinite operators.

Let $\mathcal{O}$ be a multiplicatively renormalized operator. The Callan–Symanzik equations imply that the two-point function can be written in the form

$$\langle \mathcal{O}(x)\,\mathcal{O}(0)\rangle = \frac{1}{|x|^{2d}} Z^2(\alpha(1/|x|),\alpha(\mu))G(\alpha(1/|x|)), \tag{A1}$$

where d is the canonical dimension of $\mathcal{O}$, Z is the renormalization constant and $\alpha(\lambda)$ is the running coupling constant at the energy scale λ. Now, in the UV (respectively, IR) limit, namely $|x|\to 0$ ($|x|\to\infty$), $\alpha(1/|x|)$ tends to the critical value $\alpha_{\mathrm{UV\,(IR)}}$. If $\mathcal{O}$ is not finite (i.e., $Z\neq 1$), then the limit depends on $\alpha(\mu)$ and the subtraction scheme. The values $\alpha_{\mathrm{UV\,(IR)}}$ are themselves scheme dependent.

Among the finite operators, we distinguish conserved currents, anomalous (classically conserved) currents and others. Suppressing the space–time indices, if $\mathcal{O}$ is a conserved current, the UV and IR limits of (A1) have the structure

$$\langle \mathcal{O}(x)\,\mathcal{O}(0)\rangle_{\mathrm{UV\,(IR)}} \sim \frac{G(\alpha_{\mathrm{UV\,(IR)}})}{(x^2)^d}. \tag{A2}$$

The quantities $G(\alpha_{\mathrm{UV\,(IR)}})$ (called primary central charges[12]) carry information about the conformal fixed points. The scheme dependence of $\alpha_{\mathrm{UV\,(IR)}}$ is compensated by an equal and opposite scheme dependence of G, so that $G(\alpha_{\mathrm{UV\,(IR)}})$ is scheme independent. Similar considerations extend to correlators with more insertions. When the two observers compare their results, they have to find the same answer.

Classically conserved anomalous currents can be finite. In an asymptotically free theory, for example, the renormalization constant Z_5 of the axial current J_5^μ resums nonperturbatively to a finite function $C(\alpha)$. Finiteness can be formally recovered multiplying J_5^μ by $C^{-1}(\alpha)$. Then, in (A1) the renormalization constant can be nonperturbatively replaced by unity. Scalar operators can be finite as well. An example is the topological-charge density. Details are given below. The function $G(\alpha(1/|x|))$ tends to a constant in the free-field limit and behaves like a power of $x^2\mu^2$ around the interacting critical limit. Formula (A2) is upgraded to the more general expression

$$\langle \mathcal{O}(x)\,\mathcal{O}(0)\rangle_{\mathrm{UV\,(IR)}} \sim \frac{G_{\mathrm{UV\,(IR)}}}{(x^2)^d(x^2\mu^2)^{h_{\mathrm{UV\,(IR)}}}}. \tag{A3}$$

Here the critical limits are unambiguous once the scale μ is normalized (μ plays the role of the RG invariant scale, e.g., $\Lambda_{\rm QCD}$). Two observers can compare their results, once they agree on the definition of the reference scale. It is possible to define "secondary" central charges,[12] where the μ-normalization is simplified away.

Finally, the critical limits of correlators containing insertions of nonfinite operators provide one piece of information less,[12] since a nonfinite operator needs to be normalized at some reference energy. In (A1) this is emphasized by the $\alpha(\mu)$-dependence surviving in the limits $|x|\to 0$ and $|x|\to\infty$.

These observations apply to operators whose correlators have power-behaved critical limits. Logarithmic behaviors are not infrequent, however. The improvement term of the stress tensor often exhibits a logarithmic behavior: check the $\overline{\varphi}\varphi$-two-point function in (a) the φ^4-theory around the IR and (b) supersymmetric theories with superpotential around the UV [see (3.11)].

1. Anomalous currents

Anomalous currents can be finite operators, and therefore have unambiguous critical limits, of the form (A3). This paragraph extends a discussion of Collins[13] to singlet currents and the topological-charge density.

I consider the axial current in an asymptotically free gauge theory. I assume that the current is conserved at the classical level. The inclusion of mass terms is straightforward. The anomaly equation

$$\partial_\mu J_5^\mu - \frac{g^2 N_f}{16\pi^2} F\widetilde{F} = \overline{\psi}\gamma_5 \frac{\delta_l S}{\delta\overline{\psi}} + \frac{\delta_r S}{\delta\psi}\gamma_5\psi = \text{finite} \tag{A4}$$

and the definition $[J_5^\mu] = Z_5 J_5^\mu$ imply the relations

$$[\partial_\mu J_5^\mu] = Z_5 \partial_\mu J_5^\mu, \quad \frac{g^2 N_f}{16\pi^2}[F\widetilde{F}] = (Z_5 - 1)\partial_\mu J_5^\mu + \frac{g_0^2 N_f}{16\pi^2} F\widetilde{F}.$$

Calling $\mathcal{O}_1 = \partial_\mu J_5^\mu$ and $\mathcal{O}_2 = g^2 F\widetilde{F}/(16\pi^2)$, we have

$$[\mathcal{O}_i] = Z_{ij}\mathcal{O}_j, \quad Z_{ij} = \begin{pmatrix} Z_5 & 0 \\ Z_5 - 1 & 1 \end{pmatrix}.$$

Consider the two-point function $\langle [J_5]^\mu(x)\,[J_5]^\nu(0)\rangle$. At the one-loop order it has a conformal-invariant form, namely,

$$\langle [J_5^\mu](x)\,[J_5^\nu](0)\rangle = A(g^2)\,\frac{\delta^{\mu\nu} - 2x^\mu x^\nu/x^2}{(x^2)^{3+\delta_5(g^2)}} + \mathcal{O}(g^4). \tag{A5}$$

The one-loop conformal invariance is assured by the Callan–Symanzik equations. Indeed, the conformal-violating term in

$$\mu\frac{\partial}{\partial\mu} + \beta(g)\frac{\partial}{\partial g} + 2\,\delta_5(g^2)$$

is $\beta\,\partial/\partial g$. Since $\beta = \mathcal{O}(g^3)$, this term is irrelevant at the one-loop order.

Taking two divergences of (A5), using the anomaly equation (A4) and excluding the coincident point, we get

$$\langle [\partial_\mu J_5^\mu](x)\ [\partial_\nu J_5^\nu](0)\rangle = \frac{g^4 N_f^2}{(4\pi)^4}\langle [F\widetilde{F}](x)\ [F\widetilde{F}](0)\rangle = -4A(g^2)\,\frac{\delta_5(g^2)(2+\delta_5(g^2))}{(x^2)^{4+\delta_5(g^2)}}.$$

Since $A(g^2)=\mathcal{O}(1)$, we conclude $\delta_5(g^2)=\mathcal{O}(g^4)$. This result is unaffected by the presence of masses or other super-renormalizable parameters, but does not hold when the conservation of J_5^μ is violated at the classical level by marginal operators, such as in supersymmetric theories with a superpotential: see (3.10).

Now, we observe that the renormalization constant Z_5 has a finite limit when the cut-off is sent to infinity. We can see this using the dimensional-regularization technique, but it is more explicit to write the limit in the familiar cut-off notation. Precisely,

$$\lim_{\Lambda\to\infty} Z_5(g(\Lambda),g(\mu))=\lim_{\Lambda\to\infty}\exp\left(-\int_{g(\mu)}^{g(\Lambda)}\frac{\delta_5(g')}{\beta(g')}\,dg'\right)=C(g^2)=\text{finite}.$$

This property holds because in an asymptotically free theory, $g(\Lambda)$ tends to zero when $\Lambda\to\infty$. The integral is convergent around zero, because $\delta_5(g^2)=\mathcal{O}(g^4)$ and $\beta(g)=\mathcal{O}(g^3)$.

The full matrix Z_{ij} has a finite limit $C_{ij}(g^2)$. Using the Callan–Symanzik equations, we conclude that the operators $J_5^{\mu R}\equiv C^{-1}(g^2)[J_5^\mu]$ and $\mathcal{O}_i^R\equiv C_{ij}^{-1}(g^2)[\mathcal{O}_j]$ have two-point functions of the form

$$\langle J_5^{\mu R}(x)\,J_5^{\nu R}(0)\rangle=\frac{A(g^2(1/|x|))\,\delta_{\mu\nu}+B(g^2(1/|x|))\,x^\mu x^\nu/x^2}{(x^2)^3},\quad \langle\mathcal{O}_i^R(x)\,\mathcal{O}_j^R(0)\rangle=\frac{A_{ij}(g^2(t))}{(x^2)^4},$$

and admit unambiguous critical limits, as in (A3).

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Hierarchy of Dirac, Pauli, and Klein–Gordon conserved operators in Taub-NUT background

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The algebra of conserved observables of the SO(4,1) gauge-invariant theory of the Dirac fermions in the external field of the Kaluza–Klein monopole is investigated. It is shown that the Dirac conserved operators have physical parts associated with Pauli operators that are also conserved in the sense of the Klein–Gordon theory. In this way one gets simpler methods of analyzing the properties of the conserved Dirac operators and their main algebraic structures including the representations of dynamical algebras governing the Dirac quantum modes. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1469669]

I. INTRODUCTION

The relativistic quantum mechanics, seen as the one-particle restriction of the Lagrangian quantum field theory on curved space–times, give rise to interesting mathematical problems concerning the properties of the physical observables. It is known that one of the largest algebras of conserved operators is produced by the Euclidean Taub-NUT geometry since, beside usual isometries, this has a hidden symmetry of the Kepler type.[1,2] This is related to the existence of Stäckel–Killing tensors connected with the components of an analog to the Runge–Lenz vector of the Kepler-type problem which, in addition, can be expressed in terms of four Killing–Yano tensors.[2–4]

The theory of the Dirac equation in the Kaluza–Klein monopole field was studied in the mid-1980s.[5] An attempt to take into account the Runge–Lenz vector of this problem was done in Ref. 6. We have continued this study showing that the Dirac equation is analytically solvable[7] and determining the energy eigenspinors of the central modes. Moreover, we derived all the conserved observables of this theory, including those associated with the hidden symmetries of the Taub-NUT geometry. Thus we obtained the Runge–Lenz vector-operator of the Dirac theory, pointing out its specific properties.[8] The consequences of the existence of this operator were studied in Ref. 9 showing that the dynamical algebras of the Dirac theory corresponding to different spectral domains are the same as in the scalar case[2] but involving other irreducible representations. Thus for the discrete energy spectra we obtained two irreducible representations of the $o(4)$ algebra describing distinguish quantum modes for each energy level.[9]

This new phenomenon encourages us to continue the mathematical study of the whole algebra of conserved observables of the Dirac theory in Taub-NUT background. In our opinion, the operators related to the manifest or hidden symmetries of the Taub-NUT geometry are of a special interest since they reflect the effects of the geometry on the behavior of different quantum systems, with integer or half-integer spin. However, in the Dirac case there are several complicated operators whose manipulation can be sometime extremely difficult. We hope that a general study of their action on the Dirac spinors could lead to simpler calculation methods.

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The present article is devoted to this problem. Our goal is to separate the active parts of the conserved Dirac operators, called here physical parts, which determine the effects on the Dirac energy eigenspinors. Obviously these are projections obtained with the help of the projection operator on the whole space of physical spinors. We show that these are of a specific diagonal (even) or off-diagonal (odd) form depending on Pauli operators that are also conserved in the sense of the Klein–Gordon theory. In this way we derive simpler calculation rules and identify associations among conserved Dirac and Pauli operators as those currently used in theories involving monopoles[10–12] or new others we write down here.

We start in the second section with a brief review of some previous results[7–9] we need. In the next section we study the algebra of the conserved Dirac operators and introduce a new type of even operators which help us to define the projection operator that separates the physical parts. Furthermore, we point out that the diagonal (even) physical parts of the Dirac observables can be associated with well-defined conserved Pauli operators obeying the same algebraic relations. In Sec. IV we discuss the physical parts of the main conserved Dirac operators[7–9] and we identify their associated Pauli conserved operators. Here, after presenting the simplest conserved Pauli operators, we derive those corresponding to isometries or hidden symmetries including the generators of the dynamical algebras. In this way we show that the results of Ref. 9 hold also in the case of continuous energy spectra, for $so(3,1)$ or $e(3)$ dynamical algebras. The conclusions and comments are presented in the last section and in a short Appendix some formulas involving an important Pauli operator studied in Refs. 11 and 12 are given.

We work in natural units with $\hbar = c = 1$.

II. PRELIMINARIES

The background of the gauge-invariant five-dimensional theory of the Dirac fermions in the external field of the Kaluza–Klein monopole[13] is the Taub-NUT space with the time coordinate trivially added. It is convenient to consider the static chart of Cartesian coordinates x^μ, $(\mu,\nu,\ldots=0,1,2,3,5)$, with the line element

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = dt^2 - \frac{1}{V}dl^2 - V(dx^5 + A_i dx^i)^2, \tag{1}$$

where $dl^2 = (d\vec{x})^2 = (dx^1)^2 + (dx^2)^2 + (dx^3)^2$ is the usual Euclidean three-dimensional line element in Cartesian physical space coordinates x^i $(i,j,\ldots=1,2,3)$. The other coordinates are the time, $x^0 = t$, and the Cartesian Kaluza–Klein extra-coordinate, x^5. In (1) the function $1/V(r) = 1 + \mu/r$ depends on $r = |\vec{x}|$ and the real parameter μ while A_i are the potentials of the Dirac monopole.

This background has the isometry group $G_s = \mathrm{SO}(3) \otimes \mathrm{U}(1)_5 \otimes T_t(1)$ formed by the rotations of the Cartesian space coordinates and x^5 and t translations. The $\mathrm{U}(1)_5$ symmetry is important since this eliminates the so called NUT singularity if x^5 has the period $4\pi\mu$. The Killing vectors $k_{(i)}$ $(i=1,2,3)$ and $k_{(5)}$ are directly connected with the conserved operators which appear in the scalar case. They can be expressed in terms of momentum operators $P_i = -i(\partial_i - A_i\partial_5)$ and $P_5 = -i\partial_5$.[2] The last one, for negative mass models, can be interpreted as the "relative electric charge" and it is always conserved. Moreover, the Taub-NUT geometry possesses four Killing–Yano tensors, $f^{(i)}_{\mu\nu}$ $(i=1,2,3)$ and $f^{Y}_{\mu\nu}$, of valence 2, related to the hidden symmetries of the Taub-NUT geometry reflected by the existence of the nontrivial Stäckel–Killing tensors $k^{\mu\nu}_{(i)}$.[2,4,7,14]

In this Kaluza–Klein geometry there is a pentad gauge fixing[15] where the massless Dirac field, ψ, satisfies a simple gauge-covariant Dirac equation, $\not{D}\psi = 0$, where $\not{D} = i\gamma^0\partial_t - \not{D}_s$.[16,5,7,9] In the standard representation of the Dirac matrices [with diagonal γ^0 (Ref. 17)] the Hamiltonian operator[7,9]

$$H = \gamma^0 \not{D}_s = \begin{pmatrix} 0 & \alpha^* \\ \alpha & 0 \end{pmatrix} \tag{2}$$

has manifest supersymmetry. It is expressed in terms of Pauli operators,

$$\alpha=\sqrt{V}\pi=\sqrt{V}\left(\sigma_P-\frac{iP_5}{V}\right), \tag{3}$$

$$\alpha^*=V\pi^*\frac{1}{\sqrt{V}}=V\left(\sigma_P+\frac{iP_5}{V}\right)\frac{1}{\sqrt{V}}, \tag{4}$$

where $\sigma_P=\vec{\sigma}\cdot\vec{P}$ involves the Pauli matrices, σ_i. These operators give the space part of the Klein–Gordon operator as[7,9]

$$\Delta=\alpha^*\alpha=V\pi^*\pi=V\vec{P}^2+\frac{1}{V}P_5^2. \tag{5}$$

We specify that the star superscript is a mere notation that does not represent the Hermitian conjugation because here we use a nonunitary representation of the algebra of Dirac operators. Of course, this is equivalent with the unitary representation where all of these operators are self-adjoint.[7]

Since P_5 commutes with all the other conserved observables, we settle its eigenvalue, $\hat{q}$, such that $q\equiv-\mu\hat{q}=0,\pm1/2,\pm1,\ldots$.[1,2] We denote by $\mathfrak{G}$ the space of usual and generalized energy eigenspinors of the form $U_E=(u_E,E^{-1}\alpha u_E)^T$ which solve the eigenvalue problem $HU_E=EU_E$.[7] In Refs. 7 and 9 we showed that u_E is a solution of the static Klein–Gordon equation, $\Delta u_E=E^2u_E$, that may be square integrable with respect to the specific relativistic scalar product of the Dirac theory[7] or behave as tempered distributions. The Klein–Gordon equation is analytically solvable producing continuous energy spectra, $E\geqslant|\hat{q}|$, for any real μ and discrete energy levels, E_n with $n>|q|>0$, only for $\mu<0$. These are included in the domain $(0,\hat{q})$ such that $\lim_{n\to\infty}E_n=|\hat{q}|$. Hence, there are no zero modes and the operator Δ can be considered invertible on the space of of the spinors u_E. Therefore, we can conclude that the Dirac equation produces the *same* energy spectra as the Klein–Gordon one. Moreover, since there are no zero modes the Hamiltonian operator (2) is also invertible. The meaning of this operation will be discussed in the next section.

III. THE ALGEBRA OF CONSERVED DIRAC OPERATORS

Our aim is to study here the form and the action of the *conserved* operators of the Dirac theory which, by definition, are the Dirac operators that *commute* with the Hamiltonian (2). We denote by **D** the algebra of these operators. We say that a Pauli operator $\hat{X}$ acting on the space of the two-component Pauli spinors u_E is *conserved* if it commutes with Δ. We denote by **P** the algebra of the conserved Pauli operators, including the conserved observables of the Klein–Gordon theory, called here *orbital* operators. In this section we denote systematically by capitals the operators of **D** and by hatted ones the operators of **P** without using special notations for the identity operators of these algebras.

In general, the Pauli blocks, $\hat{X}^{(ab)}$ $(a,b=1,2)$, of any conserved Dirac operator

$$X=\begin{pmatrix}\hat{X}^{(11)} & \hat{X}^{(12)}\\ \hat{X}^{(21)} & \hat{X}^{(22)}\end{pmatrix}\in\mathbf{D} \tag{6}$$

satisfy the conditions

$$\hat{X}^{(22)}\alpha=\alpha\hat{X}^{(11)},\quad \alpha^*\hat{X}^{(22)}=\hat{X}^{(11)}\alpha^*, \tag{7}$$

$$\hat{X}^{(12)}\alpha=\alpha^*\hat{X}^{(21)},\quad \alpha\hat{X}^{(12)}=\hat{X}^{(21)}\alpha^*, \tag{8}$$

which are equivalent with $[X,H]=0$. Hereby it results that

$$\hat{X}^{(21)}=\alpha\hat{X}^{(12)}\alpha\Delta^{-1} \tag{9}$$

and

$$[\hat{X}^{(11)},\Delta]=[\hat{X}^{(12)}\alpha,\Delta]=[\alpha^*\hat{X}^{(21)},\Delta]=0, \tag{10}$$

which means that $\hat{X}^{(11)}$, $\hat{X}^{(12)}\alpha$, $\alpha^*\hat{X}^{(21)}\in\mathbf{P}$.

We observe that possible solutions of Eqs. (7) and (8) are the diagonal operators

$$\mathcal{D}(\hat{X})=\begin{pmatrix}\hat{X} & 0\\ 0 & \alpha\hat{X}\Delta^{-1}\alpha^*\end{pmatrix}, \tag{11}$$

where $\hat{X}\in\mathbf{P}$. Particularly, for $\hat{X}=1$ we obtain the projection operator

$$I=\mathcal{D}(1)=\begin{pmatrix}1 & 0\\ 0 & \alpha\Delta^{-1}\alpha^*\end{pmatrix} \tag{12}$$

on the space $\mathfrak{G}$. This split the algebra $\mathbf{D}=\mathbf{D}_0\oplus\mathbf{D}_1$ in two subspaces of the projections $XI\in\mathbf{D}_0$ and $X(1-I)\in\mathbf{D}_1$ of all $X\in\mathbf{D}$. According to Eqs. (7) and (8) we find that the projections of two arbitrary operators $X,Y\in\mathbf{D}$ satisfy $(XI)(YI)=(XY)I$ and $[X(1-I)](YI)=0$ which lead to the conclusion that $\mathbf{D}_0$ is a subalgebra while $\mathbf{D}_1$ is even an ideal in $\mathbf{D}$. Obviously, I is the identity operator of $\mathbf{D}_0$. On the other hand, in Ref. 7 we introduced the $\mathcal{Q}$-operators defined as

$$\mathcal{Q}(\hat{X})=\left\{H,\begin{pmatrix}\hat{X} & 0\\ 0 & 0\end{pmatrix}\right\}=\begin{pmatrix}0 & \hat{X}\alpha^*\\ \alpha\hat{X} & 0\end{pmatrix}, \tag{13}$$

where $\hat{X}$ may be any Pauli operator. However, if $\hat{X}\in\mathbf{P}$, then $\mathcal{Q}(\hat{X})\in\mathbf{D}_0$ since $[\mathcal{Q}(\hat{X}),H]=0$ and $\mathcal{Q}(\hat{X})I=\mathcal{Q}(\hat{X})$. If $\hat{X}=1$, we obtain just the Hamiltonian operator $H=\mathcal{Q}(1)\in\mathbf{D}_0$. Consequently, the inverse of H with respect to I can be represented as $H^{-1}=\mathcal{Q}(\Delta^{-1})$. The mappings $\mathcal{D}:\mathbf{P}\rightarrow\mathbf{D}_0$ and $\mathcal{Q}:\mathbf{P}\rightarrow\mathbf{D}_0$ are linear and have the following algebraic properties,

$$\mathcal{D}(\hat{X})\mathcal{D}(\hat{Y})=\mathcal{D}(\hat{X}\hat{Y}), \tag{14}$$

$$\mathcal{Q}(\hat{X})\mathcal{Q}(\hat{Y})=\mathcal{D}(\hat{X}\hat{Y}\Delta), \tag{15}$$

$$\mathcal{D}(\hat{X})\mathcal{Q}(\hat{Y})=\mathcal{Q}(\hat{X})\mathcal{D}(\hat{Y})=\mathcal{Q}(\hat{X}\hat{Y}), \tag{16}$$

for any $\hat{X},\hat{Y}\in\mathbf{P}$. Moreover, the relations

$$[\gamma^0,\mathcal{D}(\hat{X})]=0,\quad \{\gamma^0,\mathcal{Q}(\hat{X})\}=0 \tag{17}$$

indicate that, according to the usual terminology,[17] $\mathcal{D}$ and $\gamma^0\mathcal{D}$ are *even* Dirac operators while $\mathcal{Q}$ and $\gamma^0\mathcal{Q}$ are *odd* ones. We note that there are many other odd or even operators which do not have such forms.

In general, since I is the projection operator on the space of the Dirac energy eigenspinors $\mathfrak{G}$, we say that the projection IXI of any Dirac operator X, conserved or not, represents the *physical part* of X. We can convince ourselves that if $X\in\mathbf{D}$, then

$$IXI\equiv XI=\mathcal{D}(\hat{X}^{(11)})+\mathcal{Q}(\hat{X}^{(12)}\alpha\Delta^{-1}), \tag{18}$$

which means that all the operators from $\mathbf{D}_0$ can be written as $\mathcal{D}$ or $\mathcal{Q}$-operators. Thus the action of X reduces to that of the Pauli operators involved in (18), allowing us to rewrite the problems of the Dirac theory in terms of Pauli operators.[8,9] Indeed, it is easy to show that the action of any operator $X\in\mathbf{D}$ on $U_E\in\mathfrak{G}$ is

$$XU_E=XIU_E=\begin{pmatrix}\hat{\mathcal{P}}_E(X)u_E\\ E^{-1}\alpha\hat{\mathcal{P}}_E(X)u_E\end{pmatrix}, \tag{19}$$

where, by definition,

$$\hat{\mathcal{P}}_E(X)=\hat{X}^{(11)}+E^{-1}\hat{X}^{(12)}\alpha \tag{20}$$

is the *conserved* Pauli operator *associated* to X. Since the mapping $\hat{\mathcal{P}}_E:\mathbf{D}\to\mathbf{P}$ is linear and satisfies $\hat{\mathcal{P}}_E(X)=\hat{\mathcal{P}}_E(XI)$ it results that $\mathrm{Ker}\hat{\mathcal{P}}_E=\mathbf{D}_1$. In other respects, Eqs. (7) and (8) lead to the important property

$$\hat{\mathcal{P}}_E(XY)=\hat{\mathcal{P}}_E(X)\hat{\mathcal{P}}_E(Y),\quad \forall X,Y\in\mathbf{D}, \tag{21}$$

which guarantees that $\hat{\mathcal{P}}_E$ preserves the algebraic relations, mapping any algebra or superalgebra of $\mathbf{D}_0$ into an *isomorphic* algebra or superalgebra of $\mathbf{P}$, with the same commutation and anticommutation rules.

IV. CONSERVED OBSERVABLES

In what follows we focus on the physical parts of the main Dirac conserved observables, pointing out the technical advantages of using $\mathcal{D}$ and $\mathcal{Q}$-operators that help us to identify the associated Pauli operators defined by (20). The even physical parts, $\mathcal{D}$, are associated to Pauli operators independent on E which are, therefore, well-defined physical observables. For this reason it is useful to briefly review the most important conserved Pauli operators and then turn to the physical parts of the Dirac ones.

A. Conserved orbital and Pauli operators

In general, the Pauli operators are 2×2 matrix differential operators acting on two-component Pauli spinors. There are many nonconserved operators which do not commute with Δ as, for example, $\alpha,\alpha^*,\pi,\pi^*,\sigma_r=\vec{\sigma}\cdot\vec{x}/r$ or the operator $\lambda=\vec{\sigma}\cdot(\vec{x}\times\vec{P})+1$ proposed in Ref. 11 and discussed in Ref. 12. Some algebraic properties of these operators are given in the Appendix.

By definition, the conserved operators of $\mathbf{P}$ commute with Δ, which is the static part of the Klein–Gordon operator. As mentioned, these can be the usual conserved orbital operators of the scalar fields or more complicated ones involving, in addition, the Pauli matrices which also commute with Δ.

The main conserved orbital operators are the basis generators of the natural representation of the group G_s carried by the space of scalar fields. These generators are defined up to the factor $-i$ as the Killing vector fields corresponding to isometries or the operators given by the Killing tensors associated to the hidden symmetries. The $U_5(1)$ generator is P_5 and the Killing vectors $k^\mu_{(i)}$ give the SO(3) generators which are the components L_i of the orbital angular momentum operator[7,9]

$$\vec{L}=\vec{x}\times\vec{P}-\mu\frac{\vec{x}}{r}P_5. \tag{22}$$

These commute with Δ and satisfy the canonical commutation relations among themselves and with the components of all the other vector operators (e.g. coordinates, momenta, etc.). On the other hand, the specific Killing tensors $k^{\mu\nu}_{(i)}$ of the Taub-NUT geometry allow one to define the Runge–Lenz operator for scalar particles[2]

$$\vec{K}=\frac{1}{2}(\vec{P}\times\vec{L}-\vec{L}\times\vec{P})-\frac{\mu}{2}\frac{\vec{x}}{r}\Delta+\mu\frac{\vec{x}}{r}P_5^2, \tag{23}$$

which commute with Δ and its components satisfy the commutation relations

$$[L_i,K_j]=i\varepsilon_{ijk}K_k, \quad [K_i,K_j]=i\varepsilon_{ijk}L_kF^2, \tag{24}$$

where $F^2=P_5^2-\Delta$. For given values of E and $\hat{q}$ this operator can be rescaled in order to recover the dynamical algebras corresponding to different spectral domains of the Kepler-type problems.[2] The new operators

$$R_i=\begin{cases} F^{-1}K_i & \text{for } \mu<0 \text{ and } E<|\hat{q}|, \\ K_i & \text{for any } \mu \text{ and } E=|\hat{q}|, \\ \pm iF^{-1}K_i & \text{for any } \mu \text{ and } E>|\hat{q}|, \end{cases} \tag{25}$$

and L_i $(i=1,2,3)$ generate either a representation of the $o(4)$ algebra for the discrete energy spectrum in the domain $0<E<|\hat{q}|$ or a representation of the $o(3,1)$ algebra for continuous spectrum in the domain $E>|\hat{q}|$. A special case is that of the dynamical algebra $e(3)$ which corresponds only to the ground energy of the continuous spectrum, $E=|\hat{q}|$.

The operators of **P** involving Pauli matrices can be vector operators as the total angular momentum,

$$\vec{J}=\vec{L}+\frac{\vec{\sigma}}{2}, \tag{26}$$

or scalar operators of the form $\sigma_L=\vec{\sigma}\cdot\vec{L}$, $\sigma_K=\vec{\sigma}\cdot\vec{K}$ or $\sigma_R=\vec{\sigma}\cdot\vec{R}$, involved in superalgebras as

$$\{\sigma_K,\sigma_L+1\}=0. \tag{27}$$

Other conserved Pauli operators with more complicated structure have to be derived in association with the physical parts of the conserved Dirac observables.

B. Associated Dirac and Pauli operators

We have seen that the physical parts of the conserved Dirac observables can have diagonal or off-diagonal terms; among them only the diagonal ones can be correctly associated to conserved Pauli operators independent on E. However, the off-diagonal operators can be transformed at any time in diagonal ones using the multiplication with H or H^{-1}. For example, H itself which is off-diagonal is related to the diagonal operators $H^2=\mathcal{D}(\Delta)$ or I. Thus each conserved Dirac operator can be brought in a diagonal form associated with an operator from **P**.

Let us start with the generators of the representations of the group G_s carried by the space of the Dirac spinors. The $U(1)_5$ generator remains the former operator P_5 but the SO(3) generators get the usual spin terms, $S_i=\frac{1}{2}\mathrm{diag}(\sigma_i,\sigma_i)$ of the total angular momentum whose components, $\mathcal{J}_i=L_i+S_i$, commute with H even if neither L_i nor S_i do not have this property.[7,9] However, the effect on the spinors of $\mathfrak{G}$ is due only to the physical parts which read

$$\mathcal{J}_iI=\mathcal{D}(J_i)=\mathcal{D}(L_i)+\tfrac{1}{2}\mathcal{D}(\sigma_i), \tag{28}$$

where both the orbital and the spin terms are *separately* conserved since L_i and σ_i commute with Δ. Obviously, in this case the associated Pauli operators are just J_i defined by (26).

The simplest conserved off-diagonal operators are the so called Dirac-type operators generated by the first three Killing–Yano tensors, $f^{(i)}$. We have shown[7,8] that these can be written

simply in the form $Q_i=\mathcal{Q}(\sigma_i)$, which explains why their algebraic properties are close to those of the Pauli matrices. Now, we can prove that the diagonal operators $H^{-1}Q_i=\mathcal{D}(\sigma_i)$ form a representation of the algebra of Pauli matrices with values in $\mathbf{D}_0$ since

$$H^{-1}Q_iH^{-1}Q_j=\delta_{ij}I+i\varepsilon_{ijk}H^{-1}Q_k\,. \tag{29}$$

The corresponding Dirac-type operator of the last Killing–Yano tensor, f^Y, calculated according to the general rule of Ref. 18 has been obtained in Ref. 8. This has the form

$$Q^Y=-\mathcal{Q}(\sigma_r)+\frac{2i}{\mu\sqrt{V}}\begin{pmatrix}0 & \lambda\\ -\lambda & 0\end{pmatrix}. \tag{30}$$

Using the identities presented in the Appendix one finds the equivalent forms reported in Ref. 8 and verifies that Q^Y commutes with H and P_5 and anticommutes with $\not{D}_s$ and γ^0. Moreover, after a little calculation, we obtain the remarkable identity

$$\mu P_5[Q^Y+\mathcal{Q}(\sigma_r)]=\{H,\Lambda\} \tag{31}$$

involving the operator $\Lambda=\mathrm{diag}(\lambda,\lambda)$ that is a particular version of a Biedenharn operator.[19] This is not conserved but $\Lambda^2=\vec{\mathcal{J}}^2-\mu^2P_5^2+\frac{1}{4}$ has this property. Furthermore, we observe that, according to (A1) and (A3), the physical part of Q^Y can be put in the form

$$Q^YI=\mathcal{Q}\left(-\sigma_r+\frac{2i}{\mu}\lambda\pi\Delta^{-1}\right)=\mathcal{Q}(\sigma^Y\Delta^{-1})\,, \tag{32}$$

where

$$\sigma^Y=\frac{2}{\mu}[\sigma_K+(\sigma_L+1)P_5] \tag{33}$$

is a new conserved Pauli operator associated to $HQ^Y=HQ^YI=\mathcal{D}(\sigma^Y)$.

C. The Runge–Lenz operator and dynamical algebras

These results allow us to calculate directly the physical parts of the Runge–Lenz operator of the Dirac theory (related to the Killing tensor $\vec{k}^{\mu\nu}$), following the same procedure as in Ref. 8. We start with the equivalent definition of the physical parts of the auxiliary operators[8]

$$\mathcal{N}_iI=\frac{\mu}{4}\{HQ^Y,H^{-1}Q_i\}-\mathcal{J}_iP_5I, \tag{34}$$

which can be written as

$$\mathcal{N}_iI=\mathcal{D}\left(\frac{\mu}{4}\{\sigma^Y,\sigma_i\}-J_iP_5\right)=\mathcal{D}(\hat{N}_i), \tag{35}$$

in terms of their associated conserved Pauli operators,

$$\hat{N}_i=K_i+\frac{\sigma_i}{2}P_5\,. \tag{36}$$

Furthermore, we define the physical parts of the components of the conserved Runge–Lenz operator[8,9]

$$\mathcal{K}_i I = \mathcal{N}_i I + \tfrac{1}{2}(\mathcal{F} - P_5)H^{-1}Q_i, \tag{37}$$

where $\mathcal{F}^2 = P_5^2 - H^2$. Since $\mathcal{F}^2 I = \mathcal{D}(F^2)$, we can express $\mathcal{K}_i I = \mathcal{D}(\hat{K}_i)$, now the associated conserved Pauli operators being

$$\hat{K}_i = K_i + \frac{\sigma_i}{2}F. \tag{38}$$

All these associations help us to understand the significance of the isomorphism among the algebra of the Dirac operators,[8,9]

$$[\mathcal{J}_i, \mathcal{K}_j] = i\varepsilon_{ijk}\mathcal{K}_k, \quad [\mathcal{K}_i, \mathcal{K}_j] = i\varepsilon_{ijk}\mathcal{J}_k\mathcal{F}^2, \tag{39}$$

that of the Pauli operators,

$$[J_i, \hat{K}_j] = i\varepsilon_{ijk}\hat{K}_k, \quad [\hat{K}_i, \hat{K}_j] = i\varepsilon_{ijk}J_k F^2, \tag{40}$$

and (24).

Rescaling (37) as in the case of the orbital operators (25), but using $\mathcal{F}$ instead of F, one obtains the even operators $\mathcal{R}_i \in \mathbf{D}$ (Ref. 9) having simple physical parts, $\mathcal{R}_i I = \mathcal{D}(\hat{R}_i)$, associated with the conserved Pauli operators

$$\hat{R}_i = \begin{cases} R_i + \dfrac{\sigma_i}{2} & \text{for } E \neq \hat{q}, \\ K_i & \text{for } E = \hat{q}. \end{cases} \tag{41}$$

We specify that the orbital and spin terms of $\mathcal{N}_i I$, $\mathcal{K}_i I$ and $\mathcal{R}_i I$ (for $E \neq \hat{q}$) are also separately conserved, as in the case of the angular momentum, since K_i and F commute with Δ.

The representations of the dynamical algebras $o(4)$ or $o(3,1)$ that govern the Dirac modes for $E \neq \hat{q}$ are generated by $\mathcal{J}_i$ and $\mathcal{R}_i$ (Ref. 9) whose physical parts, $\mathcal{J}_i I$ and $\mathcal{R}_i I$, have the same spin terms, $\mathcal{D}(\sigma_i)/2$. Therefore, each of these representations is the direct product between the irreducible representation of scalar modes and a spin half two-dimensional (fundamental) representation of the dynamical algebra.[9] When $E = \hat{q}$, then $\mathcal{F}$ and F vanish such that the representation of the subalgebra $so(3) \subset e(3)$ remains generated by the operators (28) while the operators $\mathcal{K}_i I$ lose their spin terms, becoming the translation generators of $e(3)$. All these representations arising from direct products are reducible. We note that this phenomenon is new since in the scalar (Klein–Gordon) case the representations of the dynamical algebras of the Kepler-type problems are irreducible.[2] However, these results could be easily obtained analyzing the *equivalent* representations generated by the associated Pauli operators J_i and $\hat{R}_i$ as we did already in Ref. 9 for the discrete energy spectrum. We recall that therein we introduced the new conserved operator $\mathcal{C} = 2\vec{\mathcal{J}}\cdot\vec{\mathcal{R}} - \frac{1}{2}$ in order to distinguish between the irreducible representations of the $o(4)$ dynamical algebra. Now we see that $\mathcal{C}I = \mathcal{D}(\sigma_R + \sigma_L + 1)$ where, according to (27), we have $\{\sigma_R, \sigma_L + 1\} = 0$.

V. CONCLUSIONS

The first conclusion is that our approach allows one to associate the conserved Dirac operators of diagonal (even) form to conserved Pauli operators independent on E. Thus for each type of symmetry we have conserved operators at three levels: Dirac, Pauli and orbital (of the Klein–Gordon theory). The following table resumes this hierarchy (K is an abbreviation for Killing, K-Y for Killing–Yano; * denotes entries which involve issues too complex to be abbreviated in the table and some comments are given below).

Geometric object	Nature	Symmetry	Dirac operator	Pauli operator	Klein–Gordon operator
$f^{(i)}_{\mu\nu}$	K-Y tensor	*	$H^{-1}Q_i$	σ_i	$\cdots$
$f^{Y}_{\mu\nu}$	K-Y tensor	*	HQ^Y	σ^Y	$\cdots$
$k^{\mu}_{(5)}$	K vector	$U(1)_5$	P_5	P_5	P_5
$k^{\mu}_{(i)}$	K vector	SO(3)	$\mathcal{J}_i$	J_i	L_i
$k^{\mu\nu}_{(i)}$	K tensor	hidden	$\mathcal{K}_i, \mathcal{R}_i$	$\hat{K}_i, \hat{R}_i$	K_i, R_i

However, there are many other even or odd conserved Dirac operators [e.g., $\mathcal{D}(\sigma_K^2)$, $\mathcal{Q}(L_i)$, $\mathcal{Q}(\sigma^Y)$, etc.] which can be constructed with the help of the conserved Pauli or orbital ones. This large collection of conserved observables is in fact a rich algebra freely generated by those related to the manifest or hidden symmetries of the Taub-NUT geometry.

In $N=1$ supersymmetric quantum models with standard supersymmetry there is a single supercharge Q that closes $Q^2=H$ on the Hamiltonian. In many of these models, and that is the case of the Taub-NUT manifold, one can find additional or hidden, nonstandard supercharges involving Killing–Yano tensors. The Killing–Yano tensors $f^{(i)}_{\mu\nu}$ $(i=1,2,3)$ give a vector representation of SO(3) and their existence is connected with the complex structures of the hyper-Kähler Taub-NUT space. The forth Killing–Yano tensor $f^{Y}_{\mu\nu}$ is a singlet and exists by virtue of the metric being type D. All four Killing–Yano tensors are invariant under the action of $U(1)_5$ which physically represents the relative electric charge of two monopoles.

For spin-$\frac{1}{2}$ particles, the Killing–Yano tensors are essential in construction of Dirac-type operators and evaluation of the spin contributions to the conserved quantities from the scalar case. The antisymmetric features of these operators make them the natural object used in description of the Dirac fermion in a curved space–time. On the other hand, the fact that the Stäckel–Killing tensors involved in the Runge–Lenz vector (23) can be expressed as symmetrized products of Killing–Yano tensors seems to be useless for scalar particles described by Schrödinger or Klein–Gordon equations. Therefore the existence of a certain square root of the Stäckel–Killing tensors becomes relevant only in the presence of fermions.

In other respects, we can eliminate many difficulties due to the spin terms of the Dirac theory if we restrict ourselves only to the physical parts XI of the operators $X\in\mathbf{D}$ giving up the projections $X(1-I)\in\mathbf{D}_1$ which can give rise sometimes to very complicated calculations. Moreover, we get the advantage of reducing the algebraic operations among the physical parts from $\mathbf{D}_0$ to calculations involving only the associated Pauli operators from $\mathbf{P}$. For example, if instead of $[\vec{Q},Q^Y]$, we calculate only its physical part, $[\vec{Q},Q^Y]I=[H^{-1}\vec{Q},HQ^Y]=\mathcal{D}([\vec{\sigma},\sigma^Y])$, we avoid a tedious algebra, easily obtaining the interesting identity

$$\frac{\mu}{4}[\vec{Q},Q^YI]=i(\vec{\mathcal{K}}+\vec{\mathcal{J}}P_5)\times(H^{-1}\vec{Q})+(\mathcal{F}+P_5)\,H^{-1}\vec{Q} \tag{42}$$

which shows that this commutator does not produce new conserved observables.

Finally, we note that our method based on the separation of the physical parts expressed in terms of $\mathcal{D}$ and $\mathcal{Q}$-operators could be used in any problem where the Hamiltonian is invertible and has manifest supersymmetry.

APPENDIX: THE OPERATOR λ

The operator

$$\lambda=\vec{\sigma}\cdot(\vec{x}\times\vec{P})+1=\sigma_L+1+\mu\sigma_rP_5 \tag{A1}$$

has the properties

$$\{\sigma_r,\lambda\}=0, \quad [\sigma_r,\sigma_P]=\frac{2i}{r}\lambda, \tag{A2}$$

and

$$\sigma_P\lambda=-\lambda\sigma_P=\frac{i}{2}\vec{\sigma}\cdot(\vec{P}\times\vec{L}-\vec{L}\times\vec{P})-\frac{i\mu}{r}\lambda P_5, \tag{A3}$$

which lead to

$$\{\alpha^*,\lambda\}=\frac{2i}{\sqrt{V}}\lambda P_5, \quad \{\alpha,\lambda\}=-\frac{2i}{\sqrt{V}}\lambda P_5. \tag{A4}$$

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Super-Grassmannian and large *N* limit of quantum field theory with bosons and fermions

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We study a large N_c limit of a two-dimensional Yang–Mills theory coupled to bosons and fermions in the fundamental representation. Extending an approach due to Rajeev we show that the limiting theory can be described as a classical Hamiltonian system whose phase space is an infinite-dimensional super-Grassmannian. The linear approximation to the equations of motion and the constraint yields the 't Hooft equations for the mesonic spectrum. Two other approximation schemes to the exact equations are discussed. © *2002 American Institute of Physics.*
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I. INTRODUCTION

To gain a better understanding of gauge theories, two-dimensional models are often used as a testing ground. In a by now classic paper, 't Hooft has shown that the large-N_c limit allows us to obtain an equation describing the meson spectrum of two-dimensional Quantum Chromodynamics (QCD).[1] The same model was analyzed using different approaches[2–5] and they confirmed the results obtained by 't Hooft.

In this article we study the large-N_c limit of certain two-dimensional (2D) theories following a general approach developed by Rajeev[6,7] (see also Refs. 8 and 9 for similar approaches). In the large N_c limit of various quantum field theories (e.g., QCD) the quantum fluctuations become small and the theories are well described by a classical limit. This classical limit however is different from the conventional one in that many of the essential nonperturbative features of the quantum theory survive the large N_c limit.[10,1,11] In the formulation of Ref. 7 the classical theory corresponding to large N_c limit of 2D QCD is described by a Hamiltonian system defined on an infinite-dimensional Grassmannian. The points of this infinite-dimensional manifold can be identified with subspaces in infinite-dimensional Hilbert space (see the main text for precise definitions). The Grassmannian is a topologically nontrivial manifold whose connected components are labeled by an integer which can be identified with the baryon number. The 't Hooft equation describing the meson mass spectrum can be obtained in the linear approximation to the equations of motion on the Grassmannian.[7] In addition to meson masses, this approach also allows one to estimate the baryon mass via a variational ansatz.[12,6] The overall scheme resembles the Skyrme model of baryons in four-dimensional QCD. However unlike the Skyrme model the Grassmannian system of Ref. 7 can be derived as a large N_c limit of an underlying gauge theory. The Grassmannian is a homogeneous manifold. It is equipped with an action of an infinite-dimensional group (which is unitary for the fermionic matter and pseudounitary in the case of bosonic matter). This fact is very important for the structure of the phase space. In particular, it can be used for

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quantization of the classical system which would allow one to get a handle on $1/N_c$ corrections (including nonperturbative ones). We believe that besides the possibility of describing baryons, not captured by the original 't Hooft approach,[10] the present approach can be made mathematically more precise. We remark that when the matter fields are in the adjoint representation, the mathematical techniques required are also very elegant and interesting, involving the Cuntz algebra in various forms. For this approach, we refer the reader to the papers of Halpern and Schwartz[13] and Rajeev and Lee.[14]

The 2D QCD interacting with bosons in the fundamental representation was also worked out following 't Hooft, partly because bosonic theory resembles the four-dimensional QCD in certain respects more than the fermionic one.[15–17] The approach of Ref. 7 was extended to the bosonic case in Ref. 18 (see also Ref. 19 for a similar approach to the problem).

In this paper we study the case when both bosonic and fermionic matter are present. One motivation for this is the fact that a dimensional reduction of four-dimensional QCD produces two-dimensional fundamental fermions and bosons in the adjoint representation coupled to the fermions via gauge fields. We do not expect that the bosons in the fundamental representation capture completely the adjoint case, but it can be used again as a testing ground. We also explore a more general case that includes the Yukawa type interaction between bosons and fermions.

The model of fundamental bosons and fermions interacting via SU(N_c) gauge field was studied, following the same ideas in the original paper of 't Hooft, by Aoki.[20,21] The more general models in the large-N_c limit are presented in a paper by Cavicchi, where he uses a bilocal field approach in the path integral picture.[22] Some of the models discussed in Ref. 22 are more general containing more complicated interactions, some of which in fact require a coupling constant renormalization.

In Refs. 20–22 it is shown that there are 't Hooft-like spectral equations for various types of mesons. In our case we have boson–boson, fermion–fermion, and boson–fermion type mesons, and they all satisfy essentially the same equation. In each case the meson spectrum is discrete and these mesons are all stable in the large-N_c approximation. One cannot say much about the baryons using these methods.

In the present work we generalize the approach of Ref. 7 to QCD for the bosonic and fermionic matter fields coupled via gauge fields. We will see that the phase space of the theory corresponds to a certain superversion of the infinite-dimensional Grassmanian. Although the original system does not have any supersymmetry the main objects describing the large N_c limit, such as the phase space, group action, symplectic form, can be described in supergeometric terms. (A similar phenomenon was observed in another two-dimensional model in Ref. 23, and indeed this is a general feature of bosons and fermions coupled via gauge fields). We obtain the equations describing the meson spectrum of the model within the linear approximation. These equations agree with the ones found by Aoki.[20,21] The theory we will present is actually nonlinear and can accommodate solitonic solutions which should describe baryons. We identify the operator which gives us the baryon number. We also propose some approximations to the spectral equations going beyond the linear approximation and discuss some consequences.

The layout of the paper is as follows. In Sec. II we reformulate the model in terms of color invariant bilinears. We further derive the Poisson brackets and the constraints imposed on the bilinear variables in large N_c limit. In Sec. III we describe this Hamiltonian system in more precise terms using the language of supergeometry. The linear approximation to the equations of motion giving the meson mass spectrum is discussed in Sec. IV. In Sec. V we propose two approximation schemes that incorporate some nonlinear corrections and give a qualitative discussion of their influence on the spectrum.

II. THE ALGEBRA OF COLOR INVARIANT OPERATORS

We start by writing the action functionals of the two theories that we are interested in. Both theories have a gauge field that can be completely eliminated in favor of static 2D Coulomb potential. We will use the light cone coordinates $x^+=(1/\sqrt{2})(t+x)$, $x^-=(1/\sqrt{2})(t-x)$ and

choose the $A_+=0$ gauge. We first look at the gauge-coupled complex bosons with a quartic self-interaction term and Dirac fermions both in the fundamental representation of SU(N_c):

$$S=\int \mathrm{d}x^+\,\mathrm{d}x^-\Big[-\frac{1}{2}\mathrm{Tr}\,F_{+-}F^{+-}+i\sqrt{2}\psi_L^{*\alpha}(\partial_-+igA_-)^\beta_\alpha\psi_{L\beta}+i\sqrt{2}\psi_R^{*\alpha}\partial_+\psi_{R\alpha}$$
$$-m_F(\psi_L^{*\alpha}\psi_{R\alpha}+\psi_R^{*\alpha}\psi_{L\alpha})-2\phi^{*\alpha}\partial_-\partial_+\phi_\alpha+ig(\partial_+\phi^{*\alpha}A^\beta_{-\alpha}\phi_\beta-\phi^{*\alpha}A^\beta_{-\alpha}\partial_+\phi_\beta)$$
$$-m_B^2\phi^{*\alpha}\phi_\alpha-\frac{\lambda^2}{4}\phi^{*\alpha}\phi_\alpha\phi^{*\beta}\phi_\beta\Big]. \tag{1}$$

In the other model we will look at parity broken and a Yukawa-type interaction is added between fermions and bosons,

$$S_Y=\int \mathrm{d}x^+\,\mathrm{d}x^-\Big[-\frac{1}{2}\mathrm{Tr}\,F_{+-}F^{+-}+i\sqrt{2}\psi_L^{*\alpha}(\partial_-+igA_-)^\beta_\alpha\psi_{L\beta}+i\sqrt{2}\psi_R^{*}\partial_+\psi_R-2\phi^{*\alpha}\partial_-\partial_+\phi_\alpha$$
$$+ig(\partial_+\phi^{*\alpha}A^\beta_{-\alpha}\phi_\beta-\phi^{*\alpha}A^\beta_{-\alpha}\partial_+\phi_\beta)-m_B^2\phi^{*\alpha}\phi_\alpha-\frac{\lambda^2}{4}\phi^{*\alpha}\phi_\alpha\phi^{*\beta}\phi_\beta+\mu(\psi_R^*\psi_{L\alpha}\phi^{*\alpha}$$
$$+\psi_L^{*\alpha}\psi_R\phi_\alpha)\Big]. \tag{2}$$

In both cases we normalize the Lie algebra generators T^a as $\mathrm{Tr}\,T^aT^b=\delta^{ab}$, and we choose them to be Hermitian. This second model is anomalous because it is not a chiral gauge theory. There exist some ideas in the literature to treat an anomalous two-dimensional model,[24] but we will not follow this path. Instead we will take the above-mentioned model at the classical level and eliminate the gauge fields which are not dynamical, and subsequently quantize the effective theory. One can check that the resulting system has a global SU(N_c) symmetry and relativistic invariance. We regard this as a toy model which is *inspired from gauge theory*.

We can further use the Gauss constraint to eliminate the gauge field A_- and the fermionic equations of motion to eliminate the right moving fermion ψ_R ($\psi_{R\alpha}$). We will do these reductions in the quantized model for the first case, and classically for the second one. The resulting action is first order in the "time direction" x^- so we can pass to Hamiltonian formalism in a straightforward way.

The Fourier mode expansions read,

$$\phi_\alpha(x^+)=\int a_\alpha(p)e^{-ipx^+}\frac{dp}{2\pi(2|p|)^{1/2}},\quad \psi_{L\alpha}(x^+)=\int \chi_\alpha(p)e^{-ipx^+}\frac{dp}{2\pi 2^{1/4}}$$

(to simpify the notation instead of p_+ we write p). The normalization factors are chosen to give the correct classical limits. The commutation/anticommutation relations for the fields in the light cone gauge take the form,[6]

$$[\chi_\alpha(p),\chi^{\dagger\beta}(q)]_+=\delta^\beta_\alpha 2\pi\delta(p-q),\quad [a_\alpha(p),a^{\dagger\beta}(q)]=\mathrm{sgn}(p)\,\delta^\beta_\alpha 2\pi\delta(p-q). \tag{3}$$

We define $\delta[p-q]=2\pi\delta(p-q)$, and use $[\mathrm{d}p]=\mathrm{d}p/2\pi$ to keep track of factors of 2π.

One defines a Fock vacuum state $|0\rangle$ by the conditions,

$$a_\alpha(p)|0\rangle=\chi_\alpha(p)|0\rangle=0\quad \text{for}\quad p>0,\quad a^{\dagger\alpha}(p)|0\rangle=\chi^{\dagger\alpha}(p)|0\rangle=0\quad \text{for}\quad p<0. \tag{4}$$

The corresponding normal orderings are defined as

$$:\chi^{\dagger\alpha}(p)\chi_\beta(q):=\begin{cases}-\chi_\beta(q)\chi^{\dagger\alpha}(p) & \text{if } p<0, q<0,\\ \chi^{\dagger\alpha}(p)\chi_\beta(q) & \text{otherwise,}\end{cases} \tag{5}$$

$$:a^{\dagger\alpha}(p)a_\beta(q):=\begin{cases} a_\beta(q)a^{\dagger\alpha}(p) & \text{if } p<0, q<0, \\ a^{\dagger\alpha}(p)a_\beta(q) & \text{otherwise.} \end{cases} \tag{6}$$

(Later on we also use the extension of normal ordering to product of four operators, and it is the standard one.) For our purposes it is most convenient to remember the normal orderings of bilinears in the following form:

$$:\chi^{\alpha\dagger}(p)\chi_\beta(q):=\chi^{\alpha\dagger}(p)\chi_\beta(q)-\frac{\delta^\alpha_\beta}{2}[1-\mathrm{sgn}(p)]\delta[p-q],$$

$$:a^{\alpha\dagger}(p)a_\beta(q):=a^{\alpha\dagger}(p)a_\beta(q)-\frac{\delta^\alpha_\beta}{2}[1-\mathrm{sgn}(p)]\delta[p-q].$$

Written as quantum operators, we have in the first model,

$$\psi_{R\alpha}=\frac{m_F}{\sqrt{2}i\partial_+}\psi_{L\alpha} \tag{7}$$

and its Hermitian conjugate, and

$$\psi_R=-\frac{\mu}{\sqrt{2}i\partial_+}\phi^{*\alpha}\psi_{L\alpha} \tag{8}$$

and its Hermitian conjugate for the second model. In the first case, A_- is given in terms of the other fields as

$$A^a_-=-\frac{g}{\partial_+^2}:(\sqrt{2}\psi^{\dagger\alpha}_L(T^a)^\beta_\alpha\psi_{L\beta}+i[\phi^{\dagger\alpha}(T^a)^\beta_\alpha\partial_+\phi_\beta-\partial_+\phi^{\dagger\alpha}(T^a)^\beta_\alpha\phi_\beta]):. \tag{9}$$

In the second model we are using the same equation to eliminate A_- at the classical level (which means without the normal ordering).

By eliminating the redundant degrees of freedom we can express the action in terms of the bilinears of the fields $\psi_{L\alpha}$ and ϕ_α only. We introduce

$$\begin{aligned} \hat{M}(p,q)&=\frac{2}{N_c}:\chi^{\dagger\alpha}(p)\chi_\alpha(q):, \\ \hat{N}(p,q)&=\frac{2}{N_c}:a^{\dagger\alpha}(p)a_\alpha(q):, \end{aligned} \tag{10}$$

and their odd counterparts,

$$\hat{Q}(p,q)=\frac{2}{N_c}\chi^{\dagger\alpha}(p)a_\alpha(q), \quad \hat{\tilde{Q}}(r,s)=\frac{2}{N_c}a^{\dagger\alpha}(r)\chi_\alpha(s). \tag{11}$$

Once the redundancies are removed the resulting action is already first order in the ''time'' variable hence we can read off the Hamiltonian, and the resulting commutation relations are consistent with the ones obtained from the conventional canonical quantization. The reduction is straightforward in principle but requires a long and careful computation. Since the details are explained in Rajeev's lecture notes[6] we only give the result:

$$H=H_0+H_I, \tag{12}$$

$$H_0=\frac{1}{4}M_B^2\int\frac{[\mathrm{d}p]}{|p|}N(p,p)+\frac{1}{4}M_F^2\int\frac{[\mathrm{d}p]}{p}M(p,p), \tag{13}$$

where for the first model we use

$$M_F^2=m_F^2-\frac{g^2}{\pi},\quad M_B^2=m_{RB}^2-\frac{g^2}{\pi}. \tag{14}$$

We employ a logarithmic renormalization on the bare mass of the bosonic field,[19] and denote the renormalized mass as m_{RB}. For the second model, since we reduce it at the classical level there are no corrections coming to the boson mass term,

$$M_F^2=0,\quad M_B^2=\frac{m_B^2}{4}. \tag{15}$$

The interaction parts are given by

$$H_I=\int[\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t]G_1(p,q;s,t)M(p,q)M(s,t)+\int[\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t]G_2(p,q;s,t)N(p,q)N(s,t)$$
$$+\int[\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t]G_3(p,q;s,t)Q(p,q)\overline{Q}(s,t),$$

where for both the first and second models,

$$G_1(p,q;s,t)=-\frac{g^2}{16}\left(\frac{1}{(p-t)^2}+\frac{1}{(q-s)^2}\right)\delta[p+s-t-q], \tag{16}$$

$$G_2(p,q;s,t)=\frac{g^2}{64}\left(\frac{1}{(p-t)^2}+\frac{1}{(q-s)^2}\right)\delta[p+s-t-q]\frac{qt+ps+st+pq}{\sqrt{|pqst|}}+\frac{\lambda^2}{64}\frac{\delta[p+s-t-q]}{\sqrt{|pqst|}}. \tag{17}$$

In the first model we use

$$G_3(p,q;s,t)=\frac{g^2}{8}\frac{q+s}{(q-s)^2}\frac{\delta[p+s-t-q]}{\sqrt{|qs|}}, \tag{18}$$

and for the second model we only have an additional term,

$$G_3(p,q;s,t)=\frac{\mu^2}{16}\frac{1}{(p-q)}\frac{1}{\sqrt{|qs|}}\delta[p-t-q+s]+\frac{g^2}{8}\frac{q+s}{(q-s)^2}\frac{\delta[p+s-t-q]}{\sqrt{|qs|}}. \tag{19}$$

Above we rescaled our coupling constants by a factor of N_c and kept the same symbols for the couplings (so $g^2N_c\mapsto g^2$, $\mu^2N_c\mapsto\mu^2$, and $\lambda^2N_c\mapsto\lambda^2$) to simplify notation. For the precise meaning of these singular integral kernels we refer to the lecture notes of Rajeev:[6] we should interpret them as Hadamard principal value. We will continue to write the ordinary integrals but keep in mind that the integrals are evaluated with this prescription.

The theory we obtained still possesses a global SU(N_c) invariance. The corresponding generator of symmetry is

$$\hat{\mathcal{Q}}^{\alpha}_{\beta}=\int [\mathrm{d}p]\left(:\chi^{\dagger\alpha}(p)\chi_{\beta}(p):-\frac{1}{N_c}\delta^{\alpha}_{\beta}:\chi^{\dagger\gamma}(p)\chi_{\gamma}(p):\right)$$
$$+\int [\mathrm{d}p]\mathrm{sgn}(p)\left(:a^{\dagger\alpha}(p)a_{\beta}(p):-\frac{1}{N_c}\delta^{\alpha}_{\beta}:a^{\dagger\gamma}(p)a_{\gamma}(p):\right). \tag{20}$$

It is known (at least for the purely spinor and purely scalar QCD_2) that in the light-like axial gauge only the color singlet sector of the model can be quantized in a way that preserves Lorentz invariance (Refs. 5, and 4). In this paper we will therefore consider only the restrictions of our models to this sector. In general for a gauge theory it is expected that in the large N_c limit any gauge invariant correlator factorizes, i.e., $\langle AB\rangle=\langle A\rangle\langle B\rangle+O(1/N_c)$. So when the two-dimensional theory is restricted to the color invariant subspace in the large N_c limit any color invariant correlator should be expressible in terms of correlators of color invariant bilinear operators, $\hat{M}$, $\hat{N}$ and $\hat{Q}$, $\hat{\bar{Q}}$ given in (10) and (11). We compute the (anti)commutation relations between these bilinears:

$$[\hat{M}(p,q),\hat{M}(r,s)]=\frac{2}{N_c}[\hat{M}(p,s)\delta[q-r]-\hat{M}(r,q)\delta[p-s]-\delta[p-s]\delta[q-r](\mathrm{sgn}(p)$$
$$-\mathrm{sgn}(q))],$$

$$[\hat{N}(p,q),\hat{N}(r,s)]=\frac{2}{N_c}[\hat{N}(p,s)\mathrm{sgn}(q)\delta[q-r]-\hat{N}(r,q)\mathrm{sgn}(p)\delta[p-s]$$
$$-\delta[q-r]\delta[p-s](\mathrm{sgn}(p)-\mathrm{sgn}(q))],$$

$$[\hat{Q}(p,q),\hat{\bar{Q}}(r,s)]_{+}=\frac{2}{N_c}[\hat{M}(p,s)\mathrm{sgn}(q)\delta[q-r]+\hat{N}(r,q)\delta[p-s]$$
$$+\delta[p-s]\delta[q-r](1-\mathrm{sgn}(p)\mathrm{sgn}(q))],$$

$$[\hat{M}(p,q),\hat{Q}(r,s)]=\frac{2}{N_c}\delta[q-r]\hat{Q}(p,s), \tag{21}$$

$$[\hat{N}(p,q),\hat{Q}(r,s)]=-\frac{2}{N_c}\delta[p-s]\mathrm{sgn}(p)\hat{Q}(r,q),$$

$$[\hat{M}(p,q),\hat{\bar{Q}}(r,s)]=-\frac{2}{N_c}\delta[p-s]\hat{\bar{Q}}(r,q),$$

$$[\hat{N}(p,q),\hat{\bar{Q}}(r,s)]=\frac{2}{N_c}\delta[q-r]\mathrm{sgn}(q)\hat{\bar{Q}}(p,s).$$

All the other (anti)commutators vanish. The first two relations were used before in Refs. 7 and 18, respectively. These (anti)commutation relations define an infinite dimensional Lie superalgebra. Its even part is isomorphic to a direct sum of central extensions of infinite-dimensional unitary and pseudounitary groups each one generated by operators $\hat{M}(p,q)$ and $\hat{N}(p,q)$, respectively (see Ref. 18 for details). We will talk more about this Lie superalgebra and the corresponding supergroup in Sec. III. As the right-hand sides of (21) all contain a factor of $1/N_c$ in the large N_c limit all of the bilinears commute (or anticommute, respectively) and can be thought of as coordinates on a classical phase space. We denote the classical variables corresponding to $\hat{M}$, $\hat{N}$, $\hat{Q}$, $\hat{\bar{Q}}$ by the same letters with carets removed. This classical phase space is an infinite-dimensional supermanifold endowed with a super-Poisson structure inherited from the (anti)commutation relations (21).

The corresponding Poisson superbrackets are obtained from the (anti)commutators in (21) by substituting $-i$ instead of $1/N_c$ factors (note that this brings an extra factor of 2). There is no simple way to decide which multiple of $1/N_c$ should be the quantum parameter. If one attempts a geometric quantization of this model, the symplectic form should be an integer multiple of the Chern character of the line bundle; the symplectic form we have in Sec. III is in fact the basic two form. The other possibility is to write the symplectic form in the action and use single valuedness of the path integral as is done in Ref. 7. (We note in passing that there is a factor of 2 missing in Ref. 18, due to an error in the conventions, but we scale the Hamiltonian with the same parameter so the large-N_c results are the same. The geometric quantization parameter instead should have been $1/N_c$).

However the super-Poisson structure corresponding to (21) only gives a local structure of the classical phase space of the theory. In addition to that there are some global constraints on the classical variables assigned to the color invariant bilinears. The constraints emerge in the large N_c limit as consequences of the color invariance condition $\hat{\mathcal{Q}}^{\alpha}_{\beta}=0$.

To write down these constraints it is convenient to introduce the following operator product convention:

$$(AB)(p,q)=\int [\mathrm{d}r]A(p,r)B(r,q),$$

where A, B stand for any of the above-mentioned (classical) bilinears. We also introduce operators 1 and ϵ as the operators with the kernels $\delta[p-q]$ and $-\mathrm{sgn}(p)\delta[p-q]$, respectively. In this notation the constraints read as follows:

$$\begin{aligned}
(M+\epsilon)^2+Q\epsilon Q^{\dagger}&=1,\\
\epsilon Q^{\dagger}M+\epsilon Q^{\dagger}\epsilon+\epsilon N\epsilon Q^{\dagger}+Q^{\dagger}&=0,\\
MQ+\epsilon Q+Q\epsilon N+Q\epsilon&=0,\\
(\epsilon N+\epsilon)^2+\epsilon Q^{\dagger}Q&=1.
\end{aligned}\tag{22}$$

For brevity we will present here a derivation only of the first constraint in (22). The derivations of all the others are very similar. We will restrict ourselves to the zero subspace of the operator $\hat{\mathcal{Q}}^{\alpha}_{\beta}$ and we define the number operators

$$\hat{F}\equiv\frac{1}{N_c}\int [\mathrm{d}p]:\chi^{\dagger\alpha}(p)\chi_{\alpha}(p):,\quad \hat{B}\equiv\frac{1}{N_c}\int [\mathrm{d}p]\mathrm{sgn}(p):a^{\dagger\alpha}(p)a_{\alpha}(p):. \tag{23}$$

(Note that these operators are scaled by a factor of $1/N_c$ so taking the limit $N_c\to\infty$ gives us zero when these operators are acting on mesonic states. They are nonzero when we look at the baryonic states as we will see shortly.)

By writing out the product of operators at hand in terms of the variables a, $a^{\dagger}$, χ and $\chi^{\dagger}$ and moving the suitable combinations to the right one can prove the identity (that holds on the whole Fock space)

$$((\hat{M}+\epsilon)^2+\hat{Q}\epsilon\hat{Q}^{\dagger})(r,s)=\delta[r-s]+\frac{2}{N_c^2}\chi^{\dagger\alpha}(r)\chi_{\beta}(s)(\hat{\mathcal{Q}}^{\beta}_{\alpha}+\delta^{\beta}_{\alpha}(\hat{F}+\hat{B})).$$

On the subspace $\hat{\mathcal{Q}}^{\beta}_{\alpha}=0$, the operator $\hat{B}+\hat{F}$ will be equal to the baryon number operator $\hat{\mathbf{B}}$. Thus when we restrict ourselves to a fixed baryon number B, we get

$$((\hat{M}+\epsilon)^2+\hat{Q}\epsilon\hat{Q}^{\dagger})(r,s)=\delta[r-s]+(\hat{M}+1-\epsilon)(r,s)\frac{B}{N_c},$$

this in the large N_c limit produces the first constraint in (22).

When we look at a possible exotic baryon state:

$$\int \epsilon_{\alpha_1 \dots \alpha_s \alpha_{s+1} \cdots \alpha_{N_c}} Z(p_1, \dots, p_s; p_{s+1}, \dots, p_{N_c}) \chi^{\dagger \alpha_1}(p_1) \dots \chi^{\dagger \alpha_s}(p_s) a^{\dagger \alpha_{s+1}}(p_{s+1}) \dots a^{\dagger \alpha_{N_c}}(p_{N_c}) |0>, \tag{24}$$

where $p_1, p_2, \dots, p_{N_c}$ are all positive, and $Z(p_1, \dots, p_s, p_{s+1}, \dots, p_{N_c})$ is symmetric in $p_1, \dots, p_s$ and antisymmetric in $p_{s+1}, \dots, p_{N_c}$. The operator $\hat{\mathbf{B}}$ gives 1 acting on such a state. On mesonic states this operator has vanishing matrix elements in the large-N_c limit. One can prove more generally therefore that this operator is the baryon number operator. If we act by this operator on a product of such exotic baryons and finite number of mesons in the large-N_c limit we get the number of baryons, B. In this discussion we see the possibility of having exotic baryons, and we will come back to the geometric meaning of this in Sec. III (and show that it is indeed an integer in our model). We will also show that just as in the purely bosonic and purely fermionic cases the constraints (22) have an elegant geometric interpretation in terms of infinite dimensional disk and Grassmannian.

III. PHASE SPACE OF THE THEORY: SUPER-GRASSMANNIAN

In this section we present the geometry of the phase space without going into the mathematical intricacies. We believe the most proper treatment requires an infinite-dimensional extension of Berezin's **Z**-graded version of supergeometry. We do not give such a complete presentation, and develop a more formal approach (in many cases we provide parenthetical remarks on the general case). We plan to provide a more detailed discussion in a later publication when we discuss geometric quantization of this system. The proper treatment of second quantization with bosons and fermions, which fits to our point of view, can be found in Refs. 25, 26, and also in Ref. 27. In order to understand the geometry of the phase space, we define an operator in supermatrix form;

$$\Phi = \begin{pmatrix} \epsilon N + \epsilon & \epsilon Q^\dagger \\ Q & M + \epsilon \end{pmatrix}, \tag{25}$$

where $\Phi: \mathcal{H}^e | \mathcal{H}^o \to \mathcal{H}^e | \mathcal{H}^o$. We think of the direct sum $\mathcal{H}^e \oplus \mathcal{H}^o$ of one-particle Hilbert spaces of bosons and fermions, respectively, as even and odd graded and the notation $\mathcal{H}^e | \mathcal{H}^o$ is used to emphasize this grading. We use $\epsilon = \left(\begin{smallmatrix} -1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ in both of these spaces. This matrix realization corresponds to the decomposition of the Hilbert spaces into positive and negative energy subspaces as $\mathcal{H}^e_+ \oplus \mathcal{H}^e_-$ for bosons and $\mathcal{H}^o_+ \oplus \mathcal{H}^o_-$ for fermions.

The constraints and the conditions that we found in Sec. II on the basic variables of our theory in terms of Φ become

$$\Phi^2 = 1, \quad E \Phi^\dagger E = \Phi, \tag{26}$$

where $E = \left(\begin{smallmatrix} \epsilon & 0 \\ 0 & 1 \end{smallmatrix}\right)$.

If we introduce a supergroup of operators acting on $\mathcal{H}^e | \mathcal{H}^o$, obeying the relations

$$g E g^\dagger = E, \quad g^\dagger E g = E, \tag{27}$$

we see that the action of this group on the variable Φ, $(g, \Phi) \mapsto g \Phi g^{-1}$ preserves the above-stated conditions on Φ. The orbit of $\hat{\epsilon} = \left(\begin{smallmatrix} \epsilon & 0 \\ 0 & \epsilon \end{smallmatrix}\right)$ under the action of this superunitary group can be parametrized by Φ.

The condition that the bilinears, originally defined on the Fock space of the quantum theory, create finite norm vectors implies that the off-diagonal components of M and N are Hilbert–Schmidt operators (see Refs. 7, 6, and 18 and for the ideals in the nonsuper case see Refs. 28 and

29). A similar computation shows that the off-diagonal components of the superoperators Q and $Q^\dagger$ also satisfy these conditions. These finite norm conditions in two dimensions can be written in an economical way as the Hilbert–Schmidt condition on the supermatrix Φ. To state these convergence conditions more properly we should decompose $\mathcal{H}^e|\mathcal{H}^o$ into negative and positive energy subspaces and think of Φ as an operator acting from $\mathcal{H}^e_+|\mathcal{H}^o_+ \oplus \mathcal{H}^e_-|\mathcal{H}^o_-$ to the same space. Thus we have the convergence conditions,

$$[\hat{\epsilon},\Phi] \in \mathcal{I}_2, \quad \hat{\epsilon}=\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{28}$$

where we write $\hat{\epsilon}$'s matrix realization with respect to this positive–negative energy decomposition. Here for the upper off-diagonal component the ideal of Hilbert–Schmidt operators $\mathcal{I}_2$ refers to the set of operators $B:\mathcal{H}^e_-|\mathcal{H}^o_- \to \mathcal{H}^e_+|\mathcal{H}^o_+$, such that $\mathrm{Tr}\, B^\dagger B$ is convergent. (This definition in the $\mathbf{Z}_2$ graded case is the usual one, since the operators have ordinary numbers as their matrix entries, in a fully $\mathbf{Z}$ graded case these questions are delicate and we have to give a precise meaning to the Hilbert–Schmidt condition. For this work we ignore this question but see Ref. 30 for further comments on it). The lower off-diagonal block will be a Hilbert–Schmidt operator $C:\mathcal{H}^e_+|\mathcal{H}^o_+ \to \mathcal{H}^e_-|\mathcal{H}^o_-$ as well. (Since the even and odd Hilbert spaces are isomorphic, it is convenient to drop the superscript when there is no confusion.) The above-mentioned considerations suggest that we should use as our symmetry group the restricted superunitary group:

$$U_1(\mathcal{H}_-,\mathcal{H}_+|\mathcal{H}) = \{g | gEg^\dagger = E, \quad g^\dagger E g = E \quad [\hat{\epsilon},g] \in \mathcal{I}_2\}, \tag{29}$$

where $\mathcal{I}_2$ denotes the ideal of Hilbert–Schmidt operators as in the above-mentioned positive–negative energy decomposition used for Φ's convergence conditions.

We look at the orbit of $\hat{\epsilon}=\left(\begin{smallmatrix} \epsilon & 0 \\ 0 & \epsilon \end{smallmatrix}\right)$, this time we write it with respect to the original decomposition $\mathcal{H}^e|\mathcal{H}^o$, under the restricted superunitary group. We notice that this orbit is in fact a homogeneous supersymplectic manifold:

$$SGr_1 = \frac{U_1(\mathcal{H}_-,\mathcal{H}_+|\mathcal{H})}{U(\mathcal{H}_-|\mathcal{H}_-)\times U(\mathcal{H}_+|\mathcal{H}_+)}. \tag{30}$$

The stability subgroup has a natural embedding into the full group. This physically means that we allow mixing of the positive energy states of bosons and fermions as well as the negative ones.

Notice that a tangent vector V_u at any point on this super-Grassmannian is given by its effect on Φ, $V_u(\Phi)=i[u,\Phi]_s$, where we use the super-Lie bracket which is defined by

$$\begin{aligned}\left[\begin{pmatrix} a_1 & \beta_1 \\ \gamma_1 & d_1 \end{pmatrix},\begin{pmatrix} a_2 & \beta_2 \\ \gamma_2 & d_2 \end{pmatrix}\right]_s &= \left[\begin{pmatrix} a_1 & 0 \\ 0 & d_1 \end{pmatrix},\begin{pmatrix} a_2 & 0 \\ 0 & d_2 \end{pmatrix}\right] + \left[\begin{pmatrix} a_1 & 0 \\ 0 & d_1 \end{pmatrix},\begin{pmatrix} 0 & \beta_2 \\ \gamma_2 & 0 \end{pmatrix}\right] \\ &\quad + \left[\begin{pmatrix} 0 & \beta_1 \\ \gamma_1 & 0 \end{pmatrix},\begin{pmatrix} a_2 & 0 \\ 0 & d_2 \end{pmatrix}\right] + \left[\begin{pmatrix} 0 & \beta_1 \\ \gamma_1 & 0 \end{pmatrix},\begin{pmatrix} 0 & \beta_2 \\ \gamma_2 & 0 \end{pmatrix}\right]_+\end{aligned}$$

for a decomposition of u into $\left(\begin{smallmatrix} a & \beta \\ \gamma & d \end{smallmatrix}\right)$, with respect to $\mathcal{H}^e|\mathcal{H}^o$. In general the super-Lie algebra element u will depend on the position Φ.

Our homogeneous manifold carries a natural two-form, this turns it into a phase space. We formally define a two-form;

$$\Omega = \frac{i}{4}\,\mathrm{Str}\,\Phi\, d\Phi \wedge d\Phi. \tag{31}$$

One can give the symplectic form explicitly via its action on vector fields, and this defines the above-mentioned two-form:

$$i_{V_u} i_{V_v} \Omega = \frac{i}{8} \mathrm{Str}\, \Phi [[u,\Phi]_s,[v,\Phi]_s]_s . \tag{32}$$

Using exactly the same methods as in Refs. 7 and 18 we can show that it is closed and nondegenerate.

In fact the above-mentioned form is also a homogeneous two-form invariant under the group action, as can be verified in a simple manner. We note that the super-Poisson brackets which we introduced in Sec. I as a result of the large-N_c limit, are precisely the ones given by this symplectic form. Therefore we may introduce a classical dynamical system defined on this super-Grassmannian with this symplectic form which gives us the same set of super-Poisson brackets. This shows that the large-N_c limit of our theory has an independent geometric formulation: the phase space is an infinite-dimensional homogeneous manifold with a natural symplectic structure on it.

The group action is generated by moment maps $F_u = -(i/2)\mathrm{Str}_\epsilon\, u(\Phi - \left(\begin{smallmatrix}\epsilon & 0\\ 0 & \epsilon\end{smallmatrix}\right))$, where we use the even–odd decomposition to write all the operators and conditional trace to be defined in the following. They satisfy the following super-Poisson realization of the super-unitary group:

$$\{F_u, F_v\} = F_{-i[u,v]_s} - \frac{i}{2} \mathrm{Str}_\epsilon \left[\begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon \end{pmatrix}, u \right]_s v, \tag{33}$$

where $[.,.]_s$ again denotes the super-commutator(super-Lie bracket). To see this, one way is to compute both sides, the other is to use general principles and evaluate both sides at $\hat{\epsilon} = \left(\begin{smallmatrix}\epsilon & 0\\ 0 & \epsilon\end{smallmatrix}\right)$ (written with respect to the even–odd decomposition). The moment function on the right vanishes there and the central term is constant on the phase space, this gives us

$$\begin{aligned}
\Sigma_s(u,v) &= -\frac{i}{8} \mathrm{Str} \begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon \end{pmatrix} \left[\left[\left[\begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon \end{pmatrix}, u \right], \left[\begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon \end{pmatrix}, v \right] \right] \right]_s \\
&= -\frac{i}{2} (\mathrm{Tr}_\epsilon [\epsilon, a(u)] a(v) - \mathrm{Tr}_\epsilon ([\epsilon, \beta(u)] \gamma(v) \\
&\quad + [\epsilon, \beta(v)] \gamma(u)) - \mathrm{Tr}_\epsilon [\epsilon, \mathrm{d}(u)] \mathrm{d}(v)) \\
&= -\frac{i}{2} \mathrm{Str}_\epsilon \left[\begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon \end{pmatrix}, u \right] v .
\end{aligned}$$

The conditional supertrace is defined by $\mathrm{Str}_\epsilon \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) = \mathrm{Tr}_\epsilon A - \mathrm{Tr}_\epsilon D$, and $\mathrm{Tr}_\epsilon A = \frac{1}{2}\mathrm{Tr}(A + \epsilon A \epsilon)$. Notice that the convergence conditions on Φ guarantees that the conditional trace exists (in fact a better convergence is possible, see the following). This can be seen most easily by using, $\Phi - \hat{\epsilon} = g \hat{\epsilon} g^{-1} - \hat{\epsilon} = -[\hat{\epsilon}, g] g^{-1}$. It is more natural to compute this with respect to the positive–negative energy decomposition (we use the subscripts $\pm$ to denote the supermatrix elements acting between various subspaces),

$$[\hat{\epsilon}, g] g^{-1} = \begin{pmatrix} 0 & g_{+-} \\ g_{-+} & 0 \end{pmatrix} \begin{pmatrix} (g^{-1})_{++} & (g^{-1})_{+-} \\ (g^{-1})_{-+} & (g^{-1})_{--} \end{pmatrix} = \begin{pmatrix} \mathcal{I}_1 & \mathcal{I}_2 \\ \mathcal{I}_2 & \mathcal{I}_1 \end{pmatrix}, \tag{34}$$

where $\mathcal{I}_1$ denotes the ideal of trace class operators and $\mathcal{I}_2$ is the ideal of Hilbert–Schmidt operators. We used the fact that the off-diagonal elements are Hilbert–Schmidt and the others are bounded, and the analog of the well-known conditions $\mathcal{I}_2 \mathcal{I}_2 \in \mathcal{I}_1$ in the supercase. If we multiply this with an element of the Lie algebra we see that the conditional traces exist. It suggests a

slightly better way to write the moment maps, $F_u = -(i/2)\mathrm{Str}_{\hat{\epsilon}} u(\Phi - \hat{\epsilon})$, which shows that the conditional convergence could be actually defined with respect to the positive–negative energy decomposition.

The previous discussion further implies that $\mathrm{Str}_{\hat{\epsilon}}(\Phi - \hat{\epsilon})$ is convergent. This expression is in fact conserved by the equations of motion of a quadratic Hamiltonian. We may understand the meaning of this number, if we think of its action on color invariant states before we take the large-N_c limit. We can prove that in this case this operator gives us twice the baryon number. Recall that the baryons in this theory can be exotic, that is we may have color singlet combinations of the form,

$$\int \epsilon_{\alpha_1 \alpha_2 \cdots \alpha_{N_c}} Z(q_1, \ldots q_s; q_{s+1}, \ldots, q_{N_c}) \chi^{\dagger \alpha_1}(q_1) \cdots \chi^{\dagger \alpha_k}(q_k) a^{\dagger \alpha_{k+1}}(q_{k+1}) \cdots a^{\dagger \alpha_{N_c}}(q_{N_c})|0\rangle, \tag{35}$$

where all the momenta are positive, and Z is symmetric in $p_1, \ldots, p_s$ and antisymmetric in $p_{s+1}, \ldots, p_{N_c}$, as we have seen in Sec. II. The negative momenta case,

$$\int \epsilon^{\alpha_1 \alpha_2 \cdots \alpha_{N_c}} \overline{Z}(q_1, \ldots, q_k; q_{k+1}, \ldots, q_{N_c}) \chi_{\alpha_1}(q_1) \ldots \chi_{\alpha_k}(q_k) a_{\alpha_{k+1}}(q_{k+1}) \ldots a_{\alpha_{N_c}}(q_{N_c})|0\rangle, \tag{36}$$

where all the momenta are negative, and similar symmetry properties for $\overline{Z}$ correspond to an antibaryon and $\hat{\mathbf{B}}$ acting on such a state gives -1. So we identify the large-N_c limit of the baryon number operator as

$$\mathbf{B} = -\tfrac{1}{2}\mathrm{Str}_{\hat{\epsilon}}(\Phi - \hat{\epsilon}). \tag{37}$$

We show in Appendix A that the baryon number operator is indeed an integer using the geometry of our phase space. We will leave the discussion of the geometry of the phase space at this point and return to the dynamics.

IV. THE LINEAR APPROXIMATION

In this section we discuss the linear approximation to the above-mentioned theory. At present we do not have a simple physical interpretation of the full equations of motion. In principle they are straightforward to compute using the Hamiltonians we have and the defining Poisson brackets. Our phase space is defined by the Poisson brackets we get from the supercommutators for this system in the large-N_c limit and the constraints which define the global nature of the phase space. We note that part of the interactions of this theory are in these constraints. We give the super-Poisson brackets that define the kinematics of our theory:

$$\begin{aligned}
\{M(p,q), M(r,s)\} &= -2i[M(p,s)\delta[q-r] - M(r,q)\delta[p-s] \\
&\quad - \delta[p-s]\delta[q-r](\mathrm{sgn}(p) - \mathrm{sgn}(q))], \\
\{N(p,q), N(r,s)\} &= -2i[N(p,s)\mathrm{sgn}(q)\delta[q-r] - N(r,q)\mathrm{sgn}(p)\delta[p-s] \\
&\quad - \delta[q-r]\delta[p-s](\mathrm{sgn}(p) - \mathrm{sgn}(q))], \\
\{Q(p,q), \overline{Q}(r,s)\}_+ &= -2i[M(p,s)\mathrm{sgn}(q)\delta[q-r] + N(r,q)\delta[p-s] \\
&\quad + \delta[p-s]\delta[q-r](1 - \mathrm{sgn}(p)\mathrm{sgn}(q))], \\
\{M(p,q), Q(r,s)\} &= -2i\,\delta[q-r]Q(p,s),
\end{aligned} \tag{38}$$

$$\{N(p,q),Q(r,s)\}=2i\delta[p-s]\mathrm{sgn}(p)Q(r,q),$$

$$\{M(p,q),\overline{Q}(r,s)\}=2i\delta[p-s]\overline{Q}(r,q),$$

$$\{N(p,q),\overline{Q}(r,s)\}=-2i\delta[q-r]\mathrm{sgn}(q)\overline{Q}(p,s).$$

We have the constraints for the basic variables given in Eq. (21).

If we are given a Hamiltonian we can compute the equations of motion using the above-mentioned super-Poisson brackets. This is a complete description of a classical system. Of course since the theory is infinite dimensional there are various delicate questions, such as, is it possible to define trajectories for any given initial data, what is the dense domain on which the Hamiltonian is defined, etc. We will not attempt to answer these questions here. In the limit $N_c\to\infty$, we can rewrite the Hamiltonians of interest in terms of these classical variables, the answers are given in Sec. II,

$$H=H_0+H_I. \tag{39}$$

Here $H_0=\int[\mathrm{d}p]h_F(p)M(p,p)+\int[\mathrm{d}p]h_B(p)N(p,p)$, and we take $h_F(p)=(M_F^2/4)(1/p)$ and $h_B(p)=(M_B^2/4)(1/|p|)$ with the interpretation that these mass terms are given by the previous expressions. H_I, the interaction part, is given generally by

$$H_I=\int[\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t]G_1(p,q;s,t)M(p,q)M(s,t)+\int[\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t]G_2(p,q;s,t)N(p,q)N(s,t)$$
$$+\int[\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t]G_3(p,q;s,t)Q(p,q)\overline{Q}(s,t).$$

In Sec. V, it will be useful to keep this general form of the Hamiltonian, but their explicit forms are given in the discussion of the models in Sec. II in (16), (17), (19); we will use them directly (in the calculations we keep μ^2 always, for the first model we must set $\mu^2=0$).

It is straightforward to find the resulting nonlinear equations of motion simply by computing

$$\frac{\partial O(x^-)}{\partial x^-}=\{O(x^-),H\}_s, \tag{40}$$

for any observable O of the theory (we allow for an odd Hamiltonian in the above-mentioned form, but in our cases, the Hamiltonians are even). However, it is simpler to first look at the linearization where everything decouples (equations for M and N were analyzed in this approximation in previous publications[7,18,6]). We will see that we get the same equations for M,N as in Refs. 7 and 18 in our linearized theory.

Let us ignore all the quadratic terms in the equations of motion and all the quadratic terms in the constraints. First let us write down the resulting constraints in this approximation:

$$\epsilon M+M\epsilon=0,$$

$$\epsilon N\epsilon+N=0,$$

$$\epsilon Q^\dagger\epsilon+Q^\dagger=0,$$

$$\epsilon Q+Q\epsilon=0.$$

We note that the last two equations are identical and the constraints on these variables decouple, hence they can be solved independently. The solutions are

$$M(u,v)=0,\quad N(u,v)=0,\quad Q(u,v)=0\quad\text{for}\quad uv>0. \tag{41}$$

The other components, that is the ones which have opposite sign momenta, are not restricted. The equations of motion one gets for the variable M in the linear approximation are (for $u>0, v<0$):

$$\frac{\partial M(u,v;x^-)}{\partial x^-}=i\frac{M_F^2}{2}\left(\frac{1}{u}-\frac{1}{v}\right)M(u,v)-\frac{ig^2}{2\pi}\int_{-(u-v)/2}^{(u-v)/2}\mathrm{d}p\,\frac{M\left(p-\frac{u-v}{2},p+\frac{u-v}{2}\right)}{\left(p-\frac{u+v}{2}\right)^2}, \quad (42)$$

which is identical with the one in Refs. 7 and 6. If we make the ansatz (see Ref. 7) $M(u,v)=\xi_M(x)e^{iP_-x^-}$, where $x=u/(u-v)$, and define the invariant mass $\Lambda_M^2=2P_-(u-v)$—recall that $(u-v)=P_+$—we get

$$\Lambda_M^2\xi_M(x)=M_F^2\left(\frac{1}{x}+\frac{1}{1-x}\right)\xi_M(x)-\frac{g^2}{\pi}\int_0^1\frac{\mathrm{d}y}{(y-x)^2}\xi_M(y). \quad (43)$$

This is the well-known 't Hooft equation.[10] Similarly for $N(u,v)$ using the same type of ansatz, $N(u,v)=\xi_N(x)e^{iP_-x^-}$, and the invariant mass $\Lambda_N^2=2P_-(u-v)$, we get

$$\Lambda_N^2\xi_N(x)=M_B^2\left(\frac{1}{x}+\frac{1}{1-x}\right)\xi_N(x)-\frac{g^2}{4\pi}\int_0^1\frac{\mathrm{d}y}{(y-x)^2}\frac{(x+y)(2-x-y)}{\sqrt{x(1-x)y(1-y)}}\xi_N(y)$$
$$+\frac{\lambda^2}{8\pi}\int_0^1\frac{\mathrm{d}y}{\sqrt{x(1-x)y(1-y)}}\xi_N(y). \quad (44)$$

This is the bosonic analog of the 't Hooft equation.[15,16,17,19] The equations for $Q,\overline{Q}$ are given in Sec. V in a slightly more general context, so we will not repeat it here. If we again use an ansatz for the $Q(u,v)$ given by $Q(u,v;x^-)=c_Q(x)e^{iP_-x^-}$ and the same interpretation of the symbols, and an invariant mass, $\Lambda_Q^2=2P_-(u-v)$, we get

$$\Lambda_Q^2c_Q(x)=\left(\frac{M_F^2}{x}+\frac{M_B^2}{1-x}\right)c_Q(x)-\frac{g^2}{2\pi}\int_0^1\frac{\mathrm{d}y}{(y-x)^2}\frac{2-x-y}{\sqrt{(1-x)(1-y)}}c_Q(y)$$
$$+\frac{\mu^2}{4\pi}\int_0^1\frac{\mathrm{d}y}{\sqrt{(1-y)(1-x)}}c_Q(y). \quad (45)$$

Setting $\mu^2=0$ we recover the equations found by Aoki.[20,21] Similarly for the complex conjugate variable $\overline{Q}$, we get

$$\Lambda_{\overline{Q}}^2c_{\overline{Q}}(x)=\left(\frac{M_B^2}{x}+\frac{M_F^2}{1-x}\right)c_{\overline{Q}}(x)-\frac{g^2}{2\pi}\int_0^1\frac{\mathrm{d}y}{(y-x)^2}\frac{x+y}{\sqrt{xy}}c_{\overline{Q}}(y)+\frac{\mu^2}{4\pi}\int_0^1\frac{\mathrm{d}y}{\sqrt{yx}}c_{\overline{Q}}(y). \quad (46)$$

We remark that the equation for $c_{\overline{Q}}$ can be obtained from the equation for c_Q if we make the change of variable $x\mapsto 1-x$, and interchange M_B and M_F and use the principal value prescription (this ultimately comes from the charge conjugation invariance).

The properties of these equations have been discussed in the literature. The two kernels above differ from the ones given in Refs. 10, 15, 20, and 21 by a relatively compact perturbation so they behave in the same way. What is remarkable about them is that they only allow for discrete spectrum, they do not have scattering states. The corresponding eigenvectors form a basis.

We make a short digression and note an interesting limit: in the second model let us set $g^2=0$. There is no coupling to gauge fields thus there is no reason to assume that the observables

of the theory are color invariant. We can study this case along the same lines assuming *it is a sort of mean-field approximation only* and we search for bound states of a fermion and a boson in the linear approximation. The Hamiltonian is quite simple,

$$H=\frac{1}{4}m_B^2\int\frac{[\mathrm{d}p]}{|p|}N(p,p)+\frac{\mu^2}{16}\int\frac{[\mathrm{d}p\ \mathrm{d}q\ \mathrm{d}s\ \mathrm{d}t]}{\sqrt{|qs|}}\frac{\delta[p-q+s-t]}{t-s}Q(p,q)\overline{Q}(s,t). \tag{47}$$

The linearization is the same as before, for the bound state solution we obtain Eq. (44) with $g^2=0$. Unfortunately this equation will not have a solution for the bound state energy. We need the opposite sign in the Hamiltonian for the coupling of $Q\overline{Q}$. It is an amusing exercise to check that the seemingly different interaction $i\mu(\phi^{*\alpha}\psi_R^*\psi_{L\alpha}-\psi_L^{*\alpha}\psi_R\phi_\alpha)$ produces the same Hamiltonian, so we will still not find a bound state for fermion–boson pair. We hope to come back to some of these issues in a separate work.

V. BEYOND THE LINEAR APPROXIMATION

In this section we will discuss the equations of motion of our theory in a semilinear approximation. The exact equations of motion can of course be written, but it is hard to grasp their meaning at this point for the most general case. It will be interesting to look at other approximations to see what new information they contain.

Our first semilinear approach is this: We will keep everything linear in the variables M and N and terms second order in Q and $Q^\dagger$ only. We will drop terms of the form MQ, NQ and M^2,N^2. Even though we have not found a justification for why this should be a good approximation, we expect that it may give us a better feeling for the system. We first show that this is a consistent approximation, that is, if the equations of motion are also kept to the same approximation, the truncated constraints are preserved.

The constraints in this new approximation become

$$M\epsilon+\epsilon M+Q\epsilon Q^\dagger=0,$$

$$Q\epsilon+\epsilon Q=0,$$

$$\epsilon N\epsilon+N+\epsilon Q^\dagger Q=0.$$

We should also obtain semilinearized equations of motion for these variables. We now show that the linearized constraints are left invariant by the semilinearized equations of motion. We will present the proof for a general quadratic Hamiltonian. The solution of the constraint on Q is simple: $Q(u,v)=0$ when u and v have the same sign. We notice that the first constraint does not impose anything on $M(u,v)$ for $u>0,v<0$ or $u<0,v>0$, and the constraint is consistent since for this case we have $\int Q(u,q)[-\mathrm{sgn}(q)]\overline{Q}(q,v)[\mathrm{d}q]=0$. Thus we should look at $u>0,v>0$ or both negative case for M in the constraint:

$$-2M(u,v)+\int Q(u,q)[-\mathrm{sgn}(q)]\overline{Q}(q,v)[\mathrm{d}q]=-2M(u,v)+\int_{-\infty}^{0}[\mathrm{d}q]Q(u,q)\overline{Q}(q,v)=0. \tag{48}$$

Let us check that it is preserved by the linearized equations of motion,

$$\frac{\partial M(u,v)}{\partial x^-}=\{M(u,v),H\}=2i(h_F(u)-h_F(v))M(u,v)+\int [\mathrm{d}p\ \mathrm{d}r\ \mathrm{d}s\ \mathrm{d}t]G_1(p,r,s,t)$$

$$\times\{M(u,v),M(p,r)M(s,t)\}+\int [\mathrm{d}p\ \mathrm{d}r\ \mathrm{d}r\ \mathrm{d}t]G_3(p,r,s,t)\{M(u,v),Q(p,r)\overline{Q}(s,t)\})$$

$$=2i(h_F(u)-h_F(v))M(u,v)+4i\int [\mathrm{d}p\ \mathrm{d}r]G_1(p,r;v,u)M(p,r)[\mathrm{sgn}(u)-\mathrm{sgn}(v)]$$

$$-2i\int [\mathrm{d}r\ \mathrm{d}s\ \mathrm{d}t]G_3(v,r,s,t)Q(u,r)\overline{Q}(s,t)$$

$$+2i\int [\mathrm{d}p\ \mathrm{d}r\ \mathrm{d}s]G_3(p,r,s,u)Q(p,r)\overline{Q}(s,v).$$

The equations of motion for Q in this approximation become

$$\frac{\partial Q(u,q)}{\partial x^-}=2ih_F(u)Q(u,q)-2i\,\mathrm{sgn}(q)h_B(q)Q(u,q)$$

$$+2i\int G_3(p,r,q,u)Q(p,r)[1-\mathrm{sgn}(u)\mathrm{sgn}(q)]. \tag{49}$$

Similarly for $Q^\dagger$,

$$\frac{\partial \overline{Q}(q,v)}{\partial x^-}=-2ih_F(v)\overline{Q}(q,v)+2i\,\mathrm{sgn}(q)h_B(q)\overline{Q}(q,v)$$

$$-2i\int G_3(v,q;s,t)\overline{Q}(s,t)[1-\mathrm{sgn}(v)\mathrm{sgn}(q)]. \tag{50}$$

Combining these equations and using the constraint again we obtain

$$2\frac{\partial M(u,v)}{\partial x^-}-\int_{-\infty}^{0}\left[\frac{\partial Q(u,q)}{\partial x^-}\overline{Q}(q,v)+Q(u,q)\frac{\partial \overline{Q}(q,v)}{\partial x^-}\right][\mathrm{d}q]=0. \tag{51}$$

Using the same equations, we can check that the condition $Q(u,v)=0$ when u, v have the same sign, is also preserved by the equations of motion, hence also for $\overline{Q}(u,v)$.

We write down the equation of motion for $N(u,v)$,

$$\frac{\partial N(u,v)}{\partial x^-}=2i[h_B(u)\mathrm{sgn}(u)-h_B(v)\mathrm{sgn}(v)]N(u,v)$$

$$+4i\int [\mathrm{d}p\ \mathrm{d}q]G_2(p,q;v,u)[\mathrm{sgn}(u)-\mathrm{sgn}(v)]N(p,q)$$

$$+2i\int [\mathrm{d}p\ \mathrm{d}q\ \mathrm{d}t][G_3(p,u;q,t)Q(p,v)\overline{Q}(q,t)\mathrm{sgn}(u)$$

$$-G_3(p,q;v,t)Q(p,q)\overline{Q}(u,t)\mathrm{sgn}(v)].$$

Using the above-mentioned equations of motion we can check that the truncated constraint on N is preserved under time evolution:

$$(1+\mathrm{sgn}(u)\mathrm{sgn}(v))\frac{\partial N(u,v)}{\partial x^-}-\mathrm{sgn}(u)\int_{-\infty}^{0}[\mathrm{d}q]\left[\frac{\partial\overline{Q}(u,q)}{\partial x^-}Q(q,v)+\overline{Q}(u,q)\frac{\partial Q(q,v)}{\partial x^-}\right]=0. \tag{52}$$

Next we discuss the equations of motion for the unconstraint components. From the above-mentioned equations we see that the equations for Q and $Q^\dagger$ are independent of M and N, therefore they can be solved independently. Furthermore, the solution acts as a source term for the M and N equations. Let us write down the equation of motion for Q in the case of $u>0$ and $v<0$ for our model:

$$\begin{aligned}\frac{\partial Q(u,v)}{\partial x^-}&=2ih_F(u)Q(u,v)+2ih_B(v)Q(u,v)\\&\quad+i\frac{\mu^2}{8(u-v)}\int_{-(u-v)/2}^{(u-v)/2}[\mathrm{d}q]\frac{Q\left(q-\frac{u-v}{2},q+\frac{u-v}{2}\right)}{\sqrt{\left|q+\frac{u-v}{2}\right||v|}}\\&\quad-i\frac{g^2}{2}\int_{-(u-v)/2}^{(u-v)/2}[\mathrm{d}p]\frac{p-\frac{u}{2}+\frac{3v}{2}}{\left(p-\frac{u+v}{2}\right)^2}\frac{Q\left(p+\frac{u-v}{2},p-\frac{u-v}{2}\right)}{\sqrt{\left|p-\frac{u-v}{2}\right||v|}}.\end{aligned}$$

A similar equation for $\overline{Q}(u,v)$ holds [which can also be found by complex conjugation of the $Q(v,u)$].

Notice that the equations of motion for $M(u,v)$ (for $u>0,v<0$) become

$$\begin{aligned}\frac{\partial M(u,v)}{\partial x^-}&=2i(h_F(u)-h_F(v))M(u,v)-ig^2\int[\mathrm{d}s]\frac{M(s+(u-v)/2,s-(u-v)/2)}{[s-(u+v)/2]^2}\\&\quad+\frac{ig^2}{4}\int[\mathrm{d}q\,\mathrm{d}s]\frac{q+s}{(q-s)^2}\frac{1}{\sqrt{|qs|}}[Q(q+u-s,q)\overline{Q}(s,v)-Q(u,q)\overline{Q}(s,v+s-q)]\\&\quad-\frac{i\mu^2}{8}\int\frac{[\mathrm{d}q\,\mathrm{d}s]}{\sqrt{|qs|}}\left[\frac{Q(u,q)\overline{Q}(s,s-v+q)}{v-q}-\frac{Q(u+q-s,q)\overline{Q}(s,v)}{u-s}\right].\end{aligned}$$

We note that in the second term on the right we should separate the constrained variables of M from the unconstrained ones. At the same time we do some shift of integration variables, and obtain

$$\begin{aligned}\frac{\partial M(u,v;x^-)}{\partial x^-}&=i\frac{M_F^2}{2}\left[\frac{1}{u}-\frac{1}{v}\right]M(u,v)-ig^2\int_{-(u-v)/2}^{(u-v)/2}[\mathrm{d}s]\frac{M(s+(u-v)/2,s-(u-v)/2)}{[s-(u+v)/2]^2}\\&\quad+f_+(u,v;x^-)+f_-(u,v;x^-)+g_+(u,v;x^-)+g_-(u,v;x^-)+Y_+(u,v;x^-)\\&\quad+Y_-(u,v;x^-),\end{aligned}$$

where all the forcing terms are functions of $Q,\overline{Q}$ and their explicit expressions are given in Appendix B. Note that once we know the solution for Q and $Q^\dagger$, f's, g's, and Y's just become-

time dependent sources for the M and N equations. Therefore we can think of this as a forced linear equation. Let us also write down the resulting equation of motion for $N(u,v)$, for $u>0$, $v<0$,

$$\frac{\partial N(u,v;x^-)}{\partial x^-}=i\frac{M_B^2}{2}\left[\frac{1}{u}-\frac{1}{v}\right]N(u,v)+i\int_{-(u-v)/2}^{(u-v)/2}[\mathrm{ds}]$$
$$\times\frac{N(s+(u-v)/2,s-(u-v)/2)}{\sqrt{\left|s-\frac{u-v}{2}\right|\left|s+\frac{u-v}{2}\right||uv|}}\left[\frac{g^2}{4}\frac{\left(s+\frac{3u}{2}-\frac{v}{2}\right)\left(s+\frac{3v}{2}-\frac{u}{2}\right)}{\left[s-\frac{(u+v)}{2}\right]^2}-\frac{\lambda^2}{8}\right]$$
$$+\tilde{f}_+(u,v;x^-)+\tilde{f}_-(u,v;x^-)+\tilde{g}_+(u,v;x^-)+\tilde{g}_-(u,v;x^-)+\tilde{Y}_+(u,v;x^-)$$
$$+\tilde{Y}_-(u,v;x^-),$$

where we again have the forcing terms determined by the variables $Q,\overline{Q}$ (the explicit formulas are given in Appendix B).

We can give a rough argument of how these equations behave. If we look at the formulas given in Appendix B, we notice that the singular looking kernels are actually harmless, since the integration regions are outside of the singular points. This means that once we have the solutions for the $Q,\overline{Q}$ variables we can treat them as small perturbations to the equations. If we could find the Green's function for these linear operator equations given the sources we should be able to solve them. Let us assume that we have the linear equation $i(\partial M/\partial x^-)=\mathbf{L}M+S(x^-)$, where $\mathbf{L}$ is a linear Hermitian operator. If we know the eigenvectors $\mathbf{L}M_\lambda=\lambda M_\lambda$ then we can use a general ansatz as $M=\Sigma_\lambda a_\lambda(x^-)M_\lambda(x^-)$, and get $a_\lambda(x^-)=-i\int_0^{x^-}\mathrm{d}x^-<M_\lambda(x^-),S(x^-)>$. (In our case the leading singular integral operators are Hermitian and have only discrete spectrum, hence the expansion makes sense). This is the full solution and represents transition probabilities among the stationary states of the operator $\mathbf{L}$. Perhaps it is better to think of the ordinary forced harmonic oscillator problem. When we have a time-dependent forcing, this causes transitions between the stationary levels of the oscillator. So, without actually solving the above equation we see that the forcing terms will cause transition between the stationary levels. That physically means that the energy levels of the mesons will have a broadening due to possible transitions.

There is another possible approximation, for which we drop all MM, NN, and $Q\overline{Q}$ terms and allow for the cross terms MQ, NQ, etc., and neglect any higher orders. In some sense this is the complementary approximation to the previous one. This implies that we should write the constraint as

$$M\epsilon+\epsilon M=0,$$

$$MQ+Q\epsilon N+\epsilon Q+Q\epsilon=0,$$

$$\epsilon N\epsilon+N=0.$$

The first and the last equations are familiar conditions. The middle one has the following solution (in the given approximation): For $u,v>0$ [recall that $\epsilon(p)=-\mathrm{sgn}(p)$],

$$-2Q(u,v)+\int_{-\infty}^{0}[\mathrm{d}q]M(u,q)Q(q,v)+\int_{-\infty}^{0}[\mathrm{d}q]Q(u,q)(-\mathrm{sgn}(q))N(q,v)=0. \qquad (53)$$

For $u>0,v<0$ we have

$$\int_{-\infty}^{0}[\mathrm{d}q]M(u,q)Q(q,v)-\int_{0}^{\infty}[\mathrm{d}q]Q(u,q)N(q,v)=0. \tag{54}$$

We satisfy the lower equation by noting that the same momenta case for Q is given by the first constraint and the integrands then become of lower order in this case. The consistency of these approximations could be checked. In fact if we write down the time derivative of the above-mentioned constraint,

$$-2\frac{\partial Q(u,v)}{\partial x^-}+\int_{-\infty}^{0}[\mathrm{d}q]\left(\frac{\partial M(u,q)}{\partial x^-}Q(q,v)+M(u,q)\frac{\partial Q(q,v)}{\partial x^-}\right)$$
$$+\int_{-\infty}^{0}[\mathrm{d}q]\left(\frac{\partial Q(u,q)}{\partial x^-}N(q,v)+Q(u,q)\frac{\partial N(q,v)}{\partial x^-}\right)=0.$$

To see this we use

$$\frac{\partial Q(u,v;x^-)}{\partial x^-}=4i\int[\mathrm{d}p\ \mathrm{d}s\ \mathrm{d}t]G_1(p,u;s,t)Q(p,v)M(s,t)$$
$$-4i\int[\mathrm{d}q\ \mathrm{d}s\ \mathrm{d}t]G_2(v,q;s,t)Q(u,q)N(s,t)\mathrm{sgn}(v)+2i(h_F(u)$$
$$-\mathrm{sgn}(v)h_B(v))Q(u,v)+2i\int[\mathrm{d}p\ \mathrm{d}q\ \mathrm{d}t]G_3(p,q;v,t)Q(p,q)M(u,t)\mathrm{sgn}(v)$$
$$+2i\int[\mathrm{d}p\ \mathrm{d}q\ \mathrm{d}s]G_3(p,q;s,u)Q(p,q)N(s,v)$$
$$+2i\int[\mathrm{d}p\ \mathrm{d}q]G_3(p,q;v,u)Q(p,q)[1-\mathrm{sgn}(u)\mathrm{sgn}(v)].$$

For the first time derivative in the constraint we insert this expression, for the time derivatives of Q inside the integral we only retain the linear terms in Q, since other combinations are of lower order by assumption. We should also use the equations of motion of M and N for the opposite momenta case and only within the linear approximation as is given in the previous semilinear case, we do not repeat them, higher order terms get multiplied by Q and become small. Then we see that the constraint is preserved within the given approximation.

This time we have decoupled linear equations for M and N for the opposite momenta case, since we ignore $Q\overline{Q}$ type terms, and in principle they can be solved independently. When we look at the equations for Q, we should again be careful. The opposite momenta case is to be treated as independent dynamical variables: if we use the constraint equation, we may express the same sign momenta in terms of the solutions of M and N and the opposite momenta terms of Q. When we look at the opposite sign momenta equation for Q we may separate the same sign momenta contributions in the integral operators. But these same momenta terms in the integral equation become of higher order, since all these terms are multiplied by other variables, and the central part vanishes in this case, hence they can be dropped. Let us denote the resulting integral equation which only acts on the opposite momenta terms by **K**, this is the expression we have found before, and write the remaining parts as an abstract integral operator $\mathbf{F}(x^-)$. Notice that it has dependence on x^- via the solutions of M and N. The time dependence of M and N is rather simple for this case, since we have singular integral equations with discrete spectra. We can in principle substitute the solutions we picked into this equation. Hence we have an integral equation

$$\frac{\partial Q(u,v;x^-)}{\partial x^-}=[\mathbf{K}Q](u,v;x^-)+[\mathbf{F}(x^-)Q](u,v;x^-). \tag{55}$$

It is most natural to think of the last term as a time-dependent perturbation. We can write this perturbation term $\mathbf{F}(x^-)$:

$$
\begin{aligned}
[\mathbf{F}(x^-)Q](u,v;x^-) = &-\frac{ig^2}{2}\left[\int_0^u [\mathrm{d}s]\int_0^{u-s}[\mathrm{d}p]+\int_{-\infty}^0[\mathrm{d}s]\int_{u-s}^{\infty}[\mathrm{d}p]\right]\frac{M(s,s+p-u;x^-)}{(s-u)^2}Q(p,v)\\
&+i\left[\int_{-\infty}^v[\mathrm{d}q]\int_0^{v-q}[\mathrm{d}t]+\int_v^0[\mathrm{d}q]\int_{v-q}^0[\mathrm{d}t]\right]\\
&\times\left[\frac{g^2}{8}\frac{(t+q)^2+(q-v)^2-2q^2}{(v-t)^2}-\frac{\lambda^2}{16}\right]\frac{N(t+q-v,t;x^-)}{\sqrt{|vq(t+q-v)|}}Q(u,q)\\
&-i\left[\int_v^0[\mathrm{d}t]\int_0^{t-v}[\mathrm{d}p]+\int_{-\infty}^v[\mathrm{d}t]\int_{t-v}^0[\mathrm{d}p]\right]\\
&\times\left(\frac{\mu^2}{8(t-v)}+\frac{g^2}{4}\frac{p-t+2v}{(p-t)^2}\right)\frac{M(u,t;x^-)}{\sqrt{|(p-t+v)v|}}Q(p,p-t+v)\\
&+i\left[\int_0^u[\mathrm{d}s]\int_0^{u-s}[\mathrm{d}p]+\int_u^{\infty}[\mathrm{d}s]\int_{u-s}^0[\mathrm{d}p]\right]\\
&\times\left(\frac{\mu^2}{8(u-s)}+\frac{g^2}{4}\frac{p+2s-u}{(p-u)^2}\right)\frac{N(s,v;x^-)}{\sqrt{|(p+s-u)s|}}Q(p,p+s-u).
\end{aligned}
$$

The method of solving such equations is known in principle. We can treat the last term as a truly time-dependent perturbation, but this time it involves the unknown itself and thus cannot be solved in closed form. However, we can solve it perturbatively. The kernels again do not become singular within the given ranges of the integrals except at the boundaries. The singularities are not as severe and we expect that the perturbations are small, so that one can obtain a reasonable answer from this approach. We will not go into further details, but the basic result is again the possibility of transitions between the different levels of the boson–fermion mesons due to the interactions.

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APPENDIX A: BARYON NUMBER

We define the Fredholm operators in a $\mathbf{Z}_2$ graded context as in the ordinary case (there is an extension to the $\mathbf{Z}$ grading which should fit to our model better: The definition of the Fredholm operator shows that the body is an ordinary Fredholm operator and the rest is compact. So in the

following use the body for all the formulas, and take the supertrace of $\Phi-\hat{\epsilon}$'s body part): a Fredholm operator is an invertible operator up to compact operators. This again implies the kernel and the cokernel are actually finite dimensional. Let us write down the kernel in a decomposition $V_e|V_o$, and define a superdimension, which is the dimension of the even part of the kernel minus the dimension of the odd part. $\mathrm{Sdim}(\mathrm{Ker}(A))=\dim(P_e\mathrm{Ker}(A)P_e)-\dim(P_o\mathrm{Ker}(A)P_o)$, where P_e and P_o denote projections onto the even and odd subspaces, respectively. Then the index should be

$$\mathrm{SInd}(A)=\mathrm{Sdim}(\mathrm{Ker}(A))-\mathrm{Sdim}(\mathrm{Coker}(A)). \tag{A1}$$

We can extend the Calderon theorem to our case (see Ref. 31 for a good introduction and the original result): If we have an operator A which is Fredholm, and assume we have an operator B such that $(I-AB)^m$ and $(I-BA)^m$ are trace class for an integer m, then we can compute the super-Fredholm index as $\mathrm{Str}(I-BA)^m-\mathrm{Str}(I-AB)^m$. Let us now see that in our problem the supertrace of Φ is indeed this index. It will be more convenient to decompose our operator with respect to the positive and negative subspaces, thus we write everything with respect to $\mathcal{H}_+|\mathcal{H}_+\oplus\mathcal{H}_-|\mathcal{H}_-$. We do not repeat odd and even superscripts, since the bar indicates this separation. In this decomposition our group conditions can be found from

$$g^\dagger Eg=E,\quad gEg^\dagger=E,\quad E=\begin{pmatrix}\epsilon & 0\\ 0 & 1\end{pmatrix}, \tag{A2}$$

so E is the same as before in this matrix representation, it is interpreted differently. The orbit is with respect to this decomposition,

$$\Phi=g\hat{\epsilon}g^{-1},\quad \hat{\epsilon}=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}. \tag{A3}$$

So if we write $g:\mathcal{H}_+|\mathcal{H}_+\oplus\mathcal{H}_-|\mathcal{H}_-\to\mathcal{H}_+|\mathcal{H}_+\oplus\mathcal{H}_-|\mathcal{H}_-$, explicitly, we have

$$g=\begin{pmatrix}A & B\\ C & D\end{pmatrix}\quad B,\quad C\in\mathcal{I}_2(\mathcal{H}_\mp|\mathcal{H}_\mp,\mathcal{H}_\pm|\mathcal{H}_\pm). \tag{A4}$$

From the first group condition we get, $A^\dagger\epsilon A+C^\dagger C=\epsilon$ and $D^\dagger D+B^\dagger\epsilon B=1$ and from the second one we get $A\epsilon A^\dagger+BB^\dagger=\epsilon$ and $DD^\dagger+C\epsilon C^\dagger=1$. Since B,C are Hilbert–Schmidt in the more generalized sense, we have A,D super-Fredholm. Further we can use the above-mentioned theorem to compute the index of A,D, for example,

$$\mathrm{SInd}(D)=\mathrm{Str}(B^\dagger\epsilon B)-\mathrm{Str}(C\epsilon C^\dagger). \tag{A5}$$

Let us compute the conditional supertrace of $\Phi-\hat{\epsilon}$, (in fact we see that this is the correct way we should be computing it), first we write it explicitly with respect to the above-given decomposition,

$$g\hat{\epsilon}g^{-1}-\hat{\epsilon}=\begin{pmatrix}-A\epsilon A^\dagger\epsilon+BB^\dagger\epsilon+1 & *\\ * & -C\epsilon C^\dagger+D\epsilon D^\dagger-1\end{pmatrix}. \tag{A6}$$

If we use the above-mentioned group properties, we get

$$\Phi-\hat{\epsilon}=\begin{pmatrix}2BB^\dagger\epsilon & *\\ * & -2C\epsilon C^\dagger\end{pmatrix}. \tag{A7}$$

The conditional supertrace of this operator gives us, $\mathrm{Str}_\epsilon(\Phi-\hat{\epsilon})=2(\mathrm{Str}(BB^\dagger\epsilon)-\mathrm{Str}(C\epsilon C^\dagger))$, which is equal to $2\,\mathrm{SInd}(D)$ (using $\mathrm{Str}(BB^\dagger\epsilon)=\mathrm{Str}(B^\dagger\epsilon B)$). Thus we prove using only the geometry of the super-Grassmanian that this is an integer.

APPENDIX B: FORCING TERMS

Here we present the forcing functions for the inhomogeneous equations of Sec. V. The ones we obtained for M in the first semilinear approximation are given by

$$f_+(u,v;x^-)=-i\frac{g^2}{2}\int_{(u-v)/2}^{\infty}[\mathrm{d}p]\int_{-\infty}^{0}[\mathrm{d}q]\frac{Q\left(p-\frac{u-v}{2},q\right)\overline{Q}\left(q,p+\frac{u-v}{2}\right)}{\left[p-\frac{u+v}{2}\right]^2},$$

$$f_-(u,v;x^-)=-i\frac{g^2}{2}\int_{-\infty}^{-(u-v)/2}[\mathrm{d}p]\int_{0}^{\infty}[\mathrm{d}q]\frac{Q\left(p-\frac{u-v}{2},q\right)\overline{Q}\left(q,p+\frac{u-v}{2}\right)}{\left[p-\frac{u+v}{2}\right]^2},$$

$$g_+(u,v;x^-)=i\frac{g^2}{4}\Bigg[\int_0^u[\mathrm{d}s]\int_{-(u-s)/2}^{(u-s)/2}[\mathrm{d}q]+\int_u^{\infty}[\mathrm{d}s]\int_{-(s-u)/2}^{(s-u)/2}[\mathrm{d}q]\Bigg]\frac{q+\frac{3s}{2}-\frac{u}{2}}{\left[q-\frac{u+s}{2}\right]^2}\frac{Q\left(q+\frac{u-s}{2},q-\frac{u-s}{2}\right)\overline{Q}(s,v)}{\sqrt{\left|q-\frac{u-s}{2}\right||s|}},$$

$$g_-(u,v;x^-)=-i\frac{g^2}{4}\Bigg[\int_v^0[\mathrm{d}s]\int_{-(s-v)/2}^{(s-v)/2}[\mathrm{d}q]+\int_{-\infty}^{v}[\mathrm{d}s]\int_{-(v-s)/2}^{(v-s)/2}[\mathrm{d}q]\Bigg]\frac{q+\frac{3s}{2}-\frac{v}{2}}{\left[q-\frac{v+s}{2}\right]^2}\frac{Q(u,s)\overline{Q}\left(q-\frac{v-s}{2},q+\frac{v-s}{2}\right)}{\sqrt{\left|q-\frac{v-s}{2}\right||s|}},$$

$$Y_-(u,v;x^-)=+\frac{i\mu^2}{8}\Bigg[\int_0^u[\mathrm{d}s]\int_{-(u-s)/2}^{(u-s)/2}[\mathrm{d}q]+\int_u^{\infty}[\mathrm{d}s]\int_{-(s-u)/2}^{(s-u)/2}[\mathrm{d}q]\Bigg]\frac{Q\left(q+\frac{u-s}{2},q-\frac{u-s}{2}\right)\overline{Q}(s,v)}{(u-s)\sqrt{\left|q-\frac{u-s}{2}\right||s|}},$$

$$Y_+(u,v;x^-)=-\frac{i\mu^2}{8}\Bigg[\int_v^0[\mathrm{d}s]\int_{-(s-v)/2}^{(s-v)/2}[\mathrm{d}q]+\int_{-\infty}^{v}[\mathrm{d}s]\int_{-(v-s)/2}^{(v-s)/2}[\mathrm{d}q]\Bigg]\frac{Q(u,s)\overline{Q}\left(q-\frac{v-s}{2},q+\frac{v-s}{2}\right)}{(v-s)\sqrt{\left|q-\frac{v-s}{2}\right||s|}}.$$

The forcing terms for the first semilinear approximation for the N variable are

$$\tilde{f}_-(u,v;x^-) = -i\int_{(u-v)/2}^{\infty}[\mathrm{d}p]\int_{-\infty}^{0}[\mathrm{d}q]\frac{\overline{Q}\left(p+\frac{u-v}{2},q\right)Q\left(q,p-\frac{u-v}{2}\right)}{\sqrt{\left|p-\frac{u-v}{2}\right|\left|p+\frac{u-v}{2}\right||uv|}}$$
$$\times\left[\frac{g^2}{8}\frac{\left(p+\frac{3u}{2}-\frac{v}{2}\right)\left(p+\frac{3v}{2}-\frac{u}{2}\right)}{\left[p-\frac{u+v}{2}\right]^2}-\frac{\lambda^2}{4}\right],$$

$$\tilde{f}_+(u,v;x^-) = i\int_{-\infty}^{-(u-v)/2}[\mathrm{d}p]\int_{0}^{\infty}[\mathrm{d}q]\frac{\overline{Q}\left(p+\frac{u-v}{2},q\right)Q\left(q,p-\frac{u-v}{2}\right)}{\sqrt{\left|p-\frac{u-v}{2}\right|\left|p+\frac{u-v}{2}\right||uv|}}$$
$$\times\left[\frac{g^2}{8}\frac{\left(p+\frac{3u}{2}-\frac{v}{2}\right)\left(p+\frac{3v}{2}-\frac{u}{2}\right)}{\left[p-\frac{u+v}{2}\right]^2}-\frac{\lambda^2}{4}\right],$$

$$\tilde{g}_+(u,v;x^-) = i\frac{g^2}{4}\left[\int_0^u[\mathrm{d}p]\int_{-(u-p)/2}^{(u-p)/2}[\mathrm{d}s]\right.$$
$$\left.+\int_u^{\infty}[\mathrm{d}p]\int_{-(p-u)/2}^{(p-u)/2}[\mathrm{d}s]\right]\frac{s-\frac{p}{2}+\frac{3u}{2}}{\left[s-\frac{u+p}{2}\right]^2}\frac{Q(p,v)Q\left(s+\frac{u-p}{2},s-\frac{u-p}{2}\right)}{\sqrt{\left|s-\frac{p-u}{2}\right||u|}},$$

$$\tilde{g}_-(u,v;x^-) = i\frac{g^2}{4}\left[\int_v^0[\mathrm{d}p]\int_{-(p-v)/2}^{(p-v)/2}[\mathrm{d}s]\right.$$
$$\left.+\int_{-\infty}^{v}[\mathrm{d}p]\int_{-(v-p)/2}^{(v-p)/2}[\mathrm{d}s]\right]\frac{q+\frac{3s}{2}-\frac{v}{2}}{\left[q-\frac{v+s}{2}\right]^2}\frac{Q\left(s-\frac{v-p}{2},s+\frac{v-p}{2}\right)\overline{Q}(u,p)}{\sqrt{\left|s-\frac{p-v}{2}\right||v|}},$$

$$\tilde{Y}_+(u,v;x^-) = -\frac{i\mu^2}{8}\left[\int_0^u[\mathrm{d}p]\int_{-(u-p)/2}^{(u-p)/2}[\mathrm{d}s]\right.$$
$$\left.+\int_u^{\infty}[\mathrm{d}p]\int_{-(p-u)/2}^{(p-u)/2}[\mathrm{d}s]\right]\frac{Q(p,v)\overline{Q}\left(s+\frac{u-p}{2},s-\frac{u-p}{2}\right)}{(p-u)\sqrt{\left|s+\frac{u-p}{2}\right||u|}},$$

$$\widetilde{Y}_{-}(u,v;x^{-})=\frac{i\mu^{2}}{8}\Bigg[\int_{v}^{0}[\mathrm{d}p]\int_{-(p-v)/2}^{(p-v)2}[\mathrm{d}s]+\int_{-\infty}^{v}[\mathrm{d}p]\int_{-(v-p)/2}^{(v-p)/2}[\mathrm{d}s]\Bigg]\frac{Q\left(s-\frac{v-p}{2},s+\frac{v-p}{2}\right)\overline{Q}(u,p)}{(p-v)\sqrt{\left|s+\frac{p-v}{2}\right||v|}}.$$

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Structure conserving parametrization of Feynman diagrams

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Using **x**-space parameters instead of Feynman parameters, dimensionally regularized Feynman diagrams are expanded with respect to the external momenta, the internal masses, the logarithms of these masses and the regularization parameter $(\nu\text{-}\frac{1}{2}n)$. A general formula for an arbitrary Feynman diagram is obtained for any dimension n. All ultraviolet divergences appear in a direct and transparent way as poles. Their residues in the limit $(\nu\text{-}\frac{1}{2}n)\to 0$ are subseries that are recognized as subdiagrams. Relations between diagrams are transparent in all orders of perturbation theory. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1475767]

I. INTRODUCTION

In the usual formalism of quantum field theory, a Feynman diagram is represented by a momentum space integral of the type[1]

$$\prod_{\substack{1\leqslant i\leqslant f\\ 1\leqslant i'<i\\ 1\leqslant j\leqslant f-1\\ d}} \int d\mathbf{k}^d_{i',i}\,\frac{P^d_{i',i}(\boldsymbol{\gamma};\mathbf{k};m)}{(\mathbf{k}^{d\,2}_{i',i}+m^{d\,2}_{i',i})^{\alpha^d_{i',i}}}\,V_i(\boldsymbol{\gamma};\mathbf{k};m)\,\delta\left(\mathbf{p}_j-\sum_{\substack{1\leqslant a\leqslant f\\ d}}\mathbf{k}^d_{a,j}\right), \tag{1.1}$$

with

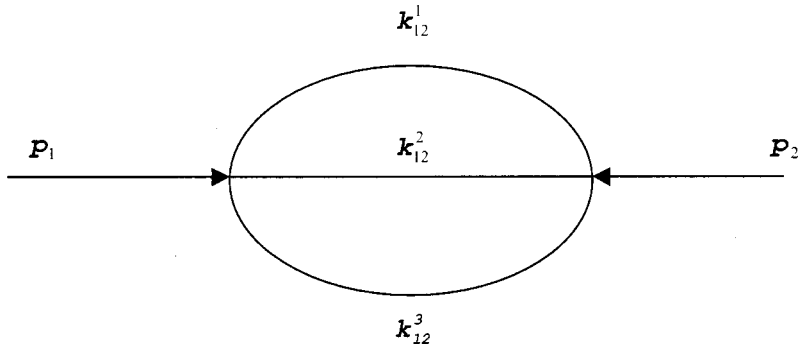
$$k^d_{a,j}=-k^d_{j,a}. \tag{1.2}$$

About the notation we remark the following points;

- Internal momenta and masses of propagators wear three indices. The two subscripts i',i indicate the vertices that they are connecting, the superscript d counts lines between these vertices.
- The exponents α in the denominator are introduced in order to clarify what happens throughout this article. In physics, they are equal to 1.
- The $i\varepsilon$-prescription of propagators has been transformed away by Wick rotations. The internal momenta, over which it is integrated, are n-dimensional Euclidean vectors.
- The numerators $P^d_{i',i}(\boldsymbol{\gamma};\mathbf{k};m)$ represent spin. They may be polynomials of matrices. In the scalar case
$$P^d_{i',i}(\boldsymbol{\gamma};\mathbf{k};m)=1, \tag{1.3}$$
and if the spin is 1/2,
$$P^d_{i',i}(\boldsymbol{\gamma};\mathbf{k};m)=\boldsymbol{\gamma}\cdot\mathbf{k}^d_{i',i}+m^d_{i',i}. \tag{1.4}$$
- The factors $V_i(\boldsymbol{\gamma};\mathbf{k};m)$ are vertex functions representing interaction. In the case of neutral scalar fields,
$$V_i(\boldsymbol{\gamma};\mathbf{k};m)=1. \tag{1.5}$$

- The number of vertices is denoted by f. The number of δ-functions, that guarantee momentum conservation in each vertex, is one less, because of overall momentum conservation:
$$\mathbf{p}_1+\mathbf{p}_2+\cdots+\mathbf{p}_f=0. \tag{1.6}$$
- Integrating away the δ-functions, the number of remaining integration vectors equals the number of independent loops.
- Remarks about notation are bulleted here and in the following sections, in order to promote legibility.

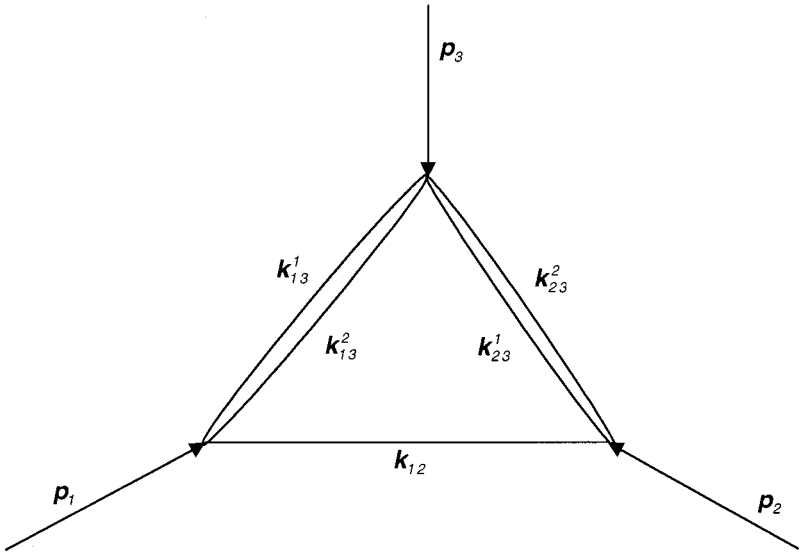
We give two diagrams as an ilustration.
The first example to be considered is the two vertice, three internal line, scalar diagram.



Its expression in momentum space is given by

$$\int d\mathbf{k}^1_{12}d\mathbf{k}^2_{12}d\mathbf{k}^3_{12}\frac{1}{(\mathbf{k}^{1\,2}_{12}+m^{1\,2}_{12})^{\alpha^1_{12}}(\mathbf{k}^{2\,2}_{12}+m^{2\,2}_{12})^{\alpha^2_{12}}(\mathbf{k}^{3\,2}_{12}+m^{3\,2}_{12})^{\alpha^3_{12}}}\,\delta(\mathbf{p}_1-\mathbf{k}^1_{12}-\mathbf{k}^2_{12}-\mathbf{k}^3_{12})$$
$$=\int d\mathbf{k}^1_{12}d\mathbf{k}^2_{12}\frac{1}{(\mathbf{k}^{1\,2}_{12}+m^{1\,2}_{12})^{\alpha^1_{12}}(\mathbf{k}^{2\,2}_{12}+m^{2\,2}_{12})^{\alpha^2_{12}}((\mathbf{p}_1-\mathbf{k}^1_{12}-\mathbf{k}^2_{12})^2+m^{3\,2}_{12})^{\alpha^3_{12}}}. \tag{1.1$'$}$$

The second example to be considered is the three vertice, five line diagram



Its momentum space representation is given by

$$\int d\mathbf{k}_{12}d\mathbf{k}_{13}^1d\mathbf{k}_{13}^2d\mathbf{k}_{23}^1d\mathbf{k}_{23}^2\delta(\mathbf{p}_1-\mathbf{k}_{12}-\mathbf{k}_{13}^1-\mathbf{k}_{13}^2)\,\delta(\mathbf{p}_2+\mathbf{k}_{12}-\mathbf{k}_{23}^1-\mathbf{k}_{23}^2)$$

$$\times\frac{1}{(\mathbf{k}_{12}{}^2+m_{12}{}^2)^{\alpha_{12}}(\mathbf{k}_{13}^1{}^2+m_{13}^1{}^2)^{\alpha_{13}^1}(\mathbf{k}_{13}^2{}^2+m_{13}^2{}^2)^{\alpha_{13}^2}(\mathbf{k}_{23}^1{}^2+m_{23}^1{}^2)^{\alpha_{23}^1}(\mathbf{k}_{23}^2{}^2+m_{23}^2{}^2)^{\alpha_{23}^2}}. \tag{1.1''}$$

In the case of charged fields, a vertex function $\mathbf{k}_a+\mathbf{k}_b$ may appear in the numerator and insertion of the identity

$$(\mathbf{k}_b-\mathbf{k}_a).\frac{(\mathbf{k}_a+\mathbf{k}_b)}{(\mathbf{k}_a{}^2+m^2)(\mathbf{k}_b{}^2+m^2)}=\frac{1}{\mathbf{k}_a{}^2+m^2}-\frac{1}{\mathbf{k}_b{}^2+m^2} \tag{1.7}$$

into (1.1) yields a relation between diagrams.

After introduction of integration parameters ρ,[2] all **k**-integrations—the ''easy integrations''—may be performed by means of Gauss integrals. Thus, (1.1′) is transformed into

$$(1.1')=\frac{(\pi^{1/2\,n})^3(4\pi)^{1/2\,n}}{(2\pi)^n}\,\frac{(m^1)^{2b^1}(m^2)^{2b^2}(m^3)^{2b^3}}{\Gamma(\alpha^1)\Gamma(\alpha^2)\Gamma(\alpha^3)}$$

$$\times\int_0^\infty d\rho^1d\rho^2d\rho^3(\rho^1)^{-b^1}(\rho^2)^{-b^2}(\rho^3)^{-b^3}\left(\frac{m^1{}^2}{\rho^1}+\frac{m^2{}^2}{\rho^2}+\frac{m^3{}^2}{\rho^3}\right)^{-(1/2)\,n}$$

$$\times\exp\left\{-\rho^1-\rho^2-\rho^3-\frac{\mathbf{p}_1^2}{m^1{}^2/\rho^1+m^2{}^2/\rho^2+m^3{}^2/\rho^3}\right\}. \tag{1.8'}$$

- The subscripts 1,2 are omitted for the sake of surveyability.

The parameter representation of (1.1′′) is

(1.1′′)

$$=\frac{(\pi^{1/2\,n})^5(4\pi)^n}{(2\pi)^{2n}}\,\frac{(m_{12})^{2b_{12}}(m'_{13})^{2b'_{13}}(m_{13}^2)^{2b_{13}^2}(m'_{23})^{2b'_{23}}(m_{23}^2)^{2b_{23}^a}}{\Gamma(\alpha_{12})\Gamma(\alpha'_{13})\Gamma(\alpha_{13}^2)\Gamma(\alpha'_{23})\Gamma(\alpha_{23}^2)}$$

$$\times\int d\rho_{12}d\rho_{13}^1d\rho_{13}^2d\rho_{23}^1d\rho_{23}^2(\rho_{12})^{-b_{12}}(\rho_{13}^1)^{-b_{13}^1}(\rho_{13}^2)^{-b_{13}^2}(\rho_{23}^1)^{-b_{23}^1}(\rho_{23}^2)^{-b_{23}^2}$$

$$\times\left\{\left(\frac{m_{13}^1{}^2}{\rho_{13}^1}+\frac{m_{13}^2{}^2}{\rho_{13}^2}\right)\left(\frac{m_{23}^1{}^2}{\rho_{23}^1}+\frac{m_{23}^2{}^2}{\rho_{23}^2}\right)+\left(\frac{m_{13}^1{}^2}{\rho_{13}^1}+\frac{m_{13}^2{}^2}{\rho_{13}^2}\right)\frac{m_{12}{}^2}{\rho_{12}}+\left(\frac{m_{23}^1{}^2}{\rho_{23}^1}+\frac{m_{23}^2{}^2}{\rho_{23}^2}\right)\frac{m_{12}{}^2}{\rho_{12}}\right\}^{-(1/2)\,n}$$

$$\times\exp\Bigg\{-\rho_{12}-\rho_{13}^1-\rho_{13}^2-\rho_{23}^1-\rho_{23}^2$$

$$-\frac{\mathbf{p}_1^2(m_{23}^1{}^2/\rho_{23}^1+m_{23}^2{}^2/\rho_{23}^2)+\mathbf{p}_2{}^2(m_{13}^1{}^2/\rho_{13}^1+m_{13}^2{}^2/\rho_{13}^2)+\mathbf{p}_3{}^2\,m_{12}{}^2/\rho_{12}}{(m_{13}^1{}^2/\rho_{13}^1+m_{13}^2{}^2/\rho_{13}^2)(m_{23}^1{}^2/\rho_{23}^1+m_{23}^2{}^2/\rho_{23}^2)+(m_{13}^1{}^2/\rho_{13}^1+m_{13}^2{}^2/\rho_{13}^2)\,m_{12}{}^2/\rho_{12}+(m_{23}^1{}^2/\rho_{23}^1+m_{23}^2{}^2/\rho_{23}^2)\,m_{12}{}^2/\rho_{12}}\Bigg\}. \tag{1.8''}$$

- The number of dimensions is denoted by n and the notation

$$b=\tfrac{1}{2}n-\alpha \tag{1.9}$$

has been used.

- The number of integration variables ρ equals the number of internal lines.

A parameter representation of the general Feynman diagram is derived in Ref. 2. A shorthand derivation is given in Appendix B.

The integrals (1.1′) and (1.1′′) are ultraviolet divergent in four dimensional space–time and so the integrals (1.8′) and (1.8′′) are divergent. They have to be regularized. Using dimensional regularization,[3] the n in (1.8′) and (1.8′′) is replaced by 2ν, which is considered to be a continuous variable.

Thus, the ultraviolet infinities in four dimensional momentum space are found back as poles at $\nu=2$ in the complex ν-plane. After a change of integration variables according to

$$\begin{aligned}\rho_1&=\rho\sigma_1,\\ \rho_2&=\rho(1-\sigma_1)\sigma_2,\\ \rho_3&=\rho(1-\sigma_1)(1-\sigma_2)\sigma_3,\\ &\text{etc.},\end{aligned}\tag{1.10}$$

the ρ-integration may be done. It yields a Γ-function being responsible for a pole at $\nu=2$. In the case of one-loop diagrams, this is the only divergence and the finite part is obtained by integration over the Feynman parameter σ.

In the case of multiple loops, integration over Feynman parameters—the ''difficult integrations''—itself may be divergent[3] and all kinds of infinities mix together. It is not easy to unravel them. It has been proposed to do it by partial integrations,[3] but even in the most simple two-loop integral (1.8′) we did not succeed. The little bit more complicated expression (1.8′′) does not look very inviting either. Anyway, there is no recipe for the general case.

The cause of this mixing of infinities is the fact that the structure of the original expression (1.1) is obscured by the Gauss integrations that were used at the derivation of (1.8′) and (1.8′′). This loss of structure is also illustrated by relation (1.7), which is not translated into a simple relation in the parameter language of (1.8′) and (1.8′′).

Dimensional regularization being introduced because the structure of the original momentum space expression is left unimpaired, it seems to be logical to combine it with a structure conserving parametrization. Because of this philosophy, it has been proposed[4] to use **x**-space parameters rather than Feynman parameters. Using these parameters, infinities were found easily in one- and two-loop diagrams.

In this article the method is extended to all orders of perturbation theory. The **x**-space parametrization is structure conserving so that relations between diagrams are transparent in all orders of perturbation theory. Moreover, all ultraviolet divergences are separated in a direct way. The **x**-parameters are a useful guide for this separation, rather than an obstacle.

Finally, the integrations over all **x**-space parameters may be done in a systematical way, partly analytically, partly numerically. In this way, a general formula, giving the expansion series with respect to external momenta, internal masses, the logarithms of these masses and the regularization parameter, is obtained in any dimension for an arbitrary Feynman diagram.

II. DIMENSIONAL REGULARIZATION IN x-SPACE

Representation (1.1) may be written by means of **x**-space integrals over polynomials, exponentials and k-functions as

$$\frac{1}{(2\pi)^{n(f-1)}}\sum_{s,t} S(s_c;s_{a,b};s^d_{a,b};t^d_{a,b})$$
$$\times\prod_{\substack{1\leqslant i\leqslant f-1\\ 1\leqslant i'<i\\ d}}\left\{\frac{2\pi^{(1/2)n}}{\Gamma(a^d_{i,f})}(m^d_{i,f})^{2b^d_{i,f}+2t^d_{i,f}}\right\}\left\{\frac{2\pi^{(1/2)n}}{\Gamma(a^d_{i',i})}(m^d_{i',i})^{2b^d_{i',i}+2t^d_{i',i}}\right\}$$
$$\times\int d\mathbf{x}_i e^{i\mathbf{p}_i\cdot\mathbf{x}_i}(x_i)^{2s_i}(\mathbf{x}_{i'}\cdot\mathbf{x}_i)^{s_{i',i}}k(b^d_{i,f}+s^d_{i,f};m^d_{i,f}x_i)k(b^d_{i',i}+s^d_{i',i};m^d_{i',i}|\mathbf{x}_i-\mathbf{x}_{i'}|). \tag{2.1}$$

- The number of **x**-space integration variables is $f-1$, one less than the number of vertices.

The functions $k(b;mx)$ differ by a factor $(mx/2)^b$ from the well known $K_b(mx)$ (Ref. 5)—the latter are named ''Bessel functions of the third kind'' or ''McDonald functions''—and are, up to another factor, the n-dimensional Fourier transform of the propagator $(\mathbf{k}^2+m^2)^{-\alpha}$:

$$\frac{2\pi^{(1/2)n}}{\Gamma(\alpha)}m^{2b}k(b;mx)=\int d\mathbf{k}e^{-i\mathbf{k}\cdot x}\frac{1}{(\mathbf{k}^2+m^2)^{\alpha}}. \tag{2.2}$$

If an internal line corresponds to mass zero, the $k(b;mx)$ has to be replaced according to

$$m^{2b}k(b;mx)\overset{m\to 0}{\to}\frac{1}{2}\Gamma(b)\left(\frac{x}{2}\right)^{-2b}. \tag{2.3}$$

Properties of the k-functions are summarized in Appendix A.

The momenta in the polynomials $P^d{}_{a,b}(\boldsymbol{\gamma};\mathbf{k};m)$ and $V_i(\boldsymbol{\gamma};\mathbf{k};m)$ become derivatives in **x**-language; the latter become, according to (A8), polynomials of $\mathbf{x}_c{}^2,\mathbf{x}_a\cdot\mathbf{x}_b$ and $(m^d{}_{a,b})^2$, in combination with higher order k-functions. The coefficients are matrices, denoted by $S(s_c;s_{a,b};s^d{}_{a,b};t^d{}_{a,b})$. In the scalar case, S is a c-number and the s_c, $s_{a,b}$, $s^d{}_{a,b}$ and $t^d{}_{a,b}$ assume only the value *0*.

If derivatives $\partial_\mu k(b;mx)$ appear, identity

$$\partial_\mu[k(b;m|\mathbf{x}-\mathbf{x}_1|)\{\partial^\mu k(b;m|\mathbf{x}-\mathbf{x}_2|)\}-\{\partial^\mu k(b;m|\mathbf{x}-\mathbf{x}_1|)\}k(b;m|\mathbf{x}-\mathbf{x}_2|)]$$
$$=(1-\alpha)m^2\{k(b;m|\mathbf{x}-\mathbf{x}_1|)k(b+1;m|\mathbf{x}-\mathbf{x}_2|)-k(b+1;m|\mathbf{x}-\mathbf{x}_1|)k(b;m|\mathbf{x}-\mathbf{x}_2|)\} \tag{2.4}$$

is obtained by using differential equation (A9). It is the translation into **x**-space language of the **p**-space relation (1.7). Equation (2.4) may be inserted into (2.1) and yields a relation between diagrams.

- The summation variables s and t of spin and complicated interaction do not impair the essence of our method and will be omitted from now on.
- The number of independent vectors $\mathbf{p}_i$ is g $(g\leqslant f-1)$ and we use the notation

$$c_{i',i}=\frac{\mathbf{x}_{i'}\cdot\mathbf{x}_i}{x_{i'}x_i},\qquad c_{i,f-1+j}=\frac{\mathbf{x}_i\cdot\mathbf{p}_j}{x_ip_j},\qquad c_{f-1+j',f-1+j}=\frac{\mathbf{p}_{j'}\cdot\mathbf{p}_j}{p_{j'}p_j} \tag{2.5}$$
$$(1\leqslant i'<i\leqslant f-1)\quad 1\leqslant i\leqslant f-1;1\leqslant j\leqslant g\qquad 1\leqslant j'<j\leqslant g$$

After introduction of appropriate coordinate systems and after calculation of the corresponding Jacobians, a number of integrations may be done and the regularized expression

$$(2.1)=\frac{1}{(2\pi)^{2\nu(f-1)}}\prod_{\substack{1\leqslant i\leqslant f-1\\ 1\leqslant i'<i\\ 1\leqslant j\leqslant g\\ d}}\left\{\frac{2\pi^{\nu}(m^d_{i,f})^{2\beta^d_{i,f}}}{\Gamma(a^d_{i,f})}\right\}\left\{\frac{2\pi^{\nu}(m^d_{i',i})^{2\beta^d_{i',i}}}{\Gamma(a^d_{i',i})}\right\}\frac{2^{f-1}\pi^{(2\nu-f-g+i+1)/2}}{\Gamma((2\nu-f-g+i+1)/2)}$$

$$\times\int_{I^2>0}dx_i dc_{i',i}dc_{i,f-1+j}x_i^{2\nu-1}e^{i\mathbf{p}_i\cdot\mathbf{x}_i}k^d_{i,f}(\beta;mx_i)$$

$$\times k^d_{i',i}(\beta;m|\mathbf{x}_i-\mathbf{x}_{i'}|)\frac{(I_{i,i+1,\ldots,f-1+g})^{2\nu-f-g+i-1}}{(I_{i+1,\ldots,f-1+g})^{2\nu-f-g+i}} \tag{2.6}$$

is obtained.

- The ν and β's are given by

$$\nu=\tfrac{1}{2}n,$$
$$\beta=\nu-\alpha, \tag{2.7}$$

  and are considered as continuous variables.

- We use the notation

$$k^d_{i,f}(\beta;mx_i)=k(\beta^d_{i,f};m^d_{i,f}x_i),$$
$$k^d_{i',i}(\beta+l+r;m\mathbf{x}_i)=k(\beta^d_{i',i}+l^d_{i',i}+r^d_{i',i};m^d_{i',i}\mathbf{x}_i). \tag{2.8}$$

- $I_{i,i+1,\ldots,f-1+g}$ is the content of an $f+g-i$ dimensional parallelopipidum formed by the unit vectors $\mathbf{x}_i/x_i,\ldots,\mathbf{x}_{f-1}/x_{f-1},\mathbf{p}_1/p_1,\ldots,\mathbf{p}_g/p_g$.

This content is the square root of a polynomial of cosines. Details are discussed in Appendix C. Integration is restricted to the area where the polynomials are positive.

We finish this section by clearing up (2.1) and (2.6) on the hand of the two example diagrams of Sec. I.

The diagram of Fig. 1 is in **x**-space given by

$$(1.1')=(1.8')$$
$$=\frac{(2\pi^{(1/2)n})^3}{(2\pi)^n}\frac{(m^1)^{2b^1}(m^2)^{2b^2}(m^3)^{2b^3}}{\Gamma(a^1)\Gamma(a^2)\Gamma(a^3)}\int d\mathbf{x}_1 e^{i\mathbf{p}_1\cdot\mathbf{x}_1}k^1(b;mx_1)k^2(b;mx_1)k^3(b;mx_1). \tag{2.1'}$$

After performance of most of the angle integrations, formula

$$(2.1')=\frac{(2\pi^{\nu})^3}{(2\pi)^{2\nu}}\frac{(m^1)^{2\beta^1}(m^2)^{2\beta^2}(m^3)^{2\beta^3}}{\Gamma(\alpha^1)\Gamma(\alpha^2)\Gamma(\alpha^3)}\frac{2\pi^{(2\nu-1)/2}}{\Gamma((2\nu-1)/2)}(ip_1)^{q_{12}}$$
$$\times\int dc_{12}(c_{12})^{q_{12}}(\sqrt{1-c_{12}{}^2})^{2\nu-3}\int dx x^{2\nu-1+q_{12}}k^1(\beta;mx)k^2(\beta;mx)k^3(\beta;mx) \tag{2.6'}$$

is obtained.

The diagram of Fig. 2 is given by

$$(1.1'')=(1.8'')$$

$$=\frac{(2\pi^{(1/2)n})^5}{(2\pi)^{2n}}\frac{(m_{13}^1)^{2b_{13}^1}(m_{13}^2)^{2b_{13}^2}(m_{23}^1)^{2b_{23}^1}(m_{23}^2)^{2b_{23}^2}(m_{12})^{2b_{12}}}{\Gamma(a_{13}^1)\Gamma(a_{13}^2)\Gamma(a_{23}^1)\Gamma(a_{23}^2)\Gamma(a_{12})}$$

$$\times\int d\mathbf{x}_1 d\mathbf{x}_2 e^{i\mathbf{p}_1\cdot\mathbf{x}_1}e^{i\mathbf{p}_2\cdot\mathbf{x}_2}k_{13}^1(b;mx_1)k_{13}^2(b;mx_1)k_{23}^1(b;mx_2)k_{23}^2(b;mx_2)k_{12}(b;m|\mathbf{x}_1-\mathbf{x}_2|), \tag{2.1''}$$

which becomes, after angle integrations,

$$(2.1'')=\frac{(2\pi^{\nu})^5}{(2\pi)^{4\nu}}\frac{(m_{12})^{2\beta_{12}}(m_{13}^1)^{2\beta_{13}^1}(m_{13}^2)^{2\beta_{13}^2}(m_{23}^1)^{2\beta_{23}^1}(m_{23}^2)^{2\beta_{23}^2}}{\Gamma(a_{12})\Gamma(a_{13}^1)\Gamma(a_{13}^2)\Gamma(a_{23}^1)\Gamma(a_{23}^2)}\frac{2^2\pi^{(2\nu-3)/2}\pi^{(2\nu-2)/2}}{\Gamma((2\nu-3)/2)\Gamma((2\nu-2)/2)}$$

$$\times\int_{I^2>0}dx_1dx_2dc_{12}dc_{13}dc_{14}dc_{23}dc_{24}{x_1}^{2\nu-1}{x_2}^{2\nu-1}e^{i\mathbf{p}_1\cdot\mathbf{x}_1}e^{i\mathbf{p}_2\cdot\mathbf{x}_2}k_{13}^1(\beta;mx_1)$$

$$\times k_{13}^2(\beta;mx_1)k_{23}^1(\beta;mx_2)k_{23}^2(\beta;mx_2)k_{12}(\beta;m|\mathbf{x}_1-\mathbf{x}_2|)\frac{(I_{1,2,3,4})^{2\nu-5}(I_{2,3,4})^{2\nu-4}}{(I_{2,3,4})^{2\nu-4}(I_{3,4})^{2\nu-3}}. \tag{2.6''}$$

- In the following sections, the notation

$$\varepsilon=\nu-\tfrac{1}{2}n=\beta_{a,b}^d-b_{a,b}^d \tag{2.9}$$

will be used and (2.6), (2.6′) and (2.6′′) will be considered in the limit $\varepsilon\to 0$.

III. SERIES EXPANSION; ANGULAR PART

The I-functions in (2.6) cancel, with the exception of the first I in the numerator and the last I in the denominator.

Furthermore, $f-1$ of the $1/2f(f-1)$ arguments of k-functions are "simple," i.e., of the form $|\mathbf{x}_i|$. The other $1/2(f-1)(f-2)$ arguments are "nonsimple:" they are absolute values of linear combinations of $\mathbf{x}_i$. The latter have to be split according to (A12). Because of condition (A13), the integration region is to be divided into $(f-1)!$ subregions:

$$(2.6)=\frac{1}{(2\pi)^{2\nu(f-1)}}\sum_{l,q,r}\prod_{\substack{1\le i\le f-1\\1\le i'<i\\1\le j\le g\\d}}(-)^{l_{i',i}^d}\left(\frac{1}{2}\right)^{2l_{i',i}^d+r_{i',i}^d}(ip_j)^{\sum_{1\le a\le f-1}q_{a,f-1+j}}$$

$$\times\frac{1}{l_{i',i}^d!q_{i,f-1+j}!r_{i',i}^d!}\left\{\frac{2\pi^{\nu}(m_{i,f}^d)^{2\beta_{i,f}^d}}{\Gamma(a_{i,f}^d)}\right\}$$

$$\times\left\{\frac{2\pi^{\nu}(m_{i',i}^d)^{2\beta_{i',i}^d+2l_{i',i}^d+2r_{i',i}^d}}{\Gamma(a_{i',i}^d)}\right\}\frac{2^{f-1}\pi^{(2\nu-f-g+i+1)/2}}{\Gamma((2\nu-f-g+i+1)/2)}$$

$$\times\int_{I^2>0}dc_{i',i}dc_{i,f-1+j}(c_{i',i})^{\sum_d r_{i',i}^d}(c_{i,f-1+j})^{q_{i,f-1+j}}\frac{(I_{1,2,\ldots,f-1+g})^{2\nu-f-g}}{(I_{f,\ldots,f-1+g})^{2\nu-g-1}}$$

$$\times\int_{0\le x_1\le x_2\le\ldots\le x_{f-1}\le\infty}dx_i{x_i}^{2\nu-1+\sum_a q_{i,f-1+a}+\sum_d^{1\le a<i}r_{a,i}^d+\sum_d^{i<a\le f-1}r_{i,a}^d+2\sum_d^{i<a\le f-1}l_{i,a}^d}$$

$$\times k_{i,f}^d(\beta;mx_i)k_{i',i}^d(\beta+l+r;mx_i)+(f-1)!-1\text{ permutations}. \tag{3.1}$$

- Multiplication is over indices $i,j,$ etc.; summation is over indices $a,b,c,$ etc., i.e.,

$$\sum_{i<a\leqslant f-1} = \sum_{a=i+1}^{f-1}, \text{ etc.} \tag{3.2}$$

If all external momenta are linearly independent,

$$g=f-1,$$
$$q_{i,f-1+j}=\delta_{i,j}q_{i,f-1+i}. \tag{3.3}$$

The angular part of (3.1) may be worked out after transformation according to Appendix C:

$$y_{i,j}=\frac{(I_{j+1,\ldots,f-1+g})^2 c_{i,j}-c_{i,j+1}c_{j,j+1}+\cdots}{I_{i,j+1,\ldots,f-1+g}I_{j,j+1,\ldots,f-1+g}}, \tag{3.4a}$$

the inverse of which is given by

$$\begin{aligned} c_{i,j}=&y_{i,j}(\sqrt{1-(y_{i,j+1})^2}\cdots\sqrt{1-(y_{i,f-1+g})^2})(\sqrt{1-(y_{j,j+1})^2}\cdots\sqrt{1-(y_{j,f-1+g})^2})\\ &+(y_{i,j+1}\sqrt{1-(y_{i,j+2})^2}\cdots\sqrt{1-(y_{i,f-1+g})^2})(y_{j,j+1}\sqrt{1-(y_{j,j+2})^2}\cdots\sqrt{1-(y_{j,f-1+g})^2})\\ &+\cdots+(y_{i,f-2+g}\sqrt{1-(y_{i,f-2+g})^2})(y_{j,f-2+g}\sqrt{1-(y_{j,f-2+g})^2})+y_{i,f-1+g}y_{j,f-1+g}. \end{aligned} \tag{3.4b}$$

It results in

$$\begin{aligned} &\prod_{\substack{1\leqslant i\leqslant f-1\\ 1\leqslant i'<i\\ 1\leqslant j<g}} \frac{2^{f-1}\pi^{(2\nu-f-g+i+1)/2}}{\Gamma((2\nu-f-g+i+1)/2)}\\ &\quad\times\int_{I^2>0} dc_{i',i}dc_{i,f-1+j}(c_{i',i})^{\Sigma_d r^d_{i',i}}(c_{i,f-1+j})^{q_{i,f-1+j}}\frac{(I_{1,2,\ldots,f-1+g})^{2\nu-f-g}}{(I_{f,\ldots,f-1+g})^{2\nu-g-1}}\\ &=\sum_q{}' \prod_{\substack{1\leqslant i'<i\\ 1\leqslant i\leqslant i''\leqslant f-1+g\\ 1\leqslant j'<j\leqslant j''\leqslant g}} \frac{(\Sigma_d r^d_{i',i})!}{q_{i',i}{}^{i''}!}\frac{q_{i,f-1+j}!}{q_{i,f-1+j}{}^{j''}!}\frac{2^{f-1}\pi^{(2\nu-f+1-g+i)/2}}{\Gamma((2\nu-f+1-g+i)/2)}\\ &\quad\times\int_{-1}^{1} dy_{i',i}(y_{i',i})^{\Sigma_{1\leqslant a<i'} q_{a,i'}{}^{i}+\Sigma_{i'<a\leqslant i}q_{i',a}{}^{i}}\\ &\quad\times(\sqrt{1-(y_{i',i})^2})^{2\nu-f-g+i-2+\Sigma_{1\leqslant a<i'\leqslant b\leqslant i-1}q_{a,i'}{}^{b}+\Sigma_{i'<a\leqslant b\leqslant i-1}q_{i',a}{}^{b}}\\ &\quad\times\int_{-1}^{1} dy_{i,f-1+j}(y_{i,f-1+j})^{\Sigma_{1\leqslant a<i}q_{a,i}{}^{f-1+j}+\Sigma_{i<a\leqslant f-1+j}q_{i,a}{}^{f-1+j}}\\ &\quad\times(\sqrt{1-(y_{i,f-1+j})^2})^{2\nu-g+j-3+\Sigma_{1\leqslant a<i\leqslant b\leqslant f-2+j}q_{a,i}{}^{b}+\Sigma_{i<a\leqslant b\leqslant f-2+j}q_{i,a}{}^{b}}\\ &\quad\times(y_{f-1+j',f-1+j})^{\Sigma_{1\leqslant a\leqslant f-1}q_{a,f-1+j'}{}^{f-1+j}}\sqrt{(1-(y_{f-1+j',f-1+j})^2}^{\Sigma^{1\leqslant a\leqslant f-1}_{f-1+j'\leqslant b\leqslant f-2+j}q_{a,f-1+j'}{}^{b}}. \end{aligned} \tag{3.5}$$

- The summation variables ${q_{a,b}}^c$ are defined in (C6). They run from 0 to ∞ under the conditions

$$\sum_{i\leqslant c\leqslant f-1+g} {q_{i',i}}^c = \sum_d r^d_{i',i},$$
$$\sum_{f-1+j\leqslant c\leqslant f-1+g} {q_{i,f-1+j}}^c = q_{i,f-1+j}, \tag{3.6}$$

  which has been indicated by the $'$ of Σ'.
- The superscript c of ${q_{a,b}}^c$ counts terms from b to $f-1+g$ in a polynomial expansion of (3.4b) to the power $q_{a,b}$.

Integrations over $y_{i',i}$ and $y_{i,f-1+j}$ yield B-functions and after a number of cancellations, the result is

(3.5)

$$\begin{aligned}
&= \sum_q{}'' \prod_{\substack{1\leqslant i'<i\\ 1\leqslant i\leqslant i''\leqslant f-1\\ 1\leqslant j'<j\leqslant j''\leqslant g}} \frac{(\Sigma_d r^d_{i',i})!\, q_{i,f-1+j}!}{{q_{i',i}}^{i''}!\, {q_{i,f-1+j}}^{j''}!} \\
&\quad\times \frac{2^{f-1}\pi^{(2\nu-f+1-g+i)/2}\Gamma((2\nu-f-g+i+1+\Sigma_{a<b\leqslant i}{q_{a,b}}^b)/2)}{\Gamma((2\nu-f-g+i+1)/2)} \\
&\quad\times \frac{\Gamma((1+\Sigma_{1\leqslant a<i'}{q_{a,i'}}^i+\Sigma_{i'<a\leqslant i}{q_{i',a}}^i)/2)\Gamma((1+\Sigma_{1\leqslant a<i}{q_{a,i}}^{f-1+j}+\Sigma_{i<a\leqslant f-1+j}{q_{i,a}}^{f-1+j})/2)}{\Gamma(2\nu+\Sigma_{1\leqslant a<i\leqslant b\leqslant f-1+g}{q_{a,i}}^b+\Sigma_{i<a\leqslant b\leqslant f-1+g}{q_{i,a}}^b/2)} \\
&\quad\times (y_{f-1+j',f-1+j})^{\Sigma_{1\leqslant a<f-1}{q_{a,f-1+j'}}^{f-1+j}} \left(\sqrt{(1-(y_{f-1+j',f-1+j})^2}\right)^{\Sigma^{1<a\leqslant f-1}_{f-1+j'<b\leqslant f-2+j}{q_{a,f-1+j'}}^b}.
\end{aligned} \tag{3.7}$$

- The summation variables in (3.7) obey both (3.6) and the subsidiary condition that the arguments of the Γ-functions in the numerator have to be half integer. This has been indicated by the $''$ of Σ''.

In order to get familiar with the notations, we shall repeat the derivation line (3.1)–(3.7) for the two example diagrams.

In the case of the example of Fig. 1, where $f-1=g=1$, (3.1) reduces to

$$\begin{aligned}
(2.6') &= \frac{(2\pi^\nu)^3}{(2\pi)^{2\nu}}(ip_1)^{q_{12}}\frac{2\pi^{(2\nu-1)/2}}{\Gamma((2\nu-1)/2)}\int dc_{12}(c_{12})^{q_{12}}\left(\sqrt{1-{c_{12}}^2}\right)^{2\nu-3} \\
&\quad\times\int_0^\infty dx x^{2\nu-1+q_{12}}k^1(\beta;mx)k^2(\beta;mx)k^3(\beta;mx),
\end{aligned} \tag{3.1'}$$

where the notation (2.5) means that

$$c_{12}=\frac{\mathbf{x}_1\cdot\mathbf{p}_1}{x_1p_1} \tag{2.5'}$$

and the transformation (3.4) becomes trivial:

$$y_{12}=c_{12}. \tag{3.4'}$$

The angular part of (3.1′) becomes

$$\frac{2\pi^{(2\nu-1)/2}}{\Gamma((2\nu-1)/2)}\int_{-1}^1 dy_{12}(y_{12})^{q_{12}}\left(\sqrt{1-{y_{12}}^2}\right)^{2\nu-3}=\frac{2\pi^{(2\nu-1)/2}\Gamma((q_{12}+1)/2)}{\Gamma((2\nu+q_{12})/2)}, \tag{3.7'}$$

if q_{12} is even. If q_{12} is odd, the integral of (3.7′) is zero.

In the case of the example of Fig. 2, where $f-1=g=2$, (3.1) reduces to

$$(2.6'')=\frac{(2\pi^{\nu})^5}{(2\pi)^{4\nu}}(ip_1)^{q_{13}}(ip_2)^{q_{24}}\frac{(m_{13}^1)^{2\beta_{13}^1}(m_{13}^2)^{2\beta_{13}^2}(m_{23}^1)^{2\beta_{23}^1}(m_{23}^2)^{2\beta_{23}^2}(m_{12})^{2\beta_{12}+2l_{12}+2r_{12}}}{l_{12}!q_{13}!q_{24}!r_{12}!\Gamma(\alpha_{13}^1)\Gamma(\alpha_{13}^2)\Gamma(\alpha_{23}^1)\Gamma(\alpha_{23}^2)\Gamma(\alpha_{12})}$$
$$\times\frac{2^2\pi^{(2\nu-3)/2}\pi^{(2\nu-2)/2}}{\Gamma((2\nu-3)/2)\Gamma((2\nu-2)/2)}(-)^{l_{12}}\left(\frac{1}{2}\right)^{2l_{12}+r_{12}}$$
$$\times\int dc_{12}dc_{13}dc_{14}dc_{23}dc_{24}(c_{12})^{r_{12}}(c_{13})^{q_{13}}(c_{24})^{q_{24}}\frac{(I_{1,2,3,4})^{2\nu-5}}{(I_{3,4})^{2\nu-3}}$$
$$\times\int_{0\leqslant x_1\leqslant x_2\leqslant\infty}dx_1dx_2{x_1}^{2\nu-1+q_{13}+r_{12}+2l_{12}}{x_2}^{2\nu-1+q_{24}+r_{12}}k_{13}^1(\beta;mx_1)k_{13}^2(\beta;mx_1)$$
$$\times k_{23}^1(\beta;mx_2)k_{23}^2(\beta;mx_2)k_{12}(\beta+l+r;mx_2)+1\text{permutation.}\qquad(3.1'')$$

- The notation (2.5) means

$$c_{12}=\frac{\mathbf{x}_1\cdot\mathbf{x}_2}{x_1x_2},\quad c_{13}=\frac{\mathbf{x}_1\cdot\mathbf{p}_1}{x_1p_1},\quad c_{14}=\frac{\mathbf{x}_1\cdot\mathbf{p}_2}{x_1p_2},$$
$$c_{23}=\frac{\mathbf{x}_2\cdot\mathbf{p}_1}{x_2p_1},\quad c_{24}=\frac{\mathbf{x}_2\cdot\mathbf{p}_2}{x_2p_2},\quad c_{34}=\frac{\mathbf{p}_1\cdot\mathbf{p}_2}{p_1p_2}\qquad(2.5'')$$

- The explicit form of $I_{1,2,3,4}$ and $I_{3,4}$ is given in (C1).

The $y\to c$ transformation (3.4) becomes in this case

$$y_{12}=\frac{(I_{3,4})^2c_{12}-c_{13}c_{32}-c_{14}c_{42}+c_{13}c_{34}c_{42}+c_{14}c_{43}c_{32}}{I_{1,3,4}I_{2,3,4}},\quad y_{13}=\frac{c_{13}-c_{14}c_{34}}{I_{1,4}I_{3,4}},$$
$$y_{14}=c_{14}\quad y_{23}=\frac{c_{23}-c_{24}c_{34}}{I_{2,4}I_{3,4}},\quad y_{24}=c_{24},\quad y_{34}=c_{34},\qquad(3.4a'')$$

and the inverse transformation $c\to y$ is, according to (C5c), given by

$$c_{12}=y_{12}\{\sqrt{1-(y_{13})^2}\sqrt{1-(y_{14})^2}\}\{\sqrt{1-(y_{23})^2}\sqrt{1-(y_{24})^2}\}$$
$$+\{y_{13}\sqrt{1-(y_{14})^2}\}\{y_{23}\sqrt{1-(y_{24})^2}\}+y_{14}y_{24},$$
$$c_{13}=y_{13}\sqrt{1-(y_{14})^2}\sqrt{1-(y_{34})^2}+y_{14}y_{34},\quad c_{14}=y_{14},$$
$$c_{23}=y_{23}\sqrt{1-(y_{24})^2}\sqrt{1-(y_{34})^2}+y_{24}y_{34},$$
$$c_{24}=y_{24},\quad c_{34}=y_{34}.\qquad(3.4b'')$$

The angular part of (3.1′′) now becomes

$$\frac{2^2\pi^{(2\nu-3)/2}\pi^{(2\nu-2)/2}}{\Gamma((2\nu-3)/2)\Gamma((2\nu-2)/2)}\int_{I^2>0}dc_{12}dc_{13}dc_{14}dc_{23}dc_{24}(c_{12})^{r_{12}}(c_{13})^{q_{13}}(c_{24})^{q_{24}}\frac{(I_{1,2,3,4})^{2\nu-5}}{(I_{3,4})^{2\nu-3}}$$
$$=\frac{2^2\pi^{(2\nu-3)/2}\pi^{(2\nu-2)/2}}{\Gamma((2\nu-3)/2)\Gamma((2\nu-2)/2)}\int_{-1}^{1}dy_{12}dy_{13}dy_{14}dy_{23}dy_{24}$$
$$\times\{\sqrt{1-(y_{12})^2}\sqrt{1-(y_{13})^2}(\sqrt{1-(y_{14})^2}\}^{2\nu-5}\{\sqrt{1-(y_{23})^2}\sqrt{1-(y_{24})^2}\}^{2\nu-4}$$

$$\times\{y_{12}\sqrt{1-(y_{13})^2}\sqrt{1-(y_{14})^2}\sqrt{1-(y_{23})^2}\sqrt{1-(y_{24})^2}+y_{13}\sqrt{1-(y_{14})^2}y_{23}\sqrt{1-(y_{24})^2}$$
$$+y_{14}y_{24}\}^{r_{12}}\{y_{13}\sqrt{1-(y_{14})^2}\sqrt{1-(y_{34})^2}+y_{14}y_{34}\}^{q_{13}}(y_{24})^{q_{24}}$$
$$=\frac{2^2\pi^{(2\nu-3)/2}\pi^{(2\nu-2)/2}}{\Gamma((2\nu-3)/2)\Gamma((2\nu-2)/2)}\sum_q{}'\frac{(r_{12})!}{q_{12}{}^2!q_{12}{}^3!q_{12}{}^4!}\frac{q_{13}!}{q_{13}{}^3!q_{13}{}^4!}\frac{q_{14}!}{q_{14}{}^4!}$$
$$\times\int_{-1}^{1}dy_{12}(y_{12})^{q_{12}{}^2}(\sqrt{1-(y_{12})^2})^{2\nu-5}\int_{-1}^{1}dy_{13}(y_{13})^{q_{12}{}^3+q_{13}{}^3}(\sqrt{1-(y_{13})^2})^{2\nu-4+q_{12}{}^2}$$
$$\times\int_{-1}^{1}dy_{14}(y_{14})^{q_{12}{}^4+q_{13}{}^4}(\sqrt{1-(y_{14})^2})^{2\nu-3+q_{12}{}^2+q_{12}{}^3+q_{13}{}^3}$$
$$\times\int_{-1}^{1}dy_{23}(y_{23})^{q_{12}{}^3}(\sqrt{1-(y_{23})^2})^{2\nu-4+q_{12}{}^2}$$
$$\times\int_{-1}^{1}dy_{24}(y_{24})^{q_{12}{}^4+q_{24}{}^4}(\sqrt{1-(y_{24})^2})^{2\nu-3+q_{12}{}^2+q_{12}{}^3}(y_{34})^{q_{13}{}^4}(\sqrt{(1-(y_{34})^2})^{q_{13}{}^3}. \tag{3.5''}$$

- The Σ' means that summation is under the subsidiary conditions

$$q_{12}{}^2+q_{12}{}^3+q_{12}{}^4=r_{12},$$
$$q_{13}{}^3+q_{13}{}^4=q_{13}, \tag{3.6''}$$
$$q_{14}{}^4=q_{14}.$$

Integration over y_{12}, y_{13}, y_{14}, y_{23}, and y_{24} yields Γ-functions, many of which cancel:

(3.5'')
$$=\frac{2^2\pi^{(2\nu-3)/2}\pi^{(2\nu-2)/2}\Gamma((2\nu-2+q_{12}{}^2)/2)}{\Gamma((2\nu-2)/2)}\sum_q{}''$$
$$\times\frac{\Gamma((1+q_{12}{}^2)/2)\Gamma((1+q_{12}{}^3+q_{13}{}^3/2)\Gamma((1+q_{12}{}^4+q_{13}{}^4)/2)\Gamma((1+q_{12}{}^3)/2)\Gamma((1+q_{12}{}^4+q_{24}{}^4)/2)}{\Gamma((2\nu+q_{12}{}^2+q_{12}{}^3+q_{13}{}^3+q_{12}{}^4+q_{13}{}^4)/2)\Gamma((2\nu+q_{12}{}^2+q_{12}{}^3+q_{12}{}^4+q_{24}{}^4)/2)}$$
$$\times(y_{34})^{q_{13}{}^4}(\sqrt{1-(y_{34})^2})^{q_{13}{}^3},$$

(3.7'')

if the arguments of all Γ-functions in the numerator are half integer, otherwise (3.5'')=0.

IV. SERIES EXPANSION; RADIAL PART

The radial part of (3.1) is transformed by insertion of expansion (A7) for k-functions with argument $x_1,x_2,\ldots,x_{f-2}$. Moreover, the integration variables x_i are transformed according to

$$\frac{x_i}{x_{i+1}}\to\xi_{i,i+1}(1\leqslant i\leqslant f-2),$$
$$x_{f-1}\to x. \tag{4.1}$$

The result is

$$\prod_{\substack{1\leqslant i\leqslant f-1\\ 1\leqslant i'<i\\ d}} \int_{0\leqslant x_1\leqslant x_2\leqslant\ldots\leqslant x_{f-1}\leqslant\infty} dx_i\; k^d_{i'i}(\beta+l+r;mx_i)k^d_{i,f}(\beta;mx_i)$$

$$\times x_i^{2\nu-1+\Sigma_{1\leqslant a\leqslant g}q_{i,f-1+a}+\sum_d{}^{1\leqslant a<i}r^d_{a,i}+\sum_d{}^{i<a\leqslant f-1}r^d_{i,a}+2\sum_d{}^{i<a\leqslant f-1}l^d_{i,a}}$$

$$=\sum_{k,u,w,\theta}\prod_{\substack{1\leqslant i\leqslant f-2\\ 1\leqslant i'<i\\ d}} K^{\theta^d}_{i',i}(b+l+r;k;u;w)K^{\theta^d}_{i,f}(b;k;u;w)\left(\frac{m^d_{i',i}}{2}\right)^{-2\theta^d_{i',i}(\beta^d_{i',i}+l^d_{i',i}+r^d_{i',i})+2k^d_{i',i}}\left(\frac{m^d_{i,f}}{2}\right)^{-2\theta^d_{i,f}\beta^d_{i,f}+2k^d_{i,f}}$$

$$\times\varepsilon^{w^d_{i',i}}\varepsilon^{w^d_{i,f}}\int_0^1 d\xi_{i,i+1}(\xi_{i,i+1})^{\Sigma_{1\leqslant a\leqslant i}N_a-1}\left\{2\ln\left(\frac{m^d_{i',i}\xi_{i,i+1}\xi_{i+1,i+2}\cdots\xi_{f-2,f-1}x}{2}\right)\right\}^{u^d_{i',i}}$$

$$\times\left\{2\ln\left(\frac{m^d_{i,f}\xi_{i,i+1}\xi_{i+1,i+2}\cdots\xi_{f-2,f-1}x}{2}\right)\right\}^{u^d_{i,f}}$$

$$\times\int_0^\infty dx\, x^{2\nu-1+\Sigma_{1\leqslant a\leqslant g}q_{f-1,f-1+a}+\sum_d{}^{1\leqslant a<f-1}r^d_{a,f-1}+\Sigma_{1\leqslant a\leqslant f-2}N_a}$$

$$\times k^d_{i,f-1}(\beta+l+r;mx)k^d_{f-1,f}(\beta;mx), \tag{4.2}$$

with the obvious notation of (2.8):

$$K^{\theta^d}_{i,f}(b;k;u;w)=K^{\theta}(b^d_{i,f};k^d_{i,f};u^d_{i,f};w^d_{i,f}),$$
$$K^{\theta^d}_{i',i}(b+l+r;k;u;w)=K^{\theta}(b^d_{i',i}+l^d_{i',i}+r^d_{i',i};k^d_{i',i};u^d_{i',i};w^d_{i',i}), \tag{4.3}$$

and with

$$N_i=2\nu+\sum_{1\leqslant a\leqslant g}q_{i,f-1+a}-2\sum_{\substack{1\leqslant a<i\\ d}}\theta^d_{a,i}(\beta^d_{a,i}+l^d_{a,i}+r^d_{a,i})-2\sum_d\theta^d_{i,f}\beta^d_{i,f}$$
$$+2\sum_{\substack{1\leqslant a<i\\ d}}k^d_{a,i}+2\sum_d k^d_{i,f}+2\sum_{\substack{i<a\leqslant f-1\\ d}}l^d_{i,a}+\sum_{\substack{1\leqslant a<i\\ d}}r^d_{a,i}+\sum_{\substack{i<a\leqslant f-1\\ d}}r^d_{i,a}. \tag{4.4}$$

The range of the summation variables is given in (A7): the θ's assume values $\theta=0$ and $\theta=1$; $k_{i',i}$ runs from 0 to ∞ if $\theta=0$ and from 0 to $b_{i',i}+l_{i',i}+r_{i',i}-1$ if $\theta=1$; $k_{i,f}$ runs from 0 to ∞ if $\theta=0$ and from 0 to $b-1$ if $\theta=1$; u runs from 0 to $w+1$ if $\theta=0$ and it takes only the value 0 if $\theta=1$; w runs from 0 to ∞.

The x-integral in (4.2) is split into two parts:

$$\int_0^\infty dx=\int_0^{1/M}dx+\int_{1/M}^\infty dx. \tag{4.5}$$

The ξ-integrations and the ${}_0\int^{1/M}dx$-integration are performed by (D2) and the result is

$$
\begin{aligned}
(4.2)=&\sum_{k,u,w,\theta}\left(\frac{1}{M}\right)^{2\nu(f-l)+\sum_{l\leqslant b\leqslant g}^{1\leqslant a\leqslant f-1}q_{a,f-1+b}+2\sum_{1\leqslant a'\leqslant a\leqslant f-1}l^d_{a',a}+2\sum_{1\leqslant a'<a\leqslant f-1}r^d_{a',a}}\\
&\times\prod_{\substack{1\leqslant i\leqslant i''\leqslant f-1\\ 1\leqslant i'<i\\ d}}K^{\theta^d}_{i',i}(b+l+r;k;u;w)K^{\theta^d}_{i,f}(b;k;u;w)\\
&\times\frac{(-)^{u^d_{i',i}\,i''+u^d_{i,f}\,i''}2^{u^d_{i',i}+u^d_{i,f}}u^d_{i',i}!u^d_{i,f}!(\sum_d{}^{1\leqslant a'<a\leqslant i}u^d_{a',a}{}^i+\sum_d{}^{1\leqslant a\leqslant i}u^d_{a,f}{}^i)!}{(u^d_{i',i}-\Sigma_{i\leqslant c\leqslant f-1}u^d_{i',i}{}^c)!(u^d_{i,f}-\Sigma_{i\leqslant c\leqslant f-1}u^d_{i,f}{}^c)!u^d_{i',i}{}^{i''}!u^d_{i,f}{}^{i''}!(\Sigma_{1\leqslant a\leqslant i}N_a)^{1+\Sigma_d^{1\leqslant a'<a\leqslant i}u^d_{a',a}{}^i+\Sigma_d^{1\leqslant a\leqslant i}u^d_{a,f}{}^i}}\\
&\times\left(\frac{m^d_{i',i}}{2M}\right)^{-2\theta^d_{i',i}(\beta^d_{i',i}+l^d_{i',i}+r^d_{i',i})+2k^d_{i',i}}\left(\frac{m^d_{i,f}}{2M}\right)^{-2\theta^d_{i,f}\beta^d_{i,f}+2k^d_{i,f}}\left\{\ln\left(\frac{m^d_{i',i}}{M}\right)\right\}^{u^d_{i',i}-\sum_{i\leqslant c\leqslant f-1}u^d_{i',i}{}^c}\left\{\ln\left(\frac{m^d_{i,f}}{M}\right)\right\}^{u^d_{i,f}-\sum_{i\leqslant c\leqslant f-1}u^d_{i,f}{}^c}\\
&\times\varepsilon^{w^d_{i',i}+w^d_{i,f}}+\sum_{k,u,w,\theta}\prod_{\substack{1\leqslant i\leqslant i''\leqslant f-2\\ 1\leqslant i'<i\\ d}}K^{\theta^d}_{i',i}(b+l+r;k;u;w)K^{\theta^d}_{i,f}(b;k;u;w)\\
&\times\frac{(-)^{u^d_{i',i}\,i''+u^d_{i,f}\,i''}2^{u^d_{i',i}+u^d_{i,f}}u^d_{i',i}!u^d_{i,f}!(\sum_d{}^{1\leqslant a'<a\leqslant i}u^d_{a',a}{}^i+\sum_d{}^{1\leqslant a\leqslant i}u^d_{a,f}{}^i)!}{(u^d_{i',i}-\Sigma_{i\leqslant c\leqslant f-2}u^d_{i',i}{}^c)!(u^d_{i,f}-\Sigma_{i\leqslant c\leqslant f-2}u^d_{i,f}{}^c)!u^d_{i',i}{}^{i''}!u^d_{i,f}{}^{i''}!(\Sigma_{1\leqslant a\leqslant i}N_a)^{1+\Sigma_d^{1\leqslant a'<a\leqslant i}u^d_{a',a}{}^i+\Sigma_d^{1\leqslant a\leqslant i}u^d_{a,f}{}^i}}\\
&\times\left(\frac{m^d_{i',i}}{2}\right)^{-2\theta^d_{i',i}(\beta^d_{i',i}+l^d_{i',i}+r^d_{i',i})+2k^d_{i',i}}\left(\frac{m^d_{i,f}}{2}\right)^{-2\theta^d_{i,f}\beta^d_{i,f}+2k^d_{i,f}}\varepsilon^{w^d_{i',i}+w^d_{i,f}}\\
&\times\int_{1/M}^{\infty}dx\,x^{2\nu-1+\Sigma_{1\leqslant a\leqslant g}q_{f-1,f-1+a}+\sum_d^{1\leqslant a\leqslant f-2}r^d_{a,f-1}+\Sigma_{1\leqslant a\leqslant f-2}N_a}\\
&\times\{\ln(m^d_{i',i}x)\}^{u^d_{i',i}-\Sigma_{i\leqslant c\leqslant f-2}u^d_{i',i}{}^c}\{\ln(m^d_{i,f}x)\}^{u^d_{i,f}-\Sigma_{i\leqslant c\leqslant f-2}u^d_{i,f}{}^c}k^d_{i,f-1}(\beta+l+r;mx)k^d_{f-1,f}(\beta;mx).
\end{aligned}
\tag{4.6}
$$

- The superscript c of $u^d_{a,b}{}^c$ appears because of a repeated integral (D2) over logarithms. It runs from b to $f-1$.
- In the ${}_0\int^{1/M}$-term of (4.6) the index f is treated differently from the other ones because of the special position of $\mathbf{x}_f$, right from the beginning.
- In the ${}_{1/M}\int^{\infty}$-term of (4.6), the index $f-1$ is treated differently as well, as the x_{f-1}-integration is the last one.

The general Feynman diagram is given by summation over all variables of a product of (3.7), (4.6) and some factors:

$$
\begin{aligned}
(3.1)=&\frac{1}{(2\pi)^{2\nu(f-1)}}\sum_{l,q,r}\prod_{\substack{1\leqslant i\leqslant f-1\\ 1\leqslant i'<i\\ 1\leqslant j\leqslant g\\ d}}(-)^{l^d_{i',i}}\left(\frac{1}{2}\right)^{2l^d_{i',i}+r^d_{i',i}}(ip_j)^{\Sigma_{1\leqslant a\leqslant f-1}q_{a,f-1+j}}\\
&\times\frac{1}{l^d_{i',i}!q_{i,f-1+j}!r^d_{i',i}!}\left\{\frac{2\pi^\nu(m^d_{i,f})^{2\beta^d_{i,f}}}{\Gamma(a^d_{i,f})}\right\}\left\{\frac{2\pi^\nu(m^d_{i',i})^{2\beta^d_{i',i}+2l^d_{i',i}+2r^d_{i',i}}}{\Gamma(a^d_{i',i})}\right\}\cdot(3.7)\cdot(4.6).
\end{aligned}
\tag{4.7}
$$

This formula may look frightening but it has to be compared with (B4), which is the general integration parameter expression. The latter might look nicer, but the integrations are mostly divergent.

On the other hand, the infinities are honestly visible in (4.6), as will be discussed in the next section. The price for it is summation variables with three or four indices. We think this price is worth paying.

The ${}_{1/M}\int^{\infty} dx$-integration may be computed numerically after insertion of the asymptotic series (A11). The splitting point $1/M$ is arbitrary and may be determined by the accuracy of the calculations.

If all u's are 0, which may happen in the limit $\varepsilon \to 0$, the logarithmic factors in the integrand disappear and the integral is recognized as the finite part of a two vertex diagram with a number of internal lines, like (3.1′). It is named ''sunset diagram,'' ''sunrise diagram'' or ''water melon diagram.'' Several authors[6–23] derived relations in order to simplify the numerical calculations in practice. Most of these authors make use of Feynman parameters which, according to the formalism of Appendix B, are correcting for a first approximation of the propagator by a Gaussian curve

$$\int d\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}} \frac{1}{(\mathbf{k}^2+m^2)^{\alpha}} \to \frac{2\pi^{\nu}(4\pi)^{\nu} m^{2\beta}}{\Gamma(\alpha)} e^{-m^2\mathbf{x}^2}. \tag{4.8}$$

Our approach starts from the propagator

$$\int d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{x}} \frac{1}{(\mathbf{k}^2+m^2)^{\alpha}} \to \frac{\pi^{\nu+1/2} 2^{\beta+1/2}}{\Gamma(\alpha)} m^{2\beta} \frac{e^{-mx}}{(mx)^{\beta+(1/2)}}, \tag{4.9}$$

which is a better first approximation at high mx. For this reason, we have good hope for better numerical results.

The formalism of this section will be elucidated by applying the derivation line (4.1)–(4.6) on our two examples.

No (4.1)-like transformation is needed for the radial part of (2.6′), the x-variable being the only one. It becomes

$$\begin{aligned}
&\int_0^{\infty} dx\, x^{2\nu-1+q_{12}} k^1(\beta;mx) k^2(\beta;mx) k^3(\beta;mx) \\
&\quad = \int_0^{1/M} dx\, x^{2\nu-1+q_{12}} k^1(\beta;mx) k^2(\beta;mx) k^3(\beta;mx) \\
&\qquad + \int_{1/M}^{\infty} dx\, x^{2\nu-1+q_{12}} k^1(\beta;mx) k^2(\beta;mx) k^3(\beta;mx).
\end{aligned} \tag{4.5′}$$

Since the θ's may assume two values, the first part of (4.5′) consists of eight subseries:

$$\begin{aligned}
&\int_0^{1/M} dx\, x^{2\nu-1+q_{12}} k^1(\beta;mx) k^2(\beta;mx) k^3(\beta;mx) \\
&\quad = \sum_{k,u,w,\theta} K^{\theta^1}(b;k;u;w) K^{\theta^2}(b;k;u;w) K^{\theta^3}(b;k;u;w) \\
&\qquad \times \left(\frac{m^1}{2}\right)^{-2\theta^1\beta^1+2k^1} \left(\frac{m^2}{2}\right)^{-2\theta^2\beta^2+2k^2} \left(\frac{m^3}{2}\right)^{-2\theta^3\beta^3+2k^2} \varepsilon^{w^1+w^2+w^3} \\
&\qquad \times \int_0^{1/M} dx\, x^{2\nu-1+q_{12}-2\theta^1\beta^1-2\theta^2\beta^2-2\theta^3\beta^3+2k^1+2k^2+2k^3} \\
&\qquad \times \left\{2\ln\left(\frac{m^1 x}{2}\right)\right\}^{u^1} \left\{2\ln\left(\frac{m^2 x}{2}\right)\right\}^{u^2} \left\{2\ln\left(\frac{m^3 x}{2}\right)\right\}^{u^3}.
\end{aligned}$$

Using (D1) we find

$$
\begin{aligned}
(4.5')=&\left(\frac{1}{M}\right)^{2\nu+q_{12}}\sum_{k,u,w}K^{0^1}(b;k;u;w)K^{0^2}(b;k;u;w)K^{0^3}(b;k;u;w)\\
&\times\frac{(-)^{u^{1,1}+u^{2,1}+u^{3,1}}2^{u^1+u^2+u^3}(u^{1,1}+u^{2,1}+u^{3,1})!}{(n+2\varepsilon+q_{12}+2k^1+2k^2+2k^3)^{1+u^{1,1}+u^{2,1}+u^{3,1}}}\\
&\times\frac{u^1!}{(u^1-u^{1,1})!u^{1,1}!}\,\frac{u^2!}{(u^2-u^{2,1})!u^{2,1}!}\,\frac{u^3!}{(u^3-u^{3,1})!u^{3,1}!}\\
&\times\left\{\ln\left(\frac{m_1}{M}\right)\right\}^{u^1-u^{1,1}}\left\{\ln\left(\frac{m_2}{M}\right)\right\}^{u^2-u^{2,1}}\left\{\ln\left(\frac{m_3}{M}\right)\right\}^{u^3-u^{3,1}}\left(\frac{m^1}{2M}\right)^{2k^1}\left(\frac{m^2}{2M}\right)^{2k^2}\left(\frac{m^3}{2M}\right)^{2k^3}\\
&\times\varepsilon^{w^1+w^2+w^3}+\left(\frac{1}{M}\right)^{2\nu+q_{12}}\sum_{k,u,w}K^{0^1}(b;k;u;w)K^{0^2}(b;k;u;w)K^{1^3}(b;k;0;w)\\
&\times\frac{(-)^{u^{1,1}+u^{2,1}}2^{u^1+u^2}(u^{1,1}+u^{2,1})!}{(2a^3+q_{12}+2k^1+2k^2+2k^3)^{1+u^{1,1}+u^{2,1}+u^{3,1}}}\,\frac{u^1!}{(u^1-u^{1,1})!u^{1,1}!}\,\frac{u^2!}{(u^2-u^{2,1})!u^{2,1}!}\\
&\times\left\{\ln\left(\frac{m_1}{M}\right)\right\}^{u^1-u^{1,1}}\left\{\ln\left(\frac{m_2}{M}\right)\right\}^{u^2-u^{2,1}}\left(\frac{m^1}{2M}\right)^{2k^1}\left(\frac{m^2}{2M}\right)^{2k^2}\left(\frac{m^3}{2M}\right)^{-2\beta^3+2k^2}\varepsilon^{w^1+w^2+w^3}\\
&+2\text{ permutations}+\left(\frac{1}{M}\right)^{2\nu+q_{12}}\sum_{k,u,w}K^{0^1}(b;k;u;w)K^{1^2}(b;k;0;w)K^{1^3}(b;k;0;w)\\
&\times\frac{(-)^{u^{1,1}}2^{u^1}(u^{1,1})!}{(2a^2+2a^3-n-2\varepsilon+q_{12}+2k^1+2k^2+2k^3)^{1+u^{1,1}}}\,\frac{u^1!}{(u^1-u^{1,1})!u^{1,1}!}\\
&\times\left\{\ln\left(\frac{m_1}{M}\right)\right\}^{u^1-u^{1,1}}\left(\frac{m^1}{2M}\right)^{2k^1}\left(\frac{m^2}{2M}\right)^{-2\beta^2+2k^2}\left(\frac{m^3}{2M}\right)^{-2\beta^3+2k^3}\varepsilon^{w^1+w^2+w^3}+2\text{ permutations}\\
&+\left(\frac{1}{M}\right)^{\nu+2q_{12}}\sum_{k,u,w}K^{1^1}(b;k;0;w)K^{1^2}(b;k;0;w)K^{1^3}(b;k;0;w)\\
&\times\frac{1}{(2a^1+2a^2+2a^3-2n-4\varepsilon+q_{12}+2k^1+2k^2+2k^3)}\left(\frac{m^1}{2M}\right)^{-2\beta^1+2k^1}\left(\frac{m^2}{2M}\right)^{-2\beta^2+2k^2}\\
&\times\left(\frac{m^3}{2M}\right)^{-2\beta^3+2k^3}\varepsilon^{w^1+w^2+w^3}+\int_{1/M}^{\infty}dx\,x^{2\nu-1+q_{12}}k^1(\beta;mx)k^2(\beta;mx)k^3(\beta;mx). \qquad (4.6')
\end{aligned}
$$

This formula, which still has to be multiplied by (3.7′), may be compared with the Feynman parameter representation (1.8′). The hidden divergences of (1.8′) are manifest via the ε's of (4.6′).

Indeed, it is seen from this formula that in four dimensional space–time ($n=4$) and in the limit $\varepsilon\to 0$

(i) the 0,0,0 subseries is finite;
(ii) the three 0,0,1 subseries too are finite;
(iii) the three 0,1,1 subseries have single poles and double poles for some values of the summation variables, as $u=0$ or $u=1$; and
(iv) the 1,1,1 subseries has a single pole for some values of the summation variables.

The radial part of our second example is obtained from (3.1′′). The radial integration variables are transformed according to

$$\frac{x_1}{x_2}\to\xi_{12},\qquad x_2\to x. \tag{4.1''}$$

After insertion of (A7)

$$\begin{aligned}&\int_{0\leqslant x_1\leqslant x_2\leqslant\infty} dx_1dx_2\,x_1^{2\nu-1+q_{13}+r_{12}+2l_{12}}x_2^{2\nu-1+q_{24}+r_{12}}\\&\quad\times k_{13}^1(\beta;x_1)k_{13}^2(\beta;mx_1)k_{23}^1(\beta;mx_2)k_{23}^2(\beta;mx_2)k_{12}(\beta+l+r;mx_2)\\&\quad=K_{13}^{\theta^1}(b;k;u;w)K_{13}^{\theta^2}(b;k;u;w)\\&\qquad\times\left(\frac{m_{13}^1}{2}\right)^{-2\theta'_{13}\beta'_{13}+2k_{13}^1}\left(\frac{m_{13}^2}{2}\right)^{-2\theta_{13}^2\beta_{13}^2+2k_{13}^2}\varepsilon^{w_{13}^1+w_{13}^2}\int_0^1 d\xi_{12}(\xi_{12})^{N_1-1}\left\{2\ln\left(\frac{m_{13}^1\xi_{12}}{2}\right)\right\}^{u_{13}^1}\\&\qquad\times\left\{2\ln\left(\frac{m_{13}^2\xi_{12}}{2}\right)\right\}^{u_{13}^2}\int_0^\infty dx\,x^{2\nu-1+q_{24}+r_{12}+N_1}k_{23}^1(\beta;mx)k_{23}^2(\beta;mx)k_{12}(\beta+l+r;mx),\end{aligned} \tag{4.2''}$$

with

$$N_1=2\nu+q_{13}-2\theta_{13}^1\beta_{13}^1-2\theta_{13}^2\beta_{13}^2+2k_{13}^1+2k_{13}^2+2l_{12}+r_{12} \tag{4.4''}$$

is obtained.

The x-integration has to be split as in (4.5′). The $\int d\xi_{12}$-integration and the ${}_0\int^{1/M}dx$-integration are done as in (4.6′) yielding 32 terms and a ${}_{1/M}\int^{\infty}dx$-integration which has to be done numerically after introduction of (A11).

Conclusion of this section and the previous one: (2.6) leads to the series expansion (3.1). Expansion with respect to external momenta, internal masses, their logarithms and the regularization parameter ε is obtained via an angular part given by (3.7) and a radial part given by (4.6) and (4.4).

V. DIVERGENCES AND THEIR UNRAVELMENT

The UV divergences of momentum space appear in **x**-space by integration in area's where the arguments of a number of the functions $k(\beta;mx)$ are zero.

Two or more of the θ's in (4.4) may assume the value 1 and, consequently, there are values of the summation variables for which

$$\sum_{1\leqslant a\leqslant i} N_a\approx\varepsilon. \tag{5.1}$$

Factor (5.1) appears after integration over x_i in the neighborhood of 0 as a factor

$$\left(\sum_{1\leqslant a\leqslant i} N_a\right)^{1+\sum\limits_{\substack{1\leqslant a'<a\leqslant i\\ d}} u_{a',a}^{d\ i}+\sum\limits_{\substack{1\leqslant a\leqslant i\\ d}} u_{a,f}^{d\ i}}$$

in the denominator and so it may lead to multiple poles at $\varepsilon=0$. The residue of such a pole at $\varepsilon=0$ is a series that is obtained by summation over the remaining variables. In the limit $\varepsilon\to0$, this subseries is recognized as a subdiagram.

All these are divergences caused by $k(\beta;m)$'s with a simple argument. If integration over nonsimple arguments does not produce infinities, the expressions of the previous sections are correct.

If $k(\beta;m)$'s with nonsimple argument do lead to infinity after integration, it will manifest by divergence of the summations over $l^d_{a,b}$ and $r^d_{a,b}$ in (3.1).

In (2.1), it is integrated over $f-1$ $\mathbf{x}$-variables and $f-1$ momenta appear in the integrand. The momentum $\mathbf{p}_f$ is not present manifestly, but is given by (1.6). Due to this momentum conservation, there is a freedom in the choice of the "dead integration variable" x_f. Translations of the kind

$$\mathbf{x}_i \to \mathbf{x}_i + \sum_{a<i} e_{a,i}\mathbf{x}_a + \sum_{b>i} e_{i,b}\mathbf{x}_b\,. \tag{5.2}$$

are allowed.

The elements of the matrix e may be chosen in such a way that any other set of $f-1$ independent arguments is made simple. The elements of e are 0 or 1 and the exponential part of (2.1) is transformed by (5.2) as

$$\sum_a \mathbf{p}_a\cdot\mathbf{x}_a \to \sum_{a,b} (e^T_{a,b}\mathbf{p}_b)\cdot\mathbf{x}_a\,, \tag{5.3}$$

where e^T is the transponed of matrix e.

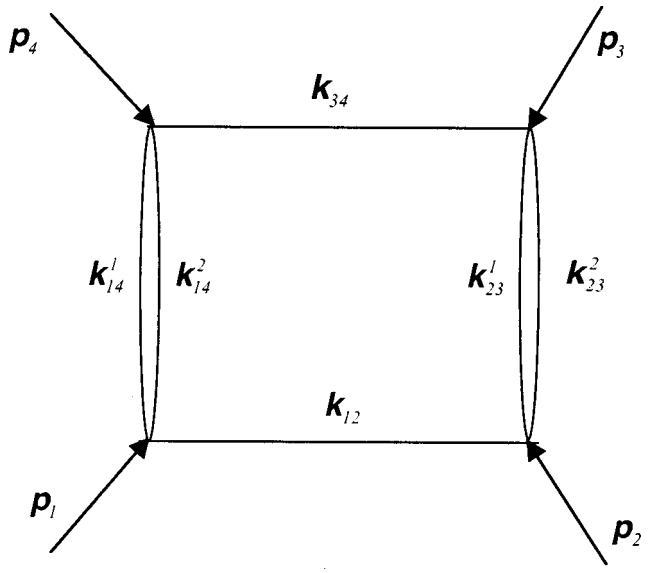
In the given examples, this freedom has been used in order to put all divergences into the integrations over simple arguments.

In the integral (2.1′) of the example of Fig. 1 there is nothing to be transformed, but the integral of (2.1′′) of the second example may be written in three forms:

$$\begin{aligned}
&\int d\mathbf{x}_1 d\mathbf{x}_2 e^{i\mathbf{p}_1\cdot\mathbf{x}_1} e^{i\mathbf{p}_2\cdot\mathbf{x}_2} k^1_{13}(b;mx_1)k^2_{13}(b;mx_1)k^1_{23}(b;mx_2)k^2_{23}(b;mx_2)k_{12}(b;m|\mathbf{x}_1-\mathbf{x}_2|)\\
&\quad=\int d\mathbf{x}_1 d\mathbf{x}_2 e^{i\mathbf{p}_1\cdot\mathbf{x}_1} e^{i(\mathbf{p}_1+\mathbf{p}_2)\cdot\mathbf{x}_2} k^1_{13}(b;m|\mathbf{x}_1+\mathbf{x}_2|)k^2_{13}(b;m|\mathbf{x}_1+\mathbf{x}_2|)\\
&\qquad\times k^1_{23}(b;mx_2)k^2_{23}(b;mx_2)k_{12}(b;mx_1)\\
&\quad=\int d\mathbf{x}_1 d\mathbf{x}_2 e^{i(\mathbf{p}_1+\mathbf{p}_2)\cdot\mathbf{x}_1} e^{i\mathbf{p}_2\cdot\mathbf{x}_2} k^1_{13}(b;mx_1)k^2_{13}(b;mx_1)k^1_{23}(b;m|\mathbf{x}_1+\mathbf{x}_2|)\\
&\qquad\times k^2_{23}(b;m|\mathbf{x}_1+\mathbf{x}_2|)k_{12}(b;mx_2).
\end{aligned} \tag{5.4}$$

Only the first integral of (5.4) satisfies the criterium that all multiple internal lines are represented

by a k-function with simple argument. In a diagram like



there are 16 integral representations where three independent internal lines are made simple. We give five of them:

$$
\begin{aligned}
&\int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 e^{i\mathbf{p}_1\cdot\mathbf{x}_1} e^{i\mathbf{p}_2\cdot\mathbf{x}_2} e^{i\mathbf{p}_3\cdot\mathbf{x}_3} k^1_{14}(\beta;mx_1) k^2_{14}(\beta;mx_1) k_{12}(\beta;m|\mathbf{x}_1-\mathbf{x}_2|)\\
&\quad\times k^1_{23}(\beta;m|\mathbf{x}_2-\mathbf{x}_3|) k^2_{23}(\beta;m|\mathbf{x}_2-\mathbf{x}_3|) k_{34}(\beta;mx_3)\\
&\quad= \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 e^{i\mathbf{p}_1\cdot\mathbf{x}_1} e^{i\mathbf{p}_2\cdot\mathbf{x}_2} e^{i(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3)\cdot\mathbf{x}_3} k^1_{14}(\beta;m|\mathbf{x}_1+\mathbf{x}_3|) k^2_{14}(\beta;m|\mathbf{x}_1+\mathbf{x}_3|)\\
&\qquad\times k_{12}(\beta;m|\mathbf{x}_1-\mathbf{x}_2|) k^1_{23}(\beta;mx_2|) k^2_{23}(\beta;mx_2|) k_{34}(\beta;mx_3)\\
&\quad= \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 e^{i\mathbf{p}_1\cdot\mathbf{x}_1} e^{i(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3)\cdot\mathbf{x}_2} e^{i\mathbf{p}_3\cdot\mathbf{x}_3} k^1_{14}(\beta;m|\mathbf{x}_1+\mathbf{x}_2|) k^2_{14}(\beta;m|\mathbf{x}_1+\mathbf{x}_2|)\\
&\qquad\times k_{12}(\beta;mx_1) k^1_{23}(\beta;mx_3|) k^2_{23}(\beta;mx_3) k_{34}(\beta;m|\mathbf{x}_2+\mathbf{x}_3|)\\
&\quad= \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 e^{i(\mathbf{p}_2+\mathbf{p}_2+\mathbf{p}_3)\cdot\mathbf{x}_2} e^{i\mathbf{p}_2\cdot\mathbf{x}_2} e^{i\mathbf{p}_3\cdot\mathbf{x}_3} k^1_{14}(\beta;mx_1|) k^2_{14}(\beta;mx_1) k_{12}(\beta;mx_2)\\
&\qquad\times k^1_{23}(\beta;m|\mathbf{x}_2-\mathbf{x}_3|) k^2_{23}(\beta;m|\mathbf{x}_2-\mathbf{x}_3|) k_{34}(\beta;m|\mathbf{x}_1+\mathbf{x}_3|)\\
&\quad= \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 e^{i\mathbf{p}_1\cdot\mathbf{x}_1} e^{i(\mathbf{p}_2+\mathbf{p}_3)\cdot\mathbf{x}_2} e^{i\mathbf{p}_3\cdot\mathbf{x}_3} k^1_{14}(\beta;mx_1) k^2_{14}(\beta;mx_1)\\
&\qquad\times k_{12}(\beta;m|\mathbf{x}_1-\mathbf{x}_2|) k^1_{23}(\beta;mx_3) k^2_{23}(\beta;mx_3|) k_{34}(\beta;m|\mathbf{x}_2+\mathbf{x}_3|). \qquad (5.5)
\end{aligned}
$$

Only the last integral satisfies the criterium that all double lines are represented by a k-function with simple argument.

However, at least in theory, there are diagrams where not all multiple lines can be made simple. For instance, if the vertices 1 and 2 of Fig. 2 would have been double connected as well, or Fig. 3 with all vertices double connected. In such cases a more delicate procedure is required.

In order to avoid zeroes of nonsimple arguments, the integration region in (3.1) is restricted to a subregion where simple arguments are smaller than the arguments that depend on them:

$$\begin{gathered} x_1 \leqslant x_2 \leqslant |\mathbf{x}_2 - \mathbf{x}_1|, \\ x_1 \leqslant x_3 \leqslant |\mathbf{x}_3 - \mathbf{x}_1|, \\ x_2 \leqslant x_3 \leqslant |\mathbf{x}_3 - \mathbf{x}_2| \\ \text{etc.} \end{gathered} \tag{5.6}$$

In terms of angles, (5.6) means that the integration is bounded by the conditions

$$\begin{gathered} x_1 \leqslant x_2 \leqslant x_3 \leqslant \cdots \leqslant x_{f-1}, \\ c_{12} \leqslant \tfrac{1}{2}\xi_{12}, \\ c_{13} \leqslant \tfrac{1}{2}\xi_{13}, \\ c_{23} \leqslant \tfrac{1}{2}\xi_{23}, \\ \text{etc.} \end{gathered} \tag{5.7}$$

with

$$\xi_{ij} = \frac{x_i}{x_j}. \tag{5.8}$$

In this way, the integration region is restricted to truncated parallelopipida. Since nonsimple arguments $|\mathbf{x}_a - \mathbf{x}_b|$ are zero only in the region where both $x_a = x_b$ and $c_{ab} = 1$, it is clear from (5.7) that dangerous regions are avoided.

Transformations like (3.4) are not useful anymore, because of the restriction conditions. Instead, the angular integrals of (3.1) in the region restricted by (5.7) are expanded directly with respect to $\xi_{a,b}$:

$$\begin{aligned} &\prod_{\substack{1 \leqslant i' < i \leqslant f=1 \\ 1 \leqslant j \leqslant g}} \int_{\substack{I^2>0 \\ c_{i',i} < 1/2\, \xi_{i',i}}} dc_{i',i} dc_{i,f-1+j} \{ (c_{i',i})^{\Sigma_d r^d_{i',i}} (c_{i,f-1+j})^{q_{i,f-1+j}} (I_{1,2,\ldots,f-1+g})^{2\nu-f-g} \} \\ &\quad = \sum_{i_{a,b}=0}^{\infty} I\left(\sum_d r^d_{a,b}; q_{a,f-1+b}; i_{a,b} \right) \frac{\left(\frac{1}{2}\xi_{1,2} \right)^{i_{1,2}}}{i_{1,2}!} \cdots \frac{\left(\frac{1}{2}\xi_{f-2,f-1} \right)^{i_{f-2,f-1}}}{i_{f-2,f-1}!}, \end{aligned} \tag{5.9}$$

where

$$\begin{aligned} &I\left(\sum_d r^d_{a,b}; q_{a,f-1+b}; i_{a,b} \right) \\ &\quad = \prod_{\substack{1 \leqslant i' < i \leqslant f-1 \\ 1 \leqslant j \leqslant g}} \int_{I^2>0} dc_{i,f-1+j} (c_{i,f-1+j})^{q_{i,f-1+j}} \\ &\qquad \times \left[(\partial_{c_{i',i}})^{i_{i',i}-1} \left\{ \prod_{1 \leqslant k' < k \leqslant f-1} (c_{k',k})^{\Sigma_d r^d_{k',k}} (I_{1,2,\ldots,f-1+g})^{2\nu-f-g} \right\} \right]_{c_{12}=c_{13}=\cdots=c_{f-2,f-1}=0}. \end{aligned} \tag{5.10}$$

The symbolical notations

$$[\partial^{-1}_{c_{i',i}} F(c_{i',i})]_{c_{i',i}=0} \equiv \int_{c_{i',i}\leqslant 0} dc_{i',i} F(c_{i',i})$$

and

$$[\partial^{0}_{c_{i',i}} F(c_{i',i})]_{c_{i',i}=0} \equiv F(0) \tag{5.11}$$

have been used. The coefficients $I(\Sigma_d {r^d}_{a,b}; q_{a,f-1+b}; i_{a,b})$ have to be computed numerically if at least one $i_{a,b}$ is zero; in all other cases they are obtained analytically.

According to (5.9), the angular integrations in the restricted area produce factors

$$(\xi_{a,b})^{i_{a,b}}.$$

These factors have to be joined to the radial part. This radial part in the truncated area now is given by (4.6) with additional summation variables $i_{i,a}$ in N_i:

$$N_i = 2\nu + \sum_{1\leqslant a\leqslant g} q_{i,f-1+a} - 2\sum_{\substack{1\leqslant a<i \\ d}} \theta^d_{a,i}(\beta^d_{a,i} + l^d_{a,i} + r^d_{a,i}) - 2\sum_d \theta^d_{i,f}\beta^d_{i,f} + 2\sum_{\substack{1\leqslant a<i \\ d}} k^d_{a,i}$$

$$+ 2\sum_d k^d_{i,f} + 2\sum_{\substack{i<a\leqslant f-1 \\ d}} l^d_{i,a} + \sum_{\substack{1\leqslant a<i \\ d}} r^d_{a,i} + \sum_{\substack{i<a\leqslant f-1 \\ d}} r^d_{i,a} + \sum_{i<a\leqslant f-1} i_{i,a}\,. \tag{5.12}$$

Conclusion of this section: Feynman diagrams in the area restricted by (5.7) may be written as an expansion (3.1); the angular part is given by (5.9)–(5.11) and the radial part is given by (4.6) and (5.12).

Finally, all possible translations (5.2) producing a set of $f-1$ independent simple arguments have to be carried out and corresponding series expansions similar to (3.1) have to be summed. In this way, integration over all space is obtained and all UV infinities are manifestly present through a factor

$$\prod_{1\leqslant i\leqslant f-1} \left(\sum_{1\leqslant a\leqslant i} N_a \right)^{1+\Sigma_d^{1\leqslant a'<a\leqslant i} u^d_{a',a} \; i \; + \Sigma_d^{1\leqslant a\leqslant i} u^d_{a,f} \; i}$$

in the denominator.

APPENDIX A

Most of the formulas of this appendix are found in the textbook by Watson[5] for the functions $K_\beta(mx)$. Because of practical reasons, functions $k(\beta;mx)$ have been introduced in this article. They differ by a factor $(mx/2)^\beta$:

$$k(\beta;mx) = \left(\frac{mx}{2}\right)^{-\beta} K_\beta(mx). \tag{A1}$$

Series expansion of $k(\beta;mx)$ is given by

$$k(\beta;mx) = \frac{1}{2}\sum_{k=0}^{\infty} \frac{(-)^k}{k!} \left\{ \Gamma(-\beta-k)\left(\frac{mx}{2}\right)^{2k} + \Gamma(\beta-k)\left(\frac{mx}{2}\right)^{-2\beta+2k} \right\}. \tag{A2}$$

The Γ-functions are infinite, when their argument is zero or a negative integer, but these infinities cancel, as may be seen after translation of the summation variable k in the second part of (A2). In this way, $k(\beta;mx)$ is split into two parts:

$$k(\beta;mx)=k^0(\beta;mx)+k^1(\beta;mx), \tag{A3}$$

where

$$k^0(\beta;mx)=\frac{(-)^b\pi}{2\sin(\pi\varepsilon)}\sum_{k=0}^{\infty}\left\{\frac{1}{\Gamma(1+k-\varepsilon)(b+k)!}\left(\frac{mx}{2}\right)^{2k-2\varepsilon}-\frac{1}{k!\Gamma(1+\varepsilon+b+k)}\left(\frac{mx}{2}\right)^{2k}\right\} \tag{A4a}$$

and

$$k^1(\beta;mx)=\frac{1}{2}\sum_{k=0}^{b-1}\frac{(-)^k}{k!}\Gamma(b+\varepsilon-k)\left(\frac{mx}{2}\right)^{-2\beta+2k}, \tag{A4b}$$

with

$$\varepsilon=\nu-\tfrac{1}{2}n=\beta-b. \tag{A5}$$

Expansion with respect to $(mx/2)$, $\ln(mx/2)$ and ε yields

$$k^0(\beta;mx)=\sum_{k=0}^{\infty}\sum_{w=0}^{\infty}\sum_{u=0}^{w+1}K^0(b;k;u;w)\left(\frac{mx}{2}\right)^{2k}\left\{2\ln\left(\frac{mx}{2}\right)\right\}^u\varepsilon^w, \tag{A6a}$$

$$k^1(\beta;mx)=\sum_{k=0}^{b-1}\sum_{w=0}^{\infty}K^1(b;k;w)\left(\frac{mx}{2}\right)^{-2\beta+2k}\varepsilon^w. \tag{A6b}$$

A combined notation of (A6a) and (A6b) is

$$k^\theta(\beta;mx)=\sum_{k,u,w,\theta}K^\theta(b;k;u;w)\left(\frac{mx}{2}\right)^{-2\theta\beta+2k}\left\{2\ln\left(\frac{mx}{2}\right)\right\}^u\varepsilon^w. \tag{A7}$$

The θ's assume values $\theta=0$ and $\theta=1$; k runs from 0 to ∞ if $\theta=0$ and from 0 to $b-1$ if $\theta=1$; u runs from 0 to $w+1$ if $\theta=0$ and it takes only the value 0 if $\theta=1$; w runs from 0 to ∞.

The $K^\theta(b;k;u;w)$ are finite coefficients that may be computed.

The functions $k(\beta;mx)$ satisfy the recursion relation

$$\frac{dk(\beta;mx)}{dx^\mu}=-\left(\frac{m^2x_\mu}{2}\right)k(\beta+1;mx) \tag{A8}$$

and the differential equations

$$\left(\partial_\mu\partial_\nu-m^2\frac{x_\mu x_\nu}{x^2}\right)k(\beta;mx)=m^2\left\{(\beta+1)\frac{x_\mu x_\nu}{x^2}-\frac{1}{2}g_{\mu\nu}\right\}k(\beta+1;mx), \tag{A9a}$$

$$(\partial_\mu\partial^\mu-m^2)k(\beta;mx)=(1-\alpha)m^2k(\beta+1;mx). \tag{A9b}$$

Their asymptotic behavior is given by

$$k(\beta;mx)=\sqrt{\pi}\sum_{h=0}^{H-1}2^{\beta-h-1/2}\frac{\Gamma(\beta+h+\frac{1}{2})}{h!\Gamma(\beta-h+\frac{1}{2})}(mx)^{-\beta-h-1/2}e^{-mx}+O(x^{-H-\beta-1/2}),\quad \text{if } x\to\infty \tag{A10}$$

from which the asymptotic expression

$$\prod_{1\leqslant d\leqslant D}\int_{1/M}^{\infty} dx\, x^{2\nu-1}\{\ln(m^d x)\}^{u^d} k(\beta^d; m^d x)$$

$$= \pi^{(1/2)\,D} \sum_{0\leqslant h^d\leqslant H^d-1} 2^{\Sigma_{1\leqslant a\leqslant D}^{(\beta_a-h_a)-(1/2)D}} \prod_{1\leqslant d\leqslant D} \frac{\Gamma(\beta^d+h^d+1/2)}{h^d!\,\Gamma(\beta^d-h^d+1/2)(m^d)^{\beta^d+h^d+1/2}}$$

$$\times \int_{1/M}^{\infty} dx\, x^{2\nu-1-\Sigma_{1\leqslant a\leqslant D}(\beta^a+h^a)-1/2D}\{\ln(m^d x)\}^{u^d} e^{-(\Sigma_{1\leqslant a\leqslant d}\, m^a)x}$$

$$+ O(M^{-2\nu+Min(H_i)+\Sigma_{1\leqslant a\leqslant D}\beta^a+1/2D}) \quad \text{if } M\to 0 \tag{A11}$$

is obtained.

The k-functions with a nonsimple argument may be split according to

$$k(\beta; m|\mathbf{x}_i-\mathbf{x}_{i'}|) = \sum_{l,r=0}^{\infty} \frac{(-)^l}{l!\,r!}\left(\frac{1}{2}\right)^{2l+r} (mx_{i'})^{2l+r}(mx_i)^r (c_{i',i})^r k(\beta+l+r; mx_i) \tag{A12}$$

if

$$x_{i'} < x_i\,. \tag{A13}$$

This formula may be obtained via the representation by Bessel functions and Gegenbauer polynomials, as shown in Ref. 4. It also is obtained by straight insertion of

$$\frac{(\mathbf{x}_i-\mathbf{x}_{i'})^{2k}}{k!} = \sum_{l,r} (-)^r \frac{(x_{i'})^{2l}(2c_{i',i}x_{i'}x_i)^r (x_i)^{2k-2l-2r}}{l!\,r!\,(k-l-r)!}$$

and

$$(\mathbf{x}_i-\mathbf{x}_{i'})^{-2\beta+2k}\Gamma(\beta-k) = \sum_{l,r} (-)^l \frac{(x_{i'})^{2l}(2c_{i',i}x_{i'}x_i)^r (x_i)^{-2\beta+2k-2l-2r}\Gamma(\beta+l+r-k)}{l!\,r!} \tag{A14}$$

into (A2).

Finally, the integral representation of $k(\beta; mx)$ is

$$k(\beta; mx) = \frac{1}{2}\int_0^{\infty} d\rho\;\; \rho^{-\beta} e^{-\rho} e^{-(mx)^2/4\rho}. \tag{A15}$$

APPENDIX B

By multiple application of the n-dimensional Gauss integral

$$G_1(\mathbf{p}^2; m^2) \equiv \int_{-\infty}^{+\infty} d\mathbf{x}\;\; e^{i\mathbf{p}\cdot\mathbf{x}} e^{-(1/4)\,m^2\mathbf{x}^2} = \frac{(4\pi)^\nu}{m^{2\nu}} e^{-\mathbf{p}^2/m^2}, \tag{B1}$$

formula

$$G_{f-1}((\Sigma_a \mathbf{p}_a)^2; m_{a,b}^2)$$
$$\equiv \prod_{1\leqslant i\leqslant f-1} \int d\mathbf{x}_i e^{i\mathbf{p}_i\cdot\mathbf{x}_i} e^{-(1/4)\sum_{1\leqslant a\leqslant i} m_{a,f}{}^2 \mathbf{x}_i^2 - 1/4 \sum_{1\leqslant a\leqslant i} m_{a,i}{}^2 (\mathbf{x}_i-\mathbf{x}_a)^2} = \frac{(4\pi)^{(f-1)\nu}}{(n_{1,2,\dots,f})^{\nu}}$$
$$\cdot \exp\left\{ - \frac{n_1 n_{2,3,\dots,f} \mathbf{p}_1{}^2 + n_2 n_{1,3,\dots,f} \mathbf{p}_2{}^2 + \cdots + n_{1,2} n_{3,4,\dots,f} (\mathbf{p}_1+\mathbf{p}_2)^2 + \cdots + n_{1,2,3} n_{4,5,\dots,f} (\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3)^2 + \cdots}{n_{1,2,\dots,f}} \right\} \tag{B2}$$

is obtained.

The coefficients $n_{1,2,\dots,f}$ are sums of products of the square masses of $f-1$ independent internal lines between the vertices $1,2,\dots,f$:

$$n_1 = 1, \quad n_2 = 1, \quad n_3 = 1, \quad \text{etc.},$$
$$n_{1,2} = m_{1,2}{}^2, \quad n_{1,3} = m_{1,3}{}^2, \quad \text{etc.}$$
$$n_{1,2,3} = m_{1,2}{}^2 m_{1,3}{}^2 + m_{1,2}{}^2 m_{2,3}{}^2 + m_{1,3}{}^2 m_{2,3}{}^2, \quad \text{etc.}, \tag{B3}$$
$$\cdots.$$
$$n_{1,2,\cdots,f} = \sum m_{1,f}{}^2 m_{2,f}{}^2 \cdots, m_{f-1,f}{}^2 + \cdots.$$

Combination of (A15) and (B2) yields

$$\prod_{\substack{1\leqslant i\leqslant f-1 \\ 1\leqslant i'<i \\ d}} \int d\mathbf{x}_i e^{i\mathbf{p}_i\cdot\mathbf{x}_i} k_{i,f}^d(\beta; m x_i) k_{i',i}^d(\beta; m|\mathbf{x}_i - \mathbf{x}_{i'}|)\}$$
$$= \prod_{\substack{1\leqslant i'<i\leqslant f \\ d}} \left(\int_0^\infty d\left(\frac{1}{2}\rho_{i',i}^d\right) (\rho_{i',i}^d)^{-\beta_{i',i}^d} e^{-\sum_d^{1\leqslant a'<a\leqslant f} \rho_{a',a}^d} G_{f-1}\left\{ (\Sigma_a \mathbf{p}_a)^2; \sum_d \frac{m_{a,b}^d{}^2}{\rho_{a,b}^d} \right\} \right). \tag{B4}$$

The rhs is, up to a factor, the parameter representation of scalar Feynman diagrams. In the case of spin, polynomials of masses and derivatives with respect to the external momenta, combined with higher β's have to be added, as explained in Sec. II.

The integration parameters ρ come straight from the textbook of Watson. Hence, Feynman parameters were known in mathematical literature long before the discovery of quantum field theory.

APPENDIX C

The expressions for the content of a unit parallelopipidum in one, two, three, and four dimensions are

$$I_1 = 1,$$
$$I_{12} = \sqrt{1 - c_{12}{}^2},$$
$$I_{123} = \sqrt{1 - c_{12}{}^2 - c_{13}{}^2 - c_{23}{}^2 + 2c_{12}c_{23}c_{31}} = I_{13} I_{23} \sqrt{1 - \left(\frac{c_{12} - c_{13}c_{23}}{I_{13} I_{23}} \right)^2},$$

$$I_{1234}$$

$$= \sqrt{1-c_{12}{}^2-c_{13}{}^2-c_{14}{}^2-c_{23}{}^2-c_{24}{}^2-c_{34}{}^2+2c_{12}c_{23}c_{31}+2c_{12}c_{24}c_{41}+2c_{13}c_{34}c_{41}+2c_{23}c_{34}c_{41} \\ +c_{12}{}^2c_{34}{}^2+c_{13}{}^2c_{24}{}^2+c_{14}{}^2c_{23}{}^2-2c_{12}c_{23}c_{34}c_{41}-2c_{13}c_{32}c_{24}c_{41}-2c_{12}c_{24}c_{43}c_{31}}$$

$$= \frac{I_{134}I_{234}}{I_{34}}\sqrt{1-\left(\frac{I_{34}{}^2c_{12}-c_{13}c_{32}-c_{14}c_{42}+c_{13}c_{34}c_{42}+c_{14}c_{43}c_{32}}{I_{134}I_{234}}\right)^2}. \tag{C1}$$

For the general case, the recursion formula

$$I_{1,2,3,,\dots,f}=\frac{I_{1,3,\dots,f}I_{2,3,\dots,f}}{I_{3,\dots,f}}\sqrt{1-y_{12}{}^2} \tag{C2}$$

is valid, with

$$y_{12}=\frac{I_{3,4,\dots,f}{}^2c_{1,2}-b_{1,2(3,4,\dots,f)}}{I_{1,3,\dots,f}I_{2,3,\dots,f}}, \tag{C3}$$

where

$$b_{1,2(3,4,\dots,f)}=c_{13}c_{32}+\cdots+c_{1f}c_{f2}-c_{13}c_{34}c_{42}-\cdots+\cdots \tag{C4}$$

is the coefficient of $2c_{12}$ in $I_{1,2,\dots,f}{}^2$.

Application of these formulas yields

$$\frac{I_{1,2,\dots,f}}{I_{2,\dots,f}}=\sqrt{1-y_{12}{}^2}\sqrt{1-y_{13}{}^2}\cdots\sqrt{1-y_{1,f}{}^2}, \tag{C5a}$$

$$\frac{dc_{12}\cdots dc_{1,f}}{I_{2\dots f}}=dy_{12}\cdots dy_{1,f}\left(\frac{I_{1,3,\dots,f}}{I_{3,4,\dots,f}}\right)\left(\frac{I_{1,4,\dots,f}}{I_{4,5,\dots,f}}\right)\dots\left(\frac{I_{1,f-1,f}}{I_{f-1,f}}\right)I_{1,f}$$
$$=dy_{12}\cdots dy_{1,f}\sqrt{1-y_{13}{}^2}(\sqrt{1-y_{14}{}^2})^2\cdots(\sqrt{1-y_{1,f}{}^2})^{f-2} \tag{C5b}$$

and

$$c_{i,j}=\frac{b_{i,j(j+1,\dots,f)}+y_{i,j}I_{i,j+1,\dots,f}I_{j,j+1,\dots,f}}{I^2_{j+1\dots f-1}}=y_{i,j}(\sqrt{1-(y_{i,j+1})^2}\cdots\sqrt{1-(y_{i,f})^2})$$
$$\times(\sqrt{1-(y_{j,j+1})^2}\cdots\sqrt{1-(y_{j,f})^2})+(y_{i,j+1}\sqrt{1-(y_{i,j+2})^2}\cdots\sqrt{1-(y_{i,f})^2})$$
$$\times(y_{j,j+1}\sqrt{1-(y_{j,j+2})^2}\cdots\sqrt{1-(y_{j,f})^2})+\dots+(y_{i,f-1}\sqrt{1-(y_{i,f})^2})(y_{j,f-1}\sqrt{1-(y_{j,f})^2})$$
$$+y_{i,f}y_{j,f}. \tag{C5c}$$

The formula

$$\frac{c_{i,j}{}^{q_{i,j}}}{q_{i,j}!}=\sum_{\substack{f\\ \sum\\ b=j}}{}_{q_{i,j}{}^b=q_{i,j}}\frac{\{y_{i,j}(\sqrt{1-(y_{i,j+1})^2}\cdots\sqrt{1-(y_{i,f})^2})(\sqrt{1-(y_{j,j+1})^2}\cdots\sqrt{1-(y_{j,f})^2})\}^{q_{i,j}{}^j}}{q_{i,j}{}^j!}\cdots$$
$$\times\left(\frac{y_{i,f}y_{j,f}}{q_{i,j}{}^f!}\right)^{q_{i,j}{}^f}, \tag{C6}$$

has been used in Section III.

APPENDIX D

By multiple application of

$$\prod_{1\leqslant i\leqslant f-1}\int_0^{\eta} d\xi\,\xi^{N-1}\{\ln(m_i\xi)\}^{u_i}=\sum_{0\leqslant u_i^{\,i}\leqslant u_i}\frac{(-)^{\Sigma_{1\leqslant a\leqslant f-1}u_a{}^a}\left(\sum_{1\leqslant a\leqslant f-1}u_a{}^a\right)!}{(N)^{1+\Sigma_{1\leqslant a\leqslant f-1}u_a{}^a}}\times\prod_{i=1}^{f-1}\frac{u_i!}{(u_i-u_i{}^i)!\,u_i{}^i!}\,\eta^N\{\ln(m_i\eta)\}^{u_i-u_i{}^i},\tag{D1}$$

the formula

$$\prod_{1\leqslant i'<i\leqslant f-1}\int_0^{\eta_i} d\xi_i(\xi_i)^{N_i-1}\{\ln(m_{i',i}\xi_i\xi_{i+1}\cdots\xi_{f-1})\}^{u_{i',i}}$$

$$=\sum_{n_{a,b}{}^c}\prod_{1\leqslant i'<i\leqslant i''\leqslant f-1}\frac{(-)^{u_{i',i}{}^{i''}}\left(\Sigma_{1\leqslant a'<a\leqslant i}u_{a',a}{}^i\right)!\,u_{i',i}!}{\left(u_{i',i}-\Sigma_{i\leqslant c\leqslant f-1}u_{i',i}{}^c\right)!\,u_{i',i}{}^{i''}!\,N_i^{1+\Sigma_{1\leqslant a'<a\leqslant i}u_{a',a^i}}}\times\eta_i^{N_i}\{\ln(m_{i',i}\eta_i\eta_{i+1}\cdots\eta_{f-1})\}^{u_{i',i}-\sum_{i\leqslant c\leqslant f-1}u_{i',i}{}^c}\tag{D2}$$

is obtained.

These formulas are obtained after a number of partial integrations. As a matter of fact, these are the partial integrations discussed in the introduction and presumably meant in Ref 3.

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Classical history theory of vector fields

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We consider the extension of classical history theory to the massive vector field and electromagnetism. It is argued that the action of the two Poincaré groups introduced by Savvidou suggests that the history fields should have five components. The extra degrees of freedom introduced to make the fields five dimensional result in an extra pair of second class constraints in the case of the massive vector field, and in an extended gauge group in the case of electromagnetism. The total gauge transformations depend on two arbitrary parameters, and contain ''internal'' and ''external'' U(1) gauge transformations as subgroups. © *2002 American Institute of Physics.*
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I. INTRODUCTION

A. Motivation

The Hamiltonian formalism provides a strong link between classical and quantum theories and is mathematically well-developed in both cases. However, a major drawback of the standard Hamiltonian approach to relativistic field theories is that it requires a splitting of space–time into space and time, thus breaking the manifest covariance of the theory. This problem becomes particularly acute when canonical methods are applied to generally covariant theories such as general relativity, and this is one aspect of the ''problem of time'' in canonical quantum gravity.

Recently a Hamiltonian formalism has been proposed by Isham and co-workers,[1–3] in which the fundamental physical entities are entire histories of the system under consideration, as opposed to Cauchy data at an instant of time. For a thorough introduction see Ref. 4. The histories formalism was originally developed in the quantum case, but there is a well-defined classical history formalism. The central object in a classical history theory is the space of histories, Π, which is defined to be a one-parameter family of single-time state spaces. An element of Π is called a history, and the space of histories carries a symplectic structure which provides the crucial link to the corresponding quantum history theory.

A particularly striking fact about history theories is that there are two notions of time evolution.[5] External time corresponds to the parameter labeling the copies of state space, and internal time is generated by Hamiltonian evolution. In this way the notion of time plays two different roles in a history theory, one corresponding to the causal ordering of logical propositions, and the second corresponding to dynamical evolution. The two times are linked together in the action principle.

The histories formalism has been applied to scalar field theory on flat[6] and curved[7,8] space–times, and in the following we discuss the extension of the classical theory to the case of vector fields. In particular we examine the massive vector field and the electromagnetic field from a histories perspective. We shall argue that, as a consequence of the two time directions, a history field should be regarded as a certain type of field on a five-dimensional space–time. We also give an analysis of the gauge transformations of histories electromagnetism.

These results are relevant to the ultimate goal of the histories program: the formulation of a histories version of general relativity.[9] First, they suggest the possibility that a covariant history

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theory of gravity should be concerned with the metric of a five-dimensional extended space–time. Second, gauge symmetry is an important feature of general relativity, particularly when formulated in terms of tetrad fields. The study of the extended gauge transformations of histories electromagnetism is relevant in this context.

B. Scalar field theory

In this section we give a brief account of the histories description of the classical scalar field on Minkowski space–time, $\mathcal{M}$, as given by Savvidou.[6] We define the Minkowski metric $\eta_{\mu\nu}$ to have signature $(+,-,-,-)$.

1. The history algebra

The canonical configuration space of the scalar field is $Q_{n,t}=C^\infty(\Sigma_{n,t})$ where $\Sigma_{n,t}$ is a Cauchy surface in $\mathcal{M}$, and $C^\infty(\Sigma_{n,t})$ denotes the set of all smooth, real-valued functions on $\Sigma_{n,t}$. The Cauchy surfaces are labeled by a future pointing timelike unit vector n normal to $\Sigma_{n,t}$, and a real number t. Each Cauchy surface represents an instant of time in a particular inertial frame. The state space $P_{n,t}$ is identified with $C^\infty(\Sigma_{n,t})\times C^\infty(\Sigma_{n,t})$ which is a dense subspace of the cotangent bundle of $Q_{n,t}$. The construction of the corresponding classical history theory begins by defining a trivial vector bundle $\xi_n : P\times\mathbb{R}\to\mathbb{R}$ such that $\xi_n^{-1}(t)=P_{n,t}$, where P is an abstract copy of the state space. The space of histories of the scalar field corresponds to the space of sections of this bundle, $\Pi_n=\Gamma(\xi_n)$. Note that Π_n could be defined directly as the space of paths $\mathbb{R}\to P_n$. However, the bundle picture is useful in more general situations (e.g., on curved space–times), and also gives a motivation for the ''internal'' / ''external'' nomenclature in history theory: internal transformations act internally to the fibers of ξ_n, while external transformations act across the fibers. The history fields satisfy the following Poisson algebra:

$$\{\phi_n(t;\mathbf{x}),\phi_n(t';\mathbf{x}')\}=0, \tag{1}$$

$$\{\pi_n(t;\mathbf{x}),\pi_n(t';\mathbf{x}')\}=0, \tag{2}$$

$$\{\phi_n(t;\mathbf{x}),\pi_n(t';\mathbf{x}')\}=\delta(t-t')\,\delta^{(3)}_{n,t}(\mathbf{x}-\mathbf{x}'), \tag{3}$$

where $\delta^{(3)}_{n,t}(\mathbf{x}-\mathbf{x}')$ is the delta function on $\Sigma_{n,t}$. The right-hand side of this equation is a space–time scalar density of weight one. In Minkowski space–time, there is no difference between a scalar density and a scalar (if we restrict attention to transformations under the connected part of the Poincaré group), which suggests that the fields can be thought of as space–time scalars. A pair $(t,\mathbf{x})\in\mathbb{R}\times\Sigma$ can be identified with a unique four-vector $X\in\mathcal{M}$ as $X=tn+x_n$, where the three-vector $\mathbf{x}$ has been associated with a corresponding four-vector x_n that is n-spatial (i.e., $n\cdot x_n := \eta_{\mu\nu}n^\mu x_n^\nu=0$). Hence we can write $\phi_n(t;\mathbf{x})$ as $\phi_n(X)$. The history algebra can then be written in the more covariant looking form

$$\{\phi_n(X),\phi_n(X')\}=0, \tag{4}$$

$$\{\pi_n(X),\pi_n(X')\}=0, \tag{5}$$

$$\{\phi_n(X),\pi_n(X')\}=\delta^{(4)}(X-X'). \tag{6}$$

Now it is tempting to drop the n label from the fields since the right-hand side of this algebra does not depend on n. However, this would be somewhat misleading in the sense that the field $\pi(X)$ has no physical meaning. This is because the conjugate momentum corresponds to the field momentum along a certain timelike *direction*, and so must be written as $\pi_n(X)$. Although the algebra (4)–(6) is independent of n, Savvidou[6] has shown that in the quantum theory n labels the physically relevant, inequivalent *representations* of the algebra on a particular Fock space. So in the analysis of the classical theory the n-labels remain on the fields under the understanding that

they are necessary for the physical interpretation of the theory and arise naturally in quantization. However, we note that it is rather unsatisfactory to have an n label on the ϕ field because, physically, the value of the field at a point in space–time *is* independent of the foliation. In this particular histories formulation of classical scalar field theory all propositions about the field are made in the context of a particular inertial reference frame.

2. Time translations

For each n, a ''Liouville'' functional can be constructed from the fields,

$$V_n := \int d^4X \pi_n n_\mu \partial^\mu \phi_n , \tag{7}$$

which generates external time translations in the n direction. In coordinates adapted to n these transformations take the form $\phi_n(t,\mathbf{x}) \mapsto \phi_n(t+\lambda,\mathbf{x})$, and similarly for $\pi_n(t,\mathbf{x})$.

There is another notion of time translation in the history theory. Intuitively the Hamiltonian at each instant of external time generates dynamical evolution *internal* to each fiber of ξ_n. More precisely, the time-averaged Hamiltonian,

$$H_n := \frac{1}{2} \int d^4X [\, \pi_n^2 + (\, \eta^{\mu\nu} - n^\mu n^\nu) \partial_\mu \phi_n \partial_\nu \phi_n + m^2 \phi_n^2], \tag{8}$$

generates transformations $\phi_n(X) \mapsto \phi_n(X,s)$.

The action operator is made up of the Liouville and Hamiltonian operators as follows:

$$S_n := V_n - H_n , \tag{9}$$

and the equations of motion can be written in the form

$$\{S_n , \phi_n(X)\} = 0, \tag{10}$$

$$\{S_n , \pi_n(X)\} = 0. \tag{11}$$

3. Poincaré covariance

Savvidou[6] has shown the existence of two Poincaré groups in the histories formulation of the scalar field. The n-spatial components of the two groups are identical, but the time translations of the internal Poincaré group are generated by the Hamiltonian while the time translations of the external Poincaré group are generated by the Liouville functional.

External boosts correspond to the following automorphism of the history algebra:

$$\phi_n(t,\mathbf{x},0) \mapsto \phi_{\Lambda n}(\Lambda(t,\mathbf{x}),0), \tag{12}$$

$$\pi_n(t,\mathbf{x},0) \mapsto \pi_{\Lambda n}(\Lambda(t,\mathbf{x}),0), \tag{13}$$

where we have used adapted coordinates to write $\phi_n(X,0) = \phi_n(t,\mathbf{x},0)$ and $\Lambda(t,\mathbf{x})$ denotes the usual Lorentz transformations acting on inertial coordinates $(t,\mathbf{x})$. We note that, in the classical case, these automorphisms cannot be generated by canonical transformations. This is because there is no momentum conjugate to the foliation vector n, and thus no way to generate changes in n. The ''multisymplectic'' approach[10] offers a solution to this problem in the classical theory, and in the quantum theory changes in n correspond to mapping between inequivalent representations of the history algebra.

Internal boosts act on the fields as follows:

$$\phi_n(0,\mathbf{x},s) \mapsto \phi_n(0,\Lambda(\mathbf{x},s)), \tag{14}$$

$$\pi_n(0,\mathbf{x},s)\mapsto\pi_n(0,\Lambda(\mathbf{x},s)). \tag{15}$$

The internal boosts leave the foliation vector fixed and can be implemented by canonical transformations. The generator of internal boosts on the hyperplane $s=\text{const}$ is

$$^{\text{int}}K_n(m)=m_\mu\int d^4X[\,\pi s\,\partial^\mu\phi-X^\mu H_n(X)], \tag{16}$$

where $H_n(X)$ is the Hamiltonian density and the integral is over the surface $s=\text{const}$.

The fields $\phi_n(X,s)$ are defined on an extended space–time $\mathcal{N}=\mathcal{M}\times\mathbb{R}$. However, the theory is not invariant under the full SO(2, 3) isometry group of this space–time. This is evident from the fact that the algebra (4)–(6) is defined on external space–time, that is the surface in $\mathcal{N}$ defined by $s=0$, and does not take the same form on internal space–time (defined by $n\cdot X=0$). This indicates that the fields are not true scalar fields on $\mathcal{N}$. However, the fields are covariant under the internal and external SO(1, 3) subgroups of SO(2, 3).

In the case of the scalar field these subtleties can be overlooked, but the construction of a history theory of vector fields acutely illustrates this issue. A particularly relevant question is whether the history vector field should have four indices, or five as it must to be a vector field on $\mathcal{N}$.

II. MASSIVE VECTOR FIELD

A. State space theory

In this section we give a brief overview of the standard state space theory of the massive vector field on $\mathcal{M}$.

We begin with the covariant theory. The covariant configuration space is $\mathcal{X}_0(\mathcal{M})$, the space of vector fields on $\mathcal{M}$ with appropriate boundary conditions. The massive vector field is described by the following Lagrangian:[11]

$$\mathcal{L}=-\tfrac{1}{4}\phi_{\mu\nu}\phi^{\mu\nu}+\tfrac{1}{2}m^2\phi_\mu\phi^\mu, \tag{17}$$

where $\phi^{\mu\nu}(X):=2\partial^{[\mu}\phi^{\nu]}(X)$ and $\phi\in\mathcal{X}_0(\mathcal{M})$. The resulting field equations are

$$(\Box+m^2)\phi^\mu(X)=0, \tag{18}$$

$$\partial_\mu\phi^\mu(X)=0. \tag{19}$$

The first of these equations shows that each component of the field behaves like a massive scalar field. The second equation is known as the Fierz–Pauli equation and it is the first indication of the presence of constraints in the theory.

To pass to the canonical theory we choose a Cauchy surface in $\mathcal{M}$ and consider the fields on this Cauchy surface. More precisely, we choose a spacelike embedding $\iota:\Sigma\to\mathcal{M}$, where $\Sigma\simeq\mathbb{R}^3$, and take the corresponding configuration space to be the space of fields $\phi^\mu_\iota(\mathbf{x})$ where $\mathbf{x}\in\Sigma$. However the fields $\phi^\mu_\iota(\mathbf{x})$ are not geometric objects on either Σ or $\mathcal{M}$. The geometrical interpretation of the fields is clarified by considering $\text{Emb}(\Sigma,\mathcal{M})$, the space of embeddings of Σ into $\mathcal{M}$. Then ϕ_ι can be thought of as an element of $T_\iota\text{Emb}(\Sigma,\mathcal{M})$ where the tangent space to $\text{Emb}(\Sigma,\mathcal{M})$ at the embedding ι is defined as

$$T_\iota\text{Emb}(\Sigma,\mathcal{M})=\{\psi:\Sigma\to T\mathcal{M}\,|\,\psi(\mathbf{x})\in T_{\iota(\mathbf{x})}\mathcal{M}\}. \tag{20}$$

The configuration space of the canonical theory is then defined as $Q_\iota:=T_\iota\text{Emb}(\Sigma,\mathcal{M})$ for some fixed ι. The cotangent space of $\text{Emb}(\Sigma,\mathcal{M})$ at ι is defined similarly:

$$T^*_\iota\text{Emb}(\Sigma,\mathcal{M})=\{l:\Sigma\to T^*\mathcal{M}\,|\,l(\mathbf{x})\in T^*_{\iota(\mathbf{x})}\mathcal{M}\} \tag{21}$$

and the pairing between these two spaces is given by

$$\langle l, \psi \rangle_\iota = \int_\Sigma \mathrm{d}\theta_{\mathbf{x}} l_\mu(\iota(\mathbf{x}))\psi^\mu(\iota(\mathbf{x})), \tag{22}$$

where $\mathrm{d}\theta_{\mathbf{x}}$ is an arbitrary volume element on Σ. The state space P_ι is defined as the Cartesian product $Q_\iota \times T^*_\iota \mathrm{Emb}(\Sigma, \mathcal{M})$.

As we are considering flat space–time, there exists a family of preferred embeddings; those which correspond to inertial frames. The space of preferred embeddings can be parametrized by pairs (n,t) where n is a future pointing unit vector in $\mathcal{M}$ and $t \in \mathbb{R}$. As we are considering a deterministic system, we choose $t=0$ without loss. We denote the configuration space and the state space corresponding to the embedding labeled by $(n,0)$ as Q_n and P_n, respectively. The state space P_n carries the following Poisson algebra:

$$\{\phi^\mu_n(\mathbf{x}), \phi^\nu_n(\mathbf{x}')\} = 0, \tag{23}$$

$$\{\pi^n_\mu(\mathbf{x}), \pi^n_\nu(\mathbf{x}')\} = 0, \tag{24}$$

$$\{\phi^\mu_n(\mathbf{x}), \pi^n_\nu(\mathbf{x}')\} = \delta^\mu_\nu \delta^{(3)}_n(\mathbf{x}-\mathbf{x}'), \tag{25}$$

where $\delta^{(3)}_n(\mathbf{x}-\mathbf{x}')$ is the delta function on Σ_n.

A field $\phi^\mu_n(\mathbf{x}) \in Q_n$ can be decomposed into the pair $(\phi^t_n(\mathbf{x}), {}^n\phi^\mu(\mathbf{x}))$ where

$$\phi^t_n(\mathbf{x}) := n_\mu \phi^\mu_n(\mathbf{x}), \tag{26}$$

$${}^n\phi^\mu(\mathbf{x}) := {}^nP^\mu_\nu \phi^\nu_n(\mathbf{x}), \tag{27}$$

and we have introduced the n-spatial projection tensor defined by

$${}^nP^\mu_\nu := \delta^\mu_\nu - n^\mu n_\nu. \tag{28}$$

It follows that $n_\mu {}^nP^\mu_\nu = 0$ and $n^\nu {}^nP^\mu_\nu = 0$. The fields $\phi^t_n(\mathbf{x})$ and ${}^n\phi^\mu(\mathbf{x})$ are defined on the space of embeddings, but $\phi^t_n(\mathbf{x})$ pulls back to give a "scalar field" on Σ_n. We can use the metric on $\mathcal{M}$ to lower the index on ${}^n\phi^\mu(\mathbf{x})$. The resulting one-form can be pulled back to Σ_n, and then the index can be raised using the metric on Σ_n to give a "vector field" on Σ_n. In a similar way, objects defined by ${}^n\pi_\mu(\mathbf{x}) := {}^nP^\nu_\mu \pi^n_\nu(\mathbf{x})$, and ${}^n\phi^{\mu\nu}(\mathbf{x}) := {}^nP^\mu_\sigma {}^nP^\nu_\rho \phi^{\sigma\rho}_n(\mathbf{x})$ can be thought of as a "one-form" and a "covariant tensor" on Σ_n.

The canonical momenta are computed from the Lagrangian and turn out to be[12]

$$\pi^n_t(\mathbf{x}) = 0, \quad {}^n\pi_\mu(\mathbf{x}) = {}^nP^\rho_\mu n^\nu \phi_{\nu\rho}(\mathbf{x}). \tag{29}$$

The first of these equations is a primary constraint. The canonical Hamiltonian is computed to be

$$H_n = \int_\Sigma \mathrm{d}\theta_{\mathbf{x}} \left[\frac{1}{2} {}^n\pi_\mu {}^n\pi^\mu + \frac{1}{4} {}^n\phi_{\mu\nu} {}^n\phi^{\mu\nu} - \frac{1}{2} m^2 (\phi^t_n)^2 + \frac{1}{2} m^2 {}^n\phi_\mu {}^n\phi^\mu - \phi^t_n {}^n\partial^\mu {}^n\pi_\mu \right], \tag{30}$$

where the n-spatial derivative is defined as ${}^n\partial^\mu = {}^nP^\mu_\nu \partial^\nu$. For the primary constraint $\pi^n_t(\mathbf{x}) = 0$ to be preserved by the dynamical evolution, it is necessary and sufficient that $\{H_n, \pi^n_t(\mathbf{x})\} = 0$. This implies the secondary constraint

$$m^2 \phi^t_n(\mathbf{x}) + {}^n\partial^\mu {}^n\pi_\mu(\mathbf{x}) = 0. \tag{31}$$

A point in the constraint surface C_n determines and is fully determined by the pair $({}^n\pi_\mu(\mathbf{x}), {}^n\phi^\nu(\mathbf{x}))$.

The constraints do not commute under the Poisson bracket and so they form a second class pair. This implies that the pull-back of the symplectic two-form on P_n to the constraint surface is nondegenerate. Therefore there is a well-defined Poisson algebra on the constraint surface which is given by the Dirac brackets:

$$\{{}^n\phi^\mu(\mathbf{x}), {}^n\pi_\nu(\mathbf{x}')\}_D = {}^nP^\mu_\nu \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{32}$$

with all other brackets vanishing.

B. Classical history theory

We begin with the abstract state space P, and follow the usual procedure of taking a one-parameter family of copies of P. This results in a trivial vector bundle $\xi_n : P\times\mathbb{R}\to\mathbb{R}$ where the fiber $\xi_n^{-1}(t) = P_{n,t}$ for each t. Sections of ξ_n correspond to histories of the vector field with respect to the foliation labeled by n. Thus a history is a map

$$h_n : t \mapsto (\phi^\mu_n(t;\mathbf{x}), \pi^n_\nu(t;\mathbf{x})). \tag{33}$$

If we choose a volume element on $\mathbb{R}$ then a symplectic structure is induced on the space of maps $\mathbb{R}\to P$ because P is a symplectic manifold. Using the Lebesgue measure, the symplectic structure defines the following algebra:

$$\{\phi^\mu_n(t;\mathbf{x}), \phi^\nu_n(t';\mathbf{x}')\} = 0, \tag{34}$$

$$\{\pi^n_\mu(t;\mathbf{x}), \pi^n_\nu(t';\mathbf{x}')\} = 0, \tag{35}$$

$$\{\phi^\mu_n(t;\mathbf{x}), \pi^n_\nu(t';\mathbf{x}')\} = \delta^\mu_\nu \delta(t-t')\,\delta^{(3)}_n(\mathbf{x}-\mathbf{x}'). \tag{36}$$

In the case of the scalar field a one-parameter family of functions on Σ_n:

$$t \mapsto \phi_n(t;\mathbf{x}) \tag{37}$$

was identified with a function $\phi_n(X)$ on $\mathcal{M}$. In a similar way, for a fixed foliation, a one-parameter family of elements of Q_n,

$$t \mapsto \phi^\mu_n(t;\mathbf{x}), \tag{38}$$

is equivalent to a unique vector field $\phi^\mu_n(X) \in \mathcal{X}(\mathcal{M})$. The one-parameter family $t\mapsto\pi^n_\mu(t;\mathbf{x})$ can be identified with a one-form $\pi^n_\mu(X) \in \Lambda^1(\mathcal{M})$ in the same way, and these fields satisfy the covariant looking algebra

$$\{\phi^\mu_n(X), \phi^\nu_n(X')\} = 0, \tag{39}$$

$$\{\pi^n_\mu(X), \pi^n_\nu(X')\} = 0, \tag{40}$$

$$\{\phi^\mu_n(X), \pi^n_\nu(X')\} = \delta^\mu_\nu \delta^{(4)}(X-X'). \tag{41}$$

In this way, the history space, Π_n, can be identified with the space $\mathcal{X}(\mathcal{M})\times\Lambda^1(\mathcal{M})$. We can decompose $\phi^\mu_n(X)$ into the pair $(\phi^t_n(X), {}^n\phi^\mu(X))$ defined by

$$\phi^t_n(X) := n_\mu \phi^\mu_n(X), \tag{42}$$

$${}^n\phi^\mu(X) := {}^nP^\mu_\nu \phi^\nu_n(X), \tag{43}$$

and we use these fields to define the generators of internal and external time translations. External time translations are generated by the ''Liouville'' functional,

$$V_n := \int d^4X \, [\, \pi_t^n n_\nu \partial^\nu \phi_n^t + {}^n\pi_\mu n_\nu \partial^\nu {}^n\phi^\mu]. \tag{44}$$

Internal time translations are generated by the time-averaged Hamiltonian

$$H_n = \int d^4X \Big[\frac{1}{2} {}^n\pi_\mu {}^n\pi^\mu + \frac{1}{4} {}^n\phi_{\mu\nu} {}^n\phi^{\mu\nu} - \frac{1}{2} m^2 (\phi_n^t)^2 \tag{45}$$

$$+ \frac{1}{2} m^2 {}^n\phi_\mu {}^n\phi^\mu - \phi_n^t {}^n\partial^\mu {}^n\pi_\mu \Big]. \tag{46}$$

The internal time translations generated by H_n take the form

$$\phi_n^\mu(X) \mapsto \phi_n^\mu(X,s). \tag{47}$$

In Sec. II C we will consider the geometric meaning of these curious objects which have four components, but depend on five space–time variables.

In the remainder of this section we discuss the history constraint surface $\mathcal{C}_n \subset \Pi_n$. An arbitrary element of Π_n will not be compatible with the constraints. The constraint submanifold, $\mathcal{C}_n$, contains all elements of Π which satisfy the constraints:

$$\pi_t^n(X) = 0, \quad m^2 \phi_n^t(X) + {}^n\partial^\mu {}^n\pi_\mu(X) = 0. \tag{48}$$

Thus a point in $\mathcal{C}_n$ is equivalent to a pair $({}^n\phi^\mu(X), {}^n\pi_\nu(X))$. The Poisson algebra induced on $\mathcal{C}_n$ by pulling back along the natural inclusion map $\mathcal{C}_n \hookrightarrow \Pi_n$ is given by

$$\{ {}^n\phi^\mu(X), {}^n\phi^\nu(X') \} = 0, \tag{49}$$

$$\{ {}^n\pi_\mu(X), {}^n\pi_\nu(X') \} = 0, \tag{50}$$

$$\{ {}^n\phi^\mu(X), {}^n\pi_\nu(X') \} = {}^nP^\mu_\nu \delta^{(4)}(X - X'), \tag{51}$$

and we note that $\mathcal{C}_n$ is symplectomorphic to the space of sections of the bundle $C_n \times \mathbb{R} \to \mathbb{R}$.

C. Poincaré covariance

As discussed in Sec. I. B. 3 for the case of the scalar field, the notion of two times leads naturally to the definition of two Poincaré groups. The external Poincaré group mixes the external time with the n-spatial variables $\mathbf{x}$ and the internal Poincaré group mixes internal time with $\mathbf{x}$. The crucial new feature of the generators for the vector field is the mixing of the time-like and space-like components of the field.

1. External Poincaré group

The generators of external space–time translations can be written in covariant looking form as

$${}^{\text{ext}}P^\mu_n = \int d^4X \, \pi^n_\nu(X) \partial^\mu \phi^\nu_n(X). \tag{52}$$

Next we define

$$M^{\mu\nu}_n = \int d^4X \, \pi^n_\rho(X) (X^\mu \partial^\nu - X^\nu \partial^\mu) \phi^\rho_n(X) + \sigma^{\mu\nu}_n, \tag{53}$$

where the "spin tensor" is

$$\sigma_n^{\mu\nu} = \int d^4X \pi_\rho^n(X)(\delta^{\rho\mu}\delta_\sigma^\nu - \delta^{\rho\nu}\delta_\sigma^\mu)\phi_n^\sigma(X). \tag{54}$$

By an "n-spatial rotation" we shall mean a rotation that leaves n fixed. n-spatial rotations can be parametrized by two vectors m^1 and m^2 satisfying $m^1 \cdot n = m^2 \cdot n = 0$ in the following way:

$$M_n(m^1, m^2) = m_\mu^1 m_\nu^2 M_n^{\mu\nu}. \tag{55}$$

As in the case of the scalar field, the external boosts cannot be implemented by canonical transformations because of the change in foliation. The natural definition of the automorphisms generated by the action of the external boosts is

$$\phi_n^\mu(t,\mathbf{x},0) \mapsto \Lambda_\nu^\mu \phi_{\Lambda n}^\nu(\Lambda(t,\mathbf{x}),0), \tag{56}$$

$$\pi_\mu^n(t,\mathbf{x},0) \mapsto \Lambda_\mu^\nu \pi_\nu^{\Lambda n}(\Lambda(t,\mathbf{x}),0). \tag{57}$$

So the external boosts mix t with $\mathbf{x}$, and the external time component $\phi_{\Lambda n}^t(t,\mathbf{x},0)$ with the space-like components ${}^{\Lambda n}\phi^\mu(t,\mathbf{x},0)$.

2. Internal Poincaré group

The n-spatial rotation and translation generators of the internal Poincaré group coincide with those for the external Poincaré group. However, internal time translations are generated by the Hamiltonian, and therefore act internally as $\phi_n^\mu(X) \mapsto \phi_n^\mu(X,s)$. We tentatively define the generator of internal Lorentz transformations on the $s = \text{const}$ hyperplane in the "obvious" way:

$${}^{\text{int}}K_n(m) := m_\mu \int d^4X[\pi_\nu^n s\partial^\mu \phi_n^\nu - X^\mu H_n(X)] + n_\mu m_\nu \sigma^{\mu\nu}, \tag{58}$$

where $H_n(X)$ is the Hamiltonian density, m is a vector satisfying $m \cdot n = 0$, and the integral is over the surface $s = \text{const}$. This functional generates the automorphisms

$$\phi_n^\mu(0,\mathbf{x},s) \mapsto \Lambda_\nu^\mu \phi_n^\nu(0,\Lambda(\mathbf{x},s)), \tag{59}$$

$$\pi_\mu^n(0,\mathbf{x},s) \mapsto \Lambda_\mu^\nu \pi_\nu^n(0,\Lambda(\mathbf{x},s)). \tag{60}$$

${}^{\text{int}}K_n(m)$ mixes s with $\mathbf{x}$, and $\phi_n^t(0,\mathbf{x},s)$ with ${}^n\phi_n^\mu(0,\mathbf{x},s)$. So in this transformation, the function $\phi_n^t(0,\mathbf{x},s)$ is associated with the *internal* time direction, whereas it was associated with the *external* time direction by the external boosts. These transformations are rather curious, and do not lead to a clear geometric interpretation of the history vector field.

D. Alternative interpretations of the history vector field

The above-presented discussion suggests that it is inappropriate to think of the history vector fields as a family of four-vectors on external space–time. We propose two alternative interpretations of the history vector fields.

1. Four-component fields

One way of thinking of the history fields is as a family of four-vectors, but with the temporal component in the $\partial_\tau := \partial_s + \partial_t$ direction,

$$\phi_n = \phi_n^\tau(X,s)\partial_\tau + \phi_n^i(X,s)\partial_i, \tag{61}$$

where $\phi_n^\tau(X,s) = \phi_n^t(X,s)$ and we have used coordinates adapted to n. From this perspective it is natural to look for a representation of the Poincaré group in which the boosts act in this direction. The internal boost generator on $s = 0$ would be

$$K_n(m) := \int d^4X[n\cdot X\pi^n_\mu(X)m_\nu\partial^\nu\phi^\mu_n(X) - m\cdot X(V_n(X)+H_n(X))], \tag{62}$$

where $V_n(X)$ is the ''Liouville'' density. However, it can be shown that

$$\{K_n(m^1),K_n(m^2)\} \neq m^1_\mu m^2_\nu M^{\mu\nu}_n, \tag{63}$$

even on the solutions to the equations of motion, and so the functionals $K_n(m)$ do not form a representation of the Poincaré group.

Thus it is not possible to eliminate the two times in favor of one ''physical'' time direction ∂_τ, in a covariant way. Nevertheless, τ does have a special significance in the theory. This is indicated by the equations of motion. Returning to the example of the scalar field for a moment, if $\phi_n(X)$ is a solution then $\{S_n,\phi_n(X)\}=0$ implies that

$$(\partial_s-\partial_t)\phi_n(X)|_{s=0}=0 \tag{64}$$

and so all the temporal change in such histories occurs in the τ direction.

2. Five-component fields

We can augment $\phi^\mu_n(X,s)$ with a new degree of freedom $\phi^s_n(X,s)$ to form $\tilde{\phi}^M_n(X,s)$, a five-component ''vector field'' on the extended space–time $\mathcal{N}=\mathcal{M}\times\mathbb{R}$. The extended fields are written

$$\tilde{\phi}_n=\tilde{\phi}^M_n(X,s)\partial_M, \quad \tilde{\pi}^n=\tilde{\pi}^n_M(X,s)\mathrm{d}x^M. \tag{65}$$

The label M runs over t, 1, 2, 3, s, where we define $M=t$ to refer to external time, $M=1,2,3$ to correspond to the spatial directions, and $M=s$ to refer to internal time.

The extended history space, $\tilde{\Pi}_n$, contains all ordered pairs $(\tilde{\phi}_n,\tilde{\pi}_n)$ that satisfy the internal field equations:

$$\partial_s\tilde{\phi}^M_n(X,s)=\{\tilde{H}_n,\tilde{\phi}^M_n(X,s)\}, \tag{66}$$

$$\partial_s\tilde{\pi}^n_M(X,s)=\{\tilde{H}_n,\tilde{\pi}^n_M(X,s)\}, \tag{67}$$

where $\tilde{H}_n$ is the Hamiltonian on extended history space, and is defined in Sec. II. E.

The history algebra can be extended to these fields in a natural way:

$$\{\tilde{\phi}^M_n(X),\tilde{\pi}^n_N(X')\}=\delta^M_N\delta^{(4)}(X-X'). \tag{68}$$

This defines the algebra of the fields on the surface $s=0$, which is a submanifold of $\mathcal{N}$. Hamiltonian evolution can be used to extend this definition to the rest of $\mathcal{N}$. The fact that the algebra is naturally defined on the hyperplane $s=0$ and not on the hyperplane $n\cdot X=0$ reflects the underlying asymmetry between the two ''modes'' of time. As a consequence of this asymmetry, the theory constructed from the fields $\tilde{\phi}_n$ will not be covariant under the full SO(2, 3) isometry group associated with $\mathcal{N}$. In particular it will not be covariant under the action of the SO(2) subgroup acting in the (s,t) plane.

In order to discuss the Poincaré transformations of the five-component fields, we make the definition:

$$\tilde{M}^{MN}_n=\int_{\mathcal{M}^{(e)}}d^4X\tilde{\pi}^n_R(X)(X^M\partial^N-X^N\partial^M)\tilde{\phi}^R_n(X)+\tilde{\sigma}^{MN}_n, \tag{69}$$

where $\mathcal{M}^{(e)} \subset \mathcal{N}$ is external space–time, defined as the surface $s=0$, and the extended spin tensor is defined as

$$\tilde{\sigma}_n^{MN} = \int_{\mathcal{M}^{(e)}} d^4X \tilde{\pi}_A^n(X)(\delta^{AM}\delta_B^N - \delta^{AN}\delta_B^M)\tilde{\phi}_n^B(X). \tag{70}$$

Using $\tilde{M}_n^{MN}$ we can write the rotation generators as

$$\tilde{M}_n(\tilde{m}^1,\tilde{m}^2) = \tilde{m}_M^1 \tilde{m}_N^2 \tilde{M}_n^{MN}, \tag{71}$$

where $\tilde{m}^1$ and $\tilde{m}^2$ are n-spatial in the sense that $\tilde{m}_M^1 \tilde{n}^M = \tilde{m}_M^1 \tilde{e}^M = 0$, and similarly for $\tilde{m}^2$.

The foliation vector n is an element of the external space–time which is a subspace of $\mathcal{N}$. Using the canonical embedding, n can be considered as a vector in $\mathcal{N}$, which we denote by $\tilde{n}$ and is given in coordinates (X,s) by $(n,0)$. Using this coordinate system the internal future pointing unit vector $\tilde{e}$ can be written as $(0,1)$. We can use these vectors to decompose an extended field $\tilde{\phi}_n^M(X,s)$ into its external and internal time components as follows:

$$\tilde{\phi}_n^t(X,s) = \tilde{n}_M \tilde{\phi}_n^M(X,s), \quad \tilde{\phi}_n^s(X,s) = \tilde{e}_M \tilde{\phi}_n^M(X,s). \tag{72}$$

Finally, given three orthogonal, n-spatial, unit vectors in $\mathcal{N}$, $\tilde{m}^i$, where $i=1,2,3$, the spatial components of $\tilde{\phi}_n^M(X,s)$ are

$$\tilde{\phi}_n^i(X,s) = \tilde{m}_M^i \tilde{\phi}_n^M(X,s). \tag{73}$$

Using this basis we write the action of the external boosts as

$$\tilde{\phi}_n^s(t,\mathbf{x},0) \mapsto \tilde{\phi}_{\Lambda n}^s(\Lambda(t,\mathbf{x}),0), \tag{74}$$

$$\tilde{\phi}_n^\mu(t,\mathbf{x},0) \mapsto \Lambda_\nu^\mu \tilde{\phi}_{\Lambda n}^\nu(\Lambda(t,\mathbf{x}),0), \tag{75}$$

$$\tilde{\pi}_s^n(t,\mathbf{x},0) \mapsto \tilde{\pi}_s^{\Lambda n}(\Lambda(t,\mathbf{x}),0), \tag{76}$$

$$\tilde{\pi}_\mu^n(t,\mathbf{x},0) \mapsto \Lambda_\mu^\nu \tilde{\pi}_\nu^{\Lambda n}(\Lambda(t,\mathbf{x}),0), \tag{77}$$

where μ takes the values t, 1, 2, 3.

Internal boosts are generated by

$${}^{\text{int}}\tilde{K}_n(\tilde{m}) := \tilde{m}_M \int_{\mathcal{M}_s^{(e)}} d^4X[\tilde{\pi}_N^n s\partial^M \tilde{\phi}_n^N - X^M \tilde{H}_n(X)] + \tilde{e}_M \tilde{m}_N \tilde{\sigma}_n^{MN}, \tag{78}$$

and the resultant automorphisms are

$$\tilde{\phi}_n^t(0,\mathbf{x},s) \mapsto \tilde{\phi}_n^t(0,\Lambda(\mathbf{x},s)), \tag{79}$$

$$\tilde{\phi}_n^{\bar{\mu}}(0,\mathbf{x},s) \mapsto \Lambda_{\bar{\nu}}^{\bar{\mu}} \tilde{\phi}_n^{\bar{\nu}}(0,\Lambda(\mathbf{x},s)), \tag{80}$$

$$\tilde{\pi}_t^n(0,\mathbf{x},s) \mapsto \tilde{\pi}_t^n(0,\Lambda(\mathbf{x},s)), \tag{81}$$

$$\tilde{\pi}_{\bar{\mu}}^n(0,\mathbf{x},s) \mapsto \Lambda_{\bar{\mu}}^{\bar{\nu}} \tilde{\pi}_{\bar{\nu}}^n(0,\Lambda(\mathbf{x},s)), \tag{82}$$

where $\bar{\mu}$ takes the values 1, 2, 3, s. Now the components of $\tilde{\phi}_n$ and $\tilde{\pi}^n$ are mixed in a way which is consistent with the mixing of the space–time variables. This indicates that the extended fields are an appropriate way of thinking about the history fields. However, it should be emphasized that

the extended fields are not covariant under SO(2, 3). Let V^M denote the vector defined by the field $\tilde{\phi}_n^M(X,s)$ at the point (X,s). Using the basis $(\tilde{n},\tilde{e},\tilde{m}^i)$, V^M can be decomposed into an "external" four-vector (V^t,V^i), or into an "internal" four-vector (V^s,V^i), and each of these four-vectors *is* a covariant object under the appropriate Poincaré group. This suggests a third interpretation of the history vector fields as *pairs* of four-component fields with identical n-spatial components. However, this identification is not preserved under the action of the boosts, so it seems that we are left with the five-vector interpretation as the only viable one.

It remains to be shown that the extra degrees of freedom can be included in the action in a way that is consistent with the symmetries and equations of motion of the theory.

E. The action

In the case of scalar field theory the physical action functional is written as $S_n = V_n - H_n$. The Liouville operator is associated with external time in the sense that it generates translations in the external time direction. In the same way, the Hamiltonian is associated with internal time, and the action functional mixes the two "modes" of time.

First we will need the following definition: The n-spatial part of $\tilde{\phi}_n^M(X,s)$ is defined as

$$ {}^n\tilde{\phi}^M(X,s) := {}^n\tilde{P}^M_N \tilde{\phi}^N(X,s), \tag{83}$$

where the extended n-spatial projection tensor is

$$ {}^n\tilde{P}^M_N := \delta^M_N - \tilde{n}^M\tilde{n}_N - \tilde{e}^M\tilde{e}_N. \tag{84}$$

Similarly we define ${}^n\partial^M := {}^n\tilde{P}^M_N\partial^N$.

Let $\tilde{V}_n$ denote the extension of the Liouville operator to the extended fields. $\tilde{V}_n$ is defined in the following natural way.

$$ \tilde{V}_n := \int_{\mathcal{M}^{(e)}} d^4X[\,\tilde{\pi}^n_s \partial^t_n \tilde{\phi}^s_n + \tilde{\pi}^n_t \partial^t_n \tilde{\phi}^t_n + {}^n\tilde{\pi}_M \partial^t_n {}^n\tilde{\phi}^M], \tag{85}$$

where $\partial^t_n := \tilde{n}_M\partial^M$ is the derivative in the external time direction defined by $\tilde{n}$. The extended Hamiltonian, $\tilde{H}_n$, is defined as

$$ \tilde{H}_n := \int_{\mathcal{M}^{(e)}} d^4X\left[\frac{1}{2}{}^n\tilde{\pi}_M\,{}^n\tilde{\pi}^M + \frac{1}{4}{}^n\tilde{\phi}_{MN}\,{}^n\tilde{\phi}^{MN} - \frac{1}{2}m^2(\tilde{\phi}^s_n)^2 \right.$$
$$ \left. - \frac{1}{2}m^2(\tilde{\phi}^t_n)^2 + \frac{1}{2}m^2\,{}^n\tilde{\phi}_M\,{}^n\tilde{\phi}^M - \tilde{\phi}^t_n\,{}^n\partial^M\,{}^n\tilde{\pi}_M\right]. \tag{86}$$

The important thing about this Hamiltonian is that $\tilde{\phi}^s_n$ and $\tilde{\phi}^t_n$ both appear in the mass term, but only $\tilde{\phi}^t_n$ appears as the coefficient of ${}^n\partial^M\,{}^n\tilde{\pi}_M$. Due to this asymmetry between $\tilde{\phi}^s_n$ and $\tilde{\phi}^t_n$, the Hamiltonian is not invariant under SO(2, 3). The action is defined to be $\tilde{S}_n := \tilde{V}_n - \tilde{H}_n$. The resulting field equations are

$$ \{\tilde{S}_n, \tilde{\phi}^s_n\} = 0 \Rightarrow \partial^t_n\tilde{\phi}^s_n = 0, \tag{87}$$

$$ \{\tilde{S}_n, \tilde{\pi}^n_s\} = 0 \Rightarrow \partial^t_n\tilde{\pi}^n_s + m^2\tilde{\phi}^s_n = 0, \tag{88}$$

$$ \{\tilde{S}_n, \tilde{\phi}^t_n\} = 0 \Rightarrow \partial^t_n\tilde{\phi}^t = 0, \tag{89}$$

$$ \{\tilde{S}_n, \tilde{\pi}^n_t\} = 0 \Rightarrow \partial^t_n\tilde{\pi}^n_t + m^2\tilde{\phi}^t_n + {}^n\partial^M\,{}^n\tilde{\pi}_M = 0, \tag{90}$$

$$\{\tilde{S}_n, {}^n\tilde{\phi}^M\}=0\Rightarrow\partial_n^t\,{}^n\tilde{\phi}^M-({}^n\tilde{\pi}^M+{}^n\partial^M\tilde{\phi}_n^t)=0, \tag{91}$$

$$\{\tilde{S}_n, {}^n\tilde{\pi}_M\}=0\Rightarrow\partial_n^t\,{}^n\tilde{\pi}_M-({}^n\partial^N\,{}^n\tilde{\phi}_{NM}+m^2\,{}^n\tilde{\phi}_M)=0. \tag{92}$$

The physical action has not been derived in the usual way from a Lagrangian, so we do not have the usual identification of primary constraints. The field equations do not determine the time-like components of the $\tilde{\pi}$ field, so we augment the equations of motion with the following equations which are interpreted as the primary constraints of the theory:

$$\tilde{\pi}_s^n(X)=0,\quad \tilde{\pi}_t^n(X)=0. \tag{93}$$

We require these constraints to be conserved in internal time which implies the following secondary constraints:

$$\tilde{\phi}_n^s(X)=0,\quad m^2\tilde{\phi}_n^t(X)+{}^n\partial^M\,{}^n\tilde{\pi}_M(X)=0, \tag{94}$$

so in the history theory of the massive vector field there are *two* pairs of second class constraints. In the state space theory a single pair of constraints allow the theory to be written in a Lorentz covariant way. In the five-component history theory where there are two SO(1, 3) symmetry groups, we have to introduce two pairs of constraints in order to have a covariant theory.

The three functionals, $\tilde{V}_n$, $\tilde{H}_n$, and $\tilde{S}_n$ are all invariant under the action of the internal Poincaré group. However, the external boosts change the foliation with respect to which $\tilde{V}_n$ and $\tilde{H}_n$ are defined, giving the transformations $\tilde{V}_n\mapsto\tilde{V}_{\Lambda n}$ and $\tilde{H}_n\mapsto\tilde{H}_{\Lambda n}$. These transformations imply $\tilde{S}_n\mapsto\tilde{S}_{\Lambda n}$, and the history theory is covariant under both Poincaré groups if we include the internal foliation dependence.

III. ELECTROMAGNETISM

A. State space theory

In this section we consider vacuum electromagnetism on $\mathcal{M}$. The covariant configuration space for electromagnetism is $Q=\Lambda^1(\mathcal{M})$, and the Lagrangian is

$$\mathcal{L}=-\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}, \tag{95}$$

where $F_{\mu\nu}(X):=2\partial_{[\mu}A_{\nu]}(X)$ for $A\in Q$. The covariant equations of motion which follow from this Lagrangian are

$$F^{\nu\mu}{}_{,\nu}(X)=0. \tag{96}$$

Given an embedding $\iota:\Sigma\to\mathcal{M}$, the canonical configuration space is $Q_\iota=T_\iota^*\mathrm{Emb}(\Sigma,\mathcal{M})$ and the state space, P_ι, can be identified with $Q_\iota\times T_\iota\mathrm{Emb}(\Sigma,\mathcal{M})$. The Poisson algebra on the state space associated with the embedding labeled by $(n,0)$ is

$$\{A_\mu^n(\mathbf{x}),A_\nu^n(\mathbf{x}')\}=0, \tag{97}$$

$$\{E_n^\mu(\mathbf{x}),E_n^\nu(\mathbf{x}')\}=0, \tag{98}$$

$$\{A_\mu^n(\mathbf{x}),E_n^\nu(\mathbf{x}')\}=\delta_\mu^\nu\delta_n^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{99}$$

The canonical momenta are computed from the Lagrangian;

$$E_n^t(\mathbf{x})=0,\quad {}^nE^\mu(\mathbf{x})={}^nP_\rho^\mu n_\nu F^{\nu\rho}(\mathbf{x}), \tag{100}$$

where we again use the decomposition into time-like and space-like parts. The canonical Hamiltonian is

$$H_n = \int_\Sigma \mathrm{d}\theta_{\mathbf{x}} \left[\frac{1}{2} {}^nE^\mu {}^nE_\mu + \frac{1}{4} {}^nF_{\mu\nu} {}^nF^{\mu\nu} - A_t^n {}^n\partial_\mu {}^nE^\mu \right]. \tag{101}$$

The equation of motion for E_n^t implies the secondary constraint

$$ {}^n\partial_\mu {}^nE^\mu(\mathbf{x}) = 0, \tag{102}$$

which can be recognized as Gauss' law. The constraints form a first class pair. The corresponding gauge freedom is manifested in the fact that the equations of motion do not determine A_t^n or A_L^n where A_L^n is the longitudinal part of A^n. The pull back of the symplectic two-form on P_n to the constraint surface C_n is degenerate because of the first class nature of the constraints. The reduced state space is obtained after gauge fixing and contains only four of the original eight degrees of freedom.

B. History theory

We follow the same procedure as before and consider sections of the trivial vector bundle $P \times \mathbb{R} \to \mathbb{R}$. So a history is a map

$$t \mapsto (A_\mu^n(t;x), E_n^\nu(t;x)), \tag{103}$$

and again, there is a unique pair $(A_\mu^n(X), E_n^\nu(X))$ corresponding to such a history so we fix an n and identify Π_n with the abstract space $\Lambda^1(\mathcal{M}) \times \mathcal{X}(\mathcal{M})$. These history fields satisfy the covariant looking algebra,

$$\{A_\mu^n(X), A_\nu^n(X')\} = 0, \tag{104}$$

$$\{E_n^\mu(X), E_n^\nu(X')\} = 0, \tag{105}$$

$$\{A_\mu^n(X), E_n^\nu(X')\} = \delta_\nu^\mu \, \delta^{(4)}(X - X'), \tag{106}$$

and the Liouville, Hamiltonian, and action operators are defined as

$$V_n := \int d^4X [E_n^t \partial_n^t A_t^n + {}^nE^\mu \partial_n^t {}^nA_\mu], \tag{107}$$

$$H_n := \int d^4X \left[\frac{1}{2} {}^nE_\mu {}^nE^\mu + \frac{1}{4} {}^nF_{\mu\nu} {}^nF^{\mu\nu} - A_t^n {}^n\partial^\mu {}^nE_\mu \right], \tag{108}$$

$$S_n := V_n - H_n . \tag{109}$$

C. Constraints

We follow the procedure detailed for the vector field and work in the extended history space $\tilde{\Pi}_n$. The extended history fields are written in the form

$$\tilde{A}^n = \tilde{A}_M^n(X,s)\mathrm{d}x^M, \quad \tilde{E}_n = \tilde{E}_n^M(X,s)\partial_M , \tag{110}$$

and using a basis we have the decomposition of $\tilde{A}^n$ into time-like and space-like components $(\tilde{A}_s^n, \tilde{A}_t^n, \tilde{A}_i^n)$. The transformations of the history electromagnetic field under the action of the

Poincaré group are very similar to the transformations of the vector field. From now on we fix an n, and work in coordinates adapted to n, dropping the n-label for typographical convenience. The new feature of electromagnetism is, of course, gauge invariance.

We extend the Liouville, Hamiltonian, and action functionals to the extended history space as

$$\tilde{V} := \int_{\mathcal{M}^{(e)}} d^4X[\tilde{E}^s \partial_t \tilde{A}_s + \tilde{E}^t \partial_t \tilde{A}_t + \tilde{E}^i \partial_t \tilde{A}_i], \tag{111}$$

$$\tilde{H} := \int_{\mathcal{M}^{(e)}} d^4X\left[\frac{1}{2}\tilde{E}_i \tilde{E}^i + \frac{1}{4}\tilde{F}_{ij}\tilde{F}^{ij} - \tilde{A}_t \partial^i \tilde{E}_i\right], \tag{112}$$

$$\tilde{S} := \tilde{V} - \tilde{H}. \tag{113}$$

As before we regard the equations

$$\tilde{E}^s(X) = 0, \quad \tilde{E}^t(X) = 0 \tag{114}$$

as the primary constraints of the theory. The corresponding secondary constraints follow from the Hamilitionian evolution of $\tilde{E}^s$ and $\tilde{E}^t$. The equation $\{\tilde{H}, \tilde{E}^s(X)\} = 0$ is identically satisfied and $\{\tilde{H}, \tilde{E}^t(X)\} = 0$ implies Gauss' law,

$$\partial_i \tilde{E}^i(X) = 0. \tag{115}$$

Gauss' law is conserved in internal time, $\{\tilde{H}, \partial_i \tilde{E}^i(X)\} = 0$, as a consequence of the antisymmetry of $\tilde{F}_{ij}$. Equations (114) and (115) are the first class constraints of the theory.

D. External local symmetries

To investigate the external local symmetries we define the extended action,[13]

$$\tilde{S}^E := \tilde{S} - \int_{\mathcal{M}^{(e)}} d^4X[\lambda_0 \tilde{E}^s + \lambda_1 \tilde{E}^t + \lambda_2 \partial_i \tilde{E}^i]. \tag{116}$$

The transformations

$$\delta \tilde{A}_s(X) = \epsilon_0(X), \tag{117}$$

$$\delta \tilde{A}_t(X) = \epsilon_1(X), \tag{118}$$

$$\delta \tilde{A}_i(X) = \partial_i \epsilon_2(X), \tag{119}$$

are generated by the functional

$$\psi = \int_{\mathcal{M}^{(e)}} d^4X[\epsilon_0 \tilde{E}^s + \epsilon_1 \tilde{E}^t + \epsilon_2 \partial_i \tilde{E}^i]. \tag{120}$$

The extended action is invariant under these transformations if

$$\delta \lambda_0(X) = \partial^t \epsilon_0(X), \tag{121}$$

$$\delta \lambda_1(X) = \partial^t \epsilon_1(X), \tag{122}$$

$$\delta \lambda_2(X) = \epsilon_1(X) - \partial^t \epsilon_2(X). \tag{123}$$

The symmetry of the total action, and therefore of the underlying Lagrangian theory is found by setting $\lambda_2=0$ (and $\delta\lambda_2=0$), thus eliminating the secondary constraint. The resulting transformations are

$$\delta\tilde{A}_s(X)=\epsilon_0(X), \tag{124}$$

$$\delta\tilde{A}_\mu(X)=\partial_\mu\epsilon_2(X), \tag{125}$$

where $\mu=t$, 1, 2, 3. These transformations contain two arbitrary real functions on external space–time. Setting $\epsilon_0=0$ we obtain "external" U(1) gauge transformations:

$$\delta\tilde{A}_\mu(X)=\partial_\mu\epsilon_2(X), \tag{126}$$

which correspond to the symmetries of the external Maxwell tensor $\tilde{F}_{\mu\nu}=2\partial_{[\mu}\tilde{A}_{\nu]}$.

E. Internal local symmetries

The map $\tilde{A}_M(X)\mapsto\tilde{A}_M(X,s)$ is one-to-many for gauge systems. This introduces an extra ambiguity into the theory which is not contained in Eqs. (124) and (125). We make this extra ambiguity explicit by introducing Lagrange multipliers to make the map $\tilde{A}_M(X)\mapsto\tilde{A}_M(X,s)$ one-to-one. To accomplish this we define the extended Hamiltonian,

$$\tilde{H}^E_s[\lambda_0,\lambda_1,\lambda_2]:=\tilde{H}-\int_{\mathcal{M}^{(e)}_s}d^4X[\lambda_0\tilde{E}^s+\lambda_1\tilde{E}^t+\lambda_2\partial_i\tilde{E}^i]. \tag{127}$$

At each moment of internal time s, the integral is over $\mathcal{M}^{(e)}_s$ (the surface $s=\text{const}$), and the Lagrange multipliers are arbitrary real valued functions $\lambda(\cdot,s):\mathcal{M}^{(e)}_s\to\mathbb{R}$. The extended Hamiltonian generates canonical transformations of the potential field

$$\partial_s\tilde{A}_M(X,s)=\{H^E_s,\tilde{A}_M(X,s)\}, \tag{128}$$

and the map $\tilde{A}_M(X)\mapsto\tilde{A}_M(X,s)$ is given by the flow of the time-dependent vector field generated by H^E_s. Thus $\tilde{A}_M(X,s)$ is the solution of the following integral equation:

$$\tilde{A}_M(X,s)=\tilde{A}_M(X,0)+\exp\left(\int_0^s ds'\{\tilde{H}^E_{s'},\tilde{A}_M(X,s')\}\right). \tag{129}$$

Because the transformation $\tilde{A}_M(X)\mapsto\tilde{A}_M(X,s)$ is canonical, it preserves the Poisson bracket so

$$\{\tilde{A}_M(X,s),\tilde{E}^N(X',s)\}=\delta^N_M\delta^{(4)}(X-X'). \tag{130}$$

Gauge-equivalent histories correspond to different choices of the Lagrange multipliers in the extended Hamiltonian. The functional defined by

$$\psi_s=\int_{\mathcal{M}^{(e)}_s}d^4X[\epsilon_0\tilde{E}^s+\epsilon_1\tilde{E}^t+\epsilon_2\partial_i\tilde{E}^i], \tag{131}$$

generates transformations on the fields on $\mathcal{M}^{(e)}_s$ as follows:

$$\delta\tilde{A}_M(X,s)=\{\psi_s,\tilde{A}_M(X,s)\}, \tag{132}$$

and these transformations take the form

$$\delta\tilde{A}_s(X,s)=\epsilon_0(X,s), \tag{133}$$

$$\delta\tilde{A}_t(X,s)=\epsilon_1(X,s), \tag{134}$$

$$\delta\tilde{A}_i(X,s)=\partial_i\epsilon_2(X,s). \tag{135}$$

In order that Eq. (128) is preserved by these transformations up to a change in the Lagrange multipliers associated with the primary constraints, the transformations must satisfy

$$\delta\tilde{A}_s(X,s)=\epsilon_0(X,s), \tag{136}$$

$$\delta\tilde{A}_t(X,s)=\partial_s\epsilon_2(X,s), \tag{137}$$

$$\delta\tilde{A}_i(X,s)=\partial_i\epsilon_2(X,s). \tag{138}$$

These are the internal local symmetry transformations of histories electromagnetism. They contain two arbitrary real valued functions on extended space–time, but are not just a trivial extension of the external local transformations to each moment of internal time. The transformation of $\tilde{A}_t$ contains a derivative with respect to internal time rather than external time. This is because the internal gauge transformations correspond to the symmetries of the internal field equations rather than the symmetries of the external field equations.

If we set $\epsilon_0=\partial^s\epsilon_2$ and restrict to a surface $t=$const, we obtain "internal" U(1) gauge transformations:

$$\delta\tilde{A}_{\bar{\mu}}(X,s)=\partial_{\bar{\mu}}\epsilon_2(X,s), \tag{139}$$

where $\bar{\mu}$ runs over $1, 2, 3, s$. These are the symmetries of the internal Maxwell tensor $\tilde{F}_{\bar{\mu}\bar{\nu}}=2\partial_{[\bar{\mu}}\tilde{A}_{\bar{\nu}]}$.

F. Internal versus external

An arbitrary history satisfies the internal equations of motion. Therefore all histories that are related by internal gauge transformations should be regarded as physically equivalent. However, most histories will not satisfy the external equations of motion, and so need not respect the external symmetry transformations. Histories which are solutions to the external equations of motion are invariant under both internal and external symmetry transformations.

An internal local symmetry transformation is also an external local symmetry transformation if and only if

$$(\partial^t-\partial^s)\epsilon_2(X,s)=0, \tag{140}$$

so the equation of motion $(\partial^t-\partial^s)\tilde{A}_\mu=0$ is conserved by these transformations. It is interesting to note that if Eq. (140) holds and we set $\epsilon_0=\partial^s\epsilon_2$ then we obtain U(1) gauge transformations on $\mathcal{N}$:

$$\delta\tilde{A}_M(X,s)=\partial_M\epsilon_2(X,s) \tag{141}$$

which are the symmetries of the five-dimensional Maxwell tensor $\tilde{F}_{MN}=\partial_{[M}\tilde{A}_{N]}$.

IV. SUMMARY AND CONCLUSION

We have shown that the global symmetry transformations of geometric objects in a history theory suggests the introduction of an extra pair of fields. The extended history fields can then be interpreted as fields on $\mathcal{N}=\mathcal{M}\times\mathbb{R}$ that are covariant under the action of two Poincaré groups, but not the SO(2, 3) group associated with $\mathcal{N}$. The history fields can be decomposed into two SO(1, 3)-vectors at each point in the extended space–time, where the spatial components of these two vectors are the same.

In the case of the massive vector field, the theory contains two pairs of second class constraints, and in the case of electromagnetism, we obtain three first class constraints. In both these examples, the extra degrees of freedom can be set to zero, and eliminated from the theory by taking Dirac brackets. It seems reasonable to expect this pattern to continue in the extension to other constrained field theories as there is no physical information in the extra degrees of freedom. So although Lorentz covariance suggests that the fields should have five components, the extra constraints allow the extra variables to be eliminated.

In conclusion, the geometry of classical history theories is not fully understood. In the state space approach the solutions to the field equations are sections of tensor bundles associated to an $\mathrm{SO}(1,3)$ principal bundle over $\mathcal{M}$. This formulation elegantly characterizes the way that the fields transform under Lorentz transformations. If the history fields were covariant under $\mathrm{SO}(2,3)$ then we would have a description of history fields in terms of sections of bundles associated to an $\mathrm{SO}(2,3)$ principal bundle over $\mathcal{N}$. However the reality of the situation appears to be more complicated. There is an $\mathrm{SO}(1,3)$ group associated to each surface of constant t, and to each surface of constant s, but the action of these two groups is intertwined in a nontrivial way. Similar remarks apply to the local symmetries in a history theory: they cannot be interpreted as the transformations of a $\mathrm{U}(1)$ connection on a principal bundle over $\mathcal{N}$.

In a subsequent paper we will discuss the quantization of histories electromagnetism using the BRST formalism.

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Poincaré invariance for continuous-time histories

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We show that the relativistic analog of the two types of time translation in a nonrelativistic history theory is the existence of two distinct *Poincaré groups*. The ''internal'' Poincaré group is analogous to the one that arises in the standard canonical quantization scheme; the ''external'' Poincaré group is similar to the group that arises in a *Lagrangian* description of the standard theory. In particular, it *performs explicit changes of the space–time foliation* that is implicitly assumed in standard canonical field theory. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The generalization of continuous-time history theory to include relativistic quantum fields raises some subtle issues that tend to be hidden in the normal canonical treatment of a quantum field.

The standard canonical quantization of a relativistic field requires the choice of a Lorentzian foliation on the background space–time: the Hamiltonian is then defined with respect to this foliation. There exist many unitarily inequivalent representations of the canonical commutation relations for this quantum field theory: the physically appropriate one is chosen by requiring that the Hamiltonian exists as a well-defined self-adjoint operator. In this sense—like the Hamiltonian itself—the physically appropriate representation is foliation dependent. Relativistic covariance is then implemented by seeking a representation of the Poincaré group on the resulting Hilbert space. However, the Poincaré group thus constructed does not explicitly perform a *change of the foliation*.

The HPO continuous-time histories approach to quantum theory[1–4] is particularly suited to deal with systems that have a nontrivial temporal structure, and therefore it should be able to provide a significant clarification of this point.

Specifically, we will show that the relativistic analog of the two types of time translation that arise in a nonrelativistic history theory is the existence of two distinct *Poincaré groups*. The ''internal'' Poincaré group is analogous to the one that arises in the standard canonical quantization scheme as sketched above.

However, the ''external'' one is a novel object: it is similar to the group that arises in the *Lagrangian* description of the field theory. In particular, it explicitly performs *changes* of the foliation. This arises from the striking property that HPO theories admit two distinct types of time transformation, each representing a distinct quality of time.[1] The first corresponds to time considered purely as a kinematical parameter of a physical system, with respect to which a history is defined as a succession of possible events. It is strongly connected with the temporal-logical structure of the theory and is related to the view of time as a parameter that determines the ordering of events. The second corresponds to the dynamical evolution generated by the Hamiltonian. For a detailed presentation of the HPO continuous-time program, see Ref. 1.

As we shall see, one of the important results of the formalism as applied to a field theory is that, even though the representations of the history algebra are foliation dependent, the physical quantities (probabilities) are *not*.

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In Sec. II, we shall give a brief description of the underlying concepts of the continuous-histories program: this is necessary for establishing the framework of the ensuing work.

In Sec. III, we present the histories version of a classical scalar field theory: in particular, we show how two Poincaré groups arise as an analog of the two types of time transformation in the nonrelativistic history theory.

The free quantum scalar field theory is presented in Sec. IV. We show that due to the histories' temporal structure previously introduced in Ref. 1, manifest Poincaré invariance is possible. Specifically, we show how different representations of the history algebra—corresponding to different choices of foliation—are realized on the *same* Fock space (notwithstanding the fact that the different representations are unitarily inequivalent), and we show that they are related in a certain way with Poincaré transformations.

II. THE HISTORY PROJECTION OPERATOR APPROACH

The history projection operator (the, so-called, ''HPO'' approach) theory was a development[2] (emphasizing quantum *temporal* logic) of the consistent-histories approach to quantum theory inaugurated by Griffiths, Omnés, Gell-Mann and Hartle.[5] However, the novel temporal structure introduced in Ref. 1 led to a departure from the original ideas on decoherence. In particular, in our approach, emphasis is placed on the distinction between (i) the temporal logic structure of the theory and (ii) the dynamics.[3]

In consistent-histories theory, a history is defined as a sequence of time-ordered propositions about properties of a physical system, each of which can be represented, as usual, by a projection operator. In normal quantum theory, it is not possible to assign a probability measure to the set of all histories. However, when a certain ''decoherence condition'' is satisfied by a set of histories, the elements of this set *can* be given probabilities.

The probability information of the theory is encoded in the decoherence functional: a complex function of pairs of histories which—in the original approach of Griffiths *et al.*—can be written as

$$d(\alpha,\beta)=\mathrm{tr}(\tilde{C}_\alpha^\dagger \rho \tilde{C}_\beta), \tag{2.1}$$

where ρ is the initial density-matrix, and where the *class operator* $\tilde{C}_\alpha$ is defined in terms of the standard Schrödinger-picture projection operators α_{t_i} as

$$\tilde{C}_\alpha := U(t_0,t_1)\alpha_{t_1}U(t_1,t_2)\alpha_{t_2}\cdots U(t_{n-1},t_n)\alpha_{t_n}U(t_n,t_0), \tag{2.2}$$

where $U(t,t')=e^{-i(t-t')H/\hbar}$ is the unitary time-evolution operator from time t to t'. Each projection operator α_{t_i} represents a proposition about the system at time t_i, and the class operator $\tilde{C}_\alpha$ represents the composite history proposition ''α_{t_1} is true at time t_1, and then α_{t_2} is true at time t_2, and then ..., and then α_{t_n} is true at time t_n.''

Isham and Linden developed the consistent-histories formalism further, concentrating on its *temporal* quantum logic structure.[2] They showed that propositions about the histories of a system could be represented by *projection operators* on a new, ''history'' Hilbert space. In particular, the history proposition ''α_{t_1} is true at time t_1, and then α_{t_2} is true at time t_2, and then ..., and then α_{t_n} is true at time t_n'' is represented by the *tensor product* $\alpha_{t_1}\otimes\alpha_{t_2}\otimes\cdots\otimes\alpha_{t_n}$ which, unlike $\tilde{C}_\alpha$, *is* a genuine projection operator that is defined on the tensor product of copies of the standard Hilbert space $\mathcal{H}_{t_1}\otimes\mathcal{H}_{t_2}\otimes\cdots\otimes\mathcal{H}_{t_n}$. Hence the ''history projection operator'' formalism extends to multiple times, the quantum logic of single-time quantum theory.

The history space. An important way of understanding the history Hilbert space $\mathcal{F}$ is in terms of the representations of the ''history group''—in elementary systems this is the history analog of the canonical group.[2] For example, for the simple case of a point particle moving on a line, the Lie algebra of the history group for a *continuous* time parameter t is described by the history commutation relations

$$[x_t, x_{t'}] = 0, \tag{2.3}$$

$$[p_t, p_{t'}] = 0, \tag{2.4}$$

$$[x_t, p_{t'}] = i\hbar\,\delta(t-t'), \tag{2.5}$$

where $-\infty \leqslant t, t' \leqslant \infty$. It is important to note that these operators are in the *Schrödinger* picture, and that the history algebra is invariant under translations of the time index of these operators.

The choice of the Dirac delta-function on the right hand side of Eq. (2.5) is associated with the requirement that time be treated as a continuous variable. One important consequence is the fact that the observables cannot be defined at sharp moments of time, but rather appear naturally as *time-averaged*.

A unique representation of this algebra can be found by requiring the existence of an operator analog of a time-averaged Hamiltonian $H = \int_{-\infty}^{\infty} dt\, H_t$, where H_t is the standard Hamiltonian defined at a moment of time t.[6]

The action and Liouville operators. One of the original problems in the development of the HPO theory was the lack of a clear notion of time evolution, in the sense that there was no natural way to express the time translations from one time slot—that refers to one copy of the Hilbert space $\mathcal{H}_t$—to another one that refers to another copy $\mathcal{H}_{t'}$. The situation changed with the introduction of the "*action*" *operator* S.

Indeed, the crucial step for constructing the temporal structure of the theory was the definition in Ref. 1 of the action operator S—a quantum analog of the Hamilton–Jacobi functional,[7] written as

$$S_\kappa := \int_{-\infty}^{+\infty} dt (p_t \dot{x}_t - \kappa(t) H_t), \tag{2.6}$$

where $\kappa(t)$ is an appropriate test function.

The first term of the action operator S_κ in Eq. (2.6) is identical to the kinematical part of the classical phase space action functional. This "Liouville" operator is formally written as

$$V := \int_{-\infty}^{\infty} dt\, (p_t \dot{x}_t) \tag{2.7}$$

so that

$$S_\kappa = V - H_\kappa. \tag{2.8}$$

A. The temporal structure

A fundamental property of the HPO form of history theory is that the Liouville operator V and the Hamiltonian operator H_κ generate two distinct types of time transformation. The Liouville operator V relates the Schrödinger-picture operators associated with different time-t labels, whereas H_t is associated with internal dynamical changes at the fixed time t (with an analogous statement for the smeared operator H_κ). The action operator S_κ is thus the generator of both types of time translation.[1]

More precisely, it was shown that there exist *two* distinct types of time transformation. One—generated by the Liouville operator V—refers to time as it appears in temporal logic, and it is related to t-label in Eqs. (2.3)–(2.5). The other—generated by the Hamiltonian—refers to time as it appears in the implementation of dynamical laws, and it is related to the label s in the "history Heisenberg picture" operator, which is hence defined in accord to the novel conceptual issues introduced with the "two modes of time,"

$$x_t(s) := e^{isH/\hbar} x_t e^{-isH/\hbar}, \tag{2.9}$$

where H is defined to be H_κ with κ set equal to 1.

We will use the notation $x_f(s)$ for these history Heisenberg-picture operators smeared with respect to the time label t, and we notice from Eq. (2.9) that these quantities behave like standard Heisenberg-picture operators with a time parameter s.

For any specific physical system these two transformations are intertwined with the aid of the action operator S as

$$e^{i\tau S/\hbar} x_f(s) e^{-i\tau S/\hbar} = x_{f_\tau}(s+\tau), \tag{2.10}$$

where $f_\tau(t) := f(t+\tau)$, and where S means S_κ with $\kappa = 1$.

B. Classical histories theory

The continuous-time histories description has a natural analog for classical histories.[3] In this scheme, the basic mathematical entity is the space $\Pi = C(\mathbb{R}, \Gamma)$ of differentiable paths taking their value in the manifold Γ of classical states. Hence an element of Π is a smooth path $\gamma: \mathbb{R} \to \Gamma$. In effect, we associate a copy of the classical state space with each moment of time, and employ differentiable sections of the ensuing bundle over $\mathbb{R}$.

The key idea in this approach to classical histories is contained in the symplectic structure on this space of temporal paths Π. For example, for a particle moving in one dimension (with configuration coordinate x and momentum coordinate p), the history space Π is equipped with a symplectic form

$$\omega = \int dt\, dp_t \wedge dx_t, \tag{2.11}$$

which generates the history Poisson brackets

$$\{x_t, x_{t'}\} = 0, \tag{2.12}$$

$$\{p_t, p_{t'}\} = 0, \tag{2.13}$$

$$\{x_t, p_{t'}\} = \delta(t - t'). \tag{2.14}$$

In general, given a function f on Γ we can define an associated family $t \mapsto F_t$ of functions on Π as

$$F_t(\gamma) := f(\gamma(t)). \tag{2.15}$$

In this way, all transformations implemented through the Poisson bracket in the normal canonical theory correspond to transformations in the history theory that *preserve the time label* t. Indeed, for two families of functions $t \mapsto F_t$ and $t \mapsto G_t$ defined through (2.15) we have

$$\{F_t, G_{t'}\} = L_t \delta(t, t'), \tag{2.16}$$

where L_t corresponds to the function l on Γ:

$$l = \{f, g\}_\Gamma. \tag{2.17}$$

In this way all relevant structures of the canonical theory can be naturally transferred to the histories framework.[3]

The Liouville, Hamilton and action functionals on Π are defined respectively as

$$V(\gamma) := \int_{-\infty}^{\infty} dt\, [p_t \dot{x}_t](\gamma), \tag{2.18}$$

$$H(\gamma) := \int_{-\infty}^{\infty} dt\,[H_t(p_t, x_t)](\gamma), \tag{2.19}$$

$$S(\gamma) := V(\gamma) - H(\gamma), \tag{2.20}$$

where $\dot{x}_t(\gamma) = (\partial x_t/\partial t)(\gamma)$ is the velocity at the time point t of the path γ. These definitions are crucial for the dynamics of the theory. In particular, V and H are the classical analogs of the generators of the two types of time transformation in the history quantum theory.[1]

The crucial result of classical histories theory is that one may deduce the equations of motion in the following way:[1] a classical history γ_{cl} is the realized path of the system—i.e., a solution of the equations of motion of the system—if it satisfies the equations

$$\{x_t, V\}(\gamma_{cl}) = \{x_t, H\}(\gamma_{cl}), \tag{2.21}$$

$$\{p_t, V\}(\gamma_{cl}) = \{p_t, H\}(\gamma_{cl}), \tag{2.22}$$

where γ_{cl} is the path $t \mapsto (x_t(\gamma_{cl}), p_t(\gamma_{cl}))$, and $x_t(\gamma_{cl})$ is the position coordinate of the realized path γ_{cl} at the time point t.

The equations (2.21)–(2.22) are the history equivalent of the canonical equations of motion. In particular, the symplectic transformation generated by the history action functional $S(\gamma)$ leaves invariant the paths that are classical solutions of the system:

$$\{x_t, S\}(\gamma_{cl}) = 0, \tag{2.23}$$

$$\{p_t, S\}(\gamma_{cl}) = 0. \tag{2.24}$$

More generally, any function F on Π satisfies the equation

$$\{F, S\}(\gamma_{cl}) = 0. \tag{2.25}$$

This is the way in which equations of motion appear in the classical history theory. Notice that the role of the action as the generator of time transformations emerges naturally in this classical case. Furthermore, the condition (2.25) above emphasizes the role of the Hamiltonian and Liouville functionals in histories theory as generators of different types of time transformation. It also clarifies the new temporal structure that arises in history theory when compared with the standard classical theory.

This result is of particular importance in the case of parameterized systems, where the notion of time is recovered *after the phase space reduction*.[3]

III. CLASSICAL SCALAR FIELD THEORY

A. Background

1. Standard canonical treatment

In the Hamiltonian description of a free scalar field ϕ with mass $\tilde{m}$ on Minkowski space–time, the first step is to choose a spacelike foliation, which can be specified by its normal—a unit timelike vector n^μ. We shall take the signature of the Minkowski metric $\eta^{\mu\nu}$ to be $(+,-,-,-)$.

The first step is to select a specific foliation, and to choose a reference leaf $\Sigma \simeq \mathbb{R}^3$ that is characterized by $t=0$, where t is the natural time label associated with the foliation.

The corresponding configuration space is the space $C^\infty(\Sigma)$ of all smooth scalar functions $\phi(x)$ on Σ, while the phase space Γ is its cotangent bundle $T^*C^\infty(\Sigma)$ defined in an appropriate way. [To make these statements mathematically rigorous it would be necessary to invoke the differential geometry of infinite-dimensional spaces like $C^\infty(\Sigma)$. However, we do not need to

become involved in such complexities here: for our purposes it suffices to postulate the basic Poisson algebra relations (3.12)–(3.14) that follow.] The key point about this structure is that the state space of fields is equipped with the Poisson brackets

$$\{\phi(\underline{x}),\phi(\underline{x}')\}=0, \tag{3.1}$$

$$\{\pi(\underline{x}),\pi(\underline{x}')\}=0, \tag{3.2}$$

$$\{\phi(\underline{x}),\pi(\underline{x}')\}=\delta(\underline{x}-\underline{x}'). \tag{3.3}$$

Poincaré group symmetry. The relativistic scalar field theory is covariant under the action of the Poincaré group.[8] For a free massive scalar field, the generators of time translations P^0, space translations P^i, spatial rotations J^i and Lorentz boosts K^i are respectively (obtained by the use of Noether's theorem on the Lagrangian theory, and a Legendre transform)

$$H=P^0=\frac{1}{2}\int d^3\underline{x}\,[\pi^2+\partial_i\phi\partial_i\phi+\tilde{m}^2\phi^2], \tag{3.4}$$

$$P^i=\int d^3\underline{x}\;\pi\partial^i\phi, \tag{3.5}$$

$$J^i=\frac{1}{2}\epsilon^{ijk}\int d^3\underline{x}\;\pi x_j\partial_k\phi, \tag{3.6}$$

$$K^i=M^{0i}=\int d^3\underline{x}\left[t\pi\partial^i\phi-x^i\frac{1}{2}(\pi^2+\partial_j\phi\partial_j\phi+\tilde{m}^2\phi^2)\right], \tag{3.7}$$

where we note that the sub/superscripts i,j,k refer to coordinates in the surface Σ that is spatial with respect to the chosen foliation vector n. Similarly, the integrals above are all defined over Σ.

If we define the partial differential operator

$$(\Gamma f)(\underline{x}):=[(\eta^{\mu\nu}-n^\mu n^\nu)\partial_\mu\partial_\nu+\tilde{m}^2]f(\underline{x}), \tag{3.8}$$

we can write the convenient expressions for the Hamiltonian and the boosts generator as

$$H=\frac{1}{2}\int d^3\underline{x}\,[\pi^2+\phi\Gamma\phi], \tag{3.9}$$

$$K^i=\int d^3\underline{x}\left[t\pi\partial^i\phi-\frac{1}{2}x^i(\pi^2+\phi\Gamma\phi)\right]. \tag{3.10}$$

For the special case of hypersurface $t=0$ the boost generator is written as

$$K^i=\int d^3\underline{x}\left[-\frac{1}{2}x^i(\pi^2+\phi\Gamma\phi)\right]. \tag{3.11}$$

B. Histories description for the classical scalar field

In the histories formalism of a scalar field, the space of phase-space histories Π is an appropriate subset of the continuous Cartesian product $\times_t\Gamma_t$ of copies of the standard state space Γ, each labeled by the time parameter t. (One may write a history version of the Lagrangian treatment, however this description is not relevant to the immediate aims of this work.) The choice of Γ depends on the choice of a foliation vector n^μ, hence the space of histories also has an implicit

dependence on n^μ and should therefore be written as ${}^n\Pi$. Furthermore, we write $\Sigma_t=(n,t)$, the spacelike surface Σ defined with respect to its normal vector n, and labeled by the parameter t.

To be more precise, for each spacelike surface Σ_t we consider the state space $\Gamma_t = T^*C^\infty(\Sigma_t)$. Then we define the fiber bundle with basis $\mathbb{R}$ and fiber Γ_t, at each $t\in\mathbb{R}$. Histories are defined as the cross-sections of the ensuing bundle, and the history space ${}^n\Pi$ is the space of all smooth cross-sections of this bundle.

The Poisson algebra relations of the history theory are

$$\{\phi(X),\phi(X')\}=0, \tag{3.12}$$

$$\{\pi(X),\pi(X')\}=0, \tag{3.13}$$

$$\{\phi(X),\pi(X')\}=\delta^4(X-X'), \tag{3.14}$$

where X and X' are space–time points. The field $\phi(X)$ and its conjugate momentum $\pi(X')$ are implicitly defined with respect to the foliation vector n^μ.

The definitions of the action S, Liouville V and "Hamiltonian" H functionals are

$$S:=V-\frac{1}{2}\int d^4X\{\pi^2(X)+\phi(X)\,{}^n\Gamma\,\phi(X)\}, \tag{3.15}$$

$$V:=\int d^4X\,\pi(X)n^\mu\partial_\mu\,\phi(X), \tag{3.16}$$

$$H:=\frac{1}{2}\int d^4X\{\pi^2(X)+\phi(X)\,{}^n\Gamma\,\phi(X)\}, \tag{3.17}$$

respectively, where again there is an implicit n label on these three quantities, and where Γ is the differential operator

$$\Gamma:=[(\eta^{\mu\nu}-n^\mu n^\nu)\partial_\mu\partial_\nu+\tilde{m}^2] \tag{3.18}$$

introduced above.

As we explained earlier, the variation of $S[\gamma]$ leaves invariant the paths γ_{cl} that are classical solutions of the system:

$$\{\phi(X),S\}(\gamma_{cl})=0, \tag{3.19}$$

$$\{\pi(X),S\}(\gamma_{cl})=0. \tag{3.20}$$

As we shall now see, H is the generator to the time averaged internal Poincaré group.

C. Poincaré symmetry

The Poincaré group is the group of isometries of the Minkowski metric. Hence, any field theory in Minkowski space–time needs to be covariant under the action of the Poincaré group. As we shall now see, in a history theory—because of its augmented temporal structure—the associated group theory leads to a particular interesting result: namely, there are *two* distinct Poincaré groups that act on the history space.

1. The internal Poincaré group

One significant feature of histories theory is that it gives a representation of the temporal logic of the system that is *independent* of the dynamics involved. Hence, propositions about the state of the system at different times are represented by appropriate subsets of the space of paths. In the context of symmetries, however, the temporal logic structure entails the following.

For each copy Γ_t of the standard state space, there exists a Poincarè group symmetry of the type one would expect in a canonical treatment of relativistic field theory. On the other hand, in the history theory the state space is heuristically the Cartesian product of such copies, and all physical quantities in the standard treatment now appear as naturally time-averaged.[1] Hence one may write time-averaged generators of the *internal* Poincaré groups, in a covariantlike notation, as

$$H=\frac{1}{2}\int d^4X\,\{\pi(X)^2+\phi(X)\,{}^n\Gamma\,\phi(X)\}, \tag{3.21}$$

$$P(m)=m_\mu\int d^4X\,\pi(X)\,\partial^\mu\,\phi(X), \tag{3.22}$$

$$J(m)=\frac{1}{2}n_\mu m_\nu\epsilon^{\mu\nu\rho\sigma}\int d^4X\,\pi(X)\,X_\rho\,\partial_\sigma\,\phi(X), \tag{3.23}$$

$$K(m)=m_\mu\int d^4X\left\{-\frac{1}{2}X^\mu[\,\pi(X)^2+\phi(X)\,{}^n\Gamma\,\phi(X)]\right\}, \tag{3.24}$$

where m^μ is an "n-spacelike" vector, i.e., one such that $n\cdot m:=n^\mu m^\nu\eta_{\mu\nu}=0$ and $K(m)$ is written for the special case of hypersurface $s=0$.

Of special interest are the groups of canonical transformations generated by the Hamiltonian generator H and the boosts generator K. Note that a space–time point X can be associated with the pair $(t,\underline{x})\in\mathbb{R}\times\mathbb{R}^3$, as $X=tn+x_n$, where the three-vector $\underline{x}$ has been associated with a corresponding n-spatial four-vector x_n (i.e., $n\cdot x_n=0$); note that $t=n\cdot X$. Then we define the classical analog of the Heisenberg picture fields as

$$\phi(X)\underset{\longrightarrow}{H}\phi(X,s) \tag{3.25}$$

or

$$\phi(t,\underline{x})\underset{\longrightarrow}{H}\phi(t,\underline{x},s):=\cos({}^n\Gamma^{1/2}s)\,\phi(X)+\frac{1}{{}^n\Gamma^{1/2}}\sin({}^n\Gamma^{1/2}s)\,\pi(X), \tag{3.26}$$

where $\phi(X):=\phi(t,\underline{x})$ and $\phi(X,s):=\phi(t,\underline{x},s)$. The square-root operator ${}^n\Gamma^{1/2}$, and functions thereof, can be defined rigorously using the spectral theory of the self-adjoint, partial differential operator ${}^n\Gamma$ on the Hilbert space $L^2(\mathbb{R}^4,d^4X)$.

Notice also that the time label t is not affected by this transformation since $[\,n\cdot\partial,\,{}^n\Gamma\,]=0$. For a fixed value of time t, the field $\phi(t,\underline{x},s)$ is the "Heisenberg-picture" field of the standard canonical treatment.

The action of boost transformations is best shown upon objects $\phi(X,s)=\phi(t,\underline{x},s)$ as

$$\phi(t,\underline{x},s)\rightarrow\phi(t,\underline{x}',s'), \tag{3.27}$$

where $(\underline{x}',s')$ and $(\underline{x},s)$ are related by the Lorentz boost parametrized by m^μ as

$$s'=\cosh|m|s+\frac{\sinh|m|}{|m|}x^i m_i\,,$$

$$x^{i\prime}=\left(\delta_{ij}-\frac{m^i m_j}{|m|^2}\right)x^j+\frac{m^i m_j}{|m|^2}\cosh|m|x^j+\frac{\sinh|m|}{|m|}m^i s, \tag{3.28}$$

where, as above, x_i is the spatial part of X with respect to n, so that $X=tn+x_n$ and $i=1,2,3$.

Hence, for each copy of the standard classical state space, there exists an ''internal'' Poincarè group that acts on the copy of standard canonical field theory that is labeled by the same t-time label.

2. The external Poincaré group

For each fixed n, there also exists an ''*external*'' Poincaré group with generators

$$\tilde{P}^{\mu}=\int d^4X\,\pi(X)\partial^{\mu}\phi(X), \tag{3.29}$$

$$\tilde{M}^{\mu\nu}=\int d^4X\,\pi(X)(X^{\mu}\partial^{\nu}-X^{\nu}\partial^{\mu})\phi(X), \tag{3.30}$$

where $\mu,\nu=0,1,2,3$ and $\tilde{P}^{\mu}$ generate space–time translations. The n-spatial parts of the tensor $\tilde{M}^{\mu\nu}$ generate spatial rotations; the time parts generate boosts.

The space translations and rotations are identical to those of the *internal* Poincaré group. However, the time translation and the boosts differ. Indeed, under $V:=\tilde{P}^0$ we have

$$\phi(t,\underline{x}) \underset{\rightarrow}{V} \phi(t+\tau,\underline{x}), \tag{3.31}$$

$$\pi(t,\underline{x}) \underset{\rightarrow}{V} \pi(t+\tau,\underline{x}), \tag{3.32}$$

where τ is the time translation generated by V. Thus, what we have shown here is that the time-translation generator for the ''external'' Poincaré group is the Liouville functional V. On the other hand, the boost generator $\tilde{K}^i=\tilde{M}^{0i}$ generates Lorentz transformations of the type

$$\phi(X)\rightarrow\phi(\Lambda X), \tag{3.33}$$

$$\pi(X)\rightarrow\pi(\Lambda X), \tag{3.34}$$

where for future convenience we write as Λ the element of the Lorentz group obtained by exponentiation of the boost parameterized by m^i.

Furthermore, under the action of this external group, the generators of the *internal* Poincaré group transform as follows

$${}^nH \underset{\rightarrow}{\tilde{K}} {}^{\Lambda n}H, \tag{3.35}$$

$${}^nK(m) \underset{\rightarrow}{\tilde{K}} {}^{\Lambda n}K(\Lambda m), \tag{3.36}$$

where we have now attached the explicit n labels that were implicit in our previous notation for these quantities. The action functional transforms in the same way

$${}^nS\rightarrow{}^{\Lambda n}S. \tag{3.37}$$

Note that the action of the two groups coincides on classical solutions γ_{cl}:

$$\{\phi(X),K(m)\}(\gamma_{cl})=\{\phi(X),\tilde{K}(m)\}(\gamma_{cl}), \tag{3.38}$$

$$\{\pi(X),K(m)\}(\gamma_{cl})=\{\pi(X),\tilde{K}(m)\}(\gamma_{cl}). \tag{3.39}$$

We must emphasize again that the definition of Π depends on the foliation vector. Hence, so will the action of the Poincaré group. Here we deal with the scalar field, for which this dependence is not explicit. However, this dependence, and analog of the Poincaré group action, is a major feature in systems where there is an explicit foliation dependence. For example, this is the case of general relativity which is discussed in Ref. 9.

IV. HISTORIES QUANTUM SCALAR FIELD THEORY

A. Background

1. Canonical quantum field theory

Canonical quantization proceeds by looking for a representation of the *canonical commutation relations*

$$[\hat{\phi}(\underline{x}),\hat{\phi}(\underline{x}')]=0, \tag{4.1}$$

$$[\hat{\pi}(\underline{x}),\hat{\pi}(\underline{x}')]=0, \tag{4.2}$$

$$[\hat{\phi}(\underline{x}),\hat{\pi}(\underline{x}')]=i\hbar\,\delta^3(\underline{x}-\underline{x}') \tag{4.3}$$

on a Hilbert space which, in practice, is selected by requiring the existence of the Hamiltonian as a genuine (essentially) self-adjoint operator.

For a free field, such a representation can be found on the Fock space $\mathcal{F}=\exp L^2(\mathbb{R}^3, d^3\underline{x})$ on which the fields can be written in terms of the creation and annihilation operators b and $b^\dagger$ that define $\mathcal{F}$

$$\hat{\phi}(\underline{x})=\frac{1}{\sqrt{2}}{}^n\Gamma^{-1/4}(\hat{b}(\underline{x})+\hat{b}^\dagger(\underline{x})), \tag{4.4}$$

$$\hat{\pi}(\underline{x})=\frac{1}{\sqrt{2}}{}^n\Gamma^{1/4}(\hat{b}(\underline{x})-\hat{b}^\dagger(\underline{x})), \tag{4.5}$$

where

$$[b(\underline{x}),b^\dagger(\underline{x}')]=\delta^3(\underline{x}-\underline{x}'). \tag{4.6}$$

The (normal-ordered) Hamiltonian then reads

$$\hat{H}=\int d^3\underline{x}\hat{b}^\dagger(\underline{x})\,{}^n\Gamma^{1/2}\,\hat{b}(\underline{x})=\sum_{\mathbf{k}}\,\omega_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}}. \tag{4.7}$$

(In momentum space we write b and $b^\dagger$ from the well known relation $b_{\mathbf{k}}=\sqrt{\omega_{\mathbf{k}}/2}\phi_{\mathbf{k}}+i/\sqrt{2\omega_{\mathbf{k}}}\pi_{\mathbf{k}}$.)

Poincaré group symmetry. A representation of the full Poincaré group exists on this Hilbert space. The starting point is the generators of the classical theory, suitably normal-ordered to correspond to well-defined operators. Substituting the fields in terms of creation and annihilation operators, the generators can be written as

$$\hat{P}^i=i\int d^3\underline{x}\hat{b}^\dagger(\underline{x})\,\partial^i\,\hat{b}(\underline{x}), \tag{4.8}$$

$$\hat{J}^i=i\,\epsilon^{ijk}\int d^3\underline{x}\hat{b}^\dagger(\underline{x})\,x_j\,\partial_k\,\hat{b}(\underline{x}), \tag{4.9}$$

$$\hat{K}^i = \int d^3\underline{x}\,\hat{b}^\dagger(\underline{x})\,{}^n\Gamma^{1/4}\,x^i\,{}^n\Gamma^{1/4}\,\hat{b}(\underline{x}). \tag{4.10}$$

These generators, together with $\hat{H}$ defined in Eq. (4.7), satisfy the Lie algebra relations of the Poincaré group.

In the canonical picture, the covariant fields are obtained by the Heisenberg equations of motion:

$$\hat{\phi}(\underline{x},s) := e^{(i/\hbar)\,s\hat{H}}\hat{\phi}(\underline{x})e^{-(i/\hbar)\,s\hat{H}} = \cos({}^n\Gamma^{1/2}s)\,\hat{\phi}(\underline{x}) + {}^n\Gamma^{-1/2}\sin({}^n\Gamma^{1/2}s)\,\hat{\pi}(\underline{x}), \tag{4.11}$$

$$\hat{\pi}(\underline{x},s) := e^{(i/\hbar)\,s\hat{H}}\hat{\pi}(\underline{x})e^{-(i/\hbar)\,s\hat{H}} = -{}^n\Gamma^{1/2}\sin({}^n\Gamma^{1/2}s)\,\hat{\phi}(\underline{x}) + \cos({}^n\Gamma^{1/2}s)\,\hat{\pi}(\underline{x}). \tag{4.12}$$

The explicit automorphisms generated by the boosts may easily be calculated for the Heisenberg picture creation and annihilation operators,

$$\hat{b}(\underline{x},s) := e^{(i/\hbar)\,s\hat{H}}\hat{b}(\underline{x})e^{-(i/\hbar)\,s\hat{H}} = e^{-is\,{}^n\Gamma}\hat{b}(\underline{x}), \tag{4.13}$$

and they give

$$e^{im_i\hat{K}^i}\hat{b}(\underline{x},s)e^{-im_i\hat{K}^i} = \hat{b}(\underline{x}',s'), \tag{4.14}$$

where the transformation $(\underline{x},s)\mapsto(\underline{x}',s')$ is given by Eq. (3.28), so that we can write

$$e^{im_i\hat{K}^i}\quad\hat{b}(\underline{x},s)e^{-im_i\hat{K}^i} = \hat{b}(\Lambda(\underline{x},s)). \tag{4.15}$$

From this, one can write the explicit transformation laws for the Heisenberg fields $\hat{\phi}(\underline{x},s)$ and $\hat{\pi}(\underline{x},s)$.

Some questions that arise in the canonical treatment. The first question that arises in this standard treatment is whether the Poincaré transformations are associated with any changes of foliation. Working canonically *there is no trace of the foliation vector* on the Fock space defined by Eq. (4.6), so this question cannot readily be answered.

Being able to talk about foliations is a necessary step if we are to elucidate the space–time character of a quantum theory, in which the parameter s of the Heisenberg-picture objects corresponds to the foliation time parameter in space–time. For example, the physical meaning of the parameter s of the Heisenberg objects depends on the choice of foliation vector.

B. Histories quantum field theory

Quantum mechanics histories. As we have already mentioned in Sec. II, the introduction of the history group[2] as an analog of the canonical group relates the spectral projectors of the generators of its Lie algebra with propositions about history phase space quantities. This algebra is infinite-dimensional and therefore there exist infinitely many representations. However, the physically appropriate representation of the smeared history algebra can be uniquely selected by the requirement that the time-averaged energy exists as a proper self-adjoint operator.[2] The resulting Hilbert space has a natural interpretation as a continuous-tensor product: hence by this means we also gain a natural mathematical implementation of the concept of ''continuous'' temporal logic.

1. Histories Hamiltonian algebra

We shall now apply the histories ideas to relativistic quantum field theory on Minkowski space–time. The representation of the history algebra is to be selected by requiring that the time-averaged energy $H_\chi = \int d^4X\,\chi(t)H_t$ (which is associated with history propositions about

temporal averages of the energy) exists as a proper essentially self-adjoint operator.[2] In what follows, for the sake of typographical simplicity we will no longer use hats to indicate quantum operators.

We start with the abstract algebra

$$[\phi(X),\phi(X')]=0, \tag{4.16}$$

$$[\pi(X),\pi(X')]=0, \tag{4.17}$$

$$[\phi(X),\pi(X')]=i\hbar\,\delta^4(X-X'), \tag{4.18}$$

where X and X' are space–time points.

In order to find suitable representations of this algebra we start with the Fock space $\mathcal{F}:=\exp L^2(\mathbb{R}^4,d^4X)$ in which there is a natural definition of creation and annihilation operators $b(X)$ and $b^\dagger(X)$ that satisfy the commutation relations

$$[b(X),b(X')]=0, \tag{4.19}$$

$$[b^\dagger(X),b^\dagger(X')]=0, \tag{4.20}$$

$$[b(X),b^\dagger(X')]=\hbar\,\delta^4(X-X'). \tag{4.21}$$

An appropriate representation of the Poincaré group can be defined by requiring

$$U(\Lambda)b(X)U(\Lambda)^\dagger=b(\Lambda X), \tag{4.22}$$

$$U(\Lambda)|0\rangle=|0\rangle, \tag{4.23}$$

where $|0\rangle$ is the cyclic ''vacuum'' state for the theory. Then clearly history fields can be defined by

$$\phi(X):=\frac{1}{\sqrt{2}}(b(X)+b^\dagger(X)), \tag{4.24}$$

$$\pi(X):=\frac{1}{i\sqrt{2}}(b(X)-b^\dagger(X)), \tag{4.25}$$

and satisfy Eqs. (4.16)–(4.18). They also transform in the obvious covariant way under the operators $U(\Lambda)$ introduced above.

It should be emphasized that the fields $\phi(X)$ and $\pi(X)$ thus defined *do not* have any foliation vector dependence. However, an operator H_χ of the time-averaged energy of the system *cannot* be well defined so that it depends functionally on these fields in the usual way.

Hence we must seek a different, and more physically appropriate, representation for the history algebra on the history Hilbert space $\mathcal{F}$.

We start by making a *fixed* choice of a unit timelike vector n which we use to foliate the four-dimensional Minkowski space–time. It is clear that the average-energy operator is itself dependent upon the choice of foliation n, and therefore this must also be true for the elements of the history algebra. Hence to emphasize that the physically appropriate representation depends on n we rewrite the history commutation relations as

$$[{}^n\phi(X),{}^n\phi(X')]=0, \tag{4.26}$$

$$[{}^n\pi(X),{}^n\pi(X')]=0, \tag{4.27}$$

$$[{}^n\phi(X),{}^n\pi(X')]=i\hbar\,\delta^4(X-X'), \tag{4.28}$$

where X and X' are space–time points. The dependence of the representation of the history algebra on the choice of the timelike foliation vector n is indicated by the upper left symbol for the field ${}^n\phi(X)$ and its "conjugate" ${}^n\pi(X)$.

One may also write the canonical version of the history algebra. Notice that—as in the discussion above of classical history theory—in relating Eqs. (4.26)–(4.28) with the canonical version of the history algebra the three-vector $\underline{x}$ may be equated with a four-vector x_n that satisfies $n\cdot x_n=0$ (the dot product is taken with respect to the Minkowski metric $\eta_{\mu\nu}$) so that the pair $(t,\underline{x})\in\mathbb{R}\times\mathbb{R}^3$ is associated with the space–time point $X=tn+x_n$ (in particular, $t=n\cdot X$). The canonical history commutation relations can be written therefore as

$$[{}^n\phi(t,\underline{x}),{}^n\phi(t',\underline{x}')]=0, \tag{4.29}$$

$$[{}^n\pi(t,\underline{x}),{}^n\pi(t',\underline{x}')]=0, \tag{4.30}$$

$$[{}^n\phi(t,\underline{x}),{}^n\pi(t',\underline{x}')]=i\hbar\,\delta(t-t')\,\delta^3(\underline{x}-\underline{x}'), \tag{4.31}$$

where, for each $t\in\mathbb{R}$, the fields ${}^n\phi(t,\underline{x})$ and ${}^n\pi(t,\underline{x})$ are associated with the spacelike hypersurface $\Sigma_t=(n,t)$, characterized by the normal vector n and by the foliation parameter t. In particular, the three-vector $\underline{x}$ in ${}^n\phi(t,\underline{x})$ or in ${}^n\pi(t,\underline{x})$ denotes a vector in this space.

A central feature of the approach that is followed in this work for the histories quantum field theory is that, for all foliation vectors n, the corresponding foliation-dependent representations of the history algebra Eqs. (4.26)–(4.28) can all be realized on the *same* Fock space $\mathcal{F}=\exp L^2(\mathbb{R}^4,d^4X)$ that also carries the "covariant" fields $\phi(X)$ and $\pi(X)$ defined in Eqs. (4.24) and (4.25).

The foliation-dependent fields ${}^n\phi(X)$ and ${}^n\pi(X)$ are expressed in terms of the covariant creation and annihilation operators of $\exp L^2(\mathbb{R}^4,d^4X)$, and the related covariant fields $\phi(X)$ and $\pi(X)$ of Eqs. (4.26)–(4.28), as

$${}^n\phi(X)=\frac{1}{\sqrt{2}}\,{}^n\Gamma^{-1/4}(b(X)+b^\dagger(X))={}^n\Gamma^{-1/4}\phi(X), \tag{4.32}$$

$${}^n\pi(X)=\frac{1}{i\sqrt{2}}\,{}^n\Gamma^{1/4}(b(X)-b^\dagger(X))={}^n\Gamma^{1/4}\pi(X), \tag{4.33}$$

and, conversely,

$$b(X)=\frac{1}{\sqrt{2}}(\phi(X)+i\,\pi(X))=\frac{1}{\sqrt{2}}({}^n\Gamma^{1/4}\,{}^n\phi(X)+i\,{}^n\Gamma^{-1/4}\,{}^n\pi(X)) \tag{4.34}$$

$$b^\dagger(X)=\frac{1}{\sqrt{2}}(\phi(X)-i\,\pi(X))=\frac{1}{\sqrt{2}}({}^n\Gamma^{1/4n}\phi(X)-i\,{}^n\Gamma^{-1/4}\,{}^n\pi(X)), \tag{4.35}$$

where ${}^n\Gamma$ denotes the partial differential operator defined in Eq. (3.18) on the Hilbert space $L^2(\mathbb{R}^4,d^4X)$.

For a fixed foliation vector n, we seek a family of "internal" Hamiltonians ${}^nH_t$, $t\in\mathbb{R}$, whose explicit formal expression may be deduced from the standard quantum field theory expression to be

$${}^nH_t:=\frac{1}{2}\int d^4X\{{}^n\pi(X)^2+(n^\mu n^\nu-\eta^{\mu\nu})\partial_\mu\,{}^n\phi(X)\partial_\nu\,{}^n\phi(X)+\tilde{m}^2\,{}^n\phi(X)^2\}\delta(t-n\cdot X). \tag{4.36}$$

The corresponding smeared expression (which must be normal-ordered to be well defined) is

$$ {}^nH_\chi := \int_{-\infty}^{\infty} dt\chi(t)\, {}^nH_t = \frac{1}{2}{:}\int d^4X\{{}^n\pi(X)^2 + (n^\mu n^\nu - \eta^{\mu\nu})\partial_\mu {}^n\phi(X)\partial_\nu {}^n\phi(X) + \tilde{m}^2\, {}^n\phi(X)^2\}\chi(n\cdot X){:}, \tag{4.37} $$

where χ is a real-valued test function.

We next augment the history algebra with the following commutation relations that would be satisfied by the operators ${}^nH(\chi)$, if they existed:

$$ [{}^nH_\chi, {}^n\phi(X)] = -i\hbar\chi(n\cdot X)\, {}^n\pi(X), \tag{4.38} $$

$$ [{}^nH_\chi, {}^n\pi(X)] = i\hbar\chi(n\cdot X)\, {}^n\Gamma\, {}^n\phi(X), \tag{4.39} $$

$$ [{}^nH_\chi, {}^nH_{\chi'}] = 0. \tag{4.40} $$

If the operators ${}^nH$ existed, the above commutation relations would give rise to the transformations

$$ e^{(i/\hbar){}^nH_\chi}\, {}^n\phi(X)\, e^{(-i/\hbar){}^nH_\chi} = \cos[\chi(n\cdot X){}^n\Gamma^{1/2}]\, {}^n\phi(X) + {}^n\Gamma^{-1/2}\sin[\chi(n\cdot X){}^n\Gamma^{1/2}]\, {}^n\pi(X), \tag{4.41} $$

$$ e^{(i/\hbar){}^nH_\chi}\, {}^n\pi(X)\, e^{(-i/\hbar){}^nH_\chi} = -{}^n\Gamma^{1/2}\sin[\chi(n\cdot X){}^n\Gamma^{1/2}]\, {}^n\phi(X) + \cos[\chi(n\cdot X){}^n\Gamma^{1/2}]\, {}^n\pi(X). \tag{4.42} $$

Note that the expression $\chi(n\cdot X){}^n\Gamma^{\frac{1}{2}}$ is unambiguous since, viewed as an operator on $L^2(\mathbb{R}^4, d^4X)$, multiplication by $\chi(n\cdot X)$ commutes with ${}^n\Gamma^{\frac{1}{2}}$.

The right hand sides of Eqs. (4.41) and (4.42) define an automorphism of the history algebra Eqs. (4.26)–(4.28), and all that remains is to show that these automorphisms are unitarily implementable in this representation. To this end, we use Eqs. (4.34) and (4.35) to prove that

$$ e^{i\,{}^nH_\chi/\hbar}\, b(X)\, e^{-i\,{}^nH_\chi/\hbar} = e^{-i\,\chi(n\cdot X){}^n\Gamma^{1/2}} b(X). \tag{4.43} $$

However, the operator defined on $L^2(\mathbb{R}^4, d^X)$ by

$$ (O(\chi)\psi)(X) := e^{-i\chi(n\cdot X){}^n\Gamma^{1/2}}\psi(X) \tag{4.44} $$

is easily seen to be unitary, and hence we conclude[2] that the desired quantities ${}^nH_\chi$ exist as self-adjoint operators on the Fock space $\mathcal{F}$ associated with the creation and annihilation operators $b^\dagger(X)$ and $b(X)$. The spectral projectors of these operators ${}^nH_\chi$ represent propositions about the time-averaged value of the energy in the space–time foliation determined by n.

To conclude: for each *fixed* choice of a foliation vector n, we have a physically meaningful representation of the history algebra Eqs. (4.26)–(4.28) on the Hilbert space $\mathcal{F} = \exp L^2(\mathbb{R}^4, d^4X)$. Thus the same Hilbert space $\mathcal{F}$ carries *all* different representations—for different choices of n—of the quantum field theory history algebra.

2. The action operator

We now define the action ${}^nS_\chi$ and the Liouville ${}^nV$ operators as normal-ordered versions of their classical analogus

$$ {}^nS_\chi = {}^nV - \frac{1}{2}{:}\int d^4X\{{}^n\pi^2(X) + {}^n\phi(X){}^n\Gamma{}^n\phi(X)\}\chi(n\cdot X){:}, \tag{4.45} $$

$$ {}^{n}V =: \int_{-\infty}^{\infty} d^4X\, {}^{n}\pi(X)\, n^{\mu}\partial_{\mu}\, {}^{n}\phi(X) :. \tag{4.46} $$

The automorphisms of the history algebra that are generated by the action and Liouville operators are

$$ e^{is\,{}^{n}S_{\chi}/\hbar}\, b(X) e^{-is\,{}^{n}S_{\chi}/\hbar} = e^{-i\int_{s'-s}^{s'+s} ds'\ \chi(nX+s')\,{}^{n}\Gamma^{1/2} - s n^{\mu}\partial_{\mu}} b(X), \tag{4.47} $$

$$ e^{is\,{}^{n}V/\hbar} b(X)\, e^{-is\,{}^{n}V/\hbar} = e^{-s\, n^{\mu}\partial_{\mu}} b(X), \tag{4.48} $$

and are easily shown to be unitarily implementable. In what follows, the real-valued smearing function χ is set equal to $\chi(t)=1$ for every $t \in \mathbb{R}$.

C. Poincaré group covariance

A significant feature of the histories formalism is the temporal structure of the theory. It introduces a new approach to the concept of time, in which time is distinguished as an ordering parameter (logical structure), and as an evolution parameter (dynamics). In particular, as we have already shown in nonrelativistic quantum mechanics,[1] the Liouville operator ${}^{n}V$ generates time translations with respect to the ''external'' t-time parameter, and the Hamiltonian operator ${}^{n}H$ generates time translations with respect to the ''internal'' evolution s-time parameter. The action operator ${}^{n}S$ generates *both* types of time transformations; it is the time generator for the histories theory for solutions of the equations of motion. [In histories theory the physical time translation generator is the action operator ${}^{n}S$; both Liouville ${}^{n}V$ and Hamiltonian ${}^{n}H$ operators are time translation generators that correspond to two different aspects (two modes) of the notion of time. However, only ${}^{n}S$ is related to the actual physical time parameter, in analogy with the standard theory where the Hamiltonian ${}^{n}H$ is the time translation generator.] The same construction is true for a histories quantum field theory.

The invariance of standard quantum field theory under the Poincaré group has been a difficult issue to address for many years. In a canonical treatment of quantum field theory, the Schrödinger-picture fields depend on the reference frame (i.e., choice of foliation). In order to demonstrate manifest independence of this choice with the aid of Heisenberg-picture fields, one still has to contend with the foliation dependence of the Hamiltonian that generates the Heisenberg fields.

In histories theory, the enhanced temporal structure enables the study of a Poincaré group transformation between different foliations. In particular we will show that different representations corresponding to different foliation vectors n are related by Lorentz boosts of the ''external'' Poincaré group,

$$ U(\Lambda)\, {}^{n}\phi(X) U(\Lambda)^{-1} = {}^{\Lambda n}\phi(\Lambda X), \tag{4.49} $$

and where the time translations generator is closely related to the ''Liouville'' operator V.

The Heisenberg-picture operators. We first define the Heisenberg-picture analog of the scalar field to illustrate the different time translations associated with the two time labels. We use a similar notation to that in the classical case: i.e., the Heisenberg-picture field is written as ${}^{n}\phi(X,s) = {}^{n}\phi(t,\underline{x},s)$, where the space–time point $X=(t,\underline{x})$ is expressed in coordinates adapted to n. Thus

$$ \begin{aligned} {}^{n}\phi(X,s) = {}^{n}\phi(t,\underline{x},s) &:= e^{(i/\hbar)\, s\, {}^{n}H}\, {}^{n}\phi(t,\underline{x}) e^{-(i/\hbar)\, s\, {}^{n}H} \\ &= \cos(s\, {}^{n}\Gamma^{1/2})\, {}^{n}\phi(X) + {}^{n}\Gamma^{-1/2} \sin(s\, {}^{n}\Gamma^{1/2})\, {}^{n}\pi(X), \end{aligned} \tag{4.50} $$

$$ \begin{aligned} {}^{n}\pi(X,s) = {}^{n}\pi(t,\underline{x},s) &:= e^{(i/\hbar)\, s\, {}^{n}H}\, {}^{n}\pi(t,\underline{x}) e^{-(i/\hbar)\, s\, {}^{n}H} \\ &= -{}^{n}\Gamma^{1/2} \sin(s\, {}^{n}\Gamma^{1/2})\, {}^{n}\phi(X) + \cos(s\, {}^{n}\Gamma^{1/2})\, {}^{n}\pi(X). \end{aligned} \tag{4.51} $$

The different types of time translation are particularly easy to see by studying the action of the Liouville ${}^nV$ and action ${}^nS$ operators on the Heisenberg-picture fields $b(X,s)$:

$$e^{i\tau {}^nH} b(t,\underline{x},s) e^{-i\tau {}^nH} := b(t,\underline{x},s+\tau), \tag{4.52}$$

$$e^{i\tau {}^nV} b(t,\underline{x},s) e^{-i\tau {}^nV} := b(t+\tau,\underline{x},s), \tag{4.53}$$

$$e^{i\tau {}^nS} b(t,\underline{x},s) e^{-i\tau {}^nS} := b(t+\tau,\underline{x},s+\tau). \tag{4.54}$$

The label s corresponds to the ''internal'' time of the unitary Hamiltonian time evolution, while t corresponds to the ''external'' time that labels the time ordering of events in a history for the Shrödinger-picture operators.

1. The internal Poincaré group

As we showed previously, each fixed choice of foliation vector n corresponds to a it *different* representation of the history algebra on the *same* Fock space $\mathcal{F}=\exp L^2(\mathbb{R}^4,d^4X)$. Hence, we may heuristically say that, for a given vector n, and for each value of the associated time t, there will be a Hilbert space $\mathcal{H}_t$ that carries an independent copy of the standard quantum field theory. (The physical quantities in histories appear naturally[1] space–time averaged, therefore they are smeared with appropriate test functions. Strictly speaking, quantities labeled at moments of time are not well-defined mathematically.) In particular, there exists a representation of the Poincaré group associated with each spacelike slice (n,t), where $t\in\mathbb{R}$.

In what follows, a particularly important role will be assigned to the averaged ''internal'' Poincaré group. For example, we define the averaged energy ${}^nH := \int d^4X\, {}^nH_t$ that generates translations on the s-time parameter of the Heisenberg-picture fields ${}^n\phi(X,s)={}^n\phi(t,\underline{x},s)$, without affecting the ''external'' t-time parameter:

$$ {}^n\phi(X,s) = \underset{\rightarrow}{{}^nH}\, {}^n\phi(X,s+s'), \tag{4.55}$$

$$ {}^n\pi(X,s) = \underset{\rightarrow}{{}^nH}\, {}^n\pi(X,s+s'). \tag{4.56}$$

The expressions for the ''internal'' Poincaré generators of spatial translations P^i, and rotations J^i, can be written in direct analogy with the expressions (3.22)–(3.24) of the classical case. We use the normal-ordered expressions

$$P(m) = :\int d^4X \pi(X) m^\mu \partial_\mu \phi(X): = i\int d^4X b^\dagger(X) m^\mu \partial_\mu b(X), \tag{4.57}$$

$$J(m) = \frac{1}{2} n_\mu m_\nu \epsilon^{\mu\nu\rho\sigma} :\int d^4X \pi(X) X_\rho \partial_\sigma \phi(X): = i\frac{1}{2} n_\mu m_\nu \epsilon^{\mu\nu\rho\sigma} \int d^4X b^\dagger(X) X_\rho \partial_\sigma b(X). \tag{4.58}$$

We have used a ''pseudo-covariant'' notation by employing an n-spacelike vector m (i.e., such that $n_\mu m^\mu = 0$). Note that the terms involving a pair of creation operators, or a pair of annihilation operators, can be shown to vanish through integration by parts.

Of particular interest is the action of the boost generator ${}^nK(m)$ defined as

$$ {}^nK(m) = \int d^4X b^\dagger(X)\, {}^n\Gamma^{1/4} X^\mu m_\mu\, {}^n\Gamma^{1/4} b(X). \tag{4.59}$$

The key feature of the boost generator ${}^{n}K(m)$ is that it mixes the it s-time parameter with the three-vectors $\underline{x}$. The action of these boost transformations is most clearly seen on the Heisenberg objects $\phi(X,s)=\phi(t,\underline{x},s)$:

$$ {}^{\mathrm{int}}U(\Lambda)\,{}^{n}\phi(t,\underline{x},s)\,{}^{\mathrm{int}}U(\Lambda)^{-1}={}^{n}\phi(t,\Lambda(\underline{x},s)), \tag{4.60}$$

where ${}^{\mathrm{int}}U(\Lambda):=e^{iK(m)}$ is the unitary operator that generates Lorentz transformations, and Λ is the Lorentz transformation generated by m.

At this point we note the action of the internal Poincaré group on the action ${}^{n}S$, Hamiltonian ${}^{n}H$ and Liouville ${}^{n}V$ operators, respectively:

$$ {}^{\mathrm{int}}U(\Lambda)\,{}^{n}H\,{}^{\mathrm{int}}U(\Lambda)^{-1}={}^{n}H, \tag{4.61}$$

$$ {}^{\mathrm{int}}U(\Lambda)\,{}^{n}V\,{}^{\mathrm{int}}U(\Lambda)^{-1}={}^{n}V, \tag{4.62}$$

$$ {}^{\mathrm{int}}U(\Lambda)\,{}^{n}S\,{}^{\mathrm{int}}U(\Lambda)^{-1}={}^{n}S. \tag{4.63}$$

As we would expect from standard canonical quantum field theory, we see that the above operators remain invariant under the ''internal'' Lorentz transformations.

2. External Poincaré group

A key result in histories classical field theory is that there also exists a second—the ''external''—Poincaré group symmetry of the theory, with generators

$$ \tilde{P}^{\mu}=:8\int d^{4}X\,\pi(X)\partial^{\mu}\phi(X):, \tag{4.64}$$

$$ \tilde{M}^{\mu\nu}=:\int d^{4}X\,\pi(X)(X^{\mu}\partial^{\nu}-X^{\nu}\partial^{\mu})\phi(X):. \tag{4.65}$$

Note that these definitions use the covariant fields $\phi(X)$ and $\pi(X)$ that satisfy the algebra (4.16)–(4.18) rather than the foliation-dependent fields ${}^{n}\phi(X)$ and ${}^{n}\pi(X)$ of Eqs. (4.26)–(4.28). However, many of the generators of the external Poincaré group are exactly the same whether one uses covariant fields expressions or foliation-dependent ones: they differ only for the case of the boosts generators ${}^{n}K(m)$.

In particular, the Liouville operator $\tilde{P}^{0}=V$, given by the expression

$$ V=:\int d^{4}X\;\pi(X)n^{\mu}\partial_{\mu}\,\phi(X):=i\int d^{4}X\,b^{\dagger}(X)n^{\mu}\partial_{\mu}b(X), \tag{4.66}$$

generates translations on the time label t.

The space translations and rotation generators are identical to those of the internal Poincaré group (4.57) and (4.58). However, the external boost generator $\tilde{K}(m)$ differs from the internal one ${}^{n}K(m)$, and hence it is of particular interest to study the action of the former.

The generator of time-translations V acts on Schrödinger picture objects as

$$ {}^{n}\phi(X)={}^{n}\phi(t,\underline{x})\underset{\rightarrow}{\overset{V}{}}{}^{n}\phi(t+\tau,\underline{x}), \tag{4.67}$$

$$ {}^{n}\pi(X)={}^{n}\pi(t,\underline{x})\underset{\rightarrow}{\overset{V}{}}{}^{n}\pi(t+\tau,\underline{x}). \tag{4.68}$$

The ''external'' boost generator $\tilde{K}(m)$ is

$$\tilde{K}(m) =: \int_{-\infty}^{\infty} d^4X \ \pi(X)\, T_m\, \phi(X): \tag{4.69}$$

$$= i \int_{-\infty}^{\infty} d^4X \ b^{\dagger}(X)\, T_m\, b(X), \tag{4.70}$$

where we define the operator T_m as

$$(T_m f)(X) := n_{\mu} m_{\nu} (X^{\mu} \partial^{\nu} - X^{\nu} \partial^{\mu}) f(X) \tag{4.71}$$

and $n \cdot m = 0$. Then the boost generator $\tilde{K}(m)$ acts on the fields ${}^n\phi(X)$ as

$${}^{\text{ext}}U(\Lambda)\, {}^n\phi(X)\, {}^{\text{ext}}U(\Lambda)^{-1} = {}^{\Lambda n}\phi(\Lambda(X)), \tag{4.72}$$

and it mixes the t-time parameter with the three-vector $\underline{x}$. However, the crucial point is that $\tilde{K}(m)$ generates Lorentz transformations *on the foliation vector n* as well.

This can be viewed as a demonstration of explicit Poincaré covariance, as we can see from the action of the external Lorentz transformations on the Heisenberg-picture fields ${}^n\phi(X,s)$ as

$${}^{\text{ext}}U(\Lambda)\, {}^n\phi(X,s)\, {}^{\text{ext}}U(\Lambda)^{-1} = {}^{\Lambda n}\phi(\Lambda(X,s)). \tag{4.73}$$

The generators of the *internal* Poincaré group transform under the action of the *external* Poincaré group as

$${}^{\text{ext}}U(\Lambda)\, {}^nH\, {}^{\text{ext}}U(\Lambda)^{-1} = {}^{\Lambda n}H, \tag{4.74}$$

$${}^{\text{ext}}U(\Lambda)\, {}^n\tilde{K}(m)\, {}^{\text{ext}}U(\Lambda)^{-1} = {}^{\Lambda n}\tilde{K}(\Lambda m). \tag{4.75}$$

Of considerable importance is the fact that the action operator ${}^nS$ transforms in the same way:

$${}^{\text{ext}}U(\Lambda)\, {}^nS\, {}^{\text{ext}}U(\Lambda)^{-1} = {}^{\Lambda n}S. \tag{4.76}$$

Hence the action of the external Poincaré group *relates* representations of the theory that *differ* with respect to the foliation vector n. As we shall see in the following section, this is crucial when we discuss the Poincaré invariance of probabilities.

In summary, we have shown that the history version of quantum field theory carries representations of two Poincaré groups. The ''internal'' Poincaré group is defined in analogy to the one in the standard canonical treatment of the theory. It corresponds to time-translations with respect to the ''internal'' s-time parameter of histories theory. The Lorentz part of the ''external'' Poincaré group intertwines representations of the theory associated with different choices of foliation, all of which, however, are realized on the *same* Fock space $\mathcal{F}$. It corresponds to time-translations with respect to the ''external'' t-time parameter.

The translation parts of these two types of Poincaré transformation—corresponding to the relations between the t time parameter and kinematics, and the s time parameter and dynamics—have very significant analogs in the case of the histories version of general relativity.[9]

3. The decoherence functional

"Classical" coherent states. In Ref. 1, we showed how a classical quantum relation can be nicely described in histories theory by using the history analog of coherent states. In the histories formalism, a non-normalized coherent state vector is written as[2]

$$|\exp z\rangle = \bigoplus_{n=0}^{\infty} (n!)^{-1/2} (\otimes |z\rangle)^n. \tag{4.77}$$

The corresponding normalized coherent states can be obtained by unitary transformations of the vacuum state as

$$|z\rangle := \frac{1}{\sqrt{\langle \exp z | \exp z\rangle}} |\exp z\rangle = U[f,h]|0\rangle, \tag{4.78}$$

where $U[f,h]$ is the Weyl operator defined as

$$U[f,h] := e^{(i/\hbar)({}^n\phi(f) - {}^n\pi(h))}, \tag{4.79}$$

and f and h are smearing functions that belong to $L^2(\mathbb{R}^4, d^4X)$. We write the normalized coherent state $|z\rangle$ corresponding to the pair f,h as $|f,h\rangle$. In this context we know that f and h correspond to classical values and therefore correspond to a path on classical phase space. In this correspondence, the functions f and h are the classical values of the field $\phi(X)$ and its conjugate momenta $\pi(X)$, respectively.

The set of all coherent states is independent of the choice of foliation since these coherent states are eigenstates of the annihilation operator $b(X)$, which is foliation independent. However, the physical identification of the vector $|z\rangle$ with a phase space path *is* foliation dependent since it depends on the Weyl operator, which itself depends on the choice of the representation of the history algebra on the Fock space $\mathcal{F}$. [Given a complex path z, the classical phase space path (f,h) is defined by the foliation-dependent expression $z = {}^n\Gamma^{1/4} f + i\,{}^n\Gamma^{-1/4} h$.] One should recall that the space of classical histories Π is itself dependent on the choice of foliation.

So far our discussion of the histories version of quantum field theory has been at the level of field algebras and group transformations. However, in histories formalism physically crucial "probabilistic" information is contained in the decoherence functional.

In this HPO formalism, the most general form for the decoherence functional of a pair of history propositions α, β is

$$d(\alpha,\beta) = Tr_{\mathcal{F}\times\mathcal{F}}(\alpha\otimes\beta\Xi), \tag{4.80}$$

in terms of an operator Ξ on $\mathcal{F}\times\mathcal{F}$.[10]

In our case, the operator Ξ reads

$$\Xi := \langle 0|\rho_{-\infty}|0\rangle (\mathcal{S}_{cts}\mathcal{U})^\dagger \otimes (\mathcal{S}_{cts}\mathcal{U}), \tag{4.81}$$

in terms of the operator $\mathcal{S}_{cts}\mathcal{U}$ that we proved in Ref. 1 that it is an implicit function of the action operator: therefore there is an implicit dependence of Ξ on the foliation vector n. The matrix elements of $\mathcal{S}_{cts}\mathcal{U}$ in a coherent state basis can written in terms of the classical action functional $S[f,h]$ as

$$\langle f,h|\mathcal{S}_{cts}\mathcal{U}|f,h\rangle = e^{iS[f,h]}. \tag{4.82}$$

The explicit relation of $\mathcal{S}_{cts}\mathcal{U}$ with the action operator ${}^nS$ is as follows. For a general operator A on $L^2(\mathbb{R}^4, d^4X)$ one can define an operator $\Gamma(A)$ on $\mathcal{F}$ as

$$\Gamma(A)|\exp z\rangle = |Az\rangle. \tag{4.83}$$

In our case we have

$$e^{is\,{}^nS} = \Gamma(e^{is\,{}^n\sigma}), \tag{4.84}$$

$$\mathcal{S}_{cts}\mathcal{U} = \Gamma(1 + i\,{}^n\sigma), \tag{4.85}$$

in terms of the operator ${}^n\sigma = n^\mu\partial_\mu - {}^n\Gamma^{1/2}$. Hence, the decoherence functional depends on the representation through the phase space action ${}^nS$.

This raises the critical issue of the physical meaning of the fact that the formalism appears to depend on a specific choice of the foliation vector n. We have seen above that the representation of the phase space quantities by Hilbert space operators depends on n, and that there exist unitary intertwiners between different representations given by the boosts of the external Poincaré group. As has been discussed in Ref. 11, a transformation law for the observables by means of a unitary operator U,

$$\alpha \rightarrow \alpha' = U\alpha U^{\dagger}, \tag{4.86}$$

implies that the operator Ξ of the decoherence functional, carrying a label for the foliation dependence n, ought to transform as

$$^{n}\Xi \rightarrow {}^{\Lambda n}\Xi = (U \otimes U)\, {}^{n}\Xi\, (U^{\dagger} \otimes U^{\dagger}) \tag{4.87}$$

so that the values of the decoherence functional (corresponding to probabilities and correlation functions of the theory) *are representation independent*,

$$^{\Lambda n}d(^{\Lambda n}\alpha, {}^{\Lambda n}\beta) = {}^{n}d(^{n}\alpha, {}^{n}\beta), \tag{4.88}$$

where $^{\Lambda n}d$ is the decoherence functional defined with reference to the operator $^{\Lambda n}\Xi$.

In our case we have $U = e^{i\tilde{K}(m)} = {}^{ext}U(\Lambda)$. This changes the foliation dependence of the fundamental fields $^{n}\phi(X)$ and $^{n}\pi(X)$, and hence of any observable $^{n}\alpha$ that depends upon them

$$^{n}\alpha \rightarrow {}^{\Lambda n}\alpha := U(\Lambda)\, {}^{n}\alpha U(\Lambda)^{\dagger}. \tag{4.89}$$

Some physically interesting examples of observables, in this sense, are integrals $\int d^{X}\, {}^{n}\phi(X) f(X)$ of fields $^{n}\phi(X)$, smeared with appropriate test functions $f(X)$, that satisfy $f(X) = f(\Lambda(X))$; another example is any space–time average of the normal-ordered polynomial functions of these fields.

In order to see how the boosts generator acts on $^{n}\Xi$, it suffices to check its action on $\mathcal{S}_{cts}\mathcal{U}$. This is

$$U\, {}^{n}\mathcal{S}_{cts}\mathcal{U}\, U^{\dagger} = \Gamma(1 + ie^{-T_m}\, {}^{n}\sigma\, e^{T_m}) = \Gamma(1 + i\, {}^{\Lambda n}\sigma). \tag{4.90}$$

Consequently, the operator $^{n}\Xi$ transforms as $^{n}\Xi \rightarrow {}^{\Lambda n}\Xi$. Hence the values of the decoherence functional are foliation independent:

$$^{n}d(^{n}\alpha, {}^{n}\beta) = {}^{\Lambda n}d(^{\Lambda n}\alpha, {}^{\Lambda n}\beta). \tag{4.91}$$

V. CONCLUSIONS

We have studied both the classical and the quantum history versions of scalar field theory. We have showed that, in both cases, the crucial feature of the history field theory is the appearance of two Poincaré groups, in direct analogy to the two types of time transformation that characterizes the history formalism. The internal Poincaré group is related to time as an ordering parameter (the Hamiltonian H is the time translations generator), and it is in analogy to the Poincaré group of standard field theory. On the other hand, the external Poincaré group is related to time as a parameter of evolution (the Liouville V is the time translations generator), and it is of particular interest for the quantum case, as it relates representations of the quantum field theory, for different choices of foliation, with Poincaré transformations.

These results will be proved to be of great importance in the study of history general relativity theory in Ref. 9. In particular, the histories formalism is suitable to deal with issues that lie at the level of the interplay between quantum theory and the space–time structure. The present work focuses on quantum field theory in a fixed space–time, however the techniques involved and the concepts introduced have been able to precisely identify the relation between the quantum me-

chanical observables and the necessary notion of the space–time foliation. Many issues are raised at the level of the meaning of reference frames in quantum theory—a foliation corresponds to a reference frame—and more importantly at the level of quantum gravity.

The latter is eventually the aim of the histories program, and this involves a further elucidation of the meaning of space–time in a quantum theory. What strikes us as relevant at present is that one might have to disentangle between the two different views of space–time transformations: the *passive* and the *active* view. This is subtly hinted by the fact that the transformations generated by the external Poincaré group should be viewed in the passive sense, since the argument X cannot be identified with a fixed, absolute space–time point *in all representations*.

In order to successfully address the above issues we must first study the history version of general relativity; this is the context of the forthcoming paper.[9]

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Large N limit of SO(N) gauge theory of fermions and Bosons

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In this paper we study the large N_c limit of SO(N_c) gauge theory coupled to a Majorana field and a real scalar field in $1+1$ dimensions extending ideas of Rajeev [Int. J. Mod. Phys. A **9**, 5583 (1994)]. We show that the phase space of the resulting classical theory of bilinears, which are the mesonic operators of this theory, is $\mathrm{OSp}_1(\mathcal{H}|\mathcal{H})/U(\mathcal{H}_+|\mathcal{H}_+)$, where $\mathcal{H}|\mathcal{H}$ refers to the underlying complex graded space of combined one-particle states of fermions and bosons and $\mathcal{H}_+|\mathcal{H}_+$ corresponds to the positive frequency subspace. In the begining to simplify our presentation we discuss in detail the case with Majorana fermions only [the purely bosonic case is treated in Toprak and Turgut, J. Math. Phys. **43**, 1340 (2002)]. In the Majorana fermion case the phase space is given by $O_1(\mathcal{H})/U(\mathcal{H}_+)$, where $\mathcal{H}$ refers to the complex one-particle states and $\mathcal{H}_+$ to its positive frequency subspace. The meson spectrum in the linear approximation again obeys a variant of the 't Hooft equation. The linear approximation to the boson/fermion coupled case brings an additonal bound state equation for mesons, which consists of one fermion and one boson, again of the same form as the well-known 't Hooft equation.
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I. INTRODUCTION

Gauge theories play a fundamental role in our description of nature. Nevertheless our understanding of confining phase of gauge theories is not so complete. In principle we should be able to calculate the hadronic spectrum starting from quantum chromodynamics (QCD), which is a gauge theory, yet this has not been possible up to now. It is believed that the hadrons are colorless excitations of the underlying gauge theory and we never see the constituent quarks as free particles. This suggests that in this case we should have an independent formulation of gauge theories in terms of color singlet operators of the original gauge theory. In general this is a very hard task.

Gauge theories in $1+1$ dimensions provide a great testing ground for many ideas about realistic theories. This is a great simplification, various difficult problems of higher dimensional theories will not be there, yet there are still interesting aspects of these theories which make them worth studying in depth. In Ref. 1, Rajeev constructed a theory of mesons in two dimensions in the limit N_c, the number of colors in SU(N_c) goes to infinity using only the color invariant variables (which correspond to the meson operators). The idea that QCD should simplify while keeping all its essential features in this limit goes back to 't Hooft[2,3] and that this limit should be a kind of classical mechanics to Migdal and Witten.[4] This is a very promising step in simplifying gauge theories, but the large-N_c theory is also quite complicated and it is not possible as yet to understand it in four dimensions.

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Originally 't Hooft studied two-dimensional QCD in the large-N_c limit to understand the meson spectrum and obtained his bound state equation in his seminal paper.[3] Soon after the scalar two-dimensional QCD was worked out by Shei and Tsao in Ref. 5 following 't Hooft, and later by Tomaras using Hamiltonian methods in Ref. 6. These works obtained the analog of the 't Hooft equation for this case. A natural extension of these would be to look at combined (fermionic) QCD and scalar QCD; this is done in a paper of Aoki,[7] where it is shown that three types of mesons are possible and they all obey a certain type of 't Hooft equation (see also Ref. 8). Cavicchi[9] using a path integral approach with bilocal fields, developed in Ref. 10, studied coupled fermions and bosons as well as some other models in two dimensions and he obtained some generalized versions of the 't Hooft equation.

To understand gauge theories better, we study the problem of bosons and fermions coupled to SO(N_c) gauge fields in $1+1$ dimensions. We will apply the methods developed by Rajeev to this toy model. We recommend his lectures for a more detailed exposition of the underlying ideas and various other directions.[11] In Ref. 1 it was shown that the phase space of the two-dimensional QCD is an infinite dimensional Grassmannian.[12] Using the same methods scalar version of QCD is worked out in Ref. 13, the phase space of the theory comes out to be an infinite dimensional disk. Recently Konechny and O.T.T. obtained the large-N_c phase space of bosons and fermions coupled to SU(N_c) gauge theory; a certain kind of super-Grassmannian.[14] The linearized equations agree with the ones found in Ref. 7. The correct equations are nonlinear and various approximation schemes are also discussed in Ref. 14. There are some ideas in the literature which suggest that gauge theories in two dimensions all behave in a very similar way,[15] therefore it will be interesting to see how much of this holds for SO(N_c) gauge theory.

The organization of our work is as follows, since we did not want to go into technical details of supergeometry immediately, we first study the purely fermionic case. The essential calculations are very similar to the ones in Rajeev's lectures[11] and for the geometry basic ideas are already in Refs. 16 and 12, we also recommend Ref. 17 for a good discussion. We show that one can formulate the large-N_c limit in terms of bilinears along the lines in Ref. 1. We obtain a variant of the 't Hooft equation in the linear approximation. We explain the geometry of the phase space and show that it is a homogeneous manifold, $O_1(\mathcal{H})/U(\mathcal{H}_+)$ (see explanations in Sec. IV), and the symplectic form is the natural one. In the second part, we study the combined system of bosons and fermions, this part is very brief—we mostly state the results. We obtain a super-Poisson structure of the bilinears in the large-N_c limit and the resulting Hamiltonian. The equations of motion in the linear approximation agree with the purely bosonic and purely fermionic ones with an additional one for the mesons made up of one fermion and one boson. This is again a variant of the well-known 't Hooft equation. The discussion on the geometry of the resulting infinite dimensional supersymplectic space requires some new ideas. This part is technically complicated; we use essentially Berezin's ideas,[18] but we do not claim that all the technicalities of the infinite dimensional case are understood. We show that the underlying phase space should be the super-homogeneous manifold $\mathrm{OSp}_1(\mathcal{H}|\mathcal{H})/U(\mathcal{H}_+|\mathcal{H}_+)$, and the supersymplectic form is the natural one on this space. We plan to come to the more mathematical aspects of this problem in a future publication.

II. THE SO(N_c) MAJORANA FERMIONS IN THE LIGHT-CONE

Since the basic philosophy was explained in Ref. 1 we can be brief and only state our conventions and define our theory. We will use the light cone coordinates $x^+=(1/\sqrt{2})(t+x)$, $x^-=(1/\sqrt{2})(t-x)$, (we recommend Ref. 19 for an introduction to light-cone quantization, and Ref. 20 for a more comprehensive review), the action functional is

$$S=\int\left[\frac{1}{2}\mathrm{Tr}\,F_{\mu\nu}F^{\mu\nu}+i\overline{\Psi}_M\gamma^\mu(\partial_\mu+gA_\mu)\Psi_M-m\overline{\Psi}_M\Psi_M\right], \tag{1}$$

where we have an SO(N_c) gauge theory for which the matter fields are in the fundamental representation and Tr denotes an invariant inner product in the Lie algebra. The Lie algebra condition for SO(N_c) implies that $A_\mu^T=-A_\mu$. To compute the variations of the action we need the

independent degress of freedom, we can expand $A_\mu = A_\mu^a T^a$, where T^a are the generators of the Lie algebra of SO(N_c), chosen such that $\mathrm{Tr}\, T^a T^b = -1/2\, \delta^{ab}$. Our conventions for the Majorana fermions are as follows: we choose the Majorana representation in which the fermions are real, i.e., $\Psi_M^\dagger = \Psi_M^T$ (transpose here also includes the color indices to simplify the notation). The gamma matrices now are given by,

$$\gamma^0 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \gamma^1 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \quad \gamma^5 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{2}$$

Note that γ^5 happens to be diagonal in $1+1$ dimensions and we set $\overline{\Psi}_M = \Psi_M^T \gamma^0$. We now rewrite the action in the light-cone coordinates and eliminate all nondynamical degrees of freedom. We write $\Psi_M = \binom{\psi_1}{\psi_2}$, and use $\gamma^+ = (1/\sqrt{2})(\gamma^0 + \gamma^1)$, $\gamma^- = (1/\sqrt{2})(\gamma^0 - \gamma^1)$. We further set $A_- = 0$ and choose x^+ as the evolution variable, which we call "time,"

$$S = \int \mathrm{d}x^+ \, \mathrm{d}x^- \left[\frac{1}{2} (\partial_- A_+^a)^2 + i\sqrt{2} \psi_1^T \partial_- \psi_1 + i\sqrt{2} \psi_2^T \partial_+ \psi_2 + i2m \psi_1^T \psi_2 + i\sqrt{2} g \psi_2^T A_+^a T^a \psi_2 \right] \tag{3}$$

(from now on T only means tranpose in the color space). We note also that we have a *real* two component fermion, they are Grassmann valued obeying $\psi_1 \psi_2 = -\psi_2 \psi_1$. We can check that the action is real if we use the following complex conjugation convention for spinors, $(\psi\xi)^* = \xi^* \psi^*$. We see that ψ_1^α is nondynamical, and hence can be eliminated using its equation of motion,

$$\psi_1^\alpha = -\frac{m}{\sqrt{2}\partial_-} \psi_2^\alpha. \tag{4}$$

Similarly we solve for the nondynamical A_+^a, and get

$$A_+^a = \frac{i\sqrt{2} g}{\partial_-^2} \psi_2^T T^a \psi_2. \tag{5}$$

A remark is in order here to clarify what we mean by "real fermions" while the action and the constraint equation for A_+^a have explicit factors of i. The resolution of this seeming paradox is that it is the equations of motion which are actually real. To see this note first that the symplectic form has a factor of i in it, and the ψ_1^α constraint only has real operators. The A_+^a constraint is also real if we choose complex conjugation of fermions to be $(\psi\xi)^* = \xi^* \psi^*$. This convention implies that the product of two real fermions is imaginary, and this is the reason for the extra factors of i in the action. The equation of motion for ψ_2^α reads

$$\partial_+ \psi_2^\alpha = \frac{m}{\sqrt{2}} \psi_1^\alpha, \tag{6}$$

which is manifestly real. This shows that the "time" evolution preserves the real valuedness condition imposed on the fermions.

If we insert the above-mentioned constraints into the action we arrive at

$$S = \int \mathrm{d}x^+ \, \mathrm{d}x^- \left[i\sqrt{2} \psi_2 \partial_+ \psi_2 - \frac{\sqrt{2} m^2}{2} \psi_2 \frac{1}{i\partial_-} \psi_2 - g^2 \psi_2^T T^a \psi_2 \frac{1}{\partial_-^2} \psi_2^T T^a \psi_2 \right]. \tag{7}$$

This defines our theory at the classical level with the redundant degrees of freedom eliminated. *Since it is written entirely in terms of ψ_2 we will refer to this field as ψ from now on.* The real fermions have a super-Poisson bracket, which can be read off from the action, given by

$$\{\psi^{\alpha}(x^{-},x^{+}),\psi^{\beta}(y^{-},x^{+})\}_{+}=\frac{-i}{2\sqrt{2}}\,\delta^{\alpha\beta}\delta(x^{-}-y^{-}). \tag{8}$$

Since our real fermions are Grassmann valued we use a symplectic structure which is i times a real symmetric operator, and the Hamiltonian is actually i times an antisymmetric one, as we will see in more detail in Sec. III. There is an ambiguity in the quantization, we follow Rajeev's original approach,[11,1] we will remove the nondynamical fields after quantizing the dynamical field, ψ^{α}. Using the Dirac rule we get an anticommutator for ψ,

$$[\psi^{\alpha}(x^{-}),\psi^{\beta}(y^{-})]_{+}=i\hbar\left(\frac{-i}{2\sqrt{2}}\,\delta^{\alpha\beta}\delta(x^{-}-y^{-})\right)=\frac{\hbar}{2\sqrt{2}}\,\delta^{\alpha\beta}\delta(x^{-}-y^{-}). \tag{9}$$

(Note that for the orthogonal group, the distinction of upper and lower indices is irrelevant, since the metric tensor is unity.) The reason for our convention of complex conjugation is to arrive at this more familiar form of the Clifford algebra. We could have chosen a convention in which the product of real fermions is real, then we would arrive at a Clifford algebra with a factor of i as in Ref. 16, but this usual form is preferable (it leads to a positive inner product, or the Hermitian conjugation is compatible with the inner product in the fermionic Fock space). Let us introduce the Fourier decomposition, which is done in a complex Hilbert space (to simplify notation we drop the subscript in p_{-}, set $\hbar=1$, and $[\mathrm{d}p]=\mathrm{d}p/2\pi$),

$$\psi^{\alpha}(x^{-})=\int_{-\infty}^{\infty}\frac{[\mathrm{d}p]}{2^{3/4}}\chi^{\alpha}(p)e^{-ipx^{-}}. \tag{10}$$

(To be precise, in the above-mentioned expansion, we should assume a cut-off ϵ_0 around zero momentum, to be taken to zero at the end of our calculations.) We see that $\chi^{\alpha}(p)$ satisfies the basic anticommutator,

$$[\chi^{\alpha}(p),\chi^{\beta}(q)]_{+}=\delta^{\alpha\beta}\delta[p+q], \tag{11}$$

where we write $\delta[p-q]=2\pi\delta(p-q)$. Real valuedness of the original field implies that $\chi^{\alpha\dagger}(p)=\chi^{\alpha}(-p)$. In standard physics notation the expansion would be written as

$$\psi^{\alpha}(x^{-})=\int_{0}^{\infty}[\chi^{\alpha}(p)e^{-ipx^{-}}+\chi^{\alpha\dagger}(p)e^{ipx^{-}}]\frac{[\mathrm{d}p]}{2^{3/4}}. \tag{12}$$

As is well known in the physics literature, to make the Hamiltonian bounded from below, we should choose a vacuum to be used to construct a fermion Fock space, and further impose a normal ordering prescription. This is done by simply requiring that $\chi^{\alpha}(p)|0>=0$ for $p>0$, and defining

$$:\chi^{\alpha}(p)\chi^{\beta}(q):=\begin{cases}-\chi^{\beta}(q)\chi^{\alpha}(p) & \text{if} \quad p>0,\ q<0,\\ \chi^{\alpha}(p)\chi^{\beta}(q) & \text{otherwise.}\end{cases} \tag{13}$$

This can be stated in one formula as

$$:\chi^{\alpha}(p)\chi^{\beta}(q):=\chi^{\alpha}(p)\chi^{\beta}(q)-\tfrac{1}{2}\,\delta^{\alpha\beta}\delta[p+q][1+\mathrm{sgn}(p)]. \tag{14}$$

For most of our calculations we need only the bilinears and the above-given expressions. (For the Hamiltonian we actually need the normal ordering of product of four such operators, and it is defined as usual all the annihilation operators are to be taken to the right of creation operators, it will be briefly explained later on.) We can reduce our Hamiltonian after this quantization process, and we get

$$H=\int \mathrm{d}x^{-}\left(\frac{m^2\sqrt{2}}{2}:\psi^{\alpha}\frac{1}{i\partial_{-}}\psi^{\alpha}:-\frac{g^2}{2}:\psi^{\alpha}(x^{-})\psi^{\beta}(x^{-}):|x^{-}-y^{-}|:\psi^{\beta}(y^{-})\psi^{\alpha}(y^{-}):\right). \quad (15)$$

Previously we used $(T^a)^{\alpha\beta}(T^a)^{\lambda\sigma}=-1/2(\delta^{\alpha\sigma}\delta^{\beta\lambda}-\delta^{\alpha\lambda}\delta^{\beta\sigma})$ and the Green function $1/2|x^{-}-y^{-}|=\partial_{-}^{-2}\delta(x^{-}-y^{-})$. The last normal orderings can be rearranged to act only on the color invariant combinations in the large-N_c limit, we will discuss this in Sec. III.

Next we introduce the algebra of color invariant bilinears and study the resulting system in the large-N_c limit following Refs. 1 and 11.

III. CLASSICAL MECHANICS OF COLOR INVARIANT OPERATORS

We define color invariant bilinears as in Refs. 1, 11, and 14 to be our dynamical variables and find the large-N_c limit by postulating Poisson algebra of these bilinears and defining the phase space to be a manifold where these Poisson brackets make sense. Since the theory is super-renormalizable we expect this to be related to the Hilbert–Schmidt ideal condition which is well-known in the literature on the Fock spaces.[12,21–23] We will see these aspects in more detail in Sec. IV when we talk about the geometry of the phase space. We define our basic dynamical variables, bilinears,

$$\hat{R}(p,q)=\frac{2}{N_c}\sum_{\alpha}:\chi^{\alpha}(p)\chi^{\alpha}(q):, \quad (16)$$

which are color invariant combinations of the fermion operators. We find it useful to define a related operator, $\hat{F}(p,q)=\hat{R}(-p,q)$, we will see that this is the correct variable for the geometry of the phase space. We assume that there are proper large-N_c limits of our operators, then they become classical variables when they are restricted to color invariant sector of the full Fock space. Following Ref. 1, we postulate the following Poisson brackets (we choose the quantization parameter to be $1/N_c$);

$$\{R(p,q),R(s,t)\}=-2i(R(p,t)\delta[q+s]-R(q,t)\delta[p+s]+R(s,p)\delta[q+t]-R(s,q)\delta[p+t]$$
$$+(\delta[q+t]\delta[p+s]-\delta[p+t]\delta[q+s])(\mathrm{sgn}(t)+\mathrm{sgn}(s))).$$

Our dynamical system is not defined completely yet, since there is still a left over global color invariance, generated by

$$\hat{Q}^{\alpha\beta}=\int[\mathrm{d}p]:\chi^{\alpha\dagger}(p)\chi^{\beta}(p):=\int_0^{\infty}[\mathrm{d}p]\chi^{\alpha\dagger}(p)\chi^{\beta}(p)-\int_0^{\infty}[\mathrm{d}p]\chi^{\beta\dagger}(p)\chi^{\alpha}(p). \quad (17)$$

The commutators of these generators satisfy the Lie algebra of SO(N_c).

If we restrict ourselves to the color invariant states, we find a constraint equation satisfied in the large-N_c limit, which can be best expressed in terms of $F(p,q)=R(-p,q)$,

$$\int[\mathrm{d}q]F(p,q)F(q,s)-\mathrm{sgn}(p)F(p,s)-F(p,s)\mathrm{sgn}(s)=0. \quad (18)$$

We define $\epsilon(p,q)=-\mathrm{sgn}(p)\delta[p-q]$, then we can rewrite this constraint as a simple quadratic operator equation,

$$(F+\epsilon)^2=1 \quad (19)$$

(we interpret F,ϵ as integral kernels acting on L_2 space of initial data). In Sec. IV we will analyze the geometric meaning of these constraints. The Hamiltonian and the above-mentioned Poisson brackets determine the evolution of our classical system; the Poisson brackets are consistent with the constraint equation.

The large-N_c Hamiltonian is obtained by dividing the original Hamiltonian by N_c and rewriting it in terms of our large-N_c variables. After certain manipulations which are sketched in the following, we obtain the following Hamiltonian,

$$H=\mathcal{P}\int \frac{1}{8}\left(m^2-\frac{g^2}{2\pi}\right)\frac{[\mathrm{d}p]}{p}R(-p,p)-\frac{g^2}{64}\mathcal{FP}\int \frac{[\mathrm{d}p\ \mathrm{d}q\ \mathrm{d}s\ \mathrm{d}t]}{(p+s)^2}R(p,q)R(s,t)\delta[p+q+s+t], \tag{20}$$

where $\mathcal{P}$ and $\mathcal{FP}$ refer to the principal value and finite part prescriptions, respectively. In the following we will often write $\int$ for $\mathcal{P}\int$ and $\mathcal{FP}\int$, but one should keep in mind that these regularization perscriptions are used to define the singular integrals. The main steps of the derivation of the above-mentioned Hamiltonian are very similar to the one in Ref. 11, although there are some small differences. Here we supply the basic ingredients to help the reader: for simplicity in many places we write x,y instead of x^-,y^-, we define $\epsilon(z)=\mathcal{P}\int_{-\infty}^{\infty}\mathrm{sgn}(p)e^{+ipz}$, note the sign of the exponent. We have the vacuum expectation value of our field product,

$$\langle 0|\psi^\alpha(x^-)\psi^\beta(y^-)|0\rangle=\frac{1}{4\sqrt{2}}[\delta(x^--y^-)-\epsilon(x^--y^-)]. \tag{21}$$

An important formula for the reduction is given in Ref. 11: If $f(x,y)=\int[\mathrm{d}p\ \mathrm{d}q]e^{ipx+iqy}\tilde{f}(p,q)$,

$$\int \epsilon(x-y)|x-y|f(x,y)=-\frac{1}{\pi}\mathcal{P}\int\frac{[\mathrm{d}p]}{p}\tilde{f}(-p,p). \tag{22}$$

We also have

$$|x-y|=\mathcal{FP}\int\frac{[\mathrm{d}p]}{p^2}e^{ip(x-y)}.$$

We use a form of Wick's theorem for normal ordered products,

$$\begin{aligned}:\psi^\alpha(x)\psi^\beta(x)::\psi^\beta(y)\psi^\alpha(y):=:\psi^\alpha(x)\psi^\beta(x)\psi^\beta(y)\psi^\alpha(y):&+\langle 0|\psi^\alpha(x)\psi^\alpha(y)|0\rangle:\psi^\beta(x)\psi^\beta(y):\\&+\langle 0|\psi^\beta(x)\psi^\beta(y)|0\rangle:\psi^\alpha(x)\psi^\alpha(y):\\&-\langle 0|\psi^\alpha(x)\psi^\beta(y)|0\rangle:\psi^\beta(x)\psi^\alpha(y):\\&-\langle 0|\psi^\beta(x)\psi^\alpha(y)|0\rangle:\psi^\alpha(x)\psi^\beta(y):+\langle 0|\psi^\alpha(x)\psi^\alpha(y)|0\rangle\\&\times\langle 0|\psi^\beta(x)\psi^\beta(y)|0\rangle-\langle 0|\psi^\beta(x)\psi^\alpha(y)|0\rangle\langle 0|\psi^\alpha(x)\psi^\beta(y)|0\rangle.\end{aligned}$$

Note that when we take the large-N_c limit we can expand the full normal ordering in the leading order to get $:\psi^\alpha(x)\psi^\alpha(y)::\psi^\beta(x)\psi^\beta(y):$. In the above-mentioned equality the fourth and fifth terms on the right are of smaller order in the large-N_c limit as well as the last term in the equality. The sixth term is an infinite vacuum expectation value, but that is a constant term which will not contribute to the equations of motion hence we can drop it. As a result,

$$\begin{aligned}:\psi^\alpha(x)\psi^\beta(x)::\psi^\beta(y)\psi^\alpha(y):=:\psi^\alpha(x)\psi^\alpha(y)::\psi^\beta(x)\psi^\beta(y):&+\langle 0|\psi^\alpha(x)\psi^\alpha(y)|0\rangle:\psi^\beta(x)\psi^\beta(y):\\&+\langle 0|\psi^\beta(x)\psi^\beta(y)|0\rangle:\psi^\alpha(x)\psi^\alpha(y):\end{aligned}$$

Using the above-given formulas we get a finite renormalization of the mass term.

Let us compute the equations of motion at the linear approximation. What we mean by this is to linearize the constraint as well as the equations of motion. The linearization of the constraint simply says that $R(u,v)=0$ if u,v have different signs. We thus restrict ourselves to $u,v>0$ and compute

$$\frac{\partial R(u,v;x^+)}{\partial x^+}=\{R(u,v;x^+);H\}. \tag{23}$$

We also put $P=u+v, x=u/P$ and make the ansatz $R(u,v;x^+)=\zeta_R(x)e^{-iP_+x^+}$. For further details we refer to Refs. 1 and 11, where similar calculations are done in more detail with the same type of ansatz; this yields an eigenvalue equation,

$$\mu^2\zeta_R(x)=\left(m^2-\frac{g^2}{2\pi}\right)\left[\frac{1}{x}+\frac{1}{1-x}\right]\zeta_R(x)-\frac{g^2}{8\pi}\int_0^1 dy\,\frac{\zeta_R(y)-\zeta_R(1-y)}{(y-x)^2}, \tag{24}$$

where $\mu^2=2P_+P$ is the invariant mass of the excitation. By looking at the behavior of this equation under $x\mapsto 1-x$, and $y\mapsto 1-y$, we see that we can choose our wave functions to be antisymmetric under $y\mapsto 1-y$, thus $\zeta(1-y)=-\zeta(y)$. This gives us

$$\mu^2\zeta_R(x)=\left(m^2-\frac{g^2}{2\pi}\right)\left[\frac{1}{x}+\frac{1}{1-x}\right]\zeta_R(x)-\frac{g^2}{4\pi}\int_0^1 dy\,\frac{\zeta_R(y)}{(y-x)^2}. \tag{25}$$

This equation is one of our main results and it is a variant of the well-known 't Hooft equation. Apart from the numerical factors this equation is the same as the original one, and this result fits to the ideas in Ref. 15. Its properties are well known, the most important one is that there are only bound state solutions.

An interesting question is the existence of ''baryon''-like excitations. These should correspond to operators of the form

$$\frac{1}{Z}\epsilon_{\alpha_1\alpha_2\ldots\alpha_{N_c}}\chi^{\alpha_1\dagger}(p_1)\chi^{\alpha_2\dagger}(p_2)\ldots\chi^{\alpha_{N_c}\dagger}(p_{N_c}), \tag{26}$$

but the meaning of these operators as $N_c\to\infty$ is not so obvious. Yet we can think about normalized states of this form when *all the momenta are positive* acting on the Fock vacuum, they should correspond to such baryon-like states. Perhaps our large-N_c theory can detect their presence. Indeed, one can check that the operator,

$$\hat{B}=\frac{1}{N_c}\int_0^\infty [dp]\chi^{\alpha\dagger}(p)\chi^{\alpha}(p), \tag{27}$$

measures the number of such excitations. This operator can be given a meaning in our theory: in the large-N_c limit therefore it is natural to expect that the operator, $B=1/2\int_0^\infty [dp]F(p,p)$ gives us this number and as we will see it is well-defined. In our classical limit we can ask if this number makes sense for our system, that is if it is a conserved quantity. The answer, not surprisingly, is no: the above-given baryon number *is not conserved* by our equations of motion. Thus there are really no baryons in this theory.

IV. GEOMETRY OF THE PHASE SPACE

To understand the geometry behind the classical system that we introduce in Sec. III, we must take a look at the finite dimensional orthogonal group. Our approach will be similar to the one in Ref. 24 where we discussed the bosonic version of this theory. The basic ideas of the quantization of free Weyl fermions and the underlying geometry is discussed in the paper of Bowick and Rajeev,[16] but we would like to expand on it and there are some differences in our conventions.

We recall that the real orthogonal group can be defined as the set of linear transformations which leave a quadratic form invariant.

$$Q(Au,Av)=Q(u,v) \tag{28}$$

[here $Q(u,v)=u^TQv$ represents this quadratic form, and superscript T denotes the ordinary transpose]. In our case the quadratic form is diagonal, so it is the standard inner product u^Tv. We work with the complexification of the original real Hilbert space, and if our Hilbert space is even dimensional, in this complex space we can use a different quadratic form, simply by using an invertible transformation S, $Q_2=S^TQS$. Assume now that we have a complex structure J acting on our original real Hilbert space, that is, a real antisymmetric matrix with respect to this form, which is also orthogonal, implying $J^2=-1$. If the quadratic form is the identity, we may think of such a matrix as $J=\left(\begin{smallmatrix}0 & 1\\ -1 & 0\end{smallmatrix}\right)$ in an appropriate basis of the *real Hilbert space*. Let us split our Hilbert space into two isomorphic pieces with respect to the above-mentioned decomposition of the complex structure, $W\oplus\tilde{W}$, and complexify the real Hilbert space, naturally we have $W\otimes\mathbf{C}\oplus\tilde{W}\otimes\mathbf{C}$. Choose with respect to this decomposition,

$$S=\begin{pmatrix} i1 & -i1 \\ 1 & 1 \end{pmatrix}. \tag{29}$$

This is the transform which we can use to diagonalize our complex structure. Of course our original quadratic form now changes as we described previously: we get

$$Q=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{30}$$

(In our problem we actually transform the inverse of this form, but one can see that as matrices these two forms are identical.) The complex orthogonal group is the set of transformations which leaves the form Q invariant. Thus a general complex matrix $g=\left(\begin{smallmatrix}a & b\\ c & d\end{smallmatrix}\right)$ is orthogonal if

$$a^Tc=-c^Ta,\quad a^Td+c^Tb=1,\quad b^Td=-d^Tb. \tag{31}$$

In finite dimensions the quadratic form is $Q(z,z)=z_1z_{m+1}+z_2z_{m+2}+\cdots+z_mz_{2m}$. We see then that the original *real orthogonal group* is embedded into the complex orthogonal group defined by this quadratic form as a set of matrices

$$g=\begin{pmatrix} a & b \\ \overline{b} & \overline{a} \end{pmatrix}, \tag{32}$$

with now a,b satisfying, $a^T\overline{a}+b^\dagger b=1$ and $a^T\overline{b}=-b^\dagger a$ (where we decomposed the matrix in the obvious way). This explicitly shows that the complex structure, which is a real orthogonal matrix, becomes diagonal,

$$J=\left(\begin{smallmatrix}-i1 & 0\\ 0 & i1\end{smallmatrix}\right).$$

In our physical example these diagonalizations will be accomplished by the Fourier transform.

An immediate consequence of this way of looking at the real orthogonal group is that the real orthogonal group actually carries a copy of the unitary group in it, corresponding to the elements, $\left(\begin{smallmatrix}a & 0\\ 0 & \overline{a}\end{smallmatrix}\right)$. The quadratic form implies $a^T\overline{a}=1$, as well as $aa^\dagger=1$, this implies $aa^\dagger=a^\dagger a=1$. It is the unitary group of $\mathcal{H}_+$, where $\mathcal{H}_+$ refers to the subspace on which J acts as i.

For our purposes we should extend these discussions to the infinite dimensional case. In the infinite dimensional one we should not use the full orthogonal group but the one with a convergence condition.[16] This condition is the well-known Hilbert–Schmidt condition in the quasifree representations of canonical anticommutation algebra. We will comment further on the convergence conditions when we make contact with our system. We define the restricted orthogonal group on the complexified Hilbert space as follows:

$$O_1(\mathcal{H})=\left\{ g^TQg=Q \,\middle|\, g=\begin{pmatrix} a & b \\ \overline{b} & \overline{a} \end{pmatrix} \quad b\in\mathcal{I}_2 \right\}, \tag{33}$$

where $\mathcal{I}_2$ is the ideal of Hilbert–Schmidt operators.[25] We can state the convergence condition more economically as $[\epsilon,g]\in\mathcal{I}_2$, where $\epsilon=\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$ with respect to the above-mentioned decomposition. This is basically the complex structure we had, except that a factor of i has been removed. The Lie algebra of this group can be found from an infinitesimal group element,

$$g=1+i\Delta u=1+i\Delta\begin{pmatrix} S & R \\ -\overline{R} & -\overline{S}\end{pmatrix}, \tag{34}$$

with $R^T=-R$ and $S^\dagger=S$ and Δ represents an infinitesimal parameter. The reader can verify that $u^TQ+Qu=0$. We would like to define a classical phase space using this infinite dimensional orthogonal group. This will be our phase space for the large-N_c theory, but for the moment let us define it as a mathematical system. We introduce a variable Φ,

$$\Phi=g\epsilon g^{-1},\quad g\in O_1(\mathcal{H}). \tag{35}$$

The orbit of ϵ under the restriced orthogonal group is parametrized by this operator. It is easy to see that the orbit is diffeomorphic to

$$O_1(\mathcal{H})/U(\mathcal{H}_+). \tag{36}$$

The operator Φ satisfies

$$\Phi^2=1,\quad \Phi=-Q^{-1}\Phi^TQ,\quad \Phi-\epsilon=\begin{pmatrix}\mathcal{I}_1 & \mathcal{I}_2\\ \mathcal{I}_2 & \mathcal{I}_1\end{pmatrix}, \tag{37}$$

where $\mathcal{I}_1$ denotes the trace class operators in the appropriate space of operators (here Q^{-1} is identical to Q as a matrix, but transforms differently). The second condition really says that Φ is in the Lie algebra of this group (it is possible to think of this space as a real subset of the restricted Grassmanian, and there is an analogous construction of a line-bundle on this space, see Ref. 26). The tangent space of this orbit is given by the infinitesimal action of the group at any point, and in fact it is a copy of the Lie algebra of this group at every point. The action of a vector field on the basic variable Φ becomes $V_u(\Phi)=i[u(\Phi),\Phi]$, for a Lie algebra element $u(\Phi)$, which changes differentiably over the orbit. So a vector field at a point $\Phi=g\epsilon g^{-1}$ comes from a Lie algebra element $g^{-1}u(\Phi)g$.

It is well-known[27] that such orbits in finite dimensions typically carry a symplectic structure. If we formally define a two form,

$$\Omega=\frac{i}{4}\operatorname{Tr}\Phi\, d\Phi\wedge d\Phi, \tag{38}$$

following the methods in Ref. 1 we can check that it is closed and nondegenerate. The form evaluated at two vector fields V_u,V_v is given by

$$\Omega(V_u,V_v)=\frac{i}{8}\operatorname{Tr}\epsilon[[\epsilon,g^{-1}u(\Phi)g],[\epsilon,g^{-1}v(\Phi)g]], \tag{39}$$

which shows that it is well-defined, due to the Hilbert–Schmidt conditions, nondegenerate, homogeneous, and Kähler. The group action on this phase space $\Phi\mapsto g^{-1}\Phi g$ is actually Hamiltonian, that is there are moment maps which generate this action, given by a conditional trace, $F_u=-1/2\operatorname{Tr}_\epsilon(\Phi-\epsilon)u$, with $\operatorname{Tr}_\epsilon(A)=1/2\operatorname{Tr}(A+\epsilon A\epsilon)$. Just for completeness we record that

$$\{F_u,F_v\}=F_{-i[u,v]}-2\,\mathfrak{Im}\operatorname{Tr}(R_1R_2^\dagger), \tag{40}$$

if we decompose u,v as above. The last term represents a central part and cannot be removed in this classical theory.

How does this tie up with our system? Recall that we had a symplectic form which was i times a quadratic form Q, and a Hamiltonian for the free theory which is the mass part, i times an antisymmetric form ω, the combination of the two provides a natural operator: $\tilde{\omega}=Q^{-1}\omega$ is a type (1,1) tensor hence a proper linear transformation. Its polar decomposition will have all the basic pieces we need. Of course we have also $\omega^{-1}Q$, so which one we choose is determined by the equations of motion. If we look at this general system in the Hamiltonian formalism,

$$S_0=\int \mathrm{d}t\,\frac{1}{2}i\psi Q\partial_t\psi-\int \mathrm{d}t\,H=\int \mathrm{d}t\,\frac{1}{2}i\psi Q\partial_t\psi-\int \mathrm{d}t\,\frac{1}{2}i\psi\omega\psi, \tag{41}$$

the equations of motion will give us

$$\partial_t\psi=Q^{-1}\omega\psi. \tag{42}$$

Hence the operator $Q^{-1}\omega$ is the one we should use. We find the polar decomposition of this operator, $\tilde{\omega}=KJ$, where K is positive symmetric and $J^TJ=1$, orthogonal (we should be using the natural inner product defined by Q to define the transpose, and in the infinite dimensional case to define underlying real Hilbert space of initial data). However $\tilde{\omega}$ is antisymmetric with respect to our quadratic form, this means that $J^2=-1$ and orthogonal, thus a complex structure (the complex structure coming from the other choice differs from this by a minus sign). In our example we see that the quadratic form is $2\sqrt{2}\,\delta(x^--y^-)\delta_{\alpha\beta}$ (thus all the calculations can be done with the usual matrix transpose), and the antisymmetric form is $-\sqrt{2}m^2\partial_-^{-1}$, so we get from the polar decomposition, $K=(m^2/2)[-\partial_-^2]^{-1/2}$, $J=-[-\partial_-^2]^{1/2}\partial_-^{-1}$ (we omit the identity in the color space). When we use a basis which diagonalizes $\tilde{\omega}$ we get solutions which oscillate in time with a frequency given by the eigenvalues of K. In our example, if we decompose the field ψ^α using a Fourier mode decomposition,

$$\psi^\alpha(x^-)=\int_{-\infty}^{\infty}\frac{[\mathrm{d}p]}{2^{3/4}}w^\alpha(p)e^{-ipx^-}, \tag{43}$$

we have

$$\begin{aligned} w^\alpha(p,x^+)&=w^\alpha(p,0)\exp\left(-i\frac{m^2}{2|p|}x^+\right) \quad \text{for } p>0,\\ w^\alpha(p,x^+)&=w^\alpha(p,0)\exp\left(+i\frac{m^2}{2|p|}x^+\right) \quad \text{for } p<0. \end{aligned} \tag{44}$$

(Note that the above-given combinations on the exponents are relativistically invariant if we recall the mass-shell condition $p_+=m^2/2p_-$.) This suggests that the i subspace of J goes to creation operators, and $-i$ subspace goes to the annihilation operators, it is better therefore to represent our Fourier coefficients as $w^\alpha(p)=\xi^\alpha(p)$ and $w^\alpha(-p)=\overline{\xi}^\alpha(p)$ for $p>0$. If we act with J on our field variables,

$$(J\psi)^\alpha(x^-)=\int_0^\infty\frac{[\mathrm{d}p]}{2^{3/4}}(-i\overline{\xi}^\alpha(p)e^{-ipx^-}+i\xi^\alpha(p)e^{ipx^-}). \tag{45}$$

We see now that this Fourier transform diagonalizes our complex structure. If we look at the inverse of the quadratic form it transforms as $\int \mathrm{d}x^-\,\mathrm{d}y^-\,2^{3/4}e^{ipx^-}(2\sqrt{2})^{-1}\delta(x^--y^-)2^{3/4}e^{iqy^-}$, which gives us $\delta[p+q]$. This is the form of Q that we wanted to obtain.

From the Fourier decomposition, creation and annihilation operators therefore are assigned according to sgn(p), $\xi(p)\mapsto\chi^{\dagger\alpha}(p)$ and $\overline{\xi}(p)\mapsto\chi^{\alpha}(p)$. The ultimate reason for the choice of Fock vacuum is to make the Hamiltonian bounded from below, if we write our Hamiltonian in the Fourier space,

$$H_0=\mathcal{P}\int\frac{[dp]}{2^{3/2}}\frac{\sqrt{2}m^2}{2|p|}\mathrm{sgn}(p):\chi^{\alpha}(-p)\chi^{\alpha}(p)$$

$$:=\int_{0^+}^{\infty}\frac{[dp]}{2^{3/2}}\frac{\sqrt{2}m^2}{2|p|}[:\chi^{\alpha\dagger}(p)\chi^{\alpha}(p):-:\chi^{\alpha}(-p)\chi^{\alpha\dagger}(-p):].$$

Notice that sgn(p) appears in the Hamiltonian, which is basically the complex structure we have, and the normal ordering (according to our choice of creation and annihilation operators) now makes the Hamiltonian bounded from below:

$$H_0=\int_{0^+}^{\infty}\frac{m^2}{2|p|}\chi^{\alpha\dagger}(p)\chi^{\alpha}(p). \tag{46}$$

We could question the effect of the interactions since we have been describing everything in terms of the free part of the Hamiltonian. Here we see a clear advantage of our light-cone point of view, the complex structure we start with using the free Hamiltonian is independent of any of the parameters of the theory, *thus the choice of quasifree representation of the canonical anticommutation relations is not affected by the change of parameters due to interactions*. In our case we explicitly keep the change of mass due to the interactions with the gauge fields, so we are not taking advantage of this property. In the more general case this property may be helpful, in fact for the scalar theory it is essential. We thus conclude our discussion on the choice of Fock space and its relation to the natural complex structure in our system.

Next we show that $\Phi-\epsilon$ really represents our basic bilinears: let us decompose the complexification of our one-particle Hilbert space as $\mathcal{H}_+\oplus\mathcal{H}_-$ according to $-\mathrm{sgn}(p)$, we can write a general bilinear as an operator acting on the one-particle space and decomposed according to this direct sum, one checks that

$$F=\begin{pmatrix} S & R \\ -\overline{R} & -\overline{S}\end{pmatrix}, \tag{47}$$

with exactly $S^{\dagger}=S$ and $R^{T}=-R$. We also know that $(F+\epsilon)^2=1$. But these are exactly the properties satisfied by Φ. Our physical system has a one-particle Hilbert space given by the initial data on the light-cone $x^{+}=0$, we complexify this space and use Fourier transform to put our operators into the desired form. Then $\mathcal{H}_-$ corresponds to the negative frequency components in the physics language. The Poisson bracket relations can be meaningfully extended to the Hilbert–Schmidt type R, so we need the convergence conditions. The convergence conditions are also a natural consequence of the super-renormalizability of this system. The time evolution of the finite N_c system should keep us in the same free Fock space, and in the large-N_c limit this should be expressible as an operator like Φ. In fact the smeared out Poisson brackets are given by the Poisson bracket relations of the moment maps. Thus the symplectic structure we have on this homogeneous manifold is the one we have found for our bilinears.

It is useful to look at the same issue from the point of view of generalized coherent states: assume that we have a Lie group which is representable on a Hilbert space by unitary operators through a highest weight vector. If we look at the orbit of this vector under the action of the group, this orbit has a natural symplectic structure, and all the vectors on the orbit correspond to the generalized coherent states.[28,29,4] In our case the group of Bogoluibov automorphisms, which do not act on the color part of our fermions, are represented on the fermion Fock space by the color invariant bilinears. The highest weight vector is the vacuum and its orbit under this group there-

fore carries a natural symplectic structure. The corresponding group is the restricted orthogonal group $O_1(\mathcal{H})$ and the orbit is our phase space. [In fact physically we should be using the projective Fock space, since the phase does not change the physical content of a state. The bilinears provide a unitary representation of the central extension $\hat{O}_1(\mathcal{H})$ of the group $O_1(\mathcal{H})$, when we use the projective Fock space, the central part disappears and we descend to the restricted orthogonal group.] The convergence conditions are now a result of the implementability of these automorphism in the Fock space, which is defined by our choice of the vacuum.[22,21,12] The large-N_c limit allows us to restrict to the bilinears and the super-normalizability keeps us in the restricted class of implementable automorphisms. Thus taking the large-N_c limit provides a classical limit in this sense.

This shows that our large-N_c limit has a well-defined classical phase space with a natural symplectic structure. This opens up various possibilities, such as studying large fluctuations of the field in this limit. There are various delicate questions, such as the domain of the Hamiltonian, existence of finite time evolution, completeness of the trajectories which we plan to come back to in the future.

V. BOSONS AND FERMIONS

This is the begining of the second part of our paper. The second part has two themes again: the construction of the phase space via the large-N_c limits of the bilinears and the geometry of the ensuing phase space. Since the bosonic theory is developed in Ref. 24 and the fermionic version is explained in detail in the previous sections the construction of the phase space and finding the Hamiltonian will be very brief. We recommend that the reader look at Ref. 24 and we use the results of the previous sections freely. The geometry part, which is in Sec. VI, will require new methods and in some sense it is not as complete. It may be helpful if the reader also consults Ref. 14, where the SU(N_c) version is discussed. We will develop these aspects as much as we can and in some cases we indicate what the idea should be.

We start our first theme: we use the same conventions as in the previous sections and our previous paper. The action functional of the combined system of bosons and fermions can be written as

$$S=\int\left[\frac{1}{2}\mathrm{Tr}\,F_{\mu\nu}F^{\mu\nu}+i\overline{\Psi}_M\gamma^\mu D_\mu\Psi_M-m_F\overline{\Psi}_M\Psi_M+\frac{1}{2}(D^\mu\phi)^T(D_\mu\phi)-\frac{1}{2}m_B^2\phi^T\phi\right], \quad (48)$$

where we use the same conventions as in Sec. IV for the Majorana fermions. The transpose refers to the color indices for the scalar field. Again the covariant derivative is $D_\mu=\partial_\mu+gA_\mu$, where A_μ has values in the Lie algebra of SO(N_c). We choose x^+ as time and set $A_-=0$ as our gauge fixing condition. Then the action in the light-cone formalism reads

$$S=\int \mathrm{d}x^+\,\mathrm{d}x^-\Bigg[i\sqrt{2}\psi_1^T\partial_-\psi_1+i\sqrt{2}\psi_2^T\partial_+\psi_2+2im_F\psi_1^T\psi_2+\frac{1}{2}\phi^T(-2\partial_-)\partial_+\phi-\frac{m_B^2}{2}\phi^T\phi$$
$$+gA_+^a\left[i\sqrt{2}\psi_2^TT^a\psi_2+\frac{1}{2}(\partial_-\phi^TT^a\phi-\phi^TT^a\partial_-\phi)\right]+\frac{1}{2}(\partial_-A_+^a)^2\Bigg].$$

The advantage of the light-cone formalism is again clear, we are already in the Hamiltonian picture. We can read off the Poisson brackets satisfied by the dynamical fields. We also see that ψ_1 is not dynamical, as well as A_+^a, therefore they can be eliminated through their equations of motion. The dynamical fermion field ψ_2^α will be called ψ^α for simplicity as in the previous sections. We will assume that the field A_+^a is eliminated after the dynamical fields are quantized, this will give us the quantized Hamiltonian of the system,

$$H=\int \mathrm{d}x^{-}\left(\frac{1}{2}m_B^2:\phi^T\phi:+\frac{1}{2}\sqrt{2}m_F^2:\psi^T\frac{1}{i\partial_-}\psi:-\frac{g^2}{2}:J^a:\frac{1}{\partial_-^2}:J^a:\right), \tag{49}$$

where

$$J^a=[i\sqrt{2}\psi^T T^a\psi+\tfrac{1}{2}(\partial_-\phi^T T^a\phi-\phi^T T^a\partial_-\phi)]. \tag{50}$$

The quantization process is defined for the Fermionic sector in Sec. II and for bosons in Ref. 24. We expand fermions and bosons into Fourier modes in a *complex* space,

$$\psi^\alpha(x^-)=\int_{-\infty}^{\infty}\frac{[\mathrm{d}p]}{2^{3/4}}\chi^\alpha(p)e^{-ipx^-},\quad \phi^\alpha(x^-)=\int_{-\infty}^{\infty}\frac{[\mathrm{d}p]}{\sqrt{2|p|}}a^\alpha(p)e^{-ipx^-}, \tag{51}$$

with now $\chi^{\alpha(p)\dagger}=\chi^\alpha(-p)$ and $a^{\alpha\dagger}(p)=a^\alpha(-p)$. (We should again assume that there is an infinitesimal cutoff around the zero momentum to be taken to zero at a later stage.) The Poisson bracket relations go to

$$[\chi^\alpha(p),\chi^\beta(q)]_+=\delta[p+q]\delta^{\alpha\beta},\quad [a^\alpha(p),a^\beta(q)]=\mathrm{sgn}(p)\,\delta[p+q]\delta^{\alpha\beta}. \tag{52}$$

These are exactly the same as before, there is one more commutator now,

$$[\chi^\alpha(p),a^\beta(q)]=0. \tag{53}$$

As we will see in Sec. VI the definition of the Fock vacuum brings new features—a larger symmetry algebra appears. We introduce the vacuum state $|0>_s$, characterized by $\chi^\alpha(p)|0>_s=0, a^\alpha(p)|0>_s=0$ for $p>0$, where we put a subscript s to emphasize that the vacuum is for the full algebra of the boson/fermion system. We repeat for the convenience of the reader the normal ordering rules of the bilinears (rewritten to fit to our needs),

$$:\chi^\alpha(p)\chi^\beta(q):=\chi^\alpha(p)\chi^\beta(q)-\tfrac{1}{2}\delta^{\alpha\beta}(1+\mathrm{sgn}(p))\,\delta[p+q],$$

$$:a^\alpha(p)a^\beta(q):=a^\alpha(p)a^\beta(q)-\tfrac{1}{2}\delta^{\alpha\beta}(1+\mathrm{sgn}(p))\,\delta[p+q].$$

There is an obvious extension of the general definition of normal ordering to the product of more than two operators, which one needs for the reduction of the Hamiltonian: set all the annihilation operators to the right of creation operators in a recursive way.

We first introduce our bilinears for the large-N_c limit and work out their Poisson brackets. Then we express our Hamiltonian in the large-N_c limit in terms of these bilinears. We can see that the basic color invariant observables are

$$\hat{F}(p,q)=\frac{2}{N_c}:\chi^{\alpha\dagger}(p)\chi^\alpha(q):,\quad \hat{B}(p,q)=\frac{2}{N_c}:a^{\alpha\dagger}(p)a^\alpha(q):,$$

$$\hat{C}(p,q)=\frac{2}{N_c}\chi^{\alpha\dagger}(p)a^\alpha(q),\quad \hat{\bar{C}}(p,q)=\frac{2}{N_c}a^{\alpha\dagger}(p)\chi^\alpha(q).$$

Note that we have no need for normal ordering in the last two operators since they consist of commuting operators. In the large-N_c limit $\hat{C}$ and $\hat{\bar{C}}$ are related, $\overline{C}=C^\dagger$, and there are similar conditions on F,B (when we represent the resulting classical observables as integral kernels and think of them as now abstract operators). For our calculational purposes it is better to introduce the following variables as in Sec. III and Ref. 24,

$$\hat{T}(p,q)=\frac{2}{N_c}:a^\alpha(p)a^\alpha(q):=\hat{B}(-p,q)\quad \hat{R}(p,q)=\frac{2}{N_c}:\chi^\alpha(p)\chi^\alpha(q):=\hat{F}(-p,q), \tag{54}$$

and also the variable,

$$\hat{S}(p,q)=\frac{2}{N_c}\chi^{\alpha}(p)a^{\alpha}(q)=\hat{C}(-p,q). \tag{55}$$

These variables in the large-N_c limit satisfy the following (super)Poisson brackets,

$$\begin{aligned}\{T(p,q),T(s,t)\}=&-2i(\mathrm{sgn}(p)\,\delta[p+s]T(q,t)+\mathrm{sgn}(q)\,\delta[q+s]T(p,t)+\mathrm{sgn}(p)\,\delta[p+t]T(s,q)\\&+\mathrm{sgn}(q)\,\delta[q+t]T(s,p)+(\mathrm{sgn}(p)+\mathrm{sgn}(q))(\delta[p+s]\delta[q+t]\\&+\delta[p+t]\delta[s+q])),\end{aligned}$$

$$\begin{aligned}\{R(p,q),R(s,t)\}=&-2i(R(p,t)\,\delta[q+s]-R(q,t)\,\delta[p+s]+R(s,p)\,\delta[q+t]-R(s,q)\,\delta[p+t]\\&+(\delta[q+t]\delta[p+s]-\delta[p+t]\delta[q+s])(\mathrm{sgn}(t)+\mathrm{sgn}(s))),\end{aligned}$$

$$\{T(p,q),S(s,t)\}=-2i(S(s,q)\mathrm{sgn}(p)\,\delta[p+t]+S(s,p)\mathrm{sgn}(q)\,\delta[q+t]),$$

$$\{R(p,q),S(s,t)\}=-2i(S(p,t)\,\delta[q+s]-S(q,t)\,\delta[p+s]),$$

$$\begin{aligned}\{S(p,q),S(s,t)\}_{+}=&-2i(T(q,t)\,\delta[p+s]-R(s,p)\mathrm{sgn}(q)\,\delta[q+t]\\&+\delta[p+s]\delta[q+t](1+\mathrm{sgn}(p)\mathrm{sgn}(q))).\end{aligned}$$

We note that the last one is symmetric in the variables and the third and fourth ones show that S behaves as a module of the algebras defined by the Poisson brackets of T,R, thus it carries a representation of these two algebras. This is the general form of a superalgebra structure. We will denote the full set of these brackets as a super-Possion bracket $\{\ ,\ \}_s$.

The conversion of the normal ordered products of noncolor invariant combinations appearing in the above Hamiltonian to the full normal ordering in the large-N_c limit can be achieved as before resulting with the same changes in the masses $m_F^2\mapsto m_F^2-g^2/2\pi$ and $m_B^2\mapsto m_R^2-g^2/2\pi$, where $m_R^2=m_B^2-g^2/4\pi\ln(\Lambda_U/\Lambda_I)$ denotes the renormalized mass of the boson. We skip the details of this reduction, since they are the extensions of the details in Ref. 11 and we have given some essential steps in Sec. III. The resulting Hamiltonian of our system in the large-N_c can be expressed as a free part and an interacting part:

$$H_0=\frac{1}{8}\left(m_R^2-\frac{g^2}{2\pi}\right)\mathcal{P}\int\frac{[\mathrm{d}p]}{|p|}T(-p,p)+\frac{1}{8}\left(m_F^2-\frac{g^2}{2\pi}\right)\mathcal{P}\int\frac{[\mathrm{d}p]}{p}R(-p,p). \tag{56}$$

The interaction part is written as

$$\begin{aligned}H_I=&\mathcal{FP}\int[\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t](G_1(p,q;s,t)T(p,q)T(s,t)+G_2(p,q;s,t)R(p,q)R(s,t)\\&+G_3(p,q;s,t)S(p,q)S(s,t)),\end{aligned}$$

where the kernels are given by

$$G_1(p,q;s,t)=\frac{g^2}{64}\frac{\delta[p+q+s+t]}{\sqrt{|pqst|}}\frac{sq-st+pt-pq}{(p+s)^2},$$

$$G_2(p,q;s,t)=-\frac{g^2}{64}\frac{\delta[p+q+s+t]}{(p+s)^2},$$

$$G_3(p,q;s,t)=\frac{g^2}{64}\,\frac{\delta[p+q+s+t]}{\sqrt{|tq|}(p+s)^2}.$$

We have not completed the definition of our large-N_c limit yet, there is a constraint. Recall that we still have a left over global color invariance, which is generated by the operator,

$$\hat{Q}^{\alpha\beta}=\int [\mathrm{d}p](:\chi^{\alpha\dagger}(p)\chi^{\beta}(p):+\mathrm{sgn}(p):a^{\alpha\dagger}(p)a^{\beta}(p):). \tag{57}$$

When we restrict our color invariant bilinears to the color invariant sector of the full Fock space, we find that

$$(F+\epsilon)^2+C\epsilon C^{\dagger}=1,$$

$$C\epsilon B+C\epsilon+FC+\epsilon C=0,$$

$$\epsilon B\epsilon C^{\dagger}+C^{\dagger}+\epsilon C^{\dagger}\epsilon+\epsilon C^{\dagger}F=0,$$

$$(\epsilon B+\epsilon)^2+\epsilon C^{\dagger}C=1,$$

where we define as in Sec. III, $\epsilon(p,q)=-\mathrm{sgn}(p)\delta[p-q]$ (here the minus sign is crucial, in our previous works that was not important, but in the super case there is a preferred choice) and we also employ the product convention as before for example $(FC)(p,s)=\int[dq]F(p,q)C(q,s)$. We warn the reader that above the two epsilons have the same matrix elements but they are acting on different spaces. The meaning of this constraint could best be understood if we introduce a superoperator,

$$\Phi=\begin{pmatrix}\epsilon B+\epsilon & \epsilon C^{\dagger}\\ C & F+\epsilon\end{pmatrix}. \tag{58}$$

The above-mentioned constraint is simply given by

$$\Phi^2=1. \tag{59}$$

It also satisfies a Lie algebra condition, it is better to write it in the following form: use a decomposition of our superspace into $\mathcal{H}_+|\mathcal{H}_+\oplus\mathcal{H}_-|\mathcal{H}_-$, according to the sign of ϵ in even and odd parts, respectively. Then we have $\hat{\epsilon}=\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$, and we introduce with respect to this decomposition

$$\hat{\omega}_s=\left(\begin{smallmatrix}0&-\overline{\epsilon}\\1&0\end{smallmatrix}\right),$$

where $-\overline{\epsilon}=\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$, and this is a supermatrix acting between positive and negative subspaces, then

$$\hat{\omega}_s\Phi^{\tau}+\Phi\hat{\omega}_s=0, \tag{60}$$

we invite the reader to verify this.

There are also convergence conditions, which come from the super-renormalizability of this system again. The time evolution should leave this system in the same Fock space. Another way to see this is to think about the smeared out operators, and see that the central terms make sense only for the restricted set of operators, for which the off-diagonal blocks are in the Hilbert–Schmidt class. We can write down these convergence conditions in an economical way as

$$[\hat{\epsilon},\Phi]\in\mathcal{I}_2, \tag{61}$$

where $\mathcal{I}_2$ refers to the ideal of Hilbert–Schmidt operators in this superspace. We have proposed elsewhere[30] a method of introducing such operators in the supercontext, and we assume this definition is used. Since these technical matters are not completely settled we are brief at this point—see also Sec. VI on the geometry. This completes the construction of our large-N_c limit: we

postulate the above-mentioned Hamiltonian, the super-Possion brackets with the constraint and this defines a classical system. The ''time'' evolution is given by the basic rule: for any observable O_s of the theory

$$\frac{\partial O_s}{\partial x^+} = \{O_s, H\}_s, \tag{62}$$

where the Hamiltonian is in general an even function of our bilinears—which we should consider as the coordinates of this phase space.

It is possible to carry out the analysis given in Ref. 14, but we will be content with describing only the linear approximation. We plan to report on these in a separate publication (they will appear in the Ph.D. thesis of E.T.).

We start with the linearization of the constraint $\Phi^2=1$, which gives us

$$F\epsilon+\epsilon F=0, \quad \epsilon B\epsilon+B=0, \quad \epsilon C+C\epsilon=0. \tag{63}$$

The first two are exactly the conditions we have found before, for mesons made up of only bosons in Ref. 24, the first one is in Sec. III, and the last one is the new condition on our odd variable. In terms of S that means we have $S(u,v)=0$ unless $u,v>0$ or $u,v<0$. If we assume $u,v>0$ and evaluate the equations of motion in the linear approximation for $S(u,v)$, $\partial_+ S(u,v;x^+) = \{S(u,v;x^+),H\}$ and furthermore we make the same type of ansatz as in Refs. 11, 24, and 14, $S(u,v;x^+)=\zeta_S(x)e^{-iP_+x^+}$, with $P=u+v, x=u/P$,

$$\mu_s^2\zeta_S(x)=\left[\frac{m_F^2-g^2/2\pi}{x}+\frac{m_R^2-g^2/2\pi}{1-x}\right]\zeta_S(x)-\frac{g^2}{8\pi}\int_0^1\frac{\mathrm{d}y}{\sqrt{xy}}\frac{x+y}{(x-y)^2}\zeta_S(1-y). \tag{64}$$

The other linearized equations are the same as before (see Sec. III and Ref. 24).

There are baryonic states that we can measure by the operator

$$\hat{\mathbf{B}}=\frac{1}{N_c}\int_0^\infty [\mathrm{d}p](\chi^{\alpha\dagger}(p)\chi^\alpha(p)+a^{\alpha\dagger}(p)a^\alpha(p)), \tag{65}$$

in the large-N_c limit this operator should go to $\mathbf{B}=1/2\int_0^\infty[\mathrm{d}p](F(p,p)+B(p,p))$. The *baryonic states* for finite N_c correspond to states of the form

$$\frac{1}{Z}\epsilon_{\alpha_1\alpha_2\cdots\ \alpha_{N_c}}\chi^{\alpha_1\dagger}(p_1)\cdots\ \chi^{\alpha_s\dagger}(p_s)a^{\alpha_{s+1}\dagger}(p_{s+1})\cdots\ a^{\alpha_{N_c}\dagger}(p_{N_c}), \tag{66}$$

where $p_1\cdots\ p_{N_c}>0$ and products of them acting on $|0>_s$.

Not surprisingly *the above-given baryon number is not a conserved quantity*, so it does not have the physical importance as it has in the case of Dirac fermions where it is a conserved number, in fact a topological number (see Ref. 11 for the discussion of this in the large-N_c limit and its extension in Ref. 14).

VI. THE GEOMETRY OF THE PHASE SPACE

Let us define a superspace $\mathcal{H}|\mathcal{H}$, where we use a splitting to even and odd according to the grading $+,-$ (we are using a $\mathbf{Z}_2$ graded *real Hilbert space*). We recall some of the conventions, following Berezin[18]: we work with the Grassmann envelope of this graded vector space (thus we acquire a $\mathbf{Z}$ grading). Its mathematical theory is delicate and we will comment on it later (some good examples of homogeneous supersymplectic manifolds are worked out in Ref. 31, this is a good reference to learn by examples). We decompose every linear transformation or tensor according to this grading, the standard matrix form of a linear transformation is

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} : \mathcal{H}|\mathcal{H} \to \mathcal{H}|\mathcal{H}, \tag{67}$$

where A,D are even and B,C are odd. This means that $A=A_B+A_S, D=D_B+D_S$ where the subscript B refers to the body that is the ordinary numbers, the subscript S refers to the soul, that is only the Grassmann part. B,C have no body, they are purely Grassmann valued.

We have the usual Hermitian conjugation of such block matrices, but the transpose has to be carefully defined. We introduce a supertranspose, τ,

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{\tau} = \begin{pmatrix} A^T & C^T \\ -B^T & D^T \end{pmatrix}, \tag{68}$$

where T denotes the ordinary matrix transpose. One can verify that this form satisfies $(AB)^{\tau} = B^{\tau}A^{\tau}$. It will be useful to record the following properties, $\mathrm{Str}(A^{\tau}) = \mathrm{Str}\, A$, if we decompose our graded space into a direct sum, for example in our case into $\mathcal{H}_+|\mathcal{H}_+ \oplus \mathcal{H}_-|\mathcal{H}_-$, the operators can also be decomposed into superoperators, say into $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$, then

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{\tau} = \begin{pmatrix} a^{\tau} & c^{\tau} \\ b^{\tau} & d^{\tau} \end{pmatrix}. \tag{69}$$

Realness is related to an involution in the Grassmann algebra, $\xi \mapsto \xi^*$ and we assume that this involution obeys $(\xi^i \xi^j)^* = (\xi^j)^*(\xi^i)^*$ and $(a\xi)^* = \overline{a}\xi^*$, where a is a complex number and the bar denotes the ordinary complex conjugation. The real Grassmann algebra is the part which is invariant under this involution. This means that there will be factors of i to make things invariant. This implies that *the real graded Hilbert space is defined residing inside a complex graded Hilbert space*.

On the space of linear transformations there is a complex conjugation operator, according to Berezin conventions it should be given by the following: write a linear transformation in its standard form, then

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^* = \begin{pmatrix} a^* & -b^* \\ c^* & d^* \end{pmatrix}. \tag{70}$$

We note that $A^{**}=A$, and $(A^{\tau})^* = \left(\begin{smallmatrix} a^{\dagger} & -c^{\dagger} \\ -b^{\dagger} & d^{\dagger} \end{smallmatrix}\right) = \tilde{E}A^{\dagger}\tilde{E}$, here $\tilde{E} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$, whereas $(A^*)^{\tau} = A^{\dagger}$.

We have the set of *real linear transformations*, this set is invariant under the above conjugation, $M^*=M$, it remains so under the product of supermatrices, thanks to $(A_1A_2)^* = A_1A_2$. The set of real linear operators thus is an algebra.

Let us assume that the even part has a symplectic form ω and the odd part has a standard quadratic form 1. On the complexification of this space we introduce a supersymplectic form,

$$\omega_s = \begin{pmatrix} \omega & 0 \\ 0 & i1 \end{pmatrix}, \quad \omega = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{71}$$

Note that multiplying the last part with an i does not really change anything as far as only the even transformations are concerned but for the full case we need this factor. We look at the space of *real transformations* which will leave this form invariant,

$$g^{\tau}\omega_s g = g\omega_s g^{\tau} = \omega_s, \tag{72}$$

this is a supergroup, and it is denoted by $\mathrm{OSp}(\mathcal{H}|\mathcal{H})$. Its even part has body isomorphic to $\mathrm{Sp}(\mathcal{H}) \oplus \mathrm{O}(\mathcal{H})$, the odd parts are modules over the Grassmann envelopes of these groups. If we write down the group conditions for an element $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) = \left(\begin{smallmatrix} a^* & -b^* \\ c^* & d^* \end{smallmatrix}\right)$, where a,d are real even, c real odd, and b imaginary odd operators,

$$a^T\omega a+ic^Tc=\omega,\quad a^T\omega b+ic^Td=0,\quad -b^T\omega a+id^Tc=0,\quad -b^T\omega b+id^Td=i1. \tag{73}$$

Since we have the complex conjugation convention $(\psi\xi)^*=-\psi^*\xi^*$, the complex conjugate of a product of odd operators become imaginary, this is why we have ic^Tc, then it becomes a real even element of the Grassmann envelope.

Decompose our spaces according to the matrix representation of ω_s, $W\oplus\tilde{W}|W\oplus\tilde{W}$. Let us assume that we also have a supercomplex structure, which is a type (1,1) tensor,

$$J_s=\begin{pmatrix} J & 0\\ 0 & J\end{pmatrix},\quad J=\begin{pmatrix} 0 & 1\\ -1 & 0\end{pmatrix}. \tag{74}$$

Assume that we extend everything to the complexification of our original Hilbert space. Then we can perform a transformation S that will put the above-mentioned complex structure into diagonal form in this complexified space. To accomplish this it is better to represent it in a slightly different way, use a decomposition $W|W\oplus\tilde{W}|\tilde{W}$, then

$$J_s=\begin{pmatrix} 0 & 1\\ -1 & 0\end{pmatrix},\quad S=\frac{1}{\sqrt{2}}\begin{pmatrix} i & -i\\ 1 & 1\end{pmatrix}. \tag{75}$$

Now compute $S^{-1}J_sS$ and see that we get $\hat{J}_s=i\hat{\epsilon}=\left(\begin{smallmatrix}-i & 0\\ 0 & i\end{smallmatrix}\right)$, which defines $\hat{\epsilon}$ in this decomposition. We use a decomposition according to the sign of i and the resulting graded Hilbert space becomes $\mathcal{H}_+|\mathcal{H}_+\oplus\mathcal{H}_-|\mathcal{H}_-$. If we compute the transformation of ω_s, it goes into $S^\tau\omega_sS$ since it is a two form, and we get

$$\hat{\omega}_s=\begin{pmatrix} 0 & -\overline{\epsilon}\\ 1 & 0\end{pmatrix},\quad \overline{\epsilon}=\begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix}, \tag{76}$$

with respect to the above-given decomposition. Obviously our real group also transformed by the same rule as J_s, so a typical group element becomes according to the above-given decomposition,

$$g=\begin{pmatrix} A & B\\ B^* & A^*\end{pmatrix}. \tag{77}$$

Note that each of the blocks are superoperators with standard decompositions, and for each one we are using Berezin definition of the complex conjugate $\left(\begin{smallmatrix}a & b\\ c & d\end{smallmatrix}\right)^*=\left(\begin{smallmatrix}a^* & -b^*\\ c^* & d^*\end{smallmatrix}\right)$. We have a full complex group which leaves invariant the above transformed version of the two form, this is the complex OSp group,

$$g^\tau\hat{\omega}_sg=\hat{\omega}_s,\quad g=\begin{pmatrix} A & B\\ C & D\end{pmatrix}, \tag{78}$$

and the real group now sits inside this complex group. Thus a complex transformation satisfies

$$A^\tau\overline{\epsilon}C-C^\tau A=0,\quad A^\tau\overline{\epsilon}D-C^\tau B=\overline{\epsilon},\quad -B^\tau\overline{\epsilon}C+D^\tau A=1,\quad B^\tau\overline{\epsilon}D-D^\tau B=0. \tag{79}$$

The reader may question the consistency of these equations. We should remember that $(M^\tau)^\tau=\overline{\epsilon}M\overline{\epsilon}$, then we can see that they are consistent. There is an interesting subgroup, given by elements of the form $g=\left(\begin{smallmatrix}A & 0\\ 0 & A^*\end{smallmatrix}\right)$ and A satisfies

$$A^\tau\overline{\epsilon}A^*=\overline{\epsilon},\quad A^{*\tau}A=1; \tag{80}$$

recall that $A^{*\tau}=A^{\dagger}$ and $(A^{\tau})^{*}=\overline{\epsilon}A^{\dagger}\overline{\epsilon}$, this is the same as before except that we express it in the subspace, so we should use $\overline{\epsilon}$ instead of $\tilde{E}$, we get $A^{\dagger}A=AA^{\dagger}=1$. Let us see what it means when we expand $A=\left(\begin{smallmatrix}a & \beta\\ \gamma & d\end{smallmatrix}\right)$,

$$a^{\dagger}a=1+\gamma^{\dagger}\gamma,\quad a^{\dagger}\beta+\gamma^{\dagger}d=0,\quad \beta^{\dagger}a+d^{\dagger}\gamma=0,\quad d^{\dagger}d=1+\beta^{\dagger}\beta. \tag{81}$$

We see that the body parts satisfy $a_B^{\dagger}a_B=1$, $d_B^{\dagger}d_B=1$, these are the ordinary unitary groups inside. Therefore we have shown that this group's even part has body $U(\mathcal{H}_+)\oplus U(\mathcal{H}_+)$. This group is denoted by $U(\mathcal{H}_+|\mathcal{H}_+)$ and it is the superunitary group of $\mathcal{H}_+$.

Let us define the orbit of $\hat{\epsilon}$, this is really the complex structure if we remove the factors of i, under the real group OSp:

$$\Phi=g^{-1}\hat{\epsilon}g. \tag{82}$$

It is immediate that $\Phi^2=1$. We will now show that we also have

$$\hat{\omega}_s\Phi^{\tau}+\Phi\hat{\omega}_s=0, \tag{83}$$

so it is an element of the Lie algebra of OSp. Define $\hat{E}=\left(\begin{smallmatrix}\overline{\epsilon} & 0\\ 0 & \epsilon\end{smallmatrix}\right)$, this is really our $\tilde{E}$ written in this splitting of the Hilbert space, and note $(\hat{\omega}_s^{\tau})^{-1}=\hat{\omega}_s$, $\hat{\omega}_s^{\tau}=\hat{\omega}_s\hat{E}$, $\hat{\omega}_s^2=\hat{E}$ and $\hat{\epsilon}\hat{\omega}_s=-\hat{\omega}_s\hat{\epsilon}$, then,

$$\begin{aligned}\Phi^{\tau}\omega_s&=(\hat{\omega}_s^{-1}g^{\tau}\hat{\omega}_s\hat{\epsilon}g)^{\tau}\omega_s=g^{\tau}\hat{\epsilon}\hat{\omega}_s\hat{E}g^{\tau\tau}\hat{E}=g^{\tau}\hat{\epsilon}\hat{\omega}_sg=-g^{\tau}\hat{\omega}_s\hat{\epsilon}g=-\hat{\omega}_s\hat{\omega}_s^{-1}g^{\tau}\hat{\omega}_s\hat{\epsilon}g=-\hat{\omega}_sg^{-1}\hat{\epsilon}g\\ &=-\hat{\omega}_s\Phi,\end{aligned}$$

where we used $\hat{E}g^{\tau\tau}\hat{E}=g$. Let us look at the stability subgroup of $\hat{\epsilon}$, that is given by operators of the form $\left(\begin{smallmatrix}A & 0\\ 0 & A^{*}\end{smallmatrix}\right)$, and we have seen that this can be identified with the unitary operators on $\mathcal{H}_+|\mathcal{H}_+$, $U(\mathcal{H}_+|\mathcal{H}_+)$. Hence we conclude that our variable Φ is actually parametrizing the space

$$\mathrm{OSp}(\mathcal{H}|\mathcal{H})/U(\mathcal{H}_+|\mathcal{H}_+). \tag{84}$$

What is the advantage of this parametrization? The above supermanifold is actually a symplectic manifold with a supersymplectic structure most naturally written in terms of the variable Φ:

$$\Omega_s=\frac{i}{4}\,\mathrm{Str}\,\Phi\,d\Phi\wedge d\Phi. \tag{85}$$

This is formally defined, but we use the rules of super analysis to define our differential forms. Clearly it is closed, use

$$\begin{aligned}d\,\mathrm{Str}\Phi\,d\Phi\wedge d\Phi&=\mathrm{Str}\,d\Phi\wedge d\Phi\wedge d\Phi=\mathrm{Str}\,\Phi^2d\Phi\wedge d\Phi\wedge d\Phi=\mathrm{Str}\,\Phi\,d\Phi\wedge d\Phi\wedge d\Phi\Phi\\ &=-\mathrm{Str}\,\Phi^2\,d\Phi\wedge d\Phi\wedge d\Phi\wedge d\Phi.\end{aligned}$$

where we used $\mathrm{Str}\,AB=\mathrm{Str}\,BA$. It is also clear that this form is homogeneous. Its nondegenaracy can be proved at $\hat{\epsilon}$, and homogeneity proves it everywhere.

Up to now we have really used a finite dimensional approach, but to identify the large-N_c phase space of Sec. V, we need to extend these notions to the infinite dimensional case. The extension is formally simple, we assume that we have super-Hilbert spaces, that is even and odd spaces each one are coming from a separable Hilbert space and we use a proper extension of the Grassmann envelope to this case(this is not so obvious and we assume our proposal in Ref. 30, this may not be the only possibility, see Refs. 32 and 33). In this infinite dimensional setting we introduce a Hilbert–Schmidt condition, the group that we use should be the restricted *real* OSp group,

$$\mathrm{OSp}_1(\mathcal{H}|\mathcal{H})=\left\{ g=\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \middle| \, g^{-1}\text{exists}, \quad g^{\tau}\hat{\omega}_s g=\hat{\omega}_s \quad [\hat{\epsilon},g]\in\mathcal{I}_2 \right\}. \tag{86}$$

The variable Φ now satisfies some convergence conditions, indeed one can check that

$$\Phi-\hat{\epsilon}\in\begin{pmatrix} \mathcal{I}_1 & \mathcal{I}_2 \\ \mathcal{I}_2 & \mathcal{I}_1 \end{pmatrix}, \tag{87}$$

where each block refers to a superoperator in the appropriate class of operator ideal. These convergence conditions imply that the supersymplectic form Ω_s we defined in the finite dimensional setting makes sense. The trace class conditions are important to write down moment maps, but we will ignore it for this work. Hence we have an infinite dimensional phase space,

$$\mathrm{OSp}_1(\mathcal{H}|\mathcal{H})/U(\mathcal{H}_+|\mathcal{H}_+), \quad \Omega_s=\frac{i}{4}\,\mathrm{Str}\,\Phi\,\mathrm{d}\Phi\wedge\mathrm{d}\Phi. \tag{88}$$

The reader can now see how this is related to our system, from the experience we have in the previous cases. In our problem we have a free action which has bosons and fermions,

$$S_0=\int \mathrm{d}x^+\,\mathrm{d}x^-\left(\frac{1}{2}\phi^T(-2\partial_-)\partial_+\phi+\frac{1}{2}i2\sqrt{2}\psi^T\partial_+\psi-\frac{1}{2}m_B^2\phi^T\phi-\frac{1}{2}\sqrt{2}m_F^2\psi^T\frac{1}{i\partial_-}\psi\right). \tag{89}$$

This action is written in the standard light-cone frame and one of the components of the Majorana field has been eliminated in favor of the other. The transpose refers to the color indices for the gauge group SO(N_c). As it stands this does not require the full content of the supergeometry, but as we have seen the interaction terms, given by the proper bilinears of field operators, make the use of supergeometry most convenient: when we reformulate our theory in terms of bilinears, we need the combinations which can only be expressed in terms of odd operators. We will now see that the Poisson algebra of these bilinears can only be formulated as a super-two form. Moreover a simple iterative solution of the constraint equation reveals that the bosonic operators should be given as an infinite series of products of odd operators, this is why we think it is most natural to use the full content of the Berezin's superanalysis. (We hope to come back to the more mathematical aspects of our system in a future publication.)

In our theory we have a supersymplectic form and a superquadratic form which is in the standard representation given by

$$\omega_s=\begin{pmatrix} -2\partial_- & 0 \\ 0 & i2\sqrt{2} \end{pmatrix} I_c, \quad Q_s=\begin{pmatrix} m_B^2 & 0 \\ 0 & -\sqrt{2}m_F^2 i\partial_-^{-1} \end{pmatrix} I_c, \tag{90}$$

where we have the identity I_c in the color space. The relevant operator is

$$\omega_s^{-1}Q_s=\begin{pmatrix} -\dfrac{m_B^2}{2}\partial_-^{-1} & 0 \\ 0 & -\dfrac{m_F^2}{2}\partial_-^{-1} \end{pmatrix} I_c. \tag{91}$$

The complex structure becomes (we drop the identity in the color space)

$$J_s=[(-\omega_s^{-1}Q_s)^2]^{-1/2}\omega_s Q_s=\begin{pmatrix} -(-\partial_-^2)^{1/2}\partial_-^{-1} & 0 \\ 0 & -(-\partial_-^2)^{1/2}\partial_-^{-1} \end{pmatrix}. \tag{92}$$

Clearly we can use the Fourier decomposition of our fields to diagonalize this and the frequency operator K_s,

$$\phi^\alpha(x^-)=\int \frac{[\mathrm{d}p]}{\sqrt{2|p|}} w^\alpha(p) e^{-ipx^-}, \quad \psi^\alpha(x^-)=\int \frac{[\mathrm{d}p]}{2^{3/4}} \zeta^\alpha(p) e^{-ipx^-}, \tag{93}$$

here we should think of w^α as even and ζ^α odd elements of the Grassmann algebra defined by a series (an infinite one) of unspecified generators $\theta^\alpha(p)$, Apply the operator J_s to the vectors of this graded space,

$$J_s\Psi = J_s\begin{pmatrix}\phi^\alpha\\ \psi^\alpha\end{pmatrix} = \int [\mathrm{d}p] e^{-ipx^-}(-i\,\mathrm{sgn}(p))\begin{pmatrix}(\sqrt{2|p|})^{-1} w^\alpha(p)\\ 2^{-3/4}\zeta^\alpha(p)\end{pmatrix}, \tag{94}$$

which we should rewrite as

$$(J_s\Psi)(x^-)=\int_0^\infty [\mathrm{d}p] e^{-ipx^-}\left[(-i)\begin{pmatrix}(\sqrt{2p})^{-1}\overline{z^\alpha}(p)\\ 2^{-3/4}\overline{\xi^\alpha}(p)\end{pmatrix}+i\begin{pmatrix}(\sqrt{2p})^{-1} z^\alpha(p)\\ 2^{-3/4}\xi^\alpha(p)\end{pmatrix}\right], \tag{95}$$

defining the superholomorphic coordinates, $(z^\alpha(p),\xi^\alpha(p))$. If we assign now our creation and annihilation operators according to the sign of i,

$$\begin{pmatrix}z^\alpha(p)\\ \xi^\alpha(p)\end{pmatrix}\mapsto\begin{pmatrix}a^{\alpha\dagger}(p)\\ \chi^{\alpha\dagger}(p)\end{pmatrix}, \quad \begin{pmatrix}\overline{z^\alpha}(p)\\ \overline{\xi^\alpha}(p)\end{pmatrix}\mapsto\begin{pmatrix}a^\alpha(p)\\ \chi^\alpha(p)\end{pmatrix}, \tag{96}$$

we get the commutation/anticommutation relations for $a^{\alpha\dagger}(p), a^\beta(q)$ and $\chi^{\alpha\dagger}(p), \chi^\alpha(q)$ respectively, and the zero commutator between the two sets. These commutation/anticommutation relations have the operator $\hat{\omega}_s$ on the right-hand side, this is what determines the algebra. Hence we see that we are in the geometric setting we were describing. Our bilinears combined in the form of Φ satisfy all the Lie algebra properties. In fact it is instructive to write down the supersymplectic form Ω_s with Φ expressed in terms of the bilinears $B,F,C,C^\dagger$. Then the reader can see that we have the same Poisson brackets satisfied by these bilinears.

From the above-given discussion we again see the remarkable fact that the geometry which is defined by the complex structure J_s is independent of the parameters of the theory in this light-cone method. This means *even though the masses change due to the interactions this will not change the representation of canonical commutation/anticommutation relations we started with*, as a result the geometry stays the same.

Our bilinears will correspond to the generators of the automorphisms of this full algebra of commutation/anticommutation relations, and it is the restricted real OSp group (for finite dimensional automorphism groups see Ref. 34, for Bogoliubov automorphisms of qausifree representations see Refs. 35–38). We can check that the bilinears we have satisfy the Lie algebra conditions and the implementability of these automorphisms will imply the convergence conditions. Therefore the evolution of the system in the large-N_c limit realizes all automorphisms of the quasifree second quantization of this system when we think of it without the color part—the color part has been averaged out and reduced the system to the bilinears. We may give an argument using the supercoherent states,[39,40] similar to the ordinary cases: there is a central extension of the automorphism group $\widehat{\mathrm{OSp}_1}$ which is realized by these bilinears on the full Fock space. When we think about the projective Fock space this descends to the OSp_1 group. The orbit of the vacuum under this group gives us a classical phase space albeit a more general one, with a supersymplectic form. The large-N_c limit provides this reduction to the space of supercoherent states. This is a natural classical phase space and the large-N_c limit corresponds to this classical limit.

Before ending our discussions we would like to make a few comments of general nature. Let us write down a superdynamical system in the Hamiltonian form

$$S_0 = \int \mathrm{d}t \frac{1}{2} \Psi^\tau \omega_s \partial_t \Psi - \int \mathrm{d}t \frac{1}{2} \Psi^\tau Q_s \Psi. \tag{97}$$

We assume that the action is an element of the even part of the Grassmann algebra. If we want this to be real we demand $(\Psi^\tau Q_s \Psi)^* = \Psi^\tau \tilde{E} Q_s^* \Psi = \Psi^\tau Q_s \Psi$, that is $Q_s = \tilde{E} Q_s^*$, we are again using $\tilde{E} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ in the standard decomposition. For the first term it implies the same $\tilde{E} \omega_s^* = \omega$. If we further note that it should be invariant under the transpose, we get for the first term using an integration by parts for the time derivative, $\Psi^\tau \omega_s \partial_t \Psi = -\Psi^\tau \omega_s^\tau \tilde{E} \partial_t \Psi$, which implies $\omega_s = -\omega_s^\tau \tilde{E}$ and the second term requires $\Psi^\tau Q_s \Psi = \Psi^\tau Q_s^\tau \tilde{E} \Psi$, which means we should have $Q_s = Q_s^\tau \tilde{E}$. The equations of motion will give us

$$\partial_t \Psi = \omega_s^{-1} Q_s \Psi. \tag{98}$$

This suggests that we should further investigate operator $\omega_s^{-1} Q_s$ which is a type (1,1) tensor, thus a true linear transformation. We note that $\omega_s^{-1} Q_s$ is real: $(\omega_s^{-1} Q_s)^* = (\omega_s^{-1})^* Q_s^* = \omega_s^{-1} \tilde{E} \tilde{E} Q_s = \omega_s^{-1} Q_s$, by using the conjugation properties of ω_s and Q. This operator is antisymmetric with respest to the form defined by Q_s:

$$Q_s^{-1} (\omega_s^{-1} Q_s)^\tau Q_s = Q_s^{-1} Q_s^\tau (\omega_s^\tau)^{-1} Q_s = -Q_s^{-1} Q_s \tilde{E} \tilde{E} \omega_s^{-1} Q_s = -\omega_s^{-1} Q_s, \tag{99}$$

as well as under ω_s. It would be most natural if we could use a generalization of the polar decomposition for $Q_s^{-1} \omega_s$, and write this operator as $\omega_s^{-1} Q_s = J_s K_s$, where $J_s^t J_s = 1$, and $K_s > 0$, $K_s^t = K_s$, with an appropriate transpose t and positivity is assumed to be given a meaning in this supercontext. Then we could claim that the basis in which J_s is diagonal, will tell us the separation of creation and annihilation operators in this full generality. This can be done in the simple case we looked at, when the operators involved only had body parts, and no Grassmann numbers. Unfortunately for the general case we do not have the proper mathematical machinery. If we could find a supertransformation S, such that $S^{-1} \omega_s^{-1} Q_s S$ is diagonal with each entry $(\pm i \lambda_k)$ for a pure number λ_k we could postulate the quantization by means of canonical commutation/anticommutation relations. To the best of our knowledge there is no such theorem. We think these questions deserve further investigations.

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The embedding of space–times in five dimensions with nondegenerate Ricci tensor

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We discuss and prove a theorem which asserts that any n-dimensional semi-Riemannian manifold can be locally embedded in an $(n+1)$-dimensional space with a nondegenerate Ricci tensor which is equal, up to a local analytic diffeomorphism, to the Ricci tensor of an arbitrary specified space. This may be regarded as a further extension of the Campbell–Magaard theorem. We highlight the significance of embedding theorems of increasing degrees of generality in the context of higher dimensional space–times theories and illustrate the new theorem by establishing the embedding of a general class of Ricci-flat space–times. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1473680]

I. INTRODUCTION

Modern physical theories which regard our space–time as a hypersurface embedded in a five-dimensional manifold constitute nowadays a branch of theoretical physics undergoing quite an active research. On the other hand, the idea of an extra fifth dimension is not new and goes back to the works of Kaluza and Klein carried out around the first quarter of the 20th century.[1,2] Kaluza–Klein's seminal work has inspired theoretical physicists to generalize their conjecture in the construction of unified theories of the fundamental interactions of nature. Subsequent developments which assume that the universe contains extra hidden dimensions include among others 11-dimensional supergravity and superstring theories.[3,4] More recently much attention has been devoted to the so-called Randall–Sundrum braneworld scenario where the space–time is viewed as a four-dimensional hypersurface embedded in a five-dimensional Einstein space.[5] Noncompactified approaches to Kaluza–Klein gravity also make use of embedding mechanisms and have been largely discussed in the literature.[6–11]

In a sense one could say that all space–time embedding theories[12] assume, implicitly or explicitly, a mathematical framework which must provide consistency for the postulates and basic principles set forth by such theories. In this connection it is of interest to know whether the embedding theorems of differential geometry are properly taken into account when constructing higher dimensional models. The analysis of the geometrical structure underlying some modern embedding theories has recently attracted the interest of some authors.[13–18] It seems that there is now a quest for embedding theorems with increasing degrees of generality, i.e., theorems ensuring that arbitrary n-dimensional space–times can be embeddable in classes of $(n+1)$-dimensional spaces the most general as possible.

Two theorems of historical importance which have played a significant role in physical theories of higher dimensions should be mentioned. The first is the well-known Janet–Cartan theorem, which asserts that if the embedding space is flat, the minimum number of extra dimensions needed to analytically embed an n-dimensional Riemannian manifold is d, with $0 \leqslant d \leqslant n(n-1)/2$.[19] An important application of this theorem may be illustrated by the isometric embedding of the Schwarzschild solution in a six-dimensional flat space.[20] Other interesting examples of isometric embeddings with application to general relativity and strings may be found in Refs. 21 and 22.

The second theorem is a little known but powerful theorem due to Campbell,[23] the proof of which was outlined by Campbell and completed by Magaard.[24] The content of the Campbell–Magaard theorem is that any n-dimensional Riemannian manifold with analytic metric, locally,

can be isometrically embedded into a certain $(n+1)$-dimensional Ricci-flat manifold. How geometric properties of the embedding space, such as extrinsic curvature, can be related to the energy-momentum tensor is discussed in Ref. 25. It is interesting to note that both theorems specify a geometry property to be satisfied by the embedding space by imposing the restrictions $R_{\mu\nu\lambda\rho}=0$ in one case and $R_{\mu\nu}=0$ in the other. It is also worth noting that by relaxing the flatness condition, assumed in the Janet–Cartan theorem, and replacing it by the weaker Ricci-flatness condition, the Campbell–Magaard theorem drastically reduces the codimension of the embedding space to $d=1$. This seems to give support to the mathematical consistency of theories in which the dynamics of the embedding space is governed by the vacuum Einstein field equations.[6] However, the view adopted by Randall–Sundrum braneworld model[5] that the embedding space, i.e., the bulk, should correspond to an Einstein space sourced by a negative cosmological constant has naturally raised the question of whether the Campbell–Magaard theorem could be extended to include embeddings in arbitrary Einstein spaces. This conjecture was shown to be, in fact, a theorem, the proof of which is given in Ref. 18. Embeddings into spaces sourced by scalar fields also have been considered and a different extension of the Campbell–Magaard theorem has been proved.[17,26] In seeking higher levels of generalization one is led to consider the more general situation of embedding spaces whose Ricci tensor is arbitrary. In this paper we shall be concerned with this problem. In Sec. II we state and prove a theorem which considers embedding spaces with arbitrary nondegenerate Ricci tensor, and, in a way, would represent a further generalization of Campbell–Magaard's result. In Sec. III we illustrate the theorem by establishing the embedding of a general class of Ricci-flat space–times in a given collection of five-dimensional spaces whose Ricci tensor is equivalent to a specified nondegenerate and nonconstant Ricci tensor.

We believe that insofar as five-dimensional embedding theories are metric theories it appears to be of relevance to allow the embedding spaces to have different geometrical properties, which must ultimately be determined by the dynamics of the theory in question. Therefore generalizations of the known embedding theorems might be helpful in building new higher dimensional models.

II. EXTENSION OF CAMPBELL–MAGAARD THEOREM: EMBEDDING SPACES WITH ARBITRARY NONDEGENERATE RICCI TENSOR

In this section we want to investigate the existence of a local analytic embedding of an n-dimensional semi-Riemannian manifold (M^n,g) into a class of $(n+1)$-dimensional spaces whose Ricci tensor is *equivalent* to the Ricci tensor of a $(n+1)$-dimensional space arbitrarily specified.

Definition: Consider a $(n+1)$*-dimensional semi-Riemannian space* $(\tilde{M}_0^{n+1},\tilde{g}_0)$ *and let* $S_{\alpha\beta}$ *denote the components of the Ricci tensor in a coordinate system* $\{x'^{\alpha}\}$. *Let* $(\tilde{M}^{n+1},\tilde{g})$ *be another* $(n+1)$*-dimensional semi-Riemannian space with* $\tilde{R}_{\alpha\beta}$ *denoting the components of the Ricci tensor in a coordinate system* $\{x^{\alpha}\}$ *which covers a neighborhood of a point* $p\in\tilde{M}^{n+1}$ *whose coordinates are* $x_p^1=\cdots=x_p^{n+1}=0$. *Then, we shall say that* $S_{\alpha\beta}$ *and* $\tilde{R}_{\alpha\beta}$ *are equivalent if there exists an analytic local diffeomorphism* $\overline{f}:\tilde{M}_0^{n+1}\to\tilde{M}^{n+1}$ *at* p *such that*

$$\tilde{R}_{\alpha\beta}(x^{\gamma})=\frac{\partial\overline{f}^{\mu}}{\partial x^{\alpha}}\frac{\partial\overline{f}^{\nu}}{\partial x^{\beta}}S_{\mu\nu}(x'^{\kappa}), \tag{1}$$

where $x'^{\kappa}=\overline{f}^{\kappa}(x^{\lambda})$. *In others words,* $S_{\alpha\beta}$ *and* $\tilde{R}_{\alpha\beta}$ *are said to be equivalent if there exists a analytic function* $\overline{f}^{\mu}=\overline{f}^{\mu}(x^{\alpha})$ *such that: (i)* $|\partial\overline{f}^{\mu}/\partial x^{\alpha}|\neq 0$ *at* $0\in\mathbb{R}^{n+1}$ *and (ii) the condition (1) holds in a neighborhood of* $0\in\mathbb{R}^{n+1}$. *In this case* $(\tilde{M}_0^{n+1},\tilde{g}_0)$ *and* $(\tilde{M}^{n+1},\tilde{g})$ *are said to be "Ricci-equivalent" spaces*. (Henceforth we shall follow the convention adopted in Ref. 18 where Latin and Greek indices run from 0 to n and $n+1$, respectively.)

Clearly, from the above, the collection $\mathcal{M}_{\tilde{g}_0}^{n+1}$ of all spaces which are Ricci-equivalent to a given space $(\tilde{M}_0^{n+1},\tilde{g}_0)$ is well defined. Therefore it makes sense to discuss the existence of the

embedding of a given arbitrary n-dimensional semi-Riemannian manifold $(\tilde{M}^n,\tilde{g})$ into the class $\mathcal{M}^{n+1}_{\tilde{g}_0}$. In what follows we shall show that if the Ricci tensor of $(\tilde{M}^{n+1}_0,\tilde{g}_0)$ is nondegenerate, i.e., the matrix formed by its components has inverse, then the existence of the embedding can be ensured.

We should note, however, that (1) defines a notion of equivalence between the covariant Ricci tensor $S_{\alpha\beta}$ and $\tilde{R}_{\alpha\beta}$. This equivalence does not imply that the contravariant Ricci tensor $S^{\alpha\beta}$ and $\tilde{R}^{\alpha\beta}$ are also equivalent. In general they are not, unless the diffeomorphism is an isometry, a condition which is more restrictive than (1).

Let us consider $(\tilde{M}^{n+1},\tilde{g})$ and choose a coordinate system in which the metric has the form

$$ds^2=\overline{g}_{ik}dx^i dx^k+\varepsilon\,\overline{\phi}^2 dy^2, \tag{2}$$

where $\varepsilon=\pm 1$. In these coordinates (1) may be written in the following equivalent form:

$$\tilde{R}_{ik}=\overline{R}_{ik}+\varepsilon\overline{g}^{jm}(\overline{\Omega}_{ik}\overline{\Omega}_{jm}-2\overline{\Omega}_{jk}\overline{\Omega}_{im})-\frac{\varepsilon}{\overline{\phi}}\frac{\partial\overline{\Omega}_{ik}}{\partial y}+\frac{1}{\overline{\phi}}\overline{\nabla_i\nabla_k\phi}=\frac{\partial\overline{f}^{\mu}}{\partial x^i}\frac{\partial\overline{f}^{\nu}}{\partial x^k}S_{\mu\nu}(\overline{f}^{\alpha}), \tag{3}$$

$$\tilde{R}^y_i=\frac{\varepsilon}{\overline{\phi}}\overline{g}^{jk}(\overline{\nabla_j\Omega_{ik}}-\overline{\nabla_i\Omega_{jk}})=\frac{\varepsilon}{\overline{\phi}^2}\frac{\partial\overline{f}^{\mu}}{\partial y}\frac{\partial\overline{f}^{\nu}}{\partial x^i}S_{\mu\nu}(\overline{f}^{\alpha}), \tag{4}$$

$$\tilde{G}^y_y=-\frac{1}{2}\overline{g}^{ik}\overline{g}^{jm}(\overline{R}_{ijkm}+\varepsilon(\overline{\Omega}_{ik}\overline{\Omega}_{jm}-\overline{\Omega}_{jk}\overline{\Omega}_{im}))=\frac{1}{2}\frac{\varepsilon}{\overline{\phi}^2}\frac{\partial\overline{f}^{\mu}}{\partial y}\frac{\partial\overline{f}^{\nu}}{\partial y}S_{\mu\nu}(\overline{f}^{\alpha})$$

$$-\frac{1}{2}\overline{g}^{jm}\frac{\partial\overline{f}^{\mu}}{\partial x^j}\frac{\partial\overline{f}^{\nu}}{\partial x^m}S_{\mu\nu}(\overline{f}^{\alpha}), \tag{5}$$

where

$$\overline{\Omega}_{ik}=-\frac{1}{2\overline{\phi}}\frac{\partial\overline{g}_{ik}}{\partial y}, \tag{6}$$

$G_{\alpha\beta}$ is the Einstein tensor and a bar is used to denote all the geometrical quantities calculated with the induced metric $\overline{g}_{ik}$ on a generic hypersurface Σ_c of the foliation $y=c=\text{const}$. Before we state the main theorem we need a few preliminaries.

We begin by defining the tensor

$$\tilde{F}^{\alpha}_{\beta}=\tilde{G}^{\alpha}_{\beta}-\left(\tilde{g}^{\alpha\gamma}\frac{\partial\overline{f}^{\mu}}{\partial x^{\gamma}}\frac{\partial\overline{f}^{\nu}}{\partial x^{\beta}}S_{\mu\nu}-\frac{1}{2}\delta^{\alpha}_{\beta}\tilde{g}^{\gamma\lambda}\frac{\partial\overline{f}^{\mu}}{\partial x^{\gamma}}\frac{\partial\overline{f}^{\nu}}{\partial x^{\lambda}}S_{\mu\nu}\right). \tag{7}$$

If we now impose that the functions $\overline{f}^{\alpha}$ satisfy the equation

$$\tilde{\nabla}_{\alpha}\left(\tilde{g}^{\alpha\gamma}\frac{\partial\overline{f}^{\mu}}{\partial x^{\gamma}}\frac{\partial\overline{f}^{\nu}}{\partial x^{\beta}}S_{\mu\nu}-\frac{1}{2}\delta^{\alpha}_{\beta}\tilde{g}^{\gamma\lambda}\frac{\partial\overline{f}^{\mu}}{\partial x^{\gamma}}\frac{\partial\overline{f}^{\nu}}{\partial x^{\lambda}}S_{\mu\nu}\right)=0, \tag{8}$$

then it is easily seen that, as the Einstein tensor G^{α}_{β} has vanishing divergence, the tensor $\tilde{F}^{\alpha}_{\beta}$ also is divergenceless for any metric $\tilde{g}_{\alpha\beta}$, even those which are not solutions of Eq. (1). Thus, we are ready to state the following lemma.

Lemma 1: Let the functions $\overline{g}_{ik}(x^1,\ldots,x^n,y),\overline{\phi}(x^1,\ldots,x^n,y)$ *and* $\overline{f}^{\alpha}(x^1,\ldots,x^n,y)$ *be analytical at* $(0,\ldots,0)\in\Sigma_0\subset\mathbb{R}^{n+1}$. *Assume that the following conditions hold:*

(i) $\overline{g}_{ik}=\overline{g}_{ki}$;
(ii) $\det(\overline{g}_{ik})\neq 0$;
(iii) $\overline{\phi}\neq 0$.

Suppose further that $\overline{g}_{ik}$ *and* $\overline{f}^{\alpha}$ *satisfy the equations (3) and (8) in an open set* $V\subset\mathbb{R}^{n+1}$ *which contains* $0\in\mathbb{R}^{n+1}$, *and (4) and (5) hold at* Σ_0. *Then,* $\overline{g}_{ik}$, $\overline{\phi}$ *and* $\overline{f}^{\alpha}$ *satisfy (4) and (5) in a neighborhood* $0\in\mathbb{R}^{n+1}$.

Proof: The key point of the proof is given by the equation $\tilde{\nabla}_{\alpha}\tilde{F}^{\alpha}_{\beta}=0$, which can be written as

$$\frac{\partial\tilde{F}^{y}_{\beta}}{\partial y}=-\frac{\partial\tilde{F}^{i}_{\beta}}{\partial x^{i}}-\tilde{\Gamma}^{\mu}_{\mu\lambda}\tilde{F}^{\lambda}_{\beta}+\tilde{\Gamma}^{\mu}_{\lambda\beta}\tilde{F}^{\lambda}_{\mu}. \tag{9}$$

On the other hand, by assumption (3) holds in $V\subset\mathbb{R}^{n+1}$. Then, it can be shown that in V we have $\tilde{F}^{i}_{k}=-\delta^{i}_{k}\tilde{F}^{y}_{y}$. After some algebra we can deduce that

$$\frac{\partial\tilde{F}^{y}_{y}}{\partial y}=-\varepsilon\overline{\phi}^{2}\overline{g}^{ij}\frac{\partial\tilde{F}^{y}_{i}}{\partial x^{j}}-2\tilde{\Gamma}^{i}_{iy}\tilde{F}^{y}_{y}+\left(-\varepsilon\frac{\partial(\overline{\phi}^{2}\overline{g}^{ij})}{\partial y^{j}}-\varepsilon\overline{\phi}^{2}\overline{g}^{ij}\tilde{\Gamma}^{k}_{kj}+\tilde{\Gamma}^{i}_{yy}\right)\tilde{F}^{y}_{i}, \tag{10}$$

$$\frac{\partial\tilde{F}^{y}_{i}}{\partial y}=\frac{\partial\tilde{F}^{y}_{y}}{\partial x^{i}}+2\tilde{\Gamma}^{y}_{yi}\tilde{F}^{y}_{y}+(\tilde{\Gamma}^{k}_{yi}+\varepsilon\overline{\phi}^{2}\overline{g}^{kj}\tilde{\Gamma}^{y}_{ij}-\tilde{\Gamma}^{\mu}_{y\mu}\delta^{k}_{i})\tilde{F}^{y}_{k}. \tag{11}$$

Since at the hypersurface Σ_0 the equations (4) and (5) also hold, it follows that $\tilde{F}^{y}_{\beta}=0$ at Σ_0 and hence $\partial\tilde{F}^{y}_{\beta}/\partial y\,|_{y=0}=0$. It is not difficult to show by mathematical induction that all the derivatives (to any order) of $\tilde{F}^{y}_{\beta}$ vanish at $y=0$. As $\tilde{F}^{y}_{\beta}$ is analytic we conclude that $\tilde{F}^{y}_{\beta}=0$ in an open set of $\mathbb{R}^{n+1}$. Hence, Eqs. (4) and (5), which are equivalent to $\tilde{F}^{y}_{\beta}=0$, also hold in an open set of $\mathbb{R}^{n+1}$ which includes the origin. This proves the lemma.

The question which now arises is: do Eqs. (3) and (8) admit solution? To answer this question we first note that (3) can be expressed in the following form:

$$\begin{aligned}\frac{\partial^{2}\overline{g}_{ik}}{\partial y^{2}}=&-2\varepsilon\overline{\phi}^{2}\left(\frac{\partial\overline{f}^{\mu}}{\partial x^{i}}\frac{\partial\overline{f}^{\nu}}{\partial x^{k}}S_{\mu\nu}(\overline{f}^{\alpha})\right)+\frac{1}{\overline{\phi}}\frac{\partial\overline{\phi}}{\partial y}\frac{\partial\overline{g}_{ik}}{\partial y}-\frac{1}{2}\overline{g}^{jm}\left(\frac{\partial\overline{g}_{ik}}{\partial y}\frac{\partial\overline{g}_{jm}}{\partial y}-2\frac{\partial\overline{g}_{im}}{\partial y}\frac{\partial\overline{g}_{jk}}{\partial y}\right)\\&-2\varepsilon\overline{\phi}\left(\frac{\partial^{2}\overline{\phi}}{\partial x^{i}\partial x^{k}}-\frac{\partial\overline{\phi}}{\partial x^{j}}\overline{\Gamma}^{j}_{ik}\right)-2\varepsilon\overline{\phi}^{2}\overline{R}_{ik}.\end{aligned} \tag{12}$$

Second, let us rewrite Eq. (8) in the form

$$\begin{aligned}&\frac{\partial}{\partial x^{\alpha}}\left(\tilde{g}^{\alpha\gamma}\frac{\partial\overline{f}^{\mu}}{\partial x^{\gamma}}\frac{\partial\overline{f}^{\nu}}{\partial x^{\beta}}S_{\mu\nu}-\frac{1}{2}\delta^{\alpha}_{\beta}\tilde{g}^{\gamma\lambda}\frac{\partial\overline{f}^{\mu}}{\partial x^{\gamma}}\frac{\partial\overline{f}^{\nu}}{\partial x^{\lambda}}S_{\mu\nu}\right)+\tilde{\Gamma}^{\alpha}_{\alpha_{\sigma}}\left(\tilde{g}^{\sigma\gamma}\frac{\partial\overline{f}^{\mu}}{\partial x^{\gamma}}\frac{\partial\overline{f}^{\nu}}{\partial x^{\beta}}S_{\mu\nu}\right)\\&-\tilde{\Gamma}^{\sigma}_{\alpha_{\beta}}\left(\tilde{g}^{\alpha\gamma}\frac{\partial\overline{f}^{\mu}}{\partial x^{\gamma}}\frac{\partial\overline{f}^{\nu}}{\partial x^{\sigma}}S_{\mu\nu}\right)=0.\end{aligned} \tag{13}$$

We now isolate the terms which contain second-order derivatives of $\overline{f}^{\alpha}$ with respect to y in the equation above. Putting $\beta=n+1$ we obtain

$$\frac{\varepsilon}{\overline{\phi}^2}\frac{\partial^2\overline{f}^\mu}{\partial y^2}\frac{\partial\overline{f}^\nu}{\partial y}S_{\mu\nu}=-\frac{1}{2}\frac{\partial\overline{f}^\mu}{\partial y}\frac{\partial\overline{f}^\nu}{\partial y}\frac{\partial}{\partial y}\left(\frac{\varepsilon}{\overline{\phi}^2}S_{\mu\nu}\right)+\frac{1}{2}\frac{\partial}{\partial y}\left(\overline{g}^{jk}\frac{\partial\overline{f}^\mu}{\partial x^j}\frac{\partial\overline{f}^\nu}{\partial x^k}S_{\mu\nu}\right)$$
$$-\frac{\partial}{\partial x^j}\left(\overline{g}^{jk}\frac{\partial\overline{f}^\mu}{\partial x^k}\frac{\partial\overline{f}^\nu}{\partial y}S_{\mu\nu}\right)-\tilde{\Gamma}^\alpha_{\alpha_\sigma}\left(\tilde{g}^{\sigma\gamma}\frac{\partial\overline{f}^\mu}{\partial x^\gamma}\frac{\partial\overline{f}^\nu}{\partial x^\beta}S_{\mu\nu}\right)+\tilde{\Gamma}^\sigma_{\alpha_\beta}\left(\tilde{g}^{\alpha\gamma}\frac{\partial\overline{f}^\mu}{\partial x^\gamma}\frac{\partial\overline{f}^\nu}{\partial x^\sigma}S_{\mu\nu}\right). \tag{14}$$

For $\beta=i$ we have

$$\frac{\varepsilon}{\overline{\phi}^2}\frac{\partial^2\overline{f}^\mu}{\partial y^2}\frac{\partial\overline{f}^\nu}{\partial x^i}S_{\mu\nu}=-\frac{\partial\overline{f}^\mu}{\partial y}\frac{\partial}{\partial y}\left(\frac{\varepsilon}{\overline{\phi}^2}\frac{\partial\overline{f}^\nu}{\partial x^i}S_{\mu\nu}\right)-\frac{\partial}{\partial x^j}\left(\overline{g}^{jk}\frac{\partial\overline{f}^\mu}{\partial x^j}\frac{\partial\overline{f}^\nu}{\partial x^i}S_{\mu\nu}\right)$$
$$+\frac{1}{2}\frac{\partial}{\partial x^i}\left(\tilde{g}^{\sigma\gamma}\frac{\partial\overline{f}^\mu}{\partial x^\gamma}\frac{\partial\overline{f}^\nu}{\partial x^\beta}S_{\mu\nu}\right)-\tilde{\Gamma}^\alpha_{\alpha_\sigma}\left(\tilde{g}^{\sigma\gamma}\frac{\partial\overline{f}^\mu}{\partial x^\gamma}\frac{\partial\overline{f}^\nu}{\partial x^\beta}S_{\mu\nu}\right)$$
$$+\tilde{\Gamma}^\sigma_{\alpha_\beta}\left(\tilde{g}^{\alpha\gamma}\frac{\partial\overline{f}^\mu}{\partial x^\gamma}\frac{\partial\overline{f}^\nu}{\partial x^\sigma}S_{\mu\nu}\right). \tag{15}$$

Clearly, the right-hand side of (14) and (15) does not contain second-order derivatives of the functions $\overline{f}^\alpha$ and $\overline{g}_{ik}$ with respect to y. Therefore, they are of the form

$$\frac{\partial^2\overline{f}^\mu}{\partial y^2}\frac{\partial\overline{f}^\nu}{\partial x^\beta}S_{\mu\nu}=Q_\beta\left(\overline{f}^\lambda,\frac{\partial\overline{f}^\lambda}{\partial x^\sigma},\frac{\partial^2\overline{f}^\lambda}{\partial x^\sigma\partial x^i},\overline{g}_{ik},\frac{\partial\overline{g}_{ik}}{\partial x^\sigma}\right). \tag{16}$$

(Of course Q_β also depends on $\overline{\phi}$ and its derivatives, however this fact is not relevant for our present reasoning.) Thus, assuming that $|\partial\overline{f}^\mu/\partial x^\alpha|\neq 0$ (we shall see later on that this assumption can always be made) we can write

$$\frac{\partial^2\overline{f}^\mu}{\partial y^2}S_{\mu\nu}=\frac{\partial x^\beta}{\partial\overline{f}^\nu}Q_\beta\left(\overline{f}^\lambda,\frac{\partial\overline{f}^\lambda}{\partial x^\sigma},\frac{\partial^2\overline{f}^\lambda}{\partial x^\sigma\partial x^i},\overline{g}_{ik},\frac{\partial\overline{g}_{ik}}{\partial x^\sigma}\right). \tag{17}$$

If we suppose that $S_{\mu\nu}$ is invertible, i.e., there exists $(S^{-1})^{\nu\lambda}$ such that

$$S_{\mu\nu}(S^{-1})^{\nu\lambda}=\delta^\lambda_\mu, \tag{18}$$

then (8) can be put into the canonical form

$$\frac{\partial^2\overline{f}^\mu}{\partial y^2}=P^\mu\left(\overline{f}^\lambda,\frac{\partial\overline{f}^\lambda}{\partial x^\sigma},\frac{\partial^2\overline{f}^\lambda}{\partial x^\sigma\partial x^i},\overline{g}_{ik},\frac{\partial\overline{g}_{ik}}{\partial x^\sigma}\right), \tag{19}$$

where each P^μ is analytic with respect to its arguments provided that $|\partial\overline{f}^\mu/\partial x^\alpha|\neq 0$, $|\overline{g}_{ik}|\neq 0$ and $\overline{\phi}\neq 0$.

It easy to see that the Cauchy–Kowalewski theorem (see the Appendix) can be applied to the equations (19) and (12), which are equivalent to (3) and (8), respectively. According to the above-mentioned theorem, if an analytic function $\overline{\phi}\neq 0$ is chosen, then there exists a unique set of analytic functions $\overline{g}_{ik}$ and $\overline{f}^\alpha$ that are solutions of (3) and (8) satisfying the initial conditions

$$\overline{g}_{ik}(x^1,\ldots,x^n,0)=g_{ik}(x^1,\ldots,x^n), \tag{20}$$

$$\frac{\partial \overline{g}_{ik}}{\partial y}(x^1,\ldots,x^n,0) = -2\,\overline{\phi}(x^1,\ldots,x^n,0)\,\Omega_{ik}(x^1,\ldots,x^n), \tag{21}$$

$$\overline{f}^{\alpha}(x^1,\ldots,x^n,0) = \xi^{\alpha}(x^1,\ldots,x^n), \tag{22}$$

$$\frac{\partial \overline{f}^{\alpha}}{\partial y}(x^1,\ldots,x^n,0) = \eta^{\alpha}(x^1,\ldots,x^n), \tag{23}$$

where g_{ik}, Ω_{ik}, ξ^{α} and η^{α} are analytic functions at the origin $0 \in \mathbb{R}^n$, and the following conditions hold: (i) $|\partial \overline{f}^{\mu}/\partial x^{\alpha}|_0 \neq 0$ and (ii) $|g_{ik}| \neq 0$. [Incidentally, we can easily verify that the condition (i) is satisfied by simply choosing: $\xi^i = x^i$; $\xi^{n+1} = 0$; $\eta^i = 0$ and $\eta^{n+1} = 1$. With this choice, $|\partial \overline{f}^{\mu}/\partial x^{\alpha}|_0 = 1$.]

We now are ready to state the following theorem.

Theorem 1: *Let M^n be an n-dimensional semi-Riemannian manifold with metric given by*

$$ds^2 = g_{ik}dx^i dx^k,$$

in a coordinate system $\{x^i\}$ of M^n. Let $p \in M^n$ have coordinates $x^1_p = \cdots = x^n_p = 0$. Then, M^n has a local isometric and analytic embedding (at the point p) in an $(n+1)$-dimensional space $(\tilde{M}^{n+1}, \tilde{g})$ whose Ricci tensor is equivalent to the symmetric, analytic and nondegenerate tensor $S_{\mu\nu}$ if and only if there exist functions $\Omega_{ik}(x^1,\ldots,x^n)$ $(i,k = 1,...,n)$, $\xi^{\alpha}(x^1,\ldots,x^n)$, $\eta^{\alpha}(x^1,\ldots,x^n)$ $(\alpha = 1,\ldots,n+1)$ and $\phi(x^1,\ldots,x^n) \neq 0$ that are analytic at $0 \in \mathbb{R}^n$, such that

$$\Omega_{ik} = \Omega_{ki}, \tag{24}$$

$$g^{jk}(\nabla_j \Omega_{ik} - \nabla_i \Omega_{jk}) = \frac{1}{\phi}\,\eta^{\mu}\frac{\partial \xi^{\nu}}{\partial x^i} S_{\mu\nu}(\xi^{\alpha}), \tag{25}$$

$$g^{ik}g^{jm}(R_{ijkm} + \varepsilon(\Omega_{ik}\Omega_{jm} - \Omega_{jk}\Omega_{im})) = -\frac{\varepsilon}{\phi^2}\,\eta^{\mu}\eta^{v} S_{\mu\nu}(\xi^{\alpha}) + g^{jm}\frac{\partial \xi^{\mu}}{\partial x^j}\frac{\partial \xi^{\nu}}{\partial x^m} S_{\mu\nu}(\xi^{\alpha}), \tag{26}$$

$$\begin{vmatrix} \dfrac{\partial \xi^1}{\partial x^1} & \cdots & \dfrac{\partial \xi^{n+1}}{\partial x^1} \\ \vdots & & \vdots \\ \dfrac{\partial \xi^1}{\partial x^n} & \cdots & \dfrac{\partial \xi^{n+1}}{\partial x^n} \\ \eta^1 & \cdots & \eta^{n+1} \end{vmatrix} \neq 0. \tag{27}$$

Proof: Let us start with the necessary condition. If (M^n, g) has an embedding in $(\tilde{M}^{n+1}, \tilde{g})$, then it can be proved that there exists a coordinate system in which the metric of the embedding space has the form[18]

$$ds^2 = \overline{g}_{ik}dx^i dx^k + \varepsilon\,\overline{\phi}^2 dy^2, \tag{28}$$

where the analytic functions $\overline{g}_{ik}(x^1,\ldots,x^n,y)$ and $\overline{\phi}(x^1,\ldots,x^n,y)$ are such that $\overline{\phi}(x^1,\ldots,x^n,y) \neq 0$ and that $\overline{g}_{ik}(x^1,\ldots,x^n,0) = g_{ik}(x^1,\ldots,x^n)$ in an open set of $\mathbb{R}^n$ which contains the origin. Given that the Ricci tensor of the embedding space $(\tilde{M}^{n+1}, \tilde{g})$ is, by assumption, equivalent to $S_{\mu\nu}$, then the equations (3), (4), (5) and (8) are satisfied in a neighborhood of 0

$\in \mathbb{R}^{n+1}$ for some functions $\overline{f}^{\mu}$. In particular, the equations (4) and (5) hold for $y=0$. Therefore, if we define Ω_{ik}, ξ^{α}, η^{α} by the relations (21), (22) and (23), and take $\phi(x^1,\ldots,x^n) = \overline{\phi}(x^1,\ldots,x^n,0)$, then the Eqs. (24)–(27) are satisfied.

Let us turn to the sufficiency. Suppose there exist functions $\Omega_{ik}(x^1,\ldots,x^n)$, $\xi^{\alpha}(x^1,\ldots,x^n)$, $\eta^{\alpha}(x^1,\ldots,x^n)$ and $\phi(x^1,\ldots,x^n)\neq 0$ which satisfy (24)–(27). Choose an analytic function $\overline{\phi}(x^1,\ldots,x^n,y)\neq 0$ such that $\overline{\phi}(x^1,\ldots,x^n,0)=\phi(x^1,\ldots,x^n)$. By virtue of the Cauchy–Kowalewski theorem there exists a unique set of analytic functions $\overline{g}_{ik}(x^1,\ldots,x^n,y)$ and $\overline{f}^{\alpha}(x^1,\ldots,x^n,y)$ satisfying the equations (3) and (8) and the initial conditions (20)–(23). Since, by assumption, the initial conditions satisfy the equations (24)–(26), then $\overline{g}_{ik}, \overline{\phi}$ and $\overline{f}^{\alpha}$ satisfy (4) and (5) at $y=0$. It follows from Lemma 1 that $\overline{g}_{ik}, \overline{\phi}$ and $\overline{f}^{\alpha}$ satisfy (1) in an open set of $\mathbb{R}^{n+1}$ which contains the origin. Further, we can say that $\overline{f}^{\alpha}$ is a diffeomorphism since by virtue of (27) we have $\left|\partial \overline{f}^{\mu}/\partial x^{\alpha}\right|\neq 0$. Therefore, we conclude that the $(n+1)$-dimensional manifold whose line element (28) is formed with the solutions $\overline{g}_{ik}$ and $\overline{\phi}$ is a space whose Ricci tensor is equivalent to $S_{\mu\nu}$, and the embedding of the manifold (M^n,g) is given by $y=0$. This completes the proof.

We now need to show that once the functions g_{ik} are given the system of equations (24)–(27) always admits solution for Ω_{ik}. For simplicity we take $\xi^i=x^i$; $\xi^{n+1}=0$; $\eta^i=0$ e $\eta^{n+1}=1$. With this choice the condition (27) is readily satisfied. The equations (24)–(26) constitute a set of n partial differential equations (25) plus a constraint equation (26) for $n(n+1)/2$ independent functions Ω_{ik}. Except for $n=1$, the number of unknown functions is greater than [or equal to $(n=2)$] the number of equations. Then, out of the set of functions Ω_{ik} we pick n functions $\Omega_{1k}(k\geqslant 2)$ and $\Omega_{r'n}$ to be regarded as the unknown. (The r' index has the following meaning. We assume, for the sake of the argument, that we are using a coordinate system in which $g_{11}\neq 0$ and $g_{1k}=0$, $k=2,\ldots,n$. Hence, there exists at least an index $r'>1$ such that $g^{r'n}\neq 0$, since $|g_{ik}| \neq 0$.) The next step is to write (25) in a suitable form for application of the Cauchy–Kowalewski theorem (first-order derivative version) to ensure the existence of the solution. For the sake of brevity we shall omit the detailed proof and refer the reader to Refs. 18 and 24 where a similar procedure is carried out. Then it can be shown that after solving (25) for Ω_{1k} $(k\geqslant 2)$ and $\Omega_{r'n}$ we obtain

$$\frac{\partial \Omega_{r'n}}{\partial x^1} = \frac{1}{g^{r'n}(\delta_{r'n}-2)}\Bigg[-\sum_{r,s>1} g^{rs}\,\Omega_{1s,r} + 2\sum_{\substack{1<r<s\\ r,s\neq r',n}} g^{rs}\,\Omega_{rs,1} + \sum_{\substack{r>1\\ r\neq r'}} g^{rr}\Omega_{rr,1} + g^{r'r'}\Omega_{r'r',1}(1-\delta_{r'n})$$
$$- \sum_{r,s>1} g^{rs}\left(\sum_{t\leqslant r}\Omega_{tr}\Gamma^{t}_{s1} + \sum_{r<t}\Omega_{rt}\Gamma^{t}_{s1} - \Omega_{11}\Gamma^{1}_{sr} - \sum_{t<1}\Omega_{1t}\Gamma^{t}_{sr}\right) + \frac{1}{\phi}S_{1y}(x^i)\Bigg], \tag{29}$$

where no sum over r' is implied, and

$$\frac{\partial \Omega_{1k}}{\partial x^1} = g_{11}\Bigg[-\sum_{r,s>1} g^{rs}\left(\sum_{s\leqslant k}\Omega_{sk,r} + \sum_{k<s}\Omega_{ks,r} - 2\sum_{r<s}\Omega_{rs,k}\right) - g^{11}\Omega_{11,k} - \sum_{r>1} g^{rr}\Omega_{rr,k}$$
$$- g^{rs}\left(\sum_{t\leqslant r}\Omega_{tr}\Gamma^{t}_{sk} + \sum_{r<t}\Omega_{rt}\Gamma^{t}_{sk} - \sum_{t\leqslant k}\Omega_{tk}\Gamma^{t}_{sr} - \sum_{k<t}\Omega_{kt}\Gamma^{t}_{sr}\right) + \frac{1}{\phi}S_{ky}(x^i)\Bigg], \quad k\geqslant 2, \tag{30}$$

where Ω_{11} must be substituted by

$$\Omega_{11}=\frac{1}{2g^{11}\underset{r,s>1}{g^{rs}}\left(\underset{r\leqslant s}{\Omega_{rs}}+\underset{s<r}{\Omega_{sr}}\right)}\left[2g^{11}\underset{r,s>1}{g^{rs}}\,\Omega_{1r}\Omega_{1s}-\underset{r,s,t,u>1}{g^{rs}g^{tu}}\left[\left(\underset{r\leqslant s}{\Omega_{rs}}+\underset{s<r}{\Omega_{sr}}\right)\left(\underset{t\leqslant u}{\Omega_{tu}}+\underset{u<t}{\Omega_{ut}}\right)-\left(\underset{r\leqslant u}{\Omega_{ru}}+\underset{u<r}{\Omega_{ur}}\right)\right.\right.$$
$$\left.\left.\times\left(\underset{s\leqslant t}{Q_{st}}+\underset{t<s}{\Omega_{ts}}\right)\right]-\varepsilon\left(R-\frac{\varepsilon}{\phi^2}S_{yy}(x^i)+g^{jm}S_{jm}(x^i)\right)\right]. \tag{31}$$

Finally, if we choose the functions Ω_{ik} $[i\leqslant k, i>1, (i,k)\neq(r',n)]$, $\phi\neq 0$ as being analytic at the origin, and since $S_{\mu\nu}(x^i)$ are also analytic, then in view of the Cauchy–Kowalewski theorem the system of equations (29) and (30) admits a solution that is analytic at the origin. Therefore, given arbitrary analytic functions $g_{ik}(x^1,\ldots,x^n)$ the existence of the functions $\Omega_{ik}(x^1,\ldots,x^n)$ $\times(i,k=1,...,n)$, $\xi^\alpha(x^1,\ldots,x^n)$, $\eta^\alpha(x^1,\ldots,x^n)$ which satisfy (24)–(27) is ensured, so Theorem 1 applies.

It should be mentioned that in the case where $S_{\mu\nu}=0$, Eq. (8) holds for any functions $\overline{f^\alpha}(x^\beta)$; hence all the results derived above apply when the space $(\tilde{M}_0^{n+1},\tilde{g}_0)$ has a vanishing Ricci tensor. Therefore, we can state the following theorem:

Theorem 2: *Let M^n be an n-dimensional semi-Riemannian manifold with metric given by*

$$ds^2=g_{ik}dx^i dx^k,$$

in a coordinate system $\{x^i\}$ of M^n. Let $p\in M^n$, have coordinates $x_p^1=\cdots=x_p^n=0$. Consider an $(n+1)$-dimensional semi-Riemannian space $(\tilde{M}_0^{n+1},\tilde{g}_0)$ whose Ricci tensor is either nondegenerate or null. If g_{ik} are analytic functions at $0\in\mathbb{R}^n$, then (M^n,g) has a local isometric and analytic embedding (at the point p) in an $(n+1)$-dimensional space which is Ricci equivalent to $(\tilde{M}_0^{n+1},\tilde{g}_0)$.

Therefore, we conclude that if the space $(\tilde{M}_0^{n+1},\tilde{g}_0)$ is a solution of the Einstein equations for some source, then Theorem 2 guarantees that there exists a space which satisfies the ''same'' Einstein equations up to a coordinate transformation [see Eq. (1)], in which the space–time (M^n,g) can be embedded.

III. A SIMPLE APPLICATION OF THEOREM 2

Up to this point we have considered the Ricci tensor only through its covariant components $\tilde{R}_{\alpha\beta}$. However, it is not difficult to realize that all the previous results we have obtained are still valid if the mixed $\tilde{R}_\beta^\alpha$ or contravariant components $\tilde{R}^{\alpha\beta}$ are considered instead.

In what follows we illustrate Theorem 2 in its Ricci tensor mixed-components version.

Consider the five-dimensional semi-Riemannian space $(\tilde{M}_0^5,\tilde{g}_0)$ with a metric given by

$${}^5ds^2=(y+1)^{4/5}(-dt^2+dx^2+dy^2+dz^2)+\tfrac{24}{25}\varepsilon dy^2. \tag{32}$$

If we calculate the mixed components of the Ricci S_ν^μ tensor for this metric we obtain

$$S_\nu^\mu=\mathrm{diag}\left(\frac{1}{4},\frac{1}{4},\frac{1}{4},\frac{1}{4},-1\right)\frac{\varepsilon}{(y+1)^2}. \tag{33}$$

We can view (32) as a five-dimensional analog of the Friedmann–Robertson–Walker cosmological metric for radiation, with an energy density given by $\rho(y)=-\varepsilon/(y+1)^2$ (as measured by observers ∂_y).

Consider now a four-dimensional space (M^4,g) with a vanishing Ricci tensor, i.e., a vacuum solution of the Einstein field equations. Let us consider the question of embedding (M^4,g) into the collection $\mathcal{M}_{\tilde{g}_0}^5$ of five-dimensional spaces that are Ricci equivalent to $(\tilde{M}_0^5,\tilde{g}_0)$. In order to work with a mixed Ricci tensor we redefine the Ricci-equivalence property by the equation

$$\tilde{R}^{\mu}_{\nu}=\frac{\partial \overline{f}^{\mu}}{\partial x^{\alpha}}\frac{\partial x^{\beta}}{\partial \overline{f}^{v}}S^{\alpha}_{\beta}. \tag{34}$$

To find the embedding we begin with the ansatz

$$\overline{g}_{ik}(x^1,\ldots,x^4,y)=u(y)g_{ik}(x^1,\ldots,x^4), \tag{35}$$

$$\overline{\phi}(x^1,\ldots,x^4,y)=1, \tag{36}$$

$$\overline{f}^{\alpha}(x^1,\ldots,x^4,y)=x^{\alpha}, \tag{37}$$

where g_{ik} is the metric of (M^4,g) and $u(y)$ is a function such that $u(0)=1$.

From Lemma 1 we can show that (34) is equivalent to the ordinary differential equation

$$u'=\frac{4}{5}\frac{u}{(y+1)}. \tag{38}$$

Therefore, after integrating (38) we conclude that (M^4,g) has a local embedding in the space

$${}^5ds^2=(y+1)^{4/5}(g_{ik}dx^i dx^k)+\tfrac{24}{25}\varepsilon dy^2, \tag{39}$$

whose Ricci tensor is the same as S^{μ}_{ν}, given by (33). Finally, it is worth mentioning that although the spaces (32) and (39) are Ricci equivalent they are not isometric. This can simply be verified since the Weyl tensor $W_{\mu\nu\lambda\rho}$ calculated from (32) vanishes while (39) may have $W_{\mu\nu\lambda\rho}\neq 0$ for some g_{ik} (choose, for example, $g_{ik}dx^i dx^k$ to be the line element of Schwarzschild space–time).

IV. FINAL COMMENTS

The restriction of the Ricci tensor being nondegenerate, as required by Theorem 2, certainly imposes a limitation on the set of possible sources of the embedding space. For example, we would have to leave out of consideration solutions of the Einstein equations such as cosmological models sourced by dust-type perfect fluid. We feel that although a great number of solutions of physical interest have nondegenerate Ricci tensor, e.g., Friedman–Robertson–Walker models sourced by incoherent radiating perfect fluids, it seems indisputable that a theorem in which the condition of nondegeneracy is relaxed would be most welcome. We are currently investigating whether this limitation can be overcome by taking into account the divergenceless condition

$${}^0\tilde{\nabla}_{\alpha}(\tilde{g}_0^{\alpha\gamma}S_{\mu\nu}-\tfrac{1}{2}\delta^{\alpha}_{\beta}\tilde{g}_0^{\gamma\lambda}S_{\mu\nu})=0, \tag{40}$$

where ${}^0\tilde{\nabla}_{\alpha}$ denotes the covariant derivative compatible with the metric $\tilde{g}_0$.

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APPENDIX: CAUCHY–KOWALEWSKI THEOREM

Theorem (Cauchy–Kowalewski): *Let us consider the set of partial differential equations:*

$$\frac{\partial^2 u^A}{\partial (y^{n+1})^2}=F^A\left(y^{\alpha},u^B,\frac{\partial u^B}{\partial y^{\alpha}},\frac{\partial^2 u^B}{\partial y^{\alpha}\partial y^{i}},\right),\quad A=1,\ldots,m, \tag{41}$$

where $u^1,\ldots,u^m$ *are* m *unknown functions of the* $n+1$ *variables* $y^1,\ldots,y^n,y^{n+1}$, $\alpha=1,\ldots,n+1$, $i=1,...,n$, $B=1,\ldots,m$. *Also, let* $v^1,\ldots,v^m,w^1,\ldots,w^m$, *functions of the variables* $y^1,\ldots,y^n$, *be analytic at* $0\in\mathbb{R}^n$. *If the functions* F^A *are analytic with respect to each of their arguments around the values evaluated at the point* $y^1=\cdots=y^n=0$, *then there exists a unique solution of Eqs. (41) which is analytic at* $0\in\mathbb{R}^{n+1}$ *and that satisfies the initial condition*

$$u^A(y^1,\ldots,y^n,0)=v^A(y^1,\ldots,y^n), \tag{42}$$

$$\frac{\partial u^A}{\partial y^{n+1}}(y^1,\ldots,y^n,0)=w^A(y^1,\ldots,y^n), \quad A=1,\ldots,m. \tag{43}$$

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New Liouville integrable noncanonical Hamiltonian systems from the AKNS spectral problem

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Liouville integrable noncanonical Hamiltonian systems with variable coefficient symplectic forms are generated from the AKNS 3×3 matrix Lax pairs by binary symmetry constraints of the AKNS hierarchy. These integrable systems provide new integrable factorization for every AKNS system in the hierarchy. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1478802]

I. INTRODUCTION

Symmetry constraints of soliton systems give us a systematic method of constructing Liouville integrable finite-dimensional Hamiltonian systems, as well as allow us to find an important class of solutions of related field systems. Moreover, most of the examples constructed so far (for example, see Refs. 1–20), both through mono nonlinearization[1] and through binary nonlinearization[13] of spectral problems of soliton systems, written down in natural coordinates, i.e., eigenfunctions of spectral problems, are Hamiltonian (or multi-Hamiltonian[5,7–12]) systems with constant coefficient symplectic forms. A natural question arises whether there are some symmetry constraints which nonlinearize spectral problems of soliton systems into Hamiltonian systems with variable coefficient symplectic forms.

In this article we give a positive answer on the basis of considering the symmetry constraints of the AKNS 2×2 matrix spectral problem as an illustrative example. The appropriate Poisson structure will be derived by the Dirac constraint method applied to the Poisson structure of binary constrained AKNS 3×3 matrix spectral problem.[18] Nevertheless, the method suggests the existence of Hamiltonian systems with variable coefficient symplectic forms by binary symmetry constraints for other spectral problems like multicomponent KdV or Kaup–Newell ones.

The article is organized as follows. In Sec. II we present a concept of factorization of a given soliton system into a pair of Hamiltonian systems with constant coefficient symplectic forms, derived through the so-called binary symmetry constraints.[13,21] Then, in Sec. III we illustrate the method by the example of binary symmetry constraints of the AKNS systems in the cases of the 2×2 matrix spectral problem and the 3×3 matrix spectral problem. In each case we obtain a respective factorization of every AKNS field system into a pair of finite-dimensional Liouville integrable Hamiltonian systems with constant coefficient symplectic forms. Finally, in Sec. IV we present a new factorization of the AKNS systems into a pair of finite-dimensional Liouville integrable Hamiltonian systems with variable coefficient symplectic forms. This new class of factorizations will be derived by using the Dirac constraint method applied to the binary symmetry constraints of the AKNS 3×3 matrix spectral problem.

II. BASIC FORMULATION OF BINARY SYMMETRY CONSTRAINTS

Let $\mathcal{B}$ denote the differential algebra of differential functions $u=u(x,t)$ and we write

$$\tilde{\mathcal{V}}^r=\mathcal{V}^r\otimes C[\lambda,\lambda^{-1}],\quad \mathcal{V}^r=\{(P^{ij})_{r\times r}|P^{ij}\in\mathcal{B}\}.$$

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A typical soliton system is related to a particular spectral problem

$$\phi_x = U\phi = U(u,\lambda)\phi, \quad U \in \tilde{\mathcal{V}}^r, \tag{1}$$

and its adjoint representation equation

$$V_x = [U,V], \quad V \in \tilde{\mathcal{V}}^r. \tag{2}$$

For an infinite set of Lax pairs

$$\phi_x = U\phi, \quad \phi_{t_n} = V^{(n)}\phi, \quad V^{(n)} = (\lambda^n V)_+ + \Delta_n, \quad n \geqslant 1, \tag{3}$$

where plus denotes the choice of the non-negative power of λ and Δ_n is some additional term which depends on a particular system under consideration, the compatibility conditions, i.e., the so-called zero-curvature equations, are equivalent to an infinite hierarchy of nonlinear partial differential equations (PDEs) in the evolutionary form under the condition that $\lambda_{t_n} = 0$:

$$U_{t_n} - V_x^{(n)} + [U,V^{(n)}] = 0 \Leftrightarrow u_{t_n} = K(u,u_x,\dots) = K[u], \quad n \geqslant 1. \tag{4}$$

Moreover, the property

$$V_{t_n}^{(m)} - V_{t_m}^{(n)} + [V^{(m)},V^{(n)}] = 0, \quad m,n \geqslant 1, \tag{5}$$

means[22] that all vector fields do commute in pairs, $[K_m,K_n] = 0$.

In fact, there is another natural set of Lax pairs related to the adjoint spectral problem

$$\psi_x = U^*\psi = -U^T\psi, \quad \psi_{t_n} = V^{*(n)}\psi = -(V^{(n)})^T\psi, \quad n \geqslant 1, \tag{6}$$

where T means the transpose of matrices. Obviously we have

$$U_{t_n} - V_x^{(n)} + [U,V^{(n)}] = 0 \Leftrightarrow U_{t_n}^* - V_x^{*(n)} + [U^*,V^{*(n)}] = 0. \tag{7}$$

There exists an additional object being very important in our theory, i.e., so-called recursion operator Φ. This second rank tensor, generally of integro-differential form, can be derived directly from the Lax representation (3) and (4), and has such a property that an action on one symmetry generator K_i produces another one K_{i+1}: $K_{i+1} = \Phi K_i$. So, the infinite hierarchy of PDEs (4) can be generated recursively: $u_{t_n} = \Phi^n K_0$. In generic cases, i.e., before different type of reductions, K_n are multi-Hamiltonian vector fields and the adjoint operator Φ^* produces a hierarchy of closed one-forms being differentials of conserved functionals (see, for example, Ref. 12).

It is well known that eigenfunctions of the recursion operator (or its adjoint) are closely related to particular solutions of systems of equations from the considered chain of PDEs. On the other hand, each eigenfunction of $\Phi(\Phi^*)$ is expressible through the respective components of eigenfunctions ϕ, ψ of isospectral problem (1) and its adjoint (6). The idea of symmetry constraints means the restriction of the kth symmetry (respectively, kth conserved one-form) to a finite number of eigenfunctions of Φ (respectively, Φ^*) and then to express each component of chosen eigenfunctions by related components of ϕ and ψ. This last step for binary symmetry constraints is carried out according to the following.

Lemma 1:[18] *Let $U(u,\lambda)$ be a square matrix of order r depending on $u,u_x,\dots$ and a parameter λ. Suppose that $\phi = (\phi_1,\phi_2,\dots,\phi_r)^T$, $\psi = (\psi_1,\psi_2,\dots,\psi_r)^T$ satisfy the spectral problem and the adjoint spectral problem*

$$\phi_x = U(u,\lambda)\phi, \quad \psi_x = -U^T(u,\lambda)\psi,$$

and set the matrix $\overline{V} = \phi\psi^T = (\phi_k\psi_l)_{r\times r}$. Then

(i) the variational derivative of the spectral parameter λ *with respect to the potential* u *can be expressed, up to a normalized constant, by*

$$\frac{\delta\lambda}{\delta u}=tr(\overline{V}\partial U/\partial u), \tag{8}$$

(ii) the matrix $\overline{V}$ *is a solution of the adjoint representation equation* $V_x=[U,V]$, *i.e.,* $\overline{V}_x=[U,\overline{V}]$.

Restriction of K_0, i.e., the simplest symmetry from the hierarchy, to a finite sum of eigenfunctions of the recursion operator allows us to express u through these eigenfunctions. Let $\tilde{u}(\phi,\psi)$ denote such a restricted potential u. Introducing N distinct eigenvalues $\lambda_1,\lambda_2,\ldots,\lambda_N$, the nth Lax pair (3) and its adjoint (6) become

$$\begin{aligned}\phi_{ix}&=U(\tilde{u},\lambda_i)\phi_i, \quad i=1,\ldots,N,\\ \psi_{ix}&=-U^T(\tilde{u},\lambda_i)\psi_i, \quad i=1,\ldots,N,\end{aligned} \tag{9}$$

$$\begin{aligned}\phi_{it_n}&=V^{(n)}(\tilde{u},\lambda_i)\phi_i, \quad i=1,\ldots,N,\\ \psi_{it_n}&=-(V^{(n)})^T(\tilde{u},\lambda_i)\psi_i, \quad i=1,\ldots,N.\end{aligned} \tag{10}$$

The compatibility condition of (9) and (10) is still the nth PDE system $\tilde{u}_{t_n}=K_n[\tilde{u}]$, but now systems (9) and (10) turn into finite-dimensional Hamiltonian systems with constant coefficient symplectic forms. Hence, such a procedure factorizes a given system of PDEs into two systems of ordinary differential equations (ODEs). Solving simultaneously both systems of ODEs, we get immediately a solution of the related PDE.

III. BINARY SYMMETRY CONSTRAINTS OF THE AKNS SYSTEMS

In the following section we illustrate the factorization procedure by binary symmetry constraints on the example of the AKNS hierarchy. These results will be important for our further considerations, when we present a factorization procedure by a new type of binary symmetry constraint which leads to noncanonical Hamiltonian systems with variable coefficient symplectic forms.

A. The case of 2×2 matrix spectral problem

Consider the AKNS 2×2 matrix spectral problem[23]

$$\phi_x=U\phi, \quad U=U(u,\lambda)=\begin{pmatrix}-\lambda & q\\ r & \lambda\end{pmatrix}, \quad \phi=\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}, \quad u=\begin{pmatrix}q\\ r\end{pmatrix}. \tag{11}$$

Take

$$V=\begin{pmatrix}a & b\\ c & -a\end{pmatrix}=\sum_{i=0}^{\infty}\begin{pmatrix}a_i & b_i\\ c_i & -a_i\end{pmatrix}\lambda^{-i} \tag{12}$$

and

$$\phi_{t_n}=V^{(n)}(u,\lambda)\phi, \quad V^{(n)}=\sum_{i=0}^{n}\begin{pmatrix}a_i & b_i\\ c_i & -a_i\end{pmatrix}\lambda^{n-i}. \tag{13}$$

The adjoint representation equation $V_x=[U,V]$ gives

$$a_0=-1,\quad b_0=c_0=0,\quad a_1=0,\quad b_1=q,\quad c_1=r,\quad a_2=\tfrac{1}{2}qr,\quad \ldots\begin{pmatrix}c_{k+1}\\ b_{k+1}\end{pmatrix}=\Phi^*\begin{pmatrix}c_k\\ b_k\end{pmatrix},$$

$$a_k=\partial^{-1}(qc_k-rb_k),\quad k=1,2,\ldots, \tag{14}$$

$$\Phi^*=\frac{1}{2}\begin{pmatrix}\partial-2r\partial^{-1}q & 2r\partial^{-1}r\\ -2q\partial^{-1}q & -\partial+2q\partial^{-1}r\end{pmatrix},\quad \partial=\frac{\partial}{\partial x},\quad \partial\partial^{-1}=\partial^{-1}\partial=1.$$

The AKNS hierarchy associated with (11) and (13) takes the form[24]

$$u_{t_n}=\begin{pmatrix}q\\ r\end{pmatrix}_{t_n}=\pi(\Phi^*)^n\begin{pmatrix}r\\ q\end{pmatrix}=\pi\frac{\delta\tilde{H}_n}{\delta u},\quad n\geqslant 0, \tag{15}$$

where

$$\pi=\begin{pmatrix}0 & -2\\ 2 & 0\end{pmatrix},\quad \tilde{H}_n=\int\frac{2}{n+1}a_{n+2}dx,\quad \begin{pmatrix}c_{n+1}\\ b_{n+1}\end{pmatrix}=\frac{\delta\tilde{H}_n}{\delta u},\quad n\geqslant 0.$$

For $n=2$ we have

$$V^{(1)}=\begin{pmatrix}-\lambda & q\\ r & \lambda\end{pmatrix}\equiv U,\quad V^{(2)}=\begin{pmatrix}-\lambda^2+\frac{1}{2}qr & q\lambda-\frac{1}{2}q_x\\ r\lambda+\frac{1}{2}r_x & \lambda^2-\frac{1}{2}qr\end{pmatrix}, \tag{16}$$

and zero curvature conditions (7) give $n=2$ AKNS systems (15):

$$\begin{aligned}q_{t_2}&=-\tfrac{1}{2}q_{xx}+q^2r,\\ r_{t_2}&=\tfrac{1}{2}r_{xx}-r^2q.\end{aligned} \tag{17}$$

According to Lemma 1, we have[13]

$$\frac{\delta\lambda}{\delta u}=\begin{pmatrix}\delta\lambda/\delta q\\ \delta\lambda/\delta r\end{pmatrix}=tr\left[\begin{pmatrix}\phi_1\psi_1 & \phi_1\psi_2\\ \phi_2\psi_1 & \phi_2\psi_2\end{pmatrix}\frac{\partial U(u,\lambda)}{\partial u}\right]=\begin{pmatrix}\phi_2\psi_1\\ \phi_1\psi_2\end{pmatrix}, \tag{18}$$

which should be read componentwise. Moreover, one can verify that under $\phi_x=U\phi$, $\psi_x=-U^T\psi$, we have

$$\Phi^*\begin{pmatrix}\phi_2\psi_1\\ \phi_1\psi_2\end{pmatrix}=\lambda\begin{pmatrix}\phi_2\psi_1\\ \phi_1\psi_2\end{pmatrix}+I\begin{pmatrix}\phi_2\psi_1\\ \phi_1\psi_2\end{pmatrix},\quad I=\frac{1}{2}\phi_1\psi_1-\frac{1}{2}\phi_2\psi_2, \tag{19}$$

where I is an integral of motion of $\phi_x=U\phi$, $\psi_x=-U^T\psi$.

Binary symmetry constraints are determined by[13,25]

$$\frac{\delta H_k}{\delta u}=\begin{pmatrix}c_{k+1}\\ b_{k+1}\end{pmatrix}=\sum_{j=1}^{N}\frac{\delta\lambda_j}{\delta u}=\begin{pmatrix}\langle Q_2,P_1\rangle\\ \langle Q_1,P_2\rangle\end{pmatrix}. \tag{20}$$

Hereafter we denote the inner product in R^N by $\langle .,.\rangle$ and

$$Q_i=(\phi_{i1},\ldots,\phi_{iN})^T,\quad P_i=(\psi_{i1},\ldots,\psi_{iN})^T,\quad i=1,2. \tag{21}$$

The simplest binary constraint for $k=0$ gives

$$\frac{\delta H_0}{\delta u}=\begin{pmatrix} c_1 \\ b_1 \end{pmatrix}=\begin{pmatrix} \langle Q_2,P_1\rangle \\ \langle Q_1,P_2\rangle \end{pmatrix}=\begin{pmatrix} r \\ q \end{pmatrix}. \tag{22}$$

Under constraint (22), for arbitrary n, and for N distinct eigenvalues $\lambda_1,\ldots,\lambda_N$, the nth Lax pair (9) and its adjoint (10),

$$\begin{aligned} &\begin{pmatrix} \phi_{1j} \\ \phi_{2j} \end{pmatrix}_x = U(\tilde{u},\lambda_j)\begin{pmatrix} \phi_{1j} \\ \phi_{2j} \end{pmatrix}, \quad j=1,\ldots,N, \\ &\begin{pmatrix} \psi_{1j} \\ \psi_{2j} \end{pmatrix}_x = -U^T(\tilde{u},\lambda_j)\begin{pmatrix} \psi_{1j} \\ \psi_{2j} \end{pmatrix}, \quad j=1,\ldots,N, \end{aligned} \tag{23}$$

$$\begin{aligned} &\begin{pmatrix} \phi_{1j} \\ \phi_{2j} \end{pmatrix}_{t_n} = V^{(n)}(\tilde{u},\lambda_j)\begin{pmatrix} \phi_{1j} \\ \phi_{2j} \end{pmatrix}, \quad j=1,\ldots,N, \\ &\begin{pmatrix} \psi_{1j} \\ \psi_{2j} \end{pmatrix}_{t_n} = -(V^{(n)})^T(\tilde{u},\lambda_j)\begin{pmatrix} \psi_{1j} \\ \psi_{2j} \end{pmatrix}, \quad j=1,\ldots,N, \end{aligned} \tag{24}$$

become two finite-dimensional Hamiltonian systems with constant coefficient symplectic forms, with evolution parameters $t_1=x$ and t_n, respectively. $2N$ pairs of canonical coordinates are given by $(\phi_{1j},\psi_{1j})_{j=1}^N$, $(\phi_{2j},\psi_{2j})_{j=1}^N$. For x-evolution we have

$$\begin{aligned} &Q_{1x}=\frac{\partial H_1}{\partial P_1}, \quad Q_{2x}=\frac{\partial H_1}{\partial P_2}, \quad P_{1x}=-\frac{\partial H_1}{\partial Q_1}, \quad P_{2x}=-\frac{\partial H_1}{\partial Q_2}, \quad x=t_1, \\ &H_1=\langle AP_2,Q_2\rangle-\langle AP_1,Q_1\rangle+\langle P_2,Q_1\rangle\langle P_1,Q_2\rangle, \end{aligned} \tag{25}$$

and for t_2-evolution

$$\begin{aligned} &Q_{1t_2}=\frac{\partial H_2}{\partial P_1}, \quad Q_{2t_2}=\frac{\partial H_2}{\partial P_2}, \quad P_{1t_2}=-\frac{\partial H_2}{\partial Q_1}, \quad P_{2t_2}=-\frac{\partial H_2}{\partial Q_2}, \\ &H_2=\langle A^2P_2,Q_2\rangle-\langle A^2P_1,Q_1\rangle+\langle P_2,Q_1\rangle\langle AP_1,Q_2\rangle+\langle AP_2,Q_1\rangle\langle P_1,Q_2\rangle-\tfrac{1}{2}(\langle P_2,Q_2\rangle \\ &\quad -\langle P_1,Q_1\rangle)\langle P_2,Q_1\rangle\langle P_1,Q_2\rangle. \end{aligned} \tag{26}$$

Hence, t_2-AKNS PDE (17) is factorized by two ODE systems (25) and (26). For $N=1$ one finds

$$\begin{aligned} \phi_{1x}&=-\lambda\phi_1+\phi_1\phi_2\psi_2, \\ \phi_{2x}&=\lambda\phi_2+\phi_1\phi_2\psi_1, \\ \psi_{1x}&=\lambda\psi_1-\phi_2\psi_1\psi_2, \\ \psi_{2x}&=-\lambda\psi_2-\phi_1\psi_1\psi_2, \end{aligned} \tag{27}$$

$$\begin{aligned} \phi_{1t_2}&=-\lambda^2\phi_1+2\lambda\phi_1\phi_2\psi_2+\phi_1^2\phi_2\psi_1\psi_2-\tfrac{1}{2}\phi_1\phi_2^2\psi_2^2, \\ \phi_{2t_2}&=\lambda^2\phi_2+2\lambda\phi_1\phi_2\psi_1-\phi_1\phi_2^2\psi_1\psi_2+\tfrac{1}{2}\phi_1^2\phi_2\psi_1^2, \end{aligned} \tag{28}$$

$$\psi_{1t_2}=\lambda^2\psi_1-2\lambda\phi_2\psi_1\psi_2-\phi_1\phi_2\psi_1^2\psi_2+\tfrac{1}{2}\phi_2^2\psi_1\psi_2^2,$$

$$\psi_{2t_2}=-\lambda^2\psi_2-2\lambda\phi_1\psi_1\psi_2+\phi_1\phi_2\psi_1\psi_2^2-\tfrac{1}{2}\phi_1^2\psi_1^2\psi_2,$$

and it is easy to verify that for any solution $(\phi_1,\phi_2,\psi_1,\psi_2)$ of two ODE systems (27) and (28) $\tilde{q}=\phi_1\psi_2$, $\tilde{r}=\phi_2\psi_1$ is a solution of the PDE system

$$\begin{aligned}\tilde{q}_{t_2}&=-\tfrac{1}{2}\tilde{q}_{xx}+\tilde{q}^2\tilde{r},\\ \tilde{r}_{t_2}&=\tfrac{1}{2}\tilde{r}_{xx}-\tilde{r}^2\tilde{q}.\end{aligned}\tag{29}$$

Both systems (25) and (26) belong to the same family of Liouville integrable systems.

As shown in Ref. 13, there is a natural set of integrals of motion generated by the relation

$$F_x=\left(\frac{1}{2}trV^2\right)_x=\frac{d}{dx}(a^2+bc)=0,\tag{30}$$

i.e., F is a generating function of integrals of motion for (25). After setting $F=\Sigma_{n\geqslant 0}F_n\lambda^{-n}$, we obtain the following expressions:

$$\begin{aligned}F_1&=-2a_1=\langle P_2,Q_2\rangle-\langle P_1,Q_1\rangle,\\ F_n&=\sum_{i=1}^{n-1}(a_ia_{n-i}+b_ic_{n-i})-2a_n\\ &=\langle A^{n-1}P_2,Q_2\rangle-\langle A^{n-1}P_1,Q_1\rangle\\ &\quad+\sum_{i=1}^{n-1}\left[\frac{1}{4}(\langle A^{i-1}P_1,Q_1\rangle-\langle A^{i-1}P_2,Q_2\rangle)(\langle A^{n-i-1}P_1,Q_1\rangle\right.\\ &\quad\left.-\langle A^{n-i-1}P_2,Q_2\rangle)+\langle A^{i-1}P_2,Q_1\rangle\langle A^{n-i-1}P_1,Q_2\rangle\right].\end{aligned}\tag{31}$$

Integrals of motion (31) are closely related to the zero boundary condition imposed on ϕ and ψ: $\lim_{|x|\to\infty}\phi_i=\lim_{|x|\to\infty}\psi_i=0$, $i=1,2$. Actually, one can then verify that

$$\Phi^*\begin{pmatrix}\phi_2\psi_1\\ \phi_1\psi_2\end{pmatrix}=\lambda\begin{pmatrix}\phi_2\psi_1\\ \phi_1\psi_2\end{pmatrix},\tag{32}$$

and under the constraint (22) we have

$$\begin{pmatrix}c_{n+1}\\ b_{n+1}\end{pmatrix}=(\Phi^*)^n\begin{pmatrix}c_1\\ b_1\end{pmatrix}=\begin{pmatrix}\langle A^nQ_2,P_1\rangle\\ \langle A^nQ_1,P_2\rangle\end{pmatrix},\tag{33}$$

where $A=\mathrm{diag}(\lambda_1,\ldots,\lambda_N)$, and thus

$$a_{n+1}=\partial^{-1}(qc_{n+1}-rb_{n+1})=\tfrac{1}{2}(\langle A^nP_1,Q_1\rangle-\langle A^nP_2,Q_2\rangle).\tag{34}$$

All Hamiltonian functions H_n are expressible through the F_k ones[13]

$$H_n=\sum_{m=0}^{n}\frac{d_m}{m+1}\sum_{i_1+\ldots+i_{m+1}=n+1}F_{i_1}\cdots F_{i_{m+1}},\quad i_1,\ldots,i_{m+1}\geqslant 1,\quad n\geqslant 0,\tag{35}$$

where constants d_m are defined by

$$d_0=1,\quad d_1=-\frac{1}{2},\quad d_2=\frac{3}{8},\quad d_m=-d_{m-1}-\frac{1}{2}\sum_{s=1}^{m-2} d_s d_{m-s-1}-\frac{1}{2}\sum_{s=1}^{m-1} d_s d_{m-s},\quad m\geqslant 3. \tag{36}$$

For example $H_1=F_2-\frac{1}{4}F_1^2$, $H_2=F_3-\frac{1}{2}F_1F_2+\frac{1}{8}F_1^3,\ldots$. Notice that $I=-\frac{1}{2}F_1$. The involutivity and functional independence of one of two sets $\{F_n\}_{n=1}^N$, $\{H_n\}_{n=1}^N$ results in the same properties of another one. Moreover, there exists an additional set of N integrals of motion

$$f_k=\phi_{1k}\psi_{1k}+\phi_{2k}\psi_{2k},\quad k=1,\ldots,N. \tag{37}$$

The set of $2N$ functions $(f_k,H_k)_{k=1}^N$ is functionally independent and all functions are in involution,[13] and hence all systems (23) and (24) are Liouville integrable. Moreover, as demonstrated in Refs. 26–28, they are also separable, so again integrable by quadratures, and give rise to explicit solutions to the related PDE systems.

B. The case of 3×3 matrix spectral problem

As was demonstrated in Ref. 18, the AKNS hierarchy can also be reconstructed from the following 3×3 matrix spectral problem:

$$\tilde{\phi}_x=\begin{pmatrix}\tilde{\phi}_1\\ \tilde{\phi}_2\\ \tilde{\phi}_3\end{pmatrix}_x=U(u\lambda)\begin{pmatrix}\tilde{\phi}_1\\ \tilde{\phi}_2\\ \tilde{\phi}_3\end{pmatrix}=\begin{pmatrix}-2\lambda & \sqrt{2}q & 0\\ \sqrt{2}r & 0 & \sqrt{2}q\\ 0 & \sqrt{2}r & 2\lambda\end{pmatrix}\begin{pmatrix}\tilde{\phi}_1\\ \tilde{\phi}_2\\ \tilde{\phi}_3\end{pmatrix}. \tag{38}$$

The standard procedure with

$$V=\begin{pmatrix}-2a & \sqrt{2}b & 0\\ \sqrt{2}c & 0 & \sqrt{2}b\\ 0 & \sqrt{2}c & 2a\end{pmatrix}=\sum_{i=0}^{\infty}\begin{pmatrix}-2a_i & \sqrt{2}b_i & 0\\ \sqrt{2}c_i & 0 & \sqrt{2}b_i\\ 0 & \sqrt{2}c_i & 2a_i\end{pmatrix}\lambda^{-i} \tag{39}$$

generates again the hierarchy (14) and (15), but binary symmetry constraints lead to another factorization, i.e., another Liouville integrable Hamiltonian system with constant coefficient symplectic forms, and, as a consequence, to a new class of solutions of the underlying AKNS systems.

Let us briefly sketch the results of Ref. 18. Following Lemma 1, for the zero boundary conditions imposed on $\tilde{\phi}$ and $\tilde{\psi}$ functions, we have the variational derivative of the spectral parameter for the spectral problem (38) and its adjoint given by

$$\frac{\delta\lambda}{\delta q}=\sqrt{2}(\tilde{\phi}_2\tilde{\psi}_1+\tilde{\phi}_3\tilde{\psi}_2),\quad \frac{\delta\lambda}{\delta r}=\sqrt{2}(\tilde{\phi}_1\tilde{\psi}_2+\tilde{\phi}_2\tilde{\psi}_3). \tag{40}$$

The simplest binary constraint (20) with $k=0$ takes the form

$$\begin{pmatrix}c_1\\ b_1\end{pmatrix}=\sqrt{2}\begin{pmatrix}\langle\tilde{P}_1,\tilde{Q}_2\rangle+\langle\tilde{P}_2,\tilde{Q}_3\rangle\\ \langle\tilde{P}_2,\tilde{Q}_1\rangle+\langle\tilde{P}_3,\tilde{Q}_2\rangle\end{pmatrix}=\begin{pmatrix}\tilde{r}\\ \tilde{q}\end{pmatrix}, \tag{41}$$

and, hence, using (38)

$$\Phi^*\begin{pmatrix}\sqrt{2}(\tilde{\phi}_2\tilde{\psi}_1+\tilde{\phi}_3\tilde{\psi}_2)\\ \sqrt{2}(\tilde{\phi}_1\tilde{\psi}_2+\tilde{\phi}_2\tilde{\psi}_3)\end{pmatrix}=\lambda\begin{pmatrix}\sqrt{2}(\tilde{\phi}_2\tilde{\psi}_1+\tilde{\phi}_3\tilde{\psi}_2)\\ \sqrt{2}(\tilde{\phi}_1\tilde{\psi}_2+\tilde{\phi}_2\tilde{\psi}_3)\end{pmatrix}+I\begin{pmatrix}\sqrt{2}(\tilde{\phi}_2\tilde{\psi}_1+\tilde{\phi}_3\tilde{\psi}_2)\\ \sqrt{2}(\tilde{\phi}_1\tilde{\psi}_2+\tilde{\phi}_2\tilde{\psi}_3)\end{pmatrix}, \tag{42}$$

$I=\tilde{\phi}_1\tilde{\psi}_1-\tilde{\phi}_3\tilde{\psi}_3$, where again $\langle .,.\rangle$ denotes the standard inner product of R^N and

$$\begin{pmatrix} \tilde{Q}_i \\ \tilde{P}_i \end{pmatrix} = \begin{pmatrix} (\tilde{\phi}_{i1}, \ldots, \tilde{\phi}_{iN})^T \\ (\tilde{\psi}_{i1}, \ldots, \tilde{\psi}_{iN})^T \end{pmatrix}, \quad i = 1,2,3. \tag{43}$$

The substitution of (41) and (38) into the corresponding Lax equations (9) and (10) yields a hierarchy of finite-dimensional Hamiltonian systems with constant coefficient symplectic forms for $n \geqslant 1$:

$$\begin{aligned} \begin{pmatrix} \tilde{\phi}_{1j} \\ \tilde{\phi}_{2j} \\ \tilde{\phi}_{3j} \end{pmatrix}_{t_n} &= V^{(n)}(\tilde{u}, \lambda_j) \begin{pmatrix} \tilde{\phi}_{1j} \\ \tilde{\phi}_{2j} \\ \tilde{\phi}_{3j} \end{pmatrix}, \quad j = 1, \ldots, N, \\ \begin{pmatrix} \tilde{\psi}_{1j} \\ \tilde{\psi}_{2j} \\ \tilde{\psi}_{3j} \end{pmatrix}_{t_n} &= -(V^{(n)})^T(\tilde{u}, \lambda_j) \begin{pmatrix} \tilde{\psi}_{1j} \\ \tilde{\psi}_{2j} \\ \tilde{\psi}_{3j} \end{pmatrix}, \quad j = 1, \ldots, N. \end{aligned} \tag{44}$$

For example, for $t_1 = x$,

$$\tilde{H}_1 = -2(\langle A\tilde{P}_1, \tilde{Q}_1\rangle - \langle A\tilde{P}_3, \tilde{Q}_3\rangle) + 2(\langle \tilde{P}_1, \tilde{Q}_2\rangle + \langle \tilde{P}_2, \tilde{Q}_3\rangle)(\langle \tilde{P}_2, \tilde{Q}_1\rangle + \langle \tilde{P}_3, \tilde{Q}_2\rangle), \tag{45}$$

and for t_2

$$\begin{aligned} H_2 = &-2(\langle A^2\tilde{P}_1, \tilde{Q}_1\rangle - \langle A^2\tilde{P}_3, \tilde{Q}_3\rangle) + 2(\langle A\tilde{P}_1, \tilde{Q}_2\rangle + \langle A\tilde{P}_2, \tilde{Q}_3\rangle)(\langle \tilde{P}_2, \tilde{Q}_1\rangle + \langle \tilde{P}_3, \tilde{Q}_2\rangle) \\ &+ 2(\langle \tilde{P}_1, \tilde{Q}_2\rangle + \langle \tilde{P}_2, \tilde{Q}_3\rangle)(\langle A\tilde{P}_2, \tilde{Q}_1\rangle + \langle A\tilde{P}_3, \tilde{Q}_2\rangle) + 2(\langle \tilde{P}_1, \tilde{Q}_2\rangle + \langle \tilde{P}_2, \tilde{Q}_3\rangle)(\langle \tilde{P}_2, \tilde{Q}_1\rangle \\ &+ \langle \tilde{P}_3, \tilde{Q}_2\rangle)(\langle \tilde{P}_1, \tilde{Q}_1\rangle - \langle \tilde{P}_3, \tilde{Q}_3\rangle). \end{aligned} \tag{46}$$

Hence, t_2-AKNS PDE system (17) is again factorized by two ODE systems (44)–(46).

For $N = 1$ one finds

$$\begin{aligned} \tilde{\phi}_{1x} &= -2\lambda\tilde{\phi}_1 + 2\tilde{\phi}_2(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3), \\ \tilde{\phi}_{2x} &= 2\tilde{\phi}_3(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3) + 2\tilde{\phi}_1(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2), \\ \tilde{\phi}_{3x} &= 2\lambda\tilde{\phi}_3 + 2\tilde{\phi}_2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2), \\ \tilde{\psi}_{1x} &= 2\lambda\tilde{\psi}_1 - 2\tilde{\psi}_2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2), \\ \tilde{\psi}_{2x} &= -2\tilde{\psi}_1(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3) - 2\tilde{\psi}_3(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2), \\ \tilde{\psi}_{3x} &= -2\lambda\tilde{\psi}_3 - 2\tilde{\psi}_2(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3), \end{aligned} \tag{47}$$

and

$$\begin{aligned} \tilde{\phi}_{1t_2} = &-2\lambda^2\tilde{\phi}_1 + 4\lambda(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)\tilde{\phi}_2 + 2(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)(\tilde{\phi}_1\tilde{\psi}_1 - \tilde{\phi}_3\tilde{\psi}_3)\tilde{\phi}_2 \\ &+ 2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)\tilde{\phi}_1, \\ \tilde{\phi}_{2t_2} = &\,4\lambda(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)\tilde{\phi}_1 + 4\lambda(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)\tilde{\phi}_3 + 2(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)(\tilde{\phi}_1\tilde{\psi}_1 - \tilde{\phi}_3\tilde{\psi}_3)\tilde{\phi}_3 \\ &+ 2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)(\tilde{\phi}_1\tilde{\psi}_1 - \tilde{\phi}_3\tilde{\psi}_3)\tilde{\phi}_1, \end{aligned}$$

$$
\begin{aligned}
\tilde{\phi}_{3t_2} &= 2\lambda^2\tilde{\phi}_3 + 4\lambda(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)\tilde{\phi}_2 + 2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)(\tilde{\phi}_1\tilde{\psi}_1 - \tilde{\phi}_3\tilde{\psi}_3)\tilde{\phi}_2 \\
&\quad - 2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)\tilde{\phi}_3, \\
\tilde{\psi}_{1t_2} &= 2\lambda^2\tilde{\psi}_1 - 4\lambda(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)\tilde{\psi}_2 - 2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)(\tilde{\phi}_1\tilde{\psi}_1 - \tilde{\phi}_3\tilde{\psi}_3)\tilde{\psi}_2 \\
&\quad - 2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)\tilde{\psi}_1, \\
\tilde{\psi}_{2t_2} &= -4\lambda(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)\tilde{\psi}_3 - 4\lambda(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)\tilde{\psi}_1 - 2(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)(\tilde{\phi}_1\tilde{\psi}_1 - \tilde{\phi}_3\tilde{\psi}_3)\tilde{\psi}_1 \\
&\quad - 2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)(\tilde{\phi}_1\tilde{\psi}_1 - \tilde{\phi}_3\tilde{\psi}_3)\tilde{\psi}_3, \\
\tilde{\psi}_{3t_2} &= -2\lambda^2\tilde{\psi}_3 - 4\lambda(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)\tilde{\psi}_2 - 2(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)(\tilde{\phi}_1\tilde{\psi}_1 - \tilde{\phi}_3\tilde{\psi}_3)\tilde{\psi}_2 \\
&\quad + 2(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)\tilde{\psi}_3,
\end{aligned}
\tag{48}
$$

and it is not difficult to verify that for an arbitrary solution $(\tilde{\phi}_1, \tilde{\phi}_2, \tilde{\phi}_3, \tilde{\psi}_1, \tilde{\psi}_2, \tilde{\psi}_3)$ of two ODE systems (47) and (48), $\tilde{q} = \sqrt{2}(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3)$, $\tilde{r} = \sqrt{2}(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2)$ is a solution of the PDE system (29). The integrals of motion (30), expressed by $\tilde{Q}, \tilde{P}$ coordinates, are

$$
\begin{aligned}
\tilde{F}_1 &= 2(\langle \tilde{P}_3, \tilde{Q}_3\rangle - \langle \tilde{P}_1, \tilde{Q}_1\rangle), \\
\tilde{F}_n &= 2(\langle A^{n-1}\tilde{P}_3, \tilde{Q}_3\rangle - \langle A^{n-1}\tilde{P}_1, \tilde{Q}_1\rangle) + \sum_{i=1}^{n-1} [(\langle A^{i-1}\tilde{P}_3, \tilde{Q}_3\rangle - \langle A^{i-1}\tilde{P}_1, \tilde{Q}_1\rangle)(\langle A^{n-i-1}\tilde{P}_3, \tilde{Q}_3\rangle \\
&\quad - \langle A^{n-i-1}\tilde{P}_1, \tilde{Q}_1\rangle) + 2(\langle A^{i-1}\tilde{P}_2, \tilde{Q}_1\rangle + \langle A^{i-1}\tilde{P}_3, \tilde{Q}_2\rangle)(\langle A^{n-i-1}\tilde{P}_1, \tilde{Q}_2\rangle \\
&\quad + \langle A^{n-i-1}\tilde{P}_2, \tilde{Q}_3\rangle)],
\end{aligned}
\tag{49}
$$

and again $I = -\frac{1}{2}\tilde{F}_1$. Integrals (49) are related to the zero boundary condition imposed on $\tilde{\phi}$ and $\tilde{\psi}$ which leads to the following relations:

$$
\Phi^* \begin{pmatrix} \sqrt{2}(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2) \\ \sqrt{2}(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3) \end{pmatrix} = \lambda \begin{pmatrix} \sqrt{2}(\tilde{\phi}_2\tilde{\psi}_1 + \tilde{\phi}_3\tilde{\psi}_2) \\ \sqrt{2}(\tilde{\phi}_1\tilde{\psi}_2 + \tilde{\phi}_2\tilde{\psi}_3) \end{pmatrix}, \tag{50}
$$

$$
\begin{aligned}
a_{i+1} &= \langle A^i\tilde{P}_1, \tilde{Q}_1\rangle - \langle A^i\tilde{P}_3, \tilde{Q}_3\rangle, \quad i \geq 0, \\
b_{i+1} &= \sqrt{2}(\langle A^i\tilde{P}_2, \tilde{Q}_1\rangle + \langle A^i\tilde{P}_3, \tilde{Q}_2\rangle), \quad i \geq 0, \\
c_{i+1} &= \sqrt{2}(\langle A^i\tilde{P}_1, \tilde{Q}_2\rangle + \langle A^i\tilde{P}_2, \tilde{Q}_3\rangle), \quad i \geq 0.
\end{aligned}
\tag{51}
$$

Again all Hamiltonian functions $\tilde{H}_n$ are expressible through the $\tilde{F}_k$ ones according to formulas (35) and (36). For example, $\tilde{H}_1 = \tilde{F}_2 - \frac{1}{4}\tilde{F}_1^2$, $\tilde{H}_2 = \frac{1}{4}\tilde{F}_3 - \frac{1}{2}\tilde{F}_1\tilde{F}_2 + \frac{1}{8}\tilde{F}_1^3, \ldots$. Moreover, there exists an additional set of N integrals of motion

$$
\tilde{f}_k = \tilde{\phi}_{1k}\tilde{\psi}_{1k} + \tilde{\phi}_{2k}\tilde{\psi}_{2k} + \tilde{\phi}_{3k}\tilde{\psi}_{3k}, \quad k = 1, \ldots, N. \tag{52}
$$

As was shown in Ref. 18, the set of $3N$ functions $(\tilde{f}_k)_{k=1}^N$, $(\tilde{H}_k)_{k=1}^{2N}$ is functionally independent and all functions are in involution, hence all systems (44) with $n \geq 1$ are Liouville integrable. Separability of these systems leads to a new class of solutions of the underlying PDEs.

IV. NEW LIOUVILLE INTEGRABLE NONCANONICAL HAMILTONIAN SYSTEMS

The importance of factorization of a given PDE system into two integrable Hamiltonian ODE systems makes the procedure of binary nonlinearization worth further investigation. A natural question arises, whether in the frames of the formalism presented one can find another factorization, different from those found till now. Of course one possibility is to search for a higher order matrix Lax representation and stay inside a binary symmetry constraint yielding integrable Hamiltonian systems with constant coefficient symplectic forms. Another one is to go beyond such a symmetry constraint. Let us come back again to the AKNS 2×2 matrix Lax representation. According to Lemma 1, we found that $(\phi_2\psi_1,\phi_1\psi_2)^T$ is an AKNS symmetry constraint. On the other hand, we also know that $f=\phi_1\psi_1+\phi_2\psi_2$ is an integral of motion $\phi_x=U\phi$, $\psi_x=-U^T\psi$, i.e., $f_x=0$. So, it is not difficult to verify that

$$\frac{\delta\lambda}{\delta u}=\begin{pmatrix}\delta\lambda/\delta q\\ \delta\lambda/\delta r\end{pmatrix}=\begin{pmatrix}2\phi_2\psi_1 f\\ 2\phi_1\psi_2 f\end{pmatrix}=\begin{pmatrix}2\phi_2\psi_1(\phi_1\psi_1+\phi_2\psi_2)\\ 2\phi_1\psi_2(\phi_1\psi_1+\phi_2\psi_2)\end{pmatrix} \tag{53}$$

is again an admissible symmetry constraint and for the zero boundary condition case it is also an eigenfunction of Φ^* with an eigenvalue λ. The constant 2 was chosen for further convenience. Let us factorize the AKNS hierarchy with respect to the constraint (53). Denoting

$$XY=(x_1y_1,\ldots,x_Ny_N)^T,\quad \text{if } X=(x_1,\ldots,x_N)^T,\quad Y=(y_1,\ldots,y_N)^T, \tag{54}$$

the simplest symmetry constraint takes the form

$$\frac{\delta H_0}{\delta u}=\begin{pmatrix}r\\ q\end{pmatrix}=\begin{pmatrix}c_1\\ b_1\end{pmatrix}=\sum_{j=1}^{N}\frac{\delta\lambda_j}{\delta u}=\begin{pmatrix}2(\langle Q_2^2,P_1P_2\rangle+\langle P_1^2,Q_1Q_2\rangle)\\ 2(\langle Q_1^2,P_1P_2\rangle+\langle P_2^2,Q_1Q_2\rangle)\end{pmatrix}. \tag{55}$$

Under the substitution (55), for N distinct eigenvalues $\lambda_1,\ldots,\lambda_N$, the $t_1=x$ spectral problem (11) and its adjoint take the form of finite-dimensional dynamical system (23), which is equivalent to the following one

$$\begin{aligned}
\phi_{1i,x}&=-\lambda_i\phi_{1i}+2\sum_{j=1}^{N}[\phi_{1j}\psi_{2j}(\phi_{1j}\psi_{1j}+\phi_{2j}\psi_{2j})]\phi_{2i},\quad i=1,\ldots,N,\\
\phi_{2i,x}&=\lambda_i\phi_{2i}+2\sum_{j=1}^{N}[\phi_{2j}\psi_{1j}(\phi_{1j}\psi_{1j}+\phi_{2j}\psi_{2j})]\phi_{1i},\quad i=1,\ldots,N,\\
\psi_{1i,x}&=\lambda_i\psi_{1i}-2\sum_{j=1}^{N}[\phi_{2j}\psi_{1j}(\phi_{1j}\psi_{1j}+\phi_{2j}\psi_{2j})]\psi_{2i},\quad i=1,\ldots,N,\\
\psi_{2i,x}&=-\lambda_i\psi_{2i}-2\sum_{j=1}^{N}[\phi_{1j}\psi_{2j}(\phi_{1j}\psi_{1j}+\phi_{2j}\psi_{2j})]\psi_{1i},\quad i=1,\ldots,N.
\end{aligned} \tag{56}$$

Contrary to the cases from the previous section, this system has no Hamiltonian structure with constant coefficient symplectic forms.[29] Actually, the system (56) was considered recently in Ref. 29, where the authors confirmed the nonexistence of some class of constant coefficient Poisson structures. As we will show later, this considered system has a coordinate dependent Poisson structure. In fact, such a Poisson structure can be attached to any finite-dimensional dynamical system (24) constructed from t_n spectral problem (13) and its adjoint, under the constraint (55).

For $N=1,t_n=t_1=x$ and $t_n=t_2$, one finds respectively

$$\begin{aligned}
\phi_{1x} &= -\lambda\phi_1 + 2\phi_1\phi_2\psi_2(\phi_1\psi_1 + \phi_2\psi_2),\\
\phi_{2x} &= \lambda\phi_2 + 2\phi_1\phi_2\psi_1(\phi_1\psi_1 + \phi_2\psi_2),\\
\psi_{1x} &= \lambda\psi_1 - 2\phi_2\psi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2),\\
\psi_{2x} &= -\lambda\psi_2 - 2\phi_1\psi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2),
\end{aligned} \tag{57}$$

and

$$\begin{aligned}
\phi_{1t} &= -\lambda^2\phi_1 + 4\lambda\phi_1\phi_2\psi_2(\phi_1\psi_1 + \phi_2\psi_2) + 4\phi_1^2\phi_2\psi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2)^2\\
&\quad - 2\phi_1\phi_2^2\psi_2^2(\phi_1\psi_1 + \phi_2\psi_2)^2,\\
\phi_{2t} &= \lambda^2\phi_2 + 4\lambda\phi_1\phi_2\psi_1(\phi_1\psi_1 + \phi_2\psi_2) - 4\phi_1\phi_2^2\psi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2)^2\\
&\quad + 2\phi_1^2\phi_2\psi_1^2(\phi_1\psi_1 + \phi_2\psi_2)^2,\\
\psi_{1t} &= \lambda^2\psi_1 - 4\lambda\phi_2\psi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2) - 4\phi_1\phi_2\psi_1^2\psi_2(\phi_1\psi_1 + \phi_2\psi_2)^2\\
&\quad + 2\phi_2^2\psi_1\psi_2^2(\phi_1\psi_1 + \phi_2\psi_2)^2,\\
\psi_{2t} &= -\lambda^2\psi_2 - 4\lambda\phi_1\psi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2) + 4\phi_1\phi_2\psi_1\psi_2^2(\phi_1\psi_1 + \phi_2\psi_2)^2\\
&\quad - 2\phi_1^2\psi_1^2\psi_2(\phi_1\psi_1 + \phi_2\psi_2)^2.
\end{aligned} \tag{58}$$

Again one can verify that when $(\phi_1, \phi_2, \psi_1, \psi_2)$ is a solution of two ODE systems (57) and (58), then

$$\tilde{q} = \phi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2), \quad \tilde{r} = \phi_2\psi_1(\phi_1\psi_1 + \phi_2\psi_2)$$

is a solution of a related PDE system (29). Moreover, one can verify that with the constraint (55) and x-evolution (57)

$$\Phi^*\begin{pmatrix} 2\phi_2\psi_1(\phi_1\psi_1 + \phi_2\psi_2) \\ 2\phi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2) \end{pmatrix} = \lambda\begin{pmatrix} 2\phi_2\psi_1(\phi_1\psi_1 + \phi_2\psi_2) \\ 2\phi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2) \end{pmatrix} + I\begin{pmatrix} 2\phi_2\psi_1(\phi_1\psi_1 + \phi_2\psi_2) \\ 2\phi_1\psi_2(\phi_1\psi_1 + \phi_2\psi_2) \end{pmatrix},$$

$$I = \phi_1^2\psi_1^2 - \phi_2^2\psi_2^2.$$

For the zero boundary condition we have

$$\begin{pmatrix} c_{n+1} \\ b_{n+1} \end{pmatrix} = (\Phi^*)^n\begin{pmatrix} c_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} 2(\langle A^n Q_2^2, P_1P_2\rangle + \langle A^n P_1^2, Q_1Q_2\rangle) \\ 2(\langle A^n Q_1^2, P_1P_2\rangle + \langle A^n P_2^2, Q_1Q_2\rangle) \end{pmatrix}, \tag{59}$$

and thus

$$a_{n+1} = \partial^{-1}(qc_{n+1} - rb_{n+1}) = (\langle A^n P_1^2, Q_1^2\rangle - \langle A^n P_2^2, Q_2^2\rangle). \tag{60}$$

Formula (30) still guarantees the existence of integrals of motion for the system (56) which now, according to relations (59) and (60), takes the form

$$\overline{F}_1 = -2a_1 = -2(\langle P_1^2, Q_1^2\rangle - \langle P_2^2, Q_2^2\rangle),$$

$$\begin{aligned}\overline{F}_n = &\sum_{i=1}^{n-1}(a_i a_{n-i} + b_i c_{n-i}) - 2a_n = -2(\langle A^{n-1}P_1^2, Q_1^2\rangle - \langle A^{n-1}P_2^2, Q_2^2\rangle)\\ &+ \sum_{i=1}^{n-1}[(\langle A^{i-1}P_1^2, Q_1^2\rangle - \langle A^{i-1}P_2^2, Q_2^2\rangle)(\langle A^{n-i-1}P_1^2, Q_1^2\rangle - \langle A^{n-i-1}P_2^2, Q_2^2\rangle)\\ &+ 4(\langle A^{i-1}Q_1^2, P_1P_2\rangle + \langle A^{i-1}P_2^2, Q_1Q_2\rangle)(\langle A^{n-i-1}Q_2^2, P_1P_2\rangle + \langle A^{n-i-1}P_1^2, Q_1Q_2\rangle)].\end{aligned} \tag{61}$$

Notice that again $I = -\frac{1}{2}\overline{F}_1$ and one can construct the alternative set of integrals of motion $\{\overline{H}_n\}$ according to formulas (35) and (36).

The question is how to relate these integrals of motion to an appropriate Hamiltonian formulation for Eqs. (56). The key observation is that the two constraints

$$\tilde{\phi}_2^2 - 2\tilde{\phi}_1\tilde{\phi}_3 = 0, \quad \tilde{\psi}_2^2 - 2\tilde{\psi}_1\tilde{\psi}_3 = 0 \tag{62}$$

imposed on the eigenfunction components of the 3×3 matrix spectral problem (38) relate it to the 2×2 matrix spectral problem. Actually, the relation between $(\tilde{\phi}_1, \tilde{\phi}_2, \tilde{\phi}_3)$, $(\tilde{\psi}_1, \tilde{\psi}_2, \tilde{\psi}_3)$ and (ϕ_1, ϕ_2), (ψ_1, ψ_2) takes the form[29]

$$(\tilde{\phi}_1, \tilde{\phi}_2, \tilde{\phi}_3) = (\phi_1^2, \sqrt{2}\phi_1\phi_2, \phi_2^2), \quad (\tilde{\psi}_1, \tilde{\psi}_2, \tilde{\psi}_3) = (\psi_1^2, \sqrt{2}\psi_1\psi_2, \psi_2^2). \tag{63}$$

One can immediately notice that under constraints (63) binary symmetry constraint (40) transforms into the one (53) yielding integrable Hamiltonian systems with variable coefficient symplectic forms. It means that the dynamical system (56) can be reconstructed by the Dirac constraint procedure applied to the Hamiltonian system (25).

Actually, let us impose on the system (44), (45) $2N$ constraints of the following form:

$$\begin{aligned}\varphi_i &= \tilde{\phi}_{2i}^2 - 2\tilde{\phi}_{1i}\tilde{\phi}_{3i}, \quad i = 1, \ldots, N,\\ \varphi_{N+i} &= \tilde{\psi}_{2i}^2 - 2\tilde{\psi}_{1i}\tilde{\psi}_{3i}, \quad i = 1, \ldots, N.\end{aligned} \tag{64}$$

The general theory due to Dirac assures that the modified Poisson structure is defined by

$$\{A,B\}_D = \{A,B\} - \{A,\varphi_i\}G_{ij}^{-1}\{\varphi_j, B\}, \quad G_{ij} = \{\varphi_i, \varphi_j\}, \quad \det G \neq 0, \quad G = (G_{ij}). \tag{65}$$

In the case considered we have

$$\begin{aligned}&\varphi_{N+i} := \overline{\varphi_i}, \quad i = 1, \ldots, N, \quad G = \begin{pmatrix} G^{11} & G^{12} \\ -(G^{12})^T & G^{22}\end{pmatrix},\\ &(G^{11})_{ij} = \{\varphi_i, \varphi_j\} = 0, \quad (G^{22})_{ij} = \{\overline{\varphi_i}, \overline{\varphi_j}\} = 0,\\ &(G^{12})_{ij} = \{\varphi_i, \overline{\varphi_j}\} = \delta_{ij}(\tilde{\phi}_{1j}\tilde{\psi}_{1j} + \tilde{\phi}_{2j}\tilde{\psi}_{2j} + \tilde{\phi}_{3j}\tilde{\psi}_{3j}),\end{aligned} \tag{66}$$

so,

$$\{A,B\}_D = \{A,B\} + \sum_{i=1}^{N}\frac{\{A,\varphi_i\}\{B,\overline{\varphi_i}\} - \{A,\overline{\varphi_i}\}\{B,\varphi_i\}}{(\tilde{\phi}_{1i}\tilde{\psi}_{1i} + \tilde{\phi}_{2i}\tilde{\psi}_{2i} + \tilde{\phi}_{3i}\tilde{\psi}_{3i})}. \tag{67}$$

The Poisson bracket $\{.,.\}_D$ is degenerated, contrary to the canonical one $\{.,.\}$, and has $2N$ Casimir functions $\varphi_i, \overline{\varphi_i}$, $i=1,\ldots,N$. Substituting for A,B the coordinates ϕ, ψ, one gets appropriate matrix elements of the Dirac Poisson tensor D. All nonzero elements are as follows:

$$\{\tilde{\phi}_{1i},\tilde{\psi}_{1i}\}_D=\tilde{\phi}_{1i}\tilde{\psi}_{1i}+\tilde{\phi}_{2i}\tilde{\psi}_{2i},\quad \{\tilde{\phi}_{1i},\tilde{\psi}_{2i}\}_D=\tilde{\phi}_{2i}\tilde{\psi}_{3i},\quad \{\tilde{\phi}_{1i},\tilde{\psi}_{3i}\}_D=-\tilde{\phi}_{1i}\tilde{\psi}_{3i},$$

$$\{\tilde{\phi}_{2i},\tilde{\psi}_{1i}\}_D=\tilde{\phi}_{3i}\tilde{\psi}_{2i},\quad \{\tilde{\phi}_{2i},\tilde{\psi}_{2i}\}_D=\tilde{\phi}_{1i}\tilde{\psi}_{1i}+\tilde{\phi}_{3i}\tilde{\psi}_{3i},\quad \{\tilde{\phi}_{2i},\tilde{\psi}_{3i}\}_D=\tilde{\phi}_{1i}\tilde{\psi}_{2i}, \tag{68}$$

$$\{\tilde{\phi}_{3i},\tilde{\psi}_{1i}\}_D=-\tilde{\phi}_{3i}\tilde{\psi}_{1i},\quad \{\tilde{\phi}_{3i},\tilde{\psi}_{2i}\}_D=\tilde{\phi}_{2i}\tilde{\psi}_{1i},\quad \{\tilde{\phi}_{3i},\tilde{\psi}_{3i}\}_D=\tilde{\phi}_{2i}\tilde{\psi}_{2i}+\tilde{\phi}_{3i}\tilde{\psi}_{3i}.$$

Now, let us perform the following coordinate transformation:

$$\begin{gathered}\phi_{1i}^2=\tilde{\phi}_{1i},\\ \phi_{2i}^2=\tilde{\phi}_{3i},\\ \psi_{1i}^2=\tilde{\psi}_{1i},\\ \psi_{2i}^2=\tilde{\psi}_{3i},\\ c_{1i}=\varphi_i(\tilde{\phi})=\tilde{\phi}_{2i}^2-2\tilde{\phi}_{1i}\tilde{\phi}_{3i},\\ c_{2i}=\overline{\varphi_i}(\tilde{\psi})=\tilde{\psi}_{2i}^2-2\tilde{\psi}_{1i}\tilde{\psi}_{3i},\quad i=1,\ldots,N.\end{gathered} \tag{69}$$

Then, on the symplectic leaf $c_{1i}=c_{2i}=0$, $i=1,\ldots,N$, parametrized by a set of coordinates $(\phi_{1i},\phi_{2i},\psi_{1i},\psi_{2i})_{i=1}^N$, we get the following nonzero elements of a nondegenerated Poisson tensor $\overline{\pi}$:

$$\begin{aligned}\{\phi_{1i},\psi_{1i}\}&=\frac{\phi_{1i}\psi_{1i}+2\phi_{2i}\psi_{2i}}{4(\phi_{1i}\psi_{1i}+\phi_{2i}\psi_{2i})^2},\quad \{\phi_{1i},\psi_{2i}\}=\frac{-\phi_{1i}\psi_{2i}}{4(\phi_{1i}\psi_{1i}+\phi_{2i}\psi_{2i})^2},\\ \{\phi_{2i},\psi_{1i}\}&=\frac{-\phi_{2i}\psi_{1i}}{4(\phi_{1i}\psi_{1i}+\phi_{2i}\psi_{2i})^2},\quad \{\phi_{2i},\psi_{2i}\}=\frac{2\phi_{1i}\psi_{1i}+\phi_{2i}\psi_{2i}}{4(\phi_{1i}\psi_{1i}+\phi_{2i}\psi_{2i})^2}.\end{aligned} \tag{70}$$

Moreover, the transformation (69) with $c_{1i}=c_{2i}=0$ relates

$$\tilde{f}_k=\tilde{\phi}_{1k}\tilde{\psi}_{1k}+\tilde{\phi}_{2k}\tilde{\psi}_{2k}+\tilde{\phi}_{3k}\tilde{\psi}_{3k}\to\overline{f_k}=(\phi_{1k}\psi_{1k}+\phi_{2k}\psi k)^2,\quad k=1,\ldots,N, \tag{71}$$

$$\tilde{F}_n(\tilde{\phi},\tilde{\psi})(49)\to\overline{F}_n(\phi,\psi)(61),\quad n\geqslant 1$$

$$\tilde{H}_n(\tilde{\phi},\tilde{\psi})\to\overline{H}_n(\phi,\psi),\quad n\geqslant 1,$$

where $\tilde{H}_n$ and $\overline{H}_n$ are constructed according to recursion formulas (35) and (36). Hence, Hamiltonian function (45) reduces to the following one:

$$\begin{aligned}\overline{H}_1&=-2(\langle AP_1^2,Q_1^2\rangle-\langle AP_2^2,Q_2^2\rangle)+4(\langle P_1P_2,Q_1^2\rangle+\langle P_2^2,Q_1Q_2\rangle)(\langle P_1P_2,Q_2^2\rangle+\langle P_1^2,Q_1Q_2\rangle)\\ &=-2\sum_{i=1}^N\lambda_i(\phi_{1i}^2\psi_{1i}^2-\phi_{2i}^2\psi_{2i}^2)+4\sum_{i,j=1}^N(\phi_{1i}^2\psi_{1i}\psi_{2i}+\phi_{1i}\phi_{2i}\psi_{2i}^2)(\phi_{1j}\phi_{2j}\psi_{1j}^2+\phi_{2j}^2\psi_{1j}\psi_{2j}),\end{aligned} \tag{72}$$

which is an appropriate Hamiltonian function of the system (56). In the simplest case of $N=1$ (57), the Hamiltonian function and the Poisson tensor are

$$\overline{H}_1=-2\lambda(\phi_1^2\psi_1^2-\phi_2^2\psi_2^2)+4\phi_1\phi_2\psi_1\psi_2(\phi_1\psi_1+\phi_2\psi_2)^2,$$

and

$$\overline{\pi}=\frac{1}{4(\phi_1\psi_1+\phi_2\psi_2)^2}\times\begin{pmatrix}0&0&\phi_1\psi_1+2\phi_2\psi_2&-\phi_1\psi_2\\0&0&-\phi_2\psi_1&2\phi_1\psi_1+\phi_2\psi_2\\-\phi_1\psi_1-2\phi_2\psi_2&\phi_2\psi_1&0&0\\\phi_1\psi_2&-2\phi_1\psi_1-\phi_2\psi_2&0&0\end{pmatrix}. \tag{73}$$

Theorem 1: *The integrals of motion* $(\overline{f}_k,\overline{F}_n)$ *and* $(\overline{f}_k,\overline{H}_n)$ *are in involution with respect to the Poisson bracket (70).*

Proof: The relation $\{\overline{f}_i,\overline{f}_j\}=0$ is obvious as $\overline{\pi}$ does not relate coordinates to different i. Noticing that $\overline{\pi}\nabla\overline{f}_i=(0,\ldots,0,\phi_{1i},\phi_{2i},-\psi_{1i},-\psi_{2i},0,\ldots,0)^T$, one immediately gets

$$\{\overline{F}_n,\overline{f}_i\}=\frac{1}{2}\left(\frac{\partial\overline{F}_n}{\partial\phi_{1i}}\phi_{1i}+\frac{\partial\overline{F}_n}{\partial\phi_{2i}}\phi_{2i}-\frac{\partial\overline{F}_n}{\partial\psi_{1i}}\psi_{1i}-\frac{\partial\overline{F}_n}{\partial\psi_{2i}}\psi_{2i}\right)=0, \tag{74}$$

which follows from the form of $\overline{F}_n$ (61). Therefore, $\{\overline{H}_n,\overline{f}_i\}=0$. According to Noether's theorem, the relation $\{\overline{H}_n,\overline{H}_m\}=0$ is equivalent to commutativity of related vector fields

$$\begin{pmatrix}\vdots\\\phi_{1i}\\\phi_{2i}\\\vdots\\\psi_{1i}\\\psi_{2i}\\\vdots\end{pmatrix}_{t_n}=\overline{V}^{(n)}(\lambda_1,\ldots,\lambda_N;\tilde{u})\begin{pmatrix}\vdots\\\phi_{1i}\\\phi_{2i}\\\vdots\\\psi_{1i}\\\psi_{2i}\\\vdots\end{pmatrix}:=K_{(n)}(\lambda;\tilde{u})=\overline{\pi}\nabla\overline{H}_n, \tag{75}$$

where $\overline{V}^{(n)}(\lambda_1,\ldots,\lambda_N;\tilde{u})=\mathrm{diag}(V^{(n)}(\lambda_1,\tilde{u}),\ldots,V^{*(n)}(\lambda_N,\tilde{u}))$. After simple calculations one gets the following form of the commutator:

$$\begin{aligned}[K_{(n)}(\lambda;\tilde{u}),K_{(m)}(\lambda;\tilde{u})]&=K'_{(n)}(\lambda;\tilde{u})[K_{(m)}(\lambda;\tilde{u})]-K'_{(m)}(\lambda;\tilde{u})[K_{(n)}(\lambda;\tilde{u})]\\&=(\overline{V}^{(n)}_{t_m}-\overline{V}^{(m)}_{t_n}+[\overline{V}^{(n)},\overline{V}^{(m)}])\begin{pmatrix}\vdots\\\phi_{1i}\\\phi_{2i}\\\vdots\\\psi_{1i}\\\psi_{2i}\\\vdots\end{pmatrix},\end{aligned} \tag{76}$$

where $'$ means a Gateaux derivative with respect to the coordinates $(\phi_{1i},\ldots,\psi_{2N})$. The commutator (76) is equal to zero if $\overline{V}^{(n)}_{t_m}-\overline{V}^{(m)}_{t_n}+[\overline{V}^{(n)},\overline{V}^{(m)}]=0$. The last equality holds if

$$V^{(n)}_{t_m}(\lambda_i,\tilde{u})-V^{(m)}_{t_n}(\lambda_i,\tilde{u})+[V^{(n)}(\lambda_i,\tilde{u}),V^{(m)}(\lambda_i,\tilde{u})]=0, \tag{77}$$

$$V^{*(n)}_{t_m}(\lambda_i,\tilde{u})-V^{*(m)}_{t_n}(\lambda_i,\tilde{u})+[V^{*(n)}(\lambda_i,\tilde{u}),V^{*(m)}(\lambda_i,\tilde{u})]=0,$$

for $i=1,\ldots,N$. As the relations (77) are true for arbitrary λ and u, they are also true for particular $\lambda=\lambda_i, u=\tilde{u}(\phi,\psi)$. Finally, $\{\overline{H}_n,\overline{H}_m\}=0$ and thus $\{\overline{F}_n,\overline{F}_m\}=0$. The proof is finished.

Theorem 2: *The functions* $\overline{f}_i$, $i=1,\ldots,N$, *and* $\overline{F}_n, n=1,\ldots,N$, *are functionally independent over some region of* R^{4N}.

Proof: We use the method established in Ref. 20. Let P_0 be a point of R^{4N} satisfying

$$\psi_{ik}=\varepsilon,\quad k=1,\ldots,N,\quad i=1,2. \tag{78}$$

At P_0 we have

$$\begin{aligned}\frac{\partial\overline{f}_k}{\partial\phi_{ij}}&=2\varepsilon^2(\phi_{1j}+\phi_{2j})\phi_{ij}\delta_{kj},\\ \frac{\partial\overline{F}_k}{\partial\phi_{ij}}&=-4\varepsilon^2\lambda_j^{k-1}\phi_{ij}+O(\varepsilon^4),\quad i=1,2,\ k,j=1,\ldots,N.\end{aligned} \tag{79}$$

Then, at the point P_0, the Jacobian of the functions $\overline{f}_k$, $\overline{F}_k$, $k=1,\ldots,N$, with respect to ϕ_{ij} can be calculated as follows

$$\begin{aligned}&\left|\frac{\partial(\overline{f}_1,\ldots,\overline{f}_N,\overline{F}_1,\ldots,\overline{F}_N)}{\partial(\phi_{11},\phi_{21},\ldots,\phi_{1N},\phi_{2N})}\right|\\ &\quad=-4\varepsilon^{4N}\\ &\quad\times\begin{vmatrix}-\frac{1}{2}(\phi_{11}+\phi_{21}) & 0 & 0 & \ldots & \ldots & 0\\ 0 & -\frac{1}{2}(\phi_{12}+\phi_{22}) & 0 & \ldots & \ldots & 0\\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots\\ 0 & 0 & 0 & \ldots & 0 & -\frac{1}{2}(\phi_{1N}+\phi_{2N})\\ \phi_{11} & \phi_{21} & \ldots & \ldots & \phi_{1N} & \phi_{2N}\\ \lambda_1\phi_{11} & \lambda_1\phi_{21} & \ldots & \ldots & \lambda_N\phi_{1N} & \lambda_N\phi_{2N}\\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots\\ \lambda_1^{N-1}\phi_{11} & \lambda_1^{N-1}\phi_{21} & & & \lambda_N^{N-1}\phi_{1N} & \lambda_N^{N-1}\phi_{2N}\end{vmatrix}\\ &\quad+O(\varepsilon^{4N+2})=-4\varepsilon^{4N}\left(-\frac{1}{2}\right)^N\prod_{k,l=1,k>l}^{N}(\lambda_k-\lambda_l)\prod_{j=1}^{N}(\phi_{1j}^2-\phi_{2j}^2)+O(\varepsilon^{4N+2}).\end{aligned} \tag{80}$$

In the evaluation of the determinant we first subtracted from the $2r-1$ column the $2r$ one for $r=1,\ldots,N$. Hence we conclude that if the $\lambda_1,\ldots,\lambda_N$ are distinct, the above Jacobian is not identically equal to zero and additionally is a polynomial function of ϕ_{ij}, therefore, the functions $\overline{f}_k$, $\overline{F}_k$, $k=1,\ldots,N$, are functionally independent at least over some dense open subset of R^{4N}. The proof is finished.

So, finally, we can summarize our results in the following way.

Theorem 3: *The binary constrained spatial system (56) is a Liouville integrable Hamiltonian system*

$$\begin{pmatrix} Q_1 \\ Q_2 \\ P_1 \\ P_2 \end{pmatrix}_x = \overline{\pi}\nabla\overline{H}_1, \tag{81}$$

with a Poisson structure given by (70) and a Hamiltonian function

$$\begin{aligned}\overline{H}_1 &= -2(\langle AP_1^2, Q_1^2\rangle - \langle AP_2^2, Q_2^2\rangle) + 4(\langle P_1P_2, Q_1^2\rangle + \langle P_2^2, Q_1Q_2\rangle)(\langle P_1P_2, Q_2^2\rangle + \langle P_1^2, Q_1Q_2\rangle) \\ &= \overline{F}_2 - \frac{1}{4}\overline{F}_1^2.\end{aligned} \tag{82}$$

Moreover, the system (81) has $2N$ *functionally independent and involutive integrals of motion* $\overline{f}_i$, $i=1,\ldots,N$, *and* $\overline{F}_n$, $n=1,\ldots,N$, *defined by (61) and (71).*

Let us mention that all other binary constrained temporal systems

$$\begin{aligned}\begin{pmatrix} \phi_{1j} \\ \phi_{2j} \end{pmatrix}_{t_n} &= V^{(n)}(\tilde{u},\lambda_j)\begin{pmatrix} \phi_{1j} \\ \phi_{2j} \end{pmatrix}, \quad j=1,\ldots,N, \\ \begin{pmatrix} \psi_{1j} \\ \psi_{2j} \end{pmatrix}_{t_n} &= -(V^{(n)})^T(\tilde{u},\lambda_j)\begin{pmatrix} \psi_{1j} \\ \psi_{2j} \end{pmatrix}, \quad j=1,\ldots,N,\end{aligned} \tag{83}$$

form a family of Hamiltonian systems with the Poisson tensor (70) and the corresponding Hamiltonian functions $\overline{H}_n$ expressible through $\overline{F}_m$. For example, $\overline{H}_2 = \overline{F}_3 - \frac{1}{2}\overline{F}_1\overline{F}_2 + \frac{1}{8}\overline{F}_1^3$.

V. CONCLUDING REMARKS

In this article we have established the Liouville integrability of a factorization of the AKNS field systems of PDEs into pairs of systems of ODEs, presented in Ref. 29. In other words, it has been shown that in a natural set of coordinates, i.e., eigenfunctions of a spectral problem, the resulting binary constrained flows defined by (56) are Liouville integrable Hamiltonian systems with variable coefficient symplectic forms. The results also provide an amendment to the answer of the question posed in Ref. 29.

The method applied suggests the existence of similar factorizations for other soliton hierarchies. However, in order to find explicit solutions of the AKNS field systems, a transformation from the set of eigenfunctions to the set of separated coordinates has to be found. This work is in progress and it will be prepared for a separate paper.

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Bruhat Poisson structure on $\mathbb{CP}^n$ and integrable systems

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In this note we present a simple formula for the Bruhat Poisson structure on complex projective spaces in terms of the momentum coordinates. We also give a simple description of a family of functions in involution on compact Hermitian symmetric spaces obtained via the bi-Hamiltonian approach using the Bruhat Poisson structure and an invariant symplectic structure. We compute these functions explicitly on $\mathbb{CP}^n$ and relate them to the Gelfand–Tsetlin coordinates. We also show how the Lenard scheme can be applied. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1477261]

I. INTRODUCTION

Let K be a compact real form of a complex semi-simple Lie group G and let $H\subset K$ be a subgroup of K defined by $H=K\cap P$, where P is a parabolic subgroup of G containing a Borel subgroup $B\subset G$. The Bruhat Poisson structure π_∞ on $X=K/H$ is constructed from a classical dynamical r-matrix and has its origin from quantum groups. It was first introduced by Lu–Weinstein[1] and Soibelman,[2] and has the property that its symplectic leaves are precisely the Bruhat cells in X. If $T=K\cap B$, a maximal torus of K, then π_∞ is T-invariant. When $X=\mathbb{CP}^n$, we use the momentum map coordinates $(x_1,\ldots,x_n)$ and the corresponding angular coordinates $(\phi_1,\ldots,\phi_n)$ to show that π_∞ is given by

$$\pi_\infty=\sum_{i=1}^{n}\Theta_i\wedge\partial_{\phi_i},$$

where

$$\Theta_i=(x_1+\cdots+x_i-1)\partial_{x_i}+\sum_{j=i+1}^{n}x_j\partial_{x_j}.$$

Let ω_s (respectively, π_s) stand for a K-invariant symplectic form (respectively, its dual bi-vector field) on X. When X is a Hermitian symmetric space, Khoroshkin, Radul, and Rubtsov[3] proved that the two Poisson structures, π_∞ and π_s form a Poisson pair, meaning that the Schouten bracket of π_∞ and π_s vanishes, $[\pi_\infty,\pi_s]=0$. In particular, any bi-vector field of the form $\alpha\pi_\infty+\beta\pi_s$, $(\alpha,\beta)\in\mathbb{R}^2$, is Poisson. In this situation, one can take $\alpha=\beta=1$ and introduce the following family $\{\sigma_k\}$ of functions:

$$\sigma_k:=((\pi_s+\pi_\infty)^{\wedge k},\omega_s^{\wedge k}),$$

obtained by the duality pairing of exterior powers of ω and $\pi_\infty+\pi_s$. If the (real) dimension of X is equal to $2n$, then we have n functions: $\sigma_1,\ldots,\sigma_n$, which may carry useful information about X. These functions are in involution with respect to either of the two Poisson structures and are related to the fundamental weights for the Lie algebra $\mathfrak{sl}(n+1,\mathbb{C})$. We show that on $\mathbb{CP}^n$ the functions that we have obtained are constant multiples of the elementary symmetric polynomials

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in the Gelfand–Tsetlin variables studied by Guillemin and Sternberg.[4] These variables define completely integrable systems on coadjoint orbits of the unitary group. In a subsequent publication we show that this statement extends to the complex Grassmannians as well as other Hermitian symmetric spaces. In the last part of the paper we make explicit computations using the Lenard scheme.[5]

II. BRUHAT POISSON STRUCTURE ON $\mathbb{CP}^n$

We recall the Bruhat Poisson structure and its properties.[1] Let K be a compact semi-simple Lie group with Lie algebra $\mathfrak{k}$, G a complexification of K with Lie algebra $\mathfrak{g}$, and $T\subset K$ a maximal torus with Lie algebra $\mathfrak{t}$. The complexification $\mathfrak{h}$ of $\mathfrak{t}$ is a Cartan in $\mathfrak{g}$. Let Δ be the set of all roots of $\mathfrak{g}$ with respect to $\mathfrak{h}$. We choose $\Delta^+\subset\Delta$ a subset of positive roots. Let $\langle,\rangle$ be the Killing form of $\mathfrak{g}$ and let H_α be the image of $\alpha\in\Delta$ under the isomorphism $\mathfrak{h}^*\to\mathfrak{h}$ which is defined by $\langle,\rangle$. For each $\alpha\in\Delta^+$ choose a root vector E_α such that $\langle E_\alpha,\theta E_\alpha\rangle=-1$, where θ is the complex conjugation on $\mathfrak{g}$ defined by $\mathfrak{k}$. Then $E_{-\alpha}:=-\theta E_\alpha$ is a root vector for $-\alpha$. Let $X_\alpha,Y_\alpha\in\mathfrak{k}$ be given by $X_\alpha=E_\alpha-E_{-\alpha}$ and $Y_\alpha=\sqrt{-1}(E_\alpha+E_{-\alpha})$. We set:

$$\Lambda=\sum_{\alpha>0}X_\alpha\wedge Y_\alpha\in\mathfrak{k}\wedge\mathfrak{k}.$$

Let Λ^l and Λ^r be the left and right invariant bivector fields on K with their value at identity equal to Λ. Then $\pi_K=\Lambda^l-\Lambda^r$ becomes a Poisson structure on K, making it into a Poisson Lie group. Let $H\subset K$ be a subgroup of K given by the intersection of K with a parabolic subgroup of G containing the Borel determined by Δ^+. There is a unique Poisson structure on $X=K/H$, denoted by π_∞ such that the natural projection $(K,\pi_K)\to(X,\pi_\infty)$ is a Poisson map. The space (X,π_∞) is a (K,π_K)-homogeneous Poisson manifold, and the symplectic leaves of π_∞ on X are precisely the Bruhat cells.

When $K=\mathrm{SU}(n+1)$, an obvious choice of H yields $X=\mathbb{CP}^n$, the complex projective space of (complex) dimension n. Let $[Z_0:Z_1:\cdots:Z_n]$ be a homogeneous coordinate system on X. We use the standard Fubini-Study form ω for the invariant symplectic form ω_s and the following description of π_∞ obtained by Lu.[6] First, we need Lu's coordinates on the largest Bruhat cell, where $Z_0\neq 0$ and we let $z_i=Z_i/Z_0$:

$$y_i:=\frac{z_i}{\sqrt{1+|z_{i+1}|^2+\cdots+|z_n|^2}},\quad 1\leqslant i\leqslant n.$$

Lu's coordinates are not holomorphic, but convenient for the Bruhat Poisson structure, which now assumes the following form:

$$\pi_\infty=\sqrt{-1}\sum_{i=1}^{n}(1+|y_i|^2)\partial_{y_i}\wedge\partial_{\overline{y_i}}.$$

In order to be able to compute with ω and π_∞, we need to move to the polar variables r_i,ϕ_j defined by $z_i=r_ie^{\sqrt{-1}\phi_i}$ and eventually to the momentum map variables x_i,ϕ_j, where x_i is defined by

$$x_i=\frac{r_i^2}{1+r_1^2+\cdots r_n^2}.$$

The functions x_i's are globally defined on $\mathbb{CP}^n$, and if one identifies $\mathbb{R}^n$ with $\mathfrak{t}^*$, then these functions define the momentum map associated with the T-action on $\mathbb{CP}^n$. One of the advantages of using the coordinates $\{x_1,\ldots,x_n\}$ is that the Fubini–Study symplectic structure and the corresponding bi-vector field have the following simple form:

$$\omega=\sum_{i=1}^{n} \mathrm{d}x_i\wedge \mathrm{d}\phi_i, \quad \pi_s=\sum_{i=1}^{n} \partial_{x_i}\wedge\partial_{\phi_i}.$$

In fact, the simplest form for the Bruhat Poisson structure is also achieved in this coordinate system.

Proposition 2.1: The Bruhat Poisson structure π_∞ on $\mathbb{CP}^n$ can be written in the coordinate system (x_j,ϕ_i) as follows:

$$\pi_\infty=\sum_{i=1}^{n} \Theta_i\wedge\partial_{\phi_i},$$

where

$$\Theta_i=(x_1+\cdots+x_i-1)\partial_{x_i}+\sum_{j=i+1}^{n} x_j\partial_{x_j}.$$

Proof: The proof of this statement is purely computational. One can introduce auxiliary variables $q_i=\log(1+|y_i|^2)$, and use these to write

$$\pi_\infty=-\sum_{i=1}^{n} \partial_{q_i}\wedge\partial_{\phi_i},$$

the action-angle form for π_∞. Eventually, one can establish the following relations: $x_1=1-e^{-q_1}$, and for $j>1$,

$$x_j=e^{-(q_1+\cdots+q_{j-1})}-e^{-(q_1+\cdots+q_j)}.$$

The rest is straightforward. □

Notice that if we take the sum $\pi_\infty+\pi_s$, the -1 in the above-given formula will disappear.

III. FAMILIES OF FUNCTIONS IN INVOLUTION

Multi-Hamiltonian structures are very important in the theory of integrable systems. Starting with the fundamental works of Magri,[5] they found many interesting and fundamental applications, as in Refs. 7–10, and references therein. We say that two Poisson structures π_0 and π_1 form a *Poisson pair* if their Schouten bracket equals zero: $[\pi_0,\pi_1]=0$. This is equivalent to the condition that for any $\alpha,\beta\in\mathbb{R}$ the bi-vector field $\alpha\pi_0+\beta\pi_1$ is also Poisson. We refer to such family $\alpha\pi_0+\beta\pi_1$ as a *Poisson pencil*.

Let M be a manifold and let π_b and π_s be two Poisson structures on M such that:

(1) The Poisson structure π_s is nondegenerate (so the subscript s stands for symplectic).
(2) The Poisson structures π_s and π_b form a Poisson pair.

If $\dim(M)=2n$, then we can define n functions $\sigma_1,\ \ldots,\ \sigma_n$ as follows:

$$\sigma_j=\frac{\pi_b^j\wedge\pi_s^{n-j}}{\pi_s^n}.$$

The operation of division by the top degree bi-vector field makes perfect sense, since π_s is nondegenerate, and thus in any local coordinate system $(x_1,\ \ldots\ x_{2n})$ the $2n$-vector field π_s^n looks like

$$\pi_s^n=h(x_1,\ldots,x_{2n})\partial_{x_1}\wedge\cdots\wedge\partial_{x_{2n}},$$

for a nonvanishing function $(hx_1, \ldots, x_{2n})$. For an equivalent definition, which only differs by a constant multiple, one can use the symplectic form ω_s dual to π_s, then one can define

$$\sigma_k=(\pi_b^{\wedge k},\omega_s^{\wedge k}),$$

where we use the duality pairing

$$\Gamma(M,\wedge^{2k}TM)\otimes\Gamma(M,\wedge^{2k}T^*M)\to C^\infty(M).$$

It turns out that this family of functions has the following property.

Proposition 3.1: The family of functions σ_i defined previously are in involution with respect to either Poisson structure, π_b or π_s.

Proof: (J.-H. Lu) Let $X_j=i_{d\sigma_j}\pi_b$ and let $Y_j=i_{d\sigma_j}\pi_s$. Then we have: $[X_j,\pi_s]=-[Y_j,\pi_b]$, $[X_j,\pi_b]=0$, and $[Y_j,\pi_s]=0$. Consider the equality $\sigma_k\pi_s^n=\pi_b^k\wedge\pi_s^{n-k}$ and compute L_{X_l} of both sides to arrive at the following identity:

$$\frac{n-k}{k+1}\{\sigma_{k+1},\sigma_l\}_s=-\{\sigma_k,\sigma_l\}_b+n\sigma_k\{\sigma_1,\sigma_l\}_s,$$

where the subscripts s and b indicate the Poisson structure with respect to which the Poisson bracket is taken. Finally, use the induction on l. □

Remark: The approach that we have followed here is intimately related to the Poisson–Nijenhuis structures, which were studied by Magri and Morosi,[11] Kosmann-Schwarzbach and Magri,[7] Vaisman,[8] and others. The set of our functions $\{\sigma_j\}$ can be expressed, polynomially, through the traces of powers of the intertwining operator corresponding to the Nijenhuis tensor.

Now let us take $M=X$ to be a coadjoint orbit in $\mathfrak{k}^*$, which we assume to be a compact Hermitian symmetric space. Let $\pi_s=\pi$ be the Kirillov–Kostant–Souriau symplectic structure and $\pi_b=\pi_\infty$ the Bruhat Poisson structure, which is obtained via an identification of X with $K/(P\cap K)$ as in Sec. I. Under this identification, π is K-invariant. The following was first proved in Ref. 3, and we offer a shorter proof due to Lu:

Proposition 3.2: If X is a Hermitian symmetric space as previously, then the Poisson structures π_s and π_∞ form a Poisson pair.

Proof: If (K,π_K) is a connected Poisson–Lie group, and (X,π_X) is a (K,π_K) Poisson homogeneous space, then for any $Y\in\mathfrak{k}$,

$$L_{\kappa(Y)}\pi_X=\kappa(\delta(Y)),$$

where $\kappa:\mathfrak{k}\to\Gamma(TX)$ is the infinitesimal action map, extended to $\kappa:\wedge^2\mathfrak{k}\to\Gamma(\wedge^2TX)$ and $\delta:\mathfrak{k}\to\wedge^2\mathfrak{k}$ is the cocycle defining π_K. Indeed, by definition of the Poisson homogeneous space,

$$\pi_X(kx)=k_*\pi_X(x)+x_*\pi_K(k),$$

where

$$k:X\to X,\ \ k(x)=k\cdot x,\quad \text{and } x:K\to X,\ \ x(k)=k\cdot x$$

are the action and the evaluation maps, respectively. Since K acts by diffeomorphisms, we can define

$$k^*(\pi_X)(x):=k_*\pi_X(k^{-1}(x)).$$

Then we see that

$$k^*(\pi_X)(x)=k_*(k_*^{-1}\pi_X(x)+x_*\pi_K(k^{-1}))=\pi_X(x)+x_*(l_{k*}\pi_K(k^{-1})),$$

where l_k is the left translation on K. Now we set $k=\exp(tY)$ and compute $\mathrm{d}/\mathrm{d}t_{|t=0}$ of both sides to conclude that

$$L_{\kappa(Y)}\pi_X(x)=\kappa(\delta(Y))(x),$$

where

$$\delta(Y)=\frac{\mathrm{d}}{\mathrm{d}t}_{|t=0} l_{\exp(tY)}\pi_K(\exp(-tY))\in\wedge^2\mathfrak{k}$$

is the Lie algebra cocycle which determines π_K.

Now since π_s is K-invariant, we can compute that for any $Y\in\mathfrak{k}$:

$$L_{\kappa(Y)}[\pi_\infty,\pi_s]=[L_{\kappa(Y)}\pi_\infty,\pi_s]+[\pi_\infty,L_{\kappa(Y)}\pi_s]=[\kappa(\delta(Y)),\pi_s]+[\pi_\infty,0]=0,$$

since $\kappa(\delta(Y))$ is the sum of wedges of generating vector fields for the K-action. This shows that $[\pi_\infty,\pi_s]$ is an invariant three-vector field.

Now we notice that in the case when $X=G/P$ is a Hermitian symmetric space, the nilradical of P is Abelian, and therefore each K-invariant nonzero differential form is closed and not exact. We also know that $H^3(X)=0$, and thus there is no nonzero K-invariant three-forms on X. Thus there is no nonzero K-invariant three-vector field on X, which implies that $[\pi_s,\pi_\infty]=0$.

Thus we have proven that π_∞ and π_s commute with respect to the Schouten bracket, and hence form a Poisson pair. □

Therefore, we have the following:

Proposition 3.3: Let X be a coadjoint orbit of K. Assume that X is a Hermitian symmetric space of complex dimension n. The above-mentioned recipe yields n functions $(\sigma_1,\ \ldots,\ \sigma_n)$ *on X, which are in involution with respect to either π_∞ or π_s.*

Now let us return to the case of $X=\mathbb{CP}^n$ with the commuting Poisson structures π_s and π_∞ introduced in Sec. II. Let us introduce the following linear change of variables on $\mathbb{R}^n$:

$$c_k=x_1+\cdots+x_k.$$

In these variables, we can easily compute the desired functions as follows:

Theorem 3.4: *The functions $\{\sigma_i\}$, $1\leqslant i\leqslant n$ on $\mathbb{CP}^n$ defined by*:

$$\sigma_i=(\omega^{\wedge i},(\pi_s+\pi_\infty)^{\wedge i}),$$

up to constant multiples, are equal to the elementary symmetric polynomials in $(c_1,\ \ldots,\ c_n)$:

$$\sigma_j=\sum_{i_1<\cdots<i_j} c_{i_1}\cdots c_{i_j}.$$

Proof: The simple linear and triagonal form of $\pi_\infty+\pi_s$ makes the computation of the functions $\{\sigma_i\}$ straightforward. □

The explicit nature of these integrals is essential in looking at the relation with the certain natural flows. So, in particular we see that

$$\sigma_1=c_1+\cdots+c_n$$

and that the Hamiltonian σ_1 in terms of the momentum map variables is given by

$$\sigma_1=nx_1+(n-1)x_2+\cdots+2x_{n-1}+x_n.$$

Then the gradient of this function in the momentum simplex has coordinates $\lambda_i=n+1-i$. If we treat these numbers as weights assigned to the vertices of the moment polytope, which correspond

to the centers of the Bruhat cells, we see the clear correspondence between these numbers and the complex dimensions of the corresponding cells. Besides, we see that the functions $\{c_i\}$ are linearly independent and satisfy $c_i - c_{i-1} = x_i$, so we conclude that:

Theorem 3.5: *The functions $\{\sigma_i\}$ are generically linearly independent on $\mathbb{CP}^n$. They Poisson commute with respect to either π_s or π_∞. The corresponding common level sets coincide with those for the standard torus action on $\mathbb{CP}^n$. The value of σ_1 at the center of a Bruhat cell equals n minus the complex dimension of that cell.*

Remark: For any compact semi-simple Lie algebra $\mathfrak{k}$ of rank l, there are l distinguished linear functions on $\mathfrak{k}^*$ defined by the fundamental weights for $\mathfrak{g} = \mathfrak{k} \otimes \mathbb{C}$. Namely, let $p: \mathfrak{k}^* \to \mathfrak{t}^*$ be the projection dual to the inclusion $\mathfrak{t} \hookrightarrow \mathfrak{k}$. The restriction of p to any co-adjoint orbit X in $\mathfrak{k}^*$ is a momentum map for the T-action on X. If we regard the l fundamental weights for $\mathfrak{g}$ as linear functions on $\mathfrak{t}^*$, then their pull-backs by p^* composed with the restriction to X define l functions on X. For $k = \mathfrak{su}(n+1)$ these functions are exactly $c_1, \ldots, c_n$.

Remark: The function σ_1 has another application. The gradient flow with respect to σ_1 on $\mathbb{CP}^n$ is just the Toda flow as explained, e.g., in Ref. 12.

The functions $(\sigma_1, \ldots, \sigma_n)$ that we have constructed turn out to be related to the Gelfan–Tsetlin coordinates in the case when $K = \mathrm{SU}(n)$, as we will see later on. In Sec. IV we will carry explicit computations of these functions on the projective spaces.

IV. RELATION WITH GELFAND–TSETLIN

When $X = \mathrm{Gr}(k)$—the Grassmannian of k-planes in $\mathbb{C}^{n+1}$, we have obtained $k(n-k+1)$ functions in involution on X. Let us recall the standard embedding

$$\Psi: F_n \hookrightarrow \mathrm{Gr}(1) \times \cdots \times \mathrm{Gr}(n),$$

where F_n is the manifold of full flags in $\mathbb{C}^{n+1}$, and the locus of the embedding is given by the incidence relations. This embedding respects the KKS Kähler structures on the manifolds involved, if we would like to view them as coadjoint orbits in $\mathfrak{k}^*$. Moreover, this embedding is equivariant with respect to the $K = \mathrm{SU}(n+1)$-action. For convenience we identify the dual of the unitary Lie algebra $\mathfrak{u}_k$ with the space of $k \times k$ complex Hermitian matrices using $-\sqrt{-1}\,\mathrm{Tr}(AB)$ as the pairing.

Recall the Gelfan–Tsetlin system on F_n. We fix the orbit type of F_n, i.e., we fix the eigenvalues λ_i of a complex Hermitian matrix A and order them, so $\lambda_1 > \lambda_2 > \cdots > \lambda_{n+1}$. For convenience and easier visualization, we will assume that $\lambda_{n+1} = 0$ (so all the eigenvalues are non-negative), which corresponds to taking $A \in \mathfrak{u}^*_{n+1}$ rather than in $\mathfrak{su}^*_{n+1}$. The Gelfand–Tsetlin system looks like:[4,13]

$$\begin{array}{c}
\lambda_1 > \lambda_2 > \cdots > \lambda_n > 0 \\
\mu_1^{(n)} \geqslant \mu_2^{(n)} \geqslant \cdots \geqslant \mu_n^{(n)} \\
\cdots \quad \cdots \quad \cdots \\
\mu_1^{(2)} \geqslant \mu_2^{(2)} \\
\mu_1^{(1)},
\end{array}$$

where in the ith row are the eigenvalues of the image $p_i(A)$ of the projection $p_i: \mathfrak{u}^*_{n+1} \to \mathfrak{u}^*_{n+2-i}$, which is dual to the embedding $U(n+2-i) \hookrightarrow U(n+1)$ as the left upper corner submatrix. The eigenvalues μ_i^j together with λ_i's satisfy the interlacing property:

$$\mu_i^{(j)} \geqslant \mu_i^{(j-1)} \geqslant \mu_{i+1}^{(j)}, \qquad \lambda_i \geqslant \mu_i^{(n)} \geqslant \lambda_{i+1}, \qquad \mu_n^{(n)} > 0.$$

The above-given picture can be adapted to any orbit, in particular to $\mathrm{Gr}(k)$, where we would take $\lambda_1=\cdots=\lambda_k>0$, and other λ's equal to zero. When k varies from 1 to n, the above-mentioned picture acquires more and more nonzero elements. At each step, while going from level k to $k+1$, we will get new integrals on $\mathrm{Gr}(k+1)$, which we can pull back to F_n using Ψ.

We also notice that if $\rho\in\sqrt{-1}\cdot\mathfrak{t}$ is given by $2\rho=\Sigma_{\alpha>0}\alpha$, then it is easy to see that the sum of all $\mu_i^{(j)}$'s is equal to the value of the momentum map for the diagonal torus action evaluated in the direction of ρ.

Our goal is to relate the integrals σ_j which we obtained in Sec. III using the bi-Hamiltonian approach on Hermitian symmetric spaces, and the Gelfand–Tsetlin coordinates for $X=\mathbb{CP}^n$.

Let B be the $(n+1)\times(n+1)$ matrix, representing an element of $\mathfrak{u}(n+1)^*$ such that the only nonzero element of B is λ, located in the very left upper place. The coadjoint orbit $\mathcal{O}_B$ of B is isomorphic to $\mathbb{CP}^n$, where the identification goes as follows. Any element in the coadjoint orbit of B can be viewed as ABA^{-1}, where $A\in U(n+1)$. Let (a_{ij}) be the entries of A. Then the identification

$$w:\ \mathcal{O}_B\to\mathbb{CP}^n$$

is given by

$$w(ABA^{-1})=[a_{11}:a_{21}:\cdots:a_{n+1,1}],$$

in terms of a homogeneous coordinate system $[Z_0:\cdots:Z_n]$ on $\mathbb{CP}^n$. We suspect that the following is well-known, and in any case, is not hard to compute, that the Gelfand–Tsetlin coordinates are:

$$\mu_r^{(k)}=0 \quad \text{for } r\neq 1,$$

$$\mu_1^{(k)}=\lambda(x_1+\cdots+x_k),$$

where $(x_1,\ldots,x_n)$ are the momentum map coordinates that we used in Sec. III. We arrive at the conclusion that the Gelfand–Tsetlin coordinates $\{\mu_1^{(k)}\}$ coincide (up to the multiple of λ, which we can assume equals one) with the coordinates $\{c_k\}$ introduced in Sec. III. Now, it remains to notice that our Theorem 3.4 from Sec. III immediately yields:

Theorem 4.1: *The complete family of integrals in involution $\{\sigma_i\}$ on $\mathbb{CP}^n$ obtained using the bi-Hamiltonian approach with respect to the Bruhat Poisson structure and an invariant symplectic structure are expressed by the elementary polynomials in the Gelfand–Tsetlin coordinates.*

We prove a similar result for other Hermitian symmetric spaces in a forthcoming paper.

V. COMPARISON TO THE LENARD SCHEME

Recall the following result.[5] If $\alpha\pi_0+\beta\pi_1$ is a Poisson pencil on a manifold M, and V a vector field, preserving this pencil, then there exists a sequence of smooth functions $\{g_i\}$ on M, such that g_1 is the Hamiltonian of V with respect to π_0 and the vector field of the π_0-Hamiltonian g_j is the same as the vector field of the π_1-Hamiltonian g_{j+1}:

$$i_{dg_j}\pi_0=i_{dg_{j+1}}\pi_1.$$

Moreover, the functions in the family $\{g_j\}$ are in involution with respect to both π_0 and π_1.

Our goal in this section is to show that if we start with $M=\mathbb{CP}^n$, and take the pencil (π_s,π_∞) as before, then there is a natural choice of V on $\mathbb{CP}^n$ leading to a completely integrable systems, and the integrals $\{g_j\}$ in question can be easily expressed in terms of the coordinates $(c_1,\ldots,c_n)$ that we introduced in Sec. III.

It is a matter of a simple computation that if we start with a Hamiltonian $g_1=a_1x_1+\cdots+a_nx_n$, where $(x_1,\ldots,x_n)$ are the momentum map coordinates as before, then on the big cell the corresponding initial vector field V is given by

$$V=i_{dg_1}\pi_\infty=\sum_j\ [a_j(x_1+\cdots x_j)+a_{j+1}x_{j+1}+\cdots+a_nx_n]\partial_{\phi_j}.$$

From this, one can compute

$$g_2=\sum_j\ \frac{a_j}{2}x_j^2+\sum_{l<k}\ a_kx_lx_k,$$

etc. An interesting choice for g_1 turns out to be

$$g_1=c_1+\cdots+c_n=nx_1+(n-1)x_2+\cdots+x_n,$$

which coincides with σ_1 from Sec. III. The reason for this choice is:

Proposition 5.1: The Lenard scheme associated with the Poisson pencil $(\pi_\infty,\ \pi_s)$ on $\mathbb{CP}^n$ *which starts with* $g_1=c_1+\cdots+c_n$ *and*

$$V=\sum_j\ [(n-j+1)(x_1+\cdots+x_j)+(n-j)x_{j+1}+\cdots+2x_{n-1}+x_n]\partial_{\phi_j},$$

yields

$$g_k=c_1^k+c_2^k+\cdots+c_n^k,$$

which determines a completely integrable bi-Hamiltonian system on $\mathbb{CP}^n$.

Proof: With all the explicit formulas that we have presented in this paper, the proof is a simple computation. □

We should remark that the constants $(a_1,\ldots,a_n)$ for the first Hamiltonian in the Lenard scheme have to be chosen with care for two reasons. First, the computations are not simple for an arbitrary choice. Second, as the next example shows, we do not always arrive at a completely integrable system.

Example. If one takes $g_1=x_1+\cdots+x_n$, and $V=\Sigma_j(x_1+\cdots+x_n)\partial_{\phi_j}$, then applying the above-mentioned scheme, one would obtain

$$g_k=(x_1+\cdots+x_n)^k=(g_1)^k.$$

The differentials of all functions in this family are clearly linearly dependent.

Remark: In fact, it was shown in Ref. 7 that in the Poisson–Nijenhuis situation the traces of the powers of the intertwining operator do satisfy the Lenard recursion relations. And, in fact, it is easy to see that in our situation for $X=\mathbb{CP}^n$, equipped with π_∞, and ω_s, the trace of the operator itself is a multiple of $c_1+\cdots+c_n$. However, the computations for the higher powers seem more complicated.

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The coupled modified Korteweg–de Vries equations: Similarity reduction, Lie–Bäcklund symmetries and integrability

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The Lie point symmetries of N-coupled modified Korteweg–de Vries equations (N-$cmKdV$) is derived and shown that the similarity reduction associated with symmetries passes the Painlevé property indicating its integrability. The nonclassical symmetry analysis of Bluman and Cole and the direct method of Clarkson and Kruskal to N-$cmKdV$ equations show that there exists no new similarity reductions. A sequence of Lie–Bäcklund symmetries for N-$cmKdV$ equations is derived explicitly, establishing its complete integrability. The question of constructing the recursion operator of N-$cmKdV$, a characteristic of integrable systems, is also discussed. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1473219]

I. INTRODUCTION

One of the most remarkable achievements in mathematics in the second half of the twentieth century is the discovery of solitons or integrable systems governed by nonlinear partial differential equations (PDEs).[1,2] The discovery of solitons exhibited by a particular class of wave equations has generated much interest to investigate different mathematical and physical aspects of nonlinear PDEs, both $(1+1)$ and higher dimensions, during the past few decades or so. It was found that these integrable nonlinear partial differential equations have rich mathematical structures with surprising features. For example, it possesses infinitely many Lie–Bäcklund (or nonpoint or generalized) symmetries, infinitely many integrals of motion (if the model is conservative), Bäcklund transformations, bilinear or trilinear structure equations, the Painlevé property (after perhaps a suitable change of variables), recursion operator, hereditary operator, master symmetries, etc.[1–7] Analytical techniques from Lie theory, group theory, differential geometry, etc., have been used in connection with these properties.[3,7–12] Among them, the Lie symmetry analysis originally advocated by Sophus Lie and later on developed by Ovsiannikov[13] and others[8,9,14] provides an effective and algorithmic technique to investigate mathematical aspects starting from finding an exact solution to deriving Kac–Moody algebras of nonlinear PDEs. The applicability of this algorithmic method has been widely illustrated to several nonlinear PDEs in different contexts.[15–17] It is well known that if a nonlinear PDE admits infinitely many Lie–Bäcklund or generalized symmetries, then it is expected to be integrable.[3] If the Lie–Bäcklund symmetries of a given nonlinear PDE are explicitly known, then it is quite often possible to construct the so called recursion and hereditary operator.[18] It is widely believed that the existence of recursion operator helps one to construct the Hamiltonian operators, if they exist, enabling one to check whether a given nonlinear PDE is a bi-Hamiltonian or tri-Hamiltonian system or not. Another systematic approach to investigate the integrability nature of nonlinear PDEs, using the symmetry consideration, is due to Shabat and his school.[11,12] In this approach, requiring the existence of a small number of symmetries (conservation laws) yields large classes of integrable nonlinear PDEs. It is well known that several scalar integrable nonlinear PDEs of $(1+1)$ dimension admit a sequence of Lie–Bäcklund symmetries.

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However, the existence of a sequence of Lie–Bäcklund symmetries for the coupled or multicomponent integrable nonlinear PDEs has not been investigated so far, perhaps except for two coupled Korteweg–de Vries equations. In this article, we consider a system of N-coupled modified Korteweg–de Vries (N-$cmKdV$) equations

$$\frac{\partial U^i}{\partial t}+6\left(\sum_{j=1}^{N}(U^j)^2\right)\frac{\partial U^i}{\partial x}+\frac{\partial^3 U^i}{\partial x^3}=0, \quad i=1,2,\ldots,N, \tag{1.1}$$

and investigate different group theoretical properties including a sequence of Lie–Bäcklund symmetries and discuss its relation with the integrability of it. Tsuchida and Wadati[19] have shown that Eq. (1.1) is solvable by inverse scattering transform technique and also derive soliton solutions of it.

The plan of the article is as follows: In Sec. II, the Lie point symmetries of N-$cmKdV$, Eqs. (1.1), is derived and shown that the similarity reduction associated with symmetries passes the Painlevé property of ordinary differential equations. Also the existence of nonclassical symmetries and other reduction to be obtained from the direct method have been investigated in detail. In Sec. III, a sequence of Lie–Bäcklund symmetries for Eqs. (1.1) is explicitly derived, establishing its integrability. The question of constructing the recursion operator for Eqs. (1.1) has been discussed in Sec. IV. Section V contains brief details of our results.

II. SIMILARITY REDUCTION AND INTEGRABILITY

A. Classical Lie symmetry analysis

Consider a one parameter (ϵ) Lie group of continuous point transformations

$$\begin{aligned} x^*&=x+\epsilon\xi(x,t,U^1,U^2,\ldots,\ U^N)+O(\epsilon^2),\\ t^*&=t+\epsilon\tau(x,t,U^1,U^2,\ldots,\ U^N)+O(\epsilon^2),\\ (U^i)^*&=U^i+\epsilon\eta^i(x,t,U^1,U^2,\ldots,\ U^N)+O(\epsilon^2), \end{aligned} \tag{2.1}$$

where $\xi,\ \tau,\ \eta^i (i=1,2,\ldots,N)$ are infinitesimal symmetries and so the infinitesimal generator is

$$X=\xi\frac{\partial}{\partial x}+\tau\frac{\partial}{\partial t}+\eta\frac{\partial}{\partial U^1}+\eta^2\frac{\partial}{\partial U^2}+\cdots+\eta^N\frac{\partial}{\partial U^N}. \tag{2.2}$$

Hereafter, the index i varies from 1,2,…,N unless otherwise specified. Equations (1.1) are invariant under the above continuous point transformations Eq. (2.1) if

$$\frac{\partial U^{*i}}{\partial t^*}+6\left(\sum_{j=1}^{N}(U^{*j})^2\right)\frac{\partial U^{*i}}{\partial x^*}+\frac{\partial^3 U^{*i}}{\partial x^{*3}}=0, \tag{2.3}$$

provided U^i satisfy Eqs. (1.1). Substituting the expressions for various derivatives of $(U^i)^*$ in Eq. (2.3) along with Eq. (2.1) and then equating different coefficients of like derivative terms of U^i to zero, we obtain a system of overdetermined linear PDEs and, solving them successively, we determine the explicit form of infinitesimals

$$\xi=\frac{\alpha}{3}x+\delta, \quad \tau=\alpha t+\gamma, \tag{2.4}$$

$$\eta^1=\frac{-\alpha}{3}U^1, \quad \eta^2=\frac{-\alpha}{3}U^2, \quad \ldots, \quad \eta^N=\frac{-\alpha}{3}U^N, \tag{2.5}$$

where $\alpha,\ \gamma,\ \delta$ are constants and so the infinitesimal generator Eq. (2.2) takes the following form:

$$X=\left(\frac{\alpha}{3}x+\delta\right)\frac{\partial}{\partial x}+(\alpha t+\gamma)\frac{\partial}{\partial t}-\frac{\alpha}{3}\left[U^1\frac{\partial}{\partial U^1}+U^2\frac{\partial}{\partial U^2}+\ldots+U^N\frac{\partial}{\partial U^N}\right]. \tag{2.6}$$

Obviously the generators are

$$\begin{gathered}X_1=\frac{x}{3}\frac{\partial}{\partial x}+t\frac{\partial}{\partial t}-\frac{1}{3}\left(U^1\frac{\partial}{\partial U^1}+U^2\frac{\partial}{\partial U^2}+\ldots+U^N\frac{\partial}{\partial U^N}\right),\\ X_2=\frac{\partial}{\partial t},\quad X_3=\frac{\partial}{\partial x}.\end{gathered} \tag{2.7}$$

The commutator relations satisfy

$$[X_1,X_2]=-X_2,\quad [X_1,X_3]=\tfrac{1}{3}X_3,\quad [X_2,X_3]=0, \tag{2.8}$$

and so the underlying symmetry algebra is a finite dimensional one.

In order to find the similarity variable and similarity transformations associated with the infinitesimal symmetries given in Eqs. (2.4) and (2.5), we solve the characteristic equation,

$$\frac{dx}{\xi}=\frac{dt}{\tau}=\frac{dU^1}{\eta^1}=\frac{dU^2}{\eta^2}=\ldots=\frac{dU^N}{\eta^N}. \tag{2.9}$$

The similarity variable ζ and the similarity transformations $f_i(\zeta)$ are

$$\zeta=\left(x+\frac{3\delta}{\alpha}\right)\left(t+\frac{\gamma}{\alpha}\right)^{-1/3}, \tag{2.10}$$

$$f_1(\zeta)=\left(t+\frac{\gamma}{\alpha}\right)^{1/3}U^1,\quad f_2(\zeta)=\left(t+\frac{\gamma}{\alpha}\right)^{1/3}U^2,\quad \ldots,\quad f_N(\zeta)=\left(t+\frac{\gamma}{\alpha}\right)^{1/3}U^N. \tag{2.11}$$

Substituting the similarity transformations, Eq. (2.11), along with the similarity variable, Eq. (2.10), in Eqs. (1.1), we find that it reduces into a system of N-coupled nonautonomous third order ordinary differential equations

$$\begin{gathered}(\zeta f_1'+f_1)-18\left(\sum_{j=1}^{n}f_j^2\right)f_1'-3f_1'''=0,\\ (\zeta f_2'+f_2)-18\left(\sum_{j=1}^{N}f_j^2\right)f_2'-3f_2'''=0,\\ \ldots\\ \ldots\\ (\zeta f_N'+f_N)-18\left(\sum_{j=1}^{N}f_j^2\right)f_N'-3f_N'''=0,\end{gathered} \tag{2.12}$$

where $f'=df/d\zeta$. Obviously Eqs. (2.12) can be transformed into the well known second Painlevé transcendental equation for $N=1$. However, for $N\geqslant 2$ it is very difficult to transform the coupled third order Eqs. (2.12) into a known integrable equation. In order to investigate the nature of the system of Eqs. (2.12), whether integrable or not, we apply the Painlevé analysis of ordinary differential equations.[6] Also, it was demonstrated by Ablowitz, Ramani, and Segur (ARS) that there exists a deep connection between the nonlinear PDEs solvable by inverse scattering trans-

form (IST) and the Painlevé equations. In fact, they have conjectured that every ordinary differential equation obtained by an exact reduction of PDEs solvable by IST is of Painlevé type, perhaps after a transformation of variable. Exploiting the Painlevé analysis (also known as ARS algorithm), several new integrable systems have been identified in recent years[2,17,20–22] (see also Refs. 23 and 24). We present below brief details of the Painlevé analysis of the similarity reduction equations (2.12).

B. Painlevé analysis of the *N*-coupled similarity reduction

The Painlevé[6] analysis essentially consists of the following three steps:

(a) determination of the leading order of the Laurent series solution of the given ordinary differential equation in the neighborhood of a movable singular point;
(b) determination of powers (called resonances) at which arbitrary constants enter into the Laurent series expansion; and
(c) verification that a sufficient number of arbitrary constants exist as that of the order of the differential equation without the introduction of movable critical points.

To apply the Painlevé analysis, we consider a solution of Eqs. (2.12) expressed as a series expansion

$$f_i(\zeta)=(\zeta-\zeta_0)^{p_i}\sum_{m=0}^{\infty} a_{im}(\zeta-\zeta_0)^m,$$

where p_i are negative integers, $a_{i0}\neq 0$ in the neighborhood of arbitrary movable singularity ζ_0.

Substituting now

$$f_i(\zeta)\approx a_{i0}\lambda^{p_i},\quad \lambda=(\zeta-\zeta_0)\to 0 \tag{2.13}$$

in Eqs. (2.12), we find from the dominating terms that

$$p_i=-1, \tag{2.14}$$

and the N equations resulting from Eqs. (2.12) reduce into a single equation

$$\sum_{j=1}^{N} a_{j0}^2=-1. \tag{2.15}$$

To obtain the resonance values, we substitute

$$f_i(\zeta)\approx a_{i0}\lambda^{p_i}+\beta_i\lambda^{p_i+r},\ \ \lambda\to 0, \tag{2.16}$$

into the leading order terms of Eqs. (2.12) and obtain a system of N-coupled linear algebraic equations for the β_i. To have a nontrivial set of solutions, we require

$$\det M_N(r)=0, \tag{2.17}$$

where

$$M_N(r)=\begin{bmatrix} -12a_{10}^2+r' & -12a_{10}a_{20} & \dots & -12a_{10}a_{N0} \\ -12a_{20}a_{10} & -12a_{20}^2+r' & \dots & -12a_{20}a_{N0} \\ \vdots & \vdots & \vdots & \vdots \\ -12a_{N0}a_{10} & -12a_{N0}a_{20} & \dots & -12a_{N0}^2+r' \end{bmatrix},$$

where $r'=r(r-1)(r-5)$. Solving Eq. (2.17) we find the following resonance values: $r=-1,0,0,\ldots(N-1)$ times, $1,1,\ldots(N-1)$ times, $3,4,5,5,\ldots(N-1)$ times.
Next, in order to identify the arbitrary constants $a_{i\mu}$, we substitute the series expansion

$$f_i(\zeta)=\sum_{\mu=1}^{5} a_{i\mu}\lambda^{\mu-1} \tag{2.18}$$

into all the terms of Eqs. (2.12) and, by equating the like coefficients of λ at each μ, we obtain an equation of the form

$$[M_{N,\mu}][a_{i\mu}]=[S_\mu], \tag{2.19}$$

where $[M_{N,\mu}]$ is an $N\times N$ matrix, and $[a_{i\mu}]$ and $[S_\mu]$ are $N\times 1$ column matrices. The matrix $[S_\mu]$ depends only on the $a_{i\mu-1}$ coefficients. The application of Cramer's rule for determinants yields a unique solution to Eq. (2.19):

$$a_{i\mu}=\det \overline{M}_{N,\mu}/\det M_{N,\mu}, \quad \det M_{N,\mu}\neq 0, \tag{2.20}$$

where the $N\times N$ matrix $[\overline{M}_{N,\mu}]$ is obtained by replacing the ith column in $[M_{N,\mu}]$ by the column matrix $[S_\mu]$.

From Eq. (2.15) we conclude that $(N-1)$ of a_{i0}'s, $i=1,2,\ldots,N$'s, are arbitrary corresponding to the resonance values $0,0,0,\ldots,(N-1)$ times. Similarly, by equating the coefficients of λ^{-3} in all the equations of Eqs. (2.12) to zero, we find that the N-equations reduce to a single equation

$$\sum_{j=1}^{N} a_{i0}a_{j1}=0, \tag{2.21}$$

and so the $(N-1)$ coefficients of a_{j1}, $j=1,2,\ldots,N$, are arbitrary associated with the resonance values $1,1,1,\ldots,(N-1)$ times. Next, by solving a system of N-equations obtained by equating the coefficient of λ^{-2} of Eqs. (2.12) to zero, we obtain

$$a_{i2}=a_{i0}\left[\sum_{j=1}^{N} a_{j1}^2-\frac{\zeta_0}{18}\right], \tag{2.22}$$

uniquely. Similarly, by solving a system of N-equations obtained from the coefficients of λ^{-1} and λ^0 in Eqs. (2.12) we find that one of coefficients of a_{i3} and a_{i4} is arbitrary corresponding to the resonance values 3 and 4, respectively. Next by equating the coefficients of λ^1 in Eqs. (2.12) we find that the N-equations reduce into a single equation and therefore $(N-1)$ coefficients of a_{i5} are arbitrary corresponding to the resonance values $5,5,5,\ldots,(N-1)$ times.

Thus the Laurent series expansion solution (2.18) of the similarity reduction (2.12) possesses the required number, $3N$, of arbitrary constants, and is free from movable critical points. Thus the Painlevé property or ARS conjecture is satisfied. Hence the similarity reduction, Eqs. (2.12), of the N-$cmKdV$ equation (1.1) is expected to be integrable.

C. Nonclassical symmetry analysis

The nonclassical symmetry analysis which is also known as method of conditional symmetries was originally proposed by Bluman and Cole[25] and illustrated its applicability through the heat equation as an example. Later on this method was applied to several nonlinear evolution equations possessing solitons by different authors and they derived similarity reductions.[25–29] In the literature, there do exist nonlinear PDEs which possess similarity reductions that are not obtained through the classical Lie group method. For instance, new similarity reductions of the Boussinesq equation were derived through the nonclassical method which cannot be obtained through classical Lie method.[28] In this subsection we apply the nonclassical symmetry analysis to Eqs. (1.1) and

investigate whether there exist any new symmetry reductions or not. Since the methodology of nonclassical symmetry analysis is presented by different authors[25–28] in detail, we refrain from presenting detailed calculations.

In the nonclassical method, N coupled systems of Eqs. (1.1) are augmented with the invariant surface conditions

$$\xi\frac{\partial U^i}{\partial x}+\tau\frac{\partial U^i}{\partial t}-\eta^i=0, \tag{2.23}$$

where $\xi(x,t,U^i)$, $\tau(x,t,U^i)$ and $\eta^i(x,t,U^i)$ are unknowns to be determined. Now we apply the standard symmetry algorithm that provides the symmetry algebra. Then there are two cases, namely $(\tau\neq 0,\xi\neq 0)$ and $(\tau=0,\xi\neq 0)$, possible.

Let us first consider the case $\tau\neq 0,\xi\neq 0$. Without loss of generality we assume that $\tau=1$ and so the invariant surface conditions, Eqs. (2.23), become

$$\frac{\partial U^i}{\partial t}+\xi\frac{\partial U^i}{\partial x}-\eta^i=0. \tag{2.24}$$

Making use of the point transformations (2.1) we obtain a system of invariant equations for Eqs. (1.1) which involves $\partial U^i/\partial t$ and $\partial^3 U^i/\partial x^3$. Using Eq. (2.24) we replaced the derivative term $\partial U^i/\partial t$ in the above mentioned invariance equation and rearranging it yields a system of overdetermined nonlinear PDEs. By solving the obtained determining equations successively we explicitly determine ξ, η^i,

$$\tau=1,\quad \xi=\frac{x}{3t},\quad \eta^1=\frac{-U^1}{3t},\quad \eta^2=\frac{-U^2}{3t},\quad \ldots,\quad \eta^N=\frac{-U^N}{3t}, \tag{2.25}$$

and the associated infinitesimal generator takes the following form:

$$X=\frac{x}{3t}\frac{\partial}{\partial x}+\frac{\partial}{\partial t}-\frac{1}{3t}\left(U^1\frac{\partial}{\partial U^1}+U^2\frac{\partial}{\partial U^2}+\ldots+U^N\frac{\partial}{\partial U^N}\right). \tag{2.26}$$

Let us compare the nonclassical symmetries of Eqs. (1.1) with the classical ones. We now multiply the invariant surface conditions (2.24) and the corresponding vector field (2.26) by t gives the following vector field:

$$Y=t\frac{\partial}{\partial t}+\frac{x}{3}\frac{\partial}{\partial x}-\frac{1}{3}\left(U^1\frac{\partial}{\partial U^1}+U^2\frac{\partial}{\partial U^2}+\ldots+U^N\frac{\partial}{\partial U^N}\right). \tag{2.27}$$

Comparing the infinitesimal generator of Eq. (2.6) obtained from the classical symmetry analysis with that of Eq. (2.27) we find that there exist no nonclassical symmetries in this case. Similar conclusions for the case $\tau=0$ and $\xi\neq 0$ can also be arrived at. Thus we conclude that no nonclassical symmetries exist for the system of N-$cmKdV$, Eqs. (1.1).

D. Direct method

The direct method of deriving similarity reductions of PDEs was originally proposed by Clarkson and Kruskal[30] and was applied to a variety of nonlinear PDEs by different researchers[2,31–33] (see also Ref. 34). The unusual characteristic of this method in comparison with the other methods is that it involves no use of group theory or Lie symmetry analysis. The basic idea of this method is to seek a solution of a nonlinear PDEs involving two independent variables in the form

$$U(x,t)=F(x,t,w(z(x,t))). \tag{2.28}$$

Then, requiring that substitution of Eq. (2.28) into the given nonlinear PDE yields an ordinary differential equation for $w(z)$. This imposes a condition upon $F(x,t,w(z))$ and its derivatives which enables one to solve for $F(t,x,w(z))$, which yields the desired reduction.

In order to use the direct method as usual we substitute

$$U^i(x,t)=A_i(x,t)+B_i(x,t)w_i(z(x,t)), \tag{2.29}$$

where $A_i(x,t)$ and $B_i(x,t)$ are unknown functions in Eqs. (1.1). We then obtain the following third order nonlinear ordinary differential equation:

$$\begin{aligned} &B_i z_x^3 w_i''' + w''(3B_{i,x}z_x^2+3B_i z_x z_{xx}) + w_i'(B_i z_t+3B_{i,xx}z_x+3B_{i,x}z_{xx}+B_i z_{xxx}+\tilde{A}B_i z_x)\\ &\quad + w_i(B_{i,t}z_t+B_{i,xxx}+\tilde{A}B_{i,x})+\tilde{B}A_{i,x}+w_i\tilde{B}B_{i,x}+w_i\tilde{C}B_{i,x}+w_i'\tilde{C}B_i z_x\\ &\quad + w_i'\tilde{B}B_i z_x+\tilde{C}A_{i,x}+A_{i,t}+A_{i,xxx}+\tilde{A}A_{i,x}=0, \end{aligned} \tag{2.30}$$

where

$$\tilde{A}=6\sum_{j=1}^{N} A_j^2, \tilde{B}=6\sum_{j=1}^{N} w_j^2 B_j^2, \tilde{C}=12\sum_{j=1}^{N} w_j A_j B_j, w'=\frac{dw}{dz}.$$

Note that the coefficient of w_i''' is $B_i z_x^3$. Using this as the normalizing coefficient and taking the other coefficient of the form $B_i z_x^3 \Gamma(z)$, where $\Gamma(z)$ is an unknown function to be determined, we obtain the following equations:

$$w_i^2 w_i' : B_i^3 z_x = B_i z_x^3 \Gamma_1, \tag{i}$$

$$w_i^2 : B_i^2 A_{i,x} = B_i z_x^3 \Gamma_2, \tag{ii}$$

$$w_i w_i' : A_i B_i^2 z_x = B_i z_x^3 \Gamma_3, \tag{iii}$$

$$w_i^3 : B_i^2 B_{i,x} = B_i z_x^3 \Gamma_4, \tag{iv}$$

$$w_i'' : B_{i,x} z_x^2 + B_i z_x z_{xx} = B_i z_x^3 \Gamma_5, \tag{v}$$

$$w_i' : B_i z_t + 3B_{i,xx}z_x + 3B_{i,x}z_{xx} + B_i z_{xxx} + 6\left(\sum_{i=1}^{N} A_j^2\right) B_i z_x = B_i z_x^3 \Gamma_6, \tag{vi}$$

$$w_i : B_{i,t} + B_{i,xxx} + 12A_i B_i A_{i,x} + 6\left(\sum_{j=1}^{N} A_j^2\right) B_{i,x} = B_i z_x^3 \Gamma_7. \tag{vii}$$

Solving the above determining equations (i)–(vii) successively, we find that the consistency condition holds only if

$$U^i(x,t)=t^{-1/3}w_i(z), z=xt^{-1/3}. \tag{2.31}$$

Thus the similarity transformation and the similarity variable obtained through the direct method are exactly the same derived through the classical Lie method. Thus we conclude that the direct method also does not yield any new similarity reductions for the system of N-$cmKdV$, Eqs. (1.1).

III. LIE–BÄCKLUND SYMMETRIES OF N-cmKdV EQUATIONS

It is well known that the existence of infinitely many commuting Lie–Bäcklund symmetries is the defining feature of complete integrability of nonlinear PDEs. It was shown by different authors

that several scalar integrable nonlinear PDEs of $(1+1)$ dimension admit a sequence of Lie–Bäcklund symmetries.[3,14,35,36] However, the existence of a sequence of Lie–Bäcklund symmetries for the coupled or multicomponent integrable PDEs has not been investigated so far. In this subsection we show that the N-coupled modified Korteweg–de Vries equations (1.1) admits a sequence of Lie–Bäcklund symmetries.

Basically the Lie–Bäcklund transformations are the generalized Lie groups of point transformations that are defined by infinitesimals depending on a finite number of derivatives of the dependent variables. Now consider a one parameter (ϵ) infinitesimal Lie–Bäcklund transformation,

$$\begin{gathered}(U^i)^*=U^i+\epsilon\eta^i(x,t,U^i_k)+O(\epsilon^2),\\ x^*=x,t^*=t,\\ (U^i_t)^*=U^i_t+\epsilon[\eta^i_t]+O(\epsilon^2),\\ (U^i_k)^*=U^i_k=\epsilon[\eta^i_x]+O(\epsilon^2),k=0,1,2,\ldots,\infty,\end{gathered}\tag{3.1}$$

where

$$\begin{gathered}U^i_0=U^i,\quad U^i_k=\frac{\partial^k U^i}{\partial x^k},\quad U^i_{kt}=\frac{\partial U^i_k}{\partial t},\quad [\eta^i_t]=D_t\eta^i,\\ [\eta^i_x]=D_x\eta^i,\quad [\eta^i_{xx}]=D^2_x\eta^i,\quad [\eta^i_{xxx}]=D^3_x\eta^i.\end{gathered}\tag{3.2}$$

Define the total derivative operators

$$D_x=\sum_{i=0}^{N}\sum_{k=0}^{\infty}U^i_{k+1}\frac{\partial}{\partial U^i_k},\quad D_t=\sum_{i=0}^{N}\sum_{k=0}^{\infty}U^i_{kt}\frac{\partial}{\partial U^i_k},\tag{3.3}$$

and the Lie–Bäcklund (LB) operator

$$X(\eta^i)=\sum_{i=0}^{N}(D_t\eta^i)\frac{\partial}{\partial U^i_t}+\sum_{i=0}^{N}\sum_{k=0}^{\infty}(D^k_x\eta^i)\frac{\partial}{\partial U^i_k}.\tag{3.4}$$

Making use of the one parameter (ϵ) Lie–Bäcklund transformations (3.1) along with the different derivatives of U^i in Eqs. (1.1) we obtain the following system of coupled invariance equations:

$$[\eta^i_t]+6\left(\sum_{j=1}^{N}(U^j)^2\right)[\eta^i_x]+12\left(\sum_{j=1}^{N}U^j\eta^j\right)U^i_x+[\eta^i_{xxx}]=0.\tag{3.5}$$

The above coupled equations can be written as a polynomial in U^i and its derivatives with respect to the variables x and t. We further assume that η^i do not depend on the independent variables x and t. Then by equating the coefficients of different derivatives of U^i in Eq. (3.5) to zero and solving them successively we find the form of η^i's explicitly. Since the calculations of obtaining the Lie–Bäcklund symmetries η^i for Eqs. (1.1) are tedious and cumbersome for arbitrary N, for clarity, we present the details for the cases $N=2$ and $N=3$. Let

$$\begin{gathered}U^1=u,\quad U^2=v,\quad U^3=w,\quad \frac{\partial U^1}{\partial x}=u_1,\quad \frac{\partial U^2}{\partial x}=v_1,\quad \frac{\partial U^3}{\partial x}=w_1,\\ \frac{\partial^2U^1}{\partial x^2}=u_2,\quad \frac{\partial^2U^2}{\partial x^2}=v_2,\quad \frac{\partial^2U^3}{\partial x^2}=w_2,\quad \frac{\partial^3U^1}{\partial x^3}=u_3,\quad \frac{\partial^3U^2}{\partial x^3}=v_3,\quad \frac{\partial^3U^3}{\partial x^3}=w_3.\end{gathered}\tag{3.6}$$

Case (i): $N=2$. The two coupled $mKdV$ equations are

$$u_t+6(u^2+v^2)u_1+u_3=0, \quad v_t+6(u^2+v^2)v_1+v_3=0, \tag{3.7}$$

and so the invariance equations (3.5) become

$$[\eta_{1,t}]+6(u^2+v^2)[\eta_{1,x}]+12(u\eta_1+v\eta_2)u_1+[\eta_{1,xxx}]=0, \tag{3.8a}$$

$$[\eta_{2,t}]+6(u^2+v^2)[\eta_{2,x}]+12(u\eta_1+v\eta_2)v_1+[\eta_{2,xxx}]=0. \tag{3.8b}$$

The trivial symmetries of the two coupled modified Korteweg–de Vries equations (3.7) are

$$\eta_I^1=u_1, \quad \eta_I^2=v_1 \tag{3.9}$$

and

$$\eta_{II}^1=u_3+6(u^2+v^2)u_1, \quad \eta_{II}^2=v_3+6(u^2+v^2)v_1. \tag{3.10}$$

Detailed calculations show that the next higher order symmetries η_{III}^1 and η_{III}^2 to be of the form

$$\eta_{III}^1=u_5+F(u,u_1,u_2,u_3,u_4,v,v_1,v_2,v_3,v_4), \tag{3.11}$$

$$\eta_{III}^2=v_5+G(u,u_1,u_2,u_3,u_4,v,v_1,v_2,v_3,v_4), \tag{3.12}$$

where F, G are unknown functions to be determined. Substituting the above Eqs. (3.11) and (3.12) along with derivative terms with respect to x and t in the two coupled invariant equations (3.8a) and (3.8b) and first equating the coefficients of u_7,u_6,u_5,u_4 and v_7,v_6,v_5,v_4 to zero yields the following determining PDEs:

$$\frac{\partial\eta_{III}^1}{\partial u_4}=0, \quad \frac{\partial\eta_{III}^2}{\partial u_4}=0, \quad \frac{\partial\eta_{III}^1}{\partial v_4}=0, \quad \frac{\partial\eta_{III}^2}{\partial v_4}=0, \quad \frac{\partial\eta_{III}^1}{\partial v_3}=0, \quad \frac{\partial\eta_{III}^2}{\partial u_3}=0, \tag{3.13}$$

$$\frac{\partial\eta_{III}^1}{\partial u_3}=10(u^2+v^2), \quad \frac{\partial\eta_{III}^2}{\partial v_3}=10(u^2+v^2). \tag{3.14}$$

Solving Eqs. (3.13) and (3.14) we obtain

$$F=10(u^2+v^2)u_3+F_1(u,u_1,u_2,v,v_1,v_2) \tag{3.15}$$

and

$$G=10(u^2+v^2)v_3+G_1(u,u_1,u_2,v,v_1,v_2), \tag{3.16}$$

where F_1, G_1 are arbitrary functions to be determined. Proceeding further we obtain the explicit forms of F_1 and G_1 and so the next order Lie–Bäcklund symmetries η_{III}^1 and η_{III}^2 are

$$\begin{aligned}\eta_{III}^1=&u_5+10(u^2+v^2)u_3+30(u^2+v^2)^2u_1+10(u_1^2+v_1^2)u_1\\&+20(uu_2+vv_2)u_1+20(uu_1+vv_1)u_2,\end{aligned} \tag{3.17}$$

$$\begin{aligned}\eta_{III}^2=&v_5+10(u^2+v^2)v_3+30(u^2+v^2)^2v_1+10(u_1^2+v_1^2)v_1\\&+20(uu_2+vv_2)v_1+20(uu_1+vv_1)v_2.\end{aligned} \tag{3.18}$$

Continuing this algorithmic procedure, we find that the two coupled modified Korteweg–de Vries equations (3.7) admit a sequence of Lie–Bäcklund symmetries.

Case (ii): $N=3$. The three coupled $mKdV$ equations are

$$u_t+6\rho^2u_1+u_3=0,\quad v_t+6\rho^2v_1+v_3=0,\quad w_t+6\rho^2w_1+w_3=0, \tag{3.19}$$

and the associated invariance equations become

$$[\eta_{1,t}]+6\rho^2[\eta_{1,x}]+12(u\eta_1+v\eta_2+w\eta_3)u_1+[\eta_{1,xxx}]=0, \tag{3.20a}$$

$$[\eta_{2,t}]+6\rho^2[\eta_{2,x}]+12(u\eta_1+v\eta_2+w\eta_3)v_1+[\eta_{2,xxx}]=0, \tag{3.20b}$$

$$[\eta_{3,t}]+6\rho^2[\eta_{3,x}]+12(u\eta_1+v\eta_2+w\eta_3)w_1+[\eta_{3,xxx}]=0, \tag{3.20c}$$

where $\rho^2=u^2+v^2+w^2$. Proceeding as before, as that of two coupled modified Korteweg–de Vries equations we obtain following Lie–Bäcklund symmetries for the three-$cmKdV$ equations:

$$\eta_I^1=u_1,\eta_{II}^1=u_3+6\rho^2u_1,\eta_I^2=v_1,\quad \eta_{II}^2=v_3+6\rho^2v_1,\quad \eta_I^3=w_1,\eta_{II}^3=w_3+6\rho^2w_1, \tag{3.21}$$

$$\eta_{III}^1=u_5+10\rho^2u_3+30\rho^4u_1+10\rho_1^2u_1+20\rho_2u_2+20\rho_3u_1, \tag{3.22}$$

$$\eta_{III}^2=v_5+10\rho2v_3+30\rho^4v_1+10\rho_1^2v_1+20\rho_2v_2+20\rho_3v_1, \tag{3.23}$$

$$\eta_{III}^3=w_5+10\rho^2w_3+30\rho^4w_1+10\rho_1^2w_1+20\rho_2w_2+20\rho_3w_1, \tag{3.24}$$

where $\rho_1^2=u_1^2+v_1^2+w_1^2$, $\rho_2=uu_1+vv_1+ww_1$ and $\rho_3=uu_2+vv_2+ww_2$. Since the procedure is algorithmic we refrain from presenting the further details of the next order Lie–Bäcklund symmetries.

Case (iii): For N-$cmKdV$, Eqs. (1.1), the Lie–Bäcklund symmetries take the following forms:

$$\eta_I^1=U_x^1,\quad \eta_I^2=U_x^2,\quad \ldots,\quad \eta_I^N=U_x^N, \tag{3.25}$$

$$\eta_{II}^1=U_{xxx}^1+6V^2U_x^1,\quad \eta_{II}^2=U_{xxx}^2+6V^2U_x^2,\quad \ldots,\quad \eta_{II}^N=U_{xxx}^N+6V^2U_x^N, \tag{3.26}$$

$$\eta_{III}^1=U_{xxxxx}^1+10V^2U_{xxx}^1+30V^4U_x^1+10V_1^2U_x^1+20V_2U_{xx}^1+20V_3U_x^1, \tag{3.27}$$

$$\eta_{III}^2=U_{xxxxx}^2+10V^2U_{xxx}^2+30V^4U_x^2+10V_1^2U_x^2+20V_2U_{xx}^2+20V_3U_x^2, \tag{3.28}$$

$$\ldots$$

$$\ldots$$

$$\eta_{III}^N=U_{xxxxx}^N+10V^2U_{xxx}^N+30V^4U_x^N+10V_1^2U_x^N+20V_2U_{xx}^N+20V_3U_x^N, \tag{3.29}$$

where $V^2=\Sigma_{j=1}^N(U^j)^2$, $V_1^2=\Sigma_{j=1}^N(U_x^j)^2$, $V_2=\Sigma_{j=1}^NU^jU_x^j$, $V_3=\Sigma_{j=1}^NU^jU_{xx}^j$.

The next higher order Lie–Bäcklund symmetries N-$cmKdV$ of Eqs. (1.1) can be obtained in a straightforward manner.

IV. RECURSION OPERATOR

In the investigation of algebraic properties of integrable nonlinear PDEs such as infinitely many symmetries, integrals of motion, existence of a bi-Hamiltonian formulation, etc., recursion operators play a central role.[3,4] If a nonlinear PDE admits a sequence of Lie–Bäcklund symmetries, it is often possible to construct its recursion operator. If the recursion operator is hereditary, then the equation possesses infinitely many symmetries. It is widely believed that the existence of recursion operators helps one to construct the Hamiltonian operators, if they exist, enabling one to check whether a given nonlinear PDE is a bi-Hamiltonian or tri-Hamiltonian system or not. There

exist different analytical techniques to construct a recursion operator for a given integrable nonlinear PDE.[4,37–40] Among them the method proposed by Aiyer[37] provides an effective technique to construct a recursion operator through group theory techniques. The advantage of this approach is that it does not require the existence of Lax representation of the concerned equation. In this subsection we use this method to construct recursion operators for the *N-cmKdV* equations (1.1). For clarity, we present the details for $N=2$ and $N=3$, which are 2×2 and 3×3 matrices, respectively.

Case (i): $N=2$

Here $U^1=u$, $U^2=v$. Let $T(u,v)$ be a 2×2 recursion operator of the two-*cmKdV* equations (3.7), connecting $(u_x,v_x)=(u_1,v_1)$ to (u_t,v_t). Then $T(u,v)$ is given by

$$T(u,v)\begin{pmatrix} u_1 \\ v_1 \end{pmatrix}=\begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}=\begin{pmatrix} u_t \\ v_t \end{pmatrix}, \tag{3.30}$$

where

$$T_{11}=-D_x^2-4(u^2+v^2)-4u_1D_x^{-1}(u);\quad T_{12}=-4u_1D_x^{-1}(v),$$

$$T_{21}=-4v_1D_x^{-1}(u);\quad T_{22}=-D_x^2-4(u^2+v^2)-4v_1D_x^{-1}(v).$$

In order to find the Lie–Bäcklund or infinitesimal transformations of the next higher order, we look for a recursion operator such that

$$T^2(u,v)\begin{pmatrix} u_1 \\ v_1 \end{pmatrix}=\begin{pmatrix} \eta^1_{III} \\ \eta^2_{III} \end{pmatrix}. \tag{3.31}$$

Then $T^2(u,v)$ takes the following form:

$$T^2(u,v)=\begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix},$$

where

$$\begin{aligned} T_{11}=&D_x^4+8(u^2+v^2)D_x^2+20uu_1D_x+10vv_1D_x+20(uu_2+vv_2)\\ &+10(u_1^2+v_1^2)+18(u^2+v^2)^2+4\{u_3+6(u^2+v^2)u_1\}D_x^{-1}(u),\\ T_{12}=&10u_2v+4\{u_3+6(u^2+v^2)u_1\}D_x^{-1}(v),\\ T_{21}=&10v_2u+4\{v_3+6(u^2+v^2)v_1\}D_x^{-1}(u),\\ T_{22}=&D_x^4+8(u^2+v^2)D_x^2+20vv_1D_x+10uu_1D_x+20(uu_2+vv_2)\\ &+10(u_1^2+v_1^2)+18(u^2+v^2)^2+4\{v_3+6(u^2+v^2)v_1\}D_x^{-1}(v). \end{aligned}$$

Thus $T(u,v)$, whose elements are given by Eq. (3.30), exists, and, acting repeatedly on $\binom{u_1}{v_1}$, generates two sets of infinitesimal transformations. Further, we get the following hierarchy of the two *cmKdV* equations (3.7):

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix}=T^n(u,v)\begin{pmatrix} u_1 \\ v_1 \end{pmatrix}=\begin{pmatrix} \eta_1^{(n+1)} \\ \eta_2^{(n+1)} \end{pmatrix}, \tag{3.32}$$

where

$$\eta_1^{(1)}=\eta_{\rm I}^1=u_1,\quad \eta_2^{(1)}=\eta_{\rm I}^2=v_1,$$

$$\eta_1^{(2)}=\eta_{\rm II}^1=u_3+6(u^2+v^2)u_1,\quad \eta_2^{(2)}=\eta_{\rm II}^2=v_3+6(u^2+v^2)v_1,\ \text{etc.}$$

Case (ii): $N=3$

Here $U^1=u$, $U^2=v$, $U^3=w$. Let $T(u,v,w)$ be a 3×3 recursion operator of the three-*cmKdV* equations, connecting (u_1,v_1,w_1) to (u_t,v_t,w_t). Then $T(u,v,w)$ is given by

$$T(u,v,w)\begin{pmatrix}u_1\\v_1\\w_1\end{pmatrix}=\begin{pmatrix}T_{11}&T_{12}&T_{13}\\T_{21}&T_{22}&T_{23}\\T_{31}&T_{32}&T_{33}\end{pmatrix}=\begin{pmatrix}u_t\\v_t\\w_t\end{pmatrix}\tag{3.33}$$

with

$$T_{11}=-D_x^2-4\rho^2-4u_1D_x^{-1}(u);\ \ T_{12}=-4u_1D_x^{-1}(v);\ \ T_{13}=-4u_1D_x^{-1}(w);$$

$$T_{21}=-4v_1D_x^{-1}(u);\ \ T_{22}=-D_x^2-4\rho^2-4v_1D_x^{-1}(v)\ \ T_{23}=-4v_1D_x^{-1}(w);$$

$$T_{31}=-4w_1D_x^{-1}(u);\ \ T_{32}=-4w_1D_x^{-1}(v);$$

$$T_{33}=-D_x^2-4\rho^2-4w_1D_x^{-1}(w);$$

where $\rho^2=u^2+v^2+w^2$.

In order to find the Lie–Bäcklund or infinitesimal transformations of the next higher order, we look for a recursion operator $T(u,v,w)$ for the three-*cmKdV* Eqs. (3.19) such that

$$T^2(u,v,w)\begin{pmatrix}u_1\\v_1\\w_1\end{pmatrix}=\begin{pmatrix}\eta^1_{III}\\\eta^2_{III}\\\eta^3_{III}\end{pmatrix}.\tag{3.34}$$

Then $T(u,v,w)$ takes the following form:

$$T(u,v,w)=\begin{pmatrix}T_{11}&T_{12}&T_{13}\\T_{21}&T_{22}&T_{23}\\T_{31}&T_{32}&T_{33}\end{pmatrix},\tag{3.35}$$

where

$$\begin{aligned}T_{11}&=D_x^4+8\rho^2D_x^2+20uu_1D_x+10(vv_1+ww_1)D_x+20(uu_2+vv_2+ww_2)\\&\quad+10\rho_1^2+18\rho^4+4\{u_3+6\rho^2u_1\}D_x^{-1}(u),\\T_{12}&=10u_2v+4\{u_3+6\rho^2u_1\}D_x^{-1}(v),\\T_{13}&=10u_2w+4\{u_3+6\rho^2u_1\}D_x^{-1}(w),\\T_{21}&=10v_2u+4\{v_3+6\rho^2v_1\}D_x^{-1}(u),\\T_{22}&=D_x^4+8\rho^2D_x^2+20vv_1D_x+10(uu_1+ww_1)D_x+20(uu_2+vv_2\\&\quad+ww_2)+10\rho_1^2+18\rho^4+4\{v_3+6\rho^2v_1\}D_x^{-1}(v),\\T_{23}&=10v_2w+4\{v_3+6\rho^2v_1\}D_x^{-1}(w),\end{aligned}\tag{3.36}$$

$$T_{31}=10w_2u+4\{w_3+6\rho^2w_1\}D_x^{-1}(u),$$

$$T_{32}=10w_2v+4\{w_3+6\rho^2w_1\}D_x^{-1}(v),$$

$$T_{33}=D_x^4+8\rho^2D_x^2+20ww_1D_x+10(uu_1+vv_1)D_x+20(uu_2+vv_2+ww_2)$$
$$+10\rho_1^2+18\rho^4+4\{w_3+6\rho^2w_1\}D_x^{-1}(w),$$

where $\rho_1^2=u_1^2+v_1^2+w_1^2$.

Here also, we get the following hierarchy of the three-$cmKdV$ equations (3.19)

$$\begin{pmatrix} u_t \\ v_t \\ w_t \end{pmatrix}=T^n(u,v,w)\begin{pmatrix} u_1 \\ v_1 \\ w_1 \end{pmatrix}=\begin{pmatrix} \eta_1^{(n+1)} \\ \eta_2^{(n+1)} \\ \eta_3^{(n+1)} \end{pmatrix},$$

where

$$\eta_1^{(1)}=\eta_{\mathrm{I}}^1=u_1,\quad \eta_2^{(1)}=\eta_{\mathrm{I}}^2=v_1,\quad \eta_3^{(1)}=\eta_{\mathrm{I}}^3=w_1,$$

$$\eta_1^{(2)}=\eta_{\mathrm{II}}^1=u_3+6\rho^2u_1,\quad \eta_2^{(2)}=\eta_{\mathrm{II}}^2=v_3+6\rho^2v_1,\quad \eta_3^{(2)}=\eta_{\mathrm{II}}^3=w_3+6\rho^2w_1,\quad \text{etc.}$$

By applying the procedure described above to N-$cmKdV$ equations (1.1), one can derive its recursion operator.

V. CONCLUSIONS

Using the classical Lie symmetry approach we derive the Lie point symmetries of N-$cmKdV$ equations and show that the similarity reduction associated with symmetries passes the Painlevé property for ordinary differential equations. Also, detailed investigations through the nonclassical symmetry approach and the direct method show that no new similarity reductions exist. Further, a sequence of Lie–Bäcklund symmetries for N-$cmKdV$ equations is derived, explicitly establishing its integrability. We have made an attempt to derive the recursion operator, a characteristic of integrable systems, for N-$cmKdV$ equations. The question of factorization of the derived recursion operator and the derivation of the well known hereditary operator is under investigation.

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Generalized symmetries in mechanics and field theories

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Generalized symmetries are introduced in a geometrical and global formalism. Such a framework applies naturally to field theories and specializes to mechanics. Generalized symmetries are characterized in a Lagrangian context by means of the transformation rules of the Poincaré–Cartan form and the (generalized) Nöther theorem is applied to obtain conserved quantities (first integrals in mechanics). In the particular case of mechanics it is shown how to use generalized symmetries to study the separation of variables of Hamilton–Jacobi equations recovering standard results by means of this new method. Supersymmetries (Wess–Zumino model) are considered as an intriguing example in field theory. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1469668]

I. INTRODUCTION

In a number of different applications, both in mechanics and in field theory, symmetries of a more general nature than the standard Lagrangian symmetries are often used (see Refs. 1–4). Ordinary Lagrangian symmetries are usually defined as transformations in the phase space which preserve the Lagrangian (or the Hamiltonian) form (see Refs. 5–8 and references quoted therein). To each one-parameter flow of Lagrangian symmetries a conserved quantity can then be associated via the so-called *Nöther theorem* (see, e.g., Refs. 6, 8, and 9). Such a theorem can be generalized in at least two physically relevant different directions.

First, one can consider transformations which do not preserve the Lagrangian form exactly, but modulo contact forms and exact differentials. Both contact forms and exact forms are, in fact, irrelevant to the Nöther theorem. Second, one can consider transformations acting on field configurations which are not induced by a transformation on the configuration space. Furthermore, since all quantities in the Nöther theorem are computed along a field configurations (and, in particular, usually along a solution) a one-parameter flow of transformations is enough to define Nöther currents by Lie dragging. In this perspective transformations on the configuration space are just a way of obtaining such a flow. More generally one can consider a transformation on the infinite jet prolongation of the configuration bundle; the infinitesimal generators of such transformations are *generalized vector fields* which will be introduced and discussed later (see Refs. 2 and 10). This approach turns out to be along the lines traced by Carter in the linear case (see Ref. 11). In the present article we develop the necessary notions and tools to deal with nonlinear systems and provide detailed examples which illustrate the relation between Lagrangian symmetries and Killing tensors.

Such a geometrical definition of generalized symmetries has been implicitly used in a number of contexts and applications. In mechanics, the first integrals of motion can often be related to separation of variables for the Hamilton–Jacobi equation and they may be generated via Nöther theorem starting from generalized symmetries. In field theory, BRST transformations, which are the most powerful tool for the quantization of gauge theories, are generalized symmetries (see Refs. 3, 4, and 12). Finally, also supersymmetries are interpretable as generalized symmetries (see Refs. 3 and 13).

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The main purpose of this article is to set these applications in the general and standard contexts of Lagrangian formalism and variational calculus. In fact, as we shall discuss in the sequel, most of the applications mentioned above in their original formulation strongly rely on Hamiltonian formalism, while we are going to set them in a purely Lagrangian context (which is certainly more standard, at least for field theories).

The plan of the article is as follows. In Sec. II we shall briefly recall the geometrical formulation of field theory which will be used extensively below. We use the geometric language of the Lagrangian framework on bundles together with the Poincaré–Cartan formulation since it is particularly suited to deal with mechanics and field theory at the same time and at any order of fields derivatives involved. In Sec. III generalized vector fields, generalized symmetries and generalized Nöther's theorem are defined. In Sec. IV we collect a number of worked out examples to mechanics and separation of variables for Hamilton–Jacobi equation. Finally, in Secs. V and VI we deal with BRST transformations and Wess–Zumino supersymmetric model as examples of application of generalized symmetries to field theory.

II. GEOMETRICAL FRAMEWORK FOR FIELD THEORY AND MECHANICS

We shall here briefly summarize the notations used in the geometrical formulation of field theory and mechanics. We assume the reader to be familiar with the basic ideas of bundle theory and classical differential geometry. Further details can be found in Refs. 6, 8, 10, and 14–17.

Let $\mathcal{C}=(C,M,\pi;F)$ be the *configuration bundle*; here C, M and F are manifolds called the *total space*, the *base* and the *standard fiber*, respectively. The map $\pi:C\to M$ is called the *projection* and it is a surjective map of maximal rank. Fiber bundles are the natural framework to deal with calculus of variations; in fact fibered coordinates on C are $(x^\mu;y^i)$ where the coordinates x^μ $[\mu=1,\ldots,\dim(M)]$ on M denote the *independent variables* while the coordinates y^i $[i=1,\ldots,\dim(F)]$ on F denote the *dependent variables*, i.e., the fields.

In mechanics one can choose $C=\mathbb{R}\times Q$ where Q is the configuration space of the system. The base manifold is $M=\mathbb{R}$ and the only independent variable is denoted by t. The fibered coordinates on $\mathbb{R}\times Q$ are (t,q^i) and q^i are the usual Lagrangian coordinates of the system.

A vector field Ξ over $\mathcal{C}$ is *projectable* if it projects over a vector field ξ of the base manifold M. Locally, projectable vector fields are hence of the form

$$\Xi=\xi^\mu(x)\partial_\mu+\xi^i(x,y)\partial_i. \tag{2.1}$$

The flow of such a projectable vector field is made of fiber preserving morphisms, i.e., a one-parameter subgroup of bundle morphisms

$$\begin{aligned} x'^\mu&=\phi_s^\mu(x),\\ y'^i&=Y_s^i(x,y). \end{aligned} \tag{2.2}$$

The vector field Ξ is the infinitesimal generator of the flow of bundle morphisms, i.e.,

$$\begin{aligned} \xi^\mu&=\frac{\mathrm{d}\phi_s^\mu}{\mathrm{d}s}(x)\bigg|_{s=0},\\ \xi^i&=\frac{\mathrm{d}Y_s^i}{\mathrm{d}s}(x,y)\bigg|_{s=0}. \end{aligned} \tag{2.3}$$

A *vertical vector field* is a vector field over $\mathcal{C}$ which projects over the zero vector field in M. Locally, a vertical vector field is in the form $\Xi=\xi^i(x,y)\partial_i$.

A *(field) configuration* is a section $\sigma:M\to C$ of the configuration bundle; locally it corresponds to a map $\sigma(x)=(x^\mu,y^i(x))$, which specifies the dependent variables as functions of the

independent variable [in mechanics $\sigma(t)=(t,q^i(t))$ represents a curve in the configuration space Q]. The transition functions of the bundle $\mathcal{C}$ encode the global topological properties of the system.

The *jet prolongation of order k* of the bundle $\mathcal{C}$ will be denoted by $J^k\mathcal{C}$, for each $k\geqslant 0$. We set $J^0\mathcal{C}\simeq\mathcal{C}$. It is a bundle over M (and over C as well as over each J^hC for $h\leqslant k$) which takes into account the fields with their derivatives up to order k included. The intermediate projections are $\pi^k_h: J^k\mathcal{C}\to J^h\mathcal{C}$, with $\pi^k_k=id$. Fibered coordinates on J^kC are denoted by $(x^\mu,y^i,y^i_\mu,y^i_{\mu\nu},\ldots,y^i_{\mu_1\ldots\mu_k})$. In mechanics the configuration bundle is isomorphic to $\mathbb{R}\times Q$ (the isomorphism being, by definition, the *observer*) and one has $J^kC\simeq\mathbb{R}\times T^kQ$ where T^kQ is the tangent bundle of order k (a point in T^kQ is an equivalence class of curves in Q having contact of order k at $t=0$). For $k=1$ the bundle T^kQ reduces to the ordinary tangent bundle TQ of the configuration space and the standard first order framework of mechanics is recovered.

The inverse limit of the inverse family $J^k\mathcal{C}$ is an infinite dimensional bundle which is denoted by $J^\infty\mathcal{C}$ and it is called the *infinite jet bundle* of $\mathcal{C}$ (see Ref. 18). All the constructions we make on finite jet bundles extend in a straighforward way to the infinite jet bundle.

If one considers a bundle morphism $\mathbf{\Phi}=(\Phi,\phi):\mathcal{C}\to\mathcal{C}'$, it can be prolonged at any order; the jet prolongation will be denoted by $J^k\mathbf{\Phi}=(j^k\Phi,\phi)$, and it makes the following diagram commutative

$$\begin{array}{ccc} J^kC & \xrightarrow{j^k\Phi} & J^kC' \\ \downarrow & & \downarrow \\ C & \xrightarrow{\Phi} & C' \\ \downarrow & & \downarrow \\ M & \xrightarrow{\phi} & M' \end{array} \tag{2.4}$$

One can also define the infinite jet prolongation $j^\infty\mathbf{\Phi}$ as the inverse limit of the family of bundle morphisms $j^k\mathbf{\Phi}$.

A section $\sigma:M\to C$ can be lifted to a section $j^k\sigma:M\to J^kC$ which is locally given by $j^k\sigma(x)=(x^\mu,y^i(x),\mathrm{d}_\mu y^i(x),\ldots,\mathrm{d}_{\mu_1\ldots\mu_k}y^i(x))$. The lift to the infinite jet bundles is obtained by the inverse limit and it is denoted by $j^\infty\sigma$.

Finally any (projectable) vector field $\Xi=\xi^\mu(x)\partial_\mu+\xi^i(x,y)\partial_i$ on $\mathcal{C}$ can be prolonged at any order to define a (projectable) vector field $j^k\Xi$ on $J^k\mathcal{C}$. The prolongation of a (projectable) vector field Ξ is the infinitesimal generator of the prolongation of the bundle morphisms (2.2). As an example, for $k=1$ the vector field $j^1\Xi=\xi^\mu\partial_\mu+\xi^i\partial_i+\xi^i_\mu\partial^\mu_i$ is locally expressed by

$$\xi^i_\mu=\mathrm{d}_\mu\xi^i-y^i_\nu\mathrm{d}_\mu\xi^\nu, \tag{2.5}$$

where the operator

$$\mathrm{d}_\mu=\partial_\mu+y^i_\mu\partial_i+y^i_{\nu\mu}\partial^\nu_i+\cdots \tag{2.6}$$

denotes (at any order k) the *formal total derivative* with respect to x^μ. Analogous but more complicated expressions hold for $k>1$ (see, e.g., Refs. 8, 17, and 18).

Contact one-forms over $J^k\mathcal{C}$ are the forms belonging to the ideal generated in $\Omega(J^k\mathcal{C})$ by

$$\begin{aligned} \omega^i&=\mathrm{d}y^i-y^i_\nu\mathrm{d}x^\nu, \\ \omega^i_\mu&=\mathrm{d}y^i_\mu-y^i_{\nu\mu}\mathrm{d}x^\nu, \\ &\cdots \end{aligned} \tag{2.7}$$

$$\omega^i_{\mu_1\dots\mu_{k-1}} = \mathrm{d}y^i_{\mu_1\dots\mu_{k-1}} - y^i_{\mu_1\dots\mu_{k-1}\nu}\mathrm{d}x^\nu.$$

Notice that all contact forms ω vanish when evaluated along the prolongation of any section, i.e., $(j^k\sigma)^*\omega = 0$.

Whenever we consider a form α over J^kC we can uniquely split its pull-back $(\pi^{k+1}_k)^*\alpha$ into the sum of a horizontal part $\mathrm{hor}(\alpha)$ and a contact part $\alpha_{(K)}$ so that $(\pi^{k+1}_k)^*\alpha = \mathrm{hor}\alpha \oplus \alpha_{(K)}$, where both $\mathrm{hor}(\alpha)$ and $\alpha_{(K)}$ are forms over $J^{k+1}C$. By an abuse of notation one identifies $(\pi^{k+1}_k)^*\alpha$ with α and simply writes $\alpha = \mathrm{hor}\alpha \oplus \alpha_{(K)}$. For example, if $\alpha = \alpha_\mu \mathrm{d}x^\mu + \alpha_i \mathrm{d}y^i + \alpha^\mu_i \mathrm{d}y^i_\mu$ is a one-form over J^1C, where all coefficients depend on (x^μ, y^i, y^i_μ), then we have the splitting

$$\alpha = (\alpha_\mu + \alpha_i y^i_\mu + \alpha^\nu_i y^i_{\mu\nu})\mathrm{d}x^\mu \oplus (\alpha_i \omega^i + \alpha^\mu_i \omega^i_\mu) = \mathrm{hor}\alpha \oplus \alpha_{(K)}. \tag{2.8}$$

We stress once again that both $\mathrm{hor}(\alpha) = (\alpha_\mu + \alpha_i y^i_\mu + \alpha^\nu_i y^i_{\mu\nu})\mathrm{d}x^\mu$ and $\alpha_{(K)} = \alpha_i \omega^i + \alpha^\mu_i \omega^i_\mu$ are one-forms over J^2C since they both involve $y^i_{\mu\nu}$. Such an example can be easily generalized to any form over any J^kC (see Ref. 19).

A *Lagrangian of order k* is a bundle morphism $L: J^kC \to A_m(M)$, where $A_m(M)$ is the bundle of m-forms over M $[\dim(M) = m]$. Locally the Lagrangian is expressed as

$$L = \mathcal{L}(x^\mu, y^i, y^i_\mu, y^i_{\mu\nu}, \dots, y^i_{\mu_1\dots\mu_k})\mathbf{ds} \tag{2.9}$$

with $\mathbf{ds} = \mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^m$. We will consider only first order Lagrangians $(k=1)$ even though most of the theory can be easily generalized to any order (see Refs. 20–23). The *Poincaré–Cartan form* of a first order Lagrangian is the m-form Θ_L over J^1C locally given by

$$\Theta_L = \mathcal{L}\mathbf{ds} + p^\mu_i \omega^i \wedge \mathbf{ds}_\mu, \quad p^\mu_i = \frac{\partial \mathcal{L}}{\partial y^i_\mu}, \tag{2.10}$$

where $\mathbf{ds}_\mu = i_{\partial_\mu}\mathbf{ds}$ and p^μ_i are the *Lagrangian momenta*.

The action functional can be recast in terms of the Poincaré–Cartan form as

$$A_D(\sigma) \equiv \int_D L \circ j^1\sigma = \int_D (j^1\sigma)^*\Theta_L, \tag{2.11}$$

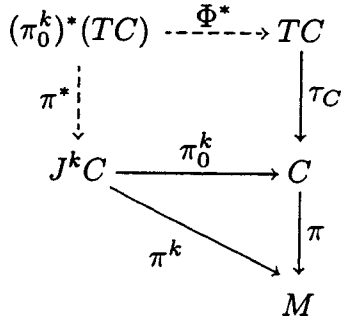
where $D \subseteq M$ is any compact domain with a regular boundary ∂D. If $X = \xi^i(x,y)\partial_i$ is any vertical vector field on C, together with its flow Φ_s and its lift j^1X to J^1C, we can drag the section σ along X by defining $\sigma_s = \Phi_s \circ \sigma$. The *variation of the action* along X is hence given by

$$\delta_X A_D(\sigma) = \frac{\mathrm{d}}{\mathrm{d}s} A_D(\sigma_s) = \int_D (j^1\sigma)^* \pounds_{j^1X}\Theta_L = \int_D (j^1\sigma)^* i_{j^1X}\mathrm{d}\Theta_L + \int_{\partial D} (j^1\sigma)^* i_{j^1X}\Theta_L, \tag{2.12}$$

where i_{j^1X} denotes contraction of forms along the vector field j^1X and $\mathrm{d}(\cdot)$ denotes the relevant exterior differential. If the vector X vanishes on the boundary ∂D of the region D, the second integral vanishes, too. By the Hamilton principle a section σ is then a *critical section* when $\delta_X A_D(\sigma) = 0$, for all regions D and any vertical vector field X which vanishes on ∂D. Equivalently, σ is a critical section if and only if $i_{j^1X}\mathrm{d}\Theta_L = 0$, for any vertical vector field X. This framework is completely equivalent to the ordinary Lagrangian framework (see Refs. 20 and 21). In fact, it can be easily shown that for X vanishing on the boundary one has $\delta_X A_D(\sigma) = \int_D (j^1\sigma)^* i_{j^1X} d\Theta_L = \int_D (j^2\sigma)^* \langle \mathbb{E}(L) | X \rangle$, where $\mathbb{E}(L)$ is the Euler–Lagrange morphism and $\langle | \rangle$ denotes the standard contraction. The Poincaré–Cartan formulation is well suited to deal with symmetries (as well as an introduction for Hamiltonian formalism and as a tool to unifying mechanics and field theory at any order). In mechanics all standard results are recovered.

III. GENERALIZED SYMMETRIES AND GENERALIZED NÖTHER THEOREM

Consider the following commutative diagram



(3.1)

The bundle $(\pi_0^k)^*(TC)$ is the pull-back of the bundle $\tau_C : TC \to C$ along the map $\pi_0^k : J^kC \to C$ and Φ^* is uniquely defined (see Refs. 10 and 19); a point in $(\pi_0^k)^*(TC)$ is a pair (p,v) where $p \in J^k\mathcal{C}$, $v \in TC$ and $\tau_C(v) = \pi_0^k(p)$, i.e., $v \in T_{\pi_0^k(p)}C$. Let Ξ be a section of the bundle $(\pi_0^k)^*(TC) \to J^k\mathcal{C}$ with local expression

$$\Xi : J^k\mathcal{C} \to (\pi_0^k)^*(TC) : p \mapsto (p, \xi^\mu(p)\partial_\mu + \xi^i(p)\partial_i). \tag{3.2}$$

The section Ξ is called a *generalized vector field* and by an abuse of notation is denoted simply by

$$\Xi = \xi^\mu(x^\mu, y^i, y^i_\mu, \ldots, y^i_{\mu_1 \ldots \mu_k})\partial_\mu + \xi^i(x^\mu, y^i, y^i_\mu, \ldots, y^i_{\mu_1 \ldots \mu_k})\partial_i . \tag{3.3}$$

Consider further a section $\sigma : M \to C$ together with its prolongation $j^k\sigma$; by composition we obtain a section $\Phi^* \circ \Xi \circ j^k\sigma$ of the bundle $TC \to M$ which is a *vector field over the section* σ. In principle, the section σ can be dragged along Ξ.

Notice that a generalized vector field Ξ is not a vector field on C (unless $k=0$) since its components depend on the derivatives of fields (see Ref. 2). Moreover, no jet prolongation $j^r\Xi$ of a generalized vector field Ξ is an ordinary vector field on any $J^s\mathcal{C}$. As an example, we can consider its prolongation to $J^1\mathcal{C}$

$$j^1\Xi = \xi^\mu\partial_\mu + \xi^i\partial_i + \xi^i_\mu\partial^\mu_i , \quad \xi^i_\mu = \mathrm{d}_\mu\xi^i - y^i_\nu \mathrm{d}_\mu\xi^\nu . \tag{3.4}$$

Clearly this is not a vector field on $J^1\mathcal{C}$ (since ξ^i_μ depends on the second order derivatives of fields) nor it is a vector field on $J^2\mathcal{C}$ [since no $\partial^{\mu\nu}_i$ is involved and the local expressions (3.4) do not glue together when changes of fibered coordinates on $\mathcal{C}$ are considered]. In other words, even if one can drag sections along a generalized vector field Ξ, such an object does not define a transformation on any finite jet bundle. Generalized vector fields can in fact be regarded as infinitesimal generators of transformations on $J^\infty C$ (see Refs. 2 and 18). We shall hereafter restrict to *projectable generalized vector fields* when the components $\xi^\mu(x)$ are independent on fields or *vertical generalized vector fields* which have $\xi^\mu = 0$.

Let σ_s be a family of sections of C and let Ξ be a projectable (generalized) vector field. The *vertical part* of $\Xi = \xi^\mu\partial_\mu + \xi^i\partial_i$ is defined by

$$\Xi_{(V)} = \xi^i - \xi^\mu y^i_\mu . \tag{3.5}$$

We remark that even when Ξ is an ordinary vector field the vertical part $\Xi_{(V)}$ is in any case a generalized (vertical) vector field. We say that σ_s is *dragged along* Ξ if and only if

$$\frac{\mathrm{d}}{\mathrm{d}s}\sigma_s = \Xi_{(V)} \circ \sigma_s . \tag{3.6}$$

A *generalized symmetry* of a Lagrangian L is a generalized vector field Ξ over C such that the Poincaré–Cartan form of L satisfies the following condition

$$\pounds_{j^1\Xi}\Theta_L = \omega + \mathrm{d}\alpha, \tag{3.7}$$

where ω is any contact form and α is any $(m-1)$-form (both possibly depending on the derivatives of fields).

Since the sum between horizontal and contact forms is direct, condition (3.7) is equivalent to

$$\mathrm{hor}(\pounds_{j^1\Xi}\Theta_L) = \mathrm{hor}\ \mathrm{d}\alpha, \tag{3.8}$$

which, since the Lie derivative of a contact form is again a contact form, is in turn equivalent to

$$\mathrm{hor}(\pounds_{j^1\Xi}(\mathrm{hor}\Theta_L)) = \mathrm{hor}(\pounds_{j^1\Xi}(\mathcal{L}\mathbf{ds})) = \mathrm{hor}\ \mathrm{d}\alpha. \tag{3.9}$$

By expanding this last equation in local fiber coordinates (x^μ, y^i, y^i_μ) over J^1C, for the jet prolongation of a (generalized) vector field $j^1\Xi = \xi^\mu\partial_\mu + \xi^i\partial_i + \xi^i_\mu\partial^\mu_i$ projecting onto $\xi = \xi^\mu\partial_\mu$, one obtains

$$[\mathrm{d}_\mu(\xi\mathcal{L}) - p_i(\xi^\mu y^i_\mu - \xi^i) - p^\mu_i(\xi^\nu y^i_{\mu\nu} - \xi^i_\mu)] = \mathrm{d}_\mu\alpha^\mu. \tag{3.10}$$

One can also regard this latter condition as a global condition expressed directly in terms of the Lagrangian (i.e., not involving the Poincaré–Cartan form); in the standard notation, see, e.g., Ref. 8, Eq. (3.10) can be in fact intrinsically expressed as

$$\pounds_\xi L - \langle \delta L | j^1\pounds_\Xi\sigma\rangle = \mathrm{Div}(\alpha). \tag{3.11}$$

In other words, a generalized symmetry leaves the Lagrangian form invariant modulo pure divergence terms plus terms which depend on the first variation δL. However, in the sequel we shall prefer to use the Poincaré–Cartan formalism which is more direct since it deals only with forms over J^kC.

If Ξ is a generalized symmetry, σ is a solution of field equations and σ_s is a dragging of σ along Ξ in the sense of (3.6), then σ_s is a solution for all s. In fact we have

$$\frac{\mathrm{d}}{\mathrm{ds}}A_D(\sigma_s) = \frac{\mathrm{d}}{\mathrm{ds}}\int_D (j^1\sigma_s)^*\Theta_L = \int_D (j^1\sigma)^*\pounds_{j^1\Xi}\Theta_L = \int_D (j^1\sigma)^*\omega + \int_D (j^1\sigma)^*\mathrm{d}\alpha. \tag{3.12}$$

The first integrand vanishes since ω is contact; by Stokes' theorem the second integral reduces to $\int_{\partial D}(j^1\sigma)^*\alpha$, which is constant with respect to deformations. In fact its variation along a vertical vector field X vanishes since $X=0$ on ∂D. Hence $(\mathrm{d}/\mathrm{ds})\,\delta_X A_D(\sigma_s) = 0$, which implies that the variation of the action is constant along the flow of the symmetry, which in turn preserves critical sections. The *generalized Nöther theorem* immediately follows. It is a constructive theorem associating to any symmetry generator Ξ a conserved current $\mathcal{E}$. In fact for any generalized symmetry generator Ξ (of order s) the following identity holds true:

$$\pounds_{j^1\Xi}\Theta_L = \omega + \mathrm{d}\alpha. \tag{3.13}$$

Expanding the Lie derivative and collecting terms it can immediately be recast as

$$\mathrm{d}(i_{j^1\Xi}\Theta_L - \alpha) = -i_{j^1\Xi}\mathrm{d}\Theta_L + \omega. \tag{3.14}$$

Define the quantities

$$\begin{cases} \mathcal{E} = (j^{2k-1}\sigma)^*(i_{j^1\Xi}\Theta_L - \alpha), \\ \mathcal{W} = -(j^{2k}\sigma)^* i_{j^1\Xi}\mathrm{d}\Theta_L. \end{cases} \tag{3.15}$$

Then the identity (3.14), pulled back on M along a section σ, can be expressed as

$$\mathrm{d}\mathcal{E}=\mathcal{W}. \tag{3.16}$$

This is the expression of Nöther's theorem; in fact, whenever σ is a solution of field equations, then $\mathcal{W}=0$ and hence the so-called *Nöther current* $\mathcal{E}$ is conserved, i.e., $\mathrm{d}\mathcal{E}=0$ which is equivalent to a continuity equation.

Equation, (3.16) is called a *weak conservation law* since it implies $\mathrm{d}\mathcal{E}=0$ on-shell (i.e., along critical sections).

For formal reasons it will be useful to define also the quantity

$$\overline{\mathcal{E}}=\mathrm{hor}(i_{j^1\Xi}\Theta_L-\alpha). \tag{3.17}$$

Because of the splitting into horizontal and contact part we have

$$(j^{2k}\sigma)^*\overline{\mathcal{E}}=\mathcal{E}. \tag{3.18}$$

IV. GENERALIZED SYMMETRIES IN MECHANICS AND SEPARATION OF VARIABLES

Let us consider a mechanical system described by a first order Lagrangian L (or, equivalently, by its Poincaré–Cartan form Θ_L) on the configuration bundle $C\simeq\mathbb{R}\times Q$ and a first order (projectable) generalized vector field

$$\Xi=\xi^\mu(t)\partial_t+\xi^i(t,q^i,\dot{q}^i)\partial_i. \tag{4.1}$$

The generator Ξ is a generalized symmetry if it leaves the Poincaré–Cartan form invariant modulo contact forms and exact forms, i.e., if

$$\pounds_{j^1\Xi}\Theta_L=\omega+\mathrm{d}\alpha, \tag{4.2}$$

where $\alpha(t,q,\dot{q})$ is a zero-form over $J^1C\simeq\mathbb{R}\times TQ$ and ω is a contact form. Then, in this case, we have for the horizontal part

$$\mathrm{hor}(\pounds_{j^1\Xi}\Theta_L)=\frac{\mathrm{d}\alpha}{\mathrm{d}t}\mathrm{d}t, \tag{4.3}$$

where $\mathrm{d}\alpha/\mathrm{d}t$ is the formal total derivative of α with respect of t and, consequently, the right hand side of Eq. (4.3) is an horizontal one-form over $J^2\mathcal{C}$. Hence Ξ is a generalized symmetry if and only if the horizontal part of the Lie derivative of the Poincaré–Cartan form is an exact differential.

Now one can consider $L'=\mathrm{hor}(\pounds_{j^1\Xi}\Theta_L)$ as an auxiliary Lagrangian. Whenever its equations of motion are identically satisfied, then L' is an exact differential. The equations of motion of the auxiliary Lagrangian L', considered as a system of partial differential equations for the components (ξ^μ,ξ^i) of the symmetry generator Ξ, are hence called the *covariance conditions for the original Lagrangian* L.

These partial differential equations are usually quite diffucult to solve, but one can try to solve them for the most general generalized symmetry and subsequently to apply the Nöther theorem with the aim of obtaining conserved quantities (i.e., first integrals in mechanics). As we shall see, such a computation leads to quite general results.

A. Free particle in the plane

Let us consider the free particle on the plane $\mathbb{R}^2$. Without loss of generality we can assume its mass to be unitary. The Lagrangian is hence

$$L=\tfrac{1}{2}(\dot{x}^2+\dot{y}^2)\mathrm{d}t. \tag{4.4}$$

The corresponding Poincaré–Cartan form reads

$$\Theta_L = -\tfrac{1}{2}(\dot{x}^2+\dot{y}^2)\mathrm{d}t+\dot{x}(\mathrm{d}x-\dot{x}\mathrm{d}t)+\dot{y}(\mathrm{d}y-\dot{y}\mathrm{d}t)=\tfrac{1}{2}(\dot{x}^2+\dot{y}^2)\mathrm{d}t+\dot{x}\mathrm{d}x+\dot{y}\mathrm{d}y. \tag{4.5}$$

Let us look for the general expression of the generators of generalized (first order) symmetries of L. A first order generalized vector field may be locally expressed as

$$\Xi = \xi(t)\partial_t+\Xi_x(t,x,y,\dot{x},\dot{y})\partial_x+\Xi_y(t,x,y,\dot{x},\dot{y})\partial_y. \tag{4.6}$$

Let us assume the components to be linear in the velocities, i.e., let us suppose that we have

$$\begin{aligned}\Xi_x(t,x,y,\dot{x},\dot{y})&=\alpha_x(t,x,y)+\xi_x(t,x,y)\dot{x}+\zeta_x(t,x,y)\dot{y},\\ \Xi_y(t,x,y,\dot{x},\dot{y})&=\alpha_y(t,x,y)+\zeta_y(t,x,y)\dot{x}+\xi_y(t,x,y)\dot{y}.\end{aligned} \tag{4.7}$$

The horizontal part of the Lie derivative of the Poincaré–Cartan form Θ_L with respect to the symmetry generator Ξ is hence

$$\begin{aligned}\mathrm{hor}(\pounds_{j^1\Xi}\Theta_L)=[&(\xi_x\dot{x}+\zeta_y\dot{y})\ddot{x}+(\zeta_x\dot{x}+\xi_y\dot{y})\ddot{y}+\dot{x}^2(\dot{x}\partial_x\xi_x+(\partial_y\xi_x+\partial_x\zeta_x+\partial_x\zeta_y)\dot{y}\\ &+\partial_t\xi_x+\partial_x\alpha_x-\tfrac{1}{2}\partial_t\xi)+\dot{y}^2(\dot{y}\partial_y\xi_y+(\partial_x\xi_y+\partial_y\zeta_y+\partial_y\zeta_x)\dot{x}+\partial_t\xi_y+\partial_y\alpha_y-\tfrac{1}{2}\partial_t\xi)\\ &+\dot{x}\dot{y}(\partial_y\alpha_x+\partial_y\alpha_x+\partial_t\zeta_x+\partial_t\zeta_y)+\dot{x}\partial_t\alpha_x+\dot{y}\partial_t\alpha_y.]\mathrm{d}t.\end{aligned} \tag{4.8}$$

To check whether (4.8) is a total derivative with respect to time we have to regard it as an auxiliary Lagrangian and see when its equations of motion identically vanish. In that way we obtain a system of partial differential equations which can be solved with respect to the symmetry generator Ξ. The result one obtains is the following general expression for the (generalized) symmetry generator:

$$\begin{aligned}\Xi=&a_0\xi(t)(\partial_t+\dot{x}\partial_x+\dot{y}\partial_y)\oplus a_1\partial_x\oplus b_1\partial_y\oplus a_2t\partial_x\oplus b_2t\partial_y\oplus a_3(xt-\dot{x}t^2)\partial_x\oplus b_3(yt+\dot{y}t^2)\partial_y\\ &\oplus a_4\dot{x}\partial_x\oplus b_4\dot{y}\partial_y\oplus a_5((tx\dot{x}-2ty\dot{x})\partial_x+(tx\dot{x}-x^2)\partial_y)\oplus b_5((ty\dot{y}-y^2)\partial_x+(ty\dot{y}-2tx\dot{y})\partial_y)\\ &\oplus a_6((y-\dot{y}t)\partial_x-t\dot{x}\partial_y)\oplus b_6(-t\dot{y}\partial_x+(x-\dot{x}t)\partial_y)\oplus a_7((x\dot{x}-2y\dot{y})\partial_x+x\dot{x}\partial_y)\\ &\oplus b_7(y\dot{y}\partial_x+(y\dot{y}-2x\dot{x})\partial_y)\oplus a_8(x-2t\dot{x})\partial_x\oplus b_8(y-2t\dot{y})\partial_y\oplus c_1(\dot{y}\partial_x+\dot{x}\partial_y)\\ &\oplus c_2((xy\dot{y}-y^2\dot{x})\partial_x+(xy\dot{x}-x^2\dot{y})\partial_y)\oplus c_3((yt-t^2\dot{y})\partial_x+(xt-t^2\dot{x})\partial_y),\end{aligned} \tag{4.9}$$

where a_1 $(i=0,1,\ldots,8)$, b_j $(j=1,2,\ldots,8)$ and c_l $(l=1,2,3)$ are 20 real constants.

Each of these generators yields a generalized symmetry for the Lagrangian L. We can now apply the Nöther theorem to obtain respectively the following 20 first integrals of motion (one of which is trivial) for the free particle in the plane:

$$\begin{aligned}E_0&=0,\\ E_1&=\dot{x},\quad E_2=\dot{y},\\ E_3&=t\dot{x}-x,\quad E_4=t\dot{y}-y,\\ E_5&=-\tfrac{1}{2}(x-t\dot{x})^2,\quad E_6=-\tfrac{1}{2}(y-t\dot{y})^2,\\ E_7&=\tfrac{1}{2}\dot{x}^2,\quad E_8=\tfrac{1}{2}\dot{y}^2,\\ E_9&=-(x-t\dot{x})(x\dot{y}-y\dot{x}),\quad E_{10}=(y-t\dot{y})(x\dot{y}-y\dot{x}),\\ E_{11}&=(x-t\dot{x})\dot{y},\quad E_{12}=(y-t\dot{y})\dot{x},\end{aligned} \tag{4.10}$$

$$E_{13}=(x\dot{y}-y\dot{x})\dot{x}, \quad E_{14}=(y\dot{x}-x\dot{y})\dot{y},$$

$$E_{15}=(x-t\dot{x})\dot{x}, \quad E_{16}=(y-t\dot{y})\dot{y},$$

$$E_{17}=\dot{x}\dot{y},$$

$$E_{18}=-\tfrac{1}{2}(x\dot{y}-y\dot{x})^2,$$

$$E_{19}=-(x-t\dot{x})(y-t\dot{y}).$$

One can easily check that all these quantities are conserved along solutions of the equations of motion of L. We should remark that the particular form of these first integrals of motion depends on the particular basis we have chosen for the symmetry generators, which in turn depends on the algorithm chosen to solve the covariance condition. One is free to change the basis, i.e., to perform any linear combination of the first integrals of motion. For example, one can consider $E_{11}-E_{12}=x\dot{y}-y\dot{x}$, and recover angular momentum.

It is known (see Refs. 1 and 24–26) that there are exactly four coordinate systems (independent on time) which lead to the separation of variables of the corresponding Hamilton–Jacobi equation in the plane; they are related to the following first integrals of motion (see Refs. 1 and 25):

$$\begin{gathered}\dot{x}^2=2E_7 \quad \text{(Cartesian coordinates)},\\ (x\dot{y}-y\dot{x})\dot{y}=-E_{14} \quad \text{(parabolic coordinates)},\\ (x\dot{y}-y\dot{x})^2=-2E_{18} \quad \text{(polar coordinates)},\\ -2E_{18}-c\dot{y}(x\dot{y}-y\dot{x})=-2E_{18}+2c^2E_7 \quad \text{(Elliptic coordinates)}.\end{gathered} \tag{4.11}$$

Consequently we can relate (modulo overall constant factors which are unessential) the four separation of variables in the plane with the following symmetry generators:

$$\begin{gathered}\Xi_1=\dot{x}\partial_x \quad \text{(Cartesian coordinates)},\\ \Xi_2=y\dot{y}\partial_x+(y\dot{y}-2x\dot{x})\partial_y \quad \text{(parabolic coordinates)},\\ \Xi_3=(x\dot{y}-y\dot{x})(y\partial_x-x\partial_y) \quad \text{(polar coordinates)}.\\ \Xi_4=\Xi_3\oplus c(y\dot{y}\partial_x+(y\dot{y}-2x\dot{x})\partial_y) \quad \text{(Elliptic coordinates)}.\end{gathered} \tag{4.12}$$

Notice that none of these is an ordinary vector field so that separation of variables is not related to ordinary vector fields and generalized symmetries are required. Explicit calculations have been carried out by using the MapleV tensor package (see Ref. 27).

B. Kepler problem

Let us consider a particle on the plane attracted to a fixed center by a Newtonian potential. We can assume its mass to be unitary. The Lagrangian is hence

$$L=\left[\frac{1}{2}(\dot{r}^2+r^2\dot{\theta}^2)+\frac{\kappa}{r}\right]\mathrm{d}t. \tag{4.13}$$

The corresponding Poincaré–Cartan form reads as

$$\Theta_L=\left[\frac{1}{2}(\dot r^2+r^2\dot\theta^2)+\frac{\kappa}{r}\right]\mathrm{d}t+\dot r(\mathrm{d}r-\dot r\,\mathrm{d}t)+r^2\dot\theta(\mathrm{d}\theta-\dot\theta\mathrm{d}t)=-\left[\frac{1}{2}(\dot r^2+r^2\dot\theta^2)-\frac{\kappa}{r}\right]\mathrm{d}t+\dot r\,\mathrm{d}r+r^2\dot\theta\,\mathrm{d}\theta. \tag{4.14}$$

Let us look for the general expression of the generators of generalized (first order) symmetries of L. A first order generalized vector field is locally expressed as

$$\Xi=\xi(t)\partial_t+\Xi_x(t,x,y,\dot x,\dot y)\partial_x+\Xi_y(t,x,y,\dot x,\dot y)\partial_y\,, \tag{4.15}$$

and the components are assumed to be linear in the velocities, i.e., we have

$$\begin{aligned}\Xi_x(t,x,y,\dot x,\dot y)&=\alpha_x(t,x,y)+\xi_x(t,x,y)\dot x+\zeta_x(t,x,y)\dot y,\\ \Xi_y(t,x,y,\dot x,\dot y)&=\alpha_y(t,x,y)+\zeta_y(t,x,y)\dot x+\xi_y(t,x,y)\dot y.\end{aligned} \tag{4.16}$$

The resulting generalized symmetry generators have the following general expression:

$$\begin{aligned}\Xi=a_0\partial_t\oplus a_1\partial_\theta\oplus a_2(r^2\dot\theta\sin\theta\partial_r+(-2r\cos\theta+\dot r\sin\theta)\partial_\theta)\\ \oplus a_3(r^2\dot\theta\cos\theta\partial_r+(-2r\sin\theta+\dot r\cos\theta)\partial_\theta)\oplus a_4r^2\dot\theta\partial_\theta\,,\end{aligned} \tag{4.17}$$

where a_i $(i=0,1,2,3,4)$ are five real constants.

All these generators can be directly checked to provide a generalized symmetry for the Lagrangian L. We can apply Nöther's theorem to obtain respectively the following five first integrals of motion

$$\begin{aligned}E_0&=\frac{1}{2}(\dot r^2+r^2\dot\theta^2)-\frac{\kappa}{r},\\ E_1&=r^2\dot\theta,\\ E_2&=r^3\dot\theta^2\cos\theta+r^2\dot r\,\dot\theta\sin\theta-\kappa\cos\theta,\\ E_3&=r^3\dot\theta^2\sin\theta+r^2\dot r\,\dot\theta\cos\theta-\kappa\sin\theta,\\ E_4&=-\tfrac{1}{2}r^4\dot\theta^2.\end{aligned} \tag{4.18}$$

The first one is total energy, the second the z-component of angular momentum; the vector $L=E_2\partial_x+E_3\partial_y=v\times(r\times v)-\kappa\partial_r$ is the so-called *Laplace vector*, also known as the *Runge–Lenz vector*, which is related to the perihelia precession.

One can easily check that all these quantities are conserved along solutions of the equations of motion. The integral E_4 leads to polar separation. The components of the Laplace vector E_2 lead to parabolic separation, while $-2E_4+2c^2E_2$ leads to elliptic separation (c is the distance between the center and the focuses) (see Refs. 1, 24 and 25).

Explicit calculations have been carried out by using the Maple V tensor package (see Ref. 27).

V. BRST TRANSFORMATIONS

As an example of generalized symmetries in field theories we shall hereafter consider BRST transformations, which are very relevant to the contemporary approach to quantum field theories (see Refs. 4, 12 and reference quoted therein).

Let us consider Minkowski space–time (M,η) on which we choose Cartesian coordinates x^μ and we define the dynamical field A^C_μ. The field A^C_μ is a Yang–Mills field, i.e., a principal

connection on a suitable (*a priori* fixed) principal bundle $\mathcal{P}$ with a semisimple gauge group G (see Ref. 28). The Cartan–Killing metric over G will be denoted by κ_{AB}. The curvature of A^C_μ is given by

$$F^A{}_{\mu\nu}=\mathrm{d}_\nu A^C_\mu-\mathrm{d}_\mu A^C_\nu+c^C{}_{AB}A^A_\mu A^B_\nu, \quad F^{\mu\nu}_A\equiv\kappa_{AB}F^B_{\rho\sigma}g^{\mu\rho}g^{\nu\sigma}. \tag{5.1}$$

The Yang–Mills Lagrangian,

$$L_{\mathrm{YM}}=-\tfrac{1}{4}F^A_{\mu\nu}F^{\mu\nu}_A\sqrt{g}\,\mathbf{ds}, \tag{5.2}$$

has very attractive symmetry properties related to gauge transformations.

From a quantum viewpoint, however, the situation does not appear so positive. The Yang–Mills Lagrangian is degenerate; as a direct consequence one cannot define the propagator of the Yang–Mills field. This is ultimately due to the fact that the gauge field A^A_μ contains both physical and unphysical degrees of freedom. One usually fixes a gauge, for example, the Lorentz gauge $g^{\mu\nu}\mathrm{d}_\mu A^A_\nu=0$. This solves the problem of propagators, but unfortunately the theory is no longer unitary, i.e. its dynamics does not conserve probability normalization (see 12). Fortunately enough unitarity can be restored by introducing a *ghost field* c^A together with its antighost field $\overline{c^A}$. In our case $(c^A,\overline{c^A})$ are scalar anticommuting fields. Another field B^A has to be introduced as a Lagrangian multiplier for the Lorentz gauge fixing.

Following Ref. 4, we consider the Lagrangian

$$L_{\mathrm{BRST}}=\left[-\frac{1}{4}F^A{}_{\mu\nu}F_A{}^{\mu\nu}+\mathrm{d}^\mu\overline{c}_A D_\mu c^A-\mathrm{d}^\mu B_A A^A_\mu+\frac{\alpha}{2}B_A B^A\right]\sqrt{g}\,\mathbf{ds}, \tag{5.3}$$

where α is a coupling constant and $D_\mu c^A=\mathrm{d}_\nu c^A+c^A{}_{BC}A^B_\mu c^A$, is the covariant derivative of the ghost field. Modulo a pure divergence term $-\mathrm{d}^\mu(B_A A^A_\mu)$, one can identify the Lagrange multiplier term $B_A\mathrm{d}^\mu A^A_\mu$ in order to introduce the Lorentz gauge and the ghost kinetic term $\mathrm{d}^\mu\overline{c}_A D_\mu c^A$. This Lagrangian is no longer gauge covariant but it yields a unitary quantum field theory and it defines good propagators which are nonetheless gauge dependent. However, propagators are not observable physical quantities. Only Green functions will be observable and one can prove that they are not affected by the gauge choice; gauge covariance is hence restored at an observational level.

The field equations are

$$\begin{gathered}
D_\nu F_C{}^{\nu\lambda}=\mathrm{d}^\lambda\overline{c}_A c^A{}_{BC}c^B+\mathrm{d}^\lambda B_C,\\
\Box\overline{c}_A+\overline{c}_C c^C{}_{AB}\mathrm{d}^\mu A^B_\mu=\mathrm{d}^\mu(\overline{c}_C c^C{}_{AB}A^B_\mu),\\
\Box c^A=\mathrm{d}^\mu(c^A{}_{BC}A^B_\mu c^C),\\
\alpha B^A+\mathrm{d}^\mu A^A_\mu=0,
\end{gathered} \tag{5.4}$$

where, as usual, we restrict to deformations which keep the background η fixed and where we denote by $\Box$ the box operator $\Box=\mathrm{d}^\mu\mathrm{d}_\mu$.

In the quantization of such a theory, which is beyond the scope of this article, it turns out to be useful to notice that the Lagrangian L_{BRST} is covariant with respect to the following generalized transformations:

$$\begin{gathered}
\delta A^A{}_\mu=\epsilon D_\mu c^A=\epsilon(\mathrm{d}_\mu c^A+c^A{}_{BC}A^B_\mu c^C),\\
\delta c^A=-\frac{\epsilon}{2}\{c,c\}^A,\\
\delta\overline{c^A}=\epsilon B^A,
\end{gathered} \tag{5.5}$$

$$\delta B^A = 0,$$

where $\{c,c\}^A = c^A{}_{BC} c^B c^C$ is the relevant (anti)-commutator. We remark that $\delta c^A \neq 0$, since c^A is an anticommuting field.

These are generalized symmetries, both since they depend on the derivatives of fields (thus they are generalized vector fields Ξ in the sense of our definition above)

$$\Xi = (D_\mu c^A) \frac{\partial}{\partial A^A{}_\mu} - \frac{1}{2}\{c,c\}^A \frac{\partial}{\partial c^A} + B^A \frac{\partial}{\partial \overline{c^A}}, \tag{5.6}$$

and since they do not leave the Poincaré–Cartan form invariant. In fact, one can easily check that the Poincaré–Cartan form is (see Ref. 4)

$$\begin{aligned}\Theta_L = \mathcal{L}\mathbf{ds} + [F_A{}^{\mu\nu}(\mathrm{d}A^A_\nu - \mathrm{d}_\lambda A^A_\nu \mathrm{d}x^\lambda) + \mathrm{d}^\mu \overline{c}_A (\mathrm{d}c^A - \mathrm{d}_\lambda c^A \mathrm{d}x^\lambda) \\ + (\mathrm{d}\overline{c}_A - \mathrm{d}_\lambda \overline{c}_A \mathrm{d}x^\lambda)(\mathrm{d}_\nu c^A + c^A{}_{BC} A^B_\nu c^C) g^{\mu\nu} - A^A_\nu g^{\mu\nu}(\mathrm{d}B^A - \mathrm{d}_\lambda B^A \mathrm{d}x^\lambda)] \wedge \mathbf{ds}_\mu .\end{aligned} \tag{5.7}$$

Its Lie derivative along Ξ is given by

$$\pounds_{j^1\Xi}\Theta = -F_A{}^{\mu\nu}(\mathrm{d}c^A_\mu - c^A_{\mu\lambda}\mathrm{d}x^\lambda) \wedge \mathbf{ds}_\nu + \mathrm{d}^\mu B_A (\mathrm{d}c^A - c^A_\lambda \mathrm{d}x^\lambda) \wedge \mathbf{ds}_\mu . \tag{5.8}$$

Hence the hypotheses of the generalized Nöther theorem are satisfied and the conserved currents are given by

$$\mathcal{E}(L,\Xi) = [F_A{}^{\mu\nu} D_\nu c^A - B_A D^\mu c^A + \tfrac{1}{2}\, \mathrm{d}^\mu \overline{c}_A \{c,c\}^A] \mathbf{ds}_\mu . \tag{5.9}$$

VI. WESS–ZUMINO MODEL

We consider finally another example of generalized symmetries in field theory (see Refs. 3, 13, 29). Let us fix a signature $\eta = (r,s)$ and a principal $\mathrm{Spin}(\eta)$-bundle Σ over the space–time M of dimension $m = r+s$. Consider the action

$$\lambda : \mathrm{Spin}(\eta) \times \mathrm{GL}(m) \to \mathrm{GL}(m), \quad \lambda(S,J) \cdot e^\mu_a = J^\mu_\nu \cdot e^\nu_b \not{\rho}^b_a (S^{-1}), \tag{6.1}$$

where $\not{\rho} : \mathrm{Spin}(\eta) \to \mathrm{SO}(\eta)$ is the covering map exhibiting the spin group as a double covering of the orthogonal group in the fixed signature. By means of the action λ we can define the associated bundle $\Sigma_\lambda = \Sigma \times_M L(M) \times_\lambda \mathrm{GL}(m)$ which admits fiber coordinates (x^μ, e^μ_a). The fields e^μ_a are called *spin frames on* Σ and they are in one-to-one correspondence with the spin structures defined on Σ (see Refs. 30 and 31 and references quoted therein). A spin frame e^μ_a induces a metric $g_{\mu\nu} = e^a_\mu \eta_{ab} e^b_\nu$ (e^b_ν being the inverse matrix of e^μ_a). Despite the fact that spin frames can be locally confused with local sections of $L(M)$, their behavior with respect to change of coordinates and their global properties differ from local frames (see Refs. 30–32). We have to warn the reader that in many cases in the literature of spinor physics when vielbein are mentioned spin frames in fact are what is meant. One can recognize this by comparing the expression for the covariant derivative of vielbein (which is there introduced as an *ad hoc* prescription) and the canonical covariant derivative for spin frames (see Refs. 33 and 34).

Let us then consider another representation of the spin group

$$\rho : \mathrm{Spin}(\eta) \times V \to V, \quad \rho(S) \cdot \psi^a = \rho^a_b(S) \psi^b, \tag{6.2}$$

induced by the choice of a set of $k \times k$ Dirac matrices γ_a such that $\{\gamma_a, \gamma_b\} = 2\eta_{ab}\mathbb{I}$, η_{ab} being the canonical diagonal matrix in signature $\eta = (r,s)$. As a further Hermitian requirement we assume that $\gamma_0 \gamma_a^\dagger \gamma_0 = \gamma_a$. The sections ψ of the associated bundle $\Sigma_\rho = \Sigma \times_\rho V$ are called *spinor fields*. The conjugation $\overline{\psi} = \psi^\dagger \gamma^0$ induces an inner product on spinors given by $\overline{\psi}\psi$. Hereafter (see also Refs. 10, 17, and 35) we shall consider $V = [\Lambda_-]^k$ modeled on the odd part of an exterior algebra

so that the local components $\psi^a: U \to \Lambda_-$ of spinors actually anticommute, i.e., $\psi^a \phi^b = -\phi^b \psi^a$. This is necessary for path integral quantization (see Refs. 3 and 36) in order to implement the Pauli principle. Hence we implement it from the very beginning also in the classical framework. For convenience we consider Majorana spinors. Recall that a spinor field ψ is called a *Majorana spinor* if it satisfies the condition $\psi = C\overline{\psi}^{\dagger}$, where C is the *charge conjugation operator*. In dimension $m=4$ and Lorentzian signature $\eta=(1,3)$ we choose a set of Dirac matrices

$$\gamma_0 = \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}, \quad \gamma_i = \begin{pmatrix} 0 & -\sigma^i \\ \sigma^i & 0 \end{pmatrix}, \tag{6.3}$$

where the σ^i two-by-two matrices denote the standard Pauli matrices. We have

$$C = \begin{pmatrix} -i\sigma^2 & 0 \\ 0 & i\sigma^2 \end{pmatrix}, \quad \psi_{\mathrm{Maj}} = \begin{pmatrix} \alpha \\ i\sigma^2 {}^t\alpha^{\dagger} \end{pmatrix}, \tag{6.4}$$

where α is any two-component spinor. The action of the spin group Spin(1,3) is compatible with the Majorana condition, so that Majorana spinors are globally well-defined.

Let us consider the following fields: a Majorana (anticommuting) field ψ and four scalar (possibly densities) commuting fields (A,B,C,D) on a space–time manifold M with a spin frame e_a^{μ} fixed on it. We shall denote by e_{μ}^{a} the spin coframe which is represented by the inverse of the matrix e_a^{μ}. As a consequence of the spin frame fixing the manifold M is endowed with an induced metric structure g and a compatible spin structure. We further consider the Lagrangian

$$\begin{aligned} L_{\mathrm{WZ}} = {} & \frac{\lambda}{2}(\nabla_{\mu} A \nabla^{\mu} A + D^2 + 2mAD) e \mathbf{ds} - \overline{\psi}(i\gamma^a \nabla_a \psi + m\psi)) e \mathbf{ds} \\ & + \frac{\lambda}{2}(\nabla_{\mu} B \nabla^{\mu} B + C^2 - 2mBC) e^3 \, \mathbf{ds}. \end{aligned} \tag{6.5}$$

Here the covariant derivatives of scalar fields are considered with respect to the Levi-Civita connection induced by the metric, which is in turn induced by the spin frame. Analogously, the covariant derivatives of spinors are with respect to the spin connection induced by the spin frame, i.e.,

$$\nabla_a \psi = e_a^{\mu}(\mathrm{d}_{\mu}\psi + \tfrac{1}{8}\, \Gamma_{\mu}^{ab}[\gamma_a, \gamma_b]\psi), \quad \Gamma_{\mu}^{ab} = e_{\rho}^{a}(\Gamma_{\sigma\mu}^{\rho} e_c^{\sigma} + \mathrm{d}_{\mu} e_c^{\rho})\, \eta^{cb}. \tag{6.6}$$

This Lagrangian is kept invariant (modulo divergence terms) by the infinitesimal transformations

$$\begin{aligned} & \delta A = \frac{a}{2}(\overline{\epsilon}\psi), \quad \delta C = -\frac{a}{2}(\overline{\epsilon}\gamma^5 \gamma^a \nabla_a \psi) e^{-1}, \\ & \delta B = -i\frac{a}{2}(\overline{\epsilon}\gamma^5 \psi) e^{-1}, \quad \delta D = i\frac{a}{2}(\overline{\epsilon}\gamma^a \nabla_a \psi), \\ & \delta\psi = \frac{a}{2}[(\gamma^a \epsilon) i \nabla_a A + (\gamma^a \gamma^5 \epsilon) e \nabla_a B + (\gamma^5 \epsilon) ieC + (\epsilon) D], \\ & \delta\overline{\psi} = \frac{a}{2}[-i\nabla_a A(\overline{\epsilon}\gamma^a) - e\nabla_a B(\overline{\epsilon}\gamma^5 \gamma^a) + ieC(\overline{\epsilon}\gamma^5) + D(\overline{\epsilon})]. \end{aligned} \tag{6.7}$$

Here the transformation parameter ϵ is a Majorana (anticommuting) spinor which is assumed to be covariantly conserved, i.e., $\nabla_{\mu}\epsilon = 0$. Further comments about spinor transformation (anticommut-

ing) parameters will follow below. Notice that the relative coupling constants appear to be fixed by the requirement that the infinitesimal transformations (6.7) are symmetries of the Lagrangian L_{WZ}. On the contrary, one could replace the fields (A,B,C,D) with scalar densities of arbitrary weight. (Of course, in this case the Lagrangian has then to undergo a number of minor changes to manitain covariance.)

We stress that the condition for ϵ to be covariantly conserved is a very strong one. It corresponds more or less to the point independent transformation on which gauge theories are based. The model we present here is a first step towards a field theory which is covariant with respect to point-dependent transformations. Such a theory is called *supergravity* and one has to redefine the Lagrangian and to introduce auxiliary fields to obtain covariance with respect to this wider class of transformations (see Ref. 13). Here we are not interested in these generalizations for which we refer the interested reader to Refs. 3 and 13. Under these conditions the transformation (6.7) is global only when trivial structure bundles $\Sigma = M \times \mathrm{Spin}(\eta)$ are considered.

One can define the infinitesimal (vertical) generalized symmetry

$$\Xi = (\delta A)\frac{\partial}{\partial A} + (\delta B)\frac{\partial}{\partial B} + (\delta C)\frac{\partial}{\partial C} + (\delta D)\frac{\partial}{\partial D} + (\delta\psi)\frac{\partial}{\partial \psi} + (\delta\overline{\psi})\frac{\partial}{\partial \overline{\psi}}, \tag{6.8}$$

which is called the *supersymmetry generator* and which can be shown to leave the Lagrangian invariant modulo the following divergence term:

$$\delta L_{\mathrm{WZ}} = \mathrm{Div}(\alpha), \tag{6.9}$$

$$\alpha = \frac{a}{4}[(2imA(\overline{\epsilon}\gamma^{\mu}\psi) + 2\nabla^{\mu}A(\overline{\epsilon}\psi) - \nabla_{\nu}A(\overline{\epsilon}\gamma^{\nu}\gamma^{\mu}\psi) + iD(\overline{\epsilon}\gamma^{\mu}\psi))e + (2mB(\overline{\epsilon}\gamma^{5}\gamma^{\mu}\psi)$$
$$- 2i\nabla^{\mu}B(\overline{\epsilon}\gamma^{5}\psi) + i\nabla_{\nu}B(\overline{\epsilon}\gamma^{5}\gamma^{\nu}\gamma^{\mu}\psi) + C(\overline{\epsilon}\gamma^{\mu}\gamma^{5}\psi))e^{2}]\mathbf{ds}_{\mu}.$$

Notice that the supersymmetry generators are not closed with respect to the commutator. One can in fact check that, given two supersymmetries generated by ϵ_1 and ϵ_2, their commutator is the Lie derivative with respect to the vector field defined on the structure bundle Σ by

$$\hat{\xi} = \xi^{\mu}(\partial_{\mu} - \Gamma_{\mu}^{ab}\sigma_{ab}) \oplus (e_{\mu}^{a}\nabla_{\nu}\xi^{\mu}e^{b\nu})\sigma_{ab}, \quad \xi^{\mu} = i\frac{a^2}{2}(\epsilon_2\gamma^{\mu}\epsilon_1). \tag{6.10}$$

We remark that the vector field (6.10) is the so-called *Kosmann lift* of the space–time vector field $\xi = \xi^{\mu}\partial_{\mu}$ (see Ref. 34).

The vector fields (6.10) and the supersymmetry generators form an algebra with the following commutation rules.

$$[\delta_1, \delta_2] = \pounds_{\hat{\xi}}, \quad [\delta_1, \pounds_{\hat{\xi}}] = 0, \quad [\pounds_{\hat{\zeta}}, \pounds_{\hat{\xi}}] = 0. \tag{6.11}$$

Of course these vector fields do not span an ordinary Lie algebra, since some of the parameters are actually anticommuting, while the ordinary Lie algebra parameters are scalars. In fact, one should regard them as generators of a graded Lie algebra (also called *superalgebra*).

VII. CONCLUSION AND PERSPECTIVES

Nöther's theorem has been generalized to include a number of cases which play a prominent role in modern applications both in mechanics and field theory. As a first application of this generalized Nöther theorem we have shown how to recover the classical results for the separation of variables of the Hamilton–Jacobi equation in mechanics. This new perspective for separation of variables is particularly interesting. In fact Nöther's theorem is stated in a purely Lagrangian context. Though of course one needs the Hamiltonian formalism to obtain the Hamilton–Jacobi

equation, its separation of variables appears to be studied both in the Hamiltonian and in the Lagrangian framework.

This is of some interest for mechanics but may turn out to be very important in field theory. In field theory there are a number of examples of separation of variables which rely on operators which commute with field equations. The relation between separation of variables in mechanics and in field theory is still unclear. Although one has a fairly general theory on separation of variables in mechanics in field theory a general framework still needs to be developed. The generalized Nöther's theorem may provide such a framework for treating the problem of separation of variables in field theory. The advantage of this perspective is that it relies completely on the Lagrangian formalism which is quite important in field theory (where there is no general agreement on what is to be regarded as Hamiltonian framework). Further investigations will therefore be devoted to separation of variables in field theory.

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Radiation of horizontal electric dipole on large dielectric sphere

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The electromagnetic field in air of a radiating electric dipole located below and tangential to the surface of a homogeneous, isotropic and optically dense sphere is studied anew. The starting point is the eigenfunction expansion for the field in spherical harmonics, which is now converted into series of integrals via the Poisson summation formula. A creeping-wave structure for all six components along the boundary is revealed that consists of waves exponentially decreasing through air and rays bouncing and circulating inside the sphere. The character of individual modes of propagation and the interplay between ''electric'' and ''magnetic'' types of polarization are investigated. Connections with and differences from standard ray optics and the cases of the radiating vertical dipole and scalar plane-wave scattering are outlined. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The scattering and diffraction of electromagnetic waves have long been understood as boundary-value problems of Maxwell's equations. In principle, the field can be determined everywhere by specifying the source and the boundary conditions. In practice, even when closed-form solutions are then obtained, the chosen representations may not be amenable to quantitative understanding. This difficulty often plagues analyses where current sources lie too close to the boundary separating two media. Such a case arises in connection with the long-distance communication along the sea surface at very low frequencies.[1,2]

In the present article, a three-dimensional idealized model is studied in which the source is an electric dipole located below and tangential to the surface of a homogeneous and isotropic, electrically large sphere surrounded by air. Of course, none of the field components can be made to vanish identically in this case. A dipole vertical to the spherical boundary,[3,4] on the other hand, introduces an axis of symmetry, having only three nonzero spherical components; these admit eigenfunction expansions of simpler structure. In both problems, the formal solution is easily attainable in terms of spherical harmonics but is not directly amenable to computations and interpretation. One of the objectives of this work is to unveil the underlying physical picture by asymptotic methods for the case of the horizontal dipole, describing the interplay between two coexisting polarizations. The assumption of an optically dense sphere is thus imposed while attention is restricted to points lying in the spherical boundary. The analysis is also intended to reveal differences from the known case of plane-wave scattering in the context of the scalar wave and Schrödinger's equations. Because the emphasis is on the physical concepts and the tools needed to expose such concepts, actual numerical calculations are beyond the scope of this article.

There is a fairly long sequence of papers in connection with the present problem. Noteworthy is Mie's formal expansion[5] in partial waves for a plane wave incident on a homogeneous sphere. Another formulation found in a later paper by Debye[6] is related to his previous studies of high-frequency plane-wave scattering by an infinitely long cylinder.[7] An exposition and discussion of

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these as well as of other works was given by van de Hulst.[8] Watson[9] appears to be the first to investigate systematically the radiation of a point source in the presence of a sphere with radius large compared to the wavelength. In his formulation the source was an electric dipole located above and vertical to the surface of a perfectly conducting sphere; his focus was on scalar potentials that furnish the electromagnetic field via successive differentiations. The merits of Watson's approach are unquestionable: the slowly converging expansion in partial waves was converted to an integral which in turn generated a rapidly converging series. This method was later invoked by other authors[10–12] in their efforts to treat the case of a finitely conducting sphere. Among these authors, Gray,[12] for example, identified a ''magnetic'' type of wave propagating and attenuating through air with an attenuation rate independent of the adjacent medium, when the source is a magnetic dipole vertical to the surface of a lossy sphere.

Being aware of these works, Norton[13] proposed simplified formulas and graphs for the field intensity of vertical and horizontal dipoles elevated over a spherical earth. Bremmer[14,15] compared the fields of the two configurations by considering the direct wave and the leading reflected wave in free space; his analysis pointed to a simple picture for wave propagation in air for distances exceeding the free-space wavelength. The radiation of a horizontal dipole above a finitely conducting sphere was investigated by Fock[16] by use of scalar potentials. He approximated the field through air in the ''shadow region'' in terms of exponentially decreasing waves, and gave the corresponding attenuation rates as solutions to two uncoupled transcendental equations. Fock started with an extension of Watson's method[9] by neglecting the field that travels through the sphere and not examining the transition to planar-earth formulas. In the same spirit, the problem was essentially revisited by Wait[17] in the 1950s; he concluded that at ''low radio frequencies'' the horizontal component of the electric field is negligibly small compared to the vertical one. On the basis of Watson's method,[9] geometrical-ray pictures were invoked in that same period of time in the study of elastic waves inside spherical cavities.[18,19] (See Refs. 20 and 21 for later developments in the theory of elastic-wave propagation.)

In a remarkable paper, Wu[22] invoked the concept of the creeping wave in order to study the high-frequency scattering of plane waves by impenetrable cylinders and spheres in the context of Schrödinger's and Maxwell's equations. He derived asymptotic expansions for the total scattering cross sections that went well beyond the standard geometrical optics, and pointed out that a mathematical tool leading to the creeping wave in the case of a sphere is the Poisson summation formula. Notably, Wu[22] extended the familiar concept of the creeping wave in two space dimensions[23–26] from high frequencies to all positive frequencies by arguments of algebraic topology.[27] The underlying physical idea was soon after generalized to other scatterers by Seshadri.[28] A similar analysis based on the Poisson summation formula was later used by Nussenzveig,[29] who referred to Ref. 22, for the study of high-frequency, plane-wave scattering by transparent spheres. Key points in his analysis were the imposition of a large index of refraction and the expansion of the total scattering amplitude in a series of the Debye type.[7] Nussenzveig provided a description in terms of waves that attenuate exponentially along the boundary and rays bouncing and circulating inside the sphere. The relevant Poisson summation formula can be written as[30]

$$\sum_{l=0}^{\infty} g(l) = \sum_{n=-\infty}^{\infty} e^{-in\pi} \int_0^{\infty} d\nu\, g\left(\nu - \frac{1}{2}\right) e^{i2\pi n\nu}, \tag{1.1}$$

where the left-hand side is the starting eigenfunction expansion. The right-hand side of this equation was interpreted in terms of ''classical paths'' by Berry and Mount.[31] This interpretation stems from noticing that for high frequencies each index n identifies a path that encircles the origin n times.[31,32] Accordingly, these authors invoked stationary-phase calculations and elaborate uniform approximations.

Recently, Houdzoumis[3,4,33] applied the Poisson summation formula in order to study the radiation of a vertical electric dipole over a sphere, by imposing the simplifying assumption of a large index of refraction. As mentioned earlier, the number of nonzero field components is reduced

to three in this case, with the corresponding polarization being termed as of the ''electric type.'' Houdzoumis placed equal emphasis on the wave that attenuates exponentially along the boundary in air and the rays that circulate around the origin inside the sphere. King *et al.*[1,2] made use of these results for the surface wave in order to calculate the field of an antenna on the sea surface in the range of very low frequencies (VLF).

In the spirit of Houdzoumis' analysis,[3,4,33] the present article has a threefold purpose. The first purpose is to give the complete solution for the field of an electric dipole located inside a sphere without recourse to scalar potentials. The dipole is taken to lie in the plane defined by a local tangent and the center of the sphere, and is parallel to the tangent. The second purpose is to evaluate all six components when the dipole approaches the boundary from below by converting the series of partial waves into integrals according to the Poisson summation formula. In this limit all series diverge in the usual sense and some care needs to be exercised. By use of asymptotics, it is found that, apart from waves that reach the observation point with the air and earth phase velocities, significant contributions may arise from rays bouncing and circulating inside the sphere. The third purpose is to compare these findings with other, known cases such as the plane-wave scattering and the radiation of a vertical electric dipole.

The remainder of the article is organized as follows. Section II starts with Maxwell's equations; the ordinary differential equations in the radial distance for the θ- and ϕ-components of the field in spherical coordinates are solved explicitly. The eigenfunction expansions in spherical harmonics are then converted into series of integrals, and both the source and the observation point are allowed to approach the boundary. In Sec. III, integral expressions are obtained with the inverse electrical radius used as the expansion parameter. The lowest-order terms are known Sommerfeld integrals.[34] Corrections to these integrals account for the finite curvature of the boundary, describing waves that travel through air and through the dense medium. Integrated expressions are given for these waves when $k_2^2 \ll |k_1^2|$, $k_2\rho \gg 1$ and the observation angle θ is sufficiently small, where k_2 is the wave number in air, assumed to be real throughout the paper, k_1 is the complex wave number in the sphere, and ρ is the cylindrical distance from the source. The expressions for the wave through the sphere are new to the author's knowledge. The accompanying zeroth-order integral terms have been evaluated via rapidly converging series elsewhere.[34,35] In Sec. IV, the aforementioned asymptotic formulas are modified to account for the transition of the planar-boundary formulas to waves decreasing exponentially through air, with the distinction of two modes of propagation pertaining to polarizations of an ''electric'' and a ''magnetic'' type. A description is also provided for the field with the phase velocity of the enclosed medium. The analysis in Sec. V shows that, for $\theta = O(1)$ and $\pi - \theta = O(1)$, the total field consists of waves that attenuate exponentially, and rays that circulate in the sphere and are multiply reflected at the boundary. The contributions of these rays are negligible for a finitely conducting sphere. A few limiting cases of the ray contributions are placed under scrutiny, an example being the case where the antipodal point at $\theta = \pi$ is approached along the boundary. The interplay between contributions of the two polarizations to the ray amplitudes as well as deviations from the ray character are discussed.

In some of the calculations presented in this article, such as those in Appendix A, the wave number in the sphere, k_1, is treated as real for the sake of simplicity. This poses no restriction on the final asymptotic formulas, however, which are usable for complex values of k_1 with $0 \leqslant \mathrm{Arg}\, k_1 \leqslant \pi/4$, and are therefore applicable to spheres of finite conductivity. The $e^{-i\omega t}$ time dependence is suppressed throughout the analysis.

II. FORMULATION

A. Formal representations

The geometry of the problem is depicted in Fig. 1. It consists of an x-directed electric dipole S of unit moment located inside a homogeneous, isotropic and nonmagnetic sphere (region 1, $r < a$) at a distance b from the origin. The sphere is surrounded by air (region 2, $r > a$). Maxwell's equations in each region j ($j = 1, 2$) read as follows:

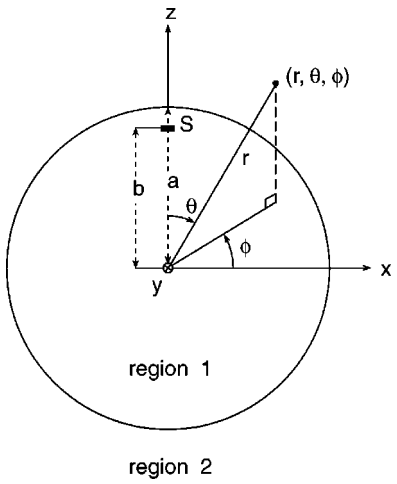

FIG. 1. Spherical coordinates and horizontal electric dipole S inside an isotropic and homogeneous sphere.

$$\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta E_{j\phi})-\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}(E_{j\theta})=i\omega B_{jr}, \tag{2.1}$$

$$\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}(E_{jr})-\frac{1}{r}\frac{\partial}{\partial r}(rE_{j\phi})=i\omega B_{j\theta}, \tag{2.2}$$

$$\frac{1}{r}\frac{\partial}{\partial r}(rE_{j\theta})-\frac{1}{r}\frac{\partial}{\partial\theta}(E_{jr})=i\omega B_{j\phi}, \tag{2.3}$$

$$\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta B_{j\phi})-\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}(B_{j\theta})=-i\frac{k_j^2}{\omega}E_{jr}, \tag{2.4}$$

$$\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}(B_{jr})-\frac{1}{r}\frac{\partial}{\partial r}(rB_{j\phi})=\mu_0 J_{j\theta}-i\frac{k_j^2}{\omega}E_{j\theta}, \tag{2.5}$$

$$\frac{1}{r}\frac{\partial}{\partial r}(rB_{j\theta})-\frac{1}{r}\frac{\partial}{\partial\theta}(B_{jr})=\mu_0 J_{j\phi}-i\frac{k_j^2}{\omega}E_{j\phi}, \tag{2.6}$$

where the current density is

$$\mathbf{J}(\mathbf{r})=\delta(x)\,\delta(y)\,\delta(z-b)\hat{\mathbf{x}}. \tag{2.7}$$

The field in region 1 is the superposition of a primary and a secondary field, viz.,

$$\mathbf{F}_1=\mathbf{F}_1^{(\mathrm{pr})}+\mathbf{F}_1^{(\mathrm{sc})},\quad \mathbf{F}=\mathbf{E},\,\mathbf{B}. \tag{2.8}$$

In order to calculate the primary field, introduce the vector potential $\mathbf{A}_1^{(\mathrm{pr})}=G(\mathbf{r};b)\hat{\mathbf{x}}$, where

$$G(\mathbf{r};b)=\frac{\mu_0}{4\pi}\frac{e^{ik_1R}}{R}=\frac{i\mu_0k_1}{4\pi}\sum_{l=0}^{\infty}(2l+1)j_l(k_1r_<)h_l^{(1)}(k_1r_>)\mathrm{P}_l(\cos\theta), \tag{2.9}$$

$R=\sqrt{r^2+b^2-2rb\cos\theta}$, $r_>$ is the larger of r and b, and $r_<$ is the smaller. j_l and $h_l^{(1)}$ denote the spherical Bessel and Hankel functions, and P_l^m is the Legendre function of the first kind.[36] Hence,

$$B_{1r}^{(\mathrm{pr})}=b_{1r}^{(\mathrm{pr})}(r,\theta)\sin\phi=-\frac{1}{r}\frac{\partial G}{\partial\theta}\sin\phi=-\frac{i\mu_0 k_1}{4\pi r}\sin\phi\sum_{l=0}^{\infty}(2l+1)j_l(k_1r_<)h_l^{(1)}(k_1r_>)\mathrm{P}_l^1(\cos\theta), \tag{2.10}$$

$$B_{1\theta}^{(\mathrm{pr})}=b_{1\theta}^{(\mathrm{pr})}(r,\theta)\sin\phi,\quad B_{1\phi}^{(\mathrm{pr})}=b_{1\phi}^{(\mathrm{pr})}(r,\theta)\cos\phi, \tag{2.11}$$

$$\begin{aligned}E_{1r}^{(\mathrm{pr})}=e_{1r}^{(\mathrm{pr})}(r,\theta)\cos\phi&=-\frac{i\omega}{k_1^2 r}\frac{\partial}{\partial\theta}\left(\frac{\partial G}{\partial b}+\frac{1}{b}G\right)\cos\phi\\&=\frac{\omega\mu_0}{4\pi b}\frac{1}{k_1 r}\cos\phi\sum_{l=0}^{\infty}(2l+1)\psi_l(k_1r)[\breve{\psi}_l(k_1b)+k_1b\,\breve{\psi}_l'(k_1b)]\mathrm{P}_l^1(\cos\theta),\end{aligned} \tag{2.12}$$

$$E_{1\theta}^{(\mathrm{pr})}=e_{1\theta}^{(\mathrm{pr})}(r,\theta)\cos\phi,\quad E_{1\phi}^{(\mathrm{pr})}=e_{1\phi}^{(\mathrm{pr})}(r,\theta)\sin\phi, \tag{2.13}$$

where $(\psi_l,\breve{\psi}_l)=(j_l,h_l^{(1)})$ if $r<b$, $(\psi_l,\breve{\psi}_l)=(h_l^{(1)},j_l)$ if $r>b$, and the prime denotes differentiation with respect to the argument. Let

$$B_{jr}=b_{jr}(r,\theta)\sin\phi,\quad B_{j\theta}=b_{j\theta}(r,\theta)\sin\phi,\quad B_{j\phi}=b_{j\phi}(r,\theta)\cos\phi, \tag{2.14}$$

$$E_{jr}=e_{jr}(r,\theta)\cos\phi,\quad E_{j\theta}=e_{j\theta}(r,\theta)\cos\phi,\quad E_{j\phi}=e_{j\phi}(r,\theta)\sin\phi. \tag{2.15}$$

It follows that

$$\frac{\partial^2}{\partial r^2}(rb_{j\phi})+k_j^2(rb_{j\phi})=\frac{1}{\sin\theta}\frac{\partial}{\partial r}(b_{jr})+\frac{ik_j^2}{\omega}\frac{\partial}{\partial\theta}(e_{jr}), \tag{2.16}$$

$$\frac{\partial^2}{\partial r^2}(re_{j\phi})+k_j^2(re_{j\phi})=-i\omega\frac{\partial}{\partial\theta}(b_{jr})-\frac{1}{\sin\theta}\frac{\partial}{\partial r}(e_{jr}), \tag{2.17}$$

$$b_{j\theta}=\frac{i}{\omega}\left[\frac{1}{r\sin\theta}e_{jr}+\frac{1}{r}\frac{\partial}{\partial r}(re_{j\phi})\right], \tag{2.18}$$

$$e_{j\theta}=\frac{i\omega}{k_j^2}\left[\frac{1}{r\sin\theta}b_{jr}-\frac{1}{r}\frac{\partial}{\partial r}(rb_{j\phi})\right]. \tag{2.19}$$

The total field must be bounded at the origin and satisfy the usual radiation conditions.[37] It is natural to set

$$e_{1r}^{(\mathrm{sc})}=-\frac{\mu_0\omega}{4\pi r}\frac{1}{k_1b}\sum_{l=0}^{\infty}(2l+1)\tilde{A}_l j_l(k_1r)[j_l(k_1b)+k_1bj_l'(k_1b)]\mathrm{P}_l^1(\cos\theta), \tag{2.20}$$

$$e_{2r}=\frac{\mu_0\omega}{4\pi r}\frac{1}{k_1b}\sum_{l=0}^{\infty}(2l+1)\tilde{B}_l h_l^{(1)}(k_2r)[j_l(k_1b)+k_1bj_l'(k_1b)]\mathrm{P}_l^1(\cos\theta), \tag{2.21}$$

$$b_{1r}^{(\mathrm{sc})}=\frac{i\mu_0 k_1}{4\pi r}\sum_{l=0}^{\infty}(2l+1)\tilde{C}_l j_l(k_1r)j_l(k_1b)\mathrm{P}_l^1(\cos\theta), \tag{2.22}$$

$$b_{2r}=-\frac{i\mu_0 k_1}{4\pi r}\sum_{l=0}^{\infty}(2l+1)\tilde{D}_l h_l^{(1)}(k_2r)j_l(k_1b)\mathrm{P}_l^1(\cos\theta), \tag{2.23}$$

where $\tilde{A}_l$, $\tilde{B}_l$, $\tilde{C}_l$, and $\tilde{D}_l$ are coefficients yet to be determined.

In region 1, Eqs. (2.16) and (2.17) split into two equations by virtue of Eq. (2.8). In compact notation, these equations are

$$\frac{\partial^2}{\partial r^2}(rw)+k^2(rw)=\frac{1}{\sin\theta}\frac{\partial g}{\partial r}, \tag{2.24a}$$

$$\frac{\partial^2}{\partial r^2}(rw)+k^2(rw)=\frac{\partial g}{\partial \theta}, \tag{2.24b}$$

where $g=g(r,\theta)$ ($g=b_{jr},e_{jr}$) is treated as known. Specifically,

$$g(r,\theta)=r^{-1}\sum_{l=0}^{\infty}(2l+1)c_l\psi_l(kr)\mathrm{P}_l^1(\cos\theta). \tag{2.25}$$

In the above, $\psi_l=j_l$ and $k=k_1$ if $r<a$, $\psi_l=h_l^{(1)}$ and $k=k_2$ if $r>a$.

A solution to Eq. (2.24a) is

$$rw(r,\theta)=\frac{1}{\sin\theta}\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}c_l w_l(r)\mathrm{P}_l^1(\cos\theta). \tag{2.26}$$

Each $w_l(r)$ ($l=0, 1, 2, \ldots$) should of course satisfy

$$\left(\frac{d^2}{dr^2}+k^2\right)w_l(r)=-\frac{l(l+1)}{r^2}[\psi_l(kr)-kr\psi_l'(kr)], \tag{2.27}$$

and therefore equals $w_l(r)=(d/dr)[r\psi_l(kr)]$. With regard to Eq. (2.24b),

$$rw(r,\theta)=\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}c_l w_l(r)\frac{\partial \mathrm{P}_l^1}{\partial\theta}, \tag{2.28}$$

where $w_l(r)$ is forced to satisfy

$$\left(\frac{d^2}{dr^2}+k^2\right)w_l(r)=\frac{l(l+1)}{r}\psi_l(kr), \tag{2.29}$$

with an admissible solution $w_l(r)=r\psi_l(kr)$. Once $b_{j\phi}$ and $e_{j\phi}$ are determined in this fashion, $b_{j\theta}$ and $e_{j\theta}$ follow from Eqs. (2.18) and (2.19).

The coefficients $\tilde{A}_l$, $\tilde{B}_l$, $\tilde{C}_l$, and $\tilde{D}_l$ in Eqs. (2.20)–(2.23) are calculated via imposition of the continuity of E_ϕ and B_θ at $r=a$. These conditions yield two independent systems of linear equations, namely, one for $\tilde{A}_l$, $\tilde{B}_l$ and one for $\tilde{C}_l$ and $\tilde{D}_l$. The former set describes a magnetic-type (H-) polarization ($B_r=0$, $E_r\neq 0$), while the latter one pertains to an electric-type (E-) polarization ($E_r=0$, $B_r\neq 0$), in correspondence to the case with a planar boundary. Explicitly,

$$\tilde{A}_l=\frac{h_l^{(1)}(k_1a)}{j_l(k_1a)}\left\{\frac{1}{k_2a}+\frac{h_l^{(1)\prime}(k_2a)}{h_l^{(1)}(k_2a)}-\frac{k_2}{k_1}\left[\frac{1}{k_1a}+\frac{h_l^{(1)\prime}(k_1a)}{h_l^{(1)}(k_1a)}\right]\right\}\frac{1}{K_l}, \tag{2.30}$$

$$\tilde{B}_l=\frac{i}{k_1k_2a^2\,j_l(k_1a)h_l^{(1)}(k_2a)\,K_l}, \tag{2.31}$$

$$\tilde{C}_l=\frac{h_l^{(1)}(k_1a)}{j_l(k_1a)}\left[\frac{h_l^{(1)'}(k_1a)}{h_l^{(1)}(k_1a)}-\frac{k_2}{k_1}\frac{h_l^{(1)'}(k_2a)}{h_l^{(1)}(k_2a)}\right]\frac{1}{M_l}, \tag{2.32}$$

$$\tilde{D}_l=-\frac{i}{(k_1a)^2 j_l(k_1a)h_l^{(1)}(k_2a)\,M_l}, \tag{2.33}$$

where the two principal denominators read as

$$K_l=\frac{h_l^{(1)'}(k_2a)}{h_l^{(1)}(k_2a)}+\frac{1}{k_2a}-\frac{k_2}{k_1}\left[\frac{1}{k_1a}+\frac{j_l'(k_1a)}{j_l(k_1a)}\right], \tag{2.34}$$

$$M_l=\frac{j_l'(k_1a)}{j_l(k_1a)}-\frac{k_2}{k_1}\frac{h_l^{(1)'}(k_2a)}{h_l^{(1)}(k_2a)}. \tag{2.35}$$

The terminology above primarily serves the purpose of distinguishing between contributions from these two denominators.

The field in region 2 is

$$E_{2r}=\frac{i\omega\mu_0}{4\pi k_1 r k_2 a^2}\cos\phi\sum_{l=0}^{\infty}(2l+1)\frac{j_l(k_1b)}{j_l(k_1a)}\frac{h_l^{(1)}(k_2r)}{h_l^{(1)}(k_2a)}\frac{1}{K_l}\left[\frac{1}{k_1b}+\frac{j_l'(k_1b)}{j_l(k_1b)}\right]\mathrm{P}_l^1(\cos\theta), \tag{2.36}$$

$$\begin{aligned}E_{2\theta}=&\frac{i\omega\mu_0}{4\pi k_1 a^2}\cos\phi\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}\frac{j_l(k_1b)}{j_l(k_1a)}\frac{h_l^{(1)}(k_2r)}{h_l^{(1)}(k_2a)}\frac{1}{K_l}\left[\frac{1}{k_1b}+\frac{j_l'(k_1b)}{j_l(k_1b)}\right]\\&\times\left[\frac{1}{k_2r}+\frac{h_l^{(1)'}(k_2r)}{h_l^{(1)}(k_2r)}\right]\frac{\partial\mathrm{P}_l^1}{\partial\theta}\\&-\frac{i\omega\mu_0}{4\pi k_1 a^2\sin\theta}\cos\phi\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}\frac{j_l(k_1b)}{j_l(k_1a)}\frac{h_l^{(1)}(k_2r)}{h_l^{(1)}(k_2a)}\frac{1}{M_l}\mathrm{P}_l^1(\cos\theta),\end{aligned} \tag{2.37}$$

$$\begin{aligned}E_{2\phi}=&-\frac{i\omega\mu_0}{4\pi k_1 a^2\sin\theta}\sin\phi\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}\frac{j_l(k_1b)}{j_l(k_1a)}\frac{h_l^{(1)}(k_2r)}{h_l^{(1)}(k_2a)}\frac{1}{K_l}\left[\frac{1}{k_1b}+\frac{j_l'(k_1b)}{j_l(k_1b)}\right]\\&\times\left[\frac{1}{k_2r}+\frac{h_l^{(1)'}(k_2r)}{h_l^{(1)}(k_2r)}\right]\mathrm{P}_l^1(\cos\theta)\\&+\frac{i\omega\mu_0}{4\pi k_1 a^2}\sin\phi\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}\frac{j_l(k_1b)}{j_l(k_1a)}\frac{h_l^{(1)}(k_2r)}{h_l^{(1)}(k_2a)}\frac{1}{M_l}\frac{\partial\mathrm{P}_l^1}{\partial\theta},\end{aligned} \tag{2.38}$$

$$B_{2r}=-\frac{\mu_0}{4\pi k_1 r a^2}\sin\phi\sum_{l=0}^{\infty}(2l+1)\frac{j_l(k_1b)}{j_l(k_1a)}\frac{h_l^{(1)}(k_2r)}{h_l^{(1)}(k_2a)}\frac{1}{M_l}\mathrm{P}_l^1(\cos\theta), \tag{2.39}$$

$$\begin{aligned}B_{2\theta}=&-\frac{\mu_0 k_2}{4\pi k_1 a^2}\sin\phi\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}\frac{j_l(k_1b)}{j_l(k_1a)}\frac{h_l^{(1)}(k_2r)}{h_l^{(1)}(k_2a)}\frac{1}{M_l}\left[\frac{1}{k_2r}+\frac{h_l^{(1)'}(k_2r)}{h_l^{(1)}(k_2r)}\right]\frac{\partial\mathrm{P}_l^1}{\partial\theta}\\&-\frac{\mu_0 k_2}{4\pi k_1 a^2\sin\theta}\sin\phi\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}\frac{j_l(k_1b)}{j_l(k_1a)}\frac{h_l^{(1)}(k_2r)}{h_l^{(1)}(k_2a)}\frac{1}{K_l}\left[\frac{1}{k_1b}+\frac{j_l'(k_1b)}{j_l(k_1b)}\right]\mathrm{P}_l^1(\cos\theta),\end{aligned} \tag{2.40}$$

$$B_{2\phi}=-\frac{\mu_0 k_2}{4\pi k_1 a^2 \sin\theta}\cos\phi\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}\frac{j_l(k_1 b)}{j_l(k_1 a)}\frac{h_l^{(1)}(k_2 r)}{h_l^{(1)}(k_2 a)}\frac{1}{M_l}\left[\frac{1}{k_2 r}+\frac{h_l^{(1)\prime}(k_2 r)}{h_l^{(1)}(k_2 r)}\right]\mathrm{P}_l^1(\cos\theta)$$
$$-\frac{\mu_0 k_2}{4\pi k_1 a^2}\cos\phi\sum_{l=0}^{\infty}\frac{2l+1}{l(l+1)}\frac{j_l(k_1 b)}{j_l(k_1 a)}\frac{h_l^{(1)}(k_2 r)}{h_l^{(1)}(k_2 a)}\frac{1}{K_l}\left[\frac{1}{k_1 b}+\frac{j_l'(k_1 b)}{j_l(k_1 b)}\right]\frac{\partial \mathrm{P}_l^1}{\partial\theta}. \tag{2.41}$$

Expansions (2.36)–(2.41) converge uniformly in all parameters if $r\neq a$ or $b\neq a$. For large l each series is majorized by a geometric series with expansion parameter $(b/a)\times(\min\{r,a\}/\max\{r,a\})$. For $k_2 a\gg 1$, the summands with $l\leqslant O(k_1 a)$ oscillate rapidly, hindering physical interpretation and rendering direct computations impractical.

B. Electromagnetic field on the surface

When the dipole and the observation point are allowed to approach the boundary ($b\to a^-$, $r\to a^+$), the series expansions for the field diverge.[38] Application of the Poisson summation formula (1.1) converts Eqs. (2.36)–(2.41) into the following series:

$$E_{2r}=\frac{i\omega\mu_0}{2\pi k_1 k_2 a^3}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\mathcal{K}(\nu)}\left[\frac{1}{2k_1 a}+\frac{J_\nu'(k_1 a)}{J_\nu(k_1 a)}\right]\mathrm{P}^1_{\nu-1/2}(\cos\theta), \tag{2.42}$$

$$E_{2\theta}=\frac{i\omega\mu_0}{2\pi k_1 a^2}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{K}(\nu)}\left[\frac{1}{2k_2 a}+\frac{H_\nu^{(1)\prime}(k_2 a)}{H_\nu^{(1)}(k_2 a)}\right]$$
$$\times\left[\frac{1}{2k_1 a}+\frac{J_\nu'(k_1 a)}{J_\nu(k_1 a)}\right]\frac{\partial \mathrm{P}^1_{\nu-1/2}}{\partial\theta}-\frac{i\omega\mu_0}{2\pi k_1 a^2\sin\theta}\cos\phi$$
$$\times\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{M}(\nu)}\mathrm{P}^1_{\nu-1/2}(\cos\theta), \tag{2.43}$$

$$E_{2\phi}=-\frac{i\omega\mu_0}{2\pi k_1 a^2\sin\theta}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{K}(\nu)}\left[\frac{1}{2k_2 a}+\frac{H_\nu^{(1)\prime}(k_2 a)}{H_\nu^{(1)}(k_2 a)}\right]$$
$$\times\left[\frac{1}{2k_1 a}+\frac{J_\nu'(k_1 a)}{J_\nu(k_1 a)}\right]\mathrm{P}^1_{\nu-1/2}(\cos\theta)$$
$$+\frac{i\omega\mu_0}{2\pi k_1 a^2}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{M}(\nu)}\frac{\partial \mathrm{P}^1_{\nu-1/2}}{\partial\theta}, \tag{2.44}$$

$$B_{2r}=-\frac{\mu_0}{2\pi k_1 a^3}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\mathcal{M}(\nu)}\mathrm{P}^1_{\nu-1/2}(\cos\theta), \tag{2.45}$$

$$B_{2\theta}=-\frac{\mu_0 k_2}{2\pi k_1 a^2}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{M}(\nu)}\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\frac{\partial \mathrm{P}^1_{\nu-1/2}}{\partial\theta}$$

$$-\frac{\mu_0 k_2}{2\pi k_1 a^2\sin\theta}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{K}(\nu)}$$

$$\times\left[\frac{1}{2k_1a}+\frac{J_\nu'(k_1a)}{J_\nu(k_1a)}\right]\mathrm{P}^1_{\nu-1/2}(\cos\theta), \tag{2.46}$$

$$B_{2\phi}=-\frac{\mu_0 k_2}{2\pi k_1 a^2\sin\theta}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{M}(\nu)}$$

$$\times\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\mathrm{P}^1_{\nu-1/2}(\cos\theta)$$

$$-\frac{\mu_0 k_2}{2\pi k_1 a^2}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{K}(\nu)}\left[\frac{1}{2k_1a}+\frac{J_\nu'(k_1a)}{J_\nu(k_1a)}\right]\frac{\partial \mathrm{P}^1_{\nu-1/2}}{\partial\theta}, \tag{2.47}$$

where

$$\mathcal{K}(\nu)=\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}+\frac{1}{2k_2a}-\frac{k_2}{k_1}\left[\frac{1}{2k_1a}+\frac{J_\nu'(k_1a)}{J_\nu(k_1a)}\right], \tag{2.48}$$

$$\mathcal{M}(\nu)=\frac{J_\nu'(k_1a)}{J_\nu(k_1a)}-\frac{k_2}{k_1}\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}. \tag{2.49}$$

The integrands in Eqs. (2.42)–(2.47) are meromorphic functions of ν. The zeros of $\mathcal{K}(\nu)$ and $\mathcal{M}(\nu)$ are sometimes called Regge poles in the literature (for example, see Ref. 29). The study of the possible resonances associated with these poles, which are often believed to give rise to various effects of absorption and scattering from spheres and other scatterers, lies beyond the scope of this analysis. A discussion on the location of the zeros of $\mathcal{K}(\nu)$ and $\mathcal{M}(\nu)$ is provided in Appendix A. Each integral diverges in the usual sense, but is interpreted unambiguously as[38]

$$\int_0^\infty d\nu\,(\cdots)=\lim_{\nu\to 0^+}\int_0^\infty d\nu\,(\cdots)\,e^{-\nu\nu}. \tag{2.50}$$

III. SOMMERFELD INTEGRALS AND LOWEST-ORDER CORRECTIONS

A. Approximate integral formulas

As $\theta\to 0^+$, Eqs. (2.42)–(2.47) should reduce to known integral formulas.[34] The following steps are taken when $\theta\ll 1$: (i) Only the $n=0$ terms are retained, since the integrands with $n\neq 0$ are highly oscillatory. (ii) The Bessel functions are replaced by asymptotic formulas that are valid outside the transitional regions.[39] (iii) The Legendre functions are replaced by MacDonald's formulas[36] that involve Bessel functions. (iv) The integration path is properly deformed in the fourth quadrant of the ν-plane, as suggested by the analysis in Appendix A.

Accordingly, $\mathcal{K}^{-1}(\nu)$ and $\mathcal{M}^{-1}(\nu)$ from Eqs. (2.48) and (2.49) are approximated as follows:

$$\frac{1}{\mathcal{K}(\nu)} \sim -i\left[\sqrt{1-\left(\frac{\nu}{k_2 a}\right)^2}+\frac{k_2}{k_1}\sqrt{1-\left(\frac{\nu}{k_1 a}\right)^2}\right]^{-1} - \frac{1}{2k_2 a}\frac{(\nu/k_2 a)^2[1-(\nu/k_2 a)^2]^{-1}-(k_2^2/k_1^2)(\nu/k_1 a)^2[1-(\nu/k_1 a)^2]^{-1}}{[\sqrt{1-(\nu/k_2 a)^2}+(k_2/k_1)\sqrt{1-(\nu/k_1 a)^2}]^2}, \tag{3.1}$$

$$\frac{1}{\mathcal{M}(\nu)} \sim i\left[\sqrt{1-\left(\frac{\nu}{k_1 a}\right)^2}+\frac{k_2}{k_1}\sqrt{1-\left(\frac{\nu}{k_2 a}\right)^2}\right]^{-1} - \frac{1}{2k_1 a}\frac{[1-(\nu/k_1 a)^2]^{-1}-[1-(\nu/k_2 a)^2]^{-1}}{\left[\sqrt{1-(\nu/k_1 a)^2}+\frac{k_2}{k_1}\sqrt{1-(\nu/k_2 a)^2}\right]^2}. \tag{3.2}$$

Note that the simplified $\mathcal{K}^{-1}(\nu=\lambda a)$ exhibits a pair of poles at

$$\lambda = \pm k_S = \pm\frac{k_1 k_2}{\sqrt{k_1^2+k_2^2}} \sim \pm\left(k_2-\frac{k_2^3}{2k_1^2}\right), \quad k_2^2 \ll |k_1^2|. \tag{3.3}$$

No poles exist in the approximation for $\mathcal{M}^{-1}(\lambda a)$.

With $\lambda=\nu/a$ and $\rho=a\theta$, the field components reduce to

$$E_{2r}^{n=0} \sim i\frac{\omega\mu_0 k_2^2}{2\pi k_1}(I_{ez}-I_{ez}^c)\cos\phi, \tag{3.4}$$

$$E_{2\theta}^{n=0} \sim -\frac{\omega\mu_0 k_2^2}{4\pi k_1}(I_{e\rho}+I_{e\rho}^c)\cos\phi, \tag{3.5}$$

$$E_{2\phi}^{n=0} \sim \frac{\omega\mu_0 k_2^2}{4\pi k_1}(I_{e\phi}+I_{e\phi}^c)\sin\phi, \tag{3.6}$$

$$B_{2r}^{n=0} \sim i\frac{\mu_0 k_2^2}{2\pi}(I_{bz}+I_{bz}^c)\sin\phi, \tag{3.7}$$

$$B_{2\theta}^{n=0} \sim -\frac{\mu_0 k_2^3}{4\pi k_1}(I_{b\rho}+I_{b\rho}^c)\sin\phi, \tag{3.8}$$

$$B_{2\phi}^{n=0} \sim -\frac{\mu_0 k_2^3}{4\pi k_1}(I_{b\phi}+I_{b\phi}^c)\cos\phi. \tag{3.9}$$

In the above, $I_{f\kappa}$ $(f=e,\ b;\ \kappa=\rho,\ \phi,\ z)$ denote the Sommerfeld integrals,[34] viz.,

$$I_{ez} = k_2^{-3}\int_0^\infty d\lambda\,\frac{\sqrt{1-(\lambda/k_1)^2}}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}\lambda^2 J_1(\lambda\rho), \tag{3.10}$$

$$I_{e\rho} = k_2^{-2}\int_0^\infty d\lambda\,\lambda\left\{\frac{\sqrt{1-(\lambda/k_1)^2}\,\sqrt{1-(\lambda/k_2)^2}}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}[J_0(\lambda\rho)-J_2(\lambda\rho)] + \frac{1}{\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}}[J_0(\lambda\rho)+J_2(\lambda\rho)]\right\}, \tag{3.11}$$

$$I_{e\phi}=k_2^{-2}\int_0^\infty d\lambda\,\lambda\left\{\frac{\sqrt{1-(\lambda/k_1)^2}\,\sqrt{1-(\lambda/k_2)^2}}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}[J_0(\lambda\rho)+J_2(\lambda\rho)]\right.$$
$$\left.+\frac{1}{\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}}[J_0(\lambda\rho)-J_2(\lambda\rho)]\right\}, \tag{3.12}$$

$$I_{bz}=k_1^{-1}k_2^{-2}\int_0^\infty d\lambda\,\frac{1}{\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}}\lambda^2 J_1(\lambda\rho), \tag{3.13}$$

$$I_{b\rho}=k_2^{-2}\int_0^\infty d\lambda\,\lambda\left\{\frac{\sqrt{1-(\lambda/k_2)^2}}{\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}}[J_0(\lambda\rho)-J_2(\lambda\rho)]\right.$$
$$\left.+\frac{\sqrt{1-(\lambda/k_1)^2}}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}[J_0(\lambda\rho)+J_2(\lambda\rho)]\right\}, \tag{3.14}$$

$$I_{b\phi}=k_2^{-2}\int_0^\infty d\lambda\,\lambda\left\{\frac{\sqrt{1-(\lambda/k_2)^2}}{\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}}[J_0(\lambda\rho)+J_2(\lambda\rho)]\right.$$
$$\left.+\frac{\sqrt{1-(\lambda/k_1)^2}}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}[J_0(\lambda\rho)-J_2(\lambda\rho)]\right\}. \tag{3.15}$$

The lowest-order corrections $I_{f\kappa}^{\mathrm{c}}$ read as

$$I_{ez}^{\mathrm{c}}=\frac{i}{2k_2^4 a}\int_0^\infty d\lambda\left\{\frac{k_2}{k_1}\frac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}\frac{1}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}\right.$$
$$\left.+\sqrt{1-(\lambda/k_1)^2}\frac{\dfrac{(\lambda/k_2)^2}{1-(\lambda/k_2)^2}-(k_2^2/k_1^2)\dfrac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}}{[\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}]^2}\right\}\lambda^2 J_1(\lambda\rho), \tag{3.16}$$

$$I_{e\rho}^{\mathrm{c}}=\frac{i}{2k_2^3 a}\int_0^\infty d\lambda\left\{\frac{\sqrt{1-(\lambda/k_1)^2}\dfrac{(\lambda/k_2)^2}{1-(\lambda/k_2)^2}-(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}\dfrac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}\right.$$
$$\left.-\sqrt{1-(\lambda/k_2)^2}\sqrt{1-(\lambda/k_1)^2}\frac{\dfrac{(\lambda/k_2)^2}{1-(\lambda/k_2)^2}-(k_2^2/k_1^2)\dfrac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}}{[\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}]^2}\right\}\lambda[J_0(\lambda\rho)$$
$$-J_2(\lambda\rho)]+\frac{i}{2k_1k_2^2a}\int_0^\infty d\lambda\,\frac{[1-(\lambda/k_1)^2]^{-1}-[1-(\lambda/k_2)^2]^{-1}}{[\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}]^2}\lambda[J_0(\lambda\rho)+J_2(\lambda\rho)], \tag{3.17}$$

$$I^{c}_{e\phi}=\frac{i}{2k_2^3a}\int_0^\infty d\lambda\left\{\frac{\sqrt{1-(\lambda/k_1)^2}\,\dfrac{(\lambda/k_2)^2}{1-(\lambda/k_2)^2}-(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}\,\dfrac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}\right.$$
$$\left.-\sqrt{1-(\lambda/k_2)^2}\sqrt{1-(\lambda/k_1)^2}\frac{\dfrac{(\lambda/k_2)^2}{1-(\lambda/k_2)^2}-(k_2^2/k_1^2)\dfrac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}}{[\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}]^2}\right\}\lambda[J_0(\lambda\rho)+J_2(\lambda\rho)]$$
$$+\frac{i}{2k_1k_2^2a}\int_0^\infty d\lambda\,\frac{[1-(\lambda/k_1)^2]^{-1}-[1-(\lambda/k_2)^2]^{-1}}{[\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}]^2}\lambda[J_0(\lambda\rho)-J_2(\lambda\rho)], \tag{3.18}$$

$$I^{c}_{bz}=\frac{i}{2k_1^2k_2^2a}\int_0^\infty d\lambda\,\frac{[1-(\lambda/k_1)^2]^{-1}-[1-(\lambda/k_2)^2]^{-1}}{[\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}]^2}\lambda^2J_1(\lambda\rho), \tag{3.19}$$

$$I^{c}_{b\rho}=\frac{i}{2k_2^3a}\int_0^\infty d\lambda\left\{\frac{(\lambda/k_2)^2}{1-(\lambda/k_2)^2}\frac{1}{\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}}\right.$$
$$\left.+\frac{k_2}{k_1}\sqrt{1-(\lambda/k_2)^2}\frac{[1-(\lambda/k_1)^2]^{-1}-[1-(\lambda/k_2)^2]^{-1}}{[\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}]^2}\right\}\lambda[J_0(\lambda\rho)-J_2(\lambda\rho)]$$
$$-\frac{i}{2k_2^3a}\int_0^\infty d\lambda\left\{\frac{k_2}{k_1}\frac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}\frac{1}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}\right.$$
$$\left.+\sqrt{1-(\lambda/k_1)^2}\frac{\dfrac{(\lambda/k_2)^2}{1-(\lambda/k_2)^2}-(k_2^2/k_1^2)\dfrac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}}{[\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}]^2}\right\}\lambda[J_0(\lambda\rho)+J_2(\lambda\rho)], \tag{3.20}$$

$$I^{c}_{b\phi}=\frac{i}{2k_2^3a}\int_0^\infty d\lambda\left\{\frac{(\lambda/k_2)^2}{1-(\lambda/k_2)^2}\frac{1}{\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}}\right.$$
$$\left.+\frac{k_2}{k_1}\sqrt{1-(\lambda/k_2)^2}\frac{[1-(\lambda/k_1)^2]^{-1}-[1-(\lambda/k_2)^2]^{-1}}{[\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}]^2}\right\}\lambda[J_0(\lambda\rho)+J_2(\lambda\rho)]$$
$$-\frac{i}{2k_2^3a}\int_0^\infty d\lambda\left\{\frac{k_2}{k_1}\frac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}\frac{1}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}\right.$$
$$\left.+\sqrt{1-(\lambda/k_1)^2}\frac{\dfrac{(\lambda/k_2)^2}{1-(\lambda/k_2)^2}-(k_2^2/k_1^2)\dfrac{(\lambda/k_1)^2}{1-(\lambda/k_1)^2}}{[\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}]^2}\right\}\lambda[J_0(\lambda\rho)-J_2(\lambda\rho)]. \tag{3.21}$$

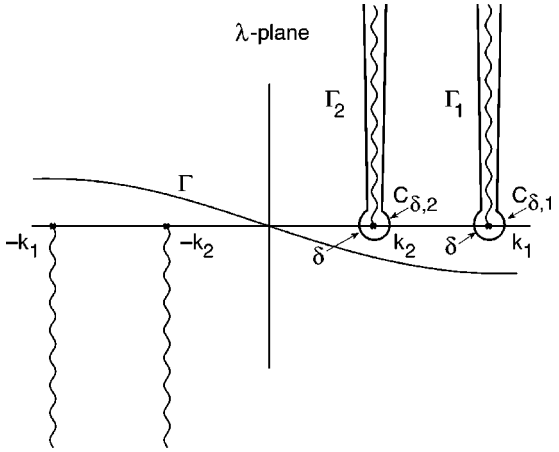

FIG. 2. Branch-cut configuration and integration paths Γ and Γ_j, $j=1,2$, pertaining to integrals (3.10)–(3.21); k_1 is taken to be real. The final formulas can be extended to complex k_1.

The first Riemann sheet is chosen so that all square roots are positive for $0<\lambda<k_2$, if k_1 is real, with the branch-cut configuration of Fig. 2; evidently, no pole lies in this sheet.

B. Integrated formulas, $k_2\rho\gg 1$, $k_2^2\ll|k_1^2|$

When $k_2\rho\gg 1$, the major contributions to integration in Eqs. (3.10)–(3.21) arise from the vicinities of branch points at $\lambda=k_j$ $(j=1,2)$. Explicit expressions for the integrals $I_{f\kappa}$ are given elsewhere.[34,35] It is noted in passing that $I_{e\rho}$, $I_{e\phi}$ and I_{bz} are evaluated exactly in terms of well-converging series that involve Fresnel and exponential integrals.[35]

Attention is now turned to $I^{c}_{f\kappa}$. By following the procedure in Appendix B of Ref. 35, let $I^{c}_{f\kappa,j}$ denote the contour integral over the path Γ_j of Fig. 2. Clearly, $I^{c}_{f,\kappa}=I^{c}_{f\kappa,2}+I^{c}_{f\kappa,1}$, since each $I^{c}_{f\kappa,j}$ follows from $I^{c}_{f\kappa}$ under

$$\int_0^\infty d\lambda\,(\cdots)J_s(\lambda\rho)\to\frac{1}{2}\int_{\Gamma_j}d\lambda\,(\cdots)H_s^{(1)}(\lambda\rho). \tag{3.22}$$

With $\lambda=k_j(1+it)$ in each side of the branch cuts in Fig. 2, it follows that

$$\sqrt{1-(\lambda/k_j)^2}=\pm e^{-i\pi/4}\sqrt{2t}\,\sqrt{1+it/2}\sim\pm e^{-i\pi/4}\sqrt{2t},\quad t\to 0^+,\quad \sqrt{t}\geqslant 0, \tag{3.23}$$

where the upper sign holds along the left-hand side and the lower sign along the right-hand side of each branch cut. Due to the factors $[1-(\lambda/k_j)^2]^{-1}$, the indentations $C_{\delta,j}$ contribute to the value of $I^{c}_{f\kappa,j}$ as δ approaches 0. For example, $I^{c}_{ez,2}$ requires the limit

$$\begin{aligned}
&\lim_{\delta\to 0^+}\int_{C_{\delta,2}}d\lambda\left\{\frac{(k_2/k_1)(\lambda/k_1)^2[1-(\lambda/k_1)^2]^{-1}}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}\right.\\
&\left.+\frac{\sqrt{1-(\lambda/k_1)^2}\{(\lambda/k_2)^2[1-(\lambda/k_2)^2]^{-1}-(k_2^2/k_1^2)(\lambda/k_1)^2[1-(\lambda/k_1)^2]^{-1}\}}{[\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}]^2}\right\}\\
&\times\lambda^2H_1^{(1)}(\lambda\rho)\\
&=2\pi i\left(\frac{-k_2}{2}\right)\sqrt{\frac{1-(k_2/k_1)^2}{[(k_2/k_1)\sqrt{1-(k_2/k_1)}]^2}}\,k_2^2H_1^{(1)}(k_2\rho)\sim-e^{i(k_2\rho-\pi/4)}k_1^2k_2\sqrt{\frac{2\pi}{k_2\rho}}.
\end{aligned} \tag{3.24}$$

Define

$$\wp = \frac{k_2^3 \rho}{2k_1^2} = \frac{k_2^2}{2k_1^2}(k_2 a)\,\theta, \tag{3.25}$$

$$F(\wp) = e^{-i\wp}\int_{\wp}^{\infty} dx\,\frac{e^{ix}}{\sqrt{2\pi x}} = e^{-i\wp}\left[\frac{1}{2}(1+i) - C(\wp) - iS(\wp)\right], \tag{3.26}$$

where $C(\wp)$ and $S(\wp)$ are the Fresnel integrals defined as[36]

$$C(\wp) = \int_0^{\wp} dx\,\frac{\cos x}{\sqrt{2\pi x}}, \quad S(\wp) = \int_0^{\wp} dx\,\frac{\sin x}{\sqrt{2\pi x}}. \tag{3.27}$$

The relevant calculations are illustrated by

$$\begin{aligned} I_{ez,2}^{c} \sim & -\frac{1}{4}e^{i(k_2\rho - 3\pi/4)}\frac{1}{k_2 a}\sqrt{\frac{2}{\pi k_2 \rho}}\int_0^{\infty} dt\left\{\frac{k_2^3}{k_1^3}\left[-\frac{1}{e^{-i\pi/4}\sqrt{2t}+k_2/k_1} + \frac{1}{-e^{-i\pi/4}\sqrt{2t}+k_2/k_1}\right]\right. \\ & \left. + \left(\frac{1}{-2it} - \frac{k_2^4}{k_1^4}\right)\left[-\frac{1}{(e^{-i\pi/4}\sqrt{2t}+k_2/k_1)^2} + \frac{1}{(-e^{-i\pi/4}\sqrt{2t}+k_2/k_1)^2}\right]\right\} e^{-k_2\rho t} \\ & + \frac{1}{2}e^{i(k_2\rho - 3\pi/4)}\frac{k_1^2}{k_2^3 a}\sqrt{\frac{\pi}{2k_2\rho}} \\ \sim & \frac{i}{2}e^{ik_2\rho}\frac{1}{k_2 a}\sqrt{\pi k_2 \rho}\left\{F(\wp) - i(2\pi\wp)^{-1/2} + (2i\wp)^{-1}\left[F(\wp) - \frac{1}{2}(1+i)\right]\right\} \end{aligned} \tag{3.28a}$$

$$\sim \begin{cases} \dfrac{1+i}{4}e^{ik_2\rho}\sqrt{\dfrac{\pi}{k_2\rho}}\,\dfrac{k_1^2}{k_2^3 a}, & |\wp| \gg 1, \\ \dfrac{1-i}{4}e^{ik_2\rho}\sqrt{\dfrac{\pi}{k_2\rho}}\,\dfrac{\rho}{a}, & |\wp| \ll 1, \end{cases} \tag{3.28b}$$

$$I_{ez,1}^{c} \sim -\frac{1}{2}e^{i(k_1\rho - \pi/4)}\frac{k_1}{k_2^2 a}\sqrt{\frac{\pi}{2k_1\rho}}. \tag{3.29}$$

From formulas (3.4)–(3.9), with $k_2 a \gg 1$, $k_2^2 \ll |k_1^2|$, $k_2 a\,\theta \gg 1$, and θ *sufficiently small*,

$$\begin{aligned} E_{2r}^{n=0} \sim & i\frac{\omega\mu_0 k_2^2}{2\pi k_1}\cos\phi\left\{-ie^{ik_2\rho}\frac{k_2}{k_1}\sqrt{\frac{\pi}{k_2\rho}}\left[F(\wp) - i(2\pi\wp)^{-1/2} + \frac{k_1\rho}{2k_2 a}\left\{F(\wp) - i(2\pi\wp)^{-1/2}\right.\right.\right. \\ & \left.\left.\left. + (2i\wp)^{-1}\left[F(\wp) - \frac{1}{2}(1+i)\right]\right\}\right] + \frac{e^{ik_1\rho}}{k_2^2\rho^2}\left(1 + \frac{1-i}{4}\sqrt{\pi k_1\rho}\frac{\rho}{a}\right)\right\}, \end{aligned} \tag{3.30}$$

$$\begin{aligned} E_{2\theta}^{n=0} \sim & \frac{\omega\mu_0 k_2^2}{2\pi k_1}\cos\phi\left\{e^{ik_2\rho}\frac{k_2^2}{k_1^2}\sqrt{\frac{\pi}{k_2\rho}}\left[F(\wp) - i(2\pi\wp)^{-1/2} + \frac{k_1\rho}{2k_2 a}\left\{F(\wp) - i(2\pi\wp)^{-1/2}\right.\right.\right. \\ & \left.\left.\left. + (2i\wp)^{-1}\left[F(\wp) - \frac{1}{2}(1+i)\right]\right\}\right] + \frac{e^{ik_1\rho}}{k_2^2\rho^2}\left(1 + \frac{1-i}{4}\sqrt{\pi k_1\rho}\frac{\rho}{a}\right)\right\}, \end{aligned} \tag{3.31}$$

$$E_{2\phi}^{n=0}\sim i\frac{\omega\mu_0 k_2^2}{2\pi k_1}\sin\phi\Bigg\{e^{ik_2\rho}\frac{k_2}{k_1^2\rho}\sqrt{\frac{\pi}{k_2\rho}}\Bigg[F(\wp)-2i(2\pi\wp)^{-1/2}+\frac{k_1\rho}{2k_2a}\Bigg\{F(\wp)-i(2\pi\wp)^{-1/2}$$
$$+(2i\wp)^{-1}\Bigg[F(\wp)-\frac{1}{2}(1+i)(1-2i\wp)\Bigg]\Bigg\}\Bigg]+i\frac{e^{ik_1\rho}}{k_2^2\rho^2}\Bigg(1+\frac{1-i}{4}\sqrt{\pi k_1\rho}\frac{\rho}{a}\Bigg)\Bigg\},\tag{3.32}$$

$$B_{2r}^{n=0}\sim\frac{\mu_0 k_2^2}{2\pi}\sin\phi\Bigg\{\frac{e^{ik_2\rho}}{k_1^2\rho^2}\Bigg(1-\frac{1-i}{4}\sqrt{\pi k_2\rho}\frac{\rho}{a}\Bigg)-\frac{e^{ik_1\rho}}{k_2^2\rho^2}\Bigg(1+\frac{1-i}{4}\sqrt{\pi k_1\rho}\frac{\rho}{a}\Bigg)\Bigg\},\tag{3.33}$$

$$B_{2\theta}^{n=0}\sim i\frac{\mu_0 k_2^3}{2\pi k_1}\sin\phi\Bigg\{\frac{e^{ik_2\rho}}{k_1\rho}\sqrt{\frac{\pi}{k_2\rho}}\Bigg[F(\wp)-2i(2\pi\wp)^{-1/2}+\frac{k_1\rho}{2k_2a}\Bigg\{F(\wp)-i(2\pi\wp)^{-1/2}$$
$$+(2i\wp)^{-1}\Bigg[F(\wp)-\frac{1}{2}(1+i)(1-2i\wp)\Bigg]\Bigg\}\Bigg]+e^{ik_1\rho}\frac{k_1}{k_2^3\rho^2}\Bigg(1+\frac{1-i}{4}\sqrt{\pi k_1\rho}\frac{\rho}{a}\Bigg)\Bigg\},\tag{3.34}$$

$$B_{2\phi}^{n=0}\sim-\frac{\mu_0 k_2^3}{2\pi k_1}\cos\phi\Bigg\{e^{ik_2\rho}\frac{k_2}{k_1}\sqrt{\frac{\pi}{k_2\rho}}\Bigg[F(\wp)-i(2\pi\wp)^{-1/2}+\frac{k_1\rho}{2k_2a}\Bigg\{F(\wp)-i(2\pi\wp)^{-1/2}$$
$$+(2i\wp)^{-1}\Bigg[F(\wp)-\frac{1}{2}(1+i)\Bigg]\Bigg\}\Bigg]+\frac{e^{ik_1\rho}}{k_2^2\rho^2}\Bigg(i\frac{k_2}{k_1}-\frac{1}{k_2\rho}\Bigg)\Bigg(1+\frac{1-i}{4}\sqrt{\pi k_1\rho}\frac{\rho}{a}\Bigg)\Bigg\}.\tag{3.35}$$

Consequently, $|I_{f\kappa,j}|\sim|I_{f\kappa,j}^{c}|$ provided that, for real k_1,

$$\rho\sim a(k_j a/2)^{-1/3}=\rho_{\mathrm{cr},j}=a\,\theta_{\mathrm{cr},j},\quad j=1,2,\tag{3.36}$$

where $\rho_{\mathrm{cr},2}$ is essentially Fock's "reduced distance."[16] Both $\rho_{\mathrm{cr},j}$, $j=1,2$, enter as parameters in the analysis for a vertical electric dipole.[3,4,33] Evidently, expressions (3.30)–(3.35) imply that

$$\theta\ll\theta_{\mathrm{cr},j}.\tag{3.37}$$

Of course, if k_1 is complex, one of these inequalities is replaced by $\theta\ll|\theta_{\mathrm{cr},1}|$.

When $1\ll k_2\rho\ll|k_1\rho|\ll|k_1\rho_{\mathrm{cr},2}|$, the maximum magnitudes in ϕ of the field components traveling with the air phase velocity satisfy

$$|E_{2r,2}^{n=0}|_m:|E_{2\theta,2}^{n=0}|_m:|E_{2\phi,2}^{n=0}|_m=O(1):O(k_2/k_1):O[(k_1\rho)^{-1}],\quad|\wp|\leqslant O(1),$$
$$=O(1):O(k_2/k_1):O(k_2^3/k_1^3),\quad|\wp|\gg 1,\tag{3.38a}$$

$$|B_{2r,2}^{n=0}|_m:|B_{2\theta,2}^{n=0}|_m:|B_{2\phi,2}^{n=0}|_m=O[(k_1\rho)^{-1}]:O[(k_2\rho)^{-1}]:O(1),\quad|\wp|\ll 1,$$
$$=O[(k_2\rho)^{-3/2}]:O[(k_2\rho)^{-1}]:O(1),\quad\wp=O(1),$$
$$=O(k_2^3/k_1^3):O(k_2^2/k_1^2):O(1),\quad|\wp|\gg 1.\tag{3.38b}$$

IV. WAVES IN THE CRITICAL RANGES, $\theta=O(\theta_{cr,j})$

When θ becomes of the order of $\theta_{\mathrm{cr},1}$ or $\theta_{\mathrm{cr},2}$ introduced in Eq. (3.36), approximations (3.4)–(3.9) break down. The approximation of Bessel functions by Airy integrals gives[39,40]

$$\mathcal{K}^{-1}(\nu)\sim-\frac{k_2}{k_1}\Bigg[1+\frac{k_2^2}{k_1^2}\Bigg(\frac{2}{k_1a}\Bigg)^{1/3}\mathcal{H}(\xi_1;0)\Bigg],\quad\xi_1=(k_1a/2)^{-1/3}(\nu-k_1a)=O(1),\tag{4.1a}$$

$$\mathcal{K}^{-1}(\nu)\sim-\left(\frac{k_2a}{2}\right)^{1/3}[\mathcal{H}(\xi_2;2\pi/3)-i\alpha]^{-1},\quad \xi_2=(k_2a/2)^{-1/3}(\nu-k_2a)=O(1), \tag{4.1b}$$

while

$$\mathcal{M}^{-1}(\nu)\sim 1+\left(\frac{2}{k_1a}\right)^{1/3}\mathcal{H}(\xi_1;0),\quad \xi_1=O(1), \tag{4.2a}$$

$$\mathcal{M}^{-1}(\nu)\sim i+\frac{k_2}{k_1}\left(\frac{2}{k_2a}\right)^{1/3}\mathcal{H}(\xi_2;2\pi/3),\quad \xi_2=O(1). \tag{4.2b}$$

In the above,

$$\mathcal{H}(\xi;\psi)=e^{i\psi}\frac{\mathrm{Ai}'(e^{i\psi}\xi)}{\mathrm{Ai}(e^{i\psi}\xi)}, \tag{4.3}$$

$$\alpha=\frac{k_2}{k_1}\left(\frac{k_2a}{2}\right)^{1/3}. \tag{4.4}$$

Notice the appearance of the Airy function $\mathrm{Ai}(z)$ and its derivative.[40] The Legendre functions are replaced by Bessel functions[36,39] of argument $\nu\theta$ where $\nu\theta\gg 1$.

By using the subscript j to denote the contribution from $\nu=k_ja$ $(j=1,2)$,

$$E_{2r,2}^{n=0}\sim-\frac{\omega\mu_0}{4\pi a}e^{i(k_2a\theta+\pi/4)}\frac{k_2}{k_1}\left(\frac{k_2a}{2}\right)^{2/3}\sqrt{\frac{2}{\pi k_2a\theta}}\mathcal{I}\cos\phi, \tag{4.5a}$$

$$E_{2r,1}^{n=0}\sim-\frac{\omega\mu_0}{4\pi a}e^{i(k_1a\theta-\pi/4)}\sqrt{\frac{2}{\pi k_1a\theta}}\mathcal{I}_1\cos\phi, \tag{4.5b}$$

$$E_{2\theta,2}^{n=0}\sim-\frac{\omega\mu_0}{4\pi a}e^{i(k_2a\theta+\pi/4)}\frac{k_2^2}{k_1^2}\left(\frac{k_2a}{2}\right)^{2/3}\sqrt{\frac{2}{\pi k_2a\theta}}\left[\mathcal{I}+\frac{i}{k_2a\theta}\left(\frac{k_2a}{2}\right)^{-2/3}\mathcal{I}_2\right]\cos\phi, \tag{4.6a}$$

$$E_{2\theta,1}^{n=0}\sim\frac{\omega\mu_0}{4\pi a}e^{i(k_1a\theta+\pi/4)}\sqrt{\frac{2}{\pi k_1a\theta}}\mathcal{I}_1\cos\phi, \tag{4.6b}$$

$$E_{2\phi,2}^{n=0}\sim-\frac{\omega\mu_0}{4\pi a}e^{i(k_2a\theta+\pi/4)}\frac{k_2^2}{k_1^2}\sqrt{\frac{2}{\pi k_2a\theta}}\left[\mathcal{I}_2+i\frac{\theta_{\mathrm{cr},2}}{2\theta}\mathcal{I}\right]\sin\phi, \tag{4.7a}$$

$$E_{2\phi,1}^{n=0}\sim-\frac{\omega\mu_0}{4\pi a}e^{i(k_1a\theta+\pi/4)}\sqrt{\frac{2}{\pi k_1a\theta}}\mathcal{I}_1\sin\phi, \tag{4.7b}$$

$$B_{2r,2}^{n=0}\sim-\frac{\mu_0k_2}{4\pi a}e^{i(k_2a\theta+\pi/4)}\frac{k_2^2}{k_1^2}\sqrt{\frac{2}{\pi k_2a\theta}}\mathcal{I}_2\sin\phi, \tag{4.8a}$$

$$B_{2r,1}^{n=0}\sim-\frac{\mu_0k_1}{4\pi a}e^{i(k_1a\theta+\pi/4)}\sqrt{\frac{2}{\pi k_1a\theta}}\mathcal{I}_1\sin\phi, \tag{4.8b}$$

$$B_{2\theta,2}^{n=0}\sim-\frac{\mu_0k_1}{4\pi a}e^{i(k_2a\theta+\pi/4)}\frac{k_2^2}{k_1^2}\sqrt{\frac{2}{\pi k_2a\theta}}\left[\mathcal{I}_2+i\frac{\theta_{\mathrm{cr},2}}{2\theta}\mathcal{I}\right]\sin\phi, \tag{4.9a}$$

$$B_{2\theta,1}^{n=0}\sim-\frac{\mu_0 k_1}{4\pi a}e^{i(k_1 a\theta-\pi/4)}\sqrt{\frac{2}{\pi k_1 a\theta}}\mathcal{I}_1\sin\phi, \tag{4.9b}$$

$$B_{2\phi,2}^{n=0}\sim\frac{\mu_0 k_2}{4\pi a}e^{i(k_2 a\theta+\pi/4)}\frac{k_2}{k_1}\left(\frac{k_2 a}{2}\right)^{2/3}\sqrt{\frac{2}{\pi k_2 a\theta}}\left[\mathcal{I}+\frac{i}{k_2 a\theta}\left(\frac{k_2 a}{2}\right)^{-2/3}\mathcal{I}_2\right]\cos\phi, \tag{4.10a}$$

$$B_{2\phi,1}^{n=0}\sim\frac{\mu_0 k_2}{4\pi a}e^{i(k_1 a\theta+\pi/4)}\left(\frac{1}{k_2 a\theta}-i\frac{k_2}{k_1}\right)\sqrt{\frac{2}{\pi k_1 a\theta}}\mathcal{I}_1\cos\phi, \tag{4.10b}$$

where

$$\mathcal{I}_1=\mathcal{I}_1(\theta)=\int_{-\infty-i\varsigma}^{\infty-i\varsigma}d\xi\, e^{i(\theta/\theta_{\mathrm{cr},1})\xi}\mathcal{H}(\xi;0), \tag{4.11}$$

$$\mathcal{I}_2=\mathcal{I}_2(\theta)=\int_{-\infty-i\varsigma}^{\infty-i\varsigma}d\xi\, e^{i(\theta/\theta_{\mathrm{cr},2})\xi}\mathcal{H}(\xi;2\pi/3), \tag{4.12}$$

$$\mathcal{I}=\mathcal{I}(\theta;\alpha)=\int_{-\infty-i\varsigma}^{\infty-i\varsigma}d\xi\frac{e^{i(\theta/\theta_{\mathrm{cr},2})\xi}}{\mathcal{H}(\xi;2\pi/3)-i\alpha},\quad \varsigma>0. \tag{4.13}$$

Because the sole singularities of the integrands are poles in the upper ξ-plane, including the real axis, terms with factors $e^{-i(\theta/\theta_{\mathrm{cr},j})\xi}$ are integrated out to zero. $\mathcal{I}$ and $\mathcal{I}_2$ describe propagation through region 2.

For $\theta\ll|\theta_{\mathrm{cr},1}|$, the leading contributions to integration in Eqs. (4.11)–(4.13) are determined by the large-ξ behavior of $\mathcal{H}(\xi;\psi)$. Accordingly,[40]

$$\mathcal{I}_1\sim-\int_{-\infty-i\varsigma}^{\infty-i\varsigma}d\xi\, e^{i(\theta/\theta_{\mathrm{cr},1})\xi}\left(\sqrt{\xi}+\frac{1}{4\xi}\right)=e^{-i\pi/4}\sqrt{\frac{2\pi}{k_1 a}}\left(\frac{\rho}{a}\right)^{-3/2}-\frac{i\pi}{2}, \tag{4.14}$$

while, for $\theta\ll\theta_{\mathrm{cr},2}$,

$$\mathcal{I}_2\sim\int_{-\infty-i\varsigma}^{\infty-i\varsigma}d\xi\, e^{i(\theta/\theta_{\mathrm{cr},2})\xi}\left(\sqrt{\xi}-\frac{1}{4\xi}\right)=-e^{-i\pi/4}\sqrt{\frac{2\pi}{k_2 a}}\left(\frac{\rho}{a}\right)^{-3/2}-\frac{i\pi}{2}, \tag{4.15}$$

$$\mathcal{I}\sim\int_{-\infty-i\varsigma}^{\infty-i\varsigma}d\xi\frac{e^{i(\theta/\theta_{\mathrm{cr},2})\xi}}{\sqrt{\xi}-1/4\xi-i\alpha}\sim i\pi e^{i\pi/4}2^{3/2}\frac{k_2}{k_1}\left(\frac{k_2 a}{2}\right)^{1/3}\left\{F(\wp)-i(2\pi\wp)^{-1/2}+\frac{k_1\rho}{2k_2 a}\left[F(\wp)\right.\right.$$
$$\left.\left.-i(2\pi\wp)^{-1/2}+(2i\wp)^{-1}\left\{F(\wp)-\frac{1}{2}(1+i)\right\}\right]\right\}, \tag{4.16}$$

in agreement with formulas (3.30)–(3.35).

A. Propagation through air

The integral $\mathcal{I}_2$ of Eq. (4.12) is expressed as a general Dirichlet series[41] over the residues associated with poles of $\mathcal{H}(\xi;2\pi/3)$. (See Appendix A for $\kappa=k_2/k_1$.) By closing the contour in the upper ξ-plane,

$$\mathcal{I}_2=2\pi i\sum_{s=1}^{\infty}e^{i(\theta/\theta_{\mathrm{cr},2})|a_s|e^{i\pi/3}}, \tag{4.17}$$

where a_s are the zeros of $\mathrm{Ai}(z)$ numbered in order of ascending magnitude.[40] Series (4.17) is approximated by its first term if $\theta \gg \theta_{\mathrm{cr},2}$.

The poles associated with $\mathcal{I}$ are obtained by solving

$$e^{i2\pi/3}\frac{\mathrm{Ai}'(\xi e^{i2\pi/3})}{\mathrm{Ai}(\xi e^{i2\pi/3})} = i\alpha, \quad \alpha = \frac{k_2}{k_1}\left(\frac{k_2 a}{2}\right)^{1/3}. \tag{4.18}$$

Let $\{\xi_s = \xi_s(\alpha)\}_{s=1,2,\ldots}$ be the sequence of these roots; $\xi_s(0)$ are numbered in order of increasing imaginary part. The integral $\mathcal{I}$ equals

$$\mathcal{I} = 2\pi i \sum_{s=1}^{\infty} \frac{e^{i(\theta/\theta_{\mathrm{cr},2})\xi_s}}{\xi_s + \alpha^2}. \tag{4.19}$$

Because $\{\xi_s\}$ do not have any finite limit, they should approach the Stokes line Arg $\xi = \pi/3$ as $s \to \infty$. Each $\xi_s(z)$ satisfies

$$\frac{d\xi_s}{dz} = \frac{i}{\xi_s + z^2}, \quad \xi_s(0) = |\check{a}_s| e^{i\pi/3}, \tag{4.20}$$

via differentiation of both sides of Eq. (4.18) in $\alpha \equiv z$. $\check{a}_s$ denote the zeros of $\mathrm{Ai}'(z)$.[40] Equation (4.20) was given by Fock[16] and has been studied numerically in the literature.[42] By integrating (4.20) along a path where $|\xi_s(z)| \gg |z^2|$,

$$\xi_s(\alpha) \sim \xi_s(0) + \frac{i\alpha}{\xi_s(0)}. \tag{4.21}$$

Clearly,

$$\mathcal{I} \sim 2\pi i \frac{e^{i(\theta/\theta_{\mathrm{cr},2})\bar{\xi}}}{\bar{\xi} + \alpha^2}, \quad \theta \gg \theta_{\mathrm{cr},2}, \tag{4.22}$$

where $\bar{\xi} = \bar{\xi}(\alpha)$ is the root of Eq. (4.18) with the smallest imaginary part. It is of interest to compare $\min_s \mathrm{Im}\, \xi_s(\alpha)$ with its limiting value for $\alpha \to \infty$. With $\alpha = te^{-i\vartheta}$ $(0 \leqslant t < \infty,\ 0 \leqslant \vartheta \leqslant \pi/4)$ and fixed ϑ, the trajectory of each $\xi_j(\alpha) = \beta_j(t) + i\gamma_j(t)$ can be described by the coupled equations

$$\frac{d\beta_j}{dt} = \frac{\gamma_j \cos\vartheta + (\beta_j - t^2)\sin\vartheta}{(\beta_j + t^2\cos 2\vartheta)^2 + (\gamma_j - t^2 \sin 2\vartheta)^2}, \tag{4.23a}$$

$$\frac{d\gamma_j}{dt} = \frac{(\beta_j + t^2)\cos\vartheta - \gamma_j \sin\vartheta}{(\beta_j + t^2\cos 2\vartheta)^2 + (\gamma_j - t^2 \sin 2\vartheta)^2}, \tag{4.23b}$$

where $\beta_j(0) = |\check{a}_j|/2$, $\gamma_j(0) = \sqrt{3}|\check{a}_j|/2$, and $|\check{a}_j| < |a_j| < |\check{a}_{j+1}|$. Of course, $\lim_{t\to\infty} \xi_j(\alpha(t)) = |a_j| e^{i\pi/3}$ uniformly in ϑ. For definiteness, consider $j = 1$. If $\vartheta = 0$, $\beta_1(t)$ and $\gamma_1(t)$ are monotonically increasing in t, and the slope of $\xi_1(\alpha(t))$ equals $\pi/6$ for $t = 0$ and approaches $\pi/2$ as $t \to \infty$. A close inspection of Eqs. (4.23) shows that $\gamma_1(t)$ remains monotonically increasing for fixed $\vartheta \in (0, \pi/6]$, while $\beta_1(t)$ reaches a maximum. For fixed $\vartheta \in (\pi/6, \pi/4]$, $\gamma_1(t)$ is monotonically decreasing and reaches a minimum, and then progresses monotonically to its limiting value. The lowest minimum of $\gamma_1(t)$ is reached for $\vartheta = \pi/4$, when the slope of $\xi_1(\alpha(t))$ is $-\pi/12$ for $t = 0$ and $3\pi/4$ as $t \to \infty$. By relaxing routine rigor, the assumed analyticity of $\xi_1(\alpha)$ in $\Delta_R = \{\alpha: 0 < |\alpha| < R,\ -\pi/4 < \mathrm{Arg}\ \alpha < 0\}$, where R is positive and arbitrarily large, entails that $\mathrm{Im}\, \xi_1(\alpha)$ is harmonic in Δ_R and hence cannot attain any maximum or minimum there. It follows from Fig. 3 that the maximum occurs along the boundary $\{\alpha: |\alpha| = R,\ \mathrm{Arg}\ \alpha = \pi/4\}$.

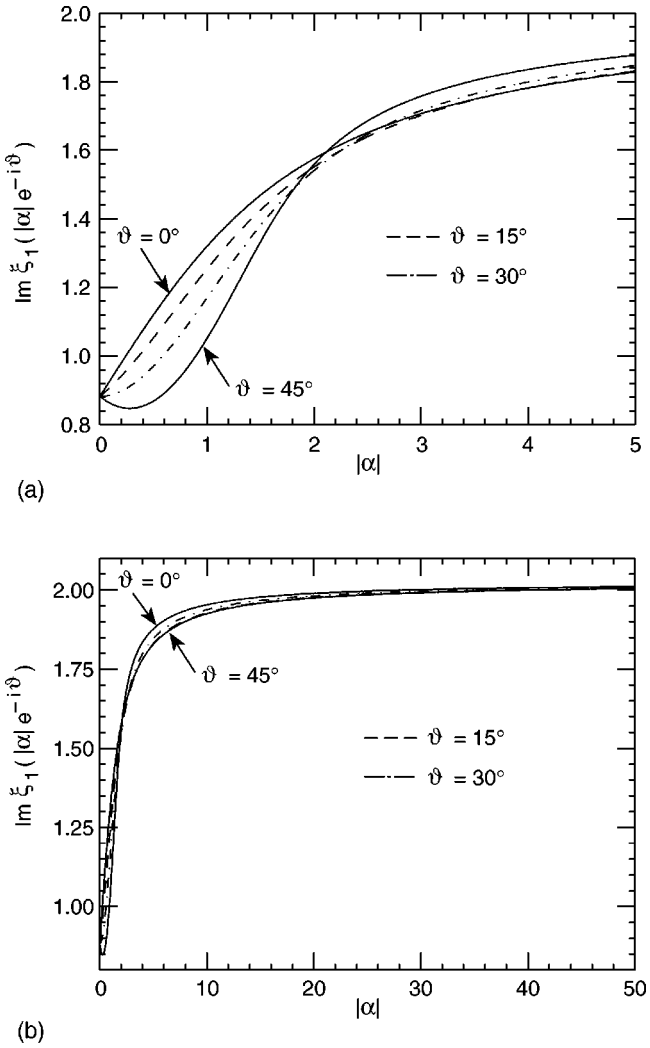

FIG. 3. Imaginary part of the root $\xi_1(\alpha)$ of (4.18) for fixed values of the phase $-\vartheta$ and varying magnitude $|\alpha|$, where $\alpha=|\alpha|e^{-i\vartheta}=(k_2/k_1)(k_2a/2)^{1/3}$, for (a) $0\leqslant|\alpha|\leqslant 5$, and (b) $0\leqslant|\alpha|\leqslant 50$.

It is therefore implied that, for $\alpha\leqslant O(1)$,

$$\mathcal{I}_2/\mathcal{I}=O[e^{-(\theta/\theta_{\mathrm{cr},2})\overline{h}}],\quad \overline{h}\equiv \tfrac{1}{2}\sqrt{3}\,|a_1|-\min_s \operatorname{Im}\xi_s(\alpha),\quad \theta\gg\theta_{\mathrm{cr},2}, \tag{4.24a}$$

while for $\alpha\to\infty$,

$$\mathcal{I}_2/\mathcal{I}=O(\alpha^2)\quad \text{as}\quad \alpha\to\infty. \tag{4.24b}$$

Formulas (4.6a) and (4.10a) are further simplified:

$$E^{n=0}_{2\theta,2}\sim -\frac{\omega\mu_0}{4\pi a}e^{i(k_2a\theta+\pi/4)}\frac{k_2^2}{k_1^2}\left(\frac{k_2a}{2}\right)^{2/3}\sqrt{\frac{2}{\pi k_2a\theta}}\,\mathcal{I}\cos\phi\sim\frac{k_2}{k_1}E^{n=0}_{2r,2}, \tag{4.25}$$

$$B^{n=0}_{2\phi,2}\sim \frac{\mu_0k_2}{4\pi a}e^{i(k_2a\theta+\pi/4)}\frac{k_2}{k_1}\left(\frac{k_2a}{2}\right)^{2/3}\sqrt{\frac{2}{\pi k_2a\theta}}\,\mathcal{I}\cos\phi\sim-\frac{1}{c}E^{n=0}_{2r,2}, \tag{4.26}$$

where c is the velocity of light in air.

From expressions (4.7a) and (4.9a),

$$E_{2\phi,2}^{n=0} \sim -i\frac{\omega\mu_0}{8\pi a}e^{i(k_2 a\theta+\pi/4)}\frac{k_2^2}{k_1^2}\sqrt{\frac{2}{\pi k_2 a\theta}}\,\frac{\theta_{\mathrm{cr},2}}{\theta}\mathcal{I}\sin\phi, \tag{4.27}$$

$$B_{2\theta,2}^{n=0} \sim -i\frac{\mu_0 k_1}{8\pi a}e^{i(k_2 a\theta+\pi/4)}\frac{k_2^2}{k_1^2}\sqrt{\frac{2}{\pi k_2 a\theta}}\,\frac{\theta_{\mathrm{cr},2}}{\theta}\mathcal{I}\sin\phi, \quad \theta \gg \theta_{\mathrm{cr},2},\ |\alpha| \leqslant O(1). \tag{4.28}$$

It is inferred that when $O(\theta_{\mathrm{cr},2}) \leqslant \theta \ll 1$, $|\alpha| \leqslant O(1)$,

$$|E_{2r,2}^{n=0}|_m : |E_{2\theta,2}^{n=0}|_m : |E_{2\phi,2}^{n=0}|_m = O(1) : O(k_2/k_1) : O[(k_1 a\theta)^{-1}], \tag{4.29a}$$

$$|B_{2r,2}^{n=0}|_m : |B_{2\theta,2}^{n=0}|_m : |B_{2\phi,2}^{n=0}|_m = O\left[\frac{\mathcal{I}_2}{\mathcal{I}}\frac{k_2}{k_1}\left(\frac{k_2 a}{2}\right)^{-2/3}\right] : O[(k_2 a\theta)^{-1}] : O(1). \tag{4.29b}$$

B. Propagation through region 1

Difficulties in the evaluation of $\mathcal{I}_1$ arise because of the presence of poles in the negative real axis. These poles stem from zeros of $\mathcal{K}(\nu)$ or $\mathcal{M}(\nu)$, as outlined in Appendix A. By use of the Wronskian of $\mathrm{Ai}(\zeta e^{-i\pi/3})$ and $\mathrm{Ai}(\zeta e^{i\pi/3})$,

$$\mathcal{I}_1 = \int_{\mathcal{L}} d\zeta\ [\mathcal{H}(-\zeta;0) - \mathcal{H}(-\zeta;-2\pi/3)]\, e^{-i(\theta/\theta_{\mathrm{cr},1})\zeta} = -\frac{e^{i\pi/6}}{2\pi}\int_{\mathcal{L}} d\zeta\,\frac{e^{-i(\theta/\theta_{\mathrm{cr},1})\zeta}}{\mathrm{Ai}(\zeta e^{i\pi/3})\,\mathrm{Ai}(-\zeta)}, \tag{4.30}$$

where $\mathcal{L}$ is a path that extends along the negative real axis, passes through zero and then extends slightly above the positive real axis. This integral can be cast in a form that is amenable to numerical computation.[33] Alternatively, rewrite $\mathcal{I}_1$ as

$$\begin{aligned}\mathcal{I}_1 &= -\frac{e^{i\pi/6}}{2\pi}\left[\int_0^\infty d\xi\,\frac{e^{i(\theta/\theta_{\mathrm{cr},1})\xi}}{\mathrm{Ai}(\xi e^{-i2\pi/3})\,\mathrm{Ai}(\xi)} + \int_0^{\infty+i\varsigma} d\zeta\,\frac{e^{-i(\theta/\theta_{\mathrm{cr},1})\zeta}}{\mathrm{Ai}(\zeta e^{i\pi/3})\,\mathrm{Ai}(-\zeta)}\right] \\ &= -\frac{i}{\pi}\left\{\int_0^\infty dy\,\frac{\exp[-(\theta/\theta_{\mathrm{cr},1})ye^{i\pi/6}] + 2\exp[(\theta/\theta_{\mathrm{cr},1})ye^{-i\pi/6}]}{\mathrm{Ai}(y)^2+\mathrm{Bi}(y)^2}\right. \\ &\quad \left. + i\int_0^\infty dy\,\frac{\exp[-(\theta/\theta_{\mathrm{cr},1})ye^{i\pi/6}]}{\mathrm{Ai}(y)^2+\mathrm{Bi}(y)^2}\,\frac{\mathrm{Bi}(y)}{\mathrm{Ai}(y)}\right\},\end{aligned} \tag{4.31}$$

by rotation of each integration path in the ξ- or ζ-plane by $2\pi/3$ or $\pi/3$ counterclockwise. The right-hand side of Eq. (4.31) involves exponentially converging integrals.

When $\theta \gg |\theta_{\mathrm{cr},1}|$, $\mathcal{I}_1$ is further simplified. By virtue of the equality

$$\mathrm{Ai}(-\zeta) + e^{i2\pi/3}\mathrm{Ai}(\zeta e^{-i\pi/3}) + e^{-i2\pi/3}\mathrm{Ai}(\zeta e^{i\pi/3}) = 0,$$

it is deduced that

$$\frac{1}{\mathrm{Ai}(\zeta e^{i\pi/3})\,\mathrm{Ai}(-\zeta)} = 2\pi e^{-i\pi/6}\frac{d}{d\zeta}\int_0^{\varpi(\zeta)}\frac{dy}{1+y}, \tag{4.32}$$

where

$$\varpi(\zeta) \equiv e^{-i2\pi/3}\,\frac{\mathrm{Ai}(\zeta e^{-i\pi/3})}{\mathrm{Ai}(\zeta e^{i\pi/3})}. \tag{4.33}$$

Note that $\varpi(\zeta)$ is bounded everywhere except near the zeros of $\mathrm{Ai}(\zeta e^{i\pi/3})$. Substitution of Eq. (4.32) into (4.30) and application of integration by parts furnish

$$\mathcal{I}_1 = -i\frac{\theta}{\theta_{\mathrm{cr},1}}\left[\sum_{p=0}^{P-1}\frac{(-1)^p}{p+1}\int_{\mathcal{L}} d\zeta\, e^{-i(\theta/\theta_{\mathrm{cr},1})\zeta}\,\varpi(\zeta)^{p+1} + \mathcal{R}_P(\theta/\theta_{\mathrm{cr},1})\right], \tag{4.34}$$

where

$$\mathcal{R}_P(x) = (-1)^P \int_{\mathcal{L}} d\zeta\, e^{-ix\zeta}\int_0^{\varpi(\zeta)} dy\,\frac{y^P}{1+y}, \quad P \gg 1, \tag{4.35}$$

$$\mathcal{R}_P(x) \sim \frac{(-1)^P}{P+1}\int_{\mathcal{L}} d\zeta\, e^{-ix\zeta}\frac{\varpi(\zeta)^{P+1}}{1+\varpi(\zeta)}, \quad P \gg 1. \tag{4.36}$$

For $\theta \gg |\theta_{\mathrm{cr},1}|$, the leading contributions in Eq. (4.34) come from points ζ_p that render the phase of $e^{-i(\theta/\theta_{\mathrm{cr},1})\zeta}\,\varpi(\zeta)^{p+1}$ stationary. Consequently, ζ_p obey

$$\frac{\varpi'(\zeta_p)}{\varpi(\zeta_p)} = i\frac{\theta}{\theta_{\mathrm{cr},1}(p+1)}, \tag{4.37}$$

or

$$\frac{1}{\pi}\frac{1}{\mathrm{Ai}(-\zeta_p)^2 + \mathrm{Bi}(-\zeta_p)^2} = \frac{\theta}{2\,\theta_{\mathrm{cr},1}(p+1)} = \chi_p\,. \tag{4.38}$$

When $p < O(\theta/\theta_{\mathrm{cr},1})$, ζ_p is positive and large,[40] viz.,

$$\zeta_p = \chi_p^2 + O(\chi_p^{-4}), \quad |\chi_p| \gg 1. \tag{4.39}$$

On the other hand, $\chi_p = O(1)$ implies $\zeta_p = O(1)$. In view of approximation (4.36), the remainder in Eq. (4.34) can be neglected if P is of the order of $\theta/\theta_{\mathrm{cr},1}$. With

$$\varpi(\zeta)^{p+1} \sim (-i)^{p+1}\exp\left[i\frac{4}{3}(p+1)\zeta^{3/2}\right], \tag{4.40}$$

an ordinary stationary-phase calculation leads to

$$\begin{aligned}\mathcal{I}_1 &\sim -i\frac{\theta}{\theta_{\mathrm{cr},1}}\sum_{p=0}^{O(\theta/\theta_{\mathrm{cr},1})}\frac{(-1)^p}{p+1}\exp\left[-\frac{i}{12}\frac{\theta^3}{\theta_{\mathrm{cr},1}^3(p+1)^2}\right](-i)^{p+1}\\ &\quad\times\int_{-\infty}^{\infty} d\zeta\exp\left\{i\frac{\theta}{\theta_{\mathrm{cr},1}}\left[\frac{\theta_{\mathrm{cr},1}(p+1)}{\theta}\right]^2(\zeta-\zeta_p)^2\right\}\\ &\sim -e^{i\pi/4}\left(\frac{\theta}{\theta_{\mathrm{cr},1}}\right)^{3/2}\sqrt{\pi}\,\mathcal{S}(k_1 a\,\theta^3),\end{aligned} \tag{4.41}$$

$$\mathcal{S}(z) = \sum_{p=0}^{\infty}\frac{i^p}{(p+1)^2}\exp\left[-\frac{i}{24}\frac{z}{(p+1)^2}\right]. \tag{4.42}$$

Finally, for $\theta \gg |\theta_{\mathrm{cr},1}|$, $k_2^2 \ll |k_1^2|$ and $k_2 a\,\theta \gg 1$,

$$E_{2r,1}^{n=0} \sim \frac{\omega\mu_0\theta}{4\pi a}e^{ik_1 a\,\theta}\,\mathcal{S}(k_1 a\,\theta^3)\cos\phi \sim iE_{2\theta,1}^{n=0}\,, \tag{4.43}$$

$$E_{2\phi,1}^{n=0}\sim\frac{i\omega\mu_0\theta}{4\pi a}e^{ik_1a\theta}\mathcal{S}(k_1a\theta^3)\sin\phi, \tag{4.44}$$

$$B_{2r,1}^{n=0}\sim\frac{i\mu_0k_1\theta}{4\pi a}e^{ik_1a\theta}\mathcal{S}(k_1a\theta^3)\sin\phi\sim iB_{2\theta,1}^{n=0}, \tag{4.45}$$

$$\begin{aligned}B_{2\phi,1}^{n=0}&\sim-\frac{i\mu_0k_2\theta}{4\pi a}e^{ik_1a\theta}\left(\frac{1}{k_2a\theta}-i\frac{k_2}{k_1}\right)\mathcal{S}(k_1a\theta^3)\cos\phi\\&\sim-\frac{\mu_0k_2^2\theta}{4\pi k_1a}e^{ik_1a\theta}\mathcal{S}(k_1a\theta^3)\cos\phi,\quad k_2a\theta\gg|k_1|/k_2.\end{aligned} \tag{4.46}$$

V. FIELD IN THE RANGE $O(\theta_{cr,j})<\theta\leqslant\pi$

A. Formulation

Consider the identity

$$\begin{aligned}\mathcal{M}(\nu)-\frac{H_\nu^{(2)'}(k_1a)}{H_\nu^{(2)}(k_1a)}&=-\frac{\mathrm{W}[H_\nu^{(1)}(k_1a),H_\nu^{(2)}(k_1a)]}{2H_\nu^{(2)}(k_1a)\,J_\nu(k_1a)}-\frac{k_2}{k_1}\frac{H_\nu^{(1)'}(k_2a)}{H_\nu^{(1)}(k_2a)}\\&=\frac{2i}{\pi k_1a\,H_\nu^{(2)}(k_1a)\,J_\nu(k_1a)}-\frac{k_2}{k_1}\frac{H_\nu^{(1)'}(k_2a)}{H_\nu^{(1)}(k_2a)},\end{aligned} \tag{5.1}$$

which is implied from Eq. (4.32) and leads to the decomposition

$$\frac{1}{\mathcal{M}(\nu)}=\frac{1}{\mathcal{D}(\nu)}-\mathcal{F}(\nu)\sum_{p=0}^{P-1}\mathcal{G}(\nu)^p-\mathcal{F}(\nu)\frac{\mathcal{G}(\nu)^P}{1-\mathcal{G}(\nu)}, \tag{5.2}$$

where

$$\mathcal{D}(\nu)=\frac{H_\nu^{(2)'}(k_1a)}{H_\nu^{(2)}(k_1a)}-\frac{k_2}{k_1}\frac{H_\nu^{(1)'}(k_2a)}{H_\nu^{(1)}(k_2a)}, \tag{5.3}$$

$$\mathcal{F}(\nu)=\frac{4i}{\pi k_1a}\frac{1}{\mathcal{D}(\nu)^2\,H_\nu^{(2)}(k_1a)^2}, \tag{5.4}$$

$$\mathcal{G}(\nu)=\frac{-H_\nu^{(1)}(k_1a)}{H_\nu^{(2)}(k_1a)}-\frac{4i}{\pi k_1a}\frac{1}{\mathcal{D}(\nu)\,H_\nu^{(2)}(k_1a)^2}. \tag{5.5}$$

When $P\to\infty$, Eq. (5.2) reduces to an expansion of the Debye type,[7] also employed by Nussenzveig.[29,32] In the lower ν-plane slightly below the positive real axis, the limit $P\to\infty$ in Eq. (5.2) is meaningful because $|\mathcal{G}(\nu)|<1$. However, care should be exercised in taking this limit under the integral sign.

A corresponding decomposition for $\mathcal{K}^{-1}(\nu)$ reads as

$$\frac{1}{\mathcal{K}(\nu)}=\frac{1}{\mathcal{A}(\nu)}+\mathcal{B}(\nu)\sum_{p=0}^{P-1}\mathcal{C}(\nu)^p+\mathcal{B}(\nu)\frac{\mathcal{C}(\nu)^P}{1-\mathcal{C}(\nu)}, \tag{5.6}$$

where

$$\mathcal{A}(\nu)=\frac{H_\nu^{(1)'}(k_2a)}{H_\nu^{(1)}(k_2a)}-\frac{k_2}{k_1}\frac{H_\nu^{(2)'}(k_1a)}{H_\nu^{(2)}(k_1a)}+\frac{1}{2k_2a}-\frac{k_2^2}{k_1^2}\frac{1}{2k_2a}, \tag{5.7}$$

$$\mathcal{B}(\nu)=\frac{4i}{\pi k_1 a}\frac{k_2}{k_1}\frac{1}{\mathcal{A}(\nu)^2 H_\nu^{(2)}(k_1 a)^2}, \tag{5.8}$$

$$\mathcal{C}(\nu)=\frac{-H_\nu^{(1)}(k_1 a)}{H_\nu^{(2)}(k_1 a)}+\frac{4i}{\pi k_1 a}\frac{k_2}{k_1}\frac{1}{\mathcal{A}(\nu) H_\nu^{(2)}(k_1 a)^2}. \tag{5.9}$$

Expressions (5.6)–(5.9) are also derived in Ref. 33 for the field of a vertical electric dipole over a spherical earth. $\mathcal{A}(\nu)$ and $\mathcal{D}(\nu)$ are entire functions of ν satisfying[39]

$$\mathcal{A}(-\nu)=\mathcal{A}(\nu), \quad \mathcal{D}(-\nu)=\mathcal{D}(\nu). \tag{5.10}$$

A brief discussion on the location of their zeros is given in Appendix B.

Residues that are associated with the poles ν_j of $\mathcal{A}^{-1}(\nu)$ and $\tilde{\nu}_j$ of $\mathcal{D}^{-1}(\nu)$ in the upper ν-plane give rise to exponentially decreasing waves that propagate through air. On the other hand, stationary-phase contributions from $\mathcal{B}(\nu)\mathcal{C}(\nu)^p$ and $\mathcal{F}(\nu)\mathcal{G}(\nu)^p$, combined with $e^{i2\pi n\nu}$ and the Legendre functions, give rise to rays that travel in region 1. Contributions from these rays become significant when $\mathrm{Im}\, k_1 a \ll 1$.

With Eqs. (C1) and (C5) of Appendix C,

$$\mathbf{E}_2=\mathbf{E}_2^{\mathrm{res}}+\mathbf{E}_2^{\mathrm{ray}}, \quad \mathbf{B}_2=\mathbf{B}_2^{\mathrm{res}}+\mathbf{B}_2^{\mathrm{ray}}, \tag{5.11}$$

where

$$E_{2r}^{\mathrm{res}}=\frac{i\omega\mu_0}{2\pi k_1 k_2 a^3}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\mathcal{A}(\nu)}\left[\frac{1}{2k_1 a}+\frac{H_\nu^{(2)\prime}(k_1 a)}{H_\nu^{(2)}(k_1 a)}\right]\mathrm{P}_{\nu-1/2}^1(\cos\theta), \tag{5.12}$$

$$\begin{aligned}E_{2\theta}^{\mathrm{res}}=&\frac{i\omega\mu_0}{2\pi k_1 a^2}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\\&\times\left\{\frac{H_\nu^{(2)\prime}(k_1 a)}{H_\nu^{(2)}(k_1 a)}+\frac{k_2}{k_1}\frac{1}{\mathcal{A}(\nu)}\left[\frac{1}{2k_1 a}+\frac{H_\nu^{(2)\prime}(k_1 a)}{H_\nu^{(2)}(k_1 a)}\right]^2\right\}\frac{\partial\mathrm{P}_{\nu-1/2}^1(\cos\theta)}{\partial\theta}\\&-\frac{i\omega\mu_0}{2\pi k_1 a^2\sin\theta}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{D}(\nu)}\mathrm{P}_{\nu-1/2}^1(\cos\theta),\end{aligned} \tag{5.13}$$

$$\begin{aligned}E_{2\phi}^{\mathrm{res}}=&-\frac{i\omega\mu_0}{2\pi k_1 a^2\sin\theta}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\\&\times\left\{\frac{H_\nu^{(2)\prime}(k_1 a)}{H_\nu^{(2)}(k_1 a)}+\frac{k_2}{k_1}\frac{1}{\mathcal{A}(\nu)}\left[\frac{1}{2k_1 a}+\frac{H_\nu^{(2)\prime}(k_1 a)}{H_\nu^{(2)}(k_1 a)}\right]^2\right\}\mathrm{P}_{\nu-1/2}^1(\cos\theta)\\&+\frac{i\omega\mu_0}{2\pi k_1 a^2}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{D}(\nu)}\frac{\partial\mathrm{P}_{\nu-1/2}^1}{\partial\theta},\end{aligned} \tag{5.14}$$

$$B_{2r}^{\mathrm{res}}=-\frac{\mu_0}{2\pi k_1 a^3}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\frac{\nu}{\mathcal{D}(\nu)}\mathrm{P}_{\nu-1/2}^1(\cos\theta), \tag{5.15}$$

$$B_{2\theta}^{\mathrm{res}}=-\frac{\mu_0}{2\pi a^2}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{D}(\nu)}\left[\frac{1}{2k_1a}+\frac{H_\nu^{(2)\prime}(k_1a)}{H_\nu^{(2)}(k_1a)}\right]$$
$$\times\frac{\partial \mathrm{P}_{\nu-1/2}^1}{\partial\theta}-\frac{\mu_0k_2}{2\pi k_1a^2\sin\theta}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{A}(\nu)}$$
$$\times\left[\frac{1}{2k_1a}+\frac{H_\nu^{(2)\prime}(k_1a)}{H_\nu^{(2)}(k_1a)}\right]\mathrm{P}_{\nu-1/2}^1(\cos\theta),\tag{5.16}$$

$$B_{2\phi}^{\mathrm{res}}=-\frac{\mu_0}{2\pi a^2\sin\theta}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{D}(\nu)}$$
$$\times\left[\frac{1}{2k_1a}+\frac{H_\nu^{(2)\prime}(k_1a)}{H_\nu^{(2)}(k_1a)}\right]\mathrm{P}_{\nu-1/2}^1(\cos\theta)-\frac{\mu_0k_2}{2\pi k_1a^2}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n$$
$$\times\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\frac{1}{\mathcal{A}(\nu)}\left[\frac{1}{2k_1a}+\frac{H_\nu^{(2)\prime}(k_1a)}{H_\nu^{(2)}(k_1a)}\right]\frac{\partial \mathrm{P}_{\nu-1/2}^1}{\partial\theta},\tag{5.17}$$

and

$$E_{2r}^{\mathrm{ray}}=\frac{i\omega\mu_0}{2\pi a}\frac{1}{(k_2a)^2}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\nu\mathcal{B}(\nu)\mathcal{C}(\nu)^p$$
$$\times\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\mathrm{P}_{\nu-1/2}^1(\cos\theta),\tag{5.18}$$

$$E_{2\theta}^{\mathrm{ray}}=\frac{i\omega\mu_0}{2\pi k_2a^2}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{B}(\nu)\mathcal{C}(\nu)^p$$
$$\times\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]^2\frac{\partial \mathrm{P}_{\nu-1/2}^1(\cos\theta)}{\partial\theta}+\frac{i\omega\mu_0}{2\pi k_1a^2\sin\theta}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n$$
$$\times\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{F}(\nu)\mathcal{G}(\nu)^p\,\mathrm{P}_{\nu-1/2}^1(\cos\theta),\tag{5.19}$$

$$E_{2\phi}^{\mathrm{ray}}=-\frac{i\omega\mu_0}{2\pi k_2a^2\sin\theta}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{B}(\nu)\mathcal{C}(\nu)^p$$
$$\times\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]^2\mathrm{P}_{\nu-1/2}^1(\cos\theta)-\frac{i\omega\mu_0}{2\pi k_1a^2}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n$$
$$\times\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{F}(\nu)\mathcal{G}(\nu)^p\frac{\partial \mathrm{P}_{\nu-1/2}^1}{\partial\theta},\tag{5.20}$$

$$B_{2r}^{\mathrm{ray}}=\frac{\mu_0}{2\pi k_1a^3}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\,e^{i2\pi n\nu}\nu\mathcal{F}(\nu)\mathcal{G}(\nu)^p\,\mathrm{P}_{\nu-1/2}^1(\cos\theta),\tag{5.21}$$

$$B_{2\theta}^{\mathrm{ray}}=\frac{\mu_0 k_2}{2\pi k_1 a^2}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{F}(\nu)\mathcal{G}(\nu)^p$$
$$\times\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\frac{\partial \mathrm{P}^1_{\nu-1/2}}{\partial\theta}-\frac{\mu_0}{2\pi a^2\sin\theta}\sin\phi\sum_{n=-\infty}^{\infty}(-1)^n$$
$$\times\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{B}(\nu)\mathcal{C}(\nu)^p\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\mathrm{P}^1_{\nu-1/2},\tag{5.22}$$

$$B_{2\phi}^{\mathrm{ray}}=\frac{\mu_0 k_2}{2\pi k_1 a^2\sin\theta}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{F}(\nu)\mathcal{G}(\nu)^p$$
$$\times\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\mathrm{P}^1_{\nu-1/2}(\cos\theta)-\frac{\mu_0}{2\pi a^2}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n$$
$$\times\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{B}(\nu)\mathcal{C}(\nu)^p\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\frac{\partial \mathrm{P}^1_{\nu-1/2}}{\partial\theta}.\tag{5.23}$$

B. Residue series

The residue contributions are illustrated by

$$E_{2r}^{\mathrm{res}}=-\frac{i\omega\mu_0}{k_1k_2a^3}\cos\phi\sum_{n=0}^{\infty}\sum_{j=1}^{\infty}\left\{e^{i(2n+1)\pi\nu}\,\nu\left[\frac{1}{2k_1a}+\frac{H_\nu^{(2)\prime}(k_1a)}{H_\nu^{(2)}(k_1a)}\right]\right.$$
$$\left.\times\mathrm{P}^1_{\nu-1/2}(-\cos\theta)\right\}_{\nu=\nu_j}\mathrm{Res}_{\nu=\nu_j}\{\mathcal{A}^{-1}(\nu)\},\tag{5.24}$$

$$B_{2r}^{\mathrm{res}}=\frac{\mu_0}{k_1a^3}\sin\phi\sum_{n=0}^{\infty}(-1)^n\sum_{j=1}^{\infty}\left[e^{i(2n+1)\pi\nu}\,\nu\,\mathrm{P}^1_{\nu-1/2}(-\cos\theta)\right]_{\nu=\tilde{\nu}_j}\mathrm{Res}_{\nu=\tilde{\nu}_j}\{\mathcal{D}^{-1}(\nu)\},\tag{5.25}$$

where the poles are numbered in order of ascending imaginary part.

If both θ and $\pi-\theta$ are $O(1)$,[36]

$$\mathrm{P}^1_{\nu-1/2}(-\cos\theta)\sim\sqrt{\frac{\nu}{2\pi\sin\theta}}\sum_{s=\pm}e^{-is[\nu(\pi-\theta)+\pi/4]}.\tag{5.26}$$

Hence, each n in Eqs. (5.24) and (5.25) represents the "winding number" of two wave paths in air, namely, one of length $\rho_n^+(\theta)=(2\pi n+\theta)a$ and another of length $\rho_n^-=\rho_n^+(2\pi-\theta)$. Both paths originate from the source and reach the observation point clockwise $(+)$ or counterclockwise $(-)$ in the plane determined by the point source, center of sphere and observation point. This plane is henceforth called the meridian plane. The configuration is shown in Fig. 4.

The approximations for the Hankel functions yield[39]

$$\mathcal{A}(\nu)\sim-\left(\frac{2}{k_2a}\right)^{1/3}[\mathcal{H}(\xi;2\pi/3)-i\alpha],\quad \alpha=(k_2/k_1)(k_2a/2)^{1/3},\tag{5.27}$$

$$\mathcal{D}(\nu)\sim\frac{k_2}{k_1}\left(\frac{2}{k_2a}\right)^{1/3}\mathcal{H}(\xi;2\pi/3)-i,\quad \xi=(\nu-k_2a)(k_2a/2)^{-1/3},\tag{5.28}$$

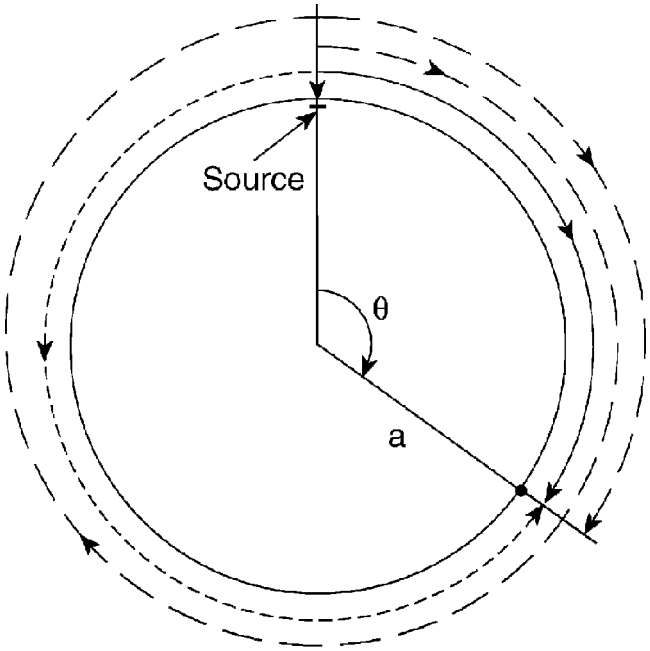

FIG. 4. Paths of lengths $\rho_n^{\pm}$ $(n\geqslant 0)$ traveled by exponentially decreasing waves that reach the observation point through the air.

where $\mathcal{H}(\xi;\psi)$ is defined by Eq. (4.3). Retainment of the $n=0$ terms in the residue series (5.24) and (5.25) and use of approximation (5.26) recover formulas (4.5a) and (4.8a), when $O(\theta_{\mathrm{cr},2})\leqslant\theta<\pi$ and $k_2a(\pi-\theta)\geqslant 1$. This procedure is also applied to the tangential field components. Care should be exercised when (i) $\theta<O(\theta_{\mathrm{cr},2})$, because the relevant residue series converge slowly, calling for the procedure of Sec. III, and (ii) $\pi-\theta\leqslant O[(k_2a)^{-1}]$, where the Legendre functions must be replaced by Bessel functions of argument $\nu(\pi-\theta)$.

By following point (ii) above and extending MacDonald's formulas[36] to the range $O(\theta_{\mathrm{cr},2})<\theta\leqslant\pi$, one gets[43]

$$E_{2r}^{\mathrm{res}}\sim-\frac{\omega\mu_0}{a}\frac{k_2}{k_1}\left(\frac{k_2a}{2}\right)^{2/3}\frac{1}{\overline{\xi}+\alpha^2}\sqrt{\frac{\pi-\theta}{\sin\theta}}e^{i\nu_1\pi}J_1(\nu_1(\pi-\theta))\cos\phi, \tag{5.29}$$

$$B_{2r}^{\mathrm{res}}\sim-\frac{\mu_0k_2}{a}\frac{k_2^2}{k_1^2}\sqrt{\frac{\pi-\theta}{\sin\theta}}e^{i\pi\tilde{\nu}_1}J_1(\tilde{\nu}_1(\pi-\theta))\sin\phi, \tag{5.30}$$

where

$$\nu_1\sim k_2a+(k_2a/2)^{1/3}\overline{\xi},\quad \tilde{\nu}_1\sim k_2a+(k_2a/2)^{1/3}|a_1|e^{i\pi/3}. \tag{5.31}$$

Bear in mind that $\overline{\xi}$ is introduced in Eq. (4.22) and a_1 is the first zero of $\mathrm{Ai}(z)$.

Evidently, for fixed $\alpha=(k_2/k_1)(k_2a/2)^{1/3}$ and $\theta\gg\theta_{\mathrm{cr},2}$, the H-type wave attenuates faster than the E-type one. Due to the factors of $\mathrm{P}^1_{\nu-1/2}(-\cos\theta)/\sin\theta$, the latter prevails for all $O(\theta_{\mathrm{cr},2})<\theta\leqslant\pi$. For example,

$$E_{2\phi}^{\mathrm{res}}\sim-\frac{i\omega\mu_0}{a}e^{ik_2a\pi}\frac{k_2^2}{k_1^2}\sqrt{\frac{\pi-\theta}{\sin\theta}}\left[\frac{1}{2\theta_{\mathrm{cr},2}}e^{i(\pi/\theta_{\mathrm{cr},2})\bar{\xi}}\frac{J_1(\nu_1(\pi-\theta))}{\sin\theta}\frac{1}{\bar{\xi}+\alpha^2}\right.$$
$$\left.+e^{i(\pi/\theta_{\mathrm{cr},2})|a_1|e^{i\pi/3}}J_1'(\tilde{\nu}_1(\pi-\theta))\right]\sin\phi$$
$$\sim-\frac{i\omega\mu_0}{2\rho_{\mathrm{cr},2}}e^{ik_2a\pi}\sqrt{\frac{\pi-\theta}{\sin\theta}}\frac{k_2^2}{k_1^2}\frac{J_1(\nu_1(\pi-\theta))}{\pi-\theta}\frac{e^{i(\pi/\theta_{\mathrm{cr},2})\bar{\xi}}}{\bar{\xi}+\alpha^2}\sin\phi. \tag{5.32}$$

C. Ray representations

1. Case $\theta=O(1)$, $\pi-\theta=O(1)$

Attention is now turned to Eqs. (5.18)–(5.23). Approximations of the Bessel functions outside the transitional regions for $k_2^2a/|k_1|\gg1$ yield[39]

$$\mathcal{A}(\nu)\sim i\sqrt{1-\left(\frac{\nu}{k_2a}\right)^2}+i\frac{k_2}{k_1}\sqrt{1-\left(\frac{\nu}{k_1a}\right)^2}, \tag{5.33}$$

$$\mathcal{B}(\nu)\sim-2i\frac{k_2}{k_1}\left[1-\left(\frac{\nu}{k_2a}\right)^2\right]^{-1/2}\mathcal{T}_E(\nu/a)\exp\left[2i\sqrt{(k_1a)^2-\nu^2}-2i\nu\arccos\left(\frac{\nu}{k_1a}\right)-i\frac{\pi}{2}\right], \tag{5.34}$$

$$\mathcal{C}(\nu)\sim R_E(\nu/a)\exp\left[2i\sqrt{(k_1a)^2-\nu^2}-2i\nu\arccos\left(\frac{\nu}{k_1a}\right)-i\frac{\pi}{2}\right], \tag{5.35}$$

$$\mathcal{D}(\nu)\sim-i\sqrt{1-\left(\frac{\nu}{k_1a}\right)^2}-i\frac{k_2}{k_1}\sqrt{1-\left(\frac{\nu}{k_2a}\right)^2}, \tag{5.36}$$

$$\mathcal{F}(\nu)\sim-2i\,\mathcal{T}_H(\nu/a)\exp\left[2i\sqrt{(k_1a)^2-\nu^2}-2i\nu\arccos\left(\frac{\nu}{k_1a}\right)-i\frac{\pi}{2}\right], \tag{5.37}$$

$$\mathcal{G}(\nu)\sim R_H(\nu/a)\exp\left[2i\sqrt{(k_1a)^2-\nu^2}-2i\nu\arccos\left(\frac{\nu}{k_1a}\right)-i\frac{\pi}{2}\right], \tag{5.38}$$

where

$$R_E(\lambda)=-\frac{\sqrt{1-(\lambda/k_2)^2}-(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}{\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}}, \tag{5.39}$$

$$R_H(\lambda)=\frac{\sqrt{1-(\lambda/k_1)^2}-(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}}{\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}}, \tag{5.40}$$

$$\mathcal{T}_E(\lambda)=\frac{\sqrt{1-(\lambda/k_1)^2}\sqrt{1-(\lambda/k_2)^2}}{[\sqrt{1-(\lambda/k_2)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_1)^2}]^2}, \tag{5.41}$$

$$\mathcal{T}_H(\lambda)=\frac{\sqrt{1-(\lambda/k_1)^2}}{[\sqrt{1-(\lambda/k_1)^2}+(k_2/k_1)\sqrt{1-(\lambda/k_2)^2}]^2}. \tag{5.42}$$

R_E and R_H are the usual Fresnel reflection coefficients. The corresponding integrands are separated into two groups as follows.

(*i*) The first group contains terms of the radial components along with integrands proportional to $\partial \mathrm{P}^1_{\nu-1/2}/\partial\theta$. For instance,

$$\nu\mathcal{B}(\nu)\,\mathcal{C}(\nu)^p\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\mathrm{P}^1_{\nu-1/2}(\cos\theta)\,e^{i2\pi n\nu}$$
$$\sim\frac{k_2}{k_1}\,\nu\,\sqrt{\frac{2\nu}{\pi\sin\theta}}\,\mathcal{T}_E(\nu/a)\,R_E(\nu/a)^p\,(e^{i\Phi_{pn+}}+e^{i\Phi_{pn-}}), \tag{5.43}$$

$$\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{B}(\nu)\,\mathcal{C}(\nu)^p\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]^2\frac{\partial\mathrm{P}^1_{\nu-1/2}}{\partial\theta}\,e^{i2\pi n\nu}$$
$$\sim i\frac{k_2}{k_1}\sqrt{\frac{2\nu}{\pi\sin\theta}}\left[1-\left(\frac{\nu}{k_2a}\right)^2\right]^{1/2}\mathcal{T}_E(\nu/a)\,R_E(\nu/a)^p\,[e^{i(\Phi_{pn+}+\pi/2)}+e^{i(\Phi_{pn-}-\pi/2)}], \tag{5.44}$$

where

$$\Phi_{pn\pm}(\nu;\theta)=2(p+1)\sqrt{(k_1a)^2-\nu^2}-2(p+1)\,\nu\,\arccos\left(\frac{\nu}{k_1a}\right)-(p+1)\,\frac{\pi}{2}+2\pi n\nu\pm\left(\nu\theta+\frac{\pi}{4}\right). \tag{5.45}$$

The phase $\Phi_{pn\pm}(\nu;\theta)$ becomes stationary at

$$\nu=\nu_{pn\pm}=k_1a\cos\psi_{pn\pm},\quad \psi_{pn\pm}=\frac{2\pi n\pm\theta}{2(p+1)},\quad 0\leqslant\psi_{pn\pm}\leqslant\pi/2, \tag{5.46}$$

where the "+" sign holds if $0\leqslant 2n\leqslant p$ and the "−" sign holds if $0<2n\leqslant p+1$. The integrals are calculated by the stationary-phase method with

$$\left.\frac{d^2\Phi_{pn\pm}}{d\nu^2}\right|_{\nu=\nu_{pn\pm}}=\frac{2(p+1)}{k_1a\sin\psi_{pn\pm}}. \tag{5.47}$$

The radial components involve the integrals

$$\int_0^\infty d\nu\,e^{i2\pi n\nu}\,\nu\mathcal{B}(\nu)\,\mathcal{C}(\nu)^p\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\mathrm{P}^1_{\nu-1/2}(\cos\theta)$$
$$\sim e^{-i\pi/4}\frac{k_1k_2a^2}{\sqrt{\sin\theta}}\,\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\cos\psi_{pns}\sqrt{\sin 2\psi_{pns}}\,\mathcal{T}_E(k_1\cos\psi_{pns})\,R_E(k_1\cos\psi_{pns})^p$$
$$\times\exp[2i(p+1)k_1a\sin\psi_{pns}+is\pi/4], \tag{5.48}$$

$$\int_0^\infty d\nu\,e^{i2\pi n\nu}\,\nu\mathcal{F}(\nu)\,\mathcal{G}(\nu)^p\,\mathrm{P}^1_{\nu-1/2}(\cos\theta)$$
$$\sim -e^{i\pi/4}\frac{(k_1a)^2}{\sqrt{\sin\theta}}\,\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\cos\psi_{pns}\sqrt{\sin 2\psi_{pns}}\,\mathcal{T}_H(k_1\cos\psi_{pns})\,R_H(k_1\cos\psi_{pns})^p$$
$$\times\exp[2i(p+1)k_1a\sin\psi_{pns}+is\pi/4]. \tag{5.49}$$

(*ii*) Terms of the second group pertain to the tangential components containing the factor $\mathrm{P}^1_{\nu-1/2}(\cos\theta)$. The respective integrals are treated similarly, but the leading contributions stem from the endpoint $\nu=0$ with width $O(1)$ and from the stationary-phase points $\nu_{pn\pm}$ with width $O(\sqrt{k_1 a})$. The former contributions are cancelled. The surviving terms are corrections $O[(k_1 a)^{-1}]$ when $\psi_{pn\pm}=O(1)$ and $\pi/2-\psi_{pn\pm}=O(1)$. For instance,

$$\sum_{n=-\infty}^{\infty}\sum_{p=0}^{\infty}\int_0^{\infty} d\nu\, e^{i2\pi n\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{F}(\nu)\,\mathcal{G}(\nu)^p\,\mathrm{P}^1_{\nu-1/2}(\cos\theta)$$

$$\sim -e^{i\pi/4}\frac{1}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}\sqrt{2\tan\psi_{pns}}$$

$$\times\mathcal{T}_H(k_1\cos\psi_{pns})\,R_H(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}+is\pi/4], \quad (5.50)$$

where

$$S_{p+}=\{n:\ 0\leqslant 2n\leqslant p\},\quad S_{p-}=\{n:\quad 0<2n\leqslant p+1\}. \quad (5.51)$$

The preceding considerations lead to the rays

$$E^{\mathrm{ray}}_{2r}\sim e^{i\pi/4}\frac{\omega\mu_0 k_1}{2\pi k_2 a}\frac{\cos\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\cos\psi_{pns}\sqrt{\sin 2\psi_{pns}}$$

$$\times\mathcal{T}_E(k_1\cos\psi_{pns})\,R_E(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}+is\pi/4], \quad (5.52)$$

$$E^{\mathrm{ray}}_{2\theta}\sim e^{-i\pi/4}\frac{\omega\mu_0}{2\pi a}\frac{\cos\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\sqrt{\sin 2\psi_{pns}}$$

$$\times\overline{\mathcal{T}}_E(k_1\cos\psi_{pns})\,R_E(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}-is\pi/4]$$

$$+\frac{1}{k_1 a}e^{-i\pi/4}\frac{\omega\mu_0}{2\pi a\sin\theta}\frac{\cos\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\sqrt{2\tan\psi_{pns}}$$

$$\times\mathcal{T}_H(k_1\cos\psi_{pns})\,R_H(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}+is\pi/4], \quad (5.53)$$

$$E^{\mathrm{ray}}_{2\phi}\sim e^{-i\pi/4}\frac{\omega\mu_0}{2\pi a}\frac{\sin\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\sqrt{\sin 2\psi_{pns}}$$

$$\times\mathcal{T}_H(k_1\cos\psi_{pns})\,R_H(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}-is\pi/4]$$

$$+\frac{1}{k_1 a}e^{-i\pi/4}\frac{\omega\mu_0}{2\pi a\sin\theta}\frac{\sin\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\sqrt{2\tan\psi_{pns}}$$

$$\times\overline{\mathcal{T}}_E(k_1\cos\psi_{pns})\,R_E(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}+is\pi/4], \quad (5.54)$$

$$B^{\mathrm{ray}}_{2r}\sim -e^{i\pi/4}\frac{\mu_0 k_1}{2\pi a}\frac{\sin\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\cos\psi_{pns}\sqrt{\sin 2\psi_{pns}}$$

$$\times\mathcal{T}_H(k_1\cos\psi_{pns})\,R_H(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}+is\pi/4], \quad (5.55)$$

$$B_{2\theta}^{\text{ray}} \sim -e^{-i\pi/4}\frac{\mu_0 k_2}{2\pi a}\frac{\sin\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\sqrt{\sin 2\psi_{pns}}$$
$$\times\overline{\mathcal{T}}_H(k_1\cos\psi_{pns})\,R_H(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}-is\pi/4]$$
$$-\frac{1}{k_1 a}e^{-i\pi/4}\frac{\mu_0 k_2}{2\pi a\sin\theta}\frac{\sin\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\sqrt{2\tan\psi_{pns}}$$
$$\times\mathcal{T}_E(k_1\cos\psi_{pns})\,R_E(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}+is\pi/4], \qquad (5.56)$$

$$B_{2\phi}^{\text{ray}} \sim e^{-i\pi/4}\frac{\mu_0 k_2}{2\pi a}\frac{\cos\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\sqrt{\sin 2\psi_{pns}}$$
$$\times\mathcal{T}_E(k_1\cos\psi_{pns})\,R_E(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}-is\pi/4]$$
$$+\frac{1}{k_1 a}e^{-i\pi/4}\frac{\mu_0 k_2}{2\pi a\sin\theta}\frac{\cos\phi}{\sqrt{\sin\theta}}\sum_{p=0}^{\infty}\frac{e^{-ip\pi/2}}{\sqrt{p+1}}\sum_{s=\pm}\sum_{n\in S_{ps}}(-1)^n\sqrt{2\tan\psi_{pns}}$$
$$\times\overline{\mathcal{T}}_H(k_1\cos\psi_{pns})\,R_H(k_1\cos\psi_{pns})^p\exp[2i(p+1)k_1 a\sin\psi_{pns}+is\pi/4], \qquad (5.57)$$

where

$$\overline{\mathcal{T}}_F(\lambda)=\sqrt{1-(\lambda/k_2)^2}\,\mathcal{T}(\lambda),\quad F=E,H. \qquad (5.58)$$

Note that corrections to the leading terms of the first group introduced above are omitted.

An inspection of the summands for $p\gg 2n>1$, $\theta=O(1)$ and $\pi-\theta=O(1)$ shows that their magnitudes decrease as $|R|^p/p^2$ when medium 1 is lossless. Of course, convergence is improved when $\mathrm{Im}\,k_1$ is positive and $O(1)$. In general, $|R(\lambda)|\leqslant 1$ for complex λ while the condition $k_2^2 \ll |k_1^2|$ forces $|R(k_1\cos\psi_{pn\pm})|$ to be nearly 1.[44]

The rays described by formulas (5.52)–(5.57) circulate around the origin in the meridian plane while they are multiply reflected at the spherical boundary, as depicted in Fig. 5; p is the number of reflections, n is the number of circulations, the sign $s=\pm$ specifies the sense of circulation, and $\psi_{pn\pm}$ is the angle between the incident ray and the corresponding local tangent. The overall phase of each ray undergoes a change of $-\pi/2$ at each reflection (see also Ref. 33).

2. Reduction to a wave through region 1, $\theta\ll 1$

When $\theta=O[(k_1 a)^{-1/3}]$ and $n=0$, the width $O(\sqrt{k_1 a\,\theta})$ of the stationary-phase contribution above becomes comparable to the width $O[(k_1 a)^{1/3}]$ of the transitional region about $\nu=k_1 a$. This suggests the transition of rays to the wave propagating in region 1 according to the integral $\mathcal{I}_1$ in Sec. IV. The two asymptotic formulas connect smoothly if $O[(k_1 a)^{-1/3}]<\theta<O[(k_1 a)^{-1/5}]$. The approximation

$$\sin\psi_{p0+}\sim\psi_{p0+}-\psi_{p0+}^3/6,\quad |k_1|a\,\theta^5\ll 2^4\,5!,$$

in the phase, along with $k_2^2 a\,\theta/|k_1|\gg 1$, $\sin(2\psi_{p0+})\sim 2\psi_{p0+}$, and

$$R(k_1\sin\psi_{p0+})\sim -1,$$

$$\mathcal{T}_E(k_1\sin\psi_{p0+})\sim -i(k_2/k_1)\,\psi_{p0+},\quad \mathcal{T}_H(k_1\sin\psi_{p0+})\sim -\psi_{p0+}$$

in the amplitude reduce the $n=0$ terms in (5.52)–(5.57) to formulas (4.42)–(4.45).

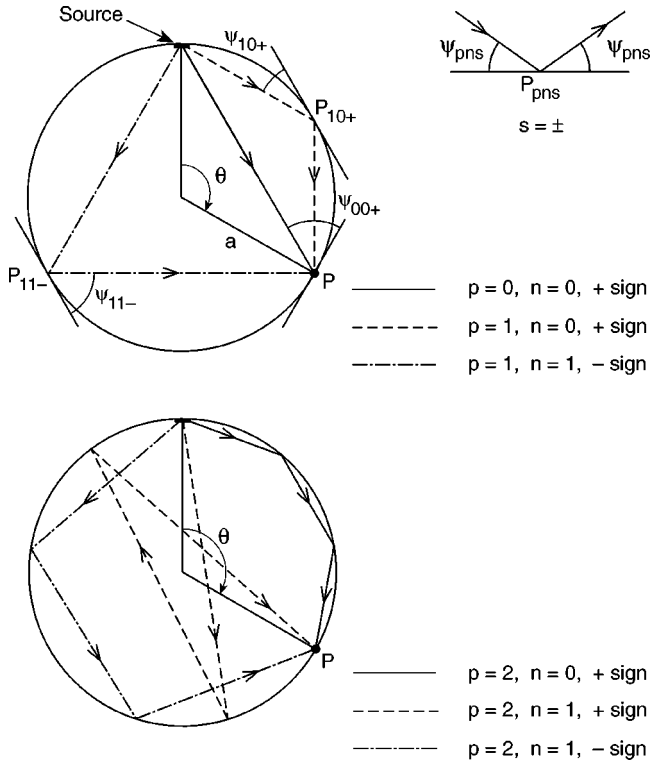

FIG. 5. Geometry of rays bouncing and circulating in the interior of the sphere. P is the observation point.

3. Field close to the antipodes, $\pi-\theta \ll 1$

Care should be exercised when $\theta \sim \pi$. This condition implies that a combination of exponentials may no longer be a reasonable approximation for the Legendre function.[36] In fact, in order to overcome this difficulty, one has to seek an alternative representation *a priori*. The identity $\mathrm{P}_l^1(\cos\theta)=(-1)^{l+1}\mathrm{P}_l^1(\cos(\pi-\theta))$ suggests the replacement

$$\mathrm{P}^1_{\nu-1/2}(\cos\theta)\to ie^{i\pi\nu}\mathrm{P}^1_{\nu-1/2}(\cos(\pi-\theta)). \tag{5.59}$$

The new representation is illustrated by

$$E^{\mathrm{ray}}_{2r}=-\frac{\omega\mu_0}{2\pi a}\frac{1}{(k_2a)^2}\cos\phi\sum_{n'=-\infty}^{\infty}(-1)^{n'}\sum_{p=0}^{\infty}\int_0^{\infty}d\nu\, e^{i\pi(2n'+1)\nu}\nu\mathcal{B}(\nu)\mathcal{C}(\nu)^p \times\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)\prime}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\mathrm{P}^1_{\nu-1/2}(-\cos\theta). \tag{5.60}$$

The ray $(n,p,s=\pm)$ of Sec. V C 1 is identified with the ray $(n'=n,p,s'=-)$ if $s=+$, or $(n'=n-1,p,s'=+)$ if $s=-$ in the present formalism. The stationary-phase points are given by

$$\tilde{\nu}_{pn'\pm}=k_1a\cos\overline{\psi}_{pn'\pm},\quad \overline{\psi}_{pn'\pm}=\frac{(2n'+1)\pi\pm\theta'}{2(p+1)},\quad 0\leqslant\overline{\psi}_{pn'\pm}\leqslant\pi/2, \tag{5.61a}$$

$$\theta'=\pi-\theta, \tag{5.61b}$$

with the sign convention $\{+:\ 0\leqslant 2n'\leqslant p-1\}$ and $\{-:\ 0\leqslant 2n'\leqslant p\}$.

An interesting case arises when $\pi-\theta \leqslant O[(k_1a)^{-1/2}]$ and $2n'=p$ $(s'=-)$, because the endpoint of integration, $\nu=0$, then falls inside the critical vicinity of a stationary-phase point. The requisite integrals for $2n'=p$ are evaluated through MacDonald's formulas[36] with $|\lambda|=|\nu/a| \ll 1$ in the radicals of expressions (5.33)–(5.42). The phase of $e^{i\pi(2n'+1)\nu}\mathcal{B}(\nu)\mathcal{C}(\nu)^p$ and $e^{i\pi(2n'+1)\nu}\mathcal{F}(\nu)\mathcal{G}(\nu)^p$ is expanded about $\nu=0$ up to $O(\nu^2)$. Let $\partial \mathrm{P}^1_{\nu-1/2}/\partial\theta' = -\partial \mathrm{P}^1_{\nu-1/2}(-\cos\theta)/\partial\theta$. The requisite integral for E_{2r} is

$$
\begin{aligned}
& i\int_0^\infty d\nu\, e^{i\pi(p+1)\nu}\,\nu\mathcal{B}(\nu)\mathcal{C}(\nu)^p\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)'}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]\mathrm{P}^1_{\nu-1/2}(\cos\theta') \\
& \quad \sim -2\frac{k_2}{k_1}e^{2i(p+1)k_1a-ip\pi/2}\int_0^\infty d\nu\left(\nu^2-\frac{1}{4}\right)J_1(\nu\theta')\,e^{i(p+1)\nu^2/(k_1a)} \\
& \quad \sim \frac{k_1k_2a^2}{2}\,\frac{e^{-ip\pi/2}}{(p+1)^2}(\pi-\theta)\exp[2i(p+1)k_1a-(i/4)k_1a(\pi-\theta)^2/(p+1)], \qquad (5.62)
\end{aligned}
$$

provided that $|k_1a|(\pi-\theta)^2 \leqslant O(1)$. Comparison with formula (5.48) shows that the character of this ray is not modified as θ approaches π, in contradistinction to the case of a vertical dipole.[33] Indeed, the approximation

$$
\sin\psi_{(2n)n+} \sim 1-\frac{(\pi-\theta)^2}{8(p+1)^2}, \quad \frac{|k_1a|\,(\pi-\theta)^4}{(p+1)^4} \ll 1,
$$

in the phase of formula (5.48), along with

$$
\cos\psi_{(2n)n+} \sim \frac{\pi-\theta}{2(p+1)}, \quad \sin 2\psi_{(2n)n+} \sim \frac{\pi-\theta}{p+1}, \quad \mathcal{T}_E \sim 1, \quad R_E \sim 1,
$$

readily furnish formula (5.62). Similar considerations apply to B^{ray}_{2r}, with the requisite integral

$$
\begin{aligned}
& i\int_0^\infty d\nu\, e^{i\pi(p+1)\nu}\,\nu\mathcal{F}(\nu)\mathcal{G}(\nu)^p\,\mathrm{P}^1_{\nu-1/2}(\cos\theta') \\
& \quad \sim -i\frac{(k_1a)^2}{2}\,\frac{e^{-ip\pi/2}}{(p+1)^2}(\pi-\theta)\exp[2i(p+1)k_1a-(i/4)k_1a(\pi-\theta)^2/(p+1)].
\end{aligned} \qquad (5.63)
$$

For $E^{\mathrm{ray}}_{2\theta}$, it suffices to compare the following integrals:[39]

$$
\begin{aligned}
e_{\theta p} &= \frac{-i}{k_2a}\int_0^\infty d\nu\, e^{i\pi(p+1)\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{B}(\nu)\mathcal{C}(\nu)^p\left[\frac{1}{2k_2a}+\frac{H_\nu^{(1)'}(k_2a)}{H_\nu^{(1)}(k_2a)}\right]^2\frac{\partial \mathrm{P}^1_{\nu-1/2}}{\partial\theta'} \\
& \sim \frac{-2i}{k_1a}e^{2i(p+1)k_1a-ip\pi/2}\frac{\partial}{\partial\theta'}\int_0^\infty d\nu\, J_1(\nu\theta')\,e^{i(p+1)\nu^2/(k_1a)} \\
& = -\left[\frac{e^{-(i/4)k_1a(\pi-\theta)^2/(p+1)}}{p+1}+2i\,\frac{1-e^{-(i/4)k_1a(\pi-\theta)^2/(p+1)}}{k_1a(\pi-\theta)^2}\right]e^{2i(p+1)k_1a-ip\pi/2} \qquad (5.64)
\end{aligned}
$$

and

$$\tilde{e}_{\theta p}=\frac{i}{k_1 a(\pi-\theta)}\int_0^\infty d\nu\, e^{i\pi(p+1)\nu}\frac{\nu}{\nu^2-\frac{1}{4}}\mathcal{F}(\nu)\mathcal{G}(\nu)^p\,\mathrm{P}^1_{\nu-1/2}(\cos\theta')$$

$$\sim 2i\,\frac{1-e^{-(i/4)k_1(\pi-\theta)^2/(p+1)}}{k_1 a(\pi-\theta)^2}\,e^{2i(p+1)k_1 a-ip\pi/2}. \tag{5.65}$$

The three terms of formula (5.64) become of the same order in magnitude if $k_1 a(\pi-\theta)^2=O(1)$. The first term is dominant if $|k_1 a|(\pi-\theta)^2\gg 1$ and then recovers the corresponding geometrical ray with $2n=p$ and $s=+$. In contrast, in formula (5.65) all terms must be retained; the second term multiplied by $k_1 a(\pi-\theta)$ connects smoothly to the correction appearing in (5.53), while the first term is the contribution from the endpoint $\nu=0$. This contribution is cancelled by the corresponding term in (5.64), viz.,

$$e_{\theta p}+\tilde{e}_{\theta p}\sim -i\,\frac{e^{-ip\pi/2}}{p+1}\exp[2i(p+1)k_1 a-(i/4)k_1 a(\pi-\theta)^2/(p+1)]. \tag{5.66}$$

These considerations can be repeated for the integral of $E^{\mathrm{ray}}_{2\phi}$ with $\mathrm{P}^1_{\nu-1/2}(\cos\theta')/\theta'$ and $\partial\mathrm{P}^1_{\nu-1/2}/\partial\theta'$ interchanged. Along the same lines is the analysis for the components of the magnetic field, because the presence of the factor $[(2k_2a)^{-1}+H_\nu^{(1)\prime}(k_2a)/H_\nu^{(1)}(k_2a)]$ amounts to multiplication by i.

The amplitudes of other rays with $2n'\leqslant p-1$ are determined by noticing that the Bessel function varies slowly over the region of width $O(\sqrt{k_1 a})$ about each stationary-phase point, and can therefore be pulled out of the corresponding integrals. This program can be carried out straightforwardly; this case is not discussed further in this article.

VI. REMARKS AND DISCUSSION

Before closing this article, it is worthwhile making the following remarks.

(*i*) The order of magnitude of the critical distance $\rho_{\mathrm{cr},j}$ in Eq. (3.36) can be obtained by postulating that, when $\rho=O(\rho_{\mathrm{cr},j})$, the difference between the arc length $\rho=a\theta$ and its projection on the tangent at $\theta=0$ becomes comparable to the wavelength in air ($j=2$) or earth ($j=1$).[3,4]

(*ii*) It is tempting to compare the field of a horizontal dipole to that of the vertical dipole with equal moment, examined, for example, in Ref. 33. The dominant components of the former field are E_{2r}, $E_{2\theta}$ and $B_{2\phi}$. These are precisely the nonzero components of a vertical dipole. The corresponding maximum magnitudes in ϕ satisfy the relations

$$|E^{\mathrm{hor}}|_m\sim\frac{k_2}{|k_1|}|E^{\mathrm{ver}}|,\quad |B^{\mathrm{hor}}_\phi|_m\sim\frac{k_2}{|k_1|}|B^{\mathrm{ver}}_\phi|. \tag{6.1}$$

(*iii*) The present analysis offers some insight into the problem of a dipole elevated at a height h ($h=b-a\ll a$). A complication in this case stems from the additional transitional point in the integrands of the Poisson summation formula. For example,

$$E_{2r}=\frac{i\mu_0\omega}{2\pi a}\left(\frac{a}{b}\right)^{1/2}\frac{1}{(k_2a)^2}\cos\phi\sum_{n=-\infty}^{\infty}(-1)^n\int_0^\infty d\nu\, e^{i2\pi n\nu}\nu\,\frac{H_\nu^{(1)}(k_2b)}{H_\nu^{(1)}(k_2a)}\,\frac{1}{\mathcal{K}(\nu)}$$

$$\times\left[\frac{1}{2k_2b}+\frac{H_\nu^{(1)\prime}(k_2b)}{H_\nu^{(1)}(k_2b)}\right]\mathrm{P}^1_{\nu-1/2}(\cos\theta). \tag{6.2}$$

It is readily concluded that elevation of the dipole results in the increase of the critical angle $\theta_{\mathrm{cr},j}$ by $O(\sqrt{2h/a})$. The analysis is simplified when $k_2h\ll(k_2a)^{1/3}$ so that the points k_2a and k_2b can be treated, in some sense, as a single transitional point.

For arbitrary h, the residue series for E_{2r} when $\theta > O(\sqrt{2h/a})$ contains the factors

$$f_j(h) = \frac{H^{(1)}_{\nu_j}(k_2 b)}{H^{(1)}_{\nu_j}(k_2 a)}, \quad j = 1, 2, \ldots, \tag{6.3}$$

where ν_j are zeros of the $\mathcal{A}(\nu)$ defined by Eq. (5.7) that lie in the vicinity of $\nu = k_2 a$. $f_j(h)$ is the "height-gain factor" introduced by Bremmer.[14] In the corresponding factor $\tilde{f}_j(h)$ for B_{2r}, the ν_j need to be replaced by the zeros $\tilde{\nu}_j$ of the $\mathcal{D}(\nu)$ defined by Eq. (5.3). These factors express the dependence of the field beyond the horizon on the parameter $(k_2 a)^{1/3}\sqrt{2h/a}$. The height-gain factors for the θ- and ϕ-components are defined in a similar fashion. With regard to $E_{2\theta}$, one needs to consider the factor

$$\frac{H^{(1)}_{\nu_j}(k_2 b)}{H^{(1)}_{\nu_j}(k_2 a)} \frac{(1/k_2 b) + [H^{(1)\prime}_{\nu_j}(k_2 b)/H^{(1)}_{\nu_j}(k_2 b)]}{(1/k_2 a) + [H^{(1)\prime}_{\nu_j}(k_2 a)/H^{(1)}_{\nu_j}(k_2 a)]}.$$

(*iv*) The method of solution here needs to be modified when the medium in region 1 or 2 contains inhomogeneities, as is the case with ionospheric effects. The ionosphere can be modeled crudely via replacement of the air for $r > d$ $(d > a)$ by a perfect conductor.

A problem of interest arises when the index of refraction near the earth's surface exhibits variations due to high moisture. This phenomenon is called "ducting" and may cause superrefraction when rays emitted from the radiating source bend downwards.[14] A model for the dielectric permittivity gives[14]

$$\epsilon_2(r) = \epsilon_0 \frac{A + B(r - r_0)^2}{r^2}. \tag{6.4}$$

(*v*) The method of stationary phase for the rays employed in Sec. V becomes questionable when $\nu_{pn\pm}$ lies in a neighborhood of width $O(\sqrt{k_1 a})$ of any pole of $\mathcal{A}^{-1}(\nu)$ or $\mathcal{D}^{-1}(\nu)$ close to the positive real axis. The value $\nu_{pn\pm} \sim k_2 a$ corresponds to a ray that undergoes total internal reflection.[45] Such a case follows, for instance, from taking $2n = p$, $s = +$ and

$$\nu_{pn+} = k_2 a(1 - \overline{\epsilon}), \quad \overline{\epsilon} = 1 - \frac{k_1}{k_2}\frac{\pi - \theta}{2(p+1)}, \quad |\overline{\epsilon}| \ll 1. \tag{6.5}$$

A remedy to this anomaly is quite elaborate, in principle involving sums of Fresnel integrals, and is provided elsewhere.[33]

VII. SUMMARY AND CONCLUSIONS

The problem of the radiating electric dipole lying just below and tangential to the surface of an electrically large, homogeneous, isotropic and nonmagnetic sphere surrounded by air has been revisited. The present analysis, however, has a different perspective from previous works, since it was guided by the physical concept of the creeping wave.[22] The Poisson summation formula, employed over 40 years ago in the study of plane-wave scattering by impenetrable objects,[22] provided a useful starting point. In the present case the creeping wave, although evidently two-dimensional, has a more intricate structure being dependent on the nature and orientation of the source.

All six components of the electromagnetic field on the boundary were determined without recourse to scalar potentials. For an optically dense sphere, each component is decomposed into waves propagating through air and through the sphere. When the polar angle θ is sufficiently lower than a critical value given by Eq. (3.36), known planar-earth formulas are recovered[34] along with simplified corrections to account for the curved boundary. In particular, the electric-type wave in

the tangential components with the air phase velocity gives rise to Fresnel integrals and surface waves,[34] and therefore has a character distinctly different from solutions to plane-wave scattering within the scalar wave and Schrödinger's equations.[29]

As θ progresses to values that are comparable to or exceed $\theta_{\mathrm{cr},2}$, the electric-type wave through air is described by series of exponentials decreasing in θ. The attenuation rates were determined to the lowest order in $(k_2 a)^{-1}$ and k_2/k_1 by solving a transcendental equation, also encountered in the problem of the vertical radiating dipole;[42] its roots depend on the widely varying parameter $\alpha=(k_2 a/2)^{1/3} k_2/k_1$. On the other hand, lowest-order attenuation constants for the magnetic-type wave are fixed numbers, in agreement with early findings by Gray.[12] Higher-order corrections to these equations are easily obtained within this scheme. By starting with the zeroth-order equations, an argument was presented to show that the H-type wave attenuates faster than the E-type one when $|\alpha| \leqslant O(1)$; a conjecture made by Fock[16] was therefore placed on firmer grounds. The electric field was found to have a dominant component perpendicular to the boundary, while the magnetic field has a dominant component in the azimuthal direction. The ensuing polarization resembles that of a vertical electric dipole, but the maximum magnitude of the field in this case is multiplied by the factor $k_2/|k_1|$. When $\theta=O(\theta_{\mathrm{cr},1})$ the wave inside the sphere is described by a well-converging integral of Airy functions.

A physical picture of waves exponentially decreasing in air and rays circulating in the interior of the sphere via their multiple reflections at the boundary was exposed when $\theta=O(1)$ and $\pi-\theta=O(1)$. These ray contributions are significant when $\mathrm{Im}\, k_1 a \ll 1$. As expected from elementary geometrical optics, only one type of wave (electric or magnetic) prevails in each component, with the amplitude of the dominant ray being described by the corresponding Fresnel reflection coefficient. There are features of both the amplitude and phase of these rays, however, that are attributed to the nature of the source and are not fully predictable by standard geometrical optics. This ray picture breaks down at the antipodal point ($\theta \sim \pi$), or any point of total internal reflection.[45] In both cases, the modified analysis unveils characteristics due to the nature of the source. For instance, the two types of polarization in the tangential components can provide comparable ray contributions if $\theta \sim \pi$, when $2n=p$, $s=+$ in the notation of Sec. V; the total amplitude then recovers the Fresnel reflection coefficient of geometrical optics. This situation is to be contrasted with the case of a vertical dipole, where the ray amplitude changes drastically at the antipodes.

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APPENDIX A: ON THE ZEROS OF $\mathcal{K}(\nu)$, $\mathcal{M}(\nu)$

To simplify the calculations in this appendix, consider k_1 to be real, unless it is stated otherwise. For $k_2 a \gg 1$, $k_2^2 \ll k_1^2$ and $k_2^2 a/k_1 \gg 1$, the terms $(2k_2 a)^{-1}$ and $k_2 k_1^{-1}(2k_1 a)^{-1}$ in $\mathcal{K}(\nu)$ are neglected. Following Refs. 29 and 33, define

$$\mathcal{P}(\nu;\kappa)=\frac{J_\nu'(k_1 a)}{J_\nu(k_1 a)}-\kappa\frac{H_\nu^{(1)\prime}(k_2 a)}{H_\nu^{(1)}(k_2 a)}, \tag{A1}$$

where $\kappa=k_1/k_2$ corresponds to $\mathcal{K}(\nu)$ and $\kappa=k_2/k_1$ corresponds to $\mathcal{M}(\nu)$. In this appendix, the task is to locate those ν that satisfy

$$\mathcal{P}(\nu;\kappa)=0. \tag{A2}$$

For $0<\nu<k_1 a$ and $|\nu-k_{1,2}a| \gg (k_{1,2}a)^{1/3}$,

$$\frac{J_\nu'(k_1a)}{J_\nu(k_1a)}\sim-\sqrt{1-\left(\frac{\nu}{k_1a}\right)^2}\tan\left[\sqrt{(k_1a)^2-\nu^2}-\nu\arccos\left(\frac{\nu}{k_1a}\right)-\frac{\pi}{4}\right], \tag{A3}$$

$$\frac{H_\nu^{(1)'}(k_2a)}{H_\nu^{(1)}(k_2a)}\sim i\sqrt{1-\left(\frac{\nu}{k_2a}\right)^2}, \tag{A4}$$

and the branch cut emanating from $\nu=k_2a$ lies in the upper ν-plane. Accordingly,

$$\mathcal{P}(\nu;\kappa)\sim-\sqrt{1-\left(\frac{\nu}{k_1a}\right)^2}\tan\left[\sqrt{(k_1a)^2-\nu^2}-\nu\arccos\left(\frac{\nu}{k_1a}\right)-\frac{\pi}{4}\right]$$
$$-i\kappa\sqrt{1-\left(\frac{\nu}{k_2a}\right)^2}. \tag{A5}$$

No zeros of the right-hand side lie in $(0,k_2a)$. The analytic continuation to (k_2a,k_1a) through the lower ν-plane does not exhibit any zeros either. More precisely,

$$\frac{H_\nu^{(1)'}(k_2a)}{H_\nu^{(1)}(k_2a)}\sim\frac{Y_\nu'(k_2a)}{Y_\nu(k_2a)}\left\{1+i\frac{\mathrm{W}[J_\nu,Y_\nu]}{Y_\nu(k_2a)\,Y_\nu'(k_2a)}\right\}, \tag{A6}$$

where $\mathrm{W}[J_\nu,Y_\nu]=(2/\pi)(k_2a)^{-1}$ denotes the Wronskian of $J_\nu(k_2a)$ and $Y_\nu(k_2a)$. This approximation produces a recessive imaginary term for $\nu>k_2a$. Hence, (A2) reads as

$$\tan\left[\sqrt{(k_1a)^2-\nu^2}-\nu\arccos\left(\frac{\nu}{k_1a}\right)-\frac{\pi}{4}\right]$$
$$\sim\kappa\sqrt{\frac{[\nu/(k_2a)]^2-1}{1-[\nu/(k_1a)]^2}}\left\{1-i\exp\left[-2\nu\cosh^{-1}\left(\frac{\nu}{k_2a}\right)+2\sqrt{\nu^2-(k_2a)^2}\right]\right\}. \tag{A7}$$

This equation cannot be satisfied by any real ν. In fact, it is satisfied only in the upper ν-plane. Let $\nu=\nu_r+i\nu_i$, where ν_r and ν_i are real, $|\nu_i|\ll\nu_r$, and $k_2a<\nu_r<k_1a$. Then,

$$\tan\left[\sqrt{(k_1a)^2-\nu_r^2}-\nu_r\arccos\left(\frac{\nu_r}{k_1a}\right)-i\nu_i\arccos\left(\frac{\nu_r}{k_1a}\right)-\frac{\pi}{4}\right]$$
$$\sim\kappa\sqrt{\frac{[\nu_r/(k_2a)]^2-1}{1-[\nu_r/(k_1a)]^2}}\left\{1-i\exp\left[-2\nu_r\cosh^{-1}\left(\frac{\nu_r}{k_2a}\right)+2\sqrt{\nu_r^2-(k_2a)^2}\right]\right\}. \tag{A8}$$

For $\kappa=k_1/k_2$,

$$\sqrt{(k_1a)^2-\nu_r^2}-\nu_r\arccos\left(\frac{\nu_r}{k_1a}\right)\sim\arctan\left\{\frac{k_1}{k_2}\sqrt{\frac{[\nu_r/(k_2a)]^2-1}{1-[\nu_r/(k_1a)]^2}}\right\}+m\pi+\frac{\pi}{4}, \tag{A9}$$

$$\nu_i\arccos\left(\frac{\nu_r}{k_1a}\right)\sim\frac{k_2}{k_1}\sqrt{\frac{1-[\nu_r/(k_1a)]^2}{[\nu_r/(k_2a)]^2-1}}\exp\left[-2\nu_r\cosh^{-1}\left(\frac{\nu_r}{k_2a}\right)+2\sqrt{\nu_r^2-(k_2a)^2}\right], \tag{A10}$$

where m is any integer. In particular, if $k_2a\ll\nu_r\ll k_1a$,

$$\nu_r\sim\frac{2k_1a}{\pi}-\left(2m+\frac{3}{2}\right),\quad \nu_i\sim\frac{4k_2}{\pi k_1}\left(\frac{k_2a}{2\nu_r}\right)^{2\nu_r+1}e^{2\nu_r}. \tag{A11}$$

For $\kappa=k_2/k_1$,

$$\sqrt{(k_1a)^2-\nu_r^2}-\nu_r\arccos\left(\frac{\nu_r}{k_1a}\right)\sim\arctan\left\{\frac{k_2}{k_1}\sqrt{\frac{[\nu_r/(k_2a)]^2-1}{1-[\nu_r/(k_1a)]^2}}\right\}+m\pi+\frac{\pi}{4}, \tag{A12}$$

$$\nu_i\arccos\left(\frac{\nu_r}{k_1a}\right)\sim\frac{k_2}{k_1}\sqrt{[\nu_r/(k_2a)]^2-1}\,\sqrt{1-[\nu_r/(k_1a)]^2}\times\exp\left[-2\nu_r\cosh^{-1}\left(\frac{\nu_r}{k_2a}\right)+2\sqrt{\nu_r^2-(k_2a)^2}\right]. \tag{A13}$$

These expressions are trivially simplified if $k_2a\ll\nu_r\ll k_1a$, i.e.,

$$\nu_r\sim\frac{2k_1a}{\pi}-\left(2m+\frac{1}{2}\right),\quad \nu_i\sim\frac{2\nu_r}{\pi k_1a}\left(\frac{k_2a}{2\nu_r}\right)^{2\nu_r}e^{2\nu_r}. \tag{A14}$$

Consider $0<\mathrm{Re}\,\nu<k_2a$. Setting the right-hand side of (A5) equal to zero in the upper ν-plane yields

$$k_1a-\frac{\nu\pi}{2}\sim m\pi+\frac{\pi}{4}-i\arctan\left[\frac{k_1}{k_2}\sqrt{1-\left(\frac{\nu}{k_2a}\right)^2}\right] \tag{A15}$$

for $\kappa=k_1/k_2$, or

$$k_1a-\frac{\nu\pi}{2}\sim m\pi+\frac{\pi}{4}-i\frac{k_2}{k_1}\sqrt{1-\left(\frac{\nu}{k_2a}\right)^2} \tag{A16}$$

for $\kappa=k_2/k_1$. With $0<|\nu|\ll k_2a$,

$$\nu\sim\frac{2k_1a}{\pi}-\left(2m+\frac{1}{2}\right)+i, \tag{A17}$$

or

$$\nu\sim\frac{2k_1a}{\pi}-\left(2m+\frac{1}{2}\right)+i\frac{2k_2}{\pi k_1}. \tag{A18}$$

In consideration of the transitional region of $H_\nu^{(1)}(k_2a)$,[39] (A2) becomes

$$\tan\left[\sqrt{(k_1a)^2-\nu^2}-\nu\arccos\left(\frac{\nu}{k_1a}\right)-\frac{\pi}{4}\right]=\kappa\left(\frac{2}{k_2a}\right)^{1/3}e^{i2\pi/3}\frac{\mathrm{Ai}'(e^{i2\pi/3}\xi)}{\mathrm{Ai}(e^{i2\pi/3}\xi)}. \tag{A19}$$

This is not satisfied by any real ν. In the lower ν-plane,

$$e^{i2\pi/3}\frac{\mathrm{Ai}'(e^{i2\pi/3}\xi)}{\mathrm{Ai}(e^{i2\pi/3}\xi)}=i\overline{\kappa}, \tag{A20}$$

where

$$\overline{\kappa}=\kappa^{-1}\left(\frac{k_2a}{2}\right)^{1/3}. \tag{A21}$$

Use of the large-argument approximation for the Airy function when $|\overline{\kappa}|\gg1$ evinces that no zeros exist for $-\pi<\mathrm{Arg}\,\xi<0$. In the upper ξ-plane, Eq. (A20) is satisfied at points ξ_s lying in the neighborhoods of zeros of the denominator:

$$\xi_s \sim (-a_s) e^{i\pi/3} [1 + e^{i\pi/6} a_s^{-1} \overline{\kappa}^{-1}], \quad |\overline{\kappa}| \gg 1, \quad s = 1, 2, \ldots, \tag{A22}$$

where a_s are the zeros of $\mathrm{Ai}(z)$ $(a_s < 0)$ numbered in order of ascending magnitude.[40] On the other hand,

$$\xi_s \sim (-\check{a}_s) e^{i\pi/3} [1 + e^{i\pi/6} \check{a}_s^{-2} \overline{\kappa}], \quad |\overline{\kappa}| \ll 1, \quad s = 1, 2, \ldots, \tag{A23}$$

where $\check{a}_s$ are zeros of $\mathrm{Ai}'(z)$.[40] A function can be constructed which is holomorphic in the sector $\{\overline{\kappa}: -\pi/4 < \mathrm{Arg}\ \overline{\kappa} < \pi/4\}$ and whose values are determined by the zeros in the lower ξ-plane given by Eq. (A20). By starting with expression (A22), it can be shown via analytic continuation that no such zeros exist. Such a construction is given in Ref. 33.

APPENDIX B: ON THE ZEROS OF $\mathcal{A}(\nu)$ AND $\mathcal{D}(\nu)$

In the spirit of Appendix A, consider the equation

$$\frac{H_\nu^{(2)'}(k_1 a)}{H_\nu^{(2)}(k_1 a)} - \kappa \frac{H_\nu^{(1)'}(k_2 a)}{H_\nu^{(1)}(k_2 a)} = 0, \tag{B1}$$

where $\kappa = k_1/k_2$ for $\mathcal{A}(\nu)$ and $\kappa = k_2/k_1$ for $\mathcal{D}(\nu)$. The following conclusions are reached.

(i) $\mathcal{A}(\nu)$ and $\mathcal{D}(\nu)$ exhibit no zeros for $0 \leqslant \mathrm{Re}\ \nu < k_2 a$ and $k_2 a < \mathrm{Re}\ \nu < k_1 a$ outside the transitional regions associated with $\nu = k_1 a$ or $\nu = k_2 a$.

(ii) The zeros inside the transitional region of $H_\nu^{(1)}(k_2 a)$ are approximated by those of the corresponding $\mathcal{K}(\nu)$ and $\mathcal{M}(\nu)$ in the upper ν-plane according to (A20) of Appendix A.

(iii) $\mathcal{A}(\nu)$ and $\mathcal{D}(\nu)$ have zeros inside the transitional region of $H_\nu^{(2)}(k_1 a)$ in the lower ν-plane. In view of Eq. (4.3), the equation there is

$$\mathcal{H}(\xi; -2\pi/3) = \kappa \frac{k_1}{k_2} \left(\frac{k_1 a}{2} \right)^{1/3}, \quad \xi = (\nu - k_1 a)(k_1 a/2)^{-1/3}, \tag{B2}$$

which is in turn approximated by

$$\mathrm{Ai}(e^{-i2\pi/3} \xi) = 0. \tag{B3}$$

APPENDIX C: AN INTEGRAL IDENTITY

In this appendix, it is shown that

$$\sum_{n=-\infty}^{\infty} (-1)^n \int_0^\infty d\nu\, e^{i2\pi n\nu} f(\nu)\, \mathrm{P}^1_{\nu-1/2}(\cos\theta)$$

$$= -2\pi \sum_{n=0}^{\infty} (-1)^n \sum_{s=\pm} \sum_{j=1}^{\infty} s\, e^{is(2n+1)\pi\nu_j^s}\, \mathrm{P}^1_{\nu_j^s - 1/2}(-\cos\theta)\, \mathrm{Res}\{f(\nu)\}\big|_{\nu=\nu_j^s}, \tag{C1}$$

where $f(\nu)$ is a meromorphic function with simple poles $\{\nu_j^s\}$ in the first $(s = +)$ and fourth $(s = -)$ quadrant $(j = 1, 2, \ldots,$ in order of ascending imaginary part), and with no singularities in the imaginary and real axes other than poles that coincide with zeros of $\mathrm{P}^1_{\nu-1/2}(\cos\theta)$. $f(\nu)$ is assumed to satisfy

$$f(-\nu) = -f(\nu) \quad \forall\ \nu, \quad f(\nu) = O(\nu^d) \quad \text{as} \quad \nu \to \infty, \ \mathrm{Re}\ \nu > 0, \tag{C2}$$

where d is a real number that may depend on Arg ν.

In the spirit of Ref. 9, the left-hand side of (C1) is written as an integral over a contour C encircling the positive real axis clockwise, as shown in Fig. 6. Then,

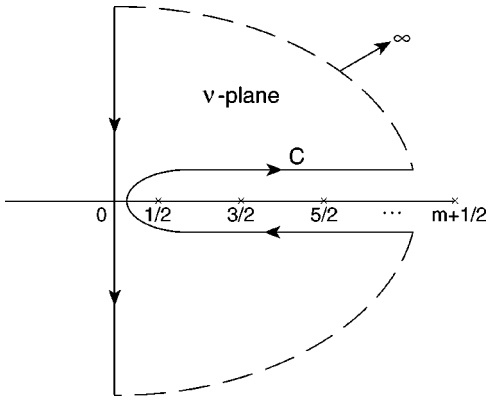

FIG. 6. Contour C that serves the derivation of identity (C1) of Appendix C; m is a non-negative integer.

$$\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\,e^{i2\pi n\nu}f(\nu)\,\mathrm{P}^1_{\nu-1/2}(\cos\theta)$$

$$=i\sum_{l=0}^{\infty}e^{i(l+1/2)\pi}f\left(l+\frac{1}{2}\right)\mathrm{P}^1_l(-\cos\theta)$$

$$=-\frac{1}{2i}\int_C\frac{d\nu}{\cos\pi\nu}f(\nu)\mathrm{P}^1_{\nu-1/2}(-\cos\theta)$$

$$=-\pi\sum_{s=\pm}\sum_{j=1}^{\infty}\frac{\mathrm{P}^1_{\nu_j^s-1/2}(-\cos\theta)}{\cos\pi\nu_j^s}\mathrm{Res}\{f(\nu)\}\big|_{\nu=\nu_j^s}-\frac{1}{2i}\int_{-i\infty}^{i\infty}\frac{d\nu}{\cos\pi\nu}f(\nu)\,\mathrm{P}^1_{\nu-1/2}(-\cos\theta), \tag{C3}$$

by employing $\mathrm{P}^1_l(\cos\theta)=(-1)^{l+1}\mathrm{P}^1_l(\cos(\pi-\theta))$ and properly closing C at infinity. By virtue of (C2) and the identity $\mathrm{P}_{-\nu-1/2}(x)=\mathrm{P}_{\nu-1/2}(x)$, the integral in the right-hand side of (C3) is identically zero. The expansion

$$\frac{1}{\cos\pi\nu}=2e^{\pm i\pi\nu}\sum_{n=0}^{\infty}(-1)^n e^{\pm i2\pi n\nu}, \tag{C4}$$

where $\mathrm{Im}\,\nu>0$ $(+)$ or $\mathrm{Im}\,\nu<0$ $(-)$, immediately yields (C1). As a corollary,

$$\sum_{n=-\infty}^{\infty}(-1)^n\int_0^{\infty}d\nu\,e^{i2\pi n\nu}f(\nu)\,\mathrm{P}^1_{\nu-1/2}(\cos\theta)=0, \tag{C5}$$

if $f(\nu)$ is holomorphic for $\mathrm{Re}\,\nu>0$.

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Plasma velocity in hydromagnetic dynamos

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Hydromagnetic dynamos are plasma configurations generating for some time an exponentially increasing magnetic field. By using a number of functional inequalities, we estimate the rate of increase of magnetic energy in terms of the plasma resistivity and diferent norms on the plasma velocity. Our bounds are proved to be optimal as far as the powers of the relevant magnitudes are concerned. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1473679]

I. INTRODUCTION

A hydromagnetic dynamo in a plasma is a configuration allowing for a finite time an exponential growth of the magnetic field. The behavior of the main magnitudes in an incompressible plasma is governed by the magnetohydrodynamic (MHD) system: the velocity **u**, magnetic field **B**, kinetic pressure p, viscosity ν and resistivity η satisfy, after the usual normalizations,

$$\frac{\partial \mathbf{u}}{\partial t} = \nu \Delta \mathbf{u} - \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{B} \cdot \nabla \mathbf{B} - \nabla p - \nabla \left(\frac{B^2}{2} \right), \tag{1}$$

$$\frac{\partial \mathbf{B}}{\partial t} = \eta \Delta \mathbf{B} - \mathbf{u} \cdot \nabla \mathbf{B} + \mathbf{B} \cdot \nabla \mathbf{u}, \tag{2}$$

$$\nabla \cdot \mathbf{u} = \nabla \cdot \mathbf{B} = 0. \tag{3}$$

The MHD system, for any boundary conditions allowing no input of energy from the outside, is dissipative (see e.g. Ref. 1). Therefore, any growth of magnetic energy must ultimately be done at the expense of the kinetic one, i.e., of the plasma velocity. Once this velocity is taken for granted, the magnetic field is governed by the induction equation (2), and the magnetic energy by the integral identity obtained making the scalar product of (2) and **B**:

$$\frac{1}{2} \frac{\partial}{\partial t} \int_\Omega B^2 dV = \eta \int_\Omega \Delta \mathbf{B} \cdot \mathbf{B} dV + \int_\Omega \mathbf{B} \cdot \nabla \mathbf{u} \cdot \mathbf{B} \, dV - \int_\Omega \mathbf{u} \cdot \nabla \mathbf{B} \cdot \mathbf{B} dV. \tag{4}$$

If we assume $\mathbf{u} \cdot \mathbf{n}|_{\partial\Omega} = 0$ (i.e., the fluid does not cross the boundary), the last integral vanishes. As for the term

$$\eta \int_\Omega \Delta \mathbf{B} \cdot \mathbf{B} dV = -\eta \int_\Omega |\nabla \mathbf{B}|^2 dV + \frac{\eta}{2} \int_{\partial\Omega} \frac{\partial B^2}{\partial n} d\sigma,$$

provided there is no input of magnetic energy from the outside,

$$\int_{\partial\Omega} \frac{\partial B^2}{\partial n} d\sigma \leqslant 0, \tag{5}$$

yields the fundamental energy inequality

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$$\frac{1}{2}\frac{\partial}{\partial t}\int_\Omega B^2 dV \leqslant -\eta\int_\Omega |\nabla \mathbf{B}|^2 dV + \int_\Omega \mathbf{B}\cdot\nabla\mathbf{u}\cdot\mathbf{B}dV. \tag{6}$$

Condition (5) holds (with an equality) for Dirichlet ($\mathbf{B}|_{\partial\Omega}=\mathbf{0}$) or perfect conductor ($\mathbf{B}\cdot\mathbf{n}|_{\partial\Omega}=0$; $(\nabla\times\mathbf{B})\times\mathbf{n}|_{\partial\Omega}=\mathbf{0}$) conditions. We will assume either periodic boundary conditions in a box Ω with

$$\int_\Omega \mathbf{u}\,dV = \int_\Omega \mathbf{B}\,dV = \mathbf{0}, \tag{7}$$

or

$$\mathbf{u}\cdot\mathbf{n}|_{\partial\Omega} = \mathbf{B}\cdot\mathbf{n}|_{\partial\Omega} = 0, \tag{8}$$

in a smooth N-dimensional domain Ω. Thus we will take (6) as the starting inequality. The first term on the right-hand side of (6) accounts for the diffusive effects of the resistivity, while the second is an advective term showing the transport of the magnetic field by the flow. In fact, in ideal plasmas ($\eta=0$) the magnetic field lines are transported by the plasma as material points and the field strength may be enhanced by this process.

From here one may ignore the diffusive term and bound the advective one by

$$\left|\int_\Omega \mathbf{B}\cdot\nabla\mathbf{u}\cdot\mathbf{B}dV\right| \leqslant \frac{1}{2}\|\nabla\mathbf{u}+(\nabla\mathbf{u})^t\|_\infty \int_\Omega B^2 dV, \tag{9}$$

where $\|\ \|_\infty$ means the maximum norm and $(\ )^t$ the transposed matrix (see, e.g., Ref. 2). Therefore, the growth parameter γ satisfies

$$\gamma \leqslant \tfrac{1}{2}\|\nabla\mathbf{u}+(\nabla\mathbf{u})^t\|_\infty. \tag{10}$$

This estimate goes back to Backus.[3] Thus the maximal exponential growth rate does not exceed the largest eigenvalue of the strain matrix $\frac{1}{2}(\nabla\mathbf{u}+(\nabla\mathbf{u})^t)$. This elementary inequality has some merits: the main one is that it does not depend on the resistivity and therefore it holds even when $\eta\to 0$. A velocity configuration yielding a dynamo even when $\eta\to 0$ [$\inf_{\eta\to 0}\gamma(\eta)>0$] is called a fast dynamo;[4] this is an extensively studied subject. On the minus side, we first note that anything involving the gradient of the velocity is somewhat unsatisfactory. This is so because in many turbulent flows there exist sharp changes in the velocity vector, whereas the velocity size remains moderate. Indeed, on general principles one may reject an extremely large plasma velocity, but there is no physical reason to exclude rapid variations of the flow: thus any norm on the velocity itself may be much smaller than the norm of the gradient. Moreover, the maximum norm is the worst possible: it could happen that the plasma remains almost quiescent except for a tiny portion which alone ensures that the maximum of the strain matrix is large. One does not expect the magnetic energy of the whole domain to be governed by a minute portion of the plasma. We will see that (9) may be significantly improved.

II. THE MAIN ESTIMATES

Certain subspaces of the Sobolev space $H^1(\Omega)$ possess the property that

$$\|f\|_{H^1} \leqslant k\|\nabla f\|_2,$$

i.e., the L^2-norm of f is dominated by the norm of its gradient. These are the so-called Poincaré inequalities. One of the most general descriptions of spaces where one of these inequalities holds is as follows (see Refs. 1 and 5): let p be a continuous seminorm [i.e., a continuous norm, except for the fact that $p(f)=0$ does not imply $f=0$] on $H^1(\Omega)$ such that for every *constant* function

$g\neq 0$, $p(g)\neq 0$. Then any subspace H of $H^1(\Omega)$, such that $p(f)=0$ for all $f\in H$, satisfies a Poincaré inequality. Among the many examples of such seminorms, we will use the following ones:

$$p(\mathbf{f})=\left|\int_\Omega \mathbf{f}dV\right|, \tag{11}$$

$$p(\mathbf{f})=\int_{\partial\Omega}|\mathbf{f}\cdot\mathbf{n}|\,d\sigma. \tag{12}$$

Equation (11) covers periodic problems because of the zero mean condition (7), while (12) covers the remaining cases, since (8) holds. That the seminorm p of (12) is continuous follows from the fact that the trace of any function $f\in H^1(\Omega)$ at the boundary belongs to $L^1(\partial\Omega)$ [and even to $L^2(\partial\Omega)$].

Our main tool will be a weak version of the Gagliardo–Nirenberg inequality (Ref. 6, pp. 65–68): denoting as usual by $\|\quad\|_p$ the norm in $L^p(\Omega)$,

$$\|f\|_p\leqslant C\|f\|_{H^1}^{\tau}\|f\|_2^{1-\tau}, \tag{13}$$

where C is a constant depending only on the domain, $\tau=(N/2)-(N/p)$. This holds provided $p\geqslant 2$, $(N/2)-(N/p)<1$, i.e., $p<2N/(N-2)$. Thus, for $N=3$, $2\leqslant p<6$; for $N=2$, any $p\geqslant 2$ is admissible.

Since

$$\int_\Omega \mathbf{B}\cdot\nabla\mathbf{u}\cdot\mathbf{B}dV=-\int_\Omega \mathbf{B}\cdot\nabla\mathbf{B}\cdot\mathbf{u}dV, \tag{14}$$

by the inequality of Cauchy–Schwarz

$$\left|\int_\Omega \mathbf{B}\cdot\nabla\mathbf{u}\cdot\mathbf{B}dV\right|\leqslant\int_\Omega|\mathbf{B}||\nabla\mathbf{B}||\mathbf{u}|dV\leqslant\|\mathbf{B}\|_p\|\nabla\mathbf{B}\|_2\|\mathbf{u}\|_q, \tag{15}$$

for any positive p, q such that $1/p+1/q=\frac{1}{2}$; hence $p,q\geqslant 2$. By (13),

$$\|\mathbf{B}\|_p\leqslant C\|\mathbf{B}\|_{H^1}^{(N/2)-(N/p)}\|\mathbf{B}\|_2^{1-(N/2)+(N/p)}=C\|\mathbf{B}\|_{H^1}^{N/q}\|\mathbf{B}\|_2^{1-(N/q)}, \tag{16}$$

provided $p<2N/(N-2)$, i.e., $q>N$. Thus,

$$\left|\int_\Omega \mathbf{B}\cdot\nabla\mathbf{u}\cdot\mathbf{B}dV\right|\leqslant C\|\mathbf{B}\|_{H^1}^{N/q}\|\mathbf{B}\|_2^{1-(N/q)}\|\nabla\mathbf{B}\|_2\|\mathbf{u}\|_q. \tag{17}$$

Let us use now the Poincaré inequality, written as

$$\|\mathbf{B}\|_{H^1}\leqslant k\|\nabla\mathbf{B}\|_2.$$

We have

$$\left|\int_\Omega \mathbf{B}\cdot\nabla\mathbf{u}\cdot\mathbf{B}dV\right|\leqslant Ck^{N/q}\|\nabla\mathbf{B}\|_2^{1+(N/q)}\|\mathbf{B}\|_2^{1-(N/q)}\|\mathbf{u}\|_q. \tag{18}$$

Let us denote

$$r=\frac{1}{2}-\frac{N}{2q}. \tag{19}$$

We may write the right-hand term as

$$Ck^{N/q}(\|\nabla\mathbf{B}\|_2^2)^{1-r}(\|\mathbf{B}\|_2^2)^r\|\mathbf{u}\|_q=(\alpha\|\nabla\mathbf{B}\|_2^2)^{1-r}((Ck^{N/q}\|\mathbf{u}\|_q)^{1/r}\alpha^{-(1-r)/r}\|\mathbf{B}\|_2^2)^r, \tag{20}$$

where α is a positive constant to be determined later. By using the classical inequality

$$x^r y^{1-r}\leqslant rx+(1-r)y,$$

for $x,y>0$ (which amounts to the convexity of the exponential function), we find

$$\left|\int_\Omega \mathbf{B}\cdot\nabla\mathbf{u}\cdot\mathbf{B}dV\right|\leqslant(1-r)\alpha\|\nabla\mathbf{B}\|_2^2+rC^{1/r}k^{N/qr}\alpha^{-(1-r)/r}\|\mathbf{u}\|_q^{1/r}\|\mathbf{B}\|_2^2. \tag{21}$$

Take now $\alpha=\eta/(1-r)$. Then the term in $\nabla\mathbf{B}$ cancels with the dissipative term in (6), and we are left with

$$\frac{1}{2}\frac{d}{dt}\|\mathbf{B}\|_2^2\leqslant r(1-r)^{(1-r)/r}(Ck^{N/q}\eta^{-(1-r)}\|\mathbf{u}\|_q)^{1/r}\|\mathbf{B}\|_2^2. \tag{22}$$

Therefore, if there exists a magnetic dynamo of exponential growth rate γ, for any $q>N$,

$$\gamma\leqslant 2r(1-r)^{(1-r)/r}(Ck^{N/q}\eta^{-(1-r)}\|\mathbf{u}\|_q)^{1/r}, \tag{23}$$

where r is given by (19). C and k are universal constants. The estimate improves with large q and η, and becomes singular as $\eta\to 0$ or $r\to 0$ (i.e., $q\to N$). For $q\to\infty$ it becomes

$$\gamma\leqslant \tfrac{1}{2}C\eta^{-1}\|\mathbf{u}\|_\infty^2, \tag{24}$$

which improves the Backus bound (10) in the sense that it does not need the velocity gradient, although the resistivity occurs. The estimate (23) is satisfactory in the sense that it involves an integral norm of the velocity and therefore it is a measure of its mean size: it shows that the dynamo cannot be governed by what happens in small regions of the plasma, although these may be relevant in the process of stretching which is basic in the dynamo process. However, the physically most important norm of the velocity is the kinetic energy $\|\mathbf{u}\|_2$, which is not reached by (23). For $N=2$ it lies at the lower limit and the constants blow there; for $N=3$ it is well beyond reach. To see that this is a physical fact and not merely the result of poor bounds, we will prove that (23) is a sharp inequality as concerns the order of the magnitudes.

III. COUNTEREXAMPLES FOR LOWER ORDER NORMS

We will consider an initial condition formed by velocity and field depending only on the radius, and radially directed. Then $\mathbf{B}\cdot\nabla\mathbf{u}$ is also radially directed and the term $\mathbf{B}\cdot\nabla\mathbf{u}\cdot\mathbf{B}$ is precisely $|\mathbf{B}|^2|\nabla\mathbf{u}|$. Specifically, assume $\mathbf{B}=B(R)\mathbf{e}_r$, $\mathbf{e}_r$ the unit radial vector, B decreasing linearly from $B=h$ at $r=0$ to $B=0$ at $r=L$: $B(r)=h-hr/L$ for $r\in[0,L]$, $B(r)=0$ for $r>L$. Take $\mathbf{u}=\mathbf{B}$. These magnitudes are not really smooth, as they fail to be differentiable at $r=0$ and $r=L$, but they can be uniformly approximated by smooth functions such that the values of all the integrals tend to the respective values for our chosen functions.

First, since the Jacobian in dimension N depends on r like r^{N-1}, the norm $\|\mathbf{u}\|_q$ behaves like $hL^{N/q}$, and $\|\mathbf{B}\|_2$ like $hL^{N/2}$. $|\nabla\mathbf{u}|$ is identical to h/L for $r\in[0,L]$, and zero otherwise; thus

$$\int_\Omega|\mathbf{B}|^2|\nabla\mathbf{u}|dV=hL^{-1}\int_\Omega|\mathbf{B}|^2dV\sim hL^{-1}h^2L^N=h^3L^{N-1}. \tag{25}$$

On the other hand,

$$\eta \int_{\Omega} |\nabla \mathbf{B}|^2 dV \sim \eta h^2 L^{N-2}, \tag{26}$$

so that the behavior of the right-hand side of Eq. (6), as a function of h and L, is

$$-\eta h^2 L^{N-2} + h^3 L^{N-1}. \tag{27}$$

Therefore, any exponential growth rate γ should be of the order of (27) divided by $h^2 L^N$, i.e.,

$$\gamma \sim -\eta L^{-2} + hL^{-1}, \tag{28}$$

while $\|\mathbf{u}\|_q \sim hL^{N/q}$.

Assume $q<N$, and take s such that $1<s<N/q$. Choose $h=L^{-s}$. Then, for L small,

$$\gamma \sim -\eta L^{-2} + L^{-1-s} \sim L^{-1-s}. \tag{29}$$

While $\|\mathbf{u}\|_q \sim L^{N/q-s}$ tends to zero with L, $\gamma \to \infty$. Thus there is no possible bound of γ in terms of $\|\mathbf{u}\|_q$.

For $q=N$, we must avoid the possible indetermination in (29) occurring for $h=L^{-1}$. Therefore, we take $h=L^{-1}\log L^{-1}$. For L small enough,

$$-\eta L^{-2} + L^{-2}\log L^{-1} \sim L^{-2}\log L^{-1}, \tag{30}$$

whereas $\|\mathbf{u}\|_q \sim \log L^{-1}$. Since obviously, for any power n,

$$(\log L^{-1})^n \ll L^{-2}\log L^{-1}, \tag{31}$$

when $L \to 0$, there cannot be any bound of γ in terms of any power of $\|\mathbf{u}\|_q$.

Logically the method fails for $q>N$, because any attempt of setting $h=L^{-s}$ would yield a negative power of L at both sides; we could choose an adequate power on the right-hand side to make the magnitudes comparable. Notice that our test functions are localized in a neigborhood of **0** and therefore satisfy our boundary conditions.

IV. CONCLUSIONS

Defining hydromagnetic dynamos as plasma configurations producing an exponential growth of the magnetic field for some time, it is desirable to bound the possible growth rates in terms of the size of the plasma velocity. Classical inequalities involve the maximum norms of the velocity gradient, which are unsuitable for several reasons. We prove a bound of the growth rate by a power of the L^q-norm of the velocity and the conductivity, for any q strictly larger than the space dimension N. The estimate blows up in the limit $q=N$ as well as in the ideal limit of zero resistivity. It is shown by examples that there cannot be analogous bounds for $q \leqslant N$.

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Symmetric periodic solutions of the anisotropic Manev problem

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We consider the Manev potential in an anisotropic space, i.e., such that the force acts differently in each direction. Using a generalization of the Poincaré continuation method we study the existence of periodic solutions for weak anisotropy. In particular we find that the symmetric periodic orbits of the Manev system are perturbed to periodic orbits in the anisotropic problem. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1469670]

I. INTRODUCTION

In this article we consider the anisotropic Manev problem (AMP) that was introduced by Diacu[1] in the early 1990s. The work on the AMP was inspired by the anisotropic Kepler problem introduced by Gutzwiller in the early 1970s. Gutzwiller aimed to find connections between classical and quantum mechanics. His interest was stimulated by an old unsolved quantum mechanical problem formulated in a paper written by Einstein:[2] even if the Born–Sommerfeld–Einstein condition (e.g., see Ref. 2) were appropriate to describe the semi-classical limit of quantum theory, it was unclear how to find a classical approximation for nonintegrable systems.

Similarly the main reason for considering the AMP is to further analyze similarities between classical mechanics and quantum theory. Moreover, as it was remarked in Ref. 1, the AMP also brings general relativity into the game, since the Manev potential explains the perihelion advance of the inner planets with the same accuracy as general relativity.[3] It should be remarked that bringing general relativity into the game is of particular importance since a satisfactory quantum theory of gravitation does not exist.

Some of the qualitative features of the anisotropic Manev problem have already been studied. In Ref. 1, a large class of capture-collision and ejection-escape solutions is studied by means of the collision and infinity manifold techniques. In particular that paper also brought arguments favoring the chaoticity and nonintegrability of the system by showing the existence of heteroclinic orbits within the zero energy manifold. In Ref. 4 the occurrence of chaos on the zero energy manifold and the nonintegrability are finally proved, putting into evidence that the AMP is a very complex problem.

In this work, to gain a better understanding of the complicated dynamics of the AMP, we find the symmetric periodic orbits. Analyzing those orbits is especially important since, by now, it is well known that studying periodic orbits is a valuable general approach to tackle complex problems in classical mechanics. The existence of periodic orbits for small values of the anisotropy is proved using generalizations of the Poincaré continuation method developed in Refs. 5–8 (see also Refs. 9–11).

The (planar) anisotropic Manev problem is described by the Hamiltonian

$$H=\frac{1}{2}\mathbf{p}^2-\frac{1}{\sqrt{x^2+\mu y^2}}-\frac{b}{x^2+\mu y^2}, \tag{1}$$

where $\mu>1$ is a constant and $\mathbf{q}=(x,y)$ is the position of one body with respect to the other

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considered fixed at the origin of the coordinate system, and $\mathbf{p}=(p_x,p_y)$ is the momentum of the moving particle. The constant μ measures the strength of the anisotropy and for $\mu=1$ we recover the classical Manev problem. Furthermore, the equation of motion can be expressed as

$$\begin{aligned}\dot{\mathbf{q}}&=\mathbf{p},\\ \dot{\mathbf{p}}&=-\frac{\partial H}{\partial \mathbf{q}}.\end{aligned} \tag{2}$$

Now consider weak anisotropies, i.e., choose the parameter $\mu>1$ close to 1. Introducing polar coordinates $x=r\cos\theta$, $y=r\sin\theta$ and the notation $\epsilon=\mu-1$ with $\epsilon\ll 1$ we can expand the Hamiltonian (1) in powers of ϵ and obtain

$$H=\frac{1}{2}\mathbf{p}^2-\frac{1}{r}-\frac{b}{r^2}+\epsilon\left(\frac{1}{2r}+\frac{b}{r^2}\right)\cos^2\theta\equiv H_0+\epsilon W(r,\theta). \tag{3}$$

It should be pointed out that the term $W(r,\theta)$ becomes unbounded as $r\to 0$ so that a perturbation analysis is not correct on the ejection-collision orbits. This means that the global dynamics of the AMP cannot be completely described by perturbations to the Manev problem even at the limit $\epsilon\to 0$. However, many interesting results concerning the Hamiltonian (1) for weak anisotropies (i.e., $\epsilon\ll 1$) can be found studying the Hamiltonian (3), some of which are presented in this article.

In the next section we describe the symmetries of the AMP and we find some properties that will be useful to find symmetric periodic orbits. In Sec. III we prove a continuation theorem for the symmetric periodic orbits of ''second kind,'' i.e., the noncircular ones. In Sec. IV we prove a continuation theorem for the orbits of ''first kind,'' i.e., the circular ones, following the method developed in Ref. 8.

II. SYMMETRIES OF THE ANISOTROPIC MANEV PROBLEM

To find periodic orbits in the anisotropic problem it is peculiarly important to know the symmetries of the system, as it was, for example observed in Refs. 5 and 6. The symmetries of the problem under discussion have been examined in Ref. 1 and they are the same as the ones found in Ref. 7 for the anisotropic Kepler problem:

$$\begin{aligned}
E &: (x,y,p_x,p_y,t)\to(x,y,p_x,p_y,t),\\
S_0 &: (x,y,p_x,p_y,t)\to(x,y,-p_x,-p_y,-t),\\
S_1 &: (x,y,p_x,p_y,t)\to(x,-y,-p_x,p_y,-t),\\
S_2 &: (x,y,p_x,p_y,t)\to(-x,y,p_x,-p_y,-t),\\
S_3 &: (x,y,p_x,p_y,t)\to(-x,-y,-p_x,-p_y,t),\\
S_4 &: (x,y,p_x,p_y,t)\to(-x,y,-p_x,p_y,t),\\
S_5 &: (x,y,p_x,p_y,t)\to(x,-y,p_x,-p_y,t),\\
S_6 &: (x,y,p_x,p_y,t)\to(-x,-y,p_x,p_y,-t),
\end{aligned} \tag{4}$$

where E is the identity.

The symmetries above can be interpreted in the following way: Let $\gamma(t)$ be a solution of (2). Then $S_i(\gamma(t))$ is another solution for $i\in\{0,1,2,3,4,5,6\}$. For $i\in\{0,1,2,3,4,5,6\}$ the orbit $\gamma(t)$ will be called symmetric if and only if $S_i(\gamma(t))=\gamma(t)$.

Let us remark that the symmetries in (4), together with the composition of functions, denoted by $\bigcirc$, form an Abelian group in which the operation acts according to the table below.

$\circ$	E	S_0	S_1	S_2	S_3	S_4	S_5	S_6
E	E	S_0	S_1	S_2	S_3	S_4	S_5	S_6
S_0	S_0	E	S_5	S_4	S_6	S_2	S_1	S_3
S_1	S_1	S_5	E	S_3	S_2	S_6	S_0	S_4
S_2	S_2	S_4	S_3	E	S_1	S_0	S_6	S_5
S_3	S_3	S_6	S_2	S_1	E	S_5	S_4	S_0
S_4	S_4	S_2	S_6	S_0	S_5	E	S_3	S_1
S_5	S_5	S_1	S_0	S_6	S_4	S_3	E	S_2
S_6	S_6	S_3	S_4	S_5	S_0	S_1	S_2	E

From the table above it is easy to deduce the following.

Proposition 1: The symmetries of the anisotropic Manev problem form an elementary Abelian group of order eight, i.e., a group isomorphic to $\mathbf{Z}_2\times\mathbf{Z}_2\times\mathbf{Z}_2$.

The symmetries in (4), (except E and S_6) are very useful to find symmetric periodic orbits, especially by means of the continuation method, as we show in the next two sections. Some important properties of the symmetric orbit, summarized in Ref. 7, are expressed in the following lemma:

Lemma 1: (i) For $i=1$ *(resp.* $i=2$*) we have that an orbit* $\gamma(t)$ *is* S_i*-symmetric if and only if it crosses the x axis (resp. y axis) orthogonally.*

(ii) An orbit $\gamma(t)$ *is* S_0*-symmetric if and only if it has a point on the zero velocity curve.*

(iii) For $i=4,5$ *an orbit* $\gamma(t)$ *is* S_i*-symmetric if and only if it is* S_0*-symmetric.*

(iv) All the S_3*-symmetric orbits are periodic.*

The properties of the S_i-symmetric orbits were first studied by Birkhoff[9] for the restricted three body problem and later by many other authors. In particular Casasayas and Llibre[7] state a proposition that gives a technique useful to obtain symmetric periodic orbits with respect to S_0, S_1, S_2 for the anisotropic Kepler problem that are verified also for the problem under discussion in this article:

Proposition 2: (i) For $i=1$ *(resp.* $i=2$*) we have that an orbit* $\gamma(t)$ *is an* S_i*-symmetric periodic orbit if and only if it crosses the x axis (resp. y axis) orthogonally at two distinct points.*

(ii) An orbit $\gamma(t)$ *is an-*S_0 *symmetric periodic orbit if and only if it meets the zero velocity curves at two distinct points.*

(iii) An orbit $\gamma(t)$ *is an-*S_1 *and* S_2*-symmetric periodic orbit if and only if it crosses the x axis and the y axis orthogonally.*

(iv) For $i=1,2$ *an orbit* $\gamma(t)$ *is a* S_0*- and* S_i*-symmetric periodic orbit if and only if it meets the zero velocity curve and crosses the x, respectively y axis, orthogonally.*

(v) For $i=4,5$*, if an orbit* $\gamma(t)$ *is* S_i*-symmetric, then it is* S_0*-symmetric and periodic.*

Now we want to find the symmetric periodic orbit for the unperturbed problem ($\epsilon=0$ or $\mu=1$) and continue them to periodic solutions of the anisotropic system (for $\epsilon\ll 1$). First we observe that, by Proposition 2, the S_i-symmetric orbits with $i=0,4,5$ must meet the zero velocity curve at two points, i.e., there must be a point where the angular momentum $K=xp_y-yp_x$ is zero, but since K is a constant of motion it must be zero along the orbit. Therefore such orbits are ejection-collision orbits, are not periodic and cannot be studied by means of the continuation method. Hence we are going to consider the symmetric periodic orbits with $i=1,2$, and also the

ones with $i=3$ that are the circular orbits of the unperturbed problem. To exploit those properties of the symmetric periodic orbits it is convenient to write the equation of motion in different coordinates.

For the S_i symmetric orbits with $i=1,2$, as it was noted in Ref. 5, it is convenient to write the canonical equations of the restricted three body problem using the Delaunay variables in the rotating frame.[5] Also the Poincaré synodic variables can be used to find symmetric periodic orbits of the restricted three body problem.[6] The anisotropic Manev problem is different since the Hamiltonian that describes it is time independent, hence the idea of using rotating coordinates in the present case cannot be applied. Moreover, our problem is nondegenerate; however, even in our case it is advantageous to perform a change of variables and apply a variation of the action angle variables used in Refs. 4 and 12. Here the nondegeneracy of the problem plays a role similar to the rotating coordinate system in the restricted three body problem.

For the S_3-symmetric orbits we can instead consider the equations in the rotating frame, and prove a theorem similar to the one proved in Ref. 8 for the anisotropic Kepler problem (in Ref. 8 the author remarks that the analysis of the Kepler problem can be redone in the Manev case, but he does not provide a proof).

III. THE S_i-SYMMETRIC ORBITS WITH $i=1,2$

We recall that the action variables introduced in Refs. 4 and 12 are given by

$$I=\frac{1}{2\pi}\oint p_r dr=-\sqrt{K^2-2b}+\frac{1}{2}\sqrt{\frac{2}{|h|}},$$
$$K=xp_y-yp_x, \tag{5}$$

where h is the energy constant and K is the angular momentum. These variables are defined for $h<0$ and $K^2>2b$, $I>0$, to avoid collision orbits as well as circular orbits. The related frequencies are

$$\omega_I=\frac{1}{(I+\sqrt{K^2-2b})^3},$$

$$\omega_K=\frac{K}{\sqrt{K^2-2b}(I+\sqrt{K^2-2b})^3},$$

and θ and ϕ are the angle variables associated to K and I, respectively.

The unperturbed Hamiltonian in the new variables can be written as

$$H_0=-\frac{1}{2(I+\sqrt{K^2-2b})^2}.$$

Now we can consider new variables that are linear combination of the previous ones. They are defined by the following canonical transformation

$$L=K+I,$$
$$G=-I,$$
$$l=\theta,$$
$$g=\theta-\phi. \tag{6}$$

Where l is the mean anomaly [where $l(t)=\omega_L(t-t_0)$ and t_0 is the time of pericenter passage], g is the longitude of pericenter as they are defined for the Manev problem in Ref. 13. Moreover, also the action variables can be written in terms of the orbital elements of the Manev problem. If we set

$$a=\frac{1}{2|h|} \quad \text{and} \quad e=\sqrt{1-2(K^2-2b)|h|}$$

as in Refs. 4 and 13, then

$$G=-a^{1/2}[1-(1-e^2)^{1/2}] \quad \text{and} \quad L=-G\pm\sqrt{a(1-e^2)+2b},$$

where a is the pseudo-semimajor axis, e is the pseudo-eccentricity, and the sign $+$ (resp. $-$) holds for $K>0$ (resp. <0). The conditions to avoid collision orbits and circular orbits, on which g becomes meaningless, can be written in terms of the orbital elements as $a>0$ and $0<e<1$. The new unperturbed Hamiltonian is

$$H_0=-\frac{1}{2(-G+\sqrt{(G+L)^2-2b})^2}, \tag{7}$$

so the perturbed equations of motion become

$$\begin{aligned}
\dot{L}&=-\frac{\partial(H_0+\epsilon W)}{\partial l}=-\epsilon\frac{\partial W}{\partial l},\\
\dot{G}&=-\frac{\partial(H_0+\epsilon W)}{\partial g}=-\epsilon\frac{\partial W}{\partial g},\\
\dot{l}&=\frac{\partial(H_0+\epsilon W)}{\partial L}=\omega_L+\epsilon\frac{\partial W}{\partial L},\\
\dot{g}&=\frac{\partial(H_0+\epsilon W)}{\partial G}=\omega_G+\epsilon\frac{\partial W}{\partial G},
\end{aligned} \tag{8}$$

where W is expressed in the new variables and

$$\omega_L=\omega_K=\frac{G+L}{(-G+\sqrt{(G+L)^2-2b})^3\sqrt{(G+L)^2-2b}}$$

$$\omega_G=\omega_K-\omega_I=\frac{G+L-\sqrt{(G+L)^2-2b}}{(-G+\sqrt{(G+L)^2-2b})^3\sqrt{(G+L)^2-2b}}$$

With these preparations, i.e., the introduction of the action angle variables (6), we are well on our way to establishing the following result:

Theorem 1: *Let $\gamma(t)$ be an S_i-symmetric periodic orbit of the Manev problem with $i=1,2$. Let the period be τ and set $\epsilon=\mu-1$ with $\epsilon\ll 1$. Then there exists a τ-periodic solution of the anisotropic Manev problem $\gamma_\epsilon(t)$ such that $\gamma_\epsilon(t)=\gamma(t)+O(\epsilon)$.*

Proof: Let us consider an S_1-symmetric orbit of period $\tau=2\pi m/k$ (m, k relatively prime integers). We remark that, since the equations of motion are autonomous, we can reduce to study the symmetric orbits that have either the pericenter or the apocenter on the positive x axis at $t=0$.

If at $t=0$, $\epsilon=0$, the pericenter of this orbit is on the positive x axis, and it is crossing the x axis perpendicularly, we have

$$g(0)=0 \quad \text{and} \quad l(0)=0. \tag{9}$$

Since the periodic orbit is S_1-symmetric, by Proposition 2, at the half period one has

$$g\left(\frac{\tau}{2}\right)=m\pi, \quad l\left(\frac{\tau}{2}\right)=k\pi, \tag{10}$$

which follows from the solution of (8) for $\epsilon=0$:

$$\begin{gathered} L=\text{const}, \quad G=\text{const} \\ l=\omega_L t, \quad g=\omega_G t. \end{gathered} \tag{11}$$

Now if, for $\epsilon\neq 0$, we consider only S_1-symmetric solutions of (8), it follows from the implicit function theorem that if the functional determinant

$$D=\det\begin{pmatrix} \dfrac{\partial l}{\partial L} & \dfrac{\partial l}{\partial G} \\ \dfrac{\partial g}{\partial L} & \dfrac{\partial g}{\partial G} \end{pmatrix} \neq 0 \tag{12}$$

at

$$t=\frac{\tau}{2}, \quad \epsilon=0, \tag{13}$$

then (10) would be satisfied for $\epsilon>0$. To compute the determinant we can by analyticity substitute (10) into (11) to find out at the time $t=\tau/2$ that

$$D=\frac{6b(\tau/2)^2}{(-G+\sqrt{(G+L)^2-2b})^7((G+L)^2-2b)^{3/2}}\neq 0. \tag{14}$$

Thus the existence of S_1-symmetric periodic orbits of period τ obtained from the τ periodic S_1-symmetric solutions of the unperturbed problem, that at $t=0$ have the pericenter on the positive x axis, is readily established.

On the other hand, if at $t=0$, $\epsilon=0$, the apocenter is on the positive x axis, and it is crossing the x axis perpendicularly, we have

$$g(0)=\frac{\pi}{\lambda} \quad \text{and} \quad l(0)=-\frac{\pi}{\lambda}, \tag{15}$$

where $\lambda=(\omega_L-\omega_G)/\omega_L$. By Proposition 1, at the half period we have

$$g\left(\frac{\tau}{2}\right)=\left(m+\frac{1}{\lambda}\right)\pi, \quad l\left(\frac{\tau}{2}\right)=\left(-\frac{1}{\lambda}+k\right)\pi. \tag{16}$$

Instead of computing the functional determinant directly, in this case, it is easier to consider the new variables given by the relations

$$\begin{gathered} \tilde{L}=L, \\ \tilde{G}=G, \\ \tilde{l}=l+\frac{\pi}{\lambda_0}, \\ \tilde{g}=g-\frac{\pi}{\lambda_0}, \end{gathered} \tag{17}$$

which define a family of canonical transformations parametrized by $\lambda_0(L_0,G_0)$. For each orbit choose a different transformation from the family (17), where $\lambda_0=\lambda$ is a fixed quantity defined by the value of the action variables along the periodic orbit under consideration.

The equations (16), expressed in the new variables, are of the same form as in (10). Thus the functional determinant, in the new variables, is exactly D, and the existence of the remaining S_1-symmetric τ-periodic orbits follows.

Now the proof for the S_2-symmetric orbits can be done along the same lines. Consider an S_2-symmetric periodic orbit of period $\tau=2\pi m/k$. If at $t=0$, $\epsilon=0$ the pericenter of the orbit is on the positive y axis and it is crossing the y axis perpendicularly, we have

$$g(0)=\frac{\pi}{2} \quad \text{and} \quad l(0)=0. \tag{18}$$

Since the periodic orbit is S_2-symmetric one has, at the half period,

$$g\left(\frac{\tau}{2}\right)=m\pi+\frac{\pi}{2}, \quad l\left(\frac{\tau}{2}\right)=k\pi. \tag{19}$$

Now we consider only S_2-symmetric solutions of (8) for $\epsilon\neq 0$. Again it follows from the implicit function theorem that if the determinant D computed at $t=\tau/2$ for $\epsilon=0$ is nonzero, then (19) would be satisfied for $\epsilon>0$. It is trivial to see from (14) that $D\neq 0$, and hence we found S_2-symmetric periodic orbits for the perturbed problem.

For the S_2-symmetric orbits having the apocenter on the positive x axis at $t=0$ the canonical transformation (17) can be used. Again we find the same expression for the functional determinant and, hence, by the implicit function theorem, the existence of the remaining S_2-symmetric periodic orbits is proved.

It is interesting to remark that Theorem 1 and its proof can be easily extended to consider any S_i-symmetric perturbation with $i=1,2$ and a very general class of nondegenerate integrable Hamiltonians, however such a generalization is trivial and not strictly related to the problem under consideration and hence it will not be discussed any further.

We can also observe that for $b=0$, i.e., for the Kepler problem, the determinant in (14) is zero. Thus in the case of the anisotropic Kepler problem, the continuation theorem proved above cannot be applied, and the existence of symmetric periodic orbits of the ''second kind'' (for weak anisotropies) remains unclear. On the other hand, the continuation theorem that we prove in the next section (for the circular orbits) can be applied to the anisotropic Kepler problem[8] and hence at least the existence of symmetric periodic orbits of the first kind is a well established fact.

IV. THE S_3-SYMMETRIC ORBITS

Again we can consider the anisotropic Manev problem taking the parameter μ close to 1. Let $\Phi(t,(\mathbf{r},\dot{\mathbf{r}}),\mu)$ be the flow of the equation of motion (1). In this section we prove the following theorem:

Theorem 2: *Let* $\mathbf{r}^0(t)$ *be an* S_3*-symmetric periodic orbit of the Manev problem, i.e., a circular one. Set* $\epsilon=\mu-1$, *and let* τ *be the period of* $\mathbf{r}^0(t)$. *Then there exists a* τ*-periodic solution* $\Phi(t,(\mathbf{r}(\epsilon),\dot{\mathbf{r}}(\epsilon)),\epsilon)$ *of the anisotropic Manev problem such that* $\Phi(t,(\mathbf{r}(0),\dot{\mathbf{r}}(0)),0)=(\mathbf{r}^0(t),\dot{\mathbf{r}}^0(t))$.

A. The equation of motion

Now using the same notation as in Ref. 8 let $\mathbf{r}^0(t)$ be a circular solution of the Manev problem which corresponds to $\mu=1$ in the xy-plane, ω its angular speed and a its radius. For $\epsilon=\mu-1\neq 0$ we set

$$\mathbf{r}(t,\epsilon)=\mathbf{r}^0(t)+\epsilon\mathbf{s}(t,\epsilon). \tag{20}$$

Expanding ∇H in powers of $\mu-1$ sufficiently small, after substituting the expression for $\mathbf{r}$ given above, considering the notation $\mathbf{r}^0(t)=x_0(t)+iy_0(t)$ and $\mathbf{s}=u+iv$ we have that $\mathbf{r}(t,\epsilon)$ is a solution of equation of motion defined by (1) if, and only if, $\mathbf{s}(t,\epsilon)$ is a solution of the equations

$$\begin{aligned}\ddot{u}&=-\left(\frac{1}{a^3}-\frac{3x_0^2}{a^5}-\frac{8bx_0^2}{a^6}+\frac{2b}{a^4}\right)u+\left(\frac{3x_0y_0}{a^5}+\frac{8bx_0y_0}{a^6}\right)v+\eta(t)+O(\epsilon),\\ \ddot{v}&=\left(\frac{3x_0y_0}{a^5}+\frac{8bx_0y_0}{a^6}\right)u-\left(\frac{1}{a^3}-\frac{8by_0^2}{a^6}-\frac{3y_0^2}{a^5}+\frac{2b}{a^4}\right)v+\xi(t)+O(\epsilon)\end{aligned} \tag{21}$$

where

$$\eta(t)=\frac{3x_0y_0^2}{a^5}+\frac{4bx_0y_0^2}{a^6}$$

$$\xi(t)=\frac{3y_0^2}{2a^5}-\frac{y_0}{a^3}+\frac{4by_0^3}{a^6}-\frac{2by_0}{a^4}.$$

Consider the orthonormal frame in $\mathbf{R}^2$, $\mathbf{e}_1(t)$ and $\mathbf{e}_2(t)$ defined by

$$\mathbf{e}_1=\frac{\mathbf{r}^0}{|\mathbf{r}^0|}=e^{i\omega t}=\cos\omega t+i\sin\omega t,\quad \mathbf{e}_2=i\mathbf{e}_1,$$

and, using the same notation as in Ref. 8 where

$$\mathbf{s}=x_1\mathbf{e}_1+x_2\mathbf{e}_2,\quad \dot{\mathbf{s}}=y_1\mathbf{e}_1+y_2\mathbf{e}_2,$$

Eq. (21) can be written in an equivalent form as

$$\dot{\mathbf{z}}=A_0(t)+A\mathbf{z}+O(\epsilon), \tag{22}$$

where $\mathbf{z}=(x_1,x_2,y_1,y_2)^T$, and

$$A_0=\begin{pmatrix}0\\0\\\alpha(t)\\\beta(t)\end{pmatrix},\quad A=\begin{pmatrix}0 & \omega & 1 & 0\\ -\omega & 0 & 0 & 1\\ 2\omega^2+2\dfrac{b}{a^4} & 0 & 0 & \omega\\ 0 & -\omega^2 & -\omega & 0\end{pmatrix},$$

where

$$\alpha(t)\cos\omega t-\beta(t)\sin\omega t=\eta(t),$$

$$\alpha(t)\sin\omega t+\beta(t)\cos\omega t=\xi(t),$$

or, equivalently,

$$\alpha(t)=\sin^2\omega t\left(\frac{1}{2a^2}+\frac{2b}{a^3}\right), \tag{23}$$

$$\beta(t) = -\sin \omega t \cos \omega t \left(\frac{1}{a^2} + \frac{2b}{a^3} \right).$$

The eigenvalues of A are 0, with multiplicity two, $i/a^{3/2}$ and $-i/a^{3/2}$. One of the two eigenvalues vanishes because the system is autonomous, and the second due to the presence of the first integral H.

Now consider the real Jordan form J of A. The matrix J is defined by the relation $J = \mathcal{T}^{-1} A \mathcal{T}$ where $\mathcal{T}$ is

$$\mathcal{T} = \begin{pmatrix} 2\,\omega^2 a^3 & 0 & \dfrac{\omega^2 a^4 + 2\,b}{a} & 0 \\ 0 & -\dfrac{\omega(3\,\omega^2 a^4 + 2\,b)}{a} & 0 & -2\,\dfrac{\omega a^2(\omega^2 a^4 + 2\,b)}{(a)^{3/2}} \\ 0 & \dfrac{1}{2}\,\dfrac{4\,a(\omega^2 a^4 + b) + 2\,(\omega^2 a^4 + 2\,b)^2}{a^5} & 0 & \dfrac{(\omega^2 a^4 + 2\,b)^2}{a^{7/2}} \\ -\dfrac{\omega(\omega^2 a^4 + 2\,b)}{a} & 0 & -\dfrac{\omega(\omega^2 a^4 + 2\,b)}{a} & 0 \end{pmatrix}$$

and the columns of $\mathcal{T}$ are the generalized eigenvectors of A.

The vector $J_0 = \mathcal{T}^{-1} A_0$ and the matrix J are

$$J_0 = \begin{pmatrix} j_1(t) \\ j_2(t) \\ j_3(t) \\ j_4(t) \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dfrac{\sqrt{a}}{a^2} \\ 0 & 0 & -\dfrac{\sqrt{a}}{a^2} & 0 \end{pmatrix},$$

where the fact that $j_1(t) = (2\omega^3 a^2 - \omega(\omega^2 a^4 + 2b)/a^2)^{-1} \beta(t)$ is the only information about J_0 that we need to retain. Furthermore, we remark that $\omega^2 a^4 - a - 2b = 0$ gives the relation between a and ω and solving this equations gives only one positive solution (for $b > 0$).

Letting $\mathbf{z} = \mathcal{T}\zeta$, the equation of motion becomes

$$\dot{\zeta} = J_0(t) + J\zeta + O(\epsilon), \tag{24}$$

and its flow is given by

$$\psi(t, \zeta, \epsilon) = \gamma(t) + e^{Jt} + O(\epsilon), \tag{25}$$

where by the variation of constants

$$\gamma(t) = e^{Jt} \int_0^t e^{-Js} J_0(s)\, ds. \tag{26}$$

Therefore, we have

$$e^{Jt}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ t & 1 & 0 & 0 \\ 0 & 0 & \cos\frac{\sqrt{a}}{a^2}t & \sin\frac{\sqrt{a}}{a^2}t \\ 0 & 0 & -\sin\frac{\sqrt{a}}{a^2}t & \cos\frac{\sqrt{a}}{a^2}t \end{pmatrix},$$

and from (26) we obtain

$$\gamma(t)=\begin{pmatrix} \gamma_1(t) \\ \gamma_2(t) \\ \gamma_3(t) \\ \gamma_4(t) \end{pmatrix}, \tag{27}$$

where we retain only the information that

$$\gamma_1(t)=\left(2\omega^3a^2-\frac{\omega(\omega^2a^4+2b)}{a^2}\right)^{-1}\int_0^t\beta(s)ds. \tag{28}$$

B. The periodicity equation

Since the Hamiltonian H of the anisotropic Manev problem is S_3-symmetric, as we have shown, we can write the periodicity equation as in[8]

$$\Phi\left(\frac{\tau}{2},(\mathbf{r},\dot{\mathbf{r}}),\epsilon\right)=-(\mathbf{r},\dot{\mathbf{r}}). \tag{29}$$

Then it easy to check that $\Phi(t,(\mathbf{r},\dot{\mathbf{r}}),\epsilon)$ is a periodic solution of the equation of motion with period τ. To find periodic solutions we have to verify that (29) is satisfied for a family of initial conditions. Equation (29) in ζ coordinates is

$$\psi\left(\frac{\tau}{2},\zeta,\epsilon\right)-\zeta=0, \tag{30}$$

where $\psi(t,\zeta,\epsilon)$ is the flow of (24). Let us denote by $\mathcal{P}(\zeta,\epsilon)$ the left hand side of the periodicity equation (29), that is, let

$$\mathcal{P}(\zeta,\epsilon)=\psi\left(\frac{\tau}{2},\zeta,\epsilon\right)-\zeta=\gamma\left(\frac{\tau}{2}\right)+(e^{J\tau/2}-I)=0. \tag{31}$$

Using (25) we notice that the requirement

$$\mathcal{P}(\zeta^*,0)=\gamma\left(\frac{\tau}{2}\right)+(e^{J\tau/2}-I)\zeta^*=0 \tag{32}$$

imposes the restrictions

$$\gamma_1\left(\frac{\tau}{2}\right)=0,\quad \zeta_1^*=-\frac{2}{\tau}\gamma_2\left(\frac{\tau}{2}\right),\quad \zeta_2^*=\text{arbitrary}, \tag{33}$$

and

$$\zeta_3^*=\frac{1}{2(1-\cos\alpha^*)}\left(-\gamma_3\left(\frac{\tau}{2}\right)(\cos\alpha^*-1)+\gamma_4\left(\frac{\tau}{2}\right)\sin\alpha^*\right)$$
$$\zeta_4^*=\frac{-1}{2(1-\cos\alpha^*)}\left(\gamma_3\left(\frac{\tau}{2}\right)\sin\alpha^*+\gamma_4\left(\frac{\tau}{2}\right)(\cos\alpha^*-1)\right), \tag{34}$$

where $\alpha^*=\pi(1+2b/a)^{-1/2}$. It easy to see from (23) and (28) that $\gamma_1(\tau/2)=0$, therefore, we take

$$\zeta^*=(\zeta_1^*,\zeta_2^*,\zeta_3^*,\zeta_4^*)^T, \tag{35}$$

with ζ_2^* arbitrary, for the moment. Now using the flow (25), we determine that the Jacobian matrix of $\mathcal{P}$ with respect to the variables ζ evaluated at the point $(\zeta^*,0)$ is given by

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ \tau/2 & 0 & 0 & 0 \\ 0 & 0 & \cos\alpha^*-1 & \sin\alpha^* \\ 0 & 0 & -\sin\alpha^* & \cos\alpha^*-1 \end{pmatrix}. \tag{36}$$

Consider the system of three equations formed by those in (31) corresponding to the indices $i=2,3,4$, and fix the variable $\zeta_2=\zeta_2^*$. Its Jacobian matrix has determinant $\tau(1-\cos\alpha^*)$ that is always positive since $0<\pi(1+2b/a)^{-1/2}\leqslant\pi$. Therefore, the implicit function theorem guarantees the existence of analytic functions $\zeta_i=\zeta_i(\epsilon)$, $i=1,3,4$, in a neighborhood of $\epsilon=0$, satisfying the equations

$$\mathcal{P}_i(\zeta,\epsilon)=0 \quad (i=2,3,4), \tag{37}$$

where

$$\zeta(\epsilon)=(\zeta_1(\epsilon),\zeta_2^*,\zeta_3(\epsilon),\zeta_4(\epsilon)) \tag{38}$$

and such that

$$\zeta_i(0)=\zeta_i^* \quad (i=1,2,3,4). \tag{39}$$

It remains to show, in order to have periodicity, that also the remaining equation

$$\mathcal{P}_1(\zeta(\epsilon),\nu(\epsilon),\epsilon)=0 \tag{40}$$

is satisfied in a possibly smaller, neighborhood of $\epsilon=0$. That will be done employing a first integral of the system under discussion, i.e., the Hamiltonian.

C. Integral of motion

Since the Hamiltonian is an integral of motion of the problem under discussion we can apply the same analysis as in Refs. 8 and 14. In particular, using the same notations as in Ref. 8 we can define

$$H_\epsilon(\mathbf{z},t)=H(\mathbf{r},\dot{\mathbf{r}},\epsilon),$$

where $H_\epsilon(\mathbf{z},t)$ is a time-dependent, τ-periodic first integral for system (22). The above integral satisfies the following relation,

$$H_\epsilon\left(\mathbf{z},t+\frac{\tau}{2}\right)=H_\epsilon(\mathbf{z},t) \tag{41}$$

for all t, since $H(-\mathbf{r},-\dot{\mathbf{r}})=H(\mathbf{r},\dot{\mathbf{r}})$, $\mathbf{r}(t)=\mathbf{r}^0(t)+\epsilon\ \mathbf{s}(t)$ and

$$\mathbf{r}^0\left(t+\frac{\tau}{2}\right)=-\mathbf{r}^0(t),\quad \mathbf{s}\left(\mathbf{z},t+\frac{\tau}{2}\right)=-\mathbf{s}(\mathbf{z},t).$$

Performing a change of coordinates we can define $\mathcal{H}_\epsilon(\zeta,t)=H_\epsilon(\mathcal{T}\zeta,t)$, hence (41) can be written as

$$\mathcal{H}_\epsilon(\zeta,t+\tau/2)=\mathcal{H}_\epsilon(\zeta,t). \tag{42}$$

Moreover, since $\mathcal{H}_\epsilon$ is an integral of motion it verifies that

$$\mathcal{H}_\epsilon(\phi(\zeta,\epsilon,t))=H_\epsilon(\zeta,0). \tag{43}$$

Thus applying Eqs. (42) and (43) it follows that

$$\mathcal{H}_\epsilon(\psi(\tau/2,\zeta,\epsilon),0)=\mathcal{H}_\epsilon(\zeta,0),$$

and by means of the mean value theorem we obtain

$$\nabla_\zeta\mathcal{H}_\epsilon(\tilde{\zeta},0)\cdot\mathcal{P}(\zeta,\epsilon)=0, \tag{44}$$

where $\nabla_\zeta\mathcal{H}_\epsilon$ is the gradient of $\mathcal{H}_\epsilon$ with respect to ζ, and $\tilde{\zeta}$ is a point on the segment joining ζ to $\psi(\tau/2,\zeta,\epsilon)$.

Expanding $\Psi(\epsilon)=\psi(\tau/2,\zeta,\epsilon)$ in power of ϵ sufficiently small it is easy to show (see Ref. 8) that $\Psi(\epsilon)=\zeta^*+O(\epsilon)$ and consequently

$$\tilde{\zeta}=s\zeta(\epsilon)+(1-s)\Psi(\epsilon)=\zeta^*+O(\epsilon)$$

for some $s\in(0,1)$. Moreover, if we also expand the Hamiltonian $H_\epsilon(\mathbf{z},0)$ in powers of ϵ we get

$$H_\epsilon(\mathbf{z},0)=H_0+\epsilon(H_1+H_2\cdot\mathbf{z})+O(\epsilon^2)$$

or, in ζ coordinates

$$\mathcal{H}_\epsilon(\zeta,0)=\mathcal{H}_0+\epsilon(\mathcal{H}_1+\mathcal{H}_2\cdot\zeta)+O(\epsilon^2), \tag{45}$$

where $\mathcal{H}_0=H_0=(1/2\,\omega^2a^2-1/a-b/a^2)$, $\mathcal{H}_1=H_1$ and $\mathcal{H}_2=\mathcal{T}^TH_2=\mathcal{T}^T(a^{-2}+2ba^{-3},0,0,a\omega)$ $=(a\omega^2\zeta_1,0,0,0)$. Hence we obtain

$$\frac{1}{\epsilon}\nabla_\zeta\mathcal{H}_\epsilon(\tilde{\zeta},0)=\mathcal{H}_2+O(\epsilon). \tag{46}$$

With these preparations Eq. (44) reduces to the equation in the unknown $\mathcal{P}_1$

$$[a\omega^2+O(\epsilon)]\mathcal{P}_1=0, \tag{47}$$

since, for small ϵ, we already found in Sec. IV B that $\mathcal{P}_i=0$ for $i=2,3,4$. It is easy to see that for $\epsilon=0$ the equation above has solution $\mathcal{P}_1=0$. Thus, by continuity, $[a\omega^2+O(\epsilon)]$ is different from zero for ϵ sufficiently small. Therefore, for such values of ϵ, this equation has a unique solution that is the trivial one. Consequently, the remaining equation,

$$\mathcal{P}_1(\zeta(\epsilon),\epsilon)=0,$$

is also satisfied in a possibly smaller neighborhood of $\epsilon=0$. Hence all the equations of the periodicity system (31) are satisfied when $\zeta=\zeta(\epsilon)$, as long as ϵ is sufficiently small. This completes the proof of Theorem 2.

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Metric-independent analysis of the stress-energy tensor

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The stress-energy tensor of field theory is defined and analyzed in a geometric setting where a metric is not available. The stress is a linear mapping that transforms the three-form representing the flux of any given property, e.g., charge-current density, to the three-form representing the flux of energy. The example of the electromagnetic stress-energy tensor is given with the additional structure of a volume element. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The introduction of the stress-energy tensor in field theory and the related analysis of conservation laws utilize the metric properties of space–time afforded by relativity theory (see, for example, Refs. 1–5). Since one cannot assume that the metric tensor is known in advance, it would be preferable, at least from the theoretical point of view, to have a formulation of the theory that does not rely on the metric structure. Such a presentation of the stress-energy tensor and conservation laws is the subject of this article.

For the electromagnetic field as a concrete example, the construction may be described simply as follows: the value of a stress-energy tensor at any event is a linear mapping that transforms the charge-current density three-form to the corresponding energy flux three-form.

The basic geometric setting is that of an m-dimensional space–time manifold $\mathcal{U}$. Space–time is assumed to be orientable and a specific orientation is assumed to be chosen. In particular, we do not use a metric or a connection in the analysis. The first part of the article, containing Secs. II and III, is concerned with the fibration of space–time induced by a conservation law for an extensive property p, for example, the electric charge. Assuming that the flux of the property p out of any region $\mathcal{R}$ in space–time is given as an integral of a flux density $(m-1)$-form $\tau_{\mathcal{R}}$, and using a generalization of the traditional Cauchy assumptions regarding the dependence of the form $\tau_{\mathcal{R}}$ on $\mathcal{R}$, there is a unique flux $(m-1)$-form J (see Ref. 6), the analog of the charge-current density three-form in electromagnetism, such that for any region $\mathcal{R}$, $\tau_{\mathcal{R}}=\imath^*(J)$, where $\imath^*$ is the restriction of forms defined on space–time to the boundary of $\mathcal{R}$. The flux density form induces a one-dimensional subbundle of the tangent bundle $T\mathcal{U}$ whose integral manifolds are the worldlines associated with the property. Thus, even in this general setting, the conservation of the property induces enough structure so the analogs of particles and velocities—worldlines and flux $(m-1)$-forms—may be defined. If a volume element θ is given on $\mathcal{U}$, the flux form induces a vector field v, the analog of the four-velocity, by the condition $J=v\lrcorner\theta$.

The next part of the article, consisting of Secs. IV–VI, presents stress theory on manifolds (see also previous works, Refs. 7 and 8). Consider a vector bundle $W\to\mathcal{U}$, whose elements are interpreted as values of generalized velocities. For a region $\mathcal{R}$ in space–time, Sec. IV is concerned with a linear functional on sections w of W that contain a ''volume'' term and a boundary term. The boundary term for a region $\mathcal{R}\subset\mathcal{U}$ is given as $\mathbf{t}_{\mathcal{R}}(w)$ where $\mathbf{t}_{\mathcal{R}}$ is a section of the bundle of linear mappings $L(W,\Lambda^{m-1}(T^*\partial\mathcal{R}))$. Again, with the Cauchy postulates for the dependence of $\mathbf{t}_{\mathcal{R}}$ on $\mathcal{R}$, there is a unique section σ of $L(W,\Lambda^{m-1}(T^*\mathcal{U}))$, the Cauchy stress, that induces by restriction of forms the vector valued forms $\mathbf{t}_{\mathcal{R}}$ for the various regions.

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Section V considers a linear functional on sections of W that may be represented as follows. Let $J^1(W)$ be the jet bundle associated with W. Then, there is a section of $L(J^1(W),\Lambda^m(T^*\mathcal{U}))$, the variational stress density, such that the value of the functional for a section w is $\int_{\mathcal{R}} S(j^1(w))$, where $j^1(w)$ is the first jet of the section w. The divergences of variational stress densities are defined and the relation between Cauchy stresses and variational stresses is presented in Sec. VI.

The values of the functionals described above are interpreted in Sec. VII as the energy variation associated with the motion of the property p as represented by the flux form J. Accordingly, $\Lambda^{m-1}(T^*\mathcal{U})$ is used for the vector bundle W over space–time. In this case, the Cauchy stress is a section of $L(\Lambda^{m-1}(T^*\mathcal{U}),\Lambda^{m-1}(T^*\mathcal{U}))$— the stress-energy tensor. It is shown in Sec. VIII that stress-energy tensors can be represented naturally by sections of the bundle of linear mappings $L(T\mathcal{U},T\mathcal{U})$.

Finally, Sec. IX presents the example of the stress-energy tensor for electromagnetism. No particular relation is used for the constitutive relation between the Maxwell and Faraday two-forms and the only additional geometric structure used is that of a volume element. Mathematically, this enables us to obtain the four-velocity vector field from the flux form. The expression for the Lorentz force we obtain is analogous to that of Ref. 2, p. 91, where a metric is used.

In Ref. 9, Gotay and Marsden present a derivation of a metric independent stress-energy tensor using a different approach. In comparison with the present article, the authors assume additional structure of a Lagrangian and a gauge group. Accordingly, the results they obtain are more comprehensive. The stress object derived in Ref. 9 is a (1,1)-tensor density, i.e., a section of $L(L(T\mathcal{U},T\mathcal{U}),\Lambda^m(T^*\mathcal{U}))$ that may be identified with a section of $L(T\mathcal{U},\Lambda^{m-1}(T^*\mathcal{U}))$. Here, allowing a slight generalization where a stress is an element of $L(L(W,T\mathcal{U}),\Lambda^m(T^*\mathcal{U}))$ for some vector bundle W, and then putting $W=\Lambda^{m-1}(T^*\mathcal{U})$ (see Sec. VII for the motivation), we arrive at a stress object that is a (1,1) tensor, i.e., a section of $L(T\mathcal{U},T\mathcal{U})$.

II. SCALAR VALUED EXTENSIVE PROPERTIES ON SPACE–TIME

We consider the conservation of an extensive property p in space–time $\mathcal{U}$. It is assumed that $\mathcal{U}$ is an m-dimensional orientable manifold with a definite orientation chosen. An m-dimensional submanifold with boundary $\mathcal{R}$ of $\mathcal{U}$ will be referred to as a *control region*.

Specifically, it is assumed that for each control region $\mathcal{R}$ there is an $(m-1)$-form $\tau_{\mathcal{R}}$ on $\partial\mathcal{R}$, the *flux density*. The integral $\int_{\partial\mathcal{R}}\tau_{\mathcal{R}}$ is interpreted as the flux of the property out of the control region in space–time relative to the positive orientation induced on $\partial\mathcal{R}$ by the orientation on $\mathcal{U}$ and the outwards pointing vectors. In case a frame is given, the flux density through a spacelike slice is interpreted as the density of the property p in space and the flux through a hyperplane containing the $\partial/\partial t$ tangent vector is interpreted as the classical flux density of p into the corresponding slice consisting of simultaneous events.

Regarding $\tau_{\mathcal{R}}$ as the value of a set function defined on the collection of control regions, Cauchy's postulates of continuum mechanics can be generalized to differentiable manifolds as follows (see Refs. 6 and 8).

GC1 There is a volume element θ on $\mathcal{U}$ such that

$$\left|\int_{\partial\mathcal{R}}\tau_{\mathcal{R}}\right|\leqslant\int_{\mathcal{R}}\theta.$$

GC2 Consider the Grassmann bundle of hyperplanes $\pi_G: G_{m-1}(T\mathcal{U})\to\mathcal{U}$ whose fiber $G_{m-1}(T_x\mathcal{U})$ at any event $x\in\mathcal{U}$ is the Grassmann manifold of hyperplanes, i.e., $(m-1)$-dimensional subspaces of the tangent space $T_x\mathcal{U}$. Let $\Lambda^{m-1}(G_{m-1}(T\mathcal{U}))^*\to G_{m-1}(T\mathcal{U})$ be the vector bundle over $G_{m-1}(T\mathcal{U})$ whose fiber over a hyperplane H is the vector space of $(m-1)$-forms on H. Then, the dependence of $\tau_{\mathcal{R}}$ on $\mathcal{R}$ is via a smooth section

$$\tau: G_{m-1}(T\mathcal{U})\to\overset{m-1}{\Lambda}(G_{m-1}(T\mathcal{U}))^*,$$

such that $\tau_{\mathcal{R}}=\tau(T_x\partial\mathcal{R})$.

Cauchy's theorem, generalized in Refs. 6 and 8 to manifolds, states that there is a unique $(m-1)$-form J on $\mathcal{U}$ such that for any control region $\mathcal{R}$,

$$\tau_{\mathcal{R}}=\tau(T_x\partial\mathcal{R})=\iota^*(J).$$

Here, $\iota:\partial\mathcal{R}\to\mathcal{U}$ is the natural inclusion and ι^* is the pull-back of forms it induces. We will refer to J as the *flux form* associated with the property p.

Usually, it is assumed that there is a source density term s for the property, an m-form on $\mathcal{U}$, so that the conservation equation of the property is

$$\int_{\partial\mathcal{R}}\tau_{\mathcal{R}}=\int_{\mathcal{R}}s.$$

In this case, Stokes' theorem implies that the conservation equation may be written in a differential form as $dJ=s$. Again, if a frame is given on space–time, then the time component of J is the density in space of the property p and the term in dJ containing it is the time derivative of that density. The spacelike components of J describe the three-dimensional flux and the terms in dJ involving the spacelike components make its $(m-1)$-dimensional divergence. In a particular frame, for every time t, the classical conservation law has the integral form

$$\int_{\mathcal{R}}\beta_{\mathcal{R}}+\int_{\partial\mathcal{R}}\tau_{\mathcal{R}}=\int_{\mathcal{R}}s,$$

where here $\mathcal{R}$ is interpreted as a region in space (a slice of space–time) and $\beta_{\mathcal{R}}$ is the rate of change of the density of the property—a three-form. In order that the previous Cauchy assumptions apply, it is usually assumed that $\beta_{\mathcal{R}}$ is actually independent of $\mathcal{R}$.

Remark 2.1: Assume the manifold $\mathcal{U}$ is given a particular volume element θ. Then, there is a vector bundle isomorphism

$$i_\theta:\ \overset{m-1}{\Lambda}\ (T_x^*\mathcal{U})\to T_x\mathcal{U}$$

such that $(i_\theta\circ J)\lrcorner\theta=J$, where $\lrcorner$ denotes the contraction (interior product) of forms by vectors. If θ is represented locally by

$$r(x^i)\,dx^1\wedge\ \cdots\wedge dx^m,$$

then $v=i_\theta\circ J$, which we will also write as $i_\theta(J)$, is represented by

$$v^i=\frac{(-1)^{i+1}J_i}{r}.$$

If J is a flux form of an extensive property p and a volume element is given, we will refer to $v=i_\theta(J)$ as the *kinematic flux* associated with p. The kinematic flux is the analog of the four-velocity field. If $\mathcal{L}$ denotes the Lie derivative, then the differential conservation equation can now be written in the form $\mathcal{L}_v\theta=s$.

III. WORLDLINES AND GENERALIZED BODY POINTS

A flux form J induces a one-dimensional distribution over the open submanifold of $\mathcal{U}$ where it does not vanish. Let $E(J)$ be the minimal enveloping subbundle associated with J, i.e., the minimal subbundle Z of $T^*\mathcal{U}$ such that $J(x)\in\Lambda^{m-1}Z_x$. We will refer to the annihilator $E(J)^\perp\subset T\mathcal{U}$ of the minimal enveloping subbundle as the *flux bundle*, that is,

$$E(J)_x^{\perp}=\{v\in T_x\mathcal{U};\phi(v)=0,\ \text{for all}\ \ \phi\in E(J)_x\}.$$

The flux bundle is one-dimensional and a tangent vector v is in the flux bundle if and only if $v\lrcorner J=0$. The flux bundle is also the one-dimensional bundle obtained by the relation $v=i_\theta(J)$ when the flux form J is kept fixed and the volume element θ is allowed to vary. Being one-dimensional, the flux bundle is integrable, and its one-dimensional integral manifolds will be referred to as (local) *worldlines*. Consider the equivalence relation $x\sim x'$ if x and x' are on the same worldline. We will refer to the collection of worldlines $\mathcal{B}=\mathcal{U}/\sim$ as the *material universe*.

The worldlines form a foliation of $\mathcal{U}$. (See Ref. 10 for a detailed treatment.) In case the foliation is regular, so $\mathcal{B}$ is an $(m-1)$-dimensional submanifold of $\mathcal{U}$ and the natural projection $\mathcal{U}\to\mathcal{B}=\mathcal{U}/\sim$ is a submersion, an element of $\mathcal{B}$ is a *material point* and a compact $(m-1)$-dimensional submanifold with boundary of $\mathcal{B}$ is a *material body*. A necessary and sufficient condition for the foliation to be regular is the existence of local slices, i.e., at every event x there exists a local $(m-1)$-dimensional submanifold P of $\mathcal{U}$ such that P intersects every worldline at one point at most and $T_x\mathcal{U}=T_xP\times T_xY$, where Y is the worldline through x.

Thus, in case the foliation by worldlines is regular, the construction we described generates a material structure in space even though the velocity field is not defined uniquely. In addition, the flux form J is an object that generalizes the velocity field even if a volume element is not given and even if the foliation it generates is not regular.

Clearly, foliated charts and slices generate frames that assign to events unique material points and ''time'' coordinates. If a volume element is given, the kinematic flux induces a unique time coordinate in the neighborhood of every event (independently of a chart). Thus, a flux form and a volume element induce together a local frame.

IV. CAUCHY'S STRESS THEORY FOR MANIFOLDS

Let $\pi:W\to\mathcal{U}$ be a vector bundle over the m-dimensional orientable manifold $\mathcal{U}$. The vector bundle is interpreted as the bundle of generalized velocities over $\mathcal{U}$. In classical continuum mechanics, if $\mathcal{U}$ is interpreted as the physical space (a slice of space–time), then in many cases W is the tangent bundle $T\mathcal{U}$. If $\mathcal{U}$ is interpreted as the material body, then W is usually the pull-back of the tangent bundle of the space manifold under the configuration mapping that embeds the material universe in space. This is the interpretation used in previous works (e.g., Refs. 7 and 8). In either case, a section of the bundle π is interpreted as a generalized velocity field from either the Eulerian or the Lagrangian points of view.

Cauchy's stress theory for manifolds, presented in Ref. 8, considers for each compact m-dimensional submanifold with boundary $\mathcal{R}$ of $\mathcal{U}$ a linear functional of the generalized velocity fields containing a volume term and a boundary term of the form

$$F_{\mathcal{R}}(w)=\int_{\mathcal{R}}\mathbf{b}_{\mathcal{R}}(w)+\int_{\partial\mathcal{R}}\mathbf{t}_{\mathcal{R}}(w).$$

Here, w is a section of W, $\mathbf{b}_{\mathcal{R}}$, the *body force*, is a section of $L(W,\Lambda^m(T^*\mathcal{R}))$ and $\mathbf{t}_{\mathcal{R}}$ the *boundary force* is a section of $L(W,\Lambda^{m-1}(T^*\partial\mathcal{R}))$ so the integrals make sense. The functional $F_{\mathcal{R}}$ is interpreted as the force, or power, functional and the value $F_{\mathcal{R}}(w)$ is classically interpreted as the power of the force for the generalized velocity field w.

We note that body forces and surface forces may be regarded as covector valued forms. For example, a surface force $\mathbf{t}_{\mathcal{R}}$ may be identified with a section $\hat{\mathbf{t}}_{\mathcal{R}}$ of $\Lambda^{m-1}(T(\partial\mathcal{R}),W^*)$ by

$$\hat{\mathbf{t}}_{\mathcal{R}}(v_1,\ldots,v_{m-1})(w)=\mathbf{t}_{\mathcal{R}}(w)(v_1,\ldots,v_{m-1}),$$

so we have an isomorphism of $\Lambda^{m-1}(T\partial\mathcal{R},W^*)$ with $L(W,\Lambda^{m-1}(T^*\partial\mathcal{R}))$.

The Cauchy postulates for forces are analogous to those pertaining to the scalar valued properties. The body term, $\mathbf{b}_{\mathcal{R}}$, is assumed to be independent of $\mathcal{R}$ (and is omitted in the space–time formulation anyhow). The local dependence on the tangent hyperplane is now provided by a section

$$\Sigma: G_{m-1}(T\mathcal{U}) \to L(\pi_G^*(W), \overset{m-1}{\Lambda}(G_{m-1}(T\mathcal{U}))^*),$$

where $\pi_G^*(W)$ is the pull-back of the vector bundle W by the projection of the Grassmann bundle onto $G_{m-1}(T\mathcal{U})$ (see diagram):

$$\begin{array}{ccccc} \pi_G^*(W) & \xrightarrow{\pi_G^*(\pi)} & G_{m-1}(T\mathcal{U}) & \longleftarrow & \Lambda^{m-1}(G_{m-1}(T\mathcal{U}))^* \\ \uparrow & & \downarrow{\scriptstyle \pi_G} & & \\ W & \xrightarrow{\pi} & \mathcal{U} & & \end{array} .$$

The boundedness postulate, the analog of GC1, requires that there is a section S of the bundle of linear mappings $L(J^1(W), \Lambda^m(T^*\mathcal{U}))$ such that

$$|F_{\mathcal{R}}(w)| = \left| \int_{\mathcal{R}} \mathbf{b}(w) + \int_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w) \right| \leqslant \int_{\mathcal{R}} |S(j^1(w))|.$$

Here, $J^1(W)$ is the first jet bundle of W, $j^1(w)$ is the first jet of the section w, and the absolute value of an m-form θ, $S(j^1(w))$, in this case, is given as

$$|\theta(x)| = \begin{cases} \theta(x) & \text{if } \theta(x) \text{ is positively oriented,} \\ -\theta(x) & \text{if } \theta(x) \text{ is negatively oriented,} \end{cases}$$

relatively to the orientation chosen on $\mathcal{U}$.

The resulting generalized version of Cauchy's theorem states that there is a unique section σ of $\Lambda^{m-1}(T\mathcal{U}, W^*) \cong L(W, \Lambda^{m-1}(T^*\mathcal{U}))$, called the *Cauchy stress*, such that $\mathbf{t}_{\mathcal{R}}(w) = \iota^*(\sigma \circ w)$. We will write $\sigma(w)$ for $\sigma \circ w$ and $\iota^*(\sigma)$ for $\iota^* \circ \sigma$ so we have the *Cauchy formula* $\mathbf{t}_{\mathcal{R}} = \iota^*(\sigma)$ in analogy with the scalar case (with the difference that the forms are vector valued now).

Using Stokes' theorem, the action of $F_{\mathcal{R}}$ may now be rewritten using an integral over $\mathcal{R}$ of $\mathcal{R}$-independent forms and without a boundary term as

$$F_{\mathcal{R}}(w) = \int_{\mathcal{R}} (d\sigma(w) + \mathbf{b}(w)).$$

Assume that (x^i, w^α) are local vector bundle coordinates in a neighborhood $\pi^{-1}(U) \subset W$, $U \subset \mathcal{U}$ with local basis elements $\{e_\alpha\}$ so a section of W is represented locally by $w^\alpha e_\alpha$. Then, denoting the dual base vectors by $\{e^\alpha\}$ a stress σ is represented locally by

$$\sigma_{\alpha 1 \ldots \hat{k} \ldots m} e^\alpha \otimes dx^1 \wedge \cdots \wedge \widehat{dx^k} \wedge \cdots \wedge dx^m,$$

where a "hat" indicates the omission of an item (an index or a factor). The value of $\sigma(w)$ is represented locally by

$$\sigma_{\alpha 1 \ldots \hat{k} \ldots m} w^\alpha dx^1 \wedge \cdots \wedge \widehat{dx^k} \wedge \cdots \wedge dx^m.$$

V. VARIATIONAL STRESSES

Let $\pi: W \to \mathcal{U}$ be a vector bundle as in the previous section. A *variational stress density* is a section of $L(J^1(W), \Lambda^m(T^*\mathcal{U}))$.

For the vector bundle coordinates $(x^i,w^\alpha), i=1,\ldots,m,\ \alpha=1,\ldots,\dim(W_x)$, the jet of a section is represented locally by the functions $\{w^\alpha(x^i),w^\beta_{,j}(x^k)\}$, where a subscript following a comma indicates partial differentiation. A variational stress density will be represented locally by the functions $\{S_{\alpha 1\ldots m},S^j_{\beta 1\ldots m}\}$ so that the single component of the m-form $S(j^1(w))$ in this coordinate system is

$$S(j^1(w))_{1\ldots m}=S_{\alpha 1\ldots m}w^\alpha+S^j_{\beta 1\ldots m}w^\beta_{,j}.$$

Note that the notation distinguishes between the components of S that are dual to the values of the section and those dual to the derivatives by the number of indices only. The next few paragraphs motivate the introduction of variational stress densities.

Variational stress theory is formulated usually in a particular frame where the space $(m-1)$-dimensional manifold $\mathcal{M}$ is a global slice of space–time and $\mathcal{U}$ is interpreted as the $(m-1)$-dimensional material universe manifold. In such a situation, for any body $\mathcal{R}$—an $(m-1)$-dimensional compact submanifold with boundary of $\mathcal{U}$—one may consider *configurations* of the body in space defined as embeddings of $\mathcal{R}$ in $\mathcal{M}$.

The rationale behind the variational formulation of stress theory is the framework for mechanical theories where a configuration manifold is constructed for the system under consideration, generalized velocities are defined as elements of the tangent bundle to the configuration manifold, and generalized forces are defined as elements of the cotangent bundle of the configuration space. For the mechanics of continuous bodies in space, the natural topology for the collection of embeddings is the C^1 topology for which the collection of embeddings is open in the collection of all C^1 mappings of the body into space. Using this topology, the tangent space to the configuration manifold at the configuration $\kappa:\mathcal{R}\to\mathcal{M}$ is $C^1(\kappa^*(T\mathcal{M}))$, the Banachable space of C^1 sections of the pull-back $\kappa^*(T\mathcal{M})$. Thus, forces in continuum mechanics are elements of $C^1(\kappa^*(T\mathcal{M}))^*$—continuous, linear functionals on the space of differentiable vector fields equipped with the C^1 topology.

The basic representation theorem (see Ref. 7) states that a force functional $F\in C^1(\kappa^*(T\mathcal{M}))^*$ may be represented by a measure on $\mathcal{U}$—the *variational stress measure*—valued in $J^1(\kappa^*(T\mathcal{M}))^*$, the dual of the first jet bundle $J^1(\kappa^*(T\mathcal{M}))\to\mathcal{U}$. The evaluation of a force $F_\mathcal{R}$ on the generalized velocity w is

$$F_\mathcal{R}(w)=\int_\mathcal{R} d\boldsymbol{\mu}(j^1(w)),$$

where $\boldsymbol{\mu}$ is the $J^1(\kappa^*T\mathcal{M})^*$-valued measure—a section Schwartz distribution.

Assuming that κ is defined on all the material universe $\mathcal{U}$, we use the notation W for $\kappa^*(T\mathcal{M})$. This vector bundle can be restricted to the individual bodies, and, with some abuse of notation, we use the same notation for both the bundle and its restrictions to the individual bodies.

In the smooth case, a variational stress measure is given in terms of a section S of $L(J^1(W),\Lambda^{m-1}(T^*\mathcal{U}))$ (recalling the $\mathcal{U}$ is now the material manifold with dimension $m-1$) so

$$F_\mathcal{R}(w)=\int_\mathcal{R} S(j^1(w)).$$

Since in the sequel we consider only the smooth case, we will use ''variational stresses'' to refer to the densities.

VI. THE RELATION BETWEEN THE CAUCHY APPROACH AND THE VARIATIONAL APPROACH

In Ref. 11 we define a canonical mapping

$$p_\sigma : L(J^1(W), \overset{m}{\Lambda}(T^*\mathcal{U})) \to L(W, \overset{m-1}{\Lambda}(T^*\mathcal{U}))$$

that assigns to a variational stress density S a Cauchy stress σ satisfying the following relation. At every $x \in \mathcal{U}$ (we suppress the evaluation at x in the notation)

$$\phi \wedge \sigma(w) = S(j_{\phi \otimes w}),$$

for any one-form ϕ. Here, $j_{\phi\otimes w}$ is roughly the jet at x of a section whose value is $0 \in W_x$ and its derivative is $\phi \otimes w$. More precisely, if $u : \mathcal{U} \to W$ is the section whose first jet at x is $j_{\phi\otimes w}$, then u satisfies the following conditions: $u(x)=0$; denoting the zero section of W by 0, $T_x u - T_x 0 \in L(T_x\mathcal{U}, T_{0(x)}W_x)$ induces the linear mapping $\phi \otimes w$ through the isomorphism of $T_{0(x)}W_x$ with W_x. The local representation of p_σ is as follows. If $\sigma = p_\sigma(S)$, then, using the local representatives of σ and S as in the previous sections,

$$\sigma_{\beta 1 \ldots \hat{\imath} \ldots m} = (-1)^{i-1} S^{+i}{}_{\beta 1 \ldots m}, \quad \text{(no sum over } i\text{)}.$$

The mapping p_σ is clearly linear and surjective.

Given a variational stress density S, its generalized divergence Div S is the section of $L(W, \Lambda^m(T^*\mathcal{U}))$ defined by

$$\mathrm{Div}\, S(w) = d(p_\sigma(S)(w)) - S(J^1(w)).$$

The local expression for $\mathrm{Div}\, S(w)$ is

$$(S^i_{\alpha 1 \ldots m, i} - S_{\alpha 1 \ldots m}) w^\alpha dx^1 \wedge \cdots \wedge dx^m,$$

which shows that Div S depends only on the values of w and not its derivative. With these definitions one obtains that

$$\int_{\mathcal{R}} S(j^1(w)) = \int_{\mathcal{R}} \mathbf{b}_{\mathcal{R}}(w) + \int_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w),$$

where $\mathbf{t}_{\mathcal{R}}(w) = \iota^*_{\mathcal{R}}(p_\sigma(S)(w))$ and $\mathrm{Div}\, S + \mathbf{b}_{\mathcal{R}} = 0$. We conclude that every variational stress induces a unique force system $\{(\mathbf{b}_{\mathcal{R}}, \mathbf{t}_{\mathcal{R}})\}$ through the Cauchy stress it induces and its divergence. Actually, we obtained a decomposition of $S(j^1(w))$ into an exact differential and a term that is linear in the values of w.

The converse is also true. If we have a force system that satisfies Cauchy's postulates, then the induced Cauchy stress enables us to define a section S of $L(J^1(W), \Lambda^m(T^*\mathcal{U}))$ by $S(j^1(w)) = \mathbf{b}(w) + d\sigma(w)$. Clearly, writing the local expression for S, it is linear in the jet of w. Hence,

$$F_{\mathcal{R}}(w) = \int_{\mathcal{R}} \mathbf{b}(w) + \int_{\mathcal{R}} d\sigma(w) = \int_{\mathcal{R}} S(j^1(w)).$$

If for a given variational stress $\mathbf{b} = \mathrm{Div}\, S = 0$, then, $S(j^1(w)) = dp_\sigma(S)(w)$.

Thus, we have a complete correspondence between the Cauchy approach and the variational approach to stress theory.

VII. STRESS-ENERGY TENSORS

Following the interpretation of the flux form J as an object generalizing the velocity vector field, we may consider stress theory on space–time $\mathcal{U}$ where we set $W=\Lambda^{m-1}(T^*\mathcal{U})$. To emphasize this we may write

$$F_{\mathcal{R}}(J)=\int_{\partial\mathcal{R}}\mathbf{t}_{\mathcal{R}}(J).$$

Here, the boundary term $\mathbf{t}_{\mathcal{R}}$ is a section of $L(\Lambda^{m-1}(T^*\mathcal{U}),\Lambda^{m-1}(T^*\partial\mathcal{R}))$. Note that for the space–time formulation the term involving $\mathbf{b}_{\mathcal{R}}$ is omitted. Assuming that the generalized Cauchy postulates hold for $\mathbf{t}_{\mathcal{R}}$, the Cauchy stress σ is a section of $L(\Lambda^{m-1}(T^*\mathcal{U}),\Lambda^{m-1}(T^*\mathcal{U}))$. Finally, $\mathrm{Div}\,S=0$ and $d\sigma(J)=S(j^1(J))$.

The situation may be described generally as follows. We started with an extensive property p, given in terms of the flux densities $\tau_{\mathcal{R}}$ for the various control regions $\mathcal{R}$ in space–time. The source term for property p is s and, assuming the Cauchy postulates are satisfied, the property p has a flux form J. We now consider a second property, the q property, whose flux densities $\tau_{\mathcal{R}}^{(q)}$ for the various control regions and source term $s^{(q)}$ satisfy the conservation equation

$$\int_{\partial\mathcal{R}}\tau_{\mathcal{R}}^{(q)}=\int_{\mathcal{R}}s^{(q)}.$$

Again, assuming the Cauchy postulates hold for the property q, we have the corresponding flux form $J^{(q)}$ satisfying $\tau_{\mathcal{R}}^{(q)}=\iota^*(J^{(q)})$ and the conservation equation has the differential representation $dJ^{(q)}=s^{(q)}$.

We will say that the property q is a *resource* for the property p if the flux density $\tau_{\mathcal{R}}^{(q)}$ depends pointwise linearly on the flux form J of the property p. Thus, there is a section $\mathbf{t}_{\mathcal{R}}$ as above such that $\tau_{\mathcal{R}}^{(q)}=\mathbf{t}_{\mathcal{R}}(J)$.

In this framework, the Cauchy theorem implies that

$$\iota^*(J^{(q)})=\tau_{\mathcal{R}}^{(q)}=\mathbf{t}_{\mathcal{R}}(J)=\iota^*(\sigma(J)),$$

for the inclusion ι of an arbitrary region, so $J^{(q)}=\sigma(J)$. In other words, the Cauchy stress transforms the flux of the property p to the flux of the resource that p uses—the property q. The source term for the property q is now given by $s^{(q)}=d\sigma(J)$.

Naturally, in the sequel we will be concerned primarily with the energy resource.

VIII. REPRESENTATIONS OF FORCE DENSITIES AND STRESS-ENERGY TENSORS

For the situation under consideration a force density (the analog of $\mathbf{b}_{\mathcal{R}}$ if considered) is given in terms of a section of $L(\Lambda^{m-1}W^*,\Lambda^mW^*)$. Such sections have simple representations as follows.

For a vector space $\mathbf{W}$ with dimension m, consider the space of linear mappings $(\Lambda^p\mathbf{W}^*)^{\mathrm{T}}=L(\Lambda^p\mathbf{W}^*,\Lambda^m\mathbf{W}^*)$. Define the mapping $\wedge^p:\Lambda^{m-p}\mathbf{W}^*\to(\Lambda^p\mathbf{W}^*)^{\mathrm{T}}$ by $\wedge^p(\alpha)(\beta)=\alpha\wedge\beta$.

Clearly $\wedge^p$ is a linear mapping between the two spaces. In addition, as $\Lambda^m\mathbf{W}^*$ is one-dimensional, $\dim(\Lambda^p\mathbf{W}^*)^{\mathrm{T}}=\dim(\Lambda^p\mathbf{W}^*)=\dim(\Lambda^{m-p}\mathbf{W}^*)$. Thus, $\wedge^p$ is an isomorphism if $\mathrm{Kernel}(\wedge^p)=\{0\}$. It is clear, however, that if $\wedge^p(\alpha)(\beta)=\alpha\wedge\beta=0$ for all β, then $\alpha=0$.

We may conclude, for example, that a body force density is of the form $A\wedge J$ for a one-form A.

As the stress-energy tensor is now a section of $L(\Lambda^{m-1}(T^*\mathcal{U}),\Lambda^{m-1}(T^*\mathcal{U}))$, it is locally represented by a matrix with respect to a local basis of $\Lambda^{m-1}(T^*\mathcal{U})$. We will make below some further observations regarding the representations of stresses.

Assume that a volume element θ is given on $\mathcal{U}$. Then, we may use the vector bundle isomorphism

$$i_\theta\colon \overset{m-1}{\Lambda}(T^*\mathcal{U})\to T\mathcal{U}$$

to represent the section σ of $L(\Lambda^{m-1}(T^*\mathcal{U}),\Lambda^{m-1}(T^*\mathcal{U}))$ by a section $\tilde{\sigma}$ of $L(T\mathcal{U},T\mathcal{U})$ satisfying $\tilde{\sigma}\circ i_\theta = i_\theta\circ\sigma$.

Let us consider the relation between the local representation of σ and the local representation $\tilde{\sigma}_i^j dx^i\otimes \partial/\partial x^j$ of $\tilde{\sigma}$. To represent σ locally, we will use the notation $\hat{e}^i$ for the basis element $dx^1\wedge\cdots\wedge\widehat{dx^i}\wedge\cdots\wedge dx^m$ of $\Lambda^{m-1}(T^*\mathcal{U})$. Thus, the flux form J is represented locally by $\hat{J}_i\hat{e}^i$, and the stress is represented locally in the form $\hat{\sigma}_i^j\hat{e}_j\otimes\hat{e}^i$, where $\{\hat{e}_j\}$ is the dual basis to $\{\hat{e}^i\}$.

If the volume element θ is represented locally by $r dx^1\wedge\cdots\wedge dx^m$, the action of i_θ is given locally by

$$\hat{J}_i\hat{e}^i \mapsto \sum_i (-1)^{i+1}\frac{1}{r}\hat{J}_i\frac{\partial}{\partial x^i}$$

(we use the summation symbol as the summation convention cannot be used on the right). Thus, $i_\theta(\sigma(J))$ is represented by

$$\sum_j (-1)^{j+1}\frac{1}{r}\hat{\sigma}_j^i\hat{J}_i\frac{\partial}{\partial x^j},$$

and $\tilde{\sigma}(i_\theta(J))$ is represented by

$$\sum_i (-1)^{i+1}\frac{1}{r}\tilde{\sigma}_i^j\hat{J}_i\frac{\partial}{\partial x^j}.$$

Hence, the relation between σ and $\tilde{\sigma}$ is represented locally as

$$\tilde{\sigma}_k^j = (-1)^{j+k}\hat{\sigma}_j^k.$$

It is interesting to note that the volume element does not enter the last relation and one may attempt to arrive at a natural isomorphism between the bundles $L(\Lambda^{m-1}(T^*\mathcal{U}),\Lambda^{m-1}(T^*\mathcal{U}))$ and $L(T\mathcal{U},T\mathcal{U})$. Such a natural isomorphism can be constructed as follows. Consider the tensor product $T^*\mathcal{U}\otimes_{\mathcal{U}}T\mathcal{U}$. This tensor product is naturally isomorphic to $L(T\mathcal{U},T\mathcal{U})$. For an element $\tilde{\sigma}=\tilde{\sigma}_i^j\phi^i\otimes v_j$ in $T^*\mathcal{U}\otimes_{\mathcal{U}}T\mathcal{U}$, $v_j\in T_x\mathcal{U}$, $\phi^i\in T_x^*\mathcal{U}$, set

$$\sigma\colon \overset{m-1}{\Lambda}(T^*\mathcal{U})\to \overset{m-1}{\Lambda}(T^*\mathcal{U})$$

by

$$(*)\qquad \sigma(J)=\tilde{\sigma}_i^j v_j\lrcorner(\phi^i\wedge J)=\tilde{\sigma}_i^j(\phi^i(v_j)J-\phi^i\wedge(v_j\lrcorner J)).$$

We note that σ is indeed linear in J. Since σ depends linearly on the v^i and on the ϕ^j, it depends linearly on the elements of the tensor product.

For the local coordinates $\{x^i\}$, let us determine the stress σ induced by the linear mapping $\tilde{\sigma}\in L(T\mathcal{U},T\mathcal{U})$ represented locally by the tensor $\tilde{\sigma}_i^j dx^i\otimes\partial/\partial x^j$. By definition, $\sigma(J)$ is represented by (the sum on i is explicitly written)

$$\sum_i \tilde{\sigma}_i^j \frac{\partial}{\partial x^j} \lrcorner (dx^i \wedge J) = \sum_i \tilde{\sigma}_i^j \frac{\partial}{\partial x^j} \lrcorner (dx^i \wedge (\hat{J}_k dx^1 \wedge \cdots \wedge \widehat{dx^k} \wedge \cdots \wedge dx^m))$$

$$= \sum_i \tilde{\sigma}_i^j \frac{\partial}{\partial x^j} \lrcorner ((-1)^{i+1} \hat{J}_i dx^1 \wedge \cdots \wedge dx^m)$$

$$= \sum_i \tilde{\sigma}_i^j (-1)^{i+j} \hat{J}_i dx^1 \wedge \cdots \wedge \widehat{dx^j} \wedge \cdots \wedge dx^m$$

$$= \sum_i \tilde{\sigma}_i^j (-1)^{i+j} \hat{J}_i \hat{e}^j = \sum_i \hat{\sigma}_j^i \hat{J}_i \hat{e}^j.$$

Hence, the matrix representing σ is $\hat{\sigma}_j^i = (-1)^{i+j} \tilde{\sigma}_i^j$. We conclude that $(*)$ is indeed the natural, invariant representation of the isomorphism between the bundles $L(\Lambda^{m-1}(T^*\mathcal{U}), \Lambda^{m-1}(T^*\mathcal{U}))$ and $L(T\mathcal{U}, T\mathcal{U})$. This motivates even further the interpretation of the Cauchy stress as a transformation operating on the flux or velocity field of the property p to give the flux form for the energy or velocity of the generalized energy points.

IX. EXAMPLE: THE MAXWELL STRESS-ENERGY TENSOR WITHOUT A METRIC

As an example for the foregoing analysis, we consider a generalization of the stress-energy tensor of classical electromagnetism to the setting where a metric is not available. We assume that there is a volume element on the four-dimensional $\mathcal{U}$. The following setting is also independent of any relation between the Maxwell two-form and the Faraday two-form such as the relations between the fields (**E**, **B**) and (**D**, **H**) in vacuum. The extensive property under consideration is of course the electric charge and J is the charge-current density—a three-form. The conservation of charge implies that $dJ = 0$ and the Maxwell two-form $\mathfrak{g}$ is a flow potential for the flux form so $J = d\mathfrak{g}$. For a one-form A, the vector potential, the energy source density is $A \wedge J$. It follows that the Faraday two-form $\mathfrak{f} = dA$ satisfies $d\mathfrak{f} = 0$.

Thus, assuming that a volume element θ is given on $\mathcal{U}$, we set $w = i_\theta(J)$ and define the stress-energy tensor as the section σ of $L(\Lambda^{m-1}(T^*\mathcal{U}), \Lambda^{m-1}(T^*\mathcal{U}))$ by (cf. Ref. 12, p. 36 for the closest expression we found)

$$\sigma(J) = (i_\theta(J) \lrcorner \mathfrak{g}) \wedge \mathfrak{f} - (i_\theta(J) \lrcorner \mathfrak{f}) \wedge \mathfrak{g}.$$

Alternatively, using

$$w \lrcorner (\mathfrak{g} \wedge \mathfrak{f}) = (w \lrcorner \mathfrak{g}) \wedge \mathfrak{f} + \mathfrak{g} \wedge (w \lrcorner \mathfrak{f}),$$

the definition of the electromagnetic stress-energy tensor may also be written as

$$\sigma(J) = i_\theta(J) \lrcorner (\mathfrak{g} \wedge \mathfrak{f}) - 2(i_\theta(J) \lrcorner \mathfrak{f}) \wedge \mathfrak{g}.$$

Note that the matrix of the Cauchy stress with respect to the natural basis of the space of $(m-1)$-forms is related to the usual matrix of the stress-energy-momentum tensor as discussed in the previous section.

We now consider the energy source term $d\sigma(J)$. Using $w = i_\theta(J)$ one obtains

$$d\sigma(J) = d((i_\theta(J) \lrcorner \mathfrak{g}) \wedge \mathfrak{f} - (i_\theta(J) \lrcorner \mathfrak{f}) \wedge \mathfrak{g})$$

$$= d(w \lrcorner \mathfrak{g}) \wedge \mathfrak{f} - (w \lrcorner \mathfrak{g}) \wedge d\mathfrak{f} + (w \lrcorner \mathfrak{f}) \wedge d\mathfrak{g} - d(w \lrcorner \mathfrak{f}) \wedge \mathfrak{g}$$

$$= d(w \lrcorner \mathfrak{g}) \wedge \mathfrak{f} + (w \lrcorner \mathfrak{f}) \wedge J - d(w \lrcorner \mathfrak{f}) \wedge \mathfrak{g},$$

where Maxwell's equations were used to arrive at the last line. Using the identity $d(w \lrcorner \alpha) = \mathcal{L}_w \alpha - w \lrcorner d\alpha$, for any differential form α, we have

$$d\sigma(J)=(w\lrcorner\mathfrak{f})\wedge J+(\mathcal{L}_w\mathfrak{g}-u\lrcorner d\mathfrak{g})\wedge\mathfrak{f}-(\mathcal{L}_w\mathfrak{f}-w\lrcorner d\mathfrak{f})\wedge\mathfrak{g}.$$

Finally, as $w\lrcorner J=0$, Maxwell's equations give

$$d\sigma(J)=(w\lrcorner\mathfrak{f})\wedge J+(\mathcal{L}_w\mathfrak{g})\wedge\mathfrak{f}-(\mathcal{L}_w\mathfrak{f})\wedge\mathfrak{g}.$$

It is noted that the term $(w\lrcorner\mathfrak{f})\wedge J$ represents the power of the Lorentz force. In addition, in the classical formulation where a metric is available and $\mathfrak{g}=*\mathfrak{f}$ ($*$ denotes the Hodge operator), the terms $(\mathcal{L}_w\mathfrak{g})\wedge\mathfrak{f}$ and $(\mathcal{L}_w\mathfrak{f})\wedge\mathfrak{g}$ are equal and the energy source density contains the power of the Lorentz force (and energy conservation) only. For an analogous expression where the constitutive relation between $\mathfrak{g}$ and $\mathfrak{f}$ is not specified but a metric is used, see Ref. 2, p. 91.

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APPENDIX: LOCAL REPRESENTATION OF THE MAXWELL STRESS-ENERGY TENSOR

We write the local representation $\hat{\mathfrak{f}}_{ij}dx^i\wedge dx^j$ of the Faraday two-form $\mathfrak{f}$ in the form

$$\{\hat{\mathfrak{f}}_{ij}\}=\begin{pmatrix}0&-E_1&-E_2&-E_3\\E_1&0&B_3&-B_2\\E_2&-B_3&0&B_1\\E_3&B_2&-B_1&0\end{pmatrix},$$

and the corresponding representation $\hat{\mathfrak{g}}_{ij}dx^i\wedge dx^j$ for the Maxwell two-form as

$$\{\hat{\mathfrak{g}}_{ij}\}=\begin{pmatrix}0&H_1&H_2&H_3\\-H_1&0&D_3&-D_2\\-H_2&-D_3&0&D_1\\-H_3&D_2&-D_1&0\end{pmatrix}.$$

For simplicity of the notation we assume that locally the volume element θ is of the form $dx^1\wedge\ \cdots\wedge dx^4$. Then, $w=i_\theta(J)$ is represented by $w^i=(-1)^{i+1}\hat{J}_i$. With this notation, the matrix $\{\hat{\sigma}_i^j\}$ representing the stress-energy tensor is

$$\{\hat{\sigma}_i^j\}=\begin{pmatrix}\{\hat{\sigma}_i^1\}&\{\hat{\sigma}_i^2\}&\{\hat{\sigma}_i^3\}&\{\hat{\sigma}_i^4\}\end{pmatrix},$$

where

$$\hat{\sigma}_i^1=\begin{Bmatrix}H_1B_1+H_2B_2+H_3B_3+D_1E_1+D_2E_2+E_3D_3\\2(E_3H_2-E_2H_3)\\2(E_3H_1-E_1H_3)\\2(E_2H_1-E_1H_2)\end{Bmatrix},$$

$$\hat{\sigma}_i^2=\begin{Bmatrix}2(B_3D_2-B_2D_3)\\H_1B_1-H_2B_2-H_3B_3+E_1D_1-E_2D_2-E_3D_3\\2(E_1D_2-B_2H_1)\\2(E_1D_3+B_3H_1)\end{Bmatrix},$$

$$\hat{\sigma}_i^3=\begin{Bmatrix} 2(B_3D_1-B_1D_3) \\ 2(B_1H_2-E_2D_1) \\ -H_1B_1+H_2B_2-H_3B_3-E_1D_1+E_2D_2-E_3D_3 \\ 2(-E_2D_3-B_3H_2) \end{Bmatrix},$$

$$\hat{\sigma}_i^4=\begin{Bmatrix} 2(B_2D_1-B_1D_2) \\ 2(B_1H_3-E_3D_1) \\ 2(-E_3D_2-B_2H_3) \\ -H_1B_1-H_2B_2+H_3B_3-E_1D_1-E_2D_2+E_3D_3 \end{Bmatrix}.$$

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Discrete version of the SHE asymptotics: multigroup neutron transport equations

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This paper is devoted to the derivation of multigroup diffusion equations from the Boltzmann equation. The limit system couples the energy levels from both zeroth-order term and diffusion currents. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Production of nuclear energy relies on the disintegration of atoms (uranium or plutonium), when subjected to collisions with neutrons. Therefore, reactor design requires an accurate description of the motion of the population of neutrons. The motion of neutrons is described through the evolution of the density $f(t,x,v)$ of neutrons occupying at time $t \geqslant 0$ the position $x \in \mathbb{R}^N$ and having velocity $v \in \mathbb{R}^N$. It will be convenient in what follows to see this last variable as $v = \sqrt{2e/m}\ \omega$, $m>0$ being the mass of the neutron, $e \geqslant 0$ its energy, and $\omega \in S^{N-1}$ the direction of the flight. The unknown f verifies a transport equation

$$\partial_t f + v \cdot \nabla_x f = Q(f) \tag{1}$$

that relates the free transport (left-hand side) to the various interaction processes undergone by the neutrons and described through the operator $Q(f)$. The latter are essentially collisions. Furthermore, the number of neutrons in any volume, at any time, remains smaller than the number of atomic nuclei (10^{11} is a typical ratio) so that it is reasonable to assume that the most probable event is an elastic collision with the surrounding medium. Consequently, the right-hand side of (1) is usually given by a Boltzmann linear operator

$$Q(f) = \int \sigma(x,v,v')\ \ f(t,x,v')\, \mathrm{d}v' - \Sigma(x,v)\ \ f(t,x,v). \tag{2}$$

The transfer function $\sigma(x,v,v') \geqslant 0$ is such that $\sigma(x,v,v')\mathrm{d}v$ represents the probability that a neutron impinging with velocity v' will have velocity in the volume $\mathrm{d}v$ around v after the collision; while $\Sigma(x,v) \geqslant 0$ is the so-called removal cross section. If the operator is conservative, i.e., $\int Q(f)\, \mathrm{d}v = 0$, which means that $\Sigma(x,v) = \int \sigma(x,v',v)\, \mathrm{d}v'$, then absorption/fission events are neglected or compensated with scattering. One also says that the reactor is critical in this case. It is worth remarking that, since the ratio of the mass of the nuclei to the mass of the neutrons is very large, then, during an elastic collision, the energy of the neutron is practically unchanged; the main effect of such a collision is only to modify the direction of the flight. Notice also that inelastic scattering, with loss of energy, remains possible, but it can only occur for highly energetic neutrons.

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On the other hand, nuclear engineers are motivated in the derivation of simplified models that describe the physics accurately enough but remain of moderate computational cost. In these applications, one encounters a very large range of energies, from 1/40 eV to some MeV; and a first simplification arises by breaking the energy range into several disjoint energy groups: $[e_{\min},e_{\max}]=\cup_{i=1}^{I}[e_i,e_{i+1}]$. In most of the situations, the total number of groups I is finite. One assumes that the cross sections do not vary too much on the energy groups and neutrons evolve according to averaged quantities, such as average scattering cross sections. Consequently, one is led to semidiscrete versions of Eqs. (1) and (2). This will be detailed in Sec. II.

Next, a commonly used strategy consists in neglecting the angular variable ω and writing a diffusion equation for a macroscopic energy distribution function $\rho(t,x,e)$, e being the energy variable (discrete or continuous). Actually, one deals in this context with systems of equations, coupled by the energy variable, which usually have the following form:

$$\partial_t\rho(t,x,e)-\mathrm{div}_x(D(x,e)\nabla_x\rho(t,x,e))=\int \tilde{\sigma}(x,e,e')\rho(t,x,e')\,de'-\tilde{\Sigma}(x,e)\rho(t,x,e), \qquad (3)$$

where the coefficients D, $\tilde{\sigma}$, $\tilde{\Sigma}$ are non-negative. Of course, one obtains similar systems in the (energy-)discretized context. These equations can be derived directly from a balance relation on the population of neutrons, through a phenomenological analysis of the scattering events. The diffusion coefficients are due to elastic scattering when neutrons do not lose energy during the collision process. Zeroth-order terms are due to absorption, inelastic scattering (i.e., collisions with loss of energy), or fission. Furthermore, system (3) can be generalized by postulating that the diffusion operator couples the energy levels as follows:

$$\mathrm{div}_x\left(\int k(x,e,e')\ \nabla_x\rho(t,x,e')\,de'\right).$$

Indeed, gradients of the density ρ at a given energy e' can have some effect on the diffusion on another energy level e.

However, it is also tempting to obtain systems like (3) from the kinetic modeling, Eqs. (1) and (2), and to identify the coefficients through an asymptotic analysis. Then, starting from the continuity equation

$$\partial_t\rho+\mathrm{div}_x j=\int_{S^{N-1}}Q(f)\,d\omega \qquad (4)$$

satisfied by the macroscopic density

$$\rho(t,x,e)=\int_{S^{N-1}}f(t,x,\sqrt{2e/m}\,\omega)\,d\omega,$$

and the macroscopic current

$$j(t,x,e)=\int_{S^{N-1}}\sqrt{2e/m}\,\omega\,f(t,x,\sqrt{2e/m}\omega)\,d\omega,$$

we search for a diffusion equation by postulating a relation between ρ and j that takes the form of a generalized Fick's law

$$j(t,x,e)=-\int k(x,e,e')\,\nabla_x\rho(t,x,e')\,de'.$$

Such an approximation is intended to apply in the limit of small mean free paths, which is related to the probability of collisions by unit length and decreases when the density of the medium increases. It leads to singular perturbation problems and this work is devoted to such a question.

For details on the physics of nuclear reactors we refer to the classical books of B. Davison,[17] E. Wigner,[41] E. Wachspress,[40] J. Bussac and P. Reuss,[12] J. Planchard,[37] and C. Cercignani.[15] The mathematical study of the vanishing mean free path limit and of the diffusion approximation is by now a classical problem with applications in various fields of physics; we refer among others to E. Larsen and J. Keller,[32] A. Bensoussan, J.-L. Lions, and G. Papanicolaou,[10] C. Bardos, R. Santos, and R. Sentis,[8] and, for recent progresses, to R. Dautray and J. L. Lions,[16] F. Malvagi, D. Levermore, and G. Pomraning,[35] F. Poupaud,[38] F. Golse,[26] C. Bardos, F. Golse, and B. Perthame,[6] C. Bardos, F. Golse, B. Perthame, and R. Sentis,[7] F. Golse and F. Poupaud,[27] P. L. Lions and G. Toscani,[34] P. Degond, T. Goudon, and F. Poupaud,[20] etc. Another difficulty in reactor physics is related to the high heterogeneity of the surrounding medium. Accordingly, the cross sections depend on the space variable and present very large oscillations. This leads to homogenization questions. Depending on the ordering, the homogenization procedure can be performed at the kinetic level, see F. Golse,[24,25] L. Dumas and F. Golse,[22] P. Gérard and F. Golse[23] or directly on the diffusion approximation as in J. Dorning, R. Uddin, and H. Zhang,[21] Y. Capdeboscq,[13,14] G. Allaire and Y. Capdeboscq,[2] and G. Allaire and F. Malige.[3] We can also combine altogether these effects as in E. Larsen,[30,31] E. Larsen and M. Williams,[33] C. Bardos, L. Dumas, P. Gérard, and F. Golse,[5] G. Allaire and G. Bal,[1] G. Bal,[4] T. Goudon and F. Poupaud,[29] and T. Goudon and A. Mellet.[28]

However, it is a well-known fact that different (formal) methods of approximation can give rise to difference on the limit coefficients, see Ref. 31 or Refs. 37, 1, and 13 for some examples. Furthermore, when starting from multigroup equations and performing the diffusion approximation limit, one usually obtains a single diffusion equation in the space variable only, see Refs. 2 and 13: the limit procedure forgets the multigroup aspect. This is because the system is considered to relax toward an equilibrium under both elastic and inelastic collisions at the same scale. However, it could be interesting to derive more complex models, which retain the energy as a variable and where the diffusion as well as the inelastic collisions couple the various energy levels. This is the goal of the present paper. To that purpose, our analysis is inspired by reasonings developed in the modeling of semiconductor devices where, instead of obtaining a drift-diffusion equation, we are led to an intermediate system, by keeping the energy as a variable, see Ben Abdallah and P. Degond,[9] and P. Degond.[18,19] We also mention the recent application to the phonons dynamics by J. P. Bourgade.[11] These so-called SHE-models have been shown to be very accurate, in particular for numerical simulations. It is worth noticing at the moment that the energy coupling can be obtained either through the zeroth-order terms when the inelastic collisions are treated as perturbations, or through the diffusion operator when inelastic processes are treated in a more intricate way, as it has been done by P. Degond,[19] in the framework of semiconductor theory, for continuous energy levels. However, the analysis developed in the present paper, though largely inspired from Ref. 19, requires less restrictive hypotheses (see in particular Sec. III and Proposition 5). Note that this work is only concerned with the diffusion approximation problem; the homogenization question will be addressed elsewhere. Note also that we have chosen to treat the evolution problem but, of course, our analysis can be applied to eigenvalue problems as well.

The paper is organized as follows. In Sec. II, we will set up precisely the multigroup aspect on the Boltzmann equation. Section III is devoted to a discussion of some properties of the collision operator. In particular, we aim at splitting the Boltzmann operator into an elastic part, which leaves the number of neutrons in a given energy level unchanged, and an inelastic part. This can be done either locally or not as far as the energy variable is concerned. In some sense, the latter retains some relevant information on the energy exchange during the collisions with the medium. In Sec. IV we formally discuss the small mean free path asymptotic limit with the requirement that elastic, or quasielastic, processes dominate. Actually, our method can be viewed as a heuristic procedure to derive macroscopic models, which are intermediate between a full kinetic description and a simple diffusion equation. Finally, Sec. V is concerned with a rigorous proof of convergence.

II. MULTIGROUP EQUATIONS

The evolution of the population of neutrons is described through an equation relating transport to interaction processes as follows:

$$\begin{gathered}(\partial_t + v\cdot\nabla_x)f = Q(f),\\ Q(f) = \frac{1}{|S^{N-1}|}\int_{\mathbb{R}^N}\sigma(x,v,v')f(v')\,\mathrm{d}v' - \Sigma(x,v)f(v),\\ \Sigma(x,v) = \frac{1}{|S^{N-1}|}\int_{\mathbb{R}^N}\sigma(x,v',v)\,\mathrm{d}v'.\end{gathered} \tag{5}$$

The third relation means that the operator Q is conservative, or critical, in the sense that, neglecting integrability questions for the time being, we have

$$\int_{\mathbb{R}^N} Q(f)\,\mathrm{d}v = 0.$$

Compared to Sec. I, we have changed the cross sections by introducing the normalization by $1/|S^{N-1}|$ for pure convenience; it will allow us to work with normalized measure and will simplify some forthcoming computations.

We write the velocity of the particles as follows:

$$\begin{gathered}v = |v|\omega = \sqrt{2e/m}\,\omega,\\ \omega = v/|v| = \text{angular variable} \in S^{N-1},\\ e = mv^2/2 = \text{energy variable} \in \mathbb{R}^+.\end{gathered}$$

Denoting by $\mathrm{d}\omega$ the normalized Euclidian measure on S^{N-1}, we have $\mathrm{d}v = |S^{N-1}|r^{N-1}\mathrm{d}r\,\mathrm{d}\omega$, with $r = |v| = \sqrt{2e/m}$, and therefore $\mathrm{d}r = \mathrm{d}e/\sqrt{2me}$. We deduce the following change of variable formula:

$$\int_{\mathbb{R}^N}\varphi(v)\,\mathrm{d}v = \int_0^\infty |S^{N-1}|\int_{S^{N-1}}\varphi(\sqrt{2e/m}\,\omega)\,(2e/m)^{N/2}\frac{\mathrm{d}e}{2e}\,\mathrm{d}\omega,$$

which applies to any integrable function φ.

Let us discretize the energy levels by introducing the energy step $\varepsilon > 0$ (we point out that ε will remain fixed throughout the paper, and will not tend to zero). We set $E_i = [i\varepsilon,(i+1)\varepsilon[$ and then we consider

$$f_i(t,x,\omega) = \frac{1}{2\varepsilon}\int_{E_i} f(t,x,\sqrt{2e/m}\,\omega)\,(2e/m)^{N/2}\frac{\mathrm{d}e}{2e},$$

which will be a new unknown. Equations for the f_i's are obtained by averaging (5). On the left-hand side, we approach v by $v_i = \sqrt{2i\varepsilon/m}\,\omega$ and the transport term is approximately $(\partial_t + v_i\cdot\nabla_x)f_i$. For the collision term, one has

$$\begin{aligned}&\frac{1}{2\varepsilon}\int_{E_i} Q(f)(t,x,|v|\omega)\,|v|^N\frac{\mathrm{d}e}{2e}\\ &\quad= \frac{1}{2\varepsilon}\int_{E_i}\Bigg(\int_0^\infty\int_{S^{N-1}}\sigma(\sqrt{2e/m}\,\omega,\sqrt{2e'/m}\,\omega')f(\sqrt{2e'/m}\omega')\,(2e'/m)^{N/2}\frac{\mathrm{d}e'}{2e'}\,\mathrm{d}\omega'\\ &\qquad-\int_0^\infty\int_{S^{N-1}}\sigma(\sqrt{2e'/m}\,\omega',\sqrt{2e/m}\,\omega)\,(2e'/m)^{N/2}\frac{\mathrm{d}e'}{2e'}\,\mathrm{d}\omega'\,f(\sqrt{2e/m}\,\omega)\Bigg)\,(2e/m)^{N/2}\frac{\mathrm{d}e}{2e}\end{aligned}$$

$$= \frac{1}{2\varepsilon} \sum_j \int_{E_j} \int_{S^{N-1}} \left(\int_{E_i} \sigma(\sqrt{2e/m}\,\omega, \sqrt{2e'/m}\,\omega') \right.$$
$$\left. \times (2e/m)^{N/2} \frac{de}{2e} \right) f(\sqrt{2e'/m}\,\omega')\,(2e'/m)^{N/2} \frac{de'}{2e'}\,d\omega' - \frac{1}{2\varepsilon} \int_{E_i} f(\sqrt{2e/m}\,\omega)$$
$$\times \left(\sum_j \int_{E_j} \int_{S^{N-1}} \sigma(\sqrt{2e'/m}\,\omega', \sqrt{2e/m}\,\omega)(2e'/m)^{N/2} \frac{de'}{2e'}\,d\omega' \right) (2e/m)^{N/2} \frac{de}{2e}.$$

Then, we suppose that σ does not vary too much as the energy variables (e,e') belong to the set $E_i \times E_j$ and we make the following approximation:

For $e' \in E_j$,

$$\sigma_{ij}(\omega,\omega') \sim \int_{E_i} \sigma(\sqrt{2e/m}\,\omega, \sqrt{2e'/m}\,\omega')(2e/m)^{N/2} \frac{de}{2e},$$

so that $Q(f)$ is replaced by

$$Q(f)_i(\omega) = \sum_j \int_{S^{N-1}} \sigma_{ij}(\omega,\omega') f_j(\omega')\,d\omega' - \Sigma_i(\omega)\, f_i(\omega), \tag{6}$$

where

$$\Sigma_i(\omega) = \sum_j \int_{S^{N-1}} \sigma_{ji}(\omega',\omega)\,d\omega'.$$

These notations lead to the following multigroup kinetic equation:

$$(\partial_t + v_i \cdot \nabla_x) f_i = Q(f)_i. \tag{7}$$

Remark 1: Of course, the subdomains E_i can be defined by using another discretization rule. For instance, one often discretizes the energy range by means of the lethargy $\lambda(e) = \ln(e_{\mathrm{ref}}/e)$ and $E_i = \{e \geqslant 0, \lambda(e) \in [\lambda_i, \lambda_{i+1}[\}$, see Ref. 41.

III. SPLITTING OF THE COLLISION OPERATOR

In this section, we introduce two different splittings of the collision operator into elastic and inelastic parts. Here and in the following "elastic" means that the operator leaves invariant the total number of neutrons on a given energy level. As in Ref. 19, we will see that it is relevant to use a convex combination of these splittings. For convenience, we skip the space dependence, having in mind that the estimates discussed in the following are uniform with respect to x. Besides, we shall only state precisely the assumptions on the cross-sections σ_{ij} and the properties of the collision operators that will be necessary later on; proofs are postponed to the Appendix.

A. First splitting

Let us split the collision operator (6) as follows:

$$Q(f)_i(\omega) = \sum_j \int_{S^{N-1}} (\sigma_{ij}(\omega,\omega') f_j(\omega') - \sigma_{ji}(\omega',\omega) f_i(\omega'))\,d\omega'$$
$$+ \int_{S^{N-1}} \left(\sum_j \sigma_{ji}(\omega',\omega) \right) (f_i(\omega') - f_i(\omega))\,d\omega'. \tag{8}$$

The first operator modifies energy while angle remains unchanged, thus, we refer to it as the inelastic part, denoted by Q_0^{inel}; the second operator modifies the velocity direction while energy is conserved, thus, we call it the elastic part, denoted by Q_0^{el}. Let us set

$$\Gamma_i(\omega',\omega)=\sum_j \sigma_{ji}(\omega',\omega), \quad \Sigma_i(\omega)=\int_{S^{N-1}}\Gamma_i(\omega',\omega)\,\mathrm{d}\omega'$$

then we have

$$Q_0^{\text{el}}(f)_i=\int_{S^{N-1}}\Gamma_i(\omega',\omega)(f_i(\omega')-f_i(\omega))\,\mathrm{d}\omega'=K(f)_i-\Sigma_i f_i.$$

Let us now state the first assumptions concerning the kernel $\sigma_{ij}(\omega,\omega')$:
$(h1)$ First symmetry assumption: $\Sigma_i(\omega)=\int_{S^{N-1}}\Gamma_i(\omega',\omega)\,\mathrm{d}\omega'=\int_{S^{N-1}}\Gamma_i(\omega,\omega')\,\mathrm{d}\omega'$.
In order to derive the coercivity properties of the operator Q_0^{el}, we also require the following hypothesis:

$$(h2)\quad \begin{cases} \text{There exists a sequence of positive reals } (\gamma_i)_{i\in\mathbb{N}} \\ \text{and a constant } M_0 \text{ such that } \gamma_i\leqslant\Gamma_i(\omega',\omega)\leqslant M_0\gamma_i. \end{cases}$$

For technical purposes now, we introduce a sequence $(B_i)_{i\in\mathbb{N}}$ of positive numbers, satisfying:
$(h3)$ Weight assumption: $(B_i)_{i\in\mathbb{N}}$ is such that $\Sigma_i B_i\gamma_i=M_1<\infty$
(it is easy to check that such a sequence always exists). Note that $(h2)$ and $(h3)$ yield

$$\sum_i B_i\int_{S^{N-1}}\Sigma_i(\omega)\mathrm{d}\omega\leqslant M_0M_1.$$

It is worth having in mind the following simple example of the isotropic Boltzmann equation, with typically $B_i=e^{-i}$:

$$\sigma_{ij}(\omega,\omega')=c_ic_jB_i, \quad c_iB_i\in\ell^1. \tag{9}$$

This leads to $\Gamma_i(\omega,\omega')=\|cB\|_{\ell^1}c_i$ and (h2) is fulfilled with $M_0=\|cB\|_{\ell^1}^2$, and $\gamma_i=c_i$.

We now introduce the following functional spaces:

$$\mathbb{E}=\left\{f:\mathbb{N}\times S^{N-1}\to\mathbb{R} \text{ such that } \|f\|_{\mathbb{E}}^2=\sum_i \int_{S^{N-1}}|f_i(\omega)|^2\frac{\Sigma_i(\omega)}{B_i}\mathrm{d}\omega<\infty\right\},$$

$$\mathbb{F}=\left\{f:\mathbb{N}\times S^{N-1}\to\mathbb{R} \text{ such that } \|f\|_{\mathbb{F}}^2=\sum_i \int_{S^{N-1}}|f_i(\omega)|^2\frac{1}{\Sigma_i(\omega)B_i}\mathrm{d}\omega<\infty\right\}.$$

We shall identify the space

$$\mathbb{L}=\left\{f:\mathbb{N}\times S^{N-1}\to\mathbb{R} \text{ such that } \|f\|_{\mathbb{L}}^2=\sum_i \int_{S^{N-1}}|f_i(\omega)|^2\frac{1}{B_i}\,\mathrm{d}\omega<\infty\right\}$$

with its dual when equipped with the inner product

$$(f,g)_{\mathbb{L}}=\sum_i \int_{S^{N-1}}f_i(\omega)g_i(\omega)\frac{1}{B_i}\,\mathrm{d}\omega.$$

Consequently, we note that

$$\left|\sum_i \int_{S^{N-1}} f_i(\omega) g_i(\omega) \frac{1}{B_i} \mathrm{d}\omega\right| \leqslant \|f\|_{\mathbb{E}} \|g\|_{\mathbb{F}}$$

for any $f \in \mathbb{E}$, $g \in \mathbb{F}$ and we can identify $\mathbb{F}$ with the dual $\mathbb{E}'$. We are now ready to establish the main properties of the elastic operator Q_0^{el}.

Proposition 1: Assume that $(h1)$ *holds. Then,* $Q_0^{\mathrm{el}} \in \mathcal{L}(\mathbb{E},\mathbb{F})$ *with* $\|Q_0^{\mathrm{el}}(f)\|_{\mathbb{F}} \leqslant 2\|f\|_E$, *and we have*

(i) Conservation property: $\int_{S^{N-1}} Q_0^{\mathrm{el}}(f)_i \mathrm{d}\omega = 0$ *(at least formally; see Remark 3),*

(ii) Dissipativity property: for all f, g *in* $\mathbb{E}$, *we set* $\mathcal{B}_0(f,g) = -\Sigma_i \int_{S_{N-1}} Q_0^{\mathrm{el}}(f)_i g_i B_i^{-1} \mathrm{d}\omega$. *Then,* $\mathcal{B}_0$ *is bilinear continuous on* $\mathbb{E}$ *and satisfies*

$$\mathcal{B}_0(f,f) = 1/2 \sum_i \int_{S^{N-1}} \int_{S^{N-1}} \Gamma_i(\omega',\omega) |f_i(\omega) - f_i(\omega')|^2 \, B_i^{-1} \, \mathrm{d}\omega' \, \mathrm{d}\omega \geqslant 1/2 \|Q_0^{\mathrm{el}}(f)\|_{\mathbb{F}}^2.$$

(iii) The eigenspace $\mathrm{Ker}(Q_0^{\mathrm{el}})$ *is the space* $\mathcal{E}_0$ *of functions in* $\mathbb{E}$ *which do not depend on the angular variable.*

Remark 2: Under Hypothesis $(h2)$, *one remarks that* $\mathcal{E}_0 = \{f : \mathbb{N} \to \mathbb{R}, \ \Sigma_i f_i^2 \gamma_i B_i^{-1} < \infty\}$ *does not reduce to* $\{0\}$. *For instance, with* $(h2)$–$(h3)$ *it contains* $\{f_i = B_i g_i, \ g \in \mathscr{C}^\infty\} \subset \mathcal{E}_0$. *Indeed, for such as* f, *we get*

$$0 \leqslant \sum_i \int_{S^{N-1}} \Sigma_i \, f_i^2 / B_i \, \mathrm{d}\omega = \sum_i \left(g_i^2 \, B_i \int_{S^{N-1}} \Sigma_i \, \mathrm{d}\omega \right) \leqslant M_1 M_0 \|g\|_{\mathscr{C}^\infty}^2 < \infty.$$

When taking into account time and space variable we will work with sequences of functions $f_i(t,x)$ *that satisfy the corresponding integrability condition.*

Remark 3: Assumption $(h3)$ *also implies that* $\mathbb{F}$ *is a subset of integrable functions, for the measure* $\mathrm{d}\omega \otimes \mathrm{d}i$, *where* $\mathrm{d}i$ *is the counting measure on* $\mathbb{N}$, *since one has*

$$\sum_i \int_{S^{N-1}} |g_i| \mathrm{d}\omega \leqslant \left(\sum_i \int_{S^{N-1}} g_i^2 / (B_i \Sigma_i) \mathrm{d}\omega \right)^{1/2} \left(\sum_i \int_{S^{N-1}} B_i \Sigma_i \, \mathrm{d}\omega \right)^{1/2} \leqslant \|g\|_{\mathbb{F}} (M_0 M_1)^{1/2}.$$

A similar conclusion holds for $f \in \mathbb{E}$ *if one assumes*

$$\sum_i \int_{S^{N-1}} B_i / \Sigma_i \, \mathrm{d}\omega < \infty.$$

For (9), this means that $B/c \in \mathscr{C}^1$.

In order to state a coercivity property in a useful setting, we introduce the following norm:

$$N(f) = \sum_i \int_{S^{N-1}} |f_i(\omega)|^2 \, \frac{\gamma_i}{B_i} \, \mathrm{d}\omega.$$

In view of Hypothesis (h2), it is readily seen that $N(f)$ defines an equivalent norm on $\mathbb{E}$. Actually we have

$$N(f)^2 \leqslant \|f\|_{\mathbb{E}}^2 \leqslant M_0 N(f)^2.$$

Corollary 1: Under Hypotheses $(h1)$–$(h3)$, *the following coercivity estimate*

$$\mathcal{B}_0(f,f) \geqslant N^2(f - \langle f \rangle)$$

holds for any $f \in \mathbb{E}$, *where one denotes* $\langle f \rangle_i = \int_{S^{N-1}} f_i(\omega) \mathrm{d}\omega$.

Remark 4: The adjoint operator of Q_0^{el} *reads*

$$Q_0^{\mathrm{el},*}(g)_i=\int_{S^{N-1}}\Gamma_i(\omega,\omega')g_i(\omega')\mathrm{d}\omega'-\Sigma_i(\omega)g_i(\omega)=\int_{S^{N-1}}\Gamma_i(\omega,\omega')(g_i(\omega')-g_i(\omega))\mathrm{d}\omega.$$

B. Second splitting

On the other hand, we can also introduce the following splitting into elastic and inelastic operators:

$$Q(f)_i=Q_1^{\mathrm{el}}(f)_i+Q_1^{\mathrm{inel}}(f)_i$$

with

$$\begin{aligned}Q_1^{\mathrm{el}}(f)_i&=\sum_j\ \int_{S^{N-1}}\sigma_{ij}(\omega,\omega')(f_j(\omega')-f_j(\omega))\mathrm{d}\omega',\\ Q_1^{\mathrm{inel}}(f)_i&=\sum_j\ \left(\int_{S^{N-1}}\sigma_{ij}(\omega,\omega')\mathrm{d}\omega'\,f_j(\omega)\right)-f_i(\omega)\sum_j\ \int_{S^{N-1}}\sigma_{ji}(\omega',\omega)\mathrm{d}\omega'.\end{aligned}\tag{10}$$

The boundedness of Q_1^{el} relies on the following assumption:

$$(h4)\quad\begin{cases}\text{There exists a constant } M_2 \text{ such that}\\ \displaystyle\sum_j\ \int_{S^{N-1}}\sigma_{ij}(\omega,\omega')B_j\,\mathrm{d}\omega'\leqslant M_2\gamma_iB_i\,.\end{cases}$$

It is worth pointing out that this assumption is a straightforward consequence of $(h2)$–$(h3)$, if we assume the following relation, known as the detailed balance principle,

$$\sigma_{ij}(\omega,\omega')B_j=\sigma_{ji}(\omega',\omega)B_i\,.\tag{11}$$

We also need the

$$(h1')\quad\text{Second symmetry condition: }\int_{S^{N-1}}\sigma_{ij}(\omega',\omega)\mathrm{d}\omega'=\int_{S^{N-1}}\sigma_{ij}(\omega,\omega')\mathrm{d}\omega'.$$

Remark that $(\mathrm{h}1')$ is stronger than $(h1)$, and that $(h4)$ as well as $(h2)$ are fulfilled if we assume $\sigma_{ij}\leqslant M\gamma_iB_i\gamma_j$.

Proposition 2: Assume that $(h1')$, $(h2)$, $(h3)$, $(h4)$ *hold. Then,* $Q_1^{\mathrm{el}}\in\mathcal{L}(\mathbb{E},\mathbb{F})$ *with* $\|Q_1^{\mathrm{el}}(f)\|_{\mathbb{F}}\leqslant 2M_2^{1/2}\|f\|_{\mathbb{E}}$, *and we have*

(i) Conservation property: $\int_{S^{N-1}}Q_1^{\mathrm{el}}(f)_i\,\mathrm{d}\omega=0$,

(ii) For all f, g *we set* $\mathcal{B}_1(f,g)=-\Sigma_i\int_{S^{N-1}}Q_1^{\mathrm{el}}(f)_ig_iB_i^{-1}\,\mathrm{d}\omega$. *Then,* $\mathcal{B}_1$ *is bilinear continuous on* $\mathbb{E}$ *and it satisfies*

$$\begin{aligned}\mathcal{B}_1(f,g)=\frac{1}{2}\sum_{i,j}\ &\int_{S^{N-1}}\int_{S^{N-1}}(f_j(\omega')-f_j(\omega))(\sigma_{ij}(\omega',\omega)g_i(\omega')\\ &-\sigma_{ij}(\omega,\omega')g_i(\omega))B_i^{-1}\mathrm{d}\omega'\,\mathrm{d}\omega.\end{aligned}$$

(iii) $\mathcal{E}_0\subset\mathrm{Ker}(Q_1^{\mathrm{el}})$, *and the following estimate holds:*

$$|\mathcal{B}_1(f,f)|\leqslant M_0\sqrt{2M_2}N(f-\langle f\rangle)^2.$$

Of course functions depending only on the energy variable belong to $\mathrm{Ker}(Q_1^{\mathrm{el}})$; however, the kernel of Q_1^{el} contains much more functions. Note that (iii) is slightly sharper than the estimate obtained by using the norm of Q_1^{el}; it can be improved under more restrictive assumptions on the kernels.

Corollary 2: Under the

$$(h1'') \quad \textit{Strong symmetry assumption: } \sigma_{ij}(\omega,\omega') = \sigma_{ij}(\omega',\omega)$$

and

$$(h2'') \quad \sigma_{ij}(\omega,\omega') \leqslant M\gamma_i B_i \gamma_j \quad \textit{with } \sum_i B_i\gamma_i = M_1 < \infty,$$

the operator Q_0^{el} is self-adjoint and, concerning Q_1^{el}, we have

$$\mathcal{B}_1(f,g) = 1/2 \sum_{i,j} \int_{S^{N-1}} \int_{S^{N-1}} \sigma_{ij}(\omega,\omega')(f_j(\omega') - f_j(\omega))(g_i(\omega') - g_i(\omega)) B_i^{-1} \mathrm{d}\omega' \, \mathrm{d}\omega.$$

As a consequence, if $\langle f \rangle = 0$, then (iii) becomes

$$|\mathcal{B}_1(f,f)| \leqslant M M_1 \, N(f)^2.$$

Remark 5: Notice that $(h1'')$ implies $(h1')$ while $(h2'')$ implies both $(h2)$ and $(h3)$ with $M_0 = M M_1$, and $(h4)$ with $M_2 = M_1$. The bound from below in $(h2)$ is fulfilled if one assumes a similar estimate from below on the σ_{ij}'s.

Remark 6: The previous symmetry conditions are included in

$$\sigma_{ij}(\omega,\omega')B_j = \sigma_{ij}(\omega',\omega)B_j = \sigma_{ji}(\omega',\omega)B_i = \sigma_{ji}(\omega,\omega')B_i, \tag{12}$$

which also implies that Q_1^{el} is self-adjoint. This corresponds to the symmetry assumption used in Ref. 19; *but here we aim at dealing with a larger class of collision kernels.*

Let us go back to the fundamental example (9). Denote $C = \Sigma_i c_i B_i < \infty$. One has in this simple case

$$Q_0^{\mathrm{el}}(f)_i = C c_i (\langle f_i \rangle - f_i),$$
$$Q_1^{\mathrm{el}}(f)_i = c_i B_i \sum_j c_j (\langle f_j \rangle - f_j).$$

Therefore, we get

$$\mathcal{B}_0(f,g) = \sum_{i,j} c_i B_i^{-1} c_j B_j (\langle f_i \rangle \langle g_i \rangle - \langle f_i g_i \rangle),$$
$$\mathcal{B}_1(f,g) = \sum_{i,j} c_i c_j (\langle f_j \rangle \langle g_i \rangle - \langle f_j g_i \rangle).$$

We write $g_i = \langle g_i \rangle + r_i$ where $\langle r_i \rangle = 0$. It yields

$$\mathcal{B}_1(f,g)=\sum_{i,j} c_i c_j(\langle f_j\rangle\langle g_i\rangle-\langle f_j\langle g_i\rangle\rangle-\langle f_j r_i\rangle)$$

$$=-\sum_{i,j} c_i c_j\langle f_j r_i\rangle$$

$$=-\sum_{i,j} c_i c_j\int_{S^{N-1}} f_j r_i\,\mathrm{d}\omega$$

$$=-\int_{S^{N-1}}\left(\sum_j c_j f_j\right)\left(\sum_i c_i r_i\right)\mathrm{d}\omega.$$

If g lies in the orthogonal set of $\mathrm{Ran}(Q_1^{\mathrm{el}})$, we deduce that $\Sigma_i c_i r_i(\omega)$ vanishes for almost all $\omega\in S^{N-1}$.

Remark 7: The adjoint operator of Q_1^{el} is given by

$$Q_1^{\mathrm{el},*}(g)_i=\sum_j \int_{S^{N-1}}\sigma_{ji}(\omega',\omega)(g_j(\omega')-g_j(\omega))\frac{B_i}{B_j}\mathrm{d}\omega'.$$

In particular, we note that, if relation (11) holds, then Q_1^{el} is a self-adjoint operator.

C. Combination of the splitting

From now on, we assume that $(h1')$, $(h2)$, $(h3)$, $(h4)$ hold and we denote by (H) this set of hypotheses. The idea will be to combine Q_1^{el} with Q_0^{el} so that the coercivity of the latter compensates the lack of positivity of the former; we are thus able to preserve the crucial dissipation properties. Let us consider the following elastic operator, obtained as a convex combination of Q_0^{el} and Q_1^{el}; for $\theta\in[0,1]$, we set

$$Q_\theta=\theta Q_1^{\mathrm{el}}+(1-\theta)Q_0^{\mathrm{el}}.$$

One deduces from Corollary 1 and Proposition 2 that

$$\mathcal{B}_\theta(f,f)=-\sum_i \int_{S^{N-1}} Q_\theta(f)_i f_i B_i^{-1}\,\mathrm{d}\omega\geqslant(1-\theta(1+M_0\sqrt{2M_2}))N(f-\langle f\rangle)^2$$

holds for any $f\in\mathbb{E}$. We are thus led to the following statement.

Proposition 3: Let $\theta\in[0,(1+M_0\sqrt{2M_2})^{-1}[$. Then, there exists a constant $\kappa_\theta>0$ such that, for any $f\in\mathbb{E}$, we have

$$\mathcal{B}_\theta(f,f)\geqslant\kappa_\theta N(f-\langle f\rangle)^2.$$

Consequently, the set of equilibria $\mathcal{E}_\theta=\mathrm{Ker}(Q_\theta)$ coincides with $\mathcal{E}_0$ (the set of functions depending only on the energy level). If one assumes $(h1'')$ and $(h2'')$, the domain for θ enlarges to $[0,(1+M_0)^{-1}[$.

One may also establish the following Fredholm alternative.

Proposition 4: For any $h\in\mathbb{F}$ the problem to find $f\in\mathbb{E}$ such that $Q_\theta(f)=h$ has a solution if and only if $\langle h\rangle=0$. The solution is unique in $\mathbb{E}_0=\{f\in\mathbb{E}$ such that $\langle f\rangle=0\}$ and satisfies

$$N(f)\leqslant(1/\sqrt{\kappa_\theta})\|h\|_{\mathbb{F}}.$$

Proof: Since the operator Q_θ is clearly conservative, the condition of null average on the data h is necessary. The problem recasts into the following variational formulation:

$$\forall \varphi \in \mathbb{E}_0, \quad \mathcal{B}_\theta(f,\varphi)=\sum_i \int_{S^{N-1}} h_i \varphi_i B_i^{-1}\, \mathrm{d}\omega = (h,\varphi)_{\mathrm{L}}$$

and we conclude by applying the Lax–Milgram theorem. □

Of course, one has a similar statement for the adjoint operator: Q_θ^* is defined by

$$Q_\theta^* = \theta Q_1^{\mathrm{el},*} + (1-\theta) Q_0^{\mathrm{el},*},$$

and fulfills the same coercivity property as Q_θ with the same constant of coercivity, since

$$\mathcal{B}_\theta(f,f) = -\sum_i \int_{S^{N-1}} Q_\theta^*(f)_i f_i B_i^{-1}\, \mathrm{d}\omega.$$

Therefore we have

Corollary 3: For any $h \in \mathbb{F}$ there exists $f \in \mathbb{E}$ such that $Q_\theta^*(f)=h$ if and only if $\langle h \rangle = 0$. Moreover, there exists a unique such function in $\mathbb{E}_0=\{f \in \mathbb{E}$ such that $\langle f \rangle = 0\}$, and this solution satisfies

$$N(f) \leqslant (1/\sqrt{\kappa_\theta}) \|h\|_{\mathbb{F}}.$$

IV. FORMAL APPROACH

The starting point of the asymptotic study is the following rescaled equation:

$$\partial_t f_i^\eta + \frac{1}{\eta} v_i \cdot \nabla_x f_i^\eta = \frac{1}{\eta^2} (Q^\eta(f^\eta))_i. \tag{13}$$

Precisely, we consider the situation where the mean free path $\eta > 0$ is small at time scale of order $1/\eta$. On the other hand, we assume that the collision operator Q^η splits as follows:

$$Q^\eta(f) = Q_\theta(f) + \eta^2 Q_\theta^{\mathrm{inel}}(f),$$

which means that inelastic collisions are of order η^2 compared to the elastic ones. This agrees with the fact that dominant scattering events are elastic. Of course, in this splitting θ is fixed and cannot be too small compared to η. In particular, it is also required that θ belongs to the range which guarantees the coercivity of the operator Q_θ, see Proposition 3. Our aim is to describe the asymptotic behavior of the solutions of (13) as $\eta \to 0$. We will obtain a set of diffusion equations, which can be viewed as a semidiscrete (with respect to the energy) version of the SHE-system of Ref. 19 for the limit macroscopic density with a coupling of the energy levels due to the action of the operator Q_1^{el} and/or the inelastic terms.

A. Formal Hilbert expansion

We can guess the limit behavior by inserting the formal ansatz

$$f^\eta = f^0 + \eta f^1 + \eta^2 f^2 + \cdots$$

into (13) and then we identify the terms that arise with the same power of η. As usual, the η^{-2} terms lead to

$$Q_\theta(f^0) = 0,$$

which means, by Proposition 3, that $(f^0)_i(\omega) = \rho_i \in \mathcal{E}_0$ does not depend on the angular variable. Hence, one expects that the asymptotic limit is entirely determined in terms of ''macroscopic'' quantities. Next, the η^{-1} equation reads

$$Q_\theta(f^1) = v \cdot \nabla_x \rho,$$

while the η^0 equation is

$$Q_\theta(f^2)+Q_\theta^{\text{inel}}(\rho)=v\cdot\nabla_x f^1+\partial_t\rho.$$

Integrating with respect to ω, we are led to the following relation:

$$\partial_t\rho_i+\operatorname{div}_x\left(\int_{S^{N-1}}\sqrt{2e_i/m}\,\omega f_i^1(\omega)\mathrm{d}\omega\right)=\int_{S^{N-1}}Q_\theta^{\text{inel}}(\rho)\mathrm{d}\omega. \tag{14}$$

The usual strategy consists in inverting the η^{-1} equation; one expects in this way to determine the current $\int_{S^{N-1}}\sqrt{2e_i/m}\,\omega f_i^1(\omega)\mathrm{d}\omega$ in the previous equation as a linear function of $\nabla_x\rho$, i.e., a Fick's relation. The difficulty of this method here comes from the action of the operator Q_1^{el} which mixes the energy levels. In particular, if ρ_i depends only on the energy and $f_i(\omega)$ depends on the two variables, in general one has

$$\begin{aligned}Q_1(\rho f)_i&=\sum_j\int_{S^{N-1}}\sigma_{ij}(\omega,\omega')\rho_j(f_j(\omega')-f_j(\omega))\mathrm{d}\omega'\\&\neq\rho_i Q_1(f)_i\\&=\rho_i\sum_j\int_{S^{N-1}}\sigma_{ij}(\omega,\omega')(f_j(\omega')-f_j(\omega))\mathrm{d}\omega'\end{aligned}$$

[while $Q_0(\rho f)_i=\rho_i Q_0(f)_i$]. However, we can solve the problem as follows. Let us define $\overrightarrow{\chi^i}\in(\mathbb{E}_0)^N$ solution of

$$Q_\theta(\overrightarrow{\chi^i})_{i_0}=-v_{i_0}\delta_{i_0 i},$$

where $\delta_{i_0 i}=1$ if $i=i_0$, and 0 if $i\neq i_0$. The equation has to be understood componentwise, and this definition makes sense thanks to Proposition 4 (since $\int_{S^{N-1}}\omega\,\mathrm{d}\omega=0$). Then one checks that

$$f_{i_0}^1=\sum_i\overrightarrow{\chi}_{i_0}^i\cdot\nabla_x\rho_i$$

provides a solution to the η^{-1} equation. Plugging this expression into (14) gives

$$\begin{aligned}\partial_t\rho_{i_0}-\nabla_x\left(\sum_i D_{i_0 i}\nabla_x\rho_i\right)&=q(\rho)_{i_0},\\q(\rho)_{i_0}&=\int_{S^{N-1}}[Q_\theta^{\text{inel}}(\rho)]_{i_0}\mathrm{d}\omega,\\D_{i_0 i}&=-\int_{S^{N-1}}v_{i_0}\otimes\overrightarrow{\chi}_{i_0}^i\mathrm{d}\omega,\end{aligned}$$

where $\otimes$ stands for the tensor product in $\mathbb{R}^N$: for $(a_1,\ldots,a_N)$ and $(b_1,\ldots,b_N)$ in $\mathbb{R}^N$, $a\otimes b$ is the $N\times N$ matrix with components $a_\alpha b_\beta$. We observe in the limit equation a coupling between the energy levels, both from the diffusion matrix and from the right-hand side.

A possible strategy to justify these computations would be to start from a solution ρ of the expected limit equation (which has to be studied independently), and to define successively f^1, f^2 in terms of ρ as solutions of the η^{-1} and η^0 equations, respectively. It remains to estimate the remainder $r^\eta=f^\eta-(\rho+\eta f^1+\eta^2 f^2)$. The drawback of this method is that it is known to require some regularity on ρ, thus on the coefficients. Such an assumption can be unrealistic for neutron transport since the physical properties of the media interacting with the neutrons are usually highly

heterogeneous. On the other hand, it could be quite delicate to carry out this strategy in the full generality considered here. Therefore, let us instead develop a duality approach, which will be close to our actual method of proof.

B. Duality interpretation

Let us assume that f^η converges to some f^0 in a suitable sense. Multiplying by η^2 and taking the limit $\eta\to 0$ in (13), we recover

$$Q_\theta(f^0)_i=0, \quad \forall i\in\mathbb{N},$$

and thus $f_i^0(t,x,\omega)=\rho_i(t,x)$.

We introduce the following macroscopic quantities

$$\begin{aligned} &\text{density of } i\text{th energy level:} \quad \rho_i^\eta(t,x)=\int_{S^{N-1}} f_i^\eta(t,x,\omega)\mathrm{d}\omega,\\ &\text{current of } i\text{th energy level:} \quad J_i^\eta(t,x)=\frac{1}{\eta}\int_{S^{N-1}}|v_i|\omega f_i^\eta(t,x,\omega)\mathrm{d}\omega. \end{aligned} \tag{15}$$

In view of the penalization of the collision term, one expects that f^η tends to belong to the kernel of Q_θ, therefore it is mainly given by its macroscopic part ρ^η, up to a formally small remainder. Hence, let us write a first-order expansion of f^η as follows:

$$f_i^\eta(t,x,\omega)=\rho_i^\eta(t,x)+\eta g_i^\eta(t,x,\omega)$$

so that $\rho^\eta\in\mathrm{Ker}(Q_\theta)$ and

$$J_i^\eta(t,x)=\int_{S^{N-1}}|v_i|\omega g_i^\eta(t,x,\omega)\mathrm{d}\omega.$$

Integrate Eq. (13) with respect to ω. Since the operator Q_θ has null average on S^{N-1}, we get for all $i\in\mathbb{N}$:

$$\partial_t\rho_i^\eta+\nabla_x\cdot J_i^\eta=\int_{S^{N-1}} Q_\theta^{\mathrm{inel}}(f^\eta)_i\mathrm{d}\omega,$$

which is the η-dependent version of the integrated η^0 equation in the above-mentioned formal expansion. As η goes to 0, we are formally led to the continuity equation

$$\partial_t\rho_i+\nabla_x\cdot J_i=\int_{S^{N-1}} Q_\theta^{\mathrm{inel}}(\rho)_i\mathrm{d}\omega.$$

It remains to find the relation between the limit current J and ρ.

Multiply (13) by some $\eta\varphi_i(\omega)$. We get

$$\sum_i \frac{1}{\eta}\int_{S^{N-1}} Q_\theta(f^\eta)_i\varphi_i\mathrm{d}\omega=\sum_i \int_{S^{N-1}}(v\cdot\nabla_x f^\eta)_i\varphi_i\mathrm{d}\omega+\eta\sum_i \int_{S^{N-1}}\partial_t f_i^\eta\varphi_i\mathrm{d}\omega,$$

and therefore

$$\sum_i \int_{S^{N-1}} Q_\theta(g^\eta)_i\varphi_i\mathrm{d}\omega=\sum_i\left(\int_{S^{N-1}}|v_i|\omega\varphi_i\mathrm{d}\omega\right)\cdot\nabla_x\rho_i^\eta+R^\eta, \tag{16}$$

where R^η is formally of order $\mathcal{O}(\eta)$.

Suppose that, for i_0 fixed in $\mathbb{N}$, we are able to find the auxiliary function $B_i\chi_i^{i_0}(\omega)\in(\mathbb{E}_0)^N$, that solves

$$Q_\theta^*(B_\cdot\chi_\cdot^{i_0})_i=v_{i_0}B_{i_0}\delta_{i_0 i}=\sqrt{2e_{i_0}/m}B_{i_0}\omega\delta_{i_0 i}. \tag{17}$$

Since v_{i_0} lies in $\mathbb{R}^N$, Eq. (17) holds for the N scalar equations with right-hand sides ω_α for $\alpha\in\{1,\ldots,N\}$. Remarking that

$$\int_{S^{N-1}}\omega\,\mathrm{d}\omega=0,$$

the existence of χ^{i_0} is given by Corollary 3.

Hence, for the test function $\varphi_i(\omega)$, we choose the components of $\chi_i^{i_0}(\omega)$ and (16) becomes

$$\sum_i\int_{S^{N-1}}g_i^\eta Q_\theta^*(B\chi^{i_0})_iB_i^{-1}\,\mathrm{d}\omega=\sum_i\left(\int_{S^{N-1}}|v_i|\chi_i^{i_0}\otimes\omega\,\mathrm{d}\omega\right)\cdot\nabla_x\rho_i^\eta+\mathcal{O}(\eta), \tag{18}$$

with

$$\sum_i\int_{S^{N-1}}g_i^\eta Q_\theta^*(B\chi^{i_0})_iB_i^{-1}\,\mathrm{d}\omega=\sum_i\int_{S^{N-1}}g_i^\eta\sqrt{2e_{i_0}/m}\,\omega\delta_{i_0 i}\,\mathrm{d}\omega=\sqrt{2e_{i_0}/m}\int_{S^{N-1}}\omega g_{i_0}^\eta\,\mathrm{d}\omega=J_{i_0}^\eta.$$

Here, we used the following fact:

$$\begin{aligned}\sum_i\int_{S^{N-1}}Q_\theta(g^\eta)_i\chi_i^{i_0}\,\mathrm{d}\omega&=(Q_\theta(g^\eta),B\chi^{i_0})_{\mathbb{L}}\\&=\sum_i\int_{S^{N-1}}g_i^\eta Q_\theta^*(B\chi^{i_0})_iB_i^{-1}\,\mathrm{d}\omega.\end{aligned}$$

Thus, passing to the limit $\eta\to0$ in (18), we are led to

$$J_{i_0}(t,x)=-\sum_i D_{i_0 i}\nabla_x\rho_i(t,x), \tag{19}$$

where the matrix D is defined through the auxiliary function χ by

$$D_{i_0 i}=-|v_i|\int_{S^{N-1}}\chi_i^{i_0}\otimes\omega\,\mathrm{d}\omega\in\mathcal{M}_{N\times N}, \tag{20}$$

where $\mathcal{M}_{N\times N}$ stands for the space of $N\times N$ matrices.

The formal limit of (13) is therefore the following macroscopic equation:

$$\partial_t\rho-\nabla_x\cdot(D(x)\nabla_x\rho)=q(\rho), \tag{21}$$

where the unknown is the sequence $\rho(t,x)=\{\rho_i(t,x),i\in\mathbb{N}\}$, D is given by (17), (20) and the right-hand side by

$$q(\rho)_i=\int_{S^{N-1}}Q_\theta^{\mathrm{inel}}(\rho)_i\,\mathrm{d}\omega=\sum_j\Lambda_{ij}\rho_j-\tilde{\Sigma}_i\rho_i, \tag{22}$$

with

$$\Lambda_{ij}=\int_{S^{N-1}}\int_{S^{N-1}}\sigma_{ij}(\omega,\omega')\mathrm{d}\omega\,\mathrm{d}\omega',$$

$$\tilde{\Sigma}_i=\sum_j\int_{S^{N-1}}\int_{S^{N-1}}\sigma_{ji}(\omega',\omega)\mathrm{d}\omega\,\mathrm{d}\omega'=\sum_j\Lambda_{ji}.$$

It is also worth splitting the matrix D as follows. The properties discussed on Q_0^{el} allow us to define a unique $\varphi^{i_0}(\omega)\in\mathbb{R}^N$ verifying

$$(1-\theta)Q_0^*(B_\cdot\varphi^{i_0}\delta_{i_0\cdot})_i=v_{i_0}B_{i_0}\delta_{i_0 i},$$

with $\int_{S^{N-1}}\varphi^{i_0}(\omega)\mathrm{d}\omega=0$. Then, we split $\chi_i^{i_0}=\varphi^{i_0}\delta_{i_0 i}+\overline{\chi}_i^{i_0}$, where

$$Q_\theta^*(B_\cdot\overline{\chi}_\cdot^{i_0})_i=-\theta Q_1^*(B_\cdot\varphi^{i_0}\delta_{i_0\cdot})_i.$$

In this way, we can rewrite

$$D_{i_0 i}=d_{i_0}\delta_{i_0 i}+\Delta_{i_0 i},$$
$$d_{i_0}=-|v_{i_0}|\int_{S^{N-1}}\varphi^{i_0}\otimes\omega\,\mathrm{d}\omega,$$
$$\Delta_{i_0 i}=-|v_i|\int_{S^{N-1}}\overline{\chi}_i^{i_0}\otimes\omega\,\mathrm{d}\omega.$$

Hence, one gets $[D\nabla_x\rho]_{i_0}=d_{i_0}\nabla_x\rho_{i_0}+\Sigma_i\Delta_{i_0 i}\nabla_x\rho_i$. Of course, we can verify readily that this definition of the diffusion matrix coincides with the one obtained in the previous section.

This limit equation (21) appears as a semidiscrete (in energy) SHE-model with a coupling of the energy levels. Actually, one obtains a hierarchy of possible limit systems:

(1) A system of uncoupled diffusion equations with respect to the space variable, energy being only a parameter. This arises when inelastic terms are negligible and $\theta=0$.

(2) A system of diffusion equations with a coupling of the energy levels through zeroth-order terms. This arises with $\theta=0$ and treating inelastic processes as a perturbation. Diffusivity remains locally defined (with respect to energy) and the coupling describes gain/loss at a given energy level due to inelastic collisions.

(3) A system of diffusion equations with a strong coupling, from both zeroth-order terms and diffusion currents which are now nonlocal: energy exchanges during the collisions induce diffusive effects.

C. Fundamental properties of the diffusivity

We are naturally led to discuss some properties of the diffusivity D. To this end, one introduces the following Hilbert space of vector-valued sequences:

$$\mathbb{H}=\left\{\Phi:\mathbb{N}\to\mathbb{R}^N;\sum_i|\Phi_i|^2\frac{2\varepsilon i}{m\gamma_i B_i}<+\infty\right\}.$$

We shall identify $\mathscr{\ell}=\{\Phi:\mathbb{N}\to\mathbb{R}^N,\Sigma_i|\Phi_i|^2B_i^{-1}<\infty\}$ with its dual; accordingly, the dual of $\mathbb{H}$ reads

$$\mathbb{H}'=\left\{J:\mathbb{N}\to\mathbb{R}^N;\sum_i|J_i|^2\frac{m\gamma_i}{2\varepsilon i B_i}<+\infty\right\},$$

with the duality relation

$$\langle J,\Phi\rangle_{\mathbb{H}',\mathbb{H}}=\left(J\sqrt{\frac{mc_i}{2\varepsilon i}},\Phi\sqrt{\frac{2\varepsilon i}{mc_i}}\right)_{\ell^2}=\sum_i J_i\Phi_i B_i^{-1}.$$

Lemma 1: Assume (H). *Let us set*

$$\mathcal{D}(\Psi,\Phi)=\sum_{i,j} D_{ij}\Psi_j\cdot\Phi_i B_i^{-1}\quad\forall\Phi,\Psi\in\mathbb{H}.$$

Then,
(i) $\mathcal{D}$ *is a bilinear continuous form on* $\mathbb{H}$;
(ii) $\mathcal{D}$ *is positive-definite (symmetric as soon as* Q_θ *is a self-adjoint operator). Furthermore, there exists a constant* $c>0$ *such that for all* $\Phi\in\mathbb{H}$,

$$\mathcal{D}(\Phi,\Phi)\geqslant c\|\Phi\|_{\mathbb{H}}^2.$$

Proof: Assuming (H), one associates to Φ in the weighted ℓ^2 space $\mathbb{H}$, the function

$$\phi:\mathbb{N}\times S^{N-1}\to\mathbb{R}$$

$$(i,\omega)\mapsto\phi_i(\omega)=v_i\cdot\Phi_i=\omega\cdot\sqrt{2\varepsilon i/m}\Phi_i.$$

One remarks that ϕ lies in $\mathbb{F}_0$, and $\|\phi\|_{\mathbb{F}}$ provides a norm equivalent to the natural norm on $\mathbb{H}$ (by using $(h2)$). Therefore, Proposition 4 allows us to define the mapping

$$K:\mathbb{H}\to\mathbb{E}_0$$

$$\Phi\mapsto K^\Phi,$$

with $Q^*(K^\Phi)_i(\omega)=v_i\cdot\Phi_i=\phi_i(\omega)$, i.e., $K^\Phi=Q^{*-1}(\phi)$. Clearly, K is a bounded linear operator from $\mathbb{H}$ to $\mathbb{E}$.

With these notations, we have the following relation, which will be proved later on,

$$B_j^{-1}K_j^\Phi(\omega)=\sum_i \chi_j^i(\omega)\cdot\Phi_i B_i^{-1}. \tag{23}$$

From the definition of D_{ij}, and (23), we can rewrite $\mathcal{D}$ as follows:

$$\begin{aligned}\mathcal{D}(\Psi,\Phi)&=\sum_{ij} D_{ij}\Psi_j\cdot\Phi_i B_i^{-1}\\&=-\sum_{ij}\int_{S^{N-1}}\chi_j^i(\omega)\cdot\Phi_i B_i^{-1}v_j\cdot\Psi_j\,d\omega\\&=-\sum_j\int_{S^{N-1}}\left(\sum_i\chi_j^i(\omega)\cdot\Phi_i B_i^{-1}\right)v_j\cdot\Psi_j\,d\omega\\&=-\sum_j\int_{S^{N-1}}B_j^{-1}K_j^\Phi(\omega)\psi_j(\omega)d\omega.\end{aligned}$$

Hence we have

$$\mathcal{D}(\Psi,\Phi)=-\sum_i\int_{S^{N-1}}\psi_i(\omega)Q^{*-1}(\phi)_i(\omega)B_i^{-1}\,d\omega=-\sum_i\left(\Psi_i\cdot\left(\int_{S^{N-1}}v_iK_i^\Phi\,d\omega\right)B_i^{-1}\right). \tag{24}$$

The lemma follows, since the first expression recasts as

$$-\sum_i \int_{S^{N-1}} Q^*(K^\Psi)_i(\omega) K_i^\Phi(\omega) B_i^{-1}\, d\omega = \mathcal{B}_\theta(K^\Phi, K^\Psi),$$

which easily leads to the conclusion by using Corollary 3.

We are thus left with the task of proving (23). However, this is a simple consequence of the linearity of Q^*, which implies that summation over i commutes with the action of this operator. We are thus able to show that Q^* acts on the right-hand side of (23) as follows:

$$Q^*\left(\sum_i B_\cdot \chi^i_\cdot \cdot \Phi_i B_i^{-1}\right)_j = \sum_i Q^*(B_\cdot \chi^i_\cdot)_j \cdot \Phi_i B_i^{-1} = \sum_i v_i B_i \delta_{ij} \cdot \Phi_i B_i^{-1} = v_j \cdot \Phi_j = \phi_j = Q^*(K^\Phi)_j .$$

□

From Lemma 1, we can deduce the following claim which will give a precise meaning to the current relation (19). It will play a key role in our rigorous analysis.

Corollary 4: We can define a linear, continuous and invertible mapping $\mathcal{J}:\mathbb{H}\to\mathbb{H}'$ *such that, for any* Φ *and* Ψ *in* $\mathbb{H}$ *one has*

$$\mathcal{D}(\Phi,\Psi) = -(\mathcal{J}(\Phi),\Psi)_{\mathcal{E}} = -\sum_i \mathcal{J}(\Phi)_i \Psi_i B_i^{-1}.$$

Proof: For any $\Phi\in\mathbb{H}$, the Riesz theorem defines a unique $\mathcal{J}(\Phi)\in\mathbb{H}'$, such that $\mathcal{D}(\Phi,\Psi) = -(\mathcal{J}(\Phi),\Psi)_{\mathcal{E}}$ for any $\Psi\in\mathbb{H}$. The corresponding mapping $\mathcal{J}:\mathbb{H}\to\mathbb{H}'$ is of course linear and continuous. Conversely, let $J\in\mathbb{H}'$. The Lax–Milgram theorem applies to solve the variational problem

find $\Phi\in\mathbb{H}$ *such that, for all* $\Psi\in\mathbb{H}$ *one has* $\mathcal{D}(\Phi,\Psi) = -(J,\Psi)_{\mathcal{E}}$.

By Proposition 4, this problem admits a unique solution $\Phi\in\mathbb{H}$ which satisfies, by its definition, $\mathcal{J}(\Phi) = J$. □

This statement will allow us to interpret the current equation (19) in a duality sense by $J = \mathcal{J}(\nabla_x\rho)$. Accordingly, one expects that J lies in $L^2(\mathbb{R}_t^+\times\mathbb{R}_x^N;\mathbb{H}')$ and $\nabla_x\rho\in L^2(\mathbb{R}_t^+\times\mathbb{R}_x^N;\mathbb{H})$. It is worth noting this gain in "regularity," both in the space and energy variables on the density, since this property is not guaranteed in general for ρ^η, for $\eta>0$. This is a usual fact when dealing with diffusion approximation, see for instance Refs. 29 and 20; the noticeable point here is that this effect also applies to the energy variable.

V. RIGOROUS DERIVATION

This section is devoted to the rigorous study of the asymptotic behavior as η goes to 0 of the solution f^η of the kinetic equation

$$\begin{aligned} &\partial_t f_i^\eta + \frac{1}{\eta} v_i \cdot \nabla_x f_i^\eta = \frac{1}{\eta^2}(Q_\theta(f^\eta))_i \quad \text{in } \mathbb{R}_t^+\times\mathbb{R}_x^N\times\mathbb{N}_i\times S_\omega^{N-1}, \\ &f^\eta(t=0) = F_I^\eta . \end{aligned} \tag{25}$$

In order to take into account time and space variables, one needs to define again some functional spaces, based on the previous ones. We set

$$\mathcal{L}^2 = \left\{ f:\mathbb{R}_x^N\times\mathbb{N}_i\times S_\omega^{N-1}\to\mathbb{R},\ \sum_i \int_{\mathbb{R}^N}\int_{S^{N-1}} f_i^2\ B_i^{-1}\, d\omega\, dx < \infty \right\}.$$

It is nothing but the L^2 space on $\mathbb{R}^N\times\mathbb{N}\times S^{N-1}$ endowed with the measure $\mathrm{d}x\otimes(B_i^{-1}\,\mathrm{d}i)\otimes\mathrm{d}\omega$, where $\mathrm{d}i$ stands for the counting measure on $\mathbb{N}$. Accordingly, we also set

$$\mathcal{E}=\left\{f:\mathbb{R}^N_x\times\mathbb{N}_i\times S^{N-1}_\omega\to\mathbb{R},\quad \sum_i\int_{\mathbb{R}^N}\int_{S^{N-1}} f_i^2\ \frac{\gamma_i}{B_i}\mathrm{d}\omega\,\mathrm{d}x<\infty\right\}=L^2(\mathbb{R}^N;\mathbb{E})$$

and

$$\mathcal{F}=\left\{f:\mathbb{R}^N_x\times\mathbb{N}_i\times S^{N-1}_\omega\to\mathbb{R},\quad \sum_i\int_{\mathbb{R}^N}\int_{S^{N-1}} f_i^2\ \frac{1}{\gamma_i B_i}\mathrm{d}\omega\,\mathrm{d}x<\infty\right\}=L^2(\mathbb{R}^N;\mathbb{F}).$$

Similarly, for vector-valued macroscopic quantities, independent on the angular variable, we set

$$\mathcal{H}=\left\{\Phi:\mathbb{R}^N_x\times\mathbb{N}_i\to\mathbb{R}^N,\quad \sum_i\int_{\mathbb{R}^N}|\Phi_i|^2\ \frac{2\varepsilon i}{m\gamma_i B_i}\mathrm{d}x<\infty\right\}=L^2(\mathbb{R}^N;\mathbb{H})$$

and

$$\mathcal{H}'=\left\{J:\mathbb{R}^N_x\times\mathbb{N}_i\to\mathbb{R},\quad \sum_i\int_{\mathbb{R}^N}|J_i|^2\ \frac{m\gamma_i}{2\varepsilon i B_i}dx<\infty\right\}=L^2(\mathbb{R}^N;\mathbb{H}'),$$

which is the dual of $\mathcal{H}$ when one identifies $L^2(\mathbb{R}^N,\not{\ell})=L^2(\mathbb{R}^N\times\mathbb{N},\mathrm{d}x\otimes B_i^{-1}\mathrm{d}i)$ with its dual, namely

$$\langle J,\Phi\rangle_{\mathcal{H}',\mathcal{H}}=\sum_i\int_{\mathbb{R}^N}\Phi_i\cdot J_i B_i^{-1}\,\mathrm{d}x.$$

We shall not detail the existence theory for the transport equation (25). With some maybe stronger assumptions on the cross sections, this can be done by means of semigroups theory. We can also use some monotonicity argument, following Petterson.[36] Instead, we shall assume from now on that there exists a function $f^\eta\in C^0(\mathbb{R}^+;\mathcal{L}^2)\cap L^\infty(\mathbb{R}^+;\mathcal{E})$ satisfying the following weak formulation of (25)

$$-\int f^\eta\partial_t\varphi\ \ B^{-1}\,\mathrm{d}\mu-\frac{1}{\eta}\int f^\eta v\cdot\nabla_x\varphi\ \ B^{-1}\,\mathrm{d}\mu+\left[\int f^\eta\varphi\ \ B^{-1}\,\mathrm{d}\nu\right]_0^T=\frac{1}{\eta^2}\int Q_\theta(f^\eta)\varphi\ \ B^{-1}\,\mathrm{d}\mu. \tag{26}$$

Here, $\mathrm{d}\mu$ indicates integration over $(0,T)\times\mathbb{R}^N\times\mathbb{N}\times S^{N-1}$ with the measure $\mathrm{d}t\otimes\mathrm{d}x\otimes\mathrm{d}i\otimes\mathrm{d}\omega$ while $\mathrm{d}\nu$ has the same meaning on $\mathbb{R}^N\times\mathbb{N}\times S^{N-1}$ with the measure $\mathrm{d}x\otimes\mathrm{d}i\otimes\mathrm{d}\omega$. Relation (26) holds for any φ in an appropriate space of admissible test functions $\mathfrak{D}$. In particular, it makes sense for $\varphi\in L^1_{\mathrm{loc}}(\mathbb{R}^+;\mathcal{E})$ such that $\partial_t\varphi$ and $\nabla_x\cdot(v\varphi)$ belong to $L^1_{\mathrm{loc}}(\mathbb{R}^+;\mathcal{L}^2)$. It is worth remarking that a sequence defined by a finite number of non zero functions $\varphi_i(t,x,\omega)$ lying in $C^1_0([0,T]\times\mathbb{R}^N;L^\infty(S^{N-1}))$ is admissible.

Remark 8: If one assumes that $0<\gamma_i\leqslant C<+\infty$, we obtain the inclusions $\mathbb{F}\subset\mathbb{L}\subset\mathbb{E}$, and therefore Q_θ can be viewed as a bounded operator on $\mathcal{L}^2$, with values in $\mathcal{L}^2$, and existence-uniqueness is easy to be established. Of course, the problem for $\eta>0$ fixed and most of our convergence analysis become easier if one deals with a finite number of energy groups.

Then, we can now state our main result.

Theorem 1: *Suppose (H) and let F_I^η be bounded in $\mathcal{L}^2$. Then, $\rho^\eta=\int_{S^{N-1}}f^\eta\,\mathrm{d}\omega$ converges weakly-$*$ in $L^\infty(0,T;L^2(\mathbb{R}^N\times\mathbb{N};B^{-1}\,\mathrm{d}i\otimes\mathrm{d}x))$ (and in $C^0([0,T],L^2(\mathbb{R}^N\times\mathbb{N};B^{-1}\,\mathrm{d}i\otimes\mathrm{d}x))$-weak) to ρ and $J^\eta=\int_{S^{N-1}}\sqrt{2\varepsilon i/m}\,\omega\ \ f^\eta\,\mathrm{d}\omega$ converges weakly-$*$ in $L^2(0,T;\mathcal{H}')$ to J (see (27) in the following). These limits satisfy*

$$\partial_t \rho + \mathrm{div}_x J = 0,$$
$$\nabla_x \rho \in L^2(0,T;\mathcal{H}), \text{ and } \mathcal{J}(\nabla_x \rho) = J.$$

The proof naturally falls into four steps.

Step 1: A priori estimates and weak convergences.

The main estimates on f^η are obtained by formally multiplying Eq. (25) by f^η/B and integrating. It yields

$$\|f^\eta(t)\|^2_{\mathcal{L}^2} + \frac{2}{\eta^2}\int_0^t \int_{\mathbb{R}^N} \mathcal{B}_\theta(f^\eta, f^\eta)\,\mathrm{d}x\,\mathrm{d}s = \|F_I^\eta\|^2_{\mathcal{L}^2}.$$

Therefore, the coercivity of $\mathcal{B}_\theta$ allows us to estimate $\|f^\eta\|_{\mathcal{L}^2}$ and $(1/\eta)\,N(f^\eta - \rho^\eta) = N(g^\eta)$ and thus leads to the following statement.

Lemma 2: Suppose that (H) *holds and let* F_I^η *be bounded in* $\mathcal{L}^2$. *Then,*

(i) f^η *is bounded in* $L^\infty(\mathbb{R}_t^+;\mathcal{L}^2)$, *with* $\|f^\eta(t)\|^2_{\mathcal{L}^2} \leqslant \|F_I^\eta\|^2_{\mathcal{L}^2} \leqslant C$.

(ii) $g^\eta = (f^\eta - \rho^\eta)/\eta$ *is bounded in* $L^2(\mathbb{R}_t^+;\mathcal{E})$,

(iii) $\rho_i^\eta(t,x) = \int_{S^{N-1}} f_i^\eta(t,x,\omega)\,\mathrm{d}\omega$ *is bounded in* $L^\infty(\mathbb{R}_t^+;L^2(\mathbb{R}^N\times\mathbb{N},\mathrm{d}x\otimes B_i^{-1}\,\mathrm{d}i))$,

(iv) $J_i^\eta(t,x) = 1/\eta \int_{S^{N-1}} v_i f^\eta(t,x,\omega)\,\mathrm{d}\omega = \int_{S^{N-1}} (2\varepsilon i)/m\ \ \omega g^\eta(t,x,\omega)\,\mathrm{d}\omega$ *is bounded in* $L^\infty(\mathbb{R}_t^+;\mathcal{H}')$.

Proof: It remains to establish the bounds on the macroscopic quantities. Clearly, one has

$$\sum_i \int_{\mathbb{R}^N} |\rho_i^\eta|^2\ \ B_i^{-1}\,\mathrm{d}x = \sum_i \int_{\mathbb{R}^N} \left|\int_{S^{N-1}} f_i^\eta\,\mathrm{d}\omega\right|^2\ \ B_i^{-1}\,\mathrm{d}x \leqslant \|f^\eta\|_{\mathcal{L}^2}.$$

Next, the current satisfies

$$\sum_i \int_{\mathbb{R}^+}\int_{\mathbb{R}^N} |J_i^\eta|^2 \frac{m\gamma_i}{2\varepsilon i B_i}\,\mathrm{d}x\,\mathrm{d}t = \sum_i \int_{\mathbb{R}^+}\int_{\mathbb{R}^N} \left|\int_{S^{N-1}} \sqrt{\frac{2\varepsilon i}{m}}\ \ \omega g_i^\eta\,\mathrm{d}\omega\right|^2 \frac{m\gamma_i}{2\varepsilon i B_i}\,\mathrm{d}x\,\mathrm{d}t$$
$$\leqslant \sum_i \int_{\mathbb{R}^+}\int_{\mathbb{R}^N}\int_{S^{N-1}} |g_i^\eta|^2 \frac{\gamma_i}{B_i}\,\mathrm{d}\omega\,\mathrm{d}x\,\mathrm{d}t \leqslant \int_{\mathbb{R}^+}\int_{\mathbb{R}^N} N(g^\eta)^2\,\mathrm{d}x\,\mathrm{d}t$$

and the boundedness of J^η is a consequence of (ii). □

Possibly at the cost of extracting subsequences, we can assume that

$$\begin{aligned} &f^\eta \rightharpoonup_* f \quad \text{weakly } * \text{ in } L^\infty(\mathbb{R}_t^+;\mathcal{L}^2),\\ &g^\eta \rightharpoonup_* g \quad \text{weakly } * \text{ in } L^2(\mathbb{R}_t^+;\mathcal{E}),\\ &\rho^\eta \rightharpoonup_* \rho \quad \text{weakly } * \text{ in } L^\infty(\mathbb{R}_t^+;L^2(\mathbb{R}^N\times\mathbb{N},\mathrm{d}x\otimes B_i^{-1}\,\mathrm{d}i)),\\ &J^\eta \rightharpoonup_* J \quad \text{weakly } * \text{ in } L^2(\mathbb{R}_t^+;\mathcal{H}'). \end{aligned} \tag{27}$$

This means, respectively,

$$\lim_{\eta\to 0}\int f^{\eta}\varphi\ \ B_i^{-1}\,\mathrm{d}\mu=\int f\varphi\ \ B^{-1}\,\mathrm{d}\mu,$$

$$\text{where}\ \ \int_{\mathbb{R}^+}\left(\int_{\mathbb{R}^N\times\mathbb{N}\times S^{N-1}}\varphi_i(t,x,\omega)^2 B_i^{-1}\,\mathrm{d}\omega\,\mathrm{d}i\,\mathrm{d}x\right)^{1/2}\mathrm{d}t<\infty,$$

$$\lim_{\eta\to 0}\int g^{\eta}\psi\ \ B_i^{-1}\,\mathrm{d}\mu=\int g\psi\ \ B^{-1}\,\mathrm{d}\mu,$$

$$\text{where}\ \ \int \psi_i(t,x,\omega)^2\ \ (\gamma_i B_i)^{-1}\,\mathrm{d}\mu<\infty,$$

$$\lim_{\eta\to 0}\int_{\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{N}}\rho^{\eta}\kappa\ \ B_i^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t=\int_{\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{N}}\rho\kappa\ \ B^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t,$$

$$\text{where}\ \ \int_{\mathbb{R}^+}\left(\int_{\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{N}}\kappa_i(t,x)^2\ \ B_i^{-1}\,\mathrm{d}i\,\mathrm{d}x\right)^{1/2}\mathrm{d}t<\infty,$$

$$\lim_{\eta\to 0}\int_{\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{N}}J^{\eta}\cdot\Phi\ \ B^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t=\int_{\mathbb{R}^N\times\mathbb{N}}J\cdot\Phi\ \ B^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t,$$

$$\text{where}\ \ \int_{\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{N}}|\Phi_i(t,x)|^2\ \ \frac{2\varepsilon i}{m\gamma_i B_i}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t<\infty.$$

Choosing, with the above-mentioned properties, $\varphi_i(t,x,\omega)=\kappa_i(t,x)$ and $\psi_i(t,x,\omega)=(2\varepsilon i/m)^{1/2}\ \ \omega\cdot\Phi_i(t,x)$, we realize that

$$\rho=\int_{S^{N-1}} f\,\mathrm{d}\omega,\ \ J=\int_{S^{N-1}}\sqrt{\frac{2\varepsilon i}{m}}\ \ \omega g\,\mathrm{d}\omega$$

holds. In fact, we obviously have $f=\rho$ by taking the limit in the distributional sense in $f^{\eta}=\rho^{\eta}+\eta g^{\eta}$.

Step 2: Continuity equation.

We wish to establish the following claim.

Lemma 3: For any i the continuity relation

$$\partial_t\rho_i+\mathrm{div}_x J_i=0$$

holds in $\mathcal{D}'((0,T)\times\mathbb{R}^N)$.

Proof: We use in (26) the test function $\kappa_i B_i\zeta(t,x)$ with $\kappa_i\in\mathscr{C}^{\infty}$ (precisely $\kappa_i=\delta_{ij}$), and $\zeta\in C_0^{\infty}((0,T)\times\mathbb{R}^N)$; then we take the limit $\eta\to 0$. □

Remark 9: Under suitable hypotheses, one could also rigorously derive the inelastic term (22). Actually, if $\sigma_{ij}(\omega,\omega')$ is such that $Q_{\theta}^{\mathrm{inel}}$ is bounded in $\mathbb{L}$, a priori estimate can still be derived by means of an application of Gronwall's lemma when $Q_{\theta}=Q_{\theta}^{\mathrm{el}}+\eta^2 Q_{\theta}^{\mathrm{inel}}$.

Step 3: Current equation.

According to our discussion in the previous section, the expected current equation $J=-\Sigma_j D_{ij}\nabla_x\rho_j$ has to be understood in the dual sense $\mathcal{J}(\nabla_x\rho)=J$, which means that

$$\mathcal{D}(\nabla_x\rho,\Phi)=-\langle J,\Phi\rangle \tag{28}$$

holds for any $\Phi\in L^2(\mathbb{R}^+,\mathcal{H})$. Of course, the notation now takes into account the time and space variables. Precisely, the right-hand side reads

$$\int\ J\cdot\Phi\ \ B^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t=\int gv\cdot\Phi\ \ B^{-1}\,\mathrm{d}\mu.$$

Since we can associate to $\Phi \in L^2(\mathbb{R}^+,\mathcal{H})$ a unique $K^\Phi \in L^2(\mathbb{R}^+,\mathcal{E})$ (with null average) such that $Q^*(K^\Phi)=v\cdot\Phi$, we get

$$(J,\Phi)=\int g Q^*(K^\Phi)\ \ B^{-1}\,\mathrm{d}\mu.$$

On the other hand, the left-hand side in (28) is

$$-\int \nabla_x\rho\cdot v K^\Phi\ \ B^{-1}\,\mathrm{d}\mu=-\int_{\mathbb{R}\times\mathbb{N}\times\mathbb{R}^N}\nabla_x\rho\left(\int_{S^{N-1}} v K^\Phi\,\mathrm{d}\omega\right)\ \ B_i^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t$$

by using (23). Then, (28) reduces to

$$\int\ g Q^*(K^\Phi)\ \ B^{-1}\,\mathrm{d}\mu=\int_{\mathbb{R}\times\mathbb{N}\times\mathbb{R}^N}\nabla_x\rho\left(\int_{S^{N-1}} v K^\Phi\,\mathrm{d}\omega\right)\ \ B^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t. \tag{29}$$

In order to justify equality (28), it thus would be tempting to use $\varphi=K^\Phi$ as a test function in (26). However, difficulties arise when we ask for such a function to belong to the admissible set $\mathfrak{D}$. We note that, for $\Phi\in L^2(0,T;\mathcal{H})$, we naturally have $K^\Phi\in L^2(0,T;\mathcal{E})$ and $\int_{S^{N-1}} vK^\Phi\,\mathrm{d}\omega \in L^2(0,T;\mathcal{H}')$. However we recall that it is required that $\nabla_x\cdot(v\varphi)\in L^2(0,T;\mathcal{L}^2)$ for φ to be an admissible test function. Space regularity is not a real difficulty, but it is not clear how it can be guaranteed that vK^Φ belongs to $L^2(0,T;\mathcal{L}^2)$. Except in some very particular cases (for instance if $2\varepsilon i\leqslant C\gamma_i$ which implies that $\mathcal{H}'$ embeds to $\not\subset$ or in some isotropic case as in Ref. 19), since Q_θ^{-1} mixes all the energy levels, it seems that a truncation of Φ on the high levels does not give such a control and it is not clear at all that the set $\{\Phi\in L^2(0,T;\mathcal{H}),\ \nabla_x\cdot vK^\Phi\in L^2(0,T;\mathcal{L}^2)\}$ is not empty in the general case. This difficulty leads to some technical restrictions on the cross sections in Ref. 19.

On the other hand, if we are able to prove that $\nabla_x\rho\in L^2(0,T;\mathcal{H})$, then, the relation (29) makes sense provided $\Phi\in L^2(0,T;\mathcal{H})$ and does not require further property on Φ. This motivates our strategy of proof: First, we establish an approximate current equation, from which we will be able to deduce that $\nabla_x\rho\in L^2(0,T;\mathcal{H})$; and then we derive the current equation (29). We are thus led to the main statement of the step.

Proposition 5: We have $\nabla_x\rho\in L^2(0,T;\mathcal{H})$, and the limit J of J^η satisfies (29).

Proof: Let Φ be a test function in $L^2(0,T;\mathcal{H})$ compactly supported with respect to time in $(0,T)$. Moreover, one assumes that $\partial_t\Phi\in L^2(0,T;\not\subset)$ and $\nabla_x\Phi\in L^2(0,T;\mathcal{H})$. This can be obtained by regularizing in time and space and eventually truncating in energy a function in $L^2(0,T;\mathcal{H})$. Then, $Q_\theta^{*-1}(v\cdot\Phi)=K^\Phi\in L^2(0,T;\mathcal{E})$ (recall that K^Φ depends on ω, though Φ does not). We introduce the function $\mu^{(n)}$ defined on $\mathbb{N}$ by

$$\mu_i^{(n)}=\begin{cases}1 & \text{if}\quad i\leqslant n\\ 0 & \text{if}\quad i>n.\end{cases}$$

The parameter n will help us in approximating (29). Then, we consider the admissible test function $\varphi_i(t,x,\omega)=\mu_i^{(n)}\ \ K_i^\Phi(t,x,\omega)\in L^2(0,T;\mathcal{E})$. We obtain from (26)

$$-\int f^\eta v\cdot\nabla_x(\mu^{(n)}K^\Phi)\ \ B^{-1}\,\mathrm{d}\mu-\eta\int f^\eta\partial_t(\mu^{(n)}K^\Phi)\ \ B^{-1}\,\mathrm{d}\mu=\frac{1}{\eta}\int Q_\theta(f^\eta)\mu^{(n)}K^\Phi\ \ B^{-1}\,\mathrm{d}\mu. \tag{30}$$

The right-hand side gives

$$\int\ Q_\theta(g^\eta)\mu^{(n)}K^\Phi\ \ B^{-1}\,\mathrm{d}\mu=\int g^\eta\ \ Q_\theta^*(\mu^{(n)}K^\Phi)\ \ B^{-1}\,\mathrm{d}\mu,$$

while the left-hand side is rewritten

$$-\int \rho^{\eta}\ \mu^{(n)} v\cdot\nabla_x K^{\Phi}\ B^{-1}\,\mathrm{d}\mu-\eta\left(\int f^{\eta}\partial_t(\mu^{(n)}K^{\Phi})\ B^{-1}\,\mathrm{d}\mu+\int g^{\eta}\ \mu^{(n)} v\cdot\nabla_x K^{\Phi}\ B^{-1}\,\mathrm{d}\mu\right).$$

Since all the sums are actually finite, there is no trouble in applying convergences (27), n being fixed. The left-hand side in (30) tends, as η goes to 0, toward

$$-\int \rho\nabla_x\cdot(v_j\mu^{(n)}vK^{\Phi})\ B^{-1}\,\mathrm{d}\mu=-\int_{\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{N}}(\mu^{(n)}\rho)\nabla_x\cdot\left(\int_{S^{N-1}}vK^{\Phi}\,\mathrm{d}\omega\right)\ B^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t.$$

Moreover, the right-hand side in (30) becomes

$$\int\ g^{\eta}Q_{\theta}^{*}(\mu^{(n)}K^{\Phi})\ B^{-1}\,\mathrm{d}\mu\to\int gQ_{\theta}^{*}(\mu^{(n)}K^{\Phi})\ B^{-1}\,\mathrm{d}\mu.$$

Thus, we are led to the equality

$$-\int_{\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{N}}(\mu^{(n)}\rho)\nabla_x\cdot\left(\int_{S^{N-1}}vK^{\Phi}\,\mathrm{d}\omega\right)B^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t=\int gQ_{\theta}^{*}(\mu^{(n)}K^{\Phi})\ B^{-1}\,\mathrm{d}\mu,\quad(31)$$

which appears as an approximate form of (28). We wish to conclude by letting n go to ∞. Let us introduce the linear mapping $J^{(n)}$ defined on the set

$$\left\{\Phi\in L^2(0,T;\mathcal{H}),\nabla_x\cdot\left(\int_{S^{N-1}}vK^{\Phi}\,\mathrm{d}\omega\right)\in L^2(0,T;\mathcal{H}')\right\}$$

by

$$J^{(n)}(\Phi)=-\int_{\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{N}}(\mu^{(n)}\rho)\nabla_x\cdot\left(\int_{S^{N-1}}vK^{\Phi}\,\mathrm{d}\omega\right)B^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t,$$

which corresponds to a weak definition of $-\mathcal{D}(\mu^{(n)}\nabla_x\rho,\Phi)$. Note that this set is obviously dense in $L^2(0,T;\mathcal{H})$ (it is only concerned with space regularization since $\int_{S^{N-1}}vK^{\Phi}\,\mathrm{d}\omega$ naturally lies in $L^2(0,T;\mathcal{H}')$). Furthermore, (31) says that one actually has

$$J^{(n)}(\Phi)=\int\ gQ_{\theta}^{*}(\mu^{(n)}K^{\Phi})\ B^{-1}\,\mathrm{d}\mu.$$

One deduces that

$$|J^{(n)}(\Phi)|\leqslant C\|g\|_{L^2(0,T;\mathcal{E})}\ \|\Phi\|_{L^2(0,T;\mathcal{H})}$$

and $J^{(n)}$ is a bounded sequence of continuous linear forms defined on the whole space $L^2(0,T;\mathcal{H})$. According to Corollary 4, we can associate a sequence $\Theta^{(n)}$ satisfying

$$\|\Theta^{(n)}\|_{L^2(0,T;\mathcal{H})}\leqslant C\|g\|_{L^2(0,T;\mathcal{E})},$$

and

$$J^{(n)}(\Phi)=-\mathcal{D}(\Theta^{(n)},\Phi)=\int_{\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{N}}\Theta_i^{(n)}(t,x)\left(\int_{S^{N-1}}v_iK_i^{\Phi}(t,x,\omega)\,\mathrm{d}\omega\right)\ B_i^{-1}\,\mathrm{d}i\,\mathrm{d}x\,\mathrm{d}t,$$

for any $\Phi\in L^2(0,T;\mathcal{H})$ [where we used (24)]. Then, coming back to (31), $\Theta^{(n)}$ is a bounded sequence in $L^2(0,T;\mathcal{H})$ which coincides with $\mu^{(n)}\nabla_x\rho$ as a linear form on the subset

$\{\int_{S^{N-1}} v K^{\Phi}\, d\omega,\ \Phi \in L^2(0,T;\mathcal{H})\} \subset L^2(0,T;\mathcal{H}')$. Hence, we will conclude that the limit of $\Theta^{(n)}$ defines $\nabla_x \rho$ as element of $L^2(0,T;\mathcal{H})$ if we are able to prove the following claim.

Lemma 4: The set $\mathbb{K} = \{\int_{S^{N-1}} v K^{\Phi} d\omega,\ \Phi \in \mathbb{H}\}$ *is dense in* $\mathbb{H}'$.

Lemma 4 yields $\mu^{(n)} \nabla_x \rho = \Theta^{(n)}$ in $L^2(0,T;\mathcal{H})$, and therefore $\mu^{(n)} \nabla_x \rho$ is bounded in this space, uniformly with respect to n. Since the sequence converges toward $\nabla_x \rho$ as $n \to \infty$ in a distributional sense, we deduce that $\mu^{(n)} \nabla_x \rho$ converges weakly toward $\nabla_x \rho$ in $L^2(0,T,\mathcal{H})$.

We end the proof by taking the limit $n \to \infty$ in the equality (31); we finally get

$$-\mathcal{D}(\nabla_x \rho, \Phi) = \int g v \cdot \Phi \ \ B^{-1}\, d\mu = \int_{\mathbb{R}^+ \times \mathbb{R}^N \times \mathbb{N}} J \cdot \Phi \ \ B^{-1}\, di\, dx\, dt.$$

Now, it remains to justify Lemma 4. □

Proof of Lemma 4: It is equivalent to prove that the orthogonal set of $\mathbb{K}$ is reduced to 0 in $\mathbb{H}$. Let $\Theta \in \mathbb{H}$ satisfy

$$\left(\Theta, \int_{S^{N-1}} v K^{\Phi}\, d\omega \right)_{\mathbb{L}} = 0, \quad \forall\, \Phi \in \mathbb{H}.$$

Then, by (24), this reads $\mathcal{D}(\Theta, \Phi) = 0$ for all $\Phi \in \mathbb{H}$, which yields $\Theta = 0$ thanks to the coercivity of the bilinear form $\mathcal{D}$. □

Step 4: Compactness in time.

We would like to recover as initial data ρ_I for the limit problem a function depending on the behavior of the sequence of data F_I^{η} for the kinetic equation. Of course this relies on a compactness in time property, at least for some weak topology. On the other hand, it can be shown a uniqueness result for the limit equation in the class of continuous functions with value in $L^2(\mathbb{R}^N \times \mathbb{N}; B^{-1}\, di \otimes dx)$ and having the gradient in $L^2(0,T;\mathcal{H})$. In turn, of course, the whole sequence ρ^{η} will converge to this ρ.

Lemma 5: The sequence $(\rho^{\eta})_{\eta > 0}$ *is sequentially compact in* $C^0([0,T]; L^2(\mathbb{R}^N \times \mathbb{N}, B_i^{-1}\, di \otimes dx)$*-weak). In particular, there exists a sequence* $(\rho^{\eta_n})_{n \in \mathbb{N}}$ *such that for any* $\phi \in L^2(\mathbb{R}^N \times \mathbb{N}, B_i^{-1}\, di \otimes dx)$

$$\int_{\mathbb{R}^N} \rho^{\eta_n} \phi \ \ B^{-1}\, di\, dx \to \int_{\mathbb{R}^N} \rho \phi \ \ B^{-1}\, di\, dx$$

as $n \to \infty$ *in* $C^0([0,T])$.

Proof: First, let $\psi \in L^2(\mathbb{R}^N \times \mathbb{N}, (1 + i/\gamma_i) B_i^{-1}\, di \otimes dx)$ with $\nabla_x \psi \in \mathcal{H}$. Looking at the continuity equation, one gets

$$\int_{\mathbb{R}^N} \rho^{\eta}(t) \psi \ \ B^{-1}\, di\, dx - \int_{\mathbb{R}^N} \rho^{\eta}(s) \psi B^{-1}\, di\, dx = \int_0^t (J^{\eta}, \nabla_x \psi)_{\mathcal{H}', \mathcal{H}}\, d\sigma$$

$$\leq C \|J^{\eta}\|_{L^2(0,T;\mathcal{H}')} \ \ \sqrt{|t-s|} \ \ \|\nabla_x \psi\|_{\mathcal{H}}.$$

The bound (iv) in Proposition 2 combined with the Arzela–Ascoli theorem allows us to deduce that $(\int \rho^{\eta}(t) \psi \ \ B^{-1}\, di\, dx)_{\eta > 0}$ lies in a compact set in $C^0([0,T])$. By considering finite series and space regularization, one sees that the above-used set of ψ's is dense into $L^2(\mathbb{R}^N \times \mathbb{N}, B_i^{-1} di \otimes dx)$. Then, let $\phi \in L^2(\mathbb{R}^N \times \mathbb{N}, B_i^{-1} di \otimes dx)$. We deduce that, for any $\varepsilon > 0$,

$$\left(\int_{\mathbb{R}^N} \rho^{\eta}(t) \phi \ \ B^{-1}\, di\, dx \right)_{\eta > 0} \subset B(0,\varepsilon) + \text{Compact Set} \quad \text{in} \ \ C^0([0,T]).$$

Hence, $(\int \rho^{\eta}(t) \phi \ \ B^{-1}\, di\, dx)_{\eta > 0}$ also lies in a compact set in $C^0([0,T])$. We conclude by using the separability of $L^2(\mathbb{R}^N \times \mathbb{N}, B_i^{-1} di \otimes dx)$ and a Cantor argument. □

Lemma 5 says that we recover as initial data for the limit equation the limit, in the weak $L^2(\mathbb{R}^N\times\mathbb{N},B_i^{-1}\mathrm{d}i\otimes\mathrm{d}x)$ sense, of $\rho_I^\eta=\int_{S^{N-1}}F_I^\eta\,\mathrm{d}\omega$. Moreover, classical reasoning gives the continuity in time for the limit problem, see for instance Ref. 16.

Lemma 6: The limit ρ is a continuous function on $[0,T]$ with values in $L^2(\mathbb{R}^N\times\mathbb{N},B_i^{-1}\mathrm{d}i\otimes\mathrm{d}x)$; and it satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\rho\|_{L^2}^2=-2\int_{\mathbb{R}^N}\mathcal{D}(\nabla_x\rho,\nabla_x\rho)\,\mathrm{d}x \tag{32}$$

in $\mathcal{D}'(]0,T[)$.

Proof: The point relies on the following facts:

$$\rho\in L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^N\times\mathbb{N},B_i^{-1}\mathrm{d}i\otimes\mathrm{d}x)),$$
$$\rho\in C^0([0,T];L^2(\mathbb{R}^N\times\mathbb{N},B_i^{-1}\mathrm{d}i\otimes\mathrm{d}x)-weak),$$
$$\nabla_x\rho\in L^2(\mathbb{R}^+;\mathcal{H}).$$

In turn, Eq. (21) implies that $\partial_t\rho$ reads as the space derivative of an element of $L^2(\mathbb{R}^+;\mathcal{H}')$. This legitimates the product with ρ. Indeed, by regularization (in time) and truncation (in energy), we can construct a sequence $\rho^{(n)}$ which lies in $C^\infty([0,T];\mathcal{H}\cap L^2(\mathbb{R}^N\times\mathbb{N},B_i^{-1}\mathrm{d}i\otimes\mathrm{d}x))$, with $\partial_t\rho^{(n)}\in C^\infty([0,T];\mathcal{H}'\cap L^2(\mathbb{R}^N\times\mathbb{N},B_i^{-1}\mathrm{d}i\otimes\mathrm{d}x))$ and satisfying

$$\rho^{(n)}\to\rho \ \text{ in } \ L^2(0,T;L^2(\mathbb{R}^N\times\mathbb{N},B_i^{-1}\mathrm{d}i\otimes\mathrm{d}x)),$$
$$\partial_t\rho^{(n)}\to\partial_t\rho \ \text{ in } \ L^2(0,T;\nabla_x\cdot(\mathcal{H}'))$$

as n goes to ∞. When dealing with regular functions, one has clearly

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\rho^{(n)}\|_{L^2}^2=2(\partial_t\rho^{(n)},\rho^{(n)})_{L^2}=2\langle\partial_t\rho^{(n)},\rho^{(n)}\rangle,$$

where the brackets stand for the duality product between $\{\rho$ such that $\nabla_x\rho\in\mathcal{H}\}$ and $\{\Sigma_{|\alpha|=1}\partial_x^\alpha J,J\in\mathcal{H}'\}$. Passing to the limit $n\to\infty$ justifies that

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\rho\|_{L^2}=2\langle\partial_t\rho,\rho\rangle$$

holds in $\mathcal{D}'(]0,T[)$, which gives (32). Therefore, one deduces that $(\mathrm{d}/\mathrm{d}t)\,\|\rho\|_{L^2}\in L^1(0,T)$ and

$$\|\rho(t)\|_{L^2}^2=\|\rho_I\|_{L^2}^2+\int_0^t 2\langle\partial_t\rho,\rho\rangle\mathrm{d}s$$

defines a continuous function on $[0,T]$. Furthermore,

$$\|\rho(t)-\rho(t_0)\|_{L^2}^2=\|\rho(t)\|_{L^2}^2+\|\rho(t_0)\|_{L^2}^2-2(\rho(t),\rho(t_0))_{L^2}$$

tends to 0 as t goes to t_0 since $\rho\in C^0([0,T],L^2-weak)$. □

In turn, one deduces the following uniqueness statement which proves that the whole sequence ρ^η converges.

Corollary 5: There exists a unique solution ρ of (21) with $\rho\in L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^N\times\mathbb{N},B_i^{-1}\mathrm{d}i\otimes\mathrm{d}x))$ and $\nabla_x\rho\in L^2(\mathbb{R}^+;\mathcal{H})$.

Proof: The previous lemma guarantees that ρ is continuous with values in $L^2(\mathbb{R}^N\times\mathbb{N},B_i^{-1}\mathrm{d}i\otimes\mathrm{d}x)$. By linearity, it suffices to consider the solution ρ corresponding to data $\rho_I=0$. Then, (32) combined to the positivity of $\mathcal{D}$ implies that $\|\rho(t)\|_{L^2}=0$. □

As a concluding remark, let us notice that we can improve the convergence of ρ^η to ρ. Indeed, using $\omega\delta_{ij}$ as test function in (26), we obtain that $\nabla_x\rho_i$ reads as a bounded term in $L^2((0,T)$

$\times\mathbb{R}^N$) plus $\eta\times$(first derivatives of bounded terms in $L^2((0,T)\times\mathbb{R}^N)$), hence it is compact in $H^{-1}((0,T)\times B(0,R))$ for any $0<T,R<\infty$. Combining this information with the continuity equation in Lemma 3, we can apply the Div-Curl argument of L. Tartar,[39] as in Refs. 34, 29, 20, and 28 and we deduce that for any $i\in\mathbb{N}$, ρ_i^η lies in a compact set of $L^2_{\rm loc}((0,T)\times\mathbb{R}^N)$. If further the B_i's tend to 0, one easily concludes that ρ^η converges to ρ strongly in $L^2((0,T)\times B(0,R)\times\mathbb{N})$, for any $0<T,R<\infty$.

APPENDIX: PROPERTIES OF THE COLLISION OPERATORS

1. Proof of Proposition 1

We write $Q_0^{\rm el}(f)_i=K(f)_i-\Sigma_i f_i$. Of course, one has $\|\Sigma f\|_{\mathbb{F}}=\|f\|_{\mathbb{E}}$. Next, using $(h1)$, we get

$$\begin{aligned}
&\sum_i \int_{S^{N-1}}|K(f)_i|^2\frac{1}{\Sigma_i B_i}\,{\rm d}\omega\\
&\quad=\sum_i \int_{S^{N-1}}\left|\int_{S^{N-1}}\Gamma_i(\omega',\omega)f_i(\omega')\,{\rm d}\omega'\right|^2\frac{1}{\Sigma_i B_i}\,{\rm d}\omega\\
&\quad\leqslant\sum_i \int_{S^{N-1}}\left\{\left(\int_{S^{N-1}}\Gamma_i(\omega',\omega)\,{\rm d}\omega\right)|f_i(\omega')|^2\,{\rm d}\omega'\int_{S^{N-1}}\Gamma_i(\omega,\omega')\,{\rm d}\omega'\frac{1}{\Sigma_i B_i}\right\}{\rm d}\omega\\
&\quad\leqslant\sum_i \int_{S^{N-1}}\Sigma_i\,(\omega')|f_i(\omega')|^2B_i^{-1}\,{\rm d}\omega'=\|f\|_{\mathbb{E}}^2. \qquad\text{(A1)}
\end{aligned}$$

It follows that $Q_0^{\rm el}\in\mathcal{L}(\mathbb{E},\mathbb{F})$, with $\|Q_0^{\rm el}(f)\|_{\mathbb{F}}\leqslant 2\|f\|_{\mathbb{E}}$.

According to Hypothesis (h1), we easily get (i)

$$\int_{S^{N-1}}Q_0^{\rm el}(f)_i\,{\rm d}\omega=\int_{S^{N-1}}f_i(\omega)\left(\int_{S^{N-1}}(\Gamma_i(\omega,\omega')-\Gamma_i(\omega',\omega))\,{\rm d}\omega'\right){\rm d}\omega=0.$$

Now, $\mathcal{B}_0$ is clearly bilinear and continuous on $\mathbb{E}\times\mathbb{E}$ and we compute

$$\begin{aligned}
\mathcal{B}_0(f,f)&=-\sum_i\int_{S^{N-1}}\int_{S^{N-1}}\Gamma_i(\omega',\omega)[f_i(\omega')-f_i(\omega)]f_i(\omega)B_i^{-1}\,{\rm d}\omega'\,{\rm d}\omega\\
&=-\sum_i\int_{S^{N-1}}\int_{S^{N-1}}\Gamma_i(\omega',\omega)f_i(\omega)f_i(\omega')B_i^{-1}\,{\rm d}\omega'\,{\rm d}\omega\\
&\quad+\frac{1}{2}\sum_i\int_{S^{N-1}}\int_{S^{N-1}}\Gamma_i(\omega',\omega)|f_i(\omega)|^2{\rm d}\omega'\,{\rm d}\omega\\
&\quad+\frac{1}{2}\sum_i\int_{S^{N-1}}\int_{S^{N-1}}\Gamma_i(\omega,\omega')|f_i(\omega')|^2{\rm d}\omega'\,{\rm d}\omega\\
&=1/2\sum_i\int_{S^{N-1}}\int_{S^{N-1}}\Gamma_i(\omega',\omega)(|f_i(\omega)|^2\\
&\quad+|f_i(\omega')|^2-2\,f_i(\omega)f_i(\omega'))B_i^{-1}\,{\rm d}\omega'\,{\rm d}\omega\\
&=1/2\sum_i\int_{S^{N-1}}\int_{S^{N-1}}\Gamma_i(\omega',\omega)|f_i(\omega)-f_i(\omega')|^2B_i^{-1}\,{\rm d}\omega'\,{\rm d}\omega.
\end{aligned}$$

This obviously leads to the characterization of the kernel of $Q_0^{\rm el}$ in (iii).

Moreover, we have

$$\sum_i \int_{S^{N-1}} |Q_0^{\mathrm{el}}(f)_i|^2 \frac{1}{\Sigma_i B_i} \mathrm{d}\omega \leqslant \sum_i \int_{S^{N-1}} \int_{S^{N-1}} \Gamma_i(\omega', \omega) |f_i(\omega) - f_i(\omega')|^2 \frac{\Sigma_i}{\Sigma_i B_i} \mathrm{d}\omega' \, \mathrm{d}\omega$$
$$\leqslant 2\mathcal{B}_0(f,f),$$

which implies the last inequality in assertion (ii). □

2. Proof of Corollary 1

Set $f = \langle f \rangle - r$. Since r has null average, assumption $(h2)$ yields

$$\mathcal{B}_0(f,f) = 1/2 \sum_i \int_{S^{N-1}} \int_{S^{N-1}} \Gamma_i(\omega' \omega) |f_i(\omega') - f_i(\omega)|^2 B_i^{-1} \, \mathrm{d}\omega' \, \mathrm{d}\omega$$
$$\geqslant 1/2 \sum_i \int_{S^{N-1}} \int_{S^{N-1}} |f_i(\omega') - f_i(\omega)|^2 \gamma_i B_i^{-1} \, \mathrm{d}\omega' \, \mathrm{d}\omega$$
$$\geqslant 1/2 \sum_i \int_{S^{N-1}} \int_{S^{N-1}} |r_i(\omega') - r_i(\omega)|^2 \gamma_i B_i^{-1} \, \mathrm{d}\omega' \, \mathrm{d}\omega$$
$$\geqslant 1/2 \sum_i \int_{S^{N-1}} \int_{S^{N-1}} (r_i^2(\omega') + r_i^2(\omega) - 2 r_i(\omega) r_i(\omega')) \gamma_i B_i^{-1} \, \mathrm{d}\omega' \, \mathrm{d}\omega$$
$$\geqslant \sum_i \int_{S^{N-1}} r_i^2(\omega) \gamma_i B_i^{-1} \, \mathrm{d}\omega = N^2(r).$$

□

3. Proof of Proposition 2

First, let us estimate

$$\|Q_1^{\mathrm{el}}(f)\|_{\mathbb{F}}^2 = \sum_i \int_{S^{N-1}} \left| \sum_j \int_{S^{N-1}} \sigma_{ij}(\omega, \omega') (f_j(\omega') - f_j(\omega)) \mathrm{d}\omega' \right|^2 (\Sigma_i(\omega) B_i)^{-1} \mathrm{d}\omega$$
$$\leqslant \sum_i \int_{S^{N-1}} \left(\sum_j \int_{S^{N-1}} \sigma_{ij}(\omega, \omega') B_j \, \mathrm{d}\omega' \right.$$
$$\left. \times \sum_j \int_{S^{N-1}} \sigma_{ij}(\omega, \omega') |f_j(\omega') - f_j(\omega)|^2 B_j^{-1} \, \mathrm{d}\omega' \right) (\Sigma_i B_i)^{-1} \mathrm{d}\omega$$
$$\leqslant M_2 \sum_j \int_{S^{N-1}} \int_{S^{N-1}} \left(\sum_i \sigma_{ij}(\omega, \omega') \right) |f_j(\omega') - f_j(\omega)|^2 B_j^{-1} \, \mathrm{d}\omega' \, \mathrm{d}\omega$$
$$\leqslant M_2 \sum_j \int_{S^{N-1}} \int_{S^{N-1}} \Gamma_j(\omega, \omega') |f_j(\omega') - f_j(\omega)|^2 B_j^{-1} \, \mathrm{d}\omega' \, \mathrm{d}\omega$$
$$\leqslant 2 M_2 \mathcal{B}_0(f,f) \leqslant 2 M_2 \|Q_0^{\mathrm{el}}(f)\|_{\mathbb{F}} \|f\|_{\mathbb{F}} \leqslant 4 M_2 \|f\|_{\mathbb{E}}^2, \tag{A2}$$

where we used the Cauchy–Schwarz inequality and the results in Proposition 1. This proves that $Q_1^{\mathrm{el}} \in \mathcal{L}(\mathbb{E}, \mathbb{F})$.

In view of Remark 2, we can integrate Q_1^{el} with respect to ω and we get

$$\int_{S^{N-1}} Q_1^{\mathrm{el}}(f)_i \mathrm{d}\omega = \sum_j \int_{S^{N-1}} f_j(\omega') \left(\int_{S^{N-1}} \sigma_{ij}(\omega,\omega') \mathrm{d}\omega \right) \mathrm{d}\omega' - \sum_j \int_{S^{N-1}} f_j(\omega) \times \left(\int_{S^{N-1}} \sigma_{ij}(\omega,\omega') \mathrm{d}\omega' \right) \mathrm{d}\omega$$
$$= \sum_j \int_{S^{N-1}} f_j(\omega) \left(\int_{S^{N-1}} (\sigma_{ij}(\omega',\omega) - \sigma_{ij}(\omega,\omega')) \mathrm{d}\omega' \right) \mathrm{d}\omega = 0,$$

by using the symmetry assumption $(h1')$.

Then, $\mathcal{B}_1$ is obviously a bilinear continuous form on $\mathbb{E}$, and a straightforward computation yields

$$\mathcal{B}_1(f,g) = -\sum_{i,j} \int_{S^{N-1}} \int_{S^{N-1}} \sigma_{ij}(\omega,\omega')(f_j(\omega') - f_j(\omega)) g_i(\omega) B_i^{-1} \mathrm{d}\omega' \, \mathrm{d}\omega$$
$$= \sum_{i,j} \int_{S^{N-1}} \int_{S^{N-1}} \sigma_{ij}(\omega',\omega)(f_j(\omega') - f_j(\omega)) g_i(\omega') B_i^{-1} \mathrm{d}\omega \, \mathrm{d}\omega'$$
$$= 1/2 \sum_{i,j} \int_{S^{N-1}} \int_{S^{N-1}} (f_j(\omega') - f_j(\omega))(\sigma_{ij}(\omega',\omega) g_i(\omega') - \sigma_{ij}(\omega,\omega') g_i(\omega)) B_i^{-1} \mathrm{d}\omega' \, \mathrm{d}\omega.$$

Finally, in view of (10), it is easy to check that $\mathcal{E}_0 \subset \mathrm{Ker}(Q_1^{\mathrm{el}})$, and writing $f = \langle f \rangle + r$, we immediately get

$$|\mathcal{B}_1(f,f)| = |(Q_1^{\mathrm{el}}(f), f)_{\mathbb{L}}| = |(Q_1^{\mathrm{el}}(r), r)_{\mathbb{L}}| \leq \|r\|_{\mathbb{E}} \|Q_1^{\mathrm{el}}(r)\|_{\mathbb{F}} \leq 2\sqrt{M_2} \|r\|_{\mathbb{E}}^2 \leq 2M_0 \sqrt{M_2} N(f - \langle f \rangle)^2.$$

We can improve this bound, by noticing that, since the average of r vanishes, (A2) and (h3) yield

$$\|Q_1^{\mathrm{el}}(r)\|_{\mathbb{F}}^2 \leq M_0 M_2 \sum_j \gamma_j B_j^{-1} \int_{S^{N-1}} \int_{S^{N-1}} |r_j(\omega') - r_j(\omega)|^2 \mathrm{d}\omega' \, \mathrm{d}\omega$$
$$\leq M_0 M_2 \sum_j \gamma_j B_j^{-1} (2\langle r_j^2 \rangle - 2\langle r_j \rangle^2)$$
$$\leq 2M_0 M_2 \sum_j \gamma_j B_j^{-1} \langle r_j^2 \rangle = 2M_0 M_2 N(r)^2,$$

and therefore

$$\mathcal{B}_1(f,f) \leq \sqrt{2M_0 M_2} \|r\|_{\mathbb{E}} N(r) \leq M_0 \sqrt{2M_2} N(f - \langle f \rangle)^2.$$

□

4. Proof of Corollary 2

By combining the symmetry condition $(h1'')$ with estimate $(h2'')$, we can dominate $|\mathcal{B}_1(f,f)|$, as given in Proposition 2(ii) by

$$M/2\sum_{ij}\ \int_{S^{N-1}}\int_{S^{N-1}}\gamma_i\gamma_j|f_j(\omega')-f_j(\omega)||f_i(\omega')-f_i(\omega)|\mathrm{d}\omega\,\mathrm{d}\omega'$$

$$\leqslant M/2\sum_{ij}\ \gamma_i\gamma_j\left(\int_{S^{N-1}}\int_{S^{N-1}}|f_j(\omega')-f_j(\omega)|^2\mathrm{d}\omega\,\mathrm{d}\omega'\right)^{1/2}$$

$$\times\left(\int_{S^{N-1}}\int_{S^{N-1}}|f_i(\omega')-f_i(\omega)|^2\mathrm{d}\omega\,\mathrm{d}\omega'\right)^{1/2}.$$

Since one assumes $\langle f\rangle=0$, the integral becomes

$$\int_{S^{N-1}}\int_{S^{N-1}}|f_i(\omega')-f_i(\omega)|^2\mathrm{d}\omega\,\mathrm{d}\omega'=2\langle f_i^2\rangle.$$

Hence, we get

$$|\mathcal{B}_1(f,f)|\leqslant M\sum_{ij}\ \gamma_i\gamma_j\langle f_j^2\rangle^{1/2}\langle f_i^2\rangle^{1/2}$$

$$\leqslant M\left(\sum_{ij}\ \gamma_i B_i^{-1}\langle f_i^2\rangle\gamma_j B_j^{-1}\langle f_j^2\rangle\right)^{1/2}\left(\sum_{ij}\ \gamma_i B_i\gamma_j B_j\right)^{1/2}$$

$$\leqslant MM_1\sum_{i}\ \gamma_i B_i^{-1}\langle f_i^2\rangle=MM_1N(f)^2.$$

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Inhomogeneous six-vertex model with domain wall boundary conditions and Bethe ansatz

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In this note, we consider the six-vertex model with domain wall boundary conditions, defined on an $M\times M$ lattice, in the inhomogeneous case where the partition function depends on $2M$ inhomogeneities λ_j and μ_k. For a particular choice of the set of λ_j we find a new determinant representation for the partition function, which allows evaluation of the bulk free energy in the thermodynamic limit. This provides a new connection between two types of determinant formulas. We also show in a special case that spin correlations on the horizontal line going through the center coincide with the ones for periodic boundary conditions. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1415430]

I. INTRODUCTION

The six-vertex model was first introduced in Ref. 1. It was solved exactly by Lieb[2] and Sutherland[3] in 1967 by means of Bethe ansatz for periodic boundary conditions (PBC). Later the six-vertex model was studied for different boundary conditions.[4–6] Domain wall boundary conditions were introduced in 1982.[7] These boundary conditions are interesting because they allow one to derive determinant representations for correlation functions[8] and the same boundary conditions help to enumerate alternating sign matrices.[9,10] Recently the bulk free energy was calculated for these boundary conditions.[11]

In this paper we show that for special choices of inhomogeneities, one can compute the free energy and some correlation functions of the system. This observation might be useful because we expect some properties of the model to be independent of the inhomogeneities, i.e., to depend only on the anisotropy parameter. In the simplest situation, the correlation functions coincide with the ones for periodic boundary conditions.

II. INHOMOGENEITIES AND BETHE ANSATZ

In this section we define the inhomogeneous six-vertex model with domain wall boundary conditions and choose the spectral parameters (inhomogeneities) to satisfy Bethe ansatz equations; this will imply special properties of the partition function.

We now introduce the notations. Given an $M\times M$ square lattice with spectral parameters λ_i and μ_k attached to the lines and columns, one defines the usual Boltzmann weights *a*, *b*, *c* to be

$$a(\lambda,\mu)=\sinh(\gamma(\lambda-\mu+i/2)),$$

$$b(\lambda,\mu)=\sinh(\gamma(\lambda-\mu-i/2)), \tag{2.1}$$

$$c(\lambda,\mu)=\sinh(i\gamma),$$

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where γ is the anisotropy. We have fixed boundary conditions for the external edges: horizontal (respectively, vertical) external edges are outgoing (respectively, incoming). The partition function is denoted by $Z_M(\{\lambda_j\},\{\mu_k\})$. Using recursion relations satisfied by the Z_M, one can show that the following determinant formula holds:[12,13]

$$Z_M(\{\lambda_j\},\{\mu_k\})=\frac{\Pi_{1\leqslant j,k\leqslant M}\sinh(\gamma(\lambda_j-\mu_k+i/2))\sinh(\gamma(\lambda_j-\mu_k-i/2))}{\Pi_{1\leqslant j\leqslant j'\leqslant M}\sinh(\gamma(\lambda_j-\lambda_{j'}))\Pi_{1\leqslant k<k'\leqslant M}\sinh(\gamma(\mu_k-\mu_{k'}))}$$
$$\times\det_{1\leqslant j,k\leqslant M}\left[\frac{\sinh(i\gamma)}{\sinh(\gamma(\lambda_j-\mu_k+i/2))\sinh(\gamma(\lambda_j-\mu_k-i/2))}\right]. \tag{2.2}$$

In the homogeneous case this representation was used in order to evaluate the bulk free energy in the thermodynamic limit.[11] In a special inhomogeneous case we shall use another determinant represention to evaluate the bulk free energy in the thermodynamic limit. Let us define our special case. We choose the spectral parameters in relation to the Bethe ansatz. In order to do that it is convenient to introduce the formalism of the algebraic Bethe ansatz. The Boltzmann weights are encoded into the L-matrix

$$L(\lambda)=\begin{pmatrix} a(\lambda) & 0 & 0 & 0\\ 0 & b(\lambda) & c(\lambda) & 0\\ 0 & c(\lambda) & b(\lambda) & 0\\ 0 & 0 & 0 & a(\lambda)\end{pmatrix}. \tag{2.3}$$

We next introduce the *monodromy matrix* $T(\lambda)$ which is an operator acting on $\mathbb{C}^{2^M}\otimes\mathbb{C}^2$ (physical space times auxiliary space) defined by

$$T(\lambda;\mu_1,\ldots,\mu_M)=L(\lambda-\mu_M)L(\lambda-\mu_{M-1})\ldots L(\lambda-\mu_1), \tag{2.4}$$

where $L(\lambda-\mu_k)$ acts on the kth factor of the tensor product in the physical space, and the auxiliary space. As an operator on the two-dimensional auxiliary space, $T(\lambda)$ can be written as

$$T(\lambda)=\begin{pmatrix}\mathbf{A}(\lambda) & \mathbf{B}(\lambda)\\ \mathbf{C}(\lambda) & \mathbf{D}(\lambda)\end{pmatrix}, \tag{2.5}$$

where **A**, **B**, **C**, **D** are operators on the physical space $\mathbb{C}^{2^M}$. The usual *transfer matrix* corresponding to periodic boundary conditions is defined as

$$\mathbf{T}(\lambda)=\mathbf{A}(\lambda)+\mathbf{D}(\lambda). \tag{2.6}$$

We shall make use of this operator later. Here, our fixed boundary conditions imply the following formal expression for the partition function:[7]

$$Z_M(\{\lambda_j\},\{\mu_k\})=\langle\downarrow|\mathbf{B}(\lambda_1;\mu_1,\ldots,\mu_M)\ldots\mathbf{B}(\lambda_M;\mu_1,\ldots,\mu_M)|\uparrow\rangle, \tag{2.7}$$

where

$$|\uparrow\rangle\equiv\begin{pmatrix}1\\0\end{pmatrix}^{\otimes M}\quad\left(\text{respectively }\ |\downarrow\rangle\equiv\begin{pmatrix}0\\1\end{pmatrix}^{\otimes M}\right)$$

is the state with all spins up (respectively, down).

Let us specify inhomogeneities. We choose the $\{\lambda_j\}$ to be divided into two sets $\{\lambda_j^1=\lambda_j,\ j=1,\ldots,m^1\}$ and $\{\lambda_j^2=\lambda_{j+m^1},\ j=1,\ldots,m^2\}$ which each satisfy the *Bethe ansatz equations:*

$$\prod_{\substack{j'=1\\ j'\neq j}}^{m^\alpha} \frac{\sinh(\gamma(\lambda_j^\alpha-\lambda_{j'}^\alpha+i))}{\sinh(\gamma(\lambda_j^\alpha-\lambda_{j'}^\alpha-i))}=\prod_{k=1}^{M}\frac{\sinh(\gamma(\lambda_j^\alpha-\mu_k+i/2))}{\sinh(\gamma(\lambda_j^\alpha-\mu_k-i/2))} \tag{2.8}$$

with $\alpha=1,2$. We define the left and right states

$$\begin{aligned}\langle 1|&=\langle\uparrow|\mathbf{C}(\lambda_1^1)\ldots\mathbf{C}(\lambda_{m^1}^1),\\ |2\rangle&=\mathbf{B}(\lambda_1^2)\ldots\mathbf{B}(\lambda_{m^2}^2)|\uparrow\rangle,\end{aligned} \tag{2.9}$$

and the *flip operator* $\mathbf{R}$ to be the operator on the physical space that flips all arrows: in terms of the usual Pauli matrices, $\mathbf{R}=\Pi_{k=1}^{M}\sigma_k^x$. Now using the overall invariance of the monodromy matrix under flip: $[T(\lambda),\mathbf{R}\sigma^x]=0$ (where the additional σ^x acts on the auxiliary space), one finds that $\mathbf{RB}(\lambda)\mathbf{R}=\mathbf{C}(\lambda)$ and therefore we can rewrite formula (2.7) in terms of the states we have defined:

$$Z_M(\{\lambda_j\},\{\mu_k\})=\langle 1|\mathbf{R}|2\rangle. \tag{2.10}$$

We now consider the situation where M is even and $m^1=m^2=M/2$. As proven in (A3), the Bethe state $|2\rangle$ is an eigenstate of $\mathbf{R}$ (with eigenvalue ±1). At this point we use orthogonality of Bethe states (A2) to conclude that

$$Z_M(\{\lambda_j\},\{\mu_k\})=\pm\,\delta_{\{\lambda_j^1\},\{\lambda_j^2\}}\langle 1|2\rangle. \tag{2.11}$$

The nonzero scalar product (square of the norm) is given by the following formula,[7] dropping the superscripts:

$$\langle 1|1\rangle=(\sin\gamma)^{M/2}\left[\prod_{j=1}^{M/2}a(\lambda_j)d(\lambda_j)\right]\left[\prod_{\substack{j,j'=1\\ j\neq j'}}^{M/2}\frac{\sinh(\gamma(\lambda_j-\lambda_{j'}+i))}{\sinh(\gamma(\lambda_j-\lambda_{j'}))}\right]\det_{1\leq j,j'\leq M/2}\left[\frac{\partial\varphi_j}{\partial\lambda_{j'}}\right] \tag{2.12}$$

with the following definitions: $a(\lambda)$ and $d(\lambda)$ are the eigenvalues of $\mathbf{A}(\lambda)$ and $\mathbf{D}(\lambda)$ acting on $|\uparrow\rangle$:

$$\begin{aligned}a(\lambda)&=\prod_{k=1}^{M}\sinh(\gamma(\lambda-\mu_k+i/2)),\\ d(\lambda)&=\prod_{k=1}^{M}\sinh(\gamma(\lambda-\mu_k-i/2)),\end{aligned} \tag{2.13}$$

and the φ_j are the logarithms of the B.A.E. (2.8):

$$\varphi_j=i\log(a(\lambda_j)/d(\lambda_j))+i\sum_{\substack{j'=1\\ j'\neq j}}^{M/2}\log\frac{\sinh(\gamma(\lambda_j-\lambda_{j'}+i))}{\sinh(\gamma(\lambda_j-\lambda_{j'}-i))}. \tag{2.14}$$

Note that the general determinant formula (2.2), in the case of two identical sets $\{\lambda_j^1\}=\{\lambda_j^2\}$, becomes

$$\begin{aligned}Z_M(\{\lambda_j\},\{\mu_k\})=&\frac{\Pi_{\substack{1\leq j\leq M/2\\ 1\leq k\leq M}}\sinh^2(\gamma(\lambda_k-\mu_k+i/2))\sinh^2(\gamma(\lambda_j-\mu_k-i/2))}{\Pi_{1\leq j<j'\leq M/2}\sinh^2(\gamma(\lambda_j-\lambda_{j'}))\Pi_{1\leq k\leq k'\leq M}\sinh(\gamma(\mu_k-\mu_{k'}))}\\ &\times\det_{\substack{1\leq j\leq M/2\\ 1\leq k\leq M}}[\phi(\lambda_j-\mu_k),\psi(\lambda_j-\mu_k)]\end{aligned} \tag{2.15}$$

with $\phi(\lambda)\equiv\sinh(i\gamma)/(\sinh(\gamma(\lambda+i/2))\sinh(\gamma(\lambda-i/2)))$ and

$$\psi(\lambda)=\frac{1}{\gamma}\frac{\mathrm{d}}{\mathrm{d}\lambda}\phi(\lambda).$$

Our new determinant representation (2.12) is quite different from Eq. (2.15); it is in particular much easier to study its thermodynamic limit.

III. CORRELATION FUNCTIONS

So far we have studied the function partition of the system; what about correlation functions?

Unfortunately it is not possible to find such a simple expression for an arbitrary correlation function; however, if we restrict ourselves to the case of special correlations which lie on a fixed horizontal line, then one can again derive determinant formulas for them.

To be specific, let us assume again that the $\{\lambda_j\}$ consist of two identical sets $\{\lambda_j, j=1\cdots M/2\}$. Then the probability that all arrows located at columns $k_1,\ldots,k_n$ and between lines $M/2$ and $M/2+1$ are up, is given by

$$\langle \pi_{k_1}\cdots\pi_{k_n}\rangle\equiv\frac{\langle\downarrow|\mathbf{B}(\lambda_1)\cdots\mathbf{B}(\lambda_{M/2})\pi_{k_1}\cdots\pi_{k_n}\mathbf{B}(\lambda_1)\cdots\mathbf{B}(\lambda_{M/2})|\uparrow\rangle}{\langle\downarrow|\mathbf{B}(\lambda_1)\cdots\mathbf{B}(\lambda_{M/2})\mathbf{B}(\lambda_1)\cdots\mathbf{B}(\lambda_{M/2})|\uparrow\rangle},\tag{3.1}$$

where $\pi_k\equiv\frac{1}{2}(1+\sigma_k^z)=\left(\begin{smallmatrix}1&0\\0&0\end{smallmatrix}\right)$ acts on the kth space.

Similarly to what was done for the partition function, one can transform Eq. (3.1) using the flip operator $\mathbf{R}$ and find:

$$\langle \pi_{k_1}\cdots\pi_{k_n}\rangle=\frac{\langle 1|\pi_{k_1}\cdots\pi_{k_2}|1\rangle}{\langle 1|1\rangle}.\tag{3.2}$$

In other words this is simply the usual correlation functions of the spin operators $\frac{1}{2}(1+\sigma^z)$ for the corresponding spin chain. The computation of these averages is a well-known problem, and the general strategy to perform it is by now well understood.[14] One must use the solution of the quantum inverse scattering problem for these operators:[15,16]

$$\pi_k=\prod_{l=1}^{k-1}\mathbf{T}(\mu_l+i/2)\mathbf{A}(\mu_k+i/2)\prod_{l=k+1}^{M}\mathbf{T}(\mu_l+i/2)\tag{3.3}$$

and then use the fact that our state $|1\rangle$ is an eigenstate of the $\mathbf{T}(\lambda)$, as well as the commutation relations satisfied by the $\mathbf{A}(\lambda)$ and $\mathbf{B}(\lambda)$. In this way we can reduce Eq. (3.1) [respectively, Eq. (3.2)] to a sum of expressions of the type $\langle\downarrow|\mathbf{B}(\tilde{\lambda}_1)\cdots\mathbf{B}(\tilde{\lambda}_{M/2})\mathbf{B}(\lambda_1)\cdots\mathbf{B}(\lambda_{M/2})|\uparrow\rangle$ (respectively $\langle\uparrow|\mathbf{C}(\tilde{\lambda}_1)\cdots\mathbf{C}(\tilde{\lambda}_{M/2})\mathbf{B}(\lambda_1)\cdots\mathbf{B}(\lambda_{M/2})|\uparrow\rangle$). These can finally be expressed as determinants either using Eq. (2.2), or according to the general formula for scalar products (p. 237 of Ref. 8).

The case $n=1$ is trivial: $|1\rangle$ is an eigenstate of $\mathbf{R}$, and therefore $\langle\pi_k\rangle=1/2$. The simplest higher correlation function is the emptiness formation probability where all k_i are nearest neighbors, in which case we obtain immediately

$$\langle \pi_{k+1}\cdots\pi_{k+n}\rangle=\prod_{l=k+1}^{k+n}\left[a(\mu_l+i/2)\prod_{j=1}^{M/2}\frac{\sinh(\gamma(\mu_l-\lambda_j+i/2))}{\sinh(\gamma(\mu_l-\lambda_j-i/2))}\right]\langle 1|\prod_{l=k+1}^{k+n}\mathbf{A}(\mu_l+i/2)|1\rangle.\tag{3.4}$$

We shall give the thermodynamic limit of this expression in a particular case.

IV. THERMODYNAMIC LIMIT

We shall show in a particular example how to take the thermodynamic limit in formulas (2.12) and (3.4). We set all μ_k to 0 and consider the critical regime, i.e., γ real. We specify the state $|1\rangle$ to be the ground state of the transfer matrices $\mathbf{T}(\lambda)$ (or of the Hamiltonian of the corresponding XXZ spin chain). In the limit $M\to\infty$ the λ_j form a continuous distribution on the real axis determined by its density $\rho(\lambda)=1/(2\cosh(\pi\lambda))$.

Let us first consider the free energy. One can show that the undetermined sign in Eq. (2.11) is $+$, and therefore we have $F=-\log\langle 1|1\rangle$. We now analyze Eq. (2.12) in the large M limit. We see that we have

$$-F\approx M^2\left[\frac{1}{2}\int d\lambda\,\rho(\lambda)\log[\sinh(\gamma(\lambda-i/2))\sinh(\gamma(\lambda+i/2))]\right.$$
$$\left.+\frac{1}{4}\int d\lambda\,\rho(\lambda)d\lambda'\rho(\lambda')\log\frac{\sinh(\gamma(\lambda-\lambda'+i))}{\sinh(\gamma(\lambda-\lambda'))}\right]+M\frac{1}{2}\log\sin\gamma+\log\det D. \quad (4.1)$$

The terms of order M^2 form the bulk free energy. In order to go further we have to analyze the behavior of the determinant. It is easy to see that the determinant of the matrix $D\equiv[\partial\varphi_j/\partial\lambda_{j'}]$ is dominated by its diagonal elements; the latter are, by definition of $\rho(\lambda)$,

$$\frac{\partial\varphi_j}{\partial\lambda_j}=2\pi\frac{M}{2}\rho(\lambda_j) \quad (4.2)$$

and therefore

$$\log\det D\approx\frac{M}{2}\log(\pi M)+\frac{M}{2}\int d\lambda\,\rho(\lambda)\log\rho(\lambda). \quad (4.3)$$

This gives us the expansion of the free energy up to linear terms in the size M. Note that similar expressions [with different densities $\rho(\lambda)$] can be found for other states, as long as they have a proper $M\to\infty$ limit.

As to the correlation functions, it is known that there is a general multiple integral representation for correlation functions in the thermodynamic limit[17] (see also Refs. 18 and 19). We shall not repeat the derivation here; let us simply mention that starting for example from (3.4), one can prove the following formula:[15,20]

$$\langle\pi_{k+1}\cdots\pi_{k+n}\rangle=2^{-n}\left(\frac{\pi}{\zeta}\right)^{n(n-1)/2}\int_{-\infty}^{+\infty}d\rho_1\cdots d\rho_n\prod_{j<k}\frac{\sinh\pi(\rho_j-\rho_k)}{\sinh\gamma(\rho_j-\rho_k-i)}$$
$$\times\prod_{j=1}^{n}\frac{\sinh^{j-1}\gamma(\rho_j-i/2)\sinh^{m-j}\gamma(\rho_j+i/2)}{\cosh^m\pi\rho_j}. \quad (4.4)$$

This result is identical to the correlation functions of the six-vertex model with periodic boundary conditions.

APPENDIX: A NONDEGENERACY PROPERTY

We assume in this appendix that $q\equiv e^{i\gamma}$ is generic (i.e., not a root of unity, except the isotropic case $q=-1$). We also assume that the spectral parameters $\{\mu_k\}$ do not form any "strings" [i.e., $\mathrm{Im}(\mu_k-\mu_l)\neq 1\ \forall k,l$]. We consider two Bethe states $|1\rangle$ and $|2\rangle$ characterized by two sets $\{\lambda_j^1, j=1,\ldots,m^1\}$ and $\{\lambda_j^2, j=1,\ldots,m^2\}$. Bethe states are eigenstates of the set of commuting transfer matrices $\mathbf{T}(\lambda)$, with corresponding eigenvalue

$$\mathbf{T}(\lambda)|\alpha\rangle=\left[\frac{Q^{\alpha}(\lambda-i)}{Q^{\alpha}(\lambda)}a(\lambda)+\frac{Q^{\alpha}(\lambda+i)}{Q^{\alpha}(\lambda)}d(\lambda)\right]|\alpha\rangle, \tag{A1}$$

where $a(\lambda)$ and $d(\lambda)$ are given by Eq. (2.13) and are independent of the state, whereas Q^{α} characterizes the $\{\lambda_j^{\alpha}\}$:

$$Q^{\alpha}(\lambda)=\prod_{j=1}^{m^{\alpha}}\sinh(\gamma(\lambda-\lambda_j^{\alpha})). \tag{A2}$$

Note that the Bethe ansatz equations are simply the equations which ensure pole cancellation in the eigenvalue of $\mathbf{T}(\lambda)$: Res $\mathbf{T}(\lambda)|\alpha\rangle_{|\lambda=\lambda_j^{\alpha}}=0$.

Because of the symmetry of the transfer matrices $\mathbf{T}(\lambda)$ under the flip operator $\mathbf{R}$, we are only considering states with $m^{\alpha}\leqslant M/2$.

We now assume that $|1\rangle$ and $|2\rangle$ have the same eigenvalue, that is

$$\frac{Q^1(\lambda+i)}{Q^1(\lambda)}a(\lambda)+\frac{Q^1(\lambda-i)}{Q^1(\lambda)}d(\lambda)=\frac{Q^2(\lambda+i)}{Q^2(\lambda)}a(\lambda)+\frac{Q^2(\lambda-i)}{Q^2(\lambda)}d(\lambda)\quad\forall\lambda. \tag{A3}$$

We rewrite this as

$$a(\lambda)[Q^1(\lambda+i)Q^2(\lambda)-Q^2(\lambda+i)Q^1(\lambda)]=d(\lambda)[Q^2(\lambda-i)Q^1(\lambda)-Q^1(\lambda-i)Q^2(\lambda)]. \tag{A4}$$

Up to an overall prefactor $e^{-2(M+m^1+m^2)\gamma\lambda}$, both the left- and right-hand sides are polynomials in $e^{2\gamma\lambda}$ of degree at most $M+m^1+m^2$. Furthermore they have the following $2M$ known zeroes: $\lambda=\mu_k\pm i/2$, $k=1,...,M$. If some μ_k coincide the zeroes have a multiplicity; however note that a $\mu_k+i/2$ cannot coincide with a $\mu_l-i/2$ (since the μ_k are not allowed to form strings). There are now two situations:

(1) $m^1+m^2<M$. In this case we conclude directly that both sides of Eq. (A4) are zero.
(2) $m^1+m^2=M$. Since $m^1\leqslant M/2$ and $m^2\leqslant M/2$, this can only happen if $m^1=m^2=M/2$. However in this case direct computation of the highest degree terms of the polynomials in Eq. (A4) shows that they are zero, and therefore they are in fact of degree at most $2M-1$. Again this means that both sides of the equation are zero.

In either case, we finally find

$$\frac{Q^1(\lambda+i)}{Q^1(\lambda)}=\frac{Q^2(\lambda+i)}{Q^2(\lambda)}\quad\forall\lambda. \tag{A5}$$

If q is not a root of unity, this implies immediately that $\{\lambda_j^1\}=\{\lambda_j^2\}$. What we have proven is the following result:

(A.1) Two Bethe states with $m\leqslant M/2$ (i.e., $S^z\geqslant 0$) correspond to the same eigenvalues of the $\mathbf{T}(\lambda)$ (for all λ) if and only if they are identical.

This has the following two immediate corollaries:

(A.2) Two distinct Bethe states are orthogonal to each other.

(A.3) A Bethe state with $m=M/2$ (i.e., $S^z=0$) is an eigenstate of the flip operator $\mathbf{R}$.

Remark: the situation is much more subtle if q is a root of unity. One way to see this is to consider Eq. (A5), and assume now that $q^{2N}=1$. One can add an extra "full string" of the form $\lambda_i=\lambda_0+ij$, $j=1,...,N$ to one of the sets without modifying the corresponding Q function. This suggests extra degeneracy can appear when q is a root of unity between states with $\Delta S^z=N$, which is precisely the phenomenon observed in Ref. 21.

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Construction of diffusion algebras

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In Isaev *et al.* [J. Phys. A **34**, 5815–5834 (2001)] diffusion algebras were introduced in the context of one-dimensional stochastic processes with exclusion in statistical mechanics. While Isaev *et al.* is based on the needs of the physicist reader and thus states results without proofs and focuses on the discussion of lower-dimensional examples, it is the purpose of this paper to present a construction formalism for diffusion algebras and to use the latter to prove the results in Isaev *et al.* © *2002 American Institute of Physics.* [DOI: 10.1063/1.1473220]

I. INTRODUCTION

Diffusion algebras play a key role in the understanding of one-dimensional stochastic processes. In the case of N species of particles with only nearest-neighbor interactions with exclusion on a one-dimensional lattice, diffusion algebras are useful tools in finding expressions for the probability distribution of the stationary state of these processes. Following the idea of matrix product states,[1,2] the latter are given in terms of monomials built from the generators of a quadratic algebra. Depending on whether the system is closed, i.e., the stochastic process is defined on a ring, or open, in which case boundary conditions at the end of the lattice come into play, this expression varies; Ref. 3 presents an exposition of these facts and the reader is referred to this reference and references within for more details about the application of diffusion algebras in physics.

It is the purpose of this work to treat diffusion algebras from the mathematician's point of view and to prove a construction theorem for diffusion algebras. We consider the following setting.

Let $\alpha<\beta\in I_N:=\{1,\ldots,N\}$ and consider quadratic relations of the form

$$g_{\alpha\beta}D_\alpha D_\beta - g_{\beta\alpha}D_\beta D_\alpha = x_\beta D_\alpha - x_\alpha D_\beta \tag{1}$$

with $g_{\alpha\beta}\in\mathbb{R}\backslash\{0\}$, $g_{\beta\alpha}\in\mathbb{R}$, and $x_\alpha\in\mathbb{C}$. [Note that dependence on all the nonvanishing coefficients x_α in (1) is easily suppressed by rescaling the elements D_α as $x_\alpha D_\alpha$. We choose to display the dependence on these coefficients here, because they are important in applications to stochastic models, which is the physical motivation for the study of this type of algebra.] Then one has

Definition 1.1: An algebra with generators $\{D_\alpha|\alpha\in I_N\}$ and relations of type (1) is called diffusion algebra, if it admits a linear PBW-basis of ordered monomials of the form

$$D_{\alpha_1}^{k_1}D_{\alpha_2}^{k_2}\cdots D_{\alpha_n}^{k_n},\quad k_j\in\mathbb{N}^0 \tag{2}$$

with $\alpha_1>\alpha_2>\cdots>\alpha_n$.

We remark that although we formulate the mathematical setting for coefficients in $\mathbb{R}$ in relation (1), for physical reasons only relations with positive coefficients $g_{\alpha\beta}\in\mathbb{R}^{>0}$ and $g_{\beta\alpha}$

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$\in \mathbb{R}^{\geqslant 0}(\alpha<\beta)$ are relevant, because they are interpreted as hopping rates in stochastic models. Since we are treating diffusion algebras from the mathematical point of view here, we will not impose this restriction, but comment on the implications of this restriction on our results after the main theorem.

The requirement of having a PBW basis (2) implies conditions on the coefficients $g_{\alpha\beta}$ and x_α in (1) according to the diamond lemma in ring theory.[4] In particular, the latter gives a criterion to check under which conditions the relations in (1) are of PBW type: it is the case if each subset of three generators $\{D_\alpha, D_\beta, D_\gamma\}$ with ordering $\alpha<\beta<\gamma$ is reduction unique with respect to the ordering, that is if the two ways of reducing the monomial $D_\alpha D_\beta D_\gamma$ to the monomial $D_\gamma D_\beta D_\alpha$ lead to the same result when expressed in the PBW basis (2).

The task of deriving all diffusion algebras with N generators thus reduces to the following two steps:

(1) Find all diffusion algebras with three generators.
(2) Find all algebras with N generators such that each subset of three generators coincides with one of the cases listed before.

The first is a trivial exercise, which amounts to finding those coefficients $g_{\alpha\beta}$ and x_α in (1) for which a set $\{D_\gamma, D_\beta, D_\alpha\}$ of three generators is reduction unique in the above-mentioned sense. The corresponding list of algebras is given in Ref. 3, and we review it here in order to set up notation and render this paper self-contained. The second is a combinatorial problem, and requires one to combine in a consistent way the three generator algebras listed before to algebras with N generators for general $N>3$.

A construction method for diffusion algebras, and thus a constructive method to approach the second point, is the so-called blending procedure in Ref. 3, which is an inductive procedure for the construction of diffusion algebras. It uses the three generator cases and augments them to larger units by attaching further generators in accordance with the requirements of the diamond lemma, then giving a prescription of how these larger building blocks may be glued (or in the terminology of Ref. 3 ''blended'') together in order to obtain a general diffusion algebra of N generators. The advantage of the inductive procedure is that it facilitates the construction of representations, which are crucial for applications in physics. The main purpose of this paper is to provide a different construction method, which is more suitable for mathematical purposes, in particular, to deliver a proof for the fact that the set of algebras obtained via the blending procedure corresponds exactly to the set of diffusion algebras in Definition 1.1.

After recalling the three-generator case in Sec. II, we present in Sec. III a derivation of diffusion algebras from first principles. Furthermore, we present in Sec. III a compact formulation for the blending procedure, and obtain the exhaustiveness of the inductive approach in Ref. 3 as a corollary to our main theorem.

II. REVIEW OF DIFFUSION ALGEBRAS WITH THREE GENERATORS

As mentioned in Sec. I, the three-generator case provides the building blocks for the derivation of diffusion algebras according to the diamond lemma and we therefore briefly recall the results of Ref. 3 for this case.

Consider a set $\{D_\alpha, D_\beta, D_\gamma\}$ of three generators with an ordering induced by the ordering of the index set $\alpha<\beta<\gamma$ and relations as in (1). Since $g_{\alpha\beta}\neq 0$ for all $\alpha<\beta\in I_N$ by assumption, we can cast the relations into the following form:

$$\begin{aligned} D_\alpha D_\beta &= q_{\beta\alpha} D_\beta D_\alpha + x_\beta^{\alpha\beta} D_\alpha - x_\alpha^{\alpha\beta} D_\beta, \\ D_\alpha D_\gamma &= q_{\gamma\alpha} D_\gamma D_\alpha + x_\gamma^{\alpha\gamma} D_\alpha - x_\alpha^{\alpha\gamma} D_\gamma, \\ D_\beta D_\gamma &= q_{\gamma\beta} D_\gamma D_\beta + x_\gamma^{\beta\gamma} D_\beta - x_\beta^{\beta\gamma} D_\gamma, \end{aligned} \tag{3}$$

where $q_{ji}:=g_{ji}/g_{ij}$, $x_k^{ij}:=x_k/g_{ij}$ for $k,\ i<j\in\{\alpha,\beta,\gamma\}$. Then, using (3), any monomial can be expressed in terms of the PBW basis (2). This is well defined, if applying (3) in different orders leads to the same result, that is if the reductions

$$D_\alpha D_\beta D_\gamma \to D_\beta D_\alpha D_\gamma \to D_\beta D_\gamma D_\alpha \to D_\gamma D_\beta D_\alpha \tag{4}$$

and

$$D_\alpha D_\beta D_\gamma \to D_\alpha D_\gamma D_\beta \to D_\gamma D_\alpha D_\beta \to D_\gamma D_\beta D_\alpha \tag{5}$$

using (3) coincide when expressed in the PBW basis (2).[4] This leads to restrictions on the coefficients $g_{\alpha\beta}$ and x_α in (1). In particular, they are constrained by a set of six equations [see (2.5)–(2.10) in Ref. 3] and their solutions determine all diffusion algebras of three generators. The latter are listed here for future convenience and in order to set up notations. Throughout this section, we assume $\alpha<\beta<\gamma$ and $x_j\neq 0$ for $j\in\{\alpha,\beta,\gamma\}$.

(1) *The case of A_I:*

$$\begin{aligned} g[D_\alpha,D_\beta]&=x_\beta D_\alpha - x_\alpha D_\beta,\\ g[D_\alpha,D_\gamma]&=x_\gamma D_\alpha - x_\alpha D_\gamma,\\ g[D_\beta,D_\gamma]&=x_\gamma D_\beta - x_\beta D_\gamma, \end{aligned} \tag{6}$$

where $g\neq 0$.

(2) *The case of A_{II}:*

$$\begin{aligned} g_{\alpha\beta}D_\alpha D_\beta&=x_\beta D_\alpha - x_\alpha D_\beta,\\ g_{\alpha\gamma}D_\alpha D_\gamma&=x_\gamma D_\alpha - x_\alpha D_\gamma,\\ g_{\beta\gamma}D_\beta D_\gamma&=x_\gamma D_\beta - x_\beta D_\gamma, \end{aligned} \tag{7}$$

where $g_{ij}:=g_i-g_j$ with $g_i\neq g_j$ for all $i<j\in\{\alpha,\beta,\gamma\}$.

(3) *The case of $B^{(1)}$:*

$$\begin{aligned} g_\beta D_\alpha D_\beta-(g_\beta-\Lambda)D_\beta D_\alpha&=-x_\alpha D_\beta,\\ gD_\alpha D_\gamma-(g-\Lambda)D_\gamma D_\alpha&=x_\gamma D_\alpha - x_\alpha D_\gamma,\\ g_\beta D_\beta D_\gamma-(g_\beta-\Lambda)D_\gamma D_\beta&=x_\gamma D_\beta, \end{aligned} \tag{8}$$

where $g\neq 0$ and $g_\beta\neq 0$. For the same ordering, we also find relations of type $B^{(1)}$ which are relations (8) with an exchange $\alpha\leftrightarrow\beta$ or $\gamma\leftrightarrow\beta$ and restrictions $g\neq 0$ and $g_\alpha\notin\{0,\Lambda\}$ or, respectively, $g\neq 0$ and $g_\gamma\notin\{0,\Lambda\}$ on the parameters.

(4) *The case of $B^{(2)}$:*

$$\begin{aligned} g_{\alpha\beta}D_\alpha D_\beta&=-x_\alpha D_\beta,\\ g_{\alpha\gamma}D_\alpha D_\gamma-g_{\gamma\alpha}D_\gamma D_\alpha&=x_\gamma D_\alpha - x_\alpha D_\gamma,\\ g_{\beta\gamma}D_\beta D_\gamma&=x_\gamma D_\beta, \end{aligned} \tag{9}$$

where $g_{\alpha\beta}$, $g_{\alpha\gamma}$ and $g_{\beta\gamma}\neq 0$.

(5) *The case of $B^{(3)}$:*

$$gD_\alpha D_\beta-(g-\Lambda)D_\beta D_\alpha=x_\beta D_\alpha - x_\alpha D_\beta,$$

$$g_\gamma D_\alpha D_\gamma = -x_\alpha D_\gamma, \tag{10}$$

$$(g_\gamma - \Lambda) D_\beta D_\gamma = -x_\beta D_\gamma,$$

where $g \neq 0$ and $g_\gamma \notin \{0, \Lambda\}$.

(6) *The case of* $B^{(4)}$*:*

$$(g_\alpha - \Lambda) D_\alpha D_\beta = x_\beta D_\alpha,$$

$$g_\alpha D_\alpha D_\gamma = x_\gamma D_\alpha, \tag{11}$$

$$g D_\beta D_\gamma - (g - \Lambda) D_\gamma D_\beta = x_\gamma D_\beta - x_\beta D_\gamma,$$

where $g \neq 0$ and $g_\alpha \notin \{0, \Lambda\}$.

(7) *The case of* $C^{(1)}$*:*

$$g_\beta D_\alpha D_\beta - (g_\beta - \Lambda) D_\beta D_\alpha = -x_\alpha D_\beta,$$

$$g_\gamma D_\alpha D_\gamma - (g_\gamma - \Lambda) D_\gamma D_\alpha = -x_\alpha D_\gamma, \tag{12}$$

$$g_{\beta\gamma} D_\beta D_\gamma - g_{\gamma\beta} D_\gamma D_\beta = 0,$$

where g_β, g_γ and $g_{\beta\gamma} \neq 0$. For the same ordering, we also find relations of type $C^{(1)}$ which are relations (12) with an exchange $\alpha \leftrightarrow \beta$ or $\alpha \to \gamma \to \beta \to \alpha$ and restrictions $g_\alpha \neq \Lambda$ and $g_\gamma, g_{\alpha\gamma} \neq 0$ or, respectively, $g_\alpha, g_\beta \neq \Lambda$ and $g_{\alpha\beta} \neq 0$ on the parameters.

(8) *The case of* $C^{(2)}$*:*

$$g_{\alpha\beta} D_\alpha D_\beta - g_{\beta\alpha} D_\beta D_\alpha = -x_\alpha D_\beta,$$

$$g_{\alpha\gamma} D_\alpha D_\gamma - g_{\gamma\alpha} D_\gamma D_\alpha = -x_\alpha D_\gamma, \tag{13}$$

$$D_\beta D_\gamma = 0,$$

where $g_{\alpha\beta}$ and $g_{\alpha\gamma} \neq 0$. For the same ordering, we also find relations of type $C^{(2)}$ which are relations (13) with an exchange $\alpha \leftrightarrow \beta$ or $\alpha \to \gamma \to \beta \to \alpha$ and restrictions $g_{\alpha\beta}, g_{\beta\gamma} \neq 0$ or, respectively, $g_{\alpha\gamma}, g_{\beta\gamma} \neq 0$ on the parameters.

(9) *The case of D:* With $q_{ji} := g_{ji}/g_{ij}$, $i, j \in \{\alpha, \beta, \gamma\}$ (recall that $g_{ij} \neq 0$ for $i < j$) we have

$$D_\alpha D_\beta - q_{\beta\alpha} D_\beta D_\alpha = 0,$$

$$D_\alpha D_\gamma - q_{\gamma\alpha} D_\gamma D_\alpha = 0, \tag{14}$$

$$D_\beta D_\gamma - q_{\gamma\beta} D_\gamma D_\beta = 0.$$

We remark that the division into algebras of type A, B, C, and D reflects the number of coefficients x_j, $j \in \{\alpha, \beta, \gamma\}$, being zero in comparison with the general form (1): for algebras of type A, B, C, and D, respectively, none, one, two, or all three of the coefficients x_i vanish. The subdivision for each type then corresponds to the different choices for the coefficients $g_{\alpha\beta}$, which are compatible with the diamond lemma.

III. THE CASE OF GENERAL *N*

This section consists of four parts: we start by providing a decomposition of the index set which later facilitates the presentation of the algebras. In other words, we decompose the whole family of algebras, which depends on the ordered set of parameters $\{g_{\alpha\beta}, x_\alpha | \alpha, \beta \in I\}$ in the

relations (1), into several subfamilies. Each subfamily is determined by a specific subset of the parameters x_α and $g_{\alpha\beta}$, which are subject to a set of conditions formulated in the following [see conditions (16), (20)–(23), (24) and (26)].

As a next step, we list some general properties specific to diffusion algebras in each of the subfamilies. They are later used in the proof of the main result. This is followed by the list of diffusion algebras and a theorem which proves the exhaustiveness of the approach. We finally comment on the counting of diffusion algebras.

A. Decomposition of the index set

The structure of the algebras in (6)–(14) suggests the following decomposition of the index set $I_N=\{1,\ldots,N\}$:

$$I_N = I \cup R, \tag{15}$$

where

$$\begin{aligned} I &:= \{\alpha \in I_N | x_\alpha \neq 0\}, \\ R &:= \{\alpha \in I_N | x_\alpha = 0\}. \end{aligned} \tag{16}$$

In the following we will use the notation $N_I := |I|$ and $N_R := |R|$ for the cardinalities of these sets.

We introduce the following terminology and notations:

Definition 3.1: Normal ordering of two generators D_α and D_β is defined as

$$:D_\alpha D_\beta: := \begin{cases} D_\alpha D_\beta & if\ \alpha < \beta \\ D_\beta D_\alpha & if\ \beta < \alpha. \end{cases} \tag{17}$$

Definition 3.2: For $\alpha<\beta$ we introduce the following short-hand notation:

$$[D_\alpha, D_\beta]_{q_{\beta\alpha}} := D_\alpha D_\beta - q_{\beta\alpha} D_\beta D_\alpha, \tag{18}$$

where the index at the commutator is referring to the coefficients $q_{\beta\alpha}$ in terms of which the commutator is defined.

Using these notations, we subdivide the set R into nonintersecting and nonempty subsets

$$R := R_1 \cup R_2 \cup \cdots \cup R_{M_R} \tag{19}$$

according to the following requirements.

(1) Relations between generators from the sets R_a and R_b for $a \neq b$ are given by

$$:D_{r_1} D_{r_2}: = 0, \quad \forall r_1 \in R_a \ \text{ and } \ \forall r_2 \in R_b. \tag{20}$$

(2) Relations within a set R_a such that $|R_a| \geqslant 2$ are given by

$$[D_{r_1}, D_{r_2}]_{q_{r_2 r_1}} = 0, \quad \forall r_1 < r_2 \in R_a, \tag{21}$$

where the coefficients in (21) are subject to the condition opposite to (20), that is: for any subdivision $R_a = R' \cup R''$ into two nonintersecting and nonempty parts R' and R'',

$$\exists r_1 \in R' \ \text{ and } \ r_2 \in R'' : g_{r_1 r_2} g_{r_2 r_1} \neq 0. \tag{22}$$

In other words, this means that for any pair of indices $r, s \in R_a$ there exists a finite sequence $\{r_k \in R_a | k = 1, \ldots, n\}$ such that $r_1 = r$, $r_n = s$ and

$$\prod_{k=1}^{n-1} g_{r_k r_{k+1}} g_{r_{k+1} r_k} \neq 0. \tag{23}$$

Thus, relations (22) and (23) may be represented graphically via a *connectivity condition* on an ordered graph the vertices of which are labeled by the indices $r \in R_a$ and the edges connect only those vertices $r_1 < r_2$ for which the condition $q_{r_2 r_1} \neq 0$ is satisfied.

Furthermore, for $N_I \geqslant 2$ we split the set R into two sets S and T as follows:

For any $R_a \subset R$ we define

$$R_a := \begin{cases} S_a & \text{if } \exists r \in R_a \text{ and } i \in I: g_{ir} g_{ri} \neq 0, \\ T_a & \text{otherwise.} \end{cases} \tag{24}$$

Suppose that the M_R sets R_a in (19) split into M_S sets S_a and M_T sets T_a in this way, thus $M_R = M_S + M_T$. We number these sets as S_a, $a = 1,\ldots,M_S$, and T_a, $a = 1,\ldots,M_T$, and introduce

$$S := \cup_{a=1}^{M_S} S_a, \quad T := \cup_{a=1}^{M_T} T_a. \tag{25}$$

Although the decomposition of the set S into subsets S_a has been used in the definition of the set S, it will not be of practical importance in what follows. Contrary to that, the structure of the set T is crucial and needs further refinement.

For any $T_a \subset T$ define

$$T_a := \begin{cases} T_a^{\bullet} & \text{if } \exists i < j \in I: \quad T_a \subset \{i+1, i+2 \ldots, j-1\} \text{ and} \\ & \qquad\qquad I \cap \{i+1, i+2, \ldots, j-1\} = \varnothing \\ T_a^{\circ} & \text{otherwise.} \end{cases} \tag{26}$$

Thus in short-hand notation $T = \{T_a^{\bullet} | a = 1,\ldots,M_T^{\bullet}\} \cup \{T_a^{\circ} | a = 1,\ldots,M_T^{\circ}\}$ with $M_T = M_T^{\bullet} + M_T^{\circ}$.

B. General structural remarks about *N*-generator diffusion algebras

Until now we have primarily discussed index sets. By an abuse of terminology, we will from now on also refer to "generators of a set I, S, T, or R," meaning the generators indexed by elements from the corresponding set.

Definition 3.3: A set of three generators $\{D_x, D_y, D_z\}$ with x, y, and $z \in X$, Y, Z, respectively, where X, Y, and Z are any of the sets I, R, S, and T or any set in their decomposition will be called a triplet (of type) $\{X,Y,Z\}$.

Note that any triplet of type $\{I,I,I\}$ in a diffusion algebra of $N \geqslant 3$ generators gives rise to a diffusion algebra of type A_I or A_{II}, any triplet of type $\{I,I,R\}$ to a diffusion algebra of type $B^{(1)}$, $B^{(2)}$, $B^{(3)}$, or $B^{(4)}$, any triplet of type $\{I,R,R\}$ to a diffusion algebra of type $C^{(1)}$ or $C^{(2)}$, and any triplet of type $\{R,R,R\}$ to a diffusion algebra of type D.

Then we have:

Lemma 3.4: For any Diffusion algebra (1) with $N \geqslant 3$ generators the following statements hold

(1) If $N_I \geqslant 3$, then all subalgebras corresponding to triplets of type $\{I,I,I\}$ are of the same type, which is either A_I (that is, $g_{ij} = g$ $\forall i,j \in I$) or A_{II} (that is, $g_{ji} = 0$, $g_{ij} = g_i - g_j$, $g_i \neq g_j$, $\forall i < j \in I$).

(2) If $N_I \geqslant 3$ and all subalgebras corresponding to triplets $\{I,I,I\}$ are of type A_I then for any $s \in S$ and for all $i \in I$ one has

$$g_{is} = g_{si} = g_s. \tag{27}$$

(3) If $N_I \geqslant 3$ and all subalgebras corresponding to triplets $\{I,I,I\}$ are of type A_{II} then $S = \varnothing$.

(4) Let $N_I \geqslant 2$.

For any $i \in I$ *and for all* $t,t' \in T_a$ *(here* T_a *means both* $T_a^{\bigcirc}$ *and* $T_a^{\bullet}$*) with* $t<i$ *and* $t'>i$ *the coefficients* g_{ti} *and* $g_{it'}$ *depend only on the index* a *of the set* T_a *and not on the individual indices* t *or* t'. *If* $t,t' \in T_a^{\bigcirc}$ *one furthermore has* $g_{ti}=-g_{it'}$.

For any $i<j \in I$ *and for all* $t,t' \in T_a : t<i$ *and* $t'>j$,

$$g_{ti}+\Lambda_{ij}=g_{tj}, \tag{28}$$

$$g_{it'}=g_{jt'}+\Lambda_{ij}, \tag{29}$$

where $\Lambda_{ij} := g_{ij}-g_{ji}$.

(5) Let $N_I=1$. *Denote the only index in* I *as* $\mathbf{i}$ *in order to stress that it is not a running index. For all* $r \in R_a$ *one has*

$$g_{\mathbf{i}r}-g_{r\mathbf{i}}=\Lambda_a. \tag{30}$$

Note that both the left- and the right-hand sides of relation (30) depend only on the index a *of the set* R_a *and not on the individual index* r.

Proof of (1): It follows from the fact that in each set $\{D_i,D_j,D_k | i,j,k \in I\}$ one has either $g_{\beta\alpha} \neq 0$ for all $\alpha<\beta \in \{i,j,k\}$, or, $g_{\beta\alpha}=0$, for all $\alpha<\beta \in \{i,j,k\}$, but no mixture thereof, which contradicts a mixing of A_I and A_{II} type algebras.

Proof of (2): Let $N_I \geqslant 3$ and $g_{ij}=g \ \forall i,j \in I$. By (25) it is enough to check (27) for any $S_a \subset S$. Consider an index $r \in S_a$ which satisfies the condition $g_{rj}g_{jr} \neq 0$ for some $j \in I$. Then, for any $i \in I$, the triplets $\{D_r,D_i,D_j\}$ are all of type $B^{(1)}$ with $\Lambda=0$ and, hence, $g_{ir}=g_{ri}=g_r$.

Next, take any $s \in S_a$. By definition, there exists a sequence $r_k \in S_a$, $k=1,\ldots,n$, such that $r_1=r$, $r_n=s$ and such that the connectivity condition (23) is satisfied. Then, for any $i \in I$, starting with the triplet $\{D_{r_1},D_{r_2},D_i\}$ one inductively proves that all the triplets $\{D_{r_k},D_{r_{k+1}},D_i\}$ are of type $C^{(1)}$ with $\Lambda=0$, and hence (27) follows.

Proof of (3): Let $N_I \geqslant 3$ and $g_{ji}=0$, $g_{ij}=g_i-g_j$, $g_i \neq g_j$, $\forall i<j \in I$ and suppose $S \neq \varnothing$. Consider some $S_a \subset S$ and take those indices $r \in S_a$ and $i_0 \in I$ for which condition $g_{i_0r}g_{ri_0} \neq 0$ is satisfied. For any $j,k \in I$ the triplets $\{D_{i_0},D_j,D_r\}$ and $\{D_{i_0},D_k,D_r\}$ are both of type $B^{(1)}$, which also implies that the triplets $\{D_j,D_k,D_r\}$, $\forall j,k \in I$, are all of type $B^{(1)}$. Now, there is no mutual ordering of any arbitrarily chosen indices $i<j<k \in I$ and the index $r \in S_p$ for which the existence of any $B^{(1)}$-type triplet $\{D_i,D_j,D_r\}$, $\{D_i,D_k,D_r\}$, and $\{D_j,D_k,D_r\}$ is compatible with the condition that $g_{ik}=g_{ij}+g_{jk}$—a contradiction.

Proof of (4): Let $N_I \geqslant 2$ and consider any three indices $i \in I$ and $t<t' \in T_a$. Exploiting the connectivity property (23) of the set T_a one can find a sequence $\{t_k | k=1,\ldots,n\}$ such that $t_1=t$, $t_n=t'$ and such that all the C-type triplets $\{D_i,D_{t_k},D_{t_{k+1}}\}$ are not of type $C^{(2)}$. Hence, their corresponding nonzero coefficients g_{it_k} (for $i<t_k$) or g_{t_ki} (for $t_k<i$) are subject to the conditions for triplets of type $C^{(1)}$ [see (12)] which together with the definition (24) of the set T_a implies $g_{it}=g_{it'}$ in the case $i<t<t'$, $g_{ti}=g_{t'i}$ in the case $t<t'<i$, and $g_{ti}=-g_{it'}$ in the case $t<i<t'$, thus proving the first part of the fourth statement in the lemma.

To prove the second part notice that for any four indices $i,j \in I$ and $t,t' \in T_a$ which are ordered as $t<i<j<t'$ their corresponding triplets $\{D_t,D_i,D_j\}$ and $\{D_i,D_j,D_{t'}\}$ are of type $B^{(4)}$ and, $B^{(3)}$, respectively. Conditions (28) and (29) then reproduce the relations between the coefficients in those triplets [see Eqs. (10) and (11)].

Proof of (5): Let $N_I=1$ and consider any pair of indices $r,r' \in R_a$. As before, for every connective set R_a there exists a chain of C-type triplets $\{D_{\mathbf{i}},D_{r_k},D_{r_{k+1}}\}$, $k=1,\ldots,n-1$, with $r_1=r$ and $r_n=r'$ which are not of type $C^{(2)}$. Hence one obtains (30) with one and the same coefficient Λ_a for all $C^{(1)}$ type triplets $\{I,R_a,R_a\}$. □

Lemma 3.4 suggests listing diffusion algebras in families according to the number of generators in the set I and provides information about the structure of relations among generators from the sets I, S, T, and R in each case.

C. List of diffusion algebras with *N* generators

In this section, we list all N-generator diffusion algebras and provide a theorem which proves the exhaustiveness of the formalism.

Diffusion algebras with N generators are listed as five families of algebras: A_I, A_{II}, B, C, and D. As in the case of $N=3$ the number of nonzero coefficients x_α or, in other words, the cardinality of the set I is used as a criterion for separating diffusion algebras into families of the types $A(N_I\geqslant 3)$, $B(N_I=2)$, $C(N_I=1)$ or $D(N_I=0)$. Type A algebras are separated further into two families A_I and A_{II} depending on the number of nonzero coefficients g_{ij} with indices i,j in the set I.

Different algebras in the families are obtained in dependence on the choice of the decomposition of the set $I_N=\{1,2,\ldots,N\}$ into *ordered subsets* I, S, T_a°, $a=1,\ldots,M_T^{\circ}$, $T_b^{\bullet}$, $b=1,\ldots,M_T^{\bullet}$ (or R_a, $a=1,\ldots,M_R$ for $N_I=1$) as well as on the choice of coefficients in their defining relations. In the following we adopt a notation for diffusion algebras where the corresponding decomposition of the set I_N is given explicitly as argument to the family symbol. To avoid any confusion let us stress that the subscript indices a and b in our notation are treated as running ones so that, e.g.,

$$A_I(I,S,T_a^{\circ},T_b^{\bullet})\equiv A_I(I,S,T_1^{\circ},\ldots,T_{M_T^{\circ}}^{\circ},T_1^{\bullet},\ldots,T_{M_T^{\bullet}}^{\bullet}),$$

where we imply $I_N=I\cup S\cup(\cup_{a=1}^{M_T^{\circ}}T_a^{\circ})\cup(\cup_{b=1}^{M_T^{\bullet}}T_b^{\bullet})$, and I, S, T_a°, and $T_b^{\bullet}$ are mutually nonintersecting ordered subsets in I_N. The values of the coefficients $g_{\alpha\beta}$ are not shown explicitly in these notations so that in fact our notation displays connnective components in a variety of diffusion algebras rather than the particular algebras.

All relations in (31)–(35) below are to be complemented by relations (20), (21) for the elements of the subset R together with the conditions (22) or (23) on the coefficients involved.

(1) *Diffusion algebras of type* $A_I(I,S,T_a^{\circ},T_b^{\bullet})$, $N_I\geqslant 3$*:*

$$\begin{aligned}
&g[D_i,D_j]=x_jD_i-x_iD_j, \quad \forall i,j\in I,\\
&g_s[D_s,D_i]=x_iD_s, \quad \forall s\in S, i\in I,\\
&g_a^{\circ}:D_iD_t:=-x_iD_t, \quad \forall a,t\in T_a^{\circ}, i\in I,\\
&g_b^{+}D_iD_t=-x_iD_t, \quad \forall b,t\in T_b^{\bullet}, i\in I: i<t,\\
&g_b^{-}D_tD_i=x_iD_t, \quad \forall b,t\in T_b^{\bullet}, i\in I: i>t,
\end{aligned} \tag{31}$$

where g, g_s, g_a°, $g_b^{\pm}\neq 0$.

(2) *Diffusion algebras of type* $A_{II}(I,T_a^{\circ},T_b^{\bullet})$, $N_I\geqslant 3$*:*

$$\begin{aligned}
&(g_i-g_j)D_iD_j=x_jD_i-x_iD_j, \quad \forall i<j\in I,\\
&(g_i+g_a^{\circ}):D_iD_t:=-x_iD_t, \quad \forall a,t\in T_a^{\circ}, i\in I,\\
&(g_i+g_b^{+})D_iD_t=-x_iD_t, \quad \forall b,t\in T_b^{\bullet}, i\in I: i<t,\\
&(g_b^{-}-g_i)D_tD_i=x_iD_t, \quad \forall b,t\in T_b^{\bullet}, i\in I: i>t,
\end{aligned} \tag{32}$$

where $g_i\neq g_j$ for $i\neq j$ and $g_i\notin\{g_a^{\circ},\mp g_b^{\pm}\}$.

(3) *Diffusion algebras of type* $B(I=\{\mathbf{i},\mathbf{j}\},S,T_a^{\circ},T_b^{\bullet})$*:*

We use the notation $\mathbf{i}$ and $\mathbf{j}$ with $\mathbf{i}<\mathbf{j}$ for the two elements of the set I to emphasize that they are not running indices. Note also that $\mathbf{i}<t<\mathbf{j}$ for all $t\in T_b^{\bullet}$ in this case.

$$
\begin{gathered}
gD_{\mathbf{i}}D_{\mathbf{j}}-(g-\Lambda)D_{\mathbf{j}}D_{\mathbf{i}}=x_{\mathbf{j}}D_{\mathbf{i}}-x_{\mathbf{i}}D_{\mathbf{j}},\\
g_sD_{\mathbf{i}}D_s-(g_s-\Lambda)D_sD_{\mathbf{i}}=-x_{\mathbf{i}}D_s,\quad \forall s\in S,\\
g_sD_sD_{\mathbf{j}}-(g_s-\Lambda)D_{\mathbf{j}}D_s=x_{\mathbf{j}}D_s,\quad \forall s\in S,\\
g_a^{\bigcirc}:D_{\mathbf{i}}D_t:=-x_{\mathbf{i}}D_t,\quad \forall t\in T_a^{\bigcirc},\\
(g_a^{\bigcirc}-\Lambda):D_{\mathbf{j}}D_t:=-x_{\mathbf{j}}D_t,\quad \forall t\in T_a^{\bigcirc},\\
g_b^{+}D_{\mathbf{i}}D_t=-x_{\mathbf{i}}D_t,\quad \forall t\in T_b^{\bullet},\\
g_b^{-}D_tD_{\mathbf{j}}=x_{\mathbf{j}}D_t,\quad \forall t\in T_b^{\bullet},
\end{gathered}
\tag{33}
$$

where $g\neq 0$, $g_s\neq 0$ for all s and $g_s\neq\Lambda$ for s such that either $s<\mathbf{i}$ or $s>\mathbf{j}$, $g_a^{\bigcirc}\notin\{0,\Lambda\}$ and $g_b^{\pm}\neq 0$.

(4) *Diffusion algebras of type* $C(I=\{\mathbf{i}\},R_a)$*:*

As in Lemma 3.4 the only element of I is denoted here as $\mathbf{i}$,

$$
g_rD_{\mathbf{i}}D_r-(g_r-\Lambda_a)D_rD_{\mathbf{i}}=-x_{\mathbf{i}}D_r,\quad \forall r\in R_a,
\tag{34}
$$

where $g_r\neq 0$ for $r<\mathbf{i}$ and $g_r\neq\Lambda_a$ for $r>\mathbf{i}$.

(5) *Diffusion algebras of type* $D(R)$*:*

$$
D_rD_s-q_{sr}D_sD_r=0,\quad \forall r<s\in R.
\tag{35}
$$

Theorem 3.5: *The previously given list of algebras is exhaustive and contains all possible diffusion algebras with N generators.*

Proof: According to the diamond lemma, an algebra of N generators with relations of type (1) is a diffusion algebra if each of its triplets $\{D_\alpha,D_\beta,D_\gamma\}$ generates a subalgebra coinciding with one of the cases listed in Sec. II. Lemma 3.4 provides information about possibile consistent combinations of several such triplets and we thus have to demonstrate that the families of algebras (31)–(35) exhaust the list of diffusion algebras which are allowed by this lemma.

Let us start with the case $N_I\geqslant 3$. According to the first statement of Lemma 3.4 there are two possible types of relations between generators from the set I. This gives rise to two families of diffusion algebras—A_I and A_{II}. Statement (2) of Lemma 3.4 describes the relations between the generators from the sets I and S in the case of the family A_I, and the third statement of Lemma 3.4 excludes the presence of a nonempty set S in the case of the family A_{II}. The coefficients in the relations between the generators from the set I and the sets $T_a^{\bigcirc}$ and $T_b^{\bullet}$ are subject to the conditions given in the fourth statement of Lemma 3.4, where $\Lambda_{ij}=0$ for the A_I family and $\Lambda_{ij}=(g_i-g_j)$ for the A_{II} family. These conditions fix the relations between the generators in the families of type A_I and A_{II} to the expressions in (31) and (32). Since the triplets of the form $\{I,S,T\}$ (occurring only for the A_I family) and $\{I,T_a,T_b\}$ for $a\neq b$ are of type $C^{(2)}$, no further conditions arise from these relations. This exhausts all possibilities, and thus no further conditions occur.

Let $N_I=2$. For each subset $S_a\subset S$ the connectivity property (23) implies relations of type $B^{(1)}$ for all triplets $\{I,I,S_a\}$, and thus for any triplet $\{I,I,S\}$. The corresponding relations are listed in the first three lines of (33). The compatibility conditions within the triplets $\{I,T_a,T_a\}$ and $\{I,I,T_a\}$ are given in the fourth statement of Lemma 3.4, where we now have $\Lambda_{\mathbf{ij}}\equiv\Lambda$. These conditions fix the form of the last four lines in (33). Since $C^{(2)}$ type relations for $\{I,S,T\}$ and $\{I,T_a,T_b\}$ $(a\neq b)$ triplets do not imply further restrictions, no further constraints arise.

In the case $N_I=1$ a decomposition of the set R into S and T is not necessary, and we thus work with the whole set R. Then the form of the relations (34) is implied by the fifth statement of Lemma 3.4, which describes the compatibility conditions for the $\{I,R_a,R_a\}$ triplets. The relations in the $C^{(2)}$ triplets $\{I,R_a,R_b\}$ for $a\neq b$ give no further constraints.

In the case $N_I=0$ all the triplets are of type D, which are compatible without any restrictions on the coefficients. □

Note that while mathematically possible, not all algebras in the families are relevant from the physicist's point of view. Due to the fact that the structure constants of diffusion algebras are interpreted as hopping rates, that is probabilities, in the framework of stochastic processes on linear lattices, only non-negative structure constants are relevant. This not only implies restrictions on the structure constants themselves, but also on the decompositions of the set I_N, because some configurations are not compatible with non-negative structure constants. In particular, due to Lemma 3.4, statement (4), part 1, non-negative structure constants throughout are possible only if the subsets $T_a^{\bigcirc}$ fulfill one of the following two requirements:

$$(1)\ \forall t \in T_a^{\bigcirc}\ \text{ and }\ \forall i \in I: t<i\ \text{ or }\ (2)\ \forall t \in T_a^{\bigcirc}\ \text{ and }\ \forall i \in I: t>i. \tag{36}$$

We conclude this section with some comments on the classification problem for diffusion algebras. To deal with the problem one should first establish criteria of equivalence, and we discuss two natural ones here.

(1) One can consider linear transformations on the set of generators $\{D_\alpha | \alpha \in I_N\}$. However, there is the difficulty that not all linear transformations respect the ansatz (1). There are two special cases: rescaling transformations $D_\alpha \to \kappa_\alpha D_\alpha$ and substitution transformations $D_\alpha \to D_{\sigma(\alpha)}$, where σ is an element of the symmetric group $\mathcal{S}_N$.

As has already been mentioned in Sec. I, rescalings may be used to fix (depending on the context of the physical application) some special values for the nonzero coefficients x_α. In particular, this implies that the values of the nonzero coefficients x_α are not relevant.

The substitution transformations clearly respect the form of the relations (1), but may contradict the requirement on the mutual ordering of the generators, that is $g_{\alpha\beta}\neq 0$ for $\alpha<\beta$. In particular, a permutation of the elements from different subsets T_a and between the subsets T and S, or T and I is strictly forbidden. In addition, one cannot permute two elements $r<s$ in the same subset R_a unless $q_{sr}\neq 0$. On the other hand, permutations inside the subset I and (in most cases) between the subsets I and S are allowed unless they contradict the above-described requirements. Thus, substitution transformations establish certain equivalence classes inside each of the families $A_I(I,S,T_a^{\bigcirc},T_b^{\bullet})$, $A_{II}(I,T_a^{\bigcirc},T_b^{\bullet})$, $B(\{\mathbf{i},\mathbf{j}\},S,T_a^{\bigcirc},T_b^{\bullet})$, $C(\{\mathbf{i}\},R_a)$, and $D(R)$. These equivalence classes can be calculated in concrete cases, but one hardly expects their complete description in the case of general N.

Note that besides the rescalings and the substitutions which always exist there may occur other types of linear transformations which relate different types of diffusion algebras. For instance, in the case of $N=3$ the $C^{(1)}$ type algebras in (12) with $\Lambda\neq 0$ can be reduced to (a subclass of) D type algebras by the transformation $D_\alpha \to D_\alpha - x_\alpha/\Lambda$. For general N, such transformations allow one to reduce the number of nonzero parameters Λ_a in the family of C type diffusion algebras in (34) by 1.

(2) One can use the algebra antihomomorphism which simultaneously inverts multiplication in the algebra, that is $D_\alpha D_\beta \to D_\beta D_\alpha$, and the order of indices, that is $\alpha<\beta \to \alpha>\beta$. This transformation amounts to a mirror reflection of the corresponding stochastic processes. For example, in the list of diffusion algebras with $N=3$ the families $B^{(3)}$ and $B^{(4)}$ are mirror symmetric. Further examples of mirror symmetry for the case $N=4$ can be found in Ref. 3 in Appendix B.

D. Description of the blending procedure

The blending procedure is a constructive method to generate diffusion algebras. The corresponding construction theorem states that any diffusion algebra can be obtained from a set of building blocks [Eqs. (4.1)–(4.7) in Ref. 3] via blending. In the following table we describe the correspondence between the building blocks from Ref. 1 (left-hand column below) and the specific subclasses of the families in Theorem 3.5 (right-hand column below):

$$
\begin{aligned}
A_I^{(1)} &: A_I(I,S), \quad T=\varnothing, \\
A_I^{(2)} &: A_I(I,T^{\bigcirc}), \text{ and } A_{II}(I,T^{\bullet}), \quad S=\varnothing, \\
A_{II} &: A_{II}(I,T^{\bigcirc}), \text{ and } A_{II}(I,T^{\bullet}), \\
B^{(1)} &: B(I=\{\mathbf{i},\mathbf{j}\},S), \quad T=\varnothing, \\
B^{(2)} &: B(I=\{\mathbf{i},\mathbf{j}\},T^{\bigcirc}), \text{ and } B(I=\{\mathbf{i},\mathbf{j}\},T^{\bullet}), \quad S=\varnothing, \\
C &: C(I=\{\mathbf{i}\},R), \\
D &: D(R).
\end{aligned}
\tag{37}
$$

Here it is understood that the sets $T^{\bigcirc}$ and $T^{\bullet}$ whenever they appear in the right-hand column are the only connective components in the decomposition (25) of the subset $T \in I_N$. The connectivity condition may be also imposed on the subsets S and R in the right-hand column of (37). We remark that the mathematical setting adopted in the present paper allow us to extract elementary building blocks for the blending procedure. They are shown in the right-hand column of (37) and the blocks listed in the left-hand column and used in Ref. 3 can be constructed by blending of an arbitrary number of the corresponding blocks from the right-hand column. Note that in the settings of Ref. 3 extracting the elementary blocks would only amount to imposing additional connectivity conditions (23) on the coefficients $g_{\alpha\beta}$ in relations (4.1)–(4.7) there and so would not suit the purposes of Ref. 3.

Furthermore we remark that in contrast to Ref. 3 we do not fix the order between $D_{\mathbf{i}}$, $D_{\mathbf{j}}$ and D_s to $\mathbf{i}<s<\mathbf{j}$ for all $s \in S$ in $B(I=\{\mathbf{i},\mathbf{j}\},S)$, because the other orders are needed when blending with $B(I=\{\mathbf{i},\mathbf{j}\},T^{\bigcirc})$ and $B(I=\{\mathbf{i},\mathbf{j}\},T^{\bullet})$ in order to obtain all diffusion algebras. This is an inaccurracy in the formulation of the construction theorem in Ref. 3. Despite that in the list of $N=4$ diffusion algebras given in Appendix B of Ref. 3 the blending of such blocks is treated correctly (see example 13 there).

Let $X_l(I,U_l)$, $l=1,\ldots,K$ denote K building blocks in the list (37), where U_l refers to the set R, S, $T^{\bigcirc}$, or $T^{\bullet}$ corresponding to the building block, and which are such that they have the same number of elements N_I in I with generators D_i, $i \in I$ satisfying in all blocks X_l the same relations among themselves.

Consider an ordered set $\mathcal{I}$ whose elements are labeled by the indices from the sets I, $U_1,\ldots,U_K$ and such that for any $l=1,\ldots,K$ the order of the elements of $\mathcal{I}$ with their labels form I and U_l is the same as the order of the indices in the block $X_l(I,U_l)$. In this situation we say that the order on $\mathcal{I}$ is *compatible* with the orders in the blocks X_l.

Let us denote as $X_{\mathcal{I}}(I,U_1,\ldots,U_K)$ the algebra with generators labeled by the elements in the set $\mathcal{I}$ and which satisfies the following conditions.

(1) For any $l=1,\ldots,K$ the generators of $X_{\mathcal{I}}$ with indices from the subsets I, $U_l \subset \mathcal{I}$ satisfy the same relations as their corresponding generators in the blocks $X_l(I,U_l)$.

(2) For any $l_1 \neq l_2 \in \{1,\ldots,K\}$ and for all $a \in U_{l_1} \subset \mathcal{I}$ and $b \in U_{l_2} \subset \mathcal{I}$ the corresponding generators D_a, $D_b \in X_{\mathcal{I}}$ satisfy the relation

$$
:D_aD_b:=0. \tag{38}
$$

The procedure of constructing the algebras $X_{\mathcal{I}}$ from their building blocks $X_l(I,U_l)$ is called *blending*. Clearly the number of different algebras $X_{\mathcal{I}}$ which are associated with the set of building blocks $\{X_l(I,U_l)\}_{l=1,\ldots,K}$, coincides with the number of different ordered sets $\mathcal{I}$ whose order is compatible with the orders in all blocks X_l.[5]

The following statement made in Ref. 1 is a corollary to the construction theorem 3.5:

Theorem 3.6: *Every diffusion algebra can be obtained via a blending of building blocks in (37).*

IV. CONCLUSION

We have presented a derivation of diffusion algebras, which has led to five different families of algebras: A_I, A_{II} B, C, and D and it has been shown that the approach is exhaustive. Since these families of algebras correspond to the algebras obtained via the blending procedure in Ref. 3, this also proves the construction theorem in Ref. 3.

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Algebraic dynamics in O^*-algebras: A perturbative approach

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In this paper the problem of recovering an algebraic dynamics in a perturbative approach is discussed. The mathematical environment in which the physical problem is considered is that of algebras of unbounded operators endowed with the quasiuniform topology. After some remarks on the domain of the perturbation, conditions are given for the dynamics to exist as the limit of a net of regularized linear maps. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1467609]

I. INTRODUCTION

In the so-called algebraic approach to quantum systems, one of the basic problems to solve consists of the rigorous definition of the algebraic dynamics, i.e., the time evolution of observables and/or states. For instance, in quantum statistical mechanics or in quantum field theory one tries to recover the dynamics by performing a certain limit of the strictly *local* dynamics. However, this can be successfully done only for few models and under quite strong topological assumptions (see, for instance, Ref. 1, and references therein). In many physical models the use of local observables corresponds, roughly speaking, to the introduction of some *cutoff* (and to its successive removal) and this is in a sense a general and frequently used procedure, see Refs. 2–4 for conservative and Refs. 5 and 6 for dissipative systems.

Introducing a cutoff means that in the description of some physical system, we know a *regularized* Hamiltonian H_L, where L is a certain parameter closely depending on the nature of the system under consideration. We assume that H_L is a bounded self-adjoint operator in the Hilbert space $\mathcal{H}$ of the physical system.

There are several possible situations of some interest. Among these we will consider the following ones:

a. H_L *converges to an operator* H. This is apparently the simplest situation. Of course we should specify the sense in which the convergence is understood. But for the moment, we want only to focus on the possible problems that arise.

For each fixed L, we know the solution of the dynamical problem, i.e., we know the solution of the Heisenberg equation

$$i\frac{\mathrm{d}\alpha_L^t(A)}{\mathrm{d}t}=[H_L,\alpha_L^t(A)]. \tag{1}$$

This solution, $\alpha_L^t(A)=e^{iH_Lt}Ae^{-iH_Lt}$, would give the *cutoff* dynamics of the system. Then it makes sense to ask the question as to whether $\alpha_L^t(A)$ converges, possibly in the same sense as H_L converges to H, to the solution $\alpha^t(A)$ of the Heisenberg equation

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$$i\frac{d\alpha^t(A)}{dt}=[H,\alpha^t(A)]. \tag{2}$$

It is worth stressing that even though H is a well-defined self-adjoint operator, it is in general, unbounded. For this reason, while the right-hand side of Eq. (1) is perfectly meaningful, the need for clarifying the right-hand side of Eq. (2) is always in order since H is certainly not everywhere defined in $\mathcal{H}$.

Of course, the analysis of the convergence of $\alpha_L^t(A)$ to $\alpha^t(A)$ [in this case where $\alpha^t(A)$ is explictly known] is significant only for deciding the accuracy of the approximation of $\alpha^t(A)$ with $\alpha_L^t(A)$.

b. H_L *does not converge*. In this case, the situation becomes more difficult and a series of questions arise whose answer is highly nontrivial.

As a first step, one could begin by considering the derivations

$$\delta_L(A)=i[H_L,A]$$

that give, at infinitesimal level, the dynamics of the system.

The first issue, of course, is if these derivations converge, in a certain sense, to a derivation δ and which properties this derivation δ enjoys. For instance, is it a spatial derivation? (i.e, is there a symmetric operator H that *implements*, at least in a generalized sense, the derivation?[7])

Further, can this derivation be integrated to some automorphisms group of the operator algebra we are dealing with? Or, conversely, since δ_L can be integrated without any problem, $\alpha_L^t(A)=e^{iH_Lt}Ae^{-iH_Lt}$, what can be said about the limit of α_L^t? And how are these two problems related? These questions are well-known not to admit an easy general solution.

In this paper we will be mainly concerned with situation (a) above, while we will only make a few comments on the more difficult situation (b), which will be considered in more detail in a future paper.

Our basic assumptions is that the Hamiltonian H of the system can be expressed in the form

$$H=H_0+B;$$

in other words, our approach is tentatively *perturbative*: indeed, we suppose that we have full knowledge of the *unperturbed system* whose Hamiltonian is H_0. In other words, given H we can extract what we call a free Hamiltonian H_0, which we know in all details, and consider $B:=H-H_0$ as a perturbation of H_0 itself.

As we have already said, handling with unbounded operators poses a problem of domain for the algebra generated by the powers of the Hamiltonian H_0. The natural choice is to take the set of C^∞-vectors of H_0. Once a perturbation B is introduced, it is natural to ask ourselves in which sense the corresponding domain for H is related to that of H_0.

This is the main subject of Sec. II, where we start with the assumption that $\mathcal{D}^\infty(H)=\mathcal{D}^\infty(H_0)$ and derive some properties of the corresponding *quasiuniform* topologies that the two operators define.

Then we give, in a quite general way, conditions on two self-adjoint operators H_0 and H for $\mathcal{D}^\infty(H)$ and $\mathcal{D}^\infty(H_0)$ to coincide.

In Sec. III, we come back to the problem of describing the dynamics of the perturbed system as limit of a cutoff dynamics. In other words, we introduce a regularized Hamiltonian $H_L=Q_L^0HQ_L^0$ where the Q_L^0's are certain spectral projections of the unperturbed Hamiltonian H_0 and we look for conditions under which the unitary group generated by H_L converges to that generated by H. A class of examples fitting our hypotheses is also given.

The main scope of the paper is to try and construct a mathematical environment where this kind of problem can be successfully treated and also to develop techniques that could be adapted for the study of the more relevant case (b) outlined previously. It is worth stressing that this is a rather common situation in physics (think of mean-field models or systems with ultraviolet

cutoff[2,3]) and a perturbative approach should also be considered for the derivations that describe the system at infinitesimal level. A short discussion on this point is made in Sec. IV.

II. THE MATHEMATICAL FRAMEWORK

We begin this section by summarizing some known facts on unbounded operator algebras and their topological properties. We refer to Refs. 4, 8–10 for full details.

Let $\mathcal{D}$ be a dense domain in Hilbert space $\mathcal{H}$; with $\mathcal{L}^\dagger(\mathcal{D})$ we denote the set of all weakly continuous endomorphisms of $\mathcal{D}$. Then to each operator $A\in\mathcal{L}^\dagger(\mathcal{D})$ we can associate an operator $A^\dagger\in\mathcal{L}^\dagger(\mathcal{D})$ with $A^\dagger=A^*_{\restriction\mathcal{D}}$ where A^* is the usual Hilbert adjoint of A. Then $\mathcal{L}^\dagger(\mathcal{D})$, under the usual operations and the involution †, is a*-algebra of unbounded operators or, simply, an O^*-algebra.

Now let S be a self-adjoint operator in $\mathcal{H}$ and

$$\mathcal{D}:=\mathcal{D}^\infty(S)=\cap_{n\geqslant 1}D(S^n).$$

Then $\mathcal{D}$ endowed with the topology t_S of $\mathcal{D}^\infty(S)$ defined by the set of seminorms

$$f\mapsto\|S^n f\|,\quad n=0,1,\ldots$$

or, equivalently

$$f\mapsto\|(1+S^{2n})^{1/2}f\|,\quad n=0,1,\ldots$$

is a reflexive Fréchet space and the topology t_S is equivalent to the topology $t_{\mathcal{L}^\dagger(\mathcal{D})}$ defined on $\mathcal{D}$ by the set of seminorms

$$f\mapsto\|Af\|,\quad A\in\mathcal{L}^\dagger(\mathcal{D}).$$

In the *-algebra $\mathcal{L}^\dagger(\mathcal{D})$ several topologies can be defined. For the purposes of this paper we will only need the *quasiuniform topology* defined on $\mathcal{L}^\dagger(\mathcal{D})$ in the following way. Put

$$\|A\|^{\mathcal{N},B}=\sup_{\phi\in\mathcal{N}}\|BA\phi\|,\quad B\in\mathcal{L}^\dagger(\mathcal{D}),\ \mathcal{N}\ \text{bounded in}\ \mathcal{D}[t_{\mathcal{L}^\dagger(\mathcal{D})}].$$

Then, the quasiuniform topology, $\tau^{\mathcal{D}}_*$ on $\mathcal{L}^\dagger(\mathcal{D})$ is defined by the set of seminorms:

$$A\in\mathcal{L}^\dagger(\mathcal{D})\to\max\{\|A\|^{\mathcal{N},B},\|A^\dagger\|^{\mathcal{N},B}\}.$$

In the case where $\mathcal{D}=\mathcal{D}^\infty(S)$, the quasiuniform topology on $\mathcal{L}^\dagger(\mathcal{D})$ can be described in an easier way.

Indeed, let $\mathcal{F}$ denote the class of all positive, bounded and continuous functions $f(x)$ on $\mathbb{R}_+$, which are decreasing faster than any inverse power of x, i.e., $\sup_{x\in\mathbb{R}_+}x^k f(x)<\infty$, $k=0,1,\ldots$.

Then, if we put

$$\mathcal{S}_f=\{f(S)\phi;\phi\in\mathcal{D},\|\phi\|=1\}$$

for $f\in\mathcal{F}$, the family $\{\mathcal{S}_f\}_{f\in\mathcal{F}}$ is a basis for the bounded sets of $\mathcal{D}[t_S]$.
In practice this means that, for each t_S-bounded set $\mathcal{N}$ in $\mathcal{D}$, there exists an $\mathcal{S}_f$ such that $\mathcal{N}\subset\mathcal{S}_f$.

This fact easily implies that the quasiuniform topology, $\tau^{\mathcal{D}}_*$ on $\mathcal{L}^\dagger(\mathcal{D})$ can be, equivalently, defined by the set of seminorms:

$$\mathcal{L}^\dagger(\mathcal{D})\ni A\mapsto\|A\|^{f,k}_*=\max\{\|S^kAf(S)\|,\|f(S)AS^k\|\}\quad f\in\mathcal{F},k\in\mathbb{N}\cup\{0\},\tag{3}$$

where the norm on the right-hand side of (3) is the usual norm in $\mathcal{B}(\mathcal{H})$. The *-algebra $\mathcal{L}^\dagger(\mathcal{D})[\tau^{\mathcal{D}}_*]$ is, in this case, a complete locally convex*-algebra, i.e., the involution and the right- and left-multiplications are continuous.

Remark: When estimating seminorms of type (3) we will often consider only the term $\|f(S)AS^k\|$; this is exactly what is needed when $A=A^\dagger$. In the general case, any $A\in\mathcal{L}^\dagger(\mathcal{D})$ is a linear combination of symmetric elements and so, as far as only estimates are concerned, the arguments go usually through.

We can now consider more concrete situations. To begin with, we consider the simplest possible example in which a physical system is described by a Hamiltonian H_0 that mathematically is a self-adjoint operator; we assume $H_0\geqslant 1$; then H_0 has a spectral decomposition

$$H_0=\int_1^\infty \lambda\, dE(\lambda).$$

We put, for $L\geqslant 1$,

$$Q_L^0=\int_1^L dE(\lambda) \tag{4}$$

and define the regularized Hamiltonian by

$$H_L=Q_L^0 H_0 Q_L^0.$$

Then if $\mathcal{D}=\mathcal{D}^\infty(H_0)$ it turns out that the operators Q_L^0 and H_L are bounded operators in $\mathcal{B}(\mathcal{H})$ which belong to $\mathcal{L}^\dagger(\mathcal{D})$ (the Q_L^0's are indeed projectors) and they commute with each other and with H_0.

This makes it quite easy to prove the following convergence properties [in what follows the topology $\tau_*^{\mathcal{D}}$ is that defined in Eq. (3) with S replaced by H_0]:

(c1) $H_L\to H_0$ with respect to the topology $\tau_*^{\mathcal{D}}$,
(c2) $e^{itH_L}\to e^{itH_0}$ with respect to the topology $\tau_*^{\mathcal{D}}$,
(c3) for each $A\in\mathcal{L}^\dagger(\mathcal{D})$, $e^{itH_L}Ae^{-itH_L}\overset{\tau_*^{\mathcal{D}}}{\to} e^{itH_0}Ae^{-itH_0}$.

All these statements can be derived from Lemma 2.2.

The next step consists in considering a Hamiltonian

$$H=H_0+B, \tag{5}$$

where B is regarded as a *perturbation* of the operator H_0. We suppose that the cutoff is determined by H_0, i.e., we assume that

$$H_L=Q_L^0(H_0+B)Q_L^0=H_0Q_L^0+Q_L^0BQ_L^0, \tag{6}$$

where Q_L^0 is defined as in Eq. (4) by the spectral family $E(\cdot)$ of H_0. The right-hand side is well defined since $Q_L^0AQ_L^0$ is bounded for any $A\in\mathcal{L}^\dagger(\mathcal{D})$.

Clearly (6) must be read as a formal expression unless the domains of the involved operators are specified. To be more definite, we make the following assumptions:

(a) $\mathcal{D}=\mathcal{D}^\infty(H_0)$,
(b) $D(H_0)\subseteq D(B)$ and $H=H_0+B$ is self-adjoint on $D(H_0)$,
(c) $\mathcal{D}^\infty(H_0)=\mathcal{D}^\infty(H)$.

Under these assumptions, we have:

Lemma 2.1: (1) The topologies t_{H_0} and t_H are equivalent on $\mathcal{D}$; (2) the topologies on $\mathcal{L}^\dagger(\mathcal{D})$ defined, respectively, by the set of seminorms

$$\mathcal{L}^\dagger(\mathcal{D})\ni A\mapsto \max\{\|H_0^kAf(H_0)\|,\|f(H_0)AH_0^k\|\}\quad f\in\mathcal{F},k\in\mathbb{N}$$

and

$$\mathcal{L}^\dagger(\mathcal{D}) \in A \mapsto \max\{\|H^k A f(H)\|, \|f(H) A H^k\|\} \quad f \in \mathcal{F}, k \in \mathbb{N}$$

are equivalent.

Proof: The statement (1) follows by taking into account that H is continuous with respect to t_{H_0} and H_0 is continuous with respect to t_H, according to the fact that the domain is reflexive.

The statement (2) follows from (1), since the family of t_H-bounded subsets of $\mathcal{D}$ and the family of t_{H_0}-bounded subsets coincide. □

By the previous Lemma, the topology $\tau_*^{\mathcal{D}}$, can be described, following the convenience, via the seminorms in H or by those in H_0. Now, we can prove the following

Lemma 2.2: For each $X \in \mathcal{L}^\dagger(\mathcal{D})$, $X = \tau_*^{\mathcal{D}} - \lim_{L\to\infty} Q_L^0 X Q_L^0$.

Proof: First, notice that, for $\ell \in \mathbb{N}^+$, we have

$$\|H_0^{-\ell}(I - Q_L^0)\phi\|^2 = \int_L^\infty \frac{1}{\lambda^{2\ell}} \mathrm{d}(E(\lambda)\phi, \phi) \leqslant \frac{1}{L^{2\ell}} \|\phi\|^2, \quad \forall \phi \in \mathcal{D}$$

and so

$$\|H_0^{-\ell}(I - Q_L^0)\| \to 0 \quad \text{as} \quad L \to \infty.$$

Now let $f \in \mathcal{F}$ and $k \in \mathbb{N}$; then we have

$$\begin{aligned}
\|f(H_0)(B - Q_L^0 B Q_L^0) H_0^k\| &\leqslant \|f(H_0) B H_0^k (I - Q_L^0)\| + \|f(H_0)(1 - Q_L^0) B H_0^k Q_L^0\| = \sup_{\|\phi\| = \|\psi\| = 1} | \\
&< H_0^{-\ell}(1 - Q_L^0)\phi, H_0^{k+\ell} B^+ f(H_0)\psi > | + \sup_{\|\phi\| = \|\psi\| = 1} | \\
&< f(H_0) H_0^\ell B H_0^k Q_L^0 \phi, H_0^{-\ell}(1 - Q_L^0)\psi > | \\
&\leqslant \|H_0^{-\ell}(1 - Q_L^0)\| \|H_0^{k+\ell} B^+ f(H_0)\| + \|H_0^\ell f(H_0) B H_0^k\| \|H_0^{-\ell}(1 - Q_L^0)\| \to 0
\end{aligned}$$

for $L \to \infty$. □

Incidentally, this lemma gives a proof of (c1) and (c2) above. The proof of (c3) requires the use of a triangular inequality of (c2) and of the commutation rule $[H_0, H_L] = 0$.

Taking into account the separate continuity of the multiplication and the previous lemma, we have:

Corollary 2.3: $\delta_L(A) := i[A, H_L]$ *converges to* $\delta(A) := i[A, H]$ *with respect to the topology* $\tau_*^{\mathcal{D}}$.

Going back to our assumptions on the domains, it is apparent that conditions (b) and (c) given previously are quite strong. It is natural to ask the question under which conditions on B they are indeed satisfied.

The domain. Our starting point is an operator

$$H = H_0 + B$$

under the assumption that the *perturbation* B is a symmetric operator and $D(B) \supseteq D(H_0)$. In general H may fail to be self-adjoint, unless B is H_0-bounded in the sense that there exist two real numbers a, b such that

$$\|B\phi\| \leqslant a\|H_0\phi\| + b\|\phi\|, \quad \forall \phi \in D(H_0). \tag{7}$$

If the inf of the numbers a for which 7 holds (the so-called *relative bound*) is smaller than 1, then the Kato–Rellich theorem[11] states that H is self-adjoint and essentially self-adjoint on any core of H_0.

This is clearly always true if B is bounded: in this case the relative bound is 0. In conclusion, the Kato–Rellich theorem gives a sufficient condition for (b) to be satisfied.

Let us now focus our attention on condition (c). We first discuss some examples.

Example 1: To begin with, we stress the fact that the conditions of the Kato–Rellich theorem are not sufficient to imply that $\mathcal{D}^\infty(H)=\mathcal{D}^\infty(H_0)$. This can be seen explicitly with a simple example. Indeed, let us consider the case where $B=P_f$ with $f\in\mathcal{H}\backslash D(H_0)$ and P_f the projection onto the one-dimensional subspace generated by f. It is quite simple to prove that, in this case:

$$D((H_0+P_f)^2)\cap D(H_0^2)=D(H_0)\cap\{f\}^\perp.$$

This equality implies that neither $\mathcal{D}^\infty(H_0+P_f)$ is a subset of $\mathcal{D}^\infty(H_0)$ nor the contrary. So, in this example, $\mathcal{D}^\infty(H)$ and $\mathcal{D}^\infty(H_0)$ do not compare.

Example 2: Let p and q be the operators in $L^2(\mathbb{R})$ defined by

$$(pf)(x)=if'(x),\quad f\in W^{1,2}(\mathbb{R}),$$

$$(qf)(x)=xf(x),\quad f\in\mathcal{F}W^{1,2}(\mathbb{R}),$$

where $\mathcal{F}$ denotes the Fourier transform. Let us consider

$$H_0=p^2+q^2,$$

then, as is known, H_0 is an essentially self-adjoint operator on $\mathcal{S}(\mathbb{R})$ and this domain is exactly $\mathcal{D}^\infty(H_0)$.

Let us now take as B the operator $-q^2$, then

$$\mathcal{D}^\infty(H)=\{f\in C^\infty(\mathbb{R})):f^{(k)}\in L^2(\mathbb{R}),\forall k\in\mathbb{N}\}.$$

Thus, in this case $\mathcal{D}^\infty(H)\supset\mathcal{D}^\infty(H_0)$.

In order to construct an example where the opposite inclusion holds, we start by taking $H_0=p^2$ and $B=q^2$. In this case,

$$\mathcal{D}^\infty(H)=\mathcal{S}(\mathbb{R})\subset\{f\in C^\infty(\mathbb{R})):f^{(k)}\in L^2(\mathbb{R}),\forall k\in\mathbb{N}\}=\mathcal{D}^\infty(H_0).$$

These examples show that all situations are possible, when comparing $\mathcal{D}^\infty(H)$ and $\mathcal{D}^\infty(H_0)$.

For shortness, we will call B a KR-perturbation if it satisfies the assumption of the Kato–Rellich theorem. Before going forth, we give the following

Proposition 2.4: Let A and B be two self-adjoint operators in Hilbert space $\mathcal{H}$. Then

$$\mathcal{D}^\infty(A)=\mathcal{D}^\infty(B)$$

if, and only if, the following two conditions hold:

(i) for each $k\in\mathbb{N}$ there exists $\ell\in\mathbb{N}$ such that $D(B^\ell)\subseteq D(A^k)$,
(ii) for each $h\in\mathbb{N}$ there exists $m\in\mathbb{N}$ such that $D(A^m)\subseteq D(B^h)$.

Proof: We put $\mathcal{D}=\mathcal{D}^\infty(A)=\mathcal{D}^\infty(B)$. Because of Lemma 2.1, the topologies t_A and t_B are equivalent. Without loss of generality we assume that $A\geqslant 0$, $B\geqslant 0$; this makes the usual families of seminorms defining the two topologies directed. This implies that for each $k\in\mathbb{N}$ there exist $\ell\in\mathbb{N}$ and $C_k>0$:

$$\|A^k\phi\|\leqslant C_k\|B^\ell\phi\|,\quad \phi\in\mathcal{D}.$$

But $\mathcal{D}$ is a core for any power of B, therefore for each $f\in D(B^\ell)$ there exists a sequence (f_n) of elements of $\mathcal{D}$ such that $f_n\to f$ and $(B^\ell f_n)$ is convergent. Then we get

$$\|A^k(f_n-f_m)\|\leqslant C_k\|B^\ell(f_n-f_m)\|\to 0$$

and therefore $f \in D(\overline{A^k_{\restriction D}}) = D(A^k)$. The proof of (ii) is similar.

Let us now assume that (i) and (ii) hold. For any $k \in \mathbb{N}$ we put

$$\ell_k = \min\{\ell \in \mathbb{N} : D(B^\ell) \subset D(A^k)\}.$$

Then we have

$$\mathcal{D}^\infty(B) \subseteq \bigcap_{k=1}^{\infty} D(B^{l_k}) \subset \bigcap_{k=1}^{\infty} D(A^k) = \mathcal{D}^\infty(A).$$

In similar way the converse inclusion can be proven. □

Example: The previous proposition easily implies the following well-known fact:

$$\mathcal{D}^\infty(A^k) = \mathcal{D}^\infty(A), \quad \forall k \in \mathbb{N}$$

since (i) and (ii) hold, as is readily seen.

Proposition 2.5: Let $A \geqslant 1$ and $B \geqslant 1$. Then if

$$\mathcal{D}^\infty(A) = \mathcal{D}^\infty(B)$$

the following two conditions hold:

(i) for each $k \in \mathbb{N}$ there exist $\ell \in \mathbb{N}$ such that $A^k B^{-\ell}$ is bounded;
(ii) for each $h \in \mathbb{N}$ there exist $m \in \mathbb{N}$ such that $B^h A^{-m}$ is bounded.

Conversely, if $D^\infty(A) \cap D^\infty(B)$ contains a common core $\mathcal{D}_0$ for all powers of A and B and both (i) and (ii) hold, then

$$\mathcal{D}^\infty(A) = \mathcal{D}^\infty(B).$$

Proof: Assume that $\mathcal{D}^\infty(A) = \mathcal{D}^\infty(B) =: \mathcal{D}$. As seen in the proof of Proposition 2.4, the equivalence of the topologies implies that for each $k \in \mathbb{N}$ there exist $\ell \in \mathbb{N}$ and $C_k > 0$:

$$\|A^k \phi\| \leqslant C_k \|B^\ell \phi\|, \quad \phi \in \mathcal{D},$$

which can be written as

$$\|A^k B^{-\ell} \phi\| \leqslant C_k \|\phi\|, \quad \phi \in \mathcal{D}.$$

The second condition can be proved in similar way.

Now, suppose that $\mathcal{D}_0$ is a common core for all powers of A and B and that (i) and (ii) hold. Then from (i) one gets that for each $k \in \mathbb{N}$ there exist $\ell \in \mathbb{N}$ and $C_k > 0$:

$$\|A^k \phi\| \leqslant C_k \|B^\ell \phi\|, \quad \phi \in \mathcal{D}_0.$$

Proceeding as in the proof of Proposition 2.4 one proves that for these k and ℓ, $D(B^\ell) \subseteq D(A^k)$. Analogously, condition (ii) implies (ii) of Proposition 2.4.

□

Proposition 2.6: Let B be a KR-perturbation and assume $B : \mathcal{D}^\infty(H_0) \to \mathcal{D}^\infty(H_0)$. Then $\mathcal{D}^\infty(H_0) \subseteq \mathcal{D}^\infty(H)$. Moreover, if the families of seminorms are directed,

$$\forall k, s \in \mathbb{N} \exists \ell \in \mathbb{N}, C_k > 0 : \|H_0^s H^k \phi\| \leqslant C_k \|H_0^\ell \phi\|, \quad \forall \phi \in \mathcal{D}^\infty(H_0).$$

Proof: In this case, $\mathcal{D}^\infty(H_0)$ is left invariant by H; but $\mathcal{D}^\infty(H)$ is the largest domain with this property. Therefore $\mathcal{D}^\infty(H_0) \subseteq \mathcal{D}^\infty(H)$.

The given inequality follows easily from the continuity of H^k in $\mathcal{D}^\infty(H_0)$. □

Remark: The above inequality also says that t_{H_0} is, in general, finer than t_H.

In order to get the equality of the two domains some stronger condition on B must be added. We have, indeed:

Proposition 2.7: Let B be a perturbation of H_0 such that $H:=H_0+B$ is self-adjoint on $D(H)=D(H_0)$. In order that

$$\mathcal{D}^\infty(H)=\mathcal{D}^\infty(H_0)$$

it is necessary and sufficient that the following conditions hold:

(i) $B:\mathcal{D}^\infty(H_0)\to\mathcal{D}^\infty(H_0)$,
(ii) *H is essentially self-adjoint in $\mathcal{D}^\infty(H_0)$,*
(iii) *the topologies t_{H_0} and t_H are equivalent on $\mathcal{D}^\infty(H_0)$.*

Proof: The necessity of (i) is obvious. As for (ii), it is well-known that $\mathcal{D}^\infty(H)$ is a core for H (and for all its powers). The necessity of (iii) follows from (1) in Lemma 2.1.

We now prove the sufficiency.

First, by Proposition 2.6 and (i) it follows that $\mathcal{D}^\infty(H_0)\subseteq\mathcal{D}^\infty(H)$ and since H is essentially self-adjoint in $\mathcal{D}^\infty(H_0)$,

$$\mathcal{D}^\infty(\overline{H_{\restriction\mathcal{D}^\infty(H_0)}})=\mathcal{D}^\infty(H).$$

But as is well known, the domain on the left-hand side is the completion of $\mathcal{D}^\infty(H_0)$ in the topology t_H. The equivalence of t_H and t_{H_0}, in turn implies that $\mathcal{D}^\infty(H_0)$ is complete under t_H and so the statement is proved. □

Remark: If B is bounded, then $H=H_0+B$ is automatically essentially self-adjoint in $\mathcal{D}^\infty(H_0)$.

Example: Let $H_0=p^2+q^2$; then $\mathcal{D}^\infty(H_0)=\mathcal{S}(\mathbb{R})$. Let $B=\alpha q$ with $\alpha\in\mathbb{R}$.
Then it is easily seen that $H=p^2+q^2+\alpha q$ leaves $\mathcal{S}(\mathbb{R})$ invariant.

Since $H=p^2+(q-\beta)^2+\beta^2$ with $\beta=\alpha/2$, it is clear that $\mathcal{S}(\mathbb{R})$ is a domain of essential self-adjointness for H.
The equivalence of the topologies t_{H_0} and t_H can be proven with easy estimates of the respective seminorms. Thus Proposition 2.7 leads us to conclude that $\mathcal{D}^\infty(H_0)=\mathcal{D}^\infty(H)$.

As a consequence of Proposition 2.7, we now consider the special case of a perturbation *weakly* commuting with H_0.

Let $\mathcal{L}^\dagger(\mathcal{D},\mathcal{H})$ denote the space of all closable operators A in $\mathcal{H}$ such that $D(A)=\mathcal{D}$, $D(A^*)\subset\mathcal{D}$. As for $\mathcal{L}^\dagger(\mathcal{D})$, we put $A^\dagger=A^*_{\restriction\mathcal{D}}$.

Now, if $\mathcal{A}$ is a $\dagger$-invariant subset of $\mathcal{L}^\dagger(\mathcal{D},\mathcal{H})$, the *weak unbounded commutant* $\mathcal{A}'_\sigma$ of $\mathcal{A}$ is defined as

$$\mathcal{A}'_\sigma=\{Y\in\mathcal{L}^\dagger(\mathcal{D},\mathcal{H}):\langle Xf,Y^\dagger g\rangle=\langle Yf,X^\dagger g\rangle,\forall f,g\in D;\forall X\in\mathcal{A}\}.$$

If T is a self-adjoint operator in $\mathcal{H}$, we can consider the O^*-algebra $\mathcal{P}(T)$ generated by T on $\mathcal{D}^\infty(T)$. It is well-known[10] that $\mathcal{P}(T)'_\sigma=\{T\}'_\sigma$. Furthermore, any $Y\in\{T\}'_\sigma$ leaves $\mathcal{D}^\infty(T)$ invariant. We now apply these facts to our situation:

Corollary 2.8: Let B be a perturbation of H_0. Assume that B satisfies the conditions:
(i) $\langle H_0f,Bg\rangle=\langle Bf,H_0g\rangle,\forall f,g\in\mathcal{D}^\infty(H_0)$,
(ii) *H is essentially self-adjoint in $\mathcal{D}^\infty(H_0)$,*
(iii) $\|H_0f\|\leqslant\|Hf\|,\forall f\in\mathcal{D}^\infty(H_0)$,

then $\mathcal{D}^\infty(H_0)=\mathcal{D}^\infty(H)$.

Proof: Condition (i) implies that B leaves $\mathcal{D}^\infty(H_0)$ invariant; therefore H is t_{H_0}-continuous (together with all its powers). So it remains to check that t_H is finer than t_{H_0} in order to apply Proposition 2.7.

We will prove by induction that

$$\|H_0^n f\| \leqslant \|H^n f\|, \quad \forall f \in \mathcal{D}^\infty(H_0).$$

The case $n=1$ is exactly condition (iii). Now we assume the statement true for $n-1$. Then we get

$$\|H_0^n f\| = \|H_0(H_0^{n-1} f)\| \leqslant \|H(H_0^{n-1} f)\| = \|H_0^{n-1} H f\| \leqslant \|H^n f\|, \quad \forall f \in \mathcal{D}^\infty(H_0).$$

since, by (i), H_0 and H commute (algebraically) on $\mathcal{D}^\infty(H_0)$. □

III. DYNAMICAL ASPECTS

We now come back to the dynamical problem posed at beginning of the paper concerning the perturbative situation and again we will consider the case where H exists. So far, we were able to prove the convergence of the dynamics only at infinitesimal level (Corollary 2.3). The problem of the convergence of $\alpha_L^t(A)$ to $\alpha^t(A)$ is not completely solved in the simple case we are dealing with. Of course, given H and its spectral projections Q_L as seen in Sec. II, we can always prove, setting $\hat{H}_L = Q_L H Q_L$, that $e^{i\hat{H}_L t} A e^{-i\hat{H}_L t}$ converges to $e^{iHt} A e^{-iHt}$ for any A in $\mathcal{L}^\dagger(\mathcal{D})$. What makes the difference here (and this is the spirit of the whole paper) is that we are defining the cut off Hamiltonian $H_L = Q_L^0 H Q_L^0$ via the spectral projections of the unperturbed Hamiltonian H_0. This is of practical interest since only in very few instances (finite discrete systems, harmonic oscillators, hydrogen atoms, etc.) the spectral projections of H are known. On the other hand, H_0 can be chosen with a sufficient freedom to guarantee the knowledge of the Q_L^0.

With this in mind, we consider the problem of finding conditions under which $e^{iH_L t}$ converges, with respect to the topology $\tau_*^{\mathcal{D}}$, to e^{iHt}.

To this aim, we define the operator function

$$g_L(t) = e^{iH_L t} - e^{iHt} = i \int_0^t e^{iH_L(t-t')} (H_L - H) e^{iHt'} \mathrm{d}t',$$

the latter equality being obtained by solving

$$\dot{g}_L(t) = iH_L g_L(t) + i(H_L - H) e^{iHt},$$

which comes directly from the definition of $g_L(t)$. Easy estimates allow one to state the following

Lemma 3.1: For each $k \in \mathbb{N}$ there exists $s \in \mathbb{N}$ such that

$$\lim_{L \to \infty} \|H_0^{-s} (H_L - H) H_0^k\| = 0,$$

then we have

Proposition 3.2: If there exists $T>0$ such that, for each $f \in \mathcal{F}$, $s \in \mathbb{N} \cup \{0\}$ there exists $M = M(T,f,s)$ such that

$$\int_0^t \|f(H_0) e^{iH_L(t-t')} H_0^s\| \mathrm{d}t' < M, \quad t \in [0,T]$$

then

$$\tau_*^{\mathcal{D}} - \lim_{L \to \infty} g_L(t) = 0.$$

Proof: We have indeed

$$\|g_L(t)\|^{f,k} \leqslant \int_0^t \|f(H)e^{iH_L(t-t')}(H_L-H)e^{-iHt'}H^k\|\mathrm{d}t'$$

$$= \int_0^t \|f(H)e^{iH_L(t-t')}(H_L-H)H^k\|\mathrm{d}t'$$

$$\leqslant C\int_0^t \|f_1(H_0)e^{iH_L(t-t')}(H_L-H)H_0^{k_1}\|\mathrm{d}t'$$

$$\leqslant C\int_0^t \|f_1(H_0)e^{iH_L(t-t')}H_0^s\|\mathrm{d}t'\cdot\|H_0^{-s}(H_L-H)H_0^{k_1}\|$$

for suitable $C>0$, $f_1\in\mathcal{F}$ and $k_1\in\mathbb{N}$ and with s chosen, correspondingly to k_1 so that Lemma 3.1 can be used. □

This proposition implies that the Schrödinger dynamics can be defined. The analysis of the Heisenberg dynamics is more complicated and will not be considered here.

The assumptions of Proposition 3.1 are indeed quite strong. They are, of course, verified if the perturbation B commutes with H_0. But this is, clearly, a trivial situation. We will now discuss a nontrivial example where they are satisfied.

Example: Let $H_0=a^\dagger a$ and $B=a^n$, n being an integer larger than 1. The conditions on the domains of the operators discussed in Sec. II are satisfied, as it is more easily seen working in the configuration space, so that our procedure can be applied. Here $Q_L^0=\Pi_0^0+\Pi_1^0+\Pi_2^0+\cdots+\Pi_L^0$, where Π_i^0 is the projection operator of H_0, $H_0=\Sigma_{l=0}^{\infty} l\Pi_l^0$. Using the algebraic rules discussed in Ref. 12, and, in particular the commutation rules $Q_L^0 a=aQ_{L+1}^0$ and $\Pi_l^0 a=a\Pi_{l+1}^0$, we find that $H_l=Q_L^0HQ_L^0=HQ_L^0$.

It is a straightforward computation now to check that for any $f\in\mathcal{F}$ and for any natural s, $\|f(H)e^{iH_L\tau}H^s\|=\|f(H)(H+(e^{iH\tau}-1)a^nP_{L,n}^0)^s\|$, where we have defined the following orthogonal projection operator

$$P_{L,n}^0=\Pi_{L+1}^0+\Pi_{L+2}^0+\cdots+\Pi_{L+n}^0=Q_{L+n}^0-Q_L^0.$$

These seminorms can be estimated for each value of s and it is not difficult to check that they are bounded by a constant which depends on f, s, and n (obviously) but not on L and τ. Therefore the main hypothesis of Proposition 3.1 is verified and so the Schrödinger dynamics can be defined. We give the estimate of the above seminorm here only in the easiest nontrivial case, $s=1$. The extension to $s>1$ only increases the length of the computation but does not affect the result,

$$\|f(H)(H+(e^{iH\tau}-1)a^nP_{L,n}^0)\|\leqslant\|f(H)H\|+\|f(H)(e^{iH\tau}-1)a^n\|\|P_{L,n}^0\|\leqslant\|f(H)H\|+2\|f(H)a^n\|,$$

which is bounded and independent of both L and τ.

The same strategy can also be applied to the more general situation when B is any given polynomial in a and $a^\dagger$.

In order to find more cases in which Proposition 3.2 can be applied, we begin with the following

Lemma 3.3: For each $f\in\mathcal{F}$ and for each $k,\ell\in\mathbb{N}$ we have

$$\lim_{L\to\infty}\|f(H)(H_L^\ell-H^\ell)H^k\|=0.$$

Proof: We proceed by induction on ℓ.

For $\ell=1$ the statement follows immediately by the equivalence of the topologies and from Lemma 2.2.

Now,

$$\|f(H)(H_L^{\ell+1}-H^{\ell+1})H^k\| \leq \|f(H)H_L(H_L^{\ell}-H^{\ell})H^k\| + \|f(H)(H_L-H)H^{\ell+k}\|$$

and the second term on the right-hand side goes to 0 because we have just proved the induction for $\ell=1$.

The first term of the right-hand side can easily be estimated, once more making use of the equivalence of the topologies, by a term of the kind

$$C'\|f_1(H_0)(H_L^{\ell}-H^{\ell})H^{k_1}\|,$$

which goes to zero again because of the induction. □

Proposition 3.4: If there exists $m \in \mathbb{N}$ *such that* $[H_L, H]_{m+1}=0$ *then*

$$\int_0^t \|f(H_0)e^{iH_L(t-t')}H_0^s\|\mathrm{d}t' < \infty, \quad t \in \mathbb{R}^+$$

for each $f \in \mathcal{F}$ *and for each* $s \in \mathbb{N}\cup\{0\}$.

Proof: By the assumption, we have

$$e^{iH_L(t-t')}He^{-iH_L(t-t')} = H + i(t-t')[H_L, H] + \cdots \frac{i^m}{m!}[H_L, H]_m. \tag{8}$$

Now, using the equivalence between the topologies produced by H_0 and H, it is easy to see that

$$\|f(H_0)e^{iH_L(t-t')}H_0^s\| \leq C\|f_1(H)(e^{iH_L(t-t')}He^{-iH_L(t-t')})^{s_1}\|.$$

Inserting (8) on the right-hand side and making use of Lemma 3.3, we finally get the estimate:

$$\|f(H_0)e^{iH_L(t-t')}H_0^s\| \leq C\|f_1(H)H^{s_1}\|,$$

and this easily implies the statement. □

Clearly, even if the conditions given previously for the $\tau_*^{\mathcal{D}}$-convergence of e^{iH_Lt} to e^{iHt} occur, the convergence of $\alpha_L^t(A)$ to $\alpha^t(A)$ is not guaranteed. For this reason we conclude this section by outlining a different possible approach.

Assume that, for each $L \in \mathbb{R}$ there exists a one-parameter family $\beta_L^t(A)$ of linear maps of $\mathcal{L}^\dagger(\mathcal{D})$ (not necessarily an automorphisms group) such that, for each $f \in \mathcal{F}$ and $k \in \mathbb{N}$,

$$\|f(H)(\beta_L^t(A)-\alpha_L^t(A))H^k\| \to 0 \quad \text{as} \quad L \to \infty. \tag{9}$$

Clearly the convergence of $\beta_L^t(A)$ to $\alpha^t(A)$ would directly lead to the solution of the dynamical problem. We want to stress that β_L^t could be rather *unusual* and, therefore, it should be only considered as a technical tool.

In general, however, the possibility of finding a good definition for the β_L^t's that allows (9) to hold is quite difficult and the lesson of the previous discussion on the convergence of e^{iH_Lt} is that strong assumptions must be imposed in order to get it.

A weaker condition on the β_L^t's, whose content of information is, nevertheless, nonempty, would consist in requiring, instead of (9), that

(a) $\beta_L^t(A)$ converges to $\alpha^t(A)$, for each $A \in \mathcal{L}^\dagger(\mathcal{D})$ together with all time derivatives. This means that an Heisenberg dynamics $e^{iHt}(\cdot)e^{-iHt}$ can be recovered.
(b) As for the Schrödinger dynamics, that is for the dynamics in the space of vectors, we ask β_L^t of being in some way (to be specified further) *generated* by a family of bounded operators which, when applied to any $\Psi \in \mathcal{D}$, is t_H-convergent together with all time derivatives.

This happens, for instance, in the case where H exists, if we define

$$\beta_L^t(A) = V_L^t A V_L^{-t},$$

where $V_L^t := Q_L^0 e^{iHt} Q_L^0$ and the Q_L^0's are the projection of H_0. (4).

Under these assumptions, V_L is a well-defined bounded operator of $\mathcal{L}^\dagger(\mathcal{D})$, and the following Proposition holds:

Proposition 3.5: In the above given conditions, the following statements hold:

(i) $t_H - \lim_{L\to\infty} V_L^t \psi = \psi(t) := e^{iHt}\psi, \quad \forall \psi \in \mathcal{D},$

(ii) $\tau_*^{\mathcal{D}} - \lim_{L\to\infty} V_L^t = e^{iHt},$

(iii) $\tau_*^{\mathcal{D}} - \lim_{L\to\infty} \beta_L^t(A) = \alpha^t(A) := e^{iHt} A e^{-iHt}, \quad \forall A \in \mathcal{L}^\dagger(\mathcal{D})$

and, more generally:

(i') $t_H - \lim_{L\to\infty} (\mathrm{d}^n/\mathrm{d}t^n)\, V_L^t \psi = (\mathrm{d}^n/\mathrm{d}t^n)\, \psi(t), \quad \forall \psi \in \mathcal{D}, n \in \mathbb{N}\cup\{0\},$

(iii') $\tau_*^{\mathcal{D}} - \lim_{L\to\infty} (\mathrm{d}^n/\mathrm{d}t^n)\, \beta_L^t(A) = (\mathrm{d}^n/\mathrm{d}t^n)\, \alpha^t(A), \quad \forall A \in \mathcal{L}^\dagger(\mathcal{D}), n \in \mathbb{N}\cup\{0\}.$

The proof of this Proposition follows from the equivalence between the topologies generated by H and H_0, proved in Lemma 2.1.

This approach, which is only one of the possible strategies when H exists, could be of a certain interest for situations when the dynamics can only be obtained via a net of operators $H_L = H_0 + B_L$, H_0 being the free Hamiltonian and B_L being a regularized perturbation. In this case the approach to the thermodynamical limit could involve the family of bounded operators $V_{L,M}^t := Q_L^0 e^{iH_M t} Q_L^0$, and one can try to extend the above results. A further analysis on this subject is currently *work in progress*.

IV. OUTCOME AND POSSIBLE DEVELOPMENTS

In this paper we have analyzed a possible approach to define an algebraic dynamics when a free Hamiltonian H_0 is perturbed by an operator B which essentially leaves the domain of all the powers of H_0 invariant.

What is still missing, as discussed in Sec. I, is the analysis of the situation where the definition of the dynamics is not straightforward since it should follow from a net of operators $\{H_L\}$ whose limit does not exist in any physical topology.[2,3] In this case a possible approach can be made in terms of derivations, for instance, in the way explained in the following.

Let us suppose that to a free spatial derivation $\delta_0(.) = i[H_0, .]$ a perturbation term δ_P is added, so that

$$\delta(A) = \delta_0(A) + \delta_P(A), \quad A \in \mathcal{L}^\dagger(\mathcal{D}).$$

In this case we define $\eta_L(A) = Q_L^0 \delta(A) Q_L^0$, with $A \in \mathcal{L}^\dagger(\mathcal{D})$ and Q_L^0 as in the previous sections. It is easy to see that η_L is not in general a derivation because the Leibniz rule may fail. Let Δ_L be a map on $\mathcal{L}^\dagger(\mathcal{D})$ which has the property that $\delta_L = \eta_L + \Delta_L$ satisfies the Leibniz rule together with the other properties of a derivation. Of course, this map is not unique since, for instance, we can always add a commutator $i[H', .]$ to Δ_L, with any self-adjoint operator H', without affecting the properties of a derivation (we should only care about domain problems in choosing H'!). From a physical point of view it is reasonable to expect that Δ_L can be chosen in such a way that $\|\Delta_L(A)\|^{f,k} \to 0$ with L since we would like to recover the original derivation δ after removing of the cutoff and we know from Corollary 2.3 that $\|(\eta_L(A) - \delta(A))\|^{f,k} \to 0$. If also δ_P is spatial, then it is not difficult to give an explicit expression for Δ_L and to check that the requirements above are satisfied. In this case in fact

$$\Delta_L(A) = \{Q_L^0 H_0, [Q_L^0, A]\} + Q_L^0 B [Q_L^0, A] + [Q_L^0, A] B Q_L^0,$$

where $\{X, Y\} = XY + YX$.

Once we have introduced δ_L the next step is to find conditions for this map to be spatial. The related operator H_L, which we expect to be of the form $Q_L^0(H_0 + B)Q_L^0$ for a suitable self-adjoint operator B, can be used to perform the same analysis as that discussed in Sec. III.

Of course this is by no means the only possibility of approaching this problem, but is the one which is closer to our previous analysis, and in this perspective, is particularly relevant for us. We hope to discuss this problem in full detail in a future paper.

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Stochastic heat and Burgers equations and their singularities. I. Geometrical properties[a)]

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Arnol'd and Thom's beautiful classification of caustics (shockwaves) for the Burgers equation suggests a similar one for the wavefronts of the corresponding heat equation. We give here a general theorem for Hamiltonian systems characterizing how the level surfaces of Hamilton's principal function (wavefronts) meet the caustic surface in both the deterministic and stochastic cases. We further show how these results can be applied to the stochastic Burgers equation by using earlier results of Truman and Zhao. The generic example of a caustic, appearing in the two-dimensional case, is the semicubical parabolic cusp with the corresponding zero level surface being a combination of a generalized hypocycloid and a line pair. We refer to these as the cusp and tricorn. The analogous butterfly caustic, in the three-dimensional case, has a cusped zero level surface, the fish, which meets the butterfly caustic in three cusped curves and touches it along a straight line. Our results explain in terms of classical mechanics the properties of the caustic and wavefront for these two archetypal examples and characterize the caustic-wavefront intersection for the general stochastic case. We discuss the application of these results to turbulence for the Burgers velocity field. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1471925]

I. INTRODUCTION

Stochastic Burgers equations have attracted a considerable amount of attention in recent years, e.g., Refs. 1–14. See also Refs. 15–20 for related works. They have been used to give models of turbulence (see especially Ref. 4) and to model the large scale structure of the universe.[21] Here we shall be interested in what has come to be called Burgulence.

Consider the stochastic viscous Burgers equation for the velocity field

$$v^{\mu}=v^{\mu}(x,t), x\in\mathbb{R}^{d}, t>0,$$

$$\frac{\partial v^{\mu}}{\partial t}+(v^{\mu}\cdot\nabla)v^{\mu}=\frac{\mu^{2}}{2}\Delta v^{\mu}-\nabla c(x)-\epsilon\nabla k(x,t)\dot{W}_{t}, \tag{1.1}$$

with initial velocity $v^{\mu}(x,0)=\nabla S_{0}(x)$ where μ^{2} is the coefficient of viscosity. Here c and k are C^{2} functions and W_{t} is a Wiener process on the probability space $\{\Omega, \mathcal{F}, P\}$. We shall be interested in the "blow-up" of $v^{0}(x,t)$ where

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$$v^0(x,t)=\lim_{\mu\to 0} v^\mu(x,t),$$

i.e., the advent of discontinuities in v^0.

The corresponding heat equation for $u^\mu=u^\mu(x,t)$ is the Stratonovich equation

$$\frac{\partial u^\mu}{\partial t}=\frac{\mu^2}{2}\Delta u^\mu+\frac{1}{\mu^2}c(x)u^\mu+\frac{\epsilon}{\mu^2}k(x,t)u^\mu\circ\dot{W}_t,$$
$$u^\mu(x,0)=\exp(-S_0(x)/\mu^2), \tag{1.2}$$

the connection between u^μ and v^μ being the Hopf–Cole logarithmic transformation $v^\mu=-\mu^2\nabla\ln u^\mu$.

Following Donsker and Freidlin *et al.*[22,23] we expect, as $\mu\to 0$,

$$-\mu^2\ln u^\mu(x,t)\to\inf_{X(0)}[A(X(0),x,t)+S_0(X(0))]=S(x,t), \tag{1.3}$$

with

$$A(X(0),x,t)=\inf_{\substack{X(s)\\X(t)=x}} A[X], \tag{1.4}$$

where $A[X]$ is the stochastic action,

$$A(X(0),x,t)=\frac{1}{2}\int_0^t\dot{X}^2(s)\,ds-\int_0^t c(X(s))\,ds-\epsilon\int_0^t k(X(s),s)\,dW_s. \tag{1.5}$$

$S(x,t)$ is the solution of the stochastic Hamilton–Jacobi equation,

$$dS_t+\frac{|\nabla S|^2}{2}dt+c(x)dt+\epsilon k(x,t)dW_t=0,\quad S(x,0)=S_0(x), \tag{1.6}$$

and so $S(x,t)$ is Hamilton's principal function for a stochastic mechanical path. To see this observe that if $\dot{X}(s)$ is a continuous process with the integration by parts property (ibp^2): for all (deterministic) $u\in C^1(0,t)$,

$$\int_0^t\dot{u}(s)\dot{X}(s)\,ds=u(t)\dot{X}(t)-u(0)\dot{X}(0)-\int_0^t u(s)\,d\dot{X}(s),$$

setting $u(t)=0$, $\mathcal{A}[X]=A[X]+S_0(X(0))$, we easily obtain for $S_0\in C^1$, $c\in C^1$, $k\in C^{1,0}$

$$-\frac{d}{d\eta}\bigg|_{\eta=0}\mathcal{A}[X+\eta u]=\int_0^t u(s)[d\dot{X}(s)+\nabla c(X(s))ds+\epsilon\nabla k(X(s),s)dW_s]$$
$$+u(0)(\dot{X}(0)-\nabla S_0(X(0))).$$

Hence necessary conditions for the extremizer are, for $s\in[0,t]$,

$$d\dot{X}(s)+\nabla c(X(s))ds+\epsilon\nabla k(X(s),s)dW_s=0,\quad \dot{X}(0)=\nabla S_0(X(0)). \tag{1.7}$$

From Eq. (1.3), as $\mu\to 0$, we expect that u^μ switches from being exponentially large to exponentially small across the level surface

$$S(x,t)=0\quad\text{(zero level surface)}.$$

If we demand that $X(t)=x$, for fixed t and x, $X(s)$ satisfying Eq. (1.7) may not be unique. Hence, we expect that shockwaves for v arise from precaustics [in (x_0,t) variables] when infinitely many of these classical mechanical paths from x_0 and a neighborhood focus in a set of zero volume centered on $X(t)$. The condition for paths starting from x_0 focusing at a point X at time t is

$$\mathrm{Det}\left(\frac{\partial X(t)}{\partial x_0}\right)=0 \quad \text{(precaustic)}. \tag{1.8}$$

Define the random map $\Phi_s:\mathbb{R}^d\to\mathbb{R}^d$ corresponding to the classical flow by the second-order stochastic differential equation

$$d_s\dot{\Phi}_s=-\nabla c(\Phi_s)ds-\epsilon\nabla k(\Phi_s,s)dW_s, \tag{1.9}$$

with $\Phi_0=I$ and $\dot{\Phi}_0=\nabla S_0$ so that $X(s)=\Phi_s\Phi_t^{-1}x$, where we accept that $x_0(x,t)=\Phi_t^{-1}x$ is not necessarily unique. Given some regularity, the global inverse function theorem gives a caustic time $T(\omega)$ such that, for $s<T(\omega)$, Φ_s is a random diffeomorphism.[24] Therefore, as we shall see,

$$v^0(x,t)=\dot{\Phi}_t\Phi_t^{-1}x=\nabla S(x,t) \tag{1.10}$$

is a formal solution of the Burgers equation with $\mu=0$, which is well defined up to the caustic time because $x_0(x,t)$ is unique.

After the caustic time, for polynomial S_0, $x_0(x,t)$ will usually have finite multiplicity. As long as the minimizing $x_0(x,t)$ is unique, Eq. (1.10) can be assumed to be true beyond the caustic time if we work with that part of the level surface of Hamilton's principal function corresponding to the minimizing $x_0(x,t)$. This is equivalent to taking the minimum entropy solution of the Burgers equation.[25] As expected, the main contribution to $\lim_{\mu\to 0}v^\mu$ will come from the minimizing $x_0(x,t)$, which we shall assume is unique. When there are a finite number (>1) of minimizing x_0's the limiting solution, v^0, is more complicated,[26] but can still be written down.

We expect the nonuniqueness of $x_0(x,t)$ to be associated with the appearance of discontinuities in $v^0(x,t)$ and $u^0(x,t)$. An obvious way for these to arise is if (as above) infinitely many paths $X(s)$ focus in zero volume centered at x. Eliminating x_0 by using $x=\Phi_t(x_0)$ gives the equation of the caustic C_t:

$$\mathrm{Det}\left(\frac{\partial X(t)}{\partial x_0}\right)\Bigg|_{x_0=\Phi_t^{-1}x}=0 \quad \text{(caustic)}. \tag{1.11}$$

The precaustic $\Phi_t^{-1}C_t$ has defining equation (1.8). Starting with the level surfaces of Hamilton's principal function H_t one can define the prelevel surfaces $\Phi_t^{-1}H_t$ in a similar way by setting $x=\Phi_t(x_0)$. The prelevel surfaces and the precaustic are just the preimages of the level surfaces and the caustic under the classical flow map Φ_t. The wavefront is the zero level set of the minimizing Hamilton function which, as we shall see, is part of H_t.

For a nondegenerate critical point, when the multiplicity of $x_0(x,t)$, $n=n(x,t)$, is finite so that $\Phi_t^{-1}\{x\}=\{x_0^1(x,t),x_0^2(x,t),\ldots,x_0^n(x,t)\}$, from Refs. 26–30 we can deduce that

$$u^\mu(x,t)\sim\sum_{i=1}^{n}\theta_i\exp\{-S_0^i(x,t)/\mu^2\}, \tag{1.12}$$

where

$$S_0^i(x,t)=S_0(x_0^i(x,t))+A(x_0^i(x,t),x,t),$$

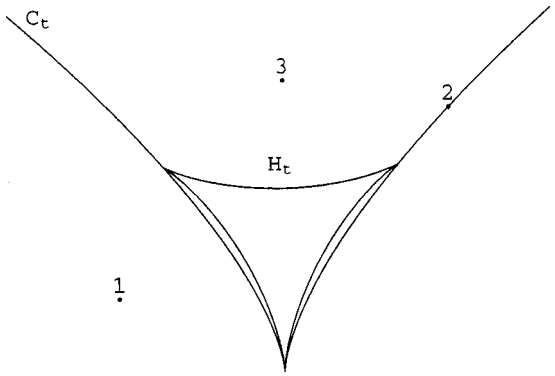

FIG. 1. Cusp and tricorn.

for $i=1,2,...,n$, and θ_i is an asymptotic series in μ^2 whose detailed structure is discussed later in this work. Here $H_t=\{x:S_0^i(x,t)=0,\ \text{some}\ i\}$ so it includes the wavefront where u^0 switches smoothly from being exponentially large to exponentially small. Needless to say, the dominant term in Eq. (1.12) comes from the minimizing $x_0(x,t)$ so that

$$S(x,t)=\min_{i=1,2,...,n} S_0^i(x,t)$$

in line with the results of Freidlin *et al.* Of course $u^0(x,t)$ can switch discontinuously from being exponentially large to exponentially small as we cross parts of the caustic since the minimizing S_0^i can disappear.

Example 1.1: The paradigm for $c=k\equiv 0$ is when $S_0(x,y)=x^2y/2$ in the two-dimensional case. This gives us the generic cusp catastrophe as shown in Fig. 1.

The caustic (shockwave), C_t, *with Eq. (4.2) is the classical semicubical parabola (cusp). This gives the surface of discontinuity of $v^0(x,t)$ with $v^0(x,0)=\nabla S_0=(xy,x^2/2)$. The corresponding zero level surface of Hamilton's principal function, H_t, is a generalized hypocycloid (tricorn) with Eq. (4.1) and line pair $x^2=0$. Only the top part of this tricorn forms the wavefront. The other two curves come from spurious zeros of S_0^i where S_0^i is not minimizing. This top part of the tricorn defines the region where u^μ switches from being exponentially large to exponentially small. We suppress the line pair in Fig. 1 to highlight how the caustic splits $\mathbb{R}^2$. The important result here is that u^0 has a sharp discontinuity on the caustic itself. Note that within the cusp there are three preimages for each point, on the cusp there are two preimages for each point, and outwith the cusp there is only one preimage for each point.*

If we fix the time t and let the point a be inside the semicubical parabolic cusp so that the multiplicity of the x_0's is three, there are three level surfaces $S_0^i(x,t)=c$, one for each $x_0^i(a,t)$, $i=1,2,3$, only one of which corresponds to the minimizer. The prelevel surfaces and their corresponding x_0's are shown in Figs. 2 and 3 with the cusp included for reference in the case of Fig. 2.

We now display all the level surfaces passing through the point a in relation to the cusp as shown in Figs. 4 and 5.

In the case when the point a is on the cusp, Fig. 6, there are only two preimage points and correspondingly only two level surfaces passing through a, one of which has a cusp at a.

The final case, Fig. 7, is where the point a lies outwith the cusp and there is only one level surface.

In Figs. 8 and 9 we see how the cusped level surfaces coalesce as the point a approaches the caustic. *The first of these figures corresponds to the two cusped level surfaces having positive S_0 and the second corresponds to the two cusped level surfaces having negative S_0. In both cases the*

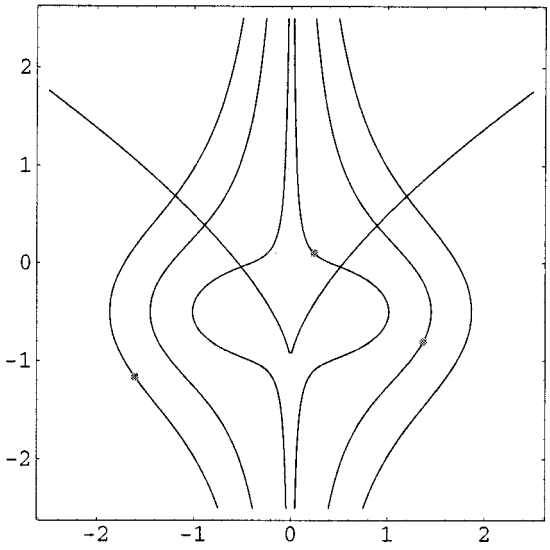

FIG. 2. Three prelevel surfaces—positive.

appearance of the cusp means that the corresponding S_0^i cannot be continued across the caustic. This is what makes u^0 discontinuous across the cusp caustic, because the cusped part of the level surface corresponds to the minimizer $x_0(x,t)$.

In the above example we see that the multiplicity of $x_0(x,t)$, n, changes by a multiple of 2 as we cross the caustic surface. We shall see that this is associated with level surfaces of Hamilton's principal function having cusps on the caustic, caused by different $x_0(x,t)$'s coalescing. Moreover, the cusp on the level surface (if it corresponds to the minimizing x_0) means that we have to take a different minimizer S_0^i on different sides of the caustic. This makes u^0 discontinuous. Thus, it is important to know when the point of intersection of a level surface and caustic is a genuine cusp, generalized cusp, or a crossover point.

In more than one dimension for $S_0 \in C^2$ there is a robust geometrical relationship between level surfaces and caustics even in the presence of noise. This is because, as we shall prove, the

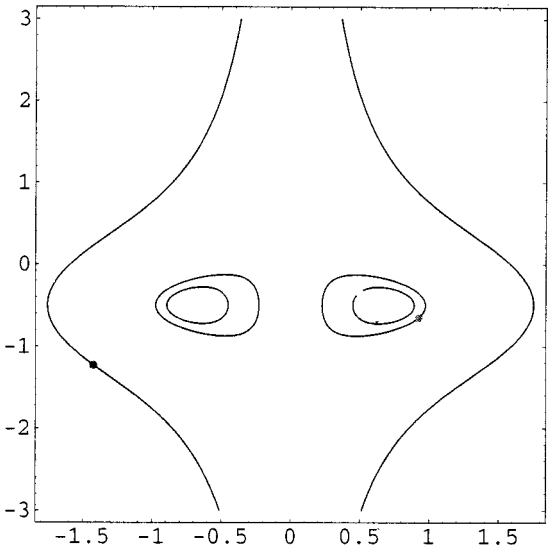

FIG. 3. Three prelevel surfaces—two negative and one positive.

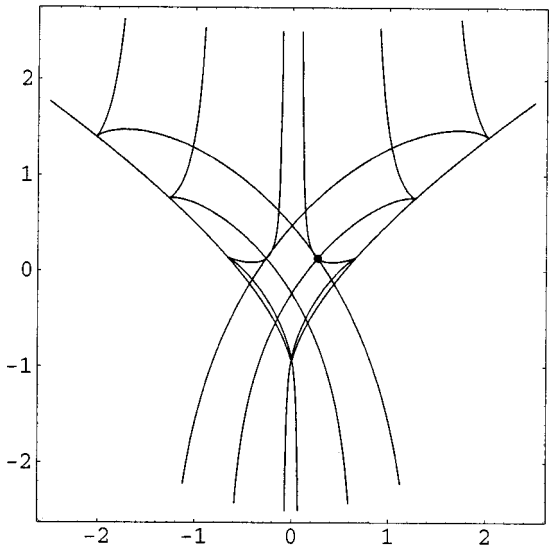

FIG. 4. Three level surfaces—positive.

tangent plane to the level surface H_t at a point x on the caustic C_t is spanned by the image of the tangent plane to the prelevel surface, where this prelevel surface tangent plane necessarily contains the kernel of the derivative of the Φ_t map if $x \in \Phi_t(\Phi_t^{-1}C_t \cap \Phi_t^{-1}H_t)$. In understanding Burgers turbulence this switches attention from C_t and H_t to their unfoldings $\Phi_t^{-1}C_t$ and $\Phi_t^{-1}H_t$. In two dimensions, at a point on the precaustic, it follows that this kernel spans the tangent plane to the prelevel surface. In three dimensions the dimension of the tangent plane to the level surface drops from two to one as we approach points on the caustic in $\Phi_t[\Phi_t^{-1}H_t \cap \Phi_t^{-1}C_t]$, which is essentially the cusped part of the level surface, $\mathrm{Cusp}(H_t)$. This manifests itself in the tangent plane to the level surface on the caustic folding back on itself—the fold being the one-dimensional tangent plane at the point of intersection. In two dimensions this is quite elementary to prove, but in three dimensions it depends on a careful analysis of the geometry of the level surface and its preimage.

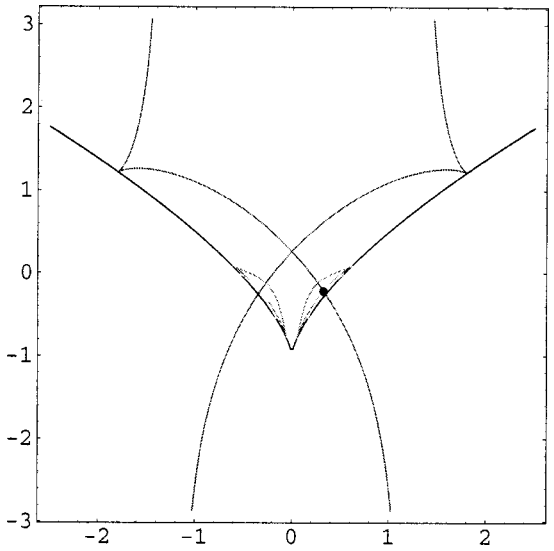

FIG. 5. Three level surfaces—two negative and one positive.

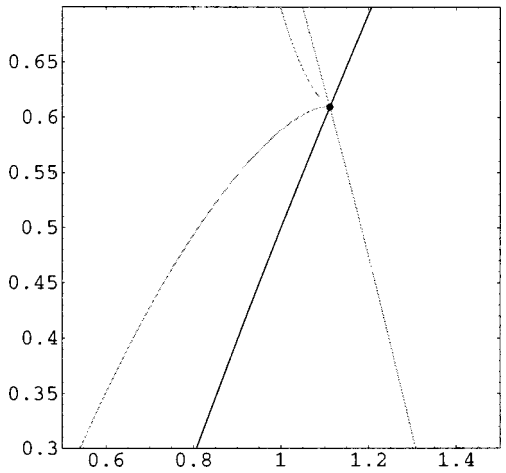

FIG. 6. Two level surfaces.

Our main theorem (in Sec. V) concerning this geometric relationship for the above stochastic Hamiltonian system, given some mild restrictions, is for fixed t:

Theorem: *Any point x on the level surface H_t, $x=\Phi_t(x_0)$ with $x_0=\Phi_t^{-1}(x)$ on the prelevel surface, can only be a generalized cusp of a curve on H_t if x_0 is a generalized cusp of the precurve on the prelevel surface or if $x_0 \in \Phi_t^{-1} C_t$ the precaustic. In three dimensions the planar cross section $y=const$ (with normal e_y) of the level surface H_t through a point x where it meets C_t, the caustic surface, will have a genuine cusp at x if $x \in \mathrm{Cusp}(H_t)$ and there is a nonzero solution δx of Eqs. (C_1), (C_2), and (C_3). The direction of the axis of the cusp will be $\widehat{\delta x}$.*

This result explains the bizarre pictures of the fish and the butterfly (Figs. 19–22) in Sec. IV and similar phenomena. In Sec. II we recapitulate our main results for the Burgers equation. This can be skipped if the reader is primarily interested in the geometrical result. An outline proof of our main geometrical result is given in Sec. III where the free case is considered in detail and proved. Section IV contains simple archetypal examples in both two and three dimensions. Section V treats the general stochastic case. In Secs. III–V we give a brief discussion of the ramifications

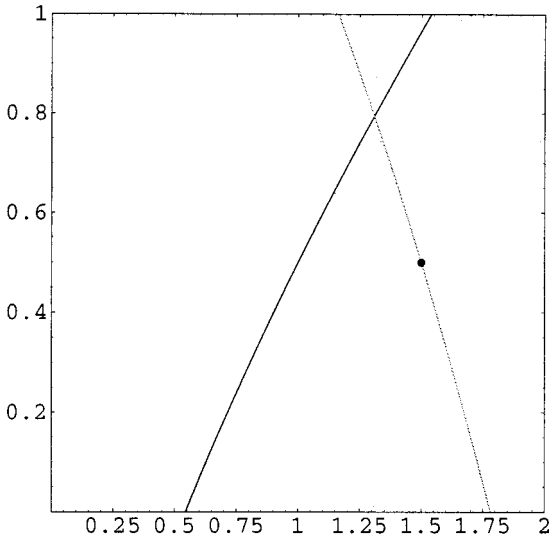

FIG. 7. One level surface.

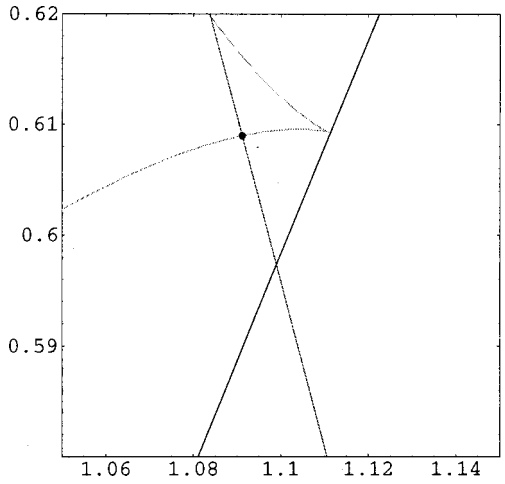

FIG. 8. Coalescing level surfaces—positive S_0.

of our results for Burgers turbulence. In particular we explain how our results give a simple model for the intermittence of turbulence for the stochastic Burgers equation at the end of Sec. V.

II. SOLUTIONS OF INVISCID BURGERS AND HEAT EQUATIONS AND ASYMPTOTIC SERIES θ

Here let $v^\mu = v^\mu(x,t)$ satisfy for $t>0$, $x \in \mathbb{R}^d$,

$$dv^\mu + (v^\mu \cdot \nabla)v^\mu dt + \nabla c dt + \epsilon \nabla k dW_t = \frac{\mu^2}{2}\Delta v^\mu dt,$$

with $v^\mu(x,0) = \nabla S_0(x)$, where $c = c(x)$, $k = k(x,t)$.

Since the convected derivative

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + v \cdot \nabla,$$

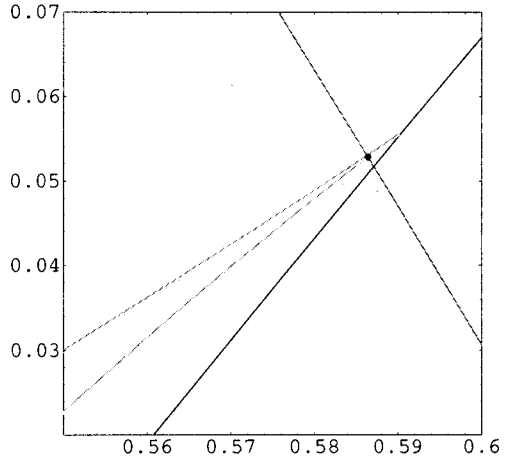

FIG. 9. Coalescing level surfaces—negative S_0.

the above Burgers equation describes a fluid where particles pass through each other with no interaction, the particles being subject to a force $(-\nabla c(x)-\epsilon\nabla k(x,t)\dot{W}_t)$ with $\dot{W}_t$ being white noise. (In fact, infinitely many pass through each other at points on the caustic and to this extent our continuation of the solution may be considered unphysical. Nevertheless, the Burgers equation has been used successfully in modeling the large-scale structure of the universe[21,31] and in studying related equations.)

Let $v^\mu=\nabla S^\mu$. Then S^μ satisfies the stochastic Hamilton–Jacobi equation

$$dS^\mu+\tfrac{1}{2}|\nabla S^\mu|^2dt+c\,dt+\epsilon k\,dW_t=\tfrac{1}{2}\mu^2\Delta S^\mu dt.$$

Formally, if $S^\mu\sim\sum_{j=0}^{\infty}\mu^{2j}S_j$, we obtain from the last equation the stochastic Hamilton–Jacobi continuity equations

$$\frac{\partial S_j}{\partial t}+\frac{1}{2}\sum_{\substack{i_1,i_2\geqslant 0\\ i_1+i_2=j}}\nabla S_{i_1}\cdot\nabla S_{i_2}=\frac{1}{2}\Delta S_{j-1},$$

for $j=0,1,2,...$, with the convention $1/2\Delta S_{-1}=-c-\epsilon k\dot{W}_t$, $\dot{W}_t$ being white noise.

The corresponding stochastic mechanical flow Φ_s satisfies

$$d\dot{\Phi}_s=-\nabla c(\Phi_s)ds-\epsilon\nabla k(\Phi_s,s)dW_s,$$

with $\Phi_0(x)=x$, $\dot{\Phi}_0(x)=\nabla S(x,0)=\nabla S_0(x)$. Now assume $\Phi_s(\omega):\mathbb{R}^d\to\mathbb{R}^d$ is a diffeomorphism for $0\leqslant s<T(\omega)$. Define

$$\tilde{S}_0(y,t)=\frac{1}{2}\int_0^t|\dot{\Phi}_s(y)|^2\,ds+S(y,0)-\int_0^t c(\Phi_s y)\,ds-\epsilon\int_0^t k(\Phi_s y,s)\,dW_s$$

and

$$S_0(x,t)=\tilde{S}_0(\Phi_t^{-1}x,t).$$

The main result of stochastic Hamilton–Jacobi theory[13,32] is the following.

Proposition 2.1: Assume $c\in C^2(\mathbb{R}^d)$, $k\in C^2(\mathbb{R}^d\times\mathbb{R})$ *and* $S_0(\cdot,0)\in C^2(\mathbb{R}^d)$. *Then*

(i) for a.e. $\omega\in\Omega$, $0\leqslant t<T(\omega)$,

$$\dot{\Phi}_t=\nabla S_0(\Phi_t,t),$$

and S_0 *satisfies the stochastic Hamilton–Jacobi equation*

$$dS_0(x,t)+\tfrac{1}{2}|\nabla S_0(x,t)|^2dt+c(x)dt+\epsilon k(x,t)dW_t=0.$$

(ii) Define $\rho(x,t)=|\mathrm{Det}((\partial/\partial x)\Phi_t^{-1}(x))|$. *Then for a.e.* $\omega\in\Omega$, *any* $x\in\mathbb{R}^d$, $0\leqslant t<T(\omega)$, ρ *satisfies the continuity equation*

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\nabla S_0)=0.$$

Suppose now that $T_0:\mathbb{R}^d\to\mathbb{R}$ is a smooth positive function whose physical role is explained later. (Eventually we will set $T_0\equiv 1$ for the applications discussed here.) Define

$$T_0(y,t)=T_0(y)$$

and, for $j=1,2,...,$

$$T_j(y,t)=\int_0^t \rho^{-1/2}(\cdot,s)\Delta_{\cdot}(\rho^{1/2}(\cdot,s)T_{j-1}(\Phi_s^{-1}\cdot,s))|_{\Phi_s y}\,ds.$$

Then for $j=0,1,2,...,$ define

$$\psi_j(x,t)=T_j(\Phi_t^{-1}x,t)\rho^{1/2}(x,t).$$

Then we have the following lemma.

Lemma 2.1:

$$\frac{\partial\psi_j}{\partial t}+\nabla\psi_j\cdot\nabla S_0=-\frac{1}{2}\psi_j\Delta S_0+\Delta\psi_{j-1}$$

for $j=0,1,2,...,$ with the convention $\psi_{-1}\equiv 0$.

We have now assembled the main tools we need. We now explain how to solve the stochastic Hamilton–Jacobi continuity equations.

Proposition 2.2: Assume that $c\in C^2(\mathbb{R}^d)$, $k\in C^2(\mathbb{R}^d\times\mathbb{R})$, $S_0\in C^2(\mathbb{R}^d)$ and Φ_t satisfies a no-caustic condition. Then for a.e. $\omega\in\Omega$ solutions of the Hamilton–Jacobi continuity equations

$$\frac{\partial S_j}{\partial t}+\frac{1}{2}\sum_{\substack{i_1,i_2\geqslant 0\\ i_1+i_2=j}}\nabla S_{i_1}\cdot\nabla S_{i_2}=\frac{1}{2}\Delta S_{j-1},\quad j\geqslant 0,$$

(with the convention $1/2\Delta S_{-1}=-c-\epsilon k\dot{W}_t$) are given by

$$S_1(x,t)=-\ln\psi_0(x,t)$$

and for $j\geqslant 2$

$$S_j(x,t)=2^{1-j}\left(-\frac{\psi_{j-1}}{\psi_0}+\sum_{\substack{i_1,i_2\geqslant 1\\ i_1+i_2=j-1}}\frac{\psi_{i_1}\psi_{i_2}}{2\psi_0^2}-\sum_{\substack{i_1,i_2,i_3\geqslant 1\\ i_1+i_2+i_3=j-1}}\frac{\psi_{i_1}\psi_{i_2}\psi_{i_3}}{3\psi_0^3}+\cdots+\frac{(-1)^{j-1}\psi_1^{j-1}}{(j-1)\psi_0^{j-1}}\right)(x,t).$$

There is an important Corollary:

Corollary 2.1:

$$\frac{\partial}{\partial t}\left(\sum_{j=0}^m\mu^{2j}S_j\right)+\frac{1}{2}\sum_{j=0}^m\mu^{2j}\left(\sum_{\substack{i_1,i_2\geqslant 0\\ i_1+i_2=j}}\nabla S_{i_1}\cdot\nabla S_{i_2}\right)+c+\epsilon k\dot{W}_t=\frac{\mu^2}{2}\Delta\sum_{j=0}^{m-1}\mu^{2j}S_j.$$

An all important role is played by the Nelson diffusion process y_s^μ with drift given by $-\nabla(\Sigma_{j=0}^m\mu^{2j}S_j(y_s^\mu,t-s))$:

$$dy_s^\mu=\mu dB(s)-\nabla\sum_{j=0}^m\mu^{2j}S_j(y_s^\mu,t-s)ds,$$

$$y_0^\mu=(x).$$

Consider the stochastic heat equation of Stratonovich type:

$$du_t^\mu(x)=\left[\frac{\mu^2}{2}\Delta u_t^\mu(x)+\mu^{-2}c(x)u_t^\mu(x)\right]dt+\epsilon\mu^{-2}k(x,t)u_t^\mu(x)\circ dW_t,$$

$$u_0^\mu(x)=T_0(x)\exp(-S_0(x)/\mu^2).$$

Proposition 2.3: For each $m\geqslant 0$,

$$u_t^\mu(x)=\exp\left\{-\mu^{-2}\sum_{j=0}^{m}\mu^{2j}S_j(x,t)\right\}\mathbb{E}\exp\left\{-\frac{\mu^{2m}}{2}\int_0^t\Delta S_m(y_s^\mu,t-s)\,ds\right.$$

$$\left.+\frac{1}{2}\sum_{j=m+1}^{2m}\mu^{2(j-1)}\sum_{\substack{0\leqslant i_1,i_2\leqslant m\\ i_1+i_2=j}}\int_0^t\nabla S_{i_1}\cdot\nabla S_{i_2}(y_s^\mu,t-s)\,ds\right\}.$$

Note that the second factor is of the form $(1+O(\mu^{2m}))$ *and the first factor gives the expansion up to* μ^{2m-2} *for each m.*

Our main result is the following.

Proposition 2.4: The solution of the viscous stochastic Burgers equation is for each $m\geqslant 0$

$$v^\mu(x,t)=\sum_{j=0}^{m}+\mu^{2j}v_j(x,t)-\mu^2\nabla\ln\mathbb{E}\left\{\exp\left\{-\frac{\mu^{2m}}{2}\int_0^t\nabla\cdot v_m(y_s^\mu,t-s)\,ds\right.\right.$$

$$\left.\left.+\frac{1}{2}\sum_{j=m+1}^{2m}\mu^{2(j-1)}\sum_{\substack{0\leqslant i_1,i_2\leqslant m\\ i_1+i_2=j}}\int_0^t v_{i_1}\cdot v_{i_2}(y_s^\mu,t-s)\,ds\right\}\right\},$$

where $v_j(x,t)=\nabla S_j(x,t)$.

Remark 2.1: When $T_0=1$, *the fluid density* ρ *is simply given by*

$$\rho^{1/2}(x,t)=e^{-S_1(x,t)}. \tag{2.1}$$

In the case $T_0\neq 1$, *we note that initially* ρ *is* T_0^2 *explaining its physical significance. Also, observe that up to the caustic time*

$$\int_{\mathbb{R}^d}\rho(x,t)\,dx=\int_{\mathbb{R}^d}T_0^2(\Phi_t^{-1}(x))|\mathrm{Det}\,(\nabla_x\Phi_t^{-1}(x))|\,dx=\int_{\mathbb{R}^d}T_0^2(y)\,dy=\int_{\mathbb{R}^d}\rho(y,0)\,dy.$$

So, mass is conserved.

In this section we have recapitulated some of the key results of Refs. 12 and 14 on stochastic Burgers equations. We have elucidated the detailed structure of the asymptotic series θ in Eq. (1.12) when Φ_s is a diffeomorphism, $0\leqslant s\leqslant t$, so that $x_0(x,t)$ is unique. If we now combine the above results with those of Davies and Truman[26,27] and Ellis and Rosen,[28–30] we can see that even when $x_0(x,t)$ is not unique, for nondegenerate critical points, θ_i has exactly the same structure as above save that we work with the ith branch of Φ_t^{-1} defined by $x_0^i(x,t)$. What breaks down here is the closed form expansion for the remainder term as a functional integral. We hope to address this in a future paper,[33] but we will not need those results here.

III. SINGULARITIES OF THE FREE BURGERS EQUATION AND HEAT EQUATION

We investigate the geometrical relationship between the level surfaces of the heat equation and the shock waves (caustics) of the Burgers equation. We find a robust geometrical relationship between curves on level surfaces and the caustics which (when suitably modified) carries over to

the general stochastic setup. In two dimensions the curves on the level surfaces are the level surfaces themselves. In three dimensions we think of these curves as arising from planar cross sections.

Definition 3.1: A curve $x=x(\gamma)$, $\gamma\in N(\gamma_0,\delta)$, *is said to have a generalized cusp at* $\gamma=\gamma_0$, γ *being arc length if*

$$\left.\frac{dx(\gamma)}{d\gamma}\right|_{\gamma=\gamma_0}=0.$$

A. A simple geometrical relationship

In this section and Sec. V we were inspired by V. I. Arnol'd's beautiful treatment of classical mechanics in Ref. 34.

Let $\mathcal{A}=\mathcal{A}(x_0,x,t)$ be the classical action for the initial momentum ∇S_0,

$$\mathcal{A}(x_0,x,t)=A(x_0,x,t)+S_0(x_0), \tag{3.1}$$

where in the deterministic case

$$A(x_0,x,t)=\inf_{\substack{X(s)\\X(t)=x\\X(0)=x_0}}\left\{\frac{1}{2}\int_0^t\dot{X}^2(s)\,ds-\int_0^t c(X(s))ds\right\},$$

c being the deterministic potential energy. The Euler–Lagrange equation for the above action reduces to

$$\ddot{X}(s)=-\nabla c(X(s)),\quad s\in[0,t],$$

and $X(t)=x$, $X(0)=x_0$. The free case corresponds to setting $c\equiv 0$ and

$$A(x_0,x,t)=\frac{(x-x_0)^2}{2t},$$

$$\mathcal{A}(x_0,x,t)=\frac{(x-x_0)^2}{2t}+S_0(x_0).$$

We assume that $\mathcal{A}(x_0,x,t)$ is at least C^4 in space variables for $t>0$. Defining the corresponding classical flow now reduces to

$$\nabla_{x_0}\mathcal{A}(x_0,x,t)=0,$$

i.e.,

$$(x_0-x)/t+\nabla S_0(x_0)=0\quad\text{or}\quad x=\Phi_t(x_0)=x_0+t\nabla S_0(x_0).$$

We sometimes write $x_0=\Phi_t^{-1}x=x_0(x,t)$ as the (possibly nonunique) solution of

$$x_0+t\nabla S_0(x_0)=x.$$

Consider the level surface equations obtained by eliminating x_0 between

$$\mathcal{A}(x_0,x,t)=0\quad\text{and}\quad\frac{\partial\mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0,\quad\alpha=1,2,...,d. \tag{3.2}$$

We obtain the prelevel surface by eliminating x in the above equations. Considering for any real constant c, the equation obtained by eliminating x_0 between

$$\mathcal{A}(x_0,x,t)=c \quad \text{and} \quad \frac{\partial \mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0, \quad \alpha=1,2,...,d, \tag{3.3}$$

gives the level surface of Hamilton's principal function $S(x,t)=c$ with $S(x,0)=S_0(x)$. We denote this level surface by H_t and the prelevel surface by $\Phi_t^{-1}H_t$.

Imitating the above, the precaustic equation and caustic equation can be obtained in a similar way by considering

$$\mathrm{Det}\left(\frac{\partial^2 \mathcal{A}}{\partial x_0{}^2}(x_0,x,t)\right)=0, \quad \frac{\partial \mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0, \quad \alpha=1,2,...,d. \tag{3.4}$$

We denote these surfaces by $\Phi_t^{-1}C_t$ and C_t, respectively.

Let $x\to\alpha$, a point on the caustic. Then, since we expect the multiplicity of the $x_0^i\in\Phi_t^{-1}\{x\}$ to change as we cross the caustic, we anticipate that $x_0^j(x,t)\to x_0^k(x,t)$ as $x\to\alpha$. Since different parts of the level surface correspond to different x_0^i, if $S_j(\alpha,t)=S_k(\alpha,t)=c$, then the parts $S_j(x,t)=c$ and $S_k(x,t)=c$ meeting at α could have a cusp. It is cusps like this which give rise to turbulent behavior of the Burgers velocity field. We therefore investigate in the free case the conditions under which we get cusps.

In the free case the equation of the zero prelevel surface is the eikonal equation

$$\frac{t}{2}|\nabla S_0(x_0)|^2+S_0(x_0)=0,$$

and the derivative map $D\Phi_t(x_0):T_{x_0}\to T_x$, mapping tangent spaces, is the linear map

$$D\Phi_t(x_0)=(I+t\nabla^2 S_0(x_0)),$$

where $\nabla^2 S_0$ is the Hessian of S_0. The following elementary identity is crucial in what follows:

$$\nabla_{x_0}\left\{\frac{t}{2}|\nabla S_0(x_0)|^2+S_0(x_0)\right\}=(I+t\nabla^2 S_0(x_0))\nabla S_0(x_0). \tag{3.5}$$

Since $D\Phi_t(x_0)$ is in this case a real symmetric matrix, we can analyse what happens very easily, especially for two dimensions.

B. Results in two dimensions

Lemma 3.1: Assume that the prelevel surface meets the precaustic at the point x_0, *where* $|(I+t\nabla^2 S_0(x_0))\nabla S_0(x_0)|\neq 0$ *and* $\dim(\mathrm{Ker}(I+t\nabla^2 S_0(x_0)))=1$. *Then the tangent plane to the prelevel surface* T_{x_0} *is spanned by* $\mathrm{Ker}(I+t\nabla^2 S_0(x_0))$.

Proof: The last displayed formula shows that where the prelevel surface meets the precaustic the nonzero normal to the prelevel surface is a linear combination of eigenvectors corresponding to the nonzero eigenvalues of $(I+t\nabla^2 S_0(x_0))$. The eigenvector of $(I+t\nabla^2 S_0(x_0))$ corresponding to eigenvalue zero, e_0, is orthogonal to these eigenvectors, so because T_{x_0} is only one dimensional, we have $T_{x_0}=\langle e_0\rangle$. □

When $\nabla S_0(x_0)=0$ at x_0 a point of the prelevel surface, the above argument shows that x_0 is a singular point of the prelevel surface, typically a node with two different directions of the tangent plane. Because the partial derivatives

$$\frac{\partial \mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0, \quad \alpha=1,2,$$

we have for $x_0 = \Phi_t^{-1} x$

$$\nabla_x \mathcal{A}(x_0, x, t) = \frac{(x - x_0)}{t} = \nabla S_0(x_0),$$

independent of dimension. (In point of fact the last result is true merely because in the free case the momentum is constant.) Hence, at the image point $x = \Phi_t(x_0)$ (independent of the dimensions of the space and independent of whether or not $x_0 \in \Phi_t^{-1} C_t$) $|\nabla_x \mathcal{A}| = 0$ so x is also a singular point. Typically then, even if we are not on the precaustic, we expect that in the free case x_0 and $\Phi_t(x_0)$ are both nodes with two or more different directions of the tangent plane. This eventuality is easy to investigate with the derivative map $D\Phi_t(x_0)$. When $x_0 \in \Phi_t^{-1} C_t$ [because $D\Phi_t(x_0)$ annihilates the zero eigenvector e_0 on the precaustic] we have only one direction for the tangent plane at $\Phi_t(x_0)$ even though there were two distinct directions for the tangent plane to the prelevel surface at x_0. This happens, for example, where the prelevel surface consists of an ellipse and a line pair crossing at x_0 where the ellipse is tangential to the parabolic precaustic. It also occurs in the three-dimensional fish and butterfly example along the straight line of intersection of the caustic and zero level surface. Both of these examples are elucidated in Sec. IV.

Lemma 3.2: Assume that the prelevel surface meets the precaustic at the point x_0 where $|\nabla S_0(x_0)| = 0$, x_0 being a node, and dim $(\mathrm{Ker}(I + t\nabla^2 S_0(x_0))) = 1$. *Then the image point $\Phi_t(x_0)$ where the level surface meets the caustic is a singular point which cannot be a node but can be a cusp. If x_0 is a node of the prelevel surface, $x_0 \notin \Phi_t^{-1} C_t$, then $x = \Phi_t(x_0)$ is a node of the level surface.*

Proof: In the first case, the two different directions t_1 and t_2 at x_0 of the tangent plane to the prelevel surface where it meets the precaustic are both mapped into $(I + t\nabla^2 S_0(x_0)) e_0^{\perp}$, $e_0^{\perp}$ being the nonzero eigenvector of $(I + t\nabla^2 S_0(x_0))$. So both t_1 and t_2 get mapped into the same direction as $e_0^{\perp}$. Moreover, $|\nabla \mathcal{A}| = 0$, so $\Phi_t(x_0)$ is a singular point so it has to be a cusp. The second case follows because the two different directions t_i get mapped into the two different directions $(I + t\nabla^2 S_0(x_0)) t_i$ for $i = 1,2$. □

Remark 3.1: Needless to say there is an analog of this lemma in d dimensions. The condition $|\nabla S_0(x_0)| = 0$ should be seen as a zero speed condition.

When $(I + t\nabla^2 S_0(x_0)) \nabla S_0(x_0)$ is nonzero, there is a simple result concerning the appearance of cusps on the level surface. We use the intrinsic equation of the prelevel surface $x_0 = x_0(\gamma)$, $\gamma \in N(\gamma_0, \delta)$, where $x_0(\gamma_0)$ is the point of intersection of the prelevel surface and precaustic. We write $x(\gamma) = \Phi_t(x_0(\gamma))$ and assume that x_0 and x are differentiable in γ.

Proposition 3.1: Assume that $|(I + t\nabla^2 S_0(x_0)) \nabla S_0(x_0)| \neq 0$, so x_0 is not a singular point of the prelevel surface. Then $\Phi_t(x_0)$ can only be a generalized cusp of the level surface if $\Phi_t(x_0) \in C_t$, the caustic. Moreover, if $x = \Phi_t(x_0) \in \Phi_t(\Phi_t^{-1} C_t \cap \Phi_t^{-1} H_t)$, x will indeed be a generalized cusp of the level surface.

Proof: We have the normal $n(x_0) = (I + t\nabla^2 S_0(x_0)) \nabla S_0(x_0) \neq 0$, $dx_0(\gamma)/d\gamma|_{\gamma = \gamma_0} \neq 0$ and from above

$$\left.\frac{dx(\gamma)}{d\gamma}\right|_{\gamma = \gamma_0} = (D\Phi_t(x_0)) \left.\frac{dx_0(\gamma)}{d\gamma}\right|_{\gamma = \gamma_0} = (I + t\nabla^2 S_0(x_0)) \left.\frac{dx_0(\gamma)}{d\gamma}\right|_{\gamma = \gamma_0}.$$

For this to be zero it is necessary that $\mathrm{Det}(I + t\nabla^2 S_0(x_0)) = 0$, so $x_0 \in \Phi_t^{-1} C_t$ i.e., it is necessary that $\Phi_t(x_0) \in C_t$. Trivially from Lemma 3.1 it follows that if $x_0 \in \Phi_t^{-1} C_t$, then $dx(\gamma)/d\gamma|_{\gamma = \gamma_0} = 0$. □

C. Results in three dimensions

Consider the above setup in three dimensions so that the wavefront H_t has the equation in x obtained by eliminating x_0 between

$$\mathcal{A}(x_0,x,t)=c \quad \text{and} \quad \frac{\partial \mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0, \quad \alpha=1,2,3,$$

and the caustic C_t by eliminating x_0 between

$$\mathrm{Det}\left(\frac{\partial^2 \mathcal{A}}{\partial x_0{}^2}(x_0,x,t)\right)=0 \quad \text{and} \quad \frac{\partial \mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0, \quad \alpha=1,2,3.$$

We define the cusped part of H_t by

$$\mathrm{Cusp}(H_t)=\{x\in H_t : x\in \Phi_t(\Phi_t^{-1}C_t\cap \Phi_t^{-1}H_t), x=\Phi_t(x_0),$$
$$x_0\in \Phi_t^{-1}C_t\cap \Phi_t^{-1}H_t, n(x_0)=(I+t\nabla^2 S_0(x_0))\nabla S_0(x_0)\neq 0\}.$$

Typical of what happens in three dimensions for which $d=3$ is the following:

Theorem 3.1: *Let $x\in \mathrm{Cusp}(H_t)$. Then T_x, the tangent plane to the level surface H_t at x, is at most one dimensional.*

Remark 3.2: The tangent plane T_x folds over onto itself at points $x\in \mathrm{Cusp}(H_t)$, the direction of the fold being the direction of the one-dimensional tangent space at x.

Proof: Let n be the unit normal to the tangent plane T_{x_0}, $x_0\in \Phi_t^{-1}C_t\cap \Phi_t^{-1}H_t$. This is the well-defined vector

$$n=|(I+t\nabla^2 S_0(x_0))\nabla S_0(x_0)|^{-1}(I+t\nabla^2 S_0(x_0))\nabla S_0(x_0),$$

which is clearly a linear combination of the nonzero eigenvectors of $(I+t\nabla^2 S_0(x_0))$. Let e_0 be an eigenvector corresponding to eigenvector zero which is orthogonal to n. Since $n\neq 0$, T_{x_0} is a well-defined two-dimensional space spanned by e_0 and $n\wedge e_0=e_0^\perp$. Because $D\Phi_t(x_0)=(I+t\nabla^2 S_0(x_0))$, T_x is spanned by $(I+t\nabla^2 S_0(x_0))e_0^\perp$. □

We now see what it takes for us to observe cusps on planar cross sections of the level surface where it meets the caustic. We shall assume, without loss of generality, that the planar cross sections are on a plane $y=\mathrm{const}$ with normal e_y. We write $x=\Phi_t(x_0)$ and

$$\nabla S_0(x_0)=\alpha_0 e_0+\alpha_1 e_1+\alpha_2 e_2=\nabla_x \mathcal{A},$$

where

$$(I+t\nabla^2 S_0(x_0))e_0=0,$$

$$(I+t\nabla^2 S_0(x_0))e_i=\lambda_i e_i, \quad i=1,2,$$

$x_0\in \Phi_t^{-1}C_t\cap \Phi_t^{-1}H_t$.

Then, from above, the unit normal

$$n=(\alpha_1\lambda_1 e_1+\alpha_2\lambda_2 e_2)\theta$$

and

$$e_0^\perp=(\alpha_2\lambda_2 e_1-\alpha_1\lambda_1 e_2)\theta,$$

where $\theta=(\alpha_1^2\lambda_1^2+\alpha_2^2\lambda_2^2)^{-1/2}$. At a point $x\in \mathrm{Cusp}(H_t)$, the axis system $\{e_0,e_0^\perp,n\}$ is well defined and intrinsically related to the geometry of the prelevel surface at $x_0\in \Phi_t^{-1}C_t\cap \Phi_t^{-1}H_t$. This is our preferred axis system for discussing cusps.

We assume that S_0 is at least C^4 and write

$$x=x_0+t\nabla S_0(x_0).$$

We work to second order

$$x+\delta x = x_0+\delta x_0 + t\nabla S_0(x_0+\delta x_0)$$
$$= x_0+\delta x_0 + t\nabla S_0(x_0) + t(\delta x_0\cdot\nabla)\nabla S_0(x_0) + \frac{t}{2}(\delta x_0\cdot\nabla)^2\nabla S_0(x_0) + O((\delta x_0)^3).$$

Hence, correct to second order,

$$\delta x = (I + t\nabla^2 S_0(x_0))\delta x_0 + \frac{t}{2}(\delta x_0\cdot\nabla)^2\nabla S_0(x_0).$$

We now set

$$\delta x_0 = \varepsilon(\lambda e_0 + \mu e_0^{\perp}) + \varepsilon^2(\xi e_0 + \eta e_0^{\perp} + \zeta n).$$

The first term gives the direction of $dx_0/d\gamma$ and the second $d^2x_0/d\gamma^2$ evaluated at $\gamma=\gamma_0$, where $x_0(\gamma_0)$ is the point of intersection. Then we obtain

$$\delta x = \varepsilon\mu\lambda_1\lambda_2(\alpha_2 e_1 - \alpha_1 e_2)\theta$$
$$+\varepsilon^2\left(\eta\lambda_1\lambda_2(\alpha_2 e_1-\alpha_1 e_2)\theta + \zeta(\alpha_1\lambda_1^2 e_1 + \alpha_2\lambda_2^2 e_2)\theta + \frac{t}{2}(\lambda\partial_0+\mu\partial_0^{\perp})^2\nabla S_0(x_0)\right),$$

∂_0 and $\partial_0^{\perp}$ being directional derivatives parallel to e_0 and $e_0^{\perp}$.

For a genuine cusp we clearly have to set $\mu=0$, for which

$$\delta x_0 = \varepsilon\lambda e_0 + \varepsilon^2(\xi e_0 + \eta e_0^{\perp} + \zeta n), \tag{C_0}$$

$$\delta x = \varepsilon^2\left(\eta\lambda_1\lambda_2(\alpha_2 e_1-\alpha_1 e_2)\theta + \zeta(\alpha_1\lambda_1^2 e_1 + \alpha_2\lambda_2^2 e_2)\theta + \frac{t}{2}\lambda^2\partial_0^2\nabla S_0(x_0)\right). \tag{C_1}$$

We now have to satisfy two further conditions:

$$\delta x\cdot e_y = 0, \tag{C_2}$$

$$\delta x\cdot\frac{\partial\mathcal{A}}{\partial x} = \delta x\cdot\nabla S_0(x_0) = \delta x\cdot(\alpha_0 e_0+\alpha_1 e_1+\alpha_2 e_2) = 0. \tag{C_3}$$

If we can choose λ, η, and ζ to satisfy the above two equations for nonzero δx, the planar cross section of the level surface H_t, $y=\text{const}$, will have a genuine cusp at $x\in\text{Cusp}(H_t)$. The axis of the cusp will be $\widehat{\delta x}$. This explains why genuine cusps are so numerous on planar cross sections.

Theorem 3.2: *Any point x on the level surface H_t, $x=\Phi_t(x_0)$ with $x_0=\Phi_t^{-1}(x)$ on the prelevel surface, can only be a generalized cusp of a curve on H_t if x_0 is a generalized cusp of the precurve on the prelevel surface or if $x_0\in\Phi_t^{-1}C_t$ the precaustic. In three dimensions, the planar cross section $y=\text{const}$ (with normal e_y) of the level surface H_t through a point x where it meets C_t will have a genuine cusp at x if $x\in\text{Cusp}(H_t)$ and there is a nonzero solution δx of Eqs. (C_0), (C_1), (C_2) and (C_3). The direction of the axis of the cusp is $\widehat{\delta x}$.*

Proof: The first part of the theorem is obvious.

Equations (C_1), (C_2) and (C_3) uniquely fix the direction of $\widehat{\delta x}$, if nonzero λ, η and ζ exist satisfying these equations. It is easy to see that Eqs. (C_0), (C_1), (C_2), and (C_3) are sufficient to solve

$$\mathcal{A}(x_0,x,t)=c,$$

$$\mathcal{A}(x_0+\delta x_0,x+\delta x,t)=c,$$

$$\frac{\partial \mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0, \quad \alpha=1,2,3,$$

$$\frac{\partial \mathcal{A}}{\partial x_0^\alpha}((x_0+\delta x_0,x+\delta x,t)=0, \quad \alpha=1,2,3,$$

correct to second order, if

$$\mathrm{Det}\left(\frac{\partial^2 \mathcal{A}}{\partial x_0^2}(x_0,x,t)\bigg|_{x=\Phi_t(x_0)}\right)=0,$$

$x_0\in\Phi_t^{-1}C_t\cap\Phi_t^{-1}H_t$, $x=\Phi_t(x_0)$, and $n(x_0)$ nonzero. □

This analysis explains the plethora of cusps which we observe in the free case. Moreover, as we shall see, the argument above can be generalized to include random and deterministic external forces i.e., nonzero c and k terms in the Burgers equation.

Remark 3.3: We make the point that

$$\Phi_t^{-1}C_t\cap\Phi_t^{-1}H_t\subset\Phi_t^{-1}(C_t\cap H_t), \tag{3.6}$$

but the opposite inclusion does not hold and so images of points in $\Phi_t^{-1}(C_t\cap H_t)\backslash(\Phi_t^{-1}C_t\cap\Phi_t^{-1}H_t)$ *give rise to cross-over points.*

D. Consequences for the Burgers fluid

Here we recapitulate a result of Truman and Zhao.[12] See Ref. 31 for more recent related results.

Theorem 3.3: *Let* $\tau(a)$ *be the first time such that there exist minimizers* $y_1\neq y_2$, y_1, $y_2\in\mathbb{R}^d$, *such that* $\Phi_\tau(y_1)=\Phi_\tau(y_2)=a$ *and* $\dot\Phi_\tau(y_1)\neq\dot\Phi_\tau(y_2)$, *i.e.,* τ *is a caustic time at point a. Then* $v^0(x,t)$ *is discontinuous at* (τ,a).

We now give a simple application of the above results to the Burgers fluid in two dimensions. For smooth S_0, in two dimensions, we can divide one side of the caustic into *hot* and *cool* parts. We consider points of intersection α with the level surface $S(x,t)=S(\alpha,t)$ cusped at α: if the part of the level surface cusped at α corresponds to the minimizing $x_0(\alpha,t)$, then the Burgers velocity field $v^0(x,t)=\nabla S(x,t)\to\nabla S(\alpha,t)=0$ as $x\to\alpha$ from the cusped side of the caustic. This is merely because the condition for $S(x,t)=S(\alpha,t)$ to have a cusp at $x=\alpha$ is $\nabla S(\alpha,t)=0$. Moreover, this entails the minimizing surface changing as we cross the caustic. Indeed the cusp occurs because the minimizing surface on the cusped side of the caustic cannot be continued across the caustic. So $u^0(x,t)$ is necessarily exponentially discontinuous as we cross such parts of the caustic. This is because here two $x_0(x,t)$'s coalesce as the minimizer at the cusp and then disappear. We call such points α cool because the Burgers fluid has zero velocity on one side of the caustic at α. The whole of one side of the generic semi-cubical parabolic cusp is cool. Not all of one side of the two-dimensional swallowtail is cool. This is discussed in the next section, where we give numerical confirmation of this result. The exponential discontinuity in u^0 can be seen by inspecting Fig. 10 which shows the number of negative S_0^i's in the different regions. Similar results apply in three dimensions.

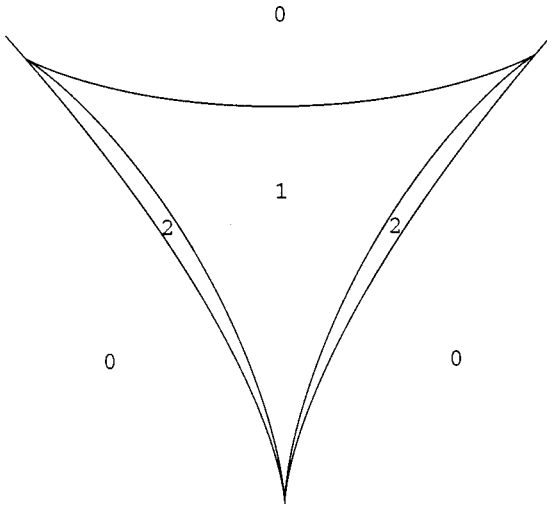

FIG. 10. Number of negative S_0.

IV. DETERMINISTIC AND ARCHETYPAL EXAMPLES

Consider S_0 given in the following table for two and three dimensions, respectively,

Shockwave	Zero Level Surface	S_0
Cusp	Tricorn	$x_0^2 y_0/2$
Swallowtail	Plough	$x_0^5+\lvert x_0\rvert^{3/2} y_0$
Butterfly	Fish	$x_0^3 y_0/3+x_0^2 z_0/2$
Swallowtail	Seagull	$\lvert x_0\rvert^5+\lvert x_0\rvert^{1+c} y_0+\lvert x_0\rvert^c z_0$

where $1/2<c<1$. The nature of the caustic (shockwave) is given in the first column and the corresponding zero level surfaces in the second. The zero level surface corresponding to the semicubical parabolic cusp is the tricorn, which has three cusps on the semi-cubical parabola, one of which coincides with the original cusp of the shockwave, and a line-pair. The zero level surface corresponding to the butterfly is the fish, which meets the butterfly in four curves (three of which are cusped and one of which is a straight line on which they touch). See Refs. 35 and 36 for further and more surprising examples.

A. A two-dimensional example

For $S_0(x_0,y_0)=x_0^2 y_0/2$ the zero prelevel surface has equation

$$x_0^2\left(\frac{(y_0+1/2t)^2}{(1/2t)^2}+\frac{x_0^2}{(1/t)^2}-1\right)=0,$$

and the precaustic has equation

$$1+ty_0=t^2x_0^2.$$

Note also that $\nabla S_0(x_0,y_0)=0$ at the point $(0,-1/t)$, so the zero speed condition is satisfied here and this point is a node of the zero prelevel surface. We now map $(x,y)=\Phi_t(x_0,y_0)$ to obtain the hypocycloid tricorn

$$x=\frac{\cos\theta(1+\sin\theta)}{2t},\quad y=\frac{\sin\theta(1-\sin\theta)}{2t}, \tag{4.1}$$

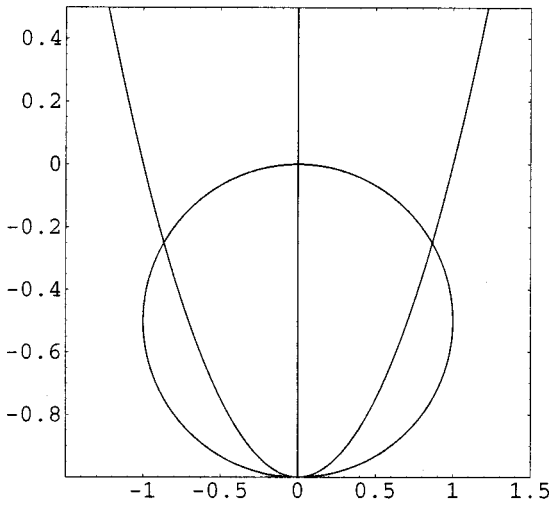

FIG. 11. Precaustic and prelevel surface.

for $0 \leqslant \theta < 2\pi$, as the zero level surface at time t for the heat equation and semi-cubical parabolic cusp

$$8(yt+1)^3 = 27t^2x^2, \tag{4.2}$$

as shockwave at time t for the corresponding Burgers velocity field.

Figures 11 and 12 illustrate the level surface $S_t(x,y)=0$. Figures 13 and 14 illustrate the level surface $S_t(x,y)=2$. Figures 15 and 16 illustrate the level surface $S_t(x,y)=-2^{-7}$.

We have verified numerically that the caustic surfaces are indeed discontinuities for the Burgers velocity field as shown in Fig. 17. Further, it is not difficult to see that the whole of one side of this cusp surface is cool. One has to note, and it is not too onerous to check, that for each point of the cusp the minimizing S_0^i corresponds to a cusp and not a crossover. The agreement with the cusp catastrophe is shown in Fig. 18.

Finally we add that in two dimensions the tricorn will be a common feature of the level surfaces of Hamilton's principal function when the corresponding prelevel surface touches the precaustic. Here the point is that the unfolding of the tricorn under the inverse classical flow map

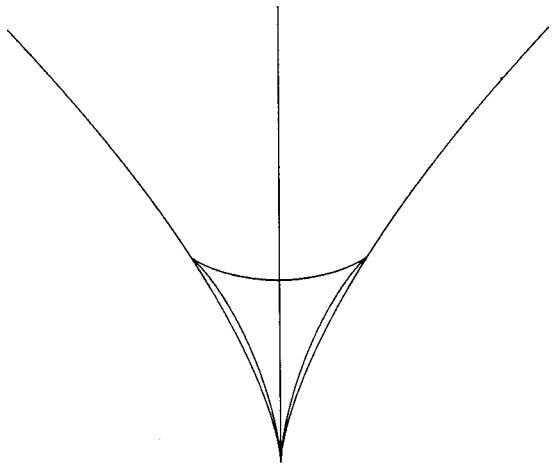

FIG. 12. Cusp and tricorn.

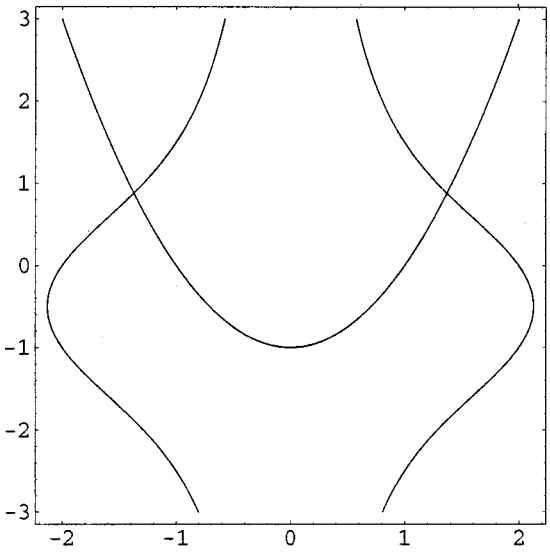

FIG. 13. Precaustic (parabola) and prelevel surface (kneecap).

Φ_t is the "halo" shown in Fig. 11. The point of contact is denoted by x_0^0 and the direction of the unit tangent vector by e_0. To see this from above we know that $\Phi_t(x_0^0 \pm \varepsilon e_0) = \Phi_t(x_0^0) + o(\varepsilon)$. If the slightly stronger result holds, namely, $\Phi_t(x_0^0 \pm \varepsilon e_0) = \Phi_t(x_0^0) + \varepsilon^2 w_0 + o(\varepsilon^2)$, then necessarily we have a tricorn with axis w_0 since both halves of the common tangent get mapped onto the half axis parallel to w_0, the other two points of intersection being mapped onto cusps.

B. A three-dimensional example

For $S_0(x_0, y_0, z_0) = x_0^3 y_0/3 + x_0^2 z_0/2$ we can quickly see the close relationship with the previous example by means of the cross sections $y = \text{const}$ shown in Figs. 19 and 20.

To see where the butterfly (Fig. 21) and fish (Fig. 22) meet, consider the classical mechanics:

$$x = x_0 + t(x_0^2 y_0 + x_0 z_0),$$

$$y = y_0 + \frac{t}{3} x_0^3,$$

$$z = z_0 + \frac{t}{2} x_0^2.$$

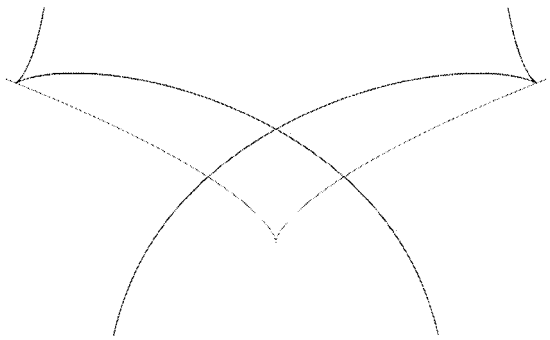

FIG. 14. Caustic (cusp) and level surface (neckline).

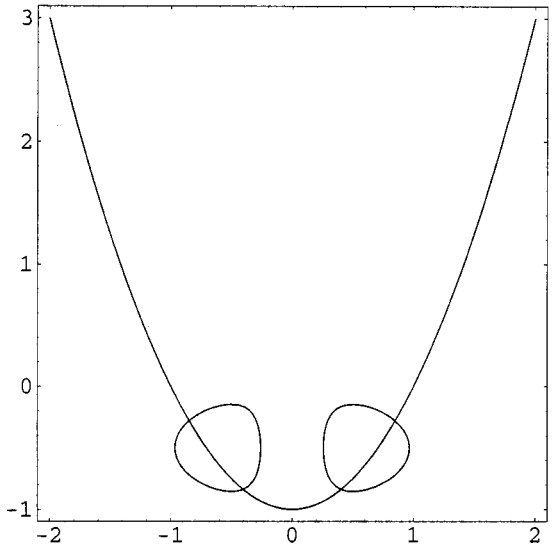

FIG. 15. Precaustic (parabola) and prelevel surface (pebble pair).

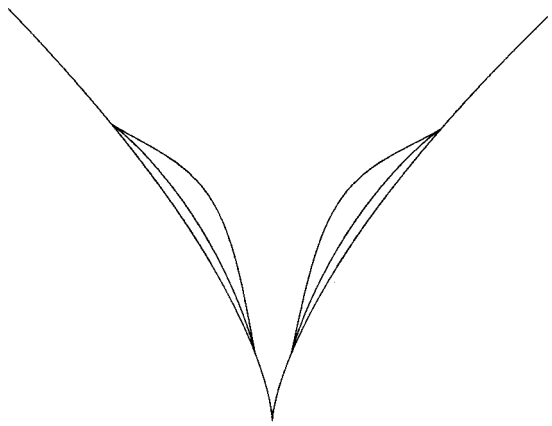

FIG. 16. Caustic (cusp) and level surface (lapel pair).

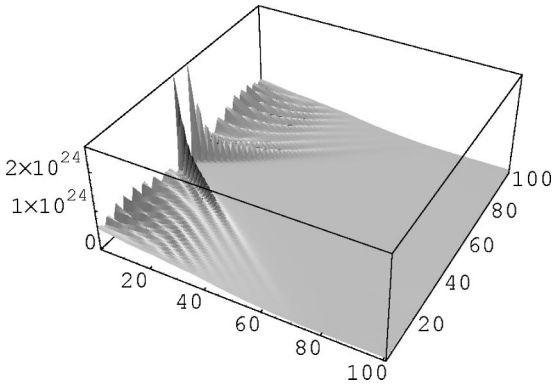

FIG. 17. $|v^{\mu}|^2$ for small μ.

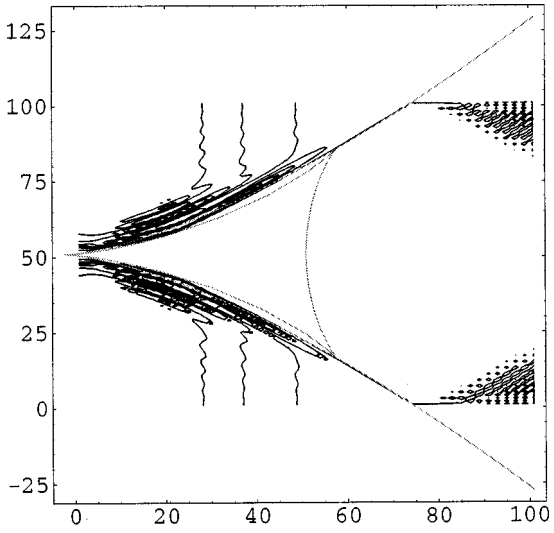

FIG. 18. Contour plot of $|v^{\mu}|^2$ with cusp and tricorn.

Solving the precaustic equation leads to

$$z_0 = -\frac{1-t^2x_0^2-t^2x_0^4+2tx_0y_0}{t},$$

and with this we simplify the zero prelevel surface equation, one solution of which is $x_0=0$ leaving a quadratic equation for y_0 with roots,

$$y_0=\frac{-2+6t^2x_0^2-6t^2x_0^4+\sqrt{4+3t^2x_0^2+8t^2x_0^4}}{6tx_0},$$

and

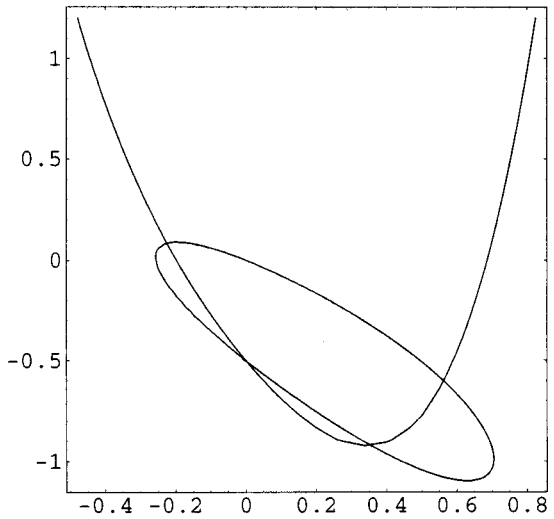

FIG. 19. Prebutterfly and fish.

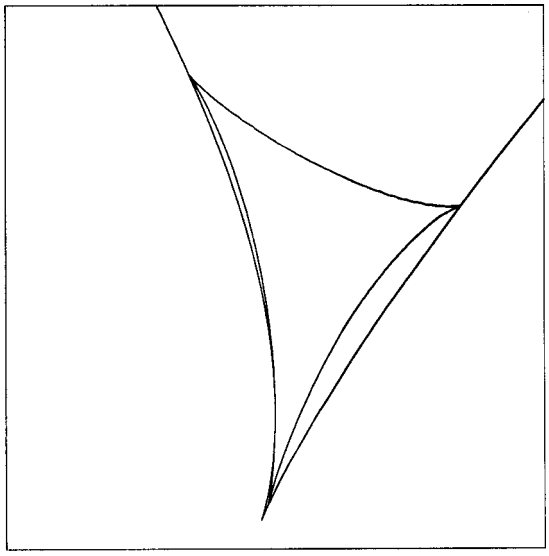

FIG. 20. Butterfly and fish.

$$y_0=\frac{-2+6t^2x_0^2+6t^2x_0^4+\sqrt{4+3t^2x_0^2+8t^2x_0^4}}{6tx_0}.$$

When $x_0=0$, we have $z_0=-1/t$ and $\nabla S_0(x_0,y_0,z_0)=0$ on this line. Hence on this line the zero speed condition is satisfied and the tangent plane to the zero prelevel surface here has two possible directions. Therefore the zero level surface and caustic meet on a straight line at

$$x=0, \quad z=-1/t, \quad y\in\mathbb{R}.$$

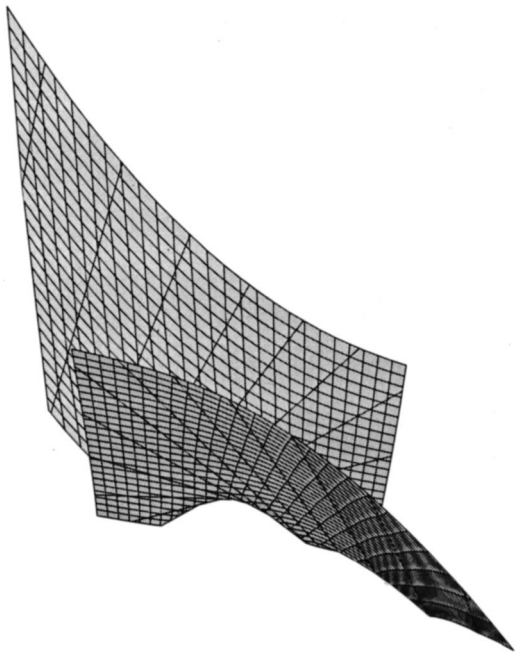

FIG. 21. The butterfly singularity for Burgers equation.

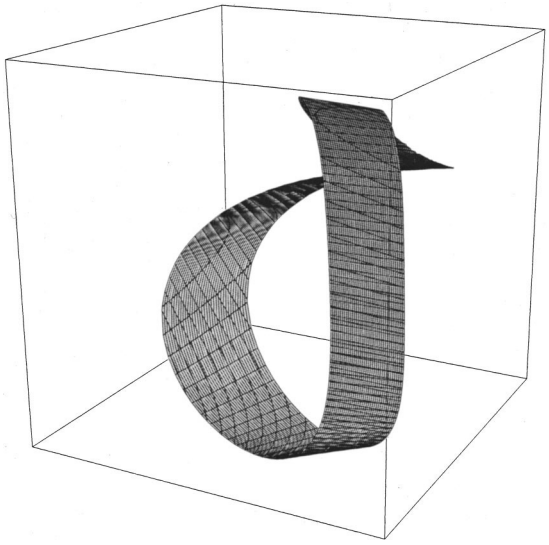

FIG. 22. The fish level surface for heat equation (a section).

It is easy to see that the two surfaces actually touch on this line because this line is on the precaustic. For one value of y_0, we obtain the parametric equations of the two curves of intersection ($x_0>0$ and $x_0<0$)

$$x=\tfrac{1}{6}x_0(2+\sqrt{4+t^2x_0^2(3+8x_0^2)}),$$

$$y=-\frac{2-2t^2x_0^2(3+4x_0^2)+\sqrt{4+t^2x_0^2(3+8t^2)}}{6tx_0},$$

$$z=\frac{-3t^2x_0^2(1+2x_0^2)+2(-1+\sqrt{4+t^2x_0^2(3+8t^2)})}{6t}.$$

For the other value of y_0 we obtain the parametric equation of one additional curve:

$$x=-\tfrac{1}{6}x_0(-2+\sqrt{4+t^2x_0^2(3+8x_0^2)}),$$

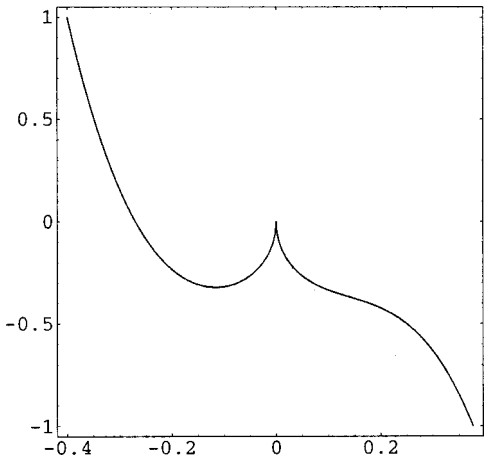

FIG. 23. Precaustic.

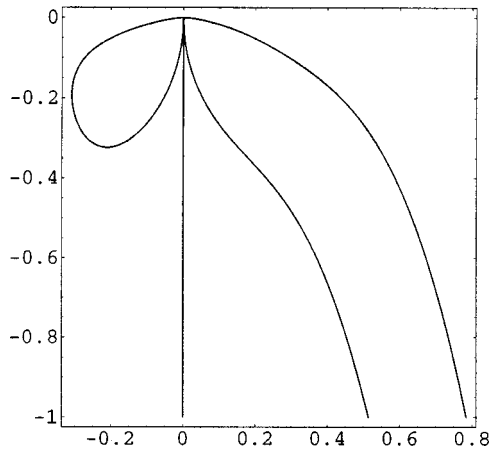

FIG. 24. Prelevel surface.

$$y=\frac{-2+2t^2x_0^2(3+4x_0^2)+\sqrt{4+t^2x_0^2(3+8t^2)}}{6tx_0},$$

$$z=-\frac{3t^2x_0^2(1+2x_0^2)+2(1+\sqrt{4+t^2x_0^2(3+8t^2)})}{6t}.$$

C. A cautionary two-dimensional example

We briefly consider the nongeneric two-dimensional swallowtail, where $S_0(x_0,y_0)=x_0^5+|x_0|^{3/2}y_0$. Here the zero level surface crosses the caustic because $\Phi_t^{-1}(C_t\cap H_t)\not\subset\Phi_t^{-1}C_t\cap\Phi_t^{-1}H_t$. This example also shows (Fig. 24) that we can have $dx_0(\gamma_0)/d\gamma=0$ occurring on the zero prelevel surface, although we should point out that S_0 is nonpolynomial in this case. We have many other cases of polynomial S_0 giving rise to two-dimensional swallowtail singularities.

Note the alignment of the generalized cusps on the zero prelevel surface and precaustic, Figs. 23 and 24, respectively. Figures 25 and 26 are the corresponding caustic and zero level surface.

We also illustrate in Fig. 27 the case where the zero level surface crosses the caustic, at the points P and Q, when Φ_t^{-1} gives distinct points on the zero prelevel surface and precaustic.

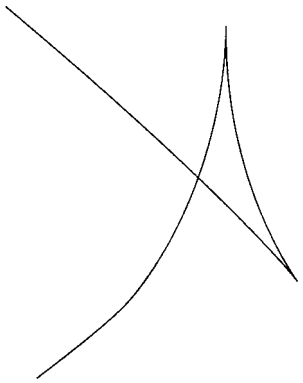

FIG. 25. Swallowtail caustic.

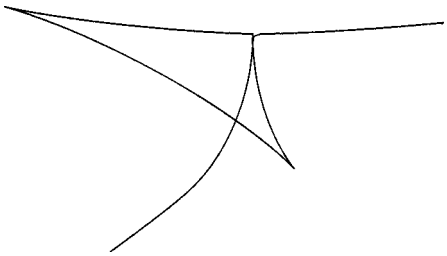

FIG. 26. Plough level surface.

D. Swallowtail

We briefly illustrate (Figs. 28 and 29), the caustic for $S_0(x_0,y_0,z_0)=|x_0|^5+|x_0|^{5/3}y_0+|x_0|^{2/3}z_0$. This was the first such S_0 found to generate the swallowtail, but we also have examples of strictly polynomial S_0 which generate the same archetypal caustic in three dimensions in analogy to the examples of the previous section.

V. THE STOCHASTIC AND GENERAL CASES

A. The stochastic action

Let $A(x_0,p_0,t)$ be defined by

$$A(x_0,p_0,t)=\frac{1}{2}\int_0^t \dot{X}^2(s)\,ds-\int_0^t [c(X(s))\,ds+\epsilon k(X(s),s)\,dW_s],$$

almost surely, where $X(s)=X_s=X(s,x_0,p_0)$ satisfies

$$d\dot{X}(s)=-\nabla c(X(s))ds-\epsilon\nabla k(X(s),s)dW_s, \quad s\in[0,t],$$

with $X(0)=x_0$ and $\dot{X}(0)=p_0,x_0,p_0\in\mathbb{R}^d$. We shall assume that X_s is unique and as usual is $\mathcal{F}_s$ measurable. We also allow for p_0 to be an as yet unspecified function of x_0.

Recall the integration by parts property (ibp^2) for the continuous process $\dot{X}(s)=\dot{X}(s,x_0,p_0)$,

$$\int_0^t u(s)\,d\dot{X}(s)=u(t)\dot{X}(t)-u(0)\dot{X}(0)-\int_0^t \dot{u}(s)\dot{X}(s)\,ds,$$

for deterministic $u\in C^1(0,t)$. This integration by parts property is also valid for random u, if the stochastic integral is of Itô's form and, $du_s d\dot{X}_s$, the corresponding Itô correction, is zero. An important case in point is when

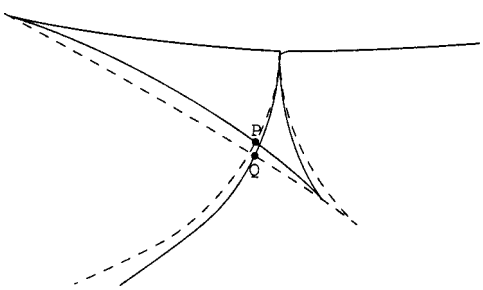

FIG. 27. Swallowtail and plough.

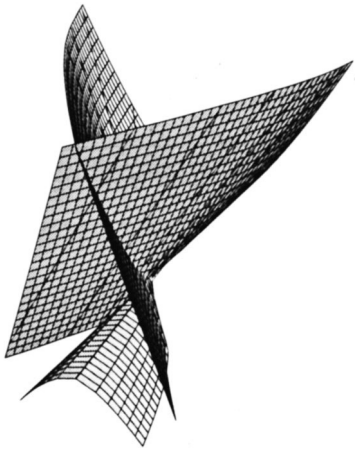

FIG. 28. The swallowtail singularity for Burgers equation.

$$u_s = \frac{\partial X_s}{\partial x_0^\alpha},$$

for $s \in [0,t]$ and $\alpha = 1,2,...,d$. Then, if we assume ∇c, ∇k are Lipschitz, with Hessians $\nabla^2 c$, $\nabla^2 k$ and all second derivatives with respect to space variables of c and k bounded, according to Kunita,[37] $\partial X_s / \partial x_0^\alpha$ satisfies

$$\frac{d}{ds}\left(\frac{\partial X_s}{\partial x_0^\alpha}\right) = \frac{\partial \dot{X}_0}{\partial x_0^\alpha} - \int_0^s \left[\nabla^2 c(X(r)) \frac{\partial X(r)}{\partial x_0^\alpha}\, dr + \epsilon \nabla^2 k(X(r),r) \frac{\partial X(r)}{\partial x_0^\alpha}\, dW_r \right].$$

So the Itô correction is zero. Hence for $u_s = \partial X_s / \partial x_0^\alpha$ we can use the ibp[2]. Moreover,

$$\dot{X}_s = \dot{X}_0 - \int_0^s [\nabla c(X(r))\, dr + \epsilon \nabla k(X(r),r)\, dW_r]. \tag{5.1}$$

Therefore, using Kunita[37] again, we obtain

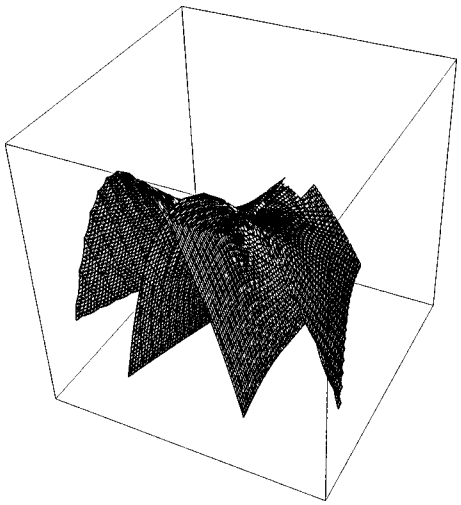

FIG. 29. The seagull level surface for heat equation.

$$\frac{d}{ds}\left(\frac{\partial X_s}{\partial x_0^\alpha}\right)=\frac{\partial \dot{X}_s}{\partial x_0^\alpha},\quad \alpha=1,2,...,d.$$

This gives the following lemma.

Lemma 5.1: Assume S_0, $c\in C^2$ and $k\in C^{2,0}$, ∇c, ∇k are Lipschitz, with Hessians $\nabla^2 c$, $\nabla^2 k$ and all second derivatives with respect to space variables of c and k bounded. If $\dot{X}_s$ satisfies Eq. (5.1) and p_0, possibly x_0 dependent, then almost surely

$$\frac{\partial A}{\partial x_0^\alpha}(x_0,p_0,t)=\dot{X}(t)\cdot\frac{\partial X(t)}{\partial x_0^\alpha}-\dot{X}_\alpha(0).$$

Proof: Arguing as above, for $\alpha=1,2,...,d$, we obtain

$$\frac{\partial A}{\partial x_0^\alpha}(x_0,p_0,t)=\int_0^t\left(\dot{X}(s)\cdot\frac{\partial \dot{X}(s)}{\partial x_0^\alpha}-\nabla c(X(s))\cdot\frac{\partial X(s)}{\partial x_0^\alpha}\right)ds-\epsilon\int_0^t\nabla k(X(s),s)\cdot\frac{\partial X(s)}{\partial x_0^\alpha}\,dW_s.$$

So using the key identity and the ibp^2 formula gives

$$\frac{\partial A}{\partial x_0^\alpha}(x_0,p_0,t)=-\int_0^t\frac{\partial X(s)}{\partial x_0^\alpha}\cdot[d\dot{X}(s)+\nabla c(X(s))\,ds+\epsilon\nabla k(X(s),s)\,dW_s]+\left[\dot{X}(s)\cdot\frac{\partial X(s)}{\partial x_0^\alpha}\right]_0^t,$$

proving the desired result. □

Remark 5.1: Observe that, if we fix $X(t)$, we obtain almost surely

$$\frac{\partial A}{\partial x_0^\alpha}(x_0,p_0,t)=-\dot{X}_\alpha(0),$$

for $\alpha=1,2,...,d$.

Let

$$X(s,x_0,x)=X(s,x_0,p_0)|_{p_0=p(x_0,x,t)},$$

where $p_0=p(x_0,x,t)$ is the (random) minimizer (assumed unique) of $A(x_0,p_0,t)$ with $X(t,x_0,p_0)=x$. Set

$$A(x_0,x,t)=A(x_0,p_0,t)|_{p_0=p(x_0,x,t)}.$$

Theorem 5.1: *Defining $A(x_0,x,t)$ as above,*

$$\left.\frac{\partial}{\partial x_0^\alpha}\right|_{\text{fixed}(x,t)}A(x_0,x,t)=-\dot{X}_\alpha(0),\quad \alpha=1,2,...d,$$

and so

$$\left.\frac{\partial}{\partial x_0^\alpha}\right|_{\text{fixed}(x,t)}[A(x_0,x,t)+S_0(x_0)]=0,\quad \alpha=1,2,...d,$$

defines the classical stochastic mechanical flow map Φ_t with $x=\Phi_t(x_0)$.

Proof: A trivial consequence of the last lemma. □

We now define the stochastic action corresponding to the initial momentum $\nabla S_0(x_0)$ by

$$\mathcal{A}(x_0,x,t)=A(x_0,x,t)+S_0(x_0).$$

B. The level surface geometry

We assume that $\mathcal{A}(x_0,x,t)$ is C^4 in space variables and that t is such that

$$\mathrm{Det}\left(\frac{\partial^2\mathcal{A}}{\partial x_0\partial x}(x_0,x,t)\right)\neq 0,\quad x_0,x\in\mathbb{R}^d.$$

The last assumption can be considerably weakened but with this last assumption the proofs are simpler. In the free case, considered previously, this assumption is valid for all $t>0$.

We now imitate the free case. We define the prelevel surface of Hamilton's principal function by eliminating x between the equations

$$\mathcal{A}(x_0,x,t)=c\quad\text{and}\quad\frac{\partial\mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0,\quad\alpha=1,2,...,d,$$

and the level surface by eliminating x_0. So the prelevel surface is $\Phi_t^{-1}H_t$. Similarly we define the caustic C_t and the precaustic $\Phi_t^{-1}C_t$ by eliminating x_0 or x between

$$\mathrm{Det}\left(\frac{\partial^2\mathcal{A}}{\partial {x_0}^2}(x_0,x,t)\right)=0\quad\text{and}\quad\frac{\partial\mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0,\quad\alpha=1,2,...,d.$$

Lemma 5.2: The classical flow map $x=\Phi_t(x_0)$ is a differentiable map from $\Phi_t^{-1}H_t$ to H_t with Frechet derivative

$$D\Phi_t(x_0)=\left(-\frac{\partial^2\mathcal{A}}{\partial x\partial x_0}(x_0,x,t)\right)^{-1}\left(\frac{\partial^2\mathcal{A}}{\partial {x_0}^2}(x_0,x,t)\right),$$

if $\mathcal{A}$ is C^3 in space derivatives.

Proof: We assume $x=\Phi_t(x_0)$, $x_0\in\Phi_t^{-1}H_t$, $x\in H_t$, so

$$\mathcal{A}(x_0,x,t)=c\quad\text{and}\quad\frac{\partial\mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0,\quad\alpha=1,2,...,d.$$

We move to a neighboring point $(x_0+\delta x_0,x+\delta x,t)$ on $\Phi_t^{-1}H_t$ and H_t, respectively. Then we obtain

$$\mathcal{A}(x_0+\delta x_0,x+\delta x,t)=c\quad\text{and}\quad\frac{\partial\mathcal{A}}{\partial x_0^\alpha}(x_0+\delta x_0,x+\delta x,t)=0,\quad\alpha=1,2,...,d,$$

i.e., correct to first order

$$\left(\frac{\partial^2\mathcal{A}}{\partial {x_0}^2}\right)\delta x_0+\left(\frac{\partial^2\mathcal{A}}{\partial x\partial x_0}\right)\delta x=0,$$

and

$$\delta x\cdot\frac{\partial\mathcal{A}}{\partial x}(x_0,x,t)=0,$$

proving the desired result. □

We can now prove the following proposition in d dimensions.

Proposition 5.1: We consider the random prelevel surface obtained by eliminating x between the equations

$$\mathcal{A}(x_0,x,t)=c \quad \text{and} \quad \frac{\partial \mathcal{A}}{\partial x_0^{\alpha}}(x_0,x,t)=0, \quad \alpha=1,2,...,d.$$

Then the normal to the prelevel surface at the point x_0 is to within a scalar multiplier given by

$$n(x_0)=-\left(\frac{\partial^2 \mathcal{A}}{\partial {x_0}^2}\right)\left(\frac{\partial^2 \mathcal{A}}{\partial x_0 \partial x}\right)^{-1}\dot{X}(t,x_0,\nabla S_0(x_0)).$$

Proof: Evidently $n(x_0)=\nabla_{x_0}\mathcal{A}(x_0,x,t)$, where $x=\Phi_t(x_0)$, the map Φ_t being defined by

$$\frac{\partial \mathcal{A}}{\partial x_0^{\alpha}}(x_0,x,t)=0, \quad \alpha=1,2,...,d.$$

Hence only the partial derivatives with respect to x contribute to $n(x_0)$, giving

$$n=(D\Phi_t(x_0))^T\frac{\partial A}{\partial x}(x_0,x,t)\bigg|_{x=\Phi_t(x_0)},$$

^{T} denoting transpose. However, following the method of Lemma 5.1, we obtain

$$\frac{\partial A}{\partial x^{\alpha}}(x_0,x,t)\bigg|_{x=\Phi_t(x_0)}=\dot{X}_{\alpha}(t,x_0,\nabla S_0(x_0)),$$

almost surely, for $\alpha=1,2,...,d$, proving the proposition. □

Corollary 5.1: In three dimensions at any point $x_0 \in \Phi_t^{-1}C_t \cap \Phi_t^{-1}H_t$ where $n(x_0)\neq 0$ and

$$\mathrm{Ker}\left(\frac{\partial^2 \mathcal{A}}{\partial {x_0}^2}(x_0,x,t)\right)\bigg|_{x=\Phi_t(x_0)}=\langle e_0\rangle,$$

e_0 being the zero eigenvector, T_{x_0} the tangent plane to the prelevel surface is spanned by e_0 and $(n(x_0)\wedge e_0)$.

Proof: We obtain by symmetry of $(\partial^2\mathcal{A}/\partial {x_0}^2)$

$$e_0\cdot n=-\left(\frac{\partial^2 \mathcal{A}}{\partial {x_0}^2}\right)e_0\cdot\left(\frac{\partial^2 \mathcal{A}}{\partial x_0 \partial x}\right)^{-1}\dot{X}(t,x_0,\nabla S_0(x_0))=0.$$

So e_0 is in the tangent plane T_{x_0}, setting $e_0^{\perp}=n\wedge e_0 \in T_{x_0}$ by definition. □

Remark 5.2: When the speed $|\dot{X}(t,x_0,\nabla S_0(x_0))|=0$, $n(x_0)=0$ and so x_0 is a singular point of the prelevel surface, either a node with two distinct directions for the tangent plane or a cusped singularity. Because $\partial\mathcal{A}/\partial x=\dot{X}$ necessarily $x=\Phi_t(x_0)$ is a singular point of the level surface even if $x_0 \notin \Phi_t^{-1}C_t$. In the case $x_0 \notin \Phi_t^{-1}C_t$ and $\dot{X}=0$ we know that this singularity can only be a node because the tangent space is fully two dimensional at this point.

Corollary 5.2: In two dimensions let the prelevel surface meet the precaustic at a point x_0 where $n(x_0)\neq 0$ and $\mathrm{Ker}(\partial^2\mathcal{A}/\partial {x_0}^2(x_0,\Phi_t(x_0),t))=\langle e_0\rangle$, e_0 being the zero eigenvector. Then the tangent plane to the prelevel surface at x_0, T_{x_0} is spanned by e_0.

Proof: This is a trivial consequence of the proposition above. □

Proposition 5.2: Assume that in two dimensions at $x_0 \in \Phi_t^{-1}H_t$ the above normal $n(x_0)\neq 0$, so that the prelevel surface does not have a generalized cusp at x_0. Then the level surface can only have a generalized cusp at $\Phi_t(x_0)$ if $\Phi_t(x_0)\in C_t$, the caustic surface. Moreover, if $x=\Phi_t(x_0) \in \Phi_t\{\Phi_t^{-1}C_t\cap\Phi_t^{-1}H_t\}$, the level surface will have a generalized cusp at x.

Proof: Because $n(x_0)$ is nonzero, the direction of the tangent to the prelevel surface curve is well defined at x_0. Hence, if the intrinsic parameterization of the curve is $x_0=x_0(\gamma)$, $\gamma \in N(\gamma_0,\delta)$ in a neighborhood of $x_0=x_0(\gamma_0)$, the tangent to the level surface

$$\left.\frac{dx(\gamma)}{d\gamma}\right|_{\gamma=\gamma_0}=\left(D\Phi_t(x_0)\left.\frac{dx_0(\gamma)}{d\gamma}\right|_{\gamma=\gamma_0}\right)=\left(-\frac{\partial^2\mathcal{A}}{\partial x\partial x_0}\right)^{-1}\left(\frac{\partial^2\mathcal{A}}{\partial {x_0}^2}\right)\frac{dx_0(\gamma_0)}{d\gamma}=0,$$

because T_{x_0} is spanned by e_0, $x_0\in\Phi_t^{-1}H_t\cap\Phi_t^{-1}C_t$. What is more $dx(\gamma_0)/d\gamma=0$ implies that necessarily $\mathrm{Det}(\partial^2\mathcal{A}/\partial {x_0}^2)=0$ if $x_0(\gamma_0)$ is not a generalized cusp. □

Needless to say, if $dx_0(\gamma_0)/d\gamma=0$, it follows from the above that $dx(\gamma_0)/d\gamma=0$. So generalized cusps map into generalized cusps regardless of whether or not $x_0\in\Phi_t^{-1}C_t$, cf. Figs. 23 and 24 for the two-dimensional swallowtail. This is true independent of the dimension of the space. We now return to the three-dimensional setup.

Definition 5.1: We define the cusped part of the level surface H_t in three dimensions by

$$\mathrm{Cusp}(H_t)=\{x\in H_t : x\in\Phi_t(\Phi_t^{-1}C_t\cap\Phi_t^{-1}H_t), x=\Phi_t(x_0), n(x_0)\neq 0\}.$$

Proposition 5.3: Let $x\in\mathrm{Cusp}(H_t)$. Then in three dimensions, T_x, the tangent space to the level surface at x, is one dimensional at most.

Proof: We know that $x=\Phi_t(x_0)$, $x_0\in\Phi_t^{-1}C_t\cap\Phi_t^{-1}H_t$ with $n(x_0)\neq 0$. It follows that there is a well-defined two-dimensional tangent plane to the prelevel surface at x_0, T_{x_0} spanned by e_0 and $(n\wedge e_0)$. However, the derivative map is given by

$$D\Phi_t(x_0)=\left(-\frac{\partial^2\mathcal{A}}{\partial x\partial x_0}\right)^{-1}\left(\frac{\partial^2\mathcal{A}}{\partial {x_0}^2}\right).$$

So $D\Phi_t(x_0)e_0=0$ and $T_x=\langle D\Phi_t(x_0)(n\wedge e_0)\rangle$ is at most one dimensional. □

Of course a similar result holds in higher dimensions.

C. A plethora of cusps

We conclude by explaining why we expect to see generalized cusps on planar cross sections of level surfaces in three dimensions. We first of all observe that, if δx is of second order of small quantities, solving

$$\frac{\partial\mathcal{A}}{\partial x_0^\alpha}(x_0,x,t)=0,\quad \alpha=1,2,3,$$

and

$$\frac{\partial\mathcal{A}}{\partial x_0^\alpha}(x_0+\delta x_0,x+\delta x,t)=0,\quad \alpha=1,2,3,$$

to second order reduces in our case to

$$\delta x=\left(-\frac{\partial^2\mathcal{A}}{\partial x\partial x_0}\right)^{-1}\left\{\left(\frac{\partial^2\mathcal{A}}{\partial {x_0}^2}\right)\delta x_0+\frac{1}{2}(\delta x_0\cdot\nabla_{x_0})^2\frac{\partial\mathcal{A}}{\partial x_0}\right\}.$$

Write

$$\left(\frac{\partial^2\mathcal{A}}{\partial x_0\partial x}\right)^{-1}\dot{X}(t,x_0,\nabla S_0(x_0))=-(\alpha_0e_0+\alpha_1e_1+\alpha_2e_2),$$

where e_0 is the zero eigenvector of $(\partial^2\mathcal{A}/\partial {x_0}^2)$ and

$$\frac{\partial^2 \mathcal{A}}{\partial x_0{}^2} e_i = \lambda_i e_i, \quad i=1,2,$$

are the remaining eigenvector equations, $\{e_0, e_1, e_2\}$ an orthonormal system. Then, from above, unit normal

$$n = (\alpha_1 \lambda_1 e_1 + \alpha_2 \lambda_2 e_2)(\alpha_1^2 \lambda_1^2 + \alpha_2^2 \lambda_2^2)^{-1/2}$$

and

$$e_0^{\perp} = n \wedge e_0 = (\alpha_2 \lambda_2 e_1 - \alpha_1 \lambda_1 e_2)(\alpha_1^2 \lambda_1^2 + \alpha_2^2 \lambda_2^2)^{-1/2}.$$

We now set

$$\delta x_0 = \varepsilon(\lambda e_0 + \mu e_0^{\perp}) + \varepsilon^2(\xi e_0 + \eta e_0^{\perp} + \zeta n).$$

The first term gives the direction of $dx_0(\gamma_0)/d\gamma$, the second term $d^2x_0(\gamma_0)/d\gamma^2$. Then

$$\delta x = \left(-\frac{\partial^2 \mathcal{A}}{\partial x \partial x_0} \right)^{-1} \left\{ [\varepsilon \mu \lambda_1 \lambda_2 (\alpha_2 e_1 - \alpha_1 e_2) + \varepsilon^2 (\eta \lambda_1 \lambda_2 (\alpha_2 e_1 - \alpha_1 e_2) + \zeta(\alpha_1 \lambda_1^2 e_1 + \alpha_2 \lambda_2^2 e_2))] \theta \right.$$
$$\left. + \frac{1}{2} (\delta x_0 \cdot \nabla_{x_0})^2 \frac{\partial \mathcal{A}}{\partial x_0} \right\},$$

where $\theta = (\alpha_1^2 \lambda_1^2 + \alpha_2^2 \lambda_2^2)^{-1/2}$. Note that there is an ε^2 term hidden within the last term of the above.

Clearly for a genuine cusp we have to set $\mu = 0$, giving

$$\delta x_0 = \varepsilon \lambda e_0 + \varepsilon^2(\xi e_0 + \eta e_0^{\perp} + \zeta n) \tag{C_0}$$

$$\delta x = \left(-\frac{\partial^2 \mathcal{A}}{\partial x \partial x_0} \right)^{-1} \left\{ \varepsilon^2 \theta (\eta \lambda_1 \lambda_2 (\alpha_2 e_1 - \alpha_1 e_2) + \zeta(\alpha_1 \lambda_1^2 e_1 + \alpha_2 \lambda_2^2 e_2)) + \frac{\varepsilon^2}{2} \lambda^2 \partial_0^2 \frac{\partial \mathcal{A}}{\partial x_0} \right\}. \tag{C_1}$$

We now have to satisfy two further conditions:

$$\delta x \cdot e_y = 0, \tag{C_2}$$

$$\delta x \cdot \frac{\partial \mathcal{A}}{\partial x} = (\alpha_0 e_0 + \alpha_1 e_1 + \alpha_2 e_2) \cdot \left(\theta (\eta \lambda_1 \lambda_2 (\alpha_2 e_1 - \alpha_1 e_2) + \zeta(\alpha_1 \lambda_1^2 e_1 + \alpha_2 \lambda_2^2 e_2)) + \frac{\lambda^2}{2} \partial_0^2 \frac{\partial \mathcal{A}}{\partial x_0} \right)$$
$$= 0. \tag{C_3}$$

Surprisingly the last condition does not depend upon η. It simplifies to give

$$(\zeta(\alpha_1^2 \lambda_1^2 + \alpha_2^2 \lambda_2^2))^{1/2} + \frac{\lambda^2}{2} (\alpha_0 e_0 + \alpha_1 e_1 + \alpha_2 e_2) \cdot \partial_0^2 \frac{\partial \mathcal{A}}{\partial x_0} = 0. \tag{C_3'}$$

The equation (C_3') determines the ratio $\zeta : \lambda^2$ and equation (C_2) determines the ratio $\eta : \lambda^2$.

Theorem 5.2: *Any point x on the level surface H_t, $x = \Phi_t(x_0)$ with $x_0 = \Phi_t^{-1}(x)$ on the prelevel surface can only be a generalized cusp of a curve on H_t if x_0 is a generalized cusp of the*

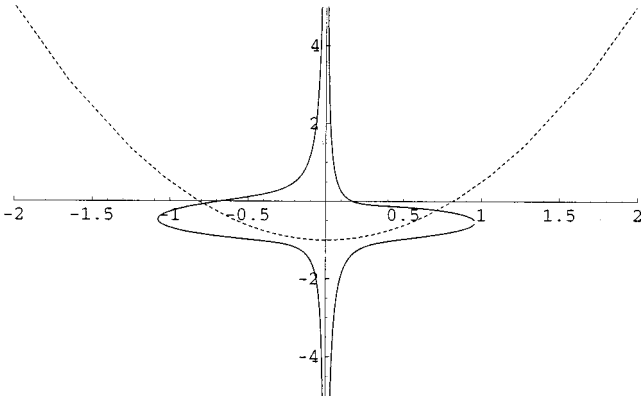

FIG. 30. Stochastic precaustic and prelevel surface.

precurve on the prelevel surface or if $x_0 \in \Phi_t^{-1} C_t$ *the precaustic. In three dimensions the planar cross section* $y = \text{const}$ *(with normal* e_y*) of the level surface* H_t *through a point x where it meets* C_t*, the caustic surface, will have a genuine cusp at x if* $x \in \text{Cusp}(H_t)$ *and there is a nonzero solution* δx *of Eqs.* (C_1)*,* (C_2)*, and* (C_3)*. The direction of the axis of the cusp will be* $\widehat{\delta x}$*.*

Proof: Similar to that of Theorem 3.2 using the generalizations expounded above. □

D. A random example

Example 5.1: Here we illustrate the random caustic and level surface for the case $S_0(x_0, y_0) = x_0^2 y_0/2$*,* $c(x) = 0$ *and* $k(x,t) = x$ *for* $\epsilon = 1/10$*. Figures 30 and 31 correspond to* $S_t(x, y, \omega) = 0$*.*

We now display Figs. 32 and 33 corresponding to $S_t(x, y, \omega) = -1/64$*.*

E. Consequences for the Burgers fluid

We now recast the comments made at the end of Sec. III in the more general setting of c and k nonzero. We emphasize that the above results hold for any finite ϵ (the strength of the white noise) as long as $\text{Det}(\partial^2 \mathcal{A}/\partial x_0 \partial x) \neq 0$. In a future paper[38] we will expound on the small ϵ case in some detail, explaining why the caustics (shockwaves) are stable and the level surfaces are unstable under noisy perturbations.

Recall that our random map $\Phi_s(\omega): \mathbb{R}^d \to \mathbb{R}^d$ satisfies

$$d_s \dot{\Phi}_s = -\nabla C(\Phi_s) ds - \epsilon \nabla k(\Phi_s, s) dW_s,$$

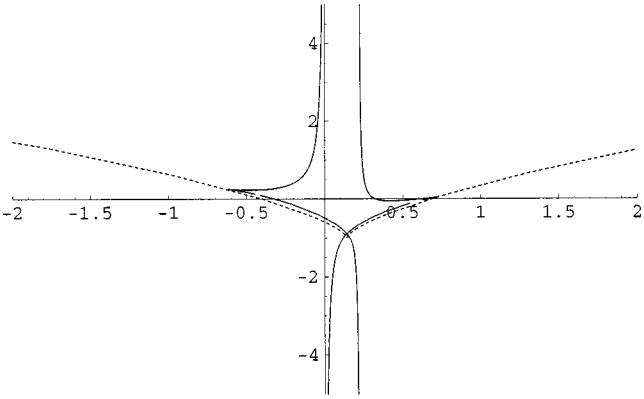

FIG. 31. Stochastic caustic and level surface.

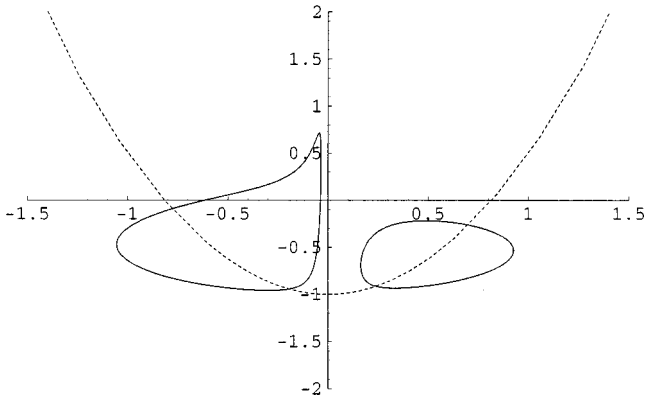

FIG. 32. Stochastic precaustic and prelevel surface.

with $\Phi_0 = I$ and $\dot{\Phi}_0 = \nabla S_0$. The global inverse function theorem[23] gives the following.

Proposition 5.4: If c, k and S_0 are smooth with bounded second order partial derivatives, there exists $T(\omega) > 0$ such that $\Phi_s(\omega): \mathbb{R}^d \to \mathbb{R}^d$ is a random diffeomorphism $0 \leqslant s \leqslant T(\omega)$.

We then have the following.

Proposition 5.5: The random Burgers velocity field in the limit of zero viscosity is

$$v^0(x,t) = v^0(\Phi_t^{-1}x,0) - \int_0^t \nabla C(\Phi_s \Phi_t^{-1}x)\, ds - \int_0^t \epsilon \nabla k(\Phi_s \Phi_t^{-1}x, s)\, dW_s,$$

with $v^0(x,0) = \nabla S_0(x)$. This v^0 is almost surely $0 \leqslant t \leqslant T(\omega)$, a classical solution of the Burgers equation. The corresponding solution of the continuity equation, the random density $\rho(x,t) = |\mathrm{Det}(\nabla \Phi_t^{-1}x)|$, is continuous almost surely for $0 \leqslant t \leqslant T(\omega)$, but v^0 has jump discontinuities on the random caustics. Evidently $\nabla \wedge v^0 \equiv 0$, almost surely.

Remark 5.3: More detailed information on the behavior of v^0 and ρ on the caustic is given in Ref. 31.

After the caustic time $T(\omega)$, we have seen how to characterize in terms of the stochastic action when the level surface meets the caustic in cusps. In two dimensions, this enables one to divide the caustic into hot and cool parts depending on whether or not the speed of the Burgers fluid is zero on one side of the caustic. We have also seen how a zero speed condition on the precaustic and prelevel surface leads to turbulent like behavior of the Burgers fluid at the corresponding points of the caustic. For instance, the large jump discontinuity in the speed of the Burgers fluid which we see in crossing the semicubical parabolic shockwave at the cusp is caused

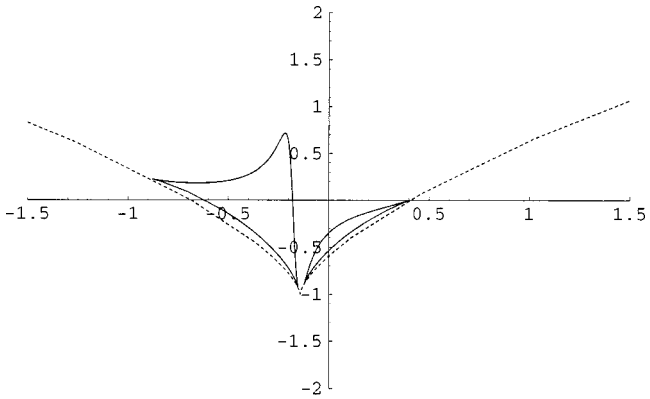

FIG. 33. Stochastic caustic and level surface.

by this zero speed condition. Here we should emphasize that the stochastic and deterministic behaviors are very similar if we take snapshots of the Burgers fluid fixed in time.

We now emphasize that new features emerge if one tries to use the above ideas to analyze the ''intermittence'' of stochastic turbulence as opposed to deterministic turbulence. We shall discuss this in detail in a future paper. The reason for the sharp contrast between stochastic and deterministic turbulence can already be seen here if we associate turbulent behavior with a change in the number of cusped curves on the level surface. According to Proposition 5.3 and Theorem 5.2, the times t when this occurs are just the times when the prelevel surfaces *touch* the precaustic. The times t when this number of curves changes in the deterministic case are simply the zeros of a deterministic function ζ, usually isolated zeros. In the stochastic case ζ is a stochastic process whose zeros usually form a perfect set, i.e., an infinite set containing no isolated points. At these times the number of cusped curves changes with infinite frequency because of the infinitely rapid oscillation of the stochastic process ζ. This is in line with what one would expect for turbulent behavior. When the stochastic process ζ is *recurrent* this turbulent behavior is ''intermittent'' so that the scale of turbulent fluctuations varies in a random periodic way.

VI. CONCLUSION

We have seen how generally the level surfaces of Hamilton's principal function meet the caustic surface in cusped curves and discussed some of the ramifications of this for Burgers turbulence. In particular, the cool part of the caustic is associated with jump discontinuities in both u^0 and v^0. The results in this article should be compared with results for Euler's equation, which is identical to the above save for the constraint that the fluid density ρ is unity. In a future paper we hope to relax the assumption that the Burgers velocity field is irrotational, when more realistic comparisons with Euler's equation can be made. Needless to say, the detailed nature of the geometry of the caustic surface and the level surface will affect the value of $v^\mu(x,t)$ on the caustic. Geometrical and analytical results are clearly relevant here for small noise in the way they relate the stochastic and deterministic situations. We will discuss some more analytical results in our future papers.[33,38]

The main object lesson of the present study is that the number of cusped curves on the wavefront will change infinitely rapidly in the stochastic case when the presurfaces touch and that this behavior will recur in a random periodic way if a certain stochastic process is recurrent. This is the ''intermittence'' of turbulence in our model. There is no analog of this for the deterministic Burgers equation. We shall discuss this in more detail in a future publication.

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Regular obstructed categories and topological quantum field theory

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A proposal of the concept of *n*-regular obstructed categories is given. The corresponding regularity conditions for mappings, morphisms, and related structures are considered. An *n*-regular topological quantum field theory is introduced. The connection of time nonivertibility with the regularity is shown. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1473681]

I. INTRODUCTION

In the generalized histories approach[1] to quantum theory the whole universe is represented by a class of ''histories.'' In this approach the standard Hamiltonian time evolution is replaced by a partial semigroup called a ''temporal support.'' A possible realization of such program can be described in terms of cobordism manifolds and corresponding categories.[2] The temporal support arises naturally as a cobordism M, where the boundary ∂M of M is a disjoint sum of the ''incoming'' boundary manifold Σ_0 and the ''outgoing'' one Σ_1. This means that the cobordism M represents certain quantum process transforming Σ_0 into Σ_1. In other words, Σ_1 is a time consequence of Σ_0. Obviously, we have two opposite possibilities to declare which boundary is the initial one.

Let N be a cobordism with the ''outgoing'' boundary of M as its ''incoming boundary'' and Σ_2 as the ''outgoing boundary.'' Then there is a cobordism $N \circ M$ whose incoming boundary is Σ_0, and the outgoing one is Σ_3. In this case we say that these two cobordisms are glued along Σ_1. Such gluing of cobordisms up to diffeomorphisms define a partial semigroup operation. One can consider cobordism with several incoming and outgoing boundary manifolds. The class of possible histories can be represented by gluing of cobordisms in several different ways. Hence there is the corresponding coherence problem for such description.

Let Cob be a category of cobordisms, where the boundary ∂M of $M \in \mathrm{Cob}$ is a disjoint sum of the incoming boundary manifold Σ_0 and the outgoing one Σ_1. There is also the cylinder cobordism $\Sigma \times [0,1]$ such that $\partial(\Sigma \times [0,1]) = \Sigma \amalg \Sigma^*$. The class of boundary components is denoted by Cob_0. According to Atiyah,[3] Baez and Dolan,[4] the topological quantum field theory (TQFT) is a functor $\mathcal{F}$ from the category Cob to the category Vect of finite-dimensional vector spaces. This means that $\mathcal{F}$ sends every manifold $\Sigma \in \mathrm{Cob}_0$ into vector space $\mathcal{F}(\Sigma)$ such that

$$\mathcal{F}(\Sigma^*) = (\mathcal{F}(\Sigma))^*, \quad \mathcal{F}(\Sigma_0 \amalg \Sigma_1) = (\mathcal{F}\Sigma_0) \otimes (\mathcal{F}\Sigma_1), \quad \mathcal{F}(\varnothing) = I, \tag{1}$$

and a cobordism $M(\Sigma_0, \Sigma_1)$ to a mapping $\Phi(M) \in \mathrm{lin}_I(\mathcal{F}\Sigma_0, \mathcal{F}\Sigma_1)$ such that $\mathcal{F}(\Sigma \times [0,1]) = id_{\mathcal{F}\Sigma}$, where I is a field, and Σ^* is the same manifold Σ but with the opposite orientation. Kerler[5] found examples of categories formed by some classes of cobordism manifolds preserving some operations like the disjoint sum or surgery. It was discussed by Baez and Dolan[4] that it is not easy to describe such categories in a coherent way. Crane[6,7] applied the category theory to an algebraic structure of the quantum gravity.

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The idea of regularity as generalized invertibility was first introduced by von Neumann[8] and applied by Penrose for matrices.[9] Let $\mathbb{R}$ be a ring. If for an element $a\in\mathbb{R}$ there is an element $a^\star$ such that

$$aa^\star a=a,\quad a^\star aa^\star=a^\star, \tag{2}$$

then a is said to be regular and $a^\star$ is called a generalized inverse inverse of a. Generalizing transition from invertibility to regularity is a widely used method of abstract extension of various algebraic structures. The intensive study of such regularity and related directions was developed in many different fields, e.g., generalized inverses theory,[10–12] semigroup theory,[13–19] supermanifold theory,[20–22] Yang–Baxter equation in endomorphism semigroup and braided almost bialgebras,[23–25] weak bialgebras, week Hopf algebras,[26] and category theory.[27]

In this paper we are going to study certain class of categories which can be useful for the study of quantum histories with noninvertible time, quantum, gravity, and field theory. The regularity concept for linear mappings and morphisms in categories are studied. Higher order regularity conditions are described. Commutative diagrams are replaced by ''semicommutative'' ones. The distinction between commutative and semicommutative cases is measured by a nonzero obstruction proportional to the difference of some self-mappings $e^{(n)}$ from the identity. This allows one to regularize the notion of categories, functions, and related algebraic structures. It is interesting that this procedure is unique up to an equivalence defined by invertible morphisms. Our regularity concept is nontrivial for equivalence classes of nonivertible morphisms. The regular version of TQFT is a natural application of the formalism presented here. In this case the n-regularity means that a time evolution is noninvertible, although repeated after n steps, but up to a classes of obstructions. Our considerations are based on the concepts of generalized inverse,[12,27] and semisupermanifolds.[20]

The paper is organized as follows. In Sec. II we consider linear mappings without requirement of ''invertibility.'' If $f:X\to Y$ is a linear mapping, then instead of the inverse mapping $f^{-1}:Y\to X$ we use less restricted ''regular'' $f^\star$ one by extending ''invertibility'' to ''regularity'' according to

$$f\circ f^\star\circ f=f,\quad f^\star\circ f\circ f^\star=f^\star. \tag{3}$$

We also propose some higher regularity conditions. In Sec. III the higher regularity notion is extended to morphisms of categories. Commutative diagrams are replaced by semicommutative ones. The concept of regular cocycles of morphisms in a category is described. An existence theorem for these cocycles is given. The corresponding generalization of certain categorical structures as tensor operation, algebras and coalgebras, etc., to our higher regularity case is given in Sec. IV. Regular equivalence classes of cobordism manifolds and the corresponding structures are considered in Sec. V. An n-regular TQFT is introduced as an n-regular obstructed category represented by some special classes of cobordisms called ''interactions.'' Our study is not complete, it is only a proposal for new algebraic structures related to topological quantum theories.

II. GENERALIZED INVERTIBILITY AND REGULARITY

Let X and Y be two linear spaces over a field k. We use the following notation. Denote by Id_X and Id_Y the identity mappings $\mathrm{Id}_X:X\to X$ and $\mathrm{Id}_Y:Y\to Y$. If $f:X\to Y$ is a linear mapping, then the image of f is denoted by $\mathrm{Im}\,f$, and the kernel by $\mathrm{Ker}\,f$.

Here we are going to study some generalizations of the standard concept of invertibility properties of mappings. Our considerations are based on the article of Nashed.[12] Let $f:X\to Y$ be a linear mapping. If $f\circ f_r^{-1}=\mathrm{Id}_Y$ for some $f_r^{-1}:Y\to X$, then f is called a *retraction*, and f_r^{-1} is the right inverse. Similarly, if $f_l^{-1}\circ f=\mathrm{Id}_X$, then it is called a *coretraction*, f_l^{-1} is the left inverse of f. A mapping f^{-1} is called an inverse of f if and only if it is both right and left inverse of f.

This standard concept of invertibility is in many cases too strong to be fulfilled. To obtain more weak conditions one has to introduce the following ''regularity'' conditions

$$f\circ f^{\star}_{\text{in}}\circ f=f, \tag{4}$$

where $f^{\star}_{\text{in}}:Y\to X$ is called an *inner inverse*, and such f is called *regular*. Similar ''reflexive regularity'' conditions

$$f^{\star}_{\text{out}}\circ f\circ f^{\star}_{\text{out}}=f^{\star}_{\text{out}} \tag{5}$$

define an *outer inverse* $f^{\star}_{\text{out}}$. Notice that in general $f^{\star}_{\text{in}}\neq f^{\star}_{\text{out}}\neq f^{-1}$ or it can be that f^{-1} does not exist at all.

Definition 1: A mapping f satisfying one of the conditions (4) or (5) is said to be regular or three-regular. A generalized inverse of a mapping f is a mapping $f^{\star}$, which is both inner and outer inverse $f^{\star}=f^{\star}_{\text{in}}=f^{\star}_{\text{out}}$.

Lemma 2: If $f^{\star}_{\text{in}}$ is an inner inverse of f, then a generalized inverse $f^{\star}$ exists, but need not be unique.

Proof: If $f^{\star}_{\text{in}}$ is an inner inverse, then

$$f^{\star}=f^{\star}_{\text{in}}\circ f\circ f^{\star}_{\text{in}} \tag{6}$$

is always both inner and outer inverse i.e., generalized inverse. It follows from (6) that both regularity conditions (4) and (5) hold. □

Definition 3: Let us define two operators $\mathcal{P}_f:Y\to Y$ and $\mathcal{P}_{f^{\star}}:X\to X$ by

$$\mathcal{P}_f:=f\circ f^{\star},\quad \mathcal{P}_{f^{\star}}:=f^{\star}\circ f. \tag{7}$$

Lemma 4: These operators satisfy

$$\begin{gathered}\mathcal{P}_f\circ\mathcal{P}_f=\mathcal{P}_f,\quad \mathcal{P}_f\circ f=f\circ\mathcal{P}_{f^{\star}}=f\\ \mathcal{P}_{f^{\star}}\circ\mathcal{P}_{f^{\star}}=\mathcal{P}_{f^{\star}},\quad \mathcal{P}_{f^{\star}}\circ f^{\star}=f^{\star}\circ\mathcal{P}_f=f^{\star}.\end{gathered} \tag{8}$$

□

Lemma 5: If $f^{\star}$ is the generalized inverse of the mapping f, then the following properties are obvious:

$$\begin{gathered}\operatorname{Im} f=\operatorname{Im}(f\circ f^{\star}),\quad \operatorname{Ker}(f\circ f^{\star})=\operatorname{Ker} f^{\star},\\ \operatorname{Im}(f^{\star}\circ f)=\operatorname{Im} f^{\star},\quad \operatorname{Ker}(f^{\star}\circ f)=\operatorname{Ker} f.\end{gathered} \tag{9}$$

In addition there are two decompositions

$$X=\operatorname{Im} f^{\star}\oplus\operatorname{Ker} f,\quad Y=\operatorname{Im} f\oplus\operatorname{Ker} f^{\star}. \tag{10}$$

The restriction $f|_{\operatorname{Im} f^{\star}}:\operatorname{Im} f^{\star}\to\operatorname{Im} f$ is one to one mapping, and operators P_f, $P_{f^{\star}}$ are projectors of Y, X onto $\operatorname{Im} f$, $\operatorname{Im} f^{\star}$, *respectively.*

Theorem 6: *Let $f:X\to Y$ be a linear mapping. If P and Q are projectors corresponding to the following two decompositions*

$$X=M\oplus\operatorname{Ker} f,\quad Y=\operatorname{Im} f\oplus N, \tag{11}$$

respectively, then there exist unique generalized inverse of f, and

$$f^{\star}:=i\circ\tilde{f}^{-1}\circ Q, \tag{12}$$

where $\tilde{f}:=f|_M$, and $i:M\hookrightarrow X$.

Here we try to construct higher analogs of generalized invertibility and regularity conditions (4) and (5). Let us consider two mappings $f:X\to Y$ and $f^{\star}:Y\to X$ and introduce two additional mappings $f^{\star\star}:X\to Y$ and $f^{\star\star\star}:Y\to X$. We propose here the following higher regularity condition:

$$f\circ f^{\star}\circ f^{\star\star}\circ f^{\star\star\star}\circ f=f. \tag{13}$$

This equation defines a four-regularity condition. By cyclic permutations we obtain

$$\begin{aligned} f^{\star}\circ f^{\star\star}\circ f^{\star\star\star}\circ f\circ f^{\star}&=f^{\star},\\ f^{\star\star}\circ f^{\star\star\star}\circ f\circ f^{\star}\circ f^{\star\star}&=f^{\star\star},\\ f^{\star\star\star}\circ f\circ f^{\star}\circ f^{\star\star}\circ f^{\star\star\star}&=f^{\star\star\star}. \end{aligned} \tag{14}$$

By recursive considerations we can propose the following formula of n-regularity:

$$\underbrace{f\circ f^{\star}\circ f^{\star\star}\ldots\circ f^{\overbrace{\star\star\ldots\star}^{n=2k+1}}\circ f}_{n+1}=f, \tag{15}$$

where $n=2k$, $k=1,2,\ldots$ and their cyclic permutations.

For the $\overbrace{\star\star\ldots\star}^{2k+1}$-operation we have the following formula:

$$(g\circ f)^{\overbrace{\star\star\ldots\star}^{2k+1}}=f^{\overbrace{\star\star\ldots\star}^{2k+1}}\circ g^{\overbrace{\star\star\ldots\star}^{2k+1}}. \tag{16}$$

We can introduce ''higher projector'' by

$$\mathcal{P}_f^{(n)}=f\circ f^{\star}\circ f^{\star\star}\cdots\circ f^{\overbrace{\star\star\ldots\star}^{2k+1}}. \tag{17}$$

It is easy to check the following properties:

$$\mathcal{P}_f^{(2k)}\circ f=f \tag{18}$$

and idempotence $\mathcal{P}_f^{(2k)}\circ\mathcal{P}_f^{(2k)}=\mathcal{P}_f^{(2k)}$.

In general case for a given $n=2k$ all $f^{\star}$, $f^{\star\star}$,$\ldots f^{\overbrace{\star\star\ldots\star}^{n}}$ are different, and, for instance, $(f^{\star})^{\star}\neq f^{\star\star}$. The existence of analogous conditions for n odd is a problem.

Theorem 7: *Let $f:X\to Y$ be a linear mapping. If P and Q are projectors corresponding to the following two decompositions*

$$X=M\oplus\operatorname{Ker} f,\quad `Y=\operatorname{Im} f\oplus N, \tag{19}$$

respectively, and

$$f^{\star}|\operatorname{Im} f=f^{\star\star\star}|_{\operatorname{Im} f}, \tag{20}$$

then the five-regularity condition of f can be reduced to the two three-regularity conditions

$$f\circ f^{\star}\circ f=f,\quad f^{\star}\circ f^{\star\star}\circ f^{\star}=f^{\star}. \tag{21}$$

III. SEMICOMMUTATIVE DIAGRAMS AND REGULAR OBSTRUCTED CATEGORIES

In Sec. II we considered mappings and regularity properties for two given spaces X and Y, because we studied various types of inverses. Now we will extend these considerations to any number of spaces and introduce semicommutative diagrams (first introduced in Ref. 20).

A *directed graph* $\mathfrak{C}$ is a pair $\{\mathfrak{C}_0,\mathfrak{C}_1\}$ and a pair of functions

$$\mathfrak{C}_0 \underset{t}{\overset{s}{\leftleftarrows}} \mathfrak{C}_1, \tag{22}$$

where elements of $\mathfrak{C}_0$ are said to be *objects*, elements of $\mathfrak{C}_1$ are said to be *arrows* or *morphisms*, sf is said to be a *domain (or source)* of f, and tf is a *codomain (or target)* of $f\in\mathfrak{C}_1$. If $sf=X\in\mathfrak{C}_0$, and $tf=Y\in\mathfrak{C}_0$, then we use the following notation $X\overset{f}{\to}Y$ and

$$\mathfrak{C}(X,Y):=\{f\in\mathfrak{C}_1: sf=X, tf=Y\}. \tag{23}$$

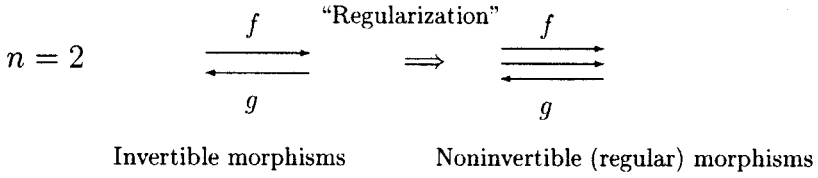
We denote by $\mathrm{End}(X)$ the collection of all morphisms defined on X into itself, i.e., $\mathrm{End}(X):=\mathfrak{C}(X,X), X\in\mathfrak{C}_0$.

Two arrows $f,g\in\mathfrak{C}_1$ such that $tf=sg$ are said to be composable. If in addition $sf=X$, $sg=tf=Y$, and $tg=Z$, then we use the notation $X\overset{f}{\to}Y\overset{g}{\to}Z$. In this case a composition $f\circ g$ of two arrows $f:X\to Y$ and $g:Y\to Z$ can be defined as an arrow $f:X\to Y$. The associativity means that $h\circ(g\circ f)=(h\circ g)\circ f=h\circ g\circ f$. An identity id in $\mathfrak{C}$ is an inclusion $X\in\mathfrak{C}_0\rightarrowtail \mathrm{id}_X\in\mathrm{End}(X)$ such that

$$f\circ \mathrm{id}_X=\mathrm{id}_Y\circ f=f \tag{24}$$

for every X, $Y\in\mathfrak{C}_1$, and $X\overset{f}{\to}Y$.

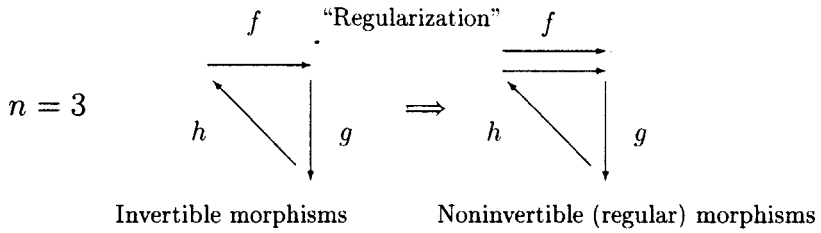
A directed graph $\mathfrak{C}$ equipped with associative composition of composable arrows and identity satisfying some natural axioms is said to be a *category*.[28,29] If $\mathfrak{C}$ is a category, then right cancellative morphisms are *epimorphisms* which satisfy $g_1\circ f=g_2\circ f\Rightarrow g_1=g_2$, where $g_{1,2}:Y\to Z$ and left cancellative morphisms are *monomorphisms* which satisfy $f\circ h_1=f\circ h_2\Rightarrow h_1=h_2$, where $h_{1,2}:Z\to X$. A morphism $X\overset{f}{\to}Y$ is invertible means that there is a morphism $Y\overset{g}{\to}X$ such that $f\circ g=\mathrm{id}_Y$ and $g\circ f=\mathrm{id}_X$. Instead of such invertibility we can use the regularity condition (4), i.e., $f\circ g\circ f=f$, where g plays the role of an inner inverse.[12]



Usually, for three objects X, Y, Z and three morphisms $f:X\to Y$ and $g:Y\to Z$ and $h:Z\to X$ one can have the "invertible" triangle commutative diagram $h\circ g\circ f=\mathrm{Id}_X$. Its regular extension has the form

$$f\circ h\circ g\circ f=f. \tag{25}$$

Such a diagram



can be called a *semicommutative diagram*. By cyclic permutations of (25) we obtain

$$h\circ g\circ f\circ h=h,$$
$$g\circ f\circ h\circ g=g. \tag{26}$$

These formulas define the concept of three-regularity.

Definition 8: A mapping $f:X\to Y$ satisfying conditions (25) and (26) is said to be three-regular. The mapping $h:Z\to X$ is called the first three-inversion and the mapping $g:Y\to Z$ the second one.

The above-given concept can be expanded to any number of objects and morphisms.

Definition 9: Let $\mathfrak{C}=(\mathfrak{C}_0,\mathfrak{C}_1)$ be a directed graph. An *n-regular cocycle* (X,f) in $\mathfrak{C}$, $n=1,2,...,$ is a sequence of composable arrows in $\mathfrak{C}$,

$$X_1\overset{f_1}{\to}X_2\overset{f_2}{\to}\cdots\overset{f_{n-1}}{\to}X_n\overset{f_n}{\to}X_1, \tag{27}$$

such that

$$f_1\circ f_n\circ\cdots\circ f_2\circ f_1=f_1,$$
$$f_2\circ f_1\circ\cdots\circ f_3\circ f_2=f_2, \tag{28}$$
$$f_n\circ f_{n-1}\circ\cdots\circ f_1\circ f_n=f_n,$$

and

$$e^{(n)}_{X_1}:=f_n\circ\cdots\circ f_2\circ f_1\in\mathrm{End}(X_1),$$
$$e^{(n)}_{X_2}:=f_1\circ\cdots\circ f_3\circ f_2\in\mathrm{End}(X_2), \tag{29}$$
$$e^{(n)}_{X_n}:=f_{n-1}\circ\cdots\circ f_1\circ f_n\in\mathrm{End}(X_n).$$

Definition 10: Let (X,f) be an n-regular cocycle in $\mathfrak{C}$, then the correspondence $e^{(n)}_X:X_i\in\mathfrak{C}_0\mapsto e^{(n)}_{X_i}\in\mathrm{End}(X_i)$, $i=1,2,...,n$, is called an n-regular cocycle obstruction structure on (X,f) in $\mathfrak{C}$.

Lemma 11: We have the following relations

$$f_i\circ e^{(n)}_{X_i}=f_i,\quad e^{(i)}_{X_{i+1}}\circ f_i=f_i,\quad e^{(n)}_{X_i}\circ e^{(n)}_{X_i}=e^{(n)}_{X_i} \tag{30}$$

for $i=1,2,...,n(\mathrm{mod}\,n)$.

Proof: The lemma simply follows from relations (28) and (29). □

Definition 12: An n-regular obstructed category is a directed graph $\mathfrak{C}$ with an associative composition and such that every object is a component of an n-regular cocycle.

Example 1: If all obstructions are equal to the identity $e^{(n)}_{X_i}=\mathrm{id}_{X_i}$, and

$$f_n\circ\cdots\circ f_2\circ f_1=\mathrm{id}_{X_1},$$

$$f_1\circ\cdots\circ f_3\circ f_2=\mathrm{id}_{X_2},\tag{31}$$

$$f_{n-1}\circ\cdots\circ f_1\circ f_n=\mathrm{id}_{X_n},$$

then the sequence (27) is trivially *n*-regular. Observe that the trivial two-regularity is just the usual invertibility, hence every grupoid *G* is a trivially two-regular obstructed category. We are interested with obstructed categories equipped with some obstruction different from the identity.

Definition 13: The minimum number $n=n_{\mathrm{obstr}}$ such that $e_X^{(n)}\neq \mathrm{id}_X$ is called the obstruction degree.

Example 2: Every inverse semigroup *S* is a nontrivial two-regular obstructed category. It has only one object, morphisms are the elements of *S*.

Theorem 14: *Let* $\mathfrak{C}$ *be a category, and*

$$X_1\xrightarrow{f_1}X_2\xrightarrow{f_2}\cdots\xrightarrow{f_{m-1}}X_n\xrightarrow{f_n}X_1\tag{32}$$

be a sequence of morphisms of category $\mathfrak{C}$*. Assume that there is a sequence*

$$Y_1\xrightarrow{\tilde f_1}Y_2\xrightarrow{\tilde f_2}\cdots\xrightarrow{\tilde f_{n-1}}Y_n\xrightarrow{\tilde f_n}Y_1,\tag{33}$$

where Y_i *is a subobject of* X_i *such that there is a collection of mappings* $\pi_i:X_i\to Y_i$ *and* $\iota:Y_i\to X_i$ *satisfying the condition* $\pi_i\circ\iota_i=\mathrm{id}_{Y_i}$ *for* $i=1,2,...,n$*. If in addition*

$$\tilde f_n\circ\cdots\tilde f_2\circ\tilde f_1=\mathrm{id}_{Y_1},$$

$$\tilde f_1\circ\cdots\tilde f_3\circ\tilde f_2=\mathrm{id}_{Y_2},$$

$$\cdots\tag{34}$$

$$\tilde f_{n-1}\circ\cdots\tilde f_1\circ\tilde f_n=\mathrm{id}_{Y_n},$$

and

$$f_i:=t_{i+1}\circ\tilde f_i\circ\pi_i\tag{35}$$

then the sequence (62) *is an n-regular cocycle.*

Proof: The corresponding obstruction structure is given by

$$e_{X_i}^{(n)}=\iota_i\circ\pi_i.\tag{36}$$

If $x\in\mathrm{Ker}\,f_1$, then the theorem is trivial, if $x\in X_i\backslash\mathrm{Ker}\,f_1$, then we obtain

$$(f_1\circ f_n\circ\cdots\circ f_2\circ f_1)(x)=\iota_2\circ\tilde f_1\circ\pi_1\circ\iota_1\circ\tilde f_n\circ\cdots\circ\tilde f_2\circ\tilde f_1\circ\pi_1(x)=\iota_2\circ\tilde f_1\circ\pi_1=f_1(x),$$

where conditions (34) and (35) have been used. We can calculate all cyclic permutations in a similar way. □

Example 3: There is an *n*-regular obstructed category $\mathfrak{C}=(\mathfrak{C}_0,\mathfrak{C}_1)$, where $\mathfrak{C}_0=\{X_i:i=1,...,n(\mathrm{mod}\,n+1)\}$ and $\mathfrak{C}_1=\{f_i:i=1,...,n(\mathrm{mod}\,n+1)\}$ are described in the above-mentioned theorem.

Definition 15: Let (X,f), (Y,g) be two *n*-regular cocycles in $\mathfrak{C}$. An *n*-regular cocycle morphism α: $(X,f)\to(Y,g)$ is a sequence of morphisms $\alpha:=(\alpha_1,\ldots,\alpha_n)$ such that the diagram

$$\begin{array}{ccccccc} X_1 & \overset{f_1}{\rightarrow} & X_2 & \overset{f_2}{\rightarrow}\cdots\overset{f_{n-1}}{\rightarrow} & X_n & \overset{f_n}{\rightarrow} & X_1 \\ \downarrow\alpha_1 & & \downarrow\alpha_2 & & \downarrow\alpha_n & & \downarrow\alpha_1 \\ Y_1 & \overset{g_1}{\rightarrow} & Y_2 & \overset{g_2}{\rightarrow}\cdots\overset{g_{n-1}}{\rightarrow} & Y_n & \overset{g_n}{\rightarrow} & Y_1 \end{array} \tag{37}$$

is commutative. If every component α_i of α is invertible, then α is said to be an n-regular cocycle equivalence.

It is obvious that the n-regular cocycle equivalence is an equivalence relation.

Definition 16: Let $\mathfrak{C}$ be an n-regular obstructed category. A collection of all equivalence classes of n-regular cocycles in $\mathfrak{C}$ and corresponding n-regular cocycle morphisms is denoted by $\mathrm{Reg}^{(n)}(\mathfrak{C})$ and is said to be an n-regularization of $\mathfrak{C}$.

Comment 17: It is obvious that the n-regular cocycle equivalence is an equivalence relation. Equivalence classes of this relation are just elements of $\mathrm{Reg}^{(n)}(\mathfrak{C})$. Our n-regular cocycles and obstruction structures are unique up to an invertible n-regular cocycle morphism. If $[(X,f)]$ is an equivalence class of n-regular cocycles, then there is the corresponding class of n-regular obstruction structures $e_X^{(n)}$ on it. The correspondence is a one to one.

IV. REGULARIZATION OF FUNCTORS AND RELATED STRUCTURES

We are going to introduce the concepts of n-regular functors, natural transformations, involution, duality, and so on. All of our definitions are in the general case the same as in the usual category theory,[29] but the preservation of the identity id_X is replaced by the requirement of preservation of obstructions $e_X^{(n)}$ up to the n-regular cocycle equivalence.

It is known that for two usual categories $\mathfrak{C}$ and $\mathfrak{D}$ a functor $\mathcal{F}:\mathfrak{C}\rightarrow\mathfrak{D}$ is defined as a pair of mappings $(\mathcal{F}_0,\mathcal{F}_1)$, where $\mathcal{F}_0$ sends objects of $\mathfrak{C}$ into objects of $\mathfrak{D}$, and $\mathcal{F}_1$ sends morphisms of $\mathfrak{C}$ into morphisms of $\mathfrak{D}$

$$\mathcal{F}_1(f\circ g)=\mathcal{F}_1(f)\circ\mathcal{F}_1(g),\quad \mathcal{F}_1\mathrm{id}_X=\mathrm{id}_{F_0X}, \tag{38}$$

for $X\in\mathfrak{C}_0$, $\mathcal{F}X\in\mathcal{D}_0$.

Let $\mathfrak{C}$ and $\mathfrak{D}$ be two n-regular obstructed categories. We postulate that all definitions are formulated on every n-regular cocycle (X,f) in $\mathfrak{C}$ up to the n-regular cocycle equivalence, and $i=1,2,\ldots \pmod n$.

Definition 18: An or n-regular cocycle functor $\mathcal{F}^{(n)}:\mathfrak{C}\rightarrow\mathfrak{D}$ is a pair of mappings $(\mathcal{F}_0^{(n)},\mathcal{F}_1^{(n)})$, where $\mathcal{F}_0^{(n)}$ sends objects of $\mathfrak{C}$ into objects of $\mathfrak{D}$, and $\mathcal{F}_1^{(n)}$ sends morphisms of $\mathfrak{C}$ into morphisms of $\mathfrak{D}$ such that

$$\mathcal{F}_1^{(n)}(f_i\circ f_{i+1})=\mathcal{F}_1^{(n)}(f_i)\circ\mathcal{F}_1^{(n)}(f_{i+1}),\quad \mathcal{F}_1^{(n)}(e_{X_i}^{(n)})=e_{\mathcal{F}_0(X_i)}^{(n)}, \tag{39}$$

where $X\in\mathfrak{C}_0$.

Lemma 19: Let $\mathfrak{C}$ and $\mathfrak{D}$ be n-regular obstructed categories, and let

$$X_1\overset{f_1}{\rightarrow}X_2\overset{f_2}{\rightarrow}\cdots\overset{f_{n-1}}{\rightarrow}X_n\overset{f_n}{\rightarrow}X_1 \tag{40}$$

be an n-regular cocycle in $\mathfrak{C}$. If $\mathcal{F}^{(n)}:\mathfrak{C}\rightarrow\mathfrak{D}$ is n-regular cocycle functor, then

$$\mathcal{F}^{(n)}(f_i)\circ e_{X_i}^{(n)}=\mathcal{F}^{(n)}(f_i). \tag{41}$$

Proof: It is a simple calculation

$$\mathcal{F}^{(n)}(f_i)=\mathcal{F}^{(n)}(f\circ e_{X_i}^{(n)})=\mathcal{F}^{(n)}(f)\circ\mathcal{F}^{(n)}(e_{X_i}^{(n)})=\mathcal{F}(f_i)\circ e_{\mathcal{F}_0X_i}^{(n)}. \tag{42}$$

□

Multifunctors can be regularized in a similar way.

Let $\mathcal{F}^{(n)}$ and $\mathcal{G}^{(n)}$ be two n-regular cocycle morphisms of the category $\mathfrak{C}$ into the category $\mathfrak{D}$.

Definition 20: An n-regular natural transformation $s:\mathcal{F}^{(n)}\to\mathcal{G}^{(n)}$ of $\mathcal{F}^{(n)}$ into $\mathcal{G}^{(n)}$ is a collection of functors $s=\{s_{X_i}:\mathcal{F}_0(X_i)\to\mathcal{G}_0(X_i)\}$ such that

$$s_{X_{i+1}}\circ\mathcal{F}_1^{(n)}(f_i)=\mathcal{G}_1^{(n)}(f_i)\circ s_{X_i}, \tag{43}$$

for $f_i:X_i\to X_{i+1}$.

Definition 21: An n-regular obstructed monoidal category $\mathfrak{C}\equiv\mathfrak{C}(\otimes,I)$ can be defined as usual, but we must remember that instead of the identity $\mathrm{id}_X\otimes\mathrm{id}_Y=\mathrm{id}_{X\otimes Y}$ we have an obstruction structure $e_X^{(n)}=\{e_{X_i}^{(n)}\in\mathrm{End}(X_i);n=1,2,...\}$ satisfying the condition

$$e_{X_i\otimes Y_i}^{(n)}=e_{X_i}^{(n)}\otimes e_{Y_i}^{(n)} \tag{44}$$

for every two n-regular cocycles (X,f) and (Y,f').

Let $\mathfrak{C}$ be an n-regular obstructed monoidal category. We introduce an *-operation in $\mathfrak{C}$ as a function which sends every object X_i into object X_i^* called the dual of X,

$$X_i^{**}=X_i,\quad (X_i\otimes Y_i)^*=X_i^*\otimes Y_i^*, \tag{45}$$

reverse all arrows

$$(f\circ g)^*=g^*\circ f^*. \tag{46}$$

The category $\mathfrak{C}$ equipped with such $*$-operation is called an *n-regular obstructed monoidal category with duals*.

Lemma 22: Let $\mathfrak{C}$ be an n-regular obstructed monoidal category with duals. If (X,f) is an n-regular cocycle in $\mathfrak{C}$, then there is a corresponding n-regular cocycle (X^*,f^*) in $\mathfrak{C}^*$, called the dual of (X,f).

Proof: If we reverse all arrows in (X,f) and replace all objects by the corresponding duals, then we obtain (X^*,f^*), where

$$X_1^*\xrightarrow{f_n^*}X_n^*\xrightarrow{f_{n-1}^*}\cdots\xrightarrow{f_2^*}X_2^*\xrightarrow{f_1^*}X_1^* \tag{47}$$

is a sequence such that

$$f_1^*\circ f_n^*\circ\cdots\circ f_2^*\circ f_1^*=f_1^*,\quad e_{X_1^*}^{(n)}:=f_n^*\circ\cdots\circ f_2^*\circ f_1^*, \tag{48}$$

where $f_i^*:X_{i+1}^*\to X_i^*$, $i=1,...,n$, and $X_{n+1}^*\equiv X_1^*$ is the dual. We have corresponding relations for all cyclic permutations. □

Definition 23: An n-regular pairing $g_{\mathfrak{C}}$ in an n-regular obstructed monoidal category $\mathfrak{C}$ can be defined in an analogy to the usual case as a collection of mappings

$$g_{\mathfrak{C}}=\{g_{X_i}\equiv\langle-|-\rangle_{X_i}:X_i^*\otimes X_i\to I\} \tag{49}$$

satisfying some natural consistency conditions and in addition the following regularity relations:

$$g_{X_{i+1}}\circ(f_i^*\otimes f_i)=g_{X_i}, \tag{50}$$

and

$$\langle e_{X_i^*}^{(n)}X_i^*|X_i\rangle_{X_i}=\langle X_i^*|e_{X_i}^{(n)}X_i\rangle_{X_i}, \tag{51}$$

where (X,f) is a regular n-cocycle in $\mathfrak{C}$, and let (X^*,f^*) be the corresponding duals.

It is known that an associative algebra in an ordinary category is an object $\mathcal{A}$ of this category such that there is a multiplication $m:\mathcal{A}\otimes\mathcal{A}\to\mathcal{A}$ which is also a morphism of this category satisfying some axioms like the associativity, the existence of the unity.

Definition 24: Let $\mathfrak{C}$ be an n-regular obstructed monoidal category. An n-regular cocycle algebra $\mathcal{A}$ in the category $\mathfrak{C}$ is an object of this category equipped with an associative multiplication $m:\mathcal{A}\otimes\mathcal{A}\to\mathcal{A}$ such that

$$m\circ(e_A^{(n)}\otimes e_A^{(n)})=e_A^{(n)}\circ m. \tag{52}$$

Obviously such multiplication does not need to be unique.

One can define an n-regular cocycle coalgebra or bialgebra in a similar way. A comultiplication $\Delta:\mathcal{A}\to\mathcal{A}\otimes\mathcal{A}$ can be regularized according to the relation

$$\Delta\circ e_{\mathcal{A}}^{(n)}=(e_{\mathcal{A}}^{(n)}\otimes e_{\mathcal{A}}^{(n)})\circ\Delta. \tag{53}$$

Definition 25: Let $\mathcal{A}$ be an n-regular cocycle algebra. If $\mathcal{A}$ is also regular coalgebra such that $\Delta(ab)=\Delta(a)\Delta(b)$, then it is said to be an n-regular cocycle almost bialgebra.

If $\mathcal{A}$ is an n-regular cocycle algebra, then we denote by $hom_m(\mathcal{A},\mathcal{A})$ the set of morphisms $s\in hom_C(\mathcal{A},\mathcal{A})$ satisfying the condition

$$s\circ m=m\circ(s\otimes s). \tag{54}$$

Let $\mathcal{A}$ be an n-regular cocycle almost bialgebra. We define the convolution product

$$s\star t:=m\circ(s\otimes t)\circ\Delta, \tag{55}$$

where $s,t\in hom_m(\mathcal{A},\mathcal{A})$. If $\mathcal{A}$ is a regular n-cocycle almost bialgebra, then the convolution product is regular.

Definition 26: A two-regular cocycle almost bialgebra $\mathcal{H}$ equipped with an element $S\in hom_m(\mathcal{H},\mathcal{H})$ such that

$$S\star\mathrm{id}_{\mathcal{H}}\star S=S,\quad \mathrm{id}_{\mathcal{H}}\star\mathrm{id}_{\mathcal{H}}=\mathrm{id}_{\mathcal{H}} \tag{56}$$

is said to be a two-regular cocycle almost Hopf algebra $\mathcal{H}$.

The above-given definition is a regular analogy of week Hopf algebras considered in Ref. 26. Similar algebras has been also considered in Ref. 30 and 31.

Lemma 27: If $\mathcal{A}$ is an n-regular cocycle algebra, then there is an n-regular cocycle coalgebra $\mathcal{A}^*$ such that[31]

$$\langle\Delta(\xi),x_1\otimes x_2\rangle=\langle\xi,m(x_1\otimes x_2)\rangle, \tag{57}$$

where $x_1,\ x_2\in\mathcal{A},\ \xi\in\mathcal{A}^*$.

Proof: Let us apply the regularity condition (52) to the above-given duality condition (57). Then the lemma follows from relations (44), (53), and (51). □

Lemma 28: Let $\mathcal{A}$ be an n-regular cocycle almost bialgebra. Then the dual $\mathcal{A}^*$ is also n-regular cocycle almost bialgebra

$$\begin{aligned}\langle\Delta(\xi),x_1\otimes x_2\rangle&=\langle\xi,m(x_1\otimes x_2)\rangle,\\ \langle\hat{m}(\xi\otimes\zeta),x_1\otimes x_2\rangle&=\langle\xi\otimes\zeta,\hat{\Delta}x\rangle.\end{aligned} \tag{58}$$

Let $\mathcal{A}$ be an n-regular cocycle algebra. Then we can define a left n-regular cocycle $\mathcal{A}$-module as an object equipped with an $\mathcal{A}$-module action $\rho_M:\mathcal{A}\otimes M\to M$ such that

$$\rho_M\circ(m\otimes \mathrm{id}_M)=\rho_M\circ(\mathrm{id}_{\mathcal{A}}\otimes\rho_M),$$
$$\rho_M\circ(e_{\mathcal{A}}^{(n)}\otimes e_M^{(n)})=e_M^{(n)}\circ\rho_M. \tag{59}$$

If $\mathcal{A}$ is an n-regular cocycle coalgebra, then one can define an n-regular cocycle comodule M in a similar way. For a coaction $\delta_M:\mathcal{A}\to\mathcal{A}\otimes M$ of $\mathcal{A}$ on M we have the following regularity condition:

$$\delta_M\circ(e_{\mathcal{A}}^{(n)}\otimes e_M^{(n)})=e_M^{(n)}\circ\varrho_M. \tag{60}$$

Remark 1: Observe that we have the following duality between $\mathcal{A}$-module action $\rho_M:\mathcal{A}\otimes M\to M$ and $\mathcal{A}^*$-comodule coactions $\delta_{M^*}:\mathcal{A}^*\to M^*\otimes\mathcal{A}^*$,

$$\langle\delta_{M^*}(\xi),a\otimes x\rangle=\langle\xi\varrho_M(a\otimes x)\rangle, \tag{61}$$

where $a\in\mathcal{A}$, $x\in M$, $\xi\in\mathcal{A}^*$.

V. REGULAR COBORDISMS AND TQFT

Let Cob be a directed graph of cobordisms whose objects Cob_0 are d-dimensional compact smooth and oriented manifolds without boundary and whose arrows are classes of cobordism manifolds with boundaries. We would like to discuss the corresponding n-regular cocycles and their meaning. For this goal we use here a parametrization such that the boundary ∂M is a multiconnected space, a disjoint sum of the ''incoming'' boundary manifold Σ_{in} and the ''outgoing'' one Σ_{out}. We call them ''physical.'' The empty boundary component is also admissible. Let Σ_0, $\Sigma_1\in\mathrm{Cob}_0$, then the disjoint sum is denoted by $\Sigma_0\amalg\Sigma_1$. For a manifold $\Sigma\in\mathrm{Cob}_0$ there is the corresponding manifold Σ^* with the opposite orientation.

We wish to represent quantum processes of certain physical system by cobordism manifolds M with the incoming boundary manifold Σ_0 (an ''input''), and the outgoing one Σ_0 (an ''output''). The incoming boundary manifold Σ_0 represents an initial condition of the system, the outgoing boundary represents the final configuration, and the cobordism manifolds represent possible interaction of the system. Note that the same cobordism manifold M but with different boundary parametrization represent different physical processes!

Definition 29: An ''interaction'' is a triple ${}_{\Sigma_0}\mathcal{M}_{\Sigma_1}$, where the incoming boundary manifold Σ_0 is multiconnected space with m components and the outgoing one Σ_1 is equipped with n components, and $\mathcal{M}$ is a class of cobordism manifolds up to parametrization preserving diffeomorfisms, Σ_0, $\Sigma_1\in\mathrm{Cob}_0$, $\mathcal{M}\in\mathrm{Cob}_1$.

Definition 30: The ''opposite interaction'' of ${}_{\Sigma_0}\mathcal{M}_{\Sigma_1}$ is the ''interaction'' ${}_{\Sigma_1}\mathcal{M}^{\mathrm{op}}_{\Sigma_0}$ with reversed boundary parametrization, i.e., the incoming boundary of $\mathcal{M}$ is the outgoing boundary of $\mathcal{M}^{\mathrm{op}}$ and vice versa.

Example 4: A ''collapsion'' of $\Sigma\in\mathrm{Cob}_0$ is an arbitrary ''interaction'' of the forms ${}_{\Sigma}\mathcal{M}_{\varnothing}$, this means the incoming boundary is Σ and the outgoing boundary is empty. The corresponding ''expansion'' of Σ is the opposite of the collapsion.

Definition 31: Let us denote by $\mathfrak{C}ob=(\mathfrak{C}ob_0,\mathfrak{C}ob_1)$ a directed graph whose objects are $\mathfrak{C}ob_0\equiv\mathrm{Cob}_0$ and arrows $\mathfrak{C}ob_1$ are ''interactions.'' A composition of two interactions ${}_{\Sigma_1}\mathcal{M}_{1\Sigma_2}$ and ${}_{\Sigma_2}\mathcal{M}_{2\Sigma_3}$ is an interaction ${}_{\Sigma_1}(\mathcal{M}_{1\Sigma_2}\mathcal{M}_2)_{\Sigma_3}$, where $\mathcal{M}_{1\Sigma_2}\mathcal{M}_2$ is a result of gluing $\mathcal{M}_1$ and $\mathcal{M}_2$ along Σ_2.

The trivial gluing along the empty boundary component is also admissible. For instance we can glue a ''collapsion'' of Σ and the corresponding ''expansion'' in the trivial way. In this way we obtain an interaction ${}_{\Sigma}(\mathcal{M}\mathcal{M}^{\mathrm{op}})_{\Sigma}$. If we glue the expansion of Σ and the collapsion of Σ along Σ, then we obtain a class of manifolds with empty boundaries.

Example 5: Classes of two-dimensional surfaces with holes provide examples of string interactions.

We wish to build the temporal support semigroup as an arbitrary sequence

$$X_1 \overset{f_1}{\to} X_2 \overset{f_2}{\to} \cdots \overset{f_{n-1}}{\to} X_n \tag{62}$$

of objects and arrows of a directed graph $\mathfrak{C}$ indexed by a discrete time. We wish to represent an interaction ${}_{\Sigma_1}\mathcal{M}_{\Sigma_2}$ as an arrow $X_1 \overset{f}{\to} X_2$ of $\mathfrak{C}$. Obviously composable arrows $X_1 \overset{f_1}{\to} X_2 \overset{f_2}{\to} X_3$ should represent the gluing ${}_{\Sigma_1}(\mathcal{M}_{1\Sigma_2}\mathcal{M}_2)_{\Sigma_3}$. Two interactions ${}_{\Sigma_1}\mathcal{M}_{\Sigma_2}$ and ${}_{\Sigma_1'}\mathcal{M}'_{\Sigma_2'}$ should be represented by the same arrow $X_1 \overset{f}{\to} X_2$ if and only if both interactions are "parallel (simultaneous) in the time."

Let us assume that the directed graph $\mathfrak{C}$ is an n-regular monoidal category with duals. Let $X_1 \overset{f_1}{\to} X_2 \overset{f_2}{\to} \cdots \overset{f_{n-1}}{\to} X_n$ be an n-regular cocycle. If there is an equivalence $\cong$ in $\mathfrak{C}$ob such that objects of the n-regular cocycle represent equivalence classes of $\cong$ and arrows represent time consequences, then we say that we have an n-regular TQFT.

What does n-regularity mean here? It is natural to assume that the opposite ${}_{\Sigma_2}\mathcal{M}^{\mathrm{op}}_{\Sigma_1}$ of ${}_{\Sigma_1}\mathcal{M}_{\Sigma_2}$ should be represented by a reversed arrow $X_1 \overset{f}{\leftarrow} X_2$. The trivial two-regularity is clear, it means that the time is invertible. We postulate that the time is directed and always runs further, never back, never stops. In other words, "our time" is not invertible in general, but it can be n-regular, where the regularity is nontrivial.

Example 6: Let us consider for instance the two-regular "interactions." Let

$${}_{\Sigma_1}\mathcal{M}_{1\Sigma_2} \text{ and } {}_{\Sigma_2}\mathcal{M}_{2\Sigma_1}$$

be two interactions, then ${}_{\Sigma_1}(\mathcal{M}_{1\Sigma_2}\mathcal{M}_2)_{\Sigma_1}$ and ${}_{\Sigma_2}(\mathcal{M}_{2\Sigma_1}\mathcal{M}_1)_{\Sigma_2}$ can be represented as arrows $X_1 \overset{f_1}{\to} X_2 \overset{f_2}{\to} X_1$, and $X_2 \overset{f_2}{\to} X_1 \overset{f_1}{\to} X_2$, respectively. Interactions ${}_{\Sigma_1}\mathcal{M}_{1\Sigma_2}\mathcal{M}_{2\Sigma_1}\mathcal{M}_{1\Sigma_2}$ and ${}_{\Sigma_2}\mathcal{M}_{2\Sigma_1}\mathcal{M}_{1\Sigma_2}\mathcal{M}_{2\Sigma_1}$ should be represented by $X_1 \overset{f_1}{\to} X_2 \overset{f_2}{\to} X_1 \overset{f_1}{\to} X_2$, and $X_2 \overset{f_2}{\to} X_1 \overset{f_1}{\to} X_2 \overset{f_2}{\to} X_1$, respectively. Now the two-regularity conditions are clear.

Observe that the regularity concept can be useful for the construction of quantum theory of the whole universe with nonivertible time evolution. In fact the nontrivial n-regularity conditions mean that all processes always go further, never back, never stop, but are cyclically repeating after n-steps up to an equivalence.

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Integrals of monomials over the orthogonal group

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A recursion formula is derived which allows one to evaluate invariant integrals over the orthogonal group $O(N)$, where the integrand is an arbitrary finite monomial in the matrix elements of the group. The value of such an integral is expressible as a finite sum of partial fractions in N. The recursion formula largely extends presently available integration formulas for the orthogonal group. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1471367]

I. INTRODUCTION

Integrals over the classical compact groups[1,2] are of interest in various fields, such as harmonic analysis[3] or random matrix theory.[4] In these applications the integrand is often a polynomial in the matrix elements of the group itself (i.e., of the true matrix representation of the group). Thus we have to integrate an arbitrary monomial of these matrix elements. Closed formulas are available only for very special cases[3,5–7] and even a new method by Prosen *et al.*[8] using computer algebras is practically limited to low degrees. For arbitrary monomials there is strong evidence that the results in Ref. 8 are exact at least up to the next leading order in N^{-1} with respect to the approximation of the group integral by independent Gaussian distributed matrix elements.[9]

In the present paper we shall address the case of the orthogonal group $O(N)$. First we rederive the well-known one-vector formula.[4,6] In this context, the terms ''R-vector formula'' or ''R-vector integral'' refer to the case where the monomial in question contains only powers of matrix elements from R rows or R columns, respectively. Next we derive a recursion formula that relates an R-vector integral to a linear combination of $(R-1)$-vector integrals. This is the central result of the present paper. Together with the one-vector formula, it allows one to calculate any integral over a monomial of finite degree in a finite number of steps. This result is then used to obtain a closed expression for general two-vector integrals that is much simpler than the one known before.[6] Besides, the older formula contains mistakes which (to the best of my knowledge) had never been corrected in the literature.

The paper is organized as follows: In Sec. II we describe the current approach to the problem. In addition, we introduce some compact nonstandard notations, which help to keep the mathematical expressions manageable. Then the one-vector result of Ullah[6] is rederived, as it is the base for the recursion formula developed later on. In passing we obtain an equally simple formula for the corresponding one-vector integral over the unitary group. In Sec. III we derive the general recursion formula. In Sec. IV some applications are presented. As an immediate consequence, we obtain a closed expression for the two-vector integral, which is then compared to the corrected old result.[6] We also illustrate the use of our general formula for $R>2$, calculating a particular three-vector integral. Section V contains the conclusions.

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II. GENERAL CONSIDERATIONS

To be specific, let us consider the orthogonal matrix $w \in O(N)$ as a point in Euclidean N^2-dimensional space. Then we are interested in integrals of monomials in the coordinates of w. These are denoted by

$$\langle M \rangle = \int \mathrm{d}\sigma(w) \quad \prod_{i,\xi=1}^{N,R} w_{i\xi}^{M_{i\xi}}. \tag{1}$$

Here σ is the normalized Haar measure[10] of $O(N)$, i.e., $\int \mathrm{d}\sigma(w) = 1$, and M is an $N \times R$ matrix of non-negative integers, with $R \leqslant N$. M is called the power matrix. In the recursion formula to be developed, R is used as the recursion parameter. Hence it is important, that R, the number of columns of M, is as small as possible.

The integral over the orthogonal group is invariant under any permutation of columns or rows of the integration variable $w \in O(N)$. It is also invariant under taking the transpose. Therefore it is sufficient to consider such monomials which contain matrix elements from the first $R \leqslant N$ columns of w only. According to Ullah[6] one may then write

$$\langle M \rangle = \frac{\mathcal{N}(M)}{\mathcal{N}(o)}, \quad \mathcal{N}(M) = \int \prod_{\xi=1}^{R} \left\{ \mathrm{d}\Omega(\vec{w}_\xi) \prod_{i=1}^{N} w_{i\xi}^{M_{i\xi}} \right\} \quad \prod_{\mu<\nu} \delta(\langle \vec{w}_\mu | \vec{w}_\nu \rangle), \tag{2}$$

where o is an $N \times R$ matrix of zeros. The integration region is the Cartesian product of R unit spheres with constant measures $\mathrm{d}\Omega(\vec{w}_\xi)$, and $\{\vec{w}_1, \ldots, \vec{w}_R\}$ are the corresponding unit vectors. The orthogonality of the unit vectors is implemented with the help of appropriately chosen δ-functions. $\langle \vec{w}_\mu | \vec{w}_\nu \rangle$ denotes the scalar product between the two vectors $\vec{w}_\mu$ and $\vec{w}_\nu$.

A. Compact notations for certain products of multinomials

In the calculations to follow, we will frequently deal with certain products of binomial and multinomial coefficients. For better legibility we use two special notations: In what follows, $\vec{x}$ and $\vec{y}$ are N-dimensional real vectors, and $\vec{m}$ and $\vec{n}$ are N-dimensional vector-indices of non-negative integers. There are two typical cases in which products of multinomials appear:

(1) Consider the expression $E = \Pi_{i=1}^{N} (x_i + y_i)^{n_i}$. Its expansion gives

$$E = \sum_{\vec{k}} \prod_{i=1}^{N} \binom{n_i}{k_i} x_i^{k_i} y_i^{n_i - k_i}, \tag{3}$$

where the sum runs over all $\vec{k}$ for which $\forall i : k_i \leqslant n_i$. In this case, the product of binomials is denoted by the following symbol:

$$\prod_{i=1}^{N} \binom{n_i}{k_i} = \binom{\vec{n}}{\vec{k}}. \tag{4}$$

(2) On other occasions, we encounter expressions of the type: $E' = \Pi_{i=1}^{N} \langle \vec{\tau} | \vec{w}_i' \rangle^{n_i}$, where $\langle \vec{\tau} | \vec{w}_i' \rangle$ is the scalar product of the two $(R-1)$-dimensional vectors $\vec{\tau}$ and $\vec{w}_i'$. In this case the expansion reads

$$E' = \sum_{K} \left\{ \prod_{i=1}^{N} (n_i | K_{i1}, \ldots, K_{i,R-1}) \right\} \quad \prod_{\xi=1}^{R-1} \bar{\tau}_\xi^{\bar{k}_\xi} \prod_{i=1}^{N} w_{i\xi}^{K_{i\xi}}. \tag{5}$$

Here we have to use the $N \times (R-1)$ matrix K as an index. The elements of K are non-negative integers. $\vec{k}_\xi$ is the ξth column vector of K, and $\bar{k}_\xi$ is the sum of its components: $\bar{k}_\xi = \Sigma_{i=1}^{N} K_{i\xi}$. The sum in Eq. (5) runs over all K for which $\forall i : \Sigma_{\xi=1}^{R-1} K_{i\xi} = n_i$. In this case, we use the following notation:

$$\prod_{i=1}^{N}(n_i|K_{i1},\ldots,K_{i,R-1})=(\vec{n}|K). \tag{6}$$

B. The one-vector integral

In the one-vector case, $R=1$, there are no orthogonality relations to respect. The power matrix M consists of one single column vector, here denoted by $\vec{m}$. According to Eq. (2) we may write

$$\langle\vec{m}\rangle=\frac{\mathcal{N}(\vec{m})}{\mathcal{N}(\vec{o})},\quad \mathcal{N}(\vec{m})=\int \mathrm{d}\Omega(\vec{w})\prod_{i=1}^{N} w_i^{m_i}, \tag{7}$$

where $\vec{o}$ is an N-dimensional vector of zeros. Following the original calculation of Ullah,[4,6] we integrate over the full vector space $\mathbb{R}^N$ and implement the normalization of the column vector with the help of a δ-function. This introduces the integration constant c_N:

$$\mathcal{N}(\vec{m})=c_N^{-1}\left\{\prod_{i=1}^{N}\int_{-\infty}^{\infty}\mathrm{d}x_i\, x_i^{m_i}\right\}\quad \delta(\|\vec{x}\|^2-1). \tag{8}$$

The next step is to remove the δ-function. Setting $x_i=u_i/\sqrt{r}$, we obtain

$$\mathcal{N}(\vec{m})r^{(N+\overline{m})/2-1}=c_N^{-1}\left\{\prod_{i=1}^{N}\int_{-\infty}^{\infty}\mathrm{d}u_i\, u_i^{m_i}\right\}\quad \delta(\|\vec{u}\|^2-r), \tag{9}$$

where $\overline{m}=\Sigma_{i=1}^{N} m_i$. The δ-function can now be removed by multiplying the *left-hand side* and the *right-hand side* with e^{-r} and integrating on r from 0 to ∞:

$$\mathcal{N}(\vec{m})\Gamma\left(\frac{N+\overline{m}}{2}\right)\quad c_N=\prod_{i=1}^{N}\int_{-\infty}^{\infty}\mathrm{d}u_i\, u_i^{m_i}e^{-u_i^2}=\prod_{i=1}^{N}\Gamma\left(\frac{1+m_i}{2}\right). \tag{10}$$

Solving this equation for $\mathcal{N}(\vec{m})$, the ratio $\mathcal{N}(\vec{m})/\mathcal{N}(\vec{o})$ can be calculated, which leads to the desired result:

$$\langle\vec{m}\rangle=\left(\frac{N}{2}\right)_{\overline{m}/2}^{-1}\prod_{i=1}^{N}\left(\frac{1}{2}\right)_{m_i/2}. \tag{11}$$

Here it is convenient to use the Pochhammer symbol $(z)_n=\Gamma(z+n)/\Gamma(z)$.[11] Note that Eq. (10) implies that the integral $\langle\vec{m}\rangle$ vanishes if at least one component of $\vec{m}$ is odd.

C. The one-vector integral over the unitary group

It is natural to consider also integrals over the unitary group $U(N)$. This is much more complicated because in general the monomials to integrate contain powers of the matrix elements and their complex conjugated counterparts. In the one-vector case, however, the integral over the unitary group can be mapped on a corresponding integral over the orthogonal group, which leads again to a simple result (it seems that such a formula has never been published elsewhere). If more vectors are involved, $R>1$, the orthogonality conditions destroy this simple correspondence.

To obtain the desired expression for one-vector integrals, it is convenient to consider monomials in the real and imaginary parts of the complex unit vector $\vec{w}$. They can be identified with the coordinates in a $2N$-dimensional Euclidean space, where the Haar measure reduces to the constant measure Ω_2 on the unit hypersphere. Denoting the one-vector integral of an arbitrary monomial by $\langle\vec{m}:\vec{n}\rangle=\langle\Pi_{i=1}^{N}x_i^{m_i}y_i^{n_i}\rangle$, where $w_i=x_i+\mathrm{i}y_i$, we may write

$$\langle \vec{m}:\vec{n}\rangle = \frac{\mathcal{M}(\vec{m},\vec{n})}{\mathcal{M}(\vec{o},\vec{o})}, \quad \mathcal{M}(\vec{m},\vec{n}) = \int \mathrm{d}\Omega_2(\vec{w}) \prod_{i=1}^{N} x_i^{m_i} y_i^{n_i}, \quad w_i = x_i + \mathrm{i}y_i . \tag{12}$$

Note the different notations: $\langle \vec{m}:\vec{n}\rangle$ stands for the one-vector integral over the unitary group, while $\langle \vec{m},\vec{n}\rangle$, used in Sec. IV, stands for the two-vector integral over the orthogonal group. As Eq. (12) shows, we may express $\langle \vec{m}:\vec{n}\rangle$ as a one-vector integral over the orthogonal group $O(2N)$: $\langle \vec{m}:\vec{n}\rangle = \langle \vec{p},\rangle$ where $\vec{p}$ is the $2N$-dimensional concatenation of $\vec{m}$ and $\vec{n}$. Then we may apply Eq. (11). This leads to

$$\langle \vec{m}:\vec{n}\rangle = (N)^{-1}_{(\overline{m}+\overline{n})/2} \prod_{i=1}^{N} \left(\frac{1}{2}\right)_{m_i/2} \left(\frac{1}{2}\right)_{n_i/2} . \tag{13}$$

Again the integral $\langle \vec{m}:\vec{n}\rangle$ vanishes, if at least one component of $\vec{m}$ or $\vec{n}$ is odd.

III. THE RECURSION FORMULA

The desired recursion formula shall express an arbitrary integral $\langle M\rangle$, where M is a power matrix with R columns, as a linear combination of simpler integrals $\langle M'\rangle$, where M' has only $R-1$ columns. Starting from Eq. (2) one may attack this problem head on, and separate the integration on the last unit vector $\vec{w}_R$ from the remaining integral:

$$\mathcal{N}(M) = \int \left\{ \prod_{\xi=1}^{R-1} \mathrm{d}\Omega(\vec{w}_\xi) \prod_{i=1}^{N} w_{i\xi}^{M_{i\xi}} \right\} \left\{ \prod_{\mu<\nu}^{R-1} \delta(\langle \vec{w}_\mu | \vec{w}_\nu \rangle) \right\} J(\vec{w}_1,\ldots,\vec{w}_{R-1};\vec{m}_R). \tag{14}$$

Here $\vec{m}_R$ is the last column vector of the power matrix M, and

$$J(\vec{w}_1,\ldots,\vec{w}_{R-1};\vec{m}_R) = \int \mathrm{d}\Omega(\vec{w}) \left\{ \prod_{i=1}^{R} w_i^{M_{iR}} \right\} \prod_{\xi=1}^{R-1} \delta(\langle \vec{w}_\xi | \vec{w} \rangle). \tag{15}$$

As shown in the following, the value of this integral can be expressed as a linear combination of monomials in the integration variables $\{w_{i\xi} | \xi \leqslant R-1\}$. If this is inserted back into Eq. (14), it obviously leads to the desired recursion formula.

To evaluate the integral (15), we replace the integration over the unit sphere by an integration over the full space $\mathbb{R}^N$, implementing the normalization condition with the help of a δ-function. This introduces the normalization constant c_N as before in Eq. (8). Then we remove the δ-function again, using the same trick as in Sec. II B. After that, we replace the remaining δ-functions (responsible for the orthogonality relations) by their respective Fourier representations. All this leads to

$$\begin{aligned} J(\vec{w}_1,\ldots,\vec{w}_{R-1};\vec{m}_R) &= c_N^{-1} \left\{ \prod_{i=1}^{N} \int \mathrm{d}x_i\, x_i^{M_{iR}} \right\} \delta(\|\vec{x}\|^2 - 1) \prod_{\xi=1}^{R-1} \delta(\langle \vec{w}_\xi | \vec{x} \rangle) \\ &= c_N^{-1} \Gamma\left(\frac{N-R+\overline{m}_R+1}{2} \right)^{-1} \left\{ \prod_{i=1}^{N} \int \mathrm{d}x_i\, x_i^{M_{iR}} e^{-x_i^2} \right\} \prod_{\xi=1}^{R-1} \delta(\langle \vec{w}_\xi | \vec{x} \rangle) \\ &= c_N^{-1} \Gamma\left(\frac{N-R+\overline{m}_R+1}{2} \right)^{-1} \int \frac{\mathrm{d}^{R-1}\vec{\tau}}{\pi^{R-1}} \prod_{i=1}^{N} \int \mathrm{d}x_i\, x_i^{M_{iR}} e^{-x_i^2 + 2i\langle \vec{\tau} | \vec{w}_i' \rangle x_i}, \end{aligned} \tag{16}$$

where $\vec{w}_i'$ stands for the row-vector $(w_{i1},\ldots,w_{i,R-1})^T$. The integrals on x_i are easily evaluated:

$$J(\cdots)\Gamma\left(\frac{N-R+\overline{m}_R+1}{2}\right)c_N=\int\frac{\mathrm{d}^{R-1}\vec{\tau}}{\pi^{R-1}}\exp^{-\Sigma_{i=1}^N\langle\vec{\tau}|\vec{w}_i'\rangle^2}\prod_{i=1}^N\left[\sum_{\kappa_i=0}^{M_{iR}}\kappa_i:\text{even}\binom{M_{iR}}{\kappa_i}\right.$$
$$\left.\times(\mathrm{i}\langle\vec{\tau}|\vec{w}_i'\rangle)^{M_{iR}-\kappa_i}\Gamma\left(\frac{1+\kappa_i}{2}\right)\right]. \tag{17}$$

Expanding the N-fold product in the second line, we obtain for the left-hand side

$$\text{l.h.s.}=\sum_{\vec{\kappa}}\binom{\vec{m}_R}{\vec{\kappa}}\mathrm{i}^{\overline{m}_R-\overline{\kappa}}\left\{\prod_{i=1}^N\Gamma\left(\frac{1+\kappa_i}{2}\right)\right\}\int\frac{\mathrm{d}^{R-1}\vec{\tau}}{\pi^{R-1}}\left\{\prod_{i=1}^N\langle\vec{\tau}|\vec{w}_i'\rangle^{M_{iR}-\kappa_i}\right\}e^{-\langle\vec{\tau}|A\vec{\tau}\rangle}, \tag{18}$$

where $\vec{\kappa}=(\kappa_1,\ldots,\kappa_N)^T$. Note that the sum runs only over such $\vec{\kappa}$, for which all components are even, and that for the product of binomials the abbreviation from Eq. (4) is used. A bar over vector quantities such as $\overline{m}_R$ and $\overline{\kappa}$ denotes the sum of all their components. The quadratic matrix A, with elements $A_{\mu\nu}=\langle\vec{w}_\mu|\vec{w}_\nu\rangle$, has dimension $R-1$.

Now, the key observation is the following: The orthogonality conditions implemented in the form of δ-functions in Eq. (14) select from the total integration region only a submanifold. There it holds that $\langle\vec{w}_\mu|\vec{w}_\nu\rangle=\delta_{\mu\nu}$, so that the matrix A may be replaced by the unit matrix. Then it is possible to evaluate the $\vec{\tau}$-integral. The expansion of the product of scalar products leads to

$$\text{l.h.s.}=\sum_{\vec{\kappa}}\binom{\vec{m}_R}{\vec{\kappa}}\mathrm{i}^{\overline{m}_R-\overline{\kappa}}\left\{\prod_{i=1}^N\Gamma\left(\frac{1+\kappa_i}{2}\right)\right\}\sum_K(\vec{m}_R-\vec{\kappa}|K)\left\{\prod_{\xi=1}^{R-1}\int\frac{\mathrm{d}\tau_\xi}{\pi}\tau_\xi^{\overline{k}_\xi}e^{-\tau_\xi^2}\prod_{i=1}^N w_{i\xi}^{K_{i\xi}}\right\}, \tag{19}$$

where K is a matrix index with $R-1$ columns, as introduced in Eq. (6) together with the abbreviation for the product of multinomials. The $\overline{k}_\xi$'s are the sums over the components of the column vectors of K. The remaining integrals are easily evaluated, which results in

$$J()=\frac{\pi^{1-R}}{c_N\Gamma\left(\frac{N-R+\overline{m}_R+1}{2}\right)}\sum_{\vec{\kappa}}\binom{\vec{m}_R}{\vec{\kappa}}(-1)^{(\overline{m}_R-\overline{\kappa})/2}\left\{\prod_{i=1}^N\Gamma\left(\frac{1+\kappa_i}{2}\right)\right\}$$
$$\times\sum_K(\vec{m}_R-\vec{\kappa}|K)\prod_{\xi=1}^{R-1}\Gamma\left(\frac{1+\overline{k}_\xi}{2}\right)\prod_{i=1}^N w_{i\xi}^{K_{i\xi}}. \tag{20}$$

Note that, as a consequence of the τ_ξ-integrals, the sum in the second line runs over such K only, for which all $\overline{k}_1,\ldots,\overline{k}_{R-1}$ are even. Inserting this expression into the initial Eq. (14) we obtain

$$\mathcal{N}(M)=\frac{\pi^{1-R}}{c_N\Gamma\left(\frac{N-R+\overline{m}_R+1}{2}\right)}\sum_{\vec{\kappa}}\binom{\vec{m}_R}{\vec{\kappa}}(-1)^{(\overline{m}_R-\overline{\kappa})/2}\left\{\prod_{i=1}^N\Gamma\left(\frac{1+\kappa_i}{2}\right)\right\}\sum_K(\vec{m}_R-\vec{\kappa}|K)$$
$$\times\left\{\prod_{\xi=1}^{R-1}\Gamma\left(\frac{1+\overline{k}_\xi}{2}\right)\right\}\left\{\prod_{\xi=1}^{R-1}\int\mathrm{d}\Omega(\vec{w}_\xi)\prod_{i=1}^N w_{i\xi}^{M_{i\xi}+K_{i\xi}}\right\}\left\{\prod_{\mu<\nu}^{R-1}\delta(\langle\vec{w}_\mu|\vec{w}_\nu\rangle)\right\}. \tag{21}$$

The integral over the normalized vectors $\vec{w}_1,\ldots,\vec{w}_{R-1}$ can be identified with $\mathcal{N}(M^{(R-1)}+K)$ which is a $(R-1)$-vector integral. In this way, we obtain a recursion formula for $\mathcal{N}(M)$. For the normalization constant, we find

$$\mathcal{N}(o)=\frac{\pi^{1-R}}{c_N\Gamma\left(\frac{N-R+1}{2}\right)}\left\{\prod_{i=1}^{N}\Gamma\left(\frac{1}{2}\right)\right\}\left\{\prod_{\xi=1}^{R-1}\Gamma\left(\frac{1}{2}\right)\right\}\mathcal{N}(o^{(R-1)}). \tag{22}$$

Thus we obtain for the R-vector integral $\langle M\rangle$, defined in Eq. (2):

$$\langle M\rangle=\left(\frac{N-R+1}{2}\right)^{-1}_{\overline{m}_R/2}\sum_{\vec{\kappa}}\binom{\vec{m}_R}{\vec{\kappa}}(-1)^{(\overline{m}_R-\overline{\kappa})/2}\left\{\prod_{i=1}^{N}\left(\frac{1}{2}\right)_{\kappa_i/2}\right\}$$
$$\times\sum_{K}(\vec{m}_R-\vec{\kappa}|K)\left\{\prod_{\xi=1}^{R-1}\left(\frac{1}{2}\right)_{\overline{k}_\xi/2}\right\}\langle M^{(R-1)}+K\rangle. \tag{23}$$

This is the desired recursion formula and the main result of the present paper. As mentioned before it is understood that the first sum runs over such $\vec{\kappa}$ only for which all components are even, while the second runs over such K only for which all $\overline{k}_\xi=\Sigma_{i=1}^{N}K_{i\xi}$ are even. Furthermore $\overline{m}_R=\Sigma_{i=1}^{N}M_{iR}$, $\overline{\kappa}=\Sigma_{i=1}^{N}\kappa_i$, and $M^{(R-1)}$ stands for the matrix consisting of the first $R-1$ columns of the matrix M.

In principle Eq. (23) allows one to evaluate integrals of arbitrary monomials of finite degree. The result is always expressible as a rational function of the dimension N, because the repeated expansion of Eq. (23) leads to nested sums of partial fractions in N. In this context it is useful to note that only the prefactor of the r.h.s. depends explicitly on N. The formula (23) can be used conveniently if either R or the degree of the monomial to be integrated is small. Otherwise Eq. (23) may lead to very lengthy expressions. However, such expressions should still be manageable with an appropriate computer algebra system. This would allow for further systematic studies of this class of integrals.

In contrast to what one might expect, the integral $\langle M\rangle$ does not necessarily vanish if the power matrix M has odd elements. It rather holds the following: If any sum over a row or column of M is odd, then $\langle M\rangle=0$. Though this is in fact well known,[12] it is still instructive to see that it follows almost immediately from the recursion relation (23).

To this end, permute columns and rows, and take the transpose if necessary, to transform M in such a way that its last column contains the row or column whose sum of components is odd. Then apply Eq. (23): The sum over $\vec{\kappa}$ is restricted to such $\vec{\kappa}$ which have only even components. Hence $\overline{\kappa}$ is even. As $\overline{m}_R$ is odd, and $\Sigma_{\xi=1}^{R-1}\overline{k}_\xi=\overline{m}_R-\overline{\kappa}$, at least one of the sums $\overline{k}_1,\ldots,\overline{k}_{R-1}$ must be odd as well. Such a term vanishes, because of what is said below Eq. (20). This implies that all terms of the sum over K vanish likewise, so that the complete integral gives zero.

IV. APPLICATIONS

In random matrix theory, many matrix ensembles are based on the concept of orthogonal invariance. Physically this corresponds to a situation where the Hamiltonian for a spinless quantum particle possesses an antiunitary symmetry, e.g., time reversal invariance. The Gaussian and circular orthogonal ensembles[4,13,14] are well-known examples based on this concept. Other examples are the Poisson orthogonal ensemble,[15] or the recently introduced matrix ensembles for semiseparable systems.[8] In those cases the orthogonal group acts directly on the Hamiltonian, and the statistical properties of the eigenvectors are uniquely determined by the orthogonal group and its invariant measure. In fact, the ensemble of eigenvectors is simply given by the orthogonal group itself. Therefore any correlators between the eigenvectors can be expressed and calculated in terms of R-vector integrals.

In what follows, we first apply our integration formula (23) to the two-vector case. In this way we obtain a closed expression for arbitrary two-vector integrals. Then we compare this result with

the corrected formula of Ref. 6. For illustration, we finally compute a simple three-vector integral, which can be evaluated with an independent method also. As it should be, we find the same answer with both methods.

A. The two-vector integral

Consider the arbitrary two-vector integral $\langle M\rangle=\langle\vec{m},\vec{n}\rangle$, where the first column vector of M is denoted by $\vec{m}$ and the second by $\vec{n}$. In this case, Eq. (23) leads directly to

$$\langle\vec{m},\vec{n}\rangle=\left(\frac{N-1}{2}\right)_{\overline{n}/2}^{-1}\sum_{\vec{\kappa}}\binom{\vec{n}}{\vec{\kappa}}(-1)^{(\overline{n}-\overline{\kappa})/2}\left\{\prod_{i=1}^{N}\left(\frac{1}{2}\right)_{\kappa_i/2}\right\}\left(\frac{1}{2}\right)_{(\overline{n}-\overline{\kappa})/2}\langle\vec{m}+\vec{n}-\vec{\kappa}\rangle. \tag{24}$$

The sum runs over such $\vec{\kappa}$ only, for which all components are even. A bar over a vector quantity denotes, as before, the sum of all its components. This formula has already been used in Ref. 16 to calculate various two-vector integrals, and numerical tests performed therein have confirmed its validity. For later purpose we use Eq. (24) to evaluate the following simple integral:

$$\left\langle\begin{pmatrix}1&1\\1&1\\0&0\\\vdots&\vdots\end{pmatrix}\right\rangle=\frac{2}{N-1}(-1)\frac{1}{2}\left\langle\begin{pmatrix}2\\2\\0\\\vdots\end{pmatrix}\right\rangle=\frac{-1}{(N-1)N(N+2)}. \tag{25}$$

Note that the same result can be obtained by an indirect method[12] also.

In principle, an integration formula for general two-vector integrals has already been published some time ago.[6] After the correction of two misprints, it reads

$$\begin{aligned}\overline{\prod_i u_i^{2m_i}v_i^{2n_i}}=\pi^{-N+1}2^{-2N+4-2\Sigma(m_i+n_i)}&\frac{\Gamma(N-1)\Gamma[N-1+\Sigma_i(m_i+n_i)]}{\Gamma[\Sigma_i m_i+(N-1)/2]\Gamma[\Sigma_i n_i+(N-1)/2]}\\&\times\sum_{k_1,\ldots,k_N,l_1,\ldots,l_N=0,\ldots,0}^{2m_1,\ldots,2m_N,2n_1,\ldots,2n_N}(-1)^{\Sigma_i l_i}\\&\times\frac{\Pi_i\binom{2m_i}{k_i}\binom{2n_i}{l_i}\Gamma[(k_i+l_i+1)/2]\Gamma[m_i+n_i-(k_i+l_i-1)/2]}{\Gamma[N/2+\Sigma_i(k_i+l_i)/2]\Gamma[N/2+\Sigma_i(m_i+n_i)-\Sigma_i(k_i+l_i)/2]},\end{aligned} \tag{26}$$

where $\forall i: k_i+l_i$ must be even. Here the original notation of Ref. 6 is used. The corrections concern the first line, where the nominator has been multiplied with $\Gamma[N-1+\Sigma_i(m_i+n_i)]$, and the sum over $k_1,\ldots,k_N,l_1,\ldots,l_N$, where the indices must start with zeros instead of ones. Finally the notation is quite unfortunate, as it seems to prohibit monomials with odd powers, though there is no reason for it. Indeed, Eq. (26) holds in those cases as well. This can be checked, for instance, by computing the integral (25) with the help of Eq. (26), setting $m_1=m_2=n_1=n_2=1/2$.

Using the notation adopted in the present work, Eq. (26) reads

$$\langle\vec{m},\vec{n}\rangle=\frac{(N-1)_{(\overline{m}+\overline{n})/2}}{2^{\overline{m}+\overline{n}}\left(\frac{N-1}{2}\right)_{\overline{m}/2}\left(\frac{N-1}{2}\right)_{\overline{n}/2}}\sum_{\vec{k},\vec{l}}\binom{\vec{m}}{\vec{k}}\binom{\vec{n}}{\vec{l}}(-1)^{\overline{l}}\langle\vec{k}+\vec{l}\rangle\langle\vec{m}-\vec{k}+\vec{n}-\vec{l}\rangle. \tag{27}$$

If we compare the integration formulas (24) and (27), they differ considerably. It seems rather difficult to prove their equivalence directly. Note moreover, that our result is much simpler, because there the sum runs over a single vector-index only.

B. A simple three-vector integral

The three-vector integral considered here is chosen because of its simplicity and because it may be evaluated using an indirect method, which allows to crosscheck the result. We will compute the integral $\langle M\rangle$ with

$$M=\begin{pmatrix} 2 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 2\\ 0 & 0 & 0\\ \vdots & \vdots & \vdots \end{pmatrix}. \tag{28}$$

Henceforth we will skip those parts of the column vectors which are zero anyway. Using our recursion formula (23) the three-vector integral $\langle M\rangle$ can be reduced to a linear combination of two-vector integrals, for which we already have a closed expression, i.e., Eq. (24). Thus, the evaluation of $\langle M\rangle$ needs only a few steps:

$$\begin{aligned}
&\left\langle \begin{pmatrix} 2 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 2 \end{pmatrix} \right\rangle \\
&\quad=\frac{2}{N-2}\left\{ -\sum_K \left(\begin{pmatrix} 0\\ 0\\ 2 \end{pmatrix} \middle| K \right) \left(\frac{1}{2}\right)_{\overline{k_1/2}} \left(\frac{1}{2}\right)_{\overline{k_2/2}} \left\langle \begin{pmatrix} 2 & 0\\ 0 & 2\\ 0 & 0 \end{pmatrix} + K \right\rangle + \frac{1}{2}\left\langle \begin{pmatrix} 2 & 0\\ 0 & 2 \end{pmatrix} \right\rangle \right\} \\
&\quad=\frac{2}{N-2}\left\{ -\frac{1}{2}\left[\left\langle \begin{pmatrix} 2 & 0\\ 0 & 2\\ 2 & 0 \end{pmatrix} \right\rangle + \left\langle \begin{pmatrix} 2 & 0\\ 0 & 2\\ 0 & 2 \end{pmatrix} \right\rangle \right] + \frac{1}{2}\,\frac{N+1}{(N-1)N(N+2)} \right\} \\
&\quad=\frac{1}{N-2}\left\{ \frac{N+1}{(N-1)N(N+2)} - 2\,\frac{N+3}{(N-1)N(N+2)(N+4)} \right\} \\
&\quad=\frac{N^2+3N-2}{(N-2)(N-1)N(N+2)(N+4)}.
\end{aligned} \tag{29}$$

The result is expressed as a rational function, where care has been taken that nominator and denominator have no more common factors.

Alternatively we may compute $\langle M\rangle$ with M as defined in Eq. (28), starting from the following identity:

$$\left(\sum_i w_{i1}^2\right)\left(\sum_j w_{j2}^2\right)\left(\sum_k w_{k3}^2\right)=1, \tag{30}$$

which holds for an arbitrary $w\in O(N)$. To this end we expand the products on the l.h.s. and integrate on both sides over the group. This gives

$$N(N-1)(N-2)\left\langle \begin{pmatrix} 2 & 0 & 0\\ 0 & 2 & 0\\ 0 & 0 & 2 \end{pmatrix} \right\rangle + 3N(N-1)\left\langle \begin{pmatrix} 2 & 0\\ 2 & 0\\ 0 & 2 \end{pmatrix} \right\rangle + N\left\langle \begin{pmatrix} 2\\ 2\\ 2 \end{pmatrix} \right\rangle = 1. \tag{31}$$

It allows one to express the three-vector integral $\langle M\rangle$ as a linear combination of a one-vector and a two-vector integral. According to Eqs. (11) and (24), these integrals are given by

$$\left\langle \begin{pmatrix} 2 \\ 2 \\ 2 \end{pmatrix} \right\rangle = \frac{1}{N(N+2)(N+4)}, \quad \left\langle \begin{pmatrix} 2 & 0 \\ 2 & 0 \\ 0 & 2 \end{pmatrix} \right\rangle = \frac{N+3}{(N-1)N(N+2)(N+4)}. \tag{32}$$

Thus we obtain

$$\left\langle \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \right\rangle = \frac{(N+2)(N+4)-3(N+3)+1}{(N-2)(N-1)N(N+2)(N+4)}$$

$$= \frac{N^2+3N-2}{(N-2)(N-1)N(N+2)(N+4)}. \tag{33}$$

As expected, the result coincides with that in Eq. (29). Here the indirect method worked so well because we first wrote down the identities (30) and (31), and then chose our particular example $\langle M \rangle$. However, if the value of a certain integral is needed, one would have to guess useful identities which allow one to express the integral by a linear combination of simpler ones, a procedure which is very difficult. In contrast to that, the recursion formula (23) always provides a well-defined finite procedure, for the computation of any integral.

V. CONCLUSIONS

To summarize, we have derived a recursion formula, which expresses an arbitrary R-vector integral over the orthogonal group as a linear combination of $(R-1)$-vector integrals. It allows one to successively evaluate the group integral of any finite monomial in the matrix elements of the group. The simplicity of the result depends primarily on R, the number of column or row vectors involved, and only secondarily on the degree of the monomial in question. The result is always given as a finite sum of partial fractions in N.

As an immediate consequence of the general result, we obtained a closed integration formula for arbitrary two-vector integrals, which is quite different and much simpler than the corrected, previously known result.

In principle a similar recursion formula can be obtained for integrals over the unitary group also. To that end one should consider monomials in the real and imaginary parts of the matrix elements. Though the derivation along the lines of the orthogonal case is rather straightforward, the resulting expressions are much more involved. It seems that the simple result for the case $R=1$ is only an exception. More work is clearly necessary to clarify the situation in this case.

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The Weierstrass representation for surfaces immersed into R^8 and CP^2 maps

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A generalization of the Weierstrass system of equations corresponding to CP^2 harmonic maps is presented. This generalization allows us to study two-dimensional surfaces immersed in a flat space R^8 with Euclidean metric. We use this system to suggest a possible geometrical interpretation of CP^2 harmonic maps.
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I. INTRODUCTION

Sigma models in two spatial dimensions are integrable and have been studied for a variety of reasons. They are low dimensional analogs of four-dimensional Yang–Mills theories which play a pivotal role in particle physics, they arise in some areas of condensed-matter physics, etc., and they are also interesting from a purely mathematical point of view. Moreover, they arise naturally in differential geometry in the investigation of immersion and deformations of surfaces.

Of course, there are many classes of σ models; particularly important amongst them are the so-called CP^{N-1} σ models. These models, all, possess topological properties and, as such, lead to the appearance of ''topological solitons.''

The models are a generalization of the, perhaps simplest, σ model, namely the S^2 model—also called the vector $SO(3)$ model. The CP^{N-1} models involve maps from R^2, or S^2 if one wants to have nontrivial topology, to CP^{N-1}. It is easiest to define them in terms of the Lagrangian density[1]

$$L=\tfrac{1}{4}(D_\mu z)^\dagger \cdot D_\mu z, \tag{1.1}$$

where z is a vector field of N components, $z=(z^1,\ldots,z^N)$, which satisfies

$$z^\dagger \cdot z=1. \tag{1.2}$$

The covariant derivative D_μ acts on $z:S^2\to CP^{N-1}$ according to

$$D_\mu z=\partial_\mu z-z(z^\dagger \cdot \partial_\mu z). \tag{1.3}$$

Here $\mu=1,2$, of course, and denotes the space coordinates x and y.

The total Lagrangian is given by

$$\mathcal{L}=\int L\, \mathrm{d}x\, \mathrm{d}y \tag{1.4}$$

and, if the model is defined over S^2, we require that $\mathcal{L}$ is finite.

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As is well known, the CP^1 sigma model ($N=2$) can be equivalently described in terms of a three-component real vector field $\vec{\phi}$ defined by

$$\vec{\phi}=z^{\dagger}\vec{\sigma}z, \tag{1.5}$$

where $\vec{\sigma}$ is a vector of Pauli's σ matrices.

Then the Lagrangian density of the CP^1 model (1) becomes

$$L=\partial_{\mu}\vec{\phi}\cdot\partial_{\mu}\vec{\phi} \tag{1.6}$$

together with the constraint

$$\vec{\phi}\cdot\vec{\phi}=1, \tag{1.7}$$

i.e., $\vec{\phi}$ lies on a unit sphere S^2.

For a model defined over S^2 all harmonic maps, i.e., solutions of the Euler Lagrange equations which follow from (1.4) are well known.[1] They come in three separate classes: those which are holomorphic, those which are antiholomorphic, and the mixed ones. The CP^1 model has only holomorphic and antiholomorphic harmonic maps but for CP^N $N\geqslant 2$ there are also mixed maps. These solutions have very different properties, e.g., holomorphic solutions are stable, as they are minima of the total Lagrangian, while the mixed solutions are not, as they are only saddle points.

Recently, there has been a lot of interest in relating CP^1 maps to the solutions of the Weierstrass problem.[2–4]

In this case, according to Ref. 4 one considers a set of first-order equations for complex fields ϕ and ψ of ζ and $\overline{\zeta}$, given by

$$\partial\psi=p\phi, \quad \overline{\partial}\phi=-p\psi, \quad p=|\phi|^2+|\psi|^2 \tag{1.8}$$

where

$$\partial=\frac{\partial}{\partial(x+iy)}=\frac{\partial}{\partial\zeta}, \quad \overline{\partial}=\frac{\partial}{\partial\overline{\zeta}}. \tag{1.9}$$

From the Weierstrass system (1.8) one constructs a geometric coordinate system of three real variables X_i, $i=1,2,3$ and, treating $X_i(x,y)$ as a map of R^2 into R^3 discusses the geometry of these surfaces.

In this paper we address the question of the generalization of these ideas to higher CP^N. Thus we consider the case of CP^2. What is the corresponding Weierstrass system and how does one construct the corresponding real quantities X_i? In Sec. II we collect together various results on the CP^1 system. We then discuss various formulations of the CP^2 model and recall some of its solutions. Next we present our generalized Weierstrass system and discuss some of its properties. We then present our ideas on how to construct a set of real-valued functions $X_i(x,y)$ and show how they describe the geometry of surfaces.

II. CP^1 MODEL

A. General properties

For the CP^1 sigma model it is convenient to introduce

$$W=\frac{z_2}{z_1}=\frac{\phi^1+i\phi^2}{1+\phi^3}. \tag{2.1}$$

In terms of W the Lagrangian becomes

$$\mathcal{L}=\int \frac{|\partial W|^2+|\partial \overline{W}|^2}{(1+|W|^2)^2}\,\mathrm{d}\zeta\,\mathrm{d}\overline{\zeta} \tag{2.2}$$

and its Euler Lagrange equations take the form

$$\partial\overline{\partial} W-2\overline{W}\frac{\partial W\overline{\partial} W}{|W|^2+1}=0. \tag{2.3}$$

In Ref. 3 it was shown that the relation between CP^1 maps W and the ϕ, ψ fields of the Weierstrass problem is given by (up to an overall multiplication of ϕ and ψ by a factor -1)

$$\psi=W\frac{(\overline{\partial W})^{1/2}}{1+|W|^2},\quad \phi=\frac{(\partial W)^{1/2}}{1+|W|^2}, \tag{2.4}$$

where

$$W=\frac{\psi}{\overline{\phi}}. \tag{2.5}$$

As is well known[5] the CP^1 equations can be written as a compatibility condition for a set of two linear spectral equations for a two component auxiliary vector Ψ,

$$\partial\Psi=\frac{2}{1+\lambda}[\partial P,P]\Psi,\quad \overline{\partial}\Psi=\frac{2}{1-\lambda}[\overline{\partial}P,P]\Psi, \tag{2.6}$$

where the 2 by 2 matrix P is a projector given by

$$P=\frac{1}{A}\begin{pmatrix}1 & \overline{W}\\ W & |W|^2\end{pmatrix},\quad A=1+|W|^2. \tag{2.7}$$

The compatibility conditions for (2.6) are, clearly,

$$[\partial\overline{\partial}P,\ P]=0 \tag{2.8}$$

which, as can be easily checked, are equivalent to (2.3).

Note that (2.8) can be written in the form of a conservation law

$$\partial[\overline{\partial}P,P]+\overline{\partial}[\partial P,P]=0 \tag{2.9}$$

or, equivalently, using the traceless matrices K and M,

$$\partial K+\overline{\partial}M=0, \tag{2.10}$$

where the matrices K and M are given by

$$K=\frac{1}{A^2}\begin{pmatrix}\overline{W\partial W}-W\overline{\partial W} & \overline{\partial W}+\overline{W}^2\overline{\partial}W\\ -\overline{\partial}W-W^2\overline{\partial W} & W\overline{\partial W}-\overline{W\partial W}\end{pmatrix} \tag{2.11}$$

and

$$M=\frac{1}{A^2}\begin{pmatrix}\overline{W}\partial W-W\partial\overline{W} & \partial\overline{W}+\overline{W}^2\partial W\\ -\partial W-W^2\partial\overline{W} & W\partial\overline{W}-\overline{W}\partial W\end{pmatrix}. \tag{2.12}$$

To proceed further it is worth recalling the existence of various quantities of the CP^{N-1} model which are holomorphic.[1] One of them is

$$T=(\overline{D}z)^{\dagger}\cdot Dz, \tag{2.13}$$

where $D=\frac{1}{2}(D_1-iD_2)$ and $\overline{D}=\frac{1}{2}(D_1+iD_2)$ denote the covariant derivative (1.3) with respect to $\zeta=x+iy$. As is easy to check, T satisfies

$$\overline{\partial}T=0 \tag{2.14}$$

and so is a function of $\zeta=x+iy$ only.

In the CP^1 case, the function T expressed in terms of W is given by

$$T=2\frac{\partial W\partial\overline{W}}{(1+|W|^2)^2}. \tag{2.15}$$

In fact, for the solutions of (2.3) which describe fields defined on S^2, W is any holomorphic or antiholomorphic function and so $T=0$.

B. Weierstrass system

Let us introduce the complex fields ϕ and ψ by (2.4) and (2.5). In Refs. 3 and 4 it was shown that

$$\partial\psi=p\phi,\quad \overline{\partial}\phi=-p\psi, \tag{2.16}$$

where

$$p=|\phi|^2+|\psi|^2=\frac{(\partial W\overline{\partial W})^{1/2}}{1+|W|^2}. \tag{2.17}$$

Now we reexpress the quantity T in terms of them using (2.4) we get

$$T=\overline{\psi}\partial\phi-\phi\partial\overline{\psi}. \tag{2.18}$$

Moreover, we also have

$$p=A|\phi|^2,\quad A=1+|W|^2 \tag{2.19}$$

and we can express the first derivatives of W in terms of ψ and ϕ:

$$\partial W=A^2\phi^2,\quad \overline{\partial}W=-\overline{T}(\overline{\phi})^{-2}. \tag{2.20}$$

This allows us to derive the explicit form of matrices K and M in terms of ϕ and ψ. So, we have

$$K=\begin{pmatrix} -(\psi\overline{\phi}+\overline{R\psi}\phi) & \overline{\phi}^2-\overline{R\psi}^2 \\ -\psi^2+\overline{R}\phi^2 & \psi\overline{\phi}+\overline{R\psi}\phi \end{pmatrix} \tag{2.21}$$

and

$$M=\begin{pmatrix} (\overline{\psi}\phi+R\psi\overline{\phi}) & \overline{\psi}^2-R\overline{\phi}^2 \\ -\phi^2+R\psi^2 & -(\overline{\psi}\phi+R\psi\overline{\phi}), \end{pmatrix} \tag{2.22}$$

where we have introduced the following notation:

$$R=\frac{T}{p^2}.$$

As a consequence of (2.9) we find that the system (2.16) possesses, at least, three further conservation laws

$$\begin{aligned}
&-\partial(\psi\overline{\phi}+\overline{R\psi}\phi)+\overline{\partial}(\overline{\psi}\phi+R\psi\overline{\phi})=0,\\
&\partial(-\psi^2+\overline{R}\phi^2)+\overline{\partial}(-\phi^2+R\psi^2)=0,\\
&\partial(\overline{\phi}^2-\overline{R\psi^2})+\overline{\partial}(\overline{\psi}^2-R\overline{\phi}^2)=0.
\end{aligned} \tag{2.23}$$

These formulas differ slightly from the conservation laws given in Ref. 4, as they contain additional terms involving R. However, if we put $R=0$ in (2.23) we recover the expressions of Ref. 4.

As a result of conservation laws (2.23) we can introduce three real-valued functions $X_i(\zeta,\overline{\zeta})$, $i=1,2,3$ given by

$$\begin{aligned}
X_1&=i\int_\gamma [\overline{\psi}^2+\phi^2-R(\psi^2+\overline{\phi}^2)]\mathrm{d}\zeta-[\psi^2+\overline{\phi}^2-\overline{R}(\overline{\psi}^2+\phi^2)]\mathrm{d}\overline{\zeta},\\
X_2&=\int_\gamma [\overline{\psi}^2-\phi^2+R(\psi^2-\overline{\phi}^2)]\mathrm{d}\zeta+[\psi^2-\overline{\phi}^2+\overline{R}(\overline{\psi}^2-\phi^2)]\mathrm{d}\overline{\zeta},\\
X_3&=-2\int_\gamma [\overline{\psi}\phi+R\psi\overline{\phi}]\mathrm{d}\zeta+[\psi\overline{\phi}+\overline{R\psi}\phi]\mathrm{d}\overline{\zeta},
\end{aligned} \tag{2.24}$$

where γ is any curve from a fixed point to ζ.

The conservation laws (2.23) guarantee that quantities X_i do not depend on the choice of the curve γ in the complex plane C (but only its end points). This is because X_i can be rewritten as

$$X_i=\int_\gamma F_i(\zeta,\overline{\zeta})\mathrm{d}\zeta+\overline{F}_i(\zeta,\overline{\zeta})\mathrm{d}\overline{\zeta},\quad i=1,2,3, \tag{2.25}$$

where F_i satisfy the following conditions:

$$\overline{\partial}F_i=\partial\overline{F}_i, \tag{2.26}$$

which shows that the integrands are total derivatives.

The functions $X_i(\zeta,\overline{\zeta})$ can be considered as components of a radius vector

$$\vec{r}(\zeta,\overline{\zeta})=(X_1(\zeta,\overline{\zeta}),X_2(\zeta,\overline{\zeta}),X_3(\zeta,\overline{\zeta})) \tag{2.27}$$

of an orientable, simply connected, surface (locally parametrized by ζ and $\overline{\zeta}$ immersed in R^3).

This allows us to calculate the tangent vectors to the surface, i.e.,

$$\partial\vec{r}=(i[\overline{\psi}^2+\phi^2-R(\psi^2+\overline{\phi}^2)],[\overline{\psi}^2-\phi^2+R(\psi^2-\overline{\phi}^2)],-2(\overline{\psi}\phi+R\psi\overline{\phi})) \tag{2.28}$$

and

$$\overline{\partial}\vec{r}=(-i[\psi^2+\overline{\phi}^2-\overline{R}(\overline{\psi}^2+\phi^2)],[\psi^2-\overline{\phi}^2+\overline{R}(\overline{\psi}^2-\phi^2)],-2(\psi\overline{\phi}+\overline{R\psi}\phi)). \tag{2.29}$$

These expressions allow us to calculate the induced metric. We find the following expressions for the components of the induced metric (written in holomorphic components):

$$g_{\zeta\zeta}=(\partial\vec{r},\partial\vec{r})=4Rp^2, \quad g_{\bar{\zeta}\bar{\zeta}}=(\bar{\partial}\vec{r},\bar{\partial}\vec{r})=4\bar{R}p^2 \tag{2.30}$$

and

$$g_{\zeta\bar{\zeta}}=(\partial\vec{r},\bar{\partial}\vec{r})=2(p^2+|R|^2p^2). \tag{2.31}$$

Hence, for the harmonic maps, $R=0$ and the only nonvanishing component of the metric is $g_{\zeta\bar{\zeta}}=2p^2$. In this case solutions of the system (2.16) are represented by expression (2.4), where $W(\zeta)$ is an arbitrary holomorphic function. As is well known[1] finiteness of the energy restricts $W(\zeta)$ to being a rational function. Geometrically, such functions parametrize an immersed sphere $S^2\in R^3$.

III. CP^2 MODEL

A. General properties

Now we consider a more general situation when the Lagrangian is given by (1.1) with a three-component vector $z=(z_1,z_2,z_3)$ (z_i, which satisfies $\bar{z}\cdot z=\Sigma_i \bar{z}_i z_i=1$). We can define two complex fields W_i, $i=1,2$ through

$$W_1=\frac{z_1}{z_3}, \quad W_2=\frac{z_2}{z_3} \tag{3.1}$$

and find that the Euler Lagrange equations take the form[6]

$$\begin{aligned}
&\bar{\partial}\partial W_1-\frac{2\bar{W}_1}{A}\partial W_1\bar{\partial}W_1-\frac{\bar{W}_2}{A}(\partial W_1\bar{\partial}W_2+\bar{\partial}W_1\partial W_2)=0,\\
&\bar{\partial}\partial W_2-\frac{2\bar{W}_2}{A}\partial W_2\bar{\partial}W_2-\frac{\bar{W}_1}{A}(\partial W_1\bar{\partial}W_2+\bar{\partial}W_1\partial W_2)=0,
\end{aligned} \tag{3.2}$$

and their respective complex conjugate equations and where

$$A=1+|W_1|^2+|W_2|^2.$$

Clearly, when, say, $W_2=0$ (i.e., $z_2=0$) the model, and its equations, reduce to the CP^1 case.

Like in the CP^1 case we still have an auxiliary spectral problem given by (2.6) but this time the auxiliary vector Φ has three components and the 3×3 projector P is given by

$$P=\frac{1}{A}\begin{pmatrix} 1 & \bar{W}_1 & \bar{W}_2 \\ W_1 & |W_1|^2 & W_1\bar{W}_2 \\ W_2 & \bar{W}_1W_2 & |W_2|^2 \end{pmatrix}. \tag{3.3}$$

As in the CP^1 case the compatibility condition for the two equations in (2.6) gives the equations of motion (2.8) which are equivalent to (3.2). Similarly as in the previous case the system (3.2) possesses a conservation law

$$\partial K+\bar{\partial}M=0 \tag{3.4}$$

with

$$K=[\bar{\partial}P,P], \quad M=[\partial P,P]. \tag{3.5}$$

The explicit forms of 3×3 traceless matrices K and M are rather complicated expressions so we shall not write them explicitly here.

In the CP^2 case the quantity T can be written in terms of W_1 and W_2 as

$$T=\frac{\partial W_1\partial\bar{W}_1+\partial W_2\partial\bar{W}_2+(\bar{W}_1\partial\bar{W}_2-\bar{W}_2\partial\bar{W}_1)(W_1\partial W_2-W_2\partial W_1)}{(1+|W_1|^2+|W_2|^2)^2}. \tag{3.6}$$

All solutions of the CP^2 model are well known. They fall into three classes; those described by analytic fields, i.e., $W_i=W_i(\zeta)$, antianalytic $[W_i=W_i(\bar{\zeta})]$, and mixed ones.

Mixed solutions can be determined from either the holomorphic or the antiholomorphic fields by the following procedure. Take arbitrary holomorphic functions $f_i=f_i(\zeta)$ and define

$$F_{ij}=f_i\partial f_j-f_j\partial f_i, \quad i,j=1,2,3. \tag{3.7}$$

Next, introduce new complex valued functions:

$$g_i=\sum_{k\neq i}\bar{f}_kF_{ki}. \tag{3.8}$$

Then we can determine W_i as ratios of the components of g_i, i.e.,

$$W_1=\frac{g_2}{g_1}, \quad W_2=\frac{g_3}{g_1}. \tag{3.9}$$

Then it can be shown[1] that all mixed solutions correspond to W_i constructed in this way from some $f_i(\zeta)$. An alternative approach starts with antiholomorphic f_i i.e., $f_i=f(\bar{\zeta})$ and constructs g_i in the same way but using $\bar{\partial}$ instead of ∂ in the definition of F_{ij}.

B. Generalized Weierstrass system

Now, according to the discussion of the previous section we can introduce two pairs of complex functions ψ_i,ϕ_i $i=1,2$, which have to satisfy

$$W_i=\frac{\psi_i}{\bar{\phi}_i}, \quad i=1,2. \tag{3.10}$$

The aim of this section is to find a system of first-order equations which is a generalization of (2.16) and which are in a one-to-one correspondence with the equations of the CP^2 sigma model (3.2).

Let us note that a possible set of equations for functions ψ_i and ϕ_i is given by

$$\bar{\partial}\phi_1=-\frac{1}{2}\left[(A+|W_1|^2)\phi_1\bar{\phi}_2\psi_2+(A+1+|W_1|^2)|\phi_1|^2\psi_1+\frac{\phi_2}{\phi_1}\bar{\psi}_2\psi_1^2+(1+|W_2|^2)\frac{|\phi_2|^4}{|\phi_1|^2}\psi_1\right], \tag{3.11}$$

$$\bar{\partial}\phi_2=-\frac{1}{2}\left[(A+|W_2|^2)\phi_2\bar{\phi}_1\psi_1+(A+1+|W_2|^2)|\phi_2|^2\psi_2+\frac{\phi_1}{\phi_2}\bar{\psi}_1\psi_2^2+(1+|W_1|^2)\frac{|\phi_1|^4}{|\phi_2|^2}\psi_2\right], \tag{3.12}$$

$$\partial\psi_1=-\frac{1}{2}\left[(A+|W_1|^2)\phi_2\overline{\psi}_2\psi_1+(A+1+|W_1|^2)|\psi_1|^2\phi_1+\frac{\overline{\phi}_2}{\overline{\phi}_1^2}\overline{\psi}_1\psi_2|\psi_1|^2\right]$$
$$-\frac{1}{2}(1+|W_2|^2)\frac{|\phi_2|^4}{\overline{\phi}_1|\phi_1|^2}|\psi_1|^2+A(1+|W_1|^2)|\phi_1|^2\phi_1+A\phi_2\psi_1\overline{\psi}_2, \tag{3.13}$$

$$\partial\psi_2=-\frac{1}{2}\left[(A+|W_2|^2)\phi_1\overline{\psi}_1\psi_2+(A+1+|W_2|^2)|\psi_2|^2\phi_2+\frac{\overline{\phi}_1}{\overline{\phi}_2^2}\overline{\psi}_2\psi_1|\psi_2|^2\right]$$
$$-\frac{1}{2}(1+|W_1|^2)\frac{|\phi_1|^4}{\overline{\phi}_2|\phi_2|^2}|\psi_2|^2+A(1+|W_2|^2)|\phi_2|^2\phi_2+A\phi_1\psi_2\overline{\psi}_1, \tag{3.14}$$

$$A=1+|W_1|^2+|W_2|^2,$$

and their respective complex conjugate equations, where we can use Eq. (3.10) to express the above-given expressions in terms of ψ_i and ϕ_i's.

It is easy to check that if we put $\phi_2=W_2=0$ then the system of equations (3.11)–(3.14) reduces to Eq. (2.16) and the system (3.2) reduces to the CP^1 model (2.3). These limits characterize some properties of solutions of the system of first-order equations (3.11)–(3.14).

Moreover, it is possible, although somewhat tedious, to show that Eqs. (3.11)–(3.14) are equivalent to (3.2). Thus Eqs. (3.11)–(3.14) can be thought of as being CP^2 analogs of (2.16); [like (2.16) they involve only first derivatives and only $\overline{\partial}\phi_i$ and $\partial\psi_i$ are given].

Here we can use the fact [the generalization of (2.4)] that

$$A^2\phi_1^2=(1+|W_2|^2)\partial W_1-W_1\overline{W}_2\partial W_2,$$
$$A^2\phi_2^2=(1+|W_1|^2)\partial W_2-W_2\overline{W}_1\partial W_1. \tag{3.15}$$

Next we address the question of the existence of real valued functions X_i's. To construct them we note that we can exploit the matrices K and M given by (3.4) and (3.5). Then the CP^2 analog of matrices (2.21) and (2.22) becomes

$$K=K_1-\frac{1}{A^2}K_2, \tag{3.16}$$

where

$$K_1=\begin{pmatrix} -(\psi_1\overline{\phi}_1+\psi_2\overline{\phi}_2) & \overline{\phi}_1^2 & \overline{\phi}_2^2 \\ -W_1(\psi_1\overline{\phi}_1+\psi_2\overline{\phi}_2) & \psi_1\overline{\phi}_1 & \dfrac{\psi_1}{\overline{\phi}_1}\overline{\phi}_2^2 \\ -W_2(\psi_1\overline{\phi}_1+\psi_2\overline{\phi}_2) & \dfrac{\psi_2}{\overline{\phi}_2}\overline{\phi}_1^2 & \psi_2\overline{\phi}_2 \end{pmatrix} \tag{3.17}$$

and

$$K_2=\begin{pmatrix} -(\overline{W}_1\overline{\partial}W_1+\overline{W}_2\overline{\partial}W_2) & -\overline{W}_1(\overline{W}_1\overline{\partial}W_1+\overline{W}_2\overline{\partial}W_2) & -\overline{W}_2(\overline{W}_1\overline{\partial}W_1+\overline{W}_2\overline{\partial}W_2) \\ \Phi_1 & \overline{W}_1\Phi_1 & \overline{W}_2\Phi_1 \\ \Phi_2 & \overline{W}_1\Phi_2 & \overline{W}_2\Phi_2 \end{pmatrix}, \tag{3.18}$$

where we have defined the following expressions:

$$\begin{aligned} \Phi_1&=(1+|W_2|^2)\overline{\partial}W_1-W_1\overline{W}_2\overline{\partial}W_2, \\ \Phi_2&=(1+|W_1|^2)\overline{\partial}W_2-W_2\overline{W}_1\overline{\partial}W_1 \end{aligned} \tag{3.19}$$

in order to abbreviate expressions (3.16) and (3.18).

Similarily, matrix M is given by

$$M=M_1-\frac{1}{A^2}M_2, \tag{3.20}$$

where

$$M_1=\begin{pmatrix} (\overline{\psi}_1\phi_1+\overline{\psi}_2\phi_2) & \overline{W}_1(\overline{\psi}_1\phi_1+\overline{\psi}_2\phi_2) & +\overline{W}_2(\overline{\psi}_1\phi_1+\overline{\psi}_2\phi_2) \\ -\phi_1^2 & -\overline{\psi}_1\phi_1 & -\dfrac{\overline{\psi}_2}{\phi_2}\phi_1^2 \\ -\phi_2^2 & -\dfrac{\overline{\psi}_1}{\phi_1}\phi_2^2 & -\overline{\psi}_2\phi_2 \end{pmatrix} \tag{3.21}$$

and

$$M_2=\begin{pmatrix} -(\overline{W}_1\overline{\partial}W_1+\overline{W}_2\overline{\partial}W_2) & \overline{\Phi}_1 & \overline{\Phi}_2 \\ -W_1(W_1\partial\overline{W}_1+W_2\partial\overline{W}_2) & W_1\overline{\Phi}_1 & W_1\overline{\Phi}_2 \\ -W_2(W_1\partial\overline{W}_1+W_2\partial\overline{W}_2) & W_2\overline{\Phi}_1 & W_2\overline{\Phi}_2 \end{pmatrix}. \tag{3.22}$$

Note that matrices K_2 and M_2 involve expressions which involve $\overline{\partial}W_i$ which are not known. In the holomorphic case $W=W_i(\zeta)$ and so $K_2=M_2=0$. In fact, this is also true in general; when the equations of motion are satisfied we can set $M_2=K_2=0$ and the conservation laws are still satisfied. Hence, in our search of real-valued functions X_i we can restrict our attention to only K_1 and M_1.

As both matrices (K_1 and M_1) are traceless we can use them to define eight new conservation laws. These in turn allow us to define nine real quantities $X_i(\zeta,\overline{\zeta})$, eight of which are linearly independent. X_i $i=1,2,3$ are constructed by taking diagonal entries of matrices M and K:

$$\begin{aligned} X_1&=-\int_\gamma[\overline{\psi}_1\phi_1+\overline{\psi}_2\phi_2]\mathrm{d}\zeta+[\psi_1\overline{\phi}_1+\psi_2\overline{\phi}_2]\mathrm{d}\overline{\zeta}, \\ X_2&=\int_\gamma\overline{\psi}_1\phi_1\mathrm{d}\zeta+\psi_1\overline{\phi}_1\,\mathrm{d}\overline{\zeta}, \\ X_3&=\int_\gamma\overline{\psi}_2\phi_2\,\mathrm{d}\zeta+\psi_2\overline{\phi}_2\,\mathrm{d}\overline{\zeta}, \end{aligned} \tag{3.23}$$

which satisfy

$$X_1+X_2+X_3=0. \tag{3.24}$$

The off-diagonal entries of matrices K and M when combined with the property that $K^{\dagger}=-M$ give us a further six real quantities X_i, $i=4,...,9$ i.e.,

$$X_4+iX_5=\int_\gamma\left[-\mu\phi_1^2+\overline{\mu}\left(\overline{\psi_1^2}+\overline{\psi_1}\,\overline{\psi_2}\,\frac{\phi_2}{\phi_1}\right)\right]d\zeta+\left[-\overline{\mu}\,\overline{\phi_1^2}+\mu\left(\psi_1^2+\psi_1\psi_2\frac{\overline{\phi_2}}{\overline{\phi_1}}\right)\right]d\overline{\zeta},$$

$$X_6+iX_7=\int_\gamma\left[-\nu\phi_2^2+\overline{\nu}\left(\overline{\psi_2^2}+\overline{\psi_1}\,\overline{\psi_2}\,\frac{\phi_1}{\phi_2}\right)\right]d\zeta+\left[-\overline{\nu}\,\overline{\phi_2^2}+\nu\left(\psi_2^2+\psi_1\psi_2\frac{\overline{\phi_1}}{\overline{\phi_2}}\right)\right]d\overline{\zeta}, \tag{3.25}$$

$$X_8+iX_9=-\int_\gamma\left[\alpha\phi_2^2\frac{\overline{\psi_1}}{\phi_1}+\overline{\alpha}\phi_1^2\frac{\overline{\psi_2}}{\phi_2}\right]d\zeta+\left[\overline{\alpha}\,\overline{\phi_2^2}\frac{\psi_1}{\overline{\phi_1}}+\alpha\,\overline{\phi_1^2}\frac{\psi_2}{\overline{\phi_2}}\right]d\overline{\zeta}.$$

Here μ, ν, and α are arbitrary constants. As in the CP^1 case the integrals in the definition of X_i do not depend on the trajectory of the curve γ (but are only on its end point ζ) in C since conditions (2.26) hold. So we can then consider function X_i as components of an eight-dimensional vector $\vec{r}$ and use it to construct and investigate two-dimensional surfaces immersed in R^8. Thus, putting it all together, we see that if the complex functions ψ_i and ϕ_i, $i=1,2$ are solutions of the system of first-order equations (3.11)–(3.14), the generalized Weierstrass formulas given by (3.23)–(3.25) determine the conformal immersion of a surface into R^8.

To see this we take $\mu=\nu=\alpha=(1+i)/2$ and consider X_i, $i=2,...,9$ as components of a radius vector in R^8,

$$\vec{r}(\xi,\overline{\xi})=(X_2,X_3,\ldots,X_9). \tag{3.26}$$

This allows us to define the induced metric [by expressions like (2.30) and (2.31)]. We find that only $g_{\xi\overline{\xi}}\neq 0$ and, in fact, is given by

$$g_{\xi\overline{\xi}}=\frac{|\partial W_1|^2+|\partial W_2|^2+|W_2\partial W_1-W_1\partial W_2|^2}{(1+|W_1|^2+|W_2|^2)^2}. \tag{3.27}$$

Having found the metric we can now study various geometrical aspects of our surfaces. This will be discussed in more detail in future work.

IV. CONCLUSIONS AND FURTHER COMMENTS

In this paper we have shown how to generalize the old ideas of Weierstrass from the CP^1 to the CP^2 case. We have found that the corresponding first-order equations have much more complicated form. We have also started discussing the geometry of the associated surfaces leaving details to a future publication. We are currently looking at the generalization of our results to CP^N.

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Nested sums, expansion of transcendental functions, and multiscale multiloop integrals

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Expansion of higher transcendental functions in a small parameter are needed in many areas of science. For certain classes of functions this can be achieved by algebraic means. These algebraic tools are based on nested sums and can be formulated as algorithms suitable for an implementation on a computer. Examples such as expansions of generalized hypergeometric functions or Appell functions are discussed. As a further application, we give the general solution of a two-loop integral, the so-called C-topology, in terms of multiple nested sums. In addition, we discuss some important properties of nested sums, in particular we show that they satisfy a Hopf algebra. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The expansion of higher transcendental functions[1,2] is a common problem occurring in many areas of science. It is of particular interest in particle physics in the calculation of higher order radiative corrections to scattering amplitudes. There, higher transcendental functions occur frequently in formal solutions for specific loop integrals. The necessary expansions of these functions are in general a highly nontrivial task. This is particularly true if the expansions are required to a very high order.

In calculations of higher order radiative corrections, classical polylogarithms,[3] as well as Nielsen's generalized polylogarithms[4] appear. However, this set of functions will not suffice, if the number of loops grows, or if several different scales are involved in the problem. Several extensions of this class of functions to multiple polylogarithms have been discussed recently.[5–8]

It is the aim of this paper to perform a systematic study of multiple nested sums appearing in the expansion of higher transcendental functions around integer values of their indices. To that end, we define so-called Z-sums, study their algebraic properties, and discuss their relation to the multiple polylogarithms introduced in the literature.[5–8] We give algorithms to solve these multiple nested sums to any order in the expansion parameter ϵ in terms of a given basis in Z-sums. All algorithms can be readily implemented on a computer. The Z-sums can be considered as certain generalizations of Euler–Zagier sums[9,10] or of harmonic sums[11–13] involving multiple ratios of scales. The latter are known in physics since the calculation of higher order Mellin moments of the deep-inelastic structure functions.[11,14–16]

At the same time, our results allow us to investigate higher loop multiscale integrals occuring for instance in pertubative corrections to four-particle scattering amplitudes. These integrals have received great attention in recent years, mainly motivated by calculations of the next-to-next-to-leading order corrections to amplitudes for Bhabha scattering,[17] for $pp \to 2$ jets[18–20] for $pp \to \gamma\gamma$,[21] and for light-by-light scattering.[22]

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The relevant master integrals at two loops with four external legs have been calculated using a variety of techniques. Analytic results were obtained either with the help of Mellin–Barnes representations[23,24] or with differential equations.[8,25] Numerical results were obtained by a numerical evaluation of the coefficients of the ϵ-expansion.[26,27] Here, we want to advocate a different point of view based on multiple nested sums. As a new result and to illustrate our approach, we discuss a specific two-loop integral, the so-called C-topology with one leg offshell, which can be reduced for arbitrary powers of the propagators and arbitrary dimensions to the aforementioned sums. This is useful for the calculation of the two-loop amplitude for $e^+e^- \to 3$ jets. Some of the techniques presented here have already been used in a recent calculation with massive fermions.[28] In addition, there exists a wide variety of related literature on higher transcendental functions occurring in loop integrals and we can only mention a few of them here.[29–35]

This paper is organized as follows. In Sec. II we introduce nested sums, show that they satisfy an algebra and summarize some important special cases of our definitions. Section III contains the main results of this paper, in particular the algorithms for solving certain classes of nested sums. In Sec. IV we give some examples for expansions of generalized hypergeometric functions, Appell functions, and the Kampé de Fériet function. As an application to higher loop multiscale integrals, we discuss the C-topology in Sec. IV D. In Appendix A we show that the algebraic structure of nested sums forms a Hopf algebra.[36,37] In Appendix B we briefly review the multiple polylogarithms of Goncharov.[5]

II. DEFINITION AND PROPERTIES OF NESTED SUMS

We define the Z-sums by

$$\begin{aligned} Z(n) &= \begin{cases} 1, & n \geqslant 0 \\ 0, & n < 0, \end{cases} \\ Z(n;m_1,\ldots,m_k;x_1,\ldots,x_k) &= \sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} Z(i-1;m_2,\ldots,m_k;x_2,\ldots,x_k), \end{aligned} \tag{1}$$

k is called the depth, $w = m_1 + \ldots + m_k$ the weight. An equivalent definition is given by

$$Z(n;m_1,\ldots,m_k;x_1,\ldots,x_k) = \sum_{n \geqslant i_1 > i_2 > \cdots > i_k > 0} \frac{x_1^{i_1}}{i_1^{m_1}} \cdots \frac{x_k^{i_k}}{i_k^{m_k}}. \tag{2}$$

In a similar way we define the S-sums by

$$\begin{aligned} S(n) &= \begin{cases} 1, & n > 0 \\ 0, & n \leqslant 0, \end{cases} \\ S(n;m_1,\ldots,m_k;x_1,\ldots,x_k) &= \sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} S(i;m_2,\ldots,m_k;x_2,\ldots,x_k). \end{aligned} \tag{3}$$

Once again an equivalent representation is given by

$$S(n;m_1,\ldots,m_k;x_1,\ldots,x_k) = \sum_{n \geqslant i_1 \geqslant i_2 \geqslant \cdots \geqslant i_k \geqslant 1} \frac{x_1^{i_1}}{i_1^{m_1}} \cdots \frac{x_k^{i_k}}{i_k^{m_k}}. \tag{4}$$

The S-sums are closely related to the Z-sums, the difference being the upper summation boundary for the nested sums: $(i-1)$ for Z-sums, i for S-sums. We introduce both Z-sums and S-sums, since some properties are more naturally expressed in terms of Z-sums while others are more naturally expressed in terms of S-sums. We can easily convert from the notation with Z-sums to the notation with S-sums and vice versa:

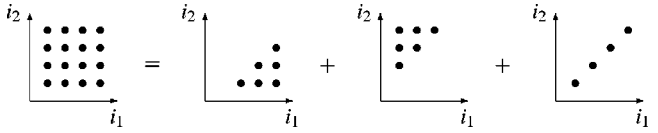


FIG. 1. Sketch of the proof for the multiplication of Z-sums. The sum over the square is replaced by the sum over the three regions on the right-hand side.

$$
\begin{aligned}
S(n;m_1,\ldots;x_1,\ldots)&=\sum_{i_1=1}^{n}\frac{x_1^{i_1}}{i_1^{m_1}}\sum_{i_2=1}^{i_1-1}\frac{x_2^{i_2}}{i_2^{m_2}}S(i_2;m_3,\ldots;x_3,\ldots)\\
&\quad+S(n;m_1+m_2,m_3,\ldots;x_1x_2,x_3,\ldots),\\
Z(n;m_1,\ldots;x_1,\ldots)&=\sum_{i_1=1}^{n}\frac{x_1^{i_1}}{i_1^{m_1}}\sum_{i_2=1}^{i_1}\frac{x_2^{i_2}}{i_2^{m_2}}Z(i_2-1;m_3,\ldots;x_3,\ldots)\\
&\quad-Z(n;m_1+m_2,m_3,\ldots;x_1x_2,x_3,\ldots).
\end{aligned}
\tag{5}
$$

The first formula allows to convert recursively an S-sum into a Z-sum. The second formula yields the conversion from a Z-sum to a S-sum. For example in terms of S-sums the Z-sum $Z(n;m_1,m_2,m_3,x_1,x_2,x_3)$ reads

$$
\begin{aligned}
Z(n;m_1,m_2,m_3,x_1,x_2,x_3)&=S(n;m_1,m_2,m_3,x_1,x_2,x_3)-S(n;m_1+m_2,m_3,x_1x_2,x_3)\\
&\quad-S(n;m_1,m_2+m_3,x_1,x_2x_3)+S(n;m_1+m_2+m_3,x_1x_2x_3).
\end{aligned}
\tag{6}
$$

Furthermore the Z-sums and the S-sums obey an algebra. A product of two Z-sums with the same upper summation limit can be written in terms of single Z-sums. A straightforward generalization of the results given by Vermaseren on the multiplication of harmonic sums yields[12]

$$
\begin{aligned}
&Z(n;m_1,\ldots,m_k;x_1,\ldots,x_k)Z(n;m_1',\ldots,m_l';x_1',\ldots,x_l')\\
&\quad=\sum_{i_1=1}^{n}\frac{x_1^{i_1}}{i_1^{m_1}}Z(i_1-1;m_2,\ldots,m_k;x_2,\ldots,x_k)Z(i_1-1;m_1',\ldots,m_l';x_1',\ldots,x_l')\\
&\quad+\sum_{i_2=1}^{n}\frac{x_1'^{i_2}}{i_2^{m_1'}}Z(i_2-1;m_1,\ldots,m_k;x_1,\ldots,x_k)Z(i_2-1;m_2',\ldots,m_l';x_2',\ldots,x_l')\\
&\quad+\sum_{i=1}^{n}\frac{(x_1x_1')^i}{i^{m_1+m_1'}}Z(i-1;m_2,\ldots,m_k;x_2,\ldots,x_k)Z(i-1;m_2',\ldots,m_l';x_2',\ldots,x_l').
\end{aligned}
\tag{7}
$$

Recursive application of Eq. (7) leads to single Z-sums. The proof of Eq. (7) follows immediately from

$$
\sum_{i=1}^{n}\sum_{j=1}^{n}a_{ij}=\sum_{i=1}^{n}\sum_{j=1}^{i-1}a_{ij}+\sum_{j=1}^{n}\sum_{i=1}^{j-1}a_{ij}+\sum_{i=1}^{n}a_{ii},
\tag{8}
$$

which is sketched in Fig. 1. Note that Eq. (7) directly translates into an algorithm for the multiplication of two Z-sums. Details on the implementation of this algorithm on a computer can be found for example in Ref. 12. We give an example for the product of two Z-sums:

$$Z(n;m_1,m_2;x_1,x_2)\times Z(n;m_3;x_3)=Z(n;m_1,m_2,m_3;x_1,x_2,x_3)+Z(n;m_1,m_3,m_2;x_1,x_3,x_2)$$
$$+Z(n;m_3,m_1,m_2;x_3,x_1,x_2)+Z(n;m_1,m_2+m_3;x_1,x_2x_3)$$
$$+Z(n;m_1+m_3,m_2;x_1x_3,x_2). \tag{9}$$

Note that the product conserves the weight. The Z-sums form actually a Hopf algebra. More details can be found in Appendix A.

The S-sums also obey an algebra. The basic formula reads

$$S(n;m_1,\ldots,m_k;x_1,\ldots,x_k)\times S(n;m_1',\ldots,m_l';x_1',\ldots,x_l')$$
$$=\sum_{i_1=1}^{n}\frac{x_1^{i_1}}{i_1^{m_1}}S(i_1;m_2,\ldots,m_k;x_2,\ldots,x_k)S(i_1;m_1',\ldots,m_l';x_1',\ldots,x_l')$$
$$+\sum_{i_2=1}^{n}\frac{x_1'^{i_2}}{i_2^{m_1'}}S(i_2;m_1,\ldots,m_k;x_1,\ldots,x_k)S(i_2;m_2',\ldots,m_l';x_2',\ldots,x_l')$$
$$-\sum_{i=1}^{n}\frac{(x_1x_1')^i}{i^{m_1+m_1'}}S(i;m_2,\ldots,m_k;x_2,\ldots,x_k)S(i;m_2',\ldots,m_l';x_2',\ldots,x_l'). \tag{10}$$

Note the minus sign in front of the last term compared to the corresponding formula for Z-sums.

Special cases. Z-sums and S-sums are generalizations of more known objects. We give here an overview of the most important special cases.

For $n=\infty$ the Z-sums are the multiple polylogarithms of Goncharov:[5]

$$Z(\infty;m_1,\ldots,m_k;x_1,\ldots,x_k)=\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1). \tag{11}$$

For $x_1=\cdots=x_k=1$ the definition reduces to the Euler–Zagier sums:[9,10]

$$Z(n;m_1,\ldots,m_k;1,\ldots,1)=Z_{m_1,\ldots,m_k}(n). \tag{12}$$

For $n=\infty$ and $x_1=\cdots=x_k=1$ the sum is a multiple ζ-value:[6]

$$Z(\infty;m_1,\ldots,m_k;1,\ldots,1)=\zeta(m_k,\ldots,m_1). \tag{13}$$

The S-sums reduce for $x_1=\cdots=x_k=1$ (and positive m_i) to harmonic sums:[12]

$$S(n;m_1,\ldots,m_k;1,\ldots,1)=S_{m_1,\ldots,m_k}(n). \tag{14}$$

The multiple polylogarithms of Goncharov contain as the notation already suggests as subsets the classical polylogarithms $\mathrm{Li}_n(x)$,[3] as well as Nielsen's generalized polylogarithms[4]

$$S_{n,p}(x)=\mathrm{Li}_{1,\ldots,1,n+1}(\underbrace{1,\ldots,1}_{p-1},x), \tag{15}$$

the harmonic polylogarithms of Remiddi and Vermaseren[7]

$$H_{m_1,\ldots,m_k}(x)=\mathrm{Li}_{m_k,\ldots,m_1}(\underbrace{1,\ldots,1}_{k-1},x) \tag{16}$$

and the two-dimensional harmonic polylogarithms introduced recently by Gehrmann and Remiddi.[8] The exact connection to the two-dimensional harmonic polylogarithms is shown in

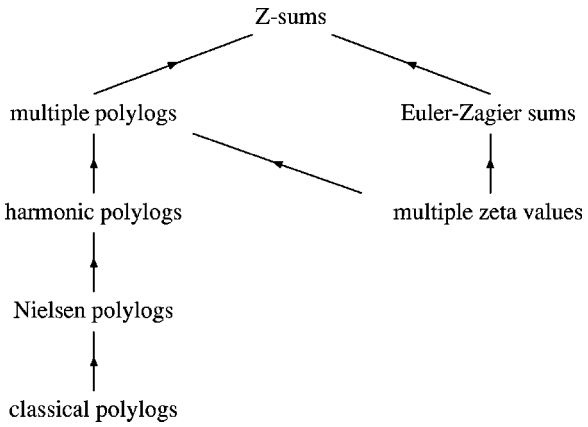


FIG. 2. The inheritance diagram for Z-sums shows the relations between the various special cases.

Appendix B together with a brief review of the multiple polylogarithms of Goncharov. Euler–Zagier sums and harmonic sums occur in the expansion of gamma functions: For positive integers n we have on the positive side

$$\Gamma(n+\epsilon)=\Gamma(1+\epsilon)\Gamma(n)(1+\epsilon Z_1(n-1)+\epsilon^2 Z_{11}(n-1)+\epsilon^3 Z_{111}(n-1) + \cdots +\epsilon^{n-1}Z_{11\ldots1}(n-1)). \tag{17}$$

On the negative side (again $n>0$) we have

$$\Gamma(-n+1+\epsilon)=\frac{\Gamma(1+\epsilon)}{\epsilon}\frac{(-1)^{n-1}}{\Gamma(n)}(1+\epsilon S_1(n-1)+\epsilon^2 S_{11}(n-1)+\epsilon^3 S_{111}(n-1)+\ldots). \tag{18}$$

The usefulness of the Z-sums lies in the fact that they interpolate between Goncharov's multiple polylogarithms and Euler–Zagier sums. In addition, the interpolation is compatible with the algebra structure. Figure 2 summarizes the relations between the various special cases.

III. ALGORITHMS

In this section we give the detailed algorithms which allow one to solve the ϵ-expansion of nested transcendental sums in terms of Z-sums or S-sums defined in Eqs. (1) and (3), respectively. By a transcendental sum we mean a sum over i of finite or infinite summation range involving the following objects.

(1) Fractions of the form

$$\frac{x^i}{(i+c)^m}, \tag{19}$$

where m is an integer, c a non-negative integer, and x a real number.

(2) Ratios of two gamma functions

$$\frac{\Gamma(i+a_1+b_1\epsilon)}{\Gamma(i+a_2+b_2\epsilon)}, \tag{20}$$

where a_1 and a_2 are integers.

(3) Z- and S-sums are also allowed to appear as subsums:

$$Z(i+c-1;m_1,\ldots;x_1,\ldots) \quad \text{or} \quad S(i+c';m_1,\ldots;x_1,\ldots). \tag{21}$$

The offsets c and c' are integers.

(4) We further allow these building blocks to occur also with index $(n-i)$, for example as in

$$S(n-i;m_1',\ldots;x_1',\ldots). \tag{22}$$

Here n denotes the upper summation limit.

(5) In addition binomials

$$\binom{n}{i} = \frac{n!}{i!(n-i)!} \tag{23}$$

may occur.

Some examples of sums which can be constructed from these building blocks are

$$\sum_{i=1}^{n} \frac{x^i}{(i+4)^3} \frac{y^i}{(i+2)^8} \frac{\Gamma(i+1+\epsilon)}{\Gamma(i+2+3\epsilon)}, \quad \sum_{i=1}^{\infty} x^i \frac{\Gamma(i+a\epsilon)}{\Gamma(i+1-c\epsilon)} \frac{\Gamma(i+b\epsilon)}{\Gamma(i+1)}. \tag{24}$$

There are some simplifications, which can be done immediately: Partial fractioning is used to reduce a product for $c_1 \neq c_2$,

$$\frac{x_1^i}{(i+c_1)^{m_1}} \frac{x_2^i}{(i+c_2)^{m_2}} = \frac{1}{c_2-c_1}\left[\frac{x_1^i}{(i+c_1)^{m_1}} \frac{x_2^i}{(i+c_2)^{m_2-1}} - \frac{x_1^i}{(i+c_1)^{m_1-1}} \frac{x_2^i}{(i+c_2)^{m_2}}\right], \tag{25}$$

to terms which involve only the first factor or only the second one, but not both.

Ratios of two gamma functions as in Eq. (20) are first reduced to the form $\Gamma(i+b_1\epsilon)/\Gamma(i+b_2\epsilon)$ with the help of the identity $\Gamma(x+1)=x\Gamma(x)$. They are then expanded in ϵ using Eq. (17). To invert the power series which is obtained in the denominator the formula

$$\begin{aligned}&(1+\epsilon Z_1(n-1)+\epsilon^2 Z_{11}(n-1)+\epsilon^3 Z_{111}(n-1)+\cdots+\epsilon^{n-1} Z_{11\ldots1}(n-1))^{-1}\\ &\quad = 1-\epsilon S_1(n-1)+\epsilon^2 S_{11}(n-1)-\epsilon^3 S_{111}(n-1)+\cdots\end{aligned} \tag{26}$$

is useful to speed up the computation on a computer.

There are also some basic operations involving Z- or S-sums. First of all we can easily convert between the two notations, using Eq. (5). Furthermore we would like to be able to relate the Z-sum $Z(n+c-1,\ldots)$ to $Z(n-1,\ldots)$ or the S-sum $S(n+c,\ldots)$ to $S(n,\ldots)$, where $c>0$ is a fixed number. This can easily be done with the help of the following formulas:

$$\begin{aligned}Z(n+c-1;m_1,\ldots;x_1,\ldots) &= Z(n-1;m_1,\ldots;x_1,\ldots)+\sum_{j=0}^{c-1} x_1^j \frac{x_1^n}{(n+j)^{m_1}}\\ &\quad \times Z(n-1+j;m_2,\ldots;x_2,\ldots),\\ S(n+c;m_1,\ldots;x_1,\ldots) &= S(n;m_1,\ldots;x_1,\ldots)+\sum_{j=1}^{c} x_1^j \frac{x_1^n}{(n+j)^{m_1}} S(n+j;m_2,\ldots;x_2,\ldots).\end{aligned} \tag{27}$$

The Z- or S-sums appearing in the last term have a reduced depth and the problem can be solved recursively.

Another situation which appears quite often is the product of two sums. If the upper summation limits of the two sums differ by some integer c we first synchronize them with the help of Eq. (27). For sums with equal upper summation limit one may use the algebra Eq. (7) or Eq. (10) to convert the product into single sums of higher weight.

Furthermore we can bring Z-sums and S-sums to a standard form by eliminating letters with negative degrees, that is positive powers of i. In general, these cases are easy to handle. We illustrate this for S-sums. We consider $S(n;-m_1,m_2,\ldots;x_1,x_2,\ldots)$, write out the outermost sum of the S-function, and then interchange the order of summation:

$$S(n;-m_1,m_2,\ldots;x_1,x_2,\ldots)=\sum_{i_2=1}^{n}\frac{x_2^{i_2}}{i_2^{m_2}}S(i_2;m_3,\ldots)\sum_{i_1=i_2}^{n}i_1^{m_1}x_1^{i_1}. \tag{28}$$

The inner sum can be evaluated for any given weight analytically. Subsequently the outer sum can be done with Eq. (3). If a negative weight occurs inside a sum, Eq. (28) is applied to the subsum starting from the negative weight.

If a binomial appears in the sum, this sum may be written as a conjugation. To any function $f(n)$ of an integer variable n one defines the conjugated function $C\circ f(n)$ as the following sum:[12]

$$C\circ f(n)=-\sum_{i=1}^{n}\binom{n}{i}(-1)^i f(i). \tag{29}$$

Conjugation satisfies the following two properties:

$$C\circ 1=1, \tag{30}$$

$$C\circ C\circ f(n)=f(n), \tag{31}$$

which can be easily verified.

We classify four types of transcendental sums, which are dealt with in the algorithms A–D.

(1) Sum over i involving only $Z(i-1;\ldots)$ (type A).
(2) Sum over i involving both $Z(i-1;\ldots)$ and $Z(n-i-1;\ldots)$ (type B).
(3) Sum over i involving $S(i;\ldots)$ and a binomial (type C).
(4) Sum over i involving both $S(i;\ldots)$, $S(n-i;\ldots)$ and a binomial (type D).

Many of the algorithms use a recursion. They relate a given problem to a simpler one, either with a reduced depth or weight of the Z-sums or S-sums involved. In these cases we only give one step in the recursion.

The algorithms presented in this paper are all suited for programming in a computer algebra system like GINAC,[38] FORM,[39] or the commercial ones like MATHEMATICA or MAPLE. Implementations within the GINAC framework and in FORM along the lines of Ref. 12 are in preparation or have been published elsewhere.[40]

A. Algorithm A

Here we consider sums of the form

$$\sum_{i=1}^{n}\frac{x^i}{(i+c)^m}\frac{\Gamma(i+a_1+b_1\epsilon)}{\Gamma(i+c_1+d_1\epsilon)}\cdots\frac{\Gamma(i+a_k+b_k\epsilon)}{\Gamma(i+c_k+d_k\epsilon)}Z(i+o-1,m_1,\ldots,m_l,x_1,\ldots,x_l) \tag{32}$$

and show how to reduce them to Z-sums. We assume that all a_j and c_j are integers, c is assumed to be a non-negative integer and o should be an integer. The upper summation limit is allowed to be infinity.

After expanding the gamma functions and synchronizing the subsum $Z(i+o-1,m_1,\ldots)$ the problem is reduced to sums of the form

$$\sum_{i=1}^{n}\frac{x^i}{(i+c)^m}Z(i-1,\ldots) \tag{33}$$

with $c \geqslant 0$. It remains to reduce the offset c to zero. If the depth of the subsum is zero, we have

$$\sum_{i=1}^{n} \frac{x^i}{(i+c)^m} = \frac{1}{x} \sum_{i=1}^{n} \frac{x^i}{(i+c-1)^m} - \frac{1}{c^m} + \frac{x^n}{(n+c)^m}. \tag{34}$$

The last term contributes only if n is not equal to infinity. If the depth of the subsum is not equal to zero, we have

$$\sum_{i=1}^{n} \frac{x^i}{(i+c)^m} Z(i-1,\ldots) = \frac{1}{x} \sum_{i=1}^{n} \frac{x^i}{(i+c-1)^m} Z(i-1,\ldots) - \sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m} \frac{x_1^i}{i^{m_1}} Z(i-1,m_2,\ldots) + \frac{x^n}{(n+c)^m} Z(n-1,\ldots). \tag{35}$$

Note that the third term only contributes if n is not equal to infinity. Finally we arrive at

$$\sum_{i=1}^{n} \frac{x^i}{i^m} Z(i-1,\ldots), \tag{36}$$

which is again a Z-sum. If the upper summation limit n equals infinity this sum yields immediately a multiple polylogarithm according to Eq. (11). In the special case where n equals infinity and the subsum is an Euler–Zagier sum we obtain a harmonic polylogarithm according to Eq. (16).

B. Algorithm B

Here we consider sums of the form

$$\begin{aligned} &\sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m} \frac{\Gamma(i+a_1+b_1\epsilon)}{\Gamma(i+c_1+d_1\epsilon)} \cdots \frac{\Gamma(i+a_k+b_k\epsilon)}{\Gamma(i+c_k+d_k\epsilon)} Z(i+o-1,m_1,\ldots,m_l,x_1,\ldots,x_l) \\ &\quad \times \frac{y^{n-i}}{(n-i+c')^{m'}} \frac{\Gamma(n-i+a_1'+b_1'\epsilon)}{\Gamma(n-i+c_1'+d_1'\epsilon)} \cdots \frac{\Gamma(n-i+a_{k'}'+b_{k'}'\epsilon)}{\Gamma(n-i+c_{k'}'+d_{k'}'\epsilon)} \\ &\quad \times Z(n-i+o'-1,m_1',\ldots,m_{l'}',x_1',\ldots,x_{l'}') \end{aligned} \tag{37}$$

and show how to reduce them to Z-sums. Here, all a_j, a_j', c_j and c_j' should be integers, c, c' should be non-negative integers and o, o' should be integers. Note that the upper summation limit is $(n-1)$. The upper summation limit should not be infinity.

Using the expansion of the gamma functions and the synchronization of the subsums, we immediately obtain sums of the form

$$\sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m} Z(i-1,m_1,\ldots) \frac{y^{n-i}}{(n-i+c')^{m'}} Z(n-i-1,m_1',\ldots). \tag{38}$$

Partial fractioning [and a change of the summation index $i \to n-i$ in sums involving the fraction with $(n-i+c')$] reduces these sums further to sums of the type

$$\sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m} Z(i-1,m_1,\ldots) Z(n-i-1,m_1',\ldots). \tag{39}$$

If the depth of $Z(n-i-1,m_1',\ldots)$ is zero, we have a sum of type A with upper summation index $(n-1)$:

$$\sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m} Z(i-1,m_1,\dots). \tag{40}$$

Otherwise we can rewrite Eq. (39) as

$$\sum_{j=1}^{n-1} \left[\sum_{i=1}^{j-1} \frac{x^i}{(i+c)^m} Z(i-1,m_1,\dots) \frac{x_1'^{j-i}}{(j-i)^{m_1'}} Z(j-i-1,m_2',\dots) \right] \tag{41}$$

and use recursion. The inner sum is again of type B, but with a reduced depth, such that the recursion will finally terminate.

C. Algorithm C

Here we consider sums of the form

$$-\sum_{i=1}^{n} \binom{n}{i} (-1)^i \frac{x^i}{(i+c)^m} \frac{\Gamma(i+a_1+b_1\epsilon)}{\Gamma(i+c_1+d_1\epsilon)} \cdots \frac{\Gamma(i+a_k+b_k\epsilon)}{\Gamma(i+c_k+d_k\epsilon)} S(i+o,m_1,\dots,m_l,x_1,\dots,x_l), \tag{42}$$

where a_j and c_j are integers, c is a non-negative integer, and o is an integer. The upper summation limit should not be infinity. These sums cannot be reduced to Z-sums with upper summation limit n alone. However, they can be reduced to Z-sums with upper summation limit n and multiple polylogarithms (which are Z-sums to infinity).

Again, we expand the gamma functions and synchronize the subsum. It is therefore sufficient to consider sums of the form

$$-\sum_{i=1}^{n} \binom{n}{i} (-1)^i \frac{x^i}{(i+c)^m} S(i,\dots) \tag{43}$$

with $c \geqslant 0$. To reduce the offset c to zero we rewrite the sum as

$$\left(-\frac{1}{x}\right) \frac{1}{n+1} (-1) \sum_{i=1}^{n+1} \binom{n+1}{i} (-1)^i \frac{x^i}{(i+c-1)^m} iS(i-1,\dots). \tag{44}$$

Repeated application of the above-given relation yields sums of the form

$$-\sum_{i=1}^{n} \binom{n}{i} (-1)^i \frac{x^i}{i^m} S(i,\dots). \tag{45}$$

If m is negative we rewrite Eq. (45) as

$$-nx(-1) \sum_{i=1}^{n-1} \binom{n-1}{i} (-1)^i \frac{x^i}{(i+1)^{m+1}} S(i+1,\dots) + nxS(1,\dots). \tag{46}$$

We can therefore assume that m is a non-negative number. Furthermore, due to Eq. (28) we may assume that in the S-sum $S(i;m_1,\dots;x_1,\dots)$ no m_j is negative and that if some m_j is zero, then the corresponding x_j is not equal to 1. The sum $S(i,\dots)$ is then rewritten as

$$
\begin{aligned}
S(i;m_1,\ldots,m_k;x_1,\ldots,x_k) = {} & S(N;m_1,\ldots,m_k;x_1,\ldots,x_k) \\
& - S(N;m_2,\ldots,m_k;x_2,\ldots,x_k)\times\left(\sum_{i_1=i+1}^{N}\frac{x_1^{i_1}}{i_1^{m_1}}\right) \\
& + S(N;m_3,\ldots,m_k;x_3,\ldots,x_k)\times\left(\sum_{i_1=i+1}^{N}\sum_{i_2=i_1+1}^{N}\frac{x_1^{i_1}}{i_1^{m_1}}\frac{x_2^{i_2}}{i_2^{m_2}}\right) \\
& - \ldots + (-1)^k\left(\sum_{i_1=i+1}^{N}\sum_{i_2=i_1+1}^{N}\cdots\sum_{i_k=i_{k-1}+1}^{N}\frac{x_1^{i_1}}{i_1^{m_1}}\frac{x_2^{i_2}}{i_2^{m_2}}\cdots\frac{x_k^{i_k}}{i_k^{m_k}}\right).
\end{aligned}
\tag{47}
$$

The proof of Eq. (47) is not too complicated and consists in repeated application of the identity

$$
\sum_{i=1}^{n}\sum_{j=1}^{i}a_{ij} = \sum_{i=1}^{N}\sum_{j=1}^{i}a_{ij} - \sum_{i=n+1}^{N}\sum_{j=1}^{N}a_{ij} + \sum_{i=n+1}^{N}\sum_{j=i+1}^{N}a_{ij}. \tag{48}
$$

Equation (47) holds for any N and in particular we may take $N=\infty$ in the end. Each term is then a product of an S-sum at infinity and a sum of a new type. The S-sum at infinity is converted to a Z-sum at infinity and expressed in terms of multiple polylogarithms. We now deal with sums of the form

$$
-\sum_{i=1}^{n}\binom{n}{i}(-1)^i\frac{x_0^i}{i^{m_0}}\sum_{i_1=i+1}^{N}\sum_{i_2=i_1+1}^{N}\cdots\sum_{i_k=i_{k-1}+1}^{N}\frac{x_1^{i_1}}{i_1^{m_1}}\frac{x_2^{i_2}}{i_2^{m_2}}\cdots\frac{x_k^{i_k}}{i_k^{m_k}}. \tag{49}
$$

We introduce raising and lowering operators as follows:

$$
\begin{aligned}
(\mathbf{x}^+)^m\cdot 1 &= \frac{1}{m!}\ln^m(x), \\
\mathbf{x}^+\cdot f(x) &= \int_0^x\frac{dx'}{x'}f(x'), \\
\mathbf{x}^-\cdot f(x) &= x\frac{d}{dx}f(x).
\end{aligned}
\tag{50}
$$

It is understood that in the second line only functions which are integrable at $x=0$ are considered. We see that $\mathbf{x}^-$ is the inverse to $\mathbf{x}^+$, e.g. $\mathbf{x}^-\mathbf{x}^+=\mathrm{id}$. However $\mathbf{x}^+\mathbf{x}^-=\mathrm{id}$ holds only if applied to nontrivial sums. For the trivial sum we have $\mathbf{x}^+\mathbf{x}^-Z(n)=0$.

With the help of the raising operators Eq. (49) may be rewritten as

$$
\begin{aligned}
& (\mathbf{x_k}^+)^{m_k}(\mathbf{x_{k-1}}^+)^{m_{k-1}}\cdots(\mathbf{x_1}^+)^{m_1}(\mathbf{x_0}^+)^{m_0}(-1)\sum_{i=1}^{n}\binom{n}{i}(-x_0)^i \\
& \quad\times\sum_{i_1=i+1}^{N}\sum_{i_2=i_1+1}^{N}\cdots\sum_{i_k=i_{k-1}+1}^{N}x_1^{i_1}x_2^{i_2}\ldots x_k^{i_k}.
\end{aligned}
\tag{51}
$$

It may happen that some x_i's are equal to one. In this case we first calculate the sum for arbitrary x_i's and then take the limit $x_i\to 1$. Some care has to be taken for the double limit $x\to 1$ and $N\to\infty$. The order is as follows: First all limits $x\to 1$ are taken, then the limit $N\to\infty$ in Eq. (47) is performed.

The sums in Eq. (51) can be performed with the help of the geometric series

$$\sum_{i=n+1}^{N} x^i = \frac{x}{1-x}x^n - \frac{x}{1-x}x^N. \tag{52}$$

It is evident that if we do not have to take the limit $x\to 1$ we can immediately neglect the second term. Also in the case $x=1$ the second term can be neglected. It gives rise to terms of the form

$$(\mathbf{x}^+)^m \frac{x}{1-x}x^N = \sum_{i=N+1}^{\infty} \frac{x^i}{i^m}. \tag{53}$$

On the right-hand side the limit $x\to 1$ may safely be performed and the resulting sum gives a vanishing contribution in the limit $N\to\infty$.

Performing the sums in Eq. (51) we therefore only have to consider expressions of the form

$$(\mathbf{x_k}^+)^{m_k}(\mathbf{x_{k-1}}^+)^{m_{k-1}}\cdots(\mathbf{x_1}^+)^{m_1}(\mathbf{x_0}^+)^{m_0}\frac{x_k}{1-x_k}\frac{x_{k-1}x_k}{1-x_{k-1}x_k}\cdots\frac{x_1\cdots x_k}{1-x_1\cdots . x_k}$$
$$\times[1-(1-x_0x_1\cdots x_k)^n]. \tag{54}$$

We then perform succesively the integrations corresponding to the raising operators. The basic formulas are

$$\mathbf{x_1}^+[1-(1-x_1x_2)^n] = \sum_{i=1}^{n}\frac{1}{i}[1-(1-x_1x_2)^i],$$

$$\mathbf{x_1}^+\frac{x_1x_2}{1-x_1x_2}[1-(1-x_0x_1x_2)^n] = -(1-x_0)^n\sum_{i=1}^{n}\frac{1}{i}\left(\frac{1}{1-x_0}\right)^i[1-(1-x_0x_1x_2)^i]$$
$$+(1-(1-x_0)^n)\sum_{i=1}^{N}\frac{(x_1x_2)^i}{i}$$
$$+\mathbf{x_1}^+\frac{x_1x_2}{1-x_1x_2}(x_1x_2)^N(1-(1-x_0)^n), \tag{55}$$

$$\mathbf{x_1}^+\frac{x_1x_2}{1-x_1x_2}[1-(1-x_1x_2)^n] = -\frac{1}{n}[1-(1-x_1x_2)^n]+\sum_{i=1}^{N}\frac{(x_1x_2)^i}{i}+(\mathbf{x_1}^+)\frac{x_1x_2}{1-x_1x_2}(x_1x_2)^N.$$

We use the first formula to reduce m_0 in Eq. (54) to zero:

$$\sum_{i=1}^{n}\frac{1}{i}(x_k^+)^{m_k}\cdots(x_1^+)^{m_1}(x_0^+)^{m_0-1}\frac{x_k}{1-x_k}\frac{x_{k-1}x_k}{1-x_{k-1}x_k}\cdots\frac{x_1\cdots x_k}{1-x_1\cdots x_k}[1-(1-x_0x_1\cdots x_k)^i]. \tag{56}$$

In the following we may therefore assume $m_0=0$ in Eq. (54). If $m_0=0$, $m_1>0$ and $x_0\neq 1$ we obtain for Eq. (54)

$$-(1-x_0)^n\sum_{i=1}^{\infty}\frac{1}{i}\left(\frac{1}{1-x_0}\right)^i(x_k^+)^{m_k}\cdots((x_0x_1)^+)^{m_1-1}\frac{x_k}{1-x_k}\frac{x_{k-1}x_k}{1-x_{k-1}x_k}\cdots\frac{x_2\cdots x_k}{1-x_2\cdots x_k}$$
$$\times[1-(1-(x_0x_1)\cdots x_k)^i]+(1-(1-x_0)^n)\sum_{i=1}^{N}\frac{x_1^i}{i^{m_1}}\sum_{i_2=i+1}^{N}\cdots\sum_{i_k=i_{k-1}+1}^{N}\frac{x_2^{i_2}}{i_2^{m_2}}\cdots\frac{x_k^{i_k}}{i_k^{m_k}}. \tag{57}$$

Here we neglected terms of the form (53). In the case $m_0=0$, $m_1>0$, and $x_0=1$ we use the third formula of Eq. (55). Again we may neglect contributions of the form (53). Doing so we obtain

$$-\frac{1}{n}(x_k^+)^{m_k}\cdots(x_1^+)^{m_1-1}\frac{x_k}{1-x_k}\frac{x_{k-1}x_k}{1-x_{k-1}x_k}\cdots\frac{x_2\cdots x_k}{1-x_2\cdots x_k}[1-(1-x_1\cdots x_k)^n]$$
$$+\sum_{i=1}^{N}\frac{x_1^i}{i^{m_1}}\sum_{i_2=i+1}^{N}\cdots\sum_{i_k=i_{k-1}+1}^{N}\frac{x_2^{i_2}}{i_2^{m_2}}\cdots\frac{x_k^{i_k}}{i_k^{m_k}}. \tag{58}$$

It remains to treat the last term to complete the recursion. The last term introduces a sum of the type

$$\sum_{i_1=n+1}^{N}\cdots\sum_{i_k=i_{k-1}+1}^{N}\frac{x_1^{i_1}}{i_1^{m_1}}\cdots\frac{x_k^{i_k}}{i_k^{m_k}}. \tag{59}$$

Using the inverse formula to Eq. (47)

$$\sum_{i_1=n+1}^{N}\cdots\sum_{i_k=i_{k-1}+1}^{N}\frac{x_1^{i_1}}{i_1^{m_1}}\cdots\frac{x_k^{i_k}}{i_k^{m_k}}$$
$$=(-1)^k S(n;m_1,\ldots,m_k;x_1,\ldots,x_k)$$
$$-(-1)^k S(N;m_1,\ldots,m_k;x_1,\ldots,x_k)+(-1)^k S(N;m_2,\ldots,m_k;x_2,\ldots,x_k)$$
$$\times\sum_{i_1=n+1}^{N}\frac{x_1^{i_1}}{i_1^{m_1}}-\cdots+(-1)^k S(N;m_k;x_k)\sum_{i_1=n+1}^{N}\cdots\sum_{i_{k-1}=i_{k-2}+1}^{N}\frac{x_1^{i_1}}{i_1^{m_1}}\cdots\frac{x_{k-1}^{i_{k-1}}}{i_{k-1}^{m_{k-1}}}, \tag{60}$$

this sum is easily related to S-sums with upper summation limit n and (after taking the limit $N\to\infty$) to multiple polylogarithms.

If $m_0=0$, $m_1=0$, and $x_1\neq 1$ we rewrite Eq. (54) as

$$-\frac{1}{1-x_1}(x_k^+)^{m_k}\cdots(x_3^+)^{m_3}((x_2x_1)^+)^{m_2}\frac{x_k}{1-x_k}\cdots\frac{x_3\cdots x_k}{1-x_3\cdots x_k}\frac{(x_1x_2)x_3\cdots x_k}{1-(x_1x_2)x_3\cdots x_k}$$
$$\times[1-(1-x_0(x_1x_2)x_3\cdots x_k)^i]+\frac{x_1}{1-x_1}(x_k^+)^{m_k}\cdots(x_2^+)^{m_2}\frac{x_k}{1-x_k}\cdots\frac{x_2x_3\cdots x_k}{1-x_2x_3\cdots x_k}$$
$$\times[1-(1-(x_0x_1)x_2x_3\cdots x_k)^i]. \tag{61}$$

The case $m_0=0$, $m_1=0$, and $x_1=1$ has to be excluded. However, with an appropriate choice of the standard form for S-sums [cf. Eq. (28)] this case never occurs.

D. Algorithm D

Here we consider sums of the form

$$-\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i\frac{x^i}{(i+c)^m}\frac{\Gamma(i+a_1+b_1\epsilon)}{\Gamma(i+c_1+d_1\epsilon)}\cdots\frac{\Gamma(i+a_k+b_k\epsilon)}{\Gamma(i+c_k+d_k\epsilon)}\times S(i+o,m_1,\ldots,m_l,x_1,\ldots,x_l)$$
$$\times\frac{y^{n-i}}{(n-i+c')^{m'}}\frac{\Gamma(n-i+a_1'+b_1'\epsilon)}{\Gamma(n-i+c_1'+d_1'\epsilon)}\cdots\frac{\Gamma(n-i+a_{k'}'+b_{k'}'\epsilon)}{\Gamma(n-i+c_{k'}'+d_{k'}'\epsilon)}$$
$$\times S(n-i+o',m_1',\ldots,m_{l'}',x_1',\ldots,x_{l'}'). \tag{62}$$

Here, all a_j, a_j', c_j, and c_j' are integers, c, c', are nonnegative integers, and o, o' are integers. Note that the upper summation limit is $(n-1)$. The upper summation limit should not be infinity. As in the case of sums of type C, we cannot relate these sums to Z-sums with upper summation limit $(n-1)$ alone, but we can reduce them to Z-sums with upper summation limit $(n-1)$ and multiple polylogarithms (which are Z-sums to infinity).

After the expansion of the gamma functions and the synchronization of the subsums we have sums of the form

$$-\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i\frac{x^i}{(i+c)^m}S(i,m_1,\dots)\frac{y^{n-i}}{(n-i+c')^{m'}}S(n-i,m_1',\dots). \tag{63}$$

Partial fractioning leads to

$$-\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i\frac{x^i}{(i+c)^m}S(i,m_1,\dots)S(n-i,m_1',\dots) \tag{64}$$

with $c\geqslant 0$. In order to reduce the offset c to zero one rewrites Eq. (64) as

$$\left(-\frac{1}{x}\right)\frac{1}{n+1}(-1)\sum_{i=1}^{n+1-1}\binom{n+1}{i}(-1)^i\frac{x^i}{(i+c-1)^m}iS(i-1,\dots)S(n+1-i,m_1',\dots). \tag{65}$$

We arrive at sums of the form

$$-\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i\frac{x^i}{i^m}S(i,m_1,\dots)S(n-i,m_1',\dots). \tag{66}$$

If the depth of $S(n-i,m_1',\dots)$ is zero, we have a sum of type C:

$$-\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i\frac{x^i}{i^m}S(i,m_1,\dots)=-\sum_{i=1}^{n}\binom{n}{i}(-1)^i\frac{x^i}{i^m}S(i,m_1,\dots)+\frac{(-x)^n}{n^m}S(n,m_1,\dots). \tag{67}$$

Otherwise, we first reduce m to zero. For $m>0$ we rewrite Eq. (66) as

$$\sum_{j=1}^{n}\frac{1}{j}\left[(-1)\sum_{i=1}^{j-1}\binom{j}{i}(-1)^i\frac{x^i}{i^{m-1}}S(i,m_1,\dots)S(j-i,m_1',\dots)\right]$$
$$+\sum_{j=1}^{n}\frac{1}{j}\left[(-1)\sum_{i=1}^{j-1}\binom{j}{i}(-1)^i\frac{x^i}{i^m}S(i,m_1,\dots)\frac{x_1'^{j-i}}{(j-i)^{m_1'-1}}S(j-i,m_2',\dots)\right]. \tag{68}$$

For $m<0$ we rewrite Eq. (66) as

$$-nx(-1)\sum_{i=1}^{n-2}\binom{n-1}{i}(-1)^i\frac{x^i}{(i+1)^{m+1}}S(i+1,m_1,\dots)S(n-1-i,m_1',\dots)$$
$$+nxS(1,m_1,\dots)S(n-1,m_1',\dots). \tag{69}$$

Having reduced m to zero we arrive at sums of the form

$$-\sum_{i=1}^{n-1}\binom{n}{i}(-1)^ix^iS(i,m_1,\dots)S(n-i,m_1',\dots). \tag{70}$$

For $x\neq 1$ we obtain after some algebra

$$-\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i x^i S(i,m_1,\ldots)S(n-i,m_1',\ldots)=(1-x)^n\sum_{j=1}^{n}\frac{1}{j}\left(\frac{1}{1-x}\right)^j(-1)\sum_{i=1}^{j-1}\binom{j}{i}$$
$$\times(-1)^i\frac{(xx_1)^i}{i^{m_1-1}}S(i,m_2,\ldots)S(j-i,m_1',\ldots)+(1-x)^n\sum_{j=1}^{n}\frac{1}{j}\left(\frac{1}{1-x}\right)^j(-1)\sum_{i=1}^{j-1}\binom{j}{i}$$
$$\times(-1)^i x^i S(i,m_1,\ldots)\frac{x_1'^{j-i}}{(n-i)^{m_1'-1}}S(j-i,m_2',\ldots), \tag{71}$$

where the original problem is reduced to one of the same type but with lower weight. In the case $x=1$ the right-hand side of Eq. (71) reduces to

$$\frac{1}{n}(-1)\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i\frac{x_1^i}{i^{m_1-1}}S(i,m_2,\ldots)S(n-i,m_1',\ldots)+\frac{1}{n}(-1)\sum_{i=1}^{n-1}\binom{n}{i}$$
$$\times(-1)^i S(i,m_1,\ldots)\frac{x_1'^{n-i}}{(n-i)^{m_1'-1}}S(n-i,m_2',\ldots). \tag{72}$$

Again, the original problem is reduced to one of the same type but with lower weight. The above-mentioned algorithm thus yields a recursion to treat sums of type D.

IV. APPLICATIONS

The algorithms given in this paper can be used for the expansion of higher transcendental functions around integer values of their indices, where the expansion parameter occurs in the Pochhammer symbols. In this section we give a few examples. Additionally, we illustrate the applicability of the algorithms for nested sums to the calculation of loop integrals, in particular to integrals with several scales. As an example, we discuss the C-topology and show that the integral can be written as a nested sum of the type previously discussed.

A. Generalized hypergeometric functions

The generalized hypergeometric functions are defined by[1,2]

$${}_{J+1}F_J(a_1,\ldots,a_{J+1};b_1,\ldots,b_J;x)=\sum_{n=0}^{\infty}\frac{(a_1)_n\cdots(a_{J+1})_n}{(b_1)_n\cdots(b_J)_n}\frac{x^n}{n!}, \tag{73}$$

where $(a)_n=\Gamma(n+a)/\Gamma(a)$ denotes a Pochhammer symbol. These functions can be rewritten as

$${}_{J+1}F_J(a_1,\ldots,a_{J+1};b_1,\ldots,b_J;x)$$
$$=1+\frac{\Gamma(b_1)\cdots\Gamma(b_J)}{\Gamma(a_1)\cdots\Gamma(a_{J+1})}\sum_{i=1}^{\infty}x^i\frac{\Gamma(i+a_1)}{\Gamma(i+b_1)}\cdots\frac{\Gamma(i+a_J)}{\Gamma(i+b_J)}\frac{\Gamma(i+a_{J+1})}{\Gamma(i+1)} \tag{74}$$

and fall therefore into the category of transcendental sums of type A. We give a few examples obtained using the algorithms given in Sec. III A:

$${}_2F_1(a\epsilon,b\epsilon;1-c\epsilon;x)=1+ab\,\mathrm{Li}_2(x)\epsilon^2+ab(c\,\mathrm{Li}_3(x)+(a+b+c)\,\mathrm{S}_{1,2}(x))\epsilon^3+O(\epsilon^4),$$
$${}_2F_1(1,-\epsilon;1-\epsilon;x)=1+\ln(1-x)\epsilon-\mathrm{Li}_2(x)\epsilon^2-\mathrm{Li}_3(x)\epsilon^3-\mathrm{Li}_4(x)\epsilon^4$$
$$-\mathrm{Li}_5(x)\epsilon^5-\mathrm{Li}_6(x)\epsilon^6-\mathrm{Li}_7(x)\epsilon^7+O(\epsilon^8), \tag{75}$$

$$
\begin{aligned}
&{}_3F_2(-2\epsilon,-2\epsilon,1-\epsilon;1-2\epsilon,1-2\epsilon;x)\\
&\quad=1+4\,\mathrm{Li}_2(x)\epsilon^2+(12\,\mathrm{Li}_3(x)-4S_{1,2}(x))\epsilon^3+(32\,\mathrm{Li}_4(x)\\
&\quad\quad+4S_{1,3}(x)-12S_{2,2}(x))\epsilon^4+(80\,\mathrm{Li}_5(x)-4S_{1,4}(x)\\
&\quad\quad+12S_{2,3}(x)-32S_{3,2}(x))\epsilon^5+O(\epsilon^6),
\end{aligned}
\tag{76}
$$

which all agree with known results in the literature.[41,42]

B. Appell functions

The first Appell function is defined by[43,2]

$$
F_1(a,b_1,b_2;c;x_1,x_2)=\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\frac{(a)_{m_1+m_2}(b_1)_{m_1}(b_2)_{m_2}}{(c)_{m_1+m_2}}\frac{x_1^{m_1}}{m_1!}\frac{x_2^{m_2}}{m_2!}.
\tag{77}
$$

It can be rewritten as

$$
\begin{aligned}
F_1(a,b_1,b_2;c;x_1,x_2)=1&+\frac{\Gamma(c)}{\Gamma(a)\Gamma(b_1)}\sum_{i=1}^{\infty}x_1^i\frac{\Gamma(i+a)\Gamma(i+b_1)}{\Gamma(i+c)\Gamma(i+1)}\\
&+\frac{\Gamma(c)}{\Gamma(a)\Gamma(b_2)}\sum_{i=1}^{\infty}x_2^i\frac{\Gamma(i+a)\Gamma(i+b_2)}{\Gamma(i+c)\Gamma(i+1)}\\
&+\frac{\Gamma(c)}{\Gamma(a)\Gamma(b_1)\Gamma(b_2)}\sum_{n=1}^{\infty}\frac{\Gamma(n+a)}{\Gamma(n+c)}\sum_{i=1}^{n-1}x_1^i\frac{\Gamma(i+b_1)}{\Gamma(i+1)}x_2^{n-i}\frac{\Gamma(n-i+b_2)}{\Gamma(n-i+1)}.
\end{aligned}
\tag{78}
$$

The inner sum of the last term is of type B. The first Appell function can therefore be expanded with the help of algorithms A and B.

The second Appell function is defined by[43,2]

$$
F_2(a,b_1,b_2;c_1,c_2;x_1,x_2)=\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\frac{(a)_{m_1+m_2}(b_1)_{m_1}(b_2)_{m_2}}{(c_1)_{m_1}(c_2)_{m_2}}\frac{x_1^{m_1}}{m_1!}\frac{x_2^{m_2}}{m_2!}.
\tag{79}
$$

It can be rewritten as

$$
\begin{aligned}
&F_2(a,b_1,b_2;c_1,c_2;x_1,x_2)\\
&\quad=1+\frac{\Gamma(c_1)}{\Gamma(a)\Gamma(b_1)}\sum_{i=1}^{\infty}x_1^i\frac{\Gamma(i+a)\Gamma(i+b_1)}{\Gamma(i+c_1)\Gamma(i+1)}+\frac{\Gamma(c_2)}{\Gamma(a)\Gamma(b_2)}\sum_{i=1}^{\infty}x_2^i\frac{\Gamma(i+a)\Gamma(i+b_2)}{\Gamma(i+c_2)\Gamma(i+1)}\\
&\quad\quad-\frac{\Gamma(c_1)\Gamma(c_2)}{\Gamma(a)\Gamma(b_1)\Gamma(b_2)}\sum_{n=1}^{\infty}\frac{\Gamma(n+a)}{\Gamma(n+1)}(-1)\sum_{i=1}^{n-1}\binom{n}{i}\\
&\quad\quad\times(-1)^i(-x_1)^i\frac{\Gamma(i+b_1)}{\Gamma(i+c_1)}x_2^{n-i}\frac{\Gamma(n-i+b_2)}{\Gamma(n-i+c_2)}.
\end{aligned}
\tag{80}
$$

The inner sum of the last term is of type D. The second Appell function can therefore be expanded with the help of algorithms A–D. As an example we give

$$
\begin{aligned}
F_2(1,1,\epsilon;1+\epsilon,1-\epsilon;x,y) = {} & \frac{1}{1-x} + \frac{1}{1-x}(2\ln(1-x) - \ln(1-x-y))\epsilon + \frac{1}{1-x}\Bigg[2\,\mathrm{Li}_2(x) \\
& + 2\,\mathrm{Li}_2(y) - \mathrm{Li}_2(x+y) + 4S_{0,2}(x) + S_{0,2}(x+y) + \mathrm{Li}_{1,1}\left(\frac{y}{x+y}, x+y\right) \\
& - 2\,\mathrm{Li}_{1,1}\left(\frac{x}{x+y}, x+y\right) - 2\,\mathrm{Li}_{1,1}\left(\frac{x+y}{x}, x\right)\Bigg]\epsilon^2 + \frac{1}{1-x}\Bigg[\mathrm{Li}_3(x+y) \\
& - 2\,\mathrm{Li}_3(x) + S_{0,3}(x+y) - 8S_{0,3}(x) - S_{1,2}(x+y) - 4S_{1,2}(x) + 4S_{1,2}(y) \\
& - H_{1,2}(x+y) - 4H_{1,2}(x) + 2\,\mathrm{Li}_{1,2}\left(\frac{x}{x+y}, x+y\right) - \mathrm{Li}_{1,2}\left(\frac{y}{x+y}, x+y\right) \\
& + 2\,\mathrm{Li}_{1,2}\left(\frac{x+y}{x}, x\right) + 2\,\mathrm{Li}_{2,1}\left(\frac{x}{x+y}, x+y\right) + 3\,\mathrm{Li}_{2,1}\left(\frac{y}{x+y}, x+y\right) \\
& + 2\,\mathrm{Li}_{2,1}\left(\frac{x+y}{x}, x\right) - 4\,\mathrm{Li}_{2,1}\left(\frac{y}{x}, x\right) + 4\,\mathrm{Li}_{1,1,1}\left(\frac{x}{x+y}, \frac{x+y}{x}, x\right) \\
& + 4\,\mathrm{Li}_{1,1,1}\left(\frac{x+y}{x}, 1, x\right) + 4\,\mathrm{Li}_{1,1,1}\left(1, \frac{x}{x+y}, x+y\right) + 2\,\mathrm{Li}_{1,1,1} \\
& \times\left(1, \frac{y}{x+y}, x+y\right) - 2\,\mathrm{Li}_{1,1,1}\left(\frac{y}{x+y}, \frac{x+y}{x}, x\right) + \mathrm{Li}_{1,1,1}\left(\frac{y}{x+y}, 1, x+y\right) \\
& - 2\,\mathrm{Li}_{1,1,1}\left(\frac{x}{x+y}, 1, x+y\right) - 2\,\mathrm{Li}_{1,1,1}\left(1, \frac{x+y}{x}, x\right) \\
& - 2\,\mathrm{Li}_{1,1,1}\left(\frac{x+y}{x}, \frac{x}{x+y}, x+y\right)\Bigg]\epsilon^3 + O(\epsilon^4). \qquad (81)
\end{aligned}
$$

After taking into account a typo in Eq. (A.47) of Ref. 44 this result agrees up to order ϵ with the one obtained along the lines of Ref. 44. Multiple polylogarithms of low weight can be expressed as products of classical polylogarithms and the result of the expansion in Eq. (81) can be simplified. However, we present here the output of our algorithm. Our algorithm gives the result as a linear combination of polylogarithms and does not generate products of polylogarithms.

C. Kampé de Fériet function

The Kampé de Fériet function is defined by[43]

$$
S_1(a_1,a_2,b_1;c,c_1;x_1,x_2) = \sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty} \frac{(a_1)_{m_1+m_2}(a_2)_{m_1+m_2}(b_1)_{m_1}}{(c)_{m_1+m_2}(c_1)_{m_1}} \frac{x_1^{m_1}}{m_1!}\frac{x_2^{m_2}}{m_2!}. \qquad (82)
$$

It can be rewritten as

$$
\begin{aligned}
S_1(a_1,a_2,b_1;c,c_1;x_1,x_2) = {} & 1 + \frac{\Gamma(c)\Gamma(c_1)}{\Gamma(a_1)\Gamma(a_2)\Gamma(b_1)}\sum_{i=1}^{\infty} x_1^i \frac{\Gamma(i+a_1)\Gamma(i+a_2)\Gamma(i+b_1)}{\Gamma(i+c)\Gamma(i+c_1)\Gamma(i+1)} \\
& + \frac{\Gamma(c)}{\Gamma(a_1)\Gamma(a_2)}\sum_{i=1}^{\infty} x_2^i \frac{\Gamma(i+a_1)\Gamma(i+a_2)}{\Gamma(i+c)\Gamma(i+1)} \\
& - \frac{\Gamma(c)\Gamma(c_1)}{\Gamma(a_1)\Gamma(a_2)\Gamma(b_1)}\sum_{n=1}^{\infty} x_2^n \frac{\Gamma(n+a_1)\Gamma(n+a_2)}{\Gamma(n+c)\Gamma(n+1)}
\end{aligned}
$$

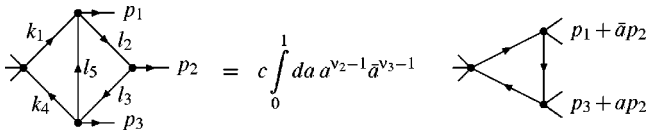


FIG. 3. The C-topology reduces to a triangle with three external masses and an additional integration over the Feynman parameter a.

$$\times(-1)\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i\left(-\frac{x_1}{x_2}\right)^i\frac{\Gamma(i+b_1)}{\Gamma(i+c_1)}. \tag{83}$$

The inner sum of the last term is of type C. The Kampé de Fériet function can therefore be expanded with the help of the algorithms A and C.

D. The C-topology

Here we study the C-topology with one massive external leg and arbitrary powers of the propagators and arbitray dimensions, which can be solved using the algorithms given in this paper. The importance of this result lies in the fact that one avoids having to solve a system of equations obtained from partial integration or Lorentz invariance. Solving such a system becomes quite difficult if one external leg is massive. The result obtained here is thus a useful ingredient for the calculation of the two-loop amplitudes with one massive external leg, such as $e^+e^-\to 3$ jets.
The second C-topology, where the massive leg is attached to the other corner, as well as all simpler topologies, can be obtained along the same lines. The two-loop C-topology with one massive external leg is defined by

$$I=\int\frac{d^Dk_1}{i\pi^{D/2}}\int\frac{d^Dl_5}{i\pi^{D/2}}\frac{1}{(-k_1^2)^{\nu_1}}\frac{1}{(-l_2^2)^{\nu_2}}\frac{1}{(-l_3^2)^{\nu_3}}\frac{1}{(-k_4^2)^{\nu_4}}\frac{1}{(-l_5^2)^{\nu_5}} \tag{84}$$

with

$$\begin{aligned} l_2&=k_1+l_5-p_1,\\ l_3&=l_2-p_2,\\ k_4&=k_1-p_{123}. \end{aligned} \tag{85}$$

Figure 3 shows the corresponding Feynman diagram. We first perform the l_5-integration. Combining with Feynman parameters first l_2^2 and l_3^2 and then the resulting propagator with l_5^2 we obtain

$$\begin{aligned} I=&\frac{\Gamma(\nu_{235}-m+\epsilon)}{\Gamma(\nu_2)\Gamma(\nu_3)\Gamma(\nu_5)}\frac{\Gamma(-\nu_{23}+m-\epsilon)\Gamma(-\nu_5+m-\epsilon)}{\Gamma(-\nu_{235}+2m-2\epsilon)}\int_0^1 da\, a^{\nu_2-1}\bar{a}^{\nu_3-1}\\ &\times\int\frac{d^Dk_1}{i\pi^{D/2}}\frac{1}{(-k_1^2)^{\nu_1}}\frac{1}{(-(k_1-p_1-\bar{a}p_2)^2)^{\nu_{235}-m+\epsilon}}\frac{1}{(-k_4^2)^{\nu_4}}. \end{aligned} \tag{86}$$

As a short-hand notation we used $D=2m-2\epsilon$, $\bar{a}=1-a$, and $\nu_{235}=\nu_2+\nu_3+\nu_5$. The second line is a one-loop triangle with three external masses. The solution for this one-loop integral with arbitrary powers of the propagators and arbitrary dimensions is known.[45] We use the solution given in Ref. 44 and perform the remaining integration. We obtain

$$
\begin{aligned}
I=&\frac{\Gamma(2m-2\epsilon-\nu_{1235})\Gamma(1+\nu_{1235}-2m+2\epsilon)\Gamma(2m-2\epsilon-\nu_{2345})\Gamma(1+\nu_{2345}-2m+2\epsilon)}{\Gamma(\nu_1)\Gamma(\nu_2)\Gamma(\nu_3)\Gamma(\nu_4)\Gamma(\nu_5)\Gamma(3m-3\epsilon-\nu_{12345})}\\
&\times\frac{\Gamma(m-\epsilon-\nu_5)\Gamma(m-\epsilon-\nu_{23})}{\Gamma(2m-2\epsilon-\nu_{235})}(-s_{123})^{2m-2\epsilon-\nu_{12345}}\sum_{i_1=0}^{\infty}\sum_{i_2=0}^{\infty}\frac{x_1^{i_1}}{i_1!}\frac{x_2^{i_2}}{i_2!}\\
&\times\Bigg[\frac{\Gamma(i_1+\nu_3)\Gamma(i_2+\nu_2)\Gamma(i_1+i_2-2m+2\epsilon+\nu_{12345})\Gamma(i_1+i_2-m+\epsilon+\nu_{235})}{\Gamma(i_1+1-2m+2\epsilon+\nu_{1235})\Gamma(i_2+1-2m+2\epsilon+\nu_{2345})\Gamma(i_1+i_2+\nu_{23})}-x_1^{2m-2\epsilon-\nu_{1235}}\\
&\times\frac{\Gamma(i_1+2m-2\epsilon-\nu_{125})\Gamma(i_2+\nu_2)\Gamma(i_1+i_2+\nu_4)\Gamma(i_1+i_2+m-\epsilon-\nu_1)}{\Gamma(i_1+1+2m-2\epsilon-\nu_{1235})\Gamma(i_2+1-2m+2\epsilon+\nu_{2345})\Gamma(i_1+i_2+2m-2\epsilon-\nu_{15})}\\
&-x_2^{2m-2\epsilon-\nu_{2345}}\\
&\times\frac{\Gamma(i_1+\nu_3)\Gamma(i_2+2m-2\epsilon-\nu_{345})\Gamma(i_1+i_2+\nu_1)\Gamma(i_1+i_2+m-\epsilon-\nu_4)}{\Gamma(i_1+1-2m+2\epsilon+\nu_{1235})\Gamma(i_2+1+2m-2\epsilon-\nu_{2345})\Gamma(i_1+i_2+2m-2\epsilon-\nu_{45})}\\
&+x_1^{2m-2\epsilon-\nu_{1235}}x_2^{2m-2\epsilon-\nu_{2345}}\frac{\Gamma(i_1+2m-2\epsilon-\nu_{125})\Gamma(i_2+2m-2\epsilon-\nu_{345})}{\Gamma(i_1+1+2m-2\epsilon-\nu_{1235})\Gamma(i_2+1+2m-2\epsilon-\nu_{2345})}\\
&\times\frac{\Gamma(i_1+i_2+2m-2\epsilon-\nu_{235})\Gamma(i_1+i_2+3m-3\epsilon-\nu_{12345})}{\Gamma(i_1+i_2+4m-4\epsilon-\nu_{12345}-\nu_5)}\Bigg],
\end{aligned}
\tag{87}
$$

where we set $x_1=(-s_{12})/(-s_{123})$ and $x_2=(-s_{23})/(-s_{123})$. Changing the summation indices as in the case of the second Appell function yields a sum of type D. For specific (integer) values of ν_i and m this expression can be expanded in ϵ with the algorithm given in Sec. III. This is a new and useful result. Up to now this integral has only been known for $m=2$ and the sets (1,1,1,1,1) and (1,1,1,1,2) for $(\nu_1,\nu_2,\nu_3,\nu_4,\nu_5)$. We have verified that our result agrees in these two specific cases with the ones given by Gehrmann and Remiddi.[8]

V. CONCLUSIONS

In this paper we studied some algebraic properties of nested sums. Based on these properties we developed a number of algorithms which can be used to expand a certain class of mathematical functions. All presented algorithms are suitable for the implementation on a computer. These algorithms allow the evaluation of integrals occurring in high-energy physics. As an application we have shown how the two-loop C-topology can be evaluated for arbitrary powers of the propagators and arbitrary dimensions. Furthermore we have shown that the nested sums satisfy a Hopf algebra and established the connection with the Hopf algebra of Kreimer.

ACKNOWLEDGMENT

The authors would like to thank Jos Vermaseren for useful discussions.

APPENDIX A: THE HOPF ALGEBRA OF *Z*-SUMS

In this section we show that the Z-sums form a Hopf algebra.[36,37] It is sufficient to demonstrate that the Z-sums form a quasishuffle algebra. A general theorem[46] guarantees then, that they also form a Hopf algebra. We also discuss the connection with the Hopf algebra of Kreimer.[47]

Before we start, we have to introduce some notation. We call a pair $(m_j;x_j)$ a letter and the set of all letters the alphabet A. We further call m_j the degree of the letter (m_j,x_j). On the alphabet A we define a multiplication

$$
\begin{aligned}
&\cdot:A\times A\to A,\\
&(m_1,x_1)\cdot(m_2,x_2)=(m_1+m_2,x_1x_2),
\end{aligned}
\tag{A1}
$$

e.g., the x_j's are multiplied and the degrees are added. As a short-hand notation we will in the following denote a letter just by $X_j=(m_j;x_j)$. A word is an ordered sequence of letters, e.g.,

$$W=X_1,X_2,\ldots,X_k. \tag{A2}$$

We denote the word of length zero by e. The sums defined in (1) are therefore completely specified by the upper summation limit n and a word W. In particular for any positive n the sum corresponding to the empty word e equals 1. A quasishuffle algebra $\mathcal{A}$ on the vector space of words is defined by[46]

$$\begin{aligned} &e\circ W=W\circ e=W,\\ &(X_1,W_1)\circ(X_2,W_2)=X_1,(W_1\circ(X_2,W_2))+X_2,((X_1,W_1)\circ W_2)+(X_1\cdot X_2),(W_1\circ W_2). \end{aligned} \tag{A3}$$

Note that "$\cdot$" denotes multiplication of letters as defined in Eq. (A1), whereas "$\circ$" denotes the product in the algebra $\mathcal{A}$, recursively defined in Eq. (A3). We observe that the formula for the multiplication of Z-sums Eq. (7) is identical to Eq. (A3). The Z-sums therefore form a quasishuffle algebra.

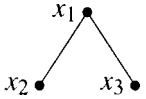
We now discuss the connection with the Hopf algebra of Kreimer.[47] Kreimer showed that the process of renormalization of UV-divergences occurring in quantum field theories can be formulated in terms of a Hopf algebra structure. We first recall the properties of an algebra and a coalgebra: An algebra has a unit and a multiplication, whereas a coalgebra has a counit and a comultiplication. A Hopf algebra is an algebra and a coalgebra at the same time, such that the two structures are compatible with each other. In addition there is an antipode. We show that the coalgebra structure of Z-sums is identical to the coalgebra structure of the Hopf algebra of Kreimer. To this aim we introduce the explicit definitions of the counit, the coproduct, and the antipode. It is convenient to phrase the coalgebra structure in terms of rooted trees. A Z-sums can be represented as rooted trees without any sidebranchings. As a concrete example we write down the pictorial representation of a sum of depth three:

$$Z(n;m_1,m_2,m_3;x_1,x_2,x_3)=\sum_{i_1=1}^{n}\sum_{i_2=1}^{i_1-1}\sum_{i_3=1}^{i_2-1}\frac{x_1^{i_1}}{i_1^{m_1}}\frac{x_2^{i_2}}{i_2^{m_2}}\frac{x_3^{i_3}}{i_3^{m_3}}= \tag{A4}$$

The pictorial representation views a Z-sum as a rooted tree without any sidebranchings. The outermost sum corresponds to the root. By convention, the root is always drawn on the top.

Trees with sidebranchings are given by nested sums with more than one subsum, e.g.,

$$\sum_{i=1}^{n}\frac{x_1^i}{i^{m_1}}Z(i-1;m_2,x_2)Z(i-1;m_3;x_3) \quad = \tag{A5}$$



Of course, due to the multiplication formula, trees with sidebranchings can always be reduced to trees without any sidebranchings:

$$\begin{aligned} \sum_{i=1}^{n}\frac{x_1^i}{i^{m_1}}Z(i-1;m_2,x_2)Z(i-1;m_3;x_3)&=Z(n;m_1,m_2,m_3;x_1,x_2,x_3)+Z(n;m_1,m_3,m_2;x_1,x_3,x_2)\\ &\quad+Z(n;m_1,m_2+m_3;x_1,x_2x_3). \end{aligned} \tag{A6}$$

The coalgebra structure is formulated in terms of rooted trees (e.g., there is no need to convert rooted trees to a basis of rooted trees without sidebranchings). We first introduce some notation how to manipulate rooted trees. We adopt the notation of Kreimer and Connes.[47,48] An elementary cut of a rooted tree is a cut at a single chosen edge. An admissible cut is any assignment of elementary cuts to a rooted tree such that any path from any vertex of the tree to the root has at most one elementary cut. An admissible cut maps a tree t to a monomial in trees $t_1\circ\cdots\circ t_{k+1}$.

Note that precisely one of these subtrees t_j will contain the root of t. We denote this distinguished tree by $R^C(t)$, and the monomial delivered by the k other factors by $P^C(t)$. The counit $\overline{e}$ is given by

$$\begin{aligned} \overline{e}(e) &= 1, \\ \overline{e}(t) &= 0, \quad t \neq e. \end{aligned} \tag{A7}$$

The coproduct Δ is defined by

$$\begin{aligned} \Delta(e) &= e \otimes e, \\ \Delta(t) &= e \otimes t + t \otimes e + \sum_{\text{adm. cuts } C \text{of } t} P^C(t) \otimes R^C(t), \\ \Delta(t_1 \circ \cdots \circ t_k) &= \Delta(t_1)(\circ \otimes \circ) \cdots (\circ \otimes \circ)\Delta(t_k). \end{aligned} \tag{A8}$$

The antipode $\mathcal{S}$ is given by

$$\begin{aligned} \mathcal{S}(e) &= e, \\ \mathcal{S}(t) &= -t - \sum_{\text{adm. cuts } C \text{ of } t} \mathcal{S}(P^C(t)) \circ R^C(t), \\ \mathcal{S}(t_1 \circ \cdots \circ t_k) &= \mathcal{S}(t_1) \circ \cdots \circ \mathcal{S}(t_k). \end{aligned} \tag{A9}$$

The proof that these definitions yield a Hopf algebra can be found in Ref. 46 and is not repeated here. The Hopf algebra of Kreimer and Connes,[47,48] which emerged in the context of renormalization of UV-divergences, has a slightly different algebra structure. There the algebra is generated by rooted trees. In this algebra a product of two rooted trees is not necessarily a rooted tree again. However, the coalgebra structures are identical, which is a remarkable observation.

Let us give some examples for the coproduct and the antipode for Z-sums:

$$\begin{aligned} \Delta Z(n;m_1;x_1) &= e \otimes Z(n;m_1;x_1) + Z(n;m_1;x_1) \otimes e, \\ \Delta Z(n;m_1,m_2;x_1,x_2) &= e \otimes Z(n;m_1,m_2;x_1,x_2) + Z(n;m_1,m_2;x_1,x_2) \otimes e + Z(n;m_2;x_2) \\ &\quad \otimes Z(n;m_1;x_1), \end{aligned} \tag{A10}$$

$$\begin{aligned} \mathcal{S}Z(n;m_1;x_1) &= -Z(n;m_1;x_1), \\ \mathcal{S}Z(n;m_1,m_2;x_1,x_2) &= Z(n;m_2,m_1;x_2,x_1) + Z(n;m_1+m_2;x_1x_2). \end{aligned} \tag{A11}$$

APPENDIX B: REVIEW OF GONCHAROV'S MULTIPLE POLYLOGARITHMS

At the end of the day we express our results in terms of Goncharov's multiple polylogarithms. They therefore form an important specialization of nested sums and we therefore review some of their properties. After the introduction by Gonacharov[5] they have been extensively studied by Borwein *et al.*[6] They use a different notation which is related to the one of Goncharov by

$$\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1) = \lambda\begin{pmatrix} m_1,\ldots,m_k \\ b_1,\ldots,b_k \end{pmatrix}, \quad b_j = \frac{1}{x_1 x_2 \cdots x_j}. \tag{B1}$$

Most of the material reviewed in this section is based on the work of Borwein *et al.*[6]

1. Integral representations

We first define the notation for iterated integrals

$$\int_0^\Lambda \frac{\mathrm{d}t}{a_n-t}\circ\cdots\circ\frac{\mathrm{d}t}{a_1-t}=\int_0^\Lambda \frac{\mathrm{d}t_n}{a_n-t_n}\int_0^{t_n}\frac{\mathrm{d}t_n-1}{a_{n-1}-t_{n-1}}\times\cdots\times\int_0^{t_2}\frac{\mathrm{d}t_1}{a_1-t_1}. \tag{B2}$$

We further use the following short-hand notation:

$$\int_0^\Lambda\left(\frac{\mathrm{d}t}{t}\circ\right)^m\frac{\mathrm{d}t}{a-t}=\int_0^\Lambda\underbrace{\frac{\mathrm{d}t}{t}\circ\cdots\frac{\mathrm{d}t}{t}}_{m\ \text{times}}\circ\frac{\mathrm{d}t}{a-t}. \tag{B3}$$

The integral representation for $\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1)$ reads

$$\begin{aligned}\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1)=&\int_0^{x_1x_2\cdots x_k}\left(\frac{\mathrm{d}t}{t}\circ\right)^{m_1-1}\frac{\mathrm{d}t}{x_2x_3\cdots x_k-t}\circ\left(\frac{\mathrm{d}t}{t}\circ\right)^{m_2-1}\\&\times\frac{\mathrm{d}t}{x_3\ldots x_k-t}\circ\cdots\circ\left(\frac{\mathrm{d}t}{t}\circ\right)^{m_k-1}\frac{\mathrm{d}t}{1-t}.\end{aligned} \tag{B4}$$

In the notation of Borwein *et al.* this representation reads

$$\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1)=(-1)^k\int_0^1\left(\frac{\mathrm{d}t}{t}\circ\right)^{m_1-1}\frac{\mathrm{d}t}{t-b_1}\circ\left(\frac{\mathrm{d}t}{t}\circ\right)^{m_2-1}\frac{\mathrm{d}t}{t-b_2}\circ\cdots\circ\left(\frac{\mathrm{d}t}{t}\circ\right)^{m_k-1}\frac{\mathrm{d}t}{t-b_k}, \tag{B5}$$

where the b_j's are related to the x_j's as in Eq. (B1). Changing the integration variables according to $t\to1-t$ yields the dual integral representation:

$$\begin{aligned}\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1)=&(-1)^k\int_0^1\frac{\mathrm{d}t}{1-b_k-t}\circ\left(\frac{\mathrm{d}t}{1-t}\circ\right)^{m_k-1}\\&\times\frac{\mathrm{d}t}{1-b_{k-1}-t}\circ\left(\frac{\mathrm{d}t}{1-t}\circ\right)^{m_{k-1}-1}\circ\cdots\circ\frac{\mathrm{d}t}{1-b_1-t}\circ\left(\frac{\mathrm{d}t}{1-t}\circ\right)^{m_1-1}.\end{aligned} \tag{B6}$$

In addition to these weight-dimensional integral representations there is also a depth-dimensional integral representation:

$$\begin{aligned}\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1)=&\frac{1}{\Gamma(m_1)\cdots\Gamma(m_k)}\int_1^\infty\frac{\mathrm{d}t_1}{t_1}\frac{(\ln t_1)^{m_1-1}}{\frac{t_1}{x_1}-1}\times\int_1^\infty\frac{\mathrm{d}t_2}{t_2}\frac{(\ln t_2)^{m_2-1}}{\frac{t_1t_2}{x_1x_2}-1}\times\cdots\\&\times\int_1^\infty\frac{\mathrm{d}t_k}{t_k}\frac{(\ln t_k)^{m_k-1}}{\frac{t_1\cdots t_k}{x_1\cdots x_k}-1}.\end{aligned} \tag{B7}$$

2. The shuffle algebra

Instead of specifying a multiple polylogarithm by the x_j's and m_j's, we may denote the function by a single string

$$(\alpha_1,\alpha_2,\ldots,\alpha_w)=(0,\ldots,0,b_1,0,\ldots,0,b_2,\ldots,0,\ldots,0,b_k), \tag{B8}$$

where (m_j-1) zeros preceed b_j. Defining further

$$\Omega(\alpha_i)=\frac{dt}{t-\alpha_i} \tag{B9}$$

allows us to rewrite the integral representation Eq. (B5) as

$$\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1)=(-1)^k\int_0^1\Omega(\alpha_1)\circ\cdots\circ\Omega(\alpha_w). \tag{B10}$$

From the iterated integral representation one deduces a second algebra structure with multiplication given by

$$\begin{aligned}&\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1)\times\mathrm{Li}_{m_{k+l},\ldots,m_{k+1}}(x_{k+l},\ldots,x_{k+1})\\&\quad=(-1)^{k+l}\int_0^1\Omega(\alpha_1)\circ\cdots\circ\Omega(\alpha_{w_k})\int_0^1\Omega(\alpha_{w_k+1})\circ\cdots\circ\Omega(\alpha_{w_k+w_l})\\&\quad=(-1)^{k+l}\sum_{\text{shuffle}}\int_0^1\Omega(\alpha_{\sigma(1)})\circ\cdots\circ\Omega(\alpha_{\sigma(w_k+w_l)}),\end{aligned} \tag{B11}$$

where $w_k=m_1+\cdots+m_k$, $w_l=m_{k+1}+\cdots+m_{k+l}$ and the sum is over all permutations, which preserve the relative order of the strings $\Omega(\alpha_1)\cdots\Omega(\alpha_{w_k})$ and $\Omega(\alpha_{w_k+1})\cdots\Omega(\alpha_{w_k+w_l})$.

3. Reduction to simpler functions

The multiple polylogarithms contain a variety of other functions as a subset. We start with depth one. As the notation already suggests, the multiple polylogarithms are in this case identical to the classical polylogarithms, e.g.,

$$\mathrm{Li}_0(x)=\frac{x}{1-x},\quad \mathrm{Li}_1(x)=-\ln(1-x) \tag{B12}$$

and

$$\mathrm{Li}_n(x)=\int_0^x dt\,\frac{\mathrm{Li}_{n-1}(t)}{t}. \tag{B13}$$

Nielsen's generalized polylogarithms,[4] defined through

$$S_{n,p}(x)=\frac{(-1)^{n-1+p}}{(n-1)!p!}\int_0^1 dt\,\frac{\ln^{n-1}(t)\ln^p(1-tx)}{t}, \tag{B14}$$

are related to the multiple polylogarithms by

$$S_{n,p}(x)=\mathrm{Li}_{1,\ldots,1,n+1}(\underbrace{1,\ldots,1}_{p-1},x), \tag{B15}$$

where $(p-1)$ one's occur before $n+1$ and x. The harmonic polylogarithms of Remiddi and Vermaseren[7] are related to the multiple polylogarithms for positive indices as

$$H_{m_1,\ldots,m_k}(x)=\mathrm{Li}_{m_k,\ldots,m_1}(\underbrace{1,\ldots,1}_{k-1},x). \tag{B16}$$

The harmonic polylogarithms are defined recursively through

$$H_0(x)=\ln(x),\quad H_1(x)=-\ln(1-x),\quad H_{-1}(x)=\ln(1+x), \tag{B17}$$

and

$$\begin{aligned} H_{m_1+1,m_2,\ldots,m_k}&=\int_0^x \mathrm{d}t\, f_0(t)H_{m_1,m_2,\ldots,m_k}(t),\\ H_{\pm 1,m_2,\ldots,m_k}&=\int_0^x \mathrm{d}t\, f_{\pm 1}(t)H_{m_2,\ldots,m_k}(t), \end{aligned} \tag{B18}$$

where the fractions $f_0(x)$, $f_1(x)$, and $f_{-1}(x)$ are given by

$$f_0(x)=\frac{1}{x},\quad f_1(x)=\frac{1}{1-x},\quad f_{-1}(x)=\frac{1}{1+x}. \tag{B19}$$

Recently Gehrmann and Remiddi[8] extended the harmonic polylogarithms to two-dimensional harmonic polylogarithms (2dHPL) by extending the fractions to

$$f(z,x)=\frac{1}{z+x},\quad f(1-z,x)=\frac{1}{1-z-x}. \tag{B20}$$

From the integral representation Eq. (B4) it is clear that the 2dHPL are a subset of Goncharov's multiple polylogarithms. If we identitfy $x=x_1x_2\times\cdots\times x_k$ we have

$$\int_0^x \mathrm{d}t\, f(z,t)\mathrm{Li}_{m_k,\ldots,m_1}\left(x_k,\ldots,x_2,\frac{t}{x_2\ldots x_k}\right)=-\mathrm{Li}_{m_k,\ldots,m_1,1}\left(x_k,\ldots,x_2,-\frac{z}{x_2\cdots x_k},-\frac{x}{z}\right), \tag{B21}$$

$$\int_0^x \mathrm{d}t\, f(1-z,t)\mathrm{Li}_{m_k,\ldots,m_1}\left(x_k,\ldots,x_2,\frac{t}{x_2\cdots x_k}\right)=\mathrm{Li}_{m_k,\ldots,m_1,1}\left(x_k,\ldots,x_2,\frac{1-z}{x_2\cdots x_k},\frac{x}{1-z}\right).$$

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Separation of variables and subgroup bases on *n*-dimensional hyperboloids

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A graphical formalism is introduced for describing subgroup type coordinates on n-dimensional Lorentzian hyperboloids imbedded into $n+1$ dimensional Minkowski spaces. The $O(n,1)$ group element is parametrized according to different subgroup chains, involving Lorentz, rotation, and Euclidean subgroups. The coordinates are then induced by the corresponding group action. Eigenfunctions of the Laplace–Beltrami operator are obtained as products of Jacobi functions, associated Legendre functions, and modified Bessel functions. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1467709]

I. INTRODUCTION

The purpose of this article is to study in a systematic manner all possible subgroup type coordinates on an n-dimensional Lorentzian hyperboloid, embedded into an $n+1$-dimensional Minkowski space. The isometry group of this space is the pseudo-orthogonal group $O(n,1)$, the Lorentz group in n space dimensions. The space itself can be identified as the quotient space $O(n,1)/O(n)$, or $O(n,1)/O(n-1,1)$, for the two-sheeted or one-sheeted hyperboloid, respectively.

By ''separable coordinates'' we mean curvlinear coordinates $(\xi_1,\xi_2,\ldots,\xi_n)$ on a hyperboloid H_n, such that the Laplace–Beltrami equation

$$\Delta_{\mathrm{LB}}\Psi(\xi_1,\xi_2,\ldots,\xi_n)=\nu(\nu+n-1)\,\Psi(\xi_1,\xi_2,\ldots,\xi_n), \tag{1.1}$$

allows the ''multiplicative'' separation

$$\Psi_{\lambda_1,\lambda_2,\ldots,\lambda_n}(\xi_1,\xi_2,\ldots,\xi_n)=\prod_{i=1}^{n}\Phi_i(\xi_i;\lambda_1,\lambda_2,\ldots,\lambda_n). \tag{1.2}$$

In Eq. (1.2) each function Φ_i depends only on one variable ξ_i, but can depend on all the separation constants λ_j.

We make use of an algebraic approach to the separation of variables in Riemannian or pseudo-Riemannian spaces.[1–10] In this approach the separated solutions $\Psi(\xi_1,\xi_2,\ldots,\xi_n)$ are simultaneous eigenfunctions of a complete set of commuting operators $\{Y_1,Y_2,\ldots,Y_n\}$, where n is the dimension of the space. The operators Y_i are second-order operators in the enveloping algebra of L, where L is the Lie algebra of the isometry group G of the corresponding space, and the Laplace–Beltrami operator Δ_{LB} is included in the set $\{Y_1,Y_2,\ldots,Y_n\}$. A classification of

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different coordinate systems corresponds to a classification of such commuting sets of operators under the action of the group G. Subgroup type coordinates are obtained when we take a chain of subgroups

$$G \equiv G_1 \supset G_2 \supset \cdots \supset G_k \tag{1.3}$$

each of which has at least one second-order Casimir operator. The commuting operators $\{Y_1, Y_2, \ldots, Y_n\}$ are then taken as Casimir operators of the groups in the chain (1.3).

Subgroup type coordinates on homogeneous spaces associated with rotation groups $O(n)$ and unitary groups $SU(n)$ were studied by Vilenkin, Kuznetsov, Smorodinsky and others.[11–15] They introduced a graphical method, the ''method of trees,'' to describe subgroup coordinates on spheres $S_n \sim O(n+1)/O(n)$ and complex ''spheres'' $C_n \sim SU(n)/U(n-1)$.

The relation between tree diagrams and subgroup chains was explored in a recent publication,[15] devoted to Lie algebra contractions and the separation of variables. The method of trees was extended from spheres to Euclidean spaces in the same article.[15]

In this article we shall adapt the method of trees to a noncompact group, namely $O(n,1)$ and introduce a graphical method for coordinates on hyperboloids. We shall relate tree diagrams to subgroup diagrams, representing chains of subgroups. We show that the subgroup chains can be used to directly generate separable coordinates by acting on a chosen ''origin'' on the homogeneous space.

In Sec. II we introduce notation and review some basic facts on maximal subgroups of pseudo-orthogonal, orthogonal, and Euclidean Lie groups. Coordinate and subgroup diagrams and all types of separable subgroup coordinates are introduced in Sec. III, first for the low-dimensional groups O(2,1) and O(3,1), then for the general case of $O(n,1)$ for n arbitrary. Section IV is devoted to the eigenfunctions of the Laplace–Beltrami operator for O(2,1) and O(3,1). Eigenfunctions for the general case of $O(n,1)$ are presented in Sec. V and are associated with the different types of subgroup and coordinate diagrams.

II. SUBGROUP CHAINS AND SUBGROUP DIAGRAMS

A. General setting

We consider the upper sheet of the two-sheeted hyperboloid H_n,

$$u \cdot u = u^2 = u_0^2 - \mathbf{u}^2 = 1, \quad \mathbf{u}^2 = u_1^2 + u_2^2 + \cdots + u_n^2, \tag{2.1}$$

where u_μ, $\mu = 0,1,\ldots,n$ are Cartesian coordinates in the ambient Minkowski space $M_{n,1}$. The Laplace–Beltrami operator in curvilinear coordinates on H_n is written as

$$\Delta_{\mathrm{LB}} \equiv \Delta(H_n) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^\mu} \sqrt{g}\, g^{\mu\nu} \frac{\partial}{\partial \xi^\nu}, \tag{2.2}$$

where the metric is

$$\mathrm{d}s^2 = g_{\mu\nu} \mathrm{d}\xi^\mu\, \mathrm{d}\xi^\nu, \quad g = |\det(g_{\mu\nu})|, \quad g_{\alpha\mu} g^{\mu\nu} = \delta_\alpha^\nu. \tag{2.3}$$

The relation between the metric tensor $G_{\mu\nu} = \mathrm{diag}(1,-1,-1,\ldots,-1)$, $(\mu,\nu = 0,1,2,\ldots,n)$ in the ambient space and $g_{\mu\nu}(\xi)$ of Eqs. (2.2) and (2.3) is

$$g_{\mu\nu}(\xi) = G_{ik} \frac{\partial u^i}{\partial \xi^\mu} \frac{\partial u^k}{\partial \xi^\nu}. \tag{2.4}$$

The isometry group is $SO(n,1)$, the proper Lorentz group. Its Lie algebra $o(n,1)$ is realized by vector fields with a standard basis $M_{\mu\nu}$, namely

$$M_{ik}=-\left(u_i\frac{\partial}{\partial u_k}-u_k\frac{\partial}{\partial u_i}\right),\quad M_{0k}=\left(u_0\frac{\partial}{\partial u_k}+u_k\frac{\partial}{\partial u_0}\right),\quad i,k=1,2,\ldots,n \tag{2.5}$$

with the commutation relations

$$[M_{\mu\nu},M_{\alpha\beta}]=G_{\nu\alpha}M_{\mu\beta}-G_{\nu\beta}M_{\mu\alpha}-G_{\mu\alpha}M_{\nu\beta}+G_{\mu\beta}M_{\nu\alpha},\quad \alpha,\beta,\mu,\nu=0,1,2,\ldots,n. \tag{2.6}$$

The Laplace–Beltrami operator and the second order Casimir operator of o(n,1) are related by

$$\Delta(H_n)=Q(n,1),\quad Q(n,1)=\sum_{i=1}^{n}M_{0i}^2-\sum_{1\leqslant i<k}^{n}M_{ik}^2. \tag{2.7}$$

B. Subgroups of O(n,1)

Since we are interested in subgroup type coordinates, we need a classification of subalgebras of the algebra o(n,1). Consider the defining representation of o(n,1), i.e., matrices X satisfying

$$XI_{1,n}+I_{1,n}X^T=0,\quad I_{n,1}=\begin{pmatrix}1 & 0\\ 0 & -I_n\end{pmatrix},\quad X\in R^{(n+1)\times(n+1)}. \tag{2.8}$$

A maximal subalgebra of o(n,1) can be embedded in this representation reducibly, or irreducibly.[16,17] A reducibly imbedded subalgebra will leave a proper vector subspace of R^{n+1} invariant, an irreducibly imbedded subalgebra will only leave R^{n+1}, and 0 invariant. Here we will only need reducibly imbedded subalgebras.

Maximal subalgebras are obtained if the invariant subspace is either completely isotropic (all vectors in the space are lightlike and mutually orthogonal with respect to the metric in the ambient space), or nondegenerate (no lightlike vectors in an orthogonal basis). For o(n,1), that means the following maximal subalgebras exist:

$$\mathrm{o}(n,1)\supset\mathrm{o}(n_1,1)\oplus\mathrm{o}(n_2),\quad n_1+n_2=n,\ n_1\geqslant 1,\ n_2\geqslant 2, \tag{2.9}$$

$$\mathrm{o}(n,1)\supset\mathrm{sim}(n-1), \tag{2.10}$$

where sim($n-1$) is the Lie algebra of the similitude group of the $n-1$ dimensional Euclidean space [the group $E(n-1)$ extended by dilations]. The subalgebra in Eq. (2.9) leaves invariant a space spanned by n_1 negative length vectors [in the metric (2.8)] and also its orthogonal complement in the Minkowski space $M_{n,1}$. We can choose the basis elements of subalgebra (2.9) to be

$$\{M_{ik},M_{j0}\},\ \{M_{ab}\}\ \ 1\leqslant i<k\leqslant n_1,\quad 1\leqslant j\leqslant n_1\ \ n_1+1\leqslant a<b\leqslant n_1+n_2=n. \tag{2.11}$$

It is to be remembered that the algebras o(1) and o(0,1) are empty. For $n_1\geqslant 1$ and $n_2\geqslant 2$ the subalgebras in Eq. (2.1) contribute two Casimir operators

$$C(n_1,1)=\sum_{i=1}^{n_1}M_{i0}^2-\sum_{1\leqslant i<k\leqslant n_1}M_{ik}^2,\quad C(n_2)=\sum_{n_1+1\leqslant a<b\leqslant n_1+n_2}M_{ab}^2. \tag{2.12}$$

The subalgebra sim($n-1$) leaves invariant a one-dimensional isotropic space in $M_{n,1}$ and is spanned by

$$\{M_{0n},M_{ik},M_{0i}+M_{ni}\},\quad 1\leqslant i<k\leqslant n-1,\quad 1\leqslant i\leqslant n-1. \tag{2.13}$$

The algebra sim($n-1$) does not have a second-order Casimir operator, but its maximal subalgebra $e(n-1)$, the Euclidean Lie algebra, does. The algebra $e(n-1)$ is obtained from (2.13) by omitting M_{0n}. The corresponding Casimir operator is

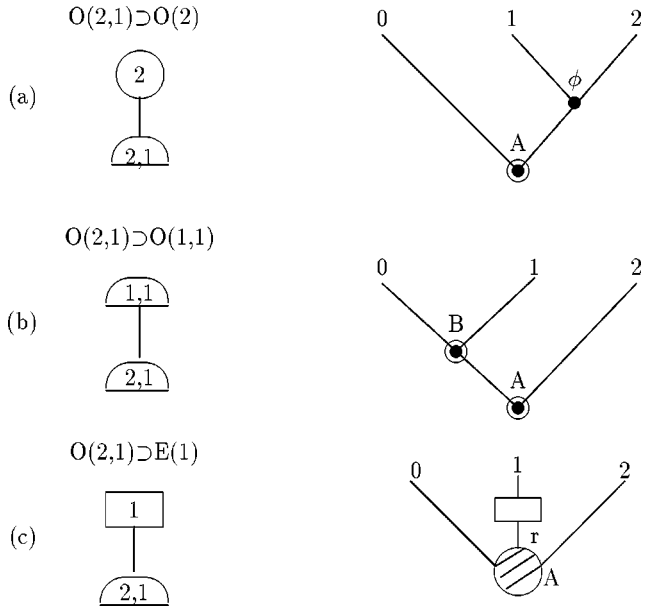

FIG. 1. All subgroup and coordinate diagrams for the O(2,1) hyperboloid.

$$P^2=(M_{01}+M_{n1})^2+(M_{02}+M_{n2})^2+\cdots+(M_{0n-1}+M_{nn-1})^2. \tag{2.14}$$

We shall use subgroup diagrams, first introduced in Ref. 3. A semicircle will denote an o(p,1) algebra with the number p indicated inside. A circle will denote an o(p) algebra, again with the number p indicated. Finally, a square with a number inside will indicate a Euclidean algebra $e(p)$.

Links in a subgroup chain can be of the following types (each indicated subgroup on the right is maximal in the group on the left):

$$\mathrm{O}(p,1)\supset \mathrm{O}(p), \quad \mathrm{O}(p,1)\supset \mathrm{O}(p-1,1), \tag{2.15}$$

$$\mathrm{O}(p,1)\supset E(p-1), \tag{2.16}$$

$$\mathrm{O}(p,1)\supset \mathrm{O}(p_1,1)\otimes \mathrm{O}(p_2), \quad p_1+p_2=p, \ p_1\geqslant 1, \quad p_2\geqslant 2, \tag{2.17}$$

$$\mathrm{O}(p)\supset \mathrm{O}(p-1), \tag{2.18}$$

$$\mathrm{O}(p)\supset \mathrm{O}(p_1)\otimes \mathrm{O}(p_2), \quad p_1+p_2=p, \quad p_1\geqslant p_2\geqslant 1, \tag{2.19}$$

$$E(p)\supset \mathrm{O}(p), \tag{2.20}$$

$$E(p)\supset E(p_1)\otimes E(p_2), \quad p_1+p_2=p, \ p_1\geqslant p_2\geqslant 1. \tag{2.21}$$

The group O(p,1) itself provides one second order operator, the Laplace operator itself. The subgroups on the right in Eqs. (2.15), (2.16), (2.18), and (2.20) provide one further Casimir operator each. The direct products on the right-hand sides of (2.17) and (2.19) provide two Casimir operators in each case. The group $E(p_1)\otimes E(p_2)$ in (2.21) provides two Casimir operators, however their sum is equal to the Casimir operator of the $E(p)$ group on the left-hand side of Eq. (2.21).

All ''allowed'' subalgebra chains and the corresponding Casimir operators for o(2,1) and o(3,1) are shown on the left-hand side of Figs. 1 and 2, respectively. The word ''allowed'' in the previous sentence means that each subalgebra has least one second-order Casimir operator and is maximal amongst those that have this property.

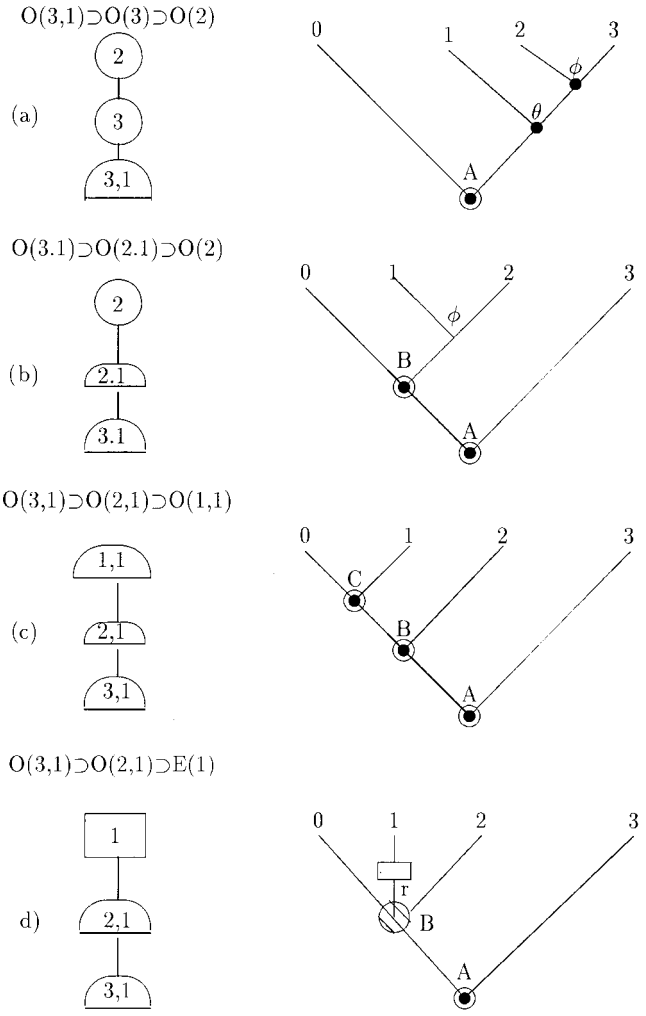

FIG. 2. All subgroup and coordinate diagrams for the O(3,1) hyperboloid.

The procedure of writing all subgroup chains for any p is recursive. From a circle, we can go to one or two circles. From a semicircle to a circle, a semicircle, a square, or a circle plus a semicircle. From a square we can go to a circle, or to two squares.

III. SUBGROUP TYPE COORDINATES AND COORDINATE DIAGRAMS

A. General procedure

Subgroup type coordinates can be interpreted quite literally. They can be obtained by successively applying a series of one-dimensional subgroups of the isometry group G to the origin of the considered space.

Let us consider the hyperboloid H_n [of Eq. (2.1)] and the isometry group O(n,1). We start from the origin which we choose to be the point $(u_0,u_1,\ldots,u_n)=(1,0,\ldots,0)\equiv\mathbb{1}$. Next, we parametrize an element of O(n,1) as

$$G=HG_1e^{M_{0k}A}G_0, \quad A\in R, \tag{3.1}$$

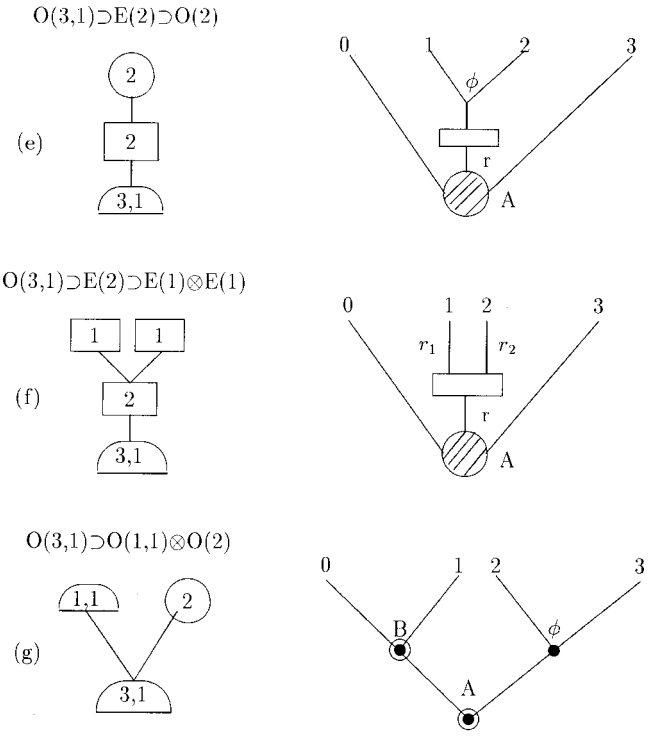

FIG. 2 (*Continued.*)

where $G_0 \sim O(n)$ is the isotropy group of the origin. The exponential represents a pseudorotation in the $(0k)$ plane. We will choose $k=n$, or $k=1$, as the case may be. The group $G_1 \sim O(n-1)$ leaves the space $\exp M_{ok}\mathbb{1}$ (a hyperbola) invariant. Finally H will act effectively on the hyperboloid and generate the coordinate system.

We will run through all different choices of the group HG_1 and relate subgroup diagrams, tree diagrams, and subgroup coordinates. We mention that H itself is not a group.

We shall first treat low dimensional examples, then return to the general case.

B. The group O(2,1)

1. O(2,1)⊃O(2)

Formula (3.1) reduces to

$$G = e^{M_{12}\phi} e^{M_{01}A} e^{M_{12}\alpha} \tag{3.2}$$

and the procedure $\mathbf{u} = G\mathbb{1}$ produces spherical coordinates $(0 \leqslant A < \infty, 0 \leqslant \phi < 2\pi)$

$$\begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} \cosh A \\ \sinh A \cos\phi \\ \sinh A \sin\phi \end{pmatrix}. \tag{3.3}$$

The commuting set of operators corresponding to this system is

$$Y_1 = M_{01}^2 + M_{02}^2 - M_{12}^2, \quad Y_2 = M_{12}^2.$$

2. O(2,1)⊃O(1,1)

We have

$$G=e^{M_{01}B}e^{M_{02}A}e^{M_{12}\alpha} \tag{3.4}$$

and we obtain hyperbolic coordinates $(-\infty<A<\infty,-\infty<B<\infty)$

$$\begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix}=\begin{pmatrix} \cosh A\cosh B \\ \cosh A\sinh B \\ \sinh A \end{pmatrix}. \tag{3.5}$$

The commuting set of operators is

$$Y_1=M_{01}^2+M_{02}^2-M_{12}^2,\quad Y_2=M_{01}^2.$$

3. O(2,1)⊃E(1)

We have

$$G=e^{(M_{01}+M_{21})r}e^{M_{02}A}e^{M_{12}\alpha} \tag{3.6}$$

and we obtain horospheric coordinates $(-\infty<A<\infty,-\infty<r<\infty)$

$$\begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix}=\begin{pmatrix} \cosh A+\dfrac{r^2}{2}e^{-A} \\ re^{-A} \\ \sinh A+\dfrac{r^2}{2}e^{-A} \end{pmatrix}. \tag{3.7}$$

The commuting set of operators is

$$Y_1=M_{01}^2+M_{02}^2-M_{12}^2,\quad Y_2=(M_{01}+M_{21})^2.$$

Notice that the group element $\exp(M_{01}A)$ in Eq. (3.2) and $\exp(M_{02}A)$ in (3.4) and (3.6) takes us onto a hyperbola in the 01 or 02 plane, respectively. The element on the left-hand side, $\exp(M_{12}\phi)$, $\exp(M_{01}B)$, or $\exp(M_{01}+M_{21})r$ completes the parametrization of the O(2,1) hyperboloid and introduces an "ignorable variable" ϕ, B, or r, respectively. Ignorable variables do not figure in the metric tensor, or in the coefficients of the Laplace–Beltrami operator. In the solutions of the Helmholtz equation they figure as exponentials.

For the group O(2,1) the group G_1 of Eq. (3.1) is $G_1=I$ and H is a one-dimensional subgroup.

In Fig. 1 we show the subgroup and coordinate diagrams for the group O(2,1) acting on the hyperboloid H_2. The coordinate diagrams of Figs. 1(a) and 1(b) are obvious extensions of the tree diagrams[13] for a sphere S_n. Each point at the top of a coordinate diagram corresponds to a point in the ambient space $M_{n,1}$ ($M_{2,1}$ in Fig. 1). The coordinate u_0 will always be chosen to be on the extreme left-hand side of the tree. All nodes on the branch leading to u_0 will be denoted by a double circle, as in Figs. 1(a) and 1(b). Nodes on branches leading to the coordinates u_i ($i=1,\ldots,n$) will be denoted by a single (full) circle [see Fig. 1(a)]. At each double circle (hyperbolic node) we introduce a hyperbolic "angle" A_i [A in Fig. 1(a), A and B in Fig. 1(b)]. At each single circle (trigonometric node) we introduce a trigonometric angle θ_i [ϕ in Fig. 1(a)]. The rules for writing coordinates corresponding to such tree diagrams are a slight modification of the rules for S_n spheres.[13] We move along a tree from the bottom to the top and write $\cos\theta_i$, or, respectively, $\cosh A_i$, when we go to the left at a node and $\sin\theta_i$, or, respectively, $\sinh A_i$ when we go to the right.

We mention that for the sphere S_2 the diagrams of Figs. 1(a) and 1(b) would be equivalent.

The subgroup diagrams involving squares (Euclidean subgroups) and the corresponding horospheric coordinates are a specific new feature arising for the noncompact group $O(n,1)$. The vertex in Fig. 1(c) is a three prong one. A variable A is asigned to the central prong. This prong leads to a rectangle, representing E_{n-1} [E_1 in Fig. 3(c)]. Further coordinates are introduced in E_{n-1}. For O(2,1) there is only one such coordinate, namely a Cartesian one which we call r. The general case $O(k,1)\supset E(k-1)$ is treated in the following.

C. The group O(3,1)

From now on we drop the groups G_0 and G_1 in Eq. (3.1) that act trivially, and hence do not produce coordinates.

1. O(3,1)⊃O(3)⊃O(2) [Fig. 2(a)]

In formula (3.1) we have

$$H=e^{M_{23}\phi}e^{M_{12}\theta}e^{M_{01}A} \tag{3.8}$$

and coordinates induced by the action $\mathbf{u}=G1$ are the spherical ones

$$\begin{aligned} u_0&=\cosh A, \quad 0\leqslant A<\infty,\\ u_1&=\sinh A\cos\theta, \quad 0\leqslant\theta\leqslant\pi,\\ u_2&=\sinh A\sin\theta\cos\phi, \quad 0\leqslant\phi<2\pi,\\ u_3&=\sinh A\sin\theta\sin\phi. \end{aligned} \tag{3.9}$$

The O(2) subgroup on the left in (3.8) provides the ignorable variable ϕ. The entire O(3) subgroup in the chain is given as $(\exp M_{23}\phi)(\exp M_{12}\theta)\ (\exp M_{23}\alpha)$, but we drop $(\exp M_{23}\alpha)$ in Eq. (3.8), since it acts trivially on the origin of the sphere $u_1^2+u_2^2+u_3^2=\sinh^2 A$.

The commuting set of operators corresponding to this system is

$$Y_1=\Delta(H_3), \quad Y_2=M_{13}^2+M_{12}^2+M_{23}^2, \quad Y_3=M_{23}^2.$$

2. O(3,1)⊃O(2,1)⊃(2) [Fig. 2(b)]

The action on the origin of H_3 is given by

$$H=e^{M_{12}\phi}e^{M_{01}B}e^{M_{03}A} \tag{3.10}$$

and the coordinates are

$$\begin{aligned} u_0&=\cosh A\cosh B, \quad -\infty<A<\infty,\\ u_1&=\sinh A\sinh B\cos\phi, \quad 0\leqslant B<\infty,\\ u_2&=\sinh A\sinh B\sin\phi, \quad 0\leqslant\phi<2\pi,\\ u_3&=\sinh A. \end{aligned} \tag{3.11}$$

The variable ϕ is ignorable, the others not. The O(2,1) subgroup is generated by M_{12}, M_{01} and M_{02}. The element $(\exp M_{02}C)$ is omitted in Eq. (3.10) since it acts trivially on $\exp M_{03}A\cdot 1$.

The commuting set of operators is

$$Y_1=\Delta(H_3), \quad Y_2=M_{01}^2+M_{02}^2-M_{12}^2, \quad Y_3=M_{12}^2.$$

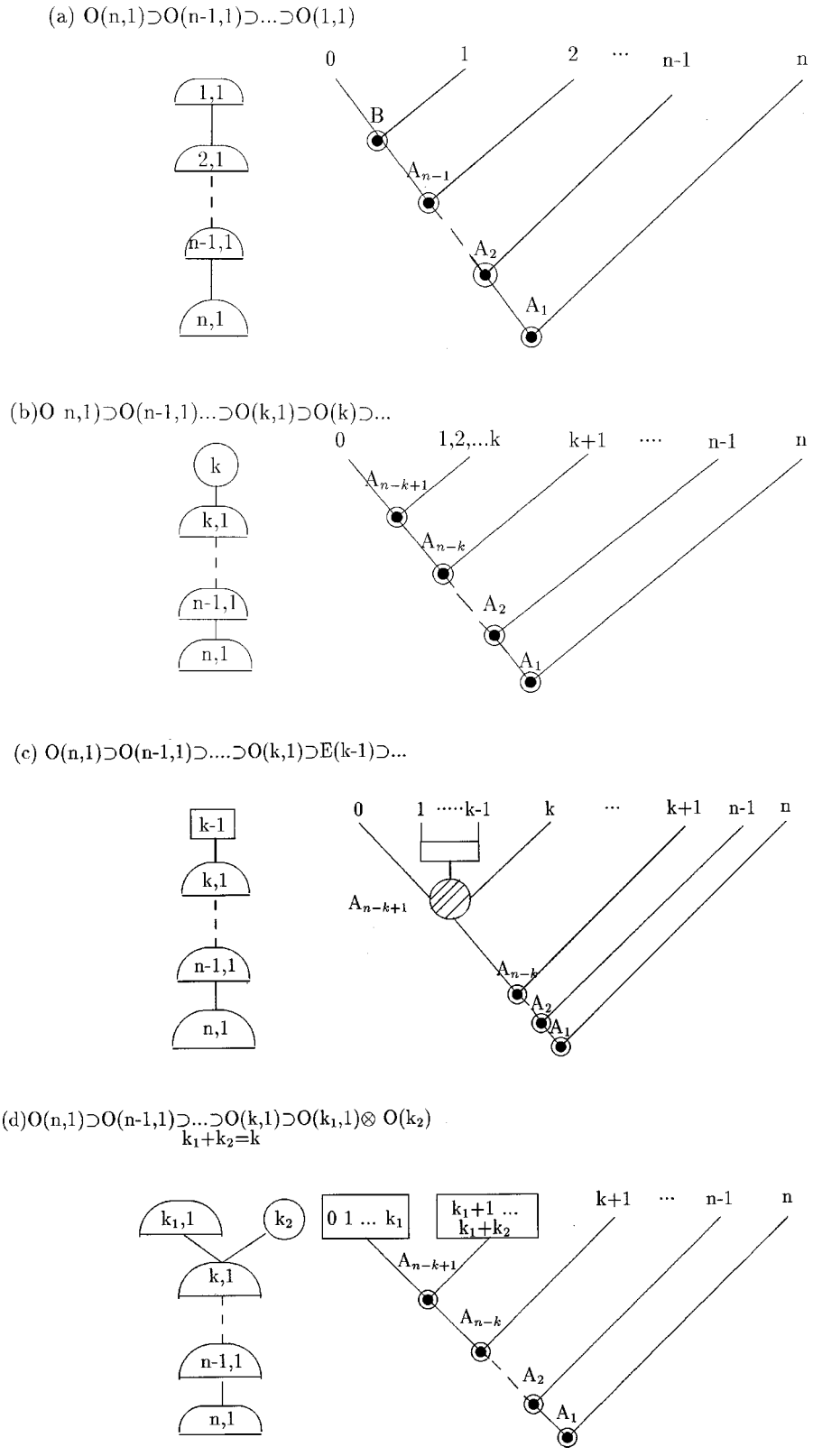

FIG. 3. Subgroup and coordinate diagrams for the O(n,1) hyperboloid.

3. O(3,1)⊃O(2,1)⊃O(1,1) [Fig. 2(c)]

The action on the origin of H_3 is given by

$$H=e^{M_{01}C}e^{M_{02}B}e^{M_{03}A} \tag{3.12}$$

and the corresponding hyperbolic coordinates are

$$\begin{gathered}u_0=\cosh A\cosh B\cosh C,\quad -\infty<A<\infty,\\ u_1=\sinh A\cosh B\sinh C,\quad -\infty<B<\infty,\\ u_2=\sinh A\sinh B,\quad -\infty<C<\infty,\\ u_3=\sinh A.\end{gathered} \tag{3.13}$$

The variable C is ignorable, A and B are not.

The commuting set of operators corresponding to this system is

$$Y_1=\Delta(H_3),\quad Y_2=M_{01}^2+M_{02}^2-M_{12}^2,\quad Y_3=M_{01}^2.$$

4. O(3,1)⊃O(2,1)⊃E(1) [Fig. 2(d)]

We take

$$H=e^{(M_{01}+M_{21})r}e^{M_{02}B}e^{M_{03}A} \tag{3.14}$$

and obtain

$$\begin{gathered}u_0=\cosh A\left(\cosh B+\frac{r^2}{2}e^{-B}\right),\quad -\infty<A<\infty,\\ u_1=\cosh A r e^{-B},\quad -\infty<B<\infty,\\ u_2=\cosh A\left(\sinh B+\frac{r^2}{2}e^{-B}\right),\quad -\infty<r<\infty,\\ u_3=\sinh A.\end{gathered} \tag{3.15}$$

The (only) ignorable variable is r. Notice that the rule for introducing the coordinates B and r coincides with that of Eq. (3.7) for O(2,1).

The commuting operators are

$$Y_1=\Delta(H_3),\quad Y_2=M_{01}^2+M_{02}^2-M_{12}^2,\quad Y_3=(M_{01}+M_{12})^2.$$

5. O(3,1)⊃E(2)⊃O(2) [Fig. 2(e)]

We have

$$H=e^{M_{12}\phi}e^{(M_{01}+M_{31})r}e^{M_{03}A} \tag{3.16}$$

and

$$\begin{gathered}u_0=\left(\cosh A+\frac{r^2}{2}e^{-A}\right),\quad -\infty<A<\infty,\\ u_1=re^{-A}\cos\phi,\quad 0\leqslant r<\infty,\end{gathered} \tag{3.17}$$

$$u_2 = re^{-A}\sin\phi, \quad 0 \leqslant \phi < 2\pi,$$

$$u_3 = \left(\sinh A + \frac{r^2}{2}e^{-A}\right)$$

where the only ignorable variable is ϕ.

The commuting set of operators are

$$Y_1 = \Delta(H_3), \quad Y_2 = M_{12}^2, \quad Y_3 = (M_{01}+M_{31})^2 + (M_{02}+M_{32})^2.$$

6. O(3,1)⊃E(2)⊃E(1)⊗E(1) [Fig. 2(f)]

The group parametrization is

$$H = e^{(M_{01}+M_{31})r_1}e^{(M_{02}+M_{32})r_2}e^{M_{03}A} \tag{3.18}$$

and we have

$$\begin{aligned} u_0 &= \cosh A + \frac{r^2}{2}e^{-A}, \quad -\infty < A < \infty, \\ u_1 &= r_1 e^{-A}, \quad -\infty < r_1 < \infty, \\ u_2 &= r_2 e^{-A}, \quad -\infty < r_2 < \infty, \\ u_3 &= \sinh A + \frac{r^2}{2}e^{-A}, \end{aligned} \tag{3.19}$$

where $r^2 = r_1^2 + r_2^2$. In this case the two exponentials on the left-hand side in Eq. (3.18) commute, i.e., $\{M_{01}+M_{31}, M_{02}+M_{32}\}$ is a (maximal) Abelian subalgebra of o(3,1). Hence we obtain two ignorable variables, r_1 and r_2.

The commuting set of operators is

$$Y_1 = \Delta(H_3), \quad Y_2 = (M_{01}+M_{31})^2, \quad Y_3 = (M_{02}+M_{32})^2.$$

7. O(3,1)⊃O(2)⊗O(1,1) [Fig. 2(g)]

The most convenient parametrization is

$$H = e^{M_{01}B}e^{M_{23}\phi}e^{M_{02}A}, \tag{3.20}$$

which yields

$$\begin{aligned} u_0 &= \cosh A \cosh B, \quad 0 \leqslant A < \infty, \\ u_1 &= \cosh A \sinh B, \quad -\infty < B < \infty, \\ u_2 &= \sinh A \cos\phi, \quad 0 \leqslant \phi < 2\pi, \\ u_3 &= \sinh A \sin\phi. \end{aligned} \tag{3.21}$$

The subalgebras M_{01} and M_{23} commute, hence both B and ϕ are ignorable variables and $\{M_{01}, M_{23}\}$ is a maximal Abelian subalgebra of O(3,1).

The commuting set of operators are

$$Y_1 = \Delta(H_3), \quad Y_2 = M_{01}^2, \quad Y_3 = M_{23}^2.$$

For a classification of maximal Abelian subalgebras of o(p,q) see Ref. 18, for those of the pseudo-Euclidean Lie algebras $e(p,q)$; see Refs. 19 and 20.

All subgroup and coordinate diagrams for O(3,1) and the hyperboloid H_3 are shown in Fig. 2. The ones that differ qualitatively from tree diagrams for O(4) are Figs. 2(d)–2(f), involving Euclidean subalgebras of O(3,1) and hence horospheric type coordinates.

Our parametrization of the group elements $G\sim$O(3,1) is such that we can read off coordinates on H_n, as in the case of O(2,1) from the coordinate diagrams (for $2\leqslant n$) as follows. For subgroup chains not involving $E(n)$ groups we start at the bottom of the coordinate diagram. When proceeding along the line leading to u_0 in the ambient space, we write $\cosh A_i$, when we go to the left, $\sinh A_i$ when we go to the right (toward a spacelike coordinate in the ambient space). When we proceed along a line toward a spacelike coordinate, then again for each vertex we write $\cos\theta_i$ when we go to the left, $\sin\theta_i$ when we go to the right [as for S_n (Refs. 13–15)]. The $E(n)$ subgroups always occur at the end of a chain. Before we come to the corresponding ''fork'' or ''tri-tail'' on the diagram we proceed as before ($\cosh A_i$ to the left, $\sinh A_i$ to the right). The fork and the box in it [see Fig. 3 for O$(n,1)$] corresponds to coordinates in a Euclidean space E_n.

D. Subgroup diagrams and coordinate diagrams for O(n,1)

The two cases considered previously, O(2,1) and O(3,1), have demonstrated two features of the general case. The first is that subgroup type coordinates are generated by successively applying the action of a chain of one-dimensional subgroups to the origin $\mathbb{1}$ of the hyperboloid. The second is that the process is recursive. To obtain all subgroup type coordinates on the hyperboloid $H_{n,1}$ we will need to know all subgroup type coordinates on hyperboloids $H_{k,1}$ $(2\leqslant k<n)$, spheres S_k $(3\leqslant k\leqslant n)$, and Euclidean spaces E_k, $(2\leqslant k\leqslant n-1)$.

The actual formula for generating the coordinates is

$$\mathbf{u}=He^{M_{0k}}\mathbb{1}, \tag{3.22}$$

where k is either $k=1$ or $k=n$ and HG_1 of Eq. (3.1) is the Lorentz group O$(n-1,1)$, the rotation group O(n), the Euclidean group $E(n-1)$, or a direct product O$(n_1,1)\otimes$O(n_2), $n_1+n_2=n$. The group $G_1\sim$O$(n-2)$ acts trivially, so we omit it in Eq. (3.22), even though H itself is not, in general, a group. Actually, H is a product of one-dimensional subgroups and we now proceed to discuss different choices of H.

1. Subgroup chain O(n,1)⊃O(n−1,1)⋯⊃O(2,1)⊃O(1,1) [see Fig. 3(a)]

We write Eq. (3.22) as

$$\mathbf{u}=e^{M_{01}B}e^{M_{02}A_{n-1}}\cdots e^{M_{0n}A_1}\mathbb{1} \tag{3.23}$$

and obtain the coordinates

$$\begin{aligned}
u_0&=\cosh A_1\cosh A_2\cdots\cosh A_{n-1}\cosh B,\\
u_1&=\cosh A_1\cosh A_2\cdots\cosh A_{n-1}\sinh B,\\
u_2&=\cosh A_1\cosh A_2\cdots\sinh A_{n-1},\\
&\cdots\\
&\cdots\\
u_{n-2}&=\cosh A_1\cosh A_2\sinh A_3,\\
u_{n-1}&=\cosh A_1\sinh A_2,\\
u_n&=\sinh A_1.
\end{aligned} \tag{3.24}$$

Only the last coordinate introduced, namely B, is ignorable.

2. Subgroup chain $O(n,1)\supset O(n-1,1)\cdots\supset O(k,1)\supset O(k)$ [see Fig. 3(b)]

Equation (3.22) in this case is

$$\mathbf{u}=Ge^{M_{01}A_{n-k+1}}e^{M_{0k+1}A_{n-k}}\cdots e^{M_{0n-1}A_2}e^{M_{0n}A_1}\rrbracket, \tag{3.25}$$

where $G\sim \mathrm{O}(k)$, $k\geqslant 2$. The coordinates are

$$\begin{aligned}
u_0&=\cosh A_1\cosh A_2\cdots\cosh A_{n-k+1},\quad 1\leqslant a\leqslant k,\\
u_a&=\cosh A_1\cosh A_2\cdots\cosh A_{n-k+1}s_a,\\
u_{k+1}&=\cosh A_1\cosh A_2\cdots\sinh A_{n-k},\\
&\cdots\\
&\cdots\\
u_{n-2}&=\cosh A_1\cosh A_2\sinh A_3,\\
u_{n-1}&=\cosh A_1\sinh A_2,\\
u_n&=\sinh A_1.
\end{aligned} \tag{3.26}$$

The variables s_a satisfy

$$s_1^2+s_2^2+\cdots+s_k^2=1 \tag{3.27}$$

and are parametrized by introducing spherical, or polyspherical coordinates on the sphere S_k.[11–15] The ignorable variables are "hidden" in s_a, $a=1,2,\ldots,k$. The number of ignorable variables N_I satisfies $1\leqslant N_I\leqslant[k/2]$ where we have $N_I=1$ for spherical coordinates on S_k, $N_I=[k/2]$ for cylindrical coordinates.

3. The subgroup chain $O(n,1)\supset O(n-1,1)\cdots\supset O(k,1)\supset E(k-1)$ [see Fig. 3(c)]

Equation (3.22) in this case

$$\mathbf{u}=Ge^{M_{0k}A_{n-k+1}}e^{M_{0n+1}A_{n-k}}\cdots e^{M_{0n}A_1}\rrbracket \tag{3.28}$$

with $G\sim E(k-1)$, $k\geqslant 2$. The coordinates are

$$\begin{aligned}
u_0&=\cosh A_1\cosh A_2\cdots\cosh A_{n-k}\left(\cosh A_{n-k+1}+\frac{r^2}{2}e^{-A_{n-k+1}}\right),\\
u_a&=\cosh A_1\cosh A_2\cdots\cosh A_{n-k}e^{-A_{n-k+1}}r_a,\quad 1\leqslant a\leqslant k-1,\\
u_k&=\cosh A_1\cosh A_2\cdots\cosh A_{n-k}\left(\sinh A_{n-k+1}+\frac{r^2}{2}e^{-A_{n-k+1}}\right),\\
u_{k+1}&=\cosh A_1\cosh A_2\cdots\sinh A_{n-k},\\
&\cdots\\
u_{n-2}&=\cosh A_1\cosh A_2\sinh A_3,
\end{aligned} \tag{3.29}$$

$$u_{n-1}=\cosh A_1 \sinh A_2,$$

$$u_n=\sinh A_1.$$

We have

$$r_1^2+r_2^2+\cdots+r_{k-1}^2=r^2, \quad -\infty<r_a<\infty \tag{3.30}$$

and r_a are coordinates in $k-1$ dimensional Euclidean space. The Euclidean Lie algebra $e(k-1)$ has the basis

$$\{M_{0a}+M_{ka}, M_{bc}\}, \quad 1\leqslant a\leqslant k-1, \quad 1\leqslant b<c\leqslant k-1. \tag{3.31}$$

Subgroup coordinates, subgroup diagrams, and coordinate diagrams (called "cluster diagrams") were discussed in detail in an earlier article.[15] In particular we can simply use r_a, $1\leqslant a\leqslant k-1$ as Cartesian coordinates, generated by $\exp(M_{0a}+M_{ka})r_a$. In this case $r_1,\ldots,r_{k-1}$ are ignorable variables since $\{M_{01}+M_{k1},\ldots,M_{0k-1}+M_{kk-1}\}$ is a maximal Abelian subalgebra[18] of O(k,1). The minimal number of ignorable variables in this case is $N_I=1$, obtained if we introduce spherical coordinates in the Euclidean space E_k.

4. The subgroup chain $O(n,1)\supset O(n-1,1)\cdots\supset O(k,1)\supset O(k_1,1)\otimes O(k_2)$, $k_1+k_2=k$, $3\leqslant k\leqslant n$, $1\leqslant k_1$, $2\leqslant k_2$

Equation (3.22) in this case

$$\mathbf{u}=G_1G_2e^{M_{0k_1+1}A_{n-k+1}}e^{M_{0k+1}A_{n-k}}\cdots e^{M_{0n-1}A_2}e^{M_{0n}A_1}\rceil \tag{3.32}$$

with $G_1\sim O(k_1,1)$, $1\leqslant k_1\leqslant k-2$, and $G_2\sim O(k_2)$, $2\leqslant k_2\leqslant k-1$,

$$u_\alpha=\cosh A_1\cosh A_2\cdots\cosh A_{n-k}\cosh A_{n-k+1}x_\alpha, \quad 0\leqslant\alpha\leqslant k_1,$$

$$u_a=\cosh A_1\cosh A_2\cdots\cosh A_{n-k}\sinh A_{n-k+1}s_a, \quad k_1+1\leqslant a\leqslant k_1+k_2=k,$$

$$u_{k+1}=\cosh A_1\cosh A_2\cdots\sinh A_{n-k},$$

$$\cdots \tag{3.33}$$

$$u_{n-2}=\cosh A_1\cosh A_2\sinh A_3,$$

$$u_{n-1}=\cosh A_1\sinh A_2,$$

$$u_n=\sinh A_1.$$

The coordinates x_α and s_a satisfy

$$x_0^2-x_1^2-x_2^2-\cdots-x_{k_1}^2=1, \tag{3.34}$$

$$s_{k_1+1}^2+s_{k_1+2}^2+\cdots+s_{k_1+k_2}^2=1. \tag{3.35}$$

The hyperboloid (3.34) must be parametrized according to some subgroup chain of $O(k_1,1)$, using the diagrams of Fig. 3 with n replaced by k_1 (a lower dimensional problem). Similarly, the sphere (3.35) is parametrized according to the "method of trees."[10–14]

The recursive character of the subgroup type coordinates is very clear in Fig. 3. The parametrization is complete only in Fig. 1(a) [see Eq. (3.24)]. In Figs. 1(b), 1(c), and 1(d) the spaces (3.27), (3.30), (3.34) and (3.35), respectively, remain to be parametrized.

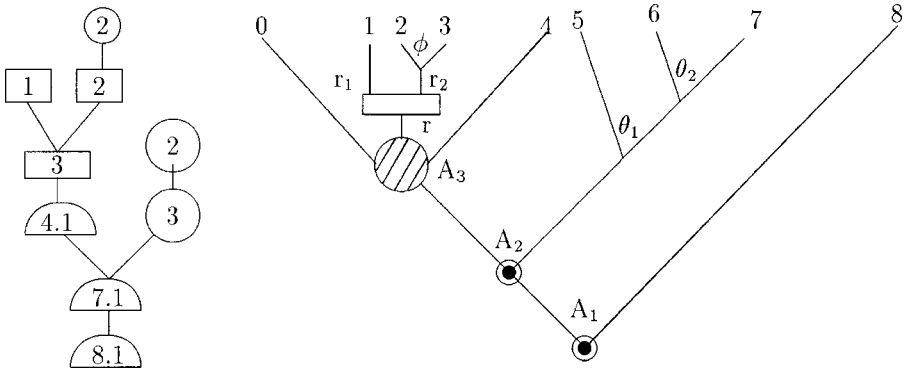

FIG. 4. Example of a subgroup and coordinate diagram for the O(8,1) hyperboloid.

The conventions are so chosen that the coordinate systems are obtained as for O(2,1) and O(3,1). We write $\cosh A_i$ when we go left at a vertex on the coordinate diagram, $\sinh A_i$ when we go right.

As an example, let us consider the subgroup and coordinate diagrams shown in Fig. 4 for the hyperboloid H_8. The coordinates and complete set of commuting operators are

$$
\begin{aligned}
u_0 &= \cosh A_1 \cosh A_2 (\cosh A_3 + \tfrac{1}{2}(r_1^2 + r_2^2) e^{-A_3}),\\
u_1 &= \cosh A_1 \cosh A_2 e^{-A_3} r_1,\\
u_2 &= \cosh A_1 \cosh A_2 e^{-A_3} r_2 \cos\phi,\\
u_3 &= \cosh A_1 \cosh A_2 e^{-A_3} r_2 \sin\phi,\\
u_4 &= \cosh A_1 \cosh A_2 (\sinh A_3 + \tfrac{1}{2}(r_1^2 + r_2^2) e^{-A_3}),\\
u_5 &= \cosh A_1 \sinh A_2 \cos\theta_1,\\
u_6 &= \cosh A_1 \sinh A_2 \sin\theta_1 \cos\theta_2,\\
u_7 &= \cosh A_1 \sinh A_2 \sin\theta_1 \sin\theta_2,\\
u_8 &= \sinh A_1,
\end{aligned}
\tag{3.36}
$$

$$
\begin{aligned}
&Y_1 = \Delta_{\mathrm{LB}}, \quad Y_2 = \sum_{i=1}^{7} M_{0i}^2 - \sum_{1 \le i < k \le 7}^{n} M_{ik}^2, \quad Y_3 = \sum_{i=1}^{4} M_{0i}^2 - \sum_{1 \le i < k \le 4}^{n} M_{ik}^2,\\
&Y_4 = \sum_{i=1}^{3} (M_{0i} + M_{4i})^2, \quad Y_5 = M_{01} + M_{41}, \quad Y_6 = M_{23}, \quad Y_7 = M_{56}^2 + M_{57}^2 + M_{67}^2, \quad Y_8 = M_{67}^2.
\end{aligned}
\tag{3.37}
$$

IV. SOLUTIONS OF THE LAPLACE–BELTRAMI EQUATION FOR THE GROUP O(2,1) AND O(3,1)

A. General comments

The general form of the Laplace–Beltrami operator for any Riemannian, or pseudo-Riemannian space is given in Eq. (2.2).

For the hyperboloid H_n we wish to solve Eq. (1.1) with Ψ as in Eq. (1.2). We will request that the function Ψ be normalizable with respect to the invariant measure for representations of the principal series of unitary representations of $O(n,1)$[12] when we have

$$\nu = -\frac{n-1}{2} + i\rho, \quad \rho \in \mathbb{R}. \tag{4.1}$$

For a (compact) rotation group $O(n+1)$ we have

$$\Delta_{LB}\Psi = \Delta(S_n)\Psi = -\ell(\ell+n-1)\Psi, \quad \ell \in I\mathbb{Z}, \tag{4.2}$$

and for a Euclidean group $E(n)$,

$$\Delta_{LB}\Psi = \Delta(E_n)\Psi = -k^2\Psi, \quad k \in \mathbb{R}, \tag{4.3}$$

where Δ is the Laplace operator.

We shall present normalizable eigenfunctions but do not give their normalization constants explicitly.

B. The group O(2,1)

The coordinates corresponding to Figs. 1(a), 1(b), and 1(c) are given in Eqs. (3.3), (3.5), and (3.7), respectively. In all cases, one coordinate is ignorable and figures only in an exponential. We take the solution as $\Psi(A,z) = f(A)e^{i\nu z}$ with $z = \phi$, B, or r, respectively. The equations for $f(A)$ and their normalizable solutions are, respectively,

(1) $O(2,1) \supset O(2)$,

$$\left[\frac{1}{\sinh A}\frac{\partial}{\partial A}\sinh A\frac{\partial}{\partial A} - \frac{m^2}{\sinh^2 A} - \nu(\nu+1)\right] f(A) = 0, \tag{4.4}$$

leading to

$$\Psi_{\nu m}(A,\phi) = P_\nu^m(\cosh A)e^{im\phi}, \quad m \in \mathbb{Z}, \quad \nu = -\tfrac{1}{2} + i\rho, \tag{4.5}$$

where $P_\nu^m(z)$ is an associated Legendre function.

(2) $O(2,1) \supset O(1,1)$,

$$\left[\frac{1}{\cosh A}\frac{\partial}{\partial A}\cosh A\frac{\partial}{\partial A} - \frac{k^2}{\cosh^2 A} - \nu(\nu+1)\right] f(A) = 0, \tag{4.6}$$

$$\Psi_{\nu k}(A,B) = \frac{1}{\sqrt{\cosh A}} P^{\nu+1/2}_{-1/2+ik}(\tanh A)e^{ikB}, \quad k \in \mathbb{R}, \quad \nu = -\frac{1}{2} + i\rho. \tag{4.7}$$

(3) $O(2,1) \supset E(1)$,

$$\left[e^A\frac{\partial}{\partial A}e^{-A}\frac{\partial}{\partial A} - k^2e^{2A} - \nu(\nu+1)\right] f(A) = 0, \tag{4.8}$$

$$\Psi_{\nu k}(A,r) = e^{A/2}K_{\nu+1/2}(ke^A)e^{ikr}, \tag{4.9}$$

where $K_\nu(z)$ is a modified Bessel function (of an imaginary argument), sometimes called a Macdonald function.[21,22]

C. The group O(3,1)

The coordinates corresponding to the diagrams in Figs. 2(a)–2(g) are (3.9), (3.11), (3.13), (3.15), (3.17), (3.19), and (3.21), respectively. The diagrams already indicate the recursive character of the procedure. The top row in the subgroup diagrams 2(a)–2(g) provides ignorable variables and hence exponentials in the solutions. The second row will provide functions that already occur in the separation of variables for the sphere S_2, the hyperboloid H_2, or the Euclidean space E_2. Figures 2(f) and 2(g) correspond to two ignorable variables. In all cases a new equation occurs only at the "ground level" of the diagrams and will involve the variable A. Let us run through all seven cases.

(1) $\mathrm{O}(3,1)\supset\mathrm{O}(3)\supset\mathrm{O}(2)$.

We put

$$\Psi_{n\ell m}(A,\theta,\phi)=f_{n\nu}(A)Y_{\ell m}(\theta,\phi). \tag{4.10}$$

In (4.10) $Y_{\ell m}(\theta,\phi)$ are spherical harmonics, coming from the O(3) subgroup with $\ell\in\mathbb{Z}$, $-\ell\leqslant m\leqslant\ell$. The function $f(A)$ satisfies

$$\left[\frac{1}{\sinh^2 A}\frac{\partial}{\partial A}\sinh^2 A\frac{\partial}{\partial A}-\frac{\ell(\ell+1)}{\sinh^2 A}-\nu(\nu+2)\right]f(A)=0, \tag{4.11}$$

and hence we obtain

$$f_{\nu\ell}(A)=\frac{1}{\sqrt{\sinh A}}P^{-\ell-1/2}_{1/2+\nu}(\cosh A),\quad \nu=-1+i\rho. \tag{4.12}$$

The negative sign in the superscript of the Legendre function was chosen to assure that the function is finite for $A=0$.

(2) $\mathrm{O}(3,1)\supset\mathrm{O}(2,1)$.

We consider diagrams of Figs. 2(b), 2(c), and 2(d) simultaneously, with $G\sim\mathrm{O}(2)$, O(1,1) and $E(1)$, respectively. We put

$$G\sim\mathrm{O}(2):\quad \Psi_{\nu_1\nu_2 m}(A,B,\phi)=f_{\nu_1\nu_2}(A)P^m_{\nu_2}(\cosh B)e^{im\phi}, \tag{4.13}$$

$$G\sim\mathrm{O}(1,1):\quad \Psi_{\nu_1\nu_2 k}(A,B,C)=f_{\nu_1\nu_2}(A)\frac{1}{\sqrt{\cosh B}}P^{\nu_2+1/2}_{-1/2+ik}(\tanh B)e^{ikC}, \tag{4.14}$$

$$G\sim E(1):\quad \Psi_{\nu_1\nu_2 k}(A,B,r)=f_{\nu_1\nu_2}(A)e^{B/2}K_{\nu_2+1/2}(ke^B)e^{ikr}. \tag{4.15}$$

The general form of the equations takes into account the results of Sec. IV B. The function $f_{\nu_1\nu_2}(A)$ is the same in all three cases. It satisfies

$$\left[\frac{1}{\cosh^2 A}\frac{\partial}{\partial A}\cosh^2 A\frac{\partial}{\partial A}+\frac{\nu_2(\nu_2+1)}{\cosh^2 A}-\nu_1(\nu_2+2)\right]f_{\nu_1\nu_2}(A)=0, \tag{4.16}$$

and is hence equal to

$$f_{\nu_1\nu_2}(A)=\frac{1}{\cosh A}P^{\nu_1+1}_{\nu_2}(\tanh A),\quad \nu_1=-1+i\rho,\quad \nu_2=-\frac{1}{2}+iq. \tag{4.17}$$

(3) $\mathrm{O}(3,1)\supset E(2)\supset G$.

We now consider diagrams of Figs. 2(e) and 2(f), with $G\sim\mathrm{O}(2)$ and $G\sim E(1)\otimes E(1)$, respectively. Subgroup coordinates in the Euclidean plane E_2 are either polar ($E(2)\supset\mathrm{O}(2)$) or Cartesian ($E(2)\supset E(1)\otimes E(1)$), so we put

$$\mathrm{O}(2): \quad \Psi_{\nu km}(A,r,\phi)=f_{\nu k}(A)J_m(kr)e^{im\phi}, \tag{4.18}$$

$$T(1)\otimes T(1): \quad \Psi_{\nu k_1 k_2}(A,r_1,r_2)=f_{\nu k}(A)e^{i(k_1 r_1+k_2 r_2)}, \quad k^2=k_1^2+k_2^2. \tag{4.19}$$

The function $f_{\nu k}(A)$ is the same in both cases and satisfies

$$\left[e^{2A}\frac{\partial}{\partial A}e^{-2A}\frac{\partial}{\partial A}-k^2e^{2A}-\nu(\nu+2)\right]f_{\nu k}(A)=0. \tag{4.20}$$

We obtain

$$f_{\nu k}(A)=e^A K_{\nu+1}(ke^A), \quad \nu=-1+i\rho. \tag{4.21}$$

(4) $\mathrm{O}(3,1)\supset \mathrm{O}(1,1)\otimes \mathrm{O}(2)$.
We have

$$\Psi_{\nu km}(A,B,\phi)=f_{\nu km}(A)e^{ikB}e^{im\phi}, \tag{4.22}$$

where $f_{\nu km}(A)$ satisfies

$$\left[\frac{1}{\sinh A\cosh A}\frac{\partial}{\partial A}\sinh A\cosh A\frac{\partial}{\partial A}-\frac{k^2}{\cosh^2 A}-\frac{m^2}{\sinh^2 A}-\nu(\nu+2)\right]f_{\nu km}(A)=0. \tag{4.23}$$

The solution can be written in terms of the hypergeometrical functions or in terms of Jacobi functions as

$$f_{\nu km}(A)=(\cosh A)^{ik}(\sinh A)^m P^{(m,ik)}_{(\nu-ik-m)/2}(\cosh 2A), \quad m\in\mathbb{Z}, \quad k\in\mathbb{R}, \quad \nu=-1+i\rho. \tag{4.24}$$

V. SOLUTIONS OF THE LAPLACE–BELTRAMI EQUATION FOR H_n

In Sec. IV we presented the separated solutions of the Laplace–Beltrami equation for all subgroup type coordinates on H_2 and H_3. The case of H_3 and the group O(3,1) illustrated the recursive character of the procedure. We will make use of this character to write out the solutions for the hyperboloid H_n for arbitrary n. To do this we need to know the basis functions for the spheres S_k, Euclidean spaces E_k, and hyperboloids H_k for $k\leqslant n-1$. The procedure depends only on the first link in the subgroup chain $\mathrm{O}(n,1)\supset G$ and we shall consider four cases separately.

A. $\mathrm{O}(n,1)\supset \mathrm{O}(n)$

This case is represented by Fig. 5(a). To the coordinates on S_{n-1} we add one hyperbolic angle A. The coordinates on H_n are

$$u_0=\cosh A, \quad u_i=s_i\sinh A, \quad s_1^2+s_2^2+\cdots+s_n^2=1. \tag{5.1}$$

The Laplace–Beltrami operator on H_n can be written as

$$\Delta(H_n)=\frac{1}{\sinh^{n-1}A}\frac{\partial}{\partial A}\sinh^{n-1}A\frac{\partial}{\partial A}+\frac{1}{\sinh^2 A}\Delta(S_{n-1}). \tag{5.2}$$

We write the solutions on H_n as

$$\Psi(A,\xi_1\cdots\xi_{n-1})=f_{\nu_n \diagup_{n-1}}(A)Y_{\diagup_{n-1},\ldots,\diagup_1}(\xi_1,\xi_2,\ldots,\xi_{n-1}) \tag{5.3}$$

where $f(A)$ satisfies

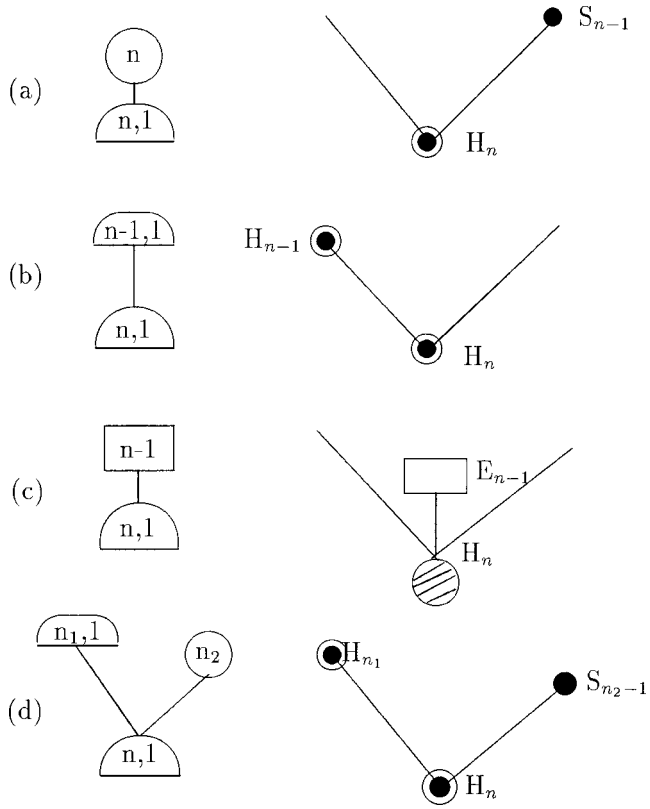

FIG. 5. Elementary links for H_n coordinate diagrams and O(n,1) subgroup diagrams.

$$\left[\frac{\partial^2}{\partial A^2}+(n-1)\coth A\frac{\partial}{\partial A}-\frac{\ell_{n-1}(\ell_{n-1}+n-2)}{\sinh^2 A}-\nu_n(\nu_n+n-1)\right]f_{\nu_n\ell_{n-1}}(A)=0. \tag{5.4}$$

The function $Y_{\ell_{n-1},\ldots,\ell_1}(\xi_1,\xi_2,\ldots,\xi_{n-1})$ is the solution of the Laplace–Beltrami equation on S_{n-1} in any one of the subgroup type coordinates on that space. That is, it corresponds to any one of the S_{n-1} tree diagrams.[13–15]

Equation (5.4) is easy to solve in terms of associated Legendre functions and we have

$$f_{\nu_n\ell_{n-1}}(A)=(\sinh A)^{(2-n)/2}P^{-\ell_{n-1}-(n-2)/2}_{\nu_n+(n-2)/2}(\cosh A). \tag{5.5}$$

The negative sign in the superscript was again chosen to assure that the function is finite for $A=0$. It should be remembered that ℓ_{n-1} refers to representations of the rotation group O(n) whereas ν_n to those of O(n,1). Hence, ℓ_{n-1} is an integer whereas ν_n satisfies $\nu_n=-(n-1)/2+ip_n$ for unitary representations of the principal series (with p_n real).

We mention that for the group O($n+1$) and the sphere S_n the corresponding formula can be written as

$$f_{l_n,l_{n-1}}(\theta)=(\sin\theta)^{(2-n)/2}P^{-l_{n-1}-(n-2)/2}_{l_n+(n-2)/2}(\cos\theta), \tag{5.6}$$

which corresponds to the diagrams in Fig. 6(a).

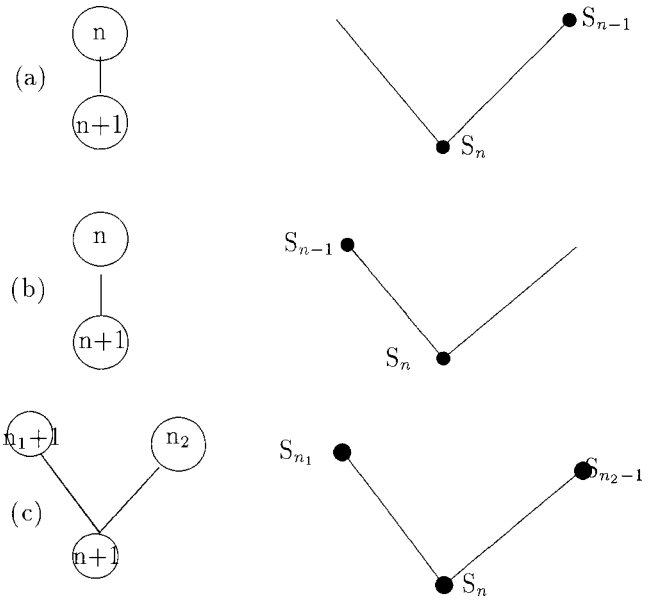

FIG. 6. Elementary links for S_n coordinate diagrams and $O(n+1)$ subgroup ones.

B. $O(n,1)\supset O(n-1,1)$

This case is represented in Fig. 5(b). We write coordinates on H_n as

$$u_\mu = x_\mu \cosh A, \quad u_n = \sinh A, \quad \mu = 0,1,2,\ldots,n-1, \quad x_0^2 - x_1^2 - \cdots - x_{n-1}^2 = 1. \tag{5.7}$$

The Laplace–Beltrami operator on H_n can be written in terms of the one on H_{n-1} as

$$\Delta(H_n) = \frac{1}{(\cosh^{n-1} A)} \frac{\partial}{\partial A}(\cosh^{n-1} A) \frac{\partial}{\partial A} + \frac{1}{\cosh^2 A} \Delta(H_{n-1}). \tag{5.8}$$

We again write the solutions on H_n as in Eq. (5.3), where $Y_{\ell_{n-1},\ldots,\ell_1}(\xi_1,\xi_2,\ldots,\xi_{n-1})$ is a set of eigenfunctions of $\Delta_{\mathrm{LB}}(H_{n-1})$ in some subgroup type coordinate system on H_{n-1}. The function $f(A)$ satisfies

$$\left[\frac{\partial^2}{\partial A^2} + (n-1)\tanh A \frac{\partial}{\partial A} + \frac{\nu_{n-1}(\nu_{n-1}+n-2)}{\cosh^2 A} - \nu_n(\nu_n+n-1)\right] f_{\nu_n \nu_{n-1}}(A) = 0. \tag{5.9}$$

The solution of this equation that is square integrable for representations of the principal series can again be expressed in terms of associated Legendre functions

$$f_{\nu_n \nu_{n-1}}(A) = (\cosh A)^{(1-n)/2} P^{\nu_n + (n-1)/2}_{\nu_{n-1} + (n-3)/2}(\tanh A). \tag{5.10}$$

Taking into account that we have $\nu_n = -(n-1)/2 + ip_n$, we can rewrite Eq. (5.10) as

$$f_{\nu_n \nu_{n-1}}(A) = (\cosh A)^{(1-n)/2} P^{ip_n}_{-1/2 + ip_{n-1}}(\tanh A). \tag{5.11}$$

For S_n, Eq. (5.10) is not convenient since the argument of the associated Legendre function would be imaginary. The contribution to the eigenfunction corresponding to the diagrams in Fig. 6(b) can be better written as

$$f_{l_n l_{n-1}}(\theta) = (\cos\theta)^{(-n+2)/2} P^{l_{n-1} + (n-2)/2}_{l_n + (n-2)/2}(\sin\theta). \tag{5.12}$$

C. $O(n,1)\supset E(n-1)$

We write coordinates corresponding to Fig. 5(c) as

$$u_0=\cosh A+\frac{r^2}{2}e^{-A},\quad r_1^2+r_2^2+\cdots+r_{n-1}^2=r^2,$$

$$u_i=r_i e^{-A},\quad i=1,2,\ldots,n-1, \tag{5.13}$$

$$u_n=\sinh A+\frac{r^2}{2}e^{-A}.$$

The Laplace–Beltrami operator on H_n is now expressed in terms of Laplace operator for the Euclidean space E_{n-1} as

$$\Delta(H_n)=e^{(n-1)A}\frac{\partial}{\partial A}e^{-(n-1)A}\frac{\partial}{\partial A}+e^{2A}\Delta(E_{n-1}). \tag{5.14}$$

The separated eigenfunctions have the form (5.3) where this time $Y_{\ell_n,\ldots,\ell_1}(\xi_1,\xi_2,\ldots,\xi_{n-1})$ are eigenfunctions of $\Delta(E_{n-1})$. The function $f_{\nu_n k}(A)$ satisfies

$$\left[\frac{\partial^2}{\partial A^2}-(n-1)\frac{\partial}{\partial A}-k^2e^{2A}-\nu_n(\nu_n+n-1)\right]f_{\nu_n k}(A)=0, \tag{5.15}$$

where we have put

$$\Delta Y=-k^2Y. \tag{5.16}$$

The function $f_{\nu_n k}$ satisfying Eq. (5.15) is best expressed in terms of modified Bessel functions as

$$f_{\nu_n k}(A)=e^{(n-1)/2A}K_{\nu_n+(n-1)/2}(ke^A) \tag{5.17}$$

or equivalently

$$f_{p_n k}(A)=e^{(n-1)/2A}K_{ip_n}(ke^A). \tag{5.18}$$

These formulas do not have an analog for the group $O(n+1)$.

D. $O(n,1)\supset O(n_1,1)\otimes O(n_2)$, $n_1+n_2=n$

We write the coordinates corresponding to Fig. 5(d) as

$$\begin{aligned} &u_\alpha=x_\alpha\cosh A,\quad \alpha=0,1,2,\ldots,n-1,\quad x_0^2-x_1^2-\cdots-x_{n_1}^2=1,\\ &u_n=s_i\sinh A,\quad i=n_1+1,..,n_1+n_2,\quad s_{n_1+1}^2+s_{n_1+2}^2+\cdots+s_{n_1+n_2}^2=1. \end{aligned} \tag{5.19}$$

The Laplace–Beltrami operator on H_n in this case is

$$\Delta(H_n)=\frac{1}{\cosh^{n_1}A\sinh^{n_2}A}\frac{\partial}{\partial A}\cosh^{n_1}A\sinh^{n_2}A\frac{\partial}{\partial A}+\frac{1}{\cosh^2 A}\Delta_{\mathrm{LB}}(H_{n_1})+\frac{1}{\sinh^2 A}\Delta_{\mathrm{LB}}(S_{n_2-1}). \tag{5.20}$$

The separated eigenfunctions of H_n have the form

$$\Psi(A,\xi_1,\ldots,\xi_{n_1},\eta_1,\ldots,\eta_{n_2-1})=f(A)\,Z(\xi_1,\ldots,\xi_{n_1})\,Y(\eta_1,\ldots,\eta_{n_2-1}), \tag{5.21}$$

where ξ_i and η_α are subgroup coordinates on H_{n_1} and S_{n_2-1}, respectively. The function $f(A)$ satisfies

$$\left[\frac{\partial^2}{\partial A^2}+[n_1\tanh A+(n_2-1)\coth A]\frac{\partial}{\partial A}+\frac{\nu_{n_1}(\nu_{n_1}+n_1-1)}{\cosh^2 A}-\frac{\ell_{n_2}(\ell_{n_2}+n_2-2)}{\sinh^2 A}-\nu_n(\nu_n+n-1)\right]f(A)=0. \tag{5.22}$$

The (normalizable) solutions of this equation can be expressed in terms of Jacobi functions as

$$f_{\nu_{n_1}\ell_{n_2}\nu_n}(A)=(\cosh A)^{\nu_{n_1}}(\sinh A)^{\ell_{n_2}}P_N^{(\alpha,\beta)}(\cosh 2A),$$
$$N=\frac{1}{2}(\nu_n-\nu_{n_1}-\ell_{n_1}),\quad \alpha=\ell_{n_2}+\frac{n_2-2}{2},\quad \beta=\nu_{n_1}+\frac{n_1-1}{2}. \tag{5.23}$$

The analog of Eq. (5.23) for the sphere S_n is

$$f_{\ell_n\ell_{n_1}\ell_{n_2}}(\theta)=(\cos\theta)^{\ell_{n_1}}(\sin\theta)^{\ell_{n_2}}P_N^{(\alpha,\beta)}(\cos 2\theta),$$
$$N=\frac{1}{2}(\ell_n-\ell_{n_1}-\ell_{n_2}),\quad \alpha=\ell_{n_2}+\frac{n_2-2}{2},\quad \beta=\ell_{n_1}+\frac{n_1-1}{2}. \tag{5.24}$$

It corresponds to the diagrams in Fig. 6(c) and $P_N^{(\alpha\beta)}$ is in this case a Jacobi polynomial.

VI. CONCLUSIONS

The main results of this article is that we have presented all separable subgroup type coordinates on a Lorentzian hyperboloid H_n, together with the corresponding separated eigenfunctions. We have introduced coordinate diagrams incorporating those introduced earlier for rotation groups[11–15] and Euclidian ones.[15] We have related the H_n coordinate diagrams to O(n,1) subgroup diagrams. Finally, we have shown that for arbitrary n the eigenfunctions of the Laplace operator involve products of the functions (5.5), (5.6), (5.10), (5.12), (5.17), (5.23) only. No new functions occur for higher dimensions, only associated Legendre functions and polynomials with various subscripts, superscripts and arguments, cylindrical functions, and Jacobi functions and polynomials.

The recursive formulas (5.2), (5.8), (5.14), and (5.20) bring out another feature of the separation of variables. Namely, they make it obvious that every separable coordinate system on the sphere S_{n-1} the hyperboloid H_{n-1}, the Euclidean space E_{n-1}, and the product space $H_{n1}\otimes S_{n_2-1}$ will provide separable coordinates on the hyperboloid H_n. We have emphasized this for subgroup type coordinates only, but we could also introduce ellipsoidal, paraboloidal, or other nonsubgroup coordinates on the lower dimentional manifolds and obtain ''semisubgroup'' [8] type coordinates on H_n.

This recursive character of separable coordinates in various spaces also gave rise to a different graphical formalism describing all coordinates in which the Laplace–Beltrami equation separates. The formalism was first introduced for the O($n+1$) spheres S_n and Euclidean spaces E_n,[23] then extended to n-dimensional hyperboloids.[10] In all cases certain ''irreducible'' types of coordinates

are introduced for any n. They are of ellipsoidal, or paraboloidal type. The graphs introduced by Kalnins and Miller then show how various coordinate systems in lower dimensions can be combined together to provide ''reducible'' type coordinates in higher dimensions. The diagrams introduced in the present paper can be directly mapped onto a proper subset of those used in Ref. 10.

The main new contributions are

(1) *The explicit relation between subgroup chains and subgroup type coordinates*.
(2) *The explicit construction of complete sets of invariant operators, their eigenfunctions, and eigenvalues*.

Finally, let us mention some directions for future research. In this article we have studied the separation of variables in the Laplace–Beltrami equation on H_n. We could also study the separation of variables in a Schrödinger equation, i.e., add a scalar potential, or scalar and a vector one to the Laplace–Beltrami operator. This would allow us to study quantum (and classical) integrable, or superintegrable, systems on hyperboloids. Another open problem is that of Lie algebra contractions in which the distance R, characterizing the hyperboloid $u_0^2-u_1^2-\cdots-u_n^2=R^2$ is subject to the limit $R\to\infty$. The hyperboloid will ''contract'' to a Euclidean, or pseudo-Euclidean space and we will obtain asymptotic formulas for the special functions involved (see Refs. 15, 24–26 for $S_n\to E_n$ contractions and Ref. 27 for $H_2\to E_2$ ones). Finally a systematic study of nonsubgroup type coordinates and their contractions is under consideration.

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Erratum: "The Fejér average and the mean value of a quantity in a quasiclassical wave packet" [J. Math. Phys. 43, 170 (2002)]

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The name of the first author, D. L. Aronstein, in Ref. 4, was mistyped. The authors apologize for this error and thank the Editor, R. G. Newton, for drawing their attention to it. Reference 4 is shown correctly below:

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Erratum: "Infinite infrared regularization and a state space for the Heisenberg algebra" [J. Math. Phys. 43, 243 (2002)]

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Time-energy coherent states and adiabatic scattering

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Coherent states in the time-energy plane provide a natural basis to study adiabatic scattering. We relate the (diagonal) matrix elements of the scattering matrix in this basis with the frozen on-shell scattering data. We describe an exactly solvable model, and show that the error in the frozen data cannot be estimated by the Wigner time delay alone. We introduce the notion of energy shift, a conjugate of Wigner time delay, and show that for incoming state $\rho(H_0)$ the energy shift determines the outgoing state. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1476952]

I. INTRODUCTION

Scattering from a slowly changing scatterer is described, to leading order, by a *time independent* scatterer frozen at the scattering time.[1] Although this seems like stating the obvious, it turns out that in trying to make precise how accurate this approximation is, one encounters both conceptual and technical difficulties. Our aim is to describe these difficulties and explain how they are resolved.

One conceptual difficulty is to understand what the frozen S matrix—a function of energy and scattering time—means. Strictly speaking, a function of both time and energy is in conflict with the uncertainty principle. A wave that is sharp in energy will have an ill-defined scattering time and, conversely, a wave with a well-defined scattering time is ill-defined in energy. What, then, is the meaning of the frozen S matrix?

The resolution of this problem is related to the fact that the adiabatic limit naturally leads to different parametrizations of time, and the right parametrization has small uncertainty. Specifically, the physical time t will parametrize the intrinsic ''fast'' dynamics and has the usual time-energy uncertainty $\hbar$. The slow variation in the external conditions will be parametrized by s. We refer to the latter as *epoch*. Since the epoch often plays the role of a parameter it is convenient to choose s dimensionless. The two parametrizations are related by $s=\omega t$, with ω a slow frequency—the adiabaticity parameter. The epoch-energy uncertainty then takes the form $\delta s\,\delta e \sim \hbar\omega$ and so arbitrarily small in the adiabatic limit.

Coherent states provide a convenient basis to analyze the semi-classical limit.[2,3] Semi-classical analysis is traditionally about the $\hbar\to 0$ limit, but is equally valid when $\hbar$ is fixed (and henceforth set equal to one) and $\omega\to 0$. Here we introduce coherent states labeled by points in the time-energy plane, with time being the scattering time. As we shall see, the frozen S matrix approximates the diagonal matrix elements of the dynamical scattering matrix in such coherent

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states. This reconciles the time-energy uncertainty with the frozen scattering data. In a further step, matrix elements of the frozen S matrix can be approximated by the on-shell data.

Another thorny issue that we address is when a description in terms of frozen data is meaningful and how accurate it is. The question can also be rephrased as a question about the intrinsic time scale relevant to scattering. If τ denotes this time scale, then $\omega\tau$ is the error in the frozen data and $\omega\tau \ll 1$ characterizes the adiabatic regime.

The Wigner time delay[14] $\tau_w(E,s)$ conveys information about the time the particle spends near the scatterer. It is a function of the energy E and scattering epoch s. It is tempting to hope that τ might be estimated by $\tau_w(E,s)$, but there is no compelling argument for doing so. One cannot argue on the basis of dimensional analysis alone, since $\dot{\tau}_w$ and $\sqrt{\tau_w'}$, with dot a derivative with respect to the epoch and prime with respect to the energy, give additional and independent time scales. In fact, since Wigner time delay is a *comparison* of the arrival time at a faraway point, relative to the time of arrival in the free dynamics, it is not even positive-definite. This suggests that it cannot quite capture τ, which is more closely related to the ''dwell time'' near the scatterer.

The way to determine τ is to consider the error in approximating the scattering data by the frozen data. The error is, to leading order, proportional to the adiabaticity parameter ω. Since the error is, in general, complex, we identify τ with the absolute value of the error divided by ω. Calculating the error, to leading order in ω, is no harder, and reminiscent of, calculating the scattering in the lowest order of the Born approximation.

We shall see that, to leading order, the adiabatic time scale τ can be estimated from the scattering data and the derivative of the Hamiltonian H with respect to the epoch, Eq. (7.4) below, but not from the Wigner time delay alone. We show this by considering an exactly soluble model where the dynamical S matrix can be computed explicitly.

We introduce the *energy shift* operator $\mathcal{E}$. This is a measure of the energy change in time dependent scattering and is a natural dual of the Wigner time delay. As we shall see, in the case that the incoming state is $\rho(H_0)$, the outgoing state is $\rho(H_0-\omega\mathcal{E})$. In the adiabatic limit, the energy shift can be approximated by the frozen energy shift, which is related to the logarithmic derivative of the on-shell scattering matrix with respect to the epoch, Eq. (4.2). The energy shift then gives a handle on the exchange of energy[4,5] and the pumping of charge in adiabatic scattering.[6,15]

II. ELEMENTS OF SCATTERING THEORY

Scattering theory is a comparison of dynamics: One is the actual dynamics generated by the time dependent $H(t)=H_s$, $(s=\omega\, t)$, the other is a fiducial dynamics generated by a *time independent* Hamiltonian H_0. The Hamiltonian H_0 is the generator of dynamics for which there is trivial scattering and the S matrix is the identity.

The results of this section are true in general, without taking the adiabatic limit $\omega\to 0$. We shall assume that H and H_0 admit good scattering. Namely, we assume the existence of wave operators and the unitarity of the S matrix. For explicit conditions on H_0 and $H(t)$ that guarantee this, see, e.g., Refs. 7 and 8.

A. The wave operator

Let $U(t'',t')$ and $U_0(t'',t')=U_0(t''-t')$ denote the evolution from time t' to t'', generated by $H(t)$ and the time-independent H_0, respectively.

Definition 2.1: The wave operators, based at epoch s, are defined by the (strong) limit

$$\Omega_{\pm}(s;H,H_0)=\lim_{t'\to\pm\infty} U(t,t')U_0(t'-t) \quad (s=\omega t). \tag{2.1}$$

The existence of the limit, and the equation of motion imply the following.

Proposition 2.2: The dependence of the wave operator on the base point s satisfy the differential equation

$$-i\omega\dot{\Omega}_{\pm}(s)=H_s\Omega_{\pm}(s,H,H_0)-\Omega_{\pm}(s,H,H_0)H_0. \tag{2.2}$$

As we shall presently see, the notion of wave operator based at epoch s is only interesting in the case of a time dependent $H(t)$.

B. The frozen wave operators

The frozen Hamiltonian H_s is *time independent* so $U(t'',t')=e^{iH_s(t''-t')}$, in this case, and $\Omega_{\pm}(s_0,H_s,H_0)$ is independent of the base point $s_0=\omega t_0$. This follows from the existence of the limit in Eq. (2.1) since $t'\to\pm\infty$ is the same as $t'-t_0\to\pm\infty$. To stress this we write $\Omega_{\pm}(H_s,H_0)$. From Eq. (2.2) then follows the standard intertwining relation of time-independent scattering theory:

Corollary 2.3: The wave operators $\Omega_{\pm}(H_s,H_0)$ relating the frozen Hamiltonian at epoch s and H_0 are independent of the base point, and intertwine the two dynamics:

$$H_s\Omega_{\pm}(H_s,H_0)=\Omega_{\pm}(H_s,H_0)H_0. \tag{2.3}$$

C. The dynamical S matrix

The (dynamical) scattering matrix based at epoch s is defined by

$$\mathcal{S}_d(s;H,H_0)=\Omega_+^{\dagger}(s;H,H_0)\Omega_-(s;H,H_0). \tag{2.4}$$

The S matrices based on different points in time are all related by conjugation generated by the free evolution. Namely, we have the following.

Proposition 2.4: Suppose that the wave operators exist. Then

$$\mathcal{S}_d(s;H,H_0)=e^{-iH_0t}\mathcal{S}_d(0;H,H_0)e^{iH_0t}\quad(s=\omega\ t). \tag{2.5}$$

This follows from $U(s,t)\Omega_{\pm}(s;H,H_0)=\Omega_{\pm}(s;H,H_0)e^{-iH_0(s-t)}$. Under a change of the reference Hamiltonian, say to the frozen Hamiltonian H_s,

$$\mathcal{S}_d(s;H,H_0)=\Omega_+^{\dagger}(H_s,H_0)\mathcal{S}_d(s;H,H_s)\Omega_-(H_s,H_0). \tag{2.6}$$

D. The frozen S matrix

In the frozen S data the epoch is decoupled from time. As such it can also be studied using time independent methods, which are normally quite powerful.[8] Its basic properties are in marked contrast with that of the dynamical S matrix, namely:

Corollary 2.5: The frozen S matrix

$$\mathcal{S}_f(H_s,H_0)=\Omega_+^{\dagger}(H_s,H_0)\Omega_-(H_s,H_0) \tag{2.7}$$

is independent of the base point. It depends on freezing time parametrically through H_s.

E. The on-shell S matrix

H_0 provides a basis that spans the Hilbert space of scattering states. Let $|E,j)$ denote the generalized eigenvectors of H_0:

$$H_0|E,j)=E|E,j),\quad (E,j|E',j')=\delta(E-E')\delta_{j,j'}. \tag{2.8}$$

E is the energy and j labels the scattering channels. $\mathcal{S}_f$ commutes with H_0, by Eq. (2.3), hence

$$(E,j|\mathcal{S}_f(H_s,H_0)|E',j')=\delta(E-E')S_{jj'}(s,E). \tag{2.9}$$

$S_{jj'}(s,E)$ is the *on-shell* scattering matrix. Note that in the frozen Hamiltonian the physical time is decoupled from the epoch, which now has been relegated to the role of a parameter. The on-shell scattering matrix therefore is not in conflict with the uncertainty principle.

III. THE ENERGY SHIFT

By taking the s-derivatives of Eq. (2.5) one gets

$$i\omega\dot{\mathcal{S}}_d(s)\mathcal{S}_d(s)^\dagger = H_0 - \mathcal{S}_d(s)H_0\mathcal{S}_d(s)^\dagger = [H_0,\mathcal{S}_d(s)]\mathcal{S}_d^\dagger(s) = [H_0,\mathcal{S}_d(s) - \mathcal{S}_f(H_s,H_0)]\mathcal{S}_d^\dagger(s). \tag{3.1}$$

This equation may be interpreted as follows. If we think of H_0 as the asymptotic observable associated with the outgoing energy, then $H_{0,in} = \mathcal{S}_d(s)H_0\mathcal{S}_d(s)^\dagger$ represents the asymptotic observable[9] corresponding to the incoming energy. This motivates calling

$$\mathcal{E}_d(s) = i\dot{\mathcal{S}}_d(s)\mathcal{S}_d^\dagger(s) \tag{3.2}$$

the operator of energy shift.

The energy shift vanishes for time independent scattering, as it must. It gives a handle on changes in (certain) quantum states. By the functional calculus applied to Eq. (3.1), for any function ρ,

$$\mathcal{S}_d(s)\rho(H_0)\mathcal{S}_d(s)^\dagger = \rho(H_0 - \omega\mathcal{E}_s(s)). \tag{3.3}$$

This is interpreted as follows: If $\rho(H_0)$ is the incoming state, then the corresponding outgoing state is $\rho(H_0 - \omega\,\mathcal{E}_s(s))$. The energy shift is a first order quantity in the adiabaticity parameter and, as we shall see, it can be approximated, to leading order, by the frozen data. This then gives a handle on the outgoing state ρ to first order in the adiabaticity parameter.

Proposition 3.1: The energy shift based on time s is conjugate to the energy shift based on time zero

$$\mathcal{E}_d(s) = e^{iH_0t}\mathcal{E}_d(0)e^{-iH_0t} \quad (s=\omega t). \tag{3.4}$$

This follows directly from Eqs. (2.5) and (3.1).

IV. THE PROBLEM OF ADIABATIC SCATTERING

The dynamical S matrix has qualitatively different properties from the frozen S matrix: The dynamical S matrix has no freezing time—it does not ''know'' when the incoming wave is going to hit the scatterer. It does depend, however, by conjugation, on a choice of a base point. In contrast, the frozen S matrix is independent of the choice of a base point and depends nontrivially on the freezing time. The frozen scattering data for one epoch know nothing *a priori* about the corresponding data at any other epoch.

Matrix elements of the scattering matrix carry information about the time that the wave is near the scatterer. For such matrix elements, the adiabatic limit can be expressed in terms of the corresponding frozen matrix elements. However, the introduction of wave packets promotes the epoch from playing the role of a parameter, to that of real, albeit slow, time. One then needs to confront the uncertainty principle. We do that by considering matrix elements between coherent states labeled by points in the energy time plane.

A. The Wigner time delay

The Wigner time delay is defined in terms of the on-shell scattering matrix. When this definition is transcribed to the frozen, on-shell, S matrix it reads

$$\tau_w(s,E) = -iS'(s,E)S^\dagger(s,E). \tag{4.1}$$

Prime denotes partial derivative with respect to the energy. With this definition, the Wigner time delay is a Hermitian matrix.

B. The frozen energy shift

For the frozen, on-shell, Hamiltonian one can associate a matrix of energy shift which is a natural conjugate of the Wigner time delay:

$$\mathcal{E}(s,E)=i\dot{S}(s,E)S^{\dagger}(s,E), \tag{4.2}$$

where dot denotes derivative with respect to the epoch.

C. Time scales

The frozen on-shell S matrix defines several time scales, among them τ_w and the (dimensionless) time scale $\mathcal{E}^{-1}$. The coherent states provide us with yet another time scale related to the time width of the coherent states. One of the problems of adiabatic scattering is to study the relation between these time scales and the time scale τ such that $\omega\tau\ll 1$ characterizes the adiabatic regime.

V. TIME-ENERGY COHERENT STATES

A. The role of dispersion

For a particle moving on the line, its energy and the time that it crosses the origin are canonical coordinates. One can therefore construct energy-time coherent states in analogy with the usual phase space coherent states. The explicit construction, however, depends on the dispersion law. For linear dispersion the construction is particularly simple.

Consider a classical particle with dispersion law $e(p)$ moving freely on the line. The velocity of the particle is $e'(p)$ so the time of passage through the origin is $t=-q/e'(p)$. Time-energy are (local) canonical coordinates since

$$de\wedge dt=dq\wedge dp. \tag{5.1}$$

The global aspects of the energy-time phase space can be complicated. For example, for a free (massive) particle, with quadratic dispersion $e(p)=p^2$, the energy-time phase space is made of two copies of the half plane $e\geqslant 0$ depending on the direction of crossing of the origin.

A simpler situation is obtained in the case of linear dispersion, $e(p)=p$. There is now no ambiguity in the direction of crossing and the energy-time phase space is again the plane. The map $(q,p)\leftrightarrow(e,t)$ is, in fact, the identity

$$e=p,\quad t=-q. \tag{5.2}$$

The usual coherent states are then also the coherent states on the energy-time plane.

B. Coherent states for linear dispersion

The time-energy coherent states are

$$|t,e;\varepsilon\rangle=e^{i(tP+eX)}|g_{\varepsilon}\rangle,\quad [P,X]=-i, \tag{5.3}$$

with g_{ε} Gaussian:

$$\langle p|g_{\varepsilon}\rangle=\frac{1}{\sqrt[4]{\pi\varepsilon^2}}e^{-p^2/2\varepsilon^2}. \tag{5.4}$$

They have the following properties:[2]

(A) The states $|t,e;\varepsilon\rangle$ are normalized.

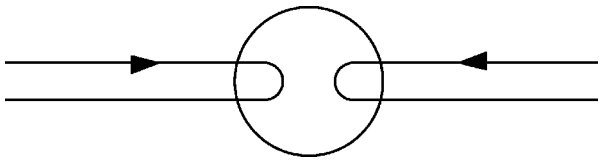

FIG. 1. A network of two channels. Each channel is chiral and lets particles propagate to and from infinity, according to the arrows. The circle denotes the region where the channels are coupled.

(B) $|t,e;\varepsilon\rangle$ have Gaussian localization in time and energy near the point (t,e) with width

$$\delta e \sim \varepsilon, \quad \delta t \sim \frac{1}{\varepsilon}, \quad \delta s \sim \frac{\omega}{\varepsilon}.$$

Hence ω plays the role of $\hbar$ in the epoch-energy plane.

(C) H_0 is the generator of shifts of the coherent states:

$$e^{-iH_0t'}|t,e;\varepsilon\rangle = e^{-it'e/2}|t-t',e;\varepsilon\rangle.$$

(D) The overlap of coherent states is

$$\langle t,e,\varepsilon|t',e',\varepsilon\rangle = e^{-(e-e')^2/4\varepsilon^2} e^{-\varepsilon^2(t-t')^2/4} e^{-i(et'-e't)/2}.$$

(E) The coherent states give a resolution of the identity

$$\int \frac{dtde}{2\pi} |t,e;\varepsilon\rangle\langle t,e;\varepsilon| = 1.$$

(F) The scalar product between coherent states and the eigenstates of $H_0 = P$ is

$$(E|t,e;\varepsilon\rangle = e^{-ite/2} e^{-itE} \frac{e^{-(E-e)^2/2\varepsilon^2}}{\sqrt[4]{\pi\varepsilon^2}}.$$

VI. SCATTERING BETWEEN CHANNELS WITH LINEAR DISPERSION

Linear dispersion approximates the low energy physics of electrons in one dimensional channels provided the Fermi energy is large. The price one pays is that the ''ultraviolet'' properties are pathological. In particular, the spectrum is unbounded below and this then leads to certain anomalies which must be correctly interpreted. With linear dispersion one can also solve certain models with interacting electrons.[10]

In the following we shall study adiabatic scattering for *noninteracting* particles with linear dispersion. The particles move on a collection of lines and are allowed to ''hop'' from one line to the other and scatter. Each line serves as an incoming and outgoing channel since the flow on it is unidirectional. An example with two channels is shown in Fig. 1. (Such models bear some resemblance to Schrödinger operators on graphs.)[11] The Hilbert space is $\oplus_{j=1}^{n} L^2(\mathbb{R})$, a finite direct sum. j labels the scattering channels. H_0 is then

$$(H_0\psi)(x,j) = -i\psi'(x,j), \quad x \in \mathbb{R}, \quad 1 \leqslant j \leqslant n.$$

For the interaction one may take, for example,

$$((H(s)-H_0)\psi)(x,j) = \sum_{j'} v_{j,j'}(x,s)\psi(x,j')$$

with $v_{jj'}$ Hermitian, and compactly supported. Alternatively, one may consider finite rank perturbations.

A. A soluble model

Here we describe a simple, time dependent, model for which the calculation of both the dynamical and frozen scattering matrices is reduced to quadrature.

Consider scattering on the line with

$$H_0 = P = -i\nabla, \quad H_s = P + f(s)V, \quad s = \omega\, t,$$

with $(V\psi)(x) = v(x)\psi(x)$ a potential (multiplication operator) which is sufficiently regular and short range so that $\int |v(x)|dx$, $\int |xv(x)|dx < \infty$. The model has one channel and should not be confused with the two-channel example pictured in Fig. 1.

To calculate the dynamical S matrix note that

$$\Omega(t,t') := U(t,t')U_0(t'-t), \tag{6.1}$$

satisfies the Volterra type equation:

$$\frac{\partial \Omega(t,t')}{\partial t'} = if(\omega t')\Omega(t,t')V(t-t'), \quad \Omega(t',t') = 1, \tag{6.2}$$

with $V(t)$ the (backward) free Heisenberg evolution of the potential, i.e.,

$$V(t) := U_0(t)VU_0(-t). \tag{6.3}$$

Since $H_0 = P$ is the generator of shifts, $V(t)$ is the shifted potential:

$$(V(t)\psi)(x) = v(x-t)\psi(x). \tag{6.4}$$

In particular, $V(t)$ at different times commute, and the solution of the Volterra type problem is given simply by

$$\Omega(t,t') = e^{-i\int_0^{t-t'} f(s-\omega t'')V(t'')dt''}, \quad s = \omega t. \tag{6.5}$$

From the definition of the wave operators based on time s, Eq. (2.1), we obtain for the dynamical wave operators

$$\Omega_-(s;H,H_0) = e^{-i\int_0^{\infty} f(s-\omega\, t')V(t')dt'}, \quad \Omega_+(s;H,H_0) = e^{i\int_{-\infty}^{0} f(s-\omega t')V(t')dt'}.$$

From this we obtain for the dynamical scattering matrix

$$S_d(s,H,H_0) = e^{-i\int_{-\infty}^{\infty} f(s-\omega t')V(t')dt'}. \tag{6.6}$$

The dynamical scattering matrix, as well as the wave operators, are local gauge transformations, i.e., multiplication by a *function* of position, of modulus one.

The wave operators and the S matrix reduce to the frozen ones upon replacing the function $f(s-\omega t')$ by its frozen value $f(s)$, hence,

$$S_f(H_s,H_0) = e^{-if(s)\int_{-\infty}^{\infty} V(t)dt} = e^{-if(s)\int_{-\infty}^{\infty} V_+(t)dt}, \tag{6.7}$$

where $2V_+(t) = V(t) + V(-t)$. S_f is just a number, not a function of position.

The frozen scattering matrix provides very little information on the potential $v(x)$, for it depends on just one number—the total weight of the potential (this is in sharp contrast with scattering problems where H_0 is the Laplacian[12]). The dynamical S matrix, in contrast, provides independent information about the potential for each value of s.

Since the frozen S matrix is independent of the incident energy, the Wigner time delay vanishes identically in this model: $\tau_w=0$. The (frozen) energy shift is just a real number (a multiple of the identity)

$$\mathcal{E}_f=\dot{f}(s)\int_{-\infty}^{\infty}v(x)dx.$$

In contrast, the dynamical energy shift is the multiplication operator:

$$\mathcal{E}_d=\int_{-\infty}^{\infty}\dot{f}(s-\omega\ t')V(t')dt'. \tag{6.8}$$

B. The on-shell scattering matrix and coherent states

For later purposes we shall need the matrix elements of the frozen S matrix. Since $\mathcal{S}_f$ commutes with H_0, the matrix elements are independent of t and are related to the on-shell matrix by

$$\langle t,e,j;\varepsilon|\mathcal{S}_f(H_s,H_0)|t,e,j';\varepsilon\rangle=\frac{1}{\sqrt{\pi}\varepsilon}\int dES_{jj'}(s,E)e^{-(E-e)^2/\varepsilon^2}=S_{jj'}(s,e)+O(\varepsilon^2\partial_{EE}S). \tag{6.9}$$

The estimate is obtained by observing that $S_{jj'}(s,E)-S_{jj'}(s,e)$ does not contribute to the integral to first order in $E-e$. Since

$$(\partial_{EE}S)S^{\dagger}=-\tau_w^2+i\tau_w'$$

(with prime denoting the derivative with respect to the energy), we see that the on-shell S matrix approximates the diagonal entries of the frozen S matrix, provided the Wigner time delay and its energy dependence are both small:

$$\varepsilon^2(\tau_w^2+|\tau_w'|)\ll 1. \tag{6.10}$$

VII. THE ADIABATIC TIME SCALE τ

In this section we compute, to leading order, the time scale τ relevant to adiabatic scattering. This time scale is defined so that $\omega\tau\ll 1$ characterizes the adiabatic regime in the sense that the frozen scattering data approximate the dynamical scattering data.

There are two results in this section, one positive and one negative. The positive result says that, at least to leading order, τ can be computed from time independent quantities alone, Eq. (7.4) below. The negative result is that τ cannot be computed from the on-shell scattering matrix and its derivatives. In particular, the Wigner time delay alone does not determine τ.

Using Eqs. (2.5)–(2.7) and property (C) in Sec. V B, one finds

$$\begin{aligned}&\langle t,e,j;\varepsilon|(\mathcal{S}_d(0;H,H_0)-\mathcal{S}_f(H_s,H_0))|t,e,j';\varepsilon\rangle\\&\quad=\langle 0,e,j;\varepsilon|\Omega_+^{\dagger}(H_s,H_0)(\mathcal{S}_d(s;H,H_s)-1)\Omega_-(H_s,H_0)|0,e,j;\varepsilon\rangle.\end{aligned} \tag{7.1}$$

The correction to the leading order of the S matrix can be approximated by an analog of the Born series:[8]

$$\mathcal{S}_d(s;H,H_s)-1\approx -i\int_{-\infty}^{\infty}e^{iH_st'}(H_{s+\omega\ t'}-H_s)e^{-iH_st'}dt'. \tag{7.2}$$

Since $H_{s+\omega t'}-H_s$ is supported near the origin, only small t' contribute to the matrix elements in Eq. (7.1). More precisely, this depends only on the time localization property of either the bra or the ket. We can therefore approximate $H_{s+\omega\, t'}-H_s \approx \omega\, t' \dot{H}_s$. Using property (C) in Sec. V B,

$$e^{-iH_s t}\Omega_-(H_s,H_0)|0,e,j;\varepsilon\rangle = e^{-iet/2}\Omega_-(H_s,H_0)|t,e,j;\varepsilon\rangle,$$

we finally get

$$\langle t,e,j;\varepsilon|(\mathcal{S}_d(0;H,H_0)-\mathcal{S}_f(H_s,H_0))|t,e,j';\varepsilon\rangle \approx -i\omega\tau(e,s;\varepsilon), \tag{7.3}$$

where

$$\tau(e,s;\varepsilon)=\int_{-\infty}^{\infty}\langle t',e,j;\varepsilon|\Omega_+^{\dagger}(H_s,H_0)\dot{H}_s\Omega_-(H_s,H_0)|t',e,j;\varepsilon\rangle t'\,dt'. \tag{7.4}$$

$\tau(e,s;\varepsilon)$ involves the frozen wave operators and the rate of change of the Hamiltonian at the epoch s. In particular, one can use methods of time-independent scattering theory to compute it. It is in general complex. The adiabatic time scale, $\tau=|\tau(e,s;\varepsilon)|$, is a measure of the error. $\omega\tau \ll 1$ then clearly characterizes the adiabatic regime.

Propagation estimates can, and have been, used[13] to bound the error in the frozen data. These estimates yield bounds on τ.

A. Example: The soluble model

For the case of one channel scattering with $H(s)=P+f(s)V$, by Eqs. (6.6) and (6.7)

$$\begin{aligned} S_d(s;H,H_0)-S_f(H_s,H_0) &= (e^{-i\int_{-\infty}^{\infty}(f(s-\omega t)-f(s))V(t)dt}-1)S_f(H_s,H_0) \\ &\approx i\omega\dot{f}(s)\left(\int_{-\infty}^{\infty} tV(t)dt\right)S_f(H_s,H_0). \end{aligned} \tag{7.5}$$

The adiabatic time scale τ is, in analogy with Eq. (7.3), the multiplication operator:

$$\tau \approx -\dot{f}(s)\left(\int_{-\infty}^{\infty} tV(t)dt\right)S_f(H_s,H_0) = -\dot{f}(s)\left(\int_{-\infty}^{\infty} tV_-(t)dt\right)S_f(H_s,H_0);$$

$$2V_-(t)=V(t)-V(-t). \tag{7.6}$$

By Eq. (6.7) the frozen S matrix only depends on V_+, while the error only depends on V_-. Since V_- and V_+ are independent this shows that the error term in the adiabatic expansion cannot be estimated in terms on the frozen scattering data alone.

Combining Eqs. (6.9) and (7.3) we obtain a relation between matrix elements of the dynamical S matrix and the on-shell S matrix:

$$\langle t,e,j;\varepsilon|\mathcal{S}_d(0;H,H_0)|t,e,j';\varepsilon\rangle = S_{jj'}(s,e)+O(\varepsilon^2(\tau_w^2+|\tau_w'|)+\omega\tau(e,s;\varepsilon)). \tag{7.7}$$

VIII. THE ENERGY SHIFT

The energy shift is a first order quantity; nevertheless, it is determined, to leading order, by the frozen data:

$$\langle t,e,j;\varepsilon|\mathcal{E}_d(0)|t,e,j';\varepsilon\rangle \approx i(\dot{S}(s,e)S^{\dagger}(s,e))_{jj'} \quad (s=\omega\, t). \tag{8.1}$$

We first remark that (7.3) and (7.4) generalize to off-diagonal matrix elements, i.e., the time t in the ket $|t,e,j';\varepsilon\rangle$ may be shifted to $t+\Delta t$ [resp. $t'+\Delta t$ in (7.4)] while leaving the bra unchanged. By the translation property of coherent states, property (C) in Sec. II B, multiplication by H_0 can be traded for derivative with respect to time. Hence

$$\begin{aligned}\langle t,e,j;\varepsilon|[H_0,\mathcal{S}_d(0;H,H_0)]|t+\Delta t,e,j';\varepsilon\rangle &= i\partial_t\langle t,e,j;\varepsilon|\mathcal{S}_d(0;H,H_0)|t+\Delta t,e,j';\varepsilon\rangle \\ &\approx i\partial_t\langle t,e,j;\varepsilon|\mathcal{S}_f(H_s,H_0)|t+\Delta t,e,j';\varepsilon\rangle \\ &= i\omega\langle t,e,j;\varepsilon|\dot{\mathcal{S}}_f(H_s,H_0)|t+\Delta t,e,j';\varepsilon\rangle. \quad (8.2)\end{aligned}$$

In principle, the order of the error in the frozen data in the passage from the second to the third line does not determine the order of the error in derivatives, but this can be justified in the present case. The last identity in the equation above can be seen from

$$\langle t,e,j;\varepsilon|\mathcal{S}_f(H_s,H_0)|t+\Delta t,e,j';\varepsilon\rangle = \frac{1}{\sqrt{\pi}\varepsilon}\int dE S_{jj'}(s,E)e^{-(E-e)^2/\varepsilon^2}e^{-i(\Delta t)e/2}e^{-i(\Delta t)E}.$$

We then multiply (8.2) with the complex conjugate of the mentioned generalization of (7.3) and integrate over Δt using property (E) of Sec. V B. The result then heuristically follows from Eq. (3.1) and the statement for $\mathcal{E}_f$ analogous to (6.9). An alternate derivation of (8.1) can be made, more directly, starting from the rhs of Eq. (3.1) and using Born's expansion.

The energy shift plays a role in the theory of adiabatic quantum pumps. In particular, the pumped charge, the entropy production and noise generation in quantum pumps can all be expressed in terms of the energy shift.[3] It is remarkable that basic properties of adiabatic quantum pumps can be understood, to leading order, in terms of the frozen scattering data alone.

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Coherent state realizations of su($n+1$) on the n-torus

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We obtain a new family of coherent state representations of SU($n+1$), in which the coherent states are Wigner functions over a subgroup of SU($n+1$). For representations of SU($n+1$) of the type (λ, 0, 0,...), the basis functions are simple products of n exponential. The corresponding coherent state representations of the algebra su($n+1$) are also obtained, and provide a polar decomposition of su($n+1$) for any $n+1$. The su($n+1$) modules thus obtained are useful in understanding contractions of su($n+1$) and su($n+1$)-phase states of quantum optics. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1479301]

I. INTRODUCTION

In this paper, we wish to present a new kind of coherent state[1] construction for the groups SU($n+1$). The construction is applicable to unitary irreducible representations (unirreps) of SU($n+1$) characterized by integral highest weights of the type (λ, 0,...) for which there is no weight multiplicity, described by Young tableaux having a single row.

Our coherent states differ from the usual coherent states in that our basis functions are functions over a subgroup $\mathfrak{k}$ of SU($n+1$) rather than polynomials in holomorphic variables. Because there is no multiplicity of weights in SU($n+1$) unirreps of the type (λ, 0,...), we can choose $\mathfrak{k}$ to be the Cartan subgroup of SU($n+1$). Basis functions for our modules are simple products of n exponential factors, and are closely related to the $\mathrm{SU}(3)\supset\mathrm{SO}(3)$ construction of Ref. 2.

The realization of su($n+1$) that we obtain is particularly well-suited for a discussion of polar decompositions of su($n+1$) generators. We consider as an application a study of phase states,[3–6] and, in particular, of SU(2) and SU(3) phase states. The general case can be inferred from the discussion of the SU(3) case and from the results of Sec. III.

Coherent states are also useful in understanding the ''semiclassical'' behavior of systems.[7] Our construction can also be used to understand some of the possible asymptotic limits of quantum systems. For SU($n+1$) unirreps of the type (λ, 0,...), which are applicable to ($n+1$)-channel interferometry,[6] the asymptotic limit corresponds to taking the number of (unpolarized) photons λ to be arbitrarily large. The parameters which enter in the explicit realization of the su($n+1$) generators will be related to the partition of λ photons between $n+1$ channels.

The construction is presented first for SU(2) in Sec. II. The general construction, valid for the irreps (λ, 0,...) of SU($n+1$) is presented in Sec. III. Section IV contains an application to SU(3) of the general formalism. Our paper ends with a discussion containing further results and a short conclusion.

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II. SU(2)

A. Coherent state representation of the su(2) algebra

A basis for A_1, the complex extension of the su(2) algebra, is given in the usual way, by the three operators $\{\hat{h}_1,\hat{e}_+,\hat{e}_-\}$ with nonzero commutation relations

$$[\hat{h}_1,\hat{e}_\pm]=\pm 2\hat{e}_\pm, \quad [\hat{e}_+,\hat{e}_-]=\hat{h}_1. \tag{1}$$

For λ any positive integer, a highest weight $|\chi_\lambda\rangle$ for an irrep of dimension $\lambda+1$ (the number λ is just twice the spin of the representation) is defined by

$$\hat{h}_1|\chi_\lambda\rangle=\lambda|\chi_\lambda\rangle, \quad \lambda\in\mathbb{Z}^+, \quad \hat{e}_+|\chi_\lambda\rangle=0. \tag{2}$$

Now it can be verified explicitly that the map Γ:

$$\begin{aligned}
&\hat{h}_1\mapsto\Gamma(\hat{h}_1)=-i\frac{\mathrm{d}}{\mathrm{d}\varphi},\\
&\hat{e}_+\mapsto\Gamma(\hat{e}_+)=-\frac{1}{2}e^{2i\varphi}(\tan\beta)^{-1}\left(\lambda+i\frac{\mathrm{d}}{\mathrm{d}\varphi}\right),\\
&\hat{e}_-\mapsto\Gamma(\hat{e}_-)=-\frac{1}{2}e^{-2i\varphi}(\tan\beta)\left(\lambda-i\frac{\mathrm{d}}{\mathrm{d}\varphi}\right),
\end{aligned} \tag{3}$$

preserves the commutation relations of su(2) and is therefore a realization of A_1. A carrier space for this representation is the span of exponential functions $\{e^{i\nu\theta},\nu=-\lambda,-\lambda+2,...,\lambda-2,\lambda\}$. The highest and lowest weight state proportional to $e^{i\lambda\theta}$ and $e^{-i\lambda\theta}$, respectively.

To obtain Eq. (3), one first chooses some fixed but otherwise arbitrary (generic) angle β in the range $0<\beta<2\pi$. With β fixed, the state $R_y(\beta)|\chi_\lambda\rangle$, where $R_y(\beta)=e^{(\hat{e}_+-\hat{e}_-)\beta}$, $R_z(\varphi)=e^{\varphi\hat{h}_1}$, is cyclic under the action of $R_z^{-1}(\varphi)$. $R_y(\beta)|\chi_\lambda\rangle$ then acts as a fiducial vector "translated" by $R_z^{-1}(\varphi)$.

Let $|\psi\rangle$ be an arbitrary state in the irrep with highest weight λ, and define the coherent state wave function for $|\psi\rangle$ by

$$|\psi\rangle\mapsto\psi_\beta(\varphi)\equiv\langle\chi_\lambda|R_y(\beta)R_z(\varphi)|\psi\rangle. \tag{4}$$

Since $\langle\chi_\lambda|\hat{e}_-=0$, it is convenient to write $R_y(\beta)$ in antinormal-ordered form, so that, ignoring a normalization and a phase factor,

$$\psi_\beta(\varphi)=\langle\chi_\lambda|R_y(\beta)R_z(\varphi)|\psi\rangle\propto\langle\chi_\lambda|e^{\tan\beta\hat{e}_+}R_z(\varphi)|\psi\rangle. \tag{5}$$

The coherent state realization $\Gamma(\hat{X})$ of an operator $\hat{X}$ in su(2) is defined by

$$\hat{X}|\psi\rangle\to[\Gamma(\hat{X})\psi]_\beta(\varphi)\equiv\langle\chi_\lambda|e^{\tan\beta\hat{e}_+}R_z(\varphi)\hat{X}|\psi\rangle. \tag{6}$$

Using $R_z(\varphi)=\exp(i\varphi\hat{h}_1)$, it follows immediately from this that

$$\hat{h}_1\mapsto\Gamma(\hat{h}_1)=-i\frac{\mathrm{d}}{\mathrm{d}\varphi}, \tag{7}$$

since

$$\Gamma(\hat{h}_1)\psi_\beta(\varphi)=\langle\chi_\lambda|e^{\tan\beta\hat{e}_+}R_z(\varphi)\hat{h}_1|\psi\rangle. \tag{8}$$

If $\hat{X}=\hat{e}_{\pm}$, we then have

$$[\Gamma(\hat{e}_{\pm})\psi_{\beta}](\varphi)=\langle\chi_{\lambda}|e^{\tan\beta\hat{e}_{+}}R_{z}(\varphi)\hat{e}_{\pm}|\psi\rangle=e^{\pm 2i\varphi}\langle\chi_{\lambda}|e^{\tan\beta\hat{e}_{+}}\hat{e}_{\pm}R_{z}(\varphi)|\psi\rangle. \tag{9}$$

The step which differentiates ours from the usual construction is to expand $\hat{e}_{\pm}$ as

$$\hat{e}_{\pm}=x_{\pm}e^{-\tan\beta\hat{e}_{+}}\hat{e}_{-}e^{\tan\beta\hat{e}_{+}}+y_{\pm}e^{-\tan\beta\hat{e}_{+}}\hat{h}_{1}e^{\tan\beta\hat{e}_{+}}+z_{\pm}\hat{h}_{1}, \tag{10}$$

where $x_{\pm}$, $y_{\pm}$, and $z_{\pm}$ are coefficients to be determined. This expansion is always possible since $\hat{e}_{\pm}$ is a traceless su(2) matrix and can therefore always be expanded in terms three linearly independent traceless matrices in A_1.

Before solving for the coefficients in Eq. (10), it is worth observing that, once substituted in Eq. (9), one obtains the simpler expression

$$\begin{aligned}[\Gamma(\hat{e}_{\pm})\psi_{\beta}](\varphi)&=e^{\pm 2i\varphi}(y_{\pm}\langle\chi_{\lambda}|\hat{h}_{1}e^{\tan\beta\hat{e}_{+}}R_{z}(\varphi)|\psi\rangle+z_{\pm}\langle\chi_{\lambda}|e^{\tan\beta\hat{e}_{+}}R_{z}(\varphi)\hat{h}_{1}|\psi\rangle)\\&=e^{\pm 2i\varphi}\left(\lambda y_{\pm}-iz_{\pm}\frac{\mathrm{d}}{\mathrm{d}\varphi}\right)\psi_{\beta}(\varphi),\end{aligned} \tag{11}$$

where Eq. (7), $\langle\chi_{\lambda}|\hat{h}_{1}=\lambda\langle\chi_{\lambda}|$ and $\langle\chi_{\lambda}|\hat{e}_{-}=0$ have been used.

Although they will depend on the parameter β, the coefficients $y_{\pm}$ and $z_{\pm}$ cannot depend on the particular choice of representation used to compute them, as long as the representation is faithful: if they did, commutation relations which would hold in a representation would not necessarily hold in another. Thus, one can compute these coefficients in the defining 2×2 representation, where

$$\hat{e}_{+}\mapsto\begin{pmatrix}0&1\\0&0\end{pmatrix},\quad \hat{e}_{-}\mapsto\begin{pmatrix}0&0\\1&0\end{pmatrix},\quad \hat{h}_{1}\mapsto\begin{pmatrix}1&0\\0&-1\end{pmatrix},\quad e^{\tan\beta\hat{e}_{+}}\mapsto\begin{pmatrix}1&\tan\beta\\0&1\end{pmatrix}. \tag{12}$$

For $\hat{X}=\hat{e}_{+}$, Eq. (10) yields the matrix system

$$\begin{pmatrix}0&1\\0&0\end{pmatrix}=x_{+}\begin{pmatrix}-\tan\beta&-\tan^{2}\beta\\1&\tan\beta\end{pmatrix}+y_{+}\begin{pmatrix}1&2\tan\beta\\0&-1\end{pmatrix}+z_{+}\begin{pmatrix}1&0\\0&-1\end{pmatrix}. \tag{13}$$

It is immediately possible to solve for x_{+}, as it multiplies the only matrix with a nonzero entry below the diagonal. Knowing x_{+}, it is then easy to solve for y_{+} and z_{+}. The solution is simply $y_{+}=-z_{+}=\frac{1}{2}(\tan\beta)^{-1}$ so that the final expression for $\Gamma(\hat{e}_{+})$ corresponds to that given in Eq. (3). Repeating the steps for $\hat{e}_{-}$ yields $x_{-}=1$ and $y_{-}=-z_{-}=\frac{1}{2}\tan\beta$ so that $\Gamma(\hat{e}_{-})$ has the form given in Eq. (3).

B. Basis functions

First, we claim that the set of states $\{R_{z}^{-1}(\varphi)R_{y}^{-1}(\beta)|\chi_{\lambda}\rangle,\ R_{z}^{-1}(\varphi)\in\mathrm{U}(1),\ \beta\ \text{fixed}\}$, obtained by U(1) rotation of the state $R_{y}^{-1}(\beta)|\chi_{\lambda}\rangle$ through all possible angle φ, spans the carrier space V_{λ} for an irrep of SU(2) with highest weight λ. To show this, recall that V_{λ} is generated from $|\chi_{\lambda}\rangle$ by repeated action of the lowering operator e_{-}. Now,

$$R_{z}^{-1}(\varphi)R_{y}^{-1}(\beta)|\chi_{\lambda}\rangle\propto R_{z}^{-1}(\varphi)e^{\tan\beta\hat{e}_{-}}|\chi_{\lambda}\rangle\propto e^{\tan\beta e^{-2i\varphi\hat{e}_{-}}}|\chi_{\lambda}\rangle e^{i\lambda\varphi} \tag{14}$$

by using the normal form of $e^{-\beta(\hat{e}_{+}-\hat{e}_{-})}$. This can be seen to indeed generate the whole of V_{λ} (provided that $\tan\beta\neq 0$, which is our assumption about β being generic).

Thus, to any state $|\psi\rangle$ in V_{λ} there corresponds a unique coherent state wave function

$$|\psi\rangle\mapsto\psi_{\beta}(\varphi)\equiv\langle\chi_{\lambda}|R_{y}(\beta)R_{z}(\varphi)|\psi\rangle, \tag{15}$$

which belongs to the set of U(1) square-integrable functions. In particular, the basis functions $|\lambda\nu\rangle$ are given by $\psi_{\beta;\lambda\nu}(\varphi)=\langle\chi_\lambda|R_y(\beta)|\lambda\nu\rangle e^{i\nu\varphi}$ and must be proportional to the only normalized function on the half-circle with weight ν:

$$\psi_{\beta;\lambda\nu}(\varphi)\propto\frac{1}{\sqrt{\pi}}e^{i\nu\varphi}. \tag{16}$$

Note that we can restrict to the half circle because the difference of two weights in an invariant subspace is always an even integer.

C. Making the representation Hermitian

The representation of su(2) given in Eq. (3) is not Hermitian with respect to the natural U(1) inner product. If, as usual, the adjoint of $\hat{e}_+$ is taken as $\hat{e}_-$, i.e., $\hat{e}_+^\dagger=\hat{e}_-$, then

$$\langle\lambda\nu'|\Gamma(\hat{e}_+)|\lambda\nu\rangle\neq\langle\lambda\nu|\Gamma(\hat{e}_-)|\lambda\nu'\rangle^* \tag{17}$$

if

$$\langle\psi_\beta|\psi'_\beta\rangle=\int_0^\pi d\varphi\,\psi^*_\beta(\varphi)\psi'_\beta(\varphi). \tag{18}$$

However, since λ is integral, the representation Γ must be equivalent to a Hermitian representation γ, i.e., there must exist an intertwining operator $\mathcal{K}$ such that

$$\mathcal{K}^{-1}\Gamma\mathcal{K}=\gamma,\quad\text{with}\quad\langle\lambda\nu'|\gamma(\hat{e}_+)|\lambda\nu\rangle=\langle\lambda\nu|\gamma(\hat{e}_-)|\lambda\nu'\rangle^*. \tag{19}$$

To construct the operator $\mathcal{K}$, note that $\Gamma(\hat{h}_1)$ is actually Hermitian in the representation of Eq. (3), so that $\mathcal{K}^{-1}\Gamma(\hat{h}_1)\mathcal{K}=\Gamma(\hat{h}_1)=\gamma(\hat{h}_1)$. Thus, $\mathcal{K}$ commutes with $\Gamma(\hat{h}_1)$ and weight eigenstates of $\Gamma(\hat{h}_1)$ are also weight eigenstates of $\mathcal{K}$. Let

$$\hat{h}_1|\lambda\nu\rangle=\nu|\lambda\nu\rangle,\quad\mathcal{K}|\lambda\nu\rangle=\mathcal{K}_\nu|\lambda\nu\rangle. \tag{20}$$

Using Eq. (19), the Hermiticity condition reads

$$\langle\lambda,\nu+2|\gamma(\hat{e}_+)|\lambda\nu\rangle=\frac{1}{2\tan\beta}(\lambda-\nu)\frac{\mathcal{K}_\nu}{\mathcal{K}_{\nu+2}}=\langle\lambda\nu|\gamma(\hat{e}_-)|\lambda,\nu+2\rangle^*=\frac{1}{2}\tan\beta(\lambda+\nu+2)\frac{\mathcal{K}^*_{\nu+2}}{\mathcal{K}^*_\nu} \tag{21}$$

from which we conclude that the ratio of $\mathcal{K}_{\nu+2}/\mathcal{K}_\nu$ must satisfy, up to a phase that we choose to be $+1$,

$$\frac{\mathcal{K}_{\nu+2}}{\mathcal{K}_\nu}=\frac{1}{\tan\beta}\sqrt{\frac{\lambda-\nu}{\lambda+\nu+2}}, \tag{22}$$

so that γ is indeed Hermitian and given explicitly by

$$\langle\lambda,\nu+2|\gamma(\hat{e}_+)|\lambda\nu\rangle=\frac{1}{2}\sqrt{(\lambda+\nu+2)(\lambda-\nu)}=\langle\lambda\nu|\gamma(\hat{e}_-)|\lambda,\nu+2\rangle. \tag{23}$$

D. Application: Phase operators and phase states

Any matrix M can be factorized in polar form $U\cdot D$, with U a unitary matrix and D a semipositive definite diagonal matrix.[8] The operator D is always well-defined. The unitary matrix U is the exponential of a Hermitian ''phase'' operator associated with the phase of the observable

described by the matrix M. The problems of constructing a phase operator in a finite or semi-infinite dimensional space are related to the lack of uniqueness in the definition of U which occurs when the rank of M is smaller than its dimension.

Our realization Γ acts in a natural way in the infinite dimensional irreducible space spanned by the set of U(1) functions (phase functions) $V_{\sigma_2}=\{e^{i(2p+\sigma_2)\varphi}/\sqrt{\pi}, p\in\mathbb{Z}\}$, where σ_2 is the "duality" of the representation: $\sigma_2=0$ for bosons and $\sigma_2=1$ for fermions. Furthermore, the realization Γ of $\hat{e}_+$ or $\hat{e}_-$ can obviously be factored as a product of two operators. One may easily show that the "diagonal" part of the decomposition of $\Gamma(\hat{e}_\pm)$ obtained, to within a sign, from $\sqrt{\Gamma^\dagger(\hat{e}_\pm)\Gamma(\hat{e}_\pm)}$.

We are primarily interested in the matrix representation of the operator $\hat{E}_\varphi \equiv e^{2i\varphi}$. In the infinite-dimensional space V_{σ_2}, the matrix representation of $\hat{E}_\varphi$ contains zeroes everywhere, except immediately above the diagonal. $\hat{E}_\varphi$ is unitary with respect to the inner product of Eq. (18). Since $[\Gamma(\hat{h}_1),\hat{E}_\varphi]=\hat{E}_\varphi, \hat{E}_\varphi$ is the exponential of an Hermitian "phase" operator that is conjugate to $\hat{h}_1$.

The eigenstates of $\hat{E}_\varphi$, known as phase states,[3] are labeled by the continuous variable $\theta_\circ$ and given by

$$|\theta_\circ\rangle=\sum_{p=-\infty}^{\infty} e^{i(2p+\sigma_2)(\theta_\circ+\varphi)}, \quad \hat{E}_\varphi|\theta_\circ\rangle=e^{-2i\theta_\circ}|\theta_\circ\rangle. \tag{24}$$

To obtain a finite dimensional Hermitian representation of su(2), we project from V_{σ_2} a finite dimensional subspace V^λ spanned by an appropriate subset of exponential functions. Rowe[9] has already observed that the appropriate projection operator is the intertwining operator $\mathcal{K}$ of Eq. (19). Since $\mathcal{K}_\nu=0$ for $|\nu|>\lambda$, $\mathcal{K}$ isolates from the set of all U(1) functions $\{e^{ip\varphi}, p=-\infty,\ldots,\infty\}$ a subset of pertinent functions which form a basis for the *physical* $SU(2)$ *subspace* for the representation. $\mathcal{K}$ also adjusts the matrix elements of the various generators of the algebra so as to make γ Hermitian. Thus, the expression of γ in terms of an intertwining operator which acts as a projector ties in nicely with the work by Popov and collaborators[10] on phase operators in a finite dimensional subspace.

The restriction of $\hat{E}_\varphi$ to the finite-dimensional space V^λ is no longer unitary: the highest weight is annihilated by $\hat{E}_\varphi$ so that $\hat{E}_\varphi$ is now nilpotent, with the last line of its matrix representation containing only zeroes:

$$\hat{E}_\varphi=\begin{pmatrix} 0 & 1 & 0 & \ldots & \\ & 0 & 1 & 0 & \\ \vdots & & \ddots & 1 & \ddots \\ & & & & 1 \\ 0 & 0 & \ldots & & 0 \end{pmatrix}. \tag{25}$$

We would like to transform $\hat{E}_\varphi$ into a unitary matrix, but that transformation is not unique, as the rank of the matrix representation of $\gamma(\hat{e}_\pm)$ in V^λ is less than the dimension of this matrix. It is nevertheless possible to obtain a unitary operator closely related to $\hat{E}_\varphi$. The choice

$$E_{\hat{\varphi}}(\xi)=\begin{pmatrix} 0 & 1 & 0 & \ldots & \\ & 0 & 1 & 0 & \\ \vdots & & \ddots & 1 & \ddots \\ & & & & 1 \\ e^{i\xi} & 0 & \ldots & & 0 \end{pmatrix} \tag{26}$$

will produce a unitary matrix with determinant $e^{i\xi}$. The factor ξ is related to the phase of the vacuum state, which cannot be determined.

Vourdas[4] has done an extensive analysis of the case where $\xi=0$, which amounts to imposing a cyclic boundary condition by identifying $|\lambda,\lambda+2\rangle\sim|\lambda,-\lambda\rangle$. The case of general ξ does not differ significantly from this particular case where $\xi=0$: the eigenvalues and eigenvectors of the matrix of Eq. (26) are simply shifted by inessential phase factors. Thus, we set $\xi=0$ and define

$$E_{\hat{\varphi}}\equiv E_{\hat{\varphi}}(0), \tag{27}$$

so that $\det(E_{\hat{\varphi}})=1$. The notation indicates that $E_{\hat{\varphi}}$ is the exponential of a Hermitian "phase" operator $\hat{\varphi}$.

Phase states in the finite dimensional subspace V^{λ} are eigenstates of $E_{\hat{\varphi}}$. They are obtained by restricting the sum in Eq. (24) to those values of ν that correspond to states occurring in the su(2) irrep with highest weight λ:

$$|\lambda;\theta_\lambda\rangle=\sum_{\nu=-\lambda,-\lambda+2,\ldots,\lambda} e^{i\nu\theta_\lambda}|\lambda\,\nu\rangle=\frac{\sin((\lambda+1)(\varphi+\theta_\lambda))}{\sin(\varphi+\theta_\lambda)},\quad \theta_\lambda=2\pi/(\lambda+1), \tag{28}$$

using $|\lambda\,\nu\rangle\mapsto e^{i\nu\varphi}$. The state $|\lambda;\theta_\lambda\rangle$ behaves like a periodic δ function as $\lambda\to\infty$, in accordance with the requirement of Ref. 5.

E. Application: Asymptotic SU(2) Wigner function

Let $\lambda\to\infty$ and set $\nu_0=\lambda\cos 2\beta$, i.e., set $\cos 2\beta=\nu_0/\lambda$ to its "classical value." Then

$$\lim_{\lambda\to\infty}\frac{\mathcal{K}_{\nu_0+p+2}}{\mathcal{K}_{\nu_0+p}}=\lim_{\lambda\to\infty}\tan\beta\sqrt{\frac{(\lambda+\nu_0+p+2)}{(\lambda-\nu_0-p)}}=\tan\beta\sqrt{\frac{1+\cos 2\beta}{1-\cos 2\beta}}=1+O(p/\lambda). \tag{29}$$

For finite values of p, we can therefore solve for $\mathcal{K}_{\nu_0+p}$ as $\mathcal{K}_{\nu_0+p}=1$. For finite p, the operators $\hat{e}_{\pm}$ are now represented by

$$\begin{aligned}\gamma(\hat{e}_+)&\to-\tfrac{1}{2}e^{2i\varphi}\lambda(1-\cos 2\beta)\operatorname{cotan}\beta=-\tfrac{1}{2}\lambda e^{2i\varphi}\sin 2\beta,\\ \gamma(\hat{e}_-)&\to-\tfrac{1}{2}e^{-2i\varphi}\lambda(1+\cos 2\beta)\tan\beta=-\tfrac{1}{2}\lambda e^{-2i\varphi}\sin 2\beta,\end{aligned} \tag{30}$$

and, in particular, we have $\gamma(\hat{L}_y)=i(\gamma(\hat{e}_+)-\gamma(\hat{e}_-))=\lambda\sin 2\beta\sin 2\varphi$. The reduced SU(2)-Wigner function, $\langle\lambda\,\nu|\exp(i\theta\hat{L}_y)|\lambda\,\nu'\rangle$, can therefore be written, in the limit, as

$$\begin{aligned}&\lim_{\lambda\to\infty}\langle\tfrac{1}{2}\lambda,\tfrac{1}{2}(\nu_0+p)|\exp(i\theta(\gamma(\hat{e}_+)-\gamma(\hat{e}_-)))|\tfrac{1}{2}\lambda,\tfrac{1}{2}(\nu_0+q)\rangle\\ &\quad\to\frac{1}{\pi}\int_0^{\pi}e^{i((1/2)(p-q))2\varphi}e^{i\theta\lambda\sin 2\beta\sin 2\varphi}\mathrm{d}\varphi\\ &\quad=J_{p-q}((-\lambda\sin 2\beta)\theta),\end{aligned} \tag{31}$$

where J_ν is a Bessel function and we have used an integral expression for J_ν found in Ref. 11. This result has been further investigated in Ref. 12.

III. GENERALIZATION TO SU($N+1$) IRREPS OF TYPE (λ, 0,...)

A. Algebraic formulation

In this section we generalize the above-mentioned construction to obtain a representation of su($n+1$) on the n-torus. We start by going to the complex extension of u($n+1$), spanned by the $(n+1)^2$ operators $\{\hat{C}_{ij}, i,j=1,...,n+1\}$ which satisfy the commutation relations

$$[\hat{C}_{ij},\hat{C}_{kl}]=\delta_{jk}\hat{C}_{il}-\delta_{il}\hat{C}_{kj}. \tag{32}$$

The complex extension of su($n+1$) is obtained by selecting from the above set the operators $\hat{C}_{ij}$, $i\neq j$ and $\hat{h}_k$, where

$$\hat{h}_k=\hat{C}_{kk}-\hat{C}_{k+1,k+1}, \quad k=1,...,n. \tag{33}$$

Let $\mathfrak{h}$ be the Cartan subalgebra of $\mathfrak{g}=sl(n+1,\mathbb{C})$ consisting of diagonal matrices. Let (λ, 0, ...) be a dominant integral weight (with respect to $\mathfrak{h}$) and $|\chi_\lambda\rangle$ the highest weight vector of a representation on the space V which has only trivial weight multiplicities. Let $\mathfrak{s}$ be the stabilizer subalgebra of $\langle\chi_\lambda|$, i.e.,

$$\mathfrak{s}=\{s\in g \quad s.t. \quad \langle\chi_\lambda|s=\alpha(s)\langle\chi_\lambda|\}, \tag{34}$$

where $\alpha(s)\in\mathbb{C}$. Note that the Cartan subalgebra $h\subset\mathfrak{s}$.

Choose and fix a generic element g in $SL(n+1,\mathbb{C})$ and construct another ''twisted'' copy of the Cartan subalgebra $g\mathfrak{h}g^{-1}$. The only condition on g must be that

$$\mathfrak{g}=\mathfrak{s}+g\mathfrak{h}g^{-1}, \tag{35}$$

i.e., it must be possible to expand an arbitrary element in $\mathfrak{g}$ as a sum of an element in $\mathfrak{s}$ and an element in $g\mathfrak{h}g^{-1}$. The coherent state representation of an operator $\hat{X}\in\mathfrak{g}$ is then defined by

$$\Gamma(\hat{X})\psi_g(k)\equiv\langle\chi_\lambda|g\,k\,\hat{X}|\psi\rangle, \quad k\in H. \tag{36}$$

Since H is just an n-dimensional torus, the group element $k\in H$ is parametrized by n angles $\varphi_1,\ldots,\varphi_n$ as in $k=\exp(i\Sigma_p\varphi_p\hat{h}_p)$, where p runs from $p=1,...,n$. We will abuse the notation and write the coherent state as a function of $\underline{\varphi}=[\varphi_1,\ldots,\varphi_n]$. With this notation we find that, for $\hat{X}=\hat{h}_k\in\mathfrak{h}$,

$$\Gamma(\hat{h}_k)=-i\frac{\partial}{\partial\varphi_k}. \tag{37}$$

If $\hat{X}=\hat{C}_{j\ell}$, $\ell\neq j$ so that $\hat{X}\notin\mathfrak{h}$, then we have

$$\begin{aligned}\Gamma(\hat{C}_{j\ell})\psi_g(\varphi)&=\langle\chi_\lambda|g\exp(i\Sigma_k\varphi_k\hat{h}_k)\hat{C}_{j\ell}|\psi\rangle,\\&=\exp(i\Sigma_k m^k_{j\ell}\varphi_k)\langle\chi_\lambda|g\hat{C}_{j\ell}\exp(i\Sigma\varphi_k\hat{h}_k)|\psi\rangle\\&=\exp(i\Sigma_k m^k_{j\ell}\varphi_k)\langle\chi_\lambda|(g\hat{C}_{j\ell}g^{-1})g\exp(i\Sigma_k\varphi_k\hat{h}_k)|\psi\rangle,\end{aligned} \tag{38}$$

where k runs from 1 to n and where

$$[\hat{h}_k,\hat{C}_{j\ell}]=m^k_{j\ell}\hat{C}_{j\ell}=\delta_{kj}\hat{C}_{k\ell}-\delta_{k+1,j}\hat{C}_{k+1,\ell}-\delta_{k\ell}\hat{C}_{jk}+\delta_{k+1,\ell}\hat{C}_{j,k+1} \tag{39}$$

for $j\neq k=1,...,n+1$. With the understanding that $\varphi_0=\varphi_{n+1}=0$, the sum $\Sigma_{k=1}^n m^k_{j\ell}\varphi_k$ can be rewritten as

$$\sum_{k=1}^{n} m_{j\ell}^{k}\varphi_k = \varphi_j - \varphi_{j-1} - \varphi_\ell + \varphi_{\ell-1}. \tag{40}$$

In order to complete the description of our coherent state representation of $\mathfrak{g}$, we need to compute explicitly, for every $(j\ell)$, the decomposition

$$g\hat{C}_{j\ell}g^{-1} = \overbrace{\hat{s}_{j\ell}}^{\epsilon_{\mathfrak{s}}} + \overbrace{g\hat{d}_{j\ell}g^{-1}}^{\epsilon_{g\mathfrak{h}g^{-1}}}, \quad \hat{d}_{j\ell} = \sum_{k=1}^{n} d_{j\ell}^{k}\hat{h}_k, \tag{41}$$

as per Eq. (35). It is simpler (and equivalent) to compute

$$\hat{C}_{j\ell} = g^{-1}\hat{s}_{j\ell g} + \hat{d}_{j\ell}. \tag{42}$$

Substitution of (42) into Eq. (38) then yields

$$\begin{aligned}\Gamma(\hat{C}_{j\ell})\psi_g(\varphi) &= \exp(i\Sigma_k m_{j\ell}^{k}\varphi_k)\langle\chi_\lambda|(\hat{s}_{j\ell}g + \hat{d}_{j\ell})\exp(i\Sigma_k\varphi_k\hat{h}_k)|\psi\rangle,\\ &= \exp(i\Sigma_k m_{j\ell}^{k}\varphi_k)\langle\chi_\lambda|(\hat{s}_{j\ell}g\,\exp(i\Sigma_k\varphi_k\hat{h}_k) + g\,\exp(i\Sigma_k\varphi_k\hat{h}_k)\hat{d}_{j\ell})|\psi\rangle.\end{aligned} \tag{43}$$

It follows therefore that, in accordance with Eq. (37), $\hat{d}_{j\ell}$ will be a sum of differential operators in the variables φ_k, while the action on the left of $\hat{s}_{j\ell}$ will yield back $\langle\chi_\lambda|$ to within a normalization factor.

Again we observe that the expansion coefficients cannot depend on the choice of representation, so that we choose to work in the $(n+1)\times(n+1)$ representation where $|\chi_\lambda\rangle = (1,0,...,0)^t$. The computation is further facilitated if we observe that the dependence on g is actually only up to left multiplication of $\mathcal{S}$; hence we can write $g = S\cdot\overline{g}$, with $S\in\mathcal{S}$ in the stabilizer subgroup and $\overline{g}$ a conveniently chosen coset representative in $\mathcal{S}\backslash G$; a different choice of the representative $g' = s\cdot g$ will produce equivalent representations in which the coherent states are multiplied by a character $\chi(s)$. Then,

$$\hat{C}_{j\ell} = (\overline{g})^{-1}\hat{s}_{j\ell}\,\overline{g} + \hat{d}_{j\ell}. \tag{44}$$

If the highest weight vector $\langle\chi_\lambda|$ is the vector (1, 0,..., 0), then a general element $\hat{s}\in\mathfrak{s}$ and coset representative $\overline{g}$ have respective the matrix forms

$$\hat{s}\mapsto\begin{pmatrix} y & \mathbf{0}\\ \mathbf{x}^t & Y\end{pmatrix}, \quad \overline{g} = \begin{pmatrix} 1 & -\mathbf{v}\\ \mathbf{0}^t & \mathbb{1}\end{pmatrix}, \tag{45}$$

where Y is an $n\times n$ complex matrix, $\mathbf{x} = (x_2, x_3, \ldots, x_{n+1})$ is a complex $1\times n$ vector, $\mathbf{0}$ is the $\mathbf{1}\times n$ null vector, $y = -\mathrm{Tr}(Y)$, $\mathbf{v} = (v_2, v_3, \ldots, v_{n+1})$ is a complex vector, and $\mathbb{1}$ is the $n\times n$ unit matrix. [The matrix form of $\overline{g}$ can be compared with Eq. (12).]

The product $\overline{g}^{-1}\hat{s}\overline{g}$ is a matrix of the form

$$\begin{pmatrix} y + \mathbf{v}\cdot\mathbf{x} & -(y + \mathbf{v}\cdot\mathbf{x})\mathbf{v} + \mathbf{v}Y\\ \mathbf{x}^t & -\mathbf{x}\otimes\mathbf{v} + Y\end{pmatrix}, \tag{46}$$

where $\mathbf{v}\cdot\mathbf{x}$ is the usual scalar product and $\otimes$ denotes the outer product so that $\mathbf{x}\otimes\mathbf{v}$ is an $n\times n$ matrix.

We therefore seek to match the matrix expression of $\hat{C}_{j\ell}$ with the expansion

$$\begin{pmatrix} y + \mathbf{v}\cdot\mathbf{x} & -(y + \mathbf{v}\cdot\mathbf{x})\mathbf{v} + \mathbf{v}Y\\ \mathbf{x}^t & -\mathbf{x}\otimes\mathbf{v} + Y\end{pmatrix} + d, \tag{47}$$

where d is a diagonal matrix $d=\mathrm{diag}(d^1,...,d^{n+1})$ of zero trace.

For every different pair of indices (j,ℓ), $j\neq\ell$, and with $\mathbf{v}$ appearing as parameter (which does not depend on j, ℓ), we need to solve the above-given equation for y, Y, $\mathbf{x}$, d. These unknowns depend on j, ℓ but, to avoid overburdening the notation, we will keep writing y for $y_{j\ell}$, d^k for $d^k_{j\ell}$, etc., until we reach final formulas.

Using the form of $\hat{s}$, the highest weight state $(1,0,...)^t$ and Eq. (43), we find that the only coefficient in $\hat{s}$ that enters in the expression of $\Gamma(\hat{C}_{j\ell})$ is y. The only element in $\mathfrak{s}$ to have nonzero entry in position (1,1) is $\hat{h}_1$. As $\langle\chi_\lambda|\hat{h}_1=\langle\chi_\lambda|\lambda$, Eq. (43) simplies to

$$\Gamma(\hat{C}_{j\ell})=y_{j\ell}\exp(i\Sigma_k m_k^{j\ell}\varphi_k)\left(\lambda-i\sum_{k=1}^{n}z^k\frac{\partial}{\partial\varphi_k}\right),\quad y_{j\ell}z^k=d^k. \tag{48}$$

We divide the straightforward search for the solution into three subcases. It is also useful at this point to introduce an auxiliary set of $n+1$ vectors in the Cartan Lie-algebra $\mathfrak{h}$, given by

$$\hat{\rho}_k=-\sum_{j=1}^{k-1}j\hat{h}_j+\sum_{j=k}^{n}(n-j+1)\hat{h}_j=\mathrm{diag}(-1,...,-1,\overbrace{\quad n\quad}^{k\text{th-term}},-1,...,-1),\quad k=1,...,n+1, \tag{49}$$

$$\Gamma(\hat{\rho}_k)=-i\left(\sum_{j=1}^{k-1}j\frac{\partial}{\partial\varphi_j}-\sum_{j=k}^{n}(n-j+1)\frac{\partial}{\partial\varphi_j}\right). \tag{50}$$

Note that, for $\hat{\rho}_{n+1}$, there is no contribution from the second sum in Eq. (49).

1. Case 1: $\hat{C}_{1\ell}$

Let $j=1$, $\mathbf{c}$ be the vector of components $(\mathbf{c})_k=\delta_{\ell k}$, $k=2,3,...,n+1$ and write

$$\hat{C}_{1\ell}=\begin{pmatrix}0 & \mathbf{c}\\ \mathbf{0}^t & \mathbf{0}\end{pmatrix}, \tag{51}$$

From Eq. (47), $\mathbf{x}=\mathbf{0}$, $y+d^1=0$, and $Y+d=0$; Y is a diagonal matrix with entries $y=Y_{kk}=-d^k$.

From $\mathbf{v}(-y\mathbb{1}+Y)=\mathbf{c}$, we find first that $Y_{kk}=y$ for $k\neq\ell$, and, using the condition $y_{1\ell}+\mathrm{Tr}(Y)=0$, that $Y_{\ell\ell}=-ny$. Finally, from the nonzero component $\ell=k$ of $\mathbf{c}$, one obtains

$$y=\frac{-1}{(n+1)v_\ell}. \tag{52}$$

If Eq. (35) is to hold, then we must have $v_\ell\neq 0\ \forall\ell$. The matrix d is given by

$$d=\mathrm{diag}\left(-y,-y,...,-y,\overbrace{\quad ny\quad}^{\ell\text{th}-\text{term}},-y...,-y\right)=-y\hat{\rho}_\ell=\frac{-1}{(n+1)v_\ell}\hat{\rho}_\ell. \tag{53}$$

Therefore we finally have

$$\Gamma(\hat{C}_{1\ell})=y_{1\ell}\,e^{i(\varphi_1-\varphi_\ell+\varphi_{\ell-1})}(\lambda+\Gamma(\hat{\rho}_\ell)),\quad y_{1\ell}=\frac{-1}{(n+1)v_\ell}, \tag{54}$$

where we have found $\Sigma_{k=1}^{n}m_k^{1\ell}\varphi_k=\varphi_1-\varphi_\ell+\varphi_{\ell-1}$ using $\varphi_{n+1}=0$ and Eq. (40).

2. Case 2: $\hat{C}_{j\ell}$, $\ell \neq j$, $\ell, j \geqslant 2$

We now write

$$\hat{C}_{j\ell} = \begin{pmatrix} 0 & \mathbf{0} \\ \mathbf{0}^t & c_{j\ell} \end{pmatrix}, \tag{55}$$

where $(c_{j\ell})_{mn} = \delta_{jm}\delta_{\ell n}$. Using Eq. (47), $\mathbf{x} = \mathbf{0}$ once more, so that $y + d^1 = 0$. Thus, the diagonal elements of Y are such that $Y_{kk} + d^k = 0$. The only off-diagonal entry in Y is a 1 in the jth row, ℓth column. (For consistency it is convenient to enumerate the entries of the $n \times n$ matrix Y_{jk} with j, $k = 2,...,n+1$.) From $\mathbf{v}(-y\mathbb{1} + Y) = 0$, we obtain the equations

$$v_k(-y + Y_{kk}) + v_j\delta_{\ell k} = 0, \tag{56}$$

from which we conclude that, if $k \neq \ell$, $Y_{kk} = y$. The coefficient $Y_{\ell\ell}$ is fixed by $y + \mathrm{tr}(Y) = 0$ to be $Y_{\ell\ell} = -ny$. Finally, from Eq. (56) with $\ell = k$, we conclude that

$$y = \frac{v_j}{(n+1)v_\ell}, \tag{57}$$

where $v_j \neq 0 \neq v_\ell$ by assumption. The diagonal matrix d is given by

$$d = \mathrm{diag}\Big(-y, -y, \ldots, -y, \overbrace{ny}^{\ell\text{th-term}}, -y \ldots, -y \Big) = -y\hat{\rho}_\ell = -\frac{v_j}{(n+1)v_\ell}\hat{\rho}_\ell \tag{58}$$

Summarizing, we find, using Eq. (40),

$$\Gamma(\hat{C}_{j\ell}) = y_{j\ell} e^{i(\varphi_j - \varphi_{j-1} - \varphi_\ell + \varphi_{\ell-1})}(\lambda + \Gamma(\hat{\rho}_\ell)), \quad y_{j\ell} = \frac{v_j}{(n+1)v_\ell}. \tag{59}$$

3. Case 3: $\hat{C}_{\ell 1}$, $\ell \neq 1$

In this case, the vector $\mathbf{x}^t$ has components $x_j = \delta_{\ell j}$. Thus, the scalar product $\mathbf{v}\cdot\mathbf{x} = v_\ell$, and the equation $y + v_\ell + d^1 = 0$ gives

$$d^1 = -(v_\ell + y). \tag{60}$$

From $\mathbf{v}(-y\mathbb{1} + v_\ell\mathbb{1} + \mathbf{Y}) = 0$, we conclude that

$$(-y - v_\ell)v_m + \sum_{k=1}^{n} v_k Y_{km} = 0, \quad m = 2,3,...,n+1. \tag{61}$$

Now, $(\mathbf{x}\otimes\mathbf{v})_{pm} = x_p v_m = \delta_{\ell p} v_m$. Thus, we have

$$0 = -(\mathbf{x}\otimes\mathbf{v})_{pm} + Y_{pm} + d^m\delta_{pm} = -\delta_{\ell p}v_m + Y_{pm} + d^m\delta_{pm}, \quad m = 2,3,...,n+1. \tag{62}$$

Multiplying Eq. (62) by v_p and summing over p, we obtain

$$0 = \sum_p (-\delta_{\ell p}v_p v_m) + \sum_p v_p Y_{pm} + \sum_p v_p d^m \delta_{pm}, \quad m = 2,3,...,n+1. \tag{63}$$

Using Eq. (61) and the fact that $v_m \neq 0$, this can be simplified to

$$0 = -v_\ell + y + v_\ell + d^m = y + d^m, \quad m = 2,3,...,n+1. \tag{64}$$

Now using the fact that $\Sigma_{k=1}^{n+1} d^k = 0$, we immediately find

$$y=-\frac{v_\ell}{n+1}, \tag{65}$$

so that, using Eq. (60), we find the matrix d to be

$$d=\mathrm{diag}(ny,-y,\ldots,-y)=-y\hat{\rho}_1=-\frac{v_\ell}{n+1}\hat{\rho}_1. \tag{66}$$

Hence,

$$\Gamma(\hat{C}_{\ell 1})=y_{\ell 1}e^{i(\varphi_\ell-\varphi_{\ell-1}-\varphi_1)}(\lambda+\Gamma(\hat{\rho}_1)),\quad y_{\ell 1}=\frac{v_\ell}{n+1},\quad \ell=2,\ldots,n+1,\quad \varphi_{n+1}\equiv 0. \tag{67}$$

B. Evaluating the v_k coefficients

The coefficients v_k are related to SU($n+1$) Wigner functions as follows. If $\nu=(\nu_1,\nu_2,\ldots,\nu_{n+1})$ denotes an ordered partition of λ, i.e., $\nu_1+\nu_2+\ldots+\nu_{n+1}=\lambda$ with ν_i a non-negative integer, then the set of states $\{\psi_\nu\}$, labeled by different partitions ν of λ, can be chosen as basis states for the irrep (λ, 0,..., 0) of su(n). These states satisfy

$$\hat{h}_k\psi_\nu=(\nu_k-\nu_{k+1})\psi_\nu, \tag{68}$$

and are uniquely identified by the set of eigenvalues of the operators $\hat{h}_k$.

Next, we need $g=\bar{g}\cdot S$, or $\bar{g}=S^{-1}g=\bar{g}$, with $\mathcal{S}^{-1}$ and G matrices of the form

$$S^{-1}=\begin{pmatrix} w & \mathbf{0} \\ \mathbf{Q}^t & X \end{pmatrix},\quad g=\begin{pmatrix} a & \mathbf{b} \\ \mathbf{c}^t & U \end{pmatrix}, \tag{69}$$

where $a=\langle\chi_\lambda|g|\chi_\lambda\rangle$ and $b_k=\langle\chi_\lambda|g|\psi_{\nu_k}\rangle$, with ψ_{χ_λ} the highest weight state of the $(n+1)$-dimensional defining representation (1, 0,..., 0) and ψ_{ν_k}, $k=2,\ldots,n+1$, the remaining basis states of this irrep. Thus we have

$$w=\frac{1}{\langle\chi_\lambda|g|\chi_\lambda\rangle},\quad v_k=\frac{\langle\chi_\lambda|g|\psi_{\nu_k}\rangle}{\langle\chi_\lambda|g|\chi_\lambda\rangle}. \tag{70}$$

C. Basis functions

We have already observed that, with $\bar{g}$ of the form of Eq. (45) and $v_j\neq 0\ \forall j$, then $(\bar{g})^{-1}|\chi_\lambda\rangle$ generates the whole representation space. Thus, the state $(\bar{g})^{-1}|\chi_\lambda\rangle$ acts as a cyclic vector for the irrep with highest weight (λ, 0, 0,...) under the action of any fixed element $k\in H$ in the Cartan subgroup. Hence, to every vector ψ in the representation space, there corresponds a unique function on H:

$$\psi\mapsto\psi_g(k)=\langle\chi_\lambda|g\,k|\psi\rangle. \tag{71}$$

The basis state ψ_ν of (λ, 0,..., 0) is mapped to the normalized element on the n-torus

$$\psi_\nu\mapsto\langle\chi_\lambda|\bar{g}k|\psi_\nu\rangle\propto\langle\chi_\lambda|\bar{g}|\psi_\nu\rangle\exp(i\Sigma_k(\nu_k-\nu_{k+1})\varphi_k)\mapsto\frac{\exp(i\Sigma_k(\nu_k-\nu_{k+1})\varphi_k)}{(2\pi)^{n/2}}. \tag{72}$$

The highest weight state ψ_{χ_λ} of (λ, 0,..., 0) is represented by $\psi_{\chi_\lambda}\mapsto e^{i\varphi_1}/(2\pi)^{n/2}$.

D. Making the representation Hermitian

States on the torus are naturally normalized with respect to the inner product

$$\langle \psi_{\nu'}|\psi_{\nu}\rangle = \frac{1}{(2\pi)^n}\int_0^{2\pi} d\varphi_1 \int_0^{2\pi} d\varphi_2 \cdots \int_0^{2\pi} d\varphi_n \exp(-i\Sigma_k(\nu'_k-\nu'_{k+1})\varphi_k)\exp(i\Sigma_p(\nu_p-\nu_{p+1})\varphi_p)$$

$$= \prod \delta_{\nu'_k-\nu_k-\nu'_{k+1}+\nu_{k+1}}. \tag{73}$$

However, with this inner product, the action of the operators $\Gamma(\hat{C}_{ij})$, $i\neq j$, is not Hermitian:

$$\langle \psi_{\nu'}|\Gamma(\hat{C}_{ij})|\psi_{\nu}\rangle \neq \langle \psi_{\nu'}|\Gamma^{\dagger}(\hat{C}_{ji})|\psi_{\nu}\rangle = \langle \psi_{\nu}|\Gamma(\hat{C}_{ji})|\psi_{\nu'}\rangle^*; \tag{74}$$

the resulting representation does not exponentiate to a unitary representation of the group. Since all representations of su$(n+1)$ having integral dominant weight are equivalent to Hermitian representations, there must exist an intertwining operator $\mathcal{K}$ that will transform Γ into a Hermitian representation γ, i.e., there exists $\mathcal{K}$

$$\gamma(\hat{C}_{ij}) = \mathcal{K}^{-1}\Gamma(\hat{C}_{ij})\mathcal{K}, \quad \text{such that} \quad \langle \psi_{\nu'}|\gamma(\hat{C}_{ij})|\psi_{\nu}\rangle = \langle \psi_{\nu}|\gamma(\hat{C}_{ji})|\psi_{\nu'}\rangle^*. \tag{75}$$

We find $\mathcal{K}$ by combining Eq. (75) with its Hermitian conjugate $\gamma^{\dagger}(\hat{C}_{ji}) = \mathcal{K}^{\dagger}\Gamma^{\dagger}(\hat{C}_{ji})(\mathcal{K}^{-1})^{\dagger}$, so that

$$\gamma(\hat{C}_{ij}) = \gamma^{\dagger}(\hat{C}_{ji}) \Rightarrow \Gamma(\hat{C}_{ij})\mathcal{S} = \mathcal{S}\Gamma^{\dagger}(\hat{C}_{ji}), \tag{76}$$

where $\mathcal{S}=\mathcal{K}\mathcal{K}^{\dagger}$ is a Hermitian operator. Noting that the Cartan elements $\hat{h}_k$ are represented under the map Γ by operators Hermitian with respect to the inner product of Eq. (73), we may take $\mathcal{S}$ to be diagonal in the weight basis: $\mathcal{S}|\psi_{\nu}\rangle = \mathcal{S}_{\nu}|\psi_{\nu}\rangle$. Thus, using Eq. (76), we obtain the condition

$$\langle \psi_{\nu'}|\Gamma(\hat{C}_{ij})\mathcal{S}|\psi_{\nu}\rangle = \langle \psi_{\nu'}|\mathcal{S}\Gamma^{\dagger}(\hat{C}_{ji})|\psi_{\nu}\rangle \Rightarrow \frac{\mathcal{S}_{\nu}}{\mathcal{S}_{\nu'}} = \frac{y^*_{ji}(\lambda+\rho_i(\nu'))}{y_{ij}(\lambda+\rho_j(\nu))} \equiv R_{\nu,\nu'}, \tag{77}$$

where $\nu_k = \nu'_k + \delta_{ik} - \delta_{jk}$ and

$$\rho_i(\nu) = \langle \psi_{\nu}|\hat{\rho}_i|\psi_{\nu}\rangle = \sum_{k=1}^{n+1} (\rho_i)_{kk}\nu_k, \tag{78}$$

where $(\rho_i)_{kk}$ is the kth entry in the diagonal matrix ρ_i defined in Eq. (49).

To construct the coefficients $\mathcal{S}_{\nu}$ from the ratios of Eq. (77), one starts by (arbitrarily) fixing to $+1$ the coefficient of the highest weight corresponding to the trivial partition $(\lambda, 0, 0,...)$; changing this would just change $\mathcal{S}$ by an overall multiplicative factor. Noting now that $\mathcal{S}=\mathcal{K}\mathcal{K}^{\dagger}$ is a positive Hermitian matrix, the ratio $\mathcal{K}_{\nu}/\mathcal{K}_{\nu'}$ can therefore be obtained, up to a phase, as the square root of the right-hand side of Eq. (77). The phase of the ratio $\mathcal{K}_{\nu}/\mathcal{K}_{\nu'}$ should be chosen so that the matrix elements of $\gamma(\hat{C}_{ij})$ are real, something that it is always possible to do. In practice, one chooses, without loss of generality, the element $g\in G$, from which y_{ij} is obtained, so that y_{ij} is always real. Assuming therefore that g is chosen in this way, we have v_k always real and

$$\frac{\mathcal{K}_{\nu}}{\mathcal{K}_{\nu'}} = \sqrt{\frac{y_{ji}(\lambda+\rho_i(\nu'))}{y_{ij}(\lambda+\rho_j(\nu))}}. \tag{79}$$

IV. APPLICATION TO SU(3)

A. Representation on the 2-torus

The su(3) Lie algebra is spanned in the usual way by the subset of u(3) operators comprising the ladder operators $\{\hat{C}_{ij}, i \neq j\}$ together with the Cartan generators $\hat{h}_1 = \hat{C}_{11} - \hat{C}_{22}$, $\hat{h}_2 = \hat{C}_{22} - \hat{C}_{33}$. The $\{\hat{C}_{ij}\}$ operators satisfy the general commutation relations $[\hat{C}_{ij}, \hat{C}_{kl}] = \delta_{jk}\hat{C}_{il} - \delta_{il}\hat{C}_{kj}$.

The highest weight state of the irrep $(\lambda,0)$ is mapped to the state $|\lambda,0,0\rangle \mapsto e^{i\lambda\varphi_1}/2\pi$. More generally, a state $|\nu_1,\nu_2,\nu_3\rangle$, with $\nu_1+\nu_2+\nu_3=\lambda$, is mapped to

$$|\nu_1,\nu_2,\nu_3\rangle \mapsto \frac{e^{i(\nu_1-\nu_2)\varphi_1 + i(\nu_2-\nu_3)\varphi_2}}{2\pi} = \frac{e^{i(\nu_1-\nu_2)\varphi_1 + i(2\nu_2+\nu_1-\lambda)\varphi_2}}{2\pi}, \tag{80}$$

where the condition $\nu_1+\nu_2+\nu_3=\lambda$ has been used.

Following the parametrization of Ref. 13 for SU(3) elements, and using the fact that we can choose g to be such that the matrix elements are real, we find

$$w = \frac{1}{\cos\frac{1}{2}\beta_2}, \quad v_2 = \cos\frac{1}{2}\beta_3 \tan\frac{1}{2}\beta_2, \quad v_3 = \sin\frac{1}{2}\beta_3 \tan\frac{1}{2}\beta_2. \tag{81}$$

Simple application of Eqs. (37), (54), (59), and (67) then yields

$$\Gamma(\hat{h}_1) = -i\frac{\partial}{\partial\varphi_1}, \quad \Gamma(\hat{h}_2) = -i\frac{\partial}{\partial\varphi_2},$$

$$\Gamma(\hat{C}_{12}) = \frac{-1}{3\cos\frac{1}{2}\beta_3 \tan\frac{1}{2}\beta_2} e^{i(2\varphi_1-\varphi_2)}\left[\lambda + i\frac{\partial}{\partial\varphi_1} - i\frac{\partial}{\partial\varphi_2}\right],$$

$$\Gamma(\hat{C}_{21}) = \frac{-\cos\frac{1}{2}\beta_3 \tan\frac{1}{2}\beta_2}{3} e^{-i(2\varphi_1-\varphi_2)}\left[\lambda - 2i\frac{\partial}{\partial\varphi_1} - \frac{\partial}{\partial\varphi_2}\right],$$

$$\Gamma(\hat{C}_{13}) = \frac{-1}{3\sin\frac{1}{2}\beta_3 \tan\frac{1}{2}\beta_2} e^{i(\varphi_1+\varphi_2)}\left[\lambda + i\frac{\partial}{\partial\varphi_1} + 2i\frac{\partial}{\partial\varphi_2}\right], \tag{82}$$

$$\Gamma(\hat{C}_{31}) = \frac{-\sin\frac{1}{2}\beta_3 \tan\frac{1}{2}\beta_2}{3} e^{-i(\varphi_1+\varphi_2)}\left[\lambda - 2i\frac{\partial}{\partial\varphi_1} - i\frac{\partial}{\partial\varphi_2}\right],$$

$$\Gamma(\hat{C}_{23}) = \frac{1}{3\tan\frac{1}{2}\beta_3} e^{i(-\varphi_1+2\varphi_2)}\left[\lambda + i\frac{\partial}{\partial\varphi_1} + 2i\frac{\partial}{\partial\varphi_2}\right],$$

$$\Gamma(\hat{C}_{32}) = \frac{\tan\frac{1}{2}\beta_3}{3} e^{i(\varphi_1-2\varphi_2)}\left[\lambda + i\frac{\partial}{\partial\varphi_1} - i\frac{\partial}{\partial\varphi_2}\right].$$

The ratios of $\mathcal{K}$ matrix elements required to compute the matrix elements of $\gamma(\hat{C}_{ij})$ are $\mathcal{K}_{\nu}/\mathcal{K}_{\nu'}$, with $\nu'_k=\nu_k+\delta_{ik}-\delta_{jk}$. Using $\nu_1+\nu_2+\nu_3=\lambda$, they are given explicitly by

$$\frac{\mathcal{K}_{\nu_1\nu_2\nu_3}}{\mathcal{K}_{\nu_1+1,\nu_2,\nu_3-1}}=v_3\sqrt{\frac{\lambda+\rho_1(\nu')}{\lambda+\rho_3(\nu)}}=\sin\frac{1}{2}\beta_3\tan\frac{1}{2}\beta_2\sqrt{\frac{\lambda+2(\nu_1+1-\nu_2)+(\nu_2-\nu_3+1)}{\lambda-(\nu_1-\nu_2)-2(\nu_2-\nu_3)}}$$
$$=\sin\frac{1}{2}\beta_3\tan\frac{1}{2}\beta_2\sqrt{\frac{\nu_1+1}{\nu_3}}, \tag{83}$$

$$\frac{\mathcal{K}_{\nu_1\nu_2\nu_3}}{\mathcal{K}_{\nu_1\nu_2-1,\nu_3+1}}=\frac{v_2}{v_3}\sqrt{\frac{\lambda+\rho_3(\nu')}{\lambda+\rho_2(\nu)}}=\frac{1}{\tan\frac{1}{2}\beta_3}\sqrt{\frac{\nu_3+1}{\nu_2}}, \tag{84}$$

$$\frac{\mathcal{K}_{\nu_1\nu_2\nu_3}}{\mathcal{K}_{\nu_1+1,\nu_2-1,\nu_3}}=v_2\sqrt{\frac{\lambda+\rho_1(\nu')}{\lambda+\rho_2(\nu)}}=\cos\frac{1}{2}\beta_3\tan\frac{1}{2}\beta_2\sqrt{\frac{\nu_1+1}{\nu_2}}. \tag{85}$$

To obtain the matrix element $\gamma(\hat{C}_{13})$, for instance, one computes

$$\begin{aligned}
&\langle\psi_{\nu_1+1,\nu_2,\nu_3-1}|\gamma(\hat{C}_{13})|\psi_{\nu_1,\nu_2,\nu_3}\rangle\\
&\quad=\int\frac{d\varphi_1}{2\pi}\int\frac{d\varphi_2}{2\pi}\exp[-i(\nu_1-\nu_2+1)\varphi_1-i(\nu_2-\nu_3-1)\varphi_2]\\
&\qquad\times(\mathcal{K}^{-1}\Gamma(\hat{C}_{13})\mathcal{K})\exp[i(\nu_1-\nu_2)\varphi_1+i(\nu_2-\nu_3)\varphi_2],\\
&\quad=\int\frac{d\varphi_1}{2\pi}\int\frac{d\varphi_2}{2\pi}\exp[-i(\nu_1-\nu_2+1)\varphi_1-i(\nu_2-\nu_3-1)\varphi_2]\\
&\qquad\times\left(\frac{1}{\mathcal{K}_{\nu_1+1,\nu_2,\nu_3-1}}e^{i(\varphi_1+\varphi_2)}\frac{-1}{3\sin\frac{1}{2}\beta_3\tan\frac{1}{2}\beta_2}\left[\lambda+i\frac{\partial}{\partial\varphi_1}+2i\frac{\partial}{\partial\varphi_2}\right]\mathcal{K}_{\nu_1,\nu_2,\nu_3}\right)\\
&\qquad\times\exp[-i(\nu_1-\nu_2)\varphi_1+i(\nu_2-\nu_3)\varphi_2]\\
&\qquad\times\frac{-1}{3\sin\frac{1}{2}\beta_3\tan\frac{1}{2}\beta_2}[\lambda-(\nu_1-\nu_2)-2(\nu_2-\nu_3)]\sin\frac{1}{2}\beta_3\tan\frac{1}{2}\beta_2\sqrt{\frac{\nu_1+1}{\nu_3}},\\
&\quad=-\sqrt{(\nu_1+1)\nu_3}.
\end{aligned} \tag{86}$$

B. Application: the SU(3)→[$\mathbb{R}^6$]U(1)^2 contraction

Consider the limit where $\lambda\to\infty$. Set

$$\overline{\nu_1}=\lambda\left(\cos\frac{1}{2}\beta_2\right)^2,\quad \overline{\nu_2}=\lambda\left(\sin\frac{1}{2}\beta_2\right)^2\left(\cos\frac{1}{2}\beta_3\right)^2,\quad \overline{\nu_3}=\lambda\left(\sin\frac{1}{2}\beta_2\right)^2\left(\sin\frac{1}{2}\beta_3\right)^2. \tag{87}$$

The angles β_2 and β_3 then provide a convenient way to parametrize the distribution of λ photons in three modes with mode i containing a large number ν_i of photons.

With this, it is readily seen that the values of the angles β_2, β_3 for which the representation Γ of Eq. (82) is singular correspond to a distribution such that at least one of the three fields contains no quanta. Provided that Γ is nonsingular, we then have, for values of ν and ν' sufficiently close to the average values $\overline{\nu}$,

$$\lim_{\lambda\to\infty}\frac{\mathcal{K}_\nu}{\mathcal{K}_{\nu'}}=1+O(1/\lambda). \tag{88}$$

The representation Γ is then Hermitian; the diagonal operators $\hat{h}_1$ and $\hat{h}_2$ remain unchanged, and the ladder generators become, in the limit where $\lambda\to\infty$,

$$\begin{aligned}
&\Gamma(\hat{C}_{12})\to -2\lambda e^{i(2\varphi_1-\varphi_2)}\sin\beta_2\cos\frac{1}{2}\beta_3,\\
&\Gamma(\hat{C}_{21})\to -2\lambda e^{-i(2\varphi_1-\varphi_2)}\sin\beta_2\cos\frac{1}{2}\beta_3,\\
&\Gamma(\hat{C}_{13})\to -2\lambda e^{i(\varphi_1+\varphi_2)}\sin\beta_2\sin\frac{1}{2}\beta_3,\\
&\Gamma(\hat{C}_{31})\to -2\lambda e^{-i(\varphi_1+\varphi_2)}\sin\beta_2\cos\frac{1}{2}\beta_3,\\
&\Gamma(\hat{C}_{23})\to 2\lambda e^{i(-\varphi_1+2\varphi_2)}\left(\sin\frac{1}{2}\beta_2\right)^2\sin\beta_3,\\
&\Gamma(\hat{C}_{32})\to 2\lambda e^{i(\varphi_1-2\varphi_2)}\left(\sin\frac{1}{2}\beta_2\right)^2\sin\beta_3.
\end{aligned} \tag{89}$$

All the ladder operators commute with one another, and the resultant algebra is $[\mathbb{R}^6]\mathrm{U}(1)^2$.

C. Application: Phase operators and SU(3) phase states

The realization Γ acts naturally in the irreducible infinite-dimensional space of functions V_{σ_3}, where a state $|n,m\rangle$, $n,m\in\mathbb{Z}$ is represented by the function over the 2-torus $|n,m\rangle\mapsto e^{i(2n-m)\varphi_1}e^{i(2m-n-\sigma_3)\varphi_2}/2\pi$. Here, $\sigma_3=0$, 1, or 2 is the "triality" of the representation.

We introduce three "phase-like" operators:

$$\hat{E}_{\varphi_{12}}=e^{i(2\varphi_1-\varphi_2)},\quad \hat{E}_{\varphi_{23}}=e^{i(-\varphi_1+2\varphi_2)},\quad \hat{E}_{\varphi_{13}}=e^{i(\varphi_1+\varphi_2)}. \tag{90}$$

In V_{σ_3}, the operators $\hat{E}_{\varphi_{12}}$ and $\hat{E}_{\varphi_{23}}$ are unitary with respect to the natural inner product over the 2-torus; they are the exponential of phase operators conjugate to $\hat{h}_1$ and $\hat{h}_2$, respectively, since

$$\left[\frac{1}{2}\Gamma(\hat{h}_1),\hat{E}_{\varphi_{12}}\right]=\hat{E}_{\varphi_{12}},\quad \left[\frac{1}{2}\Gamma(\hat{h}_2),\hat{E}_{\varphi_{23}}\right]=\hat{E}_{\varphi_{23}}. \tag{91}$$

Note that $[\frac{1}{2}\Gamma(\hat{h}_1),\hat{E}_{\varphi_{23}}]\neq 0$, $[\frac{1}{2}\Gamma(\hat{h}_2),\hat{E}_{\varphi_{12}}]\neq 0$.

The realization of an element of A_2, say, $\Gamma(\hat{C}_{12})$ can be expressed as products of a unitary and a diagonal matrix: $\Gamma(\hat{C}_{12})=-\hat{E}_{\varphi_{12}}\hat{e}_{12}$, where $\hat{e}_{12}=\sqrt{\Gamma^\dagger(\hat{C}_{12})\Gamma(\hat{C}_{12})}$.

In the infinite-dimensional space V_{σ_3}, the unitary operators $\hat{E}_{\varphi_{12}}$ and $\hat{E}_{\varphi_{23}}$ commute, and it is possible to find their common set of eigenvectors. It can be verified that, for any θ_1, θ_2, states of the type

$$|\theta_1,\theta_2\rangle = \sum_{n,m\in\mathbb{Z}} e^{i(2n-m)\theta_1} e^{i(2m-n)\theta_2} |n,m\rangle = \sum_{n,m\in\mathbb{Z}} e^{i(2n-m)(\varphi_1+\theta_1)} e^{i(2m-n)(\varphi_2+\theta_2)}, \tag{92}$$

are the simultaneous eigenstate of $\hat{E}_{\varphi_{12}}$, $\hat{E}_{\varphi_{23}}$, and $\hat{E}_{\varphi_{13}}$:

$$\begin{aligned} &\hat{E}_{\varphi_{12}}|\theta_1,\theta_2\rangle = e^{-i(2\theta_1-\theta_2)}|\theta_1,\theta_2\rangle, \quad \hat{E}_{\varphi_{23}}|\theta_1,\theta_2\rangle = e^{-i(-\theta_1+2\theta_2)}|\theta_1,\theta_2\rangle, \\ &\hat{E}_{\varphi_{13}}|\theta_1,\theta_2\rangle = e^{-i(\theta_1+\theta_2)}|\theta_1,\theta_2\rangle. \end{aligned} \tag{93}$$

The states $|\theta_1,\theta_2\rangle$ are therefore phase states.

Consider now the finite-dimensional subspace $V^\lambda \subset V_{\sigma_3}$ such that V^λ is the carrier space for a unirrep of highest weight $(\lambda, 0)$. This subspace is projected using the $\mathcal{K}$ operator from V_{σ_3}. In going from the infinite-dimensional space V_σ to the finite-dimensional V^λ, a number of problems arise in connection with the definition and properties of the phase operators.

We denote the states in V^λ by three non-negative integers as per Eq. (80). First, however, we note that it is not difficult to properly define the radial part of an operator. For instance, the radial part $\hat{J}_{12}$ of $\gamma(\hat{C}_{12})$ is found from $\hat{J}_{12} = \sqrt{\gamma^\dagger(\hat{C}_{12})\gamma(\hat{C}_{12})}$.

In V^λ, the restrictions of the operators $\hat{E}_{\varphi_{ij}}$ are nilpotent and therefore no longer unitary. The rank of $\hat{E}_{\varphi_{ij}}$ is equal to $\dim(V^\lambda)-(\lambda+1)$ as there are $(\lambda+1)$ states annihilated by $\hat{E}_{\varphi_{ij}}$ [one state in each $\mathrm{su}(2)_{ij}$ subrepresentation occurring in the su(3) irrep $(\lambda, 0)$].

In contrast with the SU(2) case, where a single entry of $\hat{E}_\varphi$ could be changed so as to obtain the unitary operator $E_{\hat{\varphi}}$, an arbitrary complex linear combination of the $(\lambda+1)$ states annihilated by $\hat{E}_{\varphi_{ij}}$ yields another state annihilated by $\hat{E}_{\varphi_{ij}}$. Thus, we are left with infinitely many ways of transforming $\hat{E}_{\varphi_{ij}}$ into a unitary phase operator $E_{\hat{\varphi}_{ij}}$, even if we insist that the determinant of $E_{\hat{\varphi}_{ij}}$ be 1. Furthermore, it can easily be verified that, for $\lambda \geqslant 2$, the restriction of $\hat{E}_{\varphi_{ij}}$ is an operator that does not necessarily commute with the other $\hat{E}_{\varphi_{kl}}$ operators: $[\hat{E}_{\varphi_{ij}}, \hat{E}_{\varphi_{kl}}] \neq 0$.

We point out that, in the matrix representation of $[\hat{E}_{\varphi_{12}}, \hat{E}_{\varphi_{23}}]$ there are precisely λ entries which are 1 rather than zero in this commutator. The ''faulty'' nonzero matrix elements appear in positions corresponding to matrix elements of the type $\langle \nu_1+1,0,\nu_3-1|\hat{E}_{\varphi_{13}}|\nu_1,0,\nu_3\rangle$, i.e., matrix elements involving vacuum states in mode 2: the familiar problems associated with the construction of unitary phase operators in the presence of vacuum states are still present.

Thus, the number of ''faulty'' nonzero matrix elements in commutators of the type $[\hat{E}_{\varphi_{ij}}, \hat{E}_{\varphi_{jk}}]$ will grow like λ, since the number of states having the vacuum in one mode grows like λ. On the other hand, the number of states in the irrep $(\lambda, 0)$ grows like λ^2. The classical limit where $\lambda \to \infty$ corresponds to the limit where the phases commute, provided that we ignore the relatively small number of ''faulty'' nonzero matrix elements compared to the number of ''correct'' zero matrix elements. This relative number grows like $1/\lambda$.

In particular, in the interpretation of Eq. (89), the realization Γ becomes singular for states near the vacuum state when $\lambda \to \infty$ limit. Hence, provided that the distribution of photons in an input state is such that the vacuum can be safely ignored, phase operators can be considered as commuting.

A similar result on the lack of commutativity between the *total* and relative su(2) phase operators in systems containing few photons has been obtained in Ref. 14. These authors found that commutativity was recovered in the classical limit. Our results are similar to those found in Ref. 14, albeit applicable to the case of noncommuting *relative* phases in a three-beam system.

The three-dimensional representation (1, 0) merits special attention. Besides providing an illustrative example for our previous discussion, this representation is the only one that allows commuting *unitary* phase operators while preserving the polar decomposition.

More precisely, in a system containing a total of $\lambda=\nu_1+\nu_2+\nu_3=1$ quantum, the explicit matrix realization of (some of) $\hat{C}_{ij}$ in terms of $\hat{E}_{\varphi_{ij}}\cdot\hat{J}_{ij}$ can easily be found:

$$
\begin{array}{lccc}
(ij) & \hat{E}_{\varphi_i} & \hat{J}_{ij} & \hat{C}_{ij}=\hat{E}_{\varphi_{ij}}\cdot\hat{J}_{ij} \\
(1,2) & \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
(2,3) & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \\
(1,3) & \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\end{array}
\tag{94}
$$

To compute $\hat{E}_{\varphi_{12}}$, for instance, one uses $\hat{E}_{\varphi_{12}}=e^{i(2\varphi_1-\varphi_2)}$, i.e., the "phase" part of $\Gamma(\hat{C}_{12})$, the basis states $\{\frac{1}{2\pi}e^{i\varphi_1},\frac{1}{2\pi}e^{i(-\varphi_1+\varphi_2)},\frac{1}{2\pi}e^{i\varphi_2}\}$, and the inner product

$$
\langle\Psi|\Phi\rangle=\int_0^{2\pi}\int_0^{2\pi}\mathrm{d}\varphi_1\,\mathrm{d}\varphi_2\,\Psi^*\Phi. \tag{95}
$$

The operators $\hat{E}_{\varphi_{ij}}$ are explicitly not unitary. Whereas $\hat{E}_{\varphi_{12}}\cdot\hat{E}_{\varphi_{23}}=\hat{E}_{\varphi_{13}}$ it is not true that $[\hat{E}_{\varphi_{12}},\hat{E}_{\varphi_{23}}]=\hat{E}_{\varphi_{13}}$: the phase operators do not commute.

There are many ways of turning $\hat{E}_{\varphi_{ij}}$ into a unitary operator $E_{\hat{\varphi}_{ij}}$ while still preserving the decomposition of $\hat{C}_{ij}$ into a phase and a diagonal part. What is unique of the (1,0) representation is that it is also possible to find unitary operators $\hat{E}_{\hat{\varphi}_{ij}}$ such that $\hat{E}_{\hat{\varphi}_{ij}}$ preserves the polar decomposition of $\hat{C}_{ij}$ and simultaneously produces commuting phase operators: $[\hat{E}_{\hat{\varphi}_{ij}},\hat{E}_{\hat{\varphi}_{kl}}]=0$. This remarkable choice is

$$
E_{\hat{\varphi}_{12}}=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},\quad E_{\hat{\varphi}_{23}}=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},\quad E_{\hat{\varphi}_{13}}=\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \tag{96}
$$

It is not possible to convert $\hat{E}_{\varphi_{ij}}$ into a unitary operator $E_{\hat{\varphi}_{ij}}$ that will have all of the above enumerated properties when the total number of photons is greater than 1.

This result on the existence of commuting unitary phase operators is expected, as the representation (1,0) is pertinent to the classical description of a three-channel interferometer,[15] for which the phases are (of course) expected to commute.

V. DISCUSSION AND CONCLUSION

In deriving the representation Γ acting over the functions defined over the maximal torus H of $G=\mathrm{SU}(n+1)$, the main hinge is the decomposition of the Lie algebra as per Eq. (35). This is equivalent to requiring that the dimension of the subgroup H or, equivalently, the rank of the group G [i.e., n in the case of $\mathrm{SU}(n+1)$] is exactly of complementary dimension to the stabilizer of the highest weight state.

The question arises now as to whether there are other representations and/or groups G which allow a similar decomposition. The answer is—unfortunately—no, i.e., we need some extensions to the above-presented picture in order to accommodate other groups. We discuss why there is such an obstruction in the Appendix.

The technique adopted in this paper has been limited in scope to unirreps of $\mathrm{SU}(n+1)$ with highest weights of the type $(\lambda, 0,...)$. However, it is possible to extend the formalism presented here to general irreps by suitably enlarging the subgroup over which the coherent states are defined. Irreps of the type $(\lambda, \mu, 0,...)$ are particularly interesting as they can be expected to have applications to the description of polarized beams. For irreps with highest weight $(\lambda, \mu, 0,...)$, the appropriate subgroup $\mathfrak{k}$ of $\mathrm{SU}(n+1)$ is $S(U(2)\times U(1)\times\ldots\times U(1))$: the basis states and the representation Γ will then be expressed[16] in terms of Wigner functions over this subgroup.

The major result of this paper is a realization of the $\mathrm{su}(n+1)$ Lie algebra (or, more precisely, of the complex extension of this algebra), appropriate for irreps with integral highest weights of the form $(\lambda, 0,...)$, for which basis functions and generators are expressed in terms of exponential functions and derivatives of phase angles. This would appear to be particularly suitable for applications to phase states, and for the study of the asymptotic limits of a representation and the appropriate limit of Wigner functions.

Although this has been done explicitly only for SU(2) and SU(3), the parameters which enter in the realization can be generally interpreted as projective coordinates, related to $\mathrm{SU}(n+1)$ Wigner functions, and understood physically as related to the distribution of λ photons between $n+1$ fields.

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APPENDIX A: HOW TO COUNT THE DIMENSION OF THE STABILIZER

In this section, we show why our construction only works for algebras which have A_n as their complexification, and for which representations of A_n our construction is possible.

Let $\mathfrak{h}$ be the Cartan subalgebra of a Lie algebra of one of the classical groups [i.e., $\mathrm{SU}(n)$, $\mathrm{SO}(2n+1)$, $\mathrm{Sp}(2n)$, $\mathrm{SO}(2n)$ or their noncompact versions]. A good comprehensive review of Lie algebra structure is Refs. 17 and 18.

Let f_α be a lowering operator corresponding to the positive root α: in order that $f_\alpha\chi_\lambda\neq 0$ it is necessary and sufficient that $(\alpha,\lambda)\geqslant 0$, where $(,)$ is the Killing form. Notice that such lowering operators form a nilpotent subalgebra: we denote by $\mathfrak{t}_\lambda$ the subset of positive roots for which $(\lambda,\alpha)>0$.

Now, let $\{\alpha_i\}_{i=1\ldots l}$ be a set of simple (positive) roots, $\{\omega_i\}_{i=1\ldots l}$ the corresponding set of weights, i.e., $(\omega_i,\alpha_j)=\delta_{ij}$.

Any dominant weight and positive root can be written as

$$\lambda=\sum_{i=1}^{n}\lambda_i\omega_i,\quad \lambda_i\in\mathbb{N}_+,\quad \alpha=\sum_{i=1}^{n}m_i\alpha_i,\quad m_i\in\mathbb{N}_+. \tag{A1}$$

Let us fix a fundamental weight ω_k (which is equivalent to choosing a node on the Dynkin diagram).

For a given Lie algebra $\mathfrak{g}$ (i.e., for a given Dynkin diagram) one can compute the number of roots in $\mathfrak{t}_{\omega_k}$ and check to see, as we choose different nodes of the Dynkin diagram, if there are sufficiently many roots to allow a decomposition of the type proposed in Eq. (35).

The results are here below (we refer to the Planches in Ref. 18).

(1) SU($n+1$) (A_n): choosing the kth node there are $k(n+1-k)$ positive roots in $\mathfrak{t}_{\omega_k}$. The minimum for $\mathfrak{t}_{\omega_k}$ is n, which occurs when $k=1$ or $k=n$. These choices correspond, respectively, to the representations $(\lambda, 0,...)$ or $(0,..., 0,\lambda)$.

(2) SO($2n+1$) ($B_n, n>1$): choosing the kth node there are $k+k(n-k)+k(n+1-k)=2k(n+1-k)$ positive roots in $\mathfrak{t}_{\omega_k}$. The minimum is $2n$, which is bigger than the rank n of the group: it is impossible to construct SO($2n+1$) on the torus.

(3) Sp($2n$) ($C_n, n>2$): choosing the kth node there are $k(n-k)+k+k=k(n+2-k)$ positive roots. The minimum is $n+1$, and this is again greater than the rank n of Sp($2n$).

(4) SO($2n$) (D_n): choosing the kth node there are $k(n-k)+k+k=k(n+2-k)$ positive roots, the minimum is $n+1$, which is also greater than the rank of the group.

As we see, the minimal number is equal to the rank of the algebra only for A_n.

APPENDIX B: A COHOMOLOGICAL PERSPECTIVE ON $\mathcal{S}$-MATRIX THEORY

We wish to draw the attention of the reader to the following interesting ''cohomological'' interpretation of the solution for the operator $\mathcal{S}$.

In the construction of the coefficients $\mathcal{S}_\nu$ of the operator $\mathcal{S}$ from the ratios of Eq. (77) as described above, it is not *a priori* clear that the coefficient $\mathcal{S}_\nu$ corresponding to a nontrivial partition ν defined starting from the trivial partition does not depend on the particular ''path'' we have followed to reach the given partition ν. Indeed—in general—there are different ways of getting to a given partition ν starting from the trivial one; for instance, we have

$$(\lambda,0,0,0,...)\overset{C_{21}}{\mapsto}(\lambda-1,1,0,0,...)\overset{C_{31}}{\mapsto}(\lambda-2,1,1,0,...) \quad \text{or} \tag{B1}$$

$$(\lambda,0,0,0,...)\overset{C_{31}}{\mapsto}(\lambda-1,0,1,0,...)\overset{C_{21}}{\mapsto}(\lambda-2,1,1,0,...). \tag{B2}$$

We have to make sure that the coefficient $\mathcal{S}_{(\lambda-2,1,1,0,...)}$ defined along these two different ''paths'' does not depend on the choice of path. We observe here that this in particular implies that the following *cocycle* condition holds

$$R_{\nu,\nu'}R_{\nu',\nu''}R_{\nu'',\nu}=1 \tag{B3}$$

for any partitions ν, ν', ν'' which are adjacent in the following sense: Two partitions ν, ν' of λ are said to be *adjacent* if there exist $i\neq j$ such that

$$\nu_k=\nu'_k+\delta_{ik}-\delta_{jk}, \quad k=1,...,n+1. \tag{B4}$$

Let us verify this fact and consider the small loop

$$\nu\overset{C_{ij}}{\to}\nu'\overset{C_{jk}}{\to}\nu''\overset{C_{ki}}{\to}\nu, \tag{B5}$$

$$\nu'_r=\nu_r+\delta_{ir}-\delta_{jr}, \quad \nu''_r=\nu'_r+\delta_{jr}-\delta_{kr}=\nu_k+\delta_{ir}-\delta_{kr}, \tag{B6}$$

and the associated cocycle condition

$$R_{\nu\nu'}R_{\nu\nu'}R_{\nu'\nu''}=\frac{y_{ji}^{*}(\lambda+\rho_i(\nu'))}{y_{ij}(\lambda+\rho_j(\nu))}\frac{y_{kj}^{*}(\lambda+\rho_j(\nu''))}{y_{jk}(\lambda+\rho_k(\nu'))}\frac{y_{ik}^{*}(\lambda+\rho_k(\nu))}{y_{ki}(\lambda+\rho_i(\nu''))}, \tag{B7}$$

which, according to Eq. (B3), should be 1.

Using the expressions for y_{ij}, it can be verified explicitly that, if we set $v_1\equiv 1$, then

$$\frac{(y_{ji})^{*}}{y_{ij}}=\left(\frac{v_j^{*}v_j}{v_i^{*}v_i}\right), \quad v_1\equiv 1. \tag{B8}$$

Using Eq. (B8), one sees at once that the y dependence drops out Eq. (B7). Moreover, since i, j, k are distinct indices, one checks also that

$$\rho_i(\nu'')=\rho_i(\nu'), \quad \rho_j(\nu'')=\rho_j(\nu), \quad \rho_k(\nu)=\rho_k(\nu'). \tag{B9}$$

Therefore Eq. (B7) is consistent with Eq. (B3). In a similar way, one can easily check that $R_{\nu,\nu'}=(R_{\nu',\nu})^{-1}$. This equation, together with Eq. (B7), define a *cocycle* over partitions.

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Integrable variant of the one-dimensional Hubbard model

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A new integrable model which is a variant of the one-dimensional Hubbard model is proposed. The integrability of the model is verified by presenting the associated quantum R-matrix which satisfies the Yang–Baxter equation. We argue that the new model possesses the SO(4) algebra symmetry, which contains a representation of the η-pairing SU(2) algebra and a spin SU(2) algebra. Additionally, the algebraic Bethe ansatz is studied by means of the quantum inverse scattering method. The spectrum of the Hamiltonian, eigenvectors, as well as the Bethe ansatz equations, are discussed. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1481956]

I. INTRODUCTION

Since the discovery of high temperature superconductivity in cuprates,[1] a tremendous effort has been made to uncover the mystery of this phenomenon. It is generally believed that the strongly correlated electron systems behaving as non-Fermi liquids are closely related to superconducting materials. This has caused an intense study in strongly correlated electron systems.[2–7] These systems possess various physical characteristics which are decisively dominated by the competing interactions; e.g., the Coulomb interaction in the Hubbard model, spin fluctuations through the antiferromagnetic coupling for the super-symmetric t-J model and current-density correlated interaction inducing hole pairs of Cooper type superconductors in the one-dimensional (1D) Bariev model. The 1D Hubbard model as a prototype among the strongly correlated electron systems has attracted a substantial deal of interest in the study of integrable quantum field theory, mathematical physics and condensed matter physics since its exact solution was achieved by Lieb and Wu[8] in 1968. Towards a complete understanding of the mathematical structure of the 1D Hubbard model in the framework of the quantum inverse scattering method (QISM), a fundamental advance was achieved by Shastry[9] in demonstrating the integrability of the model. Specifically, it was shown that a two-dimensional statistical covering model of two coupled symmetric six vertex models provides a one parameter family of transfer matrices commuting with the Hamiltonian of the 1D Hubbard model. The algebraic formulation with respect to the integrability leads to the quantum R-matrix[9–12] which facilitates not only the algebraic Bethe ansatz solution,[13] but also the construction of the boost operator[14] for the model. Remarkably, the Hamiltonian of the Hubbard model was proved to exhibit the SO(4) symmetry by Yang and Zhang[15] (see also Ref. 16). Besides the spin SU(2) algebra, the SO(4) algebra contains the η-pair SU(2) algebra with the

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raising operator creating an on-site pair of electrons with opposite spins. This can be interpreted as a localized Cooper pair. A complete set of eigenstates of the Hamiltonian can be obtained by exploiting the SO(4) symmetry.[17]

The 1D Hubbard Hamiltonian with more competing interactions may also be considered. Along this line, many extended Hubbard models have been constructed in the literature, such as a $u(2|2)$ extended Hubbard model,[5] supersymmetric $U_q(\mathrm{osp}(2|2))$ electronic systems[18] and SU(N) Hubbard models.[19] In this article, we present an alternative 1D Hubbard model such that the Hamiltonian has off-site Coulomb interaction instead of the on-site one of the standard Hubbard model. The integrability of this model is verified by presenting the associated quantum R-matrix which fulfills the Yang–Baxter equation (YBE). We show that the model exhibits the SO(4) symmetry with new representations of the η-pairing SU(2) algebra and the ζ-pairing spin SU(2) algebra. Moreover, the algebraic Bethe ansatz is formulated by means of the QISM. Though the model exhibits the same spectrum as the standard Hubbard model on a periodic lattice, the new quantum R-matrix, the hidden nesting structure associated with an asymmetric isotropic six-vertex model and the Bethe eigenvectors do distinguish this model from the standard one.[9,10] The essential differences between the two models manifest in the open lattice versions, which we will discuss in more depth in the conclusion.

The article is organized as follows. In Sec. II, we introduce a Lax operator associated with the new Hubbard model and construct a nontrivial higher conserved quantity commuting with the Hamiltonian. In Sec. III, we present the R-matrix associated with the model by solving the Yang–Baxter relation. The SO(4) symmetry is verified too. In Sec. IV, we formulate the algebraic Bethe ansatz solutions for the model with periodic boundary conditions. The eigenvectors and eigenvalues of the Hamiltonian are presented explicitly. Section V is devoted to a discussion and conclusion.

II. THE MODEL

Let us begin by introducing a variant of the 1D Hubbard model with the Hamiltonian

$$H=\sum_{j=1}^{L}\{(\sigma_j^+\sigma_{j+1}^-+\sigma_j^-\sigma_{j+1}^+)+(\sigma\to\tau)\}+\frac{U}{4}\sum_{j=1}^{L}\sigma_j^z\tau_{j+1}^z. \tag{1}$$

Above σ_j and τ_j are the two commuting species of Pauli matrices acting on site j, and U is a Coulomb coupling constant. Above and throughout, periodic boundary conditions are imposed on all summations evaluated over the lattice length L. The difference from the standard Hubbard model is that the model (1) exhibits the off-site Coulomb interaction instead of the on-site one. We shall see that it not only breaks the spin reflection symmetry but also specifies a new representation of η-pairing SU(2) algebra and spin SU(2) algebra in order to maintain the SO(4) symmetry. To verify the integrability of the model, we, at first, identify a relation between the Hamiltonian (1) and the transfer matrix which is defined by

$$\tau(u)=Tr_0T(u) \tag{2}$$

with

$$T(u)=L_{0L}(u)\cdots L_{01}(u). \tag{3}$$

The local Lax operators associated with model (1) have to be alternatively chosen as

$$L_{0j}(u)=L_{0j}^{\sigma}(u)I_0^2L_{0j}^{\tau}(u) \tag{4}$$

$$=\begin{pmatrix} e^{h(u)}P_j^+Q_j^+ & e^{h(u)}P_j^+\tau_j^- & e^{-h(u)}\sigma_j^-Q_j^+ & e^{-h(u)}\sigma_j^-\tau_j^- \\ e^{-h(u)}P_j^+\tau_j^+ & e^{-h(u)}P_j^+Q_j^- & e^{h(u)}\sigma_j^-\tau_j^+ & e^{h(u)}\sigma_j^-Q_j^- \\ e^{h(u)}\sigma_j^+Q_j^+ & e^{h(u)}\sigma_j^+\tau_j^- & e^{-h(u)}P_j^-Q_j^+ & e^{-h(u)}P_j^-\tau_j^- \\ e^{-h(u)}\sigma_j^+\tau_j^+ & e^{-h(u)}\sigma_j^+Q_j^- & e^{h(u)}P_j^-\tau_j^+ & e^{h(u)}P_j^-Q_j^- \end{pmatrix}, \tag{5}$$

where

$$P_j^{\pm}=w_4(u)\pm w_3(u)\sigma^z;$$

$$Q_j^{\pm}=w_4(u)\pm w_3(u)\tau^z$$

with a parametrization $\gamma(u)=w_4(u)-w_3(u)=\sin(u)$; $\alpha(u)=w_4(u)+w_3(u)=\cos(u)$. We would like to mention that the Lax operators

$$L_{0j}^{\sigma}(u)=w_4(u)+w_3(u)\sigma_j^z\sigma_0^z+\sigma_j^+\sigma_0^-+\sigma_0^+\sigma_j^-, \tag{6}$$

$$L_{0j}^{\tau}(u)=w_4(u)+w_3(u)\tau_j^z\tau_0^z+\tau_j^+\tau_0^-+\tau_0^+\tau_J^-, \tag{7}$$

$$I_0=\cosh\frac{h(u)}{2}+\sigma_0^z\tau_0^z\sinh\frac{h(u)}{2}, \tag{8}$$

have been chosen the same as that for the Hubbard model.[9–11] It follows that the Hamiltonian (1) is related to the transfer matrix (2) in the following way:

$$\ln\tau(u)=\ln\tau(0)+Hu+\frac{1}{2!}Ju^2+\cdots, \tag{9}$$

above the Hamiltonian $H=\Sigma_{j=1}^{L}H_{j(j+1)}$ with the Hamiltonian density

$$H_{j(j+1)}=L_{0(j+1)}(0)L_{0j}'(0)L_{0j}^{-1}(0))L_{0(j+1)}^{-1}(0), \tag{10}$$

and the second higher conserved current can be given as

$$J=\sum_{j=1}^{L}J_{j(j+1)(j+2)} \tag{11}$$

with

$$J_{j(j+1)(j+2)}=B_{j(j+1)}-H_{j(j+1)}^2-[H_{j(j+1)},H_{(j+1)(j+2)}], \tag{12}$$

$$B_{j(j+1)}=L_{0(j+1)}(0)L_{0j}''(0)L_{0j}^{-1}(0)L_{0(j+1)}^{-1}(0). \tag{13}$$

Here the prime denotes the derivative with respect to spectral parameter u. After a straightforward calculation, the equation (10) does provide us with the expression (1), whereas the second conserved quantity (11) has the form

$$J_{j(j+1)(j+2)}=\frac{U}{2}\{[-\sigma_j^+\sigma_{j+1}^-+\sigma_j^-\sigma_{j+1}^+]\tau_{j+1}^z+[-\tau_j^+\tau_{j+1}^-+\tau_{j+1}^+\tau_j^-]+\sigma_j^z[-\sigma_j^+\sigma_{j+1}^- +\sigma_j^-\sigma_{j+1}^+]\tau_{j+2}^z+[-\tau_{j+1}^+\tau_{j+2}^-+\tau_{j+2}^+\tau_{j+1}^-]\sigma_j^z\}+[-\sigma_{j+2}^+\sigma_j^-+\sigma_j^+\sigma_{j+2}^-]\sigma_{j+1}^z +[-\tau_{j+2}^+\tau_j^-+\tau_j^+\tau_{j+2}^-]\tau_{j+1}^z. \tag{14}$$

Here we would like to stress that both the Hamiltonian (1) and the conserved quantity (11) should be understood as global operators. It is meant that $[H,J]=0$ rather than $[H_{j(j+1)},J_{j(j+1)(j+2)}]=0$. The mutual commutativity of H and J convinces us of the existence of a quantum R-matrix associated with the model (1). We shall present a rigorous proof of the integrability of the model in the next section.

III. INTEGRABILITY OF THE MODEL

It has long been clarified that the existence of the quantum R-matrix which fulfills the Yang–Baxter relation is desirable for constructing integrable quantum chains. This suggests to us a way to verify the integrability of the model presented above. Indeed, following Ref. 11, we, after a cumbersome algebraic calculation, can find a class of solutions to the Yang–Baxter relation

$$\overset{\vee}{R}(u,v)L_{0j}(u)\otimes L_{0j}(v)=L_{0j}(v)\otimes L_{0j}(u)\overset{\vee}{R}(u,v), \tag{15}$$

which is given as

$$\overset{\vee}{R}(u,v) = \begin{pmatrix}
\rho_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & \rho_2^- & 0 & 0 & \rho_9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & \rho_2^+ & 0 & 0 & 0 & 0 & 0 & \rho_9 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & \rho_5 & 0 & 0 & \rho_6^+ & 0 & 0 & \rho_6^- & 0 & 0 & \rho_8 & 0 & 0 & 0\\
0 & \rho_{10} & 0 & 0 & \rho_2^+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & \rho_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & \rho_6^- & 0 & 0 & \rho_3 & 0 & 0 & \rho_7 & 0 & 0 & \rho_6^+ & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_2^- & 0 & 0 & 0 & 0 & 0 & \rho_{10} & 0 & 0\\
0 & 0 & \rho_{10} & 0 & 0 & 0 & 0 & 0 & \rho_2^- & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & \rho_6^+ & 0 & 0 & \rho_7 & 0 & 0 & \rho_3 & 0 & 0 & \rho_6^- & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_4 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_2^+ & 0 & 0 & \rho_{10} & 0\\
0 & 0 & 0 & \rho_8 & 0 & 0 & \rho_6^- & 0 & 0 & \rho_6^+ & 0 & 0 & \rho_5 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_9 & 0 & 0 & 0 & 0 & 0 & \rho_2^+ & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_9 & 0 & 0 & \rho_2^- & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho_1
\end{pmatrix}, \tag{16}$$

with the Boltzmann weights

$$\rho_1=(\cos u\cos v e^{l}+\sin v\sin u e^{-l})\rho_2,$$

$$\rho_4=(\cos u\cos v e^{-l}+\sin v\sin u e^{l})\rho_2,$$

$$\rho_9=(\sin u\cos v e^{-l}-\sin v\cos u e^{l})\rho_2,$$

$$\rho_{10}=(\sin u\cos v e^{l}-\sin v\cos u e^{-l})\rho_2,$$

$$\rho_2^{+}=e^{l}\rho_2,\quad \rho_2^{-}=e^{-l}\rho_2,$$

$$\rho_3=\frac{(\cos u\cos v e^{l}-\sin v\sin u e^{-l})}{\cos^2 u-\sin^2 v}\rho_2,$$

$$\rho_5=\frac{(\cos u\cos v e^{-l}-\sin v\sin u e^{l})}{\cos^2 u-\sin^2 v}\rho_2,$$

$$\rho_6^{+}=\frac{(\cos u\sin u e^{-l}-\sin v\cos v e^{l})}{\cos^2 u-\sin^2 v}\rho_2,$$

$$\rho_6^{-}=\frac{(\cos u\sin u e^{l}-\sin v\cos v e^{-l})}{\cos^2 u-\sin^2 v}\rho_2$$

and

$$\rho_8=\rho_3-\rho_1,$$

$$\rho_7=\rho_5-\rho_4, \tag{17}$$

$$l=h(u)-h(v),\quad i\qquad \frac{\sinh 2h(u)}{\sin 2u}=\frac{U}{2},$$

which enjoy the following identities:

$$\rho_4\rho_1+\rho_9\rho_{10}=1,$$

$$\rho_1\rho_5+\rho_3\rho_4=2,$$

$$\rho_6^{+}\rho_6^{-}=\rho_3\rho_5-1.$$

This R-matrix with more distinct Boltzmann weights is indeed different from the one for the standard Hubbard model[9–11] and a twisted version[20] which is associated with the Hubbard model with chemical potential terms. Running a Maple program we may check that the R-matrix satisfies the Yang–Baxter equation

$$R_{12}(u,v)R_{13}(u,w)R_{23}(v,w)=R_{23}(v,w)R_{13}(u,w)R_{12}(u,v). \tag{18}$$

So far we have built up the QISM mechanism for the alternative Hubbard model and concluded the integrability of the model as well. On the other hand, a fermionic model is always favorable in the study of the condensed matter physics due to the clear distinction between the fermionic degrees of freedom and bosonic degrees of freedom. By performing the Jordan–Wigner transformations,[11,21] one may obtain the Hamiltonian of a fermionic model which is equivalent to the Hubbard model (1):

$$H=-\sum_{j=1}^{N-1}\sum_{s}(a_{(j+1)s}^{\dagger}a_{js}+a_{js}^{\dagger}a_{(j+1)s})+U\sum_{j=1}^{N}\left(n_{j\uparrow}-\frac{1}{2}\right)\left(n_{(j+1)\downarrow}-\frac{1}{2}\right). \tag{19}$$

Above $a_{js}^{\dagger}$ and a_{js} are creation and annihilation operators with spins ($s=\uparrow$ or $\downarrow$) at site j satisfying the anti-commutation relations

$$\{a_{js},a_{j's'}\}=\{a_{js}^{\dagger},a_{j's'}^{\dagger}\}=0, \tag{20}$$

$$\{a_{js},a_{j's'}^{\dagger}\}=\delta_{jj'}\delta_{ss'}, \tag{21}$$

and $n_{js}=a_{js}^{\dagger}a_{js}$ is the density operator. The integrability of the fermionic model (19) requires that the graded Lax operator related to the Hamiltonian (19),

$$\mathcal{L}_{0j}(u)=\begin{pmatrix} -e^{h(u)}f_{j\uparrow}f_{j\downarrow} & -e^{h(u)}f_{j\uparrow}a_{j\downarrow} & \mathrm{i}e^{-h(u)}a_{j\uparrow}g_{j\downarrow} & \mathrm{i}e^{-h(u)}a_{j\uparrow}a_{j\downarrow} \\ -\mathrm{i}e^{-h(u)}f_{j\uparrow}a_{j\downarrow}^{\dagger} & e^{-h(u)}f_{j\uparrow}g_{j\downarrow} & e^{h(u)}a_{j\uparrow}a_{j\downarrow}^{\dagger} & \mathrm{i}e^{h(u)}a_{j\uparrow}g_{j\downarrow} \\ e^{h(u)}a_{j\uparrow}^{\dagger}f_{j\downarrow} & e^{h(u)}a_{j\uparrow}^{\dagger}a_{j\downarrow} & e^{-h(u)}g_{j\uparrow}f_{j\downarrow} & e^{-h(u)}g_{j\uparrow}a_{j\downarrow} \\ -\mathrm{i}e^{-h(u)}a_{j\uparrow}^{\dagger}a_{j\downarrow}^{\dagger} & e^{-h(u)}a_{j\uparrow}^{\dagger}g_{j\downarrow} & \mathrm{i}e^{h(u)}g_{j\uparrow}a_{j\downarrow}^{\dagger} & -e^{h(u)}g_{j\uparrow}g_{j\downarrow} \end{pmatrix}, \tag{22}$$

must generate the graded Yang–Baxter relation

$$\overset{\vee}{\mathcal{R}}(u,v)\mathcal{L}_{0j}(u)\otimes\mathcal{L}_{0j}(v)=\mathcal{L}_{0j}(v)\otimes\mathcal{L}_{0j}(u)\overset{\vee}{\mathcal{R}}(u,v), \tag{23}$$

with the graded R-matrix which is given by

$$\overset{\vee}{\mathcal{R}}(u,v)=W\overset{\vee}{R}(u,v)W^{-1}, \tag{24}$$

where

$$W=\sigma^{z}\otimes\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\mathrm{i} & 0 & 0 \\ 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\otimes I \tag{25}$$

and

$$f_{js}=\sin u-(\sin u-\mathrm{i}\cos u)n_{js},\quad g_{js}=\cos u-(\cos u+\mathrm{i}\sin u)n_{js}, \tag{26}$$

with the grading $P(1)=P(4)=0$, $P(2)=P(3)=1$. The monodromy matrix is defined by

$$\mathcal{T}(u)=\mathcal{L}_{0L}(u)\cdots\mathcal{L}_{01}(u), \tag{27}$$

such that the transfer matrices

$$\tau(u)=\mathrm{str}_{0}\mathcal{T}(u) \tag{28}$$

commute each other for different values of the parameter u. It can be verified that an expansion of the logarithm of the transfer matrix (28) in powers of u will lead to the Hamiltonian (19) as well as higher conserved quantities.

We would like to remark that the model possesses the SO(4) symmetry if we consider a new representation of the η-pair SU(2) algebra,

$$\eta=\sum_{i=1}^{L}(-1)^{i}a_{i\uparrow}a_{(i+1)\downarrow},\quad \eta^{\dagger}=(\eta)^{\dagger},\quad \eta_{z}=\frac{1}{2}\sum_{i=1}^{L}(n_{i\uparrow}+n_{i\downarrow})-\frac{1}{2}L, \tag{29}$$

and the ζ-pair spin SU(2) algebra

$$\zeta=\sum_{i=1}^{L} a_{i\uparrow}^{\dagger}a_{(i+1)\downarrow}, \quad \zeta^{\dagger}=(\zeta)^{\dagger}, \quad \zeta_z=\frac{1}{2}\sum_{i=1}^{L}(n_{(i+1)\downarrow}-n_{i\uparrow}), \tag{30}$$

which comprise the SO(4) algebra. Taking into account the globality of these operators, one may show that the Hamiltonian (19) commutes with the generators of the above two SU(2) algebras. This symmetry could be expected to complete all eigenstates of the Hubbard model like the case in the standard Hubbard model. Here the η-pairing raising operator creating a pair of electrons with opposite spin on different sites could be interpreted as a delocalized Cooper pair.

IV. ALGEBRAIC BETHE ANSATZ

Towards an exact solution of an integrable model, the algebraic Bethe ansatz seems to have more utility than the coordinate Bethe ansatz because the former not only provides us with the spectrum of all conserved quantities, but makes a close connection to the finite temperature properties of the model. There have been a lot of papers devoted to the study of the nested algebraic Bethe ansatz[22] for the multistate integrable models with Lie algebra (or Lie superalgebra) symmetry. Following the so-called ABCDF approach to solve the Hubbard-like models,[13,23] we shall formulate the algebraic Bethe ansatz for the model in that which follows. To this end, as usual, we have to perform the ansatz step by step. However, it is not necessary to restate all of the calculations used in solving our model because of the similarity to the routine proposed in Ref. 13.

In order to carry out the algebraic Bethe ansatz for this Hubbard model, we first need to find the eigenvalues and eigenvectors of the transfer matrix (28):

$$\tau|\Phi_n\rangle=\lambda|\Phi_n\rangle. \tag{31}$$

Following the prescription in Ref. 13, the eigenvectors of the transfer matrix are given by

$$|\Phi_n\rangle=\mathbf{\Phi_n}.\mathcal{F}|0\rangle, \tag{32}$$

where the components of $\mathcal{F}$ are coefficients of an arbitrary linear combination of vectors $\mathbf{\Phi_n}$ and $|0\rangle$ is the pseudovacuum state, chosen here as the standard ferromagnetic one

$$|0\rangle=\otimes_{j=1}^{N}|0\rangle_j, \tag{33}$$

where

$$|0\rangle_i=\begin{pmatrix}1\\0\end{pmatrix}_i\otimes\begin{pmatrix}1\\0\end{pmatrix}_i \tag{34}$$

which corresponds to the doubly occupied state. We write the monodromy matrix $\mathcal{T}(u)$ in (27) as

$$\mathcal{T}(u)=\begin{pmatrix} B(u) & B_1(u) & B_2(u) & F(u)\\ C_1(u) & A_{11}(u) & A_{12}(u) & E_1(u)\\ C_2(u) & A_{21}(u) & A_{22}(u) & E_2(u)\\ C_3(u) & C_4(u) & C_5(u) & D(u)\end{pmatrix} \tag{35}$$

such that the necessary commutation relations between the diagonal fields and the creation fields can be derived from the Yang–Baxter algebra

$$\mathcal{R}_{12}(u,v)\overset{1}{\mathcal{T}}(u)\overset{2}{\mathcal{T}}(v)=\overset{2}{\mathcal{T}}(v)\overset{1}{\mathcal{T}}(u)\mathcal{R}_{12}(u,v). \tag{36}$$

In the above,

$$\mathcal{R}_{12}(u,v)=\mathcal{P}\check{R}(u,v).$$

Here $\mathcal{P}$ is the graded permutation operator. Let us first display an important commutation role, which reveals to us a hidden nesting structure and the symmetry of eigenvectors,

$$\vec{B}(u)\vec{B}(v)=\frac{\rho_4(u,v)}{\rho_1(u,v)}\vec{B}(v)\vec{B}(u)\cdot\hat{r}(u,v)+\frac{\mathrm{i}}{\rho_8(u,v)\rho_1(u,v)}F(v)B(u)\vec{\xi}_1(u,v)$$
$$+\frac{\mathrm{i}}{\rho_8(u,v)}F(u)B(v)\vec{\xi}_2(u,v), \tag{37}$$

where

$$\vec{\xi}_1(u,v)=(0,f_1(u,v),f_2(u,v),0);\quad \vec{\xi}_2(u,v)=(0,\rho_6^+(u,v),\rho_6^-(u,v),0),$$

$$\hat{r}(u,v)=\begin{pmatrix}1&0&0&0\\0&a(u,v)&b(u,v)&0\\0&c(u,v)&d(u,v)&0\\0&0&0&1\end{pmatrix}, \tag{38}$$

with

$$f_1(u,v)=\rho_6^-(u,v)\rho_8(u,v)-\rho_6^+(u,v)\rho_5(u,v),$$

$$f_2(u,v)=\rho_6^-(u,v)\rho_5(u,v)-\rho_6^+(u,v)\rho_8(u,v),$$

$$a(u,v)=\frac{\rho_3(u,v)\rho_8(u,v)-\rho_6^+(u,v)^2}{\rho_4(u,v)\rho_8(u,v)},$$

$$d(u,v)=\frac{\rho_3(u,v)\rho_8(u,v)-\rho_6^-(u,v)^2}{\rho_4(u,v)\rho_8(u,v)},$$

$$b(u,v)=c(u,v)=\frac{\rho_6^+(u,v)\rho_6^-(u,v)-\rho_8(u,v)\rho_7(u,v)}{\rho_4(u,v)\rho_8(u,v)}.$$

It turns out that the auxiliary matrix $\hat{r}(u,v)$ is nothing but a gauged rational R-matrix of an isotropic six-vertex model. If we adopt the parametrization introduced in Ref. 13 or 24, explicitly,

$$\tilde{x}=-\frac{\sin x}{\cos x}e^{-2h(x)}+\frac{\cos x}{\sin x}e^{2h(x)},\quad x=u,v, \tag{39}$$

one may find that

$$a(u,v)=-\frac{Ue^{-\theta(u,v)}}{\tilde{u}-\tilde{v}-U},\quad d(u,v)=-\frac{Ue^{\theta(u,v)}}{\tilde{u}-\tilde{v}-U},$$

$$b(u,v)=c(u,v)=\frac{\tilde{u}-\tilde{v}}{\tilde{u}-\tilde{v}-U},$$

with

$$e^{-\theta(u,v)}=\frac{\cos v\,\sin u}{\sin v\cos u}.$$

We shall see that the $\hat{r}$-matrix (38) is related to the one of the isotropic six-vertex model via a proper gauge transformation, which does not change the spectrum of the spin sector. This seems to provide a new version of the R-matrix, which does not have the difference property, for the isotropic six-vertex model. In view of the commutation relation (37), the creation operators $\vec{B}_a$, $\vec{E}_a$ do not intertwine. So it is reasonable that the eigenvectors of the transfer matrices are generated only by the creation operators $\vec{B}_a(u)$ and $F(u)$. Following the argument in Ref. 13, we may find that the n-particle vector can be determined recursively by the following relation:

$$\Phi_n(v_1,\ldots,v_n)=\vec{B}(v_1)\otimes\Phi_{n-1}(v_2,\ldots,v_n)+\sum_{j=2}^{n}\frac{1}{\mathrm{i}\rho_8(v_1,v_j)}\prod_{k\neq j}^{n}\frac{\rho_1(v_k,v_j)}{\mathrm{i}\rho_9(v_k,v_j)}[\vec{\xi}_2(v_1,v_j)$$
$$\otimes F(v_1)\Phi_{n-2}(v_2,\ldots,v_{j-1},v_{j+1},\ldots,v_n)B(v_j)]\prod_{k=2}^{j-1}\frac{\rho_4(v_k,v_j)}{\rho_1(v_k,v_j)}\hat{r}_{k,k+1}(v_k,v_j). \tag{40}$$

Explicitly, the two-particle eigenvector reads

$$\Phi_2(v_1,v_2)=\vec{B}(v_1)\otimes\vec{B}(v_2)+\vec{\xi}_2(v_1,v_2)\otimes F(v_1)B(v_2)\frac{1}{\mathrm{i}\rho_8(v_1,v_2)}. \tag{41}$$

From the commutation relation (37), we can conclude that $\Phi_n(v_1,\ldots,v_n)$ satisfies an exchange symmetry relation

$$\Phi_n(v_1,\ldots,v_j,v_{j+1},\ldots,v_n)=\frac{\rho_4(v_j,v_{j+1})}{\rho_1(v_j,v_{j+1})}\Phi_n(v_1,\ldots,v_{j+1},v_j,\ldots,v_n)\cdot\hat{r}_{j,j+1}(v_j,v_{j+1}) \tag{42}$$

based on the following identity:

$$\frac{\rho_4(v_j,v_{j+1})}{\rho_1(v_{j+1},v_j)\rho_8(v_{j+1},v_j)\rho_1(v_j,v_{j+1})}\vec{\xi}_1(v_{j+1},v_j)\cdot\hat{r}(v_j,v_{j+1})$$
$$=-\frac{1}{\rho_8(v_j,v_{j+1})}\vec{\xi}_2(v_j,v_{j+1}). \tag{43}$$

In the above expressions, $\vec{\xi}$ plays the role of forbidding two spin up or two spin down electrons at same site. Also, $F(u)$ creates a local hole pair with opposite spins. In order to manipulate the eigenvalue of the transfer matrix (28) we need the commutation roles involving the diagonal fields over the creation fields. After some algebra, from the Yang–Baxter relation (36) we have

$$B(u)\vec{B}_a(v)=\frac{\rho_1(v,u)}{\mathrm{i}\rho_9(v,u)}\vec{B}_a(v)B(u)-\frac{1}{\mathrm{i}\rho_9(v,u)}\vec{B}_a(u)B(v)\cdot\hat{\eta}_1(v,u), \tag{44}$$

$$D(u)\vec{B}_a(v)=\frac{\mathrm{i}\rho_{10}(u,v)}{\rho_8(u,v)}\vec{B}_a(v)D(u)-\frac{1}{\rho_8(v,u)}F(v)\vec{C}^*_{a+3}(u)\cdot\hat{\eta}_1(u,v)$$
$$+\frac{\rho_5(u,v)}{\rho_8(u,v)}F(u)\vec{C}^*_{a+3}(v)+\frac{\mathrm{i}}{\rho_8(u,v)}\vec{\xi}_2(u,v)\cdot(\vec{E}^*(u)\otimes\hat{A}(v)), \tag{45}$$

$$\hat{A}_{ab}(u)\vec{B}_a(v)=\frac{\mathrm{i}\rho_4(u,v)}{\rho_9(u,v)}\vec{B}(v)\otimes\hat{A}(u)\cdot\hat{r}(u,v)-\frac{\mathrm{i}}{\rho_9(u,v)}\hat{\eta}_2(u,v)\cdot\vec{B}(u)\otimes\hat{A}(v)$$
$$+\frac{1}{\rho_9(u,v)\rho_8(u,v)}\{F(v)\vec{C}_{3-a}(u)\otimes\vec{\xi}_1(u,v)+\hat{\eta}_2(u,v)\cdot F(u)\vec{C}_{3-a}(v)$$
$$\otimes\vec{\xi}_2(u,v)\}+\frac{1}{\rho_8(u,v)}\vec{E}^*(u)B(v)\otimes\vec{\xi}_2(u,v). \tag{46}$$

Above we introduced the notations

$$\hat{\eta}_1(u,v)=\begin{pmatrix}\rho_2^+(u,v) & 0\\ 0 & \rho_2^-(u,v)\end{pmatrix},$$

$$\hat{\eta}_2(u,v)=\begin{pmatrix}\rho_2^-(u,v) & 0\\ 0 & \rho_2^+(u,v)\end{pmatrix},$$

$$\hat{A}(u)=\begin{pmatrix}A_{11}(u) & A_{12}(u)\\ A_{21}(u) & A_{22}(u)\end{pmatrix}, \tag{47}$$

$$\vec{B}=(B_1,B_2),\quad \vec{C}=\begin{pmatrix}C_1\\ C_2\end{pmatrix},$$

$$\vec{C}^*=(C_4,C_5),\quad \vec{E}^*=\begin{pmatrix}E_1\\ E_2\end{pmatrix}.$$

In order to determine the eigenvalue of the transfer matrix (28) acting on the mult-particle eigenstates we need to consider the commutation relations for the creation field $F(u)$:

$$B(u)F(v)=-\frac{\rho_1(v,u)}{\rho_8(v,u)}F(v)B(u)+\frac{\rho_5(v,u)}{\rho_8(v,u)}F(u)B(v)-\frac{\mathrm{i}}{\rho_8(v,u)}[\vec{B}(u)\otimes\vec{B}(v)]\cdot\vec{\xi}_2^t(v,u), \tag{48}$$

$$D(u)F(v)=-\frac{\rho_1(v,u)}{\rho_8(v,u)}F(v)D(u)+\frac{\rho_5(v,u)}{\rho_8(v,u)}F(u)D(v)+\frac{\mathrm{i}}{\rho_8(v,u)}\vec{\xi}_2(v,u)\cdot[\vec{E}^*(u)\otimes\vec{E}^*(v)], \tag{49}$$

$$\hat{A}(u)F(v)=\left[1-\frac{\rho_2^+(u,v)\rho_2^-(u,v)}{\rho_9(u,v)\rho_{10}(u,v)}\right]F(v)\hat{A}(u)+\frac{1}{\rho_9(u,v)\rho_{10}(u,v)}\hat{\eta}_2(u,v)\cdot F(u)\hat{A}(v)\cdot\hat{\eta}_2(u,v)$$
$$+\frac{1}{\mathrm{i}\rho_9(u,v)}\hat{\eta}_2(u,v)\cdot\vec{B}(u)\otimes\vec{E}^*(v)-\frac{1}{\mathrm{i}\rho_{10}(u,v)}\vec{E}^*(u)\otimes\vec{B}(v)\cdot\hat{\eta}_2(u,v), \tag{50}$$

$$\vec{B}(u)F(v)=\frac{\mathrm{i}\rho_9(u,v)}{\rho_1(u,v)}F(v)\vec{B}(u)+\frac{1}{\rho_1(u,v)}\hat{\eta}_2(u,v)\cdot\vec{B}(v)F(u), \tag{51}$$

$$F(u)\vec{B}(v)=-\frac{\mathrm{i}\rho_{10}(u,v)}{\rho_1(u,v)}\vec{B}(v)F(u)+\frac{1}{\rho_1(u,v)}\hat{\eta}_1(u,v)\cdot F(v)\vec{B}(u). \tag{52}$$

Finally, if we adopt the variables $z_\pm(v_i)$ used in Ref. 13, i.e.,

$$z_-(v_i)=\frac{\cos v_i}{\sin v_i}e^{2h(v_i)},\quad z_+(v_i)=\frac{\sin v_i}{\cos v_i}e^{2h(v_i)},\tag{53}$$

and make a shift on the spin rapidity $\tilde{\lambda}_j=\tilde{\lambda}_j+U/2$, the eigenvalue of the transfer matrix (28) is given as (up on a common factor)

$$\begin{aligned}\tau(u)|\Phi_n(v_1,\ldots,v_n)\rangle=\Bigg\{&[z_-(u)]^L\prod_{i=1}^{n}\frac{\sin u(1+z_-(v_i)/z_+(u))}{\cos u(1-z_-(v_i)/z_-(u))}\\&+[z_+(u)]^L\prod_{i=1}^{n}\frac{\sin u(1+z_-(v_i)z_-(u))}{\cos u(1-z_-(v_i)z_+(u))}\\&-\prod_{i=1}^{n}\frac{\sin u(1+z_-(v_i)/z_+(u))}{\cos u(1-z_-(v_i)/z_-(u))}\prod_{l=1}^{M}\frac{(\tilde{u}-\tilde{\lambda}_l+U/2)}{(\tilde{u}-\tilde{\lambda}_l-U/2)}\\&+\prod_{i=1}^{n}\frac{\sin u(1+z_-(v_i)z_-(u))}{\cos u(1-z_-(v_i)z_+(u))}\prod_{l=1}^{M}\frac{(\tilde{u}-\tilde{\lambda}_l-3U/2)}{(\tilde{u}-\tilde{\lambda}_l-U/2)}\Bigg\}|\Phi_n(v_1,\ldots,v_n)\rangle,\end{aligned}\tag{54}$$

provided that

$$[z_-(v_i)]^L=\prod_{l=1}^{M}\frac{(\tilde{v}_i-\tilde{\lambda}_l+U/2)}{(\tilde{v}_i-\tilde{\lambda}_l-U/2)},\tag{55}$$

$$\prod_{i=1}^{n}\frac{(\tilde{\lambda}_j-\tilde{v}_i+U/2)}{(\tilde{\lambda}_j-\tilde{v}_i-U/2)}=-\prod_{\substack{l=1,\\ l\neq j,}}^{M}\frac{(\tilde{\lambda}_j-\tilde{\lambda}_l+U)}{(\tilde{\lambda}_j-\tilde{\lambda}_l-U)},\tag{56}$$

where

$$j=1,\ldots M,\quad i=1,\ldots,n.$$

If we express the variable $z_-(u_i)$ in terms of the (hole) momenta k_i by $z_-(u_i)=e^{ik_i}$, from the relation (39), the energy is given by

$$E_n=-(N/2-n)U-\sum_{i=1}^{n}2\cos k_i.\tag{57}$$

Using the momenta k_i instead of the charge rapidity $\tilde{v}_i$ via the relation (39) and making a scaling on the spin rapidity $\tilde{\lambda}_j$ as $\lambda_j=-(i/2)\tilde{\lambda}_j$, then the Bethe equations (55) and (56) read

$$e^{iLk_i}=\prod_{l=1}^{M}\frac{(\sin k_i-\lambda_l-iU/4)}{(\sin k_i-\lambda_l+iU/4)},$$

$$\prod_{i=1}^{n}\frac{(\sin k_i-\lambda_j-iU/4)}{(\sin k_i-\lambda_j+iU/4)}=-\prod_{\substack{l=1,\\ l\neq j}}^{M}\frac{(\lambda_j-\lambda_l+iU/2)}{(\lambda_j-\lambda_l-iU/2)},\tag{58}$$

$$j=1,\ldots M,\quad i=1,\ldots,n.$$

V. CONCLUSIONS AND DISCUSSION

We have proposed an integrable variant of the Hubbard model with off-site Coulomb interaction. The integrability of the model was verified by showing that the quantum R-matrix satisfies the Yang–Baxter equation. It was argued that the model possess SO(4) symmetry, however, it contains a new representation of η-pairing SU(2) algebra and ζ-pair spin SU(2) algebra. By means of the nested Bethe ansatz, we have presented the spectrum of the Hamiltonian, eigenvectors and the Bethe ansatz equations for the model with periodic boundary conditions. We found that the model exhibits a gauged r-matrix of the isotropic XXX model, which plays a crucial role in solving the model. Under periodic boundary conditions the alternative model and the standard Hubbard model share the same spectrum and Bethe ansatz equations. However, the new R-matrix we obtained permits different boundary conditions from that for the usual one.[25,26] This is meant that there does not exist simple transformation or gauge transformation between the new R-matrix and the original one. In turn, the differences in spectrum for the two models would be apparent in the case of open boundary conditions. We would like to remark that the 1D Hubbard model with long range Coulomb interaction, i.e., $U\Sigma_{j=1}^{N}(n_{j\uparrow}-\frac{1}{2})(n_{(j+r)\downarrow}-\frac{1}{2})$, $r=1,2,\ldots$, instead of the on-site one in the standard Hubbard model would be also integrable. But this type of interaction would result in nondiagonal boundary scattering matrices which provide competing interaction terms in the Hamiltonain. This seems to open an opportunity to identify new boundary impurity effects[27–29] in a Luttinger liquid. An interesting problem is to identify the boost operator for the spectral parameter extension of this new model, which can iteratively generate all of the conserved currents, using the results of Ref. 14. We shall be focusing on these problems in the near future.

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Renormalization analysis of correlation properties in a quasiperiodically forced two-level system

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We give a rigorous renormalization analysis of the self-similarity of correlation functions in a quasiperiodically forced two-level system. More precisely, the system considered is a quantum two-level system in a time-dependent field consisting of periodic kicks with amplitude given by a discontinuous modulation function driven in a quasiperiodic manner at golden mean frequency. Mathematically, our analysis consists of a description of all piecewise-constant periodic orbits of an additive functional recurrence. We further establish a criterion for such orbits to be globally bounded functions. In a particular example, previously only treated numerically, we further calculate explicitly the asymptotic height of the main peaks in the correlation function. © *2002 American Institute of Physics.*
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I. INTRODUCTION

A number of authors have investigated the possibility of the existence of dynamics with singular continuous spectrum in quasiperiodically forced two-level quantum systems.[2,5,10] In these works, such a spectrum—suggestive of a form of weak mixing—is observed in the presence of piecewise-constant discontinuous forcing. Moreover, for the forcing frequencies considered, the autocorrelation function is observed not only neither to decay to zero nor to return to unity repeatedly, but also to possess an asymptotic self-similar structure. (We shall confine our description of the form of the dynamics to one of the nature of the autocorrelation function.) This self-similarity suggests that a renormalization analysis is appropriate to help understand this phenomenon, and this is indeed the content of the analysis of Feudel *et al.* in Ref. 5. There have, in addition, been many other studies of the response of two-level systems to quasiperiodic forcing, but we shall concentrate on the self-similarity aspects here. (See, for instance, the references in Ref. 5, and also Refs. 1, 3, and 15 to mention but a few.)

As is implicit in some of the works cited above (and is explicitly acknowledged in Ref. 5), there is much in common between the response of these quantum systems and the nature of strange nonchaotic attractors. Consequently, our work here will have important implications in that context, too.

In this article we give a rigorous renormalization analysis explaining and generalizing the numerical results in Ref. 5. Because of its number-theoretic simplicity, most analysis has been concerned with the case of forcing at golden mean frequency, and this article will be no exception. The self-similar structure is then explained by means of the additive functional recurrence

$$Z_n(x) = Z_{n-1}(-\omega x) + Z_{n-2}(\omega^2 x + \omega), \tag{1.1}$$

where $\omega = (\sqrt{5}-1)/2$ is the golden mean.

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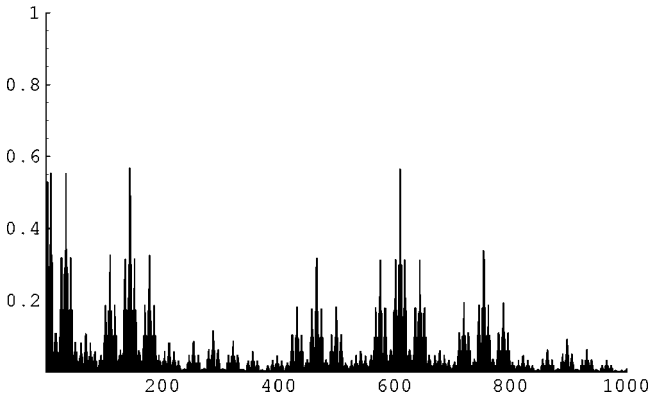

FIG. 1. Autocorrelation function K_{P_y} for modulation function (1.29) and $\kappa=\pi/2$.

The multiplicative version of (1.1) has been previously studied in some detail. It naturally appears in seemingly disparate contexts. First, it arises in the analysis of the self-similar fluctuations of the localized eigenstates of the Harper equation.[7] Second, it helps explain universal characteristics present in the birth of a strange nonchaotic attractor.[9] In Ref. 8 these two phenomena are indeed linked. It further arises in the analysis of the autocorrelation function of the orbit on a strange nonchaotic attractor.[4] (In each of these contexts the recurrence arises when the frequency parameter ω is taken to be the golden mean.)

In Ref. 11 we proved that there exists a fixed point of the multiplicative version of (1.1) of the type numerically found in Ref. 7. [To do this at times we considered the additive recurrence (1.1) in our proof.] In Ref. 12 we gave a description of all of its piecewise-constant periodic orbits, thereby providing a mathematical understanding of, and generalizing, the numerical observations in Ref. 4. In a forthcoming work[13] we give an analysis of its analytic periodic orbits, thereby explaining the beautiful ''orchid'' picture of Ketoja and Satija[7] arising in a generalized Harper equation. We expect this analysis can be adapted to the birth of a strange nonchaotic attractor scenario.[9]

In this article we describe all piecewise-constant periodic orbits of (1.1). Further, we characterize those periodic orbits which are globally bounded. As a consequence, it follows that the autocorrelation functions are indeed asymptotically self-similar for a wide class of piecewise-constant forcing functions. The precise locations of the discontinuities of these functions are, however, crucial. See Fig. 1 for an example of such an autocorrelation function. Much of our analysis of the multiplicative recurrence in Ref. 12 can be adapted to the additive case (1.1), and we begin by doing this in Sec. II. There are some important differences to be taken into account, too. The piecewise-constant periodic orbits of the multiplicative problem consist of functions taking values ± 1 only, and, as a consequence, an analysis of the discontinuities suffices to determine periodicity. In the additive problem there is no such restriction. In Sec. II F we establish a criterion to guarantee periodicity in this case. Moreover, it is quite simple to find piecewise-constant periodic orbits of the additive recurrence that are spatially unbounded. We identify the nature of the locations of the discontinuities of Z_n on the whole of $\mathbb{R}$ in Sec. III, and use this information, in Sec. IV, to establish a criterion to distinguish those periodic orbits that are spatially bounded. In Sec. V we look in detail at the particular example studied numerically by Feudel *et al.* in Ref. 5 resulting in the period-6 orbit shown in Fig. 2. For this example we calculate the averages of the function Z_n which give the asymptotic height of the main peaks in the corresponding correlation function, which is shown in Fig. 1. As a consequence, we show that the asymptotic height of the peaks in Fig. 1 is $1-1/\sqrt{5}=0.552\,786\ldots$.

In the remainder of this introduction we describe the system under consideration more precisely, and, following Ref. 5, indicate how the recurrence (1.1) arises in the analysis of its autocorrelation functions.

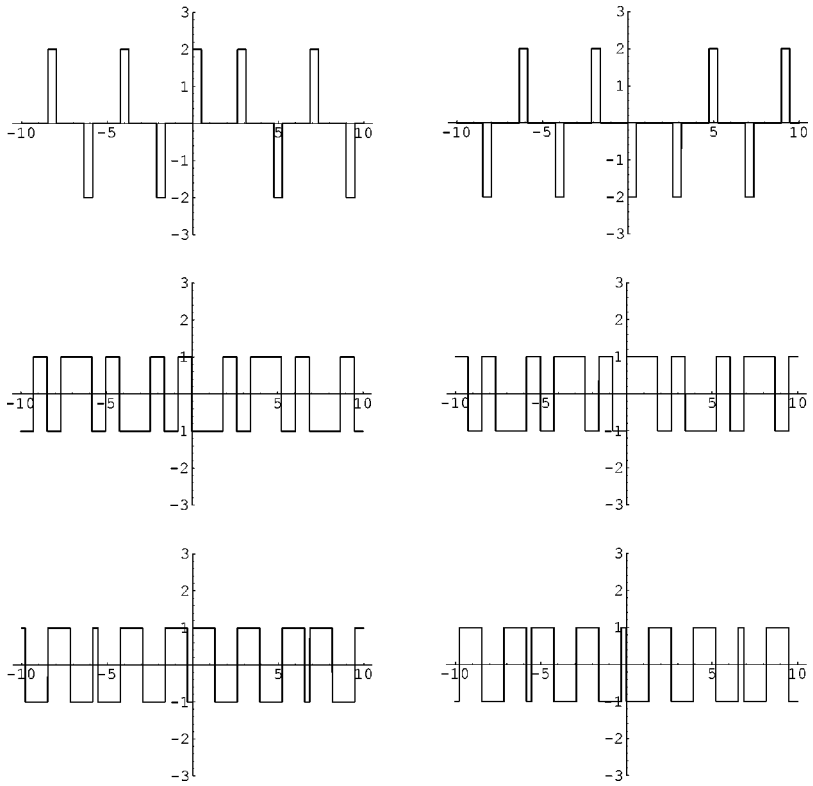

FIG. 2. Period-6 orbit of the recurrence (1.1). Left column Z_0, Z_1, Z_2 reading downwards, right column Z_3, Z_4, Z_5 reading downwards.

A. Formulation of the equations of motion

The Hamiltonian of a two-level system in a time-dependent magnetic field $B(t)$ takes the form $H=B(t)\cdot\sigma$, where $\sigma=(\sigma_x,\sigma_y,\sigma_z)$ consists of the Pauli spin matrices

$$\sigma_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{1.2}$$

Following the previous authors, we consider the special case $B(t)=(S(t)/2,0,k/2)$, which gives the Hamiltonian

$$H(t)=\tfrac{1}{2}k\sigma_z+\tfrac{1}{2}S(t)\sigma_x. \tag{1.3}$$

Schrödinger's equation for the spinor $\psi=(\psi_1,\psi_2)$ is then

$$i\dot{\psi}_1=\tfrac{1}{2}k\psi_1+\tfrac{1}{2}S(t)\psi_2,\quad i\dot{\psi}_2=-\tfrac{1}{2}k\psi_2+\tfrac{1}{2}S(t)\psi_1. \tag{1.4}$$

(We take $\hbar=1$.) This is conveniently expressed in terms of the components of the polarization vector $P=\psi^*\sigma\psi$, the so-called Bloch variables,

$$P_x=\psi_2\psi_1^*+\psi_1\psi_2^*,\quad P_y=i(\psi_1\psi_2^*-\psi_2\psi_1^*),\quad P_z=\psi_1\psi_1^*-\psi_2\psi_2^*, \tag{1.5}$$

as the first-order linear time-dependent system

$$\dot{P}_x=-kP_y,\quad \dot{P}_y=kP_x-S(t)P_z,\quad \dot{P}_z=S(t)P_y, \tag{1.6}$$

which, from the normalization $\psi_1\psi_1^*+\psi_2\psi_2^*=1$, satisfies the constraint

$$P_x^2+P_y^2+P_z^2=1. \tag{1.7}$$

We suppose that the forcing consists of period-T δ-function kicks, so that we have

$$S(t)=\sum_{n=-\infty}^{\infty} R_n\delta(t-nT), \tag{1.8}$$

with variable amplitude R_n. Between kicks we have a rotation in the (P_x,P_y) plane, and at kicks a rotation in the (P_y,P_z) plane resulting in the linear kick-to-kick mapping

$$\begin{pmatrix} P_{x,n+1} \\ P_{y,n+1} \\ P_{z,n+1} \end{pmatrix} = \begin{pmatrix} \cos kT & -\sin kT\cos R_n & \sin kT\sin R_n \\ \sin kT & \cos kT\cos R_n & -\cos kT\sin R_n \\ 0 & \sin R_n & \cos R_n \end{pmatrix} \begin{pmatrix} P_{x,n} \\ P_{y,n} \\ P_{z,n} \end{pmatrix}, \tag{1.9}$$

where $(P_{x,n},P_{y,n},P_{z,n})$ denotes the value of the polarization vector at time step n.

Although the kicks occur periodically, they do so with variable amplitude R_n which we now take to be determined in a quasiperiodic manner governed by the rotation

$$\phi_{n+1}=\phi_n+\omega \pmod 1, \tag{1.10}$$

with the rotation number $\omega\notin\mathbb{Q}$. The amplitude R_n is then defined via a period-1 *modulation function* Φ to be

$$R_n=\kappa\Phi(\phi_n), \tag{1.11}$$

where κ is an amplitude. The precise form of the modulation function Φ is crucial for the resulting dynamics. It is the case of piecewise-constant discontinuous modulation function, where a singular continuous spectrum is observed, that will concern us in this article.

To simplify matters we assume that the time between kicks, T, is commensurate with the fundamental frequency k, setting

$$kT=2\pi m, \quad m\in\mathbb{Z}, \tag{1.12}$$

thereby decoupling the variable $P_{x,n}$ so that the resulting dynamics is merely a rotation in the (P_y,P_z) plane. (Numerical work in Ref. 5 indicates that this simplification may not be essential to witness the singular continuous spectrum.) Because of the constraint (1.7), without loss of generality, we may set $P_{x,n}=0$ (otherwise we can simply rescale the remaining variables). Thus, writing

$$P_{y,n}=\cos\theta_n, \quad P_{z,n}=\sin\theta_n, \tag{1.13}$$

we arrive at the skew-product system

$$\phi_{n+1}=\phi_n+\omega \pmod 1, \tag{1.14}$$

$$\theta_{n+1}=\theta_n+\kappa\Phi(\phi_n). \tag{1.15}$$

We remark that it is in such systems that early work on the appearance of strange nonchaotic attractors was undertaken,[6] and that, in some sense, such attractors lie intermediate between regular and chaotic dynamics. In particular, the presence of a singular continuous spectrum may be mooted as a candidate for their characterization.

Of course it is straightforward to ''solve'' the system (1.14) and (1.15):

$$\phi_n=\phi_0+n\omega \pmod 1, \tag{1.16}$$

$$\theta_n = \theta_0 + \kappa \sum_{l=0}^{n-1} \Phi(\phi_0 + l\omega), \tag{1.17}$$

but this does not help illuminate the behavior of the variable θ, i.e., (P_y, P_z). To this end we turn to an analysis of correlations.

B. Renormalization analysis of the autocorrelation function

For completeness we recall here the renormalization analysis of the autocorrelation function from Feudel *et al.*[5] The autocorrelation function of the (zero mean) observable P_y is

$$K_{P_y}(t) = \frac{\langle P_{y,n} P_{y,n+t} \rangle}{\langle P_{y,n}^2 \rangle}, \tag{1.18}$$

where we have defined the average

$$\langle f(n) \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} f(n). \tag{1.19}$$

Using the trigonometric identity $2 \cos A \cos B = \cos(A+B) + \cos(A-B)$, we have

$$\langle P_{y,n} P_{y,n+t} \rangle = \langle \cos\theta_n \cos\theta_{n+t} \rangle = \tfrac{1}{2} \langle \cos(\theta_{n+t} - \theta_n) \rangle = \tfrac{1}{2} \langle \cos \kappa Q_t(\phi_n) \rangle, \tag{1.20}$$

where we have averaged over the initial phase θ_0 to remove the average of $\cos(\theta_{n+t} + \theta_n)$, and then defined

$$Q_t(\phi) = \sum_{l=0}^{t-1} \Phi(\phi + l\omega), \quad Q_0(\phi) = 0. \tag{1.21}$$

Thus

$$K_{P_y}(t) = \langle \cos \kappa Q_t(\phi_n) \rangle = \int_0^1 \cos \kappa Q_t(\phi) d\phi, \tag{1.22}$$

where we have used the fact that for irrational ω the rotation (1.14) is ergodic with respect to Lebesgue measure to replace the time average by a space average.

We now specialize to the case of golden mean rotation number, setting $\omega = (\sqrt{5}-1)/2$, and accordingly consider Fibonacci times only. Then Q_n satisfies the recurrence relation

$$Q_{F_n}(\phi) = Q_{F_{n-1}}(\phi) + Q_{F_{n-2}}(\phi + F_{n-1}\omega), \tag{1.23}$$

where the Fibonacci numbers (F_n) are defined by $F_0 = 0$, $F_1 = 1$, and $F_n = F_{n-1} + F_{n-2}$ for $n \geqslant 2$. Using the identity

$$F_{n-1}\omega = F_{n-2} - (-\omega)^{n-1}, \tag{1.24}$$

and defining the rescaled variables

$$Z_n(y) = Q_{F_n}(y(-\omega)^n), \tag{1.25}$$

results in the iterative functional recurrence

$$Z_n(x) = Z_{n-1}(-\omega x) + Z_{n-2}(\omega^2 x + \omega), \tag{1.26}$$

with initial conditions

$$Z_0(x)=0, \quad Z_1(x)=\Phi(-\omega x). \tag{1.27}$$

This recurrence is the object of study in this article.

In terms of the functions Z_n, the autocorrelation function K_{P_y} at Fibonacci times is

$$K_{P_y}(F_n)=\frac{1}{(-\omega)^{-n}}\int_0^{(-\omega)^{-n}}\cos \kappa Z_n(y)\,dy. \tag{1.28}$$

For the particular choice of modulation function

$$\Phi(\phi)=\begin{cases}+1, & 0\leqslant\{\phi\}<\frac{1}{2},\\ -1, & \frac{1}{2}\leqslant\{\phi\}<1,\end{cases} \tag{1.29}$$

where $\{\phi\}$ denotes ϕ (mod 1), with the initial conditions given by (1.27), Feudel *et al.*[5] observe that iteration of (1.1) leads to a period-6 orbit as shown in Fig. 2. The corresponding autocorrelation function K_{P_y} (with $\kappa=\pi/2$) is shown in Fig. 1. Note that the height of the largest peaks is approximately 0.55 and is numerically calculated in Ref. 5 from an average of $|Z_n|$ with $n\equiv 0$ mod 3, i.e., either of the top two figures in Fig. 2, to be asymptotically approximately 0.552 79. By carefully describing the locations of the discontinuities in Fig. 2, in Sec. V we shall show that this value is in fact $1-1/\sqrt{5}=0.552\,786\ldots$.

Our analysis shows that self-similarity of the autocorrelation function occurs for many other choices of modulation function in addition to (1.29). However, the locations of the discontinuities of the modulation function must be preperiodic points of a map of the interval to be introduced in the next section.

II. PERIODIC ORBITS AND THEIR DISCONTINUITIES

We begin this section by adapting our previous analysis[12] of the multiplicative version of (1.1) to the problem at hand. We introduce an expanding piecewise-linear map of an interval whose periodic orbits correspond to the discontinuities of the piecewise-constant periodic orbits of (1.1), and show that the dynamics of this interval map ''drives'' the global behavior of periodic orbits of (1.1). We also give a detailed analysis of the periodicity of the discontinuities. We then give a necessary and sufficient criterion for the piecewise-constant orbits of (1.1) to be periodic.

A. Iterated function system and the inverse map *F*

Defining

$$\phi_1(x)=-\omega x, \quad \phi_2(x)=\omega^2 x+\omega, \tag{2.1}$$

we may write Eq. (1.1) in the form

$$Z_n(x)=Z_{n-1}(\phi_1(x))+Z_{n-2}(\phi_2(x)), \tag{2.2}$$

where $\omega=(\sqrt{5}-1)/2$ is the golden mean,

The iterated function system (IFS) on $\mathbb{R}$ given by ϕ_1, ϕ_2 has the following properties:

(1) ϕ_1 and ϕ_2 are linear contractions with fixed points 0 and 1, respectively, and with $\phi_1'(x)=-\omega$ and $\phi_2'(x)=\omega^2$.
(2) The *fundamental interval* $I=[-\omega,1]$ is the fixed point set for the IFS. Indeed $\phi_1(I)=[-\omega,\omega^2]$, $\phi_2(I)=[\omega^2,1]$, so that $\phi_1(I)\cup\phi_2(I)=I$.
(3) The fundamental interval I is the attractor for the IFS. Indeed given any compact subset $K\subset\mathbb{R}$ and any $\varepsilon>0$, there exists $N\in\mathbb{N}$ such that for any $k\geqslant N$ and any choice $i_1,\ldots,i_k\in\{1,2\}$ we have

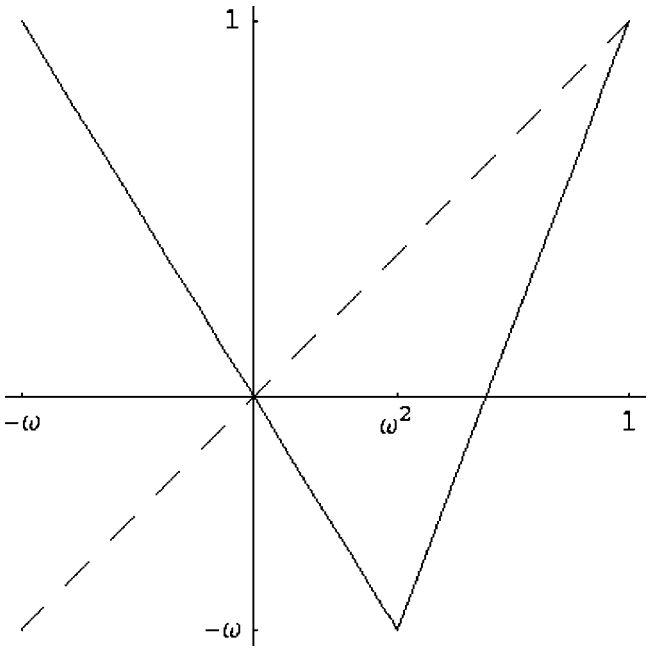

FIG. 3. The function F.

$$\phi_{i_1}\circ\cdots\circ\phi_{i_k}(x)\in[-\omega-\varepsilon,1+\varepsilon] \tag{2.3}$$

for any $x\in K$. This property will be important when we consider the behavior of Eq. (2.2) outside the fundamental interval.

Let $F:I\to I$ be defined by

$$F(x)=\begin{cases}\phi_1^{-1}(x)=-\omega^{-1}x, & x\in[-\omega,\omega^2];\\ \phi_2^{-1}(x)=\omega^{-2}x-\omega^{-1}, & x\in[\omega^2,1],\end{cases} \tag{2.4}$$

as drawn in Fig. 3. We shall see below that periodic points of F correspond to discontinuities of the periodic solutions of (2.2).

We note that for any periodic point $y\in I$, precisely one of $\phi_1(y)$, $\phi_2(y)$ is also a periodic point of F. This follows from the fact that each period point has two preimages, exactly one of which is a periodic point on the same orbit. (Note that ω^2 is not a periodic point of F.) We analyze the dynamics of F in terms of a code of a point $x\in I$. As in Ref. 12 we let the interval $[-\omega,\omega^2)$ be encoded with the symbol 1 and $(\omega^2,1]$ with the symbol 2. We define the code of $x\in I$ to be the sequence $(a_n)_{n\geqslant 0}$ in $\{1,2\}^{\mathbb{N}_0}$ given by

$$a_n=\begin{cases}1, & F^n(x)\in[-\omega,\omega^2);\\ 2, & F^n(x)\in(\omega^2,1],\end{cases} \tag{2.5}$$

and ignore the (countable) set of (nonperiodic) points whose orbits under F include the point ω^2. Hence the codes are all infinite sequences. In terms of the code $a_0a_1a_2\ldots$ of a point $x\in I$, we have

$$F(x)=(-\omega^{-1})^{a_0}x-(a_0-1)\omega^{-1}. \tag{2.6}$$

Since F is uniformly expanding ($|F'(x)|\geqslant\omega^{-1}$), every point $x\in I$ corresponds to a unique code and vice versa. In particular, periodic orbits of F correspond to periodic codes in $\{1,2\}^{\mathbb{N}_0}$ under the shift map σ:

$$\sigma(a_0a_1a_2\ldots)=a_1a_2\ldots. \tag{2.7}$$

A periodic orbit $y_0,y_1,\ldots,y_{k-1}$ of period k of F is given uniquely by a periodic code $\overline{a_0a_1\ldots a_{k-1}}$, which we henceforth denote as just $a_0a_1\ldots a_{k-1}$. Indeed, given a code $a_0a_1\ldots a_{k-1}$, it is straightforward to calculate the corresponding periodic orbit $y_0,y_1,\ldots,y_{k-1}$ of F. We have $\phi_{a_{k-1}}^{-1}\circ\cdots\circ\phi_{a_0}^{-1}(y_0)=y_0$, or, equivalently, $\phi_{a_0}\circ\cdots\circ\phi_{a_{k-1}}(y_0)=y_0$, whose (unique) solution is readily calculated to be

$$y_0=\frac{-\sum_{j=0}^{k-1}(a_j-1)(-\omega)^{1+\sum_{i=0}^{j-1}a_i}}{1-(-\omega)^{\sum a_j}}, \tag{2.8}$$

where empty sums are defined to be zero. The other points of the orbit may be calculated by applying this formula with the code $a_0a_1\ldots a_{k-1}$ cyclically permuted.

For example, $F(y)$ has two fixed points: $y=0$ with code 1, and $y=1$ with code 2. The period-2 orbit with code 21 is given by $y_0=\frac{1}{2}$ and $y_1=-\omega/2$. It is the fixed point $y=0$ and this period-2 orbit that are the discontinuity points in the fundamental interval of the period-6 orbit shown in Fig. 2.

B. Reduction of Z_n on $\mathbb{R}$ to the fundamental interval

In this section we consider Eq. (2.2) outside the fundamental interval $I=[-\omega,1]$, i.e., on the whole of $\mathbb{R}$. The fact that I is the attractor for the IFS leads to the conclusion that the global behavior of (2.2) is "driven" by its behavior in I.

The following result is a straightforward variation of the corresponding result in Ref. 12.

Lemma 1: Let Z_0, Z_1 be initial conditions for (2.2) on $\mathbb{R}$ and let $\varepsilon>0$ be such that $Z_0(x)=Z_1(x)=0$ for all $x\in[-\omega-\varepsilon,1+\varepsilon]$. Then for each $L>1$, there exists $N>0$ (depending only on L) such that $Z_n(x)=0$ for all $x\in[-L,L]$ and all $n>N$.

In other words, if the initial conditions on, and just outside, the fundamental interval are zero, then the value of Z_n at all points eventually becomes zero.

From the lemma we may prove the following proposition whose proof again follows mutatis mutandis the corresponding result in Ref. 12.

Proposition 1: Let Z_n be a piecewise-constant periodic orbit of (2.2) of period p on $\mathbb{R}$ with $Z_n(1+)=Z_n(1)$. Then Z_n is periodic with period p on the fundamental interval I. Conversely, suppose that Z_n is periodic with period p on I. Then there is a unique extension $\tilde{Z}_n$ of Z_n to $\mathbb{R}$ such that $\tilde{Z}_n$ is periodic with period p on $\mathbb{R}$.

Moreover, Lemma 1 further implies the following.

Proposition 2: Let Z_0, Z_1 be piecewise-constant initial conditions for (2.2) on $\mathbb{R}$ with $Z_0(1+)=Z_0(1)$, $Z_1(1+)=Z_1(1)$. Suppose Z_n is periodic of period p on the fundamental interval I. Then the sequence Z_n converges to the unique periodic extension $\tilde{Z}_n$ given by proposition 1, i.e., for all integers $r\geqslant 0$ we have $Z_{r+np}(x)\to\tilde{Z}_r(x)$ as $n\to\infty$.

In other words, initial data on the fundamental interval resulting in periodic behavior uniquely determines an asymptotic (right continuous at 1) global periodic behavior. It is important to realize, however, that such globally defined periodic orbits will not in general consist of bounded functions. We shall address this issue in Sec. IV.

C. Analysis of the discontinuities

In order to study the piecewise-constant periodic orbits of the recurrence (1.1) we first consider the dynamics of the discontinuities. We define, for each $x\in\mathbb{R}$ and $n\geqslant 0$,

$$D_n(x)=Z_n(x+)-Z_n(x-), \tag{2.9}$$

the difference of the right-hand limit at x to the left-hand limit at x, so that $D_n(x)\neq 0$ if and only if Z_n has a discontinuity at x. The recurrence (2.2) for Z_n naturally induces a recurrence for D_n:

$$\begin{aligned} D_n(x) &= Z_n(x+) - Z_n(x-) \\ &= Z_{n-1}(\phi_1(x+)) + Z_{n-2}(\phi_2(x+)) - Z_{n-1}(\phi_1(x-)) - Z_{n-2}(\phi_2(x-)) \\ &= Z_{n-1}(\phi_1(x)-) - Z_{n-1}(\phi_1(x)+) + Z_{n-2}(\phi_2(x)+) - Z_{n-2}(\phi_2(x)-) \\ &= -D_{n-1}(\phi_1(x)) + D_{n-2}(\phi_2(x)). \end{aligned} \tag{2.10}$$

Clearly if Z_n is periodic with period p, then D_n is also periodic with period m dividing p. Our task is to determine the possible periods m of D_n and relate m to p, the period of Z_n.

From now on we assume that Z_n is periodic with period p and that D_n is periodic with period m, and, in view of Proposition 1, we only consider the behavior of Z_n and D_n on the fundamental interval $I=[-\omega,1]$. We define the *restricted discontinuity set*

$$D=\{x\in I: D_n(x)\neq 0 \text{ for some } n\geqslant 0\}. \tag{2.11}$$

Then D is the finite set of points in I for which Z_n has a discontinuity for at least one $n\geqslant 0$. As in our analysis of the multiplicative recurrence,[12] the restricted discontinuity set D consists of finitely many periodic orbits of the map F as we now show.

Proposition 3: Let Z_n be a piecewise-constant periodic orbit of (2.2), and let D be the associated restricted discontinuity set. Then D consists of a finite collection of periodic orbits of the map F.

Proof: Suppose $y\in D$. Then $D_n(y)\neq 0$ for some $n\geqslant 0$. From (2.10) we have that $D_{n-i_1}(\phi_{i_1}(y))\neq 0$ for some $i_1\in\{1,2\}$. We therefore have $\phi_{i_1}(y)\in D$. Continuing in this way, we obtain a sequence $i_1,i_2,\ldots\in\{1,2\}$ such that $\phi_{i_k}\circ\cdots\circ\phi_{i_1}(y)\in D$ for each $k\in\mathbb{N}$. Since D is finite there exist r, $r'\in\mathbb{N}$ with $r>r'$ and $\phi_{i_{r'}}\circ\cdots\circ\phi_{i_1}(y)=\phi_{i_r}\circ\cdots\circ\phi_{i_1}(y)$. Applying F^r to this equation gives $F^{r-r'}(y)=y$, so that y is a periodic point of F of period j dividing $r-r'$.

Now let $y_0=y,y_1,\ldots,y_{k-1}$ be the points on the orbit of y_0 under F with $y_{i+1(\mathrm{mod}\,k)}=F(y_i)$ for $i=0,1,\ldots,k-1$, and let $a_0a_1\ldots a_{k-1}$ be the code of the orbit. Then for $0\leqslant i\leqslant k-1$ we have

$$\phi_{a_i}^{-1}(y_i)=y_{i+1}, \quad \text{or, equivalently,} \quad \phi_{a_{i-1}}(y_i)=y_{i-1}, \tag{2.12}$$

where here, and in what follows, we assume that expressions relating to the periodic orbit $y_0,y_1,\ldots,y_{k-1}$ are reduced modulo k.

Moreover, as we noted earlier, precisely one of $\phi_1(y_i)$, $\phi_2(y_i)$ is periodic. Thus, if $a_{i-1}=1$ then $\phi_2(y_i)\notin D$ and so $D_n(\phi_2(y_i))=0$ for all n, while if $a_{i-1}=2$, then $\phi_1(y_i)\notin D$ and so $D_{n-1}(\phi_1(y_i))=0$ for all n. The recurrence (2.10) may therefore be written

$$D_n(y_i)=\begin{cases} -D_{n-1}(y_{i-1}), & a_{i-1}=1, \\ D_{n-2}(y_{i-1}), & a_{i-1}=2, \end{cases} \tag{2.13}$$

which can be written as

$$D_n(y_i)=(-1)^{a_{i-1}}D_{n-a_{i-1}}(y_{i-1}). \tag{2.14}$$

Thus $D_{n+a_0+\cdots+a_{i-1}}(y_i)=(-1)^{a_0+\cdots+a_{i-1}}D_n(y_0)$, so that if $D_n(y_0)\neq 0$, then $D_{n+a_0+\cdots+a_{i-1}}(y_i)\neq 0$, i.e., if $y_0\in D$, then $y_i\in D$. We conclude that not only must every point $y\in D$ be a periodic point of F, but that every point on the periodic orbit of y also lies in D, so that D consists of complete orbits of F. □

D. Period of the discontinuities for a single periodic orbit of *F*

From (2.14) we see that over a complete periodic orbit with code $a_0a_1\ldots a_{k-1}$ the index n decreases by

$$l=\sum_{i=0}^{k-1} a_i, \tag{2.15}$$

and, moreover, we have $D_n(y_i)=(-1)^l D_{n-l}(y_i)$, for $0\leqslant i\leqslant k-1$. We therefore deduce the following result.

Proposition 4: Let m be the period of the discontinuity function D_n restricted to a periodic orbit $y_0,\ldots,y_{k-1}$ of F and let l *be the sum of the code over the orbit of F. Then m divides* lcm$\{2,l\}$, *i.e., if* l *is even m divides* l, *while if* l *is odd m divides* $2l$.

We define for any integer m

$$\hat{m}=\mathrm{lcm}\{2,m\}=\begin{cases} m, & m \quad \text{even;} \\ 2m, & m \quad \text{odd.} \end{cases} \tag{2.16}$$

A convenient representation of the discontinuity data is in terms of an $\hat{l}\times k$ matrix M, the *discontinuity matrix*, with entries defined by

$$M_{n,i}=D_n(y_i), \tag{2.17}$$

for $0\leqslant n\leqslant \hat{l}-1$, $0\leqslant i\leqslant k-1$, so that the entry in row n and column i is the value of D_n at the point y_i on the orbit $y_0,y_1,\ldots,y_{k-1}$.

The relation (2.14) above gives a special structure to the matrix M. Indeed (2.14) translates to

$$M_{n,i}=(-1)^{a_{i-1}}M_{n-a_{i-1},i-1}, \tag{2.18}$$

where here, and in what follows, indices referring to the periodicity of D_n are reduced modulo $\hat{l}$.

The structure of (2.18) can be more easily understood as follows. Column i of the matrix M is simply column $(i-1)$ cyclically permuted downwards by a_{i-1} single cyclic permutations with a change of sign if $a_{i-1}=1$. This observation also holds when $i=0$, for then (2.18) becomes

$$M_{n,0}=(-1)^{a_{k-1}}M_{n-a_{k-1},k-1}. \tag{2.19}$$

Let us denote the first column of M by $(X_0,X_1,\ldots,X_{\hat{l}-1})$, i.e., $M_{n,0}=X_n$ for $0\leqslant n\leqslant \hat{l}-1$. Then the relation (2.18) tells us that

$$M_{n,1}=(-1)^{a_0}M_{n-a_0,0}=(-1)^{a_0}X_{n-a_0}, \tag{2.20}$$

and, in general,

$$M_{n,i}=(-1)^{\Sigma_{j=0}^{i-1}a_j}M_{n-\Sigma_{j=0}^{i-1}a_j,0}=(-1)^{\Sigma_{j=0}^{i-1}a_j}X_{n-\Sigma_{j=0}^{i-1}a_j}, \tag{2.21}$$

so that each column of M is simply a cyclic permutation with an appropriate sign change of the first column of M. In the case of odd l, in order to satisfy (2.19), the first column of M must take the form $(X_0,X_1,\ldots,X_{l-1},-X_0,-X_1,\ldots,-X_{l-1})$.

Example 1: The period-2 orbit $\{\frac{1}{2},-\omega/2\}$ has code 21, so $k=2$, $l=3$, $\hat{l}=6$ and

$$M=\begin{pmatrix} X_0 & -X_1 \\ X_1 & -X_2 \\ X_2 & X_0 \\ -X_0 & X_1 \\ -X_1 & X_2 \\ -X_2 & -X_0 \end{pmatrix},$$

in which, since $a_0=2$, the second column is the first column shifted down two rows without sign change. Utilizing $a_1=1$ on the second column reproduces the first column by shifting down one and changing sign.

Example 2: The fixed point 0 of F has code 1 so here $k=l=1$, $\hat{l}=2$ and

$$M=\begin{pmatrix} X_0 \\ -X_0 \end{pmatrix}.$$

The combination of Examples 1 and 2 was our initial motivation for studying this problem, and enables us to give a precise description of the numerical results of Feudel *et al.*[5] We shall return again to this example later on in this article, after discussing how to treat discontinuity sets containing more than one periodic orbit of F in the next subsection.

Example 3: The fixed point 1 of F has code 2 so here $k=1$, $l=\hat{l}=2$ and

$$M=\begin{pmatrix} X_0 \\ X_1 \end{pmatrix}.$$

Example 4: When the code is 2112 we have $k=4$, $l=l'=6$ and

$$M=\begin{pmatrix} X_0 & X_4 & -X_3 & X_2 \\ X_1 & X_5 & -X_4 & X_3 \\ X_2 & X_0 & -X_5 & X_4 \\ X_3 & X_1 & -X_0 & X_5 \\ X_4 & X_2 & -X_1 & X_0 \\ X_5 & X_3 & -X_2 & X_1 \end{pmatrix}.$$

When l is even, by a suitable choice of first column, i.e., of the l numbers $X_0,X_1,\ldots,X_{l-1}$, we may arrange for the discontinuities to have any period dividing l. When l is odd, by suitably choosing X_0, $X_1,\ldots,X_{l-1}$, any period twice any divisor of l can be obtained (or the trivial period-1 case of no discontinuities). Moreover, in this latter case, the discontinuities satisfy $X_{n+l}=-X_n$.

We emphasize that our freedom of choice is in choosing the values of the discontinuities at each point of a periodic orbit of F. It is *not* the case that one may arbitrarily select the discontinuities of the initial conditions Z_0, Z_1. This would correspond to specifying the first two *rows* of the discontinuity matrix. As our analysis shows, however, the rows are not independent. However, we remark that each row of the discontinuity matrix contains each X_i at most once, and that any two adjacent rows together contain each X_i at least once. Indeed, given one row, it is clear that those entries which appear in the following row are simply those in the columns corresponding to y_i with code 1. Thus an alternative (equivalent) method of specifying a periodic discontinuity orbit may be given directly in terms of the discontinuities of Z_0 and Z_1 at each y_i. Namely, the discontinuities of Z_1, i.e., $D_1(y_i)$ may be chosen arbitrarily, as may the discontinuities $D_0(y_i)$ of Z_0 at each y_i with code 2. (This exhausts l freedoms.) The discontinuities of Z_0 at each y_i with code 1, however, are given as $D_0(y_i)=-D_1(y_{i+1})$ (with period k on the index). While useful for ensuring that initial conditions result in periodic behavior, this alternative description is less useful for determining the precise period. This description will, however, be useful in Sec. IV when we wish to analyze the global behavior of recurrence (2.2).

E. Multiple periodic orbits in *D*

In general, the restricted discontinuity set D will be composed of points of more than one periodic orbit of F. Let t be the number of periodic orbits of F in D. For $0\leqslant s\leqslant t-1$, we consider the periodic orbit s of F in D. We make the general convention that superscript s refers to the orbit s. Now, from the additive structure of (2.10), we have that a sum of solutions is again a

solution of the equation. Moreover, because the periodic orbits in D are distinct, and are never mapped to each other under the two maps ϕ_1, ϕ_2, we have that the dynamics of D_n on each of the periodic orbits in D are independent. Indeed, we may write

$$D_n(x)=\sum_{s=0}^{t-1} D_n^s(x), \tag{2.22}$$

where D_n^s is the restriction of D_n to the periodic orbit s, i.e.,

$$D_n^s(x)=\begin{cases} D_n(x), & x\in\{y_0^s,\ldots,y_{k^s-1}^s\};\\ 0, & \text{otherwise.}\end{cases} \tag{2.23}$$

We may then apply the analysis of the previous subsection to each of the functions D_n^s. This is because $D_n^s(x)=0$, except when x is one of the points on the periodic orbit $y_0^s\ldots y_{k^s-1}^s$ of F.

The theory for D_n that we discussed above carries over in a straightforward manner to the function D_n^s. In particular, for each orbit in D we can formulate an $\hat{l}^s\times k^s$ discontinuity matrix M^s, defined by $M_{n,i}^s=D_n^s(y_i^s)$ for $0\leqslant n\leqslant \hat{l}^s-1$ and $0\leqslant i\leqslant k^s-1$. To simplify notation, we adopt the convention that matrix indices are reduced modulo k^s when dealing with expressions relating to the periodic orbit $y_0^s,\ldots,y_{k^s-1}^s$ of F, while those relating to the periodicities of D_n are reduced modulo $\hat{l}^s$. These matrices are independent of each other since the dynamics of D_n on each periodic orbit in D are independent.

Thus, as in (2.18), we have

$$M_{n,i}^s=(-1)^{a_{i-1}^s}M_{n-a_{i-1}^s,i-1}^s, \tag{2.24}$$

for $0\leqslant n\leqslant \hat{l}^s-1$ and $0\leqslant i\leqslant k^s-1$, and the matrix M^s is determined by its first column $(X_0^s,X_1^s,\ldots,X_{\hat{l}^s-1}^s)$. [When l^s is odd this column takes the form $(X_0^s,X_1^s,\ldots,X_{l^s-1}^s,-X_0^s,-X_1^s,\ldots,-X_{l^s-1}^s)$.] Indeed, as in (2.21),

$$M_{n,i}^s=(-1)^{\Sigma_{j=0}^{i-1}a_j^s}X_{n-\Sigma_{j=0}^{i-1}a_j^s}^s, \tag{2.25}$$

and the period m^s of the first column is precisely the row period of M^s. We also have $m^s|\hat{l}^s$.Conversely, let $\hat{l}=\mathrm{lcm}(\hat{l}^0,\ldots,\hat{l}^{t-1})$. Then for any $m|\hat{l}$ we define $m^s=\gcd(m,\hat{l}^s)$. Then $m^s|\hat{l}^s$ and by appropriate choices of $(X_0^s,X_1^s,\ldots,X_{\hat{l}^s-1}^s)$ we may construct a matrix M^s with row period m^s if l^s is even, or $\hat{m}^s$ if l^s is odd, and, extending periodically to all $n\geqslant 0$, we have that D_n has period m^s if l^s is even, or $\hat{m}^s$ if l^s is odd, when restricted to the orbit $y_0^s,\ldots,y_{k^s-1}^s$.

We therefore have the following proposition.

Proposition 5: Let Z_n be a piecewise-constant periodic orbit of (2.2). Then the period m of the discontinuity function D_n is given by

$$m=\mathrm{lcm}(m^0,\ldots,m^{t-1}), \tag{2.26}$$

where m^s is the period of the function D_n^s, given by the period of $(X_0^s,X_1^s,\ldots,X_{\hat{l}^s-1}^s)$, i.e., the first column of the discontinuity matrix M^s. Furthermore, m divides

$$\hat{l}=\mathrm{lcm}(\hat{l}^0,\ldots,\hat{l}^{t-1}). \tag{2.27}$$

Moreover, by appropriate choices of $(X_0^s,X_1^s,\ldots,X_{\hat{l}^s-1}^s)$, for any m dividing $\hat{l}$ we may construct a periodic orbit of D_n with period $\hat{m}$ (and, if all l^s are even, we may construct a periodic orbit of odd period m).

F. The criterion for orbits to be periodic

In the previous subsection we dealt quite extensively with the periodicity of the discontinuities on the fundamental interval $I=[-\omega,1]$. It is perfectly feasible for the sequence of discontinuities D_n to be periodic while the sequence (Z_n) itself is not. The simple example $Z_0(x)=0$, $Z_1(x)=1$ for all x, with no discontinuities at all, generates the Fibonacci numbers as the values for Z_n. This sequence is clearly not periodic, growing without bound. In order to ensure that (Z_n) is itself periodic it suffices to ensure that the values at a single point are periodic. It will be convenient to choose an end point of I for this purpose. We consider then the values $Z_n(1)$. As we saw in Sec. II B, it is not just the fundamental interval, but also the right hand limit at the end point 1 of the interval that dictates the global behavior. With this in mind we take Z_n to be right continuous at 1 and write $Z_n^{1+}=Z_n(1)=Z_n(1+)$.

Iteration (2.2) gives

$$Z_n(1+)=Z_{n-1}(\phi_1(1+))+Z_{n-2}(\phi_2(1+)). \tag{2.28}$$

Now ϕ_2 is increasing and $\phi_2(1)=1$, so $\phi_2(1+)=1+$, and thus $Z_{n-2}(\phi_2(1+))=Z_{n-2}(1+)$. On the other hand ϕ_1 is decreasing and $\phi_1(1)=-\omega$, so now $\phi_1(1+)=-\omega-$. To relate $Z_{n-1}(\phi_1(1+))$ to $Z_{n-1}(1+)$ we therefore need to pass from $-\omega-$ to $1+$, which means that we need to add in the effect of all of the discontinuities of Z_{n-1} in I. Let us therefore write

$$Z_{n-1}(1+)=Z_{n-1}(-\omega-)+\Sigma_{n-1}, \tag{2.29}$$

where we denote

$$\Sigma_{n-1}=\sum_{y\in[-\omega,1]} D_{n-1}(y). \tag{2.30}$$

We thus have the following recurrence relation for Z_n^{1+}:

$$Z_n^{1+}=Z_{n-1}^{1+}+Z_{n-2}^{1+}-\Sigma_{n-1}. \tag{2.31}$$

This is a second-order inhomogeneous recurrence relation of a Fibonacci type. Its solution is

$$Z_n^{1+}=F_nZ_1^{1+}+F_{n-1}Z_0^{1+}-\sum_{i=2}^{n} F_{n+1-i}\Sigma_{i-1}. \tag{2.32}$$

If we now require Z_n to be a periodic orbit of period p of (2.2), then in particular we require Z_n^{1+} to have period p. The inhomogeneity is merely the sum of the discontinuities of Z_n and therefore this too has period p. Thus imposing periodicity of period p we can arrive at two simultaneous linear equations for Z_0^{1+} and Z_1^{1+}, namely,

$$Z_0^{1+}=Z_p^{1+}=F_pZ_1^{1+}+F_{p-1}Z_0^{1+}-\sum_{i=2}^{p} F_{p+1-i}\Sigma_{i-1}, \tag{2.33}$$

$$Z_1^{1+}=Z_{p+1}^{1+}=F_{p+1}Z_1^{1+}+F_pZ_0^{1+}-\sum_{i=2}^{p+1} F_{p+2-i}\Sigma_{i-1}. \tag{2.34}$$

When written in matrix form, the determinant of the matrix of coefficients of this system is $1+(-1)^p-F_{p+1}-F_{p-1}\neq 0$, thus these equations always possess a unique solution. The conclusion is that we may arbitrarily select the discontinuities over a set of periodic orbits of F on the fundamental interval (i.e., select the first columns of the discontinuity matrices), and then define Z_0^{1+}, Z_1^{1+}, i.e., $Z_0(1)$, $Z_1(1)$, by solving this system of linear equations, and the resulting orbit

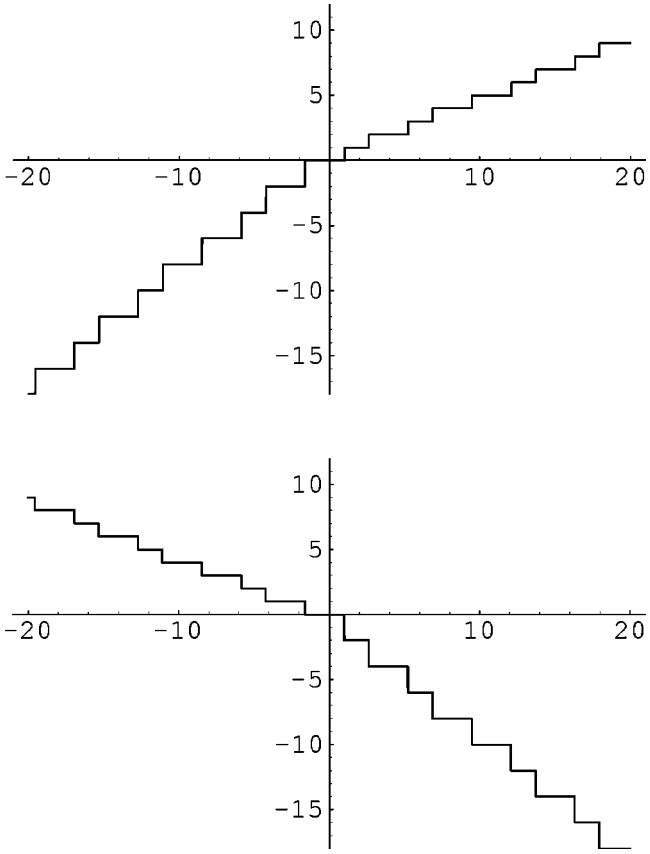

FIG. 4. Period-2 orbit of the recurrence (2.2).

is periodic on the fundamental interval. By the results of Sec. II B this local data determines the asymptotic (right continuous at 1) globally periodic orbit. In summary we have the following theorem.

Theorem 1: *A necessary and sufficient condition for a piecewise-constant, right-continuous at 1, orbit of (2.2) to be periodic (on the whole of* $\mathbb{R}$*) with period* p *is that its discontinuities have period* p *and that* Z_0^{1+}, Z_1^{1+} *satisfy Eqs. (2.33) and (2.34).*

For example, consider Example 3 above with arbitrary discontinuities X_0, X_1 at 1 of Z_0, Z_1, respectively. Solving (2.33) and (2.34) with $p=l=2$ gives $Z_0^{1+}=X_0$, $Z_1^{1+}=X_1$, i.e., that both Z_0 and Z_1 must be zero to the left of 1 on I. Figure 4 shows the case $X_0=1$, $X_1=-2$.

For the case of discontinuity set given by the union of Examples 1 and 2, $D=\{\frac{1}{2}, -\omega/2\}\cup\{0\}$, with discontinuities X_0^0, $-X_1^0$, X_0^1, and X_1^0, $-X_2^0$, $-X_0^1$ of Z_0 and Z_1 at $\frac{1}{2}$, $-\omega/2$, 0, respectively, for the period-6 orbit of the discontinuities to be a period-6 orbit of (2.2) we solve (2.33) and (2.34) with $p=6$, and thereby specify

$$Z_0^{1+}=(2X_0^0-X_1^0+X_2^0+2X_0^1)/2, \quad Z_1^{1+}=(-X_0^0+2X_1^0-X_2^0-2X_0^1)/2. \tag{2.35}$$

III. DISCONTINUITIES ON $\mathbb{R}$

Thus far we have a necessary and sufficient condition for orbits of (2.2) to be periodic on the whole of $\mathbb{R}$. We further wish to address the problem of the spatial boundedness of such orbits. The example shown in Fig. 4 demonstrates that orbits can be periodic (in time) but unbounded (in space). To find conditions for spatial boundedness we must understand both the locations and the sizes of the discontinuities of Z_n on the whole of $\mathbb{R}$, and that is the purpose of this section. The

sizes of the discontinuities will be straightforward to calculate, but identifying their locations presents some difficulty. Since recurrence (2.2) is linear, we may consider the contribution of each periodic orbit, and, indeed, each discontinuity of each periodic orbit, to the global discontinuity set of Z_n separately.

We shall return to the issue of spatial boundedness in Sec. IV. A precise identification of the locations of the discontinuities of Z_n will also enable us to calculate the autocorrelation functions. This we shall do in Sec. V.

A. Discontinuities and the field $\mathbb{Q}(\omega)$

Let L_n denote the set of locations of the discontinuities of Z_n, i.e.,

$$L_n=\{x\in\mathbb{R}:D_n(x)\neq 0\}. \tag{3.1}$$

From (2.2) it is clear that

$$L_n=\phi_1^{-1}(L_{n-1})\cup\phi_2^{-1}(L_{n-2}), \tag{3.2}$$

unless there is a cancellation of discontinuities (which, as we shall see below, may occur if both 1 and 0 are discontinuities). As we saw in Sec. II B, the global discontinuities of Z_n are generated from those in the fundamental interval I, and the latter consist of elements of periodic orbits of the map F. It is clear from (2.8) that such periodic orbits must be composed of elements of the field

$$\mathbb{Q}(\omega)=\{a+b\omega:a,b\in\mathbb{Q}\}. \tag{3.3}$$

As a consequence, the sets L_n consist of elements of $\mathbb{Q}(\omega)$, since the maps ϕ_1^{-1}, ϕ_2^{-1} act on $\mathbb{Q}(\omega)$ as

$$\phi_1^{-1}(a+b\omega)=-(a+b)-a\omega, \tag{3.4}$$

$$\phi_2^{-1}(a+b\omega)=2a+b-1+(a+b-1)\omega. \tag{3.5}$$

Rather than consider a periodic orbit itself, we shall consider initially an orbit asymptotic to it generated from discontinuity data on the fundamental interval only. By the results of Sec. II B this orbit is eventually periodic and identical to the desired periodic orbit on any bounded subset of $\mathbb{R}$.

Consider then the case of Z_0 having a single discontinuity of size X at $a+b\omega\in(-\omega,1]$, and Z_1 having discontinuity only at $\phi_1^{-1}(a+b\omega)$. This discontinuity will have size $-X$. If $a+b\omega\in(-\omega,\omega^2)$ (i.e., $a+b\omega$ has code 1), then $\phi_1^{-1}(a+b\omega)=F(a+b\omega)\in(-\omega,1)$, otherwise ($a+b\omega$ has code 2) $\phi_1^{-1}(a+b\omega)\notin(-\omega,1]$.

The first few discontinuity location sets are

$$\begin{aligned}
L_0&=\{a+b\omega\}=a+b\omega+\{0+0\omega\},\\
L_1&=\{-(a+b)-a\omega\}=-(a+b)-a\omega+\{0+0\omega\},\\
L_2&=2a+b+(a+b)\omega+\{-1-\omega,0+0\omega\},\\
L_3&=-(3a+2b)-(2a+b)\omega+\{-1-\omega,0+0\omega,2+\omega\},\\
L_4&=5a+3b+(3a+2b)\omega+\{-4-3\omega,-3-2\omega,-1-\omega,0+0\omega,2+\omega\},\\
L_5&=-(8a+5b)-(5a+3b)\omega+\{-4-3\omega,-3-2\omega,-1-\omega,0+0\omega,\\
&\quad 2+\omega,4+2\omega,5+3\omega,7+4\omega\},
\end{aligned} \tag{3.6}$$

where, when x is a number and S is a set of numbers, $x+S$ denotes the set $\{x+s:s\in S\}$. We shall write these sets in the form

$$L_n=c^{(n)}+d^{(n)}\omega+M_n. \tag{3.7}$$

We observe that the numbers $c^{(n)}$, $d^{(n)}$ obey a simple Fibonacci recurrence, and that the sets (M_n) grow in an alternating manner, appending successively on the right and left of the existing list, and that M_n contains F_{n+1} elements. Moreover, M_n consists of numbers of the form $a+b\omega$ in which b increases uniformly by 1 from $-F_{n-1}$ to F_n-1 when n is odd, and from $-F_n$ to $F_{n-1}-1$ when n is even. However, the component a has increments given by a sequence 1,2,1,2,2,1,2,..., ranging from $-(F_n-1)$ to $F_{n+1}-1$ when n is odd, and from $-(F_{n+1}-1)$ to F_n-1 when n is even. The size of each discontinuity in L_n is $(-1)^nX$.

We shall now identify the precise form of the set M_n, and then prove that the above observations hold for all n.

B. Discontinuities arising from a single discontinuity in *I*

We now state and prove the precise form of the sets L_n based on our preliminary observation in the previous subsection.

For $x\in\mathbb{R}$, we let $\lceil x\rceil$ denote the ceiling of x, namely $\min\{n\in\mathbb{Z}:n\geqslant x\}$, and $\lfloor x\rfloor$ denote the floor of x, namely $\max\{n\in\mathbb{Z}:n\leqslant x\}$. First, we have the following proposition.

Proposition 6: The discontinuity location sets (L_n) *arising from applying recurrence (2.2) to initial conditions in which* Z_0 *has a single discontinuity of size* X *at* $a+b\omega\in I$, *and* Z_1 *has a single discontinuity of size* $-X$ *at* $\phi_1^{-1}(a+b\omega)$, *are* $L_0=\{a+b\omega\}$ *and for* $n\geqslant 1$

$$L_n=c^{(n)}+d^{(n)}\omega+M_n, \tag{3.8}$$

where

$$M_n=\{\lceil i/\omega\rceil+i\omega:i=l_n,\ldots,r_n\}, \tag{3.9}$$

with

$$l_n,r_n=\begin{cases}-F_{n-1},F_n-1, & n\ \ odd,\\ -F_n,F_{n-1}-1, & n\ \ even,\end{cases} \tag{3.10}$$

and where

$$c^{(n)}=(-1)^n(F_{n+1}a+F_nb),\quad d^{(n)}=(-1)^n(F_na+F_{n-1}b). \tag{3.11}$$

Moreover, each discontinuity of L_n *is of size* $(-1)^nX$.

Proof: The proof is by induction with the base case being clear. Suppose now that L_{n-1} and L_{n-2} are given as in the statement of the proposition. As we noted earlier in (3.2) we have $L_n=\phi_1^{-1}(L_{n-1})\cup\phi_2^{-1}(L_{n-2})$. We readily calculate that

$$\phi_1^{-1}(L_{n-1})=c^{(n)}+d^{(n)}\omega+\phi_1^{-1}(M_{n-1}), \tag{3.12}$$

$$\phi_2^{-1}(L_{n-2})=c^{(n)}+d^{(n)}\omega+\phi_2^{-1}(M_{n-2}), \tag{3.13}$$

so that we need only establish that $M_n=\phi_1^{-1}(M_{n-1})\cup\phi_2^{-1}(M_{n-2})$ with M_n as given by (3.9). To do this it suffices to show that each element of M_n is in either $\phi_1^{-1}(M_{n-1})$ or $\phi_2^{-1}(M_{n-2})$, since M_n has F_{n+1} elements and $\phi_1^{-1}(M_{n-1})$, $\phi_2^{-1}(M_{n-2})$ have F_n, F_{n-1} elements, respectively. Suppose that n is even and let $i\in\{-F_n,\ldots,F_{n-1}-1\}$. Considering (3.4) and (3.5), we must show there exists either $j\in\{-F_{n-2},\ldots,F_{n-1}-1\}$ such that $i=-\lceil j/\omega\rceil$ and $\lceil i/\omega\rceil=-\lceil j/\omega\rceil-j$ or $k\in\{-F_{n-2},\ldots,F_{n-3}-1\}$ such that $i=\lceil k/\omega\rceil+k-1$ and $\lceil i/\omega\rceil=2\lceil k/\omega\rceil+k-1$.

Set $j=\lfloor -i\omega \rfloor$ so that $j+\varepsilon_1=-i\omega$, i.e.,

$$j/\omega+\varepsilon_1/\omega=-i, \tag{3.14}$$

for some $\varepsilon_1\in(0,1)$. We note that $j\in\{\lfloor -(F_{n-1}-1)\omega\rfloor,\ldots,\lfloor F_n\omega\rfloor\}$, for which the identity (1.24) (recalling that n is even) gives $\lfloor F_n\omega\rfloor=\lfloor F_{n-1}-\omega^n\rfloor=F_{n-1}-1$, and $\lfloor -(F_{n-1}-1)\omega\rfloor=\lfloor -F_{n-2}+\omega-\omega^{n-1}\rfloor=-F_{n-2}$, so that j is in the desired range.

Now (case 1) if $\varepsilon_1\in(0,\omega)$, then $\varepsilon_1/\omega\in(0,1)$ so that (3.14) gives $\lceil j/\omega\rceil=-i$, i.e., $i=-\lceil j/\omega\rceil$. We further have $i/\omega=i+i\omega=i-j-\varepsilon_1=-\lceil j/\omega\rceil-j-\varepsilon_1$, and thus $\lceil i/\omega\rceil=-\lceil j/\omega\rceil-j$ as desired.

On the other hand (case 2), if $\varepsilon_1\in(\omega,1)$, then $\varepsilon_1/\omega\in(1,\omega^{-1})$ and we deduce that $\lceil j/\omega\rceil=-i-1$, so that $i\neq-\lceil j/\omega\rceil$, and we thus need to define a suitable k. (Note that the case $\varepsilon_1=\omega$ is clearly impossible since ω is irrational. For the same reason we have $\varepsilon_1\neq 0$.) We set $k=\lfloor -j\omega\rfloor$ so that there exists $\varepsilon_2\in(0,1)$ such that

$$-j\omega=k+\varepsilon_2. \tag{3.15}$$

Since $j\in\{-F_{n-2},\ldots,F_{n-1}-1\}$, by an argument similar to that above, we deduce, as desired, that $k\in\{-F_{n-2},\ldots,F_{n-3}-1\}$. Addition of (3.14) and (3.15) gives $j+\varepsilon_1/\omega=-i+k+\varepsilon_2$ so that, since $\varepsilon_1/\omega\in(1,\omega^{-1})$ and $\varepsilon_2\in(0,1)$, we have $\varepsilon_2=\varepsilon_1/\omega-1$, and thus $\varepsilon_2\in(0,\omega)$, i.e., $\varepsilon_2/\omega\in(0,1)$. Equation (3.15) is $-j=k/\omega+\varepsilon_2/\omega$ which thus gives

$$-j=\lceil k/\omega\rceil. \tag{3.16}$$

Now addition of (3.15) and (3.16) gives $-j-j\omega-\varepsilon_2=k+\lceil k/\omega\rceil$, i.e., $-k-\lceil k/\omega\rceil=j/\omega+\varepsilon_2=\lceil j/\omega\rceil$ and so, since $\lceil j/\omega\rceil=-i-1$, we deduce that $i=\lceil k/\omega\rceil+k-1$. From $j+\varepsilon_1=-i\omega$ and $j=-\lceil k/\omega\rceil$, it immediately follows that $i/\omega=i+i\omega=i+\lceil k/\omega\rceil-\varepsilon_1=2\lceil k/\omega\rceil+k-1-\varepsilon_1$, and so $\lceil i/\omega\rceil=2\lceil k/\omega\rceil+k-1$ as desired.

The case n odd is established in a similar manner.

That each discontinuity of L_n is of size $(-1)^nX$ follows immediately from the facts that ϕ_1^{-1} is orientation reversing and ϕ_2^{-1} is orientation preserving. □

We have thus established the locations and sizes of the discontinuities of Z_n that arise from the presence of a discontinuity in Z_0 at $a+b\omega\in I$.

We must also consider the case in which Z_0 has no discontinuities and Z_1 has a single discontinuity in I. However, this situation is clearly identical to the case just considered, but with a reduction of one in all subscripts. More precisely, we have the following.

Proposition 7: The discontinuity location sets (L_n) *arising from applying recurrence (2.2) to initial conditions in which* Z_0 *has no discontinuities and* Z_1 *has a single discontinuity of size* $-X$ *at* $a+b\omega\in I$ *are* $L_0=\varnothing$, $L_1=\{a+b\omega\}$, *and for* $n\geqslant 2$

$$L_n=c^{(n-1)}+d^{(n-1)}\omega+M_{n-1}, \tag{3.17}$$

with $c^{(n)}$, $d^{(n)}$, M_n *as in the statement of Proposition 6. Moreover, each discontinuity of* L_n *is of size* $(-1)^nX$.

The proof of Proposition 7 is analogous to that of Proposition 6.

Thus far we have considered functions possessing only a finite number of discontinuities. A globally periodic orbit, however, possesses an infinite number of discontinuities, being the limit (defined by pointwise convergence) of the sets (L_n) considered thus far. It is clear from Proposition 6 what the discontinuity set generated by a single discontinuity at the fixed point zero is, namely

$$\{\lceil i/\omega\rceil+i\omega : i\in\mathbb{Z}\}, \tag{3.18}$$

this being the limit of the corresponding sets L_n with $a=b=0$, so that $c^{(n)}=d^{(n)}=0$ for all n. However, care is needed in the determination of these sets for other periodic orbits. We shall return to this issue in Sec. V where we consider the period-6 orbit of (2.2) generated by the period-2 orbit $\{\frac{1}{2},-\omega/2\}$ of F.

We remark that a symbolic formulation of the discontinuity locations is possible in terms of ''words'' with letters drawn from the ''alphabet'' {1, 2}. More precisely, a sequence of Fibonacci words with first few elements

$$\begin{gathered}1\\12\\1212\\1212212\\121221212212\end{gathered} \tag{3.19}$$

may be used to describe the increments in the elements of the discontinuity sets L_n. These words may be obtained by the following rules. We denote by $\diamondsuit$ the empty word, by S the substitution operator $1\mapsto 2$, $2\mapsto 12$, and by R the reversal operator $w_1\ldots w_k\mapsto w_k\ldots w_1$. The nth Fibonacci word w^n may be written as the concatenation $u^n v^n$ with the rule $u^1=v^1=\diamondsuit$, and, for $n\geqslant 1$, $u^{n+1}=R(S(v^n)1)$, $v^{n+1}=R(S(u^n))$. We index the ''letters'' in w^n by setting w_0^n to be the last letter of u^n and setting w_1^n to be the first letter of v^n. Then the words w^n are the words given in (3.19). As $n\to\infty$, $w^n\to w^*$, the biinfinite Fibonacci word. One may write the set (3.18) as $\{x_i+i\omega\}$ where $x_0=0$ and $x_i-x_{i-1}=w_i^*$.

IV. GLOBAL BOUNDEDNESS

In the previous section we determined the global effect of a single discontinuity in the fundamental interval. Each of the l variables $X_0,X_1,\ldots,X_{l-1}$ in the discontinuity matrix of a periodic orbit gives rise to such a discontinuity in the initial conditions Z_0, Z_1 in the form of one of the three following cases.

(1) Z_0 has a single discontinuity in I at $x\in(-\omega,\omega^2)$ and Z_1 has a single discontinuity at $F(x)\in I-\{1\}$.
(2) Z_0 has a single discontinuity in $(\omega^2,1]$ and Z_1 has no discontinuities in I.
(3) Z_0 has no discontinuities in I and Z_1 has a single discontinuity in I.

Case 1 corresponds to a discontinuity of Z_0 at a point y_i with code 1, so that y_{i+1} is a discontinuity location of Z_1 (having the same size, but opposite sign). Case 2 corresponds to a discontinuity location y_i of Z_0 with code 2. Case 3 corresponds to a discontinuity location y_i of Z_1 such that y_{i-1} has code 2. (It is illustrative to look at a discontinuity matrix such as that of Example 4 to understand these three cases.) Cases 1 and 2 are handled by Proposition 6, while Proposition 7 treats case 3.

The important thing to note from Propositions 6 and 7 is that each discontinuity generates an ordered set of discontinuities of the same size and sign in which the elements of each set have identical relative displacements: the elements of each set are separated from each other *by the same amount* $(1+\omega$ *or* $2+\omega)$ *in the same order*. Moreover, with the exception of the fixed point 1, each nonzero discontinuity causes an unbounded monotonic growth as we move further from the fundamental interval on both sides.

From Proposition 6 we see that if Z_0 has a discontinuity at 1 of size X (case 2), then this discontinuity gives rise to discontinuities in Z_n of size X at locations $\geqslant 1$ for even n and of size $-X$ at locations $\leqslant -1-\omega$ for odd n. Proposition 7 shows that if Z_1 has a discontinuity at 1 of

size $-X'$ (case 3), then *this* discontinuity gives rise to discontinuities in Z_n of size X' at locations $\leqslant -1-\omega$ for *even* n and of size $-X'$ at locations $\geqslant 1$ for *odd* n. This may be seen in Fig. 4, in which the discontinuities in the first figure (even n) are of size 1 on the right (corresponding to the discontinuity in Z_0), while those on the left are of size 2 (corresponding to the discontinuity in Z_1). The situation is reversed in the second figure (where n is odd).

For global boundedness we require there to be cumulative growth on neither the left nor the right hand sides of the fundamental interval.

Consider the case of even n. For boundedness on the right we must include the effect of 1 being a discontinuity location for Z_0. For boundedness on the left we must include the effect of 1 being a discontinuity location for Z_1.

We first look at the cumulative effect of the discontinuities contributing to growth to the right of the fundamental interval. We must consider all discontinuities from cases 1 and 2, and those of case 3 excluding the fixed point 1. The sum over all discontinuities of all periodic orbits of the type of case 2 is

$$\sum_{y\in(\omega^2,1]} D_0(y). \tag{4.1}$$

The combined contribution of all discontinuities of all periodic orbits of the type of cases 1 and 3 is

$$-\sum_{y\in(-\omega,1)} D_1(y), \tag{4.2}$$

the contributions from case 1 being of the form $+D_0(y_{i-1})=-D_1(y_i)$, and from case 3 of the form $-D_1(y_i)$. Note that 1 is excluded from the range of this sum since, as we noted above, discontinuities associated with 1 being a discontinuity of the type of case 3 are to the left of the fundamental interval for even n. Because of the same relative spacing of discontinuity locations, as we increase to the right the contributions from all three cases grow at the same rate. For boundedness we therefore require the sum of (4.1) and (4.2) to be zero, i.e., we require

$$\sum_{y\in(\omega^2,1]} D_0(y)=\sum_{y\in(-\omega,1)} D_1(y). \tag{4.3}$$

Now look to the left of the fundamental interval (with n still even). The sum over all discontinuities of all periodic orbits of the type of case 2 is now

$$\sum_{y\in(\omega^2,1)} D_0(y), \tag{4.4}$$

and the sum over all discontinuities of all periodic orbits of the type of cases 1 and 3 is

$$-\sum_{y\in(-\omega,1]} D_1(y), \tag{4.5}$$

where 1 is now excluded from the first sum since discontinuities associated with a 1 being a discontinuity of the type of case 2 are to the right of the fundamental interval for even n. For the same reasons as above, we require the sum of (4.4) and (4.5) to be zero, i.e., we require

$$\sum_{y\in(\omega^2,1)} D_0(y)=\sum_{y\in(-\omega,1]} D_1(y). \tag{4.6}$$

For even n, it is clear that if condition (4.3) is violated, there will be unbounded growth on the right, while if condition (4.6) is violated, there will be unbounded growth on the left. Thus our combined conditions are necessary and sufficient. [Consideration of boundedness for odd n results in the same two conditions (4.3) and (4.6).] We thus have the following.

Theorem 2: *A necessary and sufficient criterion for a piecewise-constant periodic orbit of (2.2) to be globally bounded is*

$$\sum_{y\in(-\omega,1]} D_1(y)=\sum_{y\in(\omega^2,1)} D_0(y) \quad \text{and} \quad \sum_{y\in(-\omega,1)} D_1(y)=\sum_{y\in(\omega^2,1]} D_0(y). \tag{4.7}$$

Note that in general the inclusion or exclusion of 1 from the intervals in these sums is crucial. (However, the points $-\omega$ and ω^2 are never discontinuities.) Further note that when 1 is not a discontinuity location these two conditions are identical. For instance, for the period-6 orbit resulting from Examples 1 and 2 the condition (4.7) is the single constraint $X_0^0-X_1^0+X_2^0+X_0^1=0$.

We remark that we may produce orbits that are unbounded, but *relatively globally bounded* by ensuring the condition of Theorem 2 is satisfied but the condition for periodicity of Sec. II F (Theorem 1) is violated. [We define the orbit (Z_n) to be relatively globally bounded if there exists a constant K such that $|Z_n(x)-Z_n(0)|\leqslant K$ for all $x\in\mathbb{R}$ and for all $n\in\mathbb{N}$.] The simplest example of such an orbit is that generated by the constant functions $Z_0(x)=0$, $Z_1(x)=1$ in which there are no discontinuities.

From the physical point of view we deduce that we may choose many forms for the modulation function in (1.11), and, provided the conditions for periodicity (Theorem 1) and global boundedness (Theorem 2) are satisfied, the resulting autocorrelation function will display asymptotic self-similarity. More precisely, provided the function Φ is chosen so that the initial conditions $Z_0(x)=0$, $Z_1(x)=\Phi(-\omega x)$ are periodic or preperiodic on the fundamental interval $[-\omega,1]$, and that two successive functions on this periodic orbit satisfy the periodicity and global boundedness conditions, then there is asymptotic self-similarity of the autocorrelation function.

We look in detail at the particular choice (1.29) in the next section.

V. THE PERIOD-6 ORBIT

As a further application of our work in Sec. III, we now look in detail at the particular example of Feudel *et al.*[5] briefly mentioned in the Introduction. The choice of modulation function (1.29) results in the period-6 orbit shown in Fig. 2. However, it is important to note that the discontinuities of the initial conditions (1.27) do not all form discontinuities of the period-6 orbit. In particular, the function $Z_1(x)=\Phi(-\omega x)$ has a discontinuity at $x=\omega^{-1}/2$ which is not periodic for F, but its image under F is $\frac{1}{2}$, which is part of the period-two orbit $\{\frac{1}{2},-\omega/2\}$. The other discontinuity of Z_1 in the fundamental interval $[-\omega,1]$ is the fixed point 0.

Henceforth, when we refer to the orbit (Z_n) we mean the global periodic orbit, and not the orbit asymptotic to it that we generate from the periodic orbit on the fundamental interval. This global period-6 orbit is generated from the restricted discontinuity set equal to the union of Examples 1 and 2, namely $\{\frac{1}{2},-\omega/2\}\cup\{0\}$ with discontinuity values $X_0^0=-2$, $X_1^0=0$, $X_2^0=0$, corresponding to $\{\frac{1}{2},-\omega/2\}$, and $X_0^1=2$ corresponding to $\{0\}$. This data means that Z_0 has discontinuities $X_0^0=-2$ at $\frac{1}{2}$, $-X_1^0=0$ at $-\omega/2$, and $X_0^1=2$ at 0, while Z_1 has discontinuities $X_1^0=0$ at $\frac{1}{2}$, $-X_2^0=0$ at $-\omega/2$, and $-X_0^1=-2$ at 0. The point 1 is not a discontinuity point, and to guarantee periodicity we specify $Z_0^{1+}=Z_0(1)=0$, and $Z_1^{1+}=Z_1(1)=-1$ according to (2.35). We further note that this data satisfies the condition $X_0^0-X_1^0+X_2^0+X_0^1=0$, which is the criterion of the previous section (Theorem 2) guaranteeing a globally bounded periodic orbit.

The value of the corresponding autocorrelation function K_{P_y} at Fibonacci times F_n will be calculated explicitly in terms of the amplitude κ. Figure 1 shows K_{P_y} for the case $\kappa=\pi/2$. In the cases $n\equiv 1, 2 \bmod 3$, since (as we shall show) $Z_n=\pm 1$, Eq. (1.28) gives us $K_{P_y}(F_n)=\cos\kappa\ (=0$

when $\kappa=\pi/2$). In the case $n\equiv 0 \bmod 3$, where now (again, as we shall show) $Z_n=0,\pm 2$, we have $K_{P_y}(F_n)=1-\alpha+\alpha\cos 2\kappa$ ($=1-2\alpha$ when $\kappa=\pi/2$) where 2α is the asymptotic average value of $|Z_n|$. In Ref. 5 it is numerically calculated that $\alpha\approx 0.2236$. In fact, this constant is $1/(2\sqrt{5})$ as we shall show in this section. As a consequence, when $\kappa=\pi/2$, for $n\equiv 0 \bmod 3$ we have $K_{P_y}(F_n)\to 1-1/\sqrt{5}=0.552\,786\ldots$ as $n\to\infty$.

A. The discontinuity location sets

1. Discontinuities arising from the fixed point 0

We have that Z_0 and Z_1 both have a single discontinuity at 0 ($=0+0\omega$) only, and so, taking the limit $n\to\infty$ in Proposition 6, the discontinuity location set associated with the fixed point 0 is

$$L^1=\{\lceil i/\omega\rceil+i\omega: i\in\mathbb{Z}\}. \tag{5.1}$$

2. Discontinuities arising from the period-two orbit $\{\frac{1}{2},-\omega/2\}$

The discontinuity location sets associated with the period-two orbit $\{\frac{1}{2},-\omega/2\}$ are generated from Z_0 having a discontinuity at $\frac{1}{2}$ and Z_1 having no discontinuities in fundamental interval $[-\omega,1]$. [Of course, Z_1 has a discontinuity at $\phi_1^{-1}(\frac{1}{2})=-\omega^{-1}/2$, but this is outside the fundamental interval.] The result is period-3 behavior. Let us define the sets

$$L^{0,0}=\{\lceil i/\omega+\tfrac{1}{2}\rceil-\tfrac{1}{2}+i\omega: i\in\mathbb{Z}\}, \tag{5.2}$$

$$L^{0,1}=\{\lceil (i-\tfrac{1}{2})/\omega+\tfrac{1}{2}\rceil-\tfrac{1}{2}+(i-\tfrac{1}{2})\omega: i\in\mathbb{Z}\}, \tag{5.3}$$

$$L^{0,2}=\{\lceil (i-\tfrac{1}{2})/\omega\rceil+(i-\tfrac{1}{2})\omega: i\in\mathbb{Z}\}. \tag{5.4}$$

Then we have the following.

Proposition 8: The discontinuity location sets L_n generated by the period-2 orbit $\{\frac{1}{2},-\omega/2\}$ satisfy

$$L^{0,0}\cap L_n=\{\lceil i/\omega+\tfrac{1}{2}\rceil-\tfrac{1}{2}+i\omega: i=l_n^0,\ldots,r_n^0\},\quad n\equiv 0 \bmod 3; \tag{5.5}$$

$$L^{0,1}\cap L_n=\{\lceil (i-\tfrac{1}{2})/\omega+\tfrac{1}{2}\rceil-\tfrac{1}{2}+(i-\tfrac{1}{2})\omega: i=l_n^1,\ldots,r_n^1\},\quad n\equiv 1 \bmod 3; \tag{5.6}$$

$$L^{0,2}\cap L_n=\{\lceil (i-\tfrac{1}{2})/\omega\rceil+(i-\tfrac{1}{2})\omega: i=l_n^2,\ldots,r_n^2\},\quad n\equiv 2 \bmod 3, \tag{5.7}$$

where, as $n\to\infty$, $l_n^k\to-\infty$, $r_n^k\to\infty$ for $k=0,1,2$, so that the sets $L^{0,0}$, $L^{0,1}$, $L^{0,2}$ are the limits as $m\to\infty$ of the sequences (L_{3m}), (L_{3m+1}), (L_{3m+2}), respectively.

Proof: We must consider the three residue classes modulo 3 separately. We shall use the readily established fact that the Fibonacci numbers have the following parity structure: $F_n\equiv 0 \bmod 2$ when $n\equiv 0 \bmod 3$, and $F_n\equiv 1 \bmod 2$ when $n\equiv 1,2 \bmod 3$.

(a) $n\equiv 0 \bmod 3$. We treat the two cases $n\equiv 0 \bmod 6$, $n\equiv 3 \bmod 6$, separately.

In the case $n\equiv 0 \bmod 6$, so that n is even, Proposition 6 gives

$$L_n=\{F_{n+1}/2+\lceil i/\omega\rceil+(F_n/2+i)\omega: i=-F_n,\ldots,F_{n-1}-1\}, \tag{5.8}$$

which by relabeling is

$$L_n=\{F_{n+1}/2+\lceil (i-F_n/2)/\omega\rceil+i\omega: i=-F_n/2,\ldots,F_n/2+F_{n-1}-1\}. \tag{5.9}$$

(Note that F_n is even.) To establish the result we must show that

$$F_{n+1}/2+\lceil (i-F_n/2)/\omega\rceil=\lceil i/\omega+\tfrac{1}{2}\rceil-\tfrac{1}{2} \tag{5.10}$$

for a suitable range of i. Now, since F_{n+1} is odd,

$$\begin{aligned}\tfrac{1}{2}+F_{n+1}/2+\lceil(i-F_n/2)/\omega\rceil&=\lceil\tfrac{1}{2}+F_{n+1}/2+(i-F_n/2)/\omega\rceil\\&=\lceil\tfrac{1}{2}+(i+(F_{n+1}\omega-F_n)/2)/\omega\rceil\\&=\lceil\tfrac{1}{2}+(i+\omega^{n+1}/2)/\omega\rceil=\lceil i/\omega+1/2+\omega^n/2)\rceil,\end{aligned}\tag{5.11}$$

where we have used the identity (1.24). We must show that for suitable i this equals $\lceil i/\omega+\frac{1}{2}\rceil$. Since $i/\omega=i+i\omega$ our desired equality may be written as $\lceil i\omega+\frac{1}{2}+\omega^n/2\rceil=\lceil i\omega+\frac{1}{2}\rceil$, which is true if, and only if, $\lceil i\omega+\frac{1}{2}\rceil-(i\omega+\frac{1}{2})\geqslant\omega^n/2$, in which we note that $\lceil i\omega+\frac{1}{2}\rceil-(i\omega+\frac{1}{2})=|i\omega+\frac{1}{2}-r|$, where $r=\lceil i\omega+\frac{1}{2}\rceil$.

Now since the ratios of successive Fibonacci numbers are the continued fraction approximants to ω we have that

$$|q\omega-p|\geqslant|F_n\omega-F_{n-1}|=\omega^n,\tag{5.12}$$

for all $p\in\mathbb{Z}$ and all integers q with $|q|\leqslant F_n$.

We thus have $|2i\omega+1-2r|\geqslant\omega^n$ for all integers i such that $2|i|\leqslant F_n$, i.e., $|i\omega+\frac{1}{2}-r|\geqslant\omega^n/2$, for all integers i such that $|i|\leqslant F_n/2$. This establishes our desired equality for a range of i of the desired type.

The case $n\equiv3$ mod 6 is similar, with minor modifications to take into account the oddness of n. Such modifications may be seen in the proof of the first part of the next case.

(b) $n\equiv1$ mod 3. We consider separately the two cases $n\equiv1$ mod 6, $n\equiv4$ mod 6.

In the case $n\equiv1$ mod 6, so that n is odd, Proposition 6 gives

$$L_n=\{-F_{n+1}/2+\lceil i/\omega\rceil+(i-F_n/2)\omega:i=-F_{n-1},\ldots,F_n-1\},\tag{5.13}$$

which by relabeling is

$$L_n=\{-F_{n+1}/2+\lceil(i+(F_n-1)/2)/\omega\rceil+(i-\tfrac{1}{2})\omega:i=-F_{n-1}-(F_n-1)/2,\ldots,(F_n-1)/2\}.\tag{5.14}$$

(Note that F_n is now odd.) To establish the result we must show that

$$-F_{n+1}/2+\lceil(i+(F_n-1)/2)/\omega\rceil=\lceil(i-\tfrac{1}{2})/\omega+\tfrac{1}{2}\rceil-\tfrac{1}{2}\tag{5.15}$$

for a suitable range of i. We now proceed as in case (a). First we have

$$1/2-F_{n+1}/2+\lceil(i+(F_n-1)/2)/\omega\rceil=\lceil i/\omega-\omega/2+\omega^n/2\rceil,\tag{5.16}$$

and so we must show that $\lceil i\omega-\omega/2+\omega^n/2\rceil=\lceil i\omega-\omega/2\rceil$ for suitable i, which is true if, and only if, $\lceil i\omega-\omega/2\rceil-(i\omega-\omega/2)>\omega^n/2$. Now $\lceil i\omega-\omega/2\rceil-(i\omega-\omega/2)=|i\omega-\omega/2-r|$, where $r=\lceil i\omega-\omega/2\rceil$, and we have $|2i\omega-\omega-2r|=|(2i-1)\omega-2r|\geqslant\omega^n$ for all integers i such that $|2i-1|<F_n$. This is just $|i\omega-\omega/2-r|>\omega^n/2$ for such a range of i as desired.

The case $n\equiv4$ mod 6 is similar.

(c) $n\equiv2$ mod 3. We omit the detail for this case which is similar to those above. □

B. Combining the discontinuities

Note that

$$L^{0,n}\subset\begin{cases}(\mathbb{Z}/2-\mathbb{Z})+\omega\mathbb{Z}, & n=0,\\(\mathbb{Z}/2-\mathbb{Z})+\omega(\mathbb{Z}/2-\mathbb{Z}), & n=1,\\\mathbb{Z}+\omega(\mathbb{Z}/2-\mathbb{Z}), & n=2,\end{cases}\tag{5.17}$$

while

$$L^1 \subset \mathbb{Z} + \omega\mathbb{Z}. \tag{5.18}$$

It follows that the discontinuity location sets generated from the period-two orbit $\{\frac{1}{2}, -\omega/2\}$ are disjoint from those associated with the fixed point 0. Thus, there can be no cancellation, or even modification, of the discontinuities generated by one periodic orbit ($\{\frac{1}{2}, -\omega/2\}$ or $\{0\}$) by the other. We further recall that the elements of each of these sets form an increasing sequence with separation either $1+\omega$ or $2+\omega$.

The initial conditions for the discontinuities are $X_0^0 = -2$, $X_1^0 = X_2^0 = 0$, and $X_0^1 = 2$. It follows that each discontinuity of Z_n due to the period-two orbit $\{\frac{1}{2}, -\omega/2\}$ is of size -2 when n is even, and of size 2 when n is odd. Each discontinuity of Z_n due to the fixed point 0 is of size 2 when n is even, and of size -2 when n is odd.

As well as specifying the initial discontinuity data, we have also specified the initial values $Z_0(1) = 0$ and $Z_1(1) = -1$, thereby giving us initial conditions asymptotic to a globally bounded periodic orbit of period-6. It is straightforward to check that $Z_2(1) = 1$, $Z_3(1) = 0$, $Z_4(1) = 1$, $Z_5(1) = -1$, so that, knowing from Sec. II that the discontinuities have period-6 satisfying $D_{n+3} = -D_n$, the periodic orbit (Z_n) itself satisfies $Z_{n+3} = -Z_n$.

C. Calculation of the autocorrelation function

Given this detailed knowledge of the locations and sizes of all discontinuities we can calculate the autocorrelation function (1.28). We denote the discontinuity locations associated with the fixed point 0 given in (5.1) as $a_i^1 + b_i^1\omega$, and those associated with the period-2 orbit $\{\frac{1}{2}, -\omega/2\}$ given in (5.2)–(5.4) as $a_i^0 + b_i^0\omega$.

We must consider the three residue classes modulo 3 separately.

1. n≡0 mod 3

When $n \equiv 0 \bmod 3$ we see from (5.1) and (5.2) that discontinuities may be matched by the coefficients of ω. The separation of matched discontinuities is then

$$a_i^1 + b_i^1\omega - (a_i^0 + b_i^0\omega) = \lceil i/\omega \rceil + i\omega - (\lceil i/\omega + \tfrac{1}{2} \rceil - \tfrac{1}{2} + i\omega) = \tfrac{1}{2} + \lceil i/\omega \rceil - \lceil i/\omega + \tfrac{1}{2} \rceil = \pm\tfrac{1}{2}, \tag{5.19}$$

and these discontinuities occur in strict alternation since the separation of elements in each sequence is either $1+\omega$ or $2+\omega$.

Now when, in addition, n is even so that $n \equiv 0 \bmod 6$, each discontinuity from $\{\frac{1}{2}, -\omega/2\}$ has size $X_0^0 = -2$, while each discontinuity from $\{0\}$ has size $X_0^1 = 2$. Moreover, we have that $Z_n(1) = 0$, so that the matched discontinuities combine to give an interval of height ± 2 and width $\frac{1}{2}$ in the graph of Z_n, as in the top two graphs in Fig. 2. For instance, the first pair after 1 is $2+\omega$ with discontinuity 2, and $\frac{5}{2}+\omega$ with discontinuity -2. Thus the graph of Z_n consists of intervals at height zero punctuated by excursions of width $\frac{1}{2}$ to a height ± 2. The analysis for odd n (i.e., so that now $n \equiv 3 \bmod 6$) is identical, but with all signs reversed.

The autocorrelation function values $K_{P_y}(F_n)$ may now be calculated.

Theorem 3: *Let* (Z_n) *be the globally bounded period-6 orbit of* (2.2) *generated by discontinuity set* $\{\frac{1}{2}, -\omega/2, 0\}$ *with initial data* $D_0(\frac{1}{2}) = -2$, $D_0(-\omega/2) = 0$, $D_0(0) = 2$, $D_1(\frac{1}{2}) = 0$, $D_1(-\omega/2) = 0$, $D_1(0) = -2$, *with* $Z_0^{1+} = Z_0(1) = 0$, *and* $Z_1^{1+} = Z_1(1) = -1$. *Then, for* $n \equiv 0 \bmod 3$,

$$\lim_{n\to\infty} K_{P_y}(F_n) = 1 - \alpha + \alpha\cos 2\kappa, \tag{5.20}$$

where

$$\alpha = \frac{1}{2\sqrt{5}}. \tag{5.21}$$

For the special case $\kappa=\pi/2$ shown in Fig. 1 we thus have $K_{P_y}(F_n)\to 1-1/\sqrt{5}=0.552\,786\ldots$ as $n\to\infty$ with $n\equiv 0 \bmod 3$.

Proof: We have already seen that Z_n takes values 0, ± 2. Note that

$$\cos \kappa Z_n(y)=\begin{cases}1, & Z_n(y)=0,\\ \cos 2\kappa, & |Z_n(y)|=2.\end{cases} \tag{5.22}$$

Thus, defining

$$\alpha_n=\frac{1}{(-\omega)^{-n}}\int_0^{(-\omega)^{-n}}\frac{|Z_n(y)|}{2}dy, \tag{5.23}$$

as the proportion of the interval $[0,\omega^{-n}]$ for even n, $[-\omega^{-n},0]$ for odd n, for which $|Z_n(y)|=2$, (1.28) becomes

$$K_{P_y}(F_n)=1-\alpha_n+\alpha_n\cos 2\kappa. \tag{5.24}$$

Now

$$F_n=\frac{\omega^{-n}}{\sqrt{5}}+O(1), \tag{5.25}$$

from which it is straightforward to deduce that

$$\omega^{-n}=F_{n+1}+F_n\omega+O(1). \tag{5.26}$$

We now recognize that $F_{n+1}+F_n\omega$, respectively $-(F_{n+1}+F_n\omega)$, is a discontinuity point generated by the fixed point 0, and thus the interval $[0,\omega^{-n}]$, respectively $[-\omega^{-n},0]$, contains $F_n+O(1)$ intervals of length $\frac{1}{2}$ with $|Z_n|=2$, and thus

$$\alpha_n=\frac{F_n+O(1)}{2\omega^{-n}}\to\frac{1}{2\sqrt{5}}. \tag{5.27}$$

Hence the result. □

2. $n\equiv 1$ mod 3

When $n\equiv 1 \bmod 3$ the discontinuity location sets are given by (5.1) and (5.3). We have

$$\begin{aligned}a_i^1+b_i^1\omega-(a_i^0+b_i^0\omega)&=\lceil i/\omega\rceil+i\omega-(\lceil(i-\tfrac{1}{2})/\omega+\tfrac{1}{2}\rceil-\tfrac{1}{2}+(i-\tfrac{1}{2})\omega)\\&=\omega^{-1}/2+\lceil i/\omega\rceil-\lceil i/\omega-\omega/2\rceil>0\end{aligned} \tag{5.28}$$

and

$$\begin{aligned}a_{i+1}^0+b_{i+1}^0\omega-(a_i^1+b_i^1\omega)&=\lceil(i+\tfrac{1}{2})/\omega+\tfrac{1}{2}\rceil-\tfrac{1}{2}+(i+\tfrac{1}{2})\omega-(\lceil i/\omega\rceil+i\omega)\\&=\lceil i/\omega+\omega/2\rceil-\lceil i/\omega\rceil+\omega^{-1}/2>0,\end{aligned} \tag{5.29}$$

so that the two sets of discontinuities alternate in a strict manner. (Note that the distance between discontinuities may be $\omega^{-1}/2$ or $1+\omega^{-1}/2$. See the second row of Fig. 2.)

When, in addition, n is odd, i.e., $n\equiv 1 \bmod 6$, each discontinuity from $\{\frac{1}{2},-\omega/2\}$ has size $-X_0^0=2$, while each discontinuity from $\{0\}$ has size $-X_0^1=-2$. We further have $Z_n(1)=-1$ in this case, and the first discontinuity after 1 is $\frac{3}{2}+\omega/2$ at which Z_n increases to $+1$. Thus Z_n oscillates between values ± 1 with discontinuity locations as calculated above.

The situation for the subcase in which n is even (i.e., $n \equiv 4 \bmod 6$) follows similarly, or more simply from the fact that $Z_{n+3} = -Z_n$.

It is a simple consequence of the fact that $Z_n = \pm 1$ that the autocorrelation function value $K_{P_y}(F_n)$ in Eq. (1.28) equals $\cos \kappa$.

3. $n \equiv 2 \bmod 3$

When $n \equiv 2 \bmod 3$ the discontinuity location sets are given by (5.1) and (5.4). We have

$$a_i^1 + b_i^1 \omega - (a_i^0 + b_i^0 \omega) = \lceil i/\omega \rceil + i\omega - (\lceil (i - \tfrac{1}{2})/\omega \rceil + (i - \tfrac{1}{2})\omega) = \omega/2 + \lceil i/\omega \rceil - \lceil i/\omega - \omega^{-1}/2 \rceil > 0 \tag{5.30}$$

and

$$a_{i+1}^0 + b_{i+1}^0 \omega - (a_i^1 + b_i^1 \omega) = \lceil (i + \tfrac{1}{2})/\omega \rceil + (i + \tfrac{1}{2})\omega - (\lceil i/\omega \rceil + i\omega) = \lceil i/\omega + \omega^{-1}/2 \rceil - \lceil i/\omega \rceil + \omega/2 > 0. \tag{5.31}$$

(Note now that the distance between discontinuities may be $\omega/2$ or $1 + \omega/2$. See the third row of Fig. 2.)

For both even and odd cases here, as in the previous case, we deduce that the two sets of discontinuities alternate in a strict manner, and, since $Z_{6l+2}(1) = -Z_{6l+5}(1) = 1$, that for all $n \equiv 2 \bmod 3$, Z_n oscillates between values ± 1 with discontinuity locations as calculated above.

Again, we immediately deduce that in this case (1.28) is simply $K_{P_y}(F_n) = \cos \kappa$.

VI. CONCLUSION

We have verified and generalized rigorously the numerical results in Ref. 5 concerning the asymptotic self-similarity of the autocorrelation function in a quasiperiodically forced two-level quantum system. As in studies of the self-similar fluctuations of the localized eigenstates of the Harper equation,[7] the birth of a strange nonchaotic attractor,[9] and of the autocorrelation function of a strange nonchaotic attractor,[4] this self-similarity is explained by means of a functional recurrence, the key to the understanding of which is the dynamics of a simple piecewise-linear map of the interval.[11–13]

To accomplish this task, a description of the piecewise-constant periodic orbits of the additive recurrence (1.1) has been completed. Moreover, a necessary and sufficient criterion for such orbits to be spatially bounded has been derived. As a consequence, provided the locations of its discontinuities are carefully chosen, a piecewise-constant modulation function gives rise to asymptotic self-similarity of the autocorrelation function. It seems likely that, as in the case of the generalized Harper equation with next-nearest-neighbor interactions,[7,13] there will be an underlying strange set on which these orbits lie. If so, an understanding of the form of the autocorrelation function in the presence of a general piecewise-constant modulation function will follow.

Our work has been in the case of golden mean frequency only, but numerical work in Ref. 5 for this problem indicates that the singular continuous spectrum is present for a wider class of irrationals. For the parallel problem of the autocorrelation function in strange nonchaotic attractors, there is evidence in Ref. 14 that, at least for certain quadratic irrational frequencies, the autocorrelation function displays self-similarity of the type studied here. Periodic orbits of a generalization of the functional recurrence (1.1) provide an explanation of this phenomenon in both settings, and will be the subject of a forthcoming paper.

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$\mathcal{N}$-fold supersymmetry in quantum mechanics—analyses of particular models

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We investigate particular models which can be $\mathcal{N}$-fold supersymmetric at specific values of a parameter in the Hamiltonians. The models to be investigated are a periodic potential and a parity-symmetric sextic triple-well potential. Through the quantitative analyses on the nonperturbative contributions to the spectra by the use of the valley method, we show how the characteristic features of $\mathcal{N}$-fold supersymmetry which have been previously reported by the authors can be observed. We also clarify the difference between quasi-exactly solvable and quasi-perturbatively solvable cases in view of the dynamical property, that is, dynamical $\mathcal{N}$-fold supersymmetry breaking. © *2002 American Institute of Physics*.
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I. INTRODUCTION

In our previous paper,[1] we have formulated in formal and abstract ways *$\mathcal{N}$-fold supersymmetry* in quantum mechanics[2–6] and investigated general properties of the models which possess this symmetry. $\mathcal{N}$-fold supersymmetry is characterized by the supercharges which are $\mathcal{N}$-th order polynomials of momentum and similar generalizations of supercharges were also investigated in different contexts.[7–23] We have shown that $\mathcal{N}$-fold supersymmetric models have a lot of significant properties similar to the ordinary supersymmetric ones[24–27] such as degenerate spectral structure between bosonic states and fermionic ones, non-renormalization theorems for the generalized Witten index and for a part of the spectra, and so on. Furthermore, we have introduced the notion of *quasi-solvability* to identify an important aspect of $\mathcal{N}$-fold supersymmetry and have proved the equivalence between $\mathcal{N}$-fold supersymmetry and quasi-solvability. Recently, we have further shown[5] that *Type A* subclass of $\mathcal{N}$-fold supersymmetry, which was first introduced in Ref. 4, is equivalent to the quasi-solvable models constructed by sl(2) generators.[28] Then, it has turned out that the equivalence between them for special cases which had been reported previously in Refs. 2, 17, and 23 holds generically.

Quasi-solvability means the existence of a finite dimensional invariant subspace under the action of the Hamiltonian. As a consequence, a part of the spectra can be solved by a finite dimensional algebraic equation. In the case where the subspace is physical, that is, L^2, these spectra give the *true* eigenvalues of the Hamiltonian. In this case, the system is often called *quasi-exactly solvable*.[28–30] On the other hand, if the subspace is not physical, solvable spectra only give *perturbative* eigenvalues at most and thus we have dubbed this case *quasi-perturbatively solvable*.[4] This distinction is quite important, especially in view of dynamical $\mathcal{N}$-fold supersymmetry breaking; $\mathcal{N}$-fold supersymmetry is broken dynamically if a system is quasi-perturbatively solvable while it is not broken if a system is quasi-exactly solvable.

In this article, we analyze particular models which can be $\mathcal{N}$-fold supersymmetric more

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quantitatively. Previously in Ref. 2, an asymmetric quartic double-well potential was investigated in detail by the valley method.[31–39] It was shown that the system possesses $\mathcal{N}$-fold supersymmetry at specific values of a parameter in the Hamiltonian where the leading Borel singularity of the perturbative corrections for the first $\mathcal{N}$-th energies disappear. This result is a consequence of a general property of $\mathcal{N}$-fold supersymmetry, namely, the non-renormalization theorem. It was also shown that the nonperturbative corrections for the first $\mathcal{N}$-th energies do not vanish even when the system becomes $\mathcal{N}$-fold supersymmetric. This result consistently reflects the fact that, in the case of an asymmetric quartic double-well potential, the solvable subspace is not physical, that is, the system is quasi-perturbatively solvable; nonvanishing nonperturbative effects break $\mathcal{N}$-fold supersymmetry dynamically.

These observations show that combining with the formal discussions in Ref. 1 quantitative analyses may give deeper and complement understanding on dynamical properties of the $\mathcal{N}$-fold supersymmetric models. As in the case of the ordinary supersymmetric models, nonperturbative analyses are quite important in the $\mathcal{N}$-fold supersymmetric case; dynamical $\mathcal{N}$-fold supersymmetry breaking can take place via purely nonperturbative effects, e.g., quantum tunneling. However, nonperturbative analyses are in general quite nontrivial even in the simple one-dimensional quantum mechanics. The valley method is one of the most successful tools for this kind of purpose. So we fully employ it in this work.

The article organizes as follows. In the next section, we summarize the general results and properties of the Type A subclass of $\mathcal{N}$-fold supersymmetry.[1,4–6] In Sec. III, we develop particular cases of the Type A models which are especially relevant for the analyses in this article. Sections IV and V are devoted to valley method analyses on a periodic and a sextic triple-well potential, respectively. We choose potentials to be investigated so that the systems can be Type A $\mathcal{N}$-fold supersymmetric at specific values of a parameter involved in the potentials. The way of the choice enables us to clarify the characteristic features of Type A $\mathcal{N}$-fold supersymmetry. The periodic potential is always quasi-exactly solvable when Type A N-fold supersymmetric while the triple-well potential can be either quasi-exactly or quasi-perturbatively solvable. In both the cases we show that the disappearance of the leading Borel singularity occurs. However, the nonperturbative corrections vanish when and only when the systems are quasi-exactly solvable. Finally, we give summary in the last section.

II. GENERAL PROPERTIES OF TYPE A $\mathcal{N}$-FOLD SUPERSYMMETRY

First of all, we summarize the general results and properties of Type A $\mathcal{N}$-fold supersymmetry. For details, e.g., derivation of the results, see Refs. 1 and 5. To define $\mathcal{N}$-fold supersymmetry, we introduce the following Hamiltonian $\mathbf{H}_{\mathcal{N}}$ and the $\mathcal{N}$-fold supercharges,

$$\mathbf{H}_{\mathcal{N}}=H_{\mathcal{N}}^{-}(p,q)\psi\psi^{\dagger}+H_{\mathcal{N}}^{+}(p,q)\psi^{\dagger}\psi, \tag{2.1}$$

$$Q_{\mathcal{N}}=P_{\mathcal{N}}^{\dagger}(p,q)\psi, \quad Q_{\mathcal{N}}^{\dagger}=P_{\mathcal{N}}(p,q)\psi^{\dagger}. \tag{2.2}$$

Here ψ and $\psi^{\dagger}$ are fermionic coordinates which satisfy

$$\{\psi,\psi\}=\{\psi^{\dagger},\psi^{\dagger}\}=0, \quad \{\psi,\psi^{\dagger}\}=1, \tag{2.3}$$

and are usually represented as the following 2×2 matrix form:

$$\psi=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}, \quad \psi^{\dagger}=\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}. \tag{2.4}$$

The component of the $\mathcal{N}$-fold supercharges $P_{\mathcal{N}}$ is given by an $\mathcal{N}$-th order polynomial of $p=-id/dq$ and thus expressed as

$$P_{\mathcal{N}}=p^{\mathcal{N}}+w_{\mathcal{N}-1}(q)p^{\mathcal{N}-1}+\cdots+w_1(q)p+w_0(q), \tag{2.5}$$

without any loss of generality. Then, the system is said to be $\mathcal{N}$-fold supersymmetric if the Hamiltonian $\mathbf{H}_{\mathcal{N}}$ commutes with the $\mathcal{N}$-fold supercharges $Q_{\mathcal{N}}$ and $Q_{\mathcal{N}}^{\dagger}$:

$$[Q_{\mathcal{N}},\mathbf{H}_{\mathcal{N}}]=[Q_{\mathcal{N}}^{\dagger},\mathbf{H}_{\mathcal{N}}]=0. \tag{2.6}$$

The Type A $\mathcal{N}$-fold supersymmetry is characterized by a particular class of the $\mathcal{N}$-fold supercharges which can be expressed as the following form:[40]

$$\begin{aligned} P_{\mathcal{N}}&=\left(D+i\frac{\mathcal{N}-1}{2}E(q)\right)\left(D+i\frac{\mathcal{N}-3}{2}E(q)\right)\cdots\left(D-i\frac{\mathcal{N}-1}{2}E(q)\right)\\ &\equiv\prod_{k=-(\mathcal{N}-1)/2}^{(\mathcal{N}-1)/2}(D+ikE(q)),\quad D=p-iW(q). \end{aligned} \tag{2.7}$$

If we restrict $H_{\mathcal{N}}^{\pm}$ to be the following Schrödinger type,

$$H_{\mathcal{N}}^{\pm}=\tfrac{1}{2}p^2+V_{\mathcal{N}}^{\pm}(q), \tag{2.8}$$

we can show[5] that necessary and sufficient conditions of the Hamiltonian (2.1) with (2.8) to be Type A $\mathcal{N}$-fold supersymmetric, that is, to satisfy the relation (2.6), are as the following:

$$V_{\mathcal{N}}^{\pm}(q)=\frac{1}{2}W(q)^2+\frac{\mathcal{N}^2-1}{24}(E(q)^2-2E'(q))\pm\frac{\mathcal{N}}{2}W'(q), \tag{2.9a}$$

$$\left(\frac{d}{dq}-E(q)\right)\frac{d}{dq}\left(\frac{d}{dq}+E(q)\right)W(q)=0\quad(\mathcal{N}\geqslant 2), \tag{2.9b}$$

$$\left(\frac{d}{dq}-2E(q)\right)\left(\frac{d}{dq}-E(q)\right)\frac{d}{dq}\left(\frac{d}{dq}+E(q)\right)E(q)=0\quad(\mathcal{N}\geqslant 3). \tag{2.9c}$$

A. The solvable subspaces

Owing to the relation Eq. (2.6), the $\mathcal{N}$-dimensional vector spaces defined by

$$\mathcal{V}_{\mathcal{N}}^{-}=\ker P_{\mathcal{N}},\quad \mathcal{V}_{\mathcal{N}}^{+}=\ker P_{\mathcal{N}}^{\dagger} \tag{2.10}$$

are invariant under the action of $H_{\mathcal{N}}^{-}$ and $H_{\mathcal{N}}^{+}$, respectively. We can therefore define the matrices $\mathbf{S}^{\pm}$ as follows:

$$H_{\mathcal{N}}^{\pm}\phi_n^{\pm}=\sum_{m=1}^{\mathcal{N}}\mathbf{S}_{n,m}^{\pm}\phi_m^{\pm}, \tag{2.11}$$

where $\phi^{\pm}$ are bases of the $\mathcal{V}_{\mathcal{N}}^{\pm}$, respectively. It can be proved[1] for general $\mathcal{N}$-fold supersymmetry that the *mother Hamiltonian* $\mathcal{H}_{\mathcal{N}}$ defined by the anticommutator of the supercharges can be expressed as

$$\mathcal{H}_{\mathcal{N}}\equiv\frac{1}{2}\{Q_{\mathcal{N}}^{\dagger},Q_{\mathcal{N}}\}=\frac{1}{2}\begin{pmatrix}\det\mathbf{M}_{\mathcal{N}}^{+}(H_{\mathcal{N}}^{+})+p^{+}P_{\mathcal{N}}^{\dagger} & 0\\ 0 & \det\mathbf{M}_{\mathcal{N}}^{-}(H_{\mathcal{N}}^{-})+p^{-\dagger}P_{\mathcal{N}}\end{pmatrix}, \tag{2.12}$$

where

$$\mathbf{M}_{\mathcal{N}}^{\pm}(\lambda)=2(\lambda\mathbf{I}-\mathbf{S}^{\pm}), \tag{2.13}$$

and $p^{\pm}$ are at most $(\mathcal{N}-1)$-th order differential operators. From the definition of the mother Hamiltonian (2.12), the elements of the subspaces $\mathcal{V}_{\mathcal{N}}^{\pm}$ are also characterized as the zero-modes of the mother Hamiltonian.

In the case of Type A, we can obtain analytic expressions for these bases:

$$\phi_n^{\pm}(q)=h(q)^{n-1}h'(q)^{-(\mathcal{N}-1)/2}U(q)^{\pm 1}, \quad (n=1,\ldots,\mathcal{N}), \tag{2.14}$$

where[41]

$$U(q)=e^{\int dq W(q)}, \tag{2.15}$$

and $h(q)$ is a solution of the following linear differential equation:

$$h''(q)-E(q)h'(q)=0, \tag{2.16}$$

and thus generically given by

$$h(q)=c_1\int dq e^{\int dq E(q)}+c_2. \tag{2.17}$$

The appearance of the two arbitrary constants $c_{1,2}$ in Eq. (2.17) reflects the fact that the spaces $\mathcal{V}_{\mathcal{N}}^{\pm}$ spanned by the bases Eq. (2.14) are invariant under any linear transformations on $h(q)$. With the aid of these bases Eq. (2.14), the components of the matrices $\mathbf{S}_{n,m}^{\pm}$ defined by Eq. (2.11) can be determined (for each fixed $n=1,\ldots,\mathcal{N}$) by the following recurrence relations:

$$\mathbf{S}_{n,\mathcal{N}-m}^{-}=\frac{P_{\mathcal{N}-m-1}(H_{\mathcal{N}}^{-}\phi_n^{-}-\Sigma_{k=\mathcal{N}-m+1}^{\mathcal{N}}\mathbf{S}_{n,k}^{-}\phi_k^{-})}{P_{\mathcal{N}-m-1}\phi_{\mathcal{N}-m}^{-}}, \tag{2.18a}$$

$$\mathbf{S}_{n,\mathcal{N}-m}^{+}=\frac{P_{\mathcal{N}-m-1}^{\dagger}(H_{\mathcal{N}}^{+}\phi_n^{+}-\Sigma_{k=\mathcal{N}-m+1}^{\mathcal{N}}\mathbf{S}_{n,k}^{+}\phi_k^{+})}{P_{\mathcal{N}-m-1}^{\dagger}\phi_{\mathcal{N}-n}^{+}}, \tag{2.18b}$$

for $m=1,\ldots,\mathcal{N}-1$ with the initial conditions

$$\mathbf{S}_{n,\mathcal{N}}^{-}=\frac{P_{\mathcal{N}-1}H_{\mathcal{N}}^{-}\phi_n^{-}}{P_{\mathcal{N}-1}\phi_{\mathcal{N}}^{-}}, \quad \mathbf{S}_{n,\mathcal{N}}^{+}=\frac{P_{\mathcal{N}-1}^{\dagger}H_{\mathcal{N}}^{+}\phi_n^{+}}{P_{\mathcal{N}-1}^{\dagger}\phi_{\mathcal{N}}^{+}}. \tag{2.19}$$

From Eq. (2.11), the spectra $E_n^{\pm}$ of the Hamiltonians $H_{\mathcal{N}}^{\pm}$ in the subspaces $\mathcal{V}_{\mathcal{N}}^{\pm}$ are given by

$$\det \mathbf{M}_{\mathcal{N}}^{\pm}(E_n^{\pm})=0. \tag{2.20}$$

If $\phi_n(q)$'s are normalizable, linear combinations of them which diagonalize the matrix $\mathbf{S}$ are the *true* eigenstates of $H_{\mathcal{N}}$. In this case, the system is often called *quasi-exactly solvable*.[28–30] On the other hand, if $\phi_n(q)$'s are not normalizable, they have, at most, restricted meanings in the perturbation theory. In this case, the spectra determined by Eq. (2.20) only give perturbatively correct ones. For this reason, we dub the case *quasi-perturbatively solvable*.[1] Then, $\mathcal{N}$-fold supersymmetry of the total system $\mathbf{H}_{\mathcal{N}}$ is dynamically broken when *both* of the systems $H_{\mathcal{N}}^{\pm}$ are quasi-perturbatively solvable. Otherwise, that is, at least one of the systems $H_{\mathcal{N}}^{\pm}$ is quasi-exactly solvable, the elements of the corresponding solvable subspace give the $\mathcal{N}$-fold supersymmetric physical states and therefore $\mathcal{N}$-fold supersymmetry is preserved.

B. A non-renormalization theorem

A kind of the non-renormalization theorem holds for the Type A models. We first assume that we can set $W(0)=0$ by the redefinition of the origin of the coordinate q and the energy. To define a perturbation theory, we then introduce a coupling constant g as

$$W(q)=\frac{1}{g}w(gq),\quad E(q)=ge(gq), \tag{2.21}$$

so that, in the leading order of g, the potential $V_{\mathcal{N}}^{\pm}$ become harmonic with frequency $|w'(0)|$,

$$V_{\mathcal{N}}^{\pm}(q)=\tfrac{1}{2}w'(0)^2q^2+O(g). \tag{2.22}$$

From Eq. (2.14) with Eqs. (2.15), (2.17) and (2.21), we can easily see that the $\phi_n^{\pm}$ behave as

$$\phi_n^{\pm}(q)=U(0)^{\pm 1}(q^{n-1}+O(g))e^{\pm w'(0)q^2/2}. \tag{2.23}$$

Here, we choose the two arbitrary constants $c_{1,2}$ in Eq. (2.17) as $h(0)=0$, $h'(0)=1$. Thus, as far as $w'(0)>0(<0)$, all the $\phi_n^-(\phi_n^+)$ remain normalizable in *any finite* order of g even if $\phi_n^-(\phi_n^+)$ themselves are *not* normalizable. So, they stay the $\mathcal{N}$-fold supersymmetric vacua in any order of the perturbation theory and therefore any perturbative corrections do not break $\mathcal{N}$-fold supersymmetry.

III. SPECIAL CASES OF TYPE A $\mathcal{N}$-FOLD SUPERSYMMETRY

In this section, we illustrate some special cases of the Type A $\mathcal{N}$-fold supersymmetry by using the general results obtained in the previous section.

A. Exponential type potentials

At first, we will consider the case where $E(q)=\lambda$ (nonzero constant). This is a trivial solution of Eq. (2.9c). From Eq. (2.9b) we yield

$$W(q)=C_1e^{\lambda q}+C_2e^{-\lambda q}+C_3. \tag{3.1}$$

In this case, the Hamiltonians and the supercharge are given by

$$H_{\pm\mathcal{N}}=\frac{1}{2}p^2+\frac{1}{2}W(q)^2+\frac{\mathcal{N}^2-1}{24}\lambda^2\pm\frac{\mathcal{N}}{2}W'(q),\quad P_{\mathcal{N}}=\prod_{k=-(\mathcal{N}-1)/2}^{(\mathcal{N}-1)/2}(D+ik\lambda). \tag{3.2}$$

The function $h(q)$ can be chosen as

$$h(q)=\frac{e^{\lambda q}}{\lambda}. \tag{3.3}$$

Bases of the solvable subspaces $\mathcal{V}_{\mathcal{N}}^{\pm}$ are calculated as

$$\phi_n^{\pm}(q)=\frac{1}{\lambda^{n-1}}\exp\left[-\frac{1}{2}(\mathcal{N}-2n+1)\lambda q\pm C_3q\pm\frac{C_1}{\lambda}e^{\lambda q}\mp\frac{C_2}{\lambda}e^{-\lambda q}\right]. \tag{3.4}$$

Thus, normalizability of $\phi_n^{\pm}$ depends on the values of the constants C_i and λ. For example, provided that all the constants C_1, C_2 and λ are nonzero real numbers, either ϕ^+ or ϕ^- is normalizable when $C_1C_2<0$ while both of $\phi^{\pm}$ are not when $C_1C_2>0$. The correspondence between quasi-exact solvability and $\mathcal{N}$-fold supersymmetry in the case of the exponential type potentials Eq. (3.1) was recently discussed in Ref. 17.

The nonzero matrix elements of $\mathbf{S}^{\pm}$ can be calculated as follows. The direct action of the Hamiltonians Eq. (2.8), with the Type A potentials Eq. (2.9a), on the bases Eq. (2.14) reads

$$H_{\mathcal{N}}^{\pm}\phi_n^{\pm}=-\frac{1}{2}(n-1)(n-2)h'^2\phi_{n-2}^{\pm}+\frac{1}{2}(n-1)[(\mathcal{N}-2)h''\mp 2Wh']\phi_{n-1}^{\pm}$$
$$-\frac{\mathcal{N}-1}{12}[(\mathcal{N}-2)(E'+E^2)\mp 6(W'+EW)]\phi_n^{\pm}. \tag{3.5}$$

From Eqs. (3.1) and (3.3), the following relations hold:

$$h'^2=\lambda^2h^2, \tag{3.6a}$$

$$h''=\lambda^2h, \tag{3.6b}$$

$$E'+E^2=\lambda^2, \tag{3.6c}$$

$$Wh'=C_1\lambda^2h^2+C_3\lambda h+C_2, \tag{3.6d}$$

$$W'+EW=2C_1\lambda^2h+C_3\lambda. \tag{3.6e}$$

Substituting the above relations (3.6) for Eq. (3.5), we obtain

$$\mathbf{S}_{n,n-1}^{\pm}=\mp(n-1)C_2, \tag{3.7a}$$

$$\mathbf{S}_{n,n}^{\pm}=-\tfrac{1}{12}[(\mathcal{N}-1)(\mathcal{N}-2)+6(n-1)(n-\mathcal{N})]\lambda^2\pm\tfrac{1}{2}(\mathcal{N}-2n+1)C_3\lambda, \tag{3.7b}$$

$$\mathbf{S}_{n,n+1}^{\pm}=\mp(n-\mathcal{N})C_1\lambda^2. \tag{3.7c}$$

All the other matrix elements are zero.

The special choices $\lambda=ig$, $C_1=1/2ig$, $C_2=-1/2ig$ and $C_3=0$ lead to

$$W(q)=\frac{1}{g}\sin(gq), \quad E(q)=ig, \tag{3.8}$$

and correspond to the periodic potential in Ref. 3. We note that Eq. (3.8) is incorporated with the perturbation theory defined by Eq. (2.21). We will later carry out nonperturbative analysis of this special case in Sec. IV.

B. Sextic oscillator potentials

Next, we will consider the case where

$$E(q)=\frac{1}{q-q_0}. \tag{3.9}$$

This is also a solution of Eq. (2.9c). This special case corresponds to (one of) the cubic type in Ref. 4. The Hamiltonians and the supercharge are given by

$$H_{\mathcal{N}}^{\pm}=\frac{1}{2}p^2+\frac{1}{2}W(q)^2+\frac{\mathcal{N}^2-1}{8(q-q_0)^2}\pm\frac{\mathcal{N}}{2}W'(q), \tag{3.10}$$

$$P_{\mathcal{N}}=\prod_{k=-(\mathcal{N}-1)/2}^{(\mathcal{N}-1)/2}\left(D+i\frac{k}{q-q_0}\right), \tag{3.11}$$

with

$$W(q)=C_1(q-q_0)^3+C_2(q-q_0)+\frac{C_3}{q-q_0}. \tag{3.12}$$

We note that the Hamiltonians (3.10) are parity symmetric. The function $h(q)$ can be chosen as

$$h(q)=\frac{(q-q_0)^2}{2}. \tag{3.13}$$

Bases of the solvable subspaces $\mathcal{V}_{\mathcal{N}}^{\pm}$ are calculated as

$$\phi_n^{\pm}(q)=\frac{1}{2^{n-1}}(q-q_0)^{2n-\mathcal{N}/2-3/2\pm C_3}\exp\left[\pm\frac{C_1}{4}(q-q_0)^4\pm\frac{C_2}{2}(q-q_0)^2\right]. \tag{3.14}$$

Thus, either ϕ^+ or ϕ^- is normalizable unless $C_1=C_2=0$ and the corresponding system $H_{\mathcal{N}}^+$ or $H_{\mathcal{N}}^-$ is quasi-exactly solvable. The correspondence between quasi-exact solvability and $\mathcal{N}$-fold supersymmetry in the case of the sextic potential Eq. (3.10) was recently pointed out in Ref. 23.

The nonzero matrix elements of $\mathbf{S}^{\pm}$ can be obtained by Eq. (3.5). From Eqs. (3.9), (3.12) and (3.13), the following relations hold:

$$h'^2=2h, \tag{3.15a}$$

$$h''=1, \tag{3.15b}$$

$$E'+E^2=0, \tag{3.15c}$$

$$Wh'=4C_1h^2+2C_2h+C_3, \tag{3.15d}$$

$$W'+EW=8C_1h+2C_2. \tag{3.15e}$$

Substituting the above relations (3.15) for Eq. (3.5) we obtain

$$\mathbf{S}_{n,n-1}^{\pm}=\tfrac{1}{2}(n-1)[(\mathcal{N}-2n+2)\mp 2C_3], \tag{3.16a}$$

$$\mathbf{S}_{n,n}^{\pm}=\pm(\mathcal{N}-2n+1)C_2, \tag{3.16b}$$

$$\mathbf{S}_{n,n+1}^{\pm}=\mp 4(n-\mathcal{N})C_1. \tag{3.16c}$$

All the other matrix elements are zero.

If we rewrite Eq. (3.12) as

$$W(q)=w(q)+\frac{C_3}{q-q_0},\quad w(q)=C_1(q-q_0)^3+C_2(q-q_0), \tag{3.17}$$

the potential parts $V_{\mathcal{N}}^{\pm}(q)$ of the Hamiltonians (3.10) are, in terms of $w(q)$,

$$V_{\mathcal{N}}^{\pm}(q)=\frac{1}{2}w(q)^2+\frac{(2C_3\mp\mathcal{N}-1)(2C_3\mp\mathcal{N}+1)}{8(q-q_0)^2}\pm\left(\frac{\mathcal{N}}{2}\pm\frac{C_3}{3}\right)w'(q)+\frac{2}{3}C_2C_3. \tag{3.18}$$

We note that in the cases when $C_3=(\mathcal{N}\pm 1)/2$ and $-(\mathcal{N}\pm 1)/2$, one of the potential-pair $V_{\mathcal{N}}^{\pm}(q)$ becomes a genuine sixth order polynomial:

$$V_{\mathcal{N}}^{+}(q)=\frac{1}{2}w(q)^2+\frac{4\mathcal{N}\pm 1}{6}w'(q)\quad\left(C_3=\frac{\mathcal{N}\pm 1}{2}\right), \tag{3.19a}$$

$$V_{\mathcal{N}}^{-}(q)=\frac{1}{2}w(q)^2-\frac{4\mathcal{N}\pm 1}{6}w'(q) \quad \left(C_3=-\frac{\mathcal{N}\pm 1}{2}\right), \tag{3.19b}$$

where irrelevant constant terms are omitted. Conversely, a sextic anharmonic oscillator or a triple-well potential (with parity symmetry) can be one of the Type A $\mathcal{N}$-fold supersymmetric pair whenever the potential can be put in one of the forms of Eq. (3.19). When $C_3=(\mathcal{N}\pm 1)/2$, the bases Eq. (3.14) for $V_{\mathcal{N}}^{+}(q)$ read

$$\phi_n^{+}(q)=\frac{1}{2^{n-1}}(q-q_0)^{2n-3/2\pm 1/2}\exp\left[\frac{C_1}{4}(q-q_0)^4+\frac{C_2}{2}(q-q_0)^2\right]\left(C_3=\frac{\mathcal{N}\pm 1}{2}\right). \tag{3.20}$$

It is worth noting that the solvable subspace $\mathcal{V}_{\mathcal{N}}^{+}$ consists of the states with definite parity [odd for $C_3=(\mathcal{N}+1)/2$ and even for $C_3=(\mathcal{N}-1)/2$]. We will later see close relation between this fact and pattern of the nonperturbative spectral shifts. When $C_3=-(\mathcal{N}\pm 1)/2$, the bases Eq. (3.14) for $V_{\mathcal{N}}^{-}(q)$ are similarly

$$\phi_n^{-}(q)=\frac{1}{2^{n-1}}(q-q_0)^{2n-3/2\pm 1/2}\exp\left[-\frac{C_1}{4}(q-q_0)^4-\frac{C_2}{2}(q-q_0)^2\right]\left(C_3=-\frac{\mathcal{N}\pm 1}{2}\right). \tag{3.21}$$

Again, the subspace $\mathcal{V}_{\mathcal{N}}^{-}$ contains only odd-parity states for $C_3=-(\mathcal{N}+1)/2$ and only even-parity states for $C_3=-(\mathcal{N}-1)/2$.

C. Quartic oscillator potentials

In the next, we will consider the case where $E(q)=0$. This is also a trivial solution of Eq. (2.9c). From Eq. (2.9b) we yield

$$W(q)=C_1q^2+C_2q+C_3. \tag{3.22}$$

In this case, the Hamiltonians and the supercharge are given by

$$H_{\pm\mathcal{N}}=\frac{1}{2}p^2+\frac{1}{2}W(q)^2\pm\frac{\mathcal{N}}{2}W'(q), \quad P_{\mathcal{N}}=D^{\mathcal{N}}. \tag{3.23}$$

The function $h(q)$ reads

$$h(q)=q. \tag{3.24}$$

Bases of the solvable subspaces $\mathcal{V}_{\mathcal{N}}^{\pm}$ are calculated as

$$\phi_n^{\pm}(q)=q^{n-1}\exp\left[\pm\frac{C_1}{3}q^3\pm\frac{C_2}{2}q^2\pm C_3q\right]. \tag{3.25}$$

Thus, both of $\phi^{\pm}$ are not normalizable and therefore the system is quasi-perturbatively solvable as far as C_1 is a nonzero real number. The relation between quasi-perturbative solvability and $\mathcal{N}$-fold supersymmetry in a special case of the models was pointed out in Ref. 2.

The nonzero matrix elements of $\mathbf{S}^{\pm}$ can be obtained by Eq. (3.5). From Eqs. (3.22) and (3.24), the following relations hold:

$$h'^2=1, \tag{3.26a}$$

$$Wh'=C_1h^2+C_2h+C_3, \tag{3.26b}$$

$$W'+EW=2C_1h+C_2. \tag{3.26c}$$

Substituting the above relations (3.26) for Eq. (3.5) we obtain

$$\mathbf{S}^{\pm}_{n,n-2} = -\tfrac{1}{2}(n-1)(n-2), \tag{3.27a}$$

$$\mathbf{S}^{\pm}_{n,n-1} = \mp(n-1)C_3, \tag{3.27b}$$

$$\mathbf{S}^{\pm}_{n,n} = \pm\tfrac{1}{2}(\mathcal{N}-2n+1)C_2, \tag{3.27c}$$

$$\mathbf{S}^{\pm}_{n,n+1} = \mp(n-\mathcal{N})C_1. \tag{3.27d}$$

All the other matrix elements are zero.

IV. ANALYSIS OF A PERIODIC POTENTIAL

A. The valley method

Before proceeding to show the results of the analyses, we briefly review the valley method[31–39] which is employed in this research. For more details about the method, see Ref. 2.

The main problem in quantum theories concerns with the evaluation of the Euclidean partition function:

$$Z = \mathcal{J}\int \mathcal{D}q\, e^{-S[q]}. \tag{4.1}$$

Since the evaluation cannot be done exactly in general, one must find out a proper method which enables one to get a good estimation of the quantity. The semi-classical approximation is known to be one of the most established methods. Especially, the uses of instantons have been succeeded in analyzing nonperturbative aspects of various quantum systems which have degenerate vacua.[42] However, validity of the approximation comes into question when the fluctuations around the classical configuration contain a negative mode. Let us consider an asymmetric double-well potential as a typical example. For this potential, there is a so-called bounce solution as the classical solution which has a negative mode in the fluctuations. The negative mode contributes nonzero imaginary part of the spectra in the approximation, showing instability of the system. Since the spectra of the model must be real, the instability in the approximation must be *fake*.

The appearance of a negative mode indicates that the classical action does not give the minimum but rather a saddle point in the functional space. In this case, one may expect that the quantity (4.1) is dominated by the configurations along the negative mode, which may intuitively constitute a *valley* in the functional space. The valley method is a natural realization of this consideration.

At first, we give a geometrical definition of the valley in the functional space $q(\tau)$:[34]

$$\frac{\delta}{\delta q(\tau)}\left[\frac{1}{2}\int d\tau'\left(\frac{\delta S[q]}{\delta q(\tau')}\right)^2 - \lambda S[q]\right] = 0. \tag{4.2}$$

The above definition (4.2) can be interpreted as follows; for each fixed "height" $S[q]$, the valley is defined at the point where the norm of the gradient vector becomes extremal. Introducing an auxiliary field $F(q)$, we can make the valley equation (4.2) a more perspicuous form:

$$\frac{\delta S[q]}{\delta q(\tau)} = F(\tau), \tag{4.3a}$$

$$\int d\tau'\, D(\tau,\tau')F(\tau') = \lambda F(\tau), \tag{4.3b}$$

where the operator D is defined as

$$D(\tau,\tau')=\frac{\delta^2 S[q]}{\delta q(\tau)\,\delta q(\tau')}. \tag{4.4}$$

It is now evident that any solution of the equation of motion is also a solution of the valley equation (4.3) with $F(\tau)\equiv 0$.

Next, we separate the integration along the valley line from the whole functional integration. We parametrize the valley line by a parameter R and denote the valley configuration by $q_R(\tau)$. We then define Faddeev–Popov determinant $\Delta[\varphi_R]$ by the following:

$$\int dR\ \delta\left(\int d\tau\,\varphi_R(\tau)G_R(\tau)\right)\Delta[\varphi_R]=1, \tag{4.5}$$

where $\varphi_R(\tau)=q(\tau)-q_R(\tau)$ is the fluctuation over which we will be doing Gaussian integrations, and $G_R(\tau)$ is the normalized gradient vector,

$$G_R(\tau)=\frac{\delta S[q_R]}{\delta q_R(\tau)}\Bigg/\sqrt{\int d\tau'\left(\frac{\delta S[q_R]}{\delta q_R(\tau')}\right)^2}. \tag{4.6}$$

Inserting Eq. (4.5) into the functional integral (4.1), expanding the action $S[q]$ around $\varphi_R(\tau)=0$ and integrating up to the second order term in $\varphi_R(\tau)$, we finally obtain the one-loop order result:

$$Z=\mathcal{J}\int dR\int \mathcal{D}q\ \delta\left(\int d\tau\,\varphi_R(\tau)G_R(\tau)\right)\Delta[\varphi_R]e^{-S[q]}\simeq\mathcal{J}\int\frac{dR}{\sqrt{2\pi\det' D_R}}\Delta[\varphi_R]e^{-S[q_R]}, \tag{4.7}$$

where the Jacobian $\Delta[\varphi_R]$ is given by, in this approximation,

$$\Delta[\varphi_R]=\frac{dS[q_R]}{dR}\Bigg/\sqrt{\int d\tau'\left(\frac{\delta S[q_R]}{\delta q_R(\tau')}\right)^2}. \tag{4.8}$$

In the above, $\det'$ denotes the determinant in the functional subspace which is perpendicular to the gradient vector $G_R(\tau)$. The valley equation (4.3) ensure that the subspace does not contain the eigenvector of the eigenvalue λ. Therefore, we can safely perform the Gaussian integrations even when we encounter a nonpositive mode. The extension to the multi-dimensional valley, which will be needed when there are multiple nonpositive eigenvalues, is straightforward.

In this article, we only deal with one-dimensional quantum mechanics where the Euclidean action is given by

$$S[q]=\int d\tau\left[\frac{1}{2}\left(\frac{dq}{d\tau}\right)^2+V(q)\right]. \tag{4.9}$$

In this case, the valley equations (4.3) are explicitly written as

$$-\frac{d^2q(\tau)}{d\tau^2}+V'(q)=F(\tau), \tag{4.10a}$$

$$\left[-\frac{d^2}{d\tau^2}+V''(q)\right]F(\tau)=\lambda F(\tau). \tag{4.10b}$$

B. Valley-instantons

At first, we will analyze a periodic potential. The form of the potential to be analyzed is the following:

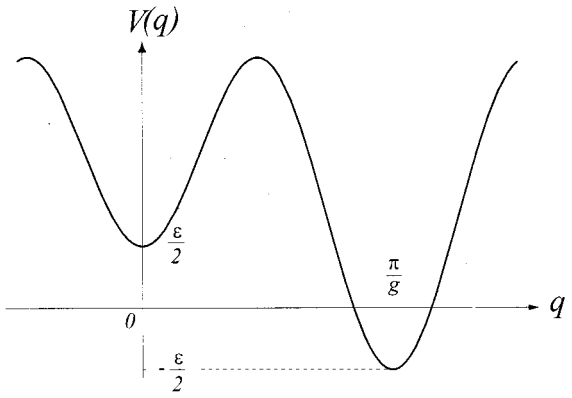

FIG. 1. The form of the periodic potential investigated in this section.

$$V(q;\epsilon)=\frac{1}{2g^2}\sin^2(gq)+\frac{\epsilon}{2}\cos(gq). \tag{4.11}$$

This is a periodic potential with periodicity $2\pi/g$ (unless $\epsilon=0$) and has two local minima at $q=2k\pi/g$ and $q=(2k+1)/g$ $(k=0,\pm1,\pm2,\ldots)$ in one period (see Fig. 1).

Comparing this potential with Eqs. (3.2) and (3.8), we find that the system has Type A $\mathcal{N}$-fold supersymmetry when

$$\epsilon=\pm\mathcal{N}. \tag{4.12}$$

Since the system is defined on a bounded region, all the bases of the solvable space $\mathcal{V}_{\mathcal{N}}^{\pm}$ are normalizable. Thus, certain linear combinations of them serve as physical eigenstates of the Hamiltonian and $\mathcal{N}$-fold supersymmetry is not broken dynamically. Therefore, we may expect that the nonperturbative corrections for certain $\mathcal{N}$ physical states will vanish and the perturbation series for the corresponding spectra will be convergent when $\epsilon=\pm\mathcal{N}$.

We note that the potential (4.11) has the following symmetry:

$$V\left(q-\frac{\pi}{g};\epsilon\right)=V(q;-\epsilon). \tag{4.13}$$

Therefore, we can restrict ϵ to be positive without any loss of generality.

In the case of $\epsilon=0$, there are (anti-)instanton solutions of the equation of motion which describe the quantum tunneling between the neighboring vacua. The instanton and anti-instanton which connect the two vacua at $q=k\pi/g$ and $q=(k+1)\pi/g$ are given by

$$q_0^{(I)}(\tau-\tau_0)=\frac{k\pi}{g}+\frac{1}{g}\arccos(-\tanh(\tau-\tau_0)), \tag{4.14a}$$

$$q_0^{\overline{(I)}}(\tau-\tau_0)=\frac{k\pi}{g}+\frac{1}{g}\arccos(\tanh(\tau-\tau_0)). \tag{4.14b}$$

When $\epsilon\neq0$, the classical solutions drastically change into the so-called bounce solutions which cause fake instability. On the other hand, the solutions of the valley equation (4.10) contain a continuously deformed (anti-)instanton which connects the two nondegenerate local minima and is called (*anti-*)*valley-instanton*.[2]

The solutions of the valley equation (4.10) also contain a family of the configurations, which tends to the trivial vacuum configuration in the one limit and tends to well-separated valley-instanton and anti-valley-instanton configuration in the other limit. The latter configuration is called $I\bar{I}$-valley. The bounce solution is also realized as an intermediate configuration of this family, which is consistent with the fact that the solution of the equation of motion is also a solution of the valley equations. For details, see the numerical result in Ref. 2. For the $I\bar{I}$-valley configuration, it turns out that $|\lambda| \ll 1$ and thus the asymptotic form of the configuration can be obtained by solving the valley equation (4.10) with perturbative expansion in λ:

$$q(\tau) = q_0(\tau) + \lambda q_1(\tau) + \cdots, \quad F(\tau) = \lambda F_1(\tau) + \lambda^2 F_2(\tau) + \cdots. \tag{4.15}$$

Indeed, if we denote the distance between the valley-instanton and the anti-valley-instanton as R, the lambda is order $\lambda \sim O(e^{-R})$ quantity. The action of the $I\bar{I}$-valley with the boundary condition $q(\pm T/2) = 2k\pi/g$ $(T \gg 1)$ is finally obtained as

$$S^{(I\bar{I})}(\tilde{R}) = S^{(\bar{I}I)}(\tilde{R}) = 2S_0^{(I)} - \frac{\epsilon}{2}\tilde{R} + \frac{\epsilon}{2}(T - \tilde{R}) - \frac{8}{g^2}e^{-\tilde{R}} + O(e^{-2\tilde{R}}), \tag{4.16}$$

while the one with $q(\pm T/2) = (2k+1)\pi/g$ $(T \gg 1)$ is

$$S^{(I\bar{I})}(R) = S^{(\bar{I}I)}(R) = 2S_0^{(I)} + \frac{\epsilon}{2}R - \frac{\epsilon}{2}(T - R) - \frac{8}{g^2}e^{-R} + O(e^{-2R}), \tag{4.17}$$

where $S_0^{(I)}$ denotes the Euclidean action of one (anti-)instanton Eq. (4.14) and amounts to

$$S_0^{(I)} = \frac{2}{g^2}. \tag{4.18}$$

In Eqs. (4.16) and (4.17), the fourth term can be interpreted as the interaction term between the valley-instanton and the anti-valley-instanton. Therefore, the minus sign indicates that the interaction is attractive.

The other type of the solutions emerges in this case, which is asymptotically composed of two successive valley-instantons or two successive anti-valley-instantons. We call them II-valley and $\overline{II}$-valley, respectively. These configurations do not appear in the case of double-well potentials since they connect every other vacuum. The Euclidean action of them with large separation R can be also calculated in the same way as

$$S^{(II)}(\tilde{R}) = S^{(\overline{II})}(\tilde{R}) = 2S_0^{(I)} - \frac{\epsilon}{2}\tilde{R} + \frac{\epsilon}{2}(T - \tilde{R}) + \frac{8}{g^2}e^{-\tilde{R}} + O(e^{-2\tilde{R}}), \tag{4.19}$$

for the configuration with $q(-T/2) = 2k\pi/g$ and $q(T/2) = (2k \pm 2)\pi/g$ $(T \gg 1)$, and

$$S^{(II)}(R) = S^{(\overline{II})}(R) = 2S_0^{(I)} + \frac{\epsilon}{2}R - \frac{\epsilon}{2}(T - R) + \frac{8}{g^2}e^{-R} + O(e^{-2R}), \tag{4.20}$$

for the one with $q(-T/2) = (2k+1)\pi/g$ and $q(T/2) = (2k+1 \pm 2)\pi/g$ $(T \gg 1)$. Note that the sign of the fourth term is plus and thus the interaction between the (anti-)valley-instantons in this case is repulsive.

C. Analysis of two-valley sector

From the results on the $I\bar{I}$-valley, the contribution of the $I\bar{I}$-valley to the partition function can be written as the following form:

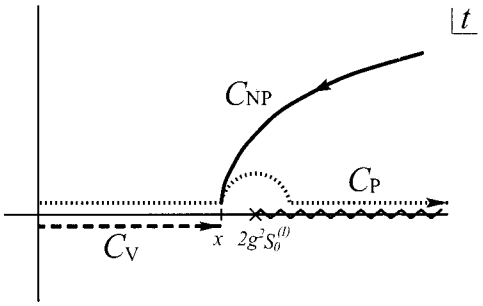

FIG. 2. Deformation of the contour C_V to the sum of C_P and C_{NP}.

$$\bar{Z^{(II)}}=\frac{4e^{-T/2}}{\pi g^2}\int_0^T dR\,(T-R)e^{-\bar{S^{II}}(R)}=\frac{4e^{-T/2}}{\pi g^2}\int_{C_V} dt\,\mathcal{F}(t)e^{-t/g^2}, \tag{4.21}$$

where we have changed the integration variable R to $t=g^2\bar{S^{II}}(R)$ in the second line. The integration contour C_V is $[0,2g^2S_0^{(I)})$ and the integrand $\mathcal{F}(t)$ has a singularity at $t=2g^2S_0^{(I)}$. The integral Eq. (4.21) contains both the perturbative contribution at $t\sim 0$ and the nonperturbative one at $t\sim 2g^2S_0^{(I)}$. To separate the perturbative and the nonperturbative contribution, we deform the contour C_V to the sum of C_P and C_{NP}:

$$\bar{Z^{(II)}}=\frac{4e^{-T/2}}{\pi g^2}\int_{C_P} dt\,\mathcal{F}(t)e^{-t/g^2}+\frac{4e^{-T/2}}{\pi g^2}\int_{C_{NP}} dt\,\mathcal{F}(t)e^{-t/g^2}=\bar{Z_P^{(II)}}(g^2)+\bar{Z_{NP}^{(II)}}(g^2), \tag{4.22}$$

as is shown in Fig. 2.

We identify the first term as the formal Borel summation of the perturbation series and the second term as the nonperturbative contribution. For the nonperturbative contribution, the following analytic property holds. If we perform the analytic continuation of $Z_{NP}(|g^2|e^{i\theta})$ from $\theta=0$ to $\theta=\pi$, the contour for Z_{NP} changes from $C_{NP}(0)$ to $C_{NP}(\pi)$, as shown in Fig. 3. In the weak coupling limit, the integral of $C_{NP}(\pi)$ can be well-approximated by that of C_V because the dominant contribution of the integral comes from $t\sim 2g^2S_0^{(I)}$. Therefore, in the case of $g^2=|g^2|e^{i\pi}$ when the interaction between valley-instantons is repulsive, the following relation holds approximately:

$$Z_{NP}(|g^2|e^{i\pi})\simeq Z(|g^2|e^{i\pi}). \tag{4.23}$$

This relation coincides with what Bogomolny suggested heuristically as a method of evaluation of the instanton–anti-instanton contribution.[43]

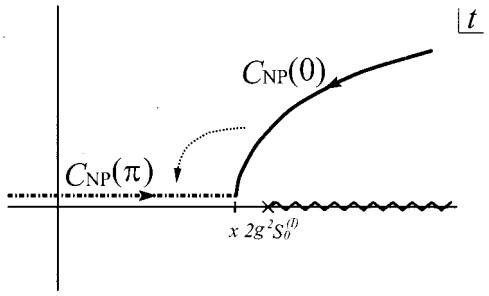

FIG. 3. The change of the contour $C_{NP}(\theta)$ as θ is changed from zero to π.

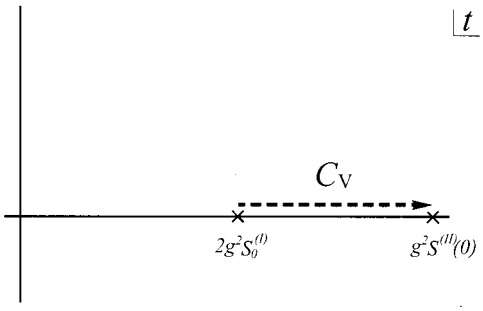

FIG. 4. The integration contour C_V in the case of the II-valley.

An immediate consequence of our decomposition of the perturbative and nonperturbative contribution is

$$\mathrm{Im}\, Z_P + \mathrm{Im}\, Z_{NP} = 0, \tag{4.24}$$

since $Z = Z_P + Z_{NP}$ is real. From the relation above, the dispersion relation becomes[2]

$$Z_P(g^2) = \frac{1}{2\pi i} \oint_{C_{g^2}} dz \frac{Z_P(z)}{z - g^2} \simeq -\frac{1}{\pi} \sum_{r=0}^{\infty} g^{2r} \int_0^{\infty} dz \frac{\mathrm{Im}\, Z_{NP}(z)}{z^{r+1}}, \tag{4.25}$$

where C_{g^2} is the counter around $z = g^2$ and we have neglected the contribution from the singularities far from the origin. The last line of Eq. (4.25) gives the relation between the coefficients of the perturbation series and the imaginary part of the nonperturbative contribution. Rewriting the above relation in terms of the energy spectra, we find for the perturbative part of the spectra $E_P(g^2) = \Sigma_{r=0}^{\infty} a^{(r)} g^{2r}$ that the coefficients $a^{(r)}$ can be estimated as

$$a^{(r)} = -\frac{1}{\pi} \int_0^{\infty} dg^2 \frac{\mathrm{Im}\, E_{NP}(g^2)}{g^{2r+2}}. \tag{4.26}$$

The situation in the case of $\overline{II}$-valley is completely the same as that in the $I\overline{I}$-valley.

On the other hand, the situation in the case of II-valley is different, reflecting the fact that the II-valley configuration cannot be deformed continuously to the trivial vacuum configuration. The contribution of the II-valley to the partition function has quite similar form to that of the $I\overline{I}$-valley:

$$Z^{(II)} = \frac{4e^{-T/2}}{\pi g^2} \int_{C_V} dt\, \mathcal{F}(t) e^{-t/g^2}. \tag{4.27}$$

However, the integration contour is now $C_V = (2g^2 S_0^{(I)}, g^2 S^{(II)}(0)]$ and thus is disconnected to the perturbative region $t \sim 0$ (see Fig. 4).

This means that Eq. (4.27) contains only the nonperturbative contribution,

$$Z_{NP}(g^2) = Z(g^2). \tag{4.28}$$

Therefore, we need not separate the integration as in the case of the $I\overline{I}$-valley. As a consequence, the II-valley configuration does not contribute to the imaginary part and also to the large order behavior of the perturbation series, which will be confirmed in the examples in Secs. IV and V. Furthermore, since the interaction for the II-valley configuration is repulsive, as has been observed in Eqs. (4.19) and (4.20), the integral is dominated around $t \sim 2g^2 S_0^{(I)}$ and can be approxi-

mated by the integral on the contour $[2g^2S_0^{(I)},\infty)$ in the weak coupling limit. Therefore, analytic continuation is not needed. The situation in the case of the $\overline{II}$-valley is completely the same as that in the II-valley.

D. Multi-valley calculus

Utilizing the knowledge of the (anti-)valley-instantons and the interactions between them obtained previously and applying the manipulation discussed in Sec. IV C, we will evaluate the partition function $Z=\mathrm{tr}\, e^{-HT}$ by summing over those configurations made of several (anti-)valley-instantons which satisfy a boundary condition in T. The periodic boundary condition for a configuration $q(\tau)$ is in general given by

$$q(\tau+T)=q(\tau). \tag{4.29}$$

For a system which has a periodic potential like Eq. (4.11), however, the condition (4.29) can be relaxed and be replaced with

$$q(\tau+T)=q(\tau)+\frac{2k\pi}{g} \quad (k=0,\pm 1,\pm 2,\ldots). \tag{4.30}$$

This condition restricts the number of the valley-instantons to be even, $2n$. The nonperturbative contributions from the multi-valley configurations satisfying Eq. (4.30) can be calculated by the extension of the technique developed in Ref. 44. We divide the time interval $0\leqslant\tau\leqslant T$ into n regions and put a valley-instanton pair on each of the region. In order to distinguish what kind of pairs, we introduce the indices ϵ_i and $\tilde{\epsilon}_i$ for the i-th region (mod n) as follows:

(i) $\epsilon_i=1$, $\tilde{\epsilon}_i=1$ for II-valley,
(ii) $\epsilon_i=1$, $\tilde{\epsilon}_i=-1$ for $I\overline{I}$-valley,
(iii) $\epsilon_i=-1$, $\tilde{\epsilon}_i=1$ for $\overline{I}I$-valley,
(iv) $\epsilon_i=-1$, $\tilde{\epsilon}_i=-1$ for $\overline{II}$-valley.

In this way, the allowed configurations for a given valley-instanton number $2n$ are exhausted by the allowed combinations of the set $\{\epsilon_i,\tilde{\epsilon}_i\}$ $(i=1,\ldots,n)$. Combining the results on well-separated valley-instanton pairs with the above conventions, the well-separated multiple valley-instanton action for given n and $\{\epsilon_i,\tilde{\epsilon}_i\}$ is expressed as

$$S_n=2nS_0^{(I)}+\frac{8}{g^2}\sum_{i=1}^{n}\epsilon_i\tilde{\epsilon}_i e^{-R_i}+\frac{8}{g^2}\sum_{i=1}^{n}\tilde{\epsilon}_i\epsilon_{i+1}e^{-\tilde{R}_i}+\frac{\epsilon}{2}\sum_{i=1}^{n}(R_i-\tilde{R}_i)+i\frac{\vartheta}{2}\sum_{i=1}^{n}(\epsilon_i+\tilde{\epsilon}_i), \tag{4.31}$$

where R_i is the distance between the $(2i-1)$-th and $2i$-th (anti-)valley-instanton and $\tilde{R}_i$ the one between the $2i$-th and the $(2i+1)$-th (anti-)valley-instanton (mod n) and $\epsilon_{n+1}=\epsilon_1$ (see Fig. 5).

The sum of the contributions from the $2n$ valley-instantons configuration can be written as

$$Z_{\mathrm{NP}}=\sum_{n=1}^{\infty}\alpha^{2n}J_n, \tag{4.32}$$

where α^2 denotes the contribution of the Jacobian and the R-independent part of the determinant for one valley-instanton-pair and is calculated as, in this case,

$$\alpha^2=\frac{4}{\pi g^2}e^{-4/g^2}. \tag{4.33}$$

The term J_n is given by

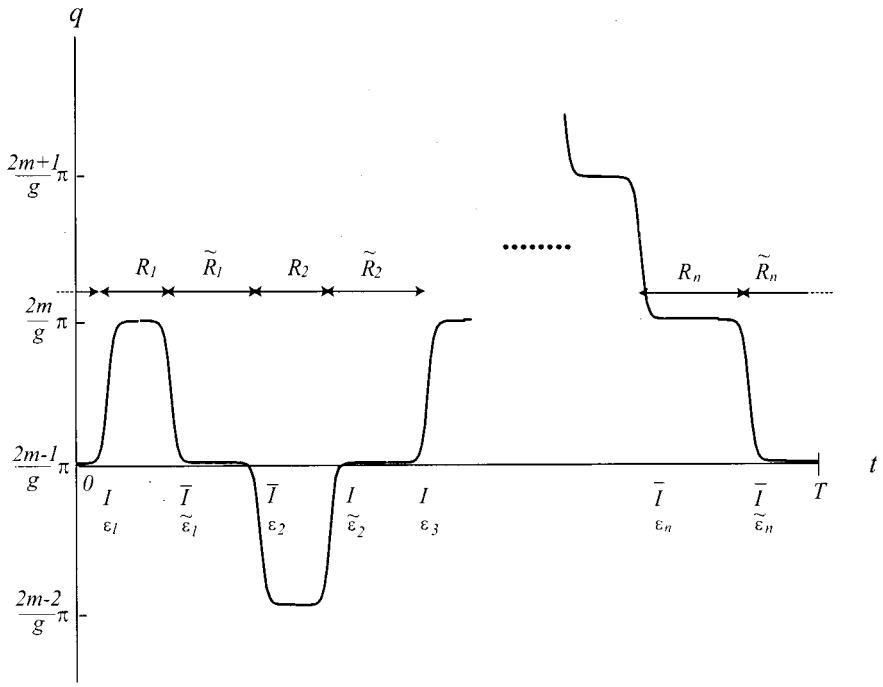

FIG. 5. The collective coordinates R_i and $\tilde{R}_i$ for a $2n$ valley-instantons configuration.

$$J_n=\frac{T}{n}\int_0^\infty\left(\prod_{i=1}^n dR_i\right)\left(\prod_{i=1}^n d\tilde{R}_i\right)\delta\left(\sum_{i=1}^n (R_i+\tilde{R}_i)-T\right)\sum_{\epsilon_i,\tilde{\epsilon}_i=\pm 1}\exp\left(-\frac{1+\epsilon}{2}\sum_{i=1}^n R_i-\frac{1-\epsilon}{2}\sum_{i=1}^n \tilde{R}_i\right.$$
$$\left.-\frac{8}{g^2}\sum_{i=1}^n \epsilon_i\tilde{\epsilon}_i e^{-R_i}-\frac{8}{g^2}\sum_{i=1}^n \tilde{\epsilon}_i\epsilon_{i+1}e^{-\tilde{R}_i}-i\frac{\vartheta}{2}\sum_{i=1}^n(\epsilon_i+\tilde{\epsilon}_i)\right). \tag{4.34}$$

To calculate the sum over the set $\{\epsilon_i,\tilde{\epsilon}_i\}$, we introduce the following transfer matrices:

$$T(R_i)=\begin{pmatrix}\exp\left(-\frac{8}{g^2}e^{-R_i}-i\vartheta\right) & \exp\left(\frac{8}{g^2}e^{-R_i}\right)\\ \exp\left(\frac{8}{g^2}e^{-R_i}\right) & \exp\left(-\frac{8}{g^2}e^{-R_i}+i\vartheta\right)\end{pmatrix}, \tag{4.35a}$$

$$\tilde{T}(\tilde{R}_i)=\begin{pmatrix}\exp\left(-\frac{8}{g^2}e^{-\tilde{R}_i}\right) & \exp\left(\frac{8}{g^2}e^{-\tilde{R}_i}\right)\\ \exp\left(\frac{8}{g^2}e^{-\tilde{R}_i}\right) & \exp\left(-\frac{8}{g^2}e^{-\tilde{R}_i}\right)\end{pmatrix}. \tag{4.35b}$$

Then, using these matrices we have

$$J_n=\frac{T}{2\pi i n}\int_{-i\infty-\eta}^{i\infty-\eta} ds\, e^{-Ts}\,\mathrm{tr}\left(\prod_{i=1}^n\int_0^\infty dR_i\, e^{(s-1/2-\epsilon/2)R_i}T(R_i)\int_0^\infty d\tilde{R}_i\, e^{(s-1/2+\epsilon/2)\tilde{R}_i}\tilde{T}(\tilde{R}_i)\right)$$
$$=\frac{T}{2\pi i n}\int_{-i\infty-\eta}^{i\infty-\eta} ds\, e^{-Ts}\,\mathrm{tr}[\mathcal{T}(s,\epsilon,\vartheta)^n], \tag{4.36}$$

where

$$\mathcal{T}(s,\epsilon,\vartheta)=\begin{pmatrix} K(s-\epsilon/2)e^{-i\vartheta} & I(s-\epsilon/2) \\ I(s-\epsilon/2) & K(s-\epsilon/2)e^{i\vartheta} \end{pmatrix}\begin{pmatrix} K(s+\epsilon/2) & I(s+\epsilon/2) \\ I(s+\epsilon/2) & K(s+\epsilon/2) \end{pmatrix}. \tag{4.37}$$

In the above, K and I are defined by

$$K(s)=\int_0^\infty dR\, e^{(s-1/2)R-(8/g^2)e^{-R}} \simeq \left(\frac{8}{g^2}\right)^{s-1/2}\Gamma\left(-s+\frac{1}{2}\right), \tag{4.38a}$$

$$I(s)=\int_0^\infty dR\, e^{(s-1/2)R+(8/g^2)e^{-R}} \simeq \left(-\frac{8}{g^2}\right)^{s-1/2}\Gamma\left(-s+\frac{1}{2}\right), \tag{4.38b}$$

where the manipulation explained in Sec. IV C is utilized for estimating each of the integration. The calculation of the trace in Eq. (4.36) can be done by diagonalizing $\mathcal{T}$. If we denote the two eigenvalues of $\mathcal{T}$ as $t_\pm$, we immediately yield

$$J_n=\frac{T}{2\pi i n}\int_{-i\infty-\eta}^{i\infty-\eta} ds\, e^{-Ts}(t_+(s)^n+t_-(s)^n). \tag{4.39}$$

From Eq. (4.37), $t_\pm$ is evaluated as

$$\begin{aligned} t_\pm(s)=&K(s+\epsilon/2)K(s-\epsilon/2)\cos\vartheta+I(s+\epsilon/2)I(s-\epsilon/2) \\ &\pm\{[I(s+\epsilon/2)^2-K(s+\epsilon/2)^2]K(s-\epsilon/2)^2\sin^2\vartheta,, \\ &+[K(s+\epsilon/2)I(s-\epsilon/2)+I(s+\epsilon/2)K(s-\epsilon/2)\cos\vartheta]^2\}^{1/2}. \end{aligned} \tag{4.40}$$

Finally, combining Eqs. (4.32) and (4.39) we obtain the nonperturbative contribution to the partition function:

$$Z_{\mathrm{NP}}=-\frac{T}{2\pi i}\int_{-i\infty-\eta}^{i\infty-\eta} ds\, e^{-Ts}\ln(1-\alpha^2 t_+(s))(1-\alpha^2 t_-(s)). \tag{4.41}$$

E. Nonperturbative contributions

From the results in Eqs. (4.38), (4.40) and (4.41), the nonperturbative contributions to the spectra are determined by the following equation:

$$\alpha^2\beta_\pm(E,\epsilon,\vartheta)\left(\frac{8}{g^2}\right)^{(E-1/2)2}\Gamma\left(-E+\frac{1}{2}-\frac{\epsilon}{2}\right)\Gamma\left(-E+\frac{1}{2}+\frac{\epsilon}{2}\right)=1, \tag{4.42}$$

where

$$\begin{aligned} \beta_\pm(E,\epsilon,\vartheta)=&\cos\vartheta+(-)^{(E-1/2)2} \\ &\pm\sqrt{(-)^{(E-1/2-\epsilon/2)2}+(-)^{(E-1/2+\epsilon/2)2}+(-)^{(E-1/2)2}2\cos\vartheta-\sin^2\vartheta}. \end{aligned} \tag{4.43}$$

We will solve the above equation by the series expansion in α:

$$E_{n_\pm}=E^{(0)}_{n_\pm}+\alpha E^{(1)}_{n_\pm}+\alpha^2 E^{(2)}_{n_\pm}+\cdots, \quad E^{(0)}_{n_\pm}=n_\pm+\frac{1}{2}\pm\frac{\epsilon}{2}, \tag{4.44}$$

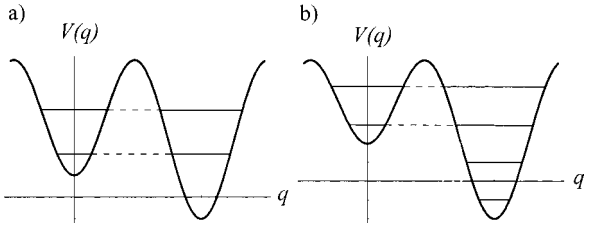

FIG. 6. Degeneracies of the harmonic spectra for (a) $\epsilon=1$ and (b) $\epsilon=2$.

where E_{n_+} stands for the spectra corresponding to, in the limit $g\to 0$, the eigenfunctions of the shallower potential wells and E_{n_-} stands for the ones corresponding to the eigenfunctions of the deeper potential wells. For $\epsilon\neq\mathcal{N}$ ($\mathcal{N}=1,2,3,\ldots$), the first order contributions vanish and the leading second order contributions are calculated as follows:

$$E^{(2)}_{n_\pm}=2[\cos\vartheta+(-)^{\pm\epsilon}]\frac{(-)^{n_\pm+1}}{n_\pm!}\left(\frac{8}{g^2}\right)^{2n_\pm\pm\epsilon}\Gamma(-n_\pm\mp\epsilon). \tag{4.45}$$

For $\epsilon=\mathcal{N}$ ($\mathcal{N}=1,2,3,\ldots$), all the harmonic spectra $E^{(0)}_{n_+}$ of the shallower wells and the higher harmonic spectra $E^{(0)}_{n_-}$ of the deeper wells degenerate for $n_-=n_++\mathcal{N}$; see Fig. 6 for $\epsilon=\mathcal{N}=1,2$. Between these degenerate states, resonant tunneling enhances the nonperturbative corrections, and results in order α^1 contributions to the spectra E_{n_-} and E_{n_+} with $n_-=n_++\mathcal{N}$:

$$E^{(1)}_{n_\pm}=\mp\sqrt{\frac{2[1+(-)^{\mathcal{N}}\cos\vartheta]}{n_+!\,n_-!}\left(\frac{8}{g^2}\right)^{n_++n_-}}, \tag{4.46}$$

$$E^{(2)}_{n_\pm}=\frac{E^{(1)2}_{n_\pm}}{2}\left[\frac{2\ln(-)}{1+(-)^{\mathcal{N}}\cos\vartheta}+2\ln\left(\frac{8}{g^2}\right)-\psi(n_++1)-\psi(n_-+1)\right], \tag{4.47}$$

where $\psi(z)=d\ln\Gamma(z)/dz$ is the digamma function. For the other spectra, say, the lower E_{n_-} with $n_-<\mathcal{N}$, the contributions are the same as Eq. (4.45). We see from Eq. (4.45) the nonperturbative corrections for these lower E_{n_-} vanish, at least up to order α^2, at $\vartheta=0(\pi)$ when $\epsilon=\mathcal{N}$ is odd(even) and thus, from Eq. (4.12), the system has $\mathcal{N}$-fold supersymmetry. This means that when the system is $\mathcal{N}$-fold supersymmetric with odd(even) $\mathcal{N}$, among the physical states for each of the lower $\mathcal{N}$ spectral bands, the state which satisfies the periodic(anti-periodic) boundary condition does not receive nonperturbative correction. From Eq. (3.4) in this case, these physical states are surely the elements of the solvable subspace $\mathcal{V}^-$. Therefore, the results are consistent with the fact that $\mathcal{N}$-fold supersymmetry in this case is not broken dynamically.

Finally, we make a remark on the resultant equation (4.42). The origin of the disappearance of the nonperturbative corrections discussed above comes from the factor $\beta_\pm$ in Eq. (4.42). Indeed, to make the lhs of Eq. (4.42) finite when $\beta_\pm=0$, the gamma functions must diverge adequately. This happens only when $E=E^{(0)}_{n_\pm}$ for certain values of $n_\pm$, and therefore the nonperturbative corrections must vanish.[45] From the derivation of Eq. (4.42), we can see that the appearance of the factor $\beta_\pm$ is achieved by taking into account both of the repulsive and attractive interactions between the valley-instantons properly. Therefore, we guess that naive application of the dilute-gas approximation can hardly lead to the correct results even for the ground-state energy.

F. Large order behavior of the perturbation series

The large order behavior of the perturbation series in g^2 for the spectra can be estimated by the same way as in the case of the double-well potential. From the nonperturbative contributions, Eqs. (4.45)–(4.47), we can easily see that the imaginary parts of them are continuous, at least up to the order α^2, in ϵ and yield

$$\mathrm{Im}\, E_{n_\pm} \sim -\alpha^2 \frac{2\pi}{n_\pm!\Gamma(n_\pm+1\pm\epsilon)}\left(\frac{8}{g^2}\right)^{2n_\pm\pm\epsilon}, \tag{4.48}$$

which are valid for arbitrary ϵ. Then, if we expand the spectra in power of g^2 such that

$$E_{n_\pm} = E^{(0)}_{n_\pm} + \sum_{r=1}^{\infty} a^{(r)}_{n_\pm} g^{2r}, \tag{4.49}$$

the large order behavior of the coefficients $a^{(r)}$ for sufficiently large r are calculated as, using Eqs. (4.26) and (4.48),

$$a^{(r)}_{n_\pm} \sim A_{n_\pm}(\epsilon)\, 4^{-r}\Gamma(r+2n_\pm+1\pm\epsilon), \tag{4.50}$$

where

$$A_{n_\pm}(\epsilon) = \frac{2}{\pi}\frac{2^{2n_\pm\pm\epsilon}}{n_\pm!\Gamma(n_\pm+1\pm\epsilon)}. \tag{4.51}$$

Equation (4.50) shows that the perturbative coefficients diverge factorially unless the prefactor $A(\epsilon)$ vanish. From Eq. (4.51), we can find the disappearance of the leading divergence takes place only when $\epsilon=\mathcal{N}$ ($\mathcal{N}=1,2,3,\ldots$). Comparing the results with Eq. (4.12) and taking the symmetry (4.13) into account, we see that the above cases completely coincide with the case where the system possesses Type A $\mathcal{N}$-fold supersymmetry. Therefore, the results of the valley method analyses are consistent with a consequence of Type A $\mathcal{N}$-fold supersymmetry, that is, the non-renormalization theorem.

V. ANALYSIS OF A TRIPLE-WELL POTENTIAL

In this section we will analyze a sextic triple-well potential. The form of the potential to be analyzed is the following:

$$V(q) = \frac{1}{2}q^2(1-g^2q^2)^2 + \frac{\epsilon}{2}(1-3g^2q^2). \tag{5.1}$$

This has three local minima at $q=0$ and $q\simeq\pm 1/g$ for $\epsilon g^2 \ll 1$ (see Fig. 7).

Comparing this potential with Eq. (3.19), C_1, C_2 and q_0 in $w(q)$ being

$$C_1 = -g^2, \quad C_2 = 1, \quad q_0 = 0, \tag{5.2}$$

we can easily see that the system has Type A $\mathcal{N}$-fold supersymmetry when

$$\epsilon = \pm\frac{4\mathcal{N}\pm 1}{3}. \tag{5.3}$$

More precisely, the system becomes one of the $\mathcal{N}$-fold supersymmetric pair $H^{\pm}_{\mathcal{N}}$; $H^{+}_{\mathcal{N}}$ when $\epsilon=(4\mathcal{N}\pm 1)/3$ and $H^{-}_{\mathcal{N}}$ when $\epsilon=-(4\mathcal{N}\pm 1)/3$. As has been explained in Sec. III B, $\mathcal{N}$-fold supersymmetry does not break in the cubic type because either bases of the solvable subspace $\mathcal{V}^{+}_{\mathcal{N}}$ or those of $\mathcal{V}^{-}_{\mathcal{N}}$ are normalizable in general. Since $C_1<0$ in this case, bases of the solvable subspace

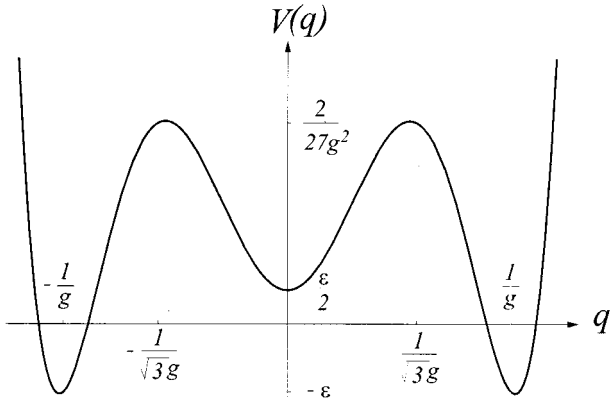

FIG. 7. The form of the triple-well potential investigated in this section.

$\mathcal{V}_{\mathcal{N}}^{+}$ are normalizable and physical while those of $\mathcal{V}_{\mathcal{N}}^{-}$ are not. Therefore, we may expect that the nonperturbative corrections for certain $\mathcal{N}$ states will vanish when $\epsilon=(4\mathcal{N}\pm 1)/3$ while those will not when $\epsilon=-(4\mathcal{N}\pm 1)/3$, though the perturbation series for the corresponding spectra will be in both the cases convergent.

As far as we know, little has been investigated for triple-well potentials. We have found only two references[46,47] on the subject, both of which employed the dilute-gas approximation. However, from the consideration mentioned at the end of Sec. IV E, we intend to analyze beyond the dilute-gas approximation using the same technique of the valley method as in Sec. IV.[48]

In the case of $\epsilon=0$, the three local minima of the potential have the same potential value. Thus, there are (anti-)instanton solutions of the equation of motion which describe the quantum tunneling between the neighboring vacua:

$$q_0^{(I)}(\tau-\tau_0)=\pm\frac{1}{g}\frac{1}{(1+e^{\mp 2(\tau-\tau_0)})^{1/2}},\quad q_0^{(\bar{I})}(\tau-\tau_0)=\pm\frac{1}{g}\frac{1}{(1+e^{\pm 2(\tau-\tau_0)})^{1/2}}. \tag{5.4}$$

When $\epsilon\neq 0$, the solutions of the valley equation now become the (anti-)valley-instantons. In this case, there are three kinds of the solutions of the valley equation which are asymptotically composed of two (anti-)valley-instantons. Contrary to the periodic potential in Sec. IV, there are two different $I\bar{I}$-valley or $\bar{I}I$-valley configurations in this case since the curvature at the central potential bottom (at $q=0$) is different, even at the leading order of g^2, from the one at the side potential bottoms (at $q\simeq\pm 1/g$); the $I\bar{I}$ ($\bar{I}I$)-valley which satisfy $q(\pm T/2)=0$ ($T\gg 1$) are different from the ones which satisfy $q(\pm T/2)\simeq 1/g$ or $-1/g$ ($T\gg 1$). The Euclidean action of the former with large separation R can be calculated by the perturbative expansion in $\lambda\sim O(e^{-2R})$ as follows:

$$S^{(I\bar{I})}(R)=S^{(\bar{I}I)}(R)=2S_0^{(I)}-\epsilon R+\frac{\epsilon}{2}(T-R)-\frac{1}{g^2}e^{-2R}+O(e^{-4R}), \tag{5.5}$$

while the one of the latter with large separation $\tilde{R}$ can be calculated in the same way as

$$S^{(I\bar{I})}(\tilde{R})=S^{(\bar{I}I)}(\tilde{R})=2S_0^{(I)}+\frac{\epsilon}{2}\tilde{R}-\epsilon(T-\tilde{R})-\frac{2}{g^2}e^{-\tilde{R}}+O(e^{-2\tilde{R}}), \tag{5.6}$$

where $S_0^{(I)}$ denotes the Euclidean action of one (anti-)instanton Eq. (5.4) and amounts to

$$S_0^{(I)}=\frac{1}{4g^2}. \tag{5.7}$$

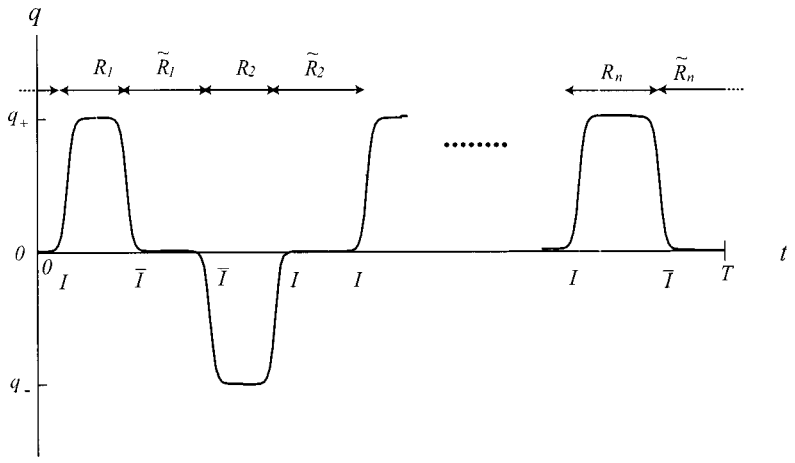

FIG. 8. The collective coordinates R_i and $\tilde{R}_i$ for a $2n$ valley-instantons configuration.

The other type is II-valley or $\overline{II}$-valley. The Euclidean action of them with large separation $\tilde{R}$ can be also calculated in the same way as

$$S^{(II)}(\tilde{R})=S^{(\overline{II})}(\tilde{R})=2S_0^{(I)}+\frac{\epsilon}{2}\tilde{R}-\epsilon(T-\tilde{R})+\frac{2}{g^2}e^{-\tilde{R}}+O(e^{-2\tilde{R}}). \tag{5.8}$$

A. Multi-valley calculus

The evaluation of the partition function $Z=\mathrm{tr}\,e^{-HT}$ by summing over multi-valley-instanton configurations can be done in the same manner as those for the double-well and the periodic potentials. One can easily see that in order to incorporate with the periodic boundary condition in T, the number of the valley-instantons in a period T must be even. For a given number $2n$ of the valley-instantons, however, there are still several configurations. If we regard a configuration as n valley-instanton pairs, we have four kinds of pair, II-, $I\bar{I}$-, $\bar{I}I$-, and $\overline{II}$-valleys. We denote the number of the II- and $\overline{II}$-valley as n_{II} and $n_{\overline{II}}$, respectively, and that of the others as $n_{I\bar{I}}$. Contrary to the periodic potential case, the particle must come back to the start point after the period T passes in this case. Therefore, we must impose Eq. (4.29) rather than Eq. (4.30). This condition results in $n_{II}=n_{\overline{II}}$. As a consequence we have

$$2n_{II}+n_{I\bar{I}}=n. \tag{5.9}$$

This restriction shows that for a given n there are $[n/2]+1$ variety of the n_{II} value. For n and n_{II} fixed, however, the configuration is not determined uniquely yet. There remains a freedom of the permutation of the pairs. The number of cases can be calculated if one notices that the configuration is uniquely determined as far as the position of the II- and $\overline{II}$-valleys among n area is fixed. We denote a set of the position as $\{i_{II}\}$. It is therefore clear that for given n and n_{II} there are ${}_nC_{2n_{II}}$ configurations of the multiple valley-instantons. Combining the results on well-separated valley-instanton pairs with the above considerations, the well-separated multi-valley-instanton action for given n, n_{II} and $\{i_{II}\}$ is expressed as

$$S^{\{i_{II}\}}_{n,n_{II}}=2nS_0^{(I)}-\epsilon\sum_{i=1}^{n}R_i+\frac{\epsilon}{2}\sum_{i=1}^{n}\tilde{R}_i-\frac{1}{g^2}\sum_{i=1}^{n}e^{-2R_i}+\frac{2}{g^2}\sum_{i\in\{i_{II}\}}e^{-\tilde{R}_i}-\frac{2}{g^2}\sum_{i\notin\{i_{II}\}}e^{-\tilde{R}_i}, \tag{5.10}$$

where R_i is the distance between the $(2i-1)$-th and $2i$-th (anti-)valley-instanton and $\tilde{R}_i$ is the one between the $2i$-th and the $(2i+1)$-th (anti-)valley-instanton (mod n) (see Fig. 8).

The sum of the contributions from the $2n$ valley-instantons configuration can be written as

$$Z_{\mathrm{NP}}=\sum_{n=1}^{\infty}\alpha^{2n}J_n,\quad J_n=\sum_{n_{II}=0}^{[n/2]}\sum_{\{i_{II}\}}\mathcal{J}_{n,n_{II}}^{\{i_{II}\}},\tag{5.11}$$

where α^2 denotes the contribution of the Jacobian and the R-independent part of the determinant for one valley-instanton-pair and is calculated as, in this case,

$$\alpha^2=\frac{\sqrt{2}}{\pi g^2}e^{-1/2g^2}.\tag{5.12}$$

The term $\mathcal{J}_{n,n_{II}}^{\{i_{II}\}}$ is given by

$$\begin{aligned}\mathcal{J}_{n,n_{II}}^{\{i_{II}\}}=\frac{T}{n}\int_0^{\infty}\left(\prod_{i=1}^{n}dR_i\right)\left(\prod_{i=1}^{n}d\tilde{R}_i\right)\delta\left(\sum_{i=1}^{n}(R_i+\tilde{R}_i)-T\right)\exp\Bigg[-(1-\epsilon)\sum_{i=1}^{n}R_i-\left(\frac{1}{2}+\frac{\epsilon}{2}\right)\sum_{i=1}^{n}\tilde{R}_i\\+\frac{1}{g^2}\sum_{i=1}^{n}e^{-2R_i}-\frac{2}{g^2}\sum_{i\in\{i_{II}\}}e^{-\tilde{R}_i}+\frac{2}{g^2}\sum_{i\notin\{i_{II}\}}e^{-\tilde{R}_i}\Bigg].\end{aligned}\tag{5.13}$$

In the above expression, we notice that for n and n_{II} fixed, the contribution $\mathcal{J}_{n,n_{II}}^{\{i_{II}\}}$ does not depend on the choice of the set $\{i_{II}\}$. This means the following equality,

$$\sum_{\{i_{II}\}}\mathcal{J}_{n,n_{II}}^{\{i_{II}\}}=\binom{n}{2n_{II}}\mathcal{J}_{n,n_{II}},\tag{5.14}$$

where $\mathcal{J}_{n,n_{II}}$ is the contribution $\mathcal{J}_{n,n_{II}}^{\{i_{II}\}}$ for a specific $\{i_{II}\}$ and is evaluated as

$$\begin{aligned}\mathcal{J}_{n,n_{II}}&=\frac{T}{n}\int_0^{\infty}\left(\prod_{i=1}^{n}dR_i\right)\left(\prod_{i=1}^{n}d\tilde{R}_i\right)\delta\left(\sum_{i=1}^{n}(R_i+\tilde{R}_i)-T\right)\exp\Bigg[-(1-\epsilon)\sum_{i=1}^{n}R_i-\left(\frac{1}{2}+\frac{\epsilon}{2}\right)\sum_{i=1}^{n}\tilde{R}_i\\&\quad+\frac{1}{g^2}\sum_{i=1}^{n}e^{-2R_i}-\frac{2}{g^2}\sum_{i=1}^{2n_{II}}e^{-\tilde{R}_i}+\frac{2}{g^2}\sum_{i=2n_{II}+1}^{n}e^{-\tilde{R}_i}\Bigg]\\&=\frac{T}{2\pi i n}\int_{-i\infty-\eta}^{i\infty-\eta}ds\,e^{-Ts}K_-(s)^nK_+^{(1)}(s)^{2n_{II}}K_+^{(2)}(s)^{n-2n_{II}}.\end{aligned}\tag{5.15}$$

In the last expression for $\mathcal{J}_{n,n_{II}}$, several K's are defined by

$$K_-(s)=\int_0^{\infty}dR\exp\left[(s-1+\epsilon)R+\frac{1}{g^2}e^{-2R}\right]\simeq\frac{1}{2}\left(-\frac{1}{g^2}\right)^{s/2-1/2+\epsilon/2}\Gamma\left(-\frac{s}{2}+\frac{1}{2}-\frac{\epsilon}{2}\right),\tag{5.16a}$$

$$K_+^{(1)}(s)=\int_0^{\infty}d\tilde{R}\exp\left[\left(s-\frac{1}{2}-\frac{\epsilon}{2}\right)\tilde{R}-\frac{2}{g^2}e^{-\tilde{R}}\right]\simeq\left(\frac{2}{g^2}\right)^{s-1/2-\epsilon/2}\Gamma\left(-s+\frac{1}{2}+\frac{\epsilon}{2}\right),\tag{5.16b}$$

$$K_+^{(2)}(s)=\int_0^{\infty}d\tilde{R}\exp\left[\left(s-\frac{1}{2}-\frac{\epsilon}{2}\right)\tilde{R}+\frac{2}{g^2}e^{-\tilde{R}}\right]\simeq\left(-\frac{2}{g^2}\right)^{s-1/2-\epsilon/2}\Gamma\left(-s+\frac{1}{2}+\frac{\epsilon}{2}\right),\tag{5.16c}$$

where the manipulation explained in Sec. IV C is again utilized for estimating each of the integrations. Eventually, from Eqs. (5.11), (5.14) and (5.15) we obtain

$$Z_{\mathrm{NP}}=\sum_{n=1}^{\infty}\alpha^{2n}\sum_{n_{II}=0}^{[n/2]}\binom{n}{2n_{II}}\mathcal{J}_{n,n_{II}}$$

$$=-\frac{T}{4\pi i}\int_{-i\infty-\eta}^{i\infty-\eta}ds e^{-Ts}\ln(1-\alpha^2K_-(s)K_+^{(+)}(s))(1-\alpha^2K_-(s)K_+^{(-)}(s)), \tag{5.17}$$

where

$$K_+^{(\pm)}(s)=K_+^{(2)}(s)\pm K_+^{(1)}(s). \tag{5.18}$$

B. Nonperturbative contributions

From the results in Eqs. (5.16)–(5.18), the nonperturbative contributions to the spectra are determined by the following equation:

$$\alpha^2\beta_{\pm}(E,\epsilon)\left(\frac{2}{g^2}\right)^{E-1/2-\epsilon/2}\Gamma\left(-E+\frac{1}{2}+\frac{\epsilon}{2}\right)\left(-\frac{1}{g^2}\right)^{E/2-1/2+\epsilon/2}\Gamma\left(-\frac{E}{2}+\frac{1}{2}-\frac{\epsilon}{2}\right)=1, \tag{5.19}$$

where

$$\beta_{\pm}(E,\epsilon)=\frac{(-)^{E-1/2-\epsilon/2}\pm 1}{2}. \tag{5.20}$$

We will solve the above equation by the series expansion in α:

$$E_{n_0}=E_{n_0}^{(0)}+\alpha E_{n_0}^{(1)}+\alpha^2E_{n_0}^{(2)}+\cdots,\quad E_{n_0}^{(0)}=n_0+\frac{1}{2}+\frac{\epsilon}{2}, \tag{5.21a}$$

$$E_{n_\pm}=E_{n_\pm}^{(0)}+\alpha E_{n_\pm}^{(1)}+\alpha^2E_{n_\pm}^{(2)}+\cdots,\quad E_{n_\pm}^{(0)}=2n_\pm+1-\epsilon, \tag{5.21b}$$

where E_{n_0} stands for the spectra corresponding to, in the limit $g\to 0$, the eigenfunctions of the center potential well and $E_{n_\pm}$ for the ones corresponding to the parity eigenstates obtained by the linear combinations of the eigenfunctions of each side potential well. For $\epsilon\neq\pm(2\mathcal{N}+1)/3$ ($\mathcal{N}=0,1,2,\ldots$), the first order contributions vanish and the leading second order contributions are calculated as follows:

$$E_{n_0}^{(2)}=-\frac{1}{n_0!}\left(\frac{2}{g^2}\right)^{n_0}\left(-\frac{1}{g^2}\right)^{n_0/2-1/4+(3/4)\epsilon}\Gamma\left(-\frac{n_0}{2}+\frac{1}{4}-\frac{3}{4}\epsilon\right), \tag{5.22}$$

$$E_{n_\pm}^{(2)}=-\left((-)^{(1-3\epsilon)/2}\pm 1\right)\frac{1}{n_\pm!}\left(\frac{2}{g^2}\right)^{2n_\pm+1/2-(3/2)\epsilon}\left(\frac{1}{g^2}\right)^{n_\pm}\Gamma\left(-2n_\pm-\frac{1}{2}+\frac{3}{2}\epsilon\right). \tag{5.23}$$

In this case, degeneracies of the harmonic oscillator spectra for each potential well only occur between both side wells. The different nonperturbative contributions for $n_\pm$ in Eq. (5.23) show the splitting of the degeneracies via the quantum tunneling as in the case of symmetric double-well potentials.

When $\epsilon=(4\mathcal{N}+1)/3$ ($\mathcal{N}=0,1,2,\ldots$), all the even-parity central harmonic spectra $E_{2m_0}^{(0)}$ and the higher side harmonic spectra $E_{n_\pm}^{(0)}$ degenerate for $n_\pm=m_0+\mathcal{N}$ [see Fig. 9(a) for $\epsilon=\frac{5}{3}$ ($\mathcal{N}=1$)].

It is interesting, however, that the interference due to the quantum tunneling only occurs between the same (even-)parity states. As a consequence, E_{2m_0} and E_{n_+} satisfying $n_+=m_0+\mathcal{N}$ acquire order α^1 contributions as follows:

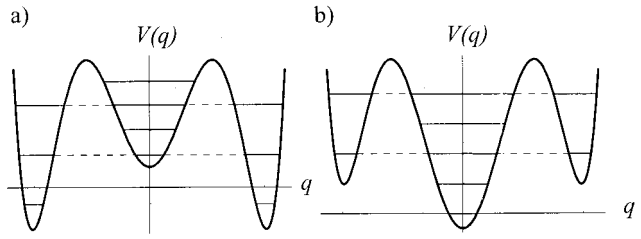

FIG. 9. Degeneracies of the harmonic spectra for (a) $\epsilon=\frac{5}{3}$ and (b) $\epsilon=-1$.

$$E^{(1)}_{n_+/2m_0}=\pm\sqrt{\frac{2}{n_+!(2m_0)!}\left(\frac{2}{g^2}\right)^{2m_0}\left(\frac{1}{g^2}\right)^{n_+}}, \tag{5.24}$$

$$E^{(2)}_{n_+/2m_0}=\frac{E^{(1)2}_{n_+/2m_0}}{4}\left[\ln\left(-\frac{2}{g^2}\right)+\ln\left(\frac{2}{g^2}\right)+\ln\left(-\frac{1}{g^2}\right)-\psi(n_++1)-2\psi(2m_0+1)\right]. \tag{5.25}$$

For the other spectra, say, E_{n_-}, E_{2m_0+1} and the lower E_{n_+} with $n_+<\mathcal{N}$, the contributions are the same as Eqs. (5.22) and (5.23). When $\epsilon=-(4\mathcal{N}-1)/3$ ($\mathcal{N}=1,2,3,\ldots$), all the side harmonic spectra $E^{(0)}_{n_\pm}$ and the higher even-parity central harmonic spectra $E^{(0)}_{2m_0}$ degenerate for $m_0=n_\pm+\mathcal{N}$ [see Fig. 9(b) for $\epsilon=-1$ ($\mathcal{N}=1$)]. In this case, the interference also occurs only between the same (even-)parity states. The contributions for E_{2m_0} and E_{n_+} satisfying $m_0=n_++\mathcal{N}$ are given by the same as Eqs. (5.24) and (5.25). For the other spectra, say, E_{n_-}, E_{2m_0+1} and the lower E_{2m_0} with $m_0<\mathcal{N}$, the contributions are the same as Eqs. (5.22) and (5.23).

When $\epsilon=(4\mathcal{N}-1)/3$ ($\mathcal{N}=1,2,3,\ldots$), all the odd-parity central harmonic spectra $E^{(0)}_{2m_0+1}$ and the higher side harmonic spectra $E^{(0)}_{n_\pm}$ degenerate for $n_\pm=m_0+\mathcal{N}$ [see Fig. 10(a) for $\epsilon=1$ ($\mathcal{N}=1$)].

In this case, only the odd-parity states interfere and yield order α^1 contributions for $n_-=m_0+\mathcal{N}$:

$$E^{(1)}_{n_-/2m_0+1}=\pm\sqrt{\frac{2}{n_-!(2m_0+1)!}\left(\frac{2}{g^2}\right)^{2m_0+1}\left(\frac{1}{g^2}\right)^{n_-}}, \tag{5.26}$$

$$E^{(2)}_{n_-/2m_0+1}=\frac{E^{(1)2}_{n_-/2m_0+1}}{4}\left[\ln\left(-\frac{2}{g^2}\right)+\ln\left(\frac{2}{g^2}\right)+\ln\left(-\frac{1}{g^2}\right)-\psi(n_-+1)-2\psi(2m_0+2)\right]. \tag{5.27}$$

The contributions for the other spectra, say, E_{n_+}, E_{2m_0} and the lower E_{n_-} with $n_-<\mathcal{N}$, are given by the same as Eqs. (5.22) and (5.23). When $\epsilon=-(4\mathcal{N}+1)/3$ ($\mathcal{N}=0,1,2,\ldots$), all the side har-

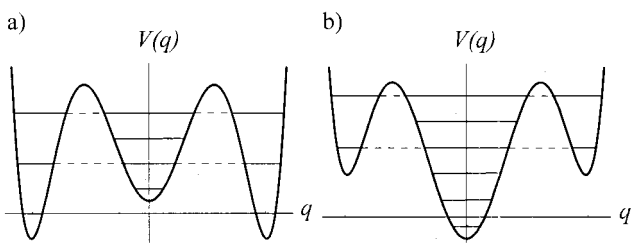

FIG. 10. Degeneracies of the harmonic spectra for (a) $\epsilon=1$ and (b) $\epsilon=-\frac{5}{3}$.

monic spectra $E^{(0)}_{n_\pm}$ and the higher odd-parity central harmonic spectra $E^{(0)}_{2m_0+1}$ degenerate for $m_0=n_\pm+\mathcal{N}$ [see Fig. 10(b) for $\epsilon=-\frac{5}{3}$ $(\mathcal{N}=1)$]. Only the odd-parity states interfere in the same way and the nonperturbative contributions for E_{2m_0+1} and E_{n_-} satisfying $m_0=n_-+\mathcal{N}$ are the same as Eqs. (5.26) and (5.27). Again, the expressions for the other spectra, say, E_{n_+}, E_{2m_0} and the lower E_{2m_0+1} with $m_0<\mathcal{N}$, are given by Eqs. (5.22) and (5.23).

From the whole result obtained here, we see that the nonperturbative corrections vanish only when $\epsilon=(4\mathcal{N}\pm1)/3$ $(\mathcal{N}=1,2,3,\ldots)$. More precisely, when $\epsilon=(4\mathcal{N}+1)/3$, Eq. (5.23) is applied for the even-parity states labeled by the quantum number n_- and results in $E^{(2)}_{n_-}=0$ for all $n_-<\mathcal{N}$. Similarly, when $\epsilon=(4\mathcal{N}-1)/3$, Eq. (5.23) is applied for the odd-parity states labeled by the quantum number n_+ and results in $E^{(2)}_{n_+}=0$ for all $n_+<\mathcal{N}$. It should be noted that in the case of $\epsilon=-(4\mathcal{N}\pm1)/3$ $(\mathcal{N}=1,2,3,\ldots)$ the nonperturbative corrections do remain although the models are $\mathcal{N}$-fold supersymmetric, reflecting the fact that they are only quasi-perturbatively solvable but are not quasi-exactly solvable. These results are just what we have expected from the general properties of $\mathcal{N}$-fold supersymmetry.

C. Large order behavior of the perturbation series

The large order behavior of the perturbation series in g^2 for the spectra can be estimated by the same way as in the case of the double-well and periodic potentials. From the nonperturbative contributions Eqs. (5.22)–(5.27), we can easily see that the imaginary parts of them are continuous, at least up to the order α^2, in ϵ and yield

$$\mathrm{Im}\,E_{n_0}\sim-\alpha^2\frac{\pi}{n_0!\Gamma\left(\frac{n_0}{2}+\frac{3}{4}+\frac{3}{4}\epsilon\right)}\left(\frac{2}{g^2}\right)^{n_0}\left(\frac{1}{g^2}\right)^{n_0/2-1/4+(3/4)\epsilon}, \tag{5.28a}$$

$$\mathrm{Im}\,E_{n_\pm}\sim-\alpha^2\frac{\pi}{n_\pm!\Gamma\left(2n_\pm+\frac{3}{2}-\frac{3}{2}\epsilon\right)}\left(\frac{2}{g^2}\right)^{2n_\pm+1/2-(3/2)\epsilon}\left(\frac{1}{g^2}\right)^{n_\pm}, \tag{5.28b}$$

which are valid for arbitrary ϵ. Then, if we expand the spectra in power of g^2 such that

$$E_{n_0/n_\pm}=E^{(0)}_{n_0/n_\pm}+\sum_{r=1}^{\infty}a^{(r)}_{n_0/n_\pm}g^{2r}, \tag{5.29}$$

the large order behavior of the coefficients $a^{(r)}$ for sufficiently large r are calculated as, using Eqs. (4.26) and (5.28),

$$a^{(r)}_{n_0}\sim A_{n_0}(\epsilon)2^r\Gamma\left(r+\frac{3}{2}n_0+\frac{3}{4}+\frac{3}{4}\epsilon\right), \tag{5.30a}$$

$$a^{(r)}_{n_\pm}\sim A_{n_\pm}(\epsilon)2^r\Gamma\left(r+3n_\pm+\frac{3}{2}-\frac{3}{2}\epsilon\right), \tag{5.30b}$$

where

$$A_{n_0}(\epsilon)=\frac{\sqrt{2}}{\pi}\frac{2^{(5/2)n_0+3/4+(3/4)\epsilon}}{n_0!\Gamma\left(\frac{n_0}{2}+\frac{3}{4}+\frac{3}{4}\epsilon\right)}, \tag{5.31a}$$

$$A_{n_\pm}(\epsilon)=\frac{\sqrt{2}}{\pi}\frac{2^{5n_\pm+2-3\epsilon}}{n_\pm!\Gamma\left(2n_\pm+\frac{3}{2}-\frac{3}{2}\epsilon\right)}. \tag{5.31b}$$

Equations (5.30) show that the perturbative coefficients diverge factorially unless the prefactor $A(\epsilon)$'s vanish. From Eq. (5.31), we can find the disappearance of the leading divergence takes place only when $\epsilon=\pm(2n+1)/3$ ($n=1,2,3,\ldots$). More precisely, we obtain the following results:

(1) $\epsilon=(4\mathcal{N}\pm1)/3(\mathcal{N}=1,2,3,\ldots)$

$$A_{n_\pm}(\epsilon)=0 \quad \text{for} \quad n_\pm<\mathcal{N}.$$

(2) $\epsilon=-(4\mathcal{N}+1)/3(\mathcal{N}=1,2,3,\ldots)$

$$A_{2m_0+1}(\epsilon)=0 \quad \text{for} \quad m_0<\mathcal{N}.$$

(3) $\epsilon=-(4\mathcal{N}-1)/3(\mathcal{N}=1,2,3,\ldots)$

$$A_{2m_0}(\epsilon)=0 \quad \text{for} \quad m_0<\mathcal{N}.$$

Comparing these results with Eq. (5.3), we see that the above cases completely coincide with the case where the system possesses Type A $\mathcal{N}$-fold supersymmetry. Again, the results of the valley method analyses are consistent with the non-renormalization theorem.

VI. SUMMARY

In this article, we have made nonperturbative analyses on the models which can be $\mathcal{N}$-fold supersymmetric at specific values of the parameter. Combining the results obtained in this article with the ones in Ref. 2, we get the following:

(1) For all the potentials investigated (double-well, triple-well, periodic), the leading divergence of the perturbation series disappears when and only when they are $\mathcal{N}$-fold supersymmetric. The non-renormalization theorem ensures that $\mathcal{N}$-fold supersymmetry is sufficient for the disappearance of the divergence. The results indicate that it may also be necessary.
(2) The nonperturbative corrections to the spectra for certain states vanish when and only when the models are quasi-exactly solvable (triple-well, periodic).
(3) For the quasi-perturbatively solvable potentials (double-well, triple-well), the nonperturbative corrections remain although they are $\mathcal{N}$-fold supersymmetric.

As was mentioned in Ref. 28 the quasi-solvable models constructed by sl(2) generators do not always have normalizable solvable states. Although the conditions on the normalizability of the models were fully investigated in Ref. 49, it remains unclear what is the role of the partial algebraization of the models without normalizable solvable states. The results listed above provide an answer to this problem. Even though the solvable wave functions are not normalizable, they can be normalizable and thus make sense in the perturbation theory. In this case, the spectra corresponding to the solvable states also make sense in the perturbation theory. As was shown in Ref. 1, the perturbation series for them are convergent since they are the solutions of a finite order algebraic equation. However, the fact that the solvable states and the corresponding spectra make sense only in the perturbation theory inevitably means the existence of the nonperturbative effects, which is in contrast to the case of the quasi-exactly solvable models. That is why we have called the case quasi-perturbatively solvable.

Finally, we would like to mention about applicability of the dilute-gas approximation. As has been mentioned previously, the dilute-gas approximation cannot give proper results, that is, con-

sistent results with $\mathcal{N}$-fold supersymmetry, for both the potentials Eqs. (4.11) and (5.1). Therefore, it seems that the success of the dilute-gas approximation for the symmetric double-well potential is rather exceptional and applicability of it is quite limited.

ACKNOWLEDGMENTS

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Quantum jump dynamics in cavity QED

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We study the stochastic dynamics of the electromagnetic field in a lossless cavity interacting with a beam of two-level atoms, given that the atomic states are measured after they have crossed the cavity. The atoms first interact at the exit of the cavity with a classical laser field $\mathcal{E}$ and then enter into a detector which measures their states. Each measurement disentangles the field and the atoms and changes in a random way the state $|\psi(t)\rangle$ of the cavity field. For weak atom-field coupling, the evolution of $|\psi(t)\rangle$ when many atoms cross the cavity and the detector is characterized by a succession of quantum jumps occurring at random times, separated by quasi-Hamiltonian evolutions, both of which depend on the laser field $\mathcal{E}$. For $\mathcal{E}=0$, the dynamics is the same as in the Monte Carlo wave function model of Dalibard *et al.* [Phys. Rev. Lett. **68**, 580 (1992)] and Carmichael, *An Open System Approach to Quantum Optics*, Lecture Notes in Physics Vol. 18 (Springer, Berlin, 1991)]. The density matrix of the quantum field, obtained by averaging the projector $|\psi(t)\rangle\langle\psi(t)|$ over all results of the measurements, is independent of $\mathcal{E}$ and follows the master equation of the damped harmonic oscillator at finite temperature. We provide numerical evidence showing that for large $\mathcal{E}$, an arbitrary initial field state $|\psi(0)\rangle$ evolves under the monitoring of the atoms and the measurements toward squeezed states $|\alpha,re^{2i\phi}\rangle$, moving in the α-complex plane but with almost constant squeezing parameters r and ϕ. The values of r and ϕ are determined analytically. On the other hand, for $\mathcal{E}=0$, the dynamics transforms the initial state into Fock states $|n\rangle$ with fluctuating numbers of photons n, as shown in Kist *et al.* [J. Opt. B: Quantum Semiclassical Opt. **1**, 251 (1999)]. In the last part, we derive the quantum jump dynamics from the linear quantum jump model proposed in Spehner and Bellissard [J. Stat. Phys. **104**, 525 (2001)], for arbitrary open quantum systems having a Lindblad-type evolution. A careful derivation of the infinite jump rates limit, where the dynamics can be approximated by a diffusion process of the quantum state, is also presented. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The dissipative dynamics of an open quantum system S can be described in two different ways. The first one consists in coupling S with a reservoir R and assuming that the total system $S+R$ is isolated. Since one is concerned by the dynamics of S only, one traces out the degrees of freedom of R in the equation of motion of $S+R$. Within the Markov approximation, the reduced density matrix of S follows a first-order differential equation with time-independent coefficients. In many cases, a separation of time scales between the Hamiltonian (R-independent) and dissipative (R-dependent) evolutions allows one to perform a local averaging in time, which kills nonresonant terms.[1,2] The coarse-grained master equation obtained in this way has the Lindblad form.[3] An alternative approach to this density matrix description has been developed in the last two

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decades in quantum optics[4–8] (see, e.g., Ref. 9), quantum measurement theory,[10–13] quantum and classical stochastic calculus,[14–17] and electronic transport in solids.[18–20] This approach is based on stochastic evolutions of pure states. The system is described by a random wave function (RW) evolving according to a linear or nonlinear *stochastic Schrödinger equation*. Consistency with the density matrix approach requires that the pure state evolution gives the master equation back after averaging over the dynamical noise. Apart from being intuitively appealing, the RW models provide quite efficient tools for solving master equations numerically, since Schrödinger equations have N components, whereas master equations have $N\times N$ components, N being the dimension of the Hilbert space of S. However, the RW models are more than simple mathematical or numerical tools: they describe the *real* evolution of single quantum systems under continuous monitoring by measurements (photon counting, homodyne or heterodyne detections).[5,8,9] In recent years, the attainment of low temperature and low dissipation regimes, as well as the improvements of detection techniques, has allowed the investigation of the dynamics of such continuously monitored systems. Remarkable examples of these are single ions[21] and Bose–Einstein condensates[22] in electromagnetic traps, probed by laser beams, and electromagnetic fields in high Q-cavities,[23] probed by beams of highly excited atoms (Rydberg atoms). This new generation of experiments, combined with the difficulties usually encountered in solving the master equation, has strongly stimulated the developments of the RW approach in quantum optics.

The aim of this paper is to investigate a specific physical realization, which could be in principle realizable experimentally (although this question is not addressed here), of a class of RW models based on quantum jumps. The system we consider is the electromagnetic field of a high Q-cavity interacting with a beam of two-level atoms, which forms the reservoir of temperature T. The states of the atoms leaving the cavity are measured by a detector. A laser field $\mathcal{E}$ is placed between the cavity and the detector. The corresponding master equation, obtained by averaging over the results of the measurement on the atoms, is, for weak atom-field coupling, the equation of the damped harmonic oscillator with finite temperature. The same problem has been considered in Ref. 24 in the reverse situation where one knows exactly the state of each atom before it crosses the cavity and no measurement is performed on it at the exit (its final state thus being unknown). It has been shown in this reference that the cavity field evolves at large times to a state which is completely controlled by the atomic initial states.

We first introduce in Sec. II the class of quantum jump models studied in this work, for arbitrary open systems having a Lindblad-type evolution. The experimental scheme is presented in Sec. III, where we also compute the random evolution of the cavity field and its corresponding average evolution. We focus in Sec. IV on single quantum trajectories, i.e., single realizations of the measurements. The numerical simulations and analytical results presented in this section show that for $T>0$ and large laser fields $\mathcal{E}$, the state of the cavity field localizes at large times to squeezed states with an almost constant squeezing amplitude r which depends only on T. Section V is devoted to the derivation, for arbitrary open systems, of the nonlinear quantum jump schemes from the corresponding linear ones introduced in Ref. 18. Their relation with the so-called quantum state diffusion stochastic Schrödinger equations[10–12,15–17] is also established. Our conclusions are presented in Sec. VI.

II. THE QUANTUM JUMP SCHEMES

Let us first recall briefly a few basic facts about the master equation approach to open quantum systems. Consider an open system S interacting with a reservoir R. The density matrix σ of the total system $S+R$ is assumed to follow the Liouville–von Neumann equation of closed systems. A state of S is specified by the reduced density matrix ρ, defined as the partial trace of σ over the reservoir's Hilbert space. By tracing out the degrees of freedom of R in the Liouville–von Neumann equation, one obtains an integro-differential equation for ρ (Nakajima–Zwanzig equation).[25] Using a Born–Markov approximation and a local time averaging on a time scale much larger than the inverse Bohr frequencies of S, this equation is transformed into a simpler first-order linear differential equation, called the *master equation*.[1,25] This coarse-grained equation has in most cases the Lindblad form:[3]

$$\frac{d\rho}{dt} = -i[H,\rho] + \frac{1}{2}\sum_m ([L_m\rho, L_m^\dagger] + [L_m, \rho L_m^\dagger]). \tag{1}$$

H is the Hamiltonian of S (including the energy shifts due to the coupling with the reservoir), and L_m are some operators acting on the Hilbert space of S. The sum over the discrete indices m can be finite or infinite, depending on the nature of the problem.

We now describe the random wave function approach of Dalibard, Castin, and Mølmer[4] and Carmichael.[5] This approach, called in the former reference the Monte Carlo wave function method, has been introduced independently by several other authors.[6,7,13] It is based on quantum jumps, i.e., on discontinuous random evolutions of the wave function of S.

At some random times, quantum jumps (QJ) occur as a result of some continuous measurement on the system S (e.g., a detection of a photon emitted by a system constituted by an atom). If a jump occurs, the wave function $|\psi\rangle$ of S is modified discontinuously as follows:

$$\text{jump } m: \quad |\psi\rangle \to \frac{L_m|\psi\rangle}{\|L_m|\psi\rangle\|}, \tag{2}$$

where L_m are the Lindblad operators appearing in (1). The probability of occurrence of a jump of type m in the time interval $[t, t+\delta t]$ is

$$\delta p_m(t) = \|L_m|\psi(t)\rangle\|^2 \delta t. \tag{3}$$

One must choose δt small enough so that $\delta p_m(t) \ll 1$ for any $|\psi\rangle$ and all m's (this is fulfilled if δt^{-1} is much bigger than the damping constants γ_m appearing in the master equation, contained in the operators L_m). If no jump occurs between t and $t+\delta t$, the wave function evolves between these two times according to Schrödinger's equation with an effective Hamiltonian $H+K$, and is then normalized at $t+\delta t$:

$$\begin{aligned} |\psi(t+\delta t)\rangle &= \frac{|\varphi(t+\delta t)\rangle}{\|\varphi(t+\delta t)\|}, \\ |\varphi(t+\delta t)\rangle &= e^{-i\delta t(H+K)}|\psi(t)\rangle. \end{aligned} \tag{4}$$

K can be computed in special cases by first determining perturbatively the wave function of the total system $S+R$ and then projecting it onto the subspace corresponding to the no-jump measurement.[4,9] An easier (though less fundamental) way to compute K is to ask directly that the average $\mathsf{M}|\psi(t)\rangle\langle\psi(t)|$ satisfies the master equation (1) (see the following). This gives[4]

$$K = K_0 \equiv \frac{1}{2i}\sum_m L_m^\dagger L_m. \tag{5}$$

Note that K_0 is *not* self-adjoint. Hence the norm of the wave function is not conserved by the evolution operator $e^{-i\delta t(H+K_0)}$. This can be interpreted by invoking the gain of information on the system provided by the measurement, namely, by the knowledge that no jump occurred between t and $t+\delta t$. For instance, in the case of an atom coupled to the quantized electromagnetic field, we may infer from a no-photon detection that the atom has not emitted spontaneously a photon.

Since the wave function is normalized at each step δt in (2) and (4), the random dynamics is norm-preserving on the time resolution δt. These normalizations make the stochastic quantum evolution nonlinear. We will see in Sec. V that it is possible to define an equivalent linear model, in which the random wave function is not normalized.[18,14] The map $t \in [0,\infty[\mapsto |\psi(t)\rangle$ for a given outcome of the jumps is called a *quantum trajectory*.[5]

Let us consider the average density matrix $\rho(t) = \mathsf{M}|\psi(t)\rangle\langle\psi(t)|$, where M is the average over all realizations of the jumps. It can be easily shown[4] that $\rho(t)$ obeys the master equation (1) to lowest order in $\|L_m\|^2\delta t$. Actually, taking $H=0$ for simplicity, one has

$$\rho(t+\delta t)=\mathsf{M}_{t+\delta t}|\psi(t+\delta t)\rangle\langle\psi(t+\delta t)|$$
$$=\mathsf{M}_t\left(\left(1-\sum_m \delta p_m(t)\right)\frac{e^{-i\delta tK_0}|\psi(t)\rangle\langle\psi(t)|e^{i\delta tK_0^\dagger}}{\|e^{-i\delta tK_0}|\psi(t)\rangle\|^2}+\sum_m \delta p_m(t)\frac{L_m|\psi(t)\langle\psi(t)|L_m^\dagger}{\|L_m|\psi(t)\rangle\|^2}\right).$$

This equation is simplified by taking

$$e^{-i\delta tK_0}=\left(1-\delta t\sum_m L_m^\dagger L_m\right)^{1/2}. \tag{6}$$

Then, by (3):

$$\rho(t+\delta t)=\left(1-\delta t\sum_m L_m^\dagger L_m\right)^{1/2}\rho(t)\left(1-\delta t\sum_m L_m^\dagger L_m\right)^{1/2}+\delta t\sum_m L_m\rho(t)L_m^\dagger. \tag{7}$$

Expanding the square roots and keeping only terms of order one in δt, one obtains (1) and K_0 is given by (5). Note that, for an arbitrary time interval δt between consecutive measurements, $\rho(t+\delta t)$ is *not* given by integrating (1) from t to $t+\delta t$ (a different result is already obtained at the next order δt^2). This should be kept in mind when dealing with real or numerical experiments, where δt is always finite.

Consider a transformation $L_m\to L_m'$ on the operators L_m which does not change (1). The quantum jumps and the effective Hamiltonian K may be modified by this replacement. This leads to a different stochastic dynamics, which unravels the same master equation. A particular transformation leaving (1) invariant is[26]

$$L_m\to L_m'=L_m+\lambda_m,\quad H\to H'=H+\frac{1}{2i}\sum_m(\lambda_m^* L_m-\lambda_m L_m^\dagger)=H'^\dagger, \tag{8}$$

where λ_m's are complex numbers. This invariance of the Lindblad equation is not related to a particular symmetry of the system or its coupling with the reservoir. It simply expresses that the separation between the Hamiltonian part $-i[H,\rho]$ and the remaining dissipative part in (1) is not unique. The transformation (8) generates a whole family of distinct QJ models depending on the set of numbers λ_m. The modification of the wave function at a jump m is now given by

$$\text{jump } m:\quad |\psi\rangle\to\frac{W_m|\psi\rangle}{\|W_m|\psi\rangle\|} \tag{9}$$

with the jump operators W_m proportional to $(L_m+\lambda_m)$:

$$W_m=\gamma_m^{-1/2}(L_m+\lambda_m). \tag{10}$$

The new generalized Hamiltonian $H+K$ is obtained by replacing L_m by L_m' in (5) and adding to it $H'-H$:

$$K=\frac{1}{2i}\sum_m(L_m^\dagger L_m+2\lambda_m^* L_m+|\lambda_m|^2). \tag{11}$$

The last term in the sum, proportional to the identity operator, is written only for convenience: it is irrelevant because of the normalization in Eq. (4) giving the evolution between jumps. The probability of occurrence of a jump of type m becomes

$$\delta p_m(t)=\|(L_m+\lambda_m)|\psi(t)\rangle\|^2\delta t=\gamma_m\delta t\,\|W_m|\psi(t)\rangle\|^2. \tag{12}$$

Note that it increases like $|\lambda_m|^2$ for large λ_m.

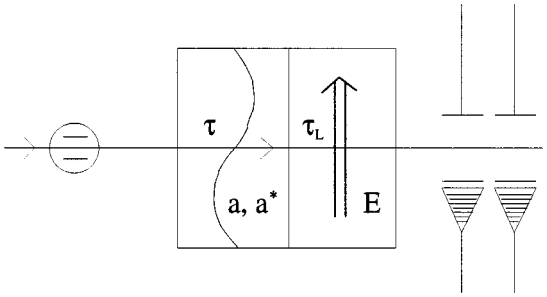

FIG. 1. The two-level atoms of the beam cross one by one a cavity containing the studied quantum field a, a second cavity containing a laser field $\mathcal{E}$, and a detector measuring their states.

III. FIELD MODE IN A CAVITY

It is shown in this section that the QJ schemes described in Sec. II can be physically realized by an atomic beam crossing a cavity with perfectly reflecting walls and interacting with the quantum field inside, which forms the system S. The measurements are performed on the outgoing atoms, after they have interacted with a classical laser field $\mathcal{E}$ placed between the cavity and the measuring apparatus.

A. Experimental scheme

Let us consider one mode of the quantized electromagnetic field of a lossless cavity coupled to its environment. The environment is a beam of atoms prepared in one of two Rydberg states $|g\rangle$ (''ground state'') and $|e\rangle$ (''excited state'') in resonance with the frequency ω of the mode. The fluxes r_g and r_e of atoms crossing the cavity, prepared, respectively, in states $|g\rangle$ and $|e\rangle$, are assumed to be such that at most one atom is in the cavity at any time. The time interval between the crossing of two consecutive atoms in the cavity is $\delta t=(r_g+r_e)^{-1}$. To simplify, all the atoms of the beam are supposed to have the same speed. They thus spend the same time $\tau<\delta t$ in the cavity, interacting with the field mode. The atom-mode interaction Hamiltonian is in the interaction picture (rotating-wave approximation):[1,2]

$$H_{\rm int}=-i\,(\lambda^*|g\rangle\langle e|\,a^\dagger-\lambda|e\rangle\langle g|\,a), \tag{13}$$

where $a^\dagger$ and a are the creation and annihilation operators of a photon. The coupling constant λ is equal to $\sqrt{q^2\omega/2\varepsilon_0 V}\,\vec{d}_{ge}\cdot\vec{\sigma}$, where $\vec{d}_{ge}$ is the matrix element of the atomic dipole, $\vec{\sigma}$ the polarization vector of the field mode, q the charge of the electron, and V the volume of the cavity.

At the exit of the cavity, the atoms enter into a second cavity, identical to the first but containing a classical laser field $\vec{\mathcal{E}}$ (Fig. 1). They spend a time $\tau_L<\delta t$ there, interacting with the laser field. Under the dipolar and rotating-wave approximations, the atom-laser interaction Hamiltonian is in the interaction picture:[1,2]

$$H_L=-\frac{i}{2}(\Omega^*|g\rangle\langle e|-\Omega|e\rangle\langle g|), \tag{14}$$

where $\Omega=i\,\vec{d}_{ge}\cdot\vec{\mathcal{E}}$ is the Rabi frequency. The Hamiltonian (14) describes the atom-laser interaction for a laser field in resonance with the atomic transition. The more general situation of nonzero detuning of the laser frequency will be discussed in the following.

Finally, the state of each atom at the exit of the second cavity is measured by a detector, telling us if it is in its ''ground'' or in its ''excited'' state. The corresponding experimental scheme is presented in Fig. 1. It has been considered in Ref. 27 without the laser field $\mathcal{E}$. The flight times of the atoms between the two cavities and between the second cavity and the detector are taken sufficiently small so that spontaneous emission of photons by the atoms can be neglected.

B. Stochastic dynamics of the field mode

Let us compute the evolution of the state of the field mode in the first cavity, for a given result of the measurements. If one looks at it with a time resolution equal or bigger than the time δt separating the entrance of consecutive atoms, the field mode is continuously monitored by the measurements on the atoms (continuous measurement). The coupling constant λ, the Rabi frequency Ω, and the interaction times τ, τ_L are assumed to satisfy

$$|\lambda|\tau \ll 1, \quad |\Omega|\tau_L \ll 1. \tag{15}$$

Let us first determine the change of the wave function $|\psi(t)\rangle$ of the field mode when one atom, initially in state $|i\rangle$, $i=g$ or e, crosses the two cavities and the detector. At the time t just prior to the entrance of the atom in the first cavity, the wave function $|\Psi(t)\rangle$ of the total system "atom+field mode" is a tensor product state $|\Psi(t)\rangle = |i\rangle|\psi(t)\rangle$ (the atom and the field did not yet interact). Since the two fields are in separated cavities, the atom interacts with the quantum field *before* interacting with the classical field $\mathcal{E}$. The total wave function at the exit of the second cavity (before the measurement) is thus, in the interaction picture,

$$|\Psi_{\text{ent}}\rangle = e^{-i\,\tau_L H_L}\, e^{-i\,\tau H_{\text{int}}} |i\rangle|\psi(t)\rangle. \tag{16}$$

Note that the evolution would be different if the laser field was placed in the first cavity (in this case, the product of exponentials must be replaced by the exponential of $H_{\text{int}}+H_L$). Because of their interaction, the quantum field and the atom are now entangled, i.e., $|\Psi_{\text{ent}}\rangle$ is not a product state. After the measurement on the atom has been performed, the field and the atom again become disentangled and the wave function of the total system is

$$|\Psi(t+\delta t)\rangle = |j\rangle|\psi(t+\delta t)\rangle, \quad |\psi(t+\delta t)\rangle = \frac{\langle j|\Psi_{\text{ent}}\rangle}{\|\langle j|\Psi_{\text{ent}}\rangle\|}, \tag{17}$$

with $j=g$ if the atom is detected in its ground state and $j=e$ if it is detected in its excited state. We have assumed for simplicity that the measurement is performed at a time $t+\tau_{\text{mes}} < t+\delta t$ earlier than the entrance of the next atom in the first cavity. Since we work in the interaction picture, $|\Psi(t+\tau_{\text{mes}})\rangle$ is then equal to $|\Psi(t+\delta t)\rangle$. The wave function $|\psi(t+\delta t)\rangle$ of the mode at the time $t+\delta t$ is thus well-defined and given by

$$\begin{aligned} |\psi(t+\delta t)\rangle &= \frac{|\varphi(t+\delta t)\rangle}{\|\varphi(t+\delta t)\|}, \\ |\varphi(t+\delta t)\rangle &= \langle j|e^{-i\tau_L H_L} e^{-i\tau H_{\text{int}}}|i\rangle|\psi(t)\rangle. \end{aligned} \tag{18}$$

The probability that the atom is detected in state $|j\rangle$, given that it enters in the cavity in state $|i\rangle$, is

$$p_{i\to j} = \|\langle j|\Psi_{\text{ent}}\rangle\|^2 = \|\varphi(t+\delta t)\|^2. \tag{19}$$

A straightforward computation leads to

$$\begin{aligned} e^{-i\tau H_{\text{int}}} = &\sum_{p=0}^{\infty} \frac{(-|\lambda|^2\tau^2)^p}{(2p)!}\left(|g\rangle\langle g|\, n^p + |e\rangle\langle e|\,(n+1)^p\right) \\ &+ \sum_{p=0}^{\infty} \frac{(-|\lambda|^2\tau^2)^p}{(2p+1)!}\left(\lambda\tau|e\rangle\langle g|\, a\, n^p - \lambda^*\tau|g\rangle\langle e|\, n^p\, a^\dagger\right), \end{aligned}$$

where $n=a^\dagger a$ is the number operator. Denoting by $n^{1/2}$ its square root, this formula can be rewritten in a more compact form:

$$e^{-i\tau H_{\rm int}} = |g\rangle\langle g|\cos(|\lambda|\tau n^{1/2}) + |e\rangle\langle e|\cos(|\lambda|\tau(n+1)^{1/2}) + \lambda\tau|e\rangle\langle g|\, a\,\mathrm{sinc}(|\lambda|\tau n^{1/2}) - \lambda^*\tau|g\rangle\langle e|\,\mathrm{sinc}(|\lambda|\tau n^{1/2})\, a^\dagger \tag{20}$$

with $\mathrm{sinc}(u) = (\sin u)/u$. Similarly,

$$e^{-i\tau H_L} = \cos\left(\frac{|\Omega|\tau_L}{2}\right) + \frac{\Omega\tau_L}{2}|e\rangle\langle g|\,\mathrm{sinc}\left(\frac{|\Omega|\tau_L}{2}\right) - \frac{\Omega^*\tau_L}{2}|g\rangle\langle e|\,\mathrm{sinc}\left(\frac{|\Omega|\tau_L}{2}\right).$$

Let us introduce the operator

$$\tilde{a} = a\,\mathrm{sinc}(|\lambda|\tau n^{1/2}) \tag{21}$$

and the complex numbers

$$\eta = \lambda\tau, \quad \epsilon = \frac{\Omega\tan(|\Omega|\tau_L/2)}{|\Omega|\lambda\tau}. \tag{22}$$

Four cases must be considered.

(1) The atom enters the first cavity in its ground state and is detected in the same state: $i=j=g$. Then,

$$|\varphi(t+\delta t)\rangle = (1+|\eta\epsilon|^2)^{-1/2}(\cos(|\eta|n^{1/2}) - |\eta|^2\epsilon^*\tilde{a})|\psi(t)\rangle \equiv (1 - i\,\delta t\, K_g)|\psi(t)\rangle. \tag{23}$$

(2) The atom enters the first cavity in its ground state and is detected in its excited state: $i=g$, $j=e$. Then,

$$|\varphi(t+\delta t)\rangle = \eta\,(1+|\eta\epsilon|^2)^{-1/2}\, W_-|\psi(t)\rangle, \quad W_- \equiv \tilde{a} + \epsilon\cos(|\eta|n^{1/2}). \tag{24}$$

(3) The atom enters the first cavity in its excited state and is detected in its ground state: $i=e$, $j=g$. Then,

$$|\varphi(t+\delta t)\rangle = -\,\eta^*(1+|\eta\epsilon|^2)^{-1/2}\, W_+|\psi(t)\rangle, \quad W_+ \equiv \tilde{a}^\dagger + \epsilon^*\cos(|\eta|(n+1)^{1/2}). \tag{25}$$

(4) The atom enters the first cavity in its excited state and is detected in the same state: $i=j=e$. Then,

$$|\varphi(t+\delta t)\rangle = (1+|\eta\epsilon|^2)^{-1/2}(\cos(|\eta|(n+1)^{1/2}) - |\eta|^2\epsilon\,\tilde{a}^\dagger)|\psi(t)\rangle \equiv (1 - i\,\delta t\, K_e)|\psi(t)\rangle. \tag{26}$$

Cases (2) and (3) correspond, respectively, to the absorption and the emission of a photon of the cavity mode or of the laser field by the atom. In order to have quantum jumps separated by ''continuous'' Hamiltonian evolutions on time scales bigger than δt, the probabilities of these events must be very small. The probability $\delta p_-(t)$ of case (2) is equal to $p_{g\to e}$ multiplied by the probability $r_g\,\delta t$ that the atom enters in the first cavity in state $|g\rangle$. With the help of (19) and (24), one gets

$$\delta p_-(t) = \frac{r_g\,\delta t\,|\eta|^2}{1+|\eta\epsilon|^2}\|W_-|\psi(t)\rangle\|^2 = r_g\,\delta t(\|\sin(|\eta|n^{1/2})|\psi(t)\rangle\|^2 + \mathcal{O}(\eta\epsilon)). \tag{27}$$

The probability $\delta p_+(t)$ of case (3) is given by a similar formula, replacing r_g by r_e, W_- by W_+, and n by $n+1$. The probabilities of cases (1) and (4) are, respectively, $r_g\,\delta t - \delta p_-(t)$ and $r_e\,\delta t - \delta p_+(t)$. We see that $\delta p_\pm(t)$ is small if $|\eta| = |\lambda|\tau \ll 1$ and $|\eta\epsilon| \simeq |\Omega|\tau_L/2 \ll 1$, provided that also

$$\langle\psi(t)|(|\eta|n^{1/2} - k\pi)^{2q}|\psi(t)\rangle = \mathcal{O}(\eta^q), \quad q = 1,2,\ldots, \tag{28}$$

with k a non-negative integer. This condition is met for $k=0$ if the maximal number of photons in the cavity is much smaller than $|\eta|^{-2}$ (of order $|\eta|^{-1}$ or smaller). This corresponds to the perturbative regime. If the condition is met for $k\geqslant 1$, the atom makes almost $k/2$ Rabi oscillations in the cavity and leaves it, with a high probability, nearly in the same state as it entered it. Indeed, neglecting terms of order η^2 and $\eta^4\epsilon^4$, it follows from (22), (23), and (26):

$$\begin{aligned}\delta t K_g &\simeq \frac{|\eta|^2}{2i}(\tilde{a}^\dagger\tilde{a}+2(-1)^k\epsilon^*\tilde{a}+|\epsilon|^2),\\ \delta t K_e &\simeq \frac{|\eta|^2}{2i}(\tilde{a}\,\tilde{a}^\dagger+2(-1)^k\epsilon\,\tilde{a}^\dagger+|\epsilon|^2),\end{aligned} \tag{29}$$

up to an irrelevant additional phase $k\pi$. When the atom is measured in the same state as its initial state [cases (1) and (4)], the normalized wave function of the mode is thus modified, up to a sign, by an amount of order $|\eta|+|\eta^{3/2}\epsilon|$. In the opposite cases (2) and (3), the mode wave function is modified by an amount of order 1. It suffers a quantum jump:

$$|\psi(t+\delta t)\rangle = \frac{W_\pm|\psi(t)\rangle}{\|W_\pm|\psi(t)\rangle\|}, \tag{30}$$

with the jump operators

$$\begin{aligned}W_- &\simeq \tilde{a}+(-1)^k\epsilon,\\ W_+ &\simeq \tilde{a}^\dagger+(-1)^k\epsilon^*.\end{aligned} \tag{31}$$

The signs $-$ and $+$ correspond to case (2) (absorption of a photon) and case (3) (emission of a photon), respectively. The probability that a jump $\pm$ occurs is of order $|\eta|+|\eta^{3/2}\epsilon|+|\eta\epsilon|^2$, see (27) and (28). It is given approximately by

$$\delta p_\pm(t) \simeq \gamma_\pm\,\delta t\|W_\pm|\psi(t)\rangle\|^2, \tag{32}$$

where we have introduced the damping rates:

$$\begin{aligned}\gamma_- &= r_g|\eta|^2 = r_g|\lambda|^2\tau^2,\\ \gamma_+ &= r_e|\eta|^2 = r_e|\lambda|^2\tau^2.\end{aligned} \tag{33}$$

The operator $\tilde{a}$ is given, up to terms of order $\eta^{1/2}$, by

$$\tilde{a} \simeq \begin{cases} a & \text{if } k=0\\ (-1)^k a\left(\dfrac{|\eta|n^{1/2}-k\pi}{k\pi}-\dfrac{(|\eta|n^{1/2}-k\pi)^2}{(k\pi)^2}\right) & \text{if } k\geqslant 1.\end{cases} \tag{34}$$

If $|\psi(t)\rangle=|n\rangle$ is a Fock state with $n=(k\pi/|\eta|)^2$ photons, the crossing of the atom of initial state $|i\rangle$ has no effect on the field if $i=g$ (since $\tilde{a}|\psi(t)\rangle=0$), and a small effect if $i=e$ and $|\eta|\ll 1$.

If condition (28) is not met, the atom strongly modifies the state of the field mode in all cases (1)–(4). Hence there is no ''continuous-like'' Hamiltonian evolution changing weakly the state of the mode, separated by unlikely jumps. For $\epsilon=0$, the evolutions for $i=g$ [Eq. (23)] and $i=e$ [Eq. (26)] have the form (6) (the jump operators $W_\pm$ are proportional to $\tilde{a}^\dagger$ and $\tilde{a}$, respectively, and $\cos^2(|\eta|n^{1/2})=1-|\eta|^2\tilde{a}^\dagger\tilde{a}$, $\cos^2(|\eta|(n+1)^{1/2})=1-|\eta|^2\tilde{a}\tilde{a}^\dagger$). Although there is *a priori* no conceptual difficulty in treating this case, the corresponding dynamics becomes cumbersome when many atoms cross the cavities. We thus restrict ourself in what follows to the simpler situation in which conditions (15) and (28) are fulfilled.

Let us determine the change of the wave function of the field mode when many atoms cross the cavities. Let Δt be such that the number $\Delta t/\delta t$ of atoms crossing the cavities in a time interval $[t,t+\Delta t]$ is large but much smaller than the inverse of the coupling strength $|\eta|$:

$$1 \ll \frac{\Delta t}{\delta t} \ll |\eta|^{-1}, |\eta^{3/2}\epsilon|^{-1}, |\eta\epsilon|^{-2}. \tag{35}$$

Assuming that r_g and r_e are of the same order of magnitude, the numbers of atoms entering in the first cavity in state $|g\rangle$ and $|e\rangle$ between t and $t+\Delta t$ are large and approximately equal to $r_g\Delta t$ and $r_e\Delta t$, respectively. Since the probabilities $\delta p_\pm(t)$ of occurrence of jumps when one atom crosses the cavities are assumed to be as small as $|\eta|+|\eta^{3/2}\epsilon|+|\eta\epsilon|^2$, the probability of occurrence of two or more jumps between t and $t+\Delta t$ is negligible. Suppose first that no jump occur between these two times, i.e., that only cases (1) and (4) occur for all atoms. Then,

$$|\varphi(t+\Delta t)\rangle = \cdots(1-i\,\delta t K_g)\cdots(1-i\,\delta t K_e)\cdots(1-i\,\delta t K_g)\cdots|\psi(t)\rangle. \tag{36}$$

There are $r_g\Delta t$ factors $(1-i\,\delta t K_g)$ and $r_e\Delta t$ factors $(1-i\,\delta t K_e)$. Let us expand the products and neglect terms of order $(\Delta t/\delta t)^2|\eta^{(4+m)/2}\epsilon^m|$, $m=0,\ldots,4$, which are small by (35). We find:

$$\begin{aligned} |\psi(t+\Delta t)\rangle &= \frac{|\varphi(t+\Delta t)\rangle}{\|\varphi(t+\Delta t)\|}, \\ |\varphi(t+\Delta t)\rangle &\simeq (1-i\Delta t K)|\psi(t)\rangle, \end{aligned} \tag{37}$$

with $K = r_g\delta t K_g + r_e\delta t K_e$. Note that the change $|\varphi(t+\Delta t)\rangle - |\varphi(t)\rangle$ is proportional to Δt. The effective Hamiltonian K is the average of the operators K_i, which describe the evolution of the quantum field as one *given* atom crosses the cavities without absorbing or emitting a photon, over its (unknown) initial state $|i\rangle$ ($i=g$ with probability $r_g\delta t$, and $i=e$ with probability $r_e\delta t$). This averaging is related to our assumption that many atoms cross the cavities between t and $t+\Delta t$; it is an average over the initial states of the atoms, and must be distinguished from the average over the results of the measurements. Equation (29) gives

$$K = \frac{1}{2i}(\gamma_-(\tilde{a}^\dagger\tilde{a} + 2(-1)^k\epsilon^*\tilde{a} + |\epsilon|^2) + \gamma_+(\tilde{a}\tilde{a}^\dagger + 2(-1)^k\epsilon\tilde{a}^\dagger + |\epsilon|^2)). \tag{38}$$

If a jump $\pm$ occurs between t and $t+\Delta t$, the change of the wave function is approximately

$$|\psi(t+\Delta t)\rangle = \frac{W_\pm|\psi(t)\rangle}{\|W_\pm|\psi(t)\rangle\|}. \tag{39}$$

Actually, the change due to atoms crossing the cavities without modifying their states [cases (1) and (4)] between t and $t+\Delta t$ is of order $(\Delta t/\delta t)(|\eta|+|\eta^{3/2}\epsilon|)$. It can be neglected with respect to the change due to an atom having emitted or absorbed a photon, of order 1. Similarly, the probability $\Delta p_\pm(t)$ of occurrence of a jump $\pm$ in the time interval $[t,t+\Delta t]$ is obtained by replacing δt by Δt in (32).

The above coarse-grained stochastic dynamics coincides for $\gamma_+ = r_e = 0$ with that considered by Wiseman and Milburn[8] for a damped mode monitored by homodyne detection. In the Schrödinger picture, the mode wave function $|\psi_S(t+\Delta t)\rangle$ is given by (39), in which $W_\pm$ is replaced by $W_\pm^S(t) = e^{-itH}W_\pm e^{itH}$, if a jump $\pm$ occurs between t and $t+\Delta t$. In the opposite (and much more probable) case, it is given by (37), with K replaced by $H+K_S(t)$, $K_S(t) = e^{-itH}Ke^{itH}$. Here $H = \omega(a^\dagger a + 1/2)$ is the free Hamiltonian of the field mode, and we have assumed $\omega\Delta t \ll 1$. The jump operators in the Schrödinger picture are, up to irrelevant phase factors, $W_-^S(t) = \tilde{a} + (-1)^k\epsilon e^{-i\omega t}$ and $W_+^S(t) = \tilde{a}^\dagger + (-1)^k\epsilon^* e^{i\omega t}$. Like the Hamiltonian $H_{\rm int}$, $W_\pm$ depends on time in the Schrödinger picture and is time-independent in the interaction picture. The dynamics in the

Schrödinger picture is the same as in the interaction picture provided that ϵ is replaced by an oscillating field $\epsilon(t)=\epsilon e^{-i\omega t}$. This is also true for the dynamics between jumps, $K_S(t)$ being obtained from (38) by the same rule.

For $\epsilon=0$, the random evolution of $|\psi_S(t)\rangle$ coincides with the random evolution in the model of Dalibard *et al.*,[4] in agreement with the results of Ref. 27. For $\epsilon\neq 0$, it coincides with the QJ evolution of Sec. II with the two Lindblad operators $L_-=\sqrt{\gamma_-}\tilde{a}$ and $L_+=\sqrt{\gamma_+}\tilde{a}^\dagger$, and with $\lambda_- = \sqrt{\gamma_-}(-1)^k\epsilon e^{-i\omega t}$, $\lambda_+=\sqrt{\gamma_+}(-1)^k\epsilon^* e^{i\omega t}$.

All the results of this section are actually valid for an arbitrary Hamiltonian H_L—describing the interaction of the two-level atoms with an arbitrary external field placed between the first cavity and the detector—such that $\|H_L\|\tau_L \ll 1$. In fact, if we define $\epsilon = \langle e|e^{-i\tau_L H_L}|g\rangle/\lambda\tau\langle e|e^{-i\tau_L H_L}|e\rangle$, the only change in the calculation is the replacement of the prefactor $(1-|\eta\epsilon|^2)^{-1/2}$ by $\langle g|e^{-i\tau_L H_L}|g\rangle$ in (23) and (25) and by $\langle e|e^{-i\tau_L H_L}|e\rangle$ in (24) and (26). In particular, the stochastic dynamics is not modified if the laser frequency is detuned from the atomic frequency by $\delta=\omega_L-\omega$, with $|\delta|\tau_L\ll 1$. This is because ϵ is independent of δ in leading order in $\|H_L\|\tau_L$, i.e., the interaction time τ_L is too short for the atoms to feel the frequency shift from the atomic transition.

C. Average dynamics of the field mode

In order to relate the random wave function dynamics with the familiar density matrix approach, let us compute the master equation satisfied by the field mode density matrix:

$$\rho(t)=\mathsf{M}|\psi(t)\rangle\langle\psi(t)|, \tag{40}$$

where M denotes the mean value over the results of the measurements on the atoms (i.e., over all quantum trajectories).

As is well known, averaging the projector $|\psi(t)\rangle\langle\psi(t)|$ over all results of the measurements is the same as not performing any measurement. One may therefore equivalently determine the differential equation for the reduced density matrix $\tilde{\rho}(t)$ of the photon mode, in the same experimental scheme as in Fig. 1 but *without the detector*. The reduced density matrix $\tilde{\rho}(t)$ is defined as the partial trace over the atomic Hilbert spaces of the density matrix $\sigma(t)$ of the total system "atoms+field mode" (see Sec. II):

$$\tilde{\rho}(t)=\operatorname*{tr}_A(\sigma(t)). \tag{41}$$

In order to justify the above-mentioned statement, let us show that the changes of $\rho(t)$ and $\tilde{\rho}(t)$ when one atom crosses the cavities are the same. The atom arrives in the first cavity in state $|i\rangle$, $i=g$ or $i=e$. Before it enters in the cavity, the total density matrix $\sigma(t)$ is a tensor product $|i\rangle\langle i|\otimes\tilde{\rho}(t)$. We assume that $\tilde{\rho}(t)=\rho(t)=\mathsf{M}|\psi(t)\rangle\langle\psi(t)|$. It follows from the second equality in (17), from (19), and from the fact that the measurements on the atoms are independent:

$$\rho(t+\delta t)=\mathsf{M}_{t+\delta t}|\psi(t+\delta t)\rangle\langle\psi(t+\delta t)|=\operatorname*{tr}_A(\mathsf{M}_t|\Psi_{\mathrm{ent}}\rangle\langle\Psi_{\mathrm{ent}}|), \tag{42}$$

where $|\Psi_{\mathrm{ent}}\rangle$ is given by (16). Thus,

$$\rho(t+\delta t)=\operatorname*{tr}_A(e^{-i\tau_L H_L}e^{-i\tau H_{\mathrm{int}}}|i\rangle\langle i|\rho(t)e^{i\tau H_{\mathrm{int}}}e^{i\tau_L H_L})=\tilde{\rho}(t+\delta t)=\operatorname*{tr}_A(e^{-i\tau H_{\mathrm{int}}}\sigma(t)e^{i\tau H_{\mathrm{int}}}). \tag{43}$$

Hence the changes of $\rho(t)$ and $\tilde{\rho}(t)$ are identical as one atom crosses the cavities. The two exponentials of H_L in (43) disappear by cyclicity of the trace, showing that $\tilde{\rho}(t+\delta t)=\rho(t+\delta t)$ does not depend on the laser field $\mathcal{E}$. This last point is actually clear, since if no measurement on the atoms is performed, their interaction with the laser field in the second cavity has no effect on the field in the first cavity.

Since they have the same time evolution, we identify in what follows $\rho(t)$ and $\tilde{\rho}(t)$ and compute the master equation for the usual density matrix (41). Two cases must be distinguished.

(1) The atom enters in the first cavity in its ground state: $i=g$. By replacing (20) into (43),

$$\rho(t+\delta t)=(1-|\eta|^2\tilde{a}^\dagger\tilde{a})^{1/2}\rho(t)(1-|\eta|^2\tilde{a}^\dagger\tilde{a})^{1/2}+|\eta|^2\tilde{a}\rho(t)\tilde{a}^\dagger\equiv(1+\delta t\mathcal{L}_g)\rho(t), \tag{44}$$

where $\tilde{a}$ is given by (21).

(2) The atom enters in the first cavity in its excited state: $i=e$. Then,

$$\rho(t+\delta t)=(1-|\eta|^2\tilde{a}\tilde{a}^\dagger)^{1/2}\rho(t)(1-|\eta|^2\tilde{a}\tilde{a}^\dagger)^{1/2}+|\eta|^2\tilde{a}^\dagger\rho(t)\tilde{a}\equiv(1+\delta t\mathcal{L}_e)\rho(t). \tag{45}$$

For a given initial state of the atom, the evolution in (44) and (45) has the general form (7). Under the conditions (15) and (28), one has

$$\begin{aligned}\delta t\mathcal{L}_g(\rho)&\simeq|\eta|^2(\tilde{a}\rho\tilde{a}^\dagger-\tfrac{1}{2}\{\tilde{a}^\dagger\tilde{a},\rho\}),\\ \delta t\mathcal{L}_e(\rho)&\simeq|\eta|^2(\tilde{a}^\dagger\rho\tilde{a}-\tfrac{1}{2}\{\tilde{a}\tilde{a}^\dagger,\rho\}),\end{aligned} \tag{46}$$

where the curly brackets denote the anticommutator $\{A,B\}=AB+BA$.

Let us determine the coarse-grained evolution of $\rho(t)$ on the time scale Δt satisfying (35). By the same arguments as in Sec. III B,

$$\rho(t+\Delta t)=\cdots(1+\delta t\mathcal{L}_g)\cdots(1+\delta t\mathcal{L}_e)\cdots(1+\delta t\mathcal{L}_g)\cdots\rho(t),$$

with $r_g\Delta t$ factors $(1+\delta t\mathcal{L}_g)$ and $r_e\Delta t$ factors $(1+\delta t\mathcal{L}_e)$. One can retain only the terms of order one in Δt in the expansion of the product:

$$\rho(t+\Delta t)\simeq\{1+\Delta t(r_g\delta t\mathcal{L}_g+r_e\delta t\mathcal{L}_e)\}\rho(t). \tag{47}$$

The superoperator inside the parentheses is the average of the superoperator $\mathcal{L}_i$ over the initial atomic states $|i\rangle$, $i=e$ or g. Writing $\Delta\rho/\Delta t=\mathrm{d}\rho/\mathrm{d}t$, the coarse-grained master equation in the interaction picture is therefore

$$\frac{\mathrm{d}\rho}{\mathrm{d}t}=\gamma_-(\tilde{a}\rho(t)\tilde{a}^\dagger-\tfrac{1}{2}\{\tilde{a}^\dagger\tilde{a},\rho(t)\})+\gamma_+(\tilde{a}^\dagger\rho(t)\tilde{a}-\tfrac{1}{2}\{\tilde{a}\tilde{a}^\dagger,\rho(t)\}). \tag{48}$$

Not surprisingly, this is the equation of the damped harmonic oscillator with finite temperature T. Here T is the temperature of the atomic beam:

$$\exp\left(-\frac{\omega}{k_BT}\right)=\frac{r_e}{r_g}=\frac{\gamma_+}{\gamma_-}, \tag{49}$$

where k_B is the Boltzmann constant. Equation (48) has the general form (1), with two Lindblad operators $L_-=\sqrt{\gamma_-}\tilde{a}$ and $L_+=\sqrt{\gamma_+}\tilde{a}^\dagger$. Recall that $\tilde{a}$ coincides with the usual annihilation operator a only if $k=0$ (perturbative regime).

In conclusion, if $|\lambda|\tau\ll1$ and condition (28) holds, i.e., if each atom modifies weakly the state of the field, the average density matrix (40) satisfies the master equation (48). Although the quantum trajectories of the mode depend on $\mathcal{E}$, the corresponding master equation is the same for all laser fields, in accordance with the general results of Sec. II.

IV. SINGLE QUANTUM TRAJECTORIES OF THE FIELD MODE

We focus in this section on single quantum trajectories of the field mode, corresponding to specific realizations of the measurements. The main question addressed in the following concerns the localization properties of the random dynamics at large times, for different laser fields $\mathcal{E}$. In the

case $\mathcal{E}=0$, i.e, for the ''standard'' Monte Carlo wave function dynamics, it has been shown in Ref. 27 that the field wave function evolves at large times toward Fock states $|n(t)\rangle$ [with a time fluctuating number of photons $n(t)$]. Note that it is straightforward to prove that Fock states form an invariant family of states under the stochastic dynamics. In fact, if $\epsilon=0$, the jump operators $W_{\pm}$ transform $|n\rangle$ into $|n\pm1\rangle$ (up to multiplicative constants), and $|n\rangle$ is an eigenvector of $H+K_0=\omega(n+1/2)-i(\gamma_-\sin^2(|\eta|n^{1/2})+\gamma_+\sin^2(|\eta|(n+1)^{1/2}))/(2|\eta|^2)$. The localization property is much more difficult to prove. For nonzero laser fields, Fock states do no longer form an invariant family and the localization is of different nature. In the case of zero temperature ($\gamma_+=0$), it has been shown in Ref. 8 that the field mode has a diffusive dynamics in the limit $\epsilon\to\infty$, given by a stochastic Schrödinger equation with real Wiener processes; we will prove in Sec. V that this remains true at any temperature. Such kind of dynamics has been widely studied in the literature.[11,12,15,26,28] It is expected that localization occurs toward coherent or squeezed states if the Lindblad operators are linear combinations of a and $a^\dagger$. However, this has only been proved in the case $L\propto(a+a^\dagger)$ as far as we are aware.[28] Here we present numerical results indicating that for $T>0$ and large enough ϵ, the mode wave function $|\psi(t)\rangle$ evolves toward squeezed states after some time $\Delta\tau$ of the order of the thermalization time in the absence of measurements. At large times, the squeezing amplitude $r(t)$ of the squeezed states is found to fluctuate slightly around a mean value $\overline{r}$, and the squeezing angle $\phi(t)$ evolves linearly in time, $\phi(t)=\overline{\phi_0}-\omega t$. Interestingly, $\overline{r}$ and $\overline{\phi_0}$ are independent of the realization and of the initial state, being, respectively, functions of the temperature T and the laser field $\mathcal{E}$ only. By letting $\epsilon\to\infty$, writing the corresponding quantum state diffusion equation (which is derived in the general case in Sec. V), and using a result due to Rigo and Gisin,[26] we obtain in Sec. IV B analytic expressions for $\overline{r}$ and $\overline{\phi_0}$ in good agreement with the numerical simulations.

A. Numerical results

Let us first look at the Husimi Q-function for the mode wave function in the interaction picture,

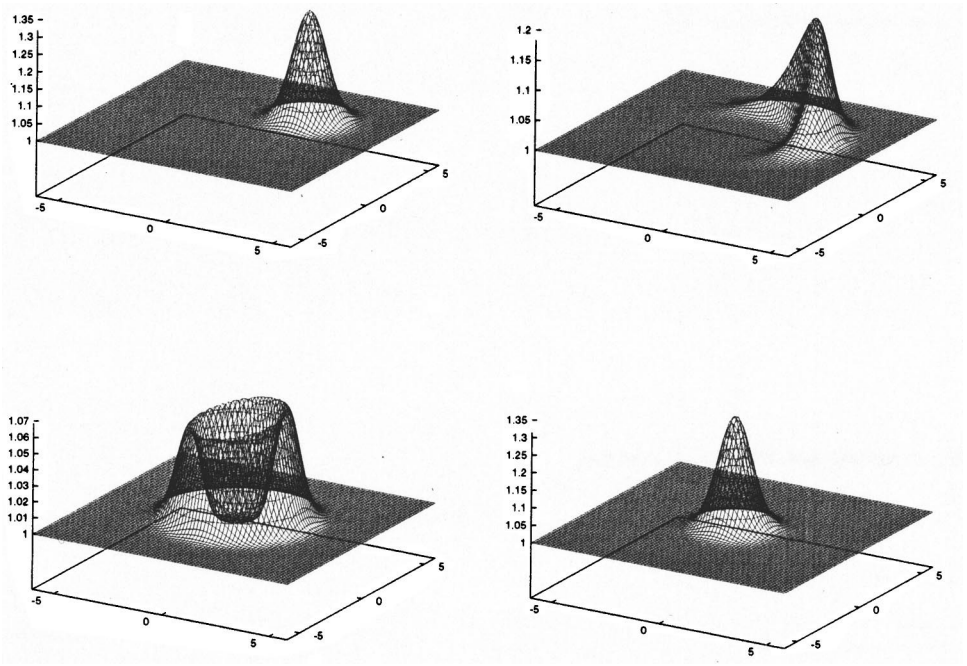

FIG. 2. $Q(\alpha,t)+1$ for $\epsilon=0$ and $\gamma_+/\gamma_-=3/4$, at four different times: $\gamma_- t=0$ (top left), $\gamma_- t=5$ (top right), $\gamma_- t=20$ (bottom left), and $\gamma_- t=60$ (bottom right).

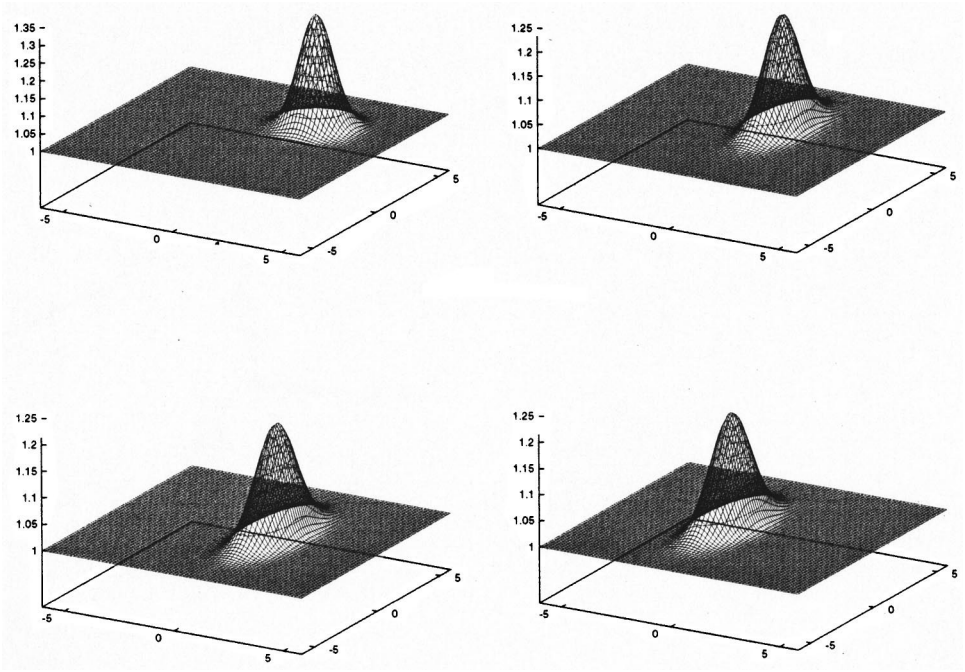

FIG. 3. $Q(\alpha,t)+1$ for $\epsilon=50$ and $\gamma_+/\gamma_-=3/4$, at the same times as in Fig. 2.

$$Q(\alpha,t)=\frac{1}{\pi}|\langle\alpha|\psi(t)\rangle|^2, \quad \alpha\in\mathbb{C}.$$

The simulations of single quantum trajectories for $\epsilon=0$ and $\epsilon=50$ give the results plotted in Figs. 2 and 3, respectively. Recall that for Fock states $|\psi\rangle=|n\rangle$, $Q(\alpha)$ is equal to $|\alpha|^{2n}\exp(-|\alpha|^2)/\pi n!$, and for squeezed states $|\psi\rangle=|\alpha_0,\xi\rangle$ with $\xi\in\mathbb{R}$, $|\xi|=r$,

$$Q(\alpha)=\frac{1}{\pi\cosh(r)}\exp\left(-\frac{2\Re(\alpha-\alpha_0)^2}{1+e^{-2r}}-\frac{2\Im(\alpha-\alpha_0)^2}{1+e^{2r}}\right)$$

(see Ref. 29). This asymmetric paraboloid becomes symmetric for a coherent state $|\psi\rangle=|\alpha_0\rangle$, which corresponds to $r=0$ in the above-mentioned formula. It is seen in Fig. 2 that in the case $\epsilon=0$, the initial coherent state $|\alpha=2+2i\rangle$ is transformed into states which are close to Fock states at times $t_3=20/\gamma_-$ $(n\neq 0)$ and $t_4=60/\gamma_-$ $(n=0)$. This is in agreement with the results of Ref. 27. On the other hand, for $\epsilon=50$, Fig. 3 shows that the same initial coherent state is transformed into states which are close to squeezed states $|\alpha,re^{i\phi}\rangle$. The squeezed states at t_3 and t_4 have approximately the same squeezing parameters r and $\phi=0$, but they have different centers α.

In order to study more precisely the localization toward squeezed states at large values of ϵ, let us follow the time evolution of the mean square deviations for a given quantum trajectory $t\mapsto|\psi(t)\rangle$:

$$\begin{aligned}\Delta x_\phi^2(t)&=\langle\psi_S(t)|X_\phi^2|\psi_S(t)\rangle-\langle\psi_S(t)|X_\phi|\psi_S(t)\rangle^2,\\ \Delta y_\phi^2(t)&=\langle\psi_S(t)|Y_\phi^2|\psi_S(t)\rangle-\langle\psi_S(t)|Y_\phi|\psi_S(t)\rangle^2.\end{aligned} \tag{50}$$

X_ϕ and Y_ϕ are the usual field quadrature operators rotated by an angle ϕ:

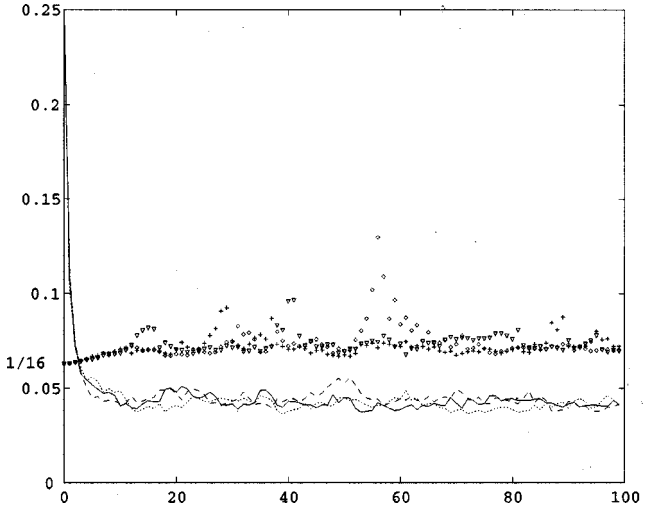

FIG. 4. $\Delta x^2(t)$ (solid, dashed, and dotted lines) and $\Delta x^2(t)\Delta y^2(t)$ [(+), ($\diamond$), and ($\triangledown$)] vs $\gamma_- t$ for three different quantum trajectories with initial coherent state. The values of the parameters are $\epsilon=20$ and $\gamma_+/\gamma_-=3/4$. The dotted line and the triangles correspond to the exact dynamics using the nonperturbative formulas (23)–(26) for K_g, $W_\pm$, and K_e, with $|\lambda|\tau=0.93\times10^{-2}$.

$$X_\phi=\frac{ae^{-i\phi}+a^\dagger e^{i\phi}}{2},\quad Y_\phi=X_{\phi+\pi/2}=\frac{ae^{-i\phi}-a^\dagger e^{i\phi}}{2i}. \tag{51}$$

We denote by $\phi_{\min}(t)$ the angle for which $\Delta x^2_\phi(t)$ is minimum. The minimum mean square deviation $\Delta x^2_{\phi_{\min}(t)}(t)$ is denoted by $\Delta x^2(t)$ and, similarly, $\Delta y^2_{\phi_{\min}(t)}(t)$ is denoted by $\Delta y^2(t)$. Obviously, $\Delta x^2(t)$ and $\Delta y^2(t)$ remain unchanged if the wave function $|\psi_S(t)\rangle$ in the Schrödinger picture is replaced in (50) by the wave function $|\psi(t)\rangle$ in the interaction picture. This replacement leads to an increase of $\phi_{\min}(t)$ by ωt.

The time evolutions of $\Delta x^2(t)$ and $\Delta x^2(t)\Delta y^2(t)$ are shown in Figs. 4 and 5, for different quantum trajectories starting from the same coherent state $|\psi(0)\rangle=|\alpha\rangle$. Note that the time scale is of order of the thermalization time of the density matrix $\rho(t)$. Figure 4 corresponds to $\epsilon=20$ and Fig. 5 to $\epsilon=100$. One sees in both Figs. 4 and 5 that $\Delta x^2(t)$ begins to fluctuate around a mean

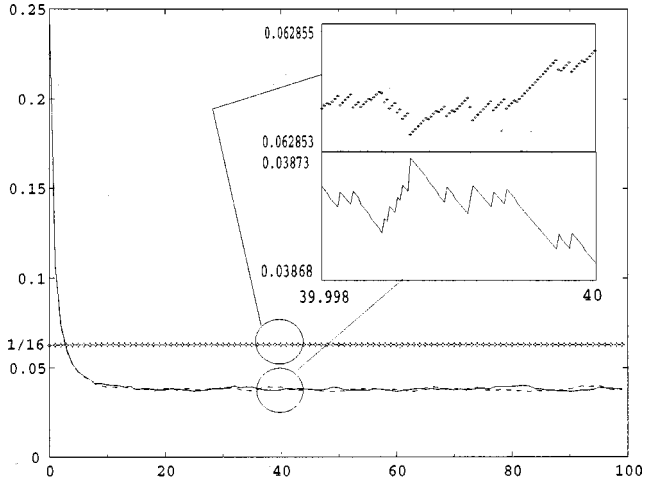

FIG. 5. Same as in Fig. 4 but with $\epsilon=100$ (the nonperturbative results are not shown but look similar). In the upper square, $\Delta x^2(t)$ and $\Delta x^2(t)\Delta y^2(t)$ are shown on a finer time scale, on which discontinuous quantum jumps can be seen separately.

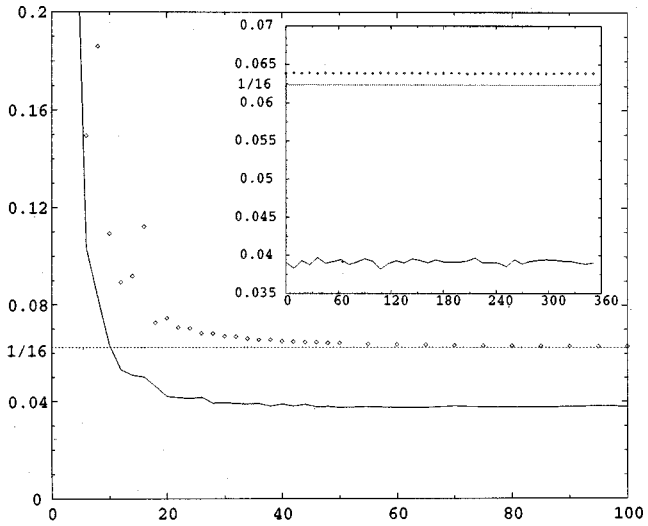

FIG. 6. Time averages $\overline{\Delta x^2}$ (plain line) and $\overline{\Delta x^2 \Delta y^2}$ ($\diamond$) for different values of $\Re\epsilon$ (shown in the horizontal axis) and $\Im\epsilon=0$. Inset: same for different values of $\arg\epsilon$ (shown in degrees in the horizontal axis) and fixed modulus $|\epsilon|=50$. The time average is taken on the interval $[10/\gamma_-, 100/\gamma_-]$ and $\gamma_+/\gamma_- = 3/4$.

value $\overline{\Delta x^2}$ after some transient time $\Delta\tau \simeq 10/\gamma_-$. The comparison of the numerical results for the different trajectories shows that $\overline{\Delta x^2}$ does not depend upon the specific realization. The fluctuations are considerably reduced in the case $\epsilon=100$ (Fig. 5) with respect to the case $\epsilon=20$ (Fig. 4). Moreover, in the former case, the product $\Delta x^2(t)\Delta y^2(t)$ is much closer to the minimum value 1/16 allowed by the Heisenberg uncertainty principle. The variation of $\overline{\Delta x^2}$ and $\overline{\Delta x^2 \Delta y^2}$ with ϵ for fixed temperature $T \simeq 0.288\omega/k_B$ is presented in Fig. 6. One observes that $\overline{\Delta x^2}$ is almost constant for $50 \leqslant \epsilon \leqslant 100$. Furthermore, the time average of $\Delta x^2(t)\Delta y^2(t)$ goes closer and closer to 1/16 as ϵ increases. The result presented in the inset shows moreover that $\overline{\Delta x^2}$ and $\overline{\Delta x^2 \Delta y^2}$ are independent of $\arg(\epsilon)$, up to small fluctuations.

Most numerical simulations were done using the approximations (31) and (38) for the jump operators $W_\pm$ and for K, together with $\tilde{a}=a$. This is justified if the maximum number of photons $n_{\max}$ is small with respect to $|\eta|^{-2}=|\lambda|^{-2}\tau^{-2}$, and $|\eta|^{-2}=|\lambda|^{-2}\tau^{-2}$, and $n_{\max}^{3/2} \ll |\eta|^{-4}|\epsilon|^{-1}$, $n_{\max}^{3/2} \ll |\eta|^{-2}|\epsilon|$ (see Sec. III B). Since we worked in the Fock states basis, $n_{\max}$ was bounded by the dimension of the Hilbert space (which was taken between 75 and 150). One may be worried, however, that, despite the smallness of the error made at each time step δt, the error made after many steps might be large and could invalidate our results in the long time limit. We checked that this is actually not the case by integrating numerically the exact dynamics, using formulas (23)–(26) for the evolution on each time step δt, and the exact possibilities of occurrence of the four cases. The curve in the dotted line and the triangles in Fig. 4 are the values of $\Delta x^2(t)$ and $\Delta x^2(t)\Delta y^2(t)$ obtained from a simulation of this nonperturbative dynamics. This means using the exact formulas (23)–(26) for the evolution on each time step δt, and the exact probabilities of occurrence of the four cases. The total number of atoms crossing the cavity in the whole time interval is 2×10^6, and $|\eta| = \sqrt{(\gamma_- + \gamma_+)\delta t} \simeq 0.0093$. The exact results show very similar fluctuations, around the same values $\overline{\Delta x^2}$ and $\overline{\Delta x^2 \Delta y^2}$, as the two trajectories obtained using the perturbative scheme. No systematic deviation increasing with time is seen. This result, together with other simulations for different values of ϵ and η,[31] shows errors in the considered time range. Note however that if $|\eta|$ is too large (for values in the range 0.06–0.09 or larger in Fig. 4, and 0.02–0.04 or larger in Fig. 5), large time fluctuations of $\Delta x^2(t)$ and $\Delta x^2(t)\Delta y^2(t)$ are observed and therefore the localization is of different nature.

In all our simulations, we found that $\overline{\Delta x^2}$ and $\overline{\Delta x^2 \Delta y^2}$ are insensitive to the initial state $|\psi(0)\rangle$ of the field mode. This is illustrated in Fig. 7 for $\epsilon=20$ and $\epsilon=20+10i$ (similar results are

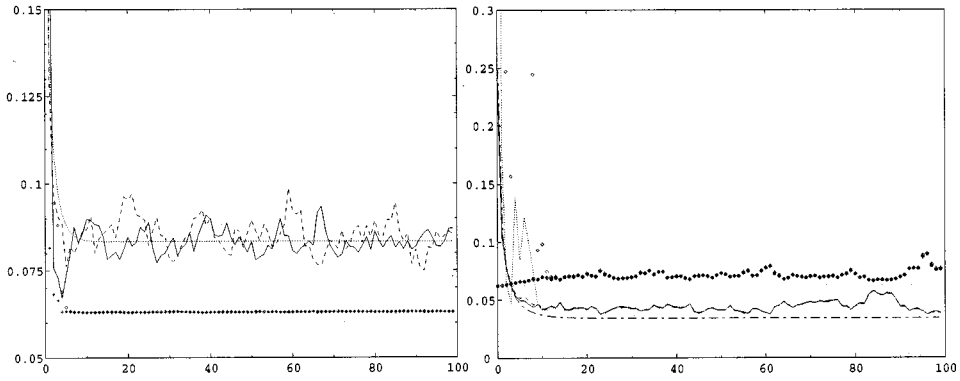

FIG. 7. $\Delta x^2(t)$ (lines) and $\Delta x^2(t)\Delta y^2(t)$ [(+), ($\diamond$), and ($\bigcirc$)] vs $\gamma_- t$ for trajectories with different initial states $|\psi(0)\rangle$. Left-hand side: in the two shown trajectories, $\langle n|\psi(0)\rangle$ is chosen randomly for $0\leqslant n\leqslant 20$ and vanishes for $n>20$; $|\psi(0)\rangle$ and the realization of the measurements are different in each trajectory; $\epsilon=20+10i$ and $\gamma_+/\gamma_-=1/2$. Right-hand side: (1) $|\psi(0)\rangle=|\alpha\rangle$ with $\alpha=\sqrt{3/2}(1+i)$ [plain line, ($\bigcirc$);] (2) id. with $\alpha=-1+5i$ [dashed line, (+);] (3) $|\psi(0)\rangle=|n=5\rangle$ [dotted line, ($\diamond$)]; in all cases, $\epsilon=20$ and $\gamma_+/\gamma_-=3/4$. The dotted line on the left-hand side and dot-dashed line on the right-hand side correspond to the theoretical result (64) for $\epsilon\to\infty$.

obtained for $\epsilon=100$). On the right-hand side of the Fig. 7, it is seen that $\Delta x^2(t)$ differs noticeably at small t's if $|\psi(0)\rangle$ is a coherent state [cases (1) and (2)] and if it is a Fock state [case (3); the first small time values are outside the range of the figure: $\Delta x^2(0)=2.75$]. However, the three curves are hard to distinguish for $\gamma_- t\gtrsim 10$. In the two trajectories shown on the left-hand side, the two distinct initial states are chosen by picking randomly the 20 first components $\langle n|\psi(0)\rangle$ in the Fock states basis (the realization of the measurements is also different in the two cases). For times bigger than $10/\gamma_-$, one observes that $\Delta x^2(t)$ fluctuates around the same value for both trajectories.

For the quantum trajectories studied in Figs. 3–5, the angle $\phi_{\min}(t)+\omega t$ is found to be zero at times $t\gtrsim\Delta\tau$. Nonvanishing angles are obtained if one considers non real ϵ's. The time dependence of $\phi_{\min}(t)+\omega t$ for $\epsilon=20+10i$ is presented in Fig. 8 for different initial states. It is seen that it evolves toward a constant value $\overline{\phi_0}$ which neither depends on $|\psi(0)\rangle$ nor on the ratio γ_+/γ_-. As shown in the inset, we obtain $\overline{\phi_0}=\arg(\epsilon)$.

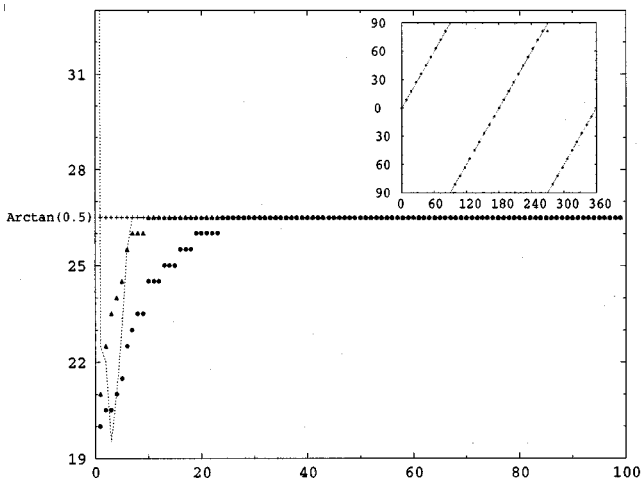

FIG. 8. Angle $\phi_{\min}(t)+\omega t$ (in degrees) vs $\gamma_- t$ for $\epsilon=20+10i$ and different initial states and temperatures: (1) $|\psi(0)\rangle=|\alpha\rangle$ with $\alpha=2-2i$; $\gamma_+/\gamma_-=1/4$ ($\triangle$); (2) $|\psi(0)\rangle=(2+2e^{-9})^{-1/2}(|\alpha\rangle+|\beta\rangle)$ with $\alpha=-3i$ and $\beta=3$; $\gamma_+/\gamma_-=3/4$ ($\bullet$); (3) $|\psi(0)\rangle=|n\rangle$ with $n=10$; $\gamma_+/\gamma_-=3/4$ (+); (4) $|\psi(0)\rangle$ is chosen randomly as in Fig. 7; $\gamma_+/\gamma_-=1/2$ (dashed line). Inset: time average of $\phi_0(t)=\phi_{\min}(t)+\omega t$ as function of $\arg\epsilon$ (both in degrees) for $|\epsilon|=50$ and $\gamma_+/\gamma_-=3/4$ (time average as in Fig. 6). The result is well fitted by the broken lines $\overline{\phi_0}=\arg(\epsilon)$ mod. 180.

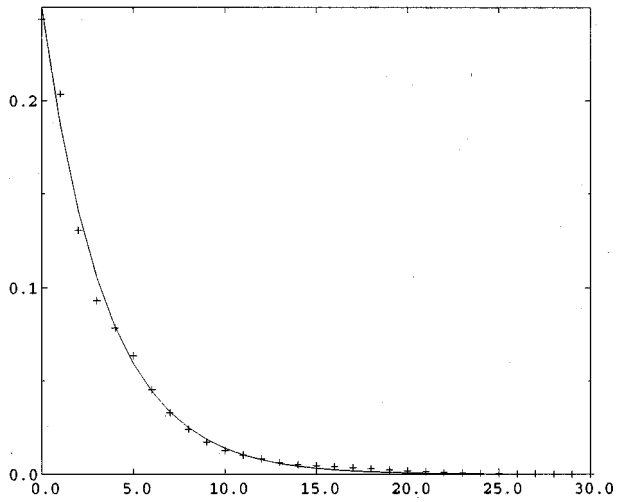

FIG. 9. Time average of the probability $|\langle n|\psi(t)\rangle|^2$ to find n photons for $\epsilon=50$, $\gamma_+/\gamma_-=3/4$ (+). The average is taken over 5000 discrete times in the interval $[0,100/\gamma_-]$. The solid line corresponds to the Bose–Einstein distribution.

Bringing together the above-mentioned results, we are led to the following conclusions. For large $|\epsilon|$ and small $|\eta|$ smaller than $\simeq 0.01$, the wave function $|\psi_S(t)\rangle$ of the field mode evolves, whatever its initial state $|\psi_S(0)\rangle$, to some almost minimum uncertainty states (MUS) at times $t \geqslant \Delta\tau$, where $\Delta\tau$ is a transient time. Moreover, if $T>0$,

$$\Delta x^2(t) \simeq \overline{\Delta x^2} < 1/4, \quad \phi_{\min}(t) \simeq \overline{\phi_0} - \omega t \tag{52}$$

at large times where both $\overline{\Delta x^2}$ and $\overline{\phi_0} = \arg(\epsilon)$ are independent of $|\psi_S(0)\rangle$ and of the realization of the measurements. Therefore, provided $|\epsilon|$ is big enough and $|\eta|$ small enough, the state of the field mode at times $t \geqslant \Delta\tau$ is close to a squeezed state:

$$|\psi_S(t)\rangle \simeq |\alpha(t), \xi(t)\rangle. \tag{53}$$

The squeezing amplitude $r(t)=|\xi(t)|$ fluctuates slightly around a time-independent value $r \simeq -\ln(4\overline{\Delta x^2})/2$ and $\arg(\xi(t)) \simeq 2(\overline{\phi_0} - \omega t)$. The center $\alpha(t)$ of the squeezed state moves around in the complex plane. Actually, by ergodicity, the time average of $|\psi_S(t)\rangle\langle\psi_S(t)|$ must coincide with the equilibrium density matrix $\rho^{(\mathrm{eq})} = Z^{-1}\exp(-\omega(a^\dagger a + 1/2)/k_B T)$. To check ergodicity, we have computed numerically the time average of $|\langle n|\psi(t)\rangle|^2$ on the interval $[0,100/\gamma_-]$ for a *single* quantum trajectory. It is indeed seen in Fig. 9 that it reproduces well the Bose–Einstein exponential distribution $\rho_{nn}^{(\mathrm{eq})}$.

B. Analytical results

The above-given numerical results suggest that the dynamics has the localization property toward squeezed states in the limit of large laser fields $|\epsilon| \to \infty$. In particular, the squeezed states should form an invariant family of states under the stochastic dynamics in this limit. The second statement can be shown analytically as follows. We restrict our analysis here to the perturbative regime where $|\eta| \ll 1$, $|\eta\epsilon| \ll 1$ and (28) holds with $k=0$, so that $\tilde{a} \simeq a$. As said previously, one can describe the mode's dynamics in the limit $|\epsilon| \to \infty$, $|\eta| \to 0$, $|\eta\epsilon| \to 0$ by a stochastic Schrödinger equation with real Wiener processes (quantum state diffusion). This is because the probability of occurrence of jumps grows like $|\epsilon|^2$ (for instance, in Figs. 4 and 5, the total number of jumps in the whole time interval $[0,100/\gamma_-]$ is close to 7×10^4 and 1.75×10^6, respectively). On the other hand, as is clear from (31) and (39), the change of the wave function during a jump is of order $1/\epsilon$. Hence there are infinitely many jumps with an infinitesimal impact on the wave function in the

limit $|\epsilon|\to\infty$. On a time scale much bigger than the inverse frequencies of jumps [but small enough so that $|\psi(t)\rangle$ does not change much on such a time scale], $|\psi(t)\rangle$ satisfies the following Itô stochastic differential equation in the limit $\epsilon\to\infty$, $\arg\epsilon=\theta$:

$$|\mathrm{d}\psi\rangle=\Big[\sqrt{\gamma_-}(e^{-i\theta}a-\Re\langle e^{-i\theta}a\rangle_t)\mathrm{d}w_-(t)+\sqrt{\gamma_+}(e^{i\theta}a^\dagger-\Re\langle e^{i\theta}a^\dagger\rangle_t)\mathrm{d}w_+(t)$$
$$+\Re\langle e^{i\theta}a^\dagger\rangle_t\Big(\gamma_-e^{-i\theta}a+\gamma_+e^{i\theta}a^\dagger-\frac{\gamma_-+\gamma_+}{2}\Re\langle e^{i\theta}a^\dagger\rangle_t\Big)\mathrm{d}t-iK_0\,\mathrm{d}t\Big]|\psi(t)\rangle. \quad (54)$$

The notation is as follows: $K_0=(\gamma_-a^\dagger a+\gamma_+aa^\dagger)/2i$, $\langle O\rangle_t=\langle\psi(t)|O|\psi(t)\rangle$ is the quantum expectation at time t and $\mathrm{d}w_\pm(t)$ are the stochastic infinitesimal increments of two independent real Wiener processes, which have zero mean and satisfy the Itô rules:[30]

$$\mathrm{d}w_\pm(t)\mathrm{d}w_\pm(t)=\mathrm{d}t,\quad \mathrm{d}w_-(t)\mathrm{d}w_+(t)=0,\quad \mathrm{d}w_\pm(t)\mathrm{d}t=0. \quad (55)$$

Equation (54) will be derived in Sec. V in the general case. It belongs to the class of stochastic Schrödinger equations studied in Refs. 11 and 12 and has been derived from the QJ dynamics by Wiseman and Milburn[8] (see also Refs. 5 and 9) in the case of a mode in a decaying cavity (corresponding here to $\gamma_+=0$). It can actually be derived directly from the stochastic dynamics of Sec. III B, Eqs. (23)–(26), with the probabilities (27), in the limit $|\epsilon|\to\infty$, $|\eta|\to0$, $|\epsilon\eta|=$const., under assumption (28) with $k=0$.[31] A related equation with complex Wiener processes has been studied in Ref. 10.

Rigo and Gisin[26] have shown that the stochastic Schrödinger equation (54) preserves squeezed states. Since (54) actually differs from the equation considered by these authors by some additional phase factors $e^{\pm i\theta}$, and the explicit solution of the evolution equations for the squeezing parameters is not given in Ref. 26, we briefly recall here their derivation. We use the Itô formalism of stochastic differential equations,[30] whereas Stratanovich formalism was used in Ref. 26. It is convenient to characterize squeezed states by the following criterion:

$$|\psi\rangle=\|\psi\||\alpha,\xi=re^{2i\phi}\rangle\Leftrightarrow(a-\Gamma a^\dagger-\beta)|\psi\rangle=0,\quad \Gamma=-e^{2i\phi}\tanh(r),\quad \beta=\alpha-\Gamma\alpha^*. \quad (56)$$

The family of the squeezed states is invariant under (54) if $|\psi\rangle+|d\psi\rangle$ remains a squeezed state for any $|\psi\rangle=|\alpha,\xi\rangle$, i.e., $(a-\Gamma a^\dagger-\mathrm{d}\Gamma\,a^\dagger-\beta-\mathrm{d}\beta)(|\psi\rangle+|\mathrm{d}\psi\rangle)=0$. This is equivalent to[26]

$$[a-\Gamma a^\dagger,D(\psi)]|\psi\rangle-(\mathrm{d}\Gamma\,a^\dagger+\mathrm{d}\beta)D(\psi)|\psi\rangle=(\mathrm{d}\Gamma\,a^\dagger+\mathrm{d}\beta)|\psi\rangle, \quad (57)$$

where $D(\psi)$ is the operator inside the square brackets in (54). The left-hand side is found to be

$$\Big(-\frac{\gamma_++\gamma_-}{2}(a+\Gamma\,a^\dagger)\mathrm{d}t+\Re\langle e^{i\theta}a^\dagger\rangle(\gamma_+e^{i\theta}\mathrm{d}t+\gamma_-e^{-i\theta}\Gamma\,\mathrm{d}t+\sqrt{\gamma_+}\mathrm{d}\beta\,\mathrm{d}w_++\sqrt{\gamma_-}\mathrm{d}\beta\,\mathrm{d}w_-)$$
$$+\sqrt{\gamma_+}\,e^{i\theta}(-a^\dagger\mathrm{d}\beta\,\mathrm{d}w_++\mathrm{d}w_+)+\sqrt{\gamma_-}e^{-i\theta}(-a\,\mathrm{d}\beta\,\mathrm{d}w_-+\Gamma\,\mathrm{d}w_-)\Big)|\psi\rangle. \quad (58)$$

We have thrown away all terms $\mathrm{d}\Gamma\,\mathrm{d}w_\pm$ since $\mathrm{d}\Gamma$ is proportional to $\mathrm{d}t$. This is because, by inspection of (58), the terms containing the noises $\mathrm{d}w_\pm$ on the left-hand side of (57) are proportional to $|\psi\rangle$. Multiplying both members of (57) by $\mathrm{d}w_\pm$ and using (55) and (58) gives

$$\mathrm{d}\beta\,\mathrm{d}w_+=\sqrt{\gamma_+}e^{i\theta}\mathrm{d}t,\quad \mathrm{d}\beta\,\mathrm{d}w_-=\sqrt{\gamma_-}e^{-i\theta}\Gamma\,\mathrm{d}t. \quad (59)$$

Now we use the well-known identity $S(-\xi)D(-\alpha)aD(\alpha)S(\xi)=a\cosh r+\Gamma\,a^\dagger\cosh r+\alpha$, where $S(\xi)=\exp(\xi^*a^2/2-\xi a^{\dagger2}/2)$ and $D(\alpha)=\exp(\alpha a^\dagger-\alpha^*a)$ are, respectively, the squeezing and the displacement operators.[2] The squeezed state $|\psi\rangle$ is equal to $D(\alpha)S(\xi)|0\rangle$. Let us multiply the two members of (57) by $S(-\xi)D(-\alpha)$ and substitute (58) and (59) into this equation. This leads to the two coupled stochastic differential equations:

$$
\begin{aligned}
d\Gamma &= -e^{2i\theta}(1+e^{-2i\theta}\Gamma)(\gamma_+ + \gamma_- e^{-2i\theta}\Gamma)dt, \\
d\beta &= -\left(\frac{\gamma_- + \gamma_+}{2} + \gamma_- e^{-2i\theta}\Gamma\right)\beta\, dt + 2\Re(e^{i\theta}a^*)(\gamma_+ e^{i\theta} + \gamma_- e^{-i\theta}\Gamma)dt \\
&\quad + \sqrt{\gamma_+}e^{i\theta}dw_+ + \sqrt{\gamma_-}e^{-i\theta}\Gamma\, dw_- .
\end{aligned}
\tag{60}
$$

These equations are equivalent to (57) and have a solution. Hence the squeezed states $|\alpha,\xi\rangle$ form an invariant family under the quantum state diffusion dynamics, and α and ξ evolve in time according to (60).

We now obtain the squeezing amplitudes $r(t)$ and angles $\phi(t)$ of the squeezed states by solving (60). They are determined by the first equation:

$$
\Gamma(t) = -e^{2i\theta}\frac{\gamma_+ e^{(\gamma_- - \gamma_+)t} + c}{\gamma_- e^{(\gamma_- - \gamma_+)t} + c} = -e^{2i\phi(t)}\tanh(r(t)), \tag{61}
$$

where c is an arbitrary complex constant. Thus $r(t)$ and $\phi(t)$ are deterministic, unlike $\alpha(t)$, which is given by the second equation. Going back to the Schrödinger picture, one has for $t(\gamma_- - \gamma_+) \gg 1$:

$$
\begin{aligned}
\tanh(r(t)) &\simeq \frac{\gamma_+}{\gamma_-} = \exp\left(-\frac{\omega}{k_B T}\right), \\
\phi(t) &\simeq \theta - \omega t.
\end{aligned}
\tag{62}
$$

It is worth noticing that perfect squeezing $[r(t)\to\infty]$ is obtained in the *high* temperature limit $k_B T \gg \omega$. The rate $(\gamma_- - \gamma_+)^{-1}$ of convergence of $\tanh r(t)$ to $\tanh \bar{r} = \exp(-\omega/k_B T)$ also tends to infinity in this limit. Since the number of photons in the cavity becomes very large at very high temperatures and long times, the perturbative approximation (28) should however break down at some point. This can put a limitation on the attainment of very large $r(t)$. A more detailed study of this apparently surprising result is the object in a separate work.[31]

As stated previously, the second equation in (62) agrees quite well with the results of the numerical simulations of Fig. 8. Using the minimum mean square deviation $\Delta x^2 = e^{-2r}/4$ of squeezed states[2] yields the time average $\overline{\Delta x^2}$:

$$
\overline{\Delta x^2} \simeq \frac{\gamma_- - \gamma_+}{4(\gamma_- + \gamma_+)}. \tag{63}
$$

In the particular case of an initial coherent state $|\psi(0)\rangle = |\alpha\rangle$, the constant c is equal to $-\gamma_+$, so that (62) is exact at all times $t \geqslant 0$ and

$$
\Delta x^2(t) \simeq \frac{\gamma_- - \gamma_+}{4\gamma_- + 4\gamma_+(1 - 2e^{-(\gamma_- - \gamma_+)t})}. \tag{64}
$$

This solution is compared in Fig. 7 with the numerical results for $|\epsilon| \sim 20$. The exact value of $\overline{\Delta x^2}$ is close to the approximated value 1/12 obtained from (63) for $\gamma_+/\gamma_- = 1/2$ (left-hand side of Fig. 7). It is a bit higher than the theoretical prediction $1/28 \simeq 0.0357$ for $\gamma_+/\gamma_- = 3/4$ (right-hand side). For $50 \leqslant \epsilon \leqslant 100$, one has a better agreement, as seen in Fig. 6. Hence the dynamics of the mode is well described by the quantum state diffusion equation (54) for $\epsilon \geqslant 50$, at this temperature.

V. STOCHASTIC SCHRÖDINGER EQUATIONS

In this section we discuss the mathematical link between the quantum jump dynamics of Sec. II and various stochastic Schrödinger equations found in the literature. The analysis is done for arbitrary open quantum systems having a Lindblad-type dynamics.

A. Linear quantum jump dynamics

A linear version of the QJ dynamics of Sec. II, in which the random wave function is not normalized at each time step δt, has been introduced in Ref. 18. The unormalized wave function $|\varphi(t)\rangle$ of the open system S satisfies the following Itô stochastic differential equation:

$$|\mathrm{d}\varphi\rangle=\left[-i(H+K)\mathrm{d}t+\sum_m\ (W_m-1)\mathrm{d}N_m(t)\right]|\varphi(t)\rangle, \tag{65}$$

where H is the Hamiltonian of S, the jump operators W_m are related to the Lindblad operators L_m by

$$L_m=\sqrt{\gamma_m}(W_m-1), \tag{66}$$

and $\mathrm{d}N_m(t)=0,1$ are the stochastic increments of independent Poisson processes N_m with parameters γ_m. These increments have mean $\mathsf{M}\,\mathrm{d}N_m(t)=\gamma_m\,\mathrm{d}t$ and satisfy the Itô rules:

$$\mathrm{d}N_m(t)\mathrm{d}N_n(t)=\delta_{n,m}\mathrm{d}N_m(t),\quad \mathrm{d}N_m(t)\mathrm{d}t=0. \tag{67}$$

Equation (65) has been first considered by Belavkin[14] with some jump operators W_m proportional to L_m [the relation with the jump operators (66) is given by the transformation (8)]. It has also been considered independently in Ref. 16. It is easy to show that $\rho(t)=\mathsf{M}|\varphi(t)\rangle\langle\varphi(t)|$ obeys the Lindblad equation (1) if K is appropriately chosen. In fact, by (65) and (67),

$$\begin{aligned}\mathrm{d}\rho&=\mathsf{M}(|\mathrm{d}\varphi\rangle\langle\varphi|+|\varphi\rangle\langle\mathrm{d}\varphi|+|\mathrm{d}\varphi\rangle\langle\mathrm{d}\varphi|)\\&=-i[H,\rho]\mathrm{d}t-iK\rho\,\mathrm{d}t+i\rho K^\dagger\,\mathrm{d}t+\sum_m\ \gamma_m((W_m-1)\rho+\rho(W_m^\dagger-1)+(W_m-1)\rho(W_m^\dagger-1))\mathrm{d}t.\end{aligned}$$

Replacing (66) into this equation yields

$$\mathrm{d}\rho=-i[H,\rho]\mathrm{d}t+\sum_m\ \left(L_m\rho L_m^\dagger-\frac{1}{2}\{L_m^\dagger L_m,\rho\}\right)\mathrm{d}t,$$

provided that

$$K=\frac{1}{2i}\sum_m\ \gamma_m(W_m^\dagger+1)(W_m-1)=\frac{1}{2i}\sum_m\ (L_m^\dagger L_m+2\sqrt{\gamma_m}L_m). \tag{68}$$

To give a physical meaning to the linear stochastic dynamics, one must choose the jump rates γ_m equal to the probability per unit time of the corresponding transitions. These are given by the Fermi golden rule to second order in perturbation theory. For instance, for the field mode considered in Sec. III, $\gamma_\pm$ are the damping rates (33) for the absorption and emission of a photon by the atoms.

Let us write (65) in the "dissipative interaction picture" $|\tilde{\varphi}(t)\rangle=U(t)|\varphi(t)\rangle$, where $U(t)=\exp(it(H+K))$. It reads $|\mathrm{d}\tilde{\varphi}\rangle=\Sigma_m(\tilde{W}_m(t)-1)\mathrm{d}N_m(t)|\tilde{\varphi}(t)\rangle$, with $\tilde{W}_m(t)=U(t)W_mU(-t)$. This implies:

$$|\tilde{\varphi}(t)\rangle=\tilde{W}_{m_p}(t_p)\cdots\tilde{W}_{m_1}(t_1)|\varphi(0)\rangle,$$

where $0\leqslant t_1\leqslant\cdots\leqslant t_p\leqslant\cdots$ are the jump times (times such that $\Sigma_m\,\mathrm{d}N_m(t)=1$), $t_p\leqslant t<t_{p+1}$, and m_q is the index of the jump occurring at time t_q ($\mathrm{d}N_{m_q}(t_q)=1$, $q=1,\ldots,p$). Hence the stochastic Schrödinger equation (65) admits the solution:

$$|\varphi(t)\rangle=e^{-i(t-t_p)(H+K)}W_{m_p}e^{-i(t_p-t_{p-1})(H+K)}\cdots W_{m_1}e^{-it_1(H+K)}|\varphi(0)\rangle,\quad t_p\leqslant t<t_{p+1}. \tag{69}$$

In other words, the evolution of the quantum state may be computed as follows.

(1) If there is a jump m between t and $t+\mathrm{d}t$, then

$$|\varphi(t+\mathrm{d}t)\rangle = W_m|\varphi(t)\rangle. \tag{70}$$

This occurs with a probability $\gamma_m \mathrm{d}t$ independent of $|\varphi(t)\rangle$.

(2) If no jump occurs between t and $t+\mathrm{d}t$, then

$$|\varphi(t+\mathrm{d}t)\rangle = (1 - i\,\mathrm{d}t(H+K))|\varphi(t)\rangle. \tag{71}$$

If $\gamma = \Sigma_m \gamma_m < \infty$, the time delays $t-t_p, t_p - t_{p-1}, \ldots, t_1$ and the jump indices $m_p, \ldots, m_1$ in (69) are independent random variables. The time delays are equally distributed, according to the exponential law $e^{-\gamma s}\,\mathrm{d}s$. Because of the independence of the Poisson processes N_m, the probability that $m_q = m$ is γ_m/γ.

It has been proven in Ref. 18 that, under appropriate hypothesis on W_m and γ_m, the wave function (69) is still well defined (as some limit of the right-hand side) if $\gamma = \infty$, in which case infinitely many jumps occur between 0 and t. This result is important for electrons in strongly disordered solids, where $m=(i,j)$ labels pairs of eigenstates $|i\rangle, |j\rangle$ of the electronic Hamiltonian, and L_{ij} is equal or "close" to $\sqrt{\gamma_{ij}}|j\rangle\langle i|$, i.e., $W_{ij} \simeq 1 + |j\rangle\langle i|$ (locality condition). Then, the number of jumps in a finite interval becomes infinite in the infinite volume limit, due to the divergence of the double sum $\Sigma_{i,j}\,\gamma_{ij}$. In this case, the presence of the identity operator inside the parentheses in (66) is necessary for the mathematical definiteness of $|\varphi(t)\rangle$.

B. Nonlinear quantum jump dynamics

The nonlinear QJ scheme of Sec. II can be deduced from the above-mentioned linear QJ dynamics in the following way. By comparing (9) and (4) with (70) and (71), it is clear that, for a given realization of the jumps, the normalized wave function

$$|\psi(t)\rangle = \frac{|\varphi(t)\rangle}{\|\varphi(t)\|} \tag{72}$$

evolves according to the nonlinear QJ scheme with $\lambda_m = \sqrt{\gamma_m}$. However, it was argued in Sec. II that the density matrix $\rho(t)$ is the mean value of $|\psi(t)\rangle\langle\psi(t)|$, whereas it has been seen earlier that $\rho(t) = \mathsf{M}|\varphi(t)\rangle\langle\varphi(t)|$. This means that the probability P' attached to $|\psi(t)\rangle$ is different from the probability P attached to $|\varphi(t)\rangle$, that is, to the Poisson processes N_m. This change of probability $P \to P'$ provides the link between the two random evolutions for $|\varphi(t)\rangle$ and $|\psi(t)\rangle$. We define it as follows. Let us denote by M' and M the mean values with respect to P' and P, respectively. Let F be an arbitrary (operator-valued) stochastic process such that $F(t)$ depends only upon the realizations of the jump times up to time t. Such F is said to be *adapted* to the filtration of the Poisson processes N_m.[33] We ask that

$$\mathsf{M}'(F(t)) = \mathsf{M}(F(t)\|\varphi(t)\|^2) \tag{73}$$

for any such process F. Taking $F(t) = |\psi(t)\rangle\langle\psi(t)|$, this implies in particular

$$\rho(t) = \mathsf{M}'|\psi(t)\rangle\langle\psi(t)| = \mathsf{M}|\varphi(t)\rangle\langle\varphi(t)|. \tag{74}$$

Let us compute the probability of occurrence of a jump m between times t and $t+\delta t$ for the new probability P':

$$\delta p_m(t) = \mathsf{M}'(\delta N_m(t)|\psi(t)). \tag{75}$$

The right-hand side is the conditional (mean) expectation of $\delta N_m(t)$ given $|\psi(t)\rangle$, for the probability P'. Indeed, the (P') probability of a jump between t and $t+\delta t$ depends upon the wave function $|\psi(t)\rangle$ at time t. Let $F(t)$ be an arbitrary stochastic force adapted to the filtration of the

N_m's. Then $F(t)\,\delta N_m(t)$ depends upon the realizations of the N_m's until time $t+\delta t$ [recall that $\delta N_m(t)=N_m(t+\delta t)-N_m(t)$]. Therefore, replacing $F(t)$ by $F(t)\,\delta N_m(t)$ in (73),

$$\mathsf{M}'(F(t)\,\delta N_m(t))=\mathsf{M}(F(t)\,\delta N_m(t)\|\varphi(t+\delta t)\|^2)=\mathsf{M}(F(t)\,\delta N_m(t)\|W_m|\varphi(t)\rangle\|^2).$$

Formula (70) together with the fact that $\delta N_m(t)=0,1$ have been used in the second line. By the independence of the forward increment $\delta N_m(t)$ and $F(t)\|W_m|\varphi(t)\rangle\|^2$, one gets

$$\mathsf{M}'(F(t)\,\delta N_m(t))=\mathsf{M}(\delta N_m(t))\mathsf{M}(F(t)\|W_m|\varphi(t)\rangle\|^2)=\gamma_m\,\delta t\,\mathsf{M}'(F(t)\|W_m|\varphi(t)\rangle\|^2\|\varphi(t)\|^{-2}). \tag{76}$$

But $F(t)$ is arbitrary, thus (76) implies the identity of the conditional expectations:

$$\delta p_m(t)=\mathsf{M}'(\delta N_m(t)|\psi(t))=\gamma_m\,\delta t\,\mathsf{M}'(\|W_m|\varphi(t)\rangle\|^2\||\varphi(t)\rangle\|^{-2}|\psi(t))=\gamma_m\,\delta t\|W_m|\psi(t)\rangle\|^2, \tag{77}$$

in accordance with (12). As a result, the stochastic evolution of the normalized wave function $|\psi(t)\rangle$ with probability P' coincides with that described in Sec. II for $\lambda_m=\sqrt{\gamma_m}$. It is moreover given by the nonlinear stochastic Schrödinger equation:[15]

$$|\mathrm{d}\psi\rangle=\left[-i\left(H+K+\frac{1}{2}\langle K^\dagger-K\rangle_t\right)\mathrm{d}t+\sum_m\left(\frac{W_m}{\sqrt{\langle W_m^\dagger W_m\rangle_t}}-1\right)\mathrm{d}N_m(t)\right]|\psi(t)\rangle, \tag{78}$$

with $\langle O\rangle_t=\langle\psi(t)|O|\psi(t)\rangle$. This equation is readily obtained by computing $|\psi(t+\mathrm{d}t)\rangle$ from (70) and (71).

C. Linear quantum state diffusion

It has been shown by Carmichael and Wiseman and Milburn[5,8] that the nonlinear QJ dynamics of the quantum field considered in Sec. III, with $\gamma_+=0$, is well described in limit $|\epsilon|\to\infty$ by a quantum state diffusion (QSD) stochastic equation involving real Wiener processes (white noise). The linear version of QSD is obtained in this section in the more general setting of arbitrary Markovian quantum open systems, by taking the limit of infinite jump rates $\gamma_m\to\infty$ in the linear QJ dynamics of Sec. V A.

Following Wiseman and Milburn,[8] we introduce a small dimensionless parameter $\varepsilon>0$ that will tend to zero. Our goal is to increase up to infinity the rates γ_m of the jumps in the linear QJ dynamics, without modifying the master equation giving the average dynamics. Hence the Lindblad operators L_m are here considered as *fixed*, i.e., independent of ε. So are the damping rates contained in the master equation, given by some ε-independent rates $\overline{\gamma}_m>0$. The jump rates γ_m are assumed to go to infinity like ε^{-4}:

$$\gamma_m=\varepsilon^{-4}\overline{\gamma}_m. \tag{79}$$

The magnitude of the negative power of ε is chosen for future convenience. Let $|\varphi(t)\rangle$ be the solution of the linear QJ stochastic equation (65). We are interested in the variation of $|\varphi(t)\rangle$ on a time interval $\Delta t\gg\gamma_m^{-1}$ such that infinitely many jumps occur between t and $t+\Delta t$ in the limit $\varepsilon\to0$. On the other hand, we want Δt to be small enough so that the change $|\Delta\varphi\rangle=|\varphi(t+\Delta t)\rangle-|\varphi(t)\rangle$ of the wave function goes to zero as $\varepsilon\to0$. A possible Δt realizing these two conditions is

$$\Delta t=\varepsilon^3\overline{\gamma}^{-1}, \tag{80}$$

where $\overline{\gamma}=\Sigma_m\,\overline{\gamma}_m$ is the sum of the fixed damping rates. Indeed, from (66),

$$W_m=1+\varepsilon^2\overline{\gamma}_m^{-1/2}L_m. \tag{81}$$

Since the L_m are ε-independent, the impact of each jump on $|\varphi\rangle$ is of order ε^2. Moreover, the number of jumps m between t and $t+\Delta t$ is of order $\gamma_m \Delta t = \varepsilon^{-1}\overline{\gamma_m}/\overline{\gamma}$. This means that the impact of the jumps between t and $t+\Delta t$ is of order $\varepsilon^{-1}\times\varepsilon^2=\varepsilon$, which is indeed small for small ε.

Let $\Delta N_m(t)$ be the number of jumps m in the time interval $[t,t+\Delta t]$. By dividing this interval into smaller intervals $[\tau_n,\tau_{n+1}]$ of length γ_m^{-1}, $\Delta N_m(t)$ can be written as a sum of $\gamma_m \Delta t = \mathcal{O}(\varepsilon^{-1})$ independent random variables $N_m([\tau_n,\tau_{n+1}])$ (number of jumps between τ_n and τ_{n+1}), which have mean and variance 1. Therefore, by the central limit theorem,

$$\Delta z_n = \frac{\Delta N_m - \gamma_m \Delta t}{\sqrt{\gamma_m}} \tag{82}$$

can be approximated for small ε by a Gaussian random variable of zero mean and variance Δt [the convergence as $\varepsilon\to 0$ actually holds for a fixed ε-independent Δt; for Δt given by (80), one gets an infinitesimal increment dz_n]. Shifting t by Δt or changing m leads to independent increments ΔN_m and Δz_m. It follows that Δz_m are the infinitesimal increments of some independent real Wiener processes z_m in the limit $\varepsilon\to 0$. Indeed, a Wiener process z is by definition a stochastic process with independent increments $\Delta z = z(t+\Delta t)-z(t)$ distributed according to a Gaussian law of variance Δt. The convergence of $(N_m-\gamma_m t)/\sqrt{\gamma_m}$ to a Wiener process can be shown more rigorously by using a theorem proven in Ref. 32.

The next step consists in evaluating both the mean and the fluctuating parts of $|\Delta\varphi\rangle$ to leading order in ε. Let $p=\Sigma_m \Delta N_m(t)$ be the total number of jumps between t and $t+\Delta t$. We denote by $s_q = t_{q+1}-t_q$, $q=1,\ldots,p-1$, the time delays between consecutive jumps and set $s_0=t_1-t$ and $s_p = t+\Delta t - t_p$. By (79) and (80), p and s_q have mean values $\gamma\Delta t$ and γ^{-1} of order ε^{-1} and ε^4, respectively. The generalized Hamiltonian (68) can be decomposed into two parts:

$$K = K_0 - i\varepsilon^{-2}R, \tag{83}$$

where K_0 and R are ε-independent:

$$K_0 = \frac{1}{2i}\sum_m L_m^\dagger L_m, \quad R = \sum_m \sqrt{\overline{\gamma_m}} L_m. \tag{84}$$

Let us set $V_q = \overline{\gamma_{m_q}}^{-1/2} L_{m_q}$ if $q=1,\ldots,p$ and $V_0=0$. With the help of (69), (81), and (83), one obtains

$$|\Delta\varphi\rangle = \left\{ \prod_{q=p}^{0} \left[\left(1-\varepsilon^{-2}s_q R + \frac{1}{2}\varepsilon^{-4}s_q^2 R^2 - i s_q (H+K_0) + \mathcal{O}(\varepsilon^6) \right)(1+\varepsilon^2 V_q) \right] - 1 \right\} |\varphi(t)\rangle, \tag{85}$$

where the product is taken in decreasing order in q. The terms of order ε in the expansion of the product are

$$\begin{aligned} |\Delta\varphi\rangle^{(f)} &= \sum_{q=0}^{p} (-\varepsilon^{-2}s_q R + \varepsilon^2 V_q)|\varphi(t)\rangle \\ &= \sum_m (-\varepsilon^{-2}\Delta t\,\overline{\gamma_m}^{1/2} + \varepsilon^2 \Delta N_m(t)\,\overline{\gamma_m}^{-1/2}) L_m |\varphi(t)\rangle = \sum_m \Delta z_m(t) L_m |\varphi(t)\rangle. \end{aligned} \tag{86}$$

These are the leading order fluctuating forces (of zero mean). Since fluctuating terms of higher order should not contribute in the limit $\varepsilon\to 0$, we may replace the product in (85) by its mean value in computing the terms of order ε^2 and more. This simplifies greatly the computation, because the order of the operators in the product then becomes of no importance. In fact, by the remark following (71), the random variables $s_0,\ldots,s_p$, $m_1,\ldots,m_p$ are independent, so that the mean of the product is the product of the means. Moreover, $\mathrm{M}V_q = \Sigma_m(\gamma_m/\gamma)\overline{\gamma_m}^{-1/2} L_m = R/\overline{\gamma}$. Therefore, one

can commute all operators in the product when computing the mean value. It is easy to show that the terms of order ε^2 cancel on average. The terms of order ε^3 are found to be proportional to Δt:

$$|\Delta\varphi\rangle^{(d)} = \mathsf{M}|\Delta\varphi\rangle = -i(H+K_0)\Delta t(1+\mathcal{O}(\varepsilon)). \tag{87}$$

This is the drift contribution to $|\Delta\varphi\rangle$.

The previous computation shows that the QJ dynamics is transformed as $\varepsilon \to 0$, if one looks at it with the time resolution $\Delta t = \overline{\gamma}^{-1}\varepsilon^3$, to a diffusive dynamics given by the linear Itô stochastic differential equation:[12,15,17]

$$|\mathrm{d}\varphi\rangle = \left[-i(H+K_0)\mathrm{d}t + \sum_m L_m \mathrm{d}z_m(t)\right]|\varphi(t)\rangle. \tag{88}$$

Here $K_0 = \Sigma_m L_m^\dagger L_m/2i$ and $\mathrm{d}z_m(t)$ are the infinitesimal increments of independent *real* Wiener processes z_m, which have zero mean and satisfy the Itô rules:

$$\mathrm{d}z_m(t)\mathrm{d}z_n(t) = \delta_{n,m}\,\mathrm{d}t, \quad \mathrm{d}z_m(t)\mathrm{d}t = 0. \tag{89}$$

D. Nonlinear quantum state diffusion

We have so far determined the linear stochastic Schrödinger equation for $|\varphi(t)\rangle$. The corresponding nonlinear equation for the normalized wave function $|\psi(t)\rangle$ is obtained by means of the above-mentioned change of probability $P \to P'$. This derivation of the nonlinear QSD equation from the linear one is actually well-known.[12,28] It is slightly more complicated than for the QJ dynamics, because $|\mathrm{d}\psi\rangle$ is to be expressed in terms of Wiener processes for the new probability P'. This can be done by using Girsanov's theorem,[33] which states that a Wiener differential $\mathrm{d}w_m$ for P' is obtained by adding an appropriate drift differential to $\mathrm{d}z_m$. For the change of probability defined by (73), the conditional (mean) expectation of $\mathrm{d}P'/\mathrm{d}P$ given $|\varphi(t)\rangle$ is $\|\varphi(t)\|^2$. The drift differential is then $-\|\varphi(t)\|^{-2}\mathrm{d}\|\varphi\|^2\mathrm{d}z_m$ (for more details, see Refs. 12, 28). From (88) and (89), one gets

$$\mathrm{d}\|\varphi\|^2 = 2\|\varphi(t)\|^2 \sum_m \Re\langle L_m\rangle_t \mathrm{d}z_m, \tag{90}$$

which implies that $\|\varphi(t)\|^2$ is a local martingale. Thus,

$$\mathrm{d}w_m(t) = \mathrm{d}z_m(t) - 2\Re\langle L_m\rangle_t \mathrm{d}t. \tag{91}$$

According to Itô's formula,[30] one has

$$\frac{|\mathrm{d}\varphi\rangle}{\|\varphi\|} = \frac{\mathrm{d}(\sqrt{\|\varphi\|^2}|\psi\rangle)}{\|\varphi\|} = |\mathrm{d}\psi\rangle + \left(\frac{\mathrm{d}\|\varphi\|^2}{2\|\varphi\|} - \frac{\mathrm{d}\|\varphi\|^2\mathrm{d}\|\varphi\|^2}{8\|\varphi\|^3}\right)\frac{|\psi\rangle + |\mathrm{d}\psi\rangle}{\|\varphi\|}.$$

The multiplication of both members by $\mathrm{d}z_m$ leads, with the help of (88)–(90), to $\mathrm{d}z_m|\mathrm{d}\psi\rangle = (L_m - \Re\langle L_m\rangle_t)|\psi\rangle\mathrm{d}t$. Going back to the original equation, it follows:

$$|\mathrm{d}\psi\rangle = \left[-i(H+K_0)\mathrm{d}t + \sum_m \Re\langle L_m\rangle_t\left(-L_m + \frac{3}{2}\Re\langle L_m\rangle_t\right)\mathrm{d}t + \sum_m (L_m - \Re\langle L_m\rangle_t)\mathrm{d}z_m\right]|\psi\rangle.$$

The nonlinear QDS equation is obtained by replacing (91) into this equation:[11,12,15]

$$|\mathrm{d}\psi\rangle = \left[-i(H+K_0)\mathrm{d}t + \sum_m \Re\langle L_m\rangle_t\left(L_m - \frac{1}{2}\Re\langle L_m\rangle_t\right)\mathrm{d}t + \sum_m (L_m - \Re\langle L_m\rangle_t)\mathrm{d}w_m(t)\right]|\psi(t)\rangle. \tag{92}$$

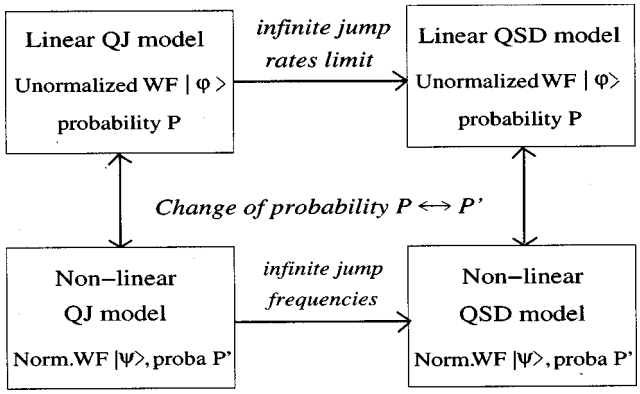

FIG. 10. The links between the different stochastic Schrödinger equations.

Let us come back to the mode dynamics of Sec. III. If one sticks to the norm-preserving QJ dynamics, the jump operators $W_{\pm}$ in (31) are defined up to a multiplicative constant. If $k=0$, $\tilde{a}\simeq a$, they can be obtained, up to such a constant, from the Lindblad operators $L_{+}=\sqrt{\overline{\gamma}_{+}}a^{\dagger}$ and $L_{-}=\sqrt{\overline{\gamma}_{-}}a$ by means of formula (66), provided that the transition rates are replaced by some effective rates $\gamma_{\pm}=\overline{\gamma}_{\pm}|\epsilon|^2$ and $L_{\pm}$ are multiplied by the phase factors $e^{\pm i\theta}$, $\theta=\arg\epsilon$. Thus the above-presented analysis can be used to compute the QSD equation for the normalized mode wave function $|\psi(t)\rangle$ in the limit of large laser fields $|\epsilon|\to\infty$. The introduction of the phase factors $e^{\pm i\theta}$ in (92) leads to the QSD equation (54).

E. Links between the stochastic Schrödinger equations

The summary of the results of this section is given in Fig. 10. The stochastic Schrödinger equations in Itô form for the linear and nonlinear QJ models are, respectively, Eqs. (65) and (78), and those for the linear and nonlinear QSD models are, respectively, Eqs. (88) and (92).

VI. CONCLUSION

We have shown that the nonlinear quantum jump (or Monte Carlo wave function) model applied to a simple optical system (damped harmonic oscillator at finite temperature T) can be generalized to describe the evolution of the quantum field in a cavity monitored by an atomic beam of two level atoms. These atoms cross one by one the cavity and interact at its exit first with a classical laser field $\mathcal{E}$, and then with a detector measuring their states. This kind of monitoring by measurements is similar to that obtained by homodyne measurement of the field in a decaying cavity,[5,8] the photon counting on the output field being replaced by the measurements on the atoms. Actually, if all atoms are sent in their ground state ($T=0$), the stochastic evolution of the wave function of the quantum field (quantum trajectories) is the same for the two kinds of monitoring. If the atoms form a beam of randomly prepared atoms with temperature $T>0$, they may also emit photons in the cavity and thus a new kind of quantum jump comes into play (creation of a photon). This has notable effects on the quantum trajectories. The effect of the laser field $\mathcal{E}$ is to modify the two jump operators. In fact, the measured atomic transitions can be driven by this field as well as by the interaction with the studied quantum field in the cavity. As a result, $\mathcal{E}$ also modifies the generalized Hamiltonian that rules the evolution between jumps. The average over all realizations of the measurements leads to an $\mathcal{E}$-independent dynamics, described by a density matrix satisfying the master equation of the damped harmonic oscillator with temperature T. Whereas the density matrix converges at large times to the Bose–Einstein equilibrium, the individual quantum trajectories for given realizations experience localization toward squeezed states at large $\mathcal{E}$. The squeezing parameters evolve to some almost constant values, up to small fluctuations going to zero in the infinite laser intensity limit. This localization occurs at large enough times, for any initial state of the quantum field. The centers of the squeezed states move

randomly in the complex plane, in such a way that the time averages of the quantum probabilities to find n-photons are distributed according to Bose–Einstein (ergodicity). The squeezing amplitude r and phase ϕ are controlled, respectively, by the temperature T and the laser field $\mathcal{E}$. r is found to increase with T, which means that the squeezing is enhanced by increasing the temperature of the atomic beam; however, the waiting time before r reaches its almost stationary value is also temperature increasing. On the other hand, no squeezing is obtained at $T=0$, and localization toward Fock states occurs if $\mathcal{E}=0$. As in the case of the homodyne measurement, the quantum trajectories are given in the infinite $\mathcal{E}$ limit by a so-called quantum state diffusion (QSD) stochastic Schrödinger equation, involving real white noise.[5,8,11,12] A precise mathematical derivation of this equation from the quantum jump dynamics was performed in Sec. V for arbitrary open quantum systems having a Lindblad-type dynamics. More precisely, this derivation starts from a linear version of the QJ dynamics proposed in Ref. 18, in which the wave function is not normalized at each step, which is proven to be related to the nonlinear QJ model by a simple change of probability.

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Quantum models related to fouled Hamiltonians of the harmonic oscillator

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We study a pair of canonoid (fouled) Hamiltonians of the harmonic oscillator which provide, at the classical level, the same equation of motion as the conventional Hamiltonian. These Hamiltonians, say K_1 and K_2, result to be explicitly time dependent and can be expressed as a formal rotation of two cubic polynomial functions, H_1 and H_2, of the canonical variables (q,p). We investigate the role of these fouled Hamiltonians at the quantum level. Adopting a canonical quantization procedure, we construct some quantum models and analyze the related eigenvalue equations. One of these models is described by a Hamiltonian admitting infinite self-adjoint extensions, each of them has a discrete spectrum on the real line. A self-adjoint extension is fixed by choosing the spectral parameter ε of the associated eigenvalue equation equal to zero. The spectral problem is discussed in the context of three different representations. For $\varepsilon=0$, the eigenvalue equation is exactly solved in all these representations, in which square-integrable solutions are explicitly found. A set of constants of motion corresponding to these quantum models is also obtained. Furthermore, the algebraic structure underlying the quantum models is explored. This turns out to be a nonlinear (quadratic) algebra, which could be applied for the determination of approximate solutions to the eigenvalue equations. [DOI: 10.1063/1.1479300]

I. INTRODUCTION

A few years ago, in Ref. 1 a method was devised to find alternative Lagrangians for the time-dependent oscillator

$$\ddot{q}+\omega(t)^2 q=0, \tag{1}$$

where $q=q(t)$, $\omega(t)$ is a given differentiable function, and the dot stands for time derivative. The method, which is based on the concept of fouling transformation,[2] is reviewed in Sec. II.

In this paper we study certain nonconventional quantum Hamiltonians corresponding to the classical fouled Hamiltonians associated with the Lagrangians derived in Ref. 1. This investigation is motivated by the fact that these nonconventional quantum Hamiltonians, having a polynomial structure in the operators a and $a^\dagger$, may play an important role in the context of quantum optics, especially in handling coherence and squeezing of multiphoton systems.

All the fouled Lagrangians of the hierarchy found in Ref. 1 lead to the same equation of motion (1) as occurs for the conventional Lagrangian $L_1=1/2(\dot{q}^2-\omega(t)^2q^2)$ [see (5)]. In Sec. III the fouled Hamiltonians $K_\pm$, related to the simplest fouled Lagrangians, $L_2^{(1)}$ and $L_2^{(2)}$, given by (23) and (24) are written down. By way of example, we have limited ourselves to considering the standard (harmonic) oscillator where $\omega(t)\equiv\lambda$ is a constant. Furthermore, it is shown that (at the classical level), as one expects, $K_\pm$ reproduce the same equation of motion coming from the conventional Hamiltonian $H_0=1/2(p^2+\lambda^2q^2)$. For brevity, we shall deal with K_+ only. It turns

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out that K_+ (see Sec. IV) can assume two possible forms, denoted by $K_+^{(1)} \equiv K_1$ and $K_+^{(2)} \equiv K_2$ [see (39) and (40)], which are independent but depend explicitly on time via the coefficients $\cos \lambda t$ and $\sin \lambda t$. Consequently, K_1 and K_2 can be formally interpreted as the result of a *rotation* (of an angle λt) of the quantities $H_1 = \sqrt{\lambda}(p^2 + \lambda^2 q^2)q$ and $H_2 = (2/3\sqrt{\lambda})p^3$, which are *not* explicitly dependent on time. In other words, we have $K_1^2 + K_2^2 = H_1^2 + H_2^2$, and

$$\{K_1, K_2\}_{q,p} = \{H_1, H_2\}_{q,p}$$

(see Sec. IV), where the symbol {,} denotes the Poisson bracket with respect to the canonical variables (q,p), namely

$$\{A,B\}_{q,p} = \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q}.$$

In Sec. V the canonical quantization procedure based on a bosonic couple of annihilation and creation operators, a and $a^\dagger$ (with $[a, a^\dagger] = 1$), is applied to the fouled Hamiltonians K_1 and K_2. In such a way K_1 and K_2 are converted into a pair of Hamiltonian operators, say $\mathcal{K}_1$ and $\mathcal{K}_2$. [Classically, as we know, K_1 and K_2 provide the same equation of motion (1).] Furthermore, since the canonical quantization procedure does affect only the cubic polynomial functions of (q,p), namely H_1 and H_2, here we limit ourselves to study the operators $\mathcal{H}_1$ and $\mathcal{H}_2$, which are the quantized versions of H_1 and H_2, respectively. The arising *quantum models* are investigated in Secs. VI and VII.

Precisely, in Sec. VI we show that the quantum model coming from $\mathcal{H}_1$ gives rise to a linear second-order eigenvalue equation of the Sturm–Liouville type (in the harmonic oscillator excitation number representation, or n-rep).

An interesting feature of the operator $\mathcal{H}_1$ is that it is connected with an undetermined Hamburger moment problem.[3–5] We show that this operator has deficiency indices (1,1) and allows a one-parameter family of self-adjoint extensions whose spectra are discrete and with no point in common. This goal has been achieved essentially by associating the operator $\mathcal{H}_1$ with a Jacobi matrix.[3,5] A possible physical interpretation of the operator $\mathcal{H}_1$ is provided by fixing, among the infinite self-adjoint extensions, the extension corresponding to $\varepsilon = 0$, where ε denotes the spectral parameter. In this case the eigenvalue equations for $\mathcal{H}_1$ can be solved exactly in all the following representations: the harmonic oscillator excitation number representation (n-rep), the coordinate space representation (q-rep), and the Fock–Bargmann holomorphic function representation (z-rep).[6–8] In all these representations, for $\varepsilon = 0$ square-integrable solutions of the eigenvalue equations are explicitly obtained.

In Sec. VII we deal with the eigenvalue equation for $\mathcal{H}_2$. The analysis of this Hamiltonian is trivial. It is exactly solvable,[9] its spectrum is on the whole line, and the related eigenfunctions can be easily found. Nevertheless, $\mathcal{H}_2$ has been involved in the construction of two quantum models described by the operators $\mathcal{H}_3$ and $\mathcal{H}_4$ [see (57) and (58)], where $\mathcal{H}_2 = \mathcal{H}_3 + \mathcal{H}_4$. One can attribute to $\mathcal{H}_3$ a physical meaning. Specifically, $\mathcal{H}_3$ can be interpreted as a special case of a class of Hamiltonians appearing in the higher order nonlinear optical processes.[5,10–12] This Hamiltonian is involved in the construction of third power squeezed states.[5,11,13]

On the other hand, as we can see in Sec. VII, the operator $\mathcal{H}_4$ is closely related to $\mathcal{H}_1$ so that the solutions of the corresponding eigenvalue equation can be derived from the solutions of the eigenvalue equation for $\mathcal{H}_1$.

In Sec. VIII some constants of motion involving the operators $\mathcal{H}_1$, $\mathcal{H}_2$, $\mathcal{H}_3$, $\mathcal{H}_4$, and $\mathcal{H}_5 \sim a^3 + a^{\dagger 3}$ are derived. Section IX contains a discussion on a possible algebraic framework which could be employed to analyze Eq. (69). This approach resorts to a quadratic algebra in terms of which the operator $\mathcal{H}_1$ can be naturally expressed. Finally, in Sec. X a few concluding remarks are presented, while in the Appendix a detail of a calculation is reported.

II. FOULED LAGRANGIANS

We recall that a fouling transformation is a transformation under which the coordinates in configuration space are preserved:

$$Q=q, \tag{2}$$

while

$$P_n=P_n(q,p,t); \tag{3}$$

P_n being a polynomial of degree n in the variables q and $p=\partial L_1/\partial\dot{q}=\dot{q}$, i.e.,

$$P_n=\sum_{j=0}^{n} a_j p^{n-j}q^j, \tag{4}$$

where

$$L_1=\tfrac{1}{2}(\dot{q}^2-\omega(t)^2q^2) \tag{5}$$

is the conventional Lagrangian, and $a_j=a_j(t)$ are (real) time-dependent coefficients.

In Ref. 1 it was proven that the function $L_n=L_n(q,\dot{q},t)$ expressed by

$$L_n=\sum_{j=0}^{n}\frac{1}{n-j+1}a_j\dot{q}^{n-j+1}q^j+(\dot{a}_n-\omega^2a_{n-1})\frac{q^{n+1}}{n+1} \tag{6}$$

satisfies

$$\frac{\partial L_n}{\partial\dot{q}}=P_n, \quad \frac{\partial L_n}{\partial q}=\dot{P}_n. \tag{7}$$

The compatibility condition for these equations provides

$$\dot{a}_0=-\frac{n-1}{n}a_1, \quad \dot{a}_j=(n-j+1)\omega^2a_{j-1}-(j+1)\frac{n-j-1}{n-j}a_{j+1}, \tag{8}$$

with $j=1,2,...,n-1$. Furthermore, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L_n}{\partial\dot{q}}-\frac{\partial L_n}{\partial q}=I_n(t)(\ddot{q}+\omega(t)^2q), \tag{9}$$

where $I_n(t)$ is a time-dependent constant of motion, viz., $(\mathrm{d}/\mathrm{d}t)I_n(t)=0$, given by

$$I_n(t)=\sum_{j=0}^{n}(n-j)a_jp^{n-j-1}q^j=\frac{\partial^2L_n}{\partial\dot{q}^2} \tag{10}$$

for any $n\geqslant 1$.

From Eq. (9) we deduce that corresponding to the solution q of the generalized oscillator (1), L_n satisfies the Euler–Lagrange equation. We notice that for $n=1$, Eq. (6) gives the conventional Lagrangian (5) (with $a_0=1$ and $a_1=0$). The related invariant is $I_1=\partial^2L_1/\partial_{\dot{q}}{}^2=1$.

Hereafter, by way of example, we are interested in the case $n=2$. Then, from (6) and (10) we obtain

$$L_2=\tfrac{1}{3}a_0\dot{q}^3+\tfrac{1}{2}a_1\dot{q}^2q+a_2\dot{q}q^2+\tfrac{1}{3}(\dot{a}_2-\omega^2a_1)q^3, \tag{11}$$

$$I_2 = 2a_0 p + a_1 q, \tag{12}$$

where [see (8)]

$$\dot{a}_0 = -\tfrac{1}{2} a_1, \quad \dot{a}_1 = 2\omega^2(t) a_0, \tag{13}$$

namely

$$\ddot{a}_0 + \omega^2(t) a_0 = 0. \tag{14}$$

The general solution of Eq. (14) can be written in the form

$$a_0 = \sqrt{2}\sigma\left(c_1 \cos\frac{\theta}{2} + c_2 \sin\frac{\theta}{2}\right). \tag{15}$$

where c_1, c_2 are constants, and σ, θ are defined by

$$\ddot{\sigma} + \omega^2(t)\sigma = \frac{1}{4\sigma^3}, \tag{16}$$

and

$$\dot{\theta} = \frac{1}{\sigma^2}. \tag{17}$$

In the following we shall limit ourselves to the choice $\omega(t) = \lambda = \text{const}$. Consequently, Eqs. (16) and (17) admit the solution

$$\sigma = \frac{1}{\sqrt{2\lambda}} \tag{18}$$

and

$$\theta = 2\lambda t. \tag{19}$$

Equation (15) has the two independent solutions

$$a_0^{(1)} = \frac{1}{\sqrt{\lambda}} \cos\lambda t, \quad a_0^{(2)} = \frac{1}{\sqrt{\lambda}} \sin\lambda t, \tag{20}$$

while the corresponding values $a_1^{(1)}$, $a_1^{(2)}$ are [see (13)]

$$a_l^{(1)} = 2\sqrt{\lambda} \sin\lambda t, \quad a_1^{(2)} = -2\sqrt{\lambda} \cos\lambda t. \tag{21}$$

On the other hand, the expressions of $a_2^{(1)}$, $a_2^{(2)}$ turn out to be (see Ref. 1)

$$a_2^{(1)} = \lambda^{3/2} \cos\lambda t, \quad a_2^{(2)} = \lambda^{3/2} \sin\lambda t. \tag{22}$$

Now, using (20)–(22), from (11) we obtain the two alternative fouled Lagrangians,

$$L_2^{(1)} = \frac{1}{3\sqrt{\lambda}} \cos\lambda t \dot{q}^3 + \sqrt{\lambda} \sin\lambda t \dot{q}^2 q + \lambda^{3/2} \cos\lambda t \dot{q} q^2 - \lambda^{5/2} \sin\lambda t q^3, \tag{23}$$

$$L_2^{(2)}=\frac{1}{3\sqrt{\lambda}}\sin\lambda t\dot{q}^3-\sqrt{\lambda}\cos\lambda t\dot{q}^2q+\lambda^{3/2}\sin\lambda t\dot{q}q^2+\lambda^{5/2}\cos\lambda tq^3, \tag{24}$$

which furnish the two independent invariants

$$I_2^{(1)}=\frac{\partial^2 L_2^{(1)}}{\partial\dot{q}^2}=\frac{2}{\sqrt{\lambda}}\cos\lambda t\dot{q}+2\sqrt{\lambda}\sin\lambda t\quad q, \tag{25}$$

$$I_2^{(2)}=\frac{\partial^2 L_2^{(2)}}{\partial\dot{q}^2}=\frac{2}{\sqrt{\lambda}}\sin\lambda t\dot{q}-2\sqrt{\lambda}\cos\lambda t\quad q, \tag{26}$$

respectively [see (10)].

Equations (25) and (26) provide the general solution q and the momentum $p=\dot{q}$ of the harmonic oscillator ($\omega\equiv\lambda$), i.e.,

$$q=\frac{1}{2\sqrt{\lambda}}(I_2^{(1)}\sin\lambda t-I_2^{(2)}\cos\lambda t), \tag{27}$$

$$p=\dot{p}=\frac{\sqrt{\lambda}}{2}(I_2^{(1)}\cos\lambda t+I_2^{(2)}\sin\lambda t), \tag{28}$$

from which, as one expects,

$$H_0=\frac{1}{2}(p^2+\lambda^2q^2)=\frac{\lambda}{8}[(I_2^{(1)})^2+(I_2^{(2)})^2]=\text{const}, \tag{29}$$

where H_0 is the conventional Hamiltonian.

III. FOULED HAMILTONIANS

At this point, we build up the Hamiltonian corresponding to the Lagrangian L_2 given by (11). Following the procedure of Ref. 1, we get

$$K_\pm=-\frac{a_1}{2a_0}qP\pm\frac{2}{3}a_0\left[\left(\frac{a_1^2}{4a_0^2}-\frac{a_2}{a_0}\right)q^2+\frac{P}{a_0}\right]^{3/2}+\left[\frac{a_1}{6a_0}\left(3a_2-\frac{a_1^2}{2a_0}\right)-\frac{1}{3}\left(\dot{a}_2-\lambda^2a_1\right)\right]q^3, \tag{30}$$

where

$$P=a_0p^2+a_1qp+a_2q^2. \tag{31}$$

For the sake of definiteness, later we shall study the Hamiltonian K_+ only.

The Hamilton equations for K_+ read

$$\dot{q}=-\frac{a_1}{2a_0}q+\frac{I_2}{2a_0}, \tag{32}$$

$$\dot{P}=\frac{a_1}{2a_0}P-\frac{a_1^2-4\lambda^2a_0^2}{4a_0^2}I_2q-3a_1\left(\lambda^2-\frac{a_1^2}{12a_0^2}\right)q^2, \tag{33}$$

where the relation

$$\left(\frac{a_1^2}{4a_0^2}-\frac{a_2}{a_0}\right)q^2+\frac{P}{a_0}=\left(\frac{I_2}{2a_0}\right)^2 \tag{34}$$

with $a_2=\lambda^2 a_0$ has been used (see Ref. 1).

By developing Eqs. (31) and (32) with the help of (12) and (30), we arrive at

$$I_2(\ddot{q}+\lambda^2 q)=0, \tag{35}$$

which tells us that the fouled Hamiltonian K_+, as it occurs for the related fouled Lagrangian L_2 [see (9)], gives rise to the same equation of motion emerging from the conventional Hamiltonian (29).

By virtue of (33), the Hamiltonians (30) take the form

$$K_+=\tfrac{1}{2}a_1(p^2+\lambda^2 q^2)q+\tfrac{2}{3}a_0 p^3, \tag{36}$$

$$K_-=-\frac{3}{2}a_1 p^2 q-\frac{a_1^2}{a_0}q^2 p+\left(\frac{a_1}{2}\lambda^2-\frac{a_1^3}{6a_0^2}\right)q^3-\frac{2}{3}a_0 p^3. \tag{37}$$

One can see that

$$K_\pm=P_p-L_2, \tag{38}$$

where P and L_2 are given by (31) and (11).

IV. THE FOULED HAMILTONIANS $K_+^{(1)}$ AND $K_-^{(2)}$

By using (20)–(22), from (36) we derive the pair of (explicitly time-dependent) Hamiltonians

$$K_+^{(1)}\equiv K_1=H_1\sin\lambda t+H_2\cos\lambda t, \tag{39}$$

$$K_+^{(2)}\equiv K_2=-H_1\cos\lambda t+H_2\sin\lambda t, \tag{40}$$

where H_1 and H_2 are defined by

$$H_1=\sqrt{\lambda}(p^2+\lambda^2 q^2)q=2\sqrt{\lambda}H_0 q, \tag{41}$$

$$H_2=\frac{2}{3\sqrt{\lambda}}p^3. \tag{42}$$

One can check straightforwardly that the following evolution equations:

$$\dot{K}_1=\{K_1,H_0\}_{q,p}+\frac{\partial K_1}{\partial t}, \tag{43}$$

$$\dot{K}_2=\{K_2,H_0\}_{q,p}+\frac{\partial K_2}{\partial t}, \tag{44}$$

$$\dot{H}_1=\{H_1,H_0\}_{q,p}, \tag{45}$$

$$\dot{H}_2=\{H_2,H_0\}_{q,p}, \tag{46}$$

hold, where H_0 is given by (29) and

$$\{H_1,H_0\}_{q,p}=2\sqrt{\lambda}pH_0, \tag{47}$$

$$\{H_2,H_0\}_{q,p}=-2\frac{\lambda^2}{\sqrt{\lambda}}p^2q. \tag{48}$$

We also have that the Poisson brackets between K_1, K_2 and H_1, H_2 concide, i.e.,

$$\{K_1,K_2\}_{q,p}=\{H_1,H_2\}_{q,p}. \tag{49}$$

This is a direct consequence of the rotation form of the transformations (39) and (40).

V. QUANTIZATION

Hereafter, we shall put for simplicity $\lambda=\hbar=1$.

In order to quantize the fouled Hamiltonians (39) and (40), let us introduce the operators

$$\hat{q}=\frac{1}{\sqrt{2}}(a+a^\dagger),\quad \hat{p}=-\frac{i}{\sqrt{2}}(a-a^\dagger), \tag{50}$$

where a and $a^\dagger$ denote a (boson) annihilation and a creation operator, respectively.

By means of (50), we can write the operators $\mathcal{H}_1$ and $\mathcal{H}_2$ corresponding to the classical functions (41) and (42). We obtain

$$\mathcal{H}_1=\sqrt{2}(a^{\dagger 2}a+a^\dagger a^2+a^\dagger+a), \tag{51}$$

$$\mathcal{H}_2=\frac{i}{\sqrt{2}}\left[\frac{1}{3}(a^3-a^{\dagger 3})+(a^{\dagger 2}a-a^\dagger a^2+a^\dagger-a)\right], \tag{52}$$

with the help of the commutation rule

$$[a,a^\dagger]=1 \tag{53}$$

or, in terms of the Heisenberg commutation relation: $[\hat{q},\hat{p}]=i$.

Now let us use the representation $\hat{q}=x$, $\hat{p}=-i(\mathrm{d}/\mathrm{d}x)$, so that the operators a and $a^\dagger$ can be written as [see (50)]

$$a=\frac{1}{\sqrt{2}}\left(x+\frac{\mathrm{d}}{\mathrm{d}x}\right),\quad a^\dagger=\frac{1}{\sqrt{2}}\left(x-\frac{\mathrm{d}}{\mathrm{d}x}\right). \tag{54}$$

In terms of these quantities, $\mathcal{H}_1$ and $\mathcal{H}_2$ take the forms

$$\mathcal{H}_1=-\left(x\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\mathrm{d}}{\mathrm{d}x}\right)+x^3, \tag{55}$$

and

$$\mathcal{H}_2=\frac{2i}{3}\frac{\mathrm{d}^3}{\mathrm{d}x^3}. \tag{56}$$

For later convenience, we shall report also in the representation (54) the following operators appearing in (52):

$$\mathcal{H}_3\equiv\frac{i}{\sqrt{2}}\frac{1}{3}(a^3-a^{\dagger 3})=\frac{i}{2}\left[\frac{1}{3}\frac{\mathrm{d}^3}{\mathrm{d}x^3}+\left(x^2\frac{\mathrm{d}}{\mathrm{d}x}+x\right)\right], \tag{57}$$

$$\mathcal{H}_4 \equiv \frac{i}{\sqrt{2}}(a^{\dagger 2}a - a^\dagger a^2 + a^\dagger - a) = \frac{i}{2}\left[\frac{\mathrm{d}^3}{\mathrm{d}x^3} - \left(x^2\frac{\mathrm{d}}{\mathrm{d}x} + x\right)\right]. \tag{58}$$

In Sec. VI, we shall study the operators $\mathcal{H}_1$ and $\mathcal{H}_2$ by dealing with the corresponding eigenvalue problems.

VI. SELF-ADJOINT EXTENSIONS OF THE OPERATOR $\mathcal{H}_1$

In order to clarify the quantum-mechanical meaning of the Hamiltonian $\mathcal{H}_1$, it is crucial to establish whether $\mathcal{H}_1$ enjoys self-adjoint type properties. In doing so, first let us recall that one can provide different representations for the operator (51), which correspond to various forms of the related eigenvalue equations. We shall consider the following representations: the harmonic oscillator excitation number representation (n-rep), the coordinate representation (q-rep), and the Fock–Bargmann holomorphic function representation (z-rep).

For reader's convenience, we shall summarize in the following the main properties of these representations.[8]

Let $\mathfrak{h}$ denote the Hilbert space where the operators $\hat{q}$, $\hat{p}$ and $a^\dagger$, a act. In the n- rep, the vectors $\{|n\rangle\}$ form a basis in $\mathfrak{h}$. The following relations

$$a = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad a^\dagger a|n\rangle = n|n\rangle \tag{59}$$

hold.

On the other hand, in the q-rep a vector $|\psi\rangle$ belonging to the space $\mathfrak{h}$ is represented by a coordinate function $\langle q|\psi\rangle = \psi(q)$ which is square-integrable:

$$\int_{-\infty}^{+\infty} |\psi(q)|^2\,\mathrm{d}q < \infty. \tag{60}$$

The basic vector $|n\rangle$ is described by the function

$$\langle q|n\rangle = \varphi_n(q) = N_n H_n(q)\exp\left(-\frac{q^2}{2}\right), \tag{61}$$

where $N_n = (\sqrt{\pi}2^n n!)^{-1/2}$ and $H_n(q)$ is the Hermite polynomial of degree n. In the q-rep, formulas (59) become the standard recursion relations for the Hermite polynomials.

In order to introduce the Fock–Bargmann representation (or z-rep), let $|\psi\rangle$ be an arbitrary normalized vector in $\mathfrak{h}$, namely

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n|n\rangle, \tag{62}$$

with $\langle\psi|\psi\rangle = \Sigma_{n=0}^{\infty}|c_n|^2 = 1$. Furthermore, taking into account the Glauber form

$$|z\rangle = \exp\left(-\frac{|z|^2}{2}\right)\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle, \tag{63}$$

the state $|\psi\rangle$ is completely determined by

$$\langle z|\psi\rangle = \exp\left(-\frac{|z|^2}{2}\right)\psi(\overline{z}), \tag{64}$$

where

$$\psi(z)=\sum_{n=0}^{\infty} c_n u_n(z), \tag{65}$$

with $u_n(z)=z^n/\sqrt{n!}$. Owing to the condition $\Sigma_{n=0}^{\infty}|c_n|^2=1$, the series in (65) converges uniformly in any compact domain of the complex z plane. Consequently, $\psi(z)$ turns out to be an entire holomorphic function in the z plane, and

$$\|\psi\|^2=\int \exp(-|z|^2)|\psi(z)|^2\,\mathrm{d}\mu(z)<\infty, \tag{66}$$

where $\mathrm{d}\mu(z)=\pi^{-1}\,\mathrm{d}x\,\mathrm{d}y$, $z=x+iy$.[8]

The scalar product of two entire functions $\psi_1(z)$ and $\psi_2(z)$ obeying the condition (66) is given by

$$\langle\psi_1|\psi_2\rangle=\int \exp(-|z|^2)\overline{\psi}_1(z)\psi_2(z)\mathrm{d}\mu(z). \tag{67}$$

As proven by Bargmann,[7] the Fock–Bargmann representation space with a scalar product provided by (67) is really a Hilbert space. We observe also that in the z-rep, the operator solution for the commutation relation $[a,a^\dagger]=1$[6] is

$$a\to\frac{\mathrm{d}}{\mathrm{dz}},\quad a^\dagger\to z. \tag{68}$$

Now let us consider the eigenvalue equation

$$(a^{\dagger 2}a+a^\dagger a^2+a+a^\dagger)|\chi\rangle=\varepsilon|\chi\rangle. \tag{69}$$

Starting from the n-rep and following the lines of Ref. 5, let us put

$$|\chi\rangle=\sum_{n=0} f_n(\varepsilon)|n\rangle \tag{70}$$

into Eq. (69). By using Eq. (59), after simple calculations we obtain the recursion formula

$$(n+1)^{3/2}f_{n+1}(\varepsilon)-\varepsilon f_n(\varepsilon)+n^{3/2}f_{n-1}(\varepsilon)=0 \tag{71}$$

for $n\geqslant 1$, and

$$f_1(\varepsilon)=\varepsilon f_0(\varepsilon) \tag{72}$$

(the boundary condition).

We remark that the sequence $\{f_n\}$ is such that the series $\Sigma_{n=0}|f_n|^2$ converges, i.e., the sequence $\{f_n\}\equiv(f_0,f_1,f_2,\ldots)$ belongs to the Hilbert space l^2.

To show this, first let us consider the case $\varepsilon=0$. Then, Eqs. (71) and (72) provide

$$f_{2n}=(-1)^n\left[\frac{(2n-1)!!}{(2n)!!}\right]^{3/2}f_0, \tag{73}$$

the odd terms being zero. Thus, from the asymptotic formula of gamma function (Ref. 14, p. 257), we deduce that for $n\to\infty$, $|f_{2n}|^2$ behaves as $n^{-3/2}$, so that $\Sigma_{n=0}|f_{2n}|^2<\infty$. In general, i.e., for $\varepsilon\neq 0$, Eq. (71) tells us that for great values of n, the sum of the first and the last term is leading with respect to the second term. This allows us to see easily that both even and odd terms, $|f_{2n}|^2$ and $|f_{2n+1}|^2$, behave asymptotically as $n^{-3/2}$. To conclude, the series $\Sigma_{n=0}|f_n|^2$ is convergent,

namely the sequence $\{f_n\}$ belongs to the Hilbert space l^2 for any value of the spectral parameter ε. Then, the equation $\mathcal{H}_1^\dagger|\chi\rangle=\varepsilon|\chi\rangle$, for $\mathrm{Im}\,\lambda\neq 0$, has nontrivial solutions (Ref. 3, p. 140).

Now, by introducing the notation $b_n=(n+1)^{3/2}$, we see that it is possible to associate with the difference equation (71) the (infinite) Jacobi matrix

$$A=\begin{pmatrix} 0 & b_0 & 0 & 0 & \cdots \\ b_0 & 0 & b_1 & 0 & \cdots \\ 0 & b_1 & 0 & b_2 & \cdots \\ 0 & 0 & b_2 & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}, \tag{74}$$

so that Eq. (69) is equivalent to the eigenvalue equation $Af=\varepsilon f$, with $f=(f_0,f_1,\ldots)^T$.

The Jacobi matrix (74) plays a crucial role in the study of the Hamburger moment problem (see, for example, Refs. 3, 5, and 15). Precisely, let us consider the moments

$$s_n=\int_{-\infty}^{+\infty} x^n\,\mathrm{d}\sigma(x), \quad n=0,1,2,..., \tag{75}$$

where σ denotes a (positive) measure on $\mathbb{R}$ (Ref. 15, p. 145). The Hamburger moment problem is to determine conditions on a sequence of real numbers $\{s_n\}_{n=0}^{\infty}$, so that there exists a measure satisfying (75). One can show that a sequence of real numbers $\{s_n\}$ are the moments of a positive measure on $\mathbb{R}$ if and only if for all N and all $\alpha_0,\alpha_1,\ldots,\alpha_N\in\mathbb{C}$, one has

$$\sum_{n,m=0}^{N} \overline{\alpha}_n\alpha_m s_{n+m}\geqslant 0. \tag{76}$$

From the Jacobi matrix (74) we get the limitations

$$\sum_{n=0}^{\infty}\frac{1}{b_n}=\sum_{n=0}^{\infty}\frac{1}{(n+1)^{3/2}}<\infty, \quad b_{n-1}b_{n+1}<b_n^2. \tag{77}$$

Consequently, the Jacobi matrix (74) belongs to the type *C* (limit circle case), and corresponds to an undetermined Hamburger moment problem (Refs. 3 and 5). So, the properties of the operator $\mathcal{H}_1\sim a^{\dagger 2}a+a^\dagger a^2+a+a^\dagger$ are similar to the properties of the operator $a^k+a^{\dagger k}$ $(k=3)$ discussed by Nagel.[5] In other words, the operator $\mathcal{H}_1$ has deficiency indices (1, 1) and allows a one-parameter family of self-adjoint extensions, each having a purely discrete spectrum on the real line.[4,16] The spectra of two different extensions turn out to have no point in common (Ref. 3, p. 152). We have that different self-adjoint extensions correspond to different dynamics.[15,17]

Since every self-adjoint extension of $\mathcal{H}_1$ has a discrete spectrum on the real line, and taking one eigenvalue determines the corresponding extension uniquely, let us choose $\varepsilon=0$.

In this case the eigenvalue equation underlying the operator $\mathcal{H}_1$ can be solved exactly in all the representations mentioned at the beginning of this section.

To show this, let us deal with the *q*-rep. With the help of (54), the eigenvalue equation (69) reads

$$x\phi''+\phi'+(\sqrt{2}\varepsilon-x^3)\phi=0, \tag{78}$$

where $\phi'\equiv(\mathrm{d}/\mathrm{d}x)\phi$.

Equation (78) can be written as the Sturm–Liouville equation (Ref. 18, p. 59)

$$\mathcal{L}[\phi(x)]=-\sqrt{2}\varepsilon\phi(x), \tag{79}$$

where $\mathcal{L}$ denotes the Sturm–Liouville operator

$$\mathcal{L}=\frac{\mathrm{d}}{\mathrm{d}x}\left[x\frac{\mathrm{d}}{\mathrm{d}x}\right]-x^3. \tag{80}$$

By using the transformation

$$\phi(x)=\exp\left(-\frac{x^2}{2}\right)\psi(x), \tag{81}$$

Eq. (78) becomes

$$x\psi''+(1-2x^2)\psi'+(\sqrt{2}\varepsilon-2x)\psi=0. \tag{82}$$

This equation is satisfied by

$$\psi(x)=\sum_{n=0}^{\infty} f_n N_n H_n(x), \tag{83}$$

where the coefficients f_n fulfill the recursion relations (71) and (72). We have already shown that $\{f_n\}\in l^2$. Then, the function $\psi(x)$ belongs to the Hilbert space $L^2_{e^{-x^2}}(-\infty,\infty)$ [$\exp(-x^2)$ is the weight function]. We point out that generally the relation (83) is not valid in the pointwise sense, but it holds in accordance with the metric of $L^2_{e^{-x^2}}(-\infty,\infty)$, namely

$$\lim_{n\to\infty}\int_{-\infty}^{+\infty}\left|\psi(x)-\sum_{k=0}^{n} f_k N_k H_k(x)\right|^2\exp(-x^2)\mathrm{d}x=0. \tag{84}$$

For $\varepsilon=0$, via the change of variable $\xi=x^2$ Eq. (82) can be written as a special case of a Kummer equation, whose independent solutions are $M(1/2,1;x^2)$ and $U(1/2,1;x^2)$ (Ref. 14, p. 504). In the case the solution $\psi(x)$ of Eq. (82) with the property $\psi(x)\in L^2_{e^{-x^2}}(-\infty,\infty)$ is given by

$$\psi(x)=cU\left(\frac{1}{2},1;x^2\right)=\sum_{n=0}^{\infty} f_{2n}N_{2n}H_{2n}(x), \tag{85}$$

where the constant c is such that $c\pi^{3/4}=f_0$, and

$$f_{2n}=f_0\pi^{-3/4}N_{2n}\int_{-\infty}^{+\infty}U\left(\frac{1}{2},1;x^2\right)H_{2n}(x)\exp(-x^2)\mathrm{d}x. \tag{86}$$

One can easily check that (86) is satisfied for any $n\in\mathbb{N}$

Finally, in the z-rep, i.e., for $|\chi\rangle\to\chi$, $a^\dagger\to z$, $a\to\mathrm{d}/\mathrm{d}z$, Eq. (69) gives

$$z\chi_{zz}+(1+z^2)\chi_z+(z-\varepsilon)\chi=0, \tag{87}$$

where

$$\chi=\sum_{n=0}^{\infty} f_n\frac{z^n}{\sqrt{n!}} \tag{88}$$

and f_n satisfies the recursion relations (71) and (72). For $\varepsilon=0$, the eigenvalue equation (87) as well can be exactly solved. In fact, by setting $z^2=y$, $\zeta=-y/2$, this equation becomes a special case of the Kummer equation.

Therefore, in the z-rep, where the eigenfunction should be a holomorphic (and normalizable) function in the whole z-plane, one has the solution $M(1/2,1;-z^2/2)$. The other solution, namely the Kummer function $U(1/2,1;-z^2/2)$, is not holomorphic at $z=0$.

To conclude this section, we observe that the solutions of the eigenvalue equation for $\mathcal{H}_1$ in the case $\varepsilon=0$ can be also found from Eqs. (71) and (72), obtained within the *n*-rep, by means of the standard integral representations of the confluent hypergeometric functions. An example of this procedure is displayed in Ref. 19.

VII. THE $\mathcal{H}_2$, $\mathcal{H}_3$, $\mathcal{H}_4$ MODELS

The eigenvalue problem for the operator $\mathcal{H}_2$ can be written as

$$\mathcal{L}\psi=\varepsilon\psi, \tag{89}$$

where $\mathcal{L}=(2i/3)D_x^3$ $(D_x=\mathrm{d}/\mathrm{d}x)$. The study of Eq. (89) is trivial. It is exactly solvable,[9] its spectrum is on the whole line, and the related eigenfunctions are of the exponential type.

The operator $\mathcal{H}_3$ [see (57)] belongs to the class of Hamiltonians

$$\mathcal{H}=i\kappa_n(a^n-a^{\dagger n}) \tag{90}$$

appearing in the higher order nonlinear optical processes. In particular, (57) describes a subharmonic generation process, in which a photon from a strong pump beam produces *n* photons of the signal beam in a nonlinear medium.[11] The constant κ_n is related to the *n*th nonlinear susceptibility coefficient and to the amplitude of the pump field, while a and $a^\dagger$ are the annihilation and the creation operators for the signal field. In this context, the evolution of an arbitrary initial state $|\Psi(0)\rangle$ of the signal field to the state $|\Psi(t)\rangle$ is governed by

$$|\psi(t)\rangle=\exp[\kappa_n t(a^n-a^{\dagger n})]|\Psi(0)\rangle. \tag{91}$$

The squeezing of this state was examined by Hillery, Zubairy, and Wódkiewicz.[11] They showed that to any order in the coupling constant κ_n, the vacuum state is not squeezed in the higher order nonlinear optical processes $(n\geqslant 3)$.

This important result stimulated the analysis of *n*th power squeezed states. Interesting (and, generally, not yet completely explored) questions arise in connection with this argument. Some of them are discussed in Refs. 5, 13, and 19, and references therein.

Now let us make some comments about the Hamiltonian $\mathcal{H}_4$. This operator is closely related to $\mathcal{H}_1$. This can be seen by means of the phase transformation $a'=ia$, $a'^\dagger=-ia^\dagger$, so that $\mathcal{H}_4$ takes the form

$$\mathcal{H}_4=-\frac{1}{\sqrt{2}}(a'^{2\dagger}a'+a'^\dagger a'^2+a'^\dagger+a'). \tag{92}$$

In other words, one has $\mathcal{H}_4=1/2\mathcal{H}_1$ (in terms of the primed operators). This corresponds to pick up $q'=-p$ and $p'=q$. In such a way $\mathcal{H}_4$ turns out to be the inverse Fourier transform of (55). Therefore, the solutions of the eigenvalue equation for the Hamiltonian operator $\mathcal{H}_4$ can be derived from the solutions of the eigenvalue equation for the Hamiltonian operator $\mathcal{H}_1$ [see (69)].

The eigenvalue equation for $\mathcal{H}_1$ $(\mathcal{H}_4)$ can be investigated by means of the algebraic approach outlined in Sec. IX.

VIII. EQUATIONS AND CONSTANTS OF MOTION RELATED TO THE OPERATORS $\mathcal{H}_j$

The equations of motion for the Hamiltonians $\mathcal{H}_j$ $(j=1,2,3,4)$ arise immediately by using the Heisenberg representation. In other words, by putting $a(t)=a(0)\exp(-it)$ and $a^\dagger(t)=a^\dagger(0)\exp(it)$ in the expressions (51) and (58), we easily find (as one expects) that $\mathcal{H}_1$ and $\mathcal{H}_4$ satisfy the same equation of motion (i.e., the equation for the harmonic oscillator of frequency $\lambda=1$):

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathcal{H}_1+\mathcal{H}_1=0, \quad \frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathcal{H}_4+\mathcal{H}_4=0. \tag{93}$$

On the other hand, for the operators $\mathcal{H}_3=(i/\sqrt{2})\frac{1}{3}(a^3-a^{\dagger 3})$ [see (57)] and $\mathcal{H}_5=(1/\sqrt{2})1/3(a^3+a^{\dagger 3})$, the same considerations made for $\mathcal{H}_1$ and $\mathcal{H}_4$ in Sec. VII hold. One has that $\mathcal{H}_3$ and $\mathcal{H}_5$ obey the same equation of motion (i.e., the equation for the harmonic oscillator of frequency 3):

$$\mathrm{d}t^2\mathcal{H}_3+9\mathcal{H}_3=0, \quad \frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathcal{H}_5+9\mathcal{H}_5=0. \tag{94}$$

Some comments on Eqs. (93) and (94) are presented in Sec. X.

At this point, we observe that in addition to the constants of motion

$$\tilde{q}=e^{-it\hat{H}_0}\hat{q}e^{it\hat{H}_0}=\hat{q}\cos t-\hat{p}\sin t, \tag{95}$$

$$\tilde{p}=e^{-it\hat{H}_0}\hat{p}e^{it\hat{H}_0}=\hat{q}\sin t+\hat{p}\cos t, \tag{96}$$

where $[\hat{q},\hat{p}]=i$, $\hat{H}_0=1/2(\hat{p}^2+\hat{q}^2)$, and $\tilde{q}=-1/2I_2^{(2)}$, $\tilde{p}=1/2I_2^{(1)}$, we obtain also the following set of constants:

$$\tilde{H}_1=\mathcal{H}_1\cos t-2\mathcal{H}_4\sin t, \tag{97}$$

$$\tilde{H}_4=\frac{1}{4}\mathcal{H}_1\sin t+\mathcal{H}_4\cos t, \tag{98}$$

$$\tilde{H}_3=\mathcal{H}_3\cos 3t-\mathcal{H}_5\sin 3t, \tag{99}$$

$$\tilde{H}_5=\mathcal{H}_3\sin 3t+\mathcal{H}_5\cos 3t. \tag{100}$$

In terms of the arbitrary constants $\tilde{H}_j(j=1,4,3,5)$, one can express the general solutions of Eqs. (93) and (94), which can be easily found by inverting the transformations (97), (98) and (99), (100), respectively.

IX. A POSSIBLE ALGEBRAIC FRAMEWORK FOR THE STUDY OF EQ. (69)

For $\varepsilon\neq 0$, Eq. (69) could be investigated following different analytical techniques. Among these, an important role is played by the algebraic approach, which allows one to express Eq. (69) in terms of the generators of a *quadratic* algebra.[20,21]

As an example of a quadratic algebra, we can consider a nonlinear deformation of the (linear) $su(1,1)$ algebra, defined by

$$[J_0,J_\pm]=\pm J_\pm, \tag{101}$$

$$[J_+,J_-]=P(J_0), \tag{102}$$

where the Jacobi indentity holds. $J_\pm$ are the ladder operators, and $P(J_0)$ is a second-degree polynomial function of the diagonal operator J_0. $P(J_0)$ can be written in the form

$$P(J_0)=\alpha_1+\alpha_2 J_0+\alpha_3 J_0^2, \tag{103}$$

where α_i $(i=1,2,3)$ are arbitrary coefficients $(\alpha_3\neq 0)$.

Now let us introduce the (bosonic) realization

$$J_0 = a^\dagger a + \tfrac{1}{2}, \tag{104}$$

$$J_- = -(a^\dagger a^2 + a), \tag{105}$$

$$J_+ = a^{\dagger 2} a + a^\dagger, \tag{106}$$

with $J_+ = -(J_-)^\dagger$. Then, the operators (104)–(106) turn out to obey the commutation relations

$$[J_0, J_\pm] = \pm J_\pm, [J_+, J_-] = \tfrac{1}{4} + 3J_0^2. \tag{107}$$

We remark that the quadratic algebra (107) is a finite $W_3^{(2)}$-algebra,[20,21] which corresponds to choosing $\alpha_1 = 1/4$, $\alpha_2 = 0$, and $\alpha_3 = 3$ in (103).

By virtue of (104)–(106), Eq. (69) can be reexpressed as

$$\Omega(\varepsilon)|\chi\rangle = 0, \tag{108}$$

with

$$\Omega(\varepsilon) = J_+ - J_- - \varepsilon. \tag{109}$$

Therefore, the eigenvalue problem (69) can be formulated in terms of the generators $J_\pm$ of a quadratic algebra of the type $W_3^{(2)}$. The Casimir operator of the quadratic algebra (107) is considered in the Appendix.

X. CONCLUSIONS

In the context of the existence of an infinite set of fouled Lagrangians and Hamiltonians for the generalized (time-dependent) oscillator, we have studied a special case where the frequency of the oscillator is assumed to be a constant λ (harmonic oscillator). By way of example, we have considered a pair of independent fouled Lagrangians $(L_2^{(1)}, L_2^{(2)})$ [see (23) and (24)] and, in correspondence, a pair of fouled independent Hamiltonians (K_1, K_2) [see (39) and (40)] which lead, at the classical level, to the same equation of motion provided by the conventional Lagrangian and Hamiltonian. Both $(L_2^{(1)}, L_2^{(2)})$ and (K_1, K_2) are explicitly time-dependent. The method followed to find these alternative Lagrangians and Hamiltonians implies the construction of two independent invariants (constants of motion), $I_2^{(1)}$ and $I_2^{(2)}$; in terms of them the canonical variables q and p can be expressed. These invariants, which are of the Nöther type,[22] are connected with the "quadrature-phase amplitudes" appearing in the problem of generation of squeezed states in certain optical devices.[23]

In this paper we have focused our attention mainly on the quantized version of the fouled Hamiltonians (K_1, K_2). Since K_1 and K_2 are related to the cubic polynomials $H_1 = \sqrt{\lambda}(p^2 + \lambda^2 q)q$ and $H_2 = (2/3\sqrt{\lambda})p^3$ by a formal rotation, the canonical quantization prescription affects essentially H_1 and H_2. Our purpose has been to study, at the quantum level, the Hamiltonians $\mathcal{H}_1$ and $\mathcal{H}_2$ [see (51) and (52)] corresponding to H_1 and H_2. The model described by $\mathcal{H}_2$ is associated with an eigenvalue problem given by a (linear) third-order differential equation, with constant coefficients, which is exactly solvable.[9] Furthermore, we have put $\mathcal{H}_2 = \mathcal{H}_3 + \mathcal{H}_4$, where $\mathcal{H}_4$ [see (58)] turns out to be closely related to the quantum model $\mathcal{H}_1$ in the sense discussed in Sec. VII. On the other hand, the quantum model $\mathcal{H}_3$ has a well-defined physical interpretation. It belongs to a class of Hamiltonians which finds applications in the field of nth power squeezed states.

Finally, the operator $\mathcal{H}_1$, considered in Sec. VI, has deficiency indices (1, 1) and allows a one-parameter family of self-adjoint extensions, each having a purely discrete spectrum on the real line. The spectra of two different extensions have no point in common. Since different self-adjoint extensions correspond to different dynamics, we needed to fix a given dynamics. This has been carried out by choosing the value $\varepsilon = 0$ for the eigenvalue parameter. In this case all the differen-

tial equations coming from (69) in all the representations: *n*-rep, *q*-rep, and *z*-rep, can be solved exactly. In this case, square-integrable solutions of the eigenvalue equations are explicitly determined.

In order to investigate some properties of the Hamiltonians $\mathcal{H}_j$ $(j=1,2,3,4)$, in Sec. VIII we have introduced the operator $\mathcal{H}_5 \sim (a^3 + a^{3\dagger})$, which is connected with $\mathcal{H}_3$, as one can see by using the transformation $a' = ia$, $a'^{\dagger} = -ia^{\dagger}$. We have built up a set of constants of motion involving $(\mathcal{H}_1, \mathcal{H}_4)$ and $(\mathcal{H}_3, \mathcal{H}_5)$. These constants play the role of the arbitrary constants present in the general solution of two equations of the harmonic oscillator-type of frequencies 1 and 3, respectively, which are satisfied by $(\mathcal{H}_1, \mathcal{H}_4)$ and $(\mathcal{H}_3, \mathcal{H}_5)$ [see (93) and (94)].

To conclude, we point out that quadratic (and, more in general, polynomially deformed algebras) take place in quantum optics in relation to the construction of coherent states and in the description of multiphoton processes (see, for example Refs. 24 and 25, and references therein). Keeping in mind these problems, it should be of interest to deal with the quantization of fouled Hamiltonians (of the generalized oscillator) expressed by polynomials in the canonical variables (q,p) of degree higher than three.

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APPENDIX: THE CASIMIR INVARIANT FOR THE QUADRATIC ALGEBRA (107)

We remind the reader that a standard form of a quadratic algebra, which is important in the treatment of coherent states of trilinear boson Hamiltonians,[26] is[24,25,27]

$$[N_0, N_\pm] = \pm N_\pm, \quad [N_+, N_-] = \pm 2N_0 + \delta N_0^2, \tag{A1}$$

where the positive (negative) sign of $2N_0$ indicates a polynomially deformed $su(2)$ $(su(1,1))$, and δ is a parameter.

The Casimir operator is given by[24,25,27]

$$C = N_- N_+ + N_0(N_0+1)\left[1 + \frac{\delta}{6}(2N_0+1)\right]. \tag{A2}$$

By setting

$$J_0 = a_0 N_0 + b_0, \tag{A3}$$

$$J_- = k_1 N_-, \tag{A4}$$

$$J_+ = k_2 N_+, \tag{A5}$$

and choosing, for example,

$$a_0 = 1, \quad b_0 = \frac{i}{2\sqrt{3}}, \quad k_1 k_2 = \frac{i\sqrt{3}}{2}, \tag{A6}$$

the commutator relations (107) are converted into

$$[N_0, N_\pm] = \pm N_\pm, \quad [N_+, N_-] = 2N_0 + \delta N_0^2, \tag{A7}$$

with $\delta = -2i\sqrt{3}$. Hence, the Casimir operator (A2) reads

$$C = N_- N_+ + N_0(N_0+1)\left[1 - \frac{i}{\sqrt{3}}(2N_0+1)\right]. \tag{A8}$$

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Redefining spinors in Lorentz-violating quantum electrodynamics

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An analysis of spinor redefinitions in the context of the Lorentz-violating quantum electrodynamics (QED) extension is performed. Certain parameters that apparently violate Lorentz invariance are found to be physically irrelevant as they can be removed from the Lagrangian using an appropriate redefinition of the spinor field components. It is shown that conserved currents may be defined using a modified action of the complex extension of the Lorentz group on the redefined spinors. This implies a natural correspondence between the apparently Lorentz-violating theory and conventional QED. Redefinitions involving derivatives are shown to relate certain terms in the QED extension to Lagrangians involving nonlocal interactions or skewed coordinate systems. The redundant parameters in the QED extension are identified and the Lagrangian is rewritten in terms of physically relevant coupling constants. The resulting Lagrangian contains only physically relevant parameters and transforms conventionally under Lorentz transformations. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1477938]

I. INTRODUCTION

The possibility of miniscule violations of Lorentz invariance arising from a more fundamental theory of nature has been of recent interest.[1] For example, such violations may arise in the low-energy limit of string theory,[2] or physically realistic noncommutative field theories.[3] The full standard model extension uses the general concept of spontaneous symmetry breaking to construct a Lagrangian consisting of all possible terms involving standard-model fields that are observer Lorentz scalars, including terms having coupling coefficients with Lorentz indices. At low energies, the relevant operators that are gauge invariant all have mass dimension $D \leqslant 4$, and are given in Ref. 4. At higher energy scales nonrenormalizable terms are expected to play a role in the theoretical consistency of the model.[5]

Various experiments have placed stringent bounds on parameters in the standard-model extension, including comparative tests of quantum electrodynamics (QED) in Penning traps and colliders,[6–11] spectroscopy of hydrogen and antihydrogen,[12,13] measurements of muon properties,[14,15] clock-comparison experiments,[16–20] observations of the behavior of a spin-polarized torsion pendulum,[21,22] measurements of cosmological birefringence,[23,4,24] studies of neutral-meson oscillations,[25–27] and observations of the baryon asymmetry.[28]

In the theoretical results involving experimentally observable quantities, some of the parameters in the standard model extension do not appear while others occur only in specific linear combinations. The reason behind this is that some parameters that apparently violate Lorentz invariance when the spinor field is assumed to transform in the standard way under the action of the Lorentz group do not in fact violate this symmetry when the action on the field is appropriately modified such that the associated Lorentz currents are conserved. The freedom to select spinor coordinates in different ways generates a natural equivalence relation on the collection of Lagrangians. Different Lagrangians in the same equivalence class are related by field redefinitions; that is, by an invertible map between fields used to describe the same physics. The explicit

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construction of the redefinition used in this paper appears in Eq. (5). All Lagrangians in the same class are physically equivalent and the spinor transformation properties can be implemented so that the Lorentz currents are as close to conserved as possible. In other words, redefinitions may be used to define the currents so that they absorb the apparently Lorentz-violating terms which are obstructions to conservation. This means that one can use the transformation properties to eliminate a subset of the parameters appearing in the standard model extension and no more.

In this paper, the effects of field redefinitions in the context of extended QED are examined in detail. Particular terms in the standard model extension are already known to be unobservable since explicit redefinitions of the spinor components have previously been considered.[4] It is the goal of this work to analyze a more general set of field redefinitions and use them to simplify the full Lorentz-violating Lagrangian as much as possible. The basic idea is to remove parameters that depend explicitly on the spinor coordinates. Once these redundant parameters have been eliminated, the remaining field transforms according to the standard action of the complex Lorentz group.

The paper is organized as follows. In Sec. II, the extended QED theory is summarized. In Sec. III, an analysis is presented of the field redefinitions that are used to generate specific terms in the QED extension. The effects of transformations which do not include terms involving differentiation as well as those that do are investigated. The currents associated with U(1) and Poincaré group transformations for the general QED extension are derived in Sec. IV. It is shown that conserved currents can be defined when only redundant parameters are present by using a similar representation to the conventional complex Lorentz group action. Section V contains the construction of the physical extended QED Lagrangian with all redundant parameters removed.

II. EXTENDED QED

To study the effects of specific field redefinitions, we restrict our attention to the QED subset involving only the electron and photon sectors of the full standard model extension presented in Ref. 4. In the pure-photon sector, there is one CPT-even (k_F) and one CPT-odd (k_{AF}) Lorentz-violating term. The free photon Lagrangian is

$$\mathcal{L}_{\text{photon}} = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} - \tfrac{1}{4}(k_F)_{\kappa\lambda\mu\nu}F^{\kappa\lambda}F^{\mu\nu} + \tfrac{1}{2}(k_{AF})^{\kappa}\epsilon_{\kappa\lambda\mu\nu}A^{\lambda}F^{\mu\nu}, \tag{1}$$

where the coupling k_F is a real, dimensionless coupling that can be taken to have the symmetries of the Riemann tensor, and the coefficient k_{AF} is real and has dimensions of mass.

Denoting the four-component electron field by ψ and the electron mass by m, the general QED Lagrangian for electrons and photons including Lorentz-violating interactions arising from a generic spontaneous symmetry breaking mechanism is

$$\mathcal{L}^{\text{QED}}_{\text{electron}} = \frac{i}{2}\bar{\psi}\Gamma_{\nu}\overleftrightarrow{D}^{\nu}\psi - \bar{\psi}M\psi, \tag{2}$$

where $D_{\mu} = \partial_{\mu} + iqA_{\mu}$ is the usual covariant derivative,

$$\Gamma_{\nu} = \gamma_{\nu} + c_{\mu\nu}\gamma^{\mu} + d_{\mu\nu}\gamma_5\gamma^{\mu} + e_{\nu} + if_{\nu}\gamma_5 + \tfrac{1}{2}g_{\lambda\mu\nu}\sigma^{\lambda\mu}, \tag{3}$$

and

$$M = m + im_5\gamma_5 + a_{\mu}\gamma^{\mu} + b_{\mu}\gamma_5\gamma^{\mu} + \tfrac{1}{2}H_{\mu\nu}\sigma^{\mu\nu}. \tag{4}$$

Note that any Lorentz-*preserving* terms that arise from spontaneous symmetry breaking can be absorbed into the bare mass terms m, m_5, and the overall normalization of the Lagrangian. The normalization is chosen such that the coefficient of the γ_{ν} term in Eq. (3) is one. The coupling coefficients a, b, c, d, e, f, g, m_5, and H are real, constant parameters related to the vacuum expectation value of contributing tensor fields in the underlying theory.

Some of these parameters (or combinations of parameters) are only apparently Lorentz-violating as the Lagrangian containing them can be shown to be equivalent to the standard Lagrangian using the appropriate field redefinition. This question is taken up in Sec. III.

III. GENERAL FERMION FIELD REDEFINITIONS

Some of the Lorentz-violating couplings in Eq. (2) can in fact be eliminated through a redefinition of the spinor field. To determine precisely which terms can be removed in this manner, it is useful to begin with the standard Dirac Lagrangian in terms of ψ with no Lorentz-violating terms and perform a field redefinition of the form $\psi = R\chi$, where R is some operator. The Lagrangian in terms of χ will contain terms included in the full Lorentz-violating Lagrangian. In this section, we examine possible choices for the field redefinition and examine the resulting terms in the Lagrangian.

To see which terms can be removed from the theory, we consider generic redefinitions of the fermion fields of the form

$$\psi(x) = [1 + f(x,\partial)]\chi(x), \tag{5}$$

where $f(x,\partial)$ represents a general 4×4 matrix function of the coordinates and derivatives. Only lowest order terms in the field redefinition parameters are retained since the Lorentz-violating couplings in the full Lagrangian are assumed small. By applying this transformation to the conventional free fermion Lagrangian (containing no Lorentz-violating parameters) we will see which terms can be eliminated from the extended theory by applying the inverse transformation.

To simplify the task, note that the Lorentz-violating terms generated by this transformation must have no explicit dependence on the coordinates and must consist of dimension $D \leqslant 4$ operators.[29] Candidate terms for $f(x,\partial)$ up to second order in x and ∂ are of the form

$$f(x,\partial) = v\cdot\Gamma + i\theta + iA_\mu x^\mu + B_\mu \partial^\mu + \gamma_5 \tilde{B}_\mu \partial^\mu + C_{\mu\nu} x^\mu \partial^\nu, \tag{6}$$

where v represents a set of arbitrary complex constants multiplying an arbitrary gamma matrix, denoted Γ, in the set $\{i\gamma_5, \gamma^\mu, \gamma_5\gamma^\mu, \sigma^{\mu\nu}\}$, θ is a complex constant, while A_μ, B_μ, $\tilde{B}_\mu$, and $C_{\mu\nu}$ are arbitrary real constants. Note that this is a generalization of the field redefinitions previously considered in Ref. 4.

The terms Re θ, B_μ and the antisymmetric part of $C_{\mu\nu}$ (together with the appropriate spin components $v_{\mu\nu}$) are simply the generators of the U(1) and Poincaré groups and are symmetries of the conventional Lagrangian. These terms do not generate any artificial Lorentz-violating parameters. The term Im θ rescales the Lagrangian and can be absorbed into the other constants. This leaves several independent transformations that may generate artificial Lorentz-violating terms. We proceed to calculate these explicitly in the rest of this section. Since we are working to lowest order in Lorentz-violating parameters, we can consider each term independently.

First, we summarize the results obtained using the v terms which have been previously described in Ref. 4. An explicit example is presented to illustrate the general method. As shown in Sec. IV, a field redefinition of this type can be interpreted as selecting a new basis in spinor space for the representations of SL(2,C), the complex extension of the Lorentz group. The standard Lagrangian expressed in terms of the redefined field is given by

$$\begin{aligned}\mathcal{L} &= \frac{i}{2}\bar{\psi}\gamma^\mu \overleftrightarrow{\partial}_\mu \psi - m\bar{\psi}\psi \\ &= \mathcal{L}_0 + \frac{i}{2}\bar{\chi}[\{\gamma^\mu, \Gamma\cdot \mathrm{Re}\, v\} + i[\gamma^\mu, \Gamma\cdot \mathrm{Im}\, v]]\overleftrightarrow{\partial}_\mu \chi - 2m\, \mathrm{Re}\, v\cdot\bar{\chi}\Gamma\chi,\end{aligned} \tag{7}$$

where $\mathcal{L}_0$ is the conventional free field Lagrangian in terms of χ. For example, consider the field redefinition induced by $v\cdot\Gamma = v_\mu\gamma^\mu$. Using the above-given relation yields

TABLE I. Summary of terms generated by field redefinitions of the form $v\cdot\Gamma$.

$\mathbf{v}\cdot\mathbf{\Gamma}$	$\mathbf{v}\in\Re$ ($v\equiv\mathrm{Re}\,\mathbf{v}$)	$\mathbf{v}\in\Im$ ($v\equiv\mathrm{Im}\,\mathbf{v}$)
$v(i\gamma_5)$	Used to eliminate m_5 term	$d_{\mu\nu}=2vg_{\mu\nu}$
$v_\mu\gamma^\mu$	$e_\mu=2v_\mu$ and $a_\mu=2mv_\mu$	$g_{\lambda\mu\nu}=2(v_\mu g_{\lambda\nu}-v_\lambda g_{\mu\nu})$
$v_\mu\gamma_5\gamma^\mu$	$g_{\lambda\mu\nu}=-2\epsilon_{\lambda\mu\nu}{}^\alpha v_\alpha$ and $b_\mu=2mv_\mu$	$f_\mu=-2v_\mu$
$v_{\mu\nu}\sigma^{\mu\nu}$	$d_{\mu\nu}=-2\epsilon_{\mu\nu}{}^{\alpha\beta}v_{\alpha\beta}$ and $\frac{1}{2}H_{\mu\nu}=2mv_{\mu\nu}$	$c_{\mu\nu}=2v_{[\mu\nu]}$

$$\mathcal{L}=\mathcal{L}_0+\mathrm{Re}\,v_\mu[i\bar{\chi}\overleftrightarrow{\partial^\mu}\chi-2m\bar{\chi}\gamma^\mu\chi]-i\,\mathrm{Im}\,v_\mu[\bar{\chi}\sigma^{\mu\nu}\overleftrightarrow{\partial}_\nu\chi]. \tag{8}$$

Inspection of the term proportional to $\mathrm{Im}\,v_\mu$ indicates that the four terms in the extended Lagrangian (2) of the form

$$g_{\lambda\mu\nu}=2\,\mathrm{Im}(v_\mu g_{\lambda\nu}-v_\lambda g_{\mu\nu}), \tag{9}$$

do not contribute in lowest order to the free fermion Lagrangian. Examination of the terms multiplying $\mathrm{Re}\,v_\mu$ indicates that the simultaneous choice of

$$e^\mu=2\,\mathrm{Re}\,v^\mu,\quad a^\mu=2m\,\mathrm{Re}\,v^\mu \tag{10}$$

can be removed from the Lagrangian. This means that the field redefinition can remove either e^μ or a^μ, but not both, unless $a^\mu=me^\mu$ happens to hold in the original Lagrangian. Similar calculations can be done for the other choices of $v\cdot\Gamma$. The results are summarized in Table I. Note that a (finite) transformation of the form $e^{iv\gamma_5}$ with $v\in\Re$ is used to remove any term of the form m_5 in the original Lagrangian to all orders. The effect is an m_5 dependent mixing of some of the Lorentz-violating parameters, but the structure is essentially unchanged.

Next, we consider the A, B, $\tilde{B}$, and C redefinitions. To lowest order in these parameters, the transformed Lagrangian becomes

$$\begin{aligned}\mathcal{L}=\mathcal{L}_0-\bar{\chi}A_\mu\gamma^\mu\chi+B_\mu\partial^\mu\mathcal{L}_0-\tilde{B}_\mu\partial^\mu\left[\frac{i}{2}\bar{\chi}\gamma_5\gamma^\nu\overleftrightarrow{\partial}_\nu\chi\right]\\ -m\bar{\chi}\gamma_5\tilde{B}_\mu\overleftrightarrow{\partial^\mu}\chi+C_{\mu\nu}x^\mu\partial^\nu\mathcal{L}_0+\frac{i}{2}\,C_{\mu\nu}\bar{\chi}\gamma^\mu\overleftrightarrow{\partial^\nu}\chi.\end{aligned} \tag{11}$$

The A term can be used to eliminate a^μ as is discussed in detail in Ref. 4. The B term is a total divergence that drops out of the action. This is a direct consequence of translational invariance since under a (finite) translation of the coordinates by B,

$$\psi(x)=e^{B\cdot\partial}\chi(x)=\chi(x+B)=\chi(x'), \tag{12}$$

and the action takes the same form in the translated coordinate system. The first C term can be partially integrated to yield a total divergence and a rescaling of $\mathcal{L}_0$. The final C term is of the form c as defined in Eq. (2).

A few remarks are in order regarding the above-mentioned transformation involving C. First, note that such a field redefinition appears equivalent to changing fermion coordinates to a system with a new (constant) metric that skews the coordinates. We can see this by examination of the transformation

$$\psi(x)=(1+C^{\mu\nu}x_\mu\partial_\nu)\chi(x)\approx e^{C^{\mu\nu}x_\mu\partial_\nu}\chi(x)=\chi(x+C\cdot x)=\chi(x'), \tag{13}$$

where $x'^\mu=x^\mu+C_\nu{}^\mu x^\nu$ are the new field coordinates. This redefinition is therefore equivalent to transforming to a skewed coordinate system with a nondiagonal metric given by

$$g'^{\mu\nu} = \eta^{\mu\nu} + C^{(\mu\nu)}. \tag{14}$$

Rewriting the transformed Lagrangian in terms of this new metric yields

$$\mathcal{L} = \frac{i}{2}\overline{\chi}(x')\tilde{\gamma}^{\mu}\overleftrightarrow{\partial}'_{\mu}\chi(x') - m\overline{\chi}(x')\chi(x'), \tag{15}$$

where the modified matrices $\tilde{\gamma}^{\mu} = (\eta^{\mu}_{\nu} + c^{\mu}_{\nu})\gamma^{\nu}$ satisfy the relations $\{\tilde{\gamma}^{\mu}, \tilde{\gamma}^{\nu}\} = 2g'^{\mu\nu}$. The resulting Lagrangian can be related to the conventional one using the vierbein formalism of general relativity by performing the appropriate general coordinate transformation. This shows that there is a natural association between the theory containing a c term and a theory formulated in a skewed coordinate system defined by the above-given metric. If the free fermions are the only component to the theory it is possible to perform the appropriate general coordinate transformation on the skewed coordinates relating it to the conventional case. This is because it is not possible to distinguish the theory in a skewed coordinate system (with a c term) from a conventional theory in an orthonormal system since fermion propagation properties are the only tool available to define the coordinate system itself.

However, when photon interactions are incorporated through the covariant derivative, it is no longer possible to perform the general coordinate transformation without affecting the photon sector. There is now an alternate way to distinguish the coordinates physically so that the skewed coordinates become observable. Under the fermion field redefinition, the fermion–photon interaction term becomes

$$\mathcal{L}_{\text{int}} = -q\overline{\psi}(x)\gamma^{\mu}A_{\mu}(x)\psi(x) \rightarrow -q\overline{\chi}(x')\tilde{\gamma}^{\mu}A'_{\mu}(x)\chi(x'), \tag{16}$$

where the photon field is expressed as a function of the conventional coordinates x, but its components are resolved in the modified coordinates x'. In this picture, the theory exhibits a form of nonlocality since the fermion fields interact with the photon field at different space–time points. If the photon field is reexpressed in terms of the new coordinates x', the Lagrangian becomes local, but picks up an extra term that breaks the natural association between the theories. Yet another approach is to redefine the physical photon field $A'_{\mu}(x) \rightarrow A'_{\mu}(x')$, but the new metric introduces corrections of the form in Eq. (1) into the kinetic photon sector. Therefore, the photon interactions prevent the trivial elimination of symmetric c terms using the above-given field redefinition. Similar problems arise when using other derivative transformations, so these are not considered in detail in subsequent sections of this paper. For example, the term $\tilde{B}$ in Eq. (6) generates a term of the form f [defined in Eq. (2)] as well as a total divergence in the transformed Lagrangian of Eq. (11). This transformation corresponds to a shift in opposite directions for the left-handed and right-handed fields due to the presence of γ_5. There is therefore a natural correspondence between the Lagrangian with an f term and the conventional theory provided the left-handed and right-handed fields can be translated independently.[30] The interaction that breaks the correspondence with the conventional theory in this case is the fermion mass term that mixes left-handed and right-handed fields. A similar situation occurs when the above-discussed C transformation is multiplied by γ_5. Symmetric components of the form d defined in Eq. (2) arise in the transformed Lagrangian, but the mass term depends explicitly on x, therefore breaking the natural correspondence between the theories.

Finite field transformations can be constructed through exponentiation of Eq. (5). The results of these transformations are often much more complicated than the infinitesimal ones since several parameters can be mixed. As an example, consider a field redefinition of the form

$$\psi = e^{v_{\mu}\gamma^{\mu}}\chi = \left(\cosh v + \frac{v_{\mu}\gamma^{\mu}}{v}\sinh v\right)\chi, \tag{17}$$

with v_μ real, timelike, and the quantity v defined by $v=\sqrt{v_\mu v^\mu}$. Application of this transformation to the standard Lagrangian in terms of ψ yields a Lagrangian for χ with apparent Lorentz-violating parameters and a modified mass given by

$$e^\mu=\frac{v^\mu}{v}\sinh 2v, \quad c^{\mu\nu}=\frac{v^\mu v^\nu}{v^2}(\cosh 2v-1),$$
$$m'=m\cosh 2v, \quad a^\mu=\frac{mv^\mu}{v}\sinh 2v. \tag{18}$$

Note that the corrections to c and m terms appear only at second order in v.

Such a choice of parameters in the QED extension leaves the dispersion relation unaltered and therefore leads to no stability problems or microcausality violations. This is true for any finite field redefinition of the form $e^{v\cdot\Gamma}$ since the field redefinition commutes with the square of the conventional Dirac equation. The set of all such transformations generates a class of Lagrangians equivalent to the conventional one.

The derivative field redefinitions may also be exponentiated to yield finite transformations. In the cases of $\tilde{B}$ and C of Eq. (6), finite transformations correspond to finite coordinate transformations, possibly different for various spinor components. As in the infinitessimal case, interactions between various spinor components and other fields limit the usefulness of these transformations due to nonlocality problems.

To gain further insight into the invariance of the physics under the above-mentioned transformations, it is useful to compute the currents associated with the generators of the Poincaré group. We will see that it is necessary to redefine the action of the complex Lorentz group along with the field in order to yield maximally conserved Lorentz generators.

IV. POINCARÉ GENERATORS

We start with a general free fermion Lagrangian of the form

$$\mathcal{L}=\frac{i}{2}\overline{\chi}\Gamma^\nu\overleftrightarrow{\partial}_\nu\chi-\overline{\chi}M\chi, \tag{19}$$

and apply Noether's theorem to obtain the divergence of the currents associated with various continuous transformations of the field. Invariance under a global U(1) phase transformation yields a conserved current of

$$j^\mu=\overline{\chi}\Gamma^\mu\chi, \tag{20}$$

satisfying $\partial_\mu j^\mu=0$. Invariance under translations yields a conserved energy momentum tensor of

$$\Theta^{\mu\nu}=\frac{i}{2}\overline{\chi}\Gamma^\mu\overleftrightarrow{\partial}^\nu\chi, \tag{21}$$

satisfying $\partial_\mu\Theta^{\mu\nu}=0$.

The Lagrangian is no longer invariant under the conventional action of the Lorentz group, so the divergences of the corresponding currents will not vanish. These can be calculated using the standard technique of writing the action over an arbitrary four-volume in terms of boosted coordinates and fields at $x'^\mu=\Lambda^\mu{}_\nu x^\nu\approx x^\mu+\epsilon^\mu{}_\nu x^\nu$ and calculating the variation to lowest order in $\epsilon^\mu{}_\nu$. A choice must be made for the induced transformation properties of the spinor components of χ under the complex extension of the Lorentz group SL(2,C). Using the standard $S(\Lambda)=1-(i/4)\sigma_{\mu\nu}\epsilon^{\mu\nu}$ yields currents given by

$$\partial_\alpha j^{\alpha\mu\nu}=X^{\mu\nu}, \tag{22}$$

where

$$j^{\alpha\mu\nu}=x^{[\mu}\Theta^{\alpha\nu]}+\tfrac{1}{4}\overline{\chi}\{\Gamma^{\alpha},\sigma^{\mu\nu}\}\chi, \tag{23}$$

and

$$\begin{aligned}X^{\mu\nu}=&-a^{[\mu}\overline{\chi}\gamma^{\nu]}\chi-b^{[\mu}\overline{\chi}\gamma_5\gamma^{\nu]}\chi-\frac{i}{2}\overline{\chi}(c^{[\nu\alpha}\gamma^{\mu]}\overleftrightarrow{\partial}_{\alpha}+c^{\alpha[\nu}\gamma_{\alpha}\overleftrightarrow{\partial}^{\mu]})\chi-\frac{i}{2}\overline{\chi}(d^{[\nu\alpha}\gamma_5\gamma^{\mu]}\overleftrightarrow{\partial}_{\alpha}\\&+d^{\alpha[\nu}\gamma_5\gamma_{\alpha}\overleftrightarrow{\partial}^{\mu]})\chi+\frac{i}{2}e^{[\mu}\overline{\chi}\overleftrightarrow{\partial}^{\nu]}\chi-\frac{1}{2}f^{[\mu}\overline{\chi}\gamma_5\overleftrightarrow{\partial}^{\nu]}\chi\\&-\frac{i}{4}\overline{\chi}(2g^{[\nu\alpha\beta}\sigma^{\mu]}{}_{\alpha}\overleftrightarrow{\partial}_{\beta}+g^{\alpha\beta[\nu}\sigma_{\alpha\beta}\overleftrightarrow{\partial}^{\mu]})\chi-\overline{\chi}H^{[\mu\alpha}\sigma^{\nu]}{}_{\alpha}\chi.\end{aligned} \tag{24}$$

All of these equations can be verified by direct calculation.

It is expected that terms which can be eliminated using a field redefinition should also be removable from $X^{\mu\nu}$ with the appropriate redefinition of the associated currents. To explicitly construct the conserved currents, the field redefinition is applied to the conventional currents written in terms of ψ, satisfying the conventional Dirac equation. These conserved currents are reexpressed in terms of χ giving the proper conserved currents for the new Lagrangian.

Alternatively, the conserved currents of the modified Lagrangian may be computed from Nöether's theorem using a modified action of the Lorentz group on the spinor fields. Using a general finite field redefinition $\psi=e^{v\cdot\Gamma}\chi$, it is found that the action of U(1) and translations is the same on ψ and χ meaning that the four-current and energy-momentum tensors are computed as in Eqs. (20) and (21). However, the action of the Lorentz transformations is in fact modified due to the field redefinition. Under an infinitesimal Lorentz transformation of the coordinates, the ψ spinor components mix according to $\delta\psi=S(\Lambda)\psi$, while the corresponding change in χ is calculated to be $\delta\chi=e^{-v\cdot\Gamma}S(\Lambda)e^{v\cdot\Gamma}\chi=\tilde{S}(\Lambda)\chi$. This means that the χ components transform according to a similar representation of the complex Lorentz group. When the associated current is computed using this modified action of SL(2,C) on χ, it is indeed conserved.

As an example, consider the field redefinition used in Eq. (8) involving $\mathrm{Re}\,v_{\mu}$. If the conventional $S(\Lambda)$ is used to find the current associated with the Lorentz transformations, the result is $j_{\chi}^{\alpha\mu\nu}$ given by Eq. (23), which is not conserved. However, if $\tilde{S}(\Lambda)$ is used to transform the field χ, then the associated current is

$$\tilde{J}_{\chi}^{\alpha\mu\nu}=x^{[\mu}\Theta^{\alpha\nu]}+\tfrac{1}{4}\overline{\chi}\{\Gamma^{\alpha},\sigma^{\mu\nu}\}\chi+\tfrac{1}{2}\overline{\chi}e^{[\mu}\sigma^{\nu]\alpha}\chi, \tag{25}$$

which is in fact conserved. This shows that one must be careful to map the correct conserved generators into the proper associated currents written in terms of χ. Similar maps between generators can be performed using the derivative transformations, however, in this case the U(1) and translation currents may also be modified.

As a practical approach, the redundant parameters can first be removed from the Lagrangian and then the conventional $S(\Lambda)$ can be used to construct the currents in the redefined Lagrangian. We perform this removal of the redundant parameters in Sec. V.

V. ELIMINATION OF REDUNDANT PARAMETERS

In this section, we start with a general Lagrangian and apply field redefinitions to remove redundant parameters. The starting point is the Lagrangian given in Eq. (2). The parameters m_5, a_{μ}, e_{μ}, f_{μ}, and $c_{[\mu\nu]}$ can all be immediately removed using a combination of the transformations described in Sec. III. The parameter $g_{\lambda\mu\nu}$ can be replaced by the traceless $\tilde{g}_{\lambda\mu\nu}$ satisfying $g^{\lambda\nu}\tilde{g}_{\lambda\mu\nu}=g^{\mu\nu}\tilde{g}_{\lambda\mu\nu}=0$. The other transformations listed in Table I involve linear combinations of parameters.

To handle these terms, the Lagrangian must be reexpressed in terms of the new, physically relevant linear combinations of parameters. For example, the combination of antisymmetric d and H terms of Eq. (2) are reexpressed as

$$\frac{i}{4}\overline{\psi}d_{[\mu\nu]}\gamma_5\gamma^\mu\overleftrightarrow{\partial}^\nu\psi-\frac{1}{2}\overline{\psi}H_{\mu\nu}\sigma^{\mu\nu}\psi=v^+_{\alpha\beta}\left[\frac{i}{2}\overline{\psi}\epsilon_{\mu\nu}{}^{\alpha\beta}\gamma_5\gamma^\mu\overleftrightarrow{\partial}^\nu\psi-m\overline{\psi}\sigma^{\alpha\beta}\psi\right]$$
$$+v^-_{\alpha\beta}\left[\frac{i}{2}\overline{\psi}\epsilon_{\mu\nu}{}^{\alpha\beta}\gamma_5\gamma^\mu\overleftrightarrow{\partial}^\nu\psi+m\overline{\psi}\sigma^{\alpha\beta}\psi\right], \tag{26}$$

where $v^\pm_{\alpha\beta}=\frac{1}{4}(\tilde{d}_{\alpha\beta}\pm 1/m\,H_{\alpha\beta})$, and $\epsilon^{\alpha\beta}_{\mu\nu}\tilde{d}_{\alpha\beta}=d_{[\mu\nu]}$. The combination $v^-_{\alpha\beta}$ can be removed using a field redefinition, leaving only $v^+_{\alpha\beta}$ terms in the Lagrangian. The g and b terms can be similarly combined using the definition $v^\pm_\alpha=\frac{1}{2}(g_\alpha\pm 1/m\,b_\alpha)$

After all of these redefinitions have been performed, the form for the Lagrangian becomes

$$\mathcal{L}=\frac{i}{2}\overline{\psi}\left(\gamma_\nu+\frac{1}{2}c_{(\mu\nu)}\gamma^\mu+\frac{1}{2}d_{(\mu\nu)}\gamma_5\gamma^\mu+\frac{1}{2}\hat{g}_{\lambda\mu\nu}\sigma^{\lambda\mu}\right)\overleftrightarrow{\partial}^\nu\psi-m\overline{\psi}\psi+\frac{1}{4}\left(\tilde{d}_{\alpha\beta}+\frac{1}{m}H_{\alpha\beta}\right)$$
$$\times\left[\frac{i}{2}\overline{\psi}\epsilon_{\mu\nu}{}^{\alpha\beta}\gamma_5\gamma^\mu\overleftrightarrow{\partial}^\nu\psi-m\overline{\psi}\sigma^{\alpha\beta}\psi\right]-\frac{1}{2}\left(g_\alpha-\frac{1}{m}b_\alpha\right)\left[\frac{i}{2}\overline{\psi}\frac{1}{2}\epsilon_{\lambda\mu}{}^{\nu\alpha}\sigma^{\lambda\mu}\overleftrightarrow{\partial}_\nu\psi-m\overline{\psi}\gamma_5\gamma^\alpha\psi\right], \tag{27}$$

where $\hat{g}_{\lambda\mu\nu}$ is a traceless coupling with a vanishing totally antisymmetric piece. The totally antisymmetric component of $\tilde{g}$ is absorbed into $g_\alpha=-\epsilon_\alpha{}^{\lambda\mu\nu}\tilde{g}_{\lambda\mu\nu}$. This Lagrangian can be written in the form

$$\mathcal{L}=\frac{i}{2}\overline{\psi}\tilde{\Gamma}_\nu\overleftrightarrow{\partial}^\nu\psi-\overline{\psi}\tilde{M}\psi, \tag{28}$$

where

$$\tilde{\Gamma}_\nu=\gamma_\nu+\tfrac{1}{2}c_{(\mu\nu)}\gamma^\mu+(\tfrac{1}{2}d_{(\mu\nu)}+\epsilon_{\mu\nu}{}^{\alpha\beta}v^+_{\alpha\beta})\gamma_5\gamma^\mu+\tfrac{1}{2}(\hat{g}_{\lambda\mu\nu}-\epsilon_{\lambda\mu\nu}{}^\alpha v^-_\alpha)\sigma^{\lambda\mu}, \tag{29}$$

and

$$\tilde{M}=m(1+v^+_{\alpha\beta}\sigma^{\alpha\beta}-v^-_\alpha\gamma_5\gamma^\alpha), \tag{30}$$

where all distinct parameters are now physically relevant.

This Lagrangian is therefore the one for which ψ can be assumed to transform under the standard representation of SL(2,C), yielding maximally conserved currents.[31] The relevant currents are given as in Sec. IV with appropriately mapped constants found by comparison of Eqs. (2) and (28). The remaining terms cannot be removed by a redefinition of spinor coordinates. Other terms may be eliminated in the free theory using transformations involving derivatives of the fields as discussed in Sec. III, but interactions between the fermion fields and other fields often break the natural correspondence between the redefined Lagrangian and the original theory. This means that if these terms are removed from the free fermion sector, they will appear as modified interaction terms and will not be removed from the theory, only shifted to another sector.

Physical quantities should therefore depend only on the combinations occurring in the Lagrangian of Eq. (28). Therefore, it is not possible to obtain experimental bounds on all Lorentz-violating parameters of Eq. (2) independently, only on the combinations present in Eq. (28). For example, it is only the linear combination $v^+_{\alpha\beta}$ of the antisymmetric part of d and H that is observable. This implies that only one parameter should in fact be used to describe this quantity.

Comparison with previous calculations within the context of this model verify that this is indeed the case. For example, in applications to electrons and positrons in Penning traps,[6–9] the relevant experimental bound is obtained from the observable cyclotron and anomaly frequencies ($\tilde{g}_{\lambda\mu\nu}=0$ in this calculation)

$$\begin{aligned}\omega_c^{e^\pm} &\approx (1-c_{00}^e-c_{11}^e-c_{22}^e)\omega_c\,,\\ \omega_c^{e^\pm} &\approx \omega_a \mp 2b_3^e+2md_{30}^e+2H_{12}^e,\end{aligned} \tag{31}$$

which can place bounds only on the combinations of parameters found in Eq. (27), not on the parameters that can be removed by the field redefinitions. As another example, a calculation of the cross section for $e^+e^-\to 2\gamma$ within the QED extension[10] only depends on the symmetric components of c. Similar results have been obtained in other QED systems.[32]

For many practical calculations it is convenient to perform another field redefinition to normalize $\tilde{\Gamma}^0\to\gamma^0$. This has the effect of removing extra time derivative couplings ensuring that the resulting Schrödinger equation has a conventional time evolution.[6,17] Starting with a general Lagrangian of the form (2), the appropriate field redefinition that removes time derivative couplings to lowest order is $\psi=A\chi$ with

$$\begin{aligned}A&=1-\tfrac{1}{2}\gamma^0(\Gamma_0-\gamma_0)\\ &=1-\tfrac{1}{2}\gamma^0(c_{\mu 0}\gamma^\mu+d_{\mu 0}\gamma_5\gamma^\mu+e_0+if_0\gamma_5+\tfrac{1}{2}g_{\lambda\mu 0}\sigma^{\lambda\mu}).\end{aligned} \tag{32}$$

Note that these are in 1–1 correspondence with the nonunitary transformations of the form $v\cdot\Gamma$ examined in Sec. III. The unitary transformations of this type can be obtained by letting the coupling constants in Eq. (32) be pure imaginary rather than real. In this case, the time derivative structure is unaffected by the field redefinition. This provides an alternative perspective on the spinor component field redefinitions. The unitary transformations preserve the time derivative terms while the nonunitary transformations modify the time derivative structure. This can be seen directly from Eq. (7) by noting that the requirement that no time derivatives are introduced is equivalent to the condition $(v\cdot\Gamma)^\dagger=-v\cdot\Gamma$, hence making the field redefinition unitary to lowest order. The unitary transformations are used in the standard Dirac theory to transition between various representations of the gamma matrices, an alternative perspective to the explicit correction terms used in this paper. In other words, any apparent Lorentz-violating terms generated by a unitary transformation may be absorbed into a modified gamma matrix representation.

As a practical method for calculation, the procedure is therefore to first remove the redundant parameters to obtain Eq. (28), then perform the field redefinition of Eq. (32) (using $\tilde{\Gamma}^0$ in place of Γ^0). The resulting Lagrangian will therefore yeild a conventional Schrödinger equation time evolution and will not contain any redundant parameters.

VI. SUMMARY

In this paper, an analysis of field redefinitions in the context of the Lorentz-violating QED extension was presented. It was shown that a variety of parameters that apparently violate Lorentz invariance can be eliminated from the Lagrangian using suitable fermionic field redefinitions.

The approach taken to find these parameters was to begin with the conventional Dirac Lagrangian, introduce an arbitrary spinor redefinition, and examine the resulting transformed Lagrangian. Any parameters generated using this procedure can be removed by the corresponding inverse transformation. The action of SL(2,C) on the spinor fields is deduced using the conventional action on the ψ spinors and performing the field redefinition to determine the corresponding action on χ. The resulting transformation matrices of the new spinor are related by a similarity transformation to the original matrices. This modified action must be taken into account when defining the conserved generators in the modified Lagrangian.

This implies a procedure for elimination of redundant parameters from the original Lagrangian. By first identifying all possible terms that can be generated from the conventional Lagrangian by a field redefinition, these terms can be omitted from the physical Lagrangian. This procedure has been carried out in Sec. V. A further transformation may be implemented to normalize the time derivative structure of the theory to obtain conventional Schrödinger time evolution and physical particle states.

The possible nonderivative field redefinitions that can be applied to the QED extension fall into two general categories, unitary and nonunitary. The nonunitary transformations modify the time derivative structure of the Lagrangian and can be used to construct a hermitian hamiltonian and a Schrödinger equation with conventional time evolution. The time derivative couplings in a general bilinear Lagrangian of the form in Eq. (2) can always be removed using a suitable nonunitary transformation. Moreover, there is a one-to-one correspondence between these nonunitary transformations and the field redefinitions used to eliminate the extra time derivative couplings.

Redefinitions involving differentiation may be useful in the free fermion theory, but often lead to nonlocal interactions or skewed coordinate systems when interactions are present. These problems make it difficult to perform a generic analysis of all possible applications of these transformations. Derivative redefinitions may be applied on a case by case basis where they might be useful in simplification of calculations.

Stability and causality issues[5] cannot be effectively addressed using the above-presented arguments since the redefinition was only carried out to lowest order in Lorentz-violating parameters. Causality and stability problems appear either when the coupling constants are large, or when the momentum is significantly large to invalidate the linear approximations involved. However, the finite field redefinition considered in Eq. (17) leads to a finite set of parameters that maintain the conventional dispersion relation. The resulting theory must therefore be stable and microcausal. A class of apparently Lorentz-violating Lagrangians that are microcausal and stable may therefore be generated by applying finite versions of the field redefinitions discussed in this paper. A complete nonperturbative analysis would be of interest, but is beyond the scope of this work.

Application of a similar analysis to the entire standard model extension would be of interest. For example, cross-generational mixings would allow for a richer structure of possible field redefinitions than in QED.

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Phase space structure and short distance behavior of local quantum field theories

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In this article a general relation between the short distance structure of quantum field theories and their phase space properties is exemplified by the simple class of generalized free fields. As is known, theories with decent phase space properties, resulting from a finite or moderately increasing infinite particle spectrum, always have non-trivial scaling (short distance) limits [cf. D. Buchholz and R. Verch, Rev. Math. Phys. **10**, 775 (1998)]. But, whereas in the finite particle case the phase space properties of the limit theories comply with strong nuclearity conditions, they violate in the infinite particle case even rather mild compactness assumptions. These results provide further evidence to the effect that relevant information on the short distance structure of a theory can be obtained by phase space analysis. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1486262]

I. INTRODUCTION

In quantum field theory the structure of a physical theory at small distances is an interesting issue in several respects. It is important for understanding the particle structure at small scales as well as the classification of the ultraviolet properties of the theory.

Recently, Buchholz and Verch presented a model independent approach to the investigation of these problems in Ref. 8, which is carried out in the framework of algebraic quantum field theory. There, they adapted the method of the renormalization group to this framework by introducing the notions of scaling algebra and scaling limit.

Before summarizing the ideas of Buchholz and Verch, let us give a brief account of the framework of algebraic quantum field theory (see, e.g., Ref. 12).

In this framework, a quantum field theory is given by the net of algebras of local observables $\mathfrak{A}$ together with a covariant action of the translation group by automorphisms $\alpha_{x,x\in\mathbb{R}^d}$. This is a map

$$\mathcal{O}\mapsto\mathfrak{A}(\mathcal{O}), \tag{1}$$

fulfilling certain properties. Here $\mathcal{O}\subset\mathbb{R}^{d=s+1}$ is an open bounded region in $d=s+1$ dimensional Minkowski-space and $\mathfrak{A}(\mathcal{O})$ is unital C^*-algebra, the algebra generated by all observables which can be measured in $\mathcal{O}$. The C^*-algebra generated by all the local algebras $\mathfrak{A}(\mathcal{O})$ (as C^*-inductive limit) is also denoted by $\mathfrak{A}$. Furthermore, we impose the following properties:

(1) *Locality:* Observables $A\in\mathfrak{A}(\mathcal{O}_1)$ and $B\in\mathfrak{A}(\mathcal{O}_2)$ corresponding to spacelike separated regions $\mathcal{O}_1$ and $\mathcal{O}_2$ should commute:

$$[A,B]=0. \tag{2}$$

(2) *Covariance:* The translation group $\mathbb{R}^d$ acts on the net by automorphisms $\alpha_x\in\mathrm{Aut}(\mathfrak{A})$, for $x\in R^d$:

$$\alpha_x(\mathfrak{A}(\mathcal{O}))=\mathfrak{A}(\mathcal{O}+x). \tag{3}$$

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Furthermore, we require the representation of the translation group to be continuous in the strong topology, i.e., the maps $x \mapsto \alpha_x(A)$ to be continuous in the norm topology, for all $A \in \mathfrak{A}$.

(3) *Vacuum state:* In general, a physical state of the theory is a positive, linear, normalized functional σ on the net $\mathfrak{A}$. Such a state allows us to get a representation π_σ of the net $\mathfrak{A}$ on a Hilbert space $\mathcal{H}_\sigma$ via GNS-construction. If the corresponding state σ is invariant under the translation group, there exists a unitary representation $U_\sigma(x)$, $x \in \mathbb{R}^d$, of the translation group on $\mathcal{H}_\sigma$ implementing the representation α:

$$U_\sigma(x)\pi_\sigma(A)U_\sigma(-x) = \pi_\sigma(\alpha_x(A)), \tag{4}$$

for all $A \in \mathfrak{A}$. Let us assume that our theory has a vacuum state, i.e., that there exist a translation-invariant state σ, such that the joint spectrum of the generators of all implementors is contained in the forward light cone.

Now, let us briefly summarize the approach of Buchholz and Verch (for details we refer to Ref. 8):

Given a local, covariant net of observables $\mathfrak{A}$, $\alpha_{x, x \in \mathbb{R}^d}$ in d space–time dimensions we construct the scaling net $\underline{\mathfrak{A}}, \underline{\alpha}_{x, x \in \mathbb{R}^d}$, again a local covariant net, by the following rule: Let $\underline{A}: \mathbb{R}^{>0} \to \mathfrak{A}$ be a bounded function. Then we set

$$\underline{\mathfrak{A}}(\mathcal{O}) := \{\underline{A} \,|\, \underline{A}_\lambda \in \mathfrak{A}(\lambda \mathcal{O}),\ x \mapsto \underline{\alpha}_x(\underline{A}) \text{ continuous in norm topology}\},$$

$$\underline{\alpha}_x(\underline{A})_\lambda := \alpha_{\lambda x}(\underline{A}_\lambda).$$

The crucial point is that the scaling net carries a representation of the dilation group τ_λ, $\lambda \in \mathbb{R}^{>0}$. Starting with the vacuum state σ on the underlying theory, we define its *canonical lift* $\underline{\sigma}$ on the scaling net: $\underline{\sigma}(\underline{A}) := \sigma(\underline{A}_1)$. Then one considers the scaled states $\underline{\sigma} \circ \tau_\lambda$. This net of states on the scaling net has limit points $\underline{\sigma}^{(0,\nu)}$, $\nu \in \Xi$ for $\lambda \searrow 0$, in the weak*-topology. Here, Ξ is a suitable index set. Via GNS-construction, we get representations $\mathfrak{A}^{(0,\nu)}$, $\nu \in \Xi$, of the scaling net $\underline{\mathfrak{A}}$ corresponding to these states. The $\mathfrak{A}^{(0,\nu)}$, $\nu \in \Xi$ are called *the scaling limit nets* of the underlying theory.

Buchholz and Verch also provided a classification of the scaling limit. Since we do not need it here, we refer to Ref. 9.

Furthermore, it was observed by Buchholz,[1] that phase space properties should play an important role for the short distance structure of a theory. This can heuristically be illustrated by the following example, which was more thoroughly investigated by Lutz:[15]

Assume we have a quantum field theory exhibiting the following behavior: The energy-momentum transfer of local observable scales with λ^{-q} with $q > 1$ under renormalization group transformations, while its localization in space–time scales with λ. Since we require Planck's constant not to vary with the scale, its scaling limit theory should be a classical theory, i.e., all observables commute.

In this article we consider a generalized free field in $d \geqslant 3$ space–time dimensions with finite or moderately increasing infinite particle spectrum. To be more precise, we impose the following condition on the mass spectrum:

$$\forall \beta > 0: \quad \sum_{i \in I} e^{-\beta m_i} < \infty, \tag{5}$$

where I is either finite or $\mathbb{N}$. It was shown by Buchholz and Verch that these theories have nontrivial scaling limit, cf. Ref. 9. As is well known,[10] these theories fulfill the nuclearity condition.

Our aim is to show that its scaling limit theories exhibit the following phase space properties: If the mass spectrum is finite, all the scaling limit theories fulfill the strong nuclearity condition. But, none of its scaling limit theories complies with the weaker compactness criterion in the infinite case. Heuristically the situation can be understood as follows: In the finite case the scaling

limit should be the massless theory with finite multiplicity, which is known to fulfill the nuclearity condition. On the other hand, in the infinite case, the scaling limit theory is expected to contain the massless free field with infinite multiplicity, which does not comply with the compactness criterion.

Our analysis will be carried out by only investigating the phase space properties of the underlying theory.

The article is organized as follows:

In Sec. II we rephrase the mathematical tools for the investigation of phase space properties in quantum field theory. Afterwards, we describe the interaction between phase space properties and the structure of the scaling limit.

The models we are dealing with are introduced in Sec. III. There we also indicate upper bounds in the scaling limit of the nuclear norms of the phase space maps of our theories. Using this we show that all the scaling limit theories in the case of a finite mass spectrum fulfill the nuclearity condition. In Sec. IV, we prove that the scaling limit in the case of an infinite mass spectrum has no decent phase space behavior, and it violates the compactness criterion. This is carried out by considering lower bounds of the ϵ-contents of the phase space maps.

II. THE PHASE SPACE AND THE SCALING LIMIT

As was already pointed out in the Introduction, the phase space properties of the underlying theory should (partially) determine its short distance behavior. In fact, a link between properties of the scaling limit and the phase space properties of a local quantum field theory was established by Buchholz (cf. Ref. 1). Here, we want to summarize the main results of his article.

Let us start by recalling the main notions for the description of phase space properties in the framework of local quantum field theory (cf. Refs. 1, 2, 4, 17, and 18).

Let T be an arbitrary bounded linear operator between two Banach spaces $\mathcal{E}$ and $\mathcal{F}$.

Definition 2.1: (i) The ϵ-content $N_T(\epsilon)$ of T is the maximal number (or infinity) of elements $E_i \in \mathcal{E}_1$, such that

$$\forall i \neq j: \quad \|T(E_i - E_j)\| > \epsilon. \tag{6}$$

(ii) T is called p-nuclear, $p \in \mathbb{R}^{>0}$, if there exist sequences $e_n \in \mathcal{E}^*$ and $F_n \in \mathcal{F}$, $n \in \mathbb{N}$, such that

$$\begin{gathered} T = \sum_{n=1}^{\infty} e_n F_n, \\ \sum_{n=1}^{\infty} \|e_n\|^p \|F_n\|^p < \infty. \end{gathered} \tag{7}$$

The first sum should converge in the strong topology. We set $\||T|\|_p := \inf(\Sigma_{n=1}^{\infty} \|e_n\|^p \|F_n\|^p)^{1/p}$ and call this the nuclear p-norm. (To be precise, it is only a quasi-norm for $0 < p < 1$.) The infimum is taken over all decompositions of T as in Eq. (7).

Furthermore, we set $\|A\|_p := (\mathrm{Tr}|A|^p)^{1/p}$ for a bounded endomorphism A of a Hilbert space, if this trace exists. This will be called the pth *trace norm of* A. For further properties of and relations between these concepts, we refer to Refs. 1 and 2.

In the fr amework of local quantum field theory, ''decent'' phase space properties of a local, covariant net $\mathfrak{A}$ are described by the compactness criterion or, a sharpened version of it, the nuclearity criterion (cf. Refs. 13, 10, and 7): First let us define the *phase space maps* $\Theta_{\beta,\mathcal{O}}$, for each bounded region $\mathcal{O} \subset \mathbb{R}^d$ and $\beta \in \mathbb{R}^{>0}$:

$$\begin{aligned} &\Theta_{\beta,\mathcal{O}} : \mathfrak{A}(\mathcal{O}) \to \mathcal{H}, \\ &A \mapsto e^{-\beta H} A \Omega. \end{aligned} \tag{8}$$

Here, H is the Hamiltonian of the theory.

Compactness condition: A local covariant net $\mathfrak{A}$ fulfills the *compactness condition*, iff the phase space maps $\Theta_{\beta,\mathcal{O}}$ are compact, for every β and $\mathcal{O}$ as above.

Nuclearity Condition: A local covariant net fulfills the *nuclearity condition*, iff the phase space maps $\Theta_{\beta,\mathcal{O}}$ are p-nuclear, for every $p>0$, bounded region $\mathcal{O}$ and sufficiently large $\beta>0$.

We should mention that these conditions have a large variety of consequences for the particle interpretation and statistical and thermodynamical properties of the underlying theory. Since we do not need them here, we refer to Refs. 13, 10, 7, 6, 14, and 19.

With these tools we are able to give an account on the interplay between phase space properties of the underlying theory and the structure of the scaling limit. We only present the results. For the proofs, we refer to Ref. 1, Proposition 4.3 and Theorems 4.5 and 4.6.

Investigating the nuclear p-norms of the phase space maps we can decide whether the scaling limit theories fulfill the nuclearity condition or not:

Theorem 2.1: *Consider a quantum field theory with p-nuclear phase space maps $\Theta_{\beta,\mathcal{O}}$ for some $0<p<\frac{1}{3}$. Furthermore, assume that* $\limsup_{\lambda\searrow 0}\|\|\Theta_{\lambda\beta,\lambda\mathcal{O}}\|\|_p<\infty$. *Then we have the following.*

The phase space maps $\Theta^{(0,\nu)}_{\beta,\mathcal{O}}$ of every scaling limit net $\mathfrak{A}^{(0,\nu)}$, $\nu\in\Xi$, are q-nuclear, for $q>2p/(2-3p.)$ Furthermore, there exists a constant c depending only on p and q, such that

$$\|\|\Theta^{(0,\nu)}_{\beta,\mathcal{O}}\|\|_q\leqslant c\limsup_{\lambda\searrow 0}\|\|\Theta_{\lambda\beta,\lambda\mathcal{O}}\|\|_p\,. \tag{9}$$

Using the ϵ-contents the following sufficient and necessary conditions for the validity of the compactness criterion of the scaling limit theories hold. Here, the ϵ-content of $\Theta_{\beta,\mathcal{O}}$ will be denoted by $N_{\beta,\mathcal{O}}(\epsilon)$.

Proposition 2.1: All scaling limit theories of a given quantum field theory fulfill the compactness criterion, if $\limsup_{\lambda\searrow 0}N_{\lambda\beta,\lambda\mathcal{O}}(\epsilon)<\infty$, *for all $\epsilon>0$ and bounded regions $\mathcal{O}$. A necessary condition for the compactness criterion is that* $\liminf_{\lambda\searrow 0}N_{\lambda\beta,\lambda\mathcal{O}}(\epsilon)<\infty$, *for all $\epsilon>0$ and bounded regions $\mathcal{O}$.*

Remark: By investigating phase space properties it is also possible to decide whether the scaling limit theories are trivial (cf. Ref. 1). Using the techniques presented in this article even the nontriviality of the scaling limit of the models under consideration can be shown (cf. Ref. 16). We will not outline this here because of the stronger results in Ref. 9, where the scaling limit nets are directly constructed.

III. THE MODELS AND UPPER BOUNDS

In this section we first give a brief description of our models. Then we show that the nuclearity condition holds in the scaling limit, in the case of a finite mass spectrum. This is done by calculating upper bounds for the nuclear p-norms of the phase space maps $\Theta_{\beta,\mathcal{O}}$ and investigating their behavior in the limit $\lambda\searrow 0$.

Let us start by giving the construction of our quantum field theories in the Cauchy data formulation.

Let $\mathcal{K}$ be the one-particle Hilbert space:

$$\mathcal{K}:=\bigoplus_{i\in I}L^2(\mathbb{R}^s,\mathbb{C}), \tag{10}$$

where $s=d-1$ is the number of space-dimensions. On $\mathcal{K}$ we have a scalar product $\langle,\rangle$ in a canonical way. In addition, there is an antilinear involution J given by componentwise complex conjugation of the functions in $\mathcal{K}$. Our vacuum Hilbert space $\mathcal{H}$ will be the symmetric Fock space over $\mathcal{K}$. Its scalar product will be denoted by $(,)$.

The creation and annihilation operators $a^*(F)$ resp. $a(F)$, $F\in\mathcal{K}$, act on $\mathcal{H}$. We define the the Weyl operators $W(F)$, $F\in\mathcal{K}$:

$$W(F) := e^{i(a^*(F)+a(F))^-}, \quad F \in \mathcal{K}. \tag{11}$$

Here, $(a^*(F)+a(F))^-$ denotes the self-adjoint operator extending the densely defined (unbounded) operator $a^*(F)+a(F)$. The Weyl operators are subject to the canonical commutation relations:

$$W(F)W(G) = e^{i\Im\langle G,F\rangle} W(F+G). \tag{12}$$

Let $\mathbf{P}$ be the momentum operator on $L^2(\mathbb{R}^s,\mathbb{C})$. Then the one particle Hamiltonian $\underline{\omega}$ acts as follows:

$$\underline{\omega} F := \bigoplus_{i\in I} \omega_i f_i, \quad \omega_i := \sqrt{|\mathbf{P}|^2 + m_i^2}. \tag{13}$$

By second quantization we get the Hamiltonian H on $\mathcal{H}$. It is the generator of the time translations of our quantum field theory.

Let $\mathcal{O}_r \in \mathbb{R}^d$ be a double cone with Basis $\mathbf{O}_r = \{\mathbf{x}\in\mathbb{R}^s, |\mathbf{x}| < r\} \subset \mathbb{R}^s$, the ball of radius r centered at 0 in the $t=0$-plane. Then we define closed subspaces of $\mathcal{K}$ [Here $\mathcal{D}(\mathbf{O}_r)$ denotes the set of test function with support contained in $\mathbf{O}_r$):

$$\mathcal{L}_\phi^{m_i}(\mathcal{O}_r) := \overline{\omega_i^{-1/2}\mathcal{D}(\mathbf{O}_r)}^{\|\cdot\|_{L^2(\mathbb{R}^s,\mathbb{C})}}, \tag{14}$$

$$\mathcal{L}_\pi^{m_i}(\mathcal{O}_r) := \overline{\omega_i^{1/2}\mathcal{D}(\mathbf{O}_r)}^{\|\cdot\|_{L^2(\mathbb{R}^s,\mathbb{C})}}, \tag{15}$$

$$\mathcal{L}_\phi(\mathcal{O}_r) := \overline{\underline{\omega}^{-1/2}\bigoplus_{i\in I}\mathcal{D}(\mathbf{O}_r)}^{\|\cdot\|_{\mathcal{K}}} = \overline{\bigoplus_{i\in I}\mathcal{L}_\phi^{m_i}(\mathcal{O}_r)}^{\|\cdot\|_{\mathcal{K}}}, \tag{16}$$

$$\mathcal{L}_\pi(\mathcal{O}_r) := \overline{\underline{\omega}^{1/2}\bigoplus_{i\in I}\mathcal{D}(\mathbf{O}_r)}^{\|\cdot\|_{\mathcal{K}}} = \overline{\bigoplus_{i\in I}\mathcal{L}_\pi^{m_i}(\mathcal{O}_r)}^{\|\cdot\|_{\mathcal{K}}}. \tag{17}$$

The corresponding projectors are denoted by $E_\phi^{m_i}(r)$, $E_\pi^{m_i}(r)$, $\underline{E}_\phi(r)$, resp. $\underline{E}_\pi(r)$. Now we consider the real linear subspace $\mathcal{L}(\mathcal{O}_r)\subset\mathcal{K}$:

$$\mathcal{L}(\mathcal{O}_r) := (1+J)\mathcal{L}_\phi(\mathcal{O}_r) \oplus (1-J)\mathcal{L}_\pi(\mathcal{O}_r). \tag{18}$$

We define the local von Neumann algebras $\mathfrak{A}(\mathcal{O})$, for $\mathcal{O}$ as above, to be the von Neumann algebras generated by all Weyl operators located in $\mathcal{O}$:

$$\mathfrak{A}(\mathcal{O}_r) := \{W(F) | \quad F \in \mathcal{L}(\mathcal{O}_r)\}''. \tag{19}$$

Here the prime denotes the commutant. The local algebras for arbitrary bounded regions are defined by use of the translation operators and additivity:

$$\mathfrak{A}(\mathcal{O}) := \left(\bigcup_{x+\tilde{\mathcal{O}}\subset\mathcal{O}} \mathfrak{A}(x+\tilde{\mathcal{O}}) \right)''. \tag{20}$$

Here, $\tilde{\mathcal{O}}$ is a double cone of the shape as above. So, $\mathfrak{A}(\mathcal{O})$ is the smallest von Neumann algebra containing all translated algebras $\mathfrak{A}(x+\tilde{\mathcal{O}})$.

Before continuing we have to deal with the following rather subtle problem: The net of von Neumann algebras we have constructed so far complies with all of the assumptions made in the Introduction except for the norm continuity of the maps $x\mapsto\alpha_x(A)$. Now, one can obtain a net of C^*-algebras $\mathcal{O}\mapsto\mathcal{A}(\mathcal{O})$ fulfilling norm continuity by ''smearing out'' with test functions. The local algebras $\mathcal{A}(\mathcal{O})$ will be weakly dense in the algebras $\mathfrak{A}(\mathcal{O})$. Now, it is not *a priori* clear how

the phase space properties behave under this procedure. The following lemma shows that they do not change. Thus, we are allowed to work with the larger von Neumann algebras.

The phase space maps and the ϵ-contents for theory using the weakly dense subalgebras $\mathcal{A}(\mathcal{O})$ are denoted with a tilde.

Lemma 3.1: We have the following.

(i) The phase space map $\Theta_{\beta,\mathcal{O}}$ is p-nuclear, iff $\tilde{\Theta}_{\beta,\mathcal{O}}$ is p-nuclear and their nuclear p-norms coincide:

$$\| |\Theta_{\beta,\mathcal{O}}| \|_p = \| |\tilde{\Theta}_{\beta,\mathcal{O}}| \|_p . \tag{21}$$

(ii) For the corresponding ϵ-contents, the following chain of inequalities holds:

$$\tilde{N}_{\beta,\mathcal{O}}(\epsilon) \leqslant N_{\beta,\mathcal{O}}(\epsilon) \leqslant \tilde{N}_{\beta,\mathcal{O}}\left(\frac{\epsilon}{2}\right). \tag{22}$$

Proof: The proof of (i) is in analogy to the proof of Lemma 2.2. in Ref. 3. It can be found in Ref. 16.

(ii) follows by use of a 3ϵ-type argument from the Kaplansky density theorem and the definition of ϵ-content. ■

Our main result of this section is the following:

Theorem 3.1: *All scaling limit theories of the generalized free field with finite mass spectrum in $d \geqslant 3$ space–time dimensions fulfill the nuclearity condition.*

Proof: In $d=3,4$ space–time dimensions the theorem follows easily from Ref. 9: There it is proven that scaling limit of the theories in question is a generalized free field of mass zero with finite multiplicity. By Ref. 5 these theories fulfill the nuclearity condition.

In higher dimensions we use Theorem 2.1 to reduce the statement of the theorem to the following proposition:

Proposition 3.1: Let $\mathcal{O} \subset \mathcal{O}_r$ *be a double cone contained in a second one with a ball of radius r centered at 0 as a basis in the $t=0$-plane.*

Then, the following upper bounds hold for the nuclear p-norms of the phase space maps:

$$\|\Theta_{\beta,\mathcal{O}}\|_p \leqslant \begin{cases} \exp\left[\mathcal{C}(p,s) \left(\frac{r}{\beta}\right)^s \sum_{i \in I} e^{-(\beta/4)\, p m_i} \right], & \beta \leqslant r, \\ \exp\left[\mathcal{C}(p,s) \left(\frac{r}{\beta}\right)^{[(s-1)/2]\, p} \sum_{i \in I} e^{-(\beta/4)\, p m_i} \right], & \beta > r. \end{cases}$$

Remark: One easily sees that these upper bounds for $\lambda r, \lambda \beta$ diverge in the limit $\lambda \searrow 0$, if the mass spectrum is infinite.

Proof of the proposition: Analogously to the proof of the theorem in the Appendix of Ref. 10 and the proofs of Theorem 2.1 and Lemma 2.2 in Ref. 5 (see also Ref. 16, Lemma 4.2.1), we get

$$\| |\Theta_{\beta,\mathcal{O}}| \|_p \leqslant \exp\left\{ \frac{2}{p} \left(\sum_{n=1}^{\infty} \frac{1}{n} \left\| |\underline{E}_{\phi}(r) e^{-\beta \underline{\omega}}|^n \right\|_p^p + \sum_{n=1}^{\infty} \frac{1}{n} \left\| |\underline{E}_{\pi}(r) e^{-\beta \underline{\omega}}|^n \right\|_p^p \right) \right\}.$$

Now, we have the direct sum decomposition $\underline{E}_{\phi}(r) = \oplus_{i \in I} E_{\phi}^{m_i}(r)$, a corresponding one for $\underline{E}_{\pi}(r)$ and the following inequalities:

$$\| |\underline{E} e^{-\beta \underline{\omega}}|^r \|_1 \leqslant \| \underline{E} e^{-r \beta \underline{\omega}} \|_1, \quad \forall r \in \{1\} \cup \mathbb{R}^{\geqslant 2}, \tag{23}$$

$$\mathrm{Tr}(|A|^r) \leqslant \mathrm{Tr}(|A|^q), \quad \forall r \geqslant q, \|A\| \leqslant 1, \tag{24}$$

of which the first one is proven in Ref. 5, Lemma 2.2, while the second is immediate. Using these equations, we derive the following upper bound for the nuclear p-norm of $\Theta_{\beta,\mathcal{O}}$:

$$\|\|\Theta_{\beta,\mathcal{O}}\|\|_p \leqslant \exp\left\{ \frac{2}{p} \sum_{i\in I} \left[\left(\sum_{n=1}^{K} \frac{1}{n} \right) (\|E_\phi^{m_i}(r)e^{-\beta\omega_i}\|_p^p + \|E_\pi^{m_i}(r)e^{-\beta\omega_i}\|_p^p) \right.\right.$$
$$\left.\left. + \sum_{n=K+1}^{\infty} \frac{1}{n} (\|E_\phi^{m_i}(r)e^{-np\beta\omega_i}\|_1 + \|E_\pi^{m_i}(r)e^{-np\beta\omega_i}\|_1) \right] \right\}, \tag{25}$$

where K is the biggest natural number with $Kp<2$.

We only need to calculate the nuclear p-norms for $p=2/N$. Because of the formula above, it is sufficient to establish upper bounds for the trace norms of the operators $E_\phi^{m_i}(r)e^{-np\beta\omega_i}$ and $E_\pi^{m_i}(r)e^{-np\beta\omega_i}$. The basic idea is to decompose the above operators into N Hilbert–Schmidt operators, whose kernels can easily be estimated. We will describe this briefly for $E_\phi^{m_i}(r)e^{-np\beta\omega_i}$: Let $\chi\in\mathcal{D}(\mathbb{R}^s)$ be a test function, which is identical to 1 on $\mathbf{O}_1$ and set χ_r by $\chi_r(\mathbf{x}):=\chi(r^{-1}\mathbf{x})$. Denote by the same symbol the corresponding multiplication operator. Let us now define the following operators:

$$h_n^{m_i,r,\beta} := \omega_i^{1/2}(1+\lambda^2\omega_i^2)^{s(n-1)}\chi_r(1+\lambda^2\omega_i^2)^{-sn}\omega_i^{-1/2}, \tag{26}$$

$$k_n^{m_i,r,\beta} := \omega_i^{1/2}(1+\lambda^2\omega_i^2)^{s(n-1)}\chi_r\omega_i^{-1/2}e^{-\beta\omega_i}. \tag{27}$$

Now, set $\lambda:=\min\{r,\beta\}$. Using the identity $E_\phi^{m_i}(r)=E_\phi^{m_i}(r)\omega_i^{1/2}\chi_r\omega_i^{-1/2}$, we obtain the following decomposition for every $N\in\mathbb{N}$:

$$E_\phi^{m_i}(r)=E_\phi^{m_i}(r)h_1^{m_i,r,\beta}\cdots h_{N-1}^{m_i,r,\beta}k_N^{m_i,r,\beta}. \tag{28}$$

By an easy, but tedious, calculation, we obtain upper bounds for the p-trace-norms of $E_\phi^{m_i}(r)e^{-\beta\omega_i}$, where the constant C is independent of r,β and m_i:

$$\|E_\phi^{m_i}(r)e^{-\beta\omega_i}\|_p^p \leqslant \begin{cases} C\left(\dfrac{r}{\beta}\right)^s e^{-(\beta/4)pm_i}, & \beta\leqslant r, \\ C\left(\dfrac{r}{\beta}\right)^{[(s-1)/2]p} e^{-(\beta/4)pm_i}, & \beta>r. \end{cases} \tag{29}$$

Inserting this and a similar estimate for the trace norms of $E_\pi^{m_i}(r)e^{-\beta\omega_i}$ into Eq. (25), the claim follows. ■

IV. THE CASE OF AN INFINITE MASS SPECTRUM

In this section we will prove that the scaling limit theories violate the compactness criterion in the case of an infinite mass spectrum. For doing this we need lower bounds of the ϵ-content of the phase space maps. Since this investigation of lower bounds does not appear in the literature so far, our discussion will be more detailed in this part. Here is our final result:

Theorem 4.1: *Let $\mathfrak{A}$ be a generalized free scalar field in $d\geqslant 3$ space–time dimensions, having a discrete infinite mass spectrum, which fulfills the condition $\Sigma_{i\in\mathbb{N}}e^{-\beta m_i}<\infty$, for all $\beta>0$.*

Then none of its scaling limit theories fulfills the compactness criterion.

For the proof of this theorem we need some auxiliary results: First, let us fix our notation. Let $\chi\in\mathcal{D}(\mathbb{R}^s)$ be a test function with $\mathrm{Supp}(\chi)\subset\mathbf{O}_1$, which is identical to 1 on $\mathbf{O}_{1/2}$. Define χ_r by $\chi_r(\mathbf{x}):=\chi(r^{-1}\mathbf{x})$. We use the same notation for the corresponding multiplication operator. Now, let us set

$$K_{\phi,m_i}^{\beta}(r) := \omega_i^{1/2}\chi_r\omega_i^{-1}e^{-2\beta\omega_i}\chi_r\omega_i^{1/2}. \tag{30}$$

We can state a first auxiliary result:

Lemma 4.1: Keeping the definitions made above, the following estimate holds:

$$\liminf_{\lambda \searrow 0} \|K^{m_i}_{\phi,\lambda\beta}(\lambda r)\| \geqslant \|K^0_{\phi,\beta}(r)\|. \tag{31}$$

Proof: To obtain this, we first present the operators $K^{m_i}_{\phi,\lambda\beta}(\lambda r)$ as integral kernels in momentum space:

$$K^{m_i}_{\phi,\lambda\beta}(\lambda r) = \int d^s\mathbf{k} \frac{(|\mathbf{p}|^2+m_i^2)^{1/4}(|\mathbf{q}|^2+m_i^2)^{1/4}}{\sqrt{|\mathbf{k}|^2+m_i^2}} e^{-2\lambda\beta\sqrt{|\mathbf{k}|^2+m_i^2}} \times (\lambda r)^{2s}\tilde{\chi}((\lambda r)(\mathbf{p}-\mathbf{k}))\tilde{\chi}((\lambda r)(\mathbf{k}-\mathbf{q})). \tag{32}$$

Here the tilde denotes the Fourier transform. Now, let $f \in \mathcal{D}(\mathbb{R}^s)$ be an arbitrary test function with $\|f\|=1$. Then we define f_λ by $f_\lambda(\mathbf{x}) := \lambda^{-s/2} f(\lambda^{-1}\mathbf{x})$. This implies $\|f_\lambda\|=1$. Using the integral kernel presentation above and the self-adjointness of $K^{m_i}_{\phi,\lambda\beta}(\lambda r)$, we get

$$\|K^{m_i}_{\phi,\lambda\beta}(\lambda r)\| \geqslant \langle f_\lambda, K^{m_i}_{\phi,\lambda\beta}(\lambda r) f_\lambda\rangle = \langle f, K^{\lambda m_i}_{\phi,\beta}(r) f\rangle, \tag{33}$$

where the last equation follows by substitution. Now, there exists an integrable upper bound, uniform in the m_i. It is, up to a positive constant, given by

$$\frac{1}{1+|\mathbf{p}-\mathbf{k}|^{2s+2}} \frac{1}{1+|\mathbf{q}|^{s+1}} \left\{ \frac{\sqrt{|\mathbf{p}|}\sqrt{|\mathbf{q}|}}{|\mathbf{k}|} + \sqrt{\frac{|\mathbf{p}|}{|\mathbf{k}|}} + \sqrt{\frac{|\mathbf{q}|}{|\mathbf{k}|}} + 1 \right\} e^{-2\beta|\mathbf{k}|}. \tag{34}$$

Thus, applying Lebesgue's theorem, we can interchange the integral with the limit $\lambda \searrow 0$ to obtain

$$\liminf_{\lambda \searrow 0} \|K^{m_i}_{\phi,\lambda\beta}(\lambda r)\| \geqslant \lim_{\lambda \to 0} \langle f, K^{\lambda m_i}_{\phi,\beta}(r) f\rangle = \langle f, K^0_{\phi,\beta}(r) f\rangle. \tag{35}$$

Since $\mathcal{D}(\mathbb{R}^s)$ is dense in $L^2(\mathbb{R}^s,\mathbb{C})$ the lemma follows. ■

Before proving the main result of this section, we still need a lemma:

Lemma 4.2: There exists a constant C independent of r,β and the mass spectrum, such that the following estimate holds:

$$\underline{\omega}^{-1/2}\chi_r\underline{\omega}\chi_r\underline{\omega}^{-1/2} \leqslant C\underline{E}_\phi(r). \tag{36}$$

Proof: The inequality is obtained as follows:

Trivially, we have $\|\underline{\omega}^{-1/2}\chi_r\underline{\omega}\chi_r\underline{\omega}^{-1/2}\| = \sup_{i\in I}\|\omega_i^{-1/2}\chi_r\omega_i\chi_r\omega_i^{-1/2}\|$. We present $\omega_i^{-1/2}\chi_r\omega_i\chi_r\omega_i^{-1/2}$ as an integral kernel in momentum space:

$$\omega_i^{-1/2}\chi_r\omega_i\chi_r\omega_i^{-1/2} := (|\mathbf{p}|^2+m^2)^{-1/4} r^{2s} \int d^s\mathbf{k}\tilde{\chi}(r(\mathbf{p}-\mathbf{k})) \times (|\mathbf{k}|^2+m^2)^{1/2}\tilde{\chi}(r(\mathbf{k}-\mathbf{q}))(|\mathbf{q}|^2+m^2)^{-1/4}.$$

Now, we can indicate, after a long but straightforward calculation, an upper bound C for its norm, uniform in m_i and r. This is achieved by using the criterion of Schur (cf. Ref. 11), which we rephrase for convenience:

Let $I = I(\mathbf{p},\mathbf{q})$ be an integral kernel, such that the following estimates are finite:

$$N_1 := \sup_{\mathbf{p}\in\mathbb{R}^s} \int d^s\mathbf{q}\,|I(\mathbf{p},\mathbf{q})| < \infty,$$

$$N_2 := \sup_{\mathbf{q}\in\mathbb{R}^s} \int d^s\mathbf{p}\,|I(\mathbf{p},\mathbf{q})| < \infty.$$

Then, I defines a bounded operator and $\|I\| \leqslant \sqrt{N_1 N_2}$. ■

Proof of the theorem: We will prove this theorem using Proposition 2.1, by showing that $\liminf_{\lambda\searrow 0} N_{\lambda\beta,\lambda\mathcal{O}}(\epsilon) = \infty$, for some $\epsilon > 0$.

By the identity $|e^{-\beta\omega}\underline{E}_\phi(r)| = \oplus_{i\in\mathbb{N}}|e^{-\beta\omega_i}E_\phi^{m_i}(r)|$ we can find orthonormal eigenfunctions $F_{\phi,i}^{(\lambda)} \in \mathcal{L}_\phi(\mathcal{O}_{\lambda r})$, $i\in\mathbb{N}$, of $|e^{-\lambda\beta\omega}\underline{E}_\phi(\lambda r)|$ corresponding to the eigenvalues $\|e^{-\lambda\beta\omega_i}E_\phi^{m_i}(\lambda r)\|$. We define local operators $A_{\phi,i}^{(\lambda)} \in \mathfrak{A}(\lambda\mathcal{O})$, $\|A_{\phi,i}^{(\lambda)}\| = 1$:

$$A_{\phi,i}^{(\lambda)} := \frac{1}{1+e^{-1/2}}\left(W(F_{\phi,i}^{(\lambda)}) - e^{-1/2}1\right). \tag{37}$$

With these definitions, the following estimate holds, for $i \neq j$:

$$\begin{aligned}\|\Theta_{\lambda\beta,\lambda\mathcal{O}}(A_{\phi,i}^{(\lambda)} - A_{\phi,j}^{(\lambda)})\|^2 &= \frac{e^{-1}}{(1+e^{-1/2})^2}\left(\exp\{\|e^{-\lambda\beta\omega_i}E_\phi^{m_i}(\lambda r)\|^2\} + \exp\{\|e^{-\lambda\beta\omega_j}E_\phi^{m_j}(\lambda r)\|^2\} - 2\right)\\ &\geqslant \frac{e^{-1}}{(1+e^{-1/2})^2}\left(\|e^{-\lambda\beta\omega_i}E_\phi^{m_i}(\lambda r)\|^2 + \|e^{-\lambda\beta\omega_j}E_\phi^{m_j}(\lambda r)\|^2\right).\end{aligned} \tag{38}$$

Applying Lemma 4.2, we conclude with C independent of r,β and m_i:

$$\|e^{-\lambda\beta\omega_i}E_\phi^{m_i}(\lambda r)\|^2 = \|e^{-\lambda\beta\omega_i}E_\phi^{m_i}(\lambda r)e^{-\lambda\beta\omega_i}\| \geqslant C\|K_{\phi,\lambda\beta}^{m_i}(\lambda r)\|. \tag{39}$$

Combining the last two equations and Lemma 4.1, we get, for $i \neq j$,

$$\liminf_{\lambda\searrow 0} \|\Theta_{\lambda\beta,\lambda\mathcal{O}}(A_{\phi,i}^{(\lambda)} - A_{\phi,j}^{(\lambda)})\|^2 \geqslant C\|K_{\phi,\beta}^0(r)\|. \tag{40}$$

The constant C does not depend on r,β and i,j. Therefore the theorem follows. ■

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Conditions for the alignment of the principal null directions of two Weyl-like tensors

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A possible means to classify the interaction between the Weyl and Ricci tensors is to look at the number of principal null directions that the Weyl and Plebanski tensors have in common. This paper presents algebraic conditions that can be used to determine this number without explicitly calculating the principal null directions themselves. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1483377]

I. INTRODUCTION

Over the past decade, considerable attention has been paid to understanding the invariants of the Riemann tensor and the relationships between them.[1–8] This renewed interest focused on the identities between the invariants and how they can be used to find information about the Riemann tensor. As a result of work by Sneddon[5–7] it is possible to write down a complete set of invariants for the Riemann tensor. Unfortunately, the number of elements required in a complete set is rather large and this limits the usefulness of such a set. Other workers[1,4] have sought to find a smaller set of invariants that is not necessarily complete, but which can be used to obtain information about all other invariants.

One reason for developing an understanding of these invariants is to enable a classification of the Riemann tensor that takes into account the interaction between the Weyl tensor and the Ricci tensor (the irreducible parts of the Riemann tensor). Most existing classifications classify each of these tensors separately. An exception is the work by Haddow,[3] who looked at the particular cases of Einstein–Maxwell fields and perfect fluids.

In Sec. II the main features of the existing classifications of the Weyl tensor and Ricci tensor are summarized. It is argued that in the first instance a classification of the interaction should be based on the principal spinors of the Weyl spinor Ψ and the Plebanski spinor L. In Sec. III the condition for Ψ and L to have at least one principal null direction (PND) in common is presented. This is essentially a condition on the scalar invariants of the Riemann tensor. In Sec. IV conditions for Ψ and L to have at least two PNDs in common are given. It is shown that these conditions can be expressed as a rotor equation, $X_{ABC}=0$. Each of the components of X can be expressed in terms of the NP components of Ψ and L, but the covariant expression for X in terms of Ψ and L is not determined at this stage. Similarly, Sec. V gives conditions for Ψ and L to have at least three PNDs in common. Also in this section, conditions for the spinors to have four PNDs in common are given. While this is really a trivial case (since then $\Psi \propto L$) it does lead to a means to find covariant expressions for the previous conditions in terms of Ψ and L. These conditions are presented in Sec. VI.

Most of the conditions were obtained using a numerical procedure rather than index manipulations. They were all checked subsequently by assigning symbolic values to the components of Ψ and L and evaluating the expressions using a computer algebra package.

Although the properties being investigated relate to principal spinors, in most instances the conditions are expressed in the language of self-dual bivectors or rotors. The main reason for this is that the smaller number of indices needed for these quantities usually leads to more compact

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expressions. On some occasions it is helpful to refer to both forms (almost interchangeably). Thus $A,B,\ldots$ will be used for rotor indices and will take values from 1 to 3. Spinor indices will be represented by $\mu,\nu,...$ and will take values 0 and 1. Finally, $k,l,\ldots$ will represent tensor indices.

II. PRELIMINARIES

The classification of the Riemann tensor proceeds by first separating the tensor into its irreducible parts, i.e.,

$$R_{klmn}=C_{klmn}+E_{klmn}+\tfrac{1}{6}g_{k[m}g_{n]l}R,$$

where C_{klmn} is the Weyl tensor, $E_{klmn}=2g_{[k[m}S_{n]l]}$ where S_{kl} is the trace-free Ricci tensor, and R is the trace of the Ricci tensor. Each of C_{klmn} and E_{klmn} (or S_{kl}) can be classified separately. There are several approaches to the classifications of these tensors. These have been described by Plebanski,[9] Kramer, Stephani and Herlt,[10] Hall,[11] Penrose and Rindler,[12] and Joly and MacCallum[13] (among others). The Weyl tensor can be classified according to the solutions of the eigenvalue equation $C^{kl}{}_{mn}V^{mn}=\lambda V^{kl}$ where V^{kl} is a bivector. Similarly, the trace free Ricci tensor can be classified by the solutions of the equation $E^{kl}{}_{mn}V^{mn}=\gamma V^{kl}$ or of $S^{k}{}_{l}v^{l}=\gamma v^{k}$.

Alternatively, the classification can be carried out on the spinor equivalents of these tensors. In the case of the Weyl tensor, the spinor equivalent is $\Psi_{\mu\nu\rho\sigma}$ which can be expressed in terms of its principal spinors by $\Psi_{\mu\nu\rho\sigma}=\alpha_{(\mu}\beta_{\nu}\gamma_{\rho}\delta_{\sigma)}$. The classification is according to the coincidences of the principal spinors and gives the same results as the approach in terms of eigenbivectors. Both approaches lead to the Petrov classification of the Weyl tensor.

The spinor equivalent of E_{klmn} is $\Phi_{\mu\nu\dot{\rho}\dot{\sigma}}$. The dotted indices appear because E_{klmn} is the anti-self-dual part of the Riemann tensor. This means that, unlike Ψ, the decomposition of Φ into principal spinors is not possible. Instead the classification can be based on the solutions of the eigenvalue equation $\Phi^{\mu\nu}{}_{\dot{\rho}\dot{\sigma}}\overline{\chi}^{\dot{\rho}\dot{\sigma}}=\gamma\chi^{\mu\nu}$, where the eigenspinor $\chi^{\mu\nu}$ can be scaled so that γ will be real. Again this gives essentially the same results as the direct classification of either E_{klmn} or S_{kl}. These approaches lead to the Plebanski classification or equivalently, a classification according to the Segré type of the Ricci tensor.

The classification of $\Phi_{\mu\nu\dot{\rho}\dot{\sigma}}$ can also be carried out according to the locus ω of complex null vectors $z^{k}\leftrightarrow\xi^{\mu}\eta^{\dot{\nu}}$ where the function

$$\Omega(\xi,\eta)=\Phi_{\mu\nu\dot{\rho}\dot{\sigma}}\xi^{\mu}\xi^{\nu}\eta^{\dot{\rho}}\eta^{\dot{\sigma}}$$

vanishes.[12] The resulting classification, together with the separation into various categories, is a refinement of the Plebanski classification.

The classification of these tensors can also be expressed in the language of complex self-dual bivectors (or rotors).[14] This is the notation that was used by Sneddon[5–7] to describe the relationships between the invariants of the Riemann tensor. A brief description of this notation is given in Ref. 5, but the main feature is that pairs of symmetric spinor indices are replaced by a single rotor index which can take values from 1 to 3. Thus $\Psi_{\mu\nu\rho\sigma}\rightarrow\Psi_{AB}$ and $\Phi_{\mu\nu\dot{\rho}\dot{\sigma}}\rightarrow\Gamma_{A\dot{B}}$, where Ψ_{AB} is symmetric and trace-free and $\Gamma_{A\dot{B}}$ is Hermitian. The metric in this space is denoted by α_{AB}. The symbols used are summarized in Table I. In this notation the relevant eigenvalue equations are

$$\Psi^{A}{}_{B}\phi^{B}=\lambda\phi^{B},\quad \Gamma^{A}{}_{\dot{B}}\overline{\chi}^{\dot{B}}=\gamma\chi^{A}.$$

One other classification scheme for the Ricci tensor is based on the Plebanski tensor

$$L_{klmn}=S_{[k[m}S_{n]l]}+g_{[k[m}S_{n]}{}^{p}S_{l]p}-\tfrac{1}{6}g_{k[m}g_{n]l}S_{pq}S^{pq}.$$

This tensor has the same symmetries as the Weyl tensor and it is trace-free. Its spinor equivalent (to within a factor) is given by $L_{\mu\nu\rho\sigma}=2\Phi_{(\mu\nu}{}^{\dot{\gamma}\dot{\delta}}\Phi_{\underline{\rho\sigma})\dot{\gamma}\dot{\delta}}$. In terms of rotors, $L_{\mu\nu\rho\sigma}$ is equivalent to L_{AB} which is the trace-free part of $K_{AB}=\Gamma_{A\dot{C}}\Gamma^{\dot{C}}{}_{B}$. It is clear that L_{AB} will have the same

TABLE I. The notation for the tensor, spinor, and rotor forms of the different entities.

	Weyl tensor	Ricci tensor	Plebanski tensor
Tensor form	C_{klmn}	S_{kl} $\downarrow$ E_{klmn}	L_{klmn}
Spinor form	$\Psi_{\mu\nu\rho\sigma}$	$\Phi_{\mu\nu\dot{\rho}\dot{\sigma}}$	$L_{\mu\nu\rho\sigma}$
Rotor form	Ψ_{AB}	$\Gamma_{A\dot{B}}$	$K_{AB}=\Gamma_{A\dot{C}}\overline{\Gamma^{C}}_{B}$ $\downarrow$ L_{AB}

symmetries as Ψ_{AB}. This means that the Petrov classification can be applied directly to the Plebanski tensor and $L_{\mu\nu\rho\sigma}$ can be expressed in terms of its principal spinors. Classifying the Ricci tensor according to the coincidences of these spinors gives rise to the Petrov–Plebanski (or PP) classification[9] of the Ricci tensor. As might be expected, the PP classification is not as fine as the Plebanski classification. Essentially, some of the detail available in Γ is lost when we take the square (and then remove the trace). However, provided $[K]$ (the trace of K) is still available, the only types that cannot be distinguished by the PP classification are the pairs

$$[11(1,1)] \text{ and } [(11)1,1], \quad [(11)(1,1)] \text{ and } [(11)2],$$

$$[1(11,1)] \text{ and } [(111),1], \quad [(111,1)] \text{ and } [(112)].$$

(See the table on page 1001 of Ref. 9.)

It should also be noted that the PP classification can be obtained from the eigenvalue equation for L (or K). The equation is $L^{A}{}_{B}\phi^{B}=\lambda\phi^{A}$. The relationship between the eigenbivectors ϕ^{A} (or their spinor equivalents) and the principal spinors of L has been given by Plebanski,[9] but it is not straightforward.

As noted by Penrose and Rindler (Ref. 12, p. 266), the separate classification of Ψ and Φ will not give the full story. There is still the interrelationship between the two parts to consider. In classifying this interrelationship, it is not essential that all possible information from the two entities be represented. An analogy might be with the classification of two matrices. Each matrix can be classified according to the nature of its eigenvalues and eigenvectors. The relationship between the matrices could then be classified according to the alignments of the two sets of eigenvectors. In that case the eigenvalues of the matrices would not affect the classification of the interrelationship.

There are two possibilities on which such a classification of Ψ and Φ might be based. These are the alignments of the eigenbivectors of Ψ and L and the coincidences between the principal spinors of Ψ and L. Given the nature of the relationship between the principal spinors and eigenbivectors, it is unlikely that the two approaches would be completely compatible. That is, neither could be seen as a refinement of the other. However, of the two approaches, it is the latter that is likely to result in a simpler classification scheme in the first instance. This is the approach taken by Haddow[3] for Einstein–Maxwell fields. In either case, it would be the properties of L, rather than Γ, that influence the classification. In other words, some of the information available in Γ would not influence the classification of the interaction between Ψ and Γ. Alternatively, the classification based on principal spinors could be viewed as asking how many of the principal spinors of $\Psi_{\mu\nu\rho\sigma}$ generate a family of complex null vectors that is tangent to (or touches) the curve ω formed from $\Phi_{\mu\nu\dot{\rho}\dot{\sigma}}$ (Ref. 12, p. 287).

With this in mind, the aim in the remainder of this paper is to find algebraic conditions for Ψ and L to have one, two, three, or four principal spinors in common.

III. THE CONDITION FOR ONE PND IN COMMON

The principal spinors (and hence the PNDs) of Ψ and L can most easily be obtained from the roots of the polynomials

$$P(z)=\Psi_0+4z\Psi_1+6z^2\Psi_2+4z^3\Psi_3+z^4\Psi_4,$$

$$Q(z)=L_0+4zL_1+6z^2L_2+4z^3L_3+z^4L_4,$$

respectively, where Ψ_i and L_i are the NP components of Ψ and L. Thus, the condition for one PND in common is just the condition that these two polynomials have a root in common. This condition is well known and is simply that the resultant of the two polynomials be zero. (See Cox, Little, and O'Shea,[15] for example.)

In our case, the quartic polynomials will have a root in common if and only if there are cubic polynomials, $A(z)$ and $B(z)$, such that

$$P(z)A(z)+Q(z)B(z)=0. \tag{1}$$

If the coefficients of $A(z)$ and $B(z)$ are $a_0\cdots a_3$ and $b_0\cdots b_3$, respectively, Eq. (1) can be expanded and the coefficients of the powers of z can be set equal to zero. This gives the following set of equations for the coefficients of $A(z)$ and $B(z)$:

$$\begin{pmatrix}
\Psi_0 & 0 & 0 & 0 & L_0 & 0 & 0 & 0\\
4\Psi_1 & \Psi_0 & 0 & 0 & 4L_1 & L_0 & 0 & 0\\
6\Psi_2 & 4\Psi_1 & \Psi_0 & 0 & 6L_2 & 4L_1 & L_0 & 0\\
4\Psi_3 & 6\Psi_2 & 4\Psi_1 & \Psi_0 & 4L_3 & 6L_2 & 4L_1 & L_0\\
\Psi_4 & 4\Psi_3 & 6\Psi_2 & 4\Psi_1 & L_4 & 4L_3 & 6L_2 & 4L_1\\
0 & \Psi_4 & 4\Psi_3 & 6\Psi_2 & 0 & L_4 & 4L_3 & 6L_2\\
0 & 0 & \Psi_4 & 4\Psi_3 & 0 & 0 & L_4 & 4L_3\\
0 & 0 & 0 & \Psi_4 & 0 & 0 & 0 & L_4
\end{pmatrix}
\begin{pmatrix} a_0\\ a_1\\ a_2\\ a_3\\ b_0\\ b_1\\ b_2\\ b_3 \end{pmatrix}
=\begin{pmatrix} 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0 \end{pmatrix}.$$

Since we need a nonzero solution, the determinant

$$R=\begin{vmatrix}
\Psi_0 & 0 & 0 & 0 & L_0 & 0 & 0 & 0\\
4\Psi_1 & \Psi_0 & 0 & 0 & 4L_1 & L_0 & 0 & 0\\
6\Psi_2 & 4\Psi_1 & \Psi_0 & 0 & 6L_2 & 4L_1 & L_0 & 0\\
4\Psi_3 & 6\Psi_2 & 4\Psi_1 & \Psi_0 & 4L_3 & 6L_2 & 4L_1 & L_0\\
\Psi_4 & 4\Psi_3 & 6\Psi_2 & 4\Psi_1 & L_4 & 4L_3 & 6L_2 & 4L_1\\
0 & \Psi_4 & 4\Psi_3 & 6\Psi_2 & 0 & L_4 & 4L_3 & 6L_2\\
0 & 0 & \Psi_4 & 4\Psi_3 & 0 & 0 & L_4 & 4L_3\\
0 & 0 & 0 & \Psi_4 & 0 & 0 & 0 & L_4
\end{vmatrix} \tag{2}$$

must be zero. This determinant is the resultant of $P(z)$ and $Q(z)$.

If the expression for R is expanded, there will be 219 terms, so this form will be quite cumbersome in the general case. Since the property of having a PND in common is an invariant property, it is to be expected that R can be written in terms of the invariants of Ψ and L. If so, this should provide a simpler expression than (2). Using a computer algebra package (in this case, MATHEMATICA) it is easy to show that R is invariant under a general Lorentz transformation as expected. For example, if $\{o^\mu,\iota^\mu\}$ forms a dyad for spin space then, under the transformation

$$o^\mu \to o^\mu + b\,\iota^\mu, \quad \iota^\mu \to \iota^\mu, \tag{3}$$

the components of Ψ undergo the transformation

$$\Psi_0 \to \Psi_0 + 4b\Psi_1 + 6b^2\Psi_2 + 4b^3\Psi_3 + b^4\Psi_4,$$

$$\Psi_1 \to \Psi_1 + 3b\Psi_2 + 3b^2\Psi_3 + b^3\Psi_4,$$

$$\Psi_2 \to \Psi_2 + 2b\Psi_3 + b^2\Psi_4,$$

$$\Psi_3 \to \Psi_3 + b\Psi_4,$$

$$\Psi_4 \to \Psi_4$$

and the components of L will change similarly. However, R is left unchanged by this transformation.

The method used to express R in terms of the invariants is the ''method of undetermined coefficients'' first used by Ouchterlony[16] and described in Ref. 7. To obtain the expression for R we start by writing down all products of invariants that have degree four in both Ψ and L. (It is sufficient to include only those invariants that belong to the complete set for Ψ and L given by Sneddon.[5]) Then R must be a linear combination of these terms. Equations for the coefficients of these terms can be found by giving random numerical values to the components of Ψ and L. These equations can be solved to give

$$\begin{aligned} R = &-48[\Psi^2L^2]^2 + 8[\Psi^2L^2][\Psi L]^2 - 32[\Psi L^2][\Psi^2 L][\Psi L] + 288\det(\Psi)\det(L)[\Psi L] \\ &- 6[\Psi^2][L^2][\Psi L]^2 - 96\det(\Psi)[\Psi L^2][L^2] - 96\det(L)[\Psi^2 L][\Psi^2] + [\Psi L]^4 \\ &+ 40[\Psi^2 L^2][\Psi^2][L^2] - 7[\Psi^2]^2[L^2]^2 + 32[L^2][\Psi^2 L]^2 + 32[\Psi^2][\Psi L^2]^2. \end{aligned} \tag{4}$$

(The notation is that $[\Psi^2 L^2]$ represents the trace of the matrix product $\Psi^2 L^2$, etc.) It can easily be confirmed that the right-hand side of this expression is equivalent to the determinant (2).

One disadvantage with this method is that it does not give any indication of the origin of this expression in terms of the components Ψ_{AB} and L_{AB} or the principal spinors of Ψ and L. In Sec. VI a covariant expression for R is obtained in terms of the components, but it is still unclear why this expression should imply that $\Psi_{\mu\nu\rho\sigma}$ and $L_{\mu\nu\rho\sigma}$ have a principal spinor in common. Presumably, if Ψ and L are each written as symmetrized products of their principal spinors, the expression for R will reduce to a product of all possible inner products of a principal spinor of Ψ with a principal spinor of L. If two such principal spinors are proportional to each other then their inner product will be zero and so R will be zero. On the other hand, if $R=0$, one of the inner products must be zero and so the corresponding spinors are proportional.

IV. THE CONDITIONS FOR TWO PNDS IN COMMON

The condition for two coincident PNDs is that there exist quadratics, $A(z)$ and $B(z)$, such that $P(z)A(z)+Q(z)B(z)=0$. (This will also include the case where the two common PNDs are actually equal.) In a similar fashion to the case for one PND in common, the equations for the coefficients of $A(z)$ and $B(z)$ will have a nonzero solution if the rank of the matrix

$$\begin{pmatrix} \Psi_0 & 0 & 0 & L_0 & 0 & 0 \\ 4\Psi_1 & \Psi_0 & 0 & 4L_1 & L_0 & 0 \\ 6\Psi_2 & 4\Psi_1 & \Psi_0 & 6L_2 & 4L_1 & L_0 \\ 4\Psi_3 & 6\Psi_2 & 4\Psi_1 & 4L_3 & 6L_2 & 4L_1 \\ \Psi_4 & 4\Psi_3 & 6\Psi_2 & L_4 & 4L_3 & 6L_2 \\ 0 & \Psi_4 & 4\Psi_3 & 0 & L_4 & 4L_3 \\ 0 & 0 & \Psi_4 & 0 & 0 & L_4 \end{pmatrix} \tag{5}$$

is less than or equal to 5. This means that the determinant of any 6×6 submatrix must be zero. While this gives seven separate conditions (one for each row that is to be removed) only two of these can be independent. The determinant of the submatrix with the $(7-i)$th row removed will be denoted by X_i.

Unlike the equation for one PND in common, the X_i are not invariant under a Lorentz transformation. This removes any hope of being able to write these conditions in terms of invariants. Instead, under the transformation (3) the X_i transform as

$$X_0 \to X_0 + 6bX_1 + 15b^2X_2 + 20b^3X_3 + 15b^4X_4 + 6b^5X_5 + b^6X_6,$$

$$X_1 \to X_1 + 5bX_2 + 10b^2X_3 + 10b^3X_4 + 5b^4X_5 + b^5X_6,$$

$$X_2 \to X_2 + 4bX_3 + 6b^2X_4 + 4b^3X_5 + b^4X_6,$$

$$X_3 \to X_3 + 3bX_4 + 3b^2X_5 + b^3X_6,$$

$$X_4 \to X_4 + 2bX_5 + b^2X_6,$$

$$X_5 \to X_5 + bX_6,$$

$$X_6 \to X_6.$$

This is precisely the transformation of the components of a six index, completely symmetric spinor $X_{\mu\nu\rho\sigma\gamma\delta}$. The corresponding rotor will be X_{ABC}, which is completely symmetric and trace-free.

In fact, X_{ABC} satisfies some other properties as well as being symmetric and trace-free. We have seen that only two of the conditions $X_i=0$ can be independent. The relations between these conditions can be found easily. For example, if the matrix (5) is augmented with the column $(\Psi_0,4\Psi_1,6\Psi_2,4\Psi_3,\Psi_4,0,0)^T$ the determinant of the resulting matrix is identically zero. Therefore,

$$\Psi_0X_6 + 4\Psi_1X_5 + 6\Psi_2X_4 + 4\Psi_3X_3 + \Psi_4X_2 \equiv 0. \tag{6}$$

Five similar identities can be found by augmenting (5) with $(0,\Psi_0,4\Psi_1,6\Psi_2,4\Psi_3,\Psi_4,0)^T$, $(0,0,\Psi_0,4\Psi_1,6\Psi_2,4\Psi_3,\Psi_4)^T$, and similar columns constructed from the components of L. In terms of rotors, these identities are

$$\Psi^{AB}X_{ABC} \equiv 0, \quad L^{AB}X_{ABC} \equiv 0.$$

There is still the task of writing X_{ABC} as a covariant expression in terms of Ψ_{AB} and L_{AB}. A sketch of one possible method for doing this is given at this stage. A different approach is used in Sec. IV, which leads to a simpler result. Each term in the expression for X_{ABC} must have three factors of Ψ_{AB} and three factors of L_{AB}. In order to get an odd number of indices the alternating tensor, e_{ABC}, must also appear in each term. Index contraction can be used to reduce the number of free indices to three. Terms of this type can have one of two possible forms. These are as follows.

TABLE II. The conditions for three coincident PNDs arranged as spinor components.

$U_{\mu\nu\rho\sigma\alpha\beta\gamma\delta}$	$V_{\mu\nu\rho\sigma}$	W
$U_0=D_{56}$		
$U_1=\frac{1}{2}D_{46}$		
$U_2=\frac{1}{14}(3D_{36}+5D_{45})$	$V_0=D_{36}-3D_{45}$	
$U_3=\frac{1}{14}(D_{26}+5D_{35})$	$V_1=\frac{1}{2}(D_{26}-2D_{35})$	
$U_4=\frac{1}{70}(D_{16}+15D_{25}+20D_{34})$	$V_2=\frac{1}{6}(D_{16}+D_{25}-8D_{34})$	$W=D_{16}-5D_{25}+10D_{34}$
$U_5=\frac{1}{14}(D_{15}+5D_{24})$	$V_3=\frac{1}{2}(D_{15}-2D_{24})$	
$U_6=\frac{1}{14}(3D_{14}+5D_{23})$	$V_4=D_{14}-3D_{23}$	
$U_7=\frac{1}{2}D_{13}$		
$U_8=D_{12}$		

(i) $se_{DEF}F^{D}{}_{(A}G^{E}{}_{B}H^{F}{}_{C)}$, where s is a scalar and F, G, and H are matrix products (all different) of Ψ and L. These matrix products can be chosen from the basis set of matrices, Eq. (3) of Sneddon.[6] It can further be shown that only terms with F equal to the identity matrix are needed.

(ii) $se_{DEF}F^{DE}G^{F}{}_{(A}H_{BC)}$ where s is a scalar, F is a skew-symmetric matrix, and H is a symmetric matrix. Again, G can be taken to be the identity.

There are a total of 62 such terms. Of these only 24 are irreducible. All other terms can be obtained from these. The method of undetermined coefficients can be used to find the coefficients of each of these terms in the expression for X_{ABC}. Unfortunately, the resulting expression gives little insight into why it should be zero if there are two PNDs in common.

V. THE CONDITIONS FOR THREE AND FOUR PNDS IN COMMON

The procedures of Secs. III and IV can be extended to the cases of three or four PNDs in common. If there are three PNDs in common the rank of the matrix

$$\begin{pmatrix} \Psi_0 & 0 & L_0 & 0 \\ 4\Psi_1 & \Psi_0 & 4L_1 & L_0 \\ 6\Psi_2 & 4\Psi_1 & 6L_2 & 4L_1 \\ 4\Psi_3 & 6\Psi_2 & 4L_3 & 6L_2 \\ \Psi_4 & 4\Psi_3 & L_4 & 4L_3 \\ 0 & \Psi_4 & 0 & L_4 \end{pmatrix} \tag{7}$$

is less than or equal to 3. Again, this means that the determinant of any 4×4 submatrix must be zero. It is clear that it cannot be a simple spinor involved on this occasion. In fact, these terms will separate into three different quantities, an eight index spinor, a four index spinor, and a scalar. These will be denoted by U, V, and W, respectively. If D_{ij} is the determinant of the submatrix obtained by removing the ith and jth rows, the components of U, V, and W are given in Table II. The terms in each of the first two columns transform as the components of a spinor under a Lorentz transformation.

The rotor equivalent of U will be a four index, completely symmetric, trace-free quantity. That of V will be a two index, completely symmetric, trace-free quantity. Again, there will be relationships connecting the conditions $U_{ABCD}=0$, $V_{AB}=0$, and $W=0$. Only three of these conditions can be independent. Also, each of these quantities will be expressible in terms of Ψ_{AB} and L_{AB}. This is not done at this stage, other than to note that the scalar W can be expressed as

$$W=24[\Psi^2L^2]-22[\Psi^2][L^2]+10[\Psi L]^2.$$

Finally, if there are four PNDs in common the rank of the matrix

$$\begin{pmatrix} \Psi_0 & L_0 \\ 4\Psi_1 & 4L_1 \\ 6\Psi_2 & 6L_2 \\ 4\Psi_3 & 4L_3 \\ \Psi_4 & L_4 \end{pmatrix} \tag{8}$$

is less than or equal to 1. The determinant of any 2×2 submatrix must be zero. This means that Ψ and L must be proportional to each other. This also follows immediately from the fact that there are four PNDs in common.

There are a total of ten conditions, not all independent. These can be arranged into a group of seven (that transform as the components of a six index spinor) and a group of three (that transform as the components of a two index spinor). The six index spinor will be equivalent to a three index rotor. The terms in the expression for this rotor must have one factor of Ψ_{AB}, one factor of L_{AB}, and one of e_{ABC}. Virtually the only quantity that meets these requirements and is symmetric is

$$Y_{ABC}=e_{DE(A}\Psi^{D}{}_{B}L^{E}{}_{C)}. \tag{9}$$

The trace-free part of this rotor gives the seven conditions that transform as a six index spinor. The trace of Y_{ABC} is $Y_A=Y_{AB}{}^{B}$. The remaining three conditions are given by $Y_A=0$. All ten conditions can be deduced from the single equation

$$Y_{ABC}=0.$$

These conditions also satisfy certain identities. An example of one such set of identities is

$$\Psi^{(A}{}_{D}Y^{BC)D}-\Psi^{(AB}Y^{C)}+\alpha^{(AB}\Psi^{C)}{}_{D}Y^{D}\equiv 0.$$

(This equation has been obtained using computer algebra rather than index manipulation.)

It turns out that Y_{ABC} also plays an important role in the expression of the conditions for one, two, and three PNDs in common. These expressions are obtained in Sec. VI.

The spinor form of rotors such as Y_{ABC}, that contain the alternating tensor, is not immediately apparent. However, because of the central role played by Y_{ABC} it is important to note its spinor equivalent. The spinor equivalent of $e_{DEA}\psi^{D}\phi^{E}$ is obtained in the Appendix. It follows that if the indices of Y_{ABC} correspond to spinor indices according to $A\leftrightarrow\mu\nu$, $B\leftrightarrow\rho\sigma$, and $C\leftrightarrow\gamma\delta$, then

$$e_{DEA}\Psi^{D}{}_{B}L^{E}{}_{C}\leftrightarrow 2\Psi_{\alpha\rho\sigma(\mu}L^{\alpha}{}_{\nu)\gamma\delta}.$$

Y_{ABC} will correspond to that part of this spinor that is symmetric under the interchange of any of the index pairs $\mu\nu$, $\rho\sigma$, and $\gamma\delta$. Note that this spinor will not be completely symmetric. Instead, the symmetric spinor $2\Psi_{\alpha(\rho\sigma\mu}L^{\alpha}{}_{\nu\gamma\delta)}$ will correspond to the trace-free part of Y which is $Y_{ABC}-\frac{3}{5}\alpha_{(AB}Y_{C)}$.

VI. COVARIANT EXPRESSIONS FOR THE CONDITIONS

The method used to obtain the conditions for coincident PNDs gives no insight into how they can be written in terms of covariant expressions. In the case of four coincidences though, it was possible to deduce that the conditions could be expressed as $Y^{ABC}=0$. It turns out that all of the conditions can be expressed in terms of Y^{ABC}.

Conditions with a certain degree in Ψ and L can be obtained by first writing down all possible combinations of Y^{ABC} that have that degree and the required number of free indices and the required symmetries. The method of undetermined coefficients can then be used to determine which linear combination of these will give the required condition. In the process, it is shown that Y^{ABC} also satisfies certain identities. These are noted along the way. Throughout, the rotor expression of the condition is given rather than the spinor form.

A. Conditions for three coincident PNDs

These conditions are all quadratic in Y. We look at the scalar W first. The only possible quadratic terms are $Y^{ABC}Y_{ABC}$ and $Y^{A}Y_{A}$. We find that

$$-\tfrac{1}{72}W=\widetilde{W}=Y^{ABC}Y_{ABC}+Y^{A}Y_{A}. \tag{10}$$

The possible quadratic two index quantities are $Y^{ABC}Y_{C}$, $Y^{ACD}Y^{B}{}_{CD}$, $Y^{A}Y^{B}$ and terms involving the metric. The components of V come from the trace-free part of $Y^{ABC}Y_{C}$. In fact,

$$\tfrac{1}{144}V^{AB}=\widetilde{V}^{AB}=Y^{ABC}Y_{C}-\tfrac{1}{3}\alpha^{AB}Y^{C}Y_{C}. \tag{11}$$

Equivalent expressions for V^{AB} can be found by using the identity

$$2Y^{ABC}Y_{C}-Y^{ACD}Y^{B}{}_{CD}+Y^{A}Y^{B}=\tfrac{1}{3}\alpha^{AB}(3Y^{C}Y_{C}-Y^{CDE}Y_{CDE}). \tag{12}$$

The four index, quadratic terms that can be formed are $Y^{E(AB}Y_{E}{}^{CD)}$, $Y^{(ABC}Y^{D)}$, and terms involving the metric. U^{ABCD} is proportional to the trace-free part of $-3Y^{E(AB}Y_{E}{}^{CD)}+4Y^{(ABC}Y^{D)}$. We have

$$\begin{aligned}\tfrac{1}{12}U^{ABCD}=\widetilde{U}^{ABCD}=&-3Y^{E(AB}Y_{E}{}^{CD)}+4Y^{(ABC}Y^{D)}+\tfrac{18}{7}\alpha^{(AB}Y^{CD)E}Y_{E}\\&+\tfrac{1}{35}\alpha^{(AB}\alpha^{CD)}(14Y^{EFG}Y_{EFG}-51Y^{E}Y_{E}).\end{aligned} \tag{13}$$

Any metric with four coincident PNDs must also have at least three coincident PNDs. Therefore, if the condition for four coincidences is satisfied, the condition for three coincidences should be automatically satisfied. In this case, it follows trivially that if $Y^{ABC}=0$ then each of U^{ABCD}, V^{AB} and W will also be zero.

B. Conditions for two coincident PNDs

These conditions are cubic in Y and have three rotor indices. There are several terms that meet this requirement. They are

$$Y^{DE(A}Y^{B}{}_{EF}Y^{C)F}{}_{D},\quad Y^{DE(A}Y^{BC)F}Y_{DEF},\quad Y^{DE(A}Y^{BC)}{}_{E}Y_{D},\quad Y^{DE(A}Y^{B}{}_{DE}Y^{C)},$$

$$Y^{D(AB}Y^{C)}Y_{D},\quad Y^{DEF}Y_{DEF}Y^{ABC},\quad Y^{D}Y_{D}Y^{ABC},\quad Y^{A}Y^{B}Y^{C},$$

and terms involving the metric. First, there are three identities connecting these terms,

$$Y^{DE(A}Y^{B}{}_{DE}Y^{C)}-2Y^{D(AB}Y^{C)}Y_{D}-Y^{A}Y^{B}Y^{C}=0,$$

$$-3Y^{DE(A}Y^{BC)F}Y_{DEF}+6Y^{DE(A}Y^{BC)}{}_{E}Y_{D}+3Y^{D(AB}Y^{C)}Y_{D}+Y^{DEF}Y_{DEF}Y^{ABC}-3Y^{D}Y_{D}Y^{ABC}=0,$$

and

$$\begin{aligned}&-6Y^{DE(A}Y^{B}{}_{EF}Y^{C)F}{}_{D}+Y^{DEF}Y_{DEF}Y^{ABC}+6Y^{A}Y^{B}Y^{C}+3Y^{D}Y_{D}Y^{ABC}\\&-\tfrac{3}{5}(-6Y^{DEF}Y_{DE}{}^{G}Y^{(A}{}_{FG}+Y^{DEF}Y_{DEF}Y^{(A}+9Y^{D}Y_{D}Y^{(A})\alpha^{BC)}=0.\end{aligned}$$

The first two can be obtained from Eq. (12), by multiplying by Y^{F} and $Y^{FG}{}_{C}$, respectively. The third identity is new and was found using the method of undetermined coefficients. The traces of the first two identities also give identities with one free index. The trace of the third is identically zero.

The expression for X^{ABC} comes from the trace-free part of $12Y^{DE(A}Y^{BC)}{}_{E}Y_{D}-Y^{DEF}Y_{DEF}Y^{ABC}-5Y^{D}Y_{D}Y^{ABC}$. We find

$$-\tfrac{1}{144}X^{ABC}=\tilde{X}^{ABC}=12Y^{DE(A}Y^{BC)}{}_{E}Y_{D}-Y^{DEF}Y_{DEF}Y^{ABC}-5Y^{D}Y_{D}Y^{ABC}$$
$$-(12Y_{E}Y_{D}Y^{ED(A}+Y^{DEF}Y_{DEF}Y^{(A}-3Y^{D}Y_{D}Y^{(A)})\alpha^{BD)}. \tag{14}$$

Again, we should be able to deduce that $X^{ABC}=0$ from the conditions for two coincident PNDs. This follows from

$$X^{ABC}=-12V^{D(A}Y^{BC)}{}_{D}-2WY^{ABC}+\tfrac{3}{5}(4V^{D(A}Y_{D}+8V^{DE}Y^{(A}{}_{DE}+2WY^{(A)})\alpha^{BC)}.$$

C. Condition for one coincident PND

In this case, there are eight possible terms in the expression for R. They are

$$Y^{ABC}Y_{ADE}Y^{DF}{}_{B}Y^{EF}{}_{C},\quad Y^{ABC}Y_{ABD}Y^{EF}{}_{A}Y^{D}{}_{EF},\quad Y^{ABC}Y^{D}{}_{BC}Y^{E}{}_{AD}Y_{E},$$
$$Y^{ABC}Y^{D}{}_{AB}Y_{C}Y_{E},\quad Y^{ABC}Y_{A}Y_{B}Y_{C},\quad (Y^{ABC}Y_{ABC})^{2},\quad (Y^{A}Y_{A})^{2},\quad (Y^{A}Y_{A})(Y^{BCD}Y_{BCD}).$$

There are four identities connecting these invariants. These are

$$6Y^{ABC}Y_{ADE}Y^{DF}{}_{B}Y^{EF}{}_{C}-24Y^{ABC}Y_{A}Y_{B}Y_{C}-(Y^{ABC}Y_{ABC})^{2}$$
$$+9(Y^{A}Y_{A})^{2}-6(Y^{A}Y_{A})(Y^{BCD}Y_{BCD})=0,$$

$$3Y^{ABC}Y_{ABD}Y^{EF}{}_{A}Y^{D}{}_{EF}-36Y^{ABC}Y_{A}Y_{B}Y_{C}-(Y^{ABC}Y_{ABC})^{2}$$
$$+6(Y^{A}Y_{A})^{2}-4(Y^{A}Y_{A})(Y^{BCD}Y_{BCD})=0,$$

$$Y^{ABC}Y^{D}{}_{BC}Y^{E}{}_{AD}Y_{E}-5Y^{ABC}Y_{A}Y_{B}Y_{C}+(Y^{A}Y_{A})^{2}-(Y^{A}Y_{A})(Y^{BCD}Y_{BCD})=0,$$

and

$$3Y^{ABC}Y^{D}{}_{AB}Y_{C}Y_{E}-6Y^{ABC}Y_{A}Y_{B}Y_{C}-(Y^{A}Y_{A})(Y^{BCD}Y_{BCD})=0.$$

The expression for R can be written as

$$-\tfrac{1}{144}R=\tilde{R}=48Y^{ABC}Y_{A}Y_{B}Y_{C}-(Y^{ABC}Y_{ABC})^{2}-9(Y^{A}Y_{A})^{2}+6(Y^{A}Y_{A})(Y^{BCD}Y_{BCD}), \tag{15}$$

although several other forms are possible.

Finally, it must be possible to obtain the condition, $R=0$, from $X_{ABC}=0$. In fact, it can be shown that

$$R=Y^{ABC}X_{ABC}. \tag{16}$$

We can also show

$$Y^{ABC}X_{ABD}=\tfrac{1}{3}R\delta^{C}{}_{D}. \tag{17}$$

VII. CONCLUSION

We have obtained algebraic conditions for the Weyl tensor and Ricci tensor to have a given number of PNDs in common. Initially, these conditions were given in terms of the determinants of certain matrices. They were also written in a covariant form in terms of rotors or complex bivectors. For one PND in common, we need $R=0$, where R is given by Eq. (15). For two PNDs in common, we need $X_{ABC}=0$ [Eq. (14)]. For three PNDs in common, we need $W=0$, $V_{AB}=0$, and $U_{ABCD}=0$ [Eqs. (10), (11), and (13)]. Finally, if $Y_{ABC}=0$ [Eq. (9)] there will be four PNDs in common. All of these conditions are expressed in terms of Y_{ABC}.

Although it is of theoretical interest that these conditions can be expressed in terms of covariant quantities, these expressions are generally fairly complex. In practice it may be the case that the expressions for these conditions in terms of the determinants will be of more use.

These results mean that it is possible to classify the Riemann tensor according to the number of PNDs the Weyl and Plebanski tensors have in common without calculating the PNDs explicitly. Such a classification would be additional to the separate classifications of the Weyl tensor and the Ricci tensor. It would be a first attempt at classifying the interaction between these tensors.

APPENDIX: ROTOR EXPRESSIONS CONTAINING e_{ABC}

It will be sufficient to consider the spinor equivalent of $e_{DEA}\psi^D\phi^E$. The notation used is that of Buchdahl[14] and is summarized in Ref. 5. The connection between spinors and rotors is given by

$$\phi_A=\lambda_{A\mu\nu}\phi^{\mu\nu}, \quad \phi_{\mu\nu}=\tfrac{1}{2}\lambda_{A\mu\nu}\phi^A.$$

In addition, we need the identities $\lambda^{A\mu\nu}\lambda_{A\alpha\rho}=2\,\delta^{(\mu}{}_{(\alpha}\delta^{\nu)}{}_{\rho)}$ and

$$\lambda^{[D}{}_{\rho\sigma}\lambda^{E]\alpha\beta}=e^{DEC}\lambda_C{}^{(\alpha}{}_{(\rho}\delta^{\beta)}{}_{\sigma)}. \tag{A1}$$

[Equation (A1) is from p. 417 of Ref. 14. It was not recorded in Ref. 5.] Then,

$$e_{DEA}\psi^D\phi^E=e_{DEA}\lambda^D{}_{\rho\sigma}\lambda^{E\alpha\beta}\psi^{\rho\sigma}\phi_{\alpha\beta}=e_{DEA}e^{DEC}\lambda_C{}^{(\alpha}{}_{(\rho}\delta^{\beta)}{}_{\sigma)}\psi^{\rho\sigma}\phi_{\alpha\beta}=2\lambda_{A\alpha\rho}\psi^\rho{}_\beta\phi^{\alpha\beta}.$$

The spinor equivalent is

$$\lambda^{A\mu\nu}\lambda_{A\alpha\rho}\psi^\rho{}_\beta\phi^{\alpha\beta}=2\,\delta^{(\mu}{}_{(\alpha}\delta^{\nu)}{}_{\rho)}\psi^\mu{}_\beta\phi^{\nu\beta}=2\,\psi^{(\mu}{}_\beta\phi^{\nu)\beta}.$$

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Modifying fractal basin boundaries by reshaping periodic terms

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A generic route is described for the modification of fractal basin boundaries in nonlinear systems by changing only the *shape* of a periodic (autonomous or non-autonomous) term in the dynamics equations. Two examples are used to illustrate the route: a non-invertible two-dimensional map, and a driven dissipative oscillator with a cubic potential that typically models a metastable system close to a fold. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1481546]

I. INTRODUCTION

The dynamics of generic physical systems is determined by their global structures such as strange attractors and the boundaries of basins of attraction. In particular, the existence of fractal basin boundaries (FBB)[1–8] has fundamental implications for the behavior since small uncertainties in initial conditions (or other system parameters) may lead to large uncertainties in the response of the system. Indeed, FBBs are of practical importance for the control of a wide class of chaotic systems such as coupled oscillator arrays. We here describe a generic route to control FBBs (i.e., to vary their fractal dimension) by solely varying the waveform of a periodic term in the dynamics equations.

To demonstrate the new technique in the simplest possible context, consider the following two-dimensional map:

$$\theta_{n+1}=\frac{4K(m)}{\pi}\theta_n \mod 2\pi, \tag{1a}$$

$$z_{n+1}=\lambda z_n+\mathrm{cn}\left[\frac{4K(m)}{\pi}\theta_n;m\right], \tag{1b}$$

where we assume $1<\lambda<2$, $0\leqslant\theta<2\pi$, $m\in[0,1[$, and where cn is the Jacobian elliptic function of parameter m and (real) period $4K(m)$, with $K(m)$ the complete elliptic integral of the first kind. When $m=0$, then $\mathrm{cn}[4K(m=0)\theta/\pi;m=0]=\cos(2\theta)$, i.e., we recover a map similar to that considered in Ref. 2. Increasing m makes the pulse given by $\mathrm{cn}[4K(m)\theta/\pi;m]$ progressively narrower. The Jacobian matrix of the map (1) has eigenvalues $4K(m)/\pi$ and λ, which are greater than 1 so that there can be no attractors with finite z. In fact, there exist only two attractors $-z=+\infty$ and $z=-\infty-$ and we wish to characterize the evolution of the fractality of their basin boundary, $z=f(\theta)$, as m varies over the range $[0,1[$. To find this boundary set, we note first that $\theta_n=[4K(m)/\pi]^n\theta_0 \mod (2\pi)$. The map (1) is two-to-one, i.e., given θ_{n+1}, it is not possible to find θ_n uniquely since there are two possible solutions of (1a), $\theta_n=\theta_{n+1}/[4K(m)/\pi]$ and $\theta_n=\pi^2/2K(m)+\theta_{n+1}/[4K(m)/\pi]$. However, we can select any z_n and find one orbit that ends at (z_N,θ_N), by using the above θ_n and taking $z_{n-1}=\lambda^{-1}z_n-\lambda^{-1}\mathrm{cn}\{[4K(m)/\pi]^n\theta_0;m\}$. For the given (z_N,θ_0) one finds that this orbit started at $z_0=\lambda^{-N}z_N-\Sigma_{i=1}^{N}\lambda^{-i}\mathrm{cn}\{[4K(m)/\pi]^i\theta_0;m\}$. The boundary between the two basins are those (z_0,θ_0) such that z_N is finite as $N\to\infty$, so these z and θ are related by

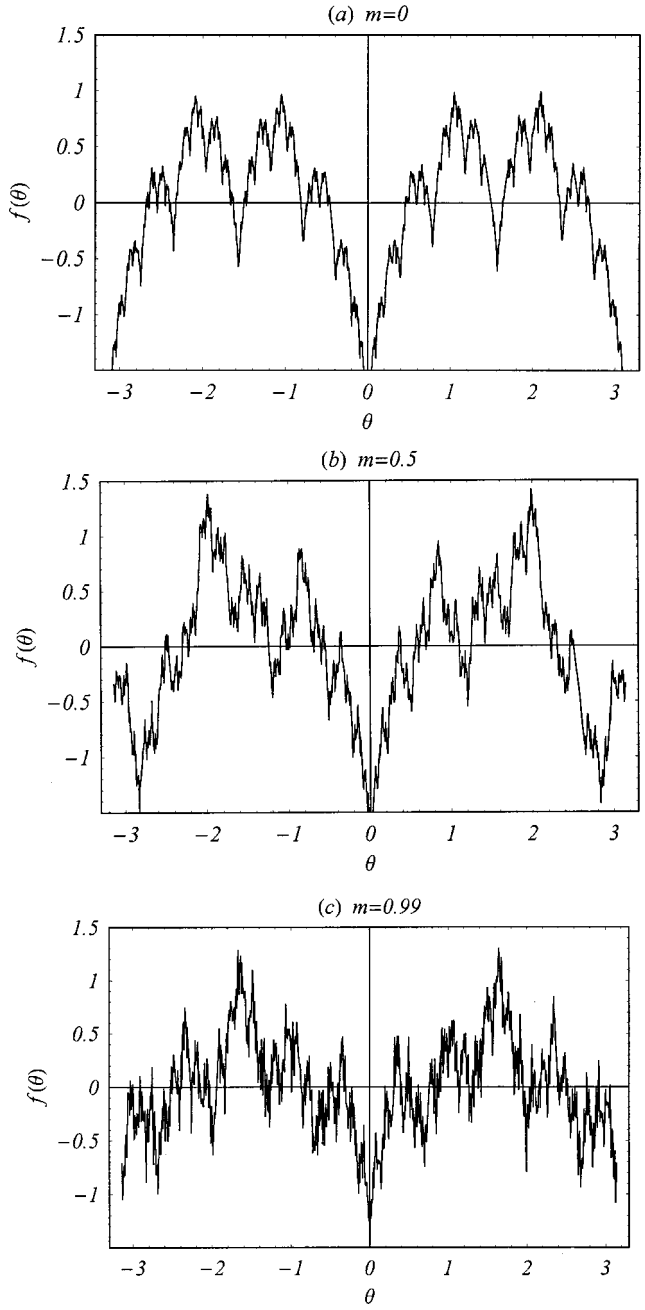

FIG. 1. Approximate plots of the fractal curve (2) (by computing the first 10^3 terms of the series) for $\lambda = 1.5$ and three values of the shape parameter m: (a) $m = 0$, (b) $m = 0.5$, and (c) $m = 0.99$.

$$z = -\sum_{n=1}^{\infty} \lambda^{-n} \mathrm{cn}\left\{\left[\frac{4K(m)}{\pi}\right]^n \theta; m\right\} \equiv f(\theta). \tag{2}$$

Since $\lambda > 1$ and $m \in [0,1[$, this sum converges absolutely and uniformly. One also has $df(\theta)/d\theta = \Sigma_{n=1}^{\infty}[4K(m)/\pi\lambda]^n \mathrm{sn}\{[4K(m)/\pi]^n\theta; m\}\mathrm{dn}\{[4K(m)/\pi]^n\theta; m\}$, where sn and dn are the Jacobian elliptic functions. The latter sum diverges $\forall m \in [0,1[$ because $\lambda < 2$. Hence $f(\theta)$ is nondifferentiable. Figure 1 shows approximate plots of the curve (2) for three values of the shape parameter $m = \{0, 0.5, 0.99\}$. It can be shown[9] that the box-counting dimension of the curve (2) is

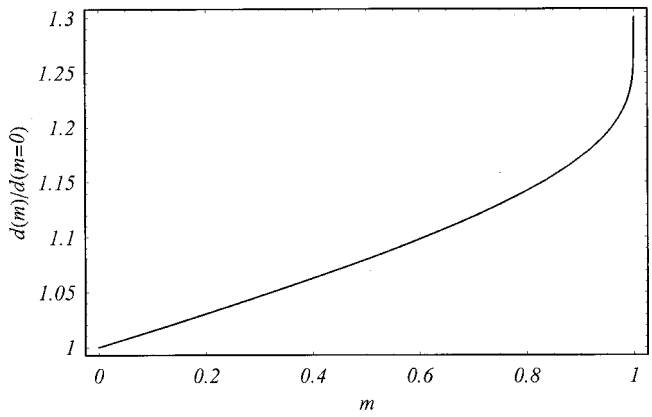

FIG. 2. Normalized fractal dimension of the curve (2), $d(m)/d(m=0)$ [cf. Eq. (3)], vs m for $\lambda=1.5$.

$$d=d(m)\equiv 2-\frac{\mathrm{Ln}\lambda}{\mathrm{Ln}[4K(m)/\pi]}. \tag{3}$$

For $m=0$, we recover the value $d(m=0)=2-(\mathrm{Ln}\lambda)(\mathrm{Ln}2)^{-1}$ reported, for a similar version of the trigonometric counterpart of the map (1), in Ref. 2, while we obtain $d(m\to 1)\to 2$ as the symmetric pulses modeled by the function $\mathrm{cn}[4K(m)\theta/\pi;m]$ become narrow. Figure 2 shows the normalized box-counting dimension $d(m)/d(m=0)$ versus m for $\lambda=\mathrm{const}$. One sees that the increase in the normalized box-counting dimension is especially noticeable for very narrow pulses ($m\lesssim 1$), which is a consequence of its dependence on $K(m)$. It is worth mentioning that similar results can be obtained[10] for other periodic functions instead of cn, i.e., the fractality of a basin boundary can be varied by reshaping a suitable periodic term in the map equations.

II. CONTROL OF CHAOTIC ESCAPE FROM A POTENTIAL WELL

To illustrate the same phenomenon in a physically motivated model equation, consider now the chaotic-escape problem of the dissipative driven oscillator

$$\ddot{x}=-x+\beta x^2-\delta\dot{x}+\gamma\,\mathrm{cn}(\omega t;m) \tag{4}$$

from the cubic potential well that typically models a metastable system close to a fold.[11,12] We assume that $\delta,\gamma\ll 1$ and $\omega=\omega(m)\equiv 4K(m)/T$, where T is the forcing period. This latter is fundamental in comparing the structural stability of the system when only the forcing shape is varied (i.e., by changing m in the range $[0,1[$). The forcing $\mathrm{cn}[4K(m)t/T;m]$ can induce escape in such a way that, before escape, chaotic transients of unpredictable duration—due to the fractal character of the basin boundary (of the attractor at infinity)—are usually observed. In order to characterize the evolution of such FBBs as the shape parameter is varied, we shall apply the Melnikov method (MM) to Eq. (4). The MM provides a criterion for the occurrence of homoclinic (and heteroclinic) chaos in a wide variety of dynamical systems. As is well known, its predictions for the appearance of strange attractors are both approximate and limited. However, it appears that the criterion for the homoclinic (and heteroclinic) orbits—accurately predicted by MM—in various systems[4,11] is coincident with the change from a smooth to an irregular FBB. This is the relevant result for our analysis of the evolution of the FBB as the shape parameter m is varied with the remaining parameters held constant. Since MM is today considered standard, we refer the interested reader to the abundant literature.[13–17]

The application of MM to Eq. (4) involves calculating the Melnikov function,

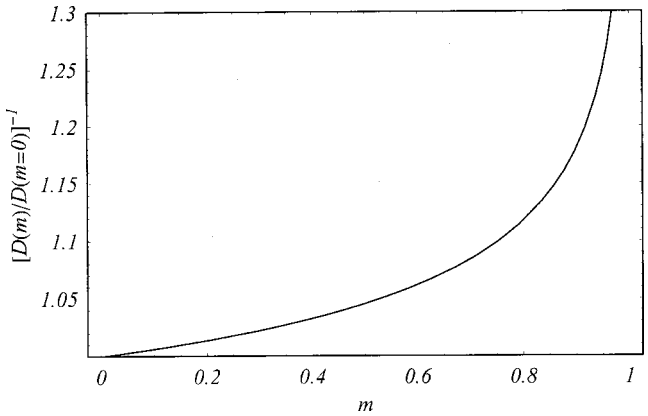

FIG. 3. Function $[D(m)/D(m=0)]^{-1}$ vs m in the range $m\in[0,m_{\text{threshold}}]$, where $D(m)\equiv U(\beta,m,T)-\delta/\gamma$ [cf. Eq. (9)], and $\delta=0.1$, $\gamma=0.08$, $\beta=1.0$, $T=2\pi/0.85$, and $m_{\text{threshold}}\approx 1$.

$$M(t_0)=\int_{-\infty}^{\infty}\left\{-\delta\dot{x}_0^2(t)+\gamma\dot{x}_0(t)\,\mathrm{cn}\left[\frac{4K(m)}{T}(t+t_0);m\right]\right\}dt, \tag{5}$$

where

$$x_0(t)=\frac{1}{\beta}\left(1-\frac{3}{1+\cosh(t)}\right),$$
$$\dot{x}_0(t)=\frac{3}{\beta}\frac{\sinh(t)}{[1+\cosh(t)]^2} \tag{6}$$

are the parametric equations of the separatrix of the underlying conservative system ($\delta=\gamma=0$).

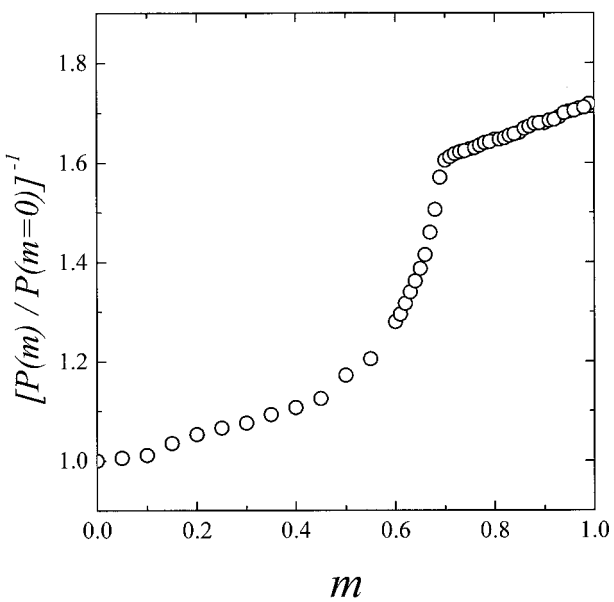

FIG. 4. Inverse normalized escape probability $[P(m)/P(m=0)]^{-1}$ vs m for the same parameters as in Fig. 3. To generate numerically the basins of attraction, we selected a grid of 300×300 starting points in the region of phase space $\{x(t=0)\in[-0.7,1.5],\dot{x}(t=0)\in[-1.0,0.7]\}$. From this grid of initial conditions, each integration was continued until either x exceeds 20, at which point the system is deemed to have escaped (i.e., to the attractor at infinity), or the maximum allowable number of cycles, here 30, is reached.

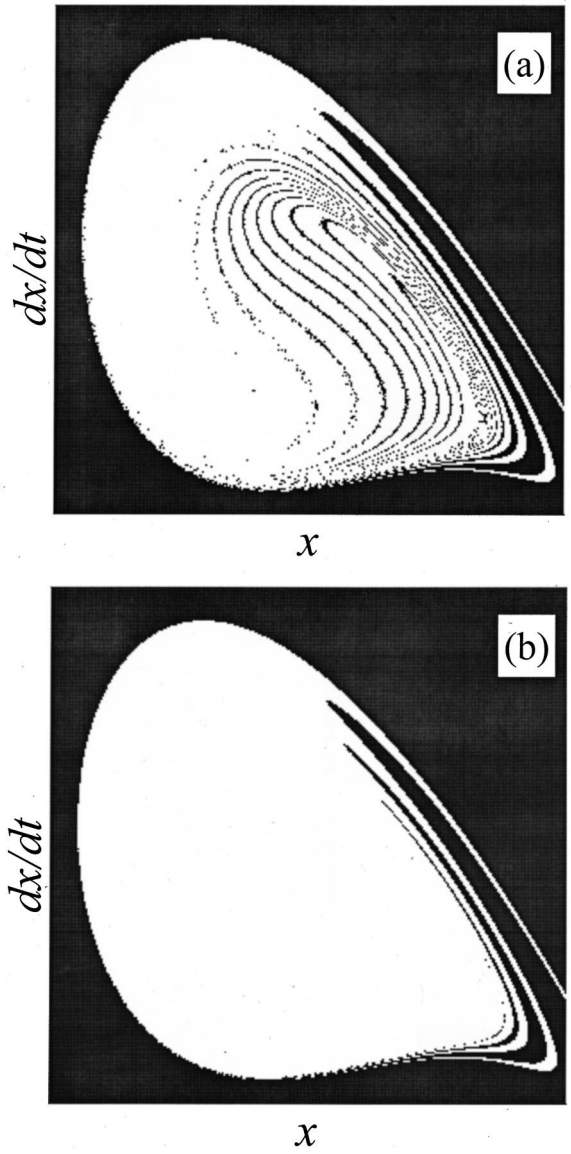

FIG. 5. Basin erosion of the system (4) for $\delta=0.1$, $\gamma=0.08$, $\beta=1.0$, and $T=2\pi/0.85$ in the window $-0.7<x<1.5$, $-1.0<\dot{x}<0.7$: (a) $m=0.68<m_c\approx 0.7$, (b) $m=0.72>m_c$.

After substituting Eq. (6) into Eq. (5), using the Fourier expansion of cn,[18] and computing the resulting integrals with the aid of standard integral tables,[19] Eq. (5) can be written as

$$M(t_0)=-\frac{6\delta}{5\beta^2}-\frac{96\pi^4\gamma}{\beta}\sum_{n=0}^{\infty}c_n(m)b_n(T)\sin\left[\frac{2\pi(2n+1)t_0}{T}\right], \tag{7}$$

with

$$\begin{aligned} c_n(m)&\equiv\frac{1}{\sqrt{m}K(m)}\operatorname{sech}\left[\left(n+\frac{1}{2}\right)\frac{\pi K(1-m)}{K(m)}\right],\\ b_n(T)&\equiv\frac{1}{T^2}\left(n+\frac{1}{2}\right)^2\operatorname{csch}\left[\left(n+\frac{1}{2}\right)\frac{4\pi^2}{T}\right]. \end{aligned} \tag{8}$$

It is straightforward to demonstrate that a homoclinic bifurcation is guaranteed if

$$\frac{\delta}{\gamma} < U(\beta,m,T) \equiv 80\beta\pi^4 \sum_{n=0}^{\infty} c_n(m) b_n(T), \tag{9}$$

where $U(\beta,m,T)$ is the threshold function. With δ,γ,β, and T constant, we can now define a "function distance" to fractality of the basin boundary, $D(m) \equiv U(\beta,m,T) - \delta/\gamma$, so that FBBs (do not) appear when $D(m) > 0 (D(m) \leqslant 0)$. Figure 3 shows a plot of the function $[D(m)/D(m=0)]^{-1}$ versus m for a set of parameters (δ,γ,β,T) such that a FBB already occurs for $m = m_{\text{threshold}}$, i.e., $D(m = m_{\text{threshold}}) > 0$, and *a fortiori* for $m \in [0, m_{\text{threshold}}]$ [cf. Eq. (9)]. It is worth noting that $D(m)$ provides a *qualitative* estimate for the variation of the fractality of the FBB (indeed, observe the similarity with Fig. 2). We can now discuss the connection between the function $D(m)/D(m=0)$ and the normalized escape probability $P(m)/P(m=0)$. We found two different regimes as m varies, as can be seen in Fig. 4. First, there is a *nonlinear* regime over the range $m \in [0, m_c]$, where the variation of the normalized escape probability is very similar to that of the function $D(m)/D(m=0)$ (compare Figs. 3 and 4). Second, there is a *linear* regime over the range $m \in]m_c, 1[$, where $P(m) = P(m=0)/(am+b)$, with a, b, m_c functions of the remaining system parameters. Note that the critical value m_c represents the threshold between having fractallike fingers protruding into the nonescaping basin [as in Fig. 5(a)] and their almost complete disappearance [as in Fig. 5(b)].

III. CONCLUSIONS

The analysis based on models (1) and (4) can be developed in two important ways.[10] First, the results extend to general nonautonomous systems with FBBs. Second, the manner of altering the geometrical shape of the periodic term can be chosen quite freely, which is fundamental in technological applications.

In sum, we have presented a generic way to reduce or increase the fractality of a FBB by only altering the waveform of a suitable periodic term. We connected it with the escape probability in a generic escape problem, where two distinct escape regimens were characterized.

ACKNOWLEDGMENT

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Complete sets of invariants for dynamical systems that admit a separation of variables

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Consider a classical Hamiltonian H in n dimensions consisting of a kinetic energy term plus a potential. If the associated Hamilton–Jacobi equation admits an orthogonal separation of variables, then it is possible to generate algorithmically a canonical basis $\mathbf{Q}$, $\mathbf{P}$ where $P_1=H, P_2,\ldots,P_n$ are the other second-order constants of the motion associated with the separable coordinates, and $\{Q_i,Q_j\}=\{P_i,P_j\}=0, \{Q_i,P_j\}=\delta_{ij}$. The $2n-1$ functions $Q_2,\ldots,Q_n,P_1,\ldots,P_n$ form a basis for the invariants. We show how to determine for exactly which spaces and potentials the invariant Q_j is a polynomial in the original momenta. We shed light on the general question of exactly when the Hamiltonian admits a constant of the motion that is polynomial in the momenta. For $n=2$ we go further and consider all cases where the Hamilton–Jacobi equation admits a second-order constant of the motion, not necessarily associated with orthogonal separable coordinates, or even separable coordinates at all. In each of these cases we construct an additional constant of the motion. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1484540]

I. INTRODUCTION

The quest for integrable systems has a long history. Basically, the question is, given a classical Hamiltonian $H=H(x,p)$ where $\mathbf{x}=(x_1,\ldots,x_n)$, $\mathbf{p}=(p_1,\ldots,p_n)$, how can one find all the solutions to the Poisson bracket condition

$$\{H,L\}=\sum_{i=1}^{n}\left(\frac{\partial H}{\partial p_i}\frac{\partial L}{\partial x_i}-\frac{\partial H}{\partial x_i}\frac{\partial L}{\partial p_i}\right)=0, \tag{1}$$

where $L=L(\mathbf{x},\mathbf{p})$.[1] There is no known comprehensive solution to this problem. However, if the associated Hamilton–Jacobi equation $H(\mathbf{x},\partial S/\partial\mathbf{x})=E$ is additively separable in the orthogonal variables $\mathbf{x}$, then a complete integral of the equation can be constructed by quadratures and one can find a basis of $2n-1$ functionally independent solutions to Eq. (1). Indeed there is an explicit canonical change of coordinates from the variables $\mathbf{x}$, $\mathbf{p}$ with $\{x_i,p_j\}=\delta_{ij}$ to variables $\mathbf{Q}$, $\mathbf{P}$ where $P_1=H, P_2,\ldots,P_n$ are the other second-order constants of the motion associated with the orthogo-

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nal separable x-coordinates, and $\{Q_i,Q_j\}=\{P_i,P_j\}=0$, $\{Q_i,P_j\}=\delta_{ij}$. Thus the $2n-1$ functions $Q_2,\ldots,Q_n,P_1,\ldots,P_n$ form a basis for the invariants. Each invariant Q_j can be expressed as a sum of the form

$$Q_j=\sum_{k=1}^{n} M_k(x_k,\mathbf{P}), \tag{2}$$

see Ref. 1.

Numerous examples have been found through this approach, but important problems remain. Many of the known interesting dynamical systems have extra constants of the motion L which are *polynomial* in the canonical momenta $p_i, i=1,\ldots,n$. This often enables global statements to be made about the system in question, e.g., the existence of closed orbits. However, though many interesting results have been obtained, e.g., Refs. 2 and 3, an algorithmic way of generating all polynomial solutions to (1) is not known. In particular, from the x-based integrals in (2) it is difficult to tell if Q_j is a polynomial in the momenta p_i. In this article we adopt a p-based approach to the calculation of the invariants Q_j in which the term M_k take the form $M_k=M(p_k,\mathbf{P})$, and we can say in advance for exactly which separable metrics and potentials Q_j is a polynomial in the momenta. We give, in principle, a complete solution to this problem. Moreover, we show how to characterize each term M_k in (2) by the Poisson brackets $\{M_k,P_j\}$. [Note: Although the term $M_k(x_k,\mathbf{P})$ always exists, there are cases where it cannot be expressed as $M_k(p_k,\mathbf{P})$, i.e., as a function of p_k alone. These are exactly the cases where x_k is an *ignorable* variable, i.e., where the components of the metric tensor in the $\mathbf{x}$-coordinates do not depend on x_k and where, also, the potential V does not depend on x_k. However, these special cases where M_k and the invariant Q_i of which it is a component term always have polynomial dependence (after multiplication by a linear combination of second-order invariants) can be handled separately or by requiring that M_k depends on a variable with some x dependence, such as $M_k(r(x_k)p_k,\mathbf{P})$ treated below.]

Of course, the system could admit a polynomial invariant

$$L=R(\mathbf{P},Q_2,\ldots,Q_n)$$

such that $L,\mathbf{P}$ is functionally independent, even if $Q_2,\ldots,Q_n$ are not polynomials. It is a much more difficult problem to classify all such possibilities for polynomial L as functions of possibly nonpolynomial Q_j. We make some progress toward the solution of this problem, through the consideration of important examples. These questions of when a system with n second-order constants of the motion (generated by an orthogonal separation of variables) admits additional polynomial constants of the motion are closely related to the concept of superintegrability.[4–18]

For dimension $n=2$ in this article, we go beyond the formulation discussed above and consider all cases where the Hamilton–Jacobi equation admits a second-order constant of the motion, not necessarily associated with orthogonal separable coordinates, or even separable coordinates at all. In each of these cases we construct an additional constant of the motion.

II. CARTESIAN SYSTEMS IN TWO DIMENSIONS

Let us first consider two dimensional Euclidean space. In Cartesian coordinates the Hamiltonian H has the form

$$H=p_x^2+p_y^2+V(x,y).$$

If we have separation of variables in Cartesian coordinates the potential must take the form

$$V(x,y)=X(x)+Y(y). \tag{3}$$

We immediately observe that there are already two invariants arising from the separation, namely $L_1=p_x^2+X(x)$ and $L_2=p_y^2+Y(y)$. Our problem is to calculate a third invariant and determine when it can be chosen to be a polynomial in the canonical momenta. To do this we compute two functions $M(x,p_x)$ and $N(y,p_y)$ that satisfy the conditions

$$\{H,M\}=1, \quad \{H,N\}=1. \tag{4}$$

These equations can be solved in principle if we know the original functions X and Y. Indeed, if we write out the first of these conditions, we obtain

$$2p_x\frac{\partial M}{\partial x}-X'\frac{\partial M}{\partial p_x}=1.$$

This equation can be readily solved to give

$$M=-\int X'^{-1}dQ,$$

where $Q=p_x$ and $L_1=p_x^2+X$. [We consider $X'^{-1}=dx/dX$ to be a function of $X=L_1-Q^2$ to compute the integral. An arbitrary function $f(L_1,L_2)$ can be added to the integral, but this makes no difference since L_1,L_2 are invariants.] Once M and N have been determined, we see that $L_3=N-M$ must be an invariant. It is immediately clear that if $X=x^{1/p}$ where p is an integer, then M is a polynomial in p_x. As examples of this consider the following.

(1) $p=3$:

$$M=-3x^{2/3}p_x-4x^{1/3}p_x^3-\tfrac{8}{5}p_x^5.$$

(2) $p=4$:

$$M=-4x^{3/4}p_x-8x^{1/2}p_x^3-\tfrac{32}{5}x^{1/4}p_x^5-\tfrac{64}{35}p_x^7.$$

It follows from these two examples that the Hamiltonian

$$H=p_x^2+p_y^2+x^{1/3}+y^{1/4}$$

has, in addition to the obvious invariants

$$L_1=p_x^2+x^{1/3}, \quad L_2=p_y^2+y^{1/4},$$

the additional invariant

$$L_3=3x^{2/3}p_x+4x^{1/3}p_x^3+\tfrac{8}{5}p_x^5-4y^{3/4}p_y-8y^{1/2}p_y^3-\tfrac{32}{5}y^{1/4}p_y^5-\tfrac{64}{35}p_y^7. \tag{5}$$

From this observation we conclude that all potentials of the form

$$V=\alpha x^{1/p}+\beta y^{1/q} \tag{6}$$

have the superintegrability property with three functionally independent invariants which are polynomial in p_x and p_y. This includes the known examples corresponding to $p=1,2$. If $X(x)$ is determined by a polynomial relation of the form

$$\sum_{j=1}^{n} a_jX^j=x,$$

we can go even further. Then the function M is always a polynomial in the canonical momentum p_x. As an example consider

$$X(x)=2^{-1/3}[\{x+\sqrt{x^2+1}\}^{1/3}-\{x+\sqrt{x^2+1}\}^{-1/3}]. \tag{7}$$

The inverse function is

$$x=X^3+\frac{3}{2^{2/3}}X$$

and the corresponding function $M(x,p_x)$ is given by

$$-M(x,p_x)=\frac{8}{5}p_x^5+4Xp_x^3+3X^2p_x+\frac{3}{2^{2/3}}p_x.$$

It is clear that all that we have done applies also to potentials that separate in n dimensions, in Cartesian coordinates. There is only one further Cartesian case for which polynomial invariants can be generated. Let us consider the case when $X(x)=\omega_1^2x^2$. The corresponding function $M(x,p_x)$ is given by

$$M(x,p_x)=\frac{1}{4\omega_1}\arcsin\left(\frac{\omega_1^2x^2-p_x^2}{\omega_1^2x^2+p_x^2}\right).$$

If $Y(y)=\omega_2^2y^2$, this establishes that the Hamiltonian

$$H=p_x^2+p_y^2+\omega_1^2x^2+\omega_2^2y^2 \tag{8}$$

has the constant of motion

$$L_3=\frac{1}{4\omega_1}\arcsin\left(\frac{\omega_1^2x^2-p_x^2}{\omega_1^2x^2+p_x^2}\right)-\frac{1}{4\omega_2}\arcsin\left(\frac{\omega_2^2y^2-p_y^2}{\omega_2^2y^2+p_y^2}\right), \tag{9}$$

in addition to the constants $L_1=p_x^2+\omega_1^2x^2$ and $L_2=p_y^2+\omega_2^2y^2$. In general this invariant is not polynomial in the canonical momenta. However, if ω_1/ω_2 is a fraction p/q for integers p,q, then $\omega_1=ps,\omega_2=qs$ and $L_3'=\sin(4spqL_3)$ will be a rational invariant whose common denominator is a product of powers of L_1 and L_2. The numerator is then an additional polynomial invariant, e.g., consider $\omega_1=1,\omega_2=2$. Then

$$L_3'=\sin(8L_3)=\frac{L_1L_2^2-2(xp_y^2-4yp_xp_y-4xy^2)^2}{L_1L_2^2},$$

which indicates that $L_3''=xp_y^2-4yp_xp_y-4xy^2$ is an additional invariant. In general, $L_1^pL_2^q\sin(4spqL_3)$ will be a polynomial invariant, functionally independent of L_1 and L_2.

III. GENERAL TWO-DIMENSIONAL SEPARABLE SYSTEMS

If we extend this problem to the case of orthogonal separable coordinates in a general Riemannian space, we know that the Hamiltonian in a given set of coordinates with a separable potential has the form

$$H=L_1=\frac{p_x^2+p_y^2+v_1(x)+v_2(y)}{f_1(x)+f_2(y)}, \tag{10}$$

and, due to the separability, there is the invariant[19–21]

$$L_2=\frac{f_2(y)(p_x^2+v_1(x))-f_1(x)(p_y^2+v_2(y))}{f_1(x)+f_2(y)}.$$

We can implement the same ansatz as we have done previously by looking for a function $M(H,x,p_x)$ which satisfies

$$\{H,M\}=\frac{1}{f_1(x)+f_2(y)}. \tag{11}$$

The condition has the form

$$(-v_1'(x)+f_1'(x)H)\frac{\partial M}{\partial p_x}+2p_x\frac{\partial M}{\partial x}=1. \tag{12}$$

Assuming that $|v_1'|+|f_1'|>0$, we see that this equation has the solution

$$M(H,L_2,p_x)=\int U'^{-1}dQ,$$

where

$$Q=p_x,\quad L_2=v_1(x)-f_1(x)H+p_x^2,\quad U(x)=-v_1(x)+f_1(x)H+L_2.$$

[We consider $U'^{-1}=dx/dU$ to be a function of $U=Q^2$. An arbitrary function $f(L_1,L_2)$ can be added to the integral, but this makes no difference since $L_1=H$ and L_2 are invariants.] There is a similar condition for the function $N(H,L_2,y,p_y)$. The new invariant is $L_3=N-M$. It is straightforward to verify the condition

$$\{L_2,L_3\}=1. \tag{13}$$

Indeed, $\{L_2,M\}=f_2/(f_1+f_2)$, $\{L_2,N\}=-f_1/(f_1+f_2)$. This implies that the set L_1,L_2,L_3 is functionally independent.

Similarly, we can construct functions $M(H,x,p_x),N(H,y,p_y)$ that satisfy

$$\{H,M\}=\frac{f_1(x)}{f_1(x)+f_2(y)},\quad \{H,N\}=\frac{-f_2(y)}{f_1(x)+f_2(y)}. \tag{14}$$

Assuming that $|v_i'|+|f_i'|>0$ for $i=1,2$, we see that these equations have the solutions

$$M(H,L_2,p_x)=\int f_1(x)U_1'^{-1}dQ,\quad N(H,L_2,p_y)=-\int f_2(y)U_2'^{-1}dQ,$$

where

$$U_i=-v_i+f_iH+L_2.$$

Setting $L_4=N-M$, we see that L_4, not an invariant, satisfies

$$\{H,L_4\}=1,\quad \{L_2,L_4\}=0. \tag{15}$$

Let us illustrate what can happen with some examples.

(1) We choose parabolic coordinates in Euclidean space[22] $x'=1/2(\xi^2-\eta^2)$, $y'=\xi\eta$. First consider the parabolic-separable Hamiltonian

$$H=L_1=\frac{p_\xi^2+p_\eta^2+\xi}{\xi^2+\eta^2}. \tag{16}$$

We can immediately associate with this the extra invariant

$$L_2=\frac{\eta^2 p_\xi^2-\xi^2 p_\eta^2+\eta^2\xi}{\xi^2+\eta^2}.$$

If we look for our functions $M(\xi,p_\xi)$ and $N(\eta,p_\eta)$, as before we obtain

$$M(\xi,p_\xi)=\frac{1}{4\sqrt{H}}\ln\left(\frac{\sqrt{H}p_\xi+\frac{1}{2}-\xi H}{-\sqrt{H}p_\xi+\frac{1}{2}-\xi H}\right),$$

$$N(\eta,p_\eta)=\frac{1}{4\sqrt{H}}\ln\left(\frac{\sqrt{H}\eta+p_\eta}{\sqrt{H}\eta-p_\eta}\right).$$

If we now consider the constant $\cosh(4(M-N)\sqrt{H})$, we find that it can be written in the form

$$4\cosh(4(M-N)\sqrt{H})=\frac{L_3^2 H}{(1-4HL_2)L_2},$$

where

$$L_3=\frac{2\xi\eta}{\xi^2+\eta^2}(p_\xi^2+p_\eta^2)-2p_\xi p_\eta+\frac{\eta(\xi^2-\eta^2)}{\xi^2+\eta^2} \tag{17}$$

is an additional invariant quadratic in the canonical momenta. This is a special case of a more general example in Ref. 23.

(2) Consider the Hamiltonian in Cartesian coordinates

$$H=p_x^2+p_y^2+\frac{x}{\sqrt{x^2+y^2}}. \tag{18}$$

In parabolic coordinates this Hamiltonian has the form

$$H=L_1=\frac{p_\xi^2+p_\eta^2+\xi^2-\eta^2}{\xi^2+\eta^2}.$$

The second-order invariant associated with this separation is

$$L_2=\frac{\xi^2 p_\eta^2-\eta^2 p_\xi^2-2\xi^2\eta^2}{\xi^2+\eta^2}.$$

The additional invariant calculated by our method is given by

$$L_3=\frac{\operatorname{arccosh}([(H-1)\xi^2+p_\xi^2]/[(H-1)\xi^2-p_\xi^2])}{\sqrt{H-1}}+\frac{\operatorname{arccosh}([(H+1)\eta^2+p_\eta^2]/[(H+1)\eta^2-p_\eta^2])}{\sqrt{H+1}}, \tag{19}$$

which is clearly transcendental.

(3) If we consider the Hamiltonian

$$H=p_x^2+p_y^2+ib(x+iy), \tag{20}$$

then using the semihyperbolic coordinates[22]

$$x+iy=i(u+w), \quad x-iy=(-i/2)(u-w)^2$$

and applying our construction, we find

$$\frac{\exp(M-N)-i}{\exp(M-N)+i}=-i\frac{\sqrt{b-iX}}{\sqrt{b+iX}},$$

thus giving rise to the additional constant $X=p_x+ip_y$.

(4) Let us now look at an example of a potential where our construction yields elliptic integrals. We consider the potential $V=2x+\beta/y^2$. If we carry out the construction using parabolic coordinates $x=(\frac{1}{2})(\xi^2-\eta^2)$, $y=\xi\eta$, then the functions M and N are given by the integrals

$$M=\frac{1}{2}\int\frac{\xi d\xi}{\sqrt{-\xi^6+H\xi^4+L\xi^2-\beta}}, \quad N=\frac{1}{2}\int\frac{\eta d\eta}{\sqrt{\eta^6+H\eta^4+L\eta^2-\beta}},$$

where L is the quadratic constant associated with the separation of variables in parabolic coordinates. If we change variables according to $u=\xi^2$, $v=-\eta^2$, then both M and N are given by integrals of the form

$$I=\frac{1}{2}\int\frac{d\lambda}{\sqrt{(a-\lambda)(b-\lambda)(c-\lambda)}},$$

where $\lambda=u,v$ and

$$abc=-\beta, \quad L=ab+bc+ac, \quad H=a+b+c.$$

There are a variety of ways of evaluating elliptic integrals of this type. We recall that all our considerations are in the complex domain. As an example, we can choose to use the complex equivalent of the integral

$$\int_{-\infty}^{u}\frac{dx}{\sqrt{(a-x)(b-x)(c-x)}}=\frac{2}{\sqrt{a-c}}F(\alpha,p),$$

valid for $a>b>c\geqslant u$ and for which

$$\sqrt{\frac{a-c}{a-u}}=\sin\alpha=\mathrm{sn}(A,p), \quad p=\sqrt{\frac{a-b}{a-c}}.$$

Then if we calculate $\mathrm{sn}^2(\sqrt{a-c}(M-N),p)$ using the addition formulas for elliptic functions we obtain

$$\mathrm{sn}^2(\sqrt{a-c}(M-N),p)=\frac{c-a}{c+b+L_1},$$

where L_1 is the second quadratic constant associated with this super-integrable system. Because of the various ways of evaluating elliptic integrals, there are a number of ways of uncovering the presence of L_1.

In analogy with the constructions (5)–(7), we can find Riemannian spaces and potentials with polynomial invariants of arbitrarily high order. Set

$$x=P_n\left(\frac{U+A}{\alpha+\beta H}\right), \quad A=\delta+\phi H-L_2, \tag{21}$$

where P_n is a polynomial of order n and α,β,δ,ϕ are constants. Then there exists a function F_n, inverse to P_n, i.e., $F_n(P_n(y))=y$, such that

$$U=(\alpha+\beta H)F_n(x)-\delta-\phi H+L_2,$$

and $v_1(x)=-\alpha F_n(x)+\delta$, $f_1(x)=\beta F_n(x)-\phi$, where $(\alpha+\beta H)^n M(x,p_x)$ is a polynomial in the momenta. The Cartesian coordinate constructions (5)–(7) correspond to the special case $\beta=0$.

The solution of the equation (11) can be understood in a more general context. We have the dual relations

$$x=F(U-L_2,H), \quad U(x,H)=-v_1(x)+f_1(x)H+L_2, \quad U_x\neq 0. \tag{22}$$

(Since U and L_2 occur only as $U-L_2$, we will, without loss of generality, set $L_2=0$ in the theoretical developments to follow, and then replace U by $U-L_2$ in the examples.) Thus we have

$$1=F_U U_x, \quad F_U U_H+F_H=0.$$

The condition that $U(x,H)$ is linear in H, i.e., $U_{HH}=0$, leads to the following necessary and sufficient conditions that the function $x=F(U,H)$ correspond to an invariant M on a Riemannian manifold with potential:

$$F_{HH}F_U^2-2F_{UH}F_UF_H+F_{UU}F_H^2=0, \quad F_U\neq 0. \tag{23}$$

This equation admits an infinite dimensional conformal symmetry group. Indeed if $V=F(U,H)$ is a solution, then $G(V)$ is also a solution, for *any* nonconstant function G. Also, this group contains the subgroup of inhomogeneous affine symmetries: if $F(U,H)$ is a solution, then so is $F([a_{11}U+a_{12}H++a_{13}]/A,[a_{21}U+a_{22}H+a_{23}+a_{23}]/A)$, where a_{ij} are constants, $\det(a_{ij})\neq 0$ and

$$A=a_{31}U+a_{32}H++a_{33}.$$

Note that the function $V_1=(U+\delta+\phi H)/(\alpha+\beta H)$ satisfies (23), so any function of V_1 must also satisfy the requirement. This puts (21) in the proper context. A more general solution is $V_2=(U+\phi H+\delta)/(\alpha U+\beta H+\gamma)$, where again any function of V_2 also satisfies the requirement. Equation (23) also occurs in the theory of level sets, used in computational geometry and computer vision,[24] since it describes the family of functions F whose level sets are always straight lines in the (U,H) plane.

We have seen that the construction (21) always leads to a polynomial invariant L_3, up to multiplication by a polynomial in H and L_2. In fact these are the *only* polynomial invariants L_3 that can be constructed directly from the integration. This follows from the following theorem.

Theorem 1: *The function $F(U,H)$ with $F_U\neq 0$ is a solution of Eq. (21) with polynomial dependence on U if and only if it is of the form*

$$F(U,H)=P\left(\frac{U+\alpha H+\beta}{\gamma H+\delta}\right),$$

where P is a (nonconstant) polynomial and $\alpha,\beta,\gamma,\delta$ are constants with $|\gamma|^2+|\delta|^2>0$.

Proof: Let

$$F=a_0(H)U^N+a_1(H)U^{N-1}+\cdots+a_{N-1}(H)U+a_N(H)$$

be a solution of (21) with $N\geqslant 1$ and $a_0\neq 0$. Substituting this expression into (21) and equating the coefficient of U^{3N-2} on both sides of the resulting expression, we find the condition $a_0''a_0=((N+1)/N)a_0'^2$, so $a_0(H)=(\gamma H+\delta)^{-N}$. Now we make the change of variables $\tilde{U}=U/(\gamma H+\delta)$, $\tilde{H}=(\phi H+{}_\rho)/(\gamma H+\delta)$, where $\phi\delta-\gamma\rho\neq 0$. It follows that

$$F=\tilde{U}^N+\tilde{a}_1(\tilde{H})\tilde{U}^{N-1}+\cdots+\tilde{a}_{N-1}(\tilde{H})\tilde{U}+\tilde{a}_N(\tilde{H})$$

in the new coordinates, and F is a solution of

$$F_{\tilde{H}\tilde{H}}F_{\tilde{U}}^2-2F_{\tilde{U}\tilde{H}}F_{\tilde{U}}F_{\tilde{H}}+F_{\tilde{U}\tilde{U}}F_{\tilde{H}}^2=0. \tag{24}$$

Substituting the polynomial into (24) and equating coefficients of $\tilde{U}^{3N-3}$, we find $\tilde{a}_1''N^2=0$ or $\tilde{a}_1=\alpha_1\tilde{H}+\beta_1$. Using this information, we return to our original expression for the polynomial and make a new change of variables of the form

$$\tilde{U}=\frac{U+\alpha H+\beta}{\gamma H+\delta},\quad \tilde{H}=\frac{\chi H+\zeta}{\gamma H+\delta}, \tag{25}$$

where $\chi\delta-\gamma\zeta\neq 0$, and α, β are chosen such that the transformed coefficient of $\tilde{U}^{N-1}$ vanishes. In these variables

$$F=\tilde{U}^N+\tilde{a}_2(\tilde{H})\tilde{U}^{N-2}+\cdots+\tilde{a}_{N-1}(\tilde{H})\tilde{U}+\tilde{a}_N(\tilde{H}).$$

We substitute this expression into (24), and equating coefficients of $\tilde{U}^{3N-4}$ we find $\tilde{a}_2''=0$, so $\tilde{a}_2$ is a polynomial in $\tilde{H}$ of order $\leqslant 1$. Proceeding in this fashion to equate coefficients of $\tilde{U}^{3N-s}$ for $s=5,6,\ldots$ in order, we find that the first occurence of $\tilde{a}_k, k\geqslant 3$ in this sequence of equations takes the form $\tilde{a}_k''=p_k(\tilde{a}_2,\ldots,\tilde{a}_{k-1})$ where p_k is a polynomial of order 3 at most. It follows by induction on k that each $\tilde{a}_k$ is a polynomial in $\tilde{H}$.

At this point we have shown that F is a polynomial in both $\tilde{U}$ and in $\tilde{H}$. Let $\tilde{H}^M$ be the maximal power of $\tilde{H}$ that occurs in F. If $M=0$, we are done. Assume $M\geqslant 1$. If we use the argument of the first paragraph of this proof with $\tilde{U}$ and $\tilde{H}$ interchanged, we see that the coefficient of $\tilde{H}^M$ in F must take the form $\alpha_0/(\beta_1\tilde{U}+1)$ with $\alpha_0\neq 0$. Since F is a polynomial in $\tilde{U}$ we must have $\beta_1=0$.

Thus

$$F=\tilde{U}^N+\tilde{a}_2(\tilde{H})\tilde{U}^{N-2}+\cdots+\tilde{a}_{N-1}(\tilde{H})\tilde{U}+\alpha_0\tilde{H}^M.$$

Now substitute this expression into (24) and equate coefficients of $\tilde{U}^n\tilde{H}^m$ where $n+m$ is maximal. Suppose $N\geqslant M$. The highest power term in $F_{\tilde{H}\tilde{H}}F_{\tilde{U}}^2$ is $\alpha_N M(M-1)N^2\tilde{H}^{M-2}\tilde{U}^{2N-2}$. The highest power term in $F_{\tilde{U}\tilde{U}}F_{\tilde{H}}^2$ is $\alpha_N^2N(N-1)M^2\tilde{H}^{2M-2}\tilde{U}^{N-2}$, but this is of lower order. The highest power term in $2F_{\tilde{U}\tilde{H}}F_{\tilde{H}}F_{\tilde{U}}$ is $t=2\alpha_N a_{N_1,M_1}N_1M_1NM\tilde{U}^{N_1+N-2}\tilde{H}^{M_1+M-2}$ where a_{N_1,M_1} is the coefficient of $\tilde{U}^{N_1}\tilde{H}^{M_1}$ in F. Here $N_1<N, M_1<M$. If $N>N_1+M_1$, then the highest power term is the coefficient of $\tilde{H}^{M-2}\tilde{U}^{2N-2}$, so $M=1$. If $N\leqslant N_1+M_1$, then $t=0$, so $a_{N_1,M_1}=0$. Thus, the only possiblity is $M=1$, so

$$F=\tilde{U}^N+\alpha_2\tilde{U}^{N-2}+\cdots+\alpha_{N-1}\tilde{U}+\alpha_N\tilde{H}.$$

Substituting this expression into the differential equation we see that $F_{\tilde{U}\tilde{U}}=0$, or $F=\tilde{U}+\alpha_N\tilde{H}$. But this is impossible since $N=1$ and the coefficient of $\tilde{U}^{N-1}$ must be 0. Hence F depends only on $\tilde{U}$. There is a similar argument for the case $M>N$. **QED**

If we limit our search for potentials to a space in which $U_H=f_1(x)$ is prescribed, then the general conditions (23) are replaced by

$$F_H+f_1(F)F_U=0, \quad F_U\neq 0. \tag{26}$$

Equation (26) admits the complete integral

$$F(U,H,\alpha,\beta)=f_1^{-1}\left(\frac{U+\alpha}{H+\beta}\right),$$

where f_1^{-1} is the function inverse to f_1. From this one can use standard techniques (method of characteristics, envelopes of solutions) from the theory of quasilinear first-order partial differential equations to construct solutions of (26) that satisfy particular initial conditions or that depend on arbitrary functions (Ref. 25, Chap. II or Ref. 26, Sec. 88).

Note: Standard Hamilton–Jacobi theory gives essentially these same constants of the motion, but from a different viewpoint.[1] Our expression for L_3, for example, is

$$L_3=\int U_x'^{-1}dp_x-\int U_y'^{-1}dp_y=M-N,$$

where $U_x=-v_1(x)+f_1(x)H+L_2$, etc. Standard Hamilton–Jacobi theory gives

$$L_3=\frac{1}{2}\int\frac{dx}{\sqrt{-v_1+f_1H+L_2}}-\frac{1}{2}\int\frac{dy}{\sqrt{-v_2+f_2H-L_2}}=\tilde{M}-\tilde{N}.$$

In the standard theory $\tilde{M}=\tilde{M}(H,L_2,x)$, etc., whereas in our approach $M=M(H,L_2,p_x)$, etc. In both cases the condition (12) is satisfied. Our approach makes it easier in some cases to determine if polynomial invariants exist. It also points out the bracket relations between M,N and the operators L_j defining the separation, e.g., (11).

Examples abound of spaces for which these constructions apply. We illustrate this with a family of surfaces in Minkowski space: $ds^2=dz^2-dy^2-dx^2$. The surfaces involve a horispherical coordinate ξ and take the form

$$\mathbf{X}(t,\xi)=(x,y,z)=(2t\xi,g(t)+(\xi^2-1)t,g(t)+(\xi^2+1)t). \tag{27}$$

The metric on the surface is

$$ds^2=4[tg'(t)dt^2-t^2d\xi^2]=4t^2[d\rho^2-d\xi^2]=(f(\rho)+1)[d\rho^2-d\xi^2],$$

where $(d\rho/dt)^2=g'(t)/t^2$, and we can construct a polynomial invariant for the surface (and for an appropriate added potential) provided that the function $t^2=F(\rho)$ has a polynomial inverse function, i.e., $\rho=G(t^2)$ where G is a polynomial. Clearly $g'(t)=4t^4G'(t^2)^2$ and any polynomial G will determine a surface with a polynomial invariant. For example, choose $G(t^2)=\frac{1}{2}t^4+t^2$. Then we can take $g(t)=\frac{4}{9}t^9+\frac{8}{7}t^7+\frac{4}{5}t^5$ and $\rho(t)=\frac{1}{2}t^4+t^2$. The resulting M will be third-order polynomial in p_ξ and p_ρ. Similarly, we can determine a potential term $v(\rho)$ with $v'\neq 0$ such that N is a polynomial in p_ξ and p_ρ.

Rather than make either of the choices p_x or x for the independent variable in (12) we could choose some other function $w(x,p_x)$, adapted to the specific problem at hand. For example, let us take $w(x,p_x)=r'(x)p_x$ for some given function r, and require $M=M(H,L_2,w)$. Solving (12) in these variables we find

$$M=\int \frac{dr(x)}{dw^2}dw, \tag{28}$$

where

$$w^2=U=r'(x)^2p_x^2=r'(x)^2(-v_1+f_1H+L_2), \quad r(x)=F(U,H,L_2).$$

This approach will work even if v_1 and f_1 are constants; it is guaranteed to yield a polynomial invariant if we require

$$r=P_n\left(\frac{U+\alpha_1H+\alpha_2L_2+\alpha_3}{\alpha_4H+\alpha_5L_2+\alpha_6}\right), \tag{29}$$

where P_n is a polynomial of order n and the α_i are constants. Then there exists a function F_n, inverse to P_n, such that

$$U=(\alpha_4H+\alpha_5L_2+\alpha_6)F_n(r)-(\alpha_1H+\alpha_2L_2+\alpha_3)=r'^2(-v_1+f_1H+L_2).$$

Equating coefficients of L_2 we find the condition $r'(x)^2=\alpha_5F_n(r)-\alpha_2$ and we can solve for $r(x)$ by quadratures. Equating coefficients of H and the constant term, we obtain expressions for f_1 and v_1:

$$f_1(x)=\frac{\alpha_4F_n(r)-\alpha_1}{\alpha_5F_n(r)-\alpha_2}, \quad v_1(x)=\frac{\alpha_3-\alpha_6F_n(r)}{\alpha_5F_n(r)-\alpha_2}.$$

It follows that $(\alpha_4H+\alpha_5L_2+\alpha_6)^nM(rp_x)$ is a polynomial in the momenta.

IV. LIE FORM AND NONORTHOGONAL SEPARATION IN TWO DIMENSIONS

We know that if a Hamiltonian

$$H=\sum_{i,j=1}^{2} g^{ij}p_ip_j$$

admits a constant of the motion L that is quadratic in the momenta

$$L=\sum_{i,j=1}^{2} a^{ij}p_ip_j, \quad \{H,L\}=0, \tag{30}$$

and if the roots of the determinant $|a^{ij}-\lambda g^{ij}|$ are distinct, then the eigenforms define new (separable) variables ρ, μ and the Hamiltonian can be written in Liouville form

$$H=\frac{p_\rho^2+p_\mu^2}{f(\rho)+g(\mu)}.$$

However, it may be that the roots of this determinant are equal. In this case H cannot be put into Liouville form, but rather Lie form, which for a suitable choice of variables (nonseparable) is

$$H=\frac{p_xp_y}{x+B(y)}. \tag{31}$$

The associated quadratic constant of the motion is

$$L=p_x^2-2yH. \tag{32}$$

We now ask the question: When the roots of L are equal, how can we calculate the third invariant? We are interested in the the same question when a potential is added to the Hamiltonian. These questions can readily be answered. Indeed if we look for a function $N(H,L,y,p_y)$ that is in involution with H, we obtain the equation

$$(x+B(y))N_y+p_yB'(y)N_{p_y}=0. \tag{33}$$

If we solve (31) and (32) for x and p_x in terms of the variables H, L, y and p_y, we obtain

$$p_x=\sqrt{L+2yH}, \quad x=\frac{p_y}{H}\sqrt{L+2yH}-B(y).$$

The equation (33) for N then has the form

$$\frac{\sqrt{L+2yH}}{HB'(y)}N_y+N_{p_y}=0.$$

From this condition a second invariant can be readily obtained in the form

$$L'=H\int\frac{B'(y)}{\sqrt{L+2yH}}dy-p_y. \tag{34}$$

We now extend these considerations by considering the possibility of adding a potential. If we do this and have an extra quadratic constant, then H and L have the forms

$$H=\frac{p_xp_y+\frac{1}{2}K(y)}{x+B(y)}+\frac{1}{2}U'(y), \quad L=p_x^2-2yH+U(y). \tag{35}$$

Solving (35) for p_x and x gives

$$p_x=\sqrt{L-U(y)+2yH}, \quad x=\frac{p_y\sqrt{L-U(y)+2yH}+\frac{1}{2}K(y)}{H-\frac{1}{2}U'(y)}-B(y).$$

Then the equation for N has the form

$$\begin{aligned}2\sqrt{L-U(y)+2yH}(2H-U'(y))N_y+[-2U''(y)\sqrt{L-U(y)+2yH}p_y+B'(y)U'(y)^2\\ +4B'(y)H^2-U''(y)K(y)-4B'(y)U'(y)H+K'(y)U'(y)-2K'(y)H]N_{p_y}=0.\end{aligned} \tag{36}$$

This equation can, in principle, be solved directly. In fact, for suitable redefinition of the variables $y\to Y$, $p_y\to P_y$, Eq. (36) can be put in the form

$$N_Y+(P_Y+s(Y))N_{P_Y}=0 \tag{37}$$

that can be solved by the further transformation

$$P_{Y'}=P_Y+t(Y), \quad Y'=Y.$$

Then, provided that

$$t'(Y)-t(Y)+s(Y)=0,$$

(37) reduces to

$$N_{Y'}+P_{Y'}N_{P_{Y'}}=0.$$

From this we immediately deduce an extra constant of the motion of the form

$$L'=e^{Y'}/P_{Y'}. \tag{38}$$

The equation for $t(Y)$ has the solution

$$t(Y)=e^{Y}\int^{Y}e^{-u}s(u)du.$$

There is one remaining possibility for a quadratic constant of the motion (30) in two dimensions: the constant may be associated with *nonorthogonal* separation of variables. In two dimensions there is only one case: separation in light cone (null) coordinates.[27] For this case the Hamiltonian takes the form

$$H=p_zp_{\bar{z}}+f(\bar{z}),$$

and there is a Killing vector p_z, so p_z^2 is a second-order constant of the motion. In addition there is a quadratic constant

$$L=Mp_z+\frac{i}{2}\int\bar{z}\frac{df}{d\bar{z}}d\bar{z}.$$

Thus we have answered the following questions.

(1) If a Hamiltonian with potential admits a quadratic constant of the motion in two dimensions how does one calculate the third constant?
(2) A subset of problem 1 is when we require separation only and ask to calculate the third constant.

V. SYSTEMS IN THREE DIMENSIONS

Let us now look at how the orthogonal separation of variable considerations extend to three dimensions. If we have a general separable coordinate system in three dimensions, we could take the Hamiltonian to be[20,28,29]

$$H=L_1=\frac{g_2-g_3}{\Phi}(p_{x_1}^2+v_1(x_1))+\frac{g_3-g_1}{\Phi}(p_{x_2}^2+v_2(x_2))+\frac{g_1-g_2}{\Phi}(p_{x_3}^2+v_3(x_3)), \tag{39}$$

where $g_i=g_i(x_i), f_i=f(x_i)$ and Φ is the determinant of the Stäckel matrix

$$\begin{pmatrix}1 & f_1 & g_1\\ 1 & f_2 & g_2\\ 1 & f_3 & g_3\end{pmatrix}. \tag{40}$$

This automatically gives us two more invariants:

$$L_2=\frac{f_3-f_2}{\Phi}(p_{x_1}^2+v_1(x_1))+\frac{f_1-f_3}{\Phi}(p_{x_2}^2+v_2(x_2))+\frac{f_2-f_1}{\Phi}(p_{x_3}^2+v_3(x_3)), \tag{41}$$

$$L_3=\frac{f_2g_3-f_3g_2}{\Phi}(p_{x_1}^2+v_1(x_1))+\frac{f_3g_1-f_1g_3}{\Phi}(p_{x_2}^2+v_2(x_2))+\frac{f_1g_2-f_2g_1}{\Phi}(p_{x_3}^2+v_3(x_3)). \tag{42}$$

We need to find an additional two invariants, such that the five form a functionally independent set.

If we look for a function M_1 such that

$$\{H,M_1\}=\frac{g_2-g_3}{\Phi}, \tag{43}$$

then this function satisfies the equation

$$2p_{x_1}\partial_{x_1}M_1+[-v_1'(x_1)+f_1'H+g_1'L_2]\partial_{p_{x_1}}M_1=1, \tag{44}$$

which looks like the form we have been using in two dimensions. There are similar equations for the corresponding functions M_i for $i=2,3$. For $M_1(H,L_2,L_3,Q_1)$ with $Q_1=p_{x_1}$ this has the solution

$$M_1=\int U_1'^{-1}dQ_1,$$

where $U_1(x_1)=-v_1(x_1)+f_1H+g_1L_2+L_3$ and $L_3=v_1-f_1H-g_1L_2+p_{x_1}^2$. (Here, we consider $U_1'^{-1}=dx_1/dU_1$ to be a function of $U_1=Q_1^2$ to compute the integral. We also assume that $|v_1'|+|f_1'|+|g_1'|>0$.) The corresponding invariant that we can calculate from these three functions is $L_3'=M_1+M_2+M_3$. This is based on the obvious identity

$$(g_2-g_3)+(g_3-g_1)+(g_1-g_2)=0.$$

Note: As in the two dimensional case, the solution of the equation (44) can be understood in a more general context. We have the dual relations

$$x=F(U-L_3,H,L_2),\quad U(x,H,L_2)=-v_1(x)+f_1(x)H+g_1(x)L_2+L_3, \tag{45}$$

where $U_x\neq 0$. (Since U and L_3 occur only as $U-L_3$ we can, without loss of generality, set $L_3=0$ in the equations immediately following, and then replace U by $U-L_3$ in the examples.) Thus we have

$$1=F_UU_x,\quad F_UU_H+F_H=0,\quad F_UU_{L_2}+F_{L_2}=0.$$

The condition that $U(x,H,L_2)$ is linear in H and L_2, i.e., $U_{HH}=U_{L_2L_2}=U_{HL_2}=0$, leads to the following necessary and sufficient conditions that the function $x=F(U,H,L_2)$ correspond to an invariant M_1 on a Riemannian manifold with potential:

$$\begin{aligned}
&F_{HH}F_U^2-2F_{UH}F_UF_H+F_{UU}F_H^2=0,\quad F_U\neq 0,\\
&F_{UU}F_{L_2}^2-2F_{L_2U}F_{L_2}F_U+F_{L_2L_2}F_U^2=0,\\
&F_{L_2L_2}F_H^2-2F_{HL_2}F_HF_{L_2}+F_{HH}F_{L_2}^2=0.
\end{aligned} \tag{46}$$

These equations admit an infinite dimensional conformal symmetry group. Indeed, if $V=F(U,H,L_2)$ is a solution, then $G(V)$ is also a solution, for *any* nonconstant function G. Also, this group contains the subgroup of inhomogeneous affine symmetries: if $F(U,H,L_2)$ is a solution, then so is $F([a_{11}U+a_{12}H+a_{13}L_2+a_{14}]/A,[a_{21}U+a_{22}H+a_{23}L_2+a_{24}]/A,[a_{31}U+a_{32}H+a_{33}L_2+a_{24}]/A)$ where a_{ij} are constants, $\det(a_{ij})\neq 0$ and

$$A=a_{41}U+a_{42}H+a_{43}L_2+a_{44}.$$

As in the two dimensional case, the only polynomial functions F of U are of a very special form.

Theorem 2: *The function $F(U,H,L_2)$ with $F_U \neq 0$ is a solution of Eqs. (46) with polynomial dependence on U if and only if it is of the form*

$$F(U,H,L_2)=P\left(\frac{U+\alpha_1 H+\alpha_2 L_2+\beta}{\gamma_1 H+\gamma_2 L_2+\delta}\right),$$

where P is a (nonconstant) polynomial and $\alpha_i,\beta,\gamma_i,\delta$ are constants with $|\gamma_1|^2+|\gamma_2|^2+|\delta|^2>0$.

Proof: The proof is similar to that of Theorem 1. It follows from this theorem and the first two equations in (46) that

$$F=P^{(1)}(U^{(1)},L_2)=P^{(2)}(U^{(2)},H),$$

where the $P^{(i)}$ are polynomials of strict order N in their first arguments and

$$U^{(1)}=\frac{U+\alpha_1^{(1)}L_2H+\beta^{(1)}L_2}{\gamma_1^{(1)}L_2H+\delta^{(1)}L_2} \quad U^{(2)}=\frac{U+\alpha_1^{(2)}HL_2+\beta^{(2)}H}{\gamma_1^{(2)}HL_2+\delta^{(2)}H}.$$

Furthermore, the coefficients of the $N-1$-st power of their first arguments can be asumed to be zero. Comparing the coefficients of the highest power U^N of U in F, we see that this coefficient must be of the form

$$(\gamma_1 H+\gamma_2 L_2+\gamma_3 HL_2+\delta)^{-N},$$

where now the γ_i,δ are constants. Substituting this into the third equation in (46) and equating coefficients of U^{3N}, we see that $\gamma_3=0$.

Equating the coefficients of U^{N-1} in the $P^{(i)}$ we see that

$$U^{(1)}=U^{(2)}=\tilde{U}=\frac{U+\alpha_1 H+\alpha_2 L_2+\phi HL_2+\beta}{\gamma_1 H+\gamma_2 L_2+\delta},$$

where the coefficients are constants. Then, substituting this result into the third equation again and comparing coefficients of U^{3N-1} we see that $\phi=0$. At this point we have shown that $F=P(\tilde{U},H,L_2)$ where P is a polynomial of order exactly N in its first argument. The proof that P is independent of its second and third arguments follows exactly as in the last part of the proof of Theorem 1. **QED**

If we limit our search for potentials to a space in which $U_H=f_1(x),U_{L_2}=g_1(x)$ are prescribed, then the general conditions (46) are replaced by

$$F_H+f_1(F)F_U=0, \quad F_{L_2}+g_1(F)F_U=0, \quad F_U\neq 0. \tag{47}$$

From this one can use standard techniques (method of characteristics, envelopes of solutions) from the theory of systems of quasilinear first order partial differential equations to construct solutions of (47) that satisfy particular initial conditions or that depend on arbitrary functions.

The invariant $L_3'=M_1+M_2+M_3$ also commutes with L_2. Indeed, from the fact that

$$\partial_{x_1}L_2=\frac{f_3-f_2}{\Phi}(v_1'-f_1'H-g_1'L_2)$$

we can verify that (44) implies

$$\{L_2,M_1\}=\frac{f_3-f_2}{\Phi}. \tag{48}$$

The corresponding conditions are satisfied by M_2 and M_3. Then the fact that $\{L_2,L_3'\}=0$ is implied by the obvious identity

$$(f_3-f_2)+(f_1-f_3)+(f_2-f_1)=0.$$

Finally, from the fact that

$$\partial_{x_1}L_3=\frac{f_2g_3-f_3g_2}{\Phi}(v_1'-f_1'H-g_1'L_2)$$

we can verify that (44) implies

$$\{L_3,M_1\}=\frac{f_2g_3-f_3g_2}{\Phi}. \tag{49}$$

The corresponding conditions are satisfied by M_2 and M_3. Then the fact that $\{L_3,L_3'\}=1$ is implied by the identity

$$(f_2g_3-f_3g_2)+(f_3g_1-f_1g_3)+(f_1g_2-f_2g_1)=\Phi. \tag{50}$$

Similarly, we can define a new invariant L_2' by requiring that a new function M_1 satisfy

$$\{L_1,M_1\}=\frac{g_1(g_2-g_3)}{\Phi}, \tag{51}$$

with analogous conditions for M_2 and M_3. For $M_1(H,L_2,L_3,Q_1)$ with $Q_1=p_{x_1}$ this has the solution

$$M_1=\int g_1U_1'^{-1}dQ_1,$$

where $U_1(x_1)=-v_1(x_1)+f_1H+g_1L_2+L_3$.

[Note that for M_1 to be a polynomial in p_x,p_y,p_z we must have $g_1(F)F_U$ a polynomial in U. If $g_1'=0$, this reduces to requiring F to be a polynomial in U. If $g_1'\neq 0$, we can replace the variable x by $\tilde{x}_1=r(x_1)=\int g_1(x_1)dx_1$ with $\tilde{x}_1=G(U,H,L_2,L_3)$. Then $g_1(F)F_U=G_U$ and our original analysis goes through with F replaced by G. It is guaranteed to yield a polynomial invariant if we require

$$r=P_n\left(\frac{U+\alpha_1H+\alpha_2L_2+\alpha_3L_3+\alpha_4}{\alpha_5H+\alpha_6L_2+\alpha_7}\right),\quad g_1=r'(x_1), \tag{52}$$

where P_n is a polynomial of order n and the α_i are constants. Then there exists a function F_n, inverse to P_n, such that

$$U=(\alpha_5H+\alpha_6L_2+\alpha_7)F_n(r)-(\alpha_1H+\alpha_2L_2+\alpha_3L_3+\alpha_4)=-v_1+f_1H+g_1L_2+L_3.$$

Equating coefficients of L_2 we find the condition $r'=\alpha_6F_n(r)-\alpha_2$ and we can solve for $r(x_1)$ by quadratures. Equating coefficients of H, L_3 and the constant term, we find $\alpha_3=-1$ and

$$f_1(x)=\alpha_5F_n(r)-\alpha_1,\quad g_1(x)=\alpha_6F_n(r)-\alpha_2,\quad v_1(x)=\alpha_4-\alpha_7F_n(r).$$

It follows that $(\alpha_5H+\alpha_6L_2+\alpha_7)^nM_1$ is a polynomial in the momenta.]

The corresponding invariant that we can calculate from these three functions is $L_2'=M_1+M_2+M_3$. This is based on the obvious identity

$$g_1(g_2-g_3)+g_2(g_3-g_1)+g_3(g_1-g_2)=0.$$

Then it follows that

$$\{L_2,M_1\}=\frac{g_1(f_3-f_2)}{\Phi},\quad \{L_3,M_1\}=\frac{g_1(f_2g_3-f_3g_2)}{\Phi},$$

with analogous results for M_2, M_3. Thus, from the definition of Φ we see that $\{L_2,L_2'\}=1$.

Finally, we define a function $L_1'=M_1+M_2+M_3$ by requiring

$$\{L_1,M_1\}=\frac{f_1(g_2-g_3)}{\Phi},\tag{53}$$

with similar conditions for M_2 and M_3. For $M_1(H,L_2,L_3,Q_1)$ with $Q_1=p_{x_1}$ this has the solution

$$M_1=\int f_1U_1'^{-1}dQ_1.$$

Then it follows that

$$\{L_2,M_1\}=\frac{f_1(f_3-f_2)}{\Phi},\quad \{L_3,M_1\}=\frac{f_1(f_2g_3-f_3g_2)}{\Phi},$$

with analogous relations for M_2 and M_3.

In summary, all brackets between the six functions L_i,L_i' are zero except that

$$\{L_3,L_3'\}=\{L_2,L_2'\}=\{L_1,L_1'\}=1.\tag{54}$$

Thus the mapping $(x_1,x_2,x_3,p_{x_1},p_{x_2},p_{x_3})\to(L_1,L_2,L_3,L_1',L_2',L_3')$ is canonical.

Note: Standard Hamilton–Jacobi theory gives exactly these same constants of the motion, from a different viewpoint.[1] Our expression for L_3', for example, is

$$L_3'=\sum_j\int U_j'^{-1}dp_{x_j}=\sum_j M_j,$$

where $U_j=-v_j(x_j)+f_jL_1+g_jL_2+L_3$ and $U_j=p_{x_j}^2$. Standard Hamilton–Jacobi theory gives

$$L_3'=\frac{1}{2}\sum_j\int\frac{dx_j}{\sqrt{-v_j+f_jL_1+g_jL_2+L_3}}=\sum_j\tilde{M}_j.$$

In the standard theory $\tilde{M}_j=\tilde{M}_j(L_1,L_2,L_3,x_j)$, whereas in our approach $M_j=M_j(L_1,L_2,L_3,p_{x_j})$. In both cases the condition (44) is satisfied. Our approach makes it straightforward to determine exactly when the L_i' are polynomials in the momenta p_{x_j}. It also points out the bracket relations between the M_i and the operators L_j defining the separation, e.g., (43), (48), (49), (51), and (53).

The generalization to n dimensions is straightforward.

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Conservation laws for a class of nonlinear equations with variable coefficients on discrete and noncommutative spaces

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The conservation laws for a class of nonlinear equations with variable coefficients on discrete and noncommutative spaces are derived. For discrete models the conserved charges are constructed explicitly. The applications of the general method include equations on quantum plane, supersymmetric equations for chiral and antichiral supermultiplets, auxiliary equations of integrable models which means various cases of nonlinear Toda lattice equations and anomalous diffusion equation. [DOI: 10.1063/1.1480449]

I. INTRODUCTION

Our aim is to present the procedure of derivation of the conservation laws and consequently the conserved charges for a certain class of nonlinear equations with variable coefficients. In the classical field theory the conserved currents and charges follow from the Noether theorem and are connected with the symmetry of the action. In the case of linear equations of motion with constant coefficients the construction of conserved currents by Takahashi and Umezawa method[1] can be applied.

In previous papers[2–5] we have extended this procedure to the linear equations on discrete and noncommutative spaces including quantum Minkowski[6–9] and braided linear spaces.[10,11] It appears, however, that we can consider in a similar way a wide class of equations with variable coefficients built within framework of any differential calculus with the Leibniz's rule for partial derivatives deformed via the transformation operator which is multiplicative and invertible. The range of admissible spaces includes the classical space–time with continuous coordinates, the discrete space, the mixed space with discrete and continuous coordinates, superspace including space–time and spinor coordinates, and quantum Minkowski and braided linear spaces (with q-Minkowski as a special case).

The equations we shall investigate have the variable coefficients which fulfill the corresponding restriction (3) including the conjugated derivatives. The possibility of derivation of the conservation laws for some equations with variable coefficients on noncommutative spaces was indicated earlier,[4,5] but the proposed conditions for coefficients were too strong to construct useful examples. In constrast the new condition (as we show explicitly in the applications) appears to be identical with the nonlinear equations of some of the integrable models for which we derive the conserved currents via the auxiliary linear equations with variable coefficients.

Resuming the proposed method can be applied to nonlinear models in two ways: namely, we can consider the equation with nonlinear term free from the derivatives (in form of the potential) or alternatively we investigate the auxiliary linear equations with variable coefficients for nonlinear integrable models.

The article is organized as follows: Sec. II contains the description of the investigated models and the derivation of the conservation laws. In Sec. III we extend the procedure to discrete and mixed discrete and continuous models, including both types of derivatives initial ∂ and its conju-

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gation $\partial^\dagger$. For this class of equations we add the construction of conserved charges following the classical method of integrating the time-component of the conserved current over the subspace excluding the time-coordinate. This result is due to the fact that for the discrete and classical differential calculi the definite integral over mentioned subspace is known to commute with time-derivative (71).

Section IV includes applications of the derived procedure. We start with a simple example of an equation of the second order with variable coefficients on quantum plane, then we consider the conserved currents and charges for a pair of chiral and antichiral supermultiplets on $D=4$, $N=1$ superspace connected via a nonlinear equation of motion. We also review the conservation laws and conserved charges for various cases of the nonlinear Toda lattice equation for which we use our results for mixed discrete and continuous spaces in order to write explicitly the conserved currents and charges. The section is closed with the derivation of the conservation law for the equation of anomalous diffusion.

II. NONLINEAR EQUATIONS WITH VARIABLE COEFFICIENTS AND THEIR CONSERVATION LAW

In the previous papers we discussed the conservation laws for linear equations with constant coefficients for discrete differential calculus[2,3] as well as for a wider category of equations acting on noncommutative spaces, namely on quantum Minkowski spaces[4,12] and the braided linear ones.[5,13,14]

Now we would like to present our results for an extended class of equations with variable coefficients of the form

$$\Lambda(\partial)\Phi=0, \tag{1}$$

$$\Lambda(\partial)=\Lambda_0+\sum_{l=1}^{N}\Lambda_{\mu_1\cdots\mu_l}\partial^{\mu_1}\cdots\partial^{\mu_l}, \tag{2}$$

where coefficients (may be matrices) fulfill the condition

$$\partial^{\dagger\,\mu_1}\Lambda_{\mu_1\cdots\mu_l}=0 \tag{3}$$

for $l=1,\ldots,N$ and with the conjugated derivative described below (30).

In addition we assume the coefficients to obey symmetry properties with respect to the permutation of indices. Their exact form is connected with the commutation relations in the algebra of partial derivatives. In the classical case this algebra is commutative, thus the coefficients for such models are fully symmetric with respect to permutation of the set of indices. In the sequel we describe the symmetry properties of the discussed equation for specific differential calculus.

We include into considerations the nonlinear equations provided the only nonlinear term does not depend on derivatives, which means

$$\Lambda_0=\Lambda_0(\Phi). \tag{4}$$

As will be shown, this class of equations contains some of the equations of motion for supersymmetric models in superfield formulation as well as auxiliary linear equations yielded by nonlinear integrable models as, for example, Toda lattice equations.

Our construction presented below in Propositions 2.1 and 2.2 holds for any differential calculus with the following deformation of Leibniz's rule:

$$\partial^i(fg)=(\partial^i f)g+(\zeta^i_j f)\partial^j g, \tag{5}$$

where ζ is the invertible transformation operator.

We shall now discuss the admissible differential calculi. They include classical, discrete, noncommutative and supersymmetric models described below.

A. Differential calculi with Leibniz's rule of the form (5)

Starting with the classical commutative differential calculus (for which ζ is the identity operator) we can also include the discrete differential calculus with derivatives defined by one of the formulas:

$$\partial^i f_k = (\zeta^i - 1) f_k = f_{k+1} - f_k, \tag{6}$$

$$\partial^i f_k = (x_{k+1} - x_k)^{-1} (\zeta^i - 1) f_k = (x_{k+1} - x_k)^{-1} (f_{k+1} - f_k), \tag{7}$$

where k denotes the position on the lattice in the direction i.

The first one is widely used in the discrete models and measures the difference between the values of the function between two points of the lattice in the given direction i while the second one (introduced in Refs. 2 and 3) is a quotient of the change of value of the function over the distance between the two neighboring points of the lattice taken in the direction i. Both types of the derivatives obey (5) with the transformation operator being the shift operator along the lattice in the direction i:

$$\zeta^i f_k = f_{k+1}, \tag{8}$$

where k in the above formula denotes the value of the ith coordinate of the point on the lattice.

It is clear that we can also include mixed models depending both on classical commutative derivatives with respect to continuous coordinates and discrete derivatives (6) or (7) with respect to lattice dimensions.

Similarly to the classical differential calculus, the algebra of discrete derivatives in the form (6) or (7) is commutative, thus we consider in these models equations with coefficients fully symmetric with respect to permutation of each of the sets of indices $(\mu_1, \ldots, \mu_l)$.

The Leibniz's rule of the form (5) is also characteristic for noncommutative spaces. We have checked[4,5] that for quantum Minkowski spaces and for braided linear spaces (including the q-Minkowski space) it is given by the formula (5) with transformation operators determined by their multiplicity property:

$$\zeta^i_j(fg) = (\zeta^i_k f)(\zeta^k_j g) \tag{9}$$

and the action on monomials of the first order:

$$\zeta^i_j x^k = R^{ik}_{aj} x^a - (RZ)^{ik}_j, \tag{10}$$

$$\zeta^i_j x_k = R^{li}_{kj} x_l. \tag{11}$$

The first of the above formulas is valid on the quantum Minkowski space and the second on the braided linear space with R being the matrices fulfilling the QYBE.[9–11] For quantum Minkowski spaces introduced by Podleś and Woronowicz the R matrix is self-invertible $R^2 = 1$ and for braided linear spaces developed by Majid it is bi-invertible:

$$(R^{-1})^{ij}_{kl} R^{kl}_{ab} = R^{ij}_{kl} (R^{-1})^{kl}_{ab} = \delta^i_a \delta^j_b, \tag{12}$$

$$\tilde{R}^{ib}_{al} R^{ak}_{jb} = R^{ib}_{al} \tilde{R}^{ak}_{jb} = \delta^i_j \delta^k_l. \tag{13}$$

Let us recall the algebra of partial derivatives for both cases:

$$\partial^l \partial^k = R^{lk}_{ij} \partial^i \partial^j, \tag{14}$$

$$\partial^l \partial^k = (R')^{lk}_{ij} \partial^j \partial^i, \tag{15}$$

with the first relation valid for the quantum Minkowski case and the second for the braided differential calculus. The above commutation relations yield respectively for coefficients of Eqs. (1) and (2) the following symmetry properties ($l=1,\ldots,N$):

$$R_{\nu\rho}^{\mu_k\mu_{k+1}}\Lambda_{\mu_1\ldots\mu_k\mu_{k+1}\ldots\mu_l}=\Lambda_{\mu_1\ldots\nu\rho\ldots\mu_l}, \tag{16}$$

$$(R')_{\nu\rho}^{\mu_k\mu_{k+1}}\Lambda_{\mu_1\ldots\mu_k\mu_{k+1}\ldots\mu_l}=\Lambda_{\mu_1\ldots\rho\nu\ldots\mu_l}. \tag{17}$$

We should here point out that also the differential calculus on finite groups investigated by Sitarz and Majid and their collaborators[15–19] includes Leibniz's rule of the form (5). The partial derivatives in this calculus read as ($i=1,\ldots,n$):

$$\partial^i f(x)=f(xx_i)-f(x), \tag{18}$$

where elements x_i numbering the basis of partial derivatives belong to the cyclic conjugacy class of a certain finite group G and the x is an arbitrary element of group G. It is clear that the transformation operator ζ is in this case

$$\zeta^i f(x)=f(xx_i). \tag{19}$$

The commutation rules for partial derivatives (18) are rather complicated so we shall discuss only the inverse operator for ζ in the next section, leaving the derivation of the conservation laws for general equation on finite groups for further investigation.

Let us notice that the important category of models on noncommutative spaces are supersymmetric models in the superspace formulation. In this framework the noncommutative space is divided into the classical commutative Minkowski space coordinates x (with corresponding indices and metric) and the spinor coordinates θ (we shall not specify below the type of spinors—Majorana or Weyl). For all equations within this class the part connected with space–time is described using the classical commutative differential calculus while for spinor coordinates we have anticommuting derivatives. The first part of the components of the transformation operator looks as follows:

$$\zeta_\nu^\mu=\delta_\nu^\mu, \quad \zeta_\nu^\alpha=\zeta_\alpha^\nu=0, \tag{20}$$

where for the supersymmetric models we have denoted the space–time indices as μ, ν while we use α and β as spinor indices (Weyl or Majorana). The only nontrivial part of the transformation operator for the supersymmetric models are the components which act between the spinor indices, namely for the monomials of the first order they are of the form

$$\zeta_\beta^\alpha x_\mu=\delta_\beta^\alpha x_\mu, \quad \zeta_\beta^\alpha\theta_\gamma=-\delta_\beta^\alpha\theta_\gamma. \tag{21}$$

We can extend the supersymmetric transformation operator to an arbitrary function by its multiplicity property (9).

Respectively the coefficients of equations (1) and (2) should be antisymmetric under permutation of two spinor indices and symmetric for all the other permutations.

B. The modification of the Leibniz's rule

For all the considered differential calculi (discrete, supersymmetric, quantum Minkowski and braided) the transformation operators have one common feature, namely, they are invertible; for discrete models with derivatives (6) or (7) the inverse operators ζ^- are simply backshift operators in the given direction while for noncommutative models the inverses are given by their multiplicity property:

$$\zeta_j^{-\,i}(fg)=(\zeta_j^{-\,k}f)(\zeta_k^{-\,i}g) \tag{22}$$

together with their action on monomials of the first order:

$$\zeta_j^{-\,i} x^k = R_{ja}^{ki} x^a + Z_j^{ki}, \tag{23}$$

$$\zeta_j^{-\,i} x_k = \tilde{R}_{kj}^{li} x_l, \tag{24}$$

where $\tilde{R}$ is the second inverse of the R matrix characteristic for braided linear spaces.[10,11]

The inverse transformation operator for differential calculus on a finite group can be derived using the definition of the cyclic conjugacy class.[19] Namely it implies the existence of the special element x_1 such that Ad_{x_1} is a cyclic permutation of $\mathcal{C}-\{x_1\}$. If $x_1^{n-1}=e$ (e being the neutral element in the group G), then also $(x_i)^{n-1}=e$ for $i=2,\ldots,n$. Thus the inverse transformation operator is given by the following formula:

$$(\zeta^i)^{-1} = (\zeta^i)^{n-2}. \tag{25}$$

Now let us discuss the supersymmetric differential calculus. The inverse operator for supersymmetric models is given by

$$\zeta_\nu^{-\,\mu} = \delta_\nu^\mu, \quad \zeta_\nu^{-\,\alpha} = \zeta_\alpha^{-\,\nu} = 0, \tag{26}$$

with the spinor–spinor part defined by the multiplicity (22) and its action on monomials of the first order:

$$\zeta_\beta^{-\,\alpha} x_\mu = \delta_\beta^\alpha x_\mu, \quad \zeta_\beta^{-\,\alpha} \theta_\gamma = -\delta_\beta^\alpha \theta_\gamma. \tag{27}$$

All the described above inverse operators fulfill the condition

$$\zeta_j^k \zeta_k^{-\,i} = \zeta_j^{-\,k} \zeta_k^i = \delta_j^i. \tag{28}$$

The properties of the transformation operators ζ and ζ^- imply the following modification of Leibniz's rule:

$$\partial^k[(\zeta_k^{-\,i} f)g] = (-\partial^{\dagger\,i} f)g + f(\partial^i g) = f(-\overleftarrow{\partial}^{\dagger\,i} + \partial^i)g, \tag{29}$$

where the conjugated derivative $\partial^\dagger$ is defined as follows:

$$\partial^{\dagger\,i} := -\partial^k \zeta_k^{-\,i}, \tag{30}$$

and we take for the given type of the derivative the connected inverse transformation operator. We see that after modification we deal with Leibniz's rule where the right-hand side is analogous to the classical differential calculus:

$$\partial^i(fg) = f(-\overleftarrow{\partial}^{\dagger\,i} + \partial^i)g$$

for which the conjugated derivative is given by: $\partial^{\dagger\,i} = -\partial^i$.

The conjugated derivatives form the conjugated equation which for the class described by conditions (1)–(3) looks as follows:

$$\Lambda(\overleftarrow{\partial}^\dagger) = \Lambda_0(\Phi) + \sum_{l=1}^{N} \overleftarrow{\partial}^{\dagger\,\mu_1} \cdots \overleftarrow{\partial}^{\dagger\,\mu_l} (\zeta_{\mu_l}^{-\,\alpha_l} \cdots \zeta_{\mu_1}^{-\,\alpha_1} \Lambda_{\alpha_1 \ldots \alpha_l}). \tag{31}$$

The following propositions hold for Eqs. (1)–(3) and are the extension of results derived in Refs. 3–5.

C. Derivation of the conservation laws for admissible differential calculi

Proposition 2.1: The unique solution of the operator equation

$$\sum_{\mu} (-\overleftarrow{\partial}^{\dagger\,\mu}+\partial^{\mu})\circ\Gamma_{\mu}(\partial,\overleftarrow{\partial}^{\dagger})=\Lambda(\partial)-\Lambda(\overleftarrow{\partial}^{\dagger}) \tag{32}$$

in the class of polynomials of derivatives $\overleftarrow{\partial}^{\dagger}$ and ∂ for the equation operator Λ fulfilling (3) is of the form

$$\Gamma_{\mu}(\partial,\overleftarrow{\partial}^{\dagger})=(\zeta_{\mu}^{-\,\alpha}\Lambda_{\alpha}) + \sum_{l=1}^{N-1}\sum_{k=0}^{l} \overleftarrow{\partial}^{\dagger\,\mu_1}\cdots\overleftarrow{\partial}^{\dagger\,\mu_k}(\zeta_{\mu}^{-\,\alpha}\zeta_{\mu_k}^{-\,\alpha_k}\cdots\zeta_{\mu_1}^{-\,\alpha_1}\Lambda_{\alpha_1\cdots\alpha_k\alpha\mu_{k+1}\cdots\mu_l})\partial^{\mu_{k+1}}\cdots\partial^{\mu_l}. \tag{33}$$

Proof: Let us explain that the "$\circ$" operation describes the way the noncommuting derivatives work on monomials of derivatives $\overleftarrow{\partial}^{\dagger}$ and ∂, namely,

$$\begin{aligned}(-\overleftarrow{\partial}^{\dagger\,\mu}+\partial^{\mu})\circ\overline{[\nu_1,\ldots,\nu_l]}a(\vec{x})[\rho_1,\ldots,\rho_k] \\ :=-\overline{[\nu_1,\ldots,\nu_l,\mu]}a(\vec{x})[\rho_1,\ldots,\rho_k]+\overline{[\nu_1,\ldots,\nu_l]}\partial^{\mu}a(\vec{x})[\rho_1,\ldots,\rho_k],\end{aligned} \tag{34}$$

where the following notation for monomials was used:

$$[\rho_1,\ldots,\rho_k]:=\partial^{\rho_1}\cdots\ \partial^{\rho_k}, \tag{35}$$

$$\overline{[\nu_1,\ldots,\nu_l]}:=\overleftarrow{\partial}^{\dagger\,\nu_1}\cdots\ \overleftarrow{\partial}^{\dagger\,\nu_l}. \tag{36}$$

The further calculations base on the assumption that we consider the general operator of the order $N-1$ with respect to the derivatives and on the associativity of the algebra of derivatives. The explicit solution of the condition (32) is enclosed in the Appendix.

We modify the Γ operator due to the deformation of Leibniz's rule [Eqs. (5) and (29)] and obtain the operator $\hat{\Gamma}$:

$$\hat{\Gamma}_{\mu}(\partial,\overleftarrow{\partial}^{\dagger})=\overleftarrow{\zeta}_{\mu}^{-\,j}(\zeta_{j}^{-\,\alpha}\Lambda_{\alpha}) + \sum_{l=1}^{N-1}\sum_{k=0}^{l} \overleftarrow{\partial}^{\dagger\,\mu_1}\cdots\ \overleftarrow{\partial}^{\dagger\,\mu_k}\overleftarrow{\zeta}_{\mu}^{-\,j}(\zeta_{j}^{-\,\alpha}\zeta_{\mu_k}^{-\,\alpha_k}\cdots\ \zeta_{\mu_1}^{-\,\alpha_1}\Lambda_{\alpha_1\cdots\alpha_k\alpha\mu_{k+1}\cdots\mu_l})\partial^{\mu_{k+1}}\cdots\ \partial^{\mu_l}, \tag{37}$$

which for a pair of arbitrary functions f and g is connected with the Γ operator by the equality

$$\sum_{\mu}\partial^{\mu}f\hat{\Gamma}_{\mu}(\partial,\overleftarrow{\partial}^{\dagger})g=\sum_{\mu} f(-\overleftarrow{\partial}^{\dagger\,\mu}+\partial^{\mu})\circ\Gamma_{\mu}(\partial,\overleftarrow{\partial}^{\dagger})g. \tag{38}$$

The immediate consequence of Proposition 2.1 is therefore the construction of conserved currents yielded by the following statement.

Proposition 2.2: Let us assume that function Φ is an arbitrary solution of Eqs. (1) and (2) with coefficients fulfilling (3), which means

$$\Lambda(\partial)\Phi=0, \tag{39}$$

and function Φ' solves the conjugated equation with the operator of the form (31):

$$\Phi' \Lambda(\overleftarrow{\partial}^{\dagger}) = 0. \tag{40}$$

Then

$$J_{\mu} = \Phi' \hat{\Gamma}_{\mu}(\partial, \overleftarrow{\partial}^{\dagger}) \Phi, \tag{41}$$

where the operator $\hat{\Gamma}_{\mu}$ *is defined by (37), is a current which obeys the conservation law:*

$$\sum_{\mu} \partial^{\mu} J_{\mu} = 0. \tag{42}$$

Proof: This is a corollary from the (38) property of the $\hat{\Gamma}$ operator, from the operator equation (32) for Γ and finally from the fact that functions Φ and Φ' fulfill the respective equations (1) and (40).

Let us notice that the auxiliary conjugated equation for the nonlinear model is now the linear one with respect to the solution Φ':

$$\Phi' \left(\Lambda_0(\Phi) + \sum_{l=1}^{N} \overleftarrow{\partial}^{\dagger \mu_1} \cdots \overleftarrow{\partial}^{\dagger \mu_l} \zeta^{-}_{\mu_l}{}^{\alpha_l} \cdots \zeta^{-}_{\mu_1}{}^{\alpha_1} \Lambda_{\alpha_1 \ldots \alpha_l} \right) = 0. \tag{43}$$

The solution Φ' depends on the solution of the initial equation Φ which defines the potential for the conjugated equation $\Lambda_0(\Phi)$.

Now the interesting question arises whether the presented construction which works on a wide class of spaces can be extended to equations with operators including both ∂ and $\partial^{\dagger}$ derivatives. As we know from discrete models (see, for example, Refs. 20 and 21) the equations depend explicitly on the forth- and backshifts along the lattice. Also the equations of motion built within the framework of generalized difference derivatives (7) (which was discussed in Refs. 3 and 22) include both initial and conjugate derivatives as a consequence of the minimal action principle. The method of derivation of the conserved currents for the discrete and mixed models shall be described in the next section. It is based on the fact that acting on functions of commutative coordinates the operators (6) and (7) yield two symmetric formulas for Leibniz's rules (both for initial and conjugated derivative).

III. CONSERVED CURRENTS AND CHARGES FOR DISCRETE AND MIXED MODELS DEPENDING ON THE ∂ AND $\partial^{\dagger}$ DERIVATIVES

Our aim is now to extend the construction described in Propositions 2.1 and 2.2 to the equations depending on the initial and conjugated derivatives of the form

$$[\Lambda(\partial) + \tilde{\Lambda}(\partial^{\dagger})] \Phi = 0, \tag{44}$$

$$\Lambda(\partial) = \Lambda_0 + \sum_{l=1}^{N} \Lambda_{\mu_1 \ldots \mu_l} \partial^{\mu_1} \cdots \partial^{\mu_l}, \tag{45}$$

$$\tilde{\Lambda}(\partial^{\dagger}) = \tilde{\Lambda}_0 + \sum_{l=1}^{\tilde{N}} \tilde{\Lambda}_{\mu_1 \ldots \mu_l} \partial^{\dagger \mu_1} \cdots \partial^{\dagger \mu_l}. \tag{46}$$

Following the previous considerations we restrict the class of equations to variable coefficients fulfilling the extended version of the condition (3):

$$\partial^{\dagger \mu_1} \Lambda_{\mu_1 \ldots \mu_l} = 0, \quad \partial^{\mu_1} \tilde{\Lambda}_{\mu_1 \ldots \mu_k} = 0, \tag{47}$$

for all $l=1,\ldots,N$ and $k=1,\ldots,\tilde{N}$.

Furthermore, the coefficients Λ and $\tilde{\Lambda}$ are symmetric under permutation of indices.

We include the nonlinear equations provided the nonlinear terms do not depend on the derivatives, which means they have a form of potential:

$$\Lambda_0=\Lambda_0(\Phi),\quad \tilde{\Lambda}_0=\tilde{\Lambda}_0(\Phi). \tag{48}$$

As we shall see in the subsequent sections the class of equations fufilling (47) contains the widely studied in different context linear auxiliary equations connected with nonlinear integrable models such as equations of nonlinear Toda lattice models.

The important factor in our calculations is the fact that for discrete (or mixed—classical and discrete) differential calculus we can write the modified Leibniz's rule symmetrically in the following form:

$$\partial^{\alpha}(\zeta_{\alpha}^{-\beta}f)g=(-\partial^{\dagger\beta}f)g+f\partial^{\beta}g=f(-\tilde{\partial}^{\dagger\beta}+\partial^{\beta})g, \tag{49}$$

$$\partial^{\dagger\alpha}(\zeta_{\alpha}^{\beta}f)g=(-\partial^{\beta}f)g+f\partial^{\dagger\beta}g=f(-\tilde{\partial}^{\beta}+\partial^{\dagger\beta})g. \tag{50}$$

Equation (50) indicates that the statement analogous to Proposition 2.1 holds for the operator $\tilde{\Lambda}(\partial^{\dagger})$; namely, we shall prove that the operator equation (51) has the unique solution by virtue of Proposition 3.1:

$$\sum_{\mu}(-\tilde{\partial}^{\mu}+\partial^{\dagger\mu})\circ\tilde{\Gamma}_{\mu}(\partial^{\dagger},\tilde{\partial})=\tilde{\Lambda}(\partial^{\dagger})-\tilde{\Lambda}(\tilde{\partial}), \tag{51}$$

where the conjugated operator $\tilde{\Lambda}(\tilde{\partial})$ looks as follows:

$$\tilde{\Lambda}(\tilde{\partial})=\tilde{\Lambda}_0(\Phi)+\sum_{l=1}^{\tilde{N}}\tilde{\partial}^{\mu_1}\cdots\tilde{\partial}^{\mu_l}(\zeta_{\mu_l}^{\alpha_l}\cdots\zeta_{\mu_1}^{\alpha_1}\Lambda_{\alpha_1\ldots\alpha_l}). \tag{52}$$

Proposition 3.1: The unique solution of (51) in the class of polynomials of derivatives $\tilde{\partial}$ and $\partial^{\dagger}$ for the equation operator $\tilde{\Lambda}$ (46) with coefficients fulfilling (47) is of the form

$$\tilde{\Gamma}_{\mu}(\partial^{\dagger},\tilde{\partial})=(\zeta_{\mu}^{\alpha}\tilde{\Lambda}_{\alpha})+\sum_{l=1}^{\tilde{N}-1}\sum_{k=0}^{l}\tilde{\partial}^{\mu_1}\cdots\tilde{\partial}^{\mu_k}(\zeta_{\mu}^{\alpha}\zeta_{\mu_k}^{\alpha_k}\cdots\zeta_{\mu_1}^{\alpha_1}\tilde{\Lambda}_{\alpha_1\ldots\alpha_k\alpha\mu_{k+1}\ldots\mu_l})\partial^{\dagger\mu_{k+1}}\cdots\partial^{\dagger\mu_l}. \tag{53}$$

Proof: The formula (53) is the immediate consequence of the proof of Proposition 2.1 enclosed in the Appendix as the following connections between derivatives and transformation operators hold:

$$\partial^{\dagger\alpha}(fg)=(\partial^{\dagger\alpha}f)g+(\zeta_{\beta}^{-\alpha}f)\partial^{\dagger\beta}g, \tag{54}$$

$$(\zeta^{-})^{-1}=\zeta, \tag{55}$$

$$(\partial^{\dagger})^{\dagger\gamma}=-(-\partial^{\beta}\zeta_{\beta}^{-\alpha})\zeta_{\alpha}^{\gamma}=\partial^{\gamma}. \tag{56}$$

We notice that ζ^{-} is the transformation operator for the derivative $\partial^{\dagger}$, the operator ζ being its inverse. Therefore, all the calculations from the proof of Proposition 2.1 can be repeated with suitable replacements. In this way we obtain the formula for the $\tilde{\Gamma}$ operator (53) which is simply the (33) operator with new derivatives $\partial^{\dagger}$ and $\tilde{\partial}$ and the operator ζ acting now as the inverse transformation operator.

We modify the operator $\tilde{\Gamma}$ similarly as in (37) and obtain the operator $\hat{\tilde{\Gamma}}$:

$$\hat{\tilde{\Gamma}}_\mu(\partial^\dagger,\tilde{\partial})=\tilde{\xi}^j_\mu(\zeta^\alpha_j\Lambda_\alpha)+\sum_{l=1}^{\tilde{N}-1}\sum_{k=0}^{l}\tilde{\partial}^{\mu_1}\cdots\tilde{\partial}^{\mu_k}\tilde{\xi}^j_\mu(\zeta^\alpha_j\zeta^{\alpha_k}_{\mu_k}\cdots\zeta^{\alpha_1}_{\mu_1}\tilde{\Lambda}_{\alpha_1\ldots\alpha_k\alpha\mu_{k+1}\ldots\mu_l})\partial^{\dagger\,\mu_{k+1}}\cdots\partial^{\dagger\,\mu_l}, \tag{57}$$

which in turn fulfills the equality

$$\sum_\mu \partial^{\dagger\,\mu}(f\hat{\tilde{\Gamma}}_\mu(\partial^\dagger,\tilde{\partial})g)=\sum_\mu f((-\tilde{\partial}^\mu+\partial^{\dagger\,\mu})\circ\tilde{\Gamma}_\mu(\partial^\dagger,\tilde{\partial}))g \tag{58}$$

for a pair of arbitrary functions f and g.

We can use the constructed operators $\hat{\Gamma}$ and $\hat{\tilde{\Gamma}}$ to derive the conserved currents by the following proposition:

Proposition 3.2: Let us assume that the function Φ is an arbitrary solution of Eq. (44) with coefficients fulfilling (47), which means

$$[\Lambda(\partial)+\tilde{\Lambda}(\partial^\dagger)]\Phi=0, \tag{59}$$

and the function Φ' solves the conjugated equation with operators (31) and (52):

$$\Phi'[\Lambda(\tilde{\partial}^\dagger)+\tilde{\Lambda}(\tilde{\partial})]=0. \tag{60}$$

Then,

$$J_\mu=\Phi'\hat{\Gamma}_\mu\Phi,\quad \tilde{J}_\mu=\Phi'\hat{\tilde{\Gamma}}_\mu\Phi, \tag{61}$$

where the operators $\hat{\Gamma}$ and $\hat{\tilde{\Gamma}}$ are given by (37) and (57) are a current that obeys the conservation law:

$$\sum_\mu \partial^\mu J_\mu+\sum_\mu \partial^{\dagger\,\mu}\tilde{J}_\mu=0. \tag{62}$$

Proof: The conservation law (62) is implied by the properties (38) and (58) of the applied operators $\hat{\Gamma}$ and $\hat{\tilde{\Gamma}}$:

$$\partial^\mu\Phi'\hat{\Gamma}_\mu\Phi+\partial^{\dagger\,\mu}\Phi'\hat{\tilde{\Gamma}}_\mu\Phi=\Phi'\left(\sum_\mu(-\tilde{\partial}^{\dagger\,\mu}+\partial^\mu)\circ\Gamma_\mu(\partial,\tilde{\partial}^\dagger)+\sum_\mu(-\tilde{\partial}^\mu+\partial^{\dagger\,\mu})\circ\tilde{\Gamma}_\mu(\partial^\dagger,\tilde{\partial})\right)\Phi$$
$$=\Phi'(\tilde{\Lambda}(\partial^\dagger)-\tilde{\Lambda}(\tilde{\partial})+\Lambda(\partial)-\Lambda(\tilde{\partial}^\dagger))\Phi=0. \tag{63}$$

Corollary 3.3: The components of the conserved current for the equation (44) fulfilling the condition (47) can be written also in the form

$$J'_\mu=\Phi'\text{`}\hat{\Gamma}_\mu\Phi-\zeta^{-\ \nu}_\mu(\Phi'\hat{\tilde{\Gamma}}_\nu\Phi). \tag{64}$$

They obey the conservation law including only the ∂ derivatives:

$$\sum_{\mu} \partial^{\mu} J'_{\mu} = 0, \tag{65}$$

provided Φ *is the solution of (44) and the function* Φ' *solves the conjugate equation with operators (31) and (52).*

Let us notice that the presented construction holds when we work within the framework of classical commutative differential calculus (for which the conjugation means $\partial^{\dagger} = -\partial$ and the transformation operator is the identity) as well as for mixed models where part of the coordinates is continuous and the other part is discrete with suitable difference derivatives in the form (6) or (7).

In the sequel we shall use the construction (37), (57), and (61) in order to derive the conserved currents and in consequence the conserved charges for the mixed discrete nonlinear Toda model and for the double discrete Toda model as well.

As we know from the classical field theory we can use the conserved currents in construction of the conserved charges. This is also the case for our discrete and mixed discrete models with derivatives defined by (6) or (7). We shall integrate the time component of the conserved current over subspace excluding the time-coordinate. We use in derivation the conserved currents given by Proposition 3.2 or accordingly by Corollary 3.3 if the conjugated derivative with respect to the time-coordinate appears in the model. Integrating we must remember to take the corresponding integral. Namely for continuous coordinates we understand $\int dx_i$ as the Lebesque integral while for the discrete derivative (6) the definite integral is given by

$$\int dx_i := \sum_{k=-\infty}^{+\infty} (\zeta_i)^k. \tag{66}$$

If the equation includes the discrete derivative of the type (7), we use the definite integral in the form

$$\int dx_i := \sum_{k=-\infty}^{+\infty} (x^i_{k+1} - x^i_k)(\zeta_i)^k. \tag{67}$$

In the above formulas for discrete integrals the ζ_i is the shift operator in the direction i along the lattice.

Let us denote the integral over subspace with excluded time-coordinate as $\int_{\text{sub}}$. Then the conserved charges for discrete and mixed discrete models with variable coefficients can be derived using the following proposition:

Proposition 3.4: Let us assume that in the model described by the equation (44) the conjugated discrete derivative with respect to the time-coordinate does not appear. Then the charge

$$Q = \int_{\text{sub}} J_t, \tag{68}$$

where J_t *is the time component of the conserved current described in Proposition 3.2, is conserved:*

$$\partial^t Q = 0. \tag{69}$$

Proof: The conservation of the charge (68) is implied by the conservation law from Proposition 3.2, namely,

$$\partial^t Q = \int_{\text{sub}} \partial^t J_t = \int_{\text{sub}} -\sum_{k \neq t} (\partial^k J_k + \partial^{\dagger\, k} \tilde{J}_k) = \text{boundary terms} = 0, \tag{70}$$

provided the currents vanish at the infinity in the corresponding spacelike dimensions. We have used here also the property of the discrete and mixed discrete differential calculus:

$$\partial^t \int_{\mathrm{sub}} = \int_{\mathrm{sub}} \partial^t. \tag{71}$$

Let us point out that the equality (71) does not apply in general to noncommutative spaces (the superspace being an exception) and this fact is the major difficulty in construction of the conserved charges for an arbitrary model on noncommutative space.[13,14]

If in equation (44) both initial and conjugate time-derivatives appear, we derive the conserved charge using Corollary 3.3, namely the following statement is then valid (with proof being the copy of the above calculations for Proposition 3.4):

Corollary 3.5: Let us assume that in the model described by the equation (44) both discrete derivatives ∂^t and $\partial^{\dagger\, t}$ appear. Then the charge

$$Q = \int_{\mathrm{sub}} J'_t, \tag{72}$$

where J'_t is the time component of the conserved current described in Corollary 3.3, is conserved:

$$\partial^t Q = 0. \tag{73}$$

IV. APPLICATIONS

A. The second order equation on quantum plane with variable coefficients

Let us start with the simple example of the second order equation on quantum plane with coefficients depending on coordinates x and y.

The commutation relations for derivatives and coordinates look as follows:[10,11]

$$yx = qxy, \quad \partial^y \partial^x = q^{-1} \partial^x \partial^y. \tag{74}$$

Leibniz's rule (5) in differential calculus is defined by the following R-matrix:

$$R = \begin{bmatrix} q^2 & 0 & 0 & 0 \\ 0 & q & q^2-1 & 0 \\ 0 & 0 & q & 0 \\ 0 & 0 & 0 & q^2 \end{bmatrix}, \quad R' = q^{-2} R. \tag{75}$$

From the above matrix we can deduce the explicit action of the transformation operator ζ on the monomials of the first order (11). It yields the following formulas for the inverse transformation ζ^-:

$$\zeta_x^{-\,x} x = q^{-2} x, \quad \zeta_x^{-\,x} y = q^{-1} y, \quad \zeta_y^{-\,x} x = (q^{-2}-1) y, \quad \zeta_y^{-\,x} y = 0, \tag{76}$$

$$\zeta_y^{-\,y} y = q^{-2} y, \quad \zeta_y^{-\,y} x = q^{-1} x, \quad \zeta_x^{-\,y} y = 0, \quad \zeta_x^{-\,y} x = 0. \tag{77}$$

The conjugated derivatives are defined using the inverse transformation operator:

$$\partial^{\dagger\, x} = -\partial^x \zeta_x^{-\,x} - \partial^y \zeta_y^{-\,x}, \quad \partial^{\dagger\, y} = -\partial^x \zeta_x^{-\,y} - \partial^y \zeta_y^{-\,y}. \tag{78}$$

Now let us discuss an arbitrary equation of the second order with the coefficients depending on x and y and check which of them fufills the condition (3):

$$\Lambda(\partial^x, \partial^y) = \Lambda_{xx} \partial^x \partial^x + \Lambda_{yx} \partial^y \partial^x + \Lambda_{xy} \partial^x \partial^y + \Lambda_{yy} \partial^y \partial^y. \tag{79}$$

The condition (3) for our simple case reads as follows:

$$\partial^{\dagger x}\Lambda_{xx}+\partial^{\dagger y}\Lambda_{yx}=0, \quad \partial^{\dagger y}\Lambda_{yy}+\partial^{\dagger x}\Lambda_{xy}=0. \tag{80}$$

Let us assume $\Lambda_{xy}=\Lambda_{yx}=0$. Then we can show that $\Lambda_{xx}=\phi(y)$ and $\Lambda_{yy}=\psi(x)$ obey the conditions (3), namely,

$$\partial^{\dagger x}\Lambda_{xx}=(-\partial^{x}\zeta_{x}^{-\,x}-\partial^{y}\zeta_{y}^{-\,x})\phi(y)=-\partial^{x}\zeta_{x}^{-\,x}\phi(y)=-\partial^{x}\phi(q^{-1}y)=0, \tag{81}$$

$$\partial^{\dagger y}\Lambda_{yy}=(-\partial^{x}\zeta_{x}^{-\,y}-\partial^{y}\zeta_{y}^{-\,y})\psi(x)=-\partial^{y}\zeta_{y}^{-\,y}\psi(x)=-\partial^{y}\psi(q^{-1}x)=0. \tag{82}$$

Now we can apply our construction to obtain the Γ operator:

$$\Gamma_{x}=\tilde{\partial}^{\dagger\ x}\phi(q^{-2}y)+\phi(q^{-1}y)\partial^{x}, \quad \Gamma_{y}=\tilde{\partial}^{\dagger\ y}\psi(q^{-2}x)+\psi(q^{-1}x)\partial^{y}. \tag{83}$$

It is easy to check that this operator fulfills the operator equation (32):

$$\begin{aligned}(-\tilde{\partial}^{\dagger\ x}+\partial^{x})\circ\Gamma_{x}+(-\tilde{\partial}^{\dagger\ y}+\partial^{y})\circ\Gamma_{y}\\ =-(\tilde{\partial}^{\dagger x}\tilde{\partial}^{\dagger\ x}\phi(q^{-2}y)+\tilde{\partial}^{\dagger y}\tilde{\partial}^{\dagger\ y}\psi(q^{-2}x))+\phi(y)\partial^{x}\partial^{x}+\psi(x)\partial^{y}\partial^{y},\end{aligned} \tag{84}$$

where the operator $\Lambda(\tilde{\partial})$ gives the conjugated equation:

$$\Lambda(\tilde{\partial})=\tilde{\partial}^{\dagger x}\tilde{\partial}^{\dagger\ x}\phi(q^{-2}y)+\tilde{\partial}^{\dagger y}\tilde{\partial}^{\dagger\ y}\psi(q^{-2}x). \tag{85}$$

The modified $\hat{\Gamma}$ operator is given by the formula

$$\hat{\Gamma}_{x}=\tilde{\partial}^{\dagger x}\tilde{\zeta}_{x}^{-\,x}\phi(q^{-2}y)+\tilde{\zeta}_{x}^{-\,x}\phi(q^{-1}y)\partial^{x}, \tag{86}$$

$$\begin{aligned}\hat{\Gamma}_{y}=\tilde{\partial}^{\dagger x}\tilde{\zeta}_{y}^{-\,x}\phi(q^{-2}y)+\tilde{\zeta}_{y}^{-\,x}\phi(q^{-1}y)\partial^{x},\\ +\tilde{\partial}^{\dagger y}\tilde{\zeta}_{y}^{-\,y}\psi(q^{-2}x)+\tilde{\zeta}_{y}^{-\,y}\psi(q^{-1}x)\partial^{y}.\end{aligned} \tag{87}$$

Having the explicit form of the Γ and $\hat{\Gamma}$ operators we can construct the conserved currents:

$$J_{x}=\Phi'\hat{\Gamma}_{x}\Phi, \quad J_{y}=\Phi'\hat{\Gamma}_{y}\Phi, \tag{88}$$

where the functions Φ' and Φ solve the respective equations:

$$\Phi'(\tilde{\partial}^{\dagger x}\tilde{\partial}^{\dagger x}\phi(q^{-2}y)+\tilde{\partial}^{\dagger y}\tilde{\partial}^{\dagger y}\psi(q^{-2}x))=0, \tag{89}$$

$$(\phi(y)\partial^{x}\partial^{x}+\psi(x)\partial^{y}\partial^{y})\Phi=0. \tag{90}$$

According to Proposition 2.2 the above current obeys the conservation law:

$$\partial^{x}J_{x}+\partial^{y}J_{y}=0, \tag{91}$$

provided functions Φ' and Φ are the solutions of the corresponding equations (89) and (90).

B. Nonlinear equation of motion for chiral and antichiral supermultiplets

The supersymmetric models in the superfield formulation yield interesting examples of the equations of motion with coefficients depending on variables.[23] Let us recall that in such a frame-

work the fields depend on superspace coordinates including the space–time and spinor variables while in construction of the action the covariant derivatives are used which explicitly depend on spinor coordinates.

We shall study in this section the $D=4$ $N=1$ chiral and antichiral superfields obeying the nonlinear equation of motion resulting from the supersymmetric action:

$$I=\int d^4x d^2\theta d^2\overline{\theta}\overline{\Phi}\Phi+\int d^4x d^2\theta\left(\frac{m}{2}\Phi^2+\frac{g}{3}\Phi^3\right)+\int d^4x d^2\overline{\theta}\left(\frac{m}{2}\overline{\Phi}^2+\frac{g}{3}\overline{\Phi}^3\right). \tag{92}$$

The integration over spinor variables θ and $\overline{\theta}$ can be expressed in terms of the covariant derivatives:

$$\int d^2\theta=-\frac{1}{4}D^2, \quad \int d^2\overline{\theta}=-\frac{1}{4}\overline{D}^2, \tag{93}$$

$$\int d^2\theta d^2\overline{\theta}=\frac{1}{16}D^2\overline{D}^2=\frac{1}{16}\overline{D}^2D^2=\frac{1}{16}D^\alpha\overline{D}^2D_\alpha=\frac{1}{16}\overline{D}_{\dot\alpha}D^2\overline{D}^{\dot\alpha}. \tag{94}$$

The covariant derivatives used in supersymmetric models are built from the basic derivatives with respect to the space–time and spinor coordinates:

$$D_\alpha=\partial_\alpha+i\sigma^\mu_{\alpha\dot\beta}\overline{\theta}^{\dot\beta}\partial_\mu, \quad D^\alpha=\epsilon^{\alpha\beta}D_\beta, \tag{95}$$

$$\overline{D}_{\dot\alpha}=-\partial_{\dot\alpha}-i\theta^\beta\sigma^\mu_{\beta\dot\alpha}\partial_\mu, \quad \overline{D}^{\dot\alpha}=\epsilon^{\dot\alpha\dot\beta}\overline{D}_{\dot\beta}. \tag{96}$$

Due to the fact that chiral Φ and antichiral $\overline{\Phi}$ superfields fulfill the following condition,

$$\overline{D}_{\dot\alpha}\Phi=0, \quad D_\alpha\overline{\Phi}=0, \tag{97}$$

we obtain from the action (92) the equations of motion in the form

$$\begin{pmatrix} \frac{1}{4}D^2 & m+g\overline{\Phi} \\ m+g\Phi & \frac{1}{4}\overline{D}^2 \end{pmatrix}\begin{pmatrix}\Phi\\ \overline{\Phi}\end{pmatrix}=0. \tag{98}$$

We have written the equations for the superfields Φ and $\overline{\Phi}$ in the matrix form. In this example we deal with the coefficients of the equation depending explicitly on θ and $\overline{\theta}$ variables due to the form of the covariant derivatives (95) and (96):

$$D^2=D^\alpha D_\alpha=-\partial^\alpha\partial_\alpha+2i\overline{\theta}^{\dot\beta}\sigma^\mu_{\alpha\dot\beta}\partial_\mu\partial^\alpha-\overline{\theta}^2\Box, \tag{99}$$

$$\overline{D}^2=\overline{D}_{\dot\alpha}\overline{D}^{\dot\alpha}=-\overline{\partial}_{\dot\alpha}\overline{\partial}^{\dot\alpha}-2i\theta^\alpha\sigma^\mu_{\alpha\dot\beta}\partial_\mu\overline{\partial}^{\dot\beta}+\theta^2\Box. \tag{100}$$

The second important feature of the chiral–antichiral superfield equation of motion is its nonlinearity for $g\neq 0$. However, the nonlinear term does not depend on the derivatives so we can apply our method of derivation to the conservation law provided the condition (3) for the kinetic part of the operator is fulfilled. Let us extract the ζ and ζ^- operators from Leibniz's rule for basic derivatives:

$$\partial^\mu(fg)=(\partial^\mu f)g+f\partial^\mu g, \tag{101}$$

$$\partial^\alpha(fg)=(\partial^\alpha f)g+(\zeta^\alpha_\beta f)\partial^\beta g, \tag{102}$$

$$\overline{\partial}^{\alpha}(fg)=(\overline{\partial}^{\alpha}f)g+(\zeta_{\dot\beta}^{\dot\alpha}f)\overline{\partial}^{\dot\beta}g. \tag{103}$$

It is clear that $\zeta_{\nu}^{\mu}=\delta_{\nu}^{\mu}$ and the following components of the transformation operator vanish:

$$\zeta_{\alpha}^{\mu}=\zeta_{\mu}^{\alpha}=0,\quad \zeta_{\dot\alpha}^{\mu}=\zeta_{\mu}^{\dot\alpha}=0,\quad \zeta_{\alpha}^{\dot\alpha}=\zeta_{\dot\alpha}^{\alpha}=0. \tag{104}$$

The remaining components of the ζ operator are defined by its action on the monomials of the first order in superspace variables:

$$\zeta_{\beta}^{\alpha}x_{\nu}=\delta_{\beta}^{\alpha}x_{\nu},\quad \zeta_{\beta}^{\alpha}\theta_{\gamma}=-\delta_{\beta}^{\alpha}\theta_{\gamma},\quad \zeta_{\beta}^{\alpha}\overline{\theta}_{\dot\gamma}=-\delta_{\beta}^{\alpha}\overline{\theta}_{\dot\gamma}. \tag{105}$$

The analogous formulas hold also for dotted indices. Hence we get for the inverse transformation operator

$$\zeta_{\beta}^{-\ \alpha}x_{\nu}=\delta_{\beta}^{\alpha}x_{\nu},\quad \zeta_{\beta}^{-\ \alpha}\theta_{\gamma}=-\delta_{\beta}^{\alpha}\theta_{\gamma},\quad \zeta_{\beta}^{-\ \alpha}\overline{\theta}_{\dot\gamma}=-\delta_{\beta}^{\alpha}\overline{\theta}_{\dot\gamma}, \tag{106}$$

with the corresponding expressions with dotted indices of the same form.

Now having the explicitly derived inverse transformation operator we arrive at the conjugated derivatives given by the formulas

$$\partial^{\dagger\,\mu}=-\partial^{\mu},\quad \partial^{\dagger\,\alpha}=-\partial^{\beta}\zeta_{\beta}^{-\ \alpha},\quad \overline{\partial}^{\dagger\,\dot\alpha}=-\overline{\partial}^{\dot\beta}\zeta_{\dot\beta}^{-\ \dot\alpha}. \tag{107}$$

Using the conjugated derivatives we obtain the condition (3) written for our equation for the chiral and antichiral superfields:

$$\partial^{\dagger\,\alpha}\Lambda_{\alpha\mu}+\overline{\partial}^{\dagger\,\dot\alpha}\Lambda_{\dot\alpha\mu}+\partial^{\dagger\,\nu}\Lambda_{\nu\mu}=0, \tag{108}$$

$$\partial^{\dagger\,\alpha}\Lambda_{\alpha\beta}+\partial^{\dagger\,\mu}\Lambda_{\mu\beta}=0, \tag{109}$$

$$\overline{\partial}^{\dagger\,\dot\alpha}\Lambda_{\dot\alpha\dot\beta}+\partial^{\dagger\,\mu}\Lambda_{\mu\dot\beta}=0. \tag{110}$$

One can easily check that the above conditions are fulfilled using the explicit form of the coefficients from Eq. (98):

$$\Lambda_{\alpha\dot\beta}=\Lambda_{\dot\beta\alpha}=\begin{pmatrix}0&0\\0&0\end{pmatrix}, \tag{111}$$

$$\Lambda_{\alpha\beta}=-\epsilon_{\alpha\beta}\begin{pmatrix}\frac{1}{4}&0\\0&0\end{pmatrix}, \tag{112}$$

$$\Lambda_{\dot\alpha\dot\beta}=-\epsilon_{\dot\alpha\dot\beta}\begin{pmatrix}0&0\\0&\frac{1}{4}\end{pmatrix}, \tag{113}$$

$$\Lambda_{\mu\alpha}=\Lambda_{\alpha\mu}=\begin{pmatrix}\frac{i}{4}\overline{\theta}^{\dot\beta}\sigma^{\nu}_{\alpha\dot\beta}&0\\0&0\end{pmatrix}g_{\nu\mu}, \tag{114}$$

$$\Lambda_{\mu\dot\alpha}=\Lambda_{\dot\alpha\mu}=\begin{pmatrix}0&0\\0&-\frac{i}{4}\theta^{\beta}\sigma^{\nu}_{\beta\dot\alpha}\end{pmatrix}g_{\nu\mu}, \tag{115}$$

$$\Lambda_{\mu\nu}=\begin{pmatrix} -\frac{1}{4}\overline{\theta^2} & 0 \\ 0 & -\frac{1}{4}\theta^2 \end{pmatrix} g_{\mu\nu}. \tag{116}$$

The next step is therefore the application of the general formula (33) for the Γ operator to our model:

$$\Gamma_\mu=\overleftarrow{\partial}^{\dagger\,\nu}\Lambda_{\nu\mu}+\Lambda_{\mu\nu}\partial^\nu, \tag{117}$$

$$\Gamma_\alpha=-\overleftarrow{\partial}^{\dagger\,\mu}\Lambda_{\mu\alpha}+\overleftarrow{\partial}^{\dagger\,\gamma}\Lambda_{\gamma\alpha}+\Lambda_{\alpha\gamma}\partial^\gamma-\Lambda_{\alpha\mu}\partial^\mu, \tag{118}$$

$$\Gamma_{\dot\alpha}=-\overleftarrow{\partial}^{\dagger\,\mu}\Lambda_{\mu\dot\alpha}+\overleftarrow{\partial}^{\dagger\,\dot\gamma}\Lambda_{\dot\gamma\dot\alpha}+\Lambda_{\dot\alpha\dot\gamma}\partial^{\dot\gamma}-\Lambda_{\dot\alpha\mu}\partial^\mu. \tag{119}$$

The operator $\hat\Gamma$ differs from the Γ by insertion of the ζ^- operator in the middle of the monomials of derivatives:

$$\hat\Gamma_\mu=\Gamma_\mu, \tag{120}$$

$$\hat\Gamma_\beta=-\overleftarrow{\partial}^{\dagger\,\mu}\overleftarrow{\zeta}^{-\,\alpha}_{\beta}\Lambda_{\mu\alpha}+\overleftarrow{\partial}^{\dagger\,\gamma}\overleftarrow{\zeta}^{-\,\alpha}_{\beta}\Lambda_{\gamma\alpha}+\overleftarrow{\zeta}^{-\,\alpha}_{\beta}\Lambda_{\alpha\gamma}\partial^\gamma-\overleftarrow{\zeta}^{-\,\alpha}_{\beta}\Lambda_{\alpha\mu}\partial^\mu, \tag{121}$$

$$\hat\Gamma_{\dot\beta}=-\overleftarrow{\partial}^{\dagger\,\mu}\overleftarrow{\zeta}^{-\,\dot\alpha}_{\dot\beta}\Lambda_{\mu\dot\alpha}+\overleftarrow{\partial}^{\dagger\,\dot\gamma}\overleftarrow{\zeta}^{-\,\dot\alpha}_{\dot\beta}\Lambda_{\dot\gamma\dot\alpha}+\overleftarrow{\zeta}^{-\,\dot\alpha}_{\dot\beta}\Lambda_{\dot\alpha\dot\gamma}\partial^{\dot\gamma}-\overleftarrow{\zeta}^{-\,\dot\alpha}_{\dot\beta}\Lambda_{\dot\alpha\mu}\partial^\mu. \tag{122}$$

We apply the obtained operator $\hat\Gamma$ to derive the currents:

$$J_\mu=(\overline{\Phi}',\Phi')\hat\Gamma_\mu\begin{pmatrix}\Phi\\ \overline{\Phi}\end{pmatrix}, \tag{123}$$

$$J_\alpha=(\overline{\Phi}',\Phi')\hat\Gamma_\alpha\begin{pmatrix}\Phi\\ \overline{\Phi}\end{pmatrix}, \tag{124}$$

$$J_{\dot\alpha}=(\overline{\Phi}',\Phi')\hat\Gamma_{\dot\alpha}\begin{pmatrix}\Phi\\ \overline{\Phi}\end{pmatrix}, \tag{125}$$

which obey the conservation law:

$$\partial^\mu J_\mu+\partial^\alpha J_\alpha+\overline{\partial^\alpha}J_{\dot\alpha}=0, \tag{126}$$

provided the fields used in construction fulfill the corresponding equation of motion (98) and the pair of superfields $\overline{\Phi}'$ and Φ' its conjugated version:

$$(\overline{\Phi}',\Phi')\begin{pmatrix}\frac{1}{4}\overleftarrow{D}^{\dagger 2} & m+g\overline{\Phi}\\ m+g\Phi & \frac{1}{4}\overleftarrow{\overline{D}}^{\dagger 2}\end{pmatrix}=0. \tag{127}$$

Let us notice that this equation is linear with respect to superfields $\overline{\Phi}'$ and Φ' and its solution depends on the potential given by the chiral and antichiral superfields Φ and $\overline{\Phi}$.

Due to the properties of covariant derivatives built from the self-conjugated operators, we conclude that the conjugated set of equations for superfields $(\overline{\Phi}', \Phi')$ has at least following solutions:

(i) For the case $g \neq 0$ we can take $\overline{\Phi}' = \Phi$ and $\Phi' = \overline{\Phi}$ where Φ and $\overline{\Phi}$ are solutions for (98).

(ii) When $g = 0$, the superfield $\overline{\Phi}'$ is an arbitrary solution of the chiral part and Φ' of the antichiral part of the set of equations (98).

The above solutions give in turn the explicit form of the conserved currents (123)–(125) where we replace the multiplet $(\overline{\Phi}', \Phi')$ with $(\Phi, \overline{\Phi})$ for $g \neq 0$ and with $(\delta\Phi, \delta\overline{\Phi})$ for $g = 0$. Let us notice that for linear model $g = 0$ we obtain the full set of conserved currents connected with symmetry operators of chiral–antichiral supermultiplet equation:

$$J_\mu = (\delta\Phi, \delta\overline{\Phi})\hat{\Gamma}_\mu \begin{pmatrix} \Phi \\ \overline{\Phi} \end{pmatrix}, \tag{128}$$

$$J_\alpha = (\delta\Phi, \delta\overline{\Phi})\hat{\Gamma}_\alpha \begin{pmatrix} \Phi \\ \overline{\Phi} \end{pmatrix}, \tag{129}$$

$$J_{\dot{\alpha}} = (\delta\Phi, \delta\overline{\Phi})\hat{\Gamma}_{\dot{\alpha}} \begin{pmatrix} \Phi \\ \overline{\Phi} \end{pmatrix}, \tag{130}$$

where the symmetries δ include supersymmetric transformations:

$$Q_\alpha = -i\partial_\alpha - \sigma^l_{\alpha\dot{\beta}}\overline{\theta}^{\dot{\beta}}\partial_l, \quad \overline{Q}^{\dot{\alpha}} = -i\overline{\partial}^{\dot{\alpha}} + \sigma^{l\,\dot{\alpha}}_{\alpha}\theta^\alpha\partial_l, \tag{131}$$

and the operators from Poincarè algebra: momenta, angular momentum and boosts for four-dimensional Minkowski space.

We can use the obtained conserved current (123)–(125) to construct the integral of motion by integrating the time-component of the current (123) over the subspace,

$$Q = \int d^3x d^2\theta d^2\overline{\theta} J_0, \tag{132}$$

as the following equality holds:

$$\partial^0 Q = \int d^3x d^2\theta d^2\overline{\theta}\partial^0 J_0 = \int d^3x d^2\theta d^2\overline{\theta}(-\partial^k J_k - \partial^\alpha J_\alpha - \partial^{\dot{\alpha}} J_{\dot{\alpha}}) = \text{boundary terms} = 0. \tag{133}$$

Let us point out that the developed method allows immediate construction of conserved charges. The obtained charges are supermultiplets built from component charges which are also conserved separately. The application of our method to the equations obeying the condition (3) is an alternative to the procedure used in supersymmetric models (see, for example, Ref. 24 for chiral superfields and Ref. 25 for supersymmetric principal chiral model) where the conservation laws include covariant spinor derivatives D and $\overline{D}$ instead of basic derivatives ∂^μ, ∂^α and $\overline{\partial}^{\dot{\alpha}}$ which we have used. The consequence of the fact that the time-derivative does not appear explicitly in the conservation law is an additional procedure required to derive the component conservation laws and conserved charges.

C. Nonlinear integrable models and their consistency conditions

1. Nonlinear Toda lattice equation

The interesting case of application of Proposition 3.2 is the linear set of equations which originates from the nonlinear Toda lattice equation. The set of auxiliary equations derived in Ref. 21 from gauged bidifferential calculus reads as follows:

$$\dot{\chi}_k=\lambda(e^{q_{k-1}-q_k}\chi_{k-1}-\chi_k)\zeta, \tag{134}$$

$$\chi_{k+1}-\chi_k=-\lambda(\dot{\chi}_k+\dot{q}_k\chi_k)\zeta, \tag{135}$$

where we have used our notation for the transformation operator which for the mixed model like the one considered in this section is simply shifting along the lattice $\zeta f_k=f_{k-1}$ with respect to the spacelike dimension. We shall discuss the consistency condition which we obtain after elimination of the parameter λ and operator ζ from the set of equations (134) and (135). It is an equation of second order including classical derivative with respect to the time-variable and the discrete one with respect to the space-lattice variable:

$$\ddot{\chi}_k+\dot{q}_k\dot{\chi}_k-e^{q_{k-1}-q_k}(\chi_{k-1}-\chi_k)-(\chi_{k+1}-\chi_k)=0. \tag{136}$$

Let us notice that this equation is free of the parameter λ and the operator ζ.

We can rewrite this equation using the notation

$$\chi_{k-1}-\chi_k=(\zeta-1)\chi_k=\partial\chi_k, \quad \chi_{k+1}-\chi_k=(\zeta^{-}-1)\chi_k=\partial^{\dagger}\chi_k, \tag{137}$$

$$q_{k-1}-q_k=(\zeta-1)q_k=\partial q_k, \quad \dot{f}=\partial^t f, \tag{138}$$

and it has the following form:

$$[\partial^t\partial^t+(\partial^t q)\partial^t-e^{(\partial q)}\partial-\partial^{\dagger}]\chi=0. \tag{139}$$

In this form we see clearly that the equation involves both ∂ and $\partial^{\dagger}$ derivatives so we should follow the construction for discrete models given in Propositions 3.1 and 3.2.

Let us observe that the discussed equation fulfills the restriction (3) and it coincides in this case with the nonlinear Toda lattice equation:

$$\partial^{\dagger\,t}\Lambda_t+\partial^{\dagger}\Lambda_x=-\ddot{q}_k-e^{q_k-q_{k+1}}+e^{q_{k-1}-q_k}=0. \tag{140}$$

We construct the Γ operator according to (33), (37), (53), and (57) taking into account that the transformation operator acts as follows:

$$\zeta_t f_k(t)=f_k(t), \quad \zeta f_k(t)=f_{k-1}(t), \quad \zeta^{-}f_k(t)=f_{k+1}(t), \tag{141}$$

$$\hat{\Gamma}_t=\Gamma_t=-\tilde{\partial}^t+\partial^t+(\partial^t q), \tag{142}$$

$$\hat{\Gamma}_x=-\tilde{\zeta}^{-}e^{-(\partial^{\dagger}q)}, \tag{143}$$

$$\hat{\tilde{\Gamma}}_x=\tilde{\zeta}. \tag{144}$$

The components of the $\hat{\Gamma}$ operator yield the corresponding components of the current:

$$J_t^{\delta}=\delta\chi'\hat{\Gamma}_t\chi, \quad J_x^{\delta}=\delta\chi'\hat{\Gamma}_x\chi, \quad \tilde{J}_x^{\delta}=\delta\chi'\hat{\tilde{\Gamma}}_x\chi, \tag{145}$$

which obeys the conservation law including the conjugated derivative:

$$\partial^t J_t^\delta + \partial J_x^\delta + \partial^\dagger \tilde{J}_x^\delta = 0, \tag{146}$$

provided the field χ fulfills the consistency condition (139), and the field χ' its conjugation:

$$\chi'[\overleftarrow{\partial}^t \overleftarrow{\partial}^t - \overleftarrow{\partial}^t(\partial^t q) - \overleftarrow{\partial}^\dagger e^{-(\partial^\dagger q)} - \overleftarrow{\partial}] = 0, \tag{147}$$

and the operator δ is now the symmetry operator of the conjugated equation (147).

We proceed taking integrals with respect to the discrete spatial variable (we have denoted it as x) and obtain the charges

$$Q^\delta = \int dx J_t = \int dx\, \delta\chi' \hat{\Gamma}_t \chi, \tag{148}$$

which are also conserved:

$$\partial^t Q = 0. \tag{149}$$

In the above formula we understand the discrete definite integral $\int dx$ as given by (66).

We can check that the following operators transform solution χ' of equation (147) into the solution $\delta\chi'$:[26]

$$\delta^0 = c\frac{\partial}{\partial\chi'}, \quad \delta^1 = e^q \frac{\partial}{\partial\chi'}, \quad \delta^2 = [-\partial^{-1}(\partial^t q) + t]\frac{\partial}{\partial\chi'}, \tag{150}$$

where the indefinite discrete integral ∂^{-1} is given by

$$\partial^{-1} = \frac{1}{\zeta - 1} = -\sum_{k=0}^{\infty} \zeta^k, \tag{151}$$

and c is a constant.

The derived symmetries of the equation (139) lead to the following expressions for charges:

$$Q^0 = \int dx c\Gamma_t \chi, \tag{152}$$

$$Q^1 = \int dx e^q \Gamma_t \chi, \tag{153}$$

$$Q^2 = \int dx[-\partial^{-1}(\partial^t q) + t]\Gamma_t \chi. \tag{154}$$

After expanding the solutions χ with respect to powers of the operators $\lambda\zeta$ we shall be able to rewrite the expressions (148) as an infinite set of conserved charges:

$$Q^{0(m)} = \int dx c\Gamma_t \chi^{(m)}, \tag{155}$$

$$Q^{1(m)} = \int dx e^q \Gamma_t \chi^{(m)}, \tag{156}$$

$$Q^{2(m)} = \int dx[-\partial^{-1}(\partial^t q) + t]\Gamma_t \chi^{(m)}, \tag{157}$$

where the components $\chi^{(m)}$ read as follows:

$$\chi^{(m)}=(-1)^{m-1}[(\partial^{\dagger})^{-1}(\partial^{t}+(\partial^{t}q))]^{m-2}(\partial^{\dagger})^{-1}(\partial^{t}q), \quad m\geqslant 2. \tag{158}$$

2. Nonlinear Toda lattice equation—generalization

Our next example is the generalization of nonlinear Toda model sketched in Ref. 21. The functions depend now smoothly on one time variable t, one spacelike variable y and one discrete spacelike coordinate x. The bidifferential calculus is in this case defined as follows:[21]

$$\delta f=[S^{-1},f]\tau-f'\xi, \quad df=\dot{f}\tau+[S,f]\xi, \tag{159}$$

$$A=X\tau+(Y-1)S\xi, \tag{160}$$

where X and Y are matrices with entries being smooth functions of t and y and discrete in the coordinate x. The condition $\delta A=0$ leads to the following generalized Toda model nonlinear equations:

$$X_k'=Y_k-Y_{k-1}, \quad \dot{Y}_k=Y_kX_{k+1}-X_kY_k. \tag{161}$$

The linear version for auxiliary field χ can be deduced following Ref. 21 from the set of equations given by

$$\delta\chi=\lambda(d+A)\chi, \tag{162}$$

and looks as follows:

$$(S^{-1}-1)\chi=\lambda[\dot{\chi}+X\chi]S, \tag{163}$$

$$-\chi'=\lambda[(S-1)\chi+(Y-1)(S\chi)]S. \tag{164}$$

We can rewrite the above set of equations using our notations:

$$S=\zeta, \quad S^{-1}=\zeta^{-}, \tag{165}$$

$$\zeta\chi_k(t,y)=\chi_{k+1}(t,y), \quad \zeta^{-}\chi_k(t,y)=\chi_{k-1}(t,y), \tag{166}$$

$$(\zeta-1)\chi=\partial\chi, \quad (\zeta^{-}-1)\chi=\partial^{\dagger}\chi, \tag{167}$$

$$\chi'=\partial^{y}\chi, \quad \dot{\chi}=\partial^{t}\chi, \tag{168}$$

and they are given by the formulas

$$\partial^{\dagger}\chi=\lambda[\partial^{t}+X]\chi\zeta, \tag{169}$$

$$-\partial^{y}\chi=\lambda[\partial\chi+(Y-1)(\zeta\chi)]\zeta. \tag{170}$$

The consistency equation (in the symmetric form) for the above set of equations reads as

$$[\tfrac{1}{2}\partial^{y}\partial^{t}+\tfrac{1}{2}\partial^{t}\partial^{y}+X\partial^{y}-Y\partial-\partial^{\dagger}]\chi=0. \tag{171}$$

Let us point out that in the derivation of the consistency equation for the generalized Toda model not only Eqs. (169) and (170), but also the second of the Toda equations (161) were used.

We check now the condition (3) for the variable coefficients of the operator of the equation:

$$\partial^{\dagger\,y}\Lambda_y+\partial^{\dagger}\Lambda_x=-\partial^{y}X+Y-\zeta^{-}Y=0. \tag{172}$$

Our equation fulfills the restriction (3) due to the fact that X and Y obey the first of the equations of nonlinear Toda model (161). The condition (47) also holds as the coefficient for the derivative $\partial^{\dagger}$ is constant.

Similarly to the previous examples we can apply Propositions 3.1 and 3.2 for the discrete models depending on initial and conjugate discrete derivatives. In this way we obtain the $\hat{\Gamma}$ operator in the form

$$\hat{\Gamma}_t=\Gamma_t=\tfrac{1}{2}(-\tilde{\partial}^y+\partial^y),\quad \hat{\Gamma}_y=\Gamma_y=\tfrac{1}{2}(-\tilde{\partial}^t+\partial^t)+X, \tag{173}$$

$$\hat{\Gamma}_x=-\tilde{\zeta}^-(\zeta^- Y),\quad \hat{\tilde{\Gamma}}_x=-\tilde{\zeta}. \tag{174}$$

We use the above components of the $\hat{\Gamma}$ and $\hat{\tilde{\Gamma}}$ operators to construct the respective components of the currents:

$$J_t^{\delta}=\delta\chi'\hat{\Gamma}_t\chi,\quad J_y^{\delta}=\delta\chi'\hat{\Gamma}_y\chi, \tag{175}$$

$$J_x^{\delta}=\delta\chi'\hat{\Gamma}_x\chi,\quad \tilde{J}_x^{\delta}=\delta\chi'\hat{\tilde{\Gamma}}_x\chi, \tag{176}$$

where we have denoted δ as the symmetry operator of the conjugated equation (177) and χ is the solution of (169)–(171) while χ' solves its conjugation:

$$[-\tfrac{1}{2}\partial^y\partial^t-\tfrac{1}{2}\partial^t\partial^y+\partial]\chi'+(\partial^y\chi')X+(\partial^{\dagger}\chi')(\zeta^- Y)=0. \tag{177}$$

As the currents fulfill the conservation law,

$$\partial^t J_t^{\delta}+\partial^y J_y^{\delta}+\partial J_x^{\delta}+\partial^{\dagger}\tilde{J}_x^{\delta}=0, \tag{178}$$

they yield the conserved charges [with the integral $\int dx$ in the sense of (66)]:

$$Q^{\delta}=\int dydx J_t^{\delta}=\int dydx\,\delta\chi'\hat{\Gamma}_t\chi. \tag{179}$$

Following the procedure applied earlier we expand the solution χ in terms of powers of the operator $\lambda\zeta$:

$$\chi=\sum_{m=0}^{\infty}\chi^{(m)}(\lambda\zeta)^m. \tag{180}$$

After assuming the first components in the form of the unital $N\times N$ matrix,

$$\chi^{(0)}=\chi'^{(0)}=\chi^{(1)}=\chi'^{(1)}=\mathbf{1}_{N\times N}, \tag{181}$$

we obtain the following equations for the subsequent components:

$$\partial^{\dagger}\chi^{(m)}=[\partial^t+X]\chi^{(m-1)},\quad m\geqslant 2, \tag{182}$$

$$-\partial^y\chi^{(m)}=[\partial+(Y-1)\zeta]\chi^{(m-1)},\quad m\geqslant 2. \tag{183}$$

Inserting the expansion (180) into the expressions for currents and charges we arrive at the infinite towers of the conserved currents and charges:

$$J_{\mu}^{\delta(m)}=\delta\chi'\hat{\Gamma}_{\mu}\chi^{(m)}, \tag{184}$$

$$Q^{\delta\ (m)}=\int dxdy\,\delta\chi'\hat{\Gamma}_t\chi^{(m)}, \tag{185}$$

with the following explicit expressions for the components of the fields χ:

$$\chi^{(2)}=(\partial^{\dagger})^{-1}X, \tag{186}$$

$$\chi^{(m)}=[(\partial^{\dagger})^{-1}(\partial^t+X)]^{m-2}(\partial^{\dagger})^{-1}X, \quad m\geqslant 2, \tag{187}$$

and the initial solutions for the conjugated equation (177) related to the symmetry operators in the form

$$\delta^0\chi'=C, \quad \delta^1\chi'=\partial^{-1}X-y, \tag{188}$$

with C being a constant $N\times N$ matrix.

3. Double discrete nonlinear Toda lattice equation

Let us end the review of the integrable models with the fully discrete Toda lattice equation. The set of auxiliary linear equations given in Ref. 20 has the following form:

$$\chi_k(n)-\chi_k(n-1)=-\frac{\gamma}{c}[g_k^{-1}(n)g_{k+1}(n)\chi_{k+1}(n)-\chi_k(n)], \tag{189}$$

$$\chi_k(n)-\chi_{k-1}(n)=-\gamma c[g_k^{-1}(n)g_k(n+1)\chi_k(n+1)-\chi_k(n)]. \tag{190}$$

We rewrite the above equations using our notation:

$$f_k(n)-f_{k-1}(n)=-\partial^x f_k(n), \quad \zeta_x^- f_k(n)=f_{k+1}(n), \tag{191}$$

$$f_k(n)-f_k(n-1)=-\partial^t f_k(n), \quad \zeta_t^- f_k(n)=f_k(n+1). \tag{192}$$

Then the set of equations (189) and (190) looks as follows:

$$-\partial^t\chi=-\frac{\gamma}{c}[g^{-1}(\zeta_x^- g)(\zeta_x^-\chi)-\chi], \tag{193}$$

$$-\partial^x\chi=-\gamma c[g^{-1}(\zeta_t^- g)(\zeta_t^-\chi)-\chi]. \tag{194}$$

The consistency equation for the above set reads as

$$-g^{-1}(\zeta_x^- g)\partial^{\dagger\,x}\chi-\partial^x\chi+c^2g^{-1}(\zeta_t^- g)\partial^{\dagger\,t}\chi+c^2\partial^t\chi=0. \tag{195}$$

The condition (47) for our example is fulfilled:

$$\partial^{\dagger\,x}\Lambda_x+\partial^{\dagger\,t}\Lambda_t=0, \tag{196}$$

$$\partial^x\tilde{\Lambda}_x+\partial^t\tilde{\Lambda}_t=-\partial^x g^{-1}(\zeta_x^- g)+c^2\partial^t g^{-1}(\zeta_t^- g)=0, \tag{197}$$

provided the double discrete nonlinear Toda lattice equation is valid for the field g:

$$\partial^x g^{-1}(\zeta_x^- g)=c^2\partial^t g^{-1}(\zeta_t^- g). \tag{198}$$

We construct the conserved currents following Propositions 3.1 and 3.2. As both initial and conjugated derivatives appear in the equation we use the Γ and $\tilde{\Gamma}$ operators:

$$\Gamma_x = -1, \quad \tilde{\Gamma}_x = -(\zeta_x g^{-1})g, \tag{199}$$

$$\Gamma_t = c^2, \quad \tilde{\Gamma}_t = c^2(\zeta_t g^{-1})g, \tag{200}$$

and obtain the $\hat{\Gamma}$ and $\hat{\tilde{\Gamma}}$ operators with the following components:

$$\hat{\Gamma}_x = -\overleftarrow{\zeta}_x^-, \quad \hat{\tilde{\Gamma}}_x = -\overleftarrow{\tilde{\zeta}}_x(\zeta_x g^{-1})g, \tag{201}$$

$$\hat{\Gamma}_x = c^2\overleftarrow{\zeta}_t^-, \quad \hat{\tilde{\Gamma}}_t = c^2\overleftarrow{\tilde{\zeta}}_t(\zeta_t g^{-1})g. \tag{202}$$

The above operators give in turn the currents:

$$J_\mu^\delta = \delta\chi' \hat{\Gamma}_\mu \chi, \quad \tilde{J}_\mu^\delta = \delta\chi' \hat{\tilde{\Gamma}}_\mu \chi, \tag{203}$$

which are conserved according to Proposition 3.2:

$$\partial^t J_t^\delta + \partial^x J_x^\delta + \partial^{\dagger\, t}\tilde{J}_t^\delta + \partial^{\dagger\, x}\tilde{J}_x^\delta = 0, \tag{204}$$

provided the function χ solves the equation (195), χ' the conjugated equation:

$$\chi'[\overleftarrow{\partial}^x(\zeta_x g^{-1})g + \overleftarrow{\partial}^{\dagger\, x} - c^2\overleftarrow{\partial}^t(\zeta_t g^{-1})g - c^2\overleftarrow{\partial}^{\dagger\, t}] = 0, \tag{205}$$

and δ is the symmetry operator for the conjugated equation.

Following Corollary 3.3 we can reformulate the currents (203) in order to obtain the conservation law including only the ∂ derivatives:

$$J_x'^{\,\delta} = J_x^\delta - \zeta_x^-(\tilde{J}_x^\delta), \quad J_t'^{\,\delta} = J_t^\delta - \zeta_t^-(\tilde{J}_t^\delta). \tag{206}$$

The current J' obeys the conservation law:

$$\partial^t J_t'^{\,\delta} + \partial^x J_x'^{\,\delta} = 0. \tag{207}$$

Now we apply the (64) version of the conserved current so as to obtain the conserved charges:

$$Q^\delta = \int dx J_t'^{\,\delta} = \int dx(\delta\chi' \hat{\Gamma}_t \chi - \zeta_t^-(\delta\chi' \hat{\tilde{\Gamma}}_t \chi)), \tag{208}$$

where the integral $\int dx$ is defined as in (66).

D. Anomalous diffusion equation

Let us close the applications with an example of the equation built within the framework of standard differential calculus. In recent years the phenomenon of anomalous diffusion attracted more and more attention. In this context the general equation for anomalous diffusion was discussed in Refs. 27–29. It contains the fractional time-derivative.[30] We shall consider here the special case with standard partial derivatives:

$$\left[\partial^t - \frac{1}{r^{D-1}}\partial^r r^{-\Theta} r^{D-1}\partial^r - \frac{\alpha}{r^2}\right]P(r,t) = 0, \tag{209}$$

where D is the Hausdorff dimension of the underlying fractal structure and Θ is connected with the anomalous diffusion parameter d_w; $\Theta = d_w - 2$ and α is an arbitrary constant.

As the above equation is the partial differential equation we work with commuting derivatives and the transformation operator is the identity. The diffusion equation (209) can be rewritten to the form

$$[r^{\Theta}\partial^t-(\partial^r)^2-V(r)]W(r,t)=0, \tag{210}$$

with the new potential

$$V(r)=-r^{-2}\left[\frac{D-1-\Theta}{2}-\frac{(D-1-\Theta)^2}{4}\right]+\alpha r^{\Theta-2} \tag{211}$$

and the new density function

$$W(r,t)=r^{(D-1-\Theta)/2}P(r,t). \tag{212}$$

The transformed equation (210) obeys the main condition (3):

$$\partial^t\Lambda_t=0, \quad \partial^r\Lambda_{rr}=0. \tag{213}$$

Analogous transformation shall be applied to the conjugated equation:

$$\left[-\partial^t-\partial^r r^{-\Theta}r^{D-1}\partial^r\frac{1}{r^{D-1}}-\frac{\alpha}{r^2}\right]P'(r,t)=0. \tag{214}$$

Using the modified density function

$$W'(r,t)=r^{(-D+1-\Theta)/2}P'(r,t), \tag{215}$$

we arrive at the corresponding form of the conjugated equation:

$$[-r^{\Theta}\partial^t-(\partial^r)^2-V(r)]W'(r,t)=0. \tag{216}$$

As both the diffusion equation (210) and its conjugation (216) fulfill the condition (3) we can apply the general method to this partial differential equation. The components of the modified $\hat{\Gamma}$ operator coincide in our case with those of the Γ operator:

$$\hat{\Gamma}_t=\Gamma_t=r^{\Theta}, \quad \hat{\Gamma}_r=\Gamma_r=\overleftarrow{\partial}^r-\partial^r. \tag{217}$$

The current looks as follows:

$$J_t=W'(r,t)\Gamma_t W(r,t), \tag{218}$$

$$J_r=W'(r,t)\Gamma_r W(r,t). \tag{219}$$

It can be expressed in terms of the probability density functions,

$$J_t=P'(r,t)P(r,t), \tag{220}$$

$$J_r=r^{-\Theta}\left[P'(r,t)(\overleftarrow{\partial}^r-\partial^r)P(r,t)-\frac{D-1}{r}P'(r,t)P(r,t)\right], \tag{221}$$

and due to Proposition 2.2 is conserved:

$$\partial^t J_t+\partial^r J_r=0, \tag{222}$$

provided the probability density functions P and P' solve respective diffusion equations (209) and (214).

The conservation law for the fractional version of the diffusion equation

$$\left[D_t^{\gamma}-\frac{1}{r^{D-1}}\partial^r r^{-\Theta}r^{D-1}\partial^r-\frac{\alpha}{r^2}\right]P(r,t)=0 \tag{223}$$

is currently under investigation. We shall follow the results developed for fractional differential equations with constant coefficients.[31]

V. FINAL REMARKS

We have discussed the method of derivation of the conservation laws for a class of equations with variable coefficients. It can be applied to models built using supersymmetric, discrete, mixed discrete and noncommutative (quantum Minkowski or braided) differential calculus.

The conserved charges were constructed explicitly for considered supersymmetric and discrete equations. The problem of derivation of such charges for noncommutative models is open. The integration over noncommutative spaces, namely braided linear space (including q-Minkowski), is well developed,[32–34] but subintegrals and commutation rules for subintegrals and derivatives need further study. In particular, the generalized version of the property (71),

$$\partial^t \int_{\mathrm{sub}} = \int_{\mathrm{sub}} \partial^t,$$

must be derived. As we have shown for models on quantum planes,[13] it is crucial in the construction of the conserved charges.

APPENDIX: PROOF OF PROPOSITION 2.1

Let us recall the notation for monomials of derivatives:

$$[\rho_1 \dots \rho_k] := \partial^{\rho_1} \cdots \partial^{\rho_k}, \quad \overleftarrow{[\nu_1 \cdots \nu_m]} := \overleftarrow{\partial}^{\dagger\,\nu_1} \cdots \overleftarrow{\partial}^{\dagger\,\nu_m}. \tag{A1}$$

Due to the modification of Leibniz's rule we are to consider the solution of the operator equation for the Γ operator in the form of the polynomial of order $N-1$:

$$\Gamma_\mu(\partial, \overleftarrow{\partial}^\dagger) = a^0_\mu + \sum_{l=1}^{N-1} \sum_{k=0}^{l} \overleftarrow{[\mu_1, \dots, \mu_k]} a^k_{\mu\mu_1 \dots \mu_l} [\mu_{k+1}, \dots, \mu_l], \tag{A2}$$

where the coefficients a^k depend on the coordinates $\vec{x}$.

The condition (32) from Sec. II applied to the above polynomial yields the equations for coefficients $a^k_{\mu\mu_1 \dots \mu_l}$:

$$\begin{aligned}
\sum_\mu (-\overleftarrow{\partial}^{\dagger\,\mu} + \partial^\mu) \circ \Gamma_\mu(\partial, \overleftarrow{\partial}^\dagger) = &- \sum_{l=1}^{N-1} \sum_{k=0}^{l} \sum_\mu \overleftarrow{[\mu_1, \dots, \mu_k, \mu]} a^k_{\mu\mu_1 \dots \mu_l} [\mu_{k+1}, \dots, \mu_l] \\
&+ \sum_{l=1}^{N-1} \sum_{k=0}^{l} \overleftarrow{[\mu_1, \dots, \mu_k]} \sum_\mu (\zeta^\mu_\nu a^k_{\mu\mu_1 \dots \mu_l})[\nu, \mu_{k+1}, \dots, \mu_l] \\
&+ \sum_{l=1}^{N-1} \sum_{k=0}^{l} \overleftarrow{[\mu_1, \dots, \mu_k]} \sum_\mu (\partial^\mu a^k_{\mu\mu_1 \dots \mu_l})[\mu_{k+1}, \dots, \mu_l] \\
&- \sum_\mu \overleftarrow{[\mu]} a^0_\mu + \sum_\mu (\zeta^\mu_\nu a^0_\mu)[\nu] + \sum_\mu (\partial^\mu a^0_\mu) = \Lambda(\partial) - \Lambda(\overleftarrow{\partial}^\dagger).
\end{aligned} \tag{A3}$$

The procedure is analogous to the one used in the proof of Proposition 4.1 from Ref. 5, which describes the derivation of conservation law for the equation with constant coefficients or fulfilling the strong condition [see (23) and (24) from Ref. 5]. Now we have decided to change the form of the conjugated equation. This results in the weaker restrictions for coefficients of equation (1) and changes the set of equations for functions $a^k_{\mu\mu_1 \dots \mu_l}$ defining the operator Γ for the following one:

$$\partial^{\mu}a^{0}_{\mu}=0, \tag{A4}$$

$$a^{0}_{\mu}=\zeta^{-\ \alpha}_{\mu}\Lambda_{\alpha}, \tag{A5}$$

$$\partial^{\alpha}a^{0}_{\alpha\mu}+\zeta^{\nu}_{\mu}a^{0}_{\nu}=\Lambda_{\mu}, \tag{A6}$$

$$\zeta^{\alpha}_{\mu}a^{0}_{\alpha\mu_1\ldots\mu_l}+\partial^{\alpha}a^{0}_{\alpha\mu\mu_1\ldots\mu_l}=\Lambda_{\mu\mu_1\ldots\mu_l}, \tag{A7}$$

$$-a^{k}_{\mu\mu_1\ldots\mu_l}+\zeta^{\alpha}_{\mu_{k+1}}a^{k+1}_{\alpha\mu_1\ldots\mu_k\mu\mu_{k+2}\ldots\mu_l}+\partial^{\alpha}a^{k+1}_{\alpha\mu_1\ldots\mu_k\mu\mu_{k+1}\ldots\mu_l}=0, \tag{A8}$$

$$a^{l}_{\mu\mu_1\ldots\mu_l}+\partial^{\alpha}a^{l}_{\alpha\mu_1\ldots\mu_l\mu}=\zeta^{-\ \alpha}_{\mu}\zeta^{-\ \alpha_l}_{\mu_l}\ldots\zeta^{-\ \alpha_1}_{\mu_1}\Lambda_{\alpha_1\ldots\alpha_l\alpha}, \tag{A9}$$

with $l=1,\ldots,N-1$ and $k=0,\ldots,l-1$.

We see that equations (A4), (A5), and (A9) yielded by the coefficients of the conjugated equation differ from the case studied earlier in Refs. 4 and 5. We begin to solve this set of equations by deriving the coefficients $a^{0}_{\mu\mu_1\ldots\mu_l}$ from Eqs. (A5)–(A7). Namely for $l=N-1$ we have

$$\zeta^{\alpha}_{\mu}a^{0}_{\alpha\mu_1\ldots\mu_{N-1}}=\Lambda_{\mu\mu_1\ldots\mu_{N-1}}. \tag{A10}$$

Applying the inverse operator ζ^{-} we obtain

$$a^{0}_{\mu\mu_1\ldots\mu_{N-1}}=\zeta^{-\ \alpha}_{\mu}\Lambda_{\alpha\mu_1\ldots\mu_{N-1}}. \tag{A11}$$

We insert this solution into (A7) for $l=N-2$ and solve the next equation:

$$\zeta^{\alpha}_{\mu}a^{0}_{\alpha\mu_1\ldots\mu_{N-2}}-\partial^{\dagger\ \alpha}\Lambda_{\alpha\mu\mu_1\ldots\mu_{N-2}}=\Lambda_{\mu\mu_1\ldots\mu_{N-2}}. \tag{A12}$$

By assumption (3) after using ζ^{-} operator and (28) we derive $a^{0}_{\mu\mu_1\ldots\mu_{N-2}}$ as

$$a^{0}_{\mu\mu_1\ldots\mu_{N-2}}=\zeta^{-\ \alpha}_{\mu}\Lambda_{\alpha\mu_1\ldots\mu_{N-2}}. \tag{A13}$$

Passing to the next equation from the subset (A7) and solving them in the similar way we obtain the unique solution for coefficients a^{0}:

$$a^{0}_{\mu_1\ldots\mu_l}=\zeta^{-\ \alpha}_{\mu_1}\Lambda_{\alpha\mu_2\ldots\mu_l},\quad l=1,\ldots,N. \tag{A14}$$

This solution for initial coefficients allows us to evaluate the remaining ones using (A8) and (A9), namely we obtain the a^{1} coefficients after writing the subset (A8) for $k=0$ and solving it the way we solved the subset (A5)–(A7) for a^{0}. The result is unique and looks as follows:

$$a^{1}_{\mu\mu_1\mu_2\ldots\mu_l}=\zeta^{-\ \alpha}_{\mu}\zeta^{-\ \alpha_1}_{\mu_1}\Lambda_{\alpha_1\alpha\mu_2\ldots\mu_l},\quad l=1,\ldots,N-1. \tag{A15}$$

The same method applied to subsets of (A8) and (A9) for $k=1,\ldots,N-2$ produces the unique solution of the set of equations for coefficients in the form

$$a^{k}_{\mu\mu_1\ldots\mu_l}=\zeta^{-\ \alpha}_{\mu}\zeta^{-\ \alpha_k}_{\mu_k}\cdots\ \zeta^{-\ \alpha_1}_{\mu_1}\Lambda_{\alpha_1\ldots\alpha_k\alpha\mu_{k+1}\ldots\mu_l},\quad l=1,\ldots,N-1. \tag{A16}$$

The derivation of the explicit formulas for unique solution of the coefficients of the operator Γ_{μ} concludes the proof of Proposition 2.1.

Let us notice once more that in the derivation of coefficients for the Γ_{μ} operator the crucial factors were the properties of coefficients of the equations (1)–(3) which enabled us to solve the equation (32) in the explicit form.

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Boundary values as Hamiltonian variables. II. Graded structures

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It is shown that the new formula for the field theory Poisson brackets arises naturally in the proposed extension of the formal variational calculus incorporating divergences. The linear spaces of local functionals, evolutionary vector fields, functional forms, multi-vectors and differential operators become graded with respect to divergences. The bilinear operations, such as the action of vector fields onto functionals, the commutator of vector fields, the interior product of forms and vectors and the Schouten–Nijenhuis bracket are compatible with the grading. A definition of the adjoint graded operator is proposed and antisymmetric operators are constructed with the help of boundary terms. The fulfilment of the Jacobi identity for the new Poisson brackets is shown to be equivalent to vanishing of the Schouten–Nijenhuis bracket of the Poisson bivector with itself. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1478144]

I. INTRODUCTION

The Hamiltonian formalism of classical mechanics may serve as the ideal model illustrating the harmony of physics and mathematics. Starting from the 1970s it was realized that a number of its mathematical constructions, for example, the Schouten–Nijenhuis bracket,[1] could be extrapolated to field theory.[2,3] This development made the search for new nonlinear integrable models much easier. More general constructions uniting the Schouten–Nijenhuis bracket with the Frolicher–Nijenhuis bracket were considered by A. Vinogradov.[4]

But these methods (initially called the formal variational calculus[5]) have some restrictions. Boundary conditions are limited by those allowing free integration by parts. As a rule, the periodic boundary conditions or the rapid decay of fields at spatial infinity are required. Of course, these are not all the physically interesting cases. For example, the Coulomb potential in electrodynamics does not tend to zero rapidly enough. The similar behavior is typical for Yang–Mills and gravitation fields. Nontrivial boundary problems arise also in the motion of material continua.

We consider the Hamiltonian treatment of nontrivial boundary problems as an interesting field of research where there is some place for new approaches and results. The field theory Poisson brackets which fulfill the Jacobi identity under arbitrary boundary conditions have been proposed in Ref. 6. Here we extend the formal variational calculus to the most general case when no one boundary term arising in integration by parts can be discarded. We present some physical applications of the methods developed here in the next paper of this series.[7] Let us also say that the interest in the role of divergences in field theory is vivid now as can be seen from related papers.[8–10]

We add that recently there has appeared a new proposal[11] for the Poisson bracket satisfying the Jacobi identity irrespective of boundary conditions. But this new formula still has no such a geometric background as the one developed here. For this reason it is not clear yet whether it can be applied, for example, to non-ultralocal brackets. We address the interested reader to Ref. 12 for a discussion.

As an example, illustrating the nonstandard nature of the problems to be considered, let us

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remind the history of the long discussion on the role of surface integrals in the canonical formulation of general relativity. During about 15 years Arnowitt, Deser and Misner,[13] Dirac,[14] Higgs,[15] Schwinger,[16] DeWitt,[17] and Regge and Teitelboim[18] were involved in it. The solution obtained in the last work[18] serves as the paradigm for the treatment of similar problems up to now. It has been proposed to work with the special class of the so-called ''differentiable'' functionals. These functionals are defined by the requirement that their variation should not have surface contributions under the prescribed boundary conditions. The Poisson brackets for these functionals are the standard ones, i.e., they are just the same as given in the formal variational calculus

$$\{F,G\}=\int_\Omega\left(\frac{\delta F}{\delta q^A(x)}\frac{\delta G}{\delta p_A(x)}-\frac{\delta G}{\delta q^A(x)}\frac{\delta F}{\delta p_A(x)}\right)d^nx,$$

but now nonzero surface contributions are allowed.

Here a natural question to ask is: do these brackets fulfill the standard axiomatic requirements, i.e., the Jacobi identity and the existence of the Poisson algebra on this space of admissible functionals? For the infinite domain of integration and the asymptotic boundary conditions the affirmative result for the second requirement was obtained by Brown and Henneaux.[19] The first requirement was partially analyzed by us and, in the case treated above, the answer is also positive.

It is more difficult to study the finite domain case. Let us take as a second example the motion of a fluid or plasma. It was shown by Lewis *et al.*[20] that the Jacobi identity for the standard Poisson bracket can be violated even in the case of fixed boundary, and so the Poisson brackets should be modified by surface terms. In the free boundary case it turns out to be natural to extend the space of admissible functionals so that their variation could include nonzero surface contributions. But according to Ref. 20 the presence of a nonzero term with δq^A in the boundary integral requires the absence of the corresponding term with δp_A and vice versa. A new formula for Poisson brackets arises as a result of a generalization of the variational derivative which is now allowed to contain a surface contribution

$$\delta H=\int_\Omega\frac{\delta^\wedge H}{\delta q^A}\delta q^A d^nx+\oint_{\partial\Omega}\frac{\delta^\vee H}{\delta q^A}\delta q^A\Big|_{\partial\Omega}dS+\int_\Omega\frac{\delta^\wedge H}{\delta p_A}\delta p_A d^nx+\oint_{\partial\Omega}\frac{\delta^\vee H}{\delta p_A}\delta p_A\Big|_{\partial\Omega}dS.$$

Unfortunately, it is not quite clear whether the Poisson bracket of the two functionals, admissible in this new sense, will be admissible functional itself.

As a third example, we would like to attract the reader's attention to consequences of the noncommutativity of the standard variational derivatives, i.e., the Euler–Lagrange derivatives. This point was discussed formally in publications by I. Anderson[21,22] and Aldersley.[23] We faced the problem independently, in the course of studying surface terms in the Poisson algebra of the Ashtekar formalism of canonical gravity.[24] There it was found that transformations of the type

$$q^A(x)\to q^A(x),\quad p_A(x)\to p_A(x)+\frac{\delta F[q]}{\delta q^A(x)},$$

were noncanonical ones if surface terms were not ignored. Tracing the connection of this calculation with the standard calculations with δ-functions,[25] we have found that the correspondence could be restored by introduction of θ_Ω—the characteristic function of the domain Ω

$$\theta_\Omega(x)=\begin{cases}1, & \text{if } x\in\Omega;\\ 0, & \text{otherwise.}\end{cases}$$

Then the standard relations

$$\left(\frac{\partial}{\partial x^i}+\frac{\partial}{\partial y^i}\right)\delta(x,y)=0$$

should be modified as

$$\left(\theta_\Omega(x)\frac{\partial}{\partial x^i}+\theta_\Omega(y)\frac{\partial}{\partial y^i}\right)\delta(x,y)=-\frac{\partial\theta_\Omega}{\partial x^i}\delta(x,y),$$

where the usually discarded surface term is preserved.

All the above examples lead us to the necessity to extend the formal variational calculus onto total divergences. This extension consists in the introduction of a new grading for the linear spaces of local functionals, vector fields, functional forms, multi-vectors and differential operators. To come back to the standard case one should put $\theta_\Omega(x)\equiv 1$ in $\mathbb{R}^n$.

The extension of the formal variational calculus naturally incorporates the new definition of local functionals (not modulo divergences now) and of their differentials (as a full variation, not restricted on the boundary). The Poisson bivectors are now defined in a more general way and they can include boundary contributions. The definition of pairing (interior product) is also revised and now the trace of two differential operators is used for it, so the pairing becomes compatible with the grading. The Poisson bracket found more or less heuristically in Ref. 6 arises now on the base of the geometrical constructions as

$$\{F,G\}=\mathrm{d}G\lrcorner\mathrm{d}F\lrcorner\Psi,$$

where Ψ is the Poisson bivector.

We show here that the Jacobi identity for the new Poisson brackets can be verified without the long calculations of binomial sums used in Ref. 6. Its fulfillment is equivalent to the vanishing of the Schouten–Nijenhuis bracket of the Poisson bivector with itself. And in its turn this condition can be easily tested along with the procedure proposed by Olver[2] with a minimal modification of it. More attention than in Ref. 6 is paid here to non-ultralocal Hamiltonian operators with non-constant coefficients, because now the technical obstacles are removed. It turns out to be that not all operators which are Hamiltonian with respect to the standard brackets remain Hamiltonian in relation to the new brackets. For example, the second structure of the Korteweg–de Vries equation is not automatically Hamiltonian with respect to the new formalism; the Jacobi identity in this case is valid only up to divergence. In this respect it strongly differs from the first KdV structure.

The content of this work is as follows. In Sec. II we introduce the grading for local functionals, and evolutionary vector fields. In Sec. III the differential, the functional m-forms, the interior product of vector fields onto m-forms and Lie derivative are defined. Section IV deals with graded differential operators and their adjoints. In Sec. V we discuss multi-vectors and the Schouten–Nijenhuis bracket. It is shown how one-vectors and evolutionary vector field spaces are isomorphic. Section VI contains the general definition of Poisson bracket, its realization in this formalism, the definition of Hamiltonian vector fields and the theorem on connection between the commutator of two Hamiltonian vector fields and the Poisson bracket of corresponding Hamiltonians. All constructions are illustrated by an example: the first Hamiltonian structure of the Korteweg–de Vries equation. The proof of Jacobi identity is postponed until Sec. VII. This new proof is applicable for all local Poisson brackets and so supersedes the proofs given earlier in Ref. 6. The proofs are easy to compare as notations are the same. At last, in Sec. VIII we consider two examples of the non-ultralocal Poisson brackets with field dependent coefficients (this class of brackets cannot be studied by the methods of Ref. 6). We show that the second structure of the Korteweg–de Vries equation is Hamiltonian only up to surface terms, whereas the two-dimensional flow of the ideal fluid is exactly described by Hamiltonian structure. This points to nontrivial character of the generalization of the formal variational calculus suggested here. A short summary is given in Sec. IX and the points remaining unclear are mentioned.

As a rule, we use below the same notations as in Ref. 6 except for a change in the notation of the Fréchet derivative (from D_f to f') and omitting the sign of summation according to the Einstein rule. We find it convenient to represent integrals over finite domain Ω through integrals over the infinite space $\mathbb{R}^n$ by inserting into all integrands the characteristic function θ_Ω. Then the formalism seems closer to the standard formal variational calculus where local functionals and functional forms are defined modulo divergences. But the formal divergences that we discard here are integrated to zero under arbitrary conditions on the boundary of the finite domain, whereas real divergences are incorporated into graded structures. All the operations introduced below are compatible both with discarding formal total divergences (if one object is a formal divergence, then the result of operation is also formal divergence) and with the grading (i.e., the same is valid for real divergences). Extension of the space of differential operators by admitting their grading permits us to use the concept of adjoint operator. So, antisymmetric operators can now be constructed and the Poisson bracket formulas become more compact than in Ref. 6, though their content is the same. Nevertheless, in the proof of the Jacobi identity we prefer to use old notations to make easier the comparison with not so general proofs of Ref. 6.

Henceforth we consider the space $\mathbb{R}^n$ and the multi-index notations $J=(j_1,\ldots,j_n)$ where $j_i\geqslant 0$:

$$\phi_A^{(J)}=\frac{\partial^{|J|}\phi_A}{\partial^{j_1}x^1\ldots\partial^{j_n}x^n},\quad |J|=j_1+\cdots+j_n.$$

The Fréchet derivative is defined as

$$f'_A=\frac{\partial f}{\partial\phi_A^{(J)}}D_J, \tag{1}$$

where

$$D_i=\frac{\partial}{\partial x^i}+\phi_A^{(J+i)}\frac{\partial}{\partial\phi_A^{(J)}},\quad D_J=D_1^{j_1}\cdots D_n^{j_n},\quad D_i^0=1,\quad D_i^{-1}=0.$$

Binomial coefficients for multi-indices are

$$\binom{J}{K}=\binom{j_1}{k_1}\ldots\binom{j_n}{k_n},$$

$$\binom{j}{k}=\begin{cases} j!/(k!(j-k)!), & \text{if } 0\leqslant k\leqslant j;\\ 0 & \text{otherwise.}\end{cases}$$

With the help of them we introduce the so-called higher Eulerian operators[2,23,26]

$$E_A^J(f)=(-1)^{|K|+|J|}\binom{K}{J}D_{K-J}\frac{\partial f}{\partial\phi_A^{(K)}}. \tag{2}$$

II. LOCAL FUNCTIONALS AND EVOLUTIONARY VECTOR FIELDS

Let us start with notions from the theory of graded spaces as they are given in Ref. 3. A *grading* in linear space L is a decomposition of it into a direct sum of subspaces, with a special value of some function p (grading function) assigned to all the elements of any subspace.

Below the function p takes its values in the set of all positive multi-indices $J=(j_1,\ldots,j_n)$ and so,

$$L=\bigoplus_{J=0}^{\infty} L^{\langle J\rangle}.$$

Elements of each subspace are called homogeneous.

A bilinear operation $x,y\mapsto x\circ y$, defined on L, is said to be *compatible with the grading* if the product of any homogeneous elements is also homogeneous, and if

$$p(x\circ y)=p(x)+p(y).$$

Now let us turn to the concrete structures.

There are two ways to write a local functional: as the integral of a smooth function $f^{\langle 0\rangle}(\phi_A^{(K)}(x))$ of fields and their derivatives up to some finite order over the prescribed domain Ω in $\mathbb{R}^n$, or as the integral over all the space $\mathbb{R}^n$ but with the characteristic function of the domain θ_Ω included into the integrand

$$F=\int_\Omega f^{\langle 0\rangle}(\phi_A^{(K)}(x))d^nx\equiv\int_{\mathbb{R}^n}\theta_\Omega f^{\langle 0\rangle}d^nx. \tag{3}$$

As in Ref. 6, let us denote the space of local functionals as $\mathcal{A}$. Here we shall call the expression given above the *canonical form of a local functional*. We formally extend that definition by allowing local functionals to be written as follows:

$$F=\int_{\mathbb{R}^n} D_J\theta_\Omega f^{\langle J\rangle}(\phi_A^{(K)}(x))d^nx\equiv\int\theta^{(J)}f^{\langle J\rangle}d^nx\equiv\int f d^nx,$$

where only a finite number of terms is allowed. Here and below we simplify the notation for derivatives of θ and remove Ω. All the integrals without the domain of integration shown explicitly are integrals over $\mathbb{R}^n$; below we shall omit d^nx. Of course, any functional can be transformed to the above form (3), exclusively used in Ref. 6, through integration by parts

$$F=\int\theta\tilde{f}^{\langle 0\rangle}\equiv\int_\Omega\tilde{f}^{\langle 0\rangle},$$

where

$$\tilde{f}^{\langle 0\rangle}=(-1)^{|J|}D_Jf^{\langle J\rangle}.$$

Evidently, the formal integration by parts over infinite space $\mathbb{R}^n$ changes the grading. It will be clear below that the general situation is the following: from one side we have the compatibility of all the bilinear operations with the grading and from the other side—with the formal integration by parts. So, basic objects (local functionals, etc.) are defined as equivalence classes modulo formal divergences (i.e., divergences of expressions containing θ-factors) and the unique decomposition into the homogeneous subspaces with the fixed grading function can be made only for representatives of these classes.

We call expressions of the form

$$\Psi=\int\theta^{(J)}D_K\psi_A^{\langle J\rangle}\frac{\partial}{\partial\phi_A^{(K)}}\equiv\int\theta^{(J)}\psi^{\langle J\rangle}\equiv\int\psi,$$

the *evolutionary vector fields*. The action of the evolutionary vector field on a local functional is given by the expression

$$\Psi F = \int \theta^{(I+J)} D_K \psi_A^{\langle J \rangle} \frac{\partial f^{\langle I \rangle}}{\partial \phi_A^{(K)}} \equiv \int \theta^{(I+J)} \psi^{\langle J \rangle} f^{\langle I \rangle} \equiv \int \psi f. \tag{4}$$

It is a straightforward calculation to check that this operation is compatible with the formal integration by parts, i.e.,

$$\psi D f = D(\psi f),$$

as it is in the standard formal variational calculus. This relation is, of course, valid for integrands.

It is easy to see that the evolutionary vector field with coefficients

$$\psi_A^{\langle J \rangle} = D_L \xi_B^{\langle I \rangle} \frac{\partial \lambda_A^{\langle J-I \rangle}}{\partial \phi_B^{(L)}} - D_L \lambda_B^{\langle I \rangle} \frac{\partial \xi_A^{\langle J-I \rangle}}{\partial \phi_B^{(L)}}$$

can be considered as the *commutator of the evolutionary vector fields* Ξ and Λ,

$$\Psi F = [\Xi, \Lambda] F = \int (\xi(\lambda f) - \lambda(\xi f)),$$

with the Jacobi identity fulfilled for the commutator operation, and so these vector fields form a Lie algebra.

Let us comment upon the representation of the evolutionary vector fields as integrals, which is different from the traditional notations.

The formal variational calculus[5] operates with the local functionals which are expressed by single integrals of functions of the specified class, for example, infinitely differentiable ones. The functional forms and multi-vectors are expressed by similar integrals. The pairing of two such objects gives us a single integral again.

At the same time, other notations are widespread, especially in physical literature, which use the δ-function and its derivatives. Then a result of the pairing of two single integrals is understood as a double integral. But as this double integral contains the δ-function, it always can be converted into the single one.

This conversion of a double integral into the single one with the help of the δ-function is trivial when no boundary terms could arise. The subject of this work is just a study of the opposite case. The new rule is necessary here and it has been proposed in Ref. 6 as Rule 4.2:

$$\int_\Omega \int_\Omega f(x) g(y) D_J^{(x)} D_K^{(y)} \delta(x,y) = \int_\Omega D_K f D_J g. \tag{5}$$

In this article we give really new and equivalent forms of these rules which help to avoid the usage of double integrals at all.

The concept of vector field appeared initially in the course of studying the evolutionary differential equations and their symmetries. In the formal variational calculus[5] functionals are, in fact, replaced by equivalence classes of functions, and so the action of evolutionary vector fields onto local functionals is replaced by their action on functions:

$$\psi f = D_K \psi_A \frac{\partial f}{\partial \phi_A^{(K)}}.$$

However, to represent functionals by integrals and to require that the result of the action of an evolutionary vector field onto a local functional is a local functional, i.e., an integral, it is absolutely natural to represent the evolutionary vector fields also as integrals,

$$\Psi = \int_\Omega D_K \psi_A(x) \frac{\partial}{\partial \phi_A^{(K)}(x)} \equiv \int \psi,$$

in combination with the standard rule

$$\frac{\partial \phi_A^{(J)}(y)}{\partial \phi_B^{(K)}(x)} = \delta(x,y)\,\delta_{AB}\delta_{JK}\,. \tag{6}$$

Another argument supporting our notations is the equivalence between evolutionary vector fields and one-vectors, which is demonstrated for the standard formal variational calculus in Ref. 2 and also for the graded case in Sec. V of this article. One-vectors as a partial case of multivectors are always written as integrals.

Apart from the notational revision we would like to mention a new feature in our treatment of the vector fields: now they are not derivations when applied to standard functions, but only to the graded ones. Of course, in the traditional approach the vector fields are not derivations when applied to functionals, because the multiplication of functionals is not defined. But these vector fields, traditionally written without the integral sign, are derivations of functions. This property is partially lost here. It can be restored formally if we consider integrands containing θ as functions and take a relation

$$D_I\theta \times D_J\theta = D_{I+J}\theta \tag{7}$$

as a definition of their multiplication.

In this context, formula (4), introduced as a definition, can be interpreted also as a consequence of the standard relation (6) and a new definition (7).

Therefore, it is evident that our ''rule for multiplication of distributions'' taken from Ref. 6, i.e., Eq. (7), is nothing more than another way to define the pairing compatible with the introduced grading.

At last, let us mention the possibility to use other notations in this formalism. It is, of course, possible to avoid θ-functions and to use integrals over the domain Ω only. Then any local functional can be given as

$$F = \int_\Omega D_J f^{\langle\langle J\rangle\rangle},$$

where

$$f^{\langle\langle J\rangle\rangle} = (-1)^{|J|} f^{\langle J\rangle},$$

with analogous rewriting of the other objects. Correspondingly, Eq. (4) will be written as

$$\Psi F = \int_\Omega D_{I+J}\left(D_K \psi_A^{\langle\langle J\rangle\rangle} \frac{\partial f^{\langle\langle I\rangle\rangle}}{\partial \phi_A^{(K)}} \right).$$

III. DIFFERENTIALS AND FUNCTIONAL FORMS

The *differential of a local functional* is simply the first variation of it,

$$\mathrm{d}F = \int \theta^{(J)} \frac{\partial f^{\langle J\rangle}}{\partial \phi_A^{(K)}}\,\delta\phi_A^{(K)} \equiv \int \theta^{(J)} \mathrm{d}f^{\langle J\rangle} \equiv \int \mathrm{d}f.$$

Here and below $\delta\phi_A^{(K)} = D_K\delta\phi_A$. It can also be expressed through the Fréchet derivative (1) or through the higher Eulerian operators (2):

$$\mathrm{d}F = \int \theta^{(J)} f^{\langle J\rangle\prime}(\delta\phi) = \int \theta^{(J)} D_K(E_A^K(f^{\langle J\rangle})\,\delta\phi_A).$$

This differential is a special example of functional one-form. A general functional one-form can be written as

$$\Sigma=\int \theta^{(J)}\sigma^{\langle J\rangle}_{AK}\delta\phi^{(K)}_{A}\equiv\int \theta^{(J)}\sigma^{\langle J\rangle}\equiv\int \sigma.$$

Of course, the coefficients $\sigma^{\langle J\rangle}_{AK}$ are not unique since we can make formal integration by parts. Let us call the following expression the *canonical form of a functional one-form*:

$$\Sigma=\int \theta^{(J)}\sigma^{\langle J\rangle}_{A}\delta\phi_{A}\,.$$

Analogously, we can define *functional m-forms* as integrals or equivalence classes modulo formal divergences of vertical m-forms:

$$\Sigma=\frac{1}{m!}\int \theta^{(J)}\sigma^{\langle J\rangle}_{A_1K_1,\ldots,A_mK_m}\delta\phi^{(K_1)}_{A_1}\wedge\cdots\wedge\delta\phi^{(K_m)}_{A_m}=\int \theta^{(J)}\sigma^{\langle J\rangle}=\int \sigma.$$

Define the *pairing* (or the *interior product*) of an evolutionary vector field and one-form as

$$\Sigma(\Xi)=\Xi\lrcorner\Sigma=\int \theta^{(I+J)}\sigma^{\langle J\rangle}_{AK}D_K\xi^{\langle I\rangle}_{A}=\int \theta^{(I+J)}\sigma^{\langle J\rangle}(\xi^{\langle I\rangle})=\int \sigma(\xi). \tag{8}$$

The interior product of an evolutionary vector field and a functional m-form will be given as follows:

$$\Xi\lrcorner\Sigma=\frac{1}{m!}(-1)^{i+1}\int \theta^{(I+J)}\sigma^{\langle J\rangle}_{A_1K_1,\ldots,A_mK_m}D_{K_i}\xi^{\langle I\rangle}_{A_i}\delta\phi^{(K_1)}_{A_1}$$

$$\wedge\cdots\wedge\delta\phi^{(K_{i-1})}_{A_{i-1}}\wedge\delta\phi^{(K_{i+1})}_{A_{i+1}}\wedge\cdots\wedge\delta\phi^{(K_m)}_{A_m}.$$

Then a value of the m-form on the m evolutionary vector fields will be defined by the formula

$$\Sigma(\Xi_1,\ldots,\Xi_m)=\Xi_m\lrcorner\cdots\Xi_1\lrcorner\Sigma.$$

It can be checked by straightforward calculation that

$$(D\sigma)(\xi_1,\ldots,\xi_m)=D(\sigma(\xi_1,\ldots,\xi_m)).$$

The *differential of the m-form*, which is given as

$$\mathrm{d}\Sigma=\frac{1}{m!}\int \theta^{(J)}\frac{\partial\sigma^{\langle J\rangle}_{A_1K_1,\ldots,A_mK_m}}{\partial\phi^{(K)}_{A}}\delta\phi^{(K)}_{A}\wedge\delta\phi^{(K_1)}_{A_1}\wedge\cdots\wedge\delta\phi^{(K_m)}_{A_m}=\int \theta^{(J)}\mathrm{d}\sigma^{\langle J\rangle}=\int \mathrm{d}\sigma,$$

satisfies standard properties

$$\mathrm{d}^2=0$$

and

$$\mathrm{d}\Sigma(\Xi_1,\ldots,\Xi_{m+1})=\sum_i(-1)^{i+1}\Xi_i\Sigma(\Xi_1,\ldots,\hat{\Xi}_i,\ldots,\Xi_{m+1})$$

$$+\sum_{i<j}(-1)^{i+j}\Sigma([\Xi_i,\Xi_j],\Xi_1,\ldots,\hat{\Xi}_i,\ldots,\hat{\Xi}_j,\ldots,\Xi_{m+1}).$$

The *Lie derivative* of a functional form Σ along the evolutionary vector field Ξ can be introduced by the standard formula

$$L_{\Xi}\Sigma = \Xi \lrcorner \mathrm{d}\Sigma + \mathrm{d}(\Xi \lrcorner \Sigma).$$

IV. GRADED DIFFERENTIAL OPERATORS AND THEIR ADJOINTS

We call linear matrix differential operators of the form

$$\hat{I}_{AB} = \theta^{(J)} I_{AB}^{\langle J \rangle N} D_N$$

the *graded differential operators*.

Let us call the linear differential operator $\hat{I}^*$ the *adjoint* to $\hat{I}$ if for an arbitrary set of smooth functions f_A, g_A

$$\int f_A \hat{I}_{AB} g_B = \int g_A \hat{I}^*_{AB} f_B .$$

For coefficients of the adjoint operator we can derive the expression

$$I^{*\langle J \rangle M}_{AB} = (-1)^{|K|} \binom{K}{L} \binom{K-L}{M} D_{K-L-M} I_{BA}^{\langle J-L \rangle K}. \tag{9}$$

It is easy to check that the relation

$$\hat{I}_{AB}(x)\,\delta(x,y) = \hat{I}^*_{BA}(y)\,\delta(x,y)$$

follows from Rule 4.2 of Ref. 6. For example, we have

$$\left(\theta(x) \frac{\partial}{\partial x^i} + \theta(y) \frac{\partial}{\partial y^i} \right) \delta(x,y) = -\theta^{(i)} \delta(x,y). \tag{10}$$

In one of our previous publications[24] we tried to connect the appearance of surface terms in Poisson brackets and the standard manipulations with the δ-function. The ansatz used there for the above simplest example coincided with (10) up to the sign. The reason for this difference laid in the other choice made there instead of Rule 4.2 of Ref. 6. That ansatz lead us to the standard Poisson brackets, which are not appropriate for nontrivial boundary problems.

Operators satisfying the relation

$$\hat{I}^* = -\hat{I}$$

will be called the *antisymmetric* ones. With the help of them it is possible to express two-forms (and also two-vectors to be defined below) in the canonical form

$$\Sigma = \frac{1}{2} \int \delta\phi_A \wedge \hat{I}_{AB} \delta\phi_B .$$

It is clear that we can consider representations of functional forms as decompositions over the basis derived as a tensor product of $\delta\phi_A$, with the totally antisymmetric multilinear operators

$$\hat{\sigma} = \theta^{(J)} \sigma^{\langle J \rangle}_{A_1 K_1, \ldots, A_m K_m} (D_{K_1} \cdot, \ldots, D_{K_m} \cdot)$$

as coefficients of these decompositions.

V. MULTI-VECTORS, MIXED TENSORS AND SCHOUTEN–NIJENHUIS BRACKET

Let us introduce dual basis to $|\delta\phi_A\rangle$ by the relation

$$\left\langle \frac{\delta}{\delta\phi_B(y)}, \delta\phi_A(x) \right\rangle = \delta_{AB}\delta(x,y) \tag{11}$$

and construct by means of the tensor product a basis

$$\frac{\delta}{\delta\phi_{B_1}(y)} \otimes \frac{\delta}{\delta\phi_{B_2}(y)} \otimes \cdots \otimes \frac{\delta}{\delta\phi_{B_m}(y)}.$$

Then by using totally antisymmetric multilinear operators described in the previous section we can define the *functional m-vectors* (or *multi-vectors*)

$$\Psi = \frac{1}{m!} \int \theta^{(J)} \psi^{\langle J\rangle}_{B_1 L_1, \ldots, B_m L_m} D_{L_1} \frac{\delta}{\delta\phi_{B_1}} \wedge \cdots \wedge D_{L_m} \frac{\delta}{\delta\phi_{B_m}} = \int \theta^{(J)} \psi^{\langle J\rangle}.$$

Here a natural question on the relation between evolutionary vector fields and one-vectors arises. Evidently, evolutionary vector fields lose their form when being integrated by parts whereas one-vectors preserve it. Let us make a partial integration in the expression of a general evolutionary vector field

$$\Xi = \int \theta^{(J)} D_K \xi^{\langle J\rangle}_A \frac{\partial}{\partial \phi^{(K)}_A}$$

by removing D_K from $\xi^{\langle J\rangle}_A$. Then we get

$$\Xi = \int \xi^{\langle J\rangle}_A \theta^{(J+L)} (-1)^{|K|} \binom{K}{L} D_{K-L} \frac{\partial}{\partial \phi^{(K)}_A}.$$

It is easy to see that by using (7), i.e., Rule 5.4 from Ref. 6, in the backward direction we can write

$$\Xi = \int (\theta^{(J)} \xi^{\langle J\rangle}_A)(\theta^{(L)} (-1)^{|L|} E^L_A) = \int \theta^{(J)} \xi^{\langle J\rangle}_A \frac{\delta}{\delta\phi_A},$$

where the higher Eulerian operators (2) and the full variational derivative (Definition 5.1 of Ref. 6)

$$\frac{\delta F}{\delta\phi_A} = \sum (-1)^{|J|} E^J_A(f) D_J \theta$$

are consequently used. Therefore, we arrive at the following statement.

Statement 5.1: There is a one-to-one correspondence between the evolutionary vector fields and the functional one-vectors. The coefficients of a one-vector in the canonical form $\xi^{\langle J\rangle}_A$ are equal to the characteristics of the evolutionary vector field.

It is not difficult to show that we can deduce the pairing (interior product) of one-forms and one-vectors and this pairing preserves the identification. Really, the definition of the dual basis (11) and (7), i.e., Rule 5.4 of Ref. 6, permits us to derive that

$$\Sigma(\Xi)=\Xi\lrcorner\Sigma=\int\int\theta^{(I)}(x)\theta^{(J)}(y)\sigma^{\langle I\rangle}_{AK}(x)\xi^{\langle J\rangle}_{BL}(y)\left\langle D_L\frac{\delta}{\delta\phi_B(y)},D_K\delta\phi_A(x)\right\rangle$$
$$=\int\theta^{(I+J)}D_L\sigma^{\langle I\rangle}_{AK}D_K\xi^{\langle J\rangle}_{AL}$$
$$=\int\theta^{(I+J)}\sigma^{\langle I\rangle}(\xi^{\langle J\rangle})=\int\sigma(\xi)=\int\theta^{(I+J)}\mathrm{Tr}(\sigma^{\langle I\rangle}\xi^{\langle J\rangle}),$$

and when a one-vector is in the canonical form (only $L=0$ term is nonzero), this result coincides with Eq. (8).

This formula for the pairing will be exploited below also for the interior product of one-vectors and m-forms or one-forms and m-vectors. Its importance comes from the fact that it is invariant under the formal partial integration both in forms and in vectors, i.e.,

$$(\mathrm{D}\sigma)(\xi)=\mathrm{D}(\sigma(\xi))=\sigma(\mathrm{D}(\xi)).$$

Evidently, it is the trace construction for convolution of differential operators (as coefficients of tensor objects in the proposed basis) that guarantees this invariance.

The interior product of a one-vector onto m-form and, analogously, of a one-form onto m-vector is defined as

$$\Xi\lrcorner\Sigma=\frac{1}{m!}(-1)^{(i+1)}\int\theta^{(I+J)}D_{K_i}\xi^{\langle I\rangle}_{A_iL}D_L(\sigma^{\langle J\rangle}_{A_1K_1,\ldots,A_mK_m}\delta\phi^{(K_1)}_{A_1}$$
$$\wedge\cdots\wedge\delta\phi^{(K_{i-1})}_{A_{i-1}}\wedge\delta\phi^{(K_{i+1})}_{A_{i+1}}\wedge\cdots\wedge\delta\phi^{(K_m)}_{A_m})$$
$$=(-1)^{(i+1)}\int\theta^{(I+J)}\xi^{\langle I\rangle}\lrcorner\sigma^{\langle J\rangle}. \tag{12}$$

Then we also can define the value of m-form on m one-vectors (or, analogously, m-vector on m one-forms)

$$\Sigma(\Xi_1,\ldots,\Xi_m)=\Xi_m\lrcorner\cdots\Xi_1\lrcorner\Sigma=\int\theta^{(J+I_1+\ldots+I_m)}\mathrm{Tr}(\sigma^{\langle J\rangle}\xi_1^{\langle I_1\rangle}\cdots\xi_m^{\langle I_m\rangle}),$$

where each entry of multilinear operator σ acts only on the corresponding ξ, whereas each derivation of the operator ξ acts on the product of σ and all the rest of the ξ's.

It is possible to define the *differential of m-vector*

$$\mathsf{d}\Psi=\frac{1}{m!}\int\theta^{(J)}\frac{\partial\psi^{\langle J\rangle}_{A_1K_1,\ldots,A_mK_m}}{\partial\phi^{(L)}_B}\delta\phi^{(L)}_BD_{K_1}\frac{\delta}{\delta\phi_{A_1}}\wedge\cdots\wedge D_{K_m}\frac{\delta}{\delta\phi_{A_m}},$$

as an example of a mixed $\binom{m}{1}$ object. Evidently, $\mathsf{d}^2\Psi=0$.

With the help of the previous constructions we can define the *Schouten–Nijenhuis bracket*

$$[\Xi,\Psi]_{SN}=\mathsf{d}\Xi\lrcorner\Psi+(-1)^{pq}\mathsf{d}\Psi\lrcorner\Xi$$

for two multi-vectors of orders p and q. The result of this operation is $p+q-1$-vector and it is analogous to the Schouten–Nijenhuis bracket in tensor analysis.[1] Its use in the formal variational calculus is described in Refs. 2 and 3. However, in cited references this bracket is usually defined for operators. We can recommend Ref. 27 as an interesting source for the treatment of the Schouten–Nijenhuis bracket of multi-vectors. Our construction of this bracket guarantees a compatibility with the equivalence modulo divergences

$$[D\xi,\psi]_{SN}=D[\xi,\psi]_{SN}=[\xi,D\psi]_{SN}.$$

Statement 5.2: The Schouten–Nijenhuis bracket of functional one-vectors up to a sign coincides with the commutator of the corresponding evolutionary vector fields.

Proof: Let us take the two one-vectors in canonical form without loss of generality,

$$\Xi=\int \theta^{(J)}\xi_A^{\langle J\rangle}\frac{\delta}{\delta\phi_A},\quad \Psi=\int \theta^{(K)}\psi_B^{\langle K\rangle}\frac{\delta}{\delta\phi_B},$$

and compute

$$[\Xi,\Psi]_{SN}=\mathsf{d}\Xi\lrcorner\Psi-\mathsf{d}\Psi\lrcorner\Xi.$$

We have

$$\mathsf{d}\Xi=\int \theta^{(J)}\xi_A^{\langle J\rangle\prime}(\delta\phi)\frac{\delta}{\delta\phi_A}=\int \theta^{(J)}\frac{\partial\xi_A^{\langle J\rangle}}{\partial\phi_C^{(L)}}\delta\phi_C^{(L)}\frac{\delta}{\delta\phi_A},$$

and

$$\mathsf{d}\Xi\lrcorner\Psi=-\int \theta^{(J+K)}\frac{\partial\xi_A^{\langle J\rangle}}{\partial\phi_B^{(L)}}D_L\psi_B^{\langle K\rangle}\frac{\delta}{\delta\phi_A}.$$

Therefore, we obtain

$$[\Xi,\Psi]_{SN}=-\int \theta^{(J+K)}\left(D_L\psi_B^{\langle K\rangle}\frac{\partial\xi_A^{\langle J\rangle}}{\partial\phi_B^{(L)}}-D_L\xi_B^{\langle K\rangle}\frac{\partial\psi_A^{\langle J\rangle}}{\partial\phi_B^{(L)}}\right)\frac{\delta}{\delta\phi_A}=-[\Xi,\Psi],$$

and the proof is completed.

Statement 5.3 (Olver's lemma[2]): The Schouten–Nijenhuis bracket for two bivectors can be expressed in the form

$$[\Lambda,\Psi]_{SN}=-\frac{1}{2}\int \xi\wedge\hat{I}'(\hat{K}\xi)\wedge\xi-\frac{1}{2}\int \xi\wedge\hat{K}'(\hat{I}\xi)\wedge\xi, \tag{13}$$

where the two differential operators $\hat{I}$, $\hat{K}$ are the coefficients of the bivectors in their canonical form.

Proof: Let us consider the Schouten–Nijenhuis bracket for the two bivectors and without loss of generality take them in the canonical form

$$\Lambda=\frac{1}{2}\int \theta^{(L)}\xi_A\wedge I_{AB}^{\langle L\rangle N}D_N\xi_B,$$

$$\Psi=\frac{1}{2}\int \theta^{(M)}\xi_C\wedge K_{CD}^{\langle M\rangle P}D_P\xi_D,$$

where $\xi_A=\delta/\delta\phi_A$ and operators $\hat{I}$, $\hat{K}$ are antisymmetric. Then we have

$$\mathsf{d}\Lambda=\frac{1}{2}\int \theta^{(L)}\frac{\partial I_{AB}^{\langle L\rangle N}}{\partial\phi_E^{(J)}}\delta\phi_E^{(J)}\xi_A\wedge D_N\xi_B$$

and

$$\mathrm{d}\Lambda \lrcorner \Psi = \frac{1}{4}\int \theta^{(L+M)} \frac{\partial I_{AB}^{\langle L\rangle N}}{\partial \phi_C^{(J)}} D_J(K_{CD}^{\langle M\rangle P} D_P \xi_D) \wedge \xi_A \wedge D_N \xi_B$$
$$- \frac{1}{4}\int \theta^{(L+M)} D_P\left(\frac{\partial I_{AB}^{\langle L\rangle N}}{\partial \phi_D^{(J)}} \xi_A \wedge D_N \xi_B \right) \wedge D_J(\xi_C K_{CD}^{\langle M\rangle P}).$$

Now let us make integration by parts in the second term:

$$\mathrm{d}\Lambda \lrcorner \Psi = -\frac{1}{4}\int \theta^{(L+M)} \xi_A \wedge (I_{AB}^{\langle L\rangle N})'(\hat{K}^{\langle M\rangle}\xi) \wedge D_N \xi_B$$
$$- \frac{1}{4}\int \theta^{(L+M+Q)} (-1)^{|P|} \binom{P}{Q} \frac{\partial I_{AB}^{\langle L\rangle N}}{\partial \phi_D^{(J)}} \xi_A \wedge D_N \xi_B \wedge D_{J+P-Q}(\xi_C K_{CD}^{\langle M\rangle P}).$$

At last we change the order of multipliers under wedge product in the second term, make a replacement $M \to M-Q$ and organize the whole expression in the form

$$\mathrm{d}\Lambda \lrcorner \Psi = -\frac{1}{4}\int \theta^{(L+M)} \xi_A \wedge (I_{AB}^{\langle L\rangle N})'_C \left(\hat{K}_{CD}^{\langle M\rangle} \xi_D + (-1)^{|P|} \binom{P}{Q} \right.$$
$$\left. \times \binom{P-Q}{R} D_{P-Q-R} K_{CD}^{\langle M-Q\rangle p} D_R \xi_C \right) \wedge D_N \xi_B .$$

Having in mind the definition of adjoint operator (9) we can represent the final result of the calculation as follows,

$$[\Lambda, \Psi]_{SN} = -\frac{1}{2}\int \theta^{(L+M)} \xi \wedge ((\hat{I}^{\langle L\rangle})'(\hat{K}^{\langle M\rangle}\xi) + (\hat{K}^{\langle M\rangle})'(\hat{I}^{\langle L\rangle}\xi)) \wedge \xi,$$

thus supporting in this extended formulation the method, proposed in Ref. 2 for testing the Jacobi identity (see Sec. VII). For the general procedure of testing Hamiltonian properties see also Ref. 28.

VI. POISSON BRACKETS AND HAMILTONIAN VECTOR FIELDS

Let us call the bivector

$$\Psi = \frac{1}{2}\int \frac{\delta}{\delta \phi_A} \wedge \hat{I}_{AB} \frac{\delta}{\delta \phi_B},$$

formed with the help of the graded antisymmetric differential operator

$$\hat{I}_{AB} = \theta^{(L)} I_{AB}^{\langle L\rangle N} D_N,$$

the *Poisson bivector* if

$$[\Psi, \Psi]_{SN} = 0.$$

The operator $\hat{I}_{AB}$ is then called the *Hamiltonian operator*. We call the value of the Poisson bivector on the differentials of two functionals F and G,

$$\{F, G\} = \Psi(\mathrm{d}F, \mathrm{d}G) = \mathrm{d}G \lrcorner \mathrm{d}F \lrcorner \Psi,$$

the *Poisson bracket* of these functionals.

The explicit form of the Poisson bracket can easily be obtained. It depends on the explicit form of the functional differential, which can be changed by the formal partial integration. Of course, all the possible forms are equivalent. Taking the extreme cases we get an expression through Fréchet derivatives,

$$\{F,G\}=\int \theta^{(J)}\mathrm{Tr}(f'_A\hat{I}^{\langle J\rangle}_{AB}g'_B), \tag{14}$$

or through higher Eulerian operators (2),

$$\{F,G\}=\int \theta^{(J)}D_{P+Q}(E^P_A(f)\hat{I}^{\langle J\rangle}_{AB}E^Q_B(g)). \tag{15}$$

Theorem 6.1: *The Poisson bracket defined above satisfies the standard requirements of the bilinearity, antisymmetry and closure on the space of local functionals $\mathcal{A}$, i.e., Definition 2.3 of Ref. 6.*

Proof: (1) From the previous formulas (14) and (15) it is clear that $\{F,G\}$ is a local functional, (2) antisymmetry of $\{F,G\}$ is evident and (3) equivalence of the Jacobi identity to the Poisson bivector property will be proved in Sec. VII.

The result of interior product of the differential of a local functional H on the Poisson bivector (up to the sign) will be called the *Hamiltonian vector field* (or the *Hamiltonian one-vector*)

$$\hat{I}\mathrm{d}H=-\mathrm{d}H\lrcorner\Psi$$

corresponding to the Hamiltonian H. Evidently, the standard relations take place:

$$\{F,H\}=\mathrm{d}F(\hat{I}\mathrm{d}H)=(\hat{I}\mathrm{d}H)F.$$

Theorem 6.2: *The Hamiltonian vector field corresponding to the Poisson bracket of the functionals F and H coincides up to the sign with the commutator of the Hamiltonian vector fields corresponding to these functionals.*

Proof: Consider a value of the commutator of Hamiltonian vector fields $\hat{I}\mathrm{d}F$ and $\hat{I}\mathrm{d}H$ on the arbitrary functional G,

$$\begin{aligned}[\hat{I}\mathrm{d}F,\hat{I}\mathrm{d}H]G&=\hat{I}\mathrm{d}F(\hat{I}\mathrm{d}H(G))-\hat{I}\mathrm{d}H(\hat{I}\mathrm{d}F(G))\\&=\hat{I}\mathrm{d}F(\{G,H\})-\hat{I}\mathrm{d}H(\{G,F\})\\&=\{\{G,H\},F\}-\{\{G,F\},H\}=-\{G,\{F,H\}\}=-\hat{I}\mathrm{d}\{F,H\}(G),\end{aligned}$$

where we have used the Jacobi identity and antisymmetry of Poisson bracket. Due to the arbitrariness of G the proof is completed.

Example 6.3: Let us consider the first structure

$$\{u(x),u(y)\}=\tfrac{1}{2}(D_x-D_y)\delta(x,y)$$

of the Korteweg–de Vries equation (Example 7.6 of Ref. 2)

$$u_t=u_{xxx}+uu_x.$$

Construct the adjoint graded operator to θD according to Eq. (9),

$$(\theta D)^*=-\theta D-D\theta,$$

and the antisymmetric operator is

$$\hat{I} = \tfrac{1}{2}(\theta D - (\theta D)^*) = \theta D + \tfrac{1}{2} D\theta.$$

The Poisson bivector has a form

$$\Psi = \frac{1}{2}\int \theta\left(\frac{\delta}{\delta u} \wedge D\frac{\delta}{\delta u}\right).$$

The differential of a local functional H (for simplicity it is written in canonical form)

$$H = \int \theta h$$

is equal to

$$\mathrm{d}H = \int \theta h'(\delta u) = \int \theta^{(k)}(-1)^k E^k(h)\,\delta u,$$

where the Fréchet derivative or higher Eulerian operators can be used. Therefore, the Hamiltonian vector field generated by H is

$$\hat{I}\mathrm{d}H = -\mathrm{d}H \lrcorner \Psi = -\frac{1}{2}\int \theta\left(h'\left(D\frac{\delta}{\delta u}\right) - Dh'\left(\frac{\delta}{\delta u}\right)\right),$$

or

$$-\frac{1}{2}\int \theta^{(k)}(-1)^k (E^k(h)D - DE^k(h))\frac{\delta}{\delta u},$$

or also

$$-\frac{1}{2}\int \theta^{(k)}(-1)^k D_i (E^k(h)D - DE^k(h))\frac{\partial}{\partial u^{(i)}}.$$

The value of this vector field on another functional F coincides with the Poisson bracket

$$-\mathrm{d}F \lrcorner \mathrm{d}H \lrcorner \Psi = \{F,H\} = \frac{1}{2}\int \theta^{(k+l)}(-1)^{k+l}(E^k(f)DE^l(h) - E^k(h)DE^l(f)).$$

VII. PROOF OF THE JACOBI IDENTITY

In this section we will prove that the Jacobi identity for the Poisson bracket is fulfilled if and only if the Schouten–Nijenhuis bracket of the corresponding Poisson bivector with itself is equal to zero. This should complete the proof of Theorem 6.1.

Let us use one of the possible forms of the Poisson brackets given in the Appendix of Ref. 6:

$$\{F,G\} = \frac{1}{2}\int \theta^{(J)}\mathrm{Tr}(f'(\hat{I}^{\langle J\rangle}g') - g'(\hat{I}^{\langle J\rangle}f')),$$

where the differential operator $\hat{I}$ is not supposed to be antisymmetric for the easier comparison of this proof with that given in Ref. 6. We remind that in less condensed notations

$$\mathrm{Tr}(f'(\hat{I}g')) = \binom{J}{M}\binom{K}{L} D_L \frac{\partial f}{\partial \phi_A^{(J)}} D_{J+K-L-M} I_{AB}^N D_{N+M} \frac{\partial g}{\partial \phi_B^{(K)}}$$

(in the Appendix of Ref. 6 the indices M and L in the binomial coefficients of the same formula are unfortunately given in the opposite order).

We will estimate the bracket

$$\{\{F,G\},H\}=\frac{1}{2}\int \theta^{(J)}\mathrm{Tr}(\{f,g\}'(\hat{I}^{\langle J\rangle}h')-h'(\hat{I}^{\langle J\rangle}\{f,g\}')),$$

where $\{f,g\}$ denotes the integrand of $\{F,G\}$. Since the Fréchet derivative is a derivation we have

$$\{f,g\}'=\tfrac{1}{2}\theta^{(K)}\mathrm{Tr}(f''(\hat{I}^{\langle K\rangle}g',\cdot)+f'\hat{I}'^{\langle K\rangle}(\cdot)g'+g''(f'\hat{I}^{\langle K\rangle},\cdot)-(f\leftrightarrow g))$$

and

$$\mathrm{Tr}(\{f,g\}'\hat{I}h')=\tfrac{1}{2}\mathrm{Tr}(f''(\hat{I}g',\hat{I}h')+f'\hat{I}'(\hat{I}h')g'+g''(f'\hat{I},\hat{I}h')-(f\leftrightarrow g)).$$

Let us explain that f'' denotes the second Fréchet derivative, i.e., the symmetric bilinear operator arising in calculation of the second variation of the local functional F (in the canonical form):

$$f''(\xi,\eta)=\frac{\partial^2 f}{\partial\phi_A^{(J)}\partial\phi_B^{(K)}}D_J\xi_A D_K\eta_B.$$

When we put into entries of f'' operators under the trace sign it should be understood that these operators act on everything except their own coefficients, for example,

$$\mathrm{Tr}(f''(\hat{I}g',\hat{I}h'))=\binom{L}{P}\binom{L-P}{Q}\binom{M}{S}\binom{M-S}{T}$$
$$\times D_{L+M-P-Q-S-T}\frac{\partial^2 f}{\partial\phi_A^{(J)}\partial\phi_B^{(K)}}D_{J+T}\left(D_P\hat{I}_{AC}\frac{\partial g}{\partial\phi_C^{(L)}}\right)D_{K+Q}\left(D_S\hat{I}_{BD}\frac{\partial h}{\partial\phi_D^{(M)}}\right)$$

and the expression remains symmetric under permutation of its entries

$$\mathrm{Tr}(f''(\hat{I}g',\hat{I}h'))=\mathrm{Tr}(f''(\hat{I}h',\hat{I}g')).$$

When the operator $\hat{I}$ stands to the right from the operator of Fréchet derivative f' as in expression

$$\mathrm{Tr}(g''(\hat{I}h',f'\hat{I})),$$

it acts on everything except f'. At last, for the Fréchet derivative of the operator we have

$$\hat{I}'(\hat{I}h')=\frac{\partial I_{AB}^K}{\partial\phi_C^{(J)}}D_J\left(I_{CD}^L D_L\frac{\partial h}{\partial\phi_D^{(M)}}D_M\right)D_K.$$

Making similar calculations we get

$$\mathrm{Tr}(h'\hat{I}\{f,g\}')=\tfrac{1}{2}\mathrm{Tr}(f''(h'\hat{I},\hat{I}g')+f'\hat{I}'(h'\hat{I})g'+g''(f'\hat{I},h'\hat{I})-(f\leftrightarrow g))$$

and therefore

$$\{\{F,G\},H\}=\frac{1}{4}\int \theta^{(J+K)}\mathrm{Tr}(f''(\hat{I}^{\langle J\rangle}g',\hat{I}^{\langle K\rangle}h')-f''(h'\hat{I}^{\langle J\rangle},\hat{I}^{\langle K\rangle}g')-f''(\hat{I}^{\langle J\rangle}h',g'\hat{I}^{\langle K\rangle})$$
$$+f''(g'\hat{I}^{\langle J\rangle},h'\hat{I}^{\langle K\rangle})+f'\hat{I}'^{\langle J\rangle}(\hat{I}^{\langle K\rangle}h'-h'\hat{I}^{\langle K\rangle})g'-(f\leftrightarrow g)).$$

Just the first four terms, apart from the fifth containing the Fréchet derivative of the operator $\hat{I}$, were present in our proof for the non-ultralocal case given in Ref. 6 (only terms with zero grading were allowed for $\hat{I}$ there). After cyclic permutation of F, G, H all terms with the symmetric operator of the second Fréchet derivative are mutually cancelled and

$$\{\{F,G\},H\}+\text{c.p.}=\frac{1}{4}\int \theta^{(J+K)}\mathrm{Tr}(f'\hat{I}'^{\langle J\rangle}(\hat{I}^{\langle K\rangle}h'-h'\hat{I}^{\langle K\rangle})g'-g'\hat{I}'^{\langle J\rangle}(\hat{I}^{\langle K\rangle}h'-h'\hat{I}^{\langle K\rangle})f'+\text{c.p.}),$$

where cyclic permutations of F, G, and H are abbreviated to c.p. When operator $\hat{I}$ is given in explicitly antisymmetric form all the four terms are equal. Taking into account Olver's Lemma (13) we get

$$\{\{F,G\},H\}+\text{c.p.}=-[\hat{I},\hat{I}]_{SN}(\mathrm{d}F,\mathrm{d}G,\mathrm{d}H),$$

so finishing the proof.

VIII. EXAMPLES: NON-ULTRALOCAL OPERATORS WITH NONCONSTANT COEFFICIENTS

The second structure of the Korteweg–de Vries equation may serve as a counterexample to the hypothesis[29] that all operators which are Hamiltonian (modulo divergences) with respect to the standard Poisson brackets should also be Hamiltonian (exactly) in the new brackets.

Example 8.1:

Let us start with the standard expression (Example 7.6 of Ref. 2)

$$\{u(x),u(y)\}=\left(\frac{d^3}{dx^3}+\frac{2}{3}u\frac{d}{dx}+\frac{1}{3}\frac{du}{dx}\right)\delta(x,y)$$

and construct the adjoint operator to

$$\hat{K}=\theta(D_3+\tfrac{2}{3}uD+\tfrac{1}{3}Du),$$

which is

$$\hat{K}^*=-\theta(D_3+\tfrac{2}{3}uD+\tfrac{1}{3}Du)-D\theta(3D_2+\tfrac{2}{3}u)-3D_2\theta D-D_3\theta.$$

Then the antisymmetric operator

$$\hat{I}=\tfrac{1}{2}(\hat{K}-\hat{K}^*)=\theta(D_3+\tfrac{2}{3}uD+\tfrac{1}{3}Du)+D\theta(\tfrac{3}{2}D_2+\tfrac{1}{3}u)+\tfrac{3}{2}D_2\theta D+\tfrac{1}{2}D_3\theta$$

can be used for forming the bivector

$$\Psi=\frac{1}{2}\int \xi\wedge\hat{I}\xi,$$

where $\delta/\delta u=\xi$. This bivector has a form

$$\Psi=\frac{1}{2}\int\left(\theta\xi\wedge D_3\xi+\frac{3}{2}D\theta\xi\wedge D_2\xi+\left(\frac{3}{2}D_2\theta+\frac{2}{3}\theta u\right)\xi\wedge D\xi\right).$$

Then evaluating the Schouten–Nijenhuis bracket for the bivector with the help of Statement 5.3,

$$[\Psi,\Psi]_{SN}=\int\left(\frac{2}{3}\theta\xi\wedge D_3\xi\wedge D\xi+D\theta\xi\wedge D_2\xi\wedge D\xi\right),$$

and integrating the first term by parts we get

$$[\Psi,\Psi]_{SN}=\frac{1}{3}\int \theta D(\xi\wedge D\xi\wedge D_2\xi).$$

Therefore, instead of the Jacobi identity we have

$$\{\{F,G\},H\}+c.p.=-\frac{1}{3}\int_\Omega D_{i+j+k+1}(E^i(f)DE^j(g)D_2E^k(h)+\text{c.p.})dx.$$

So, the second structure of KdV equation can be Hamiltonian only under special boundary conditions.

Example 8.2: Now let consider another example which is also non-ultralocal, but the operator remains to be Hamiltonian in the new brackets independently of boundary conditions. The Euler equations for the flow of ideal fluid can be written[2] in Hamiltonian form as follows (Example 7.10 of Ref. 2):

$$\frac{\partial\omega}{\partial t}=\mathcal{D}\frac{\delta H}{\delta\omega},$$

where

$$H=\int \frac{1}{2}|\mathbf{u}|^2d^2x,\quad \omega=\nabla\times\mathbf{u}.$$

Let us limit our consideration by the two-dimensional case when ω has only one component ω and

$$\mathcal{D}=\omega_xD_y-\omega_yD_x,$$

where $\omega_i=D_i\omega$, $i=(x,y)$. We can construct the antisymmetric operator

$$\hat{I}=\tfrac{1}{2}(\theta\mathcal{D}-(\theta\mathcal{D})^*)=\theta(\omega_xD_y-\omega_yD_x)+\tfrac{1}{2}(D_y\theta\omega_x-D_x\theta\omega_y),$$

and then the bivector

$$\Psi=\frac{1}{2}\int \xi\wedge\hat{I}\xi=\frac{1}{2}\int \theta(\omega_x\xi\wedge\xi_y-\omega_y\xi\wedge\xi_x),$$

where $\xi=\delta/\delta\omega$. Statement 5.3 gives us

$$[\Psi,\Psi]_{SN}=\int (\theta(\omega_x(\xi\wedge\xi_{xy}\wedge\xi_y-\xi\wedge\xi_{yy}\wedge\xi_x)+\omega_y(\xi\wedge\xi_{xy}\wedge\xi_x-\xi\wedge\xi_{xx}\wedge\xi_y))$$
$$+(D_y\theta\omega_x-D_x\theta\omega_y)\xi\wedge\xi_x\wedge\xi_y),$$

and after integration by parts the expression can be reduced to zero.

IX. CONCLUSION

We have shown that there exists an extension of the standard formal variational calculus which incorporates divergences (without any specification of boundary conditions). It would be important to understand how this formalism is related to the constructions of the variational bicomplex.[30] It seems also rather interesting to study if some physically relevant algebras can be realized with the help of new Poisson brackets as algebras of local functionals. One such example is considered in Ref. 31. This formalism may be also applied to free boundary problems as shown in the next article of this series.[7]

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Boundary values as Hamiltonian variables. III. Ideal fluid with a free surface

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An application of the approach to Hamiltonian treatment of boundary terms proposed in previous articles of this series is considered. Here the Hamiltonian formalism is constructed and the role of standard boundary conditions is revealed for a inviscid compressible fluid with surface tension which moves in a field of the Newtonian gravitational potential. It is shown that these boundary conditions guarantee absence of singular contributions to the equations of motion, i.e., to the Hamiltonian vector field. From the other side the Hamiltonian variation contains a nonzero boundary term. Such Hamiltonians are usually treated as ''nondifferentiable'' or ''inadmissible.'' We conclude that nondifferentiable functionals can be admissible Hamiltonians for non-ultralocal Poisson brackets. We give a four-sided picture of free surface dynamics: both in Lagrangian and in Eulerian variables and also both in variational and in Hamiltonian approaches. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1478145]

I. INTRODUCTION

In our previous publications[1,2] we have tried to construct a general field theory Hamiltonian formalism preserving all boundary terms arising from any integration by parts. We address the reader to these references for the detailed motivation and elaboration of the approach. The purpose of this article is to apply this formalism to a concrete problem—the ideal compressible fluid dynamics—in order to clarify the role played by boundary conditions in fixing the class of admissible functionals. A new and general result, if compared with the approach suggested by Regge and Teitelboim,[3] which is now the most popular one (see, for example, Ref. 4), is the fact that this class may differ from the class of ''differentiable'' functionals for non-ultralocal Poisson brackets. A very short and preliminary presentation of this result has already appeared in Ref. 5 with two examples considered: Ashtekar variables in canonical gravity and hydrodynamics of ideal fluid. The first example later was treated in detail in Ref. 6. Here we intend to thoroughly study the second one.

Let us remind the reader first of the history of applications of the Hamiltonian approach to surface waves in the ideal (inviscid) fluid. In 1967 Zakharov[7] was the first who suggested to apply the canonical formalism to the waves on the surface of the incompressible fluid in the case of the potential flow. Later, in 1977, this problem was discussed also by Miles[8] and Milder.[9] In 1986 Lewis, Marsden, Montgomery, and Ratiu (LMMR)[10] suggested a new approach to a more general problem where the incompressible ideal fluid flow was already not supposed to be potential. In 1988 Abarbanel *et al.*[11] treated the compressible fluid case. The approaches by these authors were rather different. It would be interesting to rederive all these results on the base of the formalism proposed in Refs. 1 and 2. But here we limit ourselves to the compressible fluid case.

Henceforth the main objective of our study will be the compressible inviscid fluid dynamics described in Eulerian coordinates and the main method will be the Hamiltonian formalism preserving all the boundary terms. For completeness of this presentation we will remind the reader here of the connections between the four possible ways of the hydrodynamics description: the

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variational approach and the Hamiltonian approach both in Lagrangian and in Eulerian coordinates. These connections may be illustrated by the following commutative diagram

Variational Principle in Lagrangian variables	*Legendre transform* $\longrightarrow$	Hamiltonian formalism in Lagrangian variables
Clebsch$\downarrow$*potentials*		$\downarrow$*reduction*
Variational Principle in Eulerian variables	*Legendre transform*+*reduction* $\longrightarrow$	Hamiltonian formalism in Eulerian variables

Our presentation is new in the part related to boundary terms. As it was already mentioned before,[11] the reduction of Hamiltonian formalism from Lagrangian variables to Eulerian ones, first made by LMMR,[10] requires here a small modification.

We will step by step consider each of the four angles and each of the four arrows of the above diagram. For every case we consider both a fixed boundary and a free boundary.

Section II concerns the variational principle in Lagrangian variables. The Lagrangian description of fluid dynamics is similar to the mechanical one and the fluid is considered as a huge number of identical mass points. The basic variables are here the coordinates of the mass points. But one needs to add to the usual potential energy of particles moving in an external field (in our case this is a field of the Newtonian gravitational potential) the internal energy which is supposed to depend on the fluid density and specific entropy. Therefore thermodynamics comes into play and a fluid temperature and pressure appear.

When dealing with the free boundary case we use the approach first proposed in Ref. 11. In particular it allows us to include into the action the surface tension energy by a suitable way for a further step to the Hamiltonian formalism.

In Sec. III we describe the transform from the Lagrangian to the Hamiltonian formalism in Lagrangian variables. Here this transformation does not create a lot of difficulties; it is only necessary to find the conjugate momenta to the coordinates of fluid particles and to make the Legendre transform.

In the case of free boundary we need not go beyond the Regge–Teitelboim criterion when deriving Hamiltonian equations of motion. This is a consequence of ultralocality of the Poisson brackets.

Section IV deals with the transform from Lagrangian variables to Eulerian ones in the framework of Hamiltonian formalism. The Eulerian description in contrast to the Lagrangian one looks like a field theory rather than mechanics. The transformation to new variables is rather nontrivial because this transformation mixes the ''dependent'' (fields) and the ''independent'' (spatial coordinates) variables. All formal calculations of the Poisson brackets are made by means of δ-functions, and this could not be understood as a rigorous deduction in the free boundary case. But results of this deduction are justified by their self-consistence. In the fixed boundary case we present explicit calculations based on our previous work[2] to demostrate the fulfillment of the Jacobi identity. This is not an easy way to prove a result as has been observed in Ref. 10. At the moment we have no such easy proof of the Jacobi identity for the free boundary case. Nevertheless, the formalism gives us the Hamiltonian equations (or the Hamiltonian vector field) by means of the internal product of the one-form (the Hamiltonian variation) and the bivector which define the Poisson bracket. At first we have a singular contribution to the Hamiltonian vector field which is proportional to the boundary δ-function. But if we put a regularity condition, i.e., require this term to be zero, we obtain the standard boundary condition for this problem (which is also the natural boundary condition following from the variational principle).

In Sec. V we construct the variational principle in Eulerian variables. The interesting story of this problem for the fixed boundary case can be found in a book by Kupershmidt.[12] After adding to the Lagrangian (which is initially taken from the Lagrangian variables approach) some constraints, there appear Clebsch variables which in the next section will serve as canonical variables of the Hamiltonian formalism.

In the free boundary case we add to the action (with minus sign) the surface energy term. But this is not enough to obtain correct boundary conditions from the variational principle and we are to add a new surface term. Then the Lagrangian density is equal to the pressure. In the particular case of the two-dimensional potential flow of incompressible fluid without surface tension the fact that the dynamical boundary conditions follow from the variational principle has been revealed by Luke.[13] Zakharov[7] has shown almost simultaneously that these boundary conditions are Hamiltonian equations.

Section VI treats the transform from the variational principle for Eulerian variables to the Hamiltonian formalism. In the fixed boundary case the Clebsch variables become canonical ones. We use here the Faddeev–Jackiw approach,[14] i.e., simply invert the symplectic matrix without looking for Dirac's "primary constraints." [15] It is easy to express the standard momenta of the Eulerian approach by means of Clebsch variables. Poisson brackets for these momenta represent the diffeomorphism algebra. The Hamiltonian also can be expressed through these momenta and a few of the Clebsch potentials: density and entropy. All this closes our diagram in its down right angle.

In the case of free boundary a new function arises which refers to the position of the boundary and so variables become noncanonical. This time we use the Dirac method for dealing with constraints and derive the Dirac brackets to construct the Poisson bivector. It is written in other variables and so differs from the one found in Sec. IV. But applying it to find the Hamiltonian vector field, i.e., to derive Hamiltonian equations, we again arrive at the result of Sec. IV. Therefore the diagram is commutative also for the free boundary case.

It is necessary to mention that recently there has appeared[16] another formula for the Poisson bracket exactly fulfilling the Jacobi identity. But this new proposal is still not general enough to include the treatment of non-ultralocal brackets and so cannot be used in this work.

II. VARIATIONAL PRINCIPLE IN LAGRANGIAN VARIABLES

The description of the continuum media in Lagrangian variables is such that the motion of each separate mass point is explicitly provided. It allows us to derive the media equations from equations of motion for mass points. Also, the thermodynamic characteristics (internal energy, temperature, pressure, entropy, etc.) are included. The particles could be numbered, for example, by their initial positions. Let the motion go on in some (fixed or changing with time) region Ω of Euclidean space $\mathbb{R}^n$, and let $\mathbf{r}\in\Omega_0$ be the particle "number," whereas $\mathbf{Y}(t)$ is its position at an arbitrary moment of time t. For simplicity we limit ourselves to Cartesian coordinates. Then the law of motion is given by the following function:

$$\mathbf{Y}=\mathbf{Y}(\mathbf{r},t), \quad \text{where} \quad \mathbf{r}\equiv\mathbf{Y}(\mathbf{r},0).$$

Classical mechanics is a deterministic theory, therefore the existence of inverse function is guaranteed:

$$\mathbf{R}=\mathbf{R}(\mathbf{x},t), \quad \text{and so} \quad \mathbf{r}\equiv\mathbf{R}(\mathbf{Y}(\mathbf{r},t),t).$$

A. Fixed boundary

It is rather natural to expect that the media Lagrangian is expressed as an integral of the difference of the kinetic and potential energy densities (with the internal energy density added to the last one) taken over the region Ω_0:

$$L=\int_{\Omega_0}\rho_0(\mathbf{r})\left[\frac{\dot{\mathbf{Y}}^2}{2}-\Phi(\mathbf{Y})-\varepsilon(\rho(\mathbf{Y}),s_0(\mathbf{r}))\right]d\mathbf{r}. \tag{1}$$

Here $\dot{\mathbf{Y}}=\partial\mathbf{Y}/\partial t(\mathbf{r},t)$; $\Phi(\mathbf{Y})$ is the potential; and $\varepsilon(\rho,s_0)$ is the internal energy per unit mass which is a function of the mass density $\rho(\mathbf{Y})$ and the specific entropy $s_0(\mathbf{r})$, where $\rho_0(\mathbf{r})$ is the mass density taken at the initial instant of time $t=0$. It is suitable to introduce the transformation matices

$$J_{ij}=\frac{\partial Y^i}{\partial r^j}, \quad J^{ij}=\frac{\partial r^i}{\partial Y^j}. \tag{2}$$

Let us denote $J=\det|J_{ij}|$. It is evident that the following relation takes place:

$$J_{ij}J^{jk}=\delta_i^k.$$

Due to the mass conservation law we have

$$\rho_0(\mathbf{r})d\mathbf{r}=\rho(\mathbf{Y})d\mathbf{Y}, \quad \text{therefore} \quad \rho_0=\rho J.$$

The entropy is supposed to be adjusted to any separate particle and additive,

$$s_0(\mathbf{r})=s(\mathbf{Y}(\mathbf{r},t),t).$$

Some additional information is given by the first law of thermodynamics

$$\delta\varepsilon=Tds_0-pd\frac{1}{\rho},$$

where T is the absolute temperature and p is the pressure, i.e.,

$$T=\frac{\partial\varepsilon}{\partial s_0}, \quad p=\rho^2\frac{\partial\varepsilon}{\partial\rho}.$$

Varying the action as a functional of $\mathbf{Y}(\mathbf{r},t)$,

$$\delta\int_{t_1}^{t_2}Ldt=\int_{t_1}^{t_2}\int_{\Omega_0}\rho_0(\mathbf{r})\left[\dot{\mathbf{Y}}\frac{\partial}{\partial t}\delta\mathbf{Y}-\frac{\partial\Phi}{\partial\mathbf{Y}}\delta\mathbf{Y}-\frac{\partial\varepsilon}{\partial\rho}\delta\rho\right]d\mathbf{r},$$

where

$$\delta\rho=\delta\left(\frac{\rho_0}{J}\right)=-\frac{\rho_0}{J^2}\delta J,$$

and therefore

$$-\rho_0\frac{\partial\varepsilon}{\partial\rho}\delta\rho=p\,\delta J$$

leads to equations of motion. Taking into account that the Jacobian variation is given by the following formula,

$$\delta J=JJ^{ji}\delta J_{ij}=JJ^{ji}\frac{\partial}{\partial r^j}\delta Y^i,$$

we obtain

$$p\,\delta J=\frac{\partial}{\partial r^j}(pJJ^{ji}\delta Y^i)-JJ^{ji}\frac{\partial p}{\partial r^j}\delta Y^i-p\frac{\partial}{\partial r^j}(JJ^{ji})\delta Y^i.$$

In the Appendix it is shown that the last term is, in fact, zero. Taking into account that

$$\frac{\partial p}{\partial Y^i}=\frac{\partial p}{\partial r^j}\frac{\partial r^j}{\partial Y^i}=J^{ji}\frac{\partial p}{\partial r^j},$$

we arrive at the following expression for the action variation:

$$\delta\int_{t_1}^{t_2}L\,dt=\int_{\Omega_0}d\mathbf{r}\rho_0\dot{\mathbf{Y}}\delta\mathbf{Y}\Big|_{t_1}^{t_2}+\int_{t_1}^{t_2}\int_{\Omega_0}\delta\mathbf{Y}\left[-\rho_0\ddot{\mathbf{Y}}-\rho_0\frac{\partial\Phi}{\partial\mathbf{Y}}-J\frac{\partial p}{\partial\mathbf{Y}}\right]d\mathbf{r}+\int_{t_1}^{t_2}dt\oint_{\partial\Omega_0}pJJ^{ji}\delta Y^i dS_j. \tag{3}$$

According to the variational principle by Hamilton we are to fix variables at the boundaries of the time interval:

$$\delta\mathbf{Y}(t_1)=\delta\mathbf{Y}(t_2)=0.$$

The term with variation $\delta\mathbf{Y}$ on the spatial boundary $\partial\Omega_0$ is zero due to the fixed boundary conditions for domain $\Omega=\Omega_0$,

$$n_jJ^{ji}\delta Y^i|_{\partial\Omega_0}=0,\quad\text{or}\quad\mathbf{n}\cdot\delta\mathbf{Y}|_{\partial\Omega}=0, \tag{4}$$

where n^j is the normal to the boundary $\partial\Omega_0$ (for the definiteness here and below it is the unit outside normal), which is supposed to be smooth; correspondingly, $\mathbf{n}$ is the same vector given in coordinates $\mathbf{Y}$.

The meaning of these boundary conditions is that particles which occur on the boundary at the initial moment of time will stay there forever.

As the volume integral in the variation of action should be zero, we obtain the Lagrangian equations of motion in Lagrangian coordinates:

$$\ddot{\mathbf{Y}}=-\frac{\partial\Phi}{\partial\mathbf{Y}}-\frac{1}{\rho}\frac{\partial p}{\partial\mathbf{Y}},\quad\text{or}\quad\ddot{Y}^i=-JJ^{ji}\frac{\partial\Phi}{\partial r^j}-\frac{JJ^{ji}}{\rho_0}\frac{\partial p}{\partial r^j}. \tag{5}$$

B. Free boundary

Suppose now that the fluid boundary or some part of it is free. Then position of the boundary $\partial\Omega=\partial\Omega_t$ is to be decribed by dynamical variables. In the Eulerian approach it requires us to introduce a new independent function, but here it is sufficient to use the same variable $\mathbf{Y}(\mathbf{r},t)$, though its variation on the boundary now is not constrained by condition (4). Moreover, some new terms given by boundary integrals may arise in the action, for example, the energy of surface tension

$$L\to L-E_{\text{surf}},$$

which is defined (up to a constant) by the following expression,

$$E_{\text{surf}}=\tau\int_{\partial\Omega_t}dS=\tau\int_{\partial\Omega_t}n^i dS_i=\tau\int_{\Omega_t}\nabla\cdot\mathbf{n}d\mathbf{Y}, \tag{6}$$

where n^i is unit outward normal to the boundary which is smoothly continued onto the whole domain Ω. It is possible to treat such problems on the base of the formalism suggested in our previous papers,[1,2] but it should be slightly generalized. Let us introduce function $P_\Omega(\mathbf{Y})$, which is positive everywhere in the region Ω, equal to zero on the boundary $\partial\Omega$ and negative outside. Then we can formally write the integral over our domain Ω as an integral over the whole space $\mathbb{R}^n$:

$$\int_{\Omega} f d\mathbf{Y} = \int \theta(P_{\Omega}) f d\mathbf{Y}. \tag{7}$$

The required generalization is that earlier[1,2] we have not treated P_{Ω} as a variable, whereas now we do so. If we suppose $\nabla P_{\Omega} \neq 0$ on $\partial\Omega$, the unit outward normal to the boundary surface is given by the following formula:

$$\mathbf{n} = -\frac{\nabla P_{\Omega}}{|\nabla P_{\Omega}|}.$$

Then the surface tension energy of the fluid (6) may be written as follows:

$$E_{\text{surf}} = \tau \int \theta(P_{\Omega}) \nabla \cdot \mathbf{n} d\mathbf{Y} = -\tau \int (\nabla \theta \cdot \mathbf{n}) d\mathbf{Y}.$$

From the other side,

$$\frac{\partial \theta(P_{\Omega})}{\partial Y^i} = \frac{d\theta(P_{\Omega})}{dP_{\Omega}} \frac{\partial P_{\Omega}}{\partial Y^i}, \quad \frac{d\theta(P_{\Omega})}{dP_{\Omega}} = \left(\nabla \theta(P_{\Omega}) \cdot \frac{\nabla P_{\Omega}}{|\nabla P_{\Omega}|^2} \right), \tag{8}$$

i.e.,

$$E_{\text{surf}} = \tau \int \frac{d\theta(P_{\Omega})}{dP_{\Omega}} |\nabla P_{\Omega}| d\mathbf{Y}.$$

Let us introduce a notion

$$K = \nabla \cdot \mathbf{n}.$$

It is easy to be convinced that on the boundary K is equal to the trace of a second fundamental form of a boundary surface. Then

$$E_{\text{surf}} = \tau \int_{\Omega_t} K d\mathbf{Y} = \tau \int \theta(P_{\Omega}) K d\mathbf{Y}.$$

To deduce a natural boundary condition we are to find a variation of this expression when function $\mathbf{Y}(\mathbf{r},t)$ is varied. First consider the surface energy variation due to varying P_{Ω}:

$$\delta E_{\text{surf}} = \tau \int \frac{d\theta(P_{\Omega})}{dP_{\Omega}} \delta P_{\Omega} K d\mathbf{Y} + \tau \int \theta(P_{\Omega}) \delta K d\mathbf{Y}.$$

Let us demonstrate that the second term is really zero (we omit $d\mathbf{Y}$),

$$\int \theta(P_{\Omega}) \delta K = \int \theta(P_{\Omega}) \delta \nabla \cdot \mathbf{n} = -\int \nabla \theta(P_{\Omega}) \delta \mathbf{n} = -\int \frac{d\theta}{dP_{\Omega}} |\nabla P_{\Omega}| (\mathbf{n} \cdot \delta \mathbf{n}) = 0, \tag{9}$$

as the only contribution to the integral comes from the boundary $\partial\Omega$, and the unit normal variation on the boundary is orthogonal to the normal itself. Therefore we obtain

$$\delta E_{\text{surf}} = \tau \int \frac{d\theta}{dP_{\Omega}} K \delta P_{\Omega} d\mathbf{Y}.$$

We will use this formula as it is when dealing with Eulerian coordinates. But here we are to find variation δE_{surf} induced by variation $\delta\mathbf{Y}$, as P_Ω is not an independent variable in the Lagrangian picture. The point is that the domain of definition for $\mathbf{r}$, i.e., Ω_0, does not change even in the case of the variable domain Ω.

Instead of function $P_\Omega(\mathbf{Y},t)$, corresponding to Ω, for the region Ω_0 we can use function

$$P_{\Omega_0}(\mathbf{r}) = P_\Omega(\mathbf{Y}(\mathbf{r},t),t)$$

or

$$P_\Omega(\mathbf{x},t) = P_{\Omega_0}(\mathbf{R}(\mathbf{x},t)).$$

Function $P_{\Omega_0}(\mathbf{r})$ should not be varied as also functions $\rho_0(\mathbf{r})$ and $s_0(\mathbf{r})$. Therefore we should take into account the following equation:

$$\delta P_\Omega = \frac{\partial P_\Omega}{\partial \mathbf{Y}}\,\delta\mathbf{Y} = \frac{\partial P_{\Omega_0}}{\partial r^j} J^{ji}\delta Y^i.$$

Then

$$\delta E_{\text{surf}} = \tau \int \frac{d\theta}{dP_\Omega}\frac{\partial P_\Omega}{\partial Y_i} K\,\delta Y^i d\mathbf{Y},$$

or, taking into account (8),

$$\delta E_{\text{surf}} = \tau \int \theta_{,j} K J J^{ji}\delta Y^i d\mathbf{r} = -\tau \int_{\Omega_0} \partial_j (K J J^{ji}\delta Y^i) d\mathbf{r}.$$

This term, together with the surface term from Eq. (3), give us the full surface contribution to the action variation in the free boundary case:

$$(\delta S)_{\text{surf}} = \int_{t_1}^{t_2} dt \int_{\Omega_0} \partial_j ((p-\tau K) J J^{ji}\delta Y^i) d\mathbf{r} = \int_{t_1}^{t_2} dt \oint_{\partial\Omega_0} (p-\tau K) J J^{ji}\delta Y^i dS_j\,.$$

The variational principle by Hamilton requires this term to be zero and as variation $\delta\mathbf{Y}$ is here arbitrary we obtain the so-called natural boundary conditions:[17,18]

$$(p-\tau K)\big|_{\partial\Omega_0} = 0. \tag{10}$$

As boundary maps to boundary after the coordinate transform $\mathbf{r}\to\mathbf{Y}(\mathbf{r},t)$, the last equality can be rewritten in the standard form:[19]

$$(p-\tau K)\big|_{\partial\Omega} = 0. \tag{11}$$

III. HAMILTONIAN FORMALISM IN LAGRANGIAN VARIABLES

A. Fixed boundary

It is easy to see from the action variation (3) that the momenta conjugated to variables $\mathbf{Y}(\mathbf{r},t)$ are as follows:

$$\mathbf{M}(\mathbf{r},t) = \rho_0(\mathbf{r})\dot{\mathbf{Y}}(\mathbf{r},t), \quad \{Y^i(\mathbf{r},t), M_j(\mathbf{r}',t)\} = \delta^i_j \delta(\mathbf{r},\mathbf{r}').$$

The standard Legendre transform of Lagrangian (1) leads to the following Hamiltonian:

$$\mathrm{H}=\int_{\Omega_0}\left(\frac{\mathbf{M}^2}{2\rho_0}+\rho_0\Phi(\mathbf{Y})+\rho_0\varepsilon(\rho(\mathbf{Y}),s_0)\right)d\mathbf{r}. \tag{12}$$

In the Hamiltonian variation

$$\delta\mathrm{H}=\int_{\Omega_0}\left(\delta\mathbf{M}\left[\frac{\mathbf{M}}{\rho_0}\right]+\delta\mathbf{Y}\left[\rho_0\frac{\partial\Phi}{\partial\mathbf{Y}}+J\frac{\partial p}{\partial\mathbf{Y}}\right]\right)d\mathbf{r}-\int_{\partial\Omega_0}pJJ^{ji}\delta Y^i dS_j$$

the last term becomes zero if boundary conditions (4) are valid. This result gives us an opportunity to treat the expressions in square brackets as variational derivatives. Then Hamiltonian equations reduce to the standard form

$$\dot{\mathbf{Y}}=\{\mathbf{Y},\mathrm{H}\}=\frac{\delta\mathrm{H}}{\delta\mathbf{M}},\quad \dot{\mathbf{M}}=\{\mathbf{M},\mathrm{H}\}=-\frac{\delta\mathrm{H}}{\delta\mathbf{Y}} \tag{13}$$

or, explicitly,

$$\dot{\mathbf{Y}}=\frac{\mathbf{M}}{\rho_0},\quad \dot{\mathbf{M}}=-\rho_0\frac{\partial\Phi}{\partial\mathbf{Y}}-J\frac{\partial p}{\partial\mathbf{Y}}. \tag{14}$$

It is easy to see that these equations are equivalent to Lagrangian ones (5). As to the Jacobi identity, canonical Poisson brackets defined in Refs. 1 and 2 satisfy it without any reference to boundary conditions as shown there.

B. Free boundary

Let us add to Hamiltonian (12) the surface energy

$$\mathrm{H}=\int_{\Omega_0}\left(\frac{\mathbf{M}^2}{2\rho_0}+\rho_0\Phi(\mathbf{Y})+\rho_0\varepsilon(\rho(\mathbf{Y}),s_0)\right)d\mathbf{r}+\tau\int_{\partial\Omega}n^i dS_i.$$

Now its variation is as follows,

$$\delta\mathrm{H}=\int_{\Omega_0}\left(\delta\mathbf{M}\left[\frac{\mathbf{M}}{\rho_0}\right]+\delta\mathbf{Y}\left[\rho_0\frac{\partial\Phi}{\partial\mathbf{Y}}+J\frac{\partial p}{\partial\mathbf{Y}}\right]\right)d\mathbf{r}-\int_{\partial\Omega_0}(p-\tau K)JJ^{ji}\delta Y^i dS_j,$$

where variation $\delta\mathbf{Y}$ is free on the boundary. Then we calculate the full variational derivatives

$$\frac{\delta\mathrm{H}}{\delta Y^i}=\theta(P_{\Omega_0})\left[\rho_0\frac{\partial\Phi}{\partial Y^i}+J\frac{\partial p}{\partial Y^i}\right]+\frac{\partial\theta(P_{\Omega_0})}{\partial r^i}[p-\tau K],$$

$$\frac{\delta\mathrm{H}}{\delta M^i}=\theta(P_{\Omega_0})\left[\frac{M^i}{\rho_0}\right].$$

The Hamiltonian vector field and equations of motion are formally the same as in the fixed boundary case (13). But now there is a singular contribution proportional to the δ-function. If we demand that this term has to be zero, we get standard boundary conditions (10). Here the Poisson bracket is canonical, and so, ultralocal,

$$\{\mathrm{F},\mathrm{G}\}=-\mathrm{d}\mathrm{F}\lrcorner\mathrm{d}\mathrm{G}\lrcorner\Psi=\int\left(\frac{\delta\mathrm{F}}{\delta Y^i}\frac{\delta\mathrm{G}}{\delta M_i}-\frac{\delta\mathrm{G}}{\delta Y^i}\frac{\delta\mathrm{F}}{\delta M_i}\right)d\mathbf{r},$$

therefore this requirement is equivalent to the disappearance of the surface term in the Hamiltonian variation, i.e., to the ''differentiability'' condition for the Hamiltonian in accordance with

Regge–Teitelboim approach.[3] Below we will see that these two requirements are not equivalent in the case of non-ultralocal Poisson brackets. As to the Jacobi identity the arguments given above for the fixed boundary are still valid because $\partial\Omega_0$ is not dynamical.

Let us mention as a curious thing that both in Ref. 10, and in our paper, Ref. 1, just similar nonzero surface terms in the Hamiltonian variation for incompressible fluid have served as a motivation to modify the standard formula for Poisson bracket. But in Ref. 11 it was reasonably stated that just this surface contribution should be zero as a consequence of boundary conditions. Such contributions, as we will see below, are important only for more complicated situations when Poisson brackets are non-ultralocal.

IV. HAMILTONIAN FORMALISM IN EULERIAN VARIABLES

A. Fixed boundary

The step from the Lagrangian description to the Eulerian one on the base of Hamiltonian formalism is a change of variables of the more general type than we used to do in the field theory. In some sense such a change is like general relativity transformations making coordinates dependent on the metric tensor (c-numbers become functions of q-numbers in quantum theory),

$$M_i(\mathbf{r},t)d\mathbf{r}=\pi_i(\mathbf{Y}(\mathbf{r},t),t)d\mathbf{Y},$$

or

$$\pi_i(\mathbf{x},t)=\int_{\Omega_0}\delta(\mathbf{x}-\mathbf{Y}(\mathbf{r},t))M_i(\mathbf{r},t)d\mathbf{r}.$$

Analogous relations are valid for mass densities in the two approaches

$$\rho_0(\mathbf{r})d\mathbf{r}=\rho(\mathbf{Y}(\mathbf{r},t),t)d\mathbf{Y},\quad \rho(\mathbf{x},t)=\int_{\Omega_0}\delta(\mathbf{x}-\mathbf{Y}(\mathbf{r},t))\rho_0(\mathbf{r})d\mathbf{r},$$

but equations for the specific entropy are different as it is a scalar, not a scalar density:

$$s(\mathbf{x},t)=s_0(\mathbf{R}(\mathbf{x},t)),\quad s(\mathbf{x},t)=\int_{\Omega_0}\delta(\mathbf{r}-\mathbf{R}(\mathbf{x},t))s_0(\mathbf{r})d\mathbf{r}. \tag{15}$$

Here

$$\mathbf{R}(\mathbf{Y}(\mathbf{r},t),t)\equiv\mathbf{r},\quad \mathbf{Y}(\mathbf{R}(\mathbf{x},t),t)\equiv\mathbf{x}.$$

Though momenta $M_i(\mathbf{r},t)$ are replaced in the Eulerian approach by an equal number of degrees of freedom $\pi_i(\mathbf{x},t)$, coordinates $Y^i(\mathbf{r},t)$ are replaced by new variables $\rho(\mathbf{x},t)$, $s(\mathbf{x},t)$, and their number in general is not equal to the spatial dimension. We will see, after all, that even for the new momenta π_i Poisson brackets are different from canonical ones.

To calculate the Poisson brackets for the new variables it is convenient to go to their linear functionals, as follows,

$$\pi(\lambda)=\int_\Omega d\mathbf{x}\lambda^i(\mathbf{x})\pi_i(\mathbf{x})=\int_\Omega d\mathbf{x}\int_{\Omega_0}d\mathbf{r}\lambda^i(\mathbf{x})\delta(\mathbf{x}-\mathbf{Y}(\mathbf{r},t))M_i(\mathbf{r},t)=\int_{\Omega_0}d\mathbf{r}\lambda^i(\mathbf{Y}(\mathbf{r},t))M_i(\mathbf{r},t).$$

Therefore

$$\{\pi(\lambda),\pi(\mu)\}=\int_{\Omega_0}d\mathbf{r}\int_{\Omega_0}d\mathbf{r}'\{\lambda^i(\mathbf{Y}(\mathbf{r},t))M_i(\mathbf{r},t),\mu^j(\mathbf{Y}(\mathbf{r}',t))M_j(\mathbf{r}',t)\}$$

$$=\int_{\Omega_0}d\mathbf{r}\int_{\Omega_0}d\mathbf{r}'\Big(\{\lambda^i(\mathbf{Y}(\mathbf{r},t)),M_j(\mathbf{r}',t)\}M_i(\mathbf{r},t)\mu^j(\mathbf{Y}(\mathbf{r}',t))$$

$$+\{M_i(\mathbf{r},t),\mu^j(\mathbf{Y}(\mathbf{r}',t))\}\lambda^i(\mathbf{Y}(\mathbf{r},t))M_j(\mathbf{r}',t)$$

$$=-\int_{\Omega_0}d\mathbf{r}[\lambda,\mu]^iM_i$$

$$=-\int_{\Omega}d\mathbf{x}[\lambda,\mu]^i\pi_i=-\pi([\lambda,\mu]),\tag{16}$$

where

$$[\lambda,\mu]^i=\lambda^j\mu^i_{,j}-\mu^j\lambda^i_{,j}.$$

In a similar way we obtain

$$\{\rho(\lambda),\pi(\mu)\}=\rho(\mu^i\lambda_{,i}).\tag{17}$$

By using results from previous papers[1,2] we come to the conclusion that Eqs. (16) and (17) locally are equivalent to the following equations:

$$\{\pi_i(\mathbf{x}),\pi_j(\mathbf{x}')\}=\pi_i(\mathbf{x}')\,\delta_{,j}(\mathbf{x}',\mathbf{x})-\pi_j(\mathbf{x})\,\delta_{,i}(\mathbf{x},\mathbf{x}'),\tag{18}$$

$$\{\rho(\mathbf{x}),\pi_i(\mathbf{x}')\}=\rho(\mathbf{x}')\,\delta_{,i}(\mathbf{x}',\mathbf{x}).\tag{19}$$

It is easy to see that these Poisson brackets correspond to the standard realization of the diffeomorphism algebra with generators given by variables $\pi_i(\mathbf{x})$.

The Poisson bracket for $\rho(\mathbf{x})$ corresponds to the scalar density transformation law. In contrast, $s(\mathbf{x})$ transforms as a scalar, i.e.,

$$\{s(\mathbf{x}),\pi(\mathbf{x}')\}=-s_{,i}\delta(\mathbf{x},\mathbf{x}').\tag{20}$$

Apparently all other brackets are zero.

Poisson brackets for arbitrary local functionals of variables $\pi_i(\mathbf{x})$, $\rho(\mathbf{x})$, $s(\mathbf{x})$ can be derived with account for all the boundary terms on the base of the Poisson bivector, interior product operation, and the full variation (differential) of local functional defined according to our formalism:[2]

$$\{\mathrm{F},\mathrm{G}\}=-\mathrm{dF}\lrcorner\mathrm{dG}\lrcorner\Psi.$$

For example, in the simplest case, if the boundary of domain Ω is fixed and if everything depends only on variables $\pi_i(\mathbf{x})$, $\rho(\mathbf{x})$, $s(\mathbf{x})$, but not on their spatial derivatives, we obtain

$$\{F,G\}=\int_{\Omega}d\mathbf{x}\Big[\rho\Big(\partial_i\Big(\frac{\partial f}{\partial\rho}\Big)\frac{\partial g}{\partial\pi_i}-\partial_i\Big(\frac{\partial g}{\partial\rho}\Big)\frac{\partial f}{\partial\pi_i}\Big)-s_{,i}\Big(\frac{\partial f}{\partial s}\frac{\partial g}{\partial\pi_i}-\frac{\partial g}{\partial s}\frac{\partial f}{\partial\pi_i}\Big)$$

$$+\pi_i\Big(\partial_j\Big(\frac{\partial f}{\partial\pi_i}\Big)\frac{\partial g}{\partial\pi_j}-\partial_j\Big(\frac{\partial g}{\partial\pi_i}\Big)\frac{\partial f}{\partial\pi_j}\Big)\Big].$$

The analytical form of the Hamiltonian practically does not change after the transform to Eulerian variables:

$$\mathrm{H}=\int_{\Omega} d\mathbf{x}\left(\frac{\pi^2}{2\rho}+\rho\Phi(\mathbf{x})+\rho\varepsilon(\rho,s)\right). \tag{21}$$

Its variational derivatives are as follows:

$$\frac{\delta \mathrm{H}}{\delta \pi_i}=\theta\frac{\pi_i}{\rho},$$

$$\frac{\delta \mathrm{H}}{\delta \rho}=\theta\left(-\frac{\pi^2}{2\rho^2}+\Phi+\varepsilon+\frac{p}{\rho}\right),$$

$$\frac{\delta \mathrm{H}}{\delta s}=\theta\rho\frac{\partial\varepsilon}{\partial s}=\theta\rho T.$$

The Hamiltonian equations are derived by means of the interior product of the Hamiltonian differential and the Poisson bivector according to the general formalism.[2] It is convenient to rewrite these equations in terms of the Eulerian velocity $v^i=\pi_i/\rho$,

$$\dot{\rho}=-(\rho v^i)_{,i}, \tag{22}$$

$$\dot{s}=-v^i s_{,i}, \tag{23}$$

$$\dot{v}^i=-v^j v^i_{,j}-\Phi_{,i}-\frac{p_{,i}}{\rho}, \tag{24}$$

where $p=\rho^2\partial\varepsilon/\partial\rho$. To test the Jacobi identity here we can exploit an approach presented and motivated in our previous work.[2] In fact, this calculation is different from the one presented, for example, in Olver's book[20] only by preserving all the boundary contributions. The bivector which determines the Poisson bracket is as follows:

$$\begin{aligned}\Psi&=\frac{1}{2}\int\int\frac{\delta}{\delta\phi_A(x)}\{\phi_A(x),\phi_B(y)\}\wedge\frac{\delta}{\delta\phi_B(y)}\\&=\frac{1}{2}\int\int\frac{\delta}{\delta\pi_i(x)}\{\pi_i(x),\pi_j(y)\}\wedge\frac{\delta}{\delta\pi_j(y)}+\frac{\delta}{\delta\rho(x)}\{\rho(x),\pi_i(y)\}\wedge\frac{\delta}{\delta\pi_i(y)}\\&\quad+\frac{\delta}{\delta\pi_i(x)}\{\pi_i(x),\rho(y)\}\wedge\frac{\delta}{\delta\rho(y)}+\frac{\delta}{\delta s(x)}\{s(x),\pi_i(y)\}\wedge\frac{\delta}{\delta\pi_i(y)}\\&\quad+\frac{\delta}{\delta\pi_i(x)}\{\pi_i(x),s(y)\}\wedge\frac{\delta}{\delta s(y)}.\end{aligned}$$

After some transformations and integrations we can get another form of it:

$$\Psi=\int\pi_i D_j\left(\frac{\delta}{\delta\pi_i}\right)\wedge\frac{\delta}{\delta\pi_j}+\rho D_i\left(\frac{\delta}{\delta\rho}\right)\wedge\frac{\delta}{\delta\pi_i}-s_{,i}\frac{\delta}{\delta s}\wedge\frac{\delta}{\delta\pi_i}.$$

Then it is easy to see that

$$\mathrm{d}\Psi=\int\delta\pi_i D_j\left(\frac{\delta}{\delta\pi_i}\right)\wedge\frac{\delta}{\delta\pi_i}+\delta\rho D_i\left(\frac{\delta}{\delta\rho}\right)\wedge\frac{\delta}{\delta\pi_i}-(\delta s)_{,i}\frac{\delta}{\delta s}\wedge\frac{\delta}{\delta\pi_i},$$

and therefore

$$\begin{aligned}\mathrm{d}\Psi \lrcorner \Psi = \int \pi_i D_k\left[D_j\left(\frac{\delta}{\delta\pi_i}\right)\wedge\frac{\delta}{\delta\pi_j}\right]\wedge\frac{\delta}{\delta\pi_k} - D_j\left(\frac{\delta}{\delta\pi_i}\right)\wedge\frac{\delta}{\delta\pi_j}\wedge\pi_k D_i\left(\frac{\delta}{\delta\pi_k}\right)\\ - D_j\left(\frac{\delta}{\delta\pi_i}\right)\wedge\frac{\delta}{\delta\pi_j}\wedge\rho D_i\left(\frac{\delta}{\delta\rho}\right) + s_{,i}D_j\left(\frac{\delta}{\delta\pi_i}\right)\wedge\frac{\delta}{\delta\pi_j}\wedge\frac{\delta}{\delta s}\\ + D_k\left[D_i\left(\frac{\delta}{\delta\rho}\right)\wedge\frac{\delta}{\delta\pi_i}\right]\wedge\rho\frac{\delta}{\delta\pi_k} + \frac{\delta}{\delta s}\wedge\frac{\delta}{\delta\pi_i}\wedge D_i\left(s_{,k}\frac{\delta}{\delta\pi_k}\right).\end{aligned}$$

By straightforward calculation, preserving all divergences, it is easy to check that this expression vanishes exactly (not up to divergences). It means that the Schouten–Nijenhuis bracket of bivector Ψ with itself becomes zero as for bivectors

$$[\Psi,\Psi]_{SN} = \mathrm{d}\Psi\lrcorner\Psi + (-1)^{2\cdot 2}\mathrm{d}\Psi\lrcorner\Psi = 2\,\mathrm{d}\Psi\lrcorner\Psi,$$

and as it has been proved in Ref. 2 that this is equivalent to the Jacobi identity fulfillment for arbitrary local functionals:

$$\{\{F,G\},H\}+\{\{H,F\},G\}+\{\{G,H\},F\} = -[\Psi,\Psi]_{SN}(\mathrm{d}F,\mathrm{d}G,\mathrm{d}H). \tag{25}$$

B. Free boundary

If we were working in Lagrangian coordinates, the same set of variables as in the case of fixed boundary was enough, but here we should add function $P_\Omega(\mathbf{x},t)$ introduced earlier in (7) as an independent dynamical variable. The following formulas analogous to (15) are valid:

$$P_\Omega(\mathbf{x},t) = P_0(\mathbf{R}(\mathbf{x},t)), \quad P_\Omega(\mathbf{x},t) = \int_{\Omega_0}\delta(\mathbf{r}-\mathbf{R}(\mathbf{x},t))P_0(\mathbf{r})d\mathbf{r},$$

therefore the Poisson brackets for $P_\Omega(\mathbf{x},t)$ are in close analogy with brackets for the entropy variable $s(\mathbf{x},t)$

$$\{P_\Omega(\mathbf{x},t),\pi^i(\mathbf{x}',t)\} = -P_{\Omega,i}\delta(\mathbf{x},\mathbf{x}'),$$

brackets of $P_\Omega(\mathbf{x},t)$ with other variables are zero.

In the free boundary case the Hamiltonian depends on function P_Ω both through the argument of θ-function and through the surface energy expression (6):

$$\mathrm{H} = \int \theta(P_\Omega)\left[\frac{\boldsymbol{\pi}^2}{2\rho}+\rho\Phi(\mathbf{x})+\rho\varepsilon(\rho,s)+\tau\nabla\cdot\mathbf{n}\right]d\mathbf{x}, \tag{26}$$

moreover in the last case it also depends on spatial derivatives of function P_Ω up to the second order. But taking into account relation (9), the full variational derivative of the Hamiltonian over function P_Ω is equal to the following expression:

$$\frac{\delta\mathrm{H}}{\delta P_\Omega} = \frac{d\theta}{dP_\Omega}\left[\frac{\pi^2}{2\rho}+\rho\Phi(\mathbf{x})+\rho\varepsilon(\rho,s)+\tau\nabla\cdot\mathbf{n}\right], \tag{27}$$

or

$$\frac{\delta\mathrm{H}}{\delta P_\Omega} = \theta_{,i}\frac{P_{\Omega,i}}{|P_{\Omega,i}|^2}\left[\frac{\pi^2}{2\rho}+\rho\Phi(\mathbf{x})+\rho\varepsilon(\rho,s)+\tau K\right].$$

The derivatives over other variables do not change if compared with the fixed boundary case.

According to our definitions,[1,2] from the Poisson bivector

$$\Psi = \frac{1}{2}\int\int \frac{\delta}{\delta\phi_A(\mathbf{x})}\wedge\frac{\delta}{\delta\phi_B(\mathbf{y})}\{\phi_A(\mathbf{x}),\phi_B(\mathbf{y})\}d\mathbf{x}d\mathbf{y}$$
$$= \int \pi_i D_j\left(\frac{\delta}{\delta\pi_i}\right)\wedge\frac{\delta}{\delta\pi_j} + \rho D_i\left(\frac{\delta}{\delta\rho}\right)\wedge\frac{\delta}{\delta\pi_i} - s_{,i}\frac{\delta}{\delta s}\wedge\frac{\delta}{\delta\pi_i} - P_{\Omega,i}\frac{\delta}{\delta P_\Omega}\wedge\frac{\delta}{\delta\pi_i},$$

and by means of the interior product operation we get the Hamiltonian vector field

$$-d\mathrm{H}\lrcorner\Psi = \int \theta[-v^i s_{,i}]\frac{\delta}{\delta s} + \theta[-v^i P_{\Omega,i}]\frac{\delta}{\delta P_\Omega} + \theta[-\pi_{i,i}]\frac{\delta}{\delta\rho}$$
$$+ \theta[-(\pi_i v_j)_{,j} - \rho\partial_i\Phi - \partial_i p]\frac{\delta}{\delta\pi_i} - \theta_{,i}[p-\tau K]\frac{\delta}{\delta\pi_i}.$$

The requirement of absence of any singular contributions to the Hamiltonian equations leads us to the already known boundary condition (11). It is easy to see that equations of motion do not change in comparison with (22), (24) and (23). But we also get the following new equation,

$$\dot{P}_\Omega = -(\mathbf{v}\cdot\nabla)P_\Omega. \tag{28}$$

Here it is evident that the requirement of disappearance of boundary terms in the Hamiltonian variation [or equivalently in the full variational derivatives (27)] leads to the boundary condition which is different from the standard one. It means that in the general statement of a problem, when the canonical choice of variables is not prescribed from the very beginning, the criterion by Regge and Teitelboim of choosing the surface contributions[3] should be replaced by the requirement of vanishing of the singular contributions to the Hamiltonian vector field, i.e., to the Hamiltonian equations of motion.

It should be stated that in the case of the dynamical domain of integration Ω we are unable to check the Jacobi identity by calculating $[\Psi,\Psi]_{SN}$ because the proof of Eq. (25) given in Ref. 2 is not valid here.

V. VARIATIONAL PRINCIPLE IN EULERIAN VARIABLES

It is natural to ask whether it is possible to derive the Hamiltonian formalism for Eulerian variables, considered in the previous section, directly from the corresponding variational principle, without appealing to the Hamiltonian formalism for Lagrangian variables. The answer will be definitely in the affirmative, but the construction of this variational principle is rather nontrivial and deserves a special discussion. It is interesting that such a discussion has been used by Kupershmidt as an intrigue for his book (see Ref. 12, Introduction). A discussion on this problem can also be found in Refs. 13, 21–23.

A. Fixed boundary

Let us first ask how to construct the Lagrangian and corresponding variables if we know a Hamiltonian [in our case as a functional of $\pi^i(\mathbf{x})$, $\rho(\mathbf{x})$ and $s(\mathbf{x})$] and Poisson brackets for Hamiltonian variables. If variables are canonical, then, certainly, it is sufficient to use the Legendre transform, but in the general case this may be a nontrivial task. Momenta $\pi^i(\mathbf{x})$ have nonzero Poisson brackets between themselves, Hamiltonian (21) does not imply variables conjugate to these momenta (''coordinates'') and the total number of variables is not in general even (for example, in case $\mathbb{R}^3$ it is equal to five). The solution may be to introduce some auxiliary variables.

Therefore, to move along the left vertical arrow of the diagram we add to the ''naive'' Lagrangian

$$L_0 = \int_\Omega d\mathbf{x}\rho\left(\frac{\mathbf{v}^2}{2} - \Phi(\mathbf{x}) - \varepsilon(\rho,s)\right),$$

derived from Lagrangian (1) by a trivial change of variables and formed as a difference of the kinetic and potential energies (with the internal energy added to the last one), some constraints together with the corresponding Lagrange multipliers.

As the first and the most evident constraint we take the continuity equation (the mass conservation law)

$$\frac{\partial\rho}{\partial t} + \mathrm{div}(\rho\mathbf{v}) = 0. \tag{29}$$

Also we use the entropy conservation law

$$\frac{\partial s}{\partial t} + (\mathbf{v}\cdot\nabla)s = 0, \tag{30}$$

which is possible to rewrite, combining with (29) also as follows:

$$\frac{\partial(\rho s)}{\partial t} + \mathrm{div}(\rho s\mathbf{v}) = 0.$$

At last, it is necessary to put a condition providing guarantee for existence of the Lagrangian coordinates. It means that any mass point having at the moment t position with coordinates $\mathbf{x}$, may be supplied by its "number" α_μ, for example, by the coordinates of its initial position $\mathbf{R}(\mathbf{x},t)$. This "number" should also be "conserved" in the process of the fluid motion

$$\frac{\partial\alpha_\mu}{\partial t} + (\mathbf{v}\cdot\nabla)\alpha_\mu = 0. \tag{31}$$

Here the number of degrees of freedom or the range for index μ, in general, does not coincide with the spatial dimension of $\mathbb{R}^n$, for example, in the case $n=3$ one variable α is enough. As a result, still up to surface terms, we arrive at the following Lagrangian,

$$L = L_0 + \int_\Omega d\mathbf{x}\left[\phi\left(\frac{\partial\rho}{\partial t} + \mathrm{div}(\rho\mathbf{v})\right) - \eta\left(\frac{\partial s}{\partial t} + (\mathbf{v}\cdot\nabla)s\right) - \beta_\mu\left(\frac{\partial\alpha_\mu}{\partial t} + (\mathbf{v}\cdot\nabla)\alpha_\mu\right)\right],$$

or at the following action

$$S = \int_{t_1}^{t_2} dt \int_\Omega d\mathbf{x}\left[\rho\left(\frac{\mathbf{v}^2}{2} - \Phi(\mathbf{x}) - \varepsilon(\rho,s)\right) + \phi\left(\frac{\partial\rho}{\partial t} + \mathrm{div}(\rho\mathbf{v})\right) - \eta\frac{Ds}{Dt} - \beta_\mu\frac{D\alpha_\mu}{Dt}\right], \tag{32}$$

where

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + (\mathbf{v}\cdot\nabla),$$

and the signs in front of η, β_μ are taken for convenience, so that we get positive signs in formula (33). By varying action (32) over ϕ, η, β_μ we evidently get supplementary conditions (29)–(31).

By varying (32) over velocity $\mathbf{v}$ we get the so-called Clebsch representation for velocity variable,

$$\mathbf{v} = \nabla\phi + \frac{\eta}{\rho}\nabla s + \frac{\beta_\mu}{\rho}\nabla\alpha_\mu, \tag{33}$$

which means that velocity may be treated as an auxiliary variable.

By varying action (32) over density ρ we get the following equation,

$$\frac{\mathbf{v}^2}{2}-\Phi(\mathbf{x})-\varepsilon(\rho,s)-\rho\frac{\partial\varepsilon}{\partial\rho}-\dot{\phi}-(\mathbf{v}\cdot\nabla)\phi=0,$$

which may be understood as an equation for evolution of potential ϕ:

$$\dot{\phi}=-(\mathbf{v}\cdot\nabla)\phi+\frac{\mathbf{v}^2}{2}-\Phi(\mathbf{x})-\varepsilon(\rho,s)-\frac{p}{\rho}. \tag{34}$$

We get new independent equations of motion by varying (32) over s,

$$\dot{\eta}=-\operatorname{div}(\eta\mathbf{v})+\rho\frac{\partial\varepsilon}{\partial s}, \tag{35}$$

and over α_μ

$$\dot{\beta}_\mu=-\operatorname{div}(\beta_\mu\mathbf{v}). \tag{36}$$

It is easy to be convinced that equations of motion for "old" variables ρ, s are still the same (22) and (23).

It is possible to demonstrate that the same is true for velocity $\mathbf{v}$, Eq. (24). For this purpose we need to differentiate (33) over time and substitute into the derived expression values of $\dot{\rho}$, $\dot{\phi}$, $\dot{s}$, $\dot{\eta}$, $\dot{\alpha}_\mu$, $\dot{\beta}_\mu$ taken from equations of motion (29), (34), (30), (35), (31), and (36), correspondingly.

Of course, we do not yet touch surface terms arising from integration by parts in the action variation (32). Let us display them explicitly:

$$(\delta S)_{\mathrm{surf}}=\int_\Omega d\mathbf{x}[\phi\delta\rho-\eta\delta s-\beta_\mu\delta\alpha_\mu]_{t_1}^{t_2}+\int_{t_1}^{t_2}dt\oint_{\partial\Omega}[\mathbf{v}(\phi\delta\rho-\eta\delta s-\beta_\mu\delta\alpha_\mu)+\rho\phi\delta\mathbf{v}]\cdot\mathbf{n}dS. \tag{37}$$

Boundary condition

$$\mathbf{n}\cdot\mathbf{v}|_{\partial\Omega}=0,$$

which means, as in previous sections, fixed edge of the domain Ω, provides vanishing of all variation contributions at the spatial part of the boundary. The contribution from variations on the time boundary disappears because variables ρ, s, α_μ must be fixed at the initial and final instants of time.

B. Free boundary

Let us add to action (32) a surface energy contribution and let us, as before, describe the free boundary dynamics by means of function $P_\Omega(\mathbf{x},t)$

$$S=\int_{t_1}^{t_2}dt\int\theta(P_\Omega)\left[\rho\left(\frac{\mathbf{v}^2}{2}-\Phi(\mathbf{x})-\varepsilon(\rho,s)\right)+\phi\left(\frac{\partial\rho}{\partial t}+\operatorname{div}(\rho\mathbf{v})\right)-\eta\frac{Ds}{Dt}-\beta_\mu\frac{D\alpha_\mu}{Dt}-\tau\nabla\cdot\mathbf{n}\right]d\mathbf{x}. \tag{38}$$

The variation of this action will differ from the variation of action (32) by some new surface terms only. Let us display them separately:

$$(\delta' S)_{\mathrm{surf}}=\int_{t_1}^{t_2}dt\int\frac{d\theta}{dP_\Omega}\Bigg(\dot{P}_\Omega(-\phi\delta\rho+\eta\delta s+\beta_\mu\delta\alpha)$$
$$+\delta P_\Omega\Bigg[\rho\Bigg(\frac{\mathbf{v}^2}{2}-\Phi(\mathbf{x})-\varepsilon(\rho,s)\Bigg)+\phi\Bigg(\frac{\partial\rho}{\partial t}+\mathrm{div}(\rho\mathbf{v})\Bigg)-\eta\frac{Ds}{Dt}-\beta_\mu\frac{D\alpha_\mu}{Dt}-\tau K\Bigg]\Bigg)d\mathbf{x}.$$

First line terms arise as a result of integration by parts of partial time derivatives. Varying over K does not contribute, as shown before [see (9)].

By combining the derived expression with the contribution (37) found above, which may be rewritten as follows,

$$(\delta'' S)_{\mathrm{surf}}=\int_{t_1}^{t_2}\int d\mathbf{x}\frac{\partial}{\partial t}[\theta(P_\Omega)(\phi\delta\rho-\eta\delta s-\beta_\mu\delta\alpha_\mu)]$$
$$-\int_{t_1}^{t_2}dt\int\nabla\theta(P_\Omega)\cdot[\mathbf{v}(\phi\delta\rho-\eta\delta s-\beta_\mu\delta\alpha_\mu)+\rho\phi\delta\mathbf{v}]d\mathbf{x},$$

we obtain

$$(\delta S)_{\mathrm{surf}}=\int\theta(P_\Omega)(\phi\delta\rho-\eta\delta s-\beta_\mu\delta\alpha_\mu)d\mathbf{x}\Big|_{t_1}^{t_2}-\int_{t_1}^{t_2}dt\int\nabla\theta(P_\Omega)\cdot(\rho\phi\delta\mathbf{v})d\mathbf{x}$$
$$-\int_{t_1}^{t_2}dt\int\frac{d\theta}{dP_\Omega}(\dot{P}_\Omega+(\mathbf{v}\cdot\nabla)P_\Omega)(\phi\delta\rho-\eta\delta s-\beta_\mu\delta\alpha_\mu)d\mathbf{x}+\int_{t_1}^{t_2}dt\int\frac{d\theta}{dP_\Omega}\delta P_\Omega$$
$$\times\Bigg[\rho\Bigg(\frac{\mathbf{v}^2}{2}-\Phi(\mathbf{x})-\varepsilon(\rho,s)\Bigg)+\phi\Bigg(\frac{\partial\rho}{\partial t}+\mathrm{div}(\rho\mathbf{v})\Bigg)-\eta\frac{Ds}{Dt}-\beta_\mu\frac{D\alpha_\mu}{Dt}-\tau K\Bigg]d\mathbf{x}.$$

Some terms here give us a boundary condition

$$\dot{P}_\Omega+(\mathbf{v}\cdot\nabla)P_\Omega=0,$$

and some other terms disappear when fields on the time boundaries are fixed. But there are other terms which do not allow us to derive the famous boundary condition (10). It is well known[17,18] that actions which differ by boundary terms lead to different natural boundary conditions. So, action (38) should be modified by some surface integral. It is easy to get convinced that we will obtain the desired action after subtracting from (38) the following expression:

$$\Delta S=\int_{t_1}^{t_2}dt\int_\Omega\Bigg(\frac{\partial}{\partial t}(\rho\phi)+\nabla\cdot(\rho\phi\mathbf{v})\Bigg)d\mathbf{x}.$$

Therefore, the action which leads to correct equations of motion and boundary conditions for the free boundary case has the following form:

$$S=\int_{t_1}^{t_2}dt\int\theta(P_\Omega)\Bigg[\rho\Bigg(\frac{\mathbf{v}^2}{2}-\Phi(\mathbf{x})-\varepsilon(\rho,s)\Bigg)-\rho\frac{D\phi}{Dt}-\eta\frac{Ds}{Dt}-\beta_\mu\frac{D\alpha_\mu}{Dt}-\tau K\Bigg]d\mathbf{x}. \qquad (39)$$

If we compare the above expression with formula (34), we can see that the Lagrangian density up to the sign is equal to the pressure when equations of motion are satisfied. In a paper by Luke[13] for the two-dimensional

$$d\mathbf{x}=dxdy,\quad P_\Omega(x,y,t)=h(x,t)-y,$$

potential flow $\mathbf{v}=\nabla\phi$ of the incompressible fluid $\rho=1$, and $s=\text{const}$ without surface tension $\tau=0$ in a constant gravitational field $\Phi(\mathbf{x})=gy$, it was first pointed out that action (39), taking the following form

$$S=-\int_{t_1}^{t_2}dt\int dx\int^{h(x,t)}dy\left(\frac{1}{2}\phi_x^2+\frac{1}{2}\phi_y^2+\dot{\phi}+gy\right),$$

allowed us to derive not only equations of motion but also the dynamical boundary conditions for the free surface. The presence of $\dot{\phi}$ in the Lagrangian density is essential as it generates the symplectic form

$$\omega=\int d\mathbf{x}\delta h\wedge\delta\phi,$$

corresponding to the Poisson bracket discovered in an almost simultaneous paper by Zakharov.[7]

It is easy to see that action (39) can be also used in the fixed boundary case for domain Ω.

VI. AN ALTERNATIVE WAY TO THE HAMILTONIAN FORMALISM FOR EULERIAN VARIABLES

Let us show that starting from the variational principle for Eulerian variables discussed in the previous section, it is possible to construct a new Hamiltonian formalism which is equivalent to the one constructed above by means of reduction of the Hamiltonian formalism for Lagrangian variables. This construction may be provided both by Dirac method,[15] and by inverting the symplectic form matrix (Faddeev–Jackiw method[14]).

A. Fixed boundary

In the Dirac approach, action (39) with variable $\mathbf{v}$ eliminated by means of Eq. (33) leads to the appearance of primary constraints

$$\pi_\phi=-\rho,\quad \pi_\rho=0,$$

$$\pi_s=-\eta,\quad \pi_\eta=0,$$

$$\pi_\alpha=-\beta,\quad \pi_\beta=0.$$

Then we look for secondary constraints, and next we derive Dirac brackets and eliminate second class constraints.

The Faddeev–Jackiw approach looks simpler here. We determine the symplectic form

$$\omega=\int\theta(P)(\delta\phi\wedge\delta\rho+\delta s\wedge\delta\eta+\delta\alpha_\mu\wedge\delta\beta_\mu)d\mathbf{x}$$

(here and below we reduce notation P_Ω to P), which is explicitly canonical, and this allows us to find the Poisson brackets

$$\{\rho(\mathbf{x}),\phi(\mathbf{x}')\}=\delta(\mathbf{x},\mathbf{x}'),\quad \{\eta(\mathbf{x}),s(\mathbf{x}')\}=\delta(\mathbf{x},\mathbf{x}'),\quad \{\beta_\mu(\mathbf{x}),\alpha_\nu(\mathbf{x}')\}=\delta_{\mu\nu}\delta(\mathbf{x},\mathbf{x}'),$$

which coincide with the Dirac brackets. Let us introduce the following quantities,

$$\pi=\rho\nabla\phi+\eta\nabla s+\beta_\mu\nabla\alpha_\mu,$$

and calculate their Poisson brackets. The result is the same as given by Eq. (18). In an analogous way we may check the correspondence with formulas (19) and (20). The Hamiltonian can be obtained by the standard Legendre transform and it coincides with expression (21) being expressed in variables π.

Therefore, by using Clebsch potentials we can maintain the correspondence between the variational principle and the Hamiltonian formalism in Eulerian coordinates.

B. Free boundary

Here for simplicity we replace α_μ by α. In the free boundary case it is necessary to consider P as a dynamical variable. Time derivatives enter action (39) in the following form,

$$\int_{t_1}^{t_2} dt \int d\mathbf{x}\theta(P)(-\rho\dot{\phi}-\eta\dot{s}-\beta\dot{\alpha}),$$

so, the corresponding symplectic form is as follows:

$$\omega=-\int d\mathbf{x}(\theta(P)(\delta\rho\wedge\delta\phi+\delta\eta\wedge\delta s+\delta\beta\wedge\delta\alpha)+\theta'(P)\delta P\wedge(\rho\delta\phi+\eta\delta s+\beta\delta\alpha)).$$

In the case of the potential flow of incompressible fluid considered by Zakharov,[7] this form reduces (for $\rho=1$) to the following expression,

$$\omega=\int d\mathbf{x}\theta'(P)\delta\phi\wedge\delta P,$$

allowing us to use the canonical Poisson brackets for the pair of conjugate variables: velocity potential on the boundary and the position of the boundary.

Here in order to come to the Hamiltonian formalism we will use Dirac approach. Let us introduce conjugate momenta for all variables

$$\{\phi(x),\pi_\phi(y)\}=\{\rho(x),\pi_\rho(y)\}=\{s(x),\pi_s(y)\}=\delta(x,y),$$

$$\{\eta(x),\pi_\eta(y)\}=\{\alpha(x),\pi_\alpha(y)\}=\{\beta(x),\pi_\beta(y)\}=\{P(x),\pi_P(y)\}=\delta(x,y),$$

and find their values from action (39) by means of the standard formula

$$\pi_i=\frac{\partial\mathcal{L}}{\partial\dot{q}_i}.$$

As the Lagrangian density depends on velocities in a linear way we get as many primary constraints as many momenta we have introduced

$$\psi_1=\pi_\phi+\theta(P)\rho,\quad \psi_4=\pi_\rho,$$

$$\psi_2=\pi_s+\theta(P)\eta,\quad \psi_5=\pi_\eta,$$

$$\psi_3=\pi_\alpha+\theta(P)\beta,\quad \psi_6=\pi_\beta,$$

$$\psi_7=\pi_P.$$

The Legendre transform gives the initial Hamiltonian

$$\mathrm{H}_0=\int d\mathbf{x}\theta(P)\left(\frac{1}{2\rho}(\rho\nabla\phi+\eta\nabla s+\beta\nabla\alpha)^2+\rho\Phi+\rho\varepsilon(\rho,s)+\tau K\right),$$

coinciding with expression (26) with the only difference: momenta π_i expressed by means of Clebsch variables. But Hamiltonian H_0 when expressed in new variables does not provide the correct equations of motion and so should be accompanied by a linear combination of the primary constraints

$$\mathrm{H}=\mathrm{H}_0+\int d\mathbf{x}\sum_{i=1}^{7}\lambda_i\psi_i\,.$$

Evidently, the first six constraints are second class. The matrix of their Poisson brackets,

$$\{\psi_i,\psi_j\}=\begin{pmatrix}0 & I\\ -I & 0\end{pmatrix}\theta(P)\,\delta(x,y),$$

has an inverse [here we are to consider $\theta(P)\,\delta(\mathbf{x},\mathbf{y})$ as a unit operator]

$$C_{ij}(\mathbf{x},\mathbf{y})=\begin{pmatrix}0 & -I\\ I & 0\end{pmatrix}\theta(P)\,\delta(\mathbf{x},\mathbf{y}),$$

so it is possible to determine the Dirac brackets by the standard formula

$$\{f(\mathbf{x}),g(\mathbf{y})\}_D=\{f(\mathbf{x}),g(\mathbf{y})\}-\sum_{i,j=1}^{6}\int d\mathbf{z}\int d\mathbf{w}\{f(\mathbf{x}),\psi_i(\mathbf{z})\}C_{ij}(\mathbf{z},\mathbf{w})\{\psi_j(\mathbf{w}),g(\mathbf{y})\}.$$

Therefore, we exclude the first six momenta, and, correspondingly, the first six constraints from the Hamiltonian

$$\mathrm{H}=\int d\mathbf{x}\left[\theta(P)\left(\frac{1}{2\rho}(\rho\nabla\phi+\eta\nabla s+\beta\nabla\alpha)^2+\rho\Phi+\rho\varepsilon(\rho,s)+\tau K\right)+\lambda_P\pi_P\right].$$

The calculation of Dirac brackets for the other eight variables gives us the following results:

$$\{\rho(\mathbf{x}),\phi(\mathbf{y})\}_D=\theta(P)\,\delta(\mathbf{x},\mathbf{y}),\quad \{\rho(\mathbf{x}),\pi_P(\mathbf{y})\}_D=-\theta'(P)\rho\,\delta(\mathbf{x},\mathbf{y}),$$

$$\{\eta(\mathbf{x}),s(\mathbf{y})\}_D=\theta(P)\,\delta(\mathbf{x},\mathbf{y}),\quad \{\eta(\mathbf{x}),\pi_P(\mathbf{y})\}_D=-\theta'(P)\,\eta\,\delta(\mathbf{x},\mathbf{y}),$$

$$\{\beta(\mathbf{x}),\alpha(\mathbf{y})\}_D=\theta(P)\,\delta(\mathbf{x},\mathbf{y}),\quad \{\beta(\mathbf{x}),\pi_P(\mathbf{y})\}_D=-\theta'(P)\beta\,\delta(\mathbf{x},\mathbf{y}),$$

$$\{P(\mathbf{x}),\pi_P(\mathbf{y})\}=\delta(\mathbf{x},\mathbf{y}).$$

Therefore, we can now relate to the initial symplectic form the following Poisson bivector:

$$\Psi=\int d\mathbf{x}\left[\theta(P)\left(\frac{\delta}{\delta\rho}\wedge\frac{\delta}{\delta\phi}+\frac{\delta}{\delta\eta}\wedge\frac{\delta}{\delta s}+\frac{\delta}{\delta\beta}\wedge\frac{\delta}{\delta\alpha}\right)+\frac{\delta}{\delta\pi_P}\wedge\left(-\frac{\delta}{\delta P}+\theta'(P)\left(\rho\frac{\delta}{\delta\rho}+\eta\frac{\delta}{\delta\eta}+\beta\frac{\delta}{\delta\beta}\right)\right)\right].$$

The differential of the Hamiltonian has the following form,

$$\mathrm{d}\mathrm{H}=\int d\mathbf{x}\frac{\delta\mathrm{H}}{\delta\phi_A}\,\delta\phi_A\,, \tag{40}$$

where some full variational derivatives have nontrivial boundary contributions

$$\frac{\delta\mathrm{H}}{\delta\rho}=\theta(P)\left(\mathbf{v}\nabla\phi-\frac{v^2}{2}+\Phi+\varepsilon+\frac{p}{\rho}\right),$$

$$\frac{\delta\mathrm{H}}{\delta\eta}=\theta(P)\mathbf{v}\cdot\nabla s,$$

$$\frac{\delta \mathrm{H}}{\delta \beta} = \theta(P)\mathbf{v}\cdot\nabla\alpha,$$

$$\frac{\delta \mathrm{H}}{\delta \phi} = -\theta'(P)\rho\mathbf{v}\cdot\nabla P - \theta(P)\nabla(\rho\mathbf{v}),$$

$$\frac{\delta \mathrm{H}}{\delta s} = -\theta'(P)\eta\mathbf{v}\cdot\nabla P - \theta(P)(\nabla(\eta\mathbf{v}) - \rho T),$$

$$\frac{\delta \mathrm{H}}{\delta \alpha} = -\theta'(P)\beta\mathbf{v}\cdot\nabla P - \theta(P)\nabla(\beta\mathbf{v}),$$

$$\frac{\delta \mathrm{H}}{\delta P} = \theta'(P)\left(\frac{\rho v^2}{2} + \rho\Phi + \rho\varepsilon + \tau K\right), \quad \frac{\delta \mathrm{H}}{\delta \pi_P} = \lambda_P .$$

The interior product of this differential onto the Poisson bivector gives (up to the sign) the following Hamiltonian vector field

$$\begin{aligned} -\mathrm{dH}\lrcorner\Psi = {} & [-\theta'(P)\rho(\lambda_P + \mathbf{v}\cdot\nabla P) - \theta(P)\nabla(\rho\mathbf{v})]\frac{\delta}{\delta\rho} + [-\theta'(P)\eta(\lambda_P + \mathbf{v}\cdot\nabla P) \\ & - \theta(P)(\nabla(\eta\mathbf{v}) - \rho T)]\frac{\delta}{\delta\eta} + [-\theta'(P)\beta(\lambda_P + \mathbf{v}\cdot\nabla P) - \theta(P)\nabla(\beta\mathbf{v})]\frac{\delta}{\delta\beta} \\ & + \theta'(P)(p - \tau K)\frac{\delta}{\delta\pi} - \theta(P)\mathbf{v}\cdot\nabla\alpha\frac{\delta}{\delta\alpha} + \lambda_P\frac{\delta}{\delta P} \\ & + \theta(P)\left[\frac{v^2}{2} - \mathbf{v}\cdot\nabla\phi - \Phi - \varepsilon - \frac{p}{\rho}\right]\frac{\delta}{\delta\phi} - \theta(P)[\mathbf{v}\cdot\nabla s]\frac{\delta}{\delta s}, \end{aligned}$$

i.e., Hamiltonian equations of motion, for example,

$$\dot{P} = \lambda_P . \tag{41}$$

If we require that all terms singular on the boundary should be zero, we get the following two equations:

$$\theta'(P)(\lambda_P + \mathbf{v}\cdot\nabla P) = 0, \tag{42}$$

$$\theta'(P)(p - \tau K) = 0. \tag{43}$$

Taking into account (41) we recognize the same standard boundary conditions (11) and (28). If we start from Regge–Teitelboim criterion,[3] i.e., if we demand cancellation of boundary terms in the Hamiltonian variation (40), then we obtain incorrect boundary conditions, in particular, the requirement of stationarity for the boundary.

After cancellation of singular terms, derived equations coincide with the Lagrangian ones.

VII. CONCLUSION

We have demonstrated that the method proposed in Refs. 1 and 2 is applicable for Hamiltonian treatment of free boundary problems. The special features of this class of problems are explicit in the approach.

It is important to stress that the most popular now Regge–Teitelboim approach[3] is not adequate for non-ultralocal Poisson brackets as the requirement of the Hamiltonian ''differentiabil-

ity'' leads to boundary conditions different from those obtained on the base of the variational principle. At the same time, it does not exclude singular boundary contributions from equations of motion.

We require that boundary conditions must exclude the contributions proportional to the δ-function and its derivatives from the Hamiltonian equations of motion, i.e., from the Hamiltonian vector fields. At the same time such terms may be present in the Hamiltonian variation or in the Poisson bivector.

These conclusions are supported by some other examples.[5,6] We hope that the method discussed here will be useful in treating various free boundary problems.

APPENDIX: A PROOF OF ONE FORMULA USED IN SEC. II

Let us prove the following formula,

$$\frac{\partial}{\partial r^j}(JJ^{ji})=0,$$

for variables given in Eq. (2).

According to the standard variational rules we have for the determinant and for the inverse matrix the following relations, correspondingly,

$$\delta J=JJ^{lk}\delta J_{kl}, \quad \delta J^{ji}=-J^{jk}J^{li}\delta J_{kl}.$$

Then we obtain

$$\frac{\partial}{\partial r^j}(JJ^{ji})=J(J^{ji}J^{lk}-J^{jk}J^{li})\frac{\partial^2 Y^k}{\partial r^j\partial r^l}=J\left(\frac{\partial r^j}{\partial Y^i}\frac{\partial r^l}{\partial Y^k}-\frac{\partial r^j}{\partial Y^k}\frac{\partial r^l}{\partial Y^i}\right)\frac{\partial^2 Y^k}{\partial r^j\partial r^l}=J\left[\frac{\partial r^l}{\partial Y^k}\frac{\partial}{\partial r^j}\left(\frac{\partial Y^k}{\partial r^l}\right)\frac{\partial r^j}{\partial Y^i}\right.$$
$$\left.-\frac{\partial r^l}{\partial Y^i}\frac{\partial}{\partial r^j}\left(\frac{\partial Y^k}{\partial r^l}\right)\frac{\partial r^j}{\partial Y^k}\right]=J\left[\frac{\partial r^l}{\partial Y^k}\frac{\partial}{\partial Y^i}\left(\frac{\partial Y^k}{\partial r^l}\right)-\frac{\partial r^l}{\partial Y^i}\frac{\partial}{\partial Y^k}\left(\frac{\partial Y^k}{\partial r^l}\right)\right]=J\left[\frac{\partial}{\partial Y^i}\left(\frac{\partial Y^k}{\partial r^l}\frac{\partial r^l}{\partial Y^k}\right)\right.$$
$$\left.-\frac{\partial Y^k}{\partial r^l}\frac{\partial^2 r^l}{\partial Y^i\partial Y^k}-\frac{\partial}{\partial Y^k}\left(\frac{\partial Y^k}{\partial r^l}\frac{\partial r^l}{\partial Y^i}\right)+\frac{\partial Y^k}{\partial r^l}\frac{\partial^2 r^l}{\partial Y^k\partial Y^i}\right]=0.$$

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On Keller theorem for anisotropic media

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The Keller theorem in the problem of effective conductivity in anisotropic two-dimensional (2D) many-component composites makes it possible to establish a simple inequality $\sigma^e_{\mathrm{is}}(\sigma_i^{-1})\cdot\sigma^e_{\mathrm{is}}(\sigma_k)>1$ for the isotropic part $\sigma^e_{\mathrm{is}}(\sigma_k)$ of the second rank symmetric tensor $\hat{\sigma}^e_{i,j}$ of effective conductivity. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1480450]

The extension of the Keller theorem[1] in the problem of effective conductivity in the infinite 2D two-component composites on the many-component case[2] poses a new question on the duality relation for the second rank symmetric tensor $\hat{\sigma}^e_{i,j}$ of effective conductivity in anisotropic media. It is related to the restrictions imposed on the linear invariant of $\hat{\sigma}^e_{i,j}$ which is called an isotropic part $\sigma^e_{\mathrm{is}}(\sigma_k)$ of effective conductivity. Recently the perturbation theory for the infinite periodic three-component 2D checkerboard with twofold rotation lattice symmetry was developed[3] where the coincidence of $\sigma^e_{\mathrm{is}}(\sigma_k)$ with solution $\sigma_B(\sigma_k)$ of the Bruggemann equation was established up to the sixth order term. This fact is curious because it gives grounds to think that effective medium approximation (EMA) describes exactly $\sigma^e_{\mathrm{is}}(\sigma_k)$ in this certain structure. Here we will discuss this conclusion.

Let us define the isotropic part of conductivity tensor

$$\sigma^e_{\mathrm{is}}(\sigma_k)=\tfrac{1}{2}\ \mathrm{Tr}\ \hat{\sigma}^e_{i,j}(\sigma_k),\quad k=1,2,\ldots,n, \tag{1}$$

which is an invariant scalar with respect to the plane rotation. We recall the extension[2] of the Keller theorem for the principal values $\hat{\sigma}^{\mathrm{xx}}_e$, $\hat{\sigma}^{\mathrm{yy}}_e$ of diagonalized matrix $\hat{\sigma}^{ij}_e$ for 2D n-component composite

$$\begin{aligned}&\hat{\sigma}^{\mathrm{xx}}_e(\sigma_1^{-1},\sigma_2^{-1},\ldots,\sigma_n^{-1})\cdot\hat{\sigma}^{\mathrm{yy}}_e(\sigma_1,\sigma_2,\ldots,\sigma_n)=1,\\&\hat{\sigma}^{\mathrm{yy}}_e(\sigma_1^{-1},\sigma_2^{-1},\ldots,\sigma_n^{-1})\cdot\hat{\sigma}^{\mathrm{xx}}_e(\sigma_1,\sigma_2,\ldots,\sigma_n)=1.\end{aligned} \tag{2}$$

Both (1) and (2) make it possible to derive a simple inequality for $\Lambda^e_{\mathrm{is}}=\sigma^e_{\mathrm{is}}(\sigma_i^{-1})\cdot\sigma^e_{\mathrm{is}}(\sigma_k)\geqslant 1$. Indeed,

$$\Lambda^e_{\mathrm{is}}=\frac{1}{4}[2+\hat{\sigma}^{\mathrm{xx}}_e(\sigma_k)\cdot\hat{\sigma}^{\mathrm{xx}}_e(\sigma_k^{-1})+\hat{\sigma}^{yy}_e(\sigma_k)\cdot\hat{\sigma}^{\mathrm{yy}}_e(\sigma_k^{-1})]=\frac{1}{4}\left[2+\frac{\hat{\sigma}^{\mathrm{xx}}_e(\sigma_k)}{\hat{\sigma}^{\mathrm{yy}}_e(\sigma_k)}+\frac{\hat{\sigma}^{\mathrm{yy}}_e(\sigma_k)}{\hat{\sigma}^{\mathrm{xx}}_e(\sigma_k)}\right]\geqslant 1, \tag{3}$$

where the only isotropic media $\hat{\sigma}^{\mathrm{xx}}_e=\hat{\sigma}^{\mathrm{yy}}_e$ corresponds to the equality in (3). At the same time another isotropic invariant $\Delta^e_{\mathrm{is}}=\det\hat{\sigma}^e_{ij}(\sigma_k)$ satisfies the duality relation

$$\Delta^e_{\mathrm{is}}(\sigma_k)\cdot\Delta^e_{\mathrm{is}}(\sigma_k^{-1})=1.$$

The EMA theory of the infinite 2D n-component isotropic composite has as its consequence the Bruggemann equation[4]

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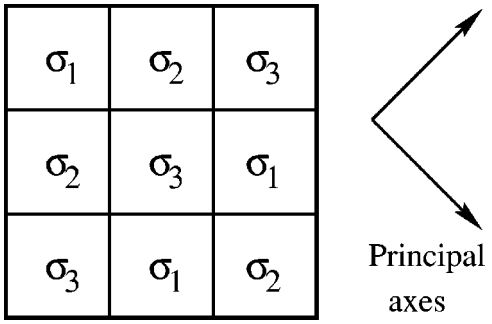

FIG. 1. A unit cell of periodic 2D three-component checkerboard considered in Ref. 3.

$$\sum_{k=1}^{n} \frac{\sigma_k - \sigma_B(\sigma_k)}{\sigma_k + \sigma_B(\sigma_k)} = 0, \tag{4}$$

which necessarily leads to the duality relation

$$\sigma_B(\sigma_k^{-1}) \cdot \sigma_B(\sigma_k) = 1. \tag{5}$$

The last formula means that σ_{is}^e can satisfy the Bruggemann equation only for isotropic S_n-permutation invariant media: $\hat{\sigma}_e^{xx} = \hat{\sigma}_e^{yy}$, $\hat{\sigma}_e^{xy} = 0$ in any reference frame $\{x,y\}$.

The infinite periodic 2D three-component checkerboard was considered in Ref. 3 for symmetrically related partial conductivities ($\sigma_1 = 1, \sigma_{2,3} = 1 \pm \delta$), see Fig. 1. Such structure does not possess an isotropy of the second rank conductivity tensor $\hat{\sigma}_e^{i,j}$ that follows from the simple crystallographical consideration[5] as well as from the straightforward calculation[3] of the nondiagonal term $\hat{\sigma}_e^{xy} \propto \delta^2$. Therefore $\sigma_{\mathrm{is}}^e(\sigma_k)$ for this structure cannot satisfy the Bruggemann equation (4) even if its coincidence with $\sigma_B(\sigma_k)$ reached the δ^6 term in the perturbation theory. In fact, the Bruggemann equation cannot provide an exact solution for the scalar linear invariant $\sigma_{\mathrm{is}}^e(\sigma_k)$ of the macroscopic conductivity tensor $\hat{\sigma}_{i,j}^e$ in any 2D problem where that tensor is nonscalar.

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Resonance dynamics and partial averaging in a restricted three-body system

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Based on the value of the orbital eccentricity of an object and also its proximity to the exact resonant orbit in a three-body system, the pendulum approximation [S. F. Dermott and C. D. Murray, Nature (London) **319**, 201 (1983)] or the second fundamental model of resonance [M. H. Andoyer, Bull. Astron. **20**, 321 (1903); J. Henrard and A. Lemaître, Celest. Mech. **30**, 197 (1983)] are commonly used to study the motion of that object near its resonant state. In this paper, we present the method of partial averaging as an analytical approach to study the dynamical evolution of a body near a resonance. To focus attention on the capabilities of this technique, a restricted, circular and planar three-body system is considered and the dynamics of its outer planet while captured in a resonance with the inner body is studied. It is shown that the first-order partially averaged system resembles a mathematical pendulum whose librational motion can be viewed as a geometrical interpretation of the resonance capture phenomenon. The driving force of this pendulum corresponds to the gravitational attraction of the inner body and its contribution, at different resonant states, is shown to be proportional to e^s, where s is the order of the resonance and e is the orbital eccentricity of the outer planet. As examples of such systems, the cases of (1:1), (1:2), and (1:3) resonances are discussed and the results are compared with known planetary systems such as the Sun–Jupiter–Trojan asteroids. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The study of the dynamical evolution of a planetary system while captured in a resonance has a long history in dynamical astronomy. Since the pioneering work of Poincaré[1] on the study of the near-resonance motions in a restricted three-body system by means of a zeroth-order resonance Hamiltonian (i.e., a Hamiltonian with no perturbing terms other than the resonant ones), the body of literature produced on this subject has become so rich and extensive that it is virtually impossible to cite all the articles here. Recent discoveries of extrasolar planetary systems such as Gliese 876,[2] where two planets are locked in a near (2:1) commensurability, have also provided rich grounds for astrodynamicists to extend such studies to the systems beyond the boundaries of our solar system.[3–7]

There are two analytical approaches that are commonly taken in the study of the dynamics of the bodies of a three-body system while captured in a resonance. For an object with high orbital eccentricity ($\geqslant 0.15$) in a first-order resonance, or for an object at any higher order resonance, the pendulum model is used when the object's orbit is sufficiently close to the real resonance location.[8] The Hamiltonian model, or as it is often called, the second fundamental model of resonance,[9,10] is usually used for small eccentricities. A comparison of the results of the application of these two models to the study of the motion of a test particle in a first-order interior resonance as well as an exterior $(1:n')$, $n'=2,3,4,5$ commensurability, with the results of numerical integrations, can be found in a series of papers by Winter and Murray.[11,12] In these articles, as

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a part of their comprehensive project CRISS-CROSS on understanding the location and origin of chaotic regions in the phase space of our solar system, Winter and Murray present a detailed analysis of the dynamics of a test particle at resonance.

The purpose of this paper is to present a relatively new approach, namely the method of partial averaging near a resonance, to study analytically the dynamics of a system near a resonant state. This technique, which is based on the averaging theorem (see Refs. 13 and 14), enables one to avoid certain complexities by studying the behavior of the system averaged over a fast angular variable.[15–17] It is necessary to mention that a complete picture of the dynamical evolution of the system can only be obtained by direct analysis of its equations of motion. The partially averaged system allows one to focus attention on the slow-changing quantities. Such an idea is commonly used in celestial mechanics: the Hamiltonian of the system is averaged over a fast variable and the resulting averaged Hamiltonian is used to study the slow dynamics of the system. A review of this technique can be found in the work of Ferraz-Mello[18] and the references cited therein. To demonstrate the capabilities of the method of partial averaging, a restricted, circular and planar three-body system is considered here and the motion of its outer planet near an $(n:n')$ resonance is studied.

Although the method of partial averaging near a resonance has long been used by mathematicians in their studies of dynamical systems near resonances,[15–17] its application to astronomical systems is quite recent. One can find such applications in papers by this author on the study of the dynamical evolution of a planetary system in a uniform and homogeneous medium of planetesimals[19,20] and also in a series of articles by Chicone, Mashhoon, and Retzloff[21–26] on their extensive study of the dynamics of a binary system subject to incident gravitational radiation as well as gravitational radiation damping.

The system of interest in this paper is a hypothetical restricted, planar and circular three-body system consisting of a star and two planets. The equations of motion of the outer planet of this system are presented in Sec. II. Section III deals with the system at resonance. In Sec. IV, the method of partial averaging near a resonance is applied and the averaged dynamics of the outer planet, in the first order of perturbation, is studied. It is shown in this section that the contribution of the gravitational attraction of the inner planet on the averaged dynamics of the outer body at different resonant states is directly proportional to the orbital eccentricity of the latter with a power equal to the order of the resonance. As examples of such cases, the (1:1), (1:2), and (1:3) resonances are studied in detail and a comparison with the system of Sun–Jupiter–Trojan asteroids as an actual case of a near (1:1) commensurability is presented. Section V concludes this study by reviewing the results and presenting remarks on their applicability to other planetary systems.

II. THE SYSTEM

The system of interest in this study is a planar three-body system consisting of a star S and two planets P_1 and P_2 where P_2 is the outer planet and P_1, the more massive planet, orbits S uniformly along a circular path. The orbital period of P_1 is considered to be known and constant. It is also assumed that the mass of S is so much larger than P_1 and P_2 that the effect of their gravitational attraction on S can be neglected.

As mentioned earlier, it is the dynamics of P_2 that is of interest here. In an inertial coordinate system with its origin at S and its axes on the plane of the system, the equation of motion of the outer planet can be written as

$$m_2\frac{d^2\vec{r}_2}{dt^2}+\mathcal{G}\frac{Mm_2}{|\vec{r}_2|^3}\vec{r}_2+\mathcal{G}\frac{m_1m_2}{|\vec{r}_2-\vec{r}_1|^3}(\vec{r}_2-\vec{r}_1)=0. \tag{1}$$

In this equation, $\mathcal{G}$ is the gravitational constant, $\vec{r}_1$ and $\vec{r}_2$ are the position vectors of the two planets, m_1 and m_2 are their corresponding masses, and M is the mass of the central star. For future purposes, it is more convenient to write Eq. (1) in a dimensionless form. Introducing r_0 and t_0 as the quantities that carry units of length and time, respectively, Eq. (1) can be written as

$$\frac{d^2\vec{\hat{r}}}{d\hat{t}^2}+\hat{k}\frac{\vec{\hat{r}}}{|\vec{\hat{r}}|^3}+\mu\,\hat{k}\frac{(\vec{\hat{r}}-\vec{\hat{r}}_1)}{|\vec{\hat{r}}-\vec{\hat{r}}_1|^3}=0, \tag{2}$$

where $\vec{\hat{r}}$, $\vec{\hat{r}}_1$, and $\hat{t}$ are dimensionless quantities given by $\vec{r}_2=r_0\,\vec{\hat{r}}$, $\vec{r}_1=r_0\,\vec{\hat{r}}_1$, and $t=t_0\,\hat{t}$. In Eq. (2), $\hat{k}=\mathcal{G}Mt_0^2/r_0^3$ and $\mu=m_1/M$. The assumption of a uniform circular motion for P_1 allows one to set $\hat{k}=1$ by choosing $r_0=r_1$ and $t_0=T_1/2\pi$ where T_1 is the orbital period of P_1.

As mentioned in Sec. I, we would like to analyze Eq. (2) using the method of partial averaging. To do so, it is necessary to write Eq. (2) in terms of appropriate action-angle variables (Appendix A). The most appropriate action-angle variables for this purpose are the Delaunay variables given by $L=a^{1/2}$, $G=\mathcal{P}_\theta=[a(1-e^2)]^{1/2}$, $\ell=u-e\sin u$, and $g=\theta-v$, where $e=\mathcal{P}_r\mathcal{P}_\theta/\sin v$ and a are the eccentricity and the semimajor axis of the osculating ellipse of P_2, θ is its plane-polar angle, $\mathcal{P}_r$ and $\mathcal{P}_\theta$ are its radial and angular momenta, and u and v are its eccentric and true anomalies related as

$$r=\frac{G^2}{1+e\cos v}=a\,(1-e\cos u). \tag{3}$$

In order to write Eq. (2) in terms of the Delaunay variables, it is more convenient to first write this equation in terms of $\mathcal{P}_r$ and $\mathcal{P}_\theta$. That is,

$$\mathcal{P}_r=\dot{r}, \tag{4}$$

$$\mathcal{P}_\theta=r^2\,\dot{\theta}, \tag{5}$$

$$\dot{\mathcal{P}}_r=\frac{1}{r^3}\mathcal{P}_\theta^2-\frac{1}{r^2}-\frac{\mu}{|\vec{r}-\vec{\mathbf{r}}_1|^3}[\vec{r}-\cos(\theta-\theta_1)], \tag{6}$$

$$\dot{\mathcal{P}}_\theta=-\frac{\mu}{|\vec{r}-\vec{\mathbf{r}}_1|^3}r\sin(\theta-\theta_1), \tag{7}$$

where $\theta_1=\omega_1\hat{t}$ and $\omega_1=1$ is the dimensionless angular velocity of P_1. In Eqs. (4)–(7), the hat signs have been dropped for the sake of simplicity and the overdot indicates a derivative with respect to the dimensionless time $\hat{t}$. The vector $\vec{\mathbf{r}}_1$ in Eqs. (6) and (7) is the unit vector along $\vec{r}_1$. In terms of the Delaunay variables, Eqs. (4)–(7) can be written as

$$\dot{G}=r\,F_\theta, \tag{8}$$

$$\dot{L}=a\,(1-e^2)^{-1/2}[F_\theta+e\,(F_r\sin v+F_\theta\cos v)], \tag{9}$$

$$\dot{g}=\frac{1}{e}[a(1-e^2)]^{1/2}\left[F_\theta\left(\frac{\sin v}{1+e\cos v}\right)-(F_r\cos v-F_\theta\sin v)\right], \tag{10}$$

$$\dot{\ell}=a^{-3/2}+\frac{r}{e}a^{-1/2}\left\{(F_r\cos v-2\,F_\theta\sin v)+\frac{1}{2}e\,[(F_r\cos 2v-F_\theta\sin 2v)-3\,F_r]\right\}, \tag{11}$$

where

$$F_r=-\mu\frac{r-\cos(\theta-\theta_1)}{|\vec{r}-\vec{\mathbf{r}}_1|^3},\quad F_\theta=-\mu\frac{\sin(\theta-\theta_1)}{|\vec{r}-\vec{\mathbf{r}}_1|^3}. \tag{12}$$

III. SYSTEM AT RESONANCE

Consider an $(n:n')$ commensurability between the angular frequency of the inner planet ω_1, and $\omega_\ell = a^{-3/2}$, the Keplerian frequency of the osculating ellipse of the outer one. That is,

$$n\,\omega_1 = n'\,\omega_\ell\,. \tag{13}$$

For our restricted circular system with this resonance condition, the Keplerian frequency ω_ℓ, and therefore, the semimajor axis of the outer planet at resonance are constant. The constant value of the semimajor axis, denoted by $a_{(n:n')}$, corresponds to the resonant value of the action variable L as $L_{(n:n')} = a^{1/2}_{(n:n')}$. We would like to study the dynamics of the outer planet when L varies in the vicinity of this value. For this purpose, we need to introduce an appropriate transformation that renders Eqs. (8)–(11) in a form that includes deviations of L from $L_{(n:n')}$. Let D be an action variable measuring these deviations. We then write (Appendix A)

$$L = a^{1/2}_{(n:n')} + \mu^{1/2} D, \tag{14}$$

and

$$\ell = a^{-3/2}_{(n:n')}\,\hat{t} + \varphi, \tag{15}$$

where φ denotes the deviations of the mean anomaly ℓ from its Keplerian value. Such transformations have been repeatedly used in application of Hamiltonian averaging techniques to resonant systems.[18] It is important to mention that the choice of $\mu^{1/2}$ in Eq. (14) is to assure equal lowest order of perturbation for $\dot{D}$ and $\dot{\varphi}$ after writing Eqs. (8)–(11) for the system near resonance. Details on this can be found in Refs. 14 and 20.

For the purpose of writing Eqs. (8)–(11) near a resonance, it is more convenient to write these equations as (Appendix B)

$$\dot{L} = -\mu \frac{\partial H}{\partial \ell}, \quad \dot{G} = -\mu \frac{\partial H}{\partial g}, \tag{16}$$

and

$$\dot{\ell} = \omega_\ell + \mu \frac{\partial H}{\partial L}, \quad \dot{g} = \mu \frac{\partial H}{\partial G}, \tag{17}$$

where $H = -|\vec{r} - \vec{\mathbf{r}}_\mathbf{1}|^{-1}$ (hereafter, *external Hamiltonian*) represents the perturbative effect of the inner planet, P_1. The dynamical equations of the system near resonance can now be written as[19]

$$\dot{D} = -\mu^{1/2}\frac{\partial H}{\partial \ell} - \mu\, D\, \frac{\partial^2 H}{\partial \ell\, \partial L} + O(\mu^{3/2}), \tag{18}$$

$$\dot{\varphi} = -3\,\mu^{1/2}\, a^{-2}_{(n:n')}\, D + \mu \left[6 a^{-5/2}_{(n:n')}\, D^2 + \frac{\partial H}{\partial L} \right] + O(\mu^{3/2}), \tag{19}$$

$$\dot{G} = -\mu \frac{\partial H}{\partial g} + O(\mu^{3/2}), \tag{20}$$

$$\dot{g} = \mu \frac{\partial H}{\partial G} + O(\mu^{3/2}). \tag{21}$$

In these equations, all partial derivatives are evaluated at $(L_{(n:n')},G,L^{-3}_{(n:n')}\hat{t}+\varphi,g)$. The averaged dynamics of the system is obtained by applying the averaging technique presented in Appendix A to Eqs. (18)–(21).

IV. FIRST-ORDER AVERAGED SYSTEM

As mentioned before, we would like to study the averaged dynamics of the outer planet near a resonance, in the first order of the perturbation parameter $\mu^{1/2}$. In that order, Eqs. (18)–(21) are written as

$$\dot{D}=-\mu^{1/2}\mathcal{F},\quad \dot{\varphi}=-\mu^{1/2}\left[\frac{3D}{a^2_{(n:n')}}\right],\quad \dot{G}=\dot{g}=0, \tag{22}$$

where $\mathcal{F}=\partial H/\partial \ell$ is evaluated at $(L_{(n:n')},G,L^{-3}_{(n:n')}\hat{t}+\varphi,g)$.

In this section, we apply the method of partial averaging, as described in Appendix A, to Eq. (22). As mentioned in Appendix A, the analysis presented there is only valid for systems with one angular variable. An inspection of the main dynamical equations of the outer planet [i.e., Eqs. (16) and (17)] reveals that these equations along with $\dot{\theta}_1=1$ represent the time variations of two action variables L and G and three angular variables ℓ, g, and θ_1. However, as shown by Eq. (22), to the first order of $\mu^{1/2}$, $\dot{g}=0$. That is, the angular variable g is a constant. Also, from the resonance condition (13) and the transformation (15), the angular variables ℓ and $\theta_1=\hat{t}$ are related as $\ell=(n/n')\hat{t}+\varphi$. These relations imply that, in fact, Eq. (22) represents a dynamical system with an action variable $D(\hat{t})$ and an angular variable $\varphi(\hat{t})$. These equations are now in the correct form for applying the partial averaging technique.

The averaged dynamics of the outer planet, to the first order of perturbation, is obtained by averaging quantities D and φ in Eq. (22) using integral (A7). The result, after eliminating $\overline{D}$, can be written as

$$\ddot{\overline{\varphi}}-3\,\mu\, a^{-2}_{(n:n')}\overline{\mathcal{F}}(L_{(n:n')},G,\overline{\varphi},g)=0, \tag{23}$$

where the overbar denotes an averaged quantity. To study this equation, it is necessary to calculate $\overline{\mathcal{F}}$. From the definition of $\mathcal{F}$, however, one has to first write the *external Hamiltonian* H in terms of the mean anomaly ℓ. To do so, we start by writing H as

$$H=-[1+r^2-2\,r\cos(\theta-\theta_1)]^{-1/2}. \tag{24}$$

The dependence of H on the mean anomaly is, in fact, implied through the dependence of r and θ on the true anomaly v. That is, in order to write H as a function of ℓ, we need to substitute for r from Eq. (3) and replace θ by $g+v$. The mean anomaly ℓ appears when $\cos v$ and $\sin v$ are replaced by

$$\cos v=-e+2\left(\frac{1-e^2}{e}\right)\sum_{j=1}^{\infty}\cos(j\ell)J_j(je), \tag{25}$$

and

$$\sin v=(1-e^2)^{1/2}\sum_{j=1}^{\infty}\sin(j\ell)[J_{j-1}(je)-J_{j+1}(je)]. \tag{26}$$

Here J_j is the Bessel function of order j. The Hamiltonian H can, therefore, be written as

$$H=-\{[1+a^2-2a\cos(\ell+g-\theta_1)]-e\,a\,[2a\cos\ell+\cos(2\ell+g-\theta_1)-3\cos(g-\theta_1)]$$
$$+\tfrac{1}{4}a\,e^2[2a(3-\cos 2\ell)+4\cos(\ell+g-\theta_1)-3\cos(3\ell+g-\theta_1)-\cos(\ell-g+\theta_1)]$$
$$+O(e^3)\}^{-1/2}. \tag{27}$$

To calculate $\mathcal{F}$, we need to differentiate H with respect to the mean anomaly ℓ. From Eq. (27), we can see that such a differentiation will result in a very complex expression for the function $\mathcal{F}$, which makes the calculation of its averaged value through integral (A7), if not impossible, quite difficult. Traditionally in celestial mechanics, such complexities are avoided by expanding the gravitational effects of the perturbing bodies in terms of the osculating orbital elements such as eccentricity.[27] Such expansions are quite customary in studies of the dynamics of the bodies, such as planets of our solar system where, except Pluto, the mean orbital eccentricities range from 3% to 8%.

In this paper, the perturbative effect of the outer planet appears as function $\mathcal{F}$ in Eq. (23). One can consider this equation as the equation of a dynamical system written according to the Newton's second law where $\mathcal{F}$ represents its associated force. After differentiating Eq. (27) with respect to the mean anomaly and expanding the results in terms of the eccentricity of the outer planet, this force can be written as

$$\mathcal{F}=\mathcal{F}^{(0)}+e\,\mathcal{F}^{(1)}+e^2\,\mathcal{F}^{(2)}+O(e^3), \tag{28}$$

where

$$\mathcal{F}^{(0)}=a\,[1+a^2-2a\cos(\ell+g-\theta_1)]^{-3/2}\sin(\ell+g-\theta_1), \tag{29}$$

$$\mathcal{F}^{(1)}=a\,[1+a^2-2a\cos(\ell+g-\theta_1)]^{-3/2}[a\sin\ell+\sin(2\ell+g-\theta_1)]$$
$$+\tfrac{3}{2}a^2[1+a^2-2a\cos(\ell+g-\theta_1)]^{-5/2}\sin(\ell+g-\theta_1)$$
$$\times[2a\cos\ell+\cos(2\ell+g-\theta_1)-3\cos(g-\theta_1)], \tag{30}$$

and

$$\mathcal{F}^{(2)}=\tfrac{1}{8}a\,[1+a^2-2\,a\cos(\ell+g-\theta_1)]^{-3/2}[4a\sin 2\ell-4\sin(\ell+g-\theta_1)+9\sin(3\ell+g-\theta_1)$$
$$+\sin(\ell-g+\theta_1)]-\tfrac{3}{16}a^2[1+a^2-2\,a\cos(\ell+g-\theta_1)]^{-5/2}[20\,a\sin(\ell+g-\theta_1)$$
$$-14\,a\sin(3\ell+g-\theta_1)+14\,a\sin(\ell-g+\theta_1)+16\sin 2(\ell+g-\theta_1)-7\sin 2(2\ell+g-\theta_1)$$
$$+2(7-4a^2)\sin 2\ell-\sin 2(g-\theta_1)]+\tfrac{15}{32}a^3[1+a^2-2a\cos(\ell+g-\theta_1)]^{-7/2}[2(4a^2$$
$$+13)\sin(\ell+g-\theta_1)+(4a^2-7)\sin(3\ell+g-\theta_1)-(4a^2-15)\sin(\ell-g+\theta_1)+\sin(5\ell+3g$$
$$-3\theta_1)+9\sin(\ell+3g-3\theta_1)+4a\sin 2(2\ell+g-\theta_1)-16\,a\sin 2\ell-12\,a\sin 2(g-\theta_1)$$
$$-8\,a\sin 2(\ell+g-\theta_1)-6\sin 3(\ell+g-\theta_1)]. \tag{31}$$

Expansion of $\mathcal{F}$ in terms of e, as given by Eq. (28), enables us to simplify the calculations of $\overline{\mathcal{F}}$ by integrating only the terms that play more significant roles. The question is now how to identify such terms. In the following, we answer this question.

To compute the averaged value of $\mathcal{F}$, we need to integrate Eq. (28) using formula (A7). From Eqs. (29)–(31) one can see that because of the terms $[1+a^2-2a\cos(\ell+g-\theta_1)]^{-\lambda}$, $\lambda=3/2,5/2,7/2$, calculation of integral (A7) may not be quite doable. This difficulty can, however, be overcome taking into account that for the outer planet $r_2>r_1$, or in a dimensionless form and in terms of the osculating elements, $a>1$. Therefore, the above-mentioned quantity can be written as $a^{-2\lambda}[1+a^{-2}-2a^{-1}\cos(\ell+g-\theta_1)]^{-\lambda}$, which can, subsequently, be expanded using the identity

$$(1-2\,\xi\cos\alpha+\xi^2)^{-\lambda}=\sum_{q=0}^{\infty} C_q^{\lambda}(\cos\alpha)\xi^q, \quad |\xi|<1. \tag{32}$$

In this equation,

$$C_q^{\lambda}(\cos\alpha)=\sum_{h=0}^{q}\frac{\Gamma(\lambda+h)\Gamma(\lambda+q-h)}{h!\,(q-h)!\,[\Gamma(\lambda)]^2}\cos[(q-2h)\alpha] \tag{33}$$

are the Gegenbauer polynomials and α and ξ are equal to $\ell+g-\theta_1$ and a^{-1}, respectively.

An inspection of Eqs. (29)–(31) reveals that quantities $\mathcal{F}^{(0)}$, $\mathcal{F}^{(1)}$, and $\mathcal{F}^{(2)}$ share a common feature; the terms $[1+a^2-2a\cos(\ell+g-\theta_1)]^{-\lambda}$ are multiplied by sinus functions with angular arguments of a general form $[\nu\ell+\nu'(g-\theta_1)]$ where ν and ν' are integers. For instance, in Eq. (29), $\nu=\nu'=1$ and in the first term of Eq. (30), $\nu=1$ and $\nu'=0$. Therefore, a general term of Eqs. (29)–(31) can be written as

$$\begin{aligned}&[1+a^2-2a\cos(\ell+g-\theta_1)]^{-\lambda}\sin[\nu\ell+\nu'(g-\theta_1)]\\&\quad=\sum_{q=0}^{\infty}\sum_{h=0}^{q} a^{-(q+2\lambda)}\frac{\Gamma(\lambda+h)\Gamma(\lambda+q-h)}{h!(q-h)!\,[\Gamma(\lambda)]^2}\cos[(q-2h)(\ell+g-\theta_1)]\sin[\nu\ell+\nu'(g-\theta_1)].\end{aligned} \tag{34}$$

Consequently, $\mathcal{F}$ will be equal to the sum of terms proportional to $e^s\cos[(q-2h)(\ell+g-\theta_1)]\sin[\nu\ell+\nu'(g-\theta_1)]$ where $s=0,1,2$.

The above-mentioned quantity appeared in Eq. (28) after the Hamiltonian (27) was differentiated with respect to the mean anomaly ℓ. That means, the three components of this quantity, $\cos[(q-2h)(\ell+g-\theta_1)]$, $\sin[\nu\ell+\nu'(g-\theta_1)]$ and e^s, have their origins in H. A deeper look at Eq. (27) indicates what the nature of these components are and how they contribute to the averaged dynamics of the outer planet.

The first term in the curly braces in Eq. (27) is the term responsible for $[1+a^2-2a\cos(\ell+g-\theta_1)]^{-\lambda}$ and consequently, for the expansion (32). As seen from Eq. (27), this term is associated with the zeroth power of eccentricity. That is, it represents the effect of the inner planet as the $\mathcal{F}^{(0)}$ component of the force of the dynamical system (23). Later in this section, we will discuss this component in more detail and explain its contribution to the dynamics of the system while captured in a (1:1) resonance.

The $\sin[\nu\ell+\nu'(g-\theta_1)]$ term in the above-mentioned coupling has its roots in all terms of the Hamiltonian H. To study this term in more details, it proves useful to evaluate the averaged value of $\mathcal{F}$ using formula (A7). Using the expansion (34), a general term of $\overline{\mathcal{F}}$ will be proportional to

$$\begin{aligned}&\int_0^{2\pi n'}\sin[(\nu+q-2h)\ell+(\nu'+q-2h)(g-\theta_1)]\mathrm{d}\hat{t}\\&\quad+\int_0^{2\pi n'}\sin[(\nu-q+2h)\ell+(\nu'-q+2h)(g-\theta_1)]\mathrm{d}\hat{t}.\end{aligned}$$

Recall that in an $(n:n')$ resonance, $\ell=(n/n')\hat{t}+\varphi$. We also have $\theta_1=\hat{t}$. Therefore, because of their harmonic natures, the above-mentioned integrals will be equal to zero except for those cases where the variable $\hat{t}$ in the integrands vanishes. In the first integral, this corresponds to $\nu+q-2h=\pm n'$ and $\nu'+q-2h=\pm n$ and in the second integral we must have $\nu-q+2h=\pm n'$ and $\nu'-q+2h=\pm n$. These four equations imply that $(q-2h)$ has to be equal to one of the four integers $\pm(\nu\pm n')$ and, at the same time, one of the four integers $\pm(\nu'\pm n)$ with the same arrangement of $+$ and $-$ signs, in order for the quantity $\mathcal{F}$ to have a nonzero averaged value. In other words, we must have

TABLE I. The angular arguments of the contributing terms of expansion (28) for a Sun–protoJupiter–protoSaturn system in a (1:2) resonance.

Angular argument of the contributing terms	(ν,ν')	$\pm(q-2h)$
ℓ	(1,0)	3,1
$g-\theta_1$	(0,1)	2,0
$\ell+2g-2\theta_1$	(1,2)	3,1
$2\ell+g-\theta_1$	(2,1)	4,2,0
$3\ell+2g-2\theta_1$	(3,2)	5,3,1

$$|\Delta\nu| = |\nu-\nu'| = n'-n. \tag{35}$$

Equation (35) is, indeed, a *selection rule*. That is, it can be used to identify the contributing terms of expansion (28) in the averaged dynamics of the outer planet in an $(n:n')$ resonance. To show this, we apply the above-mentioned analysis to a specific three-body system consisting of Sun, a proto-Jupiter, and a proto-Saturn. It was shown by Melita and Woolfson[28] and also by Haghighipour[19] that in a medium of planetesimals, the protoSaturn of the three-body system above undergo an inward migration when the dynamical friction force of the medium is taken into consideration. Recently Masset and Snellgrove[29] have also arrived at the same conclusion in their study of the migration of giant protoplanets embedded in a protoplanetary disk. As a result of this migration, the semimajor axis of the protoSaturn decreases until it is captured in a near (1:2) resonance with the protoJupiter. It has also been shown that under certain conditions, this body can migrate outward and become captured in higher order resonances of the form $(1:n')$ where $n' \geqslant 3$.[19,20,30] Equation (23) can, therefore, be used to study the averaged dynamics of the proto-Saturn above near a (1:2) and also near a higher order resonance of (1:3).

From the *selection rule* (35), it becomes evident that for the system in a (1:2) resonance, only $\mathcal{F}^{(1)}$ will have nonzero averaged value and when the system is captured in a (1:3) commensurability, only $\mathcal{F}^{(2)}$ will contribute. Tables I and II show the angular arguments of the sinus functions of the contributing terms of $\mathcal{F}^{(1)}$ and $\mathcal{F}^{(2)}$ and also their corresponding values of $(q-2h)$.

The quantity $|\Delta\nu|$ in the selection rule (35) is called the order of the resonance. The fact that $\mathcal{F}^{(1)}$ is the first contributing term of expansion (28) in a (1:2) resonance and $\mathcal{F}^{(2)}$ is its first contributing term in a (1:3) resonance imply that in a first-order exterior resonance such as (1:2), the first contributing term is proportional to e^1 and similarly, in a second-order resonance such as (1:3), the first contributing term is proportional to e^2. In general, by expanding $\mathcal{F}$ to higher orders of eccentricity, one can show that in an exterior $(n:n')$ resonance of order $|\Delta\nu|$, the first fulfillment of the condition (35) by the factor $\sin[\nu\ell+\nu'(g-\theta_1)]$ appears in a term proportional to e^s where s is equal to $|\Delta\nu|$. For instance, the contribution of expansion (28) to the averaged dynamics of the outer planet in a resonance of the form $(n:n+1)$ will first appear in its second term, $\mathcal{F}^{(1)}$, and the third term of this expansion, $\mathcal{F}^{(2)}$, will be the first term with a nonzero averaged

TABLE II. The angular arguments of the contributing terms of expansion (28) for a Sun–protoJupiter–protoSaturn system in a (1:3) resonance.

Angular argument of the contributing terms	(ν,ν')	$\pm(q-2h)$
2ℓ	(2,0)	5,1
$2(g-\theta_1)$	(0,2)	3,1
$\ell+3g-3\theta_1$	(1,3)	4,2
$\ell-g+\theta_1$	(1,−1)	4,2,0
$3\ell+g-\theta_1$	(3,1)	6,2,0
$2(2\ell+g-\theta_1)$	(4,2)	7,3,1
$5\ell+3g-3\theta_1$	(5,3)	8,4,2

value when the system is captured in an $(n:n+2)$ commensurability. The role of $\sin[\nu\ell+\nu'(g-\theta_1)]$ in the coupling term and, consequently, in the averaged dynamics of the outer planet is to differentiate the contributing terms of the expansion (28) for an $(n:n')$ resonance by determining the power of the eccentricity to which the disturbing force $\mathcal{F}$ has to be expanded, through the selection rule (35). The factor e^s in the coupling represents the strength of the contributing term associated with a resonance of order $s=\Delta\nu$. It is customary in celestial mechanics to call this resonant state an e^s-resonance.[27] For instance, the (1:2) resonant state in the Sun–protoJupiter–protoSaturn system studied previously is an e^1-resonance and the state of the system in a (1:3) commensurability corresponds to an e^2-resonance.

Let us now, just as examples of the first- and the second-order exterior resonances, study the averaged system near (1:2) and (1:3) commensurabilities. In general, after replacing ℓ by its equivalent value given by Eq. (15), substituting for $(q-2h)$ by $\pm(\nu\pm n')$ and $\pm(\nu'\pm n)$, and averaging the results, the product of $\cos[(q-2h)(\ell+g-\theta_1)]$ and $\sin[\nu\ell+\nu'(g-\theta_1)]$ will produce terms that are proportional to $\sin(n'\overline{\varphi}+ng)$. For instance, for a system near a (1:2) resonance,

$$\overline{\mathcal{F}}_{(1:2)}=\frac{e_{(1:2)}}{a^2_{(1:2)}}\sigma_{(1:2)}\sin(2\overline{\varphi}+g), \tag{36}$$

and for a (1:3) resonance,

$$\overline{\mathcal{F}}_{(1:3)}=\frac{e^2_{(1:3)}}{4a^2_{(1:3)}}\left[\sigma^{(3/2)}_{(1:3)}+3\sigma^{(5/2)}_{(1:3)}+\frac{15}{a^2_{(1:3)}}\sigma^{(7/2)}_{(3:1)}\right]\sin(3\overline{\varphi}+g). \tag{37}$$

In these equations,

$$\sigma_{(1:2)}=\sum_{h=0}^{\infty}\left[\frac{\Gamma\left(\frac{3}{2}+h\right)}{a^h_{(1:2)}h!\Gamma\left(\frac{3}{2}\right)}\right]^2\left\{1+\left(\frac{2h+3}{h+1}\right)\left[1-\frac{3}{4a^2_{(1:2)}}\left(\frac{2h+5}{h+2}\right)\right]\right\}, \tag{38}$$

$$\sigma^{(3/2)}_{(1:3)}=\sum_{h=0}^{\infty}\left[\frac{\Gamma\left(\frac{3}{2}+h\right)}{a^h_{(1:3)}h!\Gamma\left(\frac{3}{2}\right)}\right]^2\left\{\frac{9}{2}+\left(\frac{2h+3}{h+1}\right)\left[1+\frac{1}{8a^2_{(1:3)}}\left(\frac{2h+5}{h+2}\right)\right]\right\}, \tag{39}$$

$$\sigma^{(5/2)}_{(1:3)}=\sum_{h=0}^{\infty}\left[\frac{\Gamma\left(\frac{5}{2}+h\right)}{a^h_{(1:3)}h!\Gamma\left(\frac{5}{2}\right)}\right]^2\left\{\frac{7}{2}+\left[1-\frac{7}{8a^2_{(1:3)}}\right]\left(\frac{2h+5}{h+1}\right)-\frac{1}{8a^2_{(1:3)}}\left[7+\frac{1}{4a^2_{(1:3)}}\left(\frac{2h+9}{h+3}\right)\right]\frac{(2h+7)(2h+5)}{(h+2)(h+1)}\right\}, \tag{40}$$

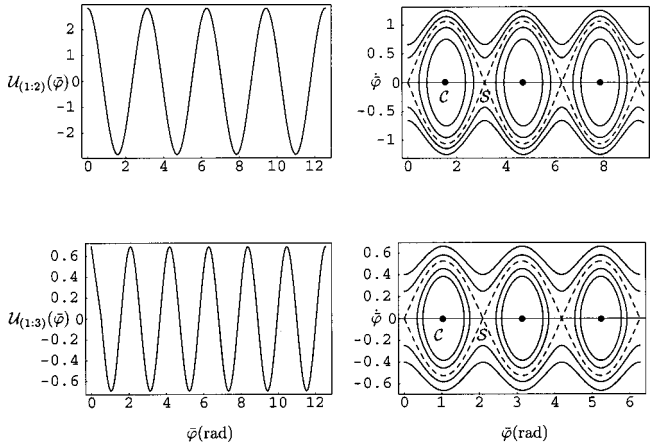

FIG. 1. Graphs of the potential function $\mathcal{U}_{(1:2)}(\overline{\varphi})$ (top left panel) and its phase diagram (top right panel) and the potential function $\mathcal{U}_{(1:3)}(\overline{\varphi})$ (bottom left panel) with its associated phase diagram (bottom right panel) for the system studied by Haghighipour (Ref. 19) at (1:2) and (1:3) resonances. The scale on all vertical axes is 0.01. The origins on the horizontal axes of the graphs of the (1:2) resonance have been shifted by -0.44(rad) and the corresponding origins of the graphs of the (1:3) resonance have been shifted by -1.7(rad).

$$\sigma^{(7/2)}_{(1:3)}=\sum_{h=0}^{\infty}\left[\frac{\Gamma\left(\frac{7}{2}+h\right)}{a^{h}_{(1:3)}h!\,\Gamma\left(\frac{7}{2}\right)}\right]^{2}\left\{\frac{1}{2}\left[a^{2}_{(1:3)}-\frac{7}{4}\right]-\frac{3}{4}\left(\frac{2h+7}{h+1}\right)\right.$$
$$+\left[\frac{1+15a^{2}_{(1:3)}-4a^{4}_{(1:3)}}{32a^{2}_{(1:3)}}\right]\frac{(2h+9)(2h+7)}{(h+2)(h+1)}$$
$$\left.+\frac{3}{16a^{2}_{(1:3)}}\left[1-\frac{3}{8a^{2}_{(1:3)}}\left(\frac{2h+13}{h+4}\right)\right]\frac{(2h+11)(2h+9)(2h+7)}{(h+3)(h+2)(h+1)}\right\}. \tag{41}$$

Because $\overline{\mathcal{F}}$ is proportional to $\sin(n'\overline{\varphi}+ng)$, Eq. (23) can be viewed as the equation of a mathematical pendulum with a potential function proportional to $\cos(n'\overline{\varphi}+ng)$ [see Eq. (A12)]. Such a pendulum, with its harmonic potential, is a characteristic of the first-order partially averaged system near a resonance where $e_{(n:n')}$ is considered to be constant.[13,14,19,31] For instance, for the cases of (1:2) and (1:3) resonances,

$$\mathcal{U}_{(1:2)}(\overline{\varphi})=\frac{3e_{(1:2)}}{2a^{4}_{(1:2)}}\sigma_{(1:2)}\cos(2\overline{\varphi}+g)+\text{constant}, \tag{42}$$

and

$$\mathcal{U}_{(1:3)}(\overline{\varphi})=\frac{e^{2}_{(1:3)}}{4a^{4}_{(1:3)}}\left[\sigma^{(3/2)}_{(1:3)}+3\,\sigma^{(5/2)}_{(1:3)}+\frac{15}{a^{2}_{(1:3)}}\sigma^{(7/2)}_{(1:3)}\right]\cos(3\overline{\varphi}+g)+\text{constant}. \tag{43}$$

Figure 1 shows the graphs of these two potential functions with their corresponding phase diagrams. In producing these graphs, the numerical values of the orbital eccentricity and the semimajor axis of P_2 have been taken from the restricted three-body system of Haghighipour[19] at (1:2) and (1:3) resonances.

The harmonic nature of the potential function of the pendulum (23) indicates that this pendulum can be in three dynamical states; stable equilibrium corresponding to the minimum of the potential function (centers $\mathcal{C}$ on the phase diagrams), unstable equilibrium corresponding to the

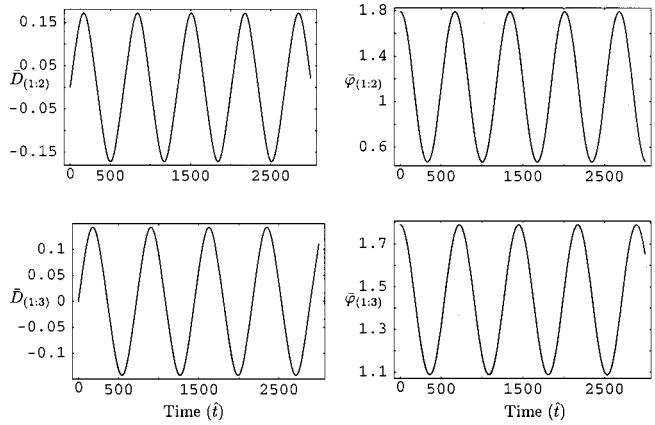

FIG. 2. Graphs of $\bar{D}(\hat{t})$ and $\bar{\varphi}(\hat{t})$ for the systems of Fig. 1, partially averaged to the first order.

maximum of the potential function (saddle points $\mathcal{S}$) or, an oscillatory (librational) motion around the stable equilibrium (the orbits inside the *separatrix*, the dashed orbit that passes through the saddle point $\mathcal{S}$). The resonance lock phenomenon is geometrically depicted by these librational motions.

The oscillatory variations in values of $\bar{\varphi}$ create a harmonic behavior for the action variable $\bar{D}$. From Eq. (22), for a system at an $(n:n')$ resonance where $\bar{\mathcal{F}}$ is proportional to $\sin(n'\bar{\varphi}+ng)$, $\bar{D}$ will be proportional to $\cos(n'\bar{\varphi}+ng)$. Figure 2 shows the graphs of $\bar{D}$ and $\bar{\varphi}$ against time for the systems of Fig. 1. As mentioned in Sec. III, D is the measure of changes in the action variable L or, in other words, an indication of the variations of the semimajor axis of the outer planet from its resonant value. From Eq. (A14), the width of the resonance band within which the semimajor axis of the outer planet varies around its resonant value is limited by the height of the separatrix and to the first order of perturbation can be written as

$$\Delta a_{(n:n')}=4\left[\tfrac{2}{3}\mu\, a^{3}_{(n:n')}\,\Delta\,\mathcal{U}_{(n:n')}(\bar{\varphi})\right]^{1/2}, \tag{44}$$

where $\Delta\,\mathcal{U}_{(n:n')}(\bar{\varphi})$ is equal to the difference between the maximum and the minimum values of $\mathcal{U}_{(n:n')}(\bar{\varphi})$.

It is necessary to mention that the procedure presented here for expansion of $[1+a^2-2a\cos(\ell+g-\theta_1)]^{-\lambda}$ using Gegenbauer polynomials, is not valid for a (1:1) resonance. At this state, from Eq. (13), the Keplerian period of the outer planet becomes nearly equal to T_1. That means, $a_{(1:1)}\simeq 1$ and expansion (32) is no longer applicable. However, it is still possible to use the method of averaging to study the dynamics of the outer planet near a (1:1) commensurability. The *external Hamiltonian* H, in this case, must be studied in its entirety as given by Eq. (25). Expanding H to the second order in eccentricity and integrating $\mathcal{F}$ in the vicinity of the (1:1) resonance, we have

$$\begin{aligned}\bar{\mathcal{F}}_{(1:1)}=&\tfrac{1}{2}a_{(1:1)}[2-e^2_{(1:1)}]\sin(\bar{\varphi}+g)\,[1+a^2_{(1:1)}-2a_{(1:1)}\cos(\bar{\varphi}+g)]^{-3/2}\\&-3\,a^2_{(1:1)}\,e^2_{(1:1)}\sin 2(\bar{\varphi}+g)\,[1+a^2_{(1:1)}-2a_{(1:1)}\cos(\bar{\varphi}+g)]^{-5/2}\\&+\tfrac{45}{4}a^3_{(1:1)}\,e^2_{(1:1)}\sin^3(\bar{\varphi}+g)[1+a^2_{(1:1)}-2a_{(1:1)}\cos(\bar{\varphi}+g)]^{-7/2}.\end{aligned} \tag{45}$$

The potential function associated with the first-order partially averaged system is given by

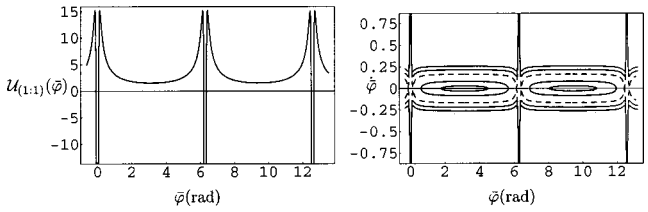

FIG. 3. Graphs of the potential function $\mathcal{U}_{(1:1)}(\bar{\varphi})$ (left panel) and its phase diagram (right panel) against $\bar{\varphi}$.

$$\mathcal{U}_{(1:1)}(\bar{\varphi})=\frac{3}{a_{(1:1)}^2}[1+a_{(1:1)}^2-2a_{(1:1)}\cos(\bar{\varphi}+g)]^{-1/2}-\frac{21}{2a_{(1:1)}}e_{(1:1)}^2\cos(\bar{\varphi}+g)$$
$$\times[1+a_{(1:1)}^2-2a_{(1:1)}\cos(\bar{\varphi}+g)]^{-3/2}+\frac{27}{4}e_{(1:1)}^2\sin^2(\bar{\varphi}+g)$$
$$\times[1+a_{(1:1)}^2-2a_{(1:1)}\cos(\bar{\varphi}+g)]^{-5/2}. \tag{46}$$

Figure 3 shows the graph of this potential for $g=0°$. The fact that $d\mathcal{U}_{(1:1)}(\bar{\varphi})/d\bar{\varphi}$ shows slight deviations from zero near the points of stable equilibrium is an indication of a slow-frequency librational motion in those neighborhoods. To see this, let us apply this analysis to the system of Sun–Jupiter–Trojan asteroid. Located at the L_4 and L_5 Lagrangian points of Jupiter's orbit, Trojan asteroids are in a near (1:1) resonance with Jupiter and have a librational motion with a period of approximately 148 years.[32,33] Substituting for a and e in Eq. (46) by the values of the semimajor axis and the eccentricity of Trojan asteroids and Taylor expanding $\mathcal{U}_{(1:1)}(\bar{\varphi})$ around its stable equilibrium, one will obtain a librational period of approximately 110 years. The difference between this period and the 148 years reported in the above-mentioned references can be attributed to several factors such as neglecting the gravitational effect of Saturn, restricting Jupiter to stay on a circular orbit, and also to the coupling between φ and the argument of the pericenter g. Studies are currently under way to extend the partially averaged equations of this system to the second order of perturbation where φ and g decouple. A closer value for the above-mentioned librational period is expected in this case.

The first-order partially averaged system near a resonance, presented by Eq. (23) is, in general, Hamiltonian. It portrays the phenomenon of resonance-lock as librational motion of a pendulum. However, with respect to an arbitrary perturbation, this Hamiltonian system is structurally unstable. In an actual system, in order to be able to draw conclusions on long-term behavior of quantities such as orbital eccentricity of the outer planet, its angular momentum and also the precession of its orbit, it is necessary to extend this analysis to higher orders of the perturbation parameter $\mu^{1/2}$. Such an extension will allow for the time variation of the angle g to be taken into consideration. This will render the system of Eqs. (18)–(21) in a set of equations with two angular variables, φ and g. In order to be able to apply the method of partial averaging near a resonance to this system, it is then necessary to introduce an averaging transformation that renders the equations of the system in a form that to the first order of perturbation, it becomes automatically equivalent to the first-order partially averaged system at resonance. The second-order partially averaged system is then obtained by averaging those equations using formula (A7). Such studies are currently in preparation for publication.

V. SUMMARY AND CONCLUDING REMARKS

Application of the method of partial averaging to the study of the dynamics of the outer body of a restricted three-body system while captured in a resonance has been presented here. Analysis of the first-order partially averaged system near a resonance has revealed that the equations of

motion of the outer planet, averaged over fast periodic motion at resonance, resemble a mathematical pendulum. Such a pendulum analogy can also be found in the comprehensive study of orbital resonances among planetary satellites by Peale[34] and also in the comprehensive study of the dynamical behavior of a test particle near an interior as well as an exterior resonance in a restricted three-body system by Winter and Murray.[11,12]

In the analysis presented here, the driving force of the pendulum-like first-order partially averaged system is obtained from the *external Hamiltonian H* [Eq. (24)] which involves the gravitational effect of the inner planet on the dynamics of the outer one. In writing the dynamical equations of the outer planet in terms of the Delaunay variables, this force appears as F_r and F_θ in Eqs. (8)–(11). It is important to mention that the form of these equations [i.e., Eqs. (8)–(11)] is quite general and independent of the physical nature of the perturbation. In a system where the perturbations are non-Hamiltonian, extra terms will be added to the functions F_r and F_θ as well as Eqs. (16) and (17). However, Eqs. (8)–(11) will keep their general form.[19,20] The procedure presented here regarding the application of the partial averaging technique and the analysis of the pendulum-like equation are also quite general and can be applied to non-Hamiltonian systems in a similar fashion. In fact, one of the most important features of the method of partial averaging near a resonance is that it presents a general analytical procedure that is equally applicable to both Hamiltonian and non-Hamiltonian systems. As examples of the systems where the method of partial averaging near a resonance has been used in conjunction with non-Hamiltonian perturbations, we refer the reader to Refs. 19, 23, and 24.

As mentioned in Sec. IV, the first-order partially averaged system near a resonance presents the first step in utilizing the method of averaging in the analytical study of the dynamics of a resonance-locked system. To this order of approximation, the argument of the pericenter g was assumed to be constant. In order to obtain a more comprehensive picture of the dynamics of a system near a resonance and the roles that perturbative effects play in its stability, one has to extend this analysis to higher orders of the perturbation parameter $\mu^{1/2}$. Such an extension is necessary to assure decoupling of the angles φ and g (see, e.g., Ref. 20). At that stage, one can apply the averaging technique presented here to the dynamics of the system at the second order of perturbation by averaging those equations over the fast-changing angular variable φ and studying the pendulum-like equation of the angular variable g. Such studies are currently under way for the case of (1:1) resonance and their applications to Trojan asteroids.

The choice of a restricted system as presented in this study was merely to focus attention on the method of partial averaging and its capabilities as another approach to analytical analysis of the dynamics of a system near a resonance. The analysis presented here is quite general and can be applied to any dynamical system at resonance. One can apply such analysis to the systems at interior resonances where $a<1$, by setting $\xi=a$ in Eq. (32) and changing the *selection rule* (35) to

$$|\Delta\nu| = n - n'. \tag{47}$$

An implication of this *selection rule* can be found in a recent paper by Michtchenko and Ferraz-Mello[35] on analytical modeling of the Jupiter–Saturn system near their (5:2) resonance. They show that at the lowest order, the contribution of the resonant part of the disturbing function appears as the third power of eccentricity, a result that is also implied by the *selection rule* (47).

Other interesting cases for application of the partial averaging technique are the study of the stability of the extrasolar planetary system Gliese 876[2] where its two planets are locked in a near (2:1) commensurability, the study of dynamical stability of P-type binary planetary systems where recent numerical integrations by Holman and Wiegert[36] have indicated the existence of islands of instabilities for eccentric binaries at $(n:1), n>3$, resonances and also the study of the dynamical evolution of pulsar planetary systems such as PSR B1257+12[37] and PSR B1620-26.[38–41] It appears that gravitational radiation reaction may play a vital role in the dynamical evolution of these system.[21–26]

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APPENDIX A: METHOD OF PARTIAL AVERAGING NEAR A RESONANCE

A short introduction to the method of partial averaging near a resonance as used in this article is presented here. For more details on this technique, the reader is referred to Refs. 13, 14, 19, and 20.

Partial averaging near a resonance is based on the application of the method of averaging to the dynamical equations of a system in the vicinity of its resonant state.[13,14] These equations are usually written in one of the several standard forms.[13] In celestial mechanics, it is customary to write the dynamical equations of the system in terms of action-angle variables.

Consider a perturbation system with an action variable $\mathcal{B}$ and an angular variable β such that

$$\dot{\mathcal{B}}=\varepsilon\,\mathcal{M}(\mathcal{B},\beta,t,\varepsilon), \tag{A1}$$

and

$$\dot{\beta}=\omega_0(\mathcal{B})+\varepsilon\,\mathcal{Q}(\mathcal{B},\beta,t,\varepsilon), \tag{A2}$$

where $\mathcal{M}$ and $\mathcal{Q}$ are periodic in time with period $\mathcal{T}$ and ω_0 is the frequency of the unperturbed $(\varepsilon=0)$ system. At resonance $\mathcal{T}$ and ω_0 are related as

$$l\,\omega_0=l'\,\omega_{\mathcal{T}}, \tag{A3}$$

where $\omega_{\mathcal{T}}$ is the angular frequency associated with $\mathcal{T}$ and l and l' are positive integers. One can show that in the vicinity of the resonance state (A3), Eqs. (A1) and (A2) can be written as[14,20]

$$\dot{\mathcal{E}}=\varepsilon^{1/2}\,\mathcal{M}(\mathcal{B}_0,\beta,t),+\varepsilon\,\mathcal{E}\frac{\partial\mathcal{M}}{\partial\mathcal{B}}(\mathcal{B}_0,\beta,t)+O(\varepsilon^{3/2}) \tag{A4}$$

and

$$\dot{\Theta}=\varepsilon^{1/2}\,\mathcal{E}\frac{\partial\omega_0}{\partial\mathcal{B}}(\mathcal{B}_0)+\varepsilon\left[\mathcal{Q}(\mathcal{B}_0,\beta,t)+\frac{1}{2}\mathcal{E}^2\frac{\partial^2\omega_0}{\partial\mathcal{B}^2}(\mathcal{B}_0)\right]+O(\varepsilon^{3/2}), \tag{A5}$$

where

$$\mathcal{E}=\varepsilon^{-1/2}(\mathcal{B}-\mathcal{B}_0),\quad \Theta=\beta-\omega_0(\mathcal{B}_0)t, \tag{A6}$$

represent deviations of $\mathcal{B}$ and β from their resonant values $\mathcal{B}_0$ and $\omega_0(\mathcal{B}_0)t$, respectively. Equations (A6) are, indeed, the necessary transformations for writing Eqs. (A1) and (A2) in the neighborhood of the $(l:l')$ resonance. The averaged dynamics of the system at this neighborhood is obtained by averaging Eqs. (A4) and (A5) using the averaging integral

$$\overline{\mathcal{R}}=\frac{1}{l\mathcal{T}}\int_0^{l\mathcal{T}}\mathcal{R}[\mathcal{B}_0,\omega_0(\mathcal{B}_0)t+\Theta,t]\,\mathrm{d}t, \tag{A7}$$

where $\mathcal{R}$ is a general function.

The first order partially averaged system near $(l:l')$ resonance is obtained by neglecting the $O(\varepsilon)$ terms in Eqs. (A4) and (A5) and is given by

$$\dot{\bar{\mathcal{E}}} = \varepsilon^{1/2}\,\bar{\mathcal{M}}(\mathcal{B}_0, \bar{\Theta}), \tag{A8}$$

and

$$\dot{\bar{\Theta}} = \varepsilon^{1/2}\,\bar{\mathcal{E}}\frac{\partial \omega_0}{\partial \mathcal{B}}(\mathcal{B}_0), \tag{A9}$$

where the overbar indicates an averaged quantity. According to the principle of averaging[13,14,19,23] the dynamics of the system of Eqs. (A1) and (A2) can be approximated by the dynamics of the system (A8) and (A9) during the time interval $\varepsilon^{-1/2}t$. It is necessary to emphasize that in order to be able to make such an approximation, it is required by the principle of averaging that the main dynamical system [i.e., Eqs. (A1) and (A2)] have only one angular variable. Extension of the method of averaging to the systems with two or more angular variables can be found in the works of Grebenikov and Ryabov,[42] Arnold, Kozlov, and Neishtadt[43] and also in a recent paper by Cucu-Dumitrescu and Selaru[44] on the study of the equations of motion around an oblate planet. In the first order of perturbation, however, such an extension is not necessary.

Introducing $\mathcal{H}$, as

$$\mathcal{H} = \varepsilon^{1/2}\left[\frac{1}{2}\bar{\mathcal{E}}^2\frac{\partial \omega_0}{\partial \mathcal{B}}(\mathcal{B}_0) - \int \bar{\mathcal{M}}(\mathcal{B}_0, \bar{\Theta}, t)\, \mathrm{d}\bar{\Theta}\right], \tag{A10}$$

one can show that Eqs. (A7) and (A8) can be written as

$$\dot{\bar{\mathcal{E}}} = -\frac{\partial \mathcal{H}}{\partial \bar{\Theta}}, \quad \dot{\bar{\Theta}} = \frac{\partial \mathcal{H}}{\partial \bar{\mathcal{E}}}. \tag{A11}$$

Equation (A11) implies that $\mathcal{H}$ can be considered as the Hamiltonian of the first-order partially averaged system at resonance. To this Hamiltonian, one can attribute a potential function given by

$$V(\bar{\Theta}) = -\int \bar{\mathcal{M}}(\mathcal{B}_0, \bar{\Theta})\, d\bar{\Theta}. \tag{A12}$$

Differentiating Eqs. (A11) with respect to t and using the Hamiltonian $\mathcal{H}$, one can write

$$\ddot{\bar{\Theta}} - \varepsilon\left[\frac{\partial \omega_0}{\partial \mathcal{B}}(\mathcal{B}_0)\right]\bar{\mathcal{M}}(\mathcal{B}_0, \bar{\Theta}) = 0. \tag{A13}$$

Equation (A13) can be regarded as the equation of a mathematical pendulum with Hamiltonian $\mathcal{H}$ and potential function $V(\bar{\Theta})$. The librational motion of this pendulum presents a geometrical interpretation for the resonance-lock phenomenon. The maximum variation of the action variable $\mathcal{B}$ associated with these librational motions is given by[14]

$$\Delta\mathcal{B} = 2\left\{2\,\varepsilon\left[\frac{\partial \omega_0}{\partial \mathcal{B}}(\mathcal{B}_0)\right]^{-1}[V_{\max}(\bar{\Theta}) - V_{\min}(\bar{\Theta})]\right\}^{1/2} + O(\varepsilon). \tag{A14}$$

APPENDIX B: PROOF OF EQUATIONS (16) AND (17)

From the definition of H, we have

$$\frac{\partial H}{\partial L} = \frac{1}{|\vec{r} - \vec{\mathbf{r}}_1|^{-3}}\left\{[r - \cos(\theta - \theta_1)]\frac{\partial r}{\partial L} + r\sin(\theta - \theta_1)\frac{\partial \theta}{\partial L}\right\}, \tag{B1}$$

$$\frac{\partial H}{\partial G}=\frac{1}{|\vec{r}-\vec{\mathbf{r}}_{\mathbf{1}}|^{-3}}\left\{[r-\cos(\theta-\theta_1)]\frac{\partial r}{\partial G}+r\sin(\theta-\theta_1)\frac{\partial \theta}{\partial G}\right\}, \tag{B2}$$

$$\frac{\partial H}{\partial \ell}=\frac{1}{|\vec{r}-\vec{\mathbf{r}}_{\mathbf{1}}|^{-3}}\left\{[r-\cos(\theta-\theta_1)]\frac{\partial r}{\partial \ell}+r\sin(\theta-\theta_1)\frac{\partial \theta}{\partial \ell}\right\}, \tag{B3}$$

$$\frac{\partial H}{\partial g}=\frac{1}{|\vec{r}-\vec{\mathbf{r}}_{\mathbf{1}}|^{-3}}r\ \sin(\theta-\theta_1)\frac{\partial \theta}{\partial g}. \tag{B4}$$

From these equations it is evident that one needs to compute derivatives of r and θ with respect to all Delaunay variables. From Eq. (3), we have

$$\frac{\partial r}{\partial L}=-\left(\frac{G}{1+e\cos v}\right)^2\left(\cos v\frac{\partial e}{\partial L}-e\sin v\frac{\partial v}{\partial L}\right), \tag{B5}$$

$$\frac{\partial r}{\partial G}=2\left(\frac{G}{1+e\cos v}\right)-\left(\frac{G}{1+e\cos v}\right)^2\left(\cos v\frac{\partial e}{\partial G}-e\sin v\frac{\partial v}{\partial G}\right), \tag{B6}$$

$$\frac{\partial r}{\partial \ell}=ea\sin u\frac{\partial u}{\partial \ell} \tag{B7}$$

and $\partial r/\partial g=0$. On the other hand, from $\theta=g+v$, $\partial\theta/\partial g=1$ and the derivatives of θ with respect to L, G and ℓ will be equal to derivatives of v with respect to these variables. Using $\ell=u-e\sin u$ and $G=L(1-e^2)^{1/2}$ along with Eq. (3), the partial derivatives of r with respect to the Delaunay variables can be written as

$$\frac{\partial r}{\partial L}=\frac{r}{e}a^{-1/2}(2e-\cos v-e\cos^3 v), \tag{B8}$$

$$\frac{\partial r}{\partial G}=\frac{1}{e}[a(1-e^2)]^{1/2}\cos v, \tag{B9}$$

$$\frac{\partial r}{\partial \ell}=ea\,(1-e^2)^{-1/2}\sin v, \tag{B10}$$

and the partial derivatives of θ with respect to L,G, and ℓ will be equal to

$$\frac{\partial \theta}{\partial L}=\frac{G^2}{e\,L^3(1-e^2)}\sin v\,(2+e\cos v), \tag{B11}$$

$$\frac{\partial \theta}{\partial G}=-\frac{1}{e}[a(1-e^2)]^{1/2}\left[\frac{1}{r}+\frac{1}{a(1-e^2)}\right]\sin v, \tag{B12}$$

$$\frac{\partial \theta}{\partial \ell}=\left(\frac{a}{r}\right)^2(1-e^2)^{1/2}. \tag{B13}$$

Replacing the derivatives of r and θ in Eqs. (B1)–(B4) by their equivalent expressions given by Eqs. (B8)–(B13), one can write

$$\frac{\partial H}{\partial L}=\frac{r}{e}a^{-1/2}\left\{\left[\frac{r-\cos(\theta-\theta_1)}{|\vec{r}-\vec{\mathbf{r}}_{\mathbf{1}}|^3}\right](2e-\cos v-e\cos^3 v)+\left[\frac{\sin(\theta-\theta_1)}{|\vec{r}-\vec{\mathbf{r}}_{\mathbf{1}}|^3}\right](2+e\cos v)\sin v\right\}, \tag{B14}$$

$$\frac{\partial H}{\partial G}=\frac{1}{e}[a(1-e^2)]^{1/2}\left\{\left[\frac{r-\cos(\theta-\theta_1)}{|\vec{r}-\vec{\mathbf{r}}_\mathbf{1}|^3}\right]\cos v-\left[\frac{\sin(\theta-\theta_1)}{|\vec{r}-\vec{\mathbf{r}}_\mathbf{1}|^3}\right]\left[\frac{1}{r}+\frac{1}{a(1-e^2)}\right]\sin v\right\}, \tag{B15}$$

$$\frac{\partial H}{\partial \ell}=a\,(1-e^2)^{-1/2}\left\{e\,\sin v\left[\frac{r-\cos(\theta-\theta_1)}{|\vec{r}-\vec{\mathbf{r}}_\mathbf{1}|^3}\right]+\frac{a}{r}(1-e^2)\left[\frac{\sin(\theta-\theta_1)}{|\vec{r}-\vec{\mathbf{r}}_\mathbf{1}|^3}\right]\right\}, \tag{B16}$$

and

$$\frac{\partial H}{\partial g}=\frac{r\,\sin(\theta-\theta_1)}{|\vec{r}-\vec{\mathbf{r}}_\mathbf{1}|^3}, \tag{B17}$$

which along with Eq. (12) immediately results in expressions (16) and (17).

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A mathematical problem of the theory of gelation

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Current theory of gelation describes this process in terms of a set of nonlinear integral equations. In this article the uniqueness of nontrivial solutions of these equations within the unit functional hypercube has been proved. Besides, the convergence to this solution of iterations from an arbitrary point of the above hypercube has been established, which is of utmost importance for calculations of particular gelation processes. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Today mathematical methods are finding ever-increasing use in chemistry.[1–4] These methods prove to be especially efficient in the solution of theoretical problems of polymer chemistry. In view of the leading positions of polymer manufacturing in modern chemical industry the role of mathematical modeling of polymerization processes is hard to overestimate. Among them the most challenging for such a modeling are the processes of obtaining polymer networks. Such a network (gel) is a giant macromolecule occupying the whole of the reaction system.

In the present article considering the formation of a gel we will focus exclusively on the processes of polycondensation of monomers, at least one of which has more than two functional groups. This condition is, however, only a necessary prerequisite of the gelation occuring in the course of a branched polycondensation. Indeed, when this process is conducted in a dilute solution of monomers along with intermolecular reactions, which lead to the enlargement of polymers, intramolecular reactions will vigorously proceed. These latter are responsible for a retardation of gelation due to the decrease in polymer molecules' functionality. At sufficiently pronounced intensity of intramolecular reactions a polymer network will not be formed at all in the course of the synthesis. In this case a suspension of colloid polymer particles will be the product of the reaction.

Our theoretical approach is based on the kinetic model which neglects intramolecular reactions in molecules of finite size. The validity of this assumption, experimentally verified for many particular polycondensation processes,[3,4] is nowadays extensively used in polymer chemistry.

Initially there is a mixture of low-molecular compounds referred to as monomers. Each of them, $R_\alpha A_1^{f_{1\alpha}} A_2^{f_{2\alpha}} \cdots A_n^{f_{n\alpha}}$, is composed of monomeric unit R_α and adjacent functional groups $A_i (i=1,\ldots,n)$ whose numbers $\{f_{i\alpha}\}$ in this αth monomer represent elements of a rectangular matrix of functionalities $\mathbf{f}$ of this monomer. In the course of the stepwise polymerization (polycondensation) functional groups react with each other to form stable chemical bonds between monomeric units. Such chemical transformations in the reaction system result in the formation of polymer molecules involving different number of monomeric units $l_1,\ldots,l_\alpha,\ldots,l_m$, which may be regarded as components of composition vector $\mathbf{l}$. The probability that a monomeric unit chosen at random in the moment t constitutes polymer molecule with given vector $\mathbf{l}$ is known as composition distribution. The problem of finding of this distribution $F(\mathbf{l};t)$ or its generating function

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$$G(\mathbf{s};t)=\sum_{l} F(\mathbf{l};t)\prod_{\alpha=1}^{m} s_{\alpha}^{l_\alpha} \tag{1}$$

represents one of the key problems of the theory of polymerization. In the course of this process the enlargement of polymer molecules takes place accompanied by the growth of their average size:

$$\overline{\mathbf{l}}(t)=\sum_{l}\sum_{\alpha=1}^{m} l_\alpha F(\mathbf{l},t)=\sum_{\alpha} s_\alpha \frac{\partial G}{\partial s_\alpha}\bigg|_{\mathbf{s}=1}. \tag{2}$$

At a certain moment $t=t^*$ the quantity $\overline{\mathbf{l}}$ turns into infinity. To such a situation there corresponds the appearance of infinite macromolecule of gel. Weight fraction $\omega_g(t)$ of this polymer network increases during the polymerization due to the decrease of the weight fraction $\omega_s(t)$ of molecules of finite sizes constituting sol:

$$\omega_s(t)=\sum_{l} F(\mathbf{l};t)=G(\mathbf{l};t). \tag{3}$$

Determination of the dependence $\omega_g(t)=1-\omega_s(t)$ along with the calculation of the gel point is a fundamental problem of the theory of gelation for polymerization processes.

The article is organized as follows. In Sec. II we give the description of the most popular kinetic model of gelation. In Sec. III we propose a convenient generalization of the main equation. In Sec. IV we prove uniqueness of a solution and in Sec. V we prove convergence of iterations.

II. MATHEMATICAL MODELS

The distribution $F(\mathbf{l};t)$ of sol molecules in a simple manner is related to the concentrations of the molecules $C(\mathbf{l};t)$ present at the instant t in the reaction system by

$$F(\mathbf{l};t)=\frac{1}{M}\sum_{\alpha} l_\alpha c(\mathbf{l};t), \quad \text{where} \quad M=\sum_{l}\sum_{\alpha} l_\alpha c(\mathbf{l};t). \tag{4}$$

The evolution of these concentrations with time can be described by material balance equations which resemble the discrete Boltzmann equation.[5] Its form is prescribed by the choice of a particular chemical model of polymerization.

The simplest among them is the ideal model[3] which suggests that the probability for every pair of groups A_i and A_j to react is controlled exclusively by their types i and j. In terms of this model monomeric units are differentiated not only by types α but by their kinds as well. Kind q of the αth type monomeric unit is specified by rectangular matrix $\mathbf{g}$ whose element $g_{i\alpha}$ equals the number of reacted groups A_i in the αth unit. Let us denote by $P_\alpha^q(t)$ the fraction of αth units of the kind q contained in polymers at moment t. Thus, the exact solution of the equation for generating function (1), obtained in Ref. 6 for the ideal model of stepwise polymerization, can be presented as follows:

$$G(\mathbf{s};t)=H(\mathbf{s};\mathbf{u}), \quad \text{where} \quad H(\mathbf{s};\mathbf{u})=\sum_{\alpha} s_\alpha \sum_{q} P_\alpha^q \prod_{i} u_i^{g_{i\alpha}}, \tag{5}$$

where the dependence of components $\{u_i\}$ of the vector $\mathbf{u}$ on components $\{s_\alpha\}$ of the vector $\mathbf{s}$ is possible to determine from the solution of the set of equations

$$u_i=\sum_{j} \pi_{ij} h_j(\mathbf{s};\mathbf{u}) (i=1,\ldots,n). \tag{6}$$

Here use is made of the following designations:

$$h_j(\mathbf{s};\mathbf{u})=\frac{H_j(\mathbf{s};\mathbf{u})}{H_j(\mathbf{1};\mathbf{1})},\quad \text{where}\quad H_j(\mathbf{s};\mathbf{u})=\frac{\partial H}{\partial u_j}, \tag{7}$$

while π_{ij} represents the fractions of all reacted groups A_i that formed chemical bond (ij) by reacting with groups A_j. Functions $P_\alpha^q(t)$ and $\pi_{ij}(t)$ can be found from the solution of the Cauchy problem for the set of the first-order ordinary differential equations whose coefficients are the parameters of ideal kinetic model which characterize the probabilities of reactions between different groups. Particular form of functions $P_\alpha^q(t)$ and $\pi_{ij}(t)$ is, however, beyond the scope of our present work. We will just make use of the fact that all their values belong to the segment [0,1] and meet obvious normalization conditions

$$\sum_\alpha \sum_q P_\alpha^q \equiv 1, \quad \sum_j \pi_{ij} \equiv 1. \tag{8}$$

Weight fraction of sol (3) is determined according to (5) and (6) by the expression

$$\omega_s = H(\mathbf{1};\mathbf{y}), \tag{9}$$

where the components of vector $\mathbf{y}$ are obtainable from the solution of the set of equations

$$y_i=\sum_j \pi_{ij} h_j(\mathbf{1};\mathbf{y})\,(i=1,\ldots,n). \tag{10}$$

It is easy to notice that in view of (8) this set always has trivial solution

$$y_1=y_2=\cdots=y_n=1, \tag{11}$$

which is the only one in unit hypercube $0\leqslant y_i\leqslant 1\,(i=1,\ldots,n)$ just up to the moment when a polymer network is formed. At this moment $t=t^*$ average size of polymers (2) becomes infinite to which there mathematically corresponds turning into unity of the largest eigenvalue of the matrix with elements

$$\theta_{ik}=\sum_j \pi_{ij}\left.\frac{\partial h_j(\mathbf{1};\mathbf{u})}{\partial u_k}\right|_{\mathbf{u}=\mathbf{1}}. \tag{12}$$

At gel point $t=t^*$ the bifurcation happens which results in forking $t>t^*$ from trivial solution (11) of the equation (6) and of a nontrivial one situated inside unit hypercube. The substitution of this solution into expression (3) enables one to find the dependence of the weight fraction of sol on time of polymerization.

The ideal model of stepwise polymerization being of prime importance in macromolecular chemistry fails, however, to describe some particular gelation processes. In such cases mathematical models normally resort to more sophisticated kinetic models. The most reputable among them is the ''substitution effect'' (SE) model,[7] which takes account of the dependence of a functional group reactivity on the number of groups of every type among its neighbors in monomeric unit which have already reacted with one or another groups of other molecules. As a result of such chemical transformations a group A_i reacts with group A_j to yield chemical bond (ij). The set of such bonds adjoined to the αth type unit characterizes in terms of the SE model the kind q of this unit. The following expression,[7]

$$G(\mathbf{s};\mathbf{t})=H(\mathbf{s};[\mathbf{u}]), \tag{13}$$

represents an extension of the expression (5) where H stands for the generating functional of the distribution P_α^q of the probabilities of *labeled* units for types α and kinds q:

$$H(\mathbf{s};[\mathbf{u}])=\sum_{\alpha} s_{\alpha}\sum_{q} \int\cdots\int P_{\alpha}^{q}(\{\tau_{\alpha}\})\prod_{\gamma} u_{\gamma}(\tau_{\gamma})d\tau_{\gamma}. \tag{14}$$

A unit is termed ''labeled'' if all bonds $\{\gamma\}=(\gamma_1,\gamma_2,\ldots,\gamma_r)$ adjoining to it are supplied by labels $\{\tau_{\gamma}\}=(\tau_{\gamma_1},\tau_{\gamma_2},\ldots,\tau_{\gamma_r})$ indicating the time of the formation of each of them. Since $P_{\alpha}^{q}(\{\tau_{\gamma}\})d\tau_1 d\tau_2\cdots d\tau_r$ has the meaning of the infinitesimal probability for a randomly chosen unit to have at instant t the type α and kind q with bonds $\{\gamma\}$ adjoining to it formed within the intervals $\{\tau_{\gamma},\tau_{\gamma}+d\tau_{\gamma}\}$, then the integration of this probability distribution over the whole possible set of variables $\{\tau_{\gamma}\}$ yields $P_{\alpha}^{q}(t)$.

The vector-function $\mathbf{u}(\tau)$ that should be substituted into functional (13) in order to get generating function (1) can be found from the solution of the set of equations

$$u_{\gamma}(\tau)=\sum_{\delta} \pi_{\gamma\delta}(\tau)h_{\delta}(\mathbf{s},[\mathbf{u}];\tau), \tag{15}$$

where the following designations are used:

$$h_{\delta}(\mathbf{s},[\mathbf{u}];\tau)=\frac{H_{\delta}(\mathbf{s},[\mathbf{u}];\tau)}{H_{\delta}(1,[1];\tau)},\quad H_{\delta}(\mathbf{s},[\mathbf{u}];\tau)=\frac{\delta H(\mathbf{s},[\mathbf{u}])}{\delta u_{\delta}(\tau)}. \tag{16}$$

Equations (15), unlike algebraic equations (6) of the ideal model, are integral ones. The structure of the first and the second equations is virtually the same with the only distinction that the role of the partial derivatives (7) is played here by variational derivatives (16).

In the case of the SE model the following expression,

$$\omega_s=H(\mathbf{1};[\mathbf{y}]), \tag{17}$$

extends the formula (9). Here the vector-function $\mathbf{y}(\tau)$ is the solution of the set of integral equations

$$y_{\gamma}(\tau)=\sum_{\delta} \pi_{\gamma\delta}(\tau)h_{\delta}(\mathbf{1},[\mathbf{y}];\tau). \tag{18}$$

Inasmuch as the matrix $\boldsymbol{\pi}(\tau)$ is stochastic one, this set always has the trivial solution (11), which as it will be proven below is unique within functional hypercube $0\leqslant y_{\gamma}(\tau)\leqslant 1$ up to the gelation moment. The attainment of unity by the largest eigenvalue of the integral operator with kernel

$$\theta_{\gamma\nu}(\tau',\tau'')=\sum_{\delta} \pi_{\gamma\delta}(\tau')\left.\frac{\delta h_{\delta}(\mathbf{1},[\mathbf{u}];\tau)}{\delta u_{\nu}(\tau'')}\right|_{\mathbf{u}(\tau)=\mathbf{1}} \tag{19}$$

will be the condition for the calculation of the gel point.

Proceeding from physical analogies the assertion was made[8] that the set of equations (18) at $t>t^*$ will have within unit functional hypercube the unique nontrivial solution $\mathbf{y}(\tau)$ whose insertion into formula (17) provides a possibility to calculate the decrease of the weight of sol with time. This assertion was verified[9] by the results of computer calculations for monomer RA^3 homopolymerization described by the SE model.

The prime objective of this work is to provide rigorous within the framework of this model mathematical proof of the validity of this assertion for arbitrary process of stepwise polymerization. Besides, we will demonstrate the convergence of the iterative process to this nontrivial solution $\mathbf{y}(\tau)$ and will prove that such a convergence is the case under numerical solution of the set of integral equations (18) irrespective of the choice of starting point within functional unit hypercube.

III. Operator *R*

Let Q be the set of continuous vector functions $\mathbf{u}(\tau)=(u_1(\tau),u_2(\tau),\ldots,u_n(\tau))$ on the segment $[0,t]$, satisfying the inequalities $0\leqslant u_k(\tau)\leqslant 1$, $k=1,\ldots,n$, $\tau\in[0;t]$.

We introduce the following notation for elements $\mathbf{u},\mathbf{v}\in Q$:

(1) $\mathbf{u}<\mathbf{v}$, if $u_k(\tau)<v_k(\tau)$ strictly for any k, τ;
(2) $\mathbf{u}=\mathbf{v}$, if $u_k(\tau)=v_k(\tau)$ for any k, τ;
(3) $\mathbf{u}\lneqq\mathbf{v}$, if $u_k(\tau)\leqslant v_k(\tau)$ for any k, τ but there exists point k',t' in which the inequality is strict;
(4) $\mathbf{u}\leqslant\mathbf{v}$, if $u_k(\tau)\leqslant v_k(\tau)$, i.e., either $\mathbf{u}=\mathbf{v}$ or $\mathbf{u}\lneqq\mathbf{v}$.

Let $\mathbf{0}\in Q$ be the vector function, for which $u_k(\tau)\equiv 0$ everywhere, and $\mathbf{1}\in Q$ is the vector function, with $u_k(\tau)\equiv 1$. We define an operator R on the set Q by the formula:

$$R_i[\mathbf{u}](\tau)=\int_{D_t} K_i(\tau,\mathbf{x},\mathbf{u}(x))dx,\quad i=1,\ldots,n. \tag{20}$$

Here $\mathbf{u}(x)=(u_1(x_1),u_2(x_2),\ldots u_n(x_n))$, $\mathbf{x}\in\mathbb{R}^n$, $D_t=\{\mathbf{x}|0\leqslant x_1\leqslant x_2\leqslant\cdots\leqslant x_n\leqslant t\}$. $K_i(\tau,x_2,x_2,\ldots x_n,r_1,r_2,\ldots,r_n)$ $i=1,\ldots,n$ are nonnegative functions possessing the following properties.

(1^0) $K_i\in\mathbb{C}^2([0,t]\times D_t\times[0,1]^n)$.

(2^0) For any i, $K_i\geqslant\mathbf{0}$ and $K_i\not\equiv\mathbf{0}$.

(3^0) $\int_{D_t}K_i(\tau,\mathbf{x},\mathbf{1})dx=1$, $i=1,\ldots,n$.

(4^0) K_i monotone increasing functions with respect to any $r_k:\partial K_i/\partial r_k>0$ for any $i=1,\ldots,n$, $k=1,\ldots,n$.

(5^0) K_i are strictly convex in non-negative directions, i.e., for any $\mathbf{b}\in\mathbb{R}^n$, $\mathbf{b}\gneqq 0$ the inequality $\Sigma_{j,k}\partial^2K_i/\partial r_j\partial r_k b_j b_k>0$ holds for any τ, $\mathbf{x}$, $\mathbf{r}$, $\mathbf{i}$.

The operator in the right-hand side of (18) has all the properties of the operator R in (20). Now we formulate the properties of R that follow from (1^0)–(5^0):

(A) $\mathbf{R}$ maps Q into Q and $\mathbf{R}[\mathbf{1}]=\mathbf{1}$.

(B) $\mathbf{R}$ is monotone: $\mathbf{u}\lneqq\mathbf{v}$ implies $\mathbf{R}[\mathbf{u}]<\mathbf{R}[\mathbf{v}]$.

(C) $\mathbf{R}$ is strictly convex in the non-negative directions, i.e., for $\theta\in[0;1]$, any $\tau\in[0;t]$, $k=1,\ldots n$ and for $\mathbf{h}\gneqq\mathbf{0}$, $\mathbf{h}\in Q$, $\mathbf{u}\in Q$, such that $\mathbf{u}+\theta\cdot\mathbf{h}\in Q$, the function $\varphi(\theta)=R_k[\mathbf{u}+\theta\cdot\mathbf{h}](\tau)$ is strictly convex: $\varphi''(\theta)>0$.

IV. A THEOREM ON THE UNIQUENESS OF A FIXED POINT

Theorem 1: If the equation

$$\mathbf{R}[\mathbf{u}]=\mathbf{u} \tag{21}$$

has a solution nonequal to $\mathbf{1}$, then this solution is unique on the set $Q\setminus\mathbf{1}$.

Proof:

Lemma 1 (on the convexity): Let $\mathbf{u}\lneqq\mathbf{v}$ and let there exist a point $(k,\aleph)$ such that $R_k[\mathbf{u}](\aleph)\leqslant u_k(\aleph)$ and $R_k[\mathbf{v}](\aleph)\leqslant v_k(\aleph)$. Let $\mathbf{w}=\mathbf{w}(\theta)=\mathbf{u}+\theta(\mathbf{v}-\mathbf{u})$ be the segment connecting $\mathbf{u}$ and $\mathbf{v}$. Then the formula $R_k[\mathbf{w}](\aleph)<\mathbf{w}_k(\aleph)$ is true for any $\theta\in(0;1)$.

Proof: Consider the function $\varphi(\theta)=R_k[\mathbf{w}(\theta)](\aleph)-\mathbf{w}_k(\theta)(\aleph)$. Clearly $\varphi(0)\leqslant 0$, $\varphi(1)\leqslant 0$ and $\varphi(\theta)$ is strictly convex due to property (C): $\varphi''(\theta)>0$, since $\mathbf{h}=\mathbf{v}-\mathbf{u}\gneqq 0$. Lemma 1 is proved.

We divide the proof of the theorem into three steps:

Step 1. Let us show that the solution $\mathbf{u}^0\neq 1$ of the equation $\mathbf{u}=R[\mathbf{u}]$ has the stronger property: $\mathbf{u}^0<1$. Let there be a point (l,λ), at which $\mathbf{u}^0_l(\lambda)=1$. Then $R_l[\mathbf{u}^0](\lambda)=1$ (since $\mathbf{u}^0$ is a solution) as well as $R_l[\mathbf{1}](\lambda)=1$. These two equalities contradict property (B) (monotonicity).

Step 2. Let us consider an element $\mathbf{u}^1<1$, which does not belong to the set $\Pi(\mathbf{u}^0)=\{\mathbf{u}|0\leqslant\mathbf{u}\lneqq\mathbf{u}^0\}$ the set of elements that are not strictly less then $\mathbf{u}^0$. We show that $\mathbf{u}^1$ is not a solution of

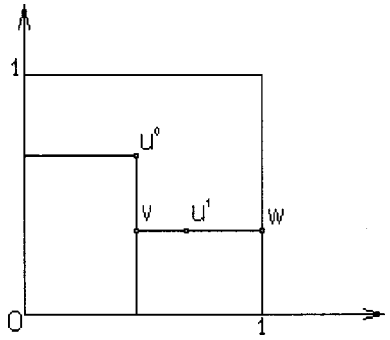

FIG. 1.

(21). Let us define **v** and **w** from Q (see Figs. 1 and 2) as follows. **v** is an element given by the formula: $v_i(\tau)=\min\{u_i^0(\tau);u_i^1(\tau)\}$; **w** is defined as an element from Q, which belongs to the straight line that connects **v** and $\mathbf{u}^1$ and is continued up to the upper bound of Q. So **w** is the point of intersection of the upper bound Q and these straight lines: $\mathbf{w}=\mathbf{v}+\theta\cdot(\mathbf{u}^1-\mathbf{v})$, $\theta>1$. Let (r,ρ) be such that $w_r(\rho)=1$.

We show that **v** and **w** satisfy the conditions of Lemma 1, i.e.,

$$R_r[\mathbf{v}](\rho)\leqslant v_r(\rho) \tag{22}$$

and

$$R_r[\mathbf{w}](\rho)\leqslant w_r(\rho). \tag{23}$$

Inequalities (22) and (23) and Lemma 1 imply the $\mathrm{R}_r[\mathbf{u}^1](\rho)<u_r^1(\rho)$. Inequality (23) is obvious since $w_r(\rho)=1$; inequality (22) follows from the monotonicity of **R** and the relation $\mathbf{v}\leqslant\mathbf{u}$: $\mathrm{R}_r[\mathbf{v}](\rho)\leqslant\mathrm{R}_r[\mathbf{u}^0](\rho)=u_r^0(\rho)=v_r(\rho)$. Thus we have proved that $\mathrm{R}[\mathbf{u}^1]\neq\mathbf{u}^1$.

Step 3. Let $\mathbf{u}^1<1$ and $\mathbf{u}^1\in\Pi(\mathbf{u}^0)$. We shall show that $\mathrm{R}[\mathbf{u}^1]\neq\mathbf{u}^1$. Assume the contrary and consider the set $\Pi(\mathbf{u}^1)$. We conclude that $\mathrm{R}[\mathbf{u}^0]\neq\mathbf{u}^0$ similar to step 2, that is a contradiction.

The theorem is proved.

Now we investigate iterations.

V. ITERATIONS

We consider the iterations $\mathbf{u}^{m+1}=\mathbf{R}[\mathbf{u}^m]$ $(m=0,1,\ldots)$ and show that the convergence properties depend strongly on the linearization $\mathbf{R}'[\mathbf{1}]$ at point **1**, fixed point of **R** ($\mathbf{R}[\mathbf{1}]=\mathbf{1}$, property (A) of the operator **R**).

Consider the linear operator $\mathbf{A}=\mathbf{R}'[\mathbf{1}]$:

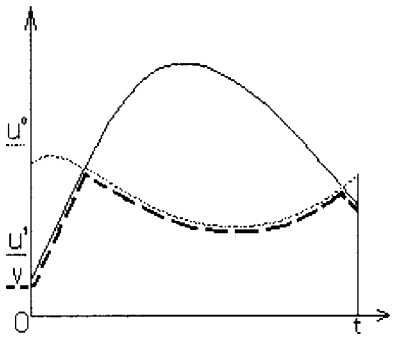

FIG. 2.

$$\mathbf{Ah}=\mathbf{R}'[\mathbf{1}]\mathbf{h}=\sum_{j=1}^{n}\int_{D_i}\frac{\partial\mathbf{K}(\tau,\mathbf{x},\mathbf{1})}{\partial r_j}h_j(x)dx. \tag{24}$$

Properties (A) and (B) of operator **R** provide the strong positivity[10,11] of operator **A** in the solid cone $K=\{\mathbf{v}=(v_1(\tau),v_2(\tau),\ldots,v_n(\tau))|v_i(\tau)\in\mathbb{C}([0,t]) \quad i=1,\ldots,n; \quad \mathbf{v}\geqslant 0\}$ of the space of continuous functions $\mathbb{C}([0,t])$. This means that every boundary point except zero is a mapping into the cone, i.e., $\mathbf{v}\gneqq\mathbf{0}$ implies $\mathbf{Av}>\mathbf{0}$. Indeed, the following decomposition is valid:

$$\mathbf{R}[\mathbf{1}]-\mathbf{R}[\mathbf{1}-\varepsilon\mathbf{v}]=\varepsilon\mathbf{R}'[\mathbf{1}]\mathbf{v}+\mathbf{O}(\varepsilon\mathbf{v})>\mathbf{0}, \quad \mathbf{v}\in \mathrm{K}\setminus\mathbf{0}.$$

Here $\mathbf{O}(\varepsilon\mathbf{v})$ is such that $\mathbf{O}(\varepsilon\mathbf{v})/\varepsilon$ tends to **0** in sup-norm as ε tends to 0. The last inequality follows from property (B). As $\varepsilon>0$ tends to zero, we have $\mathbf{R}'[\mathbf{1}]\mathbf{v}>\mathbf{0}$, i.e., $\mathbf{R}'[\mathbf{1}]\mathbf{v}\in K\setminus\partial$K.

Due to theorem 6.2 from Ref. 10 the operator A has a simple maximal positive eigenvalue (Perron eigenvalue), and the corresponding eigenfunction is positive (Perron eigenfunction).

We show below that the behavior of iterations depends upon the Perron eigenvalue ρ of **A**: cases $\rho\leqslant 1$ or $\rho>1$ specify two different types of behavior.

To prove the convergence of iterations we need the following lemma.

Lemma 2: Let ρ be an eigenvalue of a linear integral operator

$$\mathbf{A}_i[\mathbf{f}](\tau)=\sum_{j=1}^{n}\int_0^t A_{ij}(\tau,\sigma)f_j(\sigma)d\sigma$$

with positive continuous kernels $A_{ij}(\sigma,\tau)$. Let the eigenfunction **h** *corresponding to ρ be positive. And let* **g** *be an arbitrary positive element of* $[\mathbb{C}([0,t])]^n$. *Then there exists a point* (k,τ) [*respectively a point* (k',τ')], *such that* $[(\mathbf{A}-\rho\mathbf{E})\mathbf{g}]_k(\tau)\geqslant 0$ (*respectively* $[(\mathbf{A}-\rho\mathbf{E})\mathbf{g}]_{k'}(\tau')\leqslant 0$).

Proof:

Step 1. Let **f**, **f**′ be strictly positive elements of $\mathbb{C}([0,t])$. We shall show that the assertions $(\mathbf{A}-\rho\mathbf{E})\mathbf{f}>\mathbf{0}$ and $(\mathbf{A}-\rho\mathbf{E})\mathbf{f}'<\mathbf{0}$ exclude each other. Suppose that for any $i=1,\ldots,n$ and $\tau\in[0;t]$

$$-\rho f_i(\tau)+\sum_{j=0}^{n}\int_0^t A_{ij}(\tau,\sigma)f_j(\sigma)d\sigma>0, \tag{25}$$

$$\rho f_i'(\tau)-\sum_{j=0}^{n}\int_0^t A_{ij}(\tau,\sigma)f_j'(\sigma)d\sigma>0. \tag{26}$$

Define $\varepsilon_i(\tau)=f_i(\tau)/f_i'(\tau)>0$, and note that $\varepsilon_i\in\mathbb{C}([0,t])$. Multiplying (26) by $\varepsilon_i(\tau)$ and adding (25) we get

$$\sum_{j=0}^{n}\int_0^t A_{ij}(\tau,\sigma)(f_j(\sigma)-\varepsilon_i(\tau)f_j'(\sigma))d\sigma>0 \quad \text{for any} \quad (i,\tau). \tag{27}$$

Inequality (27) is violated at point (i',τ') of the maximum of $\varepsilon_i(\tau)$: if $\varepsilon_i(\tau)\leqslant\varepsilon_{i'}(\tau')$, then $f_j(\sigma)-\varepsilon_{i'}(\tau')f_j'(\sigma)\leqslant 0$ and all the terms in (27) are nonpositive.

Step 2. Suppose $(\mathbf{A}-\rho\mathbf{E})\mathbf{g}<\mathbf{0}$. Take $\mathbf{g}'=\lambda\mathbf{h}-\mathbf{g}$, where **h** is the eigenfunction of **A** and λ is large enough for $\lambda\mathbf{h}-\mathbf{g}>\mathbf{0}$. Then we get

$$(\mathbf{A}-\rho\mathbf{E})\mathbf{f}=-(\mathbf{A}-\rho\mathbf{E})\mathbf{f}',$$

consequently $(\mathbf{A}-\rho\mathbf{E})\mathbf{g}'>\mathbf{0}$. This contradicts to the step 1; hence $(\mathbf{A}-\rho\mathbf{E})\mathbf{g}'\not<\mathbf{0}$ and there exists a point (k,τ) satisfying the statement of the lemma. Similarly, supposing $(\mathbf{A}-\rho\mathbf{E})\mathbf{g}>\mathbf{0}$ we get existence of a point (k',τ') with desired properties.

There is an important property of the iterations $\mathbf{u}^{m+1}=\mathbf{R}[\mathbf{u}^m]$. If $\mathbf{u}^0 \lneqq \mathbf{u}^1$ $(\mathbf{u}^0 \leqslant \mathbf{u}^1)$, then $\mathbf{u}^k < \mathbf{u}^{k+1}$ $(\mathbf{u}^k \leqslant \mathbf{u}^{k+1})$ for $\mathbf{k}>0$. If $\mathbf{u}^0 \gneqq \mathbf{u}^1$ $(\mathbf{u}^0 \geqslant \mathbf{u}^1)$, then $\mathbf{u}^k > \mathbf{u}^{k+1}$ $(\mathbf{u}^k \geqslant \mathbf{u}^{k+1})$ for $k>0$.

Theorem 2: If $\rho \leqslant 1$, then the iterations $\mathbf{u}^{m+1}=\mathbf{R}[\mathbf{u}^m]$ $(m=0,1,\ldots)$ converge to $\mathbf{1}$ for any $\mathbf{u}^0 \in Q$.

Proof: Consider the sequence $\mathbf{v}^{m+1}=\mathbf{R}[\mathbf{v}^m]$ with $\mathbf{v}^0=\mathbf{0}$. $\mathbf{R}[\mathbf{0}] \geqslant \mathbf{0}$ and so the sequence increases monotonically $(\mathbf{v}^m \geqslant \mathbf{v}^{m-1})$. As $\mathbf{v}^m<1$ the limit $\mathbf{v}=\lim \mathbf{v}^m$ exists and is not continuous in general, and therefore it does not belong to Q. But $\mathbf{R}[\mathbf{u}](\tau)$ is equicontinuous over τ with respect to $\mathbf{u}$, in view of $|\mathrm{R}_i[u](\tau)-\mathrm{R}_i[u](\tau')| \leqslant \mathrm{M}t^n|\tau-\tau'|$ with $\mathrm{M}=\sup_{\tau,\mathbf{x},\mathbf{u}}|\partial K_i/\partial\tau|$. So $\{\mathbf{v}^m(\tau)\}$ is equicontinuous with respect to m, and $\mathbf{v} \in \mathrm{Q}$ due to the Arzela theorem (on the compactness of a subset of continuous functions[12]). Hence it follows that $\mathbf{v}$ is a fixed point of $\mathbf{R}$:$\mathbf{R}[\mathbf{v}]=\mathbf{v}$. Let us show that $\mathbf{v}=\mathbf{1}$.

If $\mathbf{v} \lneqq \mathbf{1}$, then by Lemma 1 for $\mathbf{u}(\theta)=\mathbf{v}+(\mathbf{1}-\mathbf{v})\theta$ and for any $(k,\aleph)$ $\varphi(\theta)=\mathrm{R}_k[\mathbf{u}(\theta)](\aleph) - u_k(\theta)(\aleph)$ we have $\varphi''(\theta)>0$, $\varphi(0)=\varphi(1)=0$ and hence $\varphi'(1)>0$ strictly. But $\varphi(1) =[\mathrm{R}'[\mathbf{1}]-\mathrm{E}]_k(\mathbf{1}-\mathbf{v})(\aleph)$, where E is the unit operator. In accordance with Lemma 2 the following inequality holds: $[(\mathrm{R}'[\mathbf{1}]-\rho\mathrm{E})(\mathbf{1}-\mathbf{v})]_k(\aleph) \leqslant 0$ at some point $(k,\aleph)$. Hence,

$$\varphi'(1)=[(\mathrm{R}'[\mathbf{1}]-\mathrm{E})(\mathbf{1}-\mathbf{v})]_k(\aleph) \leqslant [(\mathrm{R}'[\mathbf{1}]-\rho E)(\mathbf{1}-\mathbf{v})]_k(\aleph) \leqslant 0.$$

This contradiction shows that $\mathbf{v}=\mathbf{1}$. Any other sequence $\mathbf{u}^{m+1}=\mathrm{R}[\mathbf{u}^m]$ is bounded below by $\{\mathbf{v}^m\}$ and bounded above by $\mathbf{1}$, and hence tends to $\mathbf{1}$ as well.

Theorem 2 is proved.

Note: If $\rho<1$, then the theorem on spectrum radius[11] shows that there exists p for which $\|A^p\|<q<1$ and hence R^p is a contraction map. This shows that convergence to $\mathbf{1}$ is exponential in this case.

Theorem 3: If $\rho>1$, then the iteration $\mathbf{u}^{m+1}=\mathrm{R}[\mathbf{u}^m]$ with $\mathbf{u}^0 \neq \mathbf{1}$ converges to the unique solution in $\mathrm{Q}\setminus\mathbf{1}$ of the equation $\mathbf{u}=\mathrm{R}[\mathbf{u}]$, and $\mathbf{1}$ is a repelling fixed point.

Proof: For any $\mathbf{u}^0 \in \mathrm{Q}$ we shall construct two sequences $\{\mathbf{v}^m\}$ and $\{\mathbf{w}^m\}$ minorizing and majorizing $\{\mathbf{u}^m\}$ respectively: $\mathbf{0} \leqslant \mathbf{v}^m \leqslant \mathbf{u}^m \leqslant \mathbf{w}^m < 1$ $(m=1,2,\ldots)$.

We take $\mathbf{v}^0=\mathbf{0}$ and $\mathbf{v}^{m+1}=\mathbf{R}[\mathbf{v}^m]$. Then $\{\mathbf{v}^m\}$ is monotonically increasing: $\mathbf{v}^{m+1} \geqslant \mathbf{v}^m$ and has a limit $\mathbf{v}$, $\mathbf{v}=\mathbf{R}[\mathbf{v}]$ as in Theorem 2.

For $\mathbf{w}^1$ we take $\mathbf{w}^1=\mathbf{1}-\varepsilon\mathbf{h}$, $\mathbf{h}$ is the Perron eigenfunction of the operator A: $\mathrm{A}\mathbf{h}=\rho\mathbf{h}$. As $\mathbf{u}^1=\mathrm{R}[\mathbf{u}^0]<\mathbf{1}$ we get $\mathbf{w}^1=\mathbf{1}-\varepsilon\mathbf{h}$ for ε small enough, and so $\{\mathbf{w}^m\}$ majorizes $\{\mathbf{u}^m\}$. It decreases monotonically as $\mathrm{R}[\mathbf{w}^m]<\mathbf{w}^m$: $\mathrm{R}[\mathbf{1}-\varepsilon\mathbf{h}]=\mathbf{1}-\varepsilon\rho\mathbf{h}+\mathrm{O}(\varepsilon\mathbf{h})$.

Hence as in Theorem 2 $\{\mathbf{w}^m\}$ has the limit $\mathbf{w}$, that is the fixed point of the operator $\mathbf{R}$ also. From Theorem 1 (Sec. IV) we have $\mathbf{w}=\mathbf{v}$, and this completes the proof of the theorem.

VI. CONCLUSIONS

We have proved theorems that are infinite-dimentional analogs of ones from branching process theory.[13–15] We showed that they are useful for computations of statistical characteristics of a gel. These general results are of utmost importance for the quantitative theory of polymer networks. It would be interesting to use the correspondence between quantum Hamiltonians and kinetic equations.[16,17]

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Quadratic replica coupling in the Sherrington–Kirkpatrick mean field spin glass model

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We develop a very simple method to study the high temperature, or equivalently high external field, behavior of the Sherrington–Kirkpatrick mean field spin glass model. The basic idea is to couple two different replicas with a quadratic term, trying to push out the two replica overlap from its replica symmetric value. In the case of zero external field, our results reproduce the well known validity of the annealed approximation, up to the known critical value for the temperature. In the case of nontrivial external field, we can prove the validity of the Sherrington–Kirkpatrick replica symmetric solution up to a line, which falls short of the Almeida–Thouless line, associated to the onset of the spontaneous replica symmetry breaking, in the Parisi ansatz. The main difference with the method, recently developed by Michel Talagrand, is that we employ a quadratic coupling, and not a linear one. The resulting flow equations, with respect to the parameters of the model, turn out to be very simple, and the parameter region, where the method works, can be easily found in explicit terms. As a straightforward application of cavity methods, we show also how to determine free energy and overlap fluctuations, in the region where replica symmetry has been shown to hold. It is a major open problem to give a rigorous mathematical treatment of the transition to replica symmetry breaking, necessarily present in the model. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1483378]

I. INTRODUCTION

The mean field spin glass model, introduced by Sherrington and Kirkpatrick in Ref. 1, is here considered in the high temperature regime, or, equivalently, for a large external field. It is very well known, on physical grounds, that in this region the replica symmetric solution holds, as shown for example in Ref. 2, and references quoted there. However, due to the very large fluctuations present in the model, it is not so simple to give a complete, mathematically rigorous, characterization of this region, especially when there are external fields. Rigorous work on this subject include Refs. 3–8. For other rigorous results on the structure of the model, we refer to Refs. 9–15.

The method developed in Ref. 8, by Michel Talagrand, is particularly interesting. The starting point is given by the very sound physical idea that the spontaneous replica symmetry breaking phenomenon can be understood by exploring the properties of the model, under the application of auxiliary interactions, which explicitly break the replica symmetry. In Ref. 8, the replica symmetric solution is shown to hold in a region, which (*probably*) coincides with the region found in the theoretical physics literature, as shown for example in Ref. 2, i.e., up to the Almeida–Thouless line.[16]

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The main tool in Talagrand's treatment is an additional minimal replica coupling, linear in the overlap between two replicas. Then, a kind of quadratic stability for the so modified free energy leads immediately, through a generalization of the methods developed in Ref. 15, to establish the validity of the replica symmetric solution in a suitable parameter region.

Here we propose a very different strategy, by introducing a quadratic replica coupling, attempting to push the overlap away from its replica symmetric value. In a sense, our method is the natural extension, with applications, of the ideas put forward in Ref. 15, where sum rules were introduced for the free energy, by expressing its deviation from the replica symmetric solution in terms of appropriate quadratic fluctuations for the overlap. We choose exactly these quadratic fluctuation terms to act as additional interaction between two replicas, thus explicitly breaking replica symmetry. Then, a generalization of the sum rules, given in Ref. 15, for this modified model, allows us immediately to prove that the free energy of the original model converges, in the infinite volume limit, to its replica symmetric value, at least in a parameter region, explicitly determined.

The organization of the article is as follows. In Sec. II, we recall the basic definitions of the mean field spin glass model, and introduce the overlap distribution structure. As a first introduction of our method of quadratic coupling, in Sec. III, we treat the well known case of zero external field, by showing that the annealed approximation holds, in the infinite volume limit, up to the true critical inverse temperature $\beta_c = 1$. Our proof shows explicitly that there is a strong connection between the critical value of the transition temperature for the zero external field model, and the analogous, and numerically equivalent, temperature for the well known ferromagnetic Curie–Weiss mean field model.

In Sec. IV, we consider the model with external field, and introduce the associated model with quadratic replica coupling. Then, simple stability estimates give immediately the convergence of the free energy to its replica symmetric value, in a suitable, well defined, region of the parameters.

Section V reports about results on the free energy and overlap fluctuations, in our determined replica symmetric region. We also sketch the method of proof, based on cavity considerations, as developed for example in Refs. 2 and 5. A more complete treatment will be found in a forthcoming paper.[17]

Finally, Sec. VI is dedicated to a short outlook about open problems and further developments.

For the relevance of the mean field spin glass model for the understanding of the physical properties of realistic spin glasses, we refer to Ref. 18, but see also Ref. 19.

II. THE GENERAL STRUCTURE OF THE MEAN FIELD SPIN GLASS MODEL

The generic configuration of the mean field spin glass model is defined by Ising spin variables $\sigma_i = \pm 1$, attached to each site $i = 1,2,\ldots,N$. The external quenched disorder is given by the $N(N-1)/2$ independent and identical distributed random variables J_{ij}, defined for each couple of sites. For the sake of simplicity, we assume each J_{ij} to be a centered unit Gaussian with averages

$$E(J_{ij}) = 0, \quad E(J_{ij}^2) = 1.$$

The Hamiltonian of the model, in some external field of strength h, is given by

$$H_N(\sigma, J) = -\frac{1}{\sqrt{N}} \sum_{(i,j)} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i . \tag{1}$$

The first sum extends to all site couples, and the second to all sites. The normalizing factor $1/\sqrt{N}$ is typical of the mean field character of the model, and guarantees a good thermodynamic limit for the free energy per spin, i.e., the existence of a finite and nontrivial limit for the free energy as $N \to \infty$. The first term in (1) is a long range random two body interaction, while the second represents the interaction of the spins with a fixed external magnetic field h.

For a given inverse temperature β, we introduce the disorder dependent partition function $Z_N(\beta,J)$, the (quenched average of the) free energy per site $f_N(\beta)$, the internal energy per site $u_N(\beta)$, the Boltzmann state ω_J, and the auxiliary function $\alpha_N(\beta)$, according to the definitions

$$Z_N(\beta,J)=\sum_{\sigma_1 \dots \sigma_N} \exp(-\beta H_N(\sigma,J)), \tag{2}$$

$$-\beta f_N(\beta)=N^{-1}E \log Z_N(\beta,J)=\alpha_N(\beta), \tag{3}$$

$$\omega_J(A)=Z_N(\beta,J)^{-1}\sum_{\sigma_1 \dots \sigma_N} A \exp(-\beta H_N(\sigma,J)), \tag{4}$$

$$u_N(\beta)=N^{-1}E\omega_J(H_N(\sigma,J))=\partial_\beta(\beta f_N(\beta))=-\partial_\beta\alpha_N(\beta), \tag{5}$$

where A is a generic function of the σ's. In the notation ω_J, we have stressed the dependence of the Boltzmann state on the external noise J, but, of course, there is also a dependence on β, h and N.

We are interested in the thermodynamic limit $N\to\infty$.

Let us now introduce the important concept of replicas. Consider a generic number s of independent copies of the system, characterized by the Boltzmann variables $\sigma_i^{(1)}, \sigma_i^{(2)}, \dots$, distributed according to the product state

$$\Omega_J=\omega_J^{(1)}\omega_J^{(2)} \dots \omega_J^{(s)},$$

where all $\omega_J^{(\alpha)}$ act on each one $\sigma_i^{(\alpha)}$s, and are subject to the *same* sample J of the external noise. Clearly, the *Boltzmannfaktor* for the replicated system is given by

$$\exp(-\beta(H_N(\sigma^{(1)},J)+H_N(\sigma^{(2)},J)+\cdots+H_N(\sigma^{(s)},J))). \tag{6}$$

The overlaps between two replicas a, b are defined according to

$$q_{ab}(\sigma^{(a)},\sigma^{(b)})=\frac{1}{N}\sum_i \sigma_i^{(a)}\sigma_i^{(b)},$$

and they satisfy the obvious bounds

$$-1\leqslant q_{ab}\leqslant 1.$$

For a generic smooth function F of the overlaps, we define the $\langle\ \rangle$ averages

$$\langle F(q_{12},q_{13},\dots)\rangle=E\Omega_J(F(q_{12},q_{13},\dots)),$$

where the Boltzmann averages Ω_J act on the replicated σ variables, and E is the average with respect to the external noise J.

We remark here that the noise average E introduces correlations between different groups of replicas, which would be otherwise independent under the Boltzmann averages Ω_J, as for example q_{12} and q_{34}.

The $\langle\ \rangle$ averages are obviously invariant under permutations of the replicas.

Overlap distributions play a very important role in the theory. For example, by using integration by parts on the J integrals, a simple direct calculation[2,11] shows that

$$\partial_\beta\alpha_N(\beta)=\frac{\beta}{2}(1-\langle q_{12}^2\rangle). \tag{7}$$

In order to introduce our treatment, based on flow equations with respect to the parameters of the theory, it is convenient to start from a *Boltzmannfaktor* given by

$$\exp\left(\sqrt{\frac{t}{N}} \sum_{(i,j)} J_{ij}\sigma_i\sigma_j + \beta h \sum_i \sigma_i + \sqrt{x} \sum_i J_i\sigma_i \right). \tag{8}$$

Notice that we have introduced an auxiliary additional one body random interaction ruled by the strength $\sqrt{x}$, $x \geqslant 0$, and N quenched independent and identically distributed centered unit Gaussian random variables J_i, so that

$$E(J_i)=0, \quad E(J_i^2)=1.$$

In order to get the original model, we have to put $x=0$ at the end. Moreover, we have written $\beta=\sqrt{t}$, with $t \geqslant 0$. The variables t, and x, will play the role of time variable, and space variable, respectively, in our flow equations. Now we define the partition function Z by using the *Boltzmannfaktor* (8), and the auxiliary function $\alpha_N(x,t)$ in the form

$$\alpha_N(x,t)=N^{-1}E \log Z_N.$$

Then, as in the proof of (7), we have

$$\partial_t \alpha_N(x,t)= \tfrac{1}{4}(1-\langle q_{12}^2 \rangle), \tag{9}$$

$$\partial_x \alpha_N(x,t)= \tfrac{1}{2}(1-\langle q_{12} \rangle). \tag{10}$$

It is very simple to calculate explicitly the average $N^{-1}E \log Z_N$ for $t=0$, at a generic strength x_0 of the one body random interaction. In fact, at $t=0$, the interaction factorizes, and the spins at different sites become independent. Therefore we have

$$\alpha(x_0,0)=\log 2 + \int \log\cosh(\beta h + z\sqrt{x_0})\, d\mu(z), \tag{11}$$

independently of N, where $d\mu$ is the centered unit Gaussian, representing each single J_i,

$$d\mu(z)=\exp\left(-\frac{z^2}{2}\right) dz/\sqrt{2\pi}.$$

Starting from (11) and (10) at $t=0$, we can immediately calculate the order parameter $\overline{q}(x_0)$ according to

$$\overline{q}(x_0)=\langle q_{12} \rangle (x_0,0)= \int \tanh^2(\beta h + z\sqrt{x_0})\, d\mu(z).$$

Let us now consider linear trajectories at constant velocity given by

$$x(t)=x_0-\overline{q}(x_0)t, \tag{12}$$

where x_0 is the initial starting point. Consider the problem of inverting (12), i.e., to find the conditions such that, for a given point (x,t), $x \geqslant 0$, $t \geqslant 0$, there is only one trajectory arriving at x, at time t. A precise statement is given by the following theorem.

Theorem 1: *Consider first the case of nonzero external field h. Then, for any point (x,t), $x \geqslant 0$, $t \geqslant 0$, there exists a unique $x_0(x,t)$ such that*

$$x=x_0(x,t)-\overline{q}(x_0(x,t))t,$$

and a unique $\overline{q}(x,t)=\overline{q}(x_0(x,t))$, *such that*

$$\overline{q}(x,t)=\int \tanh^2(\beta h+z\sqrt{x+\overline{q}(x,t)t})d\mu(z).$$

If $h=0$, *then, for any point* (x,t), $x\geqslant 0$, $t\geqslant 0$, *with the exclusion of the segment* $x=0$, $0\leqslant t\leqslant 1$, *there exists a unique* $x_0(x,t)>0$, *such that the previous formulas hold.*

The proof is very simple, and can be found in Ref. 15.

By following the methods of Ref. 15, sum rules connecting α and its SK approximation can be easily found by using transport equations. They involve overlap fluctuations. In fact, let us consider α along the trajectories in (12), i.e., $\alpha(x(t),t)$. An easy calculation gives

$$\frac{d}{dt}\alpha_N(x(t),t)=\frac{1}{4}(1-\overline{q}(x_0))^2-\frac{1}{4}\langle(q_{12}-\overline{q}(x_0))^2\rangle. \tag{13}$$

Now we integrate along t, take into account the initial condition (11), and the invertibility of (12), and find the sum rule

$$\overline{\alpha}(x,t)=\alpha_N(x,t)+\frac{1}{4}\int_0^t\langle(q_{12}-\overline{q})^2\rangle_{x(t'),t'}dt'. \tag{14}$$

Here, we have defined the replica symmetric Sherrington–Kirkpatrick solution[1,2] in the form

$$\overline{\alpha}(x,t)=\log 2+\int \log\cosh(\beta h+z\sqrt{x_0})d\mu(z)+\frac{t}{4}(1-\overline{q}(x_0))^2, \tag{15}$$

where x_0 and $\overline{q}(x_0)$ are expressed in terms of (x,t), according to the invertibility assured by the previous theorem. A very simple, but important, consequence of the sum rule is that α_N is dominated by its replica symmetric solution, uniformly in N,

$$\alpha_N(x,t)=N^{-1}E\log Z_N\leqslant\overline{\alpha}(x,t). \tag{16}$$

This is a simple consequence of the positivity of the term under integration in (14). Notice that (16) is a lower bound for the free energy, so that it is not directly connected to any variational principle for the Boltzmann–Gibbs state.

It is our aim to explore the parameter region where the t'-integral in (14) can be neglected, in the thermodynamic limit.

Now, we are ready to explain our method of quadratic coupling, starting with the simple case of zero external field, and then going to the case of nontrivial external fields.

III. QUADRATIC COUPLING FOR ZERO EXTERNAL FIELD

The high temperature region ($\beta<1$) of the zero external field SK model is a very particular case where everything can be computed. As it is well known,[3] in this case the annealed approximation is exact in the infinite volume limit. In fact, we have

$$\lim_{N\to\infty}\frac{1}{N}E\ln Z_N(t,J)=\overline{\alpha}(t)\equiv\ln 2+\frac{t}{4}=\frac{1}{N}\ln EZ_N(t,J)+\frac{t}{4N}. \tag{17}$$

In this section we give a new proof of Eq. (17), based on sum rules for the free energy. Our method is very simple and can be easily extended to the case of nontrivial external field, considered in the next section.

When $h=0$, $x=0$, then also $\overline{q}=0$ and $x_0=0$. Then, the sum rule in (14) reads

$$\alpha_N(t)=\overline{\alpha}(t)-\frac{1}{4}\int_0^t\langle q_{12}^2\rangle_{t'}dt'. \tag{18}$$

The presence of $\langle q_{12}^2\rangle$, as order parameter, suggests to couple two replicas with a term proportional to the square of the overlap, the corresponding partition function being

$$\tilde{Z}_N(t,\lambda,J)=\sum_{\{\sigma,\sigma'\}}\exp\left(\sqrt{\frac{t}{N}}\sum_{(i,j)}J_{ij}(\sigma_i\sigma_j+\sigma_i'\sigma_j')+\frac{\lambda}{2}Nq_{12}^2\right), \tag{19}$$

with $\lambda\geqslant 0$. The effect of the added term is to give a larger weight to the configurations having $q_{12}\neq 0$, thus favoring non-self-averaging of the overlap. Of course, the system possesses spin-flip symmetry also for $\lambda\neq 0$, so that $\langle q_{12}\rangle=0$. Therefore, if $\langle q_{12}^2\rangle\neq 0$, then the overlap is non-self-averaging. Now replica symmetry is explicitly broken.

The basic idea of our method is to show that, as long as $t<1$ and λ is small enough, the term $\lambda N q_{12}^2$ does not change the value of the free energy in the thermodynamic limit. Therefore, ''most'' configuration must have $q_{12}=0$ and the overlap must be self-averaging. In order to implement this intuitive idea, one introduces the λ dependent auxiliary function

$$\tilde{\alpha}_N(t,\lambda)=\frac{1}{2N}E\ln\tilde{Z}_N,$$

where the normalization factor $\frac{1}{2}$ is chosen so that $\tilde{\alpha}_N(t,0)=\alpha_N(t)$. Through a simple explicit calculation, we can easily calculate the t derivative in the form

$$\partial_t\tilde{\alpha}_N=\tfrac{1}{4}(1+\langle q_{12}^2\rangle-2\langle q_{13}^2\rangle), \tag{20}$$

where now all averages $\langle\ \rangle$ involve the λ-dependent state with *Boltzmannfaktor* given in agreement with (19). Moreover, it is obvious that

$$\partial_\lambda\tilde{\alpha}_N=\tfrac{1}{4}\langle q_{12}^2\rangle.$$

Starting from some point $\lambda_0>0$, consider the linear trajectory $\lambda(t)=\lambda_0-t$, with obvious invertibility in the form $\lambda_0=\lambda+t$. Let us take the t derivative of $\tilde{\alpha}_N$ along this trajectory

$$\frac{d}{dt}\tilde{\alpha}_N(t,\lambda(t))=(\partial_t-\partial_\lambda)\tilde{\alpha}_N=\frac{1}{4}-\frac{1}{2}\langle q_{13}^2\rangle_{t,\lambda(t)}.$$

Notice that the term containing $\langle q_{12}^2\rangle$ disappeared. By integration we get the sum rule and the inequality

$$\tilde{\alpha}_N(t,\lambda)=\frac{t}{4}+\tilde{\alpha}_N(0,\lambda_0)-\frac{1}{2}\int_0^t\langle q_{13}^2\rangle_{t',\lambda(t')}dt'\leqslant\frac{t}{4}+\tilde{\alpha}_N(0,\lambda_0), \tag{21}$$

where $\langle q_{13}^2\rangle_{t',\lambda(t')}$ refers to $\lambda(t')=\lambda_0-t'=\lambda+t-t'$.

Next, we compute $\tilde{\alpha}_N(0,\lambda_0)$. We introduce an auxiliary unit Gaussian z, and perform simple rescaling, in order to obtain

$$\tilde{\alpha}_N(0,\lambda_0)=\frac{1}{2N}\ln\sum_{\{\sigma,\sigma'\}}e^{1/2\,\lambda_0 N q_{12}^2}=\frac{1}{2N}\ln\sum_{\{\sigma,\sigma'\}}\int e^{\sqrt{\lambda_0 N}q_{12}z}d\mu(z) \tag{22}$$

$$= \ln 2 + \frac{1}{2N} \ln \int \left(\cosh z \sqrt{\frac{\lambda_0}{N}} \right)^N d\mu(z)$$

$$= \ln 2 + \frac{1}{2N} \ln \int dy \sqrt{\frac{N\lambda_0}{2\pi}} \exp N \left(-\lambda_0 \frac{y^2}{2} + \ln \cosh(y\lambda_0) \right), \tag{23}$$

where we performed the change of variables z to $y\sqrt{N\lambda_0}$ in the last step. It is immediately recognized that the integral in (23) appears in the ordinary treatment of the well known ferromagnetic mean field Curie–Weiss model. The saddle point method gives immediately

$$\lim_{N\to\infty} \tilde{\alpha}_N(0,\lambda_0) = \ln 2 + \frac{1}{2} \max_y \left(-\lambda_0 \frac{y^2}{2} + \ln \cosh(y\lambda_0) \right). \tag{24}$$

Therefore, the critical value for λ_0 is $\lambda_c = 1$. For $\lambda_0 > 1$ we have

$$\lim_{N\to\infty} \tilde{\alpha}_N(0,\lambda_0) > \ln 2,$$

while for $\lambda_0 < 1$, one can use the elementary property $2 \ln \cosh x \leqslant x^2$ to find

$$\tilde{\alpha}_N(0,\lambda_0) \leqslant \ln 2 + \frac{1}{4N} \ln \frac{1}{1-\lambda_0}. \tag{25}$$

Notice that, when λ_0 approaches the value 1^-, the term of order $1/N$ diverges, since Gaussian fluctuations around the saddle point become larger and larger.

Thanks to (25), the inequality in (21) becomes

$$\tilde{\alpha}_N(t,\lambda) \leqslant \overline{\alpha}(t) + \frac{1}{4N} \ln \frac{1}{1-\lambda_0},$$

which holds for $0 \leqslant \lambda_0 < 1$, i.e., for $0 \leqslant t+\lambda < 1$.

Next, we use convexity of $\tilde{\alpha}_N(t,\lambda)$ with respect to λ and the fact that

$$\partial_\lambda \tilde{\alpha}_N(t,\lambda)|_{\lambda=0} = \tfrac{1}{4} \langle q_{12}^2 \rangle_t$$

to write

$$\alpha_N(t) + \frac{\lambda}{4} \langle q_{12}^2 \rangle_t \leqslant \tilde{\alpha}_N(t,\lambda) \leqslant \overline{\alpha}(t) + \frac{1}{4N} \ln \frac{1}{1-\lambda-t},$$

for $\lambda > 0$. For $0 \leqslant t \leqslant \overline{t} < 1$, choose $\lambda = (1-\overline{t})/2$, so that

$$\lambda + t \leqslant \overline{\lambda}_0 \equiv (1+\overline{t})/2 < 1,$$

and

$$\frac{1}{4} \langle q_{12}^2 \rangle_t \leqslant \frac{1}{\lambda} (\overline{\alpha}(t) - \alpha_N(t)) + \frac{1}{4N\lambda} \ln \frac{1}{1-\overline{\lambda}_0}. \tag{26}$$

Recalling Eq. (18), one has

$$\frac{d}{dt} (\overline{\alpha}(t) - \alpha_N(t)) = \frac{1}{4} \langle q_{12}^2 \rangle_t \leqslant \frac{1}{\lambda} (\overline{\alpha}(t) - \alpha_N(t)) + \frac{1}{4N\lambda} \ln \frac{1}{1-\overline{\lambda}_0}, \tag{27}$$

so that

$$\alpha_N(t)=\overline{\alpha}(t)+O(1/N),$$

uniformly for $0\leqslant t\leqslant\overline{t}<1$. Of course, from Eq. (21) and convexity of $\tilde{\alpha}_N$ one also has

$$\tilde{\alpha}_N(t,\lambda)=\overline{\alpha}(t)+O(1/N),$$

$$\langle q_{13}^2\rangle_{t,\lambda}=O(1/N),$$

for $0\leqslant t+\lambda\leqslant\overline{\lambda}_0<1$.

We have gained a complete control of the system in the triangular region $0\leqslant t<1$, $0\leqslant\lambda<1-t$. Note that we have not only proved Eq. (17) but we have also shown that the leading correction to annealing is of order at most $1/N$.

IV. THE GENERAL CASE

The method we follow for the general case, where the *Boltzmannfaktor* is given by (8), is a direct generalization of the one explained in the previous section. In fact, by taking into account the t derivative in (13), we are led to introduce the auxiliary function

$$\tilde{\alpha}_N(x,\lambda,t)=\frac{1}{2N}E\ln\tilde{Z}_N(x,\lambda,t;J),$$

where $\tilde{Z}_N$ is the partition function for a system of two replicas coupled by the term

$$\frac{\lambda}{2}N(q_{12}-\overline{q}(x,t))^2,$$

with $\lambda\geqslant 0$. In order to simplify notation, we omit the argument h.

Now the t derivative is given by

$$\partial_t\tilde{\alpha}_N=\frac{1}{4}(1+\langle q_{12}^2\rangle-2\langle q_{13}^2\rangle)+\frac{\lambda}{2}(\overline{q}-\langle q_{12}\rangle)\frac{\partial\overline{q}}{\partial t},$$

while the x and λ derivatives appear as

$$\partial_x\tilde{\alpha}_N=\frac{1}{2}(1+\langle q_{12}\rangle-2\langle q_{13}\rangle)+\frac{\lambda}{2}(\overline{q}-\langle q_{12}\rangle)\frac{\partial\overline{q}}{\partial x},$$

$$\partial_\lambda\tilde{\alpha}_N=\frac{1}{4}\langle(q_{12}-\overline{q}(x,t))^2\rangle.$$

Starting from points $\lambda_0>0$, x_0, consider the linear trajectories $\lambda(t)=\lambda_0-t$, $x(t)=x_0-\overline{q}(x_0)t$, as in (12), with obvious invertibility as explained before. Since $\overline{q}$ is constant along the trajectory, and therefore $\partial_t\overline{q}-\overline{q}\partial_x\overline{q}=0$, one finds for the total time derivative of $\tilde{\alpha}_N$

$$\frac{d}{dt}\tilde{\alpha}_N(x(t),\lambda(t),t)=(\partial_t-\overline{q}\partial x-\partial_\lambda)\tilde{\alpha}_N=\frac{1}{4}(1-\overline{q})^2-\frac{1}{2}\langle(q_{13}-\overline{q})^2\rangle.$$

Notice that in this case the term containing $\langle(q_{12}-\overline{q})^2\rangle$ disappeared.

By integration, we get the sum rule and the inequality

$$\tilde{\alpha}_N(x,\lambda,t)=\frac{t}{4}(1-\overline{q})^2+\tilde{\alpha}_N(x_0,\lambda_0,0)-\frac{1}{2}\int_0^t\langle(q_{13}-\overline{q})^2\rangle_{t',x(t'),\lambda(t')}dt'$$

$$\leqslant\frac{t}{4}(1-\overline{q})^2+\tilde{\alpha}_N(x_0,\lambda_0,0),$$

where $\langle(q_{13}-\overline{q})^2\rangle_{t',x(t'),\lambda(t')}$ refers to

$$\lambda(t')=\lambda_0-t'=\lambda+t-t',$$

$$x(t')=x_0-\overline{q}t'=x+\overline{q}(t-t').$$

If Ω_J is the product state for two replicas with the original *Boltzmannfaktor* given by (8), then we can write

$$\tilde{\alpha}_N(x,\lambda,t)-\alpha_N(x,t)\equiv\frac{1}{2N}E\ln\Omega_J\left(\exp\frac{1}{2}\lambda N(q_{12}-\overline{q})^2\right).$$

Therefore, by exploiting the Jensen inequality, we have, for $\lambda\geqslant 0$,

$$\frac{\lambda}{4}\langle(q_{12}-\overline{q})^2\rangle_{x,t}\leqslant\tilde{\alpha}_N(x,\lambda,t)-\alpha_N(x,t).$$

Let us also define

$$\Delta_N(x_0,\lambda_0)\equiv\tilde{\alpha}_N(x_0,\lambda_0,0)-\alpha(x_0,0)=\frac{1}{2N}E\ln\Omega_J^0\left(\exp\frac{1}{2}\lambda_0 N(q_{12}-\overline{q})^2\right),\tag{28}$$

where we have introduced the state Ω_J^0 for two replicas, corresponding to $t=0$, and $x=x_0$, in (8). Notice that Ω_J^0 is a factor state over the sites i.

By collecting all our definitions and inequalities, and taking into account the definition (15), we have

$$\frac{\lambda}{4}\langle(q_{12}-\overline{q})^2\rangle_{x,t}\leqslant\Delta_N(x_0,\lambda_0)+\overline{\alpha}(x,t)-\alpha_N(x,t).$$

Let us now introduce $\lambda_c(x_0)$ such that, for any $\lambda_0\leqslant\lambda_c(x_0)$, one has

$$\lim_{N\to\infty}\Delta_N(x_0,\lambda_0)=0.$$

Then, by the same reasoning already exploited starting from (26), and taking into account (13), we obtain the proof of the following.

Theorem 2: *For any $t\leqslant\lambda_c(x_0(x,t))$, where $x_0(x,t)$ is defined as in Theorem 1, we have the convergence*

$$\lim_{N\to\infty}\alpha_N(x,t)=\overline{\alpha}(x,t).\tag{29}$$

For the specification of $\lambda_c(x_0)$, we can easily establish the complete characterization of the Δ_N limit. In fact, the following holds.

Theorem 3: *The infinite volume limit of Δ_N is given by*

$$\lim_{N\to\infty}\Delta_N(x_0,\lambda_0)=\Delta(x_0,\lambda_0).$$

Here, $\Delta(x_0,\lambda_0)$ *is defined through the variational expression*

$$\Delta(x_0,\lambda_0)\equiv\frac{1}{2}\max_{\mu}\left(\int \ln(\cosh\mu+\tanh^2(\beta h+z\sqrt{x_0})\sinh\mu)d\rho(z)-\mu\overline{q}-\frac{\mu^2}{2\lambda_0}\right), \tag{30}$$

where $d\rho(z)$ *is the centered unit Gaussian measure.*

Of course, the expression (30) is in agreement with (24), when there are no external fields.

It is easy to realize that the value λ_c, in the general case, is strictly less than the expected value t_c, following from the Almeida–Thouless argument,

$$t_c\int \cosh^{-4}(\beta h+z\sqrt{x_0})d\mu(z)=1.$$

The proof of Theorem 3 is easy. First of all, let us establish the elementary bound, uniform in N,

$$\Delta_N(x_0,\lambda_0)\geqslant\Delta(x_0,\lambda_0). \tag{31}$$

In fact, starting from the definition of $\Delta_N(x_0,\lambda_0)$ given in (28), we can write, for $\lambda_0\neq 0$, and any μ,

$$(q_{12}-\overline{q})^2\geqslant 2\frac{\mu}{\lambda_0}(q_{12}-\overline{q})-\left(\frac{\mu}{\lambda_0}\right)^2,$$

and conclude that

$$\Delta_N(x_0,\lambda_0)\geqslant\alpha_0(\mu)-\frac{\mu^2}{4\lambda_0}, \tag{32}$$

where we have defined

$$\begin{aligned}\alpha_0(\mu)&\equiv\frac{1}{2N}E\ln\Omega_J^0(\exp\mu N(q_{12}-\overline{q}))\\&=\frac{1}{2}\int \ln(\cosh\mu+\tanh^2(\beta h+z\sqrt{x_0})\sinh\mu)d\rho(z)-\frac{1}{2}\mu\overline{q}.\end{aligned}$$

Of course, it is convenient to take the $\max_\mu$ on the rhs of (32), so that the bound in (31) is established. The proof that the bound is in effect the limit, as $N\to\infty$, can be obtained in a very simple way by using a Gaussian transformation on (28), as it was done in (22). In fact, we now have

$$\frac{1}{2N}E\ln\Omega_J^0\left(\exp\frac{1}{2}\lambda_0 N(q_{12}-\overline{q})^2\right)=\frac{1}{2N}E\ln\int\Omega_J^0(\exp\sqrt{\lambda_0 N}(q_{12}-\overline{q})z)d\rho(z). \tag{33}$$

Therefore, by exploiting the fact that also Ω_J^0 factorizes with respect to the sites i, we can write

$$\begin{aligned}\Delta_N(x_0,\lambda_0)=\frac{1}{2N}E\ln\int\prod_i&\left(\cosh\sqrt{\frac{\lambda_0}{N}}z+\tanh^2(\beta h+J_i\sqrt{x_0})\sinh\sqrt{\frac{\lambda_0}{N}}z\right)\\&\times\exp(-\sqrt{\lambda_0 N}\overline{q}z)d\rho(z).\end{aligned} \tag{34}$$

Now, we find it convenient to introduce a small $\epsilon>0$, so that

$$\frac{1}{\lambda_0}=\frac{1}{\lambda_0'}+\epsilon. \tag{35}$$

Notice that $\lambda_0<\lambda_0'$. We also introduce the auxiliary (random) function

$$\phi_N(y,\lambda_0')\equiv\frac{1}{N}\sum_i \ln(\cosh y+\tanh^2(\beta h+J_i\sqrt{x_0})\sinh y)-\overline{q}y-\frac{1}{2}\frac{y^2}{\lambda_0'}.$$

By the strong law of large numbers, as $N\to\infty$, for any y, we have the J almost sure convergence of $\phi_N(y,\lambda_0')$ to $\phi(y,\lambda_0')$ defined by

$$\phi(y,\lambda_0')\equiv\int \ln(\cosh y+\tanh^2(\beta h+z\sqrt{x_0})\sinh y)d\rho(z)-\overline{q}y-\frac{1}{2}\frac{y^2}{\lambda_0'}=E\,\phi_N(y,\lambda_0').$$

Here $d\rho(z)$ performs the averages with respect to the J_i variables. Let us also remark that the convergence is J almost surely uniform for any finite number of values of the variable y.

Now we can go back to (34), write explicitly the unit Gaussian measure $d\rho(z)$, perform the change of variables $y=z\sqrt{\lambda_0 N^{-1}}$, make the transformation (35), take the $\sup_y$ for the ϕ_N, and perform the residual Gaussian integration over y. We end up with the estimate

$$\Delta_N(x_0,\lambda_0)\leqslant\frac{1}{2}E\sup_y\phi_N(y,\lambda_0')+\frac{1}{2N}\ln\frac{1}{\sqrt{\lambda_0\epsilon}}. \tag{36}$$

Since the J-dependent $\sup_y$ is reached in some finite interval, for any fixed λ_0', and the function ϕ_N is continuous with respect to y, with bounded derivatives, we can perform the $\sup_y$ with y running over a finite discrete mesh of values, by tolerating a small error, which becomes smaller and smaller as the mesh interval is made smaller. But in this case the strong law of large numbers allows us to substitute ϕ_N with ϕ, in the infinite volume limit $N\to\infty$. On the other hand, the second term on the rhs of (36) vanishes in the limit. Therefore, we conclude that

$$\limsup_{N\to\infty}\Delta_N(x_0,\lambda_0)\leqslant\tfrac{1}{2}\sup_y\phi(y,\lambda_0').$$

From continuity with respect to λ_0, we can let λ_0' approach λ_0, and the theorem is proven.

V. FLUCTUATIONS OF OVERLAPS AND FREE ENERGY

In the previous sections we proved that, in a certain region of the parameters t, x, βh, the typical values of the free energy $\ln Z_N/N$ and of the overlap q_{ab} are the replica symmetric expressions $\overline{\alpha}$ and $\overline{q}$, respectively. In the same region, one can obtain a more precise characterization of the fluctuations of these quantities, for $N\to\infty$, showing that a central limit-type theorem holds, after suitable rescaling. This will be analyzed in detail in a subsequent paper.[17] Here, we just give the main results and sketch the ideas underlying the proof.

Concerning the fluctuations of the overlap around the Sherrington–Kirkpatrick order parameter $\overline{q}$, we prove the following.

Theorem 4:[17] *The rescaled overlap variables*

$$\xi_{ab}^N\equiv\sqrt{N}(q_{ab}-\overline{q})$$

tend in distribution, as $N\to\infty$, to centered, jointly Gaussian variables with covariances

$$\langle\xi_{ab}^2\rangle=A(t,x,h),$$

$$\langle\xi_{ab}\xi_{ac}\rangle=B(t,x,h),$$

$$\langle \xi_{ab}\xi_{cd}\rangle = C(t,x,h),$$

where $b\neq c$, $c\neq a,b$, *and* $d\neq a,b$. *The expressions of* A, B, C *are explicitly given and coincide with those found in Ref. 15.*

Recently, an analogous result was proved independently by Talagrand,[20] who computed the $N\to\infty$ limit for all moments of the ξ variables.

The scheme of our proof is as follows: The control we obtained on the coupled two replica system and concentration of measure inequalities for the free energy[21] imply that the fluctuations of q_{ab} from $\overline{q}$ are exponentially suppressed for N large. Then, by means of the cavity method[2] one can write a self-consistent closed equation for the characteristic function of the variables ξ^N_{ab}. This equation turns out to be linear, apart from error terms which vanish asymptotically for $N\to\infty$, thanks to the strong suppression of the overlap fluctuations. The solution, which is easily found, coincides with the characteristic function of a Gaussian distribution, with the correct covariance structure.

Concerning the free energy, the result we prove is the following:

Theorem 5:[17] *Define the rescaled free energy fluctuation as*

$$\hat{f}_N(t,x,h;J) \equiv \sqrt{N}\left(\frac{\ln Z_N(t,x,h;J)}{N} - \overline{\alpha}(t,x,h)\right).$$

Then,

$$\hat{f}_N(t,x,h;J) \overset{d}{\to} \mathcal{N}(0,\sigma^2(t,x,h)),$$

where $\mathcal{N}(m,\sigma^2)$ *denotes the Gaussian random variable of mean* m *and variance* σ^2, *and*

$$\sigma^2(t,x,h) = Var(\ln\cosh(z\sqrt{\overline{q}t+x}+\beta h)) - \frac{\overline{q}^2 t}{2}.$$

Here, $Var(.)$ *denotes the variance of a random variable and* $z=\mathcal{N}(0,1)$.

This result is a consequence of Theorem 4 and of concentration of measure inequalities for the free energy.

VI. OUTLOOK AND CONCLUSIONS

We obtained control on the thermodynamic limit of the model, in a region above the Almeida–Thouless line, by suitably coupling two replicas of the system and studying stability with respect to the coupling parameter. The question naturally arises, whether and how this method can be extended up to the expected critical line. This problem seems to be common to all approaches proposed so far.

The method can also be further generalized to the case where more and more replicas are mutually coupled. In this case, replica symmetry is explicitly broken at various levels, and it is possible to give a generalization of the Ghirlanda–Guerra relations.[13] We plan to report soon on these generalizations.[22]

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Wave focusing on the line

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Focusing of waves in one dimension is analyzed for the plasma-wave equation and the wave equation with variable speed. The existence of focusing causal solutions to these equations is established, and such wave solutions are constructed explicitly by deriving an orthogonality relation for the time-independent Schrödinger equation. The connection between wave focusing and inverse scattering is studied. The potential at any point is recovered from the incident wave that leads to focusing to that point. It is shown that focusing waves satisfy certain temporal-antisymmetry and support properties. Discontinuities in the spatial and temporal derivatives of the focusing waves are examined and related to the discontinuities in the potential of the Schrödinger equation. The theory is illustrated with some explicit examples. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1483894]

I. INTRODUCTION

Consider a (Dirac-delta) plane wave incident onto an inhomogeneous medium. As time progresses the plane wave is scattered by the inhomogeneity and consequently develops a ''tail'' that trails the wavefront. One of the questions considered in this article concerns the opposite process. Namely, ''Can one prepare an incident wave (consisting of a plane wave plus a tail) such that the tail vanishes at a specified instant due to the interaction with the inhomogeneity, i.e., the wave reduces to the plane wave at that instant?'' If this happens, we say that the wave focuses to the point being crossed by the wavefront at the specified instant. We are also interested in determining remotely the value of the inhomogeneity at any specified point in space from the incident wave that is going to focus to that point; this will be done by performing a measurement on the incident wave at some arbitrarily chosen moment in time before the wavefront reaches that point.

Mathematically speaking, our aim is to analyze focusing of causal solutions to the plasma-wave equation

$$\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial^2 u(x,t)}{\partial t^2} = V(x)u(x,t), \quad x,t \in \mathbf{R}, \tag{1.1}$$

where V is real valued and belongs to $L_1^1(\mathbf{R})$, the class of measurable potentials such that $\int_{-\infty}^{\infty} dx(1+|x|)|V(x)|$ is finite. In order to do this, we derive the orthogonality relation (3.6) for the associated Schrödinger equation

$$\frac{d^2\psi(k,x)}{dx^2} + k^2\psi(k,x) = V(x)\psi(k,x), \quad x \in \mathbf{R}, \tag{1.2}$$

and exploit the connection between (1.1) and (1.2) through the Fourier transformation

$$u(x,t) := \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, \psi(k,x)e^{-ikt}. \tag{1.3}$$

We use the subscript "l" to indicate waves incident from the left (i.e., coming from $x=-\infty$) and use "r" for incidence from the right. Our focusing waves consist of a (Dirac-delta distribution) wavefront and a tail lying either to the left or right of the wavefront in such a way that the tail completely disappears at a certain moment in time and thus the whole wave reduces to the wavefront at the focusing point. There is no loss of generality in choosing the focusing moment as $t=0$, and we denote the focusing point by x_0. Hence, we are interested in constructing causal solutions to (1.1) incident either from the left or right such that $u(x,0)=\delta(x-x_0)$, where $\delta(x)$ denotes the Dirac delta distribution. In Sec. VII we display $\partial u(x,0)/\partial t$ explicitly for our focusing waves and hence show that it is also possible to view them as some specific solutions to (1.1) satisfying certain initial conditions. Clearly, unless $\partial u(x,0)/\partial t\equiv 0$ when $x\in\mathbf{R}\backslash\{x_0\}$ for our focusing waves, their energy is not concentrated at x_0 when $t=0$; hence, in general, focusing of waves is not the same as focusing of the wave energy.

Our analysis helps us to understand better the connection between (1.1) and (1.2). In our treatment we include bound states of V, whereas such states are usually excluded in the analysis of (1.1) by imposing further restrictions on V such as positivity. Throughout our article, unless otherwise stated, V is only assumed to be real valued and belonging to $L_1^1(\mathbf{R})$; any other assumptions on V will be explicitly stated.

In our article we also investigate the connection between wave focusing and inverse scattering. The inverse scattering problem for (1.1) and (1.2) consists of the recovery of V from an appropriate set of scattering data. The recovery in the time domain is usually achieved by using some layer-stripping methods, see, e.g., Burridge (1980), Bube and Burridge (1983), Morawetz and Kriegsmann (1983), Bayliss *et al.* (1989), and Sacks (1993), in terms of the impulse response to a plane wave sent onto $V(x)$ either from $x=-\infty$ or from $x=+\infty$. In these techniques one considers the solution to (1.1) satisfying $u(x,t)=\delta(x-t)+o(1)$ and $\partial u(x,t)/\partial t=\delta'(x-t)+o(1)$ when $t\to-\infty$ as the wave incident from the left, or $u(x,t)=\delta(x+t)+o(1)$ and $\partial u(x,t)/\partial t=\delta'(x+t)+o(1)$ when $t\to-\infty$ as the wave incident from the right. The contrast with our focusing waves can be visualized by considering waves incident from the left especially when $V\equiv 0$ for $x<0$: our focusing wave for $x<0$ and $t<-x_0$ consists of the wavefront $\delta(x-x_0-t)$ followed by [cf. (5.19)] the nontrivial tail $K_r(x_0,x-t)$, whereas the wave in the aforementioned references is $\delta(x-t)$ for $x<0$ and $t<0$. We show in Sec. VII that the value of $V(x_0)$ for any fixed $x_0>0$ is recovered from the incident wave that is going to focus to x_0 with a measurement performed at an arbitrary moment $t<-x_0$ (i.e., before the wavefront reaches the inhomogeneity); in contrast, in the layer-stripping methods one lets the incident wave penetrate the inhomogeneity during the time interval $0<t<2x_0$ in order to recover $V(x)$ for $0<x<x_0$. A heuristic discussion of the physics connecting focusing and inverse scattering appears in Rose (2002), which is a strictly time-domain analysis that avoids reference to scattering solutions to (1.2).

This article is organized as follows. In Sec. II we introduce the Jost solutions, scattering coefficients, and normalized bound-state solutions of (1.2). In Sec. III we derive the orthogonality relation (3.6), a key result for obtaining the causal focusing wave solutions to (1.1) (incident either from the left or right) explicitly in terms of the Jost solutions, transmission coefficient, and normalized bound-state solutions of (1.2). In Sec. IV, we construct such causal waves that focus at $t=0$, namely U_l incident from the left and U_r incident from the right, and we study some of their properties; we also indicate how the value of $V(x_0)$ can be recovered by using waves focusing to x_0 and its vicinity. In Sec. V we examine the connection between wave focusing and inverse scattering problem; in particular, we analyze the relationship between wave focusing and the Marchenko inversion method, construct our focusing waves in terms of the solutions to the Marchenko integral equations, and show that wave focusing can be viewed as a consequence of the Marchenko method. In Sec. VI we explore certain temporal antisymmetries satisfied by the tails of our focusing waves; in this section we also show that, for potentials vanishing on a half line, the tail of a focusing wave may vanish in some regions at certain times and that a gap may develop between the wavefront and the tail. In Sec. VII, under more restrictive conditions on V, we analyze the discontinuities in the spatial and temporal derivatives of our focusing waves and relate such discontinuities to jump discontinuities of V; we also show that $V(x_0)$ can be recovered

solely from the incident wave leading to focusing to x_0, where the measurement can be performed at one arbitrarily chosen moment before the wavefront reaches x_0; as a corollary we obtain the interesting identities (7.22) and (7.25) for the solutions to the Marchenko equations when the corresponding potential vanishes on a half line. In Sec. VIII we present some explicit examples to illustrate various aspects of wave focusing and the recovery of $V(x_0)$ via focusing, and we also provide some snapshots of focusing waves as their tails disappear and reappear. Finally, in Sec. IX we analyze wave focusing for the variable-speed wave equation (9.14).

II. PRELIMINARIES

Let $\mathbf{C}^+$ denote the upper-half complex plane and $\overline{\mathbf{C}^+} := \mathbf{C}^+ \cup \mathbf{R}$. There are two types of solutions to (1.2). The scattering solutions consist of linear combinations of e^{ikx} and e^{-ikx} as $x \to \pm\infty$, and they occur for $k \in \mathbf{R}\backslash\{0\}$; on the other hand, the bound-state solutions decay exponentially as $x \to \pm\infty$, and they can occur only at certain k-values on the imaginary axis in $\mathbf{C}^+$. Let us use N to denote the number of bound states, which is known to be finite, and suppose that the bound states occur at $k = i\kappa_j$ with $0 < \kappa_1 < \cdots < \kappa_N$.

Among the scattering solutions to (1.2) are the Jost solution from the left, f_l, and the Jost solution from the right, f_r, satisfying the respective boundary conditions

$$e^{-ikx} f_\mathrm{l}(k,x) = 1 + o(1), \quad e^{-ikx} f_\mathrm{l}'(k,x) = ik + o(1), \quad x \to +\infty, \tag{2.1}$$

$$e^{ikx} f_\mathrm{r}(k,x) = 1 + o(1), \quad e^{ikx} f_\mathrm{r}'(k,x) = -ik + o(1), \quad x \to -\infty, \tag{2.2}$$

where the prime is used for the derivative with respect to the spatial coordinate x. From the spatial asymptotics

$$f_\mathrm{l}(k,x) = \frac{e^{ikx}}{T(k)} + \frac{L(k)e^{-ikx}}{T(k)} + o(1), \quad x \to -\infty, \tag{2.3}$$

$$f_\mathrm{r}(k,x) = \frac{e^{-ikx}}{T(k)} + \frac{R(k)e^{ikx}}{T(k)} + o(1), \quad x \to +\infty, \tag{2.4}$$

we obtain the scattering coefficients, namely, the transmission coefficient T, and the reflection coefficients L and R from the left and right, respectively.

Each bound state corresponds to a pole of T in $\mathbf{C}^+$ and vice versa. It is known that the bound states are simple and there exists only one linearly independent solution to (1.2) at each $k = i\kappa_j$ belonging to $L^2(\mathbf{R})$. The bound-state norming constants $c_{\mathrm{l}j}$ and $c_{\mathrm{r}j}$ are defined as

$$c_{\mathrm{l}j} := \left[\int_{-\infty}^{\infty} dx\, f_\mathrm{l}(i\kappa_j, x)^2 \right]^{-1/2}, \quad c_{\mathrm{r}j} := \left[\int_{-\infty}^{\infty} dx\, f_\mathrm{r}(i\kappa_j, x)^2 \right]^{-1/2}, \tag{2.5}$$

and they are related to each other via the residues of T as

$$\mathrm{Res}(T, i\kappa_j) = ic_{\mathrm{l}j}^2 \gamma_j = i\frac{c_{\mathrm{r}j}^2}{\gamma_j}, \tag{2.6}$$

where γ_j is the dependency constant given by $\gamma_j := f_\mathrm{l}(i\kappa_j, x)/f_\mathrm{r}(i\kappa_j, x)$. The sign of γ_j is the same as that of $(-1)^{N-j}$ and hence $c_{\mathrm{r}j} = (-1)^{N-j}\gamma_j c_{\mathrm{l}j}$. The normalized bound-state solution $\varphi_j(x)$ at $k = i\kappa_j$ is defined as

$$\varphi_j(x) := c_{\mathrm{l}j} f_\mathrm{l}(i\kappa_j, x) = (-1)^{N-j} c_{\mathrm{r}j} f_\mathrm{r}(i\kappa_j, x). \tag{2.7}$$

III. AN ORTHOGONALITY IDENTITY

The scattering and bound-state solutions to (1.2) satisfy the completeness relation, see, e.g., Newton (1983) and Chadan amd and Sabatier (1989),

$$\frac{1}{4\pi}\int_{-\infty}^{\infty} dk[\,\psi_{\rm l}(k,x)\psi_{\rm l}(-k,x_0)+\psi_{\rm r}(k,x)\psi_{\rm r}(-k,x_0)\,]+\sum_{j=1}^{N}\varphi_j(x)\varphi_j(x_0)=\delta(x-x_0), \quad (3.1)$$

where $\psi_{\rm l}$ and $\psi_{\rm r}$ are the physical solutions to (1.2) related to the Jost solutions as

$$\psi_{\rm l}(k,x):=T(k)f_{\rm l}(k,x), \quad \psi_{\rm r}(k,x):=T(k)f_{\rm r}(k,x). \quad (3.2)$$

In the Jost solutions, physical solutions, and scattering coefficients, for real k, replacing k by $-k$ has the same effect as taking complex conjugation. Moreover, we have

$$f_{\rm l}(-k,x)=T(k)f_{\rm r}(k,x)-R(k)f_{\rm l}(k,x), \quad k\in\mathbf{R}, \quad (3.3)$$

$$f_{\rm r}(-k,x)=-L(k)f_{\rm r}(k,x)+T(k)f_{\rm l}(k,x), \quad k\in\mathbf{R}, \quad (3.4)$$

which are consequences of the fact that either $\{f_{\rm l}(k,\cdot),f_{\rm r}(k,\cdot)\}$ or $\{f_{\rm l}(-k,\cdot),f_{\rm r}(-k,\cdot)\}$ is a linearly independent set of solutions to (1.2) when $k\in\mathbf{R}\backslash\{0\}$ and that the functions in one set can be expressed as a linear combination of those in the other. It is known that

$$R(k)T(-k)=-L(-k)T(k), \quad k\in\mathbf{R}. \quad (3.5)$$

Next we prove an orthogonality identity for (1.2) that will be useful in the analysis of wave focusing for (1.1).

Theorem 3.1: *Assume V is real valued and belongs to $L^1_1(\mathbf{R})$. Then*

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dkT(k)f_{\rm l}(k,x)f_{\rm r}(k,x_0)+\sum_{j=1}^{N}\varphi_j(x)\varphi_j(x_0)=\delta(x-x_0). \quad (3.6)$$

Proof: The proof will be given by showing that the integral term in (3.6) is identical to the integral in (3.1). From (3.2)–(3.4) we get

$$\psi_{\rm r}(k,x)=f_{\rm l}(-k,x)+R(k)f_{\rm l}(k,x), \quad k\in\mathbf{R},$$

$$\psi_{\rm l}(-k,x_0)=f_{\rm r}(k,x_0)+L(-k)f_{\rm r}(-k,x_0), \quad k\in\mathbf{R}.$$

Thus, for $k\in\mathbf{R}$ we have

$$\begin{aligned}&\psi_{\rm l}(k,x)\psi_{\rm l}(-k,x_0)+\psi_{\rm r}(k,x)\psi_{\rm r}(-k,x_0)\\ &\quad=T(k)f_{\rm l}(k,x)[f_{\rm r}(k,x_0)+L(-k)f_{\rm r}(-k,x_0)]+[f_{\rm l}(-k,x)+R(k)f_{\rm l}(k,x)]T(-k)f_{\rm r}(-k,x_0)\\ &\quad=T(k)f_{\rm l}(k,x)f_{\rm r}(k,x_0)+T(-k)f_{\rm l}(-k,x)f_{\rm r}(-k,x_0), \end{aligned} \quad (3.7)$$

where we have used (3.5) in the last step for simplification. Replacing the dummy integration variable k by $-k$, we get

$$\int_{-\infty}^{\infty} dkT(-k)f_{\rm l}(-k,x)f_{\rm r}(-k,x_0)=\int_{-\infty}^{\infty} dkT(k)f_{\rm l}(k,x)f_{\rm r}(k,x_0),$$

and hence from (3.7) we obtain

$$\int_{-\infty}^{\infty} dk[\psi_l(k,x)\psi_l(-k,x_0)+\psi_r(k,x)\psi_r(-k,x_0)]=2\int_{-\infty}^{\infty} dkT(k)f_l(k,x)f_r(k,x_0).$$

Thus, the integral on the left-hand side of (3.6) is the same as that on the left-hand side of (3.1).■

IV. WAVE FOCUSING FOR THE PLASMA-WAVE EQUATION

In this section we construct focusing waves of (1.1) incident either from the left or right in terms of the Jost solutions, transmission coefficient, and bound states for (1.2). We also relate the discontinuities at the wavefront of such focusing waves to an integral of V and show how the value of $V(x)$ at any specific point can be extracted from waves focusing to that point and its vicinity.

In terms of the Jost solutions of (1.2), let us define

$$K_l(x,t):=\frac{1}{2\pi}\int_{-\infty}^{\infty} dk[f_l(k,x)-e^{ikx}]e^{-ikt}, \tag{4.1}$$

$$K_r(x,t):=\frac{1}{2\pi}\int_{-\infty}^{\infty} dk[f_r(k,x)-e^{-ikx}]e^{ikt}. \tag{4.2}$$

Using (2.7) and the inverse Fourier transforms on (4.1) and (4.2), we obtain

$$\varphi_j(x)=(-1)^{N-j}c_{rj}\left[e^{\kappa_j x}+\int_{-\infty}^{x} dsK_r(x,s)e^{\kappa_j s}\right]=c_{lj}\left[e^{-\kappa_j x}+\int_{x}^{\infty} dsK_l(x,s)e^{-\kappa_j s}\right]. \tag{4.3}$$

The properties of K_l and K_r stated in the following theorem are already known, see, e.g., Faddeev (1967), Marchenko (1986), Chadan and Sabatier (1989), Deift and Trubowitz (1979), and they are used later in our analysis.

Theorem 4.1: *Assume V is real valued and belongs to $L^1_1(\mathbf{R})$. Then*

(i) For each fixed $x\in\mathbf{R}$, $K_l(x,\cdot)$ and $K_r(x,\cdot)$ belong to $L^2(\mathbf{R})\cap L^1(\mathbf{R})$.

(ii) For any $a\in\mathbf{R}$, $K_l(x,t)$ is uniformly bounded in (x,t) for $x\geqslant a$; similarly, $K_r(x,t)$ is uniformly bounded in (x,t) for $x\leqslant a$. Moreover, we have

$$K_l(x,t)=0, \quad t<x; \quad K_r(x,t)=0, \quad t>x. \tag{4.4}$$

(iii) K_l and K_r are continuous in (x,t) except when $t=x$, and the jumps there are related to V as

$$K_l(x,x^+)=\frac{1}{2}\int_{x}^{\infty} dzV(z), \quad K_r(x,x^-)=\frac{1}{2}\int_{-\infty}^{x} dzV(z). \tag{4.5}$$

Define

$$\hat{L}(t):=\frac{1}{2\pi}\int_{-\infty}^{\infty} dkL(k)e^{ikt}, \quad \hat{R}(t):=\frac{1}{2\pi}\int_{-\infty}^{\infty} dkR(k)e^{ikt}. \tag{4.6}$$

When V is real valued and belongs to $L^1_1(\mathbf{R})$, each of $\hat{L}$ and $\hat{R}$ is continuous and belongs to $L^2(\mathbf{R})$. In fact, they are absolutely continuous and differentiable, and for each fixed $a\in\mathbf{R}$ their derivatives satisfy $\hat{L}'\in L^1_1(-\infty,a)$ and $\hat{R}'\in L^1_1(a,+\infty)$.

Let us define

$$P_l(x,t):=\frac{1}{2\pi}\int_{-\infty}^{\infty} dk[T(k)-1]f_l(k,x)e^{-ikt}, \tag{4.7}$$

$$P_{\rm r}(x,t) := \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[T(k)-1]f_{\rm r}(k,x)e^{ikt}, \tag{4.8}$$

$$\Phi_{\rm l}(x,t) := \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[\psi_{\rm l}(k,x)-e^{ikx}]e^{-ikt}, \tag{4.9}$$

$$\Phi_{\rm r}(x,t) := \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[\psi_{\rm r}(k,x)-e^{-ikx}]e^{ikt}. \tag{4.10}$$

Proposition 4.2: Assume V is real valued and belongs to $L^1_1(\mathbf{R})$. Then, for any fixed $x\in\mathbf{R}$, each of $P_{\rm l}(x,\cdot)$, $P_{\rm r}(x,\cdot)$, $\Phi_{\rm l}(x,\cdot)$, and $\Phi_{\rm r}(x,\cdot)$ belongs to $L^2(\mathbf{R})$. Moreover, we have

$$\Phi_{\rm l}(x,t) = P_{\rm l}(x,t) + K_{\rm l}(x,t), \quad \Phi_{\rm r}(x,t) = P_{\rm r}(x,t) + K_{\rm r}(x,t), \tag{4.11}$$

$$\Phi_{\rm l}(x,t) = P_{\rm l}(x,t) = -\sum_{j=1}^{N} (-1)^{N-j} c_{{\rm r}j}\varphi_j(x)e^{\kappa_j t}, \quad t<x, \tag{4.12}$$

$$\Phi_{\rm r}(x,t) = P_{\rm r}(x,t) = -\sum_{j=1}^{N} c_{{\rm l}j}\varphi_j(x)e^{-\kappa_j t}, \quad t>x, \tag{4.13}$$

$$\Phi_{\rm l}(x,t) = K_{\rm r}(x,t) + \hat{L}(-x-t) + \int_{-\infty}^{x} ds\,\hat{L}(-t-s)K_{\rm r}(x,s), \quad t\neq x, \tag{4.14}$$

$$\Phi_{\rm r}(x,t) = K_{\rm l}(x,t) + \hat{R}(x+t) + \int_{x}^{\infty} ds\,\hat{R}(t+s)K_{\rm l}(x,s), \quad t\neq x, \tag{4.15}$$

$$P_{\rm l}(x,x_0+t) + \int_{-\infty}^{x_0} ds\,P_{\rm l}(x,s+t)K_{\rm r}(x_0,s) + \sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t} = 0, \quad x>x_0+t, \tag{4.16}$$

$$P_{\rm r}(x,x_0-t) + \int_{x_0}^{\infty} ds\,P_{\rm r}(x,s-t)K_{\rm l}(x_0,s) + \sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t} = 0, \quad x<x_0-t. \tag{4.17}$$

Proof: We obtain (4.11) by using (3.2), (4.1), (4.2), and (4.7)–(4.10). With the help of (2.6), (2.7), (4.4), (4.7), (4.8), and (4.11), by using a contour integration along the infinite semicircle enclosing $\mathbf{C}^+$, we obtain (4.12) and (4.13). Using (4.2), (4.6), and a Fourier transform on (3.4) we get (4.14). Similarly, by using (3.3), (4.1), and (4.6) we get (4.15). With the help of (4.3) and (4.12) we establish (4.16). In the same manner, using (4.3) and (4.13) we get (4.17). ■

Define

$$U_{\rm l}(x,t;x_0) := \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,\psi_{\rm l}(k,x)f_{\rm r}(k,x_0)e^{-ikt} + \sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}, \tag{4.18}$$

$$U_{\rm r}(x,t;x_0) := \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,\psi_{\rm r}(k,x)f_{\rm l}(k,x_0)e^{-ikt} + \sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}, \tag{4.19}$$

$$\Upsilon_{\rm l}(x,t;x_0) := U_{\rm l}(x,t;x_0) - \delta(x-x_0-t), \tag{4.20}$$

$$\Upsilon_{\rm r}(x,t;x_0) := U_{\rm r}(x,t;x_0) - \delta(x-x_0+t). \tag{4.21}$$

Theorem 4.3: *Assume V is real valued and belongs to $L^1_1(\mathbf{R})$. Then U_l is a causal solution to (1.1) incident from the left and focusing to $x=x_0$ when $t=0$. Similarly, U_r is a causal solution to (1.1) that is incident from the right and that focuses to $x=x_0$ when $t=0$.*

Proof: First, ψ_l, ψ_r, f_l, and f_r are solutions to (1.2) and they are transformed from the k-domain to the t-domain as in (1.3). Thus, with the help of (2.7), we see that each of U_l and U_r is a solution to (1.1). Using (4.2), (4.9), (4.11), (4.18), and (4.20) we get

$$\Upsilon_l(x,t;x_0)=K_r(x_0,x-t)+K_l(x,x_0+t)+\int_{x-t}^{x_0} ds K_l(x,s+t)K_r(x_0,s)+P_l(x,x_0+t)$$
$$+\int_{-\infty}^{x_0} ds P_l(x,s+t)K_r(x_0,s)+\sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}. \tag{4.22}$$

Similarly, using (4.1), (4.10), (4.11), (4.19), and (4.21) we obtain

$$\Upsilon_r(x,t;x_0)=K_l(x_0,x+t)+K_r(x,x_0-t)+\int_{x_0}^{x+t} ds K_r(x,s-t)K_l(x_0,s)+P_r(x,x_0-t)$$
$$+\int_{x_0}^{\infty} ds P_r(x,s-t)K_l(x_0,s)+\sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}. \tag{4.23}$$

With the help of (4.4) it follows that at any fixed moment t each of the first three terms on the right-hand side of (4.22) vanishes when $x>x_0+t$; moreover, using (4.16) it follows that the last three terms add to zero when $x>x_0+t$. Thus, U_l consists of the wavefront $\delta(x-x_0-t)$ followed by the tail Υ_l on the left, and it is incident from the left. Similarly, at any fixed moment t each of the first three terms on the right-hand side of (4.23) vanishes when $x<x_0-t$; moreover, from (4.17) it follows that the last three terms add to zero when $x<x_0-t$. Hence, U_r is a wave consisting of the wavefront $\delta(x-x_0+t)$ followed by the tail Υ_r on the right and the wave is incident from the right. Each of the waves U_l and U_r focuses to $x=x_0$ at $t=0$ because $U_l(x,0;x_0)=\delta(x-x_0)$ and $U_r(x,0;x_0)=\delta(x-x_0)$, as readily seen by comparing (4.18) and (4.19) with (3.6). ■

Since (1.1) is linear and homogeneous, any linear combination of U_l and U_r also focuses at $t=0$. In fact, for the special choice U_l-U_r even the wavefronts cancel each other and the wave vanishes on the entire x-axis at $t=0$. On the other hand, for the special choice U_l+U_r the wavefronts superimpose on top of each other at $t=0$.

Proposition 4.4: Assume V is real valued and belongs to $L^1_1(\mathbf{R})$. Then the only discontinuities of P_l and P_r can occur when $x=t$. Such discontinuities are given by

$$P_l(x,x^-)=\Phi_l(x,x^-)=-\sum_{j=1}^{N} (-1)^{N-j}c_{rj}\varphi_j(x)e^{\kappa_j x}, \tag{4.24}$$

$$P_r(x,x^+)=\Phi_r(x,x^+)=-\sum_{j=1}^{N} c_{lj}\varphi_j(x)e^{-\kappa_j x}, \tag{4.25}$$

$$P_l(x,x^+)=-\frac{1}{2}\int_{-\infty}^{\infty} ds V(s)-\sum_{j=1}^{N} (-1)^{N-j}c_{rj}\varphi_j(x)e^{\kappa_j x}, \tag{4.26}$$

$$P_r(x,x^-)=-\frac{1}{2}\int_{-\infty}^{\infty} ds V(s)-\sum_{j=1}^{N} c_{lj}\varphi_j(x)e^{-\kappa_j x}. \tag{4.27}$$

Proof: Note that (4.24) and (4.25) are equivalent to (4.12) and (4.13), respectively. Since $\hat{L}$ and $K_r(x,\cdot)$ are square integrable, their product is integrable; hence the integral term in (4.14) is

continuous in (x,t) as a result of the Lebesgue dominated convergence theorem. Similarly, from the square-integrability of $\hat{R}$ and of $K_{\rm l}(x,\cdot)$ it follows that the integral term in (4.15) is continuous in (x,t). Using the fact that $\hat{L}$ and $\hat{R}$ are continuous, from (4.11), (4.14), and (4.15) we see that the discontinuities of $P_{\rm l}$ and $P_{\rm r}$ coincide with those of $K_{\rm l}$ and $K_{\rm r}$; hence, such discontinuities can occur only when $x=t$. In fact, with the help of (4.4) we get

$$P_{\rm l}(x,x^+)-P_{\rm l}(x,x^-)=-K_{\rm r}(x,x^-)-K_{\rm l}(x,x^+), \tag{4.28}$$

$$P_{\rm r}(x,x^+)-P_{\rm r}(x,x^-)=K_{\rm l}(x,x^+)+K_{\rm r}(x,x^-). \tag{4.29}$$

Thus, using (4.5), (4.24), (4.25), (4.28), and (4.29), we get (4.26) and (4.27). ■

Theorem 4.5: *Assume V is real valued and belongs to $L^1_1(\mathbf{R})$. Then the only discontinuities of $U_{\rm l}$ and $U_{\rm r}$ occur at the wavefront, and the jumps in the tails at the wavefront are related to V as*

$$\Upsilon_{\rm l}(x_0^-+t,t;x_0)=-\frac{1}{2}\int_{x_0}^{x_0+t}dz\,V(z), \tag{4.30}$$

$$\Upsilon_{\rm r}(x_0^+-t,t;x_0)=-\frac{1}{2}\int_{x_0-t}^{x_0}dz\,V(z). \tag{4.31}$$

Proof: From (4.22) and (4.23) we see that the discontinuities in $\Upsilon_{\rm l}$ and $\Upsilon_{\rm r}$ can come only from the first, second, and fourth terms on the right-hand sides of (4.22) and (4.23), respectively; the third and fifth terms are continuous in (x,t) because the integrands there, being products of L^2-functions, are integrable in s. Thus, with the help of Proposition 4.4 and the fact that $K_{\rm r}$ and $K_{\rm l}$ can have discontinuities only when $x=t$, we conclude that the discontinuities in $\Upsilon_{\rm l}$ and $\Upsilon_{\rm r}$ can only occur at the wavefront, and we have

$$\begin{aligned}\Upsilon_{\rm l}(x_0^-+t,t;x_0)-\Upsilon_{\rm l}(x_0^++t,t;x_0)&=K_{\rm r}(x_0,x_0^-)-K_{\rm r}(x_0,x_0^+)+K_{\rm l}(x_0+t,x_0^++t)-K_{\rm l}(x_0+t,x_0^-+t)\\&\quad+P_{\rm l}(x_0+t,x_0^++t)-P_{\rm l}(x_0+t,x_0^-+t),\end{aligned} \tag{4.32}$$

$$\begin{aligned}\Upsilon_{\rm r}(x_0^+-t,t;x_0)-\Upsilon_{\rm r}(x_0^--t,t;x_0)&=K_{\rm l}(x_0,x_0^+)-K_{\rm l}(x_0,x_0^-)+K_{\rm r}(x_0-t,x_0^--t)-K_{\rm r}(x_0-t,x_0^+-t)\\&\quad+P_{\rm r}(x_0-t,x_0^--t)-P_{\rm r}(x_0-t,x_0^+-t).\end{aligned} \tag{4.33}$$

Now using (4.4), (4.5), (4.28), and (4.29) in (4.32) and (4.33) and the fact that $U_{\rm l}$ and $U_{\rm r}$ are causal, we establish (4.30) and (4.31). ■

As an application of Theorem 4.5, let us show how one can recover the value of $V(x_0)$ by using waves focusing to x_0 and its vicinity. Consider the left-hand side of (4.30) at some fixed time t in the interval $(-\infty,-x_0)$; in fact, one can even consider it when $t\to-\infty$. Let

$$\Gamma_{\rm l}(x_0,t):=\Upsilon_{\rm l}(x_0^-+t,t;x_0). \tag{4.34}$$

Thus, $\Gamma_{\rm l}(x_0,t)$ indicates the height of the tail of $U_{\rm l}$ at the wavefront at some fixed time $t<-x_0$. From (4.30), if V is continuous at x_0 and x_0+t, we see that

$$V(x_0)-V(x_0+t)=2\,\frac{\partial\Gamma_{\rm l}(x_0,t)}{\partial x_0}. \tag{4.35}$$

Note that $V(x_0+t)$ can be made as small as we want by choosing t so that either x_0+t lies to the left of the support of V (if V is supported in a right-half line) or by letting $t\to-\infty$ (if the support of V extends to $x=-\infty$). Clearly, $\partial\Gamma_{\rm l}(x_0,t)/\partial x_0$ can be obtained by using waves focusing to x_0 and its vicinity. An explicit example in Sec. VIII illustrates the recovery of $V(x_0)$ by using the technique described here.

Note that in the recovery technique outlined above, we have not made any other assumptions on V besides $V \in L_1^1(\mathbf{R})$, its realness, and its continuity at x_0 and x_0+t for some fixed $t<-x_0$. In fact, even when V is not continuous but only sectionally continuous, this technique still holds provided we replace (4.35) by

$$V(x_0^-)-V(x_0^++t)=2\frac{\partial\Gamma_l(x_0,t)}{\partial x_0}, \quad t<-x_0.$$

Under some stronger assumptions on V in Sec. VII, we will see that we can recover $V(x_0)$ by only using the wave that focuses to x_0 without needing any waves focusing near x_0.

V. CONNECTION WITH THE MARCHENKO METHOD

In this section we explore the connection between wave focusing for (1.1) and the Marchenko method to solve the inverse scattering problem for (1.2). By presenting certain representations for U_l and U_r, we show that their focusing is a direct consequence of the Marchenko method.

Let us define

$$M_r(t):=\hat{L}(-t)+\sum_{j=1}^{N} c_{rj}^2 e^{\kappa_j t}, \quad M_l(t):=\hat{R}(t)+\sum_{j=1}^{N} c_{lj}^2 e^{-\kappa_j t}, \tag{5.1}$$

where $\hat{L}$ and $\hat{R}$ are as in (4.6), and c_{rj} and c_{lj} are as in (2.5). Using (4.3), (4.4), (4.12)–(4.15), and (5.1) we get the two Marchenko equations

$$K_r(x,t)+M_r(x+t)+\int_{-\infty}^{x} dsM_r(t+s)K_r(x,s)=0, \quad t<x, \tag{5.2}$$

$$K_l(x,t)+M_l(x+t)+\int_{x}^{\infty} dsM_l(t+s)K_l(x,s)=0, \quad t>x, \tag{5.3}$$

and using (4.4), (4.14), and (4.15) we obtain the two complementary equations

$$\Phi_l(x,t)=\hat{L}(-x-t)+\int_{-\infty}^{x} ds\hat{L}(-t-s)K_r(x,s), \quad t>x, \tag{5.4}$$

$$\Phi_r(x,t)=\hat{R}(x+t)+\int_{x}^{\infty} ds\hat{R}(t+s)K_l(x,s), \quad t<x. \tag{5.5}$$

Let

$$F_l(x,t):=K_l(x,t)+M_l(x+t)+\int_{x}^{\infty} dsM_l(t+s)K_l(x,s), \tag{5.6}$$

$$F_r(x,t):=K_r(x,t)+M_r(x+t)+\int_{-\infty}^{x} dsM_r(t+s)K_r(x,s), \tag{5.7}$$

$$Z_l(x,t):=\Phi_l(x,t)-\hat{L}(-x-t)-\int_{-\infty}^{x} ds\hat{L}(-t-s)K_r(x,s), \tag{5.8}$$

$$Z_r(x,t):=\Phi_r(x,t)-\hat{R}(x+t)-\int_{x}^{\infty} ds\hat{R}(t+s)K_l(x,s). \tag{5.9}$$

Using (4.4) we can write the Marchenko equations (5.2) and (5.3) as

$$F_{\mathrm{r}}(x,t)=0, \quad t<x; \quad K_{\mathrm{r}}(x,t)=0, \quad t>x, \tag{5.10}$$

$$F_{\mathrm{l}}(x,t)=0, \quad t>x; \quad K_{\mathrm{l}}(x,t)=0, \quad t<x, \tag{5.11}$$

and the complementary equations (5.4) and (5.5) as

$$Z_{\mathrm{l}}(x,t)=0, \quad t>x; \quad Z_{\mathrm{r}}(x,t)=0, \quad t<x. \tag{5.12}$$

The following proposition shows that the focusing wave U_{l} can be constructed from the scattering data $\{L,\{\kappa_j\},\{c_{\mathrm{r}j}\}\}$ via the solution K_{r} of the Marchenko equation (5.2); similarly, the focusing wave U_{r} can be constructed from the data $\{R,\{\kappa_j\},\{c_{\mathrm{l}j}\}\}$ via the solution K_{l} of the Marchenko equation (5.3).

Proposition 5.1: The waves U_{l} and U_{r} defined in (4.18) and (4.19) can be expressed in terms of the quantities defined in (4.1), (4.2), (5.6), and (5.7) as

$$U_{\mathrm{l}}(x,t;x_0)=\delta(x-x_0-t)+K_{\mathrm{r}}(x_0,x-t)+F_{\mathrm{r}}(x,x_0+t)+\int_{-\infty}^{x_0} ds F_{\mathrm{r}}(x,t+s)K_{\mathrm{r}}(x_0,s), \tag{5.13}$$

$$U_{\mathrm{r}}(x,t;x_0)=\delta(x-x_0+t)+K_1(x_0,x+t)F_{\mathrm{l}}(x,x_0-t)+\int_{x_0}^{\infty} ds F_1(x,s-t)K_{\mathrm{l}}(x_0,s). \tag{5.14}$$

Proof: Using (4.3), (4.14), (4.22), (5.1), and (5.7), we obtain (5.13). Similarly, using (4.3), (4.15), (4.23), (5.1), and (5.6), we obtain (5.14). ■

Let us define

$$\begin{aligned} A_{\mathrm{r}}(x,t;x_0) :=& K_{\mathrm{r}}(x_0,x-t)-K_{\mathrm{r}}(x_0,x+t)-F_{\mathrm{r}}(x_0,x-t)+F_{\mathrm{r}}(x_0,x+t) \\ &-\int_{-\infty}^{x} ds K_{\mathrm{r}}(x,s)[F_{\mathrm{r}}(x_0,s-t)-F_{\mathrm{r}}(x_0,s+t)] \\ &+\int_{-\infty}^{\max\{x,x_0\}} ds[K_{\mathrm{r}}(x_0,s)K_{\mathrm{r}}(x,s+t)-K_{\mathrm{r}}(x_0,s+t)K_{\mathrm{r}}(x,s)], \end{aligned} \tag{5.15}$$

$$\begin{aligned} A_{\mathrm{l}}(x,t;x_0) :=& K_{\mathrm{l}}(x_0,x+t)-K_{\mathrm{l}}(x_0,x-t)+F_{\mathrm{l}}(x_0,x-t)-F_{\mathrm{l}}(x_0,x+t) \\ &-\int_{x}^{\infty} ds K_{\mathrm{l}}(x,s)[F_{\mathrm{l}}(x_0,s+t)-F_{\mathrm{l}}(x_0,s-t)] \\ &+\int_{\min\{x,x_0\}}^{\infty} ds[K_{\mathrm{l}}(x_0,s)K_{\mathrm{l}}(x,s-t)-K_{\mathrm{l}}(x_0,s-t)K_{\mathrm{l}}(x,s)]. \end{aligned} \tag{5.16}$$

Note that at $t=0$ both $A_{\mathrm{r}}(x,t;x_0)$ and $A_{\mathrm{l}}(x,t;x_0)$ vanish.

Proposition 5.2: The waves U_{l} and U_{r} defined in (4.18) and (4.19) can be expressed in terms of the quantities defined in (4.1), (4.2), (5.6)–(5.9), (5.15), and (5.16) as

$$U_{\mathrm{l}}(x,t;x_0)=\delta(x-x_0-t)+Z_{\mathrm{l}}(x,x_0+t)+F_{\mathrm{r}}(x_0,x-t)+\int_{x_0+t}^{x} ds F_{\mathrm{r}}(x_0,s-t)K_{\mathrm{r}}(x,s)+A_{\mathrm{r}}(x,t;x_0), \tag{5.17}$$

$$\begin{aligned} U_{\mathrm{r}}(x,t;x_0) =& \delta(x-x_0+t)+Z_{\mathrm{r}}(x,x_0-t)+F_{\mathrm{l}}(x_0,x+t) \\ &+\int_{x}^{x_0-t} ds F_{\mathrm{l}}(x_0,s+t)K_{\mathrm{l}}(x,s)+A_{\mathrm{l}}(x,t;x_0). \end{aligned} \tag{5.18}$$

Proof: We obtain (5.17) by using (4.3), (4.11), (4.14), (5.1), (5.7), and (5.8) in (4.22). Similarly, (5.18) is obtained by using (4.3), (4.11), (4.15), (5.6), and (5.9) in (4.23). ■

Theorem 5.3: *Assume that V is real valued and belongs to $L_1^1(\mathbf{R})$. Then we have the following.*

(i) The causality of U_l is a consequence of the Marchenko equation (5.2).
(ii) The causality of U_r is a consequence of the Marchenko equation (5.3).
(iii) The focusing of U_l to x_0 at $t=0$ is a consequence of (5.2) and (5.4).
(iv) The focusing of U_r to x_0 at $t=0$ is a consequence of (5.3) and (5.5).

Proof: Recall that (5.2) and (5.3) are equivalent to (5.10) and (5.11), respectively; similarly, (5.4) and (5.5) are equivalent to the first and second equations in (5.12), respectively. Note that if (5.10) holds, then the right-hand side of (5.13) vanishes when $x>x_0+t$ and hence (i) is proved. Similarly, if (5.11) holds, then the right-hand side of (5.14) vanishes for $x<x_0-t$ and hence (ii) is proved. If (5.10) and the first equation in (5.12) hold, then each of the first four terms on the right-hand side of (5.17) vanishes when $x<x_0+t$; moreover, the last term $A_r(x,t;x_0)$ vanishes at $t=0$ and hence (iii) is proved. In the same manner, if (5.11) and the second equation in (5.12) hold, then each of the first four terms on the right-hand side of (5.18) vanishes when $x>x_0-t$; moreover, the last term $A_l(x,t;x_0)$ vanishes at $t=0$ and hence (iv) is also proved. ■

Let us comment on the roles that the complementary equations (5.4) and (5.5) play in the Marchenko method. For the recovery of V by solving (5.2), one uses the ''right'' scattering data $\{L,\{\kappa_j\},\{c_{rj}\}\}$ as the input and obtains the ''right'' quantity K_r, from which the ''right'' Jost solution f_r is obtained with the help of (4.1). The complementary equation (5.4) is a means to construct the ''left'' quantity Φ_l, from which the ''left'' physical solution ψ_l can be obtained via the inverse Fourier transform on (4.9). In a similar manner, the complementary equation (5.5) is a means to construct the ''right'' quantities such as ψ_r by using only the ''left'' scattering data $\{R,\{\kappa_j\},\{c_{lj}\}\}$ as the input to the Marchenko procedure. Hence, Theorem 5.3(iii) is equivalent to the statement that the focusing of U_l is a consequence of the Marchenko method using the ''right'' scattering data as the input. Similarly, Theorem 5.3(iv) is equivalent to saying that focusing of U_r is a consequence of the Marchenko method using the ''left'' scattering data as the input.

The following result and its proof are used in the proof of Theorems 6.4 and 6.5. Even though this result is already known, we include a brief proof for convenience because we later refer to the facts stated in it.

Proposition 5.4: Assume V is real valued and belongs to $L_1^1(\mathbf{R})$. If $V\equiv 0$ for $x>0$, then $M_l(t)=0$ for $t>0$, and if $V\equiv 0$ for $x<0$, then $M_r(t)=0$ for $t<0$, where M_l and M_r are the quantities defined in (5.1).

Proof: If $V\equiv 0$ for $x>0$, then R is meromorphic in $\mathbf{C}^+$ with simple poles at the bound states $k=i\kappa_j$ having the residues $\mathrm{Res}(R,i\kappa_j)=ic_{lj}^2$, and $R(k)e^{2ikx}=o(1/k)$ as $k\to\infty$ in $\overline{\mathbf{C}^+}$ for each $x\geqslant 0$. Similarly, if $V\equiv 0$ for $x<0$, then L is meromorphic in $\mathbf{C}^+$ with simple poles at the bound states $k=i\kappa_j$ having the residues $\mathrm{Res}(L,i\kappa_j)=ic_{rj}^2$, and $L(k)e^{-2ikx}=o(1/k)$ as $k\to\infty$ in $\overline{\mathbf{C}^+}$ for each $x\leqslant 0$. Thus, from (5.1) with the help of a contour integration, we directly get the conclusion of our proposition. ■

Let us make a contrast between an incident focusing wave and an incident plane wave; the latter is often used to probe an inhomogeneous medium. For simplicity, consider the special case $V\equiv 0$ for $x<0$. In this case, from (4.2) it follows that $K_r(x,t)=0$ for $x<0$. Thus, using (5.7) and Proposition 5.4 we get $F_r(x,x_0+t)=0$ for $x<0$ and $t<-x_0$. Hence, from (5.13) it follows that our focusing wave incident from the left is given by

$$U_l(x,t;x_0)=\delta(x-x_0-t)+K_r(x_0,x-t),\quad x<0,\quad t<-x_0. \tag{5.19}$$

From (5.19) we see that, if $x_0>0$, U_l contains some information about V even before the incident wave first encounters the potential at $x=0$ and $t=-x_0$. Using $x_0+t<0$ and $V(z)=0$ for $z<0$, from (4.30) we get $\Upsilon_l(x_0^-+t,t;x_0)=(1/2)\int_0^{x_0}dzV(z)$. This is in contrast to the case where a pure

plane wave is sent onto V from $x=-\infty$, in which case the incident wave consists solely of the Dirac-delta wavefront alone and a tail is nonexistent until the wave encounters the potential at $x=0$.

VI. TEMPORAL ANTISYMMETRIES AND SUPPORT PROPERTIES

In this section we are interested in showing that the focusing waves U_l and U_r satisfy certain temporal antisymmetries and support properties that are useful in understanding their focusing. We also show that for potentials vanishing on a half line, a gap may develop between the wavefront and the tail of these focusing waves. We present our results only for U_l because the corresponding results for U_r are obtained in a similar manner.

In terms of the Jost solutions of (1.2), let us define the Faddeev functions m_l and m_r as follows:

$$m_l(k,x) := e^{-ikx} f_l(k,x), \quad m_r(k,x) := e^{ikx} f_r(k,x).$$

Then, we can write Υ_l and Υ_r defined in (4.20) and (4.21), respectively, as

$$\Upsilon_l(x,t;x_0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[T(k)m_l(k,x)m_r(k,x_0)-1]e^{ik(x-x_0-t)} + \sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}, \tag{6.1}$$

$$\Upsilon_r(x,t;x_0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[T(k)m_r(k,x)m_l(k,x_0)-1]e^{-ik(x-x_0+t)} + \sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}. \tag{6.2}$$

From Theorem 4.3 we know that U_l and U_r are causal. Hence, from (6.1) and (6.2) we conclude the following.

Corollary 6.1: Assume V is real valued and belongs to $L^1_1(\mathbf{R})$. Then for $x>x_0+t$ we have

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[T(k)m_l(k,x)m_r(k,x_0)-1]e^{ik(x-x_0-t)} = -\sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}, \tag{6.3}$$

and for $x<x_0-t$ we have

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[T(k)m_r(k,x)m_l(k,x_0)-1]e^{-ik(x-x_0+t)} = -\sum_{j=1}^{N} \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}. \tag{6.4}$$

Theorem 6.2: *Assume V is real valued and belongs to $L^1_1(\mathbf{R})$. Then, for $t<x_0-x$, the tail Υ_l defined in (4.20) satisfies*

$$\Upsilon_l(x,t;x_0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[m_l(k,x)m_l(-k,x_0)-1][e^{ik(x-x_0-t)} - e^{ik(x-x_0+t)}]. \tag{6.5}$$

Similarly, for $t<x-x_0$, the tail Υ_r defined in (4.21) satisfies

$$\Upsilon_r(x,t;x_0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[m_r(k,x)m_r(-k,x_0)-1][e^{-ik(x-x_0+t)} - e^{-ik(x-x_0-t)}]. \tag{6.6}$$

Proof: From (3.3) we get

$$T(k)m_r(k,x_0) = m_l(-k,x_0) + R(k)e^{2ikx_0}m_l(k,x_0), \quad k\in\mathbf{R},$$

and, hence, for real k, we have

$$T(k)m_l(k,x)m_r(k,x_0)=m_l(k,x)m_l(-k,x_0)+R(k)m_l(k,x)e^{2ikx_0}m_l(k,x_0). \tag{6.7}$$

From (3.3) we see that

$$R(k)m_l(k,x)=e^{-2ikx}[T(k)m_r(k,x)-m_l(-k,x)], \quad k\in\mathbf{R}. \tag{6.8}$$

Thus, using (6.8) in the second term on the right-hand side of (6.7), we obtain

$$\begin{aligned}T(k)m_l(k,x)m_r(k,x_0)=&[T(k)m_r(k,x)-m_l(-k,x)]m_l(k,x_0)e^{2ik(x_0-x)}\\&+m_l(k,x)m_l(-k,x_0), \quad k\in\mathbf{R}.\end{aligned} \tag{6.9}$$

Using (6.9) in (6.1) we get

$$\Upsilon_l(x,t;x_0)=I_1-I_2+I_3-I_4+I_5+I_6,$$

where we have defined

$$I_1:=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk m_l(k,x)m_l(-k,x_0)e^{ik(x-x_0-t)},$$

$$I_2:=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk m_l(-k,x)m_l(k,x_0)e^{-ik(x-x_0+t)},$$

$$I_3:=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk e^{-ik(x-x_0+t)}, \quad I_4:=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk e^{ik(x-x_0-t)},$$

$$I_5:=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk[T(k)m_r(k,x)m_l(k,x_0)-1]e^{-ik(x-x_0+t)},$$

$$I_6:=\sum_{j=1}^{N}\varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}.$$

Because of (6.4) we have $I_5+I_6=0$ when $x_0-t-x>0$. Changing the dummy integration variable k to $-k$ in I_2 and I_3 we obtain (6.5). The proof of (6.6) is similar to that of (6.5) and is obtained with the help of (3.4) and (6.3). ■

From (6.5) and (6.6) we get the following antisymmetry properties for Υ_l and Υ_r.

Corollary 6.3: Assume V is real valued and belongs to $L_1^1(\mathbf{R})$. *Then*

$$\Upsilon_l(x,-t;x_0)=-\Upsilon_l(x,t;x_0), \quad t\in(x-x_0,x_0-x),$$

$$\Upsilon_r(x,-t;x_0)=-\Upsilon_r(x,t;x_0), \quad t\in(x_0-x,x-x_0),$$

$$\Upsilon_l(x,-t;x_0)-\Upsilon_r(x,-t;x_0)=\Upsilon_r(x,t;x_0)-\Upsilon_l(x,t;x_0), \quad x,t,x_0\in\mathbf{R}.$$

We remark that the temporal antisymmetry is a key part of the physics underlying wave focusing. It is immediate from Corollary 6.3 that both Υ_l and Υ_r vanish at $t=0$.

Next, we present some results related to the support properties of Υ_l when the potential vanishes on a half line. Similar results hold for Υ_r although they are not listed here. In the next theorem, we show that, if the incident wave focuses to a point lying behind the support of the potential, a gap develops between the wavefront and the tail of the wave.

Theorem 6.4: *Assume V is real valued, belongs to* $L_1^1(\mathbf{R})$, *and vanishes for* $x>0$; *let* $x_0\geqslant 0$. *Then we have the following.*

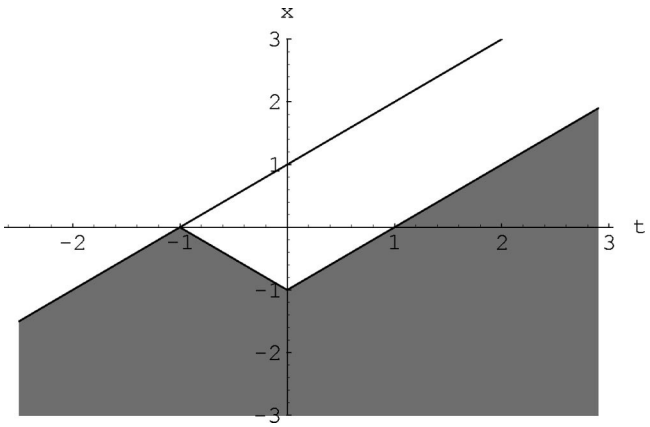

FIG. 1. The support of Υ_1 with $x_0=1$ in Theorem 6.4 is shaded in the tx-plane.

(i) *When* $t\geqslant 0$, *we have* $\Upsilon_1(x,t;x_0)=0$ *for* $x\geqslant -x_0+t$.
(ii) *When* $t\in[-x_0,0]$, *we have* $\Upsilon_1(x,t;x_0)=0$ *for* $x\geqslant -x_0-t$.
(iii) *Consequently, the wavefront* $\delta(x-x_0-t)$ *is in distance* $2x_0$ *ahead of the tail* Υ_1 *for* $t\geqslant 0$.
(iv) *Similarly, the wavefront* $\delta(x-x_0-t)$ *is in distance* $2(x_0+t)$ *ahead of the tail* Υ_1 *for* $t\in[-x_0,0]$.

Proof: The proof will be given by showing that Υ_1 vanishes on the closure of the rectangular region lying below the wavefront and above the shaded region exemplified in Fig. 1. If $V\equiv 0$ for $x>0$, then $m_1(k,x)=1$ for $x\geqslant 0$ and $T(k)m_r(k,x_0)=1+R(k)e^{2ikx_0}$. Thus, from (6.1), with the help of (2.7), we get

$$\Upsilon_1(x,t;x_0)=\hat{R}(x+x_0-t)+\sum_{j=1}^{N} c_{1j}^2 e^{-\kappa_j(x+x_0-t)}, \quad x\geqslant 0. \tag{6.10}$$

Comparing (6.10) with (5.1), we see that $\Upsilon_1(x,t;x_0)=M_1(x+x_0-t)$; hence, with the help of Proposition 5.4, we conclude that $\Upsilon_1(x,t;x_0)=0$ for $x>-x_0+t$ and $x\geqslant 0$. By the continuity of Υ_1 on the line $x=-x_0+t$, as indicated in Theorem 4.5, we get $\Upsilon_1(x,t;x_0)=0$ for $x\geqslant -x_0+t$.

On the other hand, when $x\leqslant 0$, using $T(k)m_r(k,x_0)=1+R(k)e^{2ikx_0}$, from (6.1) we get $\Upsilon_1(x,t;x_0)=I_7+I_8$, where we have defined

$$I_7:=\frac{1}{2\pi}\int_{-\infty}^{\infty} dk[m_1(k,x)-1]e^{ik(x-x_0-t)}, \tag{6.11}$$

$$I_8:=\frac{1}{2\pi}\int_{-\infty}^{\infty} dk R(k)m_1(k,x)e^{ik(x+x_0-t)}+\sum_{j=1}^{N}\varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}. \tag{6.12}$$

For $x>-x_0+t$, from (6.12) we obtain

$$I_8=i\sum_{j=1}^{N}\mathrm{Res}(R,i\kappa_j)m_1(i\kappa_j,x)e^{-\kappa_j(x+x_0-t)}+\sum_{j=1}^{N} c_{1j}^2 m_1(i\kappa_j,x)e^{-\kappa_j(x+x_0-t)}.$$

As mentioned in the proof of Proposition 5.4, we have $\mathrm{Res}(R,i\kappa_j)=ic_{1j}^2$, and hence $I_8=0$ for $x\leqslant 0$ and $x>-x_0+t$. Thus, from (4.1) and (6.11), we see that $\Upsilon_1(x,t;x_0)=K_1(x,x_0+t)$ for $x\leqslant 0$ and $x>-x_0+t$. From the Marchenko equation (5.3), we get

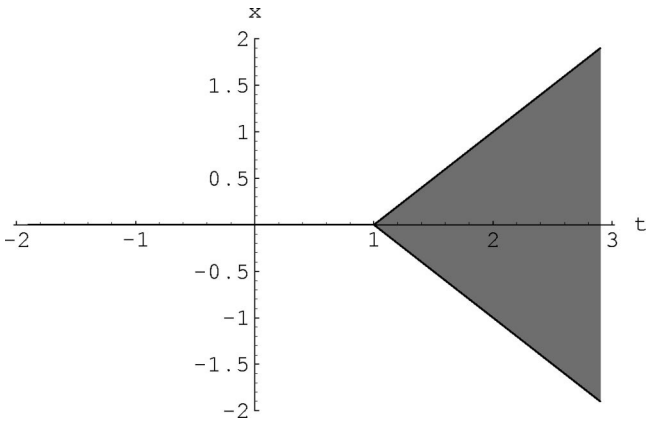

FIG. 2. The support of Υ_1 with $x_0=-1$ in Theorem 6.5 is shaded in the tx-plane.

$$K_1(x,x_0+t)+M_1(x+x_0+t)+\int_x^\infty dsM_1(x_0+t+s)K_1(x,s)=0, \quad x_0+t>x. \tag{6.13}$$

Note that in our region of interest, we have $x+x_0+t>0$, and hence by Proposition 5.4 each of the second and third terms on the left-hand side of (6.13) vanishes. Thus, from (6.13) we conclude $K_1(x,x_0+t)=0$, which in turn gives us $\Upsilon_1(x,t;x_0)=0$ for $x\leqslant 0$ and $x>\max\{-x_0-t,-x_0+t\}$. Again by the continuity of Υ_1 everywhere except at the wavefront of U_1, we get $\Upsilon_1(x,t;x_0)=0$ also on the line segment $x=-x_0+t$ for $t\in[0,x_0]$ and on the segment $x=-x_0-t$ for $t\in[-x_0,0]$. Therefore, we have proved (i) and (ii). Note that (iii) and (iv) directly follow from (i) and (ii). ■

In the next two theorems, when $V\equiv 0$ for $x<0$, we investigate the support properties of the focusing wave U_1.

Theorem 6.5: *Assume V is real valued, belongs to $L_1^1(\mathbf{R})$, and vanishes for $x<0$; let $x_0\leqslant 0$. Then we have the following.*

(i) *At each time $t\leqslant -x_0$, we have $\Upsilon_1(x,t;x_0)=0$.*
(ii) *At each time $t\geqslant -x_0$, we have $\Upsilon_1(x,t;x_0)=0$ for $x\leqslant -x_0-t$.*
(iii) *Consequently, at each fixed time $t>-x_0$, the support of $\Upsilon_1(\cdot,t;x_0)$ is the finite interval $(-x_0-t,x_0+t)$.*

Proof: The proof will be given by showing that the support of Υ_1 is confined to the interior of the region exemplified in Fig. 2. Because U_1 is a causal wave, in the region $x\leqslant \pm x_0\pm t$ we have $x\leqslant 0$; hence $T(k)m_1(k,x)=1+L(k)e^{-2ikx}$, and $m_r(k,x_0)=1$. Thus, from (6.3), with the help of (2.7), we get

$$\Upsilon_1(x,t;x_0)=\hat{L}(-x-x_0-t)+\sum_{j=1}^N c_{rj}^2 e^{\kappa_j(x+x_0+t)}, \quad x\leqslant 0. \tag{6.14}$$

From (5.1) and (6.14) we see that $\Upsilon_1(x,t;x_0)=M_r(x+x_0+t)$, and by Proposition 5.4 we conclude $\Upsilon_1(x,t;x_0)=0$ for $x<-x_0-t$. Because of the continuity of Υ_1 in the tx-plane off the wavefront, we also get $\Upsilon_1(x,t;x_0)=0$ on the line segment $x=-x_0-t$ for $t\geqslant -x_0$. ■

Theorem 6.6: *Assume V is real valued, belongs to $L_1^1(\mathbf{R})$, and vanishes for $x<0$; let $x_0\geqslant 0$. Then we have the following:*

(i) *At each time $t\leqslant 0$, we have $\Upsilon_1(x,t;x_0)=0$ for $x\leqslant -x_0+t$.*
(ii) *At each time $t\geqslant 0$, we have $\Upsilon_1(x,t;x_0)=0$ for $x\leqslant -x_0-t$.*

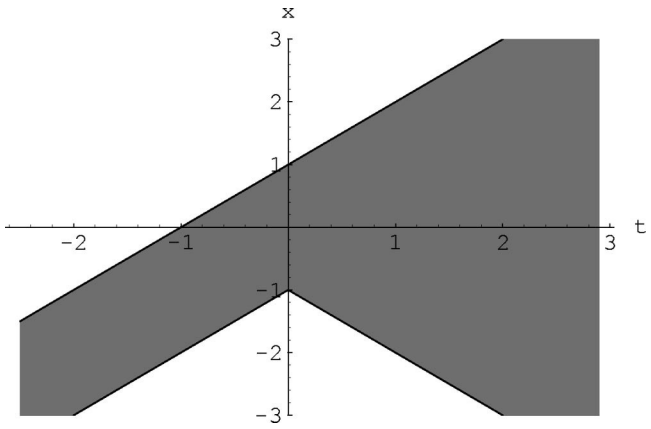

FIG. 3. The support of Υ_1 with $x_0=1$ in Theorem 6.6 is shaded in the tx-plane.

(iii) Consequently, at each fixed $t\leqslant 0$, *the support of* $\Upsilon_1(\cdot,t;x_0)$ *is the finite interval* $(-x_0+t,x_0+t)$. *Similarly, at each fixed* $t\geqslant 0$, *the support of* $\Upsilon_1(\cdot,t;x_0)$ *is the finite interval* $(-x_0-t,x_0+t)$.

Proof: The proof is obtained by using arguments similar to those used in the proof of Theorem 6.4 and by showing that the support of Υ_1 is confined to the interior of the shaded region exemplified in Fig. 3. ■

VII. DISCONTINUITIES IN DERIVATIVES OF FOCUSING WAVES

In this section, under more restrictions on V, we analyze the discontinuities in the spatial and temporal derivatives of our focusing waves, and we present some corollaries of our analysis. First, we show that we can recover $V(x_0)$ remotely by using only the wave that focuses to x_0 with a measurement taken at any fixed specified time $t<-x_0$; this complements our result in Sec. IV on the recovery of $V(x_0)$ from measurements on waves focusing to x_0 and its vicinity. Next, we examine the t-derivative of our focusing waves at $t=0$. Finally, for potentials vanishing on a half line, we derive an identity involving the temporal and spatial derivatives of the solutions to the Marchenko equations. We present the results mainly for the focusing wave incident from the left because the results for the incidence from the right can be obtained analogously.

In our analysis in the section, we put some or all of the following restrictions on V:

(H1) V is real valued and belongs to $L^1_1(\mathbf{R})$.

(H2) V is sectionally continuous with jump discontinuities at $x=a_j$ for $j=1,\ldots,n$.

(H3) V is piecewise continuously differentiable in each of the intervals $(-\infty,a_1)$, $(a_n,+\infty)$, and (a_j,a_{j+1}) with $j=1,\ldots,n-1$.

(H4) V' is integrable in each interval of its continuity.

(H5) V' is piecewise differentiable, and V'' is integrable in each interval it exists.

Paraphrasing, hypothesis (H2) states that V is continuous on $\mathbf{R}$ except perhaps at a finite number of points, and V has finite left and right limits at those points; (H3) is a similar statement for V'. Hypotheses (H4) and (H5) state that V' and V'' exist everywhere except perhaps at a finite number of points; moreover, if we remove those points from $\mathbf{R}$, V' and V'' are integrable on the resulting set.

Define

$$\alpha_l(x):=\int_x^\infty dy V(y), \quad \alpha_r(x):=\int_{-\infty}^x dy V(y), \quad \beta:=\int_{-\infty}^\infty dy V(y), \tag{7.1}$$

$$q_l(k,x):=V(x)+\sum_{a_j>x}[V(a_j^+)-V(a_j^-)]e^{2ik(a_j-x)}, \tag{7.2}$$

$$q_r(k,x) := -V(x) + \sum_{a_j^- < x} [V(a_j^+) - V(a_j^-)] e^{2ik(x-a_j)}. \tag{7.3}$$

In the next proposition we list the large-k asymptotics of the transmission coefficient and the Faddeev functions and their x-derivatives up to the orders needed in (7.15) and (7.16) [cf. p. 163 of Deift and Trubowitz(1979) where some expansions are given up to $o(1/k^2)$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$].

Proposition 7.1: (i) Assume V satisfies hypotheses (H1)–(H4). Then, as $k \to \infty$ in $\overline{\mathbf{C}^+}$ we have

$$T(k) = 1 + \frac{\beta}{2ik} - \frac{\beta^2}{8k^2} + O(1/k^3), \tag{7.4}$$

$$m_l(k,x) = 1 - \frac{\alpha_l(x)}{2ik} - \frac{1}{8k^2}[\alpha_l(x)^2 - 2q_l(k,x)] + O(1/k^3), \tag{7.5}$$

$$m_r(k,x) = 1 - \frac{\alpha_r(x)}{2ik} - \frac{1}{8k^2}[\alpha_r(x)^2 + 2q_r(k,x)] + O(1/k^3). \tag{7.6}$$

(ii) In addition, if V satisfies also hypothesis (H5), then as $k \to \infty$ in $\overline{\mathbf{C}^+}$ we have

$$m_l'(k,x) = \frac{q_l(k,x)}{2ik} + O(1/k^2), \quad m_r'(k,x) = \frac{q_r(k,x)}{2ik} + O(1/k^2). \tag{7.7}$$

Proof: The proof is straightforward. For example, (7.5) is obtained by iterating the integral representation for m_l, see, e.g., Deift and Trubowitz (1979),

$$m_l(k,x) = 1 + \frac{1}{2ik}\int_x^\infty dy [e^{2ik(y-x)} - 1] V(y) m_l(k,y), \tag{7.8}$$

and using integration by parts on $\int_x^\infty dy e^{2ik(y-x)} V(y)$. Differentiating (7.8) with respect to x and using iteration and integration by parts, we obtain the asymptotics for m_l'. Similarly, with the help of the integral representations

$$m_r(k,x) = 1 + \frac{1}{2ik}\int_{-\infty}^x dy [e^{2ik(x-y)} - 1] V(y) m_r(k,y),$$

$$\frac{1}{T(k)} = 1 - \frac{1}{2ik}\int_{-\infty}^\infty dy V(y) m_l(k,y),$$

we obtain the large-k asymptotics for m_r, m_r', and T. ■

Let $\theta(x)$ denote the Heaviside function, and with the help of (7.1)–(7.3) let us define

$$D(x,x_0) := \beta[\alpha_l(x) + \alpha_r(x_0)] - \alpha_l(x)\alpha_r(x_0) - \frac{1}{2}[\beta^2 + \alpha_l(x)^2 + \alpha_r(x_0)^2]. \tag{7.9}$$

Using (7.1) we simplify the right-hand side in (7.9) to obtain

$$D(x,x_0) = -\frac{1}{2}\left[\int_x^{x_0} dy V(y)\right]^2. \tag{7.10}$$

Theorem 7.2: *Assume that V satisfies hypotheses (H1)–(H5). Then, the discontinuous part of $\partial \Upsilon_l(x,t;x_0)/\partial x$ is given by*

$$\frac{1}{4}[V(x_0)-V(x)+D(x,x_0)]\theta(x_0+t-x)-\frac{1}{4}\theta(x_0+t-x)\sum_{a_j>x}[V(a_j^+)-V(a_j^-)]$$
$$\times\theta(x-2a_j+x_0+t)-\frac{1}{4}\theta(x_0+t-x)\sum_{a_j<x_0}[V(a_j^+)-V(a_j^-)]\theta(-x+2a_j-x_0+t), \tag{7.11}$$

where $D(x,x_0)$ is the quantity in (7.10).

Proof: Consider the representation of Υ_1 given in (6.1), from which we get

$$\frac{\partial\Upsilon_1(x,t;x_0)}{\partial x}=\theta(x_0+t-x)\left[I_{10}+I_{11}+\sum_{j=1}^{N}\varphi_j'(x)\varphi_j(x_0)e^{\kappa_j t}\right], \tag{7.12}$$

where we have defined

$$I_{10}:=\frac{i}{2\pi}\int_{-\infty}^{\infty}dk\ k[T(k)m_{\rm l}(k,x)m_{\rm r}(k,x_0)-1]e^{ik(x-x_0-t)}, \tag{7.13}$$

$$I_{11}:=\frac{1}{2\pi}\int_{-\infty}^{\infty}dkT(k)m_{\rm l}'(k,x)m_{\rm r}(k,x_0)e^{ik(x-x_0-t)}. \tag{7.14}$$

When $V\in L_1^1(\mathbf{R})$, it is known that φ_j' is continuous; hence, the summation term within the brackets in (7.12) is continuous in (x,t). From the integrands in (7.13) and (7.14) let us separate the terms that are continuous in (k,x) and integrable in k; by the Lebesgue dominated convergence theorem, the integrals of such terms are continuous in (x,t). Using (7.1)–(7.7) and (7.9), as $k\to\infty$ in $\overline{\mathbf{C}^+}$ we obtain

$$ik[T(k)m_{\rm l}(k,x)m_{\rm r}(k,x_0)-1]=-\frac{1}{2}\int_x^{x_0}dyV(y)+\frac{i}{4(k+i0^+)}[D(x,x_0)+q_{\rm l}(k,x)-q_{\rm r}(k,x_0)]$$
$$+O(1/k^2), \tag{7.15}$$

$$T(k)m_{\rm l}'(k,x)m_{\rm r}(k,x_0)=\frac{q_{\rm l}(k,x)}{2i(k+i0^+)}+O(1/k^2), \tag{7.16}$$

where the $O(1/k^2)$-terms are continuous in (k,x) and integrable in k. When $x<x_0+t$, the $O(1)$-term in (7.15) does not contribute to the integral in (7.13). Using $\int_{-\infty}^{\infty}dke^{ikz}/(k+i0^+)=-2\pi i\theta(-z)$, we evaluate the contribution of the $O(1/k)$-terms in (7.13) and (7.14) to I_{10} and I_{11}, respectively, which, with the help of (7.10), results in (7.11). ■

Let us define

$$G(x,t;x_0):=-\frac{1}{4}[V(x_0)+V(x)+D(x,x_0)]\theta(x_0+t-x)$$
$$-\frac{1}{4}\theta(x_0+t-x)\sum_{a_j>x}[V(a_j^+)-V(a_j^-)]\theta(x-2a_j+x_0+t)$$
$$+\frac{1}{4}\theta(x_0+t-x)\sum_{a_j<x_0}[V(a_j^+)-V(a_j^-)]\theta(-x+2a_j-x_0+t), \tag{7.17}$$

where $D(x,x_0)$ is the quantity in (7.10).

Theorem 7.3: *Assume that V satisfies hypotheses (H1)–(H5). Then, the discontinuous part of $\partial\Upsilon_1(x,t;x_0)/\partial t$ is equal to $G(x,t;x_0)$ defined in (7.17).*

Proof: As in (7.12) we have

$$\frac{\partial \Upsilon_l(x,t;x_0)}{\partial t} = \theta(x_0+t-x)\left[-I_{10} + \sum_{j=1}^{N} \kappa_j \varphi_j(x)\varphi_j(x_0)e^{\kappa_j t}\right]. \tag{7.18}$$

Proceeding as in the proof of Theorem 7.2, we see that the only contribution to the discontinuities comes from the $O(1/k)$-term in (7.13), which gives us (7.17). ■

As a corollary of (7.18), we see that $U_l(x,t;x_0)$ is the solution to (1.1) satisfying the initial conditions $U_l(x,0;x_0)=\delta(x-x_0)$ and

$$\frac{\partial U_l(x,0;x_0)}{\partial t} = \delta'(x-x_0) + \sum_{j=1}^{N} \kappa_j \varphi_j(x)\varphi_j(x_0) - \frac{i}{2\pi}\int_{-\infty}^{\infty} dk\; k[T(k)m_l(k,x)m_r(k,x_0)-1]e^{ik(x-x_0)}. \tag{7.19}$$

With the help of (7.11)–(7.13), it is possible to identify the discontinuities on the right-hand side of (7.19) and hence also in $\partial U_l(x,0;x_0)/\partial t$. The initial value $\partial U_r(x,0;x_0)/\partial t$ can be obtained similarly and its discontinuities can be evaluated explicitly in an analogous manner.

Next, we turn our attention to the inverse scattering problem and describe the recovery of $V(x_0)$ by using only the wave $U_l(x,t;x_0)$ focusing to x_0. Assume that V satisfies hypotheses (H1)–(H5) and that x_0 is a point of continuity of V. As stated below (4.34), we know that the height of the tail Υ_l at the wavefront at any fixed time $t<-x_0$ is given by (4.30). Furthermore, from (7.11) we see that the x-derivative from the left for the tail Υ_l at the wavefront is given by

$$\frac{\partial \Upsilon_l(x_0^- + t,t;x_0)}{\partial x} = \frac{1}{4}[V(x_0)-V(x_0+t)] - \frac{1}{8}\left(\int_{x_0+t}^{x_0} dz V(z)\right)^2. \tag{7.20}$$

Eliminating the integral term in (4.30) and (7.20), we get

$$V(x_0) = V(x_0+t) + 2\Upsilon_l(x_0^- + t,t;x_0)^2 + 4\frac{\partial \Upsilon_l(x_0^- + t,t;x_0)}{\partial x}. \tag{7.21}$$

Note that all of the three terms on the right-hand side of (7.21) can be measured at some moment $t<-x_0$, where x_0+t is a point of continuity for V; in fact, we can even make our measurement when $t\to-\infty$, in which case $V(x_0+t)\to 0$. Thus, $V(x_0)$ can be remotely determined by using only the wave that focuses to x_0.

As a corollary of the arguments leading to (5.19) and (7.21) we obtain the following property for the solution to the Marchenko equation (5.2).

Theorem 7.4: *Assume V satisfies hypotheses (H1)–(H5) and $V\equiv 0$ for $x<0$. Then, for any point $x\in\mathbf{R}$ at which V is continuous, the solution $K_r(x,t)$ of the Marchenko equation (5.2) satisfies*

$$\frac{\partial K_r(x,x^-)}{\partial x} - \frac{\partial K_r(x,x^-)}{\partial t} = K_r(x,x^-)^2, \quad x\in\mathbf{R}. \tag{7.22}$$

Proof: Note that (7.22) holds trivially for all $x\leqslant 0$ because $K_r(x,t)=0$ for $x\leqslant 0$ as indicated above (5.19). From the Marchenko method, it is known that

$$V(x_0) = 2\frac{\partial K_r(x_0,x_0^-)}{\partial x} + 2\frac{\partial K_r(x_0,x_0^-)}{\partial t}, \quad x\in\mathbf{R}. \tag{7.23}$$

From (5.19) we see that $\Upsilon_1(x,t;x_0)=K_r(x_0,x-t)$ for all $x<0$ and $t<-x_0$; hence, we can write (7.21) with $x_0>0$ and $t<-x_0$ as

$$V(x_0)=2K_r(x_0,x_0^-)^2+4\frac{\partial K_r(x_0,x_0^-)}{\partial t}, \quad x_0>0. \tag{7.24}$$

Finally, comparing (7.23) and (7.24), we see that (7.22) also holds for $x>0$. ■

We next present the analog of Theorem 7.4 for K_l without a proof. It can also be obtained from (7.22) by changing the signs of x and t.

Theorem 7.5: *Assume V satisfies hypotheses (H1)–(H5) and $V\equiv 0$ for $x>0$. Then, for any point $x\in\mathbf{R}$ at which V is continuous, the solution $K_l(x,t)$ of the Marchenko equation (5.3) satisfies*

$$\frac{\partial K_l(x,x^+)}{\partial x}-\frac{\partial K_l(x,x^+)}{\partial t}=K_l(x,x^+)^2, \quad x\in\mathbf{R}. \tag{7.25}$$

VIII. EXAMPLES

In this section we illustrate wave focusing, various properties of focusing waves, and the recovery of a potential via wave focusing. An animated example of wave focusing can be found at the web site http://www.msstate.edu/~aktosun/publications.html.

Example 8.1: Consider the wave focusing for

$$V(x)=\theta(-x)\frac{16(\sqrt{2}+1)^2e^{-2\sqrt{2}x}}{[(\sqrt{2}+1)^2e^{-2\sqrt{2}x}-1]^2}.$$

Note that V, being non-negative, does not support any bound states; moreover, it is supported in $(-\infty,0)$ and hence the region $(0,+\infty)$ is the "free region." The corresponding scattering coefficients are rational functions of k, and one can obtain explicitly the scattering coefficients and Jost solutions of (1.2). We have $f_l(k,x)=e^{ikx}$ for $x\geqslant 0$,

$$f_r(k,x)=e^{-ikx}\left[1+\frac{i}{k+\sqrt{2}i}\frac{2\sqrt{2}}{(\sqrt{2}+1)^2e^{-2\sqrt{2}x}-1}\right], \quad x\leqslant 0,$$

$$T(k)=\frac{k(k+\sqrt{2}i)}{(k+i)^2}, \quad L(k)=-\frac{1}{(k+i)^2}\frac{k+\sqrt{2}i}{k-\sqrt{2}i}, \quad R(k)=\frac{1}{(k+i)^2}.$$

Using a contour integration in (4.18), we can evaluate U_l explicitly and verify that U_l focuses to x_0 at time $t=0$. When $x_0>0$, as indicated in Theorem 6.4, a gap develops between the wavefront and the tail, which is illustrated in Fig. 4. When $x_0<0$, the corresponding wave is illustrated in Fig. 5. It can be verified directly that the discontinuity in the tail at the wavefront, the discontinuities in the x-derivative of the tail, and the discontinuities in the t-derivative of the tail agree with the results in (4.30), (7.11), and (7.17), respectively.

Next, we illustrate the recovery of $V(x_0)$ by using the technique described in Sec. IV utilizing (4.35).

Example 8.2: Consider the wave focusing for the potential

$$V(x)=\theta(x)\frac{80(\sqrt{5}+1)(\sqrt{5}+2)e^{2\sqrt{5}x}}{[(\sqrt{5}+1)(\sqrt{5}+2)e^{2\sqrt{5}x}-2]^2}. \tag{8.1}$$

The corresponding scattering coefficients and Jost solutions can be evaluated explicitly as

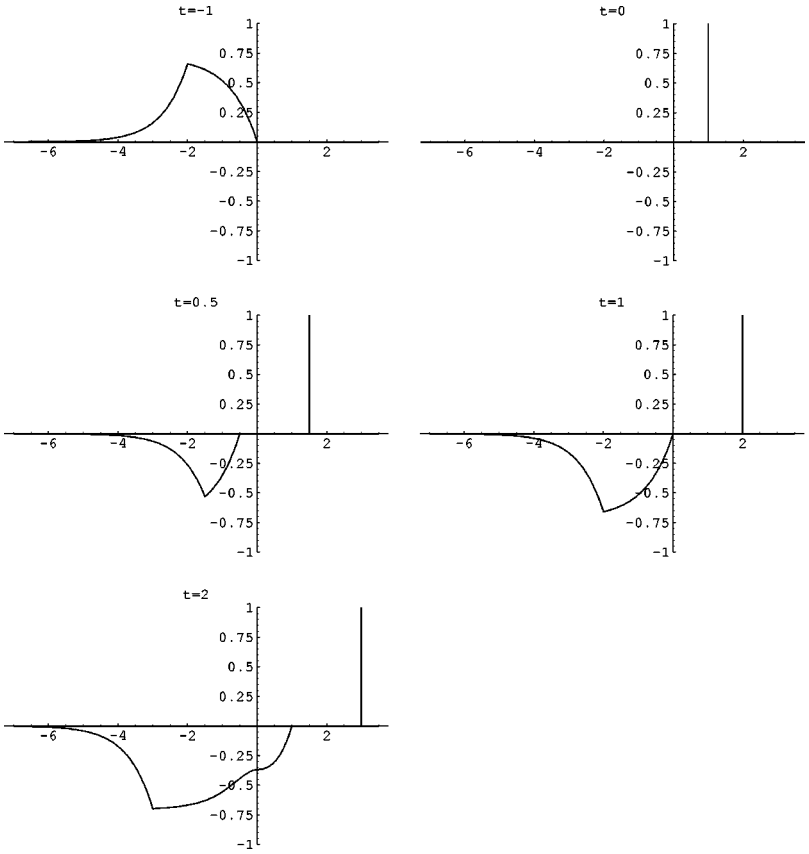

FIG. 4. The focusing wave of Example 8.1 with $x_0=1$ is shown at $t=-1,0,0.5,1,2$.

$$T(k)=\frac{k(k+\sqrt{5}i)}{(k+i)(k+2i)},\quad L(k)=\frac{2}{(k+i)(k+2i)},\quad R(k)=\frac{-2(k+\sqrt{5}i)}{(k+i)(k+2i)(k-\sqrt{5}i)},$$

$$f_{\mathrm{l}}(k,x)=e^{ikx}\left[1+\frac{iE(x)}{k+\sqrt{5}i}\right],\quad x\geqslant 0;\quad f_{\mathrm{r}}(k,x)=e^{-ikx},\quad x\leqslant 0,$$

$$f_{\mathrm{l}}(k,x)=\frac{(k+i)(k+2i)}{k(k+\sqrt{5}i)}e^{ikx}+\frac{2}{k(k+\sqrt{5}i)}e^{-ikx},\quad x\leqslant 0,$$

$$f_{\mathrm{r}}(k,x)=e^{-ikx}\left[1-\frac{iE(x)}{k-\sqrt{5}i}\right]-\frac{2(k+\sqrt{5}i)e^{ikx}}{(k+i)(k+2i)(k-\sqrt{5}i)}\left[1+\frac{iE(x)}{k+\sqrt{5}i}\right],\quad x\geqslant 0,$$

where

$$E(x):=\frac{4\sqrt{5}}{(1+\sqrt{5})(2+\sqrt{5})e^{2\sqrt{5}x}-2}.$$

Using (4.18) it is possible to construct $U_{\mathrm{l}}(x,t;x_0)$ explicitly. Since $V\equiv 0$ when $x<0$, we see that $V(x_0+t)=0$ for any fixed $t<-x_0$. Note that $\Gamma_{\mathrm{l}}(x_0,t)$ given in (4.34) can be computed as $\sqrt{5}-3+E(x_0)$. Then, using (4.35), we obtain $V(x_0)=2E'(x_0)$, agreeing with (8.1).

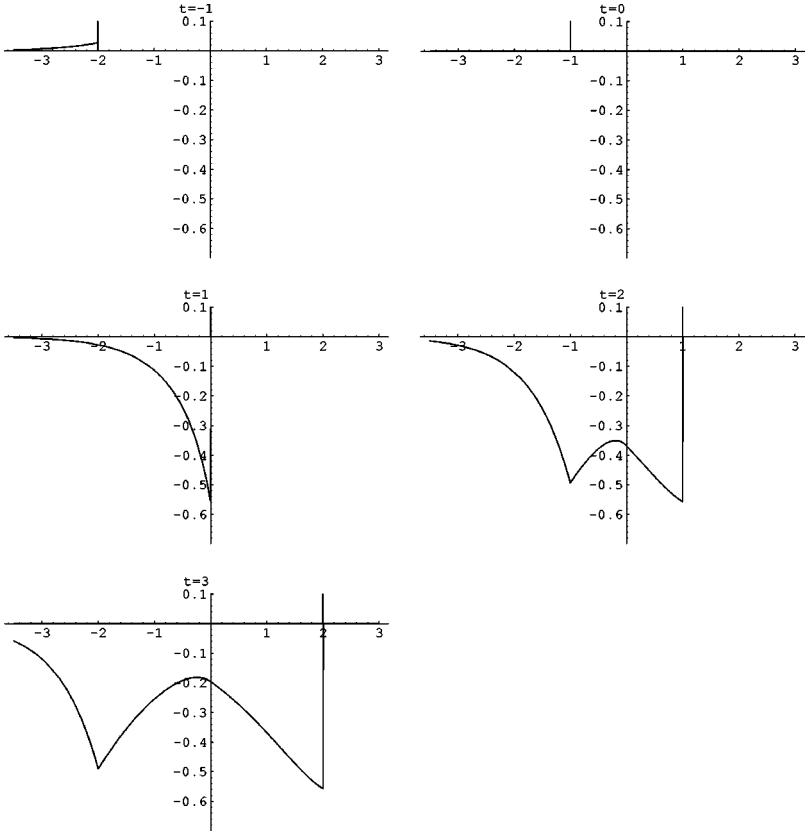

FIG. 5. The focusing wave of Example 8.1 with $x_0=-1$ is shown at $t=-1,0,1,2,3$.

Finally, we illustrate the recovery of $V(x_0)$ by using the technique described in Sec. VII utilizing (7.21).

Example 8.3: Consider the wave focusing for the potential

$$V(x)=-\frac{16c^2e^{2x}}{(2e^{2x}+c^2)^2}, \tag{8.2}$$

where $c>0$ is the bound-state norming constant. The corresponding scattering coefficients are $T(k)=(k+i)/(k-i)$, $L(k)=R(k)=0$, and the Jost solutions for $x\in\mathbf{R}$ are given by

$$f_{\rm l}(k,x)=e^{ikx}\left[1-\frac{2i}{k+i}\,\frac{c^2}{2e^{2x}+c^2}\right],\quad f_{\rm r}(k,x)=e^{-ikx}\left[1-\frac{4i}{k+i}\,\frac{e^{2x}}{2e^{2x}+c^2}\right].$$

Using (4.18) we get

$$U_{\rm l}(x,t;x_0)=\delta(x-x_0-t)+\theta(-x+x_0+t)\,\frac{4c^2e^{x+x_0}(e^t-e^{-t})}{(2e^{2x}+c^2)(2e^{2x_0}+c^2)}.$$

Hence,

$$\Upsilon_{\rm l}(x_0^-+t,t;x_0)=\frac{4c^2e^{t+x_0}(e^t-e^{-t})}{(2e^{2x_0}+c^2)(2e^{2(t+x_0)}+c^2)},$$

$$\lim_{t\to-\infty} \Upsilon_l(x_0^- + t, t; x_0) = -\frac{4e^{x_0}}{2e^{2x_0}+c^2}, \tag{8.3}$$

$$\frac{\partial \Upsilon_l(x_0^- + t, t; x_0)}{\partial x} = \frac{4c^2 e^{2x_0+t}(e^t - e^{-t})(c^2 - e^{2(t+x_0)})}{(2e^{2x_0}+c^2)(2e^{2(t+x_0)}+c^2)^2},$$

$$\lim_{t\to-\infty} \frac{\partial \Upsilon_l(x_0^- + t, t; x_0)}{\partial x} = \frac{4e^{2x_0}}{2e^{2x_0}+c^2}. \tag{8.4}$$

Since $\lim_{t\to-\infty} V(x_0+t)=0$, using (8.3) and (8.4) in (7.21), we can construct $V(x_0)$ explicitly, agreeing with its value obtained from (8.2).

IX. FOCUSING FOR THE VARIABLE-SPEED WAVE EQUATION

In this section we analyze focusing for the variable-speed wave equation given in (9.14) by using the corresponding results for (1.1).

Consider the generalized Schrödinger equation

$$\frac{d^2\psi(k,x)}{dx^2} + k^2 H(x)^2 \psi(k,x) = Q(x)\psi(k,x), \quad x \in \mathbf{R}, \tag{9.1}$$

where Q is real valued and belongs to $L^1_1(\mathbf{R})$, and H is bounded, strictly positive, $H-1 \in L^1(\mathbf{R})$, and $2HH''-3(H')^2 \in L^1_1(\mathbf{R})$. Via the Liouville transformation

$$y = y(x) := \int_0^x dz H(z), \quad \phi(k, y(x)) := \sqrt{H(x)}\,\psi(k,x), \tag{9.2}$$

we can transform (9.1) into the Schrödinger equation

$$\frac{d^2\phi(k,y)}{dy^2} + k^2\phi(k,y) = V(y)\phi(k,y), \quad y \in \mathbf{R}, \tag{9.3}$$

with

$$V(y) = V(y(x)) := \frac{Q(x)}{H(x)^2} + \frac{H''(x)}{2H(x)^3} - \frac{3H'(x)^2}{4H(x)^4}. \tag{9.4}$$

The aforementioned conditions on Q and H guarantee that V is real valued and belongs to $L^1_1(\mathbf{R})$, for which the direct and inverse scattering problems are well understood.

Let $f_l(k,x)$ and $f_r(k,x)$ denote the Jost solutions of (9.1) satisfying the boundary conditions (2.1) and (2.2), respectively. The scattering coefficients for (9.1) are obtained as in (2.3) and (2.4). For the analysis of the scattering and inverse scattering problems for (9.1), see, e.g., Aktosun *et al.* (1992a,b). It is known that the potential $V(y)$ has bound states if and only if $Q(x)$ has bound states. Since $H(x)$ is strictly positive, the mapping $x \mapsto y$ is one-to-one. Thus, for any x_0 there is a unique $y_0 := y(x_0)$, and conversely.

Let us denote the Jost solutions of (9.3) by $g_l(k,y)$ and $g_r(k,y)$, from the left and right, respectively. Let us use $\tau(k)$, $\rho(k)$, and $\ell(k)$ to denote the transmission coefficient and the reflection coefficients from the right and left, respectively, for (9.3). We have, see, e.g., Aktosun *et al.* (1992a),

$$g_l(k,y) = e^{-ikA_+}\sqrt{H(x)}\,f_l(k,x), \quad g_r(k,y) = e^{-ikA_-}\sqrt{H(x)}\,f_r(k,x), \tag{9.5}$$

$$\tau(k) = T(k)e^{ikA}, \quad \ell(k) = L(k)e^{2ikA_-}, \quad \rho(k) = R(k)e^{2ikA_+}, \tag{9.6}$$

where

$$A_{\pm} := \pm \int_0^{\pm\infty} dt[1-H(t)], \quad A := A_- + A_+ .$$

As seen from the first formula in (9.6) the bound states for (9.1) and (9.3) occur simultaneously at the same k-value on the positive imaginary axis, i.e., at the common poles of $T(k)$ and $\tau(k)$ in $\mathbf{C}^+$. We let N denote the number of bound states for (9.1) and let the bound states occur at $k = i\kappa_j$ with $0 < \kappa_1 < \cdots < \kappa_N$.

In terms of the Jost solutions of (9.3), as in (4.1) and (4.2), let us define

$$\tilde{K}_{\rm l}(y,t) := \frac{1}{2\pi} \int_{-\infty}^{\infty} dk[g_{\rm l}(k,y) - e^{iky}]e^{-ikt},$$

$$\tilde{K}_{\rm r}(y,t) := \frac{1}{2\pi} \int_{-\infty}^{\infty} dk[g_{\rm r}(k,y) - e^{-iky}]e^{ikt}.$$

As in (4.4) we have

$$\tilde{K}_{\rm l}(y,t) = 0, \quad t < y; \quad \tilde{K}_{\rm r}(y,t) = 0, \quad t > y.$$

For each fixed $y \in \mathbf{R}$, $\tilde{K}_{\rm l}(y,\cdot)$ and $\tilde{K}_{\rm r}(y,\cdot)$ belong to $L^2(\mathbf{R}) \cap L^1(\mathbf{R})$. They are discontinuous at $t = y$, and as in (4.5) the jumps there are related to V as

$$\tilde{K}_{\rm l}(y,y^+) = \frac{1}{2}\int_y^{\infty} dz V(z), \quad \tilde{K}_{\rm r}(y,y^-) = \frac{1}{2}\int_{-\infty}^{y} dz V(z).$$

Next we present the analog of Theorem 3.1 for (9.1).

Theorem 9.1: *Assume Q and H satisfy the conditions stated below (9.1). Then*

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk T(k) f_{\rm l}(k,x)\, f_{\rm r}(k,x_0) + \sum_{j=1}^{N} \frac{\varphi_j(x)\varphi_j(x_0)}{H(x)H(x_0)} = \frac{\delta(x-x_0)}{H(x)H(x_0)}, \tag{9.7}$$

where $\varphi_j(x)$ are the normalized bound-state wave functions for (9.1) corresponding to the bound states at $k = i\kappa_j$ with $j = 1,\ldots,N$.

Proof: Using (9.5) and (9.6), from (3.6) we get

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk \tau(k) g_{\rm l}(k,y) g_{\rm r}(k,y_0) + \sum_{j=1}^{N} \xi_j(y)\xi_j(y_0) = \delta(y-y_0), \tag{9.8}$$

where $\xi_j(y)$ are the normalized bound-state wave functions for (9.3). Using (9.5) and (9.6), we can write the first term on the left-hand side of (9.8) as

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk \tau(k) g_{\rm l}(k,y) g_{\rm r}(k,y_0) = \frac{\sqrt{H(x)H(x_0)}}{2\pi}\int_{-\infty}^{\infty} dk T(k) f_{\rm l}(k,x) f_{\rm r}(k,x_0). \tag{9.9}$$

As in (2.5) and (2.7), for $j = 1,\ldots,N$ we have

$$\xi_j(y) = \frac{g_{\rm l}(i\kappa_j,y)}{\sqrt{\int_{-\infty}^{\infty} dz g_{\rm l}(i\kappa_j,z)^2}}, \quad \varphi_j(x) = \frac{H(x) f_{\rm l}(i\kappa_j,x)}{\sqrt{\int_{-\infty}^{\infty} dz H(z)^2 f_{\rm l}(i\kappa_j,z)^2}}. \tag{9.10}$$

With the help of (9.5) and (9.10), we see that $\xi_j(y)$ and $\varphi_j(x)$ are related to each other as

$$\xi_j(y)=\frac{\varphi_j(x)}{\sqrt{H(x)}}, \tag{9.11}$$

and thus the summation term on the left-hand side of (9.8) is expressed as

$$\sum_{j=1}^{N}\xi_j(y)\xi_j(y_0)=\sum_{j=1}^{N}\frac{\varphi_j(x)\varphi_j(x_0)}{\sqrt{H(x)H(x_0)}}. \tag{9.12}$$

Moreover, from $dy/dx=H(x)$ and the fact that $y=y_0$ if and only if $x=x_0$, we get

$$\delta(y-y_0)=\frac{\delta(x-x_0)}{\sqrt{H(x)H(x_0)}}. \tag{9.13}$$

Hence, using (9.9), (9.12), and (9.13) in (9.8), we obtain (9.7). ■

Using the Fourier transformation (1.3), we can transform (9.1) into the variable-speed wave equation

$$\frac{\partial^2 w(x,t)}{\partial x^2}-H(x)^2\frac{\partial^2 w(x,t)}{\partial t^2}=Q(x)w(x,t),\quad x,t\in\mathbf{R}, \tag{9.14}$$

where $1/H(x)$ corresponds to the variable wave speed. We are interested in wave focusing for (9.14); in other words, we would like to construct causal solutions to (9.14) incident either from the left or right such that they focus at time $t=0$ to any specified point x_0. In particular, we want to construct solutions to (9.14) satisfying $w(x,0)=\delta(x-x_0)/H(x_0)$.

Let us define

$$W_{\mathrm{l}}(x,t;x_0):=\frac{1}{2\pi}\int_{-\infty}^{\infty}dkT(k)f_{\mathrm{l}}(k,x)f_{\mathrm{r}}(k,x_0)e^{-ikt}+\sum_{j=1}^{N}\frac{\varphi_j(x)\varphi_j(x_0)}{H(x)H(x_0)}e^{\kappa_j t}, \tag{9.15}$$

$$W_{\mathrm{r}}(x,t;x_0):=\frac{1}{2\pi}\int_{-\infty}^{\infty}dkT(k)f_{\mathrm{r}}(k,x)f_{\mathrm{l}}(k,x_0)e^{-ikt}+\sum_{j=1}^{N}\frac{\varphi_j(x)\varphi_j(x_0)}{H(x)H(x_0)}e^{\kappa_j t}, \tag{9.16}$$

where φ_j are the normalized bound-state wave functions given in (9.10).

Theorem 9.2: Assume that Q and H satisfy the conditions stated below (9.1). Then W_{l} is a causal solution to (9.14) that is incident from the left and that focuses to $x=x_0$ when $t=0$. Similarly, W_{r} is a causal solution to (9.14) that is incident from the right and that focuses to $x=x_0$ when $t=0$.

Proof: Since $g_{\mathrm{l}}(k,y)$ is a solution to (9.3), with the help of (9.2), (9.10), and (9.11) we see that W_{l} defined in (9.15) is a solution to (9.14). Using (9.5), (9.6), and (9.12) in (9.15) we get

$$\sqrt{H(x)H(x_0)}W_{\mathrm{l}}(x,t;x_0)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\tau(k)g_{\mathrm{l}}(k,y)g_{\mathrm{r}}(k,y_0)e^{-ikt}+\sum_{j=1}^{N}\xi_j(y)\xi_j(y_0)e^{\kappa_j t}. \tag{9.17}$$

By comparing the right-hand sides of (4.18) and (9.17) and applying Theorem 4.3, we see that the theorem is proved for W_{l}. The proof for W_{r} defined in (9.16) is similarly obtained. ■

We see from Theorem 9.2 that W_{l} consists of the wavefront $\delta(y-y_0-t)/\sqrt{H(x)H(x_0)}$ followed by a tail on the left and that it is incident from the left. Similarly, W_{r} consists of the wavefront $\delta(y-y_0+t)/\sqrt{H(x)H(x_0)}$ followed by a tail on the right and that it is incident from the right.

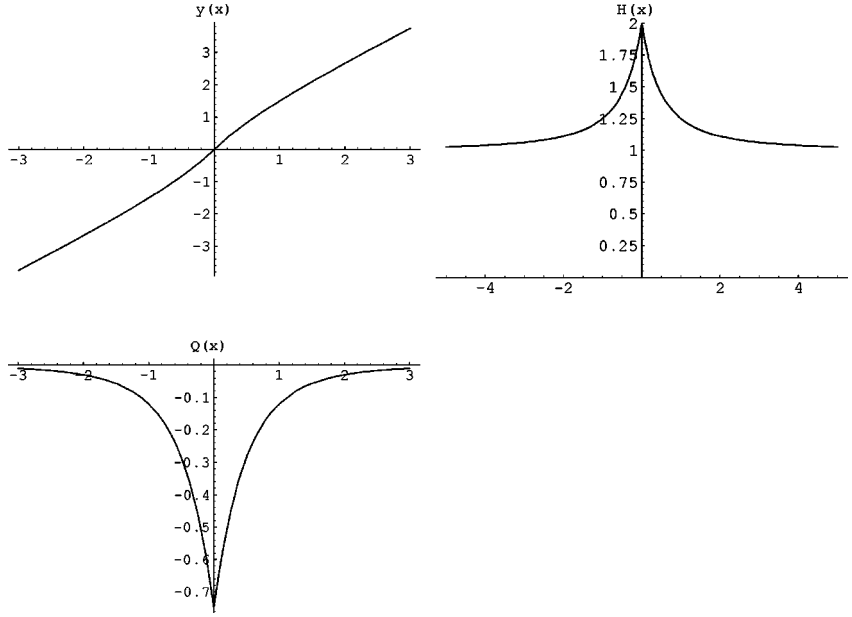

FIG. 6. The plots of $y(x)$, $H(x)$, and $Q(x)$ in Example 9.3.

The Marchenko equations associated with (9.1) were analyzed in Aktosun *et al.* (1992a). Using the results given in Secs. III and IV, it is possible to give various representations for W_l and W_r, similar to those in (4.22), (4.23), (5.13), (5.14), (5.17), and (5.18), and thus obtain the analogs of Theorems 4.5 and 5.3. We let the interested reader work out the details.

Next we present an example of focusing for (9.14).

Example 9.3: Consider

$$y(x)=\theta(-x)\left[x-1+\frac{1}{1-x}\right]+\theta(x)\left[x+1-\frac{1}{x+1}\right],$$

and hence

$$H(x)=\theta(-x)\,\frac{1+(1-x)^2}{(1-x)^2}+\theta(x)\,\frac{1+(1+x)^2}{(1+x)^2}.$$

Note that $H(x)$ is continuous, but $H'(x)$ has a discontinuity at $x=0$. Even though the focusing theory we outlined above is developed under the assumption that H'' exists, it can be extended in a straightforward manner when H'' contains some Dirac delta distributions. We have $H(0)=2$, $H'(0^+)=-2$, $H'(0^-)=2$, and hence H'' contains a delta distribution at $x=0$. Letting

$$Q(x)=\theta(-x)\,\frac{-3}{[1+(1-x)^2]^2}+\theta(x)\,\frac{-3}{[1+(1+x)^2]^2}, \tag{9.18}$$

from (9.4) we get $V(y)=-\delta(y)/2$. In Fig. 6 we show $y(x)$, $H(x)$, and $Q(x)$.

Using (9.5) and (9.6) we obtain

$$T(k)=\frac{4ke^{2ik}}{4k-i},\quad R(k)=\frac{4ie^{2ik}}{4k-i},\quad L(k)=\frac{4ie^{2ik}}{4k-i},$$

$$f_{\rm l}(k,x)=\begin{cases}\dfrac{e^{ik(y-1)}}{\sqrt{H(x)}}, & x\geqslant 0,\\ \left(1+\dfrac{1}{4ik}\right)\dfrac{e^{-ik(y+1)}}{\sqrt{H(x)}}-\dfrac{1}{4ik}\dfrac{e^{ik(y-1)}}{\sqrt{H(x)}}, & x\leqslant 0,\end{cases}$$

$$f_{\rm r}(k,x)=\begin{cases}\left(1+\dfrac{1}{4ik}\right)\dfrac{e^{-ik(y+1)}}{\sqrt{H(x)}}-\dfrac{1}{4ik}\dfrac{e^{ik(y-1)}}{\sqrt{H(x)}}, & x\geqslant 0,\\ \dfrac{e^{-ik(y+1)}}{\sqrt{H(x)}}, & x\leqslant 0.\end{cases}$$

Note that there is a bound state at $k=i/4$. Using (2.7) and (9.11) we get the normalized bound-state wave function as

$$\varphi(x)=\frac{\sqrt{H(x)}}{2}e^{-|y|/4}.$$

If the focusing point x_0 occurs in $[0,+\infty)$, with $y_0:=y(x_0)$ from (9.15) we get

$$W_{\rm l}(x,t;x_0)=\frac{\delta(y-y_0-t)}{\sqrt{H(x)H(x_0)}}+\frac{\theta(-x)w_-(x,t;x_0)+\theta(x)w_+(x,t;x_0)}{4\sqrt{H(x)H(x_0)}},$$

where

$$\begin{aligned}w_-(x,t;x_0):=&-\theta(-y+y_0+t)+\theta(y+y_0+t)+\theta(-y-y_0+t)-\theta(y-y_0+t)\\&+\theta(y-y_0+t)e^{(y-y_0+t)/4},\end{aligned}$$

$$w_+(x,t;x_0):=\theta(-y-y_0+t)e^{-(y+y_0-t)/4}.$$

It can directly be verified that $W_{\rm l}(x,0;x_0)=\delta(x-x_0)/[H(x)H(x_0)]$. This wave is illustrated in Fig. 7.

Now let us consider a slight modification of the above example.

Example 9.4: Suppose that $y(x)$ and hence $H(x)$ are as in Example 9.3. Let us assume that $Q(x)$ is given by

$$Q(x)=\delta(x)+\theta(-x)\frac{-3}{[1+(1-x)^2]^2}+\theta(x)\frac{-3}{[1+(1+x)^2]^2},$$

and hence differs from (9.18) by a delta distribution at $x=0$. From (9.4) it follows that $V(y)=0$ for all $y\in\mathbf{R}$, and hence $\tau(k)=1$ and $\rho(k)=\not{\ell}(k)=0$. Thus, we have a reflectionless case and there are no bound states. In this case, from (9.5) and (9.6) we get $T(k)=e^{2ik}$, $R(k)=L(k)=0$, and

$$f_{\rm l}(k,x)=\frac{e^{ik(y-1)}}{\sqrt{H(x)}},\quad f_{\rm r}(k,x)=\frac{e^{-ik(y+1)}}{\sqrt{H(x)}}.$$

Since Q contains a delta distribution, $f_{\rm l}'$ and $f_{\rm r}'$ are discontinuous in x at $x=0$. Using (9.15) we obtain

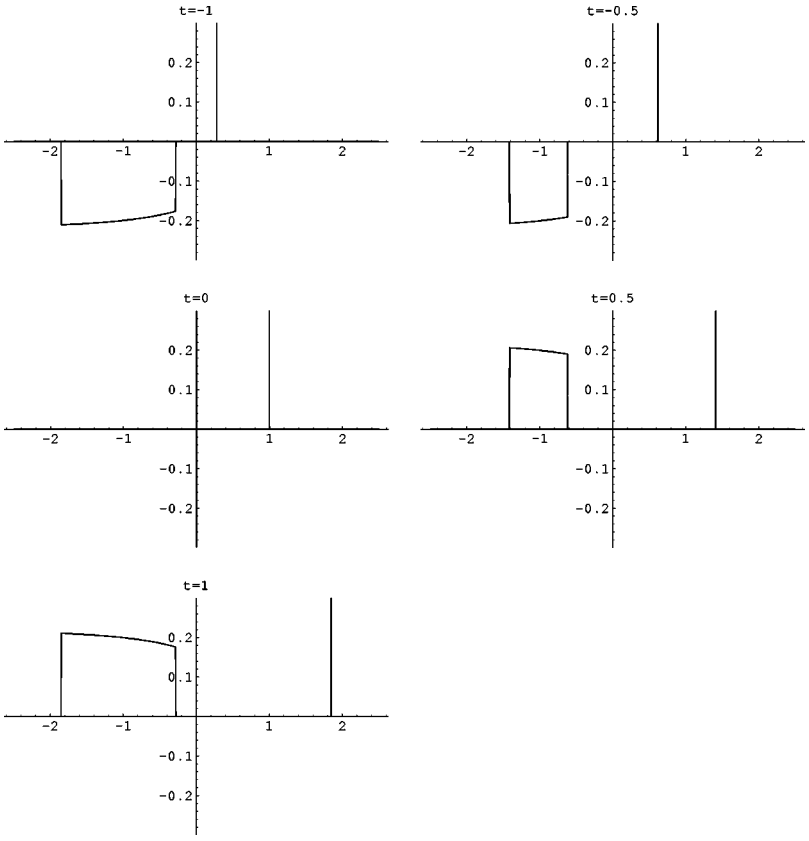

FIG. 7. The focusing wave of Example 9.3 with $x_0=1$ is shown at $t=-1,-0.5,0,0.5,1$.

$$W_1(x,t;x_0)=\frac{\delta(y-y_0-t)}{\sqrt{H(x)H(x_0)}}.$$

Thus, the wave W_1 is always focused, and there is no tail following the wave front due to the fact that there is no reflection.

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The resonance spectrum of the cusp map in the space of analytic functions

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We prove that the Frobenius–Perron operator U of the cusp map $F:[-1,1] \to [-1,1]$, $F(x)=1-2\sqrt{|x|}$ (which is an approximation of the Poincaré section of the Lorenz attractor) has no analytic eigenfunctions corresponding to eigenvalues different from 0 and 1. We also prove that for any $q \in (0,1)$ the spectrum of U in the Hardy space in the disk $\{z \in \mathbb{C}: |z-q|<1+q\}$ is the union of the segment $[0,1]$ and some finite or countably infinite set of isolated eigenvalues of finite multiplicity. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1483895]

I. INTRODUCTION

The so-called cusp map[1]

$$F:[-1,1]\to[-1,1], \quad F(x)=1-2\sqrt{|x|}$$

is an approximation of the Poincaré section of the Lorenz attractor.[2,3] This map is ergodic.[4] The unique absolutely continuous invariant probability measure μ has density $\rho(x)=(1-x)/2$.[1]

The Frobenius–Perron operator (F.P.O.) U of F is the adjoint of the Koopman operator V (Ref. 5) in the Hilbert space $L_2([-1,1],\mu)$:

$$Vf(x)=f(F(x)),$$

$$Uf(x)=\frac{1}{2}\left(1-\frac{(1-x)^2}{4}\right)f\left(\frac{(1-x)^2}{4}\right)+\frac{1}{2}\left(1+\frac{(1-x)^2}{4}\right)f\left(-\frac{(1-x)^2}{4}\right). \tag{1}$$

The spectral analysis of the F.P.O. in different function spaces is useful for the probabilistic approach to nonlinear dynamics. The spectrum of the F.P.O. known also as resonance spectrum gives estimates on the decay of correlation functions, see, e.g., Refs. 5–7. The spectral decomposition of the Koopman and Frobenius–Perron operators acquires meaning in locally convex topological spaces and allows for probabilistic prediction.[8–11]

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The cusp map is not expanding.[6] In Refs. 12–14, the following family of maps depending analytically on the parameter $\varepsilon \in (0,1/2]$ is introduced and studied:

$$F_\varepsilon : [-1,1] \to [-1,1], \quad F_\varepsilon(x) = \frac{1-\sqrt{1-4\varepsilon(1-\varepsilon-2|x|)}}{2\varepsilon}, \quad \text{for } \varepsilon \in (0,\tfrac{1}{2}]. \tag{2}$$

This family consists of piecewise analytic expanding maps and has the cusp map as the limit case for $\varepsilon = \frac{1}{2}$. For any map (2), the spectrum of the F.P.O. in the space of C^∞ functions consists of a sequence of eigenvalues of finite multiplicity converging to 0, and the corresponding eigenfunctions are analytic.[15,6] The divergence of the eigenfunctions as the maps (2) approach the cusp map has been observed numerically.[13,14,16] These numerical results indicate that the F.P.O. (1) has no analytic eigenfunctions corresponding to eigenvalues different from 0 or 1. In the present article we give an analytic proof of this fact. Our result confirms the reliability of the numerical works.[13,14,16]

The spectral properties of the F.P.O. of piecewise analytic maps with one neutral fixed point (i.e., fixed point with derivative equal to 1; this is the point $x=-1$ for the cusp map) have been addressed by Rugh.[17] For each map satisfying certain properties, Rugh has constructed a map-dependent Banach space of functions, analytic everywhere except at the neutral fixed point. The spectrum of the Frobenius–Perron operator in this Banach space is the union of the segment $[0,1]$ and some isolated eigenvalues of finite multiplicity. However, Rugh's results do not specify the spectrum of the F.P.O. in the space of everywhere analytic functions. Moreover, the cusp map does not satisfy the properties of the class of maps considered by Rugh as a result of the cusp singularity. Nevertheless, we prove in this article that for any $q \in (0,1)$ the spectrum of the F.P.O. (1) in the usual Hilbert Hardy space in the disk $\{z \in \mathbb{C}: |z-q| < 1+q\}$ is the union of the segment $[0,1]$ and a finite or countable set of isolated eigenvalues of finite multiplicity.

The article is organized as follows. In Sec. II, we summarize in Theorems 1–4 our results about spectra of the operator U, and derive Theorems 1 and 2. We prove auxiliary lemmas in Sec. III, while the main proofs are presented in Secs. IV and V.

II. THE SPECTRUM OF THE F.P.O.

We shall use the following notations. $\mathcal{A}$ is the space of real-analytic functions $f:[-1,1]\to\mathbb{C}$ and $\mathcal{E}$ is the space of entire functions of one complex variable (endowed with their natural topologies[18]). $\mathcal{P}$ is the space of polynomials of one complex variable. As usual in algebra, we assume that the degree of zero polynomial is -1.

The spectral structure of the F.P.O. in the spaces $\mathcal{A}$ and $\mathcal{E}$ is given by the following two theorems.

Theorem 1: *The spectra of both operators $U_\mathcal{E} = U|_\mathcal{E}: \mathcal{E}\to\mathcal{E}$ and $U_\mathcal{A} = U|_\mathcal{A}: \mathcal{A}\to\mathcal{A}$ coincide with the whole complex plane.*

Theorem 2: *(I) The point spectra of both operators $U_\mathcal{E}$ and $U_\mathcal{A}$ coincide with the two-point set $\{0,1\}$. The eigenvalue 1 is simple and the eigenvalue 0 has infinite multiplicity for both operators.*

(II) Let $f \in \mathcal{A}$. Then $Uf \equiv 0$ if and only if $f(x) \equiv (1+x)g(x)$ for all $x \in [-1,1]$, where $g \in \mathcal{A}$ is odd.

(III) Let $\lambda \in \mathbb{C}$, $f \in \mathcal{A}$, $n \in \mathbb{N}$ and $(U-\lambda I)^n f = 0$ (where I is the identity operator).

(i) If $\lambda \notin \{0,1\}$, then $f=0$.
(ii) If $\lambda = 1$, then f is constant.

As we have already mentioned, Rugh's theorem[17] cannot be applied for the cusp map. Moreover, one cannot use the technique of Rugh's proof to prove a similar theorem for the cusp map. Indeed, the key element of Rugh's proof is a holomorphic function φ, defined in an open simply connected set, containing all points of the segment except the neutral fixed point such that $\varphi \circ \xi \circ \varphi^{-1}(z) \equiv z+1$, where ξ is a branch of the inverse map containing the neutral fixed point

[$\xi(z)=-(1-z)^2/4$ for the cusp map]. Such a map φ obviously does not exist if ξ' vanishes somewhere on the segment, which is the case for the cusp map since $\xi'(1)=0$. Nevertheless, using similar ideas but quite different technique, we prove that U has the spectral structure as in Rugh's theorem in appropriate Hardy spaces. The definitions of the Hardy spaces H^2 in the unit disk and in the upper half-plane $\{z:\mathrm{Im}\, z\geqslant 0\}$ can be found, e.g., in Ref. 19, Chaps. 3 and 8. These spaces are separable Hilbert spaces.

Theorem 3: *Let $q\in(0,1)$ and X be the Hardy space H^2 in the disk $\{z\in\mathbb{C}:|z-q|<1+q\}$. Then U is a bounded operator on the Hilbert space X and the spectrum of $U|_X:X\to X$ is the union of the segment $[0,1]$ and a finite or countable set of isolated eigenvalues of finite multiplicity.*

The proof of Theorem 3 is given in Sec. V. The Hardy spaces in any other disk or half-plane are the results of appropriate linear change of variables applied to the Hardy space in the unit disk or the upper half-plane.

For the sake of completeness we formulate here the following theorem proved in Ref. 16.

Theorem 4: *The spectrum of the operator $U|_X:X\to X$, where X is either $L_p([-1,1],\mu)$ $(1\leqslant p\leqslant+\infty)$ or $C^k[-1,1]$ $(k=0,1,\ldots,\infty)$, is the closed unit disk. The point spectrum of $U|_X$ is the set $\{z\in\mathbb{C}:|z|<1\}\cup\{1\}$. The eigenspace corresponding to the eigenvalue 1 is the one dimensional space of constants. The eigenspace corresponding to the eigenvalues $\{z:|z|<1\}$ is infinite dimensional.*

For the proof of Theorems 1 and 2 we need the following.

Proposition: (I) Let $\lambda\in\mathbb{C}\setminus\{0\}$, $g\in\mathcal{E}$, $f\in\mathcal{A}$ and

$$Uf(x)=\lambda f(x)+g(x), \tag{3}$$

for all $x\in[-1,1]$. Then $f\in\mathcal{E}$.

(II) If additionally $g\in\mathcal{P}$, then $f\in\mathcal{P}$ and $\deg f\leqslant\deg g+1$.

(III) If $g\in\mathcal{P}$ and $\deg g=4k+1$, $k=0,1,\ldots$, then the functional equation (3) has no solutions in $\mathcal{A}$.

The proof of the Proposition is given in Sec. IV.

Proof of Theorem 1: The number 0 is an eigenvalue of $U_{\mathcal{A}}$ and $U_{\mathcal{E}}$. For example, $Uf=0$ if $f(x)=(1+x)x$. Therefore, the number 0 belongs to the spectra of these operators. Let $\lambda\in\mathbb{C}\setminus\{0\}$. According to the proposition, the functional equation (3) has in the space $\mathcal{P}$ no solutions for g with degree of the form $4k+1$. Thus, the functional equation $Uf(x)=\lambda f(x)+x$ has no analytic solutions. Therefore, the function $g(x)=x$ does not belong to the image of the operator $U_{\mathcal{A}}-\lambda I$ (and to the smaller image of $U_{\mathcal{E}}-\lambda I$) for any $\lambda\in\mathbb{C}\setminus\{0\}$. Hence, operators $U_{\mathcal{A}}-\lambda I$ and $U_{\mathcal{E}}-\lambda I$ are non-invertible. Therefore the spectra of $U_{\mathcal{A}}$ and $U_{\mathcal{E}}$ coincide with the whole complex plane.

Proof of Theorem 2: Let $z\in\mathbb{C}\setminus\{0\}$, $c\in\mathbb{C}$ and $f\in\mathcal{A}$. The proposition implies that

$$\text{if } Uf-zf\equiv c, \quad \text{then } f \text{ is a constant.} \tag{4}$$

Let $\lambda\in\mathbb{C}$, $\lambda\neq 0$, $f\in\mathcal{A}$ and $(U-\lambda I)^n f=0$. Relation (4) implies consequently that the functions $h_1=(U-\lambda I)^{n-1}f$, $h_2=(U-\lambda I)^{n-2}f,\ldots,$ $h_{k-1}=(U-\lambda I)f$, $h_k=f$ are constants. In particular, $f\equiv a$ for some $a\in\mathbb{C}$. Since $U1=1$, we have that $0=(U-\lambda I)^n f=(1-\lambda)^n\cdot a$. Therefore either $\lambda=1$ or $f=0$. This proves part III of the theorem.

Let now $f\in\mathcal{A}$. According to (1), the equality $Uf=0$ can be written in the form

$$\left(1-\frac{(1-x)^2}{4}\right)f\left(\frac{(1-x)^2}{4}\right)+\left(1+\frac{(1-x)^2}{4}\right)f\left(-\frac{(1-x)^2}{4}\right)=0, \tag{5}$$

$x\in[-1,1]$. For $x=-1$ the equality (5) implies that $f(-1)=0$. Therefore $f(x)\equiv(1+x)g(x)$ for some $g\in\mathcal{A}$. Substituting $(1+x)g(x)$ instead of $f(x)$ into (5), we obtain

$$\left(1-\frac{(1-x)^4}{16}\right)\left(g\left(\frac{(1-x)^2}{4}\right)+g\left(-\frac{(1-x)^2}{4}\right)\right)=0 \tag{6}$$

for $x\in[-1,1]$. Denoting $y=(1-x)^2/4$, we arrive to $g(y)=g(-y)$ for $y\in[0,1)$. Hence, g is odd.

Suppose now that $f(x)\equiv(1+x)g(x)$ for odd $g\in\mathcal{A}$. This implies the validity of (6) and therefore (5), which is equivalent to $Uf=0$. Part II of the theorem is proved. Part I follows immediately from parts II and III. ■

III. ANALYTIC CONTINUATION OF EIGENFUNCTIONS

First, we introduce some notations, which we shall use in Secs. III and IV without additional comments. Let λ, g, and f be as in the proposition. For $z\in\mathbb{C}$ and $r\in(0,+\infty)$ we denote

$$D(z,r)=\{w\in\mathbb{C}:|w-z|<r\},\quad \overline{D}(z,r)=\{w\in\mathbb{C}:|w-z|\leqslant r\}.$$

By $\mathbb{C}_-$ we denote the set $\mathbb{C}\setminus(-\infty,0)$. We reserve the symbol $\sqrt{z}$ for the "positive" branch of the square root on the set $\mathbb{C}_-$, i.e., $\sqrt{z}=\sqrt{r}e^{i\varphi/2}$, where $z=re^{i\varphi}$, $-\pi<\varphi<\pi$.

For an infinite connected subset $A\subseteq\mathbb{C}$ we say that a function $\varphi:A\to\mathbb{C}$ is analytic if φ admits an analytic extension to some open set, containing A. In particular, $\mathcal{A}$ is the space of all functions analytic on $[-1,1]$. For a connected set $A\subseteq\mathbb{C}$ and a subset $B\subseteq A$, having at least one limit point in A, we say that a function $\varphi:B\to\mathbb{C}$ is analytic on A if φ admits a (unique) analytic extension on A. We shall also denote by φ the extension.

We shall show that the function f admits an analytic extension to the disk $D(0,2+\sqrt{3})$ in several steps.

Lemma 1: Let A and B be subsets of $\mathbb{C}$, $\varphi_1:A\to\mathbb{C}$ and $\varphi_2:B\to\mathbb{C}$ be analytic functions, and $M\subseteq A\cap B$ be a set having at least one limit point in $A\cap B$. Let also the set $A\cap B$ be connected and $\varphi_1|_M\equiv\varphi_2|_M$. Then the function

$$\varphi:A\cup B\to\mathbb{C},\quad \varphi(z)=\begin{cases}\varphi_1(z) & \text{if } z\in A;\\ \varphi_2(z) & \text{if } z\in B\end{cases}$$

is well defined and analytic on $A\cup B$.

Proof: Since M has a limit point in the connected set $A\cap B$, then according to the uniqueness theorem[20] $\varphi_1|_{A\cap B}\equiv\varphi_2|_{A\cap B}$. Therefore φ is well defined. Analyticity of φ follows from analyticity of φ_1 and φ_2. ■

Lemma 2: The analyticity of f on $\overline{D}(0,c)$ $(c\geqslant 1)$ implies the analyticity of f on $\overline{D}(0,c)\cup\overline{D}(1,2\sqrt{c})$.

Proof: Let f be analytic on $\overline{D}(0,c)$. Consider $h:\overline{D}(1,2\sqrt{c})\to\mathbb{C}$, $h(z)=(Uf(z)-g(z))/\lambda$. Clearly h is well defined and analytic. Since (3) is valid on $[-1,1]$, we have that $h(z)=f(z)$ for $z\in[-1,1]$. Lemma 1 implies that the function

$$q(y)=\begin{cases}f(y) & \text{if } y\in\overline{D}(0,c),\\ h(y) & \text{if } z\in\overline{D}(1,2\sqrt{c}),\end{cases}$$

is well defined and analytic on $\overline{D}(0,c)\cup\overline{D}(1,2\sqrt{c})$. This is the desired analytic extension of f. ■

Lemma 3: The function f is analytic on the closed disk $\overline{D}(1,2)$ and the functional equation (3) is valid for all $x\in\overline{D}(1,2)$.

Proof: It suffices to show that f is analytic on $\overline{D}(1,2)$ [the validity of the functional equation (3) for all $x\in\overline{D}(1,2)$ follows then from the uniqueness theorem[20]]. For this goal it suffices to show that f is analytic on $\overline{D}(0,1)$. Analyticity on $\overline{D}(1,2)$ then follows from Lemma 2. For $a\in(0,1]$ let

$$K_a=\{z\in\overline{D}(0,1):|\operatorname{Im} z|<a\},\quad \overline{K_a}=\{z\in\overline{D}(0,1):|\operatorname{Im} z|\leqslant a\}.$$

Suppose that f is not analytic on $\overline{D}(0,1)$. Let us denote

$$a=\sup\{b\in(0,1): f \text{ is analytic on } K_b\}.$$

Then $a\in(0,1]$, f is analytic on K_a and f is not analytic on $\overline{K_a}$.

Let $z\in\overline{K_a}$, $x=\operatorname{Re} z$, $y=\operatorname{Im} z$ and $w=(1-z)^2/4$. Since $|z|\leqslant 1$, we have that $|w|\leqslant(1+|z|)^2/4\leqslant 1$. Since $x^2+y^2\leqslant 1$ and $|y|\leqslant a$ we have that $|\operatorname{Im} w|=|(x-1)y|/2\leqslant a|x-1|/2$. Therefore $|\operatorname{Im} w|\leqslant a$. Moreover, $|\operatorname{Im} w|=a$ if and only if $x=-1$ and $|y|=a$. But then $|z|=\sqrt{1+a^2}>1$. Hence, $|\operatorname{Im} w|<a$. Thus, we have shown that

$$\pm(1-z)^2/4\in K_a \quad \text{for any} \quad z\in\overline{K_a}. \tag{7}$$

Formulas (7) and (1) imply that the function $h(z)=(Uf(z)-g(z))/\lambda$ is well defined and analytic on $\overline{K_a}$. The equation (3) implies that $f(x)=h(x)$ for $x\in[-1,1]$. Therefore h is an analytic continuation of f, i.e., f is analytic on $\overline{K_a}$. This contradiction completes the proof. ■

Lemma 4: (I) Let $c\in[2,+\infty)$, $z\in\overline{D}(-1,c)\setminus D(1,c)$. *Then* $1-2\sqrt{-z}\in\overline{D}(-1,c)$.

(II) Let $a\in[3,+\infty)$, $z\in\overline{D}(0,a)$, $\operatorname{Re} z\geqslant 0$. *Then* $w,u\in D(0,a)$, *where* $w=2\sqrt{z}-1$ *and* $u=z-w$.

Proof: (I) According to the maximum principle,[20] it suffices to show that

$$\sqrt{z}\in\overline{D}(1,c/2) \quad \text{for any} \quad z\in\partial M, \tag{8}$$

where ∂M is the boundary of the set $M=\{z\in\overline{D}(1,c):\operatorname{Re} z\geqslant 0\}$. Clearly (8) is equivalent to

$$\sqrt{z}\in\overline{D}(1,c/2) \quad \text{for any} \quad z\in\Gamma_1=\{it: t\in[-\sqrt{c^2-1},\sqrt{c^2-1}]; \tag{9}$$

$$\sqrt{z}\in\overline{D}(1,c/2) \quad \text{for any} \quad z\in\Gamma_2=\{z\in\mathbb{C}: |z-1|=c,\ \operatorname{Re} z\geqslant 0\}. \tag{10}$$

Parametrizing $z\in\Gamma_2$ by polar coordinates $z=re^{i\varphi}$, we obtain that (9) and (10) are equivalent to

$$\max\{t+1-\sqrt{2t}: t\in[0,\sqrt{c^2-1}]\}\leqslant c^2/4; \tag{11}$$

$$r+1\leqslant 2\sqrt{r}\cos(\varphi/2)+c^2/4 \ \text{ if } \ r^2-2r\cos\varphi=c^2-1, \quad \varphi\in[-\pi/2,\pi/2], \tag{12}$$

respectively. Since $r^2-2r\cos\varphi=c^2-1$, inequality from (12) is equivalent to

$$c^4/16+c^2(\sqrt{r}\cos(\varphi/2)-1)\geqslant 0.$$

As r and $\cos(\varphi/2)$ are decreasing with respect to $\varphi\in[0,\pi/2]$ and the function $t+1-\sqrt{2t}$ on the segment $[0,\sqrt{c^2-1}]$ takes the maximal value for $t=\sqrt{c^2-1}$, we obtain that inequalities (11) and (12) are respectively equivalent to

$$4\alpha^4-8\alpha^2+8\alpha-3\geqslant 0 \quad \text{for} \quad \alpha\in[(3/4)^{1/4},+\infty); \tag{13}$$

$$4\alpha^4+16\alpha-15\geqslant 0 \quad \text{for} \quad \alpha\in[(3/4)^{1/4},+\infty). \tag{14}$$

Since $4\alpha^4-8\alpha^2+8\alpha-3=(2\alpha^2+2\alpha-3)(2\alpha^2+2\alpha+1)$ and $4\alpha^4+16\alpha-15=(2\alpha^2+2\alpha-3)(2\alpha^2-2\alpha+5)$, the number $(\sqrt{7}-1)/2<(3/4)^{1/4}$ is the maximal real zero of both polynomials $4\alpha^4-8\alpha^2+8\alpha-3$ and $4\alpha^4+16\alpha-15$. This proves (13) and (14), which imply (8).

(II) We have to prove that $|w|<a$ and $|u|<a$. According to the maximum principle, it suffices to verify this for $z\in\Gamma$, where $\Gamma=\Gamma_1\cup\Gamma_2$, $\Gamma_1=\{it: t\in[-a,a]\}$ and $\Gamma_2=\{ae^{i\varphi}: \varphi\in[-\pi/2,\pi/2]\}$.

For $z\in\Gamma_1$ we have

$$|w|^2=4|t|-2\sqrt{2|t|}+1, \quad |u|^2=t^2-2\sqrt{2}|t|^{3/2}+4|t|-2\sqrt{2}|t|^{1/2}+1.$$

For $z \in \Gamma_2$ we have

$$|w|^2 = 4a + 1 - 4\sqrt{a}\cos(\varphi/2),$$

$$|u|^2 = a^2 - 4a^{3/2}\cos(\varphi/2) + 4a + 2a\cos\varphi - 4a^{1/2}\cos(\varphi/2) + 1.$$

Differentiating these functions with respect to t and φ, we find that both $|u|^2$ and $|w|^2$ for $z \in \Gamma_1$ are maximal when $t = \pm a$ and that both $|u|^2$ and $|w|^2$ for $z \in \Gamma_2$ are maximal when $\varphi = \pm \pi/2$. Thus, in any case,

$$|w|^2 \leqslant 4a - 2\sqrt{2a} + 1 \quad \text{and} \quad |u|^2 \leqslant a^2 - 2\sqrt{2}a^{3/2} + 4a - 2\sqrt{2}a^{1/2} + 1. \tag{15}$$

Hence, it suffices to verify that

$$a^2 - 4a + 2\sqrt{2a} - 1 > 0 \quad \text{and} \quad 2\sqrt{2}a^{3/2} - 4a + 2\sqrt{2}a^{1/2} - 1 > 0 \tag{16}$$

for $a \geqslant 3$. Both functions from (16) are increasing for $a \geqslant 3$. Hence, we should only prove (16) for $a = 3$, which is a simple arithmetic exercise. ■

Lemma 5: Let $c \in [2, +\infty)$. Then the analyticity of f on $\overline{D}(1,c)$ implies the analyticity of f on $\overline{D}(1,c) \cup \overline{D}(-1,c)$.

Proof: Let f be analytic on $\overline{D}(1,c)$. Pick $\varepsilon > 0$ such that f is analytic on $\overline{D}(1,c+\varepsilon)$ and let

$$\begin{gathered} S_0 = \overline{D}(1,c+\varepsilon) \cap (\overline{D}(1,c) \cup \overline{D}(-1,c)), \\ S_{n+1} = S_n \cup \{z \in \overline{D}(-1,c) : 1 - 2\sqrt{-z} \in S_n\} = S_n \cup (\{-(1-w)^2/4 : w \in S_n\} \cap \overline{D}(-1,c)). \end{gathered} \tag{17}$$

Evidently f is analytic on S_0. It is easy to see that S_n, $n = 0,1,2...$, is an increasing sequence of subsets of $\overline{D}(1,c) \cup \overline{D}(-1,c)$.

First, we shall show that analyticity of f on S_n implies analyticity of f on S_{n+1}. Let f be analytic on S_n. Consider the function $h : A_n \to \mathbb{C}$,

$$h(z) = \frac{1+z}{z-1} f(-z) + \frac{2\lambda}{1-z} f(1 - 2\sqrt{-z}) + \frac{2}{1-z} g(1 - 2\sqrt{-z}), \tag{18}$$

where $A_n = \{z \in \overline{D}(-1,c) : z \notin [0, +\infty), 1 - 2\sqrt{-z} \in S_n\}$. Clearly h is well defined and analytic. Moreover, from (3) and the definition of h it follows that $h|_{(-1,0)} = f|_{(-1,0)}$. Lemma 1 implies that the function

$$q : S_{n+1} = A_n \cup S_n \to \mathbb{C}, \quad q(z) = \begin{cases} f(z) & \text{if } z \in S_n, \\ h(z) & \text{if } z \in A_n, \end{cases}$$

is well defined and is an analytic extension of f to S_{n+1}. Therefore f is analytic on $\bigcup_{n=0}^{\infty} S_n$. It remains to show that

$$\overline{D}(1,c) \cup \overline{D}(-1,c) = \bigcup_{n=0}^{\infty} S_n. \tag{19}$$

From the definition of S_n, the point $z \in \overline{D}(-1,c) \setminus D(1,c+\varepsilon)$ belongs to $\bigcup_{n=0}^{\infty} S_n$, if and only if there exists $m \in \mathbb{N}$ such that $z_j \in \overline{D}(-1,c) \setminus D(1,c+\varepsilon)$ for $0 \leqslant j \leqslant m$ and $z_{m+1} \in S_0$, where

$$z_0 = z, \quad z_{j+1} = 1 - 2\sqrt{-z_j}. \tag{20}$$

Suppose that there exists $z\in\overline{D}(-1,c)\setminus D(1,c+\varepsilon)$ such that $z_n\in\overline{D}(-1,c)$ for all $n\in\mathbb{N}$. Let K be the closure of the set $\{z_n : n=0,1,\dots\}$. Then K is a closed subset of the compact set $A=\overline{D}(-1,c)\setminus D(1,c+\varepsilon)$, and $\varphi(K)\subseteq K$, where $\varphi(z)=1-2\sqrt{-z}$. Since $|\varphi'(u)|<1$ for any $u\in A$, $\varphi|_K : K\to K$ is a contraction. According to the contraction map theorem, there exists a fixed point of the map $\varphi|_K$. But the unique solution (in $\mathbb{C}\setminus[1,+\infty)$) of the equation $\varphi(w)=w$ is $w=-1\notin A$. This contradiction shows that for any $z\in\overline{D}(-1,c)\setminus D(1,c+\varepsilon)$ there exists the first positive integer m for which $z_m\notin\overline{D}(-1,c)\setminus D(1,c+\varepsilon)$. Then $z_{m-1}\in\overline{D}(-1,c)\setminus D(1,c+\varepsilon)$. According to Lemma 4 $z_m=1-2\sqrt{-z_{m-1}}\in\overline{D}(-1,c)\cap\overline{D}(1,c+\varepsilon)\subset S_0$. According to the description of the set $\bigcup_{n=0}^{\infty} S_n$, we have that $z\in\bigcup_{n=0}^{\infty} S_n$. This implies (19). ■

Lemma 6: The function f is analytic on the disk $D(0,2+\sqrt{3})$.

Proof: Let $c_0=1$, $c_{n+1}=\sqrt{4c_n-1}$ for $n=1,2,\dots$. This sequence strictly increases and converges to $2+\sqrt{3}$. From Lemma 3 it follows that f is analytic on $\overline{D}(0,c_0)$. According to Lemmas 2 and 5, analyticity of f on $\overline{D}(0,c_n)$ implies analyticity of f on $\overline{D}(1,2\sqrt{c_n})\cup\overline{D}(-1,2\sqrt{c_n})\supset\overline{D}(0,c_{n+1})$. Therefore f is analytic on $\overline{D}(0,c_n)$ for any $n=0,1,\dots$. Hence, f is analytic on the set $\bigcup_{n=0}^{\infty}\overline{D}(0,c_n)=D(0,2+\sqrt{3})$. ■

IV. PROOF OF THE PROPOSITION

(I) Without loss of generality we can assume that $g(-1)=0$ and $f(-1)=0$. If this is not the case, we can achieve these conditions just by adding suitable constants to f and g. Therefore $f(x)=\varphi(x)(1+x)$, $g(x)=\psi(x)(1+x)$ and $\psi\in\mathcal{E}$, $\varphi\in\mathcal{A}$. Moreover, analyticity of f on a connected set $A\supset[-1,1]$ implies analyticity of φ on the same set A. Let

$$\begin{aligned} f_0(x)&=(\varphi(x)+\varphi(-x))/2,\quad f_1(x)=(\varphi(x)-\varphi(-x))/2;\\ g_0(x)&=(\psi(x)+\psi(-x))/2,\quad g_1(x)=(\psi(x)-\psi(-x))/2. \end{aligned} \tag{21}$$

Then $g_0,g_1\in\mathcal{E}$, $f_0,f_1\in\mathcal{A}$. The analyticity of f on a connected symmetric (with respect to 0) set $A\supset[-1,1]$ implies the analyticity of f_0,f_1 on the same set. Thus, according to Lemma 6 f_0 and f_1 are analytic on $D(0,2+\sqrt{3})$.

Evidently f_0,g_0 are even, f_1,g_1 are odd and

$$f(x)=(1+x)(f_0(x)+f_1(x)),\quad g(x)=(1+x)(g_0(x)+g_1(x)). \tag{22}$$

From (3) and (22) it follows that

$$\left(1-\frac{(1-x)^4}{16}\right)f_0\left(\frac{(1-x)^2}{4}\right)=\lambda(1+x)(f_0(x)+f_1(x))+(1+x)(g_0(x)+g_1(x))$$

for any $x\in[-1,1]$. Dividing by $(1+x)$ we obtain

$$\frac{1}{16}(15-11x+5x^2-x^3)f_0\left(\frac{(1-x)^2}{4}\right)=\lambda(f_0(x)+f_1(x))+g_0(x)+g_1(x). \tag{23}$$

Adding (23) for x with (23) for $-x$ we obtain that for any $x\in[-1,1]$,

$$\frac{1}{32}(15-11x+5x^2-x^3)f_0\left(\frac{(1-x)^2}{4}\right)+\frac{1}{32}(15+11x+5x^2+x^3)f_0\left(\frac{(1+x)^2}{4}\right)=\lambda f_0(x)+g_0(x). \tag{24}$$

Let us prove that $f_0 \in \mathcal{E}$. Suppose that $f_0 \notin \mathcal{E}$. Since f_0 is analytic on $D(0,2+\sqrt{3})$, there exists $a \in [2+\sqrt{3}, +\infty)$ such that f_0 is analytic on $D(0,a)$ and is not analytic on $\overline{D}(0,a)$. Since f_0 is even, we have that f_0 is not analytic on the set $B=\{z \in \overline{D}(0,a): z \neq 0, \mathrm{Re}\, z \geqslant 0\}$. According to Lemma 4, $x=2\sqrt{y}-1 \in D(0,a)$ and $y-x \in D(0,a)$ for any $y \in B$. Since $15+11x+5x^2+x^3 \neq 0$ for $y \in B$, the function

$$h(y)=\frac{(x^3-5x^2+11x-15)f_0(y-x)+32\lambda f_0(x)+32g_0(x)}{15+11x+5x^2+x^3},$$

where $x=x(y)=2\sqrt{y}-1$, is well defined and analytic on B. On the other hand, (24) and the definition of h imply that $h(x)=f(x)$ for all $x \in (0,1)$. The uniqueness theorem implies that h is an analytic extension of f_0 from $(0,1]$ to B, which does not exist. This contradiction proves that $f_0 \in \mathcal{E}$.

From (23) it follows that

$$f_1(x)=\frac{1}{16\lambda}(15-11x+5x^2-x^3)f_0\left(\frac{(1-x)^2}{4}\right)-f_0(x)-\frac{1}{\lambda}(g_0(x)+g_1(x)). \tag{25}$$

Therefore $f_1 \in \mathcal{E}$. Formula (22) implies that f is entire and part I is proved.

(II) Let $g \in \mathcal{P}$. We have to prove that $f \in \mathcal{P}$. According to (21) $g_0, g_1 \in \mathcal{P}$. Let $k=\deg g_0$ if $g_0 \not\equiv 0$ and $k=0$ if $g_0 \equiv 0$. Let us show that $f_0 \in \mathcal{P}$ and $\deg f_0 \leqslant k/2-1$.

The functional equation (24) can be rewritten in the form

$$f_0\left(\frac{(1+x)^2}{4}\right)=\frac{32\lambda f_0(x)}{x^3+5x^2+11x+15}+\frac{32g_0(x)}{x^3+5x^2+11x+15}+\frac{x^3-5x^2+11x-15}{x^3+5x^2+11x+15}f_0\left(\frac{(1-x)^2}{4}\right). \tag{26}$$

Since f_0 is even

$$M(R)=\max_{|x|=R}|f_0(x)|=\max_{|x|=R,\ \mathrm{Re}\, x \geqslant 0}|f_0(x)|. \tag{27}$$

Let $y \in \mathbb{C}$, $|y|=R$, $\mathrm{Re}\, y \geqslant 0$, $x=2\sqrt{y}-1$, $w=y-x$. Then $|x|=2\sqrt{R}+O(1)$ and

$$|w|=|y|\left|1-\frac{y}{x}\right|=R\left|1-\frac{2}{\sqrt{y}}+\frac{1}{y}\right|=R\left|1-\frac{2}{\sqrt{y}}\right|+O(1).$$

All O-symbols are considered here for $R \to \infty$. The number $|1-(2/\sqrt{y})|$ for $|y|=R$, $\mathrm{Re}\, y \geqslant 0$, is maximal for $y=\pm Ri$. Therefore,

$$|w| \leqslant R\left|1-\frac{\sqrt{2}(1+i)}{\sqrt{R}}\right|+O(1)=R-\sqrt{2R}+O(1)$$

and

$$|w|<R-\sqrt{R}, \quad |x|=2\sqrt{R}+O(1)<R-\sqrt{R} \tag{28}$$

for sufficiently large R. Formula (26) implies that

$$f_0(y)=\frac{32\lambda f_0(x)}{x^3+5x^2+11x+15}+\frac{32g_0(x)}{x^3+5x^2+11x+15}+\frac{x^3-5x^2+11x-15}{x^3+5x^2+11x+15}f_0(w). \tag{29}$$

Note that

$$\left|\frac{x^3-5x^2+11x-15}{x^3+5x^2+11x+15}\right|=\left|1-\frac{10}{x}+O\left(\frac{1}{x^2}\right)\right|=\left|1-\frac{5}{\sqrt{y}}\right|+O(R^{-1}).$$

The number $|1-(5/\sqrt{y})|$ for $|y|=R$, $\operatorname{Re} y\geqslant 0$, is maximal for $y=\pm Ri$. Therefore,

$$\left|\frac{x^3-5x^2+11x-15}{x^3+5x^2+11x+15}\right|\leqslant 1-\frac{5}{\sqrt{2R}}+O(R^{-1}). \tag{30}$$

Formulas (29), (27), (28) and (30) imply that

$$M(R)\leqslant M(R-\sqrt{R})\left(1-\frac{5}{\sqrt{2R}}+O(R^{-1})\right)+O(R^{(k-3)/2}).$$

If f_0 is a polynomial of degree at most $k/2-1$, we have proved the statement. Otherwise $R^{k/2}=O(M(R))$. Hence $R^{(k-3)/2}=O(M(R-\sqrt{R})/R)$, and

$$M(R)\leqslant M(R-\sqrt{R})\left(1-\frac{5}{\sqrt{2R}}+O(R^{-1})\right). \tag{31}$$

Therefore $M(R)\leqslant M(R-c\sqrt{R})$ for sufficiently large R. Hence $M(R)=O(1)$ and f_0 is a constant according to the Liouville theorem.[20] Hence $M(R)$ is constant. Formula (31) implies then that $M(R)\equiv 0$. Therefore, $f_0\equiv 0$ and $k=0$ according to (26). Thus, anyway $f_0\in\mathcal{P}$ and $\deg f_0\leqslant k/2-1$.

From (25) we find that $f_1\in\mathcal{P}$ and

$$\deg f_1\leqslant\max\{k+1,\deg g_1\}.$$

Then using (22) we find that $f\in\mathcal{P}$ and $\deg f\leqslant\deg g+1$.

(III) Suppose that $g\in\mathcal{P}$ and $f\in\mathcal{A}$ satisfies (3). According to part II of the Proposition $f(x)=\Sigma_{k=0}^{n}a_kx^k$, $a_n\neq 0$. If n is odd, then according to (1) $\deg Uf=2n+2$ and $\deg g=\deg(Uf-\lambda f)=2n+2$ is even. If n is even and $n\neq\deg Uf$, then $\deg g=\max\{\deg f,\deg Uf\}$ is even. It remains to consider the case $\deg Uf=n$. Since $\deg Uf$ is always a multiple of 4, we have that $n=4m$, $m=0,1,\ldots$. According to (1)

$$Uf(x)=\sum_{l=1}^{2m}(a_{2l}-a_{2l-1})2^{-4l}(1-x)^{4l}+a_0. \tag{32}$$

Since $\deg Uf=4m$ we have that $a_{2l}=a_{2l-1}$ if $m<l\leqslant 2m$ and $a_{2m}\neq a_{2m-1}$. Substituting (32) into (3) and taking these relations into account, we obtain that $\deg g=4m$ or $\deg g=4m-1$. In any case $\deg g$ does not have form $4j+1$.

V. PROOF OF THEOREM 3

We start with two lemmas.

Lemma 7: Let $q\in(0,1)$ *and* $z\in\overline{D}(q,1+q)$. *Then* $(1-z)^2/4\in D(q,1+q)$.

Proof: We have to prove that

$$|(z-1)^2-4q|<4+4q. \tag{33}$$

Since $z\in\overline{D}(q,1+q)$, we find that $z=q+(1+q)u$, where $|u|\leqslant 1$. Obviously (33) is equivalent to

$$|1-6q+q^2-2(1-q^2)u+(1+2q+q^2)u^2|<4+4q. \tag{34}$$

If $1-6q+q^2\geqslant 0$, we have

$$|1-6q+q^2-2(1-q^2)u+(1+2q+q^2)u^2|\leqslant 1-6q+q^2+2(1-q^2)+(1+2q+q^2)$$
$$=4-4q<4+4q.$$

If $1-6q+q^2<0$, we have

$$|1-6q+q^2-2(1-q^2)u+(1+2q+q^2)u^2|\leqslant -1+6q-q^2+2(1-q^2)+(1+2q+q^2)$$
$$=4+4q-2(1-q)^2<4+4q.$$

■

Lemma 8: Let $\mathcal{H}$ be the Hardy space H^2 in the upper half-plane $\Pi=\{z\in\mathbb{C}:\mathrm{Re}\,z>\alpha\}$, $\alpha\in\mathbb{R}$, $\nu,\varphi:\overline{\Pi}\to\mathbb{C}$ be bounded analytic functions and $c,\varepsilon\in(0,+\infty)$ be such that

$$\mathrm{Re}\,\varphi(z)\geqslant\varepsilon \quad for\ \ all\ \ z\in\Pi; \tag{35}$$

$$\int_{-\infty}^{+\infty}|\nu(\alpha+is)|^2\,ds\leqslant A<\infty; \qquad \int_{-\infty}^{+\infty}|\varphi(\alpha+is)-c|^2\,ds\leqslant A<\infty. \tag{36}$$

Then the operator $S:\mathcal{H}\to\mathcal{H}$, $Sf(z)=(1+\nu(z))f(z+\varphi(z))$ is the sum of two operators A and B, where A is bounded, self-adjoint and has purely absolutely continuous spectrum $[0,1]$ and B is a Hilbert–Schmidt operator.

Proof: Without loss of generality we assume $\alpha=0$. According to the Paley–Wiener theorem (Ref. 19, Chap. 8), the Laplace transform

$$Lg(z)=\frac{1}{\sqrt{2\pi}}\int_0^{\infty}e^{-zt}g(t)\,dt$$

is a unitary operator from $L_2[0,+\infty)$ onto $\mathcal{H}$.

Let $\mathcal{D}_+$ be the subspace of $L_2[0,+\infty)$, consisting of infinitely differentiable functions with compact support lying in $(0,+\infty)$. Consider the operator $\widetilde{S}=L^{-1}SL:L_2[0,+\infty)\to L_2[0,+\infty)$. Using the standard formula for the inverse Laplace transform we obtain that

$$\widetilde{S}g(t)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_0^{+\infty}g(\tau)e^{is(t-\tau)}e^{-\varphi(is)\tau}(1+\nu(is))\,d\tau\,ds$$

for any $g\in\mathcal{D}_+$. Therefore,

$$\widetilde{S}g(t)=g(t)e^{-ct}+\int_0^{+\infty}g(\tau)K(\tau,t)\,d\tau, \tag{37}$$

where

$$K(\tau,t)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{is(t-\tau)}[e^{-\varphi(is)\tau}(1+\nu(is))-e^{c\tau}]\,ds.$$

The existence of the last integral (in the principle value sense) for any τ and almost all t, follows from the Plancherel theorem, since formula (36) implies square integrability, with respect to s, of the function $e^{-is\tau}[e^{-\varphi(is)\tau}(1+\nu(is))-e^{c\tau}]$.

According to the Parseval identity and using formulas (35) and (36), we obtain

$$\int_{-\infty}^{+\infty}|K(\tau,t)|^2dt=\frac{1}{2\pi}\int_{-\infty}^{+\infty}|e^{-\varphi(is)\tau}(1+\nu(is))-e^{c\tau}|^2ds$$

$$\leqslant\frac{e^{-2\tau\varepsilon}}{\pi}\int_{-\infty}^{+\infty}(|e^{-(\varphi(is)-\varepsilon)\tau}-e^{(c+\varepsilon)\tau}|^2+|e^{-(\varphi(is)-\varepsilon)\tau}\nu(is)|^2)\,ds$$

$$\leqslant\frac{e^{-2\tau\varepsilon}}{\pi}\int_{-\infty}^{+\infty}(\tau^2|\varphi(is)-c|^2+|\nu(is)|^2)\,ds$$

$$\leqslant\frac{Ae^{-2\tau\varepsilon}(\tau^2+1)}{\pi}.$$

According to Fubini's theorem

$$\int_0^{+\infty}\int_0^{+\infty}|K(\tau,t)|^2dtd\tau\leqslant\int_0^{+\infty}\int_{-\infty}^{+\infty}|K(\tau,t)|^2dtd\tau\leqslant\frac{A}{\pi}\int_0^{+\infty}e^{-2\tau\varepsilon}(\tau^2+1)\,d\tau<+\infty.$$

Therefore, $K\in L_2([0,+\infty)^2)$. Since $\mathcal{D}_+$ is dense in $L_2[0,+\infty)$, formula (37) is valid for any $g\in L_2[0,+\infty)$. Therefore, $\widetilde{S}=\widetilde{A}+\widetilde{B}$, where

$$\widetilde{A}g(t)=g(t)e^{-ct}\quad\text{and}\quad\widetilde{B}g(t)=\int_0^{+\infty}g(\tau)K(\tau,t)\,d\tau,$$

the operator $\widetilde{A}$ is bounded, self-adjoint and has purely absolutely continuous spectrum $[0,1]$, and the operator $\widetilde{B}$ is a Hilbert–Schmidt operator. It remains to note that operators S and $\widetilde{S}$ are unitarily equivalent. ■

Now we can prove Theorem 3. Evidently $U=U^0+U^1$, where

$$U^0f(x)=\frac{1}{2}\left(1+\frac{(1-x)^2}{4}\right)f\left(-\frac{(1-x)^2}{4}\right),\tag{38}$$

$$U^1f(x)=\frac{1}{2}\left(1-\frac{(1-x)^2}{4}\right)f\left(\frac{(1-x)^2}{4}\right).\tag{39}$$

According to Lemma 7, there exists a $r>1+q$ such that for any $f\in X$ the function U^1f admits an analytic extension to $\overline{D}(q,r)$. Let X_r be the Hardy space in the disk $D(q,r)$. Then formula (39) defines a bounded linear operator U_r^1 from X to X_r. The operator $U_X^1:X\to X$ is the superposition of U_r^1 and the identity embedding J of X_r into X. Since the operator J is nuclear [J has the s-numbers $(1+q)^nr^{-n}$)], we find that $U_X^1=U^1|_X:X\to X$ is also nuclear and therefore compact.

Let $\mathcal{H}$ be the Hardy space in the upper half-plane $\{z\in\mathbb{C}:\mathrm{Re}\,z>(1+q)^{-1}\}$. One can easily verify that the operator $M:X\to\mathcal{H}$,

$$Mf(z)=\frac{1}{z}f\left(\frac{2}{z}-1\right),\tag{40}$$

is unitary up to a multiplication on a positive constant. Then the operators U_X^0 and $W^0=MU^0M^{-1}:\mathcal{H}\to\mathcal{H}$ are unitarily equivalent.

From the definitions of (38) and (40) we obtain that

$$M^{-1}f(z)=\frac{2}{z+1}g\left(\frac{2}{z+1}\right)\quad\text{and}\quad W^0f(z)=(1+\nu(z))f(z+\varphi(z)),$$

where

$$\nu(z)=\frac{1-z}{2z^2-z} \quad \text{and} \quad \varphi(z)=\frac{1}{2}+\frac{1}{4z-2}.$$

One can easily verify that φ and ν satisfy all conditions of Lemma 8 with $\varepsilon=c=\frac{1}{2}$. According to Lemma 8, W^0 is a sum of a self-adjoint operator with the purely absolutely continuous spectrum $[0,1]$ and a Hilbert–Schmidt operator. Since U_X^0 and W^0 are unitarily equivalent and U_X^1 is nuclear, we have that U_X is a sum of a self-adjoint operator with purely absolutely continuous spectrum $[0,1]$ and a Hilbert–Schmidt operator. Following Ref. 21, we say that $z\in\mathbb{C}$ is a normal point of a bounded linear operator on a separable Hilbert space if either z is a regular point or z is an isolated eigenvalue of finite multiplicity. According to Theorem 5.2 of Chap. 1 in Ref. 21, for any bounded self-adjoint operator A and any compact operator B acting on the same Hilbert space, the sets of normal points of A and $A+B$ coincide. It remains to apply this theorem. ■

VI. CONCLUDING REMARKS

(1) So far there exist very few results on the spectral properties of the F.P.O. of the maps with parabolic neutral fixed points. We would like to point out the result of H. Rugh,[17] who considered the F.P.O. of piecewise analytic maps, which are expanding everywhere except one parabolic fixed point. Namely, he constructed a specific map-dependent Banach space of analytic functions, where the spectrum of the F.P.O. consists of the segment $[0,1]$ and some isolated normal eigenvalues. This space is in fact the image of $L_1[0,+\infty)$ with respect to some map-dependent integral transformation similar to the Laplace transform.

The cusp map does not satisfy the conditions of Rugh's theorem because of the cusp-shaped singularity. Nevertheless, we proved that the F.P.O. of the cusp map has similar spectral properties in the Hardy spaces H^2 in the disks $D(q,1+q)$, $0<q<1$. We also conjecture that the spectrum of the F.P.O. U of the cusp map in the Hardy spaces H^2 in the disks $D(q,1+q)$, $0<q<1$ is precisely the segment $[0,1]$, i.e., the set of isolated eigenvalues of U is empty. Note that the functions of these Hardy spaces as well as the functions of Rugh's spaces are analytic in all points of the segment except at the parabolic fixed point ($x=-1$ in the case of the cusp map). However, we should notice that the spectrum of the F.P.O. of a map S in spaces of analytic functions with singularity at a fixed point of S may differ considerably from the spectrum in spaces of everywhere analytic functions. We have proved that this is precisely the case for the cusp map.

(2) The theory of the point spectrum for the maps has been recently developed in terms of locally convex topological vector spaces.[9] For different classes of observables the same evolution law may have different resonances, i.e., different rates of approach to equilibrium. However, once the class of observables is chosen, the resonance structure is unique.[9,10] In terms of the assumptions of Ref. 9, the admissible point spectra for a given map are described. Here we see that for the cusp map, we have continuous spectra in Hardy spaces. This type of spectra was not addressed in Ref. 9.

(3) We would like also to notice that Theorems 1 and 2 remain valid if one replaces the F.P.O. (1) of the cusp map by some positive transfer operator[6] of the cusp map, for example,

$$\tilde{U}f(x)=\frac{1}{2}f\left(\frac{(1-x)^2}{4}\right)+\frac{1}{2}f\left(-\frac{(1-x)^2}{4}\right).$$

Of course, Theorems 1 and 2 do not remain valid for all positive transfer operators in the class considered in Ref. 6. For example, let us consider the operator

$$Wf(x)=\left(\frac{1}{2}-\beta+\frac{a(x)}{4}\right)f(a(x))+\left(\frac{1}{2}+\beta-\frac{a(x)}{4}\right)f(-a(x)),$$

where $a(x)=(1-x)^2/4$. For the real parameter $\beta\in[-\frac{1}{4},\frac{1}{2}]$, this is a positive transfer operator for the cusp map, and $W1=1$. On the other hand, the function

$$f(x)=x-\frac{x^2}{2}+\frac{\beta}{2(1-\beta)}$$

is the eigenfunction of W corresponding to the eigenvalue β: $Wf=\beta f$. Hence Theorems 1 and 2 are not valid for the operator W.

(4) We do not consider Hardy spaces H^p, $p\neq 2$, although Theorem 3 can be generalized for such spaces. In order to do this, one has to generalize results of Chap. 1 of Ref. 21 for arbitrary continuous linear operators on Banach spaces. This can be done with minor modifications in proofs.[21]

(5) There are few questions which remain open for the cusp map. First, the question about the asymptotics of the autocorrelation function. As the eigenvalues of the F.P.O. of the family (2) tend to unity when $\varepsilon\to\frac{1}{2}$, one can expect nonexponential decrease of the autocorrelation function. The estimations in Ref. 14 show that the autocorrelation function $C(n)$ decreases as $1/n$, when $n\to\infty$. However, this conjecture has not yet been analytically proven. Another question addresses the choice of the space of analytic functions where the spectrum of the F.P.O. is naturally defined by the dynamics of the map.

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Analytic continuation of the Hurwitz zeta function with physical application

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A new formula relating the analytic continuation of the Hurwitz zeta function to the Euler gamma function and a polylogarithmic function is presented. In particular, the values of the first derivative of the real part of the analytic continuation of the Hurwitz zeta function for even negative integers and the imaginary one for odd negative integers are explicitly given. The result can be of interest both on mathematical and physical side, because we are able to apply our new formulas in the context of the spectral zeta function regularization, computing the exact pair production rate per space–time unit of massive Dirac particles interacting with a purely electric background field. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In 1951, Schwinger[1] computed the implicit effective Lagrangian for a Dirac charged spinor in a general electromagnetic background field using proper time approach. In particular, he applied the result to the physical case of a constant and uniform electric background and he was able to evaluate the exact pair-production rate per space–time unit, namely

$$w(E,e,m)=\frac{e^2E^2}{4\pi^3}\sum_{n=1}^{+\infty}\frac{e^{-n\,\pi m^2/eE}}{n^2}. \tag{1}$$

This result is well known and can be obtained by other ways (e.g., Itzykson and Zuber,[2] using the S-matrix approach, and by Beneventano and Santangelo[3]). In 1990 Blau *et al.*,[4] using the techniques of the spectral zeta function regularization, tried to obtain the same results obtained by Schwinger. However, they were able only to obtain nonexact results for the four dimensional case, using asymptotic analysis. In 1996, Soldati and Sorbo[5] obtained a new expression, but once again their methods were based on asymptotic analysis and the results were expressed in terms of asymptotic series.

The problem for general electromagnetic external field has been recently discussed by Schubert[6] and by Cho and Pak.[7] Schubert obtained the same action by Schwinger using proper time method and techniques of computation inspired by string theory. Cho and Pak obtained a renormalized action from the general one (non-renormalized) found by Schwinger, using the so-called Sitacaramachandrarao identity. Recently, Beneventano and Santangelo[8] have compared their results obtained using spectral zeta function methods with the general result obtained by Schwinger, showing that they agree.

In this article, we shall compute the imaginary part of the effective Lagrangian related to a Dirac field in a constant and uniform external electric field by making use of new formulas

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concerning the analytic continuation of the first derivative of the Hurwitz zeta function.

The content of the article is the following. In Sec. II, we briefly introduce the spectral zeta function regularization procedure and illustrate the result obtained by Blau *et al.,* which will be our starting point for the application of the new formulas. In Sec. III, we derive a new expression for the analytic continuation of the Hurwitz zeta function, viewed as an analytic function of two complex variables. In Sec. IV, we use that result to recover the rate of pair creation of Dirac particles in constant and uniform electric background.

II. ZETA FUNCTION REGULARIZATION

In this section, we shall review the relation between the mathematical problem that we have solved and the physical problem associated with the Dirac pair creation. For a review of the method, see, for example, Refs. 9–11 and references quoted therein.

Within the context of quantum field theory (QFT) interacting with a classical gauge background field, one is forced to confront with the determinants of differential operators.
In the context of a Klein Gordon field interacting with an external gauge field A, this determinant is related to some physical quantities formally obtained from the *Euclidean* functional integral:

$$Z[A_E]=\int D\varphi e^{-(1/2)\int d^4x\varphi A_E\varphi}, \tag{2}$$

where A_E is the Euclidean Klein Gordon operator. In the definition of this integral we have to analytically continue some global Minkowski temporal coordinate x^0 into imaginary value $x^0\rightarrow ix^0$ and consider the analytical continuation of all relevant quantities.

The above Gaussian functional integral could be interpreted as a Wiener measure, but, for our purposes, we may interpret it in terms of a functional determinant, and rewrite the definition of (2) as

$$Z[A_E]=\left[\det\left(\frac{A_E}{\mu}\right)\right]^{-1/2}, \tag{3}$$

where μ is a constant with the same physical dimension of the operator A_E.

It is sometime useful to introduce two physical quantities: the effective action and the effective Lagrangian. The former is defined as the logarithm of Z. The latter is a function of space–time points and gives, after an integration on the whole space–time, the effective action. The physical interpretation of this determinant is found after a reanalytical continuation of the imaginary time into a real time. The result is the vacuum to vacuum transition amplitude.

We can use zeta function regularization to give a rigorous meaning to functional determinants. This regularization technique was introduced by Ray and Singer for elliptic differential operators.[12] Within the quantum field theory, it was used by by Dowker and Chritchley[13] and Hawking.[14] Given a compact Riemannian manifold M and for elliptic and second order operators acting on $L_2(M)$, it can be proved that such definition gives a useful extension of the notion of functional determinant.

Since the square of the Euclidean Dirac operator is an elliptic second order differential operator, making use of the zeta regularization technique, Blau *et al.*[4] arrived at the following effective Lagrangian for a Dirac field in an external constant and uniform electric field:

$$L_{\rm eff}(E,0)=-\frac{e^2E^2}{2\pi^2}\left\{\left[1-\ln\left(\frac{-2ieE}{\mu^2}\right)\right]\zeta_H\left(-1;1+i\frac{m^2}{2eE}\right)+\frac{d}{ds}\zeta_H\left(s;1+i\frac{m^2}{2eE}\right)_{s=-1}\right\}$$
$$+i\frac{m^2eE}{8\pi^2}\left[\ln\frac{m^2}{\mu^2}-1\right], \tag{4}$$

where $\zeta_H(s;x)$ is the Hurwitz zeta function defined by

$$\zeta_H(s;x) \coloneqq \sum_{n=0}^{\infty} \left(\frac{1}{n+x}\right)^s, \quad \mathrm{Re}\, s>1.$$

They were not able to find an explicit form for the analytic continuation of the derivatives of the Hurwitz zeta function at $s=-1$. Thus, a direct comparison between their result and the one obtained by Schwinger was missing.

III. ANALYTIC CONTINUATION OF THE HURWITZ ZETA FUNCTION

In this section, we discuss the analytical properties of the Hurwitz zeta function. Following Ref. 15, we obtain a new identity involving the Hurwitz zeta function, the Euler $\Gamma(s)$ function and a polylogarithmic function.

Recall that the Hurwitz zeta function is defined as follows:

$$\zeta_H(s;x) \coloneqq \sum_{n=0}^{+\infty} (n+x)^{-s}, \tag{5}$$

where $\mathrm{Re}\, s>1$, $x\neq 0,-1,-2,\ldots$. One can analytically extend it into an analytic function of two complex variables s and x.

In order to search for the analytical continuation in the double complex plane, we introduce the function $F(s;z)$ defined by the following series:

$$F(s;z) \coloneqq \lim_{k\to\infty} \sum_{n=-k}^{k} (-in+z)^{-s}. \tag{6}$$

Notice that the series above is absolutely convergent for $\mathrm{Re}\, s>1$, $z\neq \pm ik, k\in N$. Thus, one may write

$$F(s;z) \coloneqq \lim_{k\to\infty}\left[\sum_{n=0}^{k} (-in+z)^{-s} + \sum_{n=0}^{k} (in+z)^{-s}\right] - z^{-s}. \tag{7}$$

Using this definition for the series (6), we proceed in searching for its analytical continuation. With regard to this issue, previous attempts can be found in Refs. 16 and 17. Here the author obtained an expression different from ours, requiring, however, as far as physical applications were concerned, an *ad hoc* finite renormalization.

It is straightforward to prove the following relation between $F(s;z)$ and $\zeta_H(s;z)$:

$$F(s;z) = i^s \zeta_H(s;iz) + i^{-s}\zeta_H(s;-iz) - z^{-s}. \tag{8}$$

First, let us investigate the function $F(s;x)$. The following theorem gives an expression for the analytic continuation of $F(s;z)$ in terms of polylogarithmic function.

Theorem: Following the definition stated above, the analytic continuation of $F(s,z)$ for each $s\in C$ and $\mathrm{Re}\, z>0$ is given by

$$F(s;z) = \frac{(2\pi)^s}{\Gamma(s)} \sum_{n=1}^{+\infty} \frac{e^{-2n\pi z}}{n^{1-s}}. \tag{9}$$

Proof: Define the sequence $F_k(s;z)$:

$$F_k(s;x) \coloneqq \sum_{n=-k}^{k} (-in+z)^{-s}, \tag{10}$$

which obviously converges to $F(s;z)$.

Recall the definition of the Euler $\Gamma(s)$ function for $\mathrm{Re}\, s>0$,

$$\Gamma(s) := \int_0^\infty t^{s-1} e^{-t} dt.$$

Consider the product of this function and the sequence $F_k(s;x)$:

$$F_k(s;z)\Gamma(s) = \sum_{n=-k}^{+k} (-in+z)^{-s} \int_0^\infty t^{s-1} e^{-t} dt = \int_0^\infty \sum_{n=-k}^{+k} (-in+z)^{-s} t^{s-1} e^{-t} dt.$$

We may change variables according to $t=\tau(-in+z)$, which is allowed for z not purely imaginary integer since $|dt/d\tau| \neq 0$, and we obtain

$$F_k(s;z) = \frac{1}{\Gamma(s)} \int_0^{+\infty} d\tau e^{-\tau z} \tau^{s-1} \sum_{n=-k}^{+k} e^{in\tau}. \tag{11}$$

The part of the integrand in (11) multiplying the series *vanishes* in $\tau=0$ for $\mathrm{Re}\, s>1$. This implies that the integration may be interpreted as the action of the **k**-element of a sequence of distributions $g_k(\tau)$,

$$g_k(\tau) := \sum_{n=-k}^{+k} e^{in\tau} \tag{12}$$

on the continuous function $e^{-\tau z}\tau^{s-1}$. It is a well-known result of the theory of distribution that this sequence converges and gives the Poisson summation formula:

$$\lim_{k\to\infty} g_k(\tau) = \lim_{k\to\infty} \sum_{n=-k}^{+k} e^{in\tau} = 2\pi \sum_{n=-\infty}^{+\infty} \delta(\tau - 2n\pi).$$

Thus we obtain in the limit $k\to\infty$:

$$F(s;z) = \frac{1}{\Gamma(s)} \int_0^{+\infty} e^{-\tau z} \tau^{s-1} \sum_{n=-\infty}^{+\infty} e^{in\tau} = \frac{(2\pi)^s}{\Gamma(s)} \sum_{n=1}^{+\infty} \frac{e^{-2n\pi z}}{n^{1-s}},$$

which, as stated in the hypotheses of the theorem, makes sense as analytic continuation for each $s\in C$ and $\mathrm{Re}\, z>0$.

Recalling the relation (8) between $F(s;z)$ and $\zeta_H(s;z)$, we have the following corollary:

Corollary: The following formula is valid for each $s\in C$ and $\mathrm{Re}\, z>0$ in the sense of the analytic continuation:

$$(i)^s \zeta_H(s;iz) + i^{-s} \zeta_H(s;-iz) - z^{-s} = \frac{(2\pi)^s}{\Gamma(s)} \sum_{n=1}^{+\infty} \frac{e^{-2n\pi z}}{n^{1-s}}. \tag{13}$$

Proof: Direct use of Eqs. (8) and (9).

Equation (13) can be checked for $s=-n$. In this case the right hand side is vanishing and Eq. (13) gives

$$i^{-n} \zeta_H(-n,iz) + i^n \zeta_H(-n,-iz) - z^{-s} = 0. \tag{14}$$

Recall that the values of the Hurwitz zeta function are known for negative integers and are related to the Bernoulli's polynomials by the following formula:

$$\zeta_H(-n,z)=-\frac{B_{n+1}(z)}{n+1}. \tag{15}$$

It is easy to show that this equation is identically fulfilled.

Remark: We now notice that the series

$$\sum_{n=1}^{+\infty}\frac{e^{-2n\pi z}}{n^{1-s}} \tag{16}$$

and its derivatives are uniformly convergent in the variable s for $\mathrm{Re}\,z>0$ and $\mathrm{Re}\,s\in(-\infty,a)$ with $a<\infty$. A straightforward computation leads to the following lemma:

Lemma 1: The following formula holds for each $s\in\mathrm{C}$ and $\mathrm{Re}\,z>0$ in the sense of the analytic continuation:

$$\begin{aligned}(i)^s\frac{d}{ds}\zeta_H(s;iz)+(i)^{-s}\frac{d}{ds}\zeta_H(s;-iz)&\\ =(2\pi)^s\left(\frac{d}{ds}\frac{1}{\Gamma(s)}\right)\sum_{n=1}^{+\infty}\frac{e^{-2n\pi z}}{n^{1-s}}+\frac{(2\pi)^s}{\Gamma(s)}\sum_{n=1}^{+\infty}\frac{e^{-2n\pi z}\ln(2n\pi)}{n^{1-s}}&\\ +i\frac{\pi}{2}\left[-2(i)^s\zeta_H(s;iz)+z^{-s}+\frac{(2\pi)^s}{\Gamma(s)}\sum_{n=1}^{+\infty}\frac{e^{-2n\pi z}}{n^{1-s}}\right]-(z)^{-s}(\ln|z|+iarg\,z).&\end{aligned} \tag{17}$$

Proof: One simply applies the derivative on both sides of the formula obtained in the corollary above, then uses the remark above to exchange the series with the derivative with respect to s, and then analytically continues the result for all the values of s.

As a result, we shall derive formulas for the real and imaginary values of the first derivative of the Hurwitz zeta function respectively for even and odd negative integers.

Using parity properties of the real and the imaginary part of this polynomials it is easy to prove the following lemma.

Lemma 2: For $x\in R$, $x>0$, and for $n\in N$, $n<0$, the Hurwitz zeta function has the following parity properties:

$$\mathrm{Re}\,\zeta_H(-n;ix)=\mathrm{Re}\,\zeta_H(-n;-ix), \tag{18}$$

$$\mathrm{Im}\,\zeta_H(-n;ix)=-\mathrm{Im}\,\zeta_H(-n;-ix). \tag{19}$$

We have the following.

Proposition: For $x\in R$ and for $m\in N$, the following two formulas are valid for any natural number:

$$\begin{aligned}\mathrm{Im}\frac{d}{ds}\zeta_H(-(2m+1);ix)=\pi\,\mathrm{Re}\frac{B_{2m+2}(ix)}{4(m+1)}+\frac{(-1)^{m+1}x^{2m+1}}{2}\ln x&\\ +\frac{(-1)^{m+1}(2m+1)!}{2(2\pi)^{2m+1}}\sum_{n=1}^{+\infty}\frac{e^{-2n\pi x}}{n^{2(m+1)}},&\end{aligned} \tag{20}$$

$$\mathrm{Re}\frac{d}{ds}\zeta_H(-2m;ix)=-\pi\,\mathrm{Im}\frac{B_{2m+1}(ix)}{2(2m+1)}+\frac{(-1)^{m+1}x^{2m}}{2}\ln x+\frac{(-1)^m(2m)!}{2(2\pi)^{2m}}\sum_{n=1}^{+\infty}\frac{e^{-2n\pi x}}{n^{1+2m}}. \tag{21}$$

Proof: Simple computation using Lemma 1 and 2.

Note: It is possible to obtain other identities involving higher order derivatives of the Hurwitz zeta function starting from (13). As a consequence, it is possible to obtain the values of higher derivatives of either the imaginary or real part of the Hurwitz zeta function for negative integers using recursive formulas.

As far as we know only asymptotic values have been found by E. Elizalde[18,19] for the analytic continuation of the derivatives of the Hurwitz zeta function. Thus (20) and (21) are new formulas. In the next section, we use the second one for the application to the study of the Dirac pair creation in the pure electrical background field.

IV. APPLICATION TO SCHWINGER PAIR CREATION

In this last section we shall apply the formula (20) to the problem of Dirac pair creation in a purely electrical background field, recovering the Schwinger result. The starting point is the effective Lagrangian obtained by Blau *et al.*

$$L_{\mathrm{eff}}(E,0)=-\frac{e^2E^2}{2\pi^2}\left\{\left[1-\ln\left(\frac{-2ieE}{\mu^2}\right)\right]\zeta_H\left(-1;1+i\frac{m^2}{2eE}\right)\frac{d}{ds}\zeta_H\left(s;1+i\frac{m^2}{2eE}\right)_{s=-1}\right\}$$
$$+i\frac{m^2eE}{8\pi^2}\left[\ln\frac{m^2}{\mu^2}-1\right]. \tag{22}$$

We have to find the imaginary part of the right-hand side of (22). Making use of Eq. (20) to $s=-1$, we obtain

$$\mathrm{Im}\frac{d}{ds}\zeta_H(-1;ix)=-\frac{1}{4\pi}\sum_{n=1}^{+\infty}\frac{e^{-2n\pi x}}{n^2}-\frac{x}{2}\ln x+\frac{\pi}{24}-\frac{\pi x^2}{4}. \tag{23}$$

If we plug this formula in the effective Lagrangian expression, we obtain the Schwinger result:

$$w(E,e,m)=\frac{e^2E^2}{4\pi^3}\sum_{n=1}^{+\infty}\frac{e^{-n\,\pi m^2/eE}}{n^2}. \tag{24}$$

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Reduction of HKT-structures

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KT-geometry is the geometry of a Hermitian connection whose torsion is a 3-form. HKT-geometry is the geometry of a hyper-Hermitian connection whose torsion is a 3-form. We identify nontrivial conditions for a reduction theory for these types of geometry. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1487443]

I. INTRODUCTION

Symplectic reduction is a novel method of constructing symplectic manifolds from others that admit a group action of symplectic diffeomorphisms. To describe the main result, let G be a compact group of symplectic diffeomorphisms acting on the symplectic manifold (M,ω) and $\mathfrak{g}$ be the Lie algebra of G. It can be shown that under certain conditions, $N=\nu^{-1}(\zeta)/G$ is also a symplectic manifold, where $\zeta\in\mathfrak{g}^*$ and $\nu:M\to\mathfrak{g}^*$ is the moment map. The manifold N is also denoted with $M//G$. It is remarkable that symplectic reduction can be generalized in various ways. First, it can be shown that if M is a Kähler manifold admitting a G-action of holomorphic isometries, then $M//G$ is also a Kähler manifold. Furthermore, it can be shown that if M is a hyper-Kähler manifold admitting an G-action of triholomorphic isometries, then $M//G=\nu^{-1}(\zeta)$ is also hyper-Kähler, where $\nu=(\nu_1,\nu_2,\nu_3):M\to\mathbf{R}^3\otimes\mathfrak{g}^*$ and $\zeta=(\zeta_1,\zeta_2,\zeta_3)\in\mathbf{R}^3\otimes\mathfrak{g}^*$.[1] In the context of hyper-Kähler reduction there are three moment maps each associated to the three complex structures. One common feature of all symplectic, Kähler and hyper-Kähler reductions is that moment maps exist because the G-action preserves some symplectic form.

More generally it has been shown that if M is a hypercomplex manifold admitting a triholomorphic group action, then $M//G$ is also hypercomplex.[2] The details of this construction will be summarized in Sec. II B. Here it is worth mentioning that in the context of hypercomplex reductions, moment maps do not arise naturally because in the generic case there are no symplectic forms which are preserved by the group action. Instead it is assumed that one can find such functions on M which have the required properties.

In the next section, we assume the existence of a G-moment map on M and study the geometry on the reduced space N. The aim is to prove that the reduction of a KT-space is a KT-space and the reduction of a HKT-space is again a HKT-space. The definition and twistor construction of HKT spaces have been given in Ref. 3. The properties of KT and HKT manifolds have been widely investigated in the literature.[3–5] The result on KT-space in Sec. II is not surprising because a Hermitian structure can easily be found on a reduced space and every Hermitian structure has a unique KT-connection. The existence of HKT-connection on the reduction of a

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HKT-space is less trivial. Examples of HKT-reduction in this regard are given at the end of this paper.

In the third section, we identify nontrivial and sufficient topological or cohomological constraints on either the manifold M or the group G to ensure the existence of a G-moment map on strong KT-manifolds and strong HKT-manifolds. In the absence of symplectic forms, this is a nontrivial result as one usually generates moment map through the Kähler form. In the fourth section, we discuss when a potential function on a HKT-space may descend to a potential function on the reduced HKT-space.

II. EXISTENCE OF HKT-STRUCTURES ON REDUCED SPACES

Assuming the existence of ''moment maps,'' we examine the geometry on the reduced space in the next two sections.

A. KT reduction

Before we explain HKT reduction, it is instructive to consider first the reduction of KT manifolds, i.e., Hermitian manifolds equipped with the hermitian connection whose torsion is a three-from.

Let M be a KT manifold and let G be a compact group of complex isometries on M. Denote the algebra of holomorphic vector fields by $\mathfrak{g}$. Next introduce a G-equivariant map $\nu: M \to \mathfrak{g}$ satisfying the transversality condition, i.e., $Id\,\nu(X) \neq 0$ for all $X \in \mathfrak{g}$. We remark that a map ν is equivariant if $\nu(g \cdot x) = \mathrm{Ad}\, g^*(\nu(x))$.

Definition 1: A map ν is called G-moment map if and only if (i) it is equivariant and (ii) it satisfies the transversality condition.

We remark that for simply connected Kähler manifolds the moment map can be constructed using the invariance of Kähler form and complex structure and it satisfies the transversality property. However additional conditions are required in order the moment map to be equivariant.

Next given a point $\zeta \in \mathfrak{g}$, denote the level set $\nu^{-1}(\zeta)$ by P. Since the map ν is G-equivariant, level sets are invariant if the group G is Abelian or if the point ς is invariant. Assuming that the level set P is invariant, and the action of G on P is free, then the quotient space $N = P/G$ is a smooth manifold. Let $\pi: P \to N$ be the quotient map.

It can be shown that in fact $N = P/G$ is a complex manifold. This construction can be done as follows. For each point m in the space P, its tangent space is

$$T_m P = \{t \in T_m M : d\nu(t) = 0\}.$$

Consider the vector subspace

$$\mathcal{U}_m = \{t \in T_m P : Id\,\nu(t) = 0\}.$$

Due to the transversality condition, this space is transversal to the vectors generated by elements in $\mathfrak{g}$. In addition, this space is a vector subspace of $T_m P$ with co-dimension $\dim \mathfrak{g}$, and hence it is a vector subspace of $T_m M$ with co-dimension $2 \dim \mathfrak{g}$. The same condition implies that, as a subbundle of $TM_{|P}$, $\mathcal{U}$ is closed under I. Moreover there is a G-invariant splitting,

$$TP = \mathcal{U} \oplus \mathcal{V}, \tag{1}$$

where $\mathcal{V}$ is the tangent space to the orbits of G and it is the bundle of kernels of $d\pi$. We use the terms ''horizontal'' and ''vertical'' for $\mathcal{U}$ and $\mathcal{V}$.

As the projection π is an isomorphism on $\mathcal{U}$, for any tangent vector $\hat{A}$ at $\pi(m)$, there exists a unique element A^u in $\mathcal{U}_m$ such that $d\pi(A^u) = \hat{A}$. We call A^u horizontal lift of $\hat{A}$. The complex structure on N is defined by

$$I\hat{A} = d\pi(IA^u), \quad \text{i.e.,} \quad (I\hat{A})^u = IA^u. \tag{2}$$

Theorem 1: *Let $(M,\mathcal{I},g)$ be a KT-manifold. Suppose that G is a compact group of complex isometries admitting a G-moment map ν. Then the complex reduced space $N=M//G$ inherits a KT structure.*

Proof: To show this, it suffices to find a complex structure I and a Hermitian metric g on N which are induced from M because for every Hermitian structure (I,g), there always exists a unique KT structure on N.[5,6]

To begin, since $\mathcal{U}$ is G-invariant, if X^u is tangent to P at m and is contained in $\mathcal{U}$, then for any element $f\in G$, $dL_f(X^u)$ is tangent to P at $f(m)$ and is contained in $\mathcal{U}$. Using $\pi\circ L_f=\pi$, if X^u is a horizontal lift of $\hat{X}$ to a point m, then $d\pi\circ dL_f(X^u)=d\pi(X^u)=\hat{X}$. Therefore, $dL_f(X^u)$ is the horizontal lift of $\hat{X}$ to $f(m)$.

Since G is also a group of isometries, $g(dL_f(X),dL_f(Y))=g(X,Y)$ for any vectors X and Y tangent to P. Define a metric $\hat{g}$ on N by

$$\hat{g}_{\pi(p)}(\hat{X},\hat{Y})=g_p(X^u,Y^u), \tag{3}$$

where X^u and Y^u are the horizontal lifts of $\hat{X}$ and $\hat{Y}$, respectively. From the analysis above, the metric $\hat{g}$ is independent from the choice of the reference point p of the orbit. Note that the "horizontal" and "vertical" spaces ARE NOT necessarily orthogonal.

To prove that $\hat{g}$ is Hermitian, we note that

$$\begin{aligned} g_{\pi(p)}(I\hat{X},I\hat{Y}) &= g_p((I\hat{X})^u,(I\hat{Y})^u) \\ &= g_p(I(\hat{X}^u),I(\hat{Y})^u)=g_p(\hat{X}^u,\hat{Y}^u)=g_{\pi(p)}(\hat{X},\hat{Y}). \end{aligned} \tag{4}$$

Q.E.D.

B. HKT reduction

We shall begin with a description of hypercomplex reduction developed by Joyce.[2] Let G be a compact group of hypercomplex automorphism on M. Denote the algebra of hyper-holomorphic vector fields by $\mathfrak{g}$. Suppose that $\nu=(\nu_1,\nu_2,\nu_3):M\to\mathbf{R}^3\otimes\mathfrak{g}$ is a G-equivariant map satisfying the following two conditions. The Cauchy–Riemann condition, $I_1d\nu_1=I_2d\nu_2=I_3d\nu_3$, and the transversality condition, $I_ad\nu_a(X)\neq 0$ for all $X\in\mathfrak{g}$. In analogy with a similar definition given in the previous section, any map satisfying these conditions is called a G-moment map. Given a point $\zeta=(\zeta_1,\zeta_2,\zeta_3)$ in $\mathbf{R}^3\otimes\mathfrak{g}$, denote the level set $\nu^{-1}(\zeta)$ by P. Assuming that the level set P is invariant, and the action of G on P is free, then the quotient space $N=P/G$ is a smooth manifold.

Joyce proved that the quotient space $N=P/G$ inherits a natural hypercomplex structure.[2] His construction runs as follows. For each point m in the space P, its tangent space is

$$T_mP=\{t\in T_mM: d\nu_1(t)=d\nu_2(t)=d\nu_3(t)=0\}.$$

Consider the vector subspace,

$$\mathcal{U}_m=\{t\in T_mP: I_1d\nu_1(t)=I_2d\nu_2(t)=I_3d\nu_3(t)=0\}. \tag{5}$$

Due to the transversality condition, this space is transversal to the vectors generated by elements in $\mathfrak{g}$. Due to the Cauchy–Riemann condition, this space is a vector subspace of T_mP with co-dimension $\dim\mathfrak{g}$, and hence it is a vector subspace of T_mM with co-dimension $4\dim\mathfrak{g}$.

The same condition implies that, as a subbundle of $TM_{|P}$, $\mathcal{U}$ is closed under I_a. Moreover there is a G-invariant splitting,

$$TP=\mathcal{U}\oplus\mathcal{V}, \tag{6}$$

where $\mathcal{V}$ is the tangent space to the orbits of G and it is the bundle of kernels of $d\pi$. Again, we use the terms ''horizontal'' and ''vertical'' for $\mathcal{U}$ and $\mathcal{V}$ although these two spaces are not necessarily orthogonal. Following techniques and notations of the last section, a hypercomplex structure on N is defined by

$$I_a\hat{A}=d\pi(I_aA^u), \quad \text{i.e.,} \quad (I_aA)^u=I_aA^u. \tag{7}$$

Theorem 2: *Let $(M,\mathcal{I},g)$ be a HKT-manifold. Suppose that G is a compact group of hypercomplex isometries admitting a G-moment map ν. Then hypercomplex reduced space $N=M//G$ inherits a HKT structure.*

Proof: Define hypercomplex structures I_a on $N=P/G$ as in (7). As in the previous section, define a metric $\hat{g}$ on N by

$$g_p(X^u,Y^u)=\hat{g}_{\pi(p)}(\hat{X},\hat{Y}), \tag{8}$$

where X^u and Y^u are the horizontal lifts of $\hat{X}$ and $\hat{Y}$, respectively. This is a hyper-Hermitian metric.

On M, define $F_a(X,Y)=g(I_aX,Y)$ and

$$\omega_1=F_2-iF_3. \tag{9}$$

This is a (0,2)-form with respect to I_1. Since the hyper-Hermitian structure on X admits a HKT-metric, $\overline{\partial}\omega_1=0$. Equivalently, the (0,3)-part of $d\omega_1$ vanishes.

Similarly, we define $\hat{\omega}_1$ on N. By (Ref. 5, Proposition 2), the hyper-Hermitian metric $\hat{g}$ is a HKT-metric if and only if $\overline{\partial}\hat{\omega}_1=0$. In other words, we need to prove that the type (0,3)-part of $d\hat{\omega}_1$ with respect to I_1 vanishes. This is equivalent to

$$\pi^*d\hat{\omega}_1(X^u,Y^u,Z^u)=0 \tag{10}$$

for any vectors X^u,Y^u,Z^u in $\mathcal{U}^{0,1}_{I_1}$. As

$$\pi^*\hat{\omega}_1(Y^u,Z^u)=\omega_1(Y^u,Z^u) \tag{11}$$

and we have the following computation:

$$\begin{aligned}
d\pi^*\hat{\omega}_1(X^u,Y^u,Z^u)&=X^u(\pi^*\hat{\omega}_1(Y^u,Z^u))-Y^u(\pi^*\hat{\omega}_1(Z^u,X^u))+Z^u(\pi^*\hat{\omega}_1(X^u,Y^u))\\
&\quad-\pi^*\hat{\omega}_1([X^u,Y^u],Z^u)-\pi^*\hat{\omega}_1([Y^u,Z^u],X^u)-\pi^*\hat{\omega}_1([Z^u,X^u],Y^u)\\
&=X^u(\omega_1(Y^u,Z^u))-Y^u(\omega_1(Z^u,X^u))+Z^u(\omega_1(X^u,Y^u))-\omega_1([X^u,Y^u]^u,Z^u)\\
&\quad-\omega_1([Y^u,Z^u]^u,X^u)-\omega_1([Z^u,X^u]^u,Y^u)=d\omega_1(X^u,Y^u,Z^u)\\
&\quad+\omega_1([X^u,Y^u]^v,Z^u)+\omega_1([Y^u,Z^u]^v,X^u)+\omega_1([Z^u,X^u]^v,Y^u)\\
&=\omega_1([X^u,Y^u]^v,Z^u)+\omega_1([Y^u,Z^u]^v,X^u)+\omega_1([Z^u,X^u]^v,Y^u).
\end{aligned}$$

To complete the proof of this theorem we claim that $[X^u,Y^u]^v=0$. Equivalently, $d_a\nu_a([X^u,Y^u])=0$ for $a=1,2,3$. Since X^u and Y^u are in the kernel of $d_a\nu_a$ for $a=1,2,3$,

$$dd_a\nu_a(X^u,Y^u)=X^u(d_a\nu_a(Y^u))-Y_a(d_a\nu_a(X^u))-d_a\nu_a([X^u,Y^u])=-d_a\nu_a([X^u,Y^u]).$$

As $dd_1\nu_1$ is of type-(1,1) with respect to I_1 and X^u and Y^u are type-(0,1) with respect to I_1, $dd_1\nu_1(X^u,Y^u)=0$. By the Cauchy–Riemann condition $d_1\nu_1=d_2\nu_2=d_3\nu_3$, our claim follows.

Q.E.D.

III. MOMENT MAPS FOR STRONG KT AND HKT SPACES

As we have seen, the construction of new HKT manifolds using HKT reduction requires the existence of a G-moment map satisfying the requirements of Theorem 2. This moment map is not specified within the theory, as it is the case for the hyper-Kähler reduction, but rather its existence is an additional assumption of the construction. However as we shall see in the special case of reduction for strong KT (and HKT) manifolds, under certain assumptions, there is such a moment map which arises naturally. The local construction of a moment map for KT and HKT geometries presented below parallels the construction of an action for two-dimensional (2,0)- and (4,0)-supersymmetric gauged sigma models with the Wess–Zumino term in Ref. 7, respectively. Again, we focus on a reduction theory for strong KT-structure first. The reduction theory for strong HKT-structures follow.

A. Local consideration

Let G a compact group of complex automorphisms on a *strong* KT manifold M. In particular G is a group of isometries on M which leaves in addition the torsion three-form H invariant. To continue we introduce a basis $\{e_a; a=1,\ldots,\dim \mathfrak{g}\}$ in the Lie algebra of $\mathfrak{g}$ and denote the associated vector fields of M with $\{X^a; a=1,\ldots,\dim \mathfrak{g}\}$; denote with $\{e^a; a=1,\ldots,\dim \mathfrak{g}^*\}$ the associated basis in the dual $\mathfrak{g}^*$ of $\mathfrak{g}$. The conditions for invariance of the KT structure can now be written as

$$\mathcal{L}_a g=0, \quad \mathcal{L}_a H=0, \quad \mathcal{L}_a I=0, \tag{12}$$

where $\mathcal{L}_a=\mathcal{L}_{X^a}$; similarly later for the inner derivation we have $i_a=i_{X^a}$.

Using the assumption that M is a strong KT manifold, $dH=0$, the last equation above implies that $d i_a H=0$ and so there is a locally defined one-form u_a such that

$$i_a H=d u_a .$$

Clearly u_a is uniquely defined up to the addition of a closed one-form.

Next let us denote with $\tilde{X}$ the one-form dual with the vector field X with respect to the KT metric. Using $\mathcal{L}_a I=0$, one can show that the two-form $d(\tilde{X}_a+u_a)$ is type-(1,1) with respect to the complex structure I. Therefore, by the $\overline{\partial}$-Poincare Lemma, there is a locally defined complex-valued function h_a on M such that $(\tilde{X}_a+u_a)^{1,0}=\partial h_a$. Let f_a be the real part of h_a. Define

$$w_a=\tilde{X}_a+u_a-d f_a . \tag{13}$$

Then $w_a^{1,0}=i\partial \nu_a$, where ν_a is a constant multiple of the imaginary part of h_a. Therefore, we can write

$$w_a=I d \nu_a . \tag{14}$$

Let $\xi=\xi^a e_a$ be any element in $\mathfrak{g}$. Define a map ν from M to $\mathfrak{g}^*$ by

$$\nu(x)(\xi) := \sum_a \xi^a \nu_a(x). \tag{15}$$

A necessary condition for ν to be well-defined on M is that the class of $i_a H$ in $H^2(M,\mathbf{R})$ should be trivial. If in addition M satisfies the $\partial\overline{\partial}$-lemma, then ν will be well-defined on M.

In the case when the group G is Abelian, the issue of equivariance is absent and hence the map ν so constructed is the moment map. Before we investigate equivariance in general, we consider the issue of nondegeneracy.

Definition 2: A holomorphic Killing vector field X is nondegenerate if $d\nu_X \neq 0$.

Therefore, a holomorphic Killing vector field is nondegenerate if its moment map is nonconstant. The following proposition is useful to determine when a holomorphic Killing vector field is nondegenerate.

Proposition 1: If the length of a holomorphic Killing vector field is nonconstant, then the vector field is nondegenerate.

Proof: Note that $d\nu_X = 0$ if and only if $d\tilde{X} + du = 0$, i.e., $d\tilde{X} + \iota_X H = 0$. It means that for any vector field Y and Z,

$$Y(g(X,Z)) - Z(g(X,Y)) - g(X,[Y,Z]) + H(X,Y,Z) = 0,$$

$$\text{i.e.,} \quad g(\nabla_Y X, Z) + g(X, \nabla_Y Z) - g(\nabla_Z X, Y) - g(X, \nabla_Z Y) - g(X,[Y,Z]) + H(X,Y,Z) = 0,$$

$$\text{or} \quad g(\nabla_Y X, Z) - g(\nabla_Z X, Y) + 2H(X,Y,Z) = 0.$$

On the other hand, since $\mathcal{L}_X g = 0$ and $\nabla g = 0$,

$$\begin{aligned} 0 &= X(g(Y,Z)) - g([X,Y],Z) - g(Y,[X,Z]) \\ &= g(\nabla_X Y, Z) + g(Y, \nabla_X Z) - g([X,Y],Z) - g(Y,[X,Z]) \\ &= g(\nabla_Y X, Z) + g([X,Y],Z) + H(X,Y,Z) + g(Y, \nabla_Z X) \\ &\quad + g(Y,[X,Z]) + H(Y,X,Z) - g([X,Y],Z) - g(Y,[X,Z]) \\ &= g(\nabla_Y X, Z) + g(Y, \nabla_Z X). \end{aligned}$$

Combining the above two identities, we find that for any vector fields Y, Z,

$$g(\nabla_Y X, Z) = -H(X,Y,Z) = -du_X(Y,Z). \tag{16}$$

In particular, $g(\nabla_Y X, X) = 0$ for any Y. Since $\nabla g = 0$. It implies that $dg(X,X) = 0$. Q.E.D.

B. Equivariance

Now we seek conditions for ν to be equivariant. This issue will be analyzed in the next few paragraphs. The map ν is equivariant if and only if $\nu(g \cdot x) = \mathrm{Ad}g^*(\nu(x))$. Let X be any element in $\mathfrak{g}$. The equivariance is determined by

$$\nu(g \cdot x)(X) = \nu(x)(\mathrm{Ad}\, g(X)). \tag{17}$$

The infinitesimal version of the above identity is

$$\mathcal{L}_Y \nu_X = \nu_{[V,X]}; \quad \text{equivalently} \quad \mathcal{L}_Y \nu_X - \nu_{[Y,X]} = 0. \tag{18}$$

Let $[X_b, X_a] = f^c_{ba} X_c$ be the structural equations for the algebra $\mathfrak{g}$ so that f^c_{ba} are constants. Apply the above formula to w_a and u_a, respectively, with respect to X_b, the equivariance conditions for w_a and u_a are

$$\mathcal{L}_b w_a - f^c_{ba} w_c = 0, \quad \mathcal{L}_b u_a - f^c_{ba} u_c = 0. \tag{19}$$

These are nontrivial conditions. Note that

$$\begin{aligned} d\mathcal{L}_b u_a &= \mathcal{L}_b du_a = \mathcal{L}_b \iota_a H = \iota_{\mathcal{L}_b X_a} H + \iota_a \mathcal{L}_b H \\ &= \iota_{\mathcal{L}_b X_a} H = f^c_{ba} \iota_c H = f^c_{ba} du_c = d(f^c_{ba} u_c). \end{aligned} \tag{20}$$

By Poincaré lemma, there exists a locally defined closed 1-form v_{ba} such that

$$\mathcal{L}_b u_a - f^c_{ba} u_c = v_{ba}. \tag{21}$$

Therefore, v_{ba} is the obstruction for u_a to be equivariant.

Next, note that $\mathcal{L}_a g = 0$,

$$\begin{aligned}(\mathcal{L}_b \tilde{X}_a)X &= \mathcal{L}_b(g(X_a, X)) - g(X_a, \mathcal{L}_b X) \\ &= g(\mathcal{L}_b X_a, X) + g(X_a, \mathcal{L}_b X) - g(X_a, \mathcal{L}_b X) \\ &= f^c_{ba} g(X_c, X) = f^c_{ba} \tilde{X}_c X.\end{aligned}$$

Therefore, the $\mathfrak{g}^*$-valued 1-form $w := w_a \eta^a$ is equivariant if and only if $u := u_a \eta^a$ is equivariant.

Assuming that u is equivariant. This implies that after a possible shift of u_a with respect to a closed one-form, u_a must satisfy the above equation. Note that even if u_a is equivariant, it is not unique but rather defined up to an equivariant *closed* one-form.

Next since dw_a is an (1,1)-form and if we assume that the $\partial\bar{\partial}$-lemma applies on the manifold M (see either Ref. 8, 5.11 or Ref. 9, Corollary 2.110), there is a function ν_a on M such that

$$dw_a = dd^c v_a = dId\nu_a. \tag{22}$$

Therefore, the 1-form,

$$z_a = w_a - Id\nu_a$$

is closed. In the above equation ν_a is not uniquely defined but rather it is defined up the addition of the real part of a *holomorphic* function.

As we have assumed that u_a is equivariant, w_a is equivariant. We obtain

$$Id\nu_{ba} + z_{ba} = 0, \tag{23}$$

where $\nu_{ba} = \mathcal{L}_b \nu_a - f_{ba}{}^c \nu_c$ and $z_{ba} = \mathcal{L}_b z_a - f_{ba}{}^c z_c$. Since $dz_{ba} = 0$, (23) implies that $dd^c \nu_{ba} = 0$. By $\partial\bar{\partial}$-Lemma again, ν_{ba} is a harmonic function and hence is the real part of a holomorphic function f_{ba}. If, in addition,

$$f_{ba} = \mathcal{L}_b F_a - f_{ba}{}^c F_c \tag{24}$$

for some holomorphic functions F_a, then redefining ν_a as $\nu_a - \mathrm{Re}\, F_a$ and z_a as $z_a - d\,\mathrm{Im}\, F_a$ both ν_a and z_a become equivariant. So there is a choice of u_a, such that $w_a = Id\nu_a$. Therefore, we have found an equivariant moment map $\nu: M \to \mathfrak{g}^*$.

C. Cohomology

The various conditions that we have found for the existence of a moment map in the previous section can be identified as classes in de-Rham H^*_{dR} and in H^*_δ cohomology, where δ will be defined shortly. Let δ_G be the map defining Lie algebra cohomology in the usual way.[10] In particular, for $\theta \in \mathfrak{g}^*$ and $\zeta,\ \eta \in \mathfrak{g}$,

$$\delta_G \theta(\zeta, \eta) = -\theta([\zeta, \eta]). \tag{25}$$

Therefore, (note the convention for wedge product) in terms of structural constants with respect to the dual basis θ^a,

$$\delta_G\theta^a=-\sum_{b,c} f^a_{bc}\theta^b\otimes\theta^c$$

$$=-\sum_{b<c} f^a_{bc}(\theta^b\otimes\theta^c-\theta^c\otimes\theta^b)=-\sum_{b<c} f^a_{bc}\theta^b\wedge\theta^c=-\frac{1}{2}\sum_{b,c} f^a_{bc}\theta^b\wedge\theta^c. \tag{26}$$

In particular, $\delta_G^2=0$. Next for ϕ in $\Lambda^l(M)$ and X in $\mathfrak{g}$, define

$$\hat{\delta}\phi(X):=\mathcal{L}_X\phi. \tag{27}$$

Equivalently, $\hat{\delta}\phi=\mathcal{L}_a\phi\cdot\theta^a$. Then we extend this operator to

$$\delta:\Lambda^l(M)\otimes\Lambda^k\mathfrak{g}^*\otimes\mathfrak{g}^*\to\Lambda^l(M)\otimes\Lambda^{k+1}\mathfrak{g}^*\otimes\mathfrak{g}^* \tag{28}$$

as follows. If ϕ is in $\Lambda^l(M)$, θ is in $\Lambda^k\mathfrak{g}^*$ and η is in $\mathfrak{g}^*$, then define

$$\begin{aligned}\delta(\phi\cdot\theta\otimes\eta):=&\hat{\delta}\phi\wedge\theta\otimes\eta+\phi\cdot\delta_G\theta\otimes\eta\\&+(-1)^k\phi\cdot\theta\wedge\delta_G\eta.\end{aligned} \tag{29}$$

This map generates a resolution.

$$\begin{aligned}\Lambda^l(M)\otimes\mathfrak{g}^*\xrightarrow{\delta_0}&\Lambda^l(M)\otimes\Lambda^1\mathfrak{g}^*\otimes\mathfrak{g}^*\cdots\\&\to\Lambda^l(M)\otimes\Lambda^k\mathfrak{g}^*\otimes\mathfrak{g}^*\\&\xrightarrow{\delta_k}\Lambda^l(M)\otimes\Lambda^{k+1}\mathfrak{g}^*\otimes\mathfrak{g}^*\cdots.\end{aligned}$$

We claim that this resolution is a complex, i.e., $\delta_k\circ\delta_{k+1}=\delta^2=0$. To check, notice that

$$\begin{aligned}\delta^2(\phi\cdot\theta\otimes\eta)=&\delta(\hat{\delta}\phi\wedge\theta)\otimes\eta+(-1)^{k+1}\hat{\delta}\phi\wedge\theta\wedge\delta_G\eta+\hat{\delta}\phi\wedge\delta_G\theta\otimes\eta\\&+\phi\cdot\delta_G^2\phi\otimes\eta+(-1)^{k+1}\phi\cdot\delta_G\theta\wedge\delta_G\eta+(-1)^k\hat{\delta}\phi\wedge\theta\wedge\delta_G\eta\\&+(-1)^k\phi\cdot\delta_G\theta\wedge\delta_G\eta+(-1)^{2k}\phi\cdot\theta\wedge\delta_G^2\eta\\=&\delta(\hat{\delta}\phi\wedge\theta)\otimes\eta+\hat{\delta}\phi\wedge\delta_G\theta\otimes\eta=(\delta(\hat{\delta}\phi\wedge\theta)+\hat{\delta}\phi\wedge\delta_G\theta)\otimes\eta\\=&(\delta(\hat{\delta}\phi)\wedge\theta-\hat{\delta}\phi\wedge\delta_G\theta+\hat{\delta}\phi\wedge\delta_G\theta)\otimes\eta\\=&(\delta(\mathcal{L}_a\phi\theta^a))\wedge\theta\otimes\eta\\=&(\mathcal{L}_b\mathcal{L}_a\phi\cdot\theta^b\wedge\theta^a+\mathcal{L}_c\phi\cdot\delta_G\theta^c)\wedge\theta\otimes\eta\\=&(\mathcal{L}_b\mathcal{L}_a\phi-\tfrac{1}{2}f^c_{ba}\mathcal{L}_c\phi)\cdot\theta^b\wedge\theta^a\wedge\theta\otimes\eta.\end{aligned}$$

Since $[\mathcal{L}_a,\mathcal{L}_a]\phi=f^c_{ba}\mathcal{L}_c\phi$ and $f^c_{ba}=-f^c_{ab}$,

$$\mathcal{L}_b\mathcal{L}_a\phi-\tfrac{1}{2}f^c_{ba}\mathcal{L}_c\phi=\mathcal{L}_a\mathcal{L}_b\phi+\tfrac{1}{2}f^c_{ba}\mathcal{L}_c\phi=\mathcal{L}_a\mathcal{L}_b\phi-\tfrac{1}{2}f^c_{ab}\mathcal{L}_c\phi. \tag{30}$$

It shows that the term $\mathcal{L}_b\mathcal{L}_a\phi-\frac{1}{2}f^c_{ba}\mathcal{L}_c\phi$ is symmetric in the indices ab while the term $\theta^b\wedge\theta^a$ is skew symmetric in ab. It follows that $\delta(\mathcal{L}_a\phi\theta^a)=0$ and hence $\delta^2=0$ as claimed.

One can now define a cohomology theory with respect to δ in the usual way and denote it with

$$H^k_\delta(\Lambda^l(M)\otimes\mathfrak{g}^*) := \frac{\ker \delta_k}{\text{image } \delta_{k-1}}. \tag{31}$$

Since δ commutes with d, one can also naturally define the cohomology groups $H^k_\delta(C^l(M)\otimes\mathfrak{g}^*)$, where $C^l(M)$ are the close l-forms on M.

A cohomology theory based on a resolution of $\mathcal{O}\otimes\mathfrak{g}^*$, where $\mathcal{O}$ is the sheaf of germs of holomorphic functions on M, is similarly defined. This is possible because the group G consists of holomorphic actions. In particular, $\overline{\partial}\circ\mathcal{L}_a=\mathcal{L}_a\circ\overline{\partial}$. This cohomology is

$$H^k_\delta(\mathcal{O}\otimes\mathfrak{g}^*) := \frac{\ker \delta:\mathcal{O}\otimes\Lambda^k\mathfrak{g}^*\otimes\mathfrak{g}^*}{\text{image } \delta:\mathcal{O}\otimes\Lambda^{k-1}\mathfrak{g}^*\otimes\mathfrak{g}^*}. \tag{32}$$

Returning now in the discussion of the previous section, we have seen a necessary condition for the existence of a moment map in the KT case is that i_aH is a trivial class in $H^2_{dR}(M)$. Now we write $i_aH=du_a$ and define $u=u_a\eta^a$. This is a section of $\Lambda^1(M)\otimes\mathfrak{g}^*$. Using (26),

$$\begin{aligned}\delta u &= (\delta u_a)\otimes\eta^a+\sum_c u_c\delta_G\eta^c \\ &= \mathcal{L}_b u_a\theta^b\otimes\eta^a-\sum_{a,b,c} f^c_{ba}u_c\theta^b\otimes\eta^a \qquad (33)\\ &= \sum_{a,b}\left(\mathcal{L}_b u_a-\sum_c f^c_{ba}u_c\right)\theta^b\otimes\eta^a. \qquad (34)\end{aligned}$$

Due to (20), the 1-form part is closed. Therefore δu is an element of $C^1(M)\otimes\Lambda^1\mathfrak{g}^*\otimes\mathfrak{g}$. Obviously, it is in the kernel of δ. It defines a class in $H^1_\delta(C^1(M)\otimes\mathfrak{g}^*)$. Since u is not necessarily a closed 1-form, this class is not necessarily trivial although it is represented by δu. Due to computation of previous paragraphs, this cohomology class is the obstruction for adjusting u by a closed 1-form so that it could be equivariant.

If this class vanishes, then as we have explained $\delta(w_a\eta^a)=0$ as well. Using this and assuming that ν_a is well-defined in $w=Id\nu+z$, where $\nu=\nu_a\eta^a$ and $z=z_a\eta^a$, we have $Id\delta\nu+\delta z=0$. As we have explained in the previous section the obstruction for both z and ν to be equivariant are δz and $\delta\nu$, respectively. The last identity implies that it suffices to find the condition for $\delta\nu=0$.

Due to identity (22), $\delta w=0$ and $\mathcal{L}_aI=0$, we have $dId\delta\nu=0$. Therefore, by $\partial\overline{\partial}$-Lemma, there exists holomorphic function f_{ba} such that $\nu_{ba}=\text{Re}\, f_{ba}$. Define

$$f := f_{ba}\theta^b\otimes\eta^a. \tag{35}$$

This is an element in $\mathcal{O}\otimes\Lambda^1\mathfrak{g}^*\otimes\mathfrak{g}^*$. The function part of δf is holomorphic as the group G consists of holomorphic actions.

However, the real part of δf is equal to $\delta\nu=0$. Therefore, δf is purely imaginary. This is possible only if $\delta f=0$. It follows that f defines a class in $H^1_\delta(\mathcal{O}\otimes\mathfrak{g}^*)$. Note that the class of f vanishes if and only if the equation $f=\delta F$ has a solution. In other words, there are solutions for Eq. (24).

Some of the conditions that we have derived above can be cast into an elegant form using equivariant cohomology.[11] In physics, it is known that the obstructions for gauging *bosonic* two-dimensional sigma models with the Wess–Zumino term[12,13] are elements of equivariant cohomology.[14] The theorem below provides sufficient conditions for KT reduction.

Theorem 3: *Let M be a strong KT manifold and G be a compact group acting on M and leaving invariant the KT structure. If the torsion three-form H admits an equivariant extension as a closed form in $EG\times_G M$, $H^1_\delta(\mathcal{O}\otimes\mathfrak{g}^*)=0$ and the $\partial\overline{\partial}$-lemma applies on M, then $M//G$ is a KT manifold.*

Proof: Note that EG is the universal classifying bundle space for the group G. It can be shown that a closed three-form H in M admits an equivariant extension in $EG\times_G M$, if H is invariant under the group action of G on M and there are equivariant one-forms $\{u_a;a=1,\ldots,\dim\mathfrak{g}\}$ on M such that

$$i_a H = du_a \quad \text{and} \quad i_a u_b + i_b u_a = 0. \tag{36}$$

Of course the one-form u_a is defined up to the addition of an equivariant closed one-form v_a. Because of this, the one-form $w_a = u_a + \tilde{X}_a$ is equivariant and dw_a is an (1,1) form on M. If the $\partial\overline{\partial}$-lemma applies, then $w_a = Id\nu_a + z_a$, where ν_a is a function on M and z_a is closed one-form. It can be shown that in fact z_a is equivariant. Indeed, since w_a is equivariant and the G-action preserves the complex structure, we have

$$Id\nu_{ba} + z_{ba} = 0, \tag{37}$$

where $\nu_{ba} = \mathcal{L}_b\nu_a - f_{ba}{}^c\nu_c$ and $z_{ba} = \mathcal{L}_b z_a - f_{ba}{}^c z_c$. We have seen that the obstruction for z_a and ν_a to be equivariant lies in $H^1_\delta(\mathcal{O}\otimes\mathfrak{g}^*)$. Since this vanishes z_a and ν_a are equivariant. So there is a choice of u_a, such that $w_a = Id\nu_a$.

It remains to prove the transversality condition. This follows from the last condition in (36) because it implies that $i_a u_b$ is skew-symmetric and so $i_a w_b$ is the sum of a nondegenerate symmetric matrix with $i_a u_b$. Therefore ν is a G-moment map and so $M//G$ is a KT manifold. Q.E.D.

D. Moment maps on strong HKT structures

The construction of G-moment maps for the reduction of strong HKT manifolds can proceed as in the case of strong KT manifolds above. The only difference is that for each complex structure $\{I_r;r=1,2,3\}$ one gets

$$w_a = I_r d(\nu^r)_a + z^r_a, \tag{38}$$

where z^r_a are again equivariant closed one-forms provided that the obstructions in $H^1_\delta(\mathcal{O}\otimes\mathfrak{g})$ vanish. In this case however it is not always possible to redefine u_a such that $w_a = I_r d(\nu^r)_a$ unless $z^1_a = z^2_a = z^3_a$. Nevertheless, we can still use the map $\nu: M\to\mathbf{R}^3\otimes\mathfrak{g}$ as defined in (38) as a moment map. This moment map is equivariant but neither transversality nor the Cauchy–Riemann conditions generically hold. Thus we have the following theorem:

Theorem 4: *Let M be a strong HKT manifold and G be a compact group acting on M and leaving invariant the HKT structure. If the torsion three-form H admits an extension as a closed form in $EG\times_G M$ such that $w_a = I_r d(\nu^r)_a$ with ν equivariant, then $M//G$ is a HKT manifold.*

Proof: The proof follows from that of reductions of strong KT manifolds and that of reductions of weak HKT manifolds. Q.E.D.

IV. POTENTIAL FUNCTIONS

Recall that if $(M,\mathcal{I},g)$ is a HKT manifold with Kähler forms ω_a, a *HKT potential* is a function ρ such that $2\omega_1 = dd_1\rho + d_2d_3\rho, 2\omega_2 = dd_2\rho + d_3d_1\rho, 2\omega_3 = dd_3\rho + d_1d_2\rho$. In this section, we follow the methods in Ref. 15 to find a potential function on reduced space. We continue to use the notations established in Sec. II B.

Theorem 5: *Let $(M,\mathcal{I},g)$ be a HKT manifold with HKT potential function ρ. Suppose that G is a compact group of hypercomplex isometries leaving ρ invariant with moment map $\nu=(\nu_1,\nu_2,\nu_3)$ such that the tangent vectors to the orbits of G in $\nu^{-1}(0)$ are in the* $\ker(d_a\rho)$, *for $a=1,2,3$. Then the function ρ induces a HKT potential function on the reduced space $N=M//G$.*

Proof: Let $P:=\nu^{-1}(0)$ and $i:P\to M$ be the inclusion map. Now we first check that $i^*dd_a\rho|_{\mathcal{U}}=dd_a i^*\rho|_{\mathcal{U}}$, where $\mathcal{U}$ is defined in (5). To this end notice that

$$i^*d\rho(X^u)=d\rho(X^u),\quad i^*d\rho([X^u,Y^u])=d\rho([X^u,Y^u]),$$

and $i^*I_a d\rho(X^u)=I_a d\rho(di(X^u))=-d\rho(I_aX^u)$ because $I_a d\rho(X)=-d\rho(I_aX)$. By direct computations after restricting on points of P we have

$$\begin{aligned}(i^*dd_a\rho)(X^u,Y^u)&=di^*d_a\rho(X^u,Y^u)\\&=X^u((i^*I_ad\rho)(Y^u))-Y^u((i^*I_ad\rho)(X^u))-i^*I_ad\rho([X^u,Y^u])\\&=-X^u(d\rho(I_aY^u))+Y^u(d\rho(I_aX^u))+d\rho(I_a[X^u,Y^u])\\&=-X^u(d\rho(I_aY^u))+Y^u(d\rho(I_aX^u))+d\rho(I_a[X^u,Y^u]^u).\end{aligned}$$

The last equality is due to $d\rho(I_a[X^u,Y^u]^v)=-d_a\rho([X^u,Y^u]^v)=0$. This is true because $[X^u,Y^u]^v$ is tangent to an orbit of G and the condition in the theorem. We shall use the same argument repeatedly and implicitly in subsequent computation.

As the map ρ is G-invariant, for x in P, we may define

$$\rho_N(\pi(x)):=\rho(x),\tag{39}$$

where π is the quotient map from P onto $N=P/G$. In other words, $\pi^*\rho_N=\rho$. It follows that

$$\begin{aligned}(\pi^*dd_a\rho_N)(X^u,Y^u)&=d\pi^*d_a\rho_N(X^u,Y^u)\\&=X^u(d_a\rho_N(d\pi(Y^u)))-Y^u(d_a\rho_N(d\pi(X^u))-d_a\rho_N(d\pi([X^u,Y^u]))\\&=-X^u(d\rho_N(I_ad\pi Y^u))+Y^u(d\rho_N(I_ad\pi X^u))+d\rho_N(I_ad\pi[X^u,Y^u]))\\&=-X^u(d\rho(I_aY^u))+Y^u(d\rho(I_aX^u))+d\rho_N(d\pi(I_a[X^u,Y^u]^u))\\&=-X^u(d\rho(I_aY^u))+Y^u(d\rho(I_aX^u))+d\rho(I_a[X^u,Y^u]^u).\end{aligned}$$

It follows that $i^*dd_a\rho_{|\mathcal{U}}=\pi^*dd_a\rho_{N|\mathcal{U}}$. Similarly,

$$\begin{aligned}(\iota^*d_ad_b\rho)(X^u,Y^u)&=(I_adI_cd\rho)(di(X^u),di(Y^u))\\&=(I_adI_cd\rho)(X^u,Y^u)\\&=dI_cd\rho(I_aX^u,I_aY^u)\\&=I_aX^u(d_c\rho(I_aY^u))-I_aY^u(d_c\rho(I_aX^u))-d_c\rho([I_aX^u,I_aY^u])\\&=I_aX^u(d_c\rho(I_aY^u))-I_aY^u(d_c\rho(I_aX^u))-d_c\rho([I_aX^u,I_aY^u]^u).\end{aligned}$$

On the other hand,

$$\begin{aligned}(\pi^*d_ad_b\rho_N)(X^u,Y^u)&=(I_adI_cd\rho_N)(d\pi(X^u),d\pi(Y^u))\\&=(dI_cd\rho_N)(I_ad\pi(X^u),I_ad\pi(Y^u))\\&=(dI_cd\rho_N)(d\pi I_a(X^u),d\pi I_a(Y^u))\\&=(\pi^*dI_cd\rho_N)(I_aX^u,I_aY^u)\\&=(d\pi^*I_cd\rho_N)(I_aX^u,I_aY^u)\\&=I_aX^u(\pi^*I_cd\rho_N(I_aY^u)-I_aY^u(\pi^*I_cd\rho_N(I_aX^u))-\pi^*I_cd\rho_N([I_aX^u,I_aY^u])\\&=I_aX^u(-d\rho_N(d\pi(I_cI_aY^u))-I_aY^u(-d\rho_N(d\pi(I_cI_aX^u))\\&\quad-d\rho_N(d\pi I_c[I_aX^u,I_aY^u])\\&=I_aX^u(I_cd\rho(I_aY^u))-I_aY^u(I_cd\rho(I_aX^u))+d\rho(d\pi I_c[I_aX^u,I_aY^u]^u)\\&=I_aX(d_c\rho(I_aY^u))-I_aY^u(d_c\rho(I_aX^u))-d_c\rho([I_aX^u,I_aY^u]^u).\end{aligned}$$

Therefore, $i^*d_bd_c\rho_{|\mathcal{U}}=\pi^*d_bd_c\rho_{N|\mathcal{U}}$ for all even permutations (abc) of (123). At the end we use the fact that the reduced Kähler forms $\overline{\omega}_a$ are characterized by the condition $(\pi^*\overline{\omega}_a)_{|\mathcal{U}}=(i^*\omega_a)_{|\mathcal{U}}$ and conclude that $2\overline{\omega}_a=dd_a\rho_N+d_bd_c\rho_N$. Q. E. D.

Remark: In the case of when the torsion vanishes the condition in the above theorem is equivalent to the one proposed by Kobak and Swann.[15] In both cases the crucial point is to ensure $i^*I_ad\rho=I_ai^*d\rho$. In both cases $d\rho(X^v)=0$ since ρ is invariant.

V. EXAMPLES

It is known that SU(3) admits invariant hypercomplex structure, constructed by Joyce. Moreover Pedersen and Poon[16] considered the deformation of this structure and succeeded to represent any ''small'' deformation as a hypercomplex reduced space of the space $S^1\times S^{11}$ under an appropriate S^1 action. As it is shown in Refs. 5 and 17, the space $S^1\times S^{11}$ is HKT and one can check that the S^1-actions considered in Ref. 16 Sec. 6.3 are HKT isometries. Now according to the theorem of Sec. II B we have:

Theorem 6: *Any small deformation of the invariant hypercomplex structure on* $SU(3)$ *admits a HKT structure*.

In the rest of this section, we will construct new HKT-metrics through a reduction process. We begin with a well-known metric, namely the Taub-NUT metric.

A. Taub-NUT metric

We use the notation of Ref. 18. Let $\mathcal{M}=\mathbb{H}\times\mathbb{H}$ with quaternionic coordinates (q,w). We identify points $(t,x,y,z)\in R^4$ with a quaternion $q\in H$: $q=t+ix+jy+kz$. The (quaternion) conjugate is $\overline{q}=t-ix-jy-kz$. The flat metric on M is

$$ds^2_{\text{flat}}=dqd\overline{q}+dwd\overline{w}. \tag{40}$$

Using left multiplication of the unit quaternions i,j, and k, we find the hypercomplex structure I,J, and K such that

$$Idt=dx,Idx=-dt,Idy=dz,Idz=-dy,$$

$$Jdt=dy,Jdx=-dz,Jdy=-dt,Jdz=dx,$$

$$Kdt=dz,Kdx=dy,Kdy=-dx,Kdz=-dt. \tag{41}$$

With respect to these complex structures, the Kähler form of the flat metric $dqd\overline{q}$ are

$$\omega_I=dt\wedge dx+dy\wedge dz,\quad \omega_J=dt\wedge dy+dz\wedge dx,\omega_K=dt\wedge dz+dx\wedge dy. \tag{42}$$

Let G be $\mathbb{R}$, $t\in\mathbb{R}$ with the action $(q,w)\to(qe^{it},w+\lambda t)$, for λ in $\mathbb{R}$. This is a group of hyper-Kähler isometries. It generates a moment map,

$$\nu=\frac{1}{2}qi\overline{q}+\frac{\lambda}{2}(w-\overline{w}). \tag{43}$$

We write $\mathbf{r}=qi\overline{q}$, $r=|\mathbf{r}|$ and $w=y+\mathbf{y}$ so $\mathbf{r}$ and $\mathbf{y}$ are in R^3. Moreover,

$$\nu=\tfrac{1}{2}\mathbf{r}+\lambda\mathbf{y}. \tag{44}$$

Define ψ by $q=\rho e^{i\psi/2}$, where ρ is a pure quaternion. Now using the coordinates $(\psi,\mathbf{r},y,\mathbf{y})$, we write the flat metric on M as

$$ds^2_{\text{flat}}=\frac{1}{4}\left(\frac{1}{r}d\mathbf{r}^2+r(d\psi+\omega\cdot d\mathbf{r})^2\right)+dy^2+d\mathbf{y}^2, \tag{45}$$

where curl $\omega = \text{grad}(1/r)$. In these coordinates the G-action is

$$(\psi, y) \to (\psi + 2t, y + \lambda t), \tag{46}$$

which leaves $\tau = \psi - 2y/\lambda$ invariant. On $\nu^{-1}(0)$, one has $\mathbf{y} = -(1/2\lambda)\,\mathbf{r}$. The induced metric in the coordinates $(\mathbf{r}, \tau, y)$ on $\nu^{-1}(0)$ is

$$ds^2_{\text{flat}} = \frac{1}{4}\left(\frac{1}{r}d\mathbf{r}^2 + r\left(d\tau + \frac{2}{\lambda}dy + \omega \cdot d\mathbf{r}\right)^2\right) + dy^2 + \frac{1}{4\lambda^2}d\mathbf{r}^2. \tag{47}$$

The quotient space $\nu^{-1}(0)/G$ is obtained by an orthogonal projection along the Killing vector field $\partial/\partial y$. It turns out that the quotient metric is the Taub–NUT metric,

$$ds^2_{\text{TN}} = \frac{1}{4}\left(\frac{1}{r} + \frac{1}{\lambda^2}\right)d\mathbf{r}^2 + \frac{1}{4}\left(\frac{1}{r} + \frac{1}{\lambda^2}\right)^{-1}(d\tau + \omega \cdot d\mathbf{r})^2. \tag{48}$$

B. A HKT-version of the Taub–NUT metric

Given the preparation of the last section, we are now ready to consider HKT-reduction. Let h be a function of r. We consider the metric on $\mathbb{H}\backslash\{0\} \times \mathbb{H}$ given by

$$ds^2_h = \frac{h(r)}{q\overline{q}}dq d\overline{q} + dw d\overline{w} = \frac{h(r)}{r}dq d\overline{q} + dw d\overline{w}. \tag{49}$$

As $[h(r)/r]\,dq d\overline{q}$ is a HKT-metric on $\mathbb{H}\backslash\{0\}$ and product of HKT metrics is again a HKT metric, ds^2 is a HKT metric. Since the hypercomplex structure does not change, the group G remains hypercomplex. It is again a group of isometries. Therefore, we again use the moment maps ν generated by the action G with respect to the hyper-Kähler metric ds^2_{flat}. On $\nu^{-1}(0)$ the induced metric with respect to ds^2_h is

$$\begin{aligned}
&\frac{h}{4r}\left(\frac{1}{r}d\mathbf{r}^2 + r\left(d\tau + \frac{2}{\lambda}dy + \omega \cdot d\mathbf{r}\right)^2\right) + dy^2 + \frac{1}{4\lambda^2}d\mathbf{r}^2 \\
&\quad = \frac{1}{4}\left(\frac{h}{r^2} + \frac{1}{\lambda^2}\right)d\mathbf{r}^2 + \left(1 + \frac{h}{\lambda^2}\right)dy^2 \\
&\qquad + \frac{h}{2\lambda}dy \odot (d\tau + \omega \cdot d\mathbf{r}) + \frac{h}{4}(d\tau + \omega \cdot d\mathbf{r})^2.
\end{aligned} \tag{50}$$

Here we used $\alpha \odot \beta = \alpha \otimes \beta + \beta \otimes \alpha$. So $\alpha \odot \alpha = 2\alpha \otimes \alpha$.

As hyper-Kähler reduction is also obtained by orthogonal projection, the horizontal distribution $\mathcal{U}$ is defined by $\ker \theta$. Therefore, the reduced metric is obtained by taking the restriction of ds^2 on $\nu^{-1}(0)$ modulo θ or μ, where

$$\theta = \iota_{\partial/\partial y} ds^2_{\text{flat}}, \quad \mu = dy + \frac{1}{2\lambda}\frac{(d\tau + \omega \cdot d\mathbf{r})}{\left(\frac{1}{r} + \frac{1}{\lambda^2}\right)}. \tag{51}$$

In other words, if $\hat{g}$ is the quotient metric, then there is a 1-form α and function a on $\nu^{-1}(0)$ such that

$$ds^2_h = a\,\mu \otimes \mu + (\alpha \otimes \mu + \mu \otimes \alpha) + \hat{g}. \tag{52}$$

It follows that $\iota_{\partial/\partial y} ds^2 = a\mu + \alpha$. In our example,

$$a=1+\frac{h}{\lambda^2},\quad \alpha=\frac{1}{2\lambda}\left(h-\left(1+\frac{h}{\lambda^2}\right)\left(\frac{1}{r}+\frac{1}{\lambda^2}\right)^{-1}\right)(d\tau+\omega\cdot d\mathbf{r}). \tag{53}$$

Therefore the quotient metric is

$$\begin{aligned}&\frac{1}{4}\left(\frac{h}{r^2}+\frac{1}{\lambda^2}\right)d\mathbf{r}^2+\left(1+\frac{h}{\lambda^2}\right)dy^2+\frac{h}{2\lambda}dy\odot(d\tau+\omega\cdot d\mathbf{r})+\frac{h}{4}(d\tau+\omega\cdot d\mathbf{r})^2\\&\quad-\left(1+\frac{h}{\lambda^2}\right)\left(dy+\frac{1}{2\lambda}\frac{(d\tau+\omega\cdot d\mathbf{r})}{\frac{1}{r}+\frac{1}{\lambda^2}}\right)^2-\left(dy+\frac{1}{2\lambda}\frac{(d\tau+\omega\cdot d\mathbf{r})}{\frac{1}{r}+\frac{1}{\lambda^2}}\right)\\&\quad\odot\frac{1}{2\lambda}\left(h-\left(1+\frac{h}{\lambda^2}\right)\left(\frac{1}{r}+\frac{1}{\lambda^2}\right)^{-1}\right)(d\tau+\omega\cdot d\mathbf{r})\\&\quad=\frac{1}{4}\left(\frac{h}{r^2}+\frac{1}{\lambda^2}\right)d\mathbf{r}^2+\frac{1}{4}\left(\frac{h}{r^2}+\frac{1}{\lambda^2}\right)\left(\frac{1}{r}+\frac{1}{\lambda^2}\right)^{-2}(d\tau+\omega\cdot d\mathbf{r})^2.\end{aligned} \tag{54}$$

$$=\left(\frac{h}{r^2}+\frac{1}{\lambda^2}\right)\left(\frac{1}{r}+\frac{1}{\lambda^2}\right)^{-1}ds^2_{\mathrm{TN}}. \tag{55}$$

In particular, the quotient metric is conformally equivalent to the Taub–NUT metric, a hyper-Kähler metric.

Amongst the class of weak HKT metrics that have been constructed above, there is a strong HKT metric which is complete. This is

$$ds^2=\left(\frac{1}{r}+\frac{1}{\lambda^2}\right)ds^2_{\mathrm{TN}}. \tag{56}$$

For this metric, the function h is

$$h(r)=1+\frac{2}{\lambda^2}r+\frac{1}{\lambda^2}\left(\frac{1}{\lambda^2}-1\right)r^2. \tag{57}$$

This metric is strong HKT because the conformal factor is a harmonic function with respect to the Taub-NUT hyper-Kähler metric. The asymptotic behavior of the metric is as follows: As $r\to\infty$, the metric (56) approaches the standard metric on $S^1\times\mathbf{R}^3$. As $r\to 0$, the metric (56) approaches

$$ds^2\sim\frac{1}{r}\left(r(d\tau+\omega\cdot d\mathbf{r})^2+\frac{1}{r}d\mathbf{r}^2\right).$$

Changing back to the quaternionic coordinates q, we find that the above metric can be rewritten as

$$ds^2=\frac{1}{q\bar{q}}dq\,d\bar{q}=du^2+ds^2(S^3)$$

with $r=q\bar{q}$ and $u=\log(|q|)$. So it is the standard metric on $\mathbf{R}\times S^3$. In physics language, the metric (56) interpolates between the ten-dimensional Kaluza–Klein vacuum and the near horizon geometry of the NS5-brane.

C. A HKT-version of the Lee–Weinberg–Yi metric

We are interested in examples beyond four-real dimension. As noted in Ref. 18, a high dimension analog of the Taub-NUT metric is the Lee–Weinberg–Yi (LWY) metric. We construct a family HKT-version of this metric. Moreover, these metrics are not conformal to the LWY-metric.

We first review the construction of the LWY-metric very briefly to fix notations. We take $\mathcal{M}=\mathbb{H}^m\times\mathbb{H}^m$ with coordinates (q_a,w_a), $a=1,\ldots,m$. Let $\Lambda=(\lambda_a^b)$ be a real nondegenerate $m\times m$-matrix. Let $V=(v_a^b)$ be the inverse matrix. For $G=\mathbb{R}^m=(t_1,\ldots,t_m)$, define an action by

$$q_a\mapsto q_a e^{it_a},\quad w_a\mapsto w_a+\sum_b \lambda_a^b t_b\,. \tag{58}$$

With respect to the flat metric $ds^2_{\text{flat}}=\Sigma_a dq_a d\overline{q}_a+\Sigma_a dw_a d\overline{w}_a$ and the hypercomplex structure defined as in (41), group G is a group hyperholomorphic isometry. The moment map

$$\nu=(\nu_1,\ldots,\nu_m):\mathcal{M}\to\mathbb{R}^m\otimes\mathbb{R}^3 \tag{59}$$

is given by

$$\nu_a=\frac{1}{2}q_a i\overline{q}_a+\frac{1}{2}\sum_b \lambda_a^b(w_b-\overline{w}_b). \tag{60}$$

Define $\mathbf{r}_a=q_a i\overline{q}_a$, $r_a=|\mathbf{r}_a|=q_a\overline{q}_a$, $\mathbf{y}_a=\frac{1}{2}(w_a-\overline{w}_a)$. It follows that $w_a=y_a+\mathbf{y}_a$. Now $\mathbf{r}_a$ and $\mathbf{y}_a$ are in $\mathbb{R}^3$ and the moment map is

$$\nu_a=\frac{1}{2}\mathbf{r}_a+\sum_b \lambda_a^b\mathbf{y}_b\,. \tag{61}$$

Define ψ_a by $q_a=\rho_a e^{i\psi_a/2}$, where ρ_a is a pure quaternion. Now using the coordinates $(\psi_a,\mathbf{r}_a,y_a,\mathbf{y}_a)$, one may construct explicitly a hyper-Kähler metric on the quotient space in the way the Taub-NUT metric is constructed. This is the LWY-metric.

For reference in subsequent computation, we note that in these coordinates the G-action is $(\psi_a,y_a)\to(\psi_a+2t_a,y_a+\Sigma_b\lambda_a^b t_b)$. It leaves the functions

$$\tau_a=\psi_a-2\sum_b v_a^b y_b \tag{62}$$

invariant. On the level set $\nu^{-1}(0)$, $\mathbf{r}_a=-2\Sigma_b\lambda_a^b\mathbf{y}_b$. Equivalently, $\mathbf{y}_a=-\frac{1}{2}\Sigma_b v_a^b\mathbf{r}_b$.

Next, consider a new metric on $\mathcal{M}$,

$$\begin{aligned} ds^2&=\sum_a f_a(q_a\overline{q}_a)dq_a d\overline{q}_a+\sum_a dw_a d\overline{w}_a\\ &=\sum_a f_a(r_a)dq_a d\overline{q}_a+\sum_a dw_a d\overline{w}_a\,. \end{aligned} \tag{63}$$

This is a HKT-metric. The group G is again a group of hyper-holomorphic isometries. We may use the G-moment map ν again to construct a quotient metric $\hat{g}$ with respect to ds^2.

The restriction of the metric ds^2 on $\nu^{-1}(0)$ with respect to the coordinates $(\mathbf{r}_a,\tau_a,y_a)$ is

$$\sum_a \left(\frac{f_a}{4r_a}d\mathbf{r}_a^2+\frac{f_a r_a}{4}\left(2\sum_b v_a^b dy_b+d\tau_a+A_a\right)^2+dy_a^2+\frac{1}{4}\left(\sum_b v_a^b d\mathbf{r}_b\right)^2\right)$$
$$=\frac{1}{4}\sum_{b,c}\left(\frac{\delta_b^c f_c}{r_c}+\sum_a v_a^b v_a^c\right)d\mathbf{r}_b\otimes d\mathbf{r}_c+\sum_{b,c}\left(\delta_b^c+\sum_a (f_a r_a v_a^b v_a^c)\right)dy_b\otimes dy_c$$
$$+\frac{1}{2}\sum_{a,b} f_a r_a v_a^b dy_b\odot(d\tau_a+A_a)+\frac{1}{4}\sum_a f_a r_a (d\tau_a+A_a)^2. \tag{64}$$

To find the quotient metric $\hat{g}$, it suffices to find functions F_{ab} and 1-forms α_a such that

$$ds^2=\sum_{a,b} F_{ab}\theta_a\otimes\theta_b+\sum_a (\theta_a\otimes\alpha_a+\alpha_a\otimes\theta_a)+\hat{g}. \tag{65}$$

Now the problem is that the Killing vector fields $\partial/\partial y_a$ generated by G on the zero level set in general are not mutually orthogonal.

From now on, we limit our discussion to the case when $\lambda_a^b=\lambda_a\delta_a^b$. Equivalently, Λ is a diagonal matrix whose nonzero entry is λ_a. Its inverse is a diagonal matrix whose non-zero entry is $v_a=1/\lambda_a$. In this case,

$$\theta_c:=\iota_{\partial/\partial y_c}ds^2=(1+r_c v_c^2)dy_c+\frac{1}{2}r_c v_c(d\tau_c+A_c)$$
$$=\left(1+\frac{r_c}{\lambda_c^2}\right)dy_c+\frac{r_c}{2\lambda_c}(d\tau_c+A_c), \tag{66}$$

where $A_c:=\omega(\mathbf{r}_a)\cdot d\mathbf{r}_a$. Since the vector fields $\partial/\partial y_a$ are mutually orthogonal with respect to ds^2,

$$\iota_{\partial/\partial y_c}ds^2=(1+r_c v_c^2)\left(\sum_a F_{ca}\theta_a+\alpha_c\right). \tag{67}$$

The restriction of the metric ds^2 on $\nu^{-1}(0)$ with respect to the coordinates $(\mathbf{r}_a,\tau_a,y_a)$ is

$$\sum_a\left(\frac{f_a}{4r_a}d\mathbf{r}_a^2+\frac{f_a r_a}{4}(2v_a dy_a+d\tau_a+A_a)^2+dy_a^2+\frac{v_a^2}{4}d\mathbf{r}_a^2\right)$$
$$=\sum_a\left(\frac{f_a}{4r_a}d\mathbf{r}_a^2+\frac{f_a r_a}{4}\left(\frac{2}{\lambda_a}dy_a+d\tau_a+A_a\right)^2+dy_a^2+\frac{1}{4\lambda_a^2}d\mathbf{r}_a^2\right)$$
$$=\sum_a\left(\tfrac{1}{4}(f_a r_a+v_a^2)d\mathbf{r}_a^2+(1+f_a r_a v_a^2)dy_a^2+\tfrac{1}{2}f_a r_a v_a dy_a\odot(d\tau_a+A_a)\right.$$
$$\left.+\tfrac{1}{4}f_a r_a(d\tau_a+A_a)^2\right).$$

Therefore,

$$\iota_{\partial/\partial y_a}ds^2=(1+f_a r_a v_a^2)dy_a+\tfrac{1}{2}v_a f_a r_a(d\tau_a+A_a)$$
$$=\frac{(1+f_a r_a v_a^2)}{(1+r_a v_a^2)}\theta_a+\tfrac{1}{2}f_a v_a r_a\left(1-\frac{1+f_a r_a v_a^2}{(1+r_a v_a^2)f_a}\right)(d\tau_a+A_a)=\frac{(1+f_a r_a v_a^2)}{(1+r_a v_a^2)}\theta_a$$
$$+\frac{v_a r_a}{2(1+r_a v_a^2)}(f_a-1)(d\tau_a+A_a).$$

It implies that the matrix (F_{ab}) is a diagonal matrix and

$$F_a = F_{aa} = \frac{(1+f_a r_a v_a^2)}{(1+r_a v_a^2)^2}, \quad \alpha_a = \frac{v_a r_a}{2(1+r_a v_a^2)^2}(f_a - 1)(d\tau_a + A_a). \tag{68}$$

Then the quotient metric is n

$$\begin{aligned}\hat{g} &= ds^2 - \sum_a (F_a \theta_a \otimes \theta_a + \theta_a \odot \alpha_a) \\ &= \frac{1}{4}\left(\frac{f_a}{r_a} + v_a^2\right) d\mathbf{r}_a^2 + \left(\frac{f_a r_a}{4} - \frac{r_a^2 v_a^2 (1+f_a r_a v_a^2)}{4(1+r_a v_a^2)^2} - \frac{v_a^2 r_a^2 (f_a - 1)}{2(1+r_a v_a^2)^2}\right)(d\tau_a + A_a)^2 \\ &= \frac{1}{4}\sum_a \left(\frac{f_a + r_a v_a^2}{1+r_a v_a^2}\right)\left(\left(\frac{1+r_a v_a^2}{r_a}\right) d\mathbf{r}_a^2 + \left(\frac{1+r_a v_a^2}{r_a}\right)^{-1} (d\tau_a + A_a)^2\right).\end{aligned} \tag{69}$$

When $f_a = 1$ for all a, we obtain a simple version of the LWY-metric,

$$ds^2_{\mathrm{LWY}} = \frac{1}{4}\sum_a \left(\left(\frac{1+r_a v_a^2}{r_a}\right) d\mathbf{r}_a^2 + \left(\frac{1+r_a v_a^2}{r_a}\right)^{-1} (d\tau_a + A_a)^2\right). \tag{70}$$

This is simple because this metric is a product metric.

In general, so long as not all the $\lambda_a = 1/v_a$ are equal, the quotient metric $\hat{g}$ is a HKT-metric. However, it is no longer conformal to the LWY-metric.

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Contact metric 5-manifolds, CR twistor spaces and integrability

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The CR twistor space is defined over a contact metric 5-manifold M. Like the 4-dim twistor theory, the integrability of the almost CR twistor structure is discussed in terms of the Weyl conformal curvature and also the scalar curvature of M. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1476953]

I. INTRODUCTION AND MAIN THEOREMS

The twistor space for 4-manifolds stems from the idea of R. Penrose developed in mathematical physics of gravity (see Ref. 15). The twistor space is endowed with the canonical almost complex structure. The integrability of this almost complex structure is exhibited by Atiyah, Hitchin and Singer in terms of conformally half flatness of a base 4-manifold.

Theorem(Atiyah, Hitchin and Singer[2,3]): Let $\mathcal{Z}^-$ be the twistor space of an oriented Riemannian 4-manifold (M,g). Then, the almost complex structure on $\mathcal{Z}^-$ is integrable if and only if (M,g) is self-dual, namely, the anti-self-dual Weyl conformal tensor W^- vanishes.

The twistor space of a 4-manifold presents a profound link between 4-dimensional conformal geometry and theory of complex manifolds. For this direction, for instance, refer to Hitchin's paper[8] and the Ward correspondence.[19]

Twistor space is defined also on odd dimensional spaces, such as a mini-twistor space for Einstein-Weyl 3-manifolds, defined by N. Hitchin in Ref. 9. LeBrun defined in this direction a CR twistor space for conformal 3-manifolds in Ref. 14 as null cones over complexified tangent bundle.

We will focus on a contact 5-manifold in this article and investigate the twistor space defined on it. So, let M be a smooth 5-manifold and suppose that M be equipped with a contact metric structure (η,ξ,ϕ,g).

M admits then a particular direction along the characteristic field ξ in each tangent space and also the rank 4 contact bundle $\mathbf{E}=\mathrm{Ker}\ \eta$ so that $TM=\mathbf{E}\oplus\langle\xi\rangle$. The bundle $\mathbf{E}$ plays a role of the tangent bundle of a 4-manifold. To $\mathbf{E}$ is associated an SO(4)-principal bundle, the oriented orthonormal frame bundle $P_{\mathbf{E}}$.

We take as the CR twistor space $\mathcal{Z}$ the sphere bundle $\mathbf{U}(\Lambda^2_-(\mathbf{E}^*))=\{\alpha\in\Lambda^2_-(\mathbf{E}^*)\,|\,|\alpha|=2\}$ for the dual $\mathbf{E}^*$ of $\mathbf{E}$. Anti-self-dual two-forms α on $\mathbf{E}$ of norm $|\alpha|=2$ are identified with orthogonal almost complex structures J of $\mathbf{E}$. So, $\mathcal{Z}$ can be regarded as the space of orthogonal almost complex structures on the contact bundle $\mathbf{E}$.

To define an almost CR structure $\mathcal{J}$ on $\mathcal{Z}$ we utilize the contact splitting of TM and the tangent space decomposition of $\mathcal{Z}$ at $\alpha\in\mathcal{Z}$ into the vertical and horizontal subspaces: $T_\alpha\mathcal{Z}=\mathcal{V}_\alpha\oplus\mathcal{H}_\alpha$, where the vertical subspace $\mathcal{V}_\alpha\cong T\boldsymbol{P}^1(\mathbf{C})$ and the horizontal subspace $\mathcal{H}_\alpha\cong T_xM$, $x=\pi(\alpha)$. Here $\pi:\mathcal{Z}\to M$ is the projection.

At $\alpha\in\mathcal{Z}$ via the identification of α with J^α, an almost complex structure of $\mathbf{E}_x$, we define

$$\mathcal{J}_\alpha:\quad \mathcal{V}_\alpha\to\mathcal{V}_\alpha;\ \ \mathcal{J}_\alpha(V)=j(V),$$

$$\mathcal{H}'_\alpha\to\mathcal{H}'_\alpha;\ \ \pi_*(\mathcal{J}_\alpha(X'))=J^\alpha(\pi_*(X')),$$

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$$\mathcal{H}''_\alpha \to \mathcal{H}''_\alpha; \quad \mathcal{J}_\alpha(X'') = 0.$$

Here j is the canonical almost complex structure of $P^1(\mathbf{C})$ and $\mathcal{H}$ has the splitting $\mathcal{H}_\alpha = \mathcal{H}'_\alpha \oplus \mathcal{H}''_\alpha$ according to the contact splitting of TM.

Set $\mathcal{E} = \mathcal{V} \oplus \mathcal{H}'$, the subbundle of the tangent bundle $T\mathcal{Z}$, on which $\mathcal{J}$ acts as an almost complex structure with the splitting $\mathcal{E} \otimes \mathbf{C} = \mathcal{E}^{1,0} \oplus \mathcal{E}^{0,1}$.

Definition: The almost CR structure $\mathcal{J}$ on $\mathcal{Z}$ is *integrable* if

$$[X - \sqrt{-1}\mathcal{J}X, Y - \sqrt{-1}\mathcal{J}Y] \in \Gamma(\mathcal{E}^{1,0})$$

for any smooth sections $X - \sqrt{-1}\mathcal{J}X, Y - \sqrt{-1}\mathcal{J}Y$ of $\mathcal{E}^{1,0}$.

The main purpose of this article is to exhibit an integrability of the almost CR structure $\mathcal{J}$ in terms of the base manifold curvature.

The curvature tensor $\mathcal{R}: \Lambda^2(T^*M) \to \Lambda^2(T^*M)$ of (M,g) enjoys the decomposition

$$\mathcal{R} = \mathcal{W} + \mathcal{B} - \frac{s}{20} id,$$

into the Weyl conformal curvature part $\mathcal{W}$, the trace free Ricci tensor part $\mathcal{B}$ and the scalar curvature part $-(s/20)\, id$.

In terms of the splitting of $\Lambda^2(T^*M)$,

$$\Lambda^2(T^*M) = \Lambda^2_+(\mathbf{E}^*) \oplus \Lambda^2_-(\mathbf{E}^*) \oplus \eta \wedge \Lambda^1(\mathbf{E}^*),$$

$\mathcal{R}$ has the block decomposition

$$\mathcal{R} = \begin{pmatrix} \mathcal{R}^+_+ & \mathcal{R}^-_+ & \mathcal{R}^0_+ \\ \mathcal{R}^+_- & \mathcal{R}^-_- & \mathcal{R}^0_- \\ \mathcal{R}^+_0 & \mathcal{R}^-_0 & \mathcal{R}^0_0 \end{pmatrix},$$

with the similar decompositions of $\mathcal{W}$, $\mathcal{B}$.[12]

The following theorem indicates the validity of contact geometrical analog of the theorem of Atiyah, Hitchin and Singer.

Theorem 1.1: Let (M, η, ξ, ϕ, g) be a K-contact 5-manifold and $\mathcal{Z} = \mathbf{U}(\Lambda^2_-(\mathbf{E}^*))$ its CR twistor space.

Then, $\mathcal{J}$ on $\mathcal{Z}$ is integrable if and only if (M,g) is self-dual contact-metric, in other words, the anti-self-dual Weyl conformal tensor $\mathcal{W}^-$ vanishes and the scalar curvature $s = -4$.

Here, a K-contact manifold is a contact metric manifold for which ξ is a Killing field (see Sec. II). The connection $\nabla^{\mathbf{E}}$, induced from the Levi-Civita connection, is utilized to define the vertical-horizontal splitting of $\mathcal{Z}$. However, it is observed that an arbitrary metric connection on $\mathbf{E}$, for example, a generalized Tanaka–Webster connection given by Tanno,[17] yields an almost CR structure on $\mathcal{Z}$, whose integrability may also be interesting.

The CR twistor space $\mathcal{Z}$ with the almost CR structure $(\mathcal{E}, \mathcal{J})$, even not integrable, admits a vector field $\tilde{\xi}$, the horizontal lift of ξ on M.

Theorem 1.2: Let $\mathcal{Z}$ be the CR twistor space of a K-contact 5-manifold (M, η, ξ, ϕ, g). Then, the following are equivalent.

(i) $\tilde{\xi}$ is a CR holomorphic vector field, i.e.,

$$[\tilde{\xi}, X - \sqrt{-1}\mathcal{J}X] \in \Gamma(\mathcal{E}^{1,0})$$

for any smooth section $X - \sqrt{-1}\mathcal{J}X$ of $\mathcal{E}^{1,0}$.

(ii) $\mathcal{R}^-_0 = \mathcal{W}^-_0 + \mathcal{B}^-_0 : \eta \wedge \Lambda^1(\mathbf{E}^*) \to \Lambda^2_-(\mathbf{E}^*)$ vanishes,

An almost CR structure $\mathcal{J}$ on $\mathcal{Z}$ induces an almost complex structure $\mathcal{I}$ on the product space $\mathcal{Z}\times\mathbf{R}$ or $\mathcal{Z}\times S^1$ such that $\mathcal{I}|_{\mathcal{E}}=\mathcal{J}$, $\mathcal{I}(\tilde{\xi})=\partial/\partial t$. It is not difficult to show that $\mathcal{I}$ on $\mathcal{Z}\times\mathbf{R}$ or $\mathcal{Z}\times S^1$ is integrable if and only if $\mathcal{J}$ on $\mathcal{Z}$ is integrable and also $\tilde{\xi}$ is CR holomorphic.

So an immediate consequence of Theorems 1.1 and 1.2 is the following integrability of the almost complex structure.

Corollary 1.1: Let (M,η,ξ,ϕ,g) be a K-contact 5-manifold. The almost complex manifold $(\mathcal{Z}\times\mathbf{R},\mathcal{I})$ is integrable if the following curvature conditions hold:

$$\mathcal{W}_-^-=0,$$

$$\mathcal{R}_0^-=\mathcal{W}_0^-+\mathcal{B}_0^-=0$$

and $s=-4$.

We exhibit certain examples of the K-contact 5-manifold for which the CR twistor space admits the integrable CR structure.

From its full curvature formula (see Ref. 4) a Sasakian 5-manifold (M,η,ξ,ϕ,g) with constant ϕ-sectional curvature $c=-3$ satisfies these three conditions in Corollary 1.1. So the CR twistor space of this manifold M admits the integrable almost CR structure with the CR holomorphic vector field $\tilde{\xi}$.

Restricting ourselves to a certain class of K-contact 5-manifolds, K-contact 5-manifolds admit an S^1-fibration with a connection η, the contact form. The above theorems are then transfered to the following.

Theorem 1.3: Let (M,η,ξ,ϕ,g) be a K-contact 5-manifold which is an S^1-principal bundle over a 4-manifold N with a connection η. Then, the CR twistor space $\mathcal{Z}$ of M is integrable if and only if N is self-dual, i.e., $W_N^-=0$ and has zero scalar curvature, $s_N=0$.

Moreover, the horizontal vector field $\tilde{\xi}$ is always CR holomorphic so that for a base 4-manifold N which is self-dual and of zero scalar curvature the product space $\mathcal{Z}\times\mathbf{R}$ or $\mathcal{Z}\times S^1$ is a complex 4-dimensional manifold.

From Boothby–Wang fibration theorem the base 4-manifold N in Theorem 1.3 must be an almost Kähler manifold with a Kähler form whose lift is $d\eta$. When M is moreover Sasakian, N is Kähler, due to the result of Hatakeyama (see Ref. 7). For a Kähler 4-manifold the scalar curvature $s=0$ if and only if the self-dual Weyl conformal tensor $W^+=0$ (see Refs. 10 and 5). Therefore the CR twistor space of a Sasakian 5-manifold M admitting a compatible S^1-bundle structure is integrable if and only if the base Kähler 4-manifold N of M is conformally flat $(W=0)$. Since N is self-dual, the twistor space $\mathcal{Z}$ of M is an S^1-fibration over the Penrose twistor space $\mathcal{Z}_N$ of N so that one gets a sequence of fibrations: $\mathcal{Z}\times\mathbf{R}\to\mathcal{Z}\to\mathcal{Z}_N$.

As a concrete example, we take a canonically defined circle bundle M over $N=S^2\times H^2$, the Riemannian product of S^2 and H^2. So, M is equipped with a Sasakian structure. N is geometrically conformally flat, Kähler and of $s_N=0$. Moreover, N is conformally equivalent to $\mathbf{R}\times(\mathbf{R}^3\backslash 0)$ and hence to $S^4\backslash C$, where C is a great circle so that $\mathcal{Z}_N$ is $P^3(\mathbf{C})\backslash\hat{C}$, where $\hat{C}$ is the set of twistor lines over C. The CR twistor space $\mathcal{Z}$ of M is then a certain circle bundle over $P^3(\mathbf{C})\backslash\hat{C}$. Namely we get the double fibration:

$$\mathcal{Z}\xrightarrow{S^1}P^3(\mathbf{C})\backslash\hat{C}\xrightarrow{P^1(\mathbf{C})}S^2\times H^2.$$

Dividing this by a certain discrete subgroup Γ of $\mathrm{SL}(2,\mathbf{R})$, one can get compact quotients. The details of the argument of Theorem 4 will be given elsewhere.[13]

Remarks: (i) Notice that $\tilde{\eta}=\pi^*\eta$, the pulled back one-form to $\mathcal{Z}$ of η, gives rise to the degeneracy of the Levi form $(Z_1,Z_2)\mapsto d\tilde{\eta}(\mathcal{J}Z_1,\overline{Z_2})$ so that our CR twistor space is not strongly pseudo-convex.

(ii) We have

$$\pi^*\Lambda^2_+(\mathbf{E}^*)=\Lambda^{(1,1)}(\mathcal{Z})\cap\pi^*\Lambda^2(\mathbf{E}^*)$$

similarly to the twistor space of a 4-manifold (see, for example, Ref. 2, p. 442), and contrarily $\Lambda^2_-(\mathbf{E}^*)$ lifts to $(\Lambda^{(2,0)}\oplus\Lambda^{(0,2)})(\mathcal{Z})$.

(iii) A contact CR analog of the Ward correspondence holds (see Ref. 2, p. 441 and Ref. 19). In fact, we easily observe that if V is a Hermitian vector bundle with a self-dual connection D, i.e., a connection D with curvature R^D satisfying $R^D\in\Gamma(\Lambda^2_+(\mathbf{E}^*)\otimes\mathrm{End}\,V)$ over a K-contact 5-manifold of $\mathcal{W}^-=0$ and $s=-4$, and if $\tilde{V}=\pi^*V$ is the pulled back bundle on $\mathcal{Z}$, then the lift $\tilde{D}=\pi^*D$ of D, a connection on $\tilde{V}$, satisfies two of the three properties of so-called Tanaka canonical connection, namely, (a) $i(\tilde{\xi})R^{\tilde{D}}=0$ and (b) $R^{\tilde{D}}\in\Gamma(\Lambda^{(1,1)}(\mathcal{Z})\otimes\mathrm{End}\,\tilde{V})$. See Refs. 16 and 18 for Tanaka canonical connection.

(iv) We can define, similarly to $\mathcal{Z}$, the positive type of CR twistor space $\mathcal{Z}^+$ over M as $\mathcal{Z}^+=\mathbf{U}(\Lambda^2_+(\mathbf{E}^*))$ which admits an almost CR structure $\mathcal{J}^+$. However, it can not be integrable, since the ϕ-invariance of $d\eta$ obstructs its integrability.

In Sec. II we will give a basic summary of contact-metric structure and almost CR structure. To investigate the integrability of the almost CR structure we take the projective spinor bundle description of the CR twistor space. We therefore provide in Sec. III a brief summary of Clifford algebra and spinors to define the projective spinor bundle. Integrability argument will be given in Sec. IV by lifting it up on the orthonormal frame bundle $P_{\mathbf{E}}$ of $\mathbf{E}$. We divide Sec. V into five small sections to accomplish a proof of Theorems 1. For this description and the argument of the integrability we owe much to Ref. 6. In Sec. VI we deal with the CR holomorphic condition of the horizontal characteristic field.

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II. CONTACT METRIC STRUCTURE AND ALMOST CR STRUCTURE

We first introduce the notion of contact metric structure. For a reference of contact metric structures see Ref. 4 and also Ref. 11.

Definition 2.1: We call a quadruplet (η,ξ,ϕ,g) of tensors on a 5-manifold M a contact metric structure, if $\eta\in\Gamma(M;\Lambda^1(M))$, $\xi\in\mathcal{X}(M)$, $\phi\in\Gamma(M;\mathrm{End}TM)$ and a smooth metric g on M satisfy

(i) $\eta\wedge(d\eta)^2\neq 0$,
(ii) $\eta(\xi)=1$, $d\eta(\xi,\cdot)=0$,
(iii) $\phi^2(X)=-X+\eta(X)\xi$, and
(iv) $g(X,\phi Y)=\frac{1}{2}d\eta(X,Y)$, $g(\phi X,\phi Y)=g(X,Y)-\eta(X)\eta(Y)$.

Then $|\xi|=1$ and $\phi(\xi)=0$. So the contact bundle $\mathbf{E}=\mathrm{Ker}\,\eta$ carries a Hermitian structure $(g|_{\mathbf{E}},\phi|_{\mathbf{E}})$ and

$$TM=\mathbf{E}\oplus\langle\xi\rangle.$$

An orthonormal frame $e=(e_1,\ldots,e_4)$ of $(\mathbf{E},g|_{\mathbf{E}})$ is called ϕ-basis, if $e_2=\phi(e_1)$, $e_4=\phi(e_3)$.

Lemma 2.1: Let $e=(e_1,\ldots,e_4)$ be a ϕ-basis. Then for any odd permutation $(i_1,\ldots,i_4)$ of (1,2,3,4) the ξ-component of $[e_{i_1},e_{i_2}]+[e_{i_3},e_{i_4}]$ vanishes.

Proof: This is obvious, since

$$d\eta(\phi(X),\phi(Y))=d\eta(X,Y),\quad X,Y\in\mathbf{E},\tag{1}$$

and that the ξ-component of $[e_j,e_k]$ is $\eta([e_j,e_k])=-d\eta(e_j,e_k)$.

The contact bundle $\mathbf{E}$ inherits a metric connection $\nabla^{\mathbf{E}}$,

$$\nabla^{\mathbf{E}}_X Y=\mathrm{pr}^{\mathbf{E}}\nabla_X Y,$$

where $\mathrm{pr}^{\mathbf{E}}$ is the projection from TM onto $\mathbf{E}$ and ∇ is the Levi-Civita connection.

Lemma 2.2:

(i) For $Z\in\Gamma(\mathbf{E})$, and $X\in TM$,

$$\nabla_X Z=\nabla^{\mathbf{E}}_X Z+\alpha_X(Z),\quad \alpha_X(Z)=-g(Z,\nabla_X\xi)\xi,$$

and

(ii) the Gauss equation for the curvature $R^{\mathbf{E}}$ of $\nabla^{\mathbf{E}}$ is

$$R^{\mathbf{E}}(X,Y)Z=(R(X,Y)Z)^{\mathbf{E}}-g(Z,\nabla_X\xi)\nabla_Y\xi+g(Z,\nabla_Y\xi)\nabla_X\xi,\quad X,Y\in TM,\ Z\in\Gamma(\mathbf{E}).$$

Here the curvature tensor is defined as $R^{\mathbf{E}}(X,Y)Z=\nabla^{\mathbf{E}}_X\nabla^{\mathbf{E}}_Y Z-\nabla^{\mathbf{E}}_Y\nabla^{\mathbf{E}}_X Z-\nabla^{\mathbf{E}}_{[X,Y]}Z$.

A contact metric structure (η,ξ,ϕ,g) is called *K-contact* if ξ is a Killing field. Basic properties of a $(2n+1)$-dimensional K-contact structure are

$$\nabla_X\xi=-\phi(X),$$

$$R(\xi,X)\xi=-X,$$

$$Ric(\xi,\xi)=2n\quad\text{for}\quad X\in\mathbf{E}_x.$$

We have from Lemma 2.2, (ii) for a K-contact 5-manifold (M,η,ξ,ϕ,g) the components $R^{\mathbf{E}}_{ijk\ell}=g(R^{\mathbf{E}}(e_i,e_j)e_k,e_\ell)$ in terms of a ϕ-basis are given as follows.

Lemma 2.3:

$$R^{\mathbf{E}}_{ijk\ell}=R_{ijk\ell}-g(\phi e_i,e_k)g(\phi e_j,e_\ell)+g(\phi e_i,e_\ell)g(\phi e_j,e_k),$$

$$i,j,k,\ell=1,2,3,4.$$

Hence the curvature $R^{\mathbf{E}}$ enjoys the symmetries

$$R^{\mathbf{E}}_{ijk\ell}=R^{\mathbf{E}}_{k\ell ij}\ \text{ for }\ i,j,k,\ell=1,2,3,4.$$

Moreover, we get

$$R^{\mathbf{E}}_{ijk\ell}=R_{ijk\ell}$$

except for

$$R^{\mathbf{E}}_{1324}=R_{1324}-1,\quad R^{\mathbf{E}}_{1423}=R_{1423}+1.$$

A contact metric manifold (M,η,ξ,ϕ,g) is called *Sasakian* when the canonically defined almost complex structure on $M\times\mathbf{R}$ is integrable (see Ref. 4). This notion is equivalent to that ϕ satisfies $(\nabla_X\phi)Y=g(X,Y)\xi-\eta(Y)X$. A Sasakian manifold is K-contact. The curvature tensor of a Sasakian manifold satisfies

$$g(R(\xi,X)Y,Z)=0,\ X,Y,Z\in\mathbf{E},$$

giving rise to the partial vanishing of $\mathcal{R}$ as $\mathcal{R}^{+}_{0}=\mathcal{R}^{-}_{0}=0$.

Let N be a smooth orientable odd dimensional manifold.

In order to define a CR structure (i.e., an integrable almost CR structure) on N we take the complexified tangent bundle $TN\otimes\mathbf{C}$ and consider a special subbundle of it.

Let $\mathcal{S}$ be a complex vector subbundle of $TN\otimes\mathbf{C}$ satisfying $\mathcal{S}\cap\overline{\mathcal{S}}=\{0\}$ and $\dim_{\mathbf{C}}TN\otimes\mathbf{C}/\mathcal{S}\oplus\overline{\mathcal{S}}=1$. Then the pair $(N,\mathcal{S})$ or $\mathcal{S}$ is called an *almost CR structure* (see Ref. 1).

$\mathcal{S}$ is called *integrable* if $[\Gamma(\mathcal{S}),\Gamma(\mathcal{S})]\subset\Gamma(\mathcal{S})$.

Real hypersurfaces of a complex manifold are prototype of the CR manifold. From the equation on the structure tensor ϕ one can see that Sasakian manifolds are CR manifolds.

A vector field ζ on N is *CR holomorphic* when $[\zeta,\Gamma(\mathcal{S})]\subset\Gamma(\mathcal{S})$. For basic references of CR structure, see, for instance, Refs. 1, 16, and 18.

III. THE PROJECTIVE SPINOR DESCRIPTION

The contact bundle $\mathbf{E}$ of a contact metric 5-manifold (M,η,ξ,ϕ,g) is rank 4, oriented and carries the fiber inner product $g|_{\mathbf{E}}$. The oriented orthonormal frame bundle $P_{\mathbf{E}}$ associated to $\mathbf{E}$ has structure group SO(4).

The spinor group $\mathrm{Spin}(4)=\mathrm{SU}(2)_+\times\mathrm{SU}(2)_-$, the universal covering group of SO(4), enjoys, via the Clifford multiplication on $S=S^+\oplus S^-\cong\mathbf{C}^2\oplus\mathbf{C}^2$, the spinor representations $\rho^{\pm}:\mathrm{Spin}(4)\to\mathrm{SU}(S^{\pm})$ yielding the action r^- of SO(4) on $P^1(\mathbf{C})$.

So, we define the projective spinor bundle $\mathbf{P}(S^-(\mathbf{E}))$ associated to $\mathbf{E}$ as

$$\mathbf{P}(S^-(\mathbf{E}))=P_{\mathbf{E}}\times_{(\mathrm{SO}(4),r^-)}P(S^-).$$

From the basic Clifford multiplication property the CR twistor space $\mathcal{Z}=\mathbf{U}(\Lambda^2_-(\mathbf{E}^*))$ can be identified with the projectified negative spinor bundle $\mathbf{P}(S^-(\mathbf{E}))$. We will explain this in a natural way in Sec. IV.

To state more precisely we let $\mathrm{Cliff}(\mathbf{R}^4)$ denote the Clifford algebra over the Euclidean 4-space with the negative inner product $(\mathbf{R}^4,-\langle,\rangle)$.

$\mathrm{Cliff}(\mathbf{R}^4)$ is 16-dimensional and generated by the orthonormal basis e_1,e_2,e_3,e_4 of $\mathbf{R}^4$ with the relations $e_i\cdot e_i=-1$ for $i=1,\ldots,4$ and $e_i\cdot e_j+e_j\cdot e_i=0$ for $i\neq j$.

As is well known in Clifford algebra theory, the complexification $\mathrm{Cliff}^{\mathbf{C}}(\mathbf{R}^4)$ is isomorphic to the algebra $C(4)$ of all 4×4 complex matrices. We denote thus obtained isomorphism by $\rho:\mathrm{Cliff}^{\mathbf{C}}(\mathbf{R}^4)\to C(4)$. Then, ρ is defined as

$$e_1\mapsto I_2\otimes g_1,\ \ e_2\mapsto I_2\otimes g_2,\ \ e_3\mapsto g_1\otimes T,\ \ e_4\mapsto g_2\otimes T, \tag{2}$$

where

$$I_2=\begin{pmatrix}1&0\\0&1\end{pmatrix},\ \ T=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\ \ g_1=\begin{pmatrix}i&0\\0&-i\end{pmatrix},\ \ g_2=\begin{pmatrix}0&i\\i&0\end{pmatrix}. \tag{3}$$

We write $\rho(X)u$ as $X\cdot u$ for brevity, for $X\in\mathrm{Cliff}^{\mathbf{C}}(\mathbf{R}^4)$ and $u\in\mathbf{C}^4$.

The group Spin(4) is generated multiplicatively by all elements $x\cdot y$ with $x,y\in\mathbf{R}^4$ and $|x|=|y|=1$. The covering homomorphism $\lambda:\mathrm{Spin}(4)\to\mathrm{SO}(4)$ is given by

$$\lambda(z)x=z\cdot x\cdot z^{-1},\quad z\in\mathrm{Spin}(4),\ \ x\in\mathbf{R}^4. \tag{4}$$

The Lie algebra $\mathfrak{spin}(4)$ of Spin(4) is identified with the linear hull of the set $\{e_i\cdot e_j|i<j\}$. On the other hand, $\{E_{ij}|i<j\}$ is the standard basis of the Lie algebra $\mathfrak{so}(4)$. The differential $\rho_*:\mathfrak{spin}(4)\to\mathfrak{so}(4)$ of the map ρ is then given by $\rho_*(e_i\cdot e_j)=2E_{ij}$. Here E_{ij}, $i<j$, is the 4×4 skew-symmetric matrix whose (i,j)-entry is -1, while the (j,i)-entry is 1, and other ones are zero.

By restricting the map ρ to Spin(4), we get a complex representaion of Spin(4) on $\mathbf{C}^4\cong S$ for which we use the same ρ. This decomposes into two irreducible unitary representations, called the spinor representations $\rho^{\pm}:\mathrm{Spin}(4)\to\mathrm{SU}(S^{\pm})$, where $S=S^+\oplus S^-\cong\mathbf{C}^2\oplus\mathbf{C}^2$.

Notice that the differential of the representation $\rho:\mathrm{Spin}(4)\to\mathrm{GL}(S)$ is given by $\rho_*=\rho$.

With respect to a certain basis of $S=S^+\oplus S^-$ we have

$$\rho^-:\sum_{i<j}a_{ij}e_i\cdot e_j\mapsto\begin{pmatrix}i(a_{34}-a_{12})&(a_{13}+a_{24})+i(a_{14}-a_{23})\\-(a_{13}+a_{24})+i(a_{14}-a_{23})&i(a_{12}-a_{34})\end{pmatrix}. \tag{5}$$

The spinor representation ρ^- induces the transitive isometric action r^- of SO(4) on the complex projective line $P(S^-)\cong P^1(\mathbf{C})$ preserving the complex structure. So, we write

$$P(S^-)=\mathrm{SO}(4)/H^-,$$

where H^- is the isotropy group of this action at the reference point $[1:0]\in P^1(\mathbf{C})$.

To exploit the integrability of the almost CR structure $\mathcal{J}$ given in Sec. I we introduce bases of the Lie algebra $\mathfrak{h}^-$ of H^- and its orthogonal complement $\mathfrak{n}^-$ in $\mathfrak{so}(4)$.

The algebra $\mathfrak{h}^-$ is the image under $\lambda:\mathfrak{spin}(4)\to\mathfrak{so}(4)$ of the inverse image $(\rho^-)^{-1}(\mathfrak{s}^1)$, where $\mathfrak{s}^1$ is the isotropy subalgebra in $\mathfrak{su}(2)$ at the point [1:0].

Thus we get the following form of $\mathfrak{h}^-$ by the aid of the precise description of the spinor representation;

$$\mathfrak{h}^-=\left\{\sum_{i<j}a_{ij}E_{ij}\,\middle|\,a_{13}+a_{24}=0,\ a_{14}=a_{23}\right\}.$$

Its orthogonal complement $\mathfrak{n}^-$ with respect to the canonical inner product is

$$\mathfrak{n}^-=\mathbf{R}(E_{13}+E_{24})\oplus\mathbf{R}(E_{14}-E_{23})$$

giving the tangent space of $P^1(\mathbf{C})$ at the origin.

The complex structure j is now written as

$$j:E_{13}+E_{24}\mapsto-(E_{14}-E_{23}),\quad E_{14}-E_{23}\mapsto E_{13}+E_{24}.$$

The detailed argument of these descriptions is referred to Ref. 6.

IV. INTEGRABILITY OF THE ALMOST CR STRUCTURE

In their paper[2] Atiyah, Hitchin, and Singer proved the integrability by reducing the problem to the integrability on the spinor bundles S^- instead of $\mathbf{P}(S^-)$.

In this article, however, we will reduce the integrability to certain conditions on the frame bundle $P_{\mathbf{E}}$ with respect to a submersion $\Phi:P_{\mathbf{E}}\to\mathbf{P}(S^-(\mathbf{E}))$. The frame of argument we adopt here is almost similar to that in Ref. 6. But our CR twistor space situation is quite different from that in Ref. 6 and so we must proceed to observe the details of the argument.

Choose a point $x\in M$ and take a small neighborhood U of x diffeomorphic to $\mathbf{R}^5$. Then, $P_{\mathbf{E}}$ over U admits the associated Spin(4)-bundle $\tilde{P}_{\mathbf{E}}$ over U and hence the spinor bundle $S^-(\mathbf{E})_U=\tilde{P}_{\mathbf{E}}\times_{\mathrm{Spin}(4)}S^-$ over U.

The projection $p:S^-\to P(S^-);u\mapsto p(u)$ yields the canonical projection

$$\mathbf{p}:S^-(\mathbf{E})_U\to\mathbf{P}(S^-(\mathbf{E}))|_U;\hat{\psi}^-=[\tilde{e},u]\mapsto\psi^-=[e,p(u)],\quad\tilde{e}\in\tilde{P}_{\mathbf{E}}|_U,$$

where $\tilde{e}$ is a lift of $e\in P_{\mathbf{E}}|_U$.

To each ψ^- of $\mathbf{P}(S^-(\mathbf{E}))|_U$ at $x\in U$ we define an almost complex structure $J^{\psi^-}:\mathbf{E}_x\to\mathbf{E}_x$ in the following way.

Choose a nonzero $\hat{\psi}^-$ in $S^-(\mathbf{E})$ such that $\mathbf{p}(\hat{\psi}^-)=\psi^-$.

Then the Clifford multiplication induces the $\mathbf{R}$-linear isomorphism

$$\mathbf{E}_x\to S^-(\mathbf{E})_x;X\mapsto X\cdot\hat{\psi}^-.$$

The complex structure of $S^-(\mathbf{E})_x$ yields canonically a $g|_{\mathbf{E}}$-orthogonal almost complex structure J^{ψ^-} of $\mathbf{E}_x$ as

$$(J^{\psi^-}(X))\cdot\hat{\psi}^-=\sqrt{-1}(X\cdot\hat{\psi}^-).$$

Remark that this definition does not depend on any choice of negative spinors $\hat{\psi}^-$ for ψ^-.

So, $\mathbf{P}(S^-(\mathbf{E}))$ is identified with the space of reversely oriented, orthogonal, almost complex structures on $\mathbf{E}$ and hence with the twistor space $\mathcal{Z}=U(\Lambda^2_-(\mathbf{E}))$.

We decompose by the aid of the connection $\nabla^{\mathbf{E}}$ on $\mathbf{E}$ the tangent bundle $TP_{\mathbf{E}}$ into

$$TP_{\mathbf{E}}=\hat{\mathcal{V}}\oplus\hat{\mathcal{H}},$$

where $\hat{\mathcal{V}}$ and $\hat{\mathcal{H}}$ are the vertical and horizontal subbundles, respectively.

We further decompose $\hat{\mathcal{V}}$ into the isotropic vertical part $\hat{\mathcal{V}}^{\mathfrak{h}^-}=\{A^*|A\in\mathfrak{h}^-\}$ and its orthogonal complement $\hat{\mathcal{V}}^{\mathfrak{n}^-}=\{B^*|B\in\mathfrak{n}^-\}$. Here A^* means the fundamental vector field on $P_{\mathbf{E}}$ generated by $A\in\mathfrak{so}(4)$.

So we have the decomposition

$$TP_{\mathbf{E}}=\hat{\mathcal{V}}^{\mathfrak{h}^-}\oplus\hat{\mathcal{V}}^{\mathfrak{n}^-}\oplus\hat{\mathcal{H}}'\oplus\hat{\mathcal{H}}'',\quad \hat{\mathcal{H}}=\hat{\mathcal{H}}'\oplus\hat{\mathcal{H}}''$$

corresponding to the contact decomposition $TM=\mathbf{E}\oplus\langle\xi\rangle$.

Now we choose a point $q\in P(S^-)$ and take a nonzero spinor $u\in S^-$ such that $p(u)=q$.

So, associated to $u\in S^-$, we have a smooth submersion $\Phi=\Phi_u$: $P_{\mathbf{E}}\to\mathbf{P}(S^-(\mathbf{E}))$, $e\mapsto\psi^-=[e,p(u)]$.

Remark that these submersions Φ_u obey

$$\Phi_u(ea)=\Phi_{\hat{a}u}(e),e\in P_{\mathbf{E}}$$

for $a\in\mathrm{SO}(4)$ and $\hat{a}\in\mathrm{Spin}(4)$ with $\lambda(\hat{a})=a$.

We define an associated endomorphism $\hat{\mathcal{J}}:T_eP_{\mathbf{E}}\to T_eP_{\mathbf{E}}$ at $e\in P_{\mathbf{E}}$ by

(1) $\hat{\mathcal{J}}=0$ on $\hat{\mathcal{V}}^{\mathfrak{h}^-}$,

(2) $\hat{\mathcal{J}}=\hat{J}$ on $\hat{\mathcal{V}}^-$, where $\hat{J}$ is canonically defined as $\hat{J}(B^*)=(jB)^*$, $B\in\mathfrak{n}^-$,

(3) for $X\in\hat{\mathcal{H}}'$ $\hat{\mathcal{J}}(X)$ is the horizontal vector in $\hat{\mathcal{H}}'$ for which

$$(\pi_P)_*(\hat{\mathcal{J}}(X))=J^{\Phi(e)}((\pi_P)_*(X)),$$

where $J^{\Phi(e)}:\mathbf{E}_x\to\mathbf{E}_x$ is the almost complex structure defined by $\Phi(e)\in\mathbf{P}(S^-(\mathbf{E}))$, and

(4) $\hat{\mathcal{J}}=0$ on $\hat{\mathcal{H}}''$, i.e., $\hat{\mathcal{J}}(\hat{\xi})=0$ for the horizontal lift $\hat{\xi}$ of ξ.

The definition of $\hat{\mathcal{J}}$ on $P_{\mathbf{E}}$ yields the relation

$$\Phi_*(\hat{\mathcal{J}}(X))=\mathcal{J}(\Phi_*(X)),X\in TP_{\mathbf{E}}.$$

Remark that $\mathrm{Ker}\Phi_*=\hat{\mathcal{V}}^{\mathfrak{h}^-}$ and further Φ_* maps the subbundle $\hat{\mathcal{E}}=\hat{\mathcal{V}}^{\mathfrak{n}^-}\oplus\hat{\mathcal{H}}'$ isomorphically onto the subbundle $\mathcal{E}=\mathcal{V}\oplus\mathcal{H}'$ of $T\mathbf{P}(S^-(\mathbf{E}))$.

With respect to $\hat{\mathcal{J}}$ the complexified bundle $\hat{\mathcal{E}}\otimes\mathbf{C}=(\hat{\mathcal{V}}^{\mathfrak{n}^-}\oplus\hat{\mathcal{H}}')\otimes\mathbf{C}$ decomposes into the (1,0)-part and (0,1)-part as

$$\hat{\mathcal{E}}\otimes\mathbf{C}=\hat{\mathcal{E}}^{(1,0)}\oplus\hat{\mathcal{E}}^{(0,1)}.$$

Since the Φ is a submersion, the bracket operation $[\cdot,\cdot]$ is preserved through Φ for φ-related vector fields. So, we can state the integrability condition of the almost CR structure as follows.

Proposition 4.1: The almost CR structure $\mathcal{J}$ on $\mathcal{Z}=\mathbf{P}(S^-(\mathbf{E}))$ is integrable if and only if, for each $p(u)\in P(S^-)$, the endomorphism $\hat{\mathcal{J}}=\hat{\mathcal{J}}^{\Phi}$ associated to the $\Phi=\Phi_u$ fulfills

$$[Z-\sqrt{-1}\hat{\mathcal{J}}Z,W-\sqrt{-1}\hat{\mathcal{J}}W]\in\Gamma(\hat{\mathcal{V}}^{\mathfrak{h}^-}\otimes\mathbf{C}\oplus\hat{\mathcal{E}}^{(1,0)})$$

for any smooth sections $Z-\sqrt{-1}\hat{\mathcal{J}}Z,W-\sqrt{-1}\hat{\mathcal{J}}W$ of $\hat{\mathcal{E}}^{(1,0)}$.

Since the pair $(\mathfrak{h}^-,\mathfrak{n}^-)$ is a symmetric pair, that is, $[\mathfrak{n}^-,\mathfrak{n}^-]\subset\mathfrak{h}^-$, Proposition 4.1 reduces to the following.

Proposition 4.2: $\mathcal{J}$ on $\mathcal{Z}^-$ is integrable if and only if, with respect to any $\hat{\mathcal{J}}=\hat{\mathcal{J}}^{\Phi}$ associated to Φ_u, the following two conditions hold
(i)

$$[V-\sqrt{-1}\hat{\mathcal{J}}V,W-\sqrt{-1}\hat{\mathcal{J}}W]\in\Gamma(\hat{\mathcal{V}}^{\mathfrak{h}^-}\otimes\mathbf{C}\oplus\hat{\mathcal{E}}^{(1,0)})$$

for any smooth sections $V-\sqrt{-1}\hat{\mathcal{J}}V$ of $(\hat{\mathcal{V}}^{\mathfrak{n}^-})^{(1,0)}$ and $W-\sqrt{-1}\hat{\mathcal{J}}W$ of $(\hat{\mathcal{H}}')^{(1,0)}$.
(ii)

$$[Z-\sqrt{-1}\hat{\mathcal{J}}Z,W-\sqrt{-1}\hat{\mathcal{J}}W]\in\Gamma(\hat{\mathcal{V}}^{\mathfrak{h}^-}\otimes\mathbf{C}\oplus\hat{\mathcal{E}}^{(1,0)})$$

for any smooth sections $Z-\sqrt{-1}\hat{\mathcal{J}}Z,W-\sqrt{-1}\hat{\mathcal{J}}W$ of the same subbundle $(\hat{\mathcal{H}}')^{(1,0)}$.

V. THE CURVATURE CONDITIONS AND THE PROOF OF THEOREM 1.1

We will verify Theorem 1.1 by investigating the integrability hypothesis given in Proposition 4.2.

1. First we show by choosing appropriate negative spinors that the integrability condition implies the curvature conditions stated in Theorem 1.1, namely, that a K-contact 5-manifold (M,η,ξ,ϕ,g) satisfies $\mathcal{W}^-=0$ for the Weyl conformal curvature tensor $\mathcal{W}$ and the scalar curvature $s=-4$.

In fact, we will take three negative spinors in $S^-(\mathbf{E})$ such that the associated almost complex structures correspond to the three anti-self-dual forms $\theta_1\wedge\theta_2-\theta_3\wedge\theta_4,\theta_1\wedge\theta_3+\theta_2\wedge\theta_4,\theta_1\wedge\theta_4-\theta_2\wedge\theta_3$, respectively. Here $\{\theta_i\}$ is the dual frame of a ϕ-basis $\{e_i\}$.

We make use of the decomposition of $\mathfrak{so}(4)=\mathfrak{h}^-\oplus\mathfrak{n}^-$ and their bases given in Sec. III and set

$$Y_1=E_{12},\quad Y_2=E_{34},\quad Y_3=E_{13}-E_{24},\quad Y_4=E_{14}+E_{23},$$

$$Y_5=E_{13}+E_{24},\quad Y_6=E_{14}-E_{23},$$

so $\mathfrak{h}^-$ is spanned by $Y_i,i=1,\ldots,4$ and $\mathfrak{n}^-$ by Y_5,Y_6.

Let $x\in M$ and choose a neighborhood U containing x. Take an orthonormal frame field $e=(e_1,e_2,e_3,e_4)$ of $\mathbf{E}$, which is a ϕ-basis.

Thus, $e=(e_1,\ldots,e_4)$ gives a smooth section of $P_{\mathbf{E}}$ over U so that $P_{\mathbf{E}}$ admits a trivialization

$$P_{\mathbf{E}}|_U=U\times\mathrm{SO}(4).$$

Fix a u in $S^-\backslash\{0\}$ with the submersion $\Phi=\Phi_u:P_{\mathbf{E}}|_U\to\mathbf{P}(S^-(\mathbf{E}))|_U$. So $\Phi(e)\in\mathbf{P}(S^-(\mathbf{E}))|_U$ yields an almost complex structure $J=J^{\Phi(e)}:\mathbf{E}_y\to\mathbf{E}_y$ at $y=\pi_P(e)\in U$.

Then $\hat{\mathcal{H}}'$ is spanned by

$$Z_i=e_i-(\omega^{\mathbf{E}}(e_i))^*=e_i-\sum_{j<k}\omega^{\mathbf{E}}_{jk}(e_i)E^*_{jk},\quad i=1,\ldots,4,$$

where $\omega^{\mathbf{E}}=(\omega^{\mathbf{E}}_{jk})=\Sigma\omega_{jk}E_{jk}$ is the connection form of $\nabla^{\mathbf{E}}$ with respect to the frame field $e=(e_i)$;

$$\nabla^{\mathbf{E}}_X e_i=\sum_{j=1}^{4}\omega^{\mathbf{E}}_{ji}(X)e_j.$$

To simplify the argument we may assume $\omega^{\mathbf{E}}_{jk}=0$ at x.

From the definition of $\hat{\mathcal{J}}$ we have

$$\hat{\mathcal{J}}Z_i = J^{\Phi(e)}e_i - \sum \omega^{\mathbf{E}}_{jk}(J^{\Phi(e)}e_i)E^*_{jk}, \quad i=1,2,3,4.$$

Hence the integrability conditions of Proposition 4.2 reduce to the following two conditions at x:

$$\text{(i)}' \quad [Y^*_6 - \sqrt{-1}Y^*_5,\ Z_i - \sqrt{-1}\hat{\mathcal{J}}Z_i] \in \Gamma((\hat{\mathcal{V}}^{\mathfrak{h}^-})\otimes\mathbf{C}\oplus(\hat{\mathcal{E}})^{(1,0)}),\ \ i=1,\ldots,4$$

and

$$\text{(ii)}' \quad [Z_i - \sqrt{-1}\hat{\mathcal{J}}Z_i,\ Z_j - \sqrt{-1}\hat{\mathcal{J}}Z_j] \in \Gamma((\hat{\mathcal{V}}^{\mathfrak{h}^-})\otimes\mathbf{C}\oplus(\hat{\mathcal{E}})^{(1,0)}),\ \ i<j$$

hold.

Remark that (ii)′ is equivalent to

$$\text{(ii)}'' \quad \hat{\mathcal{J}}([Z_i - \sqrt{-1}\hat{\mathcal{J}}Z_i, Z_j - \sqrt{-1}\hat{\mathcal{J}}Z_j]) - \sqrt{-1}[Z_i - \sqrt{-1}\hat{\mathcal{J}}Z_i, Z_j - \sqrt{-1}\hat{\mathcal{J}}Z_j] \in \Gamma((\hat{\mathcal{V}}^{\mathfrak{h}^-})\otimes\mathbf{C}),$$

since $\hat{\mathcal{E}}^{(1,0)}$ is the $\sqrt{-1}$-eigenspace of $\hat{\mathcal{J}}$.

First we remark that $(i)'$ is always satisfied.

In fact, Y^*_5, Y^*_6 and E^*_{jk} are vector fields on $U\times\mathrm{SO}(4)$ having only $\mathrm{SO}(4)$-components which are constant along U, while e_i and $J^{\Phi(e)}e_i$ have only U-components, constant along $\mathrm{SO}(4)$. So

$$[Y^*_6 - \sqrt{-1}Y^*_5, Z_i - \sqrt{-1}\hat{\mathcal{J}}Z_i] = -\sum \omega^{\mathbf{E}}_{jk}(e_i)[Y^*_6 - \sqrt{-1}Y^*_5, E^*_{jk}] + \sqrt{-1}\sum \omega^{\mathbf{E}}_{jk}(J^{\Phi(e)}e_i)[Y^*_6 - \sqrt{-1}Y^*_5, E^*_{jk}].$$

The above vanishes at x, since $\omega^{\mathbf{E}}=0$. So the condition (i)′ is fulfilled.

2. To exploit (ii)″ we choose a $u\in S^-\backslash\{0\}$ such that $J=J^{\Phi(e)}$ associated to $\Phi(e)=\Phi_u(e)$ is given by

$$J(e_1)=e_2, \quad J(e_3)=-e_4.$$

So we have $\hat{\mathcal{J}}Z_1=Z_2$ and $\hat{\mathcal{J}}Z_4=Z_3$ and then $Z_1-\sqrt{-1}\hat{\mathcal{J}}Z_1=Z_1-\sqrt{-1}Z_2$ and $Z_3-\sqrt{-1}\hat{\mathcal{J}}Z_3=Z_3+\sqrt{-1}Z_4$.

The nontrivial conditions in (ii)″ are then only the one for $(i,j)=(1,3)$, namely,

$$\hat{\mathcal{J}}[Z_1-\sqrt{-1}Z_2, Z_3+\sqrt{-1}Z_4] - \sqrt{-1}[Z_1-\sqrt{-1}Z_2, Z_3+\sqrt{-1}Z_4] \in \Gamma((\hat{\mathcal{V}}^{\mathfrak{h}^-})\otimes\mathbf{C}).$$

At the e in $P_{\mathbf{E}}$ over x the bracket $[Z_1,Z_3]$ takes the value

$$\begin{aligned}[Z_1,Z_3] &= [e_1-(\omega^{\mathbf{E}}(e_1))^*, e_3-(\omega^{\mathbf{E}}(e_3))^*] \\ &= [e_1,e_3]-[e_1,(\omega^{\mathbf{E}}(e_3))^*]+[e_3,(\omega^{\mathbf{E}}(e_1))^*]+[(\omega^{\mathbf{E}}(e_1))^*,(\omega^{\mathbf{E}}(e_3))^*] \\ &= [e_1,e_3]-\left[e_1,\sum \omega^{\mathbf{E}}_{jk}(e_3)E^*_{jk}\right]+\left[e_3,\sum \omega^{\mathbf{E}}_{jk}(e_1)E^*_{jk}\right].\end{aligned}$$

It follows then from the assumption $\omega^{\mathbf{E}}=0$ at the x that

$$[Z_1,Z_3]=[e_1,e_3]-\sum e_1(\omega^{\mathbf{E}}_{jk}(e_3)))E^*_{jk}+\sum e_3(\omega^*_{jk}(e_1))E^*_{jk}$$

$$=[e_1,e_3]-\sum_{j<k}(d\omega^{\mathbf{E}}_{jk})(e_1,e_3)E^*_{jk}$$

$$=[e_1,e_3]-\sum_{j<k}\Omega^{\mathbf{E}}_{jk}(e_1,e_3)E^*_{jk}, \tag{6}$$

where $\Omega^{\mathbf{E}}$ denotes the curvature form of $\nabla^{\mathbf{E}}$ on $\mathbf{E}$. Thus we get the following.

Lemma 5.1: At e in $P_{\mathbf{E}}=U\times \mathrm{SO}(4)$ over x

$$[Z_1-\sqrt{-1}Z_2,Z_3+\sqrt{-1}Z_4]=-\sum\{\Omega^{\mathbf{E}}_{jk}(e_1,e_3)+\Omega^{\mathbf{E}}_{jk}(e_2,e_4)+\sqrt{-1}(\Omega^{\mathbf{E}}_{jk}(e_1,e_4)$$
$$-\Omega^{\mathbf{E}}_{jk}(e_2,e_3))\}E^*_{jk}. \tag{7}$$

For brevity we write this as

$$[Z_1-\sqrt{-1}Z_2,Z_3+\sqrt{-1}Z_4]=-\sum\Omega^{\mathbf{E}}_{jk}(e_1-\sqrt{-1}e_2,e_3+\sqrt{-1}e_4)E^*_{jk}. \tag{8}$$

Proof: From (2)

$$[Z_1-\sqrt{-1}Z_2,Z_3+\sqrt{-1}Z_4]=\{[e_1,e_3]+[e_2,e_4]\}+\sqrt{-1}\{[e_1,e_4]-[e_2,e_3]\}-\sum\{\Omega^{\mathbf{E}}_{jk}(e_1,e_3)$$
$$+\Omega^{\mathbf{E}}_{jk}(e_2,e_4)+\sqrt{-1}(\Omega^{\mathbf{E}}_{jk}(e_1,e_4)-\Omega^{\mathbf{E}}_{jk}(e_2,e_3))\}E^*_{jk}. \tag{9}$$

From Lemma 2.1, the first two terms on the rhs have no ξ-component. So, they vanish at x, since $[e_1,e_3]+[e_2,e_4]+\cdots$ is given by $\nabla^{\mathbf{E}}_{e_1}e_3-\nabla^{\mathbf{E}}_{e_3}e_1+\cdots$ which vanishes at x.

We now express (5) in terms of the basis $\{Y^*_i|i=1,\ldots,6\}$ as

$$[Z_1-\sqrt{-1}Z_2,Z_3+\sqrt{-1}Z_4]=-\Omega^{\mathbf{E}}_{12}(s,t)Y^*_1-\Omega^{\mathbf{E}}_{34}(s,t)Y^*_2-\tfrac{1}{2}\{\Omega^{\mathbf{E}}_{13}(s,t)-\Omega^{\mathbf{E}}_{24}(s,t)\}Y^*_3$$
$$-\tfrac{1}{2}\{\Omega^{\mathbf{E}}_{14}(s,t)+\Omega^{\mathbf{E}}_{23}(s,t)\}Y^*_4-\tfrac{1}{2}\{\Omega^{\mathbf{E}}_{13}(s,t)+\Omega^{\mathbf{E}}_{24}(s,t)\}Y^*_5$$
$$-\tfrac{1}{2}\{\Omega^{\mathbf{E}}_{14}(s,t)-\Omega^{\mathbf{E}}_{23}(s,t)\}Y^*_6,$$

where we set $s=e_1-\sqrt{-1}e_2$ and $t=e_3+\sqrt{-1}e_4$, for brevity.

So, by the definition of $\hat{\mathcal{J}}$,

$$\hat{\mathcal{J}}[Z_1-\sqrt{-1}Z_2,Z_3+\sqrt{-1}Z_4]=\tfrac{1}{2}\{\Omega^{\mathbf{E}}_{13}(s,t)+\Omega^{\mathbf{E}}_{24}(s,t)\}Y^*_6-\tfrac{1}{2}\{\Omega^{\mathbf{E}}_{14}(s,t)-\Omega^{\mathbf{E}}_{23}(s,t)\}Y^*_5. \tag{10}$$

On the other hand,

$$\sqrt{-1}[Z_1-\sqrt{-1}Z_2,Z_3+\sqrt{-1}Z_4]=-\frac{\sqrt{-1}}{2}\{\Omega^{\mathbf{E}}_{13}(s,t)+\Omega^{\mathbf{E}}_{24}(s,t)\}Y^*_5-\frac{\sqrt{-1}}{2}\{\Omega^{\mathbf{E}}_{14}(s,t)$$
$$-\Omega^{\mathbf{E}}_{23}(s,t)\}Y^*_6 \mod \hat{\mathcal{V}}^{(1)^-}. \tag{11}$$

Therefore the condition (ii)″ for $(i,j)=(1,3)$ is equivalent to

$$\hat{\mathcal{J}}[Z_1-\sqrt{-1}Z_2,Z_3+\sqrt{-1}Z_4]-\sqrt{-1}[Z_1-\sqrt{-1}Z_2,Z_3+\sqrt{-1}Z_4]$$
$$=\left\{-\frac{1}{2}(\Omega^{\mathbf{E}}_{14}(s,t)-\Omega^{\mathbf{E}}_{23}(s,t))+\frac{\sqrt{-1}}{2}(\Omega^{\mathbf{E}}_{13}(s,t)+\Omega^{\mathbf{E}}_{24}(s,t))\right\}Y_5^*$$
$$+\left\{\frac{1}{2}(\Omega^{\mathbf{E}}_{13}(s,t)+\Omega^{\mathbf{E}}_{24}(s,t))+\frac{\sqrt{-1}}{2}(\Omega^{\mathbf{E}}_{14}(s,t)-\Omega^{\mathbf{E}}_{23}(s,t))\right\}Y_6^*\in\Gamma(\hat{\mathcal{V}}^{\flat^-}\otimes\mathbf{C}).$$

Clearly this holds if and only if

$$-\frac{1}{2}(\Omega^{\mathbf{E}}_{14}(s,t)-\Omega^{\mathbf{E}}_{23}(s,t))+\frac{\sqrt{-1}}{2}(\Omega^{\mathbf{E}}_{13}(s,t)+\Omega^{\mathbf{E}}_{24}(s,t))=0, \tag{12}$$

$$\frac{1}{2}(\Omega^{\mathbf{E}}_{13}(s,t)+\Omega^{\mathbf{E}}_{24}(s,t))+\frac{\sqrt{-1}}{2}(\Omega^{\mathbf{E}}_{14}(s,t)-\Omega^{\mathbf{E}}_{23}(s,t))=0. \tag{13}$$

Equation (13) is reduced to (12) and one can see that, when one writes $\Omega^{\mathbf{E}}_{k\ell}(e_i,e_j)=R^{\mathbf{E}}_{\ell kij}$, (12) is written as the two real equations;

$$R^{\mathbf{E}}_{1341}+R^{\mathbf{E}}_{2441}-R^{\mathbf{E}}_{1332}-R^{\mathbf{E}}_{2432}+R^{\mathbf{E}}_{1431}-R^{\mathbf{E}}_{2331}+R^{\mathbf{E}}_{1442}-R^{\mathbf{E}}_{2342}=0 \tag{14}$$

and

$$R^{\mathbf{E}}_{1441}-R^{\mathbf{E}}_{2341}-R^{\mathbf{E}}_{1432}+R^{\mathbf{E}}_{2332}-R^{\mathbf{E}}_{1331}-R^{\mathbf{E}}_{2431}-R^{\mathbf{E}}_{1342}-R^{\mathbf{E}}_{2442}=0. \tag{15}$$

From the symmetry of the curvature $R^{\mathbf{E}}_{ijk\ell}$ in (i,j) and (k,ℓ) these are

$$-R^{\mathbf{E}}_{1413}+R^{\mathbf{E}}_{1323}-R^{\mathbf{E}}_{1424}+R^{\mathbf{E}}_{2324}=0 \tag{16}$$

and

$$-R^{\mathbf{E}}_{1414}+2R^{\mathbf{E}}_{1423}-R^{\mathbf{E}}_{2323}+R^{\mathbf{E}}_{1313}+2R^{\mathbf{E}}_{1324}+R^{\mathbf{E}}_{2424}=0. \tag{17}$$

By the aid of Lemma 2.3 and the remark there they can be further written in terms of the Riemannian curvature $R_{ijk\ell}$ of (M,η,ξ,ϕ,g) as

$$-R_{1413}+R_{1323}-R_{1424}+R_{2324}=0 \tag{18}$$

and

$$-R_{1414}+2(R_{1423}+1)-R_{2323}+R_{1313}+2(R_{1324}-1)+R_{2424}=0. \tag{19}$$

We now make use of the decomposition of $R_{ijk\ell}$ in terms of the Weyl conformal tensor $W_{ijk\ell}$, the Ricci tensor $R_{ij}=\Sigma_k R_{kijk}$ and the scalar curvature s:

$$R_{ijk\ell}=W_{ijk\ell}-\frac{1}{3}(R_{ik}\delta_{j\ell}+R_{j\ell}\delta_{ik}-R_{i\ell}\delta_{jk}-R_{jk}\delta_{i\ell})-\frac{s}{12}(\delta_{jk}\delta_{i\ell}-\delta_{j\ell}\delta_{ik}).$$

We then rewrite the above as follows:

$$-W_{1414}+2W_{1423}-W_{2323}+W_{1313}+2W_{1324}+W_{2424}=0$$
$$-W_{1413}+W_{1323}-W_{1424}+W_{2324}=0, \tag{20}$$

namely

$$\mathcal{W}(\theta_1\wedge\theta_4-\theta_2\wedge\theta_3,\theta_1\wedge\theta_4-\theta_2\wedge\theta_3)=\mathcal{W}(\theta_1\wedge\theta_3+\theta_2\wedge\theta_4,\theta_1\wedge\theta_3+\theta_2\wedge\theta_4), \tag{21}$$

$$\mathcal{W}(\theta_1\wedge\theta_4-\theta_2\wedge\theta_3,\theta_1\wedge\theta_3+\theta_2\wedge\theta_4)=0. \tag{22}$$

3. We next take another $u'\in S^-\backslash\{0\}$ such that J associated with $\Phi_{u'}$ is given

$$J(e_1)=e_3,\quad J(e_2)=e_4.$$

Just like the preceding case, we get

$$\mathcal{W}(\theta_1\wedge\theta_2-\theta_3\wedge\theta_4,\theta_1\wedge\theta_4-\theta_2\wedge\theta_3)=\mathcal{W}(\theta_1\wedge\theta_3-\theta_4\wedge\theta_2,\theta_1\wedge\theta_4-\theta_2\wedge\theta_3) \tag{23}$$

and

$$\mathcal{W}(\theta_1\wedge\theta_4-\theta_2\wedge\theta_3,\theta_1\wedge\theta_4-\theta_2\wedge\theta_3)+\mathcal{W}(\theta_1\wedge\theta_2-\theta_3\wedge\theta_4,\theta_1\wedge\theta_3+\theta_2\wedge\theta_4)=\frac{s}{6}+\frac{2}{3}. \tag{24}$$

Notice a K-contact metric 5-manifold M has the scalar curvature $s=\Sigma_{i=1}^4 R_{ii}+Ric(\xi,\xi)$ and $Ric(\xi,\xi)=4$.

Further, choose a $u''\in S^-\backslash\{0\}$ such that the associated almost complex structure J satisfies

$$J(e_1)=e_4,\quad J(e_3)=e_2.$$

In this case we write similarly the integrability condition as

$$\mathcal{W}(\theta_1\wedge\theta_3-\theta_4\wedge\theta_2,\theta_1\wedge\theta_4-\theta_2\wedge\theta_3)=\mathcal{W}(\theta_1\wedge\theta_2-\theta_3\wedge\theta_4,\theta_1\wedge\theta_3+\theta_2\wedge\theta_4) \tag{25}$$

and

$$\mathcal{W}(\theta_1\wedge\theta_3-\theta_4\wedge\theta_2,\theta_1\wedge\theta_3-\theta_4\wedge\theta_2)+\mathcal{W}(\theta_1\wedge\theta_4-\theta_2\wedge\theta_3,\theta_1\wedge\theta_2-\theta_3\wedge\theta_4)=\frac{s}{6}+\frac{2}{3}. \tag{26}$$

4. From the above equations altogether, we see that $\mathcal{W}_-^-$ has only diagonal components. Further, by making use of the symmetric consideration in indices $\{1,2,3,4\}$, that is, by taking account of the even permutation invariance of the integrability, it follows that $\mathcal{W}_-^-$ is a scalar multiple $c=s/6+\frac{2}{3}$ of the standard bilinear form. Notice that the permutational invariance is based on the ambiguity in choosing the isotropy subgroup H^- representing $P^1(\mathbf{C})$ as $\mathrm{SO}(4)/H^-$.

Therefore, from the trace free property of the Weyl conformal tensor $\mathcal{W}_-^-$ must vanish and $s/6+\frac{2}{3}=0$, that is, $s=-4$. In fact, we have the following.

Lemma 5.2:

$$\mathrm{tr}\mathcal{W}_-^-=0.$$

Proof: Since $\theta_1\wedge\theta_2-\theta_3\wedge\theta_4$, $\theta_1\wedge\theta_3-\theta_4\wedge\theta_2$ and $\theta_1\wedge\theta_4-\theta_2\wedge\theta_3$ form a basis of $\Lambda_-^2(\mathbf{E}^*)$,

$$\begin{aligned}\mathrm{tr}\mathcal{W}_-^-=&\mathcal{W}(\theta_1\wedge\theta_2-\theta_3\wedge\theta_4,\theta_1\wedge\theta_2-\theta_3\wedge\theta_4)+\mathcal{W}(\theta_1\wedge\theta_3-\theta_4\wedge\theta_2,\theta_1\wedge\theta_3-\theta_4\wedge\theta_2)\\&+\mathcal{W}(\theta_1\wedge\theta_4-\theta_2\wedge\theta_3,\theta_1\wedge\theta_4-\theta_2\wedge\theta_3),\end{aligned} \tag{27}$$

which reduces to

$$\mathrm{tr}\mathcal{W}_-^-=\sum_{i,j=1,\,i<j}^{4} W_{ijij}-2(W_{1234}+W_{1342}+W_{1423}).$$

Here the second term vanishes from the first Bianchi identity, since $W_{1234}+W_{1342}+W_{1423}=R_{1234}+R_{1342}+R_{1423}$. On the other hand, from the trace free property of the Weyl conformal tensor W we have $\Sigma_{a=1}^{4}W_{a1a1}=-W_{0101}$ where 0 means the ξ-direction. So, by using again the trace free property the half of the first term is

$$\sum_a W_{a1a1}+\sum_a W_{a2a2}+\sum_a W_{a3a3}+\sum_a W_{a4a4}=-\sum_a W_{0a0a}=0.$$

5. In order to verify the converse implication of Theorem 1.1 it suffices to show that under the curvature conditions in Theorem 1.1 $\mathcal{J}$ is integrable at an arbitrary $\psi\in\mathcal{Z}=\mathbf{P}(S^-(\mathbf{E}))$. Any ψ can be represented as $[e,p(v)]$, where $e=(e_1,\ldots,e_4)$ is an orthonormal ϕ-basis at the point $\pi(\psi)=x$ and $v\in S^-$. But there is an $\hat{a}=(\mathrm{id},a_-)\in\mathrm{Spin}(4)=\mathrm{SU}(2)_+\times\mathrm{SU}(2)_-$ such that $v=\hat{a}\cdot u$ for the appropriate negative spinor $u\in S^-$ which appeared in Sec. V B.

So $\psi=[e,p(\hat{a}\cdot u)]$ is $[ea,p(u)]$, $a\in\mathrm{SO}(4)$.

Since the property of ϕ-basis is invariant under the $\mathrm{SU}(2)_-$-action, ea is again a ϕ-basis.

Renaming ea as e, we have the induced almost complex structure $J=J^{\psi}:\mathbf{E}_x\to\mathbf{E}_x$ satisfying

$$J(e_1)=e_2,\quad J(e_3)=-e_4.$$

So, the integrability of $\mathcal{J}$ at ψ reduces to the one of $\mathcal{J}$ at a particular negative spinor, which is guaranteed by the curvature condition $\mathcal{W}_-=0$ and $s=-4$, as was shown in Sec. V B.

Thus Theorem 1.1 is completely proved.

VI. THE CR HOLOMORPHICITY OF $\tilde{\xi}$

To prove Theorem 1.2 we take, similarly as in the proof of Theorem 1.1, over $P_{\mathbf{E}}$ the horizontal lift $\hat{\xi}$ of ξ and consider the CR holomorphicity of $\tilde{\xi}$ in terms of $\hat{\xi}$.

$\tilde{\xi}$ on $\mathcal{Z}$ is CR holomorphic if and only if, for each $\Phi_u:P_{\mathbf{E}}\to\mathcal{Z}$, $u\in S^-$, it holds that $[\hat{\xi},Z]$ is a section of $\hat{\mathcal{E}}^{1,0}$ mod $\Gamma(\hat{\mathcal{V}}^{\mathfrak{h}^-}\otimes\mathbf{C})$ for each section Z of $\hat{\mathcal{E}}^{1,0}$.

This is equivalent to the following:

For each Φ_u

(i) $[\hat{\xi},Y_6^*-\sqrt{-1}Y_5^*]$ is a section of $\hat{\mathcal{E}}^{1,0}$ mod $\Gamma(\hat{\mathcal{V}}^{\mathfrak{h}^-}\otimes\mathbf{C})$, and

(ii) $[\hat{\xi},Z-\sqrt{-1}\hat{\mathcal{J}}Z]$ is a section of $\hat{\mathcal{E}}^{1,0}$ mod $\Gamma(\hat{\mathcal{V}}^{\mathfrak{h}^-}\otimes\mathbf{C})$ for any $Z\in\Gamma(\hat{\mathcal{H}}')$, where $\hat{\mathcal{J}}$ is the almost complex structure associated to Φ_u.

The first condition is always fulfilled.

It suffices for the proof of Theorem 1.2 to show the following.

Proposition 6.1: Let (M,η,ξ,ϕ,g) be a K-contact metric 5-manifold and $\mathcal{Z}$ be its CR twistor space.

$\tilde{\xi}$ is CR holomorphic on $\mathcal{Z}$ if and only if the curvature R of (M,η,ξ,ϕ,g) satisfies

$$R_{0i12}-R_{0i34}=R_{0i13}+R_{0i24}=R_{0i14}-R_{0i23}=0,\ \ i=1,\ldots,4, \tag{28}$$

where $(e_1,\ldots,e_4)$ is an orthonormal ϕ-basis and $e_0=\xi$.

Proof of Proposition 6.1: We will investigate condition (ii).

Assume $\tilde{\xi}$ is CR holomorphic.

Take a point $x\in M$ and an orthonormal frame field e of $\mathbf{E}$ around x which is a ϕ-basis and choose the spinor $u\in S^-\setminus\{0\}$ again such that the associated almost complex structure J satisfies

$$J(e_1)=e_2,\quad J(e_3)=-e_4.$$

As was shown in Sec. V $Z_i=e_i-(\omega^{\mathbf{E}}(e_i))^*$ is the horizontal lift of e_i and $Z_1-\sqrt{-1}Z_2$, $Z_4-\sqrt{-1}Z_3$ span $(\hat{\mathcal{H}}')^{1,0}$.

Then, the condition (ii) for vector fields $Z_1-\sqrt{-1}Z_2$, $Z_4-\sqrt{-1}Z_3$ is written in terms of the curvature $R^{\mathbf{E}}$ as

$$-(R^{\mathbf{E}}_{1014}-R^{\mathbf{E}}_{1023})+(R^{\mathbf{E}}_{2013}+R^{\mathbf{E}}_{2024})=0,$$

$$(R^{\mathbf{E}}_{2014}-R^{\mathbf{E}}_{2023})+(R^{\mathbf{E}}_{1013}+R^{\mathbf{E}}_{1024})=0$$

and

$$-(R^{\mathbf{E}}_{4014}-R^{\mathbf{E}}_{4023})+(R^{\mathbf{E}}_{3013}+R^{\mathbf{E}}_{3024})=0,$$

$$(R^{\mathbf{E}}_{3014}-R^{\mathbf{E}}_{3023})+(R^{\mathbf{E}}_{4013}+R^{\mathbf{E}}_{4024})=0.$$

Since $\phi(\xi)=0$, from the Gauss equations in Sec. II we get

$$(R_{1014}-R_{1023})-(R_{2013}+R_{2024})=0,$$

$$(R_{2014}-R_{2023})+(R_{1013}+R_{1024})=0$$

and

$$(R_{4014}-R_{4023})-(R_{3013}+R_{3024})=0,$$

$$(R_{3014}-R_{3023})+(R_{4013}+R_{4024})=0.$$

We take another negative spinor $u'\in S^-\backslash\{0\}$. Then the conditions for u' are written similarly. So, we obtain

$$R_{0i13}+R_{0i24}=R_{0i14}-R_{0i23}=0,\quad i=0,\ldots,4.$$

By the permutational argument we have also $R_{0i12}-R_{0i34}=0$, $i=1,\ldots,4$.

The converse implication of Proposition 6.1 is obtained without difficulty, just like the proof of Theorem 1.1. So we complete the proof.

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Cyclic identities involving Jacobi elliptic functions

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We state and discuss numerous new mathematical identities involving Jacobi elliptic functions $\mathrm{sn}(x,m)$, $\mathrm{cn}(x,m)$, and $\mathrm{dn}(x,m)$, where m is the elliptic modulus parameter. In all identities, the arguments of the Jacobi functions are separated by either $2K(m)/p$ or $4K(m)/p$, where p is an integer and $K(m)$ is the complete elliptic integral of the first kind. Each p-point identity of rank r involves a cyclic homogeneous polynomial of degree r (in Jacobi elliptic functions with p equally spaced arguments) related to other cyclic homogeneous polynomials of degree $r-2$ or smaller. We algebraically demonstrate the derivation of several of our identities for specific small values of p and r by using standard properties of Jacobi elliptic functions. Identities corresponding to higher values of p and r are verified numerically using advanced mathematical software packages. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1484541]

I. INTRODUCTION

The Jacobi elliptic functions $\mathrm{sn}(x,m)$, $\mathrm{cn}(x,m)$, and $\mathrm{dn}(x,m)$ with real elliptic modulus parameter $m(0\leqslant m\leqslant 1)$ have been extensively studied and used in mathematics, science and engineering.[1,2] Recently, while studying[3,4] the properties of quantum mechanical periodic potentials,[5,6] we have discovered numerous new mathematical identities involving Jacobi elliptic functions. The purpose of this article is to tabulate, derive and discuss these identities.

To the best of our knowledge, our results are not discussed in the mathematics literature. However, we did find that geometrical constructions called the ''poristic polygons of Poncelet'' give rise to a few of our very simplest identities like Eqs. (3) and (40) involving just the Jacobi elliptic functions $\mathrm{dn}(x,m)$. For a discussion of this geometrical approach, see Refs. 7 and 8.

Our new identities play a crucial role in obtaining a large class of novel periodic solutions of both integrable and the nonintegrable nonlinear equations like the Korteweg–de Vries (KdV) and modified Korteweg–de Vries equations,[9] the nonlinear Schrödinger and KP equations, the sine–Gordon and Boussinesq equations, as well as the $\lambda\phi^4$ model.[10] The solutions obtained for the KdV equation[9] all correspond to one gap periodic potentials. This process can be generalized to obtain new solvable periodic potentials with a finite number of band gaps.[4]

If $K(m)$ denotes the complete elliptic integral of the first kind, the elliptic functions $\mathrm{sn}(x,m)$ and $\mathrm{cn}(x,m)$ have real periods $4K(m)$, whereas $\mathrm{dn}(x,m)$ has a period $2K(m)$. The $m=0$ limit gives $K(0)=\pi/2$ and trigonometric functions: $\mathrm{sn}(x,0)=\sin x$, $\mathrm{cn}(x,0)=\cos x$, $\mathrm{dn}(x,0)=1$. The $m\to 1$ limit gives $K(1)\to\infty$ and hyperbolic functions: $\mathrm{sn}(x,1)\to\tanh x$, $\mathrm{cn}(x,1)\to\mathrm{sech}\,x$, $\mathrm{dn}(x,1)\to\mathrm{sech}\,x$. Therefore, our new identities for Jacobi elliptic functions can be thought of as generalizations to arbitrary m of identities involving trigonometric and hyperbolic functions.

The plan of the article is as follows. In Sec. II, we discuss the general structure of the identities and various different ways of obtaining them. Each identity has two integer labels r and p. Here, r denotes the rank of the identity and p is the number of subdivisions of the period at which Jacobi elliptic functions are evaluated. In Sec. III, we algebraically derive some of the identities given in Tables I, II, and III for rank $r=2$, 3 and $p=2$, 3, 4. Finally, in Sec. IV, we offer several comments regarding the general patterns revealed by the identities. In Tables I and II, we have listed identities for ranks $r=2$ and 3, respectively. For clarity, we give explicit expressions

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for $p=2$, 3, 4 and then given the general structure for arbitrary p. In Table III we have given some examples of identities of rank 4 and above. The algebraic proofs of identities with large rank r and $p>4$ are tedious, but we have numerically verified the identities using the mathematical software package Maple.

II. DESCRIPTION OF THE IDENTITIES

In all the identities discussed in this article, the arguments of the Jacobi functions are separated by either $2K(m)/p$ or $4K(m)/p$, where p is an integer ($p\geqslant 2$) depending on whether the left hand side of the identity is a periodic function of period $2K(m)/p$ or $4K(m)/p$. For any given choice of p, we define the quantities s_i, c_i and d_i as follows:

$$s_i\equiv \mathrm{sn}\left[x+\frac{2(i-1)K(m)}{p},m\right],\quad c_i\equiv \mathrm{cn}\left[x+\frac{2(i-1)K(m)}{p},m\right],\quad d_i\equiv \mathrm{dn}\left[x+\frac{2(i-1)K(m)}{p},m\right]. \tag{1}$$

Similarly, we define

$$\tilde{s}_i\equiv \mathrm{sn}\left[x+\frac{4(i-1)K(m)}{p},m\right],\quad \tilde{c}_i\equiv \mathrm{cn}\left[x+\frac{4(i-1)K(m)}{p},m\right],\quad \tilde{d}_i\equiv \mathrm{dn}\left[x+\frac{4(i-1)K(m)}{p},m\right]. \tag{2}$$

Each p-point identity which we discuss will involve a cyclic homogeneous polynomial of degree r (in Jacobi elliptic functions with p equally spaced arguments) expressed as a linear combination of other cyclic homogeneous polynomials of degree $r-2n$, where $1\leqslant n\leqslant r/2$. We designate this to be a p-point identity of rank r.

Let us consider a few examples to clarify the terminology and establish the notation. A simple p-point identity of rank 2 is

$$d_1d_2+c.p.\equiv d_1d_2+d_2d_3+\cdots+d_pd_1=A, \tag{3}$$

where we have used the notation "$+c.p.$" to denote cyclic permutations of the indices 1,2,...p. Later, we have also used the notation "$-c.p.$" to denote cyclic permutations with alternating positive and negative signs in a few identities where p is an even integer. For the special case $p=4$, the quantities in Eq. (3) are

$$d_1\equiv dn(x,m), d_2\equiv \mathrm{dn}(x+K(m)/2,m), d_3\equiv \mathrm{dn}(x+K(m),m), d_4\equiv \mathrm{dn}(x+3K(m)/2,m). \tag{4}$$

As discussed in the next section, for $p=4$, the constant A can be computed and shown to be $A=2\tilde{t}(1+\tilde{t}^2)$ where

$$\tilde{t}\equiv \mathrm{dn}(K(m)/2,m)=(1-m)^{1/4}. \tag{5}$$

Similarly, two examples of three-point identities of rank 2 and rank 3 are

$$\tilde{c}_1\tilde{c}_2+c.p.=-\frac{q(q+2)}{(1+q)^2},\quad \tilde{c}_1\tilde{d}_2\tilde{d}_3+c.p.=-q^2(\tilde{c}_1+\tilde{c}_2+\tilde{c}_3), \tag{6}$$

where

$$q\equiv \mathrm{dn}(2K(m)/3,m), \tag{7}$$

and the arguments are x, $x+4K(m)/3$ and $x+8K(m)/3$, respectively. Many more examples are given in Tables I, II, and III.

Although x-independent constants like A do depend on the number of points p, the rank r, the modulus parameter m, and the specific identity involved, for simplicity, we do not usually exhibit these dependences explicitly. In fact, the symbols A and B appearing in the identities given in Tables I, II, and III are just meant to denote generic constants. They do not all have the same values.

Given any p-point identity of rank r, one way of generating a new p-point identity of rank $r+1$ is by differentiation and use of the well-known formulas

$$\frac{d}{dx}\mathrm{sn}(x,m)=\mathrm{cn}(x,m)\mathrm{dn}(x,m), \quad \frac{d}{dx}\mathrm{cn}(x,m)=-\mathrm{sn}(x,m)\mathrm{dn}(x,m),$$

$$\frac{d}{dx}\mathrm{dn}(x,m)=-m\mathrm{sn}(x,m)\mathrm{cn}(x,m), \tag{8}$$

$$\mathrm{sn}^2(x,m)+\mathrm{cn}^2(x,m)=1, \quad \mathrm{dn}^2(x,m)+m\mathrm{sn}^2(x,m)=1. \tag{9}$$

For example, differentiation of the p-point rank 2 identity

$$d_1d_2+\ldots+d_pd_1=A \tag{10}$$

yields the rank 3 identity

$$s_1c_1(d_2+d_p)+c.p.=0, \tag{11}$$

which reduces to the well-known trigonometric identity

$$\sum_{i=1}^{p}\sin\left[2x+\frac{2(i-1)\pi}{p}\right]=0 \tag{12}$$

in the limit $m=0$.

Another p-point rank r identity of interest for $r\leqslant p$ is

$$d_1d_2\cdots d_r+c.p.=A \quad (r \text{ even}), \tag{13}$$

$$d_1d_2\cdots d_r+c.p.=B\sum_{i}^{p} d_i \quad (r \text{ odd}). \tag{14}$$

One also has similar identities involving $\tilde{s}_i$ or $\tilde{c}_i$ (instead of d_i) for any odd integer value of p. All these identities have the remarkable property of reducing the degree of the polynomial in the Jacobi functions from r to 0 (1) depending on whether r is even (odd). For small values of p and r, the constants A, B in Eqs. (13) and (14) are easily evaluated. Some results are

$$A(p=2,r=2)=2\sqrt{1-m}, A(p=3,r=2)=q(q+2), A(p=4,r=2)=2\tilde{t}(1+\tilde{t}^2),$$

$$B(p=3,r=3)=3\left(\frac{m}{1-q^2}-1\right), B(p=4,r=3)=\sqrt{1-m}, \tag{15}$$

$$A(p=4,r=4)=4(1-m).$$

For the special limiting cases $m=0$ and $m=1$, one gets

$$A(m=0,p,r)=p, \;\; B(m=0,p,r)=1, \;\; A(m=1,p,r)=B(m=1,p,r)=0. \tag{16}$$

Another way of obtaining additional identities is by manipulating established identities. For example, for $p=3$ and $r=3$, Eq. (14) is

$$d_1d_2d_3=\frac{B}{3}(d_1+d_2+d_3), \tag{17}$$

where $B\equiv B(p=3,r=3)$ is as given by eq. (15). Squaring identity (3) for $p=3$ and using Eqs. (15) and (17) yields the new identity

$$d_1^2d_2^2+c.p.=-2\left(\frac{m}{1-q^2}-1\right)\sum_{i=1}^{3} d_i^2+\left[(1-q^2)^2+\frac{6m}{1-q^2}-3-4m\right]. \tag{18}$$

A similar identity is also true for any p, and in fact we have used it in a crucial manner for obtaining new periodic solutions of the KdV equation.[9] However, to establish this p-point identity, one needs a generalization of identities (3) and (14). The generalized identities are

$$d_1 d_n + c.p. = A \quad (n = 2,3,4,...), \tag{19}$$

and

$$d_1 d_{j_1} d_{j_2} + c.p. = B \sum_{i=1}^{p} d_i \quad (1 < j_1 < j_2 \leqslant p). \tag{20}$$

which we have verified to be true numerically using Maple for many specific choices of the integers n, j_1, j_2, p.

III. DERIVATION OF IDENTITIES FOR $p=2$, 3, 4

For illustrative purposes, we now outline the proof of the p-point identity $d_1 d_2 + c.p. = A$, for $p=2$, 3, 4. The left hand side of this identity contains p terms. The proof for $p=2$ is trivial, since it is well known that $d_1 d_2 \equiv \mathrm{dn}(x,m)\mathrm{dn}(x+K(m),m) = \sqrt{1-m}$.[1,2] For $p=3$, one needs to compute $d_1 d_2 + d_2 d_3 + d_3 d_1 \equiv \mathrm{dn}(x,m)\mathrm{dn}(x+2K(m)/3,m) + \mathrm{dn}(x+2K(m)/3,m)\mathrm{dn}(x+4K(m)/3,m) + \mathrm{dn}(x+4K(m)/3,m)\mathrm{dn}(x,m)$. This can be accomplished by algebraic simplification after using the addition theorem[1,2]

$$\mathrm{dn}(u+v) = (\mathrm{dn}u \ \ \mathrm{dn}v - m \ \ \mathrm{sn}u \ \ \mathrm{cn}u \ \ \mathrm{sn}v \ \ \mathrm{cn}v)/(1 - m \ \ \mathrm{sn}^2 u \ \ \mathrm{sn}^2 v), \tag{21}$$

and the fact that

$$\begin{gathered} \mathrm{dn}(4K(m)/3,m) = \mathrm{dn}(2K(m)/3,m), \ \ \mathrm{sn}(4K(m)/3,m) = \mathrm{sn}(2K(m)/3,m), \\ \mathrm{cn}(4K(m)/3,m) = -\mathrm{cn}(2K(m)/3,m). \end{gathered} \tag{22}$$

The result is the constant A for the $p=3$ case. One gets $A = q(q+2)$, where q has been defined in Eq. (7). One has also made use of the fact that q satisfies the fourth order equation

$$q^4 + 2q^3 - 2(1-m)q - (1-m) = 0, \tag{23}$$

which follows by making use of Eqs. (21) and (8) with $u = v = 2K(m)/3$. Similarly, the result for $p=4$, as discussed following Eq. (3), can be easily derived.

In principle, an analogous algebraic procedure can be used for any value of p, but the algebra becomes increasingly lengthier. We have therefore verified identity (3) numerically using the advanced mathematical software package Maple. Note that for any chosen value of p, the constant A equals p in the limit $m=0$ and vanishes for $m \to 1$.

Proceeding in this way, and using the addition theorems

$$\mathrm{cn}(u+v) = (\mathrm{cn}u \ \ \mathrm{cn}v - \mathrm{sn}u \ \ \mathrm{dn}u \ \ \mathrm{sn}v \ \ \mathrm{dn}v)/(1 - m \ \ \mathrm{sn}^2 u \ \ \mathrm{sn}^2 v), \tag{24}$$

$$\mathrm{sn}(u+v) = (\mathrm{sn}u \ \ \mathrm{cn}v \ \ \mathrm{dn}v + \mathrm{sn}v \ \ \mathrm{cn}v \ \ \mathrm{dn}u)/(1 - m \ \ \mathrm{sn}^2 u \ \ \mathrm{sn}^2 v), \tag{25}$$

for $p=2$, 3, 4, we have derived all the identities of rank 2 as given by Eqs. (31)–(34). It may be noted that the identities for $p=4$ contain identities for $p=2$ as special cases.

In the limit of $m \to 0$, two of the identities in Eq. (32) reduce to the well known trigonometric identity

$$\cos x \cos(x + 2\pi/3) + \cos(x + 2\pi/3)\cos(x + 4\pi/3) + \cos(x + 4\pi/3)\cos x = -\tfrac{3}{4}. \tag{26}$$

Let us now turn our attention to the derivation of the identities of rank $r=3$ in case $p=2$, 3, 4. For $p=2$, 4 these identities are easily derived by using the identities of rank 2 as given by Eqs. (31) and (34) and these are listed as Eqs. (39) and (60)–(63). Note that for these cases, and in fact in general for any even integer case, one obtains identities with both $+c.p.$ and $-c.p.$ As an

illustration, we start from the identity (3) with $p=4$ and $A=2\tilde{t}(1+\tilde{t}^2)$ and $\tilde{t}=(1-m)^{1/4}$. On multiplying both sides of this identity by $(d_1-d_2+d_3-d_4)$ and using the relations $d_1d_3=d_2d_4=\sqrt{1-m}$, we immediately obtain the four-point identity

$$d_1^2(d_2+d_4)-c.p.=2\tilde{t}(1+\tilde{t}+\tilde{t}^2)(d_1-c.p.). \tag{27}$$

However, for $p=3$, all the identities of rank 3 cannot be derived from those of rank 2. We find that there are four basic identities of rank 3 [say those given by Eqs. (40)–(43)] which we have derived using the addition theorems [Eqs. (21), (24), and (25)] and relations (22) and (23). As an illustration, let us consider the derivation of identity (41),

$$\tilde{c}_1\tilde{c}_2\tilde{c}_3=\frac{q^2}{1-q^2}(\tilde{c}_1+\tilde{c}_2+\tilde{c}_3), \tag{28}$$

where q is as given by Eq. (7). On using the addition theorem (24) and the fact that $\mathrm{cn}(2K(m)/3,m)=q/(1+q)$ with q satisfying Eq. (23), the identity (28) is easily derived.

Using these four basic identities and those of rank 2, one can then derive the remaining 18 identities of rank 3 (for $p=3$) as given in Table II. For example, consider the identity (57). This is easily derived by starting from the rank 2 ($p=3$) identity

$$\tilde{c}_1\tilde{c}_2+c.p.=\frac{-q(2+q)}{(1+q)^2}, \tag{29}$$

multiplying both sides by $(\tilde{c}_1+\tilde{c}_2+\tilde{c}_3)$ and using identity (28) and Eq. (27).

Finally, let us consider identities of rank 4 and higher in case $p=2$, 3, 4, some of which have been given in Table III. We find that all these identities can be derived by using the identities of rank 2 and 3 as given in Tables II and III. For example, identities (77), (79) and (80) simply follow from the basic rank 3 identities (40)–(42).

IV. DISCUSSION AND COMMENTS

By the techniques described in the previous sections, we have obtained a large number of new identities, many of which are displayed in Tables I, II, and III. It should be noted that the modulus parameter m is not transformed and remains unchanged in all identities. Although it is not easy to give a complete systematic classification, we can comment on some general properties and patterns.

(i) For any identity of rank r, the left hand side is a cyclic homogeneous polynomial expression of degree r with p terms.

(ii) If the polynomial on the left hand side is periodic with period $2K(m)/p$ $[4K(m)/p]$, then the identity involves arguments spaced by $2K(m)/p$ $[4K(m)/p]$.

(iii) The right hand side involves polynomials of rank $r-2$, $r-4$,..., which are "irreducible," some examples being Σd_i, $\Sigma\tilde{s}_i$, $\Sigma\tilde{c}_i$, $\Sigma\tilde{c}_i\tilde{d}_i$, $\Sigma\tilde{s}_i\tilde{d}_i$, Σc_is_i, $\Sigma c_is_id_i$, etc., and all these irreducibles multiplied by d_i^{2n} where $n=1,2,\ldots$.

(iv) In general, many of the identities of higher rank can be obtained from those of lower rank by either differentiation or algebraic manipulation. Similarly, many identities of a given rank r ($r>2$) can be derived from lower rank identities as well as some identities of the same rank. For example, for $p=3$, using the identities of rank 2 and three of the rank 3 identities as given by Eqs. (40)–(42) one can obtain all other identities of rank 3 as given in Table II.

(v) The generic constants A, B, C in any identity can be determined by choosing specific, convenient values of x in the arguments. The value $x=0$ is a good choice in many cases. Note that for $p\leqslant 4$, we have given explicit values for all the constants appearing in the

identities—for three-point identities, all constants are expressed in terms of $q \equiv \mathrm{dn}(2K(m)/3,m)$, and for four-point identities, all constants are expressed in terms of $\tilde{t} \equiv \mathrm{dn}(K(m)/2,m) = (1-m)^{1/4}$.

(vi) Some identities for even values of p involve alternating positive and negative signs. The symbol "$-c.p.$" in these identities refers to cyclic permutations with alternating signs. Many of these identities, like $d_1^2(d_2+d_p)-d_2^2(d_3+d_1)+\cdots-d_p^2(d_1+d_{p-1})=A(d_1-d_2+\cdots-d_p)$, play a crucial role in determining band edge wave functions of solvable quantum mechanical periodic potentials.[4]

(vii) It should be noted that our identities involve cyclic permutations $\pm c.p.$ of terms which have no clockwise or anticlockwise "handedness." For example, for even p, there is no identity of the type $(d_1^2 d_2 - c.p.)$ proportional to $(d_1 - c.p.)$, since the term $d_1^2 d_2$ has a clockwise handedness. It is only when one adds on an anticlockwise handed term $d_1^2 d_p$ that the combination $[d_1^2(d_2+d_p)-c.p.]$ is indeed proportional to $(d_1-c.p.)$.

(viii) In the limit $m \to 0$, one recovers many known nontrivial trigonometric identities. In the limit $m \to 1$, since the period $K(1) \to \infty$, one usually gets trivial hyperbolic function identities. Both these limits serve as a useful check on all the new identities involving Jacobi elliptic functions obtained in this paper. Of course, as mentioned previously, software packages like Maple or Mathematica quickly provide confirmation of any identity to typically eight digit accuracy.

(ix) Identities for a given value of p contain identities of the factors of p as special cases. For example, for even p, only half of $d_1,\ldots,d_p$ are independent since they satisfy identities

$$d_1 d_{(p+2)/2} = \cdots = d_{p/2} d_p = \sqrt{1-m}, \tag{30}$$

coming from $p=2$. Similarly, the full list of $p=6$ identities contains $p=2$, 3 identities. For example, $d_1 d_4 = d_2 d_5 = d_3 d_6 = \sqrt{1-m}$ and similarly $d_1 d_3 + d_3 d_5 + d_5 d_1 = d_2 d_4 + d_4 d_6 + d_6 d_2 = q^2 + 2q$, where q is as given by Eq. (7).

TABLE I. **Identities of rank 2.** The symbols A in Eqs. (35) and (37) are used generically to denote constants independent of x; the constants are in general all different.

p=2:

$$d_1 d_2 = \sqrt{1-m}. \tag{31}$$

p=3: $[q \equiv \mathrm{dn}(2K(m)/3,m)]$

$$d_1 d_2 + c.p. = q(q+2),\ \tilde{c}_1\tilde{c}_2 + c.p. = \frac{-q(q+2)}{(1+q)^2},\ \tilde{s}_1\tilde{s}_2 + c.p. = \frac{1}{m}(q^2-1), \tag{32}$$

$$\tilde{c}_1(\tilde{d}_2+\tilde{d}_3)+c.p. = \tilde{s}_1(\tilde{d}_2+\tilde{d}_3)+c.p. = \tilde{c}_1(\tilde{s}_2+\tilde{s}_3)+c.p. = 0. \tag{33}$$

p=4: $[\tilde{t} \equiv \mathrm{dn}(K(m)/2,m) = (1-m)^{1/4}]$

$$d_1 d_3 = d_2 d_4 = \sqrt{1-m},\ d_1 d_2 + c.p. = 2\tilde{t}(1+\tilde{t}^2). \tag{34}$$

p=even integer:

$$d_1 d_2 + c.p. = A,\ d_1 d_3 + c.p. = A,\ \ldots,\ d_1 d_{p/2} + c.p. = A, \tag{35}$$

$$d_1 d_{p/2+1} = d_2 d_{p/2+2} = \cdots = d_{p/2} d_p = \sqrt{1-m}. \tag{36}$$

p=odd integer:

$$\begin{gathered} d_1 d_2 + c.p. = A,\ \tilde{c}_1\tilde{c}_2 + c.p. = A,\ \tilde{s}_1\tilde{s}_2 + c.p. = A, \\ \vdots \\ d_1 d_{(p+1)/2} + c.p. = A,\ \tilde{c}_1\tilde{c}_{(p+1)/2} + c.p. = A,\ \tilde{s}_1\tilde{s}_{(p+1)/2} + c.p. = A, \\ \tilde{c}_1(\tilde{d}_2+\tilde{d}_p)+c.p. = 0,\ \tilde{s}_1(\tilde{d}_2+\tilde{d}_p)+c.p. = 0,\ \tilde{c}_1(\tilde{s}_2+\tilde{s}_p)+c.p. = 0, \\ \vdots \\ \tilde{c}_1(\tilde{d}_{(p+1)/2}+\tilde{d}_{(p+3)/2})+c.p. = 0,\ \tilde{s}_1(\tilde{d}_{(p+1)/2}+\tilde{d}_{(p+3)/2})+c.p. \\ = 0,\ \tilde{c}_1(\tilde{s}_{(p+1)/2}+\tilde{s}_{(p+3)/2})+c.p. = 0. \end{gathered} \tag{37, 38}$$

TABLE II. **Identities of rank 3.** The symbols A in Eqs. (66)–(73) are used generically to denote constants independent of x; the constants are in general all different.

p=2:

$$d_1^2 d_2 \pm d_2^2 d_1 = \sqrt{1-m}\,(d_1 \pm d_2), \quad c_1 s_1 d_2 + c_2 s_2 d_1 = 0. \tag{39}$$

p=3: $[q \equiv \mathrm{dn}(2K(m)/3,m)]$

$$d_1 d_2 d_3 = \frac{(q^2+m-1)}{1-q^2}(d_1+d_2+d_3), \tag{40}$$

$$\tilde{c}_1\tilde{c}_2\tilde{c}_3 = \frac{q^2}{1-q^2}(\tilde{c}_1+\tilde{c}_2+\tilde{c}_3), \tag{41}$$

$$\tilde{s}_1\tilde{s}_2\tilde{s}_3 = \frac{-1}{1-q^2}(\tilde{s}_1+\tilde{s}_2+\tilde{s}_3), \tag{42}$$

$$\tilde{c}_1(\tilde{s}_2\tilde{d}_3+\tilde{s}_3\tilde{d}_2)+c.p.=0, \tag{43}$$

$$\tilde{c}_1\tilde{d}_2\tilde{d}_3+c.p.=-q^2(\tilde{c}_1+\tilde{c}_2+\tilde{c}_3), \tag{44}$$

$$m\tilde{c}_1\tilde{s}_2\tilde{s}_3+c.p.=-(1+q)^2(\tilde{c}_1+\tilde{c}_2+\tilde{c}_3), \tag{45}$$

$$\tilde{s}_1\tilde{d}_2\tilde{d}_3+c.p.=\frac{-(1-m)}{q^2}(\tilde{s}_1+\tilde{s}_2+\tilde{s}_3), \tag{46}$$

$$\tilde{s}_1\tilde{c}_2\tilde{c}_3+c.p.=\frac{q(q+2)}{1-q^2}(\tilde{s}_1+\tilde{s}_2+\tilde{s}_3), \tag{47}$$

$$\tilde{d}_1\tilde{c}_2\tilde{c}_3+c.p.=\frac{-q^2}{(1+q)^2}(\tilde{d}_1+\tilde{d}_2+\tilde{d}_3), \tag{48}$$

$$\tilde{d}_1\tilde{s}_2\tilde{s}_3+c.p.=\frac{-1}{(1+q)^2}(\tilde{d}_1+\tilde{d}_2+\tilde{d}_3), \tag{49}$$

$$\tilde{d}_1(\tilde{d}_2\tilde{c}_2+\tilde{d}_3\tilde{c}_3)=c.p.=2q(q+1)(\tilde{c}_1+\tilde{c}_2+\tilde{c}_3), \tag{50}$$

$$m\tilde{s}_1(\tilde{s}_2\tilde{c}_2+\tilde{s}_3\tilde{c}_3)+c.p.=2q(q+1)(\tilde{c}_1+\tilde{c}_2+\tilde{c}_3), \tag{51}$$

$$\tilde{d}_1(\tilde{d}_2\tilde{s}_2+\tilde{d}_3\tilde{s}_3)+c.p.=\frac{2(q^2+2q-m+1)}{1+q}(\tilde{s}_1+\tilde{s}_2+\tilde{s}_3), \tag{52}$$

$$\tilde{c}_1(\tilde{c}_2\tilde{s}_2+\tilde{c}_3\tilde{s}_3)+c.p.=\frac{-2q(q+2)}{(1+q)(1-q^2)}(\tilde{s}_1+\tilde{s}_2+\tilde{s}_3), \tag{53}$$

$$\tilde{c}_1(\tilde{c}_2\tilde{d}_2+\tilde{c}_3\tilde{d}_3)+c.p.=\frac{-2q}{(1+q)^2}(\tilde{d}_1+\tilde{d}_2+\tilde{d}_3), \tag{54}$$

$$\tilde{s}_1(\tilde{s}_2\tilde{d}_2+\tilde{s}_3\tilde{d}_3)+c.p.=\frac{-2q}{(1+q)^2}(\tilde{d}_1+\tilde{d}_2+\tilde{d}_3), \tag{55}$$

$$d_1^2(d_2+d_3)+c.p.=\frac{2(q-m+1)}{1+q}(d_1+d_2+d_3), \tag{56}$$

$$m\tilde{c}_1^2(\tilde{c}_2+\tilde{c}_3)+c.p.=-2(1+q-m)(\tilde{c}_1+\tilde{c}_2+\tilde{c}_3), \tag{57}$$

$$m\tilde{s}_1^2(\tilde{s}_2+\tilde{s}_3)+c.p.=\frac{2(q^3+q^2-q+mq+2m-1)}{1-q^2}(\tilde{s}_1+\tilde{s}_2+\tilde{s}_3), \tag{58}$$

$$c_1 s_1(d_2+d_3)+c.p.=0, \quad \tilde{c}_1\tilde{d}_1(\tilde{s}_2+\tilde{s}_3)+c.p.=0,$$
$$\tilde{d}_1\tilde{s}_1(\tilde{c}_2+\tilde{c}_3)+c.p.=0. \tag{59}$$

p=4: $[\tilde{t} \equiv \mathrm{dn}(K(m)/2,m)=(1-m)^{1/4}]$

$$d_1 d_2 d_3 \pm d_2 d_3 d_4 + d_3 d_4 d_1 \pm d_4 d_1 d_2 = \sqrt{1-m}\,(\pm d_1 + d_2 \pm d_3 + d_4), \tag{60}$$

$$d_1^2(d_2+d_4)\pm d_2^2(d_3+d_1)+d_3^2(d_4+d_2)\pm d_4^2(d_1+d_3)=2\tilde{t}(1\mp\tilde{t}+\tilde{t}^2)(d_1\pm d_2+d_3\pm d_4), \tag{61}$$

$$d_1^2 d_3 \pm d_2^2 d_4 + d_3^2 d_1 \pm d_4^2 d_2 = \sqrt{1-m}\,(d_1 \pm d_2 + d_3 \pm d_4), \tag{62}$$

$$c_1 s_1(d_2+d_4)+c.p.=0, \quad c_1 s_1 d_3 + c_3 s_3 d_1 = 0, \quad c_2 s_2 d_4 + c_4 s_4 d_2 = 0. \tag{63}$$

p=even integer:

$$c_1 s_1(d_2+d_p)+c.p.=0, \quad c_1 s_1(d_3+d_{p-1})+c.p.=0,\ldots,c_1 s_1(d_{p/2}+d_{p/2+2}) + c.p.=0, \tag{64}$$

$$c_1 s_1 d_{p/2+1} + c_{p/2+1} s_{p/2+1} d_1 = c_2 s_2 d_{p/2+2} + c_{p/2+2} s_{p/2+2} d_2 = \cdots = c_{p/2} s_{p/2} d_p + c_p s_p d_{p/2} = 0, \tag{65}$$

TABLE II. (*Continued.*)

$$d_1^2(d_2+d_p)\pm c.p.=A(d_1\pm c.p.),\ d_1^2(d_3+d_{p-1})\pm c.p.=A(d_1\pm c.p.), \tag{66}$$

$$d_1^2(d_{p/2}+d_{p/2+2})\pm c.p.=A(d_1\pm c.p.),\ d_1^2 d_{p/2+1}\pm c.p.=\sqrt{1-m}(d_1\pm c.p.), \tag{67}$$

$$d_1d_2d_3\pm c.p.=A(d_1\pm c.p.),\ d_1d_jd_k\pm c.p.=A(d_1\pm c.p.). \tag{68}$$

p=odd integer:

For indices $1<j_1<j_2\leqslant p$:

$$d_1d_{j_1}d_{j_2}+c.p.=A(d_1+c.p.),\ \tilde{c}_1\tilde{c}_{j_1}\tilde{c}_{j_2}+c.p.=A(\tilde{c}_1+c.p.),\ \tilde{s}_1\tilde{s}_{j_1}\tilde{s}_{j_2}+c.p.=A(\tilde{s}_1+c.p.), \tag{69}$$

$$\tilde{c}_1(\tilde{s}_2\tilde{d}_p+\tilde{s}_p\tilde{d}_2)+c.p.=0,...,\tilde{c}_1(\tilde{s}_{(p+1)/2}\tilde{d}_{(p+3)/2}+\tilde{s}_{(p+3)/2}\tilde{d}_{(p+1)/2})+c.p.=0, \tag{70}$$

$$\tilde{c}_1\tilde{d}_2\tilde{d}_p+c.p.=A(\tilde{c}_1+c.p.),...,\tilde{c}_1\tilde{d}_{(p+1)/2}\tilde{d}_{(p+3)/2}+c.p.=A(\tilde{c}_1+c.p.), \tag{71}$$

$$\tilde{d}_1(\tilde{d}_2\tilde{c}_2+\tilde{d}_p\tilde{c}_p)+c.p.=A(\tilde{c}_1+c.p.),...,\tilde{d}_1(\tilde{d}_{(p+1)/2}\tilde{c}_{(p+1)/2}+\tilde{d}_{(p+3)/2}\tilde{c}_{(p+3)/2})+c.p.$$
$$=A(\tilde{c}_1+c.p.), \tag{72}$$

$$d_1^2(d_2+d_p)+c.p.=A(d_1+c.p.),...,d_1^2(d_{(p+1)/2}+d_{(p+3)/2})+c.p.=A(d_1+c.p.), \tag{73}$$

$$c_1s_1(d_2+d_p)+c.p.=0,...,c_1s_1(d_{(p+1)/2}+d_{(p+3)/2})+c.p.=0. \tag{74}$$

Note that additional identities can be obtained by changing the pair $(\tilde{c}\tilde{d})$ in Eq. (71) or (72) into any of the pairs $(\tilde{c}\tilde{s})$, $(\tilde{s}\tilde{d})$, $(\tilde{s}\tilde{c})$, $(\tilde{d}\tilde{c})$, $(\tilde{d}\tilde{s})$. Likewise, additional identities can be obtained by changing d to $\tilde{c}$ or $\tilde{s}$ in eq. (73) and by changing (c, s, d) to $(\tilde{c},\tilde{d},\tilde{s})$ or $(\tilde{d},\tilde{s},\tilde{c})$ in Eq. (74).

TABLE III. **Some indentities of rank 4 and above**. The symbols *A*, *B* in Eqs. (84)–(87) are used generically to denote constants independent of *x*; the constants are in general all different.

r=4, p=2:

$$d_1^3d_2\pm d_2^3d_1=\sqrt{1-m}(d_1^2\pm d_2^2),\ d_1^2d_2^2=1-m, \tag{75}$$

$$mc_1s_1c_2s_2=\sqrt{1-m}[1-s_1^2-s_2^2],\ c_1d_1c_2d_2=-(1-m)s_1s_2,\ s_1d_1s_2d_2$$
$$=-c_1c_2. \tag{76}$$

r=4, p=3: $[q\equiv \mathrm{dn}(2K(m)/3,m)]$

$$s_1c_1d_2d_3+c.p.=\frac{(q^2+m-1)}{1-q^2}(s_1c_1+c.p.), \tag{77}$$

$$d_1^3(d_2+d_3)+c.p.=\frac{2mq}{1-q^2}(d_1^2+c.p.)-2(1-m), \tag{78}$$

$$\tilde{s}_1\tilde{d}_1\tilde{c}_2\tilde{c}_3+c.p.=\frac{q^2}{1-q^2}(\tilde{s}_1\tilde{d}_1+c.p.), \tag{79}$$

$$\tilde{c}_1\tilde{d}_1\tilde{s}_2\tilde{s}_3+c.p.=\frac{-1}{1-q^2}(\tilde{c}_1\tilde{d}_1+c.p.), \tag{80}$$

$$m^2c_1s_1c_2s_2+c.p.=\frac{2mq}{1-q^2}(d_1^2+c.p.)+[m-(2-m)(1+q)^2]. \tag{81}$$

r=5, p=3:

$$d_1^3(s_2c_2+s_3c_3)+c.p.=\frac{-2mq}{1-q^2}(s_1c_1d_1+c.p.), \tag{82}$$

$$m\tilde{s}_1^4(\tilde{s}_2+\tilde{s}_3)+c.p.=\frac{2(q^2+m-1)}{1-q}(\tilde{s}_1^3+c.p.)+\frac{2(q^3+q^2+mq-q+2m-1)}{(1-q^2)^2}$$
$$(\tilde{s}_1+c.p.). \tag{83}$$

r=6, p=6:

$$d_1^3(d_2^2d_3+d_6^2d_5)+c.p.=A(d_1^2+c.p.)+B. \tag{84}$$

r=8, p=6:

$$c_1d_1c_2d_2s_3s_4s_5s_6+c.p.=A(s_1s_2s_3s_4s_5s_6). \tag{85}$$

r, p:

$$m^ps_1^2s_2^2\cdots s_p^2=A(s_1^2+c.p.)+B\quad(r=2p). \tag{86}$$

TABLE III. (*Continued.*)

For indices $1<j_1<j_2<\cdots<j_{r-1}\leqslant p$:

$$d_1 d_{j_1} d_{j_2}\cdots d_{j_{r-1}}+c.p.=A \ (r=\text{even},p),$$
$$d_1 d_{j_1} d_{j_2}\cdots d_{j_{r-1}}+c.p.=B(d_1+c.p.) \ (r=\text{odd},p),$$
$$\tilde{s}_1\tilde{s}_{j_1}\tilde{s}_{j_2}\cdots\tilde{s}_{j_{r-1}}+c.p.=A,\ \tilde{c}_1\tilde{c}_{j_1}\tilde{c}_{j_2}\cdots\tilde{c}_{j_{r-1}}+c.p.=A \ (r=\text{even},\ p=\text{odd}), \tag{87}$$
$$\tilde{s}_1\tilde{s}_{j_1}\tilde{s}_{j_2}\cdots\tilde{s}_{j_{r-1}}+c.p.=B(\tilde{s}_1+c.p.),\ \tilde{c}_1\tilde{c}_{j_1}\tilde{c}_{j_2}\cdots\tilde{c}_{j_{r-1}}+c.p.=B(\tilde{c}_1+c.p.)$$
$$(r=\text{odd},\ p=\text{odd}),$$
$$d_1^{r-1}(d_2+d_p)+c.p.=A(d_1^{r-2}+c.p.)+B(d_1^{r-4}+c.p.)+\cdots.$$

The last equation ends with a constant if r is odd, and with a term proportional to $(d_1+c.p.)$ if r is even.

(x) It should be noted that in many applications like finding new solutions of the KdV equation,[9] the identities needed involve summations over all combinations of many (say two) indices $i,\ j=1,...,p$. These combinations correspond to the sum of several cyclic identities discussed in the tables.

(xi) In this article, we have concentrated our attention on cyclic identities in which the arguments are separated by fractions of the periods $2K(m)$ or $4K(m)$ on the real axis. However, each one of our identities can be easily translated into a corresponding one in which the arguments are separated by fractions of the periods $i2K'$ or $i4K'$ on the imaginary axis, where $K'\equiv K(1-m)$. For example, the simple two-point identity $\mathrm{dn}(x,m)\mathrm{dn}(x+K(m),m)=\sqrt{1-m}$ translates to the new identity $\mathrm{sn}(u,m)\mathrm{sn}(u+iK',m)=1/\sqrt{m}$. The general procedure consists of first replacing m by $1-m$ [which in alternative standard notation[2] corresponds to replacing $k\equiv\sqrt{m}$ by $k'\equiv\sqrt{1-m}$ and $K(m)$ by K'], then using the well known results

$$\mathrm{sn}(x,1-m)=\frac{i\,\mathrm{cn}(ix+K,m)}{\sqrt{1-m}\,\mathrm{sn}(ix+K,m)},\quad \mathrm{cn}(x,1-m)=\frac{\mathrm{dn}(ix+K,m)}{\sqrt{1-m}\,\mathrm{sn}(ix+K,m)},$$
$$\mathrm{dn}(x,1-m)=\frac{1}{\mathrm{sn}(ix+K,m)},$$

and finally changing to a new variable $u=ix+K$.

In conclusion, even though Jacobi elliptic functions have been studied for approximately two centuries, it is exciting to discover new cyclic identities connecting them. What makes our results doubly exciting is that the identities play a vital role in the study of periodic potentials[4] and in yielding new solutions of nonlinear differential equations of physical interest.[9]

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Dispersionless scalar integrable hierarchies, Whitham hierarchy, and the quasiclassical $\bar{\partial}$-dressing method

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The quasiclassical limit of the scalar nonlocal $\bar{\partial}$-problem is derived and a quasiclassical version of the $\bar{\partial}$-dressing method is presented. Dispersionless Kadomtsev–Petviashvili (KP), modified KP, and dispersionless two-dimensional Toda lattice (2DTL) hierarchies are discussed as illustrative examples. It is shown that the universal Whitham hierarchy is nothing but the ring of symmetries for the quasiclassical $\bar{\partial}$-problem. The reduction problem is discussed and, in particular, the d2DTL equation of B type is derived. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Considerable interest has been paid recently to dispersionless or quasiclassical limits of integrable equations and hierarchies (see, e.g., Refs. 1–13, and references therein). Study of dispersionless hierarchies is of great importance since they arise in the analysis of various problems in physics, mathematics, and applied mathematics from the theory of quantum fields and strings[14–16] to the theory of conformal maps on the complex plane.[17–18]

Different methods have been used to study dispersionless equations and hierarchies.[1–13] In particular, several $1+1$-dimensional equations and systems have been analyzed by the quasiclassical version of the inverse scattering transform, including the local Riemann–Hilbert problem approach.[2,3,11–13,19] Similar study of the $2+1$-dimensional equations and hierarchies, like Kadomtsev–Petviashvili (KP) and dispersionless two-dimensional Toda lattice (2DTL), has been missing. Recently this problem has been addressed in Ref. 20 and the quasiclassical $\bar{\partial}$-dressing approach to the dispersionless KP hierarchy has been proposed.

In this paper we consider a class of scalar dispersionless integrable hierarchies governed by the scalar $\bar{\partial}$-problem with the dispersionless KP (dKP), modified dkP (mdKP), and d2DTL hierarchies as particular cases. We derived the general form of the quasiclassical $\bar{\partial}$-problem. It is given by the system

$$\frac{\partial S}{\partial \bar{\lambda}} = W\left(\lambda, \bar{\lambda}; \frac{\partial S}{\partial \lambda}\right), \tag{1.1}$$

$$\frac{\partial \varphi}{\partial \bar{\lambda}} = W'\left(\lambda, \bar{\lambda}; \frac{\partial S}{\partial \lambda}\right)\frac{\partial \varphi}{\partial \lambda} + \tilde{W}\left(\lambda, \bar{\lambda}; \frac{\partial S}{\partial \lambda}\right)\frac{\partial^2 S}{\partial \lambda^2}\varphi, \tag{1.2}$$

for $\lambda \in G$, where G is a domain in the complex plane $\mathbb{C}$ and W and $\tilde{W}$ are some functions. The type of hierarchy is specified by the undressed part $S_0(\lambda, T)$ of S and the domain G. A quasiclaszsical $\bar{\partial}$-dressing method based on the system (1.1)–(1.2) allows us to construct dispersionless integrable hierarchies and provides us a method for finding their solutions. The dKP, dmKP, and d2DTL hierarchies are considered as illustrative examples.

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Symmetries of the quasiclassical $\bar{\partial}$-problem (1.1) and (1.2) are defined by linear Beltrami-type equations and form an infinite-dimensional ring. It is shown that this ring, parametrized by symmetry parameters, is nothing but the universal Whitham hierarchy introduced in Ref. 8. In particular, the dKP, mdKP, and m2DTL hierarchies are special subrings of symmetries for problems (1.1) and (1.2).

We also discuss the reduction of the dispersionless hierarchies and present the dispersionless 2DTL equation of B type.

Equations of the form (1.1) and (1.2) are well-known in the complex-analysis; in particular, in connection with quasiconformal mappings in the plane (see, e.g., Refs. 21–23). Thus, there is a close connection between the theory of quasiclassical integrable hierarchies and the theory of quasiconformal mappings.

II. DISPERSIONLESS HIERARCHIES AND UNIVERSAL WHITHAM HIERARCHY

We begin by recalling some relevant formulas for dispersionless hierarchies and choose the Kadomtsev–Petviashili (KP) hierarchy to illustrate their main features. The usual KP hierarchy is an infinite set of the compatibility condition for the system

$$L\psi=\lambda\psi, \tag{2.1}$$

$$\frac{\partial\psi}{\partial t_n}=(L^n)_+\psi, \tag{2.2}$$

where $L=\partial+u_1\partial^{-1}+u_2\partial^{-2}+\cdots,\partial=\partial/\partial t,(L^n)_+$ denotes the pure differential part of the operator L^n, λ is a spectral parameter, and ψ is a common KP wave function. The KP equation itself is the equation for coefficient u_1 as a function of the first three times t_1,t_2,t_3. For the modified KP (mKP) hierarchy the operator L is of the form $L=\partial+u_0+u_1\partial^{-1}+u_2\partial^{-2}+\cdots$ while for the two-dimensional Toda lattice (2DTL) hierarchy one needs two operators L_1 and L_2.[10]

The dispersionless KP (dKP) hierarchy is a formal limit $\varepsilon\to 0$ of the KP hierarchy for which[1–10]

$$u_k\left(\frac{T_n}{\varepsilon}\right)\xrightarrow[\varepsilon\to 0]{} u_{k_0}(T)+O(\varepsilon), \tag{2.3}$$

and

$$\psi\left(\frac{T_n}{\varepsilon}\right)\xrightarrow[\varepsilon\to 0]{} e^{(1/\varepsilon)\,S(\lambda,T)+O(\varepsilon)}, \tag{2.4}$$

where T_n are slow times.

Under such a limit, Eq. (2.1) gives rise to the Laurent series $\mathcal{L}=p+\Sigma_{n=1}^{\infty}u_n(T)p^{-n}$, where $p=\partial S/\partial T_1$ while Eq. (2.2) becomes

$$\frac{\partial p}{\partial T_n}=\frac{\partial B_n(p)}{\partial T_1} \tag{2.5}$$

where $B_n(p)=[\mathcal{L}^n(p)]_+$ and $[\mathcal{L}^n]_+$ denotes here a polynomial part of $\mathcal{L}^n$. The compatibility conditions for (2.5) are given by the infinite set of equations

$$\frac{\partial B_n}{\partial T_m}-\frac{\partial B_n}{\partial T_m}+\{B_n,B_m\}=0 \tag{2.6}$$

where the Poisson bracket $\{,\}$ is defined as

$$\{f,g\}=\frac{\partial f}{\partial p}\frac{\partial g}{\partial T_1}-\frac{\partial f}{\partial T_1}\frac{\partial g}{\partial p}. \tag{2.7}$$

Equation (2.5) or (2.6) represent the dKP hierarchy. Similarly, the dmKP hierarchy is given by equations of the form (2.5)–(2.7) with $\mathcal{L}=p+\Sigma_{n=1}^{\infty}u_n(T)p^{-n}$.[24] The d2DTL hierarchy can be written by a set of equations similar to (2.5)–(2.7) for two Laurent series $\mathcal{L}_1$ and $\mathcal{L}_2$ (Ref. 10) with the substitution $p\to e^p$.

A more general dispersionless-like hierarchy has been introduced in Ref. 8. This universal Whitham hierarchy is given by the infinite set of equations

$$\frac{\partial\Omega_A}{\partial T_B}-\frac{\partial\Omega_B}{\partial T_A}+\{\Omega_A,\Omega_B\}=0,\quad A,B=1,2,3,\ldots, \tag{2.8}$$

where $\Omega_A(p,T)$ are arbitrary holomorphic functions of p. As has been shown in Ref. 8, the dKP, d2DTL, and Benney hierarchies are particular cases.

III. QUASICLASSICAL $\bar{\partial}$-PROBLEM

The $\vec{\partial}$-dressing method is a powerful tool to study usual integrable equations and hierarchies.[25–27] In this paper we shall formulate its quasiclassical version. We shall demonstrate that it provides an effective method to construct and study dispersionless hierarchies.

We begin with the derivation of the quasiclassical limit of the basic $\bar{\partial}$-problem.

The usual scalar integrable hierarchies are associated with the following scalar linear nonlocal problem (see Refs. 24–26):

$$\frac{\partial\chi(\lambda,\bar{\lambda};t)}{\partial\bar{\lambda}}=\int\int_{\mathbb{C}}d\mu\wedge d\bar{\mu}\chi(\mu,\bar{\mu};t)g(\mu,t)R_0(\mu,\bar{\mu};\lambda,\bar{\lambda})g^{-1}(\lambda,t), \tag{3.1}$$

where λ is a complex variable ("spectral parameter"), $\bar{\lambda}$ denotes complex conjugation of λ, $\chi(\lambda,\bar{\lambda};\mu)$ is a complex-valued function on the complex plane $\mathbb{C}$ $(\lambda,\bar{\lambda}\in\mathbb{C})$, the kernel $R_0(\mu,\bar{\mu};\lambda,\bar{\lambda})$ is the $\bar{\partial}$-data. Usually, it is assumed that the function χ has a canonical normalization i.e.,

$$\chi\to 1+\frac{\chi_1}{\lambda}+\frac{\chi_2}{\lambda^2}+\cdots,\quad \lambda\to\infty,$$

and that the problem (3.1) is uniquely solvable. Concrete integrable hierarchies are specialized by the form of the function $g(\lambda,t)=\exp(S_0(\lambda,t))$ and by the domain G of the support for the $\bar{\partial}$-data R_0 ($R_0(\mu,\bar{\mu};\lambda,\bar{\lambda})=0$ for $\mu,\lambda\in\mathbb{C}/G$.) For the KP hierarchy $S_0=\Sigma_{k=1}^{\infty}\lambda^k t_k$ and G ia a disk with center at the origin, while for the 2DTL hierarchy $S_0(\lambda;x,y,n)=n\ln\lambda+\Sigma_{k=1}^{\infty}\lambda^k x_k+\Sigma_{k=1}^{\infty}\lambda^{-k}y_k$ where x_k and y_k are continuous variables and n is an integer discrete variable. The domain G in this case is an annulus $a\leqslant|\lambda|\leqslant b$. Given $g(\lambda)$ the $\bar{\partial}$-dressing method provides us with the corresponding hierarchy of nonlinear equations and their linear problems.[24–26] Solutions of nonlinear equations are given by the function χ evaluated at certain points λ_0. For instance, for the KP hierarchy $u_1=-2(\partial\chi_1(t)/\partial t_1)$.

In order to derive the quasiclassical limit of the $\bar{\partial}$-problem (3.1) we first introduce slow variables T ($t_i=T_i/\varepsilon$ for KP and mKP, $x_i=X_i/\varepsilon$, $y_i=Y_i/\varepsilon$, $n=T/\varepsilon$ for 2DTL) for small ε and proceed to the limit $\varepsilon\to 0$. In this limit $g(T/\varepsilon)=\exp[S_0(\lambda,T)/\varepsilon]$. Motivated by the formula of the type (2.4) and by the structure of Eq. (3.1) we will look for solutions χ of the form

$$\chi\left(\lambda,\overline{\lambda};\frac{T}{\varepsilon}\right)=\hat{\chi}(\lambda,\overline{\lambda};T;\varepsilon)\exp\left(\frac{\widetilde{S}(\lambda,\overline{\lambda};T)}{\varepsilon}\right), \tag{3.2}$$

where $\widetilde{S}(\lambda,\overline{\lambda};T)$ is a certain function and

$$\hat{\chi}(\lambda,\overline{\lambda};T;\varepsilon)=\sum_{n=0}^{\infty}\hat{\chi}_n(\lambda,\overline{\lambda};T)\varepsilon^n. \tag{3.3}$$

It is clear that only for special $\overline{\partial}$-data R_0 Eq. (3.1) will have a well-defined limit as $\varepsilon\to 0$. Thus, it is not difficult to see that the $\overline{\partial}$-data of the form

$$R_0(\mu,\overline{\mu};\lambda,\overline{\lambda};\varepsilon)=\sum_{k=0}^{\infty}\Gamma_k(\mu,\overline{\mu})\varepsilon^{k-1}\delta^{(k)}(\mu-\lambda-\varepsilon\alpha_k(\lambda,\overline{\lambda})) \tag{3.4}$$

do a job. Here $\Gamma_k(\mu,\overline{\mu})$, $\alpha_k(\lambda,\overline{\lambda})$ are arbitrary functions ($\Gamma_k=0$ at $\lambda\in\mathbb{C}/G$) and $\delta^{(k)}$ is the k-derivative Dirac delta-function ($\delta^{(k)}(\lambda)=(\partial^k/\partial\lambda^k)\,\delta(\lambda)$). Indeed, in the simplest case $\alpha_k=0$, substituting (3.4) into (3.1), one gets

$$\frac{\partial\hat{\chi}(\lambda,\overline{\lambda};T,\varepsilon)}{\partial\overline{\lambda}}+\frac{1}{\varepsilon}\frac{\partial S(\lambda,\overline{\lambda};T)}{\partial\overline{\lambda}}\hat{\chi}(\lambda,\overline{\lambda},T,\varepsilon)$$

$$=\int\int_{\mathbb{C}}d\mu\wedge d\overline{\mu}\hat{\chi}(\mu,\overline{\mu},\varepsilon)\exp\left(\frac{S(\mu,T)-S(\lambda,T)}{\varepsilon}\right)\sum_{k=0}^{\infty}\Gamma_k(\mu,\overline{\mu})\varepsilon^{k-1}\delta^{(k)}(\mu-\lambda) \tag{3.5}$$

where

$$S(\lambda,\overline{\lambda};T):=\widetilde{S}(\lambda,\overline{\lambda};T)+S_0(\lambda;T).$$

Evaluating in (3.5) the terms of the order $1/\varepsilon$, one obtains

$$\frac{\partial S(\lambda,\overline{\lambda};T)}{\partial\overline{\lambda}}=W\left(\lambda,\overline{\lambda};\frac{\partial S}{\partial\lambda}\right), \tag{3.6}$$

where

$$W\left(\lambda,\overline{\lambda};\frac{\partial S}{\partial\lambda}\right)=\sum_{k=0}^{\infty}(-1)^k\Gamma_k(\lambda,\overline{\lambda})\left(\frac{\partial S}{\partial\lambda}\right)^k. \tag{3.7}$$

Furthermore, the terms of zero order in ε in (3.5) give [the contribution proportional to $\hat{\chi}_1$ disappears due to (3.6)]:

$$\frac{\partial\varphi}{\partial\overline{\lambda}}=W'\left(\lambda,\overline{\lambda};\frac{\partial S}{\partial\lambda}\right)\frac{\partial\varphi}{\partial\lambda}+\widetilde{W}\left(\lambda,\overline{\lambda};\frac{\partial S}{\partial\lambda}\right)\frac{\partial^2 S}{\partial\lambda^2}\varphi, \tag{3.8}$$

where

$$\varphi:=\hat{\chi}_0,\quad W'(\lambda,\overline{\lambda};\xi):=\frac{\partial W(\lambda,\overline{\lambda};\xi)}{\partial\xi},$$

and

$$\widetilde{W}:=(-1)^2\Gamma_2+(-1)^3\Gamma_3 3\frac{\partial S}{\partial\lambda}+\cdots=\frac{1}{2}W''\left(\lambda,\overline{\lambda};\frac{\partial S}{\partial\lambda}\right). \tag{3.9}$$

Since $\partial S_0/\partial\overline{\lambda}=0$ at $\lambda\in G$, then Eqs. (3.6)–(3.9) for $\lambda\in G$ can be rewritten as

$$\frac{\partial S}{\partial\overline{\lambda}}=W\left(\lambda,\overline{\lambda};\frac{\partial S}{\partial\lambda}\right), \tag{3.10}$$

$$\frac{\partial\varphi}{\partial\overline{\lambda}}=W'\frac{\partial\varphi}{\partial\lambda}+\widetilde{W}\frac{\partial^2 S}{\partial\lambda^2}\varphi. \tag{3.11}$$

Equations (3.10) and (3.11) are the quasiclassical limit of the nonlocal $\overline{\partial}$-problem (3.1). One gets similar equations for the kernels (3.4) with $\alpha_k\neq 0$. The derivation given above suggests that the quasiclassical limit of the $\overline{\partial}$-problem (3.1) is given by Eqs. (3.10) and (3.11) also for a more general than (3.4) $\overline{\partial}$-data R_0.

The function S is widely used in the analysis of the dispersionless limits of the integrable hierarchies.[4–10] Within the $\overline{\partial}$-approach it is a nonholomorphic function of the ''spectral'' variable λ and obeys the nonlinear $\overline{\partial}$-equation (3.10) (for $\lambda\in G$). The function $\varphi=\hat{\chi}_0$ obeys the local $\overline{\partial}$-problem (3.11) of the Beltrami type. Note that the ratio ϕ of two solutions φ_1 and φ_2 of Eq. (3.11) satisfies the Beltrami equation

$$\frac{\partial\phi}{\partial\overline{\lambda}}=W'\left(\lambda,\overline{\lambda};\frac{\partial S}{\partial\lambda}\right)\frac{\partial\phi}{\partial\lambda}. \tag{3.12}$$

For the Orlov's function $M=\partial S/\partial\lambda$ Eqs. (3.10) and (3.11) take the form of quasilinear equations

$$\frac{\partial M}{\partial\overline{\lambda}}=\frac{\partial}{\partial\lambda}W(\lambda,\overline{\lambda};M), \tag{3.13}$$

$$\frac{\partial\varphi}{\partial\overline{\lambda}}=W'(\lambda,\overline{\lambda};M)\frac{\partial\varphi}{\partial\lambda}+\widetilde{W}(\lambda,\overline{\lambda};M)\frac{\partial M}{\partial\lambda}\varphi. \tag{3.14}$$

Quasiclassical $\overline{\partial}$-problems (3.10) and (3.11) are basic equations for our approach. The equations of the type (3.10) and (3.11) are well known and widely studied in the theory of nonlinear elliptic systems with two independent variables and in complex analysis (see, e.g., Refs. 27, 21–23). One theorem from the theory of such equations will be crucial for our further constructions. This theorem (see theorem 3.32 from Ref. 27) states that, under certain mild condition on A (see the appendix), the only solution of the Beltrami equation $\partial Z/\partial\overline{\lambda}=A(\partial Z/\partial\lambda)$ in $\mathbb{C}$ which vanish as $\lambda\to\infty$ is $Z\equiv 0$.

We would like to note that the systems of the type (1.1) and (1.2) arise also within the complex Wenthel–Kramers–Brillouin method: see, e.g., the general canonical system (1.14), (1.14′) in Ref. 28. This connection and the ''elliptic'' version of Maslov's method for the system (1.1) and (1.2) will be discussed elsewhere.

IV. QUASICLASSICAL $\bar{\partial}$-DRESSING METHOD

The principal goal of the $\bar{\partial}$-dressing method based on Eqs. (3.10) and (3.11) is the same as of the original $\bar{\partial}$-dressing method.[24–26] It is to extract the nonlinear differential equations from the quasiclassical $\bar{\partial}$-problems.

Now the time dependence of the functions S and φ is encoded in the undressed functions $S_0(\lambda, T)$. Since

$$\tilde{S} = 1 + \frac{S_1}{\lambda} + \frac{S_2}{\lambda^2} + \cdots$$

at $\lambda \to \infty$ then the behavior of $\partial S/\partial T_A$ for large λ is completely defined by

$$\frac{\partial S}{\partial T_A} = \frac{\partial S_0}{\partial T_A} + \frac{1}{\lambda}\frac{\partial S_1}{\partial T_A} + \cdots, \tag{4.1}$$

where T_A is a slow time.

A basic property of the nonlinear equation (3.10) is that it implies the linear Beltrami equation for the infinitesimal variations δS (symmetries):

$$\frac{\partial}{\partial \bar{\lambda}}(\delta S) = W'\left(\lambda, \bar{\lambda}; \frac{\partial S}{\partial \lambda}\right)\frac{\partial}{\partial \lambda}(\delta S). \tag{4.2}$$

In particular, for any time T_A,

$$\frac{\partial}{\partial \bar{\lambda}}\left(\frac{\partial S}{\partial T_A}\right) = W'\left(\lambda, \bar{\lambda}; \frac{\partial S}{\partial \lambda}\right)\frac{\partial}{\partial \lambda}\left(\frac{\partial S}{\partial T_A}\right). \tag{4.3}$$

Any power of solution of the Beltrami equation is a solution too as well as any differentiable function of two solutions. So together with $\partial S/\partial T_{A_1}, \ldots, \partial S/\partial T_{A_n}$ any differentiable function

$$f\left(\frac{\partial S}{\partial T_{A_1}}, \ldots, \frac{\partial S}{\partial T_{A_n}}\right)$$

with arbitrary n is a solution of Eq. (4.3). Thus the symmetries of the problem (3.10) form a ring.

Due to (4.1), the functions

$$f\left(\frac{\partial S}{\partial T_{A_1}}, \ldots, \frac{\partial S}{\partial T_{A_n}}\right)$$

have singularities in certain points. The functions

$$f_0\left(\frac{\partial S}{\partial T_{A_1}}, \ldots, \frac{\partial S}{\partial T_{A_n}}\right)$$

which are bounded in $\mathbb{C}$ and vanish as $\lambda \to \infty$ are very special. According to the Vekua's theorem mentioned at the end of Sec. III they vanish identicaly. So we have the nonlinear equations

$$f_0\left(\frac{\partial S}{\partial T_{A_1}}, \ldots, \frac{\partial S}{\partial T_{A_n}}\right) = 0. \tag{4.4}$$

Note that in contrast to the usual hierarchies we get nonlinear equations for the ''wave function'' S (the classical action).

Now we turn to the $\bar{\partial}$-problem (3.11). It is linear one. So the construction is similar to that of the usual case. Namely, suppose that one has found a solution φ_0 to Eq. (3.11) of the form $\varphi_0 = L\varphi$ where L is a certain linear operator and φ_0 is bounded and vanishes as $\lambda \to \infty$. Since $\varphi \to 1 + \varphi_1/\lambda + \cdots$ as $\lambda \to \infty$ the ratio φ_0/φ vanishes as $\lambda \to \infty$ and obeys the Beltrami equation

$$\frac{\partial}{\partial \bar{\lambda}}\left(\frac{\varphi_0}{\varphi}\right) = W' \frac{\partial}{\partial \lambda}\left(\frac{\varphi_0}{\varphi}\right). \tag{4.5}$$

Then according to the Vekua's theorem φ_0/φ vanishes identically and, consequently,

$$L\varphi = 0 \tag{4.6}$$

that is the desired linear problem for the wave function φ. Note that one can get the same results assuming that the problem (3.11) with canonically normalized φ is uniquely solvable.

Equations (4.4) and (4.6) are the basic equations associated with the quasiclassical $\bar{\partial}$-problems (3.10) and (3.11). They are compatible by construction. Equations (4.4) and (4.6) provide us also with equations for functions $u_k(T)$ which depend only on the times T. Usually one has infinite families of equations of the type (4.4) and (4.6). So the quasiclassical $\bar{\partial}$-problems (3.10) and (3.11) give rise to an infinite hierarchy of integrable quasiclassical (or dispersionless) equations.

V. dKP AND dmKP HIERARCHIES

Let us consider concrete examples to illustrate the general scheme. We start with the dKP hierarchy. In this case $S_0(\lambda, T) = \Sigma_{n=1}^{\infty} \lambda^n T_n$ and $\partial S/\partial T_n = \lambda^n + (1/\lambda)(\partial S_1/\partial T_n) + (1/\lambda^2) \times (\partial S_2/\partial T_n) + \ldots (n = 1, 2, \ldots)$. Since $\partial S/\partial T_n$ have power singularities at infinity the desired function f_0 will be, clearly, polynomials. Taking, for instance, the derivatives $\partial S/\partial T_2$ and $\partial S/\partial T$ we readily see that the difference $\partial S/\partial T_2 - (\partial S/\partial T_1)^2$ behaves as $-2(\partial S_1/\partial T_1) + O(1/\lambda)$ as $\lambda \to \infty$. Thus, the desired function f_0 is $\partial S/\partial T_2 - (\partial S/\partial T_1)^2 + 2(\partial S_1/\partial T_1)$. So we get

$$\frac{\partial S}{\partial T_2} - \left(\frac{\partial S}{\partial T_1}\right)^2 - u = 0, \tag{5.1}$$

where $u = -2(\partial S_1/\partial T_1)$.

Analogously, taking the derivatives $\partial S/\partial T_3$ and $\partial S/\partial T_1$ one easily concludes that the combination $\partial S/\partial T_3 - (\partial S/\partial T_1)^3 - V_1(\partial S/\partial T_1) - V_0$ vanishes at $\lambda \to 0$ if $V_1 = -3(\partial S/\partial T_1)$ and $V_0 = -3(\partial S_2/\partial T_1) = -\frac{3}{2}(\partial S_1/\partial T_2)$. So one gets the other function f_0 and

$$\frac{\partial S}{\partial T_3} - \left(\frac{\partial S}{\partial T_1}\right)^3 - V_1 \frac{\partial S}{\partial T_1} - V_0 = 0 \tag{5.2}$$

where $\partial V_0/\partial T_1 = \frac{3}{4}(\partial u/\partial T_2)$.

In a similar manner one constructs an infinite family of equations

$$\frac{\partial S}{\partial T_n} - \left(\frac{\partial S}{\partial T_1}\right)^n - \sum_{k=0}^{n-2} V_{nk}(T)\left(\frac{\partial S}{\partial T_1}\right)^k = 0, \quad n = 1, 2, 3, \ldots \tag{5.3}$$

with appropriate coefficients $V_{nk}(T)$.

Equation (5.3) is nothing but the Eq. (2.5) of the dKP hierarchy. Evaluating the left-hand sides of (5.3) at $\lambda \to \infty$, taking the term of the order $1/\lambda$ and using other equations (5.3), one gets the dKP hierarchy for the function u and, in particular, the dKP equation

$$u_{T_1T_3}=\tfrac{3}{2}(u\,u_{T_1})_{T_1}+\tfrac{3}{4}u_{T_2T_2}. \tag{5.4}$$

In a usual manner Eq. (5.4) arises as the compatibility conditions for Eqs. (5.1) and (5.2). Equation (5.3) implies the hierarchy of nonlinear equations for the function S only. Indeed, eliminating all coefficients $u_{nk}(T)$ from (5.3) one gets the family of equations

$$\frac{\partial S}{\partial T_n}=F_n\left(\frac{\partial S}{\partial T_1},\frac{\partial S}{\partial T_2}\right),\quad n=3,4,5,\ldots.$$

The lowest of these equations is of the form

$$\frac{\partial^2 S}{\partial T_1\partial T_3}=\frac{3}{4}\frac{\partial^2 S}{\partial T_2^2}+\frac{3}{2}\left[\frac{\partial S}{\partial T_2}-\left(\frac{\partial S}{\partial T_1}\right)^2\right]\frac{\partial^2 S}{\partial T_1^2}.$$

Now we proceed to the $\bar{\partial}$-problem (3.11). For simplicity we restrict ourselves to the case $\tilde{W}=\frac{1}{2}W''$. It is not difficult to show, differentiating (3.11) and using Eqs. (5.1) and (5.2), that the function $Z=L\varphi=\partial\varphi/\partial T_2-2(\partial S/\partial T_1)(\partial\varphi/\partial T_1)-(\partial^2 S/\partial T_1^2)\,\varphi+\tilde{u}\varphi$ where $\tilde{u}=-2(\partial\varphi_1/\partial T_1)$ obeys

$$\frac{\partial Z}{\partial\bar{\lambda}}=W'\frac{\partial Z}{\partial\lambda}+\frac{1}{2}W''\frac{\partial^2 S}{\partial\lambda^2}Z \tag{5.5}$$

and vanish at $\lambda\to 0$. Consequently the ratio Z/φ obeys the Beltrami equation $(\partial/\partial\bar{\lambda})(Z/\varphi)=W'(\partial/\partial\lambda)(Z/\varphi)$ and $Z/\varphi=O(1/\lambda)$ as $\lambda\to\infty$. According to the Vekua's theorem this ratio vanishes identically and, consequently, we get the linear problem $Z=0$, i.e.,

$$\frac{\partial\varphi}{\partial T_2}-2\frac{\partial S}{\partial T_1}\frac{\partial\varphi}{\partial T_1}-\frac{\partial^2 S}{\partial T_1^2}\varphi+\tilde{u}\varphi=0. \tag{5.6}$$

In a similar manner, one gets

$$\frac{\partial\varphi}{\partial T_3}-6\left[2\left(\frac{\partial S}{\partial T_1}\right)^2+\tilde{u}\right]\frac{\partial\varphi}{\partial T_1}-3\left[4\frac{\partial S}{\partial T_1}\frac{\partial^2 S}{\partial T_1^2}+\frac{\partial\tilde{u}}{\partial T_1}-2\tilde{u}\frac{\partial S}{\partial T_1}+\tilde{w}\right]\varphi=0 \tag{5.7}$$

and higher-time equations

$$\frac{\partial\varphi}{\partial T_n}-A_n\frac{\partial\varphi}{\partial T_1}-B_n\varphi=0,\quad n=1,2,3,\ldots. \tag{5.8}$$

All linear problems (5.6)–(5.8) are compatible by construction.

In the particular case $\tilde{u}=\tilde{w}=0$ Eq. (5.6) is known as the transport equation within the quasiclassical approximation in quantum mechanics (see, e.g., Ref. 28). Note that in the case $\tilde{u}=\tilde{w}=0$ Eqs. (5.6) and (5.7) [and also (5.8)] take the form of conservation laws

$$\begin{aligned}&\frac{\partial\phi}{\partial T_2}-\frac{\partial}{\partial T_1}\left(\frac{\partial S}{\partial T_1}\phi\right)=0,\\ &\frac{\partial\phi}{\partial T_3}-\frac{\partial}{\partial T_1}\left(12\left(\frac{\partial S}{\partial T_1}\right)^2\phi\right)=0.\end{aligned} \tag{5.9}$$

Considering the adjoint dKP hierarchy for which $\psi^*(T)=\tilde{\chi}^*(T,\lambda;\varepsilon)e^{-S/\varepsilon}$, one gets the same equation (4.1) for S and equations for φ^* which are adjoint to (5.6) and (5.7). It is interesting that the quantity $\varphi(\lambda,T)\varphi^*(\lambda,T)$ obeys exactly Eq. (5.9).

Our second example is given by the dmKP hierarchy. In this case $S_0=\Sigma_{k=1}^{\infty}\lambda^{-k}T_k$ and

$$\frac{\partial S}{\partial T_k}=\frac{1}{\lambda^k}+\frac{\partial\tilde{S}(\lambda,T)}{\partial T_k}$$

where $\tilde{S}(\lambda,T)$ is holomorphic around $\lambda=0$. So to construct required functions f_0 one has to cancel singularities around $\lambda=0$. Taking again the derivatives $\partial S/\partial T_1$ and $\partial S/\partial T_2$ one readily sees that the combination $\partial S/\partial T_2-(\partial S/\partial T_1)^2$ has only simple pole at $\lambda=0$. To cancel it, we subtract $V(T)(\partial S/\partial T_1)$ where $V(T)=-2(\partial\tilde{S}(\lambda=0)/\partial T_2)$. Then at $\lambda=0$ one has

$$\frac{\partial S}{\partial T_2}-\left(\frac{\partial S}{\partial T_1}\right)^2-V(T)\frac{\partial S}{\partial T_1}=O\left(\frac{1}{\lambda}\right).$$

So due to the Vekua's theorem we conclude

$$\frac{\partial S}{\partial T_2}-\left(\frac{\partial S}{\partial T_1}\right)^2-V(T)\frac{\partial S}{\partial T_1}=0, \tag{5.10}$$

where $V(T)=-2(\partial\tilde{S}(\lambda=0,T)/\partial T_2)$. Taking the derivatives $\partial S/\partial T_1$ and $\partial S/\partial T_3$, one finds

$$\frac{\partial S}{\partial T_3}-\left(\frac{\partial S}{\partial T_1}\right)^3-\frac{3}{2}V\left(\frac{\partial S}{\partial T_1}\right)^2-\left(\frac{3}{4}V^2-3W\right)\frac{\partial S}{\partial T_1}=0, \tag{5.11}$$

where $\tilde{S}(\lambda)=\tilde{S}(0)+\lambda W(T)+\cdots$ as $\lambda\to 0$. Analogously, one obtains the infinite hierarchy of equations

$$\frac{\partial S}{\partial T_n}-\left(\frac{\partial S}{\partial T_1}\right)^n-\sum_{k=1}^{n-1}V_{nk}(T)\left(\frac{\partial S}{\partial T_1}\right)^k=0,\quad n=1,2,3,\ldots. \tag{5.12}$$

Equations (5.12) give us the dmKP hierarchy (see, e.g., Ref. 29). The simplest of these equations is the dmKP equation

$$V_t+\tfrac{3}{2}V^2V_x-\tfrac{3}{4}V_x\partial_x^{-1}V_y-\tfrac{3}{4}\partial_x^{-1}V_{yy}=0. \tag{5.13}$$

Analogously to the KP case, one can also construct the hierarchy of linear problems for the function φ. The simplest of them is of the form

$$\frac{\partial\varphi}{\partial T_2}-\left(2\frac{\partial S}{\partial T_1}+V\right)\frac{\partial\varphi}{\partial T_1}-\frac{\partial^2 S}{\partial T_1^2}\varphi=0. \tag{5.14}$$

Analogously to the dKP case Eq. (5.12) implies the hierarchy of equations for S only.

VI. DISPERSIONLESS TWO-DIMENSIONAL TODA LATTICE (2DTL) HIERARCHY

Our third example is the d2DTL hierarchy. In this case $S_0(\lambda;X,Y,T)=T\ln\lambda+\Sigma_{n=1}^{\infty}\lambda^nX_n+\Sigma_{n=1}^{\infty}\lambda^{-n}Y_n$ and the domain G is the ring $D_{a,b}(a\leqslant|\lambda|\leqslant b)$ with the cutted piece of the real axis. The derivatives of S now have singularities both in the origin and at the infinity:

$$\frac{\partial S}{\partial T}=\ln\lambda+\frac{\partial\tilde{S}}{\partial T},$$

$$\frac{\partial S}{\partial X_n}=\lambda^n+\frac{\partial\tilde{S}}{\partial X_n}, \tag{6.1}$$

$$\frac{\partial S}{\partial Y_n}=\lambda^{-n}+\frac{\partial \widetilde{S}}{\partial Y_n},\quad n=1,2,3,\ldots.$$

Since

$$\begin{gathered}\widetilde{S}(\lambda;X,Y,T)=1+\frac{\widetilde{S}_1}{\lambda}+\frac{\widetilde{S}_2}{\lambda^2}+\ldots,\quad \lambda\to\infty,\\ \widetilde{S}(\lambda;X,Y,T)=S_0+\lambda S_1+\lambda^2 S_2+\ldots,\quad \lambda\to 0\end{gathered}\tag{6.2}$$

one has at $\lambda\to\infty$,

$$\begin{gathered}\frac{\partial S}{\partial X_n}=\lambda^n+\frac{1}{\lambda}\frac{\partial \widetilde{S}_1}{\partial X_n}+\ldots,\\ \frac{\partial S}{\partial Y_n}=\lambda^{-n}+\frac{1}{\lambda}\frac{\partial \widetilde{S}_1}{\partial X_n}+\ldots,\quad n=1,2,3,\ldots,\\ e^{\partial S/\partial T}=\lambda+\frac{\partial \widetilde{S}_1}{\partial T}+\frac{1}{\lambda}\left[\frac{\partial \widetilde{S}_2}{\partial T}+\frac{1}{2}\left(\frac{\partial \widetilde{S}_1}{\partial T}\right)^2\right],\\ e^{-\partial S/\partial T}=\frac{1}{\lambda}-\frac{1}{\lambda^2}\frac{\partial \widetilde{S}_1}{\partial T},\end{gathered}\tag{6.3}$$

while at $\lambda\to 0$,

$$\begin{gathered}\frac{\partial S}{\partial X_n}=\frac{\partial S_0}{\partial X_n}+O(\lambda)\\ \frac{\partial S}{\partial Y_n}=\frac{1}{\lambda^n}+\frac{\partial S_0}{\partial Y_n}+O(\lambda),\quad n=1,2,3,\ldots,\\ e^{\partial S/\partial T}=\lambda e^{\partial S_0/\partial T}+\lambda^2 e^{\partial S_0/\partial T}\frac{\partial S_1}{\partial T}+O(\lambda^3),\\ e^{-\partial S/\partial T}=\frac{1}{\lambda}e^{-\partial S_0/\partial T}-\frac{\partial S_1}{\partial T}e^{-\partial S_0/\partial T}+O(\lambda).\end{gathered}\tag{6.4}$$

The required function f_0 should not have singularities at $\lambda=0$ and at $\lambda=\infty$ and should vanish at $\lambda\to\infty$. Taking the derivatives $\partial S/\partial T$, $\partial S/\partial X_n$, $\partial S\partial Y_n$ and using (6.2), (6.3), one finds the following two equations:

$$\frac{\partial S}{\partial Y_1}-Ve^{-\partial S/\partial T}=0,\tag{6.5}$$

$$\frac{\partial S}{\partial X_1}-e^{\partial S/\partial T}-U=0,\tag{6.6}$$

where $V(X,Y,T)=e^{\partial S_0/\partial T}$ and $U(X,Y,T)=-\partial \widetilde{S}_1/\partial T$. The system (6.5) and (6.6) is the simplest system of equations for the function S associated with the d2DTL hierarchy. We note that in contrast to the papers of Ref. 10 we have only one function S.

To extract from the above-mentioned system nonlinear equations for the functions $V(X,Y,T)$ and $U(X,Y,T)$ we perform the expansion of the left-hand-side of (6.5) at large λ and of the left-hand-side of Eq. (6.6) around $\lambda=0$. The terms of the order $1/\lambda$ in (6.5) give $V=1+\partial\tilde{S}/\partial Y_1$ while vanishing of the zero-order terms in Eq. (5.6) provides us with the equation $\partial S_0/\partial X_1 - U = 0$. As a result, we get the system of equations

$$1+\frac{\partial \tilde{S}_1}{\partial Y_1}=e^{\partial S_0/\partial T}, \quad \frac{\partial S_0}{\partial X_1}+\frac{\partial \tilde{S}_1}{\partial T}=0. \tag{6.7}$$

To rewrite it in a more familiar form we introduce the function $\alpha=\partial S_0/\partial T$, differentiate twice the first equation in (6.7) with respect to T, and use the second equation in (6.7). One gets

$$\frac{\partial \alpha}{\partial X_1 \partial Y_1}+\frac{\partial^2}{\partial T^2}(e^{\alpha})=0, \tag{6.8}$$

which is the standard form of the dispersionless 2DTL equation.

It is easy to show that the formal compatibility conditions for (6.5), (6.6) are equivalent to the system

$$V_{X_1}-VU_T=0, \quad U_{Y_1}+V_T=0 \tag{6.9}$$

which, of course, again gives rise to Eq. (6.8) ($\alpha=\ln V$). In the form (6.9) the 2DTL equation has been derived in Ref. 8.

Higher equations for S can be obtained analogously. Taking the times X_2 and Y_2, one finds the following:

$$\frac{\partial S}{\partial Y_2}-V_2 e^{-2(\partial S/\partial T)}-V_1 e^{-\partial S/\partial T}=0, \tag{6.10}$$

$$\frac{\partial S}{\partial X_2}-e^{2(\partial S/\partial T)}-U_1 e^{(\partial S/\partial T)}=0, \tag{6.11}$$

where

$$V_2=e^{2(\partial S_0/\partial T)}, \quad V_1=2\frac{\partial S_1}{\partial T}e^{\partial S_0/\partial T},$$

$$U_1=-2\frac{\partial \tilde{S}_1}{\partial T}, \quad U_0=-2\frac{\partial \tilde{S}_2}{\partial T}. \tag{6.12}$$

Higher d2DTL equations have, consequently, the form

$$\begin{gathered}
\frac{\partial V_2}{\partial X_2}-2V_2\frac{\partial U_0}{\partial T}=0,\\
\frac{\partial V_1}{\partial X_2}-V_1\frac{\partial U_0}{\partial T}-2V_2\frac{\partial U_1}{\partial T}-U_1\frac{\partial V_2}{\partial T}=0,\\
\frac{\partial U_0}{\partial Y_2}+\frac{\partial}{\partial T}(U_1V_1)+2\frac{\partial V_2}{\partial T}=0,\\
\frac{\partial U_1}{\partial Y_2}+2V_1\frac{\partial V_1}{\partial T}=0.
\end{gathered} \tag{6.13}$$

The hierarchy of equations for S takes the form

$$\frac{\partial S}{\partial Y_n}-\sum_{k=1}^{n} V_{nk}(X,Y,T)e^{-k(\partial S/\partial T)}=0, \tag{6.14}$$

$$\frac{\partial S}{\partial X_n}-\sum_{k=0}^{n} U_{nk}(X,Y,T)e^{k(\partial S/\partial T)}=0, \tag{6.15}$$

where V_{nk} and $U_{nk}(U_{nn}=1)$ are appropriate functions. These equations provides us with the d2DTL hierarchy for the coefficients V_{nk} and U_{nk}.

The formulas (6.14) and (6.15) shows the role of the function $e^{\partial S/\partial T}$. In the $1+1$-dimensional case this fact was first noted in Ref. 5.

The d2DTL hierarchy clearly contains the dKP and dmKP hierarchies as subhierarchies. The first arises if one consider only times X_n putting $T_n=T=0$ while the dmKP hierarchy is associated only with times $Y_n(X_n=T=0)$.

Equations (6.14) and (6.15) imply the hierarchy of equations for the function S only. The lowest of them is of the form

$$\frac{\partial^2 S}{\partial X_1 \partial Y_1}+e^{\partial S/\partial T}\frac{\partial S}{\partial Y_1}\frac{\partial^2 S}{\partial T^2}=0. \tag{6.16}$$

VII. RING OF SYMMETRIES FOR THE QUASICLASSICAL $\bar{\partial}$-PROBLEM AND UNIVERSAL WHITHAM HIERARCHY

The results of Sec. VI demonstrate that the symmetries of the quasiclassical $\bar{\partial}$-problem have a rather special property. Namely, for the dKP, dmKP, and d2DTL hierarchies different symmetries $\omega_A=\partial S/\partial T_A$ are connected by certain algebraic relations [see formulas (5.3), (5.12) and (6.14), (6.15)].

This property of the symmetries of the quasiclassical $\bar{\partial}$-problem has, in fact, a deeper background and is of general character. This background is provided by certain theorems about the solutions of the Beltrami equation (see Ref. 27).

Thus, let us start with the general quasiclassical $\bar{\partial}$-problem,

$$\frac{\partial S}{\partial \bar{\lambda}}=W\left(\lambda,\bar{\lambda};\frac{\partial S}{\partial \lambda}\right), \tag{7.1}$$

where $W(\lambda,\bar{\lambda};\xi)$ is a certain function and dependence of S on parameters (times) is not specified yet.

Infinitesimal symmetries ω of the problem (7.1) are defined by the linear Beltrami equation

$$\frac{\partial \omega}{\partial \bar{\lambda}}=W'\left(\lambda,\bar{\lambda};\frac{\partial S}{\partial \lambda}\right)\frac{\partial \omega}{\partial \lambda}. \tag{7.2}$$

Linear Beltrami equation possesses a number of interesting properties. They have been studied in detail as a part of the theory of generalized analytic functions (see Ref. 27). The first important property is formulated in Sec. 3 (Chap. II) of Ref. 27. This Theorem 1 (see the Appendix) states that for measurable and bounded on the entire complex plane $\mathbb{C}$ functions W' which satisfies the condition $|W'|\leqslant W_0<1$ and some other mild conditions, Eq. (7.2) has a solution $\omega_0(\lambda)$ (so-called, basic homeomorphism) for which

$$\omega_0(\lambda)=\lambda+O\left(\frac{1}{\lambda}\right),\quad \lambda\to\infty. \tag{7.3}$$

Another Theorem (theorem 2.16 from Ref. 27—see the Appendix) says that all solutions (in some class) of Eq. (7.2) are given by

$$\omega(\lambda,\overline{\lambda})=\Omega(\omega_0(\lambda,\overline{\lambda})), \tag{7.4}$$

where $\Omega(\xi)$ is an arbitrary analytic function in the domain $\omega(D_0)$.

These two basic results allow us to construct infinite hierarchy associated with the problem (7.1). Indeed, let us assign the time t_A for each symmetry ω_A such that $\omega_A=\partial S/\partial T_A$. So for the basic solution (7.3) $\omega_0=\partial S/\partial T_0$. The first theorem now says that there exists a symmetry of Eq. (7.1) such that

$$\frac{\partial S}{\partial T_0}=\lambda+O\left(\frac{1}{\lambda}\right). \tag{7.5}$$

Then the second theorem states that for any symmetry $\partial S/\partial T_A$ one has

$$\frac{\partial S}{\partial T_A}=\Omega_A\left(\frac{\partial S}{\partial T_0}(\lambda,\overline{\lambda}),T\right), \tag{7.6}$$

where $\Omega(\xi,T)$ is an appropriate function of the first argument. Thus the above two theorems imply that under certain conditions the $\overline{\partial}$-equation (7.1) possesses an infinite ring of symmetries (deformations) given by

$$\frac{\partial S(\lambda,\overline{\lambda};T)}{\partial T_A}=\Omega_A\left(\frac{\partial S}{\partial T_0},T\right),\quad A=0,1,2,3,\ldots, \tag{7.7}$$

where $\Omega_A(\xi,T)$ are arbitrary analytic functions of the ξ. The set of equations (7.7) is compatible by construction. Equation (7.7) gives rise to certain nonlinear equations for functions $U_k(T)$ on which S may depend. These equations can be obtained also from the equations for Ω_A which follow from (7.7). They are

$$\frac{\partial\Omega_A}{\partial T_B}-\frac{\partial\Omega_B}{\partial T_A}+\{\Omega_A,\Omega_B\}=0,\quad A,B=0,1,2,\ldots, \tag{7.8}$$

where

$$\{f,g\}=\frac{\partial f}{\partial p}\frac{\partial g}{\partial T_1}-\frac{\partial f}{\partial T_1}\frac{\partial g}{\partial p}. \tag{7.9}$$

and we denoted $p=\partial S/\partial T_0$.

So we constructed an integrable hierarchy of equations out of the $\overline{\partial}$-problem (7.1). It is an infinite ring since $\Omega_A(\xi,T)$ are arbitrary analytic functions. To get a concrete hierarchy one has to specify the set of functions Ω_A. The set of functions $\Omega_A(p(\lambda,\overline{\lambda};T),T)$ such that $\Omega_k\sim\lambda^k+O(1/\lambda)$ as $\lambda\to\infty$ with identification $T_0=T_1$, $T_k=T_{A-1}$ gives rise to the dKP hierarchy.

In the above-given construction the time T_0 has played a special role being connected with the "basic" symmetry ω_0. Infinite ring of symmetries for the problem (7.1) admits more general and symmetric formulation. It is due to the already mentioned obvious fact that any differentiable function

$$f\left(\frac{\partial S}{\partial T_{A_1}},\frac{\partial S}{\partial T_{A_2}},\dots\right)$$

of any set of symmetries $\partial S/\partial T_{A_1},\partial S/\partial T_{A_2},\dots,$ is again a symmetry [i.e., a solution of Eq. (7.2)]. Then the implicit function theorem implies that any symmetry $\partial S/\partial T_A$ can be chosen as a basic one.

So, let us take (arbitrary) symmetry $p=\partial S/\partial T_0$. The infinite hierarchy of symmetries now takes the form

$$\frac{\partial S}{\partial T_A}=\Omega_A(p,T), \tag{7.10}$$

where $\Omega_A(\xi,T)$ are arbitrary differentiable functions of ξ. The compatibility conditions for Eq. (7.10) is of the form (7.8) and (7.9) where now T_0 and $p=\partial S/\partial T_0$ are arbitrary time and the corresponding symmetry.

The infinite set of equations (7.8) in this case is nothing but the universal Whitham hierarchy introduced in the different way in Ref. 8. So in our approach the universal Whitham hierarchy is an infinite ring of symmetries of the general quasiclassical $\overline{\partial}$-problem (7.1).

VIII. DISPERSIONLESS HIERARCHIES OF THE B TYPE

Various type of reductions for the dKP hierarchy have been considered in Refs. 5 and 10. Here we will discuss the dispersionless hierarchies of the so-called B type. The dispersionless BKP hierarchy has been discussed briefly in Ref. 30. The dBKP hierarchy is characterized by the constraint[30]

$$S(-\lambda,T)=-S(\lambda,T). \tag{8.1}$$

This constraint immediately implies that only odd powers of $\partial S/\partial T_1$ are allowed in Eq. (5.3). Since in this case $S_0(\lambda,T)=\lambda T_1+\lambda^3T_3+\lambda^5T_5+\cdots$ and $\tilde{S}=1+S_1/\lambda+S_3/\lambda^3+\cdots$ as $\lambda\to\infty$, the hierarchy of equations for S takes the form

$$\frac{\partial S}{\partial T_{2n+1}}-\left(\frac{\partial S}{\partial T_1}\right)^{2n+1}-\sum_{k=0}^{n-1}U_{nk}(T)\left(\frac{\partial S}{\partial T_1}\right)^{2k+1}=0. \tag{8.2}$$

The two lowest equations (8.2) are

$$\frac{\partial S}{\partial T_3}-\left(\frac{\partial S}{\partial T_1}\right)^3-U\frac{\partial S}{\partial T_1}=0, \tag{8.3}$$

$$\frac{\partial S}{\partial T_5}-\left(\frac{\partial S}{\partial T_1}\right)^5-V_3\left(\frac{\partial S}{\partial T_1}\right)^3-V_1\frac{\partial S}{\partial T_1}=0, \tag{8.4}$$

where

$$U=-3\frac{\partial S_1}{\partial T_1},\quad V_3=\frac{5}{3}U,\quad V_1=\frac{5}{9}U^2-\frac{\partial S_3}{\partial T_1}. \tag{8.5}$$

Equations (8.3) and (8.4) imply that

$$\frac{9}{5}\frac{\partial U}{\partial T_5}+U^2\frac{\partial U}{\partial T_1}-U\frac{\partial U}{\partial T_3}-\frac{\partial U}{\partial T_1}\partial_{T_1}^{-1}\left(\frac{\partial U}{\partial T_3}\right)-\partial_{T_1}^{-1}\left(\frac{\partial^2U}{\partial T_3^2}\right)=0. \tag{8.6}$$

Equation (8.5) is the dispersionless limit of the $2+1$-dimensional Sawada–Kotera (and also Kaup-Kupershmidt) equation.[31,32]

To get the d2DTL hierarchy of the B type we shall use the universal Whitham hierarchy equation (7.10) and (7.7). Due to constraint (8.1) only odd functions $\Omega_A(-p,T)=-\Omega(p,T)$ are admissible. Taking the time $t_1=X$ as the reference one (i.e., $p=\partial S/\partial X$) and two other equations (7.10) in the form

$$\frac{\partial S}{\partial Y}=\frac{V}{p-U}-\frac{V}{p+U},\quad \frac{\partial S}{\partial T}=\ln\frac{p-U}{p+U}, \tag{8.7}$$

where u and V are functions of X,Y,T, one obtains

$$\begin{aligned} &V_T+U_Y=0,\\ &U_T+\frac{U_X}{U}-\frac{V_X}{V}=0. \end{aligned} \tag{8.8}$$

Introducing the function $\beta=\ln(V/U)$, one can rewrite the system (8.8) as

$$\begin{aligned} &\beta_{XY}+(Ue^{\beta})_{TT}=0,\\ &\beta_X+U_T=0. \end{aligned} \tag{8.9}$$

It is the d2DTL equation of the B type. The analog of Eqs. (6.5) and (6.6) for the B-d2DTL equation (8.9) is rather interesting

$$\begin{aligned} &\frac{\partial S}{\partial Y}+\frac{V}{U}\,\mathrm{sh}\left(\frac{\partial S}{\partial T}\right)=0,\\ &\frac{\partial S}{\partial X}+U\,\mathrm{cth}\left(\frac{1}{2}\,\frac{\partial S}{\partial T}\right)=0. \end{aligned} \tag{8.10}$$

The compatibility condition for this system is equivalent to the system (8.8).

Note finally that the nonlinear equation for $S(z,\bar{z};X,Y,T)$ in this case is of the form

$$\frac{S_{TT}S_XS_Y}{1+\mathrm{ch}(S_T)}-\frac{S_{TX}S_Y}{\mathrm{sh}(S_T)}+S_{XY}=0. \tag{8.11}$$

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APPENDIX: PROPERTIES OF THE BELTRAMI

There is a well-established theory of generalized solutions of the linear Beltrami equation (see for instance Refs. 21–23 and 28)

$$Z_{\bar{\lambda}}=AZ_{\lambda}, \tag{A1}$$

where A is any given measurable function $\|A\|_{\infty}<1$ on G. Obviously, for $A\equiv 0$ we get into the class of conformal mappings. To present these results we need to introduce the operators

$$Th(\lambda):=\frac{1}{2\pi i}\int\int_{\mathbb{C}\times\mathbb{C}}\frac{h(\lambda')}{\lambda'-\lambda}d\lambda'\wedge d\bar{\lambda}', \quad \Pi h(\lambda):=\frac{\partial Th}{\partial\lambda}(\lambda),$$

where the integral is taken in the sense of the Cauchy principal value. Then one has:

Lemma: For any $p>1$ *the operator* Π *defines a bounded operator in* $L^p(\mathbb{C})$ *and for any* $0\leqslant k<1$ *there exists* $\delta>0$ *such that*

$$k\|\Pi\|_p<1,$$

for all $|p-2|<\delta$.

The next theorem summarizes the properties of solutions of (A1) that we need in our discussion.

Theorem: *Given a measurable function A with compact support inside the circle* $|\lambda|<R$ *and such that* $\|A\|_\infty<k<1$. *Then, for any fixed exponent* $p=p(k)>2$ *such that* $k\|\Pi\|_p<1$, *it follows that*

(1) *There is a unique function* Z_0 *on* $\mathbb{C}$ *with distributional derivatives satisfying the Beltrami equation* (A1) *such that*

$$Z_0(\lambda)=\lambda+O\left(\frac{1}{\lambda}\right), \quad \lambda\to\infty, \tag{A2}$$

with $Z_{0,\bar{\lambda}}$ *and* $Z_{0,\lambda}-1$ *being elements of* $L^p(\mathbb{C})$.

(2) *Every solution of* (A2) *on a domain G* of $\mathbb{C}$ *can be represented as*

$$Z(\lambda)=\Phi(Z_0(\lambda)), \tag{A3}$$

where Φ *is an arbitrary analytic function on the image domain* $Z_0(G)$ *of G under* Z_0.

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3*nj*-coefficients of su(1,1) as connection coefficients between orthogonal polynomials in *n* variables

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In the tensor product of $n+1$ positive discrete series representations of su(1,1), a coupled basis vector can be described by a certain binary coupling tree. To every such binary coupling tree, polynomials $R_l^{(k)}(x)$ and $\mathcal{R}_l^{(k)}(x)$ are associated. These polynomials are n-variable Jacobi and continuous Hahn polynomials, and are orthogonal with respect to a weight function. The connection coefficients expressing such a polynomial associated with a given binary coupling tree in terms of those polynomials associated with another binary coupling tree are proportional to $3nj$-coefficients of su(1,1). © *2002 American Institute of Physics.*
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I. INTRODUCTION

The $3nj$-coefficients of su(2) [or so(3)] play a dominant role in quantum theory of angular momentum[1–5] and its applications in nuclear, atomic, and molecular physics. For $3j$- and $6j$-coefficients of su(2) there exist expressions in terms of hypergeometric series,[5–7] explaining the close relation with orthogonal polynomials such as Hahn and Racah polynomials.[7] For example, the $6j$-coefficient of su(2) is expressed in terms of a terminating balanced ${}_4F_3$ series of unit argument. The parameters of the ${}_4F_3(1)$ series are written in terms of the six representation labels (angular momenta) of the $6j$-coefficient. By the nature of these representation labels (integer or half-integer positive numbers), the parameters of the ${}_4F_3(1)$ series are integers.[6,7] When identifying the $6j$-coefficient with a Racah polynomial $R_m(\lambda(x);\alpha,\beta,\gamma,\delta)$, it is not easy to decide which parameters correspond to the degree m, which to the variable x, and which to the parameters α, β, γ, δ of the polynomial. In a way, this identification becomes easier when dealing with positive discrete series representations of su(1,1) rather than with su(2) representations. This is, for us, one of the main reasons to consider couplings of such su(1,1) representations, their $3nj$-coefficients, and the connections with orthogonal polynomials in this article.

The Lie algebra su(1,1), or so(2,1), plays itself an important role in physical models. It has been extensively used as spectrum generating algebra in many simple quantum systems, such as the nonrelativistic Coulomb problem, the isotropic harmonic oscillator, Schrödinger's relativistic equation, and the Dirac–Coulomb problem (Ref. 8, and references therein). In certain boson models,[9,10] the relevant representations are the positive discrete series representations $\mathcal{D}^+(k)$. To fix the notation, let J_0, $J_\pm$ be the generators of su(1,1) subject to

$$[J_0,J_\pm]=\pm J_\pm, \quad [J_+,J_-]=-2J_0, \tag{1.1}$$

with the conditions $J_0^\dagger=J_0$ and $J_\pm^\dagger=J_\mp$. The positive discrete series representations[7] $\mathcal{D}^+(k)$ ($k>0$) have a basis $|k,n\rangle$, with $n=0,1,2,\ldots$, and the action of the generators is given by

$$J_0|k,n\rangle=(n+k)|k,n\rangle,$$

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$$J_+|k,n\rangle=\sqrt{(n+1)(2k+n)}|k,n+1\rangle, \tag{1.2}$$

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

[In the rest of the article, we always mean ''positive discrete series representations'' whenever we say ''representations'' of su(1,1).] The tensor product of two positive discrete series representations $(k_1)=\mathcal{D}^+(k_1)$ and $(k_2)=\mathcal{D}^+(k_2)$ [or the *coupling of two representations* (k_1) and (k_2)] decomposes as follows:[7]

$$(k_1)\otimes(k_2)=\bigoplus_{j=0}^{\infty}(k_1+k_2+j). \tag{1.3}$$

The ''coupled basis vectors'' are written in terms of the uncoupled ones by means of the su(1,1) Clebsch–Gordan coefficients:

$$|(k_1k_2)k,n\rangle=\sum_{n_1,n_2}C^{k_1,k_2,k}_{n_1,n_2,n}|k_1,n_1\rangle\otimes|k_2,n_2\rangle. \tag{1.4}$$

Herein, $k=k_1+k_2+j$ for some integer $j\geqslant 0$, and the sum is such that $n_1+n_2=j+n$. Explicit expressions for the Clebsch–Gordan coefficients are given, e.g., in Refs. 7, 11, and 12, in terms of a ${}_3F_2(1)$ series.

In this article we shall be dealing with the coupling or tensor product of $n+1$ such representations, labeled by positive integers $k_1,k_2,\ldots,k_{n+1}$. For the description of coupled basis vectors in such a tensor product, the notion of binary coupling trees is essential (see Ref. 4, Topic 12 and Refs. 13 and 14). Binary couplings find their origin in the recoupling theory of $n+1$ angular momenta (Ref. 4 Topic 12) [thus in the context of tensor products of $(n+1)$ su(2) representations], but apply also to the ''recoupling theory'' of $n+1$ positive discrete series representations of su(1,1).[13,14] Binary coupling trees describe the coupling scheme (the way of taking tensor products), i.e., the sequential pairwise coupling (Ref. 4 Topic 12). A $3nj$-coefficient of su(1,1) is then the coefficient of a unitary transformation which connects two basis vectors corresponding to different binary coupling schemes of $n+1$ representations.[4,6,13,14] Thus a $3nj$-coefficient is characterized by two binary trees T_1 and T_2 (with labeled leaves and nodes), and since it is the transformation coefficient or overlap coefficient, it is usually denoted by $\langle T_1,T_2\rangle$. For the reader not familiar with binary coupling trees, their meaning will become transparent from the examples given in this article.

The motivation for the work presented here stems from interpretations of identities involving orthogonal polynomials and su(1,1) Racah coefficients [or su(1,1) $6j$-coefficients]. One such identity appears already in the seminal work of Granovskiĭ and Zhedanov [Ref. 15, Eq. (9)]: this is a convolution identity involving products of Jacobi polynomials and Racah coefficients. The identity can be interpreted as a connection coefficient identity between orthogonal polynomials in two variables, with su(1,1) Racah coefficients as connection coefficients (see Refs. 11 and 12). It was later extended to the case of continuous Hahn polynomials (Ref. 12, Theorem 3.13): here the connection coefficients are the same [namely su(1,1) Racah coefficients], but the orthogonal polynomials in two variables are certain products of two continuous Hahn polynomials.

In the present article orthogonal polynomials in n variables will be associated with the tensor product of $n+1$ representations of su(1,1). A different class of orthogonal polynomials arises depending upon the (internal) binary coupling tree. Then, the connection coefficients relating two such orthogonal polynomials associated with a different binary coupling tree are given by $3nj$-coefficients (associated with the coupling trees). For the case of three couplings Jacobi polynomials and continuous Hahn polynomials appear. Also for the n-variable case, these two families are present: the orthogonal polynomials we are dealing with are either products of certain Jacobi polynomials, or products of continuous Hahn polynomials.

In general, orthogonal polynomials in several variables give rise to certain difficulties that are not present in the one variable situation. For example, orthogonal polynomials in n variables are no longer uniquely defined by the area Ω and the weight function on the area. This is closely related to the fact that there is no obvious natural order for polynomials in several variables.

The space of all polynomials in the variables $x_1,\ldots,x_n$ with real coefficients is denoted $\mathbb{R}[x_1,\ldots,x_n]$ or Π^n for short. The degree of a polynomial $P\in\Pi^n$ is the highest degree of any of its monomials. Let $\langle\cdot,\cdot\rangle$ be an inner product defined on Π^n. Then P is an orthogonal polynomial if $\langle P,Q\rangle=0$ for all polynomials Q with $\deg Q<\deg P$. This definition does not require that P is orthogonal with other (orthogonal) polynomials of the same degree.

In our case the inner product will be defined in terms of some (classical) weight function W on some (classical) area Ω in $\mathbb{R}^n$: $\langle P,Q\rangle=\int_\Omega P(x)Q(x)W(x)dx$.

The outline of the rest of this article is as follows. In Sec. II we confine ourselves to the two variable case. The basic identities are convolution identities involving su(1,1) Racah coefficients and Jacobi polynomials[15,11] or continuous Hahn polynomials.[12] The new aspect here is that we show how to deduce these identities from the Biedenharn–Elliott identity.[4] More particularly, we show how the Biedenharn–Elliott identity yields a new convolution identity involving the Wilson and Racah polynomials. The products of Wilson polynomials on both sides of the identity are shown to be orthogonal in $\mathbb{R}^2$ with respect to some weight function. Using limiting relations between the Wilson, continuous Hahn and Jacobi polynomials, two other (known) convolution identities are (re)derived.

Section III generalizes the result involving Jacobi polynomials to n variables. With the coupling of $n+1$ representations in su(1,1) we associate a set of orthogonal polynomials on the simplex with respect to the classical weight function $x_1^{\alpha_1}\cdots x_n^{\alpha_n}(1-x_1-\cdots-x_n)^{\alpha_{n+1}}$ $(\alpha_i>-1)$. For $n=2$ these polynomials are due to Proriol.[16] For arbitrary n, but associated to a special coupling tree, these polynomials appear in Ref. 17. The more general case was also considered by Rosengren[18] in the context of multilinear Hankel forms.

Section IV does the same for the result involving continuous Hahn polynomials. In this case the area is the complete space $\mathbb{R}^n$, and the weight function is in terms of gamma functions.

In Sec. V we prove that the sets of polynomials defined in the previous sections form bases for Π^n. Moreover, we show that the generalized recoupling coefficients of su(1,1), which are essentially sums of products of Racah coefficients, are the connection coefficients between the different bases.

In the rest of this article we will use the following abbreviations: k always stands for the $(n+1)$-tuple $(k_1,\ldots,k_{n+1})\in\mathbb{R}_+^{n+1}$, and l is an n-tuple $(l_1,\ldots,l_n)\in\mathbb{N}^n$. Moreover, we use $|k|=k_1+\cdots+k_{n+1}$ and $|l|=l_1+\cdots+l_n$. The Kronecker delta symbol $\delta_{l,l'}$ then stands for the product $\delta_{l_1,l_1'},\ldots,\delta_{l_n,l_n'}$, etc.

II. A CONVOLUTION IDENTITY INVOLVING WILSON POLYNOMIALS

In general recoupling theory of su(2), the Biedenharn–Elliott identity is well known.[4,1,6] In the case of positive discrete series representations of su(1,1), the identity is essentially the same. It is easily derived by considering the overlap or transformation coefficient (Ref. 4, pp. 456–457),[13,14]

$$\langle((((k_1,k_2)k_{12},k_3)k_{13},k_4)k_{14}|(k_1,(k_2,(k_3,k_4)k_{34})k_{24})k_{14}\rangle$$

and computing this in two different ways: either directly, yielding a product of two recoupling coefficients, or in three steps, introducing a summation variable and thus yielding a sum of a product of three recoupling coefficients. Explicitly we obtain

$$\sum_{k_{23}} U^{k_1,k_2,k_{12}}_{k_3,k_{13},k_{23}} U^{k_1,k_{23},k_{13}}_{k_4,k_{14},k_{24}} U^{k_2,k_3,k_{23}}_{k_4,k_{24},k_{34}} = U^{k_{12},k_3,k_{13}}_{k_4,k_{14},k_{34}} U^{k_1,k_2,k_{12}}_{k_{34},k_{14},k_{24}}, \tag{2.1}$$

where k_{23} is restricted to some range, and U stands for a Racah coefficient (or recoupling coefficient, or $6j$-coefficient) of su(1,1). All k_i's or k_{ij}'s refer to su(1,1) representation labels and are positive real numbers. An explicit form for the recoupling coefficients in terms of terminating balanced ${}_4F_3(1)$ series is known:[7,11,12]

$$U^{k_1,k_2,k_{12}}_{k_3,k_0,k_{23}}=\begin{pmatrix} j+j_{12} \\ j_{23} \end{pmatrix}\frac{(2k_2)_{j_{12}}(2k_3)_j(2k_1+2k_2+2k_3+j+j_{12}-1)_{j_{23}}}{(2k_3,2k_2+2k_3+j_{23}-1)_{j_{23}}(2k_2+2k_3+2j_{23})_{j'}}$$
$$\times\sqrt{\frac{j'!(2k_1,2k_{23},2k_1+2k_{23}+j'-1)_{j'}\,j_{23}!(2k_2,2k_3,2k_2+2k_3+j_{23}-1)_{j_{23}}}{j!(2k_{12},2k_3,2k_{12}+2k_3+j-1)_j\,j_{12}!(2k_1,2k_2,2k_1+2k_2+j_{12}-1)_{j_{12}}}}$$
$$\times{}_4F_3\left(\begin{matrix}2k_1+2k_2+j_{12}-1,2k_2+2k_3+j_{23}-1,-j_{12},-j_{23}\\ 2k_2,2k_1+2k_2+2k_3+j+j_{12}-1,-j-j_{12}\end{matrix};1\right), \tag{2.2}$$

with the following restrictions and definitions:

$$k_{12}=k_1+k_2+j_{12},\quad k_{23}=k_2+k_3+j_{23},$$

$$k_0=k_{12}+k_3+j=k_1+k_{23}+j',\quad j_{12},j,j_{23},j'\in\mathbb{N},\ \text{and}\ j_{12}+j=j_{23}+j'.$$

In (2.2), we follow the classical notation for Pochhammer symbols $(a)_n$ and for hypergeometric series ${}_pF_q$.[19–21]

Both the Racah and Wilson polynomials are defined in terms of terminating balanced ${}_4F_3(1)$ series. We will now perform an appropriate renaming of the nine free parameters and the summation variable in (2.1) to derive a convolution identity involving Wilson and Racah polynomials.

Wilson polynomials, denoted $W_m(x^2;a,b,c,d)$, are defined as follows:

$$W_m(x^2;a,b,c,d)=(a+b)_m(a+c)_m(a+d)_m\,{}_4F_3\left(\begin{matrix}-m,m+a+b+c+d-1,a+ix,a-ix\\ a+b,a+c,a+d\end{matrix};1\right), \tag{2.3}$$

while Racah polynomials, denoted $R_m(\lambda(x);\alpha,\beta,\gamma,\delta)$, are defined by

$$R_m(\lambda(x);\alpha,\beta,\gamma,\delta)={}_4F_3\left(\begin{matrix}-m,m+\alpha+\beta+1,-x,x+\gamma+\delta+1\\ \alpha+1,\beta+\delta+1,\gamma+1\end{matrix};1\right), \tag{2.4}$$

where $\lambda(x)=x(x+\gamma+\delta+1)$ and one of the denominator parameters equals $-M$ with $M\in\mathbb{N}$ and $0\leqslant m\leqslant M$.

Here (and in the rest of the article), we use the notation of Ref. 22 for Wilson and Racah polynomials (and for all other one variable orthogonal polynomials).

Theorem 1: *The Wilson polynomials satisfy the following convolution identity:*

$$\sum_{l=0}^{m+j}\begin{pmatrix} j+m \\ l \end{pmatrix}\frac{(2k_2)_m(2k_3)_j(2k_1+2k_2+2k_3+j+m-1)_l}{(2k_3)_l(2k_2+2k_3+l-1)_l(2k_2+2k_3+2l)_{j+m-l}}R_l(\lambda(m);2k_2-1,2k_3-1,$$
$$-j-m-1,2k_1+2k_2+j+m-1)W_{m+j-l}((x_1-t)^2;k_1+it,k_2+k_3+l-is+it,k_1-it,k_2+k_3$$
$$+l+is-it)W_l((x_1+x_2-t)^2;k_2-ix_1+it,k_3-is+it,k_2+ix_1-it,k_3+is-it)$$
$$=W_m((x_1-t)^2;k_1+it,k_2-i(x_1+x_2)+it,k_1-it,k_2+i(x_1+x_2)-it)$$
$$\times W_j((x_1+x_2-t)^2;k_1+k_2+m+it,k_3-is+it,k_1+k_2+m-it,k_3+is-it), \tag{2.5}$$

where $j,\ m\in\mathbb{N},\ k_1,\ k_2,\ k_3,\ x_1,\ x_2,\ x_3,\ t\in\mathbb{R}$ *and* $s=x_1+x_2+x_3$.

Proof: In the case of su(1,1), the summation range for k_{23} in (2.1) is from k_2+k_3 to $\min(k_{13}-k_1,k_{24}-k_4)$. The summation variable k_{23} thus takes *real* values, starting with k_2+k_3 and increasing in steps of one. Substituting (2.2) in (2.1) yields an identity between terminating balanced ${}_4F_3(1)$ series:

$$\begin{aligned}
&\sum_{k_{23}=k_2+k_3}^{\min(k_{13}-k_1,k_{24}-k_4)} f\times {}_4F_3\left(\begin{matrix}k_1+k_2+k_{12}-1,k_2+k_3+k_{23}-1,k_1+k_2-k_{12},k_2+k_3-k_{23}\\ 2k_2,k_{13}+k_1+k_2+k_3-1,k_1+k_2+k_3-k_{13}\end{matrix};1\right)\\
&\quad\times {}_4F_3\left(\begin{matrix}k_1+k_{23}+k_{13}-1,k_{23}+k_4+k_{24}-1,k_1+k_{23}-k_{13},k_{23}+k_4-k_{24}\\ k_1+k_{23}+k_4-k_{14},2k_{23},k_{14}+k_1+k_{23}+k_4-1\end{matrix};1\right)\\
&\quad\times {}_4F_3\left(\begin{matrix}k_2+k_3+k_{23}-1,k_2+k_3-k_{23},k_3+k_4+k_{34}-1,k_3+k_4-k_{34}\\ k_2+k_3+k_4-k_{24},2k_3,k_{24}+k_2+k_3+k_4-1\end{matrix};1\right)\\
&\quad={}_4F_3\left(\begin{matrix}k_3+k_4+k_{34}-1,k_{12}+k_3+k_{13}-1,k_3+k_4-k_{34},k_{12}+k_3-k_{13}\\ k_{12}+k_3+k_4-k_{14},2k_3,k_{14}+k_{12}+k_3+k_4-1\end{matrix};1\right)\\
&\qquad\times {}_4F_3\left(\begin{matrix}k_1+k_2+k_{12}-1,k_1+k_2-k_{12},k_2+k_{34}+k_{24}-1,k_2+k_{34}-k_{24}\\ 2k_2,k_1+k_2+k_{34}-k_{14},k_{14}+k_1+k_2+k_{34}-1\end{matrix};1\right),
\end{aligned}$$

where f is a numerical factor that is easily calculated from (2.2). Renaming the following positive integer differences as

$$m=k_{12}-k_1-k_2,\quad j=k_{13}-k_{12}-k_3\quad\text{and}\quad l=k_{23}-k_2-k_3,$$

and performing appropriate Bailey transformations (Ref. 23, Theorem 3.3.3) on the balanced ${}_4F_3(1)$'s, yields that (when $k_{13}-k_1\leqslant k_{24}-k_4$)

$$\begin{aligned}
&\sum_{l=0}^{j+m} f'\times {}_4F_3\left(\begin{matrix}-l,l+2k_2+2k_3-1,-m,m+2k_1+2k_2-1\\ 2k_2,2k_1+2k_2+2k_3+j+m-1,-j-m\end{matrix};1\right)\\
&\quad\times {}_4F_3\left(\begin{matrix}-m-j+l,m+j+l+2k_1+2k_2+2k_3-1,k_1+k_{14}+k_{24}-1,k_1+k_{14}-k_{24}\\ 2k_1,k_1+k_2+k_3+l+k_4+k_{14}-1,k_1+k_2+k_3+l+k_{14}-k_4\end{matrix};1\right)\\
&\quad\times {}_4F_3\left(\begin{matrix}-l,l+2k_2+2k_3-1,k_2+k_{24}+k_{34}-1,k_2+k_{24}-k_{34}\\ 2k_2,k_2+k_3+k_{24}-k_4,k_{24}+k_2+k_3+k_4-1\end{matrix};1\right)\\
&\quad={}_4F_3\left(\begin{matrix}-j,j+2m+2k_1+2k_2+2k_3-1,m+k_1+k_2+k_{14}-k_{34},m+k_1+k_2+k_{14}+k_{34}-1\\ 2m+2k_1+2k_2,m+k_1+k_2+k_3+k_4+k_{14}-1,m+k_1+k_2+k_3+k_{14}-k_4\end{matrix};1\right)\\
&\qquad\times {}_4F_3\left(\begin{matrix}-m,m+2k_1+2k_2-1,k_1+k_{14}+k_{24}-1,k_1+k_{14}-k_{24}\\ 2k_1,k_1+k_2+k_{14}-k_{34},k_1+k_2+k_{14}+k_{34}-1\end{matrix};1\right),
\end{aligned}$$

where, once again, f' is a numerical factor that is easily calculated.

This last identity can be written in terms of Wilson and Racah polynomials by putting

$$ix_1=k_{14}-k_{24},\quad ix_2=k_{24}-k_{34},\quad ix_3=k_{34}-k_4\quad\text{and}\quad it=k_4+i(x_1+x_2+x_3)-\tfrac{1}{2}.$$

Note that all the renamings are invertible. Determination of the factor f' now yields the desired result. Since (2.5) is a rational identity in the parameters k_i, x_i and t, it is valid for all values of these parameters. □

From Theorem 1 we can easily rederive a convolution identity for continuous Hahn polynomials. The continuous Hahn polynomials, denoted $p_m(x;a,b,c,d)$, are defined as[22]

$$p_m(x;a,b,c,d)=i^m\frac{(a+c)_m(a+d)_m}{m!}\,{}_3F_2\left(\begin{matrix}-m,m+a+b+c+d-1,a+ix\\ a+c,a+d\end{matrix};1\right);\qquad(2.6)$$

for their orthogonality [when $\Re(a,b,c,d)>0$, $\overline{c}=a$ and $\overline{d}=b$], see Ref. 22 or (4.3). Using the limit transition,[22]

$$\lim_{t\to-\infty}\frac{W_m((x-t)^2;a+it,b+it,c-it,d-it)}{(2t)^m m!}=p_m(x;a,b,c,d), \tag{2.7}$$

in (2.5), one finds the following corollary (see also Ref. 12, Theorem 3.13).

Corollary 2: The continuous Hahn polynomials satisfy the following convolution identity:

$$\begin{aligned}&\sum_{l=0}^{m+j}\binom{j+m}{m}\frac{(2k_2)_m(2k_3)_j(2k_1+2k_2+2k_3+j+m-1)_l}{(2k_3)_l(2k_2+2k_3+l-1)_l(2k_2+2k_3+2l)_{j+m-l}}R_l(\lambda(m);2k_2-1,2k_3-1,\\&\quad -j-m-1,2k_1+2k_2+j+m-1)p_{m+j-l}(x_1;k_1,k_2+k_3+l-is,k_1,k_2+k_3+l+is)\\&\quad\times p_l(x_2;k_2,k_3-i(s-x_1),k_2,k_3+i(s-x_1))\\&\quad=p_m(x_1;k_1,k_2-i(x_1+x_2),k_1,k_2+i(x_1+x_2))\\&\qquad\times p_j(x_1+x_2;k_1+k_2+m,k_3-is,k_1+k_2+m,k_3+is),\end{aligned} \tag{2.8}$$

where $j,m\in\mathbb{N}$, $k_1,k_2,k_3,x_1,x_2,x_3\in\mathbb{R}$ and $s=x_1+x_2+x_3$. □

The classical Jacobi polynomials are defined by

$$P_m^{(\alpha,\beta)}(x)=\frac{(\alpha+1)_m}{m!}{}_2F_1\left(\begin{matrix}-m,m+\alpha+\beta+1\\ \alpha+1\end{matrix};\frac{1-x}{2}\right); \tag{2.9}$$

for $\alpha,\beta>-1$, they are orthogonal over the interval $[-1,1]$ for the weight function $(1-x)^\alpha(1+x)^\beta$. Replacing x_i by sx_i in (2.8) and letting s tend to infinity yields Corollary 3 (see also Ref. 12 Corollary 3.15, or Refs. 15 and 11):

Corollary 3: The Jacobi polynomials satisfy the following convolution identity:

$$\begin{aligned}&\sum_{l=0}^{m+j}\binom{j+m}{m}\frac{(2k_2)_m(2k_3)_j(2k_1+2k_2+2k_3+j+m-1)_l}{(2k_3)_l(2k_2+2k_3+l-1)_l(2k_2+2k_3+2l)_{j+m-l}}R_l(\lambda(m);2k_2-1,2k_3-1,\\&\quad -j-m-1,2k_1+2k_2+j+m-1)P_{m+j-l}^{(2k_1-1,2k_2+2k_3+2l-1)}(1-2x_1)\\&\quad\times(1-x_1)^l P_l^{(2k_2-1,2k_3-1)}\left(\frac{1-x_1-2x_2}{1-x_1}\right)\\&\quad=(x_1+x_2)^m P_m^{(2k_1-1,2k_2-1)}\left(\frac{x_2-x_1}{x_1+x_2}\right)P_j^{(2k_1+2k_2+2m-1,2k_3-1)}(1-2x_1-2x_2).\end{aligned}$$

□

Both Corollaries 2 and 3 can be written in a more symmetric (and unified) way using a different scaling for the continuous Hahn and Jacobi polynomials. Defining the polynomial $\mathcal{S}_m^{k_1,k_2}(x_1,x_2)$ as

$$\begin{aligned}\mathcal{S}_m^{k_1,k_2}(x_1,x_2)=&\sqrt{\frac{m!(2m+2k_1+2k_2-1)\Gamma(m+2k_1+2k_2-1)}{\Gamma(m+2k_1)\Gamma(m+2k_2)}}\\&\times p_m(x_1;k_1,k_2-i(x_1+x_2),k_1,k_2+i(x_1+x_2)),\end{aligned} \tag{2.10}$$

we have the following identity [Ref. 12, Eq. (3.15)]:

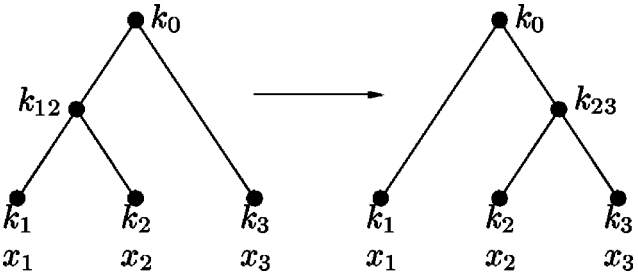

FIG. 1. Two possible ways of coupling three representations.

$$\mathcal{S}^{k_1,k_2}_{k_{12}-k_1-k_2}(x_1,x_2)\mathcal{S}^{k_{12},k_3}_{k_0-k_{12}-k_3}(x_1+x_2,x_3)$$
$$=\sum_{k_{23}=k_2+k_3}^{k_0-k_1} U^{k_1,k_2,k_{12}}_{k_3,k_0,k_{23}}\mathcal{S}^{k_2,k_3}_{k_{23}-k_2-k_3}(x_2,x_3)\mathcal{S}^{k_1,k_{23}}_{k_0-k_1-k_{23}}(x_1,x_2+x_3). \tag{2.11}$$

Formula (2.11) is easily remembered by considering two ways in which three su(1,1) representations can be coupled, as shown in Fig. 1. Notice how the left side of (2.11) follows from the tree on the left side of this figure. With each non-leaf node (i.e., with each intermediate or final coupling) one associates an $\mathcal{S}$-polynomial. The first (resp. second) variable of this $\mathcal{S}$-polynomial is the sum of all the variables associated with the leaves in the left (resp. right) subtree of the considered node. The upper parameters are determined by the value of the representation labels of the left and right child (in that order). The (positive integer) lower parameter is the difference between the value of the coupled representation label and the consisting labels. The $\mathcal{S}$-polynomials on the right side of (2.11) are formed in the same way but working with the tree on the right side of the figure. The recoupling coefficient appearing in (2.11) is that associated with a recoupling of three representations as shown in Fig. 1.

The $\mathcal{S}$-polynomials have the following property:

$$\mathcal{S}^{k_1,k_2}_m(x_1,x_2)=(-1)^m\mathcal{S}^{k_2,k_1}_m(x_2,x_1), \tag{2.12}$$

which is a direct consequence of Whipple's transformation for terminating ${}_3F_2(1)$ series (Ref. 23, p. 142).

If we define[15,11]

$$S^{k_1,k_2}_m(x_1,x_2)=(-1)^m\sqrt{\frac{m!}{(2k_1,2k_2,2k_1+2k_2+m-1)_m}}(x_1+x_2)^m P^{(2k_1-1,2k_2-1)}_m\left(\frac{x_2-x_1}{x_2+x_1}\right), \tag{2.13}$$

then relations (2.11) and (2.12) are still valid (after replacing $\mathcal{S}$ by S). This follows from the fact that

$$\lim_{u\to\infty}\frac{\mathcal{S}^{k_1,k_2}_m(ux_1,ux_2)}{u^m}=\sqrt{\frac{\Gamma(2m+2k_1+2k_2)}{\Gamma(2k_1)\Gamma(2k_2)}}S^{k_1,k_2}_m(x_1,x_2). \tag{2.14}$$

It is known[12] that the products of continuous Hahn polynomials on both the left and right sides of (2.8) [or (2.11)] are orthogonal on $\mathbb{R}^2$ for the weight function

$$\Gamma(k_1\pm ix_1)\Gamma(k_2\pm ix_2)\Gamma(k_3\pm i(s-x_1-x_2)), \tag{2.15}$$

where, for conciseness of notation, the product $\Gamma(k_j+ix)\Gamma(k_j-ix)$ is written as $\Gamma(k_j\pm ix)$. This convention is adopted throughout this article. Moreover, we will write $\Gamma(\pm k_j\mp ix)$ instead of $\Gamma(k_j-ix)\Gamma(-k_j+ix)$, etc. Observe that (2.11), with $x_3=s-x_1-x_2$, can thus be interpreted as a

connection coefficient formula between orthogonal polynomials in two variables, and the su(1,1) Racah coefficients are the connection coefficients. Similarly, replacing $\mathcal{S}$ by S in (2.11), one obtains again a connection coefficient formula. This time, the orthogonal polynomials are orthogonal on the simplex determined by $x_1, x_2 > 0$, $x_1 + x_2 < s$, and the weight function is $x_1^{2k_1-1} x_2^{2k_2-1} (s - x_1 - x_2)^{2k_3-1}$.

In this section we have shown how the Biedenharn–Elliott identity implies two connection coefficient formulas for orthogonal polynomials in two variables, one constructed with continuous Hahn polynomials, and one constructed with Jacobi polynomials. In the following sections this will be generalized to orthogonal polynomials in n variables. Finally, observe that also the products of Wilson polynomials in Theorem 1 are related to orthogonal polynomials in two variables (see Appendix A).

III. ORTHOGONAL POLYNOMIALS RELATED TO JACOBI POLYNOMIALS

When considering orthogonal polynomials in n variables, one of the classical areas is the simplex T_s^n:

$$T_s^n = \{x \in \mathbb{R}^n | 0 < x_j \text{ and } x_1 + \cdots + x_n < s\}. \tag{3.1}$$

Herein, s denotes some positive constant, and in almost all cases s is taken to be equal to 1. The classical weight function in this case is

$$x_1^{\kappa_1 - 1/2} \cdots x_n^{\kappa_n - 1/2} (s - |x|)^{\kappa_{n+1} - 1/2}, \tag{3.2}$$

where each $\kappa_i > -\frac{1}{2}$. In Ref. 24, Proposition 2.3.8, an explicit orthonormal basis is given associated with the weight function (3.2) on the simplex (3.1). Such a basis is not unique. In fact, with every binary coupling tree on $n+1$ leaves, a different basis can be constructed. In this section, an n-variable orthonormal polynomial will be constructed out of a product of n S-polynomials (2.13), and associated with a binary coupling of $n+1$ representations of su(1,1). We will show that this polynomial is orthogonal on the simplex T_s^n for the classical weight function. The outline of this proof is as follows: by a change of variables, we will transform the simplex into the cube on $\mathbb{R}^n$. This transformation will map the integral over the simplex into an integral over the cube, where one part can be interpreted as the multiple Jacobi weight function:

$$\prod_{i=1}^{n} (1 - x_i)^{a_i} (1 + x_i)^{b_i}, \tag{3.3}$$

while the other parts are the corresponding Jacobi polynomials.

Theorem 4: *With every coupling of* $(n+1)$ su(1,1) *representations labeled by* $k_1, \ldots, k_{n+1}$, *i.e., with every binary coupling tree with n internal nodes, we associate a set of polynomials* $R_l^{(k)}(x)$ *in n variables orthogonal on the simplex* T_s^n *for the weight function*

$$w^{(k)}(x) = x_1^{2k_1 - 1} \cdots x_n^{2k_n - 1} (s - |x|)^{2k_{n+1} - 1}, \tag{3.4}$$

where each $k_i > 0$. *Explicitly the orthogonality reads*

$$\int_{T_s^n} R_l^{(k)}(x) R_{l'}^{(k)}(x) w^{(k)}(x)\, dx = \delta_{l,l'} \frac{s^{2|k| + 2|l| - 1}}{\Gamma(2|k| + 2|l|)} \prod_{i=1}^{n+1} \Gamma(2k_i). \tag{3.5}$$

Note that in (3.5) *we also have orthogonality between polynomials of the same degree, which is more than the definition of orthogonality requires.*

Remark 5: In principal the notation of the polynomial should contain a reference to the binary coupling tree it corresponds to. For the moment, we can assume that the binary coupling tree is fixed, and we do not mention it in the notation of $R_l^{(k)}(x)$. When we want to emphasize the

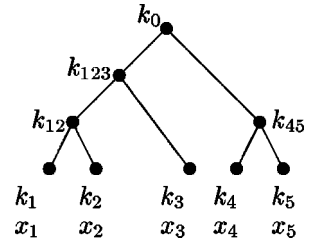

FIG. 2. Example binary coupling tree.

dependence of $R_l^{(k)}(x)$ on the given binary coupling tree T, we shall write $R_{l,T}^{(k)}(x)$. The meaning of the subscript l is related to the labeling of the internal nodes, and will soon become apparent.■

The association of a polynomial with a binary coupling tree is an extension of the method described after Eq. (2.11). For a given binary coupling tree, the polynomial $R_l^{(k)}(x)$ consists of a product of S-polynomials, each of these associated with a non-leaf node of the tree. Let us first describe an example.

Example 6: With the binary coupling tree shown in Fig. 2 we associate the following polynomial:

$$\begin{aligned}R(x_1,x_2,x_3,x_4,x_5) &= S^{k_1,k_2}_{k_{12}-k_1-k_2}(x_1,x_2)S^{k_{12},k_3}_{k_{123}-k_{12}-k_3}(x_1+x_2,x_3)S^{k_4,k_5}_{k_{45}-k_4-k_5}(x_4,x_5)\\ &\quad\times S^{k_{123},k_{45}}_{k_0-k_{123}-k_{45}}(x_1+x_2+x_3,x_4+x_5)\\ &= C\times(x_1+x_2)^{k_{12}-k_1-k_2}P^{(2k_1-1,2k_2-1)}_{k_{12}-k_1-k_2}\left(\frac{x_2-x_1}{x_2+x_1}\right)\\ &\quad\times(x_1+x_2+x_3)^{k_{123}-k_{12}-k_3}P^{(2k_{12}-1,2k_3-1)}_{k_{123}-k_{12}-k_3}\left(\frac{x_3-x_1-x_2}{x_3+x_1+x_2}\right)\\ &\quad\times(x_4+x_5)^{k_{45}-k_4-k_5}P^{(2k_4-1,2k_5-1)}_{k_{45}-k_4-k_5}\left(\frac{x_5-x_4}{x_5+x_4}\right)\\ &\quad\times(x_1+x_2+x_3+x_4+x_5)^{k_0-k_{123}-k_{45}}P^{(2k_{123}-1,2k_{45}-1)}_{k_0-k_{123}-k_{45}}\left(\frac{x_4+x_5-x_1-x_2-x_3}{x_4+x_5+x_1+x_2+x_3}\right).\end{aligned}$$

Herein, C is some numerical factor that can be determined from (2.13). ■

So the S-polynomial, associated to a non-leaf node of the tree, has as (upper) parameters the representation labels of left and right child of the node; as degree (the subindex) the difference between the representation label of the node and those of the children (this is a non-negative integer); and as left (resp. right) argument the sum of all the variables associated with the leaves in the left (resp. right) subtree of the considered node.

Such a polynomial $R(x_1,\ldots,x_{n+1})$, defined as a product of S-polynomials in this way, is homogeneous in the variables $x_1,\ldots,x_{n+1}$. So we can choose the constraint

$$x_1+x_2+\cdots+x_{n+1}=s, \tag{3.6}$$

where s is some arbitrary, positive constant. Note that this constraint is compatible with the definition of the weight function (3.4). The resulting polynomial will be denoted by $R_l^{(k)}(x)$. The subscript l in $R_l^{(k)}(x)$ stands for the sequence of degrees of the S-polynomials, in a chosen order (see later for this choice).

In order to prove (3.5), we shall transform variables from $(x_1,\ldots,x_n)$ to $(v_1,\ldots,v_n)$; determine the Jacobian and integration area for this transformation; determine the transformed weight function; and finally deduce the orthogonality. All of this can be done quite explicitly for any given binary coupling tree, and will be presented in the following subsections.

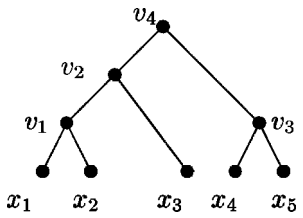

FIG. 3. Association of the variables v_i with non-leaf nodes.

A. Change of variables

We will change from variables x to variables v. The v_i are the arguments of the Jacobi polynomials appearing in the product expansion of $R_l^{(k)}(x)$ (see, for instance, Example 6).

Since each S-polynomial (and thus each Jacobi polynomial) in the product is associated with a specific non-leaf node of the tree, we can associate a variable v_i with each non-leaf node. The exact order is irrelevant but, for simplicity, we choose *postorder* (Ref. 25, Sec. 2.3.1). See Fig. 3 for an illustration.

Example 7: The arguments of the Jacobi polynomials in Example 6 are

$$\begin{aligned} v_1&=(x_2-x_1)/(x_2+x_1),\\ v_2&=(x_3-x_1-x_2)/(x_3+x_1+x_2),\\ v_3&=(x_5-x_4)/(x_5+x_4),\\ v_4&=(x_4+x_5-x_1-x_2-x_3)/(x_4+x_5+x_1+x_2+x_3). \end{aligned} \tag{3.7}$$

The set of equations (3.7), together with the constraint (3.6), has a unique solution:

$$\begin{aligned} x_1&=s(1-v_1)(1-v_2)(1-v_4)/8,\\ x_2&=s(1+v_1)(1-v_2)(1-v_4)/8,\\ x_3&=s(1+v_2)(1-v_4)/4,\\ x_4&=s(1-v_3)(1+v_4)/4,\\ x_5&=s(1+v_3)(1+v_4)/4. \end{aligned} \tag{3.8}$$

Notice how the solution (3.8) of (3.7) can easily be deduced from the tree in Fig. 3: each x_j consists of a factor s and factors $(1\pm v_i)/2$. There is a factor $(1+v_i)/2$ if x_j is in the right subtree of v_i, and there is a factor $(1-v_i)/2$ if x_j is in the left subtree of v_i. ■

This observation can be generalized to an arbitrary tree. Then we have

$$\begin{aligned} &v_i=\left(\sum_{\substack{\text{right leaves}\\ \text{of } v_i}} x_j-\sum_{\substack{\text{left leaves}\\ \text{of } v_i}} x_j\right)\Bigg/\sum_{\substack{\text{all leaves}\\ \text{of } v_i}} x_j, \quad \text{for } i=1,\ldots,n,\\ &x_1+x_2+\cdots+x_{n+1}=s. \end{aligned} \tag{3.9}$$

Lemma 8: The system (3.9) of $n+1$ (linear) equations for the variables x_j has the unique solution

$$x_j = s \prod_{\substack{\text{right ancestors} \\ \text{of } x_j}} \frac{1+v_i}{2} \prod_{\substack{\text{left ancestors} \\ \text{of } x_j}} \frac{1-v_i}{2}, \quad \text{for} \quad j=1,\ldots,n+1, \tag{3.10}$$

where we call v_i a right (resp. left) ancestor of x_j if x_j is in the right (resp. left) subtree of v_i.

Proof: By induction on n. It is easily verified that this statement is true when $n=1$. If $n>1$ and the left subtree of v_n has $0 \leqslant n_1 < n$ internal nodes, then the last two equations of (3.9) read

$$\begin{gathered} v_n = \left(\sum_{\substack{\text{right leaves} \\ \text{of } v_n}} x_j - \sum_{\substack{\text{left leaves} \\ \text{of } v_n}} x_j \right) \Bigg/ \sum_{j=1}^{n+1} x_j, \\ x_1 + x_2 + \cdots + x_{n+1} = s. \end{gathered} \tag{3.11}$$

These equations have the following unique solution for $\Sigma_{\substack{\text{right leaves} \\ \text{of } v_n}} x_j$ and $\Sigma_{\substack{\text{left leaves} \\ \text{of } v_n}} x_j$ (compare this with the case $n=1$):

$$\sum_{\substack{\text{right leaves} \\ \text{of } v_n}} x_j = s \frac{1+v_n}{2}, \qquad \sum_{\substack{\text{left leaves} \\ \text{of } v_n}} x_j = s \frac{1-v_n}{2}. \tag{3.12}$$

Using this solution for $\Sigma_{\substack{\text{left leaves} \\ \text{of } v_n}} x_j = \Sigma_{\substack{\text{leaves} \\ \text{of } v_{n_1}}} x_j$ with the first n_1 equations of (3.9), which involve only variables x that are in the left subtree of v_n, yields (by induction) the desired form of the unique solution for the variables x in the left subtree. The same applies to the variables x in the right subtree. This proves formula (3.10). We can even say more:

$$\sum_{\substack{\text{leaves} \\ \text{of } v_i}} x_j = s \prod_{\substack{\text{right ancestors} \\ \text{of } v_i}} \frac{1+v_m}{2} \prod_{\substack{\text{left ancestors} \\ \text{of } v_i}} \frac{1-v_m}{2}, \tag{3.13}$$

and

$$\sum_{\substack{\text{left leaves} \\ \text{of } v_i}} x_j = s \frac{1-v_i}{2} \prod_{\substack{\text{right ancestors} \\ \text{of } v_i}} \frac{1+v_m}{2} \prod_{\substack{\text{left ancestors} \\ \text{of } v_i}} \frac{1-v_m}{2}. \tag{3.14}$$

□

B. The Jacobian of the transformation

Example 9: The Jacobian $\partial x_j / \partial v_i$ of (the first four equations of) (3.8) is the following matrix:

$$\begin{pmatrix} -s(1-v_2)(1-v_4)/8 & -s(1-v_1)(1-v_4)/8 & 0 & -s(1-v_1)(1-v_2)/8 \\ s(1-v_2)(1-v_4)/8 & -s(1+v_1)(1-v_4)/8 & 0 & -s(1+v_1)(1-v_2)/8 \\ 0 & s(1-v_4)/4 & 0 & -s(1+v_2)/4 \\ 0 & 0 & -s(1+v_4)/4 & s(1-v_3)/4 \end{pmatrix}. \tag{3.15}$$

At first sight, this matrix is quite arbitrary. However, by taking linear combinations of rows and by swapping rows, it can be transformed into a simple upper triangular matrix. From (3.8) [or directly from (3.14)] we see that

$$\sum_{\substack{\text{left leaves}\\ \text{of } v_1}} x_j = x_1 = s(1-v_1)(1-v_2)(1-v_4)/8,$$

$$\sum_{\substack{\text{left leaves}\\ \text{of } v_2}} x_j = x_1 + x_2 = s(1-v_2)(1-v_4)/4,$$

$$\sum_{\substack{\text{left leaves}\\ \text{of } v_3}} x_j = x_4 = s(1-v_3)(1+v_4)/4,$$

$$\sum_{\substack{\text{left leaves}\\ \text{of } v_4}} x_j = x_1 + x_2 + x_3 = s(1-v_4)/2.$$

So, performing the row combinations $R_2 \leftarrow R_2 + R_1$, $R_3 \leftarrow R_3 + R_2$ and swapping the rows R_3 and R_4 of the Jacobian results in the following upper triangular matrix:

$$\begin{pmatrix} -s(1-v_2)(1-v_4)/8 & -s(1-v_1)(1-v_4)/8 & 0 & -s(1-v_1)(1-v_2)/8 \\ 0 & -s(1-v_4)/4 & 0 & -s(1-v_2)/4 \\ 0 & 0 & -s(1+v_4)/4 & s(1-v_3)/4 \\ 0 & 0 & 0 & -s/2 \end{pmatrix}. \tag{3.16}$$

The determinant of the Jacobian is thus

$$-s^4(1-v_2)(1-v_4)^2(1+v_4)/256. \tag{3.17}$$

Notice that the determinant only contains factors $s/2$ and $(1 \pm v_i)/2$. The power of each of these factors can easily be read from the tree in Fig. 3. There are four factors $s/2$, and the tree has four internal nodes. There are two factors $(1-v_4)/2$ and there are three leaves in the left subtree of v_4. There is one factor $(1+v_4)/2$ and there are two leaves in the right subtree of v_4. The same applies to v_1, v_2 and v_3.

Again, these observations can be generalized to an arbitrary tree.

Lemma 10: The absolute value of the determinant of the Jacobian, denoted J, of the transformation (3.10) (with $j=1,\ldots,n$) equals

$$J = \left| \det \frac{\partial x_j}{\partial v_i} \right| = \left(\frac{s}{2} \right)^n \prod_{i=1}^{n} \left(\frac{1+v_i}{2} \right)^{nr_i - 1} \left(\frac{1-v_i}{2} \right)^{nl_i - 1}, \tag{3.18}$$

where nr_i (resp. nl_i) is the number of leaves in the right (resp. left) subtree of v_i.

Proof: We will prove (3.18) by transforming the matrix $\partial x_j / \partial v_i$ into an upper triangular matrix by taking linear combinations of rows and by swapping rows. These manipulations do not change (up to a sign factor) the determinant of this matrix.

From (3.14) and the fact that we choose postorder, it is easily seen that $\Sigma_{\substack{\text{left leaves}\\ \text{of } v_i}} x_j$ depends on v_i but not on v_m when $m<i$. Therefore, we wish to perform row operations such that the mth row becomes

$$\frac{\partial\left(\sum_{\substack{\text{left leaves}\\ \text{of } v_m}} x_j\right)}{\partial v_i}. \tag{3.19}$$

We use induction on n to show that is possible. By the induction hypothesis, we can create the desired linear combinations in the left and right subtree. Note that the linear combinations in the right subtree do not depend on the variables $v_1,\ldots,v_{nl_n-1}$ (i.e., the variables v in the left subtree). In this process the row corresponding to the variable associated with the rightmost leaf of the left subtree is not used. For clarity, assume that this variable is x_{nl_n}. The Jacobian now has the following form:

$$x_{nl_n}\begin{array}{c} \begin{array}{ccccccccccc} v_1 & v_2 & v_3 & \cdots & v_{nl_n-1} & v_{nl_n} & v_{nl_n+1} & \cdots & v_{n-1} & v_n \end{array} \\ \left(\begin{array}{cccccccccc} * & \star & \star & \cdots & * & 0 & 0 & \cdots & 0 & * \\ 0 & * & \star & \cdots & * & 0 & 0 & \cdots & 0 & * \\ \vdots & & & & \vdots & \vdots & \vdots & & \vdots & \\ 0 & 0 & 0 & \cdots & * & 0 & 0 & \cdots & 0 & * \\ \star & \star & \star & \cdots & * & 0 & 0 & \cdots & 0 & * \\ 0 & 0 & 0 & \cdots & 0 & * & \star & \cdots & * & * \\ 0 & 0 & 0 & \cdots & 0 & 0 & * & \cdots & * & * \\ \vdots & \vdots & \vdots & & \vdots & \vdots & & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & * & * \end{array}\right) \end{array}. \tag{3.20}$$

Herein, $*$ represents a nonzero value and $\star$ an arbitrary value.

We will now use the row $\partial x_{nl_n}/\partial v_i$ to create the sum of the variables corresponding to the leaves in the left subtree of the root, i.e., the row

$$\frac{\partial\left(\sum_{\substack{\text{left leaves}\\ \text{of } v_n}} x_j\right)}{\partial v_i} = \frac{\partial\left(\sum_{\substack{\text{left leaves}\\ \text{of } v_{nl_n-1}}} x_j\right)}{\partial v_i} + \frac{\partial\left(\sum_{\substack{\text{right leaves}\\ \text{of } v_{nl_n-1}}} x_j\right)}{\partial v_i}. \tag{3.21}$$

By induction, the first term on the rhs is already a row of the matrix. If x_{nl_n} is the only leaf in the right subtree of v_{nl_n-1}, then we are finished: simply add the row corresponding to the first term to the row corresponding to x_{nl_n}. If there is more than one leaf in the right subtree of v_{nl_n-1}, we call the root of this right subtree v_m and we have

$$\frac{\partial\left(\sum_{\substack{\text{right leaves}\\ \text{of } v_{nl_n-1}}} x_j\right)}{\partial v_i} = \frac{\partial\left(\sum_{\substack{\text{left leaves}\\ \text{of } v_n}} x_j\right)}{\partial v_i} + \frac{\partial\left(\sum_{\substack{\text{right leaves}\\ \text{of } v_m}} x_j\right)}{\partial v_i}. \tag{3.22}$$

The first term of the rhs of this equation is a row of the matrix (by induction). If x_{nl_n} is the only right leaf of v_m, we are finished; add the two rows corresponding to the first terms in (3.21) and (3.22) to the row corresponding to x_{nl_n}. It is clear that we can continue in this way to create the desired row.

By swapping the rows in this matrix, we have created an upper triangular matrix with the same determinant (up to a sign) as the original matrix.

From (3.14) it is clear that the elements of this upper triangular matrix consist only of factors $s/2$, $(1\pm v_i)/2$ (and -1). Each element on the diagonal of the upper triangular matrix has a single factor $-s/2$. There is a single factor $(1+v_i)/2$ for each variable v_m that is in the right subtree of

v_i. There are nr_i-1 (i.e., the number of internal nodes in the right subtree of v_i) such variables, so there are nr_i-1 entries on the diagonal that have a factor $(1+v_i)/2$. In the same way one sees that there are nl_i-1 entries on the diagonal that have a factor $(1-v_i)/2$. Multiplying the elements on the diagonal yields formula (3.18). □

C. Transformation of the area and weight function

The cube $\square^n$ in $\mathbb{R}^n$ is defined as

$$\square^n=\{v\in\mathbb{R}^n\,|\,-1<v_j<1\}. \tag{3.23}$$

Lemma 11: When x and v are connected through (3.9) and (3.10), then $x\in T_s^n \Leftrightarrow v\in\square^n$.

Note that, although the simplex T_n^s depends on s, the cube $\square^n$ does not. An explicit proof of this lemma is given in Appendix B.

Next, we consider the transformation of the weight function (3.4), first for an example, and then for an arbitrary binary coupling tree.

Example 12: For the tree of Fig. 2 the weight function is

$$w^{(k)}(x_1,x_2,x_3,x_4)=x_1^{2k_1-1}x_2^{2k_2-1}x_3^{2k_3-1}x_4^{2k_4-1}(s-x_1-x_2-x_3-x_4)^{2k_5-1}. \tag{3.24}$$

Rewriting this weight function in terms of the variables v, using (3.8), gives

$$\begin{aligned}\tilde{w}^{(k)}(v_1,v_2,v_3,v_4)=&\,s^{2k_1+2k_2+2k_3+2k_4+2k_5-5}\\ &\times\left(\frac{1+v_1}{2}\right)^{2k_2-1}\left(\frac{1+v_2}{2}\right)^{2k_3-1}\left(\frac{1+v_3}{2}\right)^{2k_5-1}\left(\frac{1+v_4}{2}\right)^{2k_4+2k_5-2}\\ &\times\left(\frac{1-v_1}{2}\right)^{2k_1-1}\left(\frac{1-v_2}{2}\right)^{2k_1+2k_2-2}\left(\frac{1-v_3}{2}\right)^{2k_4-1}\left(\frac{1-v_4}{2}\right)^{2k_1+2k_2+2k_3-3}.\end{aligned}$$

■

Lemma 13: The transformation of the weight function (3.4) under the substitution (3.10) becomes

$$\tilde{w}^{(k)}(v)=s^{2|k|-n-1}\prod_{i=1}^{n}\left(\frac{1+v_i}{2}\right)^{\sum_{\text{right leaves of }v_i}2k_j-mr_i}\left(\frac{1-v_i}{2}\right)^{\sum_{\text{left leaves of }v_i}2k_j-nl_i}. \tag{3.25}$$

Proof: Since the weight function is essentially equal to $\Pi_{j=1}^{n+1}x_j^{2k_j-1}$, it becomes a product of factors s, and $(1\pm v_i)/2$. Each x_j has a single factor s; the power of s is thus $\Sigma_{j=1}^{n+1}(2k_j-1)=2|k|-n-1$. Furthermore, each x_j which is in the right (resp. left) subtree of v_i has a factor $(1+v_i)/2$ [resp. $(1-v_i)/2$]. □

D. Verifying the orthogonality

If two su(1,1) representations k_1 and k_2 are coupled to k_{12}, then the difference $k_{12}-k_1-k_2$ is a non-negative integer [see (1.3)]. So, with each internal node, say v_i, of a binary coupling tree we can associate a non-negative integer, say l_i. Furthermore, we can associate a real positive value with each node of the tree; for the leaves this value is simply k_j, and for an internal node v_i the value equals the value of the left child plus the value of the right child plus l_i, or explicitly

$$\sum_{\substack{\text{leaves}\\ \text{of }v_i}}k_j+\sum_{\substack{\text{nodes in}\\ \text{subtree of }v_i}}l_j+l_i. \tag{3.26}$$

Example 14: In Fig. 4 the value of each node is indicated in the tree. ■

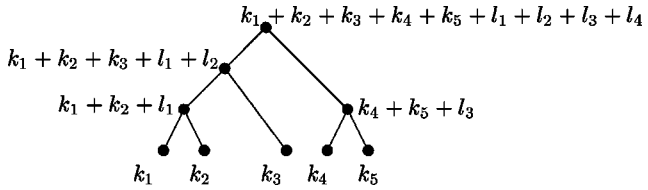

FIG. 4. Value of the nodes in the tree.

For a given binary coupling tree, the knowledge of $k=(k_1,k_2,\ldots,k_{n+1})$ and $l=(l_1,\ldots,l_n)$ completely determines the polynomial $R_l^{(k)}(x)$. Now we are in a position to prove Theorem 4.

As already mentioned, we will transform the integral over T_s^n into an integral over $\square^n$ by changing the variables from x to v. We will get a product of n integrals over the interval $(-1,1)$, each involving two Jacobi polynomials and a factor acting as weight function. Using the orthogonality of the Jacobi polynomials over this interval with respect to this weight function will yield the desired result. Explicitly, the orthogonality of the Jacobi polynomials reads

$$\int_{-1}^{1} P_m^{(a,b)}(t)P_n^{(a,b)}(t)(1-t)^a(1+t)^b dt=\delta_{m,n}h_m^{(a,b)}, \quad a,b>-1, \tag{3.27}$$

with

$$h_m^{(a,b)}=\frac{2^{a+b+1}\Gamma(m+a+1)\Gamma(m+b+1)}{(2m+a+b+1)m!\Gamma(m+a+b+1)}.$$

After transformation, using (3.13), the polynomial $R_l^{(k)}(x)$ becomes

$$\tilde{R}_l^{(k)}(v)=C\prod_{i=1}^{n}\left(s\prod_{\substack{\text{left ancestors}\\ \text{of } v_i}}\frac{1-v_m}{2}\prod_{\substack{\text{right ancestors}\\ \text{of } v_i}}\frac{1+v_m}{2}\right)^{l_i}P_{l_i}^{(a_i,b_i)}(v_i), \tag{3.28}$$

with

$$C=(-1)^{|l|}\prod_{i=1}^{n}\sqrt{\frac{l_i!}{(a_i+1,b_i+1,a_i+b_i+l_i+1)_{l_i}}}. \tag{3.29}$$

Herein, a_i equals two times the value of the node corresponding to the left child of v_i minus one, or explicitly

$$a_i=\sum_{\substack{\text{left leaves}\\ \text{of } v_i}}2k_j+\sum_{\substack{\text{nodes in left}\\ \text{subtree of } v_i}}2l_j-1. \tag{3.30}$$

Similarly, one finds

$$b_i=\sum_{\substack{\text{right leaves}\\ \text{of } v_i}}2k_j+\sum_{\substack{\text{nodes in right}\\ \text{subtree of } v_i}}2l_j-1. \tag{3.31}$$

Now we turn our attention to the transformed integrand of (3.5). Apart from the products

$$P_{l_i}^{(a_i,b_i)}(v_i)P_{l_i'}^{(a_i',b_i')}(v_i), \tag{3.32}$$

it consists of factors s and $(1\pm v_i)/2$. Let us determine the power of $(1-v_i)/2$. There are three contributing parts:

(i) the determinant of the Jacobian, yielding a term nl_i-1 [see (3.18)];
(ii) the transformed weight function, yielding a term $\sum_{\substack{\text{left leaves}\\ \text{of } v_i}} 2k_j-m_i$ [see (3.25)]; and
(iii) the transformed polynomials, yielding a term $\sum_{\substack{\text{nodes in left}\\ \text{subtree of } v_i}} l_j+\sum_{\substack{\text{nodes in left}\\ \text{subtree of } v_i}} l'_h$ [see (3.28)].

It is thus clear that the power p_i^- of $(1-v_i)/2$ is

$$p_i^-=\sum_{\substack{\text{left leaves}\\ \text{of } v_i}} 2k_j+\sum_{\substack{\text{nodes in left}\\ \text{subtree of } v_i}} l_j+\sum_{\substack{\text{nodes in left}\\ \text{subtree of } v_i}} l'_j-1. \tag{3.33}$$

In the same way one finds that the power p_i^+ of $(1+v_i)/2$ is

$$p_i^+=\sum_{\substack{\text{right leaves}\\ \text{of } v_i}} 2k_j+\sum_{\substack{\text{nodes in right}\\ \text{subtree of } v_i}} l_j+\sum_{\substack{\text{nodes in right}\\ \text{subtree of } v_i}} l'_j-1. \tag{3.34}$$

Example 15: In our example the transformed integral, denoted I, is, up to a constant factor, equal to the following product of four integrals:

$$\begin{aligned}
&\int_{-1}^{1} P_{l_1}^{(2k_1-1,2k_2-1)}(v_1)P_{l'_1}^{(2k_1-1,2k_2-1)}(v_1)\left(\frac{1-v_1}{2}\right)^{2k_1-1}\left(\frac{1+v_1}{2}\right)^{2k_2-1}dv_1\\
&\quad\times\int_{-1}^{1} P_{l_2}^{(2k_1+2k_2+2l_1-1,2k_3-1)}(v_2)P_{l'_2}^{(2k_1+2k_2+2l'_1-1,2k_3-1)}(v_2)\\
&\quad\times\left(\frac{1-v_2}{2}\right)^{2k_1+2k_2+l_1+l'_1-1}\left(\frac{1+v_2}{2}\right)^{2k_3-1}dv_2\\
&\quad\times\int_{-1}^{1} P_{l_3}^{(2k_4-1,2k_5-1)}(v_3)P_{l'_3}^{(2k_4-1,2k_5-1)}(v_3)\left(\frac{1-v_3}{2}\right)^{2k_4-1}\left(\frac{1+v_3}{2}\right)^{2k_5-1}dv_3\\
&\quad\times\int_{-1}^{1} P_{l_4}^{(2k_1+2k_2+2k_3+2l_1+2l_2-1,2k_4+2k_5+2l_3-1)}(v_4)\\
&\quad\times P_{l'_4}^{(2k_1+2k_2+2k_3+2l'_1+2l'_2-1,2k_4+2k_5+2l'_3-1)}(v_4)\\
&\quad\times\left(\frac{1-v_4}{2}\right)^{2k_1+2k_2+2k_3+l_1+l'_1+l_2+l'_2-1}\left(\frac{1+v_4}{2}\right)^{2k_4+2k_5+l_3+l'_3-1}dv_4.
\end{aligned}$$

Now, using the orthogonality (3.27) of the Jacobi polynomials, the first of these integrals is zero, except when $l_1=l'_1$. Assuming that $l_1=l'_1$, we see that the second integral is zero, except when $l_2=l'_2$. The third integral immediately implies that I is zero if $l_3\neq l'_3$. Assuming that $l_i=l'_i$, for $i=1,\ldots,3$, we see that I is zero, except when $l_4=l'_4$. We thus see that $I=\delta_{l,l'}h_l^{(k)}$, where h is some numerical constant. ■

In general, the transformation yields

$$
\begin{aligned}
I &= \int_{T_s^n} R_l^{(k)}(x) R_{l'}^{(k)}(x) w^{(k)}(x)\, dx \\
&= D \int_{\square} \prod_{i=1}^{n} P_{l_i}^{(a_i,b_i)}(v_i) P_{l_i'}^{(a_i',b_i')}(v_i) \left(\frac{1-v_i}{2}\right)^{p_i^-} \left(\frac{1+v_i}{2}\right)^{p_i^+} dv \\
&= D \prod_{i=1}^{n} \int_{-1}^{1} P_{l_i}^{(a_i,b_i)}(v_i) P_{l_i'}^{(a_i',b_i')}(v_i) \left(\frac{1-v_i}{2}\right)^{p_i^-} \left(\frac{1+v_i}{2}\right)^{p_i^+} dv_i . \qquad (3.35)
\end{aligned}
$$

Herein, the constant D equals

$$
D = C s^{|l|} \times C' s^{|l'|} \times s^{2|k|-n-1} \times \left(\frac{s}{2}\right)^n = \frac{C C' s^{|l|+|l'|+2|k|-1}}{2^n}. \qquad (3.36)
$$

The first two factors come from (3.28), the third factor comes from the transformed weight function (3.25), and the last factor originates from the Jacobian (3.18) of the transformation.

Notice that p_i^- equals a_i when $l_j = l_j'$ for the nodes in the left subtree of v_i. An analogous argument applies to p_i^+ and b_i. Suppose one computes the product of integrals (3.35) in the indicated order. At the moment that one is dealing with the integral involving v_i, the situation is so that I is zero if there is a $j<i$ so that $l_j \neq l_j'$. Therefore, we can at that moment assume that $a_i = p_i^-$ and $b_i = p_i^+$, and apply orthogonality (3.27) of the Jacobi polynomials, implying that l_i should equal l_i' in order to have a nonzero value of the integral I.

From (3.35) and (3.27) we have that

$$
\begin{aligned}
\int_{T_s^n} R_l^{(k)}(x) R_{l'}^{(k)}(x) w^{(k)}(x)\, dx &= D \prod_{i=1}^{n} \int_{-1}^{1} P_{l_i}^{(a_i,b_i)}(v_i) P_{l_i'}^{(a_i',b_i')}(v_i) \left(\frac{1-v_i}{2}\right)^{p_i^-} \left(\frac{1+v_i}{2}\right)^{p_i^+} dv_i \\
&= \delta_{l,l'} D \prod_{i=1}^{n} \frac{2\Gamma(l_i+a_i+1)\Gamma(l_i+b_i+1)}{(2l_i+a_i+b_i+1) l_i! \Gamma(l_i+a_i+b_i+1)} \\
&= \delta_{l,l'} s^{2|l|+2|k|-1} \prod_{i=1}^{n} \frac{\Gamma(l_i+a_i+1)}{(a_i+1)_{l_i}} \frac{\Gamma(l_i+b_i+1)}{(b_i+1)_{l_i}} \\
&\quad \times \frac{1}{(2l_i+a_i+b_i+1)\Gamma(l_i+a_i+b_i+1)(l_i+a_i+b_i+1)_{l_i}} \\
&= \delta_{l,l'} s^{2|l|+2|k|-1} \prod_{i=1}^{n} \frac{\Gamma(a_i+1)\Gamma(b_i+1)}{\Gamma(2l_i+a_i+b_i+2)} \\
&= \delta_{l,l'} \frac{s^{2|l|+2|k|-1}}{\Gamma(2|k|+2|l|)} \prod_{i=1}^{n+1} \Gamma(2k_i). \qquad (3.37)
\end{aligned}
$$

The last equation follows from the previous one by induction on n, using the result on the left and right subtree.

We thus have proved that with every binary coupling on n internal nodes there is an associated polynomial $R_l^{(k)}(x)$ in n variables that is orthogonal on the simplex T_s^n for the weight function $w^{(k)}(x)$.

As final comment, for $n=2$ the polynomials constructed here are due to Proriol.[16] The polynomials $R_l^{(k)}(x)$ associated with the special binary coupling tree in the shape of a *spine*[14] were already constructed in Ref. 17. The polynomials $R_l^{(k)}(x)$ associated with a general binary tree were also studied by Rosengren[18] in the context of multilinear Hankel forms. In his approach, orthogo-

nality of these polynomials follows quite easily. His methods, however, are less accessible for a mathematical physicist. Furthermore, the relation to classical $3nj$-coefficients (see Sec. V) is more explicit here.

IV. ORTHOGONAL POLYNOMIALS RELATED TO CONTINUOUS HAHN POLYNOMIALS

The notation in this section is as before, i.e., k stands for $(k_1,\ldots,k_{n+1})$ and l for $(l_1,\ldots,l_n)$. But we will also need a notation for parts of the components, so $\mathbf{k}_m=(k_1,\ldots,k_m)$, $\mathbf{k}^m=(k_m,\ldots,k_{n+1})$ [and similarly for $\mathbf{l}_m$ and $\mathbf{l}^m$, and $\mathbf{l}_m^j=(l_m,\ldots,l_j)$ $(m\leqslant j)$]. As usual, $|\mathbf{l}_m^j|=l_m+\cdots+l_j$.

In the way that a binary coupling tree defines $R_l^{(k)}(x)$ as a product of S-polynomials (Jacobi polynomials), we define new polynomials $\mathcal{R}_l^{(k)}(x)$ as the same product of $\mathcal{S}$-polynomials (continuous Hahn polynomials). In this section, we will prove the following theorem.

Theorem 16: *With every coupling of* $(n+1)$ su(1,1) *representations* $k_1,\ldots,k_{n+1}$, *i.e., with every binary coupling tree with n internal nodes, we associate a set of polynomials* $\mathcal{R}_l^{(k)}(x)$ *in n variables. This set is orthogonal on* $\mathbb{R}^n$ *for the weight function*

$$w^{(k)}(x)=\Gamma(k_1\pm ix_1)\cdots\Gamma(k_n\pm ix_n)\Gamma(k_{n+1}\pm i(s-|x|)). \tag{4.1}$$

Explicitly, the orthogonality reads

$$\int_{\mathbb{R}^n}\mathcal{R}_l^{(k)}(x)\mathcal{R}_{l'}^{(k)}(x)w^{(k)}(x)dx=\delta_{l,l'}(2\pi)^n\Gamma(|k|+|l|\pm is). \tag{4.2}$$

Recall that the $\mathcal{S}$-polynomials are defined by (2.10). The $\mathcal{S}$-polynomial in (2.10) is of degree m in the variables x_1 and x_2, but it is not homogeneous in these variables (see the proof of Lemma 19). This implies that the product $\mathcal{R}_l^{(k)}(x)$ is *not* homogeneous in the variables x_i, however, we still put $x_1+\cdots+x_{n+1}=s$. Note that this is consistent with the definition of the weight function (4.1).

Example 17: With the binary coupling tree shown in Fig. 2 we associate the following polynomial (before the replacement of x_5 by $s-x_1-x_2-x_3-x_4$):

$$\begin{aligned}
&\mathcal{R}(x_1,x_2,x_3,x_4,x_5)\\
&\quad=\mathcal{S}_{l_1}^{k_1,k_2}(x_1,x_2)\mathcal{S}_{l_2}^{k_{12},k_3}(x_1+x_2,x_3)\mathcal{S}_{l_3}^{k_4,k_5}(x_4,x_5)\mathcal{S}_{l_4}^{k_{123},k_{45}}(x_1+x_2+x_3,x_4+x_5)\\
&\quad=C\times p_{l_1}(x_1;k_1,k_2-i(x_1+x_2),k_1,k_2+i(x_1+x_2))\\
&\qquad\times p_{l_2}(x_1+x_2;k_1+k_2+l_1,k_3-i(x_1+x_2+x_3),k_1+k_2+l_1,k_3+i(x_1+x_2+x_3))\\
&\qquad\times p_{l_3}(x_4;k_4,k_5-i(x_4+x_5),k_4,k_5+i(x_4+x_5))\\
&\qquad\times p_{l_4}(x_1+x_2+x_3;k_1+k_2+k_3+l_1+l_2,k_4+k_5+l_3-i(x_1+x_2+x_3+x_4+x_5),\\
&\qquad\ k_1+k_2+k_3+l_1+l_2,k_4+k_5+l_3+i(x_1+x_2+x_3+x_4+x_5)),
\end{aligned}$$

where C is some numerical factor that can be computed from (2.10). The subscripts l_i are the same as before. ■

It is well known that the continuous Hahn polynomials, appearing in the definition of the $\mathcal{S}$-polynomials, are orthogonal on $\mathbb{R}$ for the weight function $\Gamma(a+it)\Gamma(b+it)\Gamma(c-it)\Gamma(d-it)$ when $\Re(a,b,c,d)>0$, $c=\overline{a}$ and $d=\overline{b}$:

$$\int_{\mathbb{R}} \Gamma(a+it)\Gamma(b+it)\Gamma(c-it)\Gamma(d-it)p_m(t;a,b,c,d)p_j(t;a,b,c,d)dt$$
$$= 2\pi\delta_{m,j}\frac{\Gamma(j+a+c)\Gamma(j+b+d)\Gamma(j+a+d)\Gamma(j+b+c)}{j!(2j+a+b+c+d-1)\Gamma(j+a+b+c+d-1)}. \tag{4.3}$$

Using this orthogonality relation, (4.2) is easily established in the case $n=1$.

To investigate the general case, we introduce new variables u, but use a different approach than the one in the previous section. We do not define the variables u as the arguments of the continuous Hahn polynomials in the product, but we introduce essentially only one new variable, namely $x_1+\cdots+x_{nl_n}=y$ (and thus $x_{nl_n+1}+\cdots+x_{n+1}=s-y$). Here, we assumed for simplicity that the variables associated with the leaves in the left subtree are $x_1,\ldots,x_{nl_n}$. This will enable us to use induction on n. Again, it is constructive to consider first an example.

Example 18: For the tree in Fig. 2, we define the variables u_i as follows:

$$u_1=x_1, \quad u_2=x_2, \quad u_3=x_1+x_2+x_3, \quad u_4=x_4.$$

We thus leave all the variables x unchanged, except the rightmost variable of the left subtree (in this case thus x_3). We choose the sum of all the variables in the left subtree equal to a new variable (in this case u_3). Integrating last to this variable allows this variable to be viewed as a constant in the integrands of the other integrals, enabling us to use induction.

When integrating last to u_3, the integral becomes

$$\int_{\mathbb{R}^4} \mathcal{R}_l^{(k)}(x)\mathcal{R}_{l'}^{(k)}(x)w^{(k)}(x)dx$$
$$= \sqrt{\frac{l_4!(2|l|+2|k|-1)\Gamma(l_4+2|k|+2|\mathbf{l}_3|-1)}{\Gamma(l_4+2|\mathbf{k}_3|+2|\mathbf{l}_2|)\Gamma(l_4+2|\mathbf{k}^4|+2l_3)}}$$
$$\times \sqrt{\frac{l_4'!(2|l'|+2|k|-1)\Gamma(l_4'+2|k|+2|\mathbf{l}_3'|-1)}{\Gamma(l_4'+2|\mathbf{k}_3|+2|\mathbf{l}_2'|)\Gamma(l_4'+2|\mathbf{k}^4|+2l_3')}}$$
$$\times \int_{\mathbb{R}} p_{l_4}(u_3;|\mathbf{k}_3|+|\mathbf{l}_2|,|\mathbf{k}^4|+l_3-is,|\mathbf{k}_3|+|\mathbf{l}_2|,|\mathbf{k}^4|+l_3+is)$$
$$\times p_{l_4'}(u_3;|\mathbf{k}_3|+|\mathbf{l}_2'|,|\mathbf{k}^4|+l_3'-is,|\mathbf{k}_3|+|\mathbf{l}_2'|,|\mathbf{k}^4|+l_3'+is)I_{\text{left}}I_{\text{right}}du_3,$$

with

$$I_{\text{left}}= \sqrt{\frac{l_1!(2l_1+2|\mathbf{k}_2|-1)\Gamma(l_1+2|\mathbf{k}_2|-1)}{\Gamma(l_1+2k_1)\Gamma(l_1+2k_2)}}\sqrt{\frac{l_1'!(2l_1'+2|\mathbf{k}_2|-1)\Gamma(l_1'+2|\mathbf{k}_2|-1)}{\Gamma(l_1'+2k_1)\Gamma(l_1'+2k_2)}}$$
$$\times \sqrt{\frac{l_2!(2|\mathbf{l}_2|+2|\mathbf{k}_3|-1)\Gamma(l_2+2|\mathbf{k}_3|+2l_1-1)}{\Gamma(l_2+2|\mathbf{k}_2|+2l_1)\Gamma(l_2+2k_3)}}$$
$$\times \sqrt{\frac{l_2'!(2|\mathbf{l}_2'|+2|\mathbf{k}_3|-1)\Gamma(l_2'+2|\mathbf{k}_3|+2l_1'-1)}{\Gamma(l_2'+2|\mathbf{k}_2|+2l_1')\Gamma(l_2'+2k_3)}}$$
$$\times \int_{\mathbb{R}^2} p_{l_1}(u_1;k_1,k_2-i|\mathbf{u}_2|,k_1,k_2+i|\mathbf{u}_2|)p_{l_1'}(u_1;k_1,k_2-i|\mathbf{u}_2|,k_1,k_2+i|\mathbf{u}_2|)$$
$$\times p_{l_2}(|\mathbf{u}_2|;|\mathbf{k}_2|+l_1,k_3-iu_3,|\mathbf{k}_2|+l_1,k_3+iu_3)p_{l_2'}(|\mathbf{u}_2|;|\mathbf{k}_2|+l_1',k_3-iu_3,|\mathbf{k}_2|+l_1',k_3+iu_3)$$
$$\times \Gamma(k_1\pm iu_1)\Gamma(k_2\pm iu_2)\Gamma(k_3\pm i(u_3-|\mathbf{u}_2|))du_1du_2.$$

The integral I_{left} thus corresponds to the orthogonality relation (4.2) restricted to the left subtree of the tree in Fig. 2 and with s replaced by u_3. By induction, the value of this integral is

$$I_{\text{left}}=\delta_{l_1,l_1'}\delta_{l_2,l_2'}(2\pi)^2\Gamma(|\mathbf{k}_3|+|\mathbf{l}_2|\pm iu_3).$$

The integral I_{right} equals

$$\begin{aligned}I_{\text{right}}=&\sqrt{\frac{l_3!(2l_3+2|\mathbf{k}^4|-1)\Gamma(l_3+2|\mathbf{k}^4|-1)}{\Gamma(l_3+2k_4)\Gamma(l_3+2k_5)}}\sqrt{\frac{l_3'!(2l_3'+2|\mathbf{k}^4|-1)\Gamma(l_3'+|\mathbf{k}^4|-1)}{\Gamma(l_3'+2k_4)\Gamma(l_3'+2k_5)}}\\&\times\int_{\mathbb{R}}p_{l_3}(u_4;k_4,k_5-i(s-u_3),k_4,k_5+i(s-u_3))p_{l_3'}(u_4;k_4,k_5-i(s-u_3),k_4,\\&k_5+i(s-u_3))\Gamma(k_4\pm iu_4)\Gamma(k_5\pm i(s-u_3-u_4))du_4.\end{aligned}\tag{4.4}$$

The integral I_{right} corresponds to the orthogonality relation (4.2) restricted to the right subtree with s replaced by $s-u_3$. The value of this integral is thus

$$I_{\text{right}}=\delta_{l_3,l_3'}2\pi\Gamma(|\mathbf{k}^4|+l_3\pm i(s-u_3)).$$

Using the values of I_{left} and I_{right} enables us to use the orthogonality of the continuous Hahn polynomials when integrating over u_3, yielding the following:

$$\int_{\mathbb{R}^4}\mathcal{R}_l^{(k)}(x)\mathcal{R}_{l'}^{(k)}(x)w^{(k)}(x)dx=\delta_{l,l'}(2\pi)^4\Gamma(|k|+|l|\pm is).$$ ■

In the general case, assume that the variables associated with the leaves of the tree are (from left to right) $x_1,\ldots,x_{n+1}$. Define the variables u as follows:

$$u_j=x_j,\quad j\in\{1,\ldots,n\}\backslash nl_n\quad\text{and}\quad u_{nl_n}=x_1+\cdots+x_{nl_n}.\tag{4.5}$$

It is clear that the absolute value of the Jacobian of this transformation is 1 and that $u\in\mathbb{R}^n\Leftrightarrow x\in\mathbb{R}^n$.

Continuous Hahn polynomials associated with internal nodes of the left subtree only involve variables $x_1,\ldots,x_{nl_n}$, as do the gamma functions of the weight function associated with the leaves of the left subtree. Replacing x_{nl_n} by $u_{nl_n}-u_1-\cdots-u_{nl_n-1}$ [see (4.5)] yields an integral over $\mathbb{R}^{nl_n-1}$ involving the variables $u_1,\ldots,u_{nl_n-1}$, and with u_{nl_n} playing the role of s. The way in which this integral is constructed allows induction. Denoting this integral by I_{left}, we have

$$I_{\text{left}}=\delta_{\mathbf{l}_{nl_n-1},\mathbf{l}'_{nl_n-1}}(2\pi)^{nl_n-1}\Gamma(|\mathbf{k}_{nl_n}|+|\mathbf{l}_{nl_n-1}|\pm iu_{nl_n}).\tag{4.6}$$

On the other hand, continuous Hahn polynomials associated with internal nodes in the right subtree involve variables $x_{nl_n+1},\ldots,x_n$, but may also involve variables $x_1,\ldots,x_{nl_n}$. When the latter is the case, it is always the difference $-(x_1+\cdots+x_{nl_n})=-u_{nl_n}$ which occurs. So essentially, s is replaced by $s-u_{nl_n}$; this integral involving the variables $u_{nl_n+1},\ldots,u_n$ can also be calculated by induction. Denoting this integral over $\mathbb{R}^{nr_n-1}$ by I_{right} we have

$$I_{\text{right}} = \delta_{\mathbf{l}_{nl_n}^{n-1},\mathbf{l}'^{n-1}_{nl_n}} (2\pi)^{nr_n-1} \Gamma(|\mathbf{k}^{nl_n+1}| + |\mathbf{l}_{nl_n}^{n-1}| \pm i(s-u_{nl_n})). \tag{4.7}$$

The integral I, i.e., the left side of (4.2), then reduces to

$$\begin{aligned}
I &= \sqrt{\frac{l_n!(2|l|+2|k|-1)\Gamma(l_n+2|k|+2|\mathbf{l}_{n-1}|-1)}{\Gamma(l_n+2|\mathbf{k}_{nl_n}|+2|\mathbf{l}_{nl_n-1}|)\Gamma(l_n+2|\mathbf{k}^{nl_n+1}|+2|\mathbf{l}_{nl_n}^{n-1}|)}} \\
&\quad \times \sqrt{\frac{l'_n!(2|l'|+2|k|-1)\Gamma(l'_n+2|k|+2|\mathbf{l}'_{n-1}|-1)}{\Gamma(l'_n+2|\mathbf{k}_{nl_n}|+2|\mathbf{l}'_{nl_n-1}|)\Gamma(l'_n+2|\mathbf{k}^{nl_n+1}|+2|\mathbf{l}'^{n-1}_{nl_n}|)}} \int_{\mathbb{R}} p_{l_n}(u_{nl_n};|\mathbf{k}_{nl_n}|+|\mathbf{l}_{nl_n-1}|, \\
&\quad |\mathbf{k}^{nl_n+1}|+|\mathbf{l}_{nl_n}^{n-1}|-is,|\mathbf{k}_{nl_n}|+|\mathbf{l}_{nl_n-1}|,|\mathbf{k}^{nl_n+1}|+|\mathbf{l}_{nl_n}^{n-1}|+is) p_{l'_n}(u_{nl_n};|\mathbf{k}_{nl_n}|+|\mathbf{l}'_{nl_n-1}|, \\
&\quad |\mathbf{k}^{nl_n+1}|+|\mathbf{l}'^{n-1}_{nl_n}|-is,|\mathbf{k}_{nl_n}|+|\mathbf{l}'_{nl_n-1}|,|\mathbf{k}^{nl_n+1}|+|\mathbf{l}'^{n-1}_{nl_n}|+is) \times I_{\text{left}} \times I_{\text{right}} du_{nl_n} \\
&= \delta_{\mathbf{l}_{n-1},\mathbf{l}'_{n-1}} (2\pi)^{n-1} \sqrt{\frac{l_n!(2|l|+2|k|-1)\Gamma(l_n+2|k|+2|\mathbf{l}_{n-1}|-1)}{\Gamma(l_n+2|\mathbf{k}_{nl_n}|+2|\mathbf{l}_{nl_n-1}|)\Gamma(l_n+2|\mathbf{k}^{nl_n+1}|+2|\mathbf{l}_{nl_n}^{n-1}|)}} \\
&\quad \times \sqrt{\frac{l'_n!(2|l'|+2|k|-1)\Gamma(l'_n+2|k|+2|\mathbf{l}'_{n-1}|-1)}{\Gamma(l'_n+2|\mathbf{k}_{nl_n}|+2|\mathbf{l}'_{nl_n-1}|)\Gamma(l'_n+2|\mathbf{k}^{nl_n+1}|+2|\mathbf{l}'^{n-1}_{nl_n}|)}} \int_{\mathbb{R}} p_{l_n}(u_{nl_n};|\mathbf{k}_{nl_n}|+|\mathbf{l}_{nl_n-1}|, \\
&\quad |\mathbf{k}^{nl_n+1}|+|\mathbf{l}_{nl_n}^{n-1}|-is,|\mathbf{k}_{nl_n}|+|\mathbf{l}_{nl_n-1}|,|\mathbf{k}^{nl_n+1}|+|\mathbf{l}_{nl_n}^{n-1}|+is) \\
&\quad \times p_{l'_n}(u_{nl_n};|\mathbf{k}_{nl_n}|+|\mathbf{l}'_{nl_n-1}|,|\mathbf{k}^{nl_n+1}|+|\mathbf{l}'^{n-1}_{nl_n}|-is,|\mathbf{k}_{nl_n}|+|\mathbf{l}'_{nl_n-1}|,|\mathbf{k}^{nl_n+1}|+|\mathbf{l}'^{n-1}_{nl_n}|+is) \\
&\quad \times \Gamma(|\mathbf{k}_{nl_n}|+|\mathbf{l}_{nl_n-1}| \pm iu_{nl_n}) \Gamma(|\mathbf{k}^{nl_n+1}|+|\mathbf{l}_{nl_n}^{n-1}| \pm i(s-u_{nl_n})) du_{nl_n} \\
&= \delta_{l,l'} (2\pi)^n \Gamma(|k|+|l| \pm is).
\end{aligned}$$

Once again, we have used the orthogonality (4.3) of continuous Hahn polynomials. This completes the proof of Theorem 16.

V. CONNECTION COEFFICIENTS BETWEEN DIFFERENT BASES OF ORTHOGONAL POLYNOMIALS

We will show that the set of polynomials associated with a *fixed* binary coupling tree and *fixed* leaf values k_j, but varying values l_i, form a basis for Π^n.

Lemma 19: For any binary coupling tree T the degree of the polynomial $R_l^{(k)}(x)$ (*or* $\mathcal{R}_l^{(k)}(x)$) *associated with T is* $|l|$.

Proof: In the case of Jacobi polynomials, i.e., the case of S-polynomials, the result immediately follows from the fact that $S_m^{k_1,k_2}(x_1,x_2)$ is homogeneous of degree m in the variables x_1 and x_2.

Now consider the case of continuous Hahn polynomials. Although $p_m(t;a,b,c,d)$ is a polynomial of degree m in t, we have to be careful because, in the case of $\mathcal{S}$-polynomials, the variables x_i also appear in the parameters b and d. The polynomials associated with an internal node not on the path from the leaf x_{n+1} to the root are, up to a constant factor, $p_m(x;a,b-i(x+y),a,b+i(x+y))$ (x and y stand for a sum of variables x_j). Using the definition of the continuous Hahn polynomials we have

$$
\begin{aligned}
&p_m(x;a,b-i(x+y),a,b+i(x+y))\\
&\quad=i^m\frac{(2a)_m(a+b+i(x+y))_m}{m!}\,{}_3F_2\left(\begin{matrix}-m,m+2a+2b-1,a+ix\\ 2a,a+b+i(x+y)\end{matrix};1\right)\\
&\quad=i^m\frac{(2a)_m(a+b+i(x+y))_m}{m!}\sum_{j=0}^{m}\frac{(-m)_j(m+2a+2b-1)_j(a+ix)_j}{(2a)_j(a+b+i(x+y))_j j!}\\
&\quad=i^m\frac{(2a)_m}{m!}\sum_{j=0}^{m}\frac{(-m)_j(m+2a+2b-1)_j(a+ix)_j(a+b+i(x+y)+j)_{m-j}}{(2a)_j j!}.
\end{aligned}
$$

From this last equation one sees that the degree of this polynomial is at most m. It is easy to see that the coefficient of y^m is $(i^{2m}(2a)_m/m!)\neq 0$, since in our case $a>0$. The same can be done for a polynomial associated with an internal node on the path from x_{n+1} to the root. □

Theorem 20: *The polynomials* $R_l^{(k)}(x)$ and $\mathcal{R}_l^{(k)}(x)$ *associated with a fixed binary coupling tree* T *on* n *internal nodes form a basis for* Π^n.

Proof: Theorems 4 and 16 imply that the sets of polynomials associated with T are linearly independent.

The number of polynomials associated with T that have degree m equals the number of compositions $J(m,n)$ of m into n parts, i.e., the number of ways that one can write m as a sum of n non-negative integers whereby the order of the summands is important. There are thus $\Sigma_{k=0}^{m}J(k,n)$ polynomials of degree at most m associated with T. It is not difficult to see that this is exactly the dimension of Π_m^n, the set of polynomials in n variables with degree at most m. □

We recall the two properties (2.11) and (2.12) of the $\mathcal{S}$-polynomials. We can use these two properties to determine the connection coefficients between the different bases. This is stated in the following theorem.

Theorem 21: *Consider a binary coupling tree,* T_1, *with fixed values* k_j *and* l_i. *Consider another binary coupling tree* T_2 *with the same fixed values* k_j *but varying values* l_i', *such that* $|l|=|l'|$. *Then the polynomials* $R_{l,T_1}^{(k)}(x)$ [*resp.* $\mathcal{R}_{l,T_1}^{(k)}(x)$] *can be written as a linear combination of polynomials* $R_{l',T_2}^{(k)}(x)$ (*resp.* $\mathcal{R}_{l',T_2}^{(k)}$):

$$
R_{l,T_1}^{(k)}(x)=\sum_{|l'|=|l|}C_{l'}R_{l',T_2}^{(k)}(x);\quad \mathcal{R}_{l,T_1}^{(k)}(x)=\sum_{|l'|=|l|}C_{l'}\mathcal{R}_{l',T_2}^{(k)}(x). \tag{5.1}
$$

The connection coefficient $C_{l'}$ *is equal to the* 3nj*-coefficient* $\langle T_1(l),T_2(l')\rangle$ *(which is zero anyway if* $|l|\neq|l'|$).

Proof: This follows from Theorem 20 and the two basic properties of S- and $\mathcal{S}$-polynomials. These basic properties are given in (2.11) and (2.12). Observe that (2.11) simply expresses

$$
\mathcal{R}_{(l_1,l_2),T_1}^{(k_1,k_2,k_3)}(x_1,x_2)=\sum_{|l'|=|l|}U_{k_3,|k|+|l|,k_2+k_3+l_1'}^{k_1,k_2,k_1+k_2+l_1}\mathcal{R}_{(l_1',l_2'),T_2}^{(k_1,k_2,k_3)}(x_1,x_2), \tag{5.2}
$$

where T_1 (resp. T_2) is the tree on the left hand side (resp. right hand side) of Fig. 1 with $k_{12}=k_1+k_2+l_1$ and $k_0=|k|+|l|$ (resp. with $k_{23}=k_2+k_3+l_1'$ and $k_0=|k|+|l'|$). By definition the Racah coefficient (or 6j-coefficient) can be expressed as the overlap coefficient of two binary coupling trees, i.e.,

$$
U_{k_3,|k|+|l|,k_2+k_3+l_1'}^{k_1,k_2,k_1+k_2+l_1}=\langle T_1(l),T_2(l')\rangle.
$$

In the general case, let T_1 (with fixed values k_j and l_i) and T_2 (with the same fixed values k_j) be given. The expansion of $\mathcal{R}_{l,T_1}^{(k)}(x)$ in terms of $\mathcal{S}$-polynomials is then fixed. In order to express $\mathcal{R}_{l,T_1}^{(k)}(x)$ in terms of polynomials associated with the second tree T_2, one can use (2.11) and (2.12)

a number of times. Equation (2.11) corresponds to an elementary tree operation (the flop operation of Ref. 13), depicted in Fig. 1. Equation (2.12) corresponds to an exchange operation[13] on trees. So, to express $\mathcal{R}^{(k)}_{l,T_1}(x)$ in terms of polynomials $\mathcal{R}^{(k)}_{l',T_2}(x)$, one has to perform sufficiently many elementary tree operations on T_1 until one ends up with a tree of shape T_2. Each such operation corresponds to an application of (2.11), introducing a Racah coefficient and a summation index, or to an application of (2.12), introducing only a phase factor. As a consequence, the coefficient $C_{l'}$ in (5.1) stands for a certain sum over products of Racah coefficients. But this sum over products of Racah coefficients is just the $3nj$-coefficient defined by the left and right binary coupling trees, since the ''method of trees'' [13,14] yields that the expansion of a $3nj$-coefficient in terms of Racah coefficients is obtained exactly by such elementary tree operations. □

Observe there are some alternative ways of expressing the previous results. For example, for two n-variable Jacobi polynomials corresponding to the same binary coupling tree, their inner product is given by (3.5). For two n-variable Jacobi polynomials with different binary coupling tree, the inner product is essentially given by a $3nj$-coefficient:

$$\int_{T_s^n} R^{(k)}_{l,T_1}(x) R^{(k)}_{l',T_2}(x) w^{(k)}(x)\,dx = \langle T_1(l), T_2(l')\rangle \frac{s^{2|k|+2|l|-1}}{\Gamma(2|k|+2|l|)} \prod_{i=1}^{n+1} \Gamma(2k_i), \tag{5.3}$$

where $w^{(k)}(x)$ is the classical weight function (3.4).

In the same way, we have for n-variable continuous Hahn polynomials corresponding to different binary coupling trees that

$$\int_{\mathbb{R}^n} \mathcal{R}^{(k)}_{l,T_1}(x) \mathcal{R}^{(k)}_{l',T_2}(x) w^{(k)}(x)\,dx = \langle T_1(l), T_2(l')\rangle (2\pi)^n \Gamma(|k|+|l| \pm is), \tag{5.4}$$

where in this case $w^{(k)}(x)$ is given by (4.1).

APPENDIX A: ORTHOGONALITY OF PRODUCTS OF WILSON POLYNOMIALS

In this appendix we show that the products of Wilson polynomials in (2.5) also satisfy an orthogonality relation on $\mathbb{R}^2$; thus also (2.5) can be interpreted as a connection coefficient formula.

When $\Re(a,b,c,d)>0$ and nonreal parameters occur in conjugate pairs, Wilson polynomials are orthogonal on $\mathbb{R}_+$ for the weight function $|\Gamma(a+ix)\Gamma(b+ix)\Gamma(c+ix)\Gamma(d+ix)/\Gamma(2ix)|^2$:

$$\begin{aligned}\int_0^\infty \left|\frac{\Gamma(a+ix)\Gamma(b+ix)\Gamma(c+ix)\Gamma(d+ix)}{\Gamma(2ix)}\right|^2 & W_m(x^2;a,b,c,d) W_j(x^2;a,b,c,d)\,dx \\ &= 2\pi \frac{\Gamma(j+a+b)\Gamma(j+a+c)\Gamma(j+a+d)\Gamma(j+b+c)\Gamma(j+b+d)\Gamma(j+c+d)}{\Gamma(2j+a+b+c+d)} \\ &\quad \times (j+a+b+c+d-1)_j\, j!\, \delta_{m,j},\end{aligned} \tag{A1}$$

see, e.g., Ref. 22.

Theorem 22: *The products of Wilson polynomials on both the left and right sides of Eq. (2.5) are orthogonal on* $\mathbb{R}^2$ *for the weight function*

$$\begin{aligned}&\Gamma(k_1 \pm ix_1)\Gamma(k_2 \pm ix_2)\Gamma(k_3 \pm i(s-x_1-x_2)) \\ &\quad \times \frac{\Gamma(k_1 \pm i(x_1-2t))\Gamma(k_2 \pm i(2x_1+x_2-2t))\Gamma(k_3 \pm i(s-2t+x_1+x_2))}{\Gamma(\pm 2ix_1 \mp 2it)\Gamma(\pm 2ix_1 \pm 2ix_2 \mp 2it)},\end{aligned} \tag{A2}$$

if $k_1,k_2,k_3>0$.

Following the convention mentioned earlier, each factor in (A2) stands for the product of two gamma functions.

Proof: Consider the polynomial on the right side of (2.5). The parameters of the Wilson polynomials occur in conjugate pairs and the real parts of the parameters are positive. This allows us to use the orthogonality relation (A1).

Denoting the weight function (A2) by $w(x_1,x_2)$, we want to determine the value of

$$\begin{aligned}\int \int_{\mathbb{R}^2} & w(x_1,x_2) W_m((x_1-t)^2;k_1\pm it,k_2\pm i(x_1+x_2-t)) \\ & \times W_{m'}((x_1-t)^2;k_1\pm it,k_2\pm i(x_1+x_2-t)) \\ & \times W_j((x_1+x_2-t)^2;k_1+k_2+m\pm it,k_3\pm i(s-t)) \\ & \times W_{j'}((x_1+x_2-t)^2;k_1+k_2+m'\pm it,k_3\pm i(s-t))dx_1dx_2.\end{aligned}$$

The notation is obvious: each entry of the form $k_1\pm it$ stands for two parameters of the Wilson polynomial. In order to compute the integral, introduce two new variables, namely the arguments of the Wilson polynomials: $u_1=x_1-t$ and $u_2=x_1+x_2-t$. Changing variables and integrating first with respect to u_1 and then with respect to u_2 gives a constant times $\delta_{m,m'}\delta_{j,j'}$ for the above integral, if we use the facts that $\Gamma(\overline{z})=\overline{\Gamma(z)}$ and that the integrands are even functions.

Similar arguments yield the desired result for the Wilson polynomials on the left side of (2.5). □

APPENDIX B: PROOF OF LEMMA 11

In this appendix we prove Lemma 11. First, we show that if $x\in T_s^n$, then $-1<v_i<1$ for each v_i given by (3.9). The position of the variable v_i in the binary coupling tree plays a role in its expression. For a variable v_i not on the path from x_{n+1} to the root of the tree, the equation expressing v_i in terms of x is

$$v_i=\left(\sum_{\substack{\text{right leaves}\\ \text{of } v_i}} x_j-\sum_{\substack{\text{left leaves}\\ \text{of } v_i}} x_j\right)\Bigg/\sum_{\substack{\text{all leaves}\\ \text{of } v_i}} x_j,$$

which is of the form $f(y,z)=(y-z)/(y+z)$ with $0<y$, $0<z$ (and $y+z<s$). It is easy to see that $-1<f(y,z)<1$ if $y,z>0$. On the other hand, if v_i is on the path from x_{n+1} to the root, we have, after substitution of x_{n+1} by $s-|x|$, that

$$v_i=\left(s-\sum_{\substack{\text{non-leaves}\\ \text{of } v_i}} x_j-2\sum_{\substack{\text{left leaves}\\ \text{of } v_i}} x_j\right)\Bigg/\left(s-\sum_{\substack{\text{non-leaves}\\ \text{of } v_i}} x_j\right),$$

which is of the form $g(y,z)=(s-y-2z)/(s-y)$ with $0<y$, $0<z$ and $y+z<s$. A simple examination shows that $g(y,z)$ reaches its maximum $+1$ in this area when $z=0$, and its minimum -1 when $y+z=s$. Thus $-1<g(y,z)<1$ for $y,z>0$ with $y+z<s$. So we have that $-1<v_i<1$ for each $1\leqslant i<n$. For the variable v_n a completely analogous reasoning can be given.
Before proving $v\in\square^n\Rightarrow x\in T_s^n$ in general, consider an example.

Example 23: Let $v\in\square^4$ and consider Eqs. (3.7) with x_5 replaced by $s-x_1-x_2-x_3-x_4$:

$$\begin{aligned} v_1&=(x_2-x_1)/(x_2+x_1),\\ v_2&=(x_3-x_1-x_2)/(x_3+x_1+x_2),\\ v_3&=(s-x_1-x_2-x_3-2x_4)/(s-x_1-x_2-x_3),\\ v_4&=(s-2x_1-2x_2-2x_3)/s.\end{aligned} \tag{B1}$$

Since $-1<v_4<1$, the fourth equation of (B1) implies

$$-1<v_4<1\Rightarrow 0<x_1+x_2+x_3<s. \tag{B2}$$

The denominator of the second equation of (B1) is thus positive, and

$$-1<v_2\Rightarrow x_3>0 \quad \text{and} \quad v_2<1\Rightarrow x_1+x_2>0, \tag{B3}$$

hence

$$-1<v_1\Rightarrow x_2>0 \quad \text{and} \quad v_1<1\Rightarrow x_1>0. \tag{B4}$$

From (B2) it also follows that the denominator of the third equation of (B1) is positive, implying

$$-1<v_3\Rightarrow x_1+x_2+x_3+x_4<s \quad \text{and} \quad v_3<1\Rightarrow x_4>0. \tag{B5}$$

So we clearly have $v\in\square^4\Rightarrow x\in T_s^4$. ■

In general, let $v\in\square^n$. We know that

$$v_n=\left(s-2\sum_{\substack{\text{left leaves}\\ \text{of } v_n}} x_j\right)\Big/ s,$$

with $s>0$, and thus

$$-1<v_n<1\Rightarrow 0<\sum_{\substack{\text{left leaves}\\ \text{of } v_n}} x_j<s. \tag{B6}$$

Now consider the variable associated with the left child of v_n, that is, v_{nl_n-1}:

$$v_{nl_n-1}=\left(\sum_{\substack{\text{right leaves}\\ \text{of } v_{nl_n-1}}} x_j-\sum_{\substack{\text{left leaves}\\ \text{of } v_{nl_n-1}}} x_j\right)\Big/ \sum_{\substack{\text{all leaves}\\ \text{of } v_{nl_n-1}}} x_j.$$

From (B6) we know that the denominator of the previous formula is positive, and we have

$$-1<v_{nl_n-1}\Rightarrow \sum_{\substack{\text{right leaves}\\ \text{of } v_{nl_n-1}}} x_j>0 \tag{B7}$$

and

$$v_{nl_n-1}<1\Rightarrow \sum_{\substack{\text{left leaves}\\ \text{of } v_{nl_n-1}}} x_j>0. \tag{B8}$$

Continuing in this way for all internal nodes of the left subtree (in *in-order*[25]) yields that $x_j>0$ for every variable in the left subtree, since

$$-1<\frac{y-z}{y+z}<1\Rightarrow y>0 \quad \text{and} \quad z>0,$$

if $y+z>0$.

Consider the variable associated with the right child of v_n, i.e., v_{n-1}. For v_{n-1} we have the following expression:

$$v_{n-1}=\left(s-\sum_{\substack{\text{non-leaves}\\ \text{of } v_{n-1}}}x_j-2\sum_{\substack{\text{left leaves}\\ \text{of } v_{n-1}}}x_j\right)\Big/\left(s-\sum_{\substack{\text{non-leaves}\\ \text{of } v_{n-1}}}x_j\right).$$

The ''non-leaves of v_{n-1}'' are exactly the ''left leaves of v_n,'' so from (B6) we have once again that the denominator of the previous formula is positive. We thus have

$$-1<v_{n-1}\Rightarrow\sum_{\substack{\text{non-leaves}\\ \text{of } v_{n-1}}}x_j+\sum_{\substack{\text{left leaves}\\ \text{of } v_{n-1}}}x_j<s, \tag{B9}$$

and

$$v_{n-1}<1\Rightarrow\sum_{\substack{\text{left leaves}\\ \text{of } v_{n-1}}}x_j>0. \tag{B10}$$

Starting from this last equation, we can perform the same actions as in the left subtree to conclude that $x_j>0$ for all leaves in the left subtree of v_{n-1}. Continuing in this way we get that $x_j>0$, for $j=1,\ldots,n$ and $|x|<s$, since

$$-1<\frac{s-y-2z}{s-y}<1\Rightarrow y+z<s \quad\text{and}\quad z>0,$$

if $s-y>0$. This completes the proof that $v\in\square^n\Rightarrow x\in T_s^n$.

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Jacobson generators, Fock representations and statistics of *sl*(n+1)

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The properties of A-statistics, related to the class A of simple Lie algebras [T. D. Palev, preprint JINR E17-10550 (1977); hep-th/9705032], are further investigated. The description of each $sl(n+1)$ is carried out via generators $a_1^{\pm},\ldots,a_n^{\pm}$, which we call Jacobson generators. With respect to these generators, the definition of a Fock space of $sl(n+1)$ is given. It is proved that the Fock spaces W_p, $p\in\mathbb{N}$ are the simple symmetric (finite-dimensional) modules of $sl(n+1)$. The Pauli principle of the underlying statistics is formulated. Within each W_p operators $B(p)_i^{\pm}=a_i^{\pm}/\sqrt{p}$ $(i=1,\ldots,n)$, called quasi-Bose creation and annihilation operators (CAOs), are defined. Then $\lim_{p\to\infty}B(p)_i^{\pm}=B_i^{\pm}$, where $B_i^{\pm}$ are ordinary Bose CAOs. Therefore A-statistics appears as an approximation of Bose statistics with CAOs acting in finite-dimensional state spaces. We indicate that the $p=1$ quasi-Bose operators $B(1)_1^{\pm},\ldots,B(1)_n^{\pm}$ are natural operators for the description of hard-core Bose models and of the related Heisenberg spin models. We argue that (up to a certain natural assumption) A-statistics can be interpreted as an exclusion statistics. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1481544]

I. INTRODUCTION

During the last two decades quantum statistics became a field of increasing interest among field theorists and condensed matter theorists. Various new statistics were suggested, leading to generalizations or deviations from some of the first principles in quantum physics, such as the Heisenberg commutation relations, the Pauli exclusion principle, and the commutativity of space–time.

The literature on the subject is vast, especially in the part related to quantum groups.[1–5] In a paper entitled "Twisted second quantization," [6] Pusz and Woronowicz introduced multimode deformed Bose creation and annihilation operators (CAOs), covariant under the action of the quantum group $U_q[sl(n)]$ (for n pairs of them). Another deformation with commuting modes of CAOs was proposed in Ref. 7; the link between them was established in Ref. 8. A third deformation, which for one mode of CAOs was known for many years,[9] the so-called quon algebra,[10] was defined as an associative algebra, subject to relations $a_i^- a_j^+ - q a_j^+ a_i^- = \delta_{ij}$. This generalization (note that no relations among only creation operators or among only annihilation operators are required) was in the origin of a model proposed for a verification of small violations of Bose–Fermi statistics in quantum field theory (QFT).[11] The quon statistics, which in the classification of Doplicher, Haag, and Roberts[12] belongs to the class of "infinite statistics," was studied by several authors[13] from different points of view (see Ref. 14 for further discussions and references).

Recently string theory was also involved in discussions on quantum statistics, the latter related

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to its prediction that Heisenberg's uncertainty principle has to be corrected at distances of order of the Planck length $k_P = 10^{-32}$ cm. Consequently there emerges an absolute minimum uncertainty in the measuring of any length.[15] These predictions motivated several authors to search for model independent arguments, leading to the same conclusions as string theory does (we refer to Ref. 16 for a survey on the subject). In particular it has been shown that the above-mentioned results can be reproduced on a purely kinematical level with appropriate deformations of the Heisenberg commutation relations,[17–20] i.e., of canonical quantum statistics. In all such cases the coordinates do not commute (see also Refs. 21–24), a result which is consistent with the spirit of noncommutative geometry.[25]

Turning to condensed matter physics we refer to anyons, ''particles'' with fractional statistics in two-dimensional systems.[26] The theoretical studies of this and other noncanonical statistics were strongly pushed forward after the discovery of the fractional quantum Hall effect in two-dimensional electron gases.[27] Its theoretical explanation led Laughlin[28] to the conclusion that there exist quasiparticles carrying fractional electric charges. The statistics of these particles (we write ''particles'' for the elementary excitations, the ''quasiparticles,'' when no confusion can arise) also turned out to be fractional statistics.[29]

A further breakthrough in the area of quantum statistics was marked with the 1991 paper of Haldane,[30] who proposed a generalized version of the Pauli exclusion principle. For only one kind of identical particles this new statistics, now called (fractional) exclusion statistics (ES), asserts that the change Δd in the dimension d of the single-particle Hilbert space is defined via the relation

$$\Delta d = -g \cdot \Delta N. \tag{1.1}$$

Here ΔN is an allowed increase of the number of particles. The constant g is called an exclusion statistics parameter.

Our approach to quantum statistics is strongly influenced by the ideas of Wigner, outlined in his 1950's work ''Do the equations of motion determine the quantum mechanical commutation relations?''[31] This was the first paper where it was clearly indicated that the canonical quantum statistics may, in principle, be generalized in a logically consistent way. Wigner demonstrated this on the example of a one-dimensional oscillator with a Hamiltonian $(m=\omega=\hbar=1)$ $H=\frac{1}{2}(p^2+q^2)$. Abandoning the requirement $[p,q]=-i$, Wigner was searching for all operators q and p, such that the ''classical'' equations of motion $\dot{p}=-q$, $\dot{q}=p$ are identical to the Heisenberg equations $\dot{p}=-i[p,H]$, $\dot{q}=-i[q,H]$. Apart from the canonical solution he found infinitely many other solutions. Let $\sqrt{2}B_1^{\pm}=q\mp ip$. It turns out[32] that all these different operators satisfy one and the same triple relation, namely (1.2) with $i=j=k=1$ (see the end of this section for the notation):

$$[\{B_i^{\xi},B_j^{\eta}\},B_k^{\epsilon}]=\delta_{ik}(\epsilon-\xi)B_j^{\eta}+\delta_{jk}(\epsilon-\eta)B_i^{\xi}, \quad i,j,k\in\mathbb{N}, \quad \xi,\eta,\epsilon=\pm, \quad \pm 1. \tag{1.2}$$

The operators $B_i^{\pm}$, $i=1,2,\ldots$ are para-Bose (pB) operators, discovered by Green[33] three years later as a possible generalization of statistics of tensor fields in QFT. Thus the infinitely many different solutions found by Wigner were in fact the Fock representations of one pair of para-Bose operators.

It is known that the linear span of all operators B_i^{ξ}, $\{B_j^{\eta},B_k^{\epsilon}\}$ is a Lie superalgebra[34] isomorphic to the orthosymplectic Lie superalgebra $osp(1/2n)$ for $i,j,k=1,\ldots,n$ and $\xi,\eta,\epsilon=\pm$.[35] The para-Bose operators constitute a basis in the odd subspace of this superalgebra and generate it. Consequently the representation theory of n pairs of pB operators is completely equivalent to the representation theory of $osp(1/2n)$. Hence Wigner found all Fock representations of $osp(1/2)$ long before Lie superalgebras (and supersymmetry) became of interest in physics.

Similarly, any n pairs of para-Fermi CAOs $F_1^{\pm},F_2^{\pm},\ldots,F_n^{\pm}$,[33] defined by

$$[[F_i^{\xi},F_j^{\eta}],F_k^{\epsilon}]=\tfrac{1}{2}\delta_{jk}(\epsilon-\eta)^2F_i^{\xi}-\tfrac{1}{2}\delta_{ik}(\epsilon-\xi)^2F_j^{\eta}, \quad i,j,k\in\mathbb{N}, \quad \xi,\eta,\epsilon=\pm, \quad \pm 1, \tag{1.3}$$

generate the Lie algebra $so(2n+1)$.[36,37] The key observation here is that both $so(2n+1)$ and $osp(1/2n)$ belong to class B of the basic Lie superalgebras in the classification of Kac.[38] Hence parastatistics (and in particular Bose and Fermi statistics) appear as particular Fock representations of Lie superalgebras from one and the same class, the Lie superalgebras of class B. In this sense Green's parastatistics could be called B-(para)statistics.

The clarification of the mathematical structure, hidden in parastatistics, provides a natural background for further searches of new quantum statistics. One such possibility is to consider deformations of parastatistics, namely deformations of $so(2n+1)$ and $osp(1/2n)$ in the sense of quantum groups. We refer to Ref. 39 for discussions and results along this line. Note that parastatistics associated with $so(2n+1)$ (parafermions: finite dimensional representations) and with $osp(1/2n)$ (parabosons: infinite dimensional representations) are not related to the known correspondence between $so(2n+1)$ and $osp(1/2n)$[40,41] where only finite dimensional representations play a role.

In another approach, initiated in Ref. 42, it was shown that to each infinite class A, B, C, and D of simple Lie algebras there corresponds quantum statistics. Examples from classes A and B of proper Lie superalgebras are also available. We have in mind Wigner quantum systems (WQSs).[32] Some such systems possess quite unconventional physical features. As an example we mention the $(n+1)$-particle WQS, based on the Lie superalgebra $sl(1/3n)$ from class A.[43] This WQS exhibits a quark-like structure: the composite system occupies a small volume V around the center of mass and no particles can be extracted out of V. Moreover the geometry within V is noncommutative. Another example is the $osp(3/2)$ WQS from class B.[44] It leads to a picture where two spinless point particles, ''curling'' around each other, produce an orbital (internal angular) momentum 1/2, a result which cannot be obtained in canonical quantum mechanics.

The present paper is also in the frame of quantum statistics. We study further the (microscopic) properties of A-statistics, introduced in Ref. 42 (see also Ref. 45), namely the statistics of Lie algebras $A_n \equiv sl(n+1)$, $n=1,2,\ldots$. Since Refs. 42 and 45 are not available as journal publications, we review the main issues of A-statistics in Secs. II and III and partially in Sec. IV omitting most of the proofs.

We begin (Sec. II) by recalling how the Lie algebra $sl(n+1)$ can be described via generators $a_1^{\pm},\ldots,a_n^{\pm}$ and relations; see (2.5). These generators, which we call Jacobson generators (JG), provide an alternative to the Chevalley description of $sl(n+1)$.

The Fock modules of the Jacobson generators, extended also to $gl(n+1)$-modules, are defined and classified in Sec. III. It is shown how they can be selected out of all irreducible $gl(n+1)$-modules on the ground of natural physical requirements; see Definition 1. All Fock modules W_p are finite-dimensional and are labeled by one positive integer $p \in \mathbb{N}$. More precisely, the signature (the highest weight) of the $gl(n+1)$-module W_p is $(p,0,0,\ldots,0)$, or equivalently, the representation of $gl(n+1)$ in W_p is a symmetric representation. The definition of the Fock spaces is given in such a way that within W_p each generator a_i^+ (respectively, a_i^-) can be interpreted as an operator creating (respectively, annihilating) a ''particle'' in a state i (on the orbital i).

The Pauli principle for A-statistics in W_p is formulated in Sec. IV (Corollary 3). It states that any number of particles up to p and no more than p can be distributed in an arbitrary way along the orbitals. This restriction leads to properties typical for exclusion statistics.[30] We show that under a certain natural assumption the A-statistics can be interpreted as an exclusion statistics in the form of Wu.[46]

Next, in Sec. V, representation-dependent creation and annihilation operators $B(p)_i^{\pm} = a_i^{\pm}/\sqrt{p}\,(i=1,\ldots,n)$ in W_p are defined. We prove that in an appropriate topology $\lim_{p\to\infty} B(p)_i^{\pm} = B_i^{\pm}$, where $B_1^{\pm},\ldots,B_n^{\pm}$ are Bose creation and annihilation operators. The operators $B(p)_1^{\pm},\ldots,B(p)_n^{\pm}$ possess also other Bose-type properties. For these reasons $B(p)_1^{\pm},\ldots,B(p)_n^{\pm}$ are referred to as quasi-Bose operators (of order p), the representations of $sl(n+1)$ and $gl(n+1)$ in W_p as quasiboson representations and the statistics as quasi-Bose statistics.

The Jacobson CAOs $a_1^{\pm},\ldots,a_n^{\pm}$ are ''bosonized'' in Sec. VI. These operators are expressed via n pairs of Bose CAOs $B_1^{\pm},\ldots,B_n^{\pm}$. The related realization of $gl(n+1)$ in W_p turns out to be the known Holstein–Primakoff realization.[47]

In Sec. VII we point out that the quasi-Bose operators can also be of more general interest. On the example of a two-leg $S=1/2$ Heisenberg spin ladder we show that the Bose realization of the Hamiltonian[48,49] together with the restrictions selecting the physical subspace simply means that the Bose operators related to each site have to be replaced by quasi-Bose operators of order $p=1$. This conclusion is of a more general nature. It holds for any hard-core Bose model,[50] since the $p=1$ particles are hard-core bosons (Proposition 5).

Section VIII is devoted to some conclusions and discussions.

Throughout the paper we use the following abbreviations and notation (some of them standard):

JGs	Jacobson generators;
CAOs	creation and annihilation operators;
UEA	universal enveloping algebra;
$\mathbb{N}$	all positive integers;
$\mathbb{Z}+$	all non-negative integers;
$[a,b]=ab-ba,$	$\{a,b\}=ab+ba;$
$\oplus$	direct sum of linear spaces or of Lie algebras.

II. JACOBSON GENERATORS OF $sl(n+1)$

The $sl(n+1)$-statistics, including $n=\infty$, was introduced in Ref. 42 (see also Ref. 45) as an alternative way for quantization of spinor fields in quantum field theory. References 42 and 45 are not available as journal publications. Therefore here and in Sec. III we outline the main features of this statistics in somewhat more details.

In order to define the Jacobson generators, it is convenient to consider $sl(n+1)$ as a subalgebra of the Lie algebra $gl(n+1)$. The universal enveloping algebra $U[gl(n+1)]$ of the latter can be defined as an associative algebra with unity of the generators $\{e_{ij}|i,j=0,1,\ldots,n\}$ subject to the relations

$$[e_{ij},e_{kl}]=\delta_{jk}e_{il}-\delta_{il}e_{kj}. \tag{2.1}$$

Then $gl(n+1)$ is a subalgebra of $U[gl(n+1)]$, considered as a Lie algebra, with generators e_{ij}, $i,j=0,1,\ldots,n$ and commutation relations (2.1).

The Cartan subalgebra H' of $gl(n+1)$ has a basis $h_i\equiv e_{ii}$, $i=0,1,\ldots,n$. Let $h^0,h^1,\ldots,h^n$ be the dual basis, $h^i(h_j)=\delta_{ij}$. The root vectors of both $gl(n+1)$ and $sl(n+1)$ are e_{ij}, $i\neq j=0,1,\ldots,n$. The root of each e_{ij} is h^i-h^j. Then

$$sl(n+1)=\mathrm{span}\{e_{ij},e_{ii}-e_{jj}|i\neq j=0,1,\ldots,n\}. \tag{2.2}$$

The Jacobson generators (JGs) of $sl(n+1)$ are part of the generators e_{ij}, namely

$$a_i^+=e_{i0},\quad a_i^-=e_{0i},\quad i=1,\ldots,n. \tag{2.3}$$

The correspondence with their roots reads

$$a_i^{\pm}\leftrightarrow\mp(h^0-h^i),\quad i=1,\ldots,n, \tag{2.4}$$

and therefore the JGs a_i^+ (a_i^-) are negative (positive) root vectors with respect to the natural ordering $h^0,h^1,\ldots,h^n$. Since any other root is a sum of the roots of a_j^- and a_i^+, namely

$$h^i-h^j=(h^0-h^j)-(h^0-h^i),\quad i\neq j=1,\ldots,n,$$

the JGs (2.3) generate $sl(n+1)$ in the sense of a Lie algebra.

From (2.1) and (2.3) one derives the triple relations

$$[[a_i^+,a_j^-],a_k^+]=\delta_{kj}a_i^+ + \delta_{ij}a_k^+, \tag{2.5a}$$

$$[[a_i^+,a_j^-],a_k^-]=-\delta_{ki}a_j^- - \delta_{ij}a_k^-, \tag{2.5b}$$

$$[a_i^+,a_j^+]=[a_i^-,a_j^-]=0. \tag{2.5c}$$

On the contrary, setting $e_{ij}-\delta_{ij}e_{00}=[a_i^+,a_j^-]$, one derives from (2.5) the commutation relation between all $sl(n+1)$ generators e_{ij}, $e_{ii}-e_{jj}$, $i\neq j=0,1,\ldots,n$.

The above-given description of $sl(n+1)$ via generators and relations is a particular case of describing Lie algebras via Lie triple systems, initiated by Jacobson.[51] For this reason the elements $a_i^{\pm}$ are referred to as Jacobson generators of $sl(n+1)$.

The presentation of simple Lie algebras in terms of generators and relations [as illustrated here by the JGs for $sl(n+1)$] is a topic of interest to physicists.[52,53] In fact, any simple finite dimensional Lie algebra can be generated by two elements only; this was first claimed by Jacobson (see also Ref. 54) and proved in Ref. 55. For this reason, these two generators are sometimes referred to as ''Jacobson's generators.'' We shall not use this terminology here, in order to avoid confusion with the Jacobson generators defined in this section. Observe that the nature of the relations becomes extremely complicated when using only these two generators. A simpler description was given in Ref. 56, in terms of three generators [by adding a third generator to the earlier two, which are related to a principal $sl(2)$ embedding]. The description of $sl(n)$, and other simple Lie algebras or superalgebras, is explicitly given in Ref. 56 in terms of such three generators and the corresponding relations (which are not triple relations, but of higher degree). Such a description (with three generators and a number of higher order relations) is appropriate to present the so-called Lie algebra of matrices of complex size $gl(\lambda)$, see Refs. 56 and 53, since for $gl(\lambda)$ or $sl(\lambda)$ there is no analog of a Cartan matrix or of Chevalley generators.

In the present paper, however, we shall only use the presentation of $sl(n+1)$ by means of the JGs (2.3) and the triple relations (2.5), which is essentially a description by means of Jacobson's Lie triple systems (LTSs).[51] The approach by means of LTSs was further developed to the $\mathbb{Z}_2$-graded case by Okubo.[57] Let us be more concrete. By definition[51] a Lie triple system $\mathcal{L}$ is a subspace of an associative algebra U, so that $\mathcal{L}$ is closed under the ternary operation $\omega:\mathcal{L}\otimes\mathcal{L}\otimes\mathcal{L}\to\mathcal{L}$ defined as $\omega(a\otimes b\otimes c)=[[a,b],c]$, $a,b,c\in\mathcal{L}$. The definiton of a Lie supertriple system (equivalent to the definition in Ref. 57) is similar. The difference is that $\mathcal{L}$ is a $\mathbb{Z}_2$-graded subspace of an associative superalgebra U and the commutators in the definition of ω are replaced by supercommutators.

The JGs of $sl(n+1)$ are closely related to the above-given definition. More precisely, let $\mathcal{L}_{sl}$ be the linear span of the generators (2.3) and U_{sl} be the associative unital algebra of the JGs subject to the relations (2.5). Then $\mathcal{L}_{sl}$ is a subspace of U_{sl}. Moreover $\omega:\mathcal{L}_{sl}\otimes\mathcal{L}_{sl}\otimes\mathcal{L}_{sl}\to\mathcal{L}_{sl}$ as a consequence of (2.5). Hence $\mathcal{L}_{sl}$ is a Lie triple system with a basis consisting of the JGs (2.3) and U_{sl} is the UEA of $sl(n+1)$. Similarly, the linear span $\mathcal{L}_{\rm pf}$ of para-Fermi CAOs $F_1^{\pm},F_2^{\pm},\ldots,F_n^{\pm}$ together with the associative algebra $U_{\rm pf}$ of these operators [subject to the relations (1.3)] is another example of a LTS. Hence the para-Fermi operators $F_1^{\pm},\ldots,F_n^{\pm}$ could be called JGs of $so(2n+1)$. In the same spirit the para-Bose operators $B_1^{\pm},\ldots,B_n^{\pm}$ are JGs of $osp(1/2n)$.

From a purely algebraic point of view the Jacobson generators provide an alternative to the Chevalley description of $sl(n+1)$, $so(2n+1)$, and $osp(1/2n)$. The JGs of $so(2n+1)$ and $osp(1/2n)$ however (contrary to the Chevalley generators) have a direct physical significance. These operators extend the canonical Fermi and Bose statistics to the more general parastatistics. In the following we proceed to show that the JGs of $sl(n+1)$ also introduce a new quantum statistics, different from Bose and Fermi statistics and their generalization—parastatistics. This statistics is intrinsically related to class A of simple Lie algebras in the same way as the para-Fermi statistics is related to class B of simple Lie algebras.

Typically the ''commutation relations'' between the creation and the annihilation operators (or the related position and momentum operators in case of finite degrees of freedom) are derived from (more precisely, are required to be consistent with) *the main quantization equation*

$$[H,a_i^{\pm}]=\pm\epsilon_i a_i^{\pm}, \tag{2.6}$$

where H is the Hamiltonian and i replaces all indices that may appear (momentum, spin, charge, etc.). In quantum field theory (2.6) expresses the translation invariance of the field (in infinitesimal form). In quantum mechanics the same equation appears as a compatibility condition (in the sense of Wigner[31]) between the Heisenberg equations of motion and the classical equations, if the system has a classical analog (for more details see Refs. 32 and 58). There are certainly several other conditions to be satisfied (Galilean or relativistic invariance, causality, etc.; we refer to Ref. 43 for discussions in case of noncanonical quantum mechanics). The possibility for choosing different statistics essentially depends upon the way one represents the Hamiltonian H. We are going to illustrate this on the example of para-Fermi statistics.

Consider a nonrelativistic free field locked in a finite volume. In the case of a Fermi field the Hamiltonian $\hat{H}$ is written in a normal-product form

$$\hat{H}=\sum_i \epsilon_i f_i^+ f_i^-, \tag{2.7}$$

so that the energy of the vacuum is zero. Here f_i^+ (f_i^-) are Fermi creation (annihilation) operators: $\{f_i^{\xi},f_j^{\eta}\}=\frac{1}{4}(\xi-\eta)^2\delta_{ij}$, $\xi,\eta=\pm$ or ± 1. Then (2.6) holds,

$$[\hat{H},f_i^{\pm}]=\pm\epsilon_i f_i^{\pm}, \tag{2.8}$$

and each f_i^{ξ} can be interpreted as an operator creating ($\xi=+$) or annihilating ($\xi=-$) a particle, i.e., a fermion with energy ϵ_i. Equation (2.8) is not fulfilled however, if the Fermi operators in (2.7) are replaced by para-Fermi operators (1.3): for $H=\Sigma_i \epsilon_i F_i^+ F_i^-$ the equation

$$[H,F_i^{\pm}]=\pm\epsilon_i F_i^{\pm} \tag{2.9}$$

does not hold. Why? In order to answer this question using proper Lie algebraic language assume that the sum in (2.7) is finite (finite number of Fermi oscillators),

$$\hat{H}=\sum_{i=1}^{n} \epsilon_i f_i^+ f_i^-. \tag{2.10}$$

This is only an intermediate step. The considerations in the following remain valid for $n=\infty$. Recall now that any n pairs of Fermi CAOs generate a particular Fermi representation of the Lie algebra $so(2n+1)\equiv B_n$, whereas the para-Fermi operators $F_1^{\pm},\ldots,F_n^{\pm}$ are (representation independent) generators of $so(2n+1)$.[36,37] Equation (2.8) is not preserved, when passing to other representations of B_n, because H is not an element from B_n and hence $[H,F_i^{\pm}]$ on the left-hand side of (2.9) is not a representation independent commutator. This observation also suggests the answer: one has to rewrite (2.10) in a representation independent form. In order to achieve this, represent (2.10) in the following identical form:

$$\hat{H}=\frac{1}{2}\sum_{i=1}^{n} \epsilon_i([f_i^+,f_i^-]+\{f_i^+,f_i^-\}). \tag{2.11}$$

Consider the Lie algebra generated from $f_1^{\pm},\ldots,f_n^{\pm}$ and $\{f_i^+,f_i^-\}$. Since $\{f_i^+,f_i^-\}=1$, we obtain a representation of the Lie algebra $B_n\oplus I$, where I is the one-dimensional center. Now $\hat{H}\in B_n\oplus I$ and therefore the commutation relations (2.8) hold for any other representation of $B_n\oplus I$. In other words, if we substitute $f_i^{\pm}\to F_i^{\pm}$ and $\{f_i^+,f_i^-\}\to\hat{p}$ in (2.11), i.e., set

$$H=\frac{1}{2}\sum_{i=1}^{n}\epsilon_i([F_i^+,F_i^-]+\hat{p}), \tag{2.12}$$

where $\hat{p}$ is a generator of the center I, then the quantization condition (2.8) will be fulfilled for any representation of $B_n\oplus I$ and in particular for the para-Fermi operators (1.3): $[H,F_i^{\pm}]=\pm\epsilon_i F_i^{\pm}$. The requirement $\hat{p}|0\rangle=p|0\rangle$, $p\in\mathbb{N}$ (and $F_i^-F_j^+|0\rangle=\delta_{ij}p|0\rangle$, $F_i^-|0\rangle=0$), leads to a representation with an order of the (para)statistics p.[59] Then the energy of the vacuum is also zero.

We shall now apply a similar approach for the algebra $sl(n+1)$. Let E_{ij}, $i,j=0,1,\ldots,n$, be the $(n+1)\times(n+1)$ matrix units. The map $\pi:e_{ij}\to E_{ij},i,j=0,1,\ldots,n$, gives a representation of $gl(n+1)$ (usually referred to as defining or identity representation). Its restriction to $sl(n+1)$ gives a representation of $sl(n+1)$. The operators $A_i^+=E_{i0}$, $A_i^-=E_{0i}$, $i=1,2,\ldots,n$ satisfy the triple relations (2.5). Set

$$\hat{H}=\sum_{i=1}^{n}\epsilon_i A_i^+A_i^-. \tag{2.13}$$

Then

$$[\hat{H},A_i^{\pm}]=\pm\epsilon_i A_i^{\pm}. \tag{2.14}$$

Hence A_i^{ξ} can be interpreted as an operator creating ($\xi=+$) or annihilating ($\xi=-$) a particle (quasiparticle, excitation) with energy ϵ_i for any $i=1,\ldots,n$. The representation π is an analog of the Fermi representation of para-Fermi statistics.

The commutation relations (2.14) do not hold for other representations of $sl(n+1)$. In order to extend the class of admissible representations we rewrite the Hamiltonian (2.13), like in the Fermi case, in the following identical form:

$$\hat{H}=\sum_{i=1}^{n}\epsilon_i([A_i^+,A_i^-]+E_{00}). \tag{2.15}$$

The Lie algebra generated from the operators $A_1^{\pm},\ldots,A_n^{\pm}$ and E_{00} is $gl(n+1)$ (in the representation π). Since $\hat{H}\in gl(n+1)$ (in this representation), (2.14) also holds for any other representation of $gl(n+1)$. In other words the Hamiltonian

$$H=\sum_{i=1}^{n}\epsilon_i([a_i^+,a_i^-]+e_{00})=\sum_{i=1}^{n}\epsilon_i([a_i^+,a_i^-]+h_0) \tag{2.16}$$

satisfies (2.6) for any other representation of $gl(n+1)$.

One may argue that expression (2.16) is not satisfactory, because the Hamiltonian H is not a function of the Jacobson generators only. In the following, in Corollary 1, we show that within every irreducible representation H can be written as a function of the JGs. Here we note that $[a_i^+,a_i^-]+e_{00}=h_i$ and therefore the Hamiltonian (2.16) can be represented manifestly as an element from the Cartan subalgebra of $gl(n+1)$:

$$H=\sum_{i=1}^{n}\epsilon_i h_i. \tag{2.17}$$

III. FOCK REPRESENTATIONS OF $sl(n+1)$

We proceed to outline those representations of the Jacobson generators that possess the main features of Fock space representations in ordinary quantum theory. In order to distinguish between the abstract generators and their representations, the JGs $a_1^{\pm},\ldots,a_n^{\pm}$, considered as operators in a certain $sl(n+1)$-module W, are called (Jacobson) creation and annihilation operators of $sl(n+1)$ [abbreviated also as Jacobson CAOs of $sl(n+1)$, $sl(n+1)$-CAOs, A-CAOs or simply CAOs].

Definition 1: Let $a_1^{\xi},\ldots,a_n^{\xi}$ be Jacobson creation ($\xi=+$) and annihilation ($\xi=-$) operators. The $sl(n+1)$-module W is said to be a Fock space of the algebra $sl(n+1)$ if it is a Hilbert space, so that the following conditions hold:

1. Hermiticity condition (A^* *denotes the operator conjugate to* A)

$$(a_i^+)^* = a_i^-, \quad i=1,\ldots,n. \tag{3.1}$$

2. Existence of vacuum. There exists a vacuum vector $|0\rangle \in W$ such that

$$a_i^-|0\rangle = 0, \quad i=1,\ldots,n. \tag{3.2}$$

3. The representation space W is spanned on vectors

$$a_{i_1}^+ a_{i_2}^+ \cdots a_{i_m}^+ |0\rangle, \quad m \in \mathbb{Z}_+ . \tag{3.3}$$

The Fock space of $sl(n+1)$ is also said to be an A_n-module of Fock or simply a Fock module.

Assume that W is a Fock space. Condition (3.1) asserts that any Fock representation is unitarizable with respect to this star operation, considered as an antilinear antiinvolution on $sl(n+1)$. It is known that all such representations are realized in direct sums of finite-dimensional irreducible $sl(n+1)$-modules. Then (3.3) yields that any Fock module is a finite-dimensional irreducible $sl(n+1)$-module.

We list a few propositions, proofs of which can be found in Refs. 42 and 45.

Proposition 1: The $sl(n+1)$-module W is a Fock space if and only if it is an irreducible finite-dimensional module with a highest weight Λ such that

$$a_i^- a_j^+ x_\Lambda = 0, \quad i \neq j = 1,\ldots,n. \tag{3.4}$$

The vacuum $|0\rangle$ is unique (up to a multiplicative constant) and can be identified with the highest weight vector x_Λ in W: $|0\rangle = x_\Lambda$.

For a proof see Theorem 1 in Ref. 45.

Recall that the Hamiltonian H, see (2.17), does not belong to $sl(n+1)$. It is an element from $gl(n+1)$. In order to define H as an operator in W, we extend each Fock module to an irreducible $gl(n+1)$-module. To this end we define the action of the $gl(n+1)$ central element [also $gl(n+1)$ Casimir operator] $h_0+h_1+\cdots+h_n$ in W, setting

$$(h_0+h_1+\cdots+h_n)x = px, \forall x \in W, \tag{3.5}$$

where p can be any number.

The next proposition classifies the Fock spaces. Unless otherwise stated, the roots and the weights are represented by their coordinates in the basis $h^0,h^1,\ldots,h^n$, i.e., $\lambda = \sum_{i=0}^n l_i h^i \equiv (l_0,l_1,\ldots,l_n)$.

Proposition 2: The irreducible $gl(n+1)$-module W_p is a Fock space, so that the energy of the vacuum is zero ($H|0\rangle = 0$), if and only if its highest weight (namely the weight of $|0\rangle$) is $\Lambda = ph^0 \equiv (p,0,\ldots,0)$, i.e., if

$$h_0|0\rangle = p|0\rangle, \quad h_i|0\rangle = 0, \quad i=1,\ldots,n, \tag{3.6}$$

where p is an arbitrary positive integer.

Let us add that a representation with a highest weight $(p,0,\ldots,0)$ is the pth symmetric power of the identity representation $(1,0,\ldots,0)$. It corresponds to a Young diagram with one row and p boxes.

From (2.3) and (3.5) $h_0+h_1+\cdots+h_n=p$, $h_0-h_i=[a_i^-,a_i^+]$, $i=1,\ldots,n$, which yields

$$h_0=\frac{1}{n+1}\left(p+\sum_{i=1}^{n}[a_i^-,a_i^+]\right),\quad h_i=\frac{1}{n+1}\left(p+n[a_i^+,a_i^-]-\sum_{k\neq i=1}^{n}[a_k^+,a_k^-]\right). \tag{3.7}$$

The last result shows that within any Fock module the generators e_{ij} can be expressed as functions of $a_1^{\pm},\ldots,a_n^{\pm}$. In view of this we say that $a_1^{\pm},\ldots,a_n^{\pm}$ are Jacobson CAOs of both $sl(n+1)$ and of $gl(n+1)$.

An immediate consequence of (2.16) and (3.7) is the following

Corollary 1: Within every Fock module W_p the Hamiltonian (2.16) can be expressed entirely via the Jacobson creation and annihilation operators:

$$H=\frac{1}{n+1}\sum_{i=1}^{n}\epsilon_i\left(p+n[a_i^+,a_i^-]-\sum_{k\neq i=1}^{n}[a_k^+,a_k^-]\right). \tag{3.8}$$

From (3.4), (3.6), and (3.7) one concludes:

Corollary 2: The Fock module W_p with a highest weight $\Lambda=(p,0,\ldots,0)$ is completely defined by the relations

$$a_i^-a_j^+|0\rangle=\delta_{ij}p|0\rangle,\quad a_k^-|0\rangle=0,\quad p\in\mathbb{N},\quad i,j,k=1,\ldots,n. \tag{3.9}$$

The above two conditions are the same as in the case of Green's parastatistics of order p.[33] Therefore p is referred to as an order of $sl(n+1)$-statistics (or A-statistics). The conclusion is that like in parastatistics the Fock spaces are labeled by a positive integer $p\in\mathbb{N}$. The representations corresponding to different orders of statistics have different highest weights and are therefore inequivalent.

Taking into account the second relation $a_k^-|0\rangle=0$ in (3.9), one can also define the Fock module W_p by means of the relations

$$[a_i^-a_j^+]|0\rangle=\delta_{ij}p|0\rangle,\quad a_k^-|0\rangle=0,\quad p\in\mathbb{N},\quad i,j,k=1,\ldots,n. \tag{3.10}$$

In view of this A-statistics and its Fock representations can be formulated in a somewhat more mathematical terminology. The latter is based on the observation that the linear span of all generators $[a_i^-a_j^+]$, a_i^-, $i,j=1,\ldots,n$, is a subalgebra $\mathcal{A}$ of $gl(n+1)$ [which contains as subalgebra also $gl(n)=\mathrm{span}\{[a_i^-a_j^+]|i,j=1,\ldots,n\}$]. Equation (3.10) defines one-dimensional representations of $\mathcal{A}$, spanned on the vacuum $|0\rangle$. Therefore the Fock modules W_p can be defined as those irreducible finite-dimensional $gl(n+1)$-modules, which are induced from trivial one-dimensional modules of $\mathcal{A}$ via Eq. (3.10). Then p labels the different, inequivalent one-dimensional modules of $\mathcal{A}$.

On the other hand one can define A-statistics by means of the triple relations (2.5). Then Eq. (3.9) defines completely the Fock modules W_p. All calculations can be carried out without even mentioning the underlying Lie algebraic structure of A-statistics (which is usually the case for parastatistics).

Let W_p be a Fock space with order of statistics p. From (3.3) and the fact that the creation operators commute with each other one concludes that W_p is a linear span of vectors $(a_1^+)^{l_1}(a_2^+)^{l_2}\cdots(a_n^+)^{l_n}|0\rangle$, $l_1,\ldots,l_n\in\mathbb{Z}_+$. The correspondence weight$\leftrightarrow$weight vector is one to one:

$$(a_1^+)^{l_1}(a_2^+)^{l_2}\cdots(a_n^+)^{l_n}|0\rangle \leftrightarrow \left| p-\sum_{k=1}^{n} l_k, l_1, l_2, \ldots, l_n \right\rangle, \tag{3.11}$$

i.e., all weight subspaces are one-dimensional.

Proposition 3: Let W_p be an $sl(n+1)$-module of Fock with order of statistics p. The vector

$$(a_1^+)^{l_1}(a_2^+)^{l_2}\cdots(a_n^+)^{l_n}|0\rangle \tag{3.12}$$

is not zero if and only if

$$l_1+l_2+\cdots+l_n \leqslant p. \tag{3.13}$$

The proof is a consequence of the properties of the roots in any finite-dimensional irreducible $sl(n+1)$-module W. If $\Lambda=(L_0,L_1,\ldots,L_n)$ is the highest weight in W, then for any other weight $\lambda=(l_0,l_1,\ldots,l_n)$ the following inequality holds:

$$l_{i_0}+l_{i_1}+\cdots+l_{i_m} \leqslant L_0+L_1+\cdots+L_m, \tag{3.14}$$

where $i_0 \neq i_1 \neq \ldots, \neq i_m = 0,1,\ldots,n$ and $m=0,1,\ldots,n$. Equation (3.14) is an equality for $m=n$. If W_p is a Fock space, $L_0+L_1+\cdots+L_m=p$.

Proposition 3 can be proved also by a direct, but rather long computation. One verifies that the infinite-dimensional module $\hat{W}_p$ spanned on all vectors (3.12) with $l_1,\ldots,l_n$ being arbitrary non-negative integers contains an invariant subspace V_p spanned on all vectors (3.12) with $l_1+l_2+\cdots+l_n>p$. Then W_p is the factor module $\hat{W}_p/V_p$ and all vectors (3.12), subject to (3.13) are (representatives of) the basis vectors in $W_p=\hat{W}_p/V_p$.

We proceed to recall how one defines a metric in W_p, so that it is a Hilbert space and the hermiticity condition (3.1) holds. Consider the vectors

$$(a_1^+)^{l_1}(a_2^+)^{l_2}\cdots(a_n^+)^{l_n}|0\rangle, \quad l_1+l_2+\cdots+l_n \leqslant p \tag{3.15}$$

from W_p. All such vectors have different weights. Consequently they are linearly independent and can be considered as a basis in W_p. Define a Hermitian form $(\ ,\ )$ on W_p in the usual way (for quantum theory), postulating [in addition to $a_i^-|0\rangle=0$, see (3.2)]:

$$(|0\rangle,|0\rangle) \equiv \langle 0|0\rangle = 1, \tag{3.16a}$$

$$\langle 0|a_i^+ = 0, \quad i=1,\ldots,n, \tag{3.16b}$$

$$\begin{aligned}&((a_1^+)^{m_1}(a_2^+)^{m_2}\cdots(a_n^+)^{m_n}|0\rangle,(a_1^+)^{l_1}(a_2^+)^{l_2}\cdots(a_n^+)^{l_n}|0\rangle)\\ &\quad=\langle 0|(a_n^-)^{m_n}\cdots(a_2^-)^{m_2}(a_1^-)^{m_1}(a_1^+)^{l_1}(a_2^+)^{l_2}\cdots(a_n^+)^{l_n}|0\rangle.\end{aligned} \tag{3.16c}$$

With respect to this form the vectors (3.15) are orthogonal. Moreover,

$$((a_1^+)^{l_1}(a_2^+)^{l_2}\cdots(a_n^+)^{l_n}|0\rangle,\ (a_1^+)^{l_1}(a_2^+)^{l_2}\cdots(a_n^+)^{l_n}|0\rangle) = \frac{p!}{(p-\Sigma_{j=1}^n l_j)!}\prod_{i=1}^{n} l_i! > 0. \tag{3.17}$$

Therefore all vectors

$$|p;l_1,\ldots,l_n\rangle = \sqrt{\frac{(p-\Sigma_{j=1}^n l_j)!}{p!}}\frac{(a_1^+)^{l_1}\cdots(a_n^+)^{l_n}}{\sqrt{l_1!l_2!\ldots l_n!}}|0\rangle, \quad l_1+l_2+\cdots+l_n \leqslant p \tag{3.18}$$

constitute an orthonormal basis in W_p, i.e., $(\ ,\ )$ is a scalar product. Then by construction the hermiticity condition (3.1) holds too.

The transformation of the basis (3.18) under the action of the Jacobson CAOs reads:

$$a_i^+|p;l_1,\ldots,l_i,\ldots,l_n\rangle=\sqrt{(l_i+1)\left(p-\sum_{j=1}^{n} l_j\right)}|p;l_1,\ldots,l_{i-1},l_i+1,l_{i+1}\ldots,l_n,\rangle, \tag{3.19}$$

$$a_i^-|p;l_1,\ldots,l_i,\ldots,l_n\rangle=\sqrt{l_i\left(p-\sum_{j=1}^{n} l_j+1\right)}|p;l_1,\ldots,l_{i-1},l_i-1,l_{i+1}\ldots,l_n\rangle. \tag{3.20}$$

Moreover,

$$h_0|p;l_1,l_2,\ldots,l_n\rangle=\left(p-\sum_{i=1}^{n} l_i\right)|p;l_1,l_2,\ldots,l_n\rangle, \tag{3.21}$$

$$h_i|p;l_1,l_2,\ldots,l_n\rangle=l_i|p;l_1,l_2,\ldots,l_n\rangle,\quad i=1,\ldots,n. \tag{3.22}$$

Let us consider in some more detail the $p=1$ representation. Denote by $b_i^{\pm}$ the Jacobson CAOs $a_i^{\pm}$ in this representation. In this particular case the representation space W_1 is $(n+1)$-dimensional with a basis

$$|1;l_1,\ldots,l_n\rangle,\quad l_1+\cdots+l_n\leqslant 1, \tag{3.23}$$

i.e., at most one of the labels $l_1,\ldots,l_n$ in $|1;l_1,\ldots,l_n\rangle$ is equal to 1 and all other are zeros. Then (3.19) and (3.20) reduce to

$$\begin{aligned} b_i^+|1;l_1,\ldots,l_{i-1},l_i,l_{i+1},\ldots,l_n\rangle&=(1-l_i)|1;l_1,\ldots,l_{i-1},l_i+1,l_{i+1},\ldots,l_n\rangle,\\ b_i^-|1;l_1,\ldots,l_{i-1},l_i,l_{i+1},\ldots,l_n\rangle&=l_i|1;l_1,\ldots,l_{i-1},l_i-1,l_{i+1},\ldots,l_n\rangle. \end{aligned} \tag{3.24}$$

The matrix elements of b_i^+ and b_i^-, in the basis ordered as $|1;0,0,0,\ldots,0\rangle,|1;1,0,0,\ldots,0\rangle,|1;0,1,0,\ldots,0\rangle,|1;0,0,1,\ldots,0\rangle,\ldots,|1;0,0,0,\ldots,1\rangle$ are the same as those of the matrix units E_{i0} and E_{0i} in the defining $(n+1)$-dimensional matrix representation of $gl(n+1)$. Hence the $p=1$ representation is the same as the defining representation and one can think of the operators $b_i^{\pm}$ as of matrices,

$$E_{i0}=b_i^+,\quad E_{0i}=b_i^-,\quad i=1,\ldots,n. \tag{3.25}$$

From here and (3.7) (with $p=1$) one can also express the rest of the generators via $p=1$ Jacobson creation and annihilation operators:

$$E_{00}=\frac{1}{n+1}\left(1-\sum_{i=1}^{n}[b_i^+,b_i^-]\right),\quad E_{ij}=[b_i^+,b_j^-]+\frac{\delta_{ij}}{n+1}\left(1-\sum_{k=1}^{n}[b_k^+,b_k^-]\right),\quad i,j=1,\ldots,n. \tag{3.26}$$

IV. THE PAULI PRINCIPLE FOR *A*-STATISTICS

The results obtained so far justify the terminology used. Equations (2.17) and (3.6) yield

$$H|p;l_1,\ldots,l_i,\ldots,l_n\rangle=\sum_{i=1}^{n} l_i\epsilon_i|p;l_1,\ldots,l_i,\ldots,l_n\rangle. \tag{4.1}$$

Therefore the state $|p;l_1,\ldots,l_i,\ldots,l_n\rangle$ can be interpreted as a many-particle state with l_1 particles on the first orbital, l_2 particles on the second orbital, etc. For reasons that will become clear soon,

we refer to these particles as A-particles or simply particles. The operator h_i, $i=1,\ldots,n$, see (3.22), is the number operator for the A-particles on the ith orbital, whereas $\hat{N}=h_1+\cdots+h_n$ counts all particles, accommodated in the state $|p;l_1,\ldots,l_i,\ldots,l_n\rangle$.

Since, see (3.19),

$$a_i^+|p;l_1,\ldots,l_i,\ldots,l_n\rangle\sim|p;l_1,\ldots,l_{i-1},l_i+1,l_{i+1},\ldots,l_n\rangle \quad \text{if } \sum_{i=1}^{n} l_i<p, \tag{4.2}$$

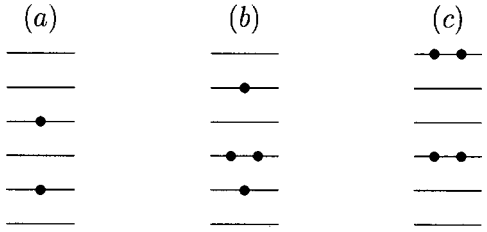
the operator a_i^+ creates an A-particle on the ith orbital, a particle with energy ϵ_i, if the state contains less than p particles. On the other hand, $a_i^+|p;l_1,\ldots,l_{i-1},l_i,l_{i+1},\ldots,l_n\rangle=0$, if $\Sigma_{i=1}^{n}l_i=p$, i.e., no more than p particles can be accommodated. Similarly, if $l_i>0$, a_i^- "kills" a particle with energy ϵ_i. Therefore, reformulating Proposition 3, one obtains:

Corollary 3 (Pauli principle for A-statistics): Let W_p be a Fock space of $sl(n+1)$, corresponding to an order of statistics p. Within W_p all states containing no more than p A-particles, namely all states

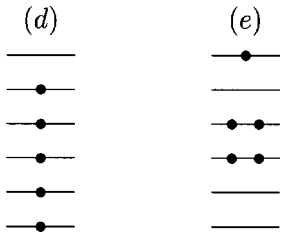
$$|p;l_1,\ldots,l_i,\ldots,l_n\rangle \quad with \quad 0\leqslant\sum_{i=1}^{n} l_i\leqslant p, \tag{4.3}$$

are allowed. There are no states accommodating more than p A-particles.

Let us consider, as an example, A-statistics of order $p=4$ with $n=6$ orbitals (for instance with six different energy levels). From (4.3), it follows that there is no restriction on the number of particles to be accommodated on a certain orbital as long as the total number of particles in any configuration does not exceed p. Hence, the following three states or configurations are allowed (the orbitals, for instance the energy levels, are represented by lines, and the particles by dots):



Note that the last two configurations (b) and (c) are already "saturated" in the sense that no more particles can be added, since the total number of them is already equal to $p=4$. The following two configurations correspond to forbidden states:



None of the states (d) and (e) is allowed since the total number of particles in the configuration exceeds $p=4$.

This example illustrates the statistical interaction between the orbitals: the filling of an orbital depends on how many particles are already accommodated on the other orbitals. This property is typical for Haldane's exclusion statistics.[30] Although Haldane's relation (1.1) does not hold for A-statistics, up to a certain natural assumption A-statistics can be viewed as a special case of exclusion statistics in the sense of Wu.

In Ref. 46 Wu proposed an "integral form" compatible with Haldane's relation (1.1):

$$d(N)=n-g(N-1). \tag{4.4}$$

This should be interpreted as follows: let n be the total number of orbitals that are available for the first particle, and suppose $N-1$ particles are already accommodated in the configuration, then $d(N)$ expresses the dimension of the single-particle space for the Nth particle (or the number of orbitals where the Nth particle can be ''loaded''). Bose statistics has $g=0$, and Fermi statistics has $g=1$.

The natural assumption mentioned previously is that the domain of definition of the function $d(N)$ consists of all *admissible* values of N, i.e., one does not require (4.4) to be applicable for values of N which the system cannot accommodate. Under this assumption A-statistics is a particular case of exclusion statistics, also with $g=0$:

$$d(N)=n, \quad \forall N\in\{1,2,\ldots,p\}. \tag{4.5}$$

If however one drops the condition for N to be an admissible value, one cannot satisfy Eq. (4.4). Indeed, (4.4) with $g=0$, does not hold for $N=p+1$, since $d(p+1)=0$.[60,61]

A-statistics is similar to Bose statistics in the sense that there is no restriction on the number of particles on an orbital apart from the general requirement that the total configuration should contain no more than p particles. This restriction leads perhaps to the simplest statistical interaction between the orbitals. Nevertheless the situation is not as easy as it sounds. As in any (nontrivial) model of an exclusion statistics (so also in this case) the orbitals cannot be considered anymore as independent (or quasiclosed) subsystems. In particular the grand partition function of the system cannot be represented anymore as a product of the partition functions of the orbitals. The latter makes the problem of studying the statistical properties of A-statistics more involved as compared to Bose or Fermi systems. From the point of view of statistical mechanics this is the main difference between A-statistics and Bose statistics.[62]

V. QUASI-BOSE CREATION AND ANNIHILATION OPERATORS

In the present section we show first approximately and then in a strict sense that A-statistics can be viewed as a good finite-dimensional approximation to Bose statistics for large values of order of statistics p. The terminology *finite-dimensional approximation* comes to remind one that the Fock spaces W_p of A-statistics are finite-dimensional linear spaces, whereas any Bose Fock space is infinite-dimensional.

Introduce new, representation-dependent, creation and annihilation operators

$$B(p)_i^{\pm}=\frac{a_i^{\pm}}{\sqrt{p}}, \quad i=1,\ldots,n, \quad p\in\mathbb{N}, \tag{5.1}$$

in W_p. The transformations following from (3.19) to (3.20) read

$$B(p)_i^{+}|p;l_1,\ldots,l_i,\ldots,l_n\rangle=\sqrt{(l_i+1)\left(1-\frac{\Sigma_{k=1}^{n}l_k}{p}\right)}|p;l_1,\ldots,l_i+1,\ldots,l_n\rangle, \tag{5.2}$$

$$B(p)_i^{-}|p;l_1,\ldots,l_i,\ldots,l_n\rangle=\sqrt{l_i\left(1+\frac{1-\Sigma_{k=1}^{n}l_k}{p}\right)}|p;l_1,\ldots,l_i-1,\ldots,l_n\rangle. \tag{5.3}$$

Consider the above-given equations for values of the order of statistics p, which are much greater than the number of accommodated particles, namely $l_1+l_2+\cdots+l_n\ll p$. In this approximation one obtains

$$B(p)_i^-|p;l_1,\ldots,l_{i-1},l_i,l_{i+1},\ldots,l_n\rangle \simeq \sqrt{l_i}|p;l_1,\ldots,l_{i-1},l_i-1,l_{i+1},\ldots,l_n\rangle,$$
$$B(p)_i^+|p;l_1,\ldots,l_{i-1},l_i,l_{i+1},\ldots,l_n\rangle \simeq \sqrt{l_i+1}|p;l_1,\ldots,l_{i-1},l_i+1,l_{i+1}\ldots,l_n\rangle, \tag{5.4}$$

which yields (an approximation to) the Bose commutation relations:

$$[B(p)_i^+,B(p)_j^+]=[B(p)_i^-,B(p)_j^-]=0 \quad \text{(exact commutators)}, \tag{5.5}$$

$$[B(p)_i^-,B(p)_j^+]\simeq \delta_{ij} \quad \text{if } l_1+l_2+\cdots+l_n \ll p. \tag{5.6}$$

Since for $l_1+l_2+\cdots+l_n\equiv\Sigma_k l_k \ll p$,

$$\frac{(p-\Sigma_k l_k)!}{p!}p^{\Sigma_k l_k}=\frac{p}{p-\Sigma_k l_k+1}\frac{p}{p-\Sigma_k l_k+2}\cdots\frac{p}{p}\simeq 1,$$

in a first approximation (3.18) reduces also to the well-known expressions for the orthonormed basis in a Fock space of n pairs of Bose creation and annihilation operators:

$$|p;l_1,\ldots,l_n\rangle=\frac{(B(p)_1^+)^{l_1}\cdots(B(p)_n^+)^{l_n}}{\sqrt{l_1!l_2!\cdots l_n!}}|0\rangle. \tag{5.7}$$

The conclusion is that the representations of $B(p)_i^{\pm}$ in (finite-dimensional) state spaces W_p with large values of p, restricted to states with a small amount $l_1+l_2+\cdots+l_n \ll p$ of accommodated particles, provide a good approximation to Bose creation and annihilation operators.[42,45] For this reason we refer to the operators $B(p)_i^{\pm}$ as *quasi-Bose creation and annihilation operators (of order p)* and to the corresponding particles as quasibosons.

In the remaining part of this section we will prove that in the limit $p\to\infty$ the quasi-Bose operators reduce to Bose creation and annihilation operators. To this end we proceed to introduce first an appropriate topology.

Let W be a Hilbert space with an orthonormed basis

$$|l_1,\ldots,l_i,\ldots,l_n\rangle\equiv|L\rangle, \quad \forall l_1,\ldots,l_n\in\mathbb{Z}_+. \tag{5.8}$$

Whenever possible we write $|L\rangle$ as an abbreviation for $|l_1,\ldots,l_i,\ldots,l_n\rangle$ and denote by $|L\rangle_{\pm i}$ a vector obtained from $|L\rangle$ by replacing l_i with $l_i\pm 1$, namely

$$|L\rangle_{\pm i}=|l_1,\ldots,l_{i-1},l_i\pm 1,l_{i+1},\ldots,l_n\rangle. \tag{5.9}$$

The space W consists of all vectors

$$\Phi=\sum_{l_1=0}^{\infty}\cdots\sum_{l_n=0}^{\infty}c(l_1,\ldots,l_n)|l_1,\ldots,l_n\rangle\equiv\sum_L c(L)|L\rangle, \tag{5.10}$$

where $c(l_1,\ldots,l_n)\equiv c(L)$ are complex numbers such that

$$\sum_{l_1=0}^{\infty}\cdots\sum_{l_n=0}^{\infty}|c(l_1,\ldots,l_n)|^2\equiv\sum_{l_1,\ldots,l_n=0}^{\infty}|c(l_1,\ldots,l_n)|^2\equiv\sum_L|c(L)|^2<\infty, \tag{5.11}$$

and this is in fact the square of the Hilbert space norm $(|\Phi|_0)^2$ of Φ.

Embed the $sl(n+1)$-module W_p in W via an identification of the basis vectors

$$|p;l_1,\ldots,l_i,\ldots,l_n\rangle\equiv|l_1,\ldots,l_i,\ldots,l_n\rangle\equiv|L\rangle, \quad \forall l_1+\cdots+l_n\leqslant p. \tag{5.12}$$

In order to turn the entire space W into an $sl(n+1)$-module, so that the restriction on $W_p \subset W$ coincides with (5.2) and (5.3), we set

$$B(p)_i^+ \Phi = \sum_{l_1+\cdots+l_n \leqslant p} c(L) \sqrt{(l_i+1)\left(1-\frac{\Sigma_{k=1}^n l_k}{p}\right)}|L\rangle_i, \tag{5.13}$$

$$B(p)_i^- \Phi = \sum_{l_1+\cdots+l_n \leqslant p} c(L) \sqrt{l_i\left(1+\frac{1-\Sigma_{k=1}^n l_k}{p}\right)}|L\rangle_{-i}, \tag{5.14}$$

where Φ is any vector (5.10) from W and $\Sigma_{l_1+\cdots+l_n \leqslant p}$ is a sum over all possible $l_1,\ldots,l_n \in \mathbb{Z}_+$ such that $l_1+\cdots+l_n \leqslant p$. Note that the sums in (5.13) and (5.14) are finite.

The transformation of the basis, following from (5.13) to (5.14), reads

$$B(p)_i^+ |L\rangle = \sqrt{(l_i+1)\left(1-\frac{\Sigma_{k=1}^n l_k}{p}\right)}|L\rangle_i, \quad \forall L \text{ such that } \sum_{k=1}^n l_k \leqslant p, \tag{5.15}$$

$$B(p)_i^- |L\rangle = \sqrt{l_i\left(1+\frac{1-\Sigma_{k=1}^n l_k}{p}\right)}|L\rangle_{-i}, \quad \forall L \text{ such that } \sum_{k=1}^n l_k \leqslant p, \tag{5.16}$$

$$B(p)_i^{\pm}|L\rangle = 0, \quad \forall L \text{ such that } \sum_{k=1}^n l_k > p. \tag{5.17}$$

Relations (5.15) and (5.16) are the same as (5.2) and (5.3) [via the identification (5.12)].

Since the quasi-Bose operators $B(p)_i^{\pm}$ take values in a finite-dimensional subspace of W, see (5.13) and (5.14), they are bounded and hence continuous linear operators in W. In view of this see (5.10), $B(p)_i^{\pm}\Phi = B(p)_i^{\pm}\Sigma_L c(L)|L\rangle = \Sigma_L c(L) B(p)_i^{\pm}|L\rangle$ and therefore (5.13) and (5.14) are a consequence of (5.15)–(5.17).

Next we proceed to define n pairs of Bose operators $B_i^{\pm}$, $i=1,\ldots,n$, in W. It is known that such operators cannot be realized as bounded operators in W (so that the corresponding position and momentum operators are selfadjoint operators in W; see, for instance, Ref. 63 or 64). Therefore care has to be taken about the common domain of definition Ω of the Bose operators. Following Ref. 65 we set Ω to be a dense subspace of W (with respect to the Hilbert space topology), consisting of all vectors (5.10) for which the series

$$(|\Phi|_r)^2 = \sum_{l_1,\ldots,l_n=0}^{\infty} \left(1+\sum_{k=1}^n l_k\right)^r |c(l_1,\ldots,l_n)|^2 \tag{5.18}$$

is convergent for any $r=0,1,2,\ldots$. Then the relations

$$B_i^-|L\rangle = \sqrt{l_i}|L\rangle_{-i}, \quad B_i^+|L\rangle = \sqrt{l_i+1}|L\rangle_i, \tag{5.19}$$

define a representation of n pairs of bosons $B_1^{\pm},\ldots,B_n^{\pm}$, namely of operators, which satisfy the relations

$$[B_i^-, B_j^+] = \delta_{ij}, \quad [B_i^+, B_j^+] = [B_i^-, B_j^-] = 0, \quad i,j=1,\ldots,n \tag{5.20}$$

in Ω (with Ω being a common domain of definition for all them). In terms of these operators

$$(|\Phi|_r)^2 = \left(\Phi, \left(1+\sum_{k=1}^n B_k^+ B_k^-\right)^r \Phi\right). \tag{5.21}$$

The norms $|\Phi|_r$, $r=0,1,2,\ldots$, turn Ω into a countably normed topological space (which can be viewed also as a metric space[66]). All balls

$$B(\Phi_0;r,\epsilon)=\{\Phi\in\Omega||\Phi-\Phi_0|_r<\epsilon\},\quad \forall\Phi_0\in\Omega,\quad \forall r\in\mathbb{Z}_+,\quad \forall\epsilon>0, \tag{5.22}$$

constitute a basis of open sets in the countably normed topological space Ω, whereas the balls (5.22) with a fixed r yield a basis in Ω, viewed as a $|\cdot|_r$-normed topological space. Clearly any $|\cdot|_r$-normed topology (*r-normed topology*) is weaker than the countably normed topology (*cn-topology*).

From now on we restrict the domain of definition of all quasi-Bose operators (5.1) to be Ω. The fact that each quasi-Bose operator maps Ω into a finite-dimensional subspace of Ω, see (5.13) and (5.14), indicates that each such operator is a bounded and hence a continuous linear operator with respect to the r-normed topology for any $r\in\mathbb{Z}_+$. A similar property however does not hold for the Bose creation and annihilation operators (5.19). These operators are not continuous with respect to any of the r-normed topologies in Ω. Therefore, if $\Sigma_{i=1}^{\infty}\Phi_i=\Phi$ converges in the sense of a certain r-normed topology, for instance in the Hilbert space topology ($r=0$), one cannot in general use relations like

$$B_i^{\pm}\sum_{i=1}^{\infty}\Phi_i=\sum_{i=1}^{\infty}B_i^{\pm}\Phi_i. \tag{5.23}$$

One of the advantages of the *cn*-topology is that it avoids the above-mentioned difficulties. Here are some of the properties of this topology, which will be relevant for the rest of the exposition:[65]

1. Ω is stable under the action of any polynomial of Bose operators,

$$P(B_1^{\pm},\ldots,B_n^{\pm})\Omega\subset\Omega. \tag{5.24}$$

2. Any polynomial of Bose CAOs is a continuous linear operator in Ω with respect to the *cn*-topology;

(5.25)

3. The scalar product in Ω is continuous with respect to the convergence defined by the *cn*-topology.

(5.26)

As a consequence, (5.23) holds for any series $\Sigma_{i=1}^{\infty}\Phi_i$ which converges in the *cn*-topology; moreover (5.26) yields $(\Sigma_{i=1}^{\infty}\Phi_i,\Psi)=\Sigma_{i=1}^{\infty}(\Phi_i,\Psi)$. The relevance of the *cn*-topology however goes far beyond the above-mentioned considerations. This topology, called nuclear topology, is of prime importance in the theory of generalized functions,[66,67] and their applications in quantum theory (see, for instance, Ref. 65).

Let $\mathcal{P}$ be the set of all linear operators in Ω defined everywhere in Ω, which are continuous in the *cn*-topology. With respect to the usual operations between operators $\mathcal{P}$ is an associative algebra.[66] According to (5.25) the Bose operators belong to $\mathcal{P}$. The quasi-Bose operators (5.1) (with domain of definition restricted to Ω) also belong to $\mathcal{P}$. Indeed $B(p)_i^{\pm}$ are bounded and hence continuous operators in Ω with respect to any r-normed topology. Let $B(\Phi_0;r,\epsilon)$ be an arbitrary open ball in the *cn*-topology; see (5.22). $B(\Phi_0;r,\epsilon)$ is an open ball also in the r-normed topology. Therefore the inverse image $O=[B(p)_i^{\pm}]^{-1}B(\Phi_0;r,\epsilon)$ of $B(\Phi_0;r,\epsilon)$ is an open set in the r-normed topology. Since the latter is weaker than the *cn*-topology, O is an open set also in the *cn*-topology. Thus, the inverse image $O=[B(p)_i^{\pm}]^{-1}B(\Phi_0;r,\epsilon)$ of any open ball (i.e., of any open set from the basis) in the *cn*-topology is an open set with respect to the same topology. Therefore $B(p)_i^{\pm}$ is a continuous operator in the *cn*-topology.

Introduce a topology on $\mathcal{P}$ in a way similar to the strong topology in the algebra $\mathcal{B}(\mathcal{H})$ of all bounded linear operators on a Hilbert space $\mathcal{H}$.[68] Let $\Phi_1,\ldots,\Phi_s$ be s different elements from Ω and ϵ be a positive number. A strong neighborhood $U(A_0;\Phi_1,\ldots,\Phi_s;\epsilon)$ of the operator $A_0\in\mathcal{P}$ is (defined as) the set of all operators $A\in\mathcal{P}$, which satisfy the inequalities

$$|(A-A_0)\Phi_k|_0<\epsilon, \quad \forall k=1,\ldots,s. \tag{5.27}$$

Definition 2: A strong topology on $\mathcal{P}$ is the topology with a basis of open sets consisting of all possible strong neighborhoods $U(A_0;\Phi_1,\ldots,\Phi_s;\epsilon)$ (namely the collection of strong neighborhoods, corresponding to any $A_0\in\mathcal{P}$, to any $\epsilon>0$, to any $s\in\mathbb{N}$, and to any sequence $\Phi_1,\ldots,\Phi_s$ of different elements from Ω).

Proposition 4: In the strong topology

$$\lim_{p\to\infty} B(p)_i^{\pm}=B_i^{\pm}, \quad i=1,\ldots,n. \tag{5.28}$$

Proof: In order to prove that (5.28) holds it is sufficient to show that every strong neighborhood $U(B_i^{\pm};\Phi_1,\ldots,\Phi_s;\epsilon)$ of $B_i^{\pm}$ contains all elements of the sequence $B(1)_i^{\pm},B(2)_i^{\pm},\ldots$ apart from a finite number of them. Since $U(B_i^{\pm};\Phi_1,\ldots,\Phi_s;\epsilon)=\cap_{k=1}^{s}U(B_i^{\pm};\Phi_k;\epsilon)$, it is sufficient to show that for any neighborhood $U(B_i^{\pm};\Phi;\epsilon)$ there exists an integer N such that $B(p)_i^{\pm}\in U(B_i^{\pm};\Phi;\epsilon)$ for any $p>N$ or, which is the same, see (5.27), that

$$|(B(p)_i^{\pm}-B_i^{\pm})\Phi|_0<\epsilon, \quad \forall p>N. \tag{5.29}$$

Equation (5.29) has to hold for any Φ and any ϵ. In general N depends on Φ and ϵ, $N=N(\Phi,\epsilon)$.

The fact that $B_i^{+}-B(p)_i^{+}$ is a continuous linear operator in Ω is essential since relations like (5.23) can be used. The latter together with (5.13)–(5.14) and (5.19) yields

$$(B_i^{+}-B(p)_i^{+})\Phi=\sum_{l_1+\cdots+l_n<p} c(L)\left(\sqrt{l_i+1}\left(1-\sqrt{1-\frac{\Sigma_k l_k}{p}}\right)|L\rangle_i+\sum_{l_1+\cdots+l_n\geqslant p} c(L)(\sqrt{l_i+1}|L\rangle_i\right). \tag{5.30}$$

The continuity of the scalar product with respect to the cn-topology and the fact that all terms on the right-hand side of (5.30) are orthogonal to each other yield

$$(|(B_i^{+}-B(p)_i^{+})\Phi|_0)^2=\sum_{l_1+\cdots+l_n<p}|c(L)|^2(l_i+1)\left(1-\sqrt{1-\frac{\Sigma_k l_k}{p}}\right)^2$$

$$+\sum_{l_1+\cdots+l_n\geqslant p}|c(L)|^2(l_i+1).$$

Let $\epsilon>0$. Select $p_0\in\mathbb{N}$ to be fixed. For any $p>p_0$,

$$\begin{aligned}(|(B_i^{+}-B(p)_i^{+})\Phi|_0)^2&=\sum_{l_1+\cdots+l_n\leqslant p_0}|c(L)|^2(l_i+1)\left(1-\sqrt{1-\frac{\Sigma_k l_k}{p}}\right)^2\\&+\sum_{p_0<l_1+\cdots+l_n<p}|c(L)|^2(l_i+1)\left(1-\sqrt{1-\frac{\Sigma_k l_k}{p}}\right)^2\\&+\sum_{l_1+\cdots+l_n\geqslant p}(1+l_i)|c(L)|^2\\&<\sum_{l_1+\cdots+l_n\leqslant p_0}|c(L)|^2(l_i+1)\left(1-\sqrt{1-\frac{\Sigma_k l_k}{p}}\right)^2\\&+\sum_{l_1+\cdots+l_n>p_0}(1+l_i)|c(L)|^2.\end{aligned} \tag{5.31}$$

Since the partial sums of $\Sigma_{l_1,\ldots,l_n=0}^{\infty}(1+l_i)|c(L)|^2$ constitute an increasing sequence of positive numbers, which is restricted from above, $\Sigma_{l_1,\ldots,l_n=0}^{\infty}(1+l_i)|c(L)|^2 \leqslant |\Phi|_1$, the series $\Sigma_{l_1,\ldots,l_n=0}^{\infty}(1+l_i)|c(L)|^2$ converges. Choose p_0 such that $\Sigma_{l_1+\cdots+l_n>p_0}(1+l_i)|c(L)|^2<\epsilon^2/2$. Then for any $p>p_0$,

$$
\begin{aligned}
(|(B_i^+ - B(p)_i^+)\Phi|_0)^2 &< \sum_{l_1+\cdots+l_n\leqslant p_0} |c(L)|^2(l_i+1)\left(1-\sqrt{1-\frac{\Sigma_k l_k}{p}}\right)^2+\frac{\epsilon^2}{2}\\
&< \sum_{l_1+\cdots+l_n\leqslant p_0} |c(L)|^2(l_i+1)\left(1-\sqrt{1-\frac{p_0}{p}}\right)^2+\frac{\epsilon^2}{2}\\
&< d\left(1-\sqrt{1-\frac{p_0}{p}}\right)^2+\frac{\epsilon^2}{2}, \qquad (5.32)
\end{aligned}
$$

where $d=\Sigma_{l_1+\cdots+l_n\leqslant p_0}|c(L)|^2(l_i+1)$ is a constant. Clearly there exists $N\in\mathbb{N}$ such that $d(1-\sqrt{1-p_0/p})^2<\epsilon^2/2$ for any $p>N$. Hence for every $\epsilon>0$ there exists a positive integer N such that $|(B_i^+ - B(p)_i^+)\Phi|_0<\epsilon$, $\forall p>N$, i.e., (5.29) holds.

In a similar way one proves that $\lim_{p\to\infty} B(p)_i^- = B_i^-$. This completes the proof. □

VI. BOSONIZATION OF *A*-STATISTICS

A simple comparison of (3.19)–(3.20) with (5.19) suggests that the Jacobson CAOs of any order p can be bosonized, namely that they can be expressed as functions of Bose CAOs $B_1^{\pm},\ldots,B_n^{\pm}$; see (5.20). Indeed, taking into account that $B_i^+B_i^-\equiv N_i$ is a number operator for bosons in a state i,

$$
N_i|L\rangle \equiv N_i|l_1,\ldots,l_i,\ldots,l_n\rangle = l_i|l_1,\ldots,l_i,\ldots,l_n\rangle, \quad i=1,\ldots,n, \qquad (6.1)
$$

one rewrites (3.19) as

$$
a_i^+|L\rangle = \sqrt{(l_i+1)\left(p-\sum_{k=1}^{n} N_k+1\right)}|L\rangle_i .
$$

In view of (5.19) the latter can also be represented as

$$
a_i^+|L\rangle = \sqrt{p+1-\sum_{k=1}^{n} N_k}\; B_i^+|L\rangle = B_i^+\sqrt{p-\sum_{k=1}^{n} B_k^+B_k^-}|L\rangle. \qquad (6.2)
$$

Since (6.2) holds for any $|L\rangle$,

$$
a_i^+ = B_i^+\sqrt{p-\sum_{k=1}^{n} B_k^+B_k^-}, \quad i=1,\ldots,n. \qquad (6.3)
$$

In a similar way one derives from (3.20):

$$
a_i^- = \sqrt{p-\sum_{k=1}^{n} B_k^+B_k^-}\; B_i^- , \quad i=1,\ldots,n. \qquad (6.4)
$$

Evidently also, see (3.21),

$$
h_0 = p-\sum_{k=1}^{n} B_k^+B_k^- . \qquad (6.5)
$$

Note that the entire Fock space W is reducible with respect to the Jacobson CAOs. Its finite-dimensional "physical" subspace W_p, see (5.12), is a simple (=irreducible) $gl(n+1)$-module and within this module $(a_i^+)^*=a_i^-$ holds.

After simple calculations and taking into account that $a_i^+=e_{i0}$, $a_i^-=e_{0i}$, $i=1,\ldots,n$, see (2.3), one can express all generators $\{e_{ij}|i,j=0,1,\ldots,n\}$ of $gl(n+1)$ via n pairs of Bose operators:

$$e_{ij}=B_i^+B_j^-, \quad i,j=1,\ldots,n, \tag{6.6a}$$

$$e_{i0}=B_i^+\sqrt{p-\sum_{k=1}^{n}B_k^+B_k^-}, \quad e_{0i}=\sqrt{p-\sum_{k=1}^{n}B_k^+B_k^-}\;B_i^-, \quad i=1,\ldots,n, \tag{6.6b}$$

$$e_{00}=p-\sum_{k=1}^{n}B_k^+B_k^-, \tag{6.6c}$$

where, we recall, p is any positive integer, $p\in\mathbb{N}$.

The above-presented bosonization of $gl(n+1)$ is not unknown. Up to a choice of notation it is the same as the so-called Holstein–Primakoff (HP) realization of $gl(n+1)$,[47] initially introduced for $sl(2)$.[69,70] Note that (6.6a) alone gives the known Jordan–Schwinger realization of $gl(n)$ via n pairs of Bose operators.

VII. QUASI-BOSE OPERATORS IN SPIN MODELS

In the present section we show that the Jacobson CAOs are implicitly present in various models. We demonstrate this on the example of a two-leg $S=1/2$ Heisenberg spin ladder.[48,49] The considerations in the following hold however for several other Heisenberg spin models (examples include lattice models with dimerization,[71–73] two-layer Heisenberg models[74–76]) and more generally for any hard-core Bose model[50] with degenerated orbitals per site (as for instance in Refs. 77 and 78).

The Hamiltonian of the model reads:

$$\hat{H}=\sum_i\,(J\hat{\mathbf{S}}_i^+\hat{\mathbf{S}}_{i+1}^++J\hat{\mathbf{S}}_i^-\hat{\mathbf{S}}_{i+1}^-+J_\perp\hat{\mathbf{S}}_i^+\hat{\mathbf{S}}_i^-). \tag{7.1}$$

Here $\hat{\mathbf{S}}_i^\pm\equiv(\hat{S}_{1i}^\pm,\hat{S}_{2i}^\pm,\hat{S}_{3i}^\pm)$ are two commuting spin-1/2 vector operators "sitting" on site i of the chain $\pm$ and the Hamiltonian is a scalar with respect to the total spin operator $\hat{\mathbf{S}}=\Sigma_i(\hat{\mathbf{S}}_i^++\hat{\mathbf{S}}_i^-)$:

$$[\hat{S}_{\alpha i}^\pm,\hat{S}_{\beta i}^\pm]=i\sum_\gamma\,\epsilon_{\alpha\beta\gamma}\hat{S}_{\gamma i}^\pm, \quad [\hat{S}_{\alpha i}^+,\hat{S}_{\beta j}^-]=0, \quad [\hat{H},\hat{\mathbf{S}}]=0. \tag{7.2}$$

Every local state space W_i related to site i is four-dimensional with a basis $|\uparrow,\uparrow\rangle$, $|\uparrow,\downarrow\rangle$, $|\downarrow,\uparrow\rangle$, $|\downarrow,\downarrow\rangle$ and $W=W_1\otimes W_2\otimes\cdots\otimes W_N$ is the global state space of the system (in the case of a ladder with N sites). The notation is standard: if A is any operator in W_i, then the operator corresponding to it in W is denoted as A_i, where $A_i\equiv id_1\otimes\ldots\otimes id_{i-1}\otimes A\otimes id_{i+1}\otimes\ldots\otimes id_N$.

If the system is in a disordered phase ($J_\perp\gg J$) its state is well described with the bond operator representation of spin operators,[71,79] which is a particular kind of bosonization:

$$\hat{S}_{\alpha i}^\pm=\tfrac{1}{2}(\pm B_{\alpha i}^-\pm B_{\alpha i}^+-i\epsilon_{\alpha\beta\gamma}B_{\beta i}^+B_{\gamma i}^-), \quad \alpha,\beta,\gamma=1,2,3. \tag{7.3}$$

Here $B_{1i}^\pm$, $B_{2i}^\pm$, $B_{3i}^\pm$ are three pairs of Bose CAOs related to site i and the vectors $|0\rangle_i$, $B_{1i}^+|0\rangle_i$, $B_{2i}^+|0\rangle_i$, $B_{3i}^+|0\rangle_i$ constitute another basis in W_i.

The treatment of the model in terms of bosonic operators is advantageous because of the simpler commutation rules of Bose statistics. However, it raises certain problems. As mentioned previously, any local state space W_i is four-dimensional, whereas the local Bose Fock space Φ_i is

infinite-dimensional. Moreover W_i is not invariant in Φ_i with respect to the Bose CAOs [and, as a result, with respect to the local spin operators (7.3)]. The physical state space W is not an invariant subspace of the global Fock space $\Phi=\Phi_1\otimes\Phi_2\otimes\cdots\otimes\Phi_N$ with respect to the Hamiltonian (7.1).

Various approaches have been proposed in order to overcome the problem. Following Ref. 71, additional scalar bosons $s_i^{\pm}$ were introduced in Ref. 48. Then the physical states are those which satisfy an additional constraint $s_i^+ s_i+\Sigma_\alpha B_{i\alpha}^+ B_{i\alpha}=1$. Another way is to keep the realization (7.3) but to introduce "by hands" a fictitious infinite on-site repulsion between the "bosons" [75] (first proposed in Ref. 50 for a nondegenerate case). This forbids configurations with two or more bosons accommodated on one and the same site. The latter leads to the "hard-core" condition $B_{\alpha i}^{\pm} B_{\beta i}^{\pm}=0$, i.e., the hard-core bosons are not quite bosons, since they satisfy fermionic-like conditions.

A third approach was worked out in Ref. 79 (see also Refs. 72–74). It proposes the Bose operators $B_{\alpha i}^{\pm}$ in (7.3) to be replaced throughout by new operators $b_{\alpha i}^{\pm}$ as follows:

$$B_{\alpha i}^+\to b_{\alpha i}^+=B_{\alpha i}^+\sqrt{1-\sum_{\beta=1}^{3} B_{\beta i}^+ B_{\beta i}^-},\quad B_{\alpha i}^-\to b_{\alpha i}^-=\sqrt{1-\sum_{\beta=1}^{3} B_{\beta i}^+ B_{\beta i}^-}\; B_{\alpha i}^-. \tag{7.4}$$

A simple comparison with (6.3) and (6.4) indicates the following.

1. The Bose operators related to site i, i.e., $B_{1i}^{\pm}$, $B_{2i}^{\pm}$, $B_{3i}^{\pm}$, are replaced by $p=1$ Jacobson CAOs (or, which is the same, by $p=1$ quasi-Bose operators),

$$B(1)_{\alpha i}^{\pm}\equiv b_{\alpha i}^{\pm},\quad \alpha=1,2,3, \tag{7.5}$$

in their Holstein–Primakov realization. Consequently (Proposition 3) the hard-core condition $b_{\alpha i}^+ b_{\beta i}^+=0$ holds.

2. The Jacobson CAOs from different sites commute:

$$[b_{\alpha i}^{\xi}, b_{\beta j}^{\eta}]=0 \quad \text{if } i\neq j \text{ for any } \xi,\eta=\pm \text{ and } \alpha,\beta=1,2,3. \tag{7.6}$$

It is essential that the substitution (7.4) does not change the commutation relations (7.2) between the new spin operators

$$S_{\alpha i}^{\pm}=\tfrac{1}{2}(\pm b_{\alpha i}^-\pm b_{\alpha i}^+-i\epsilon_{\alpha\beta\gamma} b_{\beta i}^+ b_{\gamma i}^-),\quad \alpha,\beta,\gamma=1,2,3, \tag{7.7}$$

and the corresponding new Hamiltonian

$$H=\sum_i (J\mathbf{S}_i^+\mathbf{S}_{i+1}^+ + J\mathbf{S}_i^-\mathbf{S}_{i+1}^- + J_\perp \mathbf{S}_i^+\mathbf{S}_i^-). \tag{7.8}$$

Moreover each local state space W_i is an invariant subspace of Φ_i with respect to the Jacobson CAOs and hence with respect to any function of them [in particular with respect to the spin operators (7.7)]. The Hamiltonian (7.8) is also a well-defined operator in W.

The conclusion is that replacing the Bose operators throughout the model with $p=1$ Jacobson CAOs $b_{\alpha i}^{\pm}$, which commute at different sites [see (7.6)], one obtains directly the physical state space and the correct expressions for the spin operators and the Hamiltonian.

Let us point out that the above-mentioned results can be also derived from the following proposition, which is of independent interest.

Proposition 5: Let $B_\alpha^{\pm}$, $\alpha=1,\ldots,n$, be n pairs of Bose CAOs with a Fock space $\mathcal{F}$ and a basis (5.8). Denote by $\mathcal{F}_1$ the subspace of $\mathcal{F}$ linearly spanned on the vacuum and all "single-particle" states,

$$\mathcal{F}_1=\mathrm{span}\{|l_1,\ldots,l_n\rangle | l_1+\cdots+l_n\leq 1\}. \tag{7.9}$$

Let $\mathcal{P}$ be a projection operator of $\mathcal{F}$ onto $\mathcal{F}_1$:

$$\mathcal{P}|l_1,\ldots,l_n\rangle=\begin{cases}|l_1,\ldots,l_n\rangle & if\ \ l_1+\cdots+l_n\leqslant 1\\ 0 & if\ \ l_1+\cdots+l_n>1.\end{cases} \tag{7.10}$$

Then the operators $\mathcal{P}B_\alpha^\pm\mathcal{P}$, $\alpha=1,\ldots,n$, considered as operators in $\mathcal{F}_1$, are $p=1$ Jacobson CAOs,

$$\mathcal{P}B_\alpha^\pm\mathcal{P}=B(1)_\alpha^\pm\equiv b_\alpha^\pm,\quad \alpha=1,\ldots,n. \tag{7.11}$$

Proof: One verifies directly that (2.5) and (3.24) hold. □

Coming back to the two-leg spin ladder model, introduce a projection operator $\mathcal{P}_w=\mathcal{P}_1\otimes\mathcal{P}_2\otimes\cdots\otimes\mathcal{P}_N$ of Φ onto W, where each $\mathcal{P}_i$ projects Φ_i onto W_i according to (7.10) with $n=3$. The projector $\mathcal{P}_w$ provides an alternative way for writing down the expressions for the spin operators (7.7) and the Hamiltonian (7.8). Instead of using the substitution (7.4), one can set:

$$H=\mathcal{P}_w\hat{H}\mathcal{P}_w,\quad S_{\alpha i}^\pm=\mathcal{P}_i\hat{S}_{\alpha i}^\pm\mathcal{P}_i,\quad i=1,\ldots,N. \tag{7.12}$$

The operator $\mathcal{P}_w$ is a Bose analog of the Gutzwiller projection operators,[80] extensively used in the t-J models in order to exclude the double occupation of fermions at each site (see, for instance, Ref. 81 where a similar problem, a t-J two-leg ladder is investigated).

VIII. CONCLUDING REMARKS

From a mathematical point of view the JGs $a_1^\pm,\ldots,a_n^\pm$ provide a new description of the Lie algebra $sl(n+1)$ in terms of generators and relations (2.5), based on the concept of Lie triple systems. For the same reason any n pairs of parafermions (respectively, parabosons) can be called Jacobson generators of the orthogonal Lie algebra $so(2n+1)$ [respectively, of the orthosymplectic Lie superalgebra $osp(1/2n)$]. The JGs provide an alternative to the Chevalley descriptions of these Lie (super)algebras.

From a physical point of view the interest in the JGs of $sl(n+1)$ stems from the observation that they indicate the possible existence of a new quantum statistics. Indeed, we have seen that within each Fock space W_p the operator a_i^+ (respectively, a_i^-) can be interpreted as an operator creating (respectively, annihilating) a particle in a state i (in particular with an energy ϵ_i).

In many respects the quasibosons behave as bosons. Similar to bosons, the quasibosons can be distributed along the orbitals in an arbitrary way as far as the number of accommodated particles M does not exceed p. The number of different states of $M\leqslant p$ quasibosons is the same as for bosons (the M-particle subspaces of quasibosons and bosons have one and the same dimension). There is however one essential difference: quasiboson systems of order p can accommodate at most p particles.

In order to use a proper Lie algebraic language we have restricted our consideration to finite-dimensional Lie algebras. In other words, we were studying systems with a finite number n of orbitals. Such systems certainly do exist. Examples are the local state spaces of spin systems (in particular the example considered in Sec. VII), $su(n)$ lattice models, etc. Nevertheless it is natural to ask whether A-statistics can be extended to incorporate infinitely many orbitals as this is usual in quantum theory. The answer to this question is positive and it is in fact evident from the results we have obtained so far. First of all the description of $sl(n+1)$ via generators (2.3) and relations (2.5) is well defined for $i,j,k\in\mathbb{Z}_+$, namely for $sl(\infty)=\mathrm{span}\{e_{ij}-\delta_{ij}e_{00}|i,j\in\mathbb{Z}_+\}$ [an equivalent definition is to say that $sl(\infty)$ is the algebra of all traceless infinite (in one direction) matrices containing no more than a finite number of nonzero entries]. Second, any Fock module W_p as given in Corollary 2 and in particular Eq. (3.9) are also well defined for $i,j,k\in\mathbb{N}$. In this case any W_p is an irreducible $sl(\infty)$ module, generated out of the vacuum by means of the Jacobson creation operators. Therefore each state $|p;l_1,\ldots,l_i,\ldots\rangle$ contains no more than a finite number of nonzero entries l_i. Moreover due to Proposition 3 the physical state space is a linear span of all vectors $|p;l_1,\ldots,l_i,\ldots\rangle$ with

$$\sum_{i=1}^{\infty} l_i \leqslant p. \tag{8.1}$$

All such states constitute an (orthonormal) basis in W_p. They transform according to the same relations (3.19) and (3.20) with $n=\infty$. It is straightforward to verify that any $sl(\infty)$ module W_p is a Fock space in the sense of Definition 1. Finally, the Pauli principle (Corollary 3) remains valid also for $n=\infty$: despite the infinitely many available orbitals, the infinitely many places to be occupied by the quasibosons, the system cannot accommodate more than p particles. [For an overview of commonly recognized definitions of $gl(\infty)$, see Ref. 82, where in particular several types of infinite dimensional Lie superalgebras of type gl are studied.]

We should point out that within A-statistics the main quantization equation (2.6) does not determine uniquely the creation and annihilation operators. The Jacobson generators (2.3) yield one possible solution of (2.6). For another possible choice (a causal A-statistics), we refer to Ref. 83.

The quasi-Bose operators $B(p)_1^{\pm},\ldots,B(p)_n^{\pm}$, introduced in Sec. V can be used as an approximation to Bose statistics for values of the order of statistics p, which is much bigger than the number of accommodated particles. An additional advantage of the quasi-Bose CAOs of any order p is that they are bounded linear operators, defined everywhere in the Fock space W_p. This property avoids the rather delicate questions of whether the operators under consideration can be defined on a common domain of definition Ω, so that any polynomial of them is also well defined in Ω.

The "opposite" to $p\to\infty$ case, namely the $p=1$ Jacobson CAOs (or, which is the same, the $p=1$ quasi-Bose operators) turns out to appear implicitly in various models simply because the hard-core bosons are $p=1$ quasibosons. We have illustrated this on a particular example from condensed matter physics. This observation does not lead to immediate new results as far as hard-core Bose models are concerned. Even so, we believe that the clarification of the hidden quasiboson structure of these models is of some interest. If, for instance, the Hamiltonian is written explicitly via quasibosons, then the model is representation independent. Considering instead of the hard-core bosons quasibosons with order of statistics $p=M$, one is led to a model where each site can accommodate up to M particles.

For applications of quasiboson representations in nuclear theory we refer to Ref. 60. As indicated there, the $p=1$ quasi-Bose operators reduce to Klein–Marshalek algebras,[84] which are extensively used in nuclear physics.

One way to enlarge the class of statistics studied here is to deform the relations (2.5) or, which is the same, to deform $sl(n+1)$ so that the main quantization equation (2.6) remains unaltered. The possibility for such deformations stems from the observation that the commutation relations between the Cartan elements [the Hamiltonian is a Cartan element; see (2.17)] and the root vectors [the Jacobson generators are root vectors; see (2.4)] remain unaltered upon quantum deformations (q-deformations). Therefore the problem actually is to express the known q-deformations of $sl(n+1)$ via deformed Jacobson generators. This is the first step. The second step will be to define the Fock representations and to write down the deformed analog of (3.19) and (3.20). Partial results in this respect were already announced.[85,86]

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Erratum: "Euclidean Friedman–Robertson–Walker cosmology in Brans–Dicke-like theories of gravity" [J. Math. Phys. 43, 1487 (2002)]

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In a recent paper, I have studied the cosmological model in Brans–Dicke gravity, in the matter dominated area.[1] The set of equations considered in the paper, and often considered in papers dealing with this problem, is the equation BD(0,0), obtained replacing the indices i and j by zero in the Brans–Dicke equation,[2] the scalar field equation BD(Φ), and the conservation equation BD(C). BD(C) writes $\rho a^3 = Cste$ in the problem under consideration. The conservation equation BD(C) is a consequence of the full set of cosmological equations. This full set is BD(0,0), BD(1,1) and BD(Φ). BD(1,1) is obtained replacing the indices i and j by one in the Brans–Dicke equation, which gives

$$2\frac{\ddot{a}}{a}+\left(\frac{\dot{a}}{a}\right)^2+\frac{\omega}{2}\left(\frac{\dot{\Phi}}{\Phi}\right)^2+2\frac{\dot{a}}{a}\frac{\dot{\Phi}}{\Phi}+\frac{\ddot{\Phi}}{\Phi}=0.$$

The solutions of the system [BD(0,0), BD(Φ), BD(C)], studied in the paper, are

(a) a set $S_1(A,P)$, depending on two arbitrary constants, for $\omega > -3/2$; these solutions are referenced (13) and (14) in the paper;[1]
(b) a set $S_2(A,P)$, depending on two arbitrary constants, for $\omega < -3/2$; these solutions are referenced (19) and (20) in the paper;[1]
(c) a set $S_3(A)$, depending on one arbitrary constant, for $\omega < -3/2$; these solutions are referenced (9) and (10) in the paper.[1]

By inserting these solutions in the field equation BD(1,1), it turns out that this equation is not verified by $S_3(A)$ (while it is by both $S_1(A,P)$ and $S_2(A,P)$). $S_3(A)$ is then not a set of solutions of the full set of Brans–Dicke cosmological equations.

It could be worthwhile remarking that, while the system [BD(0,0), BD(Φ), BD(C)] is not strictly equivalent to the full system [BD(0,0), BD(1,1), BD(Φ)], it is equivalent up to a subset of solutions of zero measure. This is differs from what happens in general relativity, where there is strict equivalence between the two systems [EE(0,0), EE(1,1)] and [EE(0,0), EE(C)] (EE for Einstein equation) in the framework of Friedman–Robertson–Walker cosmology.

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Symmetry breaking regime in the nonlinear Hartree equation

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The present article is concerned with minimizers of the *attractive* Hartree energy functional $\mathcal{H}_g[\overline{\psi},\psi]=\frac{1}{2}\|\nabla\psi\|_2^2+(\psi,v\psi)_2+g(\psi,V*|\psi|^2\psi)_2$ on $\mathbb{R}^d$, $d\geqslant 2$, for a general class of external potentials v and two-body interactions V of positive type, with $g<0$. We prove spontaneous symmetry breaking in the large coupling limit. A numerical investigation visualizes this regime in the example of an external double well potential. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1488673]

I. INTRODUCTION

In this article we investigate the problem of *uniqueness* of minimizers of the Hartree energy functional

$$\mathcal{H}_g[\overline{\psi},\psi]:=\tfrac{1}{2}\|\nabla\psi\|_2^2+(\psi,v\psi)_2+g\,(\psi,V*|\psi|^2\psi)_2 \tag{1}$$

in an external potential v, for *attractive* two-body interaction gV, V of positive type (e.g., the Coulomb potential),

$$g<0. \tag{2}$$

The main results of this article are described in Theorems 1 and 2 in the next section: we prove that, for *small* couplings, there exists one and only one minimizer of the Hartree functional (1), whereas, for *large* enough couplings, minimizers of (1) are *not* unique!

The *existence* of minimizers of (1) is assured by the following well known facts: minimizers exist for all $g<0$, as soon as $|g|$ exceeds some critical value $g_*\geqslant 0$, $|g|\geqslant g_*$ (for vanishing v, or for a nonzero v); the existence of a g_* follows from standard arguments in the calculus of variations, whereas the size of g_* can be determined with the help of Birman–Schwinger theory of binding in quantum mechanics. For $v=0$, it implies that, in $d=1,2$ dimensions, the critical coupling vanishes, $g_*=0$. This also holds in $d\geqslant 3$ dimensions for *long range* two-body potentials V. For *short range* potentials V, the threshold is *strictly above zero*, $g_*>0$, for $d\geqslant 3$ (e.g., by the Cwikel–Lieb–Rozenblujm bound), cf. Ref. 1. In the case of a nonvanishing *confining* external potential, $v\neq 0$, a minimizer *always* exists (i.e., for all $g\geqslant g_*=0$). Nevertheless, there is a new *strictly positive* critical coupling, g_v, say, which relates the length scale, Δ_H, set by a minimizer to the length scale, Δ_v, of the external potential by

$$\Delta_H\approx\Delta_v,\ \text{for}\ |g|<g_v,\quad \Delta_H\ll\Delta_v,\ \text{for}\ |g|>g_v,$$

and Δ_H is *independent* of the external potential v.

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We may compare the foregoing to the existence properties of minimizers of the following *local* functional (i.e., with $V=\delta$), called the *Gross–Pitaevskii functional*,

$$\mathcal{H}_g^{GP}[\overline{\psi},\psi] := \tfrac{1}{2}\|\nabla\psi\|_2^2 + g\,\|\psi\|_{p+1}^{p+1}, \quad p=3, \tag{3}$$

which does not possess any *global* minimizer for $g<0$: plugging the dilate wave function $\psi_\lambda(x) := \lambda^{d/2}\psi(\lambda x)$, $\lambda\in\mathbb{R}^+$, into (3), we arrive at

$$\mathcal{H}_g^{GP}[\overline{\psi_\lambda},\psi_\lambda] = \lambda^2\tfrac{1}{2}\|\nabla\psi\|_2^2 + g\,\lambda^{(d/2)(p-1)}\|\psi\|_{p+1}^{p+1}. \tag{4}$$

For *attractive* interaction, $g<0$, the scaled functional (4) diverges to $-\infty$ in the limit $\lambda\to\infty$ if $p>1+4/d$, in d dimensions. For $d\geqslant 3$ and $p=3$, this is the case [and (4) tends to $-\infty$ in the limit $\lambda\to\infty$, for $d=2$, provided $|g|$ is sufficiently large]!

One of our *physical motivations* for the investigation of the Hartree functional (1) comes from a description of Bose–Einstein condensation (BEC) based on an analysis of the *weak coupling limit of large bosonic systems*, cf. Refs. 2–4. In the standard BEC scenario, where the interatomic force is *repulsive* and the mean interboson distance is much larger than the range of the two-body potential V, low-energy scattering theory implies that the Hartree nonlinearity may be assumed to be *local*, $V=\delta$. However, for the case of *attractive* interatomic forces, $g<0$, e.g., for lithium ($^7_3$Li, with scattering length -1.45×10^{-9} m, cf. Ref. 5), the system undergoes a collapse, as soon as the number of condensate atoms exceeds a critical value, cf. Refs. 6 and 7. Using a nonlocal two-body potential V provides a less coarse-grained resolution of the boson–boson interaction (compared to $V=\delta$).

We stress that for a system of bosonic atoms close to collapse *collision processes* become important, see, e.g., Ref. 8. Such processes (as well as interactions of electrons and nuclei with the radiation field) are *not* taken into account in a description of the system in terms of Hartree theory. Furthermore, if we neglect short range repulsive (soft core or hard core) interactions between the atoms, such that the two-body forces are *purely attractive*, we are dealing with a system that is *not thermodynamically stable*.

Nevertheless, in the *mean-field regime*, a dilute gas of bosonic atoms is well described by Hartree theory, and, remarkably, this theory continues to be meaningful, *mathematically*, as the collapse point of a system with attractive two-body forces is approached, and even beyond that point. It may thus be expected to reproduce *qualitatively* some features of *structure formation* in a gas of bosonic atoms with attractive two-body forces, such as $^7_3$Li. One may expect that Hartree theory also provides a qualitatively valuable description of bosonic dwarf stars if the two-body potential gV is chosen to be the Newtonian gravitational potential. These features of Hartree theory contrast with the limited applicability of the *local* Gross–Pitaevskii functional, which does not have global minimizers for *attractive* two-body interactions.

In this article, we modestly study some variational problems associated with the Hartree energy functional. Our main results are rigorous, mathematically. They are important as ingredients for studies of Hartree *dynamics*. But we do not address dynamical problems in this article.

It was kindly brought to our attention that similar topics have been investigated in Refs. 9–13.

II. SYMMETRY BREAKING REGIME AT FINITE COUPLING

In this section we will prove that for large enough negative coupling g the minimizer of the functional (1) will break very general symmetries possibly induced by the external potential v. For convenience, we will formulate this statement for $N=\|\psi\|_2^2$ instead of g, which without loss of generality will be set equal to -1. Theorem 1 will be worked out for the case where V is a Coulomb potential, but at the end of the proof we will briefly discuss other potentials.

Our main theorem is the following.

Theorem 1: *Let V be the Coulomb potential in $\mathbb{R}^d$, $V=|x|^{-1}$, and $v\in C_b(\mathbb{R}^d)$, $d\geqslant 2$. Let $E(d)$ be the Euclidean group in d dimensions.*

If for some $R\in E(d)$, any minimizing sequence $x_k\in\mathbb{R}^d$ for the external potential v,

$$\lim_{k\to\infty} v(x_k) = \inf_{x\in\mathbb{R}^d} v(x), \tag{5}$$

fulfills

$$\liminf_{k\to\infty} |Rx_k - x_k| > 0,$$

then, for sufficiently large N, any minimizer Φ of the Hartree functional (1) satisfies

$$|\Phi\circ R|^2 \neq |\Phi|^2.$$

Remark: If the infimum of v is attained on its set X of minimima only, i.e., if (5) implies $\lim_{k\to\infty} \mathrm{dist}(x_k, X) = 0$, then the hypothesis simply means $\inf\{|Rx_* - x_*| \,|\, x_* \in X\} > 0$.

Corollary 1 (symmetry breaking): If $v \in C_b(\mathbb{R}^d)$ has a symmetry $R \in E(d)$, then Theorem 1 predicts symmetry breaking in the sense that no ground state wave function Φ is invariant under R.

The formulation of Theorem 1 is quite general. For illustration we consider more closely the particular cases of (a) a nonvanishing external potential consisting in a double well which has as discrete symmetry respective to the reflection at the axis orthogonal to the line between its two separate minima, (b) the Mexican hat and (c) a periodic potential. Case (a) is considered also in view of our numerical simulations. Note that Theorem 1 is not restricted to discrete symmetries at all. The corollary now tells us that for sufficiently large coupling g the ground state Φ of the case considered will not have the symmetry properties of (a) the double well, (b) the Mexican hat, resp. (c) the periodic potential. In the cases (a) and (b) this means that Φ can be localized either in one or the other well, resp. part of the Mexican hat. We mention that for a single well potential the hypotheses of the theorem are not fulfilled for any R which is a symmetry of the potential.

Proof of Theorem 1: The proof of Theorem 1 will be done in three steps corresponding to Lemma 1, Lemma 2 and the proof of the theorem itself: The first step of our proof is to show that an approximate minimizer of the *free* energy functional (i.e., without external potential),

$$\mathcal{E}_g[\overline{\psi}, \psi] = \tfrac{1}{2}\|\nabla\psi\|_2^2 + g(\psi, V*|\psi|^2\psi)_2, \quad g<0, \tag{6}$$

will be concentrated in a ball in space whose size can be arranged by varying the size of N. This is stated somewhat more accurately in the following lemma. There the term *η-approximate minimizer* (of the *free* functional) is used: Let $\eta>0$. An *η-approximate minimizer* is defined as a wave function ψ that satisfies

$$\|\psi\|_2^2 = N, \quad \mathcal{E}_{-1}[\overline{\psi}, \psi] \leqslant (1-\eta)E_N, \quad E_N := E[N, -1],$$

where

$$E[N,g] := \inf\{\mathcal{E}_g[\overline{\psi}, \psi] \,|\, \psi \in W^{1,2}(\mathbb{R}^d), \|\psi\|_2^2 = N\}.$$

Lemma 1 (concentration of approximate minimizer): Given $\delta>0$, there is $\eta>0$ such that, for N large enough, any η-approximate minimizer ψ obeys

$$\int_{B(y,\delta)} d^dx\, |\psi(x)|^2 \geqslant (1-\delta)N \quad \textit{for some} \quad y \in \mathbb{R}^d. \tag{7}$$

It will then be shown that the minimizer of the full energy functional (1) is an approximate minimizer of the free energy functional, in the sense of Lemma 1, and that they are localized around the minima of the potential:

Lemma 2 (localization): Let $v \in C_b(\mathbb{R}^d)$ and $\epsilon,\delta>0$ be fixed. Then, for N large enough, any minimizer Φ of

$$\mathcal{H}_{-1}[\overline{\psi},\psi]=\mathcal{E}_{-1}[\overline{\psi},\psi]+\int_{\mathbb{R}^d}d^dx\,v(x)|\psi(x)|^2,\quad \|\psi\|_2^2=N, \tag{8}$$

satisfies

$$\int_{B(y,\delta)}d^dx|\Phi(x)|^2\geqslant(1-\delta)N \tag{9}$$

and

$$\inf_{x\in B(y,\delta)}v(x)\leqslant\inf_{x\in\mathbb{R}^d}v(x)+\epsilon. \tag{10}$$

The last step of our proof will explicitly prove symmetry breaking.

In the following a scaling property of the wave function and the ground state energy will be used: The scaled function $\psi_{N,g}(x)=|g|^{d/2}N^{(1+d)/2}\psi_{1,1}(|g|Nx)$ satisfies for $d\geqslant 2$

$$\|\psi_{N,g}\|_2^2=N\|\psi_{1,1}\|_2^2,\quad E[N,g]=g^2N^3E[1,-1],\quad E[1,-1]<0. \tag{11}$$

The key ingredient for the proof of Lemma 1 is a partition of unity in the following form: For some $\chi\in C_0^\infty(\mathbb{R}^d)$ with $0\leqslant\chi\leqslant 1$, $\|\chi\|_2=1$, $\mathrm{supp}(\chi)\subset B(0,1)$, the ball of radius 1 with center at 0, the convolution of these approximate characteristic functions satisfies

$$\int_{\mathbb{R}^d}d^dy\,\chi^2(x-y)\chi^2(x'-y)\geqslant 1-\gamma, \tag{12}$$

for any $0<\gamma\leqslant 1$ and for $|x-x'|<\epsilon(\gamma)$ small enough. The functions

$$j_y(x)=\delta^{-d/2}\chi(\delta^{-1}(x-y))\equiv\delta^{-d/2}\chi_{y,\delta}(x)$$

indexed by $y\in\mathbb{R}^d$ form a partition of unity:

$$\int_{\mathbb{R}^d}d^dy\,j_y^2(x)=1.$$

Using the IMS-localization formula[14]

$$p^2=\int dy\,j_y p^2 j_y-\int dy(\nabla j_y)^2,$$

with p being the momentum operator, we get for the kinetic energy

$$\frac{1}{2}\|\nabla\psi\|_2^2=\frac{\delta^{-d}}{2}\int_{\mathbb{R}^d}d^dy\,\|\nabla(\chi_{y,\delta}\psi)\|_2^2-\frac{\delta^{-2}}{2}\|\nabla\chi\|_2^2\|\psi\|_2^2. \tag{13}$$

Proof of Lemma 1: Using (12) and taking $|x-x'|<\epsilon(\gamma)\delta$ we write for the nonlinearity

$$(\psi,V*|\psi|^2\psi)_2\leqslant -g\delta^{-d}\int_{|x-x'|<\epsilon\delta}\int_{\mathbb{R}^d}d^dy\,\frac{d^dx\,d^dx'}{|x-x'|}|\chi_{y,\delta}(x)\psi(x)|^2\,|\chi_{y,\delta}(x')\psi(x')|^2$$
$$+\int_{|x-x'|\geqslant\epsilon\delta}\frac{d^dx\,d^dx'}{|x-x'|}|\psi(x)|^2|\psi(x')|^2,$$

where we have set $0>g=-(1-\gamma)^{-1}$. The last term is obviously bounded by $(\epsilon\delta)^{-1}N^2$. Using (13) and extending the double integral in the first term to the whole space, which can be done because the integrand is positive, we get

$$\mathcal{E}_{-1}[\overline{\psi},\psi]\geqslant\delta^{-d}\int_{\mathbb{R}^d}d^dy\,\mathcal{E}_g[\overline{\chi_{y,\delta}\psi},\chi_{y,\delta}\psi]-(\epsilon\delta)^{-1}N^2-\frac{\delta^{-2}}{2}\|\nabla\chi\|_2^2N \tag{14}$$

with $g=-(1-\gamma)^{-1}$. Now we use (11) and obtain

$$\begin{aligned}\mathcal{E}_{-1}[\overline{\psi},\psi]+(\epsilon\delta)^{-1}N^2+\frac{\delta^{-2}}{2}\|\nabla\chi\|_2^2N&\geqslant g^2\delta^{-d}\left(\int_{\mathbb{R}^d}d^dy\,\|\chi_{y,\delta}\psi\|_2^6E[1,-1]\right)\\&\geqslant g^2\delta^{-d}\sup_y\|\chi_{y,\delta}\psi\|_2^4\left(\int_{\mathbb{R}^d}d^dy(\|\chi_{y,\delta}\psi\|_2^2)E[1,-1]\right)\\&=g^2N\sup_y\|\chi_{y,\delta}\psi\|_2^4E[1,-1].\end{aligned}$$

By assumption $(1-\eta)N^3E[1,-1]\geqslant\mathcal{E}_{-1}[\overline{\psi},\psi]$ and, since $E[1,-1]<0$,

$$N^{-2}(\sup_y\|\chi_{y,\delta}\psi\|_2)^4g^2\geqslant(1-\eta)+\left((\epsilon\delta)^{-1}N^{-1}+\frac{\delta^{-2}}{2}\|\nabla\chi\|_2^2N^{-2}\right)E[1,-1]^{-1}.$$

Choose now $\gamma(\eta)$ such that

$$g^{-2}=(1-\gamma)^2\geqslant1-\eta.$$

For $N>N_0(\eta)$ sufficiently large,

$$\left((\epsilon\delta)^{-1}N^{-1}+\frac{\delta^{-2}}{2}N^{-2}\|\nabla\chi\|_2^2\right)E[1,-1]^{-1}\geqslant-\eta.$$

So one gets

$$(\sup_y\|\chi_{y,\delta}\psi\|_2)^4N^{-2}\geqslant(1-2\eta)(1-\eta)\geqslant\left(1-\frac{\delta}{2}\right)^2$$

for $\eta(\delta)$ small enough. And, finally,

$$\int_{B(y,\delta)}d^dx|\psi(x)|^2\geqslant\|\chi_{y,\delta}\psi\|_2^2\geqslant(1-\delta)N \tag{15}$$

for some $y\in\mathbb{R}^d$.

Proof of Lemma 2: It is enough to prove this lemma for a $\delta_0=O(\epsilon)$ because it then holds for any $\delta\geqslant\delta_0$ as well.

We first show that a minimizer Φ of (1) is an approximate minimizer of (6) and so by Lemma 1 the first statement holds.

For any ψ with $\|\psi\|_2^2=N$ one has by assumption: $\mathcal{H}_{-1}[\overline{\Phi},\Phi]\leqslant\mathcal{H}_{-1}[\overline{\psi},\psi]$. This gives

$$\mathcal{E}_{-1}[\overline{\Phi},\Phi]-\mathcal{E}_{-1}[\overline{\psi},\psi]\leqslant\int_{\mathbb{R}^d}d^dx\,v(x)(|\psi(x)|^2-|\Phi(x)|^2)\leqslant2\|v\|_\infty N$$

and by passing to the infimum over ψ

$$\mathcal{E}_{-1}[\overline{\Phi},\Phi]\leqslant E_N\left(1-\frac{2\|v\|_\infty N}{(-E_N)}\right)=E_N\left(1-\frac{2\|v\|_\infty}{N^2|E[1,-1]|}\right).$$

For N large enough the bracket is $\geqslant(1-\eta)$, where η is as in Lemma 1, and so

$$\mathcal{E}_{-1}[\overline{\Phi},\Phi]\leqslant E_N(1-\eta).$$

Hence (7) holds true.

The second statement of Lemma 2 will be proved by contradiction.

In the following we denote $\inf_{x\in\mathbb{R}^d} v(x)$ by v_*. Pick $y_0\in\mathbb{R}^d$ and $\delta>0$ small enough, so that

$$v(x)\leqslant v_*+\frac{\epsilon}{2}\quad \forall x\in B(y_0,\delta),$$

and assume the second statement is false. For

$$\tilde{\Phi}(x)=\Phi(x-(y_0-y)),$$

the translate of Φ by (y_0-y), one has

$$\int_{B(y_0,\delta)} d^dx|\tilde{\Phi}(x)|^2\geqslant(1-\delta)N$$

and, since $\int_{\mathbb{R}^d\setminus B(y_0,\delta)} d^dx\,|\tilde{\Phi}(x)|^2\leqslant\delta N$,

$$\int_{\mathbb{R}^d} d^dx(v(x)-v_*)|\tilde{\Phi}(x)|^2\leqslant\frac{\epsilon}{2}N+\|v-v_*\|_\infty\delta N.$$

On the other hand, if (10) were false,

$$\int_{\mathbb{R}^d} d^dx\,(v(x)-v_*)|\Phi(x)|^2>\epsilon(1-\delta)N-\|v-v_*\|_\infty\delta N.$$

This gives

$$\begin{aligned}\mathcal{H}_{-1}[\bar{\tilde{\Phi}},\tilde{\Phi}]-\mathcal{H}_{-1}[\overline{\Phi},\Phi]&=\int_{\mathbb{R}^d} d^dx(v(x)-v_*)(|\tilde{\Phi}(x)|^2-|\Phi(x)|^2)\\&\leqslant-\frac{\epsilon}{2}(1-2\delta)N+2\|v-v_*\|_\infty\delta N\\&=-\left(\frac{\epsilon}{2}-\delta(2\|v-v_*\|_\infty+\epsilon)\right)N<0\end{aligned}$$

for $\delta<\epsilon/(4\|v-v_*\|+2\epsilon)$. This contradicts Φ being a minimizer and proves Lemma 2.

Proof of Theorem 1: By assumption, there is $0<\delta<\frac{1}{2}$ for ϵ sufficiently small such that

$$v(x)\leqslant\inf_{x'} v(x')+2\epsilon$$

implies

$$|Rx-x|>4\delta.$$

By Lemma 2,

$$\int_{B(y,\delta)} d^dx\,|\Phi(x)|^2\geqslant(1-\delta)N$$

holds for some y with

$$|Ry-y|>4\delta-2\delta=2\delta.$$

Assume $|\Phi(Rx)|\equiv|\Phi(x)|$. Then (9) also holds for y replaced by Ry. This leads to

$$N=\int_{\mathbb{R}^d}d^dx|\Phi(x)|^2\geqslant\int_{B(y,\delta)}d^dx|\Phi(x)|^2+\int_{B(Ry,\delta)}d^dx|\Phi(x)|^2\geqslant 2(1-\delta)N>N$$

since $B(y,\delta)$ and $B(Ry,\delta)$ are disjoint, which is a contradiction.

This proves Theorem 1.

We will now show how Theorem 1 can easily be extended to other potentials like the case where the two-body potential V is a potential of the form $V\in C_b(\mathbb{R}^d)$ such that $V(x)\to\sup V$ implies $x\to 0$. We first note that we have the following inequality for the energy of the minimizer:

$$E[N,-1]=E_N\leqslant -V(0)N^2+\rho,\quad \text{where}\ \ \rho=o(N^2)\ \ \text{as}\ \ N\to\infty. \tag{16}$$

The validity of this inequality can easily be seen by noting that the scaled function $\tilde{\phi}(x)=N^{1/2}a^{-d/2}\phi(a^{-1}x)$, $\|\phi\|_2^2=1$, satisfies

$$N^{-2}\mathcal{E}_g(\tilde{\phi})=a^{-2}N^{-1}\|\nabla\phi\|_2^2-\int_{\mathbb{R}^{2d}}d^d\tilde{x}d^d\tilde{x}'V(|\tilde{x}-\tilde{x}'|a)|\phi(\tilde{x})|^2|\phi(\tilde{x}')|^2,\quad \tilde{x}=a^{-1}x,$$

and $\|\tilde{\phi}\|_2=N$. Setting $a=N^{-1/3}$ and using dominated convergence in the limit of large N, one gets (16).

For the proof of Lemma 1 we note the following: We again split up the nonlinearity in (6) into two terms, one involving the integration over $|x-x'|<\epsilon\delta$ [with $\epsilon=\epsilon(\gamma)$ as in (12)] and the other over its complement. Noting that $\sup V:=V(0)>V(x)$ for $x\neq 0$ by assumption, we set $f(x,x')=|\psi(x)|^2|\psi(x')|^2$ and write

$$\begin{aligned}(\psi,V*|\psi|^2\psi)_2&\leqslant V(0)\int_{|x-x'|<\epsilon\delta}d^dxd^dx'f(x,x')+V^*\int_{|x-x'|\geqslant\epsilon\delta}d^dxd^dx'f(x,x')\\&=(V(0)-V^*)\int_{|x-x'|<\epsilon\delta}d^dxd^dx'f(x,x')+V^*N^2\\&=(V(0)-V^*)\left(\int_{|x-x'|<\epsilon\delta}d^dxd^dx'f(x,x')-N^2\right)+V(0)N^2,\end{aligned}$$

where we have set $V^*:=\sup_{|x-x'|\geqslant\epsilon\delta}V(x-x')$. Now we use (12) to get

$$(\psi,V*|\psi|^2\psi)_2\leqslant(V(0)-V^*)(-g\sup_{y\in\mathbb{R}^d}(\|\chi_{y,\delta}\psi\|_2^2)N-N^2)+V(0)N^2,$$

where again $g=-(1-\gamma)^{-1}$ and the first integral was evaluated as

$$\delta^{-d}\int_{|x-x'|<\epsilon\delta}\int_{\mathbb{R}^d}d^dyd^dxd^dx'|\chi_{y,\delta}(x)\psi(x)|^2|\chi_{y,\delta}(x')\psi(x')|^2\leqslant\sup_{y\in\mathbb{R}^d}(\|\chi_{y,\delta}\psi\|_2^2)N.$$

By assumption $(1-\eta)E[N,-1]\geqslant\mathcal{E}_{-1}(\overline{\psi},\psi)$ for an η-approximate ground state and using (16) we arrive at

$$(1-\eta)(V(0)N^2-\rho)\leqslant(V(0)-V^*)(-gN\sup_{y\in\mathbb{R}^d}(\|\chi_{y,\delta}\psi\|_2^2)-N^2)+V(0)N^2.$$

This is rewritten as

$$-g^{-1}\left(1-\frac{\eta V(0)+\rho N^{-2}}{V(0)-V^*}\right)\leqslant N^{-1}\sup_{y\in\mathbb{R}^d}(\|\chi_{y,\delta}\psi\|_2^2).$$

Setting now $\gamma=c^{-1}\delta$ with $c\gg\delta$ and choosing η small and N large enough, such that

$$\frac{\eta V(0)+\rho N^{-2}}{V(0)-V^*}<c^{-1}\delta,$$

we get

$$N^{-1}\sup_{y\in\mathbb{R}^d}(\|\chi_{y,\delta}\psi\|_2^2)\geqslant(1-c^{-1}\delta)^2\geqslant 1-\delta,$$

which gives the first lemma.

The proofs of the second lemma and of Theorem 1 are almost the same as before.

Remark: This is complemented by the following result, which conversely implies that no symmetry breaking of the ground state occurs at small coupling. This feature is reproduced by our numerical simulations.

Theorem 2: (positive critical coupling for $d\geqslant 1$): *Let the two-body potential* $V\in L^1(\mathbb{R}^d)\cap L^\infty(\mathbb{R}^d)$ *be real-valued, and the external potential* $v\in C_b(\mathbb{R}^d)$, $d\geqslant 1$, *such that*

$$H_0=-\tfrac{1}{2}\Delta+v \tag{17}$$

has an isolated ground state.

Then, for sufficiently small coupling $|g|$, *there exists a unique nonlinear ground state* ψ, $\|\psi\|_2=1$, *of*

$$H_g^{(\psi)}=H_0+gV*|\psi|^2. \tag{18}$$

This implies that, in any dimension $d\geqslant 1$, *symmetry breaking occurs above a strictly positive critical coupling* g_* *only,* $|g|>g_*$.

Proof of Theorem 2: The ground state energy E_0 of H_0 is nondegenerate by the Perron–Frobenius theorem (see, e.g., Ref. 1). Let ψ_0 (with $\|\psi_0\|\equiv\|\psi_0\|_2=1$) be the corresponding ground state, and P_0 its eigenprojection. The perturbation in (29) is bounded in operator norm since $\|V*|\psi|^2\|\leqslant\|V\|_\infty\|\psi\|^2$; hence, $H_g^{(\psi)}$ is an analytic family of type A. By the Kato–Rellich theorem[1] and its proof, we have the following.

(i) Let Γ be a circle around E_0 of small enough radius r, so that no other point in $\sigma(H_0)$ is encircled. Then

$$C\equiv\sup\|(H_g^{(\psi)}-z)^{-1}\|<\infty,$$

where the supremum is over $z\in\Gamma$, $|g|<g_*$ and $\|\psi\|\leqslant 1$, provided g_* is small enough.

(ii) For such g and ψ there is precisely one (nondegenerate) eigenvalue of $H_g^{(\psi)}$ within Γ. It is the ground state energy, and its eigenprojection is

$$P_g^{(\psi)}=-(2\pi i)^{-1}\oint_\Gamma dz(H_g^{(\psi)}-z)^{-1}.$$

A nonlinear ground state is the same (up to the phase) as a fixed point of the map

$$T:\ \mathcal{S}=\{\|\psi\|=1\}\to\mathcal{S},\quad \psi\mapsto\frac{P_g^{(\psi)}\psi_0}{\|P_g^{(\psi)}\psi_0\|}. \tag{19}$$

By the contraction mapping principle,[15] it suffices to prove that T is a *strict contraction*. Indeed,

$$P_g^{(\psi)}-P_g^{(\phi)}=(2\pi i)^{-1}\oint_\Gamma dz(H_g^{(\psi)}-z)^{-1}(gV*(|\psi|^2-|\phi|^2))(H_g^{(\phi)}-z)^{-1}$$

is estimated for $\|\psi\|,\|\phi\|\leqslant 1$ as

$$\|P_g^{(\psi)}-P_g^{(\phi)}\|\leqslant|g|C^2r\|V\|_\infty\||\psi|^2-|\phi|^2\|_1\leqslant 2|g|C^2r\|V\|_\infty\|\psi-\phi\|,$$

where the triangle inequality has been used on $|\psi|^2-|\phi|^2=\psi(\overline{\psi}-\overline{\phi})-(\psi-\phi)\overline{\phi}$. The same bound applies to

$$|\|P_g^{(\psi)}\psi_0\|-\|P_g^{(\phi)}\psi_0\||\leqslant\|(P_g^{(\psi)}-P_g^{(\phi)})\psi_0\|.$$

In particular for $\phi=0$, and hence $P_g^{(\phi)}=P_0$, $\|P_g^{(\phi)}\psi_0\|=1$, this shows that $\|P_g^{(\psi)}\psi_0\|\geqslant\frac{1}{2}$ for g_* small enough. Thus (19) is well defined. From

$$\begin{aligned}T(\psi)-T(\phi)=&\|P_g^{(\psi)}\psi_0\|^{-1}(P_g^{(\psi)}-P_g^{(\phi)})\psi_0\\&+\|P_g^{(\psi)}\psi_0\|^{-1}\|P_g^{(\phi)}\psi_0\|^{-1}(\|P_g^{(\psi)}\psi_0\|-\|P_g^{(\phi)}\psi_0\|)P_g^{(\phi)}\psi_0\end{aligned}$$

T is now seen to be a strict contraction on $\mathcal{S}$.

This proves Theorem 2.

III. NUMERICAL INVESTIGATION

The following simulation performed by a branch of our C++ HARTREE package[16] (using the extension BLITZ++, cf. Ref. 17) is built on a bilinear Lagrange finite element discretization of the numerical configuration space $\Omega\subset\mathbb{R}^2$, $\Omega=]0,D[^{\times 2}$, $D>0$, endowed with homogeneous Dirichlet boundary conditions leading to a Galerkin space of globally continuous functions in $W_0^{1,2}(\Omega)$.

Discretizing the Hartree equation by means of these bilinear finite elements, we arrive at the following nonlinear eigenvalue problem,

$$\frac{1}{(h^{(n)})^2}\left(\frac{1}{2}A^{(N)}+v^{(N)}+gW^{(N)}[\underline{\psi}^{(N)}]\right)\underline{\psi}^{(N)}=E^{(N)}\underline{\psi}^{(N)},\tag{20}$$

where $A^{(N)}$, $v^{(N)}$, and $W^{(N)}$ denote the finite element discretizations of the Laplacian $-\Delta$, the external potential v, and the Hartree energy $V*|\psi|^2$, respectively, on the square grid of $N=n^2$ vertices, and mass lumping saves us the inversion of the massmatrix. $\underline{\psi}^{(N)}$ denotes the component vector gained by expanding $\psi^{(N)}$ with respect to the finite element basis in the Galerkin space, and $h^{(n)}:=D/(n-1)$.

Since we would like to use a version of the fast Fourier transform algorithm (MFFT, cf. Ref. 18) for the fast evaluation of the Hartree energy term $W^{(N)}$, we depart from the finite element framework in the treatment of $W^{(N)}$ using a quadrature scheme for its computation. We denote by $\tilde{W}^{(N)}$ this nonconforming discretization. The two-body potentials V considered here are three-dimensional regularized Coulomb and Yukawa potentials

$$\tilde{W}^{(N)}[\underline{\psi}^{(N)}]_{(i,j),(k,l)}=\delta_{ik}\delta_{jl}(h^{(n)})^4\sum_{i',j'=0}^{n-1}|\psi_{i'j'}^{(N)}|^2\frac{e^{-(\alpha h^{(n)}\sqrt{(i-i')^2+(j-j')^2})}}{h^{(n)}\sqrt{(i-i')^2+(j-j')^2}+\delta}\tag{21}$$

depending on the falloff parameter α and the regularization δ. Here, the indices represent pairs of coordinates of the vertices in the two-dimensional grid.

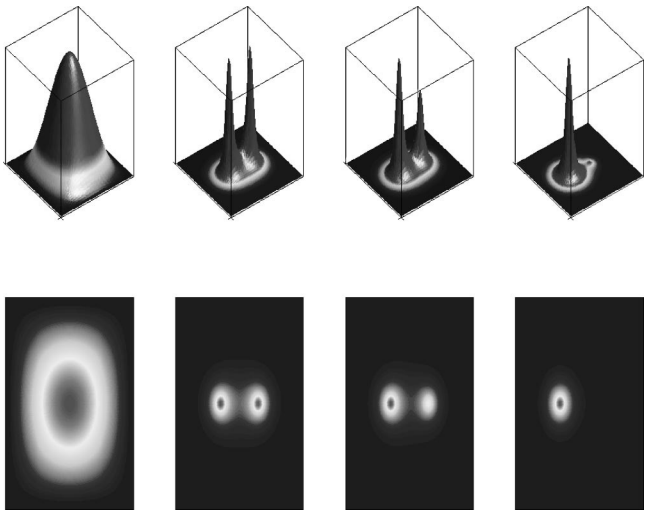

FIG. 1. Modulus squared of selected wave function iterates from the PC sequence converging to a symmetry broken minimizer. For the reason of visibility, the volumes of the boxes are determined by the maximal value of the modulus of the iterate.

The external potential v is chosen to consist of two smooth potential wells. The y-coordinates of their minima are equal whereas the x-coordinates are connected by a reflection at the axis orthogonal to the line joining the two local minimima of v. Hence, this external potential possesses a discrete symmetry, cf. Fig. 1.

The nonlinear eigenvalue problem (20) is solved by means of two interlocking iterative procedures

$$\Psi^{(N),p,q} \xrightarrow[q\to\infty]{\text{PM}} \Psi^{(N),p} \xrightarrow[p\to\infty]{\text{PC}} \Psi^{(N)} \tag{22}$$

for $\Psi^{(N),p,q} := (E^{(N),p,q}, \underline{\Phi}^{(N),p,q})$ and analogously for $\Psi^{(N),p}$ and $\Psi^{(N)}$. The superscript p is index of the Picard (PC) iteration sequence $\Psi^{(N),p}$ whose elements are the solutions of the sequence of *linearized* problems

$$\frac{1}{(h^{(n)})^2}\left(\frac{1}{2}A^{(N)} + v^{(N)} + g\tilde{W}^{(N)}[\underline{\Phi}^{(N),p}]\right)\underline{\Phi}^{(N),p+1} = E^{(N),p+1}\underline{\Phi}^{(N),p+1} \tag{23}$$

for some suitably chosen starting guess $\underline{\Phi}^{(N),0}$. Note that the Hartree energy $\tilde{W}^{(N)}$ depends on p only, and not on $p+1$!

Each element of this sequence of linear problems is solved by use of the power method (PM) consisting simply in a repeated application of the linearized operator on the rhs of (23) on a starting guess $\underline{\Phi}^{(N),p,0}$ for the linear problem, for all $p \in \mathbb{N}_0$. Subsequently, the iterate is normalized. This PM iteration is assigned the superscript q in $\Psi^{(N),p,q}$.

Although there is a *Lanczos algorithm* implemented in the HARTREE package[16] we discuss the elementary PM iteration for reasons of monitoring the iterates directly. For the Lanczos algorithm, cf. Refs. 19 and 20.

The PM iteration procedure works as follows. Given a linear real symmetric operator H on a complex finite N-dimensional Hilbert space $\mathcal{H}$ and a vector $\psi^0 \in \mathcal{H}$, PM provides us with the eigenvector whose corresponding eigenvalue is the eigenvalue with largest modulus of H restricted to the subspace determined by ψ^0. More precisely, if $\{\phi_k\}_{k=0}^{N-1}$ is an orthonormal eigenbasis of H in $\mathcal{H}$, $H\phi_k = E_k\phi_k$, in which ψ^0 may be expanded, $\psi^0 = \Sigma_{k=0}^{N-1} c_k\phi_k$, then PM computes a multiple of the eigenfunction $\phi_* \in \{\phi_k\}_{k=0}^{N-1}$ with eigenvalue E_*, for which

$$|E_*| = \max\{|E_k| | E_k \in \sigma(H|_{span\{\phi_k | c_k \neq 0\}})\} \tag{24}$$

holds (provided they are unique). This is achieved by iterating the application of H on ψ^0 with subsequent normalization of the iterate:

$$\psi^j := \frac{H^j \psi^0}{\|H^j \psi^0\|} = \sum_{k=0}^{N-1} \frac{c_k (E_k/E_*)^j}{(|c_*|^2 + \Sigma_{l=0, l\neq *}^{N-1} |c_l|^2 (E_l/E_*)^{2j})^{1/2}} \phi_k \xrightarrow{j\to\infty} \frac{c_*}{|c_*|} \phi_*, \tag{25}$$

$$(\psi^j, H\psi^j) = \sum_{k=0}^{N-1} \frac{|c_k|^2 (E_k/E_*)^{2j}}{|c_*|^2 + \Sigma_{l=0, l\neq *}^{N-1} |c_l|^2 (E_l/E_*)^{2j}} E_k \xrightarrow{j\to\infty} E_*. \tag{26}$$

As we can see in (24) the restriction to a subspace of $\mathcal{H}$ is determined by the choice of nonvanishing components in the eigenbasis expansion of the starting seed ψ^0. Now, depending on the location of the spectrum, we have to shift the linear operator H by an amount $s \in \mathbb{R}$ which, in our case, reads as

$$\begin{aligned} H_s^{(N)}[\underline{\Phi}^{(N),p}]\underline{\Phi}^{(N),p+1} &:= \left[\frac{1}{h^{(n)2}}\left(\frac{1}{2}A^{(N)} + v^{(N)} + g\tilde{W}^{(N)}[\underline{\Phi}^{(N),p}]\right) + s\mathbb{I}^{(N)}\right]\underline{\Phi}^{(N),p+1} \\ &= (E^{(N),p+1} + s)\underline{\Phi}^{(N),p+1} \end{aligned} \tag{27}$$

such that for the computation of the ground state energy, at most,

$$|\min \sigma(H_s^{(N)}[\underline{\Phi}^{(N),p}])| > |\max \sigma(H_s^{(N)}[\underline{\Phi}^{(N),p}])|. \tag{28}$$

Then, the ground state energy of $H_s^{(N)}[\underline{\Phi}^{(N),p}]$ has maximal modulus among all energies of $H_s^{(N)}[\underline{\Phi}^{(N),p}]$.

The *convergence speed characteristic* is determined by the quotient $q_{\tilde{k}}(s)$ in the numerator of (25) shifted by s, where $\hat{k} \in \{0, \ldots, N-1\}$ denotes the energy level for which the quotient $q_{\hat{k}}(s)$ is closest to one among all existing $q_k(s)$, $k \in \{0, \ldots, N-1\}$,

$$q_{\hat{k}}(s) := \left(\frac{E_{\hat{k}} + s}{E_* + s}\right)^j. \tag{29}$$

The length and energy scales l and E set by a minimizer are $l \propto |g|^{-1}$, and $E \propto g^2$. For numerical reasons, we have to allow grid resolutions with $l \gg h$ only ($h := h^{(n)}$ for some n). But the maximal kinetic energy on such a grid is roughly proportional to h^{-2}, which determines the scale of the coupling g, $|g| \ll h^{-1}$. This implies the existence of positive energy states on the grid since the depth of the Hartree energy well is $O(g^2)$. Hence,

$$\max \sigma(H^{(N)}[\underline{\Phi}^{(N),p}]) = O(h^{-2}) > 0.$$

Approximating the Hartree energy well around its minimum by a harmonic potential, we find the *level spacing* ΔE to be

$$\Delta E = O(g^2).$$

Since, on the length scale $|g|^{-1}$, the quadratic function changes as g^2 (depth of the energy well), it is of the form $O(g^4)x^2$ which results in a harmonic oscillator frequency $\omega = O(g^2)$. Therefore, we can set $E_0 = -\alpha_0 g^2$ and the first excited state $E_1 = -\alpha_1 g^2$ with $\alpha_0 - \alpha_1 > 0$. The convergence speed characteristic $q_1(s)$ from (29) is now expanded in $g^2 h^2 \ll 1$, with $(\alpha_0 - \alpha_1)$ is of order $O(1)$:

$$q_1(-h^{-2})^{1/j} = 1 - (\alpha_0 - \alpha_1) g^2 h^2 + O(g^4 h^4). \tag{30}$$

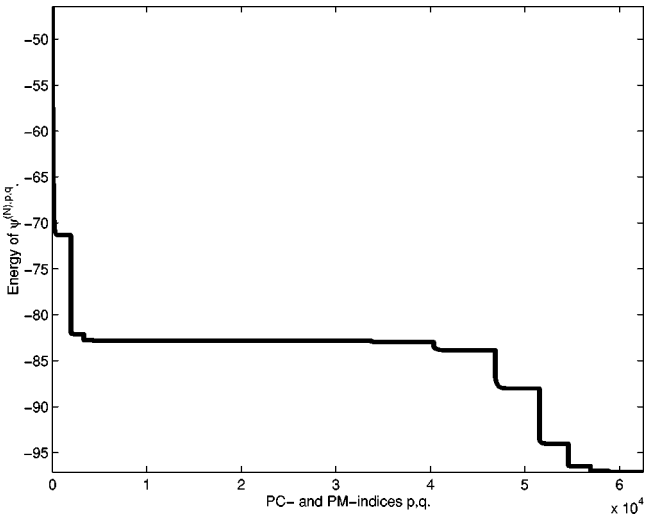

FIG. 2. Total energy of the interlocking PC iterates and PM iterates for the sequence in Fig. 1.

Now, in order to get an idea for the *size* of j, we can expand ψ^j up to first order, $k=0,1$, for example, and compute j approximately from

$$\left\| \frac{H_s\psi^j - (\psi^j, H_s\psi^j)\psi^j}{(\psi^j, (H_s - s\mathbb{1})\psi^j)} \right\| \leqslant \epsilon_{\text{rel}}, \tag{31}$$

which is the chosen *stopping criterion* for the PM iteration, given the relative error ϵ_{rel} (with $H_s := H + s1$). Note that this criterion does not depend on the shift $s \in \mathbb{R}$ if ψ^j is normalized for all j.

Clearly, (31) is satisfied for *any* eigenstate of H. But as soon as the $*$-component in the expansion of ψ^0 is nonvanishing (e.g., due to *finite precision arithmetic*), $c_* \neq 0$, the sequence ψ^j will eventually converge to a multiple of ϕ_*.

But, note that the chosen accuracy may be reached *before* a nonvanishing c_* is generated!

IV. FIGURES

In Fig. 1 we visualize some instructive elements of the PC iteration sequence $\{\Phi^{(N),p}\}_{p=0}^{\infty}$. The data specification for the simulation in Figs. 1 and 2 is as follows.

The grid is generated by six bisections leading to $n = 2^6 = 64$.

The external potential $v(x,y)$ is chosen to be a double well potential composed of two wells of the form

$$v(x,y) = V_0 / \cosh((x-x_0)^2/a^2 + (y-y_0)^2/b^2)$$

localized at

$$((x_1)_0, (y_1)_0) = (0.35, 0.5)$$

and

$$((x_2)_0, (y_2)_0) = (0.65, 0.5)$$

with widths

$$(a_1, b_1) = (a_2, b_2) = (0.03, 0.03)$$

and strengths

$$(V_1)_0=(V_2)_0=-0.1.$$

The two-body potential V has the form (21) with

$$\alpha=0 \quad \text{and} \quad \delta=0.1.$$

This Hartree energy is coupled by a coupling constant $g=-16$.

The starting guess $\Phi^{(N),0}$ for the iteration is chosen to be the ground state for the pure kinetic energy in Ω. With the additional rule

$$\underline{\Phi}^{(N),p+1,0}:=\underline{\Phi}^{(N),p,\infty}, \tag{32}$$

all the necessary starting approximations are determined, where $p\in\mathbb{N}_0$, and $\underline{\Phi}^{(N),0,\infty}:=\underline{\Phi}^{(N),0}$.

In the following simulation, $q=\infty$ means $q=O(10)-O(10^2)$ iterations, whereas $p=\infty$ is $p=O(10)$.

Figure 1 visualizes the density contours of selected iterates from the PC iteration sequence. The first picture shows the ground state for the pure kinetic energy. After a while, a state similar to the ground state of the linear operator $-\frac{1}{2}\Delta+v$ is approached. This state becomes unstable, such that, finally, one of the two possible nonlinear ground states results. The decision for the left or the right potential well is made by finite precision arithmetic.

The qualitative behavior of Fig. 1 is confirmed for different grid resolutions $n=2^m$, $m\in\mathbb{N}$, where the location and strength of the external potential v have been kept fixed.

On the chosen level of accuracy, $\epsilon_{\text{rel}}=10^{-6}$, and on this space discretization level, $n=64$, the critical coupling lies around

$$g_*\approx 16$$

(we are only interested in the qualitative behavior). Above g_*, the minimizer density looks as in the second picture of Fig. 1.

In Fig. 2 the expectation value of $H^{(N)}$ in the PC states from Fig. 1 and their underlying PM states is monitored. We note that the energy minimum for all these states is in fact reached in the final configuration.

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Bound states in straight quantum waveguides with combined boundary conditions

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We investigate the discrete spectrum of the Hamiltonian describing a quantum particle living in the two-dimensional straight strip. We impose the combined Dirichlet and Neumann boundary conditions on different parts of the boundary. Several statements on the existence or the absence of the discrete spectrum are compared for two models with combined boundary conditions. Examples of eigenfunctions and eigenvalues are computed numerically. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1491597]

I. INTRODUCTION

Quantum waveguides with Dirichlet boundary conditions were extensively studied (e.g., Refs. 1–7, and references therein). Their spectral properties essentially depend on the geometry of the waveguide, in particular the existence of bound states induced by curvature[1,2,3,5] or by coupling of straight waveguides through windows[4,6] were shown. The waveguides with Neumann boundary condition were also investigated in several papers, e.g., Refs. 8–10. The possible next generalization are waveguides with combined Dirichlet and Neumann boundary conditions on different parts of the boundary. Some very simple combinations of these conditions appear due to the symmetry of special configurations in systems studied, for example, in Refs. 4, 5, 6, 8, 10. Such ''combined'' systems might also be of interest in nanoscopic physics if interphases modeled by different conditions could be realized. The presence of different boundary conditions also gives rise to nontrivial spectral properties like the existence of bound states.

In the present paper, we compare two simple cases of straight planar waveguides of constant width with combined boundary conditions. We show the examples with[8] and without the presence of bound states. The systems we are going to study are sketched in Fig. 1. We consider a Schrödinger particle whose motion is confined to a planar strip of width d. For definiteness we assume that it is placed to the upper side of the x axis. On part of the boundary the Neumann condition is imposed (thin lines in the picture), while on the other part the Dirichlet one holds (thick lines). The length of the overlay of Neumann boundaries is 2δ and it is placed to both sides of the y axis in both cases. We shall denote this configuration space by $\Omega=\mathbb{R}\times(0,d)$ and its particular parts by $\Omega_{\mathrm{I}}=(-\infty,-\delta)\times(0,d)$, $\Omega_{\mathrm{II}}=(-\delta,\delta)\times(0,d)$ and $\Omega_{\mathrm{III}}=(\delta,\infty)\times(0,d)$.

In Sec. II we define the Hamiltonian as a Laplace operator with chosen boundary conditions with the help of a quadratic form. We also explicitly give the operator domain which contains functions not belonging to the Sobolev space $H^2(\Omega)$. For those functions $-\Delta f\in L^2(\Omega)$ but the separated second derivatives are not square integrable. Due to this fact the proof of the operator domain form is a little complicated. Similar functions are known to occur in the domains of the Dirichlet Laplacian in regions with boundaries having angles larger than π.[11] In Sec. III we study the question of bound state existence below the threshold of the essential spectrum for example A. For comparison, the known case B[8] is given to stress the different properties of two examples with

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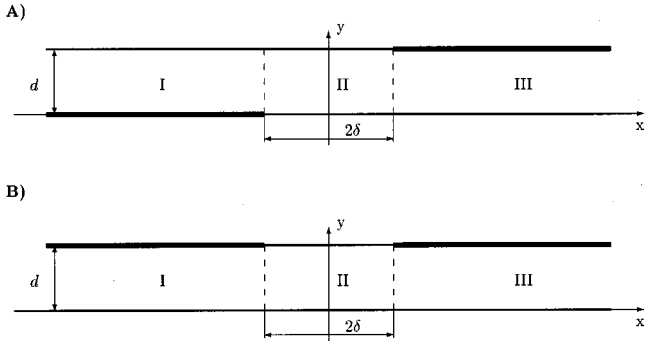

FIG. 1. Straight quantum waveguides with combined boundary conditions. The thin lines denote the Neumann boundary condition, the thick lines the Dirichlet one.

different symmetries. While in case B a bound states always exists, it appears for sufficiently large overlay 2δ only in case A. The proved results are illustrated in Sec. IV by numerical calculations. Some technical points are left to appendices.

II. THE HAMILTONIAN

As we are going to prove several statements that are valid for more general combinations of boundary conditions, let us define several objects. Let there be a finite number of points on the boundary $\partial\Omega$, where the boundary condition is changing, which we denote $P_k=\langle x_k,y_k\rangle$, $k=1,\ldots,M$. We can choose the numbering so as $y_k=d$ for $k=1,\ldots,M'$ and $x_1<x_2<\cdots<x_{M'}$ and $y_k=0$ for $k=M'+1,\ldots,M$ and $x_{M'+1}<x_{M'+2}<\cdots<x_M$. Let $\partial\Omega=\mathcal{D}\cup\mathcal{N}\cup\cup_{k=1}^{M}\{P_k\}$, where $\mathcal{D}$ is a union of finite number of intervals in $\partial\Omega$, where Dirichlet condition is imposed and $\mathcal{N}=(\partial\Omega\setminus\mathcal{D})^0$ is similar for the Neumann condition. For our examples we have
(A)

$$\mathcal{D}=\{\langle x,0\rangle|x<-\delta\}\cup\{\langle x,d\rangle|x>\delta\},$$

$$\mathcal{N}=\{\langle x,0\rangle|x>-\delta\}\cup\{\langle x,d\rangle|x<\delta\},$$

$$P_1=\langle\delta,d\rangle,\quad P_2=\langle-\delta,0\rangle,$$

(B)

$$\mathcal{D}=\{\langle x,d\rangle|(x<-\delta)\vee(x>\delta)\},$$

$$\mathcal{N}=\{\langle x,0\rangle|x\in\mathbb{R}\}\cup\{\langle x,d\rangle|-\delta<x<\delta\},$$

$$P_1=\langle-\delta,d\rangle;\quad P_2=\langle\delta,d\rangle.$$

Putting $\hbar^2/2m=1$, we may identify the particle Hamiltonian with the self-adjoint operator on the Hilbert space $L^2(\Omega)$, defined in the following way. Let us define a quadratic form

$$q_0(f,g)=\int_\Omega\overline{\nabla f}\cdot\nabla g\,\mathrm{d}^2x\quad\text{with domain}\quad Q(q_0)=\{f\in H^1(\Omega)|f\restriction\mathcal{D}=0\},\tag{2.1}$$

where $H^1(\Omega)=\{f\in L^2(\Omega)|\nabla f\in L^2(\Omega)\}$ is the standard Sobolev space and we denote as $f\restriction\mathcal{D}$ the trace of function f on $\mathcal{D}$. Now q_0 is obviously densely defined, symmetric, and below bounded quadratic form. The form q_0 is also closed as a direct consequence of Theorem 7.53 in Ref. 12.

There is the unique self-adjoint operator associated with this form (see, e.g., Ref. 13, Theorem 4.6.8). We denote this operator $-\Delta_{DN}^{\Omega}$ and its domain $D(\Omega)$. It is our Hamiltonian. We will show that this operator acts as the usual Laplace operator with the Dirichlet condition on $\mathcal{D}$ and Neumann condition on $\mathcal{N}$.

Theorem 1: *The domain of the operator* $-\Delta_{DN}^{\Omega}$ *is*

$$D(\Omega)=\left\{ f\in H^1(\Omega)\,\middle|\, -\Delta f\in L^2(\Omega), f\restriction\mathcal{D}=0, \frac{\partial f}{\partial y}\restriction\mathcal{N}=0\right\},$$
$$-\Delta_{DN}^{\Omega} f=-\Delta f \quad \text{for every} \quad f\in D(\Omega). \tag{2.2}$$

Proof: First, we know that $D(\Omega)\subset Q(q_0)$. Moreover $f\in D(\Omega)$ if and only if there exists a function $h\in L^2(\Omega)$ such that for all $g\in Q(q_0)$ the equality $q_0(g,f)=(g,h)_{L^2(\Omega)}$ holds. Then $h=-\Delta_{DN}^{\Omega} f$ (see Ref. 13, Theorem 4.6.8). Let g be any function from $C_0^{\infty}(\Omega)$. Then $g\in Q(q_0)$ and $(\nabla g,\nabla f)_{L^2(\Omega)}=(g,-\Delta f)_{L^2(\Omega)}$ using only definition of the distributional derivatives. So $-\Delta_{DN}^{\Omega} f=-\Delta f$ for all $f\in D(\Omega)$. We know now

$$D(\Omega)=\{f\in Q(q_0)\,|\,-\Delta f\in L^2(\Omega),(\forall g\in Q(q_0))((g,-\Delta f)_{L^2(\Omega)}=(\nabla g,\nabla f)_{L^2(\Omega)})\}. \tag{2.3}$$

Now we prove the implication $f\in D(\Omega)\Rightarrow \partial f/\partial y\restriction\mathcal{N}=0$. Let Ω_0 be an open subset of Ω, such that $P_k\notin\overline{\Omega}_0, k=1,\ldots,M$. We will show that every $f\in D(\Omega)$ belongs to $H^2(\Omega_0)$ for such subdomains. There exist real, positive numbers η_k, $k=1,\ldots,M$ such that the open balls $\underline{B(P_k,2\eta_k)}$ have empty intersections with Ω_0. We can choose η_k so small that even $\overline{B(P_k,2\eta_k)}\cap\overline{B(P_{k'},2\eta_{k'})}=\varnothing$ for $k\neq k'$. Let us denote

$$\omega_0=(-\infty,x_1-\eta_1)\times(d,2d),$$
$$\vdots$$
$$\omega_{M'-1}=(x_{M'-1}+\eta_{M'-1},x_{M'}-\eta_{M'})\times(d,2d),$$
$$\omega_{M'}=(x_{M'}+\eta_{M'},\infty)\times(d,2d),$$
$$\omega_{M'+1}=(-\infty,x_{M'+1}-\eta_{M'+1})\times(-d,0),$$
$$\vdots$$
$$\omega_{M+1}=(x_M+\eta_M,\infty)\times(-d,0)$$

and let $\tilde{\omega}_k$ be the reflection of ω_k to the domain Ω for $k=0,\ldots,M+1$, i.e., $\tilde{\omega}_k=\mathcal{R}_1(\omega_k)$ for $k=0,\ldots,M'$ and $\tilde{\omega}_k=\mathcal{R}_2(\omega_k)$ for $k=M'+1,\ldots,M+1$, where the bijections $\mathcal{R}_i:\mathbb{R}^2\to\mathbb{R}^2$, $i=1,2$ are defined as follows: $\mathcal{R}_1(\langle x,y\rangle)=\langle x,2d-y\rangle$ and $\mathcal{R}_2(\langle x,y\rangle)=\langle x,-y\rangle$. Let $\tilde{\Omega}=(\overline{\cup_{k=0}^{M+1}\omega_k\cup\Omega})^0$. In fact, we can say that $\tilde{\Omega}$ is the original domain Ω with its copy on each side of its boundary, from which we cut the columns $[x_k-\eta_k,x_k+\eta_k]\times[d,2d)$, respectively, $[x_k-\eta_k,x_k+\eta_k]\times(-d,0]$, above, respectively, below, the point P_k depending on which part of $\partial\Omega$ the point P_k lies. We construct a function $\tilde{f}\in L^2(\tilde{\Omega})$ as follows. For every point $\langle x,y\rangle\in\tilde{\Omega}\backslash\partial\Omega$ we define (so we see that the function will be defined almost everywhere in $\tilde{\Omega}$):

$$\tilde{f}(x,y)=\begin{cases} f(x,y) & \text{for} \quad \langle x,y\rangle\in\Omega \\ f(x,2d-y) & \text{for} \quad \langle x,2d-y\rangle\in\Omega, \quad \langle x,d\rangle\in\mathcal{N} \\ -f(x,2d-y) & \text{for} \quad \langle x,2d-y\rangle\in\Omega, \quad \langle x,d\rangle\in\mathcal{D} \\ f(x,-y) & \text{for} \quad \langle x,-y\rangle\in\Omega, \quad \langle x,0\rangle\in\mathcal{N} \\ -f(x,-y) & \text{for} \quad \langle x,-y\rangle\in\Omega, \quad \langle x,0\rangle\in\mathcal{D}. \end{cases}$$

Now for any $\varphi\in C_0^\infty(\tilde{\Omega})$ we can write

$$\begin{aligned}(-\Delta\tilde{f},\varphi)_{L^2(\tilde{\Omega})}&=(\tilde{f},-\Delta\varphi)_{L^2(\tilde{\Omega})}\\ &=(f,-\Delta\varphi)_{L^2(\Omega)}+\sum_{k=0}^{M+1}(\tilde{f},-\Delta\varphi)_{L^2(\omega_k)}\\ &=(f,-\Delta\varphi)_{L^2(\Omega)}\mp\sum_{k=0}^{M'}(-1)^k\int_{\tilde{\omega}_k}\overline{f(x,y)}\Delta\varphi(x,2d-y)\mathrm{d}^2x\\ &\quad+(-1)^s\sum_{k=M'+1}^{M+1}(-1)^k\int_{\tilde{\omega}_k}\overline{f(x,y)}\Delta\varphi(x,-y)\mathrm{d}^2x\\ &=(f,-\Delta\tilde{\varphi})_{L^2(\Omega)}, \end{aligned}\tag{2.4}$$

where we used the definition of the distributional derivatives and the substitution $y\mapsto 2d-y$, respectively, $y\mapsto -y$. The $-$ sign in $\mp$ is valid for these systems, where the Neumann condition is imposed on $\{\langle x,d\rangle|x\in(-\infty,x_1)\}$, the $+$ sign for others. The number s equals 0 or 1, so as $s+M'+1$ is odd for systems, where the Neumann condition is imposed on $\{\langle x,0\rangle|x\in(-\infty,x_{M'+1})\}$ and even for others. Finally, a new function is defined on the domain Ω as

$$\tilde{\varphi}(x,y)=\varphi(x,y)\pm\sum_{k=0}^{M'}(-1)^k\chi_{\tilde{\omega}_k}(x,y)\varphi(x,2d-y)-(-1)^s\sum_{k=M'+1}^{M+1}(-1)^k\chi_{\tilde{\omega}_k}(x,y)\varphi(x,-y),$$

where χ_ω is the standard characteristic function of the set ω. Taking into consideration the construction of the domain $\tilde{\Omega}$ and that supp $\varphi\subset\tilde{\Omega}$, we conclude that $\tilde{\varphi}\in C^\infty(\overline{\Omega})$ and it has a bounded support. Further, we know that the trace $\tilde{\varphi}\restriction\partial\Omega$ equals $\lim_{y\to d^-}\tilde{\varphi}(x,y)$ in the point $\langle x,d\rangle$ and similarly $\lim_{y\to 0^+}\tilde{\varphi}(x,y)$ in the point $\langle x,0\rangle$ for smooth functions (see the definition of traces, e.g., in Ref. 12). So the traces on $\mathcal{D}\cap\tilde{\Omega}$ are

$$(\tilde{\varphi}\restriction\partial\Omega)(x,d)=\lim_{y\to d^-}\tilde{\varphi}(x,y)=\lim_{y\to d^-}(\varphi(x,y)-\varphi(x,2d-y))=0,$$

$$(\tilde{\varphi}\restriction\partial\Omega)(x,0)=\lim_{y\to 0^+}\tilde{\varphi}(x,y)=\lim_{y\to 0^+}(\varphi(x,y)-\varphi(x,-y))=0.$$

In a similar way for parts of boundary $\partial\Omega$ with the Neumann condition inside $\tilde{\Omega}$,

$$\left(\frac{\partial\tilde{\varphi}}{\partial y}\restriction\partial\Omega\right)(x,d)=\lim_{y\to d^-}\frac{\partial\tilde{\varphi}}{\partial y}(x,y)=\lim_{y\to d^-}\frac{\partial}{\partial y}(\varphi(x,y)+\varphi(x,2d-y))=0,$$

$$\left(\frac{\partial\tilde{\varphi}}{\partial y}\restriction\partial\Omega\right)(x,0)=\lim_{y\to 0^+}\frac{\partial\tilde{\varphi}}{\partial y}(x,y)=\lim_{y\to 0^+}\frac{\partial}{\partial y}(\varphi(x,y)+\varphi(x,-y))=0.$$

On the rest of the boundary $\partial\Omega$, i.e., $\partial\Omega\backslash\tilde{\Omega}$, both Dirichlet and Neumann conditions are satisfied, which can be seen from the definition of $\tilde{\varphi}$. So it is clear that $\tilde{\varphi}\in H^2(\Omega)$ and it satisfies prescribed boundary conditions. It is easy to check that all such functions belong to $D(\Omega)$, using the Gauss theorem. Because both functions f and $\tilde{\varphi}$ are in $D(\Omega)$, which is a subset of $Q(q_0)$, we can continue the calculation from (2.4),

$$
\begin{aligned}
(f,-\Delta\tilde{\varphi})_{L^2(\Omega)}&=(\nabla f,\nabla\tilde{\varphi})_{L^2(\Omega)}=(-\Delta f,\tilde{\varphi})_{L^2(\Omega)}\\
&=(-\Delta f,\varphi)_{L^2(\Omega)}\mp\sum_{k=0}^{M'}(-1)^k\int_{\omega_k}\overline{\Delta f(x,2d-y)}\,\varphi(x,y)\,\mathrm{d}^2x\\
&\quad+(-1)^s\sum_{k=M'+1}^{M+1}(-1)^k\int_{\omega_k}\overline{\Delta f(x,-y)}\,\varphi(x,y)\,\mathrm{d}^2x=(F,\varphi)_{L^2(\tilde{\Omega})},
\end{aligned}
$$

where we used the ''reflection'' substitution again and F is a function defined by the last formula. Here $F\in L^2(\tilde{\Omega})$, because it is the sum of the finite number of L^2-functions. As we choose the function φ arbitrarily, we see that $-\Delta\tilde{f}=F\in L^2(\tilde{\Omega})$. Let $\psi\in C^\infty(\mathbb{R}^2)$, it is bounded together with its first and second derivatives, and let supp $\psi\subset\tilde{\Omega}$. Then $\psi\tilde{f}\in L^2(\mathbb{R}^2)$. Using the Leibnitz rule and several times a lemma from Sec. IX.6 in Ref. 14, we conclude that even $-\Delta(\psi\tilde{f})\in L^2(\mathbb{R}^2)$ [the Leibnitz rule itself does not give the result unless we know $\nabla\tilde{f}\in L^2(\tilde{\Omega})$]. We now use this lemma once more and we get the result that $\psi\tilde{f}\in H^2(\mathbb{R}^2)$. We can choose a function ψ so as $\psi\restriction\Omega_0=1$. It is possible, because $\Omega_0\subset\subset\tilde{\Omega}$ and our regions have a simple form at $x\to\pm\infty$. Let $r_1<r_2<r_3$ be the real positive numbers such that $[x_k-2\eta_k,x_k+2\eta_k]\subset(-r_1,r_1)$ for every $k=1,\ldots,M$ and denote $R_2=(-r_2,r_2)\times(0,d)$, $R_3=(-r_3,r_3)\times(-d,2d)$. Then using Ref. 15, Lemma XIV.2.1 we find a function $\psi_1\in C_0^\infty(\tilde{\Omega}\cap R_3)$, such that $0\leqslant\psi_1(x)\leqslant 1$ for all $x\in\tilde{\Omega}\cap R_3$ and $\psi_1(x)=1$ for $x\in\overline{\Omega_0\cap R_2}$. This function has compact support in $\tilde{\Omega}$, so its derivatives are bounded. Let now $\gamma\in C_0^\infty(-d,2d)$, such that $\gamma(y)=1$ for $y\in(0,d)$ (it can be constructed according to the same lemma as ψ_1). Let $\beta\in C^\infty(\mathbb{R})$ such that $\beta(x)=1$ for $|x|\geqslant r_2$, $\beta(x)=0$ on the interval $[-r_1,r_1]$ (we can again use the same lemma for construction of $1-\beta$). Then $\psi=\psi_1(1-\beta)+\gamma\beta$ satisfies all desired properties. Thus $\tilde{f}\psi\restriction\Omega_0=\tilde{f}\restriction\Omega_0=f\restriction\Omega_0$, so $f\in H^2(\Omega_0)$.

Now let us take any interval (a,b), such that $x_k\notin[a,b]$ for $k=1,\ldots,M$. Let $\xi\in C_0^\infty(a,b)$ be a real function. Because region $(a,b)\times(0,d)$ satisfies all conditions for Ω_0, $f\in H^2((a,b)\times(0,d))$. Using the Leibnitz rule we can see that $\xi f\in H^2((a,b)\times(0,d))$. For any $g\in Q(q_0)$ we have $g\xi\in Q(q_0)$ and

$$
\begin{aligned}
(\nabla g,\nabla(f\xi))_{L^2(\Omega)}&=(\nabla g,\xi\nabla f)_{L^2(\Omega)}+\left(\frac{\partial g}{\partial x},f\frac{d\xi}{dx}\right)_{L^2(\Omega)}\\
&=(\xi\nabla g,\nabla f)_{L^2(\Omega)}+\left(g\frac{d\xi}{dx},\frac{\partial f}{\partial x}\right)_{L^2(\Omega)}-\left(g\frac{d\xi}{dx},\frac{\partial f}{\partial x}\right)_{L^2(\Omega)}+\left(\frac{\partial g}{\partial x},f\frac{d\xi}{dx}\right)_{L^2(\Omega)}\\
&=(g\xi,-\Delta f)_{L^2(\Omega)}+\int_\Omega\frac{\partial(\overline{g(x,y)}f(x,y))}{\partial x}\frac{d\xi(x)}{dx}\mathrm{d}x\,\mathrm{d}y-2\left(g\frac{d\xi}{dx},\frac{\partial f}{\partial x}\right)_{L^2(\Omega)}\\
&=(g,-\xi\Delta f)_{L^2(\Omega)}-2\left(g,\frac{d\xi}{dx}\cdot\frac{\partial f}{\partial x}\right)_{L^2(\Omega)}-\left(g,f\frac{d^2\xi}{dx^2}\right)_{L^2(\Omega)}=(g,-\Delta(f\xi))_{L^2(\Omega)}.
\end{aligned}
\tag{2.5}
$$

Hence $\xi f\in D(\Omega)$. Using the Gauss theorem (it can be used for H^2-functions) we get for any $g\in Q(q_0)$,

$$(g,-\Delta(\xi f))_{L^2(\Omega)}=(\nabla g,\nabla(\xi f))_{L^2(\Omega)}-\int_a^b\left(\overline{g(x,d)}\xi(x)\frac{\partial f}{\partial y}(x,d)-\overline{g(x,0)}\xi(x)\frac{\partial f}{\partial y}(x,0)\right)\mathrm{d}x.$$

So due to (2.5)

$$\int_a^b\left(\overline{g(x,d)}\xi(x)\frac{\partial f}{\partial y}(x,d)-\overline{g(x,0)}\xi(x)\frac{\partial f}{\partial y}(x,0)\right)\mathrm{d}x=0$$

for any considered a,b and any $g\in Q(q_0),\xi\in C_0^\infty(a,b)$. Now we conclude that

$$\frac{\partial f}{\partial y}\restriction\mathcal{N}=0 \quad \text{a.e.}$$

This finishes the second part of proof.

It remains to show that if f satisfies all conditions from (2.2) then $f\in D(\Omega)$ [in the sense of definition (2.3)]. Let $\Omega_{0,\varepsilon}=\Omega\backslash\cup_{k=1}^M\overline{B(P_k,\varepsilon)}$, $\Omega_\varepsilon=\cup_{k=1}^M B(P_k,\varepsilon)\cap\Omega$. Because we know from the previous part of the proof that $f\in H^2(\Omega_{0,\varepsilon})$, we can use the Gauss theorem:

$$\begin{aligned}(\nabla g,\nabla f)_{L^2(\Omega)}+(g,\Delta f)_{L^2(\Omega)}&=(\nabla g,\nabla f)_{L^2(\Omega_{0,\varepsilon})}+(g,\Delta f)_{L^2(\Omega_{0,\varepsilon})}+(\nabla g,\nabla f)_{L^2(\Omega_\varepsilon)}\\&\quad+(g,\Delta f)_{L^2(\Omega_\varepsilon)}\\&=-\sum_{k=1}^M\int_0^\pi\frac{\partial\tilde f_k(\varepsilon,\theta)}{\partial r}\overline{\tilde g_k(\varepsilon,\theta)}\varepsilon\,\mathrm{d}\theta+(\nabla g,\nabla f)_{L^2(\Omega_\varepsilon)}\\&\quad+(g,\Delta f)_{L^2(\Omega_\varepsilon)},\end{aligned}\tag{2.6}$$

where $\tilde f_k$, $\tilde g_k$ are the transformations of f, g to the polar coordinates in the neighborhood of each P_k in the way, that the region $(0,\varepsilon)\times(0,\pi)\subset\Omega$, P_k is the origin of polar coordinates, and $\tilde f_k$ satisfies the Dirichlet condition for $\theta=0$. We can see that the last two terms in (2.6) go to zero as $\varepsilon\to0$, because ∇f, ∇g, $-\Delta f$, $g\in L^2(\Omega)$ and the measure of Ω_ε goes to zero. So we only have to prove that

$$\sum_{k=1}^M\int_0^\pi\frac{\partial\tilde f_k(r_n,\theta)}{\partial r}\overline{\tilde g_k(r_n,\theta)}r_n\mathrm{d}\theta\to0\quad\text{as}\quad n\to\infty\tag{2.7}$$

for some sequence $\{r_n\}_{n=0}^\infty$, $\lim_{n\to\infty}r_n=0$. We will show that each term in this sum tends to zero. For simplicity we will not write indices in the following text. We will decompose $\tilde f$ to the orthonormal transverse basis which respects our boundary conditions,

$$\tilde f(r,\theta)=\sum_{k=0}^\infty\sqrt{\frac{2}{\pi}}F_k(r)\sin\frac{2k+1}{2}\theta,\tag{2.8}$$

and in the same way

$$\tilde g(r,\theta)=\sum_{k=0}^\infty\sqrt{\frac{2}{\pi}}G_k(r)\sin\frac{2k+1}{2}\theta.\tag{2.9}$$

Let R be a small positive real number, so as $\min_{k\neq k'}\mathrm{dist}(P_k,P_{k'})>R$. It is easy to check the following equivalences:

$$f,g\in H^1(\Omega\cap B(P,R))\Leftrightarrow\tilde f,\tilde g,\frac{\partial\tilde f}{\partial r},\frac{\partial\tilde g}{\partial r},\frac{1}{r}\frac{\partial\tilde f}{\partial\theta},\frac{1}{r}\frac{\partial\tilde g}{\partial\theta}\in L^2((0,R)\times(0,\pi),r\,\mathrm{d}r\,\mathrm{d}\theta),\tag{2.10}$$

$$\Delta f\in L^2(\Omega\cap B(P,R))\Leftrightarrow\left(\frac{\partial^2\tilde f}{\partial r^2}+\frac{1}{r}\frac{\partial\tilde f}{\partial r}+\frac{1}{r^2}\frac{\partial^2\tilde f}{\partial\theta^2}\right)\in L^2((0,R)\times(0,\pi),r\,\mathrm{d}r\,\mathrm{d}\theta).\tag{2.11}$$

Using (2.10) we can decompose $(1/r)(\partial\tilde f/\partial\theta)$ to the orthonormal transverse basis

$$\frac{1}{r}\frac{\partial\tilde f}{\partial\theta}=\sum_{k=0}^{\infty}\sqrt{\frac{2}{\pi}}a_k(r)\cos\frac{2k+1}{2}\theta.$$

For almost every r we have

$$a_k(r)=\sqrt{\frac{2}{\pi}}\int_0^\pi\frac{1}{r}\frac{\partial\tilde f}{\partial\theta}(r,\theta)\cos\frac{2k+1}{2}\theta\,\mathrm{d}\theta$$

and

$$\begin{aligned}F_k(r)&=\sqrt{\frac{2}{\pi}}\int_0^\pi\tilde f(r,\theta)\sin\frac{2k+1}{2}\theta\,\mathrm{d}\theta\\&=-\sqrt{\frac{2}{\pi}}\frac{2}{2k+1}\int_0^\pi\tilde f(r,\theta)\frac{\partial}{\partial\theta}\cos\frac{2k+1}{2}\theta\,\mathrm{d}\theta\\&=\sqrt{\frac{2}{\pi}}\frac{2}{2k+1}\int_0^\pi\frac{\partial\tilde f}{\partial\theta}(r,\theta)\cos\frac{2k+1}{2}\theta\,\mathrm{d}\theta+\sqrt{\frac{2}{\pi}}\frac{2}{2k+1}\tilde f(r,0)=\frac{2}{2k+1}ra_k(r),\end{aligned}$$

due to the boundary condition $\tilde f(r,0)=0$. So

$$a_k(r)=\frac{1}{r}\frac{2k+1}{2}F_k(r).\tag{2.12}$$

Now we decompose in the same way $\partial\tilde f/\partial r$,

$$\frac{\partial\tilde f}{\partial r}=\sum_{k=0}^{\infty}\sqrt{\frac{2}{\pi}}b_k(r)\sin\frac{2k+1}{2}\theta.$$

Let $\{\xi_{k,n}\}_{n=1}^{\infty}$ be a sequence of $C_0^\infty(0,\pi)$ functions so as $\lim_{n\to\infty}\|\xi_{k,n}-\sqrt{(2/\pi)}\sin(2k+1)/2\,\theta\|_{L^2(0,\pi)}=0$ for $k=1,\ldots,M$ and let $\omega\in C_0^\infty(0,R)$. Then using twice the definition of the distributional derivatives, the definitions of F_k and b_k, and the fact that $\omega\xi_{k,n}\in C_0^\infty((0,R)\times(0,\pi))$ we get

$$\begin{aligned}\int_0^R\frac{d}{dr}F_k(r)\omega(r)\mathrm{d}r&=-\int_0^R F_k(r)\omega'(r)\mathrm{d}r\\&=-\int_0^R\omega'(r)\int_0^\pi\sqrt{\frac{2}{\pi}}\tilde f(r,\theta)\sin\frac{2k+1}{2}\theta\,\mathrm{d}\theta\,\mathrm{d}r\\&=-\lim_{n\to\infty}\int_0^R\int_0^\pi\omega'(r)\xi_{k,n}(\theta)\tilde f(r,\theta)\mathrm{d}\theta\,\mathrm{d}r\\&=\lim_{n\to\infty}\int_0^R\int_0^\pi\omega(r)\xi_{k,n}(\theta)\frac{\partial\tilde f}{\partial r}(r,\theta)\mathrm{d}\theta\,\mathrm{d}r\\&=\int_0^R\omega(r)\int_0^\pi\sqrt{\frac{2}{\pi}}\frac{\partial}{\partial r}\tilde f(r,\theta)\sin\frac{2k+1}{2}\theta\,\mathrm{d}\theta\,\mathrm{d}r=\int_0^R b_k(r)\omega(r)\mathrm{d}r.\end{aligned}$$

Because $\omega(r)$ was chosen arbitrarily, we conclude that

$$b_k(r)=\frac{dF_k(r)}{dr}=F_k'(r). \tag{2.13}$$

We can apply the same procedure to $\tilde{g}(r,\theta)$. Using (2.12) and (2.13) we know that the series (2.8) and (2.9) can be differentiated by terms. Now we use the similar derivation for Δf. Let

$$\left(\frac{\partial^2\tilde{f}}{\partial r^2}(r,\theta)+\frac{1}{r}\frac{\partial\tilde{f}}{\partial r}(r,\theta)+\frac{1}{r^2}\frac{\partial^2\tilde{f}}{\partial\theta^2}(r,\theta)\right)=\sqrt{\frac{2}{\pi}}\sum_{k=0}^{\infty}c_k(r)\sin\frac{2k+1}{2}\theta.$$

From the first part of the proof we know $\tilde{f}(r,.)\in H^2(0,\pi)$ for a.e. r and we can compute

$$\begin{aligned}
&\int_0^R\left(F_k''(r)+\frac{1}{r}F_k'(r)-\frac{1}{r^2}\left(\frac{2k+1}{2}\right)^2F_k(r)\right)r\omega(r)\,\mathrm{d}r\\
&\quad=-\int_0^R rF_k'(r)\omega'(r)\,\mathrm{d}r-\left(\frac{2k+1}{2}\right)^2\int_0^R\frac{1}{r}F_k(r)\omega(r)\,\mathrm{d}r\\
&\quad=\int_0^R(r\omega'(r))'\int_0^\pi\sqrt{\frac{2}{\pi}}\tilde{f}(r,\theta)\sin\frac{2k+1}{2}\theta\,\mathrm{d}\theta\,\mathrm{d}r\\
&\qquad-\left(\frac{2k+1}{2}\right)^2\int_0^R\frac{\omega(r)}{r}\int_0^\pi\sqrt{\frac{2}{\pi}}\tilde{f}(r,\theta)\sin\frac{2k+1}{2}\theta\,\mathrm{d}\theta\,\mathrm{d}r\\
&\quad=\lim_{n\to\infty}\int_0^R(r\omega'(r))'\int_0^\pi\tilde{f}(r,\theta)\xi_{k,n}(\theta)\mathrm{d}\theta\,\mathrm{d}r+\int_0^R\frac{\omega(r)}{r}\int_0^\pi\sqrt{\frac{2}{\pi}}\tilde{f}(r,\theta)\frac{d^2\sin\frac{2k+1}{2}\theta}{d\theta^2}\mathrm{d}\theta\,\mathrm{d}r\\
&\quad=-\lim_{n\to\infty}\int_0^R\int_0^\pi\omega'(r)\xi_{k,n}(\theta)r\frac{\partial\tilde{f}}{\partial r}(r,\theta)\mathrm{d}\theta\,\mathrm{d}r+\int_0^R\frac{\omega(r)}{r}\\
&\qquad\times\sqrt{\frac{2}{\pi}}\left(-\frac{2k+1}{2}\tilde{f}(r,0)-(-1)^k\frac{\partial\tilde{f}}{\partial\theta}(r,\pi)+\int_0^\pi\frac{\partial^2\tilde{f}}{\partial\theta^2}(r,\theta)\sin\frac{2k+1}{2}\theta\,\mathrm{d}\theta\right)\mathrm{d}r\\
&\quad=\lim_{n\to\infty}\int_0^R\int_0^\pi\omega(r)\xi_{k,n}(\theta)\frac{\partial}{\partial r}\left(r\frac{\partial\tilde{f}}{\partial r}(r,\theta)\right)\mathrm{d}\theta\,\mathrm{d}r\\
&\qquad+\int_0^R\frac{\omega(r)}{r}\sqrt{\frac{2}{\pi}}\int_0^\pi\frac{\partial^2\tilde{f}}{\partial\theta^2}(r,\theta)\sin\frac{2k+1}{2}\theta\,\mathrm{d}\theta\,\mathrm{d}r\\
&\quad=\int_0^R\int_0^\pi\sqrt{\frac{2}{\pi}}\omega(r)r\left(\frac{\partial^2\tilde{f}}{\partial r^2}(r,\theta)+\frac{1}{r}\frac{\partial\tilde{f}}{\partial r}(r,\theta)+\frac{1}{r^2}\frac{\partial^2\tilde{f}}{\partial\theta^2}(r,\theta)\right)\sin\frac{2k+1}{2}\theta\,\mathrm{d}\theta\,\mathrm{d}r\\
&\quad=\int_0^R c_k(r)r\omega(r)\mathrm{d}r,
\end{aligned}$$

so

$$c_k(r)=F_k''(r)+\frac{1}{r}F_k'(r)-\frac{1}{r^2}\left(\frac{2k+1}{2}\right)^2F_k(r)\quad\text{for a.e. } r. \tag{2.14}$$

Let us denote $\Delta_p \tilde{f}(r,\theta)=(\partial^2\tilde{f}/\partial r^2)(r,\theta)+(1/r)(\partial\tilde{f}/\partial r)(r,\theta)+(1/r^2)(\partial^2\tilde{f}/\partial\theta^2)(r,\theta)$. Taking into account (2.11) we will solve an equation $\Delta_p\tilde{f}(r,\theta)=h(r,\theta)$ for any $h\in L^2((0,R)\times(0,\pi),r\,\mathrm{d}r\,\mathrm{d}\theta)$. We are seeking, of course, only those solutions for which the function $f(x,y)$ corresponding to the function $\tilde{f}(r,\theta)$ remains in the set $H^1(B(P,R)\cap\Omega)$. If we decompose a function h to the series $h=\sqrt{(2/\pi)}\Sigma_{k=0}^{\infty}H_k(r)\sin(2k+1)/2\,\theta$ we get a set of equations:

$$F_k''(r)+\frac{1}{r}F_k'(r)-\frac{1}{r^2}\left(\frac{2k+1}{2}\right)^2F_k(r)=H_k,\quad k=0,\ldots.$$

We denote $\nu=k+1/2$. The solutions of these equations are

$$F_0=r^{1/2}\int_0^r H_0(z)z^{1/2}\mathrm{d}z-r^{-1/2}\int_0^r H_0(z)z^{3/2}\mathrm{d}z+C_1^{(0)}r^{1/2}+C_2^{(0)}r^{-1/2} \tag{2.15}$$

and for $k>0$,

$$F_k=\frac{1}{2\nu}r^{\nu}\int_R^r H_k(z)z^{-\nu+1}\mathrm{d}z-\frac{1}{2\nu}r^{-\nu}\int_0^r H_k(z)z^{\nu+1}\mathrm{d}z+C_1^{(k)}r^{\nu}+C_2^{(k)}r^{-\nu}. \tag{2.16}$$

We can compute the first derivatives

$$F_0'=\frac{1}{2}r^{-1/2}\int_0^r H_0(z)z^{1/2}\mathrm{d}z+\frac{1}{2}r^{-3/2}\int_0^r H_0(z)z^{3/2}\mathrm{d}z+\frac{1}{2}C_1^{(0)}r^{-1/2}-\frac{1}{2}C_2^{(0)}r^{-3/2} \tag{2.17}$$

and for $k>0$,

$$F_k'=\frac{1}{2}r^{\nu-1}\int_R^r H_k(z)z^{-\nu+1}\mathrm{d}z+\frac{1}{2}r^{-\nu-1}\int_0^r H_k(z)z^{\nu+1}\mathrm{d}z+\nu C_1^{(k)}r^{\nu-1}-\nu C_2^{(k)}r^{-\nu-1}. \tag{2.18}$$

Because $\tilde{f},\ \partial\tilde{f}/\partial r\in L^2((0,R)\times(0,\pi),r\,\mathrm{d}\theta\,\mathrm{d}r)$, the functions F_k and F_k' have to be in the set $L^2((0,R),r\,\mathrm{d}r)$ for all k. Taking the first two terms in (2.16) we get after application of the triangle and Schwarz inequalities

$$\begin{aligned}
&\left|\frac{1}{2\nu}r^{\nu}\int_R^r H_k(z)z^{-\nu+1}\mathrm{d}z-\frac{1}{2\nu}r^{-\nu}\int_0^r H_k(z)z^{\nu+1}\mathrm{d}z\right|\\
&\quad\leqslant\frac{1}{2\nu}\left(r^{\nu}\sqrt{\int_r^R|H_k(z)|^2z\,\mathrm{d}z}\sqrt{\int_r^R z^{-2\nu+1}\mathrm{d}z}+r^{-\nu}\sqrt{\int_0^r|H_k(z)|^2z\,\mathrm{d}z}\sqrt{\int_0^r z^{2\nu+1}\,\mathrm{d}z}\right)\\
&\quad\leqslant\frac{1}{2\nu}r\sqrt{\int_0^R|H_k(z)|^2z\,\mathrm{d}z}\left(\sqrt{\frac{1-\left(\frac{R}{r}\right)^{-2\nu+2}}{2\nu-2}}+\frac{1}{\sqrt{2\nu+2}}\right)\\
&\quad\leqslant\frac{r}{\nu\sqrt{2\nu-2}}\sqrt{\int_0^R|H_k(z)|^2z\,\mathrm{d}z}
\end{aligned}$$

for $0<r<R$. Using a similar procedure on (2.15), (2.17), and (2.18) we get the following inequalities holding for every $k=0,1,\ldots$:

$$|F_k-C_1^{(k)}r^{\nu}-C_2^{(k)}r^{-\nu}|\leqslant\frac{r}{\nu\sqrt{|2\nu-2|}}\sqrt{\int_0^R|H_k(z)|^2z\,\mathrm{d}z}, \tag{2.19}$$

$$|F_k' - \nu C_1^{(k)} r^{\nu-1} + \nu C_2^{(k)} r^{-\nu-1}| \leqslant \frac{1}{\sqrt{|2\nu-2|}} \sqrt{\int_0^R |H_k(z)|^2 z \, \mathrm{d}z}. \tag{2.20}$$

We conclude using this estimate that the first three terms in (2.16) belong to $L^2((0,R), r\,\mathrm{d}r)$ and thus the fourth term has to be in this set too. But it is obvious that $r^{-\nu} \notin L^2((0,R), r\,\mathrm{d}r)$ for $\nu \geqslant 3/2$. Hence $C_2^{(k)} = 0$ for $k \geqslant 1$. Applying the same arguments to (2.17) we have also $C_2^{(0)} = 0$. Moreover the condition $\int_0^R \Sigma_{k=0}^{\infty} |F_k'(r)|^2 r \, \mathrm{d}r < \infty$ must be satisfied. First we suppose $C_1^{(k)} = 0$ for all k. Then using estimate (2.20)

$$\begin{aligned}\int_0^R \sum_{k=0}^{\infty} |F_k'(r)|^2 r \, \mathrm{d}r &\leqslant \int_0^R r \, \mathrm{d}r \sum_{k=0}^{\infty} \frac{1}{2|\nu-1|} \int_0^R |H_k(z)|^2 z \, \mathrm{d}z \\ &\leqslant \|h\|^2_{L^2((0,R)\times(0,\pi), r\,\mathrm{d}\theta\,\mathrm{d}r)} \int_0^R r \, \mathrm{d}r \\ &= \frac{R^2}{2} \|h\|^2_{L^2((0,R)\times(0,\pi), r\,\mathrm{d}\theta\,\mathrm{d}r)}.\end{aligned}$$

Thus we must choose the constants $C_1^{(k)}$ so as

$$\sum_{k=0}^{\infty} \int_0^R |C_1^{(k)}|^2 \nu^2 r^{2\nu-2} r \, \mathrm{d}r = \sum_{k=0}^{\infty} |C_1^{(k)}|^2 \frac{\nu}{2} R^{2\nu} < \infty. \tag{2.21}$$

Now we turn our attention to the function $\tilde{g}(r,\theta)$. Using (2.10) we can write

$$u(r) := \sum_{k=0}^{\infty} \frac{1}{r^2} \left(\frac{2k+1}{2}\right)^2 |G_k(r)|^2 \in L^1((0,R), r\,\mathrm{d}r).$$

Denoting $v(r) = ru(r)$ we get a function $v \in L^1(0,R)$. Thus we can state $\liminf_{r\to 0^+} |rv(r)| = 0$. Otherwise $|rv(r)| \geqslant a > 0$ for a.e. small r, so $|v(r)| \geqslant a/r$ for some constant a and a.e. sufficiently small r, which is a contradiction of the fact that $v \in L^1(0,R)$. Hence we can find a sequence $\{r_n\}_{n=1}^{\infty}$ such that $r_n \to 0^+$ and

$$\lim_{n\to\infty} |r_n v(r_n)| = \lim_{n\to\infty} \sum_{k=0}^{\infty} \left(\frac{2k+1}{2}\right)^2 |G_k(r_n)|^2 = 0. \tag{2.22}$$

Now we are ready to return to (2.7). We rewrite the particular terms of this sum using (2.8) and (2.9),

$$\int_0^{\pi} \frac{\partial \tilde{f}_k(r_n,\theta)}{\partial r} \overline{\tilde{g}_k(r_n,\theta)} r_n \, \mathrm{d}\theta = \sum_{k=0}^{\infty} r_n F_k'(r_n) \overline{G_k(r_n)}.$$

The right-hand side of this equality can be estimated using (2.20), the triangle inequality and the Schwarz inequality in the space ℓ^2,

$$\begin{aligned}\left|\sum_{k=0}^{\infty} r_n F_k'(r_n) \overline{G_k(r_n)}\right| &\leqslant r_n \sum_{k=0}^{\infty} |G_k(r_n)| \left(\sqrt{\int_0^R |H_k(z)|^2 z \, \mathrm{d}z} \frac{1}{\sqrt{|2\nu-2|}} + \nu |C_1^{(k)}| r_n^{\nu-1} \right) \\ &\leqslant \sqrt{\sum_{k=0}^{\infty} |G_k(r_n)|^2} \left(r_n \|h\|_{L^2((0,R)\times(0,\pi), r\,\mathrm{d}\theta\,\mathrm{d}r)} + \sqrt{\sum_{k=0}^{\infty} \nu^2 |C_1^{(k)}|^2 r_n^{2\nu}} \right).\end{aligned} \tag{2.23}$$

Because of (2.22) it is enough to show that the last term in brackets in (2.23) is bounded and we will know that the statement (2.7) holds. Due to (2.21) it is sufficient to prove that the inequality $\nu r^{2\nu}<R^{2\nu}/2$ holds for all $\nu=1/2,3/2,\ldots$ and sufficiently small r. Rewriting the inequality to the form

$$\frac{r}{R}<\left(\frac{1}{2\nu}\right)^{1/2\nu} \tag{2.24}$$

we will study the function $\phi(x)=(1/x)^{1/x}$ on the interval $[1,\infty)$. It is obvious that ϕ is continuous and strictly positive on this interval. As

$$\frac{d}{dx}\phi(x)=\phi(x)\frac{\ln(x)-1}{x^2},$$

ϕ reaches its global minimum at the point $x=e$. Thus for $r/R<(1/e)^{1/e}$ the inequality (2.24) holds for every ν, which completes the proof. ■

Remark 1: The fact that all the functions from the domain of the Hamiltonian, which is defined by the quadratic form, satisfy the prescribed boundary condition is supposed to be well-known for domains with reasonable boundaries. But it is also very often supposed that the operator domain is the subset of the Sobolev space $H^2(\Omega)$, which satisfies the boundary conditions. The systems with combined boundary conditions are examples of operators for which this assertion is not true. The situation is similar to the systems studied in Ref. 11. It was shown there, that for bounded regions in the plane $\mathbb{R}^2$ with piecewise C^3-boundary, which has finite number of angles larger than π, there exists for each such angle one function, which is not in $H^2(\Omega)$ and which belongs to the operator domain with the Dirichlet boundary condition. The operator domain is then a span of the $H_0^2(\Omega)$ space and all these functions, called Guseva functions.

It is easy to check that similar functions belong to operator domain in our systems, too. Let us take the following function, written in polar coordinates with the origin in some P_k and $R<d$:

$$f(r,\theta)=\xi(r)r^{1/2}\sin\frac{\theta}{2}, \tag{2.25}$$

where $\xi(r)\in C^\infty(0,\infty)$, $\xi(r)=1$ on $(0,R/2)$, and $\xi(r)=0$ for $r>R$. This function satisfies the boundary conditions, $\Delta_p f\in L^2(\Omega)$ and $f\in H^1(\Omega)$, thus $f\in D(\Omega)$. But $f\notin H^2(\Omega)$. The trace on the part of the boundary $(-R/2,R/2)$ is

$$\frac{1}{r}\frac{\partial f}{\partial\theta}(r,\theta)=\begin{cases}\frac{1}{2}r^{-1/2} & \text{for } \theta=0\\ 0 & \text{for } \theta=\pi.\end{cases}$$

So even the trace of the normal derivatives on the boundary is not square integrable. These are the reasons why we cannot immediately use the Gauss theorem in the proof of Theorem 1.

The interesting open question arises whether all eigenfunctions have Guseva-like behavior near the points P_k.

III. BOUND STATES

Now we are going to study our specific systems from Fig. 1. First we localize the essential spectra of these systems and make the first estimate on the number of bound states below the essential spectrum threshold using the technique of the Dirichlet–Neumann bracketing (see, e.g., Ref. 14, Sec. XIII.15). Then we will continue with the specification of the number of bound states using variational methods.

A. Essential spectrum, number of bound states

The following arguments are the same for both our systems, so we do not distinguish between them in this section. Cutting the domain Ω by the additional Neumann or Dirichlet boundaries parallel to the y axis at $x=\pm\delta$, we get new operators $H^{(N)}$, $H^{(D)}$ defined in the standard way, using the quadratic form. We can decompose these operators $H^{(j)}=H_t^{(j)}\oplus H_c^{(j)}$, $j=N,D$, where the ''tail'' part corresponds to the two half strips and the rest to the central part with the Neumann and Dirichlet condition on the vertical boundaries, respectively. Using Dirichlet–Neumann bracketing we have $H_t^{(N)}\oplus H_c^{(N)}\leqslant -\Delta_{DN}^{\Omega}\leqslant H_t^{(D)}\oplus H_c^{(D)}$ in the sense of quadratic forms (see Ref. 14, Sec. XIII.15).

Now $\sigma_{\mathrm{ess}}(H_t^{(j)})=[\pi^2/4d^2,\infty)$, $j=N,D$ (we get this result after simple calculation using Example 4.9.6 in Ref. 13 and Corollary of Theorem VIII.33 in Ref. 14). By the minimax principle (see e.g., Ref. 14, Sec. XIII.1) $-\Delta_{DN}^{\Omega}$ has the same infimum of the essential spectrum. To verify that $\sigma_{\mathrm{ess}}(-\Delta_{DN}^{\Omega})$ is indeed the whole interval $[\pi^2/4d^2,\infty)$ we can use the same procedure as for $H_t^{(j)}$ (see Example 4.9.6 in Ref. 13). Possible isolated eigenvalues of $-\Delta_{DN}^{\Omega}$ are squeezed between those of $H_c^{(j)}$, $j=N,D$. Because the first eigenvalue of $H_c^{(N)}$ is zero, $-\Delta_{DN}^{\Omega}$ has an eigenvalue below the essential spectrum threshold provided $H_c^{(D)}$ does, which is true if $\delta>d$.

More generally, the number N_D of eigenvalues of $H_c^{(D)}$ smaller than $\pi^2/4d^2$ equals the largest integer number smaller than δ/d, i.e., $N_D=-[-\delta/d]-1$, where $[\cdot]$ denotes the entire part. The number of ''Neumann'' eigenvalues of $H_c^{(N)}$ is $N_N=1+N_D$. This means that the number of bound states of $-\Delta_{DN}^{\Omega}$ below the essential spectrum threshold satisfies the inequality

$$-\left[-\frac{\delta}{d}\right]-1\leqslant N\leqslant -\left[-\frac{\delta}{d}\right]. \tag{3.1}$$

We see that $-\Delta_{DN}^{\Omega}$ has isolated eigenvalues, at least for large enough δ. In the same way, one finds that the mth eigenvalue μ_m of $-\Delta_{DN}^{\Omega}$ is estimated by

$$\left(\frac{m-1}{\lambda}\right)^2\leqslant\frac{\mu_m}{\mu}\leqslant\left(\frac{m}{\lambda}\right)^2, \tag{3.2}$$

where $\lambda=\delta/d$ and $\mu=\inf(\sigma_{\mathrm{ess}})=\pi^2/4d^2$, and that the critical value $\lambda_m=\delta_m/d$ at which mth eigenvalue appears satisfies the bounds

$$m-1\leqslant\lambda_m\leqslant m. \tag{3.3}$$

To learn more about the dependence of the eigenvalues and the corresponding eigenfunctions on λ, we have to use a different technique.

B. Existence of bound states

The above-presented existence argument for $\lambda>1$ is a crude one. In fact, there is no lower bound on the length of the overlay of Neumann boundaries for case (B), which was shown in Ref. 8, Lemma 3.2. On the other hand we will show that in system (A) the discrete spectrum of the Hamiltonian is empty for small λ, but the ground state appears sooner than $\lambda=1$. We will distinguish the two cases writing $-\Delta_{DN}^{\Omega,\mathrm{A}}$, respectively, $-\Delta_{DN}^{\Omega,\mathrm{B}}$ instead of $-\Delta_{DN}^{\Omega}$ and $Q^{\mathrm{A}}(q_0)$, respectively, $Q^{\mathrm{B}}(q_0)$ instead of $Q(q_0)$.

Theorem 2: *The operator $-\Delta_{DN}^{\Omega,\mathrm{B}}$ has an isolated eigenvalue in $[0,\mu)$ for any $\delta>0$.*

The proof can be found in Ref. 8, Lemmas 2.2 and 3.1. We repeat the theorem here to show the difference with case (A), where the situation is more complicated.

Theorem 3: *There exists a real number $\Lambda_0\in(0,1)$, such that the discrete spectrum of the operator $-\Delta_{DN}^{\Omega,\mathrm{A}}(\lambda)$ is empty for all $\lambda\leqslant\Lambda_0$ and there exists at least one isolated eigenvalue in the spectrum of this operator for all $\lambda>\Lambda_0$.*

Proof: Taking into account that $\mu_1(\lambda)=\inf_{\varphi\in Q^A(q_0),\|\varphi\|=1} q_0(\varphi)$ is a nonincreasing continuous function of λ (see Appendix A) and the minimax principle,[14] it is sufficient to show that there are two real positive numbers $\Lambda_1<\Lambda_2$, Λ_1, $\Lambda_2\in(0,1)$, such that

(i) the discrete spectrum is empty for all $\lambda<\Lambda_1$,
(ii) there exists at least one isolated eigenvalue in the spectrum for all $\lambda>\Lambda_2$.

We know from Sec. III A that there exists a bound state for $\lambda>1$. Let us search for a better estimate $\Lambda_2<1$ by the variational technique. We are seeking the trial function $\Phi\in Q^A(q_0)$, for which the functional q defined by

$$q[\Phi]=q_0(\Phi,\Phi)-\mu\|\Phi\|^2_{L^2(\Omega)} \tag{3.4}$$

has a negative value (see, e.g., Ref. 16, Chap. 4). We can choose Φ continuous inside Ω, but not necessarily smooth. To make the longitudinal contribution to the kinetic energy small, we use an external scaling.

We start with the trial function

$$\Phi_\sigma(x,y)=\varphi_\sigma(x)\sin\frac{\pi y}{2d}+\psi_\sigma(x)\cos\frac{\pi y}{2d}+\eta(x)+\chi(x)\cos\frac{\pi y}{d}, \tag{3.5}$$

where

$$\varphi_\sigma(x)=\begin{cases}\varphi(x) & \text{for} \quad x\geqslant-\delta\\ \varphi(-\delta+\sigma(x+\delta)) & \text{for} \quad x\leqslant-\delta,\end{cases}$$

$$\psi_\sigma(x)=\begin{cases}\psi(x) & \text{for} \quad x\leqslant\delta\\ \psi(\delta+\sigma(x-\delta)) & \text{for} \quad x\geqslant\delta,\end{cases}$$

φ, $\psi\in\mathcal{S}(\mathbb{R})$, $\varphi(-\delta)=\psi(\delta)=1$; $\varphi(x)=0$ on $[\delta,\infty)$, $\psi(x)=0$ on $(-\infty,-\delta]$, η, $\chi\in C^\infty[-\delta,\delta]$ and $\eta(x)=\chi(x)=0$ for $|x|\geqslant\delta$. The value 1 of $\varphi(-\delta)$ and $\psi(\delta)$ is not important, it can be any constant without the influence on the result. We choose $\varphi(-\delta)=\psi(\delta)$, because we expect the ground state to be symmetric. We shall assume the functions φ, ψ, η, χ to be real. We decompose the functional q to three parts, in each of which one integrates over regions I, II, and III, respectively,

$$q[\Phi_\sigma]=q_{\mathrm{I}}[\Phi_\sigma]+q_{\mathrm{II}}[\Phi_\sigma]+q_{\mathrm{III}}[\Phi_\sigma]=\frac{d}{2}\sigma(\|\varphi'\|^2_{L^2(-\infty,-\delta)}+\|\psi'\|^2_{L^2(\delta,\infty)})+q_{\mathrm{II}}[\Phi_\sigma]. \tag{3.6}$$

We see that the first term here is always positive, but it can be arbitrarily small, due to the parameter σ, while the second term does not depend on σ. We easily compute

$$\begin{aligned}q_{\mathrm{II}}[\Phi_\sigma]=\int_{-\delta}^{\delta}\Bigg(&\frac{d}{2}(\varphi'(x)^2+\psi'(x)^2+\chi'(x)^2)+d\,\eta'(x)^2+\frac{2d}{\pi}\varphi'(x)\psi'(x)+\frac{4d}{3\pi}\chi'(x)(\psi'(x)\\&-\varphi'(x))+\frac{4d}{\pi}\eta'(x)(\varphi'(x)+\psi'(x))+\frac{\pi}{d}\chi(x)(\psi(x)-\varphi(x))+\frac{3\pi^2}{8d}\chi(x)^2\\&-\frac{\pi}{d}\varphi(x)\psi(x)-\frac{\pi^2}{4d}\eta(x)^2-\frac{\pi}{d}\eta(x)(\psi(x)+\varphi(x))\Bigg)\mathrm{d}x.\end{aligned} \tag{3.7}$$

We choose the solution of the Euler equations

$$d\varphi''(x)+\frac{2d}{\pi}\psi''(x)-\frac{4d}{3\pi}\chi''(x)+\frac{4d}{\pi}\eta''(x)+\frac{\pi}{d}(\psi(x)+\eta(x)+\chi(x))=0,$$

$$d\psi''(x)+\frac{2d}{\pi}\varphi''(x)+\frac{4d}{3\pi}\chi''(x)+\frac{4d}{\pi}\eta''(x)+\frac{\pi}{d}(\varphi(x)+\eta(x)-\chi(x))=0,$$

$$d\chi''(x)+\frac{4d}{3\pi}(\psi''(x)-\varphi''(x))-\frac{\pi}{d}(\psi(x)-\varphi(x))-\frac{3\pi^2}{4d}\chi(x)=0,$$

$$2d\eta''(x)+\frac{4d}{\pi}(\psi''(x)+\varphi''(x))+\frac{\pi}{d}(\psi(x)+\varphi(x))+\frac{\pi^2}{2d}\eta(x)=0$$

to be a trial function. By linear combinations of these equations we can obtain uncoupled second-order differential equations for $\varphi-\psi$ and $\varphi+\psi$. Then the solution with above-mentioned boundary condition is obtained,

$$\chi(x)=\frac{4}{3\pi}\left(\frac{\sinh\frac{\sqrt{3}\pi x}{2d}}{\sinh\frac{\sqrt{3}\pi\delta}{2d}}-\frac{\sinh\frac{\pi x}{d}\sqrt{3\frac{3\pi-8}{9\pi^2-18\pi-32}}}{\sinh\frac{\pi\delta}{d}\sqrt{3\frac{3\pi-8}{9\pi^2-18\pi-32}}}\right),$$

$$\varphi(x)=\frac{1}{2}\left(\frac{\cosh\frac{\pi x}{d}\sqrt{\frac{4-\pi}{\pi^2+2\pi-16}}}{\cosh\frac{\pi\delta}{d}\sqrt{\frac{4-\pi}{\pi^2+2\pi-16}}}-\frac{\sinh\frac{\pi x}{d}\sqrt{3\frac{3\pi-8}{9\pi^2-18\pi-32}}}{\sinh\frac{\pi\delta}{d}\sqrt{3\frac{3\pi-8}{9\pi^2-18\pi-32}}}\right),$$

$$\psi(x)=\frac{1}{2}\left(\frac{\cosh\frac{\pi x}{d}\sqrt{\frac{4-\pi}{\pi^2+2\pi-16}}}{\cosh\frac{\pi\delta}{d}\sqrt{\frac{4-\pi}{\pi^2+2\pi-16}}}+\frac{\sinh\frac{\pi x}{d}\sqrt{3\frac{3\pi-8}{9\pi^2-18\pi-32}}}{\sinh\frac{\pi\delta}{d}\sqrt{3\frac{3\pi-8}{9\pi^2-18\pi-32}}}\right), \tag{3.8}$$

$$\eta(x)=\frac{2}{\pi}\left(\frac{\cos\frac{\pi x}{2d}}{\cos\frac{\pi\delta}{2d}}-\frac{\cosh\frac{\pi x}{d}\sqrt{\frac{4-\pi}{\pi^2+2\pi-16}}}{\cosh\frac{\pi\delta}{d}\sqrt{\frac{4-\pi}{\pi^2+2\pi-16}}}\right).$$

As the quadratic form of the derivatives in (3.7) is positive definite this trial function is a good candidate for a minimum of the functional (3.7). Now we substitute (3.8) to (3.7) and after a tedious but straightforward calculation we obtain

$$q_{\mathrm{II}}[\Phi_\sigma]=\frac{\sqrt{(4-\pi)(\pi^2+2\pi-16)}}{2\pi}\tanh\frac{\pi\delta}{d}\sqrt{\frac{4-\pi}{\pi^2+2\pi-16}}+\frac{8}{3\sqrt{3}\pi}\coth\frac{\sqrt{3}\pi\delta}{2d}$$
$$+\frac{\sqrt{(3\pi-8)(9\pi^2-18\pi-32)}}{6\sqrt{3}\pi}\coth\frac{\pi\delta}{d}\sqrt{3\frac{3\pi-8}{9\pi^2-18\pi-32}}-\frac{4}{\pi}\tan\frac{\pi\delta}{2d}. \tag{3.9}$$

Now we can understand q_{II} like a function of a variable δ. We see that q_{II} is a continuous function on the interval $(0,d)$, $\lim_{\delta\to 0^+} q_{\mathrm{II}}(\delta)=+\infty$ and $\lim_{\delta\to d^-} q_{\mathrm{II}}(\delta)=-\infty$. So there must exist a point $\delta_0\in(0,d)$ and corresponding number $\Lambda_2=\delta_0/d$, such that $q_{\mathrm{II}}(\delta)<0$ for $\delta\in(\delta_0,d)$. Thus we can find for every δ from this interval a number σ small enough to have $q[\Phi_\sigma]<0$, which finishes the proof of the existence of Λ_2.

Now we are going to prove that the discrete spectrum of the operator $-\Delta_{DN}^{\Omega,A}(\lambda)$ is empty for all $\lambda\leqslant\Lambda_1$. It will be shown if we demonstrate that the functional $q[\Phi]\geqslant 0$ for all Φ from a suitable dense [in $H^1(\Omega)$ norm] set in $Q^A(q_0)$, say

$$\mathcal{Q}(\Omega)=\{\psi\in H^1(\Omega)\cap C(\overline{\Omega})\,|\,\psi\in C^2(\Omega_j), j=\mathrm{I,II,III}, \psi\restriction\mathcal{D}=0\},$$

where $C(\overline{\Omega})$ is just the set of functions continuous in the closure of Ω. It can be proven that this set is really dense in $Q^A(q_0)$ (See Appendix B). We again decompose q into three parts $q[\Phi]=q_{\mathrm{I}}[\Phi]+q_{\mathrm{II}}[\Phi]+q_{\mathrm{III}}[\Phi]$. The "tail" parts of $\Phi\in\mathcal{Q}(\Omega)$ we expand to the series

$$\Phi(x,y)=\sqrt{\frac{2}{d}}\sum_{k=0}^{\infty} a_k(x)\sin\frac{2k+1}{2d}\pi y \tag{3.10}$$

in the region Ω_{I} and

$$\Phi(x,y)=\sqrt{\frac{2}{d}}\sum_{k=0}^{\infty} b_k(x)\cos\frac{2k+1}{2d}\pi y \tag{3.11}$$

in region Ω_{III}. Using the same procedure like in the proof of Theorem 1, we know that these series can be differentiated by terms. Hence

$$q_{\mathrm{I}}[\Phi]=\sum_{k=0}^{\infty}\int_{-\infty}^{-\delta}\left(|a_k'(x)|^2+\frac{\pi^2}{d^2}(k^2+k)|a_k(x)|^2\right)\mathrm{d}x, \tag{3.12}$$

$$q_{\mathrm{III}}[\Phi]=\sum_{k=0}^{\infty}\int_{\delta}^{\infty}\left(|b_k'(x)|^2+\frac{\pi^2}{d^2}(k^2+k)|b_k(x)|^2\right)\mathrm{d}x, \tag{3.13}$$

and we see that $q_{\mathrm{I}}[\Phi]\geqslant 0$ and $q_{\mathrm{III}}[\Phi]\geqslant 0$ for all $\Phi\in\mathcal{Q}(\Omega)$. As we have seen previously above [similar to (3.6)] the contributions from the terms $|a_0'(x)|^2$ and $|b_0'(x)|^2$ can be arbitrarily small. We minimalize the rest of the functional using Euler equations, the general boundary conditions fixing the function values at $x=\delta$, $x=-\delta$, and the square integrability. As $\Phi\in C(\overline{\Omega})$ the Fourier coefficients a_k, b_k are continuous in $(-\infty,-\delta]$, $[\delta,\infty)$ and $a_k(-\delta)$, $b_k(\delta)$ are those of $\Phi(-\delta,\cdot)$, $\Phi(\delta,\cdot)$, respectively. The solution of the Euler equations will be really the absolute minimum of $q_{\mathrm{I}}+q_{\mathrm{III}}$. It is easy to see that for all Φ in the set $\mathcal{Q}(\Omega)$, $q_{\mathrm{I}}[\Phi]+q_{\mathrm{III}}[\Phi]=q_{\mathrm{I}}[\Phi_0]+q_{\mathrm{III}}[\Phi_0]+q_{\mathrm{I}}[\Phi-\Phi_0]+q_{\mathrm{III}}[\Phi-\Phi_0]$, where Φ_0 is given by Euler equations and we have seen previously that $q_{\mathrm{I}}[\Phi-\Phi_0]+q_{\mathrm{III}}[\Phi-\Phi_0]\geqslant 0$. For $k=1,2,\ldots$ we get

$$a_k''(x)-\frac{\pi^2}{d^2}k(k+1)a_k(x)=0,$$

$$b_k''(x)-\frac{\pi^2}{d^2}k(k+1)b_k(x)=0$$

and the square integrable solutions of these equations are

$$a_k(x)=A_k\exp\left(\frac{\pi}{d}\sqrt{k(k+1)}(x+\delta)\right), \tag{3.14}$$

$$b_k(x)=B_k\exp\left(\frac{\pi}{d}\sqrt{k(k+1)}(\delta-x)\right). \tag{3.15}$$

Putting these results to (3.12) and (3.13) we have

$$q_{\mathrm{I}}[\Phi]+q_{\mathrm{III}}[\Phi]\geqslant\frac{\pi}{d}\sum_{k=1}^{\infty}\sqrt{k(k+1)}(|A_k|^2+|B_k|^2). \tag{3.16}$$

Let us turn our attention to the functional q_{II}. First we estimate the value $\|\Phi\|^2_{L^2(\Omega_{\mathrm{II}})}$. Denoting $\Phi_-(y)=\Phi(-\delta,y)$ and $\Phi_+(y)=\Phi(\delta,y)$ we can write

$$\begin{aligned}
\|\Phi\|^2_{L^2(\Omega_{\mathrm{II}})}&=\int_0^d\int_{-\delta}^{\delta}\left|\Phi_-(y)+\int_{-\delta}^{x}\frac{\partial\Phi}{\partial x}(z,y)\,\mathrm{d}z\right|\left|\int_x^{\delta}\frac{\partial\Phi}{\partial x}(z,y)\,\mathrm{d}z-\Phi_+(y)\right|\mathrm{d}x\,\mathrm{d}y\\
&\leqslant\int_0^d\int_{-\delta}^{\delta}\left(|\Phi_-(y)|+\int_{-\delta}^{\delta}\left|\frac{\partial\Phi}{\partial x}(z,y)\right|\mathrm{d}z\right)\left(|\Phi_+(y)|+\int_{-\delta}^{\delta}\left|\frac{\partial\Phi}{\partial x}(z,y)\right|\mathrm{d}z\right)\mathrm{d}x\,\mathrm{d}y\\
&=2\delta\int_0^d\left(|\Phi_-(y)|\,|\Phi_+(y)|+(|\Phi_-(y)|+|\Phi_+(y)|)\int_{-\delta}^{\delta}\left|\frac{\partial\Phi}{\partial x}(z,y)\right|\mathrm{d}z\right.\\
&\quad\left.+\left(\int_{-\delta}^{\delta}\left|\frac{\partial\Phi}{\partial x}(z,y)\right|\mathrm{d}z\right)^2\right)\mathrm{d}y\leqslant 2\delta\left(\|\Phi_-\|_{L^2(0,d)}\|\Phi_+\|_{L^2(0,d)}+\||\Phi_-|\right.\\
&\quad\left.+|\Phi_+|\,\|_{L^2(0,d)}\sqrt{\int_0^d\left(\int_{-\delta}^{\delta}\left|\frac{\partial\Phi}{\partial x}(z,y)\right|\mathrm{d}z\right)^2\mathrm{d}y}+2\delta\left\|\frac{\partial\Phi}{\partial x}\right\|^2_{L^2(\Omega_{\mathrm{II}})}\right)\\
&\leqslant 2\delta\left(\|\Phi_-\|_{L^2(0,d)}\|\Phi_+\|_{L^2(0,d)}+\sqrt{2\delta}\||\Phi_-|+|\Phi_+|\,\|_{L^2(0,d)}\left\|\frac{\partial\Phi}{\partial x}\right\|_{L^2(\Omega_{\mathrm{II}})}\right.\\
&\quad\left.+2\delta\left\|\frac{\partial\Phi}{\partial x}\right\|^2_{L^2(\Omega_{\mathrm{II}})}\right),
\end{aligned}$$

where we used the fact that $\Phi\in C^2(\Omega_{\mathrm{II}})$ and the Schwarz inequality. Denoting $\kappa=\lambda\pi$, we use the last estimate and obtain

$$\begin{aligned}
q_{\mathrm{II}}[\Phi]&=\left\|\frac{\partial\Phi}{\partial x}\right\|^2_{L^2(\Omega_{\mathrm{II}})}+\left\|\frac{\partial\Phi}{\partial y}\right\|^2_{L^2(\Omega_{\mathrm{II}})}-\frac{\pi^2}{4d^2}\|\Phi\|^2_{L^2(\Omega_{\mathrm{II}})}\geqslant\left\|\frac{\partial\Phi}{\partial x}\right\|^2_{L^2(\Omega_{\mathrm{II}})}(1-\kappa^2)\\
&\quad-\sqrt{2\delta}\,\frac{\kappa\pi}{2d}\||\Phi_-|+|\Phi_+|\,\|_{L^2(0,d)}\left\|\frac{\partial\Phi}{\partial x}\right\|_{L^2(\Omega_{\mathrm{II}})}-\frac{\kappa\pi}{2d}\|\Phi_-\|_{L^2(0,d)}\|\Phi_+\|_{L^2(0,d)}.
\end{aligned} \tag{3.17}$$

Let us assume that there exists $\Phi\in\mathcal{Q}(\Omega)$ such that $q[\Phi]<0$. Taking into consideration (3.16) we conclude that $q_{\mathrm{II}}[\Phi]<0$ for considered $\Phi\in\mathcal{Q}$. Then also

$$\left\|\frac{\partial\Phi}{\partial x}\right\|^2_{L^2(\Omega_{\mathrm{II}})}(1-\kappa^2)-\sqrt{2\delta}\frac{\kappa\pi}{2d}\||\Phi_-|+|\Phi_+|\,\|_{L^2(0,d)}\left\|\frac{\partial\Phi}{\partial x}\right\|_{L^2(\Omega_{\mathrm{II}})}-\frac{\kappa\pi}{2d}\|\Phi_-\|_{L^2(0,d)}\|\Phi_+\|_{L^2(0,d)}<0.$$

This inequality holds obviously for $\kappa\geqslant 1$. Let us solve this inequality for $\kappa<1$. Then using the triangle inequality together with the inequality

$$2\|\Phi_-\|_{L^2(0,d)}\|\Phi_+\|_{L^2(0,d)} \leqslant \tfrac{1}{2}(\|\Phi_-\|_{L^2(0,d)}+\|\Phi_+\|_{L^2(0,d)})^2 \tag{3.18}$$

we get

$$\left\|\frac{\partial\Phi}{\partial x}\right\|_{L^2(\Omega_{\mathrm{II}})} < \frac{\kappa}{2\sqrt{2\,\delta}(1-\kappa)}(\|\Phi_-\|_{L^2(0,d)}+\|\Phi_+\|_{L^2(0,d)}). \tag{3.19}$$

We use this result in the following estimate:

$$\|\Phi_+-\Phi_-\|_{L^2(0,d)} = \sqrt{\int_0^d \left|\int_{-\delta}^{\delta}\frac{\partial\Phi}{\partial x}\mathrm{d}x\right|^2 \mathrm{d}y} \leqslant \sqrt{2\,\delta}\left\|\frac{\partial\Phi}{\partial x}\right\|_{L^2(\Omega_{\mathrm{II}})}$$

$$< \frac{\kappa}{2(1-\kappa)}(\|\Phi_-\|_{L^2(0,d)}+\|\Phi_+\|_{L^2(0,d)}). \tag{3.20}$$

Now we use estimates (3.16) and (3.17) together with inequality (3.18), the triangle inequality and

$$(\|\Phi_-\|_{L^2(0,d)}+\|\Phi_+\|_{L^2(0,d)})^2 \leqslant 2(\|\Phi_-\|^2_{L^2(0,d)}+\|\Phi_+\|^2_{L^2(0,d)}) \tag{3.21}$$

to estimate whole functional $q[\Phi]$. Denoting $A_0=a_0(-\delta)$, $B_0=b_0(\delta)$, we obtain

$$\begin{aligned} q[\Phi] &\geqslant \frac{\pi}{d}\sum_{k=1}^{\infty}\sqrt{k(k+1)}(|A_k|^2+|B_k|^2)+\left\|\frac{\partial\Phi}{\partial x}\right\|^2_{L^2(\Omega_{\mathrm{II}})}(1-\kappa^2)-\sqrt{2\,\delta}\frac{\kappa\pi}{2d}\||\Phi_-| \\ &\quad +|\Phi_+|\,\|_{L^2(0,d)}\left\|\frac{\partial\Phi}{\partial x}\right\|_{L^2(\Omega_{\mathrm{II}})}-\frac{\kappa\pi}{2d}\|\Phi_-\|_{L^2(0,d)}\,\|\Phi_+\|_{L^2(0,d)} \\ &\geqslant \frac{\pi\sqrt{2}}{d}\sum_{k=1}^{\infty}(|A_k|^2+|B_k|^2)+(1-\kappa^2)\left(\left\|\frac{\partial\Phi}{\partial x}\right\|_{L^2(\Omega_{\mathrm{II}})}-\sqrt{2\,\delta}\frac{\kappa\pi}{4d}\frac{\||\Phi_-|+|\Phi_+|\,\|_{L^2(0,d)}}{1-\kappa^2}\right)^2 \\ &\quad -\frac{\kappa^3\pi}{8d}\frac{\||\Phi_-|+|\Phi_+|\,\|^2_{L^2(0,d)}}{(1-\kappa^2)}-\frac{\kappa\pi}{4d}(\|\Phi_-\|^2_{L^2(0,d)}+\|\Phi_+\|^2_{L^2(0,d)}) \\ &\geqslant \frac{\pi\sqrt{2}}{d}\sum_{k=1}^{\infty}(|A_k|^2+|B_k|^2)-\frac{\kappa\pi}{4d(1-\kappa^2)}\sum_{k=0}^{\infty}(|A_k|^2+|B_k|^2), \end{aligned} \tag{3.22}$$

where we also used (3.10) and (3.11) together with (3.14) and (3.15). We assumed $q[\Phi]<0$, thus the same is true for the last expression in (3.22) and so we obtain for $\kappa<(\sqrt{129}-1)/8\sqrt{2}\doteq 0.92$,

$$\sum_{k=1}^{\infty}(|A_k|^2+|B_k|^2) < \frac{\kappa}{4\sqrt{2}(1-\kappa^2)-\kappa}(|A_0|^2+|B_0|^2). \tag{3.23}$$

Now we need estimates (3.21), (3.20), and (3.23) together with known inequalities for non-negative numbers

$$2ab \leqslant a^2+b^2,$$

$$(a+b+c)^2 \leqslant 3(a^2+b^2+c^2),$$

and the triangle inequality to do the last step of the proof. First notice, that

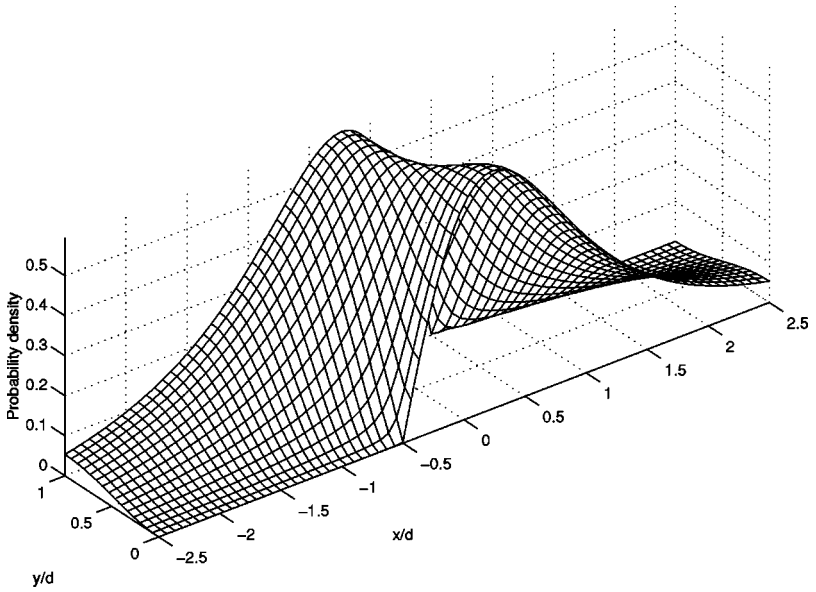

FIG. 2. Probability density $|\psi|^2$ (in units of d^{-2}) for the bound state in model A, $\lambda = 1/2$, coordinates x, y in the units of d. Only one discrete bound state exists here.

$$\frac{2}{d}\left\| A_0 \sin\frac{\pi y}{2d} - B_0 \cos\frac{\pi y}{2d}\right\|^2_{L^2(0,d)} = |A_0|^2 + |B_0|^2 - \frac{4}{\pi}\Re(A_0 B_0) \geqslant \left(1 - \frac{2}{\pi}\right)(|A_0|^2 + |B_0|^2). \tag{3.24}$$

On the other hand,

$$\begin{aligned}
&\frac{2}{d}\left\| A_0 \sin\frac{\pi y}{2d} - B_0 \cos\frac{\pi y}{2d}\right\|^2_{L^2(0,d)} \\
&\quad = \left\| \Phi_- - \Phi_+ - \sqrt{\frac{2}{d}}\sum_{k=1}^{\infty}\left(A_k \sin\frac{(2k+1)\pi y}{2d} - B_k \cos\frac{(2k+1)\pi y}{2d}\right)\right\|^2_{L^2(0,d)} \\
&\quad \leqslant \left(\|\Phi_- - \Phi_+\|_{L^2(0,d)} + \sqrt{\sum_{k=1}^{\infty}|A_k|^2} + \sqrt{\sum_{k=1}^{\infty}|B_k|^2}\right)^2 \\
&\quad \leqslant \left(\frac{\kappa}{2(1-\kappa)}(\|\Phi_-\|_{L^2(0,d)} + \|\Phi_+\|_{L^2(0,d)}) + \sqrt{\sum_{k=1}^{\infty}|A_k|^2} + \sqrt{\sum_{k=1}^{\infty}|B_k|^2}\right)^2 \\
&\quad < 3\left(\frac{\kappa^2}{2(1-\kappa)^2}\sum_{k=0}^{\infty}(|A_k|^2 + |B_k|^2) + \sum_{k=1}^{\infty}(|A_k|^2 + |B_k|^2)\right) \\
&\quad < 3\,\frac{2\sqrt{2}(1+\kappa)\kappa^2 + \kappa(1-\kappa)}{(1-\kappa)(4\sqrt{2}(1-\kappa^2) - \kappa)}(|A_0|^2 + |B_0|^2).
\end{aligned}$$

We compare this inequality with (3.24) and we have

$$1 - \frac{2}{\pi} < 3\kappa\,\frac{2\sqrt{2}(1+\kappa)\kappa + 1 - \kappa}{(1-\kappa)(4\sqrt{2}(1-\kappa^2) - \kappa)}. \tag{3.25}$$

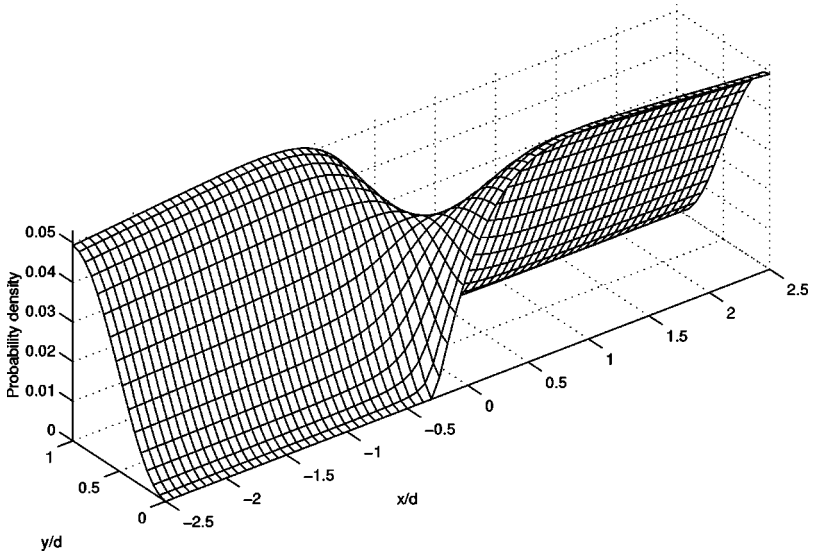

FIG. 3. The same as in Fig. 2 but $\lambda = 0.27$. It is close to the threshold for bound state appearance.

We recall that we investigate this inequality for $0 < \kappa < (\sqrt{129} - 1)/8\sqrt{2}$. The right-hand side of (3.25) is a positive, continuous function of κ on this interval and it goes to zero as κ does. Hence there must exist a number κ_0 (and so Λ_1), such that this inequality does not hold for $\kappa \in (0, \kappa_0)$, i.e., for $\lambda \in (0, \Lambda_1)$. Thus $q[\Phi] \geqslant 0$ for all $\Phi \in \mathcal{Q}(\Omega)$ for these values of the parameter λ, which has been to prove. ■

Remark 2: We also know that the discrete eigenvalues emerge at the essential spectrum threshold and they are continuous functions of λ *in both our specific cases. The rigorous formulation and the proof of this statement are given in Appendix A.*

IV. NUMERICAL RESULTS

We have solved the Schrödinger equation corresponding to our systems numerically. Since Ω consists of three rectangular regions, the easiest way to do that is the mode-matching method (see, e.g., Ref. 4). The results are shown in Figs. 2–5. In Figs. 4 and 5 we can notice that the first eigenvalue in model A appears for $\Lambda_0 > 0$. Our numerical results indicate that $\Lambda_0 \doteq 0.26$ in agreement with our analytical proofs. Solving numerically the equation $q_{\mathrm{II}}[\Phi_\sigma] = 0$ with the right-hand side given by (3.9) we get the result $\Lambda_2 \doteq 0.34$. In the same way from (3.25) we get after numerical computation $\Lambda_1 \doteq 0.08$. Hence $\Lambda_1 < \Lambda_0 < \Lambda_2$, which we have expected.

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APPENDIX A: THE CONTINUITY OF THE EIGENVALUES

First we define some notations for purposes of this appendix. Let $\lambda > 0$ then

$$Q(\lambda) = \{f \in H^1(\Omega) \mid f \restriction \mathcal{D}(\lambda) = 0\},$$

where

$$\mathcal{D}(\lambda) = \{\langle x, 0\rangle \mid x < -\lambda d\} \cup \{\langle x, d\rangle \mid x > \lambda d\}$$

or

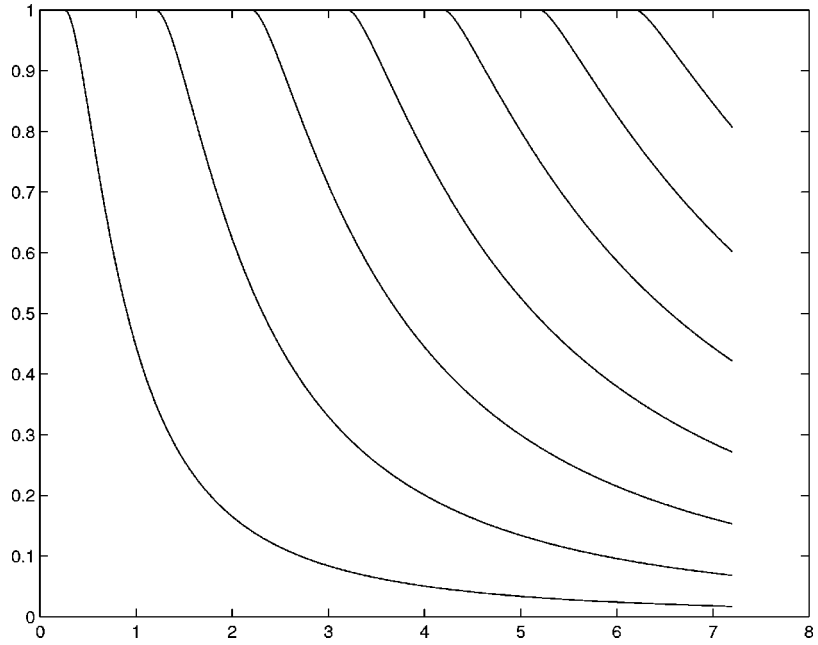

FIG. 4. Eigenvalues (in the units of $\mu = \pi^2/4d^2$) for model A in dependence on λ.

$$\mathcal{D}(\lambda) = \{\langle x,d\rangle \mid (x < -\lambda d) \vee (x > \lambda d)\}.$$

So we have stressed only the dependence of the form domain on the parameter λ. We define

$$U(\varphi_1,\ldots,\varphi_m;\lambda) = \inf_{\substack{\psi\in Q(\lambda),\psi\neq 0\\ \psi\perp\varphi_1,\ldots,\varphi_m}} \frac{\|\nabla\psi\|^2_{L^2(\Omega)}}{\|\psi\|^2_{L^2(\Omega)}},$$

$$\mu_n(\lambda) = \sup_{\varphi_1,\ldots,\varphi_{n-1}\in L^2(\Omega)} U(\varphi_1,\ldots,\varphi_{n-1};\lambda).$$

From the minimax principle,[14] we know that for every $n=1,2,\ldots$, $\mu_n(\lambda)$ is either the nth eigenvalue of the operator (counting multiplicity) or the bottom of its essential spectrum. The aim of this appendix is to show that $\mu_n(\lambda)$ are continuous functions in $(0,\infty)$.

Lemma 1: Functions $\mu_n : \lambda \mapsto \mu_n(\lambda)$ *are nonincreasing, finite, and continuous in* $(0,\infty)$ *for every* $n=1,2,\ldots$.

Proof: We know from the minimax principle and the Dirichlet–Neumann bracketing[14] that $0 \leq \mu_n(\lambda) \leq \pi^2/4d^2$ for all $\lambda > 0$ and $n=1,2,\ldots$. Let $\lambda_1 > \lambda_2$. Then $Q(\lambda_2) \subset Q(\lambda_1)$ and so for any $m=0,1,\ldots$ and any m-tuple $\varphi_1,\ldots,\varphi_m$,

$$U(\varphi_1,\ldots,\varphi_m;\lambda_1) \leq U(\varphi_1,\ldots,\varphi_m;\lambda_2) \leq \mu_{m+1}(\lambda_2).$$

Because these inequalities hold for every m-tuple $\varphi_1,\ldots,\varphi_m$ from our Hilbert space they must be fulfilled even for supremum over these m-tuples. Hence

$$\mu_{m+1}(\lambda_1) \leq \mu_{m+1}(\lambda_2) \tag{A1}$$

for every $m=0,1,\ldots$ and μ_{m+1} are thus nonincreasing.

For any $\varrho > 1$ we define $\varphi^{(\varrho)}(x,y) = \varphi(\varrho x, y)$. The equivalences $\varphi \in Q(\lambda) \Leftrightarrow \varphi^{(\varrho)} \in Q(\lambda/\varrho)$ and $\varphi \perp \psi \Leftrightarrow \varphi^{(\varrho)} \perp \psi^{(\varrho)}$ are obvious. Moreover

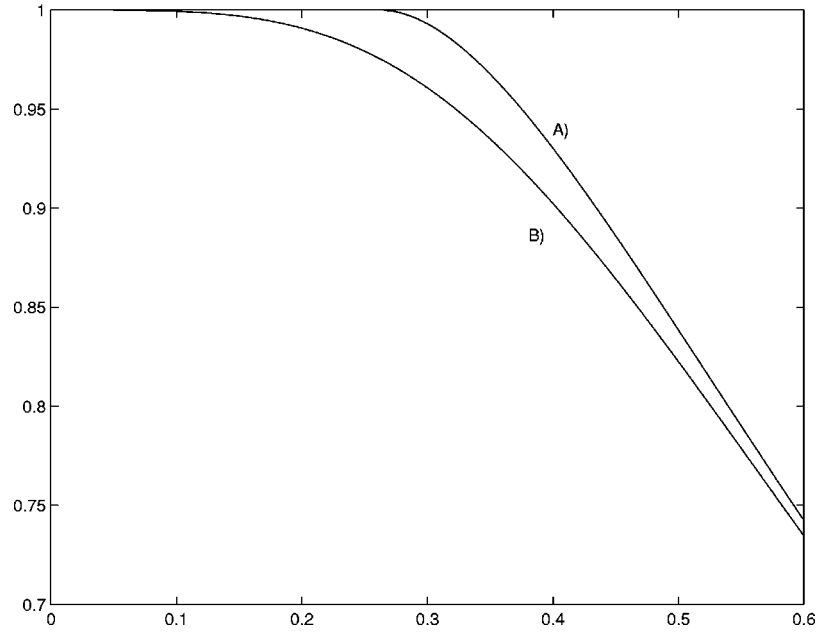

FIG. 5. First eigenvalues for models A and B in dependence of λ. While in model B the eigenvalue exists for any $\lambda>0$ in model A appears at $\Lambda>\Lambda_0$ (numerical calculations indicate $\Lambda_0\doteq 0.26$).

$$\frac{\|\nabla\varphi^{(\varrho)}\|^2_{L^2(\Omega)}}{\|\varphi^{(\varrho)}\|^2_{L^2(\Omega)}}=\frac{\varrho^2\|\dfrac{\partial\varphi}{\partial x}\|^2_{L^2(\Omega)}+\|\dfrac{\partial\varphi}{\partial y}\|^2_{L^2(\Omega)}}{\|\varphi\|^2_{L^2(\Omega)}}\leqslant\varrho^2\frac{\|\nabla\varphi\|^2_{L^2(\Omega)}}{\|\varphi\|^2_{L^2(\Omega)}}. \tag{A2}$$

Let integer $m\geqslant 0$, $\lambda>0$ and $\varphi_1,\ldots,\varphi_m\in L^2(\Omega)$ are chosen arbitrarily. Then for any $\varphi\in Q(\lambda)$ such that $\varphi\perp\varphi_1,\ldots,\varphi_m$ we know $\varphi_1^{(\varrho)},\ldots,\varphi_m^{(\varrho)}\in L^2(\Omega)$, $\varphi^{(\varrho)}\in Q(\lambda/\varrho)$, and $\varphi^{(\varrho)}\perp\varphi_1^{(\varrho)},\ldots,\varphi_m^{(\varrho)}$. Then using (A2) we get

$$U\left(\varphi_1^{(\varrho)},\ldots,\varphi_m^{(\varrho)};\frac{\lambda}{\varrho}\right)\leqslant\frac{\|\nabla\varphi^{(\varrho)}\|^2_{L^2(\Omega)}}{\|\varphi^{(\varrho)}\|^2_{L^2(\Omega)}}\leqslant\varrho^2\frac{\|\nabla\varphi\|^2_{L^2(\Omega)}}{\|\varphi\|^2_{L^2(\Omega)}}.$$

Because these inequalities hold for arbitrary m-tuple $\varphi_1,\ldots,\varphi_m$ it must hold even for the infimum of

$$\frac{\|\nabla\varphi\|^2_{L^2(\Omega)}}{\|\varphi\|^2_{L^2(\Omega)}}$$

and hence

$$U\left(\varphi_1^{(\varrho)},\ldots,\varphi_m^{(\varrho)};\frac{\lambda}{\varrho}\right)\leqslant\varrho^2U(\varphi_1,\ldots,\varphi_m;\lambda)\leqslant\varrho^2\mu_{m+1}(\lambda).$$

Passing again to the supremum over all m-tuples $\varphi_1^{(\varrho)},\ldots,\varphi_m^{(\varrho)}$ and taking into account (A1) we obtain

$$\mu_{m+1}(\lambda)\leqslant\mu_{m+1}\left(\frac{\lambda}{\varrho}\right)\leqslant\varrho^2\mu_{m+1}(\lambda), \tag{A3}$$

because $\lambda>\lambda/\varrho$. From the second inequality of (A3) and from (A1) we get

$$\frac{1}{\varrho^2}\mu_{m+1}(\lambda)\leqslant\mu_{m+1}(\lambda\varrho)\leqslant\mu_{m+1}(\lambda) \tag{A4}$$

using $\lambda\varrho>\lambda$. We recall that these inequalities hold for any $m\in\{0,1,\ldots\}$.

For any $0<\lambda'<\lambda$ we set $\varrho=\lambda/\lambda'$ and we put it to (A3)

$$\mu_{m+1}(\lambda)\leqslant\mu_{m+1}(\lambda')\leqslant\left(\frac{\lambda}{\lambda'}\right)^2\mu_{m+1}(\lambda).$$

We see that $\lim_{\lambda'\to\lambda^-}\mu_{m+1}(\lambda')=\mu_{m+1}(\lambda)$. We repeat the same procedure for $0<\lambda<\lambda'$ using the inequalities (A4) instead of (A3) and we get $\lim_{\lambda'\to\lambda^+}\mu_{m+1}(\lambda')=\mu_{m+1}(\lambda)$, which finishes the proof. ■

APPENDIX B: THE DENSE SET IN $Q^A(q_0)$

The goal of the appendix is to prove the following lemma.

Lemma 2: The set $\widetilde{Q}(\Omega)=\{\psi\in C^\infty(\overline{\Omega})\mid\psi=\widetilde{\psi}\restriction\Omega,\widetilde{\psi}\in C_0^\infty(\mathbb{R}^2),\psi\restriction\mathcal{D}=0\}$ *is dense in the set* $Q^A(q_0)$ *with respect to the* $H^1(\Omega)$ *norm.*

Proof: Let $\varphi\in Q^A(q_0)$. Then for every $\varepsilon>0$ we can find the function $\varphi_1^{(\varepsilon)}$ from the set $\{\psi\in C^\infty(\overline{\Omega})\mid\psi=\widetilde{\psi}\restriction\Omega,\widetilde{\psi}\in C_0^\infty(\mathbb{R}^2)\}$ such that $\|\varphi-\varphi_1^{(\varepsilon)}\|_{H^1(\Omega)}<\varepsilon$ (see, e.g., Ref. 12, Theorem 3.18). Due to Theorem 5.22 in Ref. 12 we can also write $\|(\varphi-\varphi_1^{(\varepsilon)})\restriction\mathcal{D}\|_{L^2(\mathcal{D})}<\sqrt{C}\varepsilon$, where C is a constant. Let γ be the function from the class $C^\infty(\mathbb{R})$ with the following properties: $0\leqslant\gamma(t)\leqslant1$ for $t\in\mathbb{R}$, $\gamma(t)=0$ for $t\leqslant1/2$, $\gamma(t)=1$ for $t\geqslant1$ and $|d\gamma(t)/dt|\leqslant\Gamma/5$ for some constant Γ and every $t\in\mathbb{R}$. For $\langle x,y\rangle\in\Omega$ and $\varepsilon<d/2$ we define

$$\omega_\varepsilon^{(1)}(x,y)=\begin{cases}\gamma\left(\dfrac{4(d-y)}{\varepsilon}\right)\gamma\left(\dfrac{\sqrt{(x-\delta)^2+(y-d)^2}}{\varepsilon}\right) & \text{for } x\geqslant\delta\\ \gamma\left(\dfrac{\sqrt{(x-\delta)^2+(y-d)^2}}{\varepsilon}\right) & \text{for } x\leqslant\delta,\end{cases}$$

$$\omega_\varepsilon^{(2)}(x,y)=\begin{cases}\gamma\left(\dfrac{4y}{\varepsilon}\right)\gamma\left(\dfrac{\sqrt{(x+\delta)^2+y^2}}{\varepsilon}\right) & \text{for } x\leqslant-\delta\\ \gamma\left(\dfrac{\sqrt{(x+\delta)^2+y^2}}{\varepsilon}\right) & \text{for } x\geqslant-\delta\end{cases}$$

and $\omega_\varepsilon=\omega_\varepsilon^{(1)}\omega_\varepsilon^{(2)}$. Obviously $\varphi_2^{(\varepsilon)}=\varphi_1^{(\varepsilon)}\omega_\varepsilon\in\widetilde{Q}(\Omega)$. Let us denote

$$\Omega_\varepsilon=\{\langle x,y\rangle\in\Omega\mid\operatorname{dist}(\langle x,y\rangle,\mathcal{D})<\varepsilon\},$$

$$\Omega_\varepsilon^1=((\delta,\infty)\times(d-\varepsilon,d))\cup((-\infty,-\delta)\times(0,\varepsilon)),$$

$$\Omega_\varepsilon^2=((\delta-\varepsilon,\delta)\times(d-\varepsilon,d))\cup((-\delta,-\delta+\varepsilon)\times(0,\varepsilon)),$$

$$\Omega_\varepsilon^3=((\delta-\varepsilon,\delta+\varepsilon)\times(d-\varepsilon,d))\cup((-\delta-\varepsilon,-\delta+\varepsilon)\times(0,\varepsilon)).$$

Now we are going to estimate $\|\varphi_2^{(\varepsilon)}-\varphi\|_{H^1(\Omega)}^2$,

$$\|\varphi_2^{(\varepsilon)}-\varphi\|_{H^1(\Omega)}^2=\|(\varphi_1^{(\varepsilon)}-\varphi)\omega_\varepsilon+\varphi(\omega_\varepsilon-1)\|_{L^2(\Omega)}^2+\|\nabla(\varphi_1^{(\varepsilon)}-\varphi)\omega_\varepsilon+\nabla\varphi(\omega_\varepsilon-1)+\varphi_1^{(\varepsilon)}\nabla\omega_\varepsilon\|_{L^2(\Omega)}^2\leqslant3\left(\|\varphi_1^{(\varepsilon)}-\varphi\|_{H^1(\Omega)}^2+\|\varphi\|_{H^1(\Omega_\varepsilon)}^2+\frac{\Gamma^2}{\varepsilon^2}\|\varphi_1^{(\varepsilon)}\|_{L^2(\Omega_\varepsilon)}^2\right).$$

Now we continue by estimating of $\|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon)}$,

$$\|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon)} \leqslant \|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon^1)} + \|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon^2)},$$

$$\|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon^1)} = \int_\delta^\infty \int_{d-\varepsilon}^d |\varphi_1^{(\varepsilon)}(x,y)|^2 \mathrm{d}y\, \mathrm{d}x + \int_{-\infty}^{-\delta} \int_0^\varepsilon |\varphi_1^{(\varepsilon)}(x,y)|^2 \mathrm{d}y\, \mathrm{d}x.$$

Because the estimates of the second term in the previous expression will be analogous to ones of the first term we will not write the second integral, but only ''second term'' instead of it,

$$\begin{aligned}
\|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon^1)} &= \int_\delta^\infty \int_{d-\varepsilon}^d \left| \varphi_1^{(\varepsilon)}(x,d) - \int_y^d \frac{\partial \varphi_1^{(\varepsilon)}}{\partial t}(x,t)\mathrm{d}t \right|^2 \mathrm{d}y\, \mathrm{d}x + \text{second term} \\
&\leqslant 2 \int_\delta^\infty \int_{d-\varepsilon}^d \left(|\varphi_1^{(\varepsilon)}(x,d)|^2 + \varepsilon \int_{d-\varepsilon}^d \left| \frac{\partial \varphi_1^{(\varepsilon)}}{\partial t}(x,t) \right|^2 \mathrm{d}t \right) \mathrm{d}y\, \mathrm{d}x + \text{second term} \\
&= 2 \left(\varepsilon \|\varphi_1^{(\varepsilon)} \restriction \mathcal{D}\|^2_{L^2(\mathcal{D})} + \varepsilon^2 \left\| \frac{\partial \varphi_1^{(\varepsilon)}}{\partial y} \right\|^2_{L^2(\Omega_\varepsilon^1)} \right) \\
&\leqslant 2\varepsilon^2 (C\varepsilon + \|\varphi_1^{(\varepsilon)}\|^2_{H^1(\Omega_\varepsilon^1)}) \leqslant 2\varepsilon^2 (C\varepsilon + 2(\|\varphi_1^{(\varepsilon)} - \varphi\|^2_{H^1(\Omega)} + \|\varphi\|^2_{H^1(\Omega_\varepsilon^1)})) \\
&\leqslant 2\varepsilon^2 (C\varepsilon + 2\varepsilon^2 + 2\|\varphi\|^2_{H^1(\Omega_\varepsilon^1)}).
\end{aligned}$$

For any $z \in (\delta, \delta+\varepsilon)$ we calculate

$$\begin{aligned}
\|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon^2)} &= \int_{\delta-\varepsilon}^\delta \int_{d-\varepsilon}^d \left| \int_x^z \frac{\partial \varphi_1^{(\varepsilon)}}{\partial t}(t,y)\mathrm{d}t + \int_y^d \frac{\partial \varphi_1^{(\varepsilon)}}{\partial s}(z,s)\mathrm{d}s - \varphi_1^{(\varepsilon)}(z,d) \right|^2 \mathrm{d}y\, \mathrm{d}x + \text{s.t.} \\
&\leqslant 3 \int_{\delta-\varepsilon}^\delta \int_{d-\varepsilon}^d \left(2\varepsilon \int_{\delta-\varepsilon}^{\delta+\varepsilon} \left| \frac{\partial \varphi_1^{(\varepsilon)}}{\partial t}(t,y) \right|^2 \mathrm{d}t + \varepsilon \int_{d-\varepsilon}^d \left| \frac{\partial \varphi_1^{(\varepsilon)}}{\partial s}(z,s) \right|^2 \mathrm{d}s \right. \\
&\quad \left. + |\varphi_1^{(\varepsilon)}(z,d)|^2 \right) \mathrm{d}y\, \mathrm{d}x + \text{second term}.
\end{aligned}$$

When we integrate the last inequality over z from δ to $\delta+\varepsilon$ we obtain

$$\varepsilon \|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon^2)} \leqslant 3 \left(2\varepsilon^3 \left\| \frac{\partial \varphi_1^{(\varepsilon)}}{\partial x} \right\|^2_{L^2(\Omega_\varepsilon^3)} + \varepsilon^3 \left\| \frac{\partial \varphi_1^{(\varepsilon)}}{\partial y} \right\|^2_{L^2(\Omega_\varepsilon^3)} + \varepsilon^2 \|\varphi_1^{(\varepsilon)} \restriction \mathcal{D}\|^2_{L^2(\mathcal{D})} \right)$$

and so

$$\|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon^2)} \leqslant 6\varepsilon^2 \|\varphi_1^{(\varepsilon)}\|^2_{H^1(\Omega_\varepsilon^3)} + 3C\varepsilon^3 \leqslant 12\varepsilon^2 (\varepsilon^2 + \|\varphi\|^2_{H^1(\Omega_\varepsilon^3)}) + 3C\varepsilon^3.$$

We give both these estimates together and we get

$$\|\varphi_1^{(\varepsilon)}\|^2_{L^2(\Omega_\varepsilon)} \leqslant 5C\varepsilon^3 + 16\varepsilon^4 + 16\varepsilon^2 \|\varphi\|^2_{H^1(\Omega_\varepsilon^1 \cup \Omega_\varepsilon^2)}.$$

Hence

$$\|\varphi_2^{(\varepsilon)} - \varphi\|^2_{H^1(\Omega)} \leqslant 3((1+16\Gamma^2)(\varepsilon^2 + \|\varphi\|^2_{H^1(\Omega_\varepsilon^1 \cup \Omega_\varepsilon^2)}) + 5C\Gamma^2\varepsilon).$$

Here $\lim_{\varepsilon\to 0^+}\|\varphi\|^2_{H^1(\Omega^1_\varepsilon\cup\Omega^2_\varepsilon)}=0$, e.g., by the dominated convergence. So $\|\varphi_2^{(\varepsilon)}-\varphi\|^2_{H^1(\Omega)}$ goes to zero as ε does which has been to show. ■

Remark 3: Our set $\tilde{Q}$ is obviously a subset of the set $\mathcal{Q}$ defined in the proof of the Theorem 3. Hence $\mathcal{Q}$ is a dense set in $Q^A(q_0)$ as well.

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Bogoliubov transformations and exact isolated solutions for simple nonadiabatic Hamiltonians

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We present a new method for finding isolated exact solutions of a class of nonadiabatic Hamiltonians of relevance to quantum optics and allied areas. Central to our approach is the use of Bogoliubov transformations of the bosonic fields in the models. We demonstrate the simplicity and efficiency of this method by applying it to the Rabi Hamiltonian. © *2002 American Institute of Physics.*
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I. INTRODUCTION

There exists a class of simple, nonintegrable, nonadiabatic Hamiltonians of the type that find application as models of light–matter interactions, for which it is possible to find exact isolated solutions. Generally these models involve some atomic system, typically characterized by a simple two-level (or multilevel) system, interacting with a number of bosonic fields. Making the familiar rotating-wave approximation usually renders these models completely soluble, but avoiding this approximation maintains the nonintegrability of the models, and gives rise to the possibility of isolated exact solutions. This was first demonstrated for the Jahn–Teller model by Judd,[1] and these solutions are often referred to as Juddian solutions. Probably the simplest model for which these solutions have been found is the Rabi Hamiltonian (RH), which describes a two-level atom interacting with a single-mode bosonic field via a dipole interaction.[2] The Juddian solutions of the RH were first discovered by Reik and co-workers,[3] where they were seen to occur at the level crossings in the energy schema of the system. This turns out to be a general and important feature of these solutions.

Apart from being of interest for what they tell us about the structure and symmetries of these models, the Juddian solutions are of considerable further value. Simple quantum optics and related models, such as the RH, have long been utilized as test cases for various calculational techniques,[4–6] and the possession of exact solutions facilitates their accurate assessment. Furthermore, the existence of isolated exact solutions in nonintegrable quantum models is also of interest from the perspective of studying possible quantum chaos in such systems.[7,8] In addition, it is hoped that these exact solutions may serve as useful starting points for perturbative treatments of the entire spectra of these models.

In this paper we present a new and more general method for finding these isolated exact solutions, which we believe to have several advantages over the methods hitherto employed. Judd and Reik, working in the Bargmann representation, have used power series and Neumann series ansätze for the field mode. Neither of these approaches is particularly intuitive and the resulting algebra can become complicated. Kuś and Lewenstein[9] have given a more concise approach which, as we describe later, is clearly related to the method that we describe here. For models such as the RH they used Bargmann representation ansätze for the field consisting of a finite number of bosonic excitations on top of a coherent state. They have also extended their method to some further systems, such as a three-level system and an auto-ionizing ion.

We believe that the method we outline in this paper is both more intuitive and more efficient

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than those discussed previously, and that it reflects the essential physics of the systems to a greater degree. At the heart of the method is a simple canonical transformation of the bosonic field operators of the models. This transformation suggests the existence of exact solutions in a most direct manner. Our method also has the advantage that it is easy to generalize, and is readily able to be extended to ''two-photon'' type interactions, in which two photons are required to induce an atomic transition.[10]

The remainder of this paper is organized as follows. In Sec. II we outline our method for finding the Juddian solutions. We describe in some detail the theory of Bogoliubov transformations of a boson mode and pay particular attention to their relation to the coherent and squeezed states. We then use these transformations to investigate the displaced and squeezed harmonic oscillators, to develop insight into the reasoning behind this approach. In Sec. III we apply this method to the Rabi Hamiltonian, as an example of the use of this method. We then finish with some conclusions and indications of further work.

II. METHODOLOGY

The models that we consider here consist of an atomic system interacting with one or more bosonic modes. Each of these modes is described by annihilation and creation operators, b and $b^\dagger$, respectively, which obey the usual commutation relation,

$$[b,b^\dagger]=1. \tag{1}$$

In general the atomic system will be described in terms of a set of matrices. For example, the two-level system in the RH is described by the SU(2) Pauli matrices.

Our method for finding exact isolated solutions for such systems involves two components. First, one must choose an appropriate representation for the atomic matrices and then, crucially, one performs a Bogoliubov transformation of the operators of the field mode. The nature of this transformation depends upon the type of interaction being considered and, with the correct choice of parameters, it leaves the Schrödinger equation in a form that admits exact solutions with very simple ansätze.

A. Bogoliubov transformations

A Bogoliubov transformation is a transformation from one description of a field mode in terms of the bosonic operators, b and $b^\dagger$, to a description in terms of new bosonic operators, $\tilde{b}$ and $\tilde{b}^\dagger$, say. This transformation is canonical so that the new operators obey the same commutation relation as the old ones, namely

$$[\tilde{b},\tilde{b}^\dagger]=1. \tag{2}$$

The most general linear Bogoliubov transformation may be viewed as a rotation plus translation of the original oscillator Hilbert space to the new oscillator space,

$$\begin{aligned}\tilde{b}&=e^{-i\beta}(1-|\sigma|^2)^{-1/2}(b-\sigma b^\dagger-z),\\ \tilde{b}^\dagger&=e^{i\beta}(1-|\sigma|^2)^{-1/2}(b^\dagger-\sigma^* b-z^*),\end{aligned} \tag{3}$$

where σ and z are complex numbers describing the amplitudes of the rotation and translation, respectively. β is a simple, and usually rather unimportant, phase factor. From the outset it is important to note the restriction $|\sigma|<1$ in order to preserve the unitarity of the transformation. In the following we consider two specializations of this transformation, namely a pure translation and a pure rotation. These transformations may be very simply related to the familiar coherent and squeezed states of quantum optics and it is from this standpoint that we introduce the transformations.

B. Coherent bosons

The usual Glauber coherent states, $|z\rangle$, may be defined as eigenkets of the single-mode bosonic annihilation operator,[11]

$$b|z\rangle = z|z\rangle, \tag{4}$$

where z is a complex number. Such states are readily constructed as the following equivalent forms:

$$|z\rangle = e^{-1/2|z|^2} e^{zb^\dagger}|0\rangle \tag{5}$$

$$= e^{(zb^\dagger - z^* b)}|0\rangle, \tag{6}$$

where we have normalized the coherent state such that $\langle z|z\rangle = 1$. The exponential operator in Eq. (6) is denoted as follows:

$$D(z) \equiv e^{(zb^\dagger - z^* b)}, \tag{7}$$

and is called the displacement operator. It is a unitary operator and we may readily use it to perform a unitary transformation of the field operators,

$$\begin{aligned} D(z) b D^\dagger(z) &= b - z \equiv a, \\ D(z) b^\dagger D^\dagger(z) &= b^\dagger - z^* \equiv a^\dagger. \end{aligned} \tag{8}$$

The operators $D(z)$ form a representation of the Weyl (or Heisenberg–Weyl) group when multiplied by a trivial phase factor $\exp(i\phi)$, with ϕ real. The operators a and $a^\dagger$ obey the same commutator relation as the original operators, and thus we see this transformation to be a Bogoliubov transformation of the type described earlier as a pure translation. Equations (4) and (8) clearly imply

$$a|z\rangle = 0, \tag{9}$$

from which we see that the operator a annihilates the coherent state $|z\rangle$. Thus $|z\rangle$ may be considered as the vacuum state of the a-type bosons, and we rewrite it accordingly as $|0;z\rangle \equiv |z\rangle$,

$$a|0;z\rangle = 0. \tag{10}$$

We shall call these a-type bosons ''coherent bosons'' and write their number states as $|n;z\rangle$, such that $a^\dagger a|n;z\rangle = n|n;z\rangle$.

C. Displaced harmonic oscillator

The simplest application of the coherent bosons is to the displaced harmonic oscillator,

$$H_D = \tfrac{1}{2}(x + \sqrt{2}\lambda)^2 + \tfrac{1}{2}p^2, \tag{11}$$

in which the center of the oscillator is shifted by an amount $-\sqrt{2}\lambda$. Introducing the harmonic oscillator operators via

$$\begin{aligned} x &\equiv \frac{1}{\sqrt{2}}(b^\dagger + b), \\ p &\equiv \frac{i}{\sqrt{2}}(b^\dagger - b), \end{aligned} \tag{12}$$

the Hamiltonian reads

$$H_D = b^\dagger b + \lambda(b^\dagger + b) + \tfrac{1}{2} + \lambda^2. \tag{13}$$

By performing a Bogoliubov transformation of the original bosonic operators to a new set of coherent bosons, $a^\dagger$ and a, such that

$$a \equiv b + \lambda, \quad a \equiv b^\dagger + \lambda, \tag{14}$$

we may rewrite the Hamiltonian of Eq. (13) in the form

$$H_D = a^\dagger a + \tfrac{1}{2}. \tag{15}$$

The eigenstates of this Hamiltonian are thus clearly seen to be the number states of the a-type bosons, with corresponding eigenenergies $E_n = n + \frac{1}{2}$.

D. Squeezed bosons

Following Bishop and Vourdas[12] we construct the most general squeezed state, $|z;\rho,\theta,\beta\rangle$, by acting upon the bosonic vacuum $|0\rangle$ first with the displacement operator $D(z)$ of Eq. (7) and then with the pure squeezing operator $S(\rho,\theta,\beta)$,

$$|z;\rho,\theta,\beta\rangle = S(\rho,\theta,\beta)D(z)|0\rangle, \tag{16}$$

The squeezing operator is given by

$$S(\rho,\theta,\beta) \equiv \exp(-\tfrac{1}{4}\rho e^{-i\theta} b^{\dagger 2} + \tfrac{1}{4}\rho e^{i\theta} b^2)\exp(i\beta b^\dagger b), \tag{17}$$

where ρ,θ,β are real parameters. It is a unitary operator, $S^\dagger S = 1$, and provides a representation of the group SU(1,1). Using a relationship given by Perelomov,[13] we are able to write the squeezing operator in the equivalent form

$$S(\sigma,\beta) = \exp(\tfrac{1}{2}\sigma b^{\dagger 2})(1-|\sigma|^2)^{b^\dagger b/2 + 1/4}\exp(-\tfrac{1}{2}\sigma^* b^2)\exp(i\beta b^\dagger b), \tag{18}$$

where β is the same real parameter as above, and σ is a complex number with modulus $|\sigma| < 1$, given by $\sigma \equiv -e^{-i\theta}\tanh(\frac{1}{2}\rho)$. Using this expression, we can use the squeezing operator to make unitary transformations of the bosonic annihilation and creation operators,

$$\begin{aligned} S(\sigma,\beta) b S^\dagger(\sigma,\beta) &= e^{-i\beta}(1-|\sigma|^2)^{-1/2}(b - \sigma b^\dagger) \equiv c, \\ S(\sigma,\beta) b^\dagger S^\dagger(\sigma,\beta) &= e^{i\beta}(1-|\sigma|^2)^{-1/2}(b^\dagger - \sigma^* b) \equiv c^\dagger. \end{aligned} \tag{19}$$

The operators c and $c^\dagger$ satisfy the commutation relation $[c,c^\dagger] = 1$ and thus the transformation $b,b^\dagger \to c,c^\dagger$ is a Bogoliubov transformation of the rotation type. From Eq. (19), it follows that for any function $f(b,b^\dagger)$,

$$S f(b,b^\dagger) S^\dagger = f(c,c^\dagger) \leftrightarrow S f(b,b^\dagger) = f(c,c^\dagger) S. \tag{20}$$

Equation (20) implies that $Sb = cS$ and hence $|z;\sigma\beta\rangle \equiv |z;\rho\theta\beta\rangle$ are eigenstates of the annihilation operator c,

$$c|z;\sigma\beta\rangle = cS(\sigma,\beta)|z\rangle = S(\sigma,\beta)b|z\rangle = z|z;\sigma\beta\rangle. \tag{21}$$

If we consider the squeezed vacuum $S|0\rangle = |0;\sigma,\beta\rangle = |0;\sigma\rangle$, we see that it is independent of β and that

$$c|0;\sigma\rangle = 0. \tag{22}$$

The number states of the c-type bosons are denoted $|n;\sigma\beta\rangle$, such that $c^\dagger c|n;\sigma\beta\rangle = n|n;\sigma\beta\rangle$. We call the c-type bosons "squeezed" bosons.

E. Squeezed harmonic oscillator

In position representation the squeezed harmonic oscillator has the form

$$H_S = \tfrac{1}{2}(1+2\lambda)x^2 + \tfrac{1}{2}(1-2\lambda)p^2, \tag{23}$$

where the real parameter λ determines the degree of squeezing, with the restriction that $|\lambda| < \frac{1}{2}$. Translating this into the standard bosonic representation defined by Eq. (12) we have

$$H_S = b^\dagger b + \tfrac{1}{2} + \lambda(b^{\dagger 2} + b^2). \tag{24}$$

We introduce squeezed c-type bosons defined by

$$c^\dagger = \frac{b^\dagger + \sigma b}{\sqrt{1-\sigma^2}}, \qquad c = \frac{b + \sigma b^\dagger}{\sqrt{1-\sigma^2}}, \tag{25}$$

and leave σ real but undetermined for the moment. Making these substitutions into Eq. (24), we have

$$H_S = \frac{1}{(1-\sigma^2)}\left\{[-\sigma+\lambda+\lambda\sigma^2](c^2+c^{\dagger 2}) + (\sigma^2+1-4\lambda\sigma)\left(c^\dagger c + \frac{1}{2}\right)\right\}. \tag{26}$$

We eliminate the first term in this Hamiltonian by choosing

$$-\sigma+\lambda+\lambda\sigma^2 = 0, \tag{27}$$

giving, as one of the two solutions,

$$\sigma = \frac{(1-\Omega)}{2\lambda}, \qquad \Omega \equiv \sqrt{1-4\lambda^2}. \tag{28}$$

With this choice, the Hamiltonian becomes

$$H_S = \{c^\dagger c + \tfrac{1}{2}\}\Omega. \tag{29}$$

The eigenstates of this Hamiltonian are clearly the number states of the squeezed c-type bosons, with eigenenergies

$$E_n = \{n + \tfrac{1}{2}\}\Omega. \tag{30}$$

We note that the other solution of Eq. (27) with $\sigma = (1+\Omega)/2\lambda$ leads to the unphysical oscillator with $H_S = -(c^\dagger c + \frac{1}{2})\Omega$, and since this Hamiltonian does not have square-integrable solutions, we discard it.

III. APPLICATION TO THE RABI HAMILTONIAN

The Rabi Hamiltonian (RH) describes a two-level atom interacting with a single mode of quantized electromagnetic radiation via a dipole interaction.[2] It is usually written in the form

$$H_{\text{Rabi}} = \tfrac{1}{2}\omega_0\sigma_z + \omega b^\dagger b + g(b^\dagger + b)(\sigma_+ + \sigma_-), \tag{31}$$

where ω_0 is the atomic level splitting, ω is the frequency of the boson mode, and g is the coupling strength of the atom to the field. The two-level atom is described by the Pauli pseudo-spin operators, which satisfy the SU(2) commutation relations

$$[\sigma_k,\sigma_l]=2i\varepsilon_{klm}\sigma_m, \tag{32}$$

where $k,l,m\in\{x,y,z\}$ with $k\neq l$ and ε_{klm} is the antisymmetric Levi-Civita symbol. We have defined the raising and lowering operators as

$$\sigma_+\equiv\sigma_x+i\sigma_y, \quad \sigma_-\equiv\sigma_x-i\sigma_y. \tag{33}$$

It is convenient to rescale the Hamiltonian as $H_{\mathrm{Rabi}}=\omega\tilde{H}_{\mathrm{Rabi}}$, where

$$\tilde{H}_{\mathrm{Rabi}}=\tilde{\omega}\sigma_z+b^\dagger b+\lambda(b^\dagger+b)\sigma_x, \tag{34}$$

and $\tilde{\omega}\equiv\omega_0/(2\omega)$ and $\lambda\equiv 2g/\omega$. There is a conserved parity Π associated with the Hamiltonian,

$$\Pi\equiv\exp[i\pi(b^\dagger b+\tfrac{1}{2}(\sigma_z+1))]=-\sigma_z\cos(\pi b^\dagger b), \tag{35}$$

such that $[H_{\mathrm{Rabi}},\Pi]=0$. The parity operator Π has two eigenvalues, $\pi=\pm 1$. The RH is not known to be integrable, but isolated exact solutions do exist. Here we use the above-outlined technique to find these Juddian solutions.

In order to do this we first require an appropriate matrix representation for the Pauli matrices, which for this model is one in which σ_x is diagonal. We shall use

$$\sigma_x=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}, \quad \sigma_y=\begin{bmatrix}0 & i\\ -i & 0\end{bmatrix}, \quad \sigma_z=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}. \tag{36}$$

In terms of the two-component wave function, $|\Psi\rangle=\binom{|\Psi_1\rangle}{|\Psi_2\rangle}$, the time-independent Schrödinger equation for the system, $\tilde{H}_{\mathrm{Rabi}}|\Psi\rangle=E|\Psi\rangle$, then reads

$$\begin{aligned}\tilde{\omega}|\Psi_2\rangle+(b^\dagger b+\lambda(b^\dagger+b)-E)|\Psi_1\rangle=0,\\ \tilde{\omega}|\Psi_1\rangle+(b^\dagger b-\lambda(b^\dagger+b)-E)|\Psi_2\rangle=0.\end{aligned} \tag{37}$$

We now make the Bogoliubov transformation to the coherent bosons, $a^\dagger$ and a, specified by

$$a^\dagger=b^\dagger-\lambda, \quad a=b-\lambda. \tag{38}$$

The vacuum state of these bosons is the coherent state $|\lambda\rangle$. It should be noted that this choice of transformation may be intuited from considering the $\tilde{\omega}=0$ limit of the Hamiltonian, where the same transformation is used to solve the model exactly in this limit, which is essentially equivalent to the displaced oscillator considered earlier. With this transformation Eq. (37) becomes

$$\begin{aligned}\tilde{\omega}|\Psi_2\rangle+\{a^\dagger a+2\lambda(a^\dagger+a)+3\lambda^2-E\}|\Psi_1\rangle=0,\\ \tilde{\omega}|\Psi_1\rangle+\{a^\dagger a-\lambda^2-E\}|\Psi_2\rangle=0,\end{aligned} \tag{39}$$

where the kets $|\Psi_{1,2}\rangle$ are now in the transformed representation. For these kets we choose the ansatz

$$|\Psi_1\rangle=\sum_{n=0}^{N-1} p_n|n;\lambda\rangle=\sum_{n=0}^{N-1} p_n\frac{(a^\dagger)^n}{\sqrt{n!}}|0;\lambda\rangle=P_{N-1}(a^\dagger)|0;\lambda\rangle,$$
$$|\Psi_2\rangle=\sum_{n=0}^{N} q_n|n;\lambda\rangle=\sum_{n=0}^{N} q_n\frac{(a^\dagger)^n}{\sqrt{n!}}|0;\lambda\rangle=Q_N(a^\dagger)|0;\lambda\rangle, \tag{40}$$

where $|n;\lambda\rangle$ are number states of the coherent bosons, $a^\dagger a|n;\lambda\rangle=n|n;\lambda\rangle$, and we have introduced the polynomials P_{N-1} and Q_N of order $N-1$ and N, respectively. Making these substitutions we have

$$\begin{aligned}&\tilde{\omega}\sum_{n=0}^{N} q_n|n;\lambda\rangle+\sum_{n=0}^{N-1} p_n(n+3\lambda^2-E)|n;\lambda\rangle\\&\quad+2\lambda\sum_{n=0}^{N-1} p_n\sqrt{n+1}|n+1;\lambda\rangle+2\lambda\sum_{n=1}^{N-1} p_n\sqrt{n}|n-1;\lambda\rangle=0,\\&\tilde{\omega}\sum_{n=0}^{N-1} p_n|n;\lambda\rangle+\sum_{n=0}^{N} q_n(n-\lambda^2-E)|n;\lambda\rangle=0.\end{aligned} \tag{41}$$

Considering the highest number state, $|N;\lambda\rangle$, in the second of these equations, we see that for this equation to hold we require

$$(N-\lambda^2-E)q_N=0. \tag{42}$$

Since $q_N\neq 0$ by ansatz, we obtain a determination of the energy

$$E=N-\lambda^2. \tag{43}$$

This equation identifies the Juddian baseline energies, along which the Juddian solutions lie. Comparing the coefficients of the remaining number states gives us $2N+1$ linear equations for the $2N+1$ coefficients $(p_m, 0\leqslant m\leqslant N-1)$ and $(q_k, 0\leqslant k\leqslant N)$. To obtain nontrivial solutions, we clearly require the determinant of this equation set to be zero. This gives the compatibility condition, providing the locations of the Juddian points. The first two conditions ($N=1,2$) have the explicit forms

$$\tilde{\omega}^2+4\lambda^2=1, \qquad \text{for} \quad N=1, \tag{44}$$

$$\tilde{\omega}^4+(12\lambda^2-5)\tilde{\omega}^2+32\lambda^4-32\lambda^2+4=0, \qquad \text{for} \quad N=2, \tag{45}$$

as have been given by Kuś and Lewenstein.[9] Thus, for a given N, we have a polynomial of Nth order in λ^2 and $\tilde{\omega}^2$. Each of these has N roots for λ^2 in terms of $\tilde{\omega}^2$, which all turn out to be real, thus giving the location of N Juddian solutions. Before we look at these results, it is of interest to consider the other possible type of finite ansatz at the Juddian points. These are found by using the coherent bosons

$$a^\dagger=b^\dagger+\lambda, \quad a=b+\lambda, \tag{46}$$

and interchanging the roles of $|\Psi_1\rangle$ and $|\Psi_2\rangle$.

Results. By solving the complementary conditions we have calculated the first ten Juddian points for the resonant RH. These are displayed in Table I, listed to ten decimal places.

TABLE I. The couplings, energies, and N, of the first ten Juddian points of the resonant Rabi Hamiltonian ($\omega=\omega_0=1$).

g	E	N
0.216 506 351 0	0.812 500 000 0	1
0.166 164 073 2	1.889 558 003 1	2
0.446 040 357 8	1.204 191 996 9	2
0.140 088 959 0	2.921 500 334 3	3
0.366 471 488 7	2.462 794 592 0	3
0.616 382 915 3	1.480 288 407 1	3
0.123 422 939 9	3.939 067 116 1	4
0.319 907 578 1	3.590 636 565 8	4
0.524 339 512 0	2.900 272 304 5	4
0.758 249 241 5	1.700 232 351 1	4

The location of these Juddian points in the energy schema of the Hamiltonian is displayed in Fig. 1, where the schema was obtained by approximate numerical diagonalization via a standard configuration-interaction method, using a basis size of the lowest 101 harmonic oscillator states.[14] Also plotted are the Juddian baselines from Eq. (43).

From Fig. 1 we see that the Juddian points occur at the level crossings in this diagram. Thus we see that they occur when two solutions of different parity Π become degenerate in energy, and this degeneracy is the key to the existence of the Juddian solutions. The coherent-boson number states $|n;\lambda\rangle$ are not eigenstates of Π, and thus the ansätze (40) is not of definite parity. It is precisely because we can construct wave functions of mixed parity that allows us to find such simple ansatz at the Juddian points.

We are now able to make explicit the connection between this method and that used by Kuś and Lewenstein[9] in investigating the RH. They worked in the Bargmann representation,[15] in which the bosonic operators are represented by

$$b^\dagger \to z; \qquad b \to \frac{d}{dz} \tag{47}$$

and postulated the following forms for the two components of the wave function:

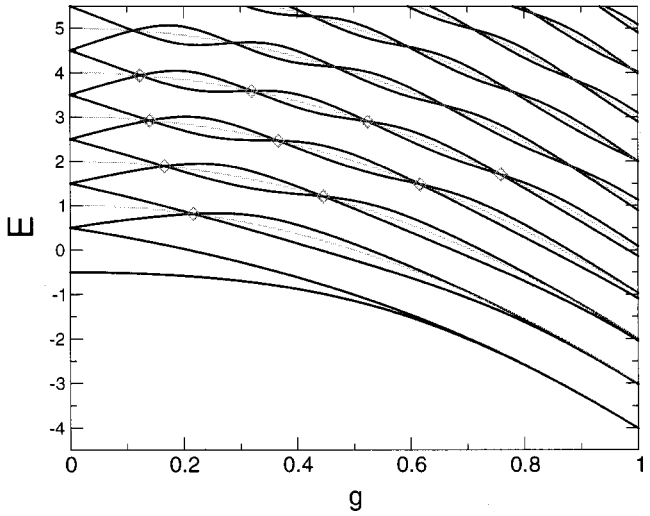

FIG. 1. The first ten Juddian points of the Rabi Hamiltonian (diamonds). Also plotted are the energy levels obtained by numerical diagonalization (dark lines), and the Juddian base lines (light lines). The Hamiltonian is resonant; $\omega=\omega_0=1$.

$$\Psi_1(z) = e^{-|z|^2/2}\langle z|\Psi_1\rangle = \tilde{P}_{N-1}(z)e^{\lambda z},$$
$$\Psi_2(z) = e^{-|z|^2/2}\langle z|\Psi_2\rangle = \tilde{Q}_N(z)e^{\lambda z}, \tag{48}$$

where $\tilde{P}_{N-1}(z)$ and $\tilde{Q}_N(z)$ are polynomials in z of order $N-1$ and N, respectively. Bearing in mind the form of the coherent state (6), these wave functions are simply seen to be of the form of polynomials in the bosonic creation operator, $b^\dagger$, acting upon a coherent state of amplitude λ. In our ansatz (40), we have the same coherent state but now being acted upon by polynomials in $a^\dagger = (b^\dagger - \lambda)$, which shares a closer connection to the coherent state than $b^\dagger$.

The polynomials of Kuś and Lewenstein are simply related to those of ansatz (40) by $\tilde{P}_N(z) = P_N(z-\lambda)$. In the present case where we have only used displacements of the boson mode, the difference between the two approaches is thus minimal. However, this is not the case when we require the use of squeezed bosons. Generally, an ansatz posited in the squeezed representation would contain polynomials of the form $P_N(c^\dagger)$, where $c^\dagger$ is the creation operator of the squeezed bosons. The analogous ansatz to Eq. (48) would still contain a polynomial in z, $\tilde{P}_N(z)$ say. If we assume the simplest type of squeezing and write $c^\dagger = (b^\dagger + \sigma b)/(\sqrt{1-\sigma^2})$ as in Eq. (25), then the Kuś and Lewenstein polynomial can be written

$$\tilde{P}_N(z) = P_N\left(\frac{z + \sigma\dfrac{d}{dz}}{\sqrt{1-\sigma^2}}\right), \tag{49}$$

which, crucially, contains both z and its derivative, and although formal relationships do exist between the polynomials of the two methods, these relationships are generally not trivial, especially if one considers the more general form of the Bogoliubov transformation. So the ansätze of the two methods are seen to be significantly different, and we conjecture that the one described here has several advantages which we shall discuss in the conclusion.

IV. CONCLUSIONS

We have presented a method for finding isolated exact solutions of a class of nonadiabatic models, of the type frequently used in quantum optics and related fields.

Compared with the original approaches of Judd and Reik, the above-mentioned method is more transparent and considerably simpler, advantages that it shares with the technique of Kuś and Lewenstein. However, we believe that the use of transformed bosons is more obviously physically meaningful than the use of wave functions in Bargmann space, especially given the connection of these bosons to the coherent and squeezed states, so important in quantum optics.

As an example of the use of this technique, we have applied it to the Rabi Hamiltonian and obtained in a simple fashion the known Juddian solutions of this model. In this example, we have used the coherent bosons to obtain Juddian solutions for a problem with an interaction of the type $\lambda(b^\dagger + b)\sigma_x$. It is hopefully now clear how one may apply this method to further problems containing the same type of interaction. We have not as yet mentioned the application of the squeezed bosons in performing this kind of calculation. This second type of Bogoliubov transformation is useful in finding Juddian solutions of models containing two-photon type interactions. An obvious example is the two-photon Rabi Hamiltonian,[16] which has the Hamiltonian

$$H = \tilde{\omega}\sigma_z + b^\dagger b + \lambda(b^{\dagger 2} + b^2)\sigma_x. \tag{50}$$

Using squeezed bosons we are able to obtain a set of Juddian solutions for this model and these results will be discussed in a future publication.

Due to the intuitive nature and simplicity of this technique it is easy to extend to other systems. For example, in view of their mode of construction we expect that our displaced and squeezed coherent states will be of particular use in any quantum field theory that has underlying

dynamical symmetry of the Weyl group or the SU(1,1) group, or to which the (inhomogeneous or homogeneous) Bogoliubov transformation may be profitably applied. The obvious group-theoretical foundations of the technique also point the way to other approximations, since, for example in the squeezed (two-photon) case, SU(1,1) is not the only relevant group. Thus, the three-dimensional Lorentz group SO(2,1), which is the group of rotations in three-dimensional Minkowski space with two space and one time dimensions, is locally isomorphic to SU(1,1). Similarly, both the groups $SL(2,\mathbb{R})$ of real second-order matrices with unit determinant and the symplectic group $Sp(2,\mathbb{R})$ are also locally isomorphic to SU(1,1).

One may also readily generalize the current approach for the two-level models involving linear or quadratic interactions with a single boson (or canonical quantum mode) to the corresponding case of linear or bilinear interactions involving several distinct bosons or modes. For the linear models involving only displacements this is essentially trivial. However, for models involving squeezing, in the case of n bosons or modes the various bilinear products of operators $b_i^\dagger b_j^\dagger$, $b_i b_j$ and $b_i^\dagger b_j$, $i,j=1,2,\ldots,n$ now form a realization of the higher symplectic algebra $Sp(2n,\mathbb{R})$. As before one can simply construct a unitary representation of this group by exponentiating the skew-adjoint operators in the algebra. For example, Bishop and Vourdas[17] have shown explicitly how to construct the most general two-mode squeezed states associated with a unitary representation of the group $Sp(4,\mathbb{R})$. Once again such states are the ordinary coherent states with respect to the new destruction operators c_1 and c_2, which are themselves general linear Bogoliubov transformations of the original destruction operators b_1, b_2 and their Hermitian-conjugate creation operators $b_1^\dagger$, $b_2^\dagger$. The $Sp(4,\mathbb{R})$ algebra has various subalgebras corresponding to different sorts of linear pairing terms. For example, whereas the single-mode paring operators $K_+^{(i)} \equiv \frac{1}{2}(b_i^\dagger)^2$; $K_-^{(i)} \equiv \frac{1}{2} b_i^2$; $K_0^{(i)} \equiv \frac{1}{2} b_i^\dagger b_i + \frac{1}{4}$ for $i=1,2$ correspond to the so-called $(\frac{1}{4}, \frac{3}{4})$ representations of SU(1,1), the mixed pairing operators $L_+ \equiv b_1^\dagger b_2^\dagger$; $L_- \equiv b_1 b_2$; $L_0 \equiv \frac{1}{2}(b_1^\dagger b_1 + b_2^\dagger b_2 + 1)$ correspond to the discrete-series representation of SU(1,1). By contrast, the mixed pairing operators $J_+ \equiv b_1^\dagger b_2$; $J_- \equiv b_1 b_2^\dagger$; $J_0 \equiv \frac{1}{2}(b_1^\dagger b_1 - b_2^\dagger b_2)$ correspond to the (Schwinger representation of) the angular momentum subalgebra SU(2). Bishop and Vourdas have shown in a separate publication[18] how squeezed (pair) coherent states can also be used in connection with a rather broad class of quantum Lagrangians which include the damped harmonic oscillator, and hence with problems involving ''quantum friction'' or fluctuation-dissipation phenomena in general. Within quantum optics for example, the quantum theory of lasers and photon detection provide obvious applications. Such problems can now also usefully be extended by our present treatment to the case of such damped systems coupled to two level atoms.

The possibility of using these solutions as the basis of a perturbative approach extends the method away from just the isolated exact points to the remainder of the spectrum of the system. The properties of such an approach are yet to be investigated. Finally we note that the extension to similar single-mode or multimode systems as considered earlier coupled to n-level atoms with $n \geqslant 2$ is also straightforward in principle.

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The Dirac operator in a fermion bag background in 1+1 dimensions and generalized supersymmetric quantum mechanics

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We show that the spectral theory of the Dirac operator $D=i\not{\partial}-\sigma(x)-i\pi(x)\gamma_5$, in a static background $(\sigma(x),\pi(x))$ in $1+1$ space–time dimensions, is underlined by a certain novel generalization of supersymmetric quantum mechanics, and we explore some of its mathematical and physical consequences. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1485114]

I. INTRODUCTION: BAGS AND RESOLVENTS

In this article we prove that the spectral theory of the Dirac operator $D=i\not{\partial}-\sigma(x)-i\pi(x)\gamma_5$ in a static scalar and pseudo-scalar background $(\sigma(x),\pi(x))$ in $1+1$ space–time dimensions is governed by a pair of isospectral Strum–Liouville operators. This observation is a generalization of the well known fact that the spectral theory of the simpler Dirac operator in a purely scalar background $i\not{\partial}-\sigma(x)$ is equivalent to one dimensional supersymmetric quantum mechanics. We then explore some of the physical and mathematical consequences of these two isospectral Sturm–Liouville operators.

The spectral theory of $i\not{\partial}-\sigma(x)-i\pi(x)\gamma_5$ is most relevant in the physics of fermion bags, which we outline briefly in the rest of this section.

A central concept in particle physics states that fundamental particles acquire their masses through interactions with vacuum condensates. Thus, a massive particle may carve out around itself a spherical region[1] or a shell[2] in which the condensate is suppressed, thus reducing the effective mass of the particle at the expense of volume and gradient energy associated with the condensate. This picture has interesting phenomenological consequences.[1,3]

This phenomenon may be studied nonperturbatively in model field theories in $1+1$ space–time dimensions such as the Gross–Neveu (GN) model[4] and the multi-flavor Nambu–Jona–Lasinio (NJL)[5] model, in the large N limit.

Explicit calculations of fermion bag profiles in the GN and NJL models were given originally in Refs. 6–8.

Following these works, fermion bags in the GN and NJL models were discussed in the literature several other times.[9–12] For a recent review on these and related matters, see Ref. 13.

Very recently, static chiral fermion bag solitons[14] in a $1+1$ dimensional model, as well as nonchiral (real scalar) fermion bag solitons,[15] were discussed, in which the scalar field that couples to the fermions was dynamical already at the classical level.

Mathematical considerations similar to those involved in studying fermion bags appear also in other branches of theoretical physics, such as the theory of inhomogeneous superconductors,[16] and the results of this paper may be applicable there as well.

Studying the physics of fermion bags necessarily involves knowledge of the resolvent of the Dirac operator in the background of the bag. As an example, let us consider the $1+1$ dimensional NJL model (which contains the GN model as a special case).

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One version of writing the action of the $1+1$ dimensional NJL model is

$$S=\int d^2x\left\{\sum_{a=1}^{N}\overline{\psi}_a[i\partial\!\!\!/-(\sigma+i\pi\gamma_5)]\psi_a-\frac{1}{2g^2}(\sigma^2+\pi^2)\right\}, \tag{1.1}$$

where the $\psi_a(a=1,\ldots,N)$ are N flavors of massless Dirac fermions, with Yukawa couplings to the scalar and pseudoscalar auxiliary fields $\sigma(x),\pi(x)$.

The partition function associated with (1.1) is

$$\mathcal{Z}=\int \mathcal{D}\sigma\mathcal{D}\pi\mathcal{D}\overline{\psi}\mathcal{D}\psi\exp i\int d^2x\left\{\overline{\psi}[i\partial\!\!\!/-(\sigma+i\pi\gamma_5)]\psi-\frac{1}{2g^2}(\sigma^2+\pi^2)\right\}. \tag{1.2}$$

Integrating over the Grassmannian variables leads to $\mathcal{Z}=\int\mathcal{D}\sigma\mathcal{D}\pi\exp\{iS_{\text{eff}}[\sigma,\pi]\}$ where the bare effective action is

$$S_{\text{eff}}[\sigma,\pi]=-\frac{1}{2g^2}\int d^2x(\sigma^2+\pi^2)-iN\,\mathrm{Tr}\log[i\partial\!\!\!/-(\sigma+i\pi\gamma_5)] \tag{1.3}$$

and the trace is taken over both functional and Dirac indices.

This theory has been studied in the limit $N\to\infty$ with Ng^2 held fixed.[4] In this limit, (1.2) is governed by saddle points of (1.3) and the small fluctuations around them. The most general saddle point condition reads

$$\begin{aligned}\frac{\delta S_{\text{eff}}}{\delta\sigma(x,t)}&=-\frac{\sigma(x,t)}{g^2}+iN\mathrm{tr}\left[\langle x,t|\frac{1}{i\partial\!\!\!/-(\sigma+i\pi\gamma_5)}|x,t\rangle\right]=0,\\ \frac{\delta S_{\text{eff}}}{\delta\pi(x,t)}&=-\frac{\pi(x,t)}{g^2}-N\mathrm{tr}\left[\gamma_5\langle x,t|\frac{1}{i\partial\!\!\!/-(\sigma+i\pi\gamma_5)}|x,t\rangle\right]=0.\end{aligned} \tag{1.4}$$

Fermion bags are the space–time dependent solutions $(\sigma(x,t),\pi(x,t))$ of (1.4), subjected to appropriate boundary conditions at spatial infinity, and on which S_{eff}/N is finite.

Thus, studying fermion bags necessarily involves the resolvent of the Dirac operator in the background of the bag.

In this article we discuss some mathematical aspects of the much simpler problem of *static* fermion bags, namely, the static solutions $(\sigma(x),\pi(x))$ of (1.4).

For the usual physical reasons, we set boundary conditions on our static fields such that $\sigma(x)$ and $\pi(x)$ start from a point on the vacuum manifold $\sigma^2+\pi^2=m^2$ (with constant σ,π of course, and where m is the dynamical mass[4]) at $x=-\infty$, wander around in the $\sigma-\pi$ plane, and then relax back to another point on the vacuum manifold at $x=+\infty$. Thus, we must have the asymptotic behavior

$$\begin{aligned}\sigma&\xrightarrow[x\to\pm\infty]{} m\cos\theta_\pm, \quad \sigma'\xrightarrow[x\to\pm\infty]{}0,\\ \pi&\xrightarrow[x\to\pm\infty]{} m\sin\theta_\pm, \quad \pi'\xrightarrow[x\to\pm\infty]{}0,\end{aligned} \tag{1.5}$$

where $\theta_\pm$ are the asymptotic chiral alignment angles. Only the difference $\theta_+-\theta_-$ is meaningful, of course, and henceforth we use the axial U(1) symmetry of (1.1) to set $\theta_-=0$, such that $\sigma(-\infty)=m$ and $\pi(-\infty)=0$. We also omit the subscript from θ_+ and denote it simply by θ from now on. As typical of solitonic configurations, we expect that $\sigma(x)$ and $\pi(x)$ tend to their asymptotic boundary values (1.5) on the vacuum manifold at an exponential rate which is determined, essentially, by the mass gap m of the model.

Thus, in order to study static fermion bags, we need to invert the Dirac operator

$$D \equiv i\partial\!\!\!/ - (\sigma(x) + i\pi(x)\gamma_5) \tag{1.6}$$

in a given background of static field configurations $\sigma(x)$ and $\pi(x)$, subjected to the boundary conditions (1.5). In particular, we have to find the diagonal resolvent of (1.6) in that background. We stress that inverting (1.6) has nothing to do with the large N approximation, and consequently our results are valid for any value of N.

The rest of the article is organized as follows: In Sec. II we show that the Dirac equation $(i\partial\!\!\!/ - (\sigma(x) + i\pi(x)\gamma_5))\psi = 0$ in a given static $\sigma(x) + i\gamma_5\pi(x)$ background is equivalent to a pair of two isospectral Sturm–Liouville equations in one dimension, which generalize the well known one dimensional supersymmetric quantum mechanics. We use this generalized supersymmetry to express all four entries of the space-diagonal Dirac resolvent (i.e., the resolvent evaluated at coincident spatial coordinates) in terms of a single function. In Sec. III, we use the results of Sec. II to derive simple expressions for various bilinear fermion condensates in the given static $\sigma(x) + i\gamma_5\pi(x)$ background. In particular, we prove that each frequency mode of the spatial current $\langle \overline{\psi}(x)\gamma^1\psi(x)\rangle$ vanishes identically in the static background.

II. RESOLVENT OF THE DIRAC OPERATOR WITH STATIC BACKGROUND FIELDS

As was explained in the Introduction, we need to invert the Dirac operator (1.6), $D \equiv i\partial\!\!\!/ - (\sigma(x) + i\pi(x)\gamma_5)$, in a given background of static field configurations $\sigma(x)$ and $\pi(x)$, subjected to the boundary conditions (1.5).

In this article we use the Majorana representation

$$\gamma^0 = \sigma_2, \quad \gamma^1 = i\sigma_3 \quad \text{and} \quad \gamma^5 = -\gamma^0\gamma^1 = \sigma_1 \tag{2.1}$$

for γ matrices. In this representation (1.6) becomes

$$D = \begin{pmatrix} -\partial_x - \sigma & -i\omega - i\pi \\ i\omega - i\pi & \partial_x - \sigma \end{pmatrix} = \begin{pmatrix} -Q & -i\omega - i\pi \\ i\omega - i\pi & -Q^\dagger \end{pmatrix}, \tag{2.2}$$

where we introduced the pair of adjoint operators

$$Q = \sigma(x) + \partial_x, \quad Q^\dagger = \sigma(x) - \partial_x. \tag{2.3}$$

[To obtain (2.2), we have naturally transformed $i\partial\!\!\!/ - (\sigma(x) + i\pi(x)\gamma_5)$ to the ω plane, since the background fields $\sigma(x), \pi(x)$ are static.]

Inverting (2.2) is achieved by solving

$$\begin{pmatrix} -Q & -i\omega - i\pi(x) \\ i\omega - i\pi(x) & -Q^\dagger \end{pmatrix} \cdot \begin{pmatrix} a(x,y) & b(x,y) \\ c(x,y) & d(x,y) \end{pmatrix} = -i\mathbf{1}\delta(x-y) \tag{2.4}$$

for the Green's function of (2.2) in a given background $\sigma(x), \pi(x)$. By dimensional analysis, we see that the quantities a, b, c and d are dimensionless.

A. Generalized "supersymmetry" in a chiral bag background

We now show that the spectral theory of the Dirac operator (2.2) is underlined by a certain generalized one dimensional supersymmetric quantum mechanics. This generalized supersymmetry is very helpful in simplifying various calculations involving the Dirac operator and its resolvent.

The diagonal elements $a(x,y), d(x,y)$ in (2.4) may be expressed in terms of the off-diagonal elements as

$$a(x,y) = \frac{-i}{\omega - \pi(x)} Q^\dagger c(x,y), \quad d(x,y) = \frac{i}{\omega + \pi(x)} Q b(x,y), \tag{2.5}$$

which in turn satisfy the second order partial differential equations

$$\left[Q^\dagger \frac{1}{\omega+\pi(x)} Q-(\omega-\pi(x))\right] b(x,y)=$$
$$-\partial_x\left[\frac{\partial_x b(x,y)}{\omega+\pi(x)}\right]+\left[\sigma(x)^2+\pi(x)^2-\sigma'(x)-\omega^2+\frac{\sigma(x)\pi'(x)}{\omega+\pi(x)}\right]\frac{b(x,y)}{\omega+\pi(x)}=\delta(x-y),$$
$$\left[Q\frac{1}{\omega-\pi(x)} Q^\dagger-(\omega+\pi(x))\right] c(x,y)= \tag{2.6}$$
$$-\partial_x\left[\frac{\partial_x c(x,y)}{\omega-\pi(x)}\right]+\left[\sigma(x)^2+\pi(x)^2+\sigma'(x)-\omega^2+\frac{\sigma(x)\pi'(x)}{\omega-\pi(x)}\right]\frac{c(x,y)}{\omega-\pi(x)}=-\delta(x-y).$$

Thus, $b(x,y)$ and $-c(x,y)$ are simply the Green's functions of the corresponding second order Sturm–Liouville operators[17]

$$L_b(\omega)b(x)=-\partial_x\left[\frac{\partial_x b(x)}{\omega+\pi(x)}\right]+\left[\sigma(x)^2+\pi(x)^2-\sigma'(x)-\omega^2+\frac{\sigma(x)\pi'(x)}{\omega+\pi(x)}\right]\frac{b(x)}{\omega+\pi(x)},$$
$$L_c(\omega)c(x)=-\partial_x\left[\frac{\partial_x c(x)}{\omega-\pi(x)}\right]+\left[\sigma(x)^2+\pi(x)^2+\sigma'(x)-\omega^2+\frac{\sigma(x)\pi'(x)}{\omega-\pi(x)}\right]\frac{c(x)}{\omega-\pi(x)}, \tag{2.7}$$

in (2.6), namely,

$$b(x,y)=\frac{\theta(x-y)b_2(x)b_1(y)+\theta(y-x)b_2(y)b_1(x)}{W_b},$$
$$c(x,y)=-\frac{\theta(x-y)c_2(x)c_1(y)+\theta(y-x)c_2(y)c_1(x)}{W_c}. \tag{2.8}$$

Here $\{b_1(x),b_2(x)\}$ and $\{c_1(x),c_2(x)\}$ are pairs of independent fundamental solutions of the two equations $L_b b(x)=0$ and $L_c c(x)=0$, subjected to the boundary conditions

$$b_1(x),c_1(x)\xrightarrow[x\to-\infty]{} A^{(1)}_{b,c}(k)e^{-ikx},\quad b_2(x),c_2(x)\xrightarrow[x\to+\infty]{} A_{b,c}(k)^{(2)}e^{ikx}, \tag{2.9}$$

with some possibly k dependent coefficients $A^{(1)}_{b,c}(k),A^{(2)}_{b,c}(k)$ and with[18]

$$k=\sqrt{\omega^2-m^2},\quad \mathrm{Im}\,k\geqslant 0. \tag{2.10}$$

The purpose of introducing the (yet unspecified) coefficients $A^{(1)}_{b,c}(k),A^{(2)}_{b,c}(k)$ will become clear following Eqs. (2.13) and (2.14). The boundary conditions (2.9) are consistent, of course, with the asymptotic behavior (1.5) of σ and π due to which both L_b and L_c tend to a free particle Hamiltonian $[-\partial_x^2+m^2-\omega^2]$ as $x\to\pm\infty$.

The Wronskians of these pairs of solutions are

$$W_b(k)=\frac{b_2(x)b_1'(x)-b_1(x)b_2'(x)}{\omega+\pi(x)},$$
$$W_c(k)=\frac{c_2(x)c_1'(x)-c_1(x)c_2'(x)}{\omega-\pi(x)}. \tag{2.11}$$

As is well known, $W_b(k)$ and $W_c(k)$ are independent of x.

Note in passing that the canonical asymptotic behavior assumed in the scattering theory of the operators L_b and L_c corresponds to setting $A^{(1)}_{b,c}=A^{(2)}_{b,c}=1$ in (2.9). Thus, the Wronskians in (2.11) are *not* the canonical Wronskians used in scattering theory. As is well known in the literature,[19] the *canonical* Wronskians are proportional (with a k independent coefficient) to $k/t(k)$, where $t(k)$ is the transmission amplitude of the corresponding operator L_b or L_c. Thus, on top of the well-known features of $t(k)$, such as the fact that $t(k)$ has simple poles on the positive imaginary k-axis (corresponding to bound states), the Wronskians in (2.11) will have additional spurious k-dependence coming from the amplitudes $A^{(1)}_{b,c}(k),A^{(2)}_{b,c}(k)$ in (2.9).

Substituting the expressions (2.8) for the off-diagonal entries $b(x,y)$ and $c(x,y)$ into (2.5), we obtain the appropriate expressions for the diagonal entries $a(x,y)$ and $d(x,y)$. We do not bother to write these expressions here. It is useful, however, to note that, despite the ∂_x's in the Q operators in (2.5) that act on the step functions in (2.8), neither $a(x,y)$ nor $d(x,y)$ contains pieces proportional to $\delta(x-y)$. Such pieces cancel one another due to the symmetry of (2.8) under $x\leftrightarrow y$.

We will now prove that the spectra of the operators L_b and L_c are essentially the same. Our proof is based on the fact that we can factorize the eigenvalue equations $L_b b(x)=0$ and $L_c c(x)=0$ as

$$\frac{1}{\omega-\pi(x)}Q^{\dagger}\frac{1}{\omega+\pi(x)}Qb=b,$$
$$\frac{1}{\omega+\pi(x)}Q\frac{1}{\omega-\pi(x)}Q^{\dagger}c=c, \tag{2.12}$$

as should be clear from (2.6) and (2.7).

The factorized Eqs. (2.12) suggest the following map between their solutions. Indeed, given that $L_b b(x)=0$, then clearly

$$c(x)=\frac{1}{\omega+\pi(x)}Qb(x) \tag{2.13}$$

is a solution of $L_c c(x)=0$. Similarly, if $L_c c(x)=0$, then

$$b(x)=\frac{1}{\omega-\pi(x)}Q^{\dagger}c(x) \tag{2.14}$$

solves $L_b b(x)=0$.

Thus, in particular, given a pair $\{b_1(x),b_2(x)\}$ of independent fundamental solutions of $L_b b(x)=0$, we can obtain from it a pair $\{c_1(x),c_2(x)\}$ of independent fundamental solutions of $L_c c(x)=0$ by using (2.13), and vice versa. Therefore, with no loss of generality, we henceforth assume that the two pairs of independent fundamental solutions $\{b_1(x),b_2(x)\}$ and $\{c_1(x),c_2(x)\}$ are related by (2.13) and (2.14).

The coefficients $A^{(1)}_{b,c}(k),A^{(2)}_{b,c}(k)$ in (2.9) are to be adjusted according to (2.13) and (2.14), and this was the purpose of introducing them in the first place.

Thus, with no loss of generality, we may make the standard choice

$$A^{(1)}_b=A^{(2)}_b=1 \tag{2.15}$$

in (2.9). The coefficients $A^{(1)}_c,A^{(2)}_c$ are then determined by (2.13):

$$A_c^{(1)}=\frac{\sigma(-\infty)-ik}{\pi(-\infty)+\omega},$$
$$A_c^{(2)}=\frac{\sigma(\infty)+ik}{\pi(\infty)+\omega}. \tag{2.16}$$

We note that these $b(x)\leftrightarrow c(x)$ mappings can break only if

$$Qb=0 \quad \text{or} \quad Q^\dagger c=0, \tag{2.17}$$

for $b(x)$ or $c(x)$ that *solve* (2.12). Do such solutions exist? Let us assume, for example, that $Qb=0$ and that $L_b b=0$. From the first equation in (2.12) [or in (2.6)], we see that this is possible if and only if $\omega\pm\pi(x)\equiv 0$, which clearly cannot hold if $\partial_x\pi(x)\neq 0$. A similar argument holds for $Q^\dagger c=0$. Thus, if $\partial_x\pi(x)\neq 0$, the mappings (2.13) and (2.14) are one-to-one. In particular, a bound state in L_b implies a bound state in L_c (at the same energy) and vice versa.

An interesting related result concerns the Wronskians W_b and W_c. From (2.11), and from (2.13) and (2.14), it follows immediately that for pairs of independent fundamental solutions $\{b_1(x),b_2(x)\}$ and $\{c_1(x),c_2(x)\}$ we have

$$W_c=\frac{c_2\partial_x c_1-c_1\partial_x c_2}{\omega-\pi(x)}=c_1b_2-c_2b_1=\frac{b_2\partial_x b_1-b_1\partial_x b_2}{\omega+\pi(x)}=W_b. \tag{2.18}$$

The Wronskians of pairs of independent fundamental solutions of L_b and L_c, which are related via (2.13) and (2.14), are equal!

To summarize, if $\partial_x\pi(x)\neq 0$, L_b and L_c have the same set of energy eigenvalues and their eigenfunctions are in one-to-one correspondence.

If, however, $\pi=$const, then we are back to the familiar ''supersymmetric'' factorization

$$Q^\dagger Qb=(\omega^2-\pi^2)b, \quad QQ^\dagger c=(\omega^2-\pi^2)c, \tag{2.19}$$

and mappings

$$c(x)=\frac{1}{\omega+\pi}Qb(x), \quad b(x)=\frac{1}{\omega-\pi}Q^\dagger c(x). \tag{2.20}$$

As is well known from the literature on supersymmetric quantum mechanics, the mappings (2.20) break down if either $Qb=0$ or $Q^\dagger c=0$, in which case the two operators $Q^\dagger Q$ and $QQ^\dagger$ are isospectral, but only up to a ''zero-mode'' (or, rather, an $\omega^2=\pi^2$ mode), which belongs to the spectrum of only one of the operators.[20] The case $\pi(x)\equiv 0$ brings us back to the GN model. Supersymmetric quantum mechanical considerations were quite useful in the study of fermion bags in Ref. 10.

The ''Witten index'' associated with the pair of isospectral operators L_b and L_c is always null for backgrounds in which $\partial_x\pi(x)\neq 0$, since they are absolutely isospectral, and not only up to zero modes. There is no interesting topology associated with spectral mismatches of L_b and L_c. This is not surprising at all, since the NJL model, with its continuous axial symmetry, does not support topological solitons. This is in contrast to the GN model, for which $\pi\equiv 0$, which contains topological kinks, whose topological charge is essentially the Witten index of the pair of operators (2.19).

We note in passing that isospectrality of L_b and L_c, which we have just proved, is consistent with the γ_5 symmetry of the system of equations in (2.4), which relates the resolvent of D with that of $\tilde{D}=-\gamma_5 D\gamma_5$. Due to this symmetry, we can map the pair of equations $L_b b(x,y)=\delta(x-y)$ and $L_c c(x,y)=-\delta(x-y)$ [Eqs. (2.6)] on each other by

$$b(x,y)\leftrightarrow -c(x,y) \quad \text{together with} \quad (\sigma,\pi)\rightarrow(-\sigma,-\pi). \tag{2.21}$$

[Note that under these reflections we also have $a(x,y)\leftrightarrow -d(x,y)$, as we can see from (2.5).] The reflection $(\sigma,\pi)\rightarrow(-\sigma,-\pi)$ just shifts both asymptotic chiral angles $\theta_{\pm}$ by the same amount π, and clearly does not change the physics. Since this reflection interchanges $b(x,y)$ and $c(x,y)$ without affecting the physics, these two objects must have the same singularities as functions of ω, consistent with isospectrality of L_b and L_c.

Isospectrality of L_b and L_c realizes a concrete generalization of SUSY quantum mechanics. We should mention, in passing, the recent discussion in Ref. 21, made in a different context, with other generalizations of SUSY quantum mechanics.

B. The diagonal resolvent

Following Refs. 22 and 11 we define the diagonal resolvent $\langle x|iD^{-1}|x\rangle$ symmetrically as

$$\langle x|-iD^{-1}|x\rangle\equiv\begin{pmatrix} A(x) & B(x) \\ C(x) & D(x)\end{pmatrix}=\frac{1}{2}\lim_{\epsilon\rightarrow 0+}\begin{pmatrix} a(x,y)+a(y,x) & b(x,y)+b(y,x) \\ c(x,y)+c(y,x) & d(x,y)+d(y,x)\end{pmatrix}_{y=x+\epsilon}. \tag{2.22}$$

Here $A(x)$ through $D(x)$ stand for the entries of the diagonal resolvent, which following (2.5) and (2.8) have the compact representation[23]

$$\begin{aligned} B(x)&=\frac{b_1(x)b_2(x)}{W_b}, \quad D(x)=\frac{i}{2}\frac{[\partial_x+2\sigma(x)]B(x)}{\omega+\pi(x)}, \\ C(x)&=-\frac{c_1(x)c_2(x)}{W_c}, \quad A(x)=\frac{i}{2}\frac{[\partial_x-2\sigma(x)]C(x)}{\omega-\pi(x)}. \end{aligned} \tag{2.23}$$

We now use the generalized ''supersymmetry'' of the Dirac operator, which we discussed in the previous subsection, to deduce some important properties of the functions $A(x)$ through $D(x)$.

From (2.23) and from (2.3) we have

$$A(x)=\frac{i}{2}\frac{\partial_x-2\sigma(x)}{\omega-\pi(x)}\left(-\frac{c_1c_2}{W_c}\right)=\frac{i}{2W_c}\frac{c_2Q^{\dagger}c_1+c_1Q^{\dagger}c_2}{\omega-\pi(x)}.$$

Using (2.14) first, and then (2.13), we rewrite this expression as

$$A(x)=\frac{i}{2W_c}(c_2b_1+c_1b_2)=\frac{i}{2W_c}\frac{b_1Qb_2+b_2Qb_1}{\omega+\pi(x)}.$$

Then, using the fact that $W_c=W_b$ [Eq. (2.18)] and (2.23), we rewrite the last expression as

$$A(x)=\frac{i}{2}\frac{\partial_x+2\sigma}{\omega+\pi(x)}\left(\frac{b_1b_2}{W_b}\right)=\frac{i}{2}\frac{(\partial_x+2\sigma)B(x)}{\omega+\pi(x)}.$$

Thus, finally,

$$A(x)=D(x). \tag{2.24}$$

Supersymmetry renders the diagonal elements A and D equal.

Due to (2.23), $A=D$ is also a first order differential equation relating B and C. We can also relate the off diagonal elements B and C to each other more directly. From (2.23) and from (2.13) we find

$$C(x)=-\frac{c_1c_2}{W_c}=-\frac{(Qb_1)(Qb_2)}{(\omega+\pi)^2W_c}. \tag{2.25}$$

After some algebra, and using (2.18), we can rewrite this as

$$-(\omega+\pi)^2 C=\sigma^2 B+\sigma B'+\frac{b_1' b_2'}{W_b}.$$

The combination $b_1' b_2'/W_b$ appears in $B''=(b_1 b_2/W_b)''$. After using $L_b b_{1,2}=0$ to eliminate b_1'' and b_2'' from B'', we find

$$\frac{b_1' b_2'}{W_b}=\frac{1}{2}B''-\frac{\pi' B'}{2(\omega+\pi)}-\left(\sigma^2+\pi^2-\sigma'-\omega^2+\frac{\sigma\pi'}{\omega+\pi}\right)B.$$

Thus, finally, we have

$$-(\omega+\pi)^2 C=\frac{1}{2}B''+\left(\sigma-\frac{\pi'}{2(\omega+\pi)}\right)B'-\left(\pi^2-\sigma'-\omega^2+\frac{\sigma\pi'}{\omega+\pi}\right)B. \tag{2.26}$$

In a similar manner we can prove that

$$(\omega-\pi)^2 B=-\frac{1}{2}C''+\left(\sigma-\frac{\pi'}{2(\omega-\pi)}\right)C'+\left(\pi^2+\sigma'-\omega^2+\frac{\sigma\pi'}{\omega-\pi}\right)C. \tag{2.27}$$

We can simplify (2.26) and (2.27) further. After some algebra, and using (2.23), we arrive at

$$\begin{aligned} C(x)&=\frac{i}{\omega+\pi(x)}\partial_x D(x)-\frac{\omega-\pi(x)}{\omega+\pi(x)}B(x),\\ B(x)&=\frac{i}{\omega-\pi(x)}\partial_x A(x)-\frac{\omega+\pi(x)}{\omega-\pi(x)}C(x). \end{aligned} \tag{2.28}$$

Supersymmetry, namely, isospectrality of L_b and L_c, enables us to relate the diagonal resolvents of these operators, B and C, to each other.

Thus, we can use (2.23), (2.24) and (2.28) to eliminate three of the entries of the diagonal resolvent in (2.23), in terms of the fourth.

Note that the two relations in (2.28) transform into each other under

$$B\leftrightarrow -C \quad \text{simultaneously with} \quad (\sigma,\pi)\rightarrow(-\sigma,-\pi), \tag{2.29}$$

in consistency with (2.21). The relations in (2.28) are linear and homogeneous, with coefficients that for $\partial_x\pi(x)\neq 0$ do not introduce additional singularities in the ω plane. Thus, we see, once more, that B and C have the same singularities in the ω plane. We refer the reader to Sec. IV in Ref. 11 for concrete examples of such resolvents.

The case $\pi(x)\equiv 0$ brings us back to the GN model. In the GN model, our B and C coincide, respectively, with ωR_- and $-\omega R_+$ defined in Eqs. (9) and (10) in Ref. 10. With these identifications, the relation $A=D$ [Eq. (2.24)] coincides essentially with Eq. (18) of Ref. 10. The relations (2.26) and (2.27) were not discussed in Ref. 10, but one can verify them, for example, for the resolvents corresponding to the kink case $\sigma(x)=m\tanh mx$ [Eq. (29) in Ref. 10], for which

$$C=-\frac{\omega}{2\sqrt{m^2-\omega^2}}, \quad B=\left[\left(\frac{m\,\mathrm{sech}\,mx}{\omega}\right)^2-1\right]C.$$

III. BILINEAR FERMION CONDENSATES AND VANISHING OF THE SPATIAL FERMION CURRENT

Following basic principles of quantum field theory, we may write the most generic flavor-singlet bilinear fermion condensate in our static background as

$$\langle \overline{\psi}_{a\alpha}(t,x)\Gamma_{\alpha\beta}\psi_{a\beta}(t,x)\rangle_{\rm reg} = N\int \frac{d\omega}{2\pi}\,{\rm tr}\left[\Gamma\langle x|\,\frac{-i}{\omega\gamma^0 + i\gamma^1\partial_x - (\sigma + i\pi\gamma_5)}\,|x\rangle_{\rm reg}\right]$$
$$= N\int \frac{d\omega}{2\pi}\,{\rm tr}\left\{\Gamma\left[\begin{pmatrix} A(x) & B(x) \\ C(x) & D(x)\end{pmatrix} - \begin{pmatrix} A & B \\ C & D\end{pmatrix}_{\rm VAC}\right]\right\}, \qquad (3.1)$$

where we have used (2.22). Here $a=1,\ldots,N$ is a flavor index, and the trace is taken over Dirac indices α,β. As usual, we regularized this condensate by subtracting from it a short distance divergent piece embodied here by the diagonal resolvent

$$\langle x|-iD^{-1}|x\rangle_{\rm VAC} = \begin{pmatrix} A & B \\ C & D\end{pmatrix}_{\rm VAC} = \frac{1}{2\sqrt{m^2-\omega^2}}\begin{pmatrix} im\cos\theta & \omega + m\sin\theta \\ -\omega + m\sin\theta & im\cos\theta\end{pmatrix} \qquad (3.2)$$

of the Dirac operator in a vacuum configuration $\sigma_{\rm VAC} = m\cos\theta$ and $\pi_{\rm VAC} = m\sin\theta$.

In our convention for γ matrices (2.1) we have

$$\begin{pmatrix} A(x) & B(x) \\ C(x) & D(x)\end{pmatrix} = \frac{A(x)+D(x)}{2}\mathbf{1} + \frac{A(x)-D(x)}{2i}\gamma^1 + i\frac{B(x)-C(x)}{2}\gamma^0 + \frac{B(x)+C(x)}{2}\gamma_5. \qquad (3.3)$$

An important condensate is the expectation value of the fermion current $\langle j^\mu(x)\rangle$. In particular, consider its spatial component. In our static background $(\sigma(x),\pi(x))$, it must, of course, vanish identically

$$\langle j^1(x)\rangle = 0. \qquad (3.4)$$

Thus, substituting $\Gamma=\gamma^1$ in (3.1) and using (3.3) we find

$$\langle j^1(x)\rangle = iN\int \frac{d\omega}{2\pi}[A(x)-D(x)]. \qquad (3.5)$$

But we have already proved that $A(x)=D(x)$ in *any* static background $(\sigma(x),\pi(x))$ (Eq. (2.24)). Thus, each frequency component of $\langle j^1\rangle$ vanishes separately, and (3.4) holds identically. It is remarkable that the generalized supersymmetry of the Dirac operator guarantees the consistency of any static $(\sigma(x),\pi(x))$ background.

Expressions for other bilinear condensates may be derived in a similar manner (here we write the unsubtracted quantities). Thus, substituting $\Gamma=\gamma^0$ in (3.1) and using (3.3), (2.24) and (2.28), we find that the fermion density is

$$\langle j^0(x)\rangle = iN\int \frac{d\omega}{2\pi}[B(x)-C(x)] = iN\int \frac{d\omega}{2\pi}\,\frac{2\omega B(x) - i\partial_x D(x)}{\omega+\pi(x)}. \qquad (3.6)$$

Similarly, the scalar and pseudoscalar condensates are

$$\langle \overline{\psi}(x)\psi(x)\rangle = N\int \frac{d\omega}{2\pi}[A(x)+D(x)] = 2N\int \frac{d\omega}{2\pi}D(x), \qquad (3.7)$$

and

$$\langle \overline{\psi}(x)\gamma^5\psi(x)\rangle = N\int \frac{d\omega}{2\pi}[B(x)+C(x)] = N\int \frac{d\omega}{2\pi}\,\frac{2\pi(x)B(x)+i\partial_x D(x)}{\omega+\pi(x)}. \tag{3.8}$$

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Stabilization of impurity states in crossed magnetic and electric fields

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It is shown that the renormalizability of the zero-range interaction in the two-dimensional space is always followed by the existence of a bound state, which is not true for odd-dimensional spaces. A renormalization procedure is defined and the exact retarded Green's function for electrons moving in two dimensions and interacting with both crossed magnetic and electric fields and an attractive zero-range interaction is constructed. Imaginary parts of poles of this Green's function determine lifetimes of quasibound (resonance) states. It is shown that for some particular parameters the stabilization against decay occurs even for strong electric fields. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1491596]

I. INTRODUCTION

The observations of the integer and fractional quantum Hall effects[1,2] are among the most important discoveries of recent years and have had a profound impact on both applied and fundamental physics. Many aspects of these discoveries are presented in the books edited by Prange and Girvin[3] and by Das Sarma and Pinczuk,[4] and in the monographs.[5,6] From the theoretical point of view the quantum Hall phenomenon is due to the two-dimensional dynamics of electrons moving under the influence of crossed magnetic and electric fields in the presence of impurities. Since the de Broglie wavelength of electrons scattered by impurities is much larger then the interaction range, therefore, it is legitimated to describe a scatterer by a zero-range potential. This, in fact, has been already proposed by Prange[7] shortly after the discovery of the quantum Hall effect, and discussed further in Refs. 8 and 9. In his seminal paper Prange studied electron states in two dimensions in perpendicular magnetic and in-plane electric fields in the presence of a single repulsive ''delta-like'' scatterer. Prange's model, with an attractive zero-range potential and zero electric field, has been reconsidered by Perez and Coutinho,[10] and by Cavalcanti and de Carvalho.[11] They showed that the attractive zero-range interaction can be rigorously defined by renormalizing the strength of the δ-function. Such a procedure cannot be developed for a repulsive two-dimensional δ-function (as it will follow shortly), for which an artificial cutoff has to be introduced, as described for instance in Ref. 12. The problem of electron scattering by a single impurity represented by a repulsive short-range potential in the presence of both magnetic and electric fields has been further studied from the classical point of view in Ref. 13, whereas the quantum description has been developed in Ref. 12 for a repulsive, and in Ref. 14 for an attractive δ-function potential. Both these quantum analyses show that due to external magnetic and electric fields new long living quasibound states appear in the positive part of the energy spectrum, the existence of which appears to be crucial for the explanation of the robustness of the quantum Hall effect.[7,12]

There has been shown[12,14] that in the limit of a very weak electric field the lifetime of these quasibound states tends to infinity and grow in a Gaussian way as the electric field tends to zero. This finding, not taking into account, however, the precisely determined functional dependence of the lifetime on the strength of the electric field, agrees with our common understanding of the decay problem in a weak electric field. The aim of this paper is to analyze this problem for strong electric fields. It is usually believed that with an increasing electric field the lifetimes of these quasibound states should decrease to zero. It appears, however, that such a behavior is not gen-

erally true and that for some particular values of magnetic and electric fields one observes a new phenomenon, the stabilization of these new quasibound states. We demonstrate this phenomenon for an attractive δ-function potential considered in Ref. 14.

In this paper we use units in which $\hbar=1$.

II. ATTRACTIVE δ-FUNCTION POTENTIAL

In this section we shall define the renormalized attractive δ-function potential for one-, two-, and three-dimensional cases. To this end let us assume that a quantum system without this interaction is described by the hamiltonian H_0. We introduce further a regularization of a zero-range potential such that the total hamiltonian is equal to

$$H=H_0+\lambda_\sigma\delta_\sigma(\mathbf{r}), \tag{1}$$

in which σ is a regularization parameter, λ_σ is a bare coupling constant, and $\delta_\sigma(\mathbf{r})$ tends to the Dirac distribution $\delta(\mathbf{r})$ in a d-dimensional space. Our aim is to construct the retarded Green's function satisfying the equation,

$$(E-H)G^{(+)}(\mathbf{r},\mathbf{r}';E)=\delta(\mathbf{r}-\mathbf{r}'), \tag{2}$$

provided that the range of a regularized potential is *very* small, i.e., is much smaller than the electron's de Broglie wavelength or the size of a bound state wave function. This means that in the Lippmann–Schwinger equation

$$G^{(+)}(\mathbf{r},\mathbf{r}';E)=G_0^{(+)}(\mathbf{r},\mathbf{r}';E) + \lambda_\sigma\int \mathrm{d}^d\mathbf{r}''G_0^{(+)}(\mathbf{r},\mathbf{r}'';E)\,\delta_\sigma(\mathbf{r}'')G^{(+)}(\mathbf{r}'',\mathbf{r}';E), \tag{3}$$

in which $G_0^{(+)}(\mathbf{r},\mathbf{r}';E)$ is the Green's function for the Hamiltonian H_0, we can approximate under the integral the full Green's function $G^{(+)}(\mathbf{r}'',\mathbf{r}';E)$ by $G^{(+)}(\mathbf{0},\mathbf{r}';E)$. This allows us to calculate $G^{(+)}(\mathbf{0},\mathbf{r}';E)$ and to arrive at the following expression for the retarded Green's function:

$$G^{(+)}(\mathbf{r},\mathbf{r}';E)=G_0^{(+)}(\mathbf{r},\mathbf{r}';E) + \frac{G_0^{(+)}(\mathbf{r},\mathbf{0};E)G_0^{(+)}(\mathbf{0},\mathbf{r}';E)}{\lambda_\sigma^{-1}-\int \mathrm{d}^d\mathbf{r}''G_0^{(+)}(\mathbf{0},\mathbf{r}'';E)\,\delta_\sigma(\mathbf{r}'')}. \tag{4}$$

In order to proceed further let us choose a particular regularization prescription for which all the space and momentum integrals, that will appear below, can be carried out and expressed in terms of elementary functions, namely,

$$\delta_\sigma(\mathbf{r})=\int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d}\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}-\sigma^2\mathbf{k}^2). \tag{5}$$

Let us also assume for a moment that H_0 describes free electrons of a reduced mass m^*. For such a hamiltonian the retarded Green's function adopts the form

$$G_0^{(+)}(\mathbf{r},\mathbf{r}';E)=-\mathrm{i}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}(E+\mathrm{i}\varepsilon)t} \times\int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d}\exp\left(\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')-\mathrm{i}\frac{\mathbf{k}^2}{2m^*}t\right), \tag{6}$$

in which ε is an infinitesimally small positive real number. Thus, after performing the Gauss integration over $\mathbf{k}$, the denominator in Eq. (4) becomes

$$D(E)=\lambda_\sigma^{-1}+\mathrm{i}\left(\frac{m^*}{2\pi\mathrm{i}}\right)^{d/2}\int_0^\infty \mathrm{d}t\,\frac{\mathrm{e}^{\mathrm{i}(E+\mathrm{i}\varepsilon)t}}{(t-2\mathrm{i}m^*\sigma^2)^{d/2}}. \tag{7}$$

As we see, for $d=1$ the last integral exists for $\sigma=0$, i.e., there is no need for the renormalization of a coupling constant λ_σ. On the other hand, for $d>1$ the integral in the equation above diverges for small t in the limit of a vanishing regularization parameter σ. It can be shown, however, that the divergent part of this integral can be absorbed into the bare coupling constant λ_σ. To this end let us consider in the beginning the case of $d=2$. Integrating by parts we end up in the limit of vanishing σ with

$$D(E)=\lambda_R^{-1}+\frac{m^*}{2\pi}\left(\ln(\mathrm{i})-\mathrm{i}E\int_0^\infty \mathrm{d}t\mathrm{e}^{\mathrm{i}(E+\mathrm{i}\varepsilon)t}\ln(t/t_0)\right), \tag{8}$$

where t_0 is an arbitrary positive real number of the same dimensionality as t, introduced only for dealing with a dimensionless argument of the logarithm function, and λ_R is the renormalized coupling constant,

$$\lambda_R^{-1}=\lim_{\sigma\to 0}\left[\lambda_\sigma^{-1}-\frac{m^*}{2\pi}\ln\left(\frac{2m^*\sigma^2}{t_0}\right)\right]. \tag{9}$$

As it follows from the equation above the bare coupling constant λ_σ has to be negative in order to carry out the renormalization procedure. Hence, the zero-range limit exists only for an attractive interaction. Performing the remaining integration we finally arrive at

$$D(E)=\lambda_R^{-1}+\frac{m^*}{2\pi}\ln\left(\frac{\mathrm{e}^{-\gamma}}{-Et_0}\right), \tag{10}$$

where γ is the Euler's constant. Since the energy of a bound state, $E_B<0$, supported by this interaction is determined by the zero of $D(E)$, therefore

$$E_B=-\frac{1}{t_0}\mathrm{e}^{-\gamma+2\pi/\lambda_R m^*}. \tag{11}$$

As one sees, the expression above is always negative, independently weather the renormalized coupling constant is negative or positive. This means that the zero-range potential in two-dimensional space always supports one bound state. Combining (10) with (11) we arrive at the following expression for the denominator $D(E)$:

$$D(E)=\frac{m^*}{2\pi}\ln\left(\frac{E_B}{E}\right), \tag{12}$$

in which an artificial parameter t_0 does not appear any more.

The existence of a bound state for a zero-range interaction, irrespectively of the sign of a renormalized coupling constant, can only happen for $d=2$. In order to show this let us consider the case of $d=3$. Now we do not need to introduce t_0 and end up with

$$D(E)=\lambda_R^{-1}+\frac{m^*}{2\pi}\sqrt{-2m^*E}, \tag{13}$$

where the renormalized coupling constant is equal to

$$\lambda_R^{-1}=\lim_{\sigma\to 0}\left(\lambda_\sigma^{-1}+\frac{m^*}{2\pi^{3/2}\sigma}\right). \tag{14}$$

Hence, it is clearly seen that again the renormalization procedure can be only performed for a negative bare coupling constant. Nevertheless, contrary to the two-dimensional case, a bound state exists only for a negative renormalized coupling constant λ_R. A similar situation occurs for the one-dimensional δ-function potential supporting one bound state just for negative coupling constants (renormalized and bare coupling constants are equal here and amount to $-\sqrt{2|E_B|/m^*}$).

Summarizing, for the two-dimensional zero-range interaction the renormalizability is followed by the existence of a bound state, irrespectively of the sign of the renormalized coupling constant. In our further discussion we shall limit ourselves to the two-dimensional renormalizable zero-range interaction. Let us also note in closing this section that the zero-range potential for an arbitrary dimensional space has been studied by Wódkiewicz[15] who also emphasized the difference between odd and even dimensions.

III. QUASIBOUND STATES IN CROSSED MAGNETIC AND ELECTRIC FIELDS

We can now include into our two-dimensional model external magnetic and electric fields. For this we need the exact form of the retarded Green's function for the Hamiltonian,

$$H_0=\frac{1}{2m^*}(-\mathrm{i}\boldsymbol{\nabla}-e\mathbf{A}(\mathbf{r}))^2-e\boldsymbol{\mathcal{E}}\cdot\mathbf{r}. \tag{15}$$

Let us assume that electrons move in the xy-plane, the magnetic field $\boldsymbol{\mathcal{B}}$ is perpendicular to this plane and the electric field $\boldsymbol{\mathcal{E}}$ points into the x-direction. For such a geometry and for the vector potential in the symmetric gauge, i.e., $\mathbf{A}=\frac{1}{2}\boldsymbol{\mathcal{B}}\times\mathbf{r}$,

$$H_0=\frac{1}{2m^*}\left[\left(-\mathrm{i}\partial_x+\frac{e\mathcal{B}}{2}y\right)^2+\left(-\mathrm{i}\partial_y-\frac{e\mathcal{B}}{2}x\right)^2\right]-e\mathcal{E}x, \tag{16}$$

and the Green's function adopts the form

$$\begin{aligned}G_0^{(+)}(\mathbf{r},\mathbf{r}';E)=&-\frac{m^*\omega}{4\pi}\int_0^\infty \mathrm{d}t\,\frac{\mathrm{e}^{\mathrm{i}(E+\mathrm{i}\varepsilon)t}}{\sin\dfrac{\omega t}{2}}\\&\times\exp\left[\frac{\mathrm{i}m^*\omega}{4}((x-x')^2+(y-y')^2)\cot\frac{\omega t}{2}+\frac{\mathrm{i}m^*\omega}{2}(xy'-x'y)+\frac{\mathrm{i}e\mathcal{E}t}{2}(x+x')\right.\\&\left.+\frac{\mathrm{i}e\mathcal{E}}{\omega}\left(\frac{\omega t}{2}\cot\frac{\omega t}{2}-1\right)\left(-y+y'+\frac{e\mathcal{E}t}{2m^*\omega}\right)\right],\end{aligned} \tag{17}$$

with $\omega=|e|\mathcal{B}/m^*$ being the cyclotron frequency. Since lifetimes of quasibound states are determined by poles of the Green's function, therefore, we shall concentrate in our further discussion on the denominator in Eq. (4). One can find that in this particular case $D(E)$ can be expressed as follows:

$$\begin{aligned}D(E)=&\lambda_\sigma^{-1}+\frac{m^*\omega}{4\pi}\int_0^\infty \mathrm{d}t\,\frac{\mathrm{e}^{\mathrm{i}(E+\mathrm{i}\varepsilon)t}}{\sin\dfrac{\omega t}{2}-\mathrm{i}m^*\omega\sigma^2\cos\dfrac{\omega t}{2}}\\&\times\exp\left[\frac{\mathrm{i}t}{2m^*}\left(\frac{e\mathcal{E}}{\omega}\right)^2\left(\frac{\omega t}{2}\cot\frac{\omega t}{2}-1\right)-\sigma^2\left(\frac{e\mathcal{E}}{\omega}\right)^2\frac{\left(\dfrac{\omega t}{2}\right)^2+\left(\dfrac{\omega t}{2}\cot\dfrac{\omega t}{2}-1\right)^2}{1-\mathrm{i}m^*\omega\sigma^2\cot\dfrac{\omega t}{2}}\right],\end{aligned} \tag{18}$$

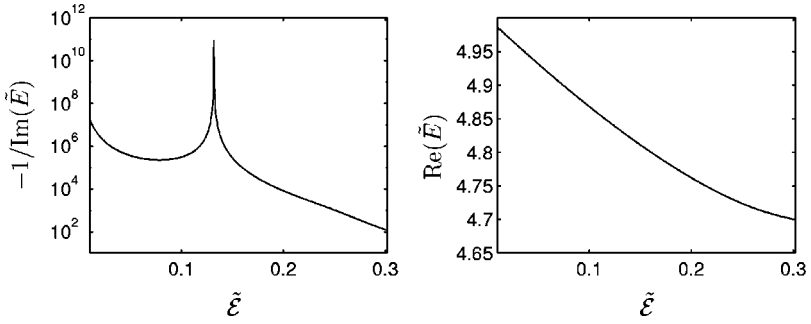

FIG. 1. Presents the dependence of the lifetime $\tau=-1/\mathrm{Im}(\tilde{E})$ and the real part of $\tilde{E}$ on the scaled electric field $\tilde{\mathcal{E}}$ for an impurity which supports one bound state of energy $\tilde{E}_B=-6.4$. For $\tilde{\mathcal{E}}=0.132$ we observe the stabilization of a resonance state located just below the third Landau level.

where the integral above diverges logarithmically for small values of t in the zero-range limit. However, as we have proved it in the previous section, this singularity can be removed by combining the divergent term with the bare coupling constant λ_σ.

For our further analysis it is convenient to introduce dimensionless variables, in which the length is measured in the units of $1/\sqrt{m^*\omega}$, whereas the electric field and the energy are scaled as $\tilde{\mathcal{E}}=|e|\mathcal{E}/\sqrt{m^*\omega^3}$ and $\tilde{E}=2E/\omega$, respectively. Changing the integration variable to $s=\omega t/2$ we obtain finally for $\sigma\to 0$,

$$D(E)=\frac{m^*}{2\pi}\left[\ln\left(\frac{\tilde{E}_B}{\tilde{E}}\right)+\int_0^\infty \mathrm{d}s\,\mathrm{e}^{\mathrm{i}(\tilde{E}+\mathrm{i}\varepsilon)s}\left(\frac{\exp(\mathrm{i}\tilde{\mathcal{E}}^2 s(s\cot s-1))}{\sin s}-\frac{1}{s}\right)\right]. \tag{19}$$

We shall demonstrate now that even in strong electric fields one can observe long living quasibound states. This nonperturbative result follows from the numerical determination of zeros of $D(E)$. It appears that for some particular values of the electric field and the binding energy there exist zeros of (19) with very small imaginary parts, although real parts remain positive. This phenomenon, which we call the stabilization, is presented in Figs. 1, 2, and 3. In Figs. 1 and 2 we draw the dependence of lifetimes, $\tau=-(2\,\mathrm{Im}(E))^{-1}=-(\omega\,\mathrm{Im}(\tilde{E}))^{-1}$, and real parts of E, $\mathrm{Re}(E)=(\omega/2)\mathrm{Re}(\tilde{E})$, in units of ω^{-1} and $\omega/2$, respectively. We see that with the increasing electric field the lifetime initially decreases, which is a commonly accepted result. We observe, however, that at a particular value for the electric field the lifetime starts increasing, approaches its maximum, and then monotonically decreases. In both presented cases the real part of E remains positive and is just below the third Landau level of energy $5\omega/2$ or above the second one of energy $3\omega/2$. In Fig. 3 we show the position of these poles of the Green's function in the complex energy plane. Only

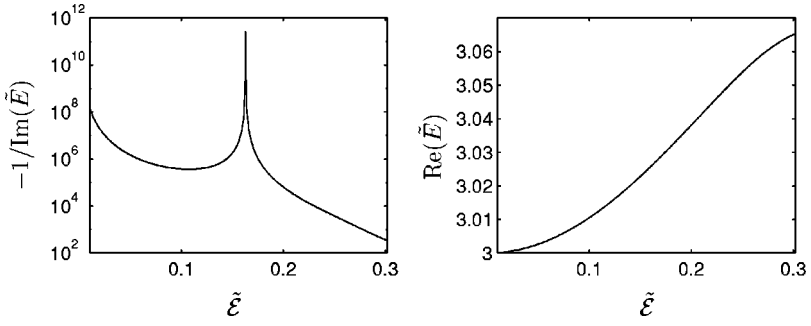

FIG. 2. The same as in Fig. 1 but for $\tilde{E}_B=-2.8$. The stabilization occurs for $\tilde{\mathcal{E}}=0.163$ for a resonance state located just above the second Landau level.

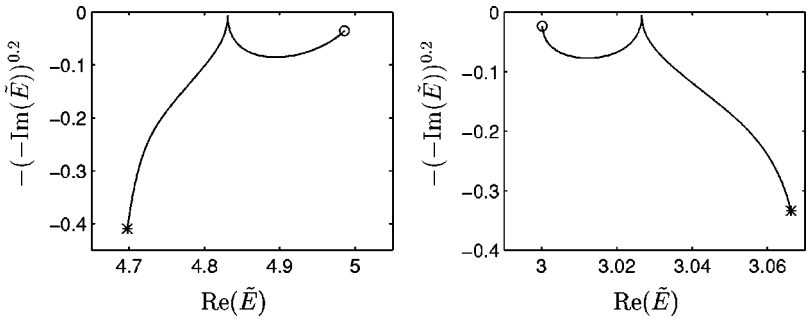

FIG. 3. Shows the trajectories of two resonances considered in Figs. 1 and 2 in the complex energy plane. For the visual purpose the imaginary part is raised to the power 1/5. The left frame corresponds to the binding energy $\tilde{E}_B=-6.4$ and the right one to $\tilde{E}_B=-2.8$. The circle marks the minimum value $\tilde{\mathcal{E}}=0.01$, whereas the asterisk indicates the maximum value $\tilde{\mathcal{E}}=3.1$. The stabilization occurs for $\tilde{\mathcal{E}}=0.132$, $\mathrm{Re}(\tilde{E})=4.83$, $\mathrm{Im}(\tilde{E})=-0.111\times10^{-10}$ and $\tilde{\mathcal{E}}=0.163$, $\mathrm{Re}(\tilde{E})=3.0266$, $\mathrm{Im}(\tilde{E})=-0.398\times10^{-11}$, respectively.

for the visual purpose the imaginary part is raised to the power 1/5. We see that with an increasing electric field the poles in the beginning depart from the real axis, but afterward start approaching it, reach minimum for the absolute value of the imaginary part of E (which appears to be almost equal to zero within the accuracy of our numerical calculation) and then again migrate downward. Such an unexpected nonmonotonic behavior happens for some particular values of the binding energies as well as the applied fields. At this point let us only mention that estimations of magnetic and electric fields show that they can be generated easily in experimental setups.

What we have checked in our numerical investigations is that the stabilization occurs only for states which are close to the excited Landau levels and does not appear for states near the first Landau level. Indeed, for very small electric fields resonances considered in this paper approach the second and the third Landau levels, i.e., the excited ones. This appears to be a general rule that the electric field generates new resonance states in a close vicinity of *excited* Landau levels. These states differ from the ones considered by Prange[7] and reinvestigated by Cavalcanti and de Carvalho.[11] In their case, when the electric field is switched off, the point interaction modifies only Landau states with the vanishing angular momentum, because only for these states the wave function does not vanish at the origin. The states with a nonzero angular momentum, i.e., the vortex Landau states, for which the wave functions explicitly depend on the polar angle φ and vanish at the origin, are not affected by a point interaction. The situation changes if a small electric field is applied. Then the vortex Landau states acquire small contributions which do not vanish at the origin, as follows for instance from perturbation theory. Hence, the interaction with a contact potential does not vanish, and apart from the well-known states considered previously[7,11] new resonance states emerge close to the excited Landau levels. These are the states for which the stabilization takes place. Since the wave function of them for small electric fields is predominantly composed of the vortex Landau states of nonzero angular momentum, therefore, one can call them the vortex resonance states. This fact suggests that the stabilization presented in this paper is due to the angular motion of electrons around the impurity, as it also happens in the classical considerations for a repulsive potential.[13] The analysis presented above can be applied to weak electric fields. For strong nonperturbative electric fields we can rather rely on the exact numerical analysis of this problem with the hope that the picture above still remains valid. However, the almost total suppression of ionization rates for some particular values of the electric field hardly can be explained only in terms of classical physics and we expect that its origin is due to complicated quantum interference effects which can only be studied numerically.

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Pseudo-Hermiticity versus *PT*-symmetry III: Equivalence of pseudo-Hermiticity and the presence of antilinear symmetries

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We show that a diagonalizable (non-Hermitian) Hamiltonian H is pseudo-Hermitian if and only if it has an antilinear symmetry, i.e., a symmetry generated by an invertible antilinear operator. This implies that the eigenvalues of H are real or come in complex conjugate pairs if and only if H possesses such a symmetry. In particular, the reality of the spectrum of H implies the presence of an antilinear symmetry. We further show that the spectrum of H is real if and only if there is a positive-definite inner-product on the Hilbert space with respect to which H is Hermitian or alternatively there is a pseudo-canonical transformation of the Hilbert space that maps H into a Hermitian operator. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1489072]

I. INTRODUCTION

The main reason for the recent interest in PT-symmetry[1] is that the eigenvalues of every PT-symmetric Hamiltonian are real or come in complex conjugate pairs. In particular, if the PT-symmetry is exact, the spectrum of the Hamiltonian is real. In Ref. 2, we introduced the concept of a pseudo-Hermitian operator and showed that the remarkable spectral properties of the PT-symmetric Hamiltonians follow from their pseudo-Hermiticity. Under the assumption of the diagonalizability (equivalently the existence of a complete biorthonormal set of energy eigenvectors), we obtained in Ref. 3 a complete characterization of all the (non-Hermitian) Hamiltonians that have a real spectrum. Here we also pointed out that the spectral properties of the PT-symmetric Hamiltonians are common to all Hamiltonians possessing an antilinear symmetry (a symmetry generated by an invertible antilinear operator). Therefore, at least for the class of diagonalizable Hamiltonians, presence of an antilinear symmetry implies pseudo-Hermiticity of the Hamiltonian. The main purpose of the present article is to show that the converse of this statement holds as well, that is, pseudo-Hermiticity of a Hamiltonian implies the existence of an antilinear symmetry. A direct consequence of this result is that if the spectrum of the Hamiltonian is real, then the system has an antilinear symmetry, PT-symmetry being the prime example.

The organization of the article is as follows. Section II includes a brief review of the necessary results reported in the companion articles.[2,3] Section III examines anti-pseudo-Hermiticity (pseudo-Hermiticity with an antilinear automorphism.) Here we prove that every (non-Hermitian) diagonalizable Hamiltonian is anti-pseudo-Hermitian and that the pseudo-Hermiticity of the Hamiltonian implies the presence of an antilinear symmetry. Section IV offers a description of the Hamiltonians with a real spectrum in terms of certain associated Hermitian operators. Section V presents a summary of the main results and the concluding remarks.

Throughout this article we shall consider (non-Hermitian) Hamiltonians H that are diagonalizable and have a discrete spectrum. As we explain below, this means that these Hamiltonians admit a complete biorthonormal set of eigenvectors $\{(|\psi_n,a\rangle,|\phi_n,a\rangle)\}$. The latter satisfy the following defining relations:[4]

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$$H|\psi_n,a\rangle=E_n|\psi_n,a\rangle,\quad H^\dagger|\phi_n,a\rangle=E_n^*|\phi_n,a\rangle, \tag{1}$$

$$\langle\phi_m,b|\psi_n,a\rangle=\delta_{mn}\delta_{ab}, \tag{2}$$

$$\sum_n\sum_{a=1}^{d_n}|\psi_n,a\rangle\langle\phi_n,a|=1, \tag{3}$$

where n and a are, respectively, the spectral and degeneracy labels, d_n is the multiplicity (degree of degeneracy) of E_n, $\dagger$ and $*$, respectively, denote the adjoint and complex-conjugate, δ_{mn} stands for the Kronecker delta function, and 1 is the identity operator. In view of Eqs. (1)–(3), we also have

$$H=\sum_n\sum_{a=1}^{d_n}E_n|\psi_n,a\rangle\langle\phi_n,a|,\quad H^\dagger=\sum_n\sum_{a=1}^{d_n}E_n^*|\phi_n,a\rangle\langle\psi_n,a|. \tag{4}$$

In order to see the equivalence of the existence of a complete biorthonormal set of eigenvectors of H and its diagonalizability, we note that by definition a diagonalizable Hamiltonian H satisfies $A^{-1}HA=H_0$ for an invertible linear operator A and a diagonal linear operator H_0, i.e., there is an orthonormal basis $\{|n,\alpha\rangle\}$ in the Hilbert space and complex numbers E_n such that $H_0=\Sigma_n\Sigma_\alpha E_n|n,\alpha\rangle\langle n,\alpha|$. Then letting $|\psi_n,\alpha\rangle:=A|n,\alpha\rangle$ and $|\phi_n,\alpha\rangle:=(A^{-1})^\dagger|n,\alpha\rangle$, we can easily check that $\{|\psi_n,\alpha\rangle,|\psi_n,\alpha\rangle\}$ is a complete biorthonormal system for H. The converse is also true, for if such a system exists we may set $A:=\Sigma_n\Sigma_\alpha|\psi_n,\alpha\rangle\langle n,\alpha|$ for some orthonormal basis $\{|n,\alpha\rangle\}$ and check that $A^{-1}=\Sigma_n\Sigma_\alpha|n,\alpha\rangle\langle\phi_n,\alpha|$ and $A^{-1}HA=H_0$, i.e., H is diagonalizable.

We would like to emphasize that the diagonalizability condition may be viewed as a physical requirement without which an energy eigenbasis would not exist. To our knowledge all known non-Hermitian Hamiltonians that are used in physical applications are diagonalizable and therefore admit a complete biorthonormal set of eigenvectors. This in particular includes all the Hermitian Hamiltonians as well as the non-Hermitian Hamiltonians used in ionization optics,[5] the study of dissipative systems and resonant states,[6] two-component formulation of the minisuperspace quantum cosmology,[7] and also the PT-symmetric Hamiltonians whose spectral properties have been obtained using numerical methods.

II. PSEUDO-HERMITICITY

Let $H:\mathcal{H}\to\mathcal{H}$ be a linear operator acting in a Hilbert space $\mathcal{H}$ and $\eta:\mathcal{H}\to\mathcal{H}$ be a linear Hermitian automorphism (invertible transformation). Then the η-pseudo-Hermitian adjoint of H is defined by[2]

$$H^\sharp:=\eta^{-1}H^\dagger\eta. \tag{5}$$

H is said to be pseudo-Hermitian with respect to η or simply η-pseudo-Hermitian if $H^\sharp=H$. H is said to be pseudo-Hermitian if it is pseudo-Hermitian with respect to some linear Hermitian automorphism η.

The basic properties of pseudo-Hermitian operators are discussed in Refs. 2 and 3. Here we survey the properties that we shall make use of in this article. Let $H:\mathcal{H}\to\mathcal{H}$ be a diagonalizable linear operator. Then

(i) H is pseudo-Hermitian if and only if its eigenvalues are real or come in complex-conjugate pairs;[2] and

(ii) if H is pseudo-Hermitian with respect to two linear Hermitian automorphisms η_1 and η_2, then $\eta_1^{-1}\eta_2$ generates a symmetry of H, i.e., $[H,\eta_1^{-1}\eta_2]=0$.[2]

III. ANTI-PSEUDO-HERMITICITY

We first recall that a function $\tau:\mathcal{H}\to\mathcal{H}$ acting in a (complex) Hilbert space $\mathcal{H}$ is said to be an antilinear operator if for all $a,b\in\mathbb{C}$ and $|\xi\rangle,|\zeta\rangle\in\mathcal{H}$,

$$\tau(a|\xi\rangle+b|\zeta\rangle)=a^*\tau|\xi\rangle+b^*\tau|\zeta\rangle. \tag{6}$$

An antilinear operator $\tau:\mathcal{H}\to\mathcal{H}$ is said to be anti-Hermitian[8] if for all $|\xi\rangle,|\zeta\rangle\in\mathcal{H}$,

$$\langle\zeta|\tau|\xi\rangle=\langle\xi|\tau|\zeta\rangle. \tag{7}$$

Definition 1: A linear operator $H:\mathcal{H}\to\mathcal{H}$ acting in a Hilbert space $\mathcal{H}$ is said to be anti-pseudo-Hermitian if there is an antilinear anti-Hermitian automorphism $\tau:\mathcal{H}\to\mathcal{H}$ satisfying

$$H^\dagger=\tau H\tau^{-1}. \tag{8}$$

We begin our analysis by giving a characterization of antilinear anti-Hermitian operators with respect to which a given linear operator is anti-pseudo-Hermitian.

Theorem 1: Let $\mathcal{H}$ be a Hilbert space and $H:\mathcal{H}\to\mathcal{H}$ be a diagonalizable linear operator with a discrete spectrum and a complete biorthonormal set of eigenvectors $\{(|\psi_n,a\rangle,|\phi_n,a\rangle)\}$. Then $\tau:\mathcal{H}\to\mathcal{H}$ is an antilinear anti-Hermitian operator and H is τ-anti-pseudo-Hermitian if and only if there are symmetric invertible matrices $c^{(n)}$ with entries $c^{(n)}_{ab}$ such that for all $|\zeta\rangle\in\mathcal{H}$,

$$\tau|\zeta\rangle=\sum_n\sum_{a,b=1}^{d_n}c^{(n)}_{ab}\langle\zeta|\phi_n,a\rangle\,|\phi_n,b\rangle. \tag{9}$$

Proof: Suppose that $\tau:\mathcal{H}\to\mathcal{H}$ is a given antilinear anti-Hermitian operator and H is τ-anti-pseudo-Hermitian, i.e., (8) or equivalently

$$H^\dagger\tau=\tau H \tag{10}$$

holds. Letting both sides of (10) act on $|\psi_n,a\rangle$ and using (1) and (6), we have

$$H^\dagger(\tau|\psi_n,a\rangle)=E_n^*(\tau|\psi_n,a\rangle).$$

Comparing this equation with the second equation in (1), we find

$$\tau|\psi_n,a\rangle=\sum_{b=1}^{d_n}c^{(n)}_{ba}|\phi_n,b\rangle, \tag{11}$$

where $c^{(n)}_{ab}$ are defined by

$$c^{(n)}_{ab}:=\langle\psi_{n,a}|\tau|\psi_n,a\rangle. \tag{12}$$

We can also express (11) in the form

$$\langle\psi_m,b|\tau|\psi_n,a\rangle=\delta_{mn}c^{(n)}_{ba}. \tag{13}$$

Next note that because τ is an invertible operator, the matrix $c^{(n)}=(c^{(n)}_{ab})$ formed by $c^{(n)}_{ab}$ is nonsingular. In fact, applying $\langle\phi_{n,c}|\tau^{-1}$ to both sides of (11) and using (6) and the fact that τ^{-1} is also antilinear, we have

$$(c^{(n)^{-1}})_{ab}=\langle\phi_n,a|\tau^{-1}|\phi_n,b\rangle^*. \tag{14}$$

Furthermore, in view of (12) and (7), $c^{(n)}$ is a symmetric matrix. Now let $|\zeta\rangle$ be an arbitrary element of $\mathcal{H}$ and use (13), (3) and (7) to compute

$$\sum_n \sum_{a,b=1}^{d_n} c^{(n)}_{ab} \langle \zeta | \phi_n, a\rangle \, |\phi_n, b\rangle = \sum_{n,m} \sum_{a,b=1}^{d_n} |\phi_m, b\rangle \langle \zeta | \phi_n, a\rangle \langle \psi_n, a | \tau | \psi_m, b\rangle$$

$$= \sum_m \sum_b |\phi_m, b\rangle \langle \zeta | \tau | \psi_m, b\rangle$$

$$= \sum_m \sum_b |\phi_m, b\rangle \langle \psi_m, b | \tau | \zeta\rangle$$

$$= \tau |\zeta\rangle.$$

This establishes (9). Next, suppose that $c^{(n)}$ are given invertible symmetric matrices and τ is defined by (9). Then the antilinearity of τ follows from the antilinearity of the inner-product in its first entry. The following simple calculation shows that τ is anti-Hermitian. For all $|\xi\rangle, |\zeta\rangle \in \mathcal{H}$,

$$\langle \xi | \tau | \zeta\rangle = \sum_n \sum_{a,b=1}^{d_n} c^{(n)}_{ab} \langle \zeta | \phi_n, a\rangle \langle \xi | \phi_n, b\rangle$$

$$= \sum_n \sum_{a,b=1}^{d_n} c^{(n)}_{ab} \langle \zeta | \phi_n, b\rangle \langle \xi | \phi_n, a\rangle$$

$$= \sum_n \sum_{a,b=1}^{d_n} c^{(n)}_{ab} \langle \xi | \phi_n, a\rangle \langle \zeta | \phi_n, b\rangle$$

$$= \langle \zeta | \tau | \xi\rangle,$$

where we used (9) and the fact that $c^{(n)}$ are symmetric. In order to establish the τ-anti-pseudo-Hermiticity of H we first observe that (9) implies

$$\tau^{-1} |\zeta\rangle = \sum_n \sum_{a,b=1}^{d_n} (c^{(n)})^{-1*}_{ab} \langle \zeta | \psi_n, a\rangle \, |\psi_n, b\rangle. \tag{15}$$

This can be easily checked by applying τ to the right-hand side of (15) and using (9), (2), and (3) to show that the result is $|\zeta\rangle$. Next, we note that applying both sides of (9) to $|\psi_n, a\rangle$ we recover (11). Finally, we use (9), (15), (6), (1), (4), and (11) to compute, for all $|\zeta\rangle \in \mathcal{H}$,

$$\tau H \tau^{-1} |\zeta\rangle = \tau \sum_n \sum_{a,b=1}^{d_n} c^{(n)-1*}_{ab} \langle \zeta | \psi_n, a\rangle \, E_n |\psi_n, b\rangle$$

$$= \sum_n \sum_{a,b=1}^{d_n} E^*_n c^{(n)-1}_{ab} \langle \zeta | \psi_n, a\rangle^* \tau |\psi_n, b\rangle$$

$$= \sum_n \sum_{a,b,c=1}^{d_n} E^*_n \langle \psi_n, a | \zeta\rangle c^{(n)}_{ca} c^{(n)-1}_{ab} |\phi_n, c\rangle$$

$$= \sum_n \sum_{b=1}^{d_n} E^*_n |\phi_n, b\rangle \langle \psi_n, b | \zeta\rangle = H^\dagger |\zeta\rangle.$$

Therefore, $\tau H \tau^{-1} = H^\dagger$. □

We should emphasize that, unlike the case of pseudo-Hermitian Hamiltonians, the anti-pseudo-Hermiticity does not restrict the energy spectrum. In fact, we can use Theorem 1 to prove the following.

Corollary 1: Every diagonalazable linear operator $H:\mathcal{H}\to\mathcal{H}$ with a discrete spectrum is anti-pseudo-Hermitian.

Proof: Let $\{(|\psi_n,a\rangle,|\phi_n,a\rangle)\}$ be a complete biorthonormal set of eigenvectors, and $\tau:\mathcal{H}\to\mathcal{H}$ be defined by (9) with $c^{(n)}=1$ for all n, i.e., for all $|\zeta\rangle\in\mathcal{H}$,

$$\tau|\zeta\rangle:=\sum_n\sum_{a=1}^{d_n}\langle\zeta|\phi_n,a\rangle\,|\phi_n,a\rangle. \tag{16}$$

Then according to Theorem 1, τ is an antilinear anti-Hermitian operator and H is τ-anti-pseudo-Hermitian. □

Corollary 2: Every diagonalizable pseudo-Hermitian linear operator $H:\mathcal{H}\to\mathcal{H}$ with a discrete spectrum has an antilinear symmetry.

Proof: Let H be pseudo-Hermitian. Then according to Corollary 1 it is also anti-pseudo-Hermitian, i.e., there are a linear Hermitian automorphism $\eta:\mathcal{H}\to\mathcal{H}$ and an antilinear anti-Hermitian automorphism $\tau:\mathcal{H}\to\mathcal{H}$ such that

$$\eta H\eta^{-1}=H^\dagger=\tau H\tau^{-1}. \tag{17}$$

Hence, $[H,\eta^{-1}\tau]=0$. Clearly $\eta^{-1}\tau$ is an antilinear operator. □

Theorem 2: Let $H:\mathcal{H}\to\mathcal{H}$ be a diagonalizable linear operator acting in a Hilbert space $\mathcal{H}$ with a discrete spectrum. Then the following are equivalent.

(1) The eigenvalues of H are real or come in complex-conjugate pairs.
(2) H is pseudo-Hermitian.
(3) H has an antilinear symmetry.

Proof: The equivalence of (1) and (2) was established in Ref. 2; Corollary 2 shows that (2) implies (3); the fact that (3) implies (1) follows from a simple calculation given in Ref. 3. □

A class of PT-symmetric Hamiltonians is given by

$$H=\frac{p^2}{2m}+V_1(x)+iV_2(x), \tag{18}$$

where V_1 and V_2 are, respectively, even and odd real-valued functions and the classical phase space is assumed to be real, i.e., x and p are the standard Hermitian operators representing the position and momentum of a particle of mass m. As we point out in Ref. 2, the Hamiltonian (18) is P-pseudo-Hermitian. It is also easy to check that it is T-anti-pseudo-Hermitian. The P-pseudo-Hermiticity and T-anti-pseudo-Hermiticity of this Hamiltonian implies its $P^{-1}T=PT$ symmetry. In general, there are PT-symmetric Hamiltonians H that are neither P-pseudo-Hermitian nor T-anti-pseudo-Hermitian. According to Theorem 2, if we make the physical assumption that H is diagonalizable, so that it admits a complete biorthonormal set of energy eigenvectors, then H must be pseudo-Hermitian with respect to a linear Hermitian automorphism η. It turns out that the choice of η is not unique. But fixing an antilinear anti-Hermitian operator τ with respect to which H is anti-pseudo-Hermitian [namely, (9)], we can express η in terms of PT and τ according to

$$\eta=\tau PT. \tag{19}$$

One can easily check that PT-symmetry ($[PT,H]=0$) and anti-pseudo-Hermiticity (8) imply pseudo-Hermiticity of H with respect to (19).

Next we consider a general diagonalizable Hamiltonian H with a discrete spectrum and a symmetry generated by a general invertible antilinear operator X,

$$[H,X]=0. \tag{20}$$

The antilinearity of X implies η-pseudo-Hermiticity of H with respect to some linear Hermitian automorphism η. The anti-pseudo-Hermiticity of H with respect to an antilinear automorphism of the form (9) always holds. Hence Eqs. (17) are valid. Taking the adjoint of both sides of (20) and making use of (17), we can easily show that $X_\eta^\sharp := \eta^{-1} X \eta$ and $X_\tau^\sharp := \tau^{-1} X \tau$ commute with H, i.e., they generate antilinear symmetries of the system as well.

IV. NON-HERMITIAN HAMILTONIANS WITH A REAL SPECTRUM

We first recall the following results which we reported in Refs. 2 and 3.

(1) The (indefinite) inner-product defined by

$$\forall |\xi\rangle, |\zeta\rangle \in \mathcal{H}, \quad \langle\langle \xi|\zeta\rangle\rangle := \langle \xi|\eta|\zeta\rangle, \tag{21}$$

is invariant under the evolution generated by an η-pseudo-Hermitian Hamiltonian H.[2] It is also easy to check that such a Hamiltonian is Hermitian with respect to the (indefinite) inner-product (21). See also Ref. 9.

(2) A diagonalizable (non-Hermitian) Hamiltonian has a real spectrum if and only if it is pseudo-Hermitian with respect to a linear Hermitian automorphism of the form

$$\eta = OO^\dagger, \tag{22}$$

where $O:\mathcal{H}\to\mathcal{H}$ is a linear automorphism.[3]

These statements suggest the following characterization of the (non-Hermitian) Hamiltonians with a real spectrum. See also Ref. 10.

Theorem 3: A diagonalizable Hamiltonian H acting in a Hilbert space $\mathcal{H}$ has a real spectrum if and only if there is a positive-definite inner-product on $\mathcal{H}$ with respect to which H is Hermitian.

Proof: Suppose H has a real spectrum so that it is $OO^\dagger$-pseudo-Hermitian for a linear automorphism $O:\mathcal{H}\to\mathcal{H}$. Then the inner-product (21) with $\eta = OO^\dagger$ is clearly a positive-definite inner-product with respect to which H is Hermitian. Conversely, suppose that there is a positive-definite inner-product $(\ ,\ )$ with respect to which H is Hermitian. Then treating the spectral problem for H in the Hilbert space $\mathcal{H}$ with the inner-product $(\ ,\ )$, we find that H has a real spectrum.

Corollary: Suppose that H has an antilinear symmetry X. If X is an exact symmetry of H, then there is a positive-definite inner product on $\mathcal{H}$ with respect to which H is Hermitian. □

Proof: Exactness of an antilinear symmetry implies reality of the spectrum of H.[3] The conclusion then follows from Theorem 3. □

Next we give an alternative and in a sense equivalent characterization of the (non-Hermitian) Hamiltonians with a real spectrum.

Definition 2: Consider a quantum system with the Hilbert space $\mathcal{H}$ and the Hamiltonian $H:\mathcal{H}\to\mathcal{H}$. Then a linear automorphism $A:\mathcal{H}\to\mathcal{H}$ is said to be a *pseudo-canonical transformation* for the system if for all $|\zeta\rangle \in \mathcal{H}$ the transformation

$$|\zeta\rangle \to |\tilde{\zeta}\rangle := A|\zeta\rangle \tag{23}$$

leaves the Schrödinger equation,

$$i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle \tag{24}$$

form-invariant. A unitary pseudo-canonical transformation is called a (quantum) canonical transformation.[11]

Clearly the defining condition for a pseudo-canonical transformation implies the following transformation rule for the Hamiltonian:

$$H \to \tilde{H} := AHA^{-1} + i\dot{A}A^{-1}, \tag{25}$$

where a dot denotes a time-derivative. For a time-independent pseudo-canonical transformation A, the second term on the right-hand side of (25) drops and H transforms as

$$H\to\tilde{H}:=AHA^{-1}. \tag{26}$$

Theorem 4: A diagonalizable time-independent Hamiltonian H has a real spectrum if and only if there is a pseudo-canonical transformation that maps H into a Hermitian operator.

Proof: Suppose that H has a real spectrum. Then it is $OO^\dagger$-pseudo-Hermitian for a linear automorphism $O:\mathcal{H}\to\mathcal{H}$, i.e., $H^\dagger=OO^\dagger H(OO^\dagger)^{-1}$. Let $A:=O^\dagger$. Then, in view of (26) and the preceding equation, we have

$$\tilde{H}^\dagger=(AHA^{-1})^\dagger=(A^{-1})^\dagger H^\dagger A^\dagger=(A^{-1})^\dagger A^\dagger AHA^{-1}(A^\dagger)^{-1}A^\dagger=AHA^{-1}=\tilde{H}.$$

Hence the transformed Hamiltonian is Hermitian. Conversely suppose that there is a pseudo-canonical transformation $A:\mathcal{H}\to\mathcal{H}$ under which H transforms to a Hermitian Hamiltonian $\tilde{H}$ and let $O:=A^\dagger$. Then using (26) and $\tilde{H}^\dagger=\tilde{H}$, we have

$$OO^\dagger H(OO^\dagger)^{-1}=A^\dagger AA^{-1}\tilde{H}A(A^\dagger A)^{-1}=A^\dagger\tilde{H}^\dagger(A^\dagger)^{-1}=(A^{-1}\tilde{H}A)^\dagger=H^\dagger.$$

Therefore, H is $OO^\dagger$-pseudo-Hermitian, and its spectrum is real. □

Corollary: Suppose that H has an antilinear symmetry X. If X is an exact symmetry of H, then there is a pseudo-canonical transformation that maps H into a Hermitian operator.

Proof: Exactness of an antilinear symmetry implies reality of the spectrum of H.[3] The conclusion then follows from Theorem 4. □

V. DISCUSSION AND CONCLUSION

In this article we established the equivalence of the notion of pseudo-Hermiticity and presence of an antilinear symmetry for the class of diagonalizable (non-Hermitian) Hamiltonians. This required the study of pseudo-Hermiticity with respect to antilinear anti-Hermitian automorphisms. It turned that the latter does not restrict the choice of the Hamiltonian and such antilinear automorphisms always exist. In fact, we obtained the general form of these automorphisms. For a fixed complete biorthonormal eigenbasis, they are determined in terms of a sequence of complex symmetric matrices $c^{(n)}$. The choice of unity for all these matrices leads to a canonical antilinear anti-Hermitian automorphism, namely (16). Under an invertible transformation u of the basis

$$|\psi_n,a\rangle\to\sum_{b=1}^{d_n}u_{ba}|\psi_n,b\rangle,\quad |\phi_n,a\rangle\to\sum_{b=1}^{d_n}(u^{-1\dagger})_{ba}|\phi_n,b\rangle$$

that preserves its completeness and biorthonormality, the matrices $c^{(n)}$ transform according to

$$c^{(n)}\to u^{*t}c^{(n)}u^*=u^\dagger c^{(n)}u^{\dagger t},$$

where ^{t} denotes the transpose. We can transform to a basis where a general τ has the canonical form (16) if we can find invertible matrices $v=u^{-1\dagger}$ satisfying $c^{(n)}=vv^t$. As shown in Ref. 12 this is always possible. Therefore, up to the choice of the biorthonormal eigenbasis, τ is actually unique.

A simple consequence of our findings is that the reality of the spectrum of a Hamiltonian implies the presence of an antilinear symmetry. In view of the proof of Corollary 2 and Eq. (9) of this article and Eq. (23) of Ref. 2, we have in fact an explicit expression for the generator of such a symmetry in terms of the biorthonormal eigenvectors of the Hamiltonian. We also gave two characterizations of Hamiltonians with real spectrum. These characterizations show how a Hamiltonian with a real spectrum may be related to an associated Hermitian Hamiltonian. Another simple implication of our analysis is that every Hermitian Hamiltonian has an antilinear symmetry.

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Energy levels and wave functions of vector bosons in a homogeneous magnetic field

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We aimed to obtain the energy levels of massive spin-1 particles moving in a constant magnetic field. The method used here is completely algebraic. In the process to obtain the energy levels the wave function is expressed in terms of Laguerre polynomials. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The problem of finding the states of a spinning particle moving in an external field has been solved for many different situations. The relativistic wave equation of spin-1 particles was at first derived by Kemmer in 1939.[1] Kemmer theory gives an entirely different aspect of the mesons. It is similar to the Dirac's equation of the electron. The similarity is very striking and the method investigated by Kemmer yields more than a mere restatement of the others. Kemmer equation is a Dirac type equation but involves matrices obeying a different scheme of commutation rules. These rules were first given by Duffin.[2] The theory can be developed in strikingly close correspondence to Dirac's electron theory; practically all the definitions of physical quantities like spin, magnetic moment etc., have their exact counterpart.

There are various wave equations to describe the spin-1 particles given in literature.[3–6] The methods used in these equations are quite complicated and give different results when they are compared. The method of Shay and Good is to expand the six-component wave function in terms of complete set of functions. This method leads to an invariant way to find the matrix elements, and it allows for arbitrary magnetic dipole moment and electric quadrupole moment of the particle. The eigenvalues of Shay and Good's equation have been obtained by Krase, Lu, and Good by using the quite complicated conventional method of solving the differential equation. A general method of obtaining the energy levels of any spin theory has been proposed by Tsai and Yildiz. They went on to obtain the energy levels of the spin-1 theory of Proca and Kemmer and observed that spin-1 theory is consistent only when there is no anomalous magnetic moment coupling.

The generally accepted method of approach is to define the Lagrange equation of motion and use the differential equation techniques to solve for the eigenfunctions and eigenvalues of the system. This method becomes complicated when higher spinning particles are handled.

In this study by starting from the Kemmer equation we used an algebraic method for obtaining the energy levels of massive spin-1 particles without anomolous magnetic moment moving in a homogeneous magnetic field.

The method we used does not require an explicit solution of the equation. The massive spin-1 particle will be considered as a two-identical particle system of spin-1/2 instead of a single spin-1 particle. This is the second quantization approach of Schrödinger applied to this problem. In the process to obtain the energy levels of the massive spin-1 particles, the solutions of spin-1/2 particles moving in a homogeneous magnetic field are used. The solutions of the Dirac equation in a magnetic field have been found in terms of Laguerre polynomials.[7] Since Kemmer matrices are expressed in terms of Dirac matrices and a massive spin-1 particle is considered as a two-identical fermion system, we used the Kemmer equation for obtaining the energy spectrum. To introduce

the method we first used it to obtain the energy levels of spin-1/2 particles moving in a homogeneous magnetic field in Sec. II. In the Conclusion we compared our results with the previous results and saw that they were in agreement with them.

The vector potential we used is

$$\vec{A}=-\tfrac{1}{2}yB\hat{x}+\tfrac{1}{2}xB\hat{y}, \tag{1}$$

where B is constant.

II. ENERGY SPECTRUM OF SPIN-1/2 PARTICLES

Covariant form of the Dirac equation for a spin-1/2 particle moving in an external field is

$$(\gamma^{\mu}\pi_{\mu}-M)\Psi(x)=0, \tag{2}$$

where γ^{μ} are 4×4 Dirac matrices; $\pi_{\mu}=(P_0-eA_0,\vec{P}-e\vec{A})$ is electrodynamical four-momentum vector; M is the mass of spin-1/2 particle, $\Psi(x)$ is the four-component spinor; $A^{\mu}=(A_0,\vec{A})$ is the four-vector electromagnetic potential and e is the charge of the electron. In the writing of the equation the Heaviside units $c=\hbar=1$ were used. The gamma matrices are given in the form

$$\gamma^0=\beta=\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \vec{\gamma}=\beta\vec{\alpha}, \tag{3}$$

$$\vec{\alpha}=\gamma^0\vec{\gamma}=\begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}. \tag{4}$$

Equation (2) can be written as

$$(\vec{\alpha}\cdot\vec{\pi}+\beta M+e\Phi)\Psi(x)=\pi_0\Psi(x). \tag{5}$$

For steady states if we choose the wave function in the form

$$\Psi(x_0=t,\ \vec{x})=e^{-iEt}\begin{pmatrix} \varphi(\vec{x}) \\ \chi(\vec{x}) \end{pmatrix} \tag{6}$$

and use $\vec{\alpha}$ matrices, Eq. (5) takes the following form

$$\begin{pmatrix} M+e\Phi & \vec{\sigma}\cdot\vec{\pi} \\ \vec{\sigma}\cdot\vec{\pi} & -M+e\Phi \end{pmatrix}\begin{pmatrix} \varphi(\vec{x}) \\ \chi(\vec{x}) \end{pmatrix}=E\begin{pmatrix} \varphi(\vec{x}) \\ \chi(\vec{x}) \end{pmatrix}. \tag{7}$$

If the particle is chosen to be moving in a homogeneous magnetic field then $A_0=\Phi=0$. Since the particle is rotating around z-axis with a θ angle in the xy-plane and going forward in the z direction the geometry of the problem is cylindrically symmetrical.

By defining φ and χ as

$$\varphi=\begin{pmatrix} \varphi_+ \\ \varphi_- \end{pmatrix}, \quad \chi=\begin{pmatrix} \chi_+ \\ \chi_- \end{pmatrix}, \tag{8}$$

Eq. (7) takes the following form:

$$\begin{pmatrix} (E-M) & 0 & -P_z & -\pi_- \\ 0 & (E-M) & -\pi_+ & P_z \\ -P_z & -\pi_- & (E+M) & 0 \\ -\pi_+ & P_z & 0 & (E+M) \end{pmatrix}\begin{pmatrix} \varphi_+ \\ \varphi_- \\ \chi_+ \\ \chi_- \end{pmatrix}=0, \tag{9}$$

where φ_+ and χ_+ are the solutions with positive frequency and φ_- and χ_- are with negative frequency. Helicity raising and lowering operators are defined in cylindrical coordinates as

$$\pi_+ = \pi_1 + i\pi_2 = e^{i\theta}\left[-i\frac{\partial}{\partial\rho} + \frac{1}{\rho}\frac{\partial}{\partial\theta} - \frac{iB\rho e}{2}\right], \tag{10}$$

$$\pi_- = \pi_1 - i\pi_2 = e^{-i\theta}\left[-i\frac{\partial}{\partial\rho} - \frac{1}{\rho}\frac{\partial}{\partial\theta} + \frac{iB\rho e}{2}\right]. \tag{11}$$

The exact solutions of Dirac equation for a homogeneous magnetic field are given in terms of Laguerre polynomials. Before obtaining the energy levels of spin-1/2 particles we must note that the effect of helicity raising and lowering operators on Laguerre polynomials are given as follows:

(i) for $m>0$,

$$\pi_+ L_N^{|m|}(x)F_m(\rho,\theta,z) = 2i\omega^{1/2}x^{1/2}L_{N-1}^{|m|+1}(x)F_{m+1}(\rho,\theta,z), \tag{12}$$

$$\pi_- L_N^{|m|}(x)F_m(\rho,\theta,z) = -2iN\omega^{1/2}x^{-1/2}L_{N+1}^{|m|-1}(x)F_{m-1}(\rho,\theta,z), \tag{13}$$

and

(ii) for $m<0$

$$\pi_+ L_N^{|m|}(x)F_m(\rho,\theta,z) = -2i(N+|m|)\omega^{1/2}x^{1/2}L_N^{|m|-1}(x)F_{m+1}(\rho,\theta,z), \tag{14}$$

$$\pi_- L_N^{|m|}(x)F_m(\rho,\theta,z) = 2i\omega^{1/2}x^{1/2}L_N^{|m|+1}(x)F_{m-1}(\rho,\theta,z), \tag{15}$$

where m is quantum number of the system and

$$F_m(\rho,\theta,z) = (\sqrt{x})^{|m|}e^{im\theta+iP_z z-(x/2)}, \tag{16}$$

$$x = \frac{eB}{2}\rho^2. \tag{17}$$

The other index of Laguerre polynomials is defined in the form

$$N = \frac{1}{4\omega}(E^2 - M^2 - P_z^2) + \frac{(m-|m|)}{2}, \quad \text{for} \quad m>0, \tag{18}$$

$$N = \frac{1}{4\omega}(E^2 - M^2 - P_z^2) + \frac{(m-|m|-2)}{2}, \text{for} \quad m<0. \tag{19}$$

There are two possible cases due to spin orientations in magnetic field and each of them are related with the positive and negative values of m quantum number. Finally we have four different situations for the spin-1/2 particle:

Situation 1: Spin is parallel to the magnetic field and $m>0$.

If we choose the wave function in the form

$$\Psi = \begin{bmatrix} L_N^{|m|}(x)F_m(\rho,\theta,z) \\ 0 \\ c_1 L_N^{|m|}(x)F_m(\rho,\theta,z) \\ d_1 L_{N-1}^{|m|+1}(x)F_{m+1}(\rho,\theta,z) \end{bmatrix} \tag{20}$$

and use it in Eq. (9) we obtain the energy spectrum and c_1, d_1 coefficients as follows:

$$E_{\uparrow,m>0}^2 = P_z^2 + M^2 + 4\omega(N-1), \tag{21}$$

$$c_1=\frac{P_z}{(E+M)}, \tag{22}$$

$$d_1=\frac{2i\omega^{1/2}x^{1/2}}{(E+M)}. \tag{23}$$

Situation 2: Spin is parallel to the magnetic field and $m<0$.
If we choose the wave function in the form

$$\Psi=\begin{bmatrix} L_N^{|m|}(x)F_m(\rho,\theta,z) \\ 0 \\ c_2L_N^{|m|}(x)F_m(\rho,\theta,z) \\ d_2L_N^{|m|-1}(x)F_{m+1}(\rho,\theta,z) \end{bmatrix} \tag{24}$$

and use it in Eq. (9) we obtain the energy spectrum and c_2, d_2 coefficients as follows:

$$E^2_{\uparrow,m<0}=P_z^2+M^2+4\omega(N+|m|), \tag{25}$$

$$c_2=\frac{P_z}{(E+M)}, \tag{26}$$

$$d_2=\frac{-2i(N+|m|)\omega^{1/2}x^{-1/2}}{(E+M)}. \tag{27}$$

Situation 3: Spin is anti-parallel to the magnetic field and $m>0$.
If we choose the wave function in the form

$$\Psi=\begin{bmatrix} 0 \\ L_N^{|m|}(x)F_m(\rho,\theta,z) \\ c_3L_{N+1}^{|m|-1}(x)F_{m-1}(\rho,\theta,z) \\ d_3L_N^{|m|}(x)F_m(\rho,\theta,z) \end{bmatrix} \tag{28}$$

and use it in Eq. (9) we obtain the energy spectrum and c_3, d_3 coefficients as follows:

$$E^2_{\downarrow,m>0}=P_z^2+M^2+4\omega N, \tag{29}$$

$$c_3=\frac{-2iN\omega^{1/2}x^{-1/2}}{(E+M)}, \tag{30}$$

$$d_3=\frac{-P_z}{(E+M)}. \tag{31}$$

Situation 4: Spin is anti-parallel to the magnetic field and $m<0$.
If we choose the wave function in the form

$$\Psi=\begin{bmatrix} 0 \\ L_N^{|m|}(x)F_m(\rho,\theta,z) \\ c_4L_N^{m+1}(x)F_{m-1}(\rho,\theta,z) \\ d_4L_N^{|m|}(x)F_m(\rho,\theta,z) \end{bmatrix} \tag{32}$$

and use it in Eq. (9) we obtain the energy spectrum and c_4, d_4 coefficients as follows:

$$E^2_{\downarrow,m<0}=P_z^2+M^2+4\omega(N+|m|+1), \tag{33}$$

$$c_4=\frac{2i\omega^{1/2}x^{1/2}}{(E+M)}, \tag{34}$$

$$d_4=\frac{-P_z}{(E+M)}. \tag{35}$$

It can be seen that these results are in agreement with the results given in Ref. 7.

III. ENERGY SPECTRUM OF MASSIVE SPIN-1 PARTICLES

For massive spin-1 particles the Kemmer equation is given in the form

$$(\beta^\mu\pi_\mu-\tilde{M})\Psi_K(x)=0, \tag{36}$$

where 16×16 Kemmer matrices β^μ are given as

$$\beta^\mu=\gamma^\mu\otimes I+I\otimes\gamma^\mu \tag{37}$$

with the usual γ^μ Dirac matrices. $\tilde{M}$ is the total mass of two identical spin-1/2 particles and $\Psi_K(x)$ is the 16-component wave function of the Kemmer equation.

Since massive spin-1 particle will be considered as two-identical spin-1/2 particles, the wave function can be rewritten in the form

$$\Psi_K(x)=\Psi_D\otimes\Psi_D=\begin{pmatrix}A\\B\\C\\D\end{pmatrix}, \tag{38}$$

where $\Psi_D(x)$ is the solution of Dirac equation which was given in Sec. II and A, B, C, D are four component spinors given as

$$A=\begin{pmatrix}A_+\\A_0\\A_{\tilde{o}}\\A_-\end{pmatrix}=\begin{pmatrix}\varphi_+\varphi_+\\\varphi_+\varphi_-\\\varphi_-\varphi_+\\\varphi_-\varphi_-\end{pmatrix},\quad B=\begin{pmatrix}B_+\\B_0\\B_{\tilde{o}}\\B_-\end{pmatrix}=\begin{pmatrix}\varphi_+\chi_+\\\varphi_+\chi_-\\\varphi_-\chi_+\\\varphi_-\chi_-\end{pmatrix}, \tag{39}$$

$$C=\begin{pmatrix}C_+\\C_0\\C_{\tilde{o}}\\C_-\end{pmatrix}=\begin{pmatrix}\chi_+\varphi_+\\\chi_+\varphi_-\\\chi_-\varphi_+\\\chi_-\varphi_-\end{pmatrix},\quad D=\begin{pmatrix}D_+\\D_0\\D_{\tilde{o}}\\D_-\end{pmatrix}=\begin{pmatrix}\chi_+\chi_+\\\chi_+\chi_-\\\chi_-\chi_+\\\chi_-\chi_-\end{pmatrix}.$$

In these matrices the left and right elements of the right matrix indicate first and second particles, respectively. In this case we can see the following equalities:

$$B_0=C_{\tilde{o}},\quad B_{\tilde{o}}=C_0,$$

$$A_0=A_{\tilde{o}},\quad D_0=D_{\tilde{o}}. \tag{40}$$

Therefore, the wave function of the massive spin-1 particle is a ten-component spinor.

After some algebra Kemmer equation takes the following form:

$$[(\gamma_1^0\otimes I_2+I_1\otimes\gamma_2^0)E-(\gamma_1^0\otimes\vec{\alpha}_2+\vec{\alpha}_1\otimes\gamma_2^0)\cdot\vec{\pi}-\tilde{M}\gamma_1^0\otimes\gamma_2^0]\begin{pmatrix}A\\B\\C\\D\end{pmatrix}=0. \tag{41}$$

We obtain four linear algebraic equations, ultimately 16 equations from Eq. (41):

$$(2E-\tilde{M})A-\vec{\sigma}_{(1)}\cdot\vec{\pi}C-\vec{\sigma}_{(2)}\cdot\vec{\pi}B=0, \tag{42}$$

$$\vec{\sigma}_{(2)}\cdot\vec{\pi}A-\vec{\sigma}_{(1)}\cdot\vec{\pi}D-\tilde{M}B=0, \tag{43}$$

$$\vec{\sigma}_{(1)}\cdot\vec{\pi}A-\vec{\sigma}_{(2)}\cdot\vec{\pi}D-\tilde{M}C=0, \tag{44}$$

$$(2E+\tilde{M})D-\vec{\sigma}_{(1)}\cdot\vec{\pi}B-\vec{\sigma}_{(2)}\cdot\vec{\pi}C=0, \tag{45}$$

where

$$\vec{\sigma}_{(1)}\cdot\vec{\pi}=(\vec{\sigma}\otimes I)\cdot\vec{\pi}=\begin{pmatrix}P_z & 0 & \pi_- & 0\\ 0 & P_z & 0 & \pi_-\\ \pi_+ & 0 & -P_z & 0\\ 0 & \pi_+ & 0 & -P_z\end{pmatrix}, \tag{46}$$

$$\vec{\sigma}_{(2)}\cdot\vec{\pi}=(I\otimes\vec{\sigma})\cdot\vec{\pi}=\begin{pmatrix}P_z & \pi_- & 0 & 0\\ \pi_+ & -P_z & 0 & 0\\ 0 & 0 & P_z & \pi_-\\ 0 & \pi_+ & \pi_+ & -P_z\end{pmatrix}. \tag{47}$$

By using these matrices in Eqs. (42)–(45) and eliminating one of the same equations we obtain ten linear algebraic equations in the form

$$(2E-\tilde{M})A_+-2P_zB_+-2\pi_-B_0=0, \tag{48}$$

$$(2E-\tilde{M})A_0-\pi_+B_+-\pi_-B_-+P_z(B_0-B_{\tilde{o}})=0, \tag{49}$$

$$(2E-\tilde{M})A_-+2P_zB_--2\pi_+B_{\tilde{o}}=0, \tag{50}$$

$$(2E-\tilde{M})D_+-2P_zB_+-2\pi_-B_{\tilde{o}}=0, \tag{51}$$

$$(2E-\tilde{M})D_0-\pi_+B_+-\pi_-B_-+P_z(B_{\tilde{o}}-B_0)=0, \tag{52}$$

$$(2E-\tilde{M})D_-+2P_zB_--2\pi_+B_0=0, \tag{53}$$

$$P_z(A_+-D_+)+\pi_-(A_0-D_0)-\tilde{M}B_+=0, \tag{54}$$

$$P_z(D_--A_-)+\pi_+(A_0-D_0)-\tilde{M}B_-=0, \tag{55}$$

$$P_z(A_0+D_0)+\pi_-A_--\pi_+D_+-\tilde{M}B_{\tilde{o}}=0, \tag{56}$$

$$P_z(A_0+D_0)-\pi_+A_++\pi_-D_-+\tilde{M}B_0=0. \tag{57}$$

In order to find the energy eigenvalues we will choose B_0 and $B_{\tilde{o}}$ in terms of Laguerre polynomials:

$$B_0 = L_N^{|m|}(x) F_m(\rho,\theta,z), \tag{58}$$

$$B_{\tilde{o}} = -L_N^{|m|}(x) F_m(\rho,\theta,z). \tag{59}$$

(i) For $m>0$:

If we use $B_0 = L_N^{|m|}(x) F_m(\rho,\theta,z)$ and $B_{\tilde{o}} = -L_N^{|m|}(x) F_m(\rho,\theta,z)$ in Eqs. (48)–(53) we find A, B, C, D spinors in the form

$$B = \begin{pmatrix} b_+ \omega^{1/2} x^{-1/2} L_{N+1}^{|m|-1}(x) F_{m-1}(\rho,\theta,z) \\ L_N^{|m|}(x) F_m(\rho,\theta,z) \\ -L_N^{|m|}(x) F_m(\rho,\theta,z) \\ b_- \omega^{1/2} x^{1/2} L_{N-1}^{|m|+1}(x) F_{m+1}(\rho,\theta,z) \end{pmatrix}, \tag{60}$$

$$C = \begin{pmatrix} b_+ \omega^{1/2} x^{-1/2} L_{N+1}^{|m|-1}(x) F_{m-1}(\rho,\theta,z) \\ -L_N^{|m|}(x) F_m(\rho,\theta,z) \\ L_N^{|m|}(x) F_m(\rho,\theta,z) \\ b_- \omega^{1/2} x^{1/2} L_{N-1}^{|m|+1}(x) F_{m+1}(\rho,\theta,z) \end{pmatrix}, \tag{61}$$

$$A = \begin{pmatrix} \dfrac{2}{2E-\tilde{M}} (P_z b_+ - 2iN) \omega^{1/2} x^{-1/2} L_{N+1}^{|m|-1}(x) F_{m-1}(\rho,\theta,z) \\ \dfrac{1}{2E-\tilde{M}} [2i\omega(b_+ - (N-1)b_-) - 2P_z] L_N^{|m|}(x) F_m(\rho,\theta,z) \\ \dfrac{1}{2E-\tilde{M}} [2i\omega(b_+ - (N-1)b_-) - 2P_z] L_N^{|m|}(x) F_m(\rho,\theta,z) \\ -\dfrac{2}{2E-\tilde{M}} (P_z b_- + 2i) \omega^{1/2} x^{1/2} L_{N-1}^{|m|+1}(x) F_{m+1}(\rho,\theta,z) \end{pmatrix}, \tag{62}$$

$$D = \begin{pmatrix} \dfrac{2}{2E+\tilde{M}} (P_z b_+ + 2iN) \omega^{1/2} x^{-1/2} L_{N+1}^{|m|-1}(x) F_{m-1}(\rho,\theta,z) \\ \dfrac{1}{2E+\tilde{M}} [2i\omega(b_+ - (N-1)b_-) + 2P_z] L_N^{|m|}(x) F_m(\rho,\theta,z) \\ \dfrac{1}{2E+\tilde{M}} [2i\omega(b_+ - (N-1)b_-) + 2P_z] L_N^{|m|}(x) F_m(\rho,\theta,z) \\ -\dfrac{2}{2E+\tilde{M}} (P_z b_- - 2i) \omega^{1/2} x^{1/2} L_{N-1}^{|m|+1}(x) F_{m+1}(\rho,\theta,z) \end{pmatrix}. \tag{63}$$

We obtain four algebraic equations given below by using these spinors in Eqs. (54)–(57):

$$\left[E^2 - P_z^2 - \frac{\tilde{M}^2}{4} - 2\omega N \right] b_+ + 2N(N-1)\omega b_- = 0, \tag{64}$$

$$\left[E^2 - P_z^2 - \frac{\tilde{M}^2}{4} - 2\omega(N-1) \right] b_- + 2\omega b_+ = 0, \tag{65}$$

$$\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}+4\omega\left(\frac{E}{\tilde{M}}-\left(N-\frac{1}{2}\right)\right)\right]+i\omega P_z(N-1)b_-+i\omega P_z b_+=0, \tag{66}$$

$$\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}-4\omega\left(\frac{E}{\tilde{M}}+\left(N-\frac{1}{2}\right)\right)\right]-i\omega P_z(N-1)b_--i\omega P_z b_+=0. \tag{67}$$

From Eqs. (64) and (66) we find

$$b_+=\frac{2N\omega\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}+4\omega\left(\frac{E}{\tilde{M}}-\left(N-\frac{1}{2}\right)\right)\right]}{i\omega P_z\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}-4\omega N\right]}, \tag{68}$$

$$b_-=\frac{-\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}+4\omega\left(\frac{E}{\tilde{M}}-\left(N-\frac{1}{2}\right)\right)\right]\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}-2\omega N\right]}{i\omega P_z(N-1)\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}-4\omega N\right].}. \tag{69}$$

If we substitute these into Eqs. (65) and (67) we obtain the energy levels as follows

$$E=\pm\frac{1}{2}\sqrt{4P_z^2+\tilde{M}^2+16\omega\left(N-\frac{1}{2}\right)}, \tag{70}$$

$$E=\frac{2\omega}{\tilde{M}}\pm\frac{1}{2}\sqrt{\frac{16\omega^2}{\tilde{M}^2}+\tilde{M}^2+4P_z^2+16\omega\left(N-\frac{1}{2}\right)}, \tag{71}$$

$$E=-\frac{2\omega}{\tilde{M}}\pm\frac{1}{2}\sqrt{\frac{16\omega^2}{\tilde{M}^2}+\tilde{M}^2+4P_z^2+16\omega\left(N-\frac{1}{2}\right)}. \tag{72}$$

(ii) For $m<0$:

If we use $B_0=L_N^{|m|}(x)F_m(\rho,\theta,z)$ and $B_{\tilde{o}}=-L_N^{|m|}(x)F_m(\rho,\theta,z)$ in Eqs. (48)–(53) we find A, B, C, D spinors in the form

$$B=\begin{pmatrix} b_+\omega^{1/2}x^{1/2}L_N^{|m|+1}(x)F_{m-1}(\rho,\theta,z) \\ L_N^{|m|}(x)F_m(\rho,\theta,z) \\ -L_N^{|m|}(x)F_m(\rho,\theta,z) \\ b_-\omega^{1/2}x^{-1/2}L_N^{|m|-1}(x)F_{m+1}(\rho,\theta,z)\end{pmatrix}, \tag{73}$$

$$C=\begin{pmatrix} b_+\omega^{1/2}x^{1/2}L_N^{|m|+1}(x)F_{m-1}(\rho,\theta,z) \\ -L_N^{|m|}(x)F_m(\rho,\theta,z) \\ L_N^{|m|}(x)F_m(\rho,\theta,z) \\ b_-\omega^{1/2}x^{-1/2}L_N^{|m|-1}(x)F_{m+1}(\rho,\theta,z)\end{pmatrix}, \tag{74}$$

$$A=\begin{pmatrix} \dfrac{2}{2E-\tilde{M}}(P_z b_+ +2i)\omega^{1/2}x^{1/2}L_N^{|m|+1}(x)F_{m-1}(\rho,\theta,z) \\ \dfrac{1}{2E-\tilde{M}}[-2i\omega(N+|m|+1)b_+ +2i\omega b_- -2P_z]L_N^{|m|}(x)F_m(\rho,\theta,z) \\ \dfrac{1}{2E-\tilde{M}}[-2i\omega(N+|m|+1)b_+ +2i\omega b_- -2P_z]L_N^{|m|}(x)F_m(\rho,\theta,z) \\ \dfrac{2}{2E-\tilde{M}}[-P_z b_- +2i(N+|m|)]\omega^{1/2}x^{-1/2}L_N^{|m|-1}(x)F_{m+1}(\rho,\theta,z) \end{pmatrix}, \tag{75}$$

$$D=\begin{pmatrix} \dfrac{2}{2E-\tilde{M}}(P_z b_+ -2i)\omega^{1/2}x^{1/2}L_N^{|m|+1}(x)F_{m-1}(\rho,\theta,z) \\ \dfrac{1}{2E-\tilde{M}}[-2i\omega(N+|m|+1)b_+ +2i\omega b_- +2P_z]L_N^{|m|}(x)F_m(\rho,\theta,z) \\ \dfrac{1}{2E-\tilde{M}}[-2i\omega(N+|m|+1)b_+ +2i\omega b_- +2P_z]L_N^{|m|}(x)F_m(\rho,\theta,z) \\ -\dfrac{2}{2E-\tilde{M}}[P_z b_- +2i(N+|m|)]\omega^{1/2}x^{-1/2}L_N^{|m|-1}(x)F_{m+1}(\rho,\theta,z) \end{pmatrix}. \tag{76}$$

We obtain four algebraic equations given below by using these spinors in Eqs. (54)–(57) in the form

$$\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}-2\omega(N+|m|+1)\right]b_+ +2\omega b_- =0 \tag{77}$$

$$\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}+4\omega\left(\frac{E}{\tilde{M}}-\left(N+|m|+\frac{1}{2}\right)\right)\right]-i\omega P_z b_- -i\omega\left(N+|m|+\frac{1}{2}\right)P_z b_+ =0, \tag{78}$$

$$\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}-4\omega\left(\frac{E}{\tilde{M}}+\left(N+|m|+\frac{1}{2}\right)\right)\right]+i\omega P_z b_- +i\omega\left(N+|m|+\frac{1}{2}\right)P_z b_+ =0, \tag{79}$$

$$\left[E^2-P_z^2-\frac{\tilde{M}^2}{4}-2\omega(N+|m|)\right]b_- +2\omega(N+|m|)(N+|m|+1)b_+ =0. \tag{80}$$

From Eqs. (77)–(79) we find

$$b_+ =\frac{2\omega\left[E^2-P_z^2-\dfrac{\tilde{M}^2}{4}-4\omega\left(\dfrac{E}{\tilde{M}}+\left(N+|m|+\dfrac{1}{2}\right)\right)\right]}{i\omega P_z\left[E^2-P_z^2-\dfrac{\tilde{M}^2}{4}-4\omega(N+|m|+1)\right]}, \tag{81}$$

$$b_- =\frac{-\left[E^2-P_z^2-\dfrac{\tilde{M}^2}{4}-4\omega\left(\dfrac{E}{\tilde{M}}+\left(N+|m|+\dfrac{1}{2}\right)\right)\right]\left[E^2-P_z^2-\dfrac{\tilde{M}^2}{4}-2\omega(N+|m|+1)\right]}{i\omega P_z\left[E^2-P_z^2-\dfrac{\tilde{M}^2}{4}-4\omega(N+|m|+1)\right]}. \tag{82}$$

If we substitute these into Eqs. (78)–(80) we obtain the energy levels as follows:

$$E=\pm\frac{1}{2}\sqrt{4P_z^2+\tilde{M}^2+16\omega\left(N+|m|+\frac{1}{2}\right)}, \tag{83}$$

$$E=\frac{2\omega}{\tilde{M}}\pm\frac{1}{2}\sqrt{\frac{16\omega^2}{\tilde{M}^2}+\tilde{M}^2+4P_z^2+16\omega\left(N+|m|+\frac{1}{2}\right)}, \tag{84}$$

$$E=-\frac{2\omega}{\tilde{M}}\pm\frac{1}{2}\sqrt{\frac{16\omega^2}{\tilde{M}^2}+\tilde{M}^2+4P_z^2+16\omega\left(N+|m|+\frac{1}{2}\right)}. \tag{85}$$

IV. CONCLUSIONS

There are several techniques developed for understanding the behavior of spin-1 particles moving in a constant magnetic field. These techniques are quite complicated. Because there is no availablity of experimental tests of these techniques we do not know which one is the best.

We used here a simple algebraic method for obtaining the energy levels of a massive spin-1 particle moving in a constant magnetic field. Spin-1 particle was considered as a two-identical fermion system and in the process to obtain the energy levels the wave functions of spin-1/2 particle which are written in terms of Laguerre polynomials were used.

The nonrelativistic approximation applies when the energies p_z^2/M and eB/M are small compared to the rest energy M. On taking the positive roots of E^2 to first order only, one finds, as approximations to Eqs. (70)–(72),

$$E=M+\frac{P_Z^2}{2M}+\frac{eB}{2M}(2N-1), \tag{86}$$

$$E=M+\frac{P_Z^2}{2M}+\frac{eB}{2M}(2N-1)+\frac{eB}{2M}(\pm 1), \tag{87}$$

and Eqs. (83)–(85),

$$E=M+\frac{P_Z^2}{2M}+\frac{eB}{2M}(2N+2|m|+1), \tag{88}$$

$$E=M+\frac{P_Z^2}{2M}+\frac{eB}{2M}(2N+2|m|+1)+\frac{eB}{2M}(\pm 1), \tag{89}$$

where we used $\tilde{M}=2M$. These are the exact results those obtained by Krase, Lu, and Good. The first of these energy spectra can be interpreted as corresponding to $m_s=0$ and the of second are for $m_s=\pm 1$. Our results are more general those were obtained by W. Tsai, W. Tsai, and A. Yildiz. They found the energy spectrum in the limit $\pi_3=0$, ultimately in two dimensions. In this limit the first of these energy spectra are the same as the result obtained by them, only $2N+2|m|$ has been replaced by $2n$ for $m<0$.

If the magnetic field is quite weak, we see that the difference of the second from the first energy level is $\pm eB/2M$. This is the interaction energy of the spin with the magnetic field. From these spectra we can see that the magnetic moment of the massive spin-1 particle is

$$\mu_s=(\pm 1)\frac{e}{\tilde{M}}. \tag{90}$$

The energy spectra given in Eqs. (87) and (89) can be interpreted as corresponding to the spins of particle and anti-particle being parallel and anti-parallel to the magnetic field, respectively. From these spectra it is seen that for all values of magnetic field the energy difference between the spin $s=1$ to $s=-1$ is equal to

$$\Delta E_{\pm}=\frac{eB}{M}. \tag{91}$$

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The propagator of the radial Dirac equation

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The propagator for the radial Dirac equation is explicitly constructed. It turns out to be a distribution of order zero, but it is shown that there exists no path-space measure associated with this equation. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1486263]

I. INTRODUCTION

It is always of interest to know whether or not there is a path-space measure associated with an initial-value problem for an evolution equation in mathematical physics, so that we may represent its solution by a path integral, that is, an integral with respect to a σ-additive set function defined on some σ-algebra of subsets of a suitable function space of ''paths.'' Then perturbations to the original equation have solutions represented by a path integral, too, and we can derive information about the solution by means of this representation.

A broad class of initial-value problems can be treated by semigroup theory, but the precise relationship of the idea of a path integral to these problems is somewhat ill-defined. Unfortunately, no such path-space measure exists as a mathematically rigorous measure associated with the Schrödinger equation, although it was with this equation in mind that Feynman conceived the very concept of *path integration* (Feynman, 1948).

However, as is well-known, for the imaginary-time Schrödinger equation, that is, the heat equation or more general evolution equations appearing in a Markov process in probability theory, the solution semigroup $S(t)$, $t\geqslant 0$, is a positivity preserving operator on some space $L^{\infty}(\Sigma)$ of bounded measurable functions on a certain set Σ, and there exists an associated path integral or path-space measure.

It is, roughly speaking, because there exists an integral kernel or transition function $p_t(x,dy)$ such that $S(t)$ is given by

$$(S(t)f)(x)=\int_{\Sigma}p_t(x,dy)f(y), \quad x\in\Sigma, \ \ t\geqslant 0,$$

for $f\in L^{\infty}(\Sigma)$ and that the bound $\|S(t)f\|_{\infty}\leqslant\|f\|_{\infty}$ holds for all $f\in L^{\infty}(\Sigma)$.

The aim of this article is to discuss this issue for the Dirac equation, in particular, the radial Dirac equation. Before going to the situation in three space dimensions, we first consider the Dirac operator D_1 with mass $m>0$ in one space dimension, defined in the space $L^2(\mathbb{R},\mathbb{C}^2)$ of $\mathbb{C}^2$-valued square-integrable functions in $\mathbb{R}$ by

$$D_1=\alpha\frac{1}{i}\frac{\partial}{\partial x}+m\beta, \tag{1}$$

for two (2×2) Hermitian matrices α and β satisfying $\alpha^2=\beta^2=1$ and $\alpha\beta+\beta\alpha=0$. Here and in the following, we are using a coordinate system where the speed of light c and Planck's constant

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$\hbar$ are equal to one. In Ichinose (1982, 1984) and Ichinose and Tamura (1984, 1987, and 1988), T. Ichinose and H. Tamura showed that the group of operators $e^{-iD_1 t}$, $t \in \mathbb{R}$, acting on $L^2(\mathbb{R},\mathbb{C}^2)$, is similar to a strongly continuous group $S(t)$ of operators for which the bound

$$\|S(t)f\|_\infty \leqslant e^{m|t|}\|f\|_\infty \tag{2}$$

holds for all $t \in \mathbb{R}$ and all bounded continuous functions $f = {}^t(f_1, f_2)$ in $L^2(\mathbb{R},\mathbb{C}^2)$, where $\|f\|_\infty = \max\{\|f_1\|_\infty, \|f_2\|_\infty\}$ stands for the norm of f as an element of the space $L^\infty(\mathbb{R},\mathbb{C}^2)$ of $\mathbb{C}^2$-valued bounded functions in $\mathbb{R}$, endowed with $\mathscr{C}^\infty$-norm on $\mathbb{C}^2$. As in the case of a Markov process above, the bound (2) is sufficient to ensure that there exist matrix-valued path-space measures $\nu_{x,t}$ such that

$$\int_\Omega \nu_{x,t}(d\omega) f(\omega(0)) = (e^{-itD_1} f)(x), \quad \text{almost all } x \in \mathbb{R}, \ t \geqslant 0, \tag{3}$$

for every bounded function f in $L^2(\mathbb{R},\mathbb{C}^2)$. It should be mentioned here that the integral kernel of e^{-itD_1} is a matrix-valued distribution of order zero or a matrix-valued *measure* in $\mathbb{R}\times\mathbb{R}$. For each $x \in \mathbb{R}$ and $t \geqslant 0$, the measure $\nu_{x,t}$, defined on the cylindrical σ-algebra of the space $\Omega_{x,t}$ of all paths $\omega:[0,t] \to \mathbb{R}$ with $\omega(t) = x$, takes values in the space $M_2(\mathbb{C})$ of (2×2) complex matrices. Further analysis in Ichinose and Tamura (1988) or Ichinose and Tamura (1987) shows that $\nu_{x,t}$ is a σ-additive Borel measure concentrated on the space $\Omega'_{x,t}$ of all Lipschitz-continuous paths $\omega:[0,t] \to \mathbb{R}$ with $\omega(t) = x$ and with velocity ± 1 and finitely many changes of direction in each finite time interval.

Initial-value problems for which the associated evolution $S(t)$, $t \geqslant 0$, satisfies a bound of the form (2) are comparatively rare. Together with the wave equation in one space dimension, the examples mentioned above are the most studied in the literature.

This article is concerned with $\mathbb{C}^2$-valued solutions $u(r,t)$ of the initial-value problem for the *radial Dirac equation*:

$$\frac{\partial u}{\partial t}(r,t) = -i(\tau_k u)(r,t), \quad u(r,0) = u_0(r), \tag{4}$$

for all $r \in \mathbb{R}_+ := (0,\infty)$ and $t \in \mathbb{R}$. The differential operator τ_k is defined for $k = \pm 1, \pm 2, \ldots$ by

$$\tau_k : u \mapsto \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_1'(r) \\ u_2'(r) \end{pmatrix} + \begin{pmatrix} m & -k/r \\ -k/r & -m \end{pmatrix} \begin{pmatrix} u_1(r) \\ u_2(r) \end{pmatrix}, \tag{5}$$

for suitably smooth $u \in L^2(\mathbb{R}_+,\mathbb{C}^2)$. The nonzero integer k represents an eigenvalue of the "spin-orbit operator" (see Thaller 1992, pp. 125–130). The radial Dirac operator (5) arises from the spin-angular momentum decomposition of the free Dirac operator in three space dimensions, defined as follows.

The *Dirac operator* D_3 in three space dimensions is defined in the space $L^2(\mathbb{R}^3,\mathbb{C}^4)$ of $\mathbb{C}^4$-valued square-integrable functions in $\mathbb{R}^3$ by means of the differential expression

$$D_3 = \sum_{j=1}^{3} \alpha_j \mathbf{p}_j + \alpha_4 m,$$

where $m > 0$ is the mass of the particle as in (1),

$$\mathbf{p}_j = \frac{1}{i}\frac{\partial}{\partial x_j}, \quad \alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \quad \text{for } j = 1,2,3,$$

with the *Pauli matrices*

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

and

$$\alpha_4=\begin{pmatrix}\sigma_0 & 0\\ 0 & -\sigma_0\end{pmatrix},\quad \text{with}\ \ \sigma_0=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.$$

Here we have taken the standard representation of the Dirac operator [Thaller, 1992), Eq. (1.213), p. 36]. Then via the spin-angular momentum decomposition, the operator D_3 is equal to the direct sum of operators unitarily equivalent to the operators (5) with $k=\pm 1,\pm 2,\ldots$.

The fact that τ_k defines a self-adjoint operator acting in $L^2(\mathbb{R}_+,\mathbb{C}^2)$ follows from the spin-angular momentum decomposition of D_3 (Thaller, 1992, Theorem 4.14), hence, $e^{-it\tau_k}$, $t\in\mathbb{R}$, is a strongly continuous unitary group of operators acting on $L^2(\mathbb{R}_+,\mathbb{C}^2)$.

The initial-value problem (4) is a worthy object of study, because on adding a Coulomb potential $\sigma_0 e/r$, $e\in\mathbb{R}$, to τ_1, we get an essentially self-adjoint operator if and only if $|e|\leqslant\sqrt{3}/2$ (Weidmann, 1987, Theorem 6.9). For $\sqrt{3}/2<|e|<1$, there is a distinguished self-adjoint extension. In this respect, the operator $\tau_1+\sigma_0 e/r$ has properties similar to the Laplacian plus an attractive potential proportional to $1/r^2$ treated by a Feynman path integral in Nelson (1964). For larger values of $|e|$ close to one, the boundary conditions near $r=0$ need to take into account the effects of the nuclear dimensions and particle pair-production in quantum field theory (Popov, 1971).

The initial-value problem (4) has a superficial appeal from the point of view of analysis by path integrals because of the following line of reasoning. The operator

$$i\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\frac{\partial}{\partial x}$$

is unitarily similar to the generator

$$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\frac{\partial}{\partial x} \tag{6}$$

of the direct sum of groups of translations acting on $L^\infty(\mathbb{R},\mathbb{C}^2)$. This is obviously a group of isometries of $L^\infty(\mathbb{R},\mathbb{C}^2)$.

For each $t\in\mathbb{R}$ and $r>0$, the matrix

$$\exp\left[-it\begin{pmatrix}m & -k/r\\ -k/r & -m\end{pmatrix}\right] \tag{7}$$

is unitary. The operator of multiplication by a function taking its values in the unitary (2×2) matrices is obviously an isometry of $L^\infty(\mathbb{R}_+,\mathbb{C}^2)$.

Thus, one might hope to apply the Trotter product formula

$$e^{-it\tau_k}=\lim_{N\to\infty}\left[\exp\left(\frac{-it}{N}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\frac{\partial}{\partial r}\right)\exp\left(\frac{-it}{N}\begin{pmatrix}m & -k/r\\ -k/r & -m\end{pmatrix}\right)\right]^N$$

to show that $e^{-it\tau_k}$ is $L^\infty(\mathbb{R}_+,\mathbb{C}^2)$-bounded and the operator norm is one. Standard arguments would then enable one to construct a σ-additive path-space measure associated with $e^{-it\tau_k}$, $t\in\mathbb{R}$. As seen in Ichinose and Tamura (1984), such a scalar measure representing $(e^{-it\tau_k}f,g)$ actually exists for states f and g with supports sufficiently separated from zero. The evidence seems to suggest that the initial-value problem (4) possesses a path-space measure.

However, the argument above is *false*. The mistake is as follows. In order that multiplication by the matrix-valued function (7) be unitary, we need to give $\mathbb{C}^2$ the usual Euclidean norm, that is, the ℓ^2-norm. But equipped with this norm, the operator

$$\exp\left[-it\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\frac{\partial}{\partial r}\right]$$

is *not* a contraction on $L^\infty(\mathbb{R}_+,\mathbb{C}^2)$ (to make sense of this exponential, a boundary condition at $r=0$ must be added). The group generated by (6) is a continuous group of isometries on $L^\infty(\mathbb{R},\mathbb{C}^2)$ only if we endow $\mathbb{C}^2$ with the *ℓ^∞-norm*.

The conflict between the two norms for $\mathbb{C}^2$ means that the Trotter product formula cannot be used in $L^\infty(\mathbb{R}_+,\mathbb{C}^2)$. Intuitively, we would *not* expect a path-space measure for (4) to exist, otherwise path-integrals would select a distinguished self-adjoint extension for *every* perturbation by a Coulomb potential $\sigma_0 e/r$ by virtue of a type of Feynman–Kac formula, whereas we know that an essentially self-adjoint perturbed operator exists only for $|e|\leqslant\sqrt{3}/2$. The main purpose of this work is to clarify the situation: we show in Sec. IV, Corollary 1, that the operator $e^{-it\tau_1}$ is not actually bounded on $L^\infty(\mathbb{R}_+,\mathbb{C}^2)$ for any $t\neq 0$.

It is not hard to see that $e^{-it\tau_1}$ *is* bounded on $L^p(\mathbb{R}_+,\mathbb{C}^2)$ for all $1<p<\infty$ and $t\in\mathbb{R}$. By contrast, for the Laplacian Δ in $\mathbb{R}^n$ and the Dirac operator D_3 in $\mathbb{R}^3$, for each $t\neq 0$, the operator $e^{it\Delta}$ is bounded on $L^p(\mathbb{R}^n)$ and the operator e^{-itD_3} is bounded on $L^p(\mathbb{R}^3,\mathbb{C}^4)$, only for $p=2$ (Hörmander, 1960; Brenner, 1966).

In order to obtain information about the group $e^{-it\tau_1}$, $t\in\mathbb{R}$, of operators, we need an explicit formula for the propagator, that is, the integral kernel $\mathcal{K}_t$ of the operator $e^{-it\tau_1}$ for each $t\in\mathbb{R}$. Although $e^{-it\tau_1}$ is a unitary operator acting on $L^2(\mathbb{R}_+,\mathbb{C}^2)$ for each $t\in\mathbb{R}$, its kernel $\mathcal{K}_t$ may well be a matrix-valued distribution defined on $\mathbb{R}_+\times\mathbb{R}_+$. Explicit formulas are known for the propagator of the group e^{-itD_3}, $t\in\mathbb{R}$ (Prosser, 1963; Vladimirov, 1971; Rosen, 1983; Brzeźniak, 1990). For each $t\neq 0$, this is a matrix-valued distribution of order one, from which it follows that there is no path-space measure associated with the Dirac equation in four space–time dimensions.

The main result of this article, given in Theorem 1 of Sec. IV, is an explicit formula for the propagator $\mathcal{K}_t$ associated with the radial Dirac equation. From this we deduce that there is no path-space measure associated with the radial Dirac equation like the one that exists for the Dirac equation in two space–time dimensions. More formally, we show that $e^{-it\tau_1}$ does not map $L^2(\mathbb{R}_+,\mathbb{C}^2)\cap L^\infty(\mathbb{R}_+,\mathbb{C}^2)$ into $L^\infty(\mathbb{R}_+,\mathbb{C}^2)$ for any $t\neq 0$. Nevertheless, a path integral approach to this equation is given in Jefferies (1994, 1996a) along the mathematical lines developed in Jefferies (1996b) for integration with respect to unbounded set functions.

Although the propagator associated with D_3 is a matrix-valued distribution of order one on $\mathbb{R}^3\times\mathbb{R}^3$, it is somewhat surprising to learn that $\mathcal{K}_t$ is a matrix-valued distribution of order *zero* on $\mathbb{R}_+\times\mathbb{R}_+$. In the course of the derivation of the formula for $\mathcal{K}_t$, it is apparent that averaging over the unit sphere smooths out the kernel.

It can be verified directly that $\partial/\partial t\mathcal{K}_t(r,\rho)=-i\tau_1\mathcal{K}_t(r,\rho)$, for all $r>0$, $\rho>0$, with $\mathcal{K}_0(r,\rho)=\delta(r-\rho)\sigma_0$ from the formula (19) for the distribution $\mathcal{K}_t$ we obtain in Sec. IV, but the proof of Theorem 1 may be applied to obtain the kernel of $e^{-it\tau_k}$ for integer values of k other than one.

A key part of our derivation is the representation (14) of the kernel of e^{-itD_3} obtained in Sec. III. The representation first appears in Rosen (1983), but we give a formal proof in Proposition 2. Using this representation, we obtain a regularization of e^{-itD_3} which preserves the reducing subspaces of D_3 with respect to the "spin-orbit" operator [Thaller, 1992, Eq. (4.105), p. 125]. The regularization simplifies our computations because we can deal with functions rather than distributions.

II. PRELIMINARIES

We first briefly fix some notation and terminology concerning function spaces and distributions.

A. Function notation

Let n be a positive integer. The sesquilinear inner product of $\mathbb{C}^n$ is denoted by $(\cdot,\cdot)$, which is linear in the first component and antilinear in the second. The corresponding inner product of two $\mathbb{C}^n$-valued functions $f(x)={}^t(f_1(x),\ldots,f_n(x))$ and $g(x)={}^t(g_1(x),\ldots,g_n(x))$ in $\mathbb{R}^d$ is denoted by

$$(f,g)=\int_{\mathbb{R}^d}(f(x),g(x))dx=\int_{\mathbb{R}^d}\sum_{j=1}^{n} f_j(x)\overline{g_j(x)}dx.$$

We shall also use the bilinear inner product $\langle\cdot,\cdot\rangle$.

For an open subset U of $\mathbb{R}^d$, $C_c^\infty(U,\mathbb{C}^n)$ denotes the space of $\mathbb{C}^n$-valued C^∞-functions with compact support in U. $\mathcal{S}(\mathbb{R}^d,\mathbb{C}^n)$ is the space of $\mathbb{C}^n$-valued rapidly decreasing C^∞ functions on $\mathbb{R}^d$. For $n=1$, they are the usual function spaces $C_c^\infty(U)$ and $\mathcal{S}(\mathbb{R}^d)$. The notation $C_0(\mathbf{R}^d,\mathbf{C}^n)$ is used for the space of $\mathbf{C}^n$-valued continuous functions vanishing at infinity on $\mathbb{R}^d$. It has the supremum norm.

For two locally convex topological linear spaces X and Y, $\mathcal{L}(X,Y)$ denotes the topological linear space of all continuous linear mappings of X into Y.

Since $\mathbb{C}^{n^2}$ is identified with the space $M_n(\mathbb{C})$ of $(n\times n)$ matrices, we denote the space of all $M_n(\mathbb{C})$-valued distributions with compact support in U by $\mathcal{L}(C_c^\infty(U),M_n(\mathbb{C}))$, which is the dual space of the space $C_c^\infty(U,M_n(\mathbb{C}))$. We denote also the space of $M_n(\mathbb{C})$-valued tempered distributions on $\mathbb{R}^d$ by $\mathcal{L}(\mathcal{S}(\mathbb{R}^d),M_n(\mathbb{C}))$, which is the dual space of the space $\mathcal{S}(\mathbb{R}^d,M_n(\mathbb{C}))$. For $n=1$, they are nothing but the usual spaces $C_c^\infty(U)'$ of Schwartz distributions in U, and $\mathcal{S}(\mathbb{R}^d)'$ of tempered distributions on $\mathbb{R}^d$.

B. Kernels of bounded linear operators

Let U be an open subset of $\mathbb{R}^d$. An $M_n(\mathbb{C})$-valued distribution K defined in $U\times U$, i.e., an element in $\mathcal{L}(C_c^\infty(U\times U),M_n(\mathbb{C}))$, is called the *integral kernel* or just the *kernel*, of a bounded linear operator T of $L^2(U,\mathbb{C}^n)$ into itself, if for every $f,g\in C_c^\infty(U)$ and $j,l=1,\ldots,n$, the equality

$$(T(fe_j),\overline{g}e_l)=(K(g\otimes f)e_j,e_l)$$

holds for the standard basis vectors $e_1,\ldots,e_n$ of $\mathbb{C}^n$. Here $g\otimes f$ is the function $(x,y)\mapsto g(x)f(y)$, $x,y\in U$. Thus, if $T:L^2(U,\mathbb{C}^n)\to L^2(U,\mathbb{C}^n)$ is a bounded linear operator and the $M_n(\mathbb{C})$-valued function $(x,y)\mapsto k(x,y)$, $x,y\in U$, is measurable and locally integrable in $U\times U$, then k is the kernel of T if, for every $f\in C_c^\infty(U)$ and $j=1,\ldots,n$, we have

$$T(fe_j)(x)=\int_U [k(x,y)e_j]f(y)dy$$

for almost all $x\in U$.

It follows that if k is a matrix-valued distribution defined in $\mathbb{R}$, i.e., an element of the space $\mathcal{L}(C_c^\infty(\mathbb{R}),M_n(\mathbb{C}))$, then the operator of convolution with respect to k has the distribution $k(x-y)$ defined in $\mathbb{R}^2$ as its kernel. The identity operator acting on $L^2(U,\mathbb{C}^n)$ has the distribution $\delta(x-y)I$ as its kernel. Here I is the $(n\times n)$ identity matrix and $\delta:f\mapsto f(0)$, $f\in C_c^\infty(\mathbb{R})$, is the Dirac distribution at zero.

III. REPRESENTATION OF THE PROPAGATOR OF THE DIRAC EQUATION

The kernel of e^{-itD_3} is known from Prosser (1963), Vladimirov (1971), Rosen (1983), and Brzeźniak (1990). It is simply obtained by applying the Dirac operator to the known propagator for the Klein–Gordon equation in four space–time dimensions [for the Klein–Gordon propagator, see, for example, De Jager (1963)].

The derivation of the kernel of $e^{-it\tau_1}$ is achieved by computing the restriction of the unitary operator e^{-itD_3} to the eigenspace corresponding to the eigenvalue $k=1$ of the "spin-orbit" operator [Thaller, 1992, Eq. (4.105), p. 125]. As we see below, the calculation is not entirely straightforward and the formula for the kernel is not simple.

We first obtain a representation of the kernel of e^{-itD_3} that simplifies the task of calculating its restriction to the eigenspace of the "spin-orbit" operator by looking at the Dirac equation in two space–time dimensions. The idea originates in Rosen (1983), where a certain one-dimensional character of the motion of a Dirac particle is emphasized.

A. The 1-D Dirac equation

The first statement is a simple consequence of perturbation theory for linear operators. It is the basis of the proof that there is a path-space measure associated with the Dirac equation in two space–time dimensions (Ichinose and Tamura, 1984). Although we have formula (9) below for the kernel of e^{-itD_1}, it is not obvious that it gives the operator bounds set out in Proposition 1 below.

Proposition 1: Let $\partial/\partial\xi$ be the operator acting in $L^2(\mathbb{R},\mathbb{C}^2)$, with domain $\mathcal{D}(\partial/\partial\xi)=H^1(\mathbb{R},\mathbb{C}^2)$ consisting of all functions $f={}^t(f_1,f_2)\in L^2(\mathbb{R},\mathbb{C}^2)$, for which f_1 and f_2 are absolutely continuous and f' is square-integrable.

Then the operator $-[\sigma_3\partial/\partial\xi+im\sigma_1]:\mathcal{D}(\partial/\partial\xi)\to L^2(\mathbb{R},\mathbb{C}^2)$ is the generator of a unitary group $e^{-t(\sigma_3\partial/\partial\xi+im\sigma_1)}$, $t\in\mathbb{R}$, such that for every $1\leqslant p\leqslant\infty$,

$$\|e^{-t(\sigma_3\partial/\partial\xi+im\sigma_1)}f\|_p\leqslant e^{m|t|}\|f\|_p,\quad t\in\mathbb{R},\tag{8}$$

for all $f\in L^2(\mathbb{R},\mathbb{C}^2)\cap L^p(\mathbb{R},\mathbb{C}^2)$.

Furthermore, the operator $e^{-t(\sigma_3\partial/\partial\xi+im\sigma_1)}$ leaves (the subspace) $C_0(\mathbb{R},\mathbb{C}^2)$ in $L^\infty(\mathbb{R},\mathbb{C}^2)$ invariant for each $t\in\mathbb{R}$.

Here note that whether a bound like (8) holds for every $1\leqslant p\leqslant\infty$ amounts essentially to the same thing as whether it holds for $p=1$ or $p=\infty$. Because if it holds for $p=1$ or $p=\infty$, by duality it also holds for the other p, and then for every $1\leqslant p\leqslant\infty$ by interpolation.

Proof of Proposition 1: The operator $\partial/\partial\xi$ is the infinitesimal generator of the group of translations on $L^2(\mathbb{R})$, so $\sigma_3\partial/\partial\xi$ acting in $L^2(\mathbb{R},\mathbb{C}^2)$ is the generator of that continuous group $T(t)$ of isometries on $L^2(\mathbb{R},\mathbb{C}^2)$ which maps the function $\xi\mapsto{}^t(f_1(\xi),f_2(\xi))$, $\xi\in\mathbb{R}$, to the function $\xi\mapsto{}^t(f_1(\xi+t),f_2(\xi-t))$, $\xi\in\mathbb{R}$.

Then $T(t)$ also defines a group of isometries $T_p(t)$ of $L^p(\mathbb{R},\mathbb{C}^2)$, for $1\leqslant p\leqslant\infty$. Clearly $T_p(t)$ is continuous for $1\leqslant p<\infty$. The group of isometries $T_\infty(t)$ leaves the space $C_0(\mathbb{R},\mathbb{C}^2)$ invariant, and defines a continuous group of isometries there.

Because $-im\sigma_1$ is a bounded perturbation of the operator $-\sigma_3\partial/\partial\xi$ acting in $L^p(\mathbb{R},\mathbb{C}^2)$ (or $C_0(\mathbb{R},\mathbb{C}^2)$), it follows from Reed and Simon (1975, Sec. X.2) that $-\sigma_3\partial/\partial\xi-im\sigma_1$ is the generator of a group $S(t)=e^{-t(\sigma_3\partial/\partial\xi+im\sigma_1)}$, $t\in\mathbb{R}$, of operators satisfying $\|S(t)\|\leqslant e^{m|t|}$, for all $t\in\mathbb{R}$. Here the same symbol $S(t)$ is used for the group of operators so defined on each space $L^p(\mathbb{R},\mathbb{C}^2)$, $1\leqslant p<\infty$, and $C_0(\mathbb{R},\mathbb{C}^2)$, and $\|\cdot\|$ denotes the operator norm of $\mathcal{L}(L^p(\mathbb{R},\mathbb{C}^2))$, for $1\leqslant p<\infty$, or of $\mathcal{L}(C_0(\mathbb{R},\mathbb{C}^2))$. □

In the following, we consider the case for $t>0$. Similar considerations apply to the case $t<0$. The integral kernel of the operator $e^{-t(\sigma_3\partial/\partial\xi+im\sigma_1)}$ is given [Ichinose and Tamura, 1984, (3.2)] by convolution with respect to the distribution

$$H(\xi,t)=\frac{1}{2}\left(\sigma_0\frac{\partial}{\partial t}-\sigma_3\frac{\partial}{\partial\xi}-im\sigma_1\right)J_0(m(t^2-\xi^2)^{1/2})\,\theta(t-|\xi|).$$

Here $J_0(t)$ is the Bessel function of order zero and θ is the Heaviside function—the characteristic function of the interval $[0,\infty)$. The distributional notation means that if $\phi:\mathbb{R}\to\mathbb{C}$ is a rapidly decreasing function, then $H(\cdot,t)(\phi)\in M_2(\mathbb{C})$ is the matrix

$$H(\cdot,t)(\phi)=\frac{1}{2}\int_{-t}^{t}\left[\left(\sigma_0\frac{\partial}{\partial t}-\sigma_3\frac{\partial}{\partial\xi}-im\sigma_1\right)J_0(m(t^2-\xi^2)^{1/2})\right]\phi(\xi)d\xi$$
$$+\frac{1}{2}(\phi(t)+\phi(-t))\sigma_0+\frac{1}{2}(\phi(t)-\phi(-t))\sigma_3. \tag{9}$$

Now the derivatives after the integral sign are interpreted in the pointwise sense. Then for each $t>0$, the convolution $H(\cdot,t)*\psi$ belongs to $C_0(\mathbb{R},\mathbb{C}^2)$ for every ψ belonging to the space $\mathcal{S}(\mathbb{R},\mathbb{C}^2)$ of rapidly decreasing $\mathbb{C}^2$-valued functions, and

$$[H(\cdot,t)*\psi](\xi)=[e^{-t(\sigma_3\partial/\partial\xi+im\sigma_1)}\psi](\xi),\quad \xi\in\mathbb{R}. \tag{10}$$

Since $dJ_0(t)/dt=-J_1(t)$ is bounded, it is clear from the representation (9) that $H(\cdot,t)$ is a matrix-valued distribution of order zero, that is, a matrix-valued measure, so we shall sometimes write $\int_{\mathbb{R}}H(d\xi,t)\phi(\xi)$ for (9) and $\int_{\mathbb{R}}H(d\eta,t)\psi(\xi-\eta)$ for (10). It follows from the representation (9) that for each $\xi\in\mathbb{R}$, the matrix-valued measure $H(d\xi,t)$ is supported by the interval $[-t,t]$.

B. The kernel of e^{-itD_3}

A bound like (8) with $p=\infty$ in Proposition 1 does not hold for the 3-D Dirac operator D_3, as noted in Ichinose (1984), because the initial-value problem for the hyperbolic system of the first order in $d+1$ space–time dimensions is L^∞ well-posed if and only if $d=1$ (cf. Brenner, 1966; Zastawniak, 1989; Brzeźniak, 1990). It is simply because the kernel of e^{-itD_3} is a distribution of order *one*, as is easily seen from the explicit representation obtained in Proposition 2 below.

It is convenient to take an equivalent representation of the Dirac operator D_3, so that

$$\alpha_j'=\begin{pmatrix}\sigma_j & 0\\ 0 & -\sigma_j\end{pmatrix},\quad \text{for } j=1,2,3,\quad \alpha_4'=\begin{pmatrix}0 & \sigma_0\\ \sigma_0 & 0\end{pmatrix}, \tag{11}$$

obtained from the Dirac matrices α_j by the similarity transformation $\alpha_j'=Q\alpha_jQ$, $j=1,2,3,4$, with

$$Q=2^{-1/2}\begin{pmatrix}\sigma_0 & \sigma_0\\ \sigma_0 & -\sigma_0\end{pmatrix}. \tag{12}$$

Let $\{e_1,e_2\}$ be the standard basis of $\mathbb{C}^2$. The tensor product $A\otimes B$ of two 2×2 matrices A and B is the 4×4 matrix of the associated linear transformation with respect to the basis $\mathcal{E}=\{e_1\otimes e_1,e_2\otimes e_1,e_1\otimes e_2,e_2\otimes e_2\}$ of $\mathbb{C}^4$. Linear transformations are identified with matrices with respect to these fixed bases. Then $\alpha_j'=\sigma_j\otimes\sigma_3$ for $j=1,2,3$ and $\alpha_4'=\sigma_0\otimes\sigma_1$ and, in this representation, the Dirac operator becomes

$$D_3=\sum_{j=1}^{3}(\sigma_j\otimes\sigma_3)\mathbf{p}_j+m\sigma_0\otimes\sigma_1. \tag{13}$$

The following result appears in Rosen (1983) in a somewhat compressed form. In the remainder of this section, we translate into the present notation and give a proof of this statement. We first give some additional notation.

Let μ_r be the uniform surface probability on the sphere S_r of radius $r>0$ in $\mathbb{R}^3$. For $r>0$, the μ_r-integral of a function f over S_r is denoted by $\mu_r(f)$. For a smooth function ϕ on $\mathbb{R}^3$, we have $\partial/\partial r\,\phi(x)=|x|^{-1}\langle x,\nabla\rangle\phi(x)$, $r=|x|\neq0$. For $r=0$, we understand $\mu_0=\delta$, the delta measure at $x=0$. For any $M_2(\mathbb{C})$-valued Borel measure λ on $\mathbb{R}$ and $M\in M_2(\mathbb{C})$, the set function $M\otimes\lambda:A\mapsto M\otimes[\lambda(A)]$, with A a Borel set in $\mathbb{R}$, is an $M_4(\mathbb{C})$-valued measure.

Proposition 2: Let D_3 be Dirac operator in the representation (13). *Then for each $t\in\mathbb{R}$, the operator e^{-itD_3} is convolution with respect to the matrix-valued distribution $K_t\in\mathcal{L}(\mathcal{S}(\mathbb{R}^3),M_4(\mathbb{C}))$ of order one, given for each test function $\phi\in\mathcal{S}(\mathbb{R}^3)$, by*

$$K_t(\phi)=\int_{-t}^{t}[\mu_{|\xi|}(\phi)+|\xi|\mu_{|\xi|}(\partial/\partial r\,\phi)][\sigma_0\otimes H(d\xi,t)]+\int_{-t}^{t}\xi\mu_{|\xi|}(\langle\sigma,\nabla\phi\rangle)\otimes H(d\xi,t), \tag{14}$$

or, as an $M_4(\mathbb{C})$*-valued distribution in* $\mathbb{R}^3$*, by*

$$K_t(x)=-\frac{1}{4\pi r}\sigma_0\otimes\left(\frac{\partial H(r,t)}{\partial r}+\frac{\partial H(-r,t)}{\partial r}\right)-\frac{1}{4\pi}\langle\sigma,\nabla\rangle\otimes\left(\frac{H(r,t)}{r}-\frac{H(-r,t)}{r}\right),\quad \text{for } r=|x|. \tag{15}$$

The representation (14) is proved by applying the Fourier transform $\mathcal{F}:L^2(\mathbb{R}^3)\to L^2(\mathbb{R}^3)$, defined for every $f\in L^2(\mathbb{R}^3)\cap L^1(\mathbb{R}^3)$ by

$$\mathcal{F}f(p)=\int_{\mathbb{R}^3}e^{-i\langle x,p\rangle}f(x)dx,\quad \text{for all } p\in\mathbb{R}^3.$$

Then $\mathcal{F}^{-1}f(x)=(2\pi)^{-3}\int_{\mathbb{R}^3}e^{i\langle x,p\rangle}f(p)\,dp$ defines the inverse operator. The same symbols are used for the operators defined on $L^2(\mathbb{R}^3,\mathbb{C}^n)$ by taking tensor products with the identity map on $\mathbb{C}^n$. Sometimes $\mathcal{F}f$ is written as $\hat{f}$ and $\mathcal{F}^{-1}f$ as $\check{f}$.

If $\Phi:\mathbb{R}^3\to M_n(\mathbb{C})$ is a matrix-valued Borel measurable function, then the operator of *multiplication* by Φ sends the element $f\in L^2(\mathbb{R}^3,\mathbb{C}^n)$ to $x\mapsto\Phi(x)f(x)$, $x\in\mathbb{R}^3$. This is a bounded linear operator on $L^2(\mathbb{R}^3,\mathbb{C}^n)$ if and only if Φ is essentially bounded.

The integral $\int_{\mathbb{R}^3}\Phi(x)\otimes\mu(dx)\in M_4(\mathbb{C})$ of a matrix-valued function $\Phi:\mathbb{R}^3\to M_2(\mathbb{C})$ with respect to an $M_2(\mathbb{C})$-valued Borel measure μ on $\mathbb{R}^3$ is taken componentwise with respect to the basis $\mathcal{E}$ of $\mathbb{C}^4$.

Lemma 1: The operator $\mathcal{F}e^{-itD_3}\mathcal{F}^{-1}$ *acting on* $L^2(\mathbb{R}^3,\mathbb{C}^4)$ *is the operator of multiplication by the matrix-valued function* $p\mapsto\int_{\mathbb{R}}e^{-i\langle\sigma,p\rangle\xi}\otimes H(d\xi,t)$, $p\in\mathbb{R}^3$, *where* $\sigma=(\sigma_1,\sigma_2,\sigma_3)$ *and* $\langle\sigma,p\rangle=\Sigma_{j=1}^{3}\sigma_j p_j$.

Proof: The integral converges because $H(d\xi,t)$ is a matrix-valued Borel measure on $\mathbb{R}$ and in the matrix norm $\|e^{-i\langle\sigma,p\rangle\xi}\|=1$ for all $\xi\in\mathbb{R}$ and $p\in\mathbb{R}^3$. By the functional calculus for the self-adjoint operator D_3, the operator $\mathcal{F}e^{-itD_3}\mathcal{F}^{-1}$ acting on $L^2(\mathbb{R}^3,\mathbb{C}^4)$ is the operator of multiplication by the matrix-valued function $p\mapsto e^{-it(\langle\sigma,p\rangle\otimes\sigma_3+m\sigma_0\otimes\sigma_1)}$, so it suffices to prove that

$$e^{-it(\langle\sigma,p\rangle\otimes\sigma_3+m\sigma_0\otimes\sigma_1)}=\int_{\mathbb{R}}e^{-i\langle\sigma,p\rangle\xi}\otimes H(d\xi,t). \tag{16}$$

To do so, rewrite the $M_4(\mathbb{C})$-valued function on the right-hand side by a formal integral with respect to $d\xi$:

$$w(p,t):=\int_{\mathbb{R}}e^{-i\langle\sigma,p\rangle\xi}\otimes H(\xi,t)d\xi,$$

each of whose (j,k) entries with $j,k=1,2$ makes sense as the bilinear inner product between a C^∞ function and a distribution with compact support in $\xi\in\mathbb{R}$. Then we have by (10)

$$\begin{aligned}\frac{\partial w(p,t)}{\partial t}&=-\int_{\mathbb{R}}e^{-i\langle\sigma,p\rangle\xi}\otimes\left(\sigma_3\frac{\partial}{\partial\xi}+im\sigma_1\right)H(\xi,t)d\xi\\&=-i\int_{\mathbb{R}}[\langle\sigma,p\rangle\otimes\sigma_3+m\sigma_0\otimes\sigma_1](e^{-i\langle\sigma,p\rangle\xi}\otimes H(\xi,t))d\xi\\&=-i[\langle\sigma,p\rangle\otimes\sigma_3+m\sigma_0\otimes\sigma_1]w(p,t).\end{aligned}$$

It follows that $w(p,t)$ is nothing but the left-hand side of Eq. (16). □

Lemma 2: The inverse Fourier transform of $p \mapsto e^{-i\langle \sigma,p\rangle \xi}$ *in the sense of distributions is* $\mu_{|\xi|} - \langle \nabla, x\rangle \mu_{|\xi|} - \xi\langle \sigma, \nabla\rangle \mu_{|\xi|}$ *for all* $\xi \in \mathbb{R}$.

Proof: The Fourier transform $p \mapsto \hat{\mu}_r(p)$, $p \in \mathbb{R}^3$, of μ_r is the function $p \mapsto \sin(r|p|)/r|p|$ [Vladimirov, 1971, p. 135, (38)] as may be seen by calculating $\hat{\mu}_r(p) = \int_{\mathbb{R}^3} e^{-i\langle x,p\rangle} \mu_r(dx)$ directly.

Suppose that $\xi \neq 0$. It follows from the commutation relations of the Pauli matrices $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ that $e^{-i\langle \sigma,p\rangle \xi} = \cos(|\xi||p|) - i\langle \sigma, p\rangle \xi \sin(|\xi||p|)/|\xi||p|$. The operation of multiplication of the Fourier transform $\hat{T}(p)$ of a distribution T by ip corresponds to taking the gradient ∇T of T, so $(i\langle \sigma, p\rangle \xi \sin(|\xi|\,|p|)/|\xi|\,|p|) = \xi\langle \sigma, \nabla\rangle \mu_{|\xi|}$.

The term $\cos(|\xi|\,|p|)$ can be expressed as

$$\cos(|\xi||p|) = \left[\frac{\partial}{\partial r} r \frac{\sin(|\xi| r)}{|\xi| r}\right]_{r=|p|} = \frac{\sin(|\xi||p|)}{|\xi||p|} + \langle p, \nabla\rangle \frac{\sin(|\xi||p|)}{|\xi||p|}.$$

The operation of forming the distribution $(1/i)\nabla \hat{T}$ from the Fourier transform $\hat{T}$ of a distribution T corresponds to multiplying the distribution $T(x)$ by $-x$, so taking the inverse Fourier transform gives $\cos(|\xi|\,|p|)^{\vee} = \mu_{|\xi|} - \langle \nabla, x\rangle \mu_{|\xi|}$ and we obtain the stated formula. In the case that $\xi = 0$, we have $-[\langle \nabla, x\rangle \mu_0](\phi) = \delta(r\partial/\partial r \phi) = 0$ for all $\phi \in \mathcal{S}(\mathbb{R}^3)$ and the formula still holds. □

Proof of Proposition 2: Let $t \in \mathbb{R}$. According to Lemma 1 the operator e^{-itD_3} corresponds to convolution with respect to the inverse Fourier transform $K_t \in \mathcal{L}(\mathcal{S}(\mathbb{R}^3), M_4(\mathbb{C}))$ of $p \mapsto \int_{\mathbb{R}} e^{-i\langle \sigma,p\rangle \xi} \otimes H(d\xi, t)$, $p \in \mathbb{R}^3$. The distribution K_t is evaluated as follows.

The map $\Phi: \xi \mapsto e^{-i\langle \sigma, \cdot\rangle \xi}$, $\xi \in \mathbb{R}$, may be viewed as a function taking its values in the space $\mathcal{L}(\mathcal{S}(\mathbb{R}^3), M_2(\mathbb{C}))$ of matrix-valued tempered distributions. An application of (the vector-valued) Fubini's theorem shows that for each $\phi \in \mathcal{S}(\mathbb{R}^3)$

$$K_t(\phi) = \int_{\mathbb{R}^3} \check{\phi}(p) \left[\int_{\mathbb{R}} e^{-i\langle \sigma,p\rangle \xi} \otimes H(d\xi, t)\right] dp = \int_{\mathbb{R}} [\Phi(\xi)^{\vee}(\phi)] \otimes H(d\xi, t).$$

By Lemma 2, $\Phi(\xi)^{\vee} = \mu_{|\xi|} - \langle \nabla, x\rangle \mu_{|\xi|} - \xi\langle \sigma, \nabla\rangle \mu_{|\xi|}$ for every $\xi \in \mathbb{R}$.

If $\phi \in \mathcal{S}(\mathbb{R}^3)$ is a test function, then

$$K_t(\phi) = \int_{\mathbb{R}} [\mu_{|\xi|}(\phi) + |\xi| \mu_{|\xi|}(\partial/\partial r \phi)] \sigma_0 \otimes H(d\xi, t) + \int_{\mathbb{R}} \xi \mu_{|\xi|}(\langle \sigma, \nabla\rangle \phi) \otimes H(d\xi, t),$$

so that Eq. (14) holds.

We now verify the representation (15) of the distribution K_t. Let $\phi \in \mathcal{S}(\mathbb{R}^3)$. In terms of the uniform probability measure μ_r on the sphere S_r with radius $r > 0$, we have

$$
\begin{aligned}
K_t(\phi) &= \int_{\mathbb{R}}\int_{S_{|\xi|}} \sigma_0 \otimes H(\xi,t)\,\phi(x)\,d\mu_{|\xi|}(x)\,d\xi + \int_{\mathbb{R}}\int_{S_{|\xi|}} |\xi|\sigma_0 \otimes H(\xi,t)\,\frac{\partial \phi}{\partial r}(x)\,d\mu_{|\xi|}(x)\,d\xi \\
&\quad + \int_{\mathbb{R}} \xi \int_{S_{|\xi|}} [(\langle \sigma,\nabla\rangle \phi)(x) \otimes H(\xi,t)]\,d\mu_{|\xi|}(x)\,d\xi \\
&= \int_0^\infty \int_{S_1} \sigma_0 \otimes [H(r,t)+H(-r,t)] \left[\frac{\partial}{\partial r} r\phi(r\omega)\right] d\mu_1(\omega)\,dr \\
&\quad + \int_0^\infty r \int_{S_1} [\langle \sigma,\nabla\rangle \phi](r\omega) \otimes [H(r,t)-H(-r,t)]\,d\mu_1(\omega)\,dr \\
&= -\int_{S_1}\int_0^\infty \sigma_0 \otimes \left[\frac{\partial H(r,t)}{\partial r} + \frac{\partial H(-r,t)}{\partial r}\right] \phi(r\omega)\,r\,dr\,d\mu_1(\omega) \\
&\quad - \int_0^\infty \int_{S_1} \phi(r\omega)(\langle \sigma,\nabla\rangle \otimes [r^{-1}H(r,t) - r^{-1}H(-r,t)])\,r^2\,d\mu_1(\omega)\,dr,
\end{aligned}
$$

using the change of variables $r=|x|$, $\omega = x/r$ for $x \in \mathbb{R}^3$ and Fubini's theorem. Here note that $d\mu_1(\omega) = (1/4\pi)\,d\omega$, with $d\omega$ the surface measure on S_1. □

IV. THE PROPAGATOR OF THE RADIAL DIRAC OPERATOR

In this section, we present the calculation of the kernel of the group generated by (the closure of) the operator $i\tau_1$ defined by (5). The characteristic function of the interval $[0,\infty)$ is denoted by θ. The open interval $(0,\infty)$ is written as $\mathbb{R}_+$.

The function $D(\xi,t) = \frac{1}{2} J_0(m\sqrt{t^2-\xi^2})\,\theta(t^2-\xi^2)$, $\xi \in \mathbb{R}$, $t \in \mathbb{R}$, is the solution, in the sense of distributions, of the initial-value problem

$$
\frac{\partial^2 g}{\partial t^2}(\xi,t) - \frac{\partial^2 g}{\partial \xi^2}(\xi,t) + m^2 g(\xi,t) = 0, \quad g(\xi,0) = 0, \quad \frac{\partial g}{\partial t}(\xi,0) = \delta(\xi), \tag{17}
$$

for the one-dimensional Klein–Gordon equation (Vladimirov, 1971).

For each $t \in \mathbb{R}$, let

$$
\begin{aligned}
E(\xi,t) &= \left(\frac{\partial}{\partial t} + im\right) D(\xi,t), \\
\overline{E}(\xi,t) &= \left(\frac{\partial}{\partial t} - im\right) D(\xi,t), \\
F(\xi,t) &= \frac{\partial D}{\partial \xi}(\xi,t)
\end{aligned} \tag{18}
$$

in the sense of distributions belonging to $C_c^\infty(\mathbb{R})'$. These distributions are of order zero and involve unit point masses at $\pm t$. Note that as $D(\cdot,t)$ is an even function, so are $E(\cdot,t)$ and $\overline{E}(\cdot,t)$, while $F(\cdot,t)$ is an odd function.

The following representation for the integral kernel $\mathcal{K}_t$ of $e^{-it\tau_1}$ holds.

Theorem 1: *For each $t \in \mathbb{R}\setminus\{0\}$, $\mathcal{K}_t$ is an $M_2(\mathbb{C})$-valued distribution defined in $\mathbb{R}_+ \times \mathbb{R}_+$, i.e., an element in $\mathcal{L}(C_c^\infty(\mathbb{R}_+ \times \mathbb{R}_+), M_2(\mathbb{C}))$ of order zero such that for all $f,g \in C_c^\infty(\mathbb{R}_+)$, the equality $\langle e^{-it\tau_1}(fe_j), \overline{g}e_k\rangle = \langle \mathcal{K}_t(g \otimes f)e_j, e_k\rangle$ holds for $j,k=1,2$ with respect to the standard basis vectors e_1, e_2 of $\mathbb{C}^2$.*

The distribution $e^{-it\tau_1}(r,\rho) := \mathcal{K}_t(r,\rho)$ is given by the matrix

$$\begin{pmatrix} \overline{E}(r-\rho,t)-\overline{E}(r+\rho,t) & iW_{12}(r,\rho;t) \\ -iW_{21}(r,\rho;t) & E(r-\rho,t)+E(r+\rho,t)-W_{22}(r,\rho;t) \end{pmatrix} \tag{19}$$

of distributions of order zero belonging to $C_c^\infty(\mathbb{R}_+\times\mathbb{R}_+)'$, *where*

$$W_{12}(r,\rho;t)=\left[F(r-\rho,t)+F(r+\rho,t)+\frac{1}{\rho}(D(r-\rho,t)-D(r+\rho,t))\right],$$

$$W_{21}(r,\rho;t)=\left[F(r-\rho,t)-F(r+\rho,t)-\frac{1}{r}(D(r-\rho,t)-D(r+\rho,t))\right],$$

$$W_{22}(r,\rho;t)=(r\rho)^{-1}\left(\frac{\partial}{\partial t}+im\right)\int_{|r-\rho|}^{r+\rho}D(\xi,t)\xi d\xi.$$

The differentiation in the t-variable is interpreted in the sense of distributions.

A. Regularization

Let $\xi\mapsto v(\xi)$ be a non-negative smooth even function in $\mathbb{R}$, with support in the interval $[-1,1]$ and with the property that $\int_{\mathbb{R}}v(\xi)d\xi=1$. Set $v(\xi)=\varepsilon^{-1}v(\xi/\varepsilon)$ for $\varepsilon>0$. Then the function $D_\varepsilon(\cdot,t)=v_\varepsilon^{*}D(\cdot,t)$ is the solution of the Klein-Gordon equation (17) but with the initial conditions $g(\xi,0)=0$ and $\partial g/\partial t(\xi,0)=v_\varepsilon(\xi)$, $\xi\in\mathbb{R}$. The function $(\xi,t)\mapsto D_\varepsilon(\xi,t)$, $\xi\in\mathbb{R}$, $t>0$, is smooth in ξ and t and for each $t>0$, the function $D_\varepsilon(\cdot,t)$ has support in the interval $[-(t+\varepsilon),t+\varepsilon]$.

Then, as $\varepsilon\to 0+$, the smooth matrix-valued function H_ε defined by

$$H_\varepsilon(\xi,t)=\left(\sigma_0\frac{\partial}{\partial t}-\sigma_3\frac{\partial}{\partial\xi}-im\sigma_1\right)D_\varepsilon(\xi,t),\quad \xi\in\mathbb{R},\ \ t\geqslant 0, \tag{20}$$

converges in the space $\mathcal{L}(\mathcal{S}(\mathbb{R}),M_2(\mathbb{C}))$ of matrix-valued distributions to the distribution $H(\xi,t)$ defined by formula (9). Furthermore, because $H(\xi,t)$ is actually a distribution of order zero with compact support, as $\varepsilon\to 0+$, the matrix-valued measure $H_\varepsilon(\xi,t)d\xi$ converges to $H(d\xi,t)$ in the topology of the Banach space $\mathcal{L}(C_b(\mathbb{R}),M_2(\mathbb{C}))$ of all continuous linear mappings of $C_b(\mathbb{R})$ into $M_2(\mathbb{C})$. Here $C_b(\mathbb{R})$ is the Banach space of all bounded continuous functions on $\mathbb{R}$.

Let $K_t^{(\varepsilon)}\in\mathcal{L}(\mathcal{S}(\mathbb{R}^3),M_4(\mathbb{C}))$ be defined by

$$K_t^{(\varepsilon)}(\phi)=\int_{\mathbb{R}}[\mu_{|\xi|}(\phi)+|\xi|\mu_{|\xi|}(\partial/\partial r\,\phi)]\sigma_0\otimes H_\varepsilon(\xi,t)d\xi+\int_{\mathbb{R}}\xi\mu_{|\xi|}(\langle\sigma,\nabla\rangle\phi)\otimes H_\varepsilon(\xi,t)d\xi, \tag{21}$$

for every test function $\phi\in\mathcal{S}(\mathbb{R}^3)$. As a consequence of the smoothing operation of convolution with respect to v_ε, we can use integration by parts in the integral above. In order to derive the representation (19) of the kernel of $e^{-it\tau_1}$, we calculate the kernel of $K_t^{(\varepsilon)}$ and take the limit as $\varepsilon\to 0+$.

Lemma 3: As $\varepsilon\to 0+$,

(i) the distribution $K_t^{(\varepsilon)}$ *converges to* K_t *in* $\mathcal{L}(\mathcal{S}(\mathbb{R}^3),M_4(\mathbb{C}))$,

(ii) for any function $\psi\in\mathcal{S}(\mathbb{R}^3,\mathbb{C}^4)$, *the convolution* $K_t^{(\varepsilon)}*\psi$ *belongs to* $\mathcal{S}(\mathbb{R}^3,\mathbb{C}^4)$ *and converges to* $e^{-itD_3}\psi=K_t*\psi$ *in the topology of* $\mathcal{S}(\mathbb{R}^3,\mathbb{C}^4)$, *and*

(iii) for any function $\psi\in L^2(\mathbb{R}^3,\mathbb{C}^4)$, *the convolution* $K_t^{(\varepsilon)}*\psi$ *belongs to* $L^2(\mathbb{R}^3,\mathbb{C}^4)$ *and converges to* $e^{-itD_3}\psi=K_t*\psi$ *in the topology of* $L^2(\mathbb{R}^3,\mathbb{C}^4)$. *The operator norm of* $\psi\mapsto K_t^{(\varepsilon)}*\psi$, $\psi\in L^2(\mathbb{R}^3,\mathbb{C}^4)$, *is bounded by* e^{mt}.

Proof: Given $\phi\in\mathcal{S}(\mathbb{R}^3)$, the function $\xi\mapsto[\mu_{|\xi|}(\phi)+|\xi|\mu_{|\xi|}(\partial/\partial r\phi)]$, $\xi\in\mathbb{R}$, is a bounded, continuous scalar-valued function and $\xi\mapsto\mu_{|\xi|}(\langle\sigma,\nabla\rangle\phi)$, $\xi\in\mathbb{R}$, is a bounded, continuous $M_2(\mathbb{C})$-valued function. The first assertion (i) now follows from the observation that $H_\varepsilon(\xi,t)d\xi$ converges to $H(d\xi,t)$ in $\mathcal{L}(C_b(\mathbb{R}),M_2(\mathbb{C}))$.

Observe that the distribution $K_t^{(\varepsilon)}$ is obtained from K_t by replacing H by H_ε. Let $T_\varepsilon(t)$ denote the operator of convolution with respect to $K_t^{(\varepsilon)}$ acting on $\mathcal{S}(\mathbb{R}^3,\mathbb{C}^4)$. The proof of Lemma 1 shows that $\mathcal{F}T_\varepsilon(t)\mathcal{F}^{-1}$ is the operator of multiplication by the matrix-valued function $p\mapsto\int_{\mathbb{R}}e^{-i\langle\sigma,p\rangle\xi}\otimes H_\varepsilon(\xi,t)\,d\xi$.

Then for every $\psi\in\mathcal{S}(\mathbb{R}^3,\mathbb{C}^4)$, the function $p\mapsto[\int_{\mathbb{R}}e^{-i\langle\sigma,p\rangle\xi}\otimes H_\varepsilon(\xi,t)\,d\xi]\psi(p)$, $p\in\mathbb{R}^3$, also belongs to $\mathcal{S}(\mathbb{R}^3,\mathbb{C}^4)$ and $\mathcal{F}T_\varepsilon(t)\mathcal{F}^{-1}\psi\to\mathcal{F}e^{-itD_3}\mathcal{F}^{-1}\psi$ in $\mathcal{S}(\mathbb{R}^3,\mathbb{C}^4)$ as $\varepsilon\to0+$ because $H_\varepsilon(\xi,t)d\xi$ converges to $H(d\xi,t)$ in $\mathcal{L}(C_b(\mathbb{R}),M_2(\mathbb{C}))$. Statement (ii) now follows from the observation that the Fourier transform leaves the space $\mathcal{S}(\mathbb{R}^3,\mathbb{C}^4)$ invariant. A similar argument proves (iii). The bound

$$\left\|\int_{\mathbb{R}}e^{-i\langle\sigma,p\rangle\xi}\otimes H_\varepsilon(\xi,t)d\xi\right\|_{\mathcal{L}(\mathbb{C}^4)}\leqslant\|v_\varepsilon*H(\cdot,t)\|_{L^1(\mathbb{R},M_2(\mathbb{C}))}\leqslant e^{mt}$$

for each $p\in\mathbb{R}^3$ follows from (20) and Proposition 1, so $\|T_\varepsilon(t)\|\leqslant e^{mt}$. □

Let $\phi\in\mathcal{S}(\mathbb{R}^3)$. In terms of the uniform probability measure μ_r on the sphere S_r with radius $r>0$, we have

$$K_t^{(\varepsilon)}(\phi)=-\int_0^\infty r\int_{S_1}\sigma_0\otimes\left[\left.\frac{\partial H_\varepsilon(\xi,t)}{\partial\xi}\right|_{\xi=r}-\left.\frac{\partial H_\varepsilon(\xi,t)}{\partial\xi}\right|_{\xi=-r}\right]\phi(r\omega)d\mu_1(\omega)dr$$
$$+\int_0^\infty r\int_{S_1}[\langle\sigma,\nabla\rangle\phi](r\omega)\otimes[H_\varepsilon(r,t)-H_\varepsilon(-r,t)]d\mu_1(\omega)dr$$

by an appeal to Fubini's theorem and integrating by parts as in the proof of Proposition 2. On converting to Cartesian coordinates, the convolution $K_t^{(\varepsilon)}*\psi(x)$ of the distribution $K_t^{(\varepsilon)}$ with $\psi\in\mathcal{S}(\mathbb{R}^3,\mathbb{C}^4)$ is equal to

$$K_t^{(\varepsilon)}*\psi(x)=-1/4\pi\int_{\mathbb{R}^3}|x-y|^{-1}\sigma_0\otimes\left[\left.\frac{\partial H_\varepsilon(\xi,t)}{\partial\xi}\right|_{\xi=|x-y|}-\left.\frac{\partial H_\varepsilon(\xi,t)}{\partial\xi}\right|_{\xi=-|x-y|}\right]\psi(y)dy \tag{22}$$

$$-1/4\pi\int_{\mathbb{R}^3}|x-y|^{-1}\sigma_0\otimes[H_\varepsilon(|x-y|,t)-H_\varepsilon(-|x-y|,t)][\langle\sigma,\nabla\rangle\otimes\sigma_0]\psi(y)dy, \tag{23}$$

for all $x\in\mathbb{R}^3$.

B. Reducing subspaces

According to Thaller (1992, Sec. 4.6.4) [see also Bjorken and Drell (1964, p. 52ff)], for every $m_k=-|k|,\ldots,|k|-1$ and $k=\pm1,\pm2,\ldots$, the operators e^{-itD_3}, $t\in\mathbb{R}$, leave the subspace $\mathcal{H}(k,m_k)$ of $L^2(\mathbb{R}^3,\mathbb{C}^4)$ invariant. The subspace $\mathcal{H}(k,m_k)$ equals the orthogonal sum $\mathcal{H}(k,m_k)_+\oplus\mathcal{H}(k,m_k)_-$ with

$$\mathcal{H}(k,m_k)_+=\left\{\Phi^{(+)}(k,m_k)\otimes\frac{u(r)}{r}:u\in L^2(\mathbb{R}_+)\right\},$$

$$\mathcal{H}(k,m_k)_-=\left\{\Phi^{(-)}(k,m_k)\otimes\frac{u(r)}{r}:u\in L^2(\mathbb{R}_+)\right\},$$

for certain $\mathbb{C}^4$-valued eigenfunctions $\Phi^{(\pm)}(k,m_k)$ on S_1. If $u={}^t(u_1,u_2)\in L^2(\mathbb{R}_+,\mathbb{C}^2)$ are functions and c_+,c_- are complex numbers such that the element

$$\psi(x)=c_+\Phi^{(+)}(k,m_k)\otimes\frac{u_1(r)}{r}+c_-\Phi^{(-)}(k,m_k)\otimes\frac{u_2(r)}{r},\quad r=|x|,$$

of $L^2(\mathbb{R}^3,\mathbb{C}^4)$ belongs to the domain of D_3, then

$$(D_3\psi)(x)=c_+\Phi^{(+)}(k,m_k)\otimes\frac{(\tau_k u)_1(r)}{r}+c_-\Phi^{(-)}(k,m_k)\otimes\frac{(\tau_k u)_2(r)}{r},\quad r=|x|,$$

for the differential operator τ_k given by formula (5). Moreover,

$$(e^{-itD_3}\psi)(x)=c_+\Phi^{(+)}(k,m_k)\otimes\frac{(e^{-it\tau_k}u)_1(r)}{r}+c_-\Phi^{(-)}(k,m_k)\otimes\frac{(e^{-it\tau_k}u)_2(r)}{r},\quad r=|x|,$$

for all $\psi\in\mathcal{H}(k,m_k)$. The function $e^{-itD_3}\psi$ is also expressed as a convolution $K_t*\psi$.

It turns out that convolution with respect to the regularized kernel $K_t^{(\varepsilon)}$ also leaves the reducing subspaces $\mathcal{H}(k,m_k)$ invariant—the first integral (22) leaves the subspaces $\mathcal{H}(k,m_k)_+$ and $\mathcal{H}(k,m_k)_-$ invariant, and the second integral (23) maps $\mathcal{H}(k,m_k)_+$ to $\mathcal{H}(k,m_k)_-$ and $\mathcal{H}(k,m_k)_-$ to $\mathcal{H}(k,m_k)_+$. We shall only prove this for the case $k=1$ and $m_k=0$. A similar argument works for $k=-1$ with only changes in signs. We compute the distributional kernel of $e^{-it\tau_1}$ by taking the limit as $\varepsilon\to 0+$ of ${K^{(\varepsilon)}}_t*\psi$ for $\psi\in\mathcal{H}(1,0)$.

In the usual representation of the Dirac matrices,

$$\Phi^{(+)}(k,m_k)=\begin{pmatrix} i\psi(k,m_k)\\ 0\\ 0\end{pmatrix},\quad \Phi^{(-)}(k,m_k)=\begin{pmatrix} 0\\ 0\\ \psi(-k,m_k)\end{pmatrix},$$

$$\psi(k,m_k)=\frac{1}{\sqrt{2k-1}}\begin{pmatrix}\sqrt{k+m_k}\,Y(k-1,m_k)\\ \sqrt{k-m_k-1}\,Y(k-1,m_k+1)\end{pmatrix},\quad \text{for } k>0,$$

$$\psi(k,m_k)=\frac{1}{\sqrt{2|k|+1}}\begin{pmatrix}\sqrt{|k|-m_k}\,Y(|k|,m_k)\\ -\sqrt{|k|+m_k+1}\,Y(|k|,m_k+1)\end{pmatrix},\quad \text{for } k<0,$$

for the spherical harmonic functions $Y(l,j)$.

For $k=1$ and $m_1=-1,0$, we have

$$\Phi^{(+)}(1,0)=\begin{pmatrix} iY(0,0)\\ 0\\ 0\\ 0\end{pmatrix},\quad \Phi^{(-)}(1,0)=\frac{1}{\sqrt{3}}\begin{pmatrix} 0\\ 0\\ Y(1,0)\\ -\sqrt{2}Y(1,1)\end{pmatrix},$$

$$\Phi^{(+)}(1,-1)=\begin{pmatrix} 0\\ iY(0,0)\\ 0\\ 0\end{pmatrix},\quad \Phi^{(-)}(1,-1)=\frac{1}{\sqrt{3}}\begin{pmatrix} 0\\ 0\\ \sqrt{2}Y(1,-1)\\ -Y(1,0)\end{pmatrix}.$$

The spherical harmonic functions in this formula are given, with $0\leqslant\theta\leqslant\pi$ and $0\leqslant\varphi\leqslant 2\pi$, by

$$Y(0,0)=\frac{1}{\sqrt{4\pi}},\quad Y(1,0)=\frac{\sqrt{3/\pi}\cos\theta}{2},$$

$$Y(1,1)=-\frac{e^{i\varphi}\sqrt{3/2\pi}\sin\theta}{2},\quad Y(1,-1)=\frac{e^{-i\varphi}\sqrt{3/2\pi}\sin\theta}{2},$$

so that

$$\Phi^{(+)}(1,0)=\frac{i}{2\sqrt{\pi}}\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\quad \Phi^{(-)}(1,0)=\frac{1}{2\sqrt{\pi}}\begin{pmatrix}0\\0\\\cos\theta\\e^{i\varphi}\sin\theta\end{pmatrix}.$$

With respect to the block-diagonal matrix representation (11) of the Dirac matrices, the new eigenvectors are $Q\Phi^{\pm}(1,0)$, $Q\Phi^{\pm}(1,-1)$, with Q in Eq. (12) used to define the α_j' in Sec. III B. For the purposes of the following computation, it is simpler to represent the tensor products $\sigma_j\otimes\sigma_3$, $j=1,2,3$ and $\sigma_0\otimes\sigma_1$ with respect to the permuted basis $\mathcal{E}'=\{e_1\otimes e_1, e_1\otimes e_2, e_2\otimes e_1, e_2\otimes e_2\}$ of $\mathbb{C}^4$ so that $\sigma_0\otimes\sigma_j=\left(\begin{smallmatrix}\sigma_j & 0\\ 0 & \sigma_j\end{smallmatrix}\right)$ for $j=1,2,3$. With respect to this new basis, the eigenvectors $Q\Phi^{\pm}(1,0)$, $Q\Phi^{\pm}(1,-1)$ are represented by the column vectors

$$\Psi^{(+)}(1,0)=\frac{i}{2\sqrt{2\pi}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix},\quad \Psi^{(-)}(1,0)=\frac{1}{2\sqrt{2\pi}}\begin{pmatrix}\cos\theta\\-\cos\theta\\e^{i\varphi}\sin\theta\\-e^{i\varphi}\sin\theta\end{pmatrix},$$

$$\Psi^{(+)}(1,-1)=\frac{i}{2\sqrt{2\pi}}\begin{pmatrix}0\\0\\1\\1\end{pmatrix},\quad \Psi^{(-)}(1,-1)=\frac{1}{2\sqrt{2\pi}}\begin{pmatrix}e^{-i\varphi}\sin\theta\\-e^{-i\varphi}\sin\theta\\-\cos\theta\\\cos\theta\end{pmatrix}.$$

Proof of Theorem 1: According to Thaller (1992, Theorem 4.1.4), the matrix elements of (19) we are trying to calculate are the limiting distributions as $\varepsilon\to 0+$ corresponding to the action of the convolutions (22) and (23) on the subspaces $\mathcal{H}(1,0)_+$ and $\mathcal{H}(1,0)_-$ of $L^2(\mathbb{R}^3,\mathbb{C}^4)$. We look at each subspace separately.

1. The subspace $\mathcal{H}(1,0)_+$

On setting $\psi(y)=\Psi^{(+)}(1,0)\otimes\rho^{-1}u(\rho)$ in polar cordinates (ρ,θ,φ) in the integral (22), we have

$$\begin{aligned}&-1/4\pi\int_0^\infty\int_0^\pi\int_0^{2\pi}|r^2+\rho^2-2r\rho\cos\theta|^{-1/2}\sigma_0\otimes\left[\left.\frac{\partial H_\varepsilon(\xi,t)}{\partial\xi}\right|_{\xi=|r^2+\rho^2-2r\rho\cos\theta|^{1/2}}\right.\\&\quad\left.-\left.\frac{\partial H_\varepsilon(\xi,t)}{\partial\xi}\right|_{\xi=-|r^2+\rho^2-2r\rho\cos\theta|^{1/2}}\right]\Psi^{(+)}(1,0)u(\rho)\,\rho\sin\theta d\varphi d\theta d\rho\\&=-1/2\int_0^\infty\int_0^\pi|r^2+\rho^2-2r\rho\cos\theta|^{-1/2}\sigma_0\otimes\left[\left.\frac{\partial H_\varepsilon(\xi,t)}{\partial\xi}\right|_{\xi=|r^2+\rho^2-2r\rho\cos\theta|^{1/2}}\right.\\&\quad\left.-\left.\frac{\partial H_\varepsilon(\xi,t)}{\partial\xi}\right|_{\xi=-|r^2+\rho^2-2r\rho\cos\theta|^{1/2}}\right]\Psi^{(+)}(1,0)u(\rho)\rho\sin\theta d\theta d\rho.\end{aligned}$$

Let $\xi=(r^2+\rho^2-2r\rho\cos\theta)^{1/2}$. Then $\xi=r+\rho$ when $\theta=\pi$ and $\xi=|r-\rho|$ when $\theta=0$. The integral (22) becomes

$$-\frac{1}{2r}\int_0^\infty\left[\int_{|r-\rho|}^{r+\rho}\sigma_0\otimes\left(\left(\frac{\partial H_\varepsilon}{\partial\xi}\right)(\xi,t)-\left(\frac{\partial H_\varepsilon}{\partial\xi}\right)(-\xi,t)\right)d\xi\right]\Psi^{(+)}(1,0)u(\rho)d\rho$$

$$=-\frac{1}{2r}\int_0^\infty\sigma_0\otimes[H_\varepsilon(r+\rho,t)-H_\varepsilon(|r-\rho|,t)+H_\varepsilon(-(r+\rho),t)$$

$$-H_\varepsilon(-|r-\rho|,t)]\Psi^{(+)}(1,0)u(\rho)d\rho.$$

Now $D(\cdot,t)$ is an even function and we chose v_ε to be even, so $D_\varepsilon(\cdot,t)$ is also an even function. In the expression (20) for H_ε, the components of $(\sigma_0\partial/\partial t-im\sigma_1)D_\varepsilon(\xi,t)$ are even functions of ξ and the components of $\sigma_3\partial D_\varepsilon(\xi,t)/\partial\xi$ are odd functions of ξ. Furthermore, in the chosen basis, the application of either of the matrices $\sigma_0\otimes\sigma_0$ and $\sigma_0\otimes\sigma_1$ does not change the vector $\Psi^{(+)}(1,0)$.

On setting $\overline{E_\varepsilon}(\xi,t)=(\partial/\partial t-im)D_\varepsilon(\xi,t)$ for $\xi\in\mathbb{R}$ and $t>0$, the integral (22) is therefore equal to

$$-\frac{\Psi^{(+)}(1,0)}{r}\int_0^\infty[\overline{E_\varepsilon}(r+\rho,t)-\overline{E_\varepsilon}(r-\rho,t)]u(\rho)d\rho.$$

The matrix element corresponding to (22) is therefore $\overline{E_\varepsilon}(r-\rho,t)-\overline{E_\varepsilon}(r+\rho,t)$.

The integrand of (23) consists of the odd components of $H_\varepsilon(\cdot,t)$. Set $F_\varepsilon(\xi,t)=\partial D_\varepsilon(\xi,t)/\partial\xi$, for all $\xi\in\mathbb{R}$ and $t\geqslant 0$. Then note that

$$H_\varepsilon(\xi,t)-H_\varepsilon(-\xi,t)=-\sigma_3(F_\varepsilon(\xi,t)-F_\varepsilon(-\xi,t))=-2\sigma_3F_\varepsilon(\xi,t).$$

Then in polar coordinates, the integral (23) becomes

$$2\int_0^\infty\left[\int_{S_1}\langle\sigma,\omega\rangle\otimes\sigma_3\Psi^{(+)}(1,0)\,\frac{F_\varepsilon([r^2+\rho^2-2r\rho\langle\omega,\hat r\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat r\rangle]^{1/2}}\,\mu_1(d\omega)\right]\left[\frac{d}{d\rho}\,\frac{u(\rho)}{\rho}\right]\rho^2d\rho \tag{24}$$

for $r=|x|$ and $\hat r=x/r$. Here we have used the fact that $\Psi^{(+)}(1,0)$ is a *constant* vector.

Suppose that $\{\hat e_1,\hat e_2,\hat r\}$ is an orthonormal basis of $\mathbb{R}^3$ and $e_j=a_{j1}\hat e_1+a_{j2}\hat e_2+a_{j3}\hat r$ for the standard basis vectors e_j, $j=1,2,3$, of $\mathbb{R}^3$. Then

$$\langle\sigma,\omega\rangle=\sum_{j=1}^3\sigma_j[a_{j1}\langle\omega,\hat e_1\rangle+a_{j2}\langle\omega,\hat e_2\rangle+a_{j3}\langle\omega,\hat r\rangle].$$

Because $\int_{S_1}f(\langle\omega,\hat r\rangle)\langle\omega,\hat e_j\rangle d\mu(\omega)=0$, for $j=1,2$ and any bounded measurable function f, only the integral over the term $\Sigma_{j=1}^3\sigma_ja_{j3}\langle\omega,\hat r\rangle$ of $\langle\sigma,\omega\rangle$ in (24) remains. But $\hat r=\Sigma_{j=1}^3e_ja_{j3}$ because $[a_{j\kappa}]_{j,\kappa=1}^3$ is an orthogonal matrix, that is, $a_{j3}=\hat r_j$ for $j=1,2,3$, so the integral (24) is equal to

$$2\int_0^\infty\left[\int_{S_1}\langle\omega,\hat r\rangle\,\frac{F_\varepsilon([r^2+\rho^2-2r\rho\langle\omega,\hat r\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat r\rangle]^{1/2}}\,\mu_1(d\omega)\right]\left[\frac{d}{d\rho}\,\frac{u(\rho)}{\rho}\right]\rho^2d\rho$$

times the vector $[\langle\sigma,\hat r\rangle\otimes\sigma_3]\Psi^{(+)}(1,0)$.

With the substitution $\xi=[r^2+\rho^2-2r\rho\cos\theta]^{1/2}$, $\cos\theta=\langle\omega,\hat r\rangle$ and integration by parts, we have

$$
\begin{aligned}
&-2\int_0^\infty d\rho\,\frac{u(\rho)}{\rho}\,\frac{\partial}{\partial\rho}\rho^2\int_{S_1}\langle\omega,\hat r\rangle\,\frac{F_\varepsilon([r^2+\rho^2-2r\rho\langle\omega,\hat r\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat r\rangle]^{1/2}}\,\mu_1(d\omega)\\
&\quad=-\frac{2}{4\pi}\int_0^\infty d\rho\,\frac{u(\rho)}{\rho}\,\frac{\partial}{\partial\rho}\rho^2\int_0^\pi\int_0^{2\pi}\cos\theta\,\frac{F_\varepsilon([r^2+\rho^2-2r\rho\cos\theta]^{1/2},t)}{[r^2+\rho^2-2r\rho\cos\theta]^{1/2}}\sin\theta d\varphi d\theta\\
&\quad=-\int_0^\infty d\rho\,\frac{u(\rho)}{\rho}\,\frac{\partial}{\partial\rho}\rho^2\int_{|r-\rho|}^{r+\rho}\frac{r^2+\rho^2-\xi^2}{2r^2\rho^2}F_\varepsilon(\xi,t)d\xi\\
&\quad=-\frac{1}{2r^2}\int_0^\infty d\rho\,\frac{u(\rho)}{\rho}\,\frac{\partial}{\partial\rho}\int_{|r-\rho|}^{r+\rho}(r^2+\rho^2-\xi^2)F_\varepsilon(\xi,t)d\xi.
\end{aligned}
$$

In the region $\rho>r$, we have

$$
\begin{aligned}
&-\frac{1}{2r^2}\int_0^\infty d\rho\,\frac{u(\rho)}{\rho}\,\frac{\partial}{\partial\rho}\int_{\rho-r}^{r+\rho}(r^2+\rho^2-\xi^2)F_\varepsilon(\xi,t)d\xi\\
&\quad=-\frac{1}{2r^2}\int_0^\infty d\rho\,\frac{u(\rho)}{\rho}\left([(r^2+\rho^2-\xi^2)F_\varepsilon(\xi,t)]_{\rho-r}^{r+\rho}+2\rho\int_{\rho-r}^{r+\rho}F_\varepsilon(\xi,t)d\xi\right)\\
&\quad=-\frac{1}{r}\int_0^\infty d\rho u(\rho)\left[-(F_\varepsilon(r+\rho,t)+F_\varepsilon(\rho-r,t))+\frac{1}{r}(D_\varepsilon(r+\rho,t)-D_\varepsilon(\rho-r,t))\right]\\
&\quad=-\frac{1}{r}\int_0^\infty d\rho u(\rho)\left[F_\varepsilon(r-\rho,t)-F_\varepsilon(r+\rho,t)+\frac{1}{r}(D_\varepsilon(r+\rho,t)-D_\varepsilon(r-\rho,t))\right],
\end{aligned}
$$

because F_ε is an odd function. The same expression is obtained for $\rho<r$.

A calculation [cf. Thaller 1992, Eq. (4.122) p. 127] shows that

$$
[\langle\sigma,\hat r\rangle\otimes\sigma_3]\Psi^{(+)}(1,0)=i\Psi^{(-)}(1,0)(\hat r). \tag{25}
$$

Indeed,

$$
\langle\sigma,\hat r\rangle\otimes\sigma_3=\begin{pmatrix}\hat r_3 & \hat r_1-i\hat r_2\\ \hat r_1+i\hat r_2 & -\hat r_3\end{pmatrix}\otimes\sigma_3=\begin{pmatrix}\hat r_3\sigma_3 & (\hat r_1-i\hat r_2)\sigma_3\\ (\hat r_1+i\hat r_2)\sigma_3 & -\hat r_3 s_3\end{pmatrix}.
$$

The sum of the first two columns of $\langle\sigma,\hat r\rangle\otimes\sigma_3$ is

$$
\begin{pmatrix}\hat r_3\\ -\hat r_3\\ \hat r_1+i\hat r_2\\ -(\hat r_1+i\hat r_2)\end{pmatrix}=\begin{pmatrix}\cos\theta\\ -\cos\theta\\ e^{i\varphi}\sin\theta\\ -e^{i\varphi}\sin\theta\end{pmatrix},
$$

which is a constant multiple of $\Psi^{(-)}(1,0)(\hat r)$. The integral (23) is equal to

$$
-i\frac{\Psi^{(-)}(1,0)(\hat r)}{r}\int_0^\infty d\rho u(\rho)\left[F_\varepsilon(r-\rho,t)-F_\varepsilon(r+\rho,t)-\frac{1}{r}(D_\varepsilon(r-\rho,t)-D_\varepsilon(r+\rho,t))\right],
$$

so that the corresponding matrix element is

$$
-iW_{21}^{(\varepsilon)}(r,\rho;t)=-i\left[F_\varepsilon(r-\rho,t)-F_\varepsilon(r+\rho,t)-\frac{1}{r}(D_\varepsilon(r-\rho,t)-D_\varepsilon(r+\rho,t))\right].
$$

2. The subspace $\mathcal{H}(1,0)_-$

On the other hand, for $\psi(y)=\Psi^{(-)}(1,0)\otimes\rho^{-1}u(\rho)$, (23) is

$$-2\int_0^\infty\left[\int_{S_1}\sigma_0\otimes\frac{\frac{\partial G_\varepsilon}{\partial\xi}([r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2}}\Psi^{(-)}(1,0)(\omega)d\mu_1(\omega)\right]u(\rho)\rho d\rho$$

for $G_\varepsilon(\xi,t)=(\sigma_0\partial/\partial t-im\sigma_1)D_\varepsilon(\xi,t)$, for all $\xi\in\mathbb{R}$ and $t>0$. Note here that

$$\frac{\partial}{\partial\xi}H_\varepsilon(\xi,t)-\frac{\partial}{\partial\xi}H_\varepsilon(-\xi,t)=2\left(\sigma_0\frac{\partial}{\partial t}-im\sigma_1\right)\frac{\partial}{\partial\xi}D_\varepsilon(\xi,t)=2\frac{\partial}{\partial\xi}G_\varepsilon(\xi,t).$$

Now

$$\begin{aligned}
&\int_{S_1}\sigma_0\otimes\frac{(\partial G_\varepsilon/\partial\xi)([r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2}}\Psi^{(-)}(1,0)(\omega)d\mu_1(\omega)\\
&\quad=-i\int_{S_1}\sigma_0\otimes\frac{(\partial G_\varepsilon/\partial\xi)([r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2}}[\langle\sigma,\omega\rangle\otimes\sigma_3]\Psi^{(+)}(1,0)d\mu_1(\omega)\\
&\quad=-i\int_{S_1}\sigma_0\otimes\frac{(\partial G_\varepsilon/\partial\xi)([r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2}}[\langle\sigma,\hat{r}\rangle\otimes\sigma_3]\Psi^{(+)}(1,0)\langle\omega,\hat{r}\rangle d\mu_1(\omega)\\
&\quad=\int_{S_1}\sigma_0\otimes\frac{(\partial G_\varepsilon/\partial\xi)([r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2}}\Psi^{(-)}(1,0)(\hat{r})\langle\omega,\hat{r}\rangle d\mu_1(\omega)\\
&\quad=\Psi^{(-)}(1,0)(\hat{r})\int_{S_1}\frac{(\partial E_\varepsilon/\partial\xi)([r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2}}\langle\omega,\hat{r}\rangle d\mu_1(\omega)\\
&\quad=4^{-1}\Psi^{(-)}(1,0)(\hat{r})(r\rho)^{-2}\int_{|r-\rho|}^{r+\rho}\frac{\partial E_\varepsilon(\xi,t)}{\partial\xi}(r^2+\rho^2-\xi^2)d\xi,
\end{aligned}$$

where we have used the identity (25) and the fact that $(\sigma_0\otimes\sigma_0)\Psi^{(-)}(1,0)=\Psi^{(-)}(1,0)$ and $(\sigma_0\otimes\sigma_1)\Psi^{(-)}(1,0)=-\Psi^{(-)}(1,0)$. Integrating by parts, we have

$$-2^{-1}(r\rho)^{-1}\int_{|r-\rho|}^{r+\rho}\frac{\partial E_\varepsilon(\xi,t)}{\partial\xi}(r^2+\rho^2-\xi^2)d\xi=E_\varepsilon(r+\rho)+E_\varepsilon(r-\rho)-(r\rho)^{-1}\int_{|r-\rho|}^{r+\rho}E_\varepsilon(\xi)\xi d\xi,$$

which is the matrix element corresponding to the convolution (22) acting on $\mathcal{H}(1,0)_-$.

For the other integral (23), appealing to the identity (25), we have

$$\begin{aligned}
[\langle\sigma,\nabla\rangle]\otimes\sigma_3]\psi(y)&=[\langle\sigma,\nabla\rangle\otimes\sigma_3][\Psi^{(-)}(1,0)(\omega)\rho^{-1}u(\rho)]\\
&=\frac{u(\rho)}{\rho}[\langle\sigma,\nabla\rangle\otimes\sigma_3]\Psi^{(-)}(1,0)(\omega)+\langle\sigma,\omega\rangle\otimes\sigma_3\Psi^{(-)}(1,0)(\omega)\frac{d}{d\rho}\frac{u(\rho)}{\rho}\\
&=\frac{1}{i}\left[\frac{u(\rho)}{\rho}[\langle\sigma,\nabla\rangle\otimes\sigma_3][\langle\sigma,\omega\rangle\otimes\sigma_3]\Psi^{(+)}(1,0)+\Psi^{(+)}(1,0)\frac{d}{d\rho}\frac{u(\rho)}{\rho}\right],
\end{aligned}$$

in coordinates $\omega=y/|y|$ and $\rho=|y|$.

The function $\Psi^{(+)}(1,0)$ is a constant vector and a calculation shows that

$$[\langle\sigma,\nabla\rangle\otimes\sigma_3]\langle\sigma,\omega\rangle\otimes\sigma_3=\frac{2}{\rho}\sigma_0\otimes\sigma_0.$$

One integral in (23) is therefore

$$
\begin{aligned}
&-2i\Psi^{(+)}(1,0)\int_0^\infty\left[\int_{S_1}\frac{F_\varepsilon([r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2}}\mu_1(d\omega)\right]\left[\frac{d}{d\rho}\frac{u(\rho)}{\rho}\right]\rho^2 d\rho\\
&=2i\Psi^{(+)}(1,0)\int_0^\infty\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho^2\left[\int_{S_1}\frac{F_\varepsilon([r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2}}\mu_1(d\omega)\right]u(\rho)d\rho\\
&=\frac{i\Psi^{(+)}(1,0)}{r}\int_0^\infty\frac{u(\rho)}{\rho}\frac{\partial}{\partial\rho}\rho\left[\int_{|r-\rho|}^{r+\rho}F_\varepsilon(\xi,t)d\xi\right]d\rho\\
&=\frac{i\Psi^{(+)}(1,0)}{r}\int_0^\infty\frac{u(\rho)}{\rho}\frac{\partial}{\partial\rho}\rho[D_\varepsilon(r+\rho,t)-D_\varepsilon(r-\rho,t)]d\rho\\
&=\frac{i\Psi^{(+)}(1,0)}{r}\int_0^\infty\left[F_\varepsilon(r-\rho,t)+F_\varepsilon(r+\rho,t)-\frac{1}{\rho}[D_\varepsilon(r-\rho,t)-D_\varepsilon(r+\rho,t)]u(\rho)d\rho\right.
\end{aligned}
$$

and the other is

$$
\begin{aligned}
&-4i\Psi^{(+)}(1,0)\int_0^\infty\left[\int_{S_1}\frac{F_\varepsilon([r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2},t)}{[r^2+\rho^2-2r\rho\langle\omega,\hat{r}\rangle]^{1/2}}\mu_1(d\omega)\right]u(\rho)d\rho\\
&=-\frac{2i\Psi^{(+)}(1,0)}{r}\int_0^\infty\frac{u(\rho)}{\rho}\int_{|r-\rho|}^{r+\rho}F_\varepsilon(\xi,t)d\xi d\rho\\
&=\frac{2i\Psi^{(+)}(1,0)}{r}\int_0^\infty\frac{u(\rho)}{\rho}[D_\varepsilon(r-\rho,t)-D_\varepsilon(r+\rho,t)]d\rho.
\end{aligned}
$$

Adding the two terms, the integral (23) becomes

$$
\frac{i\Psi^{(+)}(1,0)}{r}\int_0^\infty\left[F_\varepsilon(r-\rho,t)+F_\varepsilon(r+\rho,t)+\frac{1}{\rho}[D_\varepsilon(r-\rho,t)-D_\varepsilon(r+\rho,t)]u(\rho)d\rho,\right.
$$

so that the corresponding matrix element is

$$
iW_{12}^{(\varepsilon)}(r,\rho;t)=i\left[F_\varepsilon(r-\rho,t)+F_\varepsilon(r+\rho,t)+\frac{1}{\rho}[D_\varepsilon(r-\rho,t)-D_\varepsilon(r+\rho,t)].\right.
$$

The operator of convolution with respect to $K_t^{(\varepsilon)}$ therefore leaves the subspace $\mathcal{H}(1,0)$ invariant and its action on the radial components is the operator $e^{-it\tau_1}$ whose kernel is given by

$$
\begin{pmatrix}\overline{E_\varepsilon}(r-\rho,t)-\overline{E_\varepsilon}(r+\rho,t) & iW_{12}^{(\varepsilon)}(r,\rho;t)\\ -iW_{21}^{(\varepsilon)}(r,\rho;t) & E_\varepsilon(r-\rho,t)+E_\varepsilon(r+\rho,t)-W_{22}^{(\varepsilon)}(r,\rho;t)\end{pmatrix}, \tag{26}
$$

where

$$W_{12}^{(\varepsilon)}(r,\rho;t)=\left[F_\varepsilon(r-\rho,t)+F_\varepsilon(r+\rho,t)+\frac{1}{\rho}(D_\varepsilon(r-\rho,t)-D_\varepsilon(r+\rho,t))\right],$$

$$W_{21}^{(\varepsilon)}(r,\rho;t)=\left[F_\varepsilon(r-\rho,t)-F_\varepsilon(r+\rho,t)-\frac{1}{r}(D_\varepsilon(r-\rho,t)-D_\varepsilon(r+\rho,t))\right],$$

$$W_{22}^{(\varepsilon)}(r,\rho;t)=(r\rho)^{-1}\int_{|r-\rho|}^{r+\rho}E_\varepsilon(\xi,t)\xi d\xi.$$

By virtue of Lemma 3 and the observation that the operator of convolution with respect to $K_t^{(\varepsilon)}$ leaves the subspace $\mathcal{H}(1,0)$ invariant, the operator $e^{-it\tau_1}$ is the limit in the strong operator topology on $L^2(\mathbb{R}_+,\mathbb{C}^2)$, as $\varepsilon\to 0+$, of bounded linear operators with kernels given by (26).

It is readily verified that as $\varepsilon\to 0+$, the components of (26) converge in the space $C_c^\infty(\mathbb{R}_+\times\mathbb{R}_+)'$ of distributions to the components of (19). The proof of Theorem 1 is complete. □

The explicit form of the kernel $e^{-it\tau_1}(r,\rho)$ given in Theorem 1 enables us to show that $e^{-it\tau_1}$ is not a bounded operator on $L^\infty(\mathbb{R}_+,\mathbb{C}^2)$ for $t\neq 0$.

Proposition 3: For each $\delta>0$ *and* $t\neq 0$, $e^{-it\tau_1}(\chi_{(0,\delta)}.e_2)\notin L^\infty(\mathbb{R}_+,\mathbb{C}^2)$.

Proof: Let $t>0$. A similar argument holds for $t<0$. It is enough to show that the function

$$r\mapsto\int_0^\delta W_{12}(r,\rho;t)d\rho,\quad 0<r<t, \tag{27}$$

is not bounded near $r=t$. The distribution of order zero with the kernel $F(r-\rho,t)+F(r+\rho,t)$ is associated with the sum of convolutions with respect to measures, giving a uniformly bounded function of r, so we examine the integral

$$\int_0^\delta\frac{D(r-\rho,t)-D(r+\rho,t)}{\rho}d\rho.$$

In the region $\{(r,\rho)\in(\mathbb{R}_+)^2:|r+\rho|<t\}$, there exists a constant $C>0$ such that

$$\begin{aligned}|D(r-\rho,t)-D(r+\rho,t)|&\leqslant C|\sqrt{t^2-(r-\rho)^2}-\sqrt{t^2-(r+\rho)^2}|\\&=\frac{4Cr\rho}{\sqrt{t^2-(r-\rho)^2}+\sqrt{t^2-(r+\rho)^2}}\\&\leqslant\frac{4Cr\rho}{\sqrt{t^2-(r-\rho)^2}}.\end{aligned}$$

It follows that $r\mapsto\int_0^{\delta\wedge(t-r)}\rho^{-1}[D(r-\rho,t)-D(r+\rho,t)]\,d\rho$ is a uniformly bounded function for all $0<r<t$.

In the region $\rho>t-r$, the term $\rho^{-1}D(r+\rho,t)$ in the kernel $W_{12}(r,\rho;t)$ is zero. Suppose that $t-\delta<r<t$. Then

$$\int_{t-r}^\delta\frac{D(r-\rho,t)}{\rho}d\rho=\frac{1}{2}\int_{t-r}^{\delta\wedge(t+r)}\frac{J_0(m\sqrt{t^2-(\rho-r)^2})}{\rho}d\rho. \tag{28}$$

Because $J_0(0)=1$ and J_0 is continuous, it follows that the function (28) and hence (27) has a logarithmic divergence at $r=t$. □

Corollary 1: The operator $e^{-it\tau_1}$ *is not bounded from* $L^\infty(\mathbb{R}_+,\mathbb{C}^2)$ *to* $L^\infty(\mathbb{R}_+,\mathbb{C}^2)$ *for any* $t\neq 0$.

According to the following corollary, the group $e^{-it\tau_1}$, $t>0$, does not have path-space measures, somewhat in the same sense that the heat equation $e^{tD\Delta}$ with nonreal diffusion constant D as well as the Schrödinger group $e^{it\Delta/2}$ do not possess path-space measures (cf. Cameron, 1960/61).

The path-space $\Omega_{r,t}$ consists of all functions $\omega:[0,t]\to\mathbb{R}_+$ with $\omega(t)=r$ and we are looking for a family of $M_2(\mathbb{C})$-valued measures $\nu_{r,t}$ defined on the σ-algebra generated by cylinder sets in $\Omega_{r,t}$, such that the equations (29) below hold.

Corollary 2: There does not exist a family $\{\nu_{r,t}\}$ *of matrix-valued path-space measures on the path-space* $\Omega_{r,t}$ *such that*

$$\int_{\Omega_{r,t}} \nu_{r,t}(d\omega) f(\omega(0)) = (e^{-it\tau_1} f)(r), \quad \text{for all } r>0,\ t>0, \tag{29}$$

for every continuous function $f:[0,\infty)\to\mathbb{C}^2$ *with compact support.*

Proof: By smoothing out the function $\chi_{(0,\delta)}.e_2$ used in Proposition 3, we can find a continuous function $f:[0,\infty)\to\mathbb{C}^2$ with compact support such that $(e^{-it\tau_1}f)(r)$ diverges as $r\to t$. Hence, a formula like (29) cannot hold for *all* $r>0$. □

By duality, $e^{-it\tau_1}$ cannot be bounded from $L^1(\mathbb{R}_+,\mathbb{C}^2)$ to $L^1(\mathbb{R}_+,\mathbb{C}^2)$ either. Moreover, a construction similar to that above shows one can find a function f with an integrable singularity at $\rho=t$ such that the function

$$r\mapsto \int_{t-\delta}^{t} W_{21}(r,\rho;t) f(\rho)\, d\rho, \quad 0<r<t,$$

is not integrable at $r=0$ state.

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Properties of the symplectic structure of general relativity for spatially bounded space–time regions

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We continue a previous analysis of the covariant Hamiltonian symplectic structure of general relativity for spatially bounded regions of space–time. To allow for wide generality, the Hamiltonian is formulated using any fixed hypersurface, with a boundary given by a closed spacelike two-surface. A main result is that we obtain Hamiltonians associated with Dirichlet and Neumann boundary conditions on the gravitational field coupled to matter sources, in particular a Klein–Gordon field, an electromagnetic field, and a set of Yang–Mills–Higgs fields. The Hamiltonians are given by a covariant form of the Arnowitt–Deser–Misner (ADM) Hamiltonian modified by a surface integral term that depends on the particular boundary conditions. The general form of this surface integral involves an underlying ''energy-momentum'' vector in the space–time tangent space at the spatial boundary two-surface. We give examples of the resulting Dirichlet and Neumann vectors for topologically spherical two-surfaces in Minkowski space–time, spherically symmetric space–times, and stationary axisymmetric space–times. Moreover, we establish the relation between these vectors and the ADM energy-momentum vector for a two-surface taken in a limit to be spatial infinity in asymptotically flat space–times. We also discuss the geometrical properties of the Dirichlet and Neumann vectors and obtain several striking results relating these vectors to the mean curvature and normal curvature connection of the two-surface. Most significantly, the part of the Dirichlet vector normal to the two-surface depends only on the space–time metric at this surface and thereby defines a geometrical normal vector field on the two-surface. We show that this normal vector is orthogonal to the mean curvature vector, and its norm is the mean null extrinsic curvature, while its direction is such that there is zero expansion of the two-surface, i.e., the Lie derivative of the surface volume form in this direction vanishes. This leads to a direct relation between the Dirichlet vector and the condition for a spacelike two-surface to be (marginally) trapped.
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I. INTRODUCTION

In a previous paper[1] we began an investigation of the covariant symplectic structure associated with the Einstein equations for the gravitational field in any fixed spatially compact region $\Sigma\times\mathbb{R}$ of space–time whose spacelike slices Σ posses a closed two-surface boundary $\partial\Sigma$, with a fixed time-flow vector field tangent to the timelike boundary hypersurface $\partial\Sigma\times\mathbb{R}$. Through an analysis of boundary conditions required for the existence of a Hamiltonian variational principle, we derived Dirichlet, Neumann, and mixed type boundary conditions for the space–time metric at the spatial boundary two-surface $\partial\Sigma$. The corresponding Hamiltonians we obtained are given by a

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covariant form of the Arnowitt–Deser–Misner (ADM) Hamiltonian plus a surface integral term whose form depends on the boundary conditions. We also showed that these Hamiltonians naturally yield covariant field equations which are equivalent to a $3+1$ split of the Einstein equations into the well-known constraint equations and geometrical time-evolution equations for the space–time metric.

The present paper continues the previous analysis in two significant ways. First, in Sec. II, we investigate the covariant symplectic structure of the Einstein equations coupled to matter sources in any fixed spatially bounded region of space–time. Specifically, we consider Dirichlet and Neumann boundary conditions for a scalar field, an electromagnetic field, and a set of Yang–Mills/Higgs fields. Furthermore, we allow the fixed time-flow vector field on space–time to have an arbitrary direction (i.e., not necessarily timelike) in the space–time region. Such freedom in the choice of the time-flow vector field is useful for relating the Hamiltonian boundary terms to expressions for total energy, momentum, angular momentum associated with the gravitational and matter fields on given hypersurfaces in space–time.

Next, in Sec. III, we discuss in detail the geometrical structure of the gravitational part of the Dirichlet and Neumann Hamiltonian boundary terms. In particular, as noted in Ref. 1, these each involve an underlying locally constructed ''energy-momentum'' vector at each point in the tangent space at the two-surface. We show that the form of the boundary term vectors is closely related to the mean curvature vector and normal curvature connection one-form which describe the extrinsic geometry of the spatial boundary two-surface in space–time. Most striking, we further show that the part of the Dirichlet boundary term vector orthogonal to the two-surface yields a direction in which the two-surface has zero expansion in space–time.

Finally, through several examples, we illustrate the properties of the Dirichlet and Neumann boundary term vectors for topologically spherical two-surfaces in various physically interesting space–times in Sec. IV. As a main result, we show that in asymptotically flat space–times the Dirichlet vector at spatial infinity can be identified in a natural way with the ADM energy-momentum vector.

We make some concluding remarks in Sec. V. (The notation and conventions of Ref. 1 are used throughout.)

II. MATTER FIELDS

It is convenient here to employ the tetrad formulation of the Einstein equations, since this simplifies the analysis of boundary conditions and Hamiltonian boundary terms as shown in Ref. 1. We focus on Dirichlet and Neumann boundary conditions and make some remarks on more general boundary conditions at the end.

A. Preliminaries

On a given smooth orientable space–time (M, g_{ab}), let ξ^a be a complete, smooth time-flow vector field, allowed to be timelike, spacelike, or null. Let Σ be a region contained in a fixed hypersurface in M such that the boundary of the region is a closed orientable spacelike two-surface $\partial\Sigma$ (with the hypersurface allowed to be otherwise arbitrary).

For treatment of boundary conditions when the time-flow ξ^a is not necessarily timelike, it is helpful to introduce the following structure associated with the boundary two-surface $\partial\Sigma$.

Let $\mathcal{P}_{\partial\Sigma}$ and $\mathcal{P}^{\perp}_{\partial\Sigma}$ denote projection operators onto the tangent subspaces $T(\partial\Sigma)$ and $T(\partial\Sigma)^{\perp}$ with respect to the surface $\partial\Sigma$ in local coordinates in M. Note $\mathcal{P}_{\partial\Sigma}+\mathcal{P}^{\perp}_{\partial\Sigma}$ is the identity map on the tangent space $T(M)$ at $\partial\Sigma$. Define the metric on $\partial\Sigma$ by

$$\sigma^{ab}=\mathcal{P}_{\partial\Sigma}(g^{ab}), \quad \sigma_{ab}=g_{ac}g_{bd}\sigma^{bc}. \tag{2.1}$$

Let ϵ_{ab} be the metric volume form on $\partial\Sigma$, and define

$$*\epsilon_{ab}=\epsilon^{cd}\epsilon_{abcd}(g) \tag{2.2}$$

in terms of the space–time volume form $\epsilon_{abcd}(g)$. Note that $\mathcal{P}_{\partial\Sigma}(*\epsilon_{ab})=\mathcal{P}^{\perp}_{\partial\Sigma}(\epsilon_{ab})=0$. A useful identity is given by

$$2(\mathcal{P}_{\partial\Sigma})_{[a}{}^{c}(\mathcal{P}_{\partial\Sigma})_{b]}{}^{d}=\epsilon_{ab}\epsilon^{cd}. \tag{2.3}$$

Let

$$\zeta^a=\mathcal{P}^{\perp}_{\partial\Sigma}(\xi^a), \quad N^a=\mathcal{P}_{\partial\Sigma}(\xi^a), \tag{2.4}$$

so $\xi^a=\zeta^a+N^a$ decomposes into a sum of normal and tangential vectors with respect to $\partial\Sigma$. We now suppose ξ^a is not tangential to $\partial\Sigma$, i.e., $\zeta^a\neq 0$ everywhere on the surface $\partial\Sigma$. In this situation, much of the formalism and results given in Sec. 3 of Ref. 1 can be paralleled.

Let $\mathcal{B}$ denote the hypersurface given by the image of $\partial\Sigma$ under a one-parameter diffeomorphism generated by ξ^a on M. Note that the dual vector field $*\epsilon_{ab}\xi^b$ is hypersurface orthogonal since it is annihilated by all tangent vectors (in particular ξ^a) in $\mathcal{B}$. Define a basis $\{s_a,t_a\}$ for $T^*(\partial\Sigma)^{\perp}$ by diagonalization of the identity map

$$\delta^b_a=\sigma_a{}^b+s_a s^{*b}+t_a t^{*b}, \tag{2.5}$$

such that $s_a\propto *\epsilon_{ab}\xi^b$ is hypersurface orthogonal to $\mathcal{B}$, with $\{s^{*a},t^{*a}\}$ denoting a basis for $T(\partial\Sigma)^{\perp}$ that is dual to $\{s_a,t_a\}$. In particular, $s^{*a}s_a=t^{*a}t_a=1$, and $s^{*a}t_a=t^{*a}s_a=0$. This leads to a corresponding decomposition of the space–time metric

$$g_{ab}=\sigma_{ab}+s_a s^*_a+t_a t^*_b \tag{2.6}$$

with $s^*_a=g_{ab}s^{*b}$ and $t^*_a=g_{ab}t^{*b}$. Now, define a projection operator $\mathcal{P}_{\mathcal{B}}$ with respect to $\mathcal{B}$ by

$$h_a{}^b=\delta^b_a-s_a s^{*b} \tag{2.7}$$

satisfying

$$h_a{}^b s_b=0, \quad h_a{}^b s^{*a}=0. \tag{2.8}$$

Then

$$h_{ab}=g_{ab}-s_a s^*_a=\sigma_{ab}+t_a t^*_a \tag{2.9}$$

defines the induced metric on $\mathcal{B}$. Also, define the volume form on $\mathcal{B}$ by

$$\epsilon_{abc}(h)=\epsilon_{abcd}(g)s^{*d}=3t_{[a}\epsilon_{bc]}. \tag{2.10}$$

Finally, note that

$$*\epsilon_{ab}=4t_{[a}s_{b]}, \quad \epsilon_{abcd}=3\epsilon_{[ab}*\epsilon_{cd]}=4\epsilon_{[abc}(h)s_{d]}, \tag{2.11}$$

$$\zeta^a=-Nt^{*a}, \quad \zeta^a t_a=-N, \quad \zeta^a s_a=\zeta^a\epsilon_{ab}=0, \tag{2.12}$$

for some scalar function N. This yields the identities

$$\xi^a=-Nt^{*a}+N^a, \tag{2.13}$$

$$\xi^a\epsilon^{bc}\epsilon_{abcd}(g)=\xi^a*\epsilon_{ad}=-2Ns_d, \tag{2.14}$$

$$\xi^a\epsilon^{bc}\epsilon_{abc}(h)=-2N, \quad \mathcal{P}_{\partial\Sigma}(\xi^a\epsilon_{abc}(h))=-N\epsilon_{bc}. \tag{2.15}$$

These will be important in the analysis of boundary conditions for both the gravitational field and matter fields.

Now we introduce an orthonormal frame for g_{ab} given by

$$\theta^\mu_a = \sigma^\mu_a + s_a s^{*\mu} + t_a t^{*\mu}, \tag{2.16}$$

where $\sigma^\mu_a = \sigma_a{}^b \theta^\mu_b$ is an orthonormal frame for σ_{ab}, with the coefficients

$$s^{*\mu} = s^{*a}\theta^\mu_a, \quad t^{*\mu} = t^{*a}\theta^\mu_a \tag{2.17}$$

defined to satisfy $\mp t^{*\mu}t^{*\nu} \pm s^{*\mu}s^{*\nu} = \mathrm{diag}(-1,1,0,0)$ if ξ^a is timelike or spacelike, or $2s^{*(\mu}t^{*\nu)} = \mathrm{diag}(-1,1,0,0)$ if ξ^a is null. Consequently, the frame components of s^a, t^a, σ^{ab}, g^{ab} are given by

$$s^\mu = s^a \theta^\mu_a, \quad t^\mu = t^a \theta^\mu_a, \tag{2.18}$$

$$\sigma^{\mu\nu} = \sigma^{ab}\theta^\mu_a\theta^\nu_b = \mathrm{diag}(0,0,1,1), \quad \eta^{\mu\nu} = g^{ab}\theta^\mu_a\theta^\nu_b = \mathrm{diag}(\mp 1, \pm 1, 1, 1), \tag{2.19}$$

where $\{s^\mu, t^\mu\}$ are dual to $\{s^*_\mu = \eta_{\mu\nu}s^{*\nu}, t^*_\mu = \eta_{\mu\nu}t^{*\nu}\}$. Hereafter we fix the frame coefficients (2.17) and (2.18) to be independent of the space–time metric g_{ab}, so therefore under a variation δg_{ab}, the induced variations δs_a, δt_a, $\delta\sigma^\mu_a$, $\delta\theta^\mu_a$ satisfy

$$\delta\theta^\mu_a = \delta\sigma^\mu_a + s^{*\mu}\delta s_a + t^{*\mu}\delta t_a, \tag{2.20}$$

$$\delta s_a = s_\mu \delta\theta^\mu_a, \quad \delta t_a = t_\mu \delta\theta^\mu_a, \quad \delta\sigma^\mu_a = \sigma_\nu{}^\mu \delta\sigma^\nu_a, \tag{2.21}$$

$$\delta\sigma_{ab} = 2\sigma_{\mu\nu}\theta^\mu_{(a}\delta\theta^\nu_{b)} = \sigma^\mu_{(a}\delta\sigma_{b)\mu}, \quad \delta g_{ab} = 2\eta_{\mu\nu}\theta^\mu_{(a}\delta\theta^\nu_{b)}. \tag{2.22}$$

Note, by hypersurface orthogonality of s_a, it also follows that

$$\mathcal{P}_{\mathcal{B}}(\delta s_a) = 0, \quad \mathcal{P}_{\partial\Sigma}(\delta t_a) = 0, \quad \mathcal{P}^\perp_{\partial\Sigma}(\delta\sigma_{ab}) = 0. \tag{2.23}$$

Let

$$h^\mu_a = h_a{}^b\theta^\mu_b = \theta^\mu_a - s_a s^{*\mu}, \tag{2.24}$$

which yields a decomposition of the frame with respect to $\mathcal{B}$, satisfying

$$\mathcal{P}_{\partial\Sigma}(h^\mu_a) = \sigma^\mu_a, \quad \mathcal{P}^\perp_{\partial\Sigma}(h^\mu_a) = t_a t^{*\mu}. \tag{2.25}$$

It is convenient for later to also introduce a fixed frame adapted to $\partial\Sigma$ and ξ^a. Let

$$\vartheta^0_a = t_a, \quad \vartheta^1_a = s_a, \quad \vartheta^2_{[a}\vartheta^3_{b]} = \epsilon_{ab}, \quad \vartheta^2_a = \epsilon_a{}^b\vartheta^3_b, \tag{2.26}$$

which defines the frame ϑ^μ_a uniquely up to rotations of ϑ^2_a, ϑ^3_a. Thus, in this formalism, ϑ^μ_a is an orthonormal frame when ξ^a is timelike or spacelike, and a null frame when ξ^a is null.

In the case when ζ^a is timelike, the previous formalism reduces to that in Ref. 1. Most important, the formalism here applies equally well to the cases when ζ^a is spacelike or null.

Finally, in the case that $\zeta^a = 0$, i.e., ξ^a is tangential to $\partial\Sigma$, we simply fix any basis $\{s_a, t_a\}$ of $T^*(\partial\Sigma)^\perp$ and define a frame θ^μ_a to satisfy the previous equations (2.16)–(2.19). This yields the same formalism as in the case that ξ^a is not tangential to $\partial\Sigma$, except that there does not exist a hypersurface $\mathcal{B}$ generated by $\zeta^a = 0$.

Now, with the frame θ^μ_a used as the gravitational field variable, the Lagrangian for the vacuum Einstein equations is given by

$$L_{abcd}(\theta) = \epsilon_{abcd}(\theta)R(\theta). \tag{2.27}$$

Here $R(\theta)=\theta^b_\nu R^\nu_b(\theta)$ and $R_a{}^\mu(\theta)=\theta^b_\nu R_{ab}{}^{\mu\nu}(\theta)$ are the scalar curvature and Ricci curvature obtained from the curvature two-form

$$R_{ab}{}^{\mu\nu}(\theta)=2\partial_{[a}\Gamma_{b]}{}^{\mu\nu}(\theta)+2\Gamma_{[a}{}^{\mu\sigma}(\theta)\Gamma_{b]\sigma}{}^{\nu}(\theta) \tag{2.28}$$

in terms of the frame connection given by

$$\Gamma_a{}^{\mu\nu}=\theta^{b\mu g}\nabla_a\theta^\nu_b=2\,\theta^{b[\mu}\partial_{[a}\theta^{\nu]}_{b]}-\theta^{b\mu}\theta^{c\nu}\theta_{a\alpha}\partial_{[b}\theta^\alpha_{c]}. \tag{2.29}$$

A variation of $L_{abcd}(\theta)$ yields

$$\delta L_{abcd}(\theta)=\mathcal{E}^\mu_{[bcd}(\theta)\,\delta\theta^\mu_{a]}+\partial_{[a}\Theta_{bcd]}(\theta,\delta\theta), \tag{2.30}$$

where

$$\mathcal{E}^\mu_{bcd}(\theta)=8\epsilon_{bcda}(\theta)(R^{a\mu}(\theta)-\tfrac{1}{2}\theta^{a\mu}R(\theta))=0 \tag{2.31}$$

are the vacuum Einstein field equations for θ^μ_a, and where

$$\Theta_{bcd}(\theta,\delta\theta)=8\epsilon_{abcd}(g)\,\theta^e_\nu\theta^a_\mu\delta\Gamma_e{}^{\mu\nu}(\theta) \tag{2.32}$$

is the symplectic potential three-form. It follows that the Noether current associated with ξ^a is given by the three-form

$$J_{abc}(\xi,\theta)=\Theta_{abc}(\theta,\mathcal{L}_\xi\theta)+4\xi^dL_{abcd}(\theta)=\epsilon_{abcd}(g)(8\,\theta^e_\mu\theta^d_\nu\mathcal{L}_\xi\Gamma_e{}^{\mu\nu}(\theta)+4\xi^dR(\theta)), \tag{2.33}$$

which simplifies to

$$J_{abc}(\xi;\theta)=3\partial_{[a}Q_{bc]}(\xi;\theta)-\xi^e\theta_{e\mu}\mathcal{E}^\mu_{abc}(\theta), \tag{2.34}$$

where

$$Q_{bc}(\xi;\theta)=4\xi^e\epsilon_{bcda}(g)\,\theta^d_\mu\theta^a_\nu\Gamma_e{}^{\mu\nu}(\theta) \tag{2.35}$$

is the Noether charge potential.

The gravitational Noether charge associated with $\partial\Sigma$ is determined by the pullback of $Q_{bc}(\xi;\theta)$. A simple expression for the pullback is obtained through identities (2.2) and (2.11), yielding

$$\epsilon^{bc}\xi^a\epsilon_{debc}(g)\,\theta^d_\mu\theta^e_\theta\Gamma_a{}^{\mu\nu}(\theta)=*\epsilon_{de}\theta^d_\mu\theta^e_\nu\xi^a\Gamma_a{}^{\mu\nu}(\theta)=4t_\mu s_\nu\xi^a\theta^{e\mu g}\nabla_a\theta^\nu_e=4\xi^as_\nu t^{e\,g}\nabla_a\theta^\nu_e, \tag{2.36}$$

where, recall, ϵ_{bc} is the volume form on $\partial\Sigma$. Hence, the surface integral

$$Q_\Sigma(\xi;\theta)=\int_{\partial\Sigma}Q_{bc}(\xi;\theta)=8\int_{\partial\Sigma}\epsilon_{bc}s_\nu t^e\xi^{a\,g}\nabla_a\theta^\nu_e \tag{2.37}$$

gives the gravitational Noether charge.

When ξ^a is not tangential to $\partial\Sigma$, the pullback of $\Theta_{bcd}(\theta,\delta\theta)$ to the hypersurface $\mathcal{B}$ can be simplified similarly by the identities (2.14) and (2.11) and the frame decomposition (2.24),

$$\begin{aligned}\tfrac{1}{8}\epsilon^{ab}\xi^c\Theta_{abc}(\theta,\delta\theta)&=\epsilon^{ab}\xi^c\epsilon_{abcd}(g)\,\theta^d_\mu\theta^e_\nu\delta\Gamma_e{}^{\nu\mu}(\theta)\\&=-2Ns_\mu\theta^e_\nu\delta(\theta^{c\nu g}\nabla_e\theta^\mu_c)\\&=-2Nh^e_\nu\delta(s_\mu h_e{}^d h^{c\nu g}\nabla_d\theta^\mu_c)\\&=\epsilon^{ab}\xi^c\epsilon_{abc}(h)h^e_\nu\delta K_e{}^\nu,\end{aligned} \tag{2.38}$$

where we define

$$K_a{}^\mu = s_\nu h_a{}^d h^{c\mu\, g} \nabla_d \theta_c^\nu . \tag{2.39}$$

(Note these expressions have the same form as those obtained in Ref. 1 when ξ^a is timelike.) Hence, one obtains

$$\mathcal{P}_{\mathcal{B}} \Theta_{abc}(\theta, \delta\theta) = 8\, \epsilon_{abc}(h) h_\nu^e \delta K_e{}^\nu . \tag{2.40}$$

This expression leads to a simple form for the gravitational symplectic flux associated with $\mathcal{B}$,

$$\begin{aligned} \int_{\mathcal{B}} \omega_{abc}(\theta, \delta_1\theta, \delta_2\theta) &= \int_{\mathcal{B}} \delta_1 \Theta_{abc}(\theta, \delta_2\theta) - \delta_2 \Theta_{abc}(\theta, \delta_1\theta) \\ &= 8 \int_{\mathcal{B}} \epsilon_{abc}(h) ((\delta_1 h_\mu^d - h_\mu^d h_e^\nu \delta_1 h_\nu^e)\, \delta_2 K_d{}^\mu \\ &\quad - (\delta_2 h_\mu^d - h_\mu^d h_e^\nu \delta_2 h_\nu^e)\, \delta_1 K_d{}^\mu). \end{aligned} \tag{2.41}$$

The vanishing of this flux determines the allowed boundary conditions on the frame θ_c^μ at the boundary hypersurface $\mathcal{B}$.

We remark that in a frame (2.26) adapted to $\partial\Sigma$, one sees that $K_a{}^\mu = h^{c\mu} h_a{}^{d\, g} \nabla_d s_c$ represents the frame components of the extrinsic curvature tensor $K_{ab} = h_a{}^d h_b{}^{c\, g} \nabla_d s_c$ of the boundary hypersurface $\mathcal{B}$. Moreover, the Noether charge (2.37) is simply $Q_\Sigma(\xi;\theta) = 8 \int_{\partial\Sigma} \epsilon_{bc} \xi^a t_\mu K_a{}^\mu = 8 \int_{\partial\Sigma} \epsilon_{bc} \xi^a t^e K_{ae}$.

For the sequel, we now introduce Dirichlet and Neumann symplectic vectors,

$$P_a^{\mathrm{D}}(\theta) = s_\nu t^c \sigma_a{}^{dg} \nabla_d \theta_c^\nu - s_\nu t_a \sigma^{bd\, g} \nabla_b \theta_d^\nu + t_\nu s_a \sigma^{bd\, g} \nabla_b \theta_d^\nu = \tfrac{1}{2} \epsilon^{bc} \epsilon_{acde} \theta_\mu^d \theta_\nu^e \Gamma_b{}^{\mu\nu}(\theta), \tag{2.42}$$

$$P_a^{\mathrm{N}}(\theta) = s_\nu t^{a\, g} \nabla_a \theta_c^\nu = \tfrac{1}{4} \epsilon^{bc} \epsilon_{bcde} \theta_\mu^d \theta_\nu^e \Gamma_a{}^{\mu\nu}(\theta), \tag{2.43}$$

associated with the boundary two-surface $\partial\Sigma$ and the frame θ_a^μ. In a frame (2.26) adapted to the hypersurface $\mathcal{B}$, these vectors take the more geometrical form

$$P_a^{\mathrm{D}}(\vartheta) = t^c \sigma_a{}^{d\, g} \nabla_d s_c - t_a \sigma^{bd\, g} \nabla_b s_d + s_a \sigma^{bd\, g} \nabla_b t_d , \tag{2.44}$$

$$P_a^{\mathrm{N}}(\vartheta) = t^{cg} \nabla_a s_c . \tag{2.45}$$

Similarly to the derivation in Ref. 1 holding for the situation when $\mathcal{B}$ is timelike, here the projection of the vectors (2.42) and (2.43) along ξ^a yields the respective boundary terms required to define a covariant Hamiltonian for the vacuum Einstein equations with ξ^a as the time-flow vector field in a space–time region with spatial boundary two-surface $\partial\Sigma$, subject to Dirichlet or Neumann boundary conditions on the frame θ_a^μ, for a timelike, spacelike, or null boundary hypersurface $\mathcal{B}$. The significance and properties of the full vectors (2.42) and (2.43) will be discussed in Sec. III.

Lastly, we make some remarks on the gauge invariance of the preceeding results, which follow from the detailed gauge transformation analysis given in Sec. 3 of Ref. 1. Under a local $SO(3,1)$ transformation on the frame θ_a^μ, the Noether charge $Q_{bc}(\xi;\theta)$ transforms inhomogeneously due to its explicit dependence on the frame connection. However, the curvature $R_{ab}{}^{\mu\nu}(\theta)$ is invariant, and consequently so is the Lagrangian $L_{abcd}(\theta)$. Therefore the symplectic current $\omega_{abc}(\theta, \delta_1\theta, \delta_2\theta)$ is necessarily gauge invariant. As a result, up to addition of a locally constructed exact two-form, the symplectic current obtained here for the frame formulation of the vacuum Einstein equations must agree with the analogous current derived from the standard metric formulation. This means that the presymplectic forms $\Omega_\Sigma(\theta, \delta\theta, \mathcal{L}_\xi\theta)$ and $\Omega_\Sigma(g, \delta g, \mathcal{L}_\xi g)$ in the two formulations differ by only a boundary term (i.e., a locally constructed two-form integrated over the two-surface $\partial\Sigma$). Correspondingly, the Dirichlet and Neumann symplectic vectors associated

with $\Omega_\Sigma(g,\delta g,\mathcal{L}_\xi g)$ in the metric formulation are found to be the same as the ones given here for the frame formulation, up to certain gradient terms. Furthermore, if ξ^a is timelike and orthogonal to $\partial\Sigma$, then these gradient terms can be shown to vanish. In this situation, $\xi^a P_a^{\mathrm{D}}(\vartheta)$ and $\xi^a P_a^{\mathrm{N}}(\vartheta)$ are precisely the Dirichlet and Neumann boundary terms in the covariant Hamiltonian determined by the metric formulation of the vacuum Einstein equations (see Ref. 2 for a discussion of this Hamiltonian). Consequently, as noted in Ref. 1, we find that the expression $\xi^a P_a^{\mathrm{D}}(\vartheta)$ reduces to the boundary term derived by Brown and York[3,4] in the standard canonical formalism, with Dirichlet boundary conditions on the canonical variables in the case of a hypersurface boundary $\mathcal{B}$ where ξ^a is timelike. In comparison, the covariant formulation we have presented here applies equally well when ξ^a is null or spacelike.

B. Electromagnetic field

We start by considering a free electromagnetic field A_a on (M,g_{ab}), coupled to the gravitational field, generalizing the Minkowski background space–time considered in Sec. 2 in Ref. 1. The Lagrangian four-form for A_a is given by

$$L_{abcd}(A;\theta)=\tfrac{1}{2}\epsilon_{abcd}(g)F_{mn}F^{mn}=3F_{[ab}{}^*F_{cd]}, \tag{2.46}$$

where $F_{ab}={}^g\nabla_{[a}A_{b]}=\partial_{[a}A_{b]}$ is the electromagnetic field strength and ${}^*F_{ab}=\epsilon_{abcd}(g)F^{cd}$ is the dual field strength in terms of $F^{cd}=g^{ca}g^{db}F_{bd}$, with $g_{ab}=\theta_a^\mu\theta_b^\nu\eta_{\mu\nu}$. A useful fact here is that ${}^g\nabla_a$ reduces to ∂_a in any skew derivative expression on M. By variation of A_a and θ_a^μ in this Lagrangian, one obtains

$$\delta L_{abcd}(A;\theta)=\epsilon_{abcd}(g)({}^g\nabla_m(\delta A_n F^{mn})-\delta A_n{}^g\nabla_m F^{mn}-T_\mu{}^e(A;\theta)\,\delta\theta_e^\mu), \tag{2.47}$$

where $T_\mu{}^e(A;\theta)\,\theta_e^\mu=T_d{}^e(A;g)$ is the electromagnetic stress–energy tensor given by

$$T_a{}^b(A;g)=2F_{ac}F^{bc}-\tfrac{1}{2}\delta_a^b F_{mn}F^{mn}. \tag{2.48}$$

From the coefficient of the variation δA_a in $\delta L_{abcd}(A;\theta)$, the field equation for A_a is given by the Maxwell equations

$${}^*\mathcal{E}_a(A;g)={}^g\nabla^b F_{ba}={}^g\nabla^b\partial_{[b}A_{a]}=0. \tag{2.49}$$

The symplectic potential three-form obtained from $L_{abcd}(A;\theta)$ is given by the total derivative term in Eq. (2.47), which yields

$$\Theta_{bcd}(A,\delta A;\theta)=4\epsilon_{abcd}(g)\,\delta A_e F^{ae}. \tag{2.50}$$

Hence, the Noether current associated with ξ^a for A_a is given by the three-form

$$\begin{aligned}J_{abc}(\xi,A;g)&=\Theta_{abc}(A,\mathcal{L}_\xi A;\theta)+4\xi^d L_{abcd}(A;\theta)\\&=\epsilon_{abcd}(g)(-4F^{de}\mathcal{L}_\xi A_e+2\xi^d F_{mn}F^{mn})\\&=4\epsilon_{dabc}(g)(\xi^e T_e{}^d(A;g)+\xi^e A_e{}^*\mathcal{E}^d(A;g))+6\partial_{[a}({}^*F_{bc]}\xi^e A_e)\end{aligned} \tag{2.51}$$

by a similar derivation as in Minkowski space–time, with

$$\mathcal{L}_\xi A_a=\xi^{eg}\nabla_e A_a+A_e{}^g\nabla_a\xi^e=2\xi^{eg}\nabla_{[e}A_{a]}+{}^g\nabla_a(\xi^e A_e). \tag{2.52}$$

This yields the electromagnetic Noether charge

$$Q_\Sigma(\xi;A)=\int_\Sigma J_{abc}(\xi,A;g)=4\int_\Sigma\xi^e\epsilon_{dabc}(g)T_e{}^d(A;g)+2\int_{\partial\Sigma}\epsilon_{bcda}F^{da}\xi^e A_e \tag{2.53}$$

for solutions A_a of the Maxwell equations (2.49).

The total Lagrangian for the Maxwell equations coupled to the Einstein equations

$$R_\mu{}^a(\theta)-\tfrac{1}{2}\theta^\mu_a R(\theta)=T_\mu{}^a(A;\theta) \tag{2.54}$$

using the field variables A_a and θ^μ_a is given by $L_{abcd}(\theta,A)=L_{abcd}(\theta)-L_{abcd}(A;\theta)$ from Eqs. (2.27) and (2.46). One then obtains the total Noether current

$$\begin{aligned} J_{abc}(\xi,\theta,A)&=J_{abc}(\xi,\theta)-J_{abc}(\xi,A;\theta)\\ &=8\epsilon_{dabc}(g)\xi^e\theta^\mu_e(R_\mu{}^d(\theta)-\tfrac{1}{2}\theta^d_\mu R(\theta)-T_\mu{}^d(A;\theta))+3\partial_{[a}Q_{bc]}(\xi,\theta,A), \end{aligned} \tag{2.55}$$

where

$$Q_{bc}(\xi,\theta,A)=\xi^a\epsilon_{bcde}(g)(4\theta^d_\mu\theta^e_\nu\Gamma_a{}^{\mu\nu}(\theta)-2F^{de}A_a) \tag{2.56}$$

is the Noether charge potential. Hence, on solutions of the coupled Einstein–Maxwell equations, the total Noether charge is given by the surface integral

$$Q_\Sigma(\xi;\theta,A)=\int_{\partial\Sigma}Q_{bc}(\xi,\theta,A). \tag{2.57}$$

The electromagnetic part of this expression simplifies through identities (2.2) and (2.11), yielding

$$\epsilon^{bc}{*}F_{bc}\xi^dA_d={*}\epsilon_{bc}F^{bc}\xi^dA_d=4t_bs_cF^{bc}\xi^dA_d\,. \tag{2.58}$$

Then, substituting Eq. (2.36) for the gravitational part, one obtains

$$Q_\Sigma(\xi;\theta,A)=\int_{\partial\Sigma}\epsilon_{bc}\xi^a(8s_\nu t^{eg}\nabla_a\theta^\nu_e-4t_ds_eF^{de}A_a). \tag{2.59}$$

The Noether current gives a Hamiltonian conjugate to ξ^a on Σ under compact support variations $\delta\theta^\mu_a$ and δA_a,

$$H(\xi;\theta,A)=8\int_\Sigma\epsilon_{dabc}(g)\xi^e\theta^\mu_e(R_\mu{}^d(\theta)-\tfrac{1}{2}\theta^d_\mu R(\theta)-T_\mu{}^d(A;\theta)) \tag{2.60}$$

up to a boundary term (2.59). For variations $\delta\theta^\mu_a$ and δA_a with support on $\partial\Sigma$, after taking into account boundary terms, one has

$$\delta H(\xi;\theta,A)=\int_{\partial\Sigma}\delta Q_{ab}(\xi,\theta,A)-\xi^c\Theta_{abc}(\theta,A,\delta\theta,\delta A) \tag{2.61}$$

for Einstein–Maxwell solutions, where

$$\Theta_{abc}(\theta,A,\delta\theta,\delta A)=\Theta_{abc}(\theta,\delta\theta)-\Theta_{abc}(A,\delta A;\theta)=\epsilon_{dabc}(g)(8\theta^d_\mu\theta^e_\nu\delta\Gamma_e{}^{\mu\nu}(\theta)-4F^{de}dA_e) \tag{2.62}$$

is the total symplectic potential three-form from Eqs. (2.32) and (2.50). The electromagnetic part of the symplectic potential terms in the Hamiltonian variation (2.61) can be simplified similarly to expression (2.38) for the gravitational part, yielding

$$\tfrac{1}{4}\epsilon^{ab}\xi^c\Theta_{abc}(A,\delta A;\theta)=\epsilon^{ab}\xi^c\epsilon_{dabc}(g)F^{de}\delta A_e=2Ns_dF^{de}\delta A_e=-\epsilon^{ab}\xi^c\epsilon_{abc}(h)s_dF^{de}\delta A_e \tag{2.63}$$

through identities (2.14) and (2.15). Thus, one obtains

$$\mathcal{P}_{\partial\Sigma}(\xi^c\Theta_{abc}(\theta,A,\delta\theta,\delta A))=\mathcal{P}_{\partial\Sigma}(\xi^c\epsilon_{abc}(h)(8h^e_\nu\delta K_e{}^\nu+4s_dF^{de}\delta A_e))$$
$$=-N\epsilon_{ab}(8h^e_\nu\delta K_e{}^\nu+4s_dF^{de}\delta A_e). \tag{2.64}$$

Hence, for the existence of a Hamiltonian conjugate to ξ^a on Σ, there must exist a locally constructed three-form $\tilde{B}_{abc}(\theta,A)$ such that

$$\mathcal{P}_{\partial\Sigma}(\xi^c\Theta_{abc}(\theta,A,\delta\theta,\delta A))=\mathcal{P}_{\partial\Sigma}(\xi^c\delta\tilde{B}_{abc}(\theta,A)-\partial_{[a}\alpha_{b]}(\xi,\theta,\delta\theta,\delta A)) \tag{2.65}$$

for some locally constructed one-form $\alpha_b(\xi,\theta,A,\delta\theta,\delta A)$ in $T^*(\partial\Sigma)$. Then the total Hamiltonian is given by $H(\xi;\theta,A)$ plus a boundary term

$$H_B(\xi;\theta,A)=\int_{\partial\Sigma}Q_{ab}(\xi,\theta,A)-\xi^c\tilde{B}_{abc}(\theta,A). \tag{2.66}$$

We now consider Dirichlet and Neumann type boundary conditions on the fields θ^μ_a and A_a at $\partial\Sigma$.

First, consider the case when ξ^a is tangential to $\partial\Sigma$. Then one finds $\mathcal{P}_{\partial\Sigma}(\xi^c\Theta_{abc}(\theta,A,\delta\theta,\delta A))=0$, which leads to the following result.

Proposition 2.1: Suppose ξ^a is tangential to $\partial\Sigma$. Then no *boundary conditions are necessary for existence of a Hamiltonian conjugate to ξ^a on Σ. Consequently, a Hamiltonian is given by $H_\Sigma(\xi;\theta,A)=H(\xi;\theta,A)+Q_\Sigma(\theta,A)$.*

Next, assume ξ^a is not tangential to $\partial\Sigma$, and consider Dirichlet and Neumann boundary conditions on the electromagnetic and gravitational field variables.

Theorem 2.2: *Suppose ξ^a is nowhere tangential to $\partial\Sigma$. Let*

$$\text{(D)}\quad \delta(h_a{}^bA_b)|_{\partial\Sigma}=0,\quad \delta(h^\mu_a)|_{\partial\Sigma}=0, \tag{2.67}$$

$$\text{(N)}\quad \delta(|h|s_bh_c{}^aF^{cb})|_{\partial\Sigma}=0,\quad \delta(K_a{}^\mu)|_{\partial\Sigma}=0, \tag{2.68}$$

where $|h|=\det(h^\mu_a)$ is the determinant of the components of the frame h^μ_a associated with $\mathcal{B}$. Under Dirichlet (D) or Neumann (N) boundary conditions for both A_a and θ^μ_a, there exists a Hamiltonian $H(\xi;\theta,A)+H_B(\xi;\theta,A)$ conjugate to ξ^a on Σ, with the boundary term (2.66) given by

$$H^{\mathrm{D}}(\xi;\theta,A)=8\int_{\partial\Sigma}\xi^a(P^{\mathrm{D}}_a(\theta)-\tfrac{1}{2}t_ds_eF^{de}A_a)\mathrm{d}S, \tag{2.69}$$

$$H^{\mathrm{N}}(\xi;\theta,A)=8\int_{\partial\Sigma}\xi^a(P^{\mathrm{N}}_a(\theta)-\sigma_{[a}{}^ct_{d]}s_eF^{de}A_c)\mathrm{d}S, \tag{2.70}$$

in terms of the Dirichlet and Neumann symplectic vectors (2.42) and (2.43).

Proof: For case (D), first note from Eq. (2.63) that $\epsilon^{bc}\xi^a\Theta_{abc}(A,\delta A;\theta)=8Ns_dF^{de}h_e{}^c\delta A_c$. Now, using the boundary condition (D) on δA_a, one has

$$h_e{}^c\delta A_c=h_e{}^c\delta(s_cs^{*b}A_b)=s^{*b}A_bh_e{}^c\delta s_c=0 \tag{2.71}$$

by the hypersurface orthogonality relations (2.7) and (2.23). Thus,

$$\mathcal{P}_{\partial\Sigma}(\xi^a\Theta_{abc}(A,\delta A;\theta))=0. \tag{2.72}$$

Then, in Eq. (2.38), since $\delta\epsilon_{abc}(h)=\delta\epsilon_{bc}=0$ by the boundary condition (D) on $\delta\theta^\mu_a$, one has

$$\epsilon^{bc}\xi^a\Theta_{abc}(\theta,\delta\theta)=\epsilon^{bc}\delta(8\xi^a\epsilon_{abc}(h)K) \tag{2.73}$$

and thus,

$$\mathcal{P}_{\partial\Sigma}(\xi^a\Theta_{abc}(\theta,\delta\theta)-\delta(8\xi^a\epsilon_{abc}(h)K))=0, \tag{2.74}$$

where $K=h^e_\nu K_e{}^\nu$. Hence, substitution of Eqs. (2.72) and (2.74) into Eq. (2.65) yields

$$\xi^a\tilde{B}_{abc}(\theta,A)=8\xi^a\epsilon_{abc}(h)K \tag{2.75}$$

and $\alpha_b=0$. This leads to the boundary term (2.69) through Eq. (2.66) as follows. The pullback of $\xi^a\tilde{B}_{abc}(\theta,A)$ to $\partial\Sigma$ is given by

$$8\xi^a\epsilon^{bc}\epsilon_{abc}(h)K=8\xi^a t_a s_\nu h_d{}^e{}^g\nabla_e\theta^{d\nu}=16\xi^a t_a s_\nu h_d{}^e{}^g\nabla_e\theta^{d\nu}, \tag{2.76}$$

which, when combined with expression (2.36) for the pullback of $Q_{bc}(\xi,\theta)$, yields

$$\begin{aligned}\epsilon^{bc}(Q_{bc}(\xi,\theta)-\xi^a\tilde{B}_{abc}(\theta,A))&=16\xi^a(s_\nu t^e{}^g\nabla_a\theta^\nu_e-t_a s_\nu h_d{}^e{}^g\nabla_e\theta^{d\nu})\\&=16\xi^a s_\nu(t^d\sigma_a{}^e-t_a\sigma^{de})^g\nabla_e\theta^\nu_d=16\xi^a P^{\mathrm{D}}_a(\theta)\end{aligned} \tag{2.77}$$

by the metric decompositions (2.6) and (2.9) and the orthogonality $\xi^a s_a=0$. Finally, combining this expression with the pullback of $Q_{bc}(\xi,A)$ given by Eq. (2.58), we obtain Eq. (2.69).

For case (N), one has from Eq. (2.63) that

$$\epsilon^{bc}\xi^a\Theta_{abc}(A,\delta A;\theta)=\epsilon^{bc}\delta(4\xi^a\epsilon_{abc}(h)s_e A_d F^{de})+4\epsilon^{bc}A_e\xi^a\delta(\epsilon_{abc}(h)s_d F^{de}). \tag{2.78}$$

Now, since

$$\delta(\epsilon_{abc}(h)s_d F^{de})=\epsilon_{abc}(h)(\delta(s_d h_m{}^e F^{dm})+\delta\ln|h|s_d h_m{}^e F^{dm}), \tag{2.79}$$

this term vanishes by boundary condition (N) for δF^{ab}, and thus

$$\mathcal{P}_{\partial\Sigma}(\xi^a\Theta_{abc}(A,\delta A;\theta)-\delta(4\xi^a\epsilon_{abc}(h)s_e A_d F^{de}))=0. \tag{2.80}$$

Next, $\mathcal{P}_{\partial\Sigma}(\xi^a\Theta_{abc}(\theta,\delta\theta))=0$ holds immediately by boundary condition (N) for $\delta K_a{}^\mu$. Hence, from Eqs. (2.65) and (2.80), one has $\alpha_b=0$ and

$$\xi^a\tilde{B}_{abc}(\theta,A)=4\xi^a\epsilon_{abc}(h)s_e A_d F^{de}. \tag{2.81}$$

Then this leads to the boundary term (2.70) through Eq. (2.66) similarly to the derivation of the boundary term (2.69) above. □

C. Klein–Gordon scalar field

We next consider a free Klein–Gordon scalar field φ coupled to the gravitational field on (M,g_{ab}), with the standard Lagrangian four-form given by

$$L_{abcd}(\varphi;\theta)=\tfrac{1}{2}\epsilon_{abcd}(g)({}^g\nabla_e\varphi{}^g\nabla^e\varphi+m^2\varphi^2), \tag{2.82}$$

where $m=$const is the mass. Note, here ${}^g\nabla_a\varphi=\partial_a\varphi$, ${}^g\nabla^a\varphi=g^{ab}\partial_b\varphi$, and $g_{ab}=\theta^\mu_a\theta^\nu_b\eta_{\mu\nu}$. A variation of this Lagrangian with respect to φ and θ^μ_a yields

$$\delta L_{abcd}(\varphi;\theta)=\epsilon_{abcd}(g)({}^g\nabla_e(\delta\varphi{}^g\nabla^e\varphi)-\delta\varphi({}^g\nabla^e{}^g\nabla_e\varphi-m^2\varphi)-T_\mu{}^e(\varphi;\theta)\delta\theta^\mu_e), \tag{2.83}$$

where $T_\mu{}^e(\varphi;\theta)\theta^\mu_e=T_d{}^e(\varphi;g)$ is the Klein–Gordon stress–energy tensor given by

$$T_a{}^b(\varphi;g)={}^g\nabla^b\varphi{}^g\nabla_a\varphi-\tfrac{1}{2}\delta^b_a({}^g\nabla_e\varphi{}^g\nabla^e\varphi+m^2\varphi^2). \tag{2.84}$$

Hence, from the coefficient of the variation $\delta\varphi$ in Eq. (2.83), the Klein–Gordon field equation for φ is given by

$$*\mathcal{E}(\varphi;g) = {}^g\nabla^a\partial_a\varphi - m^2\varphi = 0. \tag{2.85}$$

The symplectic potential three-form obtained from $L_{abcd}(\varphi;\theta)$ is given by

$$\Theta_{bcd}(\varphi,\delta\varphi;\theta) = 4\epsilon_{abcd}(g)\,{}^g\nabla^a\varphi\,\delta\varphi. \tag{2.86}$$

This yields the Noether current associated with ξ^a,

$$\begin{aligned} J_{abc}(\xi,\varphi;g) &= \Theta_{abc}(\varphi,\mathcal{L}_\xi\varphi;\theta) + 4\xi^d L_{abcd}(\varphi;\theta) \\ &= \epsilon_{abcd}(g)(-4\,{}^g\nabla^d\varphi\,\mathcal{L}_\xi\varphi + 2\xi^d({}^g\nabla_e\varphi\,{}^g\nabla^e\varphi + m^2\varphi^2) \\ &= 4\epsilon_{dabc}(g)\xi^e T_e{}^d(\varphi;g), \end{aligned} \tag{2.87}$$

where $\mathcal{L}_\xi\varphi = \xi^e\,{}^g\nabla_e\varphi = \xi^e\partial_e\varphi$. Hence, one obtains the Noether charge

$$Q_\Sigma(\xi;\varphi) = \int_\Sigma J_{abc}(\xi,\varphi;g) = 4\int_\Sigma \epsilon_{dabc}(g)\xi^e T_e{}^d(\varphi;g). \tag{2.88}$$

In contrast to the situation for the electromagnetic field, here, due to the scalar nature of the Klein–Gordon field, the Noether charge does not have a surface integral term.

The total Lagrangian for the Klein–Gordon equation coupled to the Einstein equations

$$R_\mu{}^a(\theta) - \tfrac{1}{2}\theta_a^\mu R(\theta) = T_\mu{}^a(\varphi;\theta) \tag{2.89}$$

using the field variables φ and θ_a^μ is obtained through Eqs. (2.27) and (2.82) by $L_{abcd}(\theta,\varphi) = L_{abcd}(\theta) - L_{abcd}(\varphi;\theta)$. The resulting total Noether current is given by

$$\begin{aligned} J_{abc}(\xi,\theta,\varphi) &= J_{abc}(\xi,\theta) - J_{abc}(\xi,\varphi;\theta) \\ &= 8\epsilon_{dabc}(g)\xi^e\theta_e^\mu(R_\mu{}^d(\theta) - \tfrac{1}{2}\theta_\mu^d R(\theta) - T_\mu{}^d(\varphi;\theta)) + 3\partial_{[a}Q_{bc]}(\xi,\theta), \end{aligned} \tag{2.90}$$

where $Q_{bc}(\xi,\theta)$ is the gravitational Noether charge potential (2.35). Thus, there is no contribution from φ to the total Noether charge.

The Noether current gives a Hamiltonian conjugate to ξ^a on Σ under compact support variations $\delta\theta_a^\mu$ and $\delta\varphi$,

$$H(\xi;\theta,\varphi) = 8\int_\Sigma \epsilon_{dabc}(g)\xi^e\theta_e^\mu(R_\mu{}^d(\theta) - \tfrac{1}{2}\theta_\mu^d R(\theta) - T_\mu{}^d(\varphi;\theta)) \tag{2.91}$$

up to a boundary term $\int_{\partial\Sigma} Q_{ab}(\xi,\theta)$. For variations $\delta\theta_a^\mu$ and $\delta\varphi$ with support on $\partial\Sigma$, one has for Einstein–Klein–Gordon solutions,

$$\delta H(\xi;\theta,\varphi) = \int_{\partial\Sigma} \delta Q_{ab}(\xi,\theta) - \xi^c\Theta_{abc}(\theta,\delta\theta), \tag{2.92}$$

where $\Theta_{abc}(\theta,\delta\theta)$ is the expression (2.38) for the gravitational symplectic potential. Thus, there exists a Hamiltonian conjugate to ξ^a on Σ if

$$\mathcal{P}_{\partial\Sigma}(\xi^c\Theta_{abc}(\theta,\varphi,\delta\theta,\delta\varphi)) = \mathcal{P}_{\partial\Sigma}(\xi^c\delta\tilde{B}_{abc}(\theta,\varphi) - \partial_{[a}\alpha_{b]}(\xi,\theta,\varphi,\delta\theta,\delta\varphi)) \tag{2.93}$$

holds for a locally constructed three-form $\tilde{B}_{abc}(\theta,\varphi)$ and one-form $\alpha_b(\xi,\theta,\varphi,\delta\theta,\delta\varphi)$. Then the total Hamiltonian is given by $H(\xi;\theta,\varphi)$ plus a boundary term

$$H_B(\xi;\theta,\varphi)=\int_{\partial\Sigma} Q_{ab}(\xi,\theta)-\xi^c\tilde{B}_{abc}(\theta,\varphi). \tag{2.94}$$

Now, by an analysis similar to that for the Einstein–Maxwell equations, we obtain the following results.

Proposition 2.3: Suppose ξ^a *is tangential to* $\partial\Sigma$. *Then* no *boundary conditions are necessary for existence of a Hamiltonian conjugate to* ξ^a *on* Σ. *Consequently, a Hamiltonian is given by* $H_\Sigma(\xi;\theta,\varphi)=H(\xi;\theta,\varphi)+Q_\Sigma(\theta)$.

Theorem 2.4: *Suppose* ξ^a *is nowhere tangential to* $\partial\Sigma$. *Let*

$$\text{(D)}\quad \delta(\varphi)|_{\partial\Sigma}=0,\quad \delta(h_a^\mu)|_{\partial\Sigma}=0, \tag{2.95}$$

$$\text{(N)}\quad \delta(|h|s^a\partial_a\varphi)|_{\partial\Sigma}=0,\quad \delta(K_a{}^\mu)|_{\partial\Sigma}=0, \tag{2.96}$$

where $|h|=\det(h_a^\mu)$ *is the determinant of the components of the frame* h_a^μ *associated with* $\mathcal{B}$. *Under Dirichlet (D) or Neumann (N) boundary conditions for both* φ *and* θ_a^μ, *there exists a Hamiltonian* $H(\xi;\theta,\varphi)+H_B(\xi;\theta,\varphi)$ *conjugate to* ξ^a *on* Σ, *with the boundary term (2.94) given by*

$$H^{\mathrm{D}}(\xi;\theta,\varphi)=8\int_{\partial\Sigma}\xi^a P_a^{\mathrm{D}}(\theta)\mathrm{d}S, \tag{2.97}$$

$$H^{\mathrm{N}}(\xi;\theta,\varphi)=8\int_{\partial\Sigma}\xi^a(P_a^{\mathrm{N}}(\theta)-\tfrac{1}{2}t_a\varphi s^d\partial_d\varphi)\mathrm{d}S, \tag{2.98}$$

in terms of the Dirichlet and Neumann symplectic vectors (2.42) and (2.43).

D. Yang–Mills and Higgs fields

Last, we generalize the previous two examples by considering on (M,g_{ab}) a set of Yang–Mills fields A_a^{Υ} and Higgs fields φ^{Υ}, $\Upsilon=1,\ldots,n$, with a gauge group given by any n-dimensional semi-simple Lie group $\mathcal{G}$, $n\geqslant 3$. Let $C_{\Delta\Lambda}{}^{\Upsilon}$ be the commutator structure constants of the Lie algebra $\mathcal{A}$ of $\mathcal{G}$ (in a fixed basis). The structure constants are skew $C_{\Delta\Lambda}{}^{\Upsilon}=-C_{\Lambda\Delta}{}^{\Upsilon}$ and satisfy the Jacobi relation $C_{[\Delta\Lambda}{}^{\Upsilon}C_{\Pi]\Upsilon}{}^{\Phi}=0$. Let $\Gamma_{a\Delta}^{\Upsilon}(A)=C_{\Lambda\Delta}{}^{\Upsilon}A_a^{\Lambda}$ be the Yang–Mills connection, and define $k_{\Delta\Upsilon}=-1/2C_{\Delta\Lambda}{}^{\Pi}C_{\Upsilon\Pi}{}^{\Lambda}$, which denotes the positive definite Cartan–Killing metric on $\mathcal{A}$.

The Yang–Mills Lagrangian for A_a^{Υ} is given by the four-form

$$L_{abcd}(A;\theta)=\tfrac{1}{2}\epsilon_{abcd}(g)k_{\Lambda\Upsilon}F_{mn}^{\Lambda}F^{\Upsilon mn}=3k_{\Lambda\Upsilon}F_{[ab}^{\Lambda}{}^*F_{cd]}^{\Upsilon}, \tag{2.99}$$

where

$$F_{ab}^{\Lambda}={}^g\nabla_{[a}A_{b]}^{\Lambda}+\tfrac{1}{2}C_{\Delta\Upsilon}{}^{\Lambda}A_a^{\Delta}A_b^{\Upsilon} \tag{2.100}$$

is the Yang–Mills field strength, ${}^*F_{ab}^{\Lambda}=\epsilon_{abcd}(g)F^{\Lambda cd}$ is the dual field strength in terms of $F^{\Lambda cd}=g^{ca}g^{db}F_{bd}^{\Lambda}$, with $g_{ab}=\theta_a^\mu\theta_b^\nu\eta_{\mu\nu}$. For φ^{Υ}, it is convenient to introduce the gauge-covariant Higgs field strength

$$W_a^{\Lambda}={}^g\nabla_a\varphi^{\Lambda}+e\Gamma_{a\Upsilon}^{\Lambda}(A)\varphi^{\Upsilon}. \tag{2.101}$$

In terms of this field strength the Higgs Lagrangian is given by the four-form

$$L_{abcd}(\varphi;\theta)=\epsilon_{abcd}(g)(\tfrac{1}{2}k_{\Lambda\Upsilon}W_m^{\Lambda}W^{m\Upsilon}+V(|\varphi|)), \tag{2.102}$$

where $V(|\varphi|)$ is a Higgs potential with $|\varphi|^2=k_{\Lambda\Upsilon}\varphi^{\Lambda}\varphi^{\Upsilon}$, and $e=\text{const}$ is a coupling constant. These Lagrangians are gauge invariant under Yang–Mills gauge symmetries on the fields A_a^{Υ} and

φ^{Υ}. (In particular, if ${U^{\Upsilon}}_{\Lambda}$ denotes a homomorphism of $\mathcal{A}$ given by a function of the space–time coordinates x^{μ}, it is straightforward to show that the Yang–Mills gauge symmetry is then given by $A_a^{\Upsilon} \to {U^{-1\Upsilon}}_{\Lambda} A_a^{\Lambda} - {C^{*\Upsilon\Delta}}_{\Lambda} {U^{-1\Lambda}}_{\Pi} \partial_a {U^{\Pi}}_{\Delta}$ and $\varphi^{\Upsilon} \to {U^{-1\Upsilon}}_{\Lambda} \varphi^{\Lambda}$, where ${C^{*\Upsilon\Delta}}_{\Lambda} = k^{\Upsilon\Pi} C_{\Lambda\Pi}{}^{\Delta}$ denotes the structure constants of the dual Lie algebra $\mathcal{A}^*$ and $k^{\Upsilon\Pi}$ is the inverse of the Cartan–Killing metric. Under these transformations, the field strengths are gauge covariant, $F_{ab}^{\Upsilon} \to {U^{-1\Upsilon}}_{\Lambda} F_{ab}^{\Lambda}$ and $W_a^{\Upsilon} \to {U^{-1\Upsilon}}_{\Lambda} W_a^{\Lambda}$.)

To proceed, we consider the combined Yang–Mills–Higgs Lagrangian,

$$L_{abcd}(A,\varphi;\theta) = L_{abcd}(A;\theta) + L_{abcd}(\varphi;\theta). \tag{2.103}$$

First, the coefficient of the variation δA_a^{Υ} yields the Yang–Mills field equations

$$k^{\Upsilon\Lambda} {}^*\mathcal{E}_{a\Upsilon}(A;g) = {}^g\nabla^b F_{ba}^{\Lambda} + \Gamma^{b\Lambda}{}_{\Upsilon}(A) F_{ba}^{\Upsilon} - e C_{\Pi\Upsilon}{}^{\Lambda} \varphi^{\Pi} W_a^{\Upsilon} = 0, \tag{2.104}$$

where $e C_{\Pi\Upsilon}{}^{\Lambda} \varphi^{\Pi} W_a^{\Upsilon}$ has the role of a current source. The coefficient of the variation $\delta\varphi^{\Upsilon}$ similarly yields the Higgs field equations

$$k^{\Upsilon\Lambda} {}^*\mathcal{E}_{\Upsilon}(A;g) = {}^g\nabla^a W_a^{\Lambda} + \Gamma^{a\Lambda}{}_{\Upsilon}(A) W_a^{\Upsilon} - \frac{1}{|\varphi|} V'(|\varphi|) \varphi^{\Lambda} = 0. \tag{2.105}$$

Next, by variation of θ_a^{μ}, one obtains the Yang–Mills–Higgs stress–energy tensor ${T_{\mu}}^{e}(A,\varphi;\theta)\theta_e^{\mu} = {T_d}^{e}(A,\varphi;g)$ where

$${T_a}^{b}(A,\varphi;g) = k_{\Lambda\Upsilon}(2F_{ac}^{\Lambda} F^{\Upsilon bc} + W_a^{\Lambda} W^{\Upsilon b}) - \tfrac{1}{2}\delta_a^b k_{\Lambda\Upsilon}(F_{mn}^{\Lambda} F^{\Upsilon mn} + W_m^{\Lambda} W^{m\Upsilon}) - \delta_a^b V(|\varphi|). \tag{2.106}$$

The symplectic potential three-form arising from the Lagrangian (2.103) is given by

$$\Theta_{bcd}(A,\varphi,\delta A,\varphi;\theta) = 4\epsilon_{abcd}(g) k_{\Lambda\Upsilon}(\delta A_e^{\Lambda} F^{\Upsilon ae} + \delta\varphi^{\Lambda} W^{\Upsilon a}). \tag{2.107}$$

This yields the Noether current

$$\begin{aligned} J_{abc}(\xi,A,\varphi;g) &= \Theta_{abc}(A,\varphi,\mathcal{L}_{\xi}A,\mathcal{L}_{\xi}\varphi;\theta) + 4\xi^d L_{abcd}(A,\varphi;\theta) \\ &= \epsilon_{abcd}(g)(k_{\Lambda\Upsilon}(-4F^{\Lambda de}\mathcal{L}_{\xi}A_e^{\Upsilon} + \xi^d 2F_{mn}^{\Lambda} F^{\Upsilon mn}) \\ &\quad + k_{\Lambda\Upsilon}(-4W^{\Lambda d}\mathcal{L}_{\xi}\varphi^{\Upsilon} + 2W_m^{\Lambda} W^{m\Upsilon})) + 4V(|\varphi|)) \\ &= 4\epsilon_{dabc}(g)(\xi^e {T_e}^{d}(A,\varphi;g) + 6\partial_{[a}(k_{\Lambda\Upsilon} {}^*F_{bc]}^{\Lambda} \xi^e A_e^{\Upsilon}) \end{aligned} \tag{2.108}$$

for Yang–Mills–Higgs solutions. Hence, one obtains the Noether charge

$$Q_{\Sigma}(\xi;A,\varphi) = \int_{\Sigma} J_{abc}(\xi,A,\varphi;g) = 4\int_{\Sigma} \xi^e \epsilon_{dabc}(g) {T_e}^{d}(A,\varphi;g) + 2\int_{\partial\Sigma} k_{\Lambda\Upsilon}\epsilon_{bcda} F^{\Lambda da}\xi^e A_e^{\Upsilon}. \tag{2.109}$$

For the Yang–Mills–Higgs equations coupled to the Einstein equations

$$R_{\mu}^{a}(\theta) - \tfrac{1}{2}\theta_a^{\mu} R(\theta) = {T_{\mu}}^{a}(A,\varphi;\theta) \tag{2.110}$$

using the field variables A_a^{Υ}, φ^{Υ}, θ_a^{μ}, the total Lagrangian is given by $L_{abcd}(\theta,A,\varphi) = L_{abcd}(\theta) - L_{abcd}(A,\varphi;\theta)$ from Eqs. (2.27) and (2.103).

Through the same analysis as used in the Maxwell and Klein–Gordon examples, we obtain the following results.

Proposition 2.5: Suppose ξ^a is tangential to $\partial\Sigma$. Then no *boundary conditions are necessary for existence of a Hamiltonian conjugate to ξ^a on Σ. Consequently, a Hamiltonian is given by*

$$H(\xi;\theta,A,\varphi)=8\int_\Sigma \epsilon_{dabc}(g)\xi^e\theta^\mu_e(R_\mu{}^d(\theta)-\tfrac{1}{2}\theta^d_\mu R(\theta)-T_\mu{}^d(A,\varphi;\theta)) \tag{2.111}$$

up to an unessential boundary term.

Theorem 2.6: *Suppose ξ^a is nowhere tangential to $\partial\Sigma$. Let*

$$\text{(D)}\quad \delta(A^{\mathrm{Y}}_a)|_{\partial\Sigma}=0,\quad \delta(\varphi^{\mathrm{Y}})|_{\partial\Sigma}=0,\quad \delta(h^\mu_a)|_{\partial\Sigma}=0, \tag{2.112}$$

$$\text{(N)}\quad \delta(|h|s_b h_c{}^a F^{\mathrm{Y}cb})|_{\partial\Sigma}=0,\quad \delta(|h|s^a W^{\mathrm{Y}}_a)|_{\partial\Sigma}=0,\quad \delta(K_a{}^\mu)|_{\partial\Sigma}=0, \tag{2.113}$$

where $|h|=\det(h^\mu_a)$ is the determinant of the components of the frame h^μ_a associated with $\mathcal{B}$. Under Dirichlet (D) or Neumann (N) boundary conditions for both φ and θ^μ_a, there exists a Hamiltonian $H(\xi;\theta,A,\varphi)+H_B(\xi,\theta,A,\varphi)$ conjugate to ξ^a on Σ, with the boundary term given by

$$H^{\mathrm{D}}(\xi;\theta,A,\varphi)=8\int_{\partial\Sigma}\xi^a(P^{\mathrm{D}}_a(\theta)-P^{\mathrm{D}}_a(A))\mathrm{d}S, \tag{2.114}$$

$$H^{\mathrm{N}}(\xi;\theta,A,\varphi)=8\int_{\partial\Sigma}\xi^a(P^{\mathrm{N}}_a(\theta)-P^{\mathrm{N}}_a(A,\varphi))\mathrm{d},S, \tag{2.115}$$

where

$$P^{\mathrm{D}}_a(A)=\tfrac{1}{2}k_{\Lambda\mathrm{Y}}t_d s_e F^{\mathrm{Y}de}A^\Lambda_a, \tag{2.116}$$

$$P^{\mathrm{N}}_a(A,\varphi)=k_{\Lambda\mathrm{Y}}(\sigma_{[a}{}^c t_{d]}s_e F^{\mathrm{Y}de}A^\Lambda_c+\tfrac{1}{2}t_a s^d W^{\mathrm{Y}}_d\varphi^\Lambda), \tag{2.117}$$

and $P^{\mathrm{D}}_a(\theta)$, $P^{\mathrm{N}}_a(\theta)$ are the symplectic vectors given by (2.42) *and* (2.43).

E. Remarks

Clearly, the previous results when ξ^a is not tangential to $\partial\Sigma$ are easily generalized to mixed Dirichlet–Neumann boundary conditions on the tetrad and matter fields similar to Theorem 2.3 and Theorems 3.5 and 3.6 in Ref. 1. In particular, for allowed boundary conditions, note that one can have the tetrad satisfying (D) while the matter fields satisfy (N), and vice versa.

III. PROPERTIES OF THE SYMPLECTIC VECTORS

We first review some geometry of spatial two-surfaces in space–time (most of this material is standard, e.g., Ref. 5–8). Then we describe the properties of the Dirichlet and Neumann symplectic vectors regarded as locally constructed geometrical vector fields associated with a fixed spatial two-surface in space–time, independent of any Hamiltonian structure.

A. Two-surface geometry

Let (S,σ_{ab}) be a closed, orientable, smooth spacelike two-surface in a space–time (M,g_{ab}), where σ_{ab} is the pullback of g_{ab} to S. Let $T(S)$ and $T(S)^\perp$ denote, respectively, the tangent space of S and the normal space to S [defined by the orthogonal complement of $T(S)$ in $T(M)$]. Since $T(S)\oplus T(S)^\perp=T(M)$, every vector in $T(M)$ has a unique decomposition into vectors tangent and normal to $T(S)$, given by projection operators $\mathcal{P}_S:T(M)\to T(S)$, $\mathcal{P}^\perp_S:T(M)\to T(S)^\perp$.

Fix an oriented orthonormal frame $\{t^a,s^a\}$ for $T(S)^\perp$,

$$t^a s_a=0,-t^a t_a=s^a s_a=1, \tag{3.1}$$

with t^a being a future timelike unit vector and s^a being an outward spacelike unit vector. (If M is spatially noncompact, we define the ''outward'' direction by the exterior of the set $M-S$. If M is spatially compact, there is no preferred way in general to distinguish the sets S and $M-S$, so we then make an arbitrary consistent choice for an ''outward'' direction.) The metric on S is given by

$$\sigma_{ab} = g_{ab} + t_a t_b - s_a s_b . \tag{3.2}$$

The compatible volume form on S is given by

$$\epsilon_{ab} = \epsilon_{abcd}(g) s^c t^d, \tag{3.3}$$

satisfying $\sigma_{c[a}\sigma_{b]d} = \epsilon_{ab}\epsilon_{cd}$. The projection operators for $T(S)$ and $T(S)^\perp$ are given by

$$(\mathcal{P}_S)_a{}^b = \sigma_a{}^b + \epsilon_{ac}\epsilon^{bc}, \quad (\mathcal{P}_S^\perp)_a{}^b = s_a s^b - t_a t^b = \sigma_a^{\perp b} = \epsilon_{ac}^\perp \epsilon^{\perp bc}, \tag{3.4}$$

where $\epsilon_{ab}^\perp = 2 s_{[a} t_{b]}$ and

$$\sigma_{ab}^\perp = s_a s_b - t_a t_b . \tag{3.5}$$

Both σ_{ab} and ϵ_{ab} are independent of choice of the orthonormal frame. Since $\sigma_{ab}^\perp$ is a two-dimensional Lorentz metric, any two oriented orthonormal frames $\{t^a, s^a\}$ and $\{t'^a, s'^a\}$ differ by a local boost

$$t'^a = (\cosh\chi) t^a + (\sinh\chi) s^a, \quad s'^a = (\cosh\chi) s^a + (\sinh\chi) t^a, \tag{3.6}$$

where χ is a function on S. Under an arbitrary boost (3.6), σ_{ab} and ϵ_{ab} are invariant.

The intrinsic geometry of the two-surface S is completely determined by the metric σ_{ab}. In particular, the intrinsic curvature of S is given by

$$[\mathcal{D}_a, \mathcal{D}_b] v_c = \mathcal{R}_{abc}{}^d v_d , \tag{3.7}$$

where v_c is any dual tangent vector field on S, and $\mathcal{D}_a$ denotes the metric compatible (torsion-free) derivative operator on S defined by $\mathcal{D}_a \sigma_{bc} = 0$. Since S is two-dimensional, it follows that the intrinsic curvature tensor has only one linearly independent component

$$\mathcal{R}_{abc}{}^d = \tfrac{1}{2}\sigma_{c[a}\sigma_{b]}{}^d \mathcal{R} = \tfrac{1}{2}\epsilon_{ab}\epsilon_c{}^d \mathcal{R} \tag{3.8}$$

where $\mathcal{R}$ denotes the scalar curvature of S.

The two-surface S also has an extrinsic geometry with respect to (M, g_{ab}), which is characterized by the following curvatures.[5,8] Let $\nabla_a^S = \sigma_a{}^b \nabla_b$ where ∇_b is the metric compatible (torsion-free) derivative operator on (M, g_{ab}). Then ∇_a^S can be decomposed into the tangential derivative operator $\mathcal{D}_a$ and a normal derivative operator $\mathcal{D}_a^\perp$, with $\nabla_a^S = \mathcal{D}_a + \mathcal{D}_a^\perp$, defined by $\mathcal{D}_a^\perp v^b = \sigma_c^{\perp b} \nabla_a^S v^c$ for any vector field v^a in $T(M)$ at S. Now consider $\nabla_a^S t_b$ and $\nabla_a^S s_b$. The tangential parts yield the extrinsic curvature tensors of S with respect to the orthonormal frame

$$\kappa_{ab}(t) = \mathcal{D}_a t_b , \quad \kappa_{ab}(s) = \mathcal{D}_a s_b , \tag{3.9}$$

which are symmetric tensors on S. These measure the spatial rotation of the orthonormal frame in $T(S)^\perp$ under displacement on S. The normal parts of $\nabla_a^S t_b$ and $\nabla_a^S s_b$ give

$$\mathcal{D}_a^\perp t_b = s_b \mathcal{J}_a^\perp , \quad \mathcal{D}_a^\perp s_b = - t_b \mathcal{J}_a^\perp , \tag{3.10}$$

where

$$\mathcal{J}_a^\perp = s^c \nabla_a^S t_c , \tag{3.11}$$

which measures the boost of the orthonormal frame in $T(S)^\perp$ under displacement on S. The commutator of $\mathcal{D}_a^\perp$ defines the *normal curvature* of S,

$$[\mathcal{D}_a^\perp, \mathcal{D}_b^\perp] v_c = \mathcal{R}_{abc}^\perp{}^d v_d , \tag{3.12}$$

with

$$\mathcal{R}^{\perp}_{abcd} = 2\mathcal{D}_{[a}\mathcal{J}^{\perp}_{b]}\epsilon^{\perp}_{cd}, \tag{3.13}$$

where v_c is any dual normal vector field on S. Hence, $\mathcal{J}^{\perp}_a$ is geometrically a connection one-form on S associated with the normal curvature of S. Since S is two-dimensional, note $\mathcal{R}^{\perp}_{abcd}$ has only one linearly independent component, which is proportional to $\epsilon^{ab}\nabla^S_a\mathcal{J}^{\perp}_b$.

The trace of the extrinsic curvatures (3.9) of S,

$$\kappa(t) = \sigma^{ab}\kappa_{ab}(t), \quad \kappa(s) = \sigma^{ab}\kappa_{ab}(s), \tag{3.14}$$

measures how the two-surface area changes under infinitesimal dragging of S along each direction of the orthonormal frame. In particular, for any vector field v^a in $T(S)^{\perp}$,

$$\mathcal{L}_v\epsilon_{ab} = \kappa(v)\epsilon_{ab}, \tag{3.15}$$

with

$$\kappa(v) = \mathcal{D}_a v^a = \tfrac{1}{2}\sigma^{ab}\mathcal{L}_v\sigma_{ab}. \tag{3.16}$$

Thus, S is ''expanding'' or ''contracting'' in the direction v^a according to whether its trace extrinsic curvature $\kappa(v)$ is positive or negative. [More precisely, $\kappa(v)$ equals the rate of change of the area of the image of S under any diffeomorphism of M whose generator agrees with v^a at S.] We say that the expansion of S defined by (3.15) for a direction v^a is spacelike, timelike, or null, if $v^a v_a$ is, respectively, positive, negative, or zero. If v^a is non-null, we refer to $|\kappa(v)|/|v|$ as the *absolute expansion* of S in the direction v^a (with $|v| = \sqrt{|v^a v_a|}$).

A preferred direction in $T(S)^{\perp}$ is given by the mean curvature vector[5,8]

$$H^a = \kappa(s)s^a - \kappa(t)t^a. \tag{3.17}$$

If H^a is spacelike or timelike, then this is the direction of, respectively, minimum absolute spacelike or minimum absolute timelike expansion of S. Furthermore, the minimum value of the absolute expansion is given by the mean extrinsic curvature of S, $|\kappa(H)|/|H| = \sqrt{|\kappa(s)^2 - \kappa(t)^2|}$ Note, here, the norm of H^a is $H^a H_a = \kappa(s)^2 - \kappa(t)^2 \equiv H^2$.

The mean curvature vector and normal curvature tensor of S are each independent of choice of the orthonormal frame, namely, H^a and $\mathcal{R}^{\perp}_{abcd}$ are invariant under boosts (3.6) of $\{t^a, s^a\}$. In contrast, the extrinsic curvatures of S are not invariant but instead transform like the orthonormal frame, while the normal connection transforms like an SO(1, 1) connection

$$\mathcal{J}'^{\perp}_a = \mathcal{J}^{\perp}_a + \nabla^S_a\chi \tag{3.18}$$

with respect to the SO(1, 1) group generated by the boosts (3.6).

B. Dirichlet symplectic vector

It is convenient to work with a null frame for $T(S)^{\perp}$. Let

$$\sqrt{2}\,\theta^+_a = t_a + s_a, \quad \sqrt{2}\,\theta^-_a = t_a - s_a, \tag{3.19}$$

which define, respectively, outgoing and ingoing future pointing null dual vectors satisfying

$$\theta^+_a\,\theta^{-a} = -1. \tag{3.20}$$

Note that any two such oriented null frames $\{\theta^+_a, \theta^-_a\}$ and $\{\theta'^+_a, \theta'^-_a\}$ are related by a local boost

$$\theta'^+_a = e^{\chi}\theta^+_a, \quad \theta'^-_a = e^{-\chi}\theta^-_a, \tag{3.21}$$

where χ is a boost parameter given by a function on S.

The extrinsic curvatures of S in the $\theta_a^{\pm}$ directions are given by

$$\kappa_{ab}^{\pm} = \mathcal{D}_a \theta_b^{\pm} . \tag{3.22}$$

Then

$$\kappa^{\pm} = \mathcal{D}_a \theta^{\pm a} = \tfrac{1}{2} \sigma^{ab} \mathcal{L}_{\theta^{\pm}} \sigma_{ab} \tag{3.23}$$

are the trace extrinsic curvatures which measure the expansion of S in the $\theta_a^{\pm}$ directions. Specifically, $\kappa^{\pm}$ is the rate of change of two-surface area of S,

$$\mathcal{L}_{\theta^{\pm}} \epsilon_{ab} = \kappa^{\pm} \epsilon_{ab} , \tag{3.24}$$

under any diffeomorphism of M whose generator is given by $\theta_a^{\pm}$ at S. Equivalently, $\kappa^{\pm}$ measures the focusing of a congruence of null geodesics normal to S.

The mean curvature vector of S is given by

$$H^a = -(\kappa^- \theta^{+a} + \kappa^+ \theta^{-a}) \tag{3.25}$$

and the connection for the normal curvature of S is given by

$$\mathcal{J}_a^{\perp} = \theta^{+b} \nabla_a^S \theta_b^- . \tag{3.26}$$

We now consider the Dirichlet symplectic vector (2.44) associated with S in the frame $\{t^a, s^a\}$, and separate it into vectors that are normal and tangential to S,

$$(P_{\perp})^a = \mathcal{P}_S^{\perp}(P^a) = \kappa^+ \theta^{-a} - \kappa^- \theta^{+a}, \tag{3.27}$$

$$(P_{\parallel})^a = \mathcal{P}_S(P^a) = \sigma^{ac} \theta^{-b} \nabla_c^S \theta^+{}_b . \tag{3.28}$$

We call $(P_{\perp})^a$ the *Dirichlet normal vector* associated with S. It has the important property that it is independent of choice of the null frame at S.[7–9]

Proposition 3.1: $(P_{\perp})^a$ *is invariant under arbitrary boosts* (3.21) *of the oriented null frame*.

Consequently, $(P_{\perp})^a$ depends only on the two-surface S and the space–time metric g_{ab}. (In particular, its components in any coordinate system can be locally constructed out of the components of g and their partial derivatives, but not in a coordinate invariant form.) Moreover, $(P_{\perp})^a$ has three significant geometrical properties.

First of all, we consider the extrinsic curvature of S in the direction $(P_{\perp})^a$,

$$\kappa_{ab}^{\perp} = \mathcal{D}_a (P_{\perp})_b . \tag{3.29}$$

Remarkably, the trace of this extrinsic curvature vanishes

$$\kappa^{\perp} = \mathcal{D}_a (P_{\perp})^a = \kappa^+ \mathcal{D}_a \theta^{-a} - \kappa^- \mathcal{D}_a \theta^{+a} = 0 \tag{3.30}$$

by Eq. (3.23) and $\theta^{\pm a} \nabla_a^S = 0$. Then we have

$$\mathcal{L}_{P_{\perp}} \epsilon_{ab} = \kappa^+ \mathcal{L}_{\theta-} \epsilon_{ab} - \kappa^- \mathcal{L}_{\theta+} \epsilon_{ab} = \kappa^{\perp} \epsilon_{ab} = 0. \tag{3.31}$$

This result yields the following key geometrical property of $(P_{\perp})^a$.

Theorem 3.2: *The normal direction* $(P_{\perp})^a$ *to S in the space–time* (M, g_{ab}) *is area preserving, i.e., S has zero expansion in the direction* $(P_{\perp})^a$.

Moreover, this property essentially characterizes the directional part of $(P_{\perp})^a$ since there is a unique area-preserving normal direction at all points of S, except, if any, where $\kappa^+ = \kappa^- = 0$ (in which case all normal directions to S are area-preserving).

Second, we find that the norm of $(P_\perp)^a$ is given by

$$(P_\perp)^2 = 2\kappa^+\kappa^-. \tag{3.32}$$

Hence, the direction of $(P_\perp)^a$ is timelike, spacelike, or null if the expansions $\kappa^\pm$ of S are, respectively, opposite sign, same sign, or at least one is zero. (These are boost invariant properties.) In general, the signs of $\kappa^\pm$ can vary on S even if the space–time curvature satisfies positive energy conditions. Therefore, the sign of $(P_\perp)^2$ need not be the same everywhere on S. We note that the situation $(P_\perp)^2 > 0$ characterizes S as a trapped surface, related to the formation of black holes.[10] Further remarks on this aspect of $(P_\perp)^a$ will be made in Sec. V.

Third, we see that $(P_\perp)^a$ is closely related to the mean curvature vector of S.

Proposition 3.3:

$$(P_\perp)^a H_a = 0, \ (P_\perp)^2 = -H^2. \tag{3.33}$$

Thus, $(P_\perp)^a$ is, respectively, timelike, spacelike, or null as H^a is spacelike, timelike, or null. Let $|H| = \sqrt{|H^2|}$, $|P_\perp| = \sqrt{|(P_\perp)^2|}$ denote the absolute norms of H^a and $(P_\perp)^a$. Then, in the non-null case, the relations (3.33) give a unique characterization of $(P_\perp)^a$ (up to a sign) as a vector in $T(S)^\perp$ orthogonal to H^a and with the same absolute norm as H^a. Consequently, we will write $(P_\perp)^a = H^a_\perp$ and refer to

$$H^a_\perp = \kappa^+\theta^{-a} - \kappa^-\theta^{+a} \tag{3.34}$$

as the *normal mean curvature vector* of S, with $H^a_\perp H_a = 0$, $H^2_\perp = -H^2$.

Lemma 3.4: Suppose $|H| \neq 0$ or equivalently $|P_\perp| \neq 0$, i.e., H^a and $H^a_\perp = (P_\perp)^a$ are non-null. Then $\{H^a/|H|, H^a_\perp/|H|\}$ is an orthonormal frame for $T(S)^\perp$. Correspondingly, the pair of vectors

$$\hat{\theta}^{+a} \equiv \frac{1}{\sqrt{2}|H|}(H^a + H^a_\perp) = \frac{-\kappa^-}{\sqrt{|\kappa^+\kappa^-|}}\theta^{+a}, \tag{3.35}$$

$$\hat{\theta}^{-a} \equiv \frac{1}{\sqrt{2}|H|}(H^a - H^a_\perp) = \frac{-\kappa^+}{\sqrt{|\kappa^+\kappa^-|}}\theta^{-a}, \tag{3.36}$$

is a null frame for $T(S)^\perp$.

Thus, in the non-null case, H^a and $H^a_\perp = (P_\perp)^a$ determine a preferred orthonormal frame (or null frame) of $T(S)^\perp$ which depends just on the two-surface S and space–time metric g_{ab}. Then we can summarize the geometrical properties of these vectors in terms of the following orthonormal vectors in $T(S)^\perp$:

$$\hat{H}^a = \frac{1}{\sqrt{2|\kappa^+\kappa^-|}}(\kappa^-\theta^{+a} + \kappa^+\theta^{-a}), \tag{3.37}$$

$$\hat{H}^a_\perp = \frac{1}{\sqrt{2|\kappa^+\kappa^-|}}(\kappa^-\theta^{+a} - \kappa^+\theta^{-a}). \tag{3.38}$$

Theorem 3.5: *Suppose $\kappa^+\kappa^- \neq 0$ on S, i.e., H^a and $H^a_\perp$ are non-null. Then:*

(1) The expansion of S is zero in the unique normal direction $\hat{H}^a_\perp$, which is spacelike or timelike as $\kappa^+\kappa^-$ is positive or negative on S.

(2) The absolute expansion of S in the orthogonal normal direction $\hat{H}^a$ is $\sqrt{2|\kappa^+\kappa^-|}$. This is the minimum absolute spacelike expansion or minimum absolute timelike expansion where $\kappa^+\kappa^-$ is, respectively, positive or negative on S.

We now turn to consider the geometrical properties of $(P_\parallel)^a$. To begin, $(P_\parallel)^a$ can be identified[6,7] with the connection $\mathcal{J}_a^\perp$ for the normal curvature of S, in the null frame $\{\theta_a^+, \theta_a^-\}$.

Proposition 3.6:

$$(P_\parallel)^a = -\sigma^{ab}\mathcal{J}_b^\perp, \tag{3.39}$$

where

$$\mathcal{J}_a^\perp = \theta^{+c}\nabla_a^S\theta_c^-. \tag{3.40}$$

Hence, in contrast to the invariance of $(P_\perp)^a$ under boosts (3.21) of the null frame, $(P_\parallel)^a$ is not invariant but instead transforms as an SO(1, 1) connection,

$$(P_\parallel)'_a = (P_\parallel)_a - \nabla_a^S\chi, \tag{3.41}$$

where χ is a boost parameter given by a function on S. This describes a gauge transformation of $(P_\parallel)^a$ associated with the boosts (3.21) acting on $T(S)^\perp$ as an SO(1,1) gauge group. Consequently, the curl of $(P_\parallel)^a$ has the role of the gauge invariant curvature.

Proposition 3.7:

$$-\mathcal{D}_{[a}(P_\parallel)_{b]} = \tfrac{1}{4}\mathcal{R}^\perp_{abcd}\epsilon^{\perp cd} \tag{3.42}$$

is invariant under arbitrary boosts (3.21) of the null frame, where $\mathcal{R}^\perp_{abcd}$ is the normal curvature of S.

Thus, the curvature $\mathcal{D}_{[a}(P_\parallel)_{b]}$ depends only on the two-surface S and the space–time metric g_{ab}.

Interestingly, in the case when H^a is non-null, we can use the preferred orthonormal frame or null frame given by Lemma 3.4 to gauge-fix $(P_\parallel)^a$. We introduce

$$(\hat{P}_\parallel)_a = \frac{1}{H^2}H_\perp^b\mathcal{D}_a H_b = \frac{1}{H_\perp^2}H^b\mathcal{D}_a H_{\perp b} = (P_\parallel)_a + \tfrac{1}{2}\nabla_a^S\ln(\kappa^+/\kappa^-) \tag{3.43}$$

related to $(P_\parallel)_a$ by a gauge transformation (3.41) with boost parameter $\chi = \frac{1}{2}\ln(\kappa^-/\kappa^+)$ on S.

Proposition 3.8: $(\hat{P}_\parallel)_a$ *is invariant under arbitrary boosts (3.21) of the oriented null frame.*

Consequently, we call $(\hat{P}_\parallel)_a$ the *invariant Dirichlet tangent vector* associated with S. In particular, $(\hat{P}_\parallel)_a$ depends only on the two-surface S and the space–time metric g_{ab}. We now state the main geometrical property of $(\hat{P}_\parallel)_a$, which follows from Eq. (3.43).

Theorem 3.9: *Suppose $\kappa^+\kappa^- \neq 0$ on S, i.e., H^a and $H_\perp^a$ are non-null. Then the boost [with respect to $T(S)^\perp$] of the area-preserving unit normal vector $\hat{H}_\perp^a$ to S under displacement on S is a maximum in the direction $(\hat{P}_\parallel)_a$. By orthogonality of H^a and $H_\perp^a$, this is equivalent to the tangent direction on S in which the boost of the unit mean curvature vector $\hat{H}^a$ under displacement on S is a maximum.*

Finally, from Propositions 3.1 and 3.8, when the mean curvature vector is non-null we can define an invariant locally constructed Dirichlet four-vector associated with S by

$$\hat{P}^a = (P_\perp)^a + (\hat{P}_\parallel)^a = \kappa^+\theta^{-a} - \kappa^-\theta^{+a} + \sigma^{ac}\theta^{-b}\nabla_c^S\theta_b^+ + \tfrac{1}{2}\nabla_a^S\ln(\kappa^+/\kappa^-). \tag{3.44}$$

Note that this vector depends only on S and g_{ab} and is independent of the choice of null frame $\{\theta_a^+, \theta_a^-\}$. Indeed, in terms of purely geometrical structure associated with S,

$$\hat{P}^a = H_\perp^a + \frac{1}{H^2}H_\perp^b\mathcal{D}^a H_b, \tag{3.45}$$

where H^a is the mean curvature vector (3.25) and $H^a_\perp$ is the normal mean curvature vector (3.34) of S.

C. Neumann symplectic vector

Finally, we consider the Neumann symplectic vector (2.45) associated with S,

$$P^a = g^{ac}\theta^{-b}\nabla_c\theta^+_b\,. \tag{3.46}$$

Notice, first of all, the tangential part of P^a with respect to S,

$$(P_\parallel)^a = \mathcal{P}_S(P^a) = \sigma^{ac}\theta^{-b}\nabla^S_c\theta^+_b\,, \tag{3.47}$$

is identically equal to the tangential part of the Dirichlet symplectic vector (3.38). Hence, similar to Theorem 3.9, $(P_\parallel)^a$ gives the direction in which the boost of the null frame $\theta^\pm_a$ under displacement on S is a maximum. In contrast, the normal part of P^a with respect to S,

$$(P_\perp)^a = \mathcal{P}^\perp_S(P^a) = \sigma^{\perp ac}\theta^{-b}\nabla_c\theta^+_b = -\sigma^{\perp ac}\theta^{+b}\nabla_c\theta^-_b\,, \tag{3.48}$$

involves derivatives of the null frame $\theta^\pm_a$ in normal directions to S. In particular, note through substitution of

$$\sigma^{\perp b}_a = -(\theta^+_a\theta^{-b} + \theta^-_a\theta^{+b}) \tag{3.49}$$

that

$$(P_\perp)^a = -\theta^{+a}\theta^{-b}\theta^{-c}\nabla_c\theta^+_b + \theta^{-a}\theta^{+b}\theta^{+c}\nabla_c\theta^-_b = \sigma^{\perp a}_c[\theta^-,\theta^+]^c \tag{3.50}$$

since $\theta^{+b}\nabla_c\theta^+_b = \theta^{-b}\nabla_c\theta^-_b = 0$.

Proposition 3.10: $(P_\perp)^a$ *is the normal part of the commutator* $[\theta^-,\theta^+]^a$ *of the null frame,* $(P_\perp)^a = \mathcal{P}^\perp_S[\theta^-,\theta^+]^a$.

Consequently, unlike $(P_\parallel)^a$, which is well-defined given just the two-surface S and a null frame $\theta^{\pm a}$ of $T(S)^\perp$, it is necessary to consider "nearby" two-surfaces S', diffeomorphic to S, to extend the null frame $\theta^\pm_a$ of $T(S)^\perp$ off S so that $(P_\perp)^a$ is well-defined.

Let $S_{(\lambda_+,\lambda_-)}$ denote a two-parameter (λ_+,λ_-) local null congruence of two-surfaces S' diffeomorphic to S in (M,g_{ab}) with $S_{(0,0)} = S$. [The congruence is defined to be ingoing as a function of λ_- and outgoing as a function of λ_+.] Extend the null frame $\{\theta^{+a},\theta^{-a}\}$ off $T(S)^\perp$ to $T(S')^\perp$. This extension is unique up to boosts (3.21). Then $(P_\perp)^a = \sigma^{\perp ac}\theta^{-b}\nabla_c\theta^+_b$ is a well-defined normal vector at each point on S. We call $(P_\perp)^a$ the *Neumann normal vector* associated with S in a null congruence $S_{(\lambda_+,\lambda_-)} \simeq S\times(\lambda_+,\lambda_-)$. It depends, of course, on the congruence but also on the choice of null frame for $T(S_{(\lambda_+,\lambda_-)})^\perp$.

Proposition 3.11: Under boosts (3.21) of the null frame on the two-surfaces $S_{(\lambda_+,\lambda_-)} \simeq S(\lambda_+,\lambda_-)$, $(P_\perp)^a$ *transforms as*

$$(P_\perp)'_a = (P_\perp)_a - \sigma^{\perp b}_a\nabla_b\chi, \tag{3.51}$$

where χ *is a boost parameter given by a function of* (λ_+,λ_-).

By Proposition 3.6, $(P_\parallel)^a$ has a similar boost transformation property, which has the geometrical meaning of an SO(1,1) connection for the normal curvature of S. This suggests that, geometrically, $P^a = (P_\perp)^a + (P_\parallel)^a$ is also related to an SO(1, 1) connection associated with an extrinsic curvature of S.

Consider the derivative operator $\nabla^\perp_a$ defined by $\nabla^\perp_a v^b = \sigma^{\perp b}_c\nabla_a v^c$ for any normal vector field v^a on the two-surfaces $S_{(\lambda_+,\lambda_-)}$. The commutator of $\nabla^\perp_a$ gives the curvature

$$[\nabla_a^\perp, \nabla_b^\perp] v_c = R^\perp_{abc}{}^d v_d . \tag{3.52}$$

[Note that, on functions, $[\nabla_a^\perp, \nabla_b^\perp] f = 2\nabla_{[a}\nabla_{b]} f = 0$.] Clearly, $\mathcal{P}_S^\perp([\nabla_a^\perp, \nabla_b^\perp]) v_c = [\mathcal{D}_a^\perp, \mathcal{D}_b^\perp] v_c = \mathcal{R}^\perp_{abc}{}^d v_d$ yields the normal curvature of S. Hence, $R^\perp_{abcd}$ is a generalization of $\mathcal{R}^\perp_{abcd}$, which we call the *sectional curvature normal to S* in the null congruence $S_{(\lambda_+, \lambda_-)}$.

Proposition 3.12:

$$R^\perp_{abcd} = 2\nabla^\perp_{[a} J^\perp_{b]} \epsilon^\perp_{cd} , \tag{3.53}$$

where $J_a^\perp = \theta^{+b} \nabla_a \theta_b^-$.

Here $J_a^\perp$ is geometrically a connection one-form for $R^\perp_{abcd}$. In particular, boosts of the null frame act as an SO(1, 1) gauge group on $T(S_{(\lambda_+, \lambda_-)})^\perp$ under which $J_a^\perp$ transforms as $J'^\perp_a = J_a^\perp + \nabla_a \chi$ where χ is a function on $S_{(\lambda_+, \lambda_-)} \simeq S \times (\lambda_+, \lambda_-)$. Note that the curvature $R^\perp_{abcd}$ is invariant under these boosts. This leads to the main geometrical result concerning P^a.

Theorem 3.13: *In any null congruence of two-surfaces* $S_{(\lambda_+, \lambda_-)}$, $P_a = 2J_a^\perp$ *is a connection one-form for the sectional curvature normal to S,*

$$-\nabla^\perp_{[a} P_{b]} = \tfrac{1}{4} R^\perp_{abcd} \epsilon^{\perp cd} . \tag{3.54}$$

Thus the curl $\nabla^\perp_{[a} P_{b]}$ is invariant under arbitrary boosts of the null frame on $S_{(\lambda_+, \lambda_-)}$. It depends, still, on the choice of null congruence $S_{(\lambda_+, \lambda_-)} \simeq S \times (\lambda_+, \lambda_-)$.

In general, there is no unique null congruence determined just by S and g_{ab}. However, a natural choice is given by ingoing and outgoing null geodesics congruences $S_{\lambda_\pm}$ through S, with $S_{(\lambda_+, \lambda_-)}$ defined as $(S_{\lambda_+})_{\lambda_-}$ or $(S_{\lambda_-})_{\lambda_+}$ corresponding to constructing successive one-parameter ingoing and outgoing congruences.[11]

If $S_{(\lambda_+, \lambda_-)} \simeq S \times (\lambda_+, \lambda_-)$ is chosen to be a null geodesic congruence, then the geodesic equation implies that $\theta^{\pm a}$ satisfies $\theta'^{\pm b} \nabla_b \theta'^{\pm a} = 0$ where $\theta'^{\pm a}$ is given by a boost (3.21) for some function χ of (λ_+, λ_-). Thus,

$$\theta^{+b} \nabla_b \theta^{+a} = -\theta^{+a} \theta^{+b} \nabla_b \chi , \quad \theta^{-b} \nabla_b \theta^{-a} = \theta^{-a} \theta^{-b} \nabla_b \chi . \tag{3.55}$$

This leads to a simplification of $(P_\perp)^a$ from Eq. (3.50),

$$(P_\perp)^a = \theta^{+a} \theta^{+b} \theta^{-c} \nabla_c \theta_b^- - \theta^{-a} \theta^{-b} \theta^{+c} \nabla_c \theta_b^+ = -\theta^{+a} \theta^{-c} \nabla_c \chi - \theta^{-a} \theta^{+c} \nabla_c \chi . \tag{3.56}$$

Proposition 3.14: In a null geodesic congruence, $(P_\perp)^a = \sigma^{\perp ab} \nabla_b \chi$, *and consequently,* $\mathcal{P}_S^\perp(R^\perp_{abcd}) = 0$.

The converse of this result also holds, since if the normal part of $R^\perp_{abcd}$ vanishes, then $(P_\perp)_a$ is a gradient and hence $\theta^{\pm a}$ satisfies the geodesic equation (3.55) so that the congruence $S_{(\lambda_+, \lambda_-)}$ arises from null geodesics through S.

Geometrically, the boost function χ in the geodesic equation (3.55) is related to the choice of parametrization of the null congruence. Indeed, we can fix the parametrization in a natural way by $\chi = 0$, which implies a corresponding gauge-fixing of $(P_\perp)^a$,

$$(\hat{P}_\perp)^a = 0 . \tag{3.57}$$

To conclude, we remark that the use of ingoing and outgoing null congruences in defining $(P_\perp)^a$ can be replaced by using timelike and spacelike congruences, denoted S_{λ_s} and S_{λ_t}, through S. Moreover, if g_{ab} has isometries then it may be possible to fix a unique local two-parameter congruence $S_{(\lambda_s, \lambda_t)}$ constructed in a natural way from the Killing vectors and invariant surfaces of the isometries. In general, then $(P_\perp)^a$ is no longer just a gradient. This will be illustrated in the examples in Sec. IV.

Finally, it is important to note that there is no ambiguity in $(P_\perp)^a$ appearing in the Neumann Hamiltonian boundary term (2.43), since this involves only the component of $(P_\perp)^a$ in the direction of the time-flow vector, which is well-defined using the unique timelike congruence through S generated by the time-flow vector on M.

IV. EXAMPLES

We now consider examples for the Dirichlet and Neumann symplectic vectors described in Sec. III. In particular, we calculate these vectors and their properties for spacelike, topologically spherical two-surfaces in (a) Minkowski space–time, (b) spherically symmetric space–times, (c) axisymmetric space–times, (d) homogeneous isotropic space–times, (e) asymptotically flat space–times.

A. Minkowski space–time

Consider a closed orientable spacelike two-surface S embedded in a spacelike hyperplane in Minkowski space–time $(\mathbb{R}^4, \eta)$, using spherical coordinates

$$\eta_{ab} = -(\mathrm{d}t)_a(\mathrm{d}t)_b + (\mathrm{d}r)_a(\mathrm{d}r)_b + r^2((\mathrm{d}\theta)_a(\mathrm{d}\theta)_b + \sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b), \tag{4.1}$$

where S is given by $t=t_0$, $r=R(\theta,\phi)$ for some function $R(\theta,\phi)$ and constant t_0. Fix an orthonormal frame ϑ_a^μ adapted to S in (R^4,η) by

$$\vartheta_a^0 = (\mathrm{d}t)_a, \quad \vartheta_a^1 = \frac{1}{\psi}((\mathrm{d}r)_a - \partial_a R), \tag{4.2}$$

$$\vartheta_a^2 = \frac{1}{\mu}\left(r(\mathrm{d}\theta)_a + \frac{\partial_\theta R}{r}(\mathrm{d}r)_a\right), \quad \vartheta_a^3 = \frac{\mu}{\psi}\left(r\sin\theta(\mathrm{d}\phi)_a + \frac{\partial_\phi R}{\mu^2 r\sin\theta}((\mathrm{d}r)_a - \partial_\theta R(\mathrm{d}\theta)_a)\right), \tag{4.3}$$

where

$$\mu = \sqrt{1 + r^{-2}(\partial_\theta R)^2}, \quad \psi = \sqrt{1 + r^{-2}((\partial_\theta R)^2 + (\partial_\phi R/\sin\theta)^2)}. \tag{4.4}$$

Note the metric associated with S is given in spherical coordinates by

$$\begin{aligned}\sigma_{ab} = {} & (1-\psi^{-2})(\mathrm{d}r)_a(\mathrm{d}r)_b + 2\psi^{-2}(\mathrm{d}r)_{(a}\partial_{b)}R - \psi^{-2}\partial_a R\partial_b R \\ & + r^2((\mathrm{d}\theta)_a(\mathrm{d}\theta)_b + \sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b).\end{aligned} \tag{4.5}$$

The pullback of σ_{ab} to S yields the induced metric on S,

$$\sigma_{ab}|_S = (R^2 + (\partial_\theta R)^2)(\mathrm{d}\theta)_a(\mathrm{d}\theta)_b + (R^2\sin^2\theta + (\partial_\phi R)^2)(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b + 2\partial_\theta R\partial_\phi R(\mathrm{d}\theta)_{(a}(\mathrm{d}\phi)_{b)}. \tag{4.6}$$

Correspondingly, let $\psi_S = \psi|_S = \sqrt{1 + R^{-2}((\partial_\theta R)^2 + (\partial_\phi R/\sin\theta)^2)}$.

The trace of the extrinsic curvatures of (S,σ_{ab}) with respect to the frame on $T(S)^\perp$

$$t_a = \vartheta_a^0|_S = (\mathrm{d}t)_a, \quad s_a = \vartheta_a^1|_S = \frac{1}{\psi_S}((\mathrm{d}r)_a - \partial_a R), \tag{4.7}$$

are, respectively,

$$\kappa(t) = \sigma^{ab}\nabla_a t_b = -(\Gamma_2{}^{02}(\vartheta) + \Gamma_3{}^{03}(\vartheta))|_S = 0 \tag{4.8}$$

and

$$\kappa(s) = \sigma^{ab}\nabla_a s_b = -(\Gamma_2{}^{12}(\vartheta) + \Gamma_3{}^{13}(\vartheta))|_S = 2(\vartheta_1^a\vartheta_2^b\partial_{[a}\vartheta_{b]}^2 + \vartheta_1^a\vartheta_3^b\partial_{[a}\vartheta_{b]}^3)|_{r=R(\theta,\phi)}, \tag{4.9}$$

calculated in terms of the Ricci rotation coefficients

$$\Gamma_\lambda{}^{\mu\nu}(\vartheta)=\vartheta^a_\lambda\vartheta^{b\nu}\nabla_a\vartheta^\mu_b=2\,\vartheta^a_\lambda\vartheta^{b[\mu}\partial_{[a}\vartheta^{\nu]}_{b]}-\vartheta^{b\mu}\vartheta^{c\nu}\partial_{[b}\vartheta_{c]\lambda}\,. \tag{4.10}$$

Here $\kappa(s)$ is the standard Euclidean extrinsic curvature of S in $\mathbb{R}^3$.[5] [The explicit expression for $\kappa(s)$ as a function of the spherical coordinates is lengthy and will be omitted.]

A preferred direction in $T(S)^\perp$ is given by the mean curvature vector

$$H^a=s^a\kappa(s)-t^a\kappa(t)=\frac{\kappa(s)}{\psi_S}\left((\partial_r)^a-\frac{\partial_\theta R}{R^2}(\partial_\theta)^a-\frac{\partial_\phi R}{R^2\sin^2\theta}(\partial_\phi)^a\right), \tag{4.11}$$

which is spacelike. This vector gives the direction of the minimum absolute spacelike expansion of S in $(\mathbb{R}^4,\eta)$. Furthermore, the value of the expansion is the mean extrinsic curvature of S given by

$$\frac{1}{\sqrt{H^2}}\kappa(H)=|\kappa(s)|=\sqrt{H^2}. \tag{4.12}$$

Note S is convex or concave according to where the sign of $\kappa(s)$ is negative or positive.

The normal part of the Dirichlet symplectic vector is given by the normal mean curvature vector

$$(P^{\mathrm{D}}_\perp)^a=H^a_\perp=t^a\kappa(s)-s^a\kappa(t)=\kappa(s)(\partial_t)^a. \tag{4.13}$$

Note that $(P^{\mathrm{D}}_\perp)^a$ is timelike, orthogonal to H^a, with the same absolute norm as H^a. Most significant, $(P^{\mathrm{D}}_\perp)^a$ gives the direction of zero expansion of S.

A preferred orthonormal frame for $T(S)^\perp$ is

$$\hat t^a=\frac{1}{\sqrt{H^2}}H^a_\perp=(\partial_t)^a|_S,\quad \hat s^a=\frac{1}{\sqrt{H^2}}H^a=\frac{1}{\psi}\left((\partial_r)^a-\frac{\partial_\theta R}{r^2}(\partial_\theta)^a-\frac{\partial_\phi R}{r^2\sin^2\theta}(\partial_\phi)^a\right)|_S, \tag{4.14}$$

which depend only on S and η_{ab} but not on the Minkowski frame ϑ^μ_a. In the preferred frame (4.14), the tangential part of the Dirichlet symplectic vector is

$$(P^{\mathrm{D}}_\parallel)^a=\sigma^{ac}\hat t^b\nabla_c\hat s_b=-\frac{1}{\psi_S}\sigma^{ac}\left((\partial_r)^b-\frac{\partial_\theta R}{R^2}(\partial_\theta)^b-\frac{\partial_\phi R}{R^2\sin^2\theta}(\partial_\phi)^b\right)\nabla_c(\mathrm{d}t)_b=0, \tag{4.15}$$

and thus the normal curvature of S is zero.

Hence the complete Dirichlet symplectic vector is

$$P^a=(P^{\mathrm{D}}_\perp)^a+(P^{\mathrm{D}}_\parallel)^a=\kappa(s)(\partial_t)^a, \tag{4.16}$$

which depends only on S and η_{ab}. In particular, it is independent of choice of original orthonormal frame (4.2) and (4.3) on Minkowski space and of the normals (4.7) in $T(S)^\perp$.

To define the Neumann symplectic vector, it is natural to extend the preferred orthonormal frame (4.14) off S by using the obvious isometries of η_{ab}. With respect to this extension, the normal part of the Neumann symplectic vector is given by the commutator

$$(P^{\mathrm{N}}_\perp)^a=\mathcal{P}^\perp_S[\hat t,\hat s]^a=\frac{1}{\psi_S}\mathcal{P}^\perp_S\left([(\partial_t),(\partial_r)]^a-\frac{1}{R^2\sin^2\theta}[(\partial_t),\sin^2\theta\,\partial_\theta R(\partial_\theta)+\partial_\phi R(\partial_\phi)]^a\right)=0. \tag{4.17}$$

[Alternatively, the same result for $(P^{\mathrm{N}}_\perp)^a$ is obtained by extending (4.14) off S to the congruence of two-surfaces $t=\text{const}$, $r-R(\theta,\phi)=\text{const}$, which lie in parallel hyperplanes to S and are iso-

metric to S.] Then, since $(P^{\mathrm{N}}_{\parallel})^a=(P^{\mathrm{D}}_{\parallel})^a=0$, the complete Neumann symplectic vector in the congruence of two-surfaces associated with S under isometries of η_{ab} is given by

$$P^a=(P^{\mathrm{N}}_{\perp})^a+(P^{\mathrm{N}}_{\parallel})^a=0. \tag{4.18}$$

Thus the sectional curvature normal to S vanishes, reflecting the fact that S lies in a flat hyperplane.

1. Light cone two-sphere

Next, consider a closed orientable spacelike two-surface S embedded in a light cone in $(\mathbb{R}^4,\eta)$. Let $u=(t-r)/\sqrt{2}$, $v=(t+r)/\sqrt{2}$, θ, ϕ be light cone coordinates (i.e., r, θ, ϕ are spherical coordinates with respect to the origin point for the cone), with

$$\eta_{ab}=-2(\mathrm{d}u)_{(a}(\mathrm{d}v)_{b)}+\tfrac{1}{2}(v-u)^2((\mathrm{d}\theta)_a(\mathrm{d}\theta)_b+\sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b). \tag{4.19}$$

Then S is given by $u=u_0$, $v=V(\theta,\phi)$ for some function $V(\theta,\phi)$ and constant u_0. Note that $(\mathrm{d}u)_a$ and $(\mathrm{d}v)_a-\partial_a V$ are, respectively, a null normal and spacelike normal for S, while $(\partial_\theta)^a+\partial_\theta V(\partial_v)^a$ and $(\partial_\phi)^a+\partial_\phi V(\partial_v)^a$ are orthogonal tangent vectors on S.

Fix a null frame ϑ^μ_a adapted to S in $(\mathbb{R}^4,\eta)$ by

$$\vartheta^0_a=(\mathrm{d}u)_a,\quad \vartheta^1_a=\tfrac{1}{2}\psi^2(\mathrm{d}u)_a+(\mathrm{d}v)_a-\partial_a V, \tag{4.20}$$

$$\vartheta^2_a=r(\mathrm{d}\theta)_a-\frac{\partial_\theta V}{r}(\mathrm{d}u)_a,\quad \vartheta^3_a=r\sin\theta(d\phi)_a-\frac{\partial_\phi V}{r\sin\theta}(\mathrm{d}u)_a \tag{4.21}$$

satisfying $\vartheta^\mu_a\vartheta^\nu_b\eta^{ab}=-2\delta^{(\mu}_0\delta^{\nu)}_1+\delta^\mu_2\delta^\nu_2+\delta^\mu_3\delta^\nu_3$, where

$$\psi=|\mathrm{d}V|=r^{-1}\sqrt{(\partial_\theta V)^2+(\partial_\phi V/\sin\theta)^2}. \tag{4.22}$$

Note the metric associated with S is given by

$$\sigma_{ab}=\psi^2(\mathrm{d}u)_a(\mathrm{d}u)_b-2(\mathrm{d}u)_{(a}(\partial_\theta V(\mathrm{d}\theta)_{b)}+\partial_\phi V(\mathrm{d}\phi)_{b)})+r^2((\mathrm{d}\theta)_a(\mathrm{d}\theta)_b+\sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b), \tag{4.23}$$

where

$$\sigma_{ab}|_S=\tfrac{1}{2}(V-u_0)^2((\mathrm{d}\theta)_a(\mathrm{d}\theta)_b+\sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b) \tag{4.24}$$

yields the induced metric on S.

The trace of the extrinsic curvatures of (S,σ_{ab}) with respect to the null frame on $T(S)^\perp$

$$u_a=\vartheta^0_a|_S=(\mathrm{d}u)_a, \tag{4.25}$$

$$v_a=\vartheta^1_a|_S=\psi^2_S(\mathrm{d}u)_a+(\mathrm{d}v)_a-\partial_\theta V(\mathrm{d}\theta)_a-\partial_\phi V(\mathrm{d}\phi)_a, \tag{4.26}$$

are, respectively,

$$\kappa(u)=\sigma^{ab}\nabla_a u_b=-(\Gamma_2{}^{02}(\vartheta)+\Gamma_3{}^{03}(\vartheta))|_S=-\frac{2}{R} \tag{4.27}$$

and

$$\kappa(v)=\sigma^{ab}\nabla_a v_b=-(\Gamma_2{}^{12}(\vartheta)+\Gamma_3{}^{13}(\vartheta))|_S=\frac{2}{R}(1+\psi^2_S)-\frac{2\partial_\theta R}{R^2}\frac{\cos\theta}{\sin\theta}-\frac{2\partial^2_\theta R}{R^2}-\frac{2\partial^2_\phi R}{R^2\sin^2\theta}, \tag{4.28}$$

where

$$\psi_S=\frac{1}{\sqrt{2}}\,\psi|_S=R^{-1}\sqrt{(\partial_\theta R)^2+(\partial_\phi R/\sin\theta)^2},\quad R=\sqrt{2}r|_S=V-u_0. \tag{4.29}$$

A preferred direction in $T(S)^\perp$ is given by the mean curvature vector

$$H^a=-u^a\kappa(v)-v^a\kappa(u) \tag{4.30}$$

in terms of the null vectors

$$u^a=-(\partial_v)^a|_S,\quad v^a=-\left((\partial_u)^a+\frac{\psi^2}{2}(\partial_v)^a+\frac{\partial_\theta V}{r^2}(\partial_\theta)^a+\frac{\partial_\phi V}{r^2\sin^2\theta}(\partial_\phi)^a\right)\Big|_S. \tag{4.31}$$

The norm of H^a gives the mean extrinsic curvature of S,

$$\frac{1}{|H|}|\kappa(H)|=\sqrt{2|\kappa(u)\kappa(v)|}=|H|. \tag{4.32}$$

Now, the normal part of the Dirichlet symplectic vector is given by the normal mean curvature vector $(P^{\mathrm{D}}_\perp)^a=H^a_\perp=v^a\kappa(u)-u^a\kappa(v)$, which simplifies to

$$(P^{\mathrm{D}}_\perp)^a=-\kappa(u)(\partial_u)^a-(\kappa(u)\psi_S^2-\kappa(v))(\partial_v)^a-\kappa(u)\frac{2\partial_\theta R}{R^2}(\partial_\theta)^a-\kappa(u)\frac{2\partial_\phi R}{R^2\sin^2\theta}(\partial_\phi)^a. \tag{4.33}$$

This vector gives the direction of zero expansion of S in $(\mathbb{R}^4,\eta)$.

A preferred null frame for $T(S)^\perp$ consists of

$$\hat{u}^a=\frac{1}{\sqrt{2}|H|}(H^a_\perp+H^a)=\sqrt{\frac{\kappa(v)}{\kappa(u)}}(\partial_v)^a, \tag{4.34}$$

$$\hat{v}^a=\frac{1}{\sqrt{2}|H|}(H^a_\perp-H^a)=\sqrt{\frac{\kappa(u)}{\kappa(v)}}\left((\partial_u)^a+\psi_S^2(\partial_v)^a+\frac{2\partial_\theta R}{R^2}(\partial_\theta)^a+\frac{2\partial_\phi R}{R^2\sin^2\theta}(\partial_\phi)^a\right), \tag{4.35}$$

which depend only on S and η_{ab} but not on the Minkowski frame ϑ^μ_a. In the preferred frame (4.34) and (4.35), the tangential part of the Dirichlet symplectic vector is given by

$$(P^{\mathrm{D}}_\parallel)^a=\sigma^{ac}\hat{v}^b\nabla_c\hat{u}_b=\sigma^{ac}v^b\nabla_c(\mathrm{d}u)_b+\tfrac{1}{2}\sigma^{ac}\partial_c\ln(\kappa(u)/\kappa(v)). \tag{4.36}$$

This simplifies to

$$\begin{aligned}(P^{\mathrm{D}}_\parallel)^a=&\frac{1}{R^2}((\partial_\theta)^a+\partial_\theta R(\partial_v)^a)\partial_\theta\ln(\kappa(u)/\kappa(v))\\&+\frac{1}{R^2\sin^2\theta}((\partial_\phi)^a+\partial_\phi R(\partial_v)^a)\partial_\phi\ln(\kappa(u)/\kappa(v)).\end{aligned} \tag{4.37}$$

Therefore, since the dual vector $(P^{\mathrm{D}}_\parallel)_a=\nabla^S_a\ln(\kappa(u)/\kappa(v))$ is a gradient on S, the normal curvature of S is zero.

The complete Dirichlet symplectic vector is

$$P^a=(P^{\mathrm{D}}_\perp)^a+(P^{\mathrm{D}}_\parallel)^a, \tag{4.38}$$

which depends only on S and η_{ab}. In particular, it is independent of choice of the original null frame (4.20) and (4.21) on Minkowski space and of the corresponding frame (4.25) and (4.26) on $T(S)^{\perp}$. Geometrically, the dual vector $(P_{\perp}^{\mathrm{D}})_a$ provides a preferred normal direction for a family of hypersurfaces defined to cut the light cone at S, with vanishing normal curvature.

Finally, the commutator of the null frame (4.31) yields the normal part of the Neumann symplectic vector,

$$\begin{aligned}(P_{\perp}^{\mathrm{N}})^a = P_S^{\perp}[v,u]^a &= \mathcal{P}_S^{\perp}\left[\partial_u + \frac{\psi^2}{2}\partial_v + \frac{\partial_\theta V}{r^2}\partial_\theta + \frac{\partial_\phi V}{r^2\sin^2\theta}\partial_\phi, \partial_v\right]^a\Bigg|_S \\ &= \frac{\sqrt{2}}{r}\mathcal{P}_S^{\perp}\left(\frac{\psi^2}{2}(\partial_v)^a + \frac{\partial_\theta V}{r^2}(\partial_\theta)^a + \frac{\partial_\phi V}{r^2\sin^2\theta}(\partial_\phi)^a\right)\Bigg|_S \\ &= -2\,\frac{\psi_S^2}{R}(\partial_v)^a, \end{aligned} \tag{4.39}$$

through $\partial_v\psi^2 = -\sqrt{2}\psi^2/r$. The tangential part of the Neumann symplectic vector is simply $(P_{\parallel}^{\mathrm{N}})^a = (P_{\parallel}^{\mathrm{D}})^a$. Hence, this yields the complete Neumann symplectic vector

$$P^a = (P_{\perp}^{\mathrm{N}})^a + (P_{\parallel}^{\mathrm{N}})^a, \tag{4.40}$$

which depends only on the congruence of spacelike two-surfaces $u=\text{const}$, $v - V(\theta,\phi) = \text{const}$, lying on the light cones in Minkowski space.

2. Constant curvature two-sphere

In the special case of a constant curvature two-sphere S, viewed as embedded either in a hyperplane $t=t_0=\text{const}$, $r=R=r_0=\text{const}$, or in a light cone, $u=u_0=(t_0-r_0)/\sqrt{2}$, $v=V=v_0=(t_0+r_0)/\sqrt{2}$, the mean curvature vector of S is simply $H^a=(2/r_0)(\partial_r)^a$, and the complete Dirichlet symplectic vector reduces to

$$P^a = H_{\perp}^a = \frac{2}{r_0}(\partial_t)^a, \tag{4.41}$$

while the complete Neumann symplectic vector vanishes.

B. Spherically symmetric space–times

In a spherically symmetric space–time $(\mathbb{R}\times\Sigma, g_{ab})$,

$$g_{ab} = -e^{2\psi}(\mathrm{d}t)_a(\mathrm{d}t)_b + e^{-2\nu}(\mathrm{d}r)_a(\mathrm{d}r)_b + r^2((\mathrm{d}\theta)_a(\mathrm{d}\theta)_b + \sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b), \tag{4.42}$$

where $\psi=\psi(t,r)$ and $\nu=\nu(t,r)$, consider a spacelike two-surface S given by an isometry sphere $r=r_0=\text{const}$ and $t=t_0=\text{const}$. The metric on S is

$$\sigma_{ab} = r_0^2(\mathrm{d}\theta)_a(\mathrm{d}\theta)_b + r_0^2\sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b \tag{4.43}$$

and the area of S is $A(S)=4\pi r_0^2$. Fix an orthonormal frame adapted to S by

$$\vartheta_a^0 = e^{\psi}(\mathrm{d}t)_a, \quad \vartheta_a^1 = e^{-\nu}(\mathrm{d}r)_a, \quad \vartheta_a^2 = r(\mathrm{d}\theta)_a, \quad \vartheta_a^3 = r\sin\theta(\mathrm{d}\phi)_a. \tag{4.44}$$

The Ricci rotation coefficients of the frame

$$\Gamma_{\lambda}^{\mu\nu}(\vartheta) = \vartheta_{\lambda}^a\vartheta^{b\nu}\nabla_a\vartheta_b^{\mu} = 2\,\vartheta_{\lambda}^a\vartheta^{b[\mu}\partial_{[a}\vartheta_{b]}^{\nu]} - \vartheta^{b\mu}\vartheta^{c\nu}\partial_{[b}\vartheta_{c]\lambda} \tag{4.45}$$

have the following nonvanishing components:

$$\Gamma_0{}^{10} = -(\partial_r e^{\psi})e^{\nu}e^{-\psi}, \tag{4.46}$$

$$\Gamma_1{}^{01} = -(\partial_t e^{\nu})e^{-\nu}e^{-\psi}, \tag{4.47}$$

$$\Gamma_2{}^{12} = -\frac{e^{\nu}}{r} = \Gamma_3{}^{13}, \tag{4.48}$$

$$\Gamma_3{}^{23} = -\frac{\cos\theta}{r\sin\theta}. \tag{4.49}$$

The trace of the extrinsic curvatures of (S, σ_{ab}) with respect to the frame on $T(S)^{\perp}$

$$t_a = \vartheta^0_a|_S, \quad s_a = \vartheta^1_a|_S, \tag{4.50}$$

are, respectively,

$$\kappa(t) = \sigma^{ab}\nabla_a t_b = -(\Gamma_2{}^{02} + \Gamma_3{}^{03})|_S = 0, \tag{4.51}$$

and

$$\kappa(s) = \sigma^{ab}\nabla_a s_b = -(\Gamma_2{}^{12} + \Gamma_3{}^{13})|_S = \frac{2e^{\nu(t_0,r_0)}}{r_0}. \tag{4.52}$$

A preferred direction in $T(S)^{\perp}$ is given by the mean curvature vector

$$H^a = s^a\kappa(s) - t^a\kappa(t) = \frac{2e^{2\nu(t_0,r_0)}}{r_0}(\partial_r)^a, \tag{4.53}$$

which is spacelike. This vector gives the direction of the minimum absolute spacelike expansion of S. Furthermore, the value of the expansion is given by the trace extrinsic curvature of S with respect to the unit vector in the direction H^a,

$$\frac{1}{\sqrt{H^2}}\kappa(H) = |\kappa(t)| = \frac{2e^{\nu(t_0,r_0)}}{r_0}, \tag{4.54}$$

which is equal to the norm of H^a.

The normal part of the Dirichlet symplectic vector is given by the normal mean curvature vector

$$(P^{\mathrm{D}}_{\perp})^a = H^a_{\perp} = t^a\kappa(s) - s^a\kappa(t) = 2\frac{e^{\nu(t_0,r_0)}e^{-\psi(t_0,r_0)}}{r_0}(\partial_t)^a. \tag{4.55}$$

Here $(P^{\mathrm{D}}_{\perp})^a$ is timelike, orthogonal to H^a, with the same absolute norm as H^a. Most significant, $(P^{\mathrm{D}}_{\perp})^a$ gives the direction of zero expansion of S.

A preferred orthonormal frame for $T(S)^{\perp}$ is

$$\hat{t}^a = \frac{1}{\sqrt{H^2}}H^a_{\perp} = e^{-\psi}(\partial_t)^a, \quad \hat{s}^a = \frac{1}{\sqrt{H^2}}H^a = e^{\nu}(\partial_r)^a, \tag{4.56}$$

which depend only on S and η_{ab} but not on the chosen frame ϑ^{μ}_a. In the preferred frame (4.56) the tangential part of the Dirichlet symplectic vector is

$$(P^{\mathrm{D}}_{\parallel})^a = \sigma^{ac}\hat{t}^b\nabla_c\hat{s}_b = (\vartheta^{2a}\Gamma_2{}^{10} + \vartheta^{3a}\Gamma_3{}^{10})|_S = 0, \tag{4.57}$$

and thus the normal curvature of S is zero.

Hence the complete Dirichlet symplectic vector is

$$P^a=(P_\perp^{\mathrm{D}})^a+(P_\parallel^{\mathrm{D}})^a=2\,\frac{e^{\nu(t_0,r_0)-\psi(t_0,r_0)}}{r_0}(\partial_t)^a, \tag{4.58}$$

which depends only on S and η_{ab}. In particular, it is independent of choice of the original orthonormal frame (4.44) for g_{ab} and (4.50) for $\sigma^{\perp}_{ab}$.

To define the Neumann symplectic vector, it is natural to use the orthonormal frame (4.56) extended off S to the congruence of isometry spheres $t=\text{const}$, $r=\text{const}$. Then, for this extension, the normal part of the Neumann symplectic vector is given by the commutator

$$(P_\perp^{\mathrm{N}})^a=\mathcal{P}_S^{\perp}[\hat{t},\hat{s}]^a=(\hat{t}^a\Gamma_0{}^{10}+\hat{s}^a\Gamma_1{}^{10})|_S=(-(\partial_r e^{\psi})e^{\nu}e^{-2\psi}(\partial_t)^a+(\partial_t e^{\nu})e^{-\psi}(\partial_r)^a)|_S\,. \tag{4.59}$$

Since $(P_\parallel^{\mathrm{N}})^a=(P_\parallel^{\mathrm{D}})^a=0$, the complete Neumann symplectic vector with respect to the congruence of isometry spheres associated with S is given by

$$P^a=(P_\perp^{\mathrm{N}})^a+(P_\parallel^{\mathrm{N}})^a=e^{\nu(t_0,r_0)-\psi(t_0,r_0)}(-\partial_r\psi(t_0,r_0)(\partial_t)^a+\partial_t\nu(t_0,r_0)(\partial_r)^a). \tag{4.60}$$

Finally, as a special case, consider the Reissner–Nordström black hole space–time obtained for

$$e^{\psi}=e^{\nu}=\sqrt{1-2m/r+q^2/r^2}, \tag{4.61}$$

where $m=\text{const}$ and $q=\text{const}$ are the black hole mass and charge; $q=0$ yields the Schwarzschild black hole. The mean curvature vector of an isometry sphere S, $t=\text{const}$, $r=\text{const}$, is given by

$$H^a=\frac{2}{r}\left(1-\frac{2m}{r}+\frac{q^2}{r^2}\right)(\partial_r)^a, \tag{4.62}$$

which gives the direction of the minimum absolute spacelike expansion of S. Furthermore, the value of the expansion is given by the norm of H^a,

$$|\kappa(s)|=\frac{2}{r}\sqrt{1-\frac{2m}{r}+\frac{q^2}{r^2}}. \tag{4.63}$$

The complete Dirichlet symplectic vector is given by

$$P^a=\frac{2}{r}(\partial_t)^a, \tag{4.64}$$

which depends only on S and η_{ab}. Note that P^a is timelike, orthogonal to H^a, with the same absolute norm as H^a, and it gives the direction of zero expansion of S.

With respect to the congruence of isometry spheres associated to S, the complete Neumann symplectic vector is given by

$$P^a=-\left(\frac{m}{r^2}-\frac{q^2}{r^3}\right)\left(1-\frac{2m}{r}+\frac{q^2}{r^2}\right)^{-1}(\partial_t)^a. \tag{4.65}$$

The curl of this vector yields the sectional curvature normal to S.

C. Axisymmetric space–times

Now consider a stationary axisymmetric space–time $(\mathbb{R}\times\Sigma,g_{ab})$,

$$\begin{aligned} g_{ab}=&-e^{2\psi}(\mathrm{d}t)_a(\mathrm{d}t)_b+e^{-2\nu}(\mathrm{d}r)_a(\mathrm{d}r)_b+e^{-2\mu_1}(\mathrm{d}\theta)_a(\mathrm{d}\theta)_b\\ &+e^{-2\mu_2}((\mathrm{d}\phi)_a-w(\mathrm{d}t)_a)((\mathrm{d}\phi)_b-w(\mathrm{d}t)_b), \end{aligned} \tag{4.66}$$

where[12] $w=w(r,\theta)$, $\psi=\psi(r,\theta)$, $\nu=\nu(r,\theta)$, $\mu_1=\mu_1(r,\theta)$, and $\mu_2=\mu_2(r,\theta)$. Let S be a spacelike two-surface given by $r=r_0=\text{const}$ and $t=t_0=\text{const}$, which has the metric

$$\sigma_{ab}=e^{-2\mu_1(r_0,\theta)}(\mathrm{d}\theta)_a(\mathrm{d}\theta)_b)+e^{-2\mu_2(r_0,\theta)}(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b\,. \tag{4.67}$$

The area of S is $A(S)=2\pi\int_0^\pi e^{-\mu_1(r_0,\theta)-\mu_2(r_0,\theta)}\mathrm{d}\theta$. A natural orthonormal frame adapted to S is given by

$$\vartheta^0_a=e^{\psi}(\mathrm{d}t)_a\,,\quad \vartheta^1_a=e^{-\nu}(\mathrm{d}r)_a\,,\quad \vartheta^2_a=e^{-\mu_1}(\mathrm{d}\theta)_a\,,\quad \vartheta^3_a=e^{-\mu_2}((\mathrm{d}\phi)_a-w(\mathrm{d}t)_a). \tag{4.68}$$

The Ricci rotation coefficients of the frame

$$\Gamma^{\mu\nu}_{\lambda}(\vartheta)=\vartheta^a_\lambda\vartheta^{b\nu}\nabla_a\vartheta^\mu_b=2\,\vartheta^a_\lambda\vartheta^{b[\mu}\partial_{[a}\vartheta^{\nu]}_{b]}-\vartheta^{b\mu}\vartheta^{c\nu}\partial_{[b}\vartheta_{c]\lambda} \tag{4.69}$$

have the following nonvanishing components:

$$\Gamma_0{}^{01}=e^{-\psi}e^{\nu}\partial_r e^{\psi},\quad \Gamma_3{}^{01}=\tfrac{1}{2}e^{-\psi}e^{\nu}e^{-\mu_2}\partial_r w, \tag{4.70}$$

$$\Gamma_0{}^{02}=e^{-\psi}e^{\mu_1}\partial_\theta e^{\psi},\quad \Gamma_3{}^{02}=\tfrac{1}{2}e^{-\psi}e^{\mu_1}e^{-\mu_2}\partial_\theta w, \tag{4.71}$$

$$\Gamma_1{}^{03}=\tfrac{1}{2}e^{-\psi}e^{\nu}e^{-\mu_2}\partial_r w,\quad \Gamma_2{}^{03}=\tfrac{1}{2}e^{-\psi}e^{\mu_1}e^{-\mu_2}\partial_\theta w, \tag{4.72}$$

$$\Gamma_1{}^{12}=e^{\nu}e^{\mu_1}\partial_\theta e^{-\nu},\quad \Gamma_2{}^{12}=-e^{\nu}e^{\mu_1}\partial_r e^{-\mu_1}, \tag{4.73}$$

$$\Gamma_0{}^{13}=\tfrac{1}{2}e^{-\psi}e^{\nu}e^{-\mu_2}\partial_r w,\quad \Gamma_3{}^{13}=-e^{\nu}e^{\mu_2}\partial_r e^{-\mu_2}, \tag{4.74}$$

$$\Gamma_0{}^{23}=\tfrac{1}{2}e^{-\psi}e^{\mu_1}e^{-\mu_2}\partial_\theta w,\quad \Gamma_3{}^{23}=-e^{\mu_1}e^{\mu_2}\partial_\theta e^{-\mu_2}. \tag{4.75}$$

The trace of the extrinsic curvatures of (S,σ_{ab}) with respect to the frame on $T(S)^\perp$

$$t_a=\vartheta^0_a|_S\,,\quad s_a=\vartheta^1_a|_S\,, \tag{4.76}$$

are, respectively,

$$\kappa(t)=\sigma^{ab}\nabla_a t_b=-(\Gamma_2{}^{02}+\Gamma_3{}^{03})|_S=0, \tag{4.77}$$

and

$$\kappa(s)=\sigma^{ab}\nabla_a s_b=-(\Gamma_2{}^{12}+\Gamma_3{}^{13})|_S=-e^{\nu(r_0,\theta)}\partial_r\mu(r_0,\theta), \tag{4.78}$$

where $\mu(r,\theta)=\mu_1+\mu_2$. A preferred direction in $T(S)^\perp$ is given by the mean curvature vector

$$H^a=s^a\kappa(s)-t^a\kappa(t)=-e^{2\nu(r_0,\theta)}\partial_r\mu(r_0,\theta)(\partial_r)^a, \tag{4.79}$$

which is spacelike. This vector gives the direction of the minimum absolute spacelike expansion of S. Furthermore, the value of the expansion is given by the trace extrinsic curvature of S with respect to the unit vector in the direction H^a,

$$\frac{1}{\sqrt{H^2}}\,\kappa(H)=|\kappa(s)|=e^{\nu(r_0,\theta)}|\partial_r\mu(r_0,\theta)|, \tag{4.80}$$

which is equal to the norm of H^a.

The normal part of the Dirichlet symplectic vector is given by the normal mean curvature vector

$$(P^{\mathrm{D}}_\perp)^a=H^a_\perp=t^a\kappa(s)-s^a\kappa(t)=-e^{-\psi(r_0,\theta)}e^{\nu(r_0,\theta)}\partial_r\mu(r_0,\theta)((\partial_t)^a+w(\partial_\phi)^a). \tag{4.81}$$

Here $(P_\perp^{\mathrm{D}})^a$ is timelike, orthogonal to H^a, with the same absolute norm as H^a. Most significant, $(P_\perp^{\mathrm{D}})^a$ gives the direction of zero expansion of S.

A preferred orthonormal frame for $T(S)^\perp$ is

$$\hat{t}^a=\frac{1}{\sqrt{H^2}}H_\perp^a=e^{-\psi}((\partial_t)^a+w(\partial_\phi)^a),\quad \hat{s}^a=\frac{1}{\sqrt{H^2}}H^a=e^{\nu}(\partial_r)^a, \tag{4.82}$$

which depend only on S and η_{ab} but not on the chosen frame ϑ_a^μ. In the preferred frame (4.82) the tangential part of the Dirichlet symplectic vector is

$$(P_\parallel^{\mathrm{D}})^a=\sigma^{ac}\hat{t}^b\nabla_c\hat{s}_b=(\vartheta^{2a}\Gamma_2{}^{10}+\vartheta^{3a}\Gamma_3{}^{10})|_S=\tfrac{1}{2}e^{-\psi(r_0,\theta)}e^{\nu(r_0,\theta)}\partial_r w(r_0,\theta)(\partial_\phi)^a. \tag{4.83}$$

The curl of this vector yields the normal curvature of S.

Hence the complete Dirichlet symplectic vector is

$$P^a=(P_\perp^{\mathrm{D}})^a+(P_\parallel^{\mathrm{D}})^a=e^{-\psi(r_0,\theta)+\nu(r_0,\theta)}(-\partial_r\mu(r_0,\theta)((\partial_t)^a+w(\partial_\phi)^a)+\tfrac{1}{2}\partial_r w(r_0,\theta)\,(\partial_\phi)^a), \tag{4.84}$$

which depends only on S and η_{ab}. In particular, it is independent of choice of the original orthonormal frame (4.68) for g_{ab} and (4.76) for $\sigma_{ab}^\perp$.

To define the Neumann symplectic vector, it is natural to use the orthonormal frame (4.82) extended off S to the congruence of two-surfaces $t=\text{const}$, $r=\text{const}$. With respect to this extension, the normal part of the Neumann symplectic vector is given by the commutator

$$(P_\perp^{\mathrm{N}})^a=\mathcal{P}_S^\perp[\hat{t},\hat{s}]^a=(\hat{t}^a\Gamma_0{}^{10}+\hat{s}^a\Gamma_1{}^{10})|_S=-e^{-\psi(r_0,\theta)}e^{\nu(r_0,\theta)}\partial_r\psi(r_0,\theta)((\partial_t)^a+w(\partial_\phi)^a). \tag{4.85}$$

Since $(P_\parallel^{\mathrm{N}})^a=(P_\parallel^{\mathrm{D}})^a$, the complete Neumann symplectic vector in this congruence of two-surfaces associated with S is given by

$$P^a=(P_\perp^{\mathrm{N}})^a+(P_\parallel^{\mathrm{N}})^a=e^{-\psi(r_0,\theta)+\nu(r_0,\theta)}(-\partial_r\psi(r_0,\theta)((\partial_t)^a+w(\partial_\phi)^a)+\tfrac{1}{2}\partial_r w(r_0,\theta)\,(\partial_\phi)^a). \tag{4.86}$$

The curl of this vector yields the sectional curvature normal to S.

As a special case, consider the Kerr black hole space–time obtained for

$$e^{\psi}=\frac{\sqrt{\Delta}\rho}{\Upsilon},\quad e^{-\nu}=\frac{\rho}{\sqrt{\Delta}},\quad e^{-\mu_1}=\rho,\quad e^{-\mu_2}=\frac{\Upsilon\sin\theta}{\rho},\quad w=\frac{2amr}{\Upsilon^2}, \tag{4.87}$$

where

$$\Upsilon^2=(r^2+a^2)^2-a^2\Delta\sin^2\theta,\quad \Delta=r^2-2mr+a^2,\quad \rho^2=r^2+a^2\cos^2\theta. \tag{4.88}$$

Here $m=\text{const}$ and $a=\text{const}$ are the black hole mass and angular momentum; $a=0$ yields the Schwarzschild black hole. The mean curvature vector of a two-surface S, $t=\text{const}$, $r=\text{const}$, is given by

$$H^a=\frac{\Delta}{\rho^2}\frac{\partial_r\Upsilon}{\Upsilon}(\partial_r)^a=\frac{\Delta}{\rho^2\Upsilon^2}(2r(r^2+a^2)-a^2(r-m)\sin^2\theta)(\partial_r)^a, \tag{4.89}$$

which gives the direction of the minimum absolute spacelike expansion of S. Furthermore, the value of the expansion is given by the norm of H^a,

$$|\kappa(s)| = \frac{\sqrt{\Delta}}{\rho \Upsilon^2}(2r(r^2+a^2) - a^2(r-m)\sin^2\theta). \tag{4.90}$$

The complete Dirichlet symplectic vector is given by

$$\begin{aligned} P^a &= \frac{\Upsilon}{\rho^2}\left(\frac{\partial_r \Upsilon}{\Upsilon}((\partial_t)^a + w(\partial_\phi)^a) + \frac{\partial_r w}{2}(\partial_\phi)^a\right) \\ &= \frac{2r(r^2+a^2) - a^2(r-m)\sin^2\theta}{\rho^2 \Upsilon}(\partial_t)^a + \frac{am}{\rho^2 \Upsilon}(\partial_\phi)^a, \end{aligned} \tag{4.91}$$

which depends only on S and η_{ab}. Note that P^a is timelike, orthogonal to H^a, with the same absolute norm as H^a, and it gives the direction of zero expansion of S.

With respect to this congruence of two-surfaces S, the complete Neumann symplectic vector is given by

$$\begin{aligned} P^a &= \frac{\Upsilon}{\rho^2}\left(\left(\frac{\partial_r \Upsilon}{\Upsilon} - \frac{\partial_r \Delta}{2\Delta} - \frac{\partial_r \rho}{2\rho}\right)((\partial_t)^a + w(\partial_\phi)^a) + \frac{\partial_r w}{2}(\partial_\phi)^a\right) \\ &= -\frac{2m}{\rho^4 \Upsilon \Delta}((r^2+a^2)^2(r^2-a^2) + a^2((r^2+a^2)^2 - 4mr^3)\sin^2\theta)(\partial_t)^a \\ &\quad + \frac{am}{\rho^4 \Upsilon \Delta}((r^2-a^2)^2 - 4r^3(r-m) - a^2(a^2-r^2)\sin^2\theta)(\partial_\phi)^a. \end{aligned} \tag{4.92}$$

D. Homogeneous isotropic space–times

Next, consider a Friedmann–Robertson–Walker space–time $(\mathbb{R}\times\Sigma, g_{ab})$,

$$g_{ab} = -(\mathrm{d}t)_a(\mathrm{d}t)_b + a^2(t)\left(\frac{1}{1-kr^2}(\mathrm{d}r)_a(\mathrm{d}r)_b + r^2((\mathrm{d}\theta)_a(\mathrm{d}\theta)_b + \sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b)\right), \tag{4.93}$$

where $k=0, 1, -1$ [Σ is $\mathbb{R}^3$ if $k=0, -1$ or S^3 if $k=1$] corresponding to a spatially flat, spherical, or hyperbolic geometry on Σ. Let S be a spacelike two-surface given by an isometry sphere $r = r_0 = \text{const}$ and $t = t_0 = \text{const}$. The metric on S is

$$\sigma_{ab} = a^2(t_0) r_0{}^2((\mathrm{d}\theta)_a(\mathrm{d}\theta)_b + \sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b) \tag{4.94}$$

and the area of S is $A(S) = 4\pi a(t_0) r_0^2$. Fix an orthonormal frame adapted to S by

$$\vartheta^0_a = (\mathrm{d}t)_a, \quad \vartheta^1_a = \frac{a(t)}{\sqrt{1-kr^2}}(\mathrm{d}r)_a, \quad \vartheta^2_a = a(t) r (\mathrm{d}\theta)_a, \quad \vartheta^3_a = a(t) r \sin\theta (\mathrm{d}\phi)_a. \tag{4.95}$$

The Ricci rotation coefficients of the frame

$$\Gamma_\lambda{}^{\mu\nu}(\vartheta) = \vartheta^a_\lambda \vartheta^{b\nu} \nabla_a \vartheta^\mu_b = 2\vartheta^a_\lambda \vartheta^{b[\mu} \partial_{[a} \vartheta^{\nu]}_{b]} - \vartheta^{b\mu} \vartheta^{c\nu} \partial_{[b} \vartheta_{c]\lambda} \tag{4.96}$$

have the following nonvanishing components:

$$\Gamma_0{}^{01} = \frac{\dot{a}(t)}{a(t)} = \Gamma_2{}^{02} = \Gamma_3{}^{03}, \tag{4.97}$$

$$\Gamma_1{}^{12} = \frac{\sqrt{1-2kr}}{a(t) r} = \Gamma_3{}^{13}, \tag{4.98}$$

$$\Gamma_3{}^{23} = -\frac{\cos\theta}{a(t) r \sin\theta}. \tag{4.99}$$

(Here, an over-dot denotes a derivative with respect to t.)

The trace of the extrinsic curvatures of (S, σ_{ab}) with respect to the frame on $T(S)^{\perp}$

$$t_a = \vartheta^0_a|_S, s_a = \vartheta^1_a|_S, \tag{4.100}$$

are, respectively,

$$\kappa(t) = \sigma^{ab}\nabla_a t_b = -(\Gamma_2{}^{02} + \Gamma_3{}^{03})|_S = \frac{2\dot{a}(t_0)}{a(t_0)} \tag{4.101}$$

and

$$\kappa(s) = \sigma^{ab}\nabla_a s_b = -(\Gamma_2{}^{12} + \Gamma_3{}^{13})|_S = \frac{2\sqrt{1-kr_0{}^2}}{r_0 a(t_0)}. \tag{4.102}$$

A preferred direction in $T(S)^{\perp}$ is given by the mean curvature vector

$$H^a = s^a\kappa(s) - t^a\kappa(t) = 2\left(\frac{1-kr_0{}^2}{a(t_0)^2 r_0}(\partial_r)^a - \frac{\dot{a}(t_0)}{a(t_0)}(\partial_t)^a\right). \tag{4.103}$$

This vector gives the direction of the minimum absolute spacelike expansion of S. Furthermore, the value of the expansion is given by the trace extrinsic curvature of S with respect to the unit vector in the direction H^a,

$$\frac{1}{\sqrt{H^2}}\kappa(H) = |\kappa(s)| = \frac{2}{a(t_0)}\sqrt{\frac{1-kr_0{}^2}{r_0{}^2} - \dot{a}^2(t_0)}, \tag{4.104}$$

which is equal to the norm of H^a.

The normal part of the Dirichlet symplectic vector is given by the normal mean curvature vector

$$(P^{\mathrm{D}}_{\perp})^a = H^a_{\perp} = t^a\kappa(s) - s^a\kappa(t) = \frac{2\sqrt{1-kr_0{}^2}}{a(t_0)}\left(\frac{1}{r_0}(\partial_t)^a - \frac{\dot{a}(t_0)}{a(t_0)}(\partial_r)^a\right). \tag{4.105}$$

Here $(P^{\mathrm{D}}_{\perp})^a$ is orthogonal to H^a, with the same absolute norm as H^a. Most significant, $(P^{\mathrm{D}}_{\perp})^a$ gives the direction of zero expansion of S. Note that $(P^{\mathrm{D}}_{\perp})^a$ is timelike (and H^a is spacelike) if and only if the acceleration of Σ satisfies $|\dot{a}(t_0)| \leqslant \sqrt{1-kr_0{}^2}/r_0$, depending on the radius of S.

A preferred orthonormal frame for $T(S)^{\perp}$ is

$$\hat{t}^a = \frac{1}{\sqrt{H^2}}H^a_{\perp} = (\partial_t)^a, \quad \hat{s}^a = \frac{1}{\sqrt{H^2}}H^a = \frac{\sqrt{1-kr^2}}{a(t)}(\partial_r)^a, \tag{4.106}$$

which depend only on S and η_{ab} but not on the chosen frame ϑ^{μ}_a. In the preferred frame (4.56) the tangential part of the Dirichlet symplectic vector is

$$(P^{\mathrm{D}}_{\parallel})^a = \sigma^{ac}\hat{t}^b\nabla_c\hat{s}_b = (\vartheta^{2a}\Gamma_2{}^{10} + \vartheta^{3a}\Gamma_3{}^{10})|_S = 0, \tag{4.107}$$

and thus the normal curvature of S is zero.

Hence the complete Dirichlet symplectic vector is

$$P^a=(P^{\mathrm{D}}_{\perp})^a+(P^{\mathrm{D}}_{\parallel})^a=\frac{\sqrt{1-kr_0{}^2}}{a(t_o)}\left(\frac{1}{r_0}(\partial_t)^a-\frac{\dot a(t_0)}{a(t_0)}(\partial_r)^a\right), \tag{4.108}$$

which depends only on S and η_{ab}. In particular, it is independent of choice of the original orthonormal frame (4.95) for g_{ab} and (4.100) for $\sigma^{\perp}_{ab}$.

To define the Neumann symplectic vector, it is natural to use to the orthonormal frame (4.106) extended off S to the congruence of isometry spheres $t=\mathrm{const}$, $r=\mathrm{const}$. Then, for this extension, the normal part of the Neumann symplectic vector is given by the commutator

$$(P^{\mathrm{N}}_{\perp})^a=\mathcal{P}^{\perp}_S[\hat t,\hat s]^a=(\hat t^a\Gamma_0{}^{10}+\hat s^a\Gamma_1{}^{10})|_S=-\left(\frac{\sqrt{1-kr_0{}^2}}{a(t_0)^2}\right)\dot a(t_0)(\partial_r)^a. \tag{4.109}$$

Since $(P^{\mathrm{N}}_{\parallel})^a=(P^{\mathrm{D}}_{\parallel})^a=0$, the complete Neumann symplectic vector with respect to the congruence of isometry spheres associated with S is given by

$$P^a=(P^{\mathrm{N}}_{\perp})^a+(P^{\mathrm{N}}_{\parallel})^a=-\sqrt{1-kr_0{}^2}\frac{\dot a(t_0)}{a(t_0)^2}(\partial_r)^a. \tag{4.110}$$

For an isometry sphere S, $r=\mathrm{const}$, $t=\mathrm{const}$, in a time-symmetric hypersurface Σ, since $\dot a(t)=0$ it follows that H^a is spacelike, $(P^{\mathrm{D}}_{\perp})^a$ is timelike. Then the complete Dirichlet symplectic vector is

$$P^a=\frac{2\sqrt{1-kr^2}}{ra(t)}(\partial_t)^a, \tag{4.111}$$

while the complete Neumann symplectic vector vanishes.

E. Asymptotically flat space–times

Consider an asymptotically flat space–time (M,g_{ab}) with $g_{ab}=\eta_{ab}+O(1/r)$ and $\partial_c g_{ab}=O(1/r^2)$ as $r\to\infty$ at fixed t, where η_{ab} is a flat metric (4.1) in Minkowski spherical coordinates t, r, θ, ϕ. Suppose the total ADM mass, m, of the space–time (M,g_{ab}) is finite and positive. Then, the metric has the asymptotic form[13,14]

$$\begin{aligned}g_{ab}=&-(1-2m/r+O(1/r^2))(\mathrm{d}t)_a(\mathrm{d}t)_b+(1+2m/r+O(1/r^2))(\mathrm{d}r)_a(\mathrm{d}r)_b+r^2((\mathrm{d}\theta)_a(\mathrm{d}\theta)_b\\&+\sin^2\theta(\mathrm{d}\phi)_a(\mathrm{d}\phi)_b+O(1/r^3))\quad\text{as } r\to\infty \text{ at fixed } t.\end{aligned} \tag{4.112}$$

[Note that any gravitational radiation terms vanish in this limit.] We first discuss the ADM energy–momentum vector.[11] In the space–time (M,g_{ab}), spatial infinity, ι^0, can be represented as the set of asymptotic two-spheres S_∞ given by $t=\mathrm{const}$, $r=\to\infty$, which are regarded as being identified under asymptotic time translations generated by the Killing vector $(\partial_t)^a$ of η_{ab}. Now, for a spacelike hypersurface Σ_t, $t=\mathrm{const}$, the ADM energy and momentum in standard asymptotic Minkowski coordinates x^μ on M are given by[15]

$$P_\mu=\begin{cases}\displaystyle\sum_{\nu,\rho\neq 0}\frac{1}{16\pi}\int_{S_\infty}s_\nu(\partial_\rho g_{\rho\nu}-\partial_\nu g_{\rho\rho})\mathrm{d}S=m, & \mu=0\\ \displaystyle\sum_{\nu\neq 0}\frac{1}{16\pi}\int_{S_\infty}(s_\nu\partial_t g_{\mu\nu}-s_\mu\partial_t g_{\nu\nu})\mathrm{d}S=0, & \mu=1,2,3.\end{cases} \tag{4.113}$$

Hence, the ADM energy-momentum vector at spatial infinity is represented by $(P^{\mathrm{ADM}})_a=m(\mathrm{d}t)_a|_{S_\infty}$. Let $n^a=(\partial_t)^a|_{S_\infty}$. Then, geometrically, the vector

$$\frac{1}{m}(P^{\mathrm{ADM}})^a = -n^a \tag{4.114}$$

corresponds to an asymptotic stationary unit-norm Killing vector of the asymptotically flat metric (4.112).

To proceed, let S be any family of spacelike two-surfaces that approaches the two-sphere S_∞ as $r\to\infty$ at fixed t. Since the space–time metric is asymptotic to the Schwarzschild metric, we may use the results obtained in example (B) to calculate the Dirichlet and Neumann symplectic vectors in this limit.

The Dirichlet symplectic vector is given by

$$(P^{\mathrm{D}})^a = \frac{2}{r}(1-m/r)t^a + O(1/r^3), \tag{4.115}$$

where $t^a = (1+m/r+O(1/r^2))(\partial_t)^a$ is a unit timelike vector of (M,g_{ab}). For a comparison with $(P^{\mathrm{ADM}})^a$, we scale $(P^{\mathrm{D}})^a$ by the area of S, $A(S)=4\pi r^2+O(1/r)$, which yields

$$A(S)(P^{\mathrm{D}})^a = 8\pi(r-m+O(1/r))t^a. \tag{4.116}$$

Note that the first term in this expression is singular as $r\to\infty$. It corresponds to the Dirichlet symplectic vector for S_∞ with respect to the flat metric η_{ab} on M. We extend this vector in a natural geometrical manner from S_∞ to S by

$$(P^{\mathrm{D}}_{\mathrm{flat}})^a = \frac{2}{r}t^a, \tag{4.117}$$

which depends only on the radius of S and the timelike unit vector t^a with respect to g_{ab}. We now subtract $(P^{\mathrm{D}}_{\mathrm{flat}})^a$ from $(P^{\mathrm{D}})^a$ to obtain the normalized Dirichlet symplectic vector

$$(\overline{P^{\mathrm{D}}})^a = A(S)((P^{\mathrm{D}})^a - (P^{\mathrm{D}}_{\mathrm{flat}})^a) = (-8\pi m + O(1/r))t^a. \tag{4.118}$$

Then the limit $r\to\infty$ yields a well-defined (finite) vector associated to S_∞ in terms of $t^a\to n^a$. This establishes our main result.

Theorem 4.1: *For an asymptotically flat space–time (M,g_{ab}), at spatial infinity the normalized Dirichlet symplectic vector (4.118) is equal to 8π times the ADM energy-momentum vector (4.114),*

$$\frac{1}{8\pi}(\overline{P^{\mathrm{D}}})^a|_{S_\infty} = (P^{\mathrm{ADM}})^a = -mn^a. \tag{4.119}$$

[The 8π factor reflects the normalization chosen for the Hamiltonian variational principle for the Einstein equations in Sec. II.]

We remark that the ADM vector $(P^{\mathrm{ADM}})^a$ can be derived[16] directly from the symplectic structure of the Einstein equations similarly to the analysis given in Sec. 3 in Ref. 1 by using asymptotically flat boundary conditions at S_∞ in place of the Dirichlet boundary condition at S on the space–time metric.

Finally, we discuss the Neumann symplectic vector. Note that the normalized symplectic vector (4.118) is obtained from the locally constructed Dirichlet symplectic vector $(P^{\mathrm{D}})^a$ associated with a spacelike two-surface S, where $(P^{\mathrm{D}})^a$ depends only on S and g_{ab}. In contrast, the Neumann symplectic vector $(P^{\mathrm{N}})^a$ associated with S also depends on a choice of congruence of two-surfaces S' diffeomorphic to S. If a suitably parametrized null geodesic congruence through S is used to define $(P^{\mathrm{N}})^a$, it follows from Proposition 3.14 that the normal part of $(P^{\mathrm{N}})^a$ vanishes. Moreover, the tangential part of $(P^{\mathrm{N}})^a$ is equal to the tangential part of $(P^{\mathrm{D}})^a$. Thus for any

topological two-sphere S that approaches S_∞ as $r\to\infty$, by Eq. (4.115) the resulting vector $(P^{\mathrm{N}})^a$ is at most $O(1/r^3)$ and is tangential to S. Consequently, if we consider the normalized symplectic vector

$$(\overline{P}^{\mathrm{N}})^a = A(S)((P^{\mathrm{N}})^a - (P^{\mathrm{N}}_{\mathrm{flat}})^a) \tag{4.120}$$

defined analogously to $(\overline{P}^{\mathrm{D}})^a$, then

$$(\overline{P}^{\mathrm{N}})^a|_{S_\infty} = 0. \tag{4.121}$$

Note that for an asymptotically flat metric (4.112), as S approaches S_∞, all null geodesic congruences through S approach future and past null infinity, $\mathcal{I}^{\pm}$, and thereby provide a natural congruence of spacelike two-spheres $S_{\mathcal{I}^{\pm}}$ associated with the two-sphere S_∞ representing spatial infinity, $\imath^0$. In particular, $S_{\mathcal{I}^{\pm}}$ are related to S_∞ by null geodesic asymptotic isometries of g_{ab}. Hence, the normalized symplectic vector (4.121) effectively depends only on S and g_{ab} (including its asymptotic structure), similar to the vector (4.118).

V. CONCLUDING REMARKS

In this paper we have considered the covariant symplectic structure associated with the Einstein equations with matter sources. One main result is that we derive a covariant Hamiltonian under Dirichlet and Neumann type boundary conditions for both the gravitational field and matter fields in any fixed spatially bounded region of spacetime (M, g_{ab}), allowing the time-flow vector ξ^a to be timelike, spacelike, or null.

The Dirichlet and Neumann Hamiltonians evaluated on solutions of the coupled gravitational and matter field equations reduce to a surface integral over the spatial boundary two-surface, S. [In fact, this result is known to hold for any diffeomorphism covariant space–time field theory.[17]] For each of the boundary conditions this surface integral has the form of $\int_S \xi^a P_a \mathrm{d}S$ where P_a is a locally constructed dual vector field associated with the two-surface S and boundary conditions, which we call the Dirichlet and Neumann symplectic vectors. Similar results are discussed in Ref. 18.

Our principle result is to show that the purely gravitational part of the Dirichlet symplectic vector $(P^{\mathrm{D}})^a$ has very interesting geometrical properties when decomposed into its normal and tangential parts, $(P^{\mathrm{D}}_\perp)^a$ and $(P^{\mathrm{D}}_\parallel)^a$, with respect to S. First, $(P^{\mathrm{D}}_\perp)^a$ depends only on the two-surface S and space–time metric g_{ab} and thus yields a geometrical vector field normal to S in space–time. This vector $(P^{\mathrm{D}}_\perp)^a$ is shown to be orthogonal to the mean curvature vector of S and, most importantly, it gives the direction of zero expansion of S in space–time, i.e., $\mathcal{L}_{P_\perp}\epsilon_{ab}(S) = 0$ where $\epsilon_{ab}(S)$ is the area volume form of S. Furthermore, the norm of the vector $(P^{\mathrm{D}}_\perp)^a$ is equal to the product of the expansions of S with respect to ingoing and outgoing null geodesics, θ^{-a} and θ^{+a} (and is independent of parametrization of the geodesics). This expression is obviously related to the condition for a spatial two-surface S to be trapped (or marginally trapped), namely, $\kappa^+\kappa^-$ is positive (or zero) on S, where $\mathcal{L}_{\theta^\pm}\epsilon_{ab}(S) = \kappa^\pm\epsilon_{ab}(S)$. Consequently, S is trapped (or marginally trapped) precisely when $(P^{\mathrm{D}}_\perp)^a$ is spacelike (or null) on S. If this notion is applied to the ingoing and outgoing null geodesics at each point p on S [i.e., the pair of null geodesics through p is "trapped" (or "marginally trapped") if $\kappa^+\kappa^-$ is positive (or zero) at p], then, in this sense, $(P^{\mathrm{D}}_\perp)^a$ measures pointwise how close S is to being a trapped surface.

In contrast, $(P^{\mathrm{D}}_\parallel)^a$ depends not only on the two-surface S and space–time metric g_{ab} but also on a choice of orthonormal frame or null frame for the normal tangent space $T(S)^\perp$ of S. Geometrically, $(P^{\mathrm{D}}_\parallel)^a$ is shown to be a connection for the normal curvature of S in space–time and consequently changes by a gradient under a boost of the frame. However, if the normal vector $(P^{\mathrm{D}}_\perp)^a$ is non-null, then $(P^{\mathrm{D}}_\perp)^a$ and the mean curvature vector of S comprise a preferred frame for $T(S)^\perp$ and hence there exists a corresponding preferred, tangential vector $(P^{\mathrm{D}}_\parallel)^a$ (evaluated in this

frame). Thus, in this situation, the complete Dirichlet symplectic vector is a well-defined geometrical vector field depending only on S and g_{ab}. We refer to this as the invariant Dirichlet symplectic vector associated with S.

Apart from its geometrical interest, the Dirichlet symplectic vector is also related to definitions of canonical energy, momentum, and angular momentum given by the value of the Dirichlet Hamiltonian for solutions of the Einstein (and matter) equations. In particular, we have shown that in an asymptotically flat space–time in the limit of S approaching spatial infinity S_∞, the Dirichlet symplectic vector reduces in a suitable sense to the ADM energy-momentum vector. Hence, the integral $\int_{S_\infty} \xi^a (P^{\mathrm{D}})_a \mathrm{d}S$ yields total energy, momentum, angular momentum of the space–time when ξ^a is chosen to be an asymptotic Killing vector associated to time-translations, space-translations, or rotations of the asymptotic flat background metric.

In addition, for a compact spatial two-surface S in (M, g_{ab}), it follows from results in Ref. 2 that the quasilocal quantities $\int_S \xi^a (P^{\mathrm{D}})_a \mathrm{d}S$ for ξ^a chosen to be normal and tangential to S reproduce Brown and York's[3,4] quasilocal energy, momentum, and angular momentum quantities. (See also Refs. 1 and 6.) Furthermore, we have obtained matter contributions to these quantities, for an electromagnetic field and a set of Yang–Mills–Higgs fields. In a forthcoming paper we will explore geometrical quasilocal quantities defined purely in terms of $(P^{\mathrm{D}}_\perp)^a$ and $(P^{\mathrm{D}}_\parallel)^a$. We will also explore the use of $(P^{\mathrm{D}})^a$ as a time flow vector for a boundary-initial value formulation of the Einstein equations.

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On the problem of algebraic completeness for the invariants of the Riemann tensor. III.

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We study the set CZ of invariants [Zakhary and Carminati, J. Math. Phys. **42**, 1474 (2001)] for the class of space–times whose Ricci tensors possess a null eigenvector. We show that all cases are maximally backsolvable, in terms of sets of invariants from CZ, but that some cases are not completely backsolvable and these all possess an alignment between an eigenvector of the Ricci tensor with a repeated principal null vector of the Weyl tensor. We provide algebraically complete sets for each canonically different space–time and hence conclude with these results and those of a previous article [Carminati, Zakhary, and McLenaghan, J. Math. Phys. **43**, 492 (2002)] that the CZ set is determining or maximal. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1478803]

I. INTRODUCTION

In the first article of this series,[1] we introduced a new set CZ of polynomial Riemann invariants, satisfying the minimum degree property, which was claimed to be ''determining.'' The main purpose of the second article[2] in this series was to rigorously establish this fact for class A space–times whose Ricci tensors did not possess a null eigenvector. Further, for each canonically different space–time, we gave algebraically complete sets. (This was established by showing that the given sets were curvature complete and minimal in number, by a simple real count. The various new definitions which are used here were introduced in the previous articles.) In this article we will study class B space–times (Ricci tensor possesses a null eigenvector) and show that each canonically different case is maximally backsolvable in terms of sets of invariants from CZ. Interestingly, not all members of this class are completely backsolvable[3] and, in fact, we will show that such NCB space–times, in general, possess an alignment (necessary but not sufficient) between a null eigenvector of the Ricci tensor with a repeated principal null vector of the Weyl tensor. We will give, in some cases,[4] the necessary and/or sufficient invariant conditions (in terms of algebraic relations) for these to occur, together with a maximal independent set. For the NCB cases, we will also indicate, in the Ricci (or Weyl) canonical frames, the Weyl (or Ricci) information [by component(s)] which is missing. In all cases, we do provide algebraically complete sets for each canonically different space–time in class B and hence conclude with these results and those of a previous article[2] that the CZ set is determining or maximal. As before, we will establish all of our results by an implicit backsolving technique described previously.[1,2] Most of the calculations were done using Maple.

The set CZ of invariants and the relations between the various sets, in the literature, and the syzygies for the different Petrov and Segre types of the Weyl and Ricci tensors, have been given in a previous article.[1] For future use, the trace-free Ricci tensor can be written in the form

$$S_{ab} = -2[\Phi_{00} n_a n_b - 2\Phi_{01} n_{(a}\overline{m}_{b)} + \Phi_{02}\overline{m}_a\overline{m}_b - 2\Phi_{10} n_{(a} m_{b)} + 2\Phi_{11}(l_{(a} n_{b)} + m_{(a}\overline{m}_{b)}) - 2\Phi_{12} l_{(a}\overline{m}_{b)} + \Phi_{20} m_a m_b - 2\Phi_{21} l_{(a} m_{b)} + \Phi_{22} l_a l_b]. \quad (1)$$

TABLE I. Canonical frames for Segre types [2,11] and [3,1].

	PP type II, Segre type [2,11]	PP type III, Segre type [3,1]
Canonical form of R_{ab}	$R_{ab}=2\rho_1 l_{(a}n_{b)}+\lambda l_a l_b-\rho_2 x_a x_b-\rho_3 y_a y_b$, with $\rho_1\neq\rho_2$, $\rho_1\neq\rho_3$, $\rho_2\neq\rho_3$, $\lambda=\pm 2$	$R_{ab}=2\rho_1 l_{(a}n_{b)}+2\lambda l_{(a}x_{b)}-\rho_1 x_a x_b-\rho_2 y_a y_b$, with $\rho_1\neq\rho_2$, $\lambda=\pm 2\sqrt{2}$
Inner products	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\lambda l_a+\rho_1 n_a$, $R_{ab}x^b=\rho_2 x_a$, $R_{ab}y^b=\rho_3 y_a$	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\rho_1 n_a+\lambda x_a$, $R_{ab}x^b=\rho_1 x_a-\lambda l_a$, $R_{ab}y^b=\rho_2 y_a$
Eigenvectors	l^a, x^a, y^a	l^a, y^a
Eigenvalues	ρ_1, ρ_2, ρ_3	ρ_1, ρ_2
Canonical form of Φ_{ab}	$\Phi_{00}=\Phi_{01}=\Phi_{12}=0$, $\Phi_{11}=-\frac{1}{8}(2\rho_1-\rho_2-\rho_3)$, $\Phi_{02}=\Phi_{20}=\frac{1}{4}(\rho_2-\rho_3)\neq 0$, $\Phi_{22}=-\frac{1}{2}\lambda$	$\Phi_{00}=\Phi_{01}=\Phi_{22}=0$, $\Phi_{02}=-2\Phi_{11}=\Phi_{20}=\frac{1}{4}(\rho_1-\rho_2)\neq 0$, $\Phi_{12}=\dfrac{\lambda}{2\sqrt{2}}$
Remaining freedom	None	None

II. RICCI CANONICAL FRAMES FOR CLASS B

Tables I–V give the canonical forms for the Ricci tensor when it possesses a null eigenvector. A summary of the notation and complete details where the Ricci tensor does not possess a null eigenvector have been given previously.[2]

At this point, we would like to again compare our canonical forms with those as given by McIntosh *et al.*[5] and Joly and MacCallum.[6] As before,[2] apart from possible changes due to $\mathbf{l}\leftrightarrow\mathbf{n}$ interchange and other minor frame changes, our work differs from theirs in that Φ_{11} could be zero for the Segre types [2,11] and [(1,1)11], whereas they report that Φ_{11} is necessarily nonzero for these types.

III. MAXIMAL BACKSOLVING

In this section, we will prove that the CZ set is determining for class B by explicitly showing that maximal backsolving is always possible for each Segre type, with certain chosen subsets of CZ. Further, we will show that these subsets are algebraically complete. As before, regarding our method of proof, after having established that a set of invariants is maximal or determining by backsolving and if necessary using the index theorem (when the subset is not curvature complete), we then check that we have retained the minimum possible number of invariants ["minimal number" property, i.e., that it cannot be further reduced (in number[7] of invariants) and still achieve the same "measure" [8] of backsolving, after all of the possible remaining tetrad freedom which can act on the curvature components, is completely used up]. It follows that once this is done, we have

TABLE II. Canonical frames for Segre types [(1,1)11] and [(1,1)(11)].

	PP type D, Segre type [(1,1)11]	PP type D, Segre type [(1,1)(11)]
Canonical form of R_{ab}	$R_{ab}=2\rho_1 l_{(a}n_{b)}-\rho_2 x_a x_b-\rho_3 y_a y_b$, with $\rho_1\neq\rho_2$, $\rho_1\neq\rho_3$, $\rho_2\neq\rho_3$	$R_{ab}=2\rho_1 l_{(a}n_{b)}-\rho_2 x_a x_b-\rho_2 y_a y_b$, with $\rho_1\neq\rho_2$
Inner products	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\rho_1 n_a$, $R_{ab}x^b=\rho_2 x_a$, $R_{ab}y^b=\rho_3 y_a$	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\rho_1 n_a$, $R_{ab}x^b=\rho_2 x_a$, $R_{ab}y^b=\rho_2 y_a$
Eigenvectors	l^a, n^a, x^a, y^a	l^a, n^a, x^a, y^a
Eigenvalues	ρ_1, ρ_1, ρ_2, ρ_3	ρ_1, ρ_1, ρ_2, ρ_2
Canonical form of Φ_{ab}	$\Phi_{00}=\Phi_{01}=\Phi_{12}=\Phi_{22}=0$, $\Phi_{11}=-\frac{1}{8}(2\rho_1-\rho_2-\rho_3)$, $\Phi_{02}=\Phi_{20}=\frac{1}{4}(\rho_2-\rho_3)\neq 0$	$\Phi_{00}=\Phi_{01}=\Phi_{02}=\Phi_{12}=\Phi_{22}=0$, $\Phi_{11}=-\frac{1}{4}(\rho_1-\rho_2)\neq 0$
Remaining freedom	Boost: $AD=1$, $\overline{A}=A>0$, $B=C=0$	Boost and spatial rotations: $AD=1$, $B=C=0$

TABLE III. Canonical frames for Segre types [2,(11)] and [(2,1)1].

	PP type D, Segre type [2,(11)]	PP type N, Segre type [(2,1)1]
Canonical form of R_{ab}	$R_{ab}=2\rho_1 l_{(a}n_{b)}+\lambda l_a l_b-\rho_2 x_a x_b-\rho_2 y_a y_b$, with $\rho_1\neq\rho_2$, $\lambda=\pm 2$	$R_{ab}=2\rho_1 l_{(a}n_{b)}+\lambda l_a l_b-\rho_1 x_a x_b-\rho_2 y_a y_b$, with $\rho_1\neq\rho_2$, $\lambda=\pm 2$
Inner products	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\lambda l_a+\rho_1 n_a$, $R_{ab}x^b=\rho_2 x_a$, $R_{ab}y^b=\rho_2 y_a$	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\lambda l_a+\rho_1 n_a$, $R_{ab}x^b=\rho_1 x_a$, $R_{ab}y^b=\rho_2 y_a$
Eigenvectors	l^a, x^a, y^a	l^a, x^a, y^a
Eigenvalues	ρ_1, ρ_2, ρ_2	ρ_1, ρ_1, ρ_2
Canonical form of Φ_{ab}	$\Phi_{00}=\Phi_{01}=\Phi_{02}=\Phi_{12}=0$, $\Phi_{11}=-\frac{1}{4}(\rho_1-\rho_2)\neq 0$, $\Phi_{22}=-\frac{1}{2}\lambda$	$\Phi_{00}=\Phi_{01}=\Phi_{12}=0$, $\Phi_{02}=-2\Phi_{11}=\Phi_{20}=\frac{1}{4}(\rho_1-\rho_2)\neq 0$, $\Phi_{22}=-\frac{1}{2}\lambda$
Remaining freedom	Spatial rotations: $D=\bar{A}$, $A\bar{A}=1$, $B=C=0$	1-D null rotations: $A=D=1$, $\bar{C}=C$, $B=0$

established that the subset is algebraically complete. Note that if lower degree invariants (in CZ) are not used in the backsolving process, this means they are dependent for the particular case at hand (the proof of dependency will be given in a future article).

In cases where we have curvature complete sets, the minimal number property is established by simply observing that the number[7] of invariants is the same as the number of unknown functions in the curvature components (after all of the possible remaining tetrad freedom, which can act on the curvature components, is completely used up). In the cases where we do not have curvature complete sets but which are maximal, the missing amount of information is shown to be absent in all second order polynomial invariants using the index theorem. The minimal number property is then established by a simple real count modulo the mandatory missing curvature information.

We note that for the Segre types [2,11], [2,(11)], [(2,1)1] and [(2,11)], $\Phi_{22}=\pm 1$ in their respective canonical frames. In all of these cases, we have chosen $\Phi_{22}=1$ in the backsolving procedures. The backsolving when $\Phi_{22}=-1$ is identical to the case when $\Phi_{22}=1$ except for minor insignificant sign changes. Similarly, for the Segre types [3,1] and [(3,1)], we have chosen $\Phi_{12}=1$.

A. Segre type [2,11]

For this type, a complete set of invariants is $\{R, w_1, w_2, r_1, r_2, m_1, m_2, m_3\}$, and we will show that complete backsolving is always possible, at least in principle, except when $\Psi_0=\Psi_1=0$. This exceptional case occurs when the null eigenvector of the Ricci tensor aligns with the repeated

TABLE IV. Canonical frames for Segre types [(3,1)] and [(1,11)1].

	PP type N, Segre type [(3,1)]	PP type O, Segre type [(1,11)1]
Canonical form of R_{ab}	$R_{ab}=2\rho_1 l_{(a}n_{b)}+2\lambda l_{(a}x_{b)}-\rho_1 x_a x_b-\rho_1 y_a y_b$, with $\lambda=\pm 2\sqrt{2}$	$R_{ab}=2\rho_1 l_{(a}n_{b)}-\rho_1 x_a x_b-\rho_2 y_a y_b$, with $\rho_1\neq\rho_2$
Inner products	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\rho_1 n_a+\lambda x_a$, $R_{ab}x^b=\rho_1 x_a-\lambda l_a$, $R_{ab}y^b=\rho_1 y_a$	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\rho_1 n_a$, $R_{ab}x^b=\rho_1 x_a$, $R_{ab}y^b=\rho_2 y_a$
Eigenvectors	l^a, y^a	l^a, n^a, x^a, y^a
Eigenvalues	ρ_1, ρ_1	ρ_1, ρ_1, ρ_1, ρ_2
Canonical form of Φ_{ab}	$\Phi_{00}=\Phi_{01}=\Phi_{02}=\Phi_{11}=\Phi_{22}=0$, $\Phi_{12}=\dfrac{\lambda}{2\sqrt{2}}$	$\Phi_{00}=\Phi_{01}=\Phi_{12}=\Phi_{22}=0$, $\Phi_{02}=-2\Phi_{11}=\Phi_{20}=\frac{1}{4}(\rho_1-\rho_2)\neq 0$
Remaining freedom	1-D null rotations: $A=D=1$, $\bar{C}=-C$, $B=0$	3-D Lorentz group SO(1,2): $\bar{A}=A$, $\bar{B}=B$, $\bar{C}=C$, $\bar{D}=D$, $AD-BC=1$

TABLE V. Canonical frames for Segre types [(2,11)] and [(1,111)].

	PP type O, Segre type [(2,11)]	PP type O, Segre type [(1,111)]
Canonical form of R_{ab}	$R_{ab}=2\rho_1 l_{(a}n_{b)}+\lambda l_a l_b-\rho_1 x_a x_b-\rho_1 y_a y_b$, with $\lambda=\pm 2$	$R_{ab}=2\rho_1 l_{(a}n_{b)}-\rho_1 x_a x_b-\rho_1 y_a y_b$
Inner products	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\lambda l_a+\rho_1 n_a$, $R_{ab}x^b=\rho_1 x_a$, $R_{ab}y^b=\rho_1 y_a$	$R_{ab}l^b=\rho_1 l_a$, $R_{ab}n^b=\rho_1 n_a$, $R_{ab}x^b=\rho_1 x_a$, $R_{ab}y^b=\rho_1 y_a$
Eigenvectors	l^a, x^a, y^a	l^a, n^a, x^a, y^a
Eigenvalues	ρ_1, ρ_1, ρ_1	ρ_1, ρ_1, ρ_1, ρ_1
Canonical form of Φ_{ab}	$\Phi_{00}=\Phi_{01}=\Phi_{02}=\Phi_{11}=\Phi_{12}=0$, $\Phi_{22}=-\frac{1}{2}\lambda$	$\Phi_{ab}=0$
Remaining freedom	2-D null rotations and Spatial rotations: $D=\overline{A}$, $A\overline{A}=1$, $B=0$	Full Lorentz group SO(1,3): $AD-BC=1$

principal null direction of the Weyl tensor. As we shall see, for this and other Segre types, complete backsolving is, in general, not possible when such alignments occur. However, maximal backsolving is always achievable with certain invariants from CZ.

We begin with the backsolving for the Ricci components Φ_{ab}. In our canonical frame, the independent Ricci invariants are $r_1=\frac{2}{3}(\Phi_{02}^2+2\Phi_{11}^2)$ and $r_2=-2\Phi_{02}^2\Phi_{11}$. Since the Jacobian $J=-\frac{8}{3}\Phi_{02}(\Phi_{02}-2\Phi_{11})(\Phi_{02}+2\Phi_{11})\neq 0$, it follows that the Ricci invariants r_1, r_2 are always backsolvable for Φ_{ab}.

The Weyl and mixed invariants, in this case, take the form

$$w_1=\tfrac{1}{3}(\Psi_0\Psi_4-4\Psi_1\Psi_3+3\Psi_2^2),$$

$$w_2=2\Psi_1\Psi_2\Psi_3-\Psi_2^3-\Psi_0\Psi_3^2-\Psi_1^2\Psi_4+\Psi_0\Psi_2\Psi_4,$$

$$m_1=2\Psi_0\Phi_{02}+2\Psi_2\Phi_{02}^2-8\Psi_2\Phi_{11}^2,$$

$$m_2=\tfrac{2}{3}\Phi_{02}^2\Psi_0\Psi_4+\tfrac{4}{3}\Phi_{02}^2\Psi_1\Psi_3+4\Phi_{02}\Psi_0\Psi_2+8\Phi_{11}^2\Psi_2^2-\tfrac{16}{3}\Phi_{11}^2\Psi_1\Psi_3 -\tfrac{8}{3}\Phi_{11}^2\Psi_0\Psi_4-4\Phi_{02}\Psi_1^2-2\Phi_{02}^2\Psi_2^2,$$

$$m_3=-8\Phi_{11}^2\Phi_{02}\Psi_0+8\Phi_{11}^2\Phi_{02}^2\Psi_2-2\Phi_{02}^4\Psi_2.$$

Next, we begin the backsolving procedure for the Weyl components by noting that the system $\{m_1,m_3\}$, which contains only the Weyl components Ψ_0 and Ψ_2, has a Jacobian equal to $-9J^2/(16\Phi_{02})$ which is nonzero. Therefore, we may always solve for Ψ_0 and Ψ_2 in terms of m_1 and m_3 and Φ_{ab} (which in turn are determined by the Ricci invariants). We proceed by eliminating the product $\Psi_1\Psi_3$ between w_1 and m_2 to obtain an expression for Ψ_1^2 in terms of Ψ_0, Ψ_2, Ψ_4, Φ_{ab}, and invariants. This can always be done. In order to continue, we need to treat the cases when $\Psi_0=0$ separately.

Case 1: $\Psi_0\neq 0$: In this case, $m_3\neq-\Phi_{02}^2 m_1$. Since $\Psi_0\neq 0$, we may use the above expression for Ψ_1^2 and the combination of w_1 and w_2 which eliminates the product $\Psi_1\Psi_3$ to obtain an expression for Ψ_3^2 in terms of Ψ_0, Ψ_2, Ψ_4, Φ_{ab}, and invariants. Finally, solving w_1 for $\Psi_1\Psi_3$, squaring this expression and then substituting the above expressions for Ψ_1^2 and Ψ_3^2 yields a polynomial equation of degree 3 in Ψ_4 with the coefficients being polynomials in Ψ_0, Ψ_2, Φ_{ab}, and invariants. This polynomial can always be solved for Ψ_4, since the coefficient of Ψ_4^3 is $\Psi_0 J^2\neq 0$. It follows that complete backsolving has been achieved.

Case 2A: $\Psi_0=0$ & $\Psi_1\neq 0$: We note that, in this case, $m_3=-\Phi_{02}^2 m_1$. Also $(m_1^2+36r_1^2-36r_3)^2\neq 144m_2(r_2^2-r_3)$ and, together with $m_1=m_3=0$ or $m_1^3r_2^2-3m_1m_3^2r_1-2m_3^3=0$ when

$m_1 m_3 \neq 0$, provides the necessary and sufficient conditions for this case to occur. By a simple backsolving procedure, it is easily established that a complete set of invariants is $\{R, w_1, w_2, r_1, r_2, m_1, m_2\}$.

Case 2B: $\Psi_0 = \Psi_1 = 0$: The necessary and sufficient conditions for this case to occur are $w_2^2 = w_1^3$, $m_1^2 = 36(r_1^2 - r_3)w_1$, $m_2^2 = 36(r_1^2 - r_3)w_1^2$ and $m_1^3 r_2^2 - 3m_1 m_3^2 r_1 - 2m_3^3 = 0$. We can only backsolve for Ψ_2, where $\Psi_2^2 = w_1$, but cannot backsolve for Ψ_3 or Ψ_4. This is because these components do not appear in our invariants. It follows from the index theorem previously given (see the Appendix) that no other polynomial invariant formed from the Riemann tensor can contain these components (in our canonical frame). Hence, complete backsolving is not possible, in general, but maximal backsolving is possible with the (algebraically complete) set $\{R, w_1, r_1, r_2\}$.

B. Segre type [3,1]

The backsolving for this Segre type is very similar to [2,11]. A complete set of invariants is $\{R, w_1, w_2, r_1, m_1, m_2, m_3\}$ and, as will be shown below, complete backsolving is always possible, at least in principle, except when $\Psi_0 = \Psi_1 = 0$. As before, this exceptional case occurs when the null eigenvector of the Ricci tensor aligns with the repeated principal null direction of the Weyl tensor. However, maximal backsolving is always achievable using certain invariants from CZ.

In our canonical frame, the independent Ricci invariant is $r_1 = 4\Phi_{11}^2$ and, hence, $\Phi_{11} = \frac{1}{2}\sqrt{r_1}$. The Weyl and mixed invariants, in this case, take the form

$$w_1 = \tfrac{1}{3}(\Psi_0\Psi_4 - 4\Psi_1\Psi_3 + 3\Psi_2^2),$$

$$w_2 = 2\Psi_1\Psi_2\Psi_3 - \Psi_2^3 - \Psi_0\Psi_3^2 - \Psi_1^2\Psi_4 + \Psi_0\Psi_2\Psi_4,$$

$$m_1 = 16\Psi_1\Phi_{11} - 2\Psi_0,$$

$$m_2 = 4\Psi_1^2 - 4\Psi_0\Psi_2 - 16\Phi_{11}\Psi_1\Psi_2 + 16\Phi_{11}\Psi_0\Psi_3,$$

$$m_3 = -24\Phi_{11}^2\Psi_0 - 64\Phi_{11}^3\Psi_1.$$

We begin by noting that the system $\{m_1, m_3\}$ contains only the Weyl components Ψ_0 and Ψ_1. It can always be solved to give $\Psi_0 = -(m_1 r_1 + m_3)/(8r_1)$, $\Psi_1 = (3m_1 r_1 - m_3)/(32\sqrt{r_1^3})$. In order to continue, we need to treat the cases when $\Psi_0 = 0$ separately.

Case 1: $\Psi_0 \neq 0$: In this case, $m_3 \neq -m_1 r_1$. Since $\Psi_0 \neq 0$, we can solve m_2 for Ψ_3 in terms of Ψ_0, Ψ_1, Ψ_2, Φ_{11}, and m_2. Using this expression to eliminate Ψ_3 from w_1, we can solve w_1 for Ψ_4 in terms of Ψ_0, Ψ_1, Ψ_2, Φ_{11}, w_1, and m_2. Substituting these expressions for Ψ_3 and Ψ_4 into w_2 yields a polynomial equation of degree 3 in Ψ_2. This polynomial can always be solved for Ψ_2, since the coefficient of Ψ_2^3 is $\Psi_0^2\Phi_{11}^2$ which is nonzero. It follows that complete backsolving has been achieved.

Case 2A: $\Psi_0 = 0$ & $\Psi_1 \neq 0$: In this case, $m_3 = -m_1 r_1$. This condition together with $m_1 \neq 0$ provides the necessary and sufficient conditions for this case to occur. A complete set of invariants is $\{R, w_1, w_2, r_1, m_1, m_2\}$ and is completely backsolvable (CB).

Case 2B: $\Psi_0 = \Psi_1 = 0$: In this case, $w_2^2 = w_1^3$. The necessary and sufficient conditions for this case to occur are $m_1 = m_2 = m_3 = 0$. We can only backsolve for Ψ_2, where $\Psi_2^2 = w_1$, but cannot backsolve for Ψ_3 or Ψ_4. This is because these components do not appear in our invariants. It follows from the index theorem that no other polynomial invariant formed from the Riemann tensor can contain these components (see the Appendix). Hence, complete backsolving is not possible (NCB), but maximal backsolving is possible with the (algebraically complete) set $\{R, w_1, r_1\}$.

C. Segre type [(1,1)11]

In our canonical frame, the independent Ricci invariants are $r_1=\frac{2}{3}(\Phi_{02}^2+2\Phi_{11}^2)$ and $r_2=-2\Phi_{02}^2\Phi_{11}$. It follows that the Ricci invariants r_1, r_2 are always backsolvable for Φ_{ab}.

Case 1: $\Psi_0\neq 0$: In this case, we may use the tetrad freedom to make $\Psi_0\overline{\Psi}_0=1$. Further, we shall need to treat the cases where $\Psi_3=0$ or $\Psi_4=0$ separately.

Case 1A: $\Psi_3\Psi_4\neq 0$: We will now show that a complete set is $\{R,w_1,w_2,r_1,r_2,m_1,m_2,m_4\}$ and complete backsolving is always possible. The invariants in this frame are

$$w_1=\tfrac{1}{3}(\Psi_0\Psi_4-4\Psi_1\Psi_3+3\Psi_2^2),$$

$$w_2=2\Psi_1\Psi_2\Psi_3-\Psi_2^3-\Psi_0\Psi_3^2-\Psi_1^2\Psi_4+\Psi_0\Psi_2\Psi_4,$$

$$m_1=2\Psi_2(\Phi_{02}^2-4\Phi_{11}^2),$$

$$m_2=\tfrac{2}{3}(\Phi_{02}^2\Psi_0\Psi_4+2\Phi_{02}^2\Psi_1\Psi_3+12\Phi_{11}^2\Psi_2^2-4\Phi_{11}^2\Psi_0\Psi_4-3\Phi_{02}^2\Psi_2^2-8\Phi_{11}^2\Psi_1\Psi_3),$$

$$m_4=(16\Psi_2\Phi_{11}^2\overline{\Psi}_2\Psi_0+\Phi_{02}^2\Psi_4+8\Psi_3\Phi_{11}\overline{\Psi}_1\Phi_{02}\Psi_0+2\Psi_2\Phi_{02}^2\overline{\Psi}_2\Psi_0 +8\Psi_1\Phi_{11}\overline{\Psi}_3\Phi_{02}\Psi_0+\Psi_0^2\Phi_{02}^2\overline{\Psi}_4)/\Psi_0.$$

m_1 can always be solved for Ψ_2 since $\Phi_{02}^2-4\Phi_{11}^2\neq 0$. We can always solve w_1 and m_2 to get $\Psi_1=C_1/\Psi_3$ and $\Psi_4=C_4/\Psi_0$, where C_1, C_4 are given by Φ_{ab}, Ψ_2 and invariants. Substituting these expressions into w_2 we get the quadratic polynomial equation $\psi^2+(w_2-2C_1\Psi_2-C_4\Psi_2+\Psi_2^3)\psi+C_1^2C_4=0$, where $\psi=\Psi_0\Psi_3^2\neq 0$. This can always be solved for ψ in terms of Φ_{ab}, Ψ_2 and invariants. Substituting $\Psi_3=\sqrt{\psi/\Psi_0}$ into m_4, we get the following quartic polynomial equation in Ψ_0:

$$\Psi_0^4\Phi_{02}^2\overline{C}_4\sqrt{\psi\overline{\psi}}+8C_1\Phi_{02}\Psi_0^3\overline{\psi}\Phi_{11}-\sqrt{\psi\overline{\psi}}(m_4-2\Psi_2\Phi_{02}^2\overline{\Psi}_2-16\Psi_2\Phi_{11}^2\overline{\Psi}_2)\Psi_0^2 +8\psi\Psi_0\Phi_{11}\overline{C}_1\Phi_{02}+\Phi_{02}^2C_4\sqrt{\psi\overline{\psi}}=0,$$

which can always be solved for Ψ_0 since the coefficient of Ψ_0^4 is nonzero. Thus, Ψ_0 is determined in terms of Φ_{ab}, Ψ_2, ψ and invariants which in turn are all determinable by the invariants. Therefore, complete backsolving has been achieved.

Case 1B(i): $\Psi_3\Psi_1\Phi_{11}\neq 0$ & $\Psi_4=0$: For this case, a complete set is $\{R,w_1,w_2,r_1,r_2,m_1,m_4\}$ and complete backsolving is always possible. It is similar to case 1A except that m_2 is dependent (since $\Psi_4=C_4=0$).

Case 1B(ii): $\Psi_3\Phi_{11}\neq 0$ and $\Psi_1=\Psi_4=0$: A complete set is $\{R,\ w_1,\ w_2,\ r_1,\ r_2,\ \tilde{m}_5/\bar{\tilde{m}}_5\}$ and complete backsolving is again always possible. The Weyl and mixed invariants in this frame are

$$w_1=\Psi_2^2,\quad w_2=-\Psi_2^3-\Psi_0\Psi_3^2,$$

$$m_5=2(\Psi_2^2\Phi_{02}^2\overline{\Psi}_2\Psi_0-4\Psi_3\Phi_{11}\overline{\Psi}_3\Phi_{02}\Psi_0^2+8\Psi_2^2\Phi_{11}^2\overline{\Psi}_2\Psi_0+\Psi_3^2\Phi_{02}^2)/\Psi_0.$$

w_1 determines Ψ_2 and w_2 gives $\Psi_3^2=-(\Psi_2^3+w_2)/\Psi_0$. Finally, we need to determine Ψ_0. Substituting this expression into m_5 we get the cubic polynomial equation in Ψ_0: $8\Phi_{02}\Phi_{11}\overline{Q}_1\Psi_0^3-Q_0\Psi_0^2+2\Phi_{02}^2Q_1=0$ where $Q_0=[m_5+2\Psi_2^2\overline{\Psi}_2(\Phi_{02}^2+8\Phi_{11}^2)]/Q_1$ and $Q_1^2=\Psi_2^3+w_2\neq 0$. From this equation and its complex conjugate, we eliminate Ψ_0^3 (this can always be done) to obtain $\Phi_{02}Q_0\Psi_0^2-4\Phi_{11}\overline{Q}_0\Psi_0+2\Phi_{02}(16\Phi_{11}^2-\Phi_{02}^2)Q_1=0$. First, we consider the special case when $Q_0=0$. It then follows that m_5 is dependent and, from the original cubic, we obtain $\Psi_0^3=-\Phi_{02}Q_1/(4\Phi_{11}\overline{Q}_1)$ with the condition $\Phi_{02}^2=16\Phi_{11}^2$. Henceforth, we shall assume $Q_0\neq 0$. Eliminating Ψ_0^2 from the quadratic equation and its complex conjugate yields $4\Phi_{11}(Q_0^2$

$-\overline{Q}_0\overline{Q}_2)\Psi_0=\Phi_{02}(Q_0\overline{Q}_0-Q_2\overline{Q}_2)$ where $Q_2=2(16\Phi_{11}^2-\Phi_{02}^2)Q_1$. If $Q_0^2-\overline{Q}_0\overline{Q}_2=0$ (i.e., $Q_2\overline{Q}_2=Q_0\overline{Q}_0$ which is the real syzygy eliminating "half" of the information in m_5), then the quadratic equation becomes $\Phi_{02}Q_0^2\Psi_0^2-4\Phi_{11}Q_0\overline{Q}_0\Psi_0+\Phi_{02}\overline{Q}_0^2=0$ which has the two possible solutions $\Psi_0=(2\Phi_{11}\pm i\sqrt{\Phi_{02}^2-4\Phi_{11}^2})\overline{Q}_0/(\Phi_{02}Q_0)$ with the condition $\Phi_{02}^2>4\Phi_{11}^2$. In this case, $\tilde{m}_5\equiv\overline{Q}_0$. If $Q_0^2-\overline{Q}_0\overline{Q}_2\neq 0$, then we obtain $\Psi_0^2=\tilde{m}_5/\bar{\tilde{m}}_5$ where $\tilde{m}_5\equiv(Q_2\overline{Q}_2-Q_0\overline{Q}_0)/(Q_0^2-\overline{Q}_0\overline{Q}_2)$ with the real syzygy $\tilde{m}_5\bar{\tilde{m}}_5=16\Phi_{11}^2/\Phi_{02}^2$. In this case, the independent information resides in the composite invariant $\tilde{m}_5/\bar{\tilde{m}}_5$ which contains "half" of the information in m_5. The other "half" of the information in m_5 is not independent but is determined by the values of the other invariants $\{w_1,w_2,r_1,r_2\}$ via the real syzygy previously given.

Case 1B(iii): $\Psi_3\Psi_1\neq 0$ and $\Psi_4=\Phi_{11}=0$: A complete set is $\{R,w_1,w_2,r_1,m_1,\overline{m}_5^*/m_5^*\}$ and complete backsolving is always possible. The Weyl and mixed invariants in this frame are

$$w_1=\tfrac{1}{3}(3\Psi_2^2-4\Psi_1\Psi_3),\quad w_2=2\Psi_1\Psi_2\Psi_3-\Psi_2^3-\Psi_0\Psi_3^2,$$

$$m_1=2\Psi_2\Phi_{02}^2,\quad m_5=2\Phi_{02}^2(2\Psi_1\Psi_3\overline{\Psi}_2\Psi_0-3\Psi_2^2\overline{\Psi}_2\Psi_0-3\Psi_3^2)/(3\Psi_0).$$

m_1 determines Ψ_2 and then w_1 and w_2 give $\Psi_1=3(\Psi_2^2-w_1)/(4\Psi_3)$ and $\Psi_3^2=(m_1^3-12m_1w_1\Phi_{02}^4-16w_2\Phi_{02}^6)/(16\Psi_0\Phi_{02}^6)$. After substituting these expressions into m_5 and solving for Ψ_0, we obtain $\Psi_0^4=\overline{m}_5^*/m_5^*$ (or $\Psi_0^2=-\overline{m}_5^*$) where $m_5^*\overline{m}_5^*=1$ and m_5^* is defined by

$$m_5^*\equiv(8\Phi_{02}^4m_5+m_1^2\overline{m}_1+4\Phi_{02}^4w_1\overline{m}_1)/(m_1^3-12m_1w_1\Phi_{02}^4-16w_2\Phi_{02}^6).$$

In this case, the independent information resides in the composite invariant $\overline{m}_5^*/m_5^*$ which contains "half" of the information in m_5. The other "half" of the information in m_5 is not independent but is determined by the values of the other invariants $\{w_1,w_2,r_1,m_1\}$ via the real syzygy $m_5^*\overline{m}_5^*=1$.

Case 1B(iv): $\Psi_3\neq 0$ and $\Psi_1=\Psi_4=\Phi_{11}=0$: This case is similar to case 1B(iii) with basically the same equations holding, except that m_1 is now dependent because $m_1^2=4\Phi_{02}^4w_1$. Hence, a complete set is $\{R,w_1,w_2,r_1,\overline{m}_5^*/m_5^*\}$ and complete backsolving has been established.

Case 1C: $\Psi_3=0$ and $\Psi_4\neq 0$: A complete set is $\{R,w_1,w_2,r_1,r_2,m_1,m_4\}$ as complete backsolving can be easily carried out.

Case 1D: $\Psi_3=\Psi_4=0$: A maximal (complete) set in this case is $\{R,w_1,r_1,r_2\}$ and NCB. Clearly complete backsolving is impossible since only Ψ_2 can be solved for using w_1, while Ψ_0 and Ψ_1 remain undetermined (see the Appendix). All mixed invariants are dependent.

Case 2: $\Psi_0=0$ and $\Psi_1\neq 0$: We may use the tetrad freedom to make $\Psi_1\overline{\Psi}_1=1$. Further, we shall need to treat the cases where $\Psi_3=0$ or $\Psi_4=0$ separately.

Case 2A(i): $\Psi_3\Phi_{11}\neq 0$: A complete set is $\{R,w_1,w_2,r_1,r_2,m_1,m_4\}$ and is CB.

Case 2A(ii): $\Psi_3\Psi_4\neq 0$ and $\Phi_{11}=0$: A complete set is $\{R,w_1,w_2,r_1,m_1,\hat{\bar{m}}_5/\hat{m}_5\}$. The invariants in this frame are

$$w_1=\tfrac{1}{3}(3\Psi_2^2-4\Psi_1\Psi_3),\quad w_2=2\Psi_1\Psi_2\Psi_3-\Psi_2^3-\Psi_1^2\Psi_4,$$

$$m_1=2\Psi_2\Phi_{02}^2,\ \ m_5=\tfrac{2}{3}\Phi_{02}^2(2\Psi_1\overline{\Psi}_2\Psi_3-3\Psi_2^2\overline{\Psi}_2-3\Psi_1^2\overline{\Psi}_4).$$

m_1 can always be solved for Ψ_2 since $\Phi_{02}\neq 0$. We can always solve w_1 and w_2 to get $\Psi_3=3(\Psi_2^2-w_1)/(4\Psi_1)\neq 0$ and $\Psi_4=(\Psi_2^3-3\Psi_2w_1-2w_2)/(2\Psi_1^2)$. Substituting these expressions into m_5 we obtain the polynomial equation

$$\Phi_{02}^2(\overline{\Psi}_2^3-3\overline{\Psi}_2\overline{w}_1-2\overline{w}_2)\Psi_1^4+m_5+\Phi_{02}^2\overline{\Psi}_2(\Psi_2^2+w_1)=0.$$

This gives $\Psi_1^4=\hat{m}_5/\overline{Q_3}$ together with the real syzygy $\hat{m}_5\overline{\hat{m}}_5=Q_3\overline{Q_3}$, where $\hat{m}_5\equiv 18r_1^2m_5+9r_1^2w_1\overline{m}_1+m_1^2\overline{m}_1$ and $Q_3\equiv 27r_1^2w_1m_1+54r_1^3w_2-m_1^3$. Alternatively, $\Psi_1^8=\hat{m}_5Q_3/(\overline{\hat{m}}_5\overline{Q_3})$. Note that $Q_3\neq 0$ since $\Psi_4\neq 0$. Hence, backsolving is complete.

Case 2A(iii): $\Psi_3\neq 0$ and $\Psi_4=\Phi_{11}=0$: A complete set is $\{R,w_1,w_2,r_1,m_6\}$ and is CB.

Case 2B(i): $\Psi_3=0$ and $\Psi_4\neq 0$: A complete set is $\{R,w_1,w_2,r_1,r_2,\overline{m}_5'/m_5'\}$ and complete backsolving is always possible. The Weyl and mixed invariants in this frame are

$$w_1=\Psi_2^2,\quad w_2=-\Psi_2^3-\Psi_1^2\Psi_4,$$

$$m_5=2(4\Psi_4\Phi_{02}\Phi_{11}-\Psi_2^2\Phi_{02}^2\overline{\Psi}_2-8\Psi_2^2\Phi_{11}^2\overline{\Psi}_2-\Psi_1^2\Phi_{02}^2\overline{\Psi}_4).$$

The invariant w_1 determines Ψ_2 and Ψ_4 is determined, in terms of Ψ_1 and w_1 and w_2, by $\Psi_4=-(\Psi_2^3+w_2)/\Psi_1^2$. Substituting these expressions into m_5 we obtain the polynomial equation

$$2\Phi_{02}^2(\overline{w}_2+\overline{\Psi}_2^3)\Psi_1^6-Q_4\Psi_1^2-8\Phi_{02}\Phi_{11}(w_2+\Psi_2^3)=0,$$

where $Q_4\equiv m_5+2(\Phi_{02}^2+8\Phi_{11}^2)\Psi_2\overline{\Psi}_2$.

If $Q_4=0$, then necessarily $\Phi_{11}\neq 0$ and m_5 is dependent. In this case, we have $\Psi_1^6=4\Phi_{11}(w_2+\Psi_2^3)/[\Phi_{02}(\overline{w}_2+\overline{\Psi}_2^3)]$ with the condition $\Phi_{02}^2=16\Phi_{11}^2$. Henceforth, we shall assume that $Q_4\neq 0$. Combining the sixth degree equation together with its complex conjugate to eliminate Ψ_1^6 yields the quartic equation $\Phi_{02}\overline{Q}_4\Psi_1^4+4\Phi_{11}Q_4\Psi_1^2-\Phi_{02}Q_5=0$ where $Q_5\equiv 2(\Phi_{02}^2-16\Phi_{11}^2)\times(w_2+\Psi_2^3)$. If $\Phi_{11}=0$, then $Q_4Q_5\neq 0$ and $\Psi_1^8=m_5'/\overline{m}_5'$ (or $\Psi_1^4=m_5'$) together with the real syzygy $m_5'\overline{m}_5'=1$, where, in this case, $m_5'\equiv Q_4/\overline{Q}_5$. Next, we assume that $\Phi_{11}\neq 0$. It follows that if $Q_4^2+\overline{Q}_4Q_5=0\Leftrightarrow Q_4\overline{Q}_4-Q_5\overline{Q}_5=0$ (which is the real syzygy eliminating "half" of the information in m_5), then we obtain the bi-quadratic equation $\Phi_{02}\overline{Q}_4^2\Psi_1^4+4\Phi_{11}Q_4\overline{Q}_4\Psi_1^2+\Phi_{02}Q_4^2=0$ which has the two possible solutions $\Psi_0^2=(-2\Phi_{11}\pm i\sqrt{\Phi_{02}^2-4\Phi_{11}^2})Q_4/(\Phi_{02}\overline{Q}_4)$ with the condition $\Phi_{02}^2>4\Phi_{11}^2$. In this case, $m_5'=Q_4$.

Finally, we consider the case when $\Phi_{11}Q_4(Q_4\overline{Q}_4-Q_5\overline{Q}_5)\neq 0$. Combining the above quartic equation together with its complex conjugate yields $\Psi_1^4=m_5'/\overline{m}_5'$ (or equivalently $\Psi_1^2=-4\Phi_{11}m_5'/\Phi_{02}$) together with the real syzygy $16m_5'\overline{m}_5'=\Phi_{02}^2/\Phi_{11}^2$, where, in this case, $m_5'\equiv(Q_4^2+\overline{Q}_4Q_5)/(Q_4\overline{Q}_4-Q_5\overline{Q}_5)$.

Case 2B(ii): $\Psi_3=\Psi_4=0$: It immediately follows that a maximal (complete) set is $\{R,w_1,r_1,r_2\}$ and complete backsolving is impossible, since only Ψ_2 can be solved for using w_1 while the argument of Ψ_1 remains undetermined (see the Appendix).

Case 3: $\Psi_0=\Psi_1=0$ and $\Psi_3\neq 0$: We may use the tetrad freedom to make $\Psi_3\overline{\Psi}_3=1$. It follows that a maximal (complete) set is $\{R,w_1,r_1,r_2\}$ and NCB, since only Ψ_2 can be solved for using w_1 while the argument of Ψ_3 and Ψ_4 remain undetermined (see the Appendix).

Case 4: $\Psi_0=\Psi_1=\Psi_3=0$: If $\Psi_4\neq 0$, then we may use the tetrad freedom to make $\Psi_4\overline{\Psi}_4=1$. In this case, a maximal set is $\{R,w_1,r_1,r_2\}$ and NCB, since only Ψ_2 can be solved for using w_1 while the argument of Ψ_4 remains undetermined (see the Appendix). This case corresponds to an alignment between the eigenvector of the Ricci tensor and the repeated PND of the Weyl tensor. On the other hand, if $\Psi_4=0$,[3] then the set $\{R,w_1,r_1,r_2\}$ is complete.

D. Segre type [(1,1)(11)]

In our canonical frame, the only nonzero Ricci component is Φ_{11}. Hence, the only independent Ricci invariant is $r_1=4/3\Phi_{11}^2$ which determines Φ_{11}.

Case 1: $\Psi_0\neq 0$: We use the tetrad freedom to make $\Psi_0=1$. Further, we shall need to treat the cases where $\Psi_3=0$ or $\Psi_4=0$ separately.

Case 1A: $\Psi_3\neq 0$: A complete set is $\{R,w_1,w_2,r_1,m_1,m_2\}$ and is CB.

Case 1B(i): $\Psi_3=0$ and $\Psi_4\neq 0$: A complete set is $\{R,w_1,w_2,r_1,m_1\}$ and is CB.

Case 1B(ii): $\Psi_3=\Psi_4=0$: In this case all mixed invariants are dependent and $w_1=\Psi_2^2$ is the only independent Weyl invariant. Hence, a maximal (complete) set is $\{R,w_1,r_1\}$ and is NCB (see the Appendix).

Case 2: $\Psi_0=0$ and $\Psi_1\neq 0$: We use the tetrad freedom to make $\Psi_1=1$. It follows that a complete set is $\{R,w_1,w_2,r_1,m_1\}$ and is CB.

Case 3: $\Psi_0=\Psi_1=0$: If $\Psi_3=0$, we can make $\Psi_4=1$ (provided $\Psi_4\neq 0$), and then the complete set is $\{R,w_1,r_1\}$ with $w_1=\Psi_2^2$ determining Ψ_2. If $\Psi_3=\Psi_4=0$, then the same set is complete. In both of these cases, backsolving is complete. On the other hand, if $\Psi_3\neq 0$, we can make $\Psi_3=1$, and then a maximal (complete) set is $\{R,w_1,r_1\}$ with $w_1=\Psi_2^2$, while Ψ_4 is still undetermined (see the Appendix).

E. Segre type [2,(11)]

In our canonical frame, the only nonzero Ricci components are Φ_{11} and $\Phi_{22}=1$. Hence, the only independent Ricci invariant is $r_1=4/3\Phi_{11}^2$ which determines Φ_{11}.

Case 1: $\Psi_0\neq 0$: We use the tetrad freedom to make Ψ_0 real. Further, we shall need to treat the cases where $\Psi_3=0$ or $\Psi_4=0$ separately.

Case 1A: $\Psi_3\neq 0$: A complete set is $\{R,w_1,w_2,r_1,m_1,m_2,m_4\}$ and is CB.

Case 1B(i): $\Psi_3=0$ and $\Psi_4\neq 0$: In this case a complete set is $\{R,w_1,w_2,r_1,m_1,m_4\}$ since m_2 is dependent, and complete backsolving is again always possible.

Case 1B(ii): $\Psi_3=\Psi_4=0$: A complete set is $\{R,w_1,r_1,m_4,m_5\}$ and is CB.

Case 2: $\Psi_0=0$ and $\Psi_1\neq 0$: A complete set is $\{R,w_1,w_2,r_1,m_1,m_4\}$ and is CB. This is more easily established in a frame where Ψ_1 is real.

Case 3: $\Psi_0=\Psi_1=0$: In this case, a maximal (complete) set is $\{R,w_1,r_1\}$ with $w_1=\Psi_2^2$, while Ψ_3 (which can be made real if nonzero) and Ψ_4 are still undetermined (see the Appendix). Complete backsolving is not, in general, possible.

F. Segre type [(2,1)1]

In our canonical frame, the only nonzero Ricci components are $\Phi_{02}=-2\Phi_{11}=\Phi_{20}$ and $\Phi_{22}=1$. Hence, the only independent Ricci invariant is $r_1=4\Phi_{11}^2$, which determines Φ_{11}.

Case 1: $\Psi_0\neq 0$: We may use the tetrad freedom to make Ψ_1 real or imaginary, depending on the structure of Ψ_0. We note that m_1 being either not real or real invariantly distinguishes case 1A from case 1B.

Case 1A: $\mathrm{Im}(\Psi_0)\neq 0$: A complete set is $\{R,w_1,w_2,r_1,m_1,m_2,m_4\}$ and is CB. This is easily shown in a frame where Ψ_1 is real.

Case 1B: $\mathrm{Im}(\Psi_0)=0$ and $\mathrm{Re}(\Psi_0)\neq 0$: In this case m_1 is real. It can be shown that a complete set is $\{R,w_1,w_2,r_1,m_1,m_2,m_4\}$ and CB, which is more easily established in a frame where Ψ_1 is imaginary.

Case 2: $\Psi_0=0$ and $\Psi_1\neq 0$: In this case, we may use the tetrad freedom to make Ψ_2 real or imaginary, depending on the structure of Ψ_1. Also $m_1=0$ and the nature of m_2 invariantly distinguishes case 2A from case 2B.

Case 2A: $\mathrm{Im}(\Psi_1)\neq 0$: A complete set is $\{R,w_1,w_2,r_1,m_2,m_4\}$ and is CB, which is easily established in a frame where Ψ_2 is real.

Case 2B: $\mathrm{Im}(\Psi_1)=0$ and $\mathrm{Re}(\Psi_1)\neq 0$: In this case m_2 is real. It can be shown that a complete set is $\{R,w_1,w_2,r_1,m_2,m_4\}$ and is CB, which is easily established in a frame where Ψ_2 is imaginary.

Case 3: $\Psi_0=\Psi_1=0$: A maximal (complete) set is $\{R,w_1,r_1\}$ with $w_1=\Psi_2^2$, while Ψ_3 and Ψ_4 remain, in general, not completely determined (even though there still remains tetrad freedom to remove one unknown "part" of Ψ_3 or Ψ_4). Complete backsolving is, in general, not possible (see the Appendix).

G. Segre type [(3,1)]

In our canonical frame, the only nonzero Ricci components are $\Phi_{12}=\Phi_{21}=1$. All Ricci invariants vanish.

Case 1: $\Psi_0\neq 0$: We will use the tetrad freedom to make Ψ_1 real or imaginary, depending on the structure of Ψ_0. We note that m_1 being either not imaginary or imaginary invariantly distinguishes case 1A from case 1B.

Case 1A: $\mathrm{Re}(\Psi_0)\neq 0$: A complete set is $\{R,w_1,w_2,m_1,m_2,m_4\}$ and is CB. This is easily established in a frame where Ψ_1 is real.

Case 1B: $\mathrm{Re}(\Psi_0)=0$ and $\mathrm{Im}(\Psi_0)\neq 0$: In this case m_1 is imaginary. A complete set is $\{R,w_1,w_2,m_1,m_2,m_4\}$ and is CB. This is readily shown in a frame where Ψ_1 is imaginary.

Case 2: $\Psi_0=0$ and $\Psi_1\neq 0$: In this case $m_1=0$ and we may use the tetrad freedom to make Ψ_2 real or imaginary, depending on the structure of Ψ_1. We note that the nature of m_2 invariantly distinguishes case 2A from case 2B.

Case 2A: $\mathrm{Re}(\Psi_1)\neq 0$: We now use the tetrad freedom to make Ψ_2 real and will show that a complete set is $\{R,w_1,w_2,m_2,|m_5|\}$ and complete backsolving is always possible. The Weyl and mixed invariants in this frame are

$$w_1=\tfrac{1}{3}(3\Psi_2^2-4\Psi_1\Psi_3),\quad w_2=2\Psi_1\Psi_2\Psi_3-\Psi_1^2\Psi_4-\Psi_2^3,$$

$$m_2=4\Psi_1^2,\quad m_5=-8\Psi_1\Psi_2(\Psi_1+\bar{\Psi}_1).$$

This system of invariants can be solved (implicitly) for the NP Weyl components to yield

$$\Psi_1^2=m_2/4,\quad \Psi_2^2=|m_5|^2/[64\Psi_1\bar{\Psi}_1(\Psi_1+\bar{\Psi}_1)^2],$$

$$\Psi_3=3(\Psi_2^2-w_1)/(4\Psi_1)\ \text{and}\ \Psi_4=(2\Psi_1\Psi_2\Psi_3-\Psi_2^3-w_2)/\Psi_1^2.$$

Note that the invariant m_5 satisfies the real syzygy $\bar{m}_2m_5^2=m_2\bar{m}_5^2$. Also, the real invariant m_6 could be used instead of $|m_5|$.

Case 2B: $\mathrm{Re}(\Psi_1)=0$ and $\mathrm{Im}(\Psi_1)\neq 0$: In this case m_2 is real and negative and we may use the tetrad freedom to make Ψ_2 imaginary. Following the same procedure as in case 2A (with some sign differences), it can be shown that a complete set is $\{R,w_1,w_2,m_2,|m_5|\}$ and complete backsolving is always possible.

Case 3: $\Psi_0=\Psi_1=0$: A maximal (complete) set is $\{R,w_1\}$ with $w_1=\Psi_2^2$, while Ψ_3 and Ψ_4 remain, in general, not completely determined (even though there still remains tetrad freedom to remove one unknown "part" of Ψ_3 or Ψ_4). Complete backsolving is, in general, not possible (see the Appendix).

H. Segre type [(1,11)1]

For this Segre type, it is easier to use the Weyl canonical frame. The Ricci components, in general, are[9] $\Phi_{00}=\pm 2\alpha^2$, $\Phi_{01}=\pm 2\alpha\beta$, $\Phi_{02}=\pm 2\beta^2$, $\Phi_{11}=\pm(\alpha\gamma+\beta\bar{\beta})$, $\Phi_{12}=\pm 2\beta\gamma$, $\Phi_{22}=\pm 2\gamma^2$ (with the same sign all throughout) where α and γ are real, β is complex and $\alpha\gamma<\beta\bar{\beta}$. The only independent Ricci invariant is $r_1=4(\alpha\gamma-\beta\bar{\beta})^2$, therefore, $\gamma=(2\beta\bar{\beta}-\sqrt{r_1})/(2\alpha)$ if $\alpha\neq 0$, otherwise, $\beta\bar{\beta}=\frac{1}{2}\sqrt{r_1}$. In the analysis that follows, we will choose the "+" sign throughout. The analysis with the opposite sign only differs trivially in the intermediate steps, but the final conclusion does not differ.

For this Segre type and Petrov types I, II, and III, the backsolving calculations for when $\alpha\neq 0$ are virtually identical to the ones in Segre type [1,(111)] and corresponding Petrov types.[2] However, here we need to consider the case when $\alpha=0$, as well. Hence, for these Petrov types, we shall present only the backsolving for the Ricci components for when $\alpha=0$.

1. Segre type [(1,11)1], Petrov type I

Case 1: $\alpha\neq 0$: A complete set is $\{R,w_1,w_2,r_1,m_4,m_5\}$ and is CB.

Case 2: $\alpha=0$: In this case, $\beta\neq 0$, m_4 is dependent with $\beta\overline{\beta}=\frac{1}{2}\sqrt{r_1}$ and

$$m_5=8\Psi_0^2\beta^2(\overline{\Psi}_2\overline{\beta}^2+\overline{\Psi}_0\gamma^2)+8\Psi_0\Psi_2(\overline{\Psi}_0\gamma^4+\overline{\Psi}_0\beta^4+\overline{\Psi}_0\overline{\beta}^4+6\overline{\beta}^2\overline{\Psi}_2\gamma^2)$$
$$-24\Psi_2^2\beta^2(\overline{\Psi}_2\overline{\beta}^2+\overline{\Psi}_0\gamma^2).$$

Substituting $\overline{\beta}=\sqrt{r_1}/(2\beta)$ into m_5 and $\overline{m}_5$ and then eliminating γ from m_5 and $\overline{m}_5$ we get a polynomial of degree 16 in β with the coefficient of β^{16} being $256\Psi_0\overline{\Psi}_0^3\overline{\Psi}_2^2(3\Psi_2-\Psi_0)^2(3\Psi_2+\Psi_0)^2\neq 0$. Hence, we can determine β and then γ. Thus complete backsolving has been achieved.

2. Segre type [(1,11)1], Petrov type II

Case 1: $\alpha\neq 0$: A complete set is $\{R,w_1,r_1,m_4,m_5\}$ and is CB.

Case 2: $\alpha=0$: In this case, $m_4^2=36r_1w_1\overline{w}_1$, $m_5^2=36r_1w_1^2\overline{w}_1$, $\beta\overline{\beta}=\frac{1}{2}\sqrt{r_1}$ and a maximal (complete) set is $\{R,w_1,r_1\}$. We can only determine $|\beta|$ and the argument of β and γ are still undetermined, hence, is NCB. Using the index theorem, it can be shown that no invariants can determine these unknown quantities (see the Appendix). Further, we have, using (1), $S_{ab}l^b=-2\Phi_{11}l_a$. Hence, l^a is an eigenvector of the Ricci tensor as well as the repeated eigenvector of the Weyl tensor.

3. Segre type [(1,11)1], Petrov type III

Case 1: $\alpha\neq 0$: A complete set is $\{R,r_1,m_4,m_5\}$ and is CB.

Case 2: $\alpha=0$: In this case, $m_4=m_5=0$, $|\beta|=\frac{1}{2}\sqrt{r_1}$ and a maximal (complete) set is $\{R,r_1\}$. We can only determine $|\beta|$ and the argument of β, and γ are still undetermined, hence, is NCB. Using the index theorem, it can be shown that no invariants can determine these unknown quantities (see the Appendix). Again, we obtain $S_{ab}l^b=-2\Phi_{11}l_a$. Thus, l^a is an eigenvector of the Ricci tensor as well as the repeated eigenvector of the Weyl tensor.

4. Segre type [(1,11)1], Petrov type D

For this type $w_1=\Psi_2^2$ which determines Ψ_2. In our Weyl canonical frame, the only nonzero Weyl component is Ψ_2. In all type D cases below, complete backsolving is achievable.

Case 1: $\alpha\beta\neq 0$: We can make $\beta=1/\alpha$ (real) and it can be easily shown that the complete set is $\{R,w_1,r_1,m_4\}$. Note that $m_5^2=w_1m_4^2$.

Case 2: $\alpha\gamma\neq 0$ and $\beta=0$: We can make $\alpha=\pm 1$ and, hence, $\gamma=\mp\frac{1}{2}\sqrt{r_1}$. A complete set, in this case, is $\{R,w_1,r_1\}$. Note that $m_5^2=w_1m_4^2=36w_1^2\overline{w}_1r_1^2$.

Case 3: $\beta\gamma\neq 0$ and $\alpha=0$: We can make $\beta=1/\gamma$ (real) and, hence, $\beta^2=1/\gamma^2=\frac{1}{2}\sqrt{r_1}$. A complete set, in this case, is $\{R,w_1,r_1\}$. Note that $m_5^2=w_1m_4^2=36w_1^2\overline{w}_1r_1^2$.

Case 4: $\beta\neq 0$ and $\alpha=\gamma=0$: We can make β real and, hence, $\beta^2=\frac{1}{2}\sqrt{r_1}$. A complete set, in this case, is $\{R,w_1,r_1\}$. Note that $m_5^2=w_1m_4^2=36w_1^2\overline{w}_1r_1^2$.

5. Segre type [(1,11)1], Petrov type N

For this Petrov type, $w_1=w_2=0$. In our Weyl canonical frame, the only nonzero Weyl component is $\Psi_4=1$. We can use the remaining tetrad freedom to make $\beta=0$ if $\alpha\neq 0$, otherwise, we can make $\gamma=0$

Case 1: $\alpha\neq 0$ and $\beta=0$: In this case, $m_4=4\alpha^4$, $m_5=0$ and $\gamma=-\sqrt{r_1}/(2\alpha)$. Hence, a complete set is $\{R,r_1,m_4\}$ and complete backsolving is always possible.

Case 2: $\alpha=\gamma=0$ and $\beta\neq 0$: In this case, $m_4=m_5=0$, $\beta\overline{\beta}=\frac{1}{2}\sqrt{r_1}$ and a maximal (complete) set is $\{R,r_1\}$. We can only determine $|\beta|$ and the argument of β is still undetermined, in general, hence, backsolving is incomplete. Using the index theorem, it can be shown that no invariants can

TABLE VI. Algebraically complete sets for Segre type [(1,11)1] with the different Petrov types.

Petrov type	Conditions (in Weyl canonical frame)	Complete sets (and subsets thereof)	CB/NCB
I	-	$\{R,w_1,w_2,r_1,m_4,m_5\}$	CB
II	$\Phi_{00}=\Phi_{01}=0$	$\{R,w_1,r_1\}$	NCB
	Otherwise	$\{R,w_1,r_1,m_4,m_5\}$	CB
III	$\Phi_{00}=\Phi_{01}=0$	$\{R,r_1\}$	NCB
	Otherwise	$\{R,r_1,m_4,m_5\}$	CB
D	-	$\{R,w_1,r_1,m_4,m_5\}$	CB
N	$\Phi_{00}=\Phi_{01}=\Phi_{12}=\Phi_{22}=0$	$\{R,r_1\}$	NCB
	Otherwise	$\{R,r_1,m_4,m_5\}$	CB
O	-	$\{R,r_1\}$	CB

determine these unknown quantities (see the Appendix). Also, $S_{ab}l^b=-2\Phi_{11}l_a$ and, therefore, l^a is an eigenvector of the Ricci tensor as well as the repeated eigenvector of the Weyl tensor.

6. Segre type [(1,11)1], Petrov type O

For this Petrov type $w_1=w_2=0$ and $\Psi_i=0$. We can use the tetrad freedom to make $\alpha=\gamma=0$ and β real, i.e., the Ricci canonical frame as well. In this case, $m_4=m_5=0$ and $\beta^2=\frac{1}{4}r_1$. Hence, a complete set is $\{R,r_1\}$ and complete backsolving is always possible.

See Table VI for a complete summary for this Segre type.

I. Segre type [(2,11)]

In our canonical frame, the only nonzero Ricci component is $\Phi_{22}=1$. Hence, all Ricci invariants vanish.

Case 1: $\Psi_0\neq 0$: A complete set is $\{R,w_1,w_2,m_4,m_5\}$ and is CB, which is easily established in a frame where Ψ_0 is real and $\Psi_1=0$.

Case 2: $\Psi_0=0$, and $\Psi_1\neq 0$: In this case, $m_4=m_5=0$. A complete set is $\{R,w_1,w_2,m_6\}$ and is CB, which is easily established in a frame where Ψ_1 is real and $\Psi_2=0$.

Case 3: $\Psi_0=\Psi_1=0$: In this case, a maximal (complete) set is $\{R,w_1\}$ with $w_1=\Psi_2^2$. If $\Psi_2\neq 0$, we can make $\Psi_3=0$ and with Ψ_4 being real (rotation freedom if necessary), it still remains undetermined. If $\Psi_2=0$ and $\Psi_3\neq 0$, then we can make Ψ_3 real and $\Psi_4=0$. In this case Ψ_3 remains undetermined. If $\Psi_2=\Psi_3=0$ and $\Psi_4\neq 0$, then we can make Ψ_4 real and it remains undetermined[3] (also, see the Appendix).

J. Segre type [(1,111)]

We can use the tetrad freedom to reduce the Weyl components to standard forms. In this case, all Ricci and mixed invariants vanish (since all $\Phi_{ab}=0$). Complete backsolving is always possible using the Weyl invariants w_1 and w_2.[9]

Table VII summarizes our results and Fig. 1 characterizes a set S of invariants according to our definitions.

IV. CONCLUSION

In this third article on the problem of algebraic completeness for the invariants of the Riemann tensor, we have exhaustively analyzed all canonically different space–times in which the Ricci tensor does have a null eigenvector. In each case we have given algebraically complete sets. It follows from this and the previous two articles[1,2] that the set CZ is determining, as was previously claimed. Interestingly, we have also shown that complete backsolving is, in general, not possible (but maximal backsolving has been achieved) when there is an alignment between an eigenvector of the Ricci tensor with the repeated principal null direction of the Weyl tensor.[3] In such cases all the mixed invariants are either zero or always dependent. Also, there is at most one complex Weyl invariant (w_1) and two real Ricci invariants (r_1 and r_2) together with R. As previously mentioned,

TABLE VII. Algebraically complete sets for Segre types with one or two null eigenvectors.

PP type	Segre type	Conditions (in Ricci canonical frame)	Complete Sets (and subsets thereof)	CB/NCB
II	[2,11]	$\Psi_0=\Psi_1=0$	$\{R,w_1,r_1,r_2\}$	NCB
		Otherwise	$\{R,w_1,w_2,r_1,r_2,m_1,m_2,m_3\}$	CB
III	[3,1]	$\Psi_0=\Psi_1=0$	$\{R,w_1,r_1\}$	NCB
		Otherwise	$\{R,w_1,w_2,r_1,m_1,m_2,m_3\}$	CB
D	[(1,1)11]	$\Psi_0=\Psi_1=0$ or $\Psi_3=\Psi_4=0$ (not both)	$\{R,w_1,r_1,r_2\}$	NCB
		$\Psi_0=\Psi_4=\Phi_{11}=0$ & $\Psi_1\Psi_3\neq 0$	$\{R,w_1,w_2,r_1,m_6\}$	CB
		$(\Psi_0=\Psi_3=0$ & $\Psi_1\Psi_4\neq 0)$	$\{R,w_1,w_2,r_1,r_2,m_5\}$[a]	
		or	or	CB
		$(\Psi_1=\Psi_4=0$ & $\Psi_0\Psi_3\neq 0)$	$\{R,w_1,w_2,r_1,r_2,m_6\}$	
		$(\Psi_0=\Phi_{11}=0$ & $\Psi_1\Psi_3\Psi_4\neq 0)$	$\{R,w_1,w_2,r_1,m_1,m_5\}$[a]	
		or	or	CB
		$(\Phi_{11}=\Psi_4=0$ & $\Psi_0\Psi_1\Psi_3\neq 0)$	$\{R,w_1,w_2,r_1,m_1,m_6\}$	
		Otherwise	$\{R,w_1,w_2,r_1,r_2,m_1,m_2,m_4\}$	CB
	[2,(11)]	$\Psi_0=\Psi_1=0$	$\{R,w_1,r_1\}$	NCB
		$\Psi_3=\Psi_4=0$	$\{R,w_1,r_1,m_4,m_5\}$	CB
		Otherwise	$\{R,w_1,w_2,r_1,m_1,m_2,m_4\}$	CB
	[(1,1)(11)]	$\Psi_0=\Psi_1=0$ or $\Psi_3=\Psi_4=0$ (not both)	$\{R,w_1,r_1\}$	NCB
		Otherwise	$\{R,w_1,w_2,r_1,m_1,m_2\}$	CB
N	[(2,1)1]	$\Psi_0=\Psi_1=0$	$\{R,w_1,r_1\}$	NCB
		Otherwise	$\{R,w_1,w_2,r_1,m_1,m_2,m_4\}$	CB
	[(3,1)]	$\Psi_0=\Psi_1=0$	$\{R,w_1\}$	NCB
		$\Psi_0=0$	$\{R,w_1,w_2,m_2,\lvert m_5\rvert\}$	CB
		Otherwise	$\{R,w_1,w_2,m_1,m_2,m_4\}$	CB
O	[(1,11)1][b]	$\Psi_0=\Psi_1=0$ or $\Psi_3=\Psi_4=0$ (not both)	$\{R,w_1,r_1\}$	NCB
		Otherwise	$\{R,w_1,w_2,r_1,m_4,m_5\}$	CB
	[(2,11)]	$\Psi_0=\Psi_1=0$	$\{R,w_1\}$	NCB
		$\Psi_0=0$	$\{R,w_1,w_2,m_6\}$	CB
		Otherwise	$\{R,w_1,w_2,m_4,m_5\}$	CB
	[(1,111)]	-	$\{R,w_1,w_2\}$	CB

[a]With m_5 satisfying a real syzygy.
[b]See Ref. 10.

we suspect that some space–times within such classes will, in general, prove to be more difficult to distinguish as inequivalent. As a final point, there still remains to fully clarify the geometric meaning of the invariants, principally the mixed ones. This will be the main focus of our work in the next article in this series.

APPENDIX: APPLICATION OF THE INDEX THEOREM

In one of our previous articles,[1] an Index theorem was presented regarding the general structure of any invariant formed from the Weyl and Ricci spinors:

$$\Psi_{ABCD}=\Psi_0\iota_A\iota_B\iota_C\iota_D-4\Psi_1 o_{(A}\iota_B\iota_C\iota_{D)}+6\Psi_2 o_{(A}o_B\iota_C\iota_{D)}-4\Psi_3 o_{(A}o_B o_C\iota_{D)}+\Psi_4 o_A o_B o_C o_D,$$

$$\Phi_{AB\dot{A}\dot{B}}=\Phi_{00}\iota_A\iota_B\bar{\iota}_{\dot{A}}\bar{\iota}_{\dot{B}}-2\Phi_{01}\iota_A\iota_B\bar{\iota}_{(\dot{A}}\bar{o}_{\dot{B})}+\Phi_{02}\iota_A\iota_B\bar{o}_{\dot{A}}\bar{o}_{\dot{B}}-2\Phi_{10}o_{(A}\iota_{B)}\bar{\iota}_{\dot{A}}\bar{\iota}_{\dot{B}}+4\Phi_{11}\iota_{(A}o_{B)}\bar{\iota}_{(\dot{A}}\bar{o}_{\dot{B})}$$
$$-2\Phi_{12}\iota_{(A}o_{B)}\bar{o}_{\dot{A}}\bar{o}_{\dot{B}}+\Phi_{20}o_A o_B\bar{\iota}_{\dot{A}}\bar{\iota}_{\dot{B}}-2\Phi_{21}o_A o_B\bar{\iota}_{(\dot{A}}\bar{\iota}_{\dot{B})}+\Phi_{22}o_A o_B\bar{o}_{\dot{A}}\bar{o}_{\dot{B}}.$$

Index Theorem: Let a,b,c be non-negative integers and let $\boldsymbol{\Psi}^a\overline{\boldsymbol{\Psi}}^b\boldsymbol{\Phi}^c$ represent any of the complete contractions (invariant) of a copies of the Weyl spinor, b copies of its complex conjugate and c copies of the Ricci spinor. Then any term in the expansion of these invariants has the form

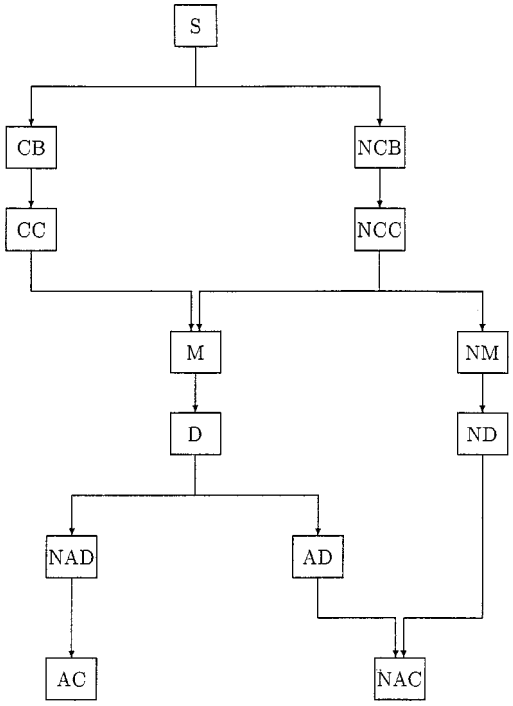

FIG. 1. Characterization of a set S of Riemann invariants. CB=completely backsolvable, NCB=not completely backsolvable, CC=curvature complete, NCC=not curvature complete, M=maximal, NM=not maximal, D=determining, ND=not determining, NAD=not always dependent, AD=always dependent, AC=algebraically complete, and NAC =not algebraically complete.

$$\Psi_0^{a_0}\Psi_1^{a_1}\Psi_2^{a_2}\Psi_3^{a_3}\Psi_4^{a_4}\overline{\Psi}_0^{b_0}\overline{\Psi}_1^{b_1}\overline{\Psi}_2^{b_2}\overline{\Psi}_3^{b_3}\overline{\Psi}_4^{b_4}\Phi_{00}^{c_{00}}\Phi_{01}^{c_{01}}\Phi_{02}^{c_{02}}\Phi_{10}^{c_{10}}\Phi_{11}^{c_{11}}\Phi_{12}^{c_{12}}\Phi_{20}^{c_{20}}\Phi_{21}^{c_{21}}\Phi_{22}^{c_{22}},$$

where $a_0,\ldots,a_4,b_0,\ldots,b_4,c_{00},\ldots,c_{22}$ are non-negative integers which must satisfy the following conditions:

$$a_0+a_1+a_2+a_3+a_4=a,\quad b_0+b_1+b_2+b_3+b_4=b,$$

$$c_{00}+c_{01}+c_{02}+c_{10}+c_{11}+c_{12}+c_{20}+c_{21}+c_{22}=c,$$

$$a_1+2a_2+3a_3+4a_4+c_{10}+c_{11}+c_{12}+2c_{20}+2c_{21}+2c_{22}=2a+c,$$

$$b_1+2b_2+3b_3+4b_4+c_{01}+2c_{02}+c_{11}+2c_{12}+c_{21}+2c_{22}=2b+c,$$

When applying the index theorem, note the following:

(1) If $\Phi_{ij}=0$ (or $\Psi_i=0$), we set $c_{ij}=0$ (or $a_i=b_i=0$).
(2) If an invariant does not include $\overline{\Psi}_i$'s, we set all $b_i=0$ and $b=0$.
(3) If $\Phi_{ij}=1$ (or $\Psi_i=1$), we do not set $c_{ij}=0$ (or $a_i=b_i=0$).
(4) If $\Phi_{ij}=\Phi_{kl}$, we do not set $c_{ij}=c_{kl}$.

We shall use this index theorem to prove the claims of non-backsolvability made above.

We begin by eliminating a, b and c to obtain the two conditions

$$2a_0+a_1+c_{00}+c_{01}+c_{02}=2a_4+a_3+c_{20}+c_{21}+c_{22}, \tag{A1}$$

$$2b_0+b_1+c_{00}+c_{10}+c_{20}=2b_4+b_3+c_{02}+c_{12}+c_{22}. \tag{A2}$$

Next, adding we obtain

$$2(a_0+b_0+c_{00})+(a_1+b_1+c_{01}+c_{10})=2(a_4+b_4+c_{22})+(a_3+b_3+c_{12}+c_{21}) \tag{A3}$$

For Segre type [2,11] with $\Psi_0=\Psi_1=0$ (in the Ricci canonical frame), we set $a_0=a_1=b_0=b_1=c_{00}=c_{01}=c_{10}=c_{12}=c_{21}=0$. Then Eq. (A3) gives $a_3+b_3+2(a_4+b_4+c_{22})=0$, which means that $a_3=b_3=a_4=b_4=c_{22}=0$, i.e., Ψ_3, $\bar{\Psi}_3$, Ψ_4 and $\bar{\Psi}_4$ (and Φ_{22}) will not appear in any invariant and hence, they cannot be determined. A similar argument can be used for the non-backsolvable cases in Segre types [3,1], [(1,1)11], [(1,1)(11)], [2,(11)], [(21)1], [(3,1)] and [(2,11)].

For Petrov type II and Segre type [(1,11)1] with $\alpha=0$, i.e., $\Phi_{00}=\Phi_{01}=0$ (in the Weyl canonical frame), we set $a_0=a_1=a_3=a_4=b_0=b_1=b_3=b_4=c_{00}=c_{01}=0$. Then Eq. (A3) gives $c_{12}+c_{21}+2c_{22}=0$, which means that $c_{12}=c_{21}=c_{22}=0$, i.e., Φ_{22}, Φ_{12}, and Φ_{21} will not appear in any invariant and hence, γ cannot be determined. Also, Eq. (A1) or (A2) gives $c_{02}=c_{20}$. Hence, any invariant will only involve $(\Phi_{02}\Phi_{20})^{c_{02}}$, which means that only $|\beta|$ can be determined. A similar argument can be used for the non-backsolvable cases in Segre type [(1,11)1] with Petrov types III and N (in the Weyl canonical frame).

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[2] J. Carminati, E. Zakhary, and R. McLenaghan, J. Math. Phys. **43**, 492 (2002).
[3] However, if further information like additional structure of the Weyl tensor is supplied, then the case could become completely backsolvable. For example, if we impose the condition that the Weyl tensor is Petrov type D and aligned, then $\Psi_3=\Psi_4=0$ and the case would become completely backsolvable. This comment would obviously also apply to other not completely backsolvable cases. Thus an alignment between an eigenvector of the Ricci tensor with a repeated principal null vector of the Weyl tensor is a necessary but not sufficient condition to prevent complete backsolving.
[4] A complete analysis of the necessary and/or sufficient conditions for all the not completely backsolvable cases to occur will be done in future work.
[5] C. B. G. McIntosh, J. M. Foyster, and A. W. C. Lun, J. Math. Phys. **22**, 2620 (1981).
[6] G. C. Joly and M. A. H. MacCallum, Class. Quantum Grav. **7**, 541 (1990).
[7] Equivalent real.
[8] Number (equivalent real) of curvature unknowns solved for in terms of the invariants and remaining, if any, curvature components.
[9] E. Zakhary, Ph.D thesis, Monash University, 1995.
[10] In the Ricci canonical frame, backsolving is not, in general, complete for Segre type [(1, 11)1] if $\Psi_0=\Psi_1=0$ or $\Psi_3=\Psi_4=0$, i.e., for degenerate Petrov types where the repeated PNDs coinside with an eigenvector of the Ricci tensor. Therefore, backsolving is always complete for Petrov type I, and also for type O (since $\Psi_a=0$). For Petrov types II, III, and N, backsolving is not, in general, always complete. On the other hand, since more conditions have been imposed on Ψ_a for Petrov type D, backsolving in this case is, understandably, complete.

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Applications of Nambu mechanics to systems of hydrodynamical type

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We show that the reduced Dubrovin–Novikov hydrodynamic type models are integrable Nambu mechanical systems admitting Lax triples. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1481955]

I. INTRODUCTION

In a remarkable paper, Nambu[1] initiated the study of multi-Hamiltonian systems. Apparently Nambu mechanics presents a new alternative view to classical mechanics. Nambu's paper was followed by a number of papers which essentially carry the idea from the physical point of view by showing that the classical part of it could be cast into the framework of classical mechanics with Dirac constraint.[2,3]

Recently, this research was revitalized and carried forward again by Takhtajan.[4] He gave rise to a beautiful theory, revealing deep and nontrivial connection with algebra and differential geometry. Note that, until now, the main activity in the theory of Nambu–Poisson geometry was concentrated around the algebraic aspects of Nambu structure—see, e.g., the papers of Alekseevsky,[5] de Azcárraga,[6,7] Grabowski, Marmo, Michor, Vaisman, Vinogradov, etc.[8–14] Somehow, the applications of Nambu dynamics is not fully explored yet. R. Chatterjee[15] had shown that several Hamiltonian systems possessing dynamical or hidden symmetries can be realized within the framework of Nambu mechanics. Among the notable examples are the SU(n) isotropic harmonic oscillator and the SO(4) Kepler problem. Most recently, Gonera and Nutku[16] showed that the Nambu structure can be extracted also from the rational Calogero–Moser system.

Some attempts have been made from the point of view of foliation theory by Dufour, Zung, and Zhitomerski.[17–19] Hence it would be rewarding to find some interesting applications of Nambu–Poisson geometry. In this article we are continuing to explore the potentiality of the application of Nambu mechanics in integrable systems.[20,21]

In this article we explore a higher dimensioanl analog of a 2D incompressible Euler equation in terms of Nambu dynamics. Thus a novel Nambu type integrable system is proposed. By generalizing Charles Li's[22,23] method we derive the corresponding linear equations or Lax triple of this equation. Surprisingly, this theory can be applied to reduced Dubrovin–Novikov type hydrodynamic systems.[24] Recently these system of equations are poping up in D-Brane theory[25–27] with the celebrated Born–Infeld action.[28]

The rest of this article is organized as follows: Since Nambu mechanics is an exotic subject, so, in the next section we will address some definitions of this subject. In Sec. III, we will discuss our Nambu integrable system.

II. PRELIMINARIES

The modern concept of Nambu–Poisson structure was proposed by Takhtajan in 1994 in order to find an axiomatic formulation for the n-bracket operation. Let M denote a smooth n-dimensional manifold and $C^{\infty}(M)$ the algebra of infinitely differentiable real valued functions on M.

Definition 2.1: A manifold M is called a Nambu–Poisson manifold if there exits a $\mathbb{R}$-multilinear map

$$\{\ ,\ldots,\ \}\ :\ [C^\infty(M)]^{\otimes n}\to C^\infty(M). \tag{1}$$

This is called Nambu–Poisson bracket of order n $\forall f_1,f_2,\ldots,f_{2n-1}\in C^\infty(M)$. *This bracket satisfies*

(1) $\{f_1,\ldots,f_n\}=(-1)^{\epsilon(\sigma)}\{f_{\sigma(1)},\ldots,f_{\sigma(n)}\}$,
(2) $\{f_1f_2,f_3,\ldots,f_{n+1}\}=f_1\{f_2,f_3,\ldots,f_{n+1}\}+\{f_1,f_3,\ldots,f_{n+1}\}f_2$, *and*
(3) fundamental identity

$$\{\{f_1,\ldots,f_{n-1},f_n\},f_{n+1},\ldots,f_{2n-1}\}+\{f_n,\{f_1,\ldots,f_{n-1},f_{n+1}\},f_{n+2},\ldots,f_{2n-1}\}+\cdots$$
$$+\{f_n,\ldots,f_{2n-2},\{f_1,\ldots,f_{n-1},f_{2n-1}\}\}=\{f_1,\ldots,f_{n-1},\{f_n,\ldots,f_{2n-1}\}\}, \tag{2}$$

where $\sigma\in S_n$*—the symmetric group of n elements—and* $\epsilon(\sigma)$ *is its parity*.

This fundamental identity is called Takhtajan identity.

Let $\{.,.,\ldots,.\}:C^\infty(M)\times C^\infty(M)\cdots\times C^\infty(M)\to C^\infty(M)$ be a multi-derivation that satisfies the Takhtajan identity if

(1) $\{.,.,.,.,.\}$ satisfies Takhtajan identity for generators
(2) satisfies quadratic identities.

$$\sum_{k=1}^{n}\{\phi,f_1,\ldots,f_{n-2},f_{n+k-1}\}\{\phi',f_n,\ldots,\widehat{f_{n+k-1}},\ldots,f_{2n-1}\}+\{\phi',f_1,\ldots,f_{n-2},f_{n+k-1}\}$$
$$\times\{\phi,f_{n+1},\ldots,\widehat{f_{n+k-1}},\ldots,f_{2n-1}\}=0. \tag{3}$$

It is known that the Nambu dynamics on a Nambu–Poisson phase space involves $n-1$ so-called Nambu–Hamiltonians $H_1,\ldots,H_{n-1}\in C^\infty(M)$ and is governed by the following equations of motion:

$$\frac{df}{dt}=\{f,H_1,\ldots,H_{n-1}\},\ \ \forall f\in C^\infty(M). \tag{4}$$

A solution to the Nambu–Hamilton equations of motion produces an evolution operator U_t which by virtue of the fundamental identity preserves the Nambu bracket structure on $C^\infty(M)$.

Definition 2.2: $f\in C^\infty(M)$ *is a first integral of* $X_{H_1,\cdots H_{n-1}}$ *if and only if*

$$\{f,H_1,H_2,\ldots,H_{n-1}\}=0.$$

III. LAX TRIPLE AND NAMBU INTEGRABLE SYSTEMS

Vladimir Arnold realized that the Euler equation is a Hamiltonian system. The Lax pair of the 2D Euler equation was first given by Friedlander and Vishik[29,30] in terms of Lagragian coordinates, and most recently by Li in terms of Eulerian coordinates.

The three-dimensional incompressible Euler equation can be expressed in vorticity form,

$$\partial_t\Omega+(u\cdot\nabla)\Omega-(\Omega\cdot\nabla)u=0, \tag{5}$$

where $u=(u_1,u_2,u_3)$ is the velocity, $\Omega=(\Omega_1,\Omega_2,\Omega_3)$ is the vorticity, $\nabla=(\partial_x,\partial_y,\partial_z)$, $\Omega=\nabla\times u$, and $\nabla\cdot u=0$.

Dropping the third subscript of Ω, the 2D euler equation can be written as

$$\partial_t\Omega+\{\Omega,\chi\}=0, \tag{6}$$

where the bracket is given by $\{f,g\}=\partial_xf\partial_yg-\partial_yf\partial_xg$, and χ is the stream function given by

$$u=-\partial_y\chi,\quad v=\partial_x\chi.$$

Thus the vorticity is connected to the stream function by

$$\Omega = \partial_x v - \partial_y u = \Delta \chi.$$

Let us introduce our Nambu integrable system. The idea of this equation is stimulated from the work of Li, Friedlander and Vishik. This equation is a higher dimensional analog of the 2D Euler equation, although it is not a 3D Euler equation (see Remark 3)

Defintion 3.1: The generalized (or Nambu) integrable system is given by

$$\partial_t \Omega + \{\Omega, \chi_1, \chi_2\} = 0,$$

where χ_1 *and* χ_2 *are two Hamiltonians and*

$$\{\Omega, \chi_1, \chi_2\} = \frac{\partial(\Omega, \chi_1, \chi_2)}{\partial(x,y,z)}.$$

Proposition 3.2: The Lax triple of the Nambu integrable equation is
(1) $\{\Omega, \phi_1, \phi_2\} = \lambda \phi_2$,
(2) $\partial \phi_1 = \{\chi_1, \chi_2, \phi_1\}$,
(3) $\partial \phi_2 = \{\chi_1, \chi_2, \phi_2\}$.

Sketch of the Proof: Let us differentiate the first equation. We obtain

$$\{\Omega_t, \phi_1, \phi_2\} + \{\Omega, \phi_{1_t}, \phi_2\} + \{\Omega, \phi_1, \phi_{2_t}\} = \{\chi_1, \chi_2, \{\Omega, \phi_1, \phi_2\}\},$$

$$\{\Omega_t, \phi_1, \phi_2\} + \{\Omega, \{\chi_1, \chi_2, \phi_1\}, \phi_2\} + \{\Omega, \phi_1, \{\chi_1, \chi_2, \phi_2\}\} = \{\chi_1, \chi_2, \{\Omega, \phi_1, \phi_2\}\}.$$

Using the Takhtajan identity

$$\{\{f_1, f_2, f_3\}, f_4, f_5\} + \{f_3, \{f_1, f_2, f_4\}, f_5\} + \{f_3, f_4, \{f_1, f_2, f_5\}\} = \{f_1, f_2, \{f_3, f_4, f_5\}\}. \quad (7)$$

we obtain our desired result. □

Remark 3.3: An ordinary Poisson integrable system is obtained from the compatibility condition of two linear equations. These equations are called the Lax pair. In the case of a Nambu (triple bracket) integrable system we need three linear equations or Lax triple.

Remark 3.4: For $n = 2$*, this coincides with the 2D Euler equation. The Lax pair of the 2D Euler equation given by Li is*

$$L\phi = \lambda \phi, \quad \partial_x \phi + A\phi = 0, \quad (8)$$

where $L\phi = \{\Omega, \phi\}$, $A\phi + \{\chi, \phi\} = 0$*, and the compatibility yields*

$$\partial_x L + [A, L] = \partial_x \Omega + \{\Omega, \chi\} = 0.$$

Remark 3.5 (Connection to n dimensional Euler equation): The higher dimensional incompressible Euler equation is given by

$$\partial_t \Omega + (u \cdot \nabla)\Omega - (\Omega \cdot \nabla)u = 0, \quad \nabla \cdot u = 0.$$

This equation can be expressed as

$$\partial_t(\partial_j u^i - \partial_i u^j) + u \cdot \nabla(\partial_j u^i - \partial_i u^j) - \sum_{k=1}^{n} (\partial_j u^k \partial_k u^i - \partial_i u^k \partial_k u^j) = 0, \quad (9)$$

where $\Omega^i_j = \partial_j u^i - \partial_i u^j$*, and* $\Omega(u) = (\Omega^i_j)_{1 \leqslant i,j \leqslant n}$.

When the dimension is equal to 2*, Eq. (9) boils down to*

$$\partial_t\Omega + u\cdot\nabla\Omega - (\partial_1 u^1\partial_1 u^2 + \partial_1 u^2\partial_2 u^2 - \partial_2 u^1\partial_1 u^1 - \partial_2 u^2\partial_2 u^1) = 0,$$

where $\Omega(u) = \partial_1 u^2 - \partial_2 u^1$. *One can express this as*

$$\partial_t\Omega + u\cdot\nabla\Omega - \Omega(\nabla\cdot u) = 0. \tag{10}$$

As the divergence of the vector field is zero, we get the well known relation

$$\partial_t\Omega + u\cdot\nabla\Omega = 0. \tag{11}$$

This equality is extremely interesting—by this one can distinguish the two dimensional case from the $n \geqslant 3$ *case.*

Hence, because of the presence of the term $(\Omega\cdot\nabla)u$ in a higher dimensional incompressible Euler equation, our Nambu integrable system does not coincide with it.

A. Applications to Dubrovin–Novikov systems

Dubrovin and Novikov considered an arbitrary $n\times n$ system of hydrodynamic type

$$u^i_t = v^i_j(x)u^j_x, \quad i,j = 1,\ldots,n, \tag{12}$$

which are nondiagonalizable but integrable.

Let us consider a special set $(n=3)$ of above hyperbolic differential equations:

$$\frac{\partial u}{\partial x_1} = u\frac{\partial u}{\partial x_4} + v\frac{\partial u}{\partial x_3} + w\frac{\partial u}{\partial x_2}, \tag{13}$$

$$\frac{\partial v}{\partial x_1} = u\frac{\partial v}{\partial x_4} + v\frac{\partial v}{\partial x_3} + w\frac{\partial v}{\partial x_2}, \tag{14}$$

$$\frac{\partial w}{\partial x_1} = u\frac{\partial w}{\partial x_4} + v\frac{\partial w}{\partial x_3} + w\frac{\partial w}{\partial x_2}. \tag{15}$$

These are examples of what Dubrovin and Novikov call ''equations of hydrodynamic type'' and these are fully integrable—for explicit solutions, any functions homogeneous of degree 1 are automatically solutions of these set, though the general solution can be found only in implicit form.

Let us combine all the equations (13)–(15). We obtain

$$\frac{\partial(u+\iota_1 v+\iota_2 w)}{\partial x_1} = u\frac{\partial(u+\iota_1 v+\iota_2 w)}{\partial x_4} + v\frac{\partial(u+\iota_1 v+\iota_2 w)}{\partial x_3} + w\frac{\partial(u+\iota_1 v+\iota_2 w)}{\partial x_2}. \tag{16}$$

Let us set $\Omega = u+\iota_1 v+\iota_2 w$:

$$\frac{\partial\Omega}{\partial x_1} = u\frac{\partial\Omega}{\partial x_4} + v\frac{\partial\Omega}{\partial x_3} + w\frac{\partial\Omega}{\partial x_2}. \tag{17}$$

Suppose

$$u = -\frac{\partial(\chi_1,\chi_2)}{\partial(x_2,x_3)}, \quad v = \frac{\partial(\chi_1,\chi_2)}{\partial(x_4,x_2)}, \quad w = \frac{\partial(\chi_1,\chi_2)}{\partial(x_3,x_4)}, \tag{18}$$

where χ_1 and χ_2 are some potential functions. Hence we obtain the reduced form of Dubrovin–Novikov equation as

$$\frac{\partial \Omega}{\partial x_1} + \{\Omega, \chi_1, \chi_2\} = 0. \tag{19}$$

Systems related 2D systems: In this case we obtain

$$\frac{\partial (u + \iota v)}{\partial x} = u \frac{\partial (u + \iota v)}{\partial z} + v \frac{\partial (u + \iota v)}{\partial y}. \tag{20}$$

Let us set $\Omega = u + \iota v$:

$$\frac{\partial \Omega}{\partial x} = u \frac{\partial \Omega}{\partial z} + v \frac{\partial \Omega}{\partial y}. \tag{21}$$

Suppose

$$u = -\frac{\partial \chi}{\partial y}, \quad v = \frac{\partial \chi}{\partial z}, \tag{22}$$

where χ is some potential function.

After this transformation the equation becomes

$$\frac{\partial \Omega}{\partial x} + \{\Omega, \chi\} = 0, \tag{23}$$

where the bracket {,} is defined as

$$\{f, g\} = (\partial_z f)(\partial_y g) - (\partial_y f)(\partial_z g).$$

The relation between Ω and χ is

$$\Omega = u + \iota v = -\partial_y \chi + \iota \partial_z \chi.$$

IV. CONCLUSION

In this article, using Nambu mechanics we have proposed a Lax representation of the reduced Dubrovin–Novikov type hydrodynamic systems. The most promising applications from this Lax triple should be along the direction of Darboux transformations, group theoretic applications, etc. Moreover, we hope that Lax representation and the Darboux transformations can be useful in investigating finite time blow up solutions of reduced Dubrovin–Novikov type systems.

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A unified treatment of quartic invariants at fixed and arbitrary energy

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Two-dimensional Hamiltonian systems admitting second invariants which are quartic in the momenta are investigated using the Jacobi geometrization of the dynamics. This approach allows for a unified treatment of invariants at both arbitrary and fixed energy. In the differential geometric picture, the quartic invariant corresponds to the existence of a fourth rank Killing tensor. Expressing the Jacobi metric in terms of a Kähler potential, the integrability condition for the existence of the Killing tensor at fixed energy is a nonlinear equation involving the Kähler potential. At arbitrary energy, further conditions must be imposed which lead to an overdetermined system with isolated solutions. We obtain several new integrable and superintegrable systems in addition to all previously known examples. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1483107]

I. INTRODUCTION

The study of Hamiltonian systems by means of geometric techniques provides fruitful clues about their integrability.[1–3] In particular, geometrization of the dynamics by using the Jacobi metric,[4,5] is a standard tool to turn a natural Hamiltonian system into a geodesic flow over a suitable Riemannian manifold. Therefore it is natural to investigate integrability of two-dimensional systems by looking for invariants corresponding to Killing tensors of a conformal Riemannian geometry. These geometric objects in fact directly produce invariants polynomial in the momenta: the degree of this polynomial is the same as the rank of the Killing tensor. Since the energy enters in the Jacobi metric as a parameter, the conditions for the existence of a Killing tensor may happen to be satisfied only at a fixed value of energy. In this case we speak of integrability at fixed energy in distinction to the usual notion of integrability which is understood to be valid at arbitrary energy.

In Ref. 2, quadratic invariants at arbitrary and fixed energy (respectively, *strongly* and *weakly* conserved phase-space functions) for two-dimensional Hamiltonian systems were treated in a unified way. The integrability condition for quadratic invariants involves an arbitrary analytic function $S(z)$. For invariants at arbitrary energy, the function $S(z)$ is a second degree polynomial with real second derivative, and the integrability condition then reduces to the classical Darboux condition for quadratic invariants at arbitrary energy.[6] Thereafter, the possibility of searching for linear and quadratic invariants at fixed energy was addressed and some examples of a system admitting a second quadratic invariant at zero energy were provided.

Weak invariants, also called *configurational invariants*, have been discussed by Hall[7] and by

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Sarlet, Leach and Cantrijn.[8] Hietarinta,[9] in his account of the direct methods for the search of the second invariant, also provides a review of all the known systems admitting one or more configurational invariants. Generalizing the approach of Ref. 2, Karlovini and Rosquist[10] have discussed the existence of invariants *cubic in the momenta* at both fixed and arbitrary energy. Beside giving a list of all known systems admitting a cubic strong invariant, they also find a superintegrable system admitting a cubic invariant related to an energy dependent linear invariant. In the present article we are going to discuss the case of the quartic invariant associated with the existence of a fourth-rank Killing tensor. Fourth-rank Killing tensors have previously been studied by one of the authors (see Ref. 11) in the Lorentzian case.

In analogy to the third-rank case, it turns out that it is natural to introduce a Kähler potential for the Jacobi metric. Expressing the conditions imposed on the geometry by Killing tensor equations in terms of this Kähler potential, there remains a system of nonlinear partial differential equations. Imposing the condition of strong integrability, it turns out that in general this system becomes overdetermined, so that, like for cubic invariants, only isolated mechanical systems exist with a second invariant quartic in the momenta. Due to the complexity of the system of equations, it is impossible to get a fully general solution. However, with our approach we are able to find some new integrable and superintegrable cases. In particular, one may wonder if the knowledge of a weak invariant can provide information about the global dynamical behavior of the system. We introduce a method which, starting from a family of weakly integrable systems, leads to finding a higher-order invariant for isolated members of the family which are therefore strongly integrable. The second invariant depends on the energy as a parameter.

The plan of the article is as follows: in Sec. II we recall the necessary and sufficient conditions for the existence of a Killing tensor in the Jacobi geometry and their application in problems of analytical mechanics. In Sec. III we examine the particular case of fourth-rank Killing tensors. In Sec. IV we analize the conditions for strong integrability with a quartic invariant. In Sec. V we present the method by which, starting from a family of weakly integrable systems, isolated examples of strongly integrable systems with quartic second invariant can be found. In Sec. VI we give tables of integrable systems admitting a quartic invariant which include new integrable and superintegrable systems in addition to all known cases. In Sec. VII we give our conclusions.

II. JACOBI GEOMETRY AND KILLING TENSORS

A. Geometric representation of the dynamics

We are interested in the classical two-dimensional systems with Hamiltonian function

$$\mathcal{H}=\tfrac{1}{2}(p_x^2+p_y^2)+V(x,y). \tag{1}$$

The approach followed in studying the integrability properties of these systems is based on the Jacobi geometrization procedure which associates to the Hamiltonian flow produced by (1), a geodesic flow on a Riemannian manifold endowed with a positive definite metric

$$ds_J^2=g_{\alpha\beta}dq^\alpha dq^\beta, \quad \alpha,\beta=1,2. \tag{2}$$

It can be shown (see, e.g., Ref. 4) that the Jacobi metric

$$g_{\alpha\beta}=2(E-V)h_{\alpha\beta}, \tag{3}$$

where $h_{\alpha\beta}$ is the metric of the flat space, generates a geodesic flow corresponding to the natural mechanical system with potential $V=V(q)$ at energy E. In fact, if we introduce the geodesic, or ''Jacobi,'' Hamiltonian

$$\mathcal{H}_J=\frac{1}{2}\,\frac{1}{2(E-V)}h^{\alpha\beta}p_\alpha p_\beta\equiv\frac{1}{2}, \tag{4}$$

the corresponding geodesic equations

$$\frac{dq^\alpha}{ds_J}=\frac{\partial \mathcal{H}_J}{\partial p_\alpha}=\frac{1}{2(E-V)}h^{\alpha\beta}p_\beta, \quad \frac{dp_\alpha}{ds_J}=-\frac{\partial \mathcal{H}_J}{\partial q^\alpha}=-\frac{1}{2(E-V)}\frac{\partial V}{\partial q^\alpha}, \tag{5}$$

are equivalent to the canonical equations of motion given by the Hamiltonian (1),

$$\frac{dq^\alpha}{dt}=\frac{\partial \mathcal{H}}{\partial p_\alpha}, \quad \frac{dp_\alpha}{dt}=-\frac{\partial \mathcal{H}}{\partial q^\alpha}, \tag{6}$$

if the natural identification of canonical coordinates

$$q^1=x, \quad q^2=y, \quad p_1=p_x, \quad p_2=p_y \tag{7}$$

is made. The phase-space trajectories are parametrized by the affine parameter s_J that is related to the standard time variable by

$$ds_J=2[E-V(q(t))]dt. \tag{8}$$

The Jacobi geometry corresponding to Hamiltonian (1) is then

$$ds^2=2G(dx^2+dy^2)=2Gdzd\overline{z}, \quad G=E-V, \tag{9}$$

where we have introduced null variables $z=x+iy$ and $\overline{z}=x-iy$.

All tensor calculations will be done in the standard null frame defined as

$$\Omega^0=\sqrt{G}dz, \quad \Omega^{\overline{0}}=\sqrt{G}d\overline{z}, \tag{10}$$

in which the metric takes the simplest possible form

$$ds^2=2d\Omega^0 d\Omega^{\overline{0}}. \tag{11}$$

We use the convention that tensor indices in this frame take the values 0 and $\overline{0}$, while in any coordinate frame the values will be the names of the coordinates (e.g., z and $\overline{z}$).

B. Invariants polynomial in the momenta and Killing tensors

One of the standard tools of the geometric approach is the investigation of integrability by looking for invariants generated by *Killing tensors*. Let us see the simple case of second-order Killing tensor equations

$$K_{(\alpha\beta;\gamma)}=0. \tag{12}$$

The existence of a second-rank Killing tensor, that is a symmetric tensor which satisfies Eq. (12), implies the existence of a conserved quadratic function

$$I_J=K^{\alpha\beta}p_\alpha p_\beta \tag{13}$$

commuting with the Jacobi Hamiltonian. In fact, it is easy to check that the vanishing of the Poisson bracket of this function with the Hamiltonian implies Eq. (12). In analogy with the theory of second order invariants, the Jacobi geometry approach leads, as it stands, to the determination of higher-order invariants. Generalizing Eq. (12), an *mth rank* Killing tensor is a symmetric tensor satisfying the equation

$$K_{(\mu_1\mu_2\ \cdots\ \mu_m;\mu_{m+1})}=0. \tag{14}$$

It gives rise to the *mth order* (in the momenta) invariant

$$I_J = K^{\mu_1 \mu_2 \cdots \mu_m} p_{\mu_1} \cdots p_{\mu_m}. \tag{15}$$

Two remarks are in order here:

(1) The function (15) is a *weak invariant*, in the sense that, in general, it is a conserved quantity in the dynamics fixed by the given value of the energy appearing in the definition of the Jacobi geometry (9). To grant it the full title of strong invariant, it must satisfy the additional requirement of satisfying the Killing tensor equations at arbitrary energy.
(2) The function (15), let us call it the *Jacobi invariant*, is a homogeneous polynomial of degree equal to the rank of the corresponding Killing tensor. To transform it into the ordinary invariant in the physical time gauge there is a straightforward recipe consisting in replacing the parameter E appearing in I_J with the corresponding Hamiltonian function (1). As a consequence, the physical invariant

$$I = I_J|_{E \to \mathcal{H}} \tag{16}$$

becomes a polynomial which is either even or odd in the momenta.

Karlovini and Rosquist[10] have discussed the existence of third-rank Killing tensors, giving a list of all known integrable or superintegrable systems admitting a cubic strong invariant. Here we are going to discuss the case of the quartic invariant associated with the existence of a fourth-rank Killing tensor. Moreover, we want to exploit the results concerning the existence of higher-order invariants to generate new solutions starting from the assumption of the existence of a second-rank Killing tensor.

III. QUARTIC INVARIANTS CORRESPONDING TO FOURTH-RANK KILLING TENSORS

In this section we derive the necessary and sufficient integrability condition for the Jacobi metric to admit a fourth-rank Killing tensor at a fixed value of the energy parameter E. In the following section we proceed by finding the conditions that ensure that the Killing tensor equations be satisfied at arbitrary values of the energy, with the restriction to the case in which the energy dependence of the Killing tensor is such that the corresponding invariant of the physical Hamiltonian is quartic in the momenta. As usual in our approach (see Ref. 11), we decompose the fourth-rank Killing tensor in the form

$$K_{\alpha\beta\gamma\delta} = P_{\alpha\beta\gamma\delta} + P_{(\alpha\beta} g_{\gamma\delta)} + \tfrac{3}{8} K g_{(\alpha\beta} g_{\gamma\delta)} \tag{17}$$

or equivalently

$$K_{\alpha\beta\gamma\delta} = P_{\alpha\beta\gamma\delta} + K_{(\alpha\beta} g_{\gamma\delta)} - \tfrac{1}{8} K g_{(\alpha\beta} g_{\gamma\delta)}, \tag{18}$$

where $K_{\alpha\beta} = K^{\gamma}_{\alpha\beta\gamma}$ and $K = K^{\gamma}_{\gamma}$. $P_{\alpha\beta\gamma\delta}$ is the trace-free (conformal) part, $P_{\alpha\beta} = P^{\gamma}_{\alpha\beta\gamma}$ its trace and K the full trace of the Killing tensor. In this way, the Killing tensor equations are split into the trace-free ''components'' and the equation for the trace

$$P_{(\alpha\beta\gamma\delta;\mu)} - \tfrac{1}{2} P^{\nu}{}_{(\alpha\beta\gamma;\nu} g_{\delta\mu)} = 0, \tag{19}$$

$$P_{(\alpha\beta;\gamma)} - \tfrac{1}{2} P^{\nu}{}_{(\alpha;\nu} g_{\gamma\delta)} + \tfrac{1}{2} P^{\nu}{}_{\alpha\beta\gamma;\nu} = 0, \tag{20}$$

$$K_{,\alpha} = -\tfrac{4}{3} P^{\beta}_{\alpha;\beta}. \tag{21}$$

It is advantageous to employ also the coordinate frame components of the conformal part and of its trace when parametrizing the five independent components of $K_{\alpha\beta\gamma\delta}$. Thus, the components of the Killing tensor can be written as

$$\begin{gathered} K_{0000}=G^2P^{\overline{zzzz}}=G^2\overline{S}, \quad K_{000\overline{0}}=\tfrac{1}{2}P_{00}=\tfrac{1}{2}GP^{\overline{zz}}=\tfrac{1}{2}G\overline{R(z,\overline{z})}, \\ K_{00\overline{00}}=\tfrac{1}{4}K, \quad K_{0\overline{000}}=\tfrac{1}{2}P_{\overline{00}}=\tfrac{1}{2}GP^{zz}=\tfrac{1}{2}GR(z,\overline{z}), \quad K_{\overline{0000}}=G^2P^{zzzz}=G^2S, \end{gathered} \tag{22}$$

where, as usual, $S=S(z)$ is a holomorphic function, so that $\overline{S}=\overline{S}(\overline{z})$ comes from (19), but the function $R=R(z,\overline{z})$ is a generic function of the arguments. With this parametrization, the equation for the trace (21) has the integrability condition

$$2(G_{,zz}R-G_{,\overline{zz}}\overline{R})+3(G_{,z}R_{,z}-G_{,\overline{z}}\overline{R}_{,\overline{z}})+G(R_{,zz}-\overline{R}_{,\overline{zz}})=0, \tag{23}$$

which is analogous to that obtained for the second-rank case (but now R is not holomorphic!).

We now proceed to solve the Killing tensor equations. Equation (20) gives

$$S^{-3/4}R_{,\overline{z}}+2(S^{1/4}G)_{,z}=0 \tag{24}$$

and its complex conjugate. In analogy with the approach followed in Refs. 2 and 10, we make a coordinate transformation to put the conformal Killing tensor in the simplest (*standard*) form. Using a conformal transformation of the form

$$w=H(z), \quad w=X+iY, \quad z=x+iy, \tag{25}$$

the transformation of the conformal tensor is such that

$$\tilde{S}(w):=P^{wwww}=[H'(z)]^4P^{zzzz}=[H'(z)]^4S(z). \tag{26}$$

If we make the standard choice

$$\tilde{S}(w):=P^{wwww}=1, \tag{27}$$

the conformal transformation is then provided by the function

$$H'(z)=[S(z)]^{-1/4}. \tag{28}$$

Equation (24) becomes

$$(S^{-1/2}R)_{,\overline{w}}+2\tilde{G}_{,w}=0, \tag{29}$$

with

$$\tilde{G}=|H'(z)|^{-2}G=\sqrt{|S|}G. \tag{30}$$

Moreover, under the conformal transformation generated by Eq. (28), the function R transforms as

$$\tilde{R}=P^{ww}=[H'(z)]^2P^{zz}=S^{-1/2}R. \tag{31}$$

Inserting $\tilde{R}$ into Eq. (29), we have the set

$$\tilde{R}_{,\overline{w}}+2\tilde{G}_{,w}=0, \quad \bar{\tilde{R}}_{,w}+2\tilde{G}_{,\overline{w}}=0. \tag{32}$$

The solution of this system can be found in terms of a real Kähler potential $\mathcal{K}(w,\overline{w})$:

$$\tilde{G}=\mathcal{K}_{,w\overline{w}}, \quad \tilde{R}=-2\mathcal{K}_{,ww}. \tag{33}$$

The integrability condition (23) determines the following equation for the Kähler potential:

$$\Im\{(\mathcal{K}_{,www}\mathcal{K}_{,w\bar{w}}+2\mathcal{K}_{,ww\bar{w}}\mathcal{K}_{,ww})_{,w}\}=0. \tag{34}$$

This is the necessary and sufficient condition for the existence of a fourth-rank Killing tensor. In analogy to the third-rank case (see Ref. 10) and in contrast to the first- and second-rank cases,[2] the condition is highly nonlinear. The same condition has been already found in Ref. 7 and treated in Ref. 9, even if not in the context of the present geometric approach. Note that in Ref. 9, Eq. (7.5.15), there is a misprint for a factor 2 missing.

In the standardized coordinate frame the second invariant can be written in the form

$$I_J=2\Re\{p_w^4+2\tilde{R}\mathcal{H}_J p_w^2\}+\tfrac{3}{2}\mathcal{H}_J^2 K, \tag{35}$$

whereas in the original null coordinate frame the second invariant is

$$I_J=2\Re\{Sp_z^4+2R\mathcal{H}_J p_z^2\}+\tfrac{3}{2}\mathcal{H}_J^2 K, \tag{36}$$

where

$$\mathcal{H}_J=\frac{1}{G}p_z p_{\bar{z}}=\frac{1}{\tilde{G}}p_w p_{\bar{w}}=p_0 p_{\bar{0}}\equiv\frac{1}{2} \tag{37}$$

is the Jacobi Hamiltonian expressed in the three different reference frames. The trace function K is found by integrating the system

$$\tfrac{3}{4}K_{,\bar{w}}+\tilde{R}_{,w}\tilde{G}+2\tilde{R}\tilde{G}_{,w}=0,\quad \tfrac{3}{4}K_{,w}+\bar{\tilde{R}}_{,\bar{w}}\tilde{G}+2\bar{\tilde{R}}\tilde{G}_{,\bar{w}}=0. \tag{38}$$

IV. ARBITRARY ENERGY INVARIANTS

Equation (34) gives the the necessary and sufficient condition for a two-dimensional Riemannian geometry to admit a fourth-rank Killing tensor. If we interpret the geometry according to Eq. (9) as that providing a natural mechanical system, we can derive the additional conditions that make the Killing tensor equations satisfied for every value of the energy E. We use the following form for the Kähler potential,

$$\mathcal{K}=E[z\bar{z}+2\Re\{\Lambda(z)\}]-\Psi, \tag{39}$$

where Λ is a holomorphic function independent of E and the real *prepotential* Ψ is such that

$$\Psi_{,z\bar{z}}=V. \tag{40}$$

In fact, no loss of generality is implied by letting the energy dependence of the Kähler potential be prescribed by Eq. (39) and by taking the function $S_4(z)$ to be energy independent, given that we only take interest in the cases for which the physical invariant I is a quartic polynomial in the momenta. Since the analogous statement was made without proving it for the cubic case,[10] we give a proof here. We begin by noting that the physical invariant I, obtained from the Jacobi invariant I_J of Eq. (36) according to prescription (16), can be written as

$$I=2\Re\{Sp_z^4+Bp_z^3 p_{\bar{z}}\}+C(p_z p_{\bar{z}})^2, \tag{41}$$

where

$$B=2RG^{-1},\quad C=\tfrac{3}{2}KG^{-2}. \tag{42}$$

Since the energy parameter E is now assumed to have been replaced by the physical Hamiltonian $\mathcal{H}$, the functions S, B and C will be dependent on the momenta p_z and $p_{\bar{z}}$, but clearly only through the combination $p_z p_{\bar{z}}$ that appears in $\mathcal{H}$. This implies that all five terms on the right hand side of Eq. (41) have to be quartic polynomials in the momenta since I is quartic by definition. This can be clearly seen by viewing I as a function of the two independent momenta functions $p_z p_{\bar{z}}$ and $p_z/p_{\bar{z}}$, rather than the momenta p_z and $p_{\bar{z}}$ themselves. Indeed, I can be recast into the form

$$I=(p_z p_{\bar{z}})^2 \sum_{k=-2}^{2} Q_k (p_z/p_{\bar{z}})^k, \tag{43}$$

where

$$Q_{-2}=\overline{Q_2}=S, \quad Q_{-1}=\overline{Q_1}=B, \quad Q_0=C. \tag{44}$$

Clearly, with the coefficients of $(p_z/p_{\bar{z}})^k$ only depending on the momenta through $p_z p_{\bar{z}}$, there can be no cancellation of possible nonquartic polynomial dependence in the individual terms. Hence, we conclude that the functions $S p_z^4$, $B p_z^4 p_{\bar{z}}$ and $C(p_z p_{\bar{z}})^2$, as well as the complex conjugates of the first two, must be quartic momenta polynomials. It immediately follows that S, B and C are polynomials in $(p_z p_{\bar{z}})^{-1}$, with coefficients depending only on z and $\bar{z}$, of degree zero, one and two, respectively. This directly proves the part of statement about S having no energy dependence. Moreover, since $G=E-V$ turns into $T=2p_z p_{\bar{z}}$ when E is replaced by $\mathcal{H}=T+V$, it now follows from Eqs. (42) that the functions R and K are restricted to be first respectively second degree polynomials in $p_z p_{\bar{z}}$, which is the same as saying that they must be the same type of polynomials in the energy parameter E, before making the substitution $E\to\mathcal{H}$. Using the second of Eqs. (33) and the conformal transformation formulas given by Eqs. (28) and (31), the function R can be expressed in terms of S and $\mathcal{K}$ according to

$$R=-2(S\mathcal{K}_{,zz}+\tfrac{1}{4}S'\mathcal{K}_{,z}), \tag{45}$$

while Eqs. (38), which notably are form invariant under conformal transformations, give that the trace K is given by integrating

$$\tfrac{3}{4}K_{,\bar{z}}+R_{,z}G+2RG_{,z}=0 \tag{46}$$

and its complex conjugate. Now, there is clearly no loss in generality to write the Kähler potential $\mathcal{K}$ as

$$\mathcal{K}=E[z\bar{z}+2\Re\{\Lambda(E,z)\}]-\Psi(z,\bar{z}), \tag{47}$$

with Λ being analytic in z and Ψ being energy independent. Moreover, since S is energy independent and R is a first degree polynomial in E, it follows from Eq. (45) that we are able to write $\Lambda(E,z)$ as

$$\Lambda(E,z)=\Lambda_0(z)+\Lambda_1(E,z), \tag{48}$$

where $\Lambda_1(E,z)$ does not contribute to Eq. (45). However, since Eq. (46) shows that $\Lambda(z)$ enters into $K_{,\bar{z}}$ only through R, we might as well set $\Lambda_1(E,z)$ to zero, which proves the fact that we could have taken $\Lambda(E,z)$ to be energy independent from the outset. We may finally note that with both R and G being first degree polynomials in E, we find from Eq. (46) that $K_{,\bar{z}}$ is a second degree polynomial in E, which indeed is a necessary and sufficient condition for K to be a second degree polynomial as well, up to addition of an irrelevant integration constant, which in principle can have an arbitrary energy dependence. This completes the proof that the form of the Kähler potential given by Eq. (39) is the most general one which is needed for full generality.

We are now in the position to solve the integrability condition at arbitrary energy. In the original z coordinates, Eq. (34) takes the form

$$\Im\{[S(\mathcal{K}_{,zzz}\mathcal{K}_{,z\bar{z}}+2\mathcal{K}_{,zz\bar{z}}\mathcal{K}_{,zz})+\tfrac{1}{2}S'(\mathcal{K}_{,zzz}\mathcal{K}_{,z}+\tfrac{5}{2}\mathcal{K}_{,zz}\mathcal{K}_{,z\bar{z}})+\tfrac{1}{4}S''\mathcal{K}_{,z\bar{z}}\mathcal{K}_{,z}]_{,z}\}=0. \tag{49}$$

Substituting the ansatz (39) into Eq. (49), this condition provides a second degree polynomial in E:

$$A_2E^2+A_1E+A_0=0. \tag{50}$$

The coefficients A_0, A_1, A_2 must vanish separately if the equation must hold for arbitrary energy. Therefore we obtain the three equations:

$$A_2=\Im\{[\Lambda'''S+\tfrac{5}{4}\Lambda''S'+\tfrac{1}{4}(\bar{z}+\Lambda')S'']_{,z}\}=0, \tag{51}$$

$$\begin{aligned}A_1=\Im\{[&S(\Psi_{,zzz}+2\Lambda'''\Psi_{,z\bar{z}}+2\Lambda''\Psi_{,zz\bar{z}})+\tfrac{1}{2}S'((\bar{z}+\Lambda')\Psi_{,zz\bar{z}}\\&+\tfrac{5}{2}(\Psi_{,zz}+\Lambda''\Psi_{,z\bar{z}}))+\tfrac{1}{4}S''(\Psi_{,z}+(\bar{z}+\Lambda')\Psi_{,z\bar{z}})]_{,z}\}=0,\end{aligned} \tag{52}$$

$$A_0=\Im\{[S(\Psi_{,zzz}\Psi_{,z\bar{z}}+2\Psi_{,zz\bar{z}}\Psi_{,zz})+\tfrac{1}{2}S'(\Psi_{,zzz}\Psi_{,z}+\tfrac{5}{2}\Psi_{,zz\bar{z}}\Psi_{,zz})+\tfrac{1}{4}S''\Psi_{,zz\bar{z}}\Psi_{,z}]_{,z}\}=0. \tag{53}$$

It turns useful to express the system of equations (51)–(53) also in the transformed coordinates since this simplifies the computations when the S function is of higher degree. Using the notation

$$F(w)=H^{-1}(z(w)) \tag{54}$$

for the inverse conformal transformation, the coefficients A_0, A_1, A_2 become

$$A_2=\Im\{[F'''\bar{F}F'\bar{F}'+2(F'')^2\bar{F}\bar{F}'+\Lambda'''F'\bar{F}'+\Lambda''F''\bar{F}']_{,w}\}, \tag{55}$$

$$A_1=\Im\{[(F'''\bar{F}+\Lambda''')\Psi_{,w\bar{w}}+2(F''\bar{F}+\Lambda'')\Psi_{,ww\bar{w}}+F'\bar{F}'\Psi_{,www}+2F''\bar{F}'\Psi_{,ww}]_{,w}\}, \tag{56}$$

$$A_0=\Im\{[\Psi_{,www}\Psi_{,w\bar{w}}+2\Psi_{,ww\bar{w}}\Psi_{,ww}]_{,w}\}. \tag{57}$$

Applying the differential operator

$$\frac{\partial^2}{\partial z\,\partial\bar{z}}$$

to Eq. (51), we get the condition

$$\Im\{S''''(z)\}=0, \tag{58}$$

so that the form allowed to the S function to have integrability at arbitrary energy is

$$S(z)=az^4+\beta z^3+\gamma z^2+\delta z+\epsilon,\quad a\in\mathbb{R},\quad \beta,\gamma,\delta,\epsilon\in\mathbb{C}. \tag{59}$$

In Ref. 2 it has been shown that, to get arbitrary energy quadratic invariants in systems with two degrees of freedom, the function $S(z)$ must satisfy the condition

$$\Im\{S_2''(z)\}=0, \tag{60}$$

that is, it must be a second degree polynomial with real second derivative. Together with the result (58) and the corresponding one obtained in the third-rank case,[10]

$$\Re\{S_3'''(z)\}=0, \tag{61}$$

we can guess that, as a general rule, the analytic function $S(z)$ representing the conformal part of a Killing tensor of arbitrary rank m is required to satisfy the condition

$$\begin{aligned}\Re\left\{\left(\frac{d}{dz}\right)^m S(z)\right\}&=0 \quad (m \text{ odd}),\\ \Im\left\{\left(\frac{d}{dz}\right)^m S(z)\right\}&=0 \quad (m \text{ even}).\end{aligned} \tag{62}$$

As a simple illustration of the solution of the above set of Equations (51)–(53), let us take

$$\Lambda=0, \quad S=b, \quad b\in\mathbb{R}.$$

Equation (51) is automatically satisfied. Equation (52) gives then the equation

$$\Psi_{,xxxy}-\Psi_{,xyyy}=0,$$

whose solution is

$$\Psi_{,xy}=F_1(x+y)+F_2(x-y).$$

Therefore

$$\Psi=f_1(x)+f_2(y)+f_3(x-y)+f_4(x+y).$$

The potential can then be written as

$$V=v_1(x)+v_2(y)+v_3(x-y)+v_4(x+y),$$

where $v_i=f_i''/4$, $i=1,2$ and $v_i=f_i''/2$, $i=3,4$. Equation (53) now gives

$$\begin{aligned}&(v_1''v_4+2v_4''v_1)+3v_1'v_4'-(v_1''v_3+2v_3''v_1)-3v_1'v_3'\\ &\quad-(v_2''v_4+2v_4''v_2)-3v_2'v_4'+(v_2''v_3+2v_3''v_2)-3v_2'v_3'=0.\end{aligned}$$

This equation coincides with that reported in the review of Hietarinta.[9] Its most relevant solutions, together with the expressions of the invariant, are listed in Table II later in this work.

In more general cases Eq. (52) is not as easily solved. The standard approach is to restrict the attention to special cases where $S(z)$ is either a homogeneous polynomial or a nonhomogeneous one which is simply a power of the corresponding function in lower rank cases. Even with such restrictions, many solutions can be obtained. Moreover, in all the solutions found it has turned out that $\Lambda(z)=\lambda z^2$, with λ a complex constant. In this way the coefficient

$$z\bar{z}+2\Re\{\Lambda(z)\}$$

of E in the Kähler potential (39) is always a Hermitian form in z. In the tables included in Sec. VI are listed all the solutions found.

V. STRONG INVARIANTS GENERATED BY LOWER-ORDER WEAK INVARIANTS

In the present section we want to introduce an alternative technique to identify classes of strongly integrable systems. This approach works only in a restricted subclass of systems, but is useful to get insight into the structure of general solutions. The key point of the idea is based on the construction of a generic weak integrable system corresponding to the existence of a second-

rank Killing tensor. Introducing the corresponding simplified Kähler potential in the general set of equations, we try to isolate single systems that satisfy them. The reader more interested in the general approach may wish to skip directly to Sec. VI with the results.

A. Quadratic invariants

The technique devised and applied in Ref. 2 amounts, in short synthesis, in a conformal transformation of the form (25). In the second-rank case, it turns out that it must be generated by an arbitrary holomorphic function $S_2(z)$ via the relation

$$H(z)=\int \frac{dz}{\sqrt{S_2(z)}}. \tag{63}$$

In the new coordinates X, Y, the Jacobi potential $G=E-V$ turns out to be of the form

$$G(X,Y)=\frac{A(X)+B(Y)}{|S_2(X,Y)|}, \tag{64}$$

where A and B are arbitrary functions of their arguments, which can be thought of as the *separation coordinates*. The conformal factor appearing in (64) can be written as

$$|S_2(X,Y)|=\sqrt{S_2(w)\overline{S_2}(\overline{w})}=F'(w)\overline{F'}(\overline{w}). \tag{65}$$

Moreover, we can write the transformation of the momenta in the form

$$p_X=Rp_x+Qp_y, \quad p_Y=-Qp_x+Rp_y, \tag{66}$$

where

$$R=\Re\{F'\}, \quad Q=\Im\{F'\}. \tag{67}$$

We can therefore write the expression of the second invariant in the Jacobi gauge as

$$I_S(p_X,p_Y,X,Y)=\tfrac{1}{2}(p_X^2-p_Y^2)+B(Y)-A(X). \tag{68}$$

As remarked in the Introduction, since to each Jacobi potential G pertains a specific dynamical system, we have that the found invariant is, in general, only a *weak* invariant for the standard Hamiltonian, in the sense that it provides a conserved quantity only at a given value of the energy (perhaps at *zero* energy). In fact, the Poisson bracket of the function (68) with the separated Hamiltonian

$$\mathcal{H}_S=\frac{\tfrac{1}{2}(p_X^2+p_Y^2)-A(X)-B(Y)}{|S_2|} \tag{69}$$

is

$$\{I_S,\mathcal{H}_S\}=\frac{E}{|S_2|}(p_X|S_2|_{,X}-p_Y|S_2|_{,Y}). \tag{70}$$

B. Quartic strong invariants generated by quadratic weak invariants

In Sec. IV, the system of equations (51)–(53) was treated and many nontrivial solutions were found. A general solution is, however, very difficult to find due to the complicated structure of the full system. Here we want instead to exploit the above results to generate new solutions simply starting from the assumption of the existence of a second-rank Killing tensor.

As a foreword to this approach, let us make the following remark. Let us suppose to have made the choice of the S_2 function generating the conformal transformation which gives the second invariant (68) satisfying Eq. (70). Denoting by $\mathcal{H}_0$ the numerator appearing in the expression (69) of the Hamiltonian, the Poisson bracket of a generic higher-order invariant with $\mathcal{H}_S$ can be written as

$$\{I_J,\mathcal{H}_S\}=\frac{1}{|S_2|}\{I_J,\mathcal{H}_0\}-\frac{\mathcal{H}_0}{|S_2|^2}\{I_J,|S_2|\}=\frac{\{I_J,\mathcal{H}_0\}-E\{I_J,|S_2|\}}{|S_2|}. \tag{71}$$

In the case of a second-order invariant in the standard form of (68), this reduces to (70). On the other hand, let us introduce the *null* Hamiltonian

$$\mathcal{H}_\mathcal{N}=(\mathcal{H}_S-E)|S_2|=\mathcal{H}_0-E|S_2|. \tag{72}$$

The Poisson bracket of the invariant with $\mathcal{H}_\mathcal{N}$ is

$$\{I_J,\mathcal{H}_\mathcal{N}\}=\{I_J,\mathcal{H}_0\}-E\{I_J,|S_2|\}. \tag{73}$$

Since $|S_2|$ is a non-null positive function everywhere, Eqs. (71) and (73) are equivalent for what concerns the conservation of I_J. The conceptual difference relies on the fact that, whereas Eq. (73) expresses the conservation of I_J in the dynamics provided by $\mathcal{H}_\mathcal{N}$ at *zero "energy,"* Eq. (71) expresses the conservation of I_J in the dynamics provided by $\mathcal{H}_S$ at *arbitrary* energy. Note that the true energy E enters into $\mathcal{H}_\mathcal{N}$ as an arbitrary parameter.

In the light of this argument, the procedure to look for new integrable systems is the following: regard the null Hamiltonian, written in the form

$$\mathcal{H}_\mathcal{N}=\tfrac{1}{2}(p_X^2+p_Y^2)-\tilde{G}(X,Y), \tag{74}$$

where

$$\tilde{G}(X,Y)=A(X)+B(Y)+E|S_2(X,Y)|, \tag{75}$$

as the system in which to find a new conserved quantity at zero energy. If the search of this new conserved quantity is successful, then *it is a strongly conserved quantity for the original Hamiltonian* $\mathcal{H}_S$, *which is therefore integrable at arbitrary energy*. Going backwards with respect to the previous approach, we take the potential of Eq. (75) and use it to solve the system (33). Once we have the solution, we can write the integrability condition (34) in the form

$$\Im\{R_{,ww}G+3R_{,w}G_{,w}+2RG_{,ww}\}=0. \tag{76}$$

Note that in the remaining part of this section we suppress the "tilde" over $\tilde{G}$ and $\tilde{R}$ to simplify the notation. The solution of this equation provides the explicit form of the functions $A(w+\overline{w})$ and $B(w-\overline{w})$ that allow for the integrability of the system. Finally, the integration of the equations for the trace (38) completes the solution.

In the development of this approach, we find it convenient to use the separating real variables. Equations (33) involving the Kähler potential therefore become

$$\begin{aligned} G(X,Y)&=\tfrac{1}{4}(\mathcal{K}_{,XX}+\mathcal{K}_{,YY}),\\ R(X,Y)&=\tfrac{1}{2}(\mathcal{K}_{,YY}-\mathcal{K}_{,XX})+i\mathcal{K}_{,XY}, \end{aligned} \tag{77}$$

and the integrability condition (76) can be written in the form

$$[(\Im\{R\})_{,XX}-(\Im\{R\})_{,YY}-2(\Re\{R\})_{,XY}]G+3[((\Im\{R\})_{,X}-(\Re\{R\})_{,Y})G_{,X}-((\Re\{R\})_{,X}+(\Im\{R\})_{,Y})G_{,Y}]+2[\Im\{R\}(G_{,XX}-G_{,YY})-2\Re\{R\}G_{,XY}]=0. \tag{78}$$

The system (38) finally becomes

$$\begin{aligned} K_{,X}&=-\tfrac{4}{3}((\Re\{R\})_{,X}+(\Im\{R\})_{,Y}))G-\tfrac{8}{3}(\Re\{R\}G_{,X}+\Im\{R\}G_{,Y}),\\ K_{,Y}&=-\tfrac{4}{3}((\Im\{R\})_{,X}-(\Re\{R\})_{,Y})G-\tfrac{8}{3}(\Im\{R\}G_{,X}-\Re\{R\}G_{,Y}). \end{aligned} \tag{79}$$

To solve system (33), we need only consider the contribution to the potential (75) coming from the conformal factor:

$$G_C=E|S_2(X,Y)|. \tag{80}$$

Recalling the relation (63) between the conformal transformation and the S_2 function in the quadratic case and the definition of the inverse transformation (54), the above source term can also be written as

$$G_C=E\sqrt{S_2(w)\overline{S_2}(\overline{w})}=EF'(w)\overline{F'}(\overline{w}). \tag{81}$$

The solutions of system (33) for this term are

$$\begin{aligned} \mathcal{K}_C&=E(F(w)\overline{F}(\overline{w})+2\Re\{\Lambda(w)\}),\\ R_C&=-2E(F''(w)\overline{F}(\overline{w})+\Lambda''(w)), \end{aligned} \tag{82}$$

so that the complete solution is therefore

$$\begin{aligned} \mathcal{K}&=4\int\left[\int AdX\right]dX+4\int\left[\int BdY\right]dY+E(F(w)\overline{F}(\overline{w})+2\Re\{\Lambda(w)\}),\\ R&=2(B(Y)-A(X))-2E(F''(w)\overline{F}(\overline{w})+\Lambda''(w)). \end{aligned} \tag{83}$$

This solution is subject to the integrability condition (76). In analogy with the general approach, substituting in it the solution (83) we get a second degree polynomial in E of the form (50). This equation must be satisfied for every value of the arbitrary parameter E, so that each coefficient must separately vanish. The three coefficients are in this case

$$\begin{aligned} A_2&=-4i\Im\{(F''''\overline{F}+\Lambda'''')F'\overline{F'}+5F'''F''\overline{F'}\,\overline{F}+3\Lambda'''F''\overline{F'}+2\Lambda''F'''\overline{F'}\},\\ A_1&=4i\Im\{3(B_{,w}-A_{,w})F''\overline{F'}-3(A_{,w}+B_{,w})(F'''\overline{F}+\Lambda''')+2(B-A)F'''\overline{F'}\\ &\quad-2(A_{,ww}+B_{,ww})(F''\overline{F}+\Lambda'')-(A+B)F''''\overline{F}\},\\ A_0&=2i\Im\{6(B_{,w}-A_{,w})(B_{,w}+A_{,w})+4(B-A)(A_{,ww}+B_{,ww})\}. \end{aligned} \tag{84}$$

From the properties of the functions A and B, A_0 is identically zero. Limiting ourselves to the simplest case $\Lambda=0$, the condition that A_2 vanishes turns out to be

$$\Im\{(F''''F'+5F'''F'')\overline{FF'}\}=0, \tag{85}$$

so that it is necessary and sufficient that

$$F''''F'+5F'''F''=6aFF',\quad a\in\mathbb{R}. \tag{86}$$

The general solution is

$$(F')^4 = aF^4 + \gamma F^2 + \delta F + \epsilon, \tag{87}$$

where β, γ, δ, ϵ are complex constants. We see that solution (87) is a subset of the general result (58) so that we can state that the simplified approach presented here consists in choosing a function in the set

$$S_2(z) = \sqrt{az^4 + \gamma z^2 + \delta z + \epsilon}. \tag{88}$$

The equation $A_1 = 0$ then picks the functions A and B that are compatible with strong integrability. The practical advantage with respect to the application of the general technique of Sec. IV is that equation $A_0 = 0$ is automatically satisfied.

C. Class iz^2 systems

To illustrate the simplified approach, in this subsection we present a class of simple systems which are strongly integrable with a quartic invariant and, at zero energy, are separable with a quadratic invariant.

Consider then the function

$$S_2(z) = iz^2. \tag{89}$$

In the solution (87) it corresponds to the choice

$$a = -1, \quad \gamma = \delta = \epsilon = 0. \tag{90}$$

This is the simplest polynomial form which does not satisfy the constraint (60) and therefore gives a potential which is not automatically integrable at arbitrary energy with a quadratic second invariant. The corresponding conformal transformation is given by

$$w = H(z) = \frac{1-i}{\sqrt{2}} \ln z. \tag{91}$$

Using polar coordinates, so that

$$\begin{gathered} z = x + iy = r \exp(i\theta), \\ r = \sqrt{x^2 + y^2}, \quad \theta = \arctan(y/x), \end{gathered} \tag{92}$$

in terms of real variables, we get

$$X = \frac{1}{\sqrt{2}}(\theta + \ln r), \quad Y = \frac{1}{\sqrt{2}}(\theta - \ln r). \tag{93}$$

We point out, in passing, that that in Ref. 2, in Eqs. (102)–(104) corresponding to Eq. (93) above, there is a misprint and the coordinate r must be substituted with its natural logarithm. It follows that the potential given by

$$V(\theta, r) = -\frac{A(\theta + \ln r) + B(\theta - \ln r)}{r^2} \tag{94}$$

is integrable at zero energy for arbitrary functions A and B. The common factor r^{-2} is due to the fact that, from the choice of Eq. (89), we have

$$|S(X,Y)| = r^2 = \mathrm{e}^{\sqrt{2}(X-Y)}. \tag{95}$$

The solutions (83) are

$$\mathcal{K}=4\int\left[\int A dX\right]dX+4\int\left[\int B dY\right]dY+E\mathrm{e}^{\sqrt{2}(X-Y)} \tag{96}$$

and

$$R=2((B(Y)-A(X))-2iE\mathrm{e}^{\sqrt{2}(X-Y)}. \tag{97}$$

The integrability condition (78) becomes

$$4E\mathrm{e}^{\sqrt{2}(X-Y)}[A''-B''+3\sqrt{2}(A'+B')+4(A-B)]=0. \tag{98}$$

This equation splits into

$$A''+3\sqrt{2}A'+4A=c,\quad B''-3\sqrt{2}B'+4B=c, \tag{99}$$

with solutions

$$A(X)=a_1\mathrm{e}^{-\sqrt{2}X}+a_2\mathrm{e}^{-2\sqrt{2}X}+\frac{c}{4},\quad B(Y)=b_1\mathrm{e}^{\sqrt{2}Y}+b_2\mathrm{e}^{2\sqrt{2}Y}+\frac{c}{4}. \tag{100}$$

The potential

$$V(r,\theta)=-\frac{c}{2r^2}-\frac{a_1\mathrm{e}^{-\theta}+b_1\mathrm{e}^{\theta}}{r^3}-\frac{a_2\mathrm{e}^{-2\theta}+b_2\mathrm{e}^{2\theta}}{r^4} \tag{101}$$

is therefore integrable. As a simple concrete example, let us take

$$a_1=b_1=c=0,\quad a_2=b_2=-\tfrac{1}{2}, \tag{102}$$

so that the potential is

$$V=\frac{\mathrm{e}^{2\theta}+\mathrm{e}^{-2\theta}}{2r^4}, \tag{103}$$

which is a known result mentioned in the review by Hietarinta. The second invariant has the form

$$I=p_\theta^4+\mathrm{ch}2\theta p_r^2+2\frac{\mathrm{sh}2\theta}{r}p_r p_\theta+3\frac{\mathrm{ch}2\theta}{r^2}p_\theta^2+2\frac{2-\mathrm{sh}2\theta}{r^4}. \tag{104}$$

VI. CLASSIFICATION OF HAMILTONIANS ADMITTING A QUARTIC INVARIANT AT ARBITRARY ENERGY

In the tables included in this section we present all the solutions we have found of systems admitting an independent invariant quartic in the momenta. Some of them are new. For all cases we present the potential V (up to linear transformations of the coordinates and a linear rescaling of the potential itself) as well as the quartic invariant I, thereby making it possible to compare directly the results with Hietarinta's classification of 1987.[9] For the cases which are superintegrable we also indicate, using the notation of Ref. 9, to which of the real quadratic cases (1), (2), (4) or (7) a given system belongs.

A peculiar property of our solutions is that all but one have a conformal factor generated by function S of even degree in z, with real coefficients. As a consequence of this, the solutions obtained can be expressed in terms of the coordinate systems of separable potentials. In fact, since from (28) and (54), the transformation is

TABLE I. Systems for which $S(z)$ is of zero degree.

$S(z)=1$

$\mathcal{K}=2Ex^2-\frac{4}{3}x^4-2bxy^2-\frac{1}{3}y^4+4c\ln|y|$

$V=4x^2+y^2+bx+cy^{-2}$

$I=p_x^4+2p_x^2p_y^2+4Vp_x^2+4byp_xp_y+16x^2p_y^2+2(2x^2+y^2)(b+4x)^2+32cx^2y^{-2}$

Superintegrable, case (4) and (7)

$S(z)=1$

$\mathcal{K}=2Ex^2-9y^{4/3}(bx+c)-\frac{3}{2}ay^4-\frac{9}{10}dy^{8/3}-\frac{8}{3}ax^4$

$V=\frac{1}{2}a(16x^2+9y^2)+(bx+c)y^{-2/3}+dy^{2/3}$

$I=p_x^4+2p_x^2p_y^2+4Vp_x^2+12by^{1/3}p_xp_y+32ax^2p_y^2+64ax^2V+16bdx-256a^2x^4+18b^2y^{2/3}+144abxy^{4/3}$

$S(z)=-1$

$\mathcal{K}=2Ex^2-2x^4y^2-\frac{1}{3}ax^4y-\frac{a^2}{12}\left(\frac{x^4}{18}+y^4\right)-\frac{16}{15}y^6-\frac{8}{15}ay^5+4d\ln|x|$

$V=x^4+6x^2y^2+8y^4+a\left(\frac{8}{3}y^3+x^2y\right)+\frac{a^2}{72}(x^2+16y^2)+\frac{d}{x^2},$

$I=p_x^4+4p_x^2\left(x^4+6x^2y^2+ax^2y+\frac{1}{72}a^2x^2+\frac{d}{x^2}\right)-\left(\frac{4}{3}ax^3+16x^3y\right)p_xp_y$

$+4x^4p_y^2+4\left(2dx^2+x^8+d^2x^{-4}+\frac{2}{3}ady+4dy^2\right)+\frac{x^6}{9}(144y^2+24ay-a^2)+\frac{x^4}{1296}(144y^2+24ay-a^2)^2$

$S(z)=-1$

$\mathcal{K}=2Ex^2-2x^4y^2-\frac{16}{15}y^6-\frac{1}{3}bx^4-\frac{4}{3}by^4+4d\ln|x|-\frac{c}{5}y^{-4}+4m\ln|y|$

$V=x^4+6x^2y^2+8y^4+b(x^2+4y^2)+\frac{d}{x^2}+\frac{m}{y^2}+\frac{c}{x^6}$ (Ref. 13)

$I=p_x^4+4p_x^2\left(x^4+6x^2y^2+bx^2+\frac{d}{x^2}+\frac{c}{x^6}\right)-16x^3yp_xp_y+4x^4p_y^2$

$+4[12cy^2x^{-4}+2dx^2+x^8+2bx^6+b^2x^4+2cx^{-2}+2cdx^{-8}+c^2x^{-12}+(d^2+2bc)x^{-4}$

$+4x^6y^2+2mx^4y^{-2}+4bx^4y^2+4x^4y^4+4dy^2]$

$$H(z)=F^{-1}(w(z))=\int dz[S_4(z)]^{-1/4}, \tag{105}$$

with S of the form

$$S_4(z)=\pm(az^2+\beta z+\gamma),\quad a\in\mathbb{R},\quad \beta,\gamma\in\mathbb{C}, \tag{106}$$

we are actually taken back to the coordinate transformations to separable variables given by an S_2 function satisfying the condition (60), for which the transformation is of the form[2]

$$H(z)=\int dz[S_2(z)]^{-1/2}. \tag{107}$$

As an exception to this situation, we have also found a solution with S_4 of third degree in z, by the method of the *coupling constant metamorphosis* (see Ref. 9) which is described in Sec. VI B.

A. Systems for which $S(z)$ is of even degree

The simplest case is that with S_4 of degree zero. This case corresponds simply to rotations and translations of the Cartesian coordinates. In Table I we list the new solutions obtained and, for comparison, the quartic integrable potential of Ref. 13. In Table II the already known solutions of this class are listed together with the proper references. The first sequence of items corresponds to

TABLE II. Systems for which $S(z)$ is of zero degree (continued).

$S(z)=1$

$\mathcal{K}=E(x^2+y^2)-f_1(x)-f_2(y)-f_3(x-y)-f_4(x+y)$

$V=v_1(x)+v_2(y)+v_3(x-y)+v_4(x+y)$

$v_i(\xi)=\frac{1}{4}f_i''(\xi)$ (for $i=1,2$), $v_i(\xi)=\frac{1}{2}f_i''(\xi)$ (for $i=3,4$) (Ref. 9)

$I=p_x^2p_y^2+2v_2p_x^2+2(v_4-v_3)p_xp_y+2v_1p_y^2+h(x,y)$

$v_1=0,\quad v_2=e^y,\quad v_3=e^{x-y},\quad v_4=0,\quad h=2e^x+e^{2(x-y)}$

$v_1=e^{-x},\quad v_2=e^y,\quad v_3=e^{x-y},\quad v_4=0,\quad h=2e^x+e^{2(x-y)}+2e^{-y}+4e^{y-x}$

$v_1=0,\quad v_2=e^y,\quad v_3=e^{x-y},\quad v_4=e^{-x-y},\quad h=2e^x+e^{2(x-y)}+2e^{-x}+e^{-2(x+y)}-2e^{-2y}$

$v_1=0,\quad v_2=e^y,\quad v_3=e^{x-y},\quad v_4=e^{-(x+y)/2},\quad h=2e^x+e^{2(x-y)}+e^{-(x+y)}-2e^{(x-3y)/2}$

$v_1=e^{-2x},\quad v_2=e^y,\quad v_3=e^{x-y},\quad v_4=0,\quad h=2e^x+e^{2(x-y)}+4e^{-2x+y}$

$v_1=\frac{a}{x^2},\ v_2=\frac{a}{y^2},\ v_3=\frac{b}{(x-y)^2},\ v_4=\frac{b}{(x+y)^2},\ h=\frac{4a^2}{x^2y^2}+\frac{16b^2x^4}{(x^2-y^2)^4}-\frac{16b^2x^2}{(x^2-y^2)^3}+\frac{16ab}{(x^2-y^2)^2}$

$S(z)=1$

$\mathcal{K}=2Ex^2-9y^{4/3}\left(cx^2+d+\frac{m}{10}y^{4/3}\right)-a\left(\frac{4}{3}x^4+3y^4\right)+4n\ln|x|$

$V=\frac{9}{2}cy^{4/3}+(cx^2+d)y^{-2/3}+my^{2/3}+a(9y^2+4x^2)+\frac{n}{x^2}$ (Ref. 13)

$I=p_x^4+2p_x^2p_y^2+4p_x^2\left((cx^2+d)y^{-2/3}+my^{2/3}+a(9y^2+4x^2)+\frac{n}{x^2}\right)+24cxy^{1/3}p_xp_y$

$+4p_y^2(4ax^2+nx^{-2})+16cmx^2+32adx^2y^{-2/3}+8\frac{dn}{x^2y^{2/3}}$

$+8\frac{cn}{y^{2/3}}+(32am+72c^2)x^2y^{2/3}+8nmx^{-2}y^{2/3}+72anx^{-2}y^2+4n^2x^{-4}+32acx^2y^{-2/3}(9y^2+x^2)+32a^2x^2(9y^2+2x^2)$

$S(z)=-1$

$\mathcal{K}=2Ex^2-a\left(\frac{1}{6}x^4+\frac{8}{3}y^4\right)-d\left(\frac{1}{3}x^4y+\frac{16}{15}y^5\right)+4h_1\ln|x|-\frac{h_2}{5x^4}$

$V=\frac{1}{2}a(x^2+16y^2)+d\left(\frac{16}{3}y^3+x^2y\right)+\frac{h_1}{x^2}+\frac{h_2}{x^6}$ (Ref. 13)

$I=p_x^4+4p_x^2\left(\frac{1}{2}ax^2+dx^2y+\frac{h_1}{x^2}+\frac{h_2}{x^6}\right)-\frac{4}{3}dx^3p_xp_y$

$+4[2dh_2yx^{-4}+2h_1h_2x^{-8}+h_2^2x^{-12}+(h_1^2+ah_2)x^{-4}+\frac{1}{4}a^2x^4-\frac{1}{18}d^2x^6-\frac{1}{3}d^2x^4y^2-\frac{1}{3}adx^4y+\frac{2}{3}dh_1y]$

the simple solution sketched at the end of Sec. IV. All solutions are generated by $S_4=\pm 1$: actually, there is nothing fundamental in the choice of sign which has been made only for sake of comparison with already known results.

We then have some solutions with S_4 of degree two and four in z. In Table III, two new interesting classes of integrable systems are presented with S_4 of degree two. They are more conveniently treated using the parabolic coordinates provided by the conformal transformation generated by $S_4=16z^2$. In Table IV, a class of integrable systems generated by $S_4=-z^4$ is presented, generalizing the separability in polar coordinates. Here, the choice of sign is dictated by the transformation used in the simplified approach of Sec. V C above, but to the same system one can also arrive with the general method using the "proper" transformation given by $S_4=z^4$.

B. A system for which $S(z)$ is of degree three

In order to describe how we get this new solution, we briefly recall the method based on the coupling constant metamorphosis.[9] We introduce a null Hamiltonian which, in analogy with Eq. (72), is defined as

$$\mathcal{H}_{\mathcal{N}}=(\mathcal{H}-E)|S_4|^2. \tag{108}$$

TABLE III. Systems for which $S(z)$ is of second degree.

$S(z)=16z^2$

$\mathcal{K}=\frac{2}{3}E(2x^2+y^2)+f(X)+g(Y)+C(XY)^{\alpha}$

$X=\sqrt{\frac{r+x}{2}},\quad Y=\sqrt{\frac{r-x}{2}},\quad r=\sqrt{x^2+y^2}=X^2+Y^2$

$f(X)=-36\,2^{-1/3}cX^{4/3}-\frac{18\,2^{1/3}}{5}aX^{8/3},\quad g(Y)=-36\,2^{-1/3}dY^{4/3}-\frac{18\,2^{1/3}}{5}bY^{8/3},\quad \alpha=4/3$

$V=\frac{a(r+x)^{1/3}+b(r-x)^{1/3}+c(r+x)^{-1/3}+d(r-x)^{-1/3}}{r}+\frac{k}{y^{2/3}},\quad k=-\frac{2^{1/3}C}{36}$

$I=J^2-8ky^{1/3}\left[p_xp_\theta-\frac{y}{r}(a(r+x)^{1/3}+b(r-x)^{1/3}+c(r+x)^{-1/3}+d(r-x)^{-1/3})\right]-8k[a(r-x)^{2/3}+b(r+x)^{2/3}]$

$J=p_yp_\theta+\frac{(r+x)[b(r-x)^{1/3}+d(r-x)^{-1/3}]-(r-x)[a(r+x)^{1/3}+c(r+x)^{-1/3}]}{r}+2\frac{kx}{y^{2/3}}$

$p_\theta=xp_y-yp_x$

$f(X)=\frac{1}{14}CX^8+8a\log X-\frac{1}{10}cX^{-4},\quad g(Y)=\frac{1}{14}CY^8+8b\log Y-\frac{1}{10}dY^{-4},\quad \alpha=4$

$V=\frac{1}{r}\left[\frac{a}{r+x}+\frac{b}{r-x}+\frac{c}{(r+x)^3}+\frac{d}{(r-x)^3}\right]+\frac{1}{2}kr^2,\quad k=-\frac{C}{2}$

$I=J^2-ky^3\left\{p_xp_\theta-\frac{y}{r}\left[\frac{a}{r+x}+\frac{b}{r-x}+\frac{c}{(r+x)^3}+\frac{d}{(r-x)^3}\right]+\frac{1}{4}kx^2y\right\}-k[a(r-x)^2+b(r+x)^2]$

$J=p_yp_\theta+\frac{1}{r}\left\{(r+x)\left[\frac{b}{r-x}+\frac{d}{(r-x)^3}\right]-(r-x)\left[\frac{a}{r+x}+\frac{c}{(r+x)^3}\right]\right\}+\frac{1}{2}kxy^2$

TABLE IV. Systems for which $S(z)$ is of third degree.

$S(z)=64z^3$

$\mathcal{K}=\frac{2}{7}E(4x^2+3y^2)+f(X)+g(Y)-\frac{4}{3}\mu(X^4+Y^4)$

$X=\sqrt{2}r^{1/4}\cos\frac{\theta}{4}=r^{1/4}\sqrt{1+\cos\frac{\theta}{2}},\quad Y=\sqrt{2}r^{1/4}\sin\frac{\theta}{4}=r^{1/4}\sqrt{1-\cos\frac{\theta}{2}}$

$r=\sqrt{x^2+y^2}=(X^2+Y^2)^2/4,\quad \theta=\arctan(y/x)$

$f(X)=32a\log X-\frac{8}{5}cX^{-4},\quad g(Y)=32b\log Y-\frac{8}{5}dY^{-4}$

$V=\frac{\mu}{r}+\frac{a}{r^2(1+\cos\theta/2)}+\frac{b}{r^2(1-\cos\theta/2)}+\frac{c}{r^3(1+\cos\theta/2)^3}+\frac{d}{r^3(1-\cos\theta/2)^3}$

$I=J^2+\Gamma_1\Pi-\Gamma_2$

$J=\Delta+B(Y)-A(X)-\mathcal{H}(X^2-Y^2)^3+4\mu(X^2-Y^2)$

$\Delta=\frac{2}{\sqrt{r}}\left[\cos\frac{\theta}{2}(r^2p_r^2-p_\theta^2)-\sin\frac{\theta}{2}rp_rp_\theta\right]$

$\Pi=\frac{2}{\sqrt{r}}\left[\sin\frac{\theta}{2}(r^2p_r^2-p_\theta^2)+\cos\frac{\theta}{2}rp_rp_\theta\right]$

$\Gamma_1=16\mathcal{H}X^3Y^3$

$\Gamma_2=16\mathcal{H}[\mathcal{H}(2X^6Y^6+3X^4Y^4(X^4+Y^4))-8\mu X^4Y^4-aY^4-bX^4]$

$\mathcal{H}$ is the Hamiltonian of the system, i.e., $\mathcal{H}=\frac{1}{2}\left(p_r^2+\frac{p_\theta^2}{r^2}\right)+V$

$p_\theta=xp_y-yp_x,\quad rp_r=xp_x+yp_y$

TABLE V. Systems for which $S(z)$ is of fourth degree.

$$S(z)=-z^4$$

$$\mathcal{K}=E\mathrm{e}^{\sqrt{2}(X-Y)}+f(X)+g(Y)-k(X^2+Y^2)$$

$$X=\frac{1}{\sqrt{2}}(\theta+\ln r),\quad Y=\frac{1}{\sqrt{2}}(\theta-\ln r)$$

$$A(X)=a_1\mathrm{e}^{-\sqrt{2}X}+a_2\mathrm{e}^{-2\sqrt{2}X},\quad A=f''/4$$

$$B(Y)=b_1\mathrm{e}^{\sqrt{2}Y}+b_2\mathrm{e}^{2\sqrt{2}Y},\quad B=g''/4$$

$$V=\frac{k}{r^2}+\frac{a\mathrm{e}^{\theta}+b\mathrm{e}^{-\theta}}{r^3}+\frac{c\mathrm{e}^{2\theta}+d\mathrm{e}^{-2\theta}}{r^4}$$

$$I=p_\theta^4+(c\mathrm{e}^{2\theta}+d\mathrm{e}^{-2\theta})p_r^2+2\left[a\mathrm{e}^{\theta}-b\mathrm{e}^{-\theta}+\frac{1}{r}(c\mathrm{e}^{2\theta}-d\mathrm{e}^{-2\theta})\right]p_rp_\theta$$
$$+\left[2k+\frac{2}{r}(a\mathrm{e}^{\theta}+b\mathrm{e}^{-\theta})+\frac{3}{r^2}(c\mathrm{e}^{2\theta}+d\mathrm{e}^{-2\theta})\right]p_\theta^2$$
$$+\frac{1}{r^2}[2k(c\mathrm{e}^{2\theta}+d\mathrm{e}^{-2\theta})-(a\mathrm{e}^{\theta}-b\mathrm{e}^{-\theta})^2]$$
$$+\frac{4}{r^3}(bc\mathrm{e}^{\theta}+ad\mathrm{e}^{-\theta})+\frac{1}{r^4}(c^2\mathrm{e}^{4\theta}+d^2\mathrm{e}^{-4\theta}+6cd)$$

The second case of Table III has a null Hamiltonian which, if expressed in the new coordinates, has the form

$$\mathcal{H}_{\mathcal{N}}=\tfrac{1}{2}(p_X^2+p_Y^2)-A(X)-B(Y)+4C(X^2+Y^2)^3-4E(X^2+Y^2). \tag{109}$$

Then, if the term $(X^2+Y^2)^3$ can be identified with the conformal factor associated to a new conformal transformation, we may interpret C as a *new* energy and E as a *new* coupling constant. We get a new potential which is strongly integrable with an invariant of the same nature as before. This is the process known as coupling constant metamorphosis.

In the present instance, we have that the transformation must be still of the form (105) or, equivalently,

$$F'(w)=S_4^{1/4}, \tag{110}$$

where, for simplicity, we still denote the new variable as $w=X+iY$, so that $|w|^2=X^2+Y^2$. Since the conformal factor is assumed to be $(X^2+Y^2)^3$, we get

$$|F'|^2\sim|w|^6. \tag{111}$$

Therefore, $F(w)$ must be of the order w^4, so that

$$w=H(z)\sim z^{1/4}. \tag{112}$$

From (105) we get

$$H'(z)\sim z^{-3/4}, \tag{113}$$

so that, finally,

$$S_4(z)\sim z^3. \tag{114}$$

We end up with a solution of third degree for S which had escaped a previous direct analysis. The new integrable Hamiltonian is

$$\mathcal{H}=\frac{1}{2}\left(p_r^2+\frac{p_\theta^2}{r^2}\right)+\frac{\mu}{r}+\frac{a}{r^2(1+\cos\theta/2)}+\frac{b}{r^2(1-\cos\theta/2)}+\frac{c}{r^3(1+\cos\theta/2)^3}+\frac{d}{r^3(1-\cos\theta/2)^3}$$
$$=\tilde{E}, \tag{115}$$

where $\tilde{E}=C$ is the new energy and $\mu=-E$ is the new coupling constant. Table V reports the form of the coordinate transformation and the expression of the second invariant.

VII. CONCLUSIONS

In this work we have explored the set of natural two-dimensional Hamiltonian systems admitting a second invariant which is a polynomial in the momenta of degree four. The approach is based on the Jacobi geometrization described in Ref. 2, where the linear and quadratic cases were also explored, and in Ref. 10, where the cubic cases were treated. The approach allows a unified treatment of integrability at fixed and arbitrary energy, even if here we have limited ourselves to obtaining the list, as complete as possible, of strongly integrable systems. There are several areas in which this approach can be still useful. The most natural seems to be that of looking for systems admitting higher order invariants of which there exist only a few known examples.

Moreover, other properties of invariants up to degree four are still worth of analysis. In Ref. 14 we have examined the properties of weakly integrable systems with quadratic second invariants and found interesting behaviors both in the integrable regime and in the generic nonintegrable one. One may wonder about the information higher order weak invariants can give on the dynamics of nonintegrable systems. It is reasonable to believe that increasing the order can improve the reliability of these functions when interpreting them as effective invariants approximately conserved in regular portions of phase-space. It would also be interesting to look for other examples of quartic invariants which correspond to lower rank Killing tensors on fixed energy surfaces.

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Multisymplectic geometry and multisymplectic Preissman scheme for the KP equation

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The multisymplectic structure of the KP equation is obtained directly from the variational principal. Using the covariant De Donder–Weyl Hamilton function theories, we reformulate the KP equation to the multisymplectic form which was proposed by Bridges. From the multisymplectic equation, we can derive a multisymplectic numerical scheme of the KP equation which can be simplified to the multisymplectic 45 points scheme. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The generalized Kadomtsev–Petviashvili (GKP) equation is

$$(u_t+\partial_x f(u)+u_{xxx})_x+\sigma u_{yy}=0 \quad (t>0,-\infty<x,y<\infty), \tag{1.1}$$

where σ is a constant, and $f(u)$ is some smooth function. The usually KP equation occurs for $f(u)$ quadratic and it is regarded as a two-dimensional generalization of the Korteweg–de Vries (KdV) equation. It describes the evolution of long water waves of small amplitude if they are weakly two dimensional. In the case of $f(u)=3u^2$ and $\sigma=-3$, Eq. (1.1) is usually called the KPI equation, whereas the KPII equation with $f(u)=3u^2$ and $\sigma=3$. As a soliton equation important from analytical and numerical point of view, the KP equation is one of the few known completely integrable equations in the multidimensional soliton equations. Thus, in the last few years, considerable attention has been paid to the KP equation. Although considerable interest has been focused on the KP equation, the numerical scheme analysis literature for the KP equation is extremely small. As far as we are aware of, Katsis proposed the explicit finite difference method,[1] the results of evolution of the lump solution for the KP equation was given by Minzoni,[2] Wang *et al.* studied the instability of a generalized KP equation,[3] Feng and Mitsui took the linearized implicit method to the KP equation.[4]

In this paper, we try to describe the KP equation in the language of multisymplectic geometry. Recently, for first order field theory, i.e., the Lagrangian density depends on the state variables and their first order derivatives, Marsden, Patrix, and Shkoller[5] derived numerical methods for the first order field theories. However the Lagrangian density of the KP equation is not first-order, therefore MPS theory cannot be applied directly. In Ref. 6, the authors focus their attention on the KdV equation whose Langrangian density is second order. The Langrangian density of the KP equation is truly third-order. In this paper, we give the multisymplectic structure of the KP equation directly from the variational principal. In Ref. 7, the author proposed that the Cartan form is not necessarily unique, and we find it was caused by the higher-order mixed multiple integral in using Stokes' formula in actual calculus variation.

In Lagrange mechanics, we know the Euler–Lagrange equation can be written as

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$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}-\frac{\partial L}{\partial q^i}=0. \tag{1.2}$$

Taking the Legendre transform of Lagrange density $L:p^i=\partial L/\partial \dot{q}^i$, we can rewrite Eq. (1.2) as regular Hamilton equation,

$$\begin{cases} \dfrac{dp^i}{dt}=-\dfrac{\partial H}{\partial q^i}, \\ \dfrac{dq^i}{dt}=\dfrac{\partial H}{\partial p^i}, \end{cases} \tag{1.3}$$

where $H=p^i\dot{q}^i-L(q^i,\dot{q}^i,t)$. With the covariant De Donder–Weyl Hamilton function theories[8] we can reformulate the partial differential equation to the following form:

$$\begin{cases} \dfrac{\partial H}{\partial \pi_i^\mu}=\partial_\mu q^i, \\ \dfrac{\partial H}{\partial q^i}=-\partial_\mu \pi_i^\mu, \end{cases} \tag{1.4}$$

where $\pi_i^\mu=\partial L/\partial\partial_\mu q^i$. According to this method, we can rewrite the KP equation to the multisymplectic form that was introduced by Bridges.[9]

Multisymplectic equations have the important multisymplectic conservation laws. In the numerical study, we also hope that the numerical approximations can preserve the multisymplectic conservation laws. Similar to the method,[10] we show that the Preissman scheme is a multisymplectic scheme for the KP equation. Though the Preissman scheme is multisymplectic, it needs more computational memory, so we reduce it to a multisymplectic 45 points scheme. Using the 45 points scheme, we get some numerical results on soliton and solitary waves over long time intervals.

In Sec. II, we describe the multisymplectic geometry of the KP equation entirely in the framework of the variational principal. Section III is devoted to the analysis of the multisymplectic Preissman scheme and reduce it to a multisymplectic 45 points scheme. In Sec. IV, some numerical results on soliton and solitary waves over long time intervals be given.

II. MULTISYMPLECTIC GEOMETRY OF THE KP EQUATION

We now review some aspects of multisymplectic geometry.

Let X be an orientable $(n+1)$-dimensional parameter space (which is usually space–time) and let $\pi_{XY}:Y\to X$ be a fiber over X. Section $\varphi:X\to Y$ of this covariant configuration bundle is the physical fields. Coordinates on X are denoted by x^μ, $\mu=1,2,\ldots,n,0$. In general, x^0 denotes the time coordinate. The parameter n denotes the number of spatial variables. In this paper, we just discuss the case of $n>0$. Adapted coordinates on Y are y^A along the fibers $Y_x=\pi_{XY}^{-1}(x), x\in X$, $A=1,2,\ldots,N$. N denotes the fiber's dimensions. Consider a kth order Lagrangian density L, viewed as a fiber-preserving map $L:J^kY\to\wedge^{n+1}X$. $J^k(Y)$ denotes the kth-order jet bundle over Y which can be induced by $J^1(\cdots(J^1(Y)))$. We let T_xX denote the tangent space of X at x, and denote the derivative of the map π_{XY} in the direction w by $T_{\pi_{XY}}\cdot w$.

At first, we introduce the first jet bundle.

Definition 2.1: The first jet bundle over Y is a fiber bundle denoted by $J^1(Y)$ whose fiber over $y\in Y_x=\pi_{XY}^{-1}(x)$, $x\in X$ consists of those linear mappings $\gamma:T_xX\to T_yY$ satisfying

$$T_{\pi_{XY}}\circ\gamma=\text{Identity}.$$

If $\varphi:X\to Y$ is a section of Y, $j^1(\varphi)$ is a section of $J^1(Y)$ and in coordinates, $j^1(\varphi)$ is given by

$$(x^\mu, \varphi^A(x^\mu), \partial_\mu \varphi^A(x^\mu)), \quad \mu = 1,2,\ldots,n,0.$$

Similarly, higher order jet bundle $J^m(Y)$ is defined by $J^1(J^{m-1}(Y))$.

Definition 2.2: The kth-order jet bundle over Y is a fiber bundle denoted by $J^k(Y)$ whose fiber over $\gamma \in J^{k-1}(Y)_y, y \in Y$ consists of those linear mappings $s: T_x X \to T_\gamma J^{k-1}(Y)$ satisfying

$$T_{\pi_{X, J^{k-1}Y}} \circ s = \text{Identity}.$$

We let $j^k(\varphi) = j^1(\cdots(j^1(\varphi))): x \to T_x j^{k-1}(\varphi)$ denote kth-order jet prolongation of the section $\varphi: X \to Y$, in which $j^{k-1}(\varphi)$ is a section of jet bundle $J^{k-1}(Y)$. Thus, $j^k(\varphi)$ is given in coordinates

$$(x^\mu, \varphi^A(x^\mu), \partial_\mu \varphi^A(x^\mu), \ldots, \partial_{\mu_n} \partial_{\mu_{n-1}} \cdots \partial_{\mu_0} \varphi^A(x^\mu)).$$

Given a kth-order Lagrangian density $L: J^k Y \to \wedge^{n+1} x$, the basis geometric object in the classical calculus of variations is the $(n+1)$-form θ_L on $J^{2k-1}(Y)$, which was called the Cartan form.

The KP equation can be written as

$$(2u_t + 6uu_x + u_{xxx})_x + \sigma u_{yy} = 0. \tag{2.1}$$

The 2 multiplying u_t is added for notational convenience, it can be eliminated by scaling t. In this paper, we consider the KPI equation.

To put the KP equation in the variational frame work, we let $\varphi_{xx} = u$, then φ satisfies equation,

$$2\varphi_{xxxt} + 6\varphi_{xx}\varphi_{xxxx} + 6\varphi_{xxx}^2 + \varphi_{xxxxxx} + \sigma \varphi_{xxyy} = 0. \tag{2.2}$$

The search for a variational principle is equivalent to the inverse problem of the calculus of variations, i.e., the existence and formulation of variational principles for systems of nonlinear partial differential equations. The existence of a variational principle for a differential equation is equivalent to determining whether or not an operator is a potential operator. According to Vainberg theorem,[11] in order that operator N be a potential operator, to summarize, it is necessary and sufficient that the Gateau derivative of the operator N is symmetry. The theorem is stated in terms of the Gateau derivative, but we assume that the Frechet derivative exists in application. Let N be an operator which defined in an appropriate function space E (typically E is Banach space), then N be a potential operator if $N'_u = \tilde{N}'_u$, where

$$N'_u \varphi = \lim_{\varepsilon \to 0} \frac{N(u + \varepsilon\varphi) - N(u)}{\varepsilon} = \left[\frac{\partial}{\partial \varepsilon} N(u + \varepsilon \varphi) \right] \Bigg|_{\varepsilon = 0},$$

and $\tilde{N}'_u$ is the adjoint operator of N'_u. If the operator is a potential operator, the potential F is given by

$$F = \int u \int_0^1 N(\lambda u) d\lambda dV,$$

where $\int dV$ represents integration over the physical domain and $\int_0^1 d\lambda$ represents integration over the scalar variable λ. We test the operator

$$N(\varphi) = 2\varphi_{xxxt} + 6\varphi_{xx}\varphi_{xxxx} + 6\varphi_{xxx}^2 + \varphi_{xxxxxx} + \sigma \varphi_{xxyy}$$

and find $N'_\varphi = \tilde{N}'_\varphi$. Hence,

$$F(\varphi)=\int \varphi\int_0^1 N(\lambda\varphi)d\lambda dV$$

$$=\int \varphi\int_0^1 [2\lambda\varphi_{xxxt}+6\lambda^2\varphi_{xx}\varphi_{xxxx}+6\lambda^2\varphi_{xxx}^2+\lambda\varphi_{xxxxxx}+\sigma\lambda\varphi_{xxyy}]d\lambda dV$$

$$=\int \varphi\left(\varphi_{xxxt}+2\varphi_{xxx}^2+2\varphi_{xx}\varphi_{xxxx}+\tfrac{1}{2}\varphi_{xxxxxx}+\frac{\sigma}{2}\varphi_{xxyy}\right)dV.$$

To obtain $F(u)$ in a more familiar form, integrate by part and discard the integration over the boundary since it has nothing with the Lagrangian density, then we get the potential

$$F(\varphi)=\int\left(\varphi_{xx}\varphi_{xt}-\tfrac{1}{2}\varphi_{xxx}^2+\frac{\sigma}{2}\varphi_{xy}^2+\varphi_{xx}^3\right)dV.$$

We can determine that the Lagrangian density for Eq. (2.2) is

$$L(j^3(\varphi))=\left(\varphi_{xx}\varphi_{xt}-\frac{1}{2}\varphi_{xxx}^2+\frac{\sigma}{2}\varphi_{xy}^2+\varphi_{xx}^3\right)dx\wedge dy\wedge dt.$$

Corresponding to Lagrangian density $L(j^3(\varphi))$, the action function is defined as the following:

$$S(\varphi)=\int_U L(j^3(\varphi)),\quad U \text{ is an open set of } X.$$

Let G be the Lie group of π_{XY} bundle automorphisms η_Y covering η_X. Denote η_Y^λ a smooth path in G such that

$$\overline{\varphi}=\eta_Y^\lambda\circ\varphi\circ(\eta_X^\lambda)^{-1}.$$

The vector field of η_Y^λ is

$$V=\left.\frac{d}{d\lambda}\right|_{\lambda=0}\overline{\varphi}=\begin{bmatrix}V^x\\V^y\\V^t\\V^\varphi\end{bmatrix}.$$

We say that φ is an extremum of S is

$$\left.\frac{d}{d\lambda}\right|_{\lambda=0}S(\overline{\varphi})=0.$$

Now we consider the variation

$$\left.\frac{d}{d\lambda}\right|_{\lambda=0}S(\overline{\varphi})=\left.\frac{d}{d\lambda}\right|_{\lambda=0}\int_{\eta_X^\lambda U}\left(\overline{\varphi_{xx}}\,\overline{\varphi_{xt}}-\frac{1}{2}\overline{\varphi}_{xxx}^2+\frac{\sigma}{2}\overline{\varphi}_{xy}^2+\overline{\varphi}_{xx}^3\right)d\overline{x}\wedge d\overline{y}\wedge d\overline{t},$$

where

$$\eta_X^\lambda\begin{bmatrix}x\\y\\t\end{bmatrix}=\begin{bmatrix}\overline{x}\\\overline{y}\\\overline{t}\end{bmatrix}.$$

A direct computation shows

$$\left.\frac{d}{d\lambda}\right|_{\lambda=0} S(\overline{\varphi}) = I_1 + I_2,$$

in which

$$I_1 = \int_U -(2\varphi_{xxxt} + 6\varphi_{xx}\varphi_{xxxx} + 6\varphi_{xxx}^2 + \varphi_{xxxxxx} + \sigma\varphi_{xxyy})(V^\varphi - \varphi_x V^x - \varphi_y V^y - \varphi_t V^t)dx\wedge dy\wedge dt, \tag{2.3}$$

$$\begin{aligned} I_2 = \int_{\partial U}\Bigg[&\left(\varphi_{xx}\varphi_{xt} - \frac{1}{2}\varphi_{xxx}^2 + \frac{\sigma}{2}\varphi_{xy}^2 + \varphi_{xx}^3\right)V^t + \varphi_{xx}(V_x^\varphi - \varphi_x V_x^x - \varphi_y V_x^y - \varphi_t V_x^t - \varphi_{xx}V^x - \varphi_{xy}V^y \\ &- \varphi_{xt}V^t)\Bigg]dx\wedge dy\Bigg[-\left(\varphi_{xx}\varphi_{xt} - \frac{1}{2}\varphi_{xxx}^2 + \frac{\sigma}{2}\varphi_{xy}^2 + \varphi_{xx}^3\right)V^y + \sigma\varphi_{xy}(V_x^\varphi - \varphi_x V_x^x - \varphi_y V_x^y - \varphi_t V_x^t \\ &- \varphi_{xx}V^x - \varphi_{xy}V^y - \varphi_{xt}V^t)\Bigg]dx\wedge dt + \Bigg[\left(\varphi_{xx}\varphi_{xt} - \frac{1}{2}\varphi_{xxx}^2 + \frac{\sigma}{2}\varphi_{xy}^2 + \varphi_{xx}^3\right)V^x + (\varphi_{xt} + 3\varphi_{xx}^2 \\ &+ \varphi_{xxxx})(V_x^\varphi - \varphi_x V_x^x - \varphi_y V_x^y - \varphi_t V_x^t - \varphi_{xx}V^x - \varphi_{xy}V^y - \varphi_{xt}V^t) - \varphi_{xxx}(V_{xx}^\varphi - \varphi_x V_{xx}^x - 2\varphi_{xx}V_x^x \\ &- \varphi_y V_{xx}^y - 2\varphi_{xy}V_x^y - \varphi_t V_{xx}^t - 2\varphi_{xt}V_x^t - \varphi_{xxy}V^y - \varphi_{xxt}V^t - \varphi_{xxx}V^x) + (-2\varphi_{xxt} - 6\varphi_{xx}\varphi_{xxx} \\ &- \sigma\varphi_{xyy} - \varphi_{xxxxx})(V^\varphi - \varphi_x V^x - \varphi_y V^y - \varphi_t V^t)\Bigg]dy\wedge dt. \end{aligned} \tag{2.4}$$

In Ref. 7, the author introduced the Lepagean equivalents which is a generalization of the Poincare–Cartan form and proposed the Carton form is not necessarily unique for higher order. The author also pointed out that every Lagrangian density has a Lepagean equivalent on $J^{2k-1}Y$. It turns out that Lepagean equivalents exists on jet bundles of order $2k-1$ or higher, but not necessarily on jet bundle of lower order. The author presented that: As being the principal part of a Lepagean equivalents, the Cartan form always exist and are typically nonunique unless $k=1$. We find it is caused by the higher-order mixed multiple integral in using Stokes' formula in actually calculus of variations. By I_2, we can define a Cartan form,

$$\begin{aligned} \theta_L = &\left(\frac{1}{2}\varphi_{xxx}^2 - \frac{\sigma}{2}\varphi_{xy}^2 + 2\varphi_x\varphi_{xxt} + 6\varphi_x\varphi_{xx}\varphi_{xxx} + \sigma\varphi_x\varphi_{xyy} + \varphi_x\varphi_{xxxxx} - \varphi_{xx}\varphi_{xt} - 2\varphi_{xx}^3 - \varphi_{xx}\varphi_{xxxx}\right)dx\wedge dy\wedge dt \\ &+ (-2\varphi_{xxt} - 6\varphi_{xx}\varphi_{xxx} - \sigma\varphi_{xyy} - \varphi_{xxxxx})d\varphi\wedge dy\wedge dt \\ &+ (\varphi_{xt} + 3\varphi_{xx}^2 + \varphi_{xxxx})d\varphi_x\wedge dy\wedge dt - \varphi_{xxx}d\varphi_{xx}\wedge dy\wedge dt - \sigma\varphi_{xy}d\varphi_x\wedge dx\wedge dt + \varphi_{xx}d\varphi_x\wedge dx\wedge dy. \end{aligned} \tag{2.5}$$

Since

$$j^5(\varphi)^*dx = dx, \quad j^5(\varphi)^*dy = dy, \quad j^5(\varphi)^*dt = dt,$$

$$j^5(\varphi)^*d\varphi = \varphi_x dx + \varphi_y dy + \varphi_t dt,$$

$$j^5(\varphi)^*d\varphi_x = \varphi_{xx}dx + \varphi_{xy}dy + \varphi_{xt}dt,$$

$$j^5(\varphi)^*d\varphi_{xx} = \varphi_{xxx}dx + \varphi_{xxy}dy + \varphi_{xxt}dt,$$

we have

$$I_2 = \int_{\partial U} j^5(\varphi)^*(j^5(V)\rfloor\theta_L).$$

Here $j^5(V)$ is the jet prolongation of the vector field V.[12] The multisymplectic form is the 4-form $\Omega_L=-d\theta_L$. Form θ_L defines a multisymplectic structure on jet bundle $J^5(Y)$.

Now, we consider the Euler–Lagrange equation for the action function $S(\varphi)$.

Since $L(j^3(\overline{\varphi}))=j^5(\overline{\varphi})^*\theta_L$, we have

$$\begin{aligned}\left.\frac{d}{d\lambda}\right|_{\lambda=0}\int_{\eta_X^\lambda U}L(j^3(\overline{\varphi}))&=\left.\frac{d}{d\lambda}\right|_{\lambda=0}\int_{\eta_X^\lambda U}j^5(\overline{\varphi})^*\theta_L\\&=\left.\frac{d}{d\lambda}\right|_{\lambda=0}\int_{\eta_X^\lambda U}j^5(\eta_Y^\lambda\circ\varphi\circ(\eta_X^\lambda)^{-1})^*\theta_L\\&=\left.\frac{d}{d\lambda}\right|_{\lambda=0}\int_{\eta_X^\lambda U}((\eta_X^\lambda)^{-1})^*j^5(\varphi)^*j^5(\eta_Y^\lambda)^*\theta_L\\&=\left.\frac{d}{d\lambda}\right|_{\lambda=0}\int_U j^5(\varphi)^*j^5(\eta_Y^\lambda)^*\theta_L=\int_U j^5(\varphi)^*\mathcal{L}_{j^5(V)}\theta_L\end{aligned}$$

in which the symbol $\mathcal{L}$ denotes the Lie derivative.

By the Cartan's Magic formula,[13]

$$\mathcal{L}_{j^5(V)}\theta_L=-j^5(V)\rfloor\Omega_L+d(j^5(V)\rfloor\theta_L).$$

We can obtain

$$\left.\frac{d}{d\lambda}\right|_{\lambda=0}S(\overline{\varphi})=-\int_U j^5(\varphi)^*(j^5(V)\rfloor\Omega_L)+\int_{\partial U}j^5(\varphi)^*(j^5(V)\rfloor\theta_L).$$

If V is a vector field with compact support, we have

$$\int_{\partial U}j^5(\varphi)^*(j^5(V)\rfloor\theta_L)=0.$$

Hence, a necessary condition for φ to be an extremum is that

$$\int_U j^5(\varphi)^*(j^5(V)\rfloor\Omega_L)=0$$

for any V with compact support. Compute the integral and obtain that

$$\begin{aligned}j^5(\varphi)^*(j^5(V)\rfloor\Omega_L)=&(2\varphi_{xxxt}+6\varphi_{xx}\varphi_{xxxx}+6\varphi_{xxx}^2+\varphi_{xxxxxx}+\sigma\varphi_{xxyy})\\&\times(V^\varphi-\varphi_xV^x-\varphi_yV^y-\varphi_tV^t).\end{aligned}\tag{2.6}$$

Remark: We can get the Euler–Lagrange equation from the vertical variation V^φ, and the V^x and V^y directions horizontal variations gives the law of conservation of momentum. The law of conservation of energy can be obtained along time-direction horizontal variation.

Taking the π_{XY}-vertical vector field V and using the standard method from the calculus of variations, we obtain that φ satisfies

$$2\varphi_{xxxt}+6\varphi_{xx}\varphi_{xxxx}+6\varphi_{xxx}^2+\varphi_{xxxxxx}+\sigma\varphi_{xxyy}=0,\tag{2.7}$$

i.e., Eq. (2.2). So, for any vector field V,

$$j^5(\varphi)^*(j^5(V)\rfloor\Omega_L)=0\tag{2.8}$$

holds. A short computation verifies that

$$j^5(\varphi)^*(P\rfloor\Omega_L)=0, \tag{2.9}$$

where $P\in TJ^5(Y)$ and is $T_{\pi_{Y,J^5(Y)}}$-vertical. For any $W\in TJ^5(Y)$, there exists the vector field V, such that

$$W=j^5(V)+P. \tag{2.10}$$

So, by (2.8)–(2.10), if φ is an extremum of S, $j^5(\varphi)^*(W\rfloor\Omega_L)$ mush vanish for any vector field $W\in TJ^5(Y)$, thus, we get the Euler–Lagrange equation,

$$j^5(\varphi)^*(W\rfloor\Omega_L)=0 \tag{2.11}$$

for any vector field $W\in TJ^5(Y)$. In the following part, we consider the multisymplectic form formula and a corollary of the multisymplectic form formula. About the multisymplectic form formula for first order field theories, please refer to Ref. 14.

Theorem 2.3: Let η_Y^λ and ξ_Y^λ demote two one-parameter symmetry groups of Eq. (2.11) and the corresponding vector fields are V and W. Then we have the multisymplectic form formula,

$$\int_{\partial U} j^5(\varphi)^*(j^5(V)\rfloor j^5(W)\rfloor\Omega_L)=0. \tag{2.12}$$

Proof: Since $j^5[W,V]=[j^5(W),j^5(V)]$, from (2.11) we have

$$\begin{aligned}0&=\int_U j^5(\varphi)^*(j^5[W,V]\rfloor\Omega_L)\\&=\int_U j^5(\varphi)^*([j^5(W),j^5(V)]\rfloor\Omega_L)\\&=\int_U j^5(\varphi)^*(\mathcal{L}_{j^5(W)}(j^5(V)\rfloor\Omega_L)-j^5(V)\rfloor\mathcal{L}_{j^5(W)}\Omega_L).\end{aligned} \tag{2.13}$$

Because η_Y^λ and ξ_Y^λ are two one-parameter symmetry groups of Eq. (2.11), so for any vector field $Q\in TJ^5(Y)$, we have

$$\left.\frac{d}{d\lambda}\right|_{\lambda=0} j^5(\eta_Y^\lambda\circ\varphi\circ(\eta_X^\lambda)^{-1})^*(Q\rfloor\Omega_L)=j^5(\varphi)^*\mathcal{L}_{j^5(V)}(Q\rfloor\Omega_L)=0, \tag{2.14}$$

$$\left.\frac{d}{d\lambda}\right|_{\lambda=0} j^5(\xi_Y^\lambda\circ\varphi\circ(\xi_X^\lambda)^{-1})^*(Q\rfloor\Omega_L)=j^5(\varphi)^*\mathcal{L}_{j^5(W)}(Q\rfloor\Omega_L)=0. \tag{2.15}$$

Thus (2.13) becomes

$$\begin{aligned}0&=-\int_U j^5(\varphi)^*(j^5(V)\rfloor\mathcal{L}_{j^5(W)}\Omega_L)\\&=-\int_U j^5(\varphi)^*(j^5(V)\rfloor d(j^5(W)\rfloor\Omega_L))\\&=\int_U j^5(\varphi)^*(j^5(V)\rfloor d(\mathcal{L}_{j^5(W)}\theta_L)).\end{aligned} \tag{2.16}$$

$j^5(V)\rfloor j^5(W)\rfloor\Omega_L$ can be written as

$$j^5(V)\rfloor j^5(W)\rfloor\Omega_L = j^5(V)\rfloor d(j^5(W)\rfloor\theta_L) - j^5(V)\rfloor\mathcal{L}_{j^5(W)}\theta_L$$
$$= \mathcal{L}_{j^5(V)}(j^5(W)\rfloor\theta_L) - j^5(V)\rfloor\mathcal{L}_{j^5(W)}\theta_L - d(j^5(V)\rfloor j^5(W)\rfloor\theta_L). \tag{2.17}$$

So from Stokes' formula we can obtain that

$$\int_{\partial U} j^5(\varphi)^*(j^5(V)\rfloor j^5(W)\rfloor\Omega_L) = \int_{\partial U} j^5(\varphi)^*(\mathcal{L}_{j^5(V)}(j^5(W)\rfloor\theta_L) - j^5(V)\rfloor\mathcal{L}_{j^5(W)}\theta_L - d(j^5(V)\rfloor j^5(W)\rfloor\theta_L))$$
$$= \int_U j^5(\varphi)^* d(\mathcal{L}_{j^5(V)}(j^5(W)\rfloor\theta_L) - j^5(V)\rfloor\mathcal{L}_{j^5(W)}\theta_L)$$
$$= \int_U j^5(\varphi)^*(\mathcal{L}_{j^5(V)}\mathcal{L}_{j^5(W)}\theta_L + \mathcal{L}_{j^5(V)}(j^5(W)\rfloor\Omega_L) - d(j^5(V)\rfloor\mathcal{L}_{j^5(W)}\theta_L)). \tag{2.18}$$

By

$$\mathcal{L}_{j^5(V)}\mathcal{L}_{j^5(W)}\theta_L = j^5(V)\rfloor d(\mathcal{L}_{j^5(W)}\theta_L) + d(j^5(V)\rfloor\mathcal{L}_{j^5(W)}\theta_L), \tag{2.19}$$

we have

$$\int_{\partial U} j^5(\varphi)^*(j^5(V)\rfloor j^5(W)\rfloor\Omega_L) = \int_U j^5(\varphi)^*(j^5(V)\rfloor d(\mathcal{L}_{j^5(W)}\theta_L) + \mathcal{L}_{j^5(V)}(j^5(W)\rfloor\Omega_L)). \tag{2.20}$$

Hence, by (2.14) and (2.16), we obtain

$$\int_{\partial U} j^5(\varphi)^*(j^5(V)\rfloor j^5(W)\rfloor\Omega_L) = 0.$$

Although the covariant Legendre transformation (or complete Legendre transformation) which transform time and space variable simultaneously are not necessarily unique, for this fixed Cartan form θ_L, we can construct corresponding covariant Lengendre transformation of Lagrangian density L. Let $v=\varphi_x$, $u=\varphi_{xx}$, $w=\varphi_{xy}$, $p=\varphi_{xt}$, taking the covariant Legendre transform of Lagrangian density L,

$$p^x = -2\varphi_{xxt} - 6\varphi_{xx}\varphi_{xxx} - \sigma\varphi_{xyy} - \varphi_{xxxxx},$$

$$p^{xx} = \varphi_{xt} + 3\varphi_{xx}^2 + \varphi_{xxxx}, \quad p^{xt} = \varphi_{xx},$$

$$p^{xy} = \sigma\varphi_{xy}, \quad p^{xxx} = -\varphi_{xxx}.$$

According to the covariant De Donder–Weyl Hamilton function theories[8] and the multisymplectic concept introduced by Bridges,[9] the KP equation can be reformulated as a system of ten first-order partial differential equations which can be written in the form,

$$M\mathbb{Z}_t + K\mathbb{Z}_x + L\mathbb{Z}_y = \nabla S(\mathbb{Z}),$$

$$\mathbb{Z} = (\varphi, v, u, w, p, p^x, p^{xx}, p^{xy}, p^{xt}, p^{xxx})^T \in \mathbb{R}^{10}, \tag{2.21}$$

where

$$M=\begin{pmatrix}
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&-1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0
\end{pmatrix},$$

$$K=\begin{pmatrix}
0&0&0&0&0&1&0&0&0&0\\
0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&1\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
-1&0&0&0&0&0&0&0&0&0\\
0&-1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&-1&0&0&0&0&0&0&0
\end{pmatrix},$$

$$L=\begin{pmatrix}
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&-1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0
\end{pmatrix},$$

$$S(\mathbb{Z})=up+\tfrac{1}{2}(p^{xxx})^2+\frac{\sigma}{2}w^2+u^3-p^xv-p^{xx}u-p^{xt}p-p^{xy}w.$$

∇S is the gradient of S with respect to the standard inner product on $\mathbb{R}^{10}$. The system (2.21) is a Hamiltonian formulation of the KP equation on a multisymplectic structure. Although this formulation is not the best, we give a constructive method to get multisymplectic form which was proposed by Bridges.[9] Attention should be paid to (2.21) that it is different from the multisymplectic form of the KP equation in Ref. 15. For Eq. (2.21), there is a conservation law,

$$\partial_t(d\mathbb{Z}\wedge Md\mathbb{Z})+\partial_x(d\mathbb{Z}\wedge Kd\mathbb{Z})+\partial_y(d\mathbb{Z}\wedge Ld\mathbb{Z})=0. \tag{2.22}$$

Substituting M, K, L into (2.22) leads to

$$\begin{aligned}&\frac{\partial}{\partial t}(d\varphi_x\wedge d\varphi_{xx})+\frac{\partial}{\partial x}(d\varphi\wedge(-6\varphi_{xxx}d\varphi_{xx}-6\varphi_{xx}d\varphi_{xxx}-\sigma d\varphi_{xyy}-2d\varphi_{xxt}-d\varphi_{xxxxx})\\&+d\varphi_x\wedge(6\varphi_{xx}d\varphi_{xx}+d\varphi_{xt}+d\varphi_{xxxx})+d\varphi_{xx}\wedge d(-\varphi_{xxx}))+\frac{\partial}{\partial y}(d\varphi_x\wedge d(\sigma\varphi_{xy}))=0.\end{aligned} \tag{2.23}$$

This multisymplectic conservation law (2.22) is consistent with our Theorem 2.3. We can regard the conservation law (2.23) as a corollary of the Theorem 2.3. Let V, W be π_{XY}-vertical and have the expressions $V^\varphi(\partial/\partial\varphi)$, $W^\varphi(\partial/\partial\varphi)$. Thus the corresponding $j^5(V)$ and $j^5(W)$ have the coordinate expressions

$$\begin{aligned}&(V^\varphi,V^\varphi_x,V^\varphi_y,V^\varphi_t,V^\varphi_{xx},V^\varphi_{yy},V^\varphi_{tt},V^\varphi_{xt},V^\varphi_{xy},V^\varphi_{yt},V^\varphi_{xxx},V^\varphi_{xtx},V^\varphi_{xxy},V^\varphi_{xtt},\\&V^\varphi_{xyy},V^\varphi_{ttt},V^\varphi_{yyy},V^\varphi_{tyy},V^\varphi_{tty},V^\varphi_{xxxx},V^\varphi_{xxyy},V^\varphi_{xxtt},V^\varphi_{xxxy},V^\varphi_{xxxt},V^\varphi_{xyyy},V^\varphi_{xttt},\\&V^\varphi_{tttt},V^\varphi_{yyyy},V^\varphi_{tyyy},V^\varphi_{ttyy},V^\varphi_{ttty},V^\varphi_{xxxxx},V^\varphi_{xxxxy},V^\varphi_{xxxxt},V^\varphi_{xxxyy},V^\varphi_{xxxtt},\\&V^\varphi_{xxyyy},V^\varphi_{xxttt},V^\varphi_{xyyyy},V^\varphi_{xtttt},V^\varphi_{yyyyy},V^\varphi_{ttttt},V^\varphi_{yyyyt},V^\varphi_{yyytt},V^\varphi_{yyttt},V^\varphi_{ytttt})\end{aligned}$$

and

$$\begin{aligned}&(W^\varphi,W^\varphi_x,W^\varphi_y,W^\varphi_t,W^\varphi_{xx},W^\varphi_{yy},W^\varphi_{tt},W^\varphi_{xt},W^\varphi_{xy},W^\varphi_{yt},W^\varphi_{xxx},W^\varphi_{xtx},W^\varphi_{xxy},W^\varphi_{xtt},\\&W^\varphi_{xyy},W^\varphi_{ttt},W^\varphi_{yyy},W^\varphi_{tyy},W^\varphi_{tty},W^\varphi_{xxxx},W^\varphi_{xxyy},W^\varphi_{xxtt},W^\varphi_{xxxy}W^\varphi_{xxxt},W^\varphi_{xyyy},W^\varphi_{xttt},\\&W^\varphi_{tttt},W^\varphi_{yyyy},W^\varphi_{tyyy},W^\varphi_{ttyy},W^\varphi_{ttty},W^\varphi_{xxxxx},W^\varphi_{xxxxy},W^\varphi_{xxxxt},W^\varphi_{xxxyy},W^\varphi_{xxxtt},W^\varphi_{xxyyy},\\&W^\varphi_{xxttt},W^\varphi_{xyyyy},W^\varphi_{xtttt},W^\varphi_{yyyyy},W^\varphi_{ttttt},W^\varphi_{yyyyt},W^\varphi_{yyytt},W^\varphi_{yyttt},W^\varphi_{ytttt}).\end{aligned}$$

We can compute

$$\begin{aligned}j^5(\varphi)^*(j^5(V)\rfloor j^5(W)\rfloor\Omega_L)=&(W^\varphi_{xx}V^\varphi_x-W^\varphi_xV^\varphi_{xx})dx\wedge dy+(\sigma W^\varphi_xV^\varphi_{xy}-\sigma W^\varphi_{xy}V^\varphi_x)dx\wedge dt\\&+[W^\varphi_{xx}V^\varphi_{xxx}-W^\varphi_{xxx}V^\varphi_{xx}-W^\varphi_x(V^\varphi_{xt}+6\varphi_{xx}V^\varphi_{xx}+V^\varphi_{xxxx})+V^\varphi_x(W^\varphi_{xt}+6\varphi_{xx}W^\varphi_{xx}+W^\varphi_{xxxx})\\&+V^\varphi(-2W^\varphi_{xxt}-6\varphi_{xx}W^\varphi_{xxx}-6\varphi_{xxx}W^\varphi_{xx}-\sigma W^\varphi_{xyy}-W^\varphi_{xxxxx})\\&+W^\varphi(2V^\varphi_{xxt}+6\varphi_{xx}V^\varphi_{xxx}+6\varphi_{xxx}V^\varphi_{xx}+\sigma V^\varphi_{xyy}+V^\varphi_{xxxxx})]dy\wedge dt.\end{aligned}$$

By the Stokes' formula, we can obtain

$$\begin{aligned}&\int_U\frac{\partial}{\partial t}(W^\varphi_{xx}V^\varphi_x-W^\varphi_xV^\varphi_{xx})dx\wedge dy\wedge dt-\frac{\partial}{\partial y}(\sigma W^\varphi_xV^\varphi_{xy}-\sigma W^\varphi_{xy}V^\varphi_x)dx\wedge dy\wedge dt+\frac{\partial}{\partial x}[W^\varphi_{xx}V^\varphi_{xxx}-W^\varphi_{xxx}V^\varphi_{xx}\\&-W^\varphi_x(V^\varphi_{xt}+6\varphi_{xx}V^\varphi_{xx}+V^\varphi_{xxxx})+V^\varphi_x(W^\varphi_{xt}+6\varphi_{xx}W^\varphi_{xx}+W^\varphi_{xxxx})+V^\varphi(-2W^\varphi_{xxt}-6\varphi_{xx}W^\varphi_{xxx}-6\varphi_{xxx}W^\varphi_{xx}\\&-\sigma W^\varphi_{xyy}-W^\varphi_{xxxxx})+W^\varphi(2V^\varphi_{xxt}+6\varphi_{xx}V^\varphi_{xxx}+6\varphi_{xxx}V^\varphi_{xx}+\sigma V^\varphi_{xyy}+V^\varphi_{xxxxx})]dx\wedge dy\wedge dt=0.\end{aligned}$$

Since U is arbitrary, we get

$$\begin{aligned}&\frac{\partial}{\partial t}(W^\varphi_{xx}V^\varphi_x-W^\varphi_xV^\varphi_{xx})-\frac{\partial}{\partial y}(\sigma W^\varphi_xV^\varphi_{xy}-\sigma W^\varphi_{xy}V^\varphi_x)+\frac{\partial}{\partial x}[W^\varphi_{xx}V^\varphi_{xxx}-W^\varphi_{xxx}V^\varphi_{xx}-W^\varphi_x(V^\varphi_{xt}+6\varphi_{xx}V^\varphi_{xx}+V^\varphi_{xxxx})\\&+V^\varphi_x(W^\varphi_{xt}+6\varphi_{xx}W^\varphi_{xx}+W^\varphi_{xxxx})+V^\varphi(-2W^\varphi_{xxt}-6\varphi_{xx}W^\varphi_{xxx}-6\varphi_{xxx}W^\varphi_{xx}-\sigma W^\varphi_{xyy}-W^\varphi_{xxxxx})\\&+W^\varphi(2V^\varphi_{xxt}+6\varphi_{xx}V^\varphi_{xxx}+6\varphi_{xxx}V^\varphi_{xx}+\sigma V^\varphi_{xyy}+V^\varphi_{xxxxx})]=0.\end{aligned} \tag{2.24}$$

If we let

$$M^t=\begin{pmatrix}0&0&0&0&0&0&0&0&0&0\\0&0&1&0&0&0&0&0&0&0\\0&-1&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\end{pmatrix},$$

$$M^x=\begin{pmatrix}0&0&-6\varphi_{xxx}&0&0&-6\varphi_{xx}&-\sigma&-2&0&-1\\0&0&6\varphi_{xx}&0&1&0&0&0&1&0\\6\varphi_{xxx}&-6\varphi_{xx}&0&0&0&-1&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&-1&0&0&0&0&0&0&0&0\\6\varphi_{xx}&0&1&0&0&0&0&0&0&0\\\sigma&0&0&0&0&0&0&0&0&0\\2&0&0&0&0&0&0&0&0&0\\0&-1&0&0&0&0&0&0&0&0\\1&0&0&0&0&0&0&0&0&0\end{pmatrix},$$

$$M^y=\begin{pmatrix}0&0&0&0&0&0&0&0&0&0\\0&0&0&\sigma&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&-\sigma&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0&0\end{pmatrix},$$

$$M^t(x,y)=x^TM^ty, M^x(x,y)=x^TM^xy, M^y(x,y)=x^TM^yy, \tag{2.25}$$

and set

$$j^5(V)=(V^\varphi,V^\varphi_x,V^\varphi_{xx},V^\varphi_{xy},V^\varphi_{xt},V^\varphi_{xxx},V^\varphi_{xyy},V^\varphi_{xxt},V^\varphi_{xxxx},V^\varphi_{xxxxx}),$$

$$j^5(W)=(W^\varphi,W^\varphi_x,W^\varphi_{xx},W^\varphi_{xy},W^\varphi_{xt},W^\varphi_{xxx},W^\varphi_{xyy},W^\varphi_{xxt},W^\varphi_{xxxx},W^\varphi_{xxxxx}),$$

the other coordinates vanish. Then conservation law (2.24) can be written as

$$\frac{\partial}{\partial t}M^t(j^5(V),j^5(W))+\frac{\partial}{\partial x}M^x(j^5(V),j^5(W))+\frac{\partial}{\partial y}M^y(j^5(V),j^5(W))=0. \tag{2.26}$$

Also, since the translation invariance of the KP equation, we choose $V=W=\varphi$ and take it into (2.26), and conservation law (2.26) becomes

$$\begin{aligned}&\frac{\partial}{\partial t}(d\varphi_x\wedge d\varphi_{xx})+\frac{\partial}{\partial x}(d\varphi\wedge(-6\varphi_{xxx}d\varphi_{xx}-6\varphi_{xx}d\varphi_{xxx}-\sigma d\varphi_{xyy}-2d\varphi_{xxt}-d\varphi_{xxxxx})\\&\quad+d\varphi_x\wedge(6\varphi_{xx}d\varphi_{xx}+d\varphi_{xt}+d\varphi_{xxxx})+d\varphi_{xx}\wedge d(-\varphi_{xxx}))+\frac{\partial}{\partial y}(d\varphi_x\wedge d(\sigma\varphi_{xy}))=0,\end{aligned} \tag{2.27}$$

i.e., the conservation law (2.23).

In the numerical study, the multisymplectic conservation law can be used to design multisymplectic numerical schemes, i.e., numerical schemes which can preserve the multisymplectic conservation law.

III. MULTISYMPLECTIC PREISSMAN SCHEME FOR THE KP EQUATION

In this section, we consider the multisymplectic Preissman scheme for the KP equation. Equation (2.21) can be reformulated as

$$\begin{cases}\dfrac{\partial p^x}{\partial x}=0,\\[2mm]\dfrac{\partial p^{xx}}{\partial x}+\dfrac{\partial p^{xy}}{\partial y}+\dfrac{\partial p^{xt}}{\partial t}=-p^x,\\[2mm]\dfrac{\partial p^{xxx}}{\partial x}=p+3u^2-p^{xx},\\[2mm]\sigma w-p^{xy}=0,\\[2mm]u-p^{xt}=0,\\[2mm]\dfrac{\partial \varphi}{\partial x}=v,\\[2mm]\dfrac{\partial v}{\partial x}=u,\\[2mm]\dfrac{\partial v}{\partial y}=w,\\[2mm]\dfrac{\partial v}{\partial t}=p,\\[2mm]\dfrac{\partial u}{\partial x}=p^{xxx}.\end{cases} \tag{3.1}$$

For convenience, we assume that the spacing of the grid points in the x,y,t directions is uniform, respectively. We apply the implicit midpoint discretization in time and in space to (3.1),

and obtain

$$
\begin{cases}
\dfrac{p^{x}_{i+1,j+(1/2),k+(1/2)}-p^{x}_{i,j+(1/2),k+(1/2)}}{\Delta x}=0,\\
\dfrac{p^{xx}_{i+1,j+(1/2),k+(1/2)}-p^{xx}_{i,j+(1/2),k+(1/2)}}{\Delta x}+\dfrac{p^{xy}_{i+(1/2),j+1,k+(1/2)}-p^{xy}_{i+(1/2),j,k+(1/2)}}{\Delta y}\\
\quad+\dfrac{p^{xt}_{i+(1/2),j+(1/2),k+1}-p^{xt}_{i+(1/2),j+(1/2),k}}{\Delta t}=-p^{x}_{i+(1/2),j+(1/2),k+(1/2)},\\
\dfrac{p^{xxx}_{i+1,j+(1/2),k+(1/2)}-p^{xxx}_{i,j+(1/2),k+(1/2)}}{\Delta x}=p_{i+(1/2),j+(1/2),k+(1/2)}+3(u_{i+(1/2),j+(1/2),k+(1/2)})^{2}\\
\qquad\qquad-p^{xx}_{i+(1/2),j+(1/2),k+(1/2)},\\
\sigma w_{i+(1/2),j+(1/2),k+(1/2)}=p^{xy}_{i+(1/2),j+(1/2),k+(1/2)},\\
u_{i+(1/2),j+(1/2),k+(1/2)}=p^{xt}_{i+(1/2),j+(1/2),k+(1/2)},\\
\dfrac{\varphi_{i+1,j+(1/2),k+(1/2)}-\varphi_{i,j+(1/2),k+(1/2)}}{\Delta x}=v_{i+(1/2),j+(1/2),k+(1/2)},\\
\dfrac{v_{i+1,j+(1/2),k+(1/2)}-v_{i,j+(1/2),k+(1/2)}}{\Delta x}=u_{i+(1/2),j+(1/2),k+(1/2)},\\
\dfrac{v_{i+(1/2),j+1,k+(1/2)}-v_{i+(1/2),j,k+(1/2)}}{\Delta y}=w_{i+(1/2),j+(1/2),k+(1/2)},\\
\dfrac{v_{i+(1/2),j+(1/2),k+1}-v_{i+(1/2),j+(1/2),k}}{\Delta t}=p_{i+(1/2),j+(1/2),k+(1/2)},\\
\dfrac{u_{i+1,j+(1/2),k+(1/2)}-u_{i,j+(1/2),k+(1/2)}}{\Delta x}=p^{xxx}_{i+(1/2),j+(1/2),k+(1/2)},
\end{cases}
\tag{3.2}
$$

where Δx is the x-direction step, Δy is the y-direction step, Δt is the time step, and $u_{i+(1/2),j+(1/2),k+(1/2)}=u(i\Delta x+(\Delta x/2),j\Delta y+(\Delta y/2),k\Delta t+(\Delta t/2)$, the others are similar.

In fact, the discretization result leads to the Preissman scheme,

$$
\begin{aligned}
&\frac{1}{\Delta}M(\mathbb{Z}_{i+(1/2),j+(1/2),k+1}-\mathbb{Z}_{i+(1/2),j+(1/2),k})+\frac{1}{\Delta x}K(\mathbb{Z}_{i+1,j+(1/2),k+(1/2)}-\mathbb{Z}_{i,j+(1/2),k+(1/2)})\\
&\quad+\frac{1}{\Delta y}L(\mathbb{Z}_{i+(1/2),j+1,k+(1/2)}-\mathbb{Z}_{i+(1/2),j,k+(1/2)})\\
&=\nabla S(\mathbb{Z}_{i+(1/2),j+(1/2),k+(1/2)}).
\end{aligned}
\tag{3.3}
$$

Equation (3.3) preserves the discrete multisymplectic conservation law,

$$
\begin{aligned}
&\frac{dv_{i+(1/2),j+(1/2),k+1}\wedge dp^{xt}_{i+(1/2),j+(1/2),k+1}-dv_{i+(1/2),j+(1/2),k}\wedge dp^{xt}_{i+(1/2),j+(1/2),k}}{\Delta t}\\
&+\frac{dv_{i+(1/2),j+1,k+(1/2)}\wedge dp^{xy}_{i+(1/2),j+1,k+(1/2)}-dv_{i+(1/2),j,k+(1/2)}\wedge dp^{xy}_{i+(1/2),j,k+(1/2)}}{\Delta y}\\
&+\frac{d\varphi_{i+1,j+(1/2),k+(1/2)}\wedge dp^{x}_{i+1,j+(1/2),k+(1/2)}-d\varphi_{i,j+(1/2),k+(1/2)}\wedge dp^{x}_{i,j+(1/2),k+(1/2)}}{\Delta x}
\end{aligned}
$$

$$+\frac{dv_{i+1,j+(1/2),k+(1/2)}\wedge dp^{xx}_{i+1,j+(1/2),k+(1/2)}-dv_{i,j+(1/2),k+(1/2)}\wedge dp^{xx}_{i,j+(1/2),k+(1/2)}}{\Delta x}$$

$$+\frac{du_{i+1,j+(1/2),k+(1/2)}\wedge dp^{xxx}_{i+1,j+(1/2),k+(1/2)}-du_{i,j+(1/2),k+(1/2)}\wedge dp^{xxx}_{i,j+(1/2),k+(1/2)}}{\Delta x}$$

$$=0. \tag{3.4}$$

Although the Preissman scheme (3.3) is multisymplectic, it took many efforts to realize. Hence we elimate the auxiliary variables $\varphi,v,w,p,p^x,p^{xx},p^{xy},p^{xt},p^{xxx}$ by a trivial computation and obtain the following multisymplectic 45 points scheme:

$$\frac{1}{2\Delta x\Delta t}\delta_y^2\Delta_t^0\{u^k_{i+2,j}+2u^k_{i+1,j}-2u^k_{i-1,j}+u^k_{i-2,j}\}+\frac{1}{\Delta x^4}\{\delta_y^2\delta_t^2(u^k_{i+2,j}-4u^k_{i+1,j}+6u^k_{i,j}-4u^k_{i-1,j}$$

$$+u^k_{i-2,j})\}+\frac{\sigma}{4\Delta y^2}\{\delta_t^2\Delta_y^2(u^k_{i+2,j}+4u^k_{i+1,j}+6u^k_{i,j}+4u^k_{i-1,j}+u^k_{i,j})\}$$

$$+\frac{2}{\Delta x^2}(\overline{\delta}f^{k+(1/2)}_{i,j+(1/2)}+\overline{\delta}f^{k+(1/2)}_{i,j-(1/2)}+\overline{\delta}f^{k-(1/2)}_{i,j+(1/2)}+\overline{\delta}f^{k-(1/2)}_{i,j-(1/2)})=0, \tag{3.5}$$

where we denote $u^k_{i,j}=u(i\Delta x,j\Delta y,k\Delta t)$, $f^k_{i,j}=3(u(i\Delta x,j\Delta y,k\Delta t))^2$ and

$$\begin{cases}\Delta_t^0u^k_{i,j}=u^{k+1}_{i,j}-u^{k-1}_{i,j},\ \delta_y^2u^k_{i,j}=u^k_{i,j+1}+2u^k_{i,j}+u^k_{i,j-1},\\ \delta_t^2u^k_{i,j}=u^{k+1}_{i,j}+2u^k_{i,j}+u^{k-1}_{i,j},\ \Delta_y^2u^k_{i,j}=u^k_{i,j+1}-2u^k_{i,j}+u^k_{i,j-1},\\ \overline{\delta}f^k_{i,j}=f^k_{i+(3/2),j}-f^k_{i+(1/2),j}-f^k_{i-(1/2),j}+f^k_{i-(3/2),j}.\end{cases} \tag{3.6}$$

IV. SOME NUMERICAL RESULTS ON SOLITON AND SOLITARY WAVES

In this section, we test the 45 points scheme on soliton and solitary waves over long time intervals.

At first, one line soliton of the KPI equation is considered. We choose the small interval in the y-direction just for computing convenience, and it has nothing to do with the scheme and result. We take the following initial conditions:

$$u(x,y,0)=2\ \mathrm{sech}^2\left(x-\frac{\sqrt{2}}{2}y-6\right) \tag{4.1}$$

and the exact boundary condition. The KPI equation has the theoretic solution,

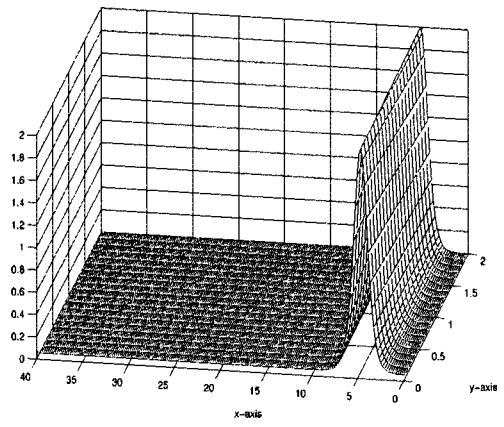

FIG. 1. One soliton at $t=0$.

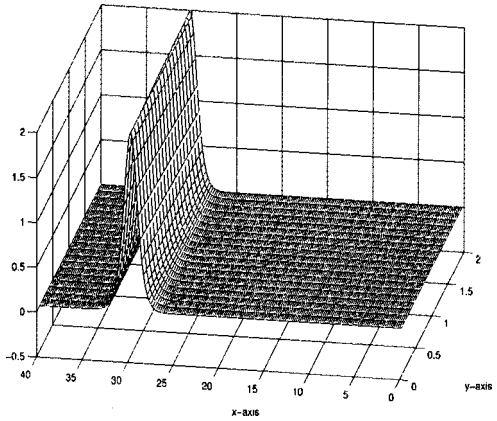

FIG. 2. One soliton at $t=10$.

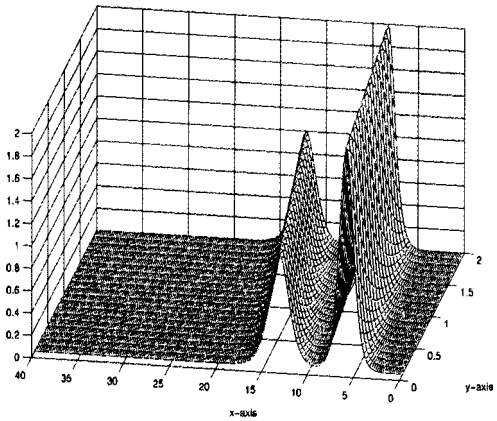

FIG. 3. Soliton interact at $t=0$.

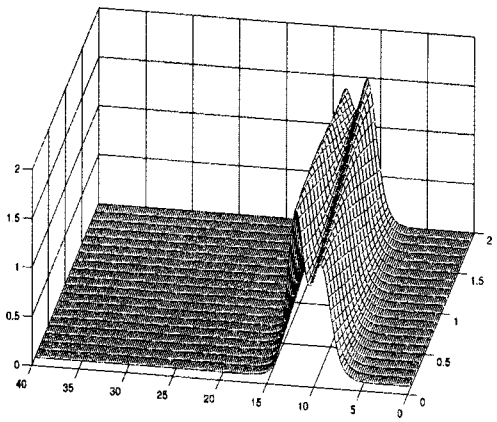

FIG. 4. Soliton interact at $t=1.5$.

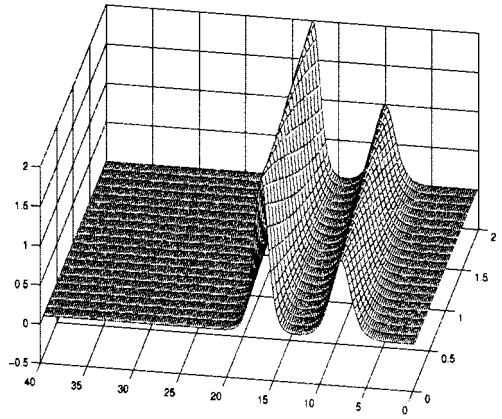

FIG. 5. Soliton interact at $t=3$.

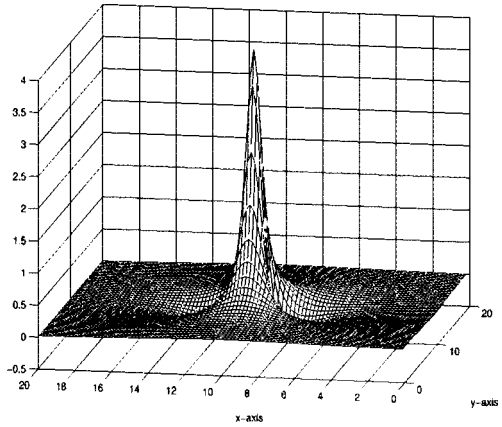

FIG. 6. Lump-type solitary wave at $t=0$.

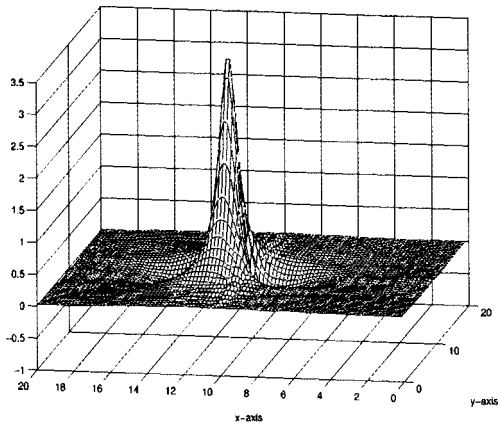

FIG. 7. Lump-type solitary wave at $t=0.5$.

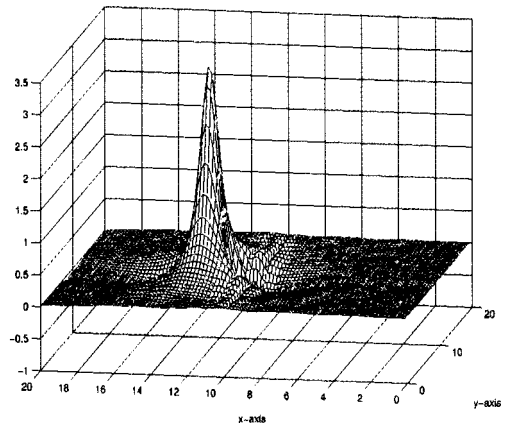

FIG. 8. Lump-type solitary wave at $t=1$.

$$u(x,y,t)=2\,\mathrm{sech}^2\left(x-\frac{\sqrt{2}}{2}y-\frac{5}{2}t-6\right),$$

which represents one line-soliton propagating with the velocity $\frac{5}{2}$ in the direction with the angle of $\tan^{-1}(\sqrt{2})$ to the positive x-axis. We take the test on the domain $[0,40]\times[0,2]$ and choose $\Delta x=0.2$, $\Delta y=0.1$, $\Delta t=0.01$. Figure 1 shows the initial condition and Fig. 2 shows the numerical solution at time $t=10$. In fact, it is the propagating 25-unit distant as we indicated.

Next we try the two line-soliton interaction.

We take the initial condition,

$$u(x,y,0)=2\sum_{i=1}^{2} k_i^2\,\mathrm{sech}^2[k_i(x+\lambda_i y-x_{0,i})], \tag{4.2}$$

where $k_1=1.0$, $k_2=1/\sqrt{2}$, $\lambda_1=-1/\sqrt{3}$, $\lambda_2=-1.0$, and $x_{0.1}=6.0$, $x_{0.2}=11.0$, and the exact boundary condition. The initial condition (4.2) corresponds to two line solitons, each with amplitude $2k_i^2$ placed initially at $x=x_{0,i}$ and moving with velocity $v_i=4k_i^2-3\lambda_i^2$ along the x-axis ($i=1,2$).

We carried out the computation on the domain $[0,40]\times[0,2]$, and choose $\Delta x=0.2$, $\Delta y=0.1$, $\Delta t=0.01$. The initial condition (4.2) is shown in Fig. 3. The larger line-soliton on the right will move with a velocity 3.0 to the positive x-direction and the smaller one on the left will move with a velocity 1.0 in the inverse direction. As time goes on, they will collide with each other, as is shown in Fig. 4. Figure 5 shows that the two line-solitons have separated completely after colliding and restored their original shape by the $t=3$.

We also consider the lump-type solitary waves of the KPI equation. The lump-type initial condition used for the test is

$$u(x,y,0)=4\,\frac{\left(-(x-x_0)^2+\mu^2(y-y_0)^2+\dfrac{1}{\mu^2}\right)}{\left((x-x_0)^2+\mu^2(y-y_0)^2+\dfrac{1}{\mu^2}\right)}, \tag{4.3}$$

where the parameters $\mu^2=1.0$, $x_0=10.0$, $y_0=10.0$, and we adopt the exact boundary condition.

We compute in a rectangle $[0,20]\times[0,20]$ and choose $\Delta x=0.1$, $\Delta y=0.2$, $\Delta t=0.01$. Figure 6 shows the initial condition and Fig. 7 shows the numerical solution at time $t=0.5$. By the time $t=1$, the result is shown in Fig. 8. The lump solution of the KPI equation can be expressed as

$$u(x,y,t)=4\frac{\left(-(x-x_0-3\mu^2t^2)^2+\mu^2(y-y_0)^2+\frac{1}{\mu^2}\right)}{\left((x-x_0-3\mu^2t^2)^2+\mu^2(y-y_0)^2+\frac{1}{\mu^2}\right)}. \tag{4.4}$$

According to (4.4), this lump type solitary wave will move to the positive x-direction with velocity $3\mu^2$. We can see the moving of the lump solitary wave from the graph.

A future task is expected to find a proper numerical boundary condition for collision of the two lump type solitary waves.

ACKNOWLEDGMENT

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(2+1)-dimensional (*M*+*N*)-component AKNS system: Painlevé integrability, infinitely many symmetries, similarity reductions and exact solutions

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The $(2+1)$-dimensional $(M+N)$-component AKNS system that is derived from the inner parameter dependent symmetry constraint of the KP equation is studied in detail. First, the Painlevé integrability of the model is proved by using the standard WTC and Kruskal approach. Using the formal series symmetry approach, the generalized KMV symmetry algebra and the related symmetry group are found. The two-dimensional similarity partial differential equation reductions and the ordinary differential equation reductions are obtained from the generalized KMV symmetry algebra and the direct method. Abundant localized coherent structures are revealed by the variable separation approach. Some special types of the localized excitations like the multiple solitoffs, dromions, lumps, ring solitons, breathers and instantons are plotted also. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In $(1+1)$-dimensions, the AKNS (Ablowitz–Kaup–Newell–Segur) system[1] is a most important physical model. The $(1+1)$-dimensional AKNS system had been extended in several different directions, say, the $(1+1)$-dimensional $(1+1)$-component AKNS system had been extended to the $(N+N)$-component $(1+1)$-dimensional AKNS system[2] and $(M+N)$-component $(1+1)$-dimensional AKNS system.[3] Several different types of $(2+1)$-dimensional integrable AKNS systems had also been obtained, say, the DS (Davey–Stewartson) type system[4] and the breaking soliton type system.[5] The $(1+1)$-dimensional AKNS system can be obtained from the usual symmetry constraint of the KP (Kadomtsev–Petviashvili) equation.[2] Recently, Lou and Hu had obtained a general $(N+M)$-component $(2+1)$-dimensional AKNS system,

$$ip_{it}+p_{ixx}+p_iu_x=0, \quad i=1,2,\ldots,N, \tag{1}$$

$$-iq_{jt}+q_{jxx}+q_ju_x=0, \quad j=1,2,\ldots,M, \tag{2}$$

$$u_y+\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}p_iq_j=0, \tag{3}$$

from the inner parameter dependent symmetry constraints of the KP equation.[3] When we take $y=x$, $N=M=1$, the system (1)–(3) is reduced to the usual $(1+1)$-dimensional AKNS system. If

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q is selected as the complex conjugate and $M=N=1$, then the system (1)–(3) can be considered as the asymmetric part of the DS system. The so-called long-wave–short-wave interaction model is linked with (1)–(3) by $N=M=1$ by

$$p(x,y,t)=L(x,y+it,it)\equiv L(x',y',t'), \quad q(x,y,t)=S(x,y+it,it)\equiv S(x',y',t').$$

The Maccari system[6] is just also a special case of (1)–(3) with $M=N=2$ and $\{q_1=p_1^*,\ q_2=p_2^*\}$.

One of the most powerful methods to prove the integrability of a model is the so-called Painlevé analysis due to WTC (Weiss–Tabor–Carnevale).[7] Furthermore, the Painlevé analysis can also be used to find some exact solutions no matter whether the model is integrable or not. If one only needs to prove the Painlevé property of a model, one may use the Kruskal simplification for the WTC approach.[8] If one hopes to find some more properties of the model, one has to use the original WTC approach or some extended forms.[9–11] In Sec. II of this article, we combine the standard WTC approach and the Kruskal simplification to study the Painlevé integrability of the model. In the symmetry study of the (2+1)-dimensional integrable models like the KP equation, Toda field theory, Davey–Stewartson (DS) equation, dispersive long wave equation, Nizhnik–Novikov–Veselov (NNV) equation, asymmetric DS (ADS) equation, asymmetric NNV (ANNV) equation, KdV-type and AKNS type breaking soliton equations and the Sawada–Kortera (SK) equation, there exist some types of generalized infinitely dimensional Kac–Moody–Virasoro (KMV) type symmetries with a common generalized centerless Virasoro symmetry subalgebra.[12] We had defined the Virasoro integrability if a model possesses an infinite dimensional centerless Virasoro symmetry algebra and a systematic method to construct the Virasoro integrable models was established.[13] Section III is devoted to investigating the Virasoro integrability by means of the formal series symmetry approach. The result shows us that the model possesses an infinite dimensional KMV symmetry algebra with two generalized centerless Virasoro symmetry subalgebra. Starting from the symmetries of a model one may obtain some exact solutions of the model in some different ways. In Sec. IV, we look for the finite transformation (symmetry group) of the related symmetry algebra. Using the finite transformation and any special simple solution, we may obtain a new generalized solution. In Sec. V, we use the general Lie point KMV symmetry algebra and the direct method to obtain the similarity solutions of the model. It is known that the famous inverse scattering transformation (IST) can be considered as an extension of the Fourier transformation in nonlinear physics. The variable separation approach (VSA) is another powerful method in linear physics. However, it is difficult to extend the VSA to nonlinear physics. Recently, two kinds of ''variable separation'' procedures were established. The first method is called the ''formal variable separation approach'' (FVSA),[14] or equivalently the symmetry constraints[2] or nonlinearization of the Lax pairs.[15] The independent variables of a reduced field in FVSA have not totally been separated though the reduced field satisfies some lower-dimensional equations. The second type of variable separation method was established first for the DS equation seven years ago[16] and the method was revisited and developed recently for the NNV equation,[17] ANNV equation,[18] DS equations,[17] ADS equation, dispersive long wave equation (DLWE) and a nonintegrable (2+1)-dimensional KdV equation.[19] In Sec. VI, we will study whether the variable separation approach can be applied to the $(N+M)$-component (2+1)-dimensional AKNS system. The positive result shows us that the (2+1)-dimensional $(N+M)$-component AKNS system possesses also abundant localized coherent structures for the quantity $\Sigma_{i=1,j=1}^{N,M} a_{ij}p_iq_j$. The abundant structures of the model are caused by the appropriate possible selections of the arbitrary functions appearing in the seed solution. Some special types of the localized excitations like the multiple solitoffs, dromions, lumps, ring solitons, breathers and instantons are studied also in this section. It is shown that the interaction between two traveling ring soliton solutions is completely elastic and a ring shape breather may ''breath'' in some different ways. The last section is a summary and discussion.

II. PAINLEVÉ INTEGRABILITY OF THE (2+1)-DIMENSIONAL (M+N) COMPONENT AKNS SYSTEM

According to the standard WTC approach, if the $(2+1)$-dimensional $(M+N)$-component AKNS system (1)–(3) is Painlevé integrable, all the possible solutions of the model can be written as

$$p_i=\sum_{k=0}^{\infty} p_{ik}f^{k+\alpha_i}, \quad i=1,2,\ldots,N, \tag{4}$$

$$q_j=\sum_{k=0}^{\infty} q_{jk}f^{k+\beta_j}, \quad j=1,2,\ldots,M, \tag{5}$$

$$u=\sum_{k=0}^{\infty} u_k f^{k+\gamma}, \tag{6}$$

with sufficient $(2M+2N)$ arbitrary functions among p_{ik}, q_{jk}, u_k in addition to f, where α_i, β_j and γ should all be the negative integers. In other words, all the solutions of the model are single valued about an arbitrary movable singularity manifold f.

To fix the constants α_i, β_j and γ, one may use the standard leading order analysis. By substituting $p_i\sim p_{i0}f^{\alpha_i}$, $q_j\sim q_{j0}f^{\beta_j}$ and $u\sim u_0 f^{\gamma}$ into (1)–(3) and comparing the leading terms for $f\sim 0$, we get the only possible branch with

$$\alpha_i=\beta_j=\gamma=-1, \tag{7}$$

$$u_0=2f_x, \quad \sum_{i=1}^{N}\sum_{j=1}^{M} a_{ij}q_{j0}p_{i0}=2f_xf_y. \tag{8}$$

Substituting (4)–(6) with (7) and (8) into (1)–(3) and vanishing all the coefficients of the powers f^k for different k, we can obtain the recursion relations to determine the functions u_k, p_{ik} and q_{jk}:

$$\begin{pmatrix} A & 0 & \cdots & 0 & 0 & \cdots & 0 & (k-1)f_xp_{10} \\ 0 & A & \cdots & 0 & 0 & \cdots & 0 & (k-1)f_xp_{20} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & A & 0 & \cdots & 0 & (k-1)f_xp_{N0} \\ 0 & 0 & \cdots & 0 & A & \cdots & 0 & (k-1)f_xq_{10} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & A & (k-1)f_xq_{M0} \\ B_1 & B_2 & \cdots & B_N & C_1 & \cdots & C_M & (k-1)f_y \end{pmatrix} \begin{pmatrix} p_{1k} \\ p_{2k} \\ \vdots \\ p_{Nk} \\ q_{1k} \\ \vdots \\ q_{Mk} \\ u_k \end{pmatrix} \equiv J\Psi = \begin{pmatrix} P_{1k} \\ P_{2k} \\ \vdots \\ P_{Nk} \\ Q_{1k} \\ \vdots \\ Q_{Mk} \\ U_k \end{pmatrix}, \tag{9}$$

where

$$A\equiv k(k-3)f_x^2,$$

$$B_i\equiv\sum_{j=1}^{M} a_{ij}q_{j0}, \quad (i=1,2,\ldots,N),$$

$$C_j\equiv\sum_{i=1}^{N} a_{ij}p_{i0}, \quad (j=1,2,\ldots,M), \tag{10}$$

$$P_{ik}=-i(p_{i(k-2)t}+(k-2)p_{i(k-1)}f_t)-p_{i(k-2)xx}-2(k-2)p_{i(k-1)x}f_x-(k-2)p_{i(k-1)}f_{xx}$$
$$-\sum_{m=0}^{k-1}u_{mx}p_{i(k-m-1)}-\sum_{m=0}^{k-1}(m-1)f_xu_mp_{i(k-m)}, \tag{11}$$

$$Q_{jk}=i(q_{j(k-2)t}+(k-2)q_{j(k-1)}f_t)-q_{j(k-2)xx}-2(k-2)q_{j(k-1)x}f_x-(k-2)q_{j(k-1)}f_{xx}$$
$$-\sum_{m=0}^{k-1}u_{mx}q_{j(k-m-1)}-\sum_{m=1}^{k-1}(m-1)f_xu_mq_{j(k-m)}, \tag{12}$$

$$U_k=-u_{(k-1)y}-\sum_{m=1}^{k-1}\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}p_{im}q_{j(k-m)} \tag{13}$$

with $p_{ik}=q_{jk}=u_k=0$ for $k<0$. From the matrix equation (9), it is easy to know that if the determinant

$$\Delta\equiv\det J=(k-1)(k(k-3)f_x^2)^{M+N-1}(k+1)(k-4)f_x^2f_y \tag{14}$$

of the coefficient matrix J is not equal to zero, the functions p_{ik}, q_{jk} and u_k can be obtained from (9) uniquely. When

$$k=-1,0,0,\ldots,0,1,3,3,\ldots,3,4, \tag{15}$$

the resonances occur. The resonance at $k=-1$ corresponds to the arbitrary singularity manifold f. If the model is Painlevé integrable, we require $(2N+2M)$ resonance conditions at $k=0$ ($M+N-1$ resonance conditions), $k=1$ (one resonance condition), $k=3$ ($M+N-1$ resonance conditions), and $k=4$ (one resonance condition) are satisfied identically such that other $2M+2N$ arbitrary functions among p_{ik}, q_{jk}, u_k can be introduced into the general series expansion (4)–(6). From the leading order analysis result (8), we know that the $M+N-1$ resonance conditions at $k=0$ are satisfied identically because only one condition exists among $M+N$ functions p_{i0} and q_{j0}. For $k=1$, we can obtain

$$p_{i1}=-\frac{ip_{i0}f_t+2p_{i0x}f_x+p_{i0}f_{xx}}{f_xu_0}, \tag{16}$$

$$q_{j1}=\frac{iq_{j0}f_t-2q_{j0x}f_x-q_{j0}f_{xx}}{f_xu_0}, \tag{17}$$

and the resonance condition

$$2u_{0y}f_x^2-\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}(2q_{j0x}f_x+q_{j0}f_{xx})p_{i0}-\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}(2p_{i0x}f_x+p_{i0}f_{xx})q_{j0}=0. \tag{18}$$

It is straightforward to see that the resonance condition (18) is satisfied identically because of (8). For $k=2$, (9) with (10)–(13) give us

$$p_{i2}=\frac{1}{12f_x^3f_y}\Bigg\{6f_xf_y(ip_{i0t}+p_{i0xx}+u_{0x}p_{i1}+u_{1x}p_{i0})-2p_{i0}f_x^2\Bigg(u_{1y}+\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}q_{m1}p_{n1}\Bigg)$$
$$-p_{i0}\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}[q_{m0}(ip_{n0t}+p_{n0xx}+u_{0x}p_{n1}+2u_{1x}p_{n0})-p_{n0}(iq_{m0t}-q_{m0xx}-u_{0x}q_{m1})]\Bigg\}, \tag{19}$$

$$q_{j2}=\frac{1}{12f_x^3f_y}\left\{6(u_{0x}q_{j1}-iq_{j0t}+u_{1x}q_{j0}+q_{j0xx})f_yf_x-2q_{j0}\left(u_{1y}+\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}q_{m1}p_{n1}\right)f_x^2\right.$$
$$\left.-\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}[(u_{0x}p_{n1}+ip_{n0t}+p_{n0xx}+2p_{n0}u_{1x})q_{m0}+(q_{m0xx}+u_{0x}q_{m1}-iq_{m0t})p_{n0}]q_{j0}\right\}, \tag{20}$$

$$u_2=\frac{1}{6f_x^2f_y}\left\{-2f_x^2u_{1y}-\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}(2u_{1x}p_{i0}+ip_{i0t}+p_{i0xx}+u_{0x}p_{i1})q_{j0}\right.$$
$$\left.+\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}[(-q_{j0xx}+iq_{j0t}-u_{0x}q_{j1})p_{i0}-2f_x^2q_{j1}p_{i1}]\right\}; \tag{21}$$

For $k=3$, the component form of (9) reads ($i=1,2,\ldots,N, j=1,2,\ldots,M$)

$$(2f_xu_3+u_{2x})p_{i0}+(f_{xx}+u_{0x}+if_t)p_{i2}+(u_{1x}+f_xu_2)p_{i1}+2p_{i2x}f_x+ip_{i1t}+p_{i1xx}=0, \tag{22}$$

$$(2f_xu_3+u_{2x})q_{j0}+(f_{xx}+u_{0x}-if_t)q_{j2}+(u_{1x}+f_xu_2)q_{j1}+2q_{j2x}f_x-iq_{j1t}+q_{j1xx}=0, \tag{23}$$

$$u_{2y}+2u_3f_y+\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}(q_{j2}p_{i1}+q_{j1}p_{i2}+q_{j3}p_{i0}+q_{j0}p_{i3})=0. \tag{24}$$

Now, to verify the remained resonance conditions at $k=3$ and $k=4$, one can use the Kruskal simplification

$$f=x+\psi(y,t),\quad p_{ik}=p_{ik}(y,t),\quad q_{jk}=q_{jk}(y,t),\quad u_k=u_k(y,t) \tag{25}$$

without loss of the generality to prove the Painlevé integrability, where $\psi(y,t)$ is an arbitrary function of $\{y,t\}$. Under the simplification (25), the known results are simplified to

$$u_0=2,\quad q_{j0}p_{i0}=2\psi_y,\quad p_{i1}=-\tfrac{1}{2}ip_{i0}\psi_t,\quad q_{j1}=\tfrac{1}{2}iq_{j0}\psi_t, \tag{26}$$

$$p_{i2}=\frac{1}{12\psi_y}\left[6i\psi_yp_{i0t}-2p_{i0}\left(u_{1y}+\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}q_{m1}p_{n1}\right)\right.$$
$$\left.+ip_{i0}\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}(p_{n0}q_{m0t}-q_{m0}p_{n0t})\right], \tag{27}$$

$$q_{j2}=\frac{1}{12\psi_y}i\left[2iq_{j0}\left(u_{1y}+\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}q_{m1}p_{n1}\right)\right.$$
$$\left.-6q_{j0t}\psi_y+\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}(q_{m0t}p_{n0}-p_{n0t}q_{m0})q_{j0}\right], \tag{28}$$

$$u_2=\frac{1}{6\psi_y}\left(\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}(iq_{m0t}p_{n0}-ip_{n0t}q_{m0})-2u_{1y}-2\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}q_{m1}p_{n1}\right). \tag{29}$$

Using (26)–(29), we can obtain

$$u_3=-\tfrac{1}{4}\psi_{tt} \tag{30}$$

from any one of (22) or (23) for fixed i or j while all the remaining equations of (22) and (23) become resonance conditions which are really satisfied identically because of (26)–(29) and (30). Under the simplification (25), Eq. (24) is simplified to

$$-2\psi_{tt}\psi_y-2\psi_{ty}\psi_t+4u_{2y}+4\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}(q_{j0}p_{i3}+4q_{j3}p_{i0})=0, \tag{31}$$

which is the only constraint condition among $M+N$ functions p_{i3} and q_{j3}. In other words, $M+N-1$ resonance conditions satisfy identically at $k=3$, and $N+M-1$ functions of p_{i3} and q_{j3} are arbitrary. For $k=4$, the resonance condition reads

$$u_{3y}+\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}\Big[q_{j3}p_{i1}+q_{j1}p_{i3}+q_{j2}p_{i2}+\frac{1}{4}(-u_2q_{j2}+iq_{j2t}+2iq_{j3}\psi_t-2u_3q_{j1})p_{i0}$$
$$+\frac{1}{4}(-u_2p_{i2}-ip_{i2t}-2ip_{i3}\psi_t-2u_3p_{i1})q_{j0}\Big]=0, \tag{32}$$

while p_{i4} and q_{j4} are expressed as

$$p_{i4}=-\tfrac{1}{4}(3u_4p_{i0}+ip_{i2t}+2ip_{i3}\psi_t+2u_3p_{i1}+u_2p_{i2}), \tag{33}$$

$$q_{j4}=\tfrac{1}{4}(iq_{j2t}-3u_4q_{j0}+2iq_{j3}\psi_t-2u_3q_{j1}-u_2q_{j2}) \tag{34}$$

for arbitrary u_4. After substituting (26)–(31) into (32), one can see that the resonance condition (32) is also satisfied identically. So the $(2+1)$-dimensional $(N+M)$-component AKNS system (1)–(3) is Painlevé integrable.

III. GENERALIZED KMV SYMMETRY ALGEBRA OF THE MODEL

In the symmetry study of the $(2+1)$-dimensional integrable models, we have found that there exists a quite universal symmetry algebra, the generalized centerless Virasoro type symmetry algebra (or named Witt algebra).[12] We had defined the Virasoro integrability if a model possesses the generalized centerless Virasoro type symmetry algebra and a system method was established to obtain the Virasoro integrable models.[13] In this section, we are interested in studying the symmetry structure of the $(2+1)$-dimensional AKNS system (1)–(3) at first and then investigating whether the $(2+1)$-dimensional AKNS system (1)–(3) is Virasoro integrable.

There are some different types of methods to find the symmetries of a model, say, the standard classical Lie approach,[20] direct Lie point symmetry ansatz[21] and the formal series symmetry approach.[12] In this article we use the formal series symmetry approach to find the symmetries of the $(2+1)$-dimensional AKNS system (1)–(3). A symmetry of the system (1)–(3) is defined as a solution of the linearized system of (1)–(3),

$$iP_{it}+P_{ixx}+P_iu_x+p_iU_x=0,\quad i=1,2,\ldots,N, \tag{35}$$

$$-iQ_{jt}+Q_{jxx}+Q_ju_x+q_jU_x=0,\quad j=1,2,\ldots,M, \tag{36}$$

$$U_y+\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}(P_iq_j+p_iQ_j)=0, \tag{37}$$

which means the system (1)–(3) is form invariant under the transformation

$$\{p_1,p_2,\ldots,q_N,q_1,q_2,\ldots,q_M,u\}\to\{p_1,p_2,\ldots,p_N,q_1,q_2,\ldots,q_M,u\}$$
$$+\epsilon\{P_1,P_2,\ldots,P_N,Q_1,Q_2,\ldots,Q_M,U\}, \tag{38}$$

where ϵ is an infinitesimal parameter. To solve the symmetry definition equations (35)–(37), we assume that $\{P_i, Q_j, U\}$ has the form

$$P_i = \sum_{k=0}^{\infty} f^{(-k)} P_i[k], \quad i = 1,2,\ldots,N, \tag{39}$$

$$Q_j = \sum_{k=0}^{\infty} f^{(-k)} Q_j[k], \quad j = 1,2,\ldots,M, \tag{40}$$

$$U = \sum_{k=0}^{\infty} f^{(-k)} U[k], \tag{41}$$

where $f \equiv f(t)$ is an arbitrary function of t, $f^{(k)} = d^k f/dt^k$, $f^{(-1)} = \int^t f \mathrm{d}t$ and the undetermined functions $P_i[k]$, $Q_j[k]$ and $U[k]$ should be determined later.

Substituting (39)–(41) into (35)–(37) and vanishing the coefficients of $f^{(-k)}$ for different k thanks to f being an arbitrary function, we can obtain the recursion relation for the functions $P_i[k]$, $Q_j[k]$ and $U[k]$:

$$P_i[k] = (-\partial_t + i\partial_x^2 + iu_x) P_i[k-1] + ip_i U_x[k-1], \quad i = 1,2,\ldots,N, \tag{42}$$

$$Q_j[k] = (-\partial_t - i\partial_x^2 - iu_x) Q_j[k-1] - iq_j U_x[k-1], \quad j = 1,2,\ldots,M, \tag{43}$$

$$U_y[k] = -\sum_{i=1}^{N} \sum_{j=1}^{M} a_{ij} (P_i[k] q_j + p_i Q_j[k]) \tag{44}$$

with

$$P_1[0] = P_2[0] = \cdots = P_N[0] = Q_1[0] = Q_2[0] = \cdots = Q_M[0] = 0, \quad U[0] = g(x,t), \tag{45}$$

and $g(x,t)$ being an arbitrary function of $\{x,t\}$. Usually the formal series symmetries (39)–(41) with (42)–(45) will not be truncated for the general $g(x,t)$. However, as in other cases (like the KP, DS and Toda equations[12,22]), if we select $g(x,t)$ as some polynomial functions of x, we may obtain some truncated symmetries. It is known that, for some types of $(2+1)$-dimensional integrable models (such as the KP and the Toda equations), one may obtain infinitely many truncated symmetries,[12] while for some other types of $(2+1)$-dimensional integrable models (like the DS and the SK equations), one can obtain only finite numbers of the truncated symmetries.[22] For the $(2+1)$-dimensional $(N+M)$-component AKNS system, we can obtain again only finite numbers of the truncated symmetries. Here are the final results obtained from the selections of the function $g(x,t)$:

$$\sigma_0 = f \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad \sigma_1 = if \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_N \\ -q_1 \\ -q_2 \\ \vdots \\ -q_M \\ 0 \end{pmatrix} + \dot{f} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ x \end{pmatrix}, \tag{46}$$

$$\sigma_2=-4f\begin{pmatrix} p_{1x}\\ p_{2x}\\ \vdots\\ p_{Nx}\\ q_{1x}\\ q_{2x}\\ \vdots\\ q_{Mx}\\ u_x\end{pmatrix}+2ix\dot{f}\begin{pmatrix} p_1\\ p_2\\ \vdots\\ p_N\\ -q_1\\ -q_2\\ \vdots\\ -q_M\\ 0\end{pmatrix}+\ddot{f}\begin{pmatrix} 0\\ 0\\ \vdots\\ 0\\ 0\\ 0\\ \vdots\\ 0\\ x^2\end{pmatrix}, \tag{47}$$

$$\sigma_3=-24f\begin{pmatrix} p_{1t}\\ p_{2t}\\ \vdots\\ p_{Nt}\\ q_{1t}\\ q_{2t}\\ \vdots\\ q_{Mt}\\ u_t\end{pmatrix}-6\dot{f}\begin{pmatrix} 2xp_{1x}+p_1\\ 2xp_{2x}+P_2\\ \vdots\\ 2xp_{Nx}+p_N\\ 2xq_{1x}+q_1\\ 2xq_{2x}+q_2\\ \vdots\\ 2xq_{Mx}+q_M\\ 2xu_x+2u\end{pmatrix}+3ix^2\ddot{f}\begin{pmatrix} p_1\\ p_2\\ \vdots\\ p_N\\ -q_1\\ -q_2\\ \vdots\\ -q_M\\ 0\end{pmatrix}+f^{(3)}\begin{pmatrix} 0\\ 0\\ \vdots\\ 0\\ 0\\ 0\\ \vdots\\ 0\\ x^2\end{pmatrix}. \tag{48}$$

Similarly, if we change the function $f\equiv f(t)$ in (39)–(41) as $h\equiv h(y)$, then we can obtain another set of formal series symmetry with two truncated ones:

$$\Sigma_0=-h\begin{pmatrix} p_1\\ p_2\\ \vdots\\ p_N\\ -q_1\\ -q_2\\ \vdots\\ -q_M\\ 0\end{pmatrix},\quad \Sigma_1=-h\begin{pmatrix} p_{1y}\\ p_{2y}\\ \vdots\\ p_{Ny}\\ q_{1y}\\ q_{2y}\\ \vdots\\ q_{My}\\ u_y\end{pmatrix}-\frac{1}{2}\dot{h}\begin{pmatrix} p_1\\ p_2\\ \vdots\\ p_N\\ q_1\\ q_2\\ \vdots\\ q_M\\ 0\end{pmatrix}. \tag{49}$$

All the truncated Lie point symmetries expressed by (46)–(49) can all be obtained by using other types of approaches like the methods described in Ref. 20 and/or in Ref. 21.

It is easy to prove that the symmetries (46)–(48) and (49) constitute the following closed symmetry algebra

$$\begin{aligned}[\sigma_0(f_1),\sigma_0(f_2)]&=[\sigma_0(f_1),\sigma_1(f_2)]=[\sigma_1(f_1),\sigma_1(f_2)]=[\Sigma_0(h_1),\Sigma_0(h_2)]=[\sigma_0(f),\Sigma_0(h)]\\ &=[\sigma_1(f),\Sigma_0(h)]=[\sigma_2(f),\Sigma_0(h)]=[\sigma_3(f),\Sigma_0(h)]=[\sigma_0(f),\Sigma_1(h)]\\ &=[\sigma_1(f),\Sigma_1(h)]=[\sigma_2(f),\Sigma_1(h)]=[\sigma_3(f),\Sigma_1(h)]=0,\end{aligned} \tag{50}$$

$$[\sigma_0(f_1),\sigma_3(f_2)]=12\sigma_0(f_2\dot{f}_1+f_1\dot{f}_2), \tag{51}$$

$$[\sigma_1(f_1),\sigma_2(f_2)]=4\sigma_0(f_2\dot{f}_1), \tag{52}$$

$$[\sigma_1(f_1),\sigma_3(f_2)]=24\sigma_1(f_2\dot{f}_1), \tag{53}$$

$$[\sigma_2(f_1),\sigma_2(f_2)]=8\sigma_1(f_2\dot{f}_1-f_1\dot{f}_2), \tag{54}$$

$$[\sigma_2(f_1),\sigma_3(f_2)]=12\sigma_2(2f_2\dot{f}_1-f_1\dot{f}_2), \tag{55}$$

$$[\sigma_3(f_1),\sigma_3(f_2)]=\sigma_3(f_2\dot{f}_1-f_1\dot{f}_2), \tag{56}$$

$$[\Sigma_1(h_1),\Sigma_0(h_2)]=\Sigma_0(h_1\dot{h}_2), \tag{57}$$

$$[\Sigma_1(h_1),\Sigma_1(h_2)]=\Sigma_1(\dot{h}_1h_2-\dot{h}_2h_1), \tag{58}$$

where the commutator $[A,B]$ $(A\equiv(A_1(p_i,q_j,u),A_2(p_i,q_j,u),\ldots,A_K(p_i,q_j,u))^T,\ K=N+M+1)$ is defined as

$$\begin{aligned}[A,B]=&\begin{pmatrix} A'_{1p_1} & A'_{1p_2} & \cdots & A'_{1p_N} & A'_{1q_1} & A'_{1q_2} & \cdots & A'_{1q_M} & A'_{1u}\\ A'_{2p_1} & A'_{2p_2} & \cdots & A'_{2p_N} & A'_{2q_1} & A'_{2q_2} & \cdots & A'_{2q_M} & A'_{2u}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ A'_{Kp_1} & A'_{Kp_2} & \cdots & A'_{Kp_N} & A'_{Kq_1} & A'_{Kq_2} & \cdots & A'_{Kq_M} & A'_{Ku}\end{pmatrix}\begin{pmatrix} B_1\\ B_2\\ \vdots\\ B_K\end{pmatrix}\\ &-\begin{pmatrix} B'_{1p_1} & B'_{1p_2} & \cdots & B'_{1p_N} & B'_{1q_1} & B'_{1q_2} & \cdots & B'_{1q_M} & B'_{1u}\\ B'_{2p_1} & B'_{2p_2} & \cdots & B'_{2p_N} & B'_{2q_1} & B'_{2q_2} & \cdots & B'_{2q_M} & B'_{2u}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ B'_{Kp_1} & B'_{Kp_2} & \cdots & B'_{Kp_N} & B'_{Kq_1} & B'_{Kq_2} & \cdots & B'_{Kq_M} & B'_{Ku}\end{pmatrix}\begin{pmatrix} A_1\\ A_2\\ \vdots\\ A_K\end{pmatrix}\end{aligned} \tag{59}$$

and the operators A'_{ig} and B'_{ig}, $(i=1,2,\ldots,K,g=p_i,q_j,u)$ are partial linearized operators, say

$$A'_{kp_i}h\equiv\lim_{\epsilon\to0}\frac{d}{d\epsilon}A_i(p_1,p_2,\ldots,p_k+\epsilon h,p_{k+1},\ldots,p_N,q_1,\ldots,q_M,u). \tag{60}$$

From the symmetry algebra (50)–(58), we see that $\sigma_0(f)$, $\sigma_1(f)$, $\sigma_2(f)$ constitute an infinite dimensional general loop algebra, $\Sigma_0(h)$ constitutes a commute algebra, and $\sigma_3(f)$ and $\Sigma_1(h)$ constitute two centerless generalized Virasoro algebra. So according to Ref. 13, the $(2+1)$-dimensional $(N+M)$-component AKNS system is Virasoro integrable.

IV. FINITE TRANSFORMATIONS

From the symmetry definition equation (38), we know that a symmetry transforms a known solution of the model to a new solution of the same model in infinitesimal form. In order to get some *exact* solutions from known ones, we should find the finite transformations from the obtained symmetries. In other words, we should find a symmetry group from the related symmetry algebra. Now starting from some special solutions and the finite transformations and using the general Lie point symmetries (46)–(49), we can find some interesting solutions. To get the general Lie symmetry group, we should solve the following ''initial'' problem:

$$\frac{\mathrm{d}t'}{\mathrm{d}\epsilon}=-24f_1(t'),\quad t'|_{\epsilon=0}=t, \tag{61}$$

$$\frac{\mathrm{d}y'}{\mathrm{d}\epsilon}=-g_1(y'),\quad y'|_{\epsilon=0}=y, \tag{62}$$

$$\frac{\mathrm{d}x'}{\mathrm{d}\epsilon}=-f_2(t')-12\frac{\mathrm{d}f_1(t')}{\mathrm{d}t'}x',\quad x'|_{\epsilon=0}=x, \tag{63}$$

$$\frac{\mathrm{d}p_i'}{\mathrm{d}\epsilon}=p_i'H(x',y',t'),\quad p'|_{i\epsilon=0}=p_i, \tag{64}$$

$$\frac{\mathrm{d}q_j'}{\mathrm{d}\epsilon}=q_j'R(x',y',t'),\quad q'|_{j\epsilon=0}=q_j, \tag{65}$$

$$\frac{\mathrm{d}u'}{\mathrm{d}\epsilon}=12u'\frac{\mathrm{d}f_1(t')}{\mathrm{d}t'}+S(x',t'),\quad u'|_{\epsilon=0}=u, \tag{66}$$

where $H(x',y',t')$, $R(x',y',t')$, $S(x',t')$ are defined as

$$H(x',y',t')=g_2(y')+\frac{1}{2}\frac{\mathrm{d}g_1(y')}{\mathrm{d}y'}-if_3(t')-3i\frac{\mathrm{d}^2f_1(t')}{\mathrm{d}t'^2}x'^2-2i\frac{\mathrm{d}f_2(t')}{\mathrm{d}t'}x'+6\frac{\mathrm{d}f_1(t')}{\mathrm{d}t'}, \tag{67}$$

$$R(x',y',t')=-H(x',y',t')+12\frac{\mathrm{d}f_1(t')}{\mathrm{d}t'}+\frac{\mathrm{d}g_1(y')}{\mathrm{d}y'}, \tag{68}$$

$$S(x',t')=-x'^3\frac{\mathrm{d}^3f_1(t')}{\mathrm{d}t'^3}-x'^2\frac{\mathrm{d}^2f_2(t')}{\mathrm{d}t'^2}-x'\frac{\mathrm{d}f_3(t')}{\mathrm{d}t'}-f_4(t'). \tag{69}$$

To solve the initial problem (61)–(66), some different situations should be considered:

(a) $f_1=g_1=0$.
(b) $f_1=0,g_1\neq 0$.
(c) $f_1\neq 0,g_1=0$.
(d) $f_1\neq 0,g_1\neq 0$.

In the first case ($f_1=g_1=0$), the general solution of (61)–(66) reads

$$t'=t,\quad y'=y,\quad x'=x-f_2(t)\epsilon, \tag{70}$$

$$p_i'(x',y',t')=[p_i(x,y',t')\exp(\epsilon H_1(\epsilon,x,y',t'))]|_{x=x'+f_2(t')\epsilon}, \tag{71}$$

$$q_j'(x',y',t')=q_j(x'+f_2(t')\epsilon,y',t')\exp(-\epsilon H_1(\epsilon,x'+f_2(t')\epsilon,y',t')), \tag{72}$$

$$u'(x',y',t')=u(x'+f_2(t')\epsilon,y',t')+S_1(\epsilon,x'+f_2(t')\epsilon,t')\epsilon, \tag{73}$$

where

$$\begin{aligned}H_1(\epsilon,x,y,t)\equiv{}&g_2(y)-4if_3(t)x^3-2if_{2t}(t)x+if_2(t)(6f_3(t)x^2+f_{2t}(t))\epsilon\\&-4if_3tf_2^2(t)\epsilon^2+if_3(t)f_2^3(t)\epsilon^3,\end{aligned} \tag{74}$$

$$S_1(\epsilon,x,t)\equiv-f_4(t)-xf_{3t}(t)-x^2f_{2tt}(t)+\tfrac{1}{2}f_2(t)(2xf_{2tt}(t)+f_2(t)f_{3t})\epsilon-\tfrac{1}{3}f_2^2(t)f_{2tt}(t)\epsilon^2. \tag{75}$$

In the second case ($f_1=0,g_1\neq 0$), the related symmetry group has the form

$$t'=t,\quad x'=x-f_2(t)\epsilon, \tag{76}$$

$$y'=G^{-1}(G(y)+\epsilon),\quad G(y)\equiv-\int^y\frac{1}{g_1(y_1)}\mathrm{d}y_1,\quad G^{-1}(G(y))=y, \tag{77}$$

$$p_i'(x',y',t') = [p_i(x,y,t')\exp(H_2(\epsilon,x,y,t'))]\Big|_{\substack{x=x'+f_2(t)\epsilon \\ y=G^{-1}(G(y')-\epsilon)}}, \tag{78}$$

$$q_j'(x',y',t') = \left[\frac{g_1(y)}{g_1(G^{-1}(G(y)+\epsilon))} q_j(x,y,t')\exp(-H_2(\epsilon,x,y,t'))\right]\Big|_{\substack{x=x'+f_2(t)\epsilon \\ y=G^{-1}(G(y')-\epsilon)}}, \tag{79}$$

$$u'(x',y',t') = (u(x,y,t') + S_1(\epsilon,x'+f_2(t)\epsilon,t')), \tag{80}$$

where

$$H_2(x,y,t) \equiv (H_1(\epsilon,x,y,t) - g_2(y))\epsilon + \int_y^{G^{-1}(G(y)+\epsilon)} \left(\frac{g_2(y_1)}{g_1(y_1)} + \frac{g_{1y_1}(y_1)}{g_1(y_1)}\right) \mathrm{d}y_1. \tag{81}$$

For the third case ($g_1 = 0$, $f_1 \neq 0$), the corresponding finite transformation becomes

$$y' = y, \quad t' = F^{-1}(F(t)+\epsilon), \quad F(t) \equiv -\frac{1}{24}\int^t \frac{1}{f_1(t_1)}\mathrm{d}t_1, \quad F^{-1}(F(t)) = t, \tag{82}$$

$$x' = \sqrt{\frac{f_1(t')}{f_1(t)}}x + \frac{\sqrt{f_1(t')}}{24}\int_t^{t'} \frac{f_2(t_1)}{f_1(t_1)^{3/2}}\mathrm{d}t_1 \equiv X_1(t',x,t), \tag{83}$$

$$p_i'(x',y',t') = \left\{ p_i(x,y,t)\exp\left(-\frac{1}{24}\int_t^{t'} \frac{H_3(t_1)}{f_1(t_1)}\mathrm{d}t_1\right)\right\}\Big|_{\substack{t=T(t') \\ y=y' \\ x=X(x',t')}}, \tag{84}$$

$$q_j'(x',y',t') = \left\{ q_j(x,y,t)\sqrt{\frac{f_1(T(t'))}{f_1(t')}}\exp\left(\frac{1}{24}\int_t^{t'} \frac{H_3(t_1)}{f_1(t_1)}\mathrm{d}t_1\right)\right\}\Big|_{\substack{t=T(t') \\ y=y' \\ x=X(x',t')}}, \tag{85}$$

$$u'(x',y',t') = \left\{ u(x,y,t)\frac{\sqrt{f_1(t)}}{\sqrt{f_1(t')}} - \frac{1}{24\sqrt{f_1(t')}}\int_t^{t'} \frac{S(t_1)}{\sqrt{f_1(t_1)}}\mathrm{d}t_1\right\}\Big|_{\substack{t=T(t') \\ y=y' \\ x=X(x',t')}}, \tag{86}$$

where

$$H_3(t_1) \equiv H(x',y',t')|_{t'=t_1,y'=y,x'=X_1(t_1,x,t)}, \tag{87}$$

$$S_3(t_1) \equiv S(x',t')|_{t'=t_1,x'=X_1(t_1,x,t)}, \tag{88}$$

$$T(t') \equiv F^{-1}(F(t')-\epsilon), \tag{89}$$

$$X(x',t') \equiv \sqrt{\frac{f_1(T(t'))}{f_1(t')}}x' - \frac{\sqrt{f_1(T(t'))}}{24}\int_{T(t')}^{t'} \frac{f_2(t_1)}{f_1(t_1)^{3/2}}\mathrm{d}t_1. \tag{90}$$

For the fourth situation, the general solution of (61)–(66) reads

$$t' = F^{-1}(F(t)+\epsilon), \quad F(t) \equiv -\frac{1}{24}\int^t \frac{1}{f_1(t_1)}\mathrm{d}t_1, \quad F^{-1}(F(t)) = t, \tag{91}$$

$$y'=G^{-1}(G(y)+\epsilon),\quad G(y)\equiv-\int^{y}\frac{1}{g_1(y_1)}\mathrm{d}y_1,\quad G^{-1}(G(y))=y, \tag{92}$$

$$x'=\sqrt{\frac{f_1(t')}{f_1(t)}}x+\frac{\sqrt{f_1(t')}}{24}\int_t^{t'}\frac{f_2(t_1)}{f_1(t_1)^{3/2}}\mathrm{d}t_1\equiv X_1(t',x,t), \tag{93}$$

$$p_i'(x',y',t')=\left\{p_i(x,y,t)\exp\left(-\frac{1}{24}\int_t^{t'}\frac{H_4(t_1)}{f_1(t_1)}\mathrm{d}t_1\right)\right\}\Bigg|_{\substack{t=T(t')\\ y=Y(y')\\ x=X(x',t')}}, \tag{94}$$

$$q_j'(x',y',t')=\left\{q_j(x,y,t)\sqrt{\frac{f_1(T(t'))}{f_1(t')}}\frac{g_1(y)}{g_1(y')}\exp\left(\frac{1}{24}\int_t^{t'}\frac{H_4(t_1)}{f_1(t_1)}\mathrm{d}t_1\right)\right\}\Bigg|_{\substack{t=T(t')\\ y=Y(y')\\ x=X(x',t')}}, \tag{95}$$

$$u'(x',y',t')=\left\{u(x,y,t)\frac{\sqrt{f_1(t)}}{\sqrt{f_1(t')}}-\frac{1}{24\sqrt{f_1(t')}}\int_t^{t'}\frac{S_3(t_1)}{\sqrt{f_1(t_1)}}\mathrm{d}t_1\right\}\Bigg|_{\substack{t=T(t')\\ y=Y(y')\\ x=X(x',t')}}, \tag{96}$$

where

$$H_4(t_1)\equiv H(x',y',t')\big|_{t'=t_1,y'=G^{-1}(G(y)+F(t_1)-F(t)),x'=X_1(t_1,x,t)}, \tag{97}$$

$$Y(y')=G^{-1}(G(y')-\epsilon). \tag{98}$$

From the above four situations, we know that if $\{p_i(x,y,t),\ q_j(x,y,t),\ u(x,y,t)\}$ is a solution of the system (1)–(3), then $\{p_i'(x',y',t'),\ q_j'(x',y',t'),\ u'(x',y',t')\}$ shown by (70)–(75), (76)–(80), (82)–(86) and (91)–(96) are all solutions of the same AKNS system (1)–(3) with the replacement $\{x,y,t,p_i,q_j,u\}\to\{x',y',t',p_i',q_j',u'\}$. Because of the entrance of the arbitrary functions $g_1(y),g_2(y),f_1(t),f_2(t),f_3(t),f_4(t)$, abundant localized structures of the (2 +1)-dimensional ($M+N$)-component AKNS system can be obtained from some simple solutions. To exhibit some interesting results explicitly, we discuss only the quantity pq of the simplest case for $M=N=1$, $p\equiv p_1$, $q\equiv q_1$. For the quantity pq, the corresponding finite transformations have the forms

$$p(x,y,t)q(x,y,t)\to p(x+f_2(t)\epsilon,y,t)q(x+f_2(t)\epsilon,y,t) \tag{99}$$

for the first case,

$$p(x,y,t)q(x,y,t)\to pq=\frac{g_1(Y(y))}{g_1(y)}p(x+\epsilon f_2(t),Y(y),t)q(x+\epsilon f_2(t),Y(y),t) \tag{100}$$

for the second case,

$$p(x,y,t)q(x,y,t)\to pq=\sqrt{\frac{f_1(T(t))}{f_1(t)}}p(X(x,t),Y(y),T(t))q(X(x,t),Y(y),T(t)) \tag{101}$$

for the third case and

$$p(x,y,t)q(x,y,t)\to pq=\sqrt{\frac{f_1(T(t))}{f_1(t)}}\frac{g_1(Y(y))}{g_1(y)}p(X(x,t),Y(y),T(t))q(X(x,t),Y(y),T(t)) \tag{102}$$

for the fourth case. In Eqs. (99)–(102), we have dropped out primes because the systems with and without primes are totally the same. Now let us write down some simple solutions of the $(2+1)$-dimensional AKNS system (1)–(3). It is straightforward to see that the system (1)–(3) possesses the n parallel (parallel to the line $x-y/c^2=0$ with constant c) bright soliton and/or n parallel (parallel to the line $x+y/c^2=0$) dark soliton solutions because the system will be reduced to the $(1+1)$-dimensional AKNS system(s):

$$ip_t+p_{\xi_\pm\xi_\pm}\mp c^2p^2q=0, \tag{103}$$

$$-iq_t+q_{\xi_\pm\xi_\pm}\mp c^2q^2p=0, \quad \xi_\pm=x\pm y/c^2. \tag{104}$$

The n dark soliton solutions of (103) and (104) with up sign and the n bright soliton solutions of (103) and (104) with lower sign are known in the literature. Now using the standard n bright soliton solutions of (103) and (104) located at

$$\xi_-=v_kt+x_{k0}, \quad k=1,2,\ldots,n, \tag{105}$$

and the transformation relation (99)–(102), we can obtain many $(2+1)$-dimensional localized structures. For instance, if we take

$$f_1(t)=\text{const.} \tag{106}$$

and $g_1(Y(y))/g_1(y)$ as m straight line (parallel to x axis) solitons, say,

$$\frac{g_1(Y(y))}{g_1(y)}=\sum_{j=1}^{m} Q_j(y-y_{0j}), \tag{107}$$

where $Q_j(y-y_{j0})$ is a straight line soliton located at $y=y_{j0}$, then pq expressed by (102) becomes a special type of $n\times m$ (or even more) dromion solution. All the dromions are located at the cross points and very closed points of the straight line solitons located at $y=y_{0j}$ and the curved line solitons located at

$$X-Y(y)/c^2=v_kt+x_{k0}, \quad k=1,2,\ldots,N, \tag{108}$$

with X and $Y(y)$ being given by (90) and (98), respectively. In high dimensions, the breather solutions may have also abundant structures. For instance, if we take the seed solution as the multi-breather solutions, then (102) with (106) and (107) becomes the breatherlike dromion solutions.

V. SIMILARITY REDUCTIONS

In this section, we try to find the solutions that are invariant under the symmetry group transformations. To find the group transformation invariant solutions of the $(2+1)$-dimensional $(M+N)$-component AKNS system, we should solve the following symmetry constraint equation,

$$\begin{pmatrix} -24f_1(t)p_{it}-(f_2(t)+12f_{1t}x)p_{ix}-g_1(y)p_{iy}+H(x,y,t) \\ -24f_1(t)q_{it}-(f_2(t)+12f_{1t}x)q_{ix}-g_1(y)q_{iy}+R(x,y,t) \\ -24f_1(t)u_t-(f_2(t)+12f_{1t}x)u_x-g_1(y)u_y+S(x,t) \end{pmatrix}=0, \tag{109}$$

at first, where $H(x,y,t)$, $R(x,y,t)$, $S(x,t)$ are given by (67)–(69). One can solve the symmetry constraint equation (109) by solving the characteristic equation

$$\frac{\mathrm{dt}}{-24f_1(t)}=\frac{\mathrm{dx}}{f_2(t)+12f_{1t}x}=\frac{\mathrm{dy}}{-g_1(y)}=\frac{\mathrm{dp_i}}{H(x,y,t)}=\frac{\mathrm{dq_j}}{R(x,y,t)}=\frac{\mathrm{du}}{S(x,t)}, \tag{110}$$

where $H(x,y,t)$, $R(x,y,t)$ and $S(x,t)$ are given by (67)–(69). It is easy to find that all the solutions of the characteristic Eq. (110) have the forms

$$p_i=\pi_i(\xi,\eta)\exp(\pi_0(x,y,t)),\quad \xi\equiv\xi(x,y,t),\quad \eta\equiv\eta(x,y,t), \tag{111}$$

$$q_j=\tau_j(\xi,\eta)\exp(\tau_0(x,y,t)), \tag{112}$$

$$u=\beta(x,y,t)u_1(\xi,\eta)+u_0(x,y,t). \tag{113}$$

The more general results but with the same forms as (111)–(113) can also be obtained by the CK (Clarkson and Kruskal) direct method[23] or the nonclassical Lie approach.[24] So, in the following, we list four general results directly with the forms (111)–(113) instead of solving the characteristic equation (110).

A. Case 1

The simplest case

$$\xi=y,\quad \eta=t,\quad \beta(x,y,t)=1, \tag{114}$$

$$u_0(x,y,t)=U_3(t)x^3+U_2(t)x^2+U_1(t)x, \tag{115}$$

$$\pi_0(x,y,t)=\tfrac{1}{2}(\tfrac{1}{2}\Gamma_1(y,t)-\tfrac{1}{2}\Omega_1(y,t))x^2+F_1(y,t)x, \tag{116}$$

$$\tau_0(x,y,t)=-\pi(x,y,t) \tag{117}$$

is related to the generalization of (110) with $f_1(t)=g_1(y)=0$. The reduction fields $\tau_j(y,t)$, $\pi_i(y,t)$ and $u_1(y,t)$ satisfy the following reduction equations

$$\Gamma_1(y,t)\pi_i(y,t)+i\pi_{it}(y,t)=0, \tag{118}$$

$$\Omega_1(y,t)\tau_j(y,t)-i\tau_{jt}(y,t)=0, \tag{119}$$

$$u_{1y}(y,t)+\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}\pi_i(y,t)\tau_j(y,t)=0, \tag{120}$$

where

$$\Omega_1(y,t)=2U_1(t)-\Gamma_1(y,t)+2F_1(y,t)^2, \tag{121}$$

while $F_1(y,t)$ and $\Gamma_1(y,t)$ are determined by

$$F_{1t}(y,t)=2i[\Gamma_1(y,t)F_1(y,t)-F_1(y,t)^3-F_1(y,t)U_1(t)+U_2(t)] \tag{122}$$

and

$$\begin{aligned}\Gamma_{1t}(y,t)=i[&6U_3(t)-2F_1(y,t)^4+4F_1(y,t)U_2(t)-iU_{1t}(t)+2\Gamma_1(y,t)^2\\&-4\Gamma_1(y,t)U_1(t)+2U_1(t)^2],\end{aligned} \tag{123}$$

and $U_1(t)$, $U_2(t)$ and $U_3(t)$ are arbitrary functions of t. When the functions $F_1(y,t)$ and $\Gamma_1(y,t)$ are fixed by (122) and (123), the general solution of the reduction equations (118)–(120) can be obtained by partial integrations:

$$\pi_i=A_i(y)\exp\left(-i\int\Gamma_1(y,t)dt\right), \tag{124}$$

$$\tau_j = B_j(y)\exp\left(i\int \Omega_1(y,t)dt\right), \tag{125}$$

$$u_1(y,t) = -\sum_{i=1}^{N}\sum_{j=1}^{M}\int a_{ij}A_iB_j\exp\left(i\int(\Omega_1(y,t)-\Gamma_1(y,t))dt\right)\mathrm{d}y, \tag{126}$$

with arbitrary functions $A_i(y)$, $i=1,2,\ldots,N$, and $B_j(y)$, $j=1,2,\ldots,M$.

B. Case 2

For the second case, we have

$$\xi = x - f_2(t)G_1(y), \quad \eta = t, \quad \beta(x,y,t)=0, \tag{127}$$

$$\pi_0(x,y,t) = \tfrac{1}{2}if_{2t}(t)G_1(y)x + A_1(y,t), \tag{128}$$

$$\tau_0(x,y,t) = -\tfrac{1}{2}if_{2t}(t)G_1(y)x - A_1(y,t) + A_2(y), \tag{129}$$

$$u_0(x,y,t) = \tfrac{1}{4}f_{2tt}(t)G_1(y)x^2 - iA_{1t}(y,t)x + \tfrac{1}{4}f_{2t}(t)^2G_1(y)^2x + A_0(y,t), \tag{130}$$

and the reduction fields $\tau_j(\xi,t)$, $\pi_i(\xi,t)$ and $u_1(\xi,t)$ satisfy the reduction equations:

$$\pi_{i\xi\xi}(\xi,t) + i\pi_{it}(\xi,t) + u_{1\xi}(\xi,t)\pi_i(\xi,t) = 0, \tag{131}$$

$$\tau_{j\xi\xi}(\xi,t) - i\tau_{jt}(\xi,t) + u_{1\xi}(\xi,t)\tau_j(\xi,t) = 0, \tag{132}$$

$$-u_{1\xi}(\xi,t)f_2(t) + \tfrac{1}{4}f_{2tt}(t)\xi^2 + H_1(t)\xi + H_0(t) + \sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}\pi_i(\xi,t)\tau_j(\xi,t) = 0, \tag{133}$$

where

$$A_0(y,t) = \tfrac{1}{12}f_{2tt}(t)f_2(t)^2G_1(y)^3 - \tfrac{1}{2}H_1(t)f_2(t)G_1(y)^2 + H_0(t)G_1(y) + H_2(t), \tag{134}$$

$$A_{1yt}(y,t) = \tfrac{1}{2}iG_{1y}(y)(-f_{2tt}(t))f_2(t)G_1(y) - f_{2t}(t)^2G_1(y) + 2H_1(t), \tag{135}$$

$$A_2(y) = \ln(G_{1y}(y)), \tag{136}$$

and $H_0(t)$, $H_1(t)$, $H_2(t)$ and $f_2(t)$ are arbitrary functions of t and $G_1(y)$ is an arbitrary function of y.

The reduction system (131)–(133) is equivalent to the $(1+1)$-dimensional $(M+N)$-component AKNS system

$$R_{iXX}(X,T) + iR_{iT}(X,T) + R_i(X,T)\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}R_n(X,T)S_m(X,T) = 0, \tag{137}$$

$$S_{jXX}(X,T) - iS_{jT}(X,T) + S_j(X,T)\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}R_n(X,T)S_m(X,T) = 0, \tag{138}$$

with

$$\pi_i(\xi,t) = R_i(X,T)\exp\left(-i\frac{h_{1t}(t)}{2h_1(t)}\xi^2 - i\frac{h_{2t}(t)}{h_1(t)}\xi + ih_3(t)\right), \tag{139}$$

$$\tau_j(\xi,t)=f_2(t)S_j(X,T)\exp\left(i\frac{h_{1t}(t)}{2h_1(t)}\xi^2+i\frac{h_{2t}(t)}{h_1(t)}\xi-ih_3(t)\right), \tag{140}$$

$$u_1(\xi,t)=\frac{1}{12f_2(t)}[f_{2tt}(t)\xi^3+6H_1(t)\xi^2+12H_0(t)\xi+12f_2(t)^2U(X,T)],$$

and $\{X,\ T,\ h_1,\ h_2,\ h_3\}$ being determined by

$$X=f_2(t)\xi+2\int^t h_{2t}(t)h_1(t)\mathrm{dt},\quad T(t)=\int^t f_2(t)^2\mathrm{dt}, \tag{141}$$

$$h_1(t)^2=f_2(t),\quad h_2(t)=-\int^t f(t')^{-3/2}\int^{t'}H_1(t_1)\mathrm{dt}_1\mathrm{dt}', \tag{142}$$

$$h_3(t)=\int^t\frac{1}{2\,f_2(t')^2}\left[if_2(t')f_{2t'}(t')+2\,f_2(t')H_0(t')-2\left(\int^{t'}H_1(t_1)\mathrm{dt}_1\right)^2\right]\mathrm{dt}'. \tag{143}$$

Actually, the second situation shown by (131)–(133) or equivalently by (137)–(138) is the generalization of that obtained by the classical Lie point symmetry approach of (110) for $f_1(t)=0$, $g_1(y)\neq 0$.

C. Case 3

The third case possesses the solution

$$\xi=F_2(t)x+F_3(t),\quad \eta=y,\quad \beta(x,y,t)=1, \tag{144}$$

$$\pi_0(x,y,t)=-\frac{iF_{2t}(t)}{4F_2(t)}x^2+\frac{iF_{3t}(t)}{2F_2(t)}x+F_1(t)+i\int H_1(y)\mathrm{dy}\int F_2(t)^2\mathrm{dt}, \tag{145}$$

$$\tau_0(x,y,t)=-\pi_0(x,y,t)+\ln(F_2(t)), \tag{146}$$

$$\begin{aligned}u_0(x,y,t)=&\left(-\frac{F_{2tt}(t)}{12F_2(t)}+\frac{1}{6}\frac{F_{2t}(t)^2}{F_2(t)^2}\right)x^3+\left(\frac{1}{4}\frac{F_{3tt}(t)}{F_2(t)}-\frac{1}{2}\frac{F_{3t}(t)F_{2t}(t)}{F_2(t)^2}\right)x^2\\&+\left(\frac{iF_{2t}(t)}{2F_2(t)}+\frac{1}{4}\frac{F_{3t}(t)^2}{F_2(t)^2}-iF_{1t}(t)+F_2(t)^2\int H_1(y)\mathrm{dy}\right)x\\&+F_2(t)\int H_0(y)\mathrm{dy}-F_2(t)F_3(t)\int H_1(y)\mathrm{dy}+F_0(t),\end{aligned} \tag{147}$$

and the reduction fields $\tau_j(\xi,y)$, $\pi_i(\xi,y)$ and $u_1(\xi,y)$ satisfy the reduction equations:

$$\pi_{i\xi\xi}(\xi,y)+u_{1\xi}(\xi,y)\pi_i(\xi,y)=0, \tag{148}$$

$$\tau_{j\xi\xi}(\xi,y)+u_{1\xi}(\xi,y)\tau_j(\xi,y)=0, \tag{149}$$

$$u_{1y}(\xi,y)+H_1(y)\xi+H_0(y)+\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}\pi_i(\xi,y)\tau_j(\xi,y)=0, \tag{150}$$

and $F_1(t)$, $F_2(t)$ $F_3(t)$, $F_0(t)$, $H_0(y)$ and $H_1(y)$ are all arbitrary functions of the indicated variables. The third case is the generalization of the solution of (110) with $f_1(t)\neq 0, g_1(y)=0$.

D. Case 4

The fourth case is related to the generalized case of (110) with $f_1(t)\neq 0, g_1(y)\neq 0$. In this case, the general solution has the form

$$\xi = F_2(t)x + F_3(t), \quad \eta = F_1(t) + G_1(y), \tag{151}$$

$$\beta(x,y,t) = F_2(t) = \sqrt{F_{1t}}, \tag{152}$$

$$\pi_0(x,y,t) = -\frac{1}{4F_2(t)}(iF_{2t}(t)x^2 + 2iF_{3t}(t)x - 2g_0(y,t)), \tag{153}$$

$$\tau_0(x,y,t) = \frac{1}{4F_2(t)}(iF_{2t}(t)x^2 + 2iF_{3t}(t)x - 2g_0(y,t) + 4F_2(t)[\ln(G_{1y}(y)\theta_1^{-1}) + \ln(F_2(t))]), \tag{154}$$

$$u_0(x,y,t) = \frac{1}{12F_2(t)^2}((2F_{2t}(t)^2 - F_2(t)F_{2tt}(t))x^3 - (3F_2(t)F_{3tt}(t) - 6F_{3t}(t)F_{2t}(t))x^2 + (-6iF_2(t)g_{0t}(y,t) + 6iF_{2t}(t)(g_0(y,t) + F_2(t)) + 3F_{3t}(t)^2)x + g_1(y,t)F_2(t)^2), \tag{155}$$

and the reduction fields $\tau_j(\xi,\eta)$, $\pi_i(\xi,\eta)$ and $u_1(\xi,\eta)$ satisfy the reduction equations:

$$\pi_{i\xi\xi}(\xi,\eta) + u_{1\xi}(\xi,\eta)\pi_i(\xi,\eta) + i\pi_{i\eta}(\xi,\eta) = 0, \tag{156}$$

$$\tau_{j\xi\xi}(\xi,\eta) + u_{1\xi}(\xi,\eta)\tau_j(\xi,\eta) - i\tau_{j\eta}(\xi,\eta) = 0, \tag{157}$$

$$u_{1\eta}(\xi,\eta)\theta_1 + \theta_{21}(\eta)\xi + \theta_{22}(\eta) + \sum_{i=1}^{N}\sum_{j=1}^{M} a_{ij}\pi_i(\xi,\eta)\tau_j(\xi,\eta) = 0, \tag{158}$$

where

$$g_1(y,t) \equiv g_1(\eta,t) = 12F_2(t)\theta_1^{-1}\int(\theta_{21}(\eta)F_3(t) + \theta_{22}(\eta))\mathrm{d}\eta + F_6(t), \tag{159}$$

$$g_0(y,t) \equiv g_0(\eta,t) = F_4(t) + F_5(\eta)F_2(t) + 2iF_2(t)\theta_1^{-1}\int\int F_2(t)^2\theta_{21}(\eta)\mathrm{d}t\mathrm{d}\eta, \tag{160}$$

while θ_1 is an arbitrary constant and $G_1(y)$, $\theta_{21}(\eta)$, $\theta_{22}(\eta)$, $F_5(\eta)$, $F_1(t)$, $F_3(t)$, $F_4(t)$ and $F_6(t)$ are all arbitrary functions of the indicated arguments.

VI. ORDINARY DIFFERENTIAL EQUATION (ODE) REDUCTIONS

To find the ODE reductions, one may directly study the ODE reductions of the original system (1)–(3) by using the CK direct method as for the KP equation.[25] However, in this section, we treat the problem alternatively. Actually, we have obtained the $(1+1)$-dimensional partial differential equation (PDE) reductions of the system (1)–(3) in the last section. If we reduce these $(1+1)$-dimensional equations further to ODEs, then the ODE reductions of the original system (1)–(3) are found at the same time thanks to the results of the last section.

Because the first type of reduction equation system (118)–(120) had been solved out and the third reduction system (148)–(150) can be considered as a special case of the fourth type of reduction system (156)–(158), we only list the ODE reductions for the $(1+1)$-dimensional systems (137) and (138) and (156)–(158).

A. ODE reductions of (137) and (138)

For the (1+1)-dimensional (M+N)-component AKNS system (137) and (138), using the standard classical and nonclassical Lie group approach and/or the direct method, we can find two types of similarity ODE reductions.

The first type of ODE reduction of the system (137) and (138) reads

$$R_i(X,T)=(T+t_0)^c\exp\left(\frac{i(X+x_0)^2}{4(T+t_0)}-\frac{ic_0(X+x_0)}{\sqrt{T+t_0}}-ic_1\sqrt{T+t_0}\right)r_i(Z), \tag{161}$$

$$S_j(X,T)=(T+t_0)^{-c-1}\exp\left(-\frac{i(X+x_0)^2}{4(T+t_0)}+\frac{ic_0(X+x_0)}{\sqrt{T+t_0}}+ic_1\sqrt{T+t_0}\right)s_j(Z), \tag{162}$$

$$i(Z-4c_0)r_{iZ}+2r_{iZZ}+(i+2ic-2c_0^2+c_0Z)r_i+2r_i\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}r_ns_m=0, \tag{163}$$

$$-i(Z-4c_0)s_{jZ}+2s_{jZZ}+(i+2ic-2c_0^2+c_0Z)s_j+2s_j\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}r_ns_m=0, \tag{164}$$

with

$$Z=\frac{(X+x_0)}{\sqrt{T+t_0}}+\frac{c_1\sqrt{T+t_0}}{c_0} \tag{165}$$

and c, c_0, x_0, t_0 and c_1 being arbitrary constants.

For the second type of ODE reduction, we have

$$R_i(X,T)=\exp\left(\frac{iX^2+4ic_1X}{4(T+t_0)}\right)r_i(T), \tag{166}$$

$$S_j(X,T)=\exp\left(-\frac{iX^2+4ic_1X}{4(T+t_0)}\right)s_j(T), \tag{167}$$

$$ir_{iT}+\left(\frac{c_1^2}{T^2}-\frac{i}{2T}\right)r_i+r_i\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}r_ns_m=0, \tag{168}$$

$$-is_{jT}+\left(\frac{c_1^2}{T^2}+\frac{i}{2T}\right)s_j+s_j\sum_{n=1}^{N}\sum_{m=1}^{M}a_{nm}r_ns_m=0, \tag{169}$$

where c_1 and t_0 are arbitrary constants.

B. ODE reductions of (156)–(158)

For the (1+1)-dimensional system (156)–(158), we can find three types of ODE reductions. The first type of ODE reduction of (156)–(158) reads

$$\pi_i(\xi,\eta)=f_0r_i(Z),\quad Z=\xi+x_0, \tag{170}$$

$$\tau_j(\xi,\eta)=(i\theta_1f_0f_{0\eta\eta}-i\theta_2f_{0\eta}^2-f_0^2\theta_{21}(\eta))\frac{s_j(Z)}{f_0^3a_1}, \tag{171}$$

$$u=u_1(Z)-i\frac{f_{0\eta}}{f_0}\xi+u_0(\eta), \tag{172}$$

$$r_{iZZ}+r_iu_{1Z}=0, \tag{173}$$

$$s_{jZZ}+s_ju_{1z}+iA_1s_j=0, \tag{174}$$

$$a_1Z+a_0+\sum_{n=1}^{N}\sum_{m=1}^{M}a_{ij}r_is_j=0, \tag{175}$$

where a_0, a_1 and A_1 are arbitrary constants and f_0 and u_0 are determined by

$$f_{0\eta\eta\eta}=-A_1\left(f_{0tt}-\frac{f_{0\eta}^2}{f_0}+\frac{if_0\theta_{21}}{\theta_1}\right)-i\frac{f_0\theta_{21\eta}}{\theta_1}+3\frac{f_{0\eta}f_{0\eta\eta}}{f_0}-2\frac{f_{0\eta}^3}{f_0^2} \tag{176}$$

and

$$u_{0\eta}=i(a_0+a_1\xi_0)\left(\frac{f_{0\eta}^2}{a_1f_0^2}-\frac{f_{0\eta\eta}}{a_1f_0}-\frac{i\theta_{21}}{a_1\theta_1}\right)-\frac{\theta_{22}}{\theta_1}. \tag{177}$$

For the second type of similarity reduction of the system (156)–(158), we have

$$\pi_i(\xi,\eta)=e^{-c_2(\eta)\xi^2-c_3(\eta)\xi}r_i(\eta),\quad \tau_j(\xi,\ \eta)=e^{c_2(\eta)\xi^2+c_3(\eta)\xi}s_j(\eta), \tag{178}$$

$$u=\tfrac{1}{3}(ic_{2\eta}-4c_2^2)\xi^3+\tfrac{1}{2}(ic_{3\eta}-4c_2c_3)\xi^2-(2c_2+c_3^2)\xi+u_0(\eta)+\xi u_1(\eta), \tag{179}$$

$$ir_{i\eta}-(4c_2-u_1)r_i=0, \tag{180}$$

$$is_{j\eta}-u_1s_j=0, \tag{181}$$

$$\theta_1u_{0\eta}+\theta_{22}+\sum_{n=1}^{N}\sum_{m=1}^{M}a_{ij}r_is_j=0, \tag{182}$$

where the functions c_2, c_3 and u_1 are given by

$$c_2=-i\frac{c_1}{4}\tanh(c_1(\eta-\eta_0)),\quad c_3=c_5\tanh(c_1(\eta-\eta_0))+c_4\,\mathrm{sech}(c_1(\eta-\eta_0)) \tag{183}$$

and

$$u_{1\eta}=c_1\,\mathrm{sech}(c_1(\eta-\eta_0))\left(2c_4c_5(2\,\mathrm{sech}^2(c_1(\eta-\eta_0))-1)-\frac{i}{2}c_1\,\mathrm{sech}(c_1(\eta-\eta_0))\right)$$

$$+2c_1(c_5^2-c_4^2)\tanh(c_1(\eta-\eta_0))\mathrm{sech}^2(c_1(\eta-\eta_0))-\frac{\theta_{21}}{\theta_1}, \tag{184}$$

and c_1, c_4, c_5 and η_0 are arbitrary constants.

The third type of ODE reduction of the system (156)–(158) has the special form

$$\pi_i=f_0\exp\left(-\frac{i}{4z_1}z_{1\eta}\xi(\xi-2\xi_0)\right)r_i(Z), \tag{185}$$

$$\tau_j=\frac{z_{1\eta}}{f_0A_2}\exp\left(\frac{i}{4z_1}z_{1\eta}\xi(\xi-2\xi_0)\right)s_j(Z), \tag{186}$$

$$u=u_0-\frac{\xi^2(\xi+3\xi_0)}{12z_1^2}(z_1z_{1\eta\eta}-2z_{1\eta}^2)-\left(\frac{if_{0\eta}}{f_0}-\frac{iz_{1\eta}}{2z_1}-\frac{\xi_0^2z_{1\eta}^2}{4z_1^2}\right)\xi, \tag{187}$$

$$Z=z_1(\xi+\xi_0)+Z_0, \tag{188}$$

$$z_1\equiv z_1(\eta)=\sqrt{\frac{c_1}{\exp(c_1(\eta-\eta_0))-A_1}}, \tag{189}$$

$$r_{iZZ}+r_iu_{1Z}=0, \tag{190}$$

$$s_{jZZ}+s_ju_{1Z}+iA_1s_j=0, \tag{191}$$

$$4A_2\theta_1(Z_0-Z)u_{1Z}-4\theta_1A_2u_1-4a_0A_2-4a_1A_2Z-\theta_1Z_0A_2A_1Z^2-4\sum_{n=1}^{N}\sum_{m=1}^{M}a_{ij}r_is_j=0, \tag{192}$$

where the functions $u_0\equiv u_0(\eta)$ and $f_0\equiv f_0(\eta)$ are determined by

$$u_{0\eta}=\frac{z_{1\eta}}{12\theta_1}[-A_1\theta_1(z_1\xi_0-2Z_0)(z_1\xi_0+Z_0)^2+12(a_0+a_1Z_0+a_1z_1\xi_0)]-\frac{\theta_{22}}{\theta_1} \tag{193}$$

and

$$f_{0\eta\eta}=\frac{if_0z_1z_{1\eta}}{4}\left(\frac{4a_1}{\theta_1}+2iA_1+A_1Z_0^2-A_1\xi_0^2z_1^2\right)+\frac{f_{0\eta}^2}{f_0}+\frac{1}{2}iA_1\xi_0^2f_0z_{1\eta}^2-\frac{\theta_{21}f_0}{\theta_1}, \tag{194}$$

while A_1, A_2, a_0, a_1, c_1, η_0, ξ_0 and Z_0 are all arbitrary constants.

VII. EXACT SOLUTIONS OF THE *M+N* COMPONENT AKNS SYSTEM OBTAINED FROM VARIABLE SEPARATION APPROACH

It is well known that the Painlevé analysis can also be used to obtain other interesting properties.[7] For instance, substituting the truncated form of the Painlevé expansion in the original system will lead to its multi-linear form. For the $(M+N)$-component AKNS system (1)–(3), substituting the truncated Painlevé expansion

$$p_i=\frac{P_i}{f}+p_{i0},\quad q_j=\frac{Q_j}{f}+q_{j0},\quad u=\frac{2f_x}{f}+u_0 \tag{195}$$

into the model yields the following bilinear form:

$$(iD_t+D_x^2+u_{0x})P_i\cdot f+p_{i0}D_x^2f\cdot f=0, \tag{196}$$

$$(-iD_t+D_x^2+u_{0x})Q_j\cdot f+q_{j0}D_x^2f\cdot f=0, \tag{197}$$

$$D_xD_yf\cdot f+\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}(P_iQ_j+p_{i0}fQ_j+q_{j0}fP_i)=0, \tag{198}$$

where D_t, D_x and D_y are the standard Hirota's bilinear operator and $\{p_{i0},q_{j0},u_0\}$ is an arbitrary seed solution of the system (1)–(3).

If we select the seed solution as

$$p_{i0}=q_{j0}=0, \quad u_0=u_0(x,t), \tag{199}$$

where $u_0=u_0(x,t)$ is an arbitrary function of x and t, then the bilinear system (196)–(198) can be solved by using the variable separation ansatz

$$f=a_1F(x,t)+a_2G(y,t)+a_3F(x,t)G(y,t), \tag{200}$$

$$P_i=F_{1i}(x,t)G_{1i}(y,t)\exp(iR_{1i}(x,t)+iS_{1i}(y,t)), \tag{201}$$

$$Q_j=F_{2j}(x,t)G_{2j}(y,t)\exp(-iR_{2j}(x,t)-iS_{2j}(y,t)), \tag{202}$$

where the space variables x and y have been totally separated into the functions $\{F,F_{1i},F_{2j},R_{1i},R_{2j}\}$ and $\{G,G_{1i},G_{2j},S_{1i},S_{2j}\}$, respectively.

Substituting the ansatz into (196)–(198) and using the fact that the space variables x and y have been separated into different functions $\{F,F_{1i},F_{2j},R_{1i},R_{2j}\}$ and $\{G,G_{1i},G_{2j},S_{1i},S_{2j}\}$, we can find that

$$G_{1i}=\frac{b_{1i}}{a_{1i}(t)}\sqrt{G_y}, \quad G_{2j}=\frac{b_{2j}}{a_{2j}(t)}\sqrt{G_y}, \tag{203}$$

$$F_{1i}=a_{1i}(t)\sqrt{F_x}, \quad F_{2j}=a_{2j}(t)\sqrt{F_x}, \tag{204}$$

$$S_{1i}=B(t)+s_{1i}(y), \quad S_{2j}=B(t)+s_{2j}(y), \tag{205}$$

$$R_{1ix}=R_{2jx}\equiv R_x=-\frac{1}{2a_1a_2F_x}(a_2^2\alpha_0(t)+a_1a_2F_t+a_2\alpha_2(t)F+\alpha_1F^2), \tag{206}$$

$$G_t=\frac{G^2}{a_1^2}(a_3^3\alpha_0(t)-a_3\alpha_2(t)+\alpha_1(t))+\frac{G}{a_1}(2a_3\alpha_0(t)-\alpha_2(t))+\alpha_0(t), \tag{207}$$

$$\begin{aligned} u_{0x}=&\frac{1}{4a_1^2a_2^2F_x^2}(a_1^2a_2^2F_t^2+2a_1a_2(a_2\alpha_0(t)+a_2\alpha_2(t)F+\alpha_1(t)F^2)F_t\\ &+a_2^2a_1^2(F_{xx}^2-2F_xF_{xxx}+4F_x^2(B_t(t)+R_t))+a_2^2\alpha_2(t)^2F^2\\ &+2a_2\alpha_2(t)F(a_2^2\alpha_0(t)+F^2\alpha_1(t))+(a_2^2\alpha_0(t)+F^2\alpha_1(t))^2), \end{aligned} \tag{208}$$

where b_{1i} and b_{2j} are arbitrary constants and $F(x,t)$,$a_{1i}(t)$, $a_{2j}(t)$, $s_{1i}(y)$, $s_{2j}(y)$, $B(t)$, $\alpha_0(t)$, $\alpha_1(t)$, $\alpha_2(t)$ are all arbitrary functions of the indicated variables with the condition

$$\sum_{i=1}^{N}\sum_{j=1}^{M}a_{ij}b_{1i}b_{2j}\exp(i(s_{1i}(y)-s_{2j}(y)))=2a_1a_2. \tag{209}$$

Hence, for the quantity $v\equiv\Sigma_{i=1}^{N}\Sigma_{j=1}^{M}a_{ij}p_iq_j$, we have

$$v=\frac{2a_1a_2F_xG_y}{(a_1F+a_2G+a_3FG)^2} \tag{210}$$

with F being an arbitrary function of x and t and $G=G(y,t)$ being an arbitrary solution of the Riccati equation (207). It is interesting that the expression (210) is valid for many $(2+1)$-dimensional models like the DS equation, NNV system, ANNV equation and ADS model and the dispersive long wave equation, etc.[4,17–19] Because of the arbitrariness of the functions F

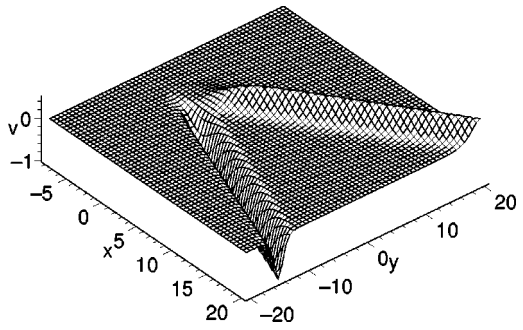


FIG. 1. A special two-solitoff solution for the quantity v shown by (210) with (211) and (212) at time $t=0$.

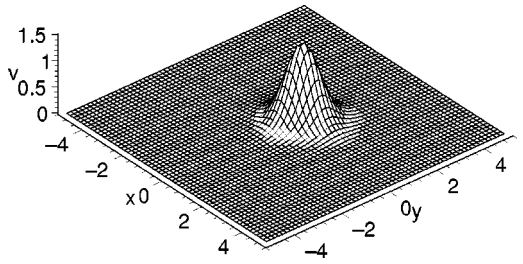


FIG. 2. A single dromion solution for the quantity v shown by (210) with (211) and (213) at time $t=0$.

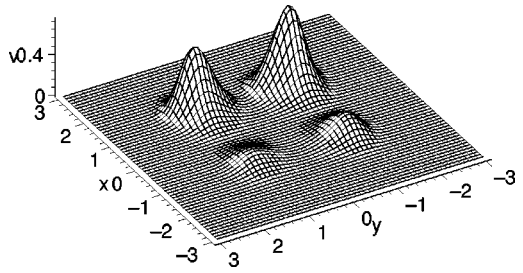


FIG. 3. A special four-dromion solution shown by (210) with (214) and (217) at time $t=0$.

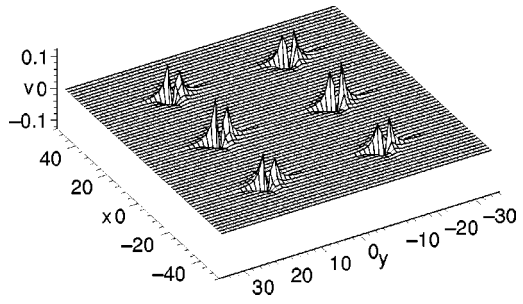


FIG. 4. A special lump solution for (210) with (219) at time $t=0$.

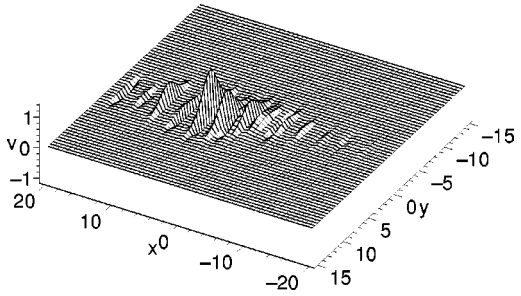


FIG. 5. A special dromion solution with the selection (221) at time $t=0$.

and G included in (210), the quantity v possesses quite rich structures. For instance, as mentioned in Refs. 4 and 17–19, if we select the functions F and G appropriately, we can obtain many kinds of localized solutions like the multi-solitoff solutions, multi-dromion and dromion lattice solutions, multiple ring soliton solutions and so on. Though these types of localized solutions have been discussed for other models, we still write down some special examples for completeness.

Example 1: Multi-solitoff solutions and multi-dromion solutions driven by straight-line solitons. If we restrict the functions F and G of (210) as

$$F=1+\sum_{i=1}^{N}\exp(k_i x+\omega_i t+x_{0i})\equiv 1+\sum_{i=1}^{N}\exp(\xi_i), \tag{211}$$

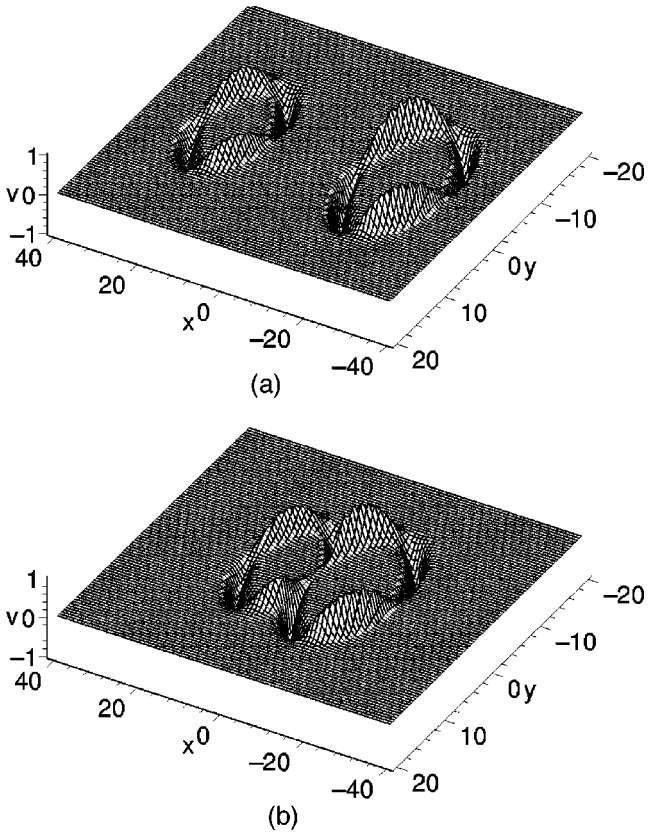
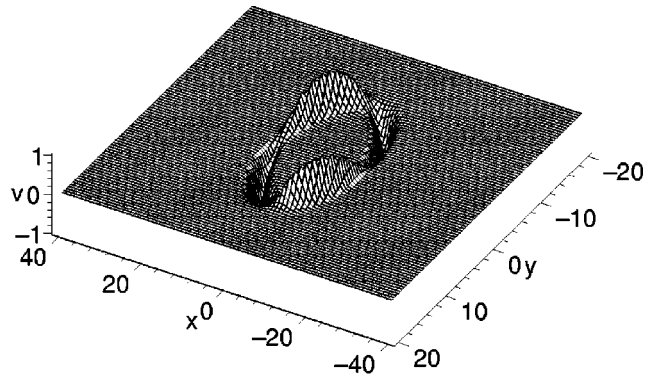
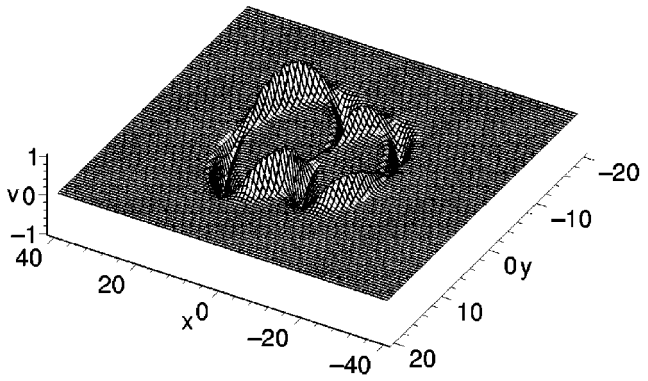


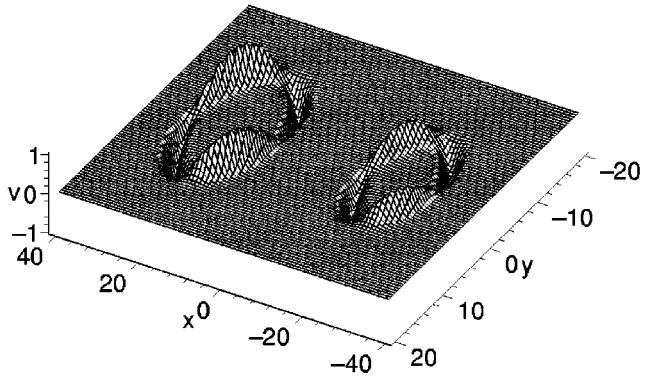
FIG. 6. The evolution of two saddle type ring soliton solution shown by (210) with the selection (222) at the times (a) $t=-1$, (b) $t=-0.4$, (c) $t=0$, (d) $t=0.4$, and (e) $t=1$.



(c)



(d)



(e)

FIG. 6. (*Continued.*)

$$G=\sum_{i=1}^{M}\exp(K_{iy}+y_{0i})\sum_{j=1}^{J}\exp(\Omega_j t),$$

where x_{0i}, y_{0i}, k_i, ω_i, K_i and Ω_i are arbitrary constants and M, N and J are arbitrary positive integers, then we have the multi-solitoff solutions (we call a half straight line soliton solution as a

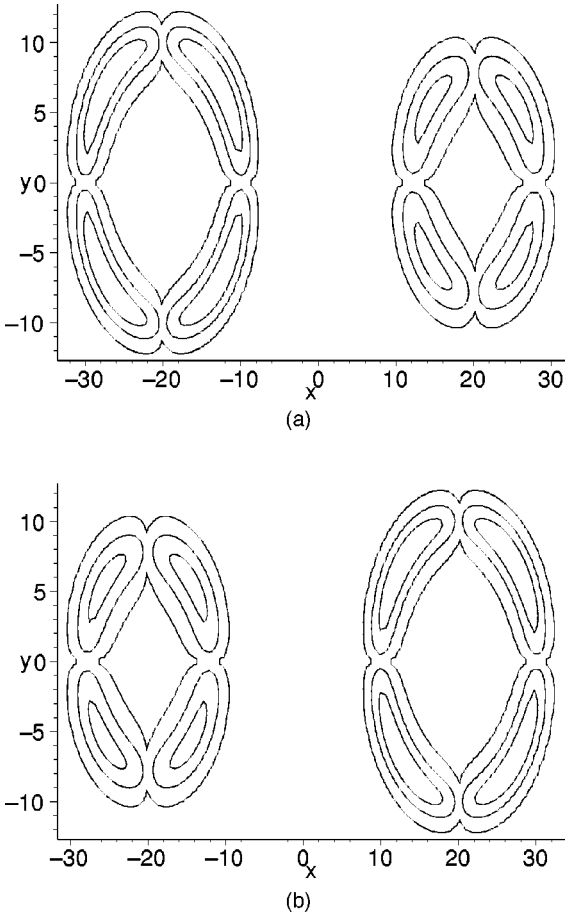


FIG. 7. (a) The contour plot related to Fig. 6(a). (b) The contour plot of Fig. 6(e). The values of the contours in these figures from the outside contours to the inside contours are $|v|=0.01$, $|v|=0.1$, and $|v|=0.4$, respectively.

solitoff which is caused by the resonance condition $a_3=0$) and the first type of special multidromion solutions ($a_3\neq 0$) driven by multiple straight line solitons. The selection (211) corresponds to

$$\alpha_0(t)=0,\quad \alpha_1(t)=a_3\alpha_2(t)=-a_1a_3\frac{\Sigma_{j=1}^{J}\Omega_j\exp(\Omega_j t)}{\Sigma_{j=1}^{J}\exp(\Omega_j t)}.$$

For the solution (211), there is no dispersion relation among k_i, ω_i, K_i and Ω_i.

Figure 1 shows the structure of a two-solitoff solution for the quantity v shown by (210) with (211) and

$$\begin{gathered}M=2,\quad N=1,\quad k_1=K_1=1,\quad K_2=-2,\quad a_1=a_2=1,\quad a_3=0,\\ x_{01}=y_{01}=0,\quad y_{02}=-9\end{gathered}\tag{212}$$

at time $t=0$.

Figure 2 shows the structure of a single dromion solution for the quantity v shown by (210) with (211) and

$$M=1,\quad N=1,\quad k_1=K_1=3,\quad a_1=10,\quad a_2=3,\quad a_3=0,\quad x_{01}=y_{01}=0\tag{213}$$

at time $t=0$.

Example 2: Multi-dromion solutions driven by curved line ghost solitons. Recently, Lou pointed out that for many (2+1)-dimensional models, a dromion may be driven not only by straight line solitons[26] but also by curved line solitons.[27] Actually, (210) can be rewritten as

$$v=\frac{Q_y P_x(a_1a_2)}{2[A_1\cosh\frac{1}{2}(P+Q+C_1)+A_2\cosh\frac{1}{2}(P-Q+C_2)]^2}, \tag{214}$$

where P and Q are related to p and q by $p=b_1\exp(P)$, $q=b_2\exp(Q)$ and

$$A_1=\sqrt{a_3(a_1b_1+a_2b_2+a_3b_1b_2)},\quad A_2=\sqrt{(a_1+a_3b_2)(a_2+a_3b_1)},$$

$$C_2=\ln\frac{a_1+a_3b_2}{a_2+a_3b_2},\quad C_1=\ln\frac{a_3}{a_1b_1+a_2b_2+a_3b_1b_2},$$

with arbitrary constants b_1 and b_2.

So the general multi-dromion solutions of the model expressed by (210) [or equivalently (214)] are driven by two sets of straight line solitons and some curved line solitons. The first set of straight line solitons appears in the factor Q_y, say, one can take

$$Q_y=\sum_{i=1}^{N} Q_i(y-y_{i0}), \tag{215}$$

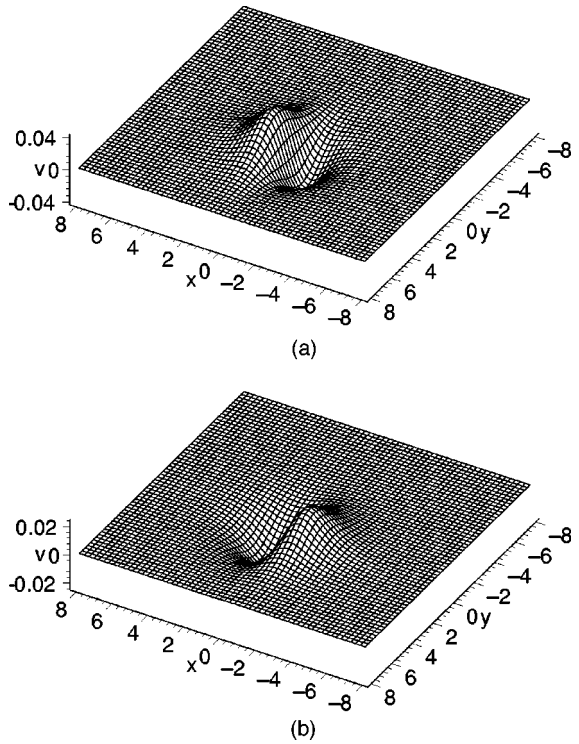


FIG. 8. The plots of the pointlike breather solution (210) with (223) and (224) and the parameters $\omega=\frac{1}{2}$, $a_1=a_2=10$, $a_3=1$, at the times (a) $t=-\pi/4$ and (b) $t=\pi/4$, respectively.

where $Q_i = Q_i(y - y_{i0})$ denotes a straight line soliton which is finite at the line $y = y_{i0}$ and decays rapidly away from the line. Similarly, the second set of straight line solitons appears in the factor P_x. Finally, the curved line solitons are determined by the factors $A_1 \cosh \frac{1}{2}(P+Q+C_1)$ and $A_2 \cosh \frac{1}{2}(P-Q+C_2)$ of (214) and the curves are determined by

$$P + Q + C_1 = \min(P + Q + C_1), \quad P - Q + C_2 = \min(P - Q + C_2), \tag{216}$$

while the number of curved line solitons is determined by the branches of the equations in (216). The dromions are located at the cross points and/or the closed points of the straight and curved lines.

Figure 3 is a plot of a multi-dromion solution driven by the curved line solitons via taking

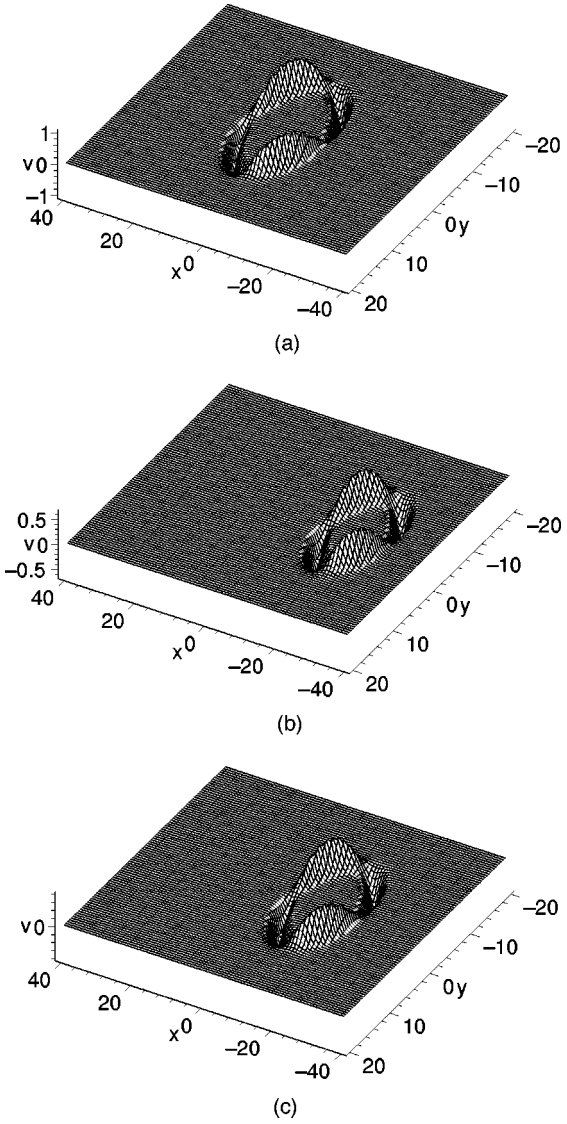


FIG. 9. The evolution of a special ring shape breather solution (210) with the selection (225) at the times (a) $t = -1$, (b) $t = -0.5$, (c) $t = -0.2$, (d) $t = 0$, (e) $t = 0.2$, and (f) $t = 1$, respectively.

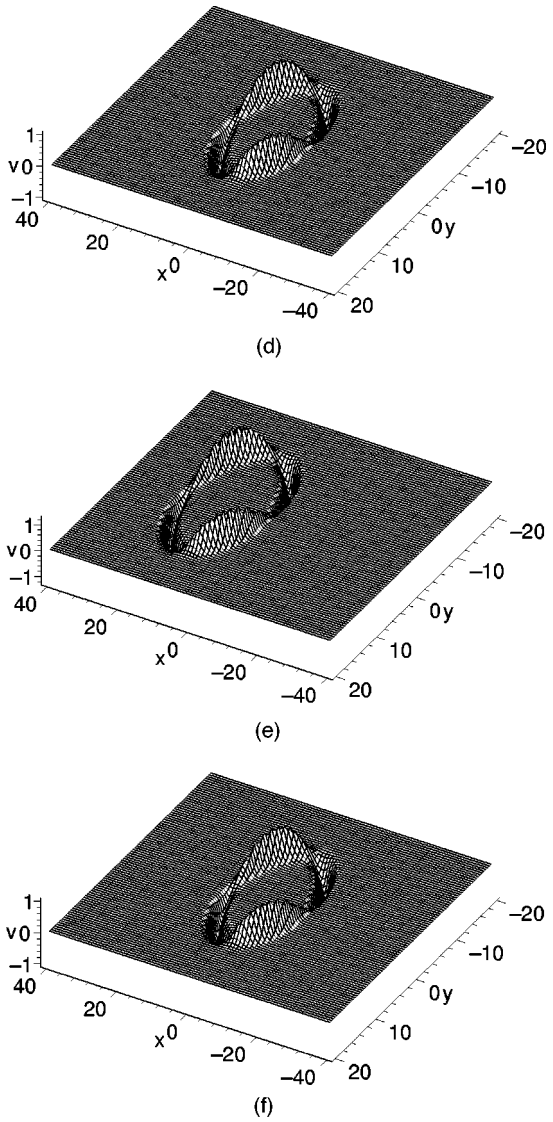


FIG. 9. (*Continued.*)

$$P=(x-v_1t)^3+\frac{x-v_1t}{15},\quad Q=\frac{(y-v_2t)^5}{20}+(y-v_2t)^3+\frac{y-v_2t}{100},$$
$$a_1=a_3=1,\quad a_2=2,b_1=3,\quad b_2=40,\quad t=0. \tag{217}$$

Example 3: Multi-lump solutions. It is also known that in high dimensions, like the KP and DSII equations, a special type of localized structure (called lump solutions) may also be formed by rational functions. Actually, the multi-lump solutions of $(2+1)$-dimensional integrable models can be found by taking the arbitrary functions appropriately.

For the $(M+N)$-component AKNS system, if we select the functions F and G of (210) as any rational functions with the conditions

$$F>0,\ \ G>0,\ \ \forall x,y,t, \tag{218}$$

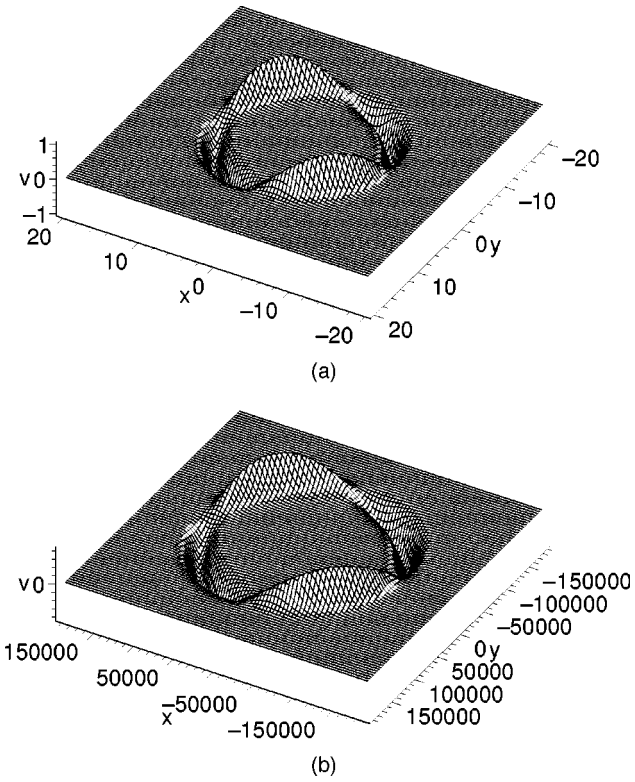


FIG. 10. (a) The evolution plots of the ring type of instanton solution (210) with (226) at the times (a) $t=0$ and (b) $t=10$.

and $a_1>0$, $a_2>0$, $a_3>0$, then we can obtain the nonsingular localized lump solutions. In Fig. 4, we plot a special lump solution (210) with

$$F=1+\frac{1}{1+(x-v_1t-30)^2}+\frac{1}{1+(x-v_2t)^2}+\frac{1}{1+(x-v_3t+30)^2}, \tag{219}$$

$$G=\frac{1}{1+(y-v_4t-15)^2}+\frac{1}{1+(y-v_5t+15)^2}, \quad a_1=10, \quad a_2=10, \quad a_3=1 \tag{220}$$

at time $t=0$.

Example 4: Oscillating dromion solutions. If some periodic functions in space variables are included in the functions p and q, we may obtain some types of multi-dromion solutions with oscillating tails. The oscillated dromion solution in Fig. 5 is related to

$$\begin{gathered} F=1+\exp((x-v_1t)\cos(2(x-v_1t))+\tfrac{5}{4}), \quad G=\exp(y-v_2t), \\ a_1=a_2=10, \quad a_3=1, \quad t=0. \end{gathered} \tag{221}$$

Example 5: Ring soliton solutions. In high dimensions, in addition to the pointlike localized coherent excitations, there may be some other types of physically significant localized excitation. For instance, in $(2+1)$-dimensional cases, there may be some types of ring soliton solutions which are not equal to zero identically at some closed curves and decay exponentially away from the closed curves.[17–19,21] In Figs. 6 and 7, we plot the interaction property of a two traveling saddle type of ring soliton solution with the selection

$$F=\exp\left(-\frac{(x-20t)^2}{10}+5\right)+\exp\left(-\frac{(x+20t)^2}{10}+1\right),\quad G=\exp\left(\frac{y^2}{10}-5\right),\quad a_1=a_2=1,\quad a_3=0. \tag{222}$$

In Fig. 6, we plot the evolution of the two ring soliton solution for the quantity v expressed by (210) with (222) at times (a) $t=-1$, (b) $t=-0.4$, (c) $t=0$, (d) $t=0.4$ and (e) $t=1$, respectively. From Figs. 6(a)–6(e), we can see that the interaction of two ring soliton solutions is elastic. To see more clearly the completely elastic interaction properties between two traveling ring soliton solutions, two counter plots related to Figs. 6(a) and 6(e) are plotted in Fig. 7.

Example 6: Multi-breatherlike soliton solutions. In $(1+1)$-dimensional cases, the breather solutions are another type of important nonlinear excitation. Because of the arbitrariness appearing in the functions F and G of (210), the breather solutions of the $(2+1)$-dimensional models may also have quite rich structures. On one hand, any $(1+1)$-dimensional breather solutions of the $(1+1)$-dimensional integrable models (like the sine-Gordon model and the nonlinear Schrödinger equation) can be used to construct the breather solutions of the higher dimensional models, say, the $(M+N)$-component AKNS system. In Fig. 8, the well known breather solution

$$F=4\arctan\left(\frac{\sqrt{1-\omega^2}\sin(\omega t)}{\omega\cosh(\sqrt{1-\omega^2}x)}\right) \tag{223}$$

of the sine-Gordon model, $F_{xx}-F_{tt}=\sin F$, is taken as the function F of (210) and while G is taken as

$$G=\exp(y) \tag{224}$$

with the parameters $\omega=\frac{1}{2}$, $a_1=a_2=10$, $a_3=1$. On the other hand, one can put any periodic functions of t into the localized excitations as shown in the examples 1–5 to construct more interesting new breatherlike solutions. Figure 9 shows the evolution behavior of a breather-like ring soliton solution shown by (210) with

$$\begin{aligned} F&=\exp\left(-\frac{1}{10}(x-20\sin(\pi t))^2+5(1.1+\sin(\pi t))\right),\\ G&=\exp\left(\frac{y^2}{10}-5+\sin(\pi t)\right),\quad a_1=a_2=1,\quad a_3=0. \end{aligned} \tag{225}$$

From Figs. 9(a)–9(e), we can see that the breatherlike ring soliton solution can ''breath'' in some different ways, say, it can breath not only in its amplitude but also in its shape (like the radius of the loop) and the position.

Example 7: Multiple instanton solution. If some types of decaying functions of time t are included in the solutions (210), then we can find some types of instanton solutions. In Fig. 10, the behavior of a special ring type of instanton solution (210) with

$$\begin{aligned} F&=\exp\left(-\frac{x^2\,\mathrm{sech}^2 t}{10}+5(1.1+\sin(\pi t))\right),\\ G&=\exp\left(\frac{y^2\,\mathrm{sech}^2 t}{10}-5\right),\quad a_1=a_2=1,\quad a_3=0 \end{aligned} \tag{226}$$

is exhibited. From Figs. 10(a) and 10(b), we can see that the amplitude of the ring type of instanton solution (210) with (226) decays rapidly from $|v|\sim 1$ to $|v|\sim 10^{-9}$ as the time increases from $t=0$ to $t=10$.

VIII. SUMMARY AND DISCUSSIONS

In summary, the $(2+1)$-dimensional $(M+N)$-component AKNS system [which is the generalization of the $(1+1)$-dimensional multi-component AKNS system and obtained from the inner parameter dependent symmetry constraints of the KP equation] possesses various interesting properties. The model is Painlevé integrable and Virasoro integrable (possesses infinitely many dimensional KMV type symmetry algebra). The finite transformation (KMV type symmetry group) is also obtained. Using the finite transformation and special seed solutions, one may obtain many types of exact solutions. The group invariant solutions of the model are obtained by means of the CK's direct method and these types of similarity solutions can all be obtained by means of the nonclassical Lie group approach.

In recent studies,[17–19] it was found that a quite universal variable separation solution with some arbitrary functions is valid for many $(2+1)$-dimensional models. For the $(2+1)$-dimensional $(M+N)$-component AKNS system, the universal expression is valid for the quantity $\Sigma_{n=1}^{N}\Sigma_{m=1}^{M}a_{mn}p_nq_m$. Then, by selecting the arbitrary functions appropriately, we may obtain many types of multi-soliton solutions like the solitoffs, dromions, positons, lumps, saddle type ring solitons, breathers, instantons, etc. Some special types of examples of these types of excitations are plotted in Sec. VI. Especially, the complete elastic interaction property between the traveling ring type of solutions is revealed in Figs. 6 and 7.

The Painlevé analysis, symmetry study and the variable separation approaches are three useful methods in the study of the nonlinear science. The idea to form the localized excitations in $(2+1)$-dimensions can be extended to obtain some types of localized excitations in $(3+1)$-dimensions. For instance, a closed camber may be used to construct a bubble like soliton. A closed line which is an intersection of two cambers may be used to form a $(3+1)$-dimensional ring soliton. Some special $(3+1)$-dimensional dromions and ring solitons have been found in some Painlevé and/or Virasoro integrable models.[28] The more about the methods and the model are worthy of studying further.

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Commensurate harmonic oscillators: Classical symmetries

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The symmetry properties of a classical N-dimensional harmonic oscillator with rational frequency ratios are studied from a global point of view. A *commensurate* oscillator possesses the same number of globally defined constants of motion as an *isotropic* oscillator. In both cases invariant phase-space functions form the *algebra* su(N) with respect to the Poisson bracket. In the isotropic case, the phase-space flows generated by the invariants can be integrated globally to a set of finite transformations isomorphic to the group SU(N). For a commensurate oscillator, however, the *group* SU(N) of symmetry transformations is found to exist only on a *reduced* phase space, due to unavoidable singularities of the flow in the full phase space. It is therefore crucial to distinguish carefully between local and global definitions of symmetry transformations in phase space. This result solves the long-standing problem of which symmetry to associate with a commensurate harmonic oscillator. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1488672]

I. INTRODUCTION

Harmonic oscillators are ubiquitous in physics. To lowest order, motion close to a stable equilibrium of a classical system is often described by a Hamiltonian of the form

$$H(q,p)=\sum_{n=1}^{N}\frac{\omega_n}{2}(p_n^2+q_n^2),\quad \omega_n\in\mathbb{R}. \tag{1}$$

Here the (appropriately rescaled) canonical coordinates and momenta have Poisson brackets $\{q_n,p_{n'}\}=\delta_{nn'}$, $n,n'=1,...,N$. If the frequencies ω_n are all equal,

$$\omega_n=\omega,\quad n=1,...,N, \tag{2}$$

the Hamiltonian (1) describes an *isotropic* N-dimensional oscillator. This system is invariant under a set of transformations isomorphic to the group SU(N): on the one hand, the quadratic form (1) in $2N$ variables is obviously invariant under proper rotations SO($2N$)—on the other hand, canonical transformations need to be symplectic, hence they are elements of Sp(N). However, any transformation in $\mathbb{R}^{2N}$ which is both (special) orthogonal and symplectic must be (special) unitary:[1] $\mathrm{SU}(N)=\mathrm{SO}(2N)\cap\mathrm{Sp}(N)$. The group SU($N$) is represented by (N^2-1) phase-space functions which, as constants of motion, generate symmetry transformations of the Hamiltonian. In fact, the isotropic oscillator is ''maximally superintegrable'' since it possesses the maximal number of $(2N-1)$ functionally independent constants of motion, exceeding by far the number of N globally defined invariants required for integrability.[2]

Suppose now that the frequency ratios $\omega_n/\omega_{n'}$ are positive rational numbers,

$$\omega_n=\frac{\omega}{m_n}, \quad m_n\in\mathbb{N}_+, \quad \omega>0. \tag{3}$$

This property defines a *commensurate* harmonic oscillator, or **m**-oscillator, with $\mathbf{m}=(m_1,\ldots,m_N)$. As shown below, it also possesses (N^2-1) globally defined phase-space invariants, apart from the Hamiltonian. Their Poisson brackets form the Lie algebra su(N), as for the isotropic oscillator. It is known that in both systems all orbits are closed. Nevertheless, some difference is to be expected, since all orbits of an isotropic oscillator have the same period, while commensurate frequencies allow for closed orbits with different periods. This is easily seen by exciting only individual degrees of freedom with frequencies ω_n.

In the following, the topological and group-theoretical impact of rational frequency ratios (different from one) will be made explicit. First, various papers dealing with commensurate oscillators are reviewed in Sec. II, which is independent of the later developments. The technical part starts with Sec. III, where, for simplicity, the class of two-dimensional **m**-oscillators will be studied in detail. The generalization to $N\geqslant 3$, given in Sec. IV, is *not* straightforward. Finally, the overall picture is summarized and conclusions are drawn. A study of *quantum mechanical* **m**-oscillators, including the classical limit to connect with the present results, will be presented elsewhere.[3]

II. SYMMETRIES OF HARMONIC OSCILLATORS

The equations of motion of N harmonic oscillators can be solved analytically for arbitrary frequency ratios. In spite of this exceptional property many authors have wrestled with the *symmetries* of such systems, the question being how their symmetries depend on the (ir-) rationality of the frequency ratios. Most contributions are fostered by the difficulty to distinguish between local and global properties of phase space. Two-dimensional oscillators with rational or irrational frequency ratios are discussed almost exclusively. Surprising claims have been made in the attempt to generalize properties of the isotropic oscillator in N dimensions.

Jauch and Hill[4] address the problem of ''accidental degeneracy'' of quantum-mechanical energy eigenvalues. The obvious invariance of the three-dimensional harmonic oscillator (as well as the hydrogen atom) under the group of rotations in configuration space is not sufficient to explain the observed degeneracy of the energy levels. They conclude that additional constants of motion must exist which account for extra degeneracies in the quantum mechanical energy spectrum. In fact, (N^2-1) Hermitian operators can be specified which commute with the Hamiltonian of the isotropic harmonic oscillator in N dimensions. Their commutation relations turn out to be those of the algebra su(N). Therefore, the oscillator is said to have the su(N) symmetry—which then leads to the correct degree of degeneracies of energy levels.

Pauli[5] and Klein[6] have pointed out that there is a connection between degeneracies of energy levels and the existence of further constants of motion in the associated *classical* system. Therefore, the result also should be manifest in the corresponding classical isotropic oscillator. Upon ''dequantizing'' the quantum invariants, one obtains indeed (N^2-1) constants of motion which constitute the su(N) algebra with respect to the Poisson bracket. Hence, the classical isotropic oscillator possesses indeed constants of motion other than the angular momentum. Its components generate obvious *geometrical* symmetry transformations while the additional constants are said to generate *dynamical* symmetry transformations. They cannot be visualized in configuration space because they mix coordinates and momenta.

However, to exhibit a set of conserved phase-space functions which form a particular algebra is *not* sufficient in order to prove invariance of the physical system in a global sense, i.e., in the entire phase space. Jauch and Hill assert that the ''system of orbits'' of a classical (m_1,m_2)-oscillator be invariant under a group of transformations isomorphic to the three-dimensional group of proper rotations SO(3). However, this claim cannot be justified by local considerations only. In other words, global invariance under a particular group of transformations does not follow from specifying phase-space functions forming the corresponding algebra.

McIntosh reviews accidental degeneracy in classical and quantum mechanics in Ref. 7. He notes that the phase space of the isotropic harmonic oscillator in two dimensions foliates into hyperspheres, being surfaces of constant energy. A discussion of the canonical transformations generated by three constants of the motion quadratic in the coordinates and momenta follows. It becomes obvious that the group of symmetry transformations is the special unitary group in two dimensions, SU(2)—*not* the group of proper three-dimensional rotations, SO(3), as Jauch and Hill suggested.

Dulock and McIntosh[8] devote a paper to the two-dimensional harmonic oscillator with arbitrary frequency ratio. Using classical variables which mimic quantum mechanical creation and annihilation operators, they write down three constants of motion with Poisson brackets isomorphic to the so(3) algebra relations. A Hopf mapping is performed in order to visualize ''how the rotational symmetry of $\mathcal{S}^2$, which is the three-dimensional rotation group, chances also to be the symmetry group of the harmonic oscillator.'' [8] Formally, this method can be applied to oscillators with *arbitrary* frequency ratio. However, one of the transformations, which is one-to-one in the isotropic case, becomes a multiple-valued map. For rational frequency ratios there is a finite ambiguity, turning to infinite multiple-valuedness if the frequencies ratios are irrationally. In spite of this result, the authors claim that the set of symmetry transformations for *all* types of oscillators investigated is isomorphic to the group SU(2)—irrespective of the multiple-valuedness. Once more, the possibility to write down formal expressions which constitute particular algebraic relations is taken as a proof of the existence of an associated *group* of transformations.

Maiella and Vitale[9] react to the claim that ''every classical system should possess a 'dynamical' symmetry larger than the 'geometrical' one.'' [9] Using action-angle variables, they provide three constants of motion for the two-dimensional oscillator which form the su(2) algebra. However, for irrational frequency ratio the invariants are not single-valued—hence they consider the ''su(2) symmetry'' to be of ''formal value'' only. It is claimed to acquire physical relevance only for commensurate and, *a fortiori*, isotropic oscillators. At the same time, no argument is given which would forbid the existence of the group SU(2) for the irrational oscillator. The authors do not investigate whether, in the commensurate case, the invariants generate indeed finite single-valued phase-space transformations in SU(2).

Maiella[10] extends this discussion to the N-dimensional oscillator and emphasizes that only single-valued constants of the motion generate actual symmetry transformations. Initially, the group of all contact transformations for a given dynamical system is considered. Any subgroup of transformations which is generated by single-valued constants of motion and leaves the Hamiltonian invariant is called an ''invariance group.'' The classical degree of degeneracy determines the number of its generators: each linear relation between the classical frequencies of the system with *rational* coefficients is accompanied by the appearance of a single-valued constant of motion. Subsequently, phase-space functions are given in action-angle variables which realize the algebra su(N) for an isotropic oscillator and the algebra su(n), $2 \leqslant n < N$, for smaller degeneracy. However, it is again not proven explicitly that the generators actually give rise to globally well-defined transformations.

In the late 1960s, successful application of group theoretical concepts in elementary particle physics renewed the interest in symmetries of classical Hamiltonian systems and stimulated more general approaches. The invariance of the three-dimensional Kepler problem under the group of four-dimensional rotations, SO(4), was explicitly shown by Moser[11] in 1970 for the first time. Already in 1965 Bacry, Ruegg and Souriau[12] proved that there exists a set of global symmetry transformations for the Kepler problem being isomorphic to the group SO(4). The transformations presented, however, do not act on variables in phase-space. The transformations of phase-space manifolds are parametrized by the components of angular momentum and of the Runge–Lenz vector. Representing only five independent constants of motion, the time t at which the particle passes the perihelion of the orbit is taken as sixth parameter.

Dulock and McIntosh[13] claim that the Kepler problem has not only the symmetry SO(4) but SU(3). Two papers by Bacry, Ruegg and Souriau[12] and by Fradkin[14] generalize this statement: all classical central potential problems should possess the dynamic symmetries O(4) *and* SU(3). This

surprising statement is subject to the same criticism as the following, even more general claim by Mukunda:[15,16] *all* classical Hamiltonian systems with N degrees of freedom have O(N) and SU(N) symmetries. If this statement were true, then there would exist just one and only one global phase-space structure for systems with N degrees of freedom—the well-established distinction between regular and chaotic systems would have no meaning at all.

Mukunda argues on the basis of a theorem by Eisenhart.[17] Consider, in a Hamiltonian system with N degrees of freedom, $n<N$ independent functions of canonically conjugate variables (subjected to weak conditions). They can always be supplemented by $(2N-n)$ phase-space functions such that N pairs of canonically conjugate variables result which define a symplectic basis of phase space. Hence, starting with the Hamiltonian of the system under consideration one can find (i) a variable being canonically conjugate to the Hamiltonian and (ii) $(N-1)$ additional pairs of phase-space functions with Poisson brackets equal to one, all commuting with the first pair and therefore with the Hamiltonian. Consequently, this theorem is a blueprint to construct $(2N-1)$ independent constants of motion in any Hamiltonian system with N degrees of freedom. The particular form of the Hamiltonian does not even enter into the construction. Next, two different sets of phase-space functions are defined in terms of the $(2N-1)$ functions of this particular basis. Their Poisson brackets realize the relations characteristic of the algebras O(N) and SU(N), respectively. In a footnote, the author restricts the applicability of the results: ''We concern ourselves only with constructing realizations of Lie algebras, not of Lie groups. Even when we talk of invariance under the O(4) group, for example, we really intend invariance under the algebra.''[15] Consequently, ''invariance under the algebra'' is a *local* concept only, so that Mukunda's construction has formal value only. Actually, the phase-space functions written down by Mukunda do not neatly map phase space onto itself: the functions become imaginary if the range of the canonical variables is not restricted artificially. The lesson to be learned is obvious: in order to establish the invariance of a system under a *group* of phase-space transformations it is not sufficient to realize specific Poisson-bracket relations with invariants.

A related position is put forward by Stehle and Han.[18,19] To identify a particular algebra by constants of motion does not guarantee the presence of a ''higher symmetry''—a single-valued, or at most finitely many-valued, realization of the group must exist in phase-space. To show this, they show that a system is classically degenerate if the Hamilton–Jacobi equation of a particular system is separable in a continuous family of coordinate systems. This property is observable. Compare the Fourier series representation of one specific orbit described with respect to two different (continuously connected) coordinate systems. For consistency, the frequencies appearing in its Fourier decomposition must be rationally related, which corresponds to a classical degeneracy. It is important to note that the transformation from one coordinate system to the other be single-valued, otherwise the argument does not hold. Any phase-space function and, consequently, any constant of motion generates a transformation of phase-space onto itself; alternatively, it can be viewed as the generator for a transition to another coordinate system such that the Hamiltonian remains invariant. Only single-valued constants of motion generate global single-valued transformations—infinitely many-valued ''constants of motion'' represent formal expressions only, not necessarily related to the existence of classical degeneracy. Therefore, they do *not* establish a higher symmetry group of the system.

To sum up, the construction of an algebra from constants of motion is only the first step in the proof of the existence of a potential higher symmetry group. It needs to be supplemented by a global investigation of the generated transformations.

III. THE TWO-DIMENSIONAL COMMENSURATE OSCILLATOR

This section deals with the symmetry properties of a two-dimensional commensurate harmonic or (m_1,m_2)-oscillator described by the Hamiltonian

$$H(q_1,q_2,p_1,p_2)=\frac{\omega}{2}\left(\frac{1}{m_1}(p_1^2+q_1^2)+\frac{1}{m_2}(p_2^2+q_2^2)\right),\quad m_1,m_2\in\mathbb{N}_+, \tag{4}$$

where the integers m_1 and m_2 have no common divisor. Two pairs of canonical variables, $q_n, p_n \in (-\infty, \infty), n=1,2$, label points in phase space $\Gamma \sim \mathbb{R}^4$, the only nonvanishing Poisson brackets being given by

$$\{q_1, p_1\} = \{q_2, p_2\} = 1. \tag{5}$$

It will be useful to introduce two other sets of canonical variables. First, combine each pair into a complex variable

$$\alpha_n = \frac{1}{\sqrt{2}}(q_n + i p_n), \quad n=1,2, \tag{6}$$

with nonvanishing brackets

$$\{\overline{\alpha}_1, \alpha_1\} = \{\overline{\alpha}_2, \alpha_2\} = i, \tag{7}$$

where $\overline{\alpha}$ denotes the complex conjugate of α. Second, action-angle variables $I_n \in [0,\infty)$ and $\varphi_n \in [0, 2\pi)$, $n=1,2$, are determined through modulus and phase of $\alpha_n = \sqrt{I_n}\exp[i\varphi_n]$. Their nonzero brackets read

$$\{I_1, \varphi_1\} = \{I_2, \varphi_2\} = 1. \tag{8}$$

These coordinates provide alternative forms of the Hamiltonian,

$$H = \omega\left(\frac{\overline{\alpha}_1 \alpha_1}{m_1} + \frac{\overline{\alpha}_2 \alpha_2}{m_2}\right) = \omega\left(\frac{I_1}{m_1} + \frac{I_2}{m_2}\right). \tag{9}$$

A. Constants of motion and Lie algebras

Commensurate harmonic oscillators possess a large number of constants of motion. The Hamiltonian itself is an invariant as $\{H,H\}=0$. Motion of the system with given energy E is thus restricted to a three-dimensional hyper-surface, an ellipsoid $\mathcal{E}(E)$ in phase space Γ. Further, the actions I_1 and I_2, having zero Poisson brackets with the Hamiltonian and among themselves, render the (m_1,m_2)-oscillator integrable. For fixed values of the actions, Arnold's theorem[2] states that the motion takes place on a two-dimensional torus $\mathcal{T}(I_1,I_2)$. In fact, the *entire* phase space is foliated by tori with radii $\sqrt{I_1}$ and $\sqrt{I_2}$, respectively. According to (9) the Hamiltonian H is a linear function of these invariants.

A third, functionally independent (complex) constant of the motion is given by the expression

$$K = \alpha_2^{m_2}(\overline{\alpha}_1)^{m_1}. \tag{10}$$

As mentioned in Ref. 4, both its real and complex parts are invariant which implies that the phase χ of the function K,

$$\chi = m_2\varphi_2 - m_1\varphi_1 \in [0, 2\pi), \tag{11}$$

is a constant of the motion, too. Considered as a generator of transformations in phase space, it connects energetically degenerate pairs of tori. The existence of a third invariant is expected to reduce the dimensionality of the accessible manifold. Indeed, fixing the values of the three invariants I_1, I_2, and K (or, equivalently, χ) singles out a one-dimensional orbit on the torus $\mathcal{T}$ if the two frequencies are rationally related. Generic orbits, $\alpha_n(t) = \sqrt{I_n}\exp(-i\omega t/m_n + \varphi_n(0))$, $n=1,2$, retrace themselves after a characteristic time $t_{\mathbf{m}} = 2\pi m_1 m_2/\omega$, with winding numbers m_2 for α_1 and m_1 for α_2. However, if the frequency ratio of the motion on the tori were *not* rational, an orbit would cover the torus $\mathcal{T}$ densely—the function K would represent a *formal* constant of the motion only, without any physical impact on the motion of the system. An important difference to the isotropic

oscillator is due to the fact that an **m**-oscillator has different types of orbits with frequencies $\omega/(2\pi m_1)$ and $\omega/(2\pi m_2)$, respectively. This allows one to distinguish experimentally the two cases.

The phase space of an **m**-oscillator has a particular *discrete* symmetry. Combine the variables α_n into a column: now the Hamiltonian is obviously invariant under $m_1 m_2$ finite rotations, $\alpha \to R_1^{r_1} R_2^{r_2} \alpha$, $r_n = 0,...,m_n - 1$, or, explicitly,

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \to \begin{pmatrix} e^{-i2\pi r_1/m_1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{-i2\pi r_2/m_2} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}. \tag{12}$$

These transformations map the phase-space Γ to itself. They form a cyclic group $\mathcal{C}_{m_1 m_2} = \mathcal{C}_{m_1} \times \mathcal{C}_{m_2}$, the direct product of two cyclic groups with m_1 and m_2 elements, respectively. In Ref. 20, $\mathcal{C}_{m_1 m_2}$ has been called *ambiguity group*.

The Poisson bracket of two invariants results in a third invariant. Therefore, the collection of all invariants is a Lie algebra. Typically, it will contain an infinite number of elements, all of which depend functionally on a smaller number of invariants. By an appropriate choice of the invariants, however, algebras with a finite number of elements can be found. The simplest example is given by the three invariants I_1, I_2, K giving rise to the following brackets:

$$\{I_1, K\} = -im_1 K, \quad \{I_2, K\} = im_2 K, \quad \{I_1, I_2\} = 0. \tag{13}$$

The algebra contains three independent elements—it is not possible to find an algebra with fewer elements since the **m**-oscillator has three invariants. It also contains two elements with vanishing Poisson bracket which, in a system with two degrees of freedom, is the maximum number of ''commuting'' functionally independent invariants.

There is an alternative set of four invariants $J = (J_0, \vec{J})$,

$$J_0 = \frac{I_1}{2m_1} + \frac{I_2}{2m_2} = \frac{1}{2\omega} H, \tag{14}$$

$$J_1 = \sqrt{\frac{I_1 I_2}{m_1 m_2}} \cos\chi, \tag{15}$$

$$J_2 = \sqrt{\frac{I_1 I_2}{m_1 m_2}} \sin\chi, \tag{16}$$

$$J_3 = \frac{I_1}{2m_1} - \frac{I_2}{2m_2}. \tag{17}$$

Only three of these invariants are functionally independent because

$$J_0^2 - \vec{J}^2 = 0. \tag{18}$$

This constraint is conveniently rephrased by saying that the ''four vector'' J is ''null'' or ''light like.'' The functions J are particularly interesting since they form the basis of a Lie algebra isomorphic to u(2),

$$\{J_0, J_j\} = 0, \quad \{J_j, J_k\} = \sum_{l=1}^{3} \epsilon_{jkl} J_l, \quad j,k = 1,2,3, \tag{19}$$

which has su(2) as a subalgebra, generated by the components of $\vec{J}$. Equations (19) have been at the origin of many attempts to associate a group SU(2) of symmetry transformations with the two-dimensional **m**-oscillator.

B. Reduced phase space and space of invariants

Consider the complex variables

$$\beta_n = \frac{|\alpha_n|}{\sqrt{m_n}}\left(\frac{\alpha_n}{|\alpha_n|}\right)^{m_n} = \sqrt{\frac{I_n}{m_n}}\exp[i m_n \varphi_n], \quad n=1,2, \tag{20}$$

which satisfy

$$\{\overline{\beta}_n, \beta_{n'}\} = i\delta_{nn'}. \tag{21}$$

In spite of these relations, the variables β_n do *not* define pairs of canonical coordinates of Γ since the map $\alpha \to \beta$ is not a one-to-one transformation. The variables β_n are, however, canonical coordinates in the *reduced* phase space $\Gamma_{\mathbf{m}}$. The reduced space is obtained from identifying those $m_1 m_2$ points of Γ which satisfy $\beta(R_1^{r_1} R_2^{r_2}\alpha) = \beta(\alpha)$, $R_n^{r_n} \in \mathcal{C}_{m_n}$. The definition of the variables (20) is motivated by the invariance of the constants of motion in (14)–(17) under the ambiguity group $\mathcal{C}_{m_1 m_2}$.

The invariants (14)–(17) take a simple form when expressed in terms of the reduced variables,

$$J_0 = \frac{1}{2}(\overline{\beta}_1\beta_1 + \overline{\beta}_2\beta_2), \tag{22}$$

$$J_1 = \frac{1}{2}(\overline{\beta}_1\beta_2 + \overline{\beta}_2\beta_1), \tag{23}$$

$$J_2 = \frac{1}{2i}(\overline{\beta}_1\beta_2 - \overline{\beta}_2\beta_1), \tag{24}$$

$$J_3 = \frac{1}{2}(\overline{\beta}_1\beta_1 - \overline{\beta}_2\beta_2). \tag{25}$$

Using the two-component "Weyl spinor" $\beta = (\beta_1, \beta_2)$, these invariants can be written

$$J_\nu = \frac{1}{2}\overline{\beta}\cdot\sigma_\nu\beta, \quad \nu = 0,...,3, \tag{26}$$

where $\sigma_0 = \mathbf{1}_2$, and the Pauli matrices σ_k, $k=1,2,3$, generate the algebra su(2). Consequently, the invariants, which span the space of invariants, Υ, turn into *sesquilinear* expressions on the reduced phase space $\Gamma_{\mathbf{m}}$. Their structure is similar to those of the isotropic or (1,1)-oscillator: in this case, the reduced phase space and the original one coincide, $\Gamma_{(1,1)} = \Gamma$. In some sense, the non-bijective map $\alpha \to \beta$ "linearizes" the invariants at the expense of accounting for a fraction of phase space only. It will be shown later that the concept of the reduced space $\Gamma_{\mathbf{m}}$ is natural in the present context as it provides appropriate setting to derive global statements about symmetry transformations.

C. Topological aspects

Turn now briefly to the topology of the spaces involved. Consider the nontrivial transformations introduced so far: first, the original phase space has been mapped to the reduced phase space,

$$\psi: \Gamma \to \Gamma_{\mathbf{m}} : \alpha \mapsto \beta(\alpha); \tag{27}$$

second, introducing the invariants J maps the reduced variables to the space of invariants, Υ,

$$\phi:\Gamma_{\mathbf{m}}\to\Upsilon:\beta\mapsto J(\beta), \tag{28}$$

which is an upper cone in $\mathbb{R}^4$ since $J_0=|\vec{J}|$.

The reduced phase space $\Gamma_{\mathbf{m}}$ has the structure of a well-known fiber bundle. To see this, consider an orbit $\alpha(t)$ in phase space Γ. Its image in the reduced space $\Gamma_{\mathbf{m}}$ is given by $\beta(t)=e^{-i\omega t}\beta(0)$. The maps $\beta\to e^{i\gamma}\beta$ form a group U(1) which leaves invariant the map ϕ, $J(e^{i\gamma}\beta)=J(\beta)$, since the phase drops out from the sesquilinear expressions given in Eqs. (26). Therefore, $\Gamma_{\mathbf{m}}$ is indeed a *fiber bundle* $(\Upsilon,\phi,\mathcal{O})$: the invariants Υ form the base, each orbit $\mathcal{O}_{\beta_0}=\{e^{i\gamma}\beta_0\,|\,\gamma\in[0,2\pi)\}$ is a fiber, and the map ϕ is the projection. The global structure of the bundle follows from the fact that the restriction of $\Gamma_{\mathbf{m}}$ to the submanifold $\Gamma_{\mathbf{m}}(E)$ with points $\overline{\beta}\cdot\beta=E/\omega$ is isomorphic to the sphere $\mathcal{S}^3$—as is obvious from the quadratic form (4). Thus, the restriction of the map ϕ to $\Gamma_{\mathbf{m}}(E)$ defines the *Hopf fibration* of $\mathcal{S}^3$. To each orbit $\mathcal{O}_\beta$ in $\mathcal{S}^3$ corresponds a point $\vec{J}(\beta)$ of the sphere of radius $J_0=E/(2\omega)$ and a circle in the tangent space at this point.

It is interesting to look at the space Υ of invariants and the transformations among them from a general perspective. To do so, consider the complex instead of the real Lie algebra su(2) which also leaves invariant the Hamiltonian $H\sim J_0$ in (22) invariant. This is the Lie algebra sl(2,C) associated with the group SL(2,C), the universal covering of the Lorentz group. The Lorentz group induced by SL(2,C) in Υ is the transitivity group of the upper (half-) cone.

The elements of SL(2,C) can be written as $u(\tau,\gamma)=\exp[g(\tau,\gamma)]$, where τ and γ are two real parameters, and each g is a traceless complex matrix,

$$g(\tau,\gamma)=\tfrac{1}{2}(\gamma\vec{\nu}\cdot\vec{\sigma}+i\tau\vec{n}\cdot\vec{\sigma}). \tag{29}$$

The matrices $u(\tau,0)$ belong to the group SU(2). Thus, they generate rotations and infinitesimal transformations which can be written in terms of a Poisson bracket:

$$\frac{d\vec{J}(\tau)}{d\tau}=\vec{n}\wedge\vec{J}(\tau)\equiv\{\vec{J},\vec{n}\cdot\vec{J}\}. \tag{30}$$

The subsets $u(0,\gamma)$ represent Lorentz boosts mapping a point β according to

$$u(0,\gamma)\beta=(\cosh(\gamma/2)+\sinh(\gamma/2)\,\vec{\nu}\cdot\vec{\sigma})\beta\equiv\beta(\gamma). \tag{31}$$

On the invariants, the transformation

$$J_\nu=\overline{\beta}\cdot\sigma_\nu\beta\mapsto J_\nu(\beta)=\overline{\beta(\gamma)}\cdot\sigma_\nu\beta(\gamma) \tag{32}$$

is induced. Hence, the sphere $\mathcal{S}^3$ of radius $J_0=H/(2\omega)$ is mapped to a sphere of radius $J_0(\gamma)$ with

$$\frac{dJ_0}{d\gamma}=\vec{\nu}\cdot\vec{J},\quad \frac{d\vec{J}}{d\gamma}=J_0\vec{\nu}. \tag{33}$$

This is an infinitesimal Lorentz transformation which maps the upper cone $\Upsilon\in\mathbb{R}^4$ to itself as is obvious from $d(J_0(\gamma)^2-\vec{J}(\gamma)^2)/d\gamma=0$ and J_0 remaining positive. Contrary to (30), it is not possible to express the right-hand sides of (33) by means of Poisson brackets. This can be understood from a quantum mechanical point of view. A classical theory can only manage Boltzmann statistics whereas in quantum (field) theory, due to the *anti*commutativity of Weyl spinors, it would be possible to find a commutator to express the derivatives $dJ_\nu/d\gamma$.

IV. GLOBAL INVARIANT VECTOR FIELDS

Each phase-space function generates a flow in phase space Γ, as well as in the reduced phase space $\Gamma_{\mathbf{m}}$, and in the space of invariants Υ. The invariants generate flows which commute with the Hamiltonian vector field. To be more specific, consider any element J_ν, $\nu=0...3$, of the Lie algebra u(2). When acting on an observable f through the Poisson bracket,

$$V_\nu=\{f,J_\nu\}, \quad \nu=0,...,3, \tag{34}$$

it defines a vector field V_ν in Γ. Its integral lines satisfy the differential equation

$$\frac{df}{d\tau}=V_\nu. \tag{35}$$

The solution of this differential equation is a map $f(\tau)$ which will be written in the form

$$f(\tau)=\mathrm{Exp}[\tau J_\nu](f)=\sum_{k=0}^{\infty}\{f,J_\nu\}_k\frac{\tau^k}{k!}, \tag{36}$$

where

$$\{g,h\}_{k+1}=\{\{g,h\}_k,h\}, \quad k=1,2,\ldots, \quad \{g,h\}_0=g, \tag{37}$$

with smooth phase-space functions g and h. In a simplified notation, the solutions (36) are written as

$$S_\nu[\tau]\equiv\mathrm{Exp}[\tau J_\nu], \quad \nu=0,...,3, \quad S_{\vec{n}}[\tau]\equiv\mathrm{Exp}[\tau\vec{n}\cdot\vec{J}], \quad |\vec{n}|=1, \tag{38}$$

each unit vector $\vec{n}$ being associated with a point of the unit sphere $\mathcal{S}^2$.

The crucial question now is to investigate whether the flow (34) and hence the maps (38) are defined everywhere in the space under consideration. Only in this case, the *algebra* formed by the closed set of Poisson brackets among the invariants integrates to a *group* of symmetry transformations. More specifically, one needs to find out whether the invariants (14)–(17) of the **m**-oscillator generate a set of transformations isomorphic to the group SU(2) [or U(2)]. This is only possible if the associated vector fields are well-defined everywhere in the space where they act. The fields will be studied separately for functions f from the spaces Γ, $\Gamma_{\mathbf{m}}$, or Υ.

A. Vector fields in the space of invariants

The simplest case to look at is the orbits generated by the first component of J, which is a multiple of the Hamiltonian, $J_0=H/(2\omega)$. Not surprisingly, one has

$$S_0[\tau](J)=J, \tag{39}$$

that is, all components of J are invariant under the action of J_0. Rotations about the 3-axis, i.e., with an axis passing through the poles $J_3=\pm J_0$, are generated by the invariant $J_3=I_1/(2m_1)-I_2/(2m_2)$,

$$S_3[\tau](J)=(J_0,R_3(\tau)\vec{J}). \tag{40}$$

Each possible orbit in Υ is generated by a linear combination of invariants $\vec{n}\cdot\vec{J}$,

$$S_{\vec{n}}[\tau](J)=(J_0,R_{\vec{n}}(\tau)\vec{J}), \tag{41}$$

where the matrix $R_{\vec{n}}(\tau)$ represents a rotation by an angle τ about an axis parallel to the vector $\vec{n}$. In other words, every point of the sphere $|\vec{J}|=J_0$ is mapped to another point of the same sphere, the energy $E=2\omega J_0$ being conserved.

These results are conveniently summarized by a group theoretical statement. The set

$$\mathcal{R}_J=\{S_{\vec{n}}[\tau]\,|\,0\leqslant\tau<2\pi,\vec{n}\in\mathcal{S}^2\} \tag{42}$$

of maps acting in Υ is a representation of the group SO(3). In other words, there is a subset of all phase-space functions, such that its elements transform according to the group SO(3). Mathematically, this group is the integrated form of the adjoint representation of the algebra (19). Consequently, one can attribute this group as a *symmetry group* to the reduced (m_1,m_2)-oscillator, for any frequency ratio. Note, however, that this symmetry does not act on points in phase space Γ but on points of the space of invariants Υ.

B. Vector fields in the reduced phase space

Again, the action of the generators J_0, J_3, and $\vec{n}\cdot\vec{J}$ will be studied, now with respect to the variables $\beta=(\beta_1,\beta_2)$. It is straightforward to see that

$$S_0[\tau](\beta)=e^{-i\tau/2}\beta, \tag{43}$$

which is just the time evolution with $\tau=2\omega t$. Similarly, the invariant J_3 generates a flow

$$S_3[\tau](\beta)=\begin{pmatrix} e^{-i\tau/2} & 0 \\ 0 & e^{i\tau/2}\end{pmatrix}\beta. \tag{44}$$

Comparison with (20) shows that the function $\chi=m_2\varphi_2-m_1\varphi_1$ is left invariant. Transformation (44) is a special case of the map

$$S_{\vec{n}}[\tau](\beta)=(\sigma_0\cos\tau/2-i\vec{n}\cdot\vec{\sigma}\sin\tau/2)\beta\equiv\beta(\tau). \tag{45}$$

No ambiguities arise when mapping points β under $S_{\vec{n}}[\tau]$, for whatever values of the parameter τ and the directions $\vec{n}$. Therefore, the set

$$\mathcal{R}_\beta=\{S_{\vec{n}}[\tau]|0\leqslant\tau<4\pi,\vec{n}\in\mathcal{S}^2\} \tag{46}$$

of maps faithfully represents the group SU(2) in $\Gamma_{\mathbf{m}}$. Consequently, an **m**-oscillator admits as symmetry not only the three-dimensional rotation group SO(3) in Υ but also the special unitary group SU(2) in $\Gamma_{\mathbf{m}}$.

In this restricted sense, and only in this one, (m_1,m_2)-oscillators are seen to possess both SO(3) and SU(2) as symmetry groups. This statement agrees with the fact that the algebras so(3) *and* su(2) are isomorphic. The next section deals with the question which groups, if any, are represented on the original phase space Γ.

C. Vector fields acting in phase space

It will be shown in this section that the vector fields associated with the invariants J are not defined globally when they act on the variables α which span phase space Γ. Consequently, it is *not* possible to implement the group SU(2) on phase space Γ. More explicitly, it will be shown that the action $S_{\vec{n}}[\tau](\alpha)=(\alpha_1(\tau),\alpha_2(\tau))$ on Γ is nonlinear, and that it is inevitably singular for some parameters $(\vec{n},\tau)$ and initial points α. Contrary to one's intuition the flows can be defined only locally, and they cannot be extended to define a *group* of symmetry transformations.

To begin with, consider the flows generated by J_0 and J_3, respectively. The resulting orbits *are* well-defined for all initial points: they are given by

$$S_0[\tau](\alpha)=\begin{pmatrix} e^{-i\tau/(2m_1)} & 0 \\ 0 & e^{-i\tau/(2m_2)} \end{pmatrix}\alpha, \tag{47}$$

and by

$$S_3[\tau](\alpha)=\begin{pmatrix} e^{-i\tau/(2m_1)} & 0 \\ 0 & e^{i\tau/(2m_2)} \end{pmatrix}\alpha, \tag{48}$$

respectively. Equation (47) describes the time evolution of the point $\alpha\in\Gamma$, hence both the energy $E=2\omega J_0$ and the torus $\mathcal{T}(I_1,I_2)$ are left invariant. Since the values of the actions change according to $I_n(0)\to I_n(\tau)=|\alpha_n(\tau)|^2$, the flow in (48) also conserves the energy while it maps a torus $\mathcal{T}(I_1,I_2)$ to a different one, $\mathcal{T}(I_1(\tau),I_2(\tau))$.

Now consider fields which are generated by *arbitrary* linear combinations of the invariants, $\vec{n}\cdot\vec{J}$. Denote potential solutions of the differential equation

$$\frac{d\alpha}{d\tau}=\{\alpha,\vec{n}\cdot\vec{J}\}\equiv V_{\vec{n}}(\alpha) \tag{49}$$

by $\alpha_{\vec{n}}(\tau)=S_{\vec{n}}[\tau](\alpha(0))$, with some initial point $\alpha(0)\in\Gamma$. Explicitly, the complex two-component field $V_{\vec{n}}$ reads

$$V_{\vec{n}}=\frac{1}{2i}\begin{pmatrix} (\vec{n}\cdot\vec{J}+im_1(\vec{n}\wedge\vec{J})_3+n_3J_0)/\overline{\alpha_1} \\ (\vec{n}\cdot\vec{J}+im_2(\vec{n}\wedge\vec{J})_3-n_3J_0)/\overline{\alpha_2} \end{pmatrix}. \tag{50}$$

It is finite but ill-defined on the hyperplanes $\mathcal{P}_1=\{\alpha|\alpha_1=0,\alpha_2\neq 0\}$ and $\mathcal{P}_2=\{\alpha|\alpha_1\neq 0,\alpha_2=0)\}$. There are points which, when transported by the flow $S_{\vec{n}}[\tau]$, hit the planes $\mathcal{P}_1$ or $\mathcal{P}_2$ for some value of τ. The associated orbits will be called *singular* since they cannot be continued unambiguously across the planes. This is due to the terms in (50) which contain J_1 and J_2,

$$J_1\pm iJ_2=\frac{|\alpha_1||\alpha_2|}{\sqrt{m_1m_2}}\exp[\pm i\chi], \tag{51}$$

while all other terms are zero on $\mathcal{P}_1$ and $\mathcal{P}_2$. Here is a toy example to illustrate the underlying problem. Consider a one-dimensional system with variable $\alpha=\sqrt{I}\exp[i\varphi]$, satisfying $\{I,\varphi\}=1$. The flow generated by $\sqrt{I}$ is ill-defined at the origin,

$$\frac{d\alpha}{d\tau}=\{\sqrt{I},\alpha\}=\frac{i}{2}\exp[i\varphi], \tag{52}$$

as its value depends on the way the point α is approached. If a trajectory were reaching the origin, it would be impossible to continue it unambiguously beyond this point. It is important to realize that this singularity as well as the one encountered in the singular planes is not due to a choice of coordinates but an intrinsic property of the flow.

To visualize the entire set of singular orbits, look at their images in Υ, that is, the orbits $S_{\vec{n}}[\tau](\vec{J})$, $\tau\in\mathbb{R}$. For given energy $E=2\omega J_0$, the points of $\mathcal{P}_1$ correspond to the north pole $(0,0,J_0=|\alpha_1|^2/2m_2)$ of the sphere $\mathcal{S}^2(J_0)$, while those of $\mathcal{P}_2$ are mapped to its south pole, $(0,0,-J_0=-|\alpha_2|^2/(2m_1))$. By $\psi\circ\phi$, an orbit $S_{\vec{n}}[\tau](\alpha)$ goes to a circle $R_{\vec{n}}(\tau)\vec{J}(\alpha)$. *Singular* orbits thus correspond to circles going through either one or both poles of the sphere, while *regular* orbits hit neither of them: for almost all flows, associated with a given vector $\vec{n}$, there exist two ''critical'' circles passing through the north pole and the south pole, respectively. These circles

coalesce into a single one passing through *both* poles if the axis of rotation is in the equatorial plane, $\vec{n}=(n_1,n_2,0)$. They degenerate to points located at the poles if $\vec{n}=\vec{e}_3=(0,0,\pm 1)$. Two conclusions can be drawn from this picture:

(1) for any given unit vector $\vec{n}\neq\pm\vec{e}_3$, the map $S_{\vec{n}}[\tau]$ has at least one singular orbit in Γ;
(2) any point $\alpha\in\Gamma$ can be sent to a singular hyperplane by a map $S_{\vec{n}}[\tau]$ with an appropriately chosen vector $\vec{n}_{\mathcal{P}}$.

In fact, the vectors $\vec{n}_{\mathcal{P}}$ can be chosen from *two* continuous sets: they only need to be in a plane (passing through the origin) which is perpendicular to either of the vectors $\vec{J}(\alpha)\pm J_0(\alpha)\vec{e}_3$, or, explicitly,

$$\vec{n}_{\mathcal{P}}^{\pm}=\frac{c_1(\vec{J}(\alpha)\pm J_0(\alpha)\vec{e}_3)\pm c_2\vec{J}(\alpha)\wedge\vec{e}_3}{|c_1(\vec{J}(\alpha)\pm J_0(\alpha)\vec{e}_3)\pm c_2\vec{J}(\alpha)\wedge\vec{e}_3|}. \tag{53}$$

Regular orbits of $S_{\vec{n}}[\tau]$ are easily computed without solving the differential equation (49). One needs to determine modulus and phase of the variables $\alpha_n, n=1,2$, as a function of τ. It is useful to write down the orbits in the reduced phase space and in the space of the invariants. According to (45), the reduced variables evolve linearly,

$$\beta_1(\tau)=(\cos\tau/2-in_3\sin\tau/2)\beta_1-(in_1+n_2)\sin(\tau/2)\beta_2, \tag{54}$$

$$\beta_2(\tau)=(\cos\tau/2+in_3\sin\tau/2)\beta_2-(in_1-n_2)\sin(\tau/2)\beta_1, \tag{55}$$

while the invariants $\vec{J}=\vec{J}(\beta)$ evolve in Υ as

$$\vec{J}(\tau)=\cos\tau\vec{J}+(1-\cos\tau)\vec{n}\circ\vec{n}\cdot\vec{J}-\sin\tau\,\vec{n}\wedge\vec{J}. \tag{56}$$

Using $|\alpha_n|^2=m_n|\beta_n|^2, n=1,2$, the τ-dependence of the moduli is simply

$$|\alpha_1(\tau)|^2=m_1(j_0+j_3(\tau)),\quad |\alpha_2(\tau)|^2=m_2(j_0-j_3(\tau)). \tag{57}$$

For the evolution of the phases, plug Eqs. (54) into

$$\exp[im_1\varphi_1(\tau)]=\left(\frac{\alpha_n(\tau)}{|\alpha_n(\tau)|}\right)^{m_n}=\frac{\beta_n(\tau)}{|\beta_n(\tau)|},\quad n=1,2, \tag{58}$$

giving

$$\exp[im_1\varphi_1(\tau)]=\frac{(\cos\tau/2-in_3\sin\tau/2)\beta_1-((in_1+n_2)\sin\tau/2)\beta_2}{|(\cos\tau/2-in_3\sin\tau/2)\beta_1-((in_1+n_2)\sin\tau/2)\beta_2|}\equiv\exp[i\Phi_1(\tau)], \tag{59}$$

and a similar equation for $\exp[im_2\varphi_2(\tau)]$. The two phases $\varphi_n(\tau)=\Phi_n(\tau)/m_n, n=1,2$, must be continuous whenever τ reaches the value 4π. They will both have a value which is a multiple of 2π when the parameter τ takes the value $4\pi m_1m_2$. This result seems to suggest that $S[\tau\vec{n}\cdot\vec{J}](\alpha)$ might be an m_1m_2-fold covering of the subgroup $S[\tau\vec{n}\cdot\vec{J}](\beta)$, $0\leqslant\tau<4\pi, \vec{n}\in\mathcal{S}^2$, of the special unitary group, SU(2). Due to the existence of singular orbits, however, this is not possible. Further, it is well-known that the only universal covering of SU(2) is this group itself. Nevertheless, one might describe the situation as a *ramified covering* of SU(2) since the maps $S[\tau\vec{n}\cdot\vec{J}]$ combine according to a group product law.

To visualize the obstruction of a global action of the group SU(2) differently, recall that a given map $S[\tau\vec{n}\cdot\vec{J}]$ sends a torus $\mathcal{T}(I_1,I_2)\in\Gamma$ to a torus $\mathcal{T}(I_1',I_2')$ such that $m_1I_1+m_2I_2=m_1I_1'+m_2I_2'$ holds. For some $\vec{n}$ and τ_0 it happens that one of the actions vanishes, I_1', say. This means that the initial two-dimensional torus $(\mathcal{S}^1\times\mathcal{S}^1)$ is mapped to a *one-dimensional torus*, i.e., a circle

$\mathcal{S}^1$, and, therefore, one of the angle variables has lost its meaning. Once this has happened, it is impossible to unambiguously continue the trajectory which has hit the singular plane, as the missing angle could take any value. The phenomenon is similar to the passage of a spherical wave through a focus.

It will be useful to give a name to the situation encountered here. A system with phase space Γ will be said to have a *faint G symmetry* if it admits a set of globally defined invariants which form an algebra $\mathcal{A}$ while the group G associated with it cannot be realized on Γ but only on a smaller part of it. Thus, all two-dimensional commensurate **m**-oscillators have a faint SU(2) symmetry.

V. THE *N*-DIMENSIONAL COMMENSURATE OSCILLATOR

To describe a commensurate harmonic oscillator in N dimensions, the present notation is straightforward to adapt. Let the label n run from 1 to N: the Hamiltonian of a commensurate **m**-oscillator with $\mathbf{m}=(m_1,\ldots,m_N)$, $m_n \epsilon \mathbb{N}_+$, reads

$$H(q,p)=\frac{\omega}{2}\sum_{n=1}^{N}\frac{1}{m_n}(p_n^2+q_n^2)=\frac{\omega}{2}\sum_{n=1}^{N}\frac{1}{m_n}\overline{\alpha}_n\alpha_n=\frac{\omega}{2}\sum_{n=1}^{N}\frac{1}{m_n}I_n. \tag{60}$$

The complex canonical variables are given by $\alpha_n=(q_n+ip_n)/\sqrt{2}$, $n=1,\ldots,N$, while actions I_n and angles φ_n are defined through $\alpha_n=\sqrt{I_n}\exp[i\varphi_n]$. Thus there are three sets of N pairs of canonical variables to choose from, with brackets

$$\{q_n,p_{n'}\}=\frac{1}{i}\{\overline{\alpha}_n,\alpha_{n'}\}=\{I_n,\varphi_{n'}\}=\delta_{nn'}, \quad n,n'=1,\ldots,N. \tag{61}$$

It will be assumed that the positive integer numbers m_n do not have an overall common divisor. For the discussion to follow, two cases will be distinguished: a commensurate oscillator is said to be *canonical* if *no* pair of numbers m_n and $m_{n'}$, $n\neq n'$, admits a common divisor but one. This class will be studied first. The presence of common divisors among subsets of the frequencies ω_n gives rise to interesting additional complications which will be considered later on.

A. Constants of motion and Lie algebras

In analogy to Eq. (10), each function

$$K_{nn'}=\alpha_n^{m_n}(\overline{\alpha}_{n'})^{m_{n'}}, \quad n,n'=1,\ldots,N, \tag{62}$$

is seen to be an invariant for the commensurate N-oscillator, $\{H,K_{nn'}\}=0$. These N^2 constants of motion depend on only $N(N+1)/2$ real invariants, namely N independent actions $I_n, n=1,\ldots,N$, and $N(N-1)/2$ relative angles

$$\chi_{nn'}=m_n\varphi_n-m_{n'}\varphi_{n'}, \quad 1\leqslant n<n'\leqslant N. \tag{63}$$

As in the two-dimensional case, the range of the functions $\chi_{nn'}$ must be restricted to the interval $[0,2\pi)$ because two values $\chi_{nn'}$ and $(\chi_{nn'}+2\pi)$, respectively, correspond to the *same* orbit. The angles $\chi_{nn'}$ satisfy $(N-1)(N-2)/2$ linear relations,

$$\chi_{nn'}+\chi_{n'n''}+\chi_{n''n}\equiv 0, \quad n,n',n'' \text{ all different.} \tag{64}$$

Therefore, there are no more than $(2N-1)$ functionally independent constants of motion, the maximum number of possibly independent invariants. As independent invariants, one may choose, for example, the N actions I_n and $(N-1)$ relative angles $\chi_{n\,n+1}, n=1,\ldots,N-1$.

The $(2N-1)$- dimensional surface of constant energy $H=E$ is an ellipsoid $\mathcal{E}(E)$ in phase space Γ. It contains the N-dimensional torus $\mathcal{T}(I_1,\ldots,I_N)$ of constant actions I_n as a submanifold. Lines of constant actions and angles are the *orbits* of the motion, winding around a torus $\mathcal{T}$. Each orbit is a one-dimensional closed loop given by

$$\alpha_n(t)=\sqrt{I_n}\exp(-i\omega t/m_n+\varphi_n(0)), \tag{65}$$

where $m_n\varphi_n(0)-m_{n+1}\varphi_{n+1}(0)=\chi_{n,n+1}(0)$. One revolution is completed after a time $t=2\pi M/\omega$, with the number M taking a value such that the *winding numbers* $w_n=M/m_n$ of each subsystem are integer without overall common divisor. In the canonical case, M is equal to $\Pi_1^N m_n$. Here is an example for $N=3$ which illustrates the noncanonical case: let $\mathbf{m}=(km_1',km_2',m_3)$. The number M would then take the value $km_1'm_2'm_3=m_1m_2m_3/k$.

It is important to note that in a canonical (but not isotropic) **m**-oscillator (i.e., all $m_n\neq 1$), there exist orbits with (2^N-1) different periods. There are N orbits corresponding to motion of a single oscillator only; there are $N(N-1)/2$ orbits winding around two-dimensional tori with frequencies $1/m_n$ and $1/m_{n'}$, $1\leqslant n<n'\leqslant N$, etc.

As in the two-dimensional case, the maps $R_n\alpha=(\alpha_1,\ldots,e^{i2\pi/m_n}\alpha_n,\ldots,\alpha_N)$ generate a cyclic group $\mathcal{C}_m=\{R_1^{r_1}\cdots R_N^{r_N}|r_n\in\mathbb{Z}\}$, the ambiguity group of the map ψ:

$$\psi(R_1^{r_1}\cdots R_N^{r_N}\alpha)=\psi(\alpha). \tag{66}$$

B. Reduced phase space and space of invariants

The $(2N-1)$ phase-space functions I_n and $\chi_{n\,n+1}$ form a basis of a Lie algebra commuting with the Hamiltonian H. Since the functions $\chi_{nn'}$ are not continuous on phase space Γ, it is natural to look at appropriate periodic functions of them. Introduce, in analogy to Eq. (20), the set of invariants

$$\beta_n=\frac{|\alpha_n|}{\sqrt{m_n}}\left(\frac{\alpha_n}{|\alpha_n|}\right)^{m_n}=\sqrt{\frac{I_n}{m_n}}\exp[im_n\varphi_n],\quad n=1,...,N. \tag{67}$$

They provide canonical coordinates on the $2N$-dimensional reduced phase space $\Gamma_{\mathbf{m}}$, now with $\mathbf{m}=(m_1,\ldots,m_N)$,

$$\{\overline{\beta}_n,\beta_{n'}\}=i\delta_{nn'}. \tag{68}$$

As before, (67) is a non-bijective map ψ: $\alpha\to\beta(\alpha)$. It is not a projection of the phase space on a subspace but should be thought of as a *ramified* cover of the reduced space $\Gamma_{\mathbf{m}}$.

Not surprisingly, Eqs. (26) have a straightforward generalization. With $\beta=(\beta_1,\ldots,\beta_N)$, one defines (N^2-1) invariants sesquilinear in the coordinates β_n by

$$J^s_{nn'}=\frac{1}{2}\,\overline{\beta}\cdot(E_{nn'}+E_{n'n})\beta=\frac{1}{2}(\overline{\beta}_n\beta_{n'}+\overline{\beta}_{n'}\beta_n),\quad 1\leqslant n<n'\leqslant N, \tag{69}$$

$$J^a_{nn'}=\frac{1}{2}\,\overline{\beta}\cdot\frac{1}{i}(E_{nn'}-E_{n'n})\beta=\frac{1}{2i}(\overline{\beta}_n\beta_{n'}-\overline{\beta}_{n'}\beta_n),\quad 1\leqslant n<n'\leqslant N, \tag{70}$$

$$J^d_{nn}=\frac{1}{2}\,\overline{\beta}\cdot(E_{nn}-E_{n+1\,n+1})\beta=\frac{1}{2}(\overline{\beta}_n\beta_n-\overline{\beta}_{n+1}\beta_{n+1}),\quad n=1,...,N-1. \tag{71}$$

The matrices $E_{nn'}$ are of size $N\times N$ with elements

$$(E_{nn'})_{kk'}=\delta_{nk}\delta_{n'k'},\quad n,n',k,k'=1,...,N, \tag{72}$$

i.e., the only nonzero elements are equal to one at position (n,n'), and they generate the Lie algebra $u(n)$ with respect to the matrix commutator.[21] This property is inherited by the N^2 phase-space functions

$$J_{nn'}=\overline{\beta}\cdot E_{nn'}\beta\equiv\overline{\beta}_n\beta_{n'}; \tag{73}$$

their Poisson brackets,

$$\{J_{nn'},J_{kk'}\}=i(\delta_{nk'}J_{kn'}-\delta_{n'k}J_{nk'}), \tag{74}$$

also realize the algebraic relations of $u(N)$.

It is possible to find (N^2-1) linear combinations of the matrices $E_{nn'}$ which are traceless and Hermitian—hence they provide a basis of the algebra su(N). In fact, these combinations have been introduced already in Eq. (69) when defining $J^s_{nn'}$, $J^a_{nn'}$, and J^d_{nn}. Therefore, these functions form a basis of the algebra su(N) with respect to the Poisson bracket. When supplemented by (a multiple of) the Hamiltonian

$$J_0=\frac{1}{2}\overline{\beta}\cdot\mathbf{1}_N\beta=\frac{1}{2}\sum_{n=1}^{N}\overline{\beta}_n\beta_n\equiv\frac{2}{\omega}H, \tag{75}$$

where $\mathbf{1}_N$ is the N-dimensional unit matrix, the algebra $u(n)$ can be recovered.

C. Vector fields

There is a first group of transformations which acts in the space of invariants Υ. As before, it is the set of finite transformations on the space generated by the real invariants (69)–(71). In other words, it arises from integrating the adjoint representation of the algebra formed by the invariants. As this group will play no role in the following, its discussion is suppressed.

Next, the invariants $J^s_{nn'}$ and $J^a_{nn'}$ generate canonical linear maps in the reduced space $\Gamma_{\mathbf{m}}$,

$$\frac{d\beta_k}{d\tau}=\{\beta_k,J^s_{nn'}\}=\frac{i}{2}(\delta_{kn}\beta_{n'}+\delta_{kn'}\beta_n)\equiv(J^s_{nn'}\beta)_k, \tag{76}$$

$$\frac{d\beta_k}{d\tau}=\{\beta_k,J^a_{nn'}\}=\frac{1}{2}(\delta_{kn}\beta_{n'}-\delta_{kn'}\beta_n)\equiv(J^a_{nn'}\beta)_k, \tag{77}$$

and similar ones follow when taking J^d_{nn} as generator. These linear equations can be integrated in the space $\Gamma_{\mathbf{m}}$ for arbitrary initial values $\beta(0)=\beta_0\in\Gamma_{\mathbf{m}}$,

$$\beta(\tau)=\exp(\tau J^{\varepsilon}_{nn'})\beta_0,\quad \varepsilon=a,s. \tag{78}$$

The solutions are unitary maps of $\Gamma_{\mathbf{m}}$ to itself. In analogy to the two-dimensional case, they will be denoted by

$$\beta(\tau)=\mathrm{Exp}[\tau J^{\varepsilon}_{nn'}](\beta),\quad \varepsilon=a,s, \tag{79}$$

and similarly for finite transformations generated by the invariants J^d_{nn}. Due to the linearity of the equations, no ambiguities arise upon integration. Therefore, the set of transformations in the reduced space $\Gamma_{\mathbf{m}}$ is isomorphic to the group SU(N). In this restricted sense, the **m**-oscillator has the special unitary group in N dimensions as a symmetry group. This group of symmetry transformations is *not* defined in the phase space Γ of the **m**-oscillator but only in $\Gamma_{\mathbf{m}}$.

Finally, a genuine ''pullback'' of SU(N) in phase space Γ does not exist, for the same reasons as in the case $N=2$. In fact, it is sufficient to consider a pair of oscillators with frequencies ω/m_n and $\omega/m_{n'}$, say, in order to see that there are obstructions which prevent the existence of a *global* symmetry group in phase space Γ. This pair of degrees of freedom is equivalent to a two-dimensional $(m_n,m_{n'})$-oscillator, and no set of transformations acting on it can be found which would be isomorphic to SU(2). If, however, the N-dimensional oscillator would have the full symmetry SU(N), a subgroup SU(2) should be associated with this pair of oscillators. Consequently, the group SU(N) cannot be identified as a symmetry group of the canonical N-dimensional commensurate oscillator. In analogy to the two-dimensional commensurate oscillator it is seen to have a *faint* SU(N) symmetry only.

D. The m-oscillator with common divisors

The canonical **m**-oscillator has been shown to be invariant under transformations isomorphic to the group SU(N) in the reduced space $\Gamma_{\mathbf{m}}$. For canonical and isotropic N-dimensional oscil-

lators, subsystems of dimension $N'<N$ are invariant only with respect to a subalgebra $\mathcal{A}_{\mathbf{m}'}$ of the algebra $\mathcal{A}_{\mathbf{m}}=\mathrm{su}(N)$. If the oscillator is neither isotropic nor canonical, other possibilities arise.

A noncanonical oscillator is characterized by frequencies $\mathbf{m}=(m_1,\ldots,m_N)$ with at least one pair (m_k,m_l) having a common integer divisor different from one. Let $N'<N$ frequencies have a common divisor. Then, for the $\mathbf{m}'$-oscillator corresponding to these frequencies, constants of motion do exist which form an algebra $\mathcal{A}_{\mathbf{m}'}=\mathrm{su}(N')$. This algebra, however, is *not* a subalgebra of $\mathcal{A}_{\mathbf{m}}$ as follows immediately from considering the $\mathbf{m}'$-oscillator as an N'-dimensional commensurate oscillator in its own right. Suppose that, after removing the common divisor, the resulting oscillator, characterized by $\mathbf{m}'=(m_1',\ldots,m_{N'}')$, is a canonical one. Then one can construct a group of symmetry transformations $\mathrm{SU}(N')$ in the reduced phase space $\Gamma_{\mathbf{m}'}$, and $\Gamma_{\mathbf{m}'}$ is *not* a subspace of $\Gamma_{\mathbf{m}}$. The Poisson brackets of the generators of $\mathrm{SU}(N')$ acting in $\Gamma_{\mathbf{m}'}$ and those of $\mathrm{SU}(N)$ acting in $\Gamma_{\mathbf{m}}$ will not be linear combinations of the initial ones. Hence, the combination of these two algebras will not close under the Lie product—the resulting algebra will be *infinite*. This property will be important for quantum mechanical commensurate oscillators since it entails additional degeneracies of energy which otherwise appear to be accidental.

Turn these results around: there is no finite algebra to account for all the symmetries of a noncanonical $\mathbf{m}$-oscillator. Obviously, this situation can arise only if $N\geqslant 3$ (if $N=2$ any common divisor can be factored out immediately). In fact, if $m_{n'}'=1$, $n'=1,\ldots,N'$, the subsystem is even an isotropic oscillator, and it has a group $\mathrm{SU}(N')$ of symmetry transformations on phase space Γ.

It is helpful to illustrate this discussion by an exhaustive list of ''classes'' for small values of N.

$\diamond$ $N=2$: A commensurate oscillator is either isotropic or canonical (a common divisor of the frequencies $m_1\neq m_2$ can be factored out).

$\diamond$ $N=3$: Five classes of commensurate oscillators can be identified. An $\mathbf{m}$-oscillator is either isotropic or canonical, or it belongs to one of the three following classes:

(1) a single pair of two frequencies have a common divisor, $\mathbf{m}=(jm_1',jm_2',m_3)$, say;
(2) two pairs have common but different divisors, $\mathbf{m}=(jm_1',jkm_2',km_3')$, say;
(3) all three pairs have common but different divisors, $\mathbf{m}=(jkm_1',klm_2',ljm_3')$, say.

For $N>3$ the number of different classes increases rapidly with N.

Consider an example of type 1 for $N=3$ in detail. The three coordinates β_n of the space $\Gamma_{\mathbf{m}}$ allow one to define eight constants of motion J. In addition, introduce coordinates of the reduced phase space $\Gamma_{\mathbf{m}'}$,

$$\beta_n'=\frac{|\alpha_n|}{\sqrt{m_n'}}\left(\frac{\alpha_n}{|\alpha_n|}\right)^{m_n'},\quad n=1,2. \tag{80}$$

The four functions

$$J_{nn'}'=\overline{\beta}_n'\beta_{n'}',\quad n,n'=1,2, \tag{81}$$

are a different set of constants of motion because the Hamiltonian of the subsystem (1,2) has an overall factor $1/k$. The constants J' are the basis of a Lie algebra $\mathcal{A}_{\mathbf{m}'}$ isomorphic to su(2) (setting aside the fourth commuting invariant), as the subsystem is an $\mathbf{m}'$-oscillator with $N=2$. The resulting algebra $\mathcal{A}_{\mathbf{m}'}$ gives rise to another faint SU(2) symmetry. It is, however, *neither* a subalgebra of the faint $\mathrm{SU}(N)$ symmetry (as it it implemented on a different reduced phase space $\Gamma_{\mathbf{m}'}$) *nor* do the generators of $\mathcal{A}_{\mathbf{m}}$ and $\mathcal{A}_{\mathbf{m}'}$ commute. Consequently, the union of both algebras gives rise to an infinite algebra. Finally, if $m_1'=m_2'=1$, three of the functions J' would generate the group SU(2) on the original phase space Γ. In other words, the faint $\mathrm{SU}(N)$ symmetry of an $\mathbf{m}$-oscillator with common divisors is compatible with the existence of smaller groups acting globally in phase space Γ.

VI. SUMMARY AND OUTLOOK

This article deals with the problem which symmetry group to associate with an N-dimensional *commensurate* harmonic oscillator. Historically, structural similarities to the isotopic oscillator seemed to indicate that the introduction of rational frequency ratios $m_n/m_{n'}$ would not affect the existence of the group SU(N) of symmetry transformations. This suggestion was based on the following observations. Arbitrary rational frequency ratios $m_n/m_{n'}$, are still compatible with the existence of $(2N-1)$ globally defined invariants. In both cases, the invariants confine trajectories to a one-dimensional manifold in phase space, the orbit. Furthermore, the invariants form an algebra su(N) with respect to the Poisson bracket. There is, however, a subtle difference between an isotropic and a commensurate oscillator: isotropy forces all orbits to have the *same* period whereas commensurate frequencies allow for orbits with *different* periods. Consequently, these system *are* distinguishable from an experimental point of view.

It has been shown that the algebra su(N) of the commensurate oscillator cannot be extended globally to a representation of the group SU(N) in phase space. Strictly speaking, it is thus not possible to attribute this group as a symmetry group to the commensurate harmonic oscillator. The group SU(N) is associated with commensurate oscillators in a restricted sense only: to do so, the action of the invariants must be considered in a *reduced* phase space the points of which are no longer in a one-to-one correspondence with the states of the system. The commensurate oscillator is said to have a *faint* SU(N) *symmetry*. Furthermore, if the rationally related frequencies have common divisors, additional sets of symmetry transformations can be found. They are not subgroups of the faint group SU(N), which acts in reduced phase, but they act in different reduced phase spaces.

To conclude, it has been shown that the symmetries of commensurate harmonic oscillators come in a surprisingly rich variety and depend in a subtle way on the frequency ratios. Classical and quantum mechanical oscillators are closely related. Therefore, it will be promising to study the impact of faint symmetries on the Hilbert-space structure of quantum mechanical commensurate oscillators.[3] In particular, a systematic group-theoretical account of their degenerate energy levels is expected to benefit from the concept of faint symmetry.

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On a low energy bound in a class of chiral field theories with solitons

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A low energy bound for static classical solutions in a class of chiral solitonic field theories related to the infrared physics of the SU(N) Yang–Mills theory is established. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1488671]

I. THE MODEL

Consider $N-1$ smooth fields $n_a=n_a(x)$ in space–time taking their values in the Lie algebra of SU(N). The fields are chosen to be commutative $[n_a,n_b]=0$ and orthonormal $(n_a,n_b)=\delta_{ab}$ with respect to the Cartan–Killing form in the Lie algebra. For any two Lie algebra elements ξ and η, the Cartan–Killing form is defined as $(\xi,\eta)=\mathrm{tr}(\hat{\xi}\hat{\eta})$ where the operator $\hat{\xi}$ acts on the Lie algebra as a Lie derivative $\hat{\xi}\eta=[\xi,\eta]$. There can only be $N-1$ mutually commutative and linearly independent elements in the Lie algebra of SU(N) because the rank of SU(N) is $r=N-1$ (the dimension of the Cartan subalgebra). If h_a form an orthonormal basis in the Cartan subalgebra in a matrix representation of SU(N), then

$$n_a(x)=U^{\dagger}(x)h_aU(x), \tag{1}$$

where $U^{\dagger}(x)\in \mathrm{SU}(N)$. In Eq. (1) U($x$) is defined modulo the left multiplication by elements from the Cartan subgroup generated by h_a [the maximal Abelian subgroup $T=U(1)^{N-1}$]. So, in fact, $U(x)\in \mathrm{SU}(N)/T$ since any group element can be represented as a product of an element of T and an element of the quotient $\mathrm{SU}(N)/T$. Under the condition that n_a approaches fixed constant values at the spatial infinity, $n_a(x)\to h_a$, i.e., $U(x)$ approaches the group unity, the fields n_a define a map of a spatial three-sphere $\mathbf{S}^3$ into the manifold $\mathrm{SU}(N)/T$ for every moment of time. The third homotopy group of this map is nontrivial $\pi_3(G/T)\sim Z$, $G=\mathrm{SU}(N)$. When $N=2$, the only field n_1 can be regarded as a unit three-vector. It is a Hopf map: $\mathbf{S}^3\to\mathbf{S}^2\sim \mathrm{SU}(2)/U(1)$. The corresponding topological number is the Hopf invariant which can also be interpreted as a linking number of two curves in $\mathbf{S}^3$ being preimages of two distinct points of $\mathbf{S}^2$. The two-forms $F^a=F^a_{jk}\,dx^j\wedge dx^k$, $j,k=1,2,3$, where

$$F^a_{jk}=iN\sum_b\,(n_a,[\partial_j n_b,\partial_k n_b]) \tag{2}$$

are closed, that is, $F^a_{jk}=\partial_jC^a_k-\partial_kC^a_j$. This is proved at the end of Sec. II. The forms F^a may not be exact. This follows from the fact that the cohomology ring $H^*(G/T)$ is rationally generated by $H^2(G/T)$.[1] The topological number of the map $\mathbf{S}^3\to G/T$ should be constructed out of the two-forms $F^a=iN(n_a,\Sigma_b[dn_b,dn_b])$ on G/T. Introducing the field $B^a_i=1/2\epsilon_{ijk}F^a_{jk}$ with ϵ_{ijk} being the Levi-Chevita tensor, the topological number of the above-mentioned map can be written as

$$Q=(16\pi^2N)^{-1}\int dx\sum_{i,a}\,C^a_iB^a_i\,. \tag{3}$$

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For SU(2), Q is a Hopf invariant. Since $\mathrm{SU}(2)/U(1)\subset G/T$, the normalization coefficient in (3) can be chosen so that Q is an integer when n_a realize a Hopf map.

An explicit realization of the Hopf map by the fields n_a is as follows. Consider the Cartan–Weyl basis in the Lie algebra. Let α be a positive root. For every positive root α, there are two basis elements e_α and $e_{-\alpha}=\overline{e_\alpha}$ such that for any element h from the Cartan subalgebra

$$[h,e_\alpha]=(h,\alpha)e_\alpha, \tag{4}$$

$$[e_\alpha,e_{-\alpha}]=\alpha, \quad [e_\alpha,e_\beta]=N_{\alpha,\beta}e_{\alpha+\beta}, \tag{5}$$

where $N_{\alpha,\beta}\neq 0$ if $\alpha+\beta$ is a root. Note that the elements α, e_α, and $e_{-\alpha}$ form a basis of an SU(2) subalgebra (associated with the root α). Let $U_\omega(x)\in \mathrm{SU}(2)/U(1)\subset \mathrm{SU}(N)/T$ where the subgroup SU(2) is associated with a simple root ω. One can always choose $h_1=N^{1/2}\omega$. The norm of any root of SU(N) is $1/N$ with respect to the Cartan–Killing form (see Sec. II). Then $n_1(x)=N^{1/2}U_\omega^\dagger\omega U_\omega$ is a Hopf map. The other fields realize a trivial map, $n_a=h_a$, $a>1$. Indeed, $U_\omega(x)=\exp[iu_\omega(x)]$ where $u_\omega(x)=\varphi_\omega(x)e_\omega+\overline{\varphi}_\omega(x)e_{-\omega}$. For $a>1$, it follows from (4) that $n_a=U_\omega^\dagger h_a U_\omega=h_a$ because $(\omega,h_a)\sim(h_1,h_a)=0$. Now, if we introduce an orthonormal basis in the SU(2) subgroup, $\tau_1=i(e_\omega-e_{-\omega})/\sqrt{2}$, $\tau_2=(e_\omega+e_{-\omega})/\sqrt{2}$, and $\tau_3=\sqrt{N}\omega$, then $[\tau_j,\tau_k]=iN^{-1/2}\epsilon_{jkn}\tau_n$. Let $\mathbf{n}$ be an isotopic unit three-vector whose components are (τ_j,n_1). It defines the Hopf map by construction. From (2) we infer that $F^a_{jk}=\delta^{a1}\sqrt{N}\mathbf{n}\cdot(\partial_j\mathbf{n}\times\partial_k\mathbf{n})$. Hence our B^a_j and C^a_j contain an extra factor $\sqrt{N}$ when the fields n_a realize a Hopf map associated with an SU(2) subgroup of SU(N). This explains the normalization factor N^{-1} in (3). Since all the roots have the same norm in SU(N), the normalization coefficient in (3) for any SU(2) subgroup has to be the same. The root system is invariant under the Weyl symmetry, and so should be Q. The sum over a in (3) provides this invariance.

The dynamics of the fields n_a is determined by the Lagrangian density

$$\mathcal{L}=m^2\sum_{\mu,a}(\partial_\mu n_a,\partial_\mu n_a)-\frac{g}{4}\sum_{\mu,\nu,a}F^a_{\mu\nu}F^a_{\mu\nu}, \tag{6}$$

$\mu,\nu=0,1,2,3$; and ∂_0 stands for the time derivative. In the case of SU(2), this Lagrangian density describes the Faddeev model[2] for knot solitons. The knot solitons have been extensively studied numerically.[3] The model (6) has been introduced in Ref. 4 and may also have solitonic solutions. The Lagrangian (6) is believed to describe (in a certain approximation) the infrared physics of the SU(N) Yang–Mills theory.[4–6] Recent analytical[7] and lattice[8,9] studies of this correspondence in the SU(2) case look promising.

Due to the Lorentz symmetry of the Langrangian density, a Lorentz transformation of a static solution is a time-dependent solution of the Euler–Lagrange equations for (6). Solutions that describe interacting solitons are not static (even modulo Lorentz transformations). In this paper a low energy bound for static solitons with a topological number Q is established:

$$E\geqslant c_N|Q|^{3/4}, \tag{7}$$

$$c_N=8\pi^2 3^{3/8}\left(\frac{2N^3}{N^2-N-1}\right)^{1/4}\sqrt{m^2 g}, \tag{8}$$

where E is the energy functional

$$E=m^2\int \mathrm{d}x\sum_{j,a}(\partial_j n_a,\partial_j n_a)+\frac{g}{2}\int \mathrm{d}x\sum_{j,a}B^a_jB^a_j \tag{9}$$

$$\equiv\int \mathrm{d}x(\mathcal{E}_2(x)+\mathcal{E}_4(x))\equiv E_2+E_4. \tag{10}$$

For the Faddeev–Hopf knot solitons the low energy bound was found in Ref. 10 and improved in Refs. 11 and 12 (meaning a larger constant c_2). Beyond conventional perturbation theory, the Yang–Mills quantum dynamics can be studied by the large N expansion method with the purpose to establish a relation (duality) to a string theory on some manifold. Therefore it is of interest to investigate the N dependence of the low energy bound for solitons in the model (6).

II. NOTATIONS AND NECESSARY FACTS

We would need the following algebraic inequalities. Let a_i, $b_i \geqslant 0$, $a=\Sigma_i a_i$, $b=\Sigma_i b_i$, and $\gamma \geqslant 1$. Then

$$a_1^\gamma + a_2^\gamma + \cdots + a_r^\gamma \leqslant a^\gamma, \tag{11}$$

$$\sqrt{a} \leqslant \sqrt{a_1} + \sqrt{a_2} + \cdots + \sqrt{a_r} \leqslant \sqrt{r}\sqrt{a}, \tag{12}$$

$$\sum_i a_i^p b_i^q \leqslant a^p b^q, \quad p+q=1. \tag{13}$$

Define $p_i = a_i/a \leqslant 1$. Then $\Sigma_i p_i = 1$. The inequality (11) follows from an obvious inequality $p_i^\gamma \leqslant p_i$ if one takes the sum over i. The second inequality is proved by squaring it and applying the basic algebraic inequality $\sqrt{a_i}\sqrt{a_j} \leqslant 1/2(a_i + a_j)$. The third inequality is an algebraic Hölder inequality (see, e.g., Ref. 13).

An arrow is used to denote vectors in space, e.g., $\vec{\partial}\phi = (\partial_1\phi, \partial_2\phi, \partial_3\phi)$ for the gradient. The scalar product for two vector fields is

$$\langle \vec{u}, \vec{v} \rangle = \int \mathrm{d}x \vec{u} \cdot \vec{v}. \tag{14}$$

The L_p norm of a vector field reads

$$\|\vec{u}\|_p = \left[\int \mathrm{d}x (\vec{u} \cdot \vec{u})^{p/2} \right]^{1/p}. \tag{15}$$

The following functional inequalities are used in the sequel

$$|\langle \vec{u}, \vec{v} \rangle| \leqslant \|\vec{u}\|_p \|\vec{v}\|_q, \quad p^{-1} + q^{-1} = 1, \tag{16}$$

$$\|\vec{u}\|_{6/5} \leqslant \|\vec{u}\|_1^{2/3} \|\vec{u}\|_2^{1/3}, \tag{17}$$

$$\|\vec{u}\|_6 \leqslant \lambda_1 \|\mathrm{curl}\, \vec{u}\|_2, \quad \lambda_1 = (48)^{1/6} (3\pi)^{-2/3}. \tag{18}$$

The first two inequalities are Hölder-type inequalities.[13] The third one follows from Rosen's result for scalar functions[14] (cf. Ref. 11)

$$\|\phi\|_6 \leqslant \lambda_1 \|\vec{\partial}\phi\|_2, \tag{19}$$

where the L_p norm for scalar functions is defined by (15) for one-dimensional vectors. Let $\phi = (\vec{u} \cdot \vec{u})^{1/2}$. We have

$$\vec{\partial}\phi \cdot \vec{\partial}\phi = \phi^{-2} \sum_j (\partial_j \vec{u} \cdot \vec{u})^2 \leqslant \sum_j \partial_j \vec{u} \cdot \partial_j \vec{u}.$$

Making use of this inequality, we infer (18) from (19):

$$\|\vec{u}\|_6=\|\phi\|_6\leqslant\lambda_1\|\vec{\partial}\phi\|_2\leqslant\lambda_1\left[\int dx\sum_{i,j}(\partial_j u_i)^2\right]^{1/2}=\lambda_1\|\mathrm{curl}\,\vec{u}\|_2. \tag{20}$$

The last equality in (20) is true if $\mathrm{div}\,\vec{u}=0$ and $\vec{u}$ decreases sufficiently fast at spatial infinity, which we require in (18). The coefficient λ_1 is the least possible coefficient in inequality (18).[14]

Let ω_a, $a=1,2,\ldots,r$, be simple roots of SU(N). They have the same norm $(\omega_a,\omega_a)\equiv\gamma^2$. The angle between ω_a and $\omega_{a\pm1}$ is $2\pi/3$, and otherwise the roots are perpendicular. Any positive root can be written in the form $\alpha=\omega_a+\omega_{a+1}+\cdots+\omega_{a+q}$ for $a+q\leqslant r$. From this it is easy to deduce that all roots have the same norm with respect to the Cartan–Killing form, $(\alpha,\alpha)=\gamma^2$. To find the actual norm γ, one should compute, say, the matrix $\hat{\omega}_1$ in the Cartan–Weyl basis and take the trace of its square. From (4) it follows that $\hat{\omega}_1$ is block diagonal. The block associated with the Cartan subalgebra is zero because ω_a commute amongst each other. The nontrivial blocks come from the subspaces spanned by e_α and $e_{-\alpha}$ where the positive root α is either equal to ω_1 or contains ω_2 or $\omega_1+\omega_2$. There are $r-1$ roots containing ω_2 and $r-1$ roots containing $\omega_1+\omega_2$. Then $\gamma^2=\mathrm{tr}\,(\hat{\omega}_1^2)=\gamma^4 N$ as is deduced from (4). Hence

$$(\omega_a,\omega_a)=N^{-1}. \tag{21}$$

As a consequence of (21), the following identity holds for any Lie algebra element v:

$$v=\sum_a n_a(n_a,v)+N\sum_a[n_a,[n_a,v]]\equiv v_\parallel+v_\perp. \tag{22}$$

The proof is based on the following observation. Relation (22) is covariant under the adjoint action of SU(N). So, according to (1), n_a can be replaced by h_a after a corresponding adjoint rotation of v. Decomposing v in the Cartan-Weyl basis, one can see that the first term in (22) is the Cartan component of v. The double commutator in the second term can be computed by means of (4) and gives rise to the factor $\Sigma_a(\alpha,h_a)^2=(\alpha,\alpha)=N^{-1}$ for every basis element e_α. Thus the second term in (22) is nothing but a projector onto the subspace orthogonal to the Cartan subalgebra spanned by n_a.

By differentiating (1) one finds

$$\partial_\mu n_a+i[A_\mu,n_a]=0, \tag{23}$$

$$i\partial_\mu U^\dagger U\equiv A_\mu-\sum_a n_a C_\mu^a,\quad (n_a,A_\mu)=0. \tag{24}$$

Equation (23) can be interpreted as: The fields n_a are transported parallel with respect to the connection A_μ. Taking a commutator of (23) with n_a, summing over a and making use of the identity (22), the connection A_μ can be explicitly written via n_a,

$$A_\mu=iN\sum_a[\partial_\mu n_a,n_a]. \tag{25}$$

The connection (25) has been introduced by Cho to study monopoles in the Yang–Mills theory for SU(2) and SU(3).[15] By multiplying (23) by n_b using the Cartan–Killing form, one deduces that the derivatives of n_a are orthogonal to the fields themselves

$$(\partial_\mu n_a,n_b)=0. \tag{26}$$

Now we show that the tensor (2) is an Abelian gauge field tensor (cf. Refs. 4 and 6), that is, the two-forms F^a are closed, $dF^a=0$. Consider the following algebraic transformations:

$$\partial_\mu A_\nu - \partial_\nu A_\mu = 2iN \sum_a [\partial_\nu n_a, \partial_\mu n_a] = 2iN \sum_a [[A_\mu, n_a], [A_\nu, n_a]], \tag{27}$$

$$= 2iN \sum_a \{[A_\nu, [n_a, [n_a, A_\mu]]] + [n_a, [[n_a, A_\mu], A_\nu]]\}, \tag{28}$$

$$= 2i[A_\nu, A_\mu] + iN \sum_a [n_a, [n_a, [A_\mu, A_\nu]]], \tag{29}$$

$$= -i[A_\mu, A_\nu] - i \sum_a n_a (n_a, [A_\mu, A_\nu]). \tag{30}$$

In (27) we have used (25); next, $\partial_\mu n_a$ has been transformed via (23); Eq. (28) follows from the Jacobi identity; to derive (29), the first term in (28) has been transformed by means of the algebraic identity (22), while the second one via the Jacobi identity; finally, by applying the algebraic identity (22) to (29), Eq. (30) has been deduced. Introducing the Yang–Mills field strength tensor

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + i[A_\mu, A_\nu], \tag{31}$$

it follows from (30) that

$$F_{\mu\nu} = i \sum_a n_a (n_a, [A_\mu, A_\nu]) = \sum_a n_a F^a_{\mu\nu}. \tag{32}$$

The last equality in (32) is deduced by multiplying (30) and the middle of (27) by n_a using the Cartan–Killing form. Now observe that the field strength (curvature) of the pure gauge connection (24) is zero. Making use of the decomposition (24) of a pure gauge connection we obtain

$$0 = F_{\mu\nu} - \sum_a n_a (\partial_\mu C^a_\nu - \partial_\nu C^a_\mu), \tag{33}$$

where the identity (23) has been used again for algebraic transformations. Thus, $F^a_{\mu\nu} = \partial_\mu C^a_\nu - \partial_\nu C^a_\mu$. Note that (24) allows one to determine C^a_μ via the group element U explicitly. In (3) the vector potential C^a_i can always be chosen to satisfy the Coulomb gauge, $\partial_i C^a_i = 0$, thanks to the gauge freedom $C^a_\mu \to C^a_\mu + \partial_\mu \xi^a$.

III. A KEY ALGEBRAIC INEQUALITY

In this section the following inequality is proved

$$\mathcal{E}_4 \leqslant \kappa_N \mathcal{E}_2^2, \quad \kappa_N = \frac{gN}{4m^4}\left(1 - \frac{1}{N^2 - N}\right). \tag{34}$$

It is used in Sec. IV to establish the low energy bound. Consider the $(N^2-1)\times(N^2-1)$ matrix

$$G = \sum_{i,b} \partial_i n_b \otimes \partial_i n_b .$$

It can be regarded as a linear operator on the Lie algebra, i.e., $G\eta = \Sigma_{i,b}\, \partial_i n_b (\partial_i n_b, \eta)$ for any Lie algebra element η. It has $N-1$ zero eigenvalues because $G n_a = 0$. The matrix G satisfies

$$\operatorname{tr} G^2 \geqslant \frac{1}{N^2 - N} (\operatorname{tr} G)^2. \tag{35}$$

The proof is simple. Let g_k, $k=1,2,\ldots,n=N^2-N$, be nonzero eigenvalues of G. They are real since $G=G^T$ with respect to the Cartan–Killing form. Consider a function of one real variable ξ, $f(\xi)=\Sigma_k(g_k-\xi)^2$. Computing the sum explicitly, one finds that $f(\xi)=\mathrm{tr}\,G^2-2\xi\,\mathrm{tr}\,G+\xi^2 n$. The function attains its absolute minimum at $\xi=\xi_0=\mathrm{tr}\,G/n$. Since $f(\xi)\geqslant 0$ for all ξ's, the inequality (35) follows from $f(\xi_0)\geqslant 0$.

Consider a local Cartan–Weyl basis which is obtained by an adjoint transformation of the basis (4), (5) with the group element $U(x)$ defined in (1). Denoting $n_\alpha=U^\dagger e_\alpha U$ and $n_{-\alpha}=U^\dagger e_{-\alpha}U=\overline{n_\alpha}$ we have

$$[n_a,n_\beta]=(h_a,\beta)n_\beta,\quad [n_\alpha,n_{-\alpha}]=U^\dagger\alpha U\equiv\alpha_U, \tag{36}$$

where $(\alpha_U,n_a)=(\alpha,h_a)$ and $(n_a,n_\beta)=0$, $(n_\alpha,n_{-\alpha})=1$, $(n_\alpha,n_\alpha)=(n_{-\alpha},n_{-\alpha})=0$.

To establish a relation between $\mathcal{E}_4$, $\mathcal{E}_2$ and G, we decompose the connection (25) in the local Cartan–Weyl basis

$$A_i=\sum_{\alpha>0}(A_i^\alpha n_\alpha+\text{c.c.})\equiv H_i+\overline{H}_i. \tag{37}$$

Then we obtain

$$\mathcal{E}_2=m^2\,\mathrm{tr}\,G=-m^2\sum_{i,b}([A_i,n_b],[A_i,n_b])=\frac{m^2}{N}\sum_i(A_i,A_i)=\frac{2m^2}{N}\sum_i(\overline{H}_i,H_i). \tag{38}$$

The second equality follows from (23); the third one is a consequence of (22) and (24). Making use of (32) we also get

$$\mathcal{E}_4=-\frac{g}{4}\sum_{a,i,j}(n_a,[A_i,A_j])^2 \tag{39}$$

$$=-\frac{g}{4}\sum_{\alpha,\beta>0}\sum_{i,j}(A_i^\alpha\overline{A}_j^\alpha-\text{c.c.})(\alpha,\beta)(A_i^\beta\overline{A}_j^\beta-\text{c.c.})$$

$$\leqslant-\frac{g}{4N}\sum_{i,j}[(H_i,\overline{H}_j)-\text{c.c.}]^2. \tag{40}$$

Note that the local Cartan component of $[A_i,A_j]$ can only come from the second commutation relation in (36). Hence the sum over a in (39) yields the factor $\Sigma_a(\alpha,h_a)(h_a,\beta)=(\alpha,\beta)=N^{-1}\cos\theta_{\alpha\beta}\leqslant N^{-1}$ for any two positive roots α and β with the angle $\theta_{\alpha\beta}$ between them. In a similar fashion we derive

$$\mathrm{tr}\,G^2=\sum_{a,b}\sum_{i,j}([A_i,n_a],[A_j,n_b])^2=\sum_{a,b}\sum_{i,j}(n_a,[[n_b,A_i],A_j])^2 \tag{41}$$

$$=\sum_{\alpha,\beta>0}\sum_{i,j}(A_i^\alpha\overline{A}_j^\alpha+\text{c.c.})(\alpha,\beta)^2(A_i^\beta\overline{A}_j^\beta+\text{c.c.})$$

$$\leqslant\frac{1}{N^2}\sum_{i,j}[(H_i,\overline{H}_j)+\text{c.c.}]^2. \tag{42}$$

Combining (42) and (40), we infer

$$4Ng^{-1}\mathcal{E}_4+N^2\,\mathrm{tr}\,G^2\leqslant 4\sum_{i,j}(H_i,\overline{H}_j)(H_j,\overline{H}_i)\leqslant 4\left(\sum_i(H_i,\overline{H}_i)\right)^2=4(\mathrm{tr}\,G)^2, \tag{43}$$

where the Schwartz inequality

$$|(H_i,\overline{H}_j)|^2 \leqslant (H_i,\overline{H}_i)(H_j,\overline{H}_j)$$

has been used. The inequality (34) immediately follows from (43), (38), and (35).

IV. THE LOW ENERGY BOUND

Let $\lambda_0=(16\pi^2 N)^{-1}$. Then Eq. (3) can be written as $Q=\lambda_0\Sigma_a\langle\vec{C}^a,\vec{B}^a\rangle$. Making use of (16) one gets (cf. the case $N=2$ in Ref. 10)

$$|Q| \leqslant \lambda_0 \sum_a \|\vec{C}^a\|_p \|\vec{B}^a\|_{p'} \tag{44}$$

$$\leqslant \lambda_0\lambda_1 \sum_a \|\mathrm{curl}\,\vec{C}^a\|_2 \|\vec{B}^a\|_{6/5} \tag{45}$$

$$= \lambda_0\lambda_1 \sum_a \|\vec{B}^a\|_2 \|\vec{B}^a\|_{6/5}$$

$$\leqslant \lambda_0\lambda_1 \sum_a \|\vec{B}^a\|_2 \|\vec{B}^a\|_2^{1/3} \|\vec{B}^a\|_1^{2/3}. \tag{46}$$

To get (45), Eq. (18) has been used, which dictated the choice $p=6$ in (44), and also $\partial_i C_i^a=0$; then the substitution $\vec{B}^a=\mathrm{curl}\,\vec{C}^a$ has been made; the last inequality (46) is a consequence of (17). The energy can be written as

$$E = m^2 \sum_a \|\vec{\partial}\, n_a\|_2^2 + \frac{g}{2}\sum_a \|\vec{B}^a\|_2^2 = \sum_a (E_{2a}+E_{4a}) = E_2+E_4. \tag{47}$$

Hence, continuing (46) we get

$$|Q| \leqslant \lambda_0\lambda_1 (2/g)^{2/3} \sum_a (E_{4a}^{4/3})^{1/2} (\|\vec{B}^a\|_1^{4/3})^{1/2} \tag{48}$$

$$\leqslant \lambda_0\lambda_1 (2/g)^{2/3} \left[\left(\sum_a E_{4a}\right)^{4/3}\right]^{1/2} \left[\left(\sum_b \|\vec{B}^b\|_1\right)^{4/3}\right]^{1/2} \tag{49}$$

$$= \lambda_0\lambda_1 (2/g)^{2/3} E_4^{2/3} \left[\sum_b \int dx \sqrt{\vec{B}_b\cdot\vec{B}_b}\right]^{2/3}$$

$$\leqslant \lambda_0\lambda_1 g^{-1} (2E_4)^{2/3} (N-1)^{1/3} \left[\int dx \sqrt{2\mathcal{E}_4}\right]^{2/3} \tag{50}$$

$$\leqslant \lambda_0\lambda_1 g^{-1} (2E_4E_2)^{2/3} [2(N-1)\kappa_N]^{1/3} \tag{51}$$

$$\leqslant \lambda_0\lambda_1 g^{-1} 2^{-2/3} [2(N-1)\kappa_N]^{1/3} E^{4/3} \tag{52}$$

$$= c_N^{-4/3} E^{4/3},$$

where the constant c_N is given in (8). To get (49), the Hölder inequality (13) for $p=q=1/2$ and then (11) for $\gamma=4/3$ have been applied; (50) follows from (12); the algebraic inequality (34) has been used to deduce (51); the final result (52), which is equivalent to (7), comes from the basic inequality $E_4E_2\leqslant E^2/4$.

If the Lagrangian (6) defines an effective theory of the SU(N) gauge fields in some approximation, then the coefficients m and g should depend on N, the Yang–Mills coupling constant and a mass scale that determines the energy range in which the approximation is valid.

The result (7) is trivially generalized to the case when the mass scales and coupling constants are different for each mode n_a, that is, m^2 and g are replaced by m_a^2 and g_a, respectively, and inserted into the corresponding sums over a in (6) (cf. Ref. 4). In this case, $m^2=\max_a\{m_a^2\}$ and $g=\max_a\{g_a\}$ in (8). Indeed, all the inequalities in Secs. III and IV still hold as a consequence of $m_a^2\leqslant m^2$ and $g_a\leqslant g$. Equality (38) becomes an inequality $m^2\,\mathrm{tr}\,G\leqslant\mathcal{E}_2$, which, however, does not affect our derivation of (34) from (43).

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The XXZ spin chain at $\Delta=-1/2$: Bethe roots, symmetric functions, and determinants

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A number of conjectures have been given recently concerning the connection between the antiferromagnetic XXZ spin chain at $\Delta=-1/2$ and various symmetry classes of alternating sign matrices. Here we use the integrability of the XXZ chain to gain further insight into these developments. In doing so we obtain a number of new results using Baxter's Q function for the XXZ chain for periodic, twisted and open boundary conditions. These include expressions for the elementary symmetric functions evaluated at the ground state solution of the Bethe roots. In this approach Schur functions play a central role and enable us to derive determinant expressions which appear in certain natural double products over the Bethe roots. When evaluated these give rise to the numbers counting different symmetry classes of alternating sign matrices. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The XXZ Heisenberg spin chain is a central and much studied model in statistical mechanics. It is arguably the best known model solved by means of the Bethe wave function Ansatz.[1] The ground state wave function at the particular anisotropy value $\Delta=-1/2$ has recently been the source of some surprising observations. At this value Razumov and Stroganov[2] observed the appearance of the numbers $A(n)=1,2,7,42,429,\ldots$, which count the number of $n\times n$ alternating sign matrices.[3–5] Here the length of the chain L is odd ($L=2n+1$) with periodic boundary conditions imposed. Alternating sign matrices are matrices whose elements are either $-1,0$ or 1 such that the elements along each row and each column alternate in sign. Furthermore, the entries in each row and column add up to $+1$. The numbers $A(n)$ are well known to enumerative combinatorialists, having appeared in other distinct problems such as the enumeration of plane partitions and generalizations of determinants. The one-to-one correspondence between vertex configurations of the square lattice ice model with domain wall boundary conditions[6] and ASM's has been well documented.[4,5] In particular it led to Kuperberg's alternate proof[7,8] of the alternating sign matrix conjecture.[3,4]

The numbers $A(n)$ appear in the ground state wave function of the XXZ Heisenberg chain at $\Delta=-1/2$ in three ways:[2] (i) as the ratio of the largest and smallest components in the ground state wave function, (ii) in the sum of the components, and (iii) in the sum of the square of the components. These observations at $\Delta=-1/2$ have been extended in a number of directions. Two other known cases are: (i) twisted boundary conditions[9] with L even,[10,11] and (ii) open boundary conditions with appropriate surface fields (the quantum $U_q[sl(2)]$ invariant chain[9,12,13]).[10] For both cases the ground state wave function is complex. Nevertheless, the sums of the wave function components and of their squares are real. The numbers $A(n)$ also appear in the twisted case. However, the open case sees the appearance of other symmetry classes. Here appear $A_V(2n+1)$, the number of $(2n+1)\times(2n+1)$ vertically symmetric alternating sign matrices when L

$=2n$ and $N_8(2n)$, the number of cyclically symmetric transpose complement plane partitions, when $L=2n-1$. The number $N_8(2n)$ is conjectured to be $A_{\mathrm{VH}}(4n+1)/A_{\mathrm{V}}(2n+1)$, where $A_{\mathrm{VH}}(4n+1)$ is the number of $(4n+1)\times(4n+1)$ vertically and horizontally symmetric alternating sign matrices.[14] These various numbers also appear in the corresponding O(1) loop model, for which the ground state wave function is real.[10] Further developments include the combinatorial interpretation[15–17] of the elements of the O(1) loop model wave function and the relation to a one-dimensional Temperley–Lieb stochastic process.[17]

The numerous conjectures made to date for the various ground state wave functions at $\Delta=-1/2$ remain to be proved. In earlier work, Stroganov and co-workers[18–20] have found an expression for Baxter's Q function[21] in each of the above cases. By definition the zeros of the Q function are the Bethe roots. However, little if any use has been made of this function. Here we use the Q function results to obtain closed form expressions for the values of the elementary symmetric functions with the ground state Bethe roots as arguments. This approach also involves the appearance of the Schur function and determinants in a natural way. Ultimately we are led to conjectures for new determinants whose values are related to the alternating sign matrix numbers. These results came from observations on the product of certain combinations of Bethe roots. Although some results can be proved along the way, the evaluation of the determinants, involving the elementary symmetric functions, remains to be done exactly.

The layout of this paper is as follows. In Sec. II we collect some necessary results on the Bethe Ansatz and symmetric polynomials. In Sec. III we give our results for the periodic (L odd), twisted and reflecting boundary cases. Some detailed working is given in the Appendix. The paper concludes with some remarks in Sec. IV.

II. PRELIMINARIES

A. XXZ spin chain and Bethe's Ansatz

We consider the periodic anisotropic quantum XXZ spin chain. A spin variable lives on each site of the chain taking either up or down values. The interaction between two neigboring spins is described in terms of Pauli spin matrices by the well known Hamiltonian,

$$H=-\frac{1}{2}\sum_{j=1}^{L}(\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y+\Delta\sigma_j^z\sigma_{j+1}^z), \tag{1}$$

where the anisotropy Δ is parametrized by

$$\Delta=-\tfrac{1}{2}(q+q^{-1}). \tag{2}$$

We denote the position of the ith down spin along the chain by x_i. The Hamiltonian (1) is diagonalized via the Ansatz,[1]

$$\psi(x_1,\ldots,x_n)=\sum_{\pi}A^{\pi_1\cdots\pi_n}\prod_{j=1}^{n}z_{\pi_j}^{x_j} \tag{3}$$

for the form of its eigenvectors. The sum over $\pi=(\pi_1,\ldots,\pi_n)$ denotes a sum over all permutations of the numbers $1,\ldots,n$. Substituting (3) into the eigenvalue equation for H one finds the eigenvalues to be given by

$$E=-\tfrac{1}{2}L\Delta-\sum_{i=1}^{n}(z_i+z_i^{-1}-2\Delta). \tag{4}$$

The amplitudes $A^{\pi_1\cdots\pi_n}$ are also expressed in the variables z_i for which the consistency equations

$$z_i^L=(-)^{n-1}\prod_{j=1}^{n}\frac{1-2\Delta z_i+z_iz_j}{1-2\Delta z_j+z_iz_j} \tag{5}$$

are derived.

It will be convenient to make the change of variables

$$z=\frac{q-w}{qw-1},\quad w=\frac{z+q}{qz+1}, \tag{6}$$

for which the Bethe equations (5) take the form

$$\left(\frac{q-w_i}{qw_i-1}\right)^L+\prod_{j=1}^{n}\frac{w_i-q^2w_j}{q^2w_i-w_j}=0. \tag{7}$$

Up to a normalization, the amplitudes are given by

$$A^{\pi_1\cdots\pi_n}=q^{n(n-1)/2}\prod_{i<j}^{n}\frac{1-2\Delta z_{\pi_i}+z_{\pi_i}z_{\pi_j}}{z_{\pi_i}-z_{\pi_j}}=\prod_{i<j}^{n}\frac{w_{\pi_i}-q^2w_{\pi_j}}{w_{\pi_i}-w_{\pi_j}}. \tag{8}$$

Note that the eigenfunctions (3) are symmetric polynomials in the variables z_i. All properties of the XXZ spin chain can therefore be expressed in symmetric functions of these variables. We will review some of the basic properties of symmetric polynomials in the next section.

From (8) we see that the amplitudes can be written in terms of the generalized Vandermonde product,

$$\det_\lambda(w_i^{n-j})=\det_\lambda(w_j^{i-1})=\prod_{i<j}^{n}(w_i+\lambda w_j), \tag{9}$$

where we have introduced the λ-determinant[22] which can be defined recursively via Dodgson's algorithm for evaluating determinants.[4] If $X^{(1)}=(x_{ij}^{(1)})$ is an $n\times n$ matrix and $Y^{(1)}$ an $(n-1)\times(n-1)$ matrix with each element equal to 1, we define new matrices $X^{(k)}$ and $Y^{(k)}$ recursively by

$$x_{ij}^{(k)}=(x_{ij}^{(k-1)}x_{i+1,j+1}^{(k-1)}+\lambda x_{i+1,j}^{(k-1)}x_{i,j+1}^{(k-1)})/y_{ij}^{(k-1)},\quad i,j=1,\ldots,n-k+1, \tag{10}$$

$$y_{ij}^{(k)}=x_{i+1,j+1}^{(k-1)},\quad i,j=1,\ldots,n-k. \tag{11}$$

The number $X^{(n)}$ thus defined is called the λ-determinant of $X^{(1)}$. For the special value $\lambda=-1$ this procedure evaluates the ordinary determinant $\det X^{(1)}$. Just as the determinant can be written as a sum over the set of permutation matrices, the λ-determinant can be written as a sum over the set of alternating sign matrices,[22]

$$\det_\lambda M=\sum_{A\in\mathcal{A}_n}\lambda^{\mathcal{I}(A)}(1+\lambda^{-1})^{N(A)}\prod_{i,j=1}^{n}m_{ij}^{a_{ij}}, \tag{12}$$

where $\mathcal{A}_n$ is the set of $n\times n$ alternating sign matrices, $\mathcal{I}(A)$ is the inversion number of A and $N(A)$ the number of -1's in A (see e.g., Ref. 4 for the definiton of $\mathcal{I}$). The total number of terms in this sum, or equivalently the number of $n\times n$ alternating sign matrices is given by

$$A(n)=\prod_{j=0}^{n-1}\frac{(3j+1)!}{(n+j)!}=\prod_{i\leqslant j}^{n}\frac{n+i+j-1}{2i+j-1}. \tag{13}$$

We will see later that this and related numbers surprisingly show up in certain combinations of the variables z_i when evaluated at a particular solution of the Bethe equations (5) for $q=e^{i\pi/3}$.

B. Symmetric polynomials

This section is included for the convenience of the reader. The results collected herein can be found in standard textbooks such as Refs. 4 or 23.

A partition μ of k is a nonincreasing set of integers $\mu_1,\ldots,\mu_l$ such that $\mu_1+\cdots+\mu_l=k$. We denote this by $\mu\vdash k$. Partitions define the shape of a semistandard tableau, which is a two-dimensional array of integers with the restriction that these integers are nondecreasing across each row of length μ_j and strictly increasing down columns. An example of a semistandard tableau of shape $(4,4,3,1,1)$ is

$$\begin{array}{cccc} 1 & 1 & 2 & 3 \\ 2 & 3 & 4 & 4 \\ 4 & 4 & 5 & \\ 5 & & & \\ 6 & & & \end{array} .$$

A conjugate partition μ' or conjugate shape is the shape obtained by reflecting the semistandard tableau of shape μ in its main diagonal. For example, the conjugate partition of $(4,4,3,1,1)$ is $(5,3,3,2)$. The integers in the semistandard tableau may be interpreted as indices of variables, and thus to every semistandard tableau is associated a monomial in which the power of each variable is the number of times its index occurs in the tableau, e.g., for the example above the monomial is given by

$$w_1^2 w_2^2 w_3^2 w_4^4 w_5^2 w_6 .$$

Given a tableau T the corresponding monomial is denoted by $\mathbf{w}^T$. In this way one may associate with every tableau of shape μ a polynomial s_μ, called the Schur polynomial, by the definition

$$s_\mu(w_1,\ldots,w_n)=\sum_T \mathbf{w}^T, \tag{14}$$

where the sum is over all semistandard tableaux of shape μ with entries chosen from $\{1,\ldots,n\}$. If $\mu\vdash k$, s_μ is a polynomial of degree k. We will see later that the Schur function is a symmetric function.

The monomial symmetric function of degree k is defined by

$$m_\mu=\sum_\pi{}' \prod_{j=1}^{n} w_j^{\pi_j}, \tag{15}$$

where the sum is over all *distinct* permutations,

$$\pi=(\pi_1,\ldots,\pi_n) \text{ of the numbers } (\mu_1,\ldots,\mu_k,0,\ldots,0).$$

The elementary symmetric function of degree k in n variables is defined as the monomial symmetric function that corresponds to the partition with k 1's,

$$\begin{aligned} e_0&=1 \\ e_1&=w_1+\cdots+w_n, \\ e_2&=w_1w_2+w_1w_3+\cdots w_{n-1}w_n \\ &\vdots \\ e_k&=\sum_{1\leqslant i_1<i_2\cdots<i_k\leqslant n} w_{i_1}\cdots w_{i_k}. \end{aligned} \tag{16}$$

Given a partition μ, this definition is extended to

$$e_\mu = e_{(\mu_1,\ldots,\mu_l)} = e_{\mu_1}\cdots e_{\mu_l}. \tag{17}$$

Finally, the complete symmetric function h_k is defined to be the sum over all monomial symmetric functions of degree k, i.e.,

$$h_k = \sum_{\mu \vdash k} m_\mu . \tag{18}$$

In a similar way as above this is extended to

$$h_\mu = h_{(\mu_1,\ldots,\mu_l)} = h_{\mu_1}\cdots h_{\mu_l}. \tag{19}$$

The following facts are well known concerning the various functions defined above:

(i) The elementary and complete symmetric functions are dual to each other in the sense,

$$e_k = \det(h_{1-i+j})_{i,j=1}^k \tag{20}$$

$$h_k = \det(e_{1-i+j})_{i,j=1}^k, \tag{21}$$

where we put by convention $e_{-k}=h_{-k}=0$ for $k>0$. Their generating functions are given by

$$\sum_{i=0}^{\infty} e_i(w_1,\ldots,w_n)t^i = \prod_{j=1}^{n}(1+w_j t), \tag{22}$$

$$\sum_{i=0}^{\infty} h_i(w_1,\ldots,w_n)t^i = \prod_{j=1}^{n}\frac{1}{1-w_j t}. \tag{23}$$

(ii) The Jacobi–Trudi identity.
Let $\mu=(\mu_1,\ldots,\mu_n)$ be a partition into at most n part, then

$$s_\mu(w_1,\ldots,w_n) = \det(h_{\mu_i+j-i})_{i,j=1}^n. \tag{24}$$

(iii) The Nägelsbach–Kostka identity.
Let μ' be the partition conjugate to μ and k the number of parts in μ', then

$$s_\mu = \det(e_{\mu_i'-i+j})_{i,j=1}^k. \tag{25}$$

(iv) The Schur function is equal to a ratio of Vandermonde determinants,

$$s_{(\mu_1,\ldots,\mu_n)}(w_1,\ldots,w_n) = \frac{\det w_i^{n-j+\mu_j}}{\det w_i^{n-j}}. \tag{26}$$

Usually (26) is taken as the definition of the Schur function.

III. RESULTS FOR $q=e^{i\pi/3}$

We now turn to the XXZ spin chain in the following cases: (i) periodic boundaries and $L=2n+1$, (ii) twisted boundaries with twist angle $\pi/3$ and $L=2n$, and (iii) reflecting boundaries. In these cases the XXZ chain has a trivial ground state energy. It is to be understood that in this section we take $q=e^{i\pi/3}$.

A. Periodic boundaries

Consider the function $Q_n(w)$, of which the zeros are the solutions of the Bethe equations (7),

$$Q_n(w) = \prod_{i=1}^{n}(w-w_i) = \sum_{l=0}^{n}(-)^l w^{n-l} e_l , \tag{27}$$

where e_l are the elementary symmetric functions (16) with the variables w_i as arguments. Stroganov showed,[20] using Baxter's T–Q relation[21] that $Q_n(w)$ can be calculated analytically in the case where the w_i are the solution of (7) with $L=2n+1$ corresponding to the lowest value of the energy (4). The answer is given as a rational function in w. Using a binomial coefficient identity, the explicit polynomial form of $Q_n(w)$ is calculated in Appendix A. Comparing expression (A7) now with the formal expansion of $Q_n(w)$ in (27) one can read off the values of the elementary symmetric functions at these particular values of w_i. We find

$$e_l=\binom{n-1/3}{n}^{-1}\sum_{p=0}^{\lfloor l/3\rfloor}\left[\binom{2n-3p+l}{2n}\binom{n-1/3}{n-p}\binom{n+1/3}{p}\right.$$
$$\left.-\binom{2n-3p+l-1}{2n}\binom{n-1/3}{p}\binom{n+1/3}{n-p}\right]. \tag{28}$$

The series in (27) with the coefficients as in (28) in general does not appear to be summable, i.e., cannot be written as a simple product, but it can be verified without too much difficulty that it satisfies the recursion relation

$$(w+1)^2(3n+2)Q_{n+1}(w)=3(w^3-1)(2n+1)Q_n(w)$$
$$-(w^2-w+1)^2(3n+1)Q_{n-1}(w). \tag{29}$$

For special values of w, $Q_n(w)$ simplifies dramatically. The results

$$q^{2n}Q_n(q^{-1})=2^n\prod_{j=1}^{n}\frac{2j-1}{3j-1},\quad Q_n(0)=(-)^n, \tag{30}$$

can for example be calculated easily from (29) when $w=q^{-1}$ and $w=0$. From this we conclude that

$$\prod_{j=1}^{n}(1+z_j+z_j^2)=\left(\frac{3}{4}\right)^n\prod_{j=1}^{n}\left(\frac{3j-1}{2j-1}\right)^2. \tag{31}$$

As another example to derive closed form expressions for symmetric combinations of Bethe roots, we consider the product

$$\prod_{i\neq j}^{n}(1+z_i+z_iz_j)=\prod_{i\neq j}^{n}\frac{\mathrm{i}\sqrt{3}(q^2w_j-w_i)}{(qw_i-1)(qw_j-1)}$$
$$=\prod_{i=1}^{n}\left(\frac{\sqrt{3}q^{-1}}{(w_i-q^{-1})^2}\right)^{n-1}\prod_{i<j}\frac{w_i^3-w_j^3}{w_i-w_j}, \tag{32}$$

where in the last step we recognize the Schur function in the ratio of the two Vandermonde determinants [see Eq. (26)]. Thus we find, using (30),

$$\prod_{i\neq j}^{n}(1+z_i+z_iz_j)=\left(\prod_{j=1}^{n}\frac{\sqrt{3}}{4}\left(\frac{3j-1}{2j-1}\right)^2\right)^{n-1}$$
$$\times s_{(2(n-1),2(n-2),\ldots,2,0)}(w_1,\ldots,w_n). \tag{33}$$

This can be rewritten using the fact that a Schur function can be written as a determinant over the elementary symmetric functions (see (25)). We now have

$$s_{(2(n-1),2(n-2),\ldots,2,0)}(w_1,\ldots,w_n)=\det(e_{n-\lfloor(i+1)/2\rfloor-i+j})_{i,j}^{2(n-1)}, \tag{34}$$

with e_l given by (28). We thus have derived a closed form expression for the product (32). When evaluated explicitly for small values of n we find

$$\prod_{i\neq j}^{n}(1+z_i+z_iz_j)=A(n)^3, \tag{35}$$

where $A(n)$ is the number of $n\times n$ alternating-sign matrices (13). Although we have not been able to evaluate the determinant in (34) analytically, we conjecture that (35) is true for all values of n.

The smallest and largest component of the groundstate wave function are given by $\psi(1,2,\ldots,n)$ and $\psi(1,3,\ldots,2n-1)$ respectively. In Ref. 2 it was conjectured that their ratio is equal to $A(n)$. Using the definitions of Sec. II A, we find by numerical calculation for small n that the smallest and largest component are given by

$$\sum_{\pi}\prod_{i<j}^{n}\frac{1+z_{\pi_i}^{-1}+z_{\pi_j}}{z_{\pi_j}-z_{\pi_i}}=\sum_{\pi}\prod_{i<j}^{n}q^{-1}\frac{qw_{\pi_i}-1}{q-w_{\pi_i}}\frac{w_{\pi_i}-q^2w_{\pi_j}}{w_{\pi_j}-w_{\pi_i}}=A(n), \tag{36}$$

$$\sum_{\pi}\prod_{i<j}^{n}\frac{z_{\pi_i}^{-1}(1+z_{\pi_i}^{-1}+z_{\pi_j})}{z_{\pi_j}-z_{\pi_i}}=\sum_{\pi}\prod_{i<j}^{n}q^{-1}\left(\frac{qw_{\pi_i}-1}{q-w_{\pi_i}}\right)^2\frac{w_{\pi_i}-q^2w_{\pi_j}}{w_{\pi_j}-w_{\pi_i}}=A(n)^2. \tag{37}$$

We conjecture that these equations are true for abitrary values of n. We see that indeed the ratio of these two components is $A(n)$. In fact, using the natural, but otherwise arbitrary, normalization of the amplitudes (8), we find that the smallest component itself is normalized to $A(n)$. Since both functions above are (up to a common factor) symmetric polynomials, we hope that these conjectures can be proven by making use of (28).

B. Twisted boundaries

For twisted boundary conditions,

$$\sigma_{L+1}^{\pm}=(\sigma_{L+1}^{x}\pm i\sigma_{L+1}^{y})=e^{\pm 2i\phi}\sigma_1^{\pm}, \tag{38}$$

the eigenvectors and eigenvalues of H are still given by (3) and (4). The equations for z_i or w_i however are modified and for the special case $\phi=\pi/3$ become

$$\left(\frac{q-w_i}{qw_i-1}\right)^L+q^{-2}\prod_{j=1}^{n}\frac{w_i-q^2w_j}{q^2w_i-w_j}=0. \tag{39}$$

Also for this case $Q_n(w)$ can be calculated analytically when the solution of (39) with $L=2n$ corresponds to the ground state.[18] We find that the elementary symmetric functions now have the values

$$e_l=\binom{n-1/3}{n}^{-1}\sum_{p=0}^{\lfloor l/3\rfloor+1}\left[\binom{2n-3p+l-1}{2n-1}\binom{n-1/3}{n-p}\binom{n-2/3}{p}\right.$$
$$\left.-\binom{2n-3p+l+1}{2n-1}\binom{n-1/3}{p-1}\binom{n-2/3}{n-p}\right]. \tag{40}$$

In a similar way as was done above for the periodic boundaries we can use this expression to evaluate symmetric polynomials in the variables z_i. For example, we find that

$$\prod_{i\neq j}^{n}(1+z_i+z_iz_j)=\left(4\mathrm{e}^{-\mathrm{i}\pi/3}3^{n/2-1}\prod_{j=1}^{n}\left(\frac{3j-1}{n+j}\right)^2\right)^{n-1}\times\det(e_{n-\lfloor(i+1)/2\rfloor-i+j})_{i,j}^{2(n-1)}. \tag{41}$$

When evaluated for small values of n we see this is equal to

$$\prod_{i\neq j}^{n}(1+z_i+z_iz_j)=\mathrm{e}^{-(n-1)\mathrm{i}\pi/3}A(n)A_{\mathrm{HT}}(2n-1), \tag{42}$$

where

$$A_{\mathrm{HT}}(2n+1)=A(n)^2\prod_{k=1}^{n}\frac{3}{4}\left(\frac{3k-1}{2k-1}\right)^2 \tag{43}$$

is the number of $(2n+1)\times(2n+1)$ half-turn symmetric alternating sign matrices. We conjecture that (42) is true for arbitrary values of n.

C. Reflecting boundaries

For the open chain with diagonal, or spin conserving, boundaries, the Hamiltonian is given by

$$H=-\tfrac{1}{2}\sum_{j=1}^{L-1}(\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y+\Delta\sigma_j^z\sigma_{j+1}^z+\tfrac{1}{2}(q-q^{-1})(\sigma_j^z-\sigma_{j+1}^z)). \tag{44}$$

The eigenvectors are now

$$\psi(x_1,\ldots,x_n)=\sum_{\pi,\sigma}A_{\sigma_1\cdots\sigma_n}^{\pi_1\cdots\pi_n}\prod_{j=1}^{n}z_{\pi_j}^{\sigma_jx_j}, \tag{45}$$

where the sum runs over all permutations $\pi=(\pi_1,\ldots,\pi_n)$ of the numbers $1,\ldots,n$ and all signs $\sigma_i=\pm1$.[12,24] In this case the energy is given by

$$E=-\tfrac{1}{2}(L-1)\Delta-\sum_{i=1}^{n}(z_i+z_i^{-1}-2\Delta). \tag{46}$$

The Bethe equations become

$$\left(\frac{q-w_i}{qw_i-1}\right)^{2L}-\prod_{\substack{j=1\\j\neq i}}^{n}\left(\frac{q^2w_j-w_i}{w_j-q^2w_i}\right)\left(\frac{q^2-w_iw_j}{1-q^2w_iw_j}\right)=0, \tag{47}$$

where z and w are again related by (6). The amplitudes are up to a normalization given by

$$A_{\sigma_1\cdots\sigma_n}^{\pi_1\cdots\pi_n}=\prod_{i=1}^{n}z_{\pi_i}^{-\sigma_iL}\frac{1+qz_{\pi_i}^{-\sigma_i}}{z_{\pi_i}^{\sigma_i}-z_{\pi_i}^{-\sigma_i}}\prod_{i<l}\frac{(q^2w_{\pi_i}^{-\sigma_i}-w_{\pi_l}^{-\sigma_l})(q^2-w_{\pi_i}^{\sigma_i}w_{\pi_l}^{\sigma_l})}{(w_{\pi_i}-w_{\pi_l})(1-w_{\pi_i}^{-1}w_{\pi_l}^{-1})}. \tag{48}$$

In this case the function Q is defined by

$$Q_n(w)=\prod_{i=1}^{n}(\tilde{w}-\tilde{w}_i)=\sum_{i=0}^{n}(-)^i\tilde{w}^{n-i}e_i(\tilde{w}_1,\ldots,\tilde{w}_n),\quad \tilde{w}=w+w^{-1}. \tag{49}$$

Also for this case $Q_n(w)$ can be given analytically when the solution of (47) corresponds to the lowest value of the energy (46).[18] The explicit polynomial form of $Q_n(w)$ is given in the Appendix, from which the e_i can be read off.

In analogy with the periodic and twisted cases we consider the product

$$\begin{aligned}\prod_{i=1}^{2n}\prod_{\substack{j=1\\ z_j\neq z_i^{\pm 1}}}^{2n}(1+z_i+z_iz_j)&=\prod_{i=1}^{2n}\prod_{\substack{j=1\\ w_j\neq w_i^{\pm 1}}}^{2n}\frac{(q-q^{-1})(q^2w_j-w_i)}{(qw_i-1)(qw_j-1)}\\ &=\prod_{i=1}^{n}\left(\frac{q-q^{-1}}{\tilde{w}_i-q-q^{-1}}\right)^{4(n-1)}\prod_{i\neq j}^{n}\frac{w_i^3+w_i^{-3}-w_j^3-w_j^{-3}}{\tilde{w}_i-\tilde{w}_j}\\ &=\prod_{i=1}^{n}\left(\frac{q-q^{-1}}{\tilde{w}_i-q-q^{-1}}\right)^{4(n-1)}\left(\frac{\det(w_i^{3(n-j)}+w_i^{-3(n-j)})}{\det(w_i^{n-j}+w_i^{-n+j})}\right)^2.\end{aligned} \tag{50}$$

Here we use the convention $w_{i+n}=w_i^{-1}$. The ratio of determinants in (50) is up to a factor a symmetric polynomial in $\tilde{w}_1\cdots\tilde{w}_n$. Unfortunately we have not succeeded in expressing it in the known basis of elementary symmetric functions. Nevertheless, numerical evaluation of (50) leads us to conjecture that

$$\prod_{i=1}^{2n}\prod_{\substack{j=1\\ z_j\neq z_i^{\pm 1}}}^{2n}(1+z_i+z_iz_j)=A_{\mathrm{V}}(2n+1)^2N_8(2n)^4, \tag{51}$$

where $A_{\mathrm{V}}(2n+1)$ is the number of $(2n+1)\times(2n+1)$ vertically symmetric alternating sign matrices (Ref. 8, Theorem 2) given by

$$A_{\mathrm{V}}(2n+1)=\prod_{j=0}^{n-1}(3j+2)\frac{(2j+1)!(6j+3)!}{(4j+2)!(4j+3)!} \tag{52}$$

and $N_8(2n)$ is the number of cyclically symmetric transpose complement plane partitions[4,22] given by

$$N_8(2n)=\prod_{j=1}^{n-1}(3j+1)\frac{(2j)!(6j)!}{(4j)!(4j+1)!}. \tag{53}$$

IV. CONCLUDING REMARKS

We have made a first step towards proving the appearance of certain numbers related to alternating sign matrices in the ground state eigenvector of the XXZ spin chain. Many of the combinatorial results concerning alternating sign matrices have been obtained using the connection with the integrable six-vertex model.[7,8] The XXZ spin chain is closely related to the six-vertex model and the methods used in this paper provide a different application of integrability. The eigenvectors of the XXZ Hamiltonian are given in the form of Bethe's Ansatz as a result of the integrability of the spin chain for each of the different boundary conditions under consideration. In fact, the normalization of the amplitudes (8) ensures that all eigenvectors are symmetric polynomials in the Bethe roots. As is well known, a basis for the space of symmetric polynomials is given by the elementary symmetric functions. Using the results of Stroganov and his collaborators[18–20]

for Baxter's Q-function, we were able to derive explicitly the values that the elementary symmetric functions take at the ground state solution of the Bethe roots. See, e.g., Eqs. (28) and (40) for the periodic and twisted cases. Although in principle possible, we were not able to re-express the ground state in terms of the elementary symmetric functions. However, we could show that certain natural double products over the Bethe roots can be rewritten in this way. Using some results from the theory of symmetric functions we could then derive determinant expressions that when evaluated give rise to the numbers counting different symmetry classes of alternating sign matrices. Our key results (35), (42), and (51) thus remain as conjectures. It is yet to be seen if such products over Bethe roots have any direct combinatorial meaning.

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APPENDIX: DETAILS

1. Periodic boundaries

Stroganov's result for $Q_n(w)$ in the case of periodic boundary conditions and odd system size is[20]

$$Q_n(w)=\prod_{i=1}^{n}(w-w_i)=\binom{n-1/3}{n}^{-1}\sum_{k=0}^{n}(-)^k\binom{n-1/3}{k}\times\binom{n+1/3}{n-k}w^{3k+1}\frac{(-1)^n+w^{3n-6k-1}}{(1+w)^{2n+1}}. \tag{A1}$$

We would like to rewrite this in the form

$$Q_n(w)=\sum_{i=0}^{n}(-)^i w^{n-i}e_i, \tag{A2}$$

where the e_i are the elementary symmetric functions with arguments $w_1,\ldots,w_n$. The right-hand side of (A1) can be expanded using

$$\sum_{m=0}^{\infty}(-)^m\binom{2n+m}{m}w^{-2n-m-1}=(1+w)^{-2n-1}. \tag{A3}$$

It follows that Q can be written as

$$Q_n(w)=\binom{n-1/3}{n}^{-1}\sum_{k=0}^{n}\sum_{m=0}^{\infty}(-)^{k+m}w^{n-3k-m}\left[\binom{2n+m}{m}\binom{n-1/3}{n-k}\binom{n+1/3}{k}-\binom{2n+m-1}{m-1}\binom{n-1/3}{k}\binom{n+1/3}{n-k}\right]. \tag{A4}$$

To show that (A4) reduces to a finite sum, we first collect terms of the form $m=3j$, $m=3j+1$ and $m=3j+2$. Then we use the following identity to rewrite (A4):

$$\sum_{k=0}^{n}\sum_{j=0}^{\infty}a_{k,j}=\sum_{l=0}^{n}\sum_{p=0}^{l}a_{l-p,p}+\sum_{l=n+1}^{\infty}\sum_{p=0}^{n}a_{p,l-p}. \tag{A5}$$

To proceed we need the result

$$\sum_{p=0}^{n}\binom{3p-n+s}{2n}\binom{n-1/3}{p}\binom{n+1/3}{n-p}=\sum_{p=0}^{n}\binom{3p-n+s-1}{2n}\binom{n-1/3}{n-p}\binom{n+1/3}{p}. \tag{A6}$$

This identity is proven by first showing that both the left and right hand sides satisfy the same recursion relation in n, i.e., both sums for $n=m+3$ can be expressed in the same sums for $n=m+2,m+1$ and $n=m$. One then shows explicitly that the identity holds for $n=0,1,2$. The recursion relation for (A6) can be easily derived using the Paule and Schorn Mathematica implementation of an algorithm of Zeilberger's.[25]

From (A6) it then follows that the infinite sum in (A5) vanishes and after recollecting terms again we can finally write

$$\begin{aligned}Q_n(w)=&\binom{n-1/3}{n}^{-1}\sum_{l=0}^{n}\sum_{p=0}^{\lfloor l/3\rfloor}(-)^l w^{n-l}\left[\binom{2n-3p+l}{2n}\binom{n-1/3}{n-p}\binom{n+1/3}{p}\right.\\&\left.-\binom{2n-3p+l-1}{2n}\binom{n-1/3}{p}\binom{n+1/3}{n-p}\right],\end{aligned} \tag{A7}$$

the desired result.

2. Twisted boundaries

In this case the result of Fridkin *et al.*[18] for $Q_n(w)$ is

$$\begin{aligned}Q_n(w)=&\binom{n-1/3}{n}^{-1}\frac{1}{(1+w)^{2n}}\sum_{k=0}^{n}(-)^k\binom{n-2/3}{n-k}\\&\times\left((-)^n\binom{n-1/3}{k}w^{3k}-\binom{n-1/3}{k-1}w^{3n-3k+2}\right).\end{aligned} \tag{A8}$$

In analogy with the periodic case we need to rewrite $Q_n(w)$ in powers of w. This can be done along the lines of the previous subsection with the help of the result

$$\sum_{p=0}^{n}\binom{3p-n+s}{2n}\binom{n-1/3}{p}\binom{n-2/3}{n-p}=\sum_{p=0}^{n}\binom{3p-n+s+2}{2n}\binom{n-1/3}{n-p-1}\binom{n-2/3}{p}. \tag{A9}$$

As in the case of (A6), this identity can be proven by showing that both the left and right-hand sides satisfy the same recursion relation in n. We then find

$$\begin{aligned}Q_n(w)=&\binom{n-1/3}{n}^{-1}\sum_{l=0}^{n}(-)^l w^{n-l}\\&\times\sum_{p=0}^{\lfloor l/3\rfloor+1}\left[\binom{2n-3p+l-1}{2n-1}\binom{n-1/3}{n-p}\binom{n-2/3}{p}-\binom{2n-3p+l+1}{2n-1}\binom{n-1/3}{p-1}\binom{n-2/3}{n-p}\right].\end{aligned} \tag{A10}$$

3. Reflecting boundaries

Following Fridkin *et al.*[18] one can prove that Q is given by

$$\binom{2n-2/3}{2n}^{-1}\sum_{k=-n}^{n}(-)^{n+k}\binom{2n+2/3}{n-k}\binom{2n-2/3}{n+k}\frac{w^{3k+1}-w^{-3k-1}}{(w-w^{-1})(2+w+w^{-1})^{2n}}. \tag{A11}$$

Using (A3) and

$$\sum_{p=0}^{\lfloor n/2\rfloor}(-)^p\binom{n-p}{p}(w+w^{-1})^{n-2p}=\frac{w^{n+1}-w^{-n-1}}{w-w^{-1}}, \tag{A12}$$

the expression for Q can be rewritten so that we can read off the values of the elementary symmetric functions with arguments $\tilde{w}_1,\ldots,\tilde{w}_n$, where $\tilde{w}=w+w^{-1}$. Namely,

$$\begin{aligned}Q_n(w)=2^{-3n}\binom{2n-2/3}{2n}^{-1}\sum_{p=0}^{n}(-2)^p\tilde{w}^{n-p}\Bigg[&\binom{3n-p-1}{n-p}\binom{2n+2/3}{n}\binom{2n-2/3}{n}\\&+\sum_{m=0}^{p}\sum_{k=1}^{n}(-)^{\lfloor(k+m+1)/2\rfloor}2^{m-1}(1+(-)^{k+m})\binom{3n-p-m-1}{2n-1}\\&\times\Bigg(\binom{2n+2/3}{n-k}\binom{2n-2/3}{n+k}\binom{\lfloor(3k+m+1)/2\rfloor}{m}\\&+\binom{2n+2/3}{n+k}\binom{2n-2/3}{n-k}\binom{\lfloor(3k+m-1)/2\rfloor}{m}\Bigg)\Bigg].\end{aligned} \tag{A13}$$

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Chiral mixtures

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An index evaluating the amount of chirality of a mixture of colored random variables is defined. Properties are established. Extreme chiral mixtures are characterized and examples are given. Connections between chirality, Wasserstein distances, and least squares Procrustes methods are pointed out. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1484559]

I. INTRODUCTION

Classifying a set as symmetric or not has been viewed as a dichotomic yes–no decision process for centuries. Attempts to evaluate the amount of symmetry has received little attention. Grünbaum (1963) noticed the difficulty to elaborate a rational approach of this problem. Physicists and chemists proposed various measures of the amount of chirality: see, for instance, Harris *et al.* (1999), Le Guennec (2000) or references cited by Petitjean (1997). Most methods handle only homogeneous solids, or only discrete sets. Many methods are limited to planar or spatial sets, and continuity properties are often ignored. E.g., for a homogeneous solid, the chiral index of Gilat (1989) is the normalized volume of the symmetric difference between the solid and its inverted image. The volume of the symmetric difference is the distance introduced by Dinghas (1957), this distance being itself the square of the $L2$-norm induced distance between the indicator functions of the solids. In this situation, continuity fails when the set becomes subdimensional. Clearly, functional distances applied to a set and its inverted image have no adequate continuity property because they are applied to densities rather than to distribution functions.

Thus, evaluating the degree of chirality of a random vector X in R^d is possible from some probability metric between the distribution of X and the distribution of its translated and rotated inverted image. The translation and the rotation are denoted respectively t and R. We consider now any two random vectors X and Y in R^d, and we look for a probability metric. For example, F being the distribution function of X, and G being the distribution function of Y, the quantity μ_K [Eq. (1.1)] is issued from the Kolmogorov metric:

$$\mu_K = \mathrm{Inf}_{\{R,t\}}(\mathrm{Sup}_{\{x\}}|F(x)-G(x)|). \tag{1.1}$$

But it was noticed previously (Petitjean, 1997, and 1999a), that some applications require us to consider colored mixtures, i.e., mixtures of colored random variables (see definition in the next section). An example is the algebraic charge density of a molecule or ion, which may be viewed as a mixture of two charge densities, namely the positive one and the negative one. As shown below, the quantity μ_K is not adequate for colored mixtures, because it is not sensitive to colors, and an extension of the Wasserstein distance will be preferred.

II. COLORED MIXTURES AND WASSERSTEIN DISTANCES

The assumption that Y is distributed as a translated and rotated inverted image of X is not used in this section.

A reason to work with the colored model is that, when evaluating the degree of chirality, Y has the distribution of a rotated inverted image of X, and therefore Y is a mixture such that each

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component $\tilde{Y}$ retains the color of its associated component $\tilde{X}$ and is distributed as the rotated inverted image of $\tilde{X}$. In other words, the mirror (in fact, the inversion operator) sees the colors, e.g., the eight vertices of a cube constitute indeed a chiral figure in R^3 when they have all different colors. Another application needing a probability metric sensitive to colors is the optimal superposition problem (see Sec. II B), the quantitative chirality evaluation being just an instance of this problem.

A. Colored mixtures

When X is a mixture of colored random variables $\tilde{X}$, the more general formulation of its distribution is written in Eq. (2.1) with the mixing distribution P_1, and, similarly, the mixture Y of colored random variables $\tilde{Y}$ is written in Eq. (2.2) with the mixing distribution P_2:

$$F(x) = \int \tilde{F}(x,c) \cdot dP_1(c), \tag{2.1}$$

$$G(y) = \int \tilde{G}(y,c) \cdot dP_2(c). \tag{2.2}$$

When all the components of a mixture have the same color, it means that there is in fact only one colored component, and the colored mixture is an ordinary random vector in R^d. A colored mixture may be viewed as an ordinary mixture of random vectors, for which a supplementary axis has been added (the space of colors), this axis not being of numeric nature.

The joint distribution W of X and Y is expressed with the mixing distribution P operating on the mixed distributions $\tilde{W}$ [Eq. (2.3)]:

$$W(x,y) = \int \int \tilde{W}(x,y,c_1,c_2) \cdot d^2P(c_1,c_2). \tag{2.3}$$

In Eqs. (2.1)–(2.3), the summations are performed over the spaces of the colors. Now, we assume that the two colored mixtures X and Y are defined on the same space of colors. Moreover, the distribution of the colors is assumed to be the same for X and Y, i.e., the respective marginal distributions of X and Y on the space of colors are identical, and therefore can be fully correlated. This correlation is indeed assumed now: $P(c_1,c_2)$ is null when $c_1 \neq c_2$, i.e., $d^2P(c_1,c_2)$ is expressed with the Dirac delta function in Eq. (2.4), and integration over c_2 is performed in (2.3) to give the expression of W in Eq. (2.5), in which P_1 is renamed P and c_1 is renamed C:

$$d^2P(c_1,c_2) = dP_1(c_1) \cdot \delta_{[c_2=c_1]} dc_2, \tag{2.4}$$

$$W(x,y) = \int \tilde{W}(x,y,C) \cdot dP(C). \tag{2.5}$$

Clearly, the independence of the mixtures X and Y cannot be assumed now, except if X has only one colored component. This ''colored model'' is such that coupling the colors of a couple of mixtures X and Y induces constraints on the existence of their joint distributions W [Eq. (2.4)], and the set of joint distributions satisfying Eq. (2.5) is a nonempty subset of the set of the joint distributions of the same couple of mixtures discarding colors.

Equations (2.4) and (2.5) are assumed to stand further.

B. Colored Wasserstein distance and Procrustes methods

A probability metric depending on the joint density is sensitive to the constraints arising from colors [see Eq. (2.5)]. The well known Wasserstein metric (Dobrushin, 1970; Dudley, 1989;

Rachev, 1991) is so. The Wasserstein metric is itself an instance of the Kantorovich functional, which is encountered in the transportation problem (see equation 1.1.25 in Rachev and Rüschendorf, 1998).

The distributions associated respectively to X and Y are P^1 and P^2, and the matricial transposition operator is denoted by the quote. We name here colored Wasserstein distance $C(P^1,P^2)$ the extension of the $L2$ Wasserstein distance μ to colored mixtures, for which the lower bound of the expectation $E[(X-Y)'\cdot(X-Y)]$ is taken for all rotations R, translations t, and joint distributions W satisfying (2.5), i.e., such that each $\tilde{W}$ belongs to the class of all joint distributions of $\tilde{X}$ and $\tilde{Y}$:

$$D^2(W)=E[(X-Y)'\cdot(X-Y)], \tag{2.6}$$

$$\mu(P^1,P^2)=\mathrm{Inf}_{\{W\}}D(W), \tag{2.7}$$

$$C(P^1,P^2)=\mathrm{Inf}_{\{R,t\}}\mu(P^1,P^2). \tag{2.8}$$

In Eq. (2.6), it should be noticed that the expectation is defined through a $2d$-dimensional Lebesgue–Stiltjes integral, rather than a d-dimensional one. On the other hand, for any joint distribution W, computing $E(X'\cdot X)$ with the $2d$-dimensional integral leads to the same value that $E(X'\cdot X)$ computed with the d-dimensional one. The same remark is valid for $E(X)$, $E(Y)$, and $E(Y'\cdot Y)$.

Data analysis methods performing an optimal superposition of a set on another one via a least squares method were named Procrustes methods by Hurley and Cattell (1962), and the sum of the least squares is named the Procrustes distance. These methods are classified with the type of transformation allowed to superpose the moving set on the fixed set: general linear transformation, orthogonal transformation, or pure rotation. The 3D instance of this latter is usually encountered in physics, chemistry and bioinformatics: see references on the RMS algorithm cited in Petitjean (1998). The translation is optional, and it is always shown that the optimal translation is obtained when the mean points are superposed at the origin before further optimizations. The null expectation condition is not required in Procrustes methods.

Clearly, minimizing the $L2$ Wasserstein distance $\mu(P^1,P^2)$ [Eq. (2.7)], for some class of affine transformations of Y, generalizes the Procrustes method, because the usual one is its instance when X and Y are finite mixtures of n colored almost constant vectors, such that there is a one to one correspondence between the n vectors $\tilde{X}_i$ and $\tilde{Y}_i$. In this discrete situation, the unique feasible joint distribution is a bistochastic matrix equal to I/n, I being the identity matrix (colors are supposed to be enumerated in the same order for X and Y), and the Procrustes distance $\mathrm{Min}(D^2)$ is just the minimized sum of the squared distances between the n pairs of vectors. The Procrustes distance is the minimum of the distance induced by the norm itself induced by the scalar product $Tr(Z_X'\cdot Z_Y)$, where Z_X and Z_Y are two (n,d) rectangular matrices. The optimal rotation is analytically known when $d=2$ (see Section 3 in Petitjean, 1997), and when $d=3$ (see appendix in Petitjean, 1999b). The optimal orthogonal transformation is analytically known for any d (Golub and van Loan 1985).

For the noncolored model, i.e., when the n colors are identical, we get the Procrustes method without prefixed correspondence, for which the minimization of D^2 involves the enumeration of at most $n!$ possible correspondences between the two sets. Looking at the probabilistic formulation, the optimal joint distribution exists and is a bistochastic matrix equal to $1/n$ times a permutation matrix, because it is an extreme point of the convex polytope of the feasible solutions of the associated linear programming problem.

To summarize, the Procrustes distance becomes an instance of the $L2$ Wasserstein distance when this latter is extended to colored mixtures and minimized for a class of affine transformations of Y. Using the colored Wasserstein distance C [Eq. (2.8)] assumes that we work in the space of finite inertia colored mixtures, but the finite inertia condition could be relaxed if other adequate Wasserstein distances (see Rachev, 1991) are extended to colored mixtures. For clarity,

we restrict the affine transformations to rotations. In this situation, C is in fact a metric for classes of equivalence of colored mixtures, the colored mixtures being in the same class when their distributions are rotated (and optionally translated) images of one of them. It is pointed out that the colored Wasserstein distance is not defined when the mixtures have different marginal distributions in the space of colors. In this situation, an attempt to work with the ''maximal common substructure'' concept rather than with distances has been done for finite discrete sets (Petitjean, 1998). Of course, when the mixture Y is distributed as $\phi(X)$, ϕ being any transform leaving unchanged the marginal of X in the space of colors, C is indeed defined.

Some immediate properties of $C(P^1,P^2)$ follow.

Let m_{X_i} and m_{Y_i} be the respective expectations of X and Y attached to the i axis, $i \in [1,...,d]$, and σ_{X_i} and σ_{Y_i} be their respective standard deviations. The covariance attached to the i axis is c_i, and the respective inertia are T_X and T_Y. Equation (2.6) is now expandable as

$$D^2 = \sum_i \left[(\sigma_{X_i}^2 + m_{X_i}^2) + (\sigma_{Y_i}^2 + m_{Y_i}^2) - 2(c_i + m_{X_i} m_{Y_i})\right].$$

And, after rearrangement,

$$D^2 = T_X + T_Y + \sum_i \left[(m_{X_i} - m_{Y_i})^2 - 2c_i\right]. \tag{2.9}$$

The inertias and the covariances do not depend on the expectations. Thus the optimal translation t is such that $E(X) = E(Y)$, and the expression of D^2 becomes

$$D^2 = T_X + T_Y - 2\sum c_i. \tag{2.10}$$

Although the optimal joint distribution is not ensured to exist (Rachev and Rüschendorf, 1998), the optimal rotation is shown to exist, but may be not unique (Appendix A). The optimal general transformation and the optimal orthogonal transformation are known (Appendix A).

III. PROPERTIES OF THE CHIRAL INDEX

Let X and Y be colored mixtures in R^d, Y having the distribution of a translated and rotated inverted image of X. W is the joint distribution of the couple X, Y and T is the inertia of X or Y, i.e., $T = E[(X - E(X))' \cdot (X - E(X))]$ and $T = E[(Y - E(Y))' \cdot (Y - E(Y))]$. We define the chiral index χ as follows:

$$\chi = \frac{d}{4T} C^2(P^1,P^2). \tag{3.1}$$

In Eq. (3.1), P^2 being function of P^1, χ depends only on the law of X. In other words, χ is the normalized squared colored Wasserstein distance between the mixtures X and Y, Y being distributed as a translated and rotated inverted image of X. The chiral index is restricted to finite non-null inertia distributions. The situation $T = 0$ arises when X is almost surely equal to some constant x_0, and offers little interest. We neglect it. The chiral index is insensitive to isometries and is size free. As noticed in the preceding section, the optimal translation is obtained when $E(X) = E(Y)$, meaning that X and Y should be centered.

For clarity, we assume without loss of generality that the condition $E(X) = E(Y) = 0$ is satisfied in all this section.

The correlation coefficient attached to the i axis is r_i. Assuming the existence of the correlation coefficients, we get from Eqs. (2.10), (3.1) and (2.8):

$$D^2 = 2T - 2\sum c_i, \tag{3.2}$$

$$\chi = \frac{d}{2}\left(1 - \frac{\mathrm{Sup}_{\{R,W\}}(\Sigma c_i)}{T}\right). \tag{3.3}$$

When $d=1$, $R=1$, Y is distributed as $-X$, and there is only one standard deviation σ, and one correlation coefficient r. Equations (3.2) and (3.3) become

$$D^2 = 2\sigma^2(1-r), \tag{3.4}$$

$$\chi = \frac{1 - \mathrm{Sup}_{\{W\}}(r)}{2}. \tag{3.5}$$

In Eq. (3.5) the chiral index depends on one parameter only. For the noncolored model, this parameter is the maximal correlation of Gebelein (1952), applied to X and $-X$.

Now we return back to the d-dimensional space, and we look for a joint distribution ensured to exist. As noticed in the previous section, the independence of the mixtures X and Y cannot be assumed, except if X has only one colored component. The chiral index is proportional to the colored Wasserstein distance between the colored mixtures X and Y, Y being distributed as a rotated inverted image X (which does not mean that Y is a rotated inverted image of X). When Y is indeed the image of X through rotation R and inversion Q, the joint distribution of (X,Y) expressed from the mixed joint distributions $\tilde{W}(x,y,C)$ in Eq. (3.6) is ensured to exist:

$$d^2\tilde{W}(x,y,C) = d\tilde{F}(x,C)\cdot h_{[y=R\cdot Q\cdot x]}dy. \tag{3.6}$$

In Eq. (3.6), $h_{[y=y_0]}$ denotes the product of the d Dirac delta functions associated to the point y_0. Expression (3.6) is reported in (2.5) for integration over C, and, using Eq. (2.1), the final expression of the joint distribution is, as for a noncolored model:

$$d^2W(x,y) = dF(x)\cdot h_{[y=R\cdot Q\cdot x]}dy. \tag{3.7}$$

Equation (2.6) is expanded for this particular joint distribution to get Eq. (3.8), in which the expectation is calculated through a d-dimensional integral:

$$D^2 = 2T - 2E(X'\cdot R\cdot Q\cdot X). \tag{3.8}$$

The chiral index being insensitive to isometries, we assume now that the covariance matrix of X is diagonal, and that Y is the image of X through the inversion of the coordinate associated to the smallest variance axis. We take $R=I$. The inertia being the sum of the variances, Eq. (3.8) becomes

$$D^2 = 4\sigma_d^2. \tag{3.9}$$

The ratio of the smallest variance to the inertia is upper bounded by $1/d$, thus χ is upper bounded by 1. This bound is the best possible because it is reached for some particular random variables, as shown in Sec. V (see also the colored Bernoulli distribution in Appendix B):

$$0 \leqslant \chi \leqslant 1. \tag{3.10}$$

We consider now the finite discrete situation. The joint distribution is expressed with the square bistochastic matrix of the probabilities W_{ij} of each couple of values $\{x_i, y_j\}$. Using Eq. (2.6), the chiral index is rewritten

$$D^2=\sum_i \sum_j W_{ij}\cdot(x_i-y_j)'\cdot(x_i-y_j), \tag{3.11}$$

$$\chi=\frac{d}{4T}\mathrm{Inf}_{\{W_{ij},R,t\}}D^2. \tag{3.12}$$

Equations (3.11) and (3.12) were proposed previously to evaluate the amount of chirality of a fnite d-dimensional set, and thus our present approach generalizes the previous one [see Eqs. (3) and (4) in Petitjean (2001)]. It was also shown that, for the mass-uniform discrete case, the bistochastic matrix associated to the joint distribution is a permutation matrix. This particular situation means that there is a one-to-one mapping between the points of the set and those of its inverted image. In general, this mapping is not symmetric.

IV. CONVERGENCE

Obtaining the convergence of the chiral index from the convergence of the random variables is desirable to ensure some kind of continuity property of the chiral index. The weakest usual type of convergence possible for random variables is the convergence in law (in distribution), e.g., convergence of densities is a stronger assumption because this latter implies convergence in law [see Scheffé's theorem in Billingsley (1995)].

We consider the noncolored model. Let X_n be a sequence of random vectors converging to X in law. We assume also the convergence of $E[X_n'\cdot X_n]$ to $E[X'\cdot X]$, this latter quantity being finite. Apart from when X is almost surely constant, the convergence properties of the chiral index will arise from the convergence of $\mathrm{Inf}_{\{R\}}(\mu^2(P_n^1,P_n^2))=\mathrm{Inf}_{\{W_n,R\}}(D_n^2)$ to $\mathrm{Inf}_{\{R\}}(\mu^2(P^1,P^2))=\mathrm{Inf}_{\{W,R\}}(D^2)$, where μ denotes the Wasserstein distance [see Eq. (2.7)]. We use the triangle inequality to write

$$\begin{aligned}
&\mu(P^1,P^2)\leqslant\mu(P^1,P_n^1)+\mu(P_n^1,P_n^2)+\mu(P_n^2,P^2),\\
&\mu(P_n^1,P_n^2)\leqslant\mu(P_n^1,P^1)+\mu(P^1,P^2)+\mu(P^2,P_n^2),\\
&|\mu(P_n^1,P_n^2)-\mu(P^1,P^2)|\leqslant\mu(P_n^1,P^1)+\mu(P_n^2,P^2).
\end{aligned} \tag{4.1}$$

The inversion matrix Q being constant, inequation (4.1) stands for any rotation R common to Y_n and Y. For clarity, we name ϵ_n the second member of inequation (4.1). Obviously, ϵ_n does not depend on R. We note respectively $\mu_n(R)=\mu(P_n^1,P_n^2)$ and $\mu_\infty(R)=\mu(P^1,P^2)$. Inequation (4.1) is rewritten

$$|\mu_n(R)-\mu_\infty(R)|\leqslant\epsilon_n. \tag{4.2}$$

Let R_n and R_∞ be optimal rotations (which are shown to exist in Appendix A), respectively associated to D_n^2 and D^2. Inequation (4.2) stands for any R, and then stands for R_n and R_∞:

$$|-\mu_n(R_n)+\mu_\infty(R_n)|\leqslant\epsilon_n, \tag{4.3}$$

$$|\mu_n(R_\infty)-\mu_\infty(R_\infty)|\leqslant\epsilon_n. \tag{4.4}$$

We deduce from addition of (4.3) and (4.4)

$$|[\mu_n(R_\infty)-\mu_n(R_n)]+[\mu_\infty(R_n)-\mu_\infty(R_\infty)]|\leqslant 2\epsilon_n. \tag{4.5}$$

We know from optimality of rotations that each of the two quantities in brackets is nonnegative. Thus both quantities are upper bounded by $2\epsilon_n$:

$$|\mu_n(R_\infty)-\mu_n(R_n)|\leqslant 2\epsilon_n, \tag{4.6}$$

$$|\mu_\infty(R_n)-\mu_\infty(R_\infty)|\leqslant 2\epsilon_n. \tag{4.7}$$

Then, adding (4.3) and (4.7),

$$|\mu_n(R_n)-\mu_\infty(R_\infty)|=|\mu_n(R_n)-\mu_\infty(R_n)+\mu_\infty(R_n)-\mu_\infty(R_\infty)|\leqslant 3\epsilon_n .$$

This inequation is rewritten in terms of Wasserstein distances:

$$|C(P_n^1,P_n^2)-C(P^1,P^2)|\leqslant 3\epsilon_n . \tag{4.8}$$

It was assumed that X_n is converging to X in distribution, and that there was convergence of $E[X_n'\cdot X_n]$ to $E[X'\cdot X]$, with $E[X'\cdot X]<\infty$. These convergences are preserved through affine transformations. Thus, the distribution of Y_n is also converging to that of Y, discarding or not the common rotation used in inequation (4.2), and $E[Y_n'\cdot Y_n]$ is converging to $E[Y'\cdot Y]$ We know from theorem 6.2.1 in Rachev (1991) that the $L2$ Wasserstein distances $\mu(P_n^1,P^1)$ and $\mu(P_n^2,P^2)$ are tending to zero. Then, $\epsilon_n\to 0$, and we get from (4.8) the convergence of $C(P_n^1,P_n^2)$ to $C(P^1,P^2)$.

Looking to the definition of the chiral index in Eq. (3.1) shows that we need also to establish the convergence of the inertia, i.e., the centered two-order moment. The convergence of the two-order moment was assumed, thus it suffices to get the convergence of $E[X_n]$ to $E[X]$. Let A be any almost surely constant random vector, and P^A its distribution. We have from the triangle inequality:

$$|\mu(P_n^1,P^A)-\mu(P^1,P^A)|\leqslant\mu(P_n^1,P^1)$$

and therefore

$$|E[X_n'\cdot X_n]-E[X'\cdot X]-2E[A]'\cdot(E[X_n]-E[X])|\to 0 .$$

Setting the constant successively equal to each of the d canonical base vectors lead to get the desired convergence for each of the d components of the first order moment.

The convergence theorem follows now for the chiral index:

Theorem: *If the sequence* (P_n) *of probability distributions converges to* P *and* $E[X_n'\cdot X_n]\to E[X'\cdot X]<\infty$, *and* $E[(X-E[X])'\cdot(X-E[X])]>0$, *then* $\chi(P_n)\to\chi(P)$.

V. EXTREME CHIRALITY RANDOM VARIABLES

The chiral index maps X onto the interval $[0;1]$. Assuming $E(X)=E(Y)=0$, we look first to the minimum of the chiral index. Let us define a mixture X as achiral when it has the distribution of one of its rotated and inverted images. In this situation, X and Y can be identically distributed, and thus they can be fully correlated, i.e., $E(X'\cdot Y)=E(X'\cdot X)=E(Y'\cdot Y)$, and $\chi=0$. Conversely, when $\chi=0$, X is almost surely equal to Y, Y having the distribution of a rotated inverted image of X, meaning that X is achiral.

Now we look to the maximum of the chiral index. We assume that X has a diagonal covariance matrix, and that Y is the image of X through inversion of the coordinate associated to the smallest variance axis. We reuse the joint distribution in Eqs. (3.7) and (3.8), and $R=I$ is set, such that Eq. (3.9) stands. The ratio of the smallest variance to the inertia being upper bounded by $1/d$; χ cannot be equal to 1 unless all the d variances are equal. Therefore, the covariance matrix of X is proportional to the identity matrix. This covariance matrix is insensitive to isometries, and any rotation R is optimal for the joint distribution. Equation (5.1) expresses thus a necessary condition to get $\chi=1$:

$$E(X\cdot X')=\sigma^2\cdot I. \tag{5.1}$$

The d-dimensional finite mixture of n almost surely constant equiprobable colored variables is such that the joint distribution in Eqs. (3.7) and (3.8) is the only one feasible when all colors are different. It has been shown (Petitjean, 1999b) that the lower bound of D^2 in Eq. (3.8) is indeed that of Eq. (3.9), and the chiral index of the mixture is d times the percentage of inertia associated to the smallest eigenvalue of the covariance matrix of X:

$$\chi = d \cdot \sigma_d^2 \Big/ \sum_i \sigma_i^2. \tag{5.2}$$

Thus, $\chi = 0$ when the set of the n equiprobable points is subdimensional, and $\chi = 1$ when Eq. (5.1) is satisfied. Well-known figures satisfy Eq. (5.1), including regular planar polygons, cube and hypercubes, octahedron and higher dimensional analogs. Regular simplices fall also in this category. It should be pointed out that when the n colors are identical, these mixtures have a null chiral index because there is a symmetry $(d-1)$-hyperplane.

Some maximal chirality random variables can be exhibited for the noncolored model. The joint distribution of the convolution product always exists, and from Eq. (3.3), it comes that the chiral index is upper bounded by $d/2$. When $d = 1$, this bound is optimal, because it cannot be lowered for the Bernoulli distribution (see Appendix B). When $d \geqslant 2$, finding the upper bound for the noncolored model is an open problem. The distribution of three equiprobable points in the plane maximizing χ has been exhibited (Petitjean, 1997).

VI. DISCUSSION AND CONCLUSION

In the definition of χ, the division by the inertia T was needed to get a size free chiral index. Thus the degenerate random variable X with a null inertia has no chiral index, because both D^2 and T are null. Viewing this degenerate situation via the limit of a family of parametrized random variables makes no sense, in general, because the result depends on how the parameters are used to get a null inertia, and because no convergence exists around the singularity $T = 0$.

Conditions under which the convergence theorem (Sec. IV) could be extended to any colored mixture are to be investigated. A consequence of this convergence theorem is that the chiral index associated to the sample converges to that of the random variable. This could be used to get Monte Carlo approximations of χ when the analytical solution is unreachable, but building consistent estimators is outside the scope of this article. Computing the chiral index of a sample is equivalent to compute it in the finite discrete mass-uniform distribution. For the latter, the unidimensional case is solved analytically, and suitable numerical techniques have been built when $d = 2$ and $d = 3$ (Petitjean, 1997, 1999a, b). Computing χ for a general finite discrete distribution is a non linearly constrained optimization problem [see Eqs. (3.11) and (3.12)]. Constraints arising from the joint distribution are linear equalities and inequalities, because the matrix associated to the joint distribution is bistochastic. Constraints arising from the rotation are quadratic, i.e., $R' \cdot R = I$, and there is the polynomial constraint on the determinant of R.

For the noncolored model, when the rotation is fixed, our optimization problem is an instance of the transportation problem, which is a linear programming one. For the latter, solving algorithms and existence conditions of optimal joint distributions have been recently reviewed in Rachev and Rüschendorf (1998) (see also Anderson and Nash, 1987), and numerous results are available in the monodimensional case.

Compared to the noncolored model, the colored model introduces additional constraints on W. These constraints are handled by the $L2$ Wasserstein metric. Extending our present approach to other color sensitive probability metrics potentially gives rise to a family of similarity measures between colored mixtures, which seems not yet to be investigated, and from which the associated family of chiral indices could be derived.

It should be noticed that monodimensional distributions, such as the Gaussian, are confusingly called symmetric in most books. They are in fact achiral. Evaluating the amount of chirality is a different concept from evaluating the amount of direct symmetry. How to extend the present approach to direct symmetry is an open problem.

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APPENDIX A: OPTIMAL PROCRUSTES TRANSFORMATIONS

The results in this appendix are valid for colored mixtures, and therefore stand for random vectors. We consider the colored Wasserstein distance $C(P^1,P^2)$ [Eqs. (2.6)–(2.8)], and we look for the lower bound of D^2 when the mixture Y is submitted to a linear transformation A and a translation t:

$$D^2=E[(X-(A\cdot Y+t))'\cdot(X-(A\cdot Y+t))], \tag{A1}$$

$$C^2=\mathrm{Inf}_{\{A,W,t\}}D^2. \tag{A2}$$

The gradient in t is null when $t=E(X)-A\cdot E(Y)$. It means that both mixtures should be centered before looking to the optimal value of A. The optional translation is further ignored, such that all results listed in this appendix remain valid, whether or not X and Y are centered prior any optimization. Now we look to the lower bound of D^2 for A. We have a quadratic expression of A, except if A is orthogonal:

$$D^2=E[(X-A\cdot Y)'\cdot(X-A\cdot Y)], \tag{A3}$$

$$C^2=\mathrm{Inf}_{\{A,W\}}D^2. \tag{A4}$$

1. The optimal general linear transformation

Derivating in (A3), we get:

$$E[2\cdot A\cdot Y\cdot Y'-2\cdot X\cdot Y']=0, \tag{A5}$$

$$A=E[X\cdot Y']\cdot(E[Y\cdot Y'])^{-1}. \tag{A6}$$

When the noncentered covariance matrix of Y is not inversible, we can try to solve by interchanging X and Y. If both noncentered covariance matrices are singular, the problem is in fact subdimensional.

2. The optimal orthogonal transformation

The solution given by Golub and van Loan (1985) is restricted to finite sets of equiprobable points (in a nonprobabilistic context). It is extended here to colored mixtures. For clarity, we set $A=Q$. Equation (A7) shows that D^2 is an affine expression of Q:

$$D^2=E[X'\cdot X+Y'\cdot Y-2\cdot X'\cdot Q\cdot Y]. \tag{A7}$$

Now we look for the upper bound of:

$$E[X'\cdot Q\cdot Y]=Tr(E[Y\cdot X']\cdot Q). \tag{A8}$$

Let us write in Eq. (A9) the singular value decomposition of the square matrix $E[Y\cdot X']$, i.e., S being the diagonal matrix containing the singular values, U being the orthonormal matrix of eigenvalues of $E[X\cdot Y']\cdot E[Y\cdot X']$, and V being the associated orthonormal matrix of eigenvalues of $E[Y\cdot X']\cdot E[X\cdot Y']$, we have

$$E[Y\cdot X']=V\cdot S\cdot U'. \tag{A9}$$

We look for the upper bound of $Tr(V\cdot S\cdot U'\cdot Q)=Tr(U'\cdot Q\cdot V\cdot S)$. The coefficients of the diagonal matrix S are non-negative, thus the trace is maximized when the coefficients of the orthogonal matrix $U'\cdot Q\cdot V$ are all equal to 1, meaning that $U'\cdot Q\cdot V=I$. The optimal matrix Q is

$$Q=U\cdot V'. \tag{A10}$$

When S is nonsingular, the determinant of Q is obtained from (A9) and (A10):

$$\det(Q) = \mathrm{sign}(\det(E[Y \cdot X'])). \tag{A11}$$

The sense of the eigenvectors of U and V are not independant, because the non-normalized matrix of eigenvalues of $E[Y \cdot X'] \cdot E[X \cdot Y']$ (which becomes V after normalization) is equal to $E[Y \cdot X'] \cdot U$. Thus, changing the sense of any eigenvector of U is still possible, but does not affect Q.

The optimal Q is unique, except when S has at least one null diagonal element.

3. The optimal *d*-dimensional rotation

As for the general orthogonal transformation [see Eqs. (A7) and (A8) in which we set $Q = R$ for clarity], we look to the upper bound of $Tr(E[Y \cdot X'] \cdot R)$, which is a linear expression of the unknown rotation. The set of rotations is closed and bounded in R^{d^2}. Our constrained maximization problem of a linear form in R^{d^2} has indeed a solution, but it may be not unique. The general expression of the solution is unknown, except in some particular situations. When $\det(E[Y \cdot X']) > 0$, the optimal rotation is given in Eq. (A10).

4. The optimal planar rotation

The planar rotation matrix is parametrized with the angle r:

$$R = I \cdot \cos(r) + \Pi \cdot \sin(r), \tag{A12}$$

where I is the identity matrix, and Π the antisymmetric matrix associated to the rotation of angle $\pi/2$. Reporting (A12) in (A3) and derivating for r gives the minimum and the maximum of D^2. The minimum is

$$\cos(r) = E[X' \cdot Y]/\mathbf{E}, \tag{A13}$$

$$\sin(r) = E[X' \cdot \Pi \cdot Y]/\mathbf{E}, \tag{A14}$$

$$\mathbf{E} = [(E[X' \cdot Y])^2 + (E[X' \cdot \Pi \cdot Y])^2]^{1/2}, \tag{A15}$$

$$D^2 = E[X' \cdot X] + E[Y' \cdot Y] - 2 \cdot \mathbf{E}. \tag{A16}$$

5. The optimal spatial rotation

The spatial rotation R is parametrized with the unit quaternion q. Its first component is the cosinus of the half rotation angle, and its other three components are the rotation axis, with length equal to the sinus of the half rotation angle. The quaternions q and $-q$ are associated to the same rotation. The optimal quaternion maximizes the quadratic form $q' \cdot B \cdot q$ in Eq. (A17) and the proof is essentially that established in the appendix of Petitjean (1999b) for finite sets of equiprobable points (in a nonprobabilistic context). It is extended here to colored mixtures. The optimal quaternion is the unit eigenvector associated to the highest eigenvalue of the symmetric matrix B:

$$D^2 = D_0^2 - 2 \cdot q' \cdot B \cdot q, \tag{A17}$$

$$D_0^2 = E[(X - Y)' \cdot (X - Y)], \tag{A18}$$

$$B = \begin{pmatrix} 0 & c' \\ c & (Z + Z' - I \cdot Tr(Z + Z')) \end{pmatrix}, \tag{A19}$$

$$Z = E[Y \cdot X'], \tag{A20}$$

$$c = E[Y \wedge X]. \tag{A21}$$

Note that the elements of c are computable from those of Z.

APPENDIX B: THE BERNOULLI DISTRIBUTION

The Bernouilli distribution is translated here to get a null expectation, i.e., the value $1-m$ has probability $P(1-m)=m$ and the value $-m$ has probabilty $P(-m)=1-m$. The rotation $R=1$, and the joint distributions between X and Y distributed as $-X$, are conveniently parametrized by only one parameter $p=P(X=-m\cap Y=m-1)$. Therefore, $P(X=1-m\cap Y=m-1)=m-p$, $P(X=-m\cap Y=m)=1-m-p$, and $P(X=1-m\cap Y=m)=p$. The covariance is $c=p-m(1-m)$, and the maximal correlation coefficient is reached for $p=m$ when $m\in[0;\frac{1}{2}]$, and for $p=1-m$ when $m\in[\frac{1}{2};1]$, i.e., $r=m/(1-m)$ and $r=(1-m)/m$, respectively. According to Eq. (2.1), $\chi=1-(\frac{1}{2})/(1-m)$ when $m\in]0;\frac{1}{2}]$, and $\chi=1-(1/2)/m$ when $m\in[\frac{1}{2};1[$. The chiral index is null when $m=\frac{1}{2}$, and is tending to $\frac{1}{2}$ when m is tending to 0 or to 1. The line $m=\frac{1}{2}$ is a symmetry axis for the graph of the function $\chi(m)$.

The colored Bernoulli distribution is, as for the noncolored one, a mixture of two random variables almost surely constant, with mixing proportions m and $1-m$. As previously, the mixture is translated to get a null expectation. However, the two components of the mixture are colored, and thus $P(X=-m\cap Y=m-1)=0$ and $P(X=1-m\cap Y=m)=0$. Setting now $p=P(X=-m\cap Y=m)$, the covariance is $c=-p\cdot m^2-(1-p)\cdot(1-m)^2$, and the maximal correlation coefficient is reached for $p=1$ when $m\in[0;\frac{1}{2}]$, and for $p=0$ when $m\in[\frac{1}{2};1]$, i.e., $r=-m/(1-m)$ and $r=(m-1)/m$, respectively. According to Eq. (2.1), $\chi=(\frac{1}{2})/(1-m)$ when $m\in]0;\frac{1}{2}]$, and $\chi=1/2m$ when $m\in[\frac{1}{2};1[$. The chiral index is equal to 1 when $m=\frac{1}{2}$, and is tending to $\frac{1}{2}$ when m is tending to 0 or to 1. The line $m=\frac{1}{2}$ is a symmetry axis for the graph of the function $\chi(m)$. This graph is the image of the previous one through the symmetry axis $\chi=\frac{1}{2}$.

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Twisted duality of the CAR-algebra

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We give a complete proof of the twisted duality property $\mathcal{M}(\mathfrak{q})' = \tilde{Z}\mathcal{M}(\mathfrak{q}^{\perp})\tilde{Z}^*$ of the (self-dual) CAR-Algebra in any Fock representation. The proof is based on the natural Halmos decomposition of the (reference) Hilbert space when two suitable closed subspaces have been distinguished. We use modular theory and techniques developed by Kato concerning pairs of projections in some essential steps of the proof. As a byproduct of the proof we obtain an explicit and simple formula for the graph of the modular operator. This formula can be also applied to fermionic free nets, hence giving a formula of the modular operator for any double cone. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1483376]

I. INTRODUCTION

Twisted duality is a structural property of the von Neumann algebra obtained from the CAR-Algebra (which is an abstract C*-algebra) in any Fock representation. The (self-dual) CAR-Algebra is uniquely given once a separable Hilbert space $\mathfrak{h}$ and an anti-unitary involution Γ are specified.[3,4] Now for any Γ-invariant subspace $\mathfrak{q}$ of $\mathfrak{h}$ and any Fock state characterized by a so-called basis projection P we can canonically construct a von Neumann algebra $\mathcal{M}(\mathfrak{q})$. Twisted duality means that the equation

$$\mathcal{M}(\mathfrak{q})' = \tilde{Z}\mathcal{M}(\mathfrak{q}^{\perp})\tilde{Z}^* \tag{1}$$

holds, where $\tilde{Z}$ is a certain unitary twist operator to be introduced in the following section and $\mathfrak{q} \oplus \mathfrak{q}^{\perp} = \mathfrak{h}$. Thus in order to formulate duality in the context of the (self-dual) CAR-Algebra one needs to distinguish two closed subspaces $\mathfrak{q}$ and $\mathfrak{p} := P\mathfrak{h}$ in the reference Hilbert space $\mathfrak{h}$. The study of two closed subspaces of a Hilbert space has a long and interesting history in functional analysis (e.g., Refs. 15, 13, 22, 30, 6, 11, and 26) as well as applications in mathematical physics.[5]

We will see how the analysis of the relative position of these subspaces will naturally suggest the strategy of the complete proof of Eq. (1) that we present in this article. Concretely, given $\mathfrak{p}$ and $\mathfrak{q}$ as before we can canonically consider the Halmos decomposition $\mathfrak{h} = \mathfrak{h}_0 \oplus \mathfrak{h}_1$ (cf. Ref. 22), where $\mathfrak{h}_0$ is the maximal subspace on which the orthoprojections corresponding to the closed subspaces commute (Ref. 11 Sec. III). Our proof of (1) in the general case is based on the corresponding property for the generic position situation where $\mathfrak{h}_0 = \{0\}$. The case where $\mathfrak{p}$ and $\mathfrak{q}$ are in generic position allows us to use modular theory[25,12] as well as results of Kato[26] for pairs of projections. In this context we will characterize the bicontinuity of different mappings that naturally appear here, e.g., the Tomita operator restricted to the one-particle Hilbert space. Further, we discuss systematically the relation of an important mapping φ (and the components of its polar decomposition) used by Araki and Dell'Antonio[2,14], to the modular objects given in our case. The mapping φ is introduced by these authors to study the type of certain local von Neumann algebras.

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The equation (1) appears naturally in the context of algebraic quantum field theory, in particular in relation with Haag duality, which is one of its central concepts (see e.g., Refs. 16, 17, 31, 21, and 7). Haag duality is a strengthening of Einstein causality for a net of von Neumann algebras indexed by suitable regions in $\mathbb{R}^4$. In the context of the CCR-Algebra (bosonic systems), one usually proceeds in two steps in order to prove this property:[2,18,23,27,29] first one shows the so-called *abstract* duality

$$\mathcal{M}(\mathfrak{m}^{\perp_\sigma}) = \mathcal{M}(\mathfrak{m})',$$

where $\mathcal{M}(\mathfrak{m})'$ is the commutant of the von Neumann algebra $\mathcal{M}(\mathfrak{m})$ which is generated by the Weyl operators associated to a closed real subspace $\mathfrak{m}$ of the one-particle Hilbert space and $\mathfrak{m}^{\perp_\sigma}$ denotes the symplectic complement of $\mathfrak{m}$. This result is then crucially used in a second step in order to reduce the proof of Haag duality to the discussion of certain real subspaces $\mathfrak{m}(\mathcal{O})$ associated to sufficiently regular regions $\mathcal{O}$ in $\mathbb{R}^4$. In the context of the CAR-Algebra (fermionic systems), and taking into account that now the generators of the algebra will anti-commute if the corresponding elements of the reference space are mutually orthogonal, one can adapt the notions of duality [cf. (1)] and Haag duality. (In the following we will avoid the use of the adjective "abstract.") Twisted duality (1) is mentioned (without proof) in Ref. 3, Remark 4.9 and proved in Ref. 20. For the special case of the generic position situation, see also Ref. 32, p. 496. An important difference between the proof we present here and those in Refs. 20 and 32 is that we will use the self-dual approach to the CAR-Algebra[3,4] and will consistently work with *complex* Hilbert subspaces. (For further details about the relation between our proof and those in Refs. 20 and 32 we refer to Remark 5.7 and to Sec. VI.) This is not only a matter of elegance, but only the *explicit* use of a basis projection P in order to specify the Fock states of the CAR-Algebra will allow us to consider the natural Halmos decomposition of the reference Hilbert space. Therefore, the whole strategy of the proof as well as various formulas we prove in Sec. IV (e.g., a simple and explicit expression for the graph of the modular operator as well as a formula for the modular conjugation, cf. Theorem 4.12 and Remark 5.7) will depend on this choice. Finally, the twisted duality property (1) of the CAR-Algebra can be applied to the fermionic free nets defined in Refs. 8, 24, and 28 in order to prove Haag duality for these models. In the mentioned references the authors present a direct way to construct nets of local C*-or von Neumann-algebras associated to massive (resp. massless) models for any half-integer spin (resp. helicity) value. The nets for these models are naturally characterized by a net of local Γ-invariant linear subspaces $\mathcal{O} \mapsto \mathfrak{q}(\mathcal{O})$ of the corresponding reference Hilbert space. Now the formulas for the graph of the modular operator and modular conjugation (cf. Theorem 4.12 and Remark 5.7) can also be applied to the localized CAR-Algebras associated with $\mathfrak{q}(\mathcal{O})$, where $\mathcal{O}$ is a double cone. We will give in Theorem 5.10 the corresponding formulas for the localized modular objects.

The article is structured in seven sections: In Sec. II we will state basic results concerning the CAR-Algebra that will be used later on. In the following section we will consider the Halmos decomposition of a Hilbert space and state necessary and sufficient conditions on the subspaces $\mathfrak{p}$ and $\mathfrak{q}$ in order that the modular theory is well defined for $\mathcal{M}(\mathfrak{q})$ and its Fock vacuum vector Ω. In Sec. IV we will systematically analyze the context defined by two projections: the first one being the orthoprojection Q onto $\mathfrak{q}$ and the other one being the basis projection P. The main goal here is to relate the objects that appear in the polar decomposition of the mapping φ and of the Tomita operator S corresponding to $(\mathcal{M}(\mathfrak{q}),\Omega)$ and restricted to the one-particle space $\mathfrak{p}$. On the way to this goal we will give simple formulas for the graphs of $\varphi^*\varphi$ and the modular operator which show a beautiful symmetry wrt the interchange $P \leftrightarrow Q$ (cf. Theorem 4.12 and Proposition 4.13). These results will be applied in the next section where (1) is proved in the case where $\mathfrak{p}$ and $\mathfrak{q}$ are in generic position. In Sec. VI the relation of the self-dual approach to the real subspace approaches in Refs. 20 and 32 are pointed out. In the last section we give a complete proof of (1) in the most general situation, i.e., for any Γ-invariant closed subspace $\mathfrak{q}$ and any Fock state. The proof is based on the results of the previous two sections.

II. BASIC STRUCTURE OF THE CAR-ALGEBRA

In order to establish our notation we will begin this section collecting some standard results concerning the CAR-Algebra that will be needed later on. For proofs and further results we refer to Refs. 3 and 4. In the following subsections we will also consider additional structure of this algebra necessary for our proof of twisted duality.

Theorem 2.1: *Let* $\mathfrak{h}$ *be a complex Hilbert space with scalar product* $\langle\cdot,\cdot\rangle$ *and let* Γ *be an anti-unitary involution on it, i.e.,* $\langle\Gamma f,\Gamma h\rangle=\langle h,f\rangle$, *for all* $f,h\in\mathfrak{h}$. *Then* $\mathrm{CAR}(\mathfrak{h},\Gamma)$ *denotes the algebraically unique* C*-*algebra generated by* $\mathbb{1}$ *and* $a(f)$, $f\in\mathfrak{h}$, *such that the following relations hold:*

(i) *The mapping* $\mathfrak{h}\ni f\mapsto a(f)$ *is antilinear.*
(ii) *For any* $f\in\mathfrak{h}$ *one has* $a(f)^*=a(\Gamma f)$.
(iii) *For any* $f,h\in\mathfrak{h}$ *the equation* $a(f)a(h)^*+a(h)^*a(f)=\langle f,h\rangle\,\mathbb{1}$ *holds.*

Next we define a class of pure states of the preceding C*-algebra. An orthoprojection P of $\mathfrak{h}$ is called a *basis projection* if it satisfies the relation $P+\Gamma P\Gamma=\mathbb{1}$. These projections uniquely characterize so-called *Fock states* ω_P by means of the equation

$$\omega_P(a(f)^*a(f)):=0 \quad \text{for any} \quad f\in\mathfrak{h} \quad \text{with} \quad Pf=f. \tag{2}$$

The antisymmetric Fock space is given by

$$\mathfrak{F}:=\bigoplus_{n=0}^{\infty}(\wedge^n P\mathfrak{h}). \tag{3}$$

In order to specify the Fock representation $\pi(a(f))$ of the generators $a(f)$ we need to introduce the usual annihilation and creation operators on $\mathfrak{F}$:

$$c(p)\Omega:=0,$$

$$c(p)(p_1\wedge\cdots\wedge p_n):=\sum_{r=1}^{n}(-1)^{r-1}\langle p,p_r\rangle_{\mathfrak{h}}p_1\wedge\cdots\wedge\hat{p}_r\wedge\cdots\wedge p_n,$$

$$c(p)^*\Omega:=p,$$

$$c(p)^*(p_1\wedge\cdots\wedge p_n):=p\wedge p_1\wedge\cdots\wedge p_n,$$

where Ω is the Fock vacuum in the subspace corresponding to $n=0$ in the definition (3) and $p,p_1,\ldots,p_n\in P\mathfrak{h}$. $\hat{p}_r$ means that the vector p_r is omitted in the wedge product. Finally, the Fock representation π is defined by

$$\pi(a(f)):=c(P\Gamma f)^*+c(Pf),\quad f\in\mathfrak{h}.$$

In the rest of the article we assume that a basis projection P is given and when no confusion arises we will also simply write $a(f)$ instead of $\pi(a(f))$. To prove twisted duality in Sec. V we will need an explicit formula for the vector $a(f_n)\cdot\cdots\cdot a(f_1)\Omega$. Let n, k, p be natural numbers with $2p+k=n$ and define the following subset of the symmetric group $\mathfrak{S}_n$:

$$\mathfrak{S}_{n,p}:=\left\{\begin{pmatrix} n & n-1 & \cdots & n-2p+2 & n-2p+1 & k & \cdots & 1\\ \alpha_1 & \beta_1 & \cdots & \alpha_p & \beta_p & j_1 & \ldots & j_k\end{pmatrix}\in\mathfrak{S}_n \,\middle|\, \alpha_1>\cdots>\alpha_p,\alpha_l>\beta_l,\right.$$
$$\left. l=1,\ldots,p \quad \text{and} \quad n\geqslant j_1>j_2>\ldots j_k\geqslant 1\right\}.$$

Note that $\mathfrak{S}_{n,p}$ contains $\binom{n}{n-2p}(2p)!/p!2^p$ elements.

Proposition 2.2: For $f_1,\ldots,f_n\in\mathfrak{h}$ the equation

$$(a(f_n)\cdot\cdots\cdot a(f_1))\Omega=\sum_{\substack{\pi\in\mathfrak{S}_{n,p}\\0\leqslant 2p\leqslant n}}(\operatorname{sgn}\pi)\prod_{l=1}^{p}\langle Pf_{\alpha_l},P\Gamma f_{\beta_l}\rangle P\Gamma f_{j_1}\wedge\cdots\wedge P\Gamma f_{j_k}$$

holds, where the indices $\alpha_l,\beta_l,j_1,..,j_k$ are given in the definition of $\mathfrak{S}_{n,p}$ and where for $n=2p$ in the preceding sum one replaces the wedge product by the vacuum Ω.

Proof: See the Appendix. ■

Let Z be the implementation on $\mathfrak{F}$ of the even-oddness automorphism associated to the Bogoljubov unitarity -1 (Ref. 4, p. 76). It satisfies $Z=Z^*=Z^{-1}$ and therefore its spectral decomposition is simply given by

$$Z=E^+-E^-. \tag{4}$$

Let further $X=X_{\text{even}}+X_{\text{odd}}$ be the unique decomposition of any $X\in\mathrm{CAR}(\mathfrak{h},\Gamma)$ into its even and odd parts. The following result will be used in Sec. VII.

Lemma 2.3: Let π be a Fock representation of $\mathrm{CAR}(\mathfrak{h},\Gamma)$ *and $Z=E^+-E^-$ as before. Then for any $X\in\mathrm{CAR}(\mathfrak{h},\Gamma)$ we have*

$$E^+\pi(X_{\text{even}})E^-=E^-\pi(X_{\text{even}})E^+=0,$$

$$E^+\pi(X_{\text{odd}})E^+=E^-\pi(X_{\text{odd}})E^-=0.$$

Proof: Recall that $Z_0\pi(X_{\text{even}})=\pi(X_{\text{even}})Z_0$. Multiplying from the left by E^+ and from the right by E^- we get

$$E^+\pi(X_{\text{even}})E^-=-E^+\pi(X_{\text{even}})E^-,$$

which implies the first two equations. Similarly we obtain the equations corresponding to the odd part. ■

A. Direct sums and tensor products

Let $(\mathfrak{h}_k,\Gamma_k)$, $k=0,1$, be two Hilbert spaces with anti-unitary involutions and let P_k be two basis projections for the corresponding spaces. We denote by π_k the Fock representations of $\mathrm{CAR}(\mathfrak{h}_k,\Gamma_k)$ on the antisymmetric Fock spaces $\mathfrak{F}_k$. Z_k are the implementers of the respective even-oddness automorphisms, $k=0,1$. Motivated by Ref. 14, p. 82 (cf. also Ref. 19, p. 219) we consider the following.

Proposition 2.4: With the preceding notation put $\mathfrak{h}:=\mathfrak{h}_0\oplus\mathfrak{h}_1$ and $\Gamma:=\Gamma_0\oplus\Gamma_1$ and consider $\mathrm{CAR}(\mathfrak{h},\Gamma)$. *The representations defined on $\mathfrak{F}_0\otimes\mathfrak{F}_1$ by*

$$\pi(a(f_0\oplus f_1)):=\pi_0(a(f_0))\otimes 1+Z_0\otimes\pi_1(a(f_1)), \tag{5}$$

$$\pi(a(f_0\oplus f_1)):=\pi_0(a(f_0))\otimes Z_1+1\otimes\pi_1(a(f_1)),\quad f_k\in\mathfrak{h}_k,\ k=0,1, \tag{6}$$

are the Fock representations of $\mathrm{CAR}(\mathfrak{h},\Gamma)$ *wrt the basis projection $P:=P_0\oplus P_1$ on* $(\mathfrak{h},\Gamma)$. *Further, the even-oddness automorphism of* $\mathrm{CAR}(\mathfrak{h},\Gamma)$ *is implemented on $\mathfrak{F}_0\otimes\mathfrak{F}_1$ by $Z:=Z_0\otimes Z_1$.*

Proof: We check first that the definition (5) is compatible with the algebraic structure of $\mathrm{CAR}(\mathfrak{h},\Gamma)$. Indeed, for any $f_k,h_k\in\mathfrak{h}_k$, $k=0,1$,

$$\pi(a(f_0\oplus f_1))^*=\pi_0(a(\Gamma_0 f_0))\otimes 1+Z_0\otimes\pi_1(a(\Gamma_1 f_1))=\pi(a(\Gamma(f_0\oplus f_1)))$$

and

$$
\begin{aligned}
&\pi(a(f_0\oplus f_1))\pi(a(h_0\oplus h_1))^*+\pi(a(h_0\oplus h_1))^*\pi(a(f_0\oplus f_1))\\
&\quad=\pi_0(a(f_0)a(h_0)^*)\otimes\mathbb{1}+\mathbb{1}\otimes\pi_1(a(f_1)a(h_1)^*)\\
&\qquad+\pi_0(a(h_0)^*a(f_0))\otimes\mathbb{1}+\mathbb{1}\otimes\pi_1(a(h_1)^*a(f_1))\\
&\qquad+\underbrace{Z_0\pi_0(a(h_0)^*)\otimes\pi_1(a(f_1))+\pi_0(a(h_0)^*)Z_0\otimes\pi_1(a(f_1))}_{=0}\\
&\qquad+\underbrace{Z_0\pi_0(a(f_0))\otimes\pi_1(a(h_1)^*)+\pi_0(a(f_0))Z_0\otimes\pi_1(a(h_1)^*)}_{=0}\\
&\quad=\langle f_0\oplus f_1,h_0\oplus h_1\rangle\mathbb{1}\otimes\mathbb{1}.
\end{aligned}
$$

Consider next the vector state associated to $\Omega_0\otimes\Omega_1$, where Ω_k are the Fock vacua in $\mathfrak{F}_k$, $k=0,1$. In this case we have

$$
\begin{aligned}
&\langle\Omega_0\otimes\Omega_1,\pi(a(f_0\oplus f_1))^*\pi(a(f_0\oplus f_1))\Omega_0\otimes\Omega_1\rangle\\
&\quad=\|\pi_0(a(f_0))\Omega_0\otimes\Omega_1+\Omega_0\otimes\pi_1(a(f_1))\Omega_1\|^2\\
&\quad=\|P_0\Gamma_0 f_0\|^2+\|P_1\Gamma_1 f_1\|^2=\|(\mathbb{1}-P)(f_0\oplus f_1)\|^2.
\end{aligned}
$$

Thus by the uniqueness of the characterizing condition (2) of a Fock state, together with the fact that the vectors $\pi(a(f_0\oplus f_1))\Omega_0\otimes\Omega_1$, $f_k\in\mathfrak{h}_k$, generate the whole space $\mathfrak{F}_0\otimes\mathfrak{F}_1$, we have that π is actually the Fock representation of CAR$(\mathfrak{h},\Gamma)$ wrt the basis projection P with Fock vacuum $\Omega_0\otimes\Omega_1$.

We still need to show that $Z_0\otimes Z_1$ implements the even-oddness automorphism of CAR$(\mathfrak{h},\Gamma)$ on $\mathfrak{F}_0\otimes\mathfrak{F}_1$. Note that $\alpha:=\mathrm{ad}(Z_0\otimes Z_1)$ satisfies $\alpha^2=\mathrm{id}$ and it is enough to consider the action of α on the generators:

$$
(Z_0\otimes Z_1)\pi(a(f_0\oplus f_1))(Z_0\otimes Z_1)=Z_0\pi_0(a(f_0))Z_0\otimes Z_1^2+Z_0^3\otimes Z_1\pi_1(a(f_1))Z_1=\pi(-a(f_0\oplus f_1)).
$$

Equation (6) is shown similarly. ■

Corollary 2.5: For $X_0\in\mathrm{CAR}(\mathfrak{h}_0,\Gamma_0)$ *and* $X_1=X_{1,\mathrm{even}}+X_{1,\mathrm{odd}}\in\mathrm{CAR}(\mathfrak{h}_1,\Gamma_1)$ *we have*

$$
\pi(X_0)=\pi_0(X_0)\otimes\mathbb{1}
$$

and

$$
\pi(X_1)=\mathbb{1}\otimes\pi_1(X_{1,\mathrm{even}})+Z_0\otimes\pi_1(X_{1,\mathrm{odd}})=E_0^+\otimes\pi_1(X_1)+E_0^-\otimes Z_1\pi_1(X_{1,\mathrm{odd}})Z_1,
$$

where $Z_0=E_0^+-E_0^-$.

B. The subspace $\mathfrak{q}$ and twisted causality

Let $(\mathfrak{q},\Gamma)$ be as in Theorem 2.1 and denote by $\mathfrak{q}$ a closed Γ-invariant subspace of $\mathfrak{h}$. We can naturally associate with the subspace $\mathfrak{q}$ a von Neumann algebra that acts on the antisymmetric Fock space characterized by the basis projection P:

$$
\mathcal{M}(\mathfrak{q}):=(\{a(q)|q\in\mathfrak{q}\})''\subset\mathcal{L}(\mathfrak{F}). \tag{7}
$$

In order to be able to formulate causality or duality in the context of the CAR-Algebra it is necessary to introduce a so-called *twist operator* $\widetilde{Z}$ on $\mathfrak{F}$. Indeed, this operator allows us to express orthogonality relations of subspaces of $\mathfrak{h}$ in terms of the commutant of a suitable von Neumann algebra. Recalling the definition of Z before Eq. (4) we define the twist operator as usual [Ref. 10, Eq. (26)]:

$$\tilde{Z} := \frac{1}{1+i}(\mathbb{1}+iZ) \quad \text{and} \quad \tilde{Z}a(f)\tilde{Z}^* = iZa(f), \quad f \in \mathfrak{h}. \tag{8}$$

Putting

$$\eta(n) := \begin{cases} 1, & \text{if } n \text{ even}, \\ -i, & \text{if } n \text{ odd}, \end{cases}$$

we may describe the action of $\tilde{Z}$ and $\tilde{Z}^*$ on $\mathfrak{F}$ by $\tilde{Z}(p_1 \wedge \cdots \wedge p_n) = \eta(n)\, p_1 \wedge \cdots \wedge p_n$ and $\tilde{Z}^*(p_1 \wedge \cdots \wedge p_n) = \overline{\eta(n)}\, p_1 \wedge \cdots \wedge p_n$. Further, considering the spectral projections $E^{\pm}$ of Z we also have the relation

$$\tilde{Z} = E^+ - iE^-. \tag{9}$$

The algebra $\tilde{Z}\,\mathcal{M}(\mathfrak{q})\,\tilde{Z}^*$ is usually called "twisted" algebra. It is now immediate to check the following inclusion, which expresses the twisted causality property in the present context.

Proposition 2.6: Let $\mathfrak{q}$ *be a closed* Γ*-invariant subspace of* $\mathfrak{h}$ *as before. Then the inclusion* $\tilde{Z}\,\mathcal{M}(\mathfrak{q}^\perp)\,\tilde{Z}^* \subseteq \mathcal{M}(\mathfrak{q})'$ *holds.*

Remark 2.7: Twisted duality strengthens this relation by turning the preceding inclusion into an equality for *any* closed Γ-invariant subspace $\mathfrak{q}$ of $\mathfrak{h}$.

Remark 2.8: Writing now explicitly the Fock representation and considering Eq. (8) as well as the even-odd grading of the CAR-Algebra we have the following ways of generating the twisted von Neumann algebra:

$$\begin{aligned} \tilde{Z}\,\mathcal{M}(\mathfrak{q}^\perp)\,\tilde{Z}^* &= \{Z\pi(a(q^\perp))\,|\,q^\perp \in \mathfrak{q}^\perp\}'' \\ &= \{\pi(Y_{\text{even}}) + iZ\pi(Y_{\text{odd}}))\,|\,Y = Y_{\text{even}} + Y_{\text{odd}} \in \mathrm{CAR}(\mathfrak{q}^\perp, \Gamma\restriction\mathfrak{q}^\perp)\}''. \end{aligned}$$

III. THE HALMOS DECOMPOSITION OF A HILBERT SPACE

From the preceding subsection we see that to formulate the duality property in the present context one needs to distinguish two closed subspaces of the reference space $\mathfrak{h}$: the subspace $\mathfrak{p}$ (one-particle Hilbert space), which is given by the basis projection P, and the Γ-invariant subspace $\mathfrak{q}$ to which we associate the orthoprojection Q. Therefore, it is natural to consider the Halmos decomposition[22] of $\mathfrak{h}$ wrt $\mathfrak{p}$ and $\mathfrak{q}$, which is given by

$$\mathfrak{h} = \mathfrak{h}_0 \oplus \mathfrak{h}_1, \tag{10}$$

where $\mathfrak{h}_0 = (\mathfrak{p}\cap\mathfrak{q}) \oplus (\mathfrak{p}\cap\mathfrak{q}^\perp) \oplus (\mathfrak{p}^\perp\cap\mathfrak{q}) \oplus (\mathfrak{p}^\perp\cap\mathfrak{q}^\perp)$ and $\mathfrak{h}_1 = \mathfrak{h} \ominus \mathfrak{h}_0$. $\mathfrak{h}_0$ is actually the maximal subspace where P and Q commute (Ref. 11, Sec. III). In $\mathfrak{h}_1$ the subspaces $\mathfrak{p}$ and $\mathfrak{q}$ are said to be in *generic position*,[22] in the sense that the preceding four mutual intersections of the subspaces $\mathfrak{p}$, $\mathfrak{q}$, $\mathfrak{p}^\perp$ and $\mathfrak{q}^\perp$ are equal to $\{0\}$.

In the present context the decomposition (10) is also natural because it allows us to separate the general situation into simpler "pieces" on $\mathfrak{h}_0$ and $\mathfrak{h}_1$:

Lemma 3.1: Consider $(\mathfrak{h},\Gamma)$ *and* P,Q *as before. Further, let* R_0 *be the orthoprojection onto the subspace* $\mathfrak{h}_0$ *in (10). Then we have*

$$R_0P = PR_0, \quad R_0Q = QR_0 \quad \text{and} \quad R_0\Gamma = \Gamma R_0.$$

Proof: The first two equations are clear from the form of $\mathfrak{h}_0$ given after (10) and recall that R_0 is the maximal orthoprojection with the property $R_0\,PQ = R_0\,QP$. Now from

$$\Gamma R_0 \Gamma\, PQ = \Gamma R_0 (\mathbb{1}-P) Q\Gamma = \Gamma R_0 \Gamma\, QP$$

and the maximality of R_0 we must have $\Gamma R_0 \Gamma \leqslant R_0$. Finally, from the Γ-invariance of $\mathfrak{h}$ and since $\Gamma^2 = \mathbb{1}$ we get $R_0 \Gamma = \Gamma R_0$. ■

Remark 3.2: The preceding result allows us to consider the following restrictions:

$$P_k := P \restriction \mathfrak{h}_k, \quad Q_k := Q \restriction \mathfrak{h}_k, \quad \text{and} \quad \Gamma_k := \Gamma \restriction \mathfrak{h}_k, \quad k = 0,1.$$

Further, P_k is a basis projection on $(\mathfrak{h}_k, \Gamma_k)$ characterizing the Fock representation π_k of CAR$(\mathfrak{h}_k, \Gamma_k)$, $k = 0,1$. This possibility to split off the general situation in an Abelian piece and a generic position piece will be essential for the proof of our main theorem in Sec. VII. In this context we will need to split again the Abelian part as $\mathfrak{h}_0 = \mathfrak{h}_{01} \oplus \mathfrak{h}_{02}$, where $\mathfrak{h}_{01} := (\mathfrak{p} \cap \mathfrak{q}^\perp) \oplus \Gamma(\mathfrak{p} \cap \mathfrak{q}^\perp)$ and $\mathfrak{h}_{02} := (\mathfrak{p} \cap \mathfrak{q}) \oplus \Gamma(\mathfrak{p} \cap \mathfrak{q})$.

A. Modular theory

Let $(\mathfrak{h}, \Gamma)$, P and $\mathfrak{q}$ be given as in Sec. II B and denote by $\mathfrak{p} := P\mathfrak{h}$ the corresponding one-particle Hilbert space. We will give in this subsection necessary and sufficient conditions on the subspaces $\mathfrak{p}$ and $\mathfrak{q}$ in order that the Fock vacuum Ω becomes a cyclic and separating vector for the von Neumann algebra $\mathcal{M}(\mathfrak{q})$ (cf. Ref. 19, p. 234). We will see that in the case where the subspaces $\mathfrak{p}$ and $\mathfrak{q}$ are in generic position we can use the results in modular theory[12,25] for the pair $(\mathcal{M}(\mathfrak{q}), \Omega)$. These techniques will be essentially used in the next two sections for the proof of the twisted duality property in the generic position context.

Lemma 3.3: Let $\mathfrak{q} \subset \mathfrak{h}$ be a closed Γ-invariant subspace. Then the following conditions are equivalent:

(i) $q \in \mathfrak{q}$ *and* $Pq = 0$ *implies* $q = 0$.
(ii) $P(\mathfrak{q}^\perp)$ *is a dense submanifold of* $\mathfrak{p}$.
(iii) $\mathfrak{q} \cap \mathfrak{p} = \{0\}$.

Proof: To show $(iii) \Rightarrow (i)$ take $q \in \mathfrak{q}$ with $Pq = 0$. From $\Gamma P \Gamma = \mathbb{1} - P$ and the Γ-invariance of $\mathfrak{q}$ we have that $\Gamma q \in \mathfrak{q} \cap \mathfrak{p} = \{0\}$, thus $q = 0$. The other implications $(i) \Rightarrow (ii) \Rightarrow (iii)$ are checked similarly. ■

Proposition 3.4: Let $\mathfrak{q}$ be a closed Γ-invariant subspace of $\mathfrak{h}$ as before. Then we have the following.

(i) The vacuum vector Ω is cyclic for $\mathcal{M}(\mathfrak{q})$ iff $P\mathfrak{q}$ is a dense submanifold of $\mathfrak{p}$.
(ii) The vacuum vector Ω is separating for $\mathcal{M}(\mathfrak{q})$ iff $P(\mathfrak{q}^\perp)$ is a dense submanifold of $\mathfrak{p}$.

Proof: (i) We assume that Ω is cyclic for $\mathcal{M}(\mathfrak{q})$ and let $p \in \mathfrak{p}$ be a vector satisfying $p \perp P\mathfrak{q}$. From this, from Proposition 2.2 and from the structure of the Fock space $\mathfrak{F}$ [recall Eq. (3)] we have

$$p \perp \operatorname{span}\{a(q_1) \cdots \cdots a(q_n)\Omega \,|\, q_1, \cdots q_n \in \mathfrak{q}, \ n \in \mathbb{N}\},$$

thus

$$p \perp \{A\Omega \,|\, A \in \mathcal{M}(\mathfrak{q})\}.$$

Now since Ω is cyclic for $\mathcal{M}(\mathfrak{q})$ we must have $p = 0$.

Assume now that $P\mathfrak{q} \subset \mathfrak{p}$ is a dense submanifold, so that $\oplus_{n=0}^{\infty}(\overset{n}{\wedge} P\mathfrak{q}) \subset \mathfrak{F}$ is also dense (here $\oplus_{n=0}^{\infty}$ denotes the algebraic direct sum). From Proposition 2.2 we obtain the inclusions

$$\bigoplus_{n=0}^{\infty} (\overset{n}{\wedge} P\mathfrak{q}) \subset \mathcal{M}(\mathfrak{q})\, \Omega \subset \mathfrak{F},$$

which imply that Ω is cyclic for $\mathcal{M}(\mathfrak{q})$.

(*ii*) Suppose now that Ω is a separating vector for $\mathcal{M}(\mathfrak{q})$. We show that this implies part (*i*) of Lemma 3.3. So, let $q \in \mathfrak{q}$ satisfy $Pq=0$. Since $0=Pq=a(\Gamma q)\Omega$ and since Ω is separating for $\mathcal{M}(\mathfrak{q})$ we must have $a(\Gamma q)=0$, which implies $q=0$.

Finally, assume that $P(\mathfrak{q}^\perp)$ is a dense submanifold of $\mathfrak{p}$. By part (*i*) of the present theorem applied to $\mathfrak{q}^\perp$, which is also Γ-invariant, we know that Ω is cyclic for $\mathcal{M}(\mathfrak{q}^\perp)$. Further, since $\tilde{Z}\Omega=\Omega$ we have that Ω is also cyclic for $\tilde{Z}\,\mathcal{M}(\mathfrak{q}^\perp)\,\tilde{Z}^*$ and consequently by Proposition 2.6 also for $\mathcal{M}(\mathfrak{q})' \supseteq \tilde{Z}\,\mathcal{M}(\mathfrak{q}^\perp)\,\tilde{Z}^*$. This shows that Ω is separating for $\mathcal{M}(\mathfrak{q})$. ■

By the preceding result we know that if $\mathfrak{q}$ is a closed Γ-invariant subspace of $\mathfrak{h}$ where $P\mathfrak{q}$ as well as $P(\mathfrak{q}^\perp)$ are dense submanifolds of $\mathfrak{p}$, then the modular theory is well-defined for the pairs $(\mathcal{M}(\mathfrak{q}),\Omega)$ and $(\mathcal{M}(\mathfrak{q}^\perp),\Omega)$. Denote by S and T the Tomita operators corresponding to these pairs respectively. We will next study their action on the submanifolds $P\mathfrak{q}$ and $P(\mathfrak{q}^\perp)$.

Lemma 3.5: With the preceding notation we have for $q \in \mathfrak{q}$ and $q^\perp \in \mathfrak{q}^\perp$

(i) $S(Pq)=P\Gamma q$,
(ii) $T(Pq^\perp)=P\Gamma q^\perp=-S^*(Pq^\perp)$.

Proof: The first two equations follow by direct computation:

$$S(Pq)=S(a(\Gamma q)\,\Omega)=a(\Gamma q)^*\,\Omega=a(q)\,\Omega=P\Gamma q,$$

and similarly for T. To prove the last equation recall that S^* is actually the Tomita operator of $\mathcal{M}(\mathfrak{q})' \supseteq \tilde{Z}\,\mathcal{M}(\mathfrak{q}^\perp)\,\tilde{Z}^*$. Note further that

$$i\,(\tilde{Z}a(\Gamma q^\perp)\tilde{Z}^*)\,\Omega=i\,\tilde{Z}a(\Gamma q^\perp)\,\Omega=i\left(\frac{1-i}{1+i}\right)Pq^\perp=Pq^\perp.$$

From this we can finally check

$$S^*(Pq^\perp)=-i\,S^*(\tilde{Z}a(\Gamma q^\perp)\tilde{Z}^*\,\Omega)=-i\,\tilde{Z}a(q^\perp)\tilde{Z}^*\,\Omega=-P\Gamma q^\perp=-T(Pq^\perp),$$

and the proof is concluded. ■

IV. PAIRS OF PROJECTIONS IN GENERIC POSITION AND THE MAPPING φ

In this section we will consider the mathematically richest situation which appears when the closed subspaces $\mathfrak{p}$ and $\mathfrak{q}$ are in generic position. Let P and Q be the corresponding orthoprojections satisfying as usual the relations $\Gamma P\Gamma=\mathbb{1}-P=P^\perp$ and $Q\Gamma=\Gamma Q$. Motivated by Proposition 3.4 we will also assume here that

$$\mathfrak{p}\cap\mathfrak{q}=\{0\}=\mathfrak{p}\cap\mathfrak{q}^\perp, \quad \text{where} \quad \mathfrak{p}:=P\mathfrak{h}, \tag{11}$$

which directly implies using the basis projection property:

$$\mathfrak{p}^\perp\cap\mathfrak{q}=\{0\}=\mathfrak{p}^\perp\cap\mathfrak{q}^\perp, \quad \text{where} \quad \mathfrak{p}^\perp=P^\perp\mathfrak{h}. \tag{12}$$

Thus in the notation of Sec. III we have the extremal case where $\mathfrak{p}$ and $\mathfrak{q}$ are already in generic position and the Halmos decomposition (10) is trivial in the sense that $\mathfrak{h}_0=\{0\}$.

Note that the properties like $\mathfrak{p}\cap\mathfrak{q}=\{0\}$ can be also expressed by the corresponding projections P and Q, because the orthoprojection onto the intersection $\mathfrak{p}\cap\mathfrak{q}$ is given by

$$\operatorname*{s-lim}_{n\to\infty}(PQ)^n=\operatorname*{s-lim}_{n\to\infty}(QP)^n.$$

Note further that by Lemma 3.3 the intersection assumptions in (11) are equivalent to the density conditions in Proposition 3.4.

Remark 4.1: The following useful density statements are immediate consequences of the assumption that $\mathfrak{p}$ and $\mathfrak{q}$ are in generic position. If $\mathfrak{r}\subseteq\mathfrak{q}$ (or $\mathfrak{r}\subseteq\mathfrak{q}^\perp$) is a dense linear submanifold in $\mathfrak{q}$ (resp. in $\mathfrak{q}^\perp$), then $P\mathfrak{r}$ is dense in $\mathfrak{p}$ and $P^\perp\mathfrak{r}$ is dense in $\mathfrak{p}^\perp$. The same holds if Q and P are interchanged. Thus we have, for example, that $Q\mathfrak{p}^\perp$ is dense in $\mathfrak{q}$, $PQ\mathfrak{p}$ is dense in $\mathfrak{p}$, etc.

We will begin next a systematic analysis of a mapping φ that can be naturally defined in the present context. Put

$$\mathfrak{H}_\varphi := \{(q,q^\perp)\in\mathfrak{q}\times\mathfrak{q}^\perp \,|\, P^\perp(q+q^\perp)=0\},$$

$$\mathfrak{H}_\rho := \{(q,q^\perp)\in\mathfrak{q}\times\mathfrak{q}^\perp \,|\, Pq=Pq^\perp\}.$$

Lemma 4.2: The sets $\mathfrak{H}_\varphi$ and $\mathfrak{H}_\rho$ are graphs of linear, injective and closed mappings $\varphi,\rho:\mathfrak{q}\to\mathfrak{q}^\perp$ with dense domains and dense images. The graphs $\operatorname{gra}\varphi=\mathfrak{H}_\varphi$ *and* $\operatorname{gra}\rho=\mathfrak{H}_\rho$ *can be parametrized by* $\mathfrak{p}$, *resp.* $\mathfrak{p}^\perp$, *as*

$$\begin{aligned}\operatorname{gra}\varphi &:= \{(Qp,Q^\perp p)\,|\,p\in\mathfrak{p}\},\\ \operatorname{gra}\rho &:= \{(Qp^\perp,-Q^\perp p^\perp)\,|\,p^\perp\in\mathfrak{p}^\perp\},\end{aligned} \tag{13}$$

where the domains and images are given explicitly. Moreover, the equation $\rho^{-1}=\varphi^*$ holds.

Proof: We consider first the mapping φ and one can similarly argue for ρ. First note that the assignment $\varphi(q):=q^\perp$ if $P^\perp(q+q^\perp)=0$ is a well-defined linear map. Indeed, if $(q,q_1^\perp)\in\mathfrak{H}_\varphi \ni (q,q_2^\perp)$, then $q_1^\perp=q_2^\perp$, because in this case $q_1^\perp-q_2^\perp\in\mathfrak{q}^\perp\cap\mathfrak{p}=\{0\}$. Injectivity is proved analogously.

Next we show Eq. (13). Let $\mathfrak{p}\ni p=Qp+Q^\perp p$, so that $P^\perp(Qp+Q^\perp p)=0$ and we have $Q\mathfrak{p}\subseteq\operatorname{dom}\varphi$ as well as $Q^\perp\mathfrak{p}\subseteq\operatorname{ima}\varphi$. To show the reverse inclusions take $q_0\in\operatorname{dom}\varphi$, i.e., $P^\perp(q_0+q_0^\perp)=0$ for some $q_0^\perp\in\mathfrak{q}^\perp$. But this implies that $q_0=Q(q_0+q_0^\perp)\in Q\mathfrak{p}$ and $q_0^\perp=Q^\perp(q_0+q_0^\perp)\in Q^\perp\mathfrak{p}$ and Eq. (13) is proved. Note that by the preceding remark the domain and image of φ are dense in $\mathfrak{q}$, resp. $\mathfrak{q}^\perp$, and it is easy to see that $\operatorname{gra}\varphi$ is closed.

Finally, it remains to show that $\rho^{-1}=\varphi^*$. Recall first that

$$\operatorname{gra}\rho^{-1}=\{(Q^\perp p^\perp,-Qp^\perp)\,|\,p^\perp\in\mathfrak{p}^\perp\}.$$

Using the isometric mapping $U:\ \mathfrak{q}\times\mathfrak{q}^\perp\to\mathfrak{q}^\perp\times\mathfrak{q}$ given by $U(q,q^\perp):=(q^\perp,-q)$ we may use the well known formula (see Ref. 1, p. 124)

$$\operatorname{gra}\varphi^*=(\mathfrak{q}^\perp\times\mathfrak{q})\ominus U(\operatorname{gra}\varphi).$$

Therefore $(q^\perp,q)\in\operatorname{gra}\varphi^*$ iff $\langle(q^\perp,q),(Q^\perp p,-Qp)\rangle=0$ for all $p\in\mathfrak{p}$ iff $\langle q^\perp,p\rangle=\langle q,p\rangle$ for all $p\in\mathfrak{p}$ iff $p^\perp:=q^\perp-q\in\mathfrak{p}^\perp$ iff $(q^\perp,q)\in\operatorname{gra}\rho^{-1}$. ∎

Remark 4.3: Note that the preceding lemma depends only on the assumption that P and Q are in generic position (the different role of P and Q wrt Γ, i.e., $Q\Gamma=\Gamma Q$ and $\Gamma P\Gamma=P^\perp$, is not used). This means that the preceding lemma remains true if we do the following replacements:

$$Q\to P \quad\text{and}\quad P\to Q^\perp.$$

Then we obtain the following.

Corollary 4.4: Put

$$\mathfrak{H}_\lambda := \{(p,p^\perp)\in\mathfrak{p}\times\mathfrak{p}^\perp \,|\, Q^\perp p=Q^\perp p^\perp\}.$$

Then $\mathfrak{H}_\lambda$ is the graph of a linear injective closed mapping $\lambda:\mathfrak{p}\to\mathfrak{p}^\perp$ with dense domain and image. $\operatorname{gra}\lambda$ *can be parametrized by* $\mathfrak{q}$:

$$\operatorname{gra}\lambda=\{(Pq,-P^\perp q)\,|\,q\in\mathfrak{q}\}.$$

The parametrization of φ and ρ in terms of $\mathfrak{p}$, resp. $\mathfrak{p}^\perp$, suggests to consider the following mappings:

$$Q:\mathfrak{p}^\perp\to\mathfrak{q}, \tag{14}$$

$$Q^\perp:\mathfrak{p}^\perp\to\mathfrak{q}^\perp, \tag{15}$$

$$Q:\mathfrak{p}\to\mathfrak{q}, \tag{16}$$

$$Q^\perp:\mathfrak{p}\to\mathfrak{q}^\perp, \tag{17}$$

where the first two are related to ρ and the last two are related to φ. For example, the parametrization of ρ in terms of $\mathfrak{p}^\perp$ means that ρ can be seen as the composition of the following mappings:

$$QP^\perp\mathfrak{h}\to P^\perp\mathfrak{h}\to Q^\perp P^\perp\mathfrak{h}.$$

Later we will also need to consider the mappings

$$P:\ \mathfrak{q}^\perp\to\mathfrak{p}, \tag{18}$$

$$P:\ \mathfrak{q}\to\mathfrak{p}. \tag{19}$$

Due to the fact that $\mathfrak{q}$ and $\mathfrak{p}$ are in generic position the mappings (14)–(19) are bounded, injective and their images are dense in the corresponding final subspaces.

We will next give a criterion for the bicontinuity of the mappings (14)–(19). First note that because P is a basis projection

$$\|PQ\|=\|QP\|=\|(\mathbb{1}-P)Q\|=\|Q(\mathbb{1}-P)\|=:\delta$$

and $0<\delta\leqslant 1$. So we can distinguish between the two cases: $\delta<1$ and $\delta=1$.

Proposition 4.5: Let P,Q and δ be given as before. If $\delta<1$, then the mappings (14)–(19) are bicontinuous, in particular their images coincide with the corresponding final spaces. Moreover, the relations

$$\|P-Q\|=\|(\mathbb{1}-Q)P\|=\|(\mathbb{1}-Q)(\mathbb{1}-P)\|=\delta$$

hold.

Proof: This result is a special case of Theorem 6.34 in Ref. 26, p. 56. Note that the second alternative stated in Kato's result cannot appear in the present situation, as a consequence of the fact that $\mathfrak{p}$ and $\mathfrak{q}$ are in generic position. ■

Remark 4.6: This situation corresponds to the case where the index of P and Q is 0 (cf. Ref. 6, Theorem 3.3).

Proposition 4.7: Let P,Q and δ be given as before. If $\delta=1$, then the inverse mappings of (14)–(19) are unbounded and densely defined, i.e., the images of (14)–(19) are nontrivial proper dense sets in the corresponding final subspaces.

Proof: We will only show the assertion for the mapping (19), since one can easily adapt the following arguments to the other cases. Put $A:=QP^\perp Q\restriction\mathfrak{q}\in\mathcal{L}(\mathfrak{q})$, so that $A=A^*$ and $A\geqslant 0$. From

$$\operatorname{spr}A=\|A\|=\|QP^\perp P^\perp Q\|=\|P^\perp Q\|^2=\delta^2=1$$

we obtain $1\in\operatorname{spec}A$. However, 1 is not an eigenvalue of A, because $Aq=q$, $q\in\mathfrak{q}$, implies $\text{s-lim}_{n\to\infty}(QP^\perp)^nq=q$ and this means $q\in\mathfrak{q}\cap\mathfrak{p}^\perp=\{0\}$. Thus $\ker(\mathbb{1}_\mathfrak{q}-A)=\{0\}$ or $(\mathbb{1}_\mathfrak{q}-A)^{-1}$ exists and is unbounded since $1\notin\operatorname{res}A$. Therefore $\vartheta:=\operatorname{dom}(\mathbb{1}_\mathfrak{q}-A)^{-1}$ is a proper dense subset in $\mathfrak{q}$ and this means $\operatorname{ima}(\mathbb{1}_\mathfrak{q}-A)=\vartheta=\operatorname{ima}(Q-QP^\perp Q)=\operatorname{ima}(QPQ)$. Finally, from the polar decomposition of PQ,

$$PQ=\operatorname{sgn}(PQ)\cdot(QPQ)^{1/2},$$

we have that $\operatorname{sgn}(PQ)$ maps $\operatorname{ima}(QPQ)^{1/2}$ isometrically onto $\operatorname{ima}(PQ)=P\mathfrak{q}$. Thus $P\mathfrak{q}$ is a proper dense set in $\mathfrak{p}$, i.e., $P:\mathfrak{q}\to\mathfrak{p}$ is unbounded invertible. ■

Remark 4.8: (*i*) Note that if $\dim\mathfrak{h}<\infty$, then the case $\|PQ\|=1$ is not possible, since the corresponding operators cannot have continuous spectrum. It is easy to show that in this case $\mathfrak{p}\cap\mathfrak{q}=\{0\}$ iff $\|PQ\|<1$.

(*ii*) Note also that $\|(\mathbb{1}-P)Q\|=1$ implies $\|(\mathbb{1}-Q)P\|=1$, because otherwise by Proposition 4.5 $\|(\mathbb{1}-Q)P\|<1$ implies $\|(\mathbb{1}-P)Q\|<1$.

Proposition 4.9: Let the projections P,Q and the mappings φ,ρ be given as before. Then $\varphi,\rho:\mathfrak{q}\to\mathfrak{q}^{\perp}$ are bicontinuous iff $\|PQ\|<1$.

Proof: Suppose that $\|PQ\|<1$, so that by Proposition 4.5 we have that the mappings (14)–(19) are bicontinuous. But as mentioned before we know that φ as well as ρ can be seen as composition of the mappings

$$\varphi:\ QP\mathfrak{h}\to P\mathfrak{h}\to Q^{\perp}P\mathfrak{h},\quad \rho:\ QP^{\perp}\mathfrak{h}\to P^{\perp}\mathfrak{h}\to Q^{\perp}P^{\perp}\mathfrak{h},$$

hence they must be bicontinuous.

In the case that ρ and φ are bicontinuous, then $\operatorname{dom}\rho=\operatorname{dom}\varphi=\mathfrak{q}$ and $\operatorname{ima}\rho=\operatorname{ima}\varphi=\mathfrak{q}^{\perp}$. Finally, Proposition 4.7 implies $\|PQ\|<1$. ■

Motivated by Lemma 3.5 we will analyze next the antilinear mappings defined by the following graphs:

$$\operatorname{gra}\beta:=\{(Pq,P\Gamma q)\in\mathfrak{p}\times\mathfrak{p}\,|\,q\in\mathfrak{q}\},$$

$$\operatorname{gra}\alpha:=\{(Pq^{\perp},-P\Gamma q^{\perp})\in\mathfrak{p}\times\mathfrak{p}\,|\,q^{\perp}\in\mathfrak{q}^{\perp}\}.$$

(Note that the rhs of the preceding equations define indeed graphs of antilinear mappings, because the assignments $q\to Pq$ and $q^{\perp}\to Pq^{\perp}$ are injective.)

Lemma 4.10: The mappings α,β defined by the preceding graphs are antilinear, injective and closed with dense domains and images $\operatorname{dom}\alpha=\operatorname{ima}\alpha=P(\mathfrak{q}^{\perp})$, $\operatorname{dom}\beta=\operatorname{ima}\beta=P\mathfrak{q}$. *Further, we have* $\alpha^2=\mathrm{id}$, $\beta^2=\mathrm{id}$ *on* $P(\mathfrak{q}^{\perp})$, *resp.* $P\mathfrak{q}$ *and* $\alpha=\beta^*$.

Proof: We will only prove the last equation, because the other statements follow immediately from the definition. Now by definition we have $(p_0,p_1)\in\operatorname{gra}\beta^*$ iff $\langle p_0,P\Gamma q\rangle=\langle Pq,p_1\rangle$ for all $q\in\mathfrak{q}$ iff $q^{\perp}:=p_0-\Gamma p_1\in\mathfrak{q}^{\perp}$ iff $(p_0,p_1)\in\operatorname{gra}\alpha$. ■

Remark 4.11: (*i*) Recall Sec. III A and denote by S the Tomita operator associated to $(\mathcal{M}(\mathfrak{q}),\Omega)$. Then from the preceding result we have $S\restriction\mathfrak{p}\supseteq\beta$ and $S^*\restriction\mathfrak{p}\supseteq\alpha$.

(*ii*) Using the mappings (18) and (19) we can now state similarly as in Proposition 4.9 a criterion for the bicontinuity of α,β: the mappings α,β are bicontinuous iff $\|PQ\|<1$.

We introduce next the notation

$$\Delta_{\mathfrak{p}}:=\beta^*\beta,$$

since it will later turn out that $\Delta_{\mathfrak{p}}$ is actually the modular operator restricted to the one-particle Hilbert space $\mathfrak{p}$.

Theorem 4.12: *The mapping $\Delta_{\mathfrak{p}}:\mathfrak{p}\to\mathfrak{p}$ is a densely defined linear positive self-adjoint operator on $\mathfrak{p}$ with graph*

$$\operatorname{gra}\Delta_{\mathfrak{p}}=\{(PQp,PQ^{\perp}p)\,|\,p\in\mathfrak{p}\}.$$

Moreover, $\Delta_{\mathfrak{p}}^{-1}=\beta\beta^*=\alpha^*\alpha$.

Proof: We will compute first the domain of $\beta^*\beta$. Recalling that $\beta^*=\alpha$ we have

$$\begin{aligned}\operatorname{dom}(\Delta_{\mathfrak{p}}) &= \{Pq \mid q \in \mathfrak{q} \text{ and } P\Gamma q \in \operatorname{dom}\alpha = P(\mathfrak{q}^{\perp})\}\\ &= \{Pq \mid q \in \mathfrak{q} \text{ and } P\Gamma q = Pq^{\perp} \text{ for some } q^{\perp} \in \mathfrak{q}^{\perp}\}\\ &= \{Pq \mid q \in \mathfrak{q} \text{ and } \Gamma q \in \operatorname{dom}\rho = Q(\mathfrak{p}^{\perp})\}\\ &= \{Pq \mid q \in \mathfrak{q} \text{ and } q \in \Gamma Q(\mathfrak{p}^{\perp}) = Q(\Gamma\mathfrak{p}^{\perp}) = Q\mathfrak{p}\} = PQ\mathfrak{p} = PQP\mathfrak{h},\end{aligned}$$

which is dense in $\mathfrak{p}$. Furthermore, since $P\Gamma Qp = -PQ^{\perp}\Gamma p$, $p \in \mathfrak{p}$ (recall $P\Gamma p = 0$, $p \in \mathfrak{p}$), we have

$$\Delta_{\mathfrak{p}}(PQp) = \alpha(P\Gamma Qp) = -\alpha(PQ^{\perp}\Gamma p) = P\Gamma Q^{\perp}\Gamma p = PQ^{\perp}p, \quad p \in \mathfrak{p}.$$

The last equations concerning the inverse of $\Delta_{\mathfrak{p}}$ follow from the preceding computation and from the fact that $\alpha^2 = \mathrm{id}$ and $\beta^2 = \mathrm{id}$ on the corresponding domains (recall Lemma 4.10). ■

Note that $\operatorname{dom}\Delta_{\mathfrak{p}} = PQ\mathfrak{p}$ is dense in $\mathfrak{p}$ and that $\Delta_{\mathfrak{p}}^{-1/2} = |\alpha|$, hence $\operatorname{dom}\Delta_{\mathfrak{p}}^{-1/2} = P(\mathfrak{q}^{\perp})$. Next we will calculate the graph of the positive self-adjoint operator $\varphi^*\varphi : \mathfrak{q} \to \mathfrak{q}$.

Proposition 4.13: The graph of $\varphi^*\varphi$ is given by

$$\operatorname{gra}\varphi^*\varphi = \{(QPq, QP^{\perp}q) \mid q \in \mathfrak{q}\}.$$

Proof: We begin computing $\operatorname{dom}(\varphi^*\varphi)$. Since by Lemma 4.2 $\varphi^* = \rho^{-1}$ we have

$$\begin{aligned}\operatorname{dom}(\varphi^*\varphi) &= \{Qp \mid p \in \mathfrak{p} \text{ and } Q^{\perp}p \in \operatorname{dom}\rho^{-1} = Q^{\perp}\mathfrak{p}^{\perp}\}\\ &= \{Qp \mid p \in \mathfrak{p} \text{ and } Q^{\perp}p = Q^{\perp}p^{\perp} \text{ for some } p^{\perp} \in \mathfrak{p}^{\perp}\}\\ &= \{Qp \mid p = Pq \text{ for some } q \in \mathfrak{q}\} = QP\mathfrak{q} = QPQ\mathfrak{h},\end{aligned}$$

where for the third equation we have used Corollary 4.4. Using again this corollary we can calculate

$$\rho^{-1}(\varphi(QPq)) = \rho^{-1}(Q^{\perp}Pq) = \rho^{-1}(Q^{\perp}(-P^{\perp}q)) = QP^{\perp}q, \quad q \in \mathfrak{q},$$

and the proof is concluded. ■

Now we can relate φ and $\varphi^*\varphi$ with $\Delta_{\mathfrak{p}}$ just computing the orthogonal decomposition of $\varphi(q)$, $q \in \operatorname{dom}\varphi$, resp. $\varphi^*\varphi(q)$, $q \in \operatorname{dom}\varphi^*\varphi$, wrt $\mathfrak{h} = \mathfrak{p} \oplus \mathfrak{p}^{\perp}$.

Corollary 4.14: Using the notation before we have the following formulas:

$$\begin{aligned}\varphi(Qp) &= \Delta_{\mathfrak{p}}(PQp) - P^{\perp}Qp, \quad p \in \mathfrak{p},\\ (\varphi^*\varphi)(QPq) &= \Delta_{\mathfrak{p}}(PQPq) + \Gamma\,\Delta_{\mathfrak{p}}^{-1}(P\Gamma QPq), \quad q \in \mathfrak{q}.\end{aligned} \tag{20}$$

Proof: From Lemma 4.2 as well as Theorem 4.12 we have

$$\varphi(Qp) = Q^{\perp}p = PQ^{\perp}p + P^{\perp}Q^{\perp}p = \Delta_{\mathfrak{p}}(PQp) - P^{\perp}Qp, \quad p \in \mathfrak{p}.$$

Further, from the preceding proposition we also have for any $q \in \mathfrak{q}$

$$\begin{aligned}(\varphi^*\varphi)(QPq) = QP^{\perp}q &= PQP^{\perp}q + P^{\perp}QP^{\perp}q\\ &= PQ^{\perp}Pq + \Gamma PQP\Gamma q\\ &= \Delta_{\mathfrak{p}}(PQPq) + \Gamma\,\Delta_{\mathfrak{p}}^{-1}(PQ^{\perp}P\Gamma q)\\ &= \Delta_{\mathfrak{p}}(PQPq) + \Gamma\,\Delta_{\mathfrak{p}}^{-1}(PQP^{\perp}\Gamma q)\\ &= \Delta_{\mathfrak{p}}(PQPq) + \Gamma\,\Delta_{\mathfrak{p}}^{-1}(P\Gamma QPq),\end{aligned}$$

which proves the second formula. ■

We will give the next two formulas in terms of $\Delta_{\mathfrak{p}}^{1/2}$ for the components of the polar decomposition of φ. Denote $\varphi=\operatorname{sgn}\varphi\cdot|\varphi|$, where as usual $|\varphi|:=(\varphi^*\varphi)^{1/2}$. Recall from the results in this section that

$$\operatorname{dom}\varphi=\operatorname{dom}|\varphi|=Q\mathfrak{p}\supseteq QP\mathfrak{q}=\operatorname{dom}(\varphi^*\varphi),$$

$$\operatorname{dom}\beta=\operatorname{dom}|\beta|=P\mathfrak{q}\supseteq PQ\mathfrak{p}=\operatorname{dom}\Delta_{\mathfrak{p}}.$$

Theorem 4.15: *With the notation above we have*

$$|\varphi|(q)=\Delta_{\mathfrak{p}}^{1/2}(Pq)+\Gamma\,\Delta_{\mathfrak{p}}^{-1/2}(P\Gamma q),\quad q\in\operatorname{dom}\varphi^*\varphi=QP\mathfrak{q}, \tag{21}$$

$$\operatorname{sgn}\varphi(q)=\Delta_{\mathfrak{p}}^{1/2}(Pq)-\Gamma\,\Delta_{\mathfrak{p}}^{1/2}(P\Gamma q),\quad q\in\mathfrak{q}. \tag{22}$$

Moreover, $\operatorname{sgn}\varphi$ *is an isometry of* $\mathfrak{q}$ *onto* $\mathfrak{q}^{\perp}$, i.e., $(\operatorname{sgn}\varphi)^*\operatorname{sgn}\varphi=Q$ *and* $\operatorname{sgn}\varphi(\operatorname{sgn}\varphi)^*=Q^{\perp}$.

Proof: From the explicit knowledge of all the domains of the mappings used before it is easily seen that the formulas are well defined. Further, recall Proposition 4.13 and Corollary 4.14 and the fact that the two terms of the rhs of the above formulas correspond to the decomposition of $\mathfrak{h}$ in terms of $P\mathfrak{h}$ and $P^{\perp}\mathfrak{h}$. Applying now for $q\in\operatorname{dom}\varphi^*\varphi$ twice the rhs of (21) we get

$$\begin{aligned}&\Delta_{\mathfrak{p}}^{1/2}P(\Delta_{\mathfrak{p}}^{1/2}(Pq)+\Gamma\,\Delta_{\mathfrak{p}}^{-1/2}(P\Gamma q))+\Gamma\,\Delta_{\mathfrak{p}}^{-1/2}P\Gamma(\Delta_{\mathfrak{p}}^{1/2}(Pq)+\Gamma\,\Delta_{\mathfrak{p}}^{-1/2}(P\Gamma q))\\&\quad=\Delta_{\mathfrak{p}}(Pq)+\Gamma\Delta_{\mathfrak{p}}^{-1}(P\Gamma q)=(\varphi^*\varphi)(q),\end{aligned}$$

which shows the first formula. To prove the second one note first that for $q'=|\varphi|(q)$, $q\in\operatorname{dom}\varphi^*\varphi$, and using Eq. (21) as well as Corollary 4.14 we obtain from a similar calculation as before that

$$(\Delta_{\mathfrak{p}}^{1/2}P-\Gamma\,\Delta_{\mathfrak{p}}^{1/2}P\Gamma)|\varphi|(q')=(\Delta_{\mathfrak{p}}P-P^{\perp})(q')=\varphi(q').$$

Thus the rhs and the lhs of (22) coincide on the dense subspace $\operatorname{ima}\varphi^*\varphi$. Finally, the fact that the rhs is also well defined for all $q\in\mathfrak{q}$ (recall that $\operatorname{dom}\Delta_{\mathfrak{p}}^{1/2}=\operatorname{dom}\beta=P\mathfrak{q}$) and that $\operatorname{sgn}\varphi$ maps isometrically the dense subspace $\operatorname{ima}|\varphi|\subseteq\mathfrak{q}$ onto the dense subspace $\operatorname{ima}\varphi=Q^{\perp}\mathfrak{p}\subseteq\mathfrak{q}^{\perp}$ proves formula (22). Therefore Q is the initial projection of $\operatorname{sgn}\varphi$ and $Q^{\perp}$ is the corresponding final projection. ■

Remark 4.16: Recall that $\operatorname{dom}\varphi^*\varphi$ is a core for $|\varphi|$ and note that the rhs of formula (21) *can not* be extended to the whole $\operatorname{dom}|\varphi|$.

Finally, we consider the mapping

$$\mathfrak{q}\ni q\mapsto Wq:=(\mathbb{1}+\Delta_{\mathfrak{p}})^{1/2}Pq\in\mathfrak{p}. \tag{23}$$

Lemma 4.17: W is an isometry from $\mathfrak{q}$ *onto* $\mathfrak{p}$.

Proof: First choose $q_1,q_2\in Q\mathfrak{p}$ which is dense in $\mathfrak{q}$. Now using

$$\langle Pq_1,\Delta_{\mathfrak{p}}(Pq_2)\rangle=\langle Pq_1,\beta^*\beta(Pq_2)\rangle=\langle\beta(Pq_2),\beta(Pq_1)\rangle=\langle P^{\perp}q_1,P^{\perp}q_2\rangle$$

we obtain

$$\langle(\mathbb{1}+\Delta_{\mathfrak{p}})^{1/2}Pq_1,(\mathbb{1}+\Delta_{\mathfrak{p}})^{1/2}Pq_2\rangle=\langle Pq_1,(\mathbb{1}+\Delta_{\mathfrak{p}})Pq_2\rangle=\langle q_1,q_2\rangle,\ q_1,q_2\in Q\mathfrak{p}.$$

Further, for any $p\in\mathfrak{p}$ we have from Theorem 4.12 that $(\mathbb{1}+\Delta_{\mathfrak{p}})(PQp)=PQp+PQ^{\perp}p=p$. This implies that $\operatorname{ima}(\mathbb{1}+\Delta_{\mathfrak{p}})^{1/2}=\mathfrak{p}$, since

$$\mathfrak{p}=\operatorname{ima}(\mathbb{1}+\Delta_{\mathfrak{p}})\subseteq\operatorname{ima}(\mathbb{1}+\Delta_{\mathfrak{p}})^{1/2}\subseteq\mathfrak{p}.$$

Therefore (23) is the isometric extension of $W\restriction Q\mathfrak{p}$. ■

Using now the isometry W we conclude this section showing the unitary equivalence of $|\varphi|$ and $\Delta_{\mathfrak{p}}^{1/2}$.

Theorem 4.18: *With the preceding notation we have*

$$W|\varphi|(q)=\Delta_{\mathfrak{p}}^{1/2}W(q),\quad q\in\mathrm{dom}\,|\varphi|.$$

Proof: For any $q\in\mathrm{dom}\,\varphi^*\varphi$, which is a core of $|\varphi|$, we may use (21) and in this case

$$W|\varphi|(q)=(\mathbb{1}+\Delta_{\mathfrak{p}})^{1/2}P(\Delta_{\mathfrak{p}}^{1/2}(Pq)+\Gamma\,\Delta_{\mathfrak{p}}^{-1/2}(P\Gamma q))=(\mathbb{1}+\Delta_{\mathfrak{p}})^{1/2}\Delta_{\mathfrak{p}}^{1/2}(Pq)=\Delta_{\mathfrak{p}}^{1/2}W(q).$$

But this implies that $W|\varphi|W^*\subseteq\Delta_{\mathfrak{p}}^{1/2}$ and since the lhs as well as the rhs of the preceding inclusion are self-adjoint operators, we must actually have the equality $W|\varphi|W^*=\Delta_{\mathfrak{p}}^{1/2}$. ■

V. TWISTED DUALITY. THE GENERIC POSITION CASE

We begin the proof of twisted duality considering first one of the extremal cases that may appear in the Halmos decomposition (10). For this assume that $(\mathfrak{h},\Gamma)$, P and Q are given as in the preceding section. In particular $\mathfrak{p}$ and $\mathfrak{q}$ are in generic position, so that by Proposition 3.4 the modular theory is well defined for the pair $(\mathcal{M}(\mathfrak{q}),\Omega)$. Denote as usual by $S=J\Delta^{1/2}$ the polar decomposition of the Tomita operator.

We prove first that the different modular objects leave the n-particle submanifolds $\overset{n}{\wedge}(P\mathfrak{q})$ invariant. This fact is well known in the context of CCR-Algebras,[27] where one can use the so-called exponential vectors which are specially well adapted to the Weyl operators.

Proposition 5.1: Let $q_1,\ldots,q_n\in\mathfrak{q}$ and $q_1^\perp,\ldots,q_n^\perp\in\mathfrak{q}^\perp$. *Then the following equations hold:*

$$S(Pq_1\wedge\cdots\wedge Pq_n)=P\Gamma q_n\wedge\cdots\wedge P\Gamma q_1=S(Pq_n)\wedge\cdots\wedge S(Pq_1),$$

$$S^*(Pq_1^\perp\wedge\cdots\wedge Pq_n^\perp)=S^*(Pq_n^\perp)\wedge\cdots\wedge S^*(Pq_1^\perp).$$

Proof: The proof is done by induction on the number of vectors in the wedge product. For $n=1$ the above equations are trivially satisfied (cf. Lemma 3.5). We will now concentrate on the first formula since one can argue similarly for S^*. Suppose that the first expression holds for a number of vectors $\leqslant n-1$. Then, applying this induction hypothesis as well as Proposition 2.2 we get

$$\begin{aligned}
&S(P\Gamma q_n\wedge\cdots\wedge P\Gamma q_1)\\
&\quad=S\left(a(q_n)\cdot\cdots\cdot a(q_1)\,\Omega-\sum_{\substack{\pi\in\mathfrak{S}_{n,p}\\ p\geqslant 1}}(\mathrm{sgn}\,\pi)\prod_{l=1}^{p}\langle Pq_{\alpha_l},P\Gamma q_{\beta_l}\rangle\,P\Gamma q_{j_1}\wedge\cdots\wedge P\Gamma q_{j_k}\right)\\
&\quad=a(\Gamma q_1)\cdot\cdots\cdot a(\Gamma q_n)\,\Omega-\sum_{\substack{\pi\in\mathfrak{S}_{n,p}\\ p\geqslant 1}}(\mathrm{sgn}\,\pi)\prod_{l=1}^{p}\langle P\Gamma q_{\beta_l},Pq_{\alpha_l}\rangle\,Pq_{j_k}\wedge\cdots\wedge Pq_{j_1},\qquad(24)
\end{aligned}$$

and recall that the indices specified by $\pi\in\mathfrak{S}_{n,p}$ satisfy $\alpha_1>\cdots>\alpha_p$, $\alpha_l>\beta_l$, $l=1,\ldots,p$ and $n\geqslant j_1>j_2>\cdots>j_k\geqslant 1$. But we can now apply again Proposition 2.2 to the first term of the preceding sum and we get

$$a(\Gamma q_1)\cdot\cdots\cdot a(\Gamma q_n)\,\Omega=Pq_1\wedge\cdots\wedge Pq_n+\sum_{\substack{\pi'\\ p\geqslant 1}}(\mathrm{sgn}\,\pi')\prod_{l=1}^{p}\langle P\Gamma q_{\alpha_l'},Pq_{\beta_l'}\rangle\,Pq_{j_1'}\wedge\cdots\wedge Pq_{j_k'},\qquad(25)$$

where now

$$\pi'=\begin{pmatrix} 1 & 2 & \cdots & 2p-1 & 2p & n-k+1 & \cdots & n \\ \alpha_1' & \beta_1' & \cdots & \alpha_p' & \beta_p' & j_1' & \cdots & j_k' \end{pmatrix}$$

with $\alpha_l'<\beta_l'$, $l=1,\ldots,p$, $1\leqslant j_1'<j_2'<\cdots<j_k'\leqslant n$ and we may reorganize the scalar products such that $\beta_1'<\cdots<\beta_p'$. We can next associate bijectively these permutations with elements in $\mathfrak{S}_{n,p}$ by means of

$$\pi'\mapsto\pi_0=\begin{pmatrix} n & n-1 & \cdots & n-2p+2 & n-2p+1 & k & \cdots & 1 \\ \beta_p' & \alpha_p' & \cdots & \beta_1' & \alpha_1' & j_k' & \cdots & j_1' \end{pmatrix}\in\mathfrak{S}_{n,p}.$$

Since $\operatorname{sgn}\pi'=\operatorname{sgn}\pi_0'$ we have inserting (25) in (24) that all vectors with particle number less than n cancel so that

$$S(P\Gamma q_n\wedge\cdots\wedge P\Gamma q_1)=Pq_1\wedge\cdots\wedge Pq_n$$

and the proof is concluded. ■

Recall from Remark 4.11 (i) $S\restriction\mathfrak{p}\supseteq\beta$ and $S^*\restriction\mathfrak{p}\supseteq\alpha$. We will show next that actually the equality holds. Let P_n denote the projection of $\mathfrak{F}$ onto the n-particle subspace $\overset{n}{\wedge}\mathfrak{p}$. Then the family of orthoprojections $\{P_n\}_{n\in\mathbb{N}}$ is mutually orthogonal and $\Sigma_{n=0}^{\infty}P_n=\mathbb{1}_{\mathfrak{F}}$. Further we define the operator S_{fin} by

$$\operatorname{dom}S_{\text{fin}}:=\operatorname{span}\{a(q_1)\cdot\cdots\cdot a(q_n)\Omega\,|\,q_1,\ldots,q_n\in\mathfrak{q},n\in\mathbb{N}\cup\{0\}\},$$

$$S_{\text{fin}}x:=Sx,\quad x\in\operatorname{dom}S_{\text{fin}}.$$

Lemma 5.2: $\operatorname{dom}S_{\text{fin}}$ *is a core for the Tomita operator* S.

Proof: Put $\mathcal{C}:=\operatorname{dom}S_{\text{fin}}$ and denote by $\mathcal{A}(\mathfrak{q})$ the*-algebra generated by $\{a(q)|q\in\mathfrak{q}\}$, so that $\mathcal{M}(\mathfrak{q})=\mathcal{A}(\mathfrak{q})''$. Further, recall that if $S_0(M\Omega):=M^*\Omega$, $M\in\mathcal{M}(\mathfrak{q})$, then the graph of the Tomita operator $S=\operatorname{clo}S_0$ can be written as

$$\operatorname{gra}S=\operatorname{clo}_w(\operatorname{gra}S_0)=\operatorname{clo}_w\{(M\Omega,M^*\Omega)|M\in\mathcal{M}(\mathfrak{q})\},$$

where clo_w denotes the closure in the weak operator topology. Thus to prove the core property of $\mathcal{C}$, i.e., $\operatorname{clo}(S\restriction\mathcal{C})=S$, we need to show that

$$\operatorname{clo}_w\{(M\Omega,M^*\Omega)|M\in\mathcal{M}(\mathfrak{q})\}=\operatorname{clo}_w\{(A\Omega,A^*\Omega)|A\in\mathcal{A}(\mathfrak{q})\}.$$

Now for each $M\in\mathcal{M}(\mathfrak{q})$ there exists a sequence $\{A_n\}_{n\in\mathbb{N}}\subset\mathcal{A}(\mathfrak{q})$ with $|\langle x,(M-A_n)y\rangle|<\epsilon$ for all $x,y\in\mathfrak{F}$ if n is sufficiently large. This implies that for all $(x,y)\in\mathfrak{F}\times\mathfrak{F}$, we have

$$|\langle(M\Omega,M^*\Omega),(x,y)\rangle-\langle(A_n\Omega,A_n^*\Omega),(x,y)\rangle|=|\langle(M-A_n)\Omega,x\rangle-\langle(M^*-A_n^*)\Omega,y\rangle|\leqslant 2\epsilon,$$

where we have used that in the weak operator topology if $A_n\to M$, then $A_n^*\to M^*$. Therefore if $(M_l\Omega,M_l^*\Omega)\overset{l}{\to}(x_0,y_0)$ weakly, then for each l there exists a sequence $\{A_{(n,l)}\}_{n\in\mathbb{N}}\subset\mathcal{A}(\mathfrak{q})$ such that $(A_{(n,l)}\Omega,A_{(n,l)}^*\Omega)\overset{n}{\to}(M_l\Omega,M_l^*\Omega)$ weakly. Finally, the estimate

$$\begin{aligned}&|\langle(A_{(n,l)}\Omega,A_{(n,l)}^*\Omega),(x,y)\rangle-\langle(x_0,y_0),(x,y)\rangle|\\&\quad\leqslant|\langle(A_{(n,l)}\Omega,A_{(n,l)}^*\Omega),(x,y)\rangle-\langle(M_l\Omega,M_l^*\Omega),(x,y)\rangle|\\&\qquad+|\langle(M_l\Omega,M_l^*\Omega),(x,y)\rangle-\langle(x_0,y_0),(x,y)\rangle|\end{aligned}$$

completes the proof. ■

From Propositions 5.1 and 2.2 we obtain further

$$P_n \operatorname{dom} S_{\mathrm{fin}} \subseteq \operatorname{dom} S_{\mathrm{fin}}, \quad n=0,1,\ldots,$$

$$P_n \operatorname{dom} S_{\mathrm{fin}} \subset P_n \mathfrak{F} \text{ is dense}, \quad n=0,1,\ldots,$$

$$P_n S_{\mathrm{fin}} P_n = S_{\mathrm{fin}} P_n, \quad n=0,1,\ldots.$$

Note that for $x \in \operatorname{dom} S_{\mathrm{fin}}$ the series $x=\Sigma_{n=0}^{\infty} P_n x$ is a finite sum. Further, we consider the operators $S_{\mathrm{fin}}(n): P_n\mathfrak{F} \to P_n\mathfrak{F}$ by $\operatorname{dom} S_{\mathrm{fin}}(n) := P_n \operatorname{dom} S_{\mathrm{fin}}$ and $S_{\mathrm{fin}}(n)x := S_{\mathrm{fin}}x, x \in \operatorname{dom} S_{\mathrm{fin}}(n)$. Recall from Lemma 4.10 that $S_{\mathrm{fin}}(1)=\beta$ is a closed densely defined operator from $\mathfrak{p}=P_1\mathfrak{F}$ into $\mathfrak{p}$ and by the preceding arguments we have

$$S_{\mathrm{fin}} = \bigoplus_{n=0}^{\infty} S_{\mathrm{fin}}(n) \quad \text{(algebraic direct sum)}. \tag{26}$$

We can now state the following.

Proposition 5.3: The Tomita operator S and its adjoint S^* can be restricted to the n-particles subspaces $P_n\mathfrak{F}$. We have

$$S \restriction P_n\mathfrak{F} = \operatorname{clo} S_{\mathrm{fin}}(n) \quad \text{and} \quad S^* \restriction P_n\mathfrak{F} = \operatorname{clo} S_{\mathrm{fin}}^*(n), \quad n=0,1,\ldots.$$

In particular $S \restriction \mathfrak{p} = \beta$ and $S^* \restriction \mathfrak{p} = \alpha$.

Proof: From (26) we obtain immediately that

$$\operatorname{gra} S = \bigoplus_{n=0}^{\infty} \operatorname{clo} \operatorname{gra} S_{\mathrm{fin}}(n) = \mathbb{C}\Omega \oplus \operatorname{gra} S_{\mathrm{fin}}(1) \oplus \sum_{n=2}^{\infty} \operatorname{clo} \operatorname{gra} S_{\mathrm{fin}}(n) \quad \text{(Hilbert sum)}. \tag{27}$$

Note that $\operatorname{clo} \operatorname{gra} S_{\mathrm{fin}}(n) = \operatorname{gra} \operatorname{clo} S_{\mathrm{fin}}(n)$, $n \geqslant 2$, and that now the direct sum (27), in contrast to (26), is the Hilbert sum of these subspaces. Equation (27) implies immediately the assertion that S can be restricted to $P_n\mathfrak{F}$ and that the restriction coincides with $\operatorname{clo} S_{\mathrm{fin}}(n)$, in particular $S \restriction \mathfrak{p} = \beta$. The statements concerning S^* are shown analogously. ■

Corollary 5.4: Let $S = J\Delta^{1/2}$ be the polar decomposition of the Tomita operator. The modular operator $\Delta = S^*S$ and the modular conjugation J can be restricted to the respective n-particle subspaces. In particular we have the following:

(i) Modular operator: $\Delta \restriction \mathfrak{p} = \Delta_{\mathfrak{p}}$ (*recall from the preceding section that* $\Delta_{\mathfrak{p}} = \beta^*\beta$), $\operatorname{dom} \Delta \restriction P_n\mathfrak{F} = \overset{n}{\wedge} \operatorname{dom} \Delta_{\mathfrak{p}}$ and

$$\Delta(p_1 \wedge \cdots \wedge p_n) = (\Delta_{\mathfrak{p}} p_1) \wedge \cdots \wedge (\Delta_{\mathfrak{p}} p_n), \quad p_1,\ldots,p_n \in \operatorname{dom} \Delta_{\mathfrak{p}} = PQ\mathfrak{p}. \tag{28}$$

(ii) Modular conjugation:

$$J(p_1 \wedge \cdots \wedge p_n) = (Jp_n) \wedge \cdots \wedge (Jp_1), \quad p_1,\ldots,p_n \in \mathfrak{p}. \tag{29}$$

Proof: Note first that from Proposition 5.3 and Lemma 4.10 we have $S^*S \restriction \mathfrak{p} = \alpha\beta = \beta^*\beta$. Further, Eq. (28) follows from Propositions 5.1 and 5.3. Next, applying formula (29) to the n-particle vectors $\Delta^{1/2}(p_1 \wedge \cdots \wedge p_n)$, where $p_k := \Delta_{\mathfrak{p}}^{1/2} p_k'$, $p_k' \in \operatorname{dom} \Delta_{\mathfrak{p}}$, $k=1,\ldots,n$, we obtain $S(p_1 \wedge \cdots \wedge p_n)$. Thus Eq. (29) coincides with $J \restriction P_n\mathfrak{F}$ on the dense set $(\operatorname{ima} \Delta_{\mathfrak{p}}) \wedge \cdots \wedge (\operatorname{ima} \Delta_{\mathfrak{p}})$, which concludes the proof. ■

For the next definition recall the formulas concerning $\operatorname{sgn} \varphi$ in Theorem 4.15.

Definition 5.5: Define the following antilinear isometry from $\mathfrak{q}$ onto $\mathfrak{q}^{\perp}$:

$$Vq := -i(\Gamma \operatorname{sgn} \varphi)(q) = i(\Delta_{\mathfrak{p}}^{1/2} P\Gamma q - \Gamma \Delta_{\mathfrak{p}}^{1/2} Pq), \quad q \in \mathfrak{q}.$$

Theorem 5.6: *With the preceding definition we have for any* $q \in \mathfrak{q}$

$$J\,a(q)\,J = \tilde{Z}\,a(Vq)\,\tilde{Z}^*. \tag{30}$$

Proof: Since $\oplus_{n=0}^{\infty} \overset{n}{\wedge} P\mathfrak{q}$ (algebraic direct sum) is dense in $\mathfrak{F}$ and the operators on both sides of Eq. (30) are bounded it is enough to show the preceding relation for the n-particle vectors in $\overset{n}{\wedge} P\mathfrak{q}$. For $q_1,\ldots,q_n \in \mathfrak{q}$ and using Corollary 5.4 (ii) the lhs of the equation reads

$$\begin{aligned}(J\,a(q)\,J)(Pq_1\wedge\cdots\wedge Pq_n) &= Pq_1\wedge\cdots\wedge Pq_n\wedge JP\Gamma q \\ &\quad + \sum_{r=n}^{1} (-1)^{n-r}\,\langle JPq, Pq_r\rangle\, Pq_1\wedge\cdots\wedge\widehat{Pq_r}\wedge\cdots\wedge Pq_n\,.\end{aligned}$$

To compute the rhs recall the definition of the function η in Sec. II B:

$$\begin{aligned}(\tilde{Z}\,a(Vq)\,\tilde{Z}^*)(Pq_1\wedge\cdots\wedge Pq_n) &= -i\,\overline{\eta(n)}\,\tilde{Z}\cdot(-c(\Delta_{\mathfrak{p}}^{1/2}Pq)^*Pq_1\wedge\cdots\wedge Pq_n \\ &\quad + c(\Delta_{\mathfrak{p}}^{1/2}P\Gamma q)Pq_1\wedge\cdots\wedge Pq_n) \\ &= Pq_1\wedge\cdots\wedge Pq_n\wedge\Delta_{\mathfrak{p}}^{1/2}Pq \\ &\quad + \sum_{r=1}^{n} (-1)^{n-r}\,\langle\Delta_{\mathfrak{p}}^{1/2}P\Gamma q, Pq_r\rangle\, Pq_1\wedge\cdots\wedge\widehat{Pq_r}\wedge\cdots\wedge Pq_n\,,\end{aligned}$$

where for the last equation we have used that $-i\,\overline{\eta(n)}\,\eta(n+1) = -i\,\overline{\eta(n)}\,\eta(n-1) = (-1)^{n+1}$. Finally, the equality of both sides follows from the fact that $\Delta_{\mathfrak{p}}^{1/2}Pq = JSPq = JP\Gamma q,\ q \in \mathfrak{q}$. ■

Remark 5.7: As expected we can relate the mapping V defined before with the mapping j (the modular conjugation restricted to the one-particle Hilbert space) used in Ref. 20, p. 738. Indeed, considering the projection onto the one-particle Hilbert space we have the relation

$$J(Pq) = \Delta_{\mathfrak{p}}^{1/2}S(Pq) = \Delta_{\mathfrak{p}}^{1/2}(P\Gamma q) = -iPV(q), \quad q \in \mathfrak{q}.$$

Theorem 5.8: (*Twisted Duality*) *Let* $\mathcal{M}(\mathfrak{q})$ *be the von Neumann algebra given at the beginning of this section. Then*

$$\mathcal{M}(\mathfrak{q})' = \tilde{Z}\,\mathcal{M}(\mathfrak{q}^{\perp})\,\tilde{Z}^*.$$

Proof: From the last theorem and using standard results in modular theory we have

$$\begin{aligned}\mathcal{M}(\mathfrak{q})' &= J\,\mathcal{M}(\mathfrak{q})\,J = J\,\{a(q)\,|\,q \in \mathfrak{q}\}''\,J \\ &= \{J\,a(q)\,J\,|\,q \in \mathfrak{q}\}'' \\ &= \{\tilde{Z}\,a(Vq)\,\tilde{Z}^*\,|\,q \in \mathfrak{q}\}'' \\ &= \tilde{Z}\,\{a(Vq)\,|\,q \in \mathfrak{q}\}''\tilde{Z}^* = \tilde{Z}\,\mathcal{M}(\mathfrak{q}^{\perp})\,\tilde{Z}^*,\end{aligned}$$

where we have used that V is an antilinear isometry from $\mathfrak{q}$ onto $\mathfrak{q}^{\perp}$. ■

Remark 5.9: If one does not want to bother about domain questions, there is possibly an alternative way to show the preceding result. Indeed, one can first prove the statements in this section for finite dimensional subspaces $\mathfrak{q}_n$ of $\mathfrak{q}$ and then apply the AFD-property of $\mathcal{M}(\mathfrak{q})$ as in the proof of Ref. 9, Theorem 15.1.3.

We will finally show that the formulas established in the previous and present sections also apply to the localized algebras that appear in the context of fermionic free nets (cf. Refs. 8 and 28). Let $\mathcal{O} \subset \mathbb{R}^4$ be a double cone in Minkowski space and denote by $\overline{\mathfrak{q}(\mathcal{O})}$ the closure of the

subspaces $\mathfrak{q}(\mathcal{O})$ of the reference Hilbert space $(\mathfrak{h},\Gamma)$. The subspaces $\mathfrak{q}(\mathcal{O})$ are defined in terms of the embeddings that characterize the free nets (essentially Fourier transformation of C^∞ functions with compact support restricted to the positive mass shell/light cone). It is easily shown that $\Gamma\mathfrak{q}(\mathcal{O})=\mathfrak{q}(\mathcal{O})$, hence $\Gamma\overline{\mathfrak{q}(\mathcal{O})}=\overline{\mathfrak{q}(\mathcal{O})}$. Further, the localized C*-algebras are again CAR-algebras, i.e.,

$$\mathcal{A}(\mathcal{O}):=\mathrm{C}^*(\{a(\varphi)\,|\,\varphi\in\mathfrak{q}(\mathcal{O})\})=\mathrm{CAR}(\mathfrak{q}(\mathcal{O}),\Gamma\restriction\mathfrak{q}(\mathcal{O}))=\mathrm{CAR}(\overline{\mathfrak{q}(\mathcal{O})},\Gamma\restriction\overline{\mathfrak{q}(\mathcal{O})})\subset\mathrm{CAR}(\mathfrak{h},\Gamma).$$

For the canonical basis projection P given in the context of free nets (see, e.g., Ref. 28, p. 1157) it is also immediate to check that for double cones

$$\mathfrak{p}\cap\overline{\mathfrak{q}(\mathcal{O})}=\mathfrak{p}\cap\overline{\mathfrak{q}(\mathcal{O})}^{\perp}=\{0\},\quad\text{where }\ \mathfrak{p}=P\mathfrak{h}.$$

This means that $\mathfrak{p}$ and $\overline{\mathfrak{q}(\mathcal{O})}$ are in generic position and we can apply the results and formulas of the previous and present sections to the corresponding localized von Neumann algebras

$$\mathcal{M}(\mathcal{O}):=\{\pi(a(\varphi))\,|\,\varphi\in\overline{\mathfrak{q}(\mathcal{O})}\}''.$$

In particular, from Proposition 5.3 and Corollary 5.4 we have that the modular operator Δ and the modular conjugation J are already characterized by their action on the one-particle Hilbert space. Finally, Theorem 4.12 and Remark 5.7 imply the following theorem.

Theorem 5.10: *Let $\mathcal{O}\subset\mathbb{R}^4$ be a double cone in Minkowski space. Denote by $Q_{\mathcal{O}}$ the orthoprojection onto $\overline{\mathfrak{q}(\mathcal{O})}$ and by P the canonical basis projection given in the context of fermionic free nets. Then the following formulas hold for the modular operator and modular conjugation on the one-particle Hilbert space $\mathfrak{p}$:*

$$\mathrm{gra}\,\Delta_{\mathfrak{p}}=\{(PQ_{\mathcal{O}}(p),PQ^{\perp}_{\mathcal{O}}(p))\,|\,p\in\mathfrak{p}\},$$

$$J(Pq)=\Delta_{\mathfrak{p}}^{1/2}(P\Gamma q),\quad q\in\overline{\mathfrak{q}(\mathcal{O})}.$$

VI. RELATION TO THE REAL SUBSPACE APPROACH

In the present section we will make explicit the relation of the real subspace approach in Refs. 20 and 32 to our consistent use of complex subspaces in the self-dual approach.

The projection $\mathcal{P}$ on the complex Hilbert space H with conjugation γ in Ref. 32 corresponds in the self-dual approach [where $\mathfrak{h}:=H\oplus H$ and $\Gamma:=\left(\begin{smallmatrix}0&\gamma\\ \gamma&0\end{smallmatrix}\right)$] to a diagonal basis projection $\mathfrak{P}:=\left(\begin{smallmatrix}\mathcal{P}&0\\ 0&\gamma\mathcal{P}^{\perp}\gamma\end{smallmatrix}\right)$. Nondiagonal basis projections are not considered in Ref. 32. Further, in that article the author extends by second quantization certain mappings on the one-particle Hilbert space. He has then to verify that these second quantized operators are the modular objects by checking the KMS condition. (In contrast to that we construct the modular objects on the whole antisymmetric Fock space and show that they restrict to the n-particle space.)

The following aspect is that in Ref. 20 (and Ref. 32) real-linear closed manifolds M (resp. K) of the one-particle (complex) space H ($\mathfrak{p}$ in our article) are used, whereas here the subalgebras of the "big" fermion algebra $\mathrm{CAR}(\mathfrak{h},\Gamma)$ are characterized by Γ-invariant complex subspaces of the reference space $\mathfrak{h}$. The relation between the two approaches is given by the following observations: first, the counterpart of the real M in our approach is given by $P(\mathrm{Re}(\mathfrak{q}))$, where $q\in\mathrm{Re}(\mathfrak{q})$ if $\Gamma q=q$. Note that $P(\mathrm{Re}(\mathfrak{q}))$ is a real-linear submanifold of $\mathfrak{p}$ and in general it is *not* closed (see the foregoing considerations). Now we still need to check that $P(\mathrm{Re}(\mathfrak{q}^{\perp}))$ corresponds in the real subspace approach of Ref. 20 to iM'. (Recall that in Ref. 20 one defines M' as the symplectic complement, i.e., $M':=\{x\in H\,|\,\mathrm{Im}\langle x,m\rangle=0,\ m\in M\}\supset M^{\perp}$.) The next result shows that indeed $P(\mathrm{Re}(\mathfrak{q}^{\perp}))$ and iM' generate the same von Neumann algebra.

Lemma 6.1: Put $M:=P(\mathrm{Re}(\mathfrak{q}))$. Then $P(\mathrm{Re}(\mathfrak{q}^{\perp}))$ is dense in (iM').

Proof: We show first that $P(\mathrm{Re}(\mathfrak{q}^{\perp}))\subseteq(iM')$. For any $(q^{\perp}+\Gamma q^{\perp})\in\mathrm{Re}(\mathfrak{q}^{\perp})$, $q^{\perp}\in\mathfrak{q}^{\perp}$, and since

$$iM' := \{p \in \mathfrak{p} | \langle q+\Gamma q, p\rangle + \langle p, q+\Gamma q\rangle = 0,\ \ q \in \mathfrak{q}\},$$

the inclusion follows from

$$\begin{aligned}\langle q+\Gamma q, P(q^\perp+\Gamma q^\perp)\rangle + \langle P(q^\perp+\Gamma q^\perp), q+\Gamma q\rangle &= (\langle q, Pq^\perp\rangle + \langle P\Gamma q^\perp, \Gamma q\rangle)\\ &\quad + (\langle \Gamma q, Pq^\perp\rangle + \langle P\Gamma q^\perp, q\rangle)\\ &\quad + (\langle q, P\Gamma q^\perp\rangle + \langle Pq^\perp, \Gamma q\rangle)\\ &\quad + (\langle \Gamma q, P\Gamma q^\perp\rangle + \langle P\Gamma q^\perp, q\rangle)\\ &= 0,\end{aligned}$$

where for the last equation we have used $\Gamma P + P\Gamma = \Gamma$. Finally, to show the density statement consider $p_0 \in iM'$, i.e.,

$$\langle q+\Gamma q, p_0\rangle + \langle p_0, q+\Gamma q\rangle = 0,\ \ q \in \mathfrak{q}, \tag{31}$$

such that $p_0 \perp P(q^\perp+\Gamma q^\perp)$ for all $q^\perp \in \mathfrak{q}^\perp$. Thus $\langle p_0, P(q^\perp+\Gamma q^\perp)\rangle = 0$, $q^\perp \in \mathfrak{q}^\perp$, and replacing $q^\perp$ by $iq^\perp$ we also obtain $\langle p_0, P(q^\perp-\Gamma q^\perp)\rangle = 0$, $q^\perp \in \mathfrak{q}^\perp$. Hence $\langle p_0, Pq^\perp\rangle = 0$, $q^\perp \in \mathfrak{q}^\perp$, and $p_0 \in \mathfrak{q} \cap \mathfrak{p}$. But according to Eq. (31) we must also have $\langle p_0+\Gamma p_0, p_0\rangle + \langle p_0, p_0+\Gamma p_0\rangle = 0$, which implies $p_0 = 0$. ■

Finally, the conditions $M \cap iM = \{0\}$ and $M + iM$ dense in H in Ref. 20 are equivalent to our conditions $\mathfrak{q} \cap \mathfrak{p} = \{0\} = \mathfrak{q}^\perp \cap \mathfrak{p}$ and the projections P_1, P_2, P_3 in Ref. 20, Proposition 1.5, correspond in the self-dual approach to the orthoprojections onto $\mathfrak{p} \cap \mathfrak{q}^\perp$, $\mathfrak{p} \cap \mathfrak{q}$, $\mathfrak{p} \ominus (\mathfrak{p} \cap \mathfrak{q}^\perp \oplus \mathfrak{p} \cap \mathfrak{q})$, respectively.

VII. TWISTED DUALITY. THE GENERAL CASE

We are now in a position to give the proof of twisted duality in the most general situation. Let $(\mathfrak{h}, \Gamma)$ be a Hilbert space with anti-unitary involution Γ, P *any* basis projection and $\mathfrak{q}$ *any* closed Γ-invariant subspace in $\mathfrak{h}$, to which we associate the orthoprojection Q. We adapt the arguments in Ref. 20, p. 735, to the self-dual approach.

Recall the Halmos decompostion $\mathfrak{h} = \mathfrak{h}_0 \oplus \mathfrak{h}_1$ given in Eq. (10), where $\mathfrak{h}_0 = (\mathfrak{p} \cap \mathfrak{q}) \oplus (\mathfrak{p} \cap \mathfrak{q}^\perp) \oplus (\mathfrak{p}^\perp \cap \mathfrak{q}) \oplus (\mathfrak{p}^\perp \cap \mathfrak{q}^\perp)$. Since $\Gamma(\mathfrak{p} \cap \mathfrak{q}^\perp) = (\mathfrak{p}^\perp \cap \mathfrak{q}^\perp)$ and $\Gamma(\mathfrak{p} \cap \mathfrak{q}) = (\mathfrak{p}^\perp \cap \mathfrak{q})$ it is also natural to consider the previous decomposition as

$$\mathfrak{h} = \mathfrak{h}_{01} \oplus \mathfrak{h}_{02} \oplus \mathfrak{h}_1, \tag{32}$$

where $\mathfrak{h}_{01} := (\mathfrak{p} \cap \mathfrak{q}^\perp) \oplus \Gamma(\mathfrak{p} \cap \mathfrak{q}^\perp)$ and $\mathfrak{h}_{02} := (\mathfrak{p} \cap \mathfrak{q}) \oplus \Gamma(\mathfrak{p} \cap \mathfrak{q})$. In particular, we have

$$Q\mathfrak{h}_{01} = \{0\}, \quad Q\mathfrak{h}_{02} = \mathfrak{h}_{02}, \tag{33}$$

$$Q^\perp \mathfrak{h}_{01} = \mathfrak{h}_{01}, \quad Q^\perp \mathfrak{h}_{02} = \{0\}, \tag{34}$$

as well as

$$\mathfrak{q} = \{0\} \oplus \mathfrak{h}_{02} \oplus Q\mathfrak{h}_1 \quad \text{and} \quad \mathfrak{q}^\perp = \mathfrak{h}_{01} \oplus \{0\} \oplus Q^\perp \mathfrak{h}_1.$$

Theorem 7.1: (*Twisted Duality*) *Let* $(\mathfrak{h}, \Gamma)$, *P and* $\mathfrak{q}$ *be given as in the beginning of this section. Then*

$$\mathcal{M}(\mathfrak{q})' = \tilde{Z}\, \mathcal{M}(\mathfrak{q}^\perp)\, \tilde{Z}^*.$$

Proof: From Proposition 2.6 it is enough to show the inclusion

$$\mathcal{M}(\mathfrak{q})' \subseteq \tilde{Z}\, \mathcal{M}(\mathfrak{q}^\perp)\, \tilde{Z}^*. \tag{35}$$

We can apply now the formulas (5) *and* (6) in Proposition 2.4 to the three-space decomposition in Eq. (32). Indeed, adapting in the obvious way the notation from Proposition 2.4 we get that

$$\pi(a(f_{01}\oplus f_{02}\oplus f_1))=\pi_{01}(a(f_{01}))\otimes Z_{02}\otimes Z_1+1\otimes\pi_{02}(a(f_{02}))\otimes 1+1\otimes Z_{02}\otimes\pi_1(a(f_1)),$$

$f_1\in\mathfrak{h}_1$, $f_{0k}\in\mathfrak{h}_{0k}$, $k=1,2$, specifies a representation of CAR$(\mathfrak{h},\Gamma)$ on the corresponding tensor product of antisymmetric Fock spaces $\mathfrak{F}=\mathfrak{F}_{01}\otimes\mathfrak{F}_{02}\otimes\mathfrak{F}_1$. Now using (33) we obtain

$$\mathcal{M}(\mathfrak{q})=\mathrm{Cl}\otimes\mathcal{L}(\mathfrak{F}_{02})\otimes\mathcal{M}(Q\mathfrak{h}_1),$$

hence

$$\mathcal{M}(\mathfrak{q})'=\mathcal{L}(\mathfrak{F}_{01})\otimes\mathrm{Cl}\otimes\mathcal{M}(Q\mathfrak{h}_1)'.$$

From (34) we also obtain

$$\mathcal{M}(\mathfrak{q}^\perp)=\mathcal{L}(\mathfrak{F}_{01})\otimes\{Z_{02}\}''\otimes\mathcal{M}(Q^\perp\mathfrak{h}_1)=\{L_{01}\otimes Z_{02}\otimes\pi_1(a(f_1))|L_{01}\in\mathcal{L}(\mathfrak{F}_{01}),\quad f_1\in Q^\perp\mathfrak{h}_1\}''.$$

Using now the result stated in Remark 2.8 we have for the twisted von Neumann algebra

$$\begin{aligned}\tilde{Z}\mathcal{M}(\mathfrak{q}^\perp)\tilde{Z}^*&=\{iZ\pi(a(q^\perp))|q^\perp\in\mathfrak{q}^\perp\}''\\&=\{(Z_{01}\otimes Z_{02}\otimes Z_1)\cdot(L_{01}\otimes Z_{02}\otimes\pi_1(a(f_1)))|L_{01}\in\mathcal{L}(\mathfrak{F}_{01}),\quad f_1\in Q^\perp\mathfrak{h}_1\}'',\end{aligned}$$

which immediately implies (35), since we have already proved twisted duality in the generic position case (cf. Theorem 5.8). ■

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APPENDIX: PROOF OF PROPOSITION 2.2

We will give in this appendix the proof of Proposition 2.2. Recall the notation and results of Sec. II.

Proposition: For $f_1,\ldots,f_n\in\mathfrak{h}$ the equation

$$(a(f_n)\cdot\cdots\cdot a(f_1))\,\Omega=\sum_{\substack{\pi\in\mathfrak{S}_{n,p}\\0\leqslant 2p\leqslant n}}(\mathrm{sgn}\,\pi)\prod_{l=1}^{p}\langle Pf_{\alpha_l},P\Gamma f_{\beta_l}\rangle\,P\Gamma f_{j_1}\wedge\cdots\wedge P\Gamma f_{j_k}$$

holds, where the indices $\alpha_l,\beta_l,j_1,\ldots,j_k$ are given in the definition of $\mathfrak{S}_{n,p}$ and where for $n=2p$ in the preceding sum one replaces the wedge product by the vacuum Ω.

Proof: The proof is done by induction on the number of generators of the CAR-Algebra. For $n=1$ the above formula is immediately verified using the definition of creation and annihilation operators. Assume that it holds for n generators and we prove that it is also true for $n+1$ generators. Take $f_{n+1},f_n,\ldots,f_1\in\mathfrak{h}$ and from the preceding assumption as well as the results stated in Sec. II we have

$$\begin{aligned}&a(f_{n+1})\,(a(f_n)\cdot\cdots\cdot a(f_1)\,\Omega)\\&\quad=(c(P\Gamma f_{n+1})^*+c(Pf_{n+1}))\,(a(f_n)\cdot\cdots\cdot a(f_1)\,\Omega)\\&\quad=\sum_{\substack{\pi\in\mathfrak{S}_{n,p}\\0\leqslant 2p\leqslant n}}(\mathrm{sgn}\,\pi)\prod_{l=1}^{p}\langle Pf_{\alpha_l},P\Gamma f_{\beta_l}\rangle\,P\Gamma f_{n+1}\wedge P\Gamma f_{j_1}\wedge\cdots\wedge P\Gamma f_{j_k}\end{aligned}$$

$$+\sum_{\substack{\pi\in\mathfrak{S}_{n,p}\\ 0\leqslant 2p\leqslant n}}\sum_{r=1}^{k}(\operatorname{sgn}\pi)(-1)^{r-1}\langle Pf_{n+1},P\Gamma f_{j_r}\rangle$$

$$\cdot\prod_{l=1}^{p}\langle Pf_{\alpha_l},P\Gamma f_{\beta_l}\rangle\, P\Gamma f_{j_1}\wedge\cdots\wedge\widehat{P\Gamma f}_{j_r}\wedge\cdots\wedge P\Gamma f_{j_k}. \tag{A1}$$

We will determine how many terms with particle number k' appear in the preceding sum. For this let $p'\in\mathbb{N}$ be such that $2p'+k'=n+1$. Now the first term in the above formula contributes by means of expressions where $k=k'-1$ (hence $p=p'$) and there are

$$\binom{n}{n-2p}\frac{(2p)!}{p!\,2^p}=\binom{n}{n-2p'}\frac{(2p')!}{p'!2^{p'}}$$

such summands. Further, the second term contributes by means of expressions where $k=k'+1$ (hence $p=p'-1$) and there are now

$$k\binom{n}{n-2p}\frac{(2p)!}{p!\,2^p}=\binom{n}{n-2p'+1}\frac{(2p')!}{p'!2^{p'}}$$

such summands. Altogether we obtain

$$\binom{n}{n-2p'}\frac{(2p')!}{p'!2^{p'}}+\binom{n}{n-2p'+1}\frac{(2p')!}{p'!2^{p'}}=\binom{n+1}{n+1-2p'}\frac{(2p')!}{p'!2^{p'}}$$

terms with particle number k' and this coincides with the number of elements in $\mathfrak{S}_{n+1,p'}$. To conclude the proof we still need to show that each term in the sum carries the correct sign. For the summands in (A1) this follows from

$$\begin{aligned}
&\operatorname{sgn}\begin{pmatrix} n & n-1 & \cdots & n-2p+2 & n-2p+1 & k & \cdots & 1\\ \alpha_1 & \beta_1 & \cdots & \alpha_p & \beta_p & j_1 & \cdots & j_k\end{pmatrix}\\
&\quad=\operatorname{sgn}\begin{pmatrix} n+1 & n & \cdots & 1\\ n+1 & \alpha_1 & \cdots & j_k\end{pmatrix}\\
&\quad=\operatorname{sgn}\begin{pmatrix} n+1 & n & \cdots & n-2p+3 & n-2p+2 & k+1 & k & \cdots & 1\\ \alpha_1 & \beta_1 & \cdots & \alpha_p & \beta_p & n+1 & j_1 & \cdots & j_k\end{pmatrix}.
\end{aligned}$$

For the remaining terms we have

$$\begin{aligned}
&(-1)^{r-1}\operatorname{sgn}\begin{pmatrix} n & n-1 & \cdots & k & \cdots & k+2-r & k+1-r & k-r & \cdots & 1\\ \alpha_1 & \beta_1 & \cdots & j_1 & \cdots & j_{r-1} & j_r & j_{r+1} & \cdots & j_k\end{pmatrix}\\
&\quad=(-1)^{r-1}\operatorname{sgn}\begin{pmatrix} n+1 & n & \cdots & 1\\ n+1 & \alpha_1 & \cdots & j_k\end{pmatrix}\\
&\quad=\operatorname{sgn}\begin{pmatrix} n+1 & n & n-1 & n-2 & \cdots & k & \cdots & k+1-r & k-r & \cdots & 1\\ n+1 & j_r & \alpha_1 & \beta_1 & \cdots & j_1 & \cdots & j_{r-1} & j_{r+1} & \cdots & j_k\end{pmatrix}.
\end{aligned}$$

Therefore, we have shown that

$$(a(f_{n+1})\cdot\cdots\cdot a(f_1))\,\Omega=\sum_{\substack{\pi\in\mathfrak{S}_{n+1,\,p'}\\ 0\leqslant 2p'\leqslant n+1}}(\operatorname{sgn}\pi)\prod_{l=1}^{p'}\langle Pf_{\alpha_l},P\Gamma f_{\beta_l}\rangle\,P\Gamma f_{j_1}\wedge\cdots\wedge P\Gamma f_{j_k},$$

which concludes the proof. ■

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Fusion bases as facets of polytopes

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A new way of constructing fusion bases (i.e., the set of inequalities governing fusion rules) out of fusion elementary couplings is presented. It relies on a polytope reinterpretation of the problem: the elementary couplings are associated with the vertices of the polytope while the inequalities defining the fusion basis are the facets. The symmetry group of the polytope associated with the lowest rank affine Lie algebras is found; it has order 24 for $\widehat{su}(2)$, 432 for $\widehat{su}(3)$ and quite surprisingly, it reduces to 36 for $\widehat{su}(4)$, while it is only of order 4 for $\widehat{sp}(4)$. This drastic reduction in the order of the symmetry group as the algebra gets more complicated is rooted in the presence of many linear relations between the elementary couplings that break most of the potential symmetries. For $\widehat{su}(2)$ and $\widehat{su}(3)$, it is shown that the fusion-basis defining inequalities can be generated from few (one and two, respectively) elementary ones. For $\widehat{su}(3)$, new symmetries of the fusion coefficients are found. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Affine fusion rules give the number of integrable representations $\hat{\nu}$ that appear in the product of two integrable representations $\hat{\lambda}$ and $\hat{\mu}$ for a given affine algebra $\hat{g}$ at fixed level k (see, e.g., Ref. 1, Chap. 16). Fusions are in fact truncated finite Lie algebra tensor products, with the degree of truncation fixed solely by the level. More precisely, fusion rules are completely characterized by the tensor-product coefficients pertaining to the corresponding finite (i.e., nonaffine) representations and the set of threshold levels.[2] The threshold level of a particular coupling representing one of the various copies of the representation $\hat{\nu}$ in the product $\hat{\lambda}\times\hat{\mu}$ is the lowest level at which this coupling appears in this fusion. (Note that only the full set of threshold levels associated with a given triple coupling is an observable; the association of a particular threshold level with a given coupling is basis dependent.)

Even for $\widehat{su}(N)$, no genuine combinatorial methods—analogous to the Littlewood–Richardson rule—have been found. The closest approach to such a goal has been obtained in Ref. 3 in which a new approach to the problem of fusion rules was introduced, centered on the notion of *fusion basis*. A fusion basis is simply a complete set of inequalities, formulated in terms of a complete set of variables needed to describe a tensor product, augmented with an extra variable, the level k. Examples of bases have been constructed for $\widehat{su}(2)$, $\widehat{su}(3)$, $\widehat{su}(4)$, and $\widehat{sp}(4)$.

The idea of the construction in Ref. 3 is the following: one starts from the tensor-product

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elementary couplings, extends this set to a complete set of fusion elementary couplings (using, for instance, the conjectural completeness under outer automorphism—but there exist other possibilities) and from these, construct the inequalities in terms of the basis variables for which the elementary couplings are the elementary solutions.

In Ref. 3, the transition from the elementary couplings to the inequalities uses Farkas' lemma. The aim of this note is to indicate another way of reconstructing the fusion basis given the fusion elementary couplings. This new construction relies on a reinterpretation of the fusion-rule computations in terms of counting points inside a polytope. A polytope can be described by its vertices or its facets. The reconstruction of the facets of a polytope from its vertices is the essential trick we want to adapt to the problem of fusion rules. In our context, the vertices are represented by the fusion elementary couplings and the facets are the inequalities for which the elementary couplings are the elementary solutions. This reformulation is not purely cosmetic: it allows us to use powerful (e.g., computer) techniques developed for the study of polytopes, for instance, for deriving the facets from its vertices.

But this conceptual shift in the description of the fusion basis has an immediate benefit: having constructed a polytope it is natural to look for its symmetries. This means looking for the symmetry group of the fusion basis and organizing the various inequalities into a number of orbits of the group. In this paper we find the symmetry group of the polytopes associated with the known fusion bases.

II. THE $\widehat{su}(2)$ EXAMPLE

As a simple illustrative example we present the $\widehat{su}(2)$ fusion basis:

$$k \geqslant \lambda_1 + n_{11}, \quad n_{12} \geqslant 0, \quad \lambda_1 \geqslant n_{12}, \quad n_{11} \geqslant 0. \tag{2.1}$$

The last three conditions define the Littlewood–Richardson (LR) basis, which is thus recovered from the fusion basis in the infinite level limit ($k \to \infty$). This basis describes the solution set of the fusion $\hat{\lambda} \times \hat{\mu}$ at fixed positive integer level k. The two Dynkin labels of $\hat{\lambda}$ are $\lambda_0 = k - \lambda_1$ and λ_1, with λ_1 being the finite Dynkin label (and we will often use the Dynkin label notation: $\hat{\lambda} = [\lambda_0, \lambda_1]$). Both Dynkin labels are assumed to be non-negative integers. The LR algorithm starts by filling the boxes of the first row of the Young tableau associated to μ with 1's, the second row with 2's, etc. For $su(2)$, μ has only one row, containing μ_1 boxes. These boxes are inserted into the tableau representing λ, which is a row of λ_1 boxes: n_{11} boxes are then added in the first row and n_{12} boxes in the second row. Therefore n_{11} and n_{12} are non-negative integers and $n_{11} + n_{12} = \mu_1$. Moreover, columns with two 1's are not permitted, which forces $\lambda_1 \geqslant n_{12}$. Finally, the tableau associated with the representation ν is read off the resulting LR tableau by taking out the columns of two boxes: $\nu_1 = \lambda_1 + n_{11} - n_{12}$. (For more details on the LR algorithm, see, e.g., Refs. 4–6.)

The elementary solutions of this system of inequalities, written in terms of vectors with entries ordered as $(k, \lambda_1, n_{11}, n_{12})$, are

$$\epsilon_0 = (1,0,0,0), \quad \hat{E}_0 : d$$

$$\epsilon_1 = (1,1,0,1), \quad \hat{E}_1 : dL_1 N_{12} : \ \begin{array}{|c|}\hline \ \\ \hline 1 \\ \hline \end{array}$$

$$\epsilon_2 = (1,1,0,0), \quad \hat{E}_2 : dL_1 : \ \begin{array}{|c|}\hline \ \\ \hline \end{array}$$

$$\epsilon_3 = (1,0,1,0), \quad \bar{E}_3 : dN_{11} : \ \begin{array}{|c|}\hline 1 \\ \hline \end{array} \tag{2.2}$$

We have also presented the corresponding LR tableau at the right and its "exponential" description in between (where the variables k, λ_1, n_{11}, n_{12} appear, respectively, as the exponents of the

dummy variables d, L_1, N_{11}, N_{12}). The problem we consider here is the following: given $\hat{E}_i$, $i=0, 1, 2, 3$, how can we reconstruct the inequalities? In other words, how to go from the vertices (2.2) to the facets (2.1)?

III. THE POLYTOPE INTERPRETATION OF FARKAS' LEMMA

As we just mentioned, for the present work we suppose that the complete set of fusion elementary couplings $\{\hat{\mathcal{E}}_i\}$ is known. These are expressed in terms of a set of variables, denoted collectively as X_j, $j=1,...,n$ (which are the dummy variables d, L_1, N_{11}, N_{12} in the previous example), that furnish a complete description of the fusion rules. These are in fact the variables that describe the tensor products with the addition of the extra variable d that keeps track of the level of the affine algebra under consideration.

A general coupling can always be decomposed into a product of elementary couplings (and that this decomposition may not be unique is irrelevant at this point). This product decomposition can be transferred into a sum decomposition by characterizing an elementary coupling by the exponents ϵ_{ij} in its decomposition in terms of the variables X_j: an elementary coupling is thereby associated with an n-dimensional vector $\boldsymbol{\epsilon}_i$.

Again, our problem is the following: what is the set of linear and homogeneous inequalities for which the $\boldsymbol{\epsilon}_i$ are the elementary solutions? These inequalities will be formulated in terms of the variables x_j, whose exponential versions are the X_j. The set $\{x_i\}$ will typically contain the finite Dynkin labels of the three affine weights entering in the fusion, together with the missing labels appropriate for a complete description of the corresponding tensor product, plus the level k.

Any coupling $\Pi_i X_i^{x_i}$ can thus be decomposed in the form $\Pi_i \hat{\mathcal{E}}_i^{a_i}$. With $\hat{\mathcal{E}}_i=\Pi_j X_j^{\epsilon_{ij}}$, reading off a particular coupling means looking for a choice set of non-negative integers $\{a_i\}$ fixed by

$$\sum_i a_i \epsilon_{ij} = x_j \tag{3.1}$$

in terms of non-negative integers x_j. We are thus searching for the conditions ensuring the existence of such a coupling. This is precisely what Farkas' lemma can do. Quite remarkably, the lemma gives existence conditions in the form of inequalities on the x_j's and these are precisely the inequalities we are looking for.

If we write $V_{ij}=\epsilon_{ji}$ (hence, the columns of the matrix V are the elementary solutions), Farkas' lemma gives existence conditions for solutions of

$$Va = x \tag{3.2}$$

(in matrix form). For instance, for $\widehat{su}(2)$, V takes the form [cf. (2.2)]:

$$V=\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{3.3}$$

In fact, we are interested in the integer solutions of (3.2).

We should stress that Farkas' lemma is true in general only in the rational case. Sufficient conditions for its application to the integer case are known (see, for instance, Ref. 7), but these are not satisfied by our matrices V. Hence, the analysis has to be completed by a verification step, that is, to check that the elementary solutions of the inequalities obtained are the elementary solutions used at the start (cf. the discussion in Sec. 3 of Ref. 3).

The polytope interpretation of (3.2) is almost immediate (see Sec. IV): modulo renormalization, (3.2) is the equation of a polytope whose vertices v_i are the columns of the matrix V without its first row, hence our elementary couplings without their first entry d.

Now it is a well-known result (the Weyl–Minkowski theorem) that a polytope can be described either in terms of its vertices or its facets. In the present case, we have the vertices; the question is thus: what are the facets of the polytopes whose vertices are our fusion elementary couplings? These facets are the sought for inequalities, which form the fusion basis.

This reformulation is made more formal in Sec. IV. The following sections are devoted to the study of the symmetry group of the fusion polytopes for the simplest affine Lie algebras.

IV. FORMALIZING THE POLYTOPE REINTERPRETATION

To recast the problem in a general setting, let $V \in \mathbb{N}^{n\times m}$ be such that

$$V=(v_1 \ldots v_m)=\begin{pmatrix} w_1 & \cdots & w_m \\ \mathbf{v}_1 & \cdots & \mathbf{v}_m \end{pmatrix}, \tag{4.1}$$

with $v_1,\ldots,v_m$ the fusion elementary couplings and $w_1,\ldots,w_m$ the entries in the first row of V. Also, let $\mathcal{S}$ denote the set of fusion couplings

$$\mathcal{S}=\{x=Va=a_1v_1+\cdots+a_mv_m | a_1,\ldots,a_m \in \mathbb{N}\},$$

which, from our central hypothesis, is the set of non-negative integral combinations of elementary couplings. It is natural to suppose that the fusion couplings are the integral points of a certain geometric object E, that is, the vectors $v_1,\ldots,v_m$ form a Hilbert basis of E. [A finite set of vectors $v_1,\ldots,v_m$ is a Hilbert basis of $C=\text{cone}(a_1,\ldots,a_t)$ if $C\cap\mathbb{Z}^n=\mathbb{N}v_1+\cdots+\mathbb{N}v_m$.] One obvious choice for E, and the one we will make, is the cone generated by $v_1,\ldots,v_m$, that is

$$E=\{x=V\lambda=\lambda_1v_1+\cdots+\lambda_mv_m | \lambda_1,\ldots,\lambda_m \in \mathbb{R}_+\}. \tag{4.2}$$

In general, $v_1,\ldots,v_m$ may or may not be a Hilbert basis of this cone. However, for our examples we find that $v_1,\ldots,v_m$ is indeed a Hilbert basis of E. This checking process is equivalent to the verification step mentioned in Sec. III. The set $\mathcal{S}$ is thus given by

$$\mathcal{S}=E\cap\mathbb{N}^m, \tag{4.3}$$

and the fusion inequalities are simply the facets of the cone E. We can therefore use Farkas' lemma (or any other method) to obtain the facets of E. Now, it turns out that the fusion inequalities are also the facets of a polytope. The remainder of this section is devoted to this reinterpretation.

If we write the vectors $x \in E$ as

$$x=\begin{pmatrix} x_0 \\ \mathbf{x} \end{pmatrix}, \tag{4.4}$$

we have that the fusion couplings at level k are the integral points of the space, $P^{(k)}$, corresponding to the intersection between the hyperplane $x_0=k$ and the cone E. If we drop the x_0 component, which has value k in $P^{(k)}$, we can describe $P^{(k)}$ as

$$P^{(k)}=\left\{\mathbf{x}\middle|\begin{pmatrix} k \\ \mathbf{x} \end{pmatrix}\in E\right\}=\left\{\mathbf{x}\middle|\begin{pmatrix} k \\ \mathbf{x} \end{pmatrix}=V\lambda,\lambda\in\mathbb{R}_+^m\right\}=\left\{\mathbf{x}=\sum_i \mathbf{v}_i\lambda_i\middle|\lambda\in\mathbb{R}_+^m,\sum_i \lambda_i w_i=k\right\}. \tag{4.5}$$

The integral points of $P^{(k)}$ are

$$\mathcal{S}^{(k)}=P^{(k)}\cap\mathbb{N}^{n-1}, \tag{4.6}$$

which are essentially the possible fusion couplings at level k (by adding to the elements of $\mathcal{S}^{(k)}$ an extra component x_0 equal to k, we recover the usual fusion couplings). Because $0<w_i<\infty$, the transformation

$$\lambda_i \to \lambda_i' = \lambda_i(w_i/k), \quad \mathbf{v}_i \to \mathbf{v}_i' = (k/w_i)\mathbf{v}_i, \quad w_i \to w_i' = (k/w_i)w_i = k, \tag{4.7}$$

is well defined, and if we further set

$$V' = \begin{pmatrix} w_1' & \cdots & w_m' \\ \mathbf{v}_1' & \cdots & \mathbf{v}_m' \end{pmatrix} = \begin{pmatrix} k & \cdots & k \\ \mathbf{v}_1' & \cdots & \mathbf{v}_m' \end{pmatrix}, \tag{4.8}$$

$P^{(k)}$ can now be given as

$$P^{(k)} = \left\{ \mathbf{x} = \sum_i \mathbf{v}_i' \lambda_i' \,\middle|\, \lambda' \in \mathbb{R}_+^m, \sum_i \lambda_i' = 1 \right\}, \tag{4.9}$$

which by definition is the *polytope* given by the convex hull of the vertices $\mathbf{v}_i'$, $i = 1,...,m$.

The main theorem of polytope theory[8] tells us that P can be equivalently described as a solution set of a finite system of ℓ linear inequalities (facets), that is

$$P^{(k)} = \{\mathbf{x} | C\mathbf{x} \leqslant -kb\} = \left\{ \mathbf{x} \,\middle|\, C' \begin{pmatrix} k \\ \mathbf{x} \end{pmatrix} \leqslant 0 \right\}, \tag{4.10}$$

where C' is the concatenation (bC) of b and C, with $C \in \mathbb{R}^{\ell \times (n-1)}$ and $b \in \mathbb{R}^{\ell \times 1}$. In the last expression, we have made explicit the fact that the polytope inequalities translate into inequalities that the fusion elements at $x_0 = k$ must satisfy. We have thus obtained that the fusion inequalities are the facets of a polytope.

From a practical point of view, we stress that there exist powerful programs that give the polytope facets from its vertices (and vice-versa). The authors have used the ''cdd'' package of Fukuda[9] for computations in this article. For a description of other methods, we refer the reader to Ref. 8.

V. THE SYMMETRY GROUP OF THE FUSION POLYTOPES: GENERALITIES

The fusion polytope is a geometrical object and so it is natural to look for its symmetry group. However, for a polytope there are several different kinds of symmetry we can consider. For example, consider the polytope E in $\mathbb{R}^2$ with vertices (0,0), (0,2), (1,2), and (1,0) which we label 1, 2, 3, and 4. This polytope is fixed by the reflections in the lines $y = 1$ and $x = 1/2$ and by a 180° rotation about the point (1/2, 1). These are examples of Euclidean (length preserving) symmetries. Except for the identity transformation, there are no other Euclidean symmetries of E. But there are additional symmetries if we consider affine transformations, for example, $x \to 1 - y/2$, $y \to 2 - 2x$ fixes the vertices 2 and 4, while exchanging 1 and 3.

In general, affine symmetries of a polytope E in $\mathbb{R}^{n-1}$ are transformations of the form

$$\overline{\zeta}: \mathbf{x} \to A\mathbf{x} + kb, \tag{5.1}$$

with $A \in \mathbb{R}^{(n-1)\times(n-1)}$ and $b \in \mathbb{R}^{(n-1)\times 1}$, such that

$$\overline{\zeta} E = E. \tag{5.2}$$

If the matrix A is orthogonal then the affine symmetry is also Euclidean.

A convenient method of finding the affine symmetries is to identify $\mathbb{R}^{n-1}$ with the plane $x_0 = k$ in $\mathbb{R}^n$. Then the affine extension of $\overline{\zeta}$, denoted ζ, is given by

$$\zeta: \begin{pmatrix} k \\ \mathbf{x} \end{pmatrix} \to \begin{pmatrix} k \\ A\mathbf{x} + kb \end{pmatrix}, \tag{5.3}$$

or, in matrix form, as

$$\zeta:\begin{pmatrix} k \\ \mathbf{x} \end{pmatrix} \to \begin{pmatrix} 1 & 0 \\ b & A \end{pmatrix} \begin{pmatrix} k \\ \mathbf{x} \end{pmatrix}. \tag{5.4}$$

Now, since any polytope is completely characterized by its vertices or its facets, a transformation that leaves E invariant has to leave its set of vertices and its set of facets invariant. That is, we must have from (4.9) and (4.10) that the action of $\overline{\zeta}$ permutes $\mathbf{v}'_1,\ldots,\mathbf{v}'_m$, so that

$$\overline{\zeta}(\mathbf{v}'_1 \ \cdots \ \mathbf{v}'_m) = (\overline{\zeta}(\mathbf{v}'_1) \ \cdots \ \overline{\zeta}(\mathbf{v}'_m)) = (\mathbf{v}'_1 \ \cdots \ \mathbf{v}'_m)\sigma, \tag{5.5}$$

for some permutation matrix σ. Using V', whose columns are vectors of the type $\binom{k}{\mathbf{x}}$, the requirement (5.5) can be put in matrix form:

$$B(\zeta)V' = V'\sigma, \tag{5.6}$$

where $B(\zeta)$ is the matrix of the transformation ζ defined in (5.4). We shall be mainly interested in finding the affine symmetries of the fusion polytopes and methods for finding these symmetries will be described in Sec. VI.

Note, however, that in general potential symmetries of a polytope can often be ruled out by considering the polytope's combinatorial structure. Consider, for example, the polytope E introduced at the beginning of this section. As mentioned previously, a symmetry of E must permute vertices and facets and so there cannot be a symmetry of any type which exchanges vertices 2 and 3 while fixing vertices 1 and 4, since vertices 1 and 2 are joined by a common edge while 1 and 3 are not.

One type of combinatorial symmetry would be to consider all permutations of the faces of the polyhedron which preserve the face lattice (see, e.g., Ref. 10, p. 128). However, a simpler type of combinatorial symmetry, which is easy to find in our examples, is to look for permutations of vertices and facets which preserve the vertex–facet incidence matrix. This matrix is easy to calculate given the vertices and the inequalities representing the facets: the incidence matrix has an entry 1 in position (i,j) if the ith-vertex saturates (i.e., satisfies with equality) the jth facet inequality and is zero otherwise.

If we label the edges 1–2, 2–3, 3–4, and 4–1 of our example polytope E as 1, 2, 3, and 4, corresponding, respectively, to the inequalities $x \geqslant 0$, $y \leqslant 2$, $x \leqslant 1$, $y \geqslant 0$, we obtain the incidence matrix:

$$\mathcal{I} = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}. \tag{5.7}$$

If permutations σ and τ of the vertices and the edges, respectively, satisfy $\sigma\mathcal{I}\tau = \mathcal{I}$ then we say that we have an incidence symmetry. If σ and τ are such symmetries then $\sigma\mathcal{I}\tau\tau^{-1}\mathcal{I}^t\sigma^{-1} = \mathcal{I}\mathcal{I}^t$ and so σ commutes with $\mathcal{I}\mathcal{I}^t$. Call any vertex permutation which commutes with $\mathcal{I}\mathcal{I}^t$ a vertex symmetry.

Note that any affine symmetry induces a combinatorial face lattice symmetry and also a combinatorial incidence symmetry and a vertex symmetry. These maps are injective since if an affine symmetry fixes all the vertices of a polytope then it fixes the whole polytope since a polytope is the convex hull of its vertices. Thus we have the inclusions: Euclidean symmetries $\subseteq$ affine symmetries $\subseteq$ combinatorial face lattice symmetries $\subseteq$ combinatorial incidence symmetries $\subseteq$ vertex symmetries. Thus finding the vertex symmetries gives a ''upper bound'' on the other types of symmetries.

For the polytope E we have

$$\mathcal{I}\mathcal{I}^t=\begin{pmatrix} 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 \end{pmatrix}. \tag{5.8}$$

Since any vertex symmetry σ commutes with $\mathcal{I}\mathcal{I}^t$, it must also map eigenvectors to eigenvectors and using this it is not difficult to show that every vertex symmetry of E arises from an affine symmetry.

In general, however, the group of combinatorial symmetries will be much larger than the group of affine symmetries. For example if we take a ''generic'' convex n-gon in $\mathbb{R}^2$, its combinatorial symmetries will be a dihedral group, but there will be no affine symmetries except for the identity transformation.

Perhaps surprisingly, we find that for our examples that every vertex symmetry comes from an affine symmetry and so the most economical method of finding the affine symmetries would be to calculate first the vertex symmetries. However, this is not the usual situation and the only real advantage in our cases turns out to be that the matrices we have to calculate have smaller entries if we use vertex symmetries. So in Sec. VI we give general methods for finding all the affine symmetries for any polytope.

In the rest of this paper we shall only be concerned with finding affine symmetries of our polytopes, and so, unless stated otherwise, by a symmetry we shall mean an affine symmetry. Similarly when we refer to a vertex permutation as being a symmetry we mean that it arises from an affine symmetry as explained at the start of Sec. VI.

VI. THE SYMMETRY GROUP OF THE FUSION POLYTOPES: TECHNICAL TOOLS

In this section we will introduce some tools for finding the affine symmetries of our fusion polytopes introduced in Sec. V. We do this by considering vertex permutations and finding which ones arise from affine symmetries. These tools, however, apply in more generality than these applications and so we start with a more general definition of a symmetry of a matrix:

Definition: Let M be an $n\times m$ matrix. An $m\times m$ permutation matrix σ is a symmetry of M iff $M\sigma=BM$ for some $n\times n$ matrix B.

The set of symmetries of $M\in\mathbb{N}^{n\times m}$ is a subset of the group of permutation matrices which is closed under multiplication, hence is a group. The corresponding set of matrices B does not necessarily form a group, but it does if the rank of M is n.

This definition is inspired by Eq. (5.6) since for the fusions of the affine Lie algebra $\hat{g}$ we will take M to be the matrix V'. So in the terminology of Sec. V, a symmetry of V' is a vertex symmetry of our fusion polytope which comes from an affine symmetry. As explained in Sec. V we will call these vertex symmetries simply symmetries to avoid tedious repetition. The group of symmetries of V' will be denoted by $G[\hat{g}]$. For all our examples the rank of V' turns out to be n, in other words the fusion polytope has ''full-dimension.''

Proposition 1: An $m\times m$ permutation matrix σ is a symmetry of the $n\times m$ matrix M iff $\sigma N(M)=N(M)$ where $N(M)=\{z|Mz=0\}$.

Proof: If $z\in N(M)$ then $M\sigma z=BMz=0$, so $\sigma N(M)\subseteq N(M)$. Also $\sigma^{-1}N(M)\subseteq N(M)$, since σ^{-1} is also a symmetry of M (because the symmetries form a group) and so $\sigma N(M)=N(M)$. Conversely, if $\sigma N(M)=N(M)$ then the matrices M and $M\sigma$ have the same null space. Thus their rows generate the annihilator of $N(M)$. In particular the rows of $M\sigma$ are contained in the span of the rows of M and so there is a matrix B such that $BM=M\sigma$. So σ is a symmetry of M.

When the kernel of M has dimension 0 or 1, this proposition is sufficient to classify the symmetries. As we will show in the following sections, this holds for the fusion polytopes for $\widehat{su}(2)$ and $\widehat{su}(3)$.

If the kernel has larger dimension, we will need another approach. However, to do so we make the additional assumptions that M has real entries and that its rank is n. As noted previously, the fusion polytope matrices V' have these properties.

With these two assumptions, using the Gram–Schmidt procedure, we can find an invertible $n\times n$ matrix L such that the rows of $W=LM$ form an orthonormal basis of the row space of M. Since $M\sigma=BM$ if and only if $W\sigma=LBL^{-1}W$, it is clear that σ is a symmetry of M if and only if σ is a symmetry of W.

Proposition 2: σ is a symmetry of M if and only if $Q\sigma=\sigma Q$, where $Q=W^{\mathsf{T}}W$.

Proof: If σ is a symmetry of M then σ is a symmetry of W and so $W\sigma=TW$ for some $n\times n$ matrix T. Moreover, since σ acts as an orthogonal transformation on the rows of W, T is an orthogonal matrix. Hence, $W\sigma=TW$ implies $\sigma^{-1}W^{\mathsf{T}}=W^{\mathsf{T}}T^{-1}$. So $Q\sigma=W^{\mathsf{T}}W\sigma=W^{\mathsf{T}}TW=\sigma W^{\mathsf{T}}W$ as required. For the converse, note that the matrix Q performs the orthogonal projection onto the row space of M. So if σ commutes with the projection matrix Q then it maps the row space of M to itself and so is a symmetry of M.

Since σ is a permutation, we can read off some of its properties directly from Q. For example a row of Q can be mapped to another row of Q by a symmetry only if the two rows have the same set of entries. A second simplification occurs by observing that if σ is a symmetry and $\sigma u=\lambda u$ for some vector u then $\sigma Qu=Q\sigma u=\lambda Qu$. In particular, if u is fixed by the symmetry group, so is Qu. We will apply these two observations when we compute the symmetries for the $\widehat{sp}(4)$ fusion polytope.

VII. THE SYMMETRY GROUP OF THE $\widehat{su}(2)_k$ POLYTOPE

For $\widehat{su}(2)$, the matrix V' takes the form kV with V given in (3.3); $N(V')$ is thus trivial. Therefore, every permutation is a symmetry. Since $n=m=4$, this gives S_4 as the symmetry group $G[\widehat{su}(2)]$. S_4 is generated by the permutations (1, 2, 3, 4) and (1, 2), where $(i,j,\ldots,k)$ stands for a cyclic permutation of $i,j,\ldots,k$. Since V' is invertible, we can easily find the corresponding transformation ζ acting on $x^{\mathsf{T}}=(k,\lambda_1,n_{11},n_{12})$. It reads:

$$\begin{aligned}(1,2,3,4):&(k,\lambda_1,n_{11},n_{12})\mapsto(k,k-\lambda_1-n_{11}+n_{12},\lambda_1-n_{12},k-\lambda_1-n_{11}),\\(1,2):&(k,\lambda_1,n_{11},n_{12})\mapsto(k,k-n_{11}-n_{12},n_{11},k-\lambda_1-n_{11}).\end{aligned}\tag{7.1}$$

The fusion basis is given in (2.1). Labeling these inequalities from 1 to 4, the symmetries (1, 2, 3, 4) and (1, 2) permute the inequalities. However, the inequalities correspond to the polytope facets, which being dual to the vertices transform by the inverse of the vertex transform. Thus if $x\mapsto Bx$ is the transformation corresponding to the vertices, then $\alpha^{\mathsf{T}}\mapsto\alpha^{\mathsf{T}}B^{-1}$ is the appropriate transformation for the facets. The necessity of this can be seen from the fact that the transformations should preserve the incidence relations of the vertices and facets and that this involves quantities of the form $\alpha^{\mathsf{T}}x$.

From this it follows that the action of (1, 2) is [[1, 2], [3], [4]], i.e., it permutes the first two inequalities and fixes the last two. Similarly the action of (1, 2, 3, 4) is [[1, 2, 3, 4]]. Thus the fusion basis is generated by any one of its inequalities under that action of the symmetry group.

Is there a simple way to understand these symmetries in terms of the symmetries of the fusion coefficients? First, notice that the fusion coefficients are described in terms of a smaller number of labels than those necessary for the complete description of the fusion basis. The complete set of labels can be split into two subsets: the Dynkin labels of the three weights under consideration and the ''missing labels.'' If some symmetries do not involve in an essential way the missing labels, they will project onto fusion-coefficient symmetries. However, if the missing labels are an essential part of the symmetry transformations, the symmetry will disappear in the projection. For instance, tensor-product coefficients can be obtained by projection of the fusion coefficients. The latter require an extra variable for their description, the level k, and fusion coefficients have more symmetries than the tensor-product coefficients. The extra symmetries are the outer automorphisms—see the next paragraph—and these involve the level in an essential way. Let us make the general situation more precise: Denote collectively the finite Dynkin labels $\{\lambda_i,\mu_i,\nu_i\}$ and k by D and the set of missing labels by γ. A facet symmetry is generically of the form $\{D,\gamma\}\to\{D'(D,\gamma),\gamma'(D,\gamma)\}$. This will be a symmetry of the fusion coefficients only when D'

does not depend upon γ. Therefore there is no simple relationship between the symmetries of the facets and the symmetries of the fusion coefficients. In this regard, each algebra has to be studied separately.

The symmetries of the fusion coefficients include those that are level-independent, i.e., the symmetries of the corresponding tensor-product coefficients; these are the conjugation of the three weights, $(\hat{\lambda},\hat{\mu},\hat{\nu})\rightarrow(\hat{\lambda}^*,\hat{\mu}^*,\hat{\nu}^*)$ and the different permutations of $\hat{\lambda}$, $\hat{\mu}$ and $\hat{\nu}^*$. The remaining symmetries are intrinsically affine. These include the outer-automorphism symmetries which take the following form: If A, A' are two arbitrary elements of the outer-automorphism group of $\hat{g}$, the fusion coefficients satisfy

$$\mathcal{N}_{A\hat{\lambda},A'\hat{\mu}}^{(k)\quad AA'\hat{\nu}}=\mathcal{N}_{\hat{\lambda}\hat{\mu}}^{(k)\,\hat{\nu}}. \tag{7.2}$$

For $\widehat{su}(N)$, this group has order N: $A^N=1$. The symmetry group can be larger than that generated by tensor product symmetries and outer automorphisms, see e.g., Refs. 11–13. There are often symmetries which exist for some, but not all levels. The method we present here will not detect this type of symmetry and from this point we will exclude them. In other words, by symmetries of the fusion coefficients we mean symmetries which exist for all levels.

For $\widehat{su}(2)$, there are no missing labels. Hence the symmetry group of the polytope must be identical to the symmetry group of the fusion coefficients which exist for all k and that leave k fixed. This group is isomorphic to the semidirect product $(S_2\times S_2)\colon S_3$. The S_3 factor comes from the permutation of the three weights, while the two factors of S_2 account for the two copies of the outer-automorphism group (one acting on the weight $\hat{\lambda}$, the other acting on $\hat{\mu}$). The conjugation action of S_3 is via the outer automorphisms of $S_2\times S_2$ which permute the nonidentity elements. The group S_4 contains a group $S_2\times S_2$ generated by the cycles of type 2^2. Any of the four S_3 subgroups act on this $S_2\times S_2$ as outer automorphisms by conjugation and so the symmetry group is isomorphic to S_4.

Let us first reexpress all the basis symmetries in terms of the Dynkin labels:

$$\begin{aligned}
&(1,2,3,4)\colon(k,\lambda_1,\mu_1,\nu_1)\rightarrow(k,k-\nu_1,k-\mu_1,\lambda_1),\\
&(1,2)\colon(k,\lambda_1,\mu_1,\nu_1)\rightarrow(k,k-\mu_1,k-\lambda_1,\nu_1),\\
&(2,3)\colon(k,\lambda_1,\mu_1,\nu_1)\rightarrow(k,\lambda_1,\nu_1,\mu_1),\\
&(3,4)\colon(k,\lambda_1,\mu_1,\nu_1)\rightarrow(k,\mu_1,\lambda_1,\nu_1).
\end{aligned} \tag{7.3}$$

(Clearly, the last two symmetries can be obtained from the first two.)

Let us make explicit the correspondence between these symmetries and symmetries of the fusion coefficients. For this, notice first that the multiplicity of the $\widehat{su}(2)_k$ product $\hat{\lambda}\times\hat{\mu}\supset\hat{\nu}$ is the same as that of $\hat{\lambda}\times\hat{\mu}\times\hat{\nu}\supset 0$. Let P_{12} be the operator that permutes the first two weights and similarly for the other permutation operators. Moreover, let a be the $\widehat{su}(2)$ automorphism that interchanges the two simple roots, hence the two Dynkin labels: $a[k-\lambda_1,\lambda_1]=[\lambda_1,k-\lambda_1]$. Therefore, the nontrivial actions on $\hat{\lambda}\times\hat{\mu}\times\hat{\nu}\supset 0$ are simply:

$$a\hat{\lambda}\times a\hat{\mu}\times\hat{\nu}\supset 0,\quad a\hat{\lambda}\times\hat{\mu}\times a\hat{\nu}\supset 0,\quad \hat{\lambda}\times a\hat{\mu}\times a\hat{\nu}\supset 0. \tag{7.4}$$

Denote these actions, respectively, as $(a,a,1)$, $(a,1,a)$, $(1,a,a)$. The fusion basis symmetries can then be related directly to a and P actions as follows:

$$
\begin{aligned}
(1,2,3,4) &\equiv (a,a,1)P_{13},\\
(1,2) &\equiv (a,a,1)P_{12},\\
(2,3) &\equiv P_{23},\\
(3,4) &\equiv P_{12}.
\end{aligned}
\tag{7.5}
$$

"Pure" finite or affine symmetries can be obtained by composition, e.g.,

$$
\begin{aligned}
(2,3,4) &\equiv P_{321},\\
(1,2)(3,4) &\equiv (a,a,1).
\end{aligned}
\tag{7.6}
$$

VIII. THE SYMMETRY GROUP OF THE $\widehat{su}(3)_k$ POLYTOPE

The situation for $\widehat{su}(2)$ is not typical in two ways. First, there are no missing labels; hence any permutation of the vertices is bound to be a symmetry of the fusion coefficients. In addition, there are no linear relations between the elementary solutions. Such relations will induce severe constraints on the possible lifts of the fusion-coefficient symmetries to polytope symmetries.

For $\widehat{su}(3)$, the elementary couplings are (using the notation $\hat{\lambda}=[\lambda_0,\lambda_1,\lambda_2]$ with $\lambda_0+\lambda_1+\lambda_2=k$ and the LR variables—cf. Ref. 3. Note that λ_1 and λ_2 are Dynkin labels and not the partition labels to which they usually refer in the Littlewood–Richardson rule as in Ref. 4, Chap. 1, for example):

$$
\begin{aligned}
\hat{E}_0&: \quad [1,0,0]\times[1,0,0]\supset[1,0,0]: \quad d \qquad (1,0,0,0,0,0,0,0) \quad (1,1)\\
\hat{E}_1&: \quad [0,1,0]\times[0,0,1]\supset[1,0,0]: \quad dL_1N_{12}N_{23} \quad (1,1,0,0,1,0,0,1) \quad (a,a^2)\\
\hat{E}_2&: \quad [0,1,0]\times[1,0,0]\supset[0,1,0]: \quad dL_1 \quad (1,1,0,0,0,0,0,0) \quad (a,1)\\
\hat{E}_3&: \quad [1,0,0]\times[0,1,0]\supset[0,1,0]: \quad dN_{11} \quad (1,0,0,1,0,0,0,0) \quad (1,a)\\
\hat{E}_4&: \quad [0,0,1]\times[0,1,0]\supset[1,0,0]: \quad dL_2N_{13} \quad (1,0,1,0,0,1,0,0) \quad (a^2,a)\\
\hat{E}_5&: \quad [0,0,1]\times[1,0,0]\supset[0,0,1]: \quad dL_2 \quad (1,0,1,0,0,0,0,0) \quad (a^2,1)\\
\hat{E}_6&: \quad [1,0,0]\times[0,0,1]\supset[0,0,1]: \quad dN_{11}N_{22} \quad (1,0,0,1,0,0,1,0) \quad (1,a^2)\\
\hat{E}_7&: \quad [0,1,0]\times[0,1,0]\supset[0,0,1]: \quad dL_1N_{12} \quad (1,1,0,0,1,0,0,0) \quad (a,a)\\
\hat{E}_8&: \quad [0,0,1]\times[0,0,1]\supset[0,1,0]: \quad dL_2N_{11}N_{23} \quad (1,0,1,1,0,0,0,1) \quad (a^2,a^2).
\end{aligned}
\tag{8.1}
$$

Besides each coupling, we have written the "exponential description," the corresponding vector ϵ_i with entries in the order $(k,\lambda_1,\lambda_2,n_{11},n_{12},n_{13},n_{22},n_{23})$, as well as the action of the outer automorphism on the first two weights of $\hat{E}_0$ [in the form (a^n,a^m)] that yields the coupling under consideration.

The corresponding facets (the fusion basis) are found to be

$$
\begin{aligned}
n_{12}&\geqslant 0, \quad \lambda_2+n_{12}-n_{13}-n_{23}\geqslant 0,\\
n_{13}&\geqslant 0, \quad n_{11}-n_{22}\geqslant 0,\\
n_{22}&\geqslant 0, \quad n_{11}+n_{12}-n_{22}-n_{23}\geqslant 0,\\
n_{23}&\geqslant 0, \quad k-\lambda_1-\lambda_2-n_{22}\geqslant 0,\\
\lambda_1-n_{12}&\geqslant 0, \quad k-\lambda_1-\lambda_2-n_{11}+n_{23}\geqslant 0,\\
\lambda_2-n_{13}&\geqslant 0, \quad k-\lambda_1-n_{13}-n_{11}\geqslant 0.
\end{aligned}
\tag{8.2}
$$

This agrees with the system of inequalities obtained in Ref. 3.

For $\widehat{su}(3)$, the matrix V' is 8×9:

$$V'=k\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{8.3}$$

and since the rank of V' is 8, $N(V')$ is one-dimensional and is spanned by

$$w^{\mathsf{T}}=(1\ \ -1\ \ 0\ \ -1\ \ 0\ \ -1\ \ 0\ \ 1\ \ 1). \tag{8.4}$$

The condition on σ is thus $\sigma w=\lambda w$ for some scalar λ and, since the eigenvalues of σ are roots of unity, λ is either 1 or -1. Thus $G[\widehat{su}(3)]$ is isomorphic to $S_3\times(S_3\wr S_2)$. The S_3 permutes the 0's of w and $S_3\wr S_2$ (the wreath product of S_3 and S_2, i.e., the direct product of *two* S_3's with S_2 acting by exchanging them) permutes and exchanges the 1's and -1's.

Let $x^{\mathsf{T}}=(k,\lambda_1,\lambda_2,n_{11},n_{12},n_{13},n_{22},n_{23})$. The action of a set of generators of the symmetry group on the variables is:

$$\begin{aligned}
(3,5,7)&:x^{\mathsf{T}}\mapsto(k,n_{12}+n_{22},\lambda_1+\lambda_2-n_{12}-n_{13},n_{11}+n_{13}-n_{22},n_{12},\lambda_1-n_{12},n_{13},n_{23}),\\
(3,5)&:x^{\mathsf{T}}\mapsto(k,n_{12}+n_{13},\lambda_1+\lambda_2-n_{12}-n_{13},n_{11},n_{12},\lambda_1-n_{12},n_{22},n_{23}),\\
(1,8,9)&:x^{\mathsf{T}}\mapsto(k,k-\lambda_2-n_{11}-n_{12}+n_{23},\lambda_2+n_{12}-n_{23},n_{11}\\
&\quad +n_{12}-n_{23},k-\lambda_1-\lambda_2-n_{11}+n_{23},n_{13},n_{22},n_{12}),\\
(1,8)&:x^{\mathsf{T}}\mapsto(k,k-\lambda_2-n_{11}-n_{12}+n_{23},\lambda_2,n_{11},k-\lambda_1-\lambda_2-n_{11}+n_{23},n_{13},n_{22},n_{23}),
\end{aligned} \tag{8.5}$$

together with

$$\begin{aligned}
(1,2)(4,8)(6,9)&:x^{\mathsf{T}}\mapsto(k,k-\lambda_2-n_{12}-n_{22},\lambda_2,\lambda_2+n_{12}-n_{13}+n_{22}\\
&\quad -n_{23},k-\lambda_1-\lambda_2-n_{22},n_{13},n_{22},k-\lambda_1-n_{13}-n_{11}).
\end{aligned} \tag{8.6}$$

The fusion basis is given by (8.2). Labeling these inequalities successively, column by column, from 1 to 12 (i.e., 8 corresponds to $n_{11}-n_{22}\geqslant 0$), we find that the action of the symmetry group on the inequalities considered as polytope facets is generated by:

$$\begin{aligned}
(3,5,7)&:[[1],[2,3,5],[4],[6],[7],[8],[9],[10],[11],[12]],\\
(3,5)&:[[1],[2,5],[3],[4],[6],[7],[8],[9],[10],[11],[12]],\\
(1,8,9)&:[[1,4,11],[2],[3],[5],[6,12,7],[8,10,9]],\\
(1,8)&:[[1,11],[2],[3],[4],[5],[6],[7,12],[8],[9,10]],\\
(1,2)(4,8)(6,9)&:[[1,10],[2],[3],[4,12],[5],[6],[7,8],[9],[11]],
\end{aligned} \tag{8.7}$$

where as before $[i,j,\ldots,k]$ stands for a cyclic permutation of the inequalities $i,j,\ldots,k$. Thus there are two orbits under the symmetry group. One consisting of the inequalities 2, 3, and 5 and the other consisting of the inequalities 1, 4, 6, 7, 8, 9, 10, 11, and 12. So the fusion basis is generated by the two inequalities $n_{12}\geqslant 0$ and $n_{13}\geqslant 0$ under the action of $G[\widehat{su}(3)]$.

Let us now try to understand these results. As already pointed out, these symmetries must be compatible with the symmetries of the fusion coefficients. But there is a further constraint on the fusion symmetries that has not been spelled out yet: in general there are linear relations among the elementary couplings and the symmetries of the facets must preserve these relations. In the $\widehat{su}(3)$ case, there is only one such linear relation, which is:

$$\hat{E}_0\hat{E}_7\hat{E}_8=\hat{E}_1\hat{E}_3\hat{E}_5. \tag{8.8}$$

This explains the existence of the three S_3 blocks: permutations among the sets $\{\hat{E}_0,\hat{E}_7,\hat{E}_8\}$ and $\{\hat{E}_1,\hat{E}_3,\hat{E}_5\}$ are symmetries that preserve each side of the relation. The third S_3 factor is bound to relate the three remaining vertices. Moreover, the S_2 group generated by (1, 2)(4, 8)(6, 9) is another transformation that leaves the relation unchanged: but instead of leaving each side invariant, it interchanges the two sides of the relation: $\hat{E}_0\leftrightarrow\hat{E}_1$, $\hat{E}_3\leftrightarrow\hat{E}_7$, $\hat{E}_5\leftrightarrow\hat{E}_8$. The occurrence of a linear relation is thus responsible for the fact that the symmetry group is not S_9 but only a subgroup thereof.

Of course, the existence of relations is intimately connected with the matrix V'. In fact, $N(V')$ is precisely the set of generating relations (in the sense of Ref. 3) out of which all the relations can be obtained.

To complete the analysis of the $\widehat{su}(3)_k$ polytope symmetries, let us investigate their explicit relation with symmetries of the fusion coefficients. For this, we first reexpress the symmetry transformations in terms of the Dynkin labels of the three weights plus n_{23}. Thus n_{23} is the missing label. We also reformulate the results in terms of the symmetrized product: $\hat{\lambda}\times\hat{\mu}\times\hat{\nu}\supset 0$. Recall that the multiplicity of $\hat{\lambda}\times\hat{\mu}\supset\hat{\nu}^*$ is the same as that of $\hat{\lambda}\times\hat{\mu}\times\hat{\nu}\supset 0$, where $*$ denotes the finite weight conjugation; for $\widehat{su}(3)$, it amounts to interchanging the two finite Dynkin labels. The precise transformation relations are as follows:

$$\begin{aligned} &n_{11}=L_2-\lambda_1-\lambda_2, \quad n_{12}=L_1-L_2+n_{23},\\ &n_{13}=L_2-\nu_1-\nu_2-n_{23}, \quad n_{22}=\mu_2-n_{23}. \end{aligned} \tag{8.9}$$

With the vector y^{T} defined as $y^{\mathsf{T}}=(k,\lambda_1,\lambda_2,\mu_1,\mu_2,\nu_1,\nu_2,n_{23})$, we can rewrite the symmetries of the fusion basis as

$$\begin{aligned} (3,5,7):&y^{\mathsf{T}}\to(k,L_2-\lambda_2-\nu_2,L_2-\mu_1-\mu_2,L_2-\lambda_2-\mu_2,L_2\\ &-\nu_1-\nu_2,L_2-\mu_2-\nu_2,L_2-\lambda_1-\lambda_2,n_{23}),\\ (3,5):&y^{\mathsf{T}}\to(k,L_1-\nu_1-\nu_2,L_2-\mu_1-\mu_2,L_2-\lambda_2-\mu_2,\mu_2,\nu_1,L_1-\lambda_1-\nu_1,n_{23}),\\ (1,8,9):&y^{\mathsf{T}}\to(k,k-L_1+\lambda_1,L_2-\mu_2-\nu_2,k-L_1+\mu_1,L_2\\ &-\lambda_2-\nu_2,k-L_1+\nu_1,L_2-\lambda_2-\mu_2,L_1-L_2+n_{23}),\\ (1,8):&y^{\mathsf{T}}\to(k,k-L_1+\lambda_1,\lambda_2,k-L_1+\mu_1,\mu_2,k-L_1+\nu_1,\nu_2,n_{23}),\\ (1,2)(4,8)(6,9):&y^{\mathsf{T}}\to(k,k-L_2+\nu_2,\lambda_2,\mu_1,k-L_1+\nu_1,L_2\\ &-\lambda_1-\lambda_2,L_1-\mu_1-\mu_2,n_{23}+k-L_1-\mu_2+\nu_1), \end{aligned} \tag{8.10}$$

where $L_i=(\lambda+\mu+\nu,\omega_i)$ with ω_i the ith fundamental weight. The remarkable feature of these symmetry transformations is that they send $y^{\mathsf{T}}\to y'^{\mathsf{T}}$ such that none of the prime variables except n'_{23} depends upon n_{23}. In other words, the new Dynkin labels, collectively denoted by D', do not depend upon n_{23}. Therefore, these symmetries map a state (i.e., a tableau) of a given fusion to another state of another fusion. The same is necessarily true for the inverted transformations. There is thus a one-to-one correspondence between the two fusions, i.e., they have the same multiplicity! In other words, the symmetries of the fusion basis are symmetries of the fusion coefficients. For instance,

$$
\begin{aligned}
&(3,5,7): \quad \mathcal{N}^{(k)}_{(\lambda_1,\lambda_2)(\mu_1,\mu_2)(\nu_1,\nu_2)} \\
&\qquad = \mathcal{N}^{(k)}_{(L_2-\lambda_2-\nu_2,L_2-\mu_1-\mu_2)(L_2-\lambda_2-\mu_2,L_2-\nu_1-\nu_2)(L_2-\mu_2-\nu_2,L_2-\lambda_1-\lambda_2)}, \\
&(3,5): \quad \mathcal{N}^{(k)}_{(\lambda_1,\lambda_2)(\mu_1,\mu_2)(\nu_1,\nu_2)} = \mathcal{N}^{(k)}_{(L_1-\nu_1-\nu_2,L_2-\mu_1-\mu_2)(L_2-\lambda_2-\mu_2,\mu_2)(\nu_1,L_1-\lambda_1-\nu_1)}, \\
&(1,8,9): \quad \mathcal{N}^{(k)}_{(\lambda_1,\lambda_2)(\mu_1,\mu_2)(\nu_1,\nu_2)} = \mathcal{N}^{(k)}_{(k-L_1+\lambda_1,L_2-\mu_2-\nu_2)(k-L_1+\mu_1,L_2-\lambda_2-\nu_2)(k-L_1+\nu_1,L_2-\lambda_2-\nu_2)}, \\
&(1,8): \quad \mathcal{N}^{(k)}_{(\lambda_1,\lambda_2)(\mu_1,\mu_2)(\nu_1,\nu_2)} = \mathcal{N}^{(k)}_{(k-L_1+\lambda_1,\lambda_2)(k-L_1+\mu_1,\mu_2)(k-L_1+\nu_1,\nu_2)}, \\
&(1,2)(4,8)(6,9): \quad \mathcal{N}^{(k)}_{(\lambda_1,\lambda_2)(\mu_1,\mu_2)(\nu_1,\nu_2)} = \mathcal{N}^{(k)}_{(k-L_2+\nu_2,\lambda_2)(\mu_1,k-L_1+\nu_1)(L_2-\lambda_1-\lambda_2,L_1-\mu_1-\mu_2)}.
\end{aligned}
\tag{8.11}
$$

In this rewriting, the dependence upon the n_{23} variable is dropped.

These are clearly new fusion symmetries as they mix the labels of the three representations. It is simple to verify that they leave the explicit expression of the $\widehat{su}(3)_k$ fusion coefficients (given in Ref. 14) invariant. Here is a numerical illustration: (1, 8) maps

$$
[4,10,12]\times[1,4,11]\times[9,3,4]\supset 0 \leftrightarrow E_0E_1^8E_3^2E_6E_7^2E_8^2, \quad E_1^8E_2E_3^2E_4E_6^2E_7E_8 \tag{8.12}
$$

onto

$$
[5,9,2]\times[2,3,11]\times[10,2,4]\supset 0 \leftrightarrow E_7E_1^8E_3^2E_6E_0^2E_8^2, \quad E_1^8E_2E_3^2E_4E_6^2E_0E_8. \tag{8.13}
$$

Both fusions have two decompositions in terms of elementary couplings, meaning that they have the same multiplicity. This symmetry is manifestly distinct from those already known. It is not a trivial symmetry in that, in terms of the elementary-coupling decompositions, it corresponds to the interchange of E_0 and E_7 in each decomposition.

The usual fusion symmetries can be obtained from various combinations of the above-mentioned symmetries of the fusion basis. For instance,

$$
\begin{aligned}
&(2,4,6)(3,5,7)\equiv P_{123}, \\
&(8,9)(5,7)(2,4)\equiv CP_{13}, \\
&(2,8)(1,4)(6,9)\equiv(1,a,a^2)P_{23},
\end{aligned}
\tag{8.14}
$$

where C is the conjugation:

$$
C\{\hat{\lambda}\times\hat{\mu}\times\hat{\nu}\supset 0\}=\hat{\lambda}^*\times\hat{\mu}^*\times\hat{\nu}^*\supset 0. \tag{8.15}
$$

We thus recover the known symmetries and additional ones.

IX. THE SYMMETRY GROUP OF THE $\widehat{sp}(4)_k$ POLYTOPE

The $\widehat{sp}(4)$ fusion rules are most conveniently described by means of the variables introduced in Ref. 15 and used in Refs. 3 and 6 (with a slight change of notation), namely $\{k,\lambda_1,\lambda_2,\mu_1,\mu_2,r_1,r_2,p,q\}$, with p, q and $r_i/2$ non-negative integers. The Dynkin labels of the third weight are

$$\nu_1=r_2-r_1-2p+\lambda_1+\mu_1, \quad \nu_2=p-q-r_2+\lambda_2+\mu_2. \tag{9.1}$$

In terms of the exponentiated variables, the elementary couplings are $\hat{E}_0=d$, together with

$$\begin{aligned}
&\hat{A}_1=dM_1, && \hat{A}_2=dL_1, && \hat{A}_3=dL_1M_1PQ,\\
&\hat{B}_1=dM_2, && \hat{B}_2=dL_2, && \hat{B}_3=dL_2M_2R_1^2R_2^2,\\
&\hat{C}_1=dL_2M_1Q, && \hat{C}_2=dL_1M_2R_2^2P, && \hat{C}_3=dL_1M_1P,\\
&\hat{D}_1=d^2L_1^2M_2R_2^2P^2, && \hat{D}_2=d^2L_2M_1^2R_1^2, && \hat{D}_3=d^2L_2M_2R_2^2.
\end{aligned} \tag{9.2}$$

Taking these to be the vertices of a polytope, the corresponding facets are found to be:

$$\begin{aligned}
k-\lambda_1-\lambda_2-\mu_2-r_1/2+r_2\geqslant 0, &\quad \mu_1-q\geqslant 0,\\
k-\lambda_1-\lambda_2-\mu_2+r_2/2\geqslant 0, &\quad \mu_1-q-r_1+r_2\geqslant 0,\\
k-\lambda_1-\mu_1-\mu_2+p\geqslant 0, &\quad \mu_1-p-r_1+r_2\geqslant 0,\\
k-\lambda_1-\lambda_2-\mu_1-\mu_2+p+q+r_1/2\geqslant 0, &\quad \mu_2-r_2/2\geqslant 0,\\
\lambda_1-p\geqslant 0, &\quad r_1\geqslant 0,\\
\lambda_2-r_1/2\geqslant 0, &\quad r_2\geqslant 0,\\
\lambda_2-r_1/2-q+p\geqslant 0, &\quad p\geqslant 0,\\
\lambda_2-r_2/2-q+p\geqslant 0, &\quad q\geqslant 0
\end{aligned} \tag{9.3}$$

in agreement with the results obtained in Ref. 3.

We next analyze the symmetries of the $\widehat{sp}(4)$ fusion polytope. The matrix V', with the column ordering $(\hat{E}_0,\hat{A}_1,\ldots,\hat{D}_3)$, reads

$$V'=k\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1\\
0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1/2 & 1/2\\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0\\
0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1/2 & 0 & 1/2\\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 1 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 0 & 1 & 0 & 1\\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0\\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}. \tag{9.4}$$

Unfortunately for this case the kernel of V' is not one-dimensional. In fact, $N(V')$ is four-dimensional, which we understand from the fact that there are four generating relations—cf. Ref. 3, Eq. (5.18). As a result, we must study the symmetries of V' via the commutant of the matrix Q that performs the orthogonal projection onto the row space of V' (cf. proposition 2 of Sec. VI). This matrix reads

$$Q=\frac{1}{108}\begin{pmatrix}
82 & 16 & 0 & 18 & 0 & 10 & -2 & -18 & -14 & -20 & 16 & 4 & 16\\
16 & 67 & 0 & -9 & 0 & -20 & -14 & 9 & 10 & 13 & -14 & 28 & 22\\
0 & 0 & 108 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
18 & -9 & 0 & 81 & 0 & -18 & 0 & 27 & 0 & 9 & 18 & 0 & -18\\
0 & 0 & 0 & 0 & 108 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
10 & -20 & 0 & -18 & 0 & 82 & -2 & 18 & -14 & 16 & 16 & 4 & 16\\
-2 & -14 & 0 & 0 & 0 & -2 & 94 & 0 & 10 & -14 & 4 & 28 & 4\\
-18 & 9 & 0 & 27 & 0 & 18 & 0 & 81 & 0 & -9 & -18 & 0 & 18\\
-14 & 10 & 0 & 0 & 0 & -14 & 10 & 0 & 70 & 10 & 28 & -20 & 28\\
-20 & 13 & 0 & 9 & 0 & 16 & -14 & -9 & 10 & 67 & 22 & 28 & -14\\
16 & -14 & 0 & 18 & 0 & 16 & 4 & -18 & 28 & 22 & 40 & -8 & 4\\
4 & 28 & 0 & 0 & 0 & 4 & 28 & 0 & -20 & 28 & -8 & 52 & -8\\
16 & 22 & 0 & -18 & 0 & 16 & 4 & 18 & 28 & -14 & 4 & -8 & 40
\end{pmatrix}. \tag{9.5}$$

As already pointed out in Sec. VI, a row of Q can be mapped to another row by a symmetry transformation σ only if the two rows have the same entries. Hence, from the explicit form of (9.5), we see that any symmetry fixes the sets {1, 6}, {2, 10}, {3, 5}, {4, 8}, {11, 13}, {7}, {9}, and {12}. It is not difficult to see that the permutation (3, 5) is a symmetry.

We can again examine Q to see that a symmetry exchanges rows 1 and 6 iff it exchanges columns 2 and 10. It exchanges rows 2 and 10 iff it exchanges columns 11 and 13 and exchanges rows 11 and 13 iff it exchanges columns 4 and 8.

It is easy to verify that (1,6)(2,10)(11,13)(4,8) is a symmetry. Thus, the symmetries of V' are

$$G[\widehat{sp}(4)]=\{(),(3,5),(1,6)(2,10)(11,13)(4,8),(3,5)(1,6)(2,10)(11,13)(4,8)\} \tag{9.6}$$

isomorphic to $S_2\times S_2$.

With $x^{\mathsf{T}}=(k,\lambda_1,\lambda_2,\mu_1,\mu_2,r_1,r_2,p,q)$, the changes of variables corresponding to the generators of the symmetry group are:

$$\begin{aligned}
&(3,5):x^{\mathsf{T}}\mapsto(k,\mu_2-r_2/2+p,\lambda_2,\mu_1,\lambda_1+r_2/2-p,r_1,r_2,p,q),\\
&(1,6)(2,10)(11,13)(4,8):x^{\mathsf{T}}\mapsto(k,\lambda_1+\mu_1-r_1+r_2-2p,k-\lambda_1-\lambda_2-\mu_1-\mu_2+r_1+p\\
&\qquad +q,\mu_1,\mu_2,r_1,r_2,\mu_1-p-r_1+r_2,q).
\end{aligned} \tag{9.7}$$

The orbits of the symmetries on the inequalities of the fusion basis are [with the inequalities (9.3) labeled consecutively, column by column, from 1 to 16]:

$$\begin{aligned}
&(3,5):[[5,12]],\\
&(1,6)(2,10)(11,13)(4,8):[[1,7],[2,8],[4,6],[11,15]],
\end{aligned} \tag{9.8}$$

where orbits of length 1 have been omitted.

As indicated in the context of the $\widehat{su}(3)$ analysis, the most severe constraints on the symmetries come from the linear relations. There is indeed a large number of relations for $\widehat{sp}(4)$:[3]

$$\begin{gathered}\hat{E}_0\hat{C}_1\hat{C}_2=\hat{A}_3\hat{D}_3,\quad \hat{E}_0\hat{C}_2\hat{C}_3=\hat{A}_1\hat{D}_1,\quad \hat{E}_0\hat{C}_3\hat{C}_1=\hat{A}_1\hat{A}_3\hat{B}_2,\\ \hat{D}_1\hat{D}_2=\hat{E}_0\hat{B}_3\hat{C}_3^2,\quad \hat{D}_2\hat{D}_3=\hat{E}_0\hat{A}_1^2\hat{B}_2\hat{B}_3,\quad \hat{D}_1\hat{D}_3=\hat{E}_0\hat{B}_2\hat{C}_2^2,\\ \hat{C}_1\hat{D}_1=\hat{A}_3\hat{B}_2\hat{C}_2,\quad \hat{C}_2\hat{D}_2=\hat{A}_1\hat{B}_3\hat{C}_3,\quad \hat{C}_3\hat{D}_3=\hat{A}_1\hat{B}_2\hat{C}_2.\end{gathered}\tag{9.9}$$

It is not difficult to check that the symmetries leave these relations invariant. In fact, $(3,5)=(\hat{A}_2,\hat{B}_1)$ (which means the interchange of $\hat{A}_2$ and $\hat{B}_1$) and these two couplings do not appear in the relations. The other symmetry reads $(\hat{E}_0,\hat{B}_2)$ $(\hat{A}_1,\hat{C}_3)$ $(\hat{D}_1,\hat{D}_3)$ $(\hat{A}_3,\hat{C}_1)$.

With the vector y^{T} defined as $y^{\mathsf{T}}=(k,\lambda_1,\lambda_2,\mu_1,\mu_2,\nu_1,\nu_2,p,q)$, we can rewrite the symmetries of the fusion basis as:

$$\begin{gathered}(3,5):y^{\mathsf{T}}\to(k,-\lambda_2/2+\mu_2/2+\nu_2/2+p/2+q/2,\lambda_2,\mu_1,\\ \lambda_1+\lambda_2/2+\mu_2/2-\nu_2/2-p/2-q/2,-\lambda_1-\lambda_2/2+\mu_2/2+\nu_1+\nu_2/2+p/2+q/2,\\ \lambda_1+\lambda_2/2-\mu_2/2+\nu_2/2-p/2-q/2,p,q),\\ (1,6)(2,10)(11,13)(4,8):y^{\mathsf{T}}\to(k,\nu_1,k-\nu_1-\nu_2,\mu_1,\mu_2,\lambda_1,k-\lambda_1-\lambda_2,-\lambda_1+\nu_1+p,q).\end{gathered}\tag{9.10}$$

The first polytope symmetry does not correspond to a fusion-coefficient symmetry. However, the second one is a combination of an outer automorphism and a permutation of two weights:

$$(1,6)(2,10)(11,13)(4,8)=(a,1,a)P_{13}.\tag{9.11}$$

This is not a new symmetry of fusion coefficients.

X. THE SYMMETRY GROUP OF THE $\widehat{su}(4)_k$ POLYTOPE

The whole set of $\widehat{su}(4)$ fusion elementary couplings can all be generated from two couplings that have no elementary finite relative:

$$\hat{E}_0=[1,0,0,0]\times[1,0,0,0]\supset[1,0,0,0],\quad \hat{F}=[0,1,0,1]\times[0,1,0,1]\supset[0,1,0,1]\tag{10.1}$$

by means of the outer-automorphism group. We can thus characterize a coupling by a pair $(a^n,a^m)_i$ where a^n and a^m act on the first and the second weight, respectively, understanding that the action on the third weight is a^{n+m}. Here a permutes the Dynkin labels of an affine $\widehat{su}(4)$ weight as $a[\lambda_0,\lambda_1,\lambda_2,\lambda_3]=[\lambda_3,\lambda_0,\lambda_1,\lambda_2]$ so that $a^4=1$. The subindex i refers to the elementary coupling $\hat{E}_0$ or $\hat{F}$ from which it is obtained; these are labeled respectively as $i=0$, 1. The remaining elementary coupling are thus

$$\begin{gathered}\hat{A}_1=(a^0,a^3)_0,\quad \hat{A}_2=(a^3,a^1)_0,\quad \hat{A}_3=(a^1,a^0)_0,\\ \hat{B}_1=(a^0,a^2)_0,\quad \hat{B}_2=(a^2a^2)_0,\quad \hat{B}_3=(a^2,a^0)_0,\\ \hat{C}_1=(a^0,a^1)_0,\quad \hat{C}_2=(a^1,a^3)_0,\quad \hat{C}_3=(a^3,a^0)_0,\\ \hat{D}_1'=(a^2,a^1)_0,\quad \hat{D}_2'=(a^1,a^1)_0,\quad \hat{D}_3'=(a^1,a^2)_0,\\ \hat{D}_1=(a^2,a^3)_0,\quad \hat{D}_2=(a^3,a^3)_0,\quad \hat{D}_3=(a^3,a^2)_0,\\ \hat{E}_1=(a^0,a^1)_1,\quad \hat{E}_2=(a^1,a^1)_1,\quad \hat{E}_3=(a^1,a^0)_1.\end{gathered}\tag{10.2}$$

(The explicit reexpression of the elementary couplings in terms of the LR variables can be found in Ref. 3).

The reconstruction of the polytope facets out of these vertices reproduce the inequalities obtained in Ref. 3. These are

$$
\begin{aligned}
k-\lambda_1-\lambda_2-\lambda_3-n_{33}\geqslant 0, \quad & \lambda_3+n_{13}-n_{14}-n_{24}\geqslant 0,\\
k-\lambda_1-\lambda_2-n_{11}-n_{14}+n_{34}\geqslant 0, \quad & \lambda_3+n_{13}+n_{23}-n_{14}-n_{24}-n_{34}\geqslant 0,\\
k-\lambda_1-n_{11}-n_{13}-n_{14}\geqslant 0, \quad & n_{11}-n_{22}\geqslant 0,\\
k-\lambda_1-\lambda_2-\lambda_3-n_{22}+n_{34}\geqslant 0, \quad & n_{11}+n_{12}-n_{22}-n_{23}\geqslant 0,\\
k-\lambda_1-\lambda_2-n_{14}-n_{22}\geqslant 0, \quad & n_{11}+n_{12}+n_{13}-n_{22}-n_{23}-n_{24}\geqslant 0,\\
k-\lambda_1-\lambda_2-\lambda_3-n_{11}+n_{24}+n_{34}\geqslant 0, \quad & n_{22}-n_{33}\geqslant 0,\\
k-\lambda_1-\lambda_2-\lambda_3+n_{12}-n_{22}-n_{23}+n_{34}\geqslant 0, \quad & n_{22}+n_{23}-n_{33}-n_{34}\geqslant 0,\\
k-\lambda_1-\lambda_2-n_{14}+n_{13}-n_{22}-n_{24}\geqslant 0, \quad & n_{12}\geqslant 0,\\
k-\lambda_1-\lambda_2-n_{11}-n_{14}+n_{23}\geqslant 0, \quad & n_{13}\geqslant 0,\\
2k-2\lambda_1-2\lambda_2-\lambda_3-n_{14}-n_{22}-n_{11}+n_{34}\geqslant 0, \quad & n_{14}\geqslant 0,\\
\lambda_1-n_{12}\geqslant 0, \quad & n_{23}\geqslant 0,\\
\lambda_2-n_{13}\geqslant 0, \quad & n_{24}\geqslant 0,\\
\lambda_2+n_{12}-n_{13}-n_{23}\geqslant 0, \quad & n_{33}\geqslant 0,\\
\lambda_3-n_{14}\geqslant 0, \quad & n_{34}\geqslant 0.
\end{aligned}
\tag{10.3}
$$

We then look for the symmetry group of the resulting polytope using the commutant of Q. The matrix V', with the column ordering $(\hat{E}_0,\hat{A}_1,\cdots,\hat{D}'_1,\cdots,\hat{D}_3,\hat{E}_1,\hat{E}_2,\hat{E}_3,\hat{F})$, is

$$V' = k \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & \frac{1}{2} & 0 & 0 & \frac{1}{2} \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \frac{1}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \frac{1}{2} & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2}
\end{pmatrix}. \tag{10.4}$$

The matrix $Q' = 3240\, Q$ reads

$$\begin{pmatrix}
2088 & 0 & 0 & 0 & 168 & 168 & 168 & 600 & 600 & 600 & -360 & -360 & -360 & -360 & -360 & -360 & 384 & 384 & 384 & -144 \\
0 & 3240 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 3240 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 3240 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
168 & 0 & 0 & 0 & 2338 & 43 & 43 & 250 & -425 & -425 & -285 & -15 & 660 & -285 & 660 & -15 & -56 & 484 & 484 & -384 \\
168 & 0 & 0 & 0 & 43 & 2338 & 43 & -425 & 250 & -425 & 660 & -285 & -15 & -15 & -285 & 660 & 484 & -56 & 484 & -384 \\
168 & 0 & 0 & 0 & 43 & 43 & 2338 & -425 & -425 & 250 & -15 & 660 & -285 & 660 & -15 & -285 & 484 & 484 & -56 & -384 \\
600 & 0 & 0 & 0 & 250 & -425 & -425 & 2050 & -245 & -245 & 255 & 525 & -420 & 255 & -420 & 525 & -200 & 340 & 340 & 480 \\
600 & 0 & 0 & 0 & -425 & 250 & -425 & -245 & 2050 & -245 & -420 & 255 & 525 & 525 & 255 & -420 & 340 & -200 & 340 & 480 \\
600 & 0 & 0 & 0 & -425 & -425 & 250 & -245 & -245 & 2050 & 525 & -420 & 255 & -420 & 525 & 255 & 340 & 340 & -200 & 480 \\
-360 & 0 & 0 & 0 & -285 & 660 & -15 & 255 & -420 & 525 & 2250 & 225 & 225 & -45 & -45 & -450 & -420 & 120 & 660 & 360 \\
-360 & 0 & 0 & 0 & -15 & -285 & 660 & 525 & 255 & -420 & 225 & 2250 & 225 & -450 & -45 & -45 & 660 & -420 & 120 & 360 \\
-360 & 0 & 0 & 0 & 660 & -15 & -285 & -420 & 525 & 255 & 225 & 225 & 2250 & -45 & -450 & -45 & 120 & 660 & -420 & 360 \\
-360 & 0 & 0 & 0 & -285 & -15 & 660 & 255 & 525 & -420 & -45 & -450 & -45 & 2250 & 225 & 225 & -420 & 660 & 120 & 360 \\
-360 & 0 & 0 & 0 & 660 & -285 & -15 & -420 & 255 & 525 & -45 & -45 & -450 & 225 & 2250 & 225 & 120 & -420 & 660 & 360 \\
-360 & 0 & 0 & 0 & -15 & 660 & -285 & 525 & -420 & 255 & -450 & -45 & -45 & 225 & 225 & 2250 & 660 & 120 & -420 & 360 \\
384 & 0 & 0 & 0 & -56 & 484 & 484 & -200 & 340 & 340 & -420 & 660 & 120 & -420 & 120 & 660 & 952 & -128 & -128 & 48 \\
384 & 0 & 0 & 0 & 484 & -56 & 484 & 340 & -200 & 340 & 120 & -420 & 660 & 660 & -420 & 120 & -128 & 952 & -128 & 48 \\
384 & 0 & 0 & 0 & 484 & 484 & -56 & 340 & 340 & -200 & 660 & 120 & -420 & 120 & 660 & -420 & -128 & -128 & 952 & 48 \\
-144 & 0 & 0 & 0 & -384 & -384 & -384 & 480 & 480 & 480 & 360 & 360 & 360 & 360 & 360 & 360 & 48 & 48 & 48 & 792
\end{pmatrix}. \tag{10.5}$$

Again, considering the sets of entries in each row of Q we find that the symmetry group fixes the

sets {1}, {2, 3, 4}, {5, 6, 7}, {8, 9, 10}, {11, 12, 13, 14, 15, 16}, {17, 18, 19}, and {20}. We notice immediately that the permutations of 2, 3, and 4 give an S_3 symmetry that commutes with all the other symmetries.

Let us suppose that σ is a symmetry and let τ be the induced permutation of {11, 12, 13, 14, 15, 16}. The submatrix of Q corresponding to rows {11, 12, 13, 14, 15, 16} and columns {5, 6, 7} is

$$U_1=\frac{1}{3240}\begin{pmatrix} -285 & 660 & -15 \\ -15 & -285 & 660 \\ 660 & -15 & -285 \\ -285 & -15 & 660 \\ 660 & -285 & -15 \\ -15 & 660 & -285 \end{pmatrix}, \tag{10.6}$$

while the submatrix for rows {11, 12, 13, 14, 15, 16} and columns {8, 9, 10} is

$$U_2=\frac{1}{3240}\begin{pmatrix} 255 & -420 & 525 \\ 525 & 255 & -420 \\ -420 & 525 & 255 \\ 255 & 525 & -420 \\ -420 & 255 & 525 \\ 525 & -420 & 255 \end{pmatrix}, \tag{10.7}$$

and for rows {11, 12, 13, 14, 15, 16} and columns {17, 18, 19} it is

$$U_3=\frac{1}{3240}\begin{pmatrix} -420 & 120 & 660 \\ 660 & -420 & 120 \\ 120 & 660 & -420 \\ -420 & 660 & 120 \\ 120 & -420 & 660 \\ 660 & 120 & -420 \end{pmatrix}. \tag{10.8}$$

Since each of these matrices have rows with distinct entries, we can deduce the action of σ on each of the sets {5, 6, 7}, {8, 9, 10}, and {17, 18, 19} from τ. Since σ fixes 1 and 20 this determines σ except for its action on 2, 3, and 4, which, as noted previously, is arbitrary.

Thus, to find all symmetries, it suffices to find all possible τ. The submatrix of Q corresponding to rows {11, 12, 13, 14, 15, 16} and columns {11, 12, 13, 14, 15, 16} is

$$K=\frac{1}{3240}\begin{pmatrix} 2550 & 225 & 225 & -45 & -45 & -450 \\ 225 & 2250 & 225 & -450 & -45 & -45 \\ 225 & 225 & 2250 & -45 & -450 & -45 \\ -45 & -450 & -45 & 2250 & 225 & 225 \\ -45 & -45 & -450 & 225 & 2250 & 225 \\ -450 & -45 & -45 & 225 & 225 & 2250 \end{pmatrix}. \tag{10.9}$$

The permutation τ commutes with K and K has an eigenvector $w^{\mathrm{T}}=(-1,-1,-1,1,1,1)$, the corresponding eigenspace being one-dimensional. τ fixes this eigenspace and so either $\tau w=w$ or $\tau w=-w$. The group of all such permutations is $S_3 \wr S_2$ with the two S_3 groups permuting {11, 12,

13} and {14, 15, 16} and the S_2 interchanging them. Thus, every σ gives a τ in $S_3 \wr S_2$, but it is not necessarily true that every element of $S_3 \wr S_2$ extends to a symmetry of V'. In fact, only a subgroup can be extended, as we now show.

By trial and error, we can find two elements

$$\alpha=(11,14)(12,16)(13,15), \quad \beta=(11,12,13)(14,15,16) \tag{10.10}$$

of $S_3 \wr S_2$ which can be extended to the two symmetries

$$(6,7)(9,10)(11,14)(12,16)(13,15)(18,19) \tag{10.11}$$

and

$$(5,6,7)(8,9,10)(11,12,13)(14,15,16)(17,18,19). \tag{10.12}$$

The group generated by α and β turns out to be isomorphic to S_3 (which does not have the standard action).

Thus, we get a group of symmetries isomorphic to $S_3 \times S_3$:

$$\begin{aligned} G[\widehat{su}(4)]=\langle &(2,3),(2,3,4),(6,7)(9,10)(11,14)(12,16)(13,15) \\ &\times(18,19),(5,6,7)(8,9,10)(11,12,13)(14,15,16)(17,18,19)\rangle. \end{aligned} \tag{10.13}$$

There are no other symmetries for the following reason. Suppose that σ is a symmetry and τ is the induced permutation on {11, 12, 13, 14, 15, 16}. Since the group generated by α and β is transitive on {11, 12, 13, 14, 15, 16}, there is some τ' such that $\tau\tau'$ fixes 11. Then, by considering the first row of U_1, $\tau\tau'$ also fixes {5, 6, 7}. Hence $\tau\tau'$ must fix U_1. But this implies $\tau\tau'$ is the identity since U_1 has distinct rows. Thus $\tau^{-1}=\tau'$ and so σ is in the group G.

With $x^{\mathsf{T}}=(k,\lambda_1,\lambda_2,\lambda_3,n_{11},n_{12},n_{13},n_{14},n_{22},n_{23},n_{24},n_{33},n_{34})$, the changes of variables corresponding to the generating symmetries are:

$$\begin{aligned} &(2,3): x^{\mathsf{T}} \mapsto (k,\lambda_1,\lambda_2,\lambda_3-n_{14}+n_{33},n_{11}+n_{14}-n_{33},n_{12},n_{13},n_{33},n_{14}+n_{22}-n_{33},n_{23},n_{24},n_{14},n_{34}), \\ &(2,3,4): x^{\mathsf{T}} \mapsto (k,n_{12}+n_{14},\lambda_2,\lambda_3-n_{14}+n_{33},\lambda_1+n_{11}-n_{12}-n_{33},n_{12},n_{13},n_{33},\lambda_1-n_{12}+n_{22} \\ &\qquad -n_{33},n_{23},n_{24},\lambda_1-n_{12},n_{34}), \\ &(11,14)(12,16)(13,15)(6,7)(18,19)(9,10): \\ &\quad x^{\mathsf{T}} \mapsto (k,\lambda_1+\lambda_3-n_{12}-n_{14},\lambda_2,n_{12}+n_{14},n_{11}+n_{12}+n_{13}-n_{24}-n_{34},\lambda_3-n_{14},\lambda_2 \\ &\qquad -n_{13},n_{14},n_{22}+n_{23}-n_{34},\lambda_3+n_{13}-n_{14}-n_{24},\lambda_2+n_{12} \\ &\qquad -n_{13}-n_{23},n_{33},\lambda_3+n_{13}+n_{23}-n_{14}-n_{24}-n_{34}), \\ &(5,6,7)(8,9,10)(11,12,13)(14,15,16)(17,18,19): \\ &\quad x^{\mathsf{T}} \mapsto (k,\lambda_1+n_{11}+n_{13}-n_{22}-n_{23}-n_{24},n_{22}+n_{23}+n_{24}-n_{33} \\ &\qquad -n_{34},n_{14}+n_{34},\lambda_2+\lambda_3-n_{13}-n_{14}+n_{33},n_{11}+n_{12}+n_{13}-n_{22}-n_{23}-n_{24},n_{22}+n_{23} \\ &\qquad -n_{33}-n_{34},n_{14},\lambda_2-n_{13}+n_{33},n_{11}+n_{12}-n_{22}-n_{23},n_{22}-n_{33},n_{33},n_{11}-n_{22}). \end{aligned} \tag{10.14}$$

Labeling the $\widehat{su}(4)$ fusion inequalities of (10.3) from 1 to 28 (row by row), the orbits on the fusion basis are:

$$
\begin{aligned}
&(2,3):[[24,27]],\\
&(2,3,4):[[11,27,24]],\\
&(11,14)(12,16)(13,15)(6,7)(18,19)(9,10):\\
&\quad [[2,9],[3,6],[4,8],[5,7],[12,23],[13,26],[14,22],[15,25],[16,28],[17,19],[20,21]],\\
&(5,6,7)(8,9,10)(11,12,13)(14,15,16)(17,18,19):\\
&\quad [[1,6,3],[2,5,4],[7,9,8],[12,20,26],[13,21,23],[14,17,28],[15,18,25],[16,19,22]],
\end{aligned}
\tag{10.15}
$$

where the orbits of length 1 have been omitted.

As already indicated, severe constraints on the symmetries come from the linear relations. And in fact there are many such relations in the $\widehat{su}(4)$ case. The full list is:[3]

$$
\begin{aligned}
&\hat{E}_0\hat{D}_j'\hat{D}_k=\hat{C}_i\hat{E}_i, \quad \hat{E}_0\hat{D}_j\hat{D}_k'=\hat{B}_i\hat{C}_j\hat{C}_k, \quad \hat{E}_i\hat{E}_j=\hat{E}_0\hat{B}_k\hat{D}_k\hat{D}_k',\\
&\hat{D}_i\hat{E}_i=\hat{C}_j\hat{B}_k\hat{D}_k, \quad \hat{D}_i'\hat{E}_i=\hat{B}_j\hat{D}_j'\hat{C}_k, \quad \hat{E}_0\hat{F}=\hat{C}_1\hat{C}_2\hat{C}_3
\end{aligned}
\tag{10.16}
$$

with *i, j, k* a cyclic permutation of 1, 2, 3. The large number of relations, and more precisely, the fact that they mix elementary couplings with different threshold levels, is responsible for the absence of symmetries involving the level. All the above-found symmetries leave this set of relations invariant. For instance, the S_3 group generated by (2, 3) and (2, 3, 4) is the permutation group of the three $\hat{A}_i$'s, which do not appear in the relations.

With the vector y^{T} defined as $y^{\mathsf{T}}=(k,\lambda_1,\lambda_2,\lambda_3,\mu_1,\mu_2,\mu_3,\nu_1,\nu_2,\nu_3,n_{12},n_{14},n_{33})$, we can rewrite the symmetries of the fusion basis as:

$$
\begin{aligned}
&(2,3):y^{\mathsf{T}}\to(k,\lambda_1,\lambda_2,\lambda_3-n_{14}+n_{33},\mu_1-n_{14}+n_{33},\mu_2,\mu_3+n_{14}-n_{33},\nu_1+n_{14}\\
&\qquad -n_{33},\nu_2,\nu_3,n_{12},n_{14}n_{33}),\\
&(2,3,4):y^{\mathsf{T}}\to(k,n_{12}+n_{33},\lambda_2,\lambda_1+\lambda_3-n_{12}-n_{14},\lambda_1+\mu_1-n_{12}-n_{14},\mu_2,\mu_3+n_{14}-n_{33},\nu_1+n_{14}\\
&\qquad -n_{33},\nu_2,-\lambda_1+\nu_3+n_{12}+n_{33},n_{12},\lambda_1-n_{12},n_{14}),\\
&\qquad (11,14)(12,16)(13,15)(6,7)(18,19)(9,10):\\
&\qquad\quad y^{\mathsf{T}}\to(k,\lambda_1+\lambda_3-n_{12}-n_{14},\lambda_2,n_{12}+n_{14},\nu_3-\lambda_1+n_{12}\\
&\qquad\qquad +n_{14},\nu_2,\nu_1,\mu_3,\mu_2,\lambda_1+\mu_1-n_{12}-n_{14},\lambda_3-n_{14},n_{14},n_{33}),\\
&(5,6,7)(8,9,10)(11,12,13)(14,15,16)(17,18,19):\\
&\quad y^{\mathsf{T}}\to(k,\lambda_1+\nu_1-n_{12}-n_{33},\nu_2,-\lambda_1+\nu_3+n_{12}+n_{14},n_{12}+n_{14},\lambda_2,\lambda_3-n_{14}+n_{33},\mu_1-n_{14}\\
&\qquad +n_{33},\mu_2,\lambda_1+\mu_3-n_{12}-n_{33},\nu_1-n_{33},n_{14},n_{33}).
\end{aligned}
\tag{10.17}
$$

These symmetries do not correspond to a fusion-coefficient symmetries.

XI. CONCLUSION

In this paper we presented the concept of fusion bases, first introduced in Ref. 3, from a novel point of view as the set of facets of a polytope. This reformulation gives access to the powerful computer programs that have been developed for generating facets out of the vertices. Moreover, by reformulating the problem in a geometrical way, we were led to the study of the affine symmetry group of the fusion polytope, introduced here for the first time. We developed simple

tools for studying this group analytically for the lowest rank affine Lie algebras. We also defined the vertex symmetry group of a polytope and noted that for fusion polytopes the affine and vertex symmetry groups appear to be the same—a property which does not hold for general polytopes.

The order of the vertex symmetry group of the fusion polytope of the lowest rank affine Lie algebras was found to be 24 for $\widehat{su}(2)$, 432 for $\widehat{su}(3)$, 36 for $\widehat{su}(4)$, and 4 for $\widehat{sp}(4)$. Comparing $\widehat{su}(2)$ and $\widehat{su}(3)$, it is natural to see an increase of the order of the group with the rank since the number of vertices increases rapidly. However, it might be surprising to observe this drastic reduction in the order when passing from $\widehat{su}(3)$ to $\widehat{su}(4)$. The reason is that the number of linear relations, which have to be preserved by the symmetry transformations, also increases rapidly with the rank.

We should stress that a fusion polytope is rather special type of polytope in that its vertices are the elementary solutions of the facets, which is far from being a generic property of polytopes.

It is an interesting open problem to try to generate the full set of fusion inequalities, or equivalently, to give a generic description of the fusion polytope, from a general Lie algebraic point of view.

On the other hand, we could ask whether the polytope we have obtained, whose description relies heavily on the LR variables, is the ''genuine'' fusion polytope or whether it is just one among a variety of polytopes. In that vein, we note that Rasmussen and Walton[16] have recently also developed a polytope interpretation of $\widehat{su}(3)$ and $\widehat{su}(4)$ fusion coefficients using a different approach from ours. Prompted by the referee we have investigated the relationship with the polytopes found in this paper. We find, perhaps surprisingly, after removing redundant variables and making a suitable change of coordinates that the two sets of polytopes coincide. This suggests that the polytopes might be in some sense unique.

Finally, concerning the symmetry analysis, we stress that we have restricted our analysis to a special class of symmetries, namely those which exist at all levels. Whether symmetries at particular levels or even symmetries that relate fusion polytopes at different levels can be unraveled by our method remains to be studied.

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Boundary-layer theory, strong-coupling series, and large-order behavior

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The introduction of a lattice converts a singular boundary-layer problem in the continuum into a regular perturbation problem. However, the continuum limit of the discrete problem is extremely nontrivial and is not completely understood. This article examines two singular boundary-layer problems taken from mathematical physics, the instanton problem and the Blasius equation, and in each case examines two strategies, Padé resummation and variational perturbation theory, to recover the solution to the continuum problem from the solution to the associated discrete problem. Both resummation procedures produce good and interesting results for the two cases, but the results still deviate from the exact solutions. To understand the discrepancy a comprehensive large-order behavior analysis of the strong-coupling lattice expansions for each of the two problems is done. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1490408]

I. INTRODUCTION

In this article we report some major advances in understanding (albeit not a complete solution to) a difficult general class of problems in mathematical physics. We consider here the conversion of a continuum problem into a discrete problem by the insertion of a lattice spacing parameter a, the solution of the continuum problem on the lattice, and the subsequent extremely subtle continuum limit $a\to 0$.

Almost every continuum physics problem is singular as a function of the parameters in the problem. As a result, only rarely does the perturbation series take the form of a Taylor series having a nonzero radius of convergence. As an elementary example, consider the algebraic polynomial equation

$$\epsilon x^3 + x - 1 = 0. \tag{1}$$

This problem is singular in the limit $\epsilon\to 0$. In this limit, the degree of the polynomial changes from three to one and thus two of the roots abruptly disappear. As a consequence, a perturbative solution to this problem [expressing the roots $x(\epsilon)$ as series in powers of ϵ] yields expressions that are more complicated than Taylor series.

A more elaborate example of a singular problem is the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2M}\nabla^2\Psi(\mathbf{x}) + [V(\mathbf{x}) - E]\Psi(\mathbf{x}) = 0. \tag{2}$$

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In the classical limit $\hbar \to 0$ this differential equation abruptly becomes an *algebraic* equation, and thus the general solution no longer contains any arbitrary constants or functions and, as a result, it can no longer satisfy the initial conditions. We know that for small $\hbar$ the solution is not Taylor-like but rather is a singular exponential in WKB form:

$$\Psi(\mathbf{x}) \sim e^{S(\mathbf{x})/\hbar} \quad (\hbar \to 0). \tag{3}$$

In the study of quantum field theory, it is well known that infinities appear in the perturbative expansion in powers of the coupling constant. There are two kinds of infinities. The first kind, which is due to the pointlike nature of the interaction, requires the use of renormalization. The second kind, which is due to singularities in the complex-coupling-constant plane, forces the perturbation series to have a zero radius of convergence.

A quantum field theory can be regulated by introducing a lattice spacing. The resulting discrete theory is completely finite and can be studied numerically by using various kinds of numerical methods such as Monte Carlo integration. However, the underlying singular nature of the continuum quantum field theory resurfaces in the continuum limit $a \to 0$. The introduction of a lattice spacing and the singular nature of the continuum limit was investigated in a series of papers by Bender *et al.*[1–9]

A quantum field theory is just one instance in which discretization regulates and eliminates the singular nature of the problem. It is also known that introducing a lattice spacing converts a boundary-layer problem, which is a singular perturbation problem, into a regular perturbation problem.[10–12] A *boundary-layer problem* is a differential-equation-boundary-value problem in which the highest derivative of the differential equation is multiplied by a small parameter ϵ. Consider as an example

$$\epsilon y''(x) + a(x)y'(x) + b(x)y(x) = c(x), \tag{4}$$

where the boundary conditions on the function $y(x)$ typically have a form such as

$$y(0) = A, \quad y(1) = B. \tag{5}$$

This boundary-value problem is singular because in the limit $\epsilon \to 0$ one of the solutions abruptly disappears and the limiting solution is not able to satisfy the two boundary conditions in (5). The usual way to solve the boundary-value problem (4) and (5) is to decompose the interval $0 \leqslant x \leqslant 1$ into two regions, an *outer region*, in which the solution varies slowly as a function of x, and an *inner region* or *boundary-layer region*, in which the solution varies rapidly as a function of x. The boundary-layer region is a narrow region whose thickness is typically of order ϵ or some power of ϵ.[13]

An important example of a boundary-layer problem is the instanton equation

$$\epsilon^2 f''(x) + f(x) - f^3(x) = 0, \tag{6}$$

with the associated boundary conditions

$$f(0) = 0, \quad f(\infty) = 1. \tag{7}$$

The exact solution to this instanton problem is

$$f(x) = \tanh \frac{x}{\epsilon\sqrt{2}}. \tag{8}$$

Note that the solution $f(x)$ varies rapidly at the origin $x = 0$ over a region of thickness ϵ; this is the boundary-layer region. The solution varies slowly (it is approximately 1) outside of this region. The outer region consists of those x not near the origin.

A novel way to solve the instanton problem is to discretize it by introducing a lattice. On the lattice, the differential equation becomes a difference equation that can easily be solved perturbatively. In the continuum limit, as the lattice spacing vanishes, we then obtain a strong-coupling expansion that must be evaluated by means of a Padé or a variational perturbation theory method. To illustrate the approach our objective will be to calculate the slope of the instanton at $x=0$, which from (8) has the value

$$f'(0)=\frac{1}{\epsilon\sqrt{2}}. \tag{9}$$

We introduce a lattice with lattice spacing a so that the real axis is discretized in steps of width a. The spatial coordinate reads $x_n=na$, where the function $f(x)$ assumes the value $f_n=f(x_n)$. On the lattice the second spatial derivative in (6) becomes

$$f''(x)\to\frac{f_{n+1}-2f_n+f_{n-1}}{a^2}. \tag{10}$$

Thus, from the instanton equation (6) we obtain the difference equation

$$\frac{\epsilon^2}{a^2}(f_{n+1}-2f_n+f_{n-1})+f_n-f_n^3=0, \tag{11}$$

where the boundary values follow from (7):

$$f_0=0, \quad f_\infty=1. \tag{12}$$

The natural expansion parameter now is ϵ^2/a^2, to which we assign the name δ:

$$\delta\equiv\frac{\epsilon^2}{a^2}. \tag{13}$$

The singular perturbation problem in the continuum [whose solution $f(x)$ in (8) does not possess a Taylor expansion in powers of ϵ] has become a *regular* perturbation problem. That is, we can now expand the solution f_n to the difference equation (11) as a *Taylor series* in powers of δ:

$$f_n=a_{n,0}+a_{n,1}\delta+a_{n,2}\delta^2+\cdots. \tag{14}$$

We impose the boundary values (12) by requiring that

$$a_{0,0}\equiv 0 \quad \text{and} \quad a_{n,0}\equiv 1 \quad (n\geqslant 1). \tag{15}$$

Inserting the *ansatz* (14) into the difference equation (11), we get the recursion relation[10]

$$a_{n,j}=\frac{1}{2}a_{n+1,j-1}+a_{n,j-1}+\frac{1}{2}a_{n-1,j-1}-\sum_{k=1}^{j-1}a_{n,k}a_{n,j-k}-\frac{1}{2}\sum_{k=1}^{j-1}\sum_{l=1}^{j-k}a_{n,k}a_{n,l}a_{n,j-k-l}. \tag{16}$$

For the first derivative at the origin $x=0$ this leads to the series

$$f'(0)=\lim_{a\to 0}\frac{f_1-f_0}{a}=\lim_{a\to 0}\frac{f_1}{a}=\lim_{a\to 0}\frac{1}{a}\sum_{j=0}^{\infty}a_{1,j}\delta^j=\lim_{a\to 0}\frac{1}{a}\left(1-\frac{\delta}{2}+\frac{\delta^2}{8}+\frac{11\delta^4}{128}+\cdots\right). \tag{17}$$

We have calculated the coefficients $a_{1,j}$ with the help of Maple V R7 up to order $j=200$. The first 20 numbers are given in Table I. A complete list of these coefficients can be found on the

TABLE I. The first 20 weak-coupling coefficients $a_{1,j}$ for the instanton problem (15) and (16).

j	$a_{1,j}$	j	$a_{1,j}$
1	$-\frac{1}{8}$	11	$-\frac{2887747}{262144}$
2	$\frac{1}{8}$	12	$\frac{99392471}{4194304}$
3	0	13	$-\frac{215798295}{4194304}$
4	$\frac{11}{128}$	14	$\frac{3781670831}{33554432}$
5	$-\frac{23}{128}$	15	$-\frac{8349041385}{33554432}$
6	$\frac{295}{1024}$	16	$\frac{1188129285795}{2147483648}$
7	$-\frac{589}{1024}$	17	$-\frac{2659104132291}{2147483648}$
8	$\frac{39203}{32768}$	18	$\frac{47890245452569}{17179869184}$
9	$-\frac{80723}{32786}$	19	$-\frac{108383753179167}{17179869184}$
10	$\frac{1354949}{262144}$	20	$\frac{39433620359113981}{274877906944}$

webpage of the author FW.[14] Note that the expansion parameter δ in (17) is not small but rather tends to infinity in the limit as the lattice spacing a approaches zero. Using the parameter δ defined in (13) we rewrite the series (17) as

$$f'(0)=\frac{1}{\epsilon}\lim_{\delta\to\infty}\sqrt{\delta}\left(1-\frac{\delta}{2}+\frac{\delta^2}{8}+\frac{11\delta^4}{128}+\cdots\right). \tag{18}$$

Taking into account the exact result (9), we obtain the identity

$$\frac{1}{\sqrt{2}}=\lim_{\delta\to\infty}\sqrt{\delta}\left(1-\frac{\delta}{2}+\frac{\delta^2}{8}+\frac{11\delta^4}{128}+\cdots\right). \tag{19}$$

The purpose of this article is to examine equations like (19). This equation shows that the singular nature of the instanton problem has resurfaced in the continuum limit $\delta\to\infty$ of the lattice expansion. The expression on the right side of (19) should have the value $1/\sqrt{2}=0.707\,106\,781\,2\ldots$, but it is not at all obvious why this is so, and the objective of this article is to analyze this difficult and subtle limit.

This article is organized as follows. In Sec. II we use Padé techniques to perform the limit in (19). We will see that while the results are not bad (the accuracy is about 1%), better methods are needed. We perform the Padé analysis to much higher order than has ever been done before and we discover a new qualitative behavior that has not yet been observed. In Sec. III we try the use of the variational perturbation theory techniques introduced by Kleinert to perform the sum in (19). These techniques increase the accuracy by a factor of about 10, but they still do not give the exact result. While variational perturbation theory works very well in summing the strong-coupling series for the ground-state energy of the anharmonic oscillator,[15] and for the critical exponents of second-order phase transitions,[16] we show that the series in (19) is at the very edge of validity for Kleinert's methods. We then examine the large-order behavior of the terms of the

sum in (19) in Sec. IV. We show definitively that the Taylor expansion has a nonzero radius of convergence and, thus, on the lattice, the instanton problem is a regular perturbation problem.

In Sec. V we turn to a more difficult singular perturbation problem, namely, the Blasius equation of fluid dynamics. We use the same approach as for the instanton equation. In Secs. VI–VIII we study the summation of the lattice perturbation expansion using Padé and variational methods and we examine the large-order behavior of the lattice perturbation series. We find that Padé methods give good but not excellent results and that variational perturbation theory is better than Padé. Again, the series we need to evaluate in the continuum limit lies at the very edge of validity for Kleinert's methods. We also find that, unlike the lattice perturbation expansion coefficients for the instanton problem, the sign pattern of the Blasius weak-coupling series does not alternate. Rather, it is governed by a cosine function with a frequency different from π.

II. PADÉ RESUMMATION FOR THE INSTANTON EQUATION

In this section we examine what happens if we attempt to evaluate the right side of (19) by using Padé techniques. Padé resummation has already been applied to the instanton problem up to 50th order.[10] However, we have been able to perform the procedures to much higher orders. We have discovered that remarkable and unsuspected new phenomena occur just a few orders beyond what has been computed.

The procedure is as follows. Consider the formal Frobenius series

$$S(\delta)=\delta^M\sum_{n=0}^{\infty} a_n\delta^n, \tag{20}$$

where M is a non-negative number. Raising this series to the power $1/M$, inverting the right hand side and reexpanding, we obtain

$$S^{1/M}(\delta)=\frac{\delta}{\sum_{n=0}^{\infty} b_n\delta^n}, \tag{21}$$

with new expansion coefficients b_n. Assuming we know the first $N+1$ terms of the original power series in (20), we raise Eq. (21) to the power N. We then truncate the summation at $n=N$, finally getting

$$S^{N/M}(\delta)=\frac{\delta^N}{\sum_{n=0}^{N} c_n^{(N)}\delta^n}, \tag{22}$$

where we have reexpanded and obtained new expansion coefficients c_n. In the limit $\delta\to\infty$, only the Nth term in the denominator survives and we obtain the approximant

$$(S_N)^{N/M}\equiv\lim_{\delta\to\infty} S^{N/M}(\delta)=\lim_{\delta\to\infty}\frac{\delta^N}{\sum_{n=0}^{N} c_n^{(N)}\delta^n}=\frac{1}{c_N^{(N)}}. \tag{23}$$

The approximant $S_N=(c_N^{(N)})^{-M/N}$ is the zeroth-order survivor of the limiting process. Also, taking into account the first-order correction we observe that, as in the case of variational perturbation theory (see Sec. III), there is an approach to scaling. In the limit $\delta\to\infty$ the Frobenius series $S(\delta)$ in Eq. (20) converges to a constant C. Additionally, the approach to scaling, following from the Padé resummation (23), reveals how fast it converges:

$$S(\delta)\sim C+C'\delta^{-1}\quad(\delta\to\infty). \tag{24}$$

We now apply this procedure to the boundary-layer problem (11). [Recall that the weak-coupling coefficients for the first 20 coefficients $a_{1,j}$ obtained from (16) are shown in Table I and that more can be found in Ref. 14.] Resumming the series (14) for $n=1$,

TABLE II. The first 20 Padé approximants for the solution to the instanton problem (19).

N	S_N	N	S_N
1	1	11	0.709 998 411
2	0.840 896 415	12	0.708 235 422
3	0.781 934 407	13	0.706 789 935
4	0.757 237 797	14	0.705 659 505
5	0.740 759 114	15	0.704 734 605
6	0.731 210 449	16	0.704 006 945
7	0.723 927 185	17	0.703 419 862
8	0.719 045 188	18	0.702 964 717
9	0.715 146 335	19	0.702 610 220
10	0.712 308 458	20	0.702 349 024

$$f_1 = \sum_{j=0}^{N} a_{1,j}\delta^j, \tag{25}$$

according to the Padé procedure (23) with $M=\frac{1}{2}$ as follows from (19) and evaluating the approximants $S_N=(c_N^{(N)})^{-M/N}$, we get the numbers listed in Table II.

Compared with the numerical solution $1/\sqrt{2}\approx 0.717\,106\,781\,2$, this strong-coupling expansion seems to converge quite well. However, when we go to higher orders, we find that the numbers drop below the exact solution and assume a minimum at $N=24$, where the approximant has the value $S_{24}\approx 0.701\,983\,19$. The approximants then rise again, cross the exact solution at $N=41$ and become complex at $N=52$. The appearance of complex numbers is a consequence of taking the Nth root in Eq. (23) when the coefficients $c_N^{(N)}$ become negative. This phenomenon has not been observed before in the course of using this Padé procedure. The imaginary part then becomes smaller and smaller as N rises. Abruptly, at $N=68$, the approximants become real again. As one can see from the spikes in Fig. 1 this pattern is repeated for higher N. Note that the figure only shows the real part of the Padé approximant S_N.

Apparently, the sequence of approximants S_N does not converge. The singular nature of the instanton equation has the effect of making the Padé approximants behave like the partial sums of a divergent (asymptotic) series; at first the partial sums appear to converge to a limit, and then they veer off. In the case of the Padé's shown in Fig. 1 the approximants approach to within 1% of the

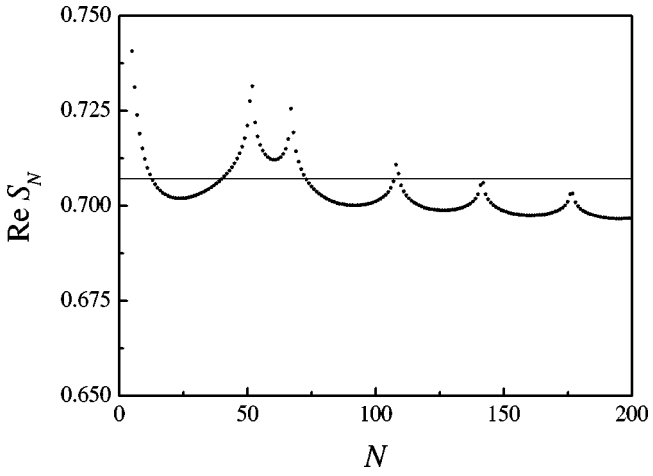

FIG. 1. The real part of the Padé approximants S_N up to 200th order. Note that the approximants do not converge to the exact solution, which is represented by the horizontal solid line. The phases where the approximants become complex are marked by spikes.

correct limit before veering off. It appears that another more powerful resummation technique is needed to treat the expression in (19). In the next section we apply a technique due to Kleinert.

III. VARIATIONAL PERTURBATION THEORY FOR THE INSTANTON EQUATION

Kleinert has developed a technique in the context of the ground-state energy of the anharmonic oscillator[15] and of critical exponents of second-order phase transitions[16] for summing divergent perturbation series. This technique, known as Kleinert's square-root trick, is described below.

Consider a weak-coupling series

$$f_N(\delta)=\sum_{n=0}^{N} f_n \delta^n, \tag{26}$$

which is truncated at order N. Rewrite this weak-coupling expansion by introducing an auxiliary scaling parameter κ:[15,16]

$$f_N(\delta)=\kappa^p \sum_{n=0}^{N} f_n \left(\frac{\delta}{\kappa^q}\right)^n \Bigg|_{\kappa=1}, \tag{27}$$

which is set to $\kappa=1$ later. The square-root trick now reads

$$\kappa \to \sqrt{K^2+\kappa^2-K^2}=K\sqrt{1+\delta r}, \tag{28}$$

where K is a ''dummy'' scaling parameter and

$$r=\frac{1}{\delta}\left(\frac{\kappa^2}{K^2}-1\right). \tag{29}$$

In the case of the anharmonic oscillator, K is the frequency Ω of a trial harmonic oscillator.[15]

Substituting (28) into the truncated weak-coupling series (27), we obtain

$$f_N(\delta)=\sum_{n=0}^{N} f_n K^{p-nq}(1+\delta r)^{(p-nq)/2}\delta^n. \tag{30}$$

The factor $(1+\delta r)^\alpha$ with $\alpha \equiv (p-nq)/2$ is expanded by means of generalized binomials:

$$(1+\delta r)^\alpha=\sum_{k=0}^{N-n}\binom{\alpha}{k}(\delta r)^k \mathcal{O}(\delta^{N-n})=\sum_{k=0}^{N-n}\binom{\alpha}{k}\left(\frac{1}{K^2}-1\right)^k \mathcal{O}(\delta^{N-n}), \tag{31}$$

where we have used (29) and finally have set $\kappa \equiv 1$. The binomial is defined as

$$\binom{\alpha}{k}\equiv \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)}. \tag{32}$$

Thus the function $f_N(\delta)$ becomes K dependent and reduces to

$$f_N(\delta,K)=\sum_{n=0}^{N}\left[\sum_{k=0}^{N-n}\binom{\frac{1}{2}(p-nq)}{k}\left(\frac{1}{K^2}-1\right)^k K^{p-nq}\right] f_n \delta^n. \tag{33}$$

To first order this expression reduces to

$$f_1(\delta,K)=\left(1-\frac{p}{2}\right)f_0K^p+\frac{p}{2}f_0K^{p-2}+f_1\delta K^{p-q}. \tag{34}$$

Applying the principle of least sensitivity[17] leaves us with

$$\frac{\partial f_1(\delta,K)}{\partial K}\sim p\left(1-\frac{p}{2}\right)f_0+\frac{p(p-2)}{2}f_0K^{-2}+(p-q)f_1\delta K^{-q}\equiv 0. \tag{35}$$

Next, making the strong-coupling ansatz

$$K^{(1)}(\delta)=\delta^{1/q}(k_0^{(1)}+k_1^{(1)}\delta^{-2/q}+\cdots), \tag{36}$$

we obtain the following equation from (35):

$$p\left(1-\frac{p}{2}\right)f_0+\frac{p(p-2)}{2}f_0(k_0^{(1)}\delta^{1/q})^{-2}+(p-q)f_1\delta(\delta^{1/q}k_0^{(1)})^{-q}=0. \tag{37}$$

The second term is a subleading contribution in the limit as the coupling δ goes to infinity which we can neglect. Solving for $k_0^{(1)}$ we then get

$$k_0^{(1)}=\left(\frac{2f_1}{f_0}\frac{p-q}{p(p-2)}\right)^{1/q}. \tag{38}$$

Assuming that the ansatz (36) for the variational parameter $K(\delta)$ also holds for higher orders we obtain from the function $f_N(\delta,K)$ in (33)

$$f_N(\delta)=\delta^{p/q}[b_0^{(N)}(k_0^{(N)})+b_1^{(N)}(k_0^{(N)},k_1^{(N)})\delta^{-2/q}+\cdots], \tag{39}$$

where the leading strong-coupling coefficient $b_0^{(N)}(k_0^{(N)})$ is given by

$$b_0^{(N)}(k_0^{(N)})=\sum_{n=0}^{N}\sum_{k=0}^{N-n}\binom{\frac{1}{2}(p-nq)}{k}(-1)^k f_n(k_0^{(N)})^{p-nq}. \tag{40}$$

The inner sum can be further simplified, using

$$\sum_{k=0}^{m}(-1)^k\binom{\alpha}{k}=(-1)^m\binom{\alpha-1}{m}. \tag{41}$$

Thus the strong-coupling coefficient (40) reduces to

$$b_0^{(N)}(k_0^{(N)})=\sum_{n=0}^{N}(-1)^{N-n}\binom{\frac{1}{2}(p-nq)-1}{N-n}f_n(k_0^{(N)})^{p-nq}. \tag{42}$$

So, looking at Eq. (39) we see that the fraction p/q tells us the leading power behavior in δ and $2/q$ indicates the approach to scaling:

$$\sum_{j=0}^{\infty}f_j\delta^j\sim\delta^{p/q}(b_0+b_1\delta^{-2/q}+\cdots)\quad(\delta\to\infty). \tag{43}$$

For the instanton equation we can determine the numbers p and q by re-obtaining the differential equation (6) from the difference equation (11). The positive real axis is discretized in steps of width a, so that we let $x_n \equiv na$. The power series expansion for the discrete function $f_n = f(x_n)$ has the form

$$f_{n\pm1} = f(x_n) \pm f'(x_n)a + \tfrac{1}{2}f''(x_n)a^2 \pm \tfrac{1}{6}f'''(x_n)a^3 + \tfrac{1}{24}f''''(x_n)a^4 \pm \cdots . \tag{44}$$

Thus, the numerator of the second derivative (10) becomes

$$f_{n+1} - 2\,f_n + f_{n-1} = f_n'' a^2 + \tfrac{1}{12}f_n''''a^4 + \cdots , \tag{45}$$

so the zeroth-, first-, and third-order contributions cancel. Translating the lattice result for f_n back to the continuous function $f(x_n) = f_n$, the difference equation (11) reads

$$\epsilon^2[f''(x) + \tfrac{1}{12}f''''(x)a^2 + \cdots] + f(x) - f^3(x) = 0. \tag{46}$$

Writing out the power series

$$f(x) = f_0(x) + a^2 f_1(x) + a^4 f_2(x) + \cdots , \tag{47}$$

and comparing even powers of a, we get from Eq. (46) for a^0

$$\epsilon^2 f_0''(x) + f_0(x) - f_0^3(x) = 0, \tag{48}$$

which is just the original instanton equation (6). For a^2 we have

$$\epsilon^2 f_1''(x) + f_1(x)(1 - 3f_0^2(x)) = -\tfrac{1}{12}\epsilon^2 f_0''''(x). \tag{49}$$

The boundary values read

$$f_0(0) = 0, \quad f_0(\infty) = 1, \tag{50}$$

and

$$f_1(0) = f_1(\infty) = 0, \tag{51}$$

respectively. The solution to Eq. (48) with the boundary values (50) is of course

$$f_0(x) = \tanh\frac{x}{\epsilon\sqrt{2}}. \tag{52}$$

So, finally from (47) we get for the derivative at the origin $x = 0$:

$$f'(0) = f_0'(0) + \frac{\epsilon^2}{\delta}f_1'(0) + \cdots = \frac{1}{\epsilon\sqrt{2}} + \frac{\epsilon^2}{\delta}f_1'(0) + \cdots . \tag{53}$$

Comparing Eq. (53) with (18), we resum the weak-coupling series in (18) as

$$1 - \frac{\delta}{2} + \frac{\delta^2}{8} + \cdots = \delta^{-1/2}\left[\frac{1}{\sqrt{2}} + \epsilon^3 f_1'(0)\,\delta^{-1} + \cdots\right]. \tag{54}$$

Also, comparing with (43), we conclude that the leading power and the approach to scaling are given by

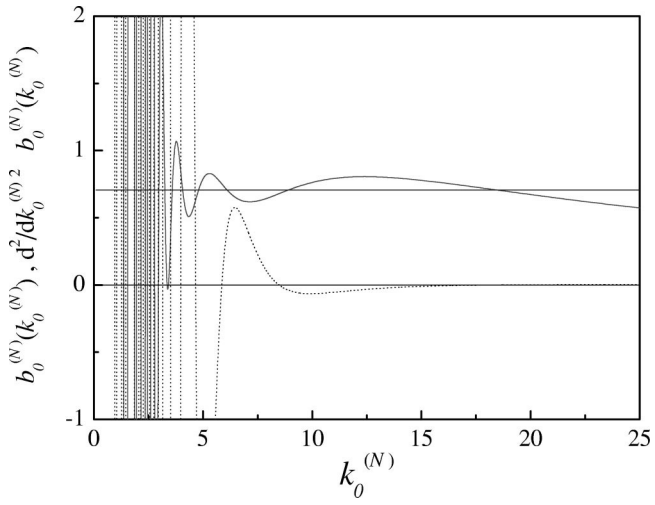

FIG. 2. The function $b_0^{(N)}(k_0^{(N)})$ from (42) for $N=200$ (solid line) and its second derivative with respect to $k_0^{(N)}$ (dotted line). The upper horizontal line equals $1/\sqrt{2}$, the correct limiting value of the instanton problem. All extrema of $b_0^{(N)}$ are far from this value. Only the inflection point on the right-hand side comes close. The value for $k_0^{(N)}$, for which the second derivative vanishes, is $k_0^{(N)}=18.425\,10$. Substituting that number into the function $b_0^{(N)}(k_0^{(N)})$, we obtain in the 200th order $b_0^{(200)}=0.707\,417$. The corresponding Richardson extrapolations can be found in Table IV.

$$\frac{p}{q}=-\frac{1}{2}, \quad \frac{2}{q}=1, \tag{55}$$

respectively. So we identify $p=-1$ and $q=2$.

We now evaluate the leading strong-coupling coefficient b_0 from (43) according to (42) with $p=-1$ and $q=2$. To that end we substitute our 200 weak-coupling coefficients from Ref. 14 into the formula using a computer algebra program. We are now confronted with the following problem: The principle of least sensitivity cannot be unambiguously applied. Optimizing with respect to extrema, inflection points, or higher derivatives does yield converging results for the strong-coupling limit. However, all these strong-coupling series converge to the wrong values.

There is one particularly unpleasant case: The second derivative with respect to $k_0^{(N)}$ for the largest $k_0^{(N)}$ where this derivative exists (see Fig. 2) gives a convergent strong-coupling series. The numbers come extremely close to $1/\sqrt{2}$ as one can see from the 20 numbers in Table III. The 200th leading strong-coupling coefficient is $b_0^{(200)}=0.707\,417\ldots$. However, a Richardson extrapolation[13] based on the first 200 orders then unfortunately shows that variational perturbation theory produces a value slightly smaller than $1/\sqrt{2}$. The first six orders of Richardson extrapola-

TABLE III. The last 20 variational strong-coupling coefficients $b_0^{(N)}$ from Eq. (42).

N	$b_0^{(N)}$	N	$b_0^{(N)}$
180	0.707 530 492	190	0.707 471 024
181	0.707 524 250	191	0.707 465 419
182	0.707 518 076	192	0.707 459 872
183	0.707 511 970	193	0.707 454 384
184	0.707 505 930	194	0.707 448 952
185	0.707 499 955	195	0.707 443 575
186	0.707 494 044	196	0.707 438 253
187	0.707 488 197	197	0.707 432 986
188	0.707 482 412	198	0.707 427 771
189	0.707 476 687	199	0.707 422 609

TABLE IV. Six orders of Richardson extrapolations for the strong-coupling coefficient $b_0^{(N)}(k_0^{(N)})$ up to $N=200$ for the instanton problem. The last value is only 0.099% away from the correct limiting value $1/\sqrt{2}=0.707\,106\,781\,2\ldots$.

Order	Value for $b_0^{(N)}$	Convergence
1	0.706 400 49	decreasing
2	0.706 399 832 00	increasing
3	0.706 399 832 082	increasing
4	0.706 399 832 085 865 8	increasing
5	0.706 399 832 085 884 411	increasing
6	0.706 399 832 085 884 464 98	increasing

tions are presented in Table IV. Hence, the strong-coupling series $b_0^{(N)}$ does converge, but it converges to the wrong number, only one part per 1000 away from the true value:

$$f_1^{(\mathrm{VPT})} \approx \lim_{\delta\to\infty} \sum_{n=0}^{200} a_{1,n}\delta^n = b_0^{(\infty)} = 0.706\,399\,832\,085\,88\,45 \pm 0.000\,000\,000\,000\,000\,1 \tag{56}$$

compared with $f'(0)=1/\sqrt{2}=0.707\,106\,781\,2\ldots$. The deviation is just 0.099%, but $1/\sqrt{2}$ can unfortunately be ruled out.

Given that $p=-1$ and $q=2$, the failure of variational perturbation theory is not surprising. According to Ref. 16 the fraction $2/q$ must lie within the open interval $(\frac{1}{2},1)$. Otherwise, one cannot prove that variational perturbation theory converges. Thus, *this problem lies exactly on the upper boundary of the region in which the summation method is known to work.*

We can understand the upper edge of the range of the parameter $2/q$ that describes the approach to scaling by looking at the standard deviation from the actual limiting value. It turns out[16] that the deviation in the limit as the perturbative order N goes to infinity assumes the shape

$$\left|\frac{b_0^{(N)}-b_0}{b_0}\right| \sim \exp(-CN^{1-2/q}) \quad (N\to\infty), \tag{57}$$

where C is a constant. So, to obtain exponential convergence for the sequence formed by the $b_0^{(N)}$, we need $1-2/q>0$. In other words, the approach to scaling $2/q$ is bounded and it must be smaller than one. The lower edge is more subtle and is discussed in Ref. 16.

In conclusion, we have applied variational perturbation theory to a case that lies at the very edge of its applicability. We see that variational perturbation theory gives better results by about a factor of 10 than the Padé approximations examined in Sec. II. However, we have not yet found a systematic method for resumming (19) that enables us to perform the continuum limit of the discrete lattice theory. Therefore, we now lay the foundation for further investigations by analyzing the large-order behavior of the instanton series.

IV. LARGE-ORDER BEHAVIOR FOR THE INSTANTON EQUATION

It can be seen from the numerical results in Ref. 14 that the instanton weak-coupling series is of Borel type. That is, it exhibits an alternating sign pattern. From the ratio test we can see that the coefficients $a_{n,j}$ do not grow factorially fast. The large-order behavior of $a_{n,j}$ has the general form

$$a_{n,j} \sim (-1)^{n+j+1} K_n^j j^{A_n} B_n \quad (j\to\infty). \tag{58}$$

The constant A_n can be obtained by evaluating the limit

$$A_n = \lim_{j\to\infty} \frac{\log[a_{n,j+2}\,a_{n,j}/(a_{n,j+1})^2]}{\log[j(j+2)/(j+1)^2]}, \tag{59}$$

TABLE V. Six orders of Richardson extrapolations for the exponent A of the large-order instanton weak-coupling coefficients, based on the first 200 weak-coupling coefficients. The value $A=-\frac{3}{2}$ is quite plausible.

Order	Value for A	Convergence
1	−1.4998	increasing
2	−1.500 017	decreasing
3	−1.500 001 1	decreasing
4	−1.499 998 74	increasing
5	−1.500 000 4	decreasing
6	−1.499 999 893	increasing

and the reciprocal of the radius of convergence is

$$K_n=-\lim_{j\to\infty}\frac{a_{n,j+1}}{a_{n,j}}\left(\frac{j}{j+1}\right)^{A_n}. \tag{60}$$

Also, the overall factor B_n is determined from

$$B_n=\lim_{j\to\infty}\frac{|a_{n,j}|}{K_n^j j^{A_n}}. \tag{61}$$

Using the 200 weak-coupling coefficients, we find that the exponent A_n and the reciprocal radius of convergence K_n are independent of n. The value of $K_2=2.466\,829\,06$ coincides with $K_1=2.466\,829\,06$ for all significant digits. The same is true for $A_1=-1.500\,000$ and $A_2=-1.500\,000$. Thus, it appears that we may omit the subscripts n for K_n and A_n. In contrast, the data suggest that B_n strongly depends on n. B_n is the numerical value associated with the largest uncertainty. In fact, Eq. (61) suggests that small deviations in K and A lead to dramatic changes in the value of B_n. We calculated A, K, B_1, and B_2 up to 200th order with the help of Maple V R7. We then extrapolated these 200 orders to infinity using Richardson extrapolation.[13] We obtained

$$\begin{aligned} A&=-1.500\,000\pm 0.000\,001,\\ K&=2.466\,829\,06\pm 0.000\,000\,1,\\ B_1&=0.0171\pm 0.0001,\\ B_2&=0.1190\pm 0.0001. \end{aligned} \tag{62}$$

Detailed numerical results for the first six Richardson extrapolations for the exponent A, the inverse radius of convergence K, and the overall factors B_1 and B_2 can be found in Tables

TABLE VI. Six orders of Richardson extrapolations for the inverse radius of convergence K of the large-order instanton weak-coupling coefficients, based on the first 200 weak-coupling coefficients under the assumption that $A=-\frac{3}{2}$.

Order	Value for K	Convergence
1	2.466 92	decreasing
2	2.466 828 3	increasing
3	2.466 829 11	decreasing
4	2.466 829 065	decreasing
5	2.466 829 059 7	increasing
6	2.466 829 063 5	decreasing

TABLE VII. Six orders of Richardson extrapolations for the overall factor B_1 of the large-order instanton weak-coupling coefficients, based on the first 200 weak-coupling coefficients under the assumption that $K=2.448\,290\,6$ and $A=-\frac{3}{2}$. The value of B_1 strongly depends on the numerical values for A and K. Changing K in the sixth decimal place influences the third significant figure of B_1. Also, all the Richardson extrapolations are increasing, so, strictly speaking, we only have a lower boundary for B_1. Thus, the accuracy of B_1 may not be very good.

Order	Value for B_1	Convergence
1	0.017 083 7	increasing
2	0.017 086 4	increasing
3	0.017 087	increasing
4	0.017 089 3	increasing
5	0.017 090 8	increasing
6	0.017 092 2	increasing

V–VIII. The calculation of B_1 is extremely delicate; changing the inverse radius of convergence in the sixth decimal place influences the third significant figure of B_1. The same is true of B_2.

Unfortunately, there is no way to derive these values by applying asymptotic analysis to the recursion relation (16). The problem is that the double summation in this equation includes small j, so we cannot let j go to infinity and use the large-order behavior (58). Substituting the *ansatz* (58) into Eq. (16) and taking the limit leads to contradictory results. For $n=1$ we get

$$Kj^A B_1=\frac{1}{2}(j-1)^A B_2+(j-1)^A B_1-\frac{3}{2}B_1^2 K\sum_{k=1}^{j-1}k^A(j-k)^A-\frac{1}{2}B_1^3 K\sum_{k=1}^{j-1}\sum_{l=1}^{j-k}k^A l^A(j-k-l)^A. \tag{63}$$

Pulling out some factors and letting $x\equiv k/j$, we obtain for the first summation

$$\lim_{j\to\infty}\sum_{k=1}^{j}\left(\frac{k}{j}\right)^A\left(1-\frac{k}{j}\right)^A=\int_0^1 dx\,[x(1-x)]^A=\frac{\Gamma^2(A+1)}{\Gamma(2A+2)}, \tag{64}$$

if and only if $A>-1$. For $A<-1$ which is strongly favored by the data we obtain

$$\int_0^1 dx\,[x(1-x)]^A=2\zeta(-A). \tag{65}$$

The double summation reduces to

$$\lim_{j\to\infty}\sum_{k=1}^{j}\sum_{l=1}^{j-k}\frac{k^A l^A}{j^{2A}}\left(1-\frac{k}{j}-\frac{l}{j}\right)=\int_0^1 dx\int_0^1 dy\,[xy(1-x-y)]^A=\frac{\Gamma^3(A+1)}{\Gamma(3A+3)}, \tag{66}$$

where $y\equiv l/j$ and $A>-1$. For $A<-1$ the result is

TABLE VIII. Six orders of Richardson extrapolations for the overall factor B_2 of the large-order instanton weak-coupling coefficients based on the first 200 weak-coupling coefficients and the same assumptions as in the case of B_1 (see Table VII). The value of B_2 depends strongly on A and K.

Order	Value for B_2	Convergence
1	0.119 069	increasing
2	0.119 083	increasing
3	0.119 093	increasing
4	0.119 054 095	increasing
5	0.119 054 125	increasing
6	0.119 054 146	increasing

$$\int_0^1 dx \int_0^1 dy\,[xy(1-x-y)]^A = 3\zeta^2(-A). \tag{67}$$

Substituting the results in (65) and (67) into (63) leads to a contradiction: The inverse radius of convergence then turns out to be

$$K = \frac{1 + B_2/2B_1}{1 + 3\zeta(\frac{3}{2})B_1 + \frac{3}{2}\zeta^2(\frac{3}{2})B_1^2}, \tag{68}$$

which would imply that, given $B_1 = 0.0171$ and $B_2 = 0.1190$, the value of K would be

$$K = 3.940. \tag{69}$$

This result can be ruled out because of the numerical result (62). Also, (68) does not contain the exponent A because all the factors j^A in (63) cancel. So A cannot be determined analytically using this asymptotic analysis.

V. BOUNDARY LAYERS ON THE LATTICE—BLASIUS EQUATION

The Blasius equation[18] arises in the study of fluid dynamics. It is a special limiting case of the Navier–Stokes equation and determines the flow of an incompressible fluid across a semi-infinite flat plate. The equation reads

$$2\epsilon y'''(x) + y(x)y''(x) = 0. \tag{70}$$

Assuming that the tangential velocity $y'(x)$ at the outer limit of the boundary layer is constant, the boundary conditions read[19]

$$y(0) = y'(0) = 0, \quad y'(\infty) = 1. \tag{71}$$

Our objective here is to calculate the second derivative $y''(0)$, which represents the stress on the plate. We discretize the Blasius equation (70) by introducing a lattice spacing a:

$$2\delta(f_{n+1} - 3f_n + 3f_{n-1} - f_{n-2}) + f_n(f_{n+1} - 2f_n + f_{n-1}) = 0, \tag{72}$$

where we define $f_n \equiv y(na)/a$ and $\delta \equiv \epsilon/a^2$. The boundary conditions (71) now read

$$f_0 = f_{-1} = 0, \quad f_n \sim n \quad (n \to \infty). \tag{73}$$

Expanding f_n as a series in powers of δ as in Eq. (14), we obtain the recursion relation[10]

$$\begin{aligned} a_{n+1,j} - 2a_{n,j} + a_{n-1,j} = &-\frac{2}{n}(a_{n+1,j-1} - 3a_{n,j-1} + 3a_{n-1,j-1} - a_{n-2,j-1}) \\ &-\frac{1}{n}\sum_{k=1}^{j-1} a_{n,k}(a_{n+1,j-k} - 2a_{n,j-k} + a_{n-1,j-k}). \end{aligned} \tag{74}$$

The boundary values are

$$\begin{aligned} a_{n,0} &= n \quad (n \geqslant 0), \\ a_{-1,0} &= 0, \\ a_{-n-1,j} &= a_{n,j} \quad (n \geqslant 0). \end{aligned} \tag{75}$$

TABLE IX. The first 20 weak-coupling coefficients for the Blasius recursion relation (74) and (75). Observe that the coefficients $a_{1,j}$ are not of Borel type (they do not alternate in sign). A cosine function with a frequency different from π governs the sign pattern (see Sec. VIII).

j	$a_{1,j}$	j	$a_{1,j}$
1	-2	11	$\frac{30868632383}{5457375}$
2	2	12	$\frac{6325029622}{637875}$
3	$\frac{8}{3}$	13	$-\frac{487693745019181}{13408770375}$
4	-6	14	$-\frac{4774319527974167}{37819608750}$
5	$-\frac{184}{15}$	15	$\frac{430321251088745734}{2212447111875}$
6	$\frac{136}{9}$	16	$\frac{796235344548876790517}{603998061541875}$
7	$\frac{11062}{105}$	17	$-\frac{22499880545067641745840 49}{677685825049983750 0}$
8	$-\frac{8162}{225}$	18	$-\frac{178060537619150189817796}{14237097164915625}$
9	$-\frac{10557416}{14175}$	19	$-\frac{132248961522197296674980 38639}{130190976834602433750 0}$
10	$-\frac{57628622}{99225}$	20	$\frac{121756993154067534451733120837029}{115321796848755734737500 0}$

Equation (74) can be solved order by order by using a computer algebra program. Table IX shows the first 20 weak-coupling coefficients $a_{1,j}$. All coefficients up to the 300th order can be found Ref. 20.

VI. PADÉ RESUMMATION FOR THE BLASIUS EQUATION

We now resum the weak-coupling coefficients using the Padé method (23) with $M=\frac{1}{2}$. This value of M will be derived in Sec. VII in Eq. (82). The exact solution[10] to the Blasius equation (70), obtained numerically up to five digits, is $y''(0)=0.332\,06$. Unfortunately, the sequence formed by the approximants S_N appears to converge, but not to the correct value. According to Table X the sequence becomes very flat and Richardson extrapolation[13] shows that the S_N ap-

TABLE X. The first 20 Padé approximants for the solution to the Blasius equation (70). The sequence formed by the S_N converges extremely slowly.

N	S_N	N	S_N
1	0.5	11	0.357 463 212 1
2	0.420 448 207 6	12	0.356 332 665 1
3	0.394 820 183 0	13	0.355 384 804 8
4	0.381 944 373 2	14	0.354 579 594 4
5	0.374 206 230 9	15	0.353 888 284 2
6	0.369 050 481 1	16	0.353 289 150 9
7	0.365 377 967 3	17	0.352 765 581 3
8	0.362 635 906 0	18	0.352 304 658 8
9	0.360 515 591 5	19	0.351 896 192 9
10	0.358 830 970 7	20	0.351 532 039 9

TABLE XI. Three orders of Richardson extrapolations for the Blasius equation (70), based on the first 70 Padé approximants S_N.

Order	Value of $y''(0)$	Convergence
1	0.3445	decreasing
2	0.3436	decreasing
3	0.3430	oscillating

proach the wrong limiting value (see Table XI). A third-order Richardson gives $S_\infty = 0.3430$, based on the first 70 weak-coupling coefficients. This value is significantly higher than the correct value $y''(0) = 0.33206$, the deviation is 3.3%.

The failure of the Padé resummation is not surprising because the Padé method assumes the approach to scaling δ^{-1} according to (24). However, in the case of the Blasius equation the approach to scaling is $\delta^{-1/2}$, as we will see in Eq. (82) in the next section.

VII. VARIATIONAL PERTURBATION THEORY FOR THE BLASIUS EQUATION

Variational perturbation theory for the Blasius equation fails to converge to the correct answer in the same way as for the instanton problem. We determined the leading strong-coupling term (42) up to 200th order and again it was impossible to find extrema, inflection points, or higher derivatives that yield the correct result. Tables XII and XIII show the last 20 strong-coupling coefficients $b_0^{(N)}$ and six orders of Richardson extrapolation. By determining the values of p and q we show why variational perturbation is likely to fail for this problem.

Consider again the Taylor expansions for $f_{n\pm1}$ in (44) together with the Taylor series for $f_{n-2} = f(x_n - 2a)$, namely,

$$f_{n-2} = f(x_n) - 2\,f'(x_n)a + 2\,f''(x_n)a^2 - \tfrac{4}{3}f'''(x_n)a^3 + \tfrac{2}{3}f''''(x_n)a^4 \pm \cdots . \tag{76}$$

Inserting these expressions into the difference equation for the Blasius problem (72) and translating back to the continuous function $f(x_n) = f_n$, we get

$$2\epsilon(f'''(x)a - \tfrac{1}{2}f''''(x)a^2 + \cdots) + f(x)(f''(x)a^2 + \tfrac{1}{2}f''''(x)a^4 + \cdots) = 0. \tag{77}$$

Next we transform back to the function $y(x) = af(x)$ and assume the Taylor series

$$y(x) = y_0(x) + ay_1(x) + a^2y_2(x) + \cdots . \tag{78}$$

To zeroth order in a we obtain

TABLE XII. The last 20 variational strong-coupling coefficients $b_0^{(N)}$ for the Blasius equation. The very last coefficient is $b_0^{(200)} = 0.336\,959\,312\,377\,13$, as opposed to the correct value $y''(0) = 0.33206$.

N	$b_0^{(N)}$	N	$b_0^{(N)}$
180	0.336 960 177 930 94	190	0.336 959 711 196 46
181	0.336 960 127 770 85	191	0.336 959 668 491 39
182	0.336 960 078 430 82	192	0.336 959 626 448 43
183	0.336 960 029 893 08	193	0.336 959 585 053 96
184	0.336 959 982 140 34	194	0.336 959 544 294 71
185	0.336 959 935 155 75	195	0.336 959 504 157 74
186	0.336 959 888 922 92	196	0.336 959 464 630 46
187	0.336 959 843 425 91	197	0.336 959 425 700 58
188	0.336 959 798 649 18	198	0.336 959 387 356 12
189	0.336 959 754 577 60	199	0.336 959 349 585 40

TABLE XIII. Six orders of Richardson extrapolations for the strong-coupling coefficient $b_0^{(N)}(k_0^{(N)})$ up to $N=200$ for the Blasius equation. The last value is 1.5% away from the correct limiting value $y''(0)=0.33206$.

Order	Value for $b_0^{(N)}$	Convergence
1	0.336 951 8	increasing
2	0.336 955 563	increasing
3	0.336 955 600 539	increasing
4	0.336 955 600 880 3	increasing
5	0.336 955 600 883 462	increasing
6	0.336 955 600 883 492 32	increasing

$$2\epsilon y_0'''(x)+y_0(x)y_0''(x)=0, \tag{79}$$

which is just the Blasius equation (70). The small parameter a, which is the lattice spacing, relates ϵ and δ by $a=\sqrt{\epsilon/\delta}$. Thus, if we evaluate the Taylor series (78) for the second derivative at the origin, we see that

$$y''(0)=y_0''(0)+ay_1''(0)+\cdots=\frac{0.332\,06}{\sqrt{\epsilon}}+\sqrt{\frac{\epsilon}{\delta}}y_1''(0)+\cdots. \tag{80}$$

Comparing this series to the original weak-coupling series

$$y''(0)=\sqrt{\frac{\delta}{\epsilon}}(1-2\delta+2\delta^2+\cdots), \tag{81}$$

we can now determine the leading power p/q and the approach to scaling $2/q$:

$$1-2\delta+2\delta^2+\cdots=\delta^{-1/2}(0.332\,06+\delta^{-1/2}\epsilon y_1''(0)+\cdots), \tag{82}$$

so we obtain $p=-2$ and $q=4$.

Again we find that the approach to scaling $2/q=\frac{1}{2}$ lies just on the boundary of the open interval $(\frac{1}{2}, 1)$, for which the proof of convergence[16] holds. This situation here is the opposite of the instanton case in that it sits at the *lower* boundary of the open interval in which variational perturbation theory works.

VIII. LARGE-ORDER BEHAVIOR FOR THE BLASIUS EQUATION

The Blasius equation exhibits a large-order behavior which is a more subtle than for the instanton problem (58). The Blasius weak-coupling coefficients are not of Borel type; that is, the sign pattern is not alternating. Rather, the sign structure is governed by a cosine function with a frequency that is significantly different from π. Remarkably, it turns out that a pure cosine $\cos(an)$ cannot reproduce all signs correctly. Up to 300th order the sign structure given by $\cos(an)$ is broken twice: The signs at $n=62$ and at $n=212$ are not correct if we optimize with respect to a. So we must consider an additional phase shift $\cos(an+b)$. The parameter b turns out to be slightly smaller than π, but it reproduces all 300 signs correctly.

In order to determine the numerical values of a and b we define

$$f(a,b)\equiv\sum_{n=1}^{N}\frac{\cos(an+b)}{|\cos(an+b)|}\frac{a_{1,n}}{|a_{1,n}|}. \tag{83}$$

The sum ends at $N=300$ because this is as high as we can calculate using Maple; we know the first 300 weak-coupling coefficients $a_{1,j}$. For the correct values of a and b the function $f(a,b)$

TABLE XIV. Examples of the parameters a and b that give the first 300 signs of the Blasius weak-coupling coefficients correctly, assuming that the sign structure of the underlying large-order behavior is of the form $\cos(an+b)$. The last two values for a can be obtained approximately by summing 2π to the first two values.

a	b
1.3941	3.09
1.3939	3.11
7.67830	3.031
7.67686	3.130

must be equal to 300. We then plot the function $f(a,b)$ over the $a-b$ plane and search for peaks. A careful study of the peaks yields values for a and b which allow the function $f(a,b)$ to assume its maximum at 300. These numbers are given in Table XIV.

The large-order behavior of the Blasius weak-coupling coefficients (unlike the large-order behavior of the instanton coefficients) has an additional overall factor $\cos(an+b)$, and we can now see that the remaining structure differs from the structure of the instanton weak-coupling coefficients. Dividing by the cosine, we observe that the coefficients

$$a_j' \equiv \frac{a_{1,j}}{\cos(aj+b)} \tag{84}$$

grow factorially fast. Thus, we also divide by $j!$:

$$b_j \equiv \frac{a_{1,j}}{\cos(aj+b)j!}. \tag{85}$$

The coefficients b_j are unstable under a ratio test. That is, the ratio b_{j+1}/b_j decreases and then begins to oscillate. This is the inaccuracy that results from the delicate sign pattern of the first 300 coefficients $a_{1,j}$.

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The Gelfand–Zeitlin selection rules and representations of quantum A_n^q algebras

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The problem of construction of irreducible representations of quantum A_n^q algebras is solved by explicit integration of the linear (inhomogeneous) system of equations in finite differences in the n-dimensional space. The general solution of this system is given explicitly, and particular solutions corresponding to the irreducible representations are selected. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In the author's recent paper,[1] the problem of construction of irreducible representations of the unimodular matrix algebra A_n—the famous result obtained by Gel'fand and Tsetlin[2]—was reformulated through explicit integration of a linear system in finite differences.

It is possible to reduce all the calculations to the solution of a linear system of equations in finite differences (or PDEs in the continuous functional group limit). What is surprising and intriguing in this approach is the fact that the results obtained at the functional group level[3,4] (the Poisson brackets of the classical Hamiltonian formalism) literally pass to those arising in the algebraic calculations. The only thing that is necessary is to replace the Poisson brackets by commutators, and canonically conjugated classical variables by elements of n-dimensional Heisenberg algebras and to choose the correct order of operators involved. All expressions retain their form at both the levels after replacing the operation of usual differentiation in the case of the functional group by discrete difference in the algebra-theoretical case.

In the present paper we apply the method of Ref. 1 to the problem of construction of irreducible representations of the quantum A_n^q algebras. We try to resolve the system of commutation relations between $3n$ generators ($2n$ generators of simple roots $X_i^{\pm}$ and n generators of the Cartan elements h_i)

$$[X_i^+, X_j^-] = \delta_{ij}\phi_i(h_i), \quad [h_i, X_j^{\pm}] = \pm k_{ji} X_j^{\pm}, \tag{1}$$

where ϕ_i are initially arbitrary functions of their arguments.

Using only the ''selection rules'' of the Gel'fand–Tsetlin paper,[2] we find that in the case of $U_q(2)$, A_1^q algebra it is possible to resolve Eq. (1) for an arbitrary function ϕ in a self-consistent way. However, already in the case of $U_q(3)$, A_2^q algebras, the self-consistency of the construction leads to a unique choice of the functions ϕ_i in the standard trigonometrical form.

The notion of coproduct was not used at any step of our construction. We try to literally conserve the text and presentation of the material as in Ref. 1, in order to simplify the comparison between these too very similar papers for the reader.

In Secs. II and III, we consider the simplest cases of $U_q(2)$, $U_q(3)$ quantum algebras with detailed calculations. In Sec. IV, we consider the case of arbitrary $U_q(n+1)$ quantum algebras. In Sec. V, we summarize the results and discuss the perspectives for further investigations.

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II. THE CASES OF $A_1^q \approx SU_q(2)$ AND $U_q(2)$

Every section will be divided into two parts: the classical case (the functional group level) and proper algebraic construction (''quantum case''). As remarked in Sec. I, the classical results can be used as good guides in further algebraic (quantum) calculations.

A. The functional algebra case

The functional $U_q(2)$ algebra contains four elements $X^{\pm}$, H, I connected by the Poisson brackets:

$$\{I,X^{\pm}\}=\{I,H\}=0, \quad \{X^{+},X^{-}\}=\phi(H), \quad \{H,X^{\pm}\}=\pm 2X^{\pm}, \tag{2}$$

where ϕ is an arbitrary function of a single argument.

In accordance with the Darboux theorem,[3] of the elements of the $U_q(2)$ functional group[3] it is possible to construct a pair of canonically conjugated variables M,m, $\{M,m\}=1$ and two cyclic variables I,L with the zero Poisson brackets with each other and with all other elements of the $U_q(2)$ functional group (clearly, up to an arbitrary canonical transformation). The explicit expression for them in terms of the functional group elements will be given a bit later.

Let us choose $M=H$ and $m=(1/4)\ln(X^{+}/X^{-})+f(H)$. With the help of Poisson brackets (2) it is not difficult to see that M,m thus constructed are really canonically conjugated variables. Resolving these relations with respect to the functional group elements leads to the following realization in terms of the canonical conjugated coordinate m and momenta M and the two cyclic momenta L_1,L_2:

$$X^{+}=\frac{1}{2}e^{2m}\left(f\left(\frac{L_1-L_2}{2}\right)-f(H)\right), \quad X^{-}=\frac{1}{2}e^{-2m}\left(f\left(\frac{L_1-L_2}{2}\right)+f(H)\right),$$
$$H=M-\frac{L_1+L_2}{2}, \quad \phi(x)=\frac{\mathrm{d}f^2}{\mathrm{d}x}. \tag{3}$$

It is not difficult to verify by direct calculations that (3) is indeed a realization of the functional group (2). If we want to restrict ourselves to the case of quantum A_1^q algebra it is necessary to put $I=L_1+L_2=0$.

B. Quantum algebra case

As always, to pass from the classical expressions to the quantum ones it is necessary to order the operators involved in a certain way and to replace the Poisson brackets by commutators. Equation (3) provides a very tempting possibility to rewrite them as

$$X^{+}=\frac{1}{2}e^{m}\left(f\left(\frac{L_1-L_2}{2}\right)-f(H)\right)e^{m}, \quad X^{-}=\frac{1}{2}e^{-m}\left(f\left(\frac{L_1-L_2}{2}\right)+f(H)\right)e^{-m}, \tag{4}$$

$$H=M-\frac{L_1+L_2}{2}, \quad I=L_1+L_2, \quad L=X^{+}X^{-}+X^{-}X^{+}+\tfrac{1}{4}(f^2(H+1)+f^2(H-1))$$

and consider now M,m as generators of the Heisenberg algebra ($[M,m]=1,[M,1]=0,[m,1]=0$), with L_1,L_2 commuting with all the generators involved in (4). Keeping in mind the operator relation of the Heisenberg algebra: $\exp(\pm x)p\exp(\mp x)=p\mp 1$, we conclude that the generators defined in (4) satisfy the commutation relations (2) of $U_q(2)$ algebra (of course with square brackets instead of the curly ones) and $\phi=1/4(f^2(H+1)-f^2(H-1))$.

Two Casimir operators under realization (4) take the constant values

$$K^{(1}=L_1+L_2, \quad K^{(2}=X^{+}X^{-}+X^{-}X^{+}+\frac{1}{4}(f^2(H+1)+f^2(H-1))=\frac{1}{2}f^2\left(\frac{L_1-L_2}{2}\right), \tag{5}$$

which proves the irreducibility of the constructed representation. In the conclusion of this section, we want to stress the fact that commutation relations themselves give no additional restrictions on the form of the f,ϕ functions.

III. $A_2^q \equiv SU_q(3)$ AND $U_q(3)$ CASES

In this case, the problem consists in resolution of the system of commutation relations

$$\begin{aligned}&[X_1^+,X_1^-]=\phi(h_1),\quad [X_1^+,X_2^-]=0,\quad [h_1,X_1^\pm]=\pm 2X_1^\pm,\quad [h_1,X_2^\pm]=\mp X_2^\pm,\\ &[X_1^+,X_2^-]=0,\quad [X_2^+,X_2^-]=\Phi(h_2),\quad [h_2,X_2^\pm]=\pm 2X_2^\pm,\quad [h_2,X_1^\pm]=\mp X_1^\pm.\end{aligned}\tag{6}$$

We choose the arbitrary functions $\phi(h_1)$, $\Phi(h_2)$ in accordance with the comments at the end of Sec. II.

The selection rules of the GZ paper allow us to try to find a resolution of this problem in the following form:

$$\begin{aligned}&X_1^+=\frac{1}{2}e^m\left(f\left(\frac{L_1-L_2}{2}\right)-f(H)\right)e^m,\quad X_2^+=e^{l_1}f^1e^{l_1}+e^{l_2}f^2e^{l_2},\\ &h_1=M-\frac{L_1+L_2}{2},\\ &X_1^-=\frac{1}{2}e^{-m}\left(f\left(\frac{L_1-L_2}{2}\right)+f(H)\right)e^{-m},\quad X_2^-=e^{-l_1}\overline{f^1}e^{-l_1}+e^{-l_2}\overline{f^2}e^{-l_2},\\ &h_2=-\frac{M}{2}+L_1+L_2-\frac{N_1+N_2+N_3}{2},\end{aligned}\tag{7}$$

where all "structural" functions $f^{1,2}$, $\overline{f}^{1,2}$ depend only on the momentum (capital letters) variables. We intentionally preserve the order of factors to avoid rewriting the same formulas several times.

A. Functional group case

In this case, it is necessary to understand all the above-mentioned relations at the functional group level. The commutators have to be replaced by the Poisson brackets understood as usual:

$$\{A,B\}=\sum_1^3\left(\frac{\partial A}{\partial p_i}\frac{\partial B}{\partial x_i}-\frac{\partial A}{\partial x_i}\frac{\partial B}{\partial p_i}\right),\quad x_i=(m,l_1,l_2),\quad p_i=(M,L_1,L_2).$$

Now all of the objects are commutative, and the order of the factors in (7) is unimportant. As a consequence of the vanishing Poisson brackets $\{X_1^+,X_2^-\}=\{X_2^+,X_1^-\}=0$, we obtain equations determining the explicit dependence of structural functions on the momentum M. Namely

$$\begin{aligned}&(\ln\overline{f^1})_M+\frac{1}{2}\frac{f_1'+f_2'}{f_1-f_2}=0,\quad (\ln\overline{f^2})_M+\frac{1}{2}\frac{-f_1'+f_2'}{f_1-f_2}=0,\\ &(\ln f^1)_M+\frac{1}{2}\frac{f_1'-f_2'}{f_1+f_2}=0,\quad (\ln f^2)_M-\frac{1}{2}\frac{f_1'+f_2'}{f_1+f_2}=0,\end{aligned}$$

where $f_1\equiv f((L_1-L_2)/2)$, $f_2\equiv f(M-(L_1+L_2)/2)$ and the prime means differentiation of the functions f_1,f_2 with respect to their arguments.

The Poisson brackets $\{X_2^+,X_2^-\}=\Phi(h_2)$ have, as their corollary, three additional equations:

$$(\ln \overline{f^1})_{L_2}+(\ln f^2)_{L_1}=0, \quad (\ln \overline{f^2})_{L_1}+(\ln f^1)_{L_2}=0$$
$$-2(f^1\overline{f^1})_{L_1}+2(f^2\overline{f^2})_{L_2}=\Phi(h_2). \tag{8}$$

The condition of self-consistency of the second pair of equations containing $\ln f$, $\ln \overline{f}$ with the first one leads to the functional equation with shifted arguments for a single unknown function ($X \equiv f(x), Y \equiv f(y)$):

$$(X_{xx}X+Y_{yy}Y)(X^2-Y^2)=(X_x^2-Y_y^2)(X^2+Y^2). \tag{9}$$

This equation allows the exact integration, and its general solution has the form (see Appendix A)

$$f(x)=\sqrt{(a+b\cosh(2\epsilon x))}. \tag{10}$$

In what follows, we will use a special choice of parameters (10) such that $f=\sinh \epsilon x$. This choice can be connected with the condition of the correct classical limit (in the sense $\epsilon \to 0$) in which the quantum functional algebra should pass into the functional algebra A_1. In this case, it is possible to perform all the calculations up to explicit expressions.

Resolution of all additional equations, except for (8), gives the following dependence of the structure functions upon the momentum M:

$$f^1=\cosh \epsilon \frac{L_1-M}{2} f^1(L_1,L_2), \quad f^2=\sinh \epsilon \frac{M-L_2}{2} f^2(L_1,L_2),$$
$$\overline{f^1}=\sinh \epsilon \frac{L_1-M}{2} \overline{f^1}(L_1,L_2), \quad \overline{f^2}=\cosh \epsilon \frac{M-L_2}{2} \overline{f^2}(L_1,L_2), \tag{11}$$

where all new structure functions (for which we reserve the same notation) depend only on two arguments $x_1 \equiv L_1, x_2 \equiv L_2$.

For two unknown functions $X^1 \equiv -f^1\overline{f^1}, X^2 \equiv f^2\overline{f^2}$, Eq. (8) (keeping in mind the form of its right-hand side) becomes the system of two equations:

$$(e^{\epsilon x_1}X^1)_{x_1}+(e^{\epsilon x_2}X^2)_{x_2}=e^{\epsilon(2x_1+2x_2-N)}(e^{-\epsilon x_1}X^1)_{x_1}+(e^{-\epsilon x_2}X^2)_{x_2}=e^{-\epsilon(2x_1+2x_2-N)}, \tag{12}$$

where $N \equiv N_1+N_2+N_3$.

In accordance with Ref. 1, we try to find a solution to the last system in the form:

$$X^1=Y^2_{x_2}, \quad X^2=Y^1_{x_1}.$$

Solving the linear algebraic system of equations that arises for the functions $Y^{1,2}$, we are led to the following solution of the initial system:

$$X^1=\frac{1}{4\epsilon^2}\left(\frac{\sinh \epsilon(2x_1+x_2-N)}{\sinh \epsilon(x_1-x_2)}\right)_{x_2}+\left(\coth \epsilon(x_1-x_2)\Theta(x_1)+\frac{\overline{\Theta}(x_2)}{\sinh \epsilon(x_1-x_2)}\right)_{x_2},$$
$$X^2=-\frac{1}{4\epsilon^2}\left(\frac{\sinh \epsilon(x_1+2x_2-N)}{\sinh \epsilon(x_1-x_2)}\right)_{x_1}-\left(\coth \epsilon(x_1-x_2)\overline{\Theta}(x_2)+\frac{\Theta(x_1)}{\sinh \epsilon(x_1-x_2)}\right)_{x_1}. \tag{13}$$

These formulas result from the exact integration of the system (12). The remaining additional conditions follow from the corresponding equations for invariant (in the sense of independence of the momentum M) structural functions. They can be summarized as follows:

$$(\ln X^1)_{x_2}+(\ln X^2)_{x_1}=0. \tag{14}$$

To satisfy them, it is natural to make a special choice of arbitrary functions $\Theta,\overline{\Theta}$ in the general solution (13).

After performing all operations of the differentiation in (13) we obtain for X^1,

$$X^1=\frac{1}{4\epsilon}\left(\frac{\sinh\epsilon(3x_1-N)}{\sinh^2\epsilon(x_1-x_2)}\right)+\frac{\Theta(x_1)}{\sinh^2\epsilon(x_1-x_2)}+\frac{\sinh\epsilon(x_1-x_2)\overline{\Theta}(x_2)_{x_2}+\cosh\epsilon(x_1-x_2)\overline{\Theta}(x_2)}{\sinh^2\epsilon(x_1-x_2)}.$$

If we want to satisfy the auxiliary condition (14), it is natural to find the solution in the form

$$X^{1,2}=\frac{\psi(x_{1,2})}{\sinh^2\epsilon(x_1-x_2)}.$$

Under this kind of assumption, for functions $\Theta,\overline{\Theta}$ we uniquely obtain $\Theta=A\cosh\epsilon x+B\sinh\epsilon x$, $\overline{\Theta}=C\cosh\epsilon x+D\sinh\epsilon x$ where A,B,C,D are arbitrary numerical constants. Finally, for the function ψ that parametrizes the solution of the system (13), we obtain

$$\psi(x)=\frac{1}{4\epsilon}\sinh\epsilon(3x-N)+(A+C)\sinh\epsilon x+(B+D)\cosh\epsilon x.$$

This expression for ψ can be parametrized in the following form:

$$\psi(x)=\frac{1}{\epsilon}\sinh\epsilon(x-N_1)\sinh\epsilon(x-N_2)\sinh\epsilon(x-N_3)$$

as one can see representing sinh as the difference of the exponentials with further multiplication term by term.

B. The quantum group case

Now in the realization (7) we consider (m,l_1,l_2) as coordinates and (M,L_1,L_2) as momenta of the three independent (commutative) Heisenberg algebras, and (N_1,N_1,N_2) as "cyclic" variables that commute with all other generators. We choose $f=a\sinh\epsilon x$, since the quantum group should have, as its classical limit, the functional group of Sec. III A.

Commutation relations $[X_1^+,X_2^-]=0$, $[X_2^+,X_1^-]=0$ allow us to reconstruct the dependence of structural functions $f^{1,2}$, $\overline{f^{1,2}}$ upon the momentum M exactly in the form (11).

The only commutation relation

$$[X_2^+,X_2^-]=a\sinh\epsilon(M-2(L_1+L_2)+N_1+N_2+N_3)$$

not used until now, together with (7), has, as its consequence, an additional system of equations determining the structural functions:

$$\begin{aligned}&f^1(L_1,L_2-1)\overline{f^2}(L_1-1,L_2)=f^1(L_1,L_2+1)\overline{f^2}(L_1+1,L_2),\\&\overline{f^1}(L_1,L_2-1)f^2(L_1-1,L_2)=\overline{f^1}(L_1,L_2+1)f^2(L_1+1,L_2).\end{aligned} \tag{15}$$

Finally, we will present the last remaining equation using the following notation: $X^1_{\pm}\equiv-f^1(L_1\pm1,L_2)\overline{f^1}(L_1\pm1,L_2)$, $X^2_{\pm}\equiv f^2(L_1,L_2\pm1)\overline{f^2}(L_1,L_2\pm1)$ for new unknown functions and $x_1\equiv L_1$, $x_2\equiv L_2$ for new coordinates. The equation takes on the form:

$$
\begin{aligned}
&-\sinh\epsilon(x_1-M-1)X^1_- + \sinh\epsilon(x_1-M+1)X^1_+ \\
&\quad -\sinh\epsilon(M-L_2+1)X^2_- + \sinh\epsilon(M-L_2-1)X^2_+ \\
&\quad = 2a\sinh\epsilon(M-2(L_1+L_2)+N_1+N_2+N_3). \qquad (16)
\end{aligned}
$$

After resolution of Eq. (16) (equating terms with $\sinh M$, $\cosh M$ on both sides), we come to the system of two equations for determining the two unknown functions $X^{1,2}$:

$$
\begin{aligned}
&-e^{\epsilon(x_1-1)}X^1_- + e^{\epsilon(x_1+1)}X^1_+ - e^{\epsilon(x_2-1)}X^2_- + e^{\epsilon(x_2+1)}X^2_+ = 2e^{\epsilon(2x_1+2x_2-N)}, \\
&-e^{-\epsilon(x_1-1)}X^1_- + e^{-\epsilon(x_1+1)}X^1_+ - e^{-\epsilon(x_2-1)}X^2_- + e^{-\epsilon(x_2+1)}X^2_+ = 2e^{-\epsilon(2x_1+2x_2+N)}, \qquad (17)
\end{aligned}
$$

where $N=N_1+N_2+N_3$.

To solve this system, we introduce the operation of discrete differentiation as

$$
\Delta_i F(x_1,\ldots,x_n) \equiv \frac{F(x_1,\ldots,x_i+1,\ldots,x_n)-F(x_1,\ldots,x_i-1,\ldots,x_n)}{2}.
$$

These operations commute with each other, $\Delta_i\Delta_j=\Delta_j\Delta_i$, and possess the linearity properties in the following sense:

$$
\Delta_i(F^1+F^2)=\Delta_iF^1+\Delta_iF^2, \quad \Delta_i(CF)=C\Delta_iF
$$

if the function C is independent of the x_i coordinate.

The system (16) and (17) can be rewritten in terms of these operations as

$$
\Delta_1(e^{\epsilon x_1}X^1)+\Delta_2(e^{\epsilon x_2}X^2)=e^{\epsilon(2x_1+2x_2-N)},
$$

$$
\Delta_1(e^{-\epsilon x_1}X^1)+\Delta_2(e^{-\epsilon x_2}X^2)=e^{-\epsilon(2x_1+2x_2-N)}.
$$

As in Sec. III A, we seek for a solution of the last system in the form

$$
X^1=\Delta_2(Y^2), \quad X^2=\Delta_1(Y^1).
$$

Keeping in mind the relation (that can be easily checked)

$$
\Delta_2\Delta_1 e^{\epsilon(2x_1+2x_2)}=(\sinh 2\epsilon)^2 e^{\epsilon(2x_1+2x_2)},
$$

we obtain the linear system of algebraic equations determining Y^1, Y^2. After resolution of this system, the solution of the initial system takes the form

$$
\begin{aligned}
X^1 &= \Delta_2\left(\frac{1}{\sinh^2 2\epsilon}\frac{\sinh\epsilon(2x_1+x_2-N)}{\sinh\epsilon(x_1-x_2)}+\coth\epsilon(x_1-x_2)\Theta(x_1)+\frac{\overline{\Theta}(x_2)}{\sinh\epsilon(x_1-x_2)}\right), \\
X^2 &= -\Delta_1\left(\frac{1}{\sinh^2 2\epsilon}\frac{\sinh\epsilon(x_1+2x_2-N)}{\sinh\epsilon(x_1-x_2)}+\coth\epsilon(x_1-x_2)\overline{\Theta}(x_2)+\frac{\Theta(x_1)}{\sinh\epsilon(x_1-x_2)}\right). \qquad (18)
\end{aligned}
$$

After all necessary calculations, from (18) we obtain the final expression:

$$
\begin{aligned}
X^1 &= \frac{1}{2\sinh 2\epsilon}\frac{\sinh\epsilon(3x_1-N)}{\sinh\epsilon(x_1-x_2-1)\sinh\epsilon(x_1-x_2+1)} \\
&\quad + \frac{\sinh 2\epsilon\Theta(x_1)+\overline{\Theta}(x_2+1)\sinh\epsilon(x_1-x_2+1)-\overline{\Theta}(x_2-1)\sinh\epsilon(x_1-x_2-1)}{\sinh\epsilon(x_1-x_2-1)\sinh\epsilon(x_1-x_2+1)} \qquad (19)
\end{aligned}
$$

and the same kind of expression for X^2. If we want to satisfy the additional condition (15) that can be rewritten in the form

$$X^1(L_1,L_2-1)X^2(L_1-1,L_2)=X^1(L_1,L_2+1)X^2(L_1+1,L_2),$$

then it is necessary to find a solution in the form

$$X^1=\frac{\psi_1(x_1)}{\phi(x_1-x_2)},\quad X^2=\frac{\psi_2(x_2)}{\phi(x_1-x_2)}. \tag{20}$$

It is easy to see that with this form of solution, the additional condition (15) is satisfied automatically. Comparing Eqs. (19) and (20), we come to the only possible choice of the function $(\Theta,\overline{\Theta})$,

$$\Theta(x)=A\sinh x+B\cosh x,\quad \overline{\Theta}(x)=C\sinh x+D\cosh x.$$

And as a consequence, we find that $\psi_1(x)=\psi_2(x)=\sinh\epsilon(3x-N)+p\sinh\epsilon x+q\cosh\epsilon x \equiv\sinh\epsilon(x-N_1)\sinh\epsilon(x-N_2)\sinh\epsilon(x-N_3)$. Finally, the solution of the initial system satisfying all necessary additional conditions can be written in the form:

$$\begin{aligned}X^1&=\frac{\sinh\epsilon(x_1-N_1)\sinh\epsilon(x_1-N_2)\sinh\epsilon(x_1-N_3)}{2\sinh 2\epsilon\sinh\epsilon(x_1-x_2-1)\sinh\epsilon(x_1-x_2+1)},\\ X^2&=\frac{\sinh\epsilon(x_2-N_1)\sinh\epsilon(x_2-N_2)\sinh\epsilon(x_2-N_3)}{2\sinh 2\epsilon\sinh\epsilon(x_1-x_2-1)\sinh\epsilon(x_1-x_2+1)}.\end{aligned} \tag{21}$$

IV. GENERAL CASE OF ARBITRARY *n*

A. The algebra representation level

Let us assume that the generators of simple roots and Cartan elements of $U(n+1)$ algebra can be represented in the form

$$\begin{aligned}X_s^+&=\sum_{k=1}^{s} e^{l_k^s}g_k^s e^{l_k^s},\quad X_s^-=\sum_{k=1}^{s} e^{-l_k^s}\overline{g}_k^s e^{-l_k^s},\\ h_s&=-\frac{1}{2}\sum_{r=1}^{s-1}L_r^{s-1}+\sum_{k=1}^{s}L_k^s-\frac{1}{2}\sum_{l=1}^{s+1}L_l^{s+1},\quad 1\leqslant s\leqslant n,\end{aligned} \tag{22}$$

where nonzero commutators of the operators involved are

$$[L_k^s,L_l^t]=\delta_{st}\delta_{kl}I.$$

We assume that the structural functions are ''factorizable'' and, as functions of their arguments, can be represented in the following form:

$$g_k^s=F_k^s(L^{s+1},L^s)f_k^s(L^{s-1},L^{s-1})\quad \overline{g}_k^s=\overline{F}_k^s(L^{s+1},L^s)\overline{f}_k^s(L^{s-1},L^{s-1}).$$

Without any difficulty, the reader can identify L^1 with M, L^2 with L_1,L_2 and L^3 with N_1,N_2,N_3 from Sec. III.

We assume also that all necessary commutation relations for $1\leqslant s\leqslant(n-1)$ are correctly satisfied and

$$(F_k^{n-1})^2=(\overline{F}_k^{n-1})^2=\frac{\Pi_{r=1}^{n}\sinh\epsilon(L_k^{n-1}-L_r^n)}{\Phi(L^{n-1})},$$

where the function Φ is translation-invariant with respect to the simultaneous shift of all the arguments L_k^{n-1}. We prove by induction that the squares of the structural functions $F_i^n=\overline{F_i^n}$ conserve their form and find the explicit expressions for the denominator.

It is obvious that under the above-mentioned restrictions, the commutation relations between generators of the Cartan subalgebra h_l and generators of simple roots $X_k^{\pm}$ are correctly satisfied. It is also clear that the generators $X_n^{\pm}$ commute with all generators $X_k^{\mp}$ with $1\leqslant k\leqslant(n-2)$, because they act on essentially different arguments. And finally, the commutation relations

$$[X_n^{\pm},X_{n-1}^{\mp}]=0$$

allow us to reconstruct the explicit dependence of structural functions f_k^n, $\overline{f_k^n}$ on their arguments L_k^{n-1}.

As a direct corollary of the last commutation relations, we arrive at the expressions: $f_k^n(L^n;\ldots,L_r^{n-1}-1,\ldots)\overline{F_r^{n-1}}(\ldots,L_k^n-1,\ldots,L^{n-1})=f_k^n(L^n;\ldots,L_r^{n-1}+1,\ldots)\overline{F_r^{n-1}}(\ldots,L_k^n+1,\ldots,L^{n-1})$ $\times\overline{f_k^n}(L^n;\ldots,L_r^{n-1}-1,\ldots)F_r^{n-1}(\ldots,L_k^n-1,\ldots,L^{n-1})=\overline{f_k^n}(L^n,\ldots,L_r^{n-1}+1,\ldots)F_r^{n-1}(\ldots,L_k^n+1,\ldots,L^{n-1})$ that should be satisfied for all the possible choices of k and r indices. Keeping in mind the explicit forms $\overline{F_k^{n-1}}$ as assumed previously, we can resolve the last equations in the form:

$$g_k^n=F_k^n(L^{n+1};L^n)\sqrt{\prod_{r=1}^{n-1}\sinh\epsilon(L_k^n-L_r^{n-1})},\quad \overline{g_k^n}=\overline{F_k^n}(L^{s+1};L^s)\sqrt{\prod_{r=1}^{s-1}\sinh\epsilon(L_k^n-L_r^{n-1})}. \tag{23}$$

The only commutation relation that is not satisfied up to now is

$$[X_n^+,X_n^-]=\sinh\epsilon(h_n). \tag{24}$$

It consists of the ''diagonal'' part (that does not contain the coordinates of Heisenberg subalgebras l_i) and the nondiagonal one (in the above-mentioned sense). The arising equation for the diagonal part can naturally be written by using the notation:

$$\begin{aligned} X_k^{\pm n}&=F_k^n(L^{n+1};\ldots L_k^n\pm1,\ldots)\overline{F_k^n}(L^{n+1};\ldots,L_k^n\pm1,\ldots)\\ \sum_{k=1}^{n}\prod_{r=1}^{n-1}\sinh\epsilon(L_k^n+1-L_r^{n-1})X_k^{+n}&-\sum_{k=1}^{n}\prod_{r=1}^{n-1}\sinh\epsilon(L_k^n-1-L_r^{n-1})X_k^{-n}\\ &=\sinh\epsilon\left(\sum_{r=1}^{n-1}L_r^{n-1}+2\sum_{k=1}^{n}L_k^n-\sum_{j=1}^{n+1}L_j^{n+1}\right). \end{aligned} \tag{25}$$

The unknown functions $X_k^{\pm n}$ depend only on L^{n+1},L^n variables (as it follows from their definition) and thus, with respect to the variables L^{n-1} (25) they are to be satisfied identically. Let us consider the structure of the product on the left-hand side of (25) representing each hyperbolic function as a sum of two exponentials:

$$\prod_{r=1}^{n-1}\sinh\epsilon(x-L_r^{n-1})=\frac{1}{2^{n-1}}\sum_{k=0}^{n-1}A_k e^{\epsilon[(n-1)-2k]x]}.$$

It is clear that $A_0=\exp(-\epsilon\Sigma_{r=1}^{n-1}L_r^{n-1})$, $A_{n-1}=(-1)^{n-1}\exp(\epsilon\Sigma_{r=1}^{n-1}L_r^{n-1})$ and all other A_k are some complicated symmetric functions constructed from the components of the $(n-1)$-dimensional vector L^{n-1}. On the right-hand side of (25) (after the decomposition of the hyperbolic function), the dependence on L^{n-1} is concentrated only in the two exponentials. Thus, equating the coefficients of such terms on both sides of (25), we come to the system of n equations for X_k^n functions (we introduce the notation: $L_k^{n-1}\equiv x_k$ and for the moment put $\epsilon=1$):

$$\sum_{k=1}^{n}\left[e^{(n-1)(x_k+1)}X_k^{+n}-e^{(n-1)(x_k-1)}X_k^{-n}\right]=2^{n-2}\exp\left(2\sum_{k=1}^{n}x_k-\sum_{j=1}^{s+1}L_j^{s+1}\right)$$

$$\sum_{k=1}^{n}\left[e^{s(x_k+1)}X_k^{+s}-e^{s(x_k+1)}X_k^{-s}\right]=0,\quad s\equiv n-1-2r,\quad r=1,2,...(n-2) \tag{26}$$

$$\sum_{k=1}^{n}\left[e^{-(n-1)(x_k+1)}X_k^{+n}-e^{-(n-1)(x_k-1)}X_k^{-n}\right]=(-1)^n2^{n-2}\exp\left(-2\sum_{k=1}^{n}x_k+\sum_{j=1}^{s+1}L_j^{s+1}\right).$$

The zero value of the ''nondiagonal'' part of (24) is equivalent to the additional conditions that should hold for the structural functions $F,\overline{F}$:

$$F_k^n(L^{n+1};\ldots,L_j^n-1,\ldots)\overline{F}_j^n(L^{n+1};\ldots,L_k^n-1,\ldots)=F_k^n(L^{n+1};\ldots,L_j^n+1,\ldots)\overline{F}_j^n(L^{n+1};\ldots,L_k^n+1,\ldots)$$

$$\overline{F}_k^n(L^{n+1};\ldots,L_j^n-1,\ldots)F_j^n(L^{n+1};\ldots,L_k^n-1,\ldots)=\overline{F}_k^n(L^{n+1};\ldots,L_j^n+1,\ldots)F_j^n(L^{n+1};\ldots,L_k^n+1,\ldots). \tag{27}$$

From (27) we see that the solution $F_j^n=\overline{F}_j^n$ is the possible one and, functions $X_k^n\equiv X^k$ [being the solution of (25)] should satisfy additional conditions:

$$X^k(L^{n+1};\ldots,L_j^n-1,\ldots)X^j(L^{n+1};\ldots,L_k^n-1,\ldots)=X^k(L^{n+1};\ldots,L_j^n+1,\ldots)X^j(L^{n+1};\ldots,L_n^s+1,\ldots). \tag{28}$$

The reader can easily obtain, from general equations of the present section, all results of Sec. III for the case $n=2$. At this point we interrupt our consideration for a moment to represent the general solution of a continuous version of equations (26).

B. General solution of linear system in the continuous limit

In this section, we give the general solution of the system (26) in the continuous limit or at the level of the functional group approach. In this limit, the system (26) can be obviously rewritten as

$$\sum_{k=1}^{n}\left(e^{(n-1)x_k}X^k\right)_{x_k}=-2^{n-2}\exp\left(2\sum_{k=1}^{n}x_k-L_{n+1}\right),$$

$$\sum_{k=1}^{n}\left(e^{sx_k}X^k\right)_{x_k}=0,\quad s\equiv n-1-2r,\quad r=1,2,...(n-2), \tag{29}$$

$$\sum_{k=1}^{n}\left(e^{-(n-1)x_k}X^k\right)_{x_k}=(-1)^{n-1}2^{n-2}\exp\left(-2\sum_{k=1}^{n}x_k+L_{n+1}\right)$$

[compare with the corresponding Eq. (12) of Sec. III A]. We have introduced the following abbreviation, $\Sigma_{j=1}^{n+1}L_j^{n+1}\equiv L_{n+1}$.

Keeping in mind the ways of resolution of the systems of that kind known for us,[1] we find the solution in the form:

$$X^i=(Y^i)_{x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_n}.$$

After substitution of these expressions into (29), we arrive at the linear system of algebraic equations with the known right-hand side (we have used the obvious relation $(\exp(2\Sigma_{k=1}^{n}x_k-L_{n+1}))_{x_1,\ldots,x_n}=2^n(\exp(2\Sigma_{k=1}^{n}x_k-L_{n+1}))$ to determine the unknown functions Y^i:

$$\sum_{k=1}^{n} e^{(n-1)x_k} Y^k = 2^{-3} \exp\left(2\sum_{k=1}^{n} x_k - L_{n+1} \right) + \Phi^{n-1},$$

$$\sum_{k=1}^{n} e^{sx_k} Y^k = \Phi^s, \quad s \equiv n-1-2r, \quad r = 1,2,...,(n-2), \tag{30}$$

$$\sum_{k=1}^{n} e^{-(n-1)x_k} Y^k = 2^{-3} \exp\left(-2\sum_{k=1}^{n} x_k + L_{n+1} \right) + \Phi^{-n+1}.$$

All functions Φ^{n-1-2s}, $0 \leqslant s \leqslant (n-1)$ are solutions of the single equation $\Phi_{x_1,\ldots,x_n} = 0$ (differentiation with respect to all arguments of the problem!).

The following notation will be useful for resolution of (30). Let W_r be a coefficient of the polynomial of $(n-1)$ degree expressed in terms of its roots:

$$P_{n-1}(z) = W_0 z^{n-1} + W_1 z^{n-2} + \cdots + W_{n-1} = \prod_{k=1}^{n-1} (z - z_k) \quad (W_0 = 1).$$

We denote the coefficients of the polynomial as $W_r^{(k}$; the $(n-1)$ roots of this polynomial coincide with the $(n-1)$ exponentials e^{2x_i} except for only one e^{2x_k}.

In this notation, the resolution of the algebraic system of equations (30) can be represented as

$$Y^k = \frac{1}{2^2} \frac{(\sinh)\cosh(2x_k + \Sigma'^{k}_{i=1} x_i - L_{n+1})}{\Pi'^{n}_{i=1} \sinh(x_k - x_i)} + \frac{\Sigma_{s=0}^{n-1} \Phi^{(n-1-2s)} W_s^{(k}}{\Pi'^{n}_{i=1} \sinh(x_k - x_i)}.$$

In the numerator of the last expression, the sign of cosh arises in the case of odd $n = 2r+1$, and the sign of sinh, in the case of even $n = 2r$, and $L_{n+1} = \Sigma_{j=1}^{n+1} L_j^{n+1}$. By consequent differentiation of Y^k with respect to all independent arguments, except for x_k, we come to the explicit solution of the initial system (30):

$$X^k = \frac{1}{2^2} \frac{(\sinh)\cosh((n+1)x_k - L_{n+1})}{\Pi'^{n}_{i=1} \sinh^2(x_k - x_i)} + \left(\frac{\Sigma_{s=0}^{n-1} \Phi^{(n-1-2s)} W_s^{(k}}{\Pi'^{n}_{i=1} \sinh^2(x_k - x_i)} \right)_{x_1,\ldots,x_{k-1}x_{k+1},\ldots,x_n}. \tag{31}$$

The first term in (31) is a particular solution of the inhomogeneous system (30), the second one is a general solution of the homogeneous part of it. Of course, after performing all the differentiations, the general solution will contain the only function that satisfies the scalar equation $(\Phi)_{x_1,\ldots,x_n} = 0$.

In the following we demonstrate only a particular solution of the homogeneous system, sufficient for the aim to satisfy all necessary additional conditions of our problem. We will directly show that

$$X^i = \frac{e^{[(n+1)-2s]x_i}}{\Pi'^{n}_{k=1} \sinh^2(x_i - x_k)} = \left(e^{[(n+1)-2s]x_i} \prod_{k=1}^{'n} \frac{e^{2x_i} + e^{2x_k}}{e^{2x_i} - e^{2x_k}} \right)_{x_1,\ldots,x_{i-1}x_{i+1},\ldots,x_n}, \quad 2 \leqslant s \leqslant (n-1). \tag{32}$$

In the above-mentioned transformation, we have used the equality $(\coth(x_i - x_k))_{x_k} = \sinh^{-2}(x_i - x_k)$ and the decomposition of sinh,cosh functions into two exponentials. Replacing X^i in that form on the left-hand side of the system (30), we have:

$$\left(\sum_{k=1}^{n} e^{[(n+1)-2s+(n-1)-2r]x_k} \prod_{i=1}^{'n} \frac{e^{2x_k} + e^{2x_i}}{e^{2x_k} - e^{2x_i}} \right)_{x_1,\ldots,x_n}, \quad 0 \leqslant r \leqslant (n-1). \tag{33}$$

In all cases from restrictions on s,r, we have $-n+2\leqslant n-r-s\leqslant n-2$. In further transformations of the last expression, it is suitable to distinguish between two different cases: $0\leqslant n-r-s\leqslant n-2$ and $-n+2\leqslant n-r-s\leqslant 0$. In the first one we introduce $\lambda_i\equiv e^{2x_i}$ and rewrite (33) in the form

$$2^n(\lambda_1,\ldots,\lambda_n)\left(\sum_{k=1}^{n}\lambda_k^{(n-s-r)}\frac{\Pi'^{n}_{i=1}(\lambda_k+\lambda_i)}{\Pi'^{n}_{i=1}(\lambda_k-\lambda_i)}\right)_{\lambda_1,\ldots,\lambda_n},\quad 0\leqslant n-r-s\leqslant n-2$$

and in the second case we will get the same expression (up to unessential factors) introducing $\lambda_i\equiv e^{-2x_i}$.

In both cases, we have a symmetric function under the sign of differentiation. Reducing to a common denominator, we obtain the ratio of two n-dimensional polynomial functions, one of which (denominator) is exactly the Wandermond determinant (the single function that is antisymmetric with respect to permutation of each pair of coordinates). Thus, the numerator must also be an antisymmetric polynomial (since the ratio is a symmetric one!). This is impossible if $n-r-s$ is less than $n-1$ (the degree of numerator in this case is less than the degree of the Wandermond determinant).

We thus prove that (32) is a particular solution of the homogeneous system (30).

Adding the particular solution (32) to the particular solution of inhomogeneous equations (31), we arrive at the following solution of the inhomogeneous system (30) that satisfies all necessary additional conditions as one can check directly:

$$X^k=\frac{1}{2^2}\frac{(\sinh)\cosh((n+1)x_k-L_{n+1})+\Sigma_{s=1}^{n-2}(A_s e^{((n+1)x_k-2s)})+B_s e^{(-(n+1)x_k+2s)}}{\Pi'^{n}_{i=1}\sinh^2(x_k-x_i)}$$
$$\equiv\frac{1}{2^2}\frac{\Pi_{j=1}^{n+1}\sinh(x_k-L_j^{n+1})}{\Pi'^{n}_{i=1}\sinh^2(x_k-x_i)}. \tag{34}$$

One can verify the validity of the last representation by decomposition of sinh into two exponentials in each factor of the product with further multiplication term by term.

The last representation for X^n accomplishes the proof of the induction procedure in the case of the functional group.

C. Solution of the problem in the discrete case

In this section, we present the solution of the finite difference system (26) together with all additional conditions (28) and thus prove the induction assumption.

As the reader will see, the most surprising feature of this approach is that both the calculations themselves and the final result are not changed essentially in comparison with the continuous functional group case.

Being rewritten in terms of the operation of discrete differentiation (see Sec. III C), the system (26) takes the form

$$\sum_{k=1}^{n}\Delta_k(e^{(n-1)x_k}X^k)=-2^{n-3}\exp\left(2\sum_{i=1}^{n}x_i-L_{n+1}\right),$$
$$\sum_{k=1}^{n}\Delta_k(e^{sx_k}X^k)=0,\quad s=\equiv(n-1-2r),\quad r=1,2,\ldots(n-2), \tag{35}$$
$$\sum_{k=1}^{n}\Delta_k(e^{-(n-1)x_k}X^k)=(-1)^n2^{n-3}\exp\left(-2\sum_{i=1}^{n}x_i+L_{n+1}\right).$$

Let us seek for the solution of this system in the conventional form:

$$X^k=(Y^k)_{x_1,\ldots,x_{k-1}x_{k+1},\ldots,x_n}.$$

Replacing this expression in (35) and using the obvious equality $\Delta_i e^{\pm 2x_i}=\pm\sinh 2e^{\pm 2x_i}$, we come to linear algebraic equations for determining the unknown functions Y^k:

$$\sum_{k=1}^{n} e^{(n-1)x_k}Y^k=2^{n-3}(\sinh 2)^{-n}\exp\left(2\sum_{k=1}^{n}x_k-L_{n+1}\right)+\Phi^{n-1},$$

$$\sum_{k=1}^{n} e^{sx_k}Y^k=\Phi^s,\quad s\equiv n-1-2r,\quad r=1,2,\ldots,(n-2), \tag{36}$$

$$\sum_{k=1}^{n} e^{-(n-1)x_k}Y^k=-2^{n-3}(\sinh 2)^{-n}\exp\left(-2\sum_{k=1}^{n}x_k+L_{n+1}\right)+\Phi^{-n+1},$$

where all Φ^a are solutions of the same equation

$$(\Delta_1,\Delta_2,\ldots,\Delta_n)\Phi^a=0.$$

In the last expression, the discrete differentiation is performed with respect to all coordinates of the problem.

The system (36) coincides with (??) up to unessential factors. Thus, its general solution (up to obvious corrections) is the same as (31) (of course, with discrete differentiation).

To conduct the last operation, the following equality is necessary:

$$\Delta_i\frac{(\cosh)\sinh(x_i+A)}{\sinh(x_i-x_k)}=\frac{\sinh 2}{2}\frac{(\cosh)\sinh(x_k+A)}{\sinh(x_i-x_k-1)\sinh(x_i-x_k+1)}.$$

Finally for the solution of (35), we obtain:

$$X^k=\frac{1}{2\sinh 2}\frac{(\sinh)\cosh((n+1)x_k-L_{n+1})}{\Pi'^{n}_{i=1}\sinh(x_k-x_i-1)\sinh(x_k-x_i+1)}+X_0^k, \tag{37}$$

where X_0^k is the general solution of the homogeneous system.

As the reader can notice, the only difference from the continuous case is the appearance of the product of sinh functions with shifted arguments in the denominator instead of the single square.

As in the continuous case, it is not difficult to verify that the form

$$X^k=\frac{\Psi(x_k)}{\Phi(x_k-x_i)}$$

is self-consistent with all additional restrictions. We want to show now that the corresponding solution of a homogeneous system [the second term in (37)] can be chosen.

By the same methods, we show that the homogeneous system possesses solutions of the form

$$X^i=\frac{e^{[(n+1)-2s]x_i}}{\Pi'^{n}_{k=1}\sinh(x_i-x_k-1)\sinh(x_i-x_k+1)}$$

$$=\Delta_1\ldots\Delta_{i-1}\Delta_{i+1}\ldots\Delta_n\left(e^{[(n+1)-2s]x_i}\prod_{k=1}^{\prime n}\frac{e^{2x_i}+e^{2x_k}}{e^{2x_i}-e^{2x_k}}\right),\quad 2\leqslant s\leqslant(n-1). \tag{38}$$

Taking the sum of this solution and the particular solution of the inhomogeneous system (37) we obtain X^k in the factorized form,

$$X^k=\frac{1}{2\sinh 2}\,\frac{\Pi_{j=1}^{n+1}\sinh(x_k-L_j^{n+1})}{\Pi_{i=1}'^{n}\sinh(x_k-x_i-1)\sinh(x_k-x_i+1)}.$$

The last expression accomplishes the proof of the induction procedure in the quantum algebra case.

V. OUTLOOK

The main result of the present paper consists in the explicit realization of irreducible representations of quantum algebras A_n^q of the semisimple series. The method we have used is essentially different from the commonly used approaches to the solution of this problem in literature.[5,6] Of the fundamental suggestions, we have used only the Gel'fand–Zeitlin selection rules and commutation relations between generators of the simple roots and Cartan elements of the A_n^q algebra with arbitrary functional dependence in the principal commutation relation $[X_i^+,X_j^-]=\delta_{ij}\phi_i(h_i)$.

Already for the case of A_2^q algebra (and for all A_n^q, $n>2$), this construction is self-consistent only for the choice of ϕ_i functions in the standard trigonometrical form. No additional assumption about the existence of a coproduct is made. In fact, the result can be obtained at the level of the functional group (classic limit), and the only thing that is necessary is to check it at the algebra-theoretical level.

From the physical point of view, this means that the quasiclassical approach in fact leads to a correct quantum result. We are in a position to describe this situation but would not like to make final conclusions at this step.

ACKNOWLEDGMENT

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APPENDIX

Choosing the new unknown function as $F^1(X)\equiv X_x^2, F^2(Y)=Y_y^2$ and $x_1=X^2, x_2=Y^2$ as new independent coordinates, we rewrite (9) in the form of linear equation:

$$(x_1F_{x_1}^1+x_2F_{x_2}^2)(x_1-x_2)=(F^1-F^2)(x_1+x_2).$$

It possesses the three obvious solutions $F=x, F=1, F=1/x$. Their linear combination with arbitrary coefficients is also a solution. This solution is the general one. Indeed, twice differentiating the last equation with respect, say, to the x_1 coordinate, we come to a system of self-consistent equations of the form presented above.

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Characterizing entanglement

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Quantum entanglement is at the heart of many tasks in quantum information. Apart from simple cases (low dimensions, few particles, pure states), however, the mathematical structure of entanglement is not yet fully understood. This tutorial is an introduction to our present knowledge about how to decide whether a given state is separable or entangled, how to characterize entanglement via witness operators, how to classify entangled states according to their usefulness (i.e., distillability), and how to quantify entanglement with appropriate measures.
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I. INTRODUCTION

The role of entanglement in quantum information processing is manifold. Rather than considering entanglement as a mystery, like in the early years of quantum mechanics, it is nowadays viewed as a resource for certain tasks that can be performed faster or in a more secure way than classically. This genuinely new aspect of quantum properties has launched intensive experimental efforts to create entangled states and theoretical efforts to understand the mathematical structure of entanglement. This tutorial presents the status regarding our understanding of entanglement.

As the number of articles about entanglement has ernomously increased during the last 10 years, it is almost impossible to give a complete overview, and this is not the purpose of this article. It will rather introduce the reader to the established knowledge and some important tools in this field, and discuss some of the questions that remain open at present.

Throughout this tutorial, we will mostly consider entanglement of just two parties, unless stated otherwise explicitly. Most concepts can be explained best with bipartite systems; some of them could then be generalized to more parties in an evident way, for others the situation changes completely for more than two parties. Not many results are known for multipartite systems. In Sec. V D some reasons for this will become clear from studying tripartite states.

Various aspects of entanglement have recently been summarized in the following review articles, which were partially used as a source for this tutorial: the ''primer'' [1] aims at introducing the nonexpert reader to the problem of separability and distillability of quantum states. The Horodecki family discusses entanglement in the context of quantum communication,[2] where the distillability properties of a given state are important. B. Terhal summarizes the use of witness operators for detecting entanglement in Ref. 3. Various entanglement measures are presented in the context of the theorem of their uniqueness in Ref. 4. Other reviews on theoretical and experimental aspects of entanglement can be found in the first issues of the newly launched journal QIC.[5]

This article is organized as follows: Section II presents various possible answers to the question ''what is entanglement?,'' thus shedding light upon different facets of quantum correlations. In Sec. III several criteria are introduced that allow us to distinguish separable from entangled states. In Sec. IV we discuss the possibility to distill entanglement, and give a distillability criterion. Finally, Sec. V concerns attempts to quantify entanglement via entanglement measures. Some important measures are defined and their properties are discussed. The classification of

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entangled states according to their Schmidt number is introduced, and a generalization to tripartite states is included.

II. WHAT *IS* ENTANGLEMENT?

It is nearly 70 years ago that Erwin Schrödinger gave the name ''Verschränkung'' to a correlation of quantum nature.[6] In colloquial German for nonphysicists this term is only used in the sense of ''folding the arms.'' It was then rather loosely translated to ''entanglement,'' with more inspiring connotations.

Over the decades the meaning of the word ''entanglement'' has changed its flavor. The following list is an attempt to sketch the attitude towards entanglement of various important persons in the fields of foundations of quantum physics and later in quantum information theory. These statements are not quotations, unless indicated explicitly.

Einstein/Podolsky/Rosen: An entangled wavefunction does not describe the physical reality in a complete way.

E. Schrödinger: For an entangled state ''the best possible knowledge of the whole does *not* include the best possible knowledge of its parts.'' [6]

Entanglement is ...

J. Bell: ...a correlation that is stronger than any classical correlation.

D. Mermin: ...a correlation that contradicts the theory of elements of reality.

A. Peres: ''...a trick that quantum magicians use to produce phenomena that cannot be imitated by classical magicians.'' [7]

C. Bennett: ...a resource that enables quantum teleportation.

P. Shor: ...a global structure of the wavefunction that allows for faster algorithms.

A. Ekert: ...a tool for secure communication.

Horodecki family: ...the need for first applications of positive maps in physics.

Our view of the nature of entanglement may continue to be modified during the coming years.

III. GIVEN A QUANTUM STATE, IS IT *SEPARABLE* OR *ENTANGLED*?

In this section we will summarize *operational* and *nonoperational* criteria that allow us to classify a given state as separable or entangled. Here the word ''operational'' is used in the sense of ''user-friendly:'' an operational criterion is a recipe that can be applied to an explicit density matrix ϱ, giving some immediate answer like ''ϱ is entangled,'' or ''ϱ is separable,'' or ''this criterion is not strong enough to decide whether ϱ is separable or entangled.''

But, first of all, we need a mathematical definition for entanglement versus separability. This is very simple for *pure states:* a pure state $|\psi\rangle$ is called *separable* iff it can be written as $|\psi\rangle = |a\rangle \otimes |b\rangle$, otherwise it is *entangled*. (Remember that throughout most of this article we talk about bipartite entanglement. In some cases the generalization to more particles is straightforward, like here.) An example for a pure separable state is $|\psi\rangle = |00\rangle$; examples for pure entangled states are the *Bell states*

$$|\Phi^{\pm}\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle), \tag{1}$$

$$|\Psi^{\pm}\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle). \tag{2}$$

A *mixed state* is called separable if it can be prepared by the two parties (which are traditionally called Alice and Bob) in a ''classical'' way, that is, by agreeing over the phone on the *local* preparation of states. A density matrix that has been created in this way can only contain classical correlations. Mathematically this means: a mixed state ϱ is called *separable* iff it can be written as[8]

$$\varrho = \sum_i p_i |a_i\rangle\langle a_i| \otimes |b_i\rangle\langle b_i|, \tag{3}$$

otherwise it is *entangled*. Here the coefficients p_i are probabilities, i.e., $0 \leqslant p_i \leqslant 1$ and $\Sigma_i p_i = 1$. Note that in general $\langle a_i|a_j\rangle \neq \delta_{ij}$, and also Bob's states need not be orthogonal. This decomposition is not unique. An example for a mixed separable state that contains classical correlations, but no quantum correlations, is $\varrho = 1/2(|00\rangle\langle 00| + |11\rangle\langle 11|)$. An example for a mixed entangled state is a Werner state, an admixture of a Bell state as in (1) or (2) to the identity: $\varrho_W = (1-p)1/4\,\mathbb{1} + p|\Phi^+\rangle\langle\Phi^+|$ with $\frac{1}{3} < p \leqslant 1$. The lower limit of p for ϱ_W to be entangled can be easily found with the operational criteria discussed below. In fact, any density matrix that is ''close enough'' to the identity is separable.[9]

Finding a decomposition as in (3) for a given ϱ, or proving that it does not exist, is a nontrivial task which has been solved explicitly only for a few cases. Therefore, this simple-looking definition of separability is by no means ''user-friendly,'' and we are in demand of criteria that are easier to test.

A. Operational separability criteria

Here we present some separability criteria that are easy to check in an explicit case. In the following we will assume that $\varrho \in \mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim \mathcal{H}_A = M$ and $\dim \mathcal{H}_B = N \geqslant M$, without loss of generality.

For *pure states* there is a very simple necessary and sufficient criterion for separability, the **Schmidt decomposition**. A pure state has Schmidt rank $r \leqslant M$ if it can be decomposed as the biorthogonal sum

$$|\psi^r\rangle = \sum_{i=1}^{r} a_i |e_i\rangle |f_i\rangle, \tag{4}$$

with $a_i > 0$ and $\Sigma_i^r a_i^2 = 1$, where $\langle e_i|e_j\rangle = \delta_{ij} = \langle f_i|f_j\rangle$. Note that a_i^2 are the eigenvalues of the reduced density matrices, and therefore the Schmidt rank is easy to compute. A given pure state $|\psi\rangle$ is separable iff $r = 1$.

For *mixed states* the situation is less simple. There are several operational separability criteria for this case. Here they are ordered in decreasing strength, i.e., the last criterion fails to detect an entangled state as entangled in more cases than the previous ones:

(1) **Peres-Horodecki criterion (positive partial transpose):**[10,11] The partial transpose of a composite density matrix is given by transposing only one of the subsystems. Thus, the entries of a density matrix that is partially transposed with respect to Alice are given by

$$(\varrho^{T_A})_{m\mu,n\nu} = \varrho_{n\mu,m\nu}, \tag{5}$$

where Latin indices are referring to Alice's subsystem and Greek ones to Bob's subsystem. As any separable state can be decomposed according to (3), its partial transpose is given by

$$\varrho_{\mathrm{sep}}^{T_A}=\sum_i p_i(|a_i\rangle\langle a_i|)^T\otimes|b_i\rangle\langle b_i|. \tag{6}$$

Since the $(|a_i\rangle\langle a_i|)^T$ are again valid density matrices for Alice, one finds immediately that $\varrho_{\mathrm{sep}}^{T_A}\geqslant 0$. The same holds for partial transposition with respect to Bob (or any other party for multipartite systems). In conclusion, the partial transpose of a separable state ϱ with respect to any subsystem is positive.[10] (In our terminology a positive operator has positive or vanishing eigenvalues—more precisely it should be called positive semidefinite. The expectation value of a positive operator with any state is positive or zero.)

It was shown in Ref. 11 for bipartite systems that the converse (i.e., if $\varrho^{T_A}\geqslant 0$, then ϱ is separable) is true only for low-dimensional systems, namely for composite states of dimension 2×2 and 2×3. In this case the positivity of the partial transpose (PPT) is a necessary and sufficient condition for separability. For higher dimensions it is only necessary, and the existence of entangled PPT states has been shown[12]—these states have been called *bound entangled states*, as their entanglement does not seem to be "useful," as explained in Sec. IV.

(2) **Reduction criterion:**[13] According to the reduction criterion, if ϱ is separable, then

$$\varrho_A\otimes\mathbb{1}-\varrho\geqslant 0 \quad \text{and} \quad \mathbb{1}\otimes\varrho_B-\varrho\geqslant 0, \tag{7}$$

where ϱ_A is Alice's reduced density matrix, and ϱ_B is Bob's. In order to understand why the positivity of the left-hand sides in (7) is a separability criterion, one has to note that they correspond to the application of the positive map $\Lambda(\sigma)=(\mathrm{Tr}\sigma)\mathbb{1}-\sigma$ to Bob's subsystem, or to Alice's subsystem. (The important role of positive maps will be discussed in the next subsection, Sec. III B.) A positive map applied to one subsystem of a separable state preserves the properties of a density matrix—therefore the resulting density matrix has to remain positive.

Like the partial transpose criterion, the reduction criterion is a necessary and sufficient separability condition only for dimensions 2×2 and 2×3, and a necessary condition otherwise.

(3) **Majorization criterion:**[14] The majorization criterion says that if a state ϱ is separable, then

$$\lambda_\varrho^\downarrow\prec\lambda_{\varrho_A}^\downarrow \quad \text{and} \quad \lambda_\varrho^\downarrow\prec\lambda_{\varrho_B}^\downarrow \tag{8}$$

has to be fulfilled. Here $\lambda_\varrho^\downarrow$ denotes the vector consisting of the eigenvalues of ϱ, in decreasing order, and a vector $x^\downarrow$ is *majorized* by a vector $y^\downarrow$, denoted as $x^\downarrow\prec y^\downarrow$, when $\Sigma_{j=1}^k x_j^\downarrow\leqslant\Sigma_{j=1}^k y_j^\downarrow$ holds for $k=1,\ldots,d-1$, and the equality holds for $k=d$, with d being the dimension of the vector. Zeros are appended to the vectors $\lambda_{\varrho_{A,B}}^\downarrow$ in (8), in order to make their dimension equal to the one of $\lambda_\varrho^\downarrow$.

Thus, for a separable state the ordered vector of eigenvalues for the whole density matrix is majorized by the ones of the reduced density matrices. This is was summarized by Nielsen and Kempe as "Separable states are more disordered globally than locally."[14] Note that the spectra of a density matrix and its reduced density matrices do not allow us to distinguish separable and entangled states. The majorization criterion is only a necessary, not a sufficient condition for separability.

The logical ordering of the separability criteria introduced in this section is as follows:

(i) *dimension 2×2 and 2×3:* ϱ is separable$\Leftrightarrow$satisfies PPT$\Leftrightarrow$satisfies reduction criterion$\Rightarrow$satisfies majorization criterion, and

(ii) *higher dimensions:* ϱ is separable$\Rightarrow$satisfies PPT$\Rightarrow$satisfies reduction criterion$\overset{?}{\Rightarrow}$satisfies majorization criterion

B. Nonoperational separability criteria

In this subsection we will discuss two nonoperational separability criteria. Both are necessary and sufficient criteria for any bipartite system. They bear the major problem, however, that they do not provide us with a simple procedure to check the separability properties of a given state. This will become clear from their description.

(1) **Positive maps:** It was shown in Ref. 11 that ϱ *is separable iff for any positive map* Λ

$$(\mathbb{1}\otimes\Lambda)(\varrho)\geqslant 0 \tag{9}$$

holds.

A positive map is a map that takes positive operators to positive operators. A positive map Λ is called *completely positive* (CP) if any extension to a larger Hilbert space, i.e., $\mathbb{1}_x\otimes\Lambda$, is a positive map. Here x denotes the dimension of the extension and is arbitrary. It is clear from Eq. (9) that, for the purpose of finding separability criteria, only those maps are interesting which are positive, but *not* CP, as a CP map will fulfill (9) for any given ϱ.

In the previous section we have already studied two examples for positive maps that are not CP and the extensions of which provide separability criteria: the transpose and the map $\Lambda(\sigma)=(\mathrm{Tr}\sigma)\mathbb{1}-\sigma$. There we have already explained the reason why (9) has to hold for separable states: it is the possibility to decompose a separable state into a sum of tensor products according to (3). Applying a positive map to one of the subsystems will keep each term positive, and therefore also their sum.

Note that the problem about the nonoperational criterion of positive maps lies in the little word ''any'' just before (9): we do not have a complete characterization of the set of all positive maps.

(2) **Entanglement witnesses:** The criterion of the so-called entanglement witnesses was given in Ref. 11 and studied in Ref. 15:

A density matrix ϱ *is entangled iff there exists a Hermitian operator* $\mathcal{W}$ *with* $Tr(\mathcal{W}\varrho)<0$ *and* $Tr(\mathcal{W}\varrho_{sep})\geqslant 0$ *for any separable state* ϱ_{sep}.

We say that the witness $\mathcal{W}$ ''detects'' the entanglement of ϱ.

Correspondence between (1) and (2): These two criteria are not independent—there is the Jamiołkowski isomorphism[16] that provides us with a correspondence between an entanglement witness and a positive map,

$$\mathcal{W}=(\mathbb{1}\otimes\Lambda)(P_+), \tag{10}$$

where $P_+=(1/M)\,(\Sigma_{i=1}^{M}|ii\rangle)(\Sigma_{j=1}^{M}\langle jj|)$ is the projector onto the maximally entangled state.

Let us for the rest of this subsection pursue the concept of entanglement witnesses. What seems at first sight to be a rather abstract theorem will prove to be a powerful tool, as it allows us to answer explicit questions about entanglement properties of certain states (see, e.g., Sec. V E).

The existence of entanglement witnesses is a consequence of the Hahn–Banach theorem, which states the following:

Let S *be a convex, compact set, and let* $\varrho\notin S$. *Then there exists a hyper-plane that separates* ϱ *from* S.

This fact is illustrated in Fig. 1: the bigger ''egg''-shaped set symbolizes the convex, compact set of all density matrices. The smaller one stands for the separable density matrices, and is a convex, compact subset of the bigger one. The state ϱ is entangled and therefore $\notin S$. The dotted line sketches the hyper-plane that separates ϱ from S, and is given by those σ that fulfill $\mathrm{Tr}(\mathcal{W}\sigma)=0$.

It is helpful to realize that $\mathrm{Tr}(\mathcal{W}\varrho)$ defines a scalar product. Let us for a moment look at a scalar product which is familiar to everybody, the scalar product of two vectors of unit length with common origin. Let us call them $\vec{w}$ and $\vec{r}$. Their scalar product $\vec{w}\cdot\vec{r}$ is equal to $\cos\alpha$, where α is

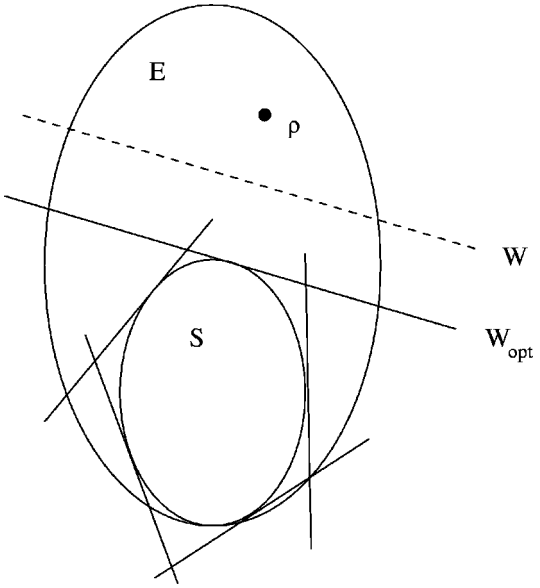

FIG. 1. Intuitive picture of entanglement witnesses and their optimization.

the relative angle between the two vectors. A *fixed* $\vec{w}$ defines a certain plane—the one to which $\vec{w}$ is orthogonal. Vectors $\vec{r}$ from this plane have a vanishing scalar product with $\vec{w}$. All vectors $\vec{r}$ that are ''on one side'' of this plane have a positive scalar product with $\vec{w}$; all vectors $\vec{r}$ ''on the other side'' a negative one—due to the properties of the cosine function. The scalar product $\mathrm{Tr}(\mathcal{W}\varrho)$ has the same property: all density operators on one side of the hyper-plane lead to a positive outcome; the ones on the other side to a negative one.

This intuitive picture of entanglement witnesses also helps to understand how they can be optimized:[17] performing a parallel transport of the hyper-plane such that it becomes tangent to the set of separable states means that the corresponding optimized witness $\mathcal{W}_{\mathrm{opt}}$ detects more entangled states than before. This is also indicated in Fig. 1.

In order to completely characterize the set S one would in principle need infinitely many witnesses, unless the shape of S is a polytope. This is not known nowadays. But several witnesses can already give a good approximation of the set of separable states. Methods to construct entanglement witnesses in a canonical way have been provided in Ref. 17.

IV. GIVEN AN ENTANGLED STATE, IS THE ENTANGLEMENT *USEFUL*?

In an ideal experiment an initially prepared maximally entangled state would remain maximally entangled. In reality, the resource of entanglement is very fragile, due to interaction with the environment. As entanglement is the foundation of many quantum information processing tasks, it would therefore be desirable to concentrate nonmaximal entanglement. A central question is: given several copies of a nonmaximally entangled state, is there a process that allows us to locally ''distill'' its entanglement, i.e., to retrieve a maximally entangled state?

This is a straightforward motivation to study entanglement distillation. In addition, this concept is useful in any other quantum communication task: assume that Alice wants to send a quantum message to Bob. As a simple illustration she will send a polarized photon along an optical fiber. Interaction with the environment disturbs the original quantum state—in general one has to deal with ''noisy channels.'' An initial pure state $|\psi\rangle$ will arrive as some disturbed mixed state ϱ. This situation is sketched in Figs. 2(a) and 2(b).

In the wide field of error correction one deals with this problem by ''repairing the state,'' i.e., via encoding, finding the error and then restoring the original state. The idea of distillation of

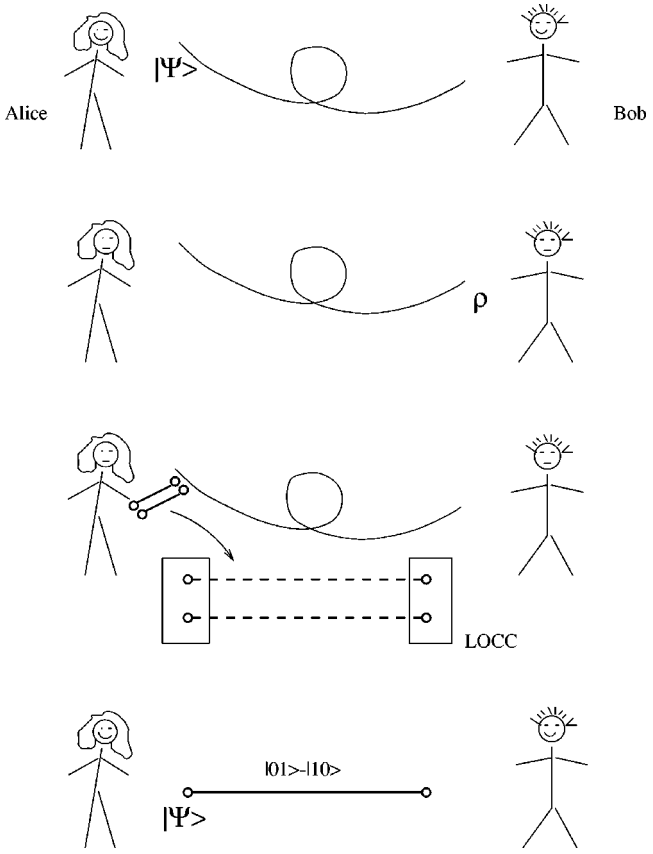

FIG. 2. Providing a noiseless channel via distillation: (a) Alice wants to send the message $|\psi\rangle$ to Bob. (b) Bob receives ϱ instead, as the channel is noisy. (c) Alice sends one subsystem of a maximally entangled state through the noisy channel to Bob, and repeats this with a second pair. They employ a distillation protocol. (d) Alice and Bob have created a maximally entangled singlet which they can use as a noiseless teleportation channel.

nonmaximally entangled states pursues a different path, by ''providing a noiseless channel,'' as explained below.

Figure 2(c) visualizes this concept: Alice sends one subsystem of a maximally entangled state through the noisy channel to Bob. The resulting state will not be maximally entangled and mixed, due to the noise. She repeats this with a second pair or more pairs. Alice and Bob then operate locally on their respective qubits and communicate classically (LOCC=local operations and classical communication), thus employing a distillation protocol. One explicit protocol will be introduced below. Thus they create a maximally entangled state as indicated in Fig. 2(d). This state can now be used as a noiseless channel via teleportation.

In summary, it is an essential question to ask: Given an entangled density matrix ϱ, can its entanglement be *distilled*?

A. A distillation protocol

The following distillation protocol for nonmaximally entangled mixed states was proposed in Ref. 18. It is designed for the case that Alice and Bob share a supply of many identical entangled bipartite systems of qubits. They can always convert them by local operations to the isotropic state $\varrho_{iso}=(1-p)1/4\,\mathbb{1}+p|\Phi^+\rangle\langle\Phi^+|$, with $\frac{1}{3}<p\leqslant 1$.

In the first step Alice and Bob use two ϱ's, as illustrated in Fig. 3. Each of them applies a local CNOT-gate to his/her two qubits. The action of this gate is given by $U_{\mathrm{CNOT}}|a_1\rangle|a_2\rangle=|a_1\rangle|(a_1+a_2)\mathrm{mod}\,2\rangle$.

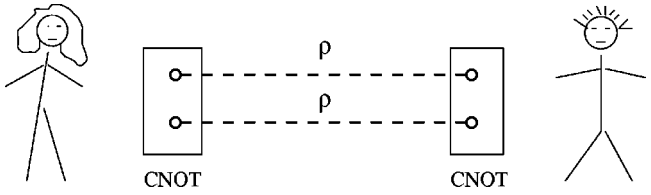

FIG. 3. First step in the distillation protocol: applying local CNOT's.

In the next step, both Alice and Bob do a measurement on their second qubit, as shown in Fig. 4. They only keep the first density matrix, which had changed to some ϱ', if their outcomes are identical. Otherwise the two pairs have to be discarded.

This process has increased the overlap of the new density matrix ϱ' with the maximally entangled state. Thus both entanglement and purity are enhanced. The new fidelity is defined as $F'=\langle\Phi^+|\varrho'|\Phi^+\rangle$ and is plotted in Fig. 5, as a function of the original fidelity $F=\langle\Phi^+|\varrho|\Phi^+\rangle = (1+3p)/4$. This procedure is then repeated with new pairs of the higher fidelity. In this way the entanglement is increased in successive steps, finally being maximal when enough original pairs were available. A distillation protocol is successful, i.e., enhances the entanglement, whenever the curve for the new fidelity lies above the line $F'=F$ (dashed line in Fig. 5).

B. Which states can be *distilled*?

For the general reasons discussed at the beginning of Sec. IV it is a very fundamental question to ask: which entangled states can be distilled? For two-qubit states the answer was given in Ref. 19: *all* entangled two-qubit states are distillable.

In general, this question is unsolved, however. A necessary and sufficient criterion for distillability of a given ϱ was proved in Ref. 20:

The state ϱ *is distillable iff there exists* $|\psi^2\rangle=a_1|e_1\rangle|f_1\rangle+a_2|e_2\rangle|f_2\rangle$ *such that* $\langle\psi^2|(\varrho^{T_A})^{\otimes n}|\psi^2\rangle<0$ *for some* n.

In other words, if for a certain number n of copies the partial transpose of the total state has a negative expectation value with some vector of Schmidt rank 2, then ϱ can be distilled (one says: ϱ is n-distillable), and vice versa. From this theorem it follows immediately that a state with a positive partial transpose cannot be distilled: if $\varrho^{T_A}\geqslant 0$, then $(\varrho^{T_A})^{\otimes n}\geqslant 0$, and thus PPT states are undistillable. As mentioned above, entangled PPT states are therefore called ''bound entangled.''

It is an open question whether the reverse of the statement ''PPT states are undistillable'' is also true, i.e., if a state is undistillable, does it have to be PPT? For the dimension $2\times N$ this is indeed true.[21] For higher dimensions there is a strong conjecture that it is false, i.e., that there are undistillable states with a nonpositive partial transpose (NPT). A family of such states in dimension $N\times N$ was discussed in Refs. 21 and 22. This family consists of a convex combination of projectors onto the symmetric and the antisymmetric subspace, where the relative weight of these two contributions is the only free parameter. Depending on the value of this parameter, the state is PPT or NPT. The undistillability of NPT states with a certain constant finite range of this param-

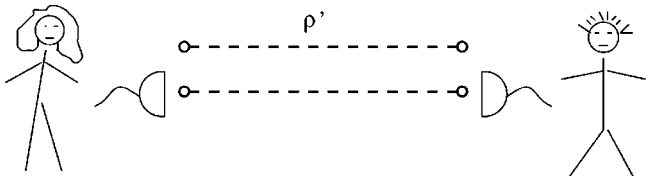

FIG. 4. Second step in the distillation protocol: measurement.

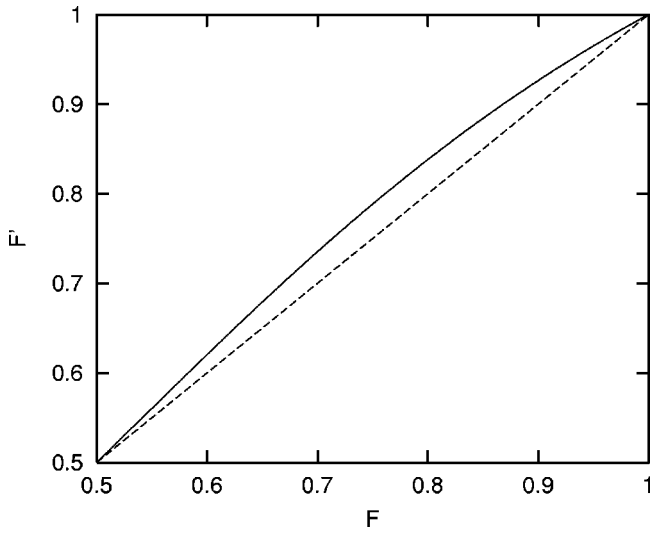

FIG. 5. New fidelity after one distillation step, as a function of the fidelity in the previous step.

eter was shown numerically for up to three copies in the case $N=3$. The problem in finding a rigorous answer to the question of distillability for these NPT states lies in the fact that one has to consider the limit $n\to\infty$.

Our present understanding of how the set of all states is decomposed into separable, entangled undistillable and distillable states is summarized in Fig. 6.

V. GIVEN AN ENTANGLED STATE, *HOW MUCH* IS IT ENTANGLED?

So far we have shown that it is still an open question how to *qualify* a given state as separable versus entangled or undistillable versus distillable. How can we hope to answer the question of *quantifying* the amount of entanglement of a given state? It is not surprising that there is no simple answer to that. We will summarize the requirements for a good entanglement measure, and introduce the reader to some important entanglement measures, without making the attempt to discuss all existing entanglement measures.

In Sec. V C we will explain the concept of Schmidt witnesses, which us allows to classify entangled states in classes according to their Schmidt number. In the final two subsections we will study composite systems of three qubits, showing that the question of quantification of entanglement has to be reformulated in that case.

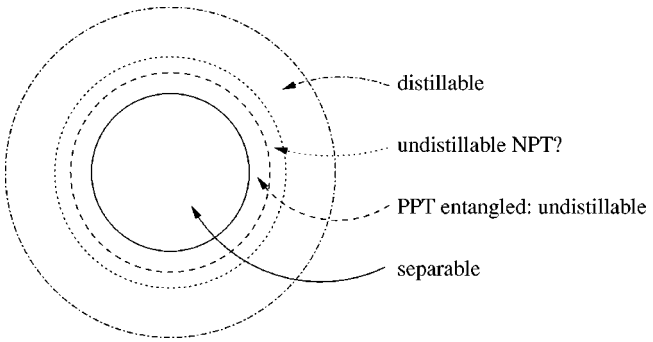

FIG. 6. Decomposition of the set of all states into distillable and undistillable states.

TABLE I. Properties of entanglement measures.

	E_C	E_F	E_R	E_D
continuity	?	√	√	?
additivity	√	?	no[a]	√
convexity	√	√	√	no (?)[b]

[a]Reference 24.
[b]Reference 25.

A. Requirements for entanglement measures

A good entanglement measure E has to fulfill several requirements. However, it is still an open question whether all of these conditions are indeed necessary. In fact, some of the entanglement measures that are introduced below do not fulfill the whole list of properties (see Table I).

(1) If ϱ is *separable*, then $E(\varrho)=0$.
(2) *Normalization:* The entanglement of a maximally entangled state of two d-dimensional systems is given by

$$E(P_+^d)=\log d. \tag{11}$$

(3) *No increase under LOCC:* Applying local operations to ϱ and classically communicating cannot increase the entanglement of ϱ, i.e.,

$$E(\Lambda_{\mathrm{LOCC}}(\varrho))\leqslant E(\varrho). \tag{12}$$

(4) *Continuity:* In the limit of vanishing distance between two density matrices the difference between their entanglement should tend to zero, i.e.,

$$E(\varrho)-E(\sigma)\to 0 \quad \text{for } \|\varrho-\sigma\|\to 0. \tag{13}$$

(5) *Additivity:* A certain number n of identical copies of the state ϱ should contain n times the entanglement of one copy,

$$E(\varrho^{\otimes n})=nE(\varrho). \tag{14}$$

(6) *Subadditivity:* The entanglement of the tensor product of two states ϱ and σ should not be larger than the sum of the entanglement of each of the states,

$$E(\varrho\otimes\sigma)\leqslant E(\varrho)+E(\sigma). \tag{15}$$

(7) *Convexity:* The entanglement measure should be a convex function, i.e.,

$$E(\lambda\varrho+(1-\lambda)\sigma)\leqslant\lambda E(\varrho)+(1-\lambda)E(\sigma) \tag{16}$$

for $0<\lambda<1$.

B. Some important entanglement measures

For a pure bipartite state $|\psi\rangle$ a good entanglement measure is the von Neumann entropy of its reduced density matrix, $S(\varrho_{\mathrm{red}})=-\mathrm{Tr}(\varrho_{\mathrm{red}}\log\varrho_{\mathrm{red}})$. For mixed states there is no unique entanglement measure, but all entanglement measures should coincide on pure bipartite states and be equal to the von Neumann entropy of the reduced density matrix (uniqueness theorem).[5] Some important entanglement measures are defined as follows:

Entanglement cost: The entanglement cost tells us how expensive it is to create an entangled state ϱ, i.e., what is the ratio of the number of maximally entangled input states $|\Phi^+\rangle$ over the produced output states ϱ, minimized over all LOCC operations. In the limit of infinitely many outputs this reads

$$E_C(\varrho)=\inf_{\{\Lambda_{\mathrm{LOCC}}\}}\lim_{n_\varrho\to\infty}\frac{n^{in}_{|\Phi^+\rangle}}{n^{\mathrm{out}}_{\varrho}}. \tag{17}$$

Entanglement of formation: Any state ϱ can be decomposed as a convex combination of projectors onto pure states, $\varrho=\Sigma_i p_i|\psi_i\rangle\langle\psi_i|$. The entanglement of formation is the averaged von Neumann entropy of the reduced density matrices of the pure states $|\psi_i\rangle$, minimized over all possible decompositions,

$$E_F(\varrho)=\inf_{\{\mathrm{dec}\}}\sum_i p_i S(\varrho_{i,\mathrm{red}}). \tag{18}$$

Relative entropy of entanglement: The relative entropy can be seen intuitively as the ''distance'' of the entangled ϱ to the closest separable state σ, although it is not a distance in the mathematical sense,

$$E_R(\varrho)=\inf_{\sigma\in S}\mathrm{tr}[\varrho(\log\varrho-\log\sigma)]. \tag{19}$$

Distillable entanglement: The distillable entanglement tells us how much entanglement we can extract from an entangled state ϱ, i.e., what is the ratio of the number of maximally entangled output states $|\Phi^+\rangle$ over the needed input states ϱ, maximized over all LOCC operations. In the limit of infinitely many inputs this reads

$$E_D(\varrho)=\sup_{\{\Lambda_{\mathrm{LOCC}}\}}\lim_{n_\varrho\to\infty}\frac{n^{\mathrm{out}}_{|\Phi^+\rangle}}{n^{\mathrm{in}}_{\varrho}}. \tag{20}$$

There are some known relations between these entanglement measures: the distillable entanglement (entanglement cost) is a lower (upper) bound for *any* entanglement measure, i.e., $E_D(\varrho)\leqslant E(\varrho)\leqslant E_C(\varrho)$. For any bound entangled state $E_D(\varrho)<E_C(\varrho)$ holds, but there is also an example for a free entangled state, i.e., a distillable state, with the same property.[23] It is conjectured that the entanglement of formation and the entanglement cost are identical, i.e., $E_F(\varrho)\overset{?}{=}E_C(\varrho)$.

Some known and unknown properties of the entanglement measures discussed above are given in Table I.[24,25]

C. Schmidt witnesses

A slightly different question from ''how much entangled is a state ϱ?'' can be addressed via the generalization of entanglement witnesses to so-called Schmidt witnesses. They give an answer to the question ''how many degrees of freedom are entangled in ϱ?'' This corresponds to a finer classification of entangled states.

The Schmidt rank for pure bipartite states, as defined in Eq. (4), was generalized to the so-called Schmidt number k for mixed bipartite states in Ref. 26. For a given decomposition of ϱ into a convex combination of projectors onto pure states, let us call the highest occurring Schmidt rank $r_{\max}$. The Schmidt number is the minimization of this highest Schmidt rank over all possible decompositions:

$$\varrho=\sum_i p_i|\Psi_i^{r_i}\rangle\langle\Psi_i^{r_i}|,\quad k=\min_{\{\mathrm{dec}\}}(r_{\max}). \tag{21}$$

The Schmidt number cannot be higher than M, the smaller of the dimensions of the two subsystems.

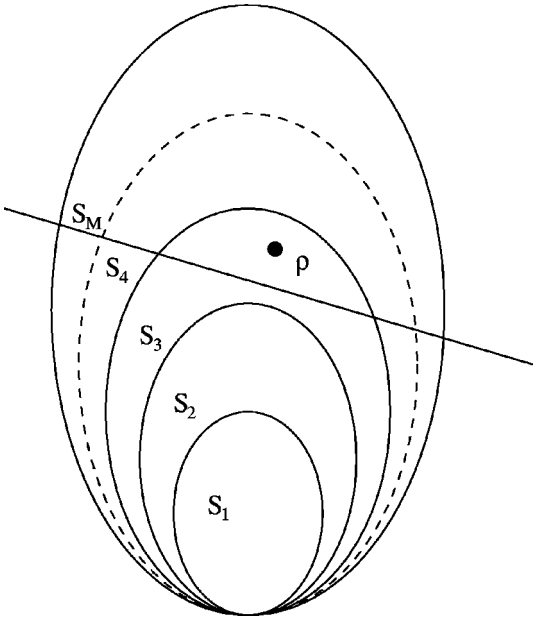

FIG. 7. Schmidt classes and the detection of the Schmidt number by a Schmidt witness.

Entangled states can now be classified according to Schmidt classes:[27] the Schmidt class S_k is a subset of the set of all density matrices and contains all density matrices with Schmidt number $\leqslant k$. The Schmidt classes are successively embedded into each other, as visualized in Fig. 7: $S_1 \subset S_2 \subset \ldots \subset S_M$.

A Schmidt witness $\mathcal{W}_k$ for the Schmidt class S_k is defined as a straightforward generalization of the entanglement witnesses discussed in Sec. III B. A Schmidt witness $\mathcal{W}_k$ is a Hermitian operator for which

$$\exists \varrho \in S_k \quad \text{with} \quad \mathrm{Tr}(\mathcal{W}_k \varrho) < 0, \tag{22}$$

$$\forall \varrho_{k-1} \in S_{k-1}: \quad \mathrm{Tr}(\mathcal{W}_k \varrho_{k-1}) \geqslant 0. \tag{23}$$

Constructive methods for Schmidt witnesses have been shown; they can be optimized in analogy with entanglement witnesses, and they can be used for example as a tool to study properties of bound entangled states.

D. "Many" systems: Pure three-qubit states

So far we have only considered bipartite systems. Unfortunately, according to current knowledge one already has to call three subsystems ''many.'' Can we generalize the concepts that were introduced so far to tripartite states? Again, one can ask whether a given state is separable or entangled. But now one can also specify the kind of entanglement: is it genuine three-particle entanglement or are just two of the three subsystems entangled? Like for bipartite states, one can ask whether a given tripartite state can be distilled. This question will not be addressed here, however. And, finally, does it make sense to ask ''how much is a given tripartite state entangled?''

For *pure* three-qubit states the situation is as follows:

A *separable* state can be written as

$$|\psi_S\rangle = |\phi_A\rangle \otimes |\phi_B\rangle \otimes |\phi_C\rangle. \tag{24}$$

A *biseparable* state is a state where only two out of the three systems are entangled, and the third system is a tensor product with the entangled ones, e.g., A–BC:

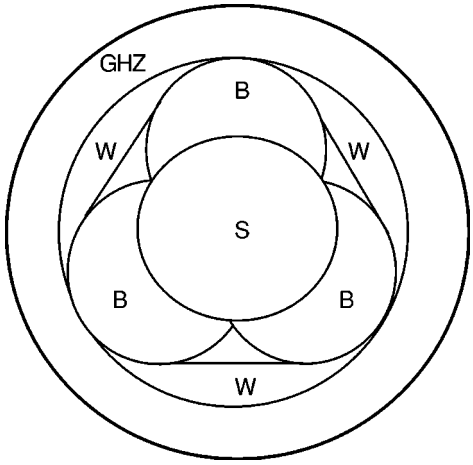

FIG. 8. Schematic structure of the set of all three-qubit states. *S*: separable class; *B*: biseparable class (convex hull of biseparable states with respect to any partition); *W*-class and GHZ-class.

$$|\psi_B\rangle = |\phi_A\rangle \otimes \sum_{i=1}^{2} a_i |e_i\rangle |f_i\rangle. \tag{25}$$

The other two possible partitions for biseparable states are B–AC and C–AB.

A *three-qubit correlated* state is one with genuine entanglement of all three subsystems. It was shown in Ref. 28 that there exist two classes of *inequivalent* states:

$$|\psi_{\mathrm{GHZ}}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle), \tag{26}$$

$$|\psi_W\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle). \tag{27}$$

Any three-qubit correlated pure state $|\psi\rangle$ can be transformed into either $|\psi_{\mathrm{GHZ}}\rangle$ or $|\psi_W\rangle$ by local reversible operations $\mathcal{A}\otimes\mathcal{B}\otimes\mathcal{C}$.

Therefore, it is not enough to ask whether a given three-qubit state is separable or biseparable or three-party entangled, but also whether a genuinely three-qubit entangled state belongs to the GHZ- or *W*-class. For mixed states, the tool of witness operators is again useful for this purpose, as will be discussed in the following subsection.

E. Classification of mixed three-qubit states

Let us introduce entanglement classes for mixed three-qubit states.[29] A mixed three-qubit state ϱ can be written as convex combination of pure states: if ϱ can be decomposed as a sum of projectors onto pure separable states $|\psi_S\rangle\langle\psi_S|$, then it belongs to the convex compact set S. If one needs at least one biseparable state $|\psi_B\rangle\langle\psi_B|$ in the sum, but no genuine tripartite entanglement, then ϱ belongs to the class B, more precisely to $B\setminus S$. In the same way we define the *W*-class (needs at least one *W*-state in the decomposition) and the GHZ-class (at least one GHZ-state needed).

These sets are embedded into each other: $S\subset B\subset W\subset \mathrm{GHZ}$. This is schematically shown in Fig. 8. It is important to note that $W\subset\mathrm{GHZ}$ and not the other way round: otherwise the class GHZ would not be compact, as can be seen by studying the most general form of a *W*-versus a GHZ-state, as given in Ref. 30.

In analogy to entanglement witnesses and Schmidt witnesses one can construct tripartite witnesses. A GHZ witness $\mathcal{W}_{\mathrm{GHZ}}$ is an Hermitian operator with $\mathrm{Tr}(\mathcal{W}_{\mathrm{GHZ}}\varrho)<0$ for some $\varrho \in \mathrm{GHZ}\setminus W$, and $\mathrm{Tr}(\mathcal{W}_{\mathrm{GHZ}}\varrho_W)\geqslant 0$ for all $\varrho_W \in W$. An example for a GHZ witness is given by

$$\mathcal{W}_{\mathrm{GHZ}}=\tfrac{3}{4}\mathbb{1}-P_{\mathrm{GHZ}}, \tag{28}$$

where P_{GHZ} is the projector onto $|\psi_{\mathrm{GHZ}}\rangle$, given in (26). It is straightforward to show that this operator has the desired properties, when one realizes that the maximal squared overlap between a pure W-state and $|\psi_{\mathrm{GHZ}}\rangle$ is given by $\frac{3}{4}$.

In a similar manner one can define a W-witness. An example for such a witness that detects a W-state, but has a positive or vanishing expectation value for all states in B, is given by

$$\mathcal{W}_W=\tfrac{2}{3}\mathbb{1}-P_W, \tag{29}$$

where P_W is the projector onto $|\psi_W\rangle$, given in (27), and $\frac{2}{3}$ is the maximal squared overlap between $|\psi_W\rangle$ and a pure biseparable state.

Using the witness in (29), one can show that the set of mixed $W\setminus B$-states is not of measure zero. This is contrary to the pure case, where W-states are of measure zero.[28] The idea of the proof is to show that there is a finite ball around a state from the family

$$\varrho=\frac{1-p}{8}\mathbb{1}+pP_W, \tag{30}$$

for a certain given parameter p, such that the ball is contained in the W-class. This is an example where the concept of witnesses helps to answer an explicit question about the structure of the set of entangled states.

Another interesting topic in this context is the properties of bound entangled states. Using again the tool of witness operators, there is some evidence that bound entangled three-qubit states cannot be in $\mathrm{GHZ}\setminus W$, i.e., they are at most in W.[29]

By studying mixed three-qubit states we have realized that in this case it is not enough to ask ''how much a given state is entangled.'' As there are different inequivalent entanglement classes, this question makes sense only within a given class W or GHZ. For more than three qubits the number of inequivalent classes grows fast.[28]

VI. SUMMARY

The section headings in this tutorial were phrased as questions. Let us summarize some answers.

What is entanglement?

There are many possible answers, maybe as many as there are researchers in this field.

Given a state ϱ, is it separable or entangled?

This question is easy to answer for pure states, and for low dimensions (2×2 and 2×3). It is very difficult to answer otherwise. Several separability criteria have been explained.

Given an entangled ϱ, is the entanglement useful?

We have discussed that states with a positive partial transpose are undistillable, most states with a nonpositive partial transpose (NPT) are distillable; but some NPT states are conjectured to be undistillable.

Given an entangled ϱ, how much is it entangled?

There are several different bipartite entanglement measures which quantify the degree of entanglement. For multipartite systems there are inequivalent entanglement classes, and therefore the above question has to be rephrased accordingly.

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The uniqueness theorem for entanglement measures

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We explore and develop the mathematics of the theory of entanglement measures. After a careful review and analysis of definitions, of preliminary results, and of connections between conditions on entanglement measures, we prove a sharpened version of a uniqueness theorem which gives necessary and sufficient conditions for an entanglement measure to coincide with the reduced von Neumann entropy on pure states. We also prove several versions of a theorem on extreme entanglement measures in the case of mixed states. We analyze properties of the asymptotic regularization of entanglement measures proving, for example, convexity for the entanglement cost and for the regularized relative entropy of entanglement. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1495917]

I. INTRODUCTION

Quantifying entanglement[1–4] is one of the central topics of quantum information theory. Any function that quantifies entanglement is called an entanglement measure. Entanglement is a complex property of a state and, for arbitrary states, there is no unique definitive measure. In general, there are two ''regimes'' under which entanglement can be quantified: they may be called the ''finite'' and the ''asymptotic'' regimes. The first deals with the entanglement of a single copy of a quantum state. In the second, one is interested in how entanglement behaves when one considers tensor products of a large number of identical copies of a given state. It turns out that by studying the asymptotic regime it is possible to obtain a clearer physical understanding of the nature of entanglement. This is seen, for example, in the so-called ''uniqueness theorem'' [3–6] which states that, under appropriate conditions, all entanglement measures coincide on pure bipartite states and are equal to the von Neumann entropy of the corresponding reduced density operator. However, this theorem was never rigorously proved under unified assumptions and definitions. Rather, there are various versions of the argument scattered through the literature.

In Ref. 4, the uniqueness theorem was put into a more general perspective. Namely, there are two basic measures of entanglement[1]—entanglement of distillation (E_D) and entanglement cost (E_C)—having the following dual meanings:

(i) $E_D(\varrho)$ is the maximal number of singlets that can be produced from the state ϱ by means of local quantum operations and classical communication (LQCC operations).
(ii) $E_C(\varrho)$ is the minimal number of singlets needed to produce the state ϱ by LQCC operations.

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[More precisely (cf. Definitions 16 and 17): $E_D(\varrho)$ ($E_C(\varrho)$) is the maximal (minimal) number of singlets *per copy* distillable from the state ϱ (needed to form ϱ) by LQCC operations in the asymptotic regime of $n\to\infty$ copies.] It is important here that the conversion is not required to be perfect: the transformed state needs to converge to the required state only in the limit of large n. Now, in Ref. 4 it was shown that the two basic measures of entanglement are, respectively, a lower and an upper bound for any entanglement measure satisfying appropriate postulates in the asymptotic regime.[7] This suggests the following clear picture: entanglement cost and entanglement of distillation are extreme measures, and provided they coincide on pure states, all other entanglement measures coincide with them on pure states as well. However, as mentioned above, the fact that E_D and E_C coincide on pure states was not proven rigorously. Moreover, it turned out that the postulates are too strong. They include convexity, and some additivity and continuity requirements. It is not known whether any measure exists which satisfies all the requirements. E_D and E_C satisfy the additivity requirement, but it is not known whether or not they are continuous in the sense of Ref. 4. There are also indications that the entanglement of distillation is not convex.[8] On the other hand, two other important measures, the *entanglement of formation* (denoted by E_F) and the *relative entropy of entanglement* (denoted by E_R) are continuous[6,9] and convex, but there are problems with additivity. The relative entropy of entanglement is certainly not additive,[10] and we do not know about the entanglement of formation.

In this situation it is desirable to prove the uniqueness theorem from first principles, and to study to what extent we can relax the assumptions and still get uniqueness of entanglement measures on pure states. In the present article we have solved the problem completely by providing *necessary and sufficient* conditions for a measure of entanglement to be equal to the von Neumann entropy of the reduced density operator for pure states. We also show that if we relax the postulate of asymptotic continuity, then any measure of entanglement (not unique any longer) for pure states must lie between the two analogs of E_D and E_C corresponding to *perfect* fidelity of conversion. These are $\tilde{E}_C(\psi)=S_0(\varrho)$ and $\tilde{E}_D(\psi)=S_\infty(\varrho)$, where ϱ is the reduced density matrix of $|\psi\rangle$, and S_0, S_∞ are Rènyi entropies. In Refs. 11 and 12, one of us has studied entanglement measures based on cross norms and proved an alternative uniqueness theorem for entanglement measures stemming from the Khinchin–Faddeev characterization of Shannon entropy.

The present article also contains further developments on the problem of extreme measures. We provide two useful new versions of the theorem of Ref. 4. In one of them, we show that for any (suitably normalized) function E for which the regularization $E^\infty(\varrho)=\lim_{n\to\infty}E(\varrho^{\otimes n})/n$ exists and which is (i) nonincreasing under local quantum operations and classical communication (LQCC operations) and (ii) asymptotically continuous, the regularization E^∞ must lie between E_D and E_C. The theorem and its proof can easily be generalized by replacing the class of LQCC operations by other classes of operations, or by considering conversions between any two states. Moreover, it is valid for multipartite cases. Therefore, the result will be an important tool for analyzing asymptotic conversion rates between different states. In particular, it follows from our result that to establish irreversibility of conversion between two states (see Ref. 13), one needs to compare regularizations of asymptotically continuous entanglement measures for these states.

In the other new version of the extreme measures theorem, we are able to weaken the postulates of Ref. 4, so that they are at least satisfied by E_C. On the other hand, we do not have a proof that E_D is asymptotically continuous for mixed states, although there is strong evidence that this is the case. If it is, then we would finally have a form of the theorem, in which both E_D and E_C could be called extreme measures, not only in the sense provided by the inequalities we prove, but also in the sense that they belong to the set described by the postulates.

To obtain our results we perform a detailed study of possible postulates for entanglement measures in the finite and the asymptotic regime. In particular, we examine which postulates survive the operation of regularization. We show that if a function is convex and subadditive [i.e., $f(\varrho\otimes\sigma)\leqslant f(\varrho)+f(\sigma)$], then its regularization is convex, too. Hence, both the regularization of the relative entropy of entanglement[2] as well as of the entanglement of formation[1] are convex.

It should be emphasized that our results are stated and proved in language accessible for mathematicians or mathematical physicists who have not previously been involved in quantum

information theory. This is in contrast to many papers in this field, where many implicit assumptions are obstacles for understanding the meaning of the theorems and their proofs by nonspecialists. For this reason, we devote Secs. II and III to careful statements of some essential definitions and results. In Sec. IV we present a self-contained and straightforward proof of the difficult implication in Nielsen's theorem. This is a theorem which we shall use several times. Properties of entanglement measures and relations between them are analyzed in Sec. V. The most prominent entanglement measures—entanglement of distillation, entanglement cost, entanglement of formation and relative entropy of entanglement—are defined and studied in Sec. VI. In Sec. VII we present our versions of the theorem on extreme measures. Finally, Sec. VIII contains our version of the uniqueness theorem for entanglement measures, stating necessary and sufficient conditions for a functional to coincide with the reduced von Neumann entropy on pure states.

II. PRELIMINARIES

Throughout this article, all spaces considered are assumed to be finite dimensional. The set of trace class operators on a Hilbert space $\mathcal{H}$ is denoted by $\mathcal{T}(\mathcal{H})$ and the set of bounded operators on $\mathcal{H}$ by $\mathcal{B}(\mathcal{H})$. A density operator (or *state*) is a positive trace class operator with trace one. The set of states on $\mathcal{H}$ is denoted by $\Sigma(\mathcal{H})$ and the set of pure states by $\Sigma_p(\mathcal{H})$. The trace class norm on $\mathcal{T}(\mathcal{H})$ is denoted by $\|\cdot\|_1$. For a wavefunction $|\psi\rangle \in \mathcal{H}$ the corresponding state will be denoted by $P_\psi \equiv |\psi\rangle\langle\psi|$. The *support* of a trace class operator is the subspace spanned by its eigenvectors with nonzero eigenvalues.

In the present article we restrict ourselves mainly to the situation of a composite quantum system consisting of two subsystems with Hilbert space $\mathcal{H}^A \otimes \mathcal{H}^B$ where $\mathcal{H}^A$ and $\mathcal{H}^B$ denote the Hilbert spaces of the subsystems. Often these systems are to be thought of as being spatially separate and accessible to two independent observers, Alice and Bob.

Definition 1: Let $\mathcal{H}^A$ and $\mathcal{H}^B$ be Hilbert spaces. A density operator ϱ on the tensor product $\mathcal{H}^A \otimes \mathcal{H}^B$ is called separable *or* disentangled *if there exist a sequence (r_i) of positive real numbers, a sequence (ρ_i^A) of density operators on $\mathcal{H}^A$ and a sequence (ρ_i^B) of density operators on $\mathcal{H}^B$ such that*

$$\varrho = \sum_i r_i \rho_i^A \otimes \rho_i^B, \tag{1}$$

where the sum converges in trace class norm.

The Schmidt decomposition[14] is of central importance in the characterization and quantification of entanglement associated with pure states.

Lemma 2: Let $\mathcal{H}^A$ and $\mathcal{H}^B$ be Hilbert spaces and let $|\psi\rangle \in \mathcal{H}^A \otimes \mathcal{H}^B$. Then there exist a sequence of non-negative real numbers $(p_i)_i$ summing to one and orthonormal bases $(|a_i\rangle)_i$ and $(|b_i\rangle)_i$ of $\mathcal{H}^A$ and $\mathcal{H}^B$, respectively, such that

$$|\psi\rangle = \sum_i \sqrt{p_i} |a_i \otimes b_i\rangle.$$

■

By $S(\varrho)$ we will denote von Neumann entropy of the state ϱ given by

$$S(\varrho) := -\operatorname{tr}\varrho \log_2 \varrho. \tag{2}$$

The *von Neumann reduced entropy* for a pure state σ on a tensor product Hilbert space $\mathcal{H}^A \otimes \mathcal{H}^B$ is defined as

$$S_{\mathrm{vN}}(\sigma) := -\operatorname{tr}_A((\operatorname{tr}_B \sigma)\log_2(\operatorname{tr}_B \sigma)), \tag{3}$$

where tr_A and tr_B denote the partial traces over $\mathcal{H}^A$ and $\mathcal{H}^B$, respectively. For $\sigma = P_\psi = |\psi\rangle\langle\psi|$, it is a straightforward consequence of Lemma 2 that

$$-\mathrm{tr}_A((\mathrm{tr}_B P_\psi)\log_2(\mathrm{tr}_B P_\psi)) = -\mathrm{tr}_B((\mathrm{tr}_A P_\psi)\log_2(\mathrm{tr}_A P_\psi)) = -\sum_i p_i \log_2 p_i,$$

where $(p_i)_i$ denotes the sequence of Schmidt coefficients of $|\psi\rangle$. However, for a general mixed state σ, $\mathrm{tr}_A((\mathrm{tr}_B\sigma)\log_2(\mathrm{tr}_B\sigma))$ may not equal $\mathrm{tr}_B((\mathrm{tr}_A\sigma)\log_2(\mathrm{tr}_A\sigma))$.

III. CLASSES OF QUANTUM OPERATIONS

In quantum information theory it is important to distinguish between the class of quantum operations on a composite quantum system which can be realized by separate *local* actions on the subsystems (i.e., separate actions by ''Alice'' and by ''Bob'') and those which cannot. The class of local quantum operations assisted by classical communication (LQCC) is of central importance in quantum cryptography and the emerging theory of quantum entanglement.

An *operation* is a positive linear map $\Lambda:\mathcal{T}(\mathcal{H}_1)\to\mathcal{T}(\mathcal{H}_2)$ such that $\mathrm{tr}(\Lambda(\sigma))\leqslant 1$ for all $\sigma\in\Sigma(\mathcal{H}_1)$. *Quantum operations* are operations which are *completely positive*.[15,16] We shall be interested in the trace preserving quantum operations. By the Choi–Kraus representation,[15–18] these are precisely the linear maps $\Lambda:\mathcal{T}(\mathcal{H}_1)\to\mathcal{T}(\mathcal{H}_2)$ which can be written in the form $\Lambda(B)=\Sigma_{i=1}^{n_1 n_2} W_i B W_i^\dagger$ for $B\in\mathcal{T}(\mathcal{H}_1)$ with operators $W_i:\mathcal{H}_1\to\mathcal{H}_2$ satisfying $\Sigma_{i=1}^{n_1 n_2} W_i^\dagger W_i = 1_1$, where $n_1\equiv\dim\mathcal{H}_1$, $n_2\equiv\dim\mathcal{H}_2$, and 1_1 is the identity operator on $\mathcal{H}_1$. These can also be characterized as precisely the linear maps which can be composed out of the following elementary operations.

(O1) Adding an uncorrelated ancilla:
$\Lambda_1:\mathcal{T}(\mathcal{H}_1)\to\mathcal{T}(\mathcal{H}_1\otimes\mathcal{K}_1)$, $\Lambda_1(\rho):=\rho\otimes\sigma$, where $\mathcal{H}_1$ and $\mathcal{K}_1$ denote the Hilbert spaces of the original quantum system and of the ancilla, respectively, and where $\sigma\in\Sigma(\mathcal{K}_1)$.

(O2) Tracing out part of the system:
$\Lambda_2:\mathcal{T}(\mathcal{H}_2\otimes\mathcal{K}_2)\to\mathcal{T}(\mathcal{H}_2)$, $\Lambda_2(\rho):=\mathrm{tr}_{\mathcal{K}_2}(\rho)$, where $\mathcal{H}_2\otimes\mathcal{K}_2$ and $\mathcal{K}_2$ denote the Hilbert spaces of the full original quantum system and of the dismissed part, respectively, and where $\mathrm{tr}_{\mathcal{K}_2}$ denotes the partial trace over $\mathcal{K}_2$.

(O3) Unitary transformations:
$\Lambda_3:\mathcal{T}(\mathcal{H}_3)\to\mathcal{T}(\mathcal{H}_3)$, $\Lambda_3(\rho):=U\rho U^\dagger$, where U is a unitary operator on $\mathcal{H}_3$.

A discussion of this material with complete proofs from first principles may be found in the initial archived draft of this article.[19]

Defining a local operation as quantum operation on a individual subsystem, we now turn to the definition of local operations assisted by classical communication. As always in this article we consider a quantum system consisting of two (possibly separate) subsystems A and B with (initial) Hilbert spaces $\mathcal{H}^A$ and $\mathcal{H}^B$, respectively. There are three cases: the communication between A and B can be unidirectional (in either direction) or bidirectional.

Let us first define the class of local quantum operations (LO) assisted by unidirectional classical communication (operations in this class will be called one-way LQCC operations) with direction from system A (Alice) to system B (Bob). In this case, the operations performed by Bob depend on Alice's operations, but not conversely.

Definition 3: A completely positive map $\Lambda:\mathcal{T}(\mathcal{H}_1^A\otimes\mathcal{H}_1^B)\to\mathcal{T}(\mathcal{H}_2^A\otimes\mathcal{H}_2^B)$ is called a one-way LQCC *operation from A to B if it can be written in the form*

$$\Lambda(\sigma)=\sum_{i,j=1}^{K,L}(1_2^A\otimes W_{ji}^B)(V_i^A\otimes 1_1^B)\sigma(V_i^{A\dagger}\otimes 1_1^B)(1_2^A\otimes W_{ji}^{B\dagger}) \tag{4}$$

for all $\sigma\in\mathcal{T}(\mathcal{H}_1^A\otimes\mathcal{H}_1^B)$ and some sequences of operators $(V_i^A:\mathcal{H}_1^A\to\mathcal{H}_2^A)_i$ and $(W_{ji}^B:\mathcal{H}_1^B\to\mathcal{H}_2^B)_{ji}$ with $\Sigma_{i=1}^K V_i^{A\dagger}V_i^A=1_1^A$ and $\Sigma_{j=1}^L W_{ji}^{B\dagger}W_{ji}^B=1_1^B$ for each i, where 1_1^A, 1_1^B and 1_2^A are the unit operators acting on the Hilbert spaces $\mathcal{H}_1^A$, $\mathcal{H}_1^B$ and $\mathcal{H}_2^A$, respectively.

Of course, by the Choi–Kraus representation any operation Λ of the form

$$\Lambda=\Lambda^A\otimes I_1^B, \tag{5}$$

where $\Lambda^A:\mathcal{T}(\mathcal{H}_1^A)\to\mathcal{T}(\mathcal{H}_2^A)$ is a completely positive trace preserving map and I_1^B is the identity operator on $\mathcal{T}(\mathcal{H}_1^B)$, is a one-way LQCC operation from A to B.

Let us now define local quantum operations assisted by bidirectional classical communication (LQCC operations).

Definition 4: A completely positive map $\Lambda:\mathcal{T}(\mathcal{H}^A\otimes\mathcal{H}^B)\to\mathcal{T}(\mathcal{K}^A\otimes\mathcal{K}^B)$ is called an LQCC *operation if there exist $n>0$ and sequences of Hilbert spaces $(\mathcal{H}_k^A)_{k=1}^{n+1}$ and $(\mathcal{H}_k^B)_{k=1}^{n+1}$ with $\mathcal{H}_1^{A(B)}=\mathcal{H}^{A(B)}$ and $\mathcal{H}_{n+1}^{A(B)}=\mathcal{K}^{A(B)}$, such that Λ can be written in the following form,*

$$\Lambda(\sigma)=\sum_{i_1,\ldots,i_{2n}=1}^{K_1,\ldots,K_{2n}} V_{i_1,\ldots,i_{2n}}^{AB}\sigma V_{i_1,\ldots,i_{2n}}^{AB\,\dagger} \tag{6}$$

for all $\sigma\in\mathcal{T}(\mathcal{H}^A\otimes\mathcal{H}^B)$ where $V_{i_1,\ldots,i_{2n}}^{AB}:\mathcal{H}^A\otimes\mathcal{H}^B\to\mathcal{K}^A\otimes\mathcal{K}^B$ is given by

$$V_{i_1,\ldots,i_{2n}}^{AB}:=(\mathbb{1}_{n+1}^A\otimes W_{2n}^{i_{2n},\ldots,i_1})(V_{2n-1}^{i_{2n-1},\ldots,i_1}\otimes\mathbb{1}_n^B)(\mathbb{1}_n^A\otimes W_{2n-2}^{i_{2n-2},\ldots,i_1})\cdots(\mathbb{1}_2^A\otimes W_2^{i_2,i_1})(V_1^{i_1}\otimes\mathbb{1}_1^B)$$

with families of operators

$$(V_{2k-1}^{i_{2k-1},\ldots,i_1}:\mathcal{H}_k^A\to\mathcal{H}_{k+1}^A)_{k=1}^n, \tag{7a}$$

$$(W_{2k}^{i_{2k},\ldots,i_1}:\mathcal{H}_k^B\to\mathcal{H}_{k+1}^B)_{k=1}^n, \tag{7b}$$

such that for $k=0,\ldots,n-1$ and each sequence of indices $(i_{2k},\ldots,i_1)$,

$$\sum_{i_{2k+1}=1}^{K_{2k+1}}(V_{2k+1}^{i_{2k+1},\ldots,i_1})^\dagger V_{2k+1}^{i_{2k+1},\ldots,i_1}=\mathbb{1}_{k+1}^A, \tag{8a}$$

and for $k=1,\ldots,n$ and each sequence of indices $(i_{2k-1},\ldots,i_1)$,

$$\sum_{i_{2k}=1}^{K_{2k}}(W_{2k}^{i_{2k},\ldots,i_1})^\dagger W_{2k}^{i_{2k},\ldots,i_1}=\mathbb{1}_k^B, \tag{8b}$$

where for all $k>0$, $\mathbb{1}_k^A$ and $\mathbb{1}_k^B$ denote the unit operator on $\mathcal{H}_k^A$ and $\mathcal{H}_k^B$, respectively.

Obviously the class of one-way LQCC operations is a subclass of the class of LQCC operations. There is another important class: separable operations. A separable operation is an operation of the form

$$\Lambda:\mathcal{T}(\mathcal{H}^A\otimes\mathcal{H}^B)\to\mathcal{T}(\mathcal{K}^A\otimes\mathcal{K}^B),\quad \Lambda(\sigma)\equiv\sum_{i=1}^k (V_i\otimes W_i)\sigma(V_i\otimes W_i)^\dagger, \tag{9}$$

with $\Sigma_{i=1}(V_i\otimes W_i)^\dagger V_i\otimes W_i=\mathbb{1}^{AB}$ where $\mathbb{1}^{AB}$ denotes the unit operator acting on $\mathcal{H}^A\otimes\mathcal{H}^B$. The class of separable operations is strictly larger than the LQCC class.[20]

One can also consider a small class obtained by taking the convex hull C of the set of all maps of the form $\Lambda^A\otimes\Lambda^B$. Such operations require in general one-way classical communication, but they do not cover the whole class of one-way LQCC operations.

All the classes above are closed under tensor multiplication, convex combinations, and composition. The results of our article apply in principle to all the classes apart from the last (i.e., apart from the class of all operations in the convex hull C of the set of all maps of the form $\Lambda^A\otimes\Lambda^B$). For definiteness, in the sequel we will use LQCC operations.

Finally, we conclude this section with a useful technical lemma.

Lemma 5: Let $\Lambda:\mathcal{T}(\mathcal{H}_1)\to\mathcal{T}(\mathcal{H}_2)$ be a positive trace-preserving map and suppose that $B\in\mathcal{T}(\mathcal{H}_1)$ with $B=B^\dagger$. Then $\|\Lambda(B)\|_1\leqslant\|B\|_1$.

Proof: Suppose that B has eigenvalue expansion $B=\Sigma_{i=1}^{n_1}\beta_i|\psi_i\rangle\langle\psi_i|$. Then

$$\|\Lambda(B)\|_1 \leqslant \sum_{i=1}^{n_1} |\beta_i| \|\Lambda(|\psi_i\rangle\langle\psi_i|)\|_1 = \|B\|_1$$

as $\|B\|_1 = \Sigma_{i=1}^{n_1} |\beta_i|$ and $\Lambda(|\psi_i\rangle\langle\psi_i|)$ is a positive trace class operator with unit trace. ■

IV. NIELSEN'S THEOREM

A beautiful and powerful result of entanglement theory is Nielsen's theorem.[21] In one direction, the proof is straightforward, and we refer to Ref. 21. The other direction is more difficult. We present here an entirely self-contained, simple, and direct proof. Alternative proofs have previously been given by Hardy[22] and by Jensen and Schack.[23]

Before we state the theorem we need the following definition.

Definition 6: Let $(p_i)_{i=1}^{m_1}$ *and* $(q_i)_{i=1}^{m_2}$ *be two probability distributions with probabilities arranged in decreasing order, i.e.,* $p_1 \geqslant p_2 \geqslant \cdots \geqslant p_{m_1}$ *and similarly for* $(q_i)_i$. *Then we will say that* $(q_i)_i$ majorizes $(p_i)_i$ [*in symbols* $(q_i)_i \succ (p_i)_i$] *if for all* $k \leqslant \min\{m_1, m_2\}$ *we have*

$$\sum_{i=1}^{k} q_i \geqslant \sum_{i=1}^{k} p_i . \tag{10}$$

Theorem 7 (Nielsen): *Let* $\mathcal{H}^A$ *and* $\mathcal{H}^B$ *be Hilbert spaces and let* $(|\chi_m\rangle)_{m=1}^M$ *and* $(|\kappa_m\rangle)_{m=1}^M$ *be orthonormal bases for* $\mathcal{H}^A$ *and* $\mathcal{H}^B$, *respectively. Let* $|\Psi\rangle = \Sigma_{m=1}^M \sqrt{p_m}|\chi_m \kappa_m\rangle$ *and* $|\Phi\rangle = \Sigma_{m=1}^M \sqrt{q_m}|\chi_m \kappa_m\rangle$ *be Schmidt decompositions of normalized vectors* $|\Psi\rangle$ *and* $|\Phi\rangle$ *in* $\mathcal{H}^A \otimes \mathcal{H}^B$ *with* $p_1 \geqslant p_2 \geqslant \cdots \geqslant p_M$ *and* $q_1 \geqslant q_2 \geqslant \cdots \geqslant q_M$. *Then* $|\Psi\rangle\langle\Psi|$ *can be converted into* $|\Phi\rangle\langle\Phi|$ *by* LQCC *operations if and only if* (q_i) *majorizes* (p_i).

Proof: (One direction only.) Suppose that (q_i) majorizes (p_i). Set $\rho \equiv |\Psi\rangle\langle\Psi|$ and $\sigma \equiv |\Phi\rangle\langle\Phi|$. We shall prove that there is a sequence $(\Lambda_n)_{n=1}^N$ with $N < M$ of completely positive maps on $\mathcal{T}(\mathcal{H}^A \otimes \mathcal{H}^B)$ of the form

$$\Lambda_n(\omega) = (C_n \otimes U_n)\omega(C_n \otimes U_n)^\dagger + (D_n \otimes V_n)\omega(D_n \otimes V_n)^\dagger, \tag{11}$$

where U_n, $V_n \in \mathcal{B}(\mathcal{H}^B)$ are unitary and C_n, $D_n \in \mathcal{B}(\mathcal{H}^A)$ satisfy $C_n^\dagger C_n + D_n^\dagger D_n = \mathbb{1}^A$ such that $\Lambda_1 \circ \Lambda_2 \circ \cdots \circ \Lambda_N(\rho) = \sigma$. Note that all the Λ_n are one-way LQCC operations from A to B and hence their composition also is. As the Schmidt decomposition is symmetrical between A and B, we could also use one-way LQCC operations from B to A. Set $\delta_k \equiv \Sigma_{m=1}^k q_m - \Sigma_{m=1}^k p_m$ for $k = 1,2,\ldots,M$. Then $\delta_M = 0$. Let $N = N(|\Psi\rangle, |\Phi\rangle)$ be the number of nonzero δ_k. We shall prove the result by induction on N. $|\Psi\rangle = |\Phi\rangle$ if and only if $\delta_1 = \delta_2 = \cdots = \delta_{M-1} = 0$. In this case $N(|\Psi\rangle, |\Phi\rangle) = 0$, $\rho = \sigma$, and the result is certainly true.

Suppose that the result holds for all pairs $(|\Psi\rangle, |\Phi\rangle)$ satisfying the conditions of the proposition with $N(|\Psi\rangle, |\Phi\rangle) = 0,\ldots,L$ and that $(|\Psi\rangle, |\Phi\rangle)$ is a pair with $N(|\Psi\rangle, |\Phi\rangle) = L+1$. Then there exists $J \geqslant 1$ such that $\delta_1 = \delta_2 = \cdots = \delta_{J-1} = 0$ and $\delta_J > 0$. Setting $\delta_0 := 0$, we have $q_j - p_j = \delta_{j-1} + q_j - p_j = \delta_j$ for $j = 1,\ldots,J$. This implies that $p_j = q_j$ for $j = 1,\ldots,J-1$ and that $q_J > p_J$. Suppose that $\delta_k > 0$ for $k = J, J+1,\ldots,K-1$ and that $\delta_K = 0$. $p_K - q_K = p_K - q_K + \delta_K = \delta_{K-1}$ and $p_K > q_K$. Moreover, if $K < M$, then $q_{K+1} - p_{K+1} = \delta_K + q_{K+1} - p_{K+1} = \delta_{K+1} \geqslant 0$. Summarizing, we have

$$p_{J-1} = q_{J-1} \geqslant q_J > p_J \geqslant p_K > q_K \geqslant q_{K+1} \geqslant p_{K+1}.$$

Define $(r_m)_{m=1}^M$ by $r_m := p_m$ for $m \neq J, K$ and by $r_J := p_J + \delta$, $r_K := p_K - \delta$ where $\delta := \min\{\delta_k : k = J,\ldots,K-1\}$. By construction $\delta > 0$. Now $\delta \leqslant \delta_J$ implies $q_J \geqslant r_J \geqslant p_J$, and $\delta \leqslant \delta_{K-1}$ implies $p_K \geqslant r_K \geqslant q_K$. This in turn implies that $r_1 \geqslant r_2 \geqslant \cdots \geqslant r_M$. Thus for $k = 1,\ldots,J-1$ and for $k = K,\ldots,M$,

$$\sum_{m=1}^{k} r_m = \sum_{m=1}^{k} p_m \leqslant \sum_{m=1}^{k} q_m .$$

For $k=J,\ldots,K-1$, $\Sigma_{m=1}^{k} r_m = \Sigma_{m=1}^{k} p_m + \delta$ and so, as $0<\delta\leqslant\delta_k$,

$$\sum_{m=1}^{k} p_m < \sum_{m=1}^{k} r_m \leqslant \sum_{m=1}^{k} q_m .$$

Define $|\Xi\rangle := \Sigma_{m=1}^{M} \sqrt{r_m}|\chi_m \kappa_m\rangle$. Then $N(|\Xi\rangle,|\Phi\rangle)\leqslant L$ so that, by the inductive hypothesis, there is a sequence $(\Lambda_n)_{n=1}^{N}$ of maps of the required form with $N=N(|\Xi\rangle,|\Phi\rangle)$ such that

$$\Lambda_1 \circ \Lambda_2 \circ \cdots \circ \Lambda_N(|\Xi\rangle\langle\Xi|) = \sigma.$$

Thus to complete the proof, we need only find a completely positive map Λ of the required form such that

$$\Lambda(|\Psi\rangle\langle\Psi|) = |\Xi\rangle\langle\Xi|. \tag{12}$$

To this end set $P := \Sigma_{m\neq J,K}|\chi_m\rangle\langle\chi_m|$. Set

$$C := \sqrt{\frac{r_J p_J - r_K p_K}{r_J^2 - r_K^2}}\left(P + \sqrt{\frac{r_J}{p_J}}|\chi_J\rangle\langle\chi_J| + \sqrt{\frac{r_K}{p_K}}|\chi_K\rangle\langle\chi_K| \right)$$

and $U := 1^B$. Set

$$D := \sqrt{\frac{r_J p_K - r_K p_J}{r_J^2 - r_K^2}}\left(P + \sqrt{\frac{r_K}{p_J}}|\chi_K\rangle\langle\chi_J| + \sqrt{\frac{r_J}{p_K}}|\chi_J\rangle\langle\chi_K| \right)$$

and

$$V := |\kappa_K\rangle\langle\kappa_J| + |\kappa_J\rangle\langle\kappa_K| + \sum_{m\neq J,K} |\kappa_m\rangle\langle\kappa_m|.$$

Note that $p_J \geqslant p_K > q_K \geqslant 0$, that $r_J > r_K$, that $r_J p_J > r_K p_K$, and that $r_J p_K - r_K p_J = (p_J+\delta)p_K - (p_K-\delta)p_J = \delta(p_K+p_J) > 0$. Note also that $r_J^2 - r_K^2 = (r_J - r_K)(r_J + r_K) = (r_J - r_K)(p_J + p_K)$ so that

$$\frac{r_J p_J - r_K p_K}{r_J^2 - r_K^2} + \frac{r_J p_K - r_K p_J}{r_J^2 - r_K^2} = 1.$$

With these definitions and notes, the completion of the proof is straightforward. ■

V. ENTANGLEMENT MEASURES

Definition 8: Consider a bipartite composite quantum system with Hilbert space of the form $\mathcal{H}^A \otimes \mathcal{H}^B$ where $\mathcal{H}^A \equiv \mathcal{H}^B \equiv \mathbb{C}^d$. Assume that isomorphisms between $\mathbb{C}^d$, $\mathcal{H}^A$, and $\mathcal{H}^B$ are chosen. For a chosen orthonormal basis $(|\psi_i\rangle)_{i=1}^{d}$ of $\mathbb{C}^d$, we let

$$|\Psi_+(\mathbb{C}^d)\rangle \equiv \sum_{i=1}^{d} \frac{1}{\sqrt{d}}|\psi_i \otimes \psi_i\rangle \in \mathcal{H}^A \otimes \mathcal{H}^B.$$

$|\Psi_+(\mathbb{C}^d)\rangle$ *is a* maximally entangled *wavefunction. All other maximally entangled wavefunctions in* $\mathcal{H}^A\otimes\mathcal{H}^B$ *can be obtained by applying a unitary operator of the form* $\mathbb{1}^A\otimes U^B$ *to* $|\Psi_+(\mathbb{C}^d)\rangle$ *where* U^B *is a unitary operator on* $\mathcal{H}^B$. *The pure state corresponding to* $|\Psi_+(\mathbb{C}^d)\rangle$ *will be denoted by* $P_+(\mathbb{C}^d)\equiv|\Psi_+(\mathbb{C}^d)\rangle\langle\Psi_+(\mathbb{C}^d)|$.

In an arbitrary bipartite composite system, we shall refer to any wavefunction with the same Schmidt coefficients as $|\Psi_+(\mathbb{C}^d)\rangle$ *as a* representative *of* $|\Psi_+(\mathbb{C}^d)\rangle$ *and to the corresponding state as a* representative *of* $P_+(\mathbb{C}^d)$.

A. Conditions on mixed states

The degree of entanglement of a density operator on the Hilbert space of a bipartite composite quantum system can be expressed by an ''entanglement measure.'' This is a non-negative real-valued functional E defined on $\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$ for all finite-dimensional Hilbert spaces $\mathcal{H}^A$ and $\mathcal{H}^B$. Any of the following conditions might be imposed on E.[1–4,24]

(E0) If σ is separable, then $E(\sigma)=0$.

(E1) (Normalization) If P_+^d is any representative of $P_+(\mathbb{C}^d)$, then $E(P_+^d)=\log_2 d$ for $d=1,2,\ldots$.

A weaker condition is the following.

(E1′) $E(P_+(\mathbb{C}^2))=1$.

(E2) (LQCC Monotonicity) Entanglement cannot increase under procedures consisting of local operations on the two quantum systems and classical communication. If Λ is an LQCC operation, then

$$E(\Lambda(\sigma))\leqslant E(\sigma) \tag{13}$$

for all $\sigma\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$.

A condition which, as we shall confirm below (Lemma 9), is weaker than (E2), is the following.

(E2′) $E(\Lambda(\sigma))=E(\sigma)$ whenever $\sigma\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$ and Λ is a strictly local operation which is either unitary or which adds extraneous dimensions. On Alice's side, these local operations take the form of either $\Lambda_1(\varrho)=(U^A\otimes I^B)\varrho(U^A\otimes I^B)^\dagger$ where $U^A:\mathcal{H}^A\to\mathcal{H}^A$ is unitary or $\Lambda_2(\varrho)=(W^A\otimes I^B)\varrho(W^A\otimes I^B)^\dagger$ where $\mathcal{H}^A\subset\mathcal{K}^A$ and $W^A:\mathcal{H}^A\to\mathcal{K}^A$ is the inclusion map. There are equivalent local operations on Bob's side.

(E2″) $E(\Lambda(\sigma))=E(\sigma)$ whenever $\sigma\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$ and Λ is a strictly local unitary operation. Without further remark, we shall always assume that all our measures satisfy (E2″).

(E3) (Continuity) Let $(\mathcal{H}_n^A)_{n\in\mathbb{N}}$ and $(\mathcal{H}_n^B)_{n\in\mathbb{N}}$ be sequences of Hilbert spaces and let $\mathcal{H}_n\equiv\mathcal{H}_n^A\otimes\mathcal{H}_n^B$ for all n. For all sequences $(\varrho_n)_{n\in\mathbb{N}}$ and $(\sigma_n)_{n\in\mathbb{N}}$ of states with $\varrho_n,\sigma_n\in\Sigma(\mathcal{H}_n^A\otimes\mathcal{H}_n^B)$, such that $\|\varrho_n-\sigma_n\|_1\to 0$, we require that

$$\frac{E(\varrho_n)-E(\sigma_n)}{1+\log_2\dim\mathcal{H}_n}\to 0.$$

A weaker condition deals only with approximations to pure states:

(E3′) Same as (E3) but with $\varrho_n\in\Sigma_p(\mathcal{H}_n^A\otimes\mathcal{H}_n^B)$ for all n.

Sometimes we are interested in entanglement measures which satisfy an additivity property:

(E4) (Additivity) For all $n\geqslant 1$ and all $\varrho\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$

$$\frac{E(\varrho^{\otimes n})}{n}=E(\varrho).$$

Here $\varrho^{\otimes n}$ denotes the n-fold tensor product of ϱ by itself which acts on the tensor product $(\mathcal{H}^A)^{\otimes n}\otimes(\mathcal{H}^B)^{\otimes n}$.

An apparently weaker property, which as we shall see in Lemma 10 is actually equivalent to (E4), is the following.

(E4′) (Asymptotic Additivity) Given $\epsilon>0$ and $\varrho\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$, there exists an integer $N>0$ such that $n\geqslant N$ implies

$$\frac{E(\varrho^{\otimes n})}{n}-\epsilon\leqslant E(\varrho)\leqslant\frac{E(\varrho^{\otimes n})}{n}+\epsilon.$$

(E5) (Subadditivity) For all $\varrho,\sigma\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$,

$$E(\varrho\otimes\sigma)\leqslant E(\varrho)+E(\sigma).$$

(E5′) For all $\varrho\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$ and $m,n\geqslant 1$,

$$E(\varrho^{\otimes(m+n)})\leqslant E(\varrho^{\otimes m})+E(\varrho^{\otimes n}).$$

(E5″) (Existence of a regularization) For all $\varrho\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$, the limit

$$E^\infty(\varrho)\equiv\lim_{n\to\infty}\frac{E(\varrho^{\otimes n})}{n}$$

exists.

In Lemma 12 we shall prove the well-known result that (E5′) is a sufficient condition for (E5″). When (E5″) holds, we shall refer to E^∞ as the regularization of E. We shall discuss some general properties of E^∞ in Proposition 13.

(E6) (Convexity) Mixing of states does not increase entanglement:

$$E(\lambda\varrho+(1-\lambda)\sigma)\leqslant\lambda E(\varrho)+(1-\lambda)E(\sigma)$$

for all $0\leqslant\lambda\leqslant 1$ and all $\varrho,\sigma\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$.

(E6) might seem to be essential for a measure of entanglement. Nevertheless, there is some evidence that an important entanglement measure (the entanglement of distillation) which describes asymptotic properties of multiple copies of identical states may not be convex.[8] A weaker condition is to require convexity only on decompositions into pure states. We shall prove below that this property is satisfied by the entanglement of distillation.

(E6′) For any state $\varrho\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$ and any decomposition $\varrho=\Sigma_i p_i|\psi_i\rangle\langle\psi_i|$ with $|\psi_i\rangle\in\mathcal{H}^A\otimes\mathcal{H}^B$, $p_i\geqslant 0$ for all i and $\Sigma_i p_i=1$, we require

$$E(\varrho)\leqslant\sum_i p_i E(P_{\psi_i}).$$

B. Conditions on pure states

The conditions imposed on an entanglement measure can be weakened by requiring that they only apply for pure states. Indeed, it might not even be required that the measure is defined except on pure states. Recall that $\Sigma_p(\mathcal{H}^A\otimes\mathcal{H}^B)$ denotes the set of pure states on the composite space.

(P0) If $\sigma\in\Sigma_p(\mathcal{H}^A\otimes\mathcal{H}^B)$ is separable, then $E(\sigma)=0$.

(P1)=(E1) (Normalization) If P_+^d is any representative of $P_+(\mathbb{C}^d)$, then $E(P_+^d)=\log_2 d$ for $d=1,2,\ldots$.

(P1′)=(E1′) $E(P_+(\mathbb{C}^2))=1$.

(P2) Let Λ be an operation which can be realized by means of local operations and classical communications. If $\sigma\in\Sigma_p(\mathcal{H}^A\otimes\mathcal{H}^B)$ is such that $\Lambda(\sigma)$ is also pure, then

$$E(\Lambda(\sigma))\leqslant E(\sigma).$$

(P2′) For $\sigma\in\Sigma_p(\mathcal{H}^A\otimes\mathcal{H}^B)$, $E(\sigma)$ depends only on the nonzero coefficients of a Schmidt decomposition of σ.

By Nielsen's theorem and the proof of Lemma 9 below, (P2) is equivalent to assuming (P2′) and that if the Schmidt coefficients of ϱ majorize those of σ, then $E(\varrho)\leqslant E(\sigma)$. Our proof of the theorem shows that, given (P2′), only local operations and operations of the specific form of Eq. (11) need be considered for (P2) (cf. Ref. 25).

Below we will in particular be interested in entanglement measures satisfying the following additional conditions:

(P3) Let $(\mathcal{H}_n^A)_{n\in\mathbb{N}}$ and $(\mathcal{H}_n^B)_{n\in\mathbb{N}}$ be sequences of Hilbert spaces and let $\mathcal{H}_n\equiv\mathcal{H}_n^A\otimes\mathcal{H}_n^B$ for all n. For all sequences $(\varrho_n)_{n\in\mathbb{N}}$ and $(\sigma_n)_{n\in\mathbb{N}}$ of states with $\varrho_n,\sigma_n\in\Sigma_p(\mathcal{H}_n^A\otimes\mathcal{H}_n^B)$, such that $\|\varrho_n-\sigma_n\|_1\to 0$, we require that

$$\frac{E(\varrho_n)-E(\sigma_n)}{1+\log_2\dim\mathcal{H}_n}\to 0.$$

(P4) For all $n\geqslant 1$ and all $\varrho\in\Sigma_p(\mathcal{H}^A\otimes\mathcal{H}^B)$,

$$\frac{E(\varrho^{\otimes n})}{n}=E(\varrho).$$

Of course, when ϱ is pure, so is $\varrho^{\otimes n}$.

(P4′) Given $\epsilon>0$ and $\varrho\in\Sigma_p(\mathcal{H}^A\otimes\mathcal{H}^B)$, there exists an integer $N>0$ such that $n\geqslant N$ implies

$$\frac{E(\varrho^{\otimes n})}{n}-\epsilon\leqslant E(\varrho)\leqslant\frac{E(\varrho^{\otimes n})}{n}+\epsilon.$$

(P5″) (Existence of a regularization on pure states) For all $\varrho\in\Sigma_p(\mathcal{H}^A\otimes\mathcal{H}^B)$, the limit

$$E^\infty(\varrho)\equiv\lim_{n\to\infty}\frac{E(\varrho^{\otimes n})}{n}$$

exists.

C. Some connections between the conditions

Lemma 9: (*E2′*) *is implied by* (*E2*).

Proof: By Eq. (5), the operations considered in (E2′) are LQCC. To see this for Λ_2, note that $W^{A\dagger}W^A=1_{\mathcal{H}^A}$. Thus (E2) implies $E(\Lambda_i(\sigma))\leqslant E(\sigma)$ for $i=1,2$. Unitary maps are invertible and so $E(\Lambda_1(\sigma))\geqslant E(\sigma)$. On the other hand, if $\mathcal{H}^A\subset\mathcal{K}^A$ and P^A is the projection onto $\mathcal{H}^A$, then, for any $\tau^A\in\Sigma_p(\mathcal{H}^A)$, the map $\Lambda_3^A:\Sigma(\mathcal{K}^A)\to\Sigma(\mathcal{H}^A)$ defined by $\Lambda_3^A(\varrho):=P^A\varrho P^{A\dagger}+\mathrm{tr}(\varrho(1-P^A))\tau^A$ is completely positive and trace preserving, so by Eq. (5), the map on $\Sigma(\mathcal{K}^A\otimes\mathcal{H}^A)$ defined by $\Lambda_3=\Lambda_3^A\otimes I^B$ is LQCC.

$\Lambda_3(\Lambda_2(\sigma))=\sigma$ and hence (E2) implies $E(\sigma)\leqslant E(\Lambda_2(\sigma))$. ■

Lemma 10: (*E4′*) *is equivalent to* (*E4*) *and* (*P4′*) *is equivalent to* (*P4*).

Proof: That (E4) implies (E4′) is immediate. Suppose (E4′) and choose m, ϱ, and ϵ.

By (E4′), there exists N such that $n\geqslant N$ implies $|E(\varrho)-E(\varrho^{\otimes n})/n|\leqslant\epsilon$ and $|E(\varrho^{\otimes m})-(E(\varrho^{\otimes m})^{\otimes n})/n|\leqslant\epsilon$. But, by definition, $(\varrho^{\otimes m})^{\otimes n}=\varrho^{\otimes mn}$ where the equality relates equivalent density matrices on products of isomorphic local spaces. Thus $n\geqslant N$ implies

$$\left|E(\varrho)-\frac{E(\varrho^{\otimes m})}{m}\right|\leqslant\left|E(\varrho)-\frac{E(\varrho^{\otimes mn})}{mn}\right|+\left|\frac{E(\varrho^{\otimes mn})}{mn}-\frac{E(\varrho^{\otimes m})}{m}\right|\leqslant 2\epsilon.$$

(E4) follows. The same proof shows the equivalence of (P4′) and (P4). ■

Lemma 11: Let E be an entanglement measure which satisfies $(P1')$, $(P2)$, and $(P4)$. Then E satisfies $(P0)$ and $(P1)$. Moreover, if E is defined on mixed states and satisfies either $(E2)$ or $(E6')$, then $(E0)$ is satisfied.

Proof: First we deal with separable states.

Choose $\epsilon>0$. Any pair of separable pure states is interconvertible by local unitary operators. If σ is such a state, then so is $\sigma^{\otimes n}$, and so, by (P2), $E(\sigma)=E(\sigma^{\otimes n})$. But (P4) implies that $E(\sigma)=E(\sigma^{\otimes n})/n$ and hence $E(\sigma)=0$. This gives (P0) and the $d=1$ case of (P1).

Now let $\varrho\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$ be a mixed separable state. Expanding the states ϱ_i^A and ϱ_i^B of Eq. (1) into pure components shows that σ is a convex combination of pure separable states: $\sigma=\Sigma_i p_i\sigma_i$.

Thus (E6′) is sufficient to go from (P0) to (E0). But (E2) is also sufficient, because if $\Lambda_i:\mathcal{T}(\mathcal{H}^A\otimes\mathcal{H}^B)\to\mathcal{T}(\mathcal{H}^A\otimes\mathcal{H}^B)$ is a local operation such that $\Lambda_i(\sigma_1)=\sigma_i$, then $\Lambda:=\Sigma_i p_i\Lambda_i$ is a LQCC operation such that $\Lambda(\sigma_1)=\sigma$ and so (E2) and (P0) yield $E(\sigma)\leqslant E(\sigma_1)=0$.

Now we turn to showing that, for $d\geqslant 2$, $E(P_+^d)=\log_2 d$ follows from (P1′), (P2), and (P4). By (P2′), $E(P_+^d)$ is independent of the representative of $P_+(\mathbb{C}^d)$ considered.

Choose $\epsilon>0$ and $d\geqslant 2$. Choose $N>1/\epsilon$. Set $w(n)\equiv E(P_+^n)$.

By Nielsen's theorem, (P2) implies that $w(d_1)\leqslant w(d_2)$ whenever $d_1\leqslant d_2$.

Up to local isomorphisms, $(P_+^d)^{\otimes n}=P_+^{d^n}$, so that, by (P4), $w(d)=w(d^n)/n$ for all n and, by (P1′), $w(2)=w(2^n)/n=1$.

Choose $n_1,n_2>N$ such that $2^{n_2+1}\geqslant d^{n_1}\geqslant 2^{n_2}$. Then $\log_2 d\geqslant n_2/n_1$, $|n_2/n_1-\log_2 d|\leqslant 1/n_1<\epsilon$, and, using (P4),

$$|w(d)-\log_2 d|\leqslant|w(d^{n_1})-n_2|/n_1+|n_2/n_1-\log_2 d|\leqslant|w(d^{n_1})-n_2w(2)|/n_1+\epsilon$$

and

$$|w(d^{n_1})-n_2w(2)|/n_1=|w(d^{n_1})-w(2^{n_2})|/n_1\leqslant|w(2^{n_2+1})-w(2^{n_2})|/n_1=1/n_1\leqslant\epsilon.$$

It follows that $w(d)$ is arbitrarily close to $\log_2 d$. ■

Lemma 12: $(E5')$ implies $(E5'')$. Indeed, $(E5')$ implies that

$$E(\varrho^{\otimes m})/m\to\inf\{E(\varrho^{\otimes m})/m:m\geqslant 1\}.$$

Proof: (See Ref. 26, Theorem 4.9.) Fix $k>0$. Every $m\geqslant 1$ can be written $m=nk+r$ with $0\leqslant r<k$. Then for all $m>0$ set $f(m):=E(\varrho^{\otimes m})$. $(E5')$ implies that

$$\frac{f(m)}{m}\leqslant\frac{nf(k)+f(r)}{nk+r}\leqslant\frac{nf(k)}{nk}+\frac{f(r)}{nk}=\frac{f(k)}{k}+\frac{f(r)}{nk}.$$

As $m\to\infty$ then $n\to\infty$ so $\limsup_{m\to\infty}f(m)/m\leqslant f(k)/k$ and thus $\limsup_{m\to\infty}f(m)/m\leqslant\inf_{k\geqslant 1}f(k)/k$. Now $\inf_{k\geqslant 1}f(k)/k\leqslant\liminf_{m\to\infty}f(m)/m$ shows that $\lim_{m\to\infty}f(m)/m$ exists and equals $\inf_{m\geqslant 1}f(m)/m$. ■

Proposition 13: Let E be an entanglement measure which satisfies $(E5'')$. Then we have the following.

(1) *E^∞ satisfies $(E4)$*
(2) *If E satisfies $(E0)$, then so does E^∞.*
(3) *If E satisfies $(E1)$, then so does E^∞.*
(4) *If E satisfies $(E2)$, then so does E^∞.*
(5) *If E satisfies $(E5)$, then so does E^∞.*
(6) *If E satisfies $(E5)$ and $(E6)$, then so does E^∞.*

Proof:

(1) For all m and ϱ,

$$\frac{E^{\infty}(\varrho^{\otimes m})}{m}=\lim_{n\to\infty}\frac{E(\varrho^{\otimes nm})}{nm}=E^{\infty}(\varrho).$$

(2) If σ is separable, then so is $\sigma^{\otimes n}$ for all n.
(3) If P_+^d is a representative of $P_+(\mathbb{C}^d)$, then $(P_+^d)^{\otimes n}$ is a representative of $P_+(\mathbb{C}^{d^n})$.
(4) If Λ is LQCC, then so is $\Lambda^{\otimes n}$ and $\Lambda(\sigma)^{\otimes n}=\Lambda^{\otimes n}(\sigma^{\otimes n})$.
(5) For all ϱ,σ and $k\geqslant 1$, (E5) implies that

$$\frac{E((\varrho\otimes\sigma)^{\otimes k})}{k}\leqslant\frac{E(\varrho^{\otimes k})}{k}+\frac{E(\sigma^{\otimes k})}{k}.$$

(6) Suppose that E satisfies (E5) and (E6). Let $\varrho,\sigma\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$ and choose $x_1,x_2\in[0,1]$ with $x_1+x_2=1$. Let $\omega=x_1\varrho+x_2\sigma$. Expanding $\omega^{\otimes n}$ as a sum of products, using convexity of E, and then using local isomorphisms to reorder the terms in each product gives

$$E(\omega^{\otimes n})\leqslant\sum_{k=0}^{n}\binom{n}{k}x_1^k x_2^{n-k}E(\varrho^{\otimes k}\otimes\sigma^{\otimes(n-k)})\leqslant\sum_{k=0}^{n}\binom{n}{k}x_1^k x_2^{n-k}(E(\varrho^{\otimes k})+E(\sigma^{\otimes(n-k)})),$$

where the second inequality is a consequence of (E5). To complete the proof, we need the following lemma:

Lemma 14: As $n\to\infty$, $(1/n)\sum_{k=0}^{n}\binom{n}{k}x_1^k x_2^{n-k}E(\varrho^{\otimes k})\to x_1E^{\infty}(\varrho)$ *and* $(1/n)\sum_{k=0}^{n}\binom{n}{k}x_1^k x_2^{n-k}\times E(\sigma^{\otimes(n-k)})\to x_2E^{\infty}(\sigma)$.

Proof: It is sufficient to prove the first limit. Set $g(m)=E(\varrho^{\otimes m})/m$ and $L=E^{\infty}(\varrho)$. Choose $\epsilon>0$. By Lemma 12, there exists K such that $k\geqslant K$ implies $|g(k)-L|<\epsilon/2$ and there is a constant $C>0$ such that $|g(k)-L|<C$ for all k. $N>K$ implies that

$$\frac{1}{N}\sum_{k=0}^{K}\binom{N}{k}kx_1^k x_2^{N-k}\leqslant\frac{K}{N}\sum_{k=0}^{N}\binom{N}{k}x_1^k x_2^{N-k}=\frac{K}{N}.$$

Set $h(x)=(x+y)^n=\sum_{k=0}^{n}\binom{n}{k}x^k y^{n-k}$. $xh'(x)=nx(x+y)^{n-1}=\sum_{k=0}^{n}\binom{n}{k}kx^k y^{n-k}$. Thus $x_1+x_2=1$ implies that $\sum_{k=0}^{n}\binom{n}{k}kx_1^k x_2^{n-k}=nx_1$.

Choose $N_0>K$ such that $KC/N_0<\epsilon/2$. Then $N>N_0$ implies

$$\begin{aligned}\left|\frac{1}{N}\sum_{k=0}^{N}\binom{N}{k}x_1^k x_2^{N-k}E(\varrho^{\otimes k})-x_1E^{\infty}(\varrho)\right|&=\left|\frac{1}{N}\sum_{k=0}^{N}\binom{N}{k}kx_1^k x_2^{N-k}g(k)-x_1L\right|\\&=\left|\frac{1}{N}\sum_{k=0}^{N}\binom{N}{k}kx_1^k x_2^{N-k}(g(k)-L)\right|\\&\leqslant\frac{1}{N}\sum_{k=0}^{K}\binom{N}{k}kx_1^k x_2^{N-k}C\\&\quad+\frac{1}{N}\sum_{k=K+1}^{N}\binom{N}{k}kx_1^k x_2^{N-k}(g(k)-L)\\&\leqslant KC/N+\epsilon/2\sum_{k=K+1}^{N}\binom{N}{k}x_1^k x_2^{N-k}\\&\leqslant\epsilon.\end{aligned}$$

■

Continuity (E3) is not mentioned in Proposition 13, although we could use Lemma 12 to deduce upper-semicontinuity from (E3) and (E5′), as the infimum of a family of real continuous

functions is upper-semicontinuous. For an example which may be relevant, consider the sequence of functions on [0,1] defined by $f_n(x)=nx^n$. Clearly $f_{m+n}(x)\leqslant f_m(x)+f_n(x)$. $g_n(x)=x^n$ converges (pointwise) as $n\to\infty$ to a discontinuous but upper-semicontinuous function.

VI. EXAMPLES OF IMPORTANT ENTANGLEMENT MEASURES

In this section we will present some important entanglement measures and check which of the postulates from Sec. V they satisfy.

A. Operational measures

Here we shall describe two entanglement measures, *entanglement of distillation* and *entanglement cost*[1] (see also Refs. 27 and 28), which are defined in terms of specific state conversions.

Lemma 15: Let $\varrho\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$ *with* $\mathcal{H}^A\equiv\mathcal{H}^B\equiv\mathcal{H}$ *and* $\dim\mathcal{H}=d$. *Let* $|\phi\rangle=|\phi^A\rangle\otimes|\phi^B\rangle\in\mathcal{H}^A\otimes\mathcal{H}^B$ *be a separable wavefunction and* P_+^d *be a representative of* $P_+(\mathbb{C}^d)$ *on* $\mathcal{H}^A\otimes\mathcal{H}^B$. *Then there exist* LQCC *operations* Λ_1 *and* Λ_2 *such that* $\Lambda_1(\varrho)=|\phi\rangle\langle\phi|$ *and* $\Lambda_2(P_+^d)=\varrho$.

Proof: Let $(\psi_i^A)_{i=1}^d$ [resp. $(\psi_i^B)_{i=1}^d$] be an orthonormal basis for $\mathcal{H}^A$ [resp. $\mathcal{H}^B$] and define Λ_1 by

$$\Lambda_1(\sigma)\equiv\sum_{j=1}^d (1^A\otimes|\phi^B\rangle\langle\psi_j^B|)\left(\sum_{i=1}^d (|\phi^A\rangle\langle\psi_i^A|\otimes 1^B)\sigma(|\psi_i^A\rangle\langle\phi^A|\otimes 1^B)\right)(1^A\otimes|\psi_j^B\rangle\langle\phi^B|)$$

$$=\sum_{i,j=1}^d |\phi^A\otimes\phi^B\rangle\langle\psi_i^A\otimes\psi_j^B|\sigma|\psi_i^A\otimes\psi_j^B\rangle\langle\phi^A\otimes\phi^B|=|\phi\rangle\mathrm{tr}(\sigma)\langle\phi|=|\phi\rangle\langle\phi|$$

for all $\sigma\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$.

For Λ_2, we note that if $|\Psi\rangle\langle\Psi|\in\Sigma(\mathcal{H}^A\otimes\mathcal{H}^B)$ is any pure state, then, by Nielsen's theorem, there exists an LQCC operation mapping P_+^d to $|\Psi\rangle\langle\Psi|$ because the distribution $(1/d)_{i=1}^d$ is majorized by any probability distribution on $\{1,\ldots,d\}$. Now, as in the proof of Lemma 11, we can construct Λ_2 as a convex combination of operations mapping P_+^d to pure components of ϱ.■

Given a state ϱ on $\mathcal{H}^A\otimes\mathcal{H}^B$, consider a sequence of LQCC operations (Λ_n) with $\Lambda_n:\mathcal{T}((\mathcal{H}^A)^{\otimes n}\otimes(\mathcal{H}^B)^{\otimes n})\to\mathcal{T}((\mathcal{H}^A)^{\otimes n}\otimes(\mathcal{H}^B)^{\otimes n})$. Suppose that $\sigma_n\equiv\Lambda_n(\varrho^{\otimes n})$ satisfies

$$\|P_+^{d_n}-\sigma_n\|_1\to 0$$

for some representative $P_+^{d_n}$ of $P_+(\mathbb{C}^{d_n})$ on $(\mathcal{H}^A)^{\otimes n}\otimes(\mathcal{H}^B)^{\otimes n}$. We call such a sequence (Λ_n) an LQCC *distillation protocol*. The asymptotic ratio attainable via this protocol is then defined by

$$E_D((\Lambda_n),\varrho)\equiv\limsup_{n\to\infty}\frac{\log_2 d_n}{n}. \tag{14}$$

Lemma 15 shows that, for any state, a distillation protocol always exists with $d_n\equiv 1$.

Definition 16: The distillable entanglement *or* entanglement of distillation E_D *is defined as the supremum of Eq. (14) over all possible* LQCC *distillation protocols:*

$$E_D(\varrho)\equiv\sup_{(\Lambda_n)} E_D((\Lambda_n),\varrho). \tag{15}$$

By construction E_D satisfies the properties (E2) and (E4) of entanglement measures. The proof is analogous to the proof of Lemma 1 in Ref. 28. It is not known whether E_D satisfies (E3) or (E6). (Indeed, as already mentioned, there is evidence that (E6) may not be satisfied.[8]) We shall confirm in Lemma 24 that (E0) and (E1) are satisfied.

The so-called *entanglement cost* E_C is defined in a complementary way. Given a state ϱ, consider a sequence of LQCC operations $\Lambda_n:\mathcal{T}(\mathbb{C}^{d_n}\otimes\mathbb{C}^{d_n})\to\mathcal{T}((\mathcal{H}^A)^{\otimes n}\otimes(\mathcal{H}^B)^{\otimes n})$ transforming a representative of $P_+(\mathbb{C}^{d_n})$ into a state σ_n such that

$$\|\sigma_n - \varrho^{\otimes n}\|_1 \to 0.$$

The asymptotic ratio attainable via this *formation*-protocol is then given by

$$E_C((\Lambda_n), \varrho) \equiv \liminf_{n\to\infty} \frac{\log_2 d_n}{n}. \tag{16}$$

Once again Lemma 15 shows that, for any state, a formation protocol always exists with $d_n \equiv d^n$ where $d = \max\{\dim\mathcal{H}^A, \dim\mathcal{H}^B\}$.

Definition 17: The entanglement cost E_C *is defined as the infimum of Eq. (16) over all possible* LQCC *formation protocols:*

$$E_C(\varrho) \equiv \inf_{\{\Lambda_n\}} E_C((\Lambda_n), \varrho). \tag{17}$$

By construction E_C satisfies property (E2). As we shall discuss in the next section, by Ref. 28 and Proposition 13, it also satisfies (E0), (E1), (E2), (E4), (E5), and (E6). It is not known whether it satisfies (E3). We shall also prove below that for pure states both E_D and E_C are equal to the reduced von Neumann entropy given by Eq. (3). (This was first realized in Ref. 29 and a rigorous proof was sketched in Ref. 21.)

B. Abstract measures

The entanglement measures discussed in this subsection quantify entanglement mathematically, but their definitions do not admit a direct operational interpretation in terms of entanglement manipulations. The first one is the so-called *entanglement of formation*[1] which is defined as follows:

Definition 18: Let $\mathcal{H}^A$ *and* $\mathcal{H}^B$ *be finite dimensional Hilbert spaces and let* $|\psi\rangle \in \mathcal{H}^A \otimes \mathcal{H}^B$. *Then the* entanglement of formation *is defined for pure states as*

$$E_F(P_\psi) := S_{\mathrm{vN}}(P_\psi), \tag{18a}$$

where $S_{\mathrm{vN}}(P_\psi)$ [*defined in Eq. (3)*] *is the von Neumann entropy of either of the reduced density matrices of* $|\psi\rangle$. *For mixed states* $\varrho \in \Sigma(\mathcal{H}^A \otimes \mathcal{H}^B)$ *we define*

$$E_F(\varrho) := \inf \sum_i p_i E_F(P_{\psi_i}), \tag{18b}$$

where the infimum is taken over all possible decompositions of ϱ *of the form* $\varrho = \Sigma_i p_i |\psi_i\rangle\langle\psi_i|$ *with* $p_i \geqslant 0$ *for all* i *and* $\Sigma_i p_i = 1$.

The entanglement of formation satisfies (E0)–(E3), (E5), and (E6). In particular, (E2) was shown in Ref. 1, (E3) in Ref. 6, and (E0), (E1), (E5), and (E6) follow directly from the definition of E_F.

The entanglement of formation E_F is believed but not known to be equal to the entanglement cost E_C. However, it is known that the *regularized* entanglement of formation E_F^∞ [which exists by (E5′)] is equal to the entanglement cost.[28] This allows us to apply Proposition 13 to E_C.

Let us now present another important measure, namely, the *relative entropy of entanglement*.[24,2] It is defined as follows:

$$E_R(\varrho) \equiv \inf_\sigma S_{\mathrm{rel}}(\varrho|\sigma), \tag{19}$$

where $S_{\mathrm{rel}}(\varrho|\sigma) \equiv \mathrm{tr}\varrho \log_2 \varrho - \mathrm{tr}\varrho \log_2 \sigma$ is the quantum relative entropy, and where the infimum is taken over all separable states σ. One can consider variations of the above measure, by changing the set of states over which the infimum is taken (this set should be closed under LQCC

operations though). Like the entanglement of formation, E_R satisfies (E0)–(E3), (E5), and (E6). In particular, (E1) and (E2) were shown in Ref. 24, (E3) in Ref. 9, (E0) follows immediately and (E5) almost immediately from the definition of E_R, and (E6) follows from the convexity of the quantum relative entropy S_{rel}.

The properties of E_R and Proposition 13 show that the *regularized* relative entropy of entanglement E_R^∞ exists and satisfies (E0), (E1), (E2), (E4), (E5), and (E6). It is shown in Ref. 10 that E_R does *not* satisfy (E4). This implies, of course, that E_R and E_R^∞ are not always equal (cf. Ref. 30).

Finally, let us note that for pure states both the entanglement of formation (by definition) and the relative entropy of entanglement (as shown in Refs. 2 and 31) are equal to the reduced von Neumann entropy S_{vN} [defined in Eq. (3)]. An immediate consequence of the additivity of S_{vN} is that $E_F^\infty = E_C$ and E_R^∞ are also equal to S_{vN} on pure states (see also Theorem 23).

VII. ENTANGLEMENT OF DISTILLATION AND ENTANGLEMENT COST AS EXTREME MEASURES

In this section we improve the theorem of Ref. 4 by giving precise conditions under which E_D and E_C are lower and upper bounds for entanglement measures. We propose three versions of the theorem.

Proposition 19: Suppose that E is an entanglement measure defined on mixed states which satisfies (E1)–(E4). Then for all states $\varrho \in \Sigma(\mathcal{H}^A \otimes \mathcal{H}^B)$

$$E_D(\varrho) \leqslant E(\varrho) \leqslant E_C(\varrho). \tag{20}$$

Proof: Choose $\epsilon > 0$. We shall prove the result in three steps:

(**I**) First we prove that, having if necessary passed to a subsequence, there exists an integer $N_1 > 0$ such that $n \geqslant N_1$ implies

$$\frac{E(\varrho^{\otimes n})}{n} \geqslant E_D(\varrho) - \epsilon. \tag{21}$$

Consider a near-optimal LQCC protocol $(\Lambda_n)_n$. By the definition of distillable entanglement, there exists a LQCC protocol $(\Lambda_n)_n$ such that, after possibly passing to a subsequence,

$$\| P_+^{d_n} - \Lambda_n(\varrho^{\otimes n}) \|_1 \to 0 \tag{22a}$$

and

$$\left| E_D(\varrho) - \frac{\log_2 d_n}{n} \right| \leqslant \frac{\epsilon}{2} \tag{22b}$$

for all $n \geqslant N_1'$. (E3) implies that

$$\left| \frac{E(\Lambda_n(\varrho^{\otimes n})) - E(P_+^{d_n})}{1 + n \log_2 d} \right| \to 0 \tag{23}$$

as $n \to \infty$ where $d = \dim \mathcal{H}^A \otimes \mathcal{H}^B$. It follows that we can choose $N_1'' > 0$ such that $n \geqslant N_1''$ implies

$$\left| \frac{E(\Lambda_n(\varrho^{\otimes n}))}{n} - \frac{E(P_+^{d_n})}{n} \right| \leqslant \frac{\epsilon}{2}, \tag{24}$$

and, so, using (E2), for $n \geqslant N_1 = \max\{N_1', N_1''\}$,

$$\frac{E(\varrho^{\otimes n})}{n} \geqslant \frac{E(\Lambda_n(\varrho^{\otimes n}))}{n} \geqslant \frac{E(P_+^{d_n})}{n} - \frac{\epsilon}{2} = \frac{\log_2 d_n}{n} - \frac{\epsilon}{2} \geqslant E_D(\varrho) - \epsilon. \tag{25}$$

(**II**) As a second step, we prove that, having if necessary passed to another (perhaps disjoint) subsequence, there exists an integer $N_2 \geqslant N_1$ such that $n \geqslant N_2$ implies

$$\frac{E(\varrho^{\otimes n})}{n} \leqslant E_C(\varrho) + \epsilon. \tag{26}$$

This is similar to the first step. Consider a near-optimal protocol $(\Lambda_n)_n$ for ϱ. We have [after possibly passing to a suitable subsequence of $(\Lambda_n)_n$], for all sufficiently large n,

$$\frac{E(\varrho^{\otimes n})}{n} \leqslant \frac{E(\Lambda_n(P_+^{d_n}))}{n} + \frac{\epsilon}{2} \leqslant \frac{E(P_+^{d_n})}{n} + \frac{\epsilon}{2} = \frac{\log_2 d_n}{n} + \frac{\epsilon}{2} \leqslant E_C(\varrho) + \epsilon. \tag{27}$$

(**III**) The final step is to invoke (E4) to give

$$E_D(\varrho) - \epsilon \leqslant E(\varrho) = \frac{E(\varrho^{\otimes n})}{n} \leqslant E_C(\varrho) + \epsilon. \tag{28}$$

■

Unfortunately, as we do not at present know of any function for which we can prove that postulates (E1)–(E4) hold for all states, it is possible that Proposition 19 may be empty. Nevertheless, by modifying the final step of the proof, we can obtain the following:

Proposition 20: Let E be an entanglement measure defined on mixed states and satisfying (E1), (E2), (E3), and (E5″). Then for all states $\varrho \in \Sigma(\mathcal{H}^A \otimes \mathcal{H}^B)$,

$$E_D(\varrho) \leqslant E^\infty(\varrho) \leqslant E_C(\varrho). \tag{29}$$

Proof: Without using condition (E4) or any properties of E^∞ except its existence, we can maintain the structure of the previous proof, simply by replacing $E(\varrho)$ in (28) by $E^\infty(\varrho)$. ■

Proposition 20 is certainly nonempty. Indeed, as mentioned in the previous section, both the entanglement of formation and the relative entropy of entanglement satisfy all assumptions of the proposition. We obtain the following corollary.

Corollary 21: The entanglement of distillation E_D is less than or equal to the entanglement cost E_C for all states.

Although, in physical terms, Corollary 21 seems almost necessary, a rigorous proof requires some control both over changes in state and over changes in dimension.

Let us now consider yet another version, where we weaken the assumptions in the theorem on extreme measures of Ref. 4. We impose the condition (E3′), which is stronger than (P3) but weaker than (E3).

One mechanism for deriving condition (E3′) for a given function E might be to establish the inequalities

$$f(\varrho) \leqslant E(\varrho) \leqslant g(\varrho), \tag{30}$$

where f, g are functions satisfying (E3′) which coincide on pure states. We will take $f(\varrho) \equiv S(\varrho_A) - S(\varrho)$ and $g(\varrho) \equiv S(\varrho_A)$ (where $\varrho_A := \mathrm{tr}_{\mathcal{H}_B}\varrho$). Both of these functions f and g do satisfy (E3′). This follows immediately from two facts:

(i) Fannes inequality[32,33]

$$|S(\sigma) - S(\varrho)| \leqslant \|\sigma - \varrho\|_1 \log_2 \dim\mathcal{H} + \eta(\|\sigma - \varrho\|_1), \tag{31}$$

which holds for any two states σ and ϱ acting on the Hilbert space $\mathcal{H}$ and satisfying $\|\sigma-\varrho\|_1 \leqslant 1/3$; here $\eta(s)\equiv -s\log s$ and S denotes the standard von Neumann entropy as above.

(ii) $\|\sigma_A-\varrho_A\|_1 \leqslant \|\sigma-\varrho\|_1$, where σ_A and ϱ_A are the reduced density operators of ϱ and σ, respectively.

With the above choices for f and g one can show that E_F and E_R satisfy the inequalities in (30) (see Refs. 1, 2, 31, and 34). Then, E_R^∞ and E_F^∞ also satisfy inequalities (30), because the additivity of the von Neumann entropy implies that both f and g satisfy (E4). E_D also satisfies the inequality $E_D \leqslant g$, but we do not know whether or not it satisfies the second inequality. However, a stronger inequality (the so-called *hashing inequality*), which would have many interesting implications, was conjectured in Ref. 35. Strong evidence for this conjecture was collected there.

We shall also use the weak form of convexity (E6′).

Proposition 22: Let E be an entanglement measure defined on mixed states and satisfying (E1), (E2), (E3′), and (E6′). Then for all states $\varrho \in \Sigma(\mathcal{H}^A \otimes \mathcal{H}^B)$ *we have*

$$E_D(\varrho) \leqslant E(\varrho) \leqslant E_C(\varrho) \tag{32}$$

if (E4) holds and

$$E_D(\varrho) \leqslant E^\infty(\varrho) \leqslant E_C(\varrho) \tag{33}$$

if (E5) holds.

Proof: Step I of the proof of Proposition 19 goes through with (E3′) replacing (E3) in inequality (24).

To replace step II, we use the estimate $E_C \geqslant E_F^\infty$. This follows from Proposition 20 (but also, of course, from Ref. 28, where it was shown that $E_C = E_F^\infty$). For any state ϱ consider its finite decompositions into pure states

$$\varrho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

for which

$$E_F(\varrho) = \sum_i p_i S_{\mathrm{vN}}(P_{\psi_i}).$$

In Ref. 36 it was shown that such a decomposition exists.

As (E1)=(P1)⇒(P1′), (E2)⇒(P2), and (E3′)⇒(P3), we can apply Theorem 23 (to follow) to show that $E(P_{\psi_i}) = S_{\mathrm{vN}}(P_{\psi_i})$ if E satisfies (E4) and $E^\infty(P_{\psi_i}) = S_{\mathrm{vN}}(P_{\psi_i})$ if E satisfies (E5).

Now (E6′) implies, in the first case, that $E(\varrho) \leqslant E_F(\varrho)$ (cf. Ref. 36) and hence

$$E(\varrho) = \frac{E(\varrho^{\otimes n})}{n} \leqslant \frac{E_F(\varrho^{\otimes n})}{n},$$

which yields the required upper bound when $n \to \infty$. For the second case, we can use the proof of part (6) of Proposition 13 to show that (E6′) holds for E^∞. This yields $E^\infty(\varrho) \leqslant E_F(\varrho)$ and

$$E^\infty(\varrho) = \frac{E^\infty(\varrho^{\otimes n})}{n} \leqslant \frac{E_F(\varrho^{\otimes n})}{n}.$$

Again the required bound follows on taking $n \to \infty$. ■

VIII. THE UNIQUENESS THEOREM FOR ENTANGLEMENT MEASURES

Theorem 23: *Let E be a functional on pure states. Then the following are equivalent:*

(1) *E satisfies $(P1')$, $(P2)$, $(P3)$, and $(P4')$.*
(2) *E satisfies $(P0)$, $(P1)$, $(P2)$, $(P3)$, and $(P4)$.*
(3) *E coincides with the reduced von Neumann entropy $E=S_{\mathrm{vN}}$.*

On the other hand, if E satisfies $(P0)$, $(P1)$, $(P2)$, and $(P3)$, then E satisfies $(P5'')$ and, on pure states, $E^{\infty}=S_{\mathrm{vN}}$.

Proof: The equivalence of (1) and (2) is proved in Lemmas 10 and 11.

It is clear that the reduced von Neumann entropy satisfies (P0), (P1), and (P4). (P3) follows from the facts (i) and (ii) of the previous section. Finally (P2) is a consequence of Nielsen's theorem and the fact that the von Neumann entropy is a Schur-concave function.[37] Indeed, with the inductive decomposition of LQCC operations introduced in our proof of Nielsen's theorem, we can prove (P2) just by showing, in the notation of Eq. (12), that $S_{\mathrm{vN}}(\Lambda(|\Psi\rangle\langle\Psi|))\leqslant S_{\mathrm{vN}}(|\Psi\rangle\times\langle\Psi|)$. This amounts to proving that, for $p_J\geqslant p_K$ and suitable δ,

$$-(p_J+\delta)\log_2(p_J+\delta)-(p_K-\delta)\log_2(p_K-\delta)\leqslant -p_J\log_2 p_J-p_K\log_2 p_K,$$

and this is easily confirmed by differentiating with respect to δ.

Now suppose that E satisfies (P0), (P1), (P2), and (P3). Using $(P2')$, we may assume that $\mathcal{H}^A\equiv\mathcal{H}^B\equiv\mathcal{H}$. Suppose that $\dim\mathcal{H}=d$ and let $|\psi\rangle\in\mathcal{H}\otimes\mathcal{H}$. Write $\mathsf{S}\equiv S_{\mathrm{vN}}(|\psi\rangle\langle\psi|)$ for the von Neumann entropy of the reduced density matrix of $|\psi\rangle$. Consider n copies of the wavefunction $|\psi\rangle$: $|\psi^{\otimes n}\rangle\in\mathcal{H}_{\mathrm{tot}}\equiv\mathcal{H}^{\otimes n}\otimes\mathcal{H}^{\otimes n}$. Let $\{q_j:j=1,\ldots,d\}$ be the set of eigenvalues of the reduced density matrix of $|\psi\rangle$ and $\{p_i:i=1,\ldots,d^{2n}\}$ be the set of eigenvalues of the reduced density matrix of $|\psi^{\otimes n}\rangle$. Again using $(P2')$, we may adjust d so that $q_j>0$ for $j=1,\ldots,d$. In view of (P0), we may also assume that $\mathsf{S}>0$. Considered as a probability distribution, $\{p_i\}$ is the distribution for n independent trials each with distribution $\{q_j\}$. Choose bases $(e_i)\subset\mathcal{H}^{\otimes n}$ and $(f_i)\subset\mathcal{H}^{\otimes n}$ such that

$$|\psi^{\otimes n}\rangle=\sum_i\sqrt{p_i}|e_i\rangle\otimes|f_i\rangle.$$

Choose $\epsilon>0$. By the asymptotic equipartition theorem (Ref. 38, Theorem 3.1.2), there exists an integer $N\equiv N(\epsilon)$ such that, for all $n\geqslant N$, one can find a subset $\mathsf{TYP}\equiv\mathsf{TYP}(n,\epsilon)$ of the set of indices $\{i\}_{i=1}^{d^{2n}}$ with the following properties:

$$2^{-n(\mathsf{S}+\epsilon)}\leqslant p_i\leqslant 2^{-n(\mathsf{S}-\epsilon)},\quad \text{for } i\in\mathsf{TYP}, \tag{34a}$$

$$p\equiv\sum_{i\in\mathsf{TYP}}p_i\geqslant 1-\epsilon, \tag{34b}$$

$$\#\mathsf{TYP}\leqslant 2^{n(\mathsf{S}+\epsilon)}. \tag{34c}$$

Here #TYP denotes the number of elements in TYP.

Introduce another wavefunction $|\phi_n\rangle\in\mathcal{H}_{\mathrm{tot}}$ given by

$$|\phi_n\rangle\equiv\frac{1}{\sqrt{p}}\sum_{i\in\mathsf{TYP}}\sqrt{p_i}|e_i\rangle\otimes|f_i\rangle.$$

This wavefunction satisfies

$$|\langle\psi^{\otimes n}|\phi_n\rangle|^2=p\geqslant 1-\epsilon \tag{35}$$

and so

$$\| |\psi^{\otimes n}\rangle\langle\psi^{\otimes n}| - |\phi_n\rangle\langle\phi_n| \|_1 = 2\sqrt{(1-|\langle\psi^{\otimes n}|\phi_n\rangle|^2)} \leqslant 2\sqrt{\epsilon}. \tag{36}$$

Now, the crucial observation (cf. Ref. 21) is that for $\epsilon < \min\{1/2\mathsf{S}, 1/2\}$ and n sufficiently large, there exist completely positive maps Λ_n and Λ_n' such that

$$\Lambda_n(|\phi_n\rangle\langle\phi_n|) = P_+^a \tag{37a}$$

for P_+^a a representative of $P_+(\mathbb{C}^a)$ in $\mathcal{H}_{\text{tot}}$ with $|(\log_2 a)/n - \mathsf{S}| < \epsilon + 2/n$ and

$$\Lambda_n'(P_+^b) = |\phi_n\rangle\langle\phi_n| \tag{37b}$$

for P_+^b a representative of $P_+(\mathbb{C}^b)$ in $\mathcal{H}_{\text{tot}}$ with $|(\log_2 b)/n - \mathsf{S}| < \epsilon + 1/n$. Indeed, to see Eq. (37a), set $a \equiv \lfloor p2^{n(\mathsf{S}-\epsilon)} \rfloor$, i.e., a is the largest integer smaller than or equal to $p2^{n(\mathsf{S}-\epsilon)}$. Then $a \leqslant p2^{n(\mathsf{S}-\epsilon)} \leqslant p/p_i$ and we see that the distribution $(p_i/p)_{i \in \mathsf{TYP}}$ is majorized by $(1/a)_{i=1}^a$, hence Eq. (37a) follows from Nielsen's theorem. Equation (37b) follows by a similar argument when we take $b \equiv \lceil p2^{n(\mathsf{S}+\epsilon)} \rceil$, i.e., b is the smallest integer larger than or equal to $p2^{n(\mathsf{S}+\epsilon)}$. The conditions on ϵ and n are sufficient to go from $a \equiv \lfloor p2^{n(\mathsf{S}-\epsilon)} \rfloor$ to $|(\log_2 a)/n - \mathsf{S}| < \epsilon + 2/n$ and from $b \equiv \lceil p2^{n(\mathsf{S}+\epsilon)} \rceil$ to $|(\log_2 b)/n - \mathsf{S}| < \epsilon + 1/n$, ensuring, for example, that $a \neq 0$.

Now choose a sequence $(\epsilon_j)_{j \in \mathbb{N}}$ of positive numbers such that $\epsilon_j \to 0$ for $j \to \infty$. Suppose that $(n_k)_{k \in \mathbb{N}}$ is a sequence of integers such that $n_k \to \infty$ and $E(|\psi^{\otimes n_k}\rangle\langle\psi^{\otimes n_k}|)/n_k \to L$ for some L.

For each j, choose $n_{k_j} \geqslant \max\{N(\epsilon_j), 1/\epsilon_j\}$. We can apply the postulates (P0)–(P3) to obtain the following estimates:

$$\begin{aligned}
\frac{E(|\psi^{\otimes n_{k_j}}\rangle\langle\psi^{\otimes n_{k_j}}|)}{n_{k_j}} &= \frac{E(|\psi^{\otimes n_{k_j}}\rangle\langle\psi^{\otimes n_{k_j}}|) - E(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|)}{n_{k_j}} + \frac{E(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|)}{n_{k_j}} \\
&\geqslant \frac{E(|\psi^{\otimes n_{k_j}}\rangle\langle\psi^{\otimes n_{k_j}}|) - E(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|)}{n_{k_j}} + \frac{E(\Lambda_{n_{k_j}}(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|))}{n_{k_j}} \\
&= \frac{E(|\psi^{\otimes n_{k_j}}\rangle\langle\psi^{\otimes n_{k_j}}|) - E(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|)}{n_{k_j}} + \frac{E(P_+^{a_{n_{k_j}}})}{n_{k_j}} \\
&= \frac{E(|\psi^{\otimes n_{k_j}}\rangle\langle\psi^{\otimes n_{k_j}}|) - E(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|)}{n_{k_j}} + \frac{\log_2 a_{n_{k_j}}}{n_{k_j}}.
\end{aligned}$$

As $j \to \infty$, the first term vanishes due to (P3) and the second approaches $S_{\text{vN}}(P_\psi)$ (cf. Ref. 6). This implies that $L \geqslant S_{\text{vN}}(|\psi\rangle\langle\psi|)$. The proof of the inequality $L \leqslant S_{\text{vN}}(|\psi\rangle\langle\psi|)$ is similar:

$$\begin{aligned}
\frac{E(|\psi^{\otimes n_{k_j}}\rangle\langle\psi^{\otimes n_{k_j}}|)}{n_{k_j}} &= \frac{E(|\psi^{\otimes n_{k_j}}\rangle\langle\psi^{\otimes n_{k_j}}|) - E(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|)}{n_{k_j}} + \frac{E(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|)}{n_{k_j}} \\
&\leqslant \frac{E(|\psi^{\otimes n_{k_j}}\rangle\langle\psi^{\otimes n_{k_j}}|) - E(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|)}{n_{k_j}} + \frac{E(P_+^{b_{n_{k_j}}})}{n_{k_j}} \\
&= \frac{E(|\psi^{\otimes n_{k_j}}\rangle\langle\psi^{\otimes n_{k_j}}|) - E(|\phi_{n_{k_j}}\rangle\langle\phi_{n_{k_j}}|)}{n_{k_j}} + \frac{\log_2 b_{n_{k_j}}}{n_{k_j}}.
\end{aligned}$$

We have now shown that every limit point of the sequence $E(|\psi^{\otimes n}\rangle\langle\psi^{\otimes n}|)/n$ has the value $L = S_{\text{vN}}(|\psi\rangle\langle\psi|)$. But, by (P1), (P2), and Lemma 15, this sequence is bounded, and so (P5″) holds

with $E^{\infty}(|\psi\rangle\langle\psi|)=L=S_{\mathrm{vN}}(|\psi\rangle\langle\psi|)$. This proves the final statement of the theorem. On the other hand, if (P4) holds, then $L=E(|\psi\rangle\langle\psi|)$, and so we have proved that (2) implies (3). This completes the proof of Theorem 23. ■

It is natural to wonder whether the conditions in Theorem 23 can be weakened, and, in particular, whether (P3) is necessary. That it is has been noted by Vidal.[3] Consider the entanglement measures defined on pure states by $S_{\infty}(\sigma)=-\log_2 p_1(\sigma)$ where $p_1(\sigma)$ is the largest coefficient in a Schmidt decomposition of σ and by $S_0(\sigma)=\log d(\sigma)$, where d is the number of nonzero coefficients. S_0 and S_{∞} both satisfy (P0), (P1), (P2) (by Nielsen's theorem), and (P4). S_{∞} is even trace norm continuous on Hilbert spaces of fixed dimension. (P3), however, does not hold for either. This is, of course, a consequence of Theorem 23. An explicit example of the failure of (P3) for S_{∞} is provided by the states $\sigma_n\equiv|\Psi_n\rangle\langle\Psi_n|$, $\varrho_n\equiv|\Phi_n\rangle\langle\Phi_n|$ with Schmidt decompositions $|\Psi_n\rangle\equiv\sqrt{1/2^n}|\psi_1\psi_1\rangle+\Sigma_{i=2}^{4^n-2^{n+1}}(1/2^n)|\psi_i\psi_i\rangle$ and $|\Phi_n\rangle\equiv\Sigma_{i=1}^{4^n}(1/2^n)|\psi_i\psi_i\rangle$ for some orthonormal family $(|\psi_i\rangle)$ of wavefunctions. In fact, any entanglement measure E defined on pure states and satisfying (P0), (P1), (P2), and (P4) will satisfy $S_{\infty}(\sigma)\leqslant E(\sigma)\leqslant S_0(\sigma)$ for all pure σ. The upper bound here is a consequence of Lemma 15 while, for the lower bound, we modify the proof of Theorem 23 using the fact that $|\psi^{\otimes n}\rangle\langle\psi^{\otimes n}|$ can always be converted without approximation into P_+^c where c is the largest integer smaller than or equal to $1/p_1$.

An example of a measure on pure states satisfying (P0), (P1), (P2), and (P3), but not (P4), is given by $E(\sigma)=2(1-p_1(\sigma))S_{\mathrm{vN}}(\sigma)$ for $p_1(\sigma)\geqslant 1/2$, $E(\sigma)=S_{\mathrm{vN}}(\sigma)$ for $p_1(\sigma)\leqslant 1/2$.

Finally, let us consider entanglement of distillation and entanglement cost in the above context. Using the maps constructed in Theorem 23, we show that they are equal to S_{vN}. We have already noted that for E_C this also follows from Ref. 28.

Lemma 24: The entanglement of distillation E_D and the entanglement cost E_C both coincide on pure states with the von Neumann reduced entropy $E_D(P_\psi)=E_C(P_\psi)=S_{\mathrm{vN}}(P_\psi)$ for all $|\psi\rangle\in\mathcal{H}\otimes\mathcal{H}$.

Proof: From Sec. VII we know that $E_D\leqslant E_C$. It suffices to show that on pure states $E_D\geqslant S_{\mathrm{vN}}$ and $E_C\leqslant S_{\mathrm{vN}}$. We will continue to use the notation from the proof of Theorem 23.

That $E_C(P_\psi)\leqslant S_{\mathrm{vN}}(P_\psi)$ follows directly from the definition of E_C, using the operations defined by the Λ'_{n_j} which satisfy Eq. (37b) and estimate (36).

To show that $E_D(P_\psi)\geqslant S_{\mathrm{vN}}(P_\psi)$, let us apply the map Λ_{n_j} from Eq. (37a) to the state $|\psi^{\otimes n_j}\rangle\langle\psi^{\otimes n_j}|$. We only need check that the resulting state $\Lambda_{n_j}(|\psi^{\otimes n_j}\rangle\langle\psi^{\otimes n_j}|)$ approaches P_+^a as $j\to\infty$. But, by Lemma 5,

$$\begin{aligned}\|\Lambda_{n_j}(|\psi^{\otimes n_j}\rangle\langle\psi^{\otimes n_j}|)-P_+^a\|_1&=\|\Lambda_{n_j}(|\psi^{\otimes n_j}\rangle\langle\psi^{\otimes n_j}|)-\Lambda_{n_j}(|\phi_{n_j}\rangle\langle\phi_{n_j}|)\|_1\\&\leqslant\||\psi^{\otimes n_j}\rangle\langle\psi^{\otimes n_j}|-|\phi_{n_j}\rangle\langle\phi_{n_j}|\|_1\end{aligned}$$

and once again estimate (36) is sufficient. ■

With the results obtained in this article, we can now prove that E_D is convex on pure decompositions, i.e., we have the following Lemma.

Lemma 25:

$$E_D\left(\sum_i p_i|\psi_i\rangle\langle\psi_i|\right)\leqslant\sum_i p_i E_D(|\psi_i\rangle\langle\psi_i|),\tag{38}$$

where $p_i\geqslant 0$ for all i and $\Sigma_i p_i=1$.

Proof: We have seen that E_C is convex and satisfies $E_D\leqslant E_C$. Using Lemma 24 gives

$$E_D\left(\sum_i p_i|\psi_i\rangle\langle\psi_i|\right) \leqslant E_C\left(\sum_i p_i|\psi_i\rangle\langle\psi_i|\right)$$
$$\leqslant \sum_i p_i E_C(|\psi_i\rangle\langle\psi_i|)$$
$$= \sum_i p_i S_{\mathrm{vN}}(P_{\psi_i})$$
$$= \sum_i p_i E_D(|\psi_i\rangle\langle\psi_i|). \tag{39}$$

■

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Global entanglement in multiparticle systems

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We define a polynomial measure of multiparticle entanglement which is scalable, i.e., which applies to any number of spin-$\frac{1}{2}$ particles. By evaluating it for three particle states, for eigenstates of the one dimensional Heisenberg antiferromagnet and on quantum error correcting code subspaces, we illustrate the extent to which it quantifies global entanglement. We also apply it to track the evolution of entanglement during a quantum computation. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1497700]

Although entanglement has been recognized as a remarkable feature of quantum mechanics since Schrödinger introduced the word[1] in response to Einstein, Podolsky and Rosen's famous paper,[2] it remains only incompletely understood. In fact, for more than two particles—even of only spin-$\frac{1}{2}$—there is no complete classification of entanglement. To be more precise, a *measure of entanglement* is a function on the space of states of a multiparticle system which is invariant under local unitary operators, i.e., unitary transformations on individual particles. Thus a complete classification of entanglement for a multiparticle system is a characterization of all such functions. Under the most general local operations assisted by classical communication (LOCC[3]), entanglement can change. A measure of entanglement which decreases under LOCC is called an *entanglement monotone*.[4]

On two particle pure states, for example, all measures of entanglement are functions of the eigenvalues of the reduced density matrix (obtained by tracing the density matrix for the whole system over the degrees of freedom of one of the particles), and sums of the k smallest eigenvalues are entanglement monotones.[5] The same information—in somewhat less familiar, but more algebraically convenient form—is contained in the coefficients of the characteristic polynomial of the reduced density matrix. These coefficients are polynomials in the components of the state vector and their complex conjugates. They generate the ring of polynomial functions invariant under the action of local unitary transformations; thus they completely classify two particle pure state entanglement.

As the number of particles n increases, however, the number of independent invariants—measures of entanglement—grows exponentially. Complete classification rapidly becomes impractical. Our goal in this article is more modest: we seek a measure of entanglement which is *scalable*, i.e., which is defined for any number of particles; which is easily calculated; and which provides physically relevant information. We concentrate on the case of spin-$\frac{1}{2}$ particles (*qubits*) and begin by defining a family (parametrized by n) of functions on $(\mathbb{C}^2)^{\otimes n}$. We show that each function is a measure of entanglement, vanishing exactly on product states. Next we evaluate this measure for several example states which illustrate its properties, most importantly that it measures *global* entanglement. This is perhaps best exemplified by its values on eigenstates of the antiferromagnetic Hamiltonian, for which we show that it is maximal only on the ground state. In a less traditional context, quantum computation relies heavily on multiparticle entangled states, particularly for error correction. We show that quantum error correcting code states also maximize

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our measure of entanglement. Finally, we illustrate its use in a dynamical setting, tracking the evolution of entanglement during a specific quantum computation.

The Hilbert space $(\mathbb{C}^2)^{\otimes n}$ of n qubits has a basis labeled by the 2^n n-bit strings: $|b_1\cdots b_n\rangle$, $b_j\in\{0,1\}$. For $b\in\{0,1\}$, define

$$\imath_j(b)|b_1\cdots b_n\rangle=\delta_{bb_j}|b_1\cdots\hat{b}_j\cdots b_n\rangle,$$

where $\hat{}$ denotes absence. We extend $\imath_j$ by linearity to be a map $\mathbb{C}^2\otimes(\mathbb{C}^2)^{\otimes n}\to(\mathbb{C}^2)^{\otimes n-1}$. For $u,v\in(\mathbb{C}^2)^{\otimes n-1}$ we can write $u=\Sigma u_x|x\rangle$ and $v=\Sigma v_y|y\rangle$, where $0\leqslant x,y<2^{n-1}$ are $(n-1)$-bit strings. Next, let

$$D(u,v)=\sum_{x<y}|u_xv_y-u_yv_x|^2,$$

the norm-squared of the wedge product of u and v. Finally, for $\psi\in(\mathbb{C}^2)^{\otimes n}$, define

$$Q(\psi)=\frac{4}{n}\sum_{j=1}^{n}D(\imath_j(0)\psi,\imath_j(1)\psi).$$

As we will see shortly, the $4/n$ factor provides a convenient normalization for Q.

Proposition 1: For each $n\in\mathbb{Z}_{\geqslant 2}$, $Q:(\mathbb{C}^2)^{\otimes n}\to\mathbb{R}$ is a measure of entanglement.

Proof: For $u,v\in(\mathbb{C}^2)^{\otimes n-1}$, $D(u,v)$ is invariant under $U(2^{n-1})$. A transformation of the jth qubit in $\psi\in(\mathbb{C}^2)^{\otimes n}$ multiplies the jth summand in Q by the norm squared of its determinant. Thus each summand is invariant under $\mathrm{TSL}(2)\times\mathrm{U}(2^{n-1})$, where T denotes the unit scalars. The intersection of these groups for all the summands is $\mathrm{U}(2)^n$, i.e., the local unitary transformations. ■

The most basic property that a measure of entanglement can have is to identify completely unentangled, i.e., product states. Q has this property:

Proposition 2: $Q(\psi)=0$ iff ψ is a product state.

Proof: Two vectors $u,v\in(\mathbb{C}^2)^{\otimes n-1}$, are linearly dependent iff $D(u,v)=0$. Thus $Q(\psi)=0$ implies the existence of $\alpha_j\in\mathbb{C}$ such that $\imath_j(1)\psi=\alpha_j\imath_j(0)\psi$ for all $1\leqslant j\leqslant n$. In particular,

$$\psi=|0\rangle\otimes\imath_1(0)\psi+|1\rangle\otimes\imath_1(1)\psi=(|0\rangle+\alpha_1|1\rangle)\otimes\imath_1(0)\psi=(g\otimes I)\cdot(|0\rangle\otimes\psi')$$

for some $g\in\mathrm{SU}(2)$, $\psi'\in(\mathbb{C}^2)^{\otimes n-1}$. By Proposition 1, Q is invariant under the local unitary transformation $g\otimes I$, so

$$0=Q(\psi)=Q(|0\rangle\otimes\psi')=0+\sum_{j=2}^{n}D(\imath_j(0)[|0\rangle\otimes\psi'],\imath_j(1)[|0\rangle\otimes\psi'])=Q(\psi').$$

Then, by induction, ψ is a product state.

Conversely, if ψ is a product state, then for all $1\leqslant j\leqslant n$, $\imath_j(0)\psi$ is parallel to $\imath_j(1)\psi$. Thus $Q(\psi)=0$. ■

Having demonstrated that Q vanishes on product states, we should now calculate it for some entangled states. First consider the EPR-Bohm[2,6] state $(|01\rangle-|10\rangle)/\sqrt{2}$, or, equivalently, $\gamma_2=(|00\rangle+|11\rangle)/\sqrt{2}$. It is straightforward to calculate:

$$Q(\gamma_2)=2\cdot\frac{4}{2}\left[\det\frac{1}{\sqrt{2}}\begin{pmatrix}1&0\\0&1\end{pmatrix}\right]^2=1.$$

Next, the three qubit GHZ-Mermin[7,8] state is $\gamma_3=(|000\rangle+|111\rangle)/\sqrt{2}$. Calculating the invariant, we again find

$$Q(\gamma_3)=3\cdot\frac{4}{3}\left[\det\frac{1}{\sqrt{2}}\begin{pmatrix}1&0\\0&1\end{pmatrix}\right]^2=1.$$

Finally, it is now clear that for the n qubit state $\gamma_n=(|0\cdots0\rangle+|1\cdots1\rangle)/\sqrt{2}$, $Q(\gamma_n)=1$. These examples demonstrate that the $4/n$ factor provides a natural normalization for Q.

Proposition 3: With this normalization, $0\leqslant Q\leqslant 1$.

Proof: Since $D(u,v)$ is the norm-squared of the wedge product of the two vectors u and v, it is bounded above by $\|u\|^2\|v\|^2$, which takes its maximal value of $\frac{1}{4}$ when $\|u\|^2=\|v\|^2=\frac{1}{2}$ for vectors $\psi=|0\rangle\otimes\imath_1(0)\psi+|1\rangle\otimes\imath_1(1)\psi$ with $\|\psi\|^2=1$. Since there are n summands in Q, it is bounded above by $n\cdot(4/n)\cdot\frac{1}{4}=1$. ■

Proposition 2 and the calculations above show that these bounds are saturated on, respectively, product states and the entangled states γ_n. Of course, Q does take other values: Under the action of $\mathrm{U}(2)\times\mathrm{U}(2)\times\mathrm{U}(2)$, the Hilbert space for three qubits, $\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^2$, decomposes into multiple orbits.[9–15] Representative states are $|000\rangle$ (product states), $|0\rangle\otimes\gamma_2=|0\rangle(|00\rangle+|11\rangle)/\sqrt{2}$ (and cyclic permutations), $(|100\rangle+|010\rangle+|001\rangle)/\sqrt{3}$, and γ_3. By Proposition 2, $Q(|000\rangle)=0$. By Proposition 2 and the calculation above, $Q(|0\rangle\otimes\gamma_2)=\frac{4}{3}\cdot\frac{1}{2}=\frac{2}{3}$. A straightforward calculation gives $Q((|100\rangle+|010\rangle+|001\rangle)/\sqrt{3})=\frac{8}{9}$. And we have already calculated $Q(\gamma_3)=1$. Thus for three qubits our measure of entanglement behaves in the way we would want, decreasing through states we would consider successively less globally entangled (and taking different values on each of these states, unlike the "tangle,"[16] for example, which vanishes on all but γ_3). In fact, on three qubits Q is an entanglement monotone and numerical evidence indicates that this is true in general.[17]

The traditional context in which globally entangled multiparticle states occur is lattice spin systems. Consider, for example, the one-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet[18,19] on a lattice of size n, with periodic boundary conditions, defined by the Hamiltonian

$$H_n=\sum_{j=1}^{n}X_jX_{j+1}+Y_jY_{j+1}+Z_jZ_{j+1},$$

where the subscripts are to be interpreted mod n, and X, Y, Z denote the Pauli matrices σ_x, σ_y, σ_z, respectively. H_n commutes with $S_z=\Sigma Z_j$, so the eigenstates of H_n can be labeled by their total spin S_z, i.e., each eigenstate of H_n is a superposition of basis vectors $|b_1\cdots b_n\rangle$ with $|\{j|b_j=1\}|=s$ for some fixed $0\leqslant s\leqslant n$. When $s=1$, the translation invariance of H_n implies that the eigenstates are plane waves

$$\psi_n^{(k)}=\frac{1}{\sqrt{n}}\sum_{j=0}^{n-1}e^{ikj}|0\cdots010\cdots0\rangle,$$

where the jth summand has a single 1 at the jth bit and the wave number $k=2\pi m/n$ for some integer $0\leqslant m\leqslant n-1$. For $n=3$ these plane waves are equivalent under local unitary transformations to the state $(|100\rangle+|010\rangle+|001\rangle)/\sqrt{3}$, for which we calculated $Q=\frac{8}{9}$ above. In fact, for arbitrary n the entanglement of these plane waves is simply

$$Q(\psi_n^{(k)})=\frac{4}{n}\cdot n\cdot(n-1)\frac{1}{n^2}=\frac{4(n-1)}{n^2}.$$

For $s>1$ the eigenstates of H_n can be computed using the Bethe *Ansatz*; the ground state has $s=n/2$ (for even n).[20] Using the translation invariance of these eigenstates we can evaluate Q easily. The result is

$$Q(S_z=s\ \text{ eigenstate of }H_n)=\frac{4}{n}\cdot n\cdot\binom{n-1}{s}\binom{n-1}{s-1}\binom{n}{s}^{-2}=\frac{4s(n-s)}{n^2}.$$

Notice that for the ground state this entanglement measure is maximal, $Q=1$. This result contrasts with O'Connor and Wootters' calculations of the ''concurrence'' C in these states:[21] they find that C is not maximal on the ground state, but rather for $s/n\approx 0.3$ as $n\to\infty$. This difference is due to the fact that C is really a measure of two particle entanglement, even when generalized to multiparticle states, while Q is a global measure of multiparticle entanglement.

Highly entangled multiparticle states also occur in the relatively new context of quantum error correcting codes. In fact, the code subspace for an additive code can be described as the space of ground states of the Hamiltonian formed by the sum of the stabilizers.[22] For example, the code subspace for a 5 qubit code [5,1,3] encoding 1 qubit against single bit errors[23,24] is the space of ground states of the translation invariant Hamiltonian on a one-dimensional lattice of five qubits:

$$H_{[5,1,3]}=\sum_{j=1}^{5} X_j Z_{j+1} Z_{j+2} X_{j+3},$$

where the subscripts are to be interpreted mod 5. The space of ground states is two dimensional—which is why it can encode 1 qubit. A basis is

$$|0\rangle\mapsto[|00000\rangle-(|11000\rangle+\text{cyc})+(|10100\rangle+\text{cyc})-(|11110\rangle+\text{cyc})]/4,$$

$$|1\rangle\mapsto[|11111\rangle-(|00111\rangle+\text{cyc})+(|01011\rangle+\text{cyc})-(|00001\rangle+\text{cyc})]/4,$$

where ''cyc'' indicates cyclic permutations. From these equations it is straightforward to calculate that $Q=1$ for all states in this code space. Here the difference from the concurrence is even more dramatic: C vanishes on the code subspace since tracing over all but two qubits leaves a reduced density matrix proportional to the identity.[25]

Shor's original 9 qubit code protecting 1 qubit against single qubit errors[26] can also be described as the ground state subspace of a lattice Hamiltonian—for a lattice triangulating $\mathbb{R}P^2$.[27] In this case a basis for the code space is

$$|0\rangle\mapsto(|000\rangle+|111\rangle)^{\otimes 3}/3,$$

$$|1\rangle\mapsto(|000\rangle-|111\rangle)^{\otimes 3}/3.$$

Calculating Q for the states in this subspace we find that again it is maximal, despite the fact that these states decompose into products of three qubit factors. So Q does not distinguish all subglobal entanglements; this is a consequence of using a single invariant. Finer resolution requires a more complete set of invariants, and, in general, higher degree polynomials.[9,10,12,15,28]

Nevertheless, as we have seen, Q provides useful information about global entanglement in certain contexts. Furthermore, in dynamical problems, Q quantifies the evolution of entanglement. Consider Grover's algorithm,[29] for example: Given $a_j\in\{0,1\}$, $1\leqslant j\leqslant n$, define

$$U_a|b_1\cdots b_n\rangle=(-1)^{\Pi\delta_{a_j b_j}}|b_1\cdots b_n\rangle$$

and then extend U_a by linearity to a map $(\mathbb{C}^2)^{\otimes n}\to(\mathbb{C}^2)^{\otimes n}$. The goal of Grover's algorithm is to convert an initial state of n qubits, say $|0\cdots 0\rangle$, to a state with probability bounded above $\frac{1}{2}$ of being in the state $|a_1\cdots a_n\rangle$, using U_a the fewest times possible. Grover showed that it can be done with $O(\sqrt{2^n})$ uses of U_a by preparing the state

$$\frac{1}{\sqrt{2^n}}\sum_{x=0}^{2^n-1}|x\rangle=H^{\otimes n}|0\cdots 0\rangle,\quad\text{where}\quad H=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix},$$

and then iterating the transformation $H^{\otimes n}U_0H^{\otimes n}U_a$ on this state.[29] The initial state is a product state, as is the target state $|a_1\cdots a_n\rangle$, but intermediate states $\psi(k)$ are entangled for $k>0$ iterations. We can evaluate Q on these states to quantify this entanglement:

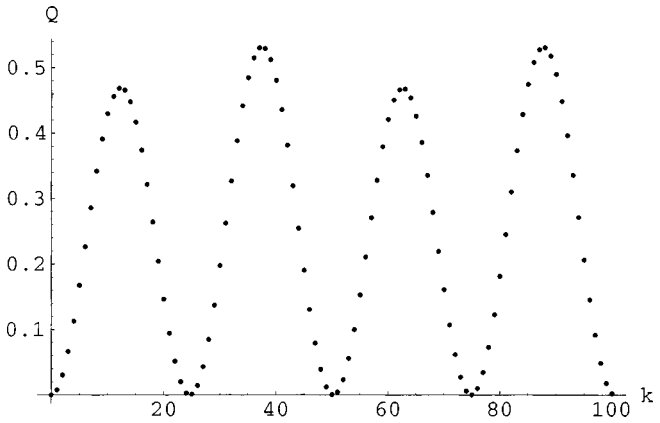

FIG. 1. Entanglement in Grover's algorithm for ten qubits as a function of number of iterations.

$$Q(\psi(k))=4\left(\frac{N}{2}-1\right)\frac{\cos^2\theta_k}{N-1}\left(\sin\theta_k-\frac{\cos\theta_k}{\sqrt{N-1}}\right)^2,$$

where $\theta_k=(2k+1)\csc^{-1}(\sqrt{N})$ and $N=2^n$. The results are plotted in Fig. 1 for $n=10$: the entanglement oscillates, first returning to close to 0 at

$$k=\left\lfloor\frac{1}{2}\left(\frac{\pi}{2\csc^{-1}(\sqrt{N})}-1\right)\right\rceil\sim\left\lfloor\frac{\pi}{4}\sqrt{N}\right\rceil \quad \text{as} \quad N\to\infty,$$

where $\lfloor\cdot\rceil$ denotes "closest integer to"; this is when the probability of measuring $|a_1\cdots a_n\rangle$ is first close to 1.

Three qubit states, eigenstates of lattice Hamiltonians, quantum error correcting code subspaces, and the intermediate states in Grover's algorithm all illustrate how a measure of multiparticle entanglement such as Q provides insight into global properties of quantum multiparticle systems. While Q has the satisfactory properties of Propositions 2 and 3, is an entanglement monotone on three qubits, and is a straightforwardly computable polynomial, it is in no sense a unique measure of multiparticle entanglement. A more complete (but still partial) characterization can be obtained by also using some of the other measures which have been proposed, like the concurrence,[21] the closely related n-tangle,[30] the Schmidt rank,[31] the negativity,[32] etc. Each emphasizes a specific feature of multiparticle entanglement and describes a different physical property. We anticipate that multiparticle entanglement measures—whose current development is largely motivated by quantum computation—will contribute to the understanding of the physics of quantum multiparticle systems more generally.[33–35]

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Entanglement and perfect quantum error correction

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The entanglement of formation gives a necessary and sufficient condition for the existence of a perfect quantum error correction procedure. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1497183]

I. QUANTUM ERROR CORRECTION

Suppose a composite quantum system RQ is initially in a pure joint input state $|\Psi^{RQ}\rangle$. The subsystem Q undergoes a dynamical evolution described by a trace-preserving, completely positive (CP) map $\mathcal{E}$. The joint output state is therefore

$$\rho^{RQ'} = I \otimes \mathcal{E}(|\Psi^{RQ}\rangle\langle\Psi^{RQ}|). \tag{1}$$

This situation describes the transmission of ''quantum information'' (the entanglement between R and Q) via a noisy quantum channel. For example, imagine that RQ is a quantum computing device. The overall state of the device is entangled. Subsystem Q is imperfectly isolated from the environment, and thus experiences noise and distortion given by $\mathcal{E}$. The problem of sending entanglement through a channel in this way is closely related to other tasks of quantum information transfer, such as the transmission of an unknown quantum state of Q.[1]

We are interested in the question of whether the original input state $|\Psi^{RQ}\rangle$ can be restored by some possible operation on Q alone. Such a restoring operation is called a ''quantum error correction'' procedure.[2] We say that *perfect* quantum error correction is possible when there exists a trace preserving CP map $\mathcal{D}$ on Q such that

$$|\Psi^{RQ}\rangle\langle\Psi^{RQ}| = I \otimes \mathcal{D}(\rho^{RQ'}). \tag{2}$$

If no such $\mathcal{D}$ exists, we may still be able to do *approximate* quantum error correction, in which case we restore $\rho^{RQ'}$ to a state close to the original. (''Close'' here is usually defined in terms of the fidelity or some equivalent measure.) In this article, we will mostly be concerned with the question of perfect (unit fidelity) error correction.

We first note that, if the input state of RQ is a product state, then it is always possible to restore the input state by means of an operation on Q. Thus, the problem of error correction is only nontrivial when $|\Psi^{RQ}\rangle$ is entangled. The entanglement of a pure state of RQ is measured by the entropy S^Q of the subsystem Q:

$$S^Q = -\operatorname{Tr}\rho^Q \log \rho^Q. \tag{3}$$

Of course, since RQ is in a pure state, then $S^Q = S^R$.

The output state $\rho^{RQ'}$ is generally not pure. Schumacher and Nielsen[3] defined the ''coherent information'' to be

$$I = S^{Q'} - S^{RQ'}. \tag{4}$$

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This quantity has a number of significant properties. It is positive only if the output state $\rho^{RQ'}$ is entangled. Furthermore, it cannot be increased by any operation on Q alone. Since the initial coherent information is just S^Q, this means that $I \leqslant S^Q$ after the action of $\mathcal{E}$. Furthermore, any loss of I due to the action of $\mathcal{E}$ is irreversible, i.e., cannot be reversed by any subsequent evolution of Q. It follows that $I = S^Q$ is a necessary condition for the existence of a perfect quantum error correction operation $\mathcal{D}$.

In Ref. 3, it is shown that the condition $I = S^Q$ is also *sufficient* for the existence of such an operation. In outline, we imagine a larger quantum system RQE that includes the environment E with which Q interacts. The initial state of the environment is a pure state $|0^E\rangle$, and the interaction of Q and E is described by the unitary operator U^{QE}. (Since the operation $\mathcal{E}$ is a trace-preserving CP map, it must always be realizable in this way as a unitary evolution on a larger system.) The condition $I = S^Q$ implies that the output state of the subsystem RE is a product state. From this product structure, a perfect error correction procedure can be constructed. In short, the lack of any correlation between R and E after the evolution is sufficient to permit the restoration of the original QE state by an error-correction operation $\mathcal{D}$.

Although the error-correction operation $\mathcal{D}$ is constructed for a particular input entangled state $|\Psi^{RQ}\rangle$, the same procedure will also work for any other state $|\Phi^{RQ}\rangle$ whose support in Q lies within the Q-support for $|\Psi^{RQ}\rangle$. Furthermore, if we have an ensemble of pure input Q states within this subspace, $\mathcal{D}$ will restore these states with unit average fidelity.[3]

II. ENTANGLEMENT OF FORMATION

The coherent information I is a measure of the entanglement of Q with R after it has undergone its noisy evolution. There are, however, many other ways to measure the entanglement of the output state $\rho^{RQ'}$. One of the most fundamental is the "entanglement of formation,"[4] denoted $\mathbf{E}$. The entanglement of formation of a pure state $|\psi^{AB}\rangle$ is just $\mathbf{E} = S^A$, the entropy of one of the subsystems. A mixed state ρ^{AB} has an entanglement of formation

$$\mathbf{E} = \min \sum_k p_k \mathbf{E}_k , \tag{5}$$

where $\mathbf{E}_k$ is the entanglement of the pure state $|\phi_k^{AB}\rangle$ and the minimum is taken over all pure-state ensembles such that $\rho^{AB} = \Sigma_k\, p_k |\phi_k^{AB}\rangle\langle\phi_k^{AB}|$. $\mathbf{E}$ has the property that it cannot be increased by local quantum operations on, or the exchange of classical information between, the two subsystems.

The entanglement of formation is related to the "entanglement resources" necessary to create the quantum state. However, to make this connection sharp one must define an *asymptotic* entanglement of formation

$$\mathbf{E}_\infty(\rho^{AB}) = \lim_{n\to\infty} \frac{1}{n} \mathbf{E}((\rho^{AB})^{\otimes n}). \tag{6}$$

$\mathbf{E}_\infty$ is the asymptotic number of maximally entangled qubit pairs needed to create the state ρ^{AB} by local operations and classical communication—that is, for large n, about $n\mathbf{E}_\infty$ pairs are required to make n copies of the state ρ^{AB}. Though the definitions of $\mathbf{E}_\infty$ and $\mathbf{E}$ are distinct, and we can see that $\mathbf{E}_\infty \leqslant \mathbf{E}$, it is not known whether or not these are actually equal in general.[5] We will here use the "single system" definition of the entanglement of formation $\mathbf{E}$, since we are not primarily concerned with asymptotic questions.

The coherent information I and the entanglement of formation $\mathbf{E}$ of the output state $\rho^{RQ'}$ satisfy $I \leqslant \mathbf{E}$. To see this, suppose we have an ensemble of RQ states such that $\rho^{RQ'} = \Sigma_k\, p_k \rho_k^{RQ}$, then

$$S^{Q'} - \sum_k p_k S_k^Q \leqslant S^{RQ'} - \sum_k p_k S_k^{RQ}. \tag{7}$$

(This follows from the strong subadditivity of the entropy functional.[6]) For any ensemble of pure states, $S_k^{RQ}=0$ and so

$$S^{Q'} - S^{RQ'} \leqslant \sum_k p_k S_k^Q. \tag{8}$$

If we choose the pure state ensemble that minimizes the right-hand side, we obtain $I \leqslant \mathbf{E}$.

For the input pure state of RQ, both $\mathbf{E}$ and I are equal to S^Q. For the output state, the condition that $\mathbf{E}=S^Q$ is weaker than the condition that $I=S^Q$, since we can have $I<\mathbf{E}$. Thus, $\mathbf{E}=S^Q$ is a necessary condition for the existence of a perfect quantum error correction operation $\mathcal{D}$. Remarkably, it turns out that this is also a sufficient condition. We now show this. Suppose that $\mathbf{E}=S^Q$ for our output state $\rho^{RQ'}$. Our argument is based on three facts.

Fact 1: Concavity of the entropy. Suppose we write a mixed state as an ensemble of states: $\rho=\Sigma_k p_k \rho_k$. Then

$$S \geqslant \sum_k p_k S_k \tag{9}$$

with equality if and only if $\rho_k=\rho$ for all k with $p_k>0$.[7] In our context, the condition that $\mathbf{E}=S^Q$ means that

$$0 = S^{R'} - \min \sum_k p_k S_k^R, \tag{10}$$

where the minimum is taken over all pure state ensembles for $\rho^{RQ'}$, and where we have recalled that $S^Q=S^R=S^{R'}$. Equation (9) then tells us that

$$0 = S^{R'} - \sum_k p_k S_k^R \tag{11}$$

for *any* pure state ensemble for $\rho^{RQ'}$, and therefore all of the elements of such an ensemble have $\rho_k^R=\rho^{R'}$. Since we can consider any mixed state to be made up of pure states, this is also true for $\rho^{RQ'}$ ensembles that include mixed states.

Fact 2: Choice of ensemble is choice of ancilla measurement. Hughston, Jozsa and Wootters[8] give a useful characterization of all the pure state ensembles that can lead to a particular density operator ρ^A for a system A. We "purify" the state by envisioning a pure state $|\psi^{AB}\rangle$ of a larger composite system AB such that $\rho^A=\mathrm{Tr}_B|\psi^{AB}\rangle\langle\psi^{AB}|$. A measurement on system B will lead to an ensemble of relative states of A. In Ref. 8 it is shown that, given a purification $|\psi^{AB}\rangle$ of ρ^A, we can realize *any* ensemble for ρ^A as an ensemble of relative states for some measurement on B. In other words, the choice of ρ^A ensemble is exactly the same as the choice of measurement on the purifying system B.

In our context, we can include the environment system E as before, with the whole system RQE in the pure state $|\Psi^{RQE'}\rangle$ after the interaction of Q and E. E purifies RQ, so an ensemble of RQ states corresponds to a measurement on E. From fact 1, we know that every element of an ensemble for $\rho^{RQ'}$ yields the same state $\rho^{R'}$ on R alone. Thus, for any possible outcome of any measurement on E, the relative state of R will be $\rho^{R'}$. This means that the probabilities of the outcomes of possible R-measurements are unaffected by the particular outcomes of an E-measurement.

Fact 3: No correlation implies product state. Quantum state tomography[2] allows the reconstruction of a quantum state ρ from the outcome distributions of a finite number of possible measurements on the quantum system. This procedure, when applied to a composite quantum system AB, has two important features. First, it is sufficient to consider only product measurements of A and B to do tomography of the joint state. Second, if no statistical correlations appear between the outcomes of the A and B measurements, the resulting joint state must be a product state $\rho^A \otimes \sigma^B$. Thus, a necessary and sufficient condition for A and B to be in a product state is that no correlations arise in any product measurement of the systems.

Since we have shown that $\mathbf{E}=S^Q$ implies no statistical correlations between E- and R-measurements on the output state, we can conclude that the output state of the subsystem RE is a product state $\rho^{R'} \otimes \sigma^{E'}$. Given such a product state, we can apply the procedure in Ref. 3 to give an explicit error correction operation $\mathcal{D}$ that will restore the input state $|\Psi^{RQ}\rangle$ of RQ with perfect fidelity. Therefore, perfect quantum error correction is possible if and only if $\mathbf{E}=S^Q$.

III. INTRINSIC EXPRESSIONS FOR *I* AND E

Both the coherent information I and the entanglement of formation $\mathbf{E}$ are "intrinsic" quantities to the system Q—that is, they can be expressed entirely in terms of the input state ρ^Q of Q alone and the trace-preserving CP map $\mathcal{E}$ that describes Q's dynamics. First, we note that the map $\mathcal{E}$ can be given an "operator sum" representation:[2]

$$\mathcal{E}(\rho^Q)=\sum_k A_k \rho^Q A_k^\dagger, \tag{12}$$

where the A_k operators satisfy $\Sigma_k A_k^\dagger A_k = 1$. A given $\mathcal{E}$ always has many different operator sum representations. Suppose we have a unitary matrix V_{kl}, and define some operators B_k as linear combinations of the A_k's:

$$B_k=\sum_l V_{kl} A_l. \tag{13}$$

Then the B_k's give an alternate operator sum representation for $\mathcal{E}$.

The operator sum representation is closely related to the unitary representation for $\mathcal{E}$, in which $\mathcal{E}$ is given via unitary evolution on a larger system that includes the environment E. Once again, E is taken to be initially in a pure state $|0^E\rangle$, and the interaction of Q and E is given by the unitary operator U^{QE}. Let $|k^E\rangle$ be a basis of E states, and define the operator A_k on Q by the "partial inner product"

$$A_k|\psi^Q\rangle=\langle k^E|U^{QE}|\psi^Q 0^E\rangle, \tag{14}$$

where $|\psi^Q 0^E\rangle$ is shorthand for $|\psi^Q\rangle\otimes|0^E\rangle$. We can use the $|k^E\rangle$ basis to do a partial trace over the E system, so that

$$\mathcal{E}(\rho^Q)=\mathrm{Tr}_E[U^{QE}(\rho^Q\otimes|0^E\rangle\langle 0^E|)U^{QE\dagger}]=\sum_k \langle k^E|U^{QE}(\rho^Q\otimes|0^E\rangle\langle 0^E|)U^{QE\dagger}|k^E\rangle=\sum_k A_k\rho^Q A_k^\dagger. \tag{15}$$

The unitary freedom in the operator sum representation is the same as the freedom to choose a basis for the environment system E.

The operator sum representation of $\mathcal{E}$ gives the output state $\rho^{Q'}=\mathcal{E}(\rho^Q)$ as an ensemble of Q states. If we let

$$p_k=\mathrm{Tr}A_k\rho^Q A_k^\dagger,$$

$$\rho_k^Q = \frac{1}{p_k}(A_k \rho^Q A_k^\dagger), \tag{16}$$

then $\rho^{Q'} = \Sigma_k p_k \rho_k^Q$. Different operator sum representations yield different ensembles for the same output state.

The entanglement of formation $\mathbf{E}$ of the $\rho^{RQ'}$ state can be written

$$\mathbf{E} = \min \sum_k p_k S_k^Q, \tag{17}$$

where S_k^Q is the entropy of ρ_k^Q (as defined above) and the minimum is taken over all operator sum representations for $\mathcal{E}$. In a similar way, the coherent information I can be written

$$I = S^{Q'} - \min H(\vec{p}), \tag{18}$$

where $H(\vec{p}) = -\Sigma_k p_k \log p_k$ and the minimum is once again taken over all operator sum representations.[1] We can see why this is true by appealing to a unitary representation. The p_k's are the diagonal entries of the output density matrix for the environment E, and $S^{E'} = \min H(\vec{p})$ (where we minimize over basis states). Since the global state of RQE is pure, $S^{E'} = S^{RQ'}$.

IV. GENERALIZATION

We pointed out that both I and $\mathbf{E}$ were measures of entanglement of the state $\rho^{RQ'}$, and that $I = \mathbf{E} = S^Q$ for the input pure state $|\Psi^{RQ}\rangle$. We now consider other possible measures of the entanglement of $\rho^{RQ'}$. Suppose M is such a measure, and that it satisfies the following conditions:

(1) $M = S^Q$ when RQ is in a pure state.

(2) M is additive if we have many copies of $\rho^{RQ'}$; that is,

$$M((\rho^{RQ'})^{\otimes n}) = nM(\rho^{RQ'}). \tag{19}$$

(3) M does not increase on average under local operations on, or classical communication between, R and Q.

The requirement that M be nonincreasing ''on average'' allows us to include nondeterministic operations, such as local measurements. Though M may increase conditionally for some measurement outcomes, we require that, if M is averaged over all outcomes, then it cannot increase.

Coherent information satisfies (1) and (2) but not (3); the asymptotic entanglement of formation $\mathbf{E}_\infty$ satisfies all three; it is not known whether the ''single system'' entanglement of formation $\mathbf{E}$ satisfies (2) (for this is exactly the question of whether $\mathbf{E} = \mathbf{E}_\infty$). Conditions (1)–(3) are similar to those discussed in Ref. 9.

We will now show that perfect quantum error correction is possible if and only if $M = S^Q$ for the output state $\rho^{RQ'}$.

''Only if'' is easy to see. Initially, $M = S^Q$. If M decreases under the action of $\mathcal{E}$ on Q, then this loss cannot be made up by any error correction procedure, which must be a local operation on Q. Thus, the original state can be restored only if $M = S^Q$ after $\mathcal{E}$ acts.

To show that $M = S^Q$ is sufficient to allow perfect error correction, we will show that $M \leqslant \mathbf{E}$. Imagine that we begin with $n\mathbf{E}_\infty$ maximally entangled qubit pairs, for which $M_n = n\mathbf{E}_\infty$. We know that, if n is large, we can use these pairs to make about n copies of our state $\rho^{RQ'}$ by local operations and classical communication. Since M cannot increase in this process, $nM \leqslant M_n$, and so $M \leqslant \mathbf{E}_\infty$. But we have seen that $\mathbf{E}_\infty \leqslant \mathbf{E}$, so $M \leqslant \mathbf{E}$.

We know that $\mathbf{E} \leqslant S^Q$. Thus, if $M = S^Q$, then $\mathbf{E} = S^Q$. As we have seen, this is sufficient to guarantee the existence of a perfect error correction operation $\mathcal{D}$ for Q. $M = S^Q$ is therefore both necessary and sufficient for the existence of $\mathcal{D}$.

Remarkably, inequivalent entanglement measures lead to equivalent conditions for perfect quantum error correction. The coherent information I, the entanglement of formation $\mathbf{E}$ (or its asymptotic form $\mathbf{E}_\infty$), and entanglement measures M satisfying our properties all share the feature that they are conserved by the evolution $\mathcal{E}$ on Q only when that evolution produces no correlations between R and E.

V. REMARKS

We have assumed that Q may interact with environment, while R remains untouched. Suppose instead that both Q and R independently interact with separate parts of the environment, so that

$$\rho^{RQ\prime} = \mathcal{E}^R \otimes \mathcal{E}^Q(|\Psi^{RQ}\rangle\langle\Psi^{RQ}|). \tag{20}$$

We say in this case that perfect quantum error correction is possible if the original state of RQ can be restored by local operations and classical communication. It turns out that this can be done if and only if $\mathbf{E}=S^Q$; furthermore, if error correction is possible at all, then no classical communication between R and Q is necessary.

Once again, $\mathbf{E}=S^Q$ is plainly a necessary condition, and we must show that it is also sufficient. Suppose $\mathbf{E}=S^Q$ after the operation $\mathcal{E}^R\otimes\mathcal{E}^Q$. We can imagine that this operation occurs in two stages:

$$\rho^{RQ\prime} = (\mathcal{E}^R \otimes I^Q)\circ(I^R \otimes \mathcal{E}^Q)(|\Psi^{RQ}\rangle\langle\Psi^{RQ}|). \tag{21}$$

After the first stage, in which $I^R\otimes\mathcal{E}^Q$ acts, we must have $\mathbf{E}=S^Q$. Therefore, at this stage there exists an operation $\mathcal{D}^Q$ on Q that can accomplish perfect error correction. That is,

$$|\Psi^{RQ}\rangle\langle\Psi^{RQ}| = (I^R \otimes \mathcal{D}^Q)\circ(I^R \otimes \mathcal{E}^Q)(|\Psi^{RQ}\rangle\langle\Psi^{RQ}|). \tag{22}$$

Alternately, we note that

$$\rho^{RQ\prime} = (I^R \otimes \mathcal{E}^Q)\circ(\mathcal{E}^R \otimes I^Q)(|\Psi^{RQ}\rangle\langle\Psi^{RQ}|), \tag{23}$$

in which case $\mathbf{E}=S^Q=S^R$ after the first operation, and an error-correction operation $\mathcal{D}^R$ exists at this stage:

$$|\Psi^{RQ}\rangle\langle\Psi^{RQ}| = (\mathcal{D}^R \otimes I^Q)\circ(\mathcal{E}^R \otimes I^Q)(|\Psi^{RQ}\rangle\langle\Psi^{RQ}|). \tag{24}$$

Now we can see that $\mathcal{D}^R\otimes\mathcal{D}^Q$ will correct the complete operation:

$$\begin{aligned}
&(\mathcal{D}^R \otimes \mathcal{D}^Q)\circ(\mathcal{E}^R \otimes \mathcal{E}^Q)(|\Psi^{RQ}\rangle\langle\Psi^{RQ}|) \\
&\quad = (I^R \otimes \mathcal{D}^Q)\circ(\mathcal{D}^R \otimes I^Q)\circ(I^R \otimes \mathcal{E}^Q)\circ(\mathcal{E}^R \otimes I^Q)(|\Psi^{RQ}\rangle\langle\Psi^{RQ}|) \\
&\quad = (I^R \otimes \mathcal{D}^Q)\circ(I^R \otimes \mathcal{E}^Q)\circ(\mathcal{D}^R \otimes I^Q)\circ(\mathcal{E}^R \otimes I^Q)(|\Psi^{RQ}\rangle\langle\Psi^{RQ}|) \\
&\quad = |\Psi^{RQ}\rangle\langle\Psi^{RQ}|.
\end{aligned} \tag{25}$$

Thus, $\mathbf{E}=S^Q$ is a necessary and sufficient condition for local correction of the quantum state, even if both subsystems have experienced independent noisy evolutions.

Throughout this article, we have focused our attention on the issue of *perfect* error correction. What about *approximate* error correction? We have elsewhere[10] shown that, if the loss of coherent information is small, then an operation $\mathcal{D}$ exists that will nearly restore the original state $|\Psi^{RQ}\rangle$. To be precise, if $S^Q - I < \epsilon$, then there exists an operation $\mathcal{D}$ on Q that will restore the input state with fidelity $F > 1-2\sqrt{\epsilon}$. Is there an analogous theorem for the entanglement of formation $\mathbf{E}$? That is, suppose $S^Q - \mathbf{E} < \epsilon$. With what fidelity can error correction be performed? This and many other questions remain unresolved.

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The entanglement of purification

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We introduce a measure of both quantum as well as classical correlations in a quantum state, the entanglement of purification. We show that the (regularized) entanglement of purification is equal to the entanglement cost of creating a state ρ asymptotically from maximally entangled states, with negligible communication. We prove that the classical mutual information and the quantum mutual information divided by two are lower bounds for the regularized entanglement of purification. We present numerical results of the entanglement of purification for Werner states in $\mathcal{H}_2 \otimes \mathcal{H}_2$. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The theory of quantum entanglement aims at quantifying and characterizing uniquely quantum correlations. It does so by analyzing how entangled quantum states can be processed and transformed by quantum operations. A crucial role in the theory is played by the class of local operations and classical communication (LOCC), since quantum entanglement is nonincreasing under these operations. Indeed, by considering this class of operations we are able to neatly distinguish between the quantum entanglement and the classical correlations that are present in the quantum state.

Given the success of this theory, we may be daring enough to ask whether we can similarly construct a theory of purely classical correlations in quantum states and their behavior under local or nonlocal processing. At first sight, such an effort seems doomed to fail since merely local actions can convert quantum entanglement into classical correlations. Namely, Alice and Bob who possess an entangled state $|\psi\rangle = \Sigma_i \sqrt{\lambda_i} |a_i\rangle \otimes |b_i\rangle$ with Schmidt coefficients λ_i can, by local measurements, obtain a joint probability distribution with mutual information equal to $H(\lambda)$. Thus it does not seem possible to separate the classical correlations from the entanglement if we try to do this in an operational way. Note that it may be possible to separate quantum and classical correlations in a nonoperational way (see, for example, Ref. 1 or 2. The drawback of such an approach is that no connection is made to the dynamical processing of quantum information, which is precisely what has made the theory of quantum entanglement so elegant and innovative. An

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operational approach to the quantification of quantum and classical correlations was recently formulated in Ref. 3.

In this article we propose to treat quantum entanglement and classical correlation in a unified framework, namely we express both correlations in units of entanglement. Such a theory of ''all'' correlations may have potential applications outside quantum information theory as well. Researchers have started to look at entanglement properties of many-particle systems for example at (quantum) phase transitions (see, for example, Ref. 4 and references therein). Instead of considering the entanglement of formation in these studies, one may choose to look at the behavior of a complete correlation measure. In this article we introduce such a measure, called the entanglement of purification. We would like to emphasize that our correlation measure is *not* an entanglement measure, but a measure of correlations expressed in terms of the entanglement of a pure state.

It has been the experience in (quantum) information theory that questions in the asymptotic approximate regime are easier to answer than exact nonasymptotic queries. Thus we ask how to create a bipartite quantum state ρ in the asymptotic regime, allowing approximation, from an initial supply of EPR-pairs by means of *local operations and asymptotically vanishing communication*. This latter class of operations will be denoted as LOq [local operations with $o(n)$ communication in the asymptotic regime] versus the class LO for strictly local operations. We can properly define this formation cost E_{LOq} as follows:

$$E_{LOq}(\rho)=\lim_{\epsilon\to 0}\inf\left\{\frac{m}{n}\;\middle|\;\exists\,\mathcal{L}_{LOq}, D(\mathcal{L}_{LOq}(|\Psi_-\rangle\langle\Psi_-|^{\otimes m}),\rho^{\otimes n})\leq\epsilon\right\}. \tag{1}$$

Here $|\Psi_-\rangle$ is the singlet state in $\mathcal{H}_2\otimes\mathcal{H}_2$ and $\mathcal{L}_{LOq}$ is a local superoperator using $o(n)$ quantum communication. D is the Bures distance $D(\rho,\rho')=2\sqrt{1-F(\rho,\rho')}$ and the square-root-fidelity is defined as $F(\rho,\rho')=\mathrm{Tr}(\sqrt{\rho^{1/2}\rho'\rho^{1/2}})$.[5] We could have allowed classical instead of quantum communication in our definition (our results will not depend on this choice), so we may as well call all communication quantum communication.

Before we consider this entanglement cost for mixed states, we observe that by allowing asymptotically vanishing communication, we have preserved the interconvertibility result for pure states.[6] This is due to the fact that both the process of entanglement dilution as well as entanglement concentration can be accomplished with no more than asymptotically vanishing amount of communication, see Ref. 7.

We see that the cost $E_{LOq}(\rho)$ of creating the state ρ is defined analogously to the entanglement cost $E_c(\rho)$,[8,9] with the restriction that Alice and Bob can only do a negligible amount of communication. It is immediate that $E_{LOq}(\rho)$ will in general be larger than $E_c(\rho)$. In particular, for a separable density matrix, $E_c(\rho)=0$, whereas we will show that for any correlated (i.e., not of the form $\rho_{AB}=\rho_A\otimes\rho_B$) density matrix $E_{LOq}(\rho)>0$. The entanglement cost E_c was found[9] to be equal to

$$E_c(\rho)=\lim_{n\to\infty}\frac{E_f(\rho^{\otimes n})}{n}, \tag{2}$$

where $E_f(\rho)$ is the entanglement of formation.[8] We will similarly find an expression for E_{LOq},

$$E_{LOq}=\lim_{n\to\infty}\frac{E_p(\rho^{\otimes n})}{n}\equiv E_p^{\infty}(\rho), \tag{3}$$

where $E_p(\rho)$ is a new quantity, the entanglement of purification of ρ.

Our article is organized in the following manner. We start by defining the entanglement of purification and deriving some basic properties of this new function, such as continuity and monotonicity under local operations. We will relate the entanglement of purification to the problem of minimizing the entropy of a state under a local TCP (trace-preserving completely positive) map. With these tools in hand, we can prove our main result, Theorem 2. Then we spend some

time proving the mutual information lower bounds for $E_{LOq}(\rho)$. We also compare our correlation measure with the induced Holevo correlation measures $C_{A/B}$ that were introduced in Ref. 1. We prove that for Bell-diagonal states the correlation measure C_A is equal to the classical capacity of the related one-qubit Pauli channel. At the end of the article we present our numerical results for $E_p(\rho)$ where ρ is a Werner state on $\mathcal{H}_2 \otimes \mathcal{H}_2$. The proofs of the lemmas and theorems in this article are all fairly straightforward and use many basic properties of entropy and mutual information (concavity, subadditivity of entropy, nonincrease of mutual information under local actions, etc.).

II. ENTANGLEMENT OF PURIFICATION

We define the entanglement of purification:

Definition 1: Let ρ be a bipartite density matrix on $\mathcal{H}_A \otimes \mathcal{H}_B$. Let $|\psi\rangle \in \mathcal{H}_{AA'} \otimes \mathcal{H}_{BB'}$. The entanglement of purification $E_p(\rho)$ is defined as

$$E_p(\rho) = \min_{\psi: \mathrm{Tr}_{A'B'}|\psi\rangle\langle\psi| = \rho} E_f(|\psi\rangle\langle\psi|), \tag{4}$$

where $E_f(|\psi\rangle\langle\psi|)$ is the entanglement of $|\psi\rangle$ which is equal to the von Neumann entropy $S(\sigma_{BB'}) = -\mathrm{Tr}\sigma_{BB'} \log \sigma_{BB'}$ where $\sigma_{BB'} = \mathrm{Tr}_{AA'}|\psi\rangle\langle\psi|$. Let $\{\lambda_i, |\psi_i\rangle\}$ be the eigenvalues and eigenvectors of ρ_{AB}. The "standard purification" of ρ is defined as

$$|\psi_s\rangle = \sum_i \sqrt{\lambda_i} |\psi_i\rangle_{AB} \otimes |0\rangle_{A'} |i\rangle_{B'}. \tag{5}$$

Every purification of ρ can be written as $|\psi\rangle = (I_{AB} \otimes U_{A'B'})|\psi_s\rangle$ for some unitary operator $U_{A'B'}$ on A' and B'. Therefore, Eq. (4) can be rephrased as

$$E_p(\rho) = \min_{U_{A'B'}} E((I_{AB} \otimes U_{A'B'})|\psi_s\rangle\langle\psi_s|(I_{AB} \otimes U_{A'B'})^\dagger) \tag{6}$$

$$= \min_{U_{A'B'}} S(\mathrm{Tr}_{AA'}(I_{AB} \otimes U_{A'B'})|\psi_s\rangle\langle\psi_s|(I_{AB} \otimes U_{A'B'})^\dagger))$$

$$= \min_{\Lambda_{B'}} S((I_B \otimes \Lambda_{B'})(\mu_{BB'}(\rho))), \tag{7}$$

where we have taken the trace over A and A' to obtain Eq. (7),

$$\mu_{BB'}(\rho) = \mathrm{Tr}_{AA'}|\psi_s\rangle\langle\psi_s|, \tag{8}$$

and $\Lambda_{B'}(\nu) \equiv \mathrm{Tr}_{A'} U_{A'B'}(\nu_{B'} \otimes |0\rangle\langle 0|_{A'}) U^\dagger_{A'B'}$. The minimization in Eq. (7) is over all possible TCP maps $\Lambda_{B'}$ since every TCP map can be implemented by performing a unitary transformation on the system and some ancilla and tracing over the ancilla. Note that the minimizations over $U_{A'B'}$ and $\Lambda_{B'}$ are equivalent. Equations (6) and (7) provide two different formulations of the same minimization. Conceptually the first formulation is based on purifications of ρ and variation over $U_{A'B'}$. The second formulation is based on extensions of ρ, $\sigma_{ABB'}$, such that $\mathrm{Tr}_{B'}\sigma_{ABB'} = \rho_{AB}$, and variation over $\Lambda_{B'}(\nu)$. Both formulations will be used throughout the article.

The idea of bipartite purifications was considered in Ref. 10 where the authors proved that every correlated state has, in our language, a nonzero entanglement of purification. If we would have included mixed states in the minimization in Eq. (4) and used the entanglement of formation as the entanglement measure, then the defined quantity would be equal to the entanglement of formation of ρ, since the optimal extension of ρ is ρ itself.

We put some simple bounds on $E_p(\rho)$. Intuitively, "the amount of quantum correlation in a state is smaller than or equal to the total amount of correlation," or $E_f(\rho) \leqslant E_p(\rho)$. To prove this lower bound, let $|\psi_\rho\rangle = \Sigma_{i,j}|i\rangle_{A'}|j\rangle_{B'} \otimes |\psi_{ij}\rangle$ be the purification that achieves the minimum in Eq.

(4). Alice and Bob locally measure the labels $i_{A'}$ and $j_{B'}$ of the state $|\psi_\rho\rangle$ such that they obtain $|\psi_{ij}\rangle$ with probability $p_{ij}=\langle\psi_{ij}|\psi_{ij}\rangle$. Since entanglement is nonincreasing under local operations, we have

$$E_f(\rho)\leqslant\sum_{ij} p_{ij}E\left(\frac{|\psi_{ij}\rangle\langle\psi_{ij}|}{p_{ij}}\right)\leqslant E_p(\rho). \tag{9}$$

It is immediate that we have equality between the entanglement of formation and the entanglement of purification for pure states, where the optimal purification of a pure state is the pure state itself.

An easy upper bound is $E_p(\rho)\leqslant E(|\psi_s\rangle\langle\psi_s|)=S(\rho_A)$, where $\rho_A=\mathrm{Tr}_B(\rho)$ is the reduced density matrix in A. This corresponds to $U_{A'B'}=I_{A'B'}$ or equivalently $\Lambda_{B'}=I_{B'}$ on the rhs of Eq. (6) or (7). Applying the same argument with AA' and BB' interchanged, we obtain

$$E_p(\rho)\leqslant\min(S(\rho_A),S(\rho_B)), \tag{10}$$

where the purifications correspond to either completely purifying the state on A' or on B'. In general this is not the optimal purification, as we will see in Sec. V.

The entanglement of purification is neither convex nor concave, unlike the entanglement of formation. For instance, a mixture of product states, each with zero entanglement of purification, need not have zero entanglement of purification (for example, consider an equal mixture of $|00\rangle$ and $|11\rangle$). On the other hand, the completely mixed state has zero entanglement of purification equal to zero yet it is a mixture of four Bell states, each with one ebit of entanglement of purification.

Before we present continuity bounds for the entanglement of purification, we analyze the optimization problem of Eq. (4) in more detail. We can omit doubly stochastic maps $\Lambda_{B'}$ in the optimization in Eq. (7) since they never decrease the entropy. Furthermore, the von Neumann entropy is concave, so that the optimum in Eq. (7) can always be achieved when $\Lambda_{B'}$ is an *extremal* TCP map. An extremal TCP map is a TCP map that cannot be expressed as a convex combination of other TCP maps. Choi[11] has proved that an extremal TCP map with input dimension d has at most d operation elements in its operator-sum representation. This result will allow us to upper bound the dimensions of the optimal purifying Hilbert spaces, as stated in the following lemma.

Lemma 1: Let ρ act on a Hilbert space of dimension $d_{AB}=d_Ad_B$. The minimum of Eq. (4) can always be achieved by a state ψ for which the dimension of A' is $d_{A'}=d_{AB}$ and the dimension of B' is $d_{B'}=d_{AB}^2$ (or vice versa).

Proof: We use the formulation of the entanglement of purification as an optimization of a TCP map in Eq. (7). Since the density matrix $\mu_{BB'}(\rho)$ is on $\mathcal{H}_{d_B}\otimes\mathcal{H}_{d_{AB}}$, the optimal map $\Lambda_{B'}$ maps $\mathcal{H}_{d_{AB}}$ into a space of some unspecified dimension. The optimal map $\Lambda_{B'}$ can be assumed to be extremal. Theorem 5 of Ref. 11 shows that an extremal TCP map $\Lambda:B(\mathcal{H}_{d_1})\to B(\mathcal{H}_{d_2})$ (Refs. 12 and 13) can be written with at most d_1 operations elements, that is, has the form

$$\Lambda(\rho)=\sum_{i=1}^{d_1} V_i\rho V_i^\dagger. \tag{11}$$

In our case $d_1=d_{AB}$. Consider implementing the TCP map by applying a unitary operation U to the input state with an ancilla appended. In our case, this ancilla can be taken as Alice's purifying system A', and U acts on $A'B'$. The dimension of the ancilla A' can always be taken to be the number of operation elements. Thus we have $d_{A'}=d_{AB}$. The B' dimension is equal to the output dimension d_2 of the optimal map Λ, which is unconstrained by the extremality condition. However, we note that the operator $\Lambda(\rho)$ of Eq. (11) has a rank of at most d_{AB}^2. This is obtained by observing that the range of this operator is exactly that of the vectors given by all the columns of the matrices V_i for all i (the V_i matrices have d_1 columns and d_2 rows). Thus, there exists a unitary operator U that permits the construction of a new map $\Lambda'=U\Lambda$ whose output is confined

to the first d_1^2 dimensions of the output space. The operator U may be obtained explicitly via a Gram–Schmidt procedure applied to the column vectors of the V_i matrices. Λ' is also optimal, since the entropy of Eq. (7) is not changed by a unitary operation. Since the output space of Λ' has dimension d_1^2, we conclude that $d_{B'}$ can be taken to be $d_{B'}=d_{AB}^2$. □

It is interesting to note that a similar minimization problem was encountered in Ref. 14. There the goal was to use a set of noisy states for classical information transmission and we wanted to minimize the coherent information divided by the entropy of a quantum state under the action of a local map.

Theorem 1 (continuity of the entanglement of purification): *Let ρ and σ be two density matrices on $\mathcal{H}_{d_A}\otimes\mathcal{H}_{d_B}$ with Bures distance $D(\rho,\sigma)\leqslant\epsilon$. Then*

$$|E_p(\rho)-E_p(\sigma)|\leqslant 20D(\rho,\sigma)\log d_{AB}-D(\rho,\sigma)\log D(\rho,\sigma), \tag{12}$$

for small enough ϵ.

Proof: Let $|\psi'_\sigma\rangle$ and $|\psi'_\rho\rangle$ be the purifications of ρ and σ which achieve the maximum[5] in

$$F(\rho,\sigma)=\max_{\psi_\sigma,\psi_\rho}|\langle\psi_\sigma|\psi_\rho\rangle|. \tag{13}$$

Let $|\phi_\rho\rangle$ and $|\phi_\sigma\rangle$ correspond to the optimal purifications of ρ and σ with respect to E_p. There exists a unitary transformation U relating $|\psi'_\rho\rangle$ to $|\phi_\rho\rangle$, i.e., $(U\otimes\mathbf{1})|\psi'_\rho\rangle=|\phi_\rho\rangle$. We define the (nonoptimal) purification $|\psi_\sigma\rangle$ as $(U\otimes\mathbf{1})|\psi'_\sigma\rangle=|\psi_\sigma\rangle$. Now we have

$$E_p(\sigma)-E_p(\rho)=E(|\phi_\sigma\rangle\langle\phi_\sigma|)-E(|\phi_\rho\rangle\langle\phi_\rho|)\leqslant E(|\psi_\sigma\rangle\langle\psi_\sigma|)-E(|\phi_\rho\rangle\langle\phi_\rho|). \tag{14}$$

We use continuity of entanglement,[15,16] Lemma 1 (which indicates that the pure state has support on a space of dimension at most d_{AB}^4), and the fact that $|\langle\psi_\sigma|\phi_\rho\rangle|=|\langle\psi'_\sigma|\psi'_\rho\rangle|=F(\rho,\sigma)$ to bound

$$E_p(\sigma)-E_p(\rho)\leqslant 5D(\rho,\sigma)\log d_{AB}^4-2D(\rho,\sigma)\log D(\rho,\sigma) \tag{15}$$

for small enough $D(\rho,\sigma)$. We can obtain the full bound in Eq. (12) by alternatively relating $|\psi'_\sigma\rangle$ to the optimal purification $|\phi_\sigma\rangle$ by a unitary transformation U. □

It is fairly straightforward to prove monotonicity of the entanglement of purification from monotonicity of entanglement:

Lemma 2 (monotonicity of the entanglement of purification): The entanglement of purification of a density matrix ρ is nonincreasing under strictly local operations. Let Alice carry out a local TCP map $\mathcal{S}_A$ on the state ρ. We have

$$E_p((\mathcal{S}_A\otimes\mathbf{1})(\rho))\leqslant E_p(\rho). \tag{16}$$

Let Alice carry out a local measurement on ρ through which she obtains the state ρ_i with probability p_i. We have

$$\sum_i p_i E_p(\rho_i)\leqslant E_p(\rho). \tag{17}$$

Let $\mathcal{L}_{LOq}$ be a local operation assisted by m qubits of communication. The entanglement of purification obeys the equation

$$E_p(\mathcal{L}_{LOq}(\rho))\leqslant E_p(\rho)+m. \tag{18}$$

Proof: Let $|\psi_\rho\rangle$ be the optimal purification of ρ. This optimal purification is related to *some* purification of $(\mathcal{S}_A\otimes\mathbf{1})(\rho)$ by a unitary transformation on Alice's system only. Then Eq. (16) follows from the fact that entanglement is nonincreasing under local partial traces. The state

$|\psi_i\rangle = A_i \otimes I_B |\psi\rangle / \sqrt{\langle\psi|A_i^\dagger A_i \otimes I_B|\psi\rangle}$, where A_i corresponds to a measurement outcome of Alice, is some purification of ρ_i. The entanglement is nonincreasing under local operations and thus

$$E_p(\rho) = E(|\psi_\rho\rangle\langle\psi_\rho|) \geqslant \sum_i p_i E(|\psi_i\rangle\langle\psi_i|) \geqslant \sum_i p_i E_p(\rho_i). \tag{19}$$

For the last inequality, let Alice and Bob start with the entangled state $|\psi_\rho\rangle$ and carry out their LOq protocol. By subadditivity of entropy, the entanglement of this state can increase by at most m bits when m qubits of communication are sent (back and forth). Thus the entanglement of the final state which is some purification of $\mathcal{L}_{LOq}(\rho)$ is smaller than or equal to $E_p(\rho)+m$. □

Now we are ready to prove our main theorem:

Theorem 2: *The entanglement cost of ρ on $\mathcal{H}_d \otimes \mathcal{H}_d$ without classical communication equals* $E_{LOq}(\rho) = E_p^\infty(\rho)$.

Proof: The inequality $E_{LOq}(\rho) \leqslant E_p^\infty(\rho)$ uses entanglement dilution. Let k be the number of copies of ρ for which the regularized entanglement of purification E_p^∞ is achieved. One way of making many (p) copies of $\rho^{\otimes k}$ out of EPR pairs and $o(p) \leqslant o(pk)$ classical communication is to first perform entanglement dilution on the EPR pairs so as to create (an approximation to) the purification $|\psi\rangle^{\otimes p}$ and then trace over the additional registers to get $\rho^{\otimes kp}$. The other inequality $E_p^\infty(\rho) \leqslant E_{LOq}(\rho)$ can be proved from monotonicity and continuity of the entanglement of purification. We start with n EPR pairs which have E_p equal to n. The LOq process for creating an approximation $\tilde{\rho}_k$ to $\rho^{\otimes k}$ using $o(k)$ qubits of communication increases the entanglement of purification by at most $o(k)$ bits, see Lemma 2, or $E_p(\tilde{\rho}_k) \leqslant n + o(k)$. Using the continuity of Theorem 1 and dividing the last inequality by k and taking the limit $k \to \infty$ gives $E_p^\infty(\rho) \leqslant E_{LOq}(\rho)$. □

III. MUTUAL INFORMATION LOWER BOUNDS

The entanglement cost E_{LOq} is a measure of the quantum and classical correlations in a quantum state. The quantum and classical mutual information of a quantum state are similar measures that capture correlations in a quantum state. How do these measures relate to the new correlation measure? The quantum mutual information $I_q(\rho_{AB})$ is defined as

$$I_q(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}). \tag{20}$$

We define the classical mutual information of a quantum state $I_c(\rho_{AB})$ as

$$I_c(\rho_{AB}) = \max_{M_A : p_A, M_B : p_B} H(p_A) + H(p_B) - H(p_{AB}). \tag{21}$$

Here local measurements M_A and M_B give rise to local probability distributions p_A and p_B. The classical mutual information of a quantum state is the maximum classical mutual information that can be obtained by local measurements by Alice and Bob. Both quantum as well as classical mutual information share the important property that they are nonincreasing under local operations (LO) by Alice and Bob. For the classical mutual information, this basically follows from the definition Eq. (21). The definition itself as a maximum over local measurements makes sense since the classical mutual information of a probability distribution is nonincreasing under local manipulations of the distribution. The proof of this well known fact is analogous to the proof for the quantum mutual information which we will give here for completeness.

We can write the quantum mutual information as

$$I_q(\rho_{AB}) = S(\rho_{AB} || \rho_A \otimes \rho_B), \tag{22}$$

where $S(.||.)$ is the relative entropy. The relative entropy is nonincreasing under any map Λ (cf. Ref. 17), i.e.,

$$S(\Lambda(\rho_{AB})||\Lambda(\rho_A\otimes\rho_B))\leqslant S(\rho_{AB}||\rho_A\otimes\rho_B). \tag{23}$$

When Λ is of a local form, i.e., $\Lambda_A\otimes\Lambda_B$, the lhs of this equation equals the quantum mutual information of the state $(\Lambda_A\otimes\Lambda_B)(\rho_{AB})$ and thus the inequality $I_q((\Lambda_A\otimes\Lambda_B)(\rho_{AB}))\leqslant I_q(\rho_{AB})$ is proved.

Proof of lower bounds

We show that the quantities $I_q(\rho)/2$ and the regularized classical information $I_c^\infty(\rho)=\lim_{n\to\infty}(I_c(\rho^{\otimes n})/n)$ are both lower bounds for the entanglement cost E_{LOq}. The argument is similar to the proof of the E_p^∞ lower bound on E_{LOq} in Theorem 2. [The reasoning is in fact a special case of Theorem 4 in Ref. 18 (cf. Ref. 19) applied to the class LOq instead of the original LOCC.]

We start with a number, say k, of EPR pairs which have $I_q=2k$ and I_c equal to k.[20] In the limit of large n, the ratio k/n is the entanglement cost $E_{LOq}(\rho)$. We apply the LOq map $\mathcal{L}$ which uses $o(n)$ communication to obtain an approximation $\tilde{\rho}_n$ to $\rho^{\otimes n}$. Since the quantum mutual information and the classical mutual information can only increase by $o(n)$ by the process $\mathcal{L}$ applied to the initial EPR pairs, see Lemma 3, it follows that

$$I_q(\tilde{\rho}_n)\leqslant o(n)+2k, \tag{24}$$

and similarly

$$I_c(\tilde{\rho}_n)\leqslant o(n)+k. \tag{25}$$

The last step is to relate the mutual informations of $\tilde{\rho}_n$ to the mutual information of $\rho^{\otimes n}$. For this, we need a continuity result of the form

$$|I_{q/c}(\sigma)-I_{q/c}(\rho)|\leqslant C\log d\|\rho-\sigma\|_1+O(1) \tag{26}$$

for ρ, σ on $\mathcal{H}_d$, $\|\rho-\sigma\|_1$ sufficiently small and C is some constant.[21] Below we will prove these desired continuity results. We can divide Eqs. (24) and (25) by n and take the limit of large n. We use the continuity relation of Eq. (26) and the fact that in the large n limit $\tilde{\rho}_n$ tends to $\rho^{\otimes n}$. Thus we have

$$\lim_{n\to\infty}\frac{I_q(\rho^{\otimes n})}{n}=I_q(\rho)\leqslant 2E_{LOq}(\rho), \tag{27}$$

where we used that the quantum mutual information is additive, and similarly

$$I_c^\infty(\rho)\leqslant E_{LOq}(\rho). \tag{28}$$

What remains is to prove the continuity relations and the nonincrease modulo $o(n)$ under LOq operations.

Continuity of mutual information

The continuity of the quantum mutual information $I_q(\rho)$ can be proved by invoking Fannes' inequality[22] and Ruskai's proof of nonincrease of the trace-distance under TCP maps.[23] Let ρ and σ be two density matrices which are close, i.e., $\|\rho-\sigma\|_1=\mathrm{Tr}|\rho-\sigma|\leqslant\epsilon$ for sufficiently small ϵ. We have

$$|I_q(\rho_{AB})-I_q(\sigma_{AB})|\leqslant|S(\rho_A)-S(\sigma_A)|+|S(\rho_B)-S(\sigma_B)|+|S(\sigma_{AB})-S(\rho_{AB})|, \tag{29}$$

which can be bounded as

$$|I_q(\rho_{AB})-I_q(\sigma_{AB})|\leqslant 3\log d_{AB}\|\rho_{AB}-\sigma_{AB}\|_1+3\,\eta(\|\rho_{AB}-\sigma_{AB}\|_1), \tag{30}$$

where $\eta(x)=-x\log x$ and $\|\rho-\sigma\|_1\leqslant\frac{1}{3}$.

It is not hard to prove the continuity of the classical information of a quantum state, again using the nonincrease of $\|.\|_1$ under TCP maps. Let M_A^ρ and M_B^ρ be the optimal measurement achieving the classical mutual information $I_c(\rho)$. Under this measurement the states ρ and σ, which is, say, close to ρ, go to probability distributions $p^\rho(i,j)$ and $p^\sigma(i,j)$ which are close again, i.e., $\|p^\rho-p^\sigma\|_1\leqslant\|\rho-\sigma\|_1$. We have that

$$I_c(\sigma)-I_c(\rho)\leqslant I(p^\sigma)-I(p^\rho)\leqslant\log k\|p^\rho-p^\sigma\|_1+O(1), \tag{31}$$

where k is the number of joint outcomes in the optimal measurement (M_A^ρ,M_B^ρ) and I is the classical mutual information of a joint probability distribution. The last inequality in Eq. (31) could in principle be derived from Fannes' inequality, using diagonal matrices, but it is a standard continuity result in information theory[24] as well. To finish the argument, we should argue that k, the number of joint measurement outcomes, is bounded. The classical mutual information I is a concave function of the joint probability $p(i,j)$.[24] Therefore only extremal measurements M_A and M_B need to be considered in the optimization over measurements. An extremal measurement has at most d^2 outcomes when acting on a space of dimension d (Ref. 25) and thus $k\leqslant d_{AB}^2$. The same argument, interchanging σ and ρ, can be used to upperbound $I_c(\rho)-I_c(\sigma)$.

Lemma 3 (monotonicity properties of mutual information): Let $\mathcal{L}$ consist of a series of local operations assisted by m qubits of two-way communication. The quantum mutual information obeys the inequality

$$I_q(\mathcal{L}(\sigma))\leqslant I_q(\sigma)+2m, \tag{32}$$

for all states σ. For the classical mutual information we have

$$I_c(\mathcal{L}(|\psi\rangle\langle\psi|)\leqslant I_c(|\psi\rangle\langle\psi|)+m, \tag{33}$$

for all pure states $|\psi\rangle$.

Proof: Let us first consider the quantum mutual information. We can decompose the two-way scheme $\mathcal{L}$ into a sequence of one-way schemes. It is sufficient to prove for such a one-way scheme using m qubits of communication, say from Alice to Bob, that

$$I_q(\mathcal{L}(\sigma))\leqslant I_q(\sigma)+2m. \tag{34}$$

Alice's local action can consist of adding an ancilla A' in some state and apply a TCP map to the systems AA' thus obtaining the state $\sigma_{AA':B}$. Such an action does not increase the quantum nor classical mutual information as we showed before. Now Alice sends system A' to Bob. We have

$$\begin{aligned} I_q(\sigma_{AB})\geqslant I_q(\sigma_{AA':B}) &= S(AA')+S(B)-S(AA'B)\\ &\geqslant S(AA')-S(A')+S(BA')-S(AA'B)\\ &\geqslant S(A)-2S(A')+S(BA')-S(AA'B)\\ &= I_q(\sigma_{A:BA'})-2S(A'), \end{aligned} \tag{35}$$

where we used $|S(A)-S(B)|\leqslant S(AB)\leqslant S(A)+S(B)$. The quantum mutual information of the final state is $I_q(\sigma_{A:BA'})$. Since $S(A')\leqslant m$, we obtain the needed inequality. Alice could send only a part of ancilla A', but this does not change the bound.

Let us now consider the classical mutual information. We may convert the entire process $\mathcal{L}$ into a coherent process $\mathcal{L}$ where all the measurements are deferred to the end; this does not change the amount of communication that Alice and Bob carry out. Thus, prior to the measurements Alice and Bob have converted the pure state $|\psi\rangle$ into some pure state $|\phi\rangle$ whose local entropy is at most $E+m$ where E is the entanglement of the state $|\psi\rangle$, which is equal to $I_c(|\psi\rangle\langle\psi|)$ (see Ref. 20). Now Alice and Bob locally measure and/or trace out some registers which are operations that do

not increase the classical mutual information. Therefore the final state $\mathcal{L}(|\psi\rangle\langle\psi|)$ has a classical mutual information that is bounded by the initial classical mutual information plus m. □

Remark: Note that Eq. (32) for the quantum mutual information applies to both pure and mixed states while we have found mixed states that violate Eq. (33) for the classical mutual information.

Let us state the final result once more:

Corollary 1: $E_{LOq}(\rho) \geq I_q(\rho)/2$ *and* $E_{LOq} \geq I_c^{\infty}(\rho)$.

With this corollary we can show that the LOq-entanglement cost of any correlated density matrix ρ is nonzero.[26] Indeed, the quantum mutual information $I_q(\rho)$ of a correlated density matrix is strictly larger than zero, since $S(\rho_{AB})$ is strictly less than $S(\rho_A)+S(\rho_B)$ (equality is only obtained when $\rho_{AB}=\rho_A \otimes \rho_B$) and therefore $E_{LOq}(\rho)>0$.

We present a simple example for which $E_{LOq}(\rho)=E_p^{\infty}(\rho)>I_q(\rho)/2$.

Example 1 (All correlation is classical correlation): Consider the separable state $\rho = \Sigma_i p_i |a_i\rangle\langle a_i| \otimes |b_i\rangle\langle b_i|$ *where* $\langle a_i|a_j\rangle = \delta_{ij}$ *and* $\langle b_i|b_j\rangle = \delta_{ij}$. *In this case* $I_q(\rho)/2 = H(p)/2$. *However, we can show that* $E_p(\rho) \geq H(p)$. *We have* [*cf. Eq. (8)*] $\mu(\rho) = \Sigma_i p_i |b_i\rangle\langle b_i| \otimes |i\rangle\langle i|$. *Under some local TCP map* Λ *we obtain a state* $\mu' = \Sigma_i p_i |b_i\rangle\langle b_i| \otimes \rho_i$ *where* ρ_i *are density matrices. The entropy of* μ' *equals* $S(\mu') = \Sigma_i p_i S(\rho_i) + H(p) \geq H(p)$. *The entanglement of purification* $E_p(\rho)$ *may be nonadditive, so we have to consider* $E_p(\rho^{\otimes n})$. *We have* $\mu(\rho^{\otimes n}) = \mu^{\otimes n}$ *and now* $\mu' = \Sigma_{i_1,\ldots,i_n} p_{i_1} \cdots p_{i_n} |i_1,\ldots,i_n\rangle\langle i_1,\ldots,i_n| \otimes \rho_{i_1,\ldots,i_n}$. *Again the von Neumann entropy of* μ' *is larger than or equal to* $nH(p)$. *Note that in this example we do achieve the classical mutual information lower bound.*

Here is an example where the upper and lower bounds fix the (regularized) entanglement of purification:

Example 2: Let ρ *be an equal mixture of the state* $|\Psi_0\rangle = (1/\sqrt{2})(|00\rangle + |11\rangle)$ *and* $|\Psi_1\rangle = (1/\sqrt{2})(|00\rangle - |11\rangle)$. *Alice and Bob can get one bit of classical mutual information by both measuring in the* $\{0,1\}$ *basis. Thus* $E_{LOq}(\rho) \geq I_c(\rho) = 1$, *but* $E_{LOq}(\rho) \leq S(\rho_A) \leq 1$, *Eq. (10). Therefore* $E_{LOq} = 1$.

IV. OTHER CORRELATION MEASURES: THE LOCALLY INDUCED HOLEVO INFORMATION

In Ref. 1 the authors considered the locally induced Holevo information as a measure of classical correlations in the state. It is defined either with respect to Alice's measurement (C_A) or Bob's measurement (C_B)

$$C_{A/B}(\rho) = \max_{M_A/M_B} S\left(\sum_i p_i^{B/A} \rho_i^{B/A}\right) - \sum_i p_i^{B/A} S(\rho_i^{B/A}), \tag{36}$$

where $M_A(M_B)$ on ρ gives reduced density matrices $\rho_i^B(\rho_i^A)$ with probability $p_i^B(p_i^A)$. The classical mutual information $I_c^{\infty}(\rho)$ will in general be less than these quantities, since to achieve the Holevo information one may have to do coding. In Ref. 1 it was shown that $C_{A/B}$ are nonincreasing under local operations. We leave it as an exercise for the reader to prove continuity and nonincrease modulo $o(n)$ under LOq operations (applied to some pure state), thus showing that the regularized versions of these two quantities are also lower bounds for E_{LOq}.

Bell-diagonal states

We show that for Bell-diagonal states ρ_{Bell} the quantity C_A (equal to C_B by symmetry of the Bell-diagonal states) is equal to the classical capacity of the corresponding qubit channels. By the previous arguments this give us some lower bounds on the regularized entanglement of purification of these states. The Bell-diagonal states are of the following form,

$$\rho_{\text{Bell}} = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|, \tag{37}$$

where $\Psi_{0\ldots3}$ are the four Bell states where $|\Psi_0\rangle$ is $(1/\sqrt{2})(|00\rangle+|11\rangle)$. The corresponding channel, the so called generalized depolarizing channel, or Pauli channel, is of the form

$$\Lambda_\rho(\cdot)=\sum_i p_i\sigma_i(\cdot)\sigma_i, \tag{38}$$

where $\sigma_0=\mathbf{1}$, and $\sigma_{1,2,3}$ are the three Pauli matrices. It is known[27] that all two qubit states with maximally mixed subsystems are Bell-diagonal, up to a unitary transformation $U_A\otimes U_B$. From the isomorphism between states and channels,[8,11,28] it follows that all unital channels are of the form (38) (cf. Ref. 29), up to unitary transformations applied before and after the action of the channel. The classical one-shot capacity of the quantum channel Λ is given by[30,31]

$$C_1(\Lambda)=\sup_{\{q_i,\rho_i\}}\chi(\{q_i,\Lambda(\rho_i)\}), \tag{39}$$

where χ is the Holevo function of the ensemble

$$\chi(\{q_i,\rho_i\})=S\left(\sum_i q_i\rho_i\right)-\sum_i q_iS(\rho_i). \tag{40}$$

The optimal states ρ_i that achieve the capacity C_1 are always pure states, moreover it can be shown[29] that the ensemble $\{q_i,|\psi_i\rangle\}$ that achieves C_1 for unital one-qubit channels satisfies

$$\sum_i q_i|\psi_i\rangle\langle\psi_i|=\frac{1}{2}\mathbf{1}. \tag{41}$$

Let us argue that $C_A(\rho)=C_1(\Lambda)$ for a Bell-diagonal state $\rho_{\mathrm{Bell}}=(\mathbf{1}_A\otimes\Lambda_\rho)(|\Psi_0\rangle\langle\Psi_0|)$. Alice's POVM measurement on this state commutes with the channel Λ_ρ. By doing a measurement on $|\Psi_0\rangle$ she can create any pure-state-ensemble on system B, obeying the relation Eq. (41). This ensemble is then sent through the channel Λ_ρ. If the ensemble is optimal for C_1, then its Holevo information χ equals C_1 and thus $C_A=C_1$.

For unital one-qubit channels C_1 is given by[29,32]

$$C_1(\Lambda)=1-\min_\psi S(\Lambda(|\psi\rangle\langle\psi|)). \tag{42}$$

We can perform the minization in the last inequality and we obtain the following formula for the capacity of a Pauli channel or the induced Holevo information of the Bell-diagonal states,

$$C_A(\rho_{Bell})=C_1(\Lambda_\rho)=1-H(1-\lambda), \tag{43}$$

where λ is the sum of the two largest probabilities p_i and $H(.)$ is the binary entropy function $H(x)=-x\log x-(1-x)\log(1-x)$. For two-qubit Werner states of the form

$$\rho_W=e|\Psi_0\rangle\langle\Psi_0|+(1-e)/3\sum_{i=1}^{3}|\Psi_i\rangle\langle\Psi_i|, \tag{44}$$

we obtain

$$\begin{aligned} C_A&=1-H\left(\frac{1+2e}{3}\right)\quad \text{for } e\in\left[\frac{1}{4},1\right],\\ C_A&=1-H\left(\frac{2-2e}{3}\right)\quad \text{for } e\in\left[0,\frac{1}{4}\right]. \end{aligned} \tag{45}$$

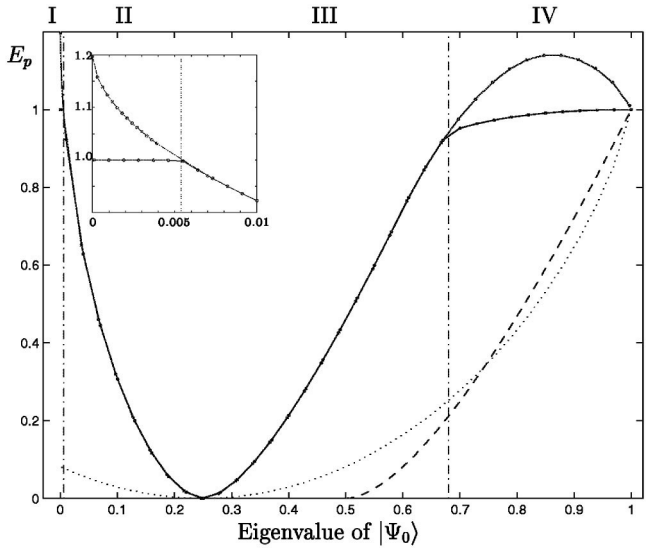

FIG. 1. Numerical bounds on E_p for Werner states. In the upper curve we restrict to $\dim(A')=\dim(B')=2$; for the next curve, we permit $\dim(A')=\dim(B')=4$. The inset shows the curious behavior of E_p around the point where the eigenvalue of $|\Psi_0\rangle$ approaches zero. The dotted curve is the C_A lower bound of Sec. IV A. The dashed curve is the entanglement of formation lower bound which vanishes when the eigenvalue is smaller than or equal to $\frac{1}{2}$.

It was shown by King[32] that the classical capacity of unital one-qubit channels is equal to the one shot capacity, or $C_1=C_1^{\infty}\equiv\lim_{n\to\infty}(1/n)\,C_1(\rho^{\otimes n})$. Therefore $C_A=C_A^{\infty}=C_1$, which is a lower bound on E_{LOq}.

V. WERNER STATES

A numerical minimization based on Eq. (6) was performed for the Werner states Eq. (44) for E_p. We plot the results as a function of the $|\Psi_0\rangle$ eigenvalue e in Fig. 1. We permitted various output dimensions; The two curves shown have $\dim(A')=\dim(B')=2$ and $\dim(A')=\dim(B')=4$. In the first case, the initial variable of the minimization was determined by a random 4×4 unitary $U_{A'B'}$ picked according to the Haar measure. In the second case, the initial point was determined by a random 16×4 isometry picked according to a parameterization derived from Ref. 33. We did not explore the largest dimensions permitted by Lemma 1, which would have required an optimization over a 64×4 isometry.

It is evident from the numerics presented in the figure that the C_A bound of Eq. (45) is not achieved for the Werner states: the C_A lower bound is only tight at the trivial points $e=\frac{1}{4}$ and $e=1$. Our results indicate that E_p is a very complex function, neither concave nor convex, with several distinct regimes. In fact, we find four different regimes in our numerics: (I) In this regime the standard purification of Eq. (5) appears to be optimal, so the U of Eq. (6) is the identity, and the purifying dimensions are $\dim(A')=1$ and $\dim(B')=4$. This regime only extends over a tiny range, approximately $0\leqslant e\leqslant0.005$. (II) In the range $0.005\leqslant e\leqslant0.25$ we find an optimal purification of the form

$$\sqrt{e}|\Psi_0\rangle_{AB}|\Psi_0\rangle_{A'B'}+\sqrt{\frac{1-e}{3}}(|\Psi_1\rangle_{AB}|\Psi_1\rangle_{A'B'}+|\Psi_2\rangle_{AB}|\Psi_2\rangle_{A'B'}+|\Psi_3\rangle_{AB}|\Psi_3\rangle_{A'B'}). \tag{46}$$

In this region the E_p curve is given by $E_p=-x\log x-(1-x)\log((1-x)/3)$, with $x=(1+2e-2\sqrt{3}\sqrt{e(1-e)})/12$. Here the purifying dimensions are $\dim(A')=2$ and $\dim(B')=2$. Of course E_p drops to zero for the completely mixed state at $e=\frac{1}{4}$. (III) In the range $0.25\leqslant e\leqslant0.69$ we also find purifying dimensions $\dim(A')=2$ and $\dim(B')=2$, but we were unable to determine the

analytical form of the purifying state or of E_p. (IV) In the range $0.69 \leqslant e \leqslant 1$ the purifying dimensions were $\dim(A')=2$ and $\dim(B')=3$. Again, we were unable to come to any analytical understanding of the result. Of course, $E_p=1$ for $e=1$, corresponding to the pure maximally entangled state.

VI. CONCLUSION

We have shown that the entanglement cost $E_{LOq}(\rho)$ is equal to the regularized entanglement of purification. It is an open question whether the entanglement of purification is additive:

$$E_p(\rho\otimes\rho) \stackrel{?}{=} E_p(\rho)+E_p(\rho). \tag{47}$$

In the alternative formulation using the state $\mu(\rho)$ the additivity question is the following. Is the minimum in

$$\min_{\Lambda_{CD}} S((I_{AB}\otimes\Lambda_{CD})(\mu_{AC}\otimes\mu_{BD})), \tag{48}$$

achieved by a TCP map $\Lambda_{CD}=\mathcal{S}\otimes\mathcal{S}$? This problem is similar again to the additivity question encountered in Ref. 14 where a local map could possibly lower the ratio of the coherent information and the entropy of many copies of a state together.

It is interesting not only to ask the formation question with respect to this class LOq, but also consider ''the distillation'' question. One can consider different versions. For example, how much entanglement can we distill from ρ using $o(n)$ communication? One would expect that this quantity $D_{LOq}(\rho)$ is always zero for states for which the entanglement cost E_c (using *LOCC*) is lower than the distillable entanglement D. We do not have a proof of this statement, relating irreversibility to a need for classical communication.

Instead of trying to convert the correlations in ρ back to entanglement, we may ask what classical correlations Alice and Bob can establish using ρ. We could allow Alice and Bob to perform an asymptotically vanishing amount of communication in this extraction process. A little bit of communication could potentially increase the classical mutual information in a quantum state by a large amount (when the classical correlation is initially ''hidden''), thus this may not be the best problem to pose. Researchers[34,35] have investigated the possibly more interesting problem of the *secret* key K that Alice and Bob can establish given ρ where one allows arbitrary public classical communication between the parties. There is again more than one version of this problem, one in which Eve possesses the purification of the density matrix[34] and a situation in which Eve is initially uncorrelated with the density matrix. In Ref. 36 a general framework is developed to address these issues also in the multipartite setting.

Quite recently, entanglement properties of bipartite density matrices were studied by looking at mixed extensions of the density matrix.[37] It would be interesting to explore the connection between our results here on the entanglement of purification and this other approach.

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Conditional entropies and their relation to entanglement criteria

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We discuss conditional Rényi and Tsallis entropies for bipartite quantum systems of finite dimension. We investigate the relation between the positivity of conditional entropies and entanglement properties. It is in particular shown that any state having a negative conditional entropy with respect to any value of the entropic parameter is distillable since it violates the reduction criterion. Moreover, we show that the entanglement of Werner states in odd dimensions can neither be detected by entropic criteria nor by any other spectral criterion. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1498490]

I. INTRODUCTION

Entanglement has always been a key issue in the ongoing debate about the foundations and interpretation of quantum mechanics since Einstein[1] and Schrödinger[2] expressed their deep dissatisfaction about this astonishing part of quantum theory. Whereas for the long period from 1935 to 1964, until Bell[3] published his famous work, discussions about entanglement were purely meta-theoretical, nowadays quantum information theory has established entanglement as a physical resource and key ingredient for quantum computation and quantum information processing. This led to a dramatic increase of general structural knowledge about entanglement in the last few years, and the resource point of view often led to results that are reminiscent of those known from thermodynamics: *free entanglement* is distinguished from *bound entanglement*,[4] irreversibility can be observed in the process of preparing and distilling entangled states[5] and entanglement itself is defined in a way that it must not increase by means of local operations and classical communication (LOCC). Moreover, there is recent effort in order to quantify quantum correlations through heat engines.[6]

Entropies lay at the heart of both theories, thermodynamics and entanglement theory. Concerning the latter it was shown that a few reasonable assumptions lead to a unique measure of entanglement[7] for pure bipartite quantum states, which is just the *von Neumann entropy* of the reduced state. Hence, it is obvious that the two subsystems of a pure entangled state exhibit more disorder than the system as a whole, so that the respective conditional entropy is negative. This is a remarkable property of entangled states, which is impossible for classical systems (i.e., classical random variables).

The present article is primarily devoted to settling the relationship between the negativity of conditional Rényi and Tsallis entropies and other entanglement properties. We will in particular show how the property of having a positive conditional entropy enters into the known implication chain of entanglement, resp., separability criteria.

In the second part we will then follow the result of Nielsen and Kempe[8] and give examples of entangled states having the property that their entanglement can neither be detected by entropic criteria nor by any other spectral criterion. In Sec. IV we show that this is indeed the case for symmetric *Werner states* (in odd dimensions), which play a crucial role in entanglement theory.

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II. PRELIMINARIES ON SEPARABILITY CRITERIA

To fix ideas we will start by recalling some of the basic notions and previous results concerning separability, resp., entanglement criteria.

A bipartite quantum state described by its density matrix ρ acting on a Hilbert space $\mathcal{H}=\mathcal{H}^{(A)}\otimes\mathcal{H}^{(B)}$ is said to be *separable*, unentangled or classically correlated if it can be written as a convex combination of tensor product states[9]

$$\rho=\sum_j p_j\rho_j^{(A)}\otimes\rho_j^{(B)}, \tag{1}$$

where the positive weights p_j sum up to one and $\rho^{(A)}$ ($\rho^{(B)}$) describes a state on $\mathcal{H}^{(A)}$ ($\mathcal{H}^{(B)}$). This means in particular that pure states are separable if and only if they are product states. Moreover, all entanglement properties of pure states, which can always be written in their Schmidt form (cf. Ref. 10) as $|\Psi\rangle=\Sigma_i\sqrt{\lambda_i}|i\rangle\otimes|i\rangle$, are completely determined by the eigenvalues $\{\lambda_i\}$ of the reduced state $\rho_A=\mathrm{tr}_B|\Psi\rangle\langle\Psi|$. The unique measure of entanglement for pure states is then given by the *von Neumann entropy* of the reduced state:

$$S_1(\rho_A)=-\mathrm{tr}(\rho_A\log\rho_A). \tag{2}$$

For mixed quantum states, however, the situation is much more difficult and deciding whether a state is entangled or separable is not yet feasible in general. Currently, the most efficient necessary criterion for separability is the positivity of the partial transpose (PPT), i.e., the condition that ρ^{T_A} has to be a positive semi-definite operator.[11] The partial transpose of the state is thereby defined in terms of its matrix elements with respect to some basis by $\langle kl|\rho^{T_A}|mn\rangle=\langle ml|\rho|kn\rangle$. For the smallest nontrivial systems with 2×2, resp., 2×3, dimensional Hilbert spaces and a few other special cases the PPT criterion also turned out to be sufficient.[12] In higher dimensional systems, however, so-called *bound entangled* states exist, which satisfy the PPT condition without being separable.[4]

Another well known condition is given by the *reduction criterion*[13,14]

$$\rho_A\otimes\mathbf{1}-\rho\geqslant0 \qquad \text{and} \qquad \mathbf{1}\otimes\rho_B-\rho\geqslant0, \tag{3}$$

which is implied by the PPT criterion but is nevertheless an important condition since its violation implies the possibility of recovering entanglement by distillation (which is yet unclear for PPT violating states). For the case of two qubits (and 2×3) the reduction criterion is also known to be sufficient for separability.[13,14] Moreover, it was shown in Ref. 15 that Eq. (3) implies that the rank of the reduced state has to be smaller than or equal to the rank of ρ. The general line of implication is then

$$\begin{array}{c}\rho \text{ separable}\\ \Downarrow\\ \rho^{T_A}\geqslant0\\ \Downarrow\\ \rho \text{ undistillable}\\ \Downarrow\\ \rho_A\otimes\mathbf{1}-\rho\geqslant0\wedge\mathbf{1}\otimes\rho_B-\rho\geqslant0\\ \Downarrow\\ \max[\mathrm{rank}(\rho_A),\mathrm{rank}(\rho_B)]\leqslant\mathrm{rank}(\rho).\end{array} \tag{4}$$

The last condition we want to mention was recently derived by Nielsen and Kempe[8] and is based on majorization. However, it is yet not known how the *majorization criterion* enters into the above implication chain. Since it is closely related to conditional entropies we will discuss it in more detail in the following section.

III. CONDITIONAL ENTROPIES

The idea to use entropic inequalities as separability, resp., entanglement, criteria for mixed states goes back to the mid-1990s when Cerf and Adami[16] and the Horodecki family[17] recognized that certain conditional Rényi entropies are non-negative for separable states, and it was recently resurrected by several groups[18–23] in the form of conditional Tsallis entropies.

The quantum *Rényi entropy* depending on the entropic parameter $\alpha \in \mathbb{R}$ is given by

$$S_\alpha(\rho) = \frac{\log \mathrm{tr}(\rho^\alpha)}{1-\alpha}, \tag{5}$$

where S_0, S_1, S_∞ reduce to the logarithm of the rank, the von Neumann entropy and the negative logarithm of the operator norm, respectively. For the case of separable states it was shown in Refs. 15–17 that the conditional entropy[24]

$$S_\alpha(B|A;\rho) := S_\alpha(\rho) - S_\alpha(\rho_A) \tag{6}$$

is non-negative for $\alpha = 0, \infty$ and $\alpha \in [1,2]$.

In Refs. 18 and 20 essentially the same criterion was expressed in terms of the *Tsallis entropy*

$$T_\alpha(\rho) = \frac{1-\mathrm{tr}(\rho^\alpha)}{\alpha-1}, \tag{7}$$

which is non-negative, concave (convex) for $\alpha > 0$ ($\alpha < 0$) and becomes the von Neumann entropy in the limit $\alpha \to 1$. The *conditional Tsallis entropy* defined in Ref. 18 reads

$$T_\alpha(B|A;\rho) := \frac{\mathrm{tr}(\rho_A^\alpha) - \mathrm{tr}(\rho^\alpha)}{(\alpha-1)\mathrm{tr}(\rho_A^\alpha)}. \tag{8}$$

Concerning positivity, however, the two conditional entropies are equivalent, i.e.,

$$T_\alpha(B|A;\rho) \geqslant 0 \Leftrightarrow S_\alpha(B|A;\rho) \geqslant 0, \tag{9}$$

which is in turn equivalent to $\mathrm{tr}(\rho_A^\alpha) \geqslant \mathrm{tr}(\rho^\alpha)$ for $\alpha > 1$, $\mathrm{tr}(\rho_A^\alpha) \leqslant \mathrm{tr}(\rho^\alpha)$ for $0 \leqslant \alpha < 1$, and the positivity of the conditional von Neumann entropy for $\alpha = 1$.

Obviously, for pure states the conditional entropies are negative if and only if the state is entangled.

A. Monotonicity counterexample

It was conjectured in Ref. 20 that $T_\alpha(B|A;\rho)$ is monotonically decreasing in α, such that it would be sufficient to calculate $T_\infty(B|A;\rho)$ in order to decide positivity. However, monotonicity does not hold in general and can most easily be ruled out by low rank examples like

$$\rho = \frac{1}{2}(|\Phi_+\rangle\langle\Phi_+| + |01\rangle\langle 01|), \quad |\Phi_+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle),$$

for which the reduced state has eigenvalues $\frac{1}{4}, \frac{3}{4}$ and therefore $T_0 = T_\infty = 0 \neq T_2 = \frac{1}{5}$. We note that similar counterexamples can be found for the monotonicity of the conditional Rényi entropy as well. Fortunately, however, monotonicity is not necessary for proving the positivity of the conditional Tsallis/Rényi entropies for separable states for other values than $\alpha = 0, \infty$, $\alpha \in [1,2]$.[25]

B. Majorization and convex functions

Majorization turned out to be a powerful tool in the discussion of quantum state transformations by means of LOCC operations (cf. Ref. 26), and it was recently proven to yield the strongest

separability criterion, which is based on the spectra of a state and one of its reductions. It was proven in Ref. 8 that any separable state ρ acting on $\mathbb{C}^d\otimes\mathbb{C}^d$ is majorized by its reduced state ρ_A:

$$\rho_A \succ \rho, \quad \text{i.e.,} \quad \forall k \leqslant d: \sum_{i=1}^{k} \lambda_i^{(A)} \geqslant \sum_{i=1}^{k} \lambda_i, \tag{10}$$

where $\{\lambda_i\}$ and $\{\lambda_i^{(A)}\}$ are the decreasingly ordered eigenvalues of ρ, resp., ρ_A.

It is a well known result in the theory of majorization that $x \succ y$ iff $\mathrm{tr}(f(x)) \geqslant \mathrm{tr}(f(y))$ for all convex functions $f:\mathbb{R}\to\mathbb{R}$.[27] Since $f(x)=x^\alpha$ is convex for $\alpha \geqslant 1$ and concave on $\mathbb{R}^+$ for $0 \leqslant \alpha \leqslant 1$ and the von Neumann entropy is concave (needed for $\alpha=1$), this immediately implies (cf. Ref. 28) the following.

Theorem 1: *Let ρ be a bipartite quantum state, which is majorized by its reduction $\rho_A \succ \rho$. Then for every $\alpha \geqslant 0$ the conditional Tsallis/Rényi entropies of ρ are non-negative, i.e.,*

$$S_\alpha(B|A;\rho) \geqslant 0 \quad \textit{and} \quad T_\alpha(B|A;\rho) \geqslant 0. \tag{11}$$

The result of Nielsen and Kempe implies that this holds in particular for any separable state.

It is yet not known how the majorization criterion (10) is related to other separability criteria like PPT, undistillability and the reduction criterion. However, we will show in the next subsection how the positivity of conditional entropies is related to these properties.

C. Conditional entropies and the reduction criterion

Positivity of the conditional entropies for $\alpha=0$ reduces to the rank criterion in the implication chain (4). The following theorem will show, however, that all the other properties stated in (4) in turn imply positivity of the conditional entropies for every value of the entropic parameter α.

Theorem 2: *Let ρ be a bipartite quantum state satisfying the reduction criterion $\rho_A\otimes\mathbf{1} \geqslant \rho$. Then for every $\alpha \geqslant 0$ the conditional Tsallis/Rényi entropies are non-negative*:

$$S_\alpha(B|A;\rho) \geqslant 0 \quad \textit{and} \quad T_\alpha(B|A;\rho) \geqslant 0. \tag{12}$$

We note that Theorem 2 implies, in particular, that states with negative conditional entropies are distillable.

Proof: We will divide the proof into three steps depending on the value of the entropic parameter.

For $\alpha > 1$ the proof is essentially based on the Golden–Thompson inequality (cf. Ref. 29) stating that

$$\mathrm{tr}(e^A e^B) \geqslant \mathrm{tr}(e^{A+B}) \tag{13}$$

for Hermitian matrices A,B. Utilizing the definition of the reduced state, i.e.,

$$\forall P \geqslant 0: \mathrm{tr}(\rho(P\otimes\mathbf{1})) \equiv \mathrm{tr}(\rho_A P), \tag{14}$$

this leads to

$$\begin{aligned}\mathrm{tr}(\rho_A^\alpha) &= \mathrm{tr}[\rho(\rho_A^{\alpha-1}\otimes\mathbf{1})] = \mathrm{tr}[\exp(\ln\rho)\exp((\alpha-1)\ln(\rho_A\otimes\mathbf{1}))] \\ &\geqslant \mathrm{tr}[\exp(\ln(\rho)+(\alpha-1)\ln(\rho_A\otimes\mathbf{1}))].\end{aligned} \tag{15}$$

At this point we need two monotonicity properties in order to exploit the validity of the reduction criterion. First of all we use the fact that the logarithm is operator monotone,[30] i.e.,

$$A \geqslant B \Rightarrow \ln A \geqslant \ln B. \tag{16}$$

Thus, for $\alpha > 1$ the reduction criterion $\rho_A\otimes\mathbf{1} \geqslant \rho$ implies

$$\ln(\rho)+(\alpha-1)\ln(\rho_A\otimes\mathbf{1})\geqslant\ln(\rho)+(\alpha-1)\ln(\rho)=\alpha\ln(\rho). \tag{17}$$

In the second step we utilize the fact that the exponential function is monotone under the trace. This can be seen by noting that for any A Hermitian, $P\geqslant 0$ and $B=(A+\epsilon P)$ with $\epsilon\geqslant 0$:

$$\frac{\partial}{\partial\epsilon}\mathrm{tr}(e^B)=\mathrm{tr}(e^B P)\geqslant 0. \tag{18}$$

Hence $\mathrm{tr}(e^B)\geqslant\mathrm{tr}(e^A)$ is implied by $B\geqslant A$. Combining (15) and (17), this leads to

$$\mathrm{tr}(\rho_A^\alpha)\geqslant\mathrm{tr}[\exp(\alpha\ln\rho)]=\mathrm{tr}(\rho^\alpha). \tag{19}$$

For $0\leqslant\alpha<1$ the reduction criterion can immediately be applied since $f(A)=A^r$ is an operator decreasing function for $-1\leqslant r\leqslant 0$, $A\geqslant 0$ (cf. Ref. 31) and thus

$$\mathrm{tr}(\rho_A^\alpha)=\mathrm{tr}[\rho(\rho_A^{\alpha-1}\otimes\mathbf{1})]\leqslant\mathrm{tr}(\rho^\alpha). \tag{20}$$

For the case $\alpha=1$ we have to look at the conditional von Neumann entropy $S_1(\rho)-S_1(\rho_A)$, for which positivity is directly implied by the reduction criterion and the operator monotonicity of the logarithm:

$$S_1(\rho_A)=-\mathrm{tr}\rho_A\log\rho_A \tag{21}$$

$$=-\mathrm{tr}\rho\log\rho_A\otimes\mathbf{1} \tag{22}$$

$$\leqslant-\mathrm{tr}\rho\log\rho \tag{23}$$

$$=S_1(\rho), \tag{24}$$

which completes the proof. □

D. Negative entropic parameters

So far we have only discussed conditional entropies for non-negative values of the entropic parameter α. For these cases we know that they can become negative for entangled states, the simplest examples being pure entangled states. However, for $\alpha<0$ (and states of full rank) the sign of the conditional entropy contains no information

Theorem 3: *Let ρ be a bipartite quantum state of full rank. Then for every $\alpha<0$ the conditional Tsallis/Rényi entropies are non-negative*:

$$\forall\,\alpha<0: S_\alpha(B|A;\rho)\geqslant 0 \quad \textit{and} \quad T_\alpha(B|A;\rho)\geqslant 0. \tag{25}$$

Proof: Let $\{|a\rangle\}$ be an eigenbasis of ρ_A. Then

$$\mathrm{tr}(\rho_A^\alpha)=\sum_a\langle a|\rho_A|a\rangle^\alpha \tag{26}$$

$$=\sum_a\left[\sum_i\langle a\otimes i|\rho|a\otimes i\rangle\right]^\alpha \tag{27}$$

$$\leqslant\sum_{a,i}\langle a\otimes i|\rho|a\otimes i\rangle^\alpha$$

$$\leqslant\mathrm{tr}(\rho^\alpha), \tag{28}$$

where Eqs. (27) and (28) use that $(\Sigma_i b_i)^\alpha \leqslant \Sigma_i b_i^\alpha$ holds for $b_i \geqslant 0$, $\alpha \leqslant 0$, and the last inequality is implied by the convexity of negative powers on $\mathbb{R}^+$.

IV. ISOSPECTRAL STATES

The fact that positivity of conditional entropies is implied by the reduction criterion (Theorem 2) shows already that such an entropic criterion cannot be sufficient for separability. In fact, it was shown in Ref. 8 that no spectral property is capable of distinguishing any entangled state from separable ones.

We will in this section follow the idea of Ref. 8 and construct particular examples of states, such that their entanglement cannot be detected by any spectral criterion, since there exist separable states having the same spectrum and the same reductions.

Werner states[9] have always played an important and paradigmatic role in quantum information theory. Their characteristic property is that they commute with all unitaries of the form $U \otimes U$ and they can be expressed as

$$\rho(p) = (1-p)\frac{P_+}{r_+} + p\frac{P_-}{r_-}, \quad 0 \leqslant p \leqslant 1, \tag{29}$$

where P_+ (P_-) is the projector onto the symmetric (antisymmetric) subspace of $\mathbb{C}^d \otimes \mathbb{C}^d$ and $r_\pm = \mathrm{tr}[P_\pm] = (d^2 \pm d)/2$ are the respective dimensions. Werner showed that these states are entangled iff $p > \frac{1}{2}$ independent of the dimension d. The following shows, however, that none of these entangled states for odd dimension d can be detected by any separability criterion, which is based on the spectrum of the state and its reductions.

Theorem 4: *Any entangled state in $\mathbb{C}^d \otimes \mathbb{C}^d$ with maximal chaotic reductions and eigenvalues having multiplicities, which are multiples of d, has a separable isospectral counterpart, which is locally undistinguishable as it has the same reductions.*

Proof: Let us consider a special basis of maximally entangled states in $\mathbb{C}^d \otimes \mathbb{C}^d$:[32]

$$|\Psi_{jk}\rangle = \frac{1}{\sqrt{d}} \sum_{n=1}^{d} \exp\left(\frac{2\pi i}{d} jn\right) |n, n \oplus k\rangle, \tag{30}$$

where $j,k = 1,\ldots,d$ and $\oplus$ means addition modulo d. Any equal weight combination of all states of the form (30), which belong to the same value of k, is then a projector onto a separable state since

$$\begin{aligned} P_k &= \sum_{j=1}^{d} |\Psi_{jk}\rangle\langle\Psi_{jk}| \\ &= \frac{1}{d} \sum_{j,n,m=1}^{d} \exp\left[\frac{2\pi i}{d} j(n-m)\right] |n, n\oplus k\rangle\langle m, m\oplus k| \\ &= \sum_{n=1}^{d} |n\rangle\langle n| \otimes |n\oplus k\rangle\langle n\oplus k| \end{aligned} \tag{31}$$

is an equal weight combination of product states. Here we have used that $(1/d)\,\Sigma_{j=1}^{d} \exp[(2\pi i/d)\, j(n-m)] = \delta_{n,m}$. Moreover, the reductions of the respective states P_k/d are maximally chaotic, i.e., $\rho_A = \mathbf{1}/d$, just as the reductions of any maximally entangled state.

If we now have a state with multiplicities being multiples of d, we can replace the projectors onto its eigenspaces with sufficiently many projectors of the form P_k. The resulting state will then be again a convex combination of product states, i.e., separable, having the same spectrum and maximal chaotic reductions. □

For the case of Werner states we note that the unitary invariance of the state $\rho(p)$ in Eq. (29) implies that its reductions are $\rho_A = \mathbf{1}/d$. Moreover, $\rho(p)$ has two eigenvalues $(1-p)/r_+$ and p/r_- with multiplicities r_+, r_- which are indeed multiples of d in odd dimensions.

Following Proposition 2 we can now construct a state

$$\rho'(p) = \frac{(1-p)}{r_+} \sum_{k=1}^{r_+/d} P_k + \frac{p}{r_-} \sum_{l=1}^{r_-/d} P_{l+r_+/d}, \tag{32}$$

which has then both, the same spectrum and the same reductions as $\rho(p)$. However, as a convex combination of separable states, it is itself separable for any $0 \leqslant p \leqslant 1$.

V. CONCLUSION

We discussed conditional Rényi and Tsallis entropies and the relation between their positivity and other separability properties. We showed in particular that states having a negative conditional entropy are distillable since they violate the reduction criterion.

Conditional entropies are a special instance of criteria using just the spectra of a state and its reductions. Concerning the detection of entanglement, it was shown in Ref. 8 that majorization is the strongest spectral criterion, which uses the spectra of a state and just one of its reductions. Its relation to other separability criteria is yet not known. The present result and numerical evidence may indicate that majorization is also implied by the reduction criterion. However, the proof presented in Sec. III C does not work for arbitrary convex functions and, in fact, majorization is not implied by the conditional entropy criteria.

Concerning separability, the most efficient criterion is still the PPT criterion, which is also a spectral criterion, however, for the partially transposed state. One interesting question in this context would therefore be: how can other (easy calculable) invariants provide information about the separability of a state, which is not yet encoded in the smallest eigenvalue of its partial transpose?

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Parallel transport in an entangled ring

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This article defines a notion of parallel transport in a lattice of quantum particles, such that the transformation associated with each link of the lattice is determined by the quantum state of the two particles joined by that link. We focus particularly on a one-dimensional lattice—a ring—of entangled *rebits*, which are binary quantum objects confined to a *real* state space. We consider states of the ring that maximize the correlation between nearest neighbors, and show that some correlation must be sacrificed in order to have nontrivial parallel transport around the ring. An analogy is made with lattice gauge theory, in which nontrivial parallel transport around closed loops is associated with a reduction in the *probability* of the field configuration. We discuss the possibility of extending our result to qubits and to higher dimensional lattices. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In lattice gauge theory, the gauge field assigns to every pair of neighboring lattice sites a transformation that tells how to ''transport'' a vector, representing an internal property such as quark color, from one site to the other. That is, with every ordered pair $\langle j,k\rangle$ of neighboring sites, or link, one associates a transformation $U(k,j)$ which is an element of the gauge group. Indeed, this assignment of transformations to links *constitutes* the configuration of the gauge field. If we apply $U(k,j)$ to a vector v associated with site j, we can interpret the image vector, $v' = U(k,j)v$, as the result of moving v from site j to site k. (It helps to read the arguments of U from right to left. This notation makes sense when combined with the usual notation for a sequence of operations, in which the operator on the right acts first.) This process is called parallel transport, and the transformation $U(k,j)$ is sometimes called a parallel transporter.

This article is not about lattice gauge theory but about actual lattices consisting of simple quantum particles, in which each particle is correlated with its nearest neighbors. As we will see later in this work, for typical states of the lattice, one can use the state itself to specify a notion of parallel transport. Our conception is distinct from the more familiar notion of quantum parallel transport (expressible in terms of gauge fields[1,2]), in which a quantum particle is physically moved either in actual space or in a parameter space.[2–4] In our approach there is no physical motion or evolution; rather, the transformation that we associate with a link expresses something about the relationship between the particles joined by that link. The present work is an initial exploration into a possible analogy between the quantum state of a lattice of quantum particles and the configuration of the gauge field in a lattice gauge theory. Roughly, the analogy we are looking for would be along the following lines (it will be spelled out more precisely in later sections of the article).

A lattice gauge theory assigns a probability distribution to the set of possible field configurations, the probability density of a configuration $\mathcal{A}$ being proportional to $\exp[-S(\mathcal{A})]$ where the real function $S(\mathcal{A})$ is the action. The action depends on the effect of parallel transport around each of the elementary plaquettes of the lattice; that is, it depends on the transformations that the field configuration associates with these elementary closed paths. The more these transformations differ from the identity, the higher the action, and therefore the lower the probability of that particular field configuration. Let us call this effect ''the probability cost of twisting.'' I am looking for something similar in a lattice of correlated quantum objects, but instead of a probability cost, I am

looking for a ''correlation cost.'' We will be focusing our attention on states in which nearest neighbors are maximally correlated. The question is whether this maximal correlation must be reduced if there is to be nontrivial parallel transport around closed loops (that is, transport whose net effect is not null), and, if so, whether the reduction in correlation becomes more severe as the effect of such parallel transport differs further from the identity. In other words, in an entangled lattice, is there a correlation cost of twisting?

In fact this article only begins to answer this question. Although we set up the problem for lattices of arbitrary dimension, the one concrete example we work out in detail is the case of a one-dimensional ring. Moreover, for most of the article we will restrict our attention to the simplest possible quantum object, namely, a *rebit*, a fictitious object whose state space is a two-dimensional vector space over the *real* numbers.[5] Thus we will mostly be analyzing a closed ring of rebits. At the end of the article I discuss the generalization to qubits and to higher-dimensional lattices.

This research is related to a recent line of work on ''entanglement sharing,'' concerning the ways in which quantum entanglement can be shared among several objects. A number of authors have found constraints on the sharing of entanglement that follow directly from the structure of quantum mechanics itself and not from any particular Hamiltonian. For example, it has been shown that any entanglement that might exist between a pair of qubits limits the extent to which either of them can be entangled with a third qubit.[6,7] There are similar limits for n qubits all entangled with each other.[8–10] Another example is an entangled ring: in a translationally invariant state of a ring of qubits, there is a certain maximum possible entanglement between nearest neighbors.[11] (The measure of entanglement used in all of these studies is the entanglement of formation.[12,13]) In this article we are putting a different sort of condition on the quantum state of a multipartite system—we are imposing a certain configuration of twists in the nearest-neighbor correlations—and we are asking what constraint this condition places on the strength of the correlations.

I hope that the results of this research will ultimately be useful in analyzing systems of entangled particles on a lattice, such as magnetic systems. If there are simple laws of quantum correlations that transcend any particular Hamiltonian, then these laws might lead to the identification of interesting generic properties of quantum many-body systems. Arguments along these lines, particularly focusing on entanglement, have appeared recently in the literature.[14–17] But at least as much of the actual motivation for the present work comes from pure curiosity: I wonder how close an analogy one can draw between the degree of correlation between particles in a quantum lattice and the probability density of a field configuration in lattice gauge theory. Of course there are many connections between lattice gauge theory and the theory of many-body systems—see, for example, Ref. 18 and references cited therein—but I am looking for an analogy along the particular lines traced out above.

The reader may have noticed that in describing the work to be presented here (as opposed to earlier work), I have been using the word ''correlation'' rather than ''entanglement.'' Though they are related, the two concepts are not the same. In this article I focus on correlation because it seems natural in this context and it is easy to work with. But it would also be interesting to explore the same questions using one of the standard measures of entanglement. I might add that the states we will primarily be concerned with are in fact highly entangled, hence the reference to an ''entangled ring'' in the title.

The article is organized as follows. First we review briefly those aspects of lattice gauge theory that have suggested our main question. We then define a rebit more precisely and develop our notion of parallel transport. We analyze in some detail the case of a ring of rebits and determine whether nontrivial parallel transport does indeed entail a ''correlation cost.'' Finally, we ask how the problem and the results are likely to change when extended to more complex systems.

II. LATTICE GAUGE THEORY AND A SIMPLE ANALOGY

Ideally, lattice gauge theory is done on a four-dimensional lattice representing space–time, except that the fourth dimension represents *imaginary* time, so that it acts in many respects like

another spatial dimension. The results of a calculation can be interpreted in terms of *real* time by means of analytic continuation. One consequence of the use of imaginary time is this: in computing the expectation value of an observable, one does not sum up complex amplitudes associated with different histories; rather, one takes a weighted average of the observable of interest using *real* weights.[19] As mentioned above, the weighting function is proportional to $\exp(-S)$, where the action S is a real function of the field configuration. More precisely, in a pure gauge theory, in which there are no matter fields but only the gauge field itself, the expectation value of an observable B is

$$\langle B\rangle = \frac{1}{Z}\int Be^{-S(\mathcal{A})}\prod_{\langle j,k\rangle} dU(k,j). \tag{1}$$

Here $\mathcal{A}$ is the configuration of the gauge field, which assigns a parallel transporter $U(k,j)$ to each link $\langle j,k\rangle$. Each such transformation U is an element of the gauge group, e.g., U(1) for electrodynamics or SU(3) for chromodynamics. The integral in Eq. (1) is over all field configurations, that is, over all possible parallel transporters for each link, and $dU(k,j)$ indicates the invariant measure over the gauge group. In the integral, the parallel transporters for different links are independent, except that $U(k,j)=U(j,k)^{-1}$, so that only one of these two ordered pairs needs to be represented in the integral. The normalizing constant Z is simply

$$Z = \int e^{-S(\mathcal{A})}\prod_{\langle j,k\rangle} dU(k,j). \tag{2}$$

The action S depends only on the results of parallel transport around plaquettes of the lattice, e.g., elementary squares in a cubic lattice. Let $\mathcal{P}$ be a plaquette, which we can think of as a sequence of lattice sites; for a cubic lattice $\mathcal{P}$ would consist of four sites j,k,l,m. Let $U(\mathcal{P})$ be the net effect of parallel transport around plaquette $\mathcal{P}$; in the square example, $U(\mathcal{P})$ would be $U(j,m)U(m,l)U(l,k)U(k,j)$ (the right-most operator acting first). S is defined so that it increases as the plaquette transformations $U(\mathcal{P})$ get farther from the identity. Various action functions with this property have been used in the literature; the one originally proposed by Wilson for an SU(N) gauge field is[20]

$$S \propto -\sum_{\mathcal{P}} \mathrm{Re}(\mathrm{Tr}(U(\mathcal{P}))), \tag{3}$$

where the sum is over all plaquettes in the lattice. Note that if $\mathcal{P}'$ consists of the same set of points as $\mathcal{P}$, but with a different starting point or with the points taken in the opposite order, then $\mathrm{Re}(\mathrm{Tr}(U(\mathcal{P}')))=\mathrm{Re}(\mathrm{Tr}(U(\mathcal{P})))$. Thus we need include in the above sum only one ordered set $\mathcal{P}$ representing each geometric plaquette.

A gauge transformation associates with each lattice point j a group element $\Lambda(j)$, and under such a transformation each parallel transporter $U(k,j)$ transforms according to

$$U(k,j)\rightarrow \Lambda(k)U(k,j)\Lambda(j)^{-1}. \tag{4}$$

It is easy to see that, though a gauge transformation changes the field configuration, it does not change any of the plaquette transformations $U(\mathcal{P})$. Therefore, it does not affect the action S and so has no physical consequences.

This invariance under gauge transformations provides a simple analogy between the configuration of a gauge field and the state of a lattice of quantum particles. Consider, for example, a lattice of qubits. Rotating each of the individual qubits separately is analogous to a gauge transformation. The state of the lattice changes under such rotations, but certain physical properties do not change. In particular, any reasonable measure of the degree of *entanglement* or *correlation* between two qubits does not change. So at least in this one modest respect, the degree of corre-

lation in a quantum lattice is similar to the action or the probability density of a field configuration in a lattice gauge theory. We want to see whether the similarity goes any further than this.

III. WHAT IS A REBIT?

As we have said, the quantum object we will mostly be concerned with in this article is the *rebit*. We now define this object more precisely.

A pure state $|\psi\rangle$ of a single rebit is simply a normalized vector in a two-dimensional real vector space. A mixed state of a rebit is a mixture of pure states:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \tag{5}$$

where $p_i > 0$ and $\Sigma_i p_i = 1$. Equivalently, a mixed state can be represented as a real, symmetric 2×2 matrix with unit trace and no negative eigenvalues.

Of course any rebit state is also a qubit state, and for our purposes it will be helpful to think of rebits simply as restricted qubits. On the Bloch sphere, the restriction to real density matrices becomes a restriction to the x-z plane. But it will be more useful to change the representation by rotating the Bloch sphere. Let us rotate all states by 90° in the left-handed sense around the positive x axis, so that our rebit states now lie in the x-y plane. A general mixed state lying in this plane can be written as

$$\rho = \tfrac{1}{2}[I + a\sigma_x + b\sigma_y], \tag{6}$$

where the σ's are Pauli matrices and the real numbers a and b satisfy $a^2 + b^2 \leqslant 1$. Let us call this representation of rebit states the ''horizontal representation,'' as opposed to the original ''real-number representation.'' Given a rebit density matrix ρ expressed in the horizontal representation, we can always reexpress it as a *real* density matrix ρ_{real} simply by reversing the rotation around the x axis:

$$\rho_{\text{real}} = U\rho U^\dagger, \tag{7}$$

where

$$U = e^{-i(\pi/4)\sigma_x} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}. \tag{8}$$

Here we have written the matrix in the basis of eigenstates of σ_z, $\{|\uparrow\rangle, |\downarrow\rangle\}$. Note that $U\sigma_y U^\dagger = \sigma_z$ and $U\sigma_x U^\dagger = \sigma_x$.

In the real-number representation, a pure state of n rebits is a real vector in 2^n dimensions, and a mixed state of such a system is a real, symmetric $2^n \times 2^n$ density matrix. But again we will usually work in the horizontal representation, in which each rebit has been rotated by 90° around the x axis. It will be helpful to have a simple way of recognizing whether a given n-qubit state is a legitimate n-rebit state expressed in the horizontal representation. Conceptually, the test is straightforward: apply the above transformation U to each qubit—that is, rotate each qubit by 90° (in the right-handed sense) around the positive x axis—and see whether the resulting state has only real components. Thus for a pure state $|\Psi\rangle$, we insist that $U^{\otimes n}|\Psi\rangle$ be real in the standard up–down basis. But this is the same as saying that $U^{\otimes n}|\Psi\rangle = (U^{-1})^{\otimes n}|\Psi^*\rangle$, where the asterisk indicates complex conjugation in the standard basis. Multiplying both sides of this equation by $U^{\otimes n}$ and noting that $U^2 = -i\sigma_x$, we arrive at the following criterion:

$$(-i\sigma_x)^{\otimes n}|\Psi\rangle = |\Psi^*\rangle. \tag{9}$$

In practice it will be simplest if we also allow ourselves to use state vectors of the form $\exp(i\alpha)|\Psi\rangle$, where α is real and $|\Psi\rangle$ satisfies Eq. (9). Though such state vectors do not become real when they are transformed by $U^{\otimes n}$, their density matrices do become real. Allowing this possibility leads to the following weaker condition on an n-qubit state $|\Psi\rangle$,

$$\sigma_x^{\otimes n}|\Psi\rangle = e^{i\beta}|\Psi^*\rangle, \tag{10}$$

β being any real phase. Note that the matrix σ_x simply interchanges $|\uparrow\rangle$ and $|\downarrow\rangle$. Thus we can recognize a pure n-qubit state $|\Psi\rangle$ as a legitimate horizontal representation of an n-rebit state by checking to see that the coefficient of each basis state, e.g., $|\uparrow\uparrow\downarrow\uparrow\rangle$, is the complex conjugate of the coefficient of the opposite state, in this case $|\downarrow\downarrow\uparrow\downarrow\rangle$, multiplied by a phase factor that is the same for all basis states. Let us call Eq. (10) the ''rebit condition'' for pure states. The corresponding test for mixed states can be obtained by a similar argument; one finds that a density matrix ρ of n qubits is the horizontal representation of a legitimate n-rebit state if and only if

$$\sigma_x^{\otimes n}\rho\sigma_x^{\otimes n} = \rho^*, \tag{11}$$

the complex conjugation again being in the standard basis.

We conclude this section with a word about *rotations* of a rebit. Viewing the states of a rebit as qubit states confined to the equatorial plane of the Bloch sphere, we could take as the allowed rotations all the unitary transformations that represent rotations around the z axis, that is, all transformations of the form

$$R = \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{i\beta} \end{pmatrix}. \tag{12}$$

However, our definition of parallel transport will not be able to distinguish unitary transformations that are different only by an overall phase factor; so we will call such transformations identical. For definiteness we pick a standard representative from each of the resulting equivalence classes: a rotation by an angle ξ around the z axis, with $0 \leqslant \xi < 2\pi$, will be represented by the matrix

$$R = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\xi} \end{pmatrix}. \tag{13}$$

IV. PARALLEL TRANSPORT IN A LATTICE OF REBITS

We now consider a lattice of rebits, on which we want to define a notion of parallel transport. For now the structure of the lattice does not matter, as long as any two rebits are identified as either being neighbors or not. Thus the lattice is simply a graph. The mathematical object that is to be parallel transported is a pure state of a single rebit, which we can picture as a direction in the horizontal plane. The parallel transporter associated with a link in the lattice will be a rebit rotation—represented in the form (13)—which we can identify with an element of U(1). We want the assignment of parallel transporters to links to be determined by the quantum state of the lattice itself.

We begin with the following scenario. Consider a pair of neighboring rebits labeled j and k. They are in some joint state $\rho^{(jk)}$, a 4×4 density matrix obtained from the state of the whole lattice by tracing over all the other particles. Imagine performing an arbitrary orthogonal measurement on particle j. In the standard von Neumann model this measurement brings particle j into a certain pure state—one of the eigenstates of the measurement—and it also brings particle k into some state, typically a mixed state, determined as follows. Let $|\psi^{(j)}\rangle$ be the eigenstate into which particle j is brought by the measurement. Then the postmeasurement state of particle k is the 2×2 density matrix

$$\omega^{(k)}=\frac{1}{P}\langle\psi^{(j)}|\rho^{(jk)}|\psi^{(j)}\rangle, \tag{14}$$

where $P=\langle\psi^{(j)}|\mathrm{Tr}_k\rho^{(jk)}|\psi^{(j)}\rangle$ is the probability with which that particular outcome occurs. In Eq. (14) the matrix operations are done only in the space of particle j. To be more explicit, if $r=0,1$ and $s=0,1$ are indices associated with particles j and k, respectively, we can write the components of $\omega^{(k)}$ in terms of the components of $|\psi^{(j)}\rangle$ and $\rho^{(jk)}$ as

$$\omega^{(k)}_{ss'}=\frac{1}{P}\sum_{r,r'}\psi^{(j)*}_r\rho^{(jk)}_{rs,r's'}\psi^{(j)}_{r'}. \tag{15}$$

We want to use this measurement scenario to associate with the two-particle state $\rho^{(jk)}$ a simple rotation $U(k,j)$. First, let $\mathcal{M}$ (for "measurement") be the mapping defined by Eq. (14), which takes each pure state of particle j for which $P\neq 0$ into a pure or mixed state of particle k; that is, $\mathcal{M}(\psi^{(j)})=\omega^{(k)}$. If $P=0$, let us say for definiteness that $\mathcal{M}(\psi^{(j)})=\mathrm{Tr}_j\rho^{(jk)}$, though it will not actually matter in what follows. For an arbitrary rebit rotation R, we define a function $F(R)$ by

$$F(R)=\frac{\int\langle\psi|R^\dagger\mathcal{M}(\psi)R|\psi\rangle P\,d\psi}{\int P\,d\psi}. \tag{16}$$

Here P is the probability given above, and $d\psi$ indicates the uniform measure over the circle of pure rebit states, normalized so that $\int d\psi=1$. Thus $F(R)$ is an average fidelity of $\mathcal{M}(\psi)$, not with respect to $|\psi\rangle$ itself but with respect to a rotated version of $|\psi\rangle$. As we will see in the next paragraph, depending on the density matrix $\rho^{(jk)}$, one of the following two conditions will hold: (i) $F(R)$ is independent of R or (ii) there is a unique rotation $R=U$ that maximizes $F(R)$. In case (i), we say that there is no correlation between particles j and k. In case (ii), we take the special rotation U that maximizes $F(R)$ to be the parallel transporter associated with the link $\langle j,k\rangle$. In a certain sense, U is the rotation that most closely approximates the action of $\mathcal{M}$.

Combining Eqs. (14) and (16) and the definition of P, we have

$$F(R)=\frac{\int(\langle\psi|\otimes\langle\psi|R^\dagger)\rho^{(jk)}(|\psi\rangle\otimes R|\psi\rangle)\,d\psi}{\int\langle\psi|\mathrm{Tr}_k\rho^{(jk)}|\psi\rangle\,d\psi}. \tag{17}$$

It is not hard to show that the denominator is always $\frac{1}{2}$. Also, in the horizontal representation, the integral in the numerator involves rotating $|\psi\rangle$ around the z axis, so that we can rewrite Eq. (17) as

$$F(R)=2(\langle\psi_0|\otimes\langle\psi_0|R^\dagger)\left[\frac{1}{2\pi}\int_0^{2\pi}e^{i\gamma S_z}\rho^{(jk)}e^{-i\gamma S_z}d\gamma\right](|\psi_0\rangle\otimes R|\psi_0\rangle), \tag{18}$$

where $S_z=(\sigma_z^{(j)}+\sigma_z^{(k)})/2$ and $|\psi_0\rangle$ is some fixed reference state which for definiteness we take to be $|\psi_0\rangle=(|\uparrow\rangle+|\downarrow\rangle)/\sqrt{2}$. Now, a general two-particle density matrix satisfying the rebit condition (11) is of the form

$$\rho^{(jk)}=\begin{pmatrix} a & x_1 & x_2 & x_3\\ x_1^* & b & c & x_2\\ x_2^* & c^* & b & x_1\\ x_3^* & x_2^* & x_1^* & a\end{pmatrix}, \tag{19}$$

the representation being in the standard basis $\{|\uparrow\uparrow\rangle,|\uparrow\downarrow\rangle,|\downarrow\uparrow\rangle,|\downarrow\downarrow\rangle\}$. The average over γ in Eq. (18) has the effect of replacing the x_i's in $\rho^{(jk)}$ with zero and leaving the matrix elements a, b, and c unchanged. To evaluate $F(R)$, we write R explicitly as a rotation around the z axis by some angle ξ:

$$R=\begin{pmatrix} 1 & 0 \\ 0 & e^{i\xi} \end{pmatrix}. \tag{20}$$

Inserting this matrix into Eq. (18) we find that

$$F(R)=\tfrac{1}{2}[1+2|c|\cos(\xi-\phi)], \tag{21}$$

where ϕ is the phase of the matrix element c; that is, $c=|c|e^{i\phi}$. If c is zero, then we find ourselves in case (i) mentioned above: $F(R)$ is independent of R. Otherwise F is maximized when the angle of rotation ξ is equal to the phase ϕ. According to our prescription, then, the parallel transporter $U(k,j)$ is the rotation given in Eq. (20) with $\xi=\phi$.

We will take as our measure of the degree of correlation between particles j and k the quantity $2|c|$, which ranges from 0 to 1. Equation (21) makes it clear that $2|c|$ measures the degree of angular correlation between the two particles. We can also interpret this quantity in terms of the more standard correlation matrix $\tau_{\mu\nu}=\mathrm{Tr}[\rho^{(jk)}(\sigma_\mu\otimes\sigma_\nu)]$, in which both μ and ν take as values the axis labels x and y. One finds that $(2|c|)^2=[(\tau_{xx}+\tau_{yy})^2+(\tau_{xy}-\tau_{yx})^2]/4=[2\det\tau+\mathrm{Tr}(\tau^T\tau)]/4$.

Note that the single complex number c determines both the parallel transporter (through its phase) and the degree of correlation (through its magnitude). Typically we will be trying to maximize the magnitude of c for a given value of its phase. The fact that it is possible for a link $\langle j,k\rangle$ to have an undefined parallel transporter $U(k,j)$ [case (i) above, where $c=0$] will not cause any difficulties for the problem we will be studying. We will be considering the set of all states that are consistent with a given specification of the parallel transporters, i.e., the phases of the c's. If a link has $c=0$, then we simply say that that link is consistent with any specified phase.

Our notion of parallel transport has a particularly simple interpretation if $\rho^{(jk)}$ has the form (19) with all the x_i's equal to zero. This will happen, for example, if the state of the lattice is invariant under identical rotations of all the rebits. If $\rho^{(jk)}$ has this form, then Eq. (14) yields

$$\omega^{(k)}=pU(k,j)|\psi^{(j)}\rangle\langle\psi^{(j)}|U(k,j)^\dagger+(1-p)(I/2), \tag{22}$$

where I is the 2×2 identity and $p=2|c|$. Thus the postmeasurement state of particle k is simply a rotated and partially depolarized version of $|\psi^{(j)}\rangle$, and the weight p of the pure rotated state is our measure of correlation.

Let us now imagine transporting, mathematically, a rebit state around a closed loop in accordance with the above prescription. As we will see, the final state in such a process need not be the same as the initial state but could be rotated by some angle θ. One might ask: How does one interpret physically this process of transport, and what is the meaning of the rotation angle θ? I regard our concept of parallel transport primarily as a mathematical notion; nothing is being physically transported. However, in the special case considered above, in which the state of the lattice is rotationally invariant, one can extract from our definition a simple physical interpretation of the net rotation angle. Consider a closed loop of n lattice sites $j_0,j_1,\ldots,j_{n-1}$. At each of the sites $j_0,\ldots,j_{n-2}$, that is, at all but the last site, perform an orthogonal measurement, with outcomes labeled "0" and "1," choosing the measurement at j_m so that it maximizes the probability of getting the same outcome (0 or 1) as at site j_{m-1}. That is, we are trying to minimize the expected number of flips from 0 to 1 or from 1 to 0 as we go around the loop. Now, at the last site, j_{n-1}, one is faced with a dilemma: there will be a measurement that maximizes the probability of agreement between j_{n-2} and j_{n-1}, and there will be a (possibly different) measurement that maximizes the probability of agreement between j_{n-1} and j_0. The angle between these two

measurements, that is, between their ''0'' eigenstates, is the angle θ associated with parallel transport around the loop. We can think of this angle as measuring the net ''twist'' in the nearest-neighbor correlations.

When the state of the lattice is not rotationally invariant, the angle between the two competing optimal measurements at the last site (the two being reckoned optimal from different directions) may depend on the choice of the initial measurement on the first particle. So the interpretation in this case is not as simple. Still, it is reasonable to think of the net rotation angle as a measure of the net twist in the correlations. In the following section where we analyze the case of a rebit ring, we will find that the optimal states, which are the states most relevant to our problem, are in fact rotationally invariant, so that the above interpretation applies.

V. ANALYSIS OF A REBIT RING

So far we have not made any assumptions about the structure of the lattice. In order to obtain a concrete result, we now specialize to the simplest possible lattice for which our general question can be addressed, namely, a closed one-dimensional ring. Let the ring consist of n rebits with $n \geqslant 2$, labeled by $j=0,1,\ldots,n-1$; the labeling is mod n, so that $j=n$ is the same as $j=0$. Let c_j be the matrix element c of Eq. (19) when the two particles in question are particles j and $j+1$. The quantity $K=(2/n)\,\Sigma_j|c_j|$ will be the measure of average nearest-neighbor correlation that we will be trying to maximize; note that $0\leqslant K\leqslant 1$. The product $\Pi_j(c_j/|c_j|)$, which we will call $e^{i\theta}$, is the net phase factor associated with transport around the whole ring, and θ (defined only mod 2π) is the net rotation angle. Our question is this: what is the maximum possible value of K for a fixed value of θ? Let us call this maximum value $K_{\max}(\theta)$. If $K_{\max}(\theta)$ decreases as $e^{i\theta}$ gets farther from unity, then we can say that there is a correlation cost associated with nontrivial parallel transport.

As we have stated the problem so far, the phases of the different c_j's, that is, the phases that define the individual parallel transporters, need not be the same for all links in the ring. However, for our purpose there is no loss of generality in assuming that these phases are all equal. This is because if they were not equal, we could always apply local rotations to the individual rebits (analogous to a gauge transformation) so as to make them equal. Local rotations can change neither the magnitude of any c_j nor the overall phase factor $e^{i\theta}$. So the restriction to equal phases does not eliminate any states that might change the answer to our question. That is, states with maximal K for any given θ are still represented in the restricted set.

With this restriction, we can simplify our problem by expressing the average correlation K and the overall phase θ in terms of creation and annihilation operators. Let a_j be an operator on particle j defined by $a_j|\uparrow\rangle=|\downarrow\rangle$ and $a_j|\downarrow\rangle=0$. Then for the link between the jth and the $(j+1)$st rebits, we can write c_j as

$$c_j=\mathrm{Tr}(\rho a_{j+1}^{\dagger}a_j), \tag{23}$$

ρ being the density matrix of the ring. Now if we define the operator Γ to be

$$\Gamma=\frac{1}{n}\sum_{j=0}^{n-1} a_{j+1}^{\dagger}a_j \tag{24}$$

and write $\langle\Gamma\rangle=\mathrm{Tr}\rho\Gamma$, it follows (assuming that each c_j has the same phase) that

$$K=2|\langle\Gamma\rangle|, \tag{25}$$

and that the overall phase θ (mod 2π) is simply

$$\theta=n\arg(\langle\Gamma\rangle). \tag{26}$$

Γ is not a Hermitian operator—so its eigenvalues may be complex and indeed must be complex if θ is to take any nontrivial value—but Γ does commute with its adjoint, which implies that eigenvectors corresponding to distinct eigenvalues are orthogonal. Note also that Γ commutes with

the total z component of spin; so the eigenstates of Γ can be taken to be states with a definite number u of up spins. Our immediate goal is to find the eigenvalues of Γ, from which we will be able to determine the set of possible values of $\langle\Gamma\rangle$, which in turn will give us $K_{\max}(\theta)$.

The a operators are not quite fermionic creation and annihilation operators, because the operators associated with different sites commute with each other rather than anticommute. However, we can use a standard trick[21] to define genuinely fermionic operators b_j:

$$b_j = \exp\left[i\pi \sum_{k=0}^{j-1} a_k^\dagger a_k \right] a_j . \tag{27}$$

The operators b_j satisfy the usual fermionic anticommutation relations:

$$\{b_j, b_k\} = \{b_j^\dagger, b_k^\dagger\} = 0; \quad \{b_j, b_k^\dagger\} = \delta_{jk} . \tag{28}$$

We now express Γ in terms of the b's. The expression depends on whether u, the number of up spins in the ring, is even or odd; that is, the expression is different in different subspaces. For odd values of u, Γ looks the same in terms of the b's as it does in terms of the a's:

$$\Gamma = \frac{1}{n} \sum_{j=0}^{n-1} b_{j+1}^\dagger b_j . \tag{29}$$

For even values of u, there is a sign change in the last term:

$$\Gamma = \frac{1}{n} \left[\sum_{j=0}^{n-2} b_{j+1}^\dagger b_j - b_0^\dagger b_{n-1} \right]. \tag{30}$$

In either case, we can diagonalize Γ and find its exact single-fermion eigenvalues. From these we can obtain the eigenvalues of Γ for an arbitrary value of u by summing u of the single-fermion eigenvalues.

For odd u, the single-fermion eigenstates of Γ are $|\omega_m\rangle = d_m^\dagger |0\rangle$, $m = 0, \ldots, n-1$, where $|0\rangle$ is the vacuum state, that is, the state with all spins down, and the creation operator $d_m^\dagger$ is given by

$$d_m^\dagger = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} e^{-2m\pi ij/n} b_j^\dagger . \tag{31}$$

The corresponding eigenvalues of Γ are

$$g_m = (1/n) e^{2m\pi i/n}. \tag{32}$$

For even u, the creation operators for the single-fermion eigenstates are

$$d_m^\dagger = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} e^{-(2m+1)\pi ij/n} b_j^\dagger , \quad m = 0, \ldots, n-1, \tag{33}$$

and the corresponding eigenvalues are

$$g_m = (1/n) e^{(2m+1)\pi i/n}. \tag{34}$$

Regardless of the value of u, the single-fermion eigenvalues of Γ are complex numbers of length $1/n$, with phases uniformly spaced around the complex plane.

The eigenvalues of Γ corresponding to a system of u fermions (that is, u up spins) are all the possible sums of u of the g_m's. That is, we can write each such eigenvalue as

$$G(M)=\sum_{m\in M} g_m, \tag{35}$$

where M is a set of exactly u integers chosen from the set $\{0,\ldots,n-1\}$. (We cannot use the same value of m twice in this sum because no two identical fermions can be in the same state, and all the single-fermion eigenvalues are nondegenerate.)

As we will see, the most important eigenvalues $G(M)$ for our purpose will be the ones with the greatest magnitude. For even values of n, these are the ones for which $u=n/2$ and the set M consists of a string of consecutive integers (mod n), so that the corresponding values g_m constitute a "fan" of complex numbers spread out over half of the complex plane. Performing the sum in Eq. (35), we find that these extreme eigenvalues are

$$G_r=\frac{e^{2r\pi i/n}}{n\sin(\pi/n)}, \quad r=0,\ldots,n-1 \quad (\text{even } n), \tag{36}$$

an equation that holds for all even values of n (even though $u=n/2$ might be even or odd). For odd values of n, the eigenvalues with largest magnitude are obtained by setting u equal to either $(n+1)/2$ or $(n-1)/2$, and again letting M consist of a string of consecutive integers mod n. For either of these choices of u, the eigenvalues thereby obtained are

$$G_r=\frac{e^{2r\pi i/n}}{n\sin(\pi/n)}\cos(\pi/(2n)), \quad r=0,\ldots,n-1 \quad (\text{odd } n). \tag{37}$$

For either even or odd n, each eigenstate corresponding to one of the eigenvalues G_r can be written as

$$|\Omega_{r,u}\rangle=d^\dagger_{m_0}d^\dagger_{m_0+1}\cdots d^\dagger_{m_0+u-1}|0\rangle, \tag{38}$$

where $m_0=r-\lfloor u/2\rfloor$ mod n. (Here and below, addition in the subscript of d is always mod n.) This value of m_0 places $\exp(2r\pi i/n)$ in the center of the fan of complex eigenvalues $g_{m_0},\ldots,g_{m_0+u-1}$. For later convenience, we define the following density matrices based on these eigenstates. For even n,

$$\rho_r=|\Omega_{r,n/2}\rangle\langle\Omega_{r,n/2}|, \tag{39}$$

and for odd n,

$$\rho_r=\tfrac{1}{2}[|\Omega_{r,(n+1)/2}\rangle\langle\Omega_{r,(n+1)/2}|+|\Omega_{r,(n-1)/2}\rangle\langle\Omega_{r,(n-1)/2}|]. \tag{40}$$

As we will see shortly, both of these density matrices satisfy the rebit condition, even though $|\Omega_{r,(n+1)/2}\rangle$ and $|\Omega_{r,(n-1)/2}\rangle$ do not. Note also that for both even and odd n, $\mathrm{Tr}\,\rho_r\Gamma=G_r$.

One can check that ρ_r is translationally invariant and thus is in accord with the assumption we made earlier, that the matrix element c_j has the same phase for each link of the ring. But we also want to check that ρ_r is a legitimate rebit state, i.e., that it satisfies Eq. (11). Let us do this first for even values of n, in which case we are dealing with a pure state $|\Omega_{r,n/2}\rangle$.

We begin by noting that

$$\sigma_x^{\otimes n}b_j^\dagger=(-1)^j b_j\sigma_x^{\otimes n}, \tag{41}$$

which can be seen directly from the definition of b_j. It follows that

$$\sigma_x^{\otimes n}d^\dagger_{m_1}\cdots d^\dagger_{m_u}|0\rangle=[d_{m_1+n/2}\cdots d_{m_u+n/2}\sigma_x^{\otimes n}|0\rangle]^*, \tag{42}$$

where $m_1,\ldots,m_u$ are any distinct values chosen from the set $\{0,\ldots,n-1\}$. [The addition of $n/2$ in the subscripts on the right-hand side comes from $(-1)^j$ in the preceding equation.] In general, a state of the form $d^\dagger_{m_1}\cdots d^\dagger_{m_u}|0\rangle$ will not satisfy the rebit condition, even if $u=n/2$. However, for the special case in which $m_1,\ldots,m_u$ are $n/2$ *consecutive* integers, as they are in the definition of $|\Omega_{r,n/2}\rangle$, the subscripts on the right-hand side of Eq. (42) are precisely those elements of $\{0,\ldots,n-1\}$ that are not included in $\{m_1,\ldots,m_u\}$. Therefore, when those annihilation operators are applied to the all-up-spin state $\sigma_x^{\otimes n}|0\rangle$, which within a phase factor is the same as $d_0^\dagger d_1^\dagger\cdots d_{n-1}^\dagger|0\rangle$, the resulting state, again up to an overall phase factor, is $d^\dagger_{m_1}\cdots d^\dagger_{m_u}|0\rangle$. We have thus shown that

$$\sigma_x^{\otimes n}|\Omega_{r,n/2}\rangle = e^{i\beta}|\Omega^*_{r,n/2}\rangle \tag{43}$$

for some phase β, so that ρ_r satisfies the rebit condition (10) for even values of n.

Turning now to the case of odd n, one can use an argument like the one in the preceding paragraph to show that

$$\sigma_x^{\otimes n}|\Omega_{r,(n-1)/2}\rangle\langle\Omega_{r,(n-1)/2}|\sigma_x^{\otimes n} = |\Omega^*_{r,(n+1)/2}\rangle\langle\Omega^*_{r,(n+1)/2}|, \tag{44}$$

and vice versa, so that

$$\sigma_x^{\otimes n}\rho_r\sigma_x^{\otimes n} = \rho_r^* . \tag{45}$$

So ρ_r satisfies the rebit condition for odd values of n as well.

We are now in position to find the set—call it $\mathcal{G}$—of possible values of $\langle\Gamma\rangle$, from which we will be able to determine $K_{\max}(\theta)$. The complex numbers G_r given by Eq. (36) or (37), being values of $\langle\Gamma\rangle$ corresponding to the legitimate rebit states ρ_r, are elements of $\mathcal{G}$. By taking mixtures of these states, we can obtain other possible values of $\langle\Gamma\rangle$. Let

$$\rho = \sum_r q_r\rho_r , \tag{46}$$

where the q's are non-negative numbers summing to 1. For this state we have

$$\langle\Gamma\rangle = \mathrm{Tr}\ \rho\Gamma = \sum_r q_r G_r . \tag{47}$$

The complex numbers G_r are the vertices of a regular n-gon in the complex plane, and Eq. (47) shows that this n-gon and its interior are contained in $\mathcal{G}$.

In fact, it is easy to see that $\mathcal{G}$ contains no other points. Any complex number $\langle\Gamma\rangle$ in $\mathcal{G}$ must be a weighted average of eigenvalues of Γ:

$$\langle\Gamma\rangle = \sum_M q_M G(M). \tag{48}$$

But one can show that each eigenvalue $G(M)$, regardless of the value of u, lies on or inside the n-gon defined by the special eigenvalues discussed above. Therefore it is impossible for the average to get outside this region.

For the special case $n=2$, the interior of the "n-gon" is simply a segment of the real axis, running from $-\frac{1}{2}$ to $+\frac{1}{2}$. Thus the only possible phases of $\langle\Gamma\rangle$ are zero and π, so that according to Eq. (26) the only possible value of $\exp(i\theta)$ is 1. (This is because there is no real loop to traverse; to return to the starting place, one has to retrace one's steps.) For all other values of n, all values of θ from 0 to 2π are possible. To see this, it is enough to consider a single side of the n-gon; let us take the side consisting of the line segment joining the point G_0, on the positive real axis, with

the point $G_1 = e^{2\pi i/n} G_0$. As we travel along this segment, the phase of $\langle \Gamma \rangle$ varies from 0 to $2\pi/n$, so that θ varies from 0 to 2π. The range of values of $|\langle \Gamma \rangle|$ as a function of θ is the same for each of the other sides of the n-gon.

It thus becomes a simple geometric problem to find $K_{\max}(\theta)$. For $n > 2$, consider the line segment just described, connecting G_0 to G_1, and note that for any θ in the range $0 \leq \theta \leq 2\pi$, $K_{\max}(\theta)$ is twice the magnitude of the unique point along this segment whose phase is θ/n. Doing the geometry, and using the values of G_r given in Eqs. (36) and (37), one finds that for even n,

$$K_{\max}(\theta) = \frac{2\cos(\pi/n)}{n \sin(\pi/n)\cos[(\pi-\theta)/n]}, \tag{49}$$

and for odd n,

$$K_{\max}(\theta) = \frac{2\cos(\pi/n)\cos(\pi/(2n))}{n \sin(\pi/n)\cos[(\pi-\theta)/n]}. \tag{50}$$

It is clear both from the geometric picture and from Eqs. (49) and (50) that $K_{\max}$ is largest at $\theta = 0$ and $\theta = 2\pi$ and smallest at $\theta = \pi$. Indeed, the value of $K_{\max}$ becomes smaller the more $e^{i\theta}$ differs from unity. In this sense there is a correlation cost of nontrivial parallel transport around the ring.

It is not hard to interpret the states ρ_r physically. The state ρ_0, which entails no twisting as one goes around the ring, is the ground state, or, in the case of odd n an equal mixture of the two degenerate ground states, of the ferromagnetic XY model[21] on a one-dimensional ring, whose Hamiltonian is $H = -\Sigma_j (a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) = -n(\Gamma^\dagger + \Gamma)$. The state ρ_r can be obtained from ρ_0 by rotating each rebit, the rotation angle at site j being $2\pi r j/n$. These rotations do not change the strength of the nearest-neighbor correlations, but for each site j they change the phase of the matrix element c_j from zero to $2\pi r/n$. Still, this does not change the *overall* phase factor $e^{i\theta}$ associated with the whole ring. When one creates a mixture of two of these differently rotated states, e.g., ρ_0 and ρ_1, the resulting matrix element c_j is an average of two complex numbers with different phases. It is this averaging process that allows the possibility of a nontrivial net phase change around the ring.

In the case of even n, where ρ_r represents the pure state $|\Omega_{r,n/2}\rangle$, one could achieve the same averaging effect by creating coherent superpositions of eigenstates of Γ rather than incoherent mixtures. I have chosen to use mixtures because superpositions of these eigenstates are not necessarily translationally invariant. However, just to demonstrate that it is possible for a translationally invariant pure state to have a nonzero rotation angle θ associated with parallel transport around the ring, I offer the following example for $n = 6$:

$$|\Psi\rangle = \frac{i}{\sqrt{12}}[e^{i\phi/2}(|\uparrow\uparrow\downarrow\uparrow\downarrow\downarrow\rangle + \cdots) + e^{-i\phi/2}(|\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\rangle + \cdots)]. \tag{51}$$

Here each ellipsis stands for all possible translations of the given state. [Though we are not paying particular attention to the overall phase factors of pure states, I have chosen the overall phase in Eq. (51) to satisfy Eq. (9).] One finds that the matrix element c_j for each link in this ring is $(\frac{1}{6})\exp(i\phi)$, so that the overall rotation angle is $\theta = 6\phi$ and the average correlation is $K = \frac{1}{3}$. Thus any value of θ can be realized with a translationally invariant pure state. But the value $K = \frac{1}{3}$ is not optimal. To obtain the optimal value $K_{\max}(\theta)$ in a translationally invariant state, one must typically use mixed states rather than pure states.

We finish this section by giving asymptotic expressions for $K_{\max}(\theta)$ as the number of rebits in the ring gets very large. For even n, Eq. (49) to order $1/n^2$ becomes (for $0 \leq \theta \leq 2\pi$)

$$K_{\max}(\theta) = \frac{2}{\pi}\left[1 + \frac{1}{n^2}\left(\frac{\pi^2}{6} - \pi\theta + \frac{\theta^2}{2}\right)\right], \tag{52}$$

while for odd n we have

$$K_{\max}(\theta)=\frac{2}{\pi}\left[1+\frac{1}{n^2}\left(\frac{\pi^2}{24}-\pi\theta+\frac{\theta^2}{2}\right)\right]. \tag{53}$$

Thus the correlation cost of nontrivial parallel transport becomes smaller as the size of the ring increases.

VI. OTHER LATTICES

Let us now think about how the above problem might be generalized to a finite or infinite lattice of higher dimension (still using rebits as our basic objects). We can state the problem as follows. As in Sec. IV, let $\rho^{(jk)}$ be the density matrix of the pair of rebits at the neighboring sites j and k, and let $c_{j,k}$ be the coefficient of $|\uparrow\downarrow\rangle\langle\downarrow\uparrow|$ in this density matrix. (This $c_{j,k}$ is analogous to the c_j of the preceding section.) Now suppose that the phases of all the c's, for all the links $\langle j,k\rangle$, are specified. We will call this complete specification $\mathcal{A}$, since it is analogous to a field configuration in the U(1) gauge theory. Given this specification, we have two questions: (i) Is it possible to find a lattice state for which the numbers $c_{j,k}$ are all nonzero and have the chosen phases? (One can always find a state in which all the $c_{j,k}$'s are zero, making the state consistent with any phases, but such a state is not very interesting.) (ii) What is the maximum possible value of

$$K=\frac{2}{L}\sum_{\langle j,k\rangle}|c_{j,k}|, \tag{54}$$

consistent with the specification $\mathcal{A}$? Here L is the number of links in the lattice. In the case of an infinite lattice, K can be defined as a limit over a sequence of finite lattices. Let us call the maximum value $K_{\max}(\mathcal{A})$.

For definiteness let us consider a specific lattice, namely, an infinite square lattice in two dimensions. Let us consider first the configuration $\mathcal{A}_0$ in which the phases of all the $c_{j,k}$'s are zero. In this case it is again helpful to invoke the Hamiltonian of the ferromagnetic XY model:

$$H=-\sum_{\langle j,k\rangle}(a_k^\dagger a_j+a_j^\dagger a_k). \tag{55}$$

Here the sum is over all links in the square lattice. The optimal value of K is the infinite-lattice limit of $(-E_0/L)$, E_0 being the minimum eigenvalue of this Hamiltonian. In the thermodynamic limit, the ground state of the XY model on a square lattice breaks the SO(2) symmetry of the problem and picks out a preferred direction of magnetization in the x-y plane,[22,23] which can be characterized by a single angle α. But if we choose to do so (in order to simplify the interpretation of parallel transport), we can easily generate a rotationally invariant state with the same energy—or in our context, with the same degree of correlation—simply by averaging the ground state density matrix $\rho(\alpha)$ over all angles: $\rho_0=(1/2\pi)\int\rho(\alpha)d\alpha$. The ground-state energy has been evaluated numerically,[24–26] and one finds that $K_{\max}(\mathcal{A}_0)=0.549$. Notice that this value is smaller than the corresponding value for a rebit ring in the limit $n\to\infty$ [see Eqs. (52) and (53) or Ref. 21], which is $2/\pi=0.637$.

Given a different specification of the phases, it is not immediately obvious whether there exists a state that has all nonzero $c_{j,k}$'s—let us call such a state "fully connected"—and that is also consistent with the given phases. Consider, for example, the configuration $\mathcal{A}$ in which all the phases are zero except at a specific link $\langle j,k\rangle$, where the phase is required to be ϕ. Can one find a fully connected state of the lattice consistent with these phases? The following method will work, though it is not likely to be optimal. Start with the state ρ_0 defined in the preceding paragraph, in which all the phases are zero. Construct the following sum:

$$\rho(j,k,\phi)=\tfrac{1}{3}[V_j\rho_0 V_j^\dagger+V_k^\dagger\rho_0 V_k+(V_j^\dagger\otimes V_k)\rho_0(V_j\otimes V_k^\dagger)], \tag{56}$$

where V_j is the matrix

$$V_j=\begin{pmatrix}1 & 0\\ 0 & e^{i\xi}\end{pmatrix} \tag{57}$$

applied to particle j and V_k is the same matrix applied to particle k. Here ξ will be a function of ϕ to be determined later. Because the rotations in Eq. (56) affect only particles j and k, all links not involving either of these particles will continue to have zero phase. Moreover, any link involving only one of the two special sites will likewise have its phase unchanged. Consider, for example, the link $\langle j,l\rangle$ where $l\neq k$. The value of $c_{j,l}$ is

$$c_{j,l}=\frac{1}{3}(c_0e^{-i\xi}+c_0+c_0e^{i\xi})=\left(\frac{1+2\cos(\xi)}{3}\right)c_0, \tag{58}$$

so that the phase has not been affected. On the other hand, the value of c associated with the link $\langle j,k\rangle$ is

$$c_{j,k}=\left(\frac{2e^{-i\xi}+e^{2i\xi}}{3}\right)c_0, \tag{59}$$

which has a phase that can be made equal to ϕ by a proper choice of the value of ξ.

An even simpler strategy, which is surely not optimal, shows that *any* phase configuration $\mathcal{A}$ can be realized in a fully connected quantum state of the lattice. Let us imagine the two dimensions of the lattice to be horizontal and vertical. Start with a state in which each vertical column of lattice sites is in the ground state of the ferromagnetic XY model for an infinite chain. Call this state $|\phi_V\rangle$. Now rotate each of the rebits in each of these chains so as to achieve the desired phases for the vertical links. This can be done with no loss of correlation, because we are simply performing local rotations. Similarly, consider the state $|\phi_H\rangle$ in which each *horizontal* row is in the XY ground state, and rotate the rebits so as to achieve the desired phases for the horizontal links. Let $|\phi_V'\rangle$ and $|\phi_H'\rangle$ be the states resulting from these rotations. Then the mixed state

$$\rho=\tfrac{1}{2}(|\phi_V'\rangle\langle\phi_V'|+|\phi_H'\rangle\langle\phi_H'|) \tag{60}$$

completely matches the phase configuration $\mathcal{A}$. We can even compute the value of K for the state ρ: it is equal to half of $K_{\max}$ for the infinite chain, independent of the configuration $\mathcal{A}$. That is, $K=1/\pi=0.318$. For the special configuration considered above, in which only one link has nonzero phase, this value is smaller than what one can achieve with the specialized method of Eq. (57). Nevertheless, the method we have just described does answer our first question: all configurations $\mathcal{A}$ can be achieved without making any $c_{j,k}$ vanish. Notice also that this construction gives us a lower bound on $K_{\max}(\mathcal{A})$ for all configurations $\mathcal{A}$: $K_{\max}(\mathcal{A})\geqslant 1/\pi$.

Actually finding $K_{\max}(\mathcal{A})$, even for simple configurations $\mathcal{A}$, is probably a very hard problem. If one uses strategies similar in spirit to the one given in Eq. (57), then it would seem that the value of $K_{\max}(\mathcal{A})$ must decrease in order to achieve nontrivial parallel transport around a loop. [One can see the decrease in the values of $|c_{j,l}|$ and $|c_{j,k}|$ in Eqs. (58) and (59).] But it is conceivable that a completely different strategy could do much better; so we must leave this basic question unanswered.

VII. LATTICES OF QUBITS

In our definition of parallel transport for rebits, developed in Sec. III, we implicitly made use of the fact that for rebits, there exists a two-particle state $\rho^{(+)}$ such that if particles j and k are in this state, and if particle j is measured and found to be in the state $|\psi\rangle$, then particle k will always be brought to the *same* state $|\psi\rangle$. Mathematically,

$$\omega = \frac{1}{P}\langle\psi|\rho^{(+)}|\psi\rangle = |\psi\rangle\langle\psi|. \tag{61}$$

The state $\rho^{(+)}$ is in fact $|\Psi^{(+)}\rangle\langle\Psi^{(+)}|$, with $|\Psi^{(+)}\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$. So for this state, the parallel transporter is the identity and the degree of correlation is 1. In effect, our definition of parallel transport compares other two-particle states to this special state; when the parallel transporter U is not the identity, it is because one of the particles has been rotated (and possibly distorted in other ways as well) compared to the standard state $\rho^{(+)}$.

For qubits, there is no two-particle state with this property. The most closely analogous state is the singlet state $|\Psi^{(-)}\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$. It has the property that if a measurement on one of the particles brings it to the state $|\psi\rangle$, the other particle will be brought to the *orthogonal* state $|\tilde{\psi}\rangle = \sigma_y|\psi^*\rangle$, where the complex conjugation is in the standard basis. In defining parallel transport for qubits, we will take the singlet state as our standard state, for which the parallel transporter is defined to be the identity. All other states will then be compared with this one. A general parallel transporter will be a rotation of the Bloch sphere, that is, an element of SO(3); as in the case of rebits, our definition will not allow us to distinguish overall phases. We will usually represent such a rotation as a 2×2 unitary matrix, keeping in mind that the overall phase is irrelevant.

We start again with Eq. (14):

$$\omega^{(k)} = \frac{1}{P}\langle\psi^{(j)}|\rho^{(jk)}|\psi^{(j)}\rangle, \tag{62}$$

and again let $\mathcal{M}$ be the map that takes $|\psi^{(j)}\rangle$ to $\omega^{(k)}$. But now we define our generalized fidelity as

$$F(R) = \frac{\int\langle\tilde{\psi}|R^\dagger\mathcal{M}(\psi)R|\tilde{\psi}\rangle P\,d\psi}{\int P\,d\psi}, \tag{63}$$

where $d\psi$ refers to the uniform measure over the surface of the Bloch sphere. Note that F compares $\mathcal{M}(\psi)$ with a rotated version of $|\tilde{\psi}\rangle$ rather than a rotated version of $|\psi\rangle$. If there is a unique rotation $R=U$ (up to an overall phase) that maximizes $F(R)$, then we will take this U to be the parallel transporter for the link $\langle j,k\rangle$. Thus, if $\rho^{(jk)}$ happens to be the singlet state, we have $U(k,j)=I$.

The fact that we base our notion of parallel transport for qubits on *antiparallel* states has the following consequence when we consider a closed loop. If the loop consists of an odd number of qubits, then the expression "no net twist," by our definition, implies a net reflection of the state. This is not what we intend to convey by this expression; so, I regard our definition as appropriate only for loops consisting of an *even* number of qubits. In a cubic lattice, every loop is of this sort. This restriction to even numbers of qubits is less than perfectly satisfying, but it is hard to see how it can be avoided, since there is no two-qubit state expressing a perfect *positive* correlation along every axis.

Carrying out the integrals in Eq. (63), we find that

$$F(R) = \tfrac{1}{3} + \tfrac{2}{3}\langle\Psi^{(-)}|(I\otimes R^\dagger)\rho^{(jk)}(I\otimes R)|\Psi^{(-)}\rangle. \tag{64}$$

Now, it is a fact that any maximally entangled state of two qubits can be written as $(I\otimes R)|\Psi^{(-)}\rangle$. So maximizing $F(R)$ over all rotations R is the same as finding the maximally entangled state that has the greatest overlap with $\rho^{(jk)}$. The quantity

$$f=\max_R \langle\Psi^{(-)}|(I\otimes R^\dagger)\rho^{(jk)}(I\otimes R)|\Psi^{(-)}\rangle \tag{65}$$

has been called the ''fully entangled fraction'' of $\rho^{(jk)}$.[13] It ranges from $\frac{1}{4}$ (for the completely mixed state) to 1 (for a maximally entangled state).[27] We will take $(4f-1)/3$, which ranges from 0 to 1, as our measure of the degree of correlation between particles j and k, and define K_q (q for ''qubit'') to be the average of this quantity over all the links of the lattice. As has been mentioned, the rotation R that achieves this maximum value, if it is unique, will be our parallel transporter $U(k,j)$.[28] We would like to maximize K_q for a fixed set of parallel transporters.

Our notion of parallel transport for qubits is particularly simple if $\rho^{(jk)}$ happens to be a ''twisted Werner state,'' that is, a state of the form[29]

$$p(I\otimes V)|\Psi^{(-)}\rangle\langle\Psi^{(-)}|(I\otimes V^\dagger)+(1-p)(I/4). \tag{66}$$

Here $0<p\leqslant 1$, $|\Psi^{(-)}\rangle$ is the singlet state, I is the 4×4 identity matrix, and V is a unitary transformation acting on particle k. If $\rho^{(jk)}$ is of this form, then the parallel transporter $U(k,j)$ works out, not surprisingly, to be the transformation V. Moreover, the weight p appearing in Eq. (66) is none other than our measure of correlation $(4f-1)/3$. Thus both the parallel transporter and the degree of correlation are particularly easy to interpret in this case. One can show that the six-rebit state of Eq. (51), reinterpreted as the state of a six-qubit ring, has the property that each pair of nearest neighbors is of the twisted Werner form.

A more interesting example of a qubit ring exhibiting nontrivial parallel transport—but whose pairs are not necessarily of the twisted Werner form—is given by the following state of six qubits,

$$\begin{aligned}|\psi\rangle=\alpha(|\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\rangle-\cdots)+\beta[e^{-i\xi}(|\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\rangle-\cdots)+e^{i\xi}(|\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\rangle-\cdots)]\\ +\gamma(|\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle-|\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\rangle).\end{aligned} \tag{67}$$

Here each ellipsis indicates all the translations of the given state, but with *alternating* signs. For example, the coefficient α multiplies

$$|\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\rangle-|\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\rangle+|\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\rangle-|\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle+|\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\rangle-|\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\rangle. \tag{68}$$

The coefficients α, β and γ are real and positive; their values will be specified shortly. Note that each pair of nearest neighbors in this state has the same density matrix, so that each has the same degree of correlation and the same parallel transporter. Because the state $|\psi\rangle$ is an eigenstate of S_z with eigenvalue zero, the density matrix of each pair is of the form (19) with all the x_i's equal to zero. (It is convenient to introduce a negative sign in the off-diagonal elements since our standard state is now the singlet.)

$$\rho^{(jk)}=\begin{pmatrix} a & 0 & 0 & 0\\ 0 & b & -c & 0\\ 0 & -c^* & b & 0\\ 0 & 0 & 0 & a\end{pmatrix}. \tag{69}$$

Carrying out the trace of $|\psi\rangle\langle\psi|$ over the other particles, one finds that $a=2\alpha^2+2\beta^2$, $b=\alpha^2+4\beta^2+\gamma^2$, and $c=2\beta[(\alpha+\gamma)e^{i\xi}+\beta e^{-2i\xi}]$. The correlation K_q is $(4f-1)/3$, where

$$f=b+|c|=\alpha^2+4\beta^2+\gamma^2+2\beta|(\alpha+\gamma)e^{i\xi}+\beta e^{-2i\xi}|, \tag{70}$$

and the parallel transporter is

$$U=\begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}, \tag{71}$$

where ϕ is the phase of c, that is, the phase of $(\alpha+\gamma)e^{i\xi}+\beta e^{-2i\xi}$. The fact that K_q depends on the matrix element b, while the analogous quantity K for rebits depended only on c, ultimately comes from the fact that in Eq. (63) we average over the entire surface of the Bloch sphere and not just over the equator.

In the spirit of our main problem, we would like to choose α, β and γ so as to maximize K_q. Let us do this extremization for the special case $\xi=0$, for which the parallel transporter given in Eq. (71) is the identity. In this case one finds that the optimal values are $\alpha=(130+34\sqrt{13})^{-1/2}$, $\beta=(1/2)(3+\sqrt{13})\alpha$, and $\gamma=(4+\sqrt{13})\alpha$, which satisfy the normalization condition $6\alpha^2+12\beta^2+2\gamma^2=1$. (By no accident, the state $|\psi\rangle$ with these values of the coefficients is the ground state of the antiferromagnetic Heisenberg model for a ring of six qubits.) In what follows we will assume that α, β and γ have these values. One finds then that for $\xi=0$, each pair of nearest neighbors is in a Werner state, and the correlation K_q is $(2+\sqrt{13})/9=0.623$. Let us call this value $K_q^{(0)}$.

How do K_q and U for the state $|\psi\rangle$ change as ξ departs from zero? Let us first look at U. To lowest order in ξ, the angle ϕ, which is the rotation angle associated with parallel transport across a link, is

$$\phi=\arg[(\alpha+\gamma)(1+i\xi)+\beta(1-2i\xi)]=\left(\frac{\alpha+\gamma-2\beta}{\alpha+\gamma+\beta}\right)\xi. \tag{72}$$

Note that $\alpha+\gamma-2\beta>0$, so that this linear contribution to ϕ does not vanish. Meanwhile, the correlation K_q diminishes by an amount proportional to the square of ξ:

$$K_q=K_q^{(0)}-\left(\frac{12\beta^2(\alpha+\gamma)}{\alpha+\gamma+\beta}\right)\xi^2. \tag{73}$$

Letting $\theta=6\phi$ be the net rotation associated with parallel transport around the whole ring, we can see how K_q depends on θ to lowest order:

$$K_q=K_q^{(0)}-\left(\frac{\beta^2(\alpha+\gamma)(\alpha+\gamma+\beta)}{3(\alpha+\gamma-2\beta)^2}\right)\theta^2=0.623-(0.369)\theta^2. \tag{74}$$

Notice that the reduction in correlation is of second order in θ, whereas in the case of rebits it is of first order as seen in Eqs. (52) and (53). Of course we have not done the thorough optimization for qubits that we have done for rebit rings, but this example indicates that there is a significant difference between the two cases.

VIII. DISCUSSION

We have shown, first of all, that there is a sense in which certain quantum states exhibit nontrivial parallel transport around a closed loop, which is to say that the nearest-neighbor correlations exhibit a net twist as one goes around the loop. One might regard this result as somewhat surprising, since there is, after all, only a single quantum state for the whole loop, and one might think that the local twists would therefore have to cancel each other out. We have also shown that in the case of the rebit ring, there is a loss of nearest-neighbor correlation associated with nontrivial parallel transport around the ring. For other lattices or for lattices of qubits, we do not know whether there is such a correlation cost, though it is certainly plausible that there would be.

As we have seen, there is a close relationship between our rebit problem and the XY model, a model that has been very well studied. Studies of spin stiffness in this model (see, for example, Ref. 26) have a certain similarity with the problem we have been considering in that in both cases one enforces a twist between neighboring spins. What distinguishes the present work is the fact

that we have not actually specified any Hamiltonian. Though it has been helpful for us to use an operator similar to the Hamiltonian of the XY model, we are really working with what might be called the *kinematics* of quantum mechanics. We are asking what correlation properties of quantum states follow from certain other correlation properties—specifically, we are asking what one can say about the *strength* of correlations given some information about the *twist* in the correlations—and this question is independent of any considerations of energy.

I introduced the subject by relating it to lattice gauge theory. To what extent, then, have we found an analogy between the state of a quantum lattice and the configuration of a lattice gauge field? In a qualitative sense, the reduction in correlation that we have observed in a rebit ring can be compared to the reduction in probability that one finds in a lattice gauge theory. But for this rebit case, the analogy must be regarded as quite rough, because there is a significant lack of congruence in the details. In gauge theory, the initial decrease in the probability is of *second order* in the net rotation angle θ associated with transport around a plaquette. In the U(1) theory, for example, the function $\exp(-S)$, with S given by Eq. (3), decreases in proportion to θ^2 for small values of θ. In contrast, in the rebit ring, the average correlation K, as given by Eqs. (49) and (50), decreases in proportion to θ itself. The second-order dependence is in fact important in lattice gauge theory for taking the continuum limit. Moreover, our first-order dependence makes $K_{\max}(\theta)$ a nonanalytic function, since near $\theta=0$ it takes the form $a-b|\theta|$. So this difference is not trivial.

On the other hand, we have just seen that the *qubit* correlation as we have defined it does seem to diminish quadratically in θ, at least for a ring of six qubits. It is interesting to ask whether in the case of a two-dimensional or higher-dimensional lattice, the dependence of $K_{\max}(\mathcal{A})$ is of second order in the rotation angles. In the one relevant example we have considered for a rebit lattice, namely, the strategy given in Eq. (57), the value of K decreases as $\phi^{2/3}$, which is an even sharper dependence than in the rebit ring. But we have not explored at all fully the range of possible states that one might consider for these higher-dimensional lattices.

It is worth commenting on the fact that in the case of qubits, our approach makes the parallel transporters elements of SO(3), whereas one might have expected SU(2). The nature of our definition does not allow us to pick out a relative phase in the relation between neighboring qubits. For example, we cannot distinguish between the identity operation and a rotation by 2π, even though a pure qubit state experiencing the latter rotation picks up a phase factor of -1. It is conceivable that by taking into account the density matrix of an entire loop, in addition to the density matrices of the neighboring pairs, one might be able to make sense of this distinction as it applies to the *net* rotation associated with the loop as a whole.

There are other ways in which one might modify the problem we have been considering. One could use a different measure of correlation or entanglement. Moreover, even if one continues to use the quantity $2|c|$ for rebits and the quantity $(4f-1)/3$ for qubits as the measure of nearest-neighbor correlation, one could combine the correlations from all the links in a different way. For example, in the case of a ring it would make some sense to consider the *product* of the individual correlations rather that the average; this measure has the pleasing feature that it vanishes if any of the links in the ring is broken.

Again, our main conclusion is this: in the one example we have worked out in detail, if there is a nontrivial twist in the nearest-neighbor correlations, that is, a twisting that cannot be undone by local rotations, then there is a corresponding reduction in the maximum possible magnitude of these correlations. That is, in this one example at least, twisted correlations are weaker correlations. This conclusion follows from the structure of the quantum state space and is true irrespective of the system's Hamiltonian.

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On entanglement-assisted classical capacity

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We give a modified proof of the recent result of C. H. Bennett, P. W. Shor, J. A. Smolin, and A. V. Thapliyal concerning entanglement-assisted classical capacity of a quantum channel and discuss the relation between entanglement-assisted and unassisted classical capacities. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The classical capacity of a quantum channel is the capacity of transmission of classical information through the channel. It is well known that the classical capacity can be increased if there is an additional resource in the form of an entangled state shared between the input A and the output B of the channel. While entanglement itself cannot serve for transmission of information from A to B, it may enhance the transmission provided there is a quantum channel connecting the systems. If the channel is ideal (i.e., the identity map Id from A to B), then the entanglement-assisted capacity is twice as great as the unassisted classical capacity, the enhancement being realized by the dense coding protocol.[1]

Recently C. H. Bennett, P. W. Shor, J. A. Smolin, and A. V. Thapliyal (BSST) studied the effect of the shared entanglement on the classical capacity of a quantum nonideal (noisy) channel[2,3] and obtained a remarkably simple formula for the entanglement-assisted capacity in terms of the maximal mutual quantum information between A and B. The proof, which is by no means trivial, involves in particular a rather tricky derivation of an important continuity property of quantum entropy. In this article we give a modified proof of the BSST theorem, including a more transparent proof of this property; moreover, we make further simplifications by using heavily properties of conditional quantum entropy rather than the underlying strong subadditivity.

In Ref. 2 it was shown that the enhancement in the classical capacity can achieve arbitrarily large values. To this end the case of a d-dimensional depolarizing channel in the limit of strong noise ($p\to 1$) was considered; we remark that the enhancement is even greater for the extreme case $p=d^2/(d^2-1)$. Moreover, we derive a general inequality between entanglement-assisted and unassisted capacities which may be relevant to the additivity problem in quantum information theory.

II. THE BSST THEOREM

We refer the reader to Refs. 4 and 5 for some basic definitions and results of quantum information theory used in this article.

Consider the following protocol for the classical information transmission through a quantum channel Φ. Systems A and B of the same dimension share an entangled (pure) state S_{AB}. A does some encoding $i\to\mathcal{E}_A^i$ depending on a classical signal i with probabilities π_i and sends its part of this shared state through the channel Φ to B. Thus B gets the states $(\Phi\otimes \mathrm{Id}_B)[S_{AB}^i]$, where $S_{AB}^i=(\mathcal{E}_A^i\otimes \mathrm{Id}_B)[S_{AB}]$, with probabilities π_i, and B is trying to extract the maximal classical information by doing measurements on these states. This is similar to the dense coding, but instead of the ideal channel, A uses a noisy channel Φ. We now look for the classical capacity of this protocol, which is called the *entanglement-assisted classical capacity* of the channel Φ.

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The maximum over measurements of B can be evaluated using the coding theorem for the classical capacity.[6] First we have the it *one-shot entanglement-assisted classical capacity*

$$C_{ea}^{(1)}(\Phi)=\max_{\pi_i,\mathcal{E}_A^i,S_{AB}}\left[H\left(\sum_i \pi_i(\Phi\otimes \mathrm{Id}_B)[S_{AB}^i]\right)-\sum_i \pi_i H((\Phi\otimes \mathrm{Id}_B)[S_{AB}^i])\right], \tag{1}$$

where $H(S)$ denotes the von Neumann entropy of the density operator S. Using the channel n times and allowing entangled measurements on B's side, one gets

$$C_{ea}^{(n)}(\Phi)=C_{ea}^{(1)}(\Phi^{\otimes n}). \tag{2}$$

The full entanglement-assisted classical capacity is then

$$C_{ea}(\Phi)=\lim_{n\to\infty}\frac{1}{n}C_{ea}^{(1)}(\Phi^{\otimes n}). \tag{3}$$

The following result was announced in Ref. 2, and a proof was given in Ref. 3:

$$C_{ea}(\Phi)=\max_{S_A} I(S_A;\Phi), \tag{4}$$

where

$$I(S_A;\Phi)=H(S_A)+H(\Phi(S_A))-H(S_A;\Phi) \tag{5}$$

is the quantum mutual information, with $H(S_A;\Phi)$ denoting the entropy exchange (see Refs. 4 and 5). Below we give a simplified proof of this remarkable formula.

Proof of the inequality:

$$C_{ea}(\Phi)\geqslant \max_{S_A} I(S_A;\Phi). \tag{6}$$

It is shown in Ref. 3 by generalizing the dense coding protocol that

$$C_{ea}^{(1)}(\Phi^{\otimes n})\geqslant I\left(\frac{P}{\dim P},\Phi^{\otimes n}\right) \tag{7}$$

for arbitrary projection P in $\mathcal{H}_A^{\otimes n}$. We give this proof for completeness here. Indeed, let $P=\Sigma_{k=1}^m |e_k\rangle\langle e_k|$, where $\{e_k;k=1,\ldots,m=\dim P\}$ is an orthonormal system. Define unitary operators in $\mathcal{H}_A$ acting as

$$V|e_k\rangle=\exp\left(\frac{2\pi i k}{m}\right)|e_k\rangle,\quad U|e_k\rangle=|e_{k+1(\mathrm{mod}m)}\rangle,\quad k=1,\ldots,m,$$

$$W_{\alpha\beta}=U^\alpha V^\beta,\quad \alpha,\beta=1,\ldots,m,$$

on the subspace generated by $\{e_k\}$, and as the identity onto its orthogonal complement. The operators $W_{\alpha\beta}$ are a finite-dimensional version of the Weyl–Segal operators for Boson systems (see, e.g., Ref. 5). Let

$$|\psi_{AB}\rangle=\frac{1}{\sqrt{m}}\sum_{k=1}^m |e_k\rangle\otimes|e_k\rangle.$$

Then it is easy to show the following.

(1) $(W_{\alpha\beta}\otimes I_B)|\psi_{AB}\rangle$; $\alpha,\beta=1,\ldots,m$, is an orthonormal system in $\mathcal{H}_A\otimes\mathcal{H}_B$. In particular, if $m=\dim\mathcal{H}_A$, it is a basis.
(2) $\Sigma_{\alpha,\beta=1}^{m}(W_{\alpha\beta}\otimes I_B)|\psi_{AB}\rangle\langle\psi_{AB}|(W_{\alpha\beta}\otimes I_B)^*=P\otimes P$.

Thus operators $\{W_{\alpha\beta};\alpha,\beta=1,\ldots,m\}$ play a role similar to Pauli matrices in the dense coding protocol for qubits.

Take the classical signal to be transmitted as $i=(\alpha,\beta)$ with equal probabilities $1/m^2$, the entangled state $|\psi_{AB}\rangle\langle\psi_{AB}|$, and the unitary encodings $\mathcal{E}_A^i[S]=W_{\alpha\beta}SW_{\alpha\beta}^*$. Then we have

$$C_{ea}^{(1)}(\Phi^{\otimes n})\geqslant H\left(\frac{1}{m^2}\sum_{\alpha\beta}(\Phi\otimes\mathrm{Id}_B)[S_{AB}^{\alpha\beta}]\right)-\frac{1}{m^2}\sum_{\alpha\beta}H((\Phi\otimes\mathrm{Id}_B)[S_{AB}^{\alpha\beta}]),$$

where $S_{AB}^{\alpha\beta}=(W_{\alpha\beta}\otimes I_B)|\psi_{AB}\rangle\langle\psi_{AB}|(W_{\alpha\beta}\otimes I_B)^*$. Then by the property (2) the first term on the right hand side is equal to $H((\Phi\otimes\mathrm{Id}_B)[P/m\otimes P/m])=H(P/m)+H(\Phi[P/m])$. Since $S_{AB}^{\alpha\beta}$ is a purification of P/m in $\mathcal{H}_B$, the entropies in the second term are all equal to $H(P/m,\Phi)$. By the expression for quantum mutual information (5) this proves (7). For future use, note that the last term in the quantum mutual information—the entropy exchange $H(S_A;\Phi)$—is equal to the final environment entropy $H(\Phi_E[S_A])$, where Φ_E is a channel from the system space $\mathcal{H}_A$ to the environment space $\mathcal{H}_E$, the actual form of which we need not know (see Ref. 5).

Now let $S_A=S$ be an arbitrary state in $\mathcal{H}_A$, and let $P^{n,\delta}$ be the typical projection of the state $S^{\otimes n}$ in $\mathcal{H}_A^{\otimes n}$. It was suggested in Ref. 2 that for *arbitrary* channel Ψ from $\mathcal{H}_A$ to possibly other Hilbert space $\tilde{\mathcal{H}}$

$$\lim_{\delta\to 0}\lim_{n\to\infty}\frac{1}{n}H\left(\Psi^{\otimes n}\left(\frac{P^{n,\delta}}{\dim P^{n,\delta}}\right)\right)=H(\Psi(S)),$$

which would imply, by the expressions for the mutual information and the entropy exchange, that

$$\lim_{\delta\to 0}\lim_{n\to\infty}\frac{1}{n}I\left(\frac{P^{n,\delta}}{\dim P^{n,\delta}};\Phi^{\otimes n}\right)=I(S;\Phi),\tag{8}$$

and, hence, by (7), the required inequality (6). We shall prove (8) with $P^{n,\delta}$ being the *strongly typical projection* of the state $S^{\otimes n}$.

Let us fix small positive δ, and let λ_j be the eigenvalues and $|e_j\rangle$ be the eigenvectors of the density operator S. Then the eigenvalues and eigenvectors of $S^{\otimes n}$ are $\lambda_J=\lambda_{j_1}\cdot\cdots\cdot\lambda_{j_n}$, $|e_J\rangle=|e_{j_1}\rangle\otimes\cdots\otimes|e_{j_n}\rangle$ where $J=(j_1,\ldots,j_n)$. The sequence J is called *strongly typical*[7] if the numbers $N(j|J)$ of appearance of the symbol j in J satisfy the condition

$$\left|\frac{N(j|J)}{n}-\lambda_j\right|<\delta,\quad j=1,\ldots,d,$$

and $N(j|J)=0$ if $\lambda_j=0$. Let us denote the collection of all strongly typical sequences as $B^{n,\delta}$, and let P^n be the probability distribution given by the eigenvalues λ_J. Then by the Law of Large Numbers, $\mathsf{P}^n(\mathsf{B}^{n,\delta})\to 1$ as $n\to\infty$. It is shown in Ref. 7 that the size of $B^{n,\delta}$ satisfies

$$2^{n[H(S)-\Delta_n(\delta)]}<|B^{n,\delta}|<2^{n[H(S)+\Delta_n(\delta)]},\tag{9}$$

where $H(S)=-\Sigma_{j=1}^{d}\lambda_j\log\lambda_j$, and $\lim_{\delta\to 0}\lim_{n\to\infty}\Delta_n(\delta)=0$.

For arbitrary function $f(j)$, $j=1,\ldots,d$, and $J=(j_1,\ldots,j_n)\in B^{n,\delta}$, we have

$$\left|\frac{f(j_1)+\cdots+f(j_n)}{n}-\sum_{j=1}^{d}\lambda_j f(j)\right|<\delta\max f. \tag{10}$$

In particular, any strongly typical sequence is (entropy) typical: taking $f(j)=-\log\lambda_j$ gives

$$n[H(S)-\delta_1]<-\log\lambda_J<n[H(S)+\delta_1], \tag{11}$$

where $\delta_1=\delta\max_{\lambda_j>0}(-\log\lambda_j)$. The converse is not true—not every typical sequence is strongly typical.

The strongly typical projector is defined as the following spectral projector of $S^{\otimes n}$:

$$P^{n,\delta}=\sum_{J\in B^{n,\delta}}|e_J\rangle\langle e_J|.$$

We denote $d_{n,\delta}=\dim P^{n,\delta}=|B^{n,\delta}|$ and $\overline{S}^{n,\delta}=P^{n,\delta}/d_{n,\delta}$ and we are going to prove that

$$\lim_{\delta\to 0}\lim_{n\to\infty}\frac{1}{n}H(\Psi^{\otimes n}(\overline{S}^{n,\delta}))=H(\Psi(S)) \tag{12}$$

for arbitrary channel Ψ.

We have

$$\begin{aligned}nH(\Psi(S))-H(\Psi^{\otimes n}(\overline{S}^{n,\delta}))&=H(\Psi(S)^{\otimes n})-H(\Psi^{\otimes n}(\overline{S}^{n,\delta}))\\&=H(\Psi^{\otimes n}(\overline{S}^{n,\delta})|\Psi^{\otimes n}(S^{\otimes n}))\\&\quad+\mathrm{Tr}\log\Psi(S)^{\otimes n}(\Psi^{\otimes n}(\overline{S}^{n,\delta})-\Psi(S)^{\otimes n}),\end{aligned} \tag{13}$$

where $H(\cdot|\cdot)$ is relative entropy. Strictly speaking, this formula is correct if the density operator $\Psi(S)^{\otimes n}$ is nondegenerate, which we assume for a moment. Later we shall show how the argument can be modified to the general case.

For the first term we have the estimate by the fundamental property of monotonicity of the relative entropy

$$H(\Psi^{\otimes n}(\overline{S}^{n,\delta})|\Psi^{\otimes n}(S^{\otimes n}))\leqslant H(\overline{S}^{n,\delta}|S^{\otimes n}),$$

with the right-hand side computed explicitly as

$$H(\overline{S}^{n,\delta}|S^{\otimes n})=\sum_{J\in B^{n,\delta}}\frac{1}{d_{n,\delta}}\log\frac{1}{d_{n,\delta}\lambda_J}=-\log d_{n,\delta}-\sum_{J\in B^{n,\delta}}\frac{1}{d_{n,\delta}}\log\lambda_J,$$

which is less than or equal to $n(\delta_1+\Delta_n(\delta))$ by (11) and (9), giving sufficient estimate.

By using the identity

$$\log\Psi(S)^{\otimes n}=\log\Psi(S)\otimes I\otimes\cdots\otimes I+\cdots+I\otimes\cdots\otimes I\otimes\log\Psi(S),$$

and introducing the operator $F=\Psi^*(\log\Psi(S))$ where Ψ^* is the dual channel, we can rewrite the second term as

$$\begin{aligned}&n\,\mathrm{Tr}\frac{(F\otimes I\otimes\cdots\otimes I+\cdots+I\otimes\cdots\otimes I\otimes F)}{n}(\overline{S}^{n,\delta}-S^{\otimes n})\\&=\frac{n}{d_{n,\delta}}\sum_{J\in B^{n,\delta}}\left[\frac{f(j_1)+\cdots+f(j_n)}{n}-\sum_{j=1}^{d}\lambda_j f(j)\right],\end{aligned}$$

where $f(j)=\langle e_j|F|e_j\rangle$, which is evaluated by $n\delta\max f$ via (10). This establishes (12) in the case of a nondegenerate $\Psi(S)$.

Coming back to the general case, let us denote by P_Ψ the supporting projector of $\Psi(S)$. Then the supporting projector of $\Psi(S)^{\otimes n}$ is $P_\Psi^{\otimes n}$, and the support of $\Psi^{\otimes n}(\overline{S^{n,\delta}})$ is contained in the support of $\Psi(S)^{\otimes n}=\Psi^{\otimes n}(S^{\otimes n})$, because the support of $\overline{S^{n,\delta}}$ is contained in the support of $S^{\otimes n}$. Thus the second term in (13) should be understood as

$$\mathrm{Tr}P_\Psi^{\otimes n}\log[P_\Psi^{\otimes n}\Psi(S)^{\otimes n}P_\Psi^{\otimes n}]P_\Psi^{\otimes n}(\Psi^{\otimes n}(\overline{S^{n,\delta}})-\Psi(S)^{\otimes n}),$$

where now we have log of a nondegenerate operator in $P_\Psi^{\otimes n}\mathcal{H}_A^{\otimes n}$. We can then repeat the argument with F defined as $\Psi^*(P_\Psi[\log P_\Psi\Psi(S)P_\Psi]P_\Psi)$. This fulfills the proof of (8), from which (6) follows.

Proof of the inequality:

$$C_{ea}(\Phi)\leqslant\max_{S_A} I(S_A,\Phi). \tag{14}$$

We first prove that

$$C_{ea}^{(1)}(\Phi)\leqslant\max_{S_A} I(S_A,\Phi). \tag{15}$$

The proof is a modification of that from Ref. 3, using properties of conditional quantum entropy which are known to follow from the strong subadditivity of the entropy (see, e.g., Refs. 8 and 4), rather than the strong subadditivity itself.

Let us denote $\mathcal{E}_A^i$ the encodings used by A. Let S_{AB} be the pure state initially shared by A and B. Then the state of the system AB (resp. A) after the encoding is

$$S_{AB}^i=(\mathcal{E}_A^i\otimes\mathrm{Id}_B)[S_{AB}],\quad \text{resp.}\quad S_A^i=\mathcal{E}_A^i[S_A]. \tag{16}$$

Note that the partial state of B does not change after the encoding, $S_B^i=S_B$. We are going to prove that

$$H\left(\sum_i \pi_i(\Phi\otimes\mathrm{Id}_B)[S_{AB}^i]\right)-\sum_i \pi_i H((\Phi\otimes\mathrm{Id}_B)[S_{AB}^i])\leqslant I\left(\sum_i \pi_i S_A^i;\Phi\right). \tag{17}$$

By the quantum coding theorem, the maximum of the left-hand side with respect to all possible $\pi_i,\mathcal{E}_A^i$ is just $C_{ea}^{(1)}(\Phi)$, whence (15) will follow.

By using subadditivity of quantum entropy, we can evaluate the first term on the left-hand side of (17) as

$$H\left(\sum_i \pi_i\Phi[S_A^i]\right)+H(S_B)=H\left(\Phi\left[\sum_i \pi_i S_A^i\right]\right)+\sum_i \pi_i H(S_B).$$

Here the first term already gives the output entropy from $I(\Sigma_i\pi_i S_A^i;\Phi)$. Let us proceed with evaluation of the remainder

$$\sum_i \pi_i[H(S_B)-H((\Phi\otimes\mathrm{Id}_B)[S_{AB}^i])].$$

We first show that the term in square brackets does not exceed $H(S_A^i)-H((\Phi\otimes\mathrm{Id}_{R^i})[S_{AR^i}^i])$, where R^i is the purifying (reference) system for S_A^i, and $S_{AR^i}^i$ is the purified state. To this end consider the unitary extension of the encoding $\mathcal{E}_A^i$ with the environment E_i, which is initially in

a pure state. From (16) we see that we can take $R^i=BE_i$ (after the unitary interaction which involves only AE_i). Then, again denoting with primes the states after the application of the channel Φ, we have

$$H(S_B)-H((\Phi\otimes \mathrm{Id}_B)[S^i_{AB}])=H(S_B)-H(S^i_{A'B})=-H_i(A'|B), \tag{18}$$

where the lower index i of the conditional entropy points out to the joint state $S^i_{A'B}$. Similarly

$$H(S^i_A)-H((\Phi\otimes \mathrm{Id}_{R^i})[S^i_{AR^i}])=H(S^i_{R^i})-H(S^i_{A'R^i})=-H_i(A'|R^i)=-H_i(A'|BE_i),$$

which is greater than or equal to (18) by monotonicity of the conditional entropy.

Using the concavity of the function $S_A\to H(S_A)-H((\Phi\otimes \mathrm{Id}_R)[S_{AR}])$ to be shown below, we get

$$\sum_i \pi_i[H(S^i_A)-H((\Phi\otimes \mathrm{Id}_{R^i})[S^i_{AR^i}])]\leqslant H\left(\sum_i \pi_i S^i_A\right)-H((\Phi\otimes \mathrm{Id}_R)[\hat{S}_{AR}]),$$

where $\hat{S}_{AR}$ is the state purifying $\Sigma_i\pi_i S^i_A$ with a reference system R.

To complete this proof it remains to show the above concavity. By introducing the environment E for the channel Φ, we have

$$H(S_A)-H((\Phi\otimes \mathrm{Id}_R)[S_{AR}])=H(S_R)-H(S_{A'R})=H(S_{A'E'})-H(S_{E'})=H(A'|E').$$

The conditional entropy $H(A'|E')$ is a concave function of $S_{A'E'}$. The map $S_A\to S_{A'E'}$ is affine and therefore $H(A'|E')$ is a concave function of S_A.

Applying the same argument to the channel $\Phi^{\otimes n}$ gives

$$C^{(n)}_{ea}(\Phi)\leqslant \max_{S^n_A} I(S^n_A;\Phi^{\otimes n}). \tag{19}$$

Then from subadditivity of quantum mutual information,[9] we have

$$\max_{S_{12}} I(S_{12};\Phi_1\otimes\Phi_2)=\max_{S_1} I(S_1;\Phi_1)+\max_{S_2} I(S_2;\Phi_2),$$

implying the remarkable additivity property

$$\max_{S^n_A} I(S^n_A;\Phi^{\otimes n})=n\max_{S_A} I(S_A;\Phi).$$

Therefore, finally we obtain (14).

III. RELATION BETWEEN ENTANGLEMENT-ASSISTED AND UNASSISTED CAPACITIES

The definition of $C^{(1)}_{ea}(\Phi)$ and hence of $C_{ea}(\Phi)$ can be formulated without explicit introduction of the encoding operations $\mathcal{E}^i_A$, namely,

$$C^{(1)}_{ea}(\Phi)=\max_{\pi_i,\{S^i_{AB}\}\in\Sigma_B}\left[H\left(\sum_i \pi_i(\Phi\otimes \mathrm{Id}_B)[S^i_{AB}]\right)-\sum_i \pi_i H((\Phi\otimes \mathrm{Id}_B)[S^i_{AB}])\right], \tag{20}$$

where Σ_B is the collection of families of the states $\{S^i_{AB}\}$ satisfying the condition that their partial states S^i_B do not depend on i, $S^i_B=S_B$. This follows from the next lemma.

Lemma: Let $\{S^i_{AB}\}$ be a family of the states satisfying the condition $S^i_B=S_B$. Then there exist a pure state S_{AB} and encodings $\mathcal{E}^i_A$ such that

$$S_{AB}^i=(\mathcal{E}_A^i\otimes \mathrm{Id}_B)[S_{AB}]. \tag{21}$$

Proof: For simplicity assume that S_B is nondegenerate. Then

$$S_B=\sum_{k=1}^{d}\lambda_k|e_k^B\rangle\langle e_k^B|,$$

where $\lambda_k>0$ and $\{|e_k^B\rangle\}$ is an orthonormal basis in $\mathcal{H}_B$. Let $\{|e_k^A\rangle\}$ be an orthonormal basis in $\mathcal{H}_A$. For a vector $|\psi^A\rangle=\Sigma_{k=1}^d c_k|e_k^A\rangle$ we denote $|\overline{\psi}^B\rangle=\Sigma_{k=1}^d\overline{c_k}|e_k^B\rangle$. The map $|\psi^A\rangle\to|\overline{\psi}^B\rangle$ is an anti-isomorphism of $\mathcal{H}_A$ and $\mathcal{H}_B$. Put

$$|\psi_{AB}\rangle=\sum_{k=1}^{d}\sqrt{\lambda_k}|e_k^A\rangle\otimes|e_k^B\rangle,$$

so that $S_{AB}=|\psi_{AB}\rangle\langle\psi_{AB}|$ and define encodings by the relation

$$\mathcal{E}_A^i[|\psi^A\rangle\langle\phi^A|]=\langle\overline{\psi}^B|S_B^{-1/2}S_{AB}^iS_B^{-1/2}|\overline{\phi}^B\rangle,\quad |\psi^A\rangle,|\phi^A\rangle\in\mathcal{H}_A.$$

Then one can check that $\mathcal{E}_A^i$ are indeed channels fulfilling the formula (21).

In the case S_B is degenerate, the above construction should be modified by replacing $S_B^{-1/2}S_{AB}^iS_B^{-1/2}$ in the formula above with $\sqrt{S_B^-}S_{AB}^i\sqrt{S_B^-}+P_B^0$ where S_B^- is the generalized inverse of S_B and P_B^0 is the projection onto the null subspace of S_B.

We now observe an inequality relating the asymptotic entanglement-assisted and unassisted capacities. Apparently,

$$C_{ea}^{(1)}(\Phi)\leqslant\max_{\pi_i,S_{AB}^i}\left[H\left(\sum_i\pi_i(\Phi\otimes\mathrm{Id}_B)[S_{AB}^i]\right)-\sum_i\pi_iH((\Phi\otimes\mathrm{Id}_B)[S_{AB}^i])\right], \tag{22}$$

where S_{AB}^i are already arbitrary states, not necessarily of the form (21). The quantity on the right hand side is nothing but the one-shot classical capacity $C^{(1)}(\Phi\otimes\mathrm{Id}_B)$ of the channel $\Phi\otimes\mathrm{Id}_B$. It was shown in Ref. 10 that $C^{(1)}(\Phi\otimes\mathrm{Id}_B)=C^{(1)}(\Phi)+C^{(1)}(\mathrm{Id}_B)=C^{(1)}(\Phi)+\log d$. Applying the same argument to $\Phi^{\otimes n}$ instead of Φ, we have

$$C_{ea}^{(1)}(\Phi^{\otimes n})\leqslant C^{(1)}(\Phi^{\otimes n})+n\log d.$$

Dividing by n and taking limit $n\to\infty$, we obtain

$$C_{ea}(\Phi)\leqslant C(\Phi)+\log d.$$

One can expect that a similar inequality,

$$C_{ea}(\Phi)\leqslant C^{(1)}(\Phi)+\log d,$$

holds generally for the one-shot classical capacity; if it breaks for some channel Φ, then for this channel $C^{(1)}(\Phi)<C(\Phi)$, which would imply a negative answer to the long-standing question concerning additivity of the classical capacity.

It is not difficult to check that the inequality indeed holds for all unital qubit channels and for d-depolarizing channel

$$\Phi[\mathcal{S}]=(1-p)S+p\frac{I}{d}\mathrm{Tr}S. \tag{23}$$

Here $\dim\mathcal{H}=d$ and the parameter p should lie in the range $0\leqslant p\leqslant d^2/(d^2-1)$, as can be seen from the Kraus representation

$$\Phi[\mathcal{S}]=\left(1-p\frac{d^2-1}{d^2}\right)S+p\frac{1}{d^2}\sum_{\alpha,\beta\neq d}W_{\alpha\beta}SW_{\alpha\beta}^{*}, \tag{24}$$

with $W_{\alpha\beta};\alpha,\beta=1,\ldots,d$ built upon an arbitrary orthonormal basis in $\mathcal{H}$.

The quantity $C_{ea}(\Phi)$ can be computed by using unitary covariance of the depolarizing channel and concavity of the function $S\rightarrow I(S;\Phi)$. It follows that it achieves the maximum at the chaotic state $\overline{S}=I/d$. We have $H(\overline{S})=H(\Phi[\overline{S}])=\log d$. The entropy exchange $H(\overline{S};\Phi)$ can be computed by as the entropy of the matrix $[\mathrm{Tr}\overline{S}A_{\alpha\beta}^{*}A_{\alpha\beta}]$, where $A_{\alpha\beta}=(\sqrt{p}/d)W_{\alpha\beta};\alpha,\beta\neq d;A_{dd}=\sqrt{1-p\,[(d^2-1)/d^2]}\,I$ are the Kraus operators from the representation (24). We thus obtain

$$C_{ea}(\Phi)=\log d^2+\left(1-p\frac{d^2-1}{d^2}\right)\log\left(1-p\frac{d^2-1}{d^2}\right)+p\frac{d^2-1}{d^2}\log\frac{p}{d^2}. \tag{25}$$

This should be compared with the unassisted classical capacity, which is equal to

$$C^{(1)}(\Phi)=\log d+\left(1-p\frac{d-1}{d}\right)\log\left(1-p\frac{d-1}{d}\right)+p\frac{d-1}{d}\log\frac{p}{d}, \tag{26}$$

and is achieved for an ensemble of equiprobable pure states taken from an orthonormal basis in $\mathcal{H}$. One then sees as in Ref. 2 that $C_{ea}(\Phi)/C^{(1)}(\Phi)\rightarrow d+1$ in the limit of strong noise $p\rightarrow 1$. (Note that both capacities tend to zero!)

Moreover, taking the maximal possible value $p=d^2/(d^2-1,)$ we obtain

$$C_{ea}=\log\frac{d^2}{d^2-1},$$

$$C^{(1)}=\frac{1}{d+1}\log\frac{d}{d+1}+\frac{d}{d+1}\log\frac{d^2}{d^2-1}.$$

Here the ratio $C_{ea}/C^{(1)}$ monotonically increases from the value 5.0798 for $d=2$, approaching tightly the asymptotic line $2(d+1)$ as d grows to infinity.

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Additivity of the classical capacity of entanglement-breaking quantum channels

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We show that for the tensor product of an entanglement-breaking quantum channel with an arbitrary quantum channel, both the minimum entropy of an output of the channel and the Holevo–Schumacher–Westmoreland capacity are additive. In addition, for the tensor product of two arbitrary quantum channels, we give a bound involving entanglement of formation for the amount of subadditivity (for minimum entropy output) or superadditivity (for classical capacity) that can occur. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1498000]

One of the more important open questions of quantum information theory is the determination of the capacity of a quantum channel for carrying classical information. This question has been only partially resolved. If entanglement between multiple inputs to the channel is not allowed, a formula for the classical capacity of a quantum channel has indeed been discovered.[1,2] This capacity formula for a quantum channel Ψ is

$$\chi^*(\Psi)=\max_{p_i,\rho_i} H\left(\sum_i \Psi(p_i\rho_i)\right)-\sum_i p_i H(\Psi(\rho_i)), \tag{1}$$

where H is the von Neumann entropy $H(\rho)=-\mathrm{Tr}\,\rho\log\rho$, and where the maximization is over probability distributions p_i on density matrices ρ_i over the input space of the channel. This maximum can be attained because we need at most d^2 density matrices ρ_i to achieve any attainable value of

$$\chi(\{p_i,\rho_i\})=H\left(\sum_i \Psi(p_i\rho_i)\right)-\sum_i p_i H(\Psi(\rho_i)) \tag{2}$$

and are thus maximizing over a compact space. The general capacity of a quantum channel Ψ, without feedback or prior entanglement between sender and receiver, but possibly using entangled inputs, is

$$C(\Psi)=\lim_{n\to\infty}\frac{1}{n}\chi^*(\Psi^{\otimes n}), \tag{3}$$

i.e., the limit for large n of the capacity when we permit the input to be entangled over blocks of n channel uses. This limit can be shown to exist because χ^* satisfies the superadditivity condition

$$\chi^*(\Psi\otimes\Phi)\geqslant\chi^*(\Psi)+\chi^*(\Phi). \tag{4}$$

It is conjectured that equality holds, i.e., that χ^* is additive, in which case χ^* would give the classical capacity of a quantum channel without feedback. Substantial work has been done on this conjecture,[3,4] and it has been proven for several special cases. In particular, it has been proven

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when one of the channels is the identity channel,[4,5] when one of the channels is what A. S. Holevo calls a c-q or q-c channel (these terms will be defined later),[6,7] and when one of the channels is a unital qubit channel.[8]

We will prove additivity for the special case where one of the two channels is entanglement breaking. Entanglement breaking channels are channels which destroy entanglement with other quantum systems. That is, when the input state is entangled between the input space $\mathcal{H}_{\text{in}}$ and another quantum system $\mathcal{H}_{\text{ref}}$, the output of the channel is no longer entangled with the system $\mathcal{H}_{\text{ref}}$. Both c-q and q-c channels are special cases of entanglement breaking channels. A c-q channel is a channel which can be expressed by the composition of a complete von Neumann measurement on the input space followed by an arbitrary completely positive trace-preserving (CPT) map. A q-c channel can be expressed as the composition of a CPT map followed by a complete von Neumann measurement on the output space. Stated more intuitively, for c-q maps, the input can be treated as being classical, and for q-c maps, the output can be taken to be classical. In either case, the von Neumann measurement eliminates any entanglement between the input space and another system, so c-q and q-c maps are both special cases of entanglement breaking channels. In a conversation with the author, Michal Horodecki[9] gave a simple proof that any entanglement breaking channel can be expressed as a q-c-q channel; that is, the composition of a CPT operator followed by a complete von Neumann measurement followed by another CPT operator. (See also Ref. 10 for details of this proof.) As a consequence, the action of an entanglement breaking channel Φ on a state ρ can always be written in the following form introduced by Holevo:[6]

$$\Phi(\rho)=\sum_i \operatorname{Tr}(X_i\rho)\,\theta_i \tag{5}$$

where $\{X_i\}$ form a general POVM and $\{\theta_i\}$ are arbitrary states. For a c-q map, $X_i=|i\rangle\langle i|$ where $|i\rangle$ form an orthonormal basis, and for a q-c map $\theta_i=|i\rangle\langle i|$.

The additivity problem for capacity is closely related to another additivity problem, that of the minimum entropy output of a channel.[11] For the case of entanglement breaking channels, we first found the additivity proof for the minimum entropy output, and then discovered a straightforward way to extend this additivity proof to cover the classical capacity. In this article, we first give the proof for additivity of minimum entropy output, as this proof contains the important ideas for the capacity proof, but has significantly fewer technicalities.

Theorem 1: *For an arbitrary quantum channel Ψ and an entanglement breaking channel Φ*

$$\min_{\rho_{AB}} H((\Psi\otimes\Phi)(\rho_{AB}))=\min_{\rho_A} H(\Psi(\rho_A))+\min_{\rho_B} H(\Phi(\rho_B)). \tag{6}$$

Proof: The left-hand side is clearly at most the right-hand side, as can be seen by choosing $\rho_{AB}=\rho_A\otimes\rho_B$. We would like to show that it is at least the right-hand side. We use the strong subadditivity property of von Neumann entropy.[12] Consider the minimum obtainable value of $H((\Psi\otimes\Phi)(\rho_{AB}))$. Because Φ is entanglement breaking,

$$(I\otimes\Phi)(\rho_{AB})=\sum_j q_j|a_j\rangle\langle a_j|\otimes|b_j\rangle\langle b_j| \tag{7}$$

for some q_j, $|a_j\rangle\in\mathcal{H}_A$ and $|b_j\rangle\in\mathcal{H}_B$. Now, we apply to the state

$$\sigma_{ABC}=\sum_j q_j\Psi(|a_j\rangle\langle a_j|)\otimes|b_j\rangle\langle b_j|\otimes|j\rangle\langle j| \tag{8}$$

the property of strong subadditivity in the form

$$H(\sigma_{AB})\geqslant H(\sigma_{ABC})-H(\sigma_{BC})+H(\sigma_B). \tag{9}$$

We have

$$\sigma_{AB}=\sum_j q_j\Psi(|a_j\rangle\langle a_j|)\otimes|b_j\rangle\langle b_j|=(\Psi\otimes\Phi)(\rho_{AB}), \tag{10}$$

the quantity for the entropy of which we would like a lower bound. Now, note that

$$H(\sigma_{ABC})-H(\sigma_{BC})=H(\sigma_{AC})-H(\sigma_C)=\sum_j q_j H(\Psi(|a_j\rangle\langle a_j|)). \tag{11}$$

The first equality above follows from the facts that the $|j\rangle$ form an orthonormal set and ρ_B is in a pure state, so that $H(\sigma_{ABC})=H(\sigma_{AC})$ and $H(\sigma_{BC})=H(\sigma_C)$. The second equality follows from the chain rule for entropy, namely,

$$H\left(\sum_j q_j\gamma_j\otimes|j\rangle\langle j|\right)-\sum_j H(q_j|j\rangle\langle j|)=\sum_j q_j H(\gamma_j), \tag{12}$$

for a probability distribution q_j, orthonormal states $|j\rangle$, and arbitrary density matrices γ_j. Now, note that

$$\sigma_B=\sum_j q_j|b_j\rangle\langle b_j|=\mathrm{Tr}_A(I\otimes\Phi)(\rho_{AB})=\Phi(\mathrm{Tr}_A\rho_{AB}). \tag{13}$$

Putting the above equalities together, we see that

$$H((\Psi\otimes\Phi)(\rho_{AB}))\geqslant\sum_j q_j H(\Psi(|a_j\rangle\langle a_j|))+H(\Phi(\mathrm{Tr}_A\rho_{AB})). \tag{14}$$

Since $\Sigma_j q_j=1$, the right-hand side is clearly at least the sum of the minimum output entropies of Ψ and of Φ. We have thus shown that the minimum output entropy is additive for the tensor product of two channels if one of the channels is an entanglement breaking channel. □

We now prove the corresponding additivity result for the Holevo–Schumacher–Westmoreland capacity χ^*; recall

$$\chi^*(\Psi)=\max_{p_i,\rho_i} H\left(\Psi\left(\sum_i p_i\rho_i\right)\right)-\sum_i p_i H(\Psi(\rho_i)) \tag{15}$$

over probability distributions p_i and density matrices ρ_i.

Theorem 2: *For an arbitrary quantum channel Ψ and an entanglement breaking channel Φ,*

$$\chi^*(\Psi\otimes\Phi)=\chi^*(\Psi)+\chi^*(\Phi). \tag{16}$$

Proof: The capacity χ^* is composed of two terms. We will be treating these two terms separately. For the second term, additivity is shown in essentially the same way as in the proof of additivity for minimum entropy, and, for the first term, additivity follows from the subadditivity of von Neumann entropy.

Again, we assume that we have an arbitrary quantum channel Ψ and an entanglement breaking channel Φ. We use strong subadditivity. Consider the optimal signal states for $\Psi\otimes\Phi$, i.e., the p_i and ρ_i such that

$$\chi^*(\Psi\otimes\Phi)=H((\Psi\otimes\Phi)(\rho))-\sum p_i H((\Psi\otimes\Phi)(\rho_i)), \tag{17}$$

where $\rho=\Sigma p_i\rho_i$. Let us consider the state $(I\otimes\Phi)(\rho_i)$. Because Φ is an entanglement breaking map, this state is separable, and so

$$(I\otimes\Phi)(\rho_i)=\sum_j q_{ij}|a_{ij}\rangle\langle a_{ij}|\otimes|b_{ij}\rangle\langle b_{ij}| \tag{18}$$

for some q_{ij}, $|a_{ij}\rangle$, $|b_{ij}\rangle$. Now, we apply strong subadditivity to the state

$$\sigma_{ABC}=\sum_j q_{ij}\Psi(|a_{ij}\rangle\langle a_{ij}|)\otimes|b_{ij}\rangle\langle b_{ij}|\otimes|j\rangle\langle j|. \tag{19}$$

To simplify notation, we let the dependence of σ on i be implicit. Again, we apply strong subadditivity in the form

$$H(\sigma_{AB})\geqslant H(\sigma_{ABC})-H(\sigma_{BC})+H(\sigma_B). \tag{20}$$

As before,

$$H(\sigma_{AB})=H((\Psi\otimes\Phi)(\rho_i)). \tag{21}$$

We also have that

$$H(\sigma_B)=H(\Phi(\mathrm{Tr}_A\rho_i)) \tag{22}$$

and

$$H(\sigma_{ABC})-H(\sigma_{BC})=\sum_j q_{ij}H(\Psi(|a_{ij}\rangle\langle a_{ij}|)). \tag{23}$$

We let $|a_{ij}\rangle\langle a_{ij}|=\tau_{ij}$. Then $\mathrm{Tr}_B\rho_i=\Sigma q_{ij}\tau_{ij}$. Combining the terms, we observe

$$H((\Psi\otimes\Phi)(\rho_i))\geqslant\sum_j q_{ij}H(\Psi(\tau_{ij}))+H(\Phi(\mathrm{Tr}_A\rho_i)). \tag{24}$$

Now, let us sum over all the states ρ_i. We obtain

$$\sum_i p_iH((\Psi\otimes\Phi)(\rho_i))\geqslant\sum_{i,j} p_iq_{ij}H(\Psi(\tau_{ij}))+\sum_i p_iH(\Phi(\mathrm{Tr}_A\rho_i)). \tag{25}$$

Using subadditivity of von Neumann entropy and the above inequality (25), we get that

$$\begin{aligned}\chi^*(\Psi\otimes\Phi)&=H((\Psi\otimes\Phi)(\rho))-\sum_i p_iH((\Psi\otimes\Phi)(\rho_i))\\&\leqslant H(\Psi(\mathrm{Tr}_B\rho))+H(\Phi(\mathrm{Tr}_A\rho))-\sum_{i,j} p_iq_{ij}H(\Psi(\tau_{ij}))-\sum_i p_iH(\Phi(\mathrm{Tr}_A\rho_i)).\end{aligned} \tag{26}$$

However, since

$$\sum_{i,j} p_iq_{ij}\tau_{ij}=\sum_i p_i\mathrm{Tr}_B\rho_i=\mathrm{Tr}_B\rho \quad\text{and}\quad \sum_i p_i\mathrm{Tr}_A\rho_i=\mathrm{Tr}_A\rho, \tag{27}$$

we see that

$$\chi^*(\Psi\otimes\Phi)\leqslant\chi^*(\Psi)+\chi^*(\Phi). \tag{28}$$

As the opposite inequality is easy, we have additivity of χ^* for entanglement breaking channels.□

We finally give a bound on the amount of superadditivity for general channels. For this, we need to define the entanglement of formation of a bipartite state. This is another quantity that is conjectured to be additive, but for which additivity has not been proved. Entanglement of formation for a bipartite state ρ_{AB} is defined

$$E_F(\rho_{AB}) = \min_{\substack{p_i,\rho_i \\ \Sigma_i p_i \rho_i = \rho_{AB}}} \sum p_i H(\mathrm{Tr}_A \rho_i), \tag{29}$$

where the minimization is over probability distributions p_i on rank-one density matrices ρ_i such that $\Sigma_i p_i \rho_i = \rho_{AB}$. The theorem is

Theorem 3: *Suppose we have two quantum channels, i.e., completely positive trace preserving maps, Ψ and Φ. Then*

$$\min_{\rho_{AB}} H((\Psi\otimes\Phi)(\rho_{AB})) \geqslant \min_{\rho_A} H(\Psi(\rho_A)) + \min_{\rho_B} H(\Phi(\rho_B)) - \max_{\rho_{AB}} E_F((I\otimes\Phi)(\rho_{AB})) \tag{30}$$

and

$$\chi^*(\Psi\otimes\Phi) \leqslant \chi^*(\Psi) + \chi^*(\Phi) + \max_{\rho_{AB}} E_F((I\otimes\Phi)(\rho_{AB})). \tag{31}$$

Note that the formulation of the theorem is asymmetric with respect to Ψ and Φ. Thus, to bound the amount of sub- or superadditivity, one can use either the entanglement of formation of $(I\otimes\Phi)(\rho_{AB})$ or of $(\Psi\otimes I)(\rho_{AB})$, whichever is smaller.

Proof: We first give the proof of the first part of Theorem 3 Let

$$(I\otimes\Phi)(\rho_{AB}) = \sum_i q_i \nu_i \tag{32}$$

be the decomposition of $(I\otimes\Phi)(\rho_{AB})$ into pure states ν_i that minimizes entanglement of formation, i.e., so that $\Sigma_j q_j H(\mathrm{Tr}_A \nu_j)$ is minimum. Now, we consider

$$\sigma_{ABC} = \sum_j q_j (\Psi\otimes I)(\nu_j)\otimes |j\rangle\langle j| \tag{33}$$

and apply strong subadditivity to this state. We obtain

$$H(\sigma_{AB}) \geqslant (H(\sigma_{ABC}) - H(\sigma_C)) + (H(\sigma_B)) - (H(\sigma_{BC}) - H(\sigma_C)). \tag{34}$$

As in (10), we have

$$H(\sigma_{AB}) = H((\Psi\otimes\Phi)(\rho_{AB})). \tag{35}$$

Similar to (13), we get

$$H(\sigma_B) = H\left(\sum_j q_j \mathrm{Tr}_A \nu_j\right) = H(\Phi(\mathrm{Tr}_A \rho_{AB})). \tag{36}$$

Furthermore, the choice of ν_j and the definition of E_F give

$$H(\sigma_{BC}) - H(\sigma_C) = E_F((I\otimes\Phi)(\rho_{AB})). \tag{37}$$

Finally, application of the entropy chain rule (12) gives

$$H(\sigma_{ABC})-H(\sigma_C)=\sum_j q_j H((\Psi\otimes I)(\nu_j)). \tag{38}$$

The expression (36) is bounded below by $\min_\rho H(\Phi(\rho))$. The second expression (37) is bounded above by $\max_\rho E_F((I\otimes\Phi)(\rho))$. The third expression (38) is bounded below by $\min_\rho H((\Psi\otimes I)(\rho))$, which is known to equal $\min_\rho H(\Psi(\rho))$. Combining these three expressions give the first part of Theorem 3.

To prove the second part of the theorem, (38) must be replaced by

$$H(\sigma_{ABC})-H(\sigma_C)\geqslant\sum_{jk} q_j r_{jk} H(\Psi(|v_{jk}\rangle\langle v_{jk}|)) \tag{39}$$

for states $|v_{jk}\rangle$ and probabilities $q_j r_{jk}$ such that

$$\sum_{j,k} q_j r_{jk}|v_{jk}\rangle\langle v_{jk}|=\mathrm{Tr}_B\nu_j. \tag{40}$$

We then consider the signal states ρ_i and the associated probabilities p_i which give the value of $\chi^*(\Psi\otimes\Phi)$ in Eq. (1), and let $\Sigma_i p_i\rho_i=\rho$. We now use expressions (36), (37), and (39) with ρ_i in the place of ρ_{AB}. Combining these three expressions yields

$$H((\Psi\otimes\Phi)(\rho_i))\geqslant H(\Phi(\mathrm{Tr}_A\rho_i))+\sum_{j,k} q_{ij}r_{ijk}H(\Psi(|v_{ijk}\rangle\langle v_{ijk}|))-E_F((I\otimes\Phi)(\rho_i)). \tag{41}$$

The second part of Theorem 3 then follows in a way entirely analogous to the proof of Theorem 2. We use the equalities

$$\mathrm{Tr}_B\rho=\sum_i p_i\mathrm{Tr}_A\rho_i \tag{42}$$

and

$$\mathrm{Tr}_A\rho=\sum_{i,j,k} p_i q_{ij} r_{ijk}|v_{ijk}\rangle\langle v_{ijk}|, \tag{43}$$

and expand $\chi^*(\Psi\otimes\Phi)$ similarly to Eq. (26) to obtain Eq. (31).

We still must prove the inequality (39). The left-hand side of (39) is

$$\sum_j q_j H((\Psi\otimes I)(\nu_j)). \tag{44}$$

Now, ν_j is a purification of $\mathrm{Tr}_B\nu_j$, and $H((\Psi\otimes I)(\nu_j))=H((\Psi\otimes I)(\tau))$ for any quantum state τ which is a purification of $\sigma_j=\mathrm{Tr}_B\nu_j$. Let $\sigma_j=\Sigma_k q_{jk}|v_{jk}\rangle\langle v_{jk}|$ be the eigenvector decomposition of σ_j. A different purification is

$$\tau_j=\left(\sum_k q_{jk}|v_{jk}\rangle\otimes|k\rangle\otimes|k\rangle\right)\left(\sum_k q_{jk}\langle v_{jk}|\otimes\langle k|\otimes\langle k|\right). \tag{45}$$

It suffices to show that

$$H((\Psi\otimes I)(\tau_j))\geqslant H(\mathrm{Tr}_3(\Psi\otimes I)(\tau_j))-H(\mathrm{Tr}_{12}(\Psi\otimes I)(\tau_j)) \tag{46}$$

as the first term in the above equation is $H((\Psi\otimes I)(\nu_j))$, the second is $H(\{q_{jk}\}_k)+\Sigma_k q_{jk}H(\Psi(|v_{jk}\rangle\langle v_{jk}|))$, and the third is $H(\{q_{jk}\}_k)$. However, the above equation follows from

the inequality $H(\rho_{34}) \geqslant H(\rho_3) - H(\rho_4)$, which is a consquence (after another purification) of the subadditivity property of entropy.[13] □

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Scalable programmable quantum gates and a new aspect of the additivity problem for the classical capacity of quantum channels

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We consider two apparently separated problems: in the first part of the article we study the concept of a *scalable (approximate) programmable quantum gate* (SPQG). These are special (approximate) programmable quantum gates, with nice properties that could have implications on the theory of universal computation. Unfortunately, as we prove, such objects do not exist in the domain of usual quantum theory. In the second part the problem of noisy dense coding (and generalizations) is addressed. We observe that the additivity problem for the classical capacity obtained is of apparently greater generality than for the usual quantum channel (completely positive maps): i.e., the latter occurs as a special case of the former, but, as we shall argue with the help of the nonexistence result of the first part, the former cannot be reduced to an instance of the latter. We conclude by suggesting that the additivity problem for the classical capacity of quantum channels, as posed until now, may conceptually not be in its appropriate generality. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1498489]

I. INTRODUCTION

The present article brings together two subjects in the realm of quantum information theory that might at first glance seem far apart: the theory of universal computation in a quantum computer, and noise resistant coding of classical information in quantum channels.

The former deals with implementing arbitrary transformation of the (quantum) data in the memory of a computer by a sequence of commands (a *program*) that are themselves presented to the machine as data. From the first days of the theory of quantum computation this issue was of central importance, as a tool to show that there is essentially only one quantum Turing machine, and to parallel Turing's insight of the existence of universal classical machines (see Refs. 1 and 2). A great deal of work has been invested into finding small universal sets of ''quantum gates,'' acting on only a few qubits at a time, so that by concatenation any multi-qubit unitary can be approximated arbitrarily.[3–7] This concatenation (represented as a certain directed graph with labeled nodes) can be given to a machine as classical data, which then interprets it as a series of controlled actions on the quantum data.

The universality problem was studied abstractly by Nielsen and Chuang[8] in the notion of *programmable quantum gate* (PQG), where one allows *arbitrary quantum* data for a program, their results being further developed by Vidal, Masanes, and Cirac.[9,10] We review these studies, as far as they are relevant for the present purpose, in Sec. II. Then, in Sec. III, the notion of *scalability* is introduced, which captures the idea that a sufficiently powerful universal programmable quantum gate might give a universal gate if tensored with itself and fed with entangled programs. Unfortunately, it turns out that such objects do not exist, and we point out some implications for the general theory of universal computation.

Then, we switch to the apparently completely distinct problem of quantum channel coding of

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classical data: a quantum channel usually is modeled by a completely positive, trace preserving, linear map $\varphi:\mathcal{B}(\mathcal{H}_1)\to\mathcal{B}(\mathcal{H}_2)$. We may use this channel to communicate by choosing states σ_i on $\mathcal{H}_1$ at the sender's side, the receiver getting $\varphi(\sigma_i)$. By the result of Holevo[11] and Schumacher and Westmoreland[12] the maximum rate at which classical information can be transmitted asymptotically reliably (the *capacity*) is given by

$$C(\varphi)=\max_{\{\sigma_i,p_i\}} I(p;\varphi(\sigma)), \tag{1}$$

with the *Holevo mutual information*

$$I(p;\varphi(\sigma))=H\left(\sum_i p_i\varphi(\sigma_i)\right)-\sum_i p_i H(\varphi(\sigma_i)),$$

H being the von Neumann entropy on density operators. This holds when in the block coding (implicit in the statement) for $\varphi^{\otimes n}$ one is restricted to using product states $\sigma_{i_1}\otimes\cdots\otimes\sigma_{i_n}$. Strictly speaking, we should write "sup" over *all* probability distributions p on states, and integrals instead of finite sums. However, we restrict our attention to finite dimensional spaces, and there it is possible to show that the supremum is achieved by a finitely supported measure p (see Ref. 12).

Unfortunately it is unknown whether it is sufficient to restrict coding to product states. It would be if the additivity conjecture

$$C(\varphi\otimes\vartheta)=C(\varphi)+C(\vartheta)$$

is true. To show this one would need to consider input state ensembles with entangled states, and prove that the corresponding Holevo information can be achieved by an ensemble without entangled states, or, more directly, that a code using entangled states can be modified to an equally good code (in terms of error probability and rate) without entangled states. Neither of these has been achieved in generality so far, though there have been advances recently: see Refs. 13–17.

In Sec. IV we present an example of a special classical–quantum channel as a case study: dense coding in the presence of noisy entanglement, and by use of a general quantum channel, in particular a noiseless one. Here, coding is done by selecting not a state of a system, to be sent down the channel, but by selecting an operation on a given state. This is a more general concept of coding, as we demonstrate in Sec. V. It appears that the coding of such a channel can be approximated by programmable quantum gates (in this sense the new model is a special case of the old one), but that the parallel use of these systems cannot: there will always be actions on the combined space that cannot be mimicked by entangled inputs to the PQG-augmented channel.

We conclude with the suggestion that the additivity problem for classical capacities of quantum channels has not been posed until now in its appropriate generality.

II. PROGRAMMABLE QUANTUM GATES

In classical computers there is no fundamental distinction in a univeral machine's memory between data and program. In fact, a program may modify itself during the computation (a feature considered essential by von Neumann when he designed his computer model). To which extent can a quantum computer memory be used to modify other parts of the memory in a programlike fashion? More precisely (following Ref. 8), assume that a unitary process G acts on $\mathcal{H}_D\otimes\mathcal{H}_P$, with the *data register* $\mathcal{H}_D$ and the *program register* $\mathcal{H}_P$:

$$|\zeta\rangle\otimes|\psi\rangle\mapsto G(|\zeta\rangle\otimes|\psi\rangle).$$

We call $|\psi\rangle$ a *program* if it has the property that

$$\forall|\zeta\rangle\quad G(|\zeta\rangle\otimes|\psi\rangle)=U_\psi|\zeta\rangle\otimes|\psi'\rangle. \tag{2}$$

Note that—though *a priori* $|\psi'\rangle$ could also depend on $|\zeta\rangle$—for $|\zeta_1\rangle$, $|\zeta_2\rangle \in \mathcal{H}_D$ the corresponding $|\psi_1'\rangle$, $|\psi_2'\rangle$ are linearly dependent:

$$G((\alpha|\zeta_1\rangle+\beta|\zeta_2\rangle)\otimes|\psi\rangle)=\alpha U_\psi|\zeta_1\rangle\otimes|\psi_1'\rangle+\beta U_\psi|\zeta_2\rangle\otimes|\psi_2'\rangle,$$

which generally is entangled unless $|\psi_1'\rangle \in \mathbb{C}|\psi_2'\rangle$.

(We thus *can* have a global phase—which we shall systematically ignore.) Henceforth, we assume that $|\psi'\rangle$ is independent of $|\zeta\rangle$, just as Eq. (2) suggests. It follows that U_ψ is unitary, which is encoded (via G) in the program $|\psi\rangle$. How many unitaries can be implemented in this way?

Theorem 1 (Nielsen and Chuang[8]): *If* $U_{\psi_1} \neq \gamma U_{\psi_2}$ *for all* $\gamma \in \mathbb{C}$, *then* $|\psi_1\rangle \perp |\psi_2\rangle$.

Proof: Let

$$G(|\zeta\rangle\otimes|\psi_1\rangle)=U_{\psi_1}|\zeta\rangle\otimes|\psi_1'\rangle,$$

$$G(|\zeta\rangle\otimes|\psi_2\rangle)=U_{\psi_2}|\zeta\rangle\otimes|\psi_2'\rangle.$$

Hence

$$\langle\psi_1|\psi_2\rangle=(\langle\zeta|\otimes\langle\psi_1|)G^*G(|\zeta\rangle\otimes|\psi_2\rangle)=\langle\psi_1'|\psi_2'\rangle\langle\zeta|U_{\psi_1}^*U_{\psi_2}|\zeta\rangle.$$

If $\langle\psi_1'|\psi_2'\rangle=0$, also $\langle\psi_1|\psi_2\rangle=0$, and we are done. Else $\langle\zeta|U_{\psi_1}^*U_{\psi_2}|\zeta\rangle$ is a constant, independent of $|\zeta\rangle$, hence $U_{\psi_1}^*U_{\psi_2}=\gamma\mathbb{1}$, contradicting the assumption. □

As a consequence we have only at most $\dim\mathcal{H}_P$ many essentially different programs. There is no way to encode all possible unitaries on $\mathcal{H}_D$ by "quantum code" unless we allow for an infinite-dimensional $\mathcal{H}_P$.

We have already in the Introduction pointed out that it is well possible to implement arbitarily good approximations to all unitaries (at the cost of ever increasing $\dim\mathcal{H}_P$). In Ref. 8, however, there was proposed a more interesting solution: a *probabilistic* programmable quantum gate, i.e., an encoding of unitaries in a state, and a process that performs the encoded unitary with some probability, and otherwise fails (does something else): the process is able to report which of the two events happened. This result was refined in subsequent work of Vidal, Masanes, and Cirac,[9,10] but we will not follow this line of research here.

To fix notions, let us define our concept of approximation: a (unitary) gate G on $\mathcal{H}_D\otimes\mathcal{H}_P$ is said to be *ϵ-approximating* if for every unitary U on $\mathcal{H}_D$ there is a state vector $|\psi\rangle \in \mathcal{H}_P$ (it is easily seen that pure state program register contents suffice) such that

$$\forall|\zeta\rangle \quad \|U|\zeta\rangle\langle\zeta|U^*-\mathrm{Tr}_{\mathcal{H}_P}(G(|\zeta\rangle\langle\zeta|\otimes|\psi\rangle\langle\psi|)G^*)\|_1\leq\epsilon.$$

Of course there are ϵ-approximating gates such that the approximating induced maps

$$\Gamma_\psi(\sigma)=\mathrm{Tr}_{\mathcal{H}_P}(G(\sigma\otimes|\psi\rangle\langle\psi|)G^*)$$

in the above equation all may be chosen unitary, but the present formulation has the appropriate generality for the nonexistence theorem of the following section.

A sequence $(G^{(n)})_{n\in\mathbb{N}}$ of programmable quantum gates $G^{(n)}$ on $\mathcal{H}_{P_n}\otimes\mathcal{H}_D$ is called *approximating for* $\mathcal{H}_D$ if each $G^{(n)}$ is ϵ_n-approximating, with $\epsilon_n\to 0$ for $n\to\infty$.

III. SCALABLE PROGRAMMABLE QUANTUM GATES

Given $\epsilon>0$ we can devise ϵ-approximating quantum gates G_1 and G_2 for given data registers $\mathcal{H}_{D_1}$ and $\mathcal{H}_{D_2}$, respectively, by allowing for sufficiently large program registers.

Programming, however, is about making data act together in a potentially unlimited number of registers. In general, to approximately perform an arbitary unitary on $\mathcal{H}_{D_1}\otimes\mathcal{H}_{D_2}$ it is necessary to define a new quantum gate G.

This motivates us to the following definition: we say that two sequences $(G_1^{(n)})_{n\in\mathbb{N}}$ and $(G_2^{(n)})_{n\in\mathbb{N}}$ of programmable quantum gates that are approximating for $\mathcal{H}_{D_1}$ and $\mathcal{H}_{D_2}$, respectively, are *scalable*, if the sequence $(G_1^{(n)}\otimes G_2^{(n)})_{n\in\mathbb{N}}$ is approximating for $\mathcal{H}_{D_1}\otimes\mathcal{H}_{D_2}$.

Such approximating gate sequences thus spare us the task to find and implement new programmable quantum gates when we scale up our computing system.

Unfortunately, nature does not supply us with such objects:

Theorem 2: *Let $(G_1^{(n)})_{n\in\mathbb{N}}$ and $(G_2^{(n)})_{n\in\mathbb{N}}$ be sequences of programmable quantum gates with fixed data registers $\mathcal{H}_{D_1}$ and $\mathcal{H}_{D_2}$, respectively. Assume that the unitary U on $\mathcal{H}_{D_1}\otimes\mathcal{H}_{D_2}$ is approximated arbitarily close by programs $\psi^{(n)}\in\mathcal{H}_{P_{1n}}\otimes\mathcal{H}_{P_{2n}}$, i.e.,*

$$\mathrm{Tr}_{\mathcal{H}_{P_{1n}}\otimes\mathcal{H}_{P_{2n}}}[G_1^{(n)}\otimes G_2^{(n)}(|\zeta\rangle\langle\zeta|\otimes|\psi^{(n)}\rangle\langle\psi^{(n)}|)G_1^{(n)*}\otimes G_2^{(n)*}]\to U|\zeta\rangle\langle\zeta|U^* \tag{3}$$

as $n\to\infty$. Then U is not entangling, i.e., it is of the form $U=U_1\otimes U_2$.

Proof: Consider the expressions of Eq. (3) for data of the form $|\zeta\rangle=|\zeta_1\rangle\otimes|\zeta_2\rangle$. The first claim is that the reduced state of the left hand side on $\mathcal{H}_{D_1}$ is independent of ζ_2: this becomes clear by first tracing out $\mathcal{H}_{D_2}\otimes\mathcal{H}_{P_{2n}}$ and then $\mathcal{H}_{P_{2n}}$. Then the same applies to the limit at the right hand side.

So, for fixed $|\zeta_1\rangle$ we have

$$\mathrm{Tr}_{\mathcal{H}_{D_2}}U(|\zeta_1\rangle\langle\zeta_1|\otimes|\zeta_2\rangle\langle\zeta_2|)U^*=\rho_0=\sum_i \lambda_i|e_i\rangle\langle e_i|, \tag{4}$$

with a constant state ρ_0 (that we wrote in diagonalized form), regardless of $|\zeta_2\rangle$.

Now assume that U is entangling, and choose $|\zeta_1\rangle$ such that there exists $|\zeta_2\rangle$ so that $U|\zeta_1\rangle\otimes|\zeta_2\rangle$ is entangled. Then ρ_0 is mixed, and its diagonalization contains at least two terms. We shall derive a contradiction from this: first observe that for arbitrary $|\zeta_2\rangle$ the state $U|\zeta_1\rangle\otimes|\zeta_2\rangle$ is a purification of ρ_0, hence, by Eq. (4) there exists an orthonormal basis $\{|f_i\rangle\}$ of $\mathcal{H}_{D_2}$ such that

$$U|\zeta_1\rangle\otimes|\zeta_2\rangle=\sum_i \sqrt{\lambda_i}|e_i\rangle\otimes|f_i\rangle.$$

For $|\zeta_2'\rangle$ orthogonal to $|\zeta_2\rangle$ there is another such basis $\{|f_i'\rangle\}$ with

$$U|\zeta_1\rangle\otimes|\zeta_2'\rangle=\sum_i \sqrt{\lambda_i}|e_i\rangle\otimes|f_i'\rangle.$$

By linearity we get thus

$$U|\zeta_1\rangle\otimes(\alpha|\zeta_2\rangle+\beta|\zeta_2'\rangle)=\sum_i \sqrt{\lambda_i}|e_i\rangle\otimes(\alpha|f_i\rangle+\beta|f_i'\rangle),$$

for $|\alpha|^2+|\beta|^2=1$. This again must be a purification of ρ_0, so the resulting $\{\alpha|f_i\rangle+\beta|f_i'\rangle\}$ must form an orthonormal basis: this leads quickly to the condition (for all i, j)

$$\overline{\alpha}\beta\langle f_i|f_j'\rangle+\alpha\overline{\beta}\langle f_i'|f_j\rangle=0,$$

implying $\langle f_i|f_j'\rangle=\langle f_i'|f_j\rangle=0$, otherwise z and $\overline{z}$ would be linearly dependent over the complex field.

As a consequence, to each orthonormal system of $|\zeta_2\rangle$'s of $\mathcal{H}_{D_2}$ we would get an orthonormal system of $|f_i\rangle$'s of at least double size, contradicting the finite dimension of $\mathcal{H}_{D_2}$. Thus U cannot be entangling, forcing $U=U_1\otimes U_2$. To see this either consult Ref. 18 or follow this simple argument: since

$$\sigma_{12}\mapsto U\sigma_{12}U^*$$

maps product states to product states, the map

$$T_1:\sigma\mapsto \mathrm{Tr}_2 U(\sigma\otimes|\zeta_2\rangle\langle\zeta_2|)U^*$$

maps pure states to pure states and is completely positive and trace preserving, entailing that it has to be of the form $T_1(\sigma)=U_1\sigma U_1^*$, or is constant which cannot occur. Here U_1 is a unitary which cannot—except for a global phase—depend on $|\zeta_2\rangle$, or else there would be entangled states $U(\sigma_1\otimes\sigma_2)U^*$. The same applies to the second factor, yielding a unitary U_2. In total we have that the unitary $U_1\otimes U_2$ coincides with U on the pure states, hence $U=U_1\otimes U_2$ (again except for an unimportant global phase). □

Observe the following peculiarity of the argument: it is not true that the reduced state on the left hand side of Eq. (3) is always a product (if it is, our proof is simplified drastically). For example, G_1 and G_2 may be swapping operations, so their product may be used to swap in any entangled state! What is true, however, is that entangled states cannot occur as a result of a unitary action on the data registers.

This nonexistence should not be mixed up with the existence of the beautiful model of *one-way quantum computer* by Raussendorf and Briegel:[19] there, too, a single state is prepared and acted on locally (even only by measurements), to produce any given effect on the data register. There is no contradiction, however, to our result, as there is implied *classical* communication between the sites of these quantum operations, which we had to exclude.

In a sense, the result had to be expected: it reproduces on a somewhat different level the insight in universal computation that single qubit actions are not sufficient for universality, but one needs interacting gates like the C–NOT gate.

We shall show in the following, however, that this nonexistence result has some bearing on quantum channel coding.

IV. NOISY DENSE CODING CAPACITY

Consider the following communication scenario: a sender A and a receiver B share a state ρ on the $d_A\times d_B$-system $\mathcal{H}_A\otimes\mathcal{H}_B$, i.e., $\dim\mathcal{H}_A=d_A$, $\dim\mathcal{H}_B=d_B$. They have at their disposal a quantum channel from A to B that allows noiseless transmission of an arbitrary quantum state in $\mathcal{H}\simeq\mathbb{C}^d$. They want to use this channel to communicate classical information, taking advantage of the correlation (or even entanglement) of ρ. The most general thing possible for A to do is to subject her share of the state to an operation, and send the result through the channel. It is well known that, if ρ supplies only classical correlation (for instance, if

$$\rho=\sum_{i=0}^{d_A-1}\sum_{j=0}^{d_B-1} p_{ij}|i\rangle\langle i|\otimes|j\rangle\langle j|,$$

for orthogonal bases $\{|i\rangle: i=0,\ldots,d_A-1\}$ and $\{|j\rangle: j=0,\ldots,d_B-1\}$ of $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively), then this is of no help at all, and the capacity is just that of the noiseless channel: $\log d$ (in this article log and exp are to basis 2).

However, for entangled ρ the phenomenon of *dense coding* arises, which was first described in Ref. 20: there $d_A=d_B=d=2$ was considered, with the joint singlet state

$$\rho=|\Psi^-\rangle\langle\Psi^-|=\tfrac{1}{2}(|01\rangle-|10\rangle)(\langle 01|-\langle 10|).$$

It was demonstrated that by applying one of the three Pauli unitaries σ_x, σ_y, σ_z, or the identity $\mathbb{1}$, A can drive the state to any of the four Bell states, hence can encode 2 bits. It is quite clear that by starting with any maximally entangled state, e.g.,

$$\rho=|\Phi\rangle\langle\Phi|, \text{ with } |\Phi\rangle=\frac{1}{\sqrt{d}}\sum_{i=0}^{d-1}|i\rangle\otimes|i\rangle$$

on the system $\mathbb{C}^d\otimes\mathbb{C}^d$, i.e., $d_A=d_B=d$, one can devise a scheme to transmit $2\log d=\log d^2$ bits (see Ref. 21 for a detailed discussion).

It is less clear what happens if the state is not maximally entangled, or even mixed: however, since the protocol A and B have to follow depends even in the maximally mixed case on the actual state, we allow them to use *the protocol optimally adapted to* ρ. Formally, A chooses an operation (i.e., a completely positive, trace preserving linear map)

$$T:\mathfrak{L}(\mathcal{H}_A)\to\mathfrak{L}(\mathcal{H}),$$

and applies it to her part of ρ, after which she sends the resulting state to B. He thus receives the signal state

$$\rho^T:=(T\otimes\mathrm{id})\rho.$$

We here assume that one copy of ρ is available per use of the noiseless channel. Below we will discuss the case of more or unlimited many copies per round.

Then we can compute the mutual information

$$I(\mu;\rho):=H\left(\int \mathrm{d}\mu(T)\rho^T\right)-\int \mathrm{d}\mu(T)H(\rho^T),$$

with respect to a probability measure μ on the space $\mathbf{CP}(\mathcal{H}_A,\mathcal{H})$ of quantum operations (i.e., completely positive, trace preserving, linear maps) from $\mathcal{B}(\mathcal{H}_A)$ to $\mathcal{B}(\mathcal{H})$. By the quantum channel coding theorem, Eq. (1), of Refs. 11 and 12, the *dense coding capacity*

$$DC(d,\rho):=\sup_{\mu} I(\mu;\rho)$$

is the classical capacity of the channel with signal states ρ^T, when block coding using product states

$$\rho^{T_1}\otimes\cdots\otimes\rho^{T_n}=((T_1\otimes\mathrm{id})\rho)\otimes\cdots\otimes((T_n\otimes\mathrm{id})\rho)=((T_1\otimes\cdots\otimes T_n)\otimes\mathrm{id}^{\otimes n})\rho^{\otimes n}$$

is allowed.

If we impose no restriction on the block coding, i.e., all states

$$(\mathbf{T}\otimes\mathrm{id}^{\otimes n})\rho^{\otimes n},$$

with $\mathbf{T}\in\mathbf{CP}(\mathcal{H}_A^{\otimes n},\mathcal{H}^{\otimes n})$ are admissible, we get the *ultimate dense coding capacity*

$$\overline{DC}(d,\rho)=\lim_{n\to\infty}\frac{1}{n}DC(d^n,\rho^{\otimes n}).$$

Note that the limit exists by the trivial superadditivity of DC:

$$DC(d_1d_2,\rho\otimes\sigma)\geqslant DC(d_1,\rho)+DC(d_2,\sigma).$$

Our first task is the evaluation of $DC(d,\rho)$:

Assume any probability distribution μ on $\mathbf{CP}(\mathcal{H}_A,\mathcal{H})$, and denote the Haar measure on the group $\mathcal{U}(d)$ of unitaries on $\mathcal{H}$ as $\mathrm{d}U$. Then for every unitary U we have (by unitary invariance of entropy)

$$H\left(\int \mathrm{d}\mu(T)\rho^T\right)=H\left(\int \mathrm{d}\mu(T)(U\otimes\mathbb{1})\rho^T(U\otimes\mathbb{1})^*\right),$$

$$H(\rho^T)=H((U\otimes\mathbb{1})\rho^T(U\otimes\mathbb{1})^*),$$

i.e., $I(\mu;\rho)=I(\mu^U;\rho)$, with the translated measure

$$\mu^U(F)=\mu(U^*FU),\ \text{for measureable}\ F\subset\mathbf{CP}(\mathcal{H}_A,\mathcal{H}).$$

With concavity of H we find

$$I(\mu;\rho)=\int_{\mathcal{U}(d)}\mathrm{d}U\left[H\left(\int \mathrm{d}\mu(T)(U\otimes\mathbb{1})\rho^T(U\otimes\mathbb{1})^*\right)-\int \mathrm{d}\mu(T)H((U\otimes\mathbb{1})\rho^T(U\otimes\mathbb{1})^*)\right]$$

$$\leqslant H\left(\int \mathrm{d}\mu(T)\int \mathrm{d}U(U\otimes\mathbb{1})\rho^T(U\otimes\mathbb{1})^*\right)-\int \mathrm{d}\mu(T)H(\rho^T).$$

The latter quantity is exactly $I(\overline{\mu};\rho)$, with $\overline{\mu}=\int \mathrm{d}U\mu^U$.

Now it is straightforward to prove (essentially by Schur's lemma) that

$$\int \mathrm{d}U(U\otimes\mathbb{1})\rho^T(U\otimes\mathbb{1})^*=\frac{1}{d}\mathbb{1}\otimes\rho_B,$$

where we observed that by definition

$$\mathrm{Tr}_A\rho^T=\mathrm{Tr}_A((T\otimes\mathrm{id})\rho)=\mathrm{Tr}_A\rho=\rho_B.$$

Hence maximization yields

$$DC(d,\rho)=\log d+H(\rho_B)-\inf_{\mu}\int \mathrm{d}\mu(T)H(\rho^T).$$

This infimum in turn is achieved at the point mass on a T minimizing $H(\rho^T)$.

Hence we arrive at the following result.

Theorem 3: *The dense coding capacity of the state ρ and a d-level noiseless transmission system, using one copy of ρ per round and product states for coding, is given by*

$$DC(d,\rho)=\log d+H(\rho_B)-\min_{T}H((T\otimes\mathrm{id})\rho),$$

where the minimization is over all quantum operations $T:\mathcal{B}(\mathcal{H}_A)\to\mathcal{B}(\mathcal{H})$. □

As a consequence we obtain the following.

Theorem 4: *Without the restriction on product state encoding, but still using one copy of ρ per round, the capacity is*

$$\overline{DC}(d,\rho)=\log d+H(\rho_B)-\lim_{n\to\infty}\frac{1}{n}\min_{\mathbf{T}}H((\mathbf{T}\otimes\mathrm{id}^{\otimes n})\rho^{\otimes n}),$$

where the minimization is over all quantum operations $\mathbf{T}:\mathcal{B}(\mathcal{H}_A^{\otimes n})\to\mathcal{B}(\mathcal{H}^{\otimes n})$. □

Note that the argument describes at the same time a distribution on $\mathbf{CP}(\mathcal{H}_A,\mathcal{H})$ that achieves the capacity: A should apply a fixed minimizing T, followed by uniformly distributed unitary rota-

tions. The effect of the latter can be achieved equally by a uniform distribution on an orthogonal basis of unitaries [with respect to the Hilbert–Schmidt inner product $(A,B)=\mathrm{Tr}A^*B$ on operators] (see Ref. 21).

As applications of the theorem we can see immediately that for pure states $|\psi\rangle$

$$DC(d,|\psi\rangle\langle\psi|)=\log d+E(\psi)=\log d+H(\mathrm{Tr}_B|\psi\rangle\langle\psi|),$$

a result already reported in Refs. 22 and 23, and that $DC(d,\rho)=\log d$ if ρ is separable (later in this work, Theorem 7, we will see that this holds true even for *nondistillable* ρ): in the first case the optimizing T is any unitary map, in the second case it is the projection onto any pure state [note that $DC(d,\rho)\leqslant\log d$ follows from the inequality $H(\sigma_B)-H(\sigma)\leqslant 0$ for separable σ]. This latter choice shows that always $DC(d,\rho)\geqslant\log d$ (it amounts to ignoring the correlation provided by ρ).

In general, however, the minimization required by the theorem seems not an easy task itself.

Remark 5: The quantity $H(\sigma_B)-H(\sigma)$, $\sigma=(T\otimes 1)\rho$, from Theorem 3 has appeared in another context before: it is the coherent information *of Schumacher*.[24]

Remark 6: Until now we stuck to using one copy of ρ per use of the noiseless channel. In recent work by Horodecki et al.[25] *this restriction was lifted: unlimited many copies of ρ were assumed to be available. Of course, the theorem can be used to obtain a formula for that case, too, which we give, because it interestingly differs from the one in Ref. 25 (though of course the numbers coincide):*

Assume k copies of ρ may be used per round. Obviously the resulting dense coding capacity is

$$DC^{(k)}(d,\rho)=DC(d,\rho^{\otimes k}),$$

and for unlimited use of ρ we get

$$DC^{(\infty)}(d,\rho)=\lim_{k\to\infty}DC(d,\rho^{\otimes k}).$$

Similarly, for the ultimate dense coding capacity with k copies of ρ per round,

$$\overline{DC^{(k)}}(d,\rho)=\overline{DC}(d,\rho^{\otimes k})=\lim_{n\to\infty}\frac{1}{n}DC(d^n,\rho^{\otimes kn}),$$

and with unlimited use of ρ

$$\begin{aligned}\overline{DC^{(\infty)}}(d,\rho)=\lim_{k\to\infty}\overline{DC^{(k)}}(d,\rho)&=\lim_{k\to\infty}\lim_{n\to\infty}\frac{1}{n}DC(d^n,\rho^{\otimes kn})\\&=\lim_{n\to\infty}\lim_{k\to\infty}\frac{1}{n}DC(d^n,\rho^{\otimes kn})\\&=\lim_{n\to\infty}\frac{1}{n}DC^{(\infty)}(d,\rho)=\overline{DC}^{(\infty)}(d,\rho).\end{aligned}$$

(*The limits are exchangeable because the double* lim *is actually a joint* sup *over n and k, because of monotonicity*.)

In Ref. 25 the differently looking expression (*for the case $d=2$*)

$$\overline{DC}(\rho)=\sup_n\sup_{\mathbf{T}}\left\{1+\frac{nH(\rho_B)-H((\mathbf{T}\otimes\mathrm{id}^{\otimes n})(\rho^{\otimes n}))}{H(\mathbf{T}(\rho_A^{\otimes n}))}\right\}$$

was given, the sup *being over all quantum operations* **T** *defined on* $\mathcal{B}(\mathcal{H}_A^{\otimes n})$. *However, the derivation in that work is sufficiently close to ours so as to see the identity of the results*.

Let us comment here a bit on other related work, and the relation of $DC(d,\rho)$ to entanglement:

In Refs. 26 and 27 the relation of the dense coding capacity to entanglement measures was stressed. With our results, it is easy to reproduce the observations of these papers, and go even a little further:

We use the following inequality from Ref. 28: for a (two–way) nondistillable state σ

$$H(\rho_B)-H(\rho)\leqslant D(\rho\|\sigma).$$

Applying $T\otimes\mathrm{id}$ to both ρ and σ, and invoking the monotonicity of relative entropy under completely positive maps,[29,30] we find

$$H(\rho_B)-H((T\otimes\mathrm{id})\rho)\leqslant D((T\otimes\mathrm{id})\rho\|(T\otimes\mathrm{id})\sigma)\leqslant D(\rho\|\sigma).$$

Now minimize over T and nondistillable σ: this proves the following.

Theorem 7: *For all states* ρ *one has*

$$DC(d,\rho)\leqslant\log d+E_{\mathrm{re}}(\rho),$$

where $E_{\mathrm{re}}(\rho)=\inf_{\sigma\in\mathcal{D}}D(\rho\|\sigma)$ *is the relative entropy of entanglement with respect to the set* $\mathcal{D}$ *of nondistillable states*. □

In particular, when ρ is nondistillable, $DC(d,\rho)=\log d$ (see also Ref. 25 for this observation). One may wonder whether the inverse is true, too: when ρ is distillable, does $DC(d,\rho)>\log d$ follow?

To compare this result to the statements in Refs. 26 and 27 and the result of the recently published Ref. 31 we have to note that in these works only *unitary* encodings were considered. Hence our $DC(d,\rho)$ is typically a strict upper bound to the capacity in the cited works. Still, questions raised in Refs. 26 and 27 receive answers: the conjectured capacity formulas and inequalities from these works follow immediately, by the same method of Haar averaging we employed above (see also Ref. 31).

To get a bound in the other direction is not so easy. We might try to go further on the road of entanglement, and find an entanglement measure lower bound. For example, if we could prove that

$$f(\rho)=\overline{DC}^{(\infty)}(d,\rho)-\log d$$

is an entanglement measure itself, we would find the lower bound

$$\overline{DC}^{(\infty)}(d,\rho)\geqslant\log d+E_D(\rho),$$

with the *distillable entanglement* $E_D(\rho)$: this follows from general inequalities in Ref. 32. We leave this question, however, to another occasion.

We would like now to discuss the additivity of D, i.e., whether for states ρ, σ

$$DC(d_1d_2,\rho\otimes\sigma)=DC(d_1,\rho)+DC(d_2,\sigma). \tag{5}$$

Note that if this is true for ρ and all $\sigma=\rho^{\otimes n}$ (e.g., inductively), it immediately follows that $\overline{DC}(d,\rho)=DC(d,\rho)$. In particular, all ultimate capacities in Remark 6 are identical to their ''unbarred'' versions. The capacity with unlimited use of ρ from Ref. 25 would then read

$$\overline{DC}^{(\infty)}(d,\rho)=DC^{(\infty)}(d,\rho)=\log d+H(\rho_B)-\inf_k\min_T H((T\otimes\mathrm{id}^{\otimes k})\rho^{\otimes k}),$$

where the minimization is over all quantum operations $T:\mathcal{B}(\mathcal{H}_A^{\otimes k})\to\mathcal{B}(\mathcal{H})$.

By Theorem 3, the statement of Eq. (5) is equivalent to asking if

$$\min_{T_{12}} H((T_{12}\otimes \mathrm{id}^{\otimes 2})(\rho\otimes\sigma)) = \min_{T_1} H((T_1\otimes \mathrm{id})\rho) + \min_{T_2} H((T_2\otimes \mathrm{id})\sigma).$$

Obviously, and fitting with the superadditivity of D, "$\leqslant$" (subadditivity) is trivial, and the question is if "$<$" can occur. Note that in this generality it is quite easy to come up with states that violate the additivity property (see the discussion below). The problem is rather to find conditions where additivity holds.

Generalizing, one may assume not a noiseless but a noisy channel $\varphi:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ between A and B, and consider the dense coding capacities

$$DC(\varphi,\rho), \quad \overline{DC}(\varphi,\rho),$$

$$DC^{(k)}(\varphi,\rho), \quad \overline{DC}^{(k)}(\varphi,\rho),$$

$$DC^{(\infty)}(\varphi,\rho), \quad \overline{DC}^{(\infty)}(\varphi,\rho).$$

For example, we can define

$$DC(\varphi,\rho) = \sup_{\mu} I(\mu;\varphi\circ\rho)$$

over all probability distributions μ on $\mathbf{CP}(\mathcal{H}_A,\mathcal{H})$, with

$$I(\mu;\varphi\circ\rho) := H\left(\int \mathrm{d}\mu(T)\rho^{\varphi\circ T}\right) - \int \mathrm{d}\mu(T) H(\rho^{\varphi\circ T}).$$

Observe that our previous $DC(d,\rho)$ is reproduced in the new definition as $DC(\mathrm{id}_d,\rho)$. Further, observe that for a pure entangled state ρ the definition relates to the entanglement assisted classical capacity[33] of the quantum channel φ: in fact, $\overline{DC}^{(\infty)}(\varphi,\rho)$ *is* this latter quantity.

Again, the superadditivity

$$DC(\varphi\otimes\vartheta,\rho\otimes\sigma) \geqslant DC(\varphi,\rho) + DC(\vartheta,\sigma) \tag{6}$$

trivially holds, and we may study conditions for equality in Eq. (6), i.e., additivity.

Note that it is fairly easy to come up with situations $(\varphi, \vartheta, \rho, \sigma)$ where strict superadditivity holds. In fact, one can even have either $\varphi=\vartheta$ or $\rho=\sigma$: e.g., consider

$$\varphi=\vartheta=\mathrm{id}_{\mathcal{B}(\mathbb{C}^2)}, \quad \begin{cases} \rho = |00\rangle\langle 00| \text{(un-entangled)}, \\ \sigma = |\Psi^-\rangle\langle\Psi^-|^{\otimes 2}, \end{cases}$$

or alternatively

$$\left.\begin{aligned} &\varphi = \mathrm{id}_{\mathcal{B}(\mathbb{C}^4)}, \\ &\vartheta = \tfrac{1}{2}\mathbb{1} \ \text{(constant map)}, \end{aligned}\right\} \quad \rho=\sigma=|\Psi^-\rangle\langle\Psi^-|.$$

But with both these conditions simultaneously it seems not so easy. It may even be that *weak additivity* holds, i.e.,

$$DC(\varphi^{\otimes n},\rho^{\otimes n}) = nDC(\varphi,\rho),$$

for all channels φ and joint states ρ, but we could not reach a conclusive result on this question.

V. REDUCTIONS AMONG ADDITIVITY QUESTIONS

We have encountered two paradigms of coding in quantum channels, the first in the established discussion (a good overview is in Ref. 34, and some recent developments are reviewed in Ref. 13), the second in the previous section:

(1) State preparation: The encoder may prepare any state on the input system space $\mathcal{H}_1$ for the quantum channel $\varphi:\mathcal{B}(\mathcal{H}_1)\to\mathcal{B}(\mathcal{H}_2)$.

(2) Action on given state: On the input system a state is given in advance (possibly entangled with the receiver), and the encoder may act on it in an arbitary way, and the result is sent down the channel φ.

It is quite obvious that method 1 can be reduced to method 2: the previously given state is just any state not entangled with the receiver (say, a pure state). Then by executing an appropriate operation the encoder can drive the input into any desired state.

Less obvious, but still quite canonical, is the converse reduction: any operation T: $\mathcal{B}(\mathcal{H}_A)\to\mathcal{B}(\mathcal{H}_1)$ can be implemented as a unitary

$$U:\mathcal{H}_A\otimes\mathcal{H}'\to\mathcal{H}_1\otimes\mathcal{H}'',$$

followed by a partial trace over $\mathcal{H}''$, the system $\mathcal{H}'$ being prepared initially in a null state σ_0. This is a formulation of the Stinespring dilation theorem,[35] and it is quite easy to see that $\dim\mathcal{H}'$ can be chosen fixed and finite for all possible T. Now pick an ϵ-approximating quantum gate G_ϵ for $\mathcal{H}_A\otimes\mathcal{H}'$, with program register $\mathcal{H}_{P_\epsilon}$: by choosing ψ in the program register appropriately one obtains (using monotonicity of the trace norm under partial trace), for all states σ on $\mathcal{H}_A$,

$$\|T(\sigma)-\mathrm{Tr}_{\mathcal{H}''\otimes\mathcal{H}_{P_\epsilon}}(G_\epsilon(\sigma\otimes|0\rangle\langle 0|\otimes|\psi\rangle\langle\psi|)G_\epsilon^*)\|_1\leq\epsilon. \tag{7}$$

Thus every coding process by acting on the input system can be arbitrarily well approximated by coding via choice of $|\psi\rangle\in\mathcal{H}_{P_\epsilon}$.

These two reductions, however, are of a very different nature, as we can see by considering their behavior under tensor products of channels: while the reduction $1\to 2$ scales correctly (any entangled input state can be obtained by a suitable entangling operation on the product of the initial states), the reduction $2\to 1$ that we proposed does not. In fact, as we have seen in Theorem 2, on a product $\mathcal{H}_{A1}\otimes\mathcal{H}_{A2}$ of two input systems we can never implement an entangling operation, once we have chosen approximating quantum gates for each of them individually according to Eq. (7), and tensor them.

We have seen that there are channels where classical information is encoded after method 1 (these are just the operations φ), and that there are channels where it is encoded after method 2 (the generalized noisy dense coding channels). The above reductions show that the two approaches are equivalent in the sense that a channel of the one kind can be simulated to arbitary accuracy by one of the other kind.

However, for the additivity question of channel capacity one has to look at higher tensor products of the channel at hand. By the above argument the reduction $1\to 2$ provides a reduction of the additivity question for channels of the first type to those of the second type. It is unknown to us if the additivity question can be reduced in the other direction: the construction above, summarized in Eq. (7), at least does not provide this, as we have seen. On the other hand, it appears to be most natural: it seems the most reasonable thing to do to associate a channel of the first type to the given channel of the second type that has the same properties with respect to classical information transmission, by simply enabling to emulate the effect of any encoding transformation T by a suitable input state.

VI. CONCLUSION

By studying entanglement assisted classical communication via quantum channels, attention was drawn towards channels which require *actions* for signaling rather than *state preparations* like

the usual quantum dynamics, represented by completely positive maps. An attempted reduction of the more general scenario to the usual one was shown to fail, because no *scalable programmable quantum gates* exist. This was taken to indicate that the new concept is strictly more general, which leads us to conjecture that the additivity question for quantum channel capacity really is not about ''whether entangled inputs help,'' but rather ''whether *entangling* inputs help.'' It must be stressed that in the more general vista we presented, additivity is not a mere matter of ''right'' or ''false.'' Rather, it becomes (as we demonstrated by examples) a question of *characterization* of the situations where it holds. Note finally that the very occurrence of the above mentioned distinction in coding concepts is a purely quantum phenomenon.

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Counterexample to an additivity conjecture for output purity of quantum channels

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A conjecture arising naturally in the investigation of additivity of classical information capacity of quantum channels states that the maximal purity of outputs from a quantum channel, as measured by the p-norm, should be multiplicative with respect to the tensor product of channels. We disprove this conjecture for $p>4.79$. The same example (with $p=\infty$) also disproves a conjecture for the multiplicativity of the injective norm of Hilbert space tensor products. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1498491]

I. STATEMENT OF THE PROBLEM

A. Multiplicativity of output purity

In many applications of quantum information theory the entanglement of states or the capacity of channels appear as resources, which are needed to perform a task and are used up in the process. Therefore, it is natural to expect that certain entanglement or capacity measures should be *additive* in the sense that preparing two pairs of entangled particles should give us twice the entanglement of one pair and, similarly, using a channel twice doubles its capacity. However, such additivity properties have turned out to be notoriously difficult to prove, and in some cases folk conjectures claiming additivity have turned out to be wrong.

The purpose of this work is to provide a counterexample of this kind, i.e., to show that a family of quantities, which had been conjectured to be additive in an earlier paper by the present authors,[1] actually is not. The quantities considered all characterize the highest purity of the outputs of a channel. That is, if S is a completely positive map, taking density operators on a finite dimensional Hilbert space $\mathcal{H}_1$ to density operators on another finite dimensional Hilbert space $\mathcal{H}_2$, and $1<p<\infty$, we defined

$$\nu_p(S)=\sup\|S(\rho)\|_p, \tag{1}$$

where the supremum is over all input density operators, and $\|\rho\|_p=(\mathrm{tr}|\rho|^p)^{1/p}$ is the standard p-norm. The conjecture in Ref. 1 was that $\log\nu_p$ is additive in the sense that

$$\nu_p(S_1\otimes S_2)=\nu_p(S_1)\,\nu_p(S_2) \tag{2}$$

for arbitrary channels S_1, S_2.

This conjecture was supported by some numerical evidence (the inequality "$\geqslant$" being trivial anyhow), and a proof for very noisy and almost noiseless channels in Ref. 1, as well as some depolarizing channels. Further supporting evidence was given by C. King.[2,3] The main application would probably have been in the limit $p\to 1$, where it would be the additivity of "maximal purity

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as measured by entropy." This in turn is closely related[1,3,4] to the question of additivity of classical channel capacity, i.e., whether transmission of classical information over multiple quantum channels can sometimes be improved by using entangled signal states.

B. Injective tensor norm for Hilbert space vectors

The case $p=\infty$, i.e., when $\|\cdot\|_\infty$ is the ordinary operator norm, is implied by another additivity conjecture, namely for the *injective tensor norm* of Hilbert space vectors. For any vector $\Phi \in \mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_N$ we define this norm as

$$\mu_N(\Phi)=\sup|\langle\Phi,\phi_1\otimes\cdots\otimes\phi_N\rangle|, \tag{3}$$

where the supremum is over all tuples of vectors $\phi_\alpha\in\mathcal{H}_\alpha$ with $|\phi_\alpha|=1$. The conjectured property for this quantity was that $\mu_N(\Phi\otimes\Psi)=\mu_N(\Phi)\mu_N(\Psi)$, where $\Phi\in\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_N$ and $\Psi\in\mathcal{K}_1\otimes\cdots\otimes\mathcal{K}_N$ may be in different N-fold Hilbert space tensor products, and the supremum in $\mu_N(\Phi\otimes\Psi)$ is taken over unit vectors $\phi_\alpha\in\mathcal{H}_\alpha\otimes\mathcal{K}_\alpha$. Again, the inequality "$\geqslant$" and the case $N=2$ are trivial. The connection with the previous problem is seen by writing S in Kraus form $S(\rho)=\Sigma_x A_x\rho A_x^*$. Then

$$\langle\varphi,S(|\phi\rangle\langle\phi|)\varphi\rangle=\sum_x\ |\langle\varphi,A_x\phi\rangle|^2=\sup_\psi\left|\sum_x\ \overline{\psi_x}\langle\varphi,A_x\phi\rangle\right|^2, \tag{4}$$

where at the last equality we consider the $\langle\varphi,A_x\phi\rangle$ as the components of a Hilbert space vector, whose norm can also be written as the largest scalar product with a unit vector. Accordingly, the supremum in the last line is over all unit vectors ψ. Taking the supremum over the unit vectors ϕ and φ, too, we find that

$$\nu_\infty(S)=\mu_3(\tilde{A})^2, \tag{5}$$

where $\tilde{A}$ denotes the vector in a threefold Hilbert space tensor product with components $\langle h_j,A_x e_k\rangle$, where h_j and e_k are orthonormal bases of the appropriate spaces. In particular, since the tensor product of channels S corresponds to the tensor product of vectors $\tilde{A}$, the conjectured multiplicativity of μ_3 would imply the multiplicativity of ν_∞. Conversely, the counterexample given to the latter disproves the multiplicativity of μ_N for all $N\geqslant 3$.

II. THE COUNTEREXAMPLE

We give an explicit example of a channel violating conjecture (2) for large values of p. It is the channel S on the $d\times d$-matrices defined as

$$S(\rho)=\frac{1}{d-1}(\mathrm{tr}(\rho)\mathbb{1}-\rho^T) \tag{6}$$

$$=\frac{1}{2(d-1)}\sum_{ij}\ (|i\rangle\langle j|-|j\rangle\langle i|)^*\rho(|i\rangle\langle j|-|j\rangle\langle i|). \tag{7}$$

Here ρ^T denotes the matrix transpose with respect to some fixed basis. In the first form it is easy to verify that S is linear and trace preserving, in the second it becomes clear that it is also completely positive. The equality of the two forms is a straightforward exercise. Further interesting properties are that S is Hermitian with respect to the Hilbert–Schmidt scalar product $(A,B)\mapsto\mathrm{tr}(A^*B)$ on $d\times d$-matrices, and covariant for arbitrary unitary transformations in the sense that $S\circ\mathrm{ad}_U=\mathrm{ad}_{\overline{U}}\circ S$, $\mathrm{ad}_U(X)=UXU^*$, where $\overline{U}$ denotes the matrix element-wise complex conjugate of a unitary in the fixed basis. We remark that S is the dual of the state which provided the counterexample to the additivity of the relative entropy of entanglement for bipartite states in

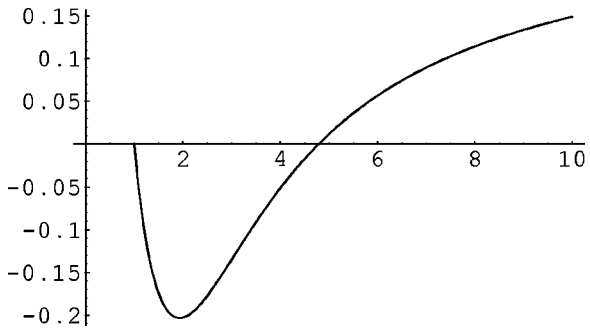

FIG. 1. $\Delta(p,\Phi_m)$ over p, as explained in the text.

Ref. 5, i.e., that state, the normalized projection onto the Fermi subspace of $\mathbb{C}^d\otimes\mathbb{C}^d$ $(d\geqslant 3)$, is obtained by acting with S on one partner of a maximally entangled pair on $\mathbb{C}^d\otimes\mathbb{C}^d$.

Now $\rho\mapsto\|S(\rho)\|_p$ is a convex function, and hence takes its maximum on the extremal states. Therefore it suffices to take pure input states, for which

$$S(|\phi\rangle\langle\phi|)=\frac{1}{d-1}(\mathbb{1}-|\overline{\phi}\rangle\langle\overline{\phi}|). \tag{8}$$

Clearly, the p-norm is the same for all pure inputs, and we get

$$\nu_p(S)=(d-1)^{-(1-1/p)}. \tag{9}$$

On the other hand, let us consider $S\otimes S$ acting on a pure state Φ. Due to covariance we may take Φ in Schmidt diagonal form $\Phi=\Sigma_\alpha c_\alpha|\alpha\alpha\rangle$. Then with the reduced density operator $\rho=\Sigma_\alpha c_\alpha^2|\alpha\rangle\langle\alpha|$ we get

$$S\otimes S(|\Phi\rangle\langle\Phi|)=\frac{1}{(d-1)^2}(\mathbb{1}-\mathbb{1}\otimes\rho-\rho\otimes\mathbb{1}+|\Phi\rangle\langle\Phi|). \tag{10}$$

We now specialize further to *maximally entangled* $\Phi=\Phi_m$, i.e., all $c_\alpha=1/\sqrt{d}$ and $\rho=(1/d)\mathbb{1}$, all terms in this expression commute, and the operator in parenthesis has one eigenvalue $(1-2/d)$ with multiplicity (d^2-1) and a nondegenerate eigenvalue $(1-2/d+1)$. From this we find, for $d=3$,

$$\|S\otimes S(|\Phi_m\rangle\langle\Phi_m|)\|_p=\tfrac{1}{3}(1+2^{3-2p})^{1/p}. \tag{11}$$

If additivity were true, the following quantity should be negative, becoming zero upon maximization with respect to Φ:

$$\Delta(p,\Phi)=\log\|S\otimes S(|\Phi\rangle\langle\Phi|)\|_p-2\log\nu_p(S). \tag{12}$$

However, inserting for Φ the maximally entangled state we get

$$\Delta(p,\Phi_m)=\log\frac{4}{3}+\frac{1}{p}\log\left(\frac{1}{4}+2^{1-2p}\right). \tag{13}$$

This quantity is plotted in Fig. 1. Thus additivity is violated for $p>p_0$, where the zero p_0 is numerically determined as $p_0=4.7823$. In particular, we get $\Delta(\infty,\Phi_m)=\log(\frac{4}{3})>0$, so additivity fails for $p=\infty$. Transcribed to the problem for injective Hilbert space norms, the counterexample

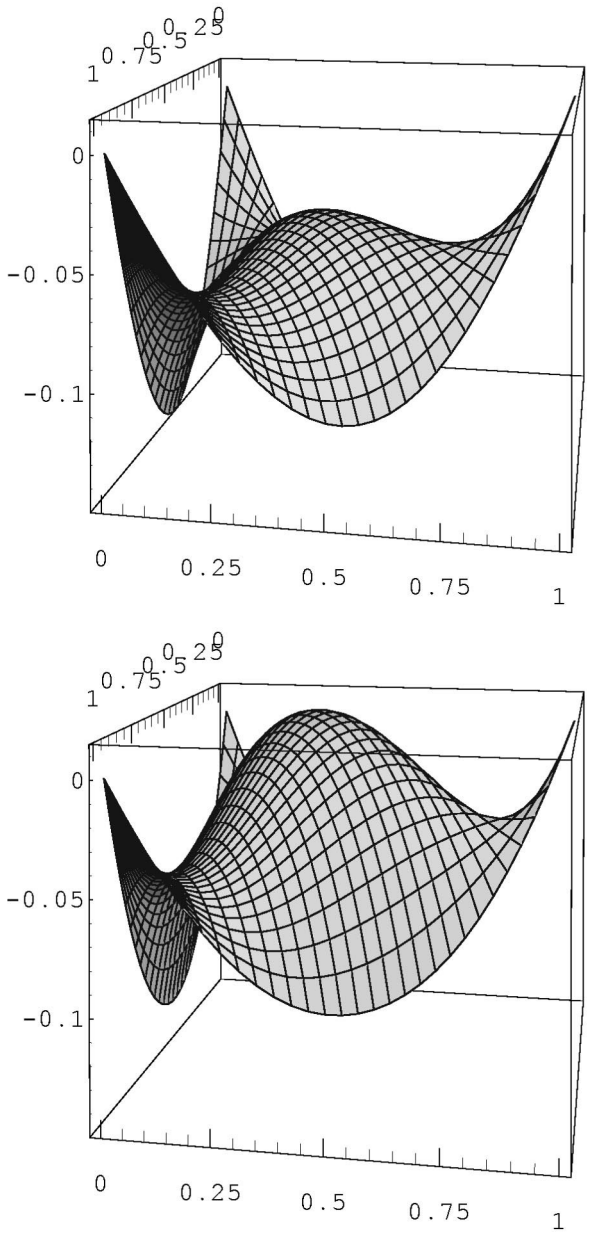

FIG. 2. $\Delta(p,\Phi)$ for $d=3$ over the Schmidt parameters c_1^2 and c_2^2 of Φ, for $p=4$ (top) and for $p=5$ (bottom).

is the unique antisymmetric vector Φ on $\mathbb{C}^3\otimes\mathbb{C}^3\otimes\mathbb{C}^3$, tensored with itself. On the other hand, for $p\to 1$ we have $\Delta(p,\Phi_m)<0$, so in this case, which is of main interest for classical channel capacity, the additivity conjecture survives.

The boundary point p_0 cannot be improved by choosing another vector Φ, i.e., the maximizing Φ in the definition of $\nu_p(S\otimes S)$ jumps discontinuously from a product state to a maximally entangled state, as p increases beyond p_0. This is seen by plotting Δ for fixed p over the Schmidt parameters of Φ. There is little difference between the plots for $p=4$ and $p=5$ (see Fig. 2) except that the global maximum switches from corners (Φ a product vector) to the center ($\Phi=\Phi_m$).

III. CONCLUDING REMARKS

We have seen that multiplicativity of maximal purity depends crucially on how we measure purity: if we use p-norms for large p, it fails. But the conjecture remains open for small p, and in particular for purity as measured by entropy. There seems to be no simple modification of the example given here to improve the critical value of p. On the other hand, it is hardly expected to be optimal.

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Inequalities for quantum entropy: A review with conditions for equality

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This article presents self-contained proofs of the strong subadditivity inequality for von Neumann's quantum entropy, $S(\rho)$, and some related inequalities for the quantum relative entropy, most notably its convexity and its monotonicity under stochastic maps. Moreover, the approach presented here, which is based on Klein's inequality and Lieb's theorem that the function $A \to \mathrm{Tr}\, e^{K+\log A}$ is concave, allows one to obtain conditions for equality. In the case of strong subadditivity, which states that $S(\rho_{123})+S(\rho_2) \leqslant S(\rho_{12})+S(\rho_{23})$ where the subscripts denote subsystems of a composite system, equality holds if and only if $\log \rho_{123} = \log \rho_{12} - \log \rho_2 + \log \rho_{23}$. Using the fact that the Holevo bound on the accessible information in a quantum ensemble can be obtained as a consequence of the monotonicity of relative entropy, we show that equality can be attained for that bound only when the states in the ensemble commute. The article concludes with an Appendix giving a short description of Epstein's elegant proof of Lieb's theorem. [DOI: 10.1063/1.1497701]

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I. INTRODUCTION

A. Quantum entropy

Quantum information science[32] is the study of the information carrying and processing properties of quantum mechanical systems. Recent work in this area has generated renewed interest in the properties of the quantum mechanical entropy. It is interesting to note that von Neumann[45,46] introduced the notion of mixed state, represented by a density matrix ρ (a positive semi-definite operator with $\mathrm{Tr}\rho=1$), into quantum theory and defined its entropy as $S(\rho)\equiv-\mathrm{Tr}(\rho\log\rho)$ in 1927, well before the corresponding classical quantity was introduced in Shannon's seminal work[41] on "The Mathematical Theory of Communication" in 1948. (Admittedly, von Neumann's motivation was the extension of the classical theory of statistical mechanics, developed by Gibbs *et al.* to the quantum domain rather than the development of a theory of quantum communication.) Many fundamental properties of the quantum entropy were proved in a remarkable, but little-known, 1936 paper of Delbrück and Molèiere.[9] For further discussion of the history of quantum entropy, see Refs. 33, 38 and 47 and the introductory remarks in Ref. 40.

One important class of inequalities relates the entropy of subsystems to that of a composite system, whose Hilbert space is a tensor product $\mathcal{H}_{12}=\mathcal{H}_1\otimes\mathcal{H}_2$ of the Hilbert spaces for the subsystems. When the state of the composite system is described by the density matrix ρ_{12}, the states of the subsystems are given by the reduced density matrices, e.g., $\rho_1=T_2(\rho_{12})$, obtained by taking the partial trace. The subadditivity inequality

$$S(\rho_{12})\leqslant S(\rho_1)+S(\rho_2) \tag{1}$$

was proved in Refs. 9 and 24. [It should not be confused with the concavity

$$S(x\rho'+(1-x)\rho'')\geqslant xS(\rho')+(1-x)S(\rho''), \tag{2}$$

which can actually be obtained *from* subadditivity by considering block matrices.[27,28,47]] In the more complex situation in which the composite system is composed of three subsystems, the following stronger inequality, known as strong subadditivity (SSA), holds:

$$S(\rho_{123})+S(\rho_2)\leqslant S(\rho_{12})+S(\rho_{23}). \tag{3}$$

This inequality was conjectured by Lanford and Robinson in Ref. 24 and proved in Refs. 28 and 29. In this article, we review its proof in a form that easily yields the following condition for equality.

Theorem 1: *Equality holds in strong subadditivity (3) if and only if*

$$\log\rho_{123}-\log\rho_{12}=\log\rho_{23}-\log\rho_2. \tag{4}$$

We have suppressed implicit tensor products with the identity so that, e.g., $\log\rho_{12}$ means $(\log\rho_{12})\otimes I_3$. Rewriting (4) as $\log\rho_{123}+\log\rho_2=\log\rho_{12}+\log\rho_{23}$, multiplying by ρ_{123} and taking the trace immediately establishes the sufficiency of this equality condition. In Sec. IV, we will show that it is also necessary.

B. Relative entropy

The SSA inequality can be restated as a property of the *quantum relative entropy* which is defined as

$$H(\rho,\gamma)\equiv \mathrm{Tr}\rho(\log\rho-\log\gamma). \tag{5}$$

It is usually assumed that ρ, γ are density matrices, although (5) is well-defined for any pair of positive semi-definite matrices for which $\ker(\gamma)\subset\ker(\rho)$. Strong subadditivity can now be restated as

$$H(\rho_{12},\rho_2)\leqslant H(\rho_{123},\rho_{23}), \tag{6}$$

where we again write, e.g., ρ_{23} for $I_1\otimes\rho_{23}$. More generally, the relative entropy is monotone under completely positive, trace-preserving maps (also known as ''quantum operations'' [32] and ''stochastic maps'' [1,20] and discussed in more detail in Sec. III D), i.e.,

$$H[\Phi(\rho),\Phi(\gamma)]\leqslant H(\rho,\gamma). \tag{7}$$

This monotonicity implies (6) when $\Phi=T_3$ is the partial trace operation; perhaps surprisingly, the converse is also true.[31] This, and other connections between strong subadditivity and relative entropy, are discussed in Sec. V C.

The approach to SSA presented here can also be used to obtain conditions for equality in properties of relative entropy, including its joint convexity and monotonicity. The explicit statements are postponed to later sections. Since the monotonicity can be used to give a simple proof of the celebrated Holevo bound[14,32] on accessible information, we show how our results can be used to recover the equality conditions in that bound. As discussed in Sec. II C, Petz[33,36] has also obtained several equality conditions in different, but equivalent, forms. However, Theorem 8, which applies to the most general form of monotonicity, appears to be new.

C. Lieb's convex trace functions

One of the most frequently cited approaches to strong subadditivity is to present it as a consequence of the concavity of a quantity known as the Wigner–Yanase–Dyson entropy.[49] This property, conjectured by Bauman,[6] is equivalent to the joint concavity in A and B of the map

$$(A,B)\to \mathrm{Tr}A^sK^\dagger B^{(1-s)}K \quad \text{for} \quad A,B>0,\ 0<s<1 \tag{8}$$

(where † is used to denote the adjoint). Lieb's proof[26] of the concavity of the WYD function (8) and his realization of a connection between SSA and Bauman's concavity conjecture was a crucial breakthrough. However, concavity of the WYD function was only one of several concave trace functions studied in Ref. 26; the following result was also established by Lieb.

Theorem 2: *For any fixed self-adjoint matrix K, the function* $A\mapsto F(A)=\mathrm{Tr}\ e^{K+\log A}$ *is concave in* $A>0$.

This result played a fundamental role in the original proof[28,29] of SSA and the closely related property of joint concavity of the relative entropy.[28–30] Although SSA is a deep theorem, a complete proof is not as forbidding as is sometimes implied. Therefore, for completeness, we include Epstein's elegant proof[11] of Theorem 2 in the Appendix, and then follow the original strategies of Lieb and Ruskai[29] to show how it implies SSA.

D. Overview

Although this article grew out of questions about the conditions for equality in strong subadditivity and related inequalities, it seems useful to present these conditions within a more comprehensive exposition. For simplicity, we confine our discussion to finite dimensions, and assume that, unless otherwise stated, the density matrices under consideration are strictly positive.

The remainder of the article is structured as follows. In Sec. II we discuss some consequences and interpretations of the SSA equality condition. In Sec. III we summarize some mathematical results needed for the proofs in the sections that follow. Section IV, which might be regarded as the heart of the paper, presents the proof of strong subadditivity in a form which easily yields the equality conditions. (A reader primarily interested in this proof can proceed directly to Sec. IV with a willingness to accept the results of Sec. III.) Section V presents proofs with equality conditions for the monotonicity of the relative entropy under partial traces, the joint convexity of the relative entropy, and the general monotonicity under stochastic maps. This section also contains a discussion of the connection between these properties, SSA and their proofs. Section VI contains the proof of the equality conditions for monotonicity of relative entropy. Section VII considers bounds, most notably the Holevo bound, on the accessible information that can be extracted from an ensemble of quantum states, and the conditions under which they can be attained. The article concludes with some additional historical comments in Sec. VIII.

II. IMPLICATIONS OF THE EQUALITY CONDITIONS FOR SSA

A. Classical conditions

To describe the corresponding classical inequalities, let the subsystems A, B and C correspond to classical random variables. One can recover the classical Shannon entropy $-\Sigma_a p(a)\log p(a)$ from the von Neumann entropy by taking ρ to be a diagonal matrix with elements $p(a)$ on the diagonal. Employing a slight abuse of notation, we write $S[p(a)]$ for this quantity. Then the classical strong subadditivity inequality can be stated as

$$S[p(a,b,c)]+S[p(b)]\leqslant S[p(a,b)]+S[p(b,c)]. \tag{9}$$

The classical relative entropy of the distribution $q(a)$ with respect to $p(a)$ is $H[p(a),q(a)]=\Sigma_a p(a)\log p(a)/q(a)$. It is well-known (see, e.g., Ref. 23) that the convexity of the function $f(x)=x\log x$ implies that $H[p(a),q(a)]\geqslant 0$ and its strict convexity implies that equality holds if and only if $p(a)=q(a)\forall a$. (The generalization of this result to quantum situations is discussed in Sec. III A.)

The classical form (9) of SSA is equivalent to $H[p(a,b,c),q(a,b,c)]\geqslant 0$ when the second distribution is $q(a,b,c)=p(a,b)[p(b)]^{-1}p(b,c)$. Thus, equality holds in (9) if and only if

$$p(a,b,c)=p(a,b)[p(b)]^{-1}p(b,c)\quad \forall a,b,c, \tag{10}$$

which can be rewritten as

$$\log p(a,b,c)-\log p(a,b)=\log p(b,c)-\log p(b)\quad \forall a,b,c, \tag{11}$$

which is identical to what one would obtain from Theorem 1. Using $p(c|b)$ to denote the classical conditional probability distribution, (11) can be rewritten as

$$p(c|a,b)=p(c|b), \tag{12}$$

which is precisely the condition that the sequence $A\rightarrow B\rightarrow C$ forms a Markov chain.

B. Special cases of SSA equality

Some insight into equality condition (4) may be obtained by looking at special cases in which it is satisfied. The most obvious is when ρ_{123} is a tensor product of its three reduced density matrices. However, it is readily verified that (4) also holds when either $\rho_{123}=\rho_1\otimes\rho_{23}$ *or* $\rho_{123}=\rho_{12}\otimes\rho_3$. One can generalize this slightly further. If the subsystem 2 can be partitioned further into two subsystems $2'$ and $2''$, then one can verify equality holds if $\rho_{123}=\rho_{12'}\otimes\rho_{2''3}$, where $\rho_{12'}$ and $\rho_{2''3}$ are states of the composite systems 1, $2'$ and $2''$, 3 respectively.

However, such a decomposition into tensor products is not necessary; indeed, we have already seen that equality also holds for the case of classical Markov processes. Moreover, by comparison to (12) it is natural to regard (4) as a kind of quantum Markov condition. Thus, the conditions in Theorem 1 can also be viewed as a natural noncommutative analog of the conditions for equality in classical SSA. Another way of regarding (4) is as a concise statement of a subtle intertwining condition discussed below. Unfortunately, we have not found explicit examples which satisfy it other than the two classes discussed above, that is, a partial decomposition into tensor products or a classical Markov chain.

C. Petz's conditions

Using a completely different approach, Petz[33,36] gave conditions for equality in (7) when Φ can be identified with a mapping of an algebra onto a subalgebra, a situation which includes (6). In that case Petz's conditions become

$$\rho_{12}^{it}\rho_{2}^{-it}=\rho_{123}^{it}\rho_{23}^{-it}. \tag{13}$$

Taking the derivative of both sides of (13) at $t=0$ yields (4). Although (13) appears stronger than (4), it is not since, as noted above, (4) is sufficient for equality in (6). Moreover, since (4) implies

$$e^{it\log(\rho_{123})}=e^{it[\log\rho_{12}-\log\rho_{12}+\log\rho_{23}]}, \tag{14}$$

our results can be combined with those of Petz to see that equality holds in SSA$\Leftrightarrow$(4)$\Leftrightarrow$(13) and that any of these conditions suffices to imply

$$e^{it[\log\rho_{12}-\log\rho_{2}+\log\rho_{23}]}=e^{it\log(\rho_{12})}e^{-it\log(\rho_{2})}e^{it\log(\rho_{23})}. \tag{15}$$

Note that one can also relate Petz's conditions to those for equality in classical SSA by rewriting (10) as $p(a,b,c)[p(b,c)]^{-1}=p(a,b)[p(b)]^{-1}$ and then raising to the *it* power.

III. FUNDAMENTAL MATHEMATICAL TOOLS

A. Klein's inequality

The fact that the relative entropy is positive, i.e., $H(\rho,\gamma)\geqslant 0$ when $\mathrm{Tr}\rho=\mathrm{Tr}\gamma$, is an immediate consequence of the following fundamental convexity result due to Klein.[22,32,47]

Theorem 3 (Klein's inequality): *For A, B>0*

$$\mathrm{Tr}\ \ A(\log A-\log B)\geqslant \mathrm{Tr}(A-B), \tag{16}$$

with equality if and only if A=B.

The closely related Peierls–Bogoliubov inequality[33,47] is sometimes used instead of Klein's inequality. However, the equality conditions in Theorem 3 play a critical role in the sections that follow.

B. Lieb's golden corollary

The proofs in Sec. IV do not use Theorem 2 directly, but a related result generalizing the following inequality, which we will also need.

Theorem 4 (Golden–Thompson–Symanzik): *For self-adjoint matrices A and B,* $\mathrm{Tr}\ e^{A+B}\leqslant \mathrm{Tr}\ e^{A}e^{B}$ *with equality if and only if A and B commute*.

Although this inequality is extremely well-known, the conditions for equality do not appear explicitly in such standard references as Refs. 16, 42 and 47. However, one method of proof is based on the observation that $\mathrm{Tr}[e^{A/2^k}e^{B/2^k}]^{2^k}$ is monotone decreasing in k, yielding e^{A+B} in the limit as $k\to\infty$. The equality conditions then follow easily from those for the Schwarz inequality for the Hilbert–Schmidt inner product $\mathrm{Tr}C^{\dagger}D$. Indeed, $k=1$ yields

$$\mathrm{Tr}(e^{A/2}e^{B/2})(e^{A/2}e^{B/2})\leqslant[\mathrm{Tr}\ \ e^{B/2}e^{A}e^{B/2}]^{1/2}[\mathrm{Tr}\ \ e^{A/2}e^{B}e^{A/2}]^{1/2}=\mathrm{Tr}\ \ e^{A}e^{B}$$

with $C=e^{B/2}e^{A/2}$ and $D=e^{A/2}e^{B/2}$. The equality condition that C is a multiple of D implies $e^{B/2}e^{A/2}=e^{A/2}e^{B/2}$ which holds if and only if A and B commute. One reference[33] that does discuss equality does so by making the interesting observation that (as shown in Ref. 37) Theorem 4 and its equality conditions can be derived as a consequence of the monotonicity of relative entropy, Theorem 7.

The natural extension to three matrices $\mathrm{Tr}\ e^{A+B+C}\leqslant|\mathrm{Tr}\ e^{A}e^{B}e^{C}|$, fails; see, for example, Problem 20 on pp. 512–513 of Ref. 16. Therefore, the following result of Lieb[26] is particularly noteworthy.

Theorem 5 (Lieb): *For any R,S,T>0*

$$\mathrm{Tr}\ \ e^{\log R-\log S+\log T}\geqslant\mathrm{Tr}\int_0^\infty R\,\frac{1}{S+uI}\,T\,\frac{1}{S+uI}\,du. \tag{17}$$

One might expect that equality holds if and only if R,S,T commute. Although this is sufficient, it is not necessary. One easily checks that both sides of (17) equal $\mathrm{Tr}\rho_1\otimes\rho_{23}$ when $R=\rho_1\otimes\rho_2\otimes I_3$, $S=I_1\otimes\rho_2\otimes I_3$, and $T=I_1\otimes\rho_{23}$, even when T does not commute with R or S.

Proof: Lieb's proof of (17) begins with the easily established fact[39] that if $F(A)$ is concave and homogeneous in the sense $F(xA)=xF(A)$, then

$$\lim_{x\to0}\frac{F(A+xB)-F(A)}{x}\geqslant F(B). \tag{18}$$

Applying this to the functions in Theorem 2 with $A=S$, $B=T$, $K=\log R-\log S$ yields

$$\mathrm{Tr}\ \ e^{\log R-\log S+\log T}\leqslant\lim_{x\to0}\frac{\mathrm{Tr}\ \ e^{\log R-\log S+\log(S+xT)}-\mathrm{Tr}R}{x}. \tag{19}$$

To complete the proof, we need the well-known integral representation

$$\log(S+xT)-\log S=\int_0^\infty\frac{1}{S+uI}\,xT\,\frac{1}{S+xT+uI}\,du. \tag{20}$$

Substituting (20) into (19) and noting that

$$\mathrm{Tr}\ e^{\log R+x\int_0^\infty[1/(S+uI)]T[1/(S+xT+uI)]du}=\mathrm{Tr}R+x\mathrm{Tr}R\int_0^\infty\frac{1}{S+uI}\,T\,\frac{1}{S+uI}\,du+O(x^2)$$

yields the desired result. Q.E.D.

C. Purification

Araki and Lieb[5,27] observed that one could obtain useful new entropy inequalities by applying what is now known as the ''purification process'' to known inequalities. Any density ρ_1 can be extended to a pure state density matrix ρ_{12} on a tensor product space; moreover, $S(\rho_1)=S(\rho_2)$. Applying this to the subadditivity inequality (1), i.e., $S(\rho_{12})\leqslant S(\rho_1)+S(\rho_2)$, yields the equivalent result $S(\rho_3)\leqslant S(\rho_{23})+S(\rho_2)$ which can be combined with (1) to give the triangle inequality[5,27]

$$|S(\rho_1)-S(\rho_2)|\leqslant S(\rho_{12})\leqslant S(\rho_1)+S(\rho_2). \tag{21}$$

By purifying ρ_{123} to ρ_{1234} one can similarly show that SSA (3) is equivalent to

$$S(\rho_4)+S(\rho_2)\leqslant S(\rho_{12})+S(\rho_{14}). \tag{22}$$

D. Lindblad's representation of stochastic maps

Stochastic maps arise naturally in quantum information as a description of the effect on a subsystem A interacting with the environment in the pure state $\gamma_B=|\psi_B\rangle\langle\psi_B|$ via the unitary operation U_{AB},

$$\rho_A \to \mathrm{Tr}_B(U_{AB}\rho_A\otimes\gamma_B U_{AB}^\dagger). \tag{23}$$

Lindblad[31] used Stinespring's representation to show that any completely positive trace-preserving map Φ which maps an algebra into itself can be represented as if it arose in this way. That is, given such a map Φ one can always find an auxiliary system, $\mathcal{H}_B$, a density matrix γ_B on $\mathcal{H}_B$, and a unitary map U_{AB} on the combined system $\mathcal{H}_A\otimes\mathcal{H}_B$ (where A denotes the original system) such that

$$\Phi(\rho)=\mathrm{Tr}_B(U_{AB}\rho\otimes\gamma_B U_{AB}^\dagger) \tag{24}$$

where Tr_B denotes the partial trace over the auxiliary system.

Using the Kraus representation $\Phi(\rho)=\Sigma_k F_k\rho F_k^\dagger$ (and noting that the requirement that Φ be trace-preserving is equivalent to $\Sigma_k F_k^\dagger F_k=I$), one can give a construction equivalent to Lindblad's by initially defining U_{AB} as

$$U_{AB}|\psi\rangle\otimes|\beta\rangle\equiv\sum_k F_k|\psi\rangle\otimes|k\rangle, \tag{25}$$

where $|\beta\rangle$ is a fixed normalized state of the auxiliary system, and $\{|k\rangle\}$ is some orthonormal basis for the auxiliary system. Then U_{AB} is a partial isometry from $\mathcal{H}_A\otimes|\beta\rangle\langle\beta|$ to $\mathcal{H}_A\otimes\mathcal{H}_B$ which can be extended to a unitary operator on all of $\mathcal{H}_A\otimes\mathcal{H}_B$. This yields (24) with $\gamma_B=|\beta\rangle\langle\beta|$ a pure state.

However, U_{AB} can also be extended to $\mathcal{H}_A\otimes\mathcal{H}_B$ in other ways. In particular, it can be extended, instead, to the partial isometry for which $U_{AB}^\dagger U_{AB}$ is the projection onto $\mathcal{H}_A\otimes|\beta\rangle\langle\beta|$ so that $U_{AB}=0$ on the orthogonal complement of $\mathcal{H}_A\otimes|\beta\rangle\langle\beta|$. We describe this in more detail when Φ requires at most m Kraus operators F_k, in which case one can choose the auxiliary system to be $\mathbf{C}^m$. One can also choose $|k\rangle=|e_k\rangle$, and $|\beta\rangle=|e_1\rangle$ with $|e_k\rangle$ the standard basis of column vectors with elements $c_j=\delta_{jk}$. Then (25) depends only on the first column of U_{AB} which we denote V and regard as a map from $\mathcal{H}$ to $\mathcal{H}\otimes\mathbf{C}^m$. In block form

$$V_\rho V^\dagger=U_{AB}\rho\otimes|e_1\rangle\langle e_1|U_{AB}^\dagger=\begin{pmatrix}F_1\\F_2\\\vdots\\F_m\end{pmatrix}\rho(F_1^\dagger\ F_2^\dagger\ \cdots\ F_m^\dagger)=\begin{pmatrix}F_1\rho F_1^\dagger & F_1\rho F_2^\dagger & \cdots & F_1\rho F_m^\dagger\\F_2\rho F_1^\dagger & F_2\rho F_2^\dagger & \cdots & F_2\rho F_m^\dagger\\\vdots & \vdots & & \vdots\\F_m\rho F_1^\dagger & & \cdots & F_m\rho F_m^\dagger\end{pmatrix} \tag{26}$$

from which it easily follows that $\mathrm{Tr}_B(V\rho V^\dagger)=\Sigma_k F_k\rho F_k^\dagger=\Phi(\rho)$. The requirement that Φ be trace-preserving gives $V^\dagger V=\Sigma_k F_k^\dagger F_k=I$ which again implies that V is a partial isometry. Moreover, $V\rho V^\dagger$ has the same nonzero eigenvalues as $(V\sqrt{\rho})^\dagger(V\sqrt{\rho})=\rho$ so that $S[V\rho V^\dagger]=S(\rho)$.

This construction can be readily extended to situations in which Φ maps operators acting on one Hilbert space $\mathcal{H}_A$ to those acting on another space $\mathcal{H}_{A'}$, e.g., $\Phi:\mathcal{B}(\mathcal{H}_A)\mapsto\mathcal{B}(\mathcal{H}_{A'})$. In this case, the Kraus operators $F_k:\mathcal{H}_A\mapsto\mathcal{H}_{A'}$, and U_{AB} is a partial isometry from $\mathcal{H}_A\otimes|\beta\rangle\langle\beta|$ to a subspace of $\mathcal{H}_{A'}\otimes\mathcal{H}_B$. Alternatively, V can be defined as a partial isometry from $\mathcal{H}_A$ to $\mathcal{H}_{A'}\otimes\mathbf{C}^m$.

E. Measurements and their representations

A von Neumann or *projective measurement* is a partition of the identity $I=\Sigma_b E_b$ into mutually orthogonal projections, i.e., $E_b E_c=\delta_{bc}E_b$. A positive operator valued measurement (POVM) is a set of positive semi-definite operators E_b such that $\Sigma_b E_b=I$, i.e., the orthogonality condition is dropped. It is well-known that a general POVM can be represented as a projective measurement on a tensor product space.[32]

In fact, by noting that the map $\rho\mapsto\Sigma_b\sqrt{E_b}\rho\sqrt{E_b}$ is completely positive and trace-preserving with Kraus operators $F_b=\sqrt{E_b}$ one can use the construction above. Write $V=\Sigma_b\sqrt{E_b}\otimes|b\rangle$ where $|b\rangle$ is an orthonormal basis for $\mathbf{C}^M$ and M is the number of measurements in the POVM, i.e., $b=1,...,M$. Then $V\rho V^\dagger=\Sigma_{b,c}\sqrt{E_b}\rho\sqrt{E_c}\otimes|b\rangle\langle c|$. Now, if $F_b=I\otimes|b\rangle\langle b|$, then $\{F_b\}$ is a projective measurement on $\mathcal{H}\otimes\mathbf{C}^M$ and $\mathrm{Tr}F_b(V\rho V^\dagger)=\mathrm{Tr}E_b\rho$.

F. Adjoint maps

It is sometimes useful to consider the adjoint, which we denote $\widehat{\Phi}$, of a stochastic map Φ with respect to the Hilbert–Schmidt inner product $\langle A,B\rangle=\mathrm{Tr}A^\dagger B$. When Φ acts on $n\times n$ matrices, this adjoint (or dual) is fully defined by the requirement

$$\mathrm{Tr}[\Phi(A)]^\dagger B=\mathrm{Tr}A^\dagger\widehat{\Phi}(B) \tag{27}$$

for all $n\times n$ matrices, A,B. Indeed, when $\Phi(\rho)=\Sigma_k F_k\rho F_k^\dagger$, the adjoint is given by $\widehat{\Phi}(\rho)=\Sigma_k F_k^\dagger\rho F_k$. Moreover, Φ is trace-preserving if and only if $\widehat{\Phi}$ is unital, i.e., $\widehat{\Phi}(I)=I$. When Φ is the partial trace, T_2, its adjoint takes $A\mapsto A\otimes I_2$.

IV. SUBADDITIVITY PROOFS

To understand the proof of strong subadditivity, it is instructive to first understand how Klein's inequality can be used to prove two weaker inequalities. First, we consider the subadditivity inequality (1). Substituting $A=\rho_{12}$ and $B=\rho_1\otimes\rho_2$ into Klein's inequality (16) yields

$$-S(\rho_{12})+S(\rho_1)+S(\rho_2)\geqslant\mathrm{Tr}(\rho_{12}-\rho_1\otimes\rho_2)=0, \tag{28}$$

which is equivalent to subadditivity. Furthermore, the well-known conditions for equality in subadditivity follow from the conditions for equality in Klein's inequality, namely that equality holds if and only if ρ_{12} is a tensor product, that is, $\rho_{12}=\rho_1\otimes\rho_2$.

A second, more powerful subadditivity inequality was obtained by Araki and Lieb,[5]

$$S(\rho_{123})\leqslant S(\rho_{12})+S(\rho_{23}) \tag{29}$$

under the constraint $\mathrm{Tr}\rho_{123}=1$. To prove this, choose $A=\rho_{123}$ and $B=e^{\log\rho_{12}+\log\rho_{23}}$ in Klein's inequality to obtain

$$-S(\rho_{123})+S(\rho_{12})+S(\rho_{23})\geqslant 1-\mathrm{Tr}\ e^{\log\rho_{12}+\log\rho_{23}}. \tag{30}$$

Applying Theorem 4 to the right-hand side gives

$$-S(\rho_{123})+S(\rho_{12})+S(\rho_{23})\geqslant 1-\mathrm{Tr}_{123}\rho_{12}\rho_{23}=1-\mathrm{Tr}_2(\rho_2)^2\geqslant 1-\mathrm{Tr}_2\rho_2=0,$$

where the last line follows from $(\rho_2)^2\leqslant\rho_2$ (which is the *only* place the normalization condition $\mathrm{Tr}\rho_{123}=1$ is needed). Q.E.D.

The strategy for proving SSA is similar to that above, but with Theorem 4 replaced by Theorem 5. Let $A=\rho_{123}$ and choose B so that $\log B=\log\rho_{12}-\log\rho_2+\log\rho_{23}$. Then Klein's inequality implies

$$-S(\rho_{123})+S(\rho_{12})-S(\rho_2)+S(\rho_{23})\geqslant\mathrm{Tr}(\rho_{123}-e^{\log\rho_{12}-\log\rho_2+\log\rho_{23}}). \tag{31}$$

Applying Lieb's result (17) to the right-hand side above, we obtain

$$-S(\rho_{123})+S(\rho_{12})-S(\rho_2)+S(\rho_{23}) \geqslant \mathrm{Tr}\left(\rho_{123} - \int_0^\infty \rho_{12}\frac{1}{\rho_2+uI}\rho_{23}\frac{1}{\rho_2+uI}\,du \right)$$

$$= \mathrm{Tr}_{123}\rho_{123} - \mathrm{Tr}_2 \int_0^\infty \rho_2\frac{1}{\rho_2+uI}\rho_2\frac{1}{\rho_2+uI}\,du$$

$$= (\mathrm{Tr}_{123}\rho_{123} - \mathrm{Tr}_2\rho_2) = 0.$$

This proves SSA. Moreover, this approach allows us to easily determine the conditions for equality, and thus complete the proof of Theorem 1. The first inequality in the derivation above is satisfied with equality if and only if $A=B$, which is just the condition (4). Although the conditions for equality in (17) are more difficult to analyze, this is not necessary here. When $A=B$, it immediately follows that $\mathrm{Tr}A=\mathrm{Tr}B$ so that the second inequality in the above derivation automatically becomes an equality when (4) holds.

V. INEQUALITIES FOR RELATIVE ENTROPY

A. Monotonicity under partial trace

We now show how the same strategy can be applied to obtain a proof with equality conditions for the monotonicity of relative entropy under partial trace.

Theorem 6: *When* $\rho_{12},\gamma_{12}>0$ *and* $\mathrm{Tr}\rho_{12}=\mathrm{Tr}\gamma_{12}$,

$$H(\rho_2,\gamma_2) \leqslant H(\rho_{12},\gamma_{12}) \tag{32}$$

with equality if and only if $\log\rho_{12}-\log\gamma_{12}=\log\gamma_2+\log\rho_2$.

This condition should be interpreted as $\log\rho_{12}-\log\gamma_{12}=I_1\otimes[\log\gamma_2-\log\rho_2]$. Since, as noted in Sec. III F, when $\Phi=T_1$, the action $\hat{\Phi}$ is precisely $I_1\otimes$, the equality condition can be written as $\log\rho_{12}-\log\gamma_{12}=\hat{T}_1[\log T_1(\gamma_{12})-\log T_1(\rho_{12})]$ which is a special case of the more general form (40) developed later.

SSA can be regarded as a special case of this monotonicity result via the correspondence $\rho_{12}\to\rho_{123}$, $\gamma_{12}\to\rho_{12}$, and Petz's form of the equality condition becomes $\rho_2^{it}\gamma_2^{-it}=\rho_{12}^{it}\gamma_{12}^{-it}$. It is interesting to note that in Ref. 29, Lieb and Ruskai actually obtained Eq. (32) *from* SSA using the convexity of the conditional entropy $S(\rho_1)-S(\rho_{12})$ and the inequality (18).

Proof: Let $A=\rho_{12}$, $\log B=\log\gamma_{12}-\log\gamma_2+\log\rho_2$. Then Klein's inequality and (17) imply

$$H(\rho_{12},\gamma_{12})-H(\rho_2,\gamma_2) \geqslant \mathrm{Tr}_{12}(\rho_{12}-e^{\log\gamma_{12}-\log\gamma_2+\log\rho_2})$$

$$\geqslant \mathrm{Tr}_{12}\left(\rho_{12} - \int_0^\infty \gamma_{12}\frac{1}{\gamma_2+uI}\rho_2\frac{1}{\gamma_2+uI}\,du \right)$$

$$= \mathrm{Tr}_{12}\rho_{12} - \mathrm{Tr}_2\int_0^\infty \gamma_2\frac{1}{\gamma_2+uI}\rho_2\,\frac{1}{\gamma_2+uI}\,du = \mathrm{Tr}_{12}\rho_{12}-\mathrm{Tr}_2\rho_2 = 0.$$

The equality condition is again precisely the condition $A=B$. Q.E.D.

B. Joint convexity of the relative entropy

The joint convexity of relative entropy can be obtained directly from Theorem 6 by choosing ρ_{12} (and similarly γ_{12}) to be a block diagonal matrix with blocks $\lambda_k\rho^{(k)}$ (and $\lambda_k\gamma^{(k)}$). We can interpret the partial trace as a sum over blocks so that $\rho\equiv\rho_2=\Sigma_k\lambda_k\rho^{(k)}$. However, it is worth giving a direct proof of the joint convexity since it demonstrates the central role of Theorem 2.

Theorem 7: *The relative entropy is jointly convex in its arguments, i.e., if* $\rho=\Sigma_k\lambda_k\rho^{(k)}$ *and* $\gamma=\Sigma_k\lambda_k\gamma^{(k)}$, *then*

$$H(\rho,\gamma)\leqslant\sum_k \lambda_k H(\rho^{(k)},\gamma^{(k)}) \tag{33}$$

with equality if and only if $\log\rho-\log\gamma=\log\rho^{(k)}-\log\gamma^{(k)}$ *for all k.*

Proof: Let $A=\rho^{(k)}$ and $\log B=\log\rho-\log\gamma+\log\gamma^{(k)}$ with $\rho=\Sigma_k\lambda_k\rho^{(k)}$ and $\gamma=\Sigma_k\lambda_k\gamma^{(k)}$. Then Klein's inequality implies

$$H(\rho^{(k)},\gamma^{(k)})-\mathrm{Tr}\rho^{(k)}[\log\rho-\log\gamma]\geqslant\mathrm{Tr}(\rho-e^{\log\rho-\log\gamma+\log\gamma^{(k)}}). \tag{34}$$

Multiplying this by λ_k with $\lambda_k>0$ and $\Sigma_k\lambda_k=1$ yields, after summation,

$$\begin{aligned}\sum_k \lambda_k H(\rho^{(k)},\gamma^{(k)})-H(\rho,\gamma)&\geqslant\mathrm{Tr}\left(\rho-\sum_k \lambda_k e^{\log\rho-\log\gamma+\log\gamma^{(k)}}\right)\\&\geqslant\mathrm{Tr}\left(\rho-e^{\log\rho-\log\gamma+\log\sum_k \lambda_k\gamma^{(k)}}\right)\\&=\mathrm{Tr}(\rho-e^{\log\rho})=0,\end{aligned}$$

where the second inequality is precisely the concavity of $C\to F(C)=\mathrm{Tr}\ e^{K+\log C}$ with $K=\log\rho-\log\gamma$ and $C=\Sigma_k\lambda_k\gamma^{(k)}$. Q.E.D.

C. Relationships among inequalities

We make some additional remarks about connections between SSA and various properties of relative entropy. To facilitate the discussion, we will use MONO to denote the general monotonicity inequality (7), MPT to denote the special case of monotonicity under partial traces, i.e., Theorem 6, and JC to denote the joint convexity, Theorem 7. Using the restatement of SSA in the form (6), it is easy to see that MONO⇒MPT⇒SSA. Before Theorem 7, we showed that MPT⇒JC. Similarly, by choosing ρ_{123} to be block diagonal with blocks ρ^k_{123} one can show that SSA implies that the map $\rho_{12}\mapsto S(\rho_1)-S(\rho_{12})$ is convex. In Ref. 29 it was observed that applying the convexity inequality (18) to this map (with $A+xB=\rho_{12}+x\gamma_{12}$) yields (32). This shows that SSA⇒MPT, so that we have the chain of implications

$$\mathrm{MONO}\Rightarrow\mathrm{MPT}\Leftrightarrow\mathrm{SSA}\Rightarrow\mathrm{JC}. \tag{35}$$

One can show that JC⇒MPT by using Uhlmann's observation[43] that the partial trace can be written as a convex combination of unitary transformations.

One can also show directly that JC⇒SSA by using the purification process described in Sec. III C to show that SSA is equivalent to

$$\rho_4+\rho_2\leqslant\rho_{12}+\rho_{14}. \tag{36}$$

Moreover, if ρ_{124} is pure, then $\rho_4=\rho_{12}$ and $\rho_2=\rho_{14}$ so that equality holds in (36). Since the extreme points of the convex set of density matrices are pure states, the inequality (36) then follows from the joint convexity, Theorem 7. Thus we have

$$\mathrm{MONO}\Rightarrow\mathrm{MPT}\Leftrightarrow\mathrm{SSA}\Leftrightarrow\mathrm{JC}. \tag{37}$$

Lindblad[31] completed this circuit by showing that MPT⇒MONO.

Using the representation described in Sec. III D, with V the partial isometry from $\mathcal{H}$ to $\mathcal{H}\otimes\mathbf{C}^m$ as in (26), one finds

$$H[\Phi(\rho),\Phi(\gamma)] = H[\mathrm{Tr}_B(V\rho V^\dagger),\ \mathrm{Tr}_B(V\gamma V^\dagger)]$$
$$\leqslant H[V\rho V^\dagger, V\gamma V^\dagger] \tag{38}$$
$$= H(\rho,\gamma). \tag{39}$$

since $\mathrm{Tr}V\rho V^\dagger \log(V\gamma V^\dagger) = \mathrm{Tr}\rho \log \gamma$ for a partial isometry V.

VI. EQUALITY IN MONOTONICITY UNDER STOCHASTIC MAPS

Conditions for equality in the general monotonicity inequality (7) may be more subtle since it is not always possible to achieve equality. Indeed, it was noted in Ref. 25 that $\sup_{\rho\neq\gamma} H[\Phi(\rho),\Phi(\gamma)]/H(\rho,\gamma)$ can be strictly less than 1. Using the reformulation (38) above, we prove the following result.

Theorem 8: *Equality holds in (7), $H[\Phi(\rho),\Phi(\gamma)] \leqslant H(\rho,\gamma)$, if and only if*

$$\log\rho - \log\gamma = \widehat{\Phi}\,[\log\Phi(\rho) - \log\Phi(\gamma)] \tag{40}$$

where $\widehat{\Phi}$ denotes the adjoint of Φ with respect to the Hilbert–Schmidt inner product as defined in (27).

To verify sufficiency, multiply (40) by ρ and take the trace to obtain

$$H(\rho,\gamma) = \mathrm{Tr}\rho\,\widehat{\Phi}\,[\log\Phi(\rho) - \log\Phi(\gamma)] = \mathrm{Tr}\Phi(\rho)[\log\Phi(\rho) - \log\Phi(\gamma)] = H[\Phi(\rho),\Phi(\gamma)].$$

It is tempting to follow our previous strategy and choose $A=\rho$, $\log B = \log\gamma + \widehat{\Phi}[\log\Phi(\rho) - \log\Phi(\gamma)]$. However, we have been unable to verify that $\mathrm{Tr}\, e^{\log\gamma + \widehat{\Phi}[\log\Phi(\rho) - \log\Phi(\gamma)]} \leqslant 1$ as required by this approach.

Instead, we use the representation (24) or (26). Rather than applying the equality conditions in Theorem 6 directly to (38), it is useful to repeat the argument for an appropriate choice of A and B.

Proof: Choose $A = V\rho V^\dagger$, $\log B = \log(V\gamma V^\dagger) + \log \mathrm{Tr}_2(V\rho V^\dagger) - \log \mathrm{Tr}_2(V\gamma V^\dagger)$ where V is again the partial isometry as in (26) of Sec. III D. B is defined so that the last two terms in $\log B$ are extended from $\mathcal{H}$ to $\mathcal{H}\otimes\mathbf{C}^m$ so that $\ker(B)\subset\ker(A)$. The condition for equality in (38) is then

$$\log(V\rho V^\dagger) - \log(V\gamma V^\dagger) = \log \mathrm{Tr}_2(V\rho V^\dagger) - \log \mathrm{Tr}_2(V\gamma V^\dagger) = \log\Phi(\rho) - \log\Phi(\gamma). \tag{41}$$

We can put this into a more useful form by noting that for a partial isometry V,

$$\log(V\rho V^\dagger) - \log(V\gamma V^\dagger) = V[\log\rho - \log\gamma]V^\dagger, \tag{42}$$

from which it follows that (41) is equivalent to

$$V[\log\rho - \log\gamma]V^\dagger = \log\Phi(\rho) - \log\Phi(\gamma). \tag{43}$$

Multiplying by $V^\dagger$ on the left and V on the right and using that $V^\dagger V = I$, one sees that (43) implies

$$\log\rho - \log\gamma = V^\dagger[\log\Phi(\rho) - \log\Phi(\gamma)]V. \tag{44}$$

Taking the partial trace Tr_2 over the auxiliary space in (44) yields (40) since $\widehat{\Phi}(P) = \Sigma_k F_k^\dagger P F_k = V^\dagger P V$ for all P in $\mathcal{H}$. Q.E.D.

Another useful necessary condition for equality in (7) can be obtained by multiplying both sides of (43) by the projection $VV^\dagger$. Since $V^\dagger V = I$, one finds

$$VV^\dagger[\log\Phi(\rho) - \log\Phi(\gamma)] = V[\log\rho - \log\gamma]V^\dagger = [\log\Phi(\rho) - \log\Phi(\gamma)]VV^\dagger, \tag{45}$$

i.e., the projection $VV^\dagger$ commutes with $[\log\Phi(\rho)-\log\Phi(\gamma)]$. Taking the partial trace and noting that $\Phi(I)=\mathrm{Tr}_2 VV^\dagger$ we can summarize this discussion in the following.

Corollary 9: If equality holds in (7), then

$$\Phi(\log\rho-\log\gamma)=\Phi(I)[\log\Phi(\rho)-\log\Phi(\gamma)]=[\log\Phi(\rho)-\log\Phi(\gamma)]\Phi(I). \tag{46}$$

Moreover, $\log\Phi(\rho)-\log\Phi(\gamma)$ *commutes with the projection* $VV^\dagger=\Sigma_{k,\ell}|k\rangle\langle\ell|F_k F_\ell^\dagger$ *where* $\{F_k\}$ *is a set of Kraus operators for* Φ*, i.e.,* $\Phi(\rho)=\Sigma_k F_k\rho F_k^\dagger$ *and* $|k\rangle$ *is an orthonormal basis for the auxiliary space* $\mathcal{H}_2$.

The results of this section also hold in the more general situation when $\Phi:\mathcal{B}(\mathcal{H}_A)\mapsto\mathcal{B}(\mathcal{H}'_A)$ maps operators on one Hilbert space to those on another, in which case $F_k:\mathcal{H}_A)\mapsto\mathcal{H}'_A$.

VII. THE HOLEVO BOUND

A. Background

One reason for studying conditions for equality is that other results, such as Holevo's celebrated bound[14] on the accessible information, can be obtained rather easily from SSA or some form of the monotonicity of relative entropy. However, obtaining the corresponding conditions for equality is not as straightforward as one might hope because of the need to introduce an auxiliary system. Although Holevo's bound is quite general, it is often applied in situations where $\tilde\rho_j=\Phi(\rho_j)$ is the output of a noisy quantum channel Φ with input ρ_j. We use the tilde $\tilde{}$ as a reminder of this, as well as to ensure a distinction from other density matrices which arise.

For any fixed POVM and density matrix γ, $p(b)=\mathrm{Tr}(\gamma E_b)$ defines a classical probability distribution whose entropy we denote $S[\mathrm{Tr}\gamma E_b]$. The Holevo bound states that for any ensemble of density matrices $\mathcal{E}=\{\pi_j\tilde\rho_j\}$ with average density matrix $\tilde\rho=\Sigma_j\pi_j\tilde\rho_j$, the accessible information in the ensemble satisfies

$$I(\mathcal{E},\mathcal{M})\equiv S[\mathrm{Tr}\tilde\rho E_b]-\sum_j \pi_j S[\mathrm{Tr}\tilde\rho_j E_b] \tag{47}$$

$$\leqslant S(\tilde\rho)-\sum_j \pi_j S(\tilde\rho_j) \tag{48}$$

for any POVM $\mathcal{M}=\{E_b\}$. If all of the $\tilde\rho_j$ commute, then it is easy to see that equality can be achieved by choosing the E_b to be the spectral projections which simultaneously diagonalize the density matrices $\tilde\rho_j$. We wish to show that this condition is also necessary, i.e., equality can only be achieved in (48) if all the $\tilde\rho_j$ commute.

It is known[21,50] that (48) can be obtained from (7). First, observe that

$$S(\tilde\rho)-\sum_j \pi_j S(\tilde\rho_j)=\sum_j \pi_j H(\tilde\rho_j,\tilde\rho). \tag{49}$$

Now let $\Omega_{\mathcal{M}}$ be the map $\Omega_{\mathcal{M}}(A)=\Sigma_b|b\rangle\langle b|\mathrm{Tr}(AE_b)$ where $\mathcal{M}=\{E_b\}$. Then $\Omega_{\mathcal{M}}$ is a stochastic map of the special type known as a Q-C channel[15] and the Holevo bound (48) follows immediately from (49) and

$$H[\Omega_{\mathcal{M}}(\tilde\rho_j),\Omega_{\mathcal{M}}(\tilde\rho)]\leqslant H(\tilde\rho_j,\tilde\rho). \tag{50}$$

B. Equality conditions

We will henceforth assume that $\{\pi_j,\tilde\rho_j\}$ is a fixed ensemble and seek conditions under which we can find a POVM satisfying the equality requirements. Since $\widehat{\Omega}_{\mathcal{M}}(D)=\Sigma_b E_b\langle b,Db\rangle$, applying Theorem 8 yields conditions for equality in (50). For equality in (48) these conditions must hold for every j and reduce to

$$\log\tilde{\rho}_j - \log\tilde{\rho} = \sum_b E_b \log\frac{\mathrm{Tr}E_b\tilde{\rho}_j}{\mathrm{Tr}E_b\tilde{\rho}}\,\forall j, \tag{51}$$

where this should be interpreted as a condition on $\ker(\tilde{\rho}_j)^\perp$ in which case all terms are well-defined. (Indeed, since the condition arises from the use of Klein's inequality and the requirement $A=B$, the operators in B must be defined to be zero on $\ker(A)$, which reduces to $\ker(\tilde{\rho}_j)$ in the situation considered here.) If the POVM $\{E_b\}$ consists of a set of mutually orthogonal projections, then it is immediate that the operators $Z_j \equiv \log\tilde{\rho}_j - \log\tilde{\rho}$ commute, since (51) can be regarded as the spectral decomposition of Z_j. To show that the $\tilde{\rho}_j$ themselves commute, observe that

$$\begin{aligned}
1 = \mathrm{Tr}\tilde{\rho}_j &= \mathrm{Tr}\ \ e^{\log\tilde{\rho}+[\log\tilde{\rho}_j-\log\tilde{\rho}]} \\
&\leqslant \mathrm{Tr}\tilde{\rho}e^{\log\tilde{\rho}_j-\log\tilde{\rho}} \\
&= \mathrm{Tr}\tilde{\rho}e^{\Sigma_b E_b \log(\mathrm{Tr}E_b\tilde{\rho}_j/\mathrm{Tr}E_b\rho)} \\
&= \mathrm{Tr}\tilde{\rho}\ \sum_b E_b\frac{\mathrm{Tr}E_b\tilde{\rho}_j}{\mathrm{Tr}E_b\tilde{\rho}} = \sum_b \mathrm{Tr}E_b\tilde{\rho}_j = 1,
\end{aligned}$$

where we have used Theorem 4 with $A=\log\tilde{\rho}$, $B=\log\tilde{\rho}_j-\log\tilde{\rho}$, and the fact that for orthogonal projections $e^{\Sigma_b a_b E_b}=\Sigma_b e^{a_b}E_b$. The conditions for equality in Theorem 4 then imply that $\log\tilde{\rho}_j$ and $\log\tilde{\rho}$ commute for all j. Hence $\tilde{\rho}_j$ and $\tilde{\rho}_k$ also commute for all j,k when the POVM consists of mutually orthogonal projections.

Using King's observation in the next section, one can reduce the general case to that of projective measurements. However, we prefer to use the equality conditions to show directly that the elements of the POVM must be orthogonal. Moreover, the commutativity condition involving $VV^\dagger$ is reminiscent of the more sophisticated Connes cocyle approach used by Petz, and thus of some interest.

Since the Kraus operators for the Q-C map $\Omega_{\mathcal{M}}$ can be chosen as $F_{kb}=|b\rangle\langle k|\sqrt{E_b}$ where $|b\rangle$ and $|k\rangle$ are orthonormal bases, one finds

$$VV^\dagger = \sum_{b,c}\ \sum_{k,\ell}\ |b\rangle\langle c|\langle k\sqrt{E_b}\sqrt{E_c}\ell\rangle = \sum_{b,c}\ |b\rangle\langle c|\langle\phi\sqrt{E_b}\sqrt{E_c}\phi\rangle, \tag{52}$$

where $|\phi\rangle=\Sigma_k|k\rangle$. By (45), this must commute for all j with $\log\Omega_{\mathcal{M}}(\tilde{\rho}_j)-\log\Omega_{\mathcal{M}}(\tilde{\rho}_j)$ which can be written in the form $\Sigma_b z_{bj}|b\rangle\langle b|$ with $z_{bj}=\log(\mathrm{Tr}E_b\tilde{\rho}_j/\mathrm{Tr}E_b\rho)$. A diagonal operator of the form $\Sigma_b z_b|b\rangle\langle b|$ with all $z_b\neq 0$ will commute with the projection in (52) if and only if all off-diagonal terms are zero. This will hold if the POVM is a projective measurement, since then $\sqrt{E_b}\sqrt{E_c}=E_bE_c=E_b\delta_{bc}$. To see that this is necessary, note that the possibility that the vector ϕ is orthogonal to all E_b is precluded by the condition that $\Sigma_b E_b=I$. Moreover, since the orthonormal basis $|k\rangle$ is arbitrary, ϕ can be chosen to be arbitrary. The restriction that (51) hold only on $\ker(\tilde{\rho}_j)^\perp$ may permit some $z_{bj}=0$; however, for each b there will always be at least one j for which $z_{bj}\neq 0$, and this suffices. Q.E.D.

One can obtain an alternate form of the equality conditions from Corollary 9. Since $\Phi(I)=\Sigma_b|b\rangle\langle b|\mathrm{Tr}E_b$, another necessary condition for equality in (48) is

$$\mathrm{Tr}E_b[\log\tilde{\rho}_j-\log\tilde{\rho}] = \mathrm{Tr}E_b(\log\mathrm{Tr}E_b\tilde{\rho}_j-\log\mathrm{Tr}E_b\tilde{\rho})\ \ \forall j,b. \tag{53}$$

Inserting this in (51) yields the requirement

$$\log\tilde{\rho}_j-\log\tilde{\rho} = \sum_b \frac{1}{\mathrm{Tr}E_b}E_b\mathrm{Tr}E_b[\log\tilde{\rho}_j-\log\tilde{\rho}], \tag{54}$$

which can be rewritten as

$$Z_j = \sum_b \frac{|E_b\rangle}{\mathrm{Tr}E_b}\langle E_b, Z_j\rangle \quad \forall j, \tag{55}$$

where $Z_j = \log\tilde{\rho}_j - \log\tilde{\rho}$ and the bra-ket now refer to the Hilbert–Schmidt inner product. This implies that $\Sigma_b|E_b\rangle\langle E_b|/\mathrm{Tr}E_b$ projects onto the span($\{Z_j\}$). However, this alone is not sufficient to imply that the E_b form a projective measurement.

C. Other approaches

Chris King has observed[19] that when the POVM is a projective measurement of the form $E_b = |b\rangle\langle b|$, one can obtain the Holevo bound from the joint convexity of relative entropy. Let $\beta(\tilde{\rho}) = \Sigma_b|b\rangle\langle b|\mathrm{Tr}E_b\tilde{\rho}$. Then applying Theorem 7 to $H[\tilde{\rho}, \beta(\tilde{\rho})]$ yields

$$-S(\tilde{\rho}) + S(\mathrm{Tr}E_b\tilde{\rho}) \leqslant \sum_j \pi_j[-S(\tilde{\rho}_j) + S(\mathrm{Tr}E_b\tilde{\rho}_j)] \tag{56}$$

or

$$S(\mathrm{Tr}E_b\tilde{\rho}) - \sum_j \pi_j S(\mathrm{Tr}E_b\tilde{\rho}_j) \leqslant S(\tilde{\rho}) - \sum_j \pi_j S(\tilde{\rho}_j)$$

with equality if and only if

$$\log\tilde{\rho} - \sum_b |b\rangle\langle b|\log \mathrm{Tr}E_b\tilde{\rho} = \log\tilde{\rho}_j - \sum_b |b\rangle\langle b|\log \mathrm{Tr}E_b\tilde{\rho}_j \quad \forall j. \tag{57}$$

This is equivalent to (51) when $E_b = |b\rangle\langle b|$, and the argument can be extended to more general projective measurements.

King also pointed out that if $\{E_b\}$ is an arbitrary POVM, the construction in Sec. III E can be used to show that (48) and (51) are equivalent to the equalities obtained when $\tilde{\rho}_j$ is replaced by $V\tilde{\rho}_j V^\dagger$ and E_b by F_b. Since the $\{F_b\}$ form a projective measurement, we can conclude from the argument above that equality implies that all $V\tilde{\rho}_j V^\dagger$ commute, which implies that all $\tilde{\rho}_j$ also commute since $V^\dagger V = I$.

It should be noted that Petz was able to use his equality conditions to find the conditions for equality in the Holevo bound and this is sketched in Ref. 34. Indeed, Petz's analog of (57) is $\tilde{\rho}^{it}D^{-it} = \tilde{\rho}_j^{it}D_j^{-it} \forall j$ where D, D_j denotes the diagonal parts of $\tilde{\rho}$, $\tilde{\rho}_j$, respectively. Then

$$\tilde{\rho}_j^{it} = \tilde{\rho}^{it}D^{-it}D_j^{it}. \tag{58}$$

Since (58) holds for all real t, as well as all j, it also implies $\tilde{\rho}_j^{-it} = \tilde{\rho}^{-it}D^{it}D_j^{-it}$. However, taking the adjoint of (58) yields $\tilde{\rho}_j^{-it} = D_j^{-it}D^{it}\tilde{\rho}^{-it}$. Therefore, $\tilde{\rho}^{-it}$ commutes with the diagonal matrix $D^{it}D_j^{-it} = D_j^{-it}D^{it}$ and must also be diagonal. This gives a simultaneous diagonalization of all $\tilde{\rho}_j^{it}$ which means that all $\tilde{\rho}_j$ commute.

Holevo's original longer derivation[14] of the bound (48) also concluded that commutativity was necessary and sufficient for equality. Some simplifications of this argument were given by Fuchs[12] in his thesis.

D. Another bound on accessible information

When ρ is a density matrix, the mapping $A \mapsto \rho^{-1/2}A\rho^{-1/2}$ and its inverse gives a duality between ensembles and POVMs. Hall[13] observed that this duality can be used to give another upper bound on the accessible information (47) in terms of the POVM and average density ρ, i.e.,

$$I(\mathcal{E},\mathcal{M}) \leqslant S(\rho) - \sum_b \tau_b S\left(\frac{1}{\tau_b}\sqrt{\rho}E_b\sqrt{\rho}\right) \tag{59}$$

$$= \sum_b \tau_b H\left(\frac{1}{\tau_b}\sqrt{\rho}E_b\sqrt{\rho},\rho\right), \tag{60}$$

where $\tau_b = \mathrm{Tr}\, E_b\rho$. This inequality can be obtained from the monoticity of relative entropy under the Q-C map $\Omega_{\mathcal{E}}(A) = \Sigma_j |j\rangle\langle j| \pi_j \rho^{-1/2}\rho_j\rho^{-1/2}$ applied to $H((1/\tau_b)\sqrt{\rho}E_b\sqrt{\rho},\rho)$ as in (50); or as in Ref. 21 where an equivalent bound was given. The argument in Sec. VII B can then be used to show that equality can be achieved in (59) if and only if all $\sqrt{\rho}E_b\sqrt{\rho}$ commute. Hall[13] also found this condition and noted that it implies that ρ commutes with every E_b in the POVM.

One is often interested in (48) and (59) when one wants to optimize the accessible information after using a noisy quantum channel, Φ. It was observed in Ref. 21 that, since $\mathrm{Tr}\Phi(\rho_j)E_b = \mathrm{Tr}\rho_j\,\widehat{\Phi}(E_b)$, one can regard the noise as either acting to transform pure inputs ρ_j to mixed state outputs $\Phi(\rho_j)$ or as acting through the adjoint $\widehat{\Phi}$ on the POVM with uncorrupted outputs. In the first case, one can bound the right side of (59) by choosing the E_b to be the spectral projections of the average output state $\Phi(\rho)$ to yield $I[\Phi(\mathcal{E}),\mathcal{M}] \leqslant S[\Phi(\rho)]$ which is weaker than the corresponding Holevo bound. Moreover, since the optimal choice for $\Phi(\rho_j)$ need not be in the image of Φ, it is not necessarily achievable even though the commutativity condition holds. Hall[13] discussed other situations in which the bound can not be achieved despite the fact that all $\sqrt{\rho}E_b\sqrt{\rho}$ commute.

Viewing the noise as acting on the POVM, King and Ruskai[21] defined

$$U_{EP}(\Phi) = \sup_{\rho,\mathcal{M}}\left[S(\rho) - \sum_b \tau_b S\left(\frac{1}{\tau_b}\sqrt{\rho}\,\widehat{\Phi}(E_b)\sqrt{\rho}\right)\right] \tag{61}$$

with $\tau_b = \mathrm{Tr}\rho\,\widehat{\Phi}(E_b) = \mathrm{Tr}\Phi(\rho)E_b$. If the supremum in (61) is achieved with an average density and POVM for which $\sqrt{\rho}\,\widehat{\Phi}(E_b)\sqrt{\rho}$ do not commute, then $U_{EP}(\Phi)$ is strictly greater than the accessible information. The questions of whether or not (61) can actually exceed the optimal accessible information, and how it might then be interpreted, are under investigation.

VIII. CONCLUDING REMARKS

The proof presented here for each inequality, SSA, Theorem 6, Theorem 7 and the general monotonicity (7), is quite short—only half a page using results from Sec. III which require less than one additional page *and* Theorem 2. However, as shown in the Appendix, even this result does *not* require a long argument if one is permitted to use some powerful tools of complex analysis.

It is certainly not unusual to find that complex analysis can be extremely useful, even when the functions of interest are real-valued. Indeed, Lieb's original proof of the concavity of WYD entropy used a complex interpolation argument. In his influential book[42] on trace ideals, Simon (extracting ideas from Uhlmann[44]) gave a longer ''elementary'' proof using the Schwarz inequality, perhaps inadvertently reinforcing the notion that any complete proof of SSA is long and forbidding. Similar ideas are implicit in Ando,[3] who restates the result in terms of tensor product spaces and block matrices. Uhlmann[44] again demonstrated the power of complex interpolation by using it to prove the monotonicity of relative entropy under trace-preserving maps which satisfy the slightly weaker condition of two-positivity (rather than complete positivity). SSA then follows immediately as a special case. However, Uhlmann's approach, which has been extended by Petz,[35,33] was developed within the framework of the relative modular operator formalism introduced by Araki[4,7,33] for much more general situations. Recently, Lesniewski and Ruskai[25] observed that within this relative modular operator framework, monotonicity can be established directly using an argument based on the Schwarz inequality.

The approach of this review is similar to that of Wehrl[47] in that we view Theorem 2 as the ''essential ingredient.'' Indeed, Uhlmann,[43,47] using a completely different approach, had independently recognized that Theorem 2 would imply SSA. However, Wehrl's otherwise excellent review stated (at the end of Sec. III B) that ''Unfortunately, the proof of [this] is not easy at all.'' Later (in Sec. III C) Wehrl again states that ''...the proof is surprisingly complicated. I want to indicate only that the concavity of Tr $e^{K+\log A}$ can be obtained from Lieb's theorem [on concavity of the WYD entropy] through a sequence of lemmas.'' Although aware that Epstein's approach,[11] which was developed shortly after Lieb announced his results, permitted a ''direct'' proof of Theorem 2, Wehrl does not seem to have fully appreciated it. The utility of Epstein's technique may have been underestimated, in part, because he presented his results in a form which applied to the full collection of convex trace functions studied in Ref. 26. Checking Epstein's hypotheses for the WYD function requires some nontrivial mapping theorems. This may have obscured the elegance of the argument in Appendix A.

It is worth noting that if the concavity of WYD entropy is regarded as the key result, it is not necessary to use the long sequence of lemmas Wehrl refers to in order prove SSA. Lindblad[30] gave a direct proof of the joint convexity, Theorem 7, directly by differentiating the WYD function. Once this is done, SSA follows via the purification argument sketched after Eq. (36) or, alternatively, the variant of Uhlmann's argument described in Refs. 42 and 47. Combining this with Lieb's original complex interpolation proof of the concavity of the WYD function yields another ''short'' proof of SSA, albeit one which does not appear to be well-suited to establishing conditions for equality.

Finally, we mention that Carlen and Lieb[8] obtained another proof of SSA by using Epstein's technique to prove some Minkowski type inequalities for L_p trace norms. Using a different approach, King[17,18] recently proved several additivity results for the minimal entropy and Holevo capacity of a noisy channel by using L_p inequalities in which Epstein's technique provided a critical estimate. This suggests that connections with L_p inequalities, as advocated by Amosov, Holevo and Werner,[2] may be a promising avenue for studying entropy and capacity in quantum information. Despite the results mentioned above, many open conjectures remain; see Refs. 2, 8, 17, 18, and 48 for further details.

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APPENDIX: EPSTEIN'S PROOF OF CONCAVITY OF $A \to \mathrm{Tr}\, e^{K+\log A}$

Let $f(x) = \mathrm{Tr}\, e^{K+\log(A+xB)}$ with $A > 0$ strictly positive and K, B self-adjoint. For sufficiently small x, the function $f(x)$ is well-defined and the concavity of $F(A)$ in Theorem 2 follows immediately if $f''(0) < 0$ for all choices of $B = B^*$.

Instead of dealing with f directly, Epstein considered the function $g(x)=xf(x^{-1})$ which is well-defined for $|x|>\mu^{-1}\equiv\|A^{-1}\|\|B\|$ and can be analytically continued to the upper half plane so that

$$g(z)=\mathrm{Tr}\ \ e^{K+\log(zA+B)}. \tag{A1}$$

There are a number of equivalent (when meaningful) ways of defining functions of matrices. For the purposes needed here it is natural to assume that the spectrum $\sigma(A)$ of the operator A is contained in the domain of an analytic function $F(z)$ and that

$$F(A)=\frac{1}{2\pi i}\oint\frac{F(z)}{zI-A}dz. \tag{A2}$$

One can then use the spectral mapping theorem $\sigma[F(A)]\subset F[\sigma(A)]$ for an appropriate sequence of functions to verify that

$$\begin{aligned}
&\Im z>0 \Rightarrow \Im\ \omega(zA+B) > 0\\
&\Rightarrow\ \pi > \Im\ \omega[\log(zA+B)] > 0\\
&\Rightarrow\ \pi > \Im\ \omega[K+\log(zA+B)] > 0\\
&\Rightarrow \Im\ \omega[e^{K+\log(zA+B)}] > 0\\
&\Rightarrow \Im\ \mathrm{Tr}\ \ e^{K+\log(zA+B)} > 0,
\end{aligned}$$

where $\Im$ denotes the imaginary part of a complex number and ω is used to denote an arbitrary element of the spectrum of the indicated operator. Thus, $g(z)$ maps the upper half plane into the upper half plane. Functions with this property have been studied extensively under various names, including, ''operator monotone,'' ''Herglotz'' or ''Pick.'' (See, for example, Refs. 3, 10 and 33.) It then follows that g has an integral representation of the form

$$g(z)=a+bz+\int_{-\mu}^{\mu}\frac{1}{t-z}dm(t) \tag{A3}$$

for some positive measure $\mu(t)$. This yields (via the change of variables $s=t^{-1}$)

$$f(x)=ax+b+\int_{-\mu}^{\mu}\frac{x^2}{tx-1}dm(t). \tag{A4}$$

Differentiation under the integral sign can then be used to establish that $f''(0)<0$ as desired by observing $x^2/(tx-1)=t^{-2}[(xt+1)+(xt-1)^{-1}]$. Q.E.D.

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Quantum operations that cannot be implemented using a small mixed environment

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To implement any quantum operation (a.k.a. ''superoperator'' or ''CP map'') on a d-dimensional quantum system, it is enough to apply a suitable overall unitary transformation to the system and a d^2-dimensional environment which is initialized in a fixed pure state. It has been suggested that a d-dimensional environment might be enough if we could initialize the environment in a mixed state of our choosing. In this note we show with elementary means that certain explicit quantum operations cannot be realized in this way. Our counterexamples map some pure states to pure states, giving strong and easily manageable conditions on the overall unitary transformation. Everything works in the more general setting of quantum operations from d-dimensional to d'-dimensional spaces, so we place our counterexamples within this more general framework. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1499763]

I. QUANTUM OPERATIONS

Quantum operations (see, e.g., Schumacher, 1996) are also known as ''superoperators,'' ''superscattering operators'' or ''completely positive maps'' (''CP maps''). They can be viewed as a generalization of unitary transformations and are the most general transformations that can be applied to a quantum system in an unknown (possibly mixed) state. More precisely, quantum operations are the most general transformations that can be implemented deterministically, thus excluding operations which only succeed with a certain probability, like those depending on a measurement outcome. Under a quantum operation pure states are frequently mapped to mixed states.

All quantum operations on a d-dimensional system can be implemented as the partial trace of a unitary operator acting on the system together with an auxiliary system (the ''environment''). The question is how small an environment suffices to implement all possible quantum operations on a d-dimensional system. The answer is easy, and has long been known, for the case in which the environment is initialized in a pure state. The answer is more interesting when the environment can be initialized in a mixed state.

II. INITIALIZING THE ENVIRONMENT IN A PURE STATE

The environment is initialized in a standard pure state (let's call it $|0\rangle$). We apply an overall unitary transformation to the system plus environment (which typically involves interaction between the two). Finally, we are only interested in the (now generally mixed) state of the system alone, thus we ''trace over'' the environment. Decoherence is a typical example of such a process. It is easy to see that quantum operations act linearly on density matrices.

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We will think of quantum operations as given in the above way, as overall unitary transformations on a system together with an environment. For example, a quantum operation on a single-qubit system can be given by the action of an overall unitary transformation on basis vectors for the space consisting of the system together with the environment. As the environment starts out in the state $|0\rangle$, we need only to give the images of the vectors $|i\rangle|0\rangle$ (where the first vector corresponds to the system and the second to the environment):

$$|0\rangle|0\rangle \rightarrow |0\rangle|\psi_{00}\rangle + |1\rangle|\psi_{01}\rangle,$$

$$|1\rangle|0\rangle \rightarrow |0\rangle|\psi_{10}\rangle + |1\rangle|\psi_{11}\rangle,$$

where the environment vectors $|\psi_{ij}\rangle$ have to be such that the two right-hand sides are orthonormal.

The action of the quantum operation on (density) operators is obtained by first lifting the above overall unitary transformation to the level of density operators and then tracing over the environment (using $tr|\varphi\rangle\langle\psi| = \langle\psi|\varphi\rangle$). Thus

$$|i\rangle|0\rangle\langle 0|\langle i'| \overset{U}{\rightarrow} \sum_{jj'} |j\rangle|\psi_{ij}\rangle\langle\psi_{i'j'}|\langle j'| \overset{tr_{env}}{\rightarrow} \sum_{jj'} |j\rangle\langle j'|\langle\psi_{i'j'}|\psi_{ij}\rangle.$$

Since only the inner product of the $|\psi_{ij}\rangle$ matter, we may assume that $|0\rangle = |\psi_{00}\rangle$. Thus we see that any quantum operation on a single-qubit system can be implemented with a four-dimensional environment, as the $|\psi_{ij}\rangle$ span at most a four-dimensional space. For a d-dimensional system we have d^2 environment vectors $|\psi_{ij}\rangle$, so an environment of that dimension will always do. It is also not hard to show that in this setting some quantum operations really need an environment of this size.

A. Initializing the environment in a mixed state

While it does not matter in which pure state we initialize the environment, initializing in a mixed state rather than a pure state does matter. A mixed state is not unitarily equivalent to a pure state, rather the unitary equivalence is characterized by the eigenvalues p_i of the density matrix of the state. The question at hand is whether we could implement any quantum operation with an environment smaller than d^2 if, for each map we want to implement, we are allowed to initialize the environment in a mixed state of our choosing.

Without loss of generality we can assume the initial state of the environment to be of the form $\rho_{\text{env,initial}} = \Sigma_i p_i |i\rangle\langle i|$. Because the environment now is smaller, the overall unitary transformation has fewer parameters, but more of them matter; it is no longer sufficient to know only the action on the subspace in which the environment is in state $|0\rangle$.

A parameter count (including the choice of the p_i) suggests that an environment of the same dimension as the system might just be enough to implement any quantum operation were we allowed to choose the initial mixed state of the environment, thus the conjecture in Lloyd (1996 [see Eq. (2)]). We give a more general version of the parameter count in Sec. II B 1.

It has been shown (Terhal, 1999) for the qubit case ($d=2$) that this conjecture is not true; there are quantum operations which cannot be implemented with a mixed single-qubit environment. The proof in Terhal (1999) was rather "brute force," as it used computer algebra to show that a system of equations does not have a solution. Here we give a simple proof using only elementary means that also generalizes to arbitrary dimensions.

Thus we show the following: There are quantum operations on a d-dimensional system which cannot be implemented using an environment which is only of the same dimension. In particular, this statement remains true even if we can initialize the environment in a mixed state of our choosing.

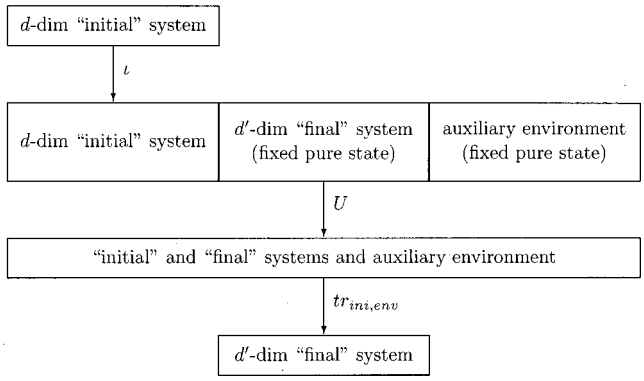

FIG. 1. Map from d-dimensional "initial" system to d'-dimensional "final" system induced by unitary transformation U acting on the two systems and an auxiliary environment. The "final" system and the auxiliary environment are initialized in fixed pure states.

B. General framework

In general we consider maps between systems of (possibly) different dimensions d and d'. We embed the "initial" d-dimensional system in a larger system, apply a unitary operator, and then take the partial trace over everything except the d'-dimensional "final" system. Thus physically we start with a system in some (generally mixed) state and end with a different system in some state. Note that the dimension can increase or decrease.

When the larger system contains a d'-dimensional system and an auxiliary environment initialized in pure states (see Fig. 1), the same argument as in Sec. II shows that besides the d-dimensional initial system and the d'-dimensional final system, a d-dimensional environment is enough (and in general necessary) to realize general quantum operations between the two systems.

Were we to initialize the "final" system in a mixed state, a parameter count (misleadingly) suggests that the d-dimensional auxiliary environment could simply be left away. We place our counterexamples in this general framework of maps from a d-dimensional "initial" system to a d'-dimensional final (or "target") system initialized in a mixed state of our choosing. An overall unitary transformation is applied to the initial plus final system, and, then, as we are only interested in the state of the final system, we "trace over" the initial one. (See Fig. 2.)

Note that the question we were initially interested in, of whether a d-dimensional environment that can be initialized in a mixed state is sufficient to implement any quantum operation on a d-dimensional system, can be answered in this general framework by looking at initial and final systems of the same dimension d and then swapping them at the end.

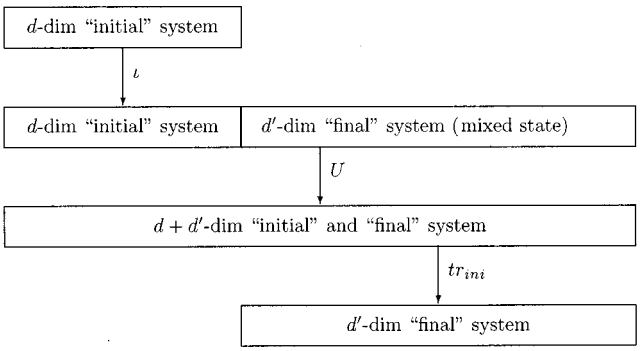

FIG. 2. General framework: map from d-dimensional "initial" system to d'-dimensional "final" system induced by unitary transformation U. The "final" system is initialized in a mixed state.

1. A sketch of the parameter count

Here is a sketch of the parameter count that leads to the wrong conjecture. The d'-dimensional mixed state in the standard form is given by $d'-1$ (real) parameters. Note that it is invariant under diagonal (special) unitary transformations (''rephasings''). The overall (special) unitary transformation has $d^2d'^2-1$ parameters. Finally, we have to take into account that after this overall transformation, a (special) unitary transformation just on the initial system alone does not matter. In the end we get $(d'-1)-(d'-1)+(d^2d'^2-1)-(d^2-1)=d^2(d'^2-1)$ real parameters, which is the correct number for a quantum operation $d\to d'$.

III. THE COUNTEREXAMPLE

A. The basic idea

We explain the basic idea behind the counterexamples in the simple setting of a map from a d-dimensional system to itself induced by a unitary map on the system together with a d'-dimensional environment. Imagine we initialize the d'-dimensional environment in a mixed state, say $\rho_{\text{ini}}=p|0\rangle\langle 0|+(1-p)|1\rangle\langle 1|$. The resulting map (quantum operation) will be a probabilistic mixture (convex linear combination) of the two ''pure-environment'' maps we would get by initializing the environment either in state $|0\rangle$ or $|1\rangle$. A convex linear combination of quantum operations is defined through the convex linear combination of the density matrices to which they map. Also note that given one of these maps, the other has to fulfill certain conditions because they come from the same overall unitary transformation.

The main idea of our counterexample is as follows: A pure state cannot be written as a nontrivial mixture of two pure states. This gives us strong restrictions on maps that take certain pure system states to pure states. For example, consider a quantum operation that maps $|0\rangle \to|0\rangle$. Then any ''pure-environment'' maps that make up part of a convex linear combination that gives this map must also map $|0\rangle$ to $|0\rangle$.

B. The counterexample

As announced, we use the general framework of a quantum operation from an ''initial'' d-dimensional system to a ''final'' d'-dimensional system (Fig. 2). We will mark vectors in the final system with a prime: $|\ldots\rangle'$.

In our counterexample, we require that all but one of the initial system basis states go to one pure state, say $|0\rangle'$,

$$|i\rangle\langle i|\to|0\rangle'\langle 0|', \quad i=0,\ldots,d-2.$$

Before further specifying the counterexample, let us look at the consequences of this condition. If the target system has been initialized in a (truly, thus nonpure) mixed state, say $\rho'_{\text{ini}}=p|0\rangle'\langle 0|' +(1-p)|1\rangle'\langle 1|'$ with $0<p<1$, we get for the overall unitary transformation

$$|i\rangle|0\rangle'\to|\psi_i\rangle|0\rangle' \quad \text{and} \quad |i\rangle|1\rangle'\to|\xi_i\rangle|0\rangle', \quad i=0,\ldots,d-2.$$

All $2(d-1)$ states on the right-hand side have to be orthonormal, thus the $|\psi_i\rangle$ and $|\xi_i\rangle$ have to be orthonormal. But for $d>2$ their number exceeds the dimension of the system. It is clear that were we to initialize the final system in a mixed state of rank >2, things would only be worse. It follows that the final system cannot start out in a mixed state, thus we assume it is initialized in the pure state $|0\rangle'$. (We treat the special case $d=2$ below.)

Without loss of generality we set $|\psi_i\rangle=|i\rangle$. We have $|i\rangle|0\rangle'\to|i\rangle|0\rangle'$ for $i=0,\ldots,d-2$. The image of the remaining basis state $|d-1\rangle$ can be written

$$|d-1\rangle|0\rangle'\to\sum_{i=0}^{d-1}|i\rangle|\varphi_i\rangle'.$$

Now we require that the image of $|d-1\rangle$ be a truly mixed state ρ'_{d-1}. Furthermore, we require that under the quantum operation, $|d-1\rangle$ should "totally decohere" from the other basis states $|i\rangle$, meaning that a superposition should go to a mixture of the individual images of the states, so $(\alpha|i\rangle+\beta|d-1\rangle)(\overline{\alpha}\langle i|+\overline{\beta}\langle d-1|)\rightarrow|\alpha|^2|0\rangle'\langle 0|'+|\beta|^2\rho'_{d-1}$ $(i=0,\ldots,d-2)$. But the "totally decohere" condition means that $|\varphi_i\rangle'=0$ for all $i\neq d-1$, from which it follows that the image of $|d-1\rangle$ would have to be pure after all.

C. The special case $d\rightarrow d'$ with $d=2$

For $d=2$ we still have to consider the case in which the final system is initialized in a mixed state, although from above it is clear that it would have to be a mixed state of rank 2, thus a mixture of just two different pure states. Thus $\rho'_{\mathrm{ini}}=p|0\rangle'\langle 0|'+(1-p)|1\rangle'\langle 1|'$ with $0<p<1$. Then we have for the overall unitary transformation

$$|0\rangle|0\rangle'\rightarrow|0\rangle|0\rangle' \quad \text{and} \quad |0\rangle|1\rangle'\rightarrow|1\rangle|0\rangle'.$$

It follows that $|1\rangle|0\rangle'\rightarrow\alpha|0\rangle|0^{\perp}\rangle'+\beta|1\rangle|0'^{\perp}\rangle'$ where both $|0^{\perp}\rangle'$ and $|0'^{\perp}\rangle'$ are vectors orthogonal to $|0\rangle'$ and similarly for the image of $|1\rangle|1\rangle'$. We can now make our counterexample above work also for $d=2$ by additionally requiring that the (truly mixed) image of $|d-1\rangle$ have some overlap with $|0\rangle'$, thus we require that

$$\langle 0|'\rho'_{d-1}|0\rangle'\neq 0.$$

D. Summary of the counterexample

In summary we give the counterexample map by its action on pure states:

$$\left(\sum_{i=0}^{d-2}\alpha_i|i\rangle+\beta|d-1\rangle\right)\left(\sum_{i=0}^{d-2}\overline{\alpha_i}\langle i|+\overline{\beta}\langle d-1|\right)\rightarrow\left(\sum_{i=0}^{d-2}|\alpha_i|^2\right)|0\rangle'\langle 0|'+|\beta|^2\rho'_{d-1},$$

where ρ'_{d-1} is not a pure state. For $d=2$ we must additionally require that $\langle 0|'\rho'_{d-1}|0\rangle'\neq 0$. (Actually for $d'=2$ this is always true.)

E. The counterexample is a quantum operation

Finally we show that the counterexample is a possible quantum operation, thus that with a large enough environment it can be implemented. So besides the initial and final systems we also have an environment. The map is simple, but for completeness we show it. The following overall unitary transformation implements the counterexample map (including the additional property required for the case $d=2$), with $\alpha,\beta\neq 0$:

$$|i\rangle|0\rangle'|0\rangle_{\mathrm{env}}\rightarrow|i\rangle|0\rangle'|0\rangle_{\mathrm{env}}, \quad i=0,\ldots,d-2,$$

$$|d-1\rangle|0\rangle'|0\rangle_{\mathrm{env}}\rightarrow\alpha|d-1\rangle|0\rangle'|0\rangle_{\mathrm{env}}+\beta|d-1\rangle|1\rangle'|1\rangle_{\mathrm{env}}.$$

IV. FURTHER REMARKS

A. How many counterexamples are there?

Once a single counterexample has been found, basic topological properties of the (convex) set of all quantum operations and the (also convex) subset of those that can be realized with a d-dimensional (possibly) mixed environment imply that the set of counterexamples contains balls and thus is a set of nonzero measure. All that is needed is that the subset of maps that can be realized with a d-dimensional mixed environment is closed, and that the "outer" set is a regular

set, thus it is a closure of its inner points. The latter is simply because the set of all quantum operations is a ''closed voluminous'' convex set, thus one which does not happen to lie in some hyperplane.

Note that our counterexample lies on the boundary of the set of quantum operations, so we must take the intersection of a ball around it with the set of quantum operations to find inner points of the set of counterexamples. Around these points there will then be balls of counterexamples.

Also note that the counterexample given in Terhal (1999), for the single-qubit case ($d=2$), is unital and thus very different from ours.

A complete characterization of exactly which maps can be realized with a d-dimensional mixed environment and which cannot has yet to be found even in the single-qubit case. Ruskai (2001) gives a parameterization of the space of all quantum operations for the single-qubit space that might be useful here.

B. How big an environment is necessary?

From the counterexamples for $d>2$ we can see that more could be said about how large a mixed environment has to be, but we have not investigated further.

C. Implications for simulating quantum operations (?)

It looks like our subject is mostly a mathematical challenge. In Terhal (1999) it was said that one may want to simulate quantum operations (e.g., on a quantum computer) with as few resources as possible (see also Bacon, 2001). But Choi (1975) shows that every extremal map of the convex set of quantum operations can be realized with a d-dimensional environment initialized in a pure state. To achieve any mixture of such extremal maps (and thus any map) one can simply carry out each of them with a certain probability, using a probabilistic protocol. On the other hand, certain extremal maps do need an environment of dimension d, thus this probably is a necessary resource.

D. What about ''Markovian'' quantum operations?

By ''Markovian'' quantum operations we mean those quantum operations that can be ''generated'' from ones that are infinitesimally close to the identity. Of course this notion makes sense only for dimension preserving quantum operations. It is known that not all quantum operations can be generated in this way, so we may wonder whether all those maps could be implemented with a ''small'' mixed environment.

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A lower bound on the quantum capacity of channels with correlated errors

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The highest fidelity of quantum error-correcting codes of length n and rate R is proven to be lower bounded by $1-\exp[-nE(R)+o(n)]$ for some function $E(R)$ on noisy quantum channels that are subject to not necessarily independent errors. The $E(R)$ is positive below some threshold R_0, which implies R_0 is a lower bound on the quantum capacity. This work is an extension of the author's previous works [M. Hamada, Phys. Rev. A, **65**, 052305 (2002); quant-ph/0109114, LANL (2001); M. Hamada, quant-ph/0112103, LANL (2001)], which presented the bound for channels subject to independent errors, or channels modeled as tensor products of copies of a completely positive linear map. The relation of the channel class treated in this article to those in the previous works is similar to that of Markov chains to sequences of independent identically distributed random variables. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1495537]

I. INTRODUCTION

Quantum error-correcting codes (simply called quantum codes or *codes* in this work) were discovered by Shor[1] and Steane[2] as schemes that protect quantum states from decoherence during quantum computation. Shor[1] not only gave the first quantum code but also posed a problem of determining the quantum analog of Shannon's channel capacity. In classical information theory, channels with independent errors are called memoryless channels and channels with correlated errors are called channels with memory,[3] which will be applied to quantum channels as well in the present work. On quantum memoryless channels, several bounds on the quantum capacity have been known,[1,4–7] and also exponential convergence of fidelity of codes was recently proved by the present author.[8,9] It is natural to ask whether such bounds and exponential convergence hold true or not on channels with memory, which will be answered affirmatively in this work.

While one of the greatest incentives to investigate quantum codes is need in quantum computing, we are not sure which devices to use for this purpose currently. Hence, we do not know which channel models are appropriate, so that treating general channels may be among what we can proceed to now. Thus, this article analyzes the code performance on a class of quantum channels that is much wider than was treated in the literature.

In the proof of the main result below, the method of types, which is a powerful tool from classical information theory, plays an important role.[10,11] This method was exploited by the Hungarian mathematician (information theorist) Csiszár and co-workers around 1980 to present the strongest coding theorems such as the one showing the existence of universal channel codes asymptotically as good as any codes.[10,11] It has often produced results in elementary enumerative manners, which is also the case in this article.

II. MAIN RESULT FOR SIMPLE CASE

As usual, all quantum channels and decoding (state-recovery) operations in coding systems are described in terms of *trace-preserving completely positive* (TPCP) linear maps.[4,7,12–14] Given

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a Hilbert space H of finite dimension, let $\mathsf{L}(\mathsf{H})$ denote the set of linear operators on H. In general, every CP linear map $\mathcal{M}:\mathsf{L}(\mathsf{H})\to\mathsf{L}(\mathsf{H})$ has an operator-sum representation $\mathcal{M}(\rho)=\Sigma_{i\in\mathcal{I}}M_i\rho M_i^\dagger$ for some $M_i\in\mathsf{L}(\mathsf{H})$, $i\in\mathcal{I}$.[4,12–14] When $\mathcal{M}$ is specified by a set of operators $\{M_i\}_{i\in\mathcal{I}}$ in this way, we write $\mathcal{M}\sim\{M_i\}_{i\in\mathcal{I}}$.

Hereafter, H denotes an arbitrarily fixed Hilbert space of dimension d, which is a prime number. A quantum channel is a sequence of TPCP linear maps $\{\mathcal{A}_n:\mathsf{L}(\mathsf{H}^{\otimes n})\to\mathsf{L}(\mathsf{H}^{\otimes n})\}$. We want a large subspace $\mathcal{C}_n\subseteq\mathsf{H}^{\otimes n}$, every state vector in which remains almost unchanged after the effect of a channel followed by some suitable recovery operation $\mathcal{R}_n:\mathsf{L}(\mathsf{H}^{\otimes n})\to\mathsf{L}(\mathsf{H}^{\otimes n})$. A pair $(\mathcal{C}_n,\mathcal{R}_n)$ consisting of such a subspace $\mathcal{C}_n$ and a TPCP map $\mathcal{R}_n$ is called a *code* and its performance is evaluated in terms of minimum fidelity[6,7,15]

$$F(\mathcal{C}_n,\mathcal{R}_n\mathcal{A}_n)=\min_{|\psi\rangle\in\mathcal{C}_n}\langle\psi|\mathcal{R}_n\mathcal{A}_n(|\psi\rangle\langle\psi|)|\psi\rangle,$$

where $\mathcal{R}_n\mathcal{A}_n$ denotes the composition of $\mathcal{A}_n$ and $\mathcal{R}_n$. Throughout, bras $\langle\cdot|$ and kets $|\cdot\rangle$ are assumed normalized. A subspace $\mathcal{C}_n$ alone is also called a code assuming implicitly some recovery operator.

Let $F^\star_{n,k}(\mathcal{A}_n)$ denote the supremum of $F(\mathcal{C}_n,\mathcal{R}_n\mathcal{A}_n)$ such that there exists a code $(\mathcal{C}_n,\mathcal{R}_n)$ with $\log_d\dim\mathcal{C}_n\geqslant k$, where n is a positive integer and k is a non-negative real number. Our goal is to estimate $F^\star_{n,k}(\mathcal{A}_n)$ as precisely as possible.

First, we state the main result for an easy case, and give a more general statement later. Fix an orthonormal basis $\{|0\rangle,\ldots,|d-1\rangle\}$ of H. Put $\mathcal{X}=\{0,\ldots,d-1\}^2$ and $N_{(i,j)}=X^iZ^j$ for $(i,j)\in\mathcal{X}$. Here, $X,Z\in\mathsf{L}(\mathsf{H})$ are Weyl's unitaries, which could be viewed as generalized Pauli operators, and are defined by

$$X|j\rangle=|(j-1)\mod d\rangle,\quad Z|j\rangle=\omega^j|j\rangle,\tag{1}$$

where ω is a primitive dth root of unity.[16–20] From the $\mathsf{L}(\mathsf{H})$ basis $\{N_{(i,j)}\}$, we obtain a basis $\mathsf{N}_n=\{N_x|x\in\mathcal{X}^n\}$ of $\mathsf{L}(\mathsf{H}^{\otimes n})$, where $N_x=N_{x_1}\otimes\cdots\otimes N_{x_n}$ for $x=(x_1,\ldots,x_n)\in\mathcal{X}^n$. The first channel class to be considered here consists of those $\{\mathcal{A}_n\}$ such that $\mathcal{A}_n\sim\{\sqrt{P_n(x)}N_x\}_{x\in\mathcal{X}^n}$, where we assume that P_n are the probability distributions of a (first-order) homogeneous Markov chain, i.e., that P_n has the form

$$P_n(x_1,\ldots,x_n)=p(x_1)\prod_{j=1}^{n-1}P(x_{j+1}|x_j)\tag{2}$$

with some transition probabilities $P(v|u)$, $u,v\in\mathcal{X}$, and some initial distribution p. These are generalizations of the so-called depolarizing channel;[5,6] see Ref. 21 for a thorough analysis of memoryless channels with $d=2$.

Given a probability distribution Q on $\mathcal{X}^2$, we let $\overline{Q}$ and $\bar{\bar{Q}}$ denote the two marginal distributions:

$$\overline{Q}(u)=\sum_{v\in\mathcal{X}}Q(u,v),\quad \bar{\bar{Q}}(u)=\sum_{v\in\mathcal{X}}Q(v,u),\quad u\in\mathcal{X}.$$

The classical (conditional) Kullback–Leibler information (informational divergence or relative entropy) is denoted by D and entropy by H.[10,11,22] Specifically, for a probability distribution Q on $\mathcal{X}^2$, transition (or conditional) probabilities $P(v|u)$, $u,v\in\mathcal{X}$, and a probability distribution p on $\mathcal{X}$, we define $\tilde{Q}(\cdot|\cdot)$ by $\tilde{Q}(v|u)=Q(u,v)/\overline{Q}(u)$ for $\overline{Q}(u)>0$, $D(Q\|P)$ by

$$D(Q\|P)=\sum_{u\in\mathcal{X}:Q(u)>0}\sum_{v\in\mathcal{X}}Q(u,v)\log_d\frac{\tilde{Q}(v|u)}{P(v|u)},$$

and $H(P|p)$ by

$$H(P|p)=-\sum_{u\in\mathcal{X}:\ p(u)>0}\ \sum_{v\in\mathcal{X}} p(u)P(v|u)\log_d P(v|u),$$

which is called the entropy of $P(\cdot|\cdot)$ conditional on p. We remark that $D(Q\|P)$ is a conditional Kullback–Leibler information, so that in a more consistent notation,[10] it would be denoted by $D(\tilde{Q}\|P|\overline{Q})$.

By convention, we assume $\log(a/0)=\infty$ for $a>0$, $0\log 0=0\log(0/0)=0$. The first form of this work's main result is the next one.

Theorem 1: *Let a channel* $\mathcal{A}_n\sim\{\sqrt{P_n(x)}N_x\}_{x\in\mathcal{X}^n}$, $n=1,2,\ldots$, *be specified by (2) with some* $P(\cdot|\cdot)$ *and* p. *Then, for* $0\leqslant R\leqslant 1$, *we have*

$$\liminf_{n\to\infty}-\frac{1}{n}\log_d[1-F^{\star}_{n,Rn}(\mathcal{A}_n)]\geqslant E(R,P), \tag{3}$$

where

$$E(R,P)=\min_{Q:\overline{Q}=\bar{\bar{Q}}}[D(Q\|P)+|1-H(\tilde{Q}|\overline{Q})-R|^{+}],$$

$|x|^{+}=\max\{x,0\}$, *and the minimization with respect to* Q *is taken over all probability distributions on* $\mathcal{X}^2$ *with* $\overline{Q}=\bar{\tilde{Q}}$.

Remarks: Roughly speaking, the theorem says $F^{\star}_{n,Rn}(\mathcal{A}_n)\overset{>}{\approx}1-\exp_d[-nE(R,P)]$. An immediate consequence of the theorem is that when the Markov chain is irreducible, the quantum capacity[1,4–7] of $\{\mathcal{A}_n\}$ is lower bounded by $1-H(P|q)$, where q is the unique stationary (steady state, or equilibrium) distribution of the Markov chain.[23] To see this, observe that $E(R,P)$ is positive for $R<1-H(P|q)$ due to an easily established inequality $D(Q\|P)\geqslant 0$ where equality occurs if and only if $Q(u,v)=q(u)P(v|u)$ for all $u,v\in\mathcal{X}$ under the constraint $\overline{Q}=\bar{\tilde{Q}}$.

Example: Let us assume $d=2$, rename the elements (0,0),(1,0),(0,1),(1,1) in $\mathcal{X}$ as $\underline{0}$, $\underline{1}$, $\underline{2}$, $\underline{3}$, and define $P(v|u)$, $u,v\in\mathcal{X}$, by

$$P(v|u)=\begin{cases}1-\varepsilon & \text{if } u=\underline{0} \text{ and } v=\underline{0},\\ \varepsilon/3 & \text{if } u=\underline{0} \text{ and } v\neq\underline{0},\\ 1-\gamma & \text{if } u\neq\underline{0} \text{ and } v=\underline{0},\\ \gamma/3 & \text{if } u\neq\underline{0} \text{ and } v\neq\underline{0}.\end{cases}$$

In this case, $\{A_n\}$ is analogous to the channel with memory discussed by Gilbert[24] in the context of classical channel coding (see also Ref. 3, Sec. 4.6). If we brought Gilbert's idea into our quantum case innocently, we might assume $0<\varepsilon\leqslant\gamma<1$ and interpret $\underline{0}$ as "good state," $\underline{1}$, $\underline{2}$, $\underline{3}$ as "bad ones," where a state means that of the Markov chain, not a quantum state, and ε (resp., γ) as the probability of going into a "bad state" provided the current state be "good (resp., bad)." For the above quantum channel, the lower bound $1-H(P|q)$ becomes

$$1-\frac{(1-\gamma)[h(\varepsilon)+\varepsilon\log_2 3]+\varepsilon[h(\gamma)+\gamma\log_2 3]}{1-\gamma+\varepsilon},$$

where h is the binary entropy function $h(z)=-z\log_2 z-(1-z)\log_2(1-z)$. Note that when $\varepsilon=\gamma$, the channel becomes the depolarizing channel and the lower bound on the capacity becomes the known one.[5,8]

III. PROOF OF THEOREM 1

A. Codes based on symplectic geometry

The codes to be proven to have the desired performance are *symplectic (stabilizer, or additive) codes*.[25–27] Let us recall first the basics of symplectic codes. We can regard the index of $N_{(i,j)} = X^i Z^j$, $(i,j) \in \mathcal{X}$, as a pair of elements from the field $\mathsf{F} = \mathbb{F}_d = \mathbb{Z}/d\mathbb{Z}$, the finite field consisting of d elements. Recall we put $N_x = N_{x_1} \otimes \cdots \otimes N_{x_n}$ for $x = (x_1, \ldots, x_n) \in (\mathsf{F}^2)^n$. We write N_J for $\{N_x \in \mathsf{N}_n | x \in J\}$ where $J \subseteq (\mathsf{F}^2)^n$. The index $((u_1, v_1), \ldots, (u_n, v_n)) \in (\mathsf{F}^2)^n$ of a basis element can be regarded as the plain $2n$-dimensional vector

$$x = (u_1, v_1, \ldots, u_n, v_n) \in \mathsf{F}^{2n}.$$

We can equip the vector space F^{2n} over F with a *symplectic bilinear form* (symplectic paring), which is defined by

$$(x,y)_{\mathrm{sp}} = \sum_{i=1}^{n} u_i v_i' - v_i u_i'$$

for the above x and $y = (u_1', v_1', \ldots, u_n', v_n') \in \mathsf{F}^{2n}$.[28–30] Given a subspace $L \subseteq \mathsf{F}^{2n}$, let

$$L^{\perp} = \{x \in \mathsf{F}^{2n} | \forall y \in L, \quad (x,y)_{\mathrm{sp}} = 0\}.$$

Lemma 1:[25,27] *Let a subspace $L \subseteq \mathsf{F}^{2n}$ satisfy*

$$L \subseteq L^{\perp} \quad \textit{and} \quad \dim\ L = n - k.$$

In addition, let $J_0 \subseteq \mathsf{F}^{2n}$ be a set satisfying

$$\forall x, y \in J_0, \quad [y - x \in L^{\perp} \Rightarrow x = y]. \tag{4}$$

Then, there exist d^k-dimensional N_{J_0}-correcting codes.

In fact, given a subspace L as above, there are d^k subspaces of the form

$$\{\psi \in \mathsf{H}^{\otimes n} | \forall M \in N_L, M\psi = \tau(M)\psi\},$$

with some scalars $\tau(M)$ (eigenvalues of $M \in N_L$), and each of them, together with a suitable recovery operator, serves as an N_{J_0}-correcting quantum code of dimension d^k. Note that the direct sum of these subspaces is the whole space $\mathsf{H}^{\otimes n}$. The precise meaning of N_{J_0}-correcting can be found, e.g., in Ref. 15. Originally, Lemma 1 was claimed for the case where $d = 2$, and has been generalized to the case where d is a general prime.[18–20,31]

By definition, for an N_{J_0}-correcting code $(\mathcal{C}_n, \mathcal{R}_n)$ and the channel $\{\mathcal{A}_n\}$ in the theorem, it holds

$$1 - F(\mathcal{C}) \leqslant \sum_{x \notin J_0} P_n(x), \tag{5}$$

where $F(\mathcal{C}) = F(\mathcal{C}, \mathcal{R}_n \mathcal{A}_n)$. We remark that, as is usually done in the literature, it is assumed in this article that when we speak of an N_{J_0}-correcting code $(\mathcal{C}_n, \mathcal{R}_n)$, the $\mathcal{R}_n$ indicates the one constructed by Knill and Laflamme.[15] Note that $\mathcal{R}_n$ is determined from J_0 and $\mathcal{C}$. The premise (4) of Lemma 1 is restated as that J_0 is a set of representatives of cosets of $L^{\perp}$ in F^{2n}. A natural choice for J_0 would be a set consisting of representatives each of which maximizes the probability $P_n(x)$ in its coset[27] since it is analogous to maximum likelihood decoding, which is an optimum strategy for classical coding (see Ref. 32 or any textbook of information theory). In the proof below, we

choose another set of representatives, the classical counterpart of which (minimum entropy decoding) asymptotically yields the same performance as maximum likelihood decoding.[10,33]

B. The method of types

The theorem can be proved along the lines of Ref. 8, which employed the method of types.[10,11,22,33] In the present case, second-order (Markov) types rather than the usual types are used. Needed technical tools from the method of types in the Markov case can be found in Ref. 22 and papers cited therein. We collect here a few basic facts on this method to be used below.

For $x=(x_1,\ldots,x_n)\in\mathcal{X}^n$, $n>1$, define a probability distribution M_x on $\mathcal{X}^2$ by

$$\mathsf{M}_x(u,v)=\frac{|\{i|1\leqslant i\leqslant n-1,(x_i,x_{i+1})=(u,v)\}|}{n-1},\quad u\in\mathcal{X},$$

which is called the second-order *type* or Markov type of x. With $\mathcal{X}$ and an element $u\in\mathcal{X}$ fixed, the set of all possible Markov types of sequences $(x_1,\ldots,x_n)$ from $\mathcal{X}^n$ satisfying $x_1=u$ is denoted by $\mathcal{Q}_n(\mathcal{X},u)$ or simply by $\mathcal{Q}_n(u)$, and $\mathcal{Q}_n$ stands for $\cup_{u\in\mathcal{X}}\mathcal{Q}_n(u)$. For a type $Q\in\mathcal{Q}_n(u)$, $\mathcal{T}_Q^n(u)$ is defined as $\{(x_1,\ldots,x_n)\in\mathcal{X}^n|x_1=u \text{ and } \mathsf{M}_x=Q\}$, and $\mathcal{T}_Q^n$ denotes $\cup_{u\in\mathcal{X}}\mathcal{T}_Q^n(u)$.

In what follows, we use

$$|\mathcal{T}_Q^n(u)|\leqslant\exp_d[(n-1)H(\tilde{Q}|\overline{Q})],\quad u\in\mathcal{X}. \tag{6}$$

Note that if $x=(x_1,\ldots,x_n)\in\mathcal{X}^n$ with $x_1=u$ has type Q, then $P_n(x)=p(u)\Pi_{(a,b)\in\mathcal{X}^2}P(b|a)^{(n-1)Q(a,b)}=p(u)\exp_d\{-(n-1)[H(\tilde{Q}|\overline{Q})+D(Q\|P)]\}$ and, hence, (6) is equivalent to the latter inequality in (39) of Ref. 22, i.e.,

$$\Pr\{\mathsf{M}_{\mathbf{X}}=Q|\mathbf{X}_1=u\}\leqslant\exp_d\{-(n-1)D(Q\|P)\}, \tag{7}$$

where the sequence of random variables $\mathbf{X}=(\mathbf{X}_1,\ldots,\mathbf{X}_n)$ represents the Markov chain in the theorem, i.e., $\Pr\{\mathbf{X}_1=x_1,\ldots,\mathbf{X}_n=x_n\}=P_n(x_1,\ldots,x_n)$ with P_n defined in (2). Equation (6) or (7) is a consequence of Whittle's formula for $|\mathcal{T}_Q^n(u)|$, a simple proof of which was given by Billingsley.[34] The upper bound in (6) can be proved more easily with a simple way of enumeration (Ref. 35 or the paragraph containing (9) of Ref. 36).

C. Proof of theorem I

The case where $R=1$ is trivial, so we assume $R<1$ from now on. Putting $k=\lceil Rn\rceil$, we apply Lemma 1, where we choose J_0 as follows. Assume dim $L=n-k$. Then, dim $L^{\perp}=n+k$.[28,30] For notational simplicity, we write $H_c(Q)$ in place of $H(\tilde{Q}|\overline{Q})$ for a probability distribution Q on $\mathcal{X}^2$. From each of the d^{n-k} cosets of $L^{\perp}$ in F^{2n}, select a vector that minimizes $H_c(\mathsf{M}_x)$, i.e., a vector x satisfying $H_c(\mathsf{M}_x)\leqslant H_c(\mathsf{M}_y)$ for any y in the coset. This selection uses the idea of the minimum entropy decoder known in the classical information theory literature.[33]

Let $J_0(L)$ denote the set of the d^{n-k} selected vectors, let

$$\mathsf{A}=\{L\subseteq\mathsf{F}^{2n}|L \text{ linear},\quad L\subseteq L^{\perp},\quad \dim L=n-k\},$$

and, for each $L\in\mathsf{A}$, let $\mathcal{C}(L)$ be an $N_{J_0(L)}$-correcting code, the existence of which is ensured by Lemma 1. Putting

$$\overline{F}=\frac{1}{|\mathsf{A}|}\sum_{L\in\mathsf{A}}F(\mathcal{C}(L)),$$

we will show $\liminf_n -n^{-1}\log_d(1-\overline{F})\geqslant E(R,P)$, which implies that, at least, one sequence of codes has fidelity as high as promised in the theorem. Such a method for a proof is referred to as random coding.[10,37]

As in the proof of Theorem 1 of Ref. 8, we have

$$1-\overline{F}\leqslant \sum_{x\in \mathsf{F}^{2n}} P_n(x)\frac{|\mathsf{B}(x)|}{|\mathsf{A}|}, \tag{8}$$

where

$$\mathsf{B}(x)=\{L\in \mathsf{A}|x\notin J_0(L)\},\quad x\in \mathsf{F}^{2n}.$$

The fraction $|\mathsf{B}(x)|/|\mathsf{A}|$ is trivially bounded as

$$\frac{|\mathsf{B}(x)|}{|\mathsf{A}|}\leqslant 1,\quad x\in \mathsf{F}^{2n}. \tag{9}$$

We use the next inequality.[9] Let

$$\mathsf{A}(x)=\{L\in \mathsf{A}|x\in L^{\perp}\backslash\{0\}\}.$$

Then, $|\mathsf{A}(0)|=0$ and

$$\frac{|\mathsf{A}(x)|}{|\mathsf{A}|}=\frac{d^{n+k}-1}{d^{2n}-1}\leqslant \frac{1}{d^{n-k}},\quad x\in \mathsf{F}^{2n},\quad x\neq 0. \tag{10}$$

This is a variant of the relation established by Calderbank *et al.*,[25] or its analog proved by Matsumoto and Uyematsu[38] with an explicit use of the Witt lemma[28,29] from the theory of bilinear forms.

Since $\mathsf{B}(x)\subseteq\{L\in \mathsf{A}|\exists y\in \mathsf{F}^{2n}, H_{\mathrm{c}}(\mathsf{M}_y)\leqslant H_{\mathrm{c}}(\mathsf{M}_x), y-x\in L^{\perp}\backslash\{0\}\}$ from the design of $J_0(L)$ specified above (cf. Ref. 37), it follows that

$$|\mathsf{B}(x)|\leqslant \sum_{y\in \mathsf{F}^{2n}:H_{\mathrm{c}}(\mathsf{M}_y)\leqslant H_{\mathrm{c}}(\mathsf{M}_x),\ y\neq x}|\mathsf{A}(y-x)|\leqslant \sum_{y\in \mathsf{F}^{2n}:H_{\mathrm{c}}(\mathsf{M}_y)\leqslant H_{\mathrm{c}}(\mathsf{M}_x),\ y\neq x}|\mathsf{A}|d^{-n+k}, \tag{11}$$

where we have used (10) for the latter inequality. Combining (8), (9), and (11), we obtain the following chain of inequalities with the aid of the basic inequalities in (6) and (7) as well as the inequality $\min\{a+b,1\}\leqslant\min\{a,1\}+\min\{b,1\}$ for $a,b\geqslant 0$:

$$\begin{aligned}
1-\overline{F}&\leqslant \sum_{x\in \mathsf{F}^{2n}} P_n(x)\ \min\left\{\sum_{y\in \mathsf{F}^{2n}:H_{\mathrm{c}}(\mathsf{M}_y)\leqslant H_{\mathrm{c}}(\mathsf{M}_x),\ y\neq x} d^{-(n-k)},\ 1\right\}\\
&\leqslant \sum_{u\in \mathcal{X}} p(u)\sum_{Q\in \mathcal{Q}_n(u)}\Pr\{\mathsf{M}_{\mathbf{X}}=Q|\mathbf{X}_1=u\}\min\left\{\sum_{Q'\in \mathcal{Q}_n:H_{\mathrm{c}}(Q')\leqslant H_{\mathrm{c}}(Q)}\frac{|\mathcal{T}^n_{Q'}|}{d^{n(1-R)-1}},\ 1\right\}\\
&\leqslant d^3\sum_{u\in \mathcal{X}} p(u)\sum_{Q\in \mathcal{Q}_n}\exp_d[-(n-1)D(Q\|P)]\\
&\quad\times\sum_{Q'\in \mathcal{Q}_n:H_{\mathrm{c}}(Q')\leqslant H_{\mathrm{c}}(Q)}\exp_d[-(n-1)|1-R-H_{\mathrm{c}}(Q')|^{+}]\\
&\leqslant d^3\sum_{Q\in \mathcal{Q}_n}\exp_d[-(n-1)D(Q\|P)]|\mathcal{Q}_n|\max_{Q'\in \mathcal{Q}_n:H(Q')\leqslant H(Q)}\\
&\quad\exp_d[-(n-1)|1-R-H_{\mathrm{c}}(Q')|^{+}]
\end{aligned}$$

$$\leqslant d^3 \sum_{Q \in \mathcal{Q}_n} \exp_d[-(n-1)D(Q\|P)]\,|\mathcal{Q}_n| \exp_d[-(n-1)|1-R-H_c(Q)|^+]$$

$$\leqslant d^3 |\mathcal{Q}_n|^2 \exp_d\{-(n-1) \min_{Q \in \mathcal{Q}_n} [D(Q\|P)+|1-R-H_c(Q)|^+]\}.$$

Since $|\mathcal{Q}_n|$ is polynomial in n, the remaining task is to show that

$$\liminf_{n\to\infty} \min_{Q \in \mathcal{Q}_n} [D(Q\|P)+|1-R-H_c(Q)|^+]$$

is not less than

$$\min_{Q:\|\overline{Q}-\bar{\bar{Q}}\|=0} [D(Q\|P)+|1-R-H_c(Q)|^+],$$

which is $E(R,P)$. One sees this holds immediately, noticing that any $Q \in \mathcal{Q}_n$ satisfies $\|\overline{Q}-\bar{\bar{Q}}\| \leqslant 1/(n-1)$ for the norm $\|(z_1,\ldots,z_{|\mathcal{X}|})\| = \max_i |z_i|$,[22] the set of all probability distributions is compact, and $D(Q)=D(Q\|P)$ is continuous in its effective domain $\{Q|D(Q)<\infty\}$ (cf. the proof of Lemma 2 in Ref. 22). This completes the proof.

IV. MAIN RESULT FOR GENERAL CASE

Theorem 1 actually holds for a wider class of channels. To evaluate the fidelity of codes on a more general channel $\{\mathcal{A}_n\}$, we first associate a sequence of probability distributions $\{P_{\mathcal{A}_n}\}$ with the channel $\{\mathcal{A}_n\}$ as in Ref. 9.

Definition 1: For each n, let $\mathcal{A}_n \sim \{A_x^{(n)}\}_{x \in \mathcal{X}^n}$, *expand* $A_x^{(n)}$ *as* $A_x^{(n)} = \Sigma_{y \in \mathcal{X}^n} a_{xy} N_y$, $x \in \mathcal{X}^n$, *and define a probability distribution* $P_{\mathcal{A}_n}$ *on* $\mathcal{X}^n$ *by*

$$P_{\mathcal{A}_n}(y) = \sum_x |a_{xy}|^2, \quad y \in \mathcal{X}^n.$$

Example: Let $\{\mathcal{A}_n\}$ be a memoryless channel $\mathcal{A}_n = \mathcal{A}^{\otimes n}$, $n=1,2,\ldots$. It is easy to see that $P_{\mathcal{A}_n}(y_1,\ldots,y_n) = \Pi_{i=1}^n P_{\mathcal{A}}(y_i)$.

The case of memoryless channels as above was discussed in this author's previous work.[9] This work claims the next.

Theorem 2: *Consider a channel* $\{\mathcal{A}_n\}$ *whose* $\{P_n = P_{\mathcal{A}_n}\}$ *satisfies (2) with some* $P(\cdot|\cdot)$ *and* p. *Then, again, for* $0 \leqslant R \leqslant 1$, *(3) in Theorem 1 holds*.

The above theorem can be proved along the lines of this author's previous work,[9] which treated general memoryless quantum channels. Namely, Theorem 1 can be generalized to Theorem 2 in the same way as the result in Ref. 8 was strengthened in Ref. 9. Here it is briefly described how to prove Theorem 2. First, we evaluate the minimum average fidelity $F_a(\mathcal{C})$, which is another performance measure for a code $\mathcal{C}$ introduced in Ref. 9, instead of the minimum fidelity $F(\mathcal{C})$. Actually, we evaluate the average of $F_a(\mathcal{C})$ over the whole ensemble of quantum codes $\{\mathcal{C}(L,i)|L \in \mathsf{A}, 0 \leqslant i < d^{n-k}\}$, where $\mathcal{C}(L,i)$, $i=0,\ldots,d^{n-k}-1$, are the d^{n-k} quantum codes associated with L as in Lemma 1; compare the proof of Theorem 1 above, where using an arbitrarily chosen code $\mathcal{C}(L,i)$ for each L was enough. The average of $F_a(C(L,i))$ turns out to be lower bounded by $1-\exp_d[-nE(R,P)+o(n)]$. Then, at least, one code $\mathcal{C}(L,i)$ has this performance or higher. As proved in Ref. 9, if we have a code with $1-F_a(\mathcal{C}) \leqslant G$, we can choose a subcode $\mathcal{C}'$ of half the dimension with $1-F(\mathcal{C}') \leqslant 2G$, which implies Theorem 2.

The major difficulty in the analysis on general channels lies in the fact that (5) is no longer true in the general case; this was resolved in Ref. 9 by proving that (5) holds true if we replace $F(\mathcal{C})=F(\mathcal{C}(L))$ by $F_a(\mathcal{C}(L,i))$ averaged over $0 \leqslant i < d^{n-k}$.

We remark that the result of this article readily extends to the case where P_n is the probability distribution of a higher-order Markov chain. For this extension, we have only to use higher-order types instead of second-order types.[11,22]

V. CONCLUDING REMARKS

It should be remarked that the lower bound $1-H(P|q)$ on the quantum capacity is not tight in general since there is an example of a code which slightly goes beyond the bound for some very noisy memoryless channels.[6] This work, however, seems the first to demonstrate that standard error correction schemes work reliably even in the presence of correlated errors with positive information rate for all large enough code lengths. Moreover, the established convergence of the fidelity is exponential. Research in this direction is yet to be developed in quantum information theory, while exponent problems have already been central issues in other fields including large-deviation theory[39] and classical information theory.[40,41]

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Lower bound for the quantum capacity of a discrete memoryless quantum channel

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We generalize the random coding argument of stabilizer codes and derive a lower bound on the quantum capacity of an arbitrary discrete memoryless quantum channel. For the depolarizing channel, our lower bound coincides with that obtained by Bennett *et al.* We also slightly improve the quantum Gilbert–Varshamov bound for general stabilizer codes, and establish an analog of the quantum Gilbert–Varshamov bound for linear stabilizer codes. Our proof is restricted to the binary quantum channels, but its extension of to l-adic channels is straight forward. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1497999]

I. INTRODUCTION

The quantum capacity of a quantum channel is the amount of quantum states that can be reliably transmitted through the channel. It is one of the fundamental unsolved problems in the quantum information theory. Except for the quantum erasure channel, we know only lower and upper bounds for the quantum capacity of a quantum channel, and, in addition, a tight lower bound is not known for a general memoryless quantum channel. In this article we shall demonstrate a lower bound on the capacity of a general memoryless quantum channel. A quantum channel is said to be memoryless if the state change of one transmitted quantum system (of the fixed degree of freedom) is statistically independent of the state change of another.

The problem of quantum capacity has attracted great attention, and rapid progress has been made. To be precise, the quantum capacity of a binary memoryless channel Γ is the maximum number $Q(\Gamma)$ such that for any rate $R<Q(\Gamma)$ and any $\epsilon>0$ there exists an $[[n,k]]$ quantum code Q with $k/n \geqslant R$ such that the fidelity between the recovered state and the original state $|\varphi\rangle \in Q$ is at least $1-\epsilon$ for any $|\varphi\rangle$.[1,2] In Refs. 1 and 2, the authors obtained the exact capacity of the quantum erasure channel, and showed lower and upper bounds for that of the quantum depolarizing channel. The same lower bounds for those channels were also obtained in Ref. 3 by using random coding of the stabilizer codes introduced in Refs. 4–6. After that, DiVincenzo *et al.*[7] improved the lower bound for a depolarizing channel by using nonrandom stabilizer codes. The upper bound of the depolarizing channel was improved in Refs. 8–10, and generalized to asymmetric depolarizing channels in Ref. 11. An apparently different definition of the quantum capacity was formalized in Ref. 12, in which an upper bound of a general memoryless quantum channel was established by using the notion of coherent information introduced in Ref. 13. It is informally argued in Ref. 14 that the upper bound in Ref. 12 is achieved by random coding over a general memoryless channel. Barnum *et al.*[15] showed that the definitions of quantum capacity in Refs. 1, 2, and 12 were equivalent.

It is the random coding that is the most commonly used technique in classical information theory to show that a specific rate is achieved by a code in a specific class of codes. For example, Elias showed that the capacity of the binary symmetric channel is achieved by binary linear codes

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using random coding[16] (a readable proof of this fact can be found in Sec. 6.2 of Ref. 17). A proof by random coding usually proceeds as follows: one first calculates the average of error probability of all codes in a specific class of codes of the same rate and the same code length, then shows that the average converges to 0 as the code length increases, and finally concludes that there exists at least one sequence of codes of the fixed rate with which the error probability converges to 0.

The technique of random coding is also used in the quantum information theory. Gottesman[3] showed using random coding that the lower bound on the quantum capacity of the depolarizing channel[2] can be achieved by stabilizer codes. However, his proof does not seem to extend easily to the case of general memoryless channel. The aim of the present article is to derive a lower bound on the quantum capacity of a general memoryless channel by using random coding of stabilizer codes. In our argument of random coding, we shall use the fidelity[18,19] as a replacement of error probability in the classical random coding, and use the idea behind the proof of the quantum Gilbert–Varshamov bound for the stabilizer codes.[4] As a byproduct, we also improve the quantum Gilbert–Varshamov bound for stabilizer codes. Our improved bound (Remark 10) is slightly better than the quantum Gilbert–Varshamov bound for general codes.[20]

As a natural consequence of the quantum Gilbert–Varshamov bound[4,20] and the fidelity bound of t-error correcting quantum codes,[21–23] we can also derive lower bounds for the quantum capacity of a general memoryless quantum channel. However, for the depolarizing channel, the derived lower bounds are much smaller than that obtained in Ref. 2. In contrast to this, our lower bound coincides with the bound in Ref. 2 for the depolarizing channel.

It is interesting whether the proposed lower bound is achieved by a subclass of general stabilizer codes. We also show that the random coding of linear stabilizer codes yields the same lower bound on the quantum capacity. As a byproduct we obtain an analog of the quantum Gilbert–Varshamov bound for linear stabilizer codes (Remark 13), which is asymptotically the same as that for general quantum codes.[20]

The quantum channel considered in this article is discrete in the sense that the channel carries finite-dimensional quantum systems, and we do not touch the quantum capacity of a continuous quantum channel recently studied in Refs. 24 and 25. Our proof is restricted to the binary quantum channels for the simplicity of presentation, but its extension to l-adic channels is straightforward for prime l.

This article is organized as follows: In Sec. II we introduce notations and review relevant research results. In Sec. III we derive a lower bound [Eq. (16)] for the quantum capacity of an arbitrary discrete memoryless quantum channel by random coding of stabilizer codes.

II. NOTATIONS AND PRELIMINARIES

In this section we fix notations used in this article, and review known research results that are necessary to establish our results.

A. Quantum channel and its quantum capacity

For a finite-dimensional complex Hilbert space $\mathcal{H}$, let $\mathcal{S}(\mathcal{H})$ be the set of density operators on $\mathcal{H}$ and $\mathcal{L}(\mathcal{H})$ be the set of linear operators on $\mathcal{H}$. The standard description of a quantum channel is the completely positive trace-preserving map (CP map).[26–28] Suppose that we send a state $\rho \in \mathcal{S}(\mathcal{H})$. The statistical ensemble of the received states is described as $\Gamma(\rho)$ by a CP map Γ.

Suppose that we send a state $\rho \in \mathcal{S}(\mathcal{H}^{\otimes n})$ through a quantum channel. The quantum channel is said to be *memoryless* if the received state is described as $\Gamma^{\otimes n}(\rho)$ for all $\rho \in \mathcal{S}(\mathcal{H}^{\otimes n})$ and for some CP map Γ on $\mathcal{L}(\mathcal{H})$.

Fidelity is a measure of closeness between two quantum states. The fidelity F between a pure state $|\varphi\rangle \in \mathcal{H}$ and a state $\rho \in \mathcal{S}(\mathcal{H})$ is defined by $\langle\varphi|\rho|\varphi\rangle$.[18,19] We have $0 \leqslant F \leqslant 1$ and two states are closer if the fidelity between them is larger.

Let H_2 be the two-dimensional complex Hilbert space. Unless otherwise stated we consider the binary memoryless quantum channel, that is, when we send $\rho \in \mathcal{S}(H_2^{\otimes n})$ we receive $\Gamma^{\otimes n}(\rho)$, where Γ is a CP map on $\mathcal{L}(H_2)$. We shall identify a binary memoryless channel with a CP map on $\mathcal{L}(H_2)$.

A binary $[[n,k]]$ quantum code Q is a 2^k-dimensional subspace of $H_2^{\otimes n}$. The rate of an $[[n,k]]$ quantum code is k/n. The quantum capacity of a binary memoryless channel Γ is the maximum number $Q(\Gamma)$ such that for any rate $R<Q(\Gamma)$ and any $\epsilon>0$ there exists an $[[n,k]]$ quantum code Q with $k/n \geqslant R$ such that the fidelity between the recovered state and the original state $|\varphi\rangle \in Q$ is at least $1-\epsilon$ for any $|\varphi\rangle$.[1,2]

B. Fidelity bound of the quantum error correction

In this subsection we review Preskill's lower bound on the fidelity of quantum error correction in terms of the set of uncorrectable errors of a quantum code. Let

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and $\mathcal{E}=\{w_1 \otimes \cdots \otimes w_n\}$, where w_i is either I, σ_x, σ_z or $\sigma_x\sigma_z$. For a quantum code Q and a fixed error correction process for Q, an operator $M \in \mathcal{E}$ is said to be correctable if the error correction process of Q recovers $M|\varphi\rangle$ to $|\varphi\rangle$ for all $|\varphi\rangle \in Q$. An operator M is uncorrectable if it is not correctable. Let $\mathcal{E}_{\mathrm{unc}} \subset \mathcal{E}$ be the set of uncorrectable errors of a quantum code $Q \subset H_2^{\otimes n}$. Suppose that we send a pure state $|\varphi\rangle \in Q$ through a binary memoryless channel described by a CP map Γ on $\mathcal{L}(H_2)$. By a unitary representation of a CP map,[29] there exists a finite-dimensional Hilbert space H_{env}, a pure state $|0_{\mathrm{env}}\rangle \in H_{\mathrm{env}}$ and a unitary operator U on $H_2^{\otimes n} \otimes H_{\mathrm{env}}$ such that

$$\Gamma(\rho) = \mathrm{Tr}_{H_{\mathrm{env}}}(U(\rho \otimes |0_{\mathrm{env}}\rangle\langle 0_{\mathrm{env}}|)U^*) \tag{1}$$

for all $\rho \in \mathcal{S}(H_2^{\otimes n})$, where $\mathrm{Tr}_{H_{\mathrm{env}}}$ is the partial trace over H_{env}. Since $\mathcal{E}$ is a basis of $\mathcal{L}(H_2^{\otimes n})$ we can write U in Eq. (1) as

$$U = \sum_{M \in \mathcal{E}} M \otimes L_M,$$

where L_M is a linear operator on H_{env}. Preskill proved the following theorem in Sec. 7.4 of Ref. 23.

Theorem 1: *Let Q and $\mathcal{E}_{\mathrm{unc}}$ be as above. When we send a pure state $|\varphi\rangle \in Q$, the fidelity between $|\varphi\rangle$ and the recovered state is not less than*

$$1 - \left\| \sum_{M \in \mathcal{E}_{\mathrm{unc}}} M|\varphi\rangle \otimes L_M|0_{\mathrm{env}}\rangle \right\|^2,$$

where $\|\cdot\|$ denotes the norm of a vector.

C. Stabilizer codes and their error correction process

In this subsection we review stabilizer quantum codes introduced in Refs. 4–6. Let $E = \{\pm w_1 \otimes \cdots \otimes w_n\}$, where w_i is either I, σ_x, σ_z or $\sigma_x\sigma_z$, S is a commutative subgroup of E, and

$$S' = \{M \in E : \forall N \in S, \quad MN = NM\}.$$

A stabilizer code Q is defined as a simultaneous eigenspace of all matrices in S. If S' has 2^{n+k+1} elements, then $\dim Q = 2^k$. The set of simultaneous eigenspaces of S is equal to $\{MQ: \ M \in \mathcal{E}\}$, where $MQ = \{M|\varphi\rangle : |\varphi\rangle \in Q\}$.

We shall describe the error correction process of a stabilizer code. Suppose that we send a pure state $|\varphi\rangle \in Q$ and received $\rho \in \mathcal{S}(H_2^{\otimes n})$. We measure an observable of $H_2^{\otimes n}$ whose eigenspaces are the same as those of S. Then the received state ρ is projected to a state ρ' that is an ensemble of pure states in some eigenspace Q' of S. For $M = \pm w_1 \otimes \cdots \otimes w_n \in E$ we define the weight $w(M)$ of M by $\sharp\{i : w_i \neq I\}$, where $\sharp$ denotes the number of elements in a set. Let

$M \in \mathcal{E}$ such that $MQ = Q'$ and that, if $MQ = M'Q$ for $M' \in \mathcal{E}$, then $w(M) \leqslant w(M')$. We recover ρ' to $M^{-1}\rho'(M^{-1})^*$. With this error correction process the set of uncorrectable errors is contained in

$$\{M \in \mathcal{E}: \text{ there exists } M' \in \mathcal{E} \text{ such that } w(M') \leqslant w(M),$$
$$M'Q = MQ, \text{ and } MS \neq \pm M'S\} = \{M \in \mathcal{E}: \text{ there exists } M' \in \mathcal{E} \text{ such that } w(M') \leqslant w(M), \tag{2}$$
$$M'S' = MS', \text{ and } MS \neq \pm M'S\}.$$

Hamada[30] showed the following theorem based on Theorem 1.

Theorem 2: *Notations as in Theorem 1. Let Q be a stabilizer code with the decoding process described above. Then there exists a subspace $Q' \subset Q$ such that* $\dim Q' = \dim Q/2$ *and that for all pure state $|\varphi\rangle \in Q'$, the fidelity between $|\varphi\rangle$ and the recovered state is not less than*

$$1 - 2 \sum_{M \in \mathcal{E}_{\text{unc}}} \| L_M |0_{\text{env}}\rangle \|^2. \tag{3}$$

Observe that the information rates of Q and Q' in Theorem 2 differ by $\log 2/n$, which becomes negligible as $n \to \infty$. We call a subspace Q' as a subcode of Q as in the classical coding theory. We shall consider the subcode Q' of a stabilizer code Q in the discussion of Sec. III.

D. Symplectic geometry

In this subsection we review the symplectic geometric interpretation of stabilizer codes introduced in Refs. 4 and 5. A symplectic geometry is a linear space with a nondegenerate symplectic form.[31] Let $\mathbf{F}_2$ be the finite field with two elements. For $\vec{a} = (a_1, \ldots, a_n) \in \mathbf{F}_2^n$ and $\vec{b} = (b_1, \ldots, b_n) \in \mathbf{F}_2^n$, we define $(\vec{a}|\vec{b})$ by $(a_1, \ldots, a_n, b_1, \ldots, b_n) \in \mathbf{F}_2^{2n}$ and

$$f(\pm \sigma_x^{a_1}\sigma_z^{b_1} \otimes \cdots \otimes \sigma_x^{a_n}\sigma_z^{b_n}) = (\vec{a}|\vec{b}).$$

We also define the standard symplectic form of $(\vec{a}|\vec{b})$ and $(\vec{a}'|\vec{b}') \in \mathbf{F}_2^{2n}$ by

$$\langle \vec{a}, \vec{b}' \rangle - \langle \vec{a}', \vec{b} \rangle, \tag{4}$$

where $\langle \cdot, \cdot \rangle$ denotes the standard inner product in $\mathbf{F}_2^n$. For a subspace $C \subseteq \mathbf{F}_2^{2n}$ we denote by $C^\perp$ the orthogonal space of C with respect to (4). For a subgroup $S \subseteq E$, S is commutative if and only if $f(S) \subseteq (f(S))^\perp$, and $S' = f^{-1}((f(S))^\perp)$.

E. Linear stabilizer codes and unitary geometry

Calderbank *et al.*[5] related stabilizer codes to classical error-correcting codes and unitary geometry, which is a linear space with a nondegenerate hermitian form.[31] Let ω be a primitive element in $\mathbf{F}_4$, and define

$$g(\pm \sigma_x^{a_1}\sigma_z^{b_1} \otimes \cdots \otimes \sigma_x^{a_n}\sigma_z^{b_n}) = \omega\vec{a} + \omega^2\vec{b} \in \mathbf{F}_4^n.$$

For vectors $\vec{x}, \vec{y} \in \mathbf{F}_4^n$ we define an $\mathbf{F}_2$-bilinear map

$$\langle \vec{x}^2, \vec{y} \rangle - \langle \vec{x}, \vec{y}^2 \rangle, \tag{5}$$

where $\langle , \rangle$ denotes the standard inner product in $\mathbf{F}_4^n$ and $\vec{x}^2 = (x_1^2, \ldots, x_n^2)$. For an $\mathbf{F}_2$-linear subspace C of $\mathbf{F}_4^n$, let $C^\perp$ denotes the orthogonal space of C with respect to (5). For a subgroup $S \subseteq E$, S is commutative if and only if $g(S) \subseteq (g(S))^\perp$, and $S' = g^{-1}((g(S))^\perp)$.

For $\vec{x}$, $\vec{y} \in \mathbf{F}_4^n$, we define the standard Hermitian form of $\vec{x}$, $\vec{y}$ by

$$\tau(\vec{x},\vec{y}) = \langle \vec{x}^2, \vec{y} \rangle, \tag{6}$$

which is used only in Sec. III D. If C is an $\mathbf{F}_4$-linear subspace of $\mathbf{F}_4^n$, $C^\perp$ is equal to the orthogonal space of C with respect to (6). A stabilizer code constructed from an $\mathbf{F}_2$-linear self-orthogonal space $C \subset \mathbf{F}_4^n$ is said to be linear if C is $\mathbf{F}_4$-linear. This connection between binary stabilizer codes and classical codes over $\mathbf{F}_4$ is generalized to nonbinary case in Refs. 32–34.

III. LOWER BOUND ON THE QUANTUM CAPACITY

As described in the Introduction, we have to calculate the average of fidelity over all the stabilizer codes, and show that the average converges to 1. Strictly speaking, we shall use the subcode of a stabilizer code introduced in Theorem 2. This section is organized as follows: In Sec. III A we introduce a definition of the distance of a quantum channel from the identity channel. In Sec. III B we calculate the average of fidelity over subcodes of general stabilizer codes of the fixed rate. In Sec. III C we deduce a sufficient condition for the rate to let the average of fidelity converge to 1. In Sec. III D we indicate that a small modification of the argument in Secs. III B and III C shows that the same lower bound on the capacity is obtained from the random coding of linear stabilizer codes.

A. A definition of distance of a quantum channel from the identity channel

We give a lower bound on the quantum capacity in terms of the distance of a quantum channel from the identity channel. Let us first review a definition of the distance of a quantum channel from the identity channel introduced in Ref. 22, then show some properties of the definition. Let Γ be a CP map on $\mathcal{L}(H_2)$.

Definition 3: Suppose that there exist a four-dimensional space H_E, $|e_0\rangle \in H_E$, and a unitary operator U on $H_2 \otimes H_E$ such that

$$\Gamma(\rho) = \mathrm{Tr}_E[U(\rho \otimes |e_0\rangle\langle e_0|)U^*] \tag{7}$$

for all $\rho \in \mathcal{S}(H_2)$. Write U as

$$U = I \otimes L_I + \sigma_x \otimes L_x + \sigma_z \otimes L_z + \sigma_x\sigma_z \otimes L_{xz},$$

where L_I, L_x, L_z, and L_{xz} are linear operators on H_E. Then the distance $p(\Gamma)$ and $q(\Gamma)$ of the channel Γ from the identity channel are defined by

$$q(\Gamma) = \| L_I |e_0\rangle \|^2,$$

$$p(\Gamma) = \| L_x |e_0\rangle \|^2 + \| L_z |e_0\rangle \|^2 + \| L_{xz} |e_0\rangle \|^2.$$

It is not clear whether the values of $p(\Gamma)$ and $q(\Gamma)$ are uniquely determined by Γ alone, that is, whether they are independent of choice of U and $|e_0\rangle$ in Eq. (7). In order to answer this question in Corollary 5, we shall represent $p(\Gamma)$ and $q(\Gamma)$ using the operator-sum representation of Γ induced by U and $|e_0\rangle$.

Proposition 4: Let $|e_0\rangle, \ldots, |e_3\rangle$ be an orthonormal basis of H_E, and

$$A_i = \langle e_i | U | e_0 \rangle.$$

By Eq. (8.10) of Ref. 35,

$$\Gamma(\rho) = \sum_{i=0}^{3} A_i \rho A_i^*$$

for all $\rho \in \mathcal{S}(H_2)$. Write A_i as

$$A_i = a_{i,I} I + a_{i,x}\sigma_x + a_{i,z}\sigma_z + a_{i,xz}\sigma_x\sigma_z .$$

Then we have another representations of $p(\Gamma)$ *and* $q(\Gamma)$ *as*

$$p(\Gamma) = \sum_{i=0}^{3} |a_{i,x}|^2 + |a_{i,z}|^2 + |a_{i,xz}|^2,$$

$$q(\Gamma) = \sum_{i=0}^{3} |a_{i,I}|^2.$$

Proof: By definition of A_i,

$$A_i = \langle e_i|L_I|e_0\rangle I + \langle e_i|L_x|e_0\rangle\sigma_x + \langle e_i|L_z|e_0\rangle\sigma_z + \langle e_i|L_{xz}|e_0\rangle\sigma_x\sigma_z .$$

Therefore,

$$a_{i,I} = \langle e_i|L_I|e_0\rangle, \quad a_{i,x} = \langle e_i|L_x|e_0\rangle, \quad a_{i,z} = \langle e_i|L_z|e_0\rangle, \quad a_{i,xz} = \langle e_i|L_{xz}|e_0\rangle.$$

Since $|e_0\rangle,\ldots,|e_3\rangle$ are an orthonormal basis, we have

$$q(\Gamma) = \| L_I|e_0\rangle \|^2 = \sum_{i=0}^{3} |a_{i,I}|^2.$$

The equality of $p(\Gamma)$ can be shown in a similar way. ■

Corollary 5: The values of $p(\Gamma)$ *and* $q(\Gamma)$ *do not depend on choice of* U *and* $|e_0\rangle$ *in Eq. (7).*

Proof: Let

$$\Gamma(\rho) = \sum_{i=0}^{3} B_i \rho B_i^*$$

be another operator-sum representation of Γ. By Theorem 8.2 of Ref. 35, there exists a 4×4 unitary matrix V such that

$$\begin{pmatrix} B_0 \\ \vdots \\ B_3 \end{pmatrix} = V \begin{pmatrix} A_0 \\ \vdots \\ A_3 \end{pmatrix}.$$

Write B_i as

$$B_i = b_{i,I} I + b_{i,x}\sigma_x + b_{i,z}\sigma_z + b_{i,xz}\sigma_x\sigma_z ,$$

and define $\vec{a}_I = (a_{0,I},\ldots,a_{3,I})^T$, $\vec{b}_I = (b_{0,I},\ldots,b_{3,I})^T$. Since I, σ_x, σ_z, and $\sigma_x\sigma_z$ are linearly independent, we have $\vec{b}_I = V\vec{a}_I$. Since V is unitary, $\|\vec{b}_I\| = \|\vec{a}_I\|$, which shows that $q(\Gamma)$ does not depend on choice of representation. The independence of $p(\Gamma)$ can be shown in a similar way. ■

The following corollary drastically simplifies the formula for the lower bound in Eq. (16).

Corollary 6: $p(\Gamma) + q(\Gamma) = 1$.

Proof: Notations as in Proposition 4. We have

$$I = \sum_{i=0}^{3} A_i^* A_i .$$

Taking trace on the both side, we have

$$\begin{aligned}\mathrm{Tr}[I] &= \sum_{i=0}^{3} \mathrm{Tr}[A_i^* A_i] \\ &= \sum_{i=0}^{3} \mathrm{Tr}[(a_{i,I} I + a_{i,x}\sigma_x + a_{i,z}\sigma_z + a_{i,xz}\sigma_x\sigma_z)^* \times (a_{i,I} I + a_{i,x}\sigma_x + a_{i,z}\sigma_z + a_{i,xz}\sigma_x\sigma_z)] \\ &= \mathrm{Tr}[I] \sum_{i=0}^{3} |a_{i,I}|^2 + |a_{i,x}|^2 + |a_{i,z}|^2 + |a_{i,xz}|^2 = \mathrm{Tr}[I](p(\Gamma) + q(\Gamma)).\end{aligned}$$

■

B. Average of the fidelity over all the stabilizer codes

In this subsection we shall prove that the average fidelity of the subcodes of all $[[n,\lfloor Rn \rfloor]]$ stabilizer codes converges to 1 as $n \to \infty$ under the conditions (8) and (9). The proof is proceeded as follows:

(1) For every stabilizer code, there exists its subcode whose fidelity of error correction is lower bounded by Eq. (3). The lower bound (3) is expressed as a sum indexed by error operators. The average of the sum will be divided according to the weight of error operators in Eq. (10).
(2) It is easy to see the part indexed by operators of larger weights converges to 0 as $n \to \infty$.
(3) We shall show that the other part indexed by operators of smaller weights converges to 0 by the fact that most of stabilizer codes can correct an error of small weight, which will be rigorously proved in Eq. (13) from Lemma 9.

Let δ and R be real numbers such that

$$\lim_{n\to\infty} \sum_{i=\lfloor \delta n \rfloor + 1}^{n} \binom{n}{i} p(\Gamma)^i q(\Gamma)^{n-i} = 0, \tag{8}$$

$$1 - \lim_{n\to\infty} \frac{\log_2 [\sum_{i=1}^{\lfloor \delta n \rfloor} \binom{n}{i} p(\Gamma)^i q(\Gamma)^{n-i} \Sigma_{j=0}^{i} \binom{n}{j} 3^j]}{n} > R, \tag{9}$$

where $\lfloor x \rfloor$ denotes the largest integer $\leqslant x$.

Let

$$A_n = \{C \subset \mathbf{F}_2^{2n} : \ C \text{ is linear}, \quad \dim C = n - \lfloor Rn \rfloor, C \subseteq C^{\perp}\}.$$

Recall that we can construct an $[[n,\lfloor Rn \rfloor]]$ stabilizer code from every $C \in A_n$. Note that A_n is not empty because there exists a self-orthogonal subspace of dimension n in $\mathbf{F}_2^{2n}$.[31] This subsection is devoted to show the following.

Proposition 7: If R satisfies Eq. (9), then there exists a sequence of subcodes of stabilizer codes whose rates are greater than or equal to R and whose fidelity converges to 1 as $n \to \infty$.

Since the information rates of the subcode Q' and Q in Theorem 2 are asymptotically the same as $n \to \infty$, it is sufficient to show that the average of the fidelity bound (3) of Q' over all the stabilizer codes in A_n converges to 1 as $n \to \infty$.

Let $|0_{\mathrm{env}}\rangle = |e_0\rangle^{\otimes n}$, and for $M = \sigma_{i_1} \otimes \cdots \otimes \sigma_{i_n} \in \mathcal{E}$ let

$$L_M = L_{i_1} \otimes \cdots \otimes L_{i_n},$$

where $\sigma_I = I$ and $|e_0\rangle$, L_I, L_x, L_z, and L_{xz} are as defined in Definition 3. For $C \in A_n$ we denote the set of uncorrectable errors of C in $\mathcal{E}$ by $\mathcal{E}_{\mathrm{unc}}(C)$. The average of the fidelity bound (3) of Q' over all the stabilizer codes in A_n is not less than

$$\frac{1}{\sharp A_n}\sum_{C\in A_n}\left(1-2\sum_{M\in\mathcal{E}_{\mathrm{unc}}(C)}\|L_M|0_{\mathrm{env}}\rangle\|^2\right)$$
$$=1-\frac{2}{\sharp A_n}\sum_{C\in A_n}\left(\sum_{\substack{M\in\mathcal{E}_{\mathrm{unc}}(C)\\1\leqslant w(M)\leqslant\lfloor\delta n\rfloor}}\|L_M|0_{\mathrm{env}}\rangle\|^2+\sum_{\substack{M\in\mathcal{E}_{\mathrm{unc}}(C)\\w(M)>\lfloor\delta n\rfloor}}\|L_M|0_{\mathrm{env}}\rangle\|^2\right)$$
$$\geqslant 1-\left(\frac{2}{\sharp A_n}\sum_{C\in A_n}\sum_{\substack{M\in\mathcal{E}_{\mathrm{unc}}(C)\\1\leqslant w(M)\leqslant\lfloor\delta n\rfloor}}\|L_M|0_{\mathrm{env}}\rangle\|^2\right)-2\sum_{\substack{M\in\mathcal{E}\\w(M)>\lfloor\delta n\rfloor}}\|L_M|0_{\mathrm{env}}\rangle\|^2. \tag{10}$$

By the same argument as Ref. 22, one can show that

$$\sum_{\substack{M\in\mathcal{E}\\w(M)>\lfloor\delta n\rfloor}}\|L_M|0_{\mathrm{env}}\rangle\|\leqslant\sum_{i=\lfloor\delta n\rfloor+1}^{n}\binom{n}{i}p(\Gamma)^i q(\Gamma)^{n-i},$$

which converges to 0 as $n\to\infty$ by the condition (8).

We shall calculate an upper bound for the second term in Eq. (10). For $M\in\mathcal{E}$ we define

$$B_n(M)=\{C\in A_n : M\in\mathcal{E}_{\mathrm{unc}}(C)\}.$$

It follows that

$$\frac{1}{\sharp A_n}\sum_{C\in A_n}\sum_{\substack{M\in\mathcal{E}_{\mathrm{unc}}(C)\\1\leqslant w(M)\leqslant\lfloor\delta n\rfloor}}\|L_M|0_{\mathrm{env}}\rangle\|^2\leqslant\frac{1}{\sharp A_n}\sum_{\substack{M\in\mathcal{E}\\1\leqslant w(M)\leqslant\lfloor\delta n\rfloor}}\sharp B_n(M)\|L_M|0_{\mathrm{env}}\rangle\|^2. \tag{11}$$

Note that we omitted the factor 2 from Eq. (10) for simplicity, because we shall show that the right-hand side of Eq. (11) converges to 0 and factor 2 is negligible.

We shall give an upper bound for $\sharp B_n(M)$. To estimate $\sharp B_n(M)$ we shall introduce Lemma 9. In the proof of Lemma 9 we use the Witt theorem, so we review it.

Theorem 8 (Witt): *Let K be a field, V_1, V_2 finite-dimensional K-linear spaces, and τ_1, τ_2 symplectic forms on V_1, V_2, respectively. An injective linear map $T:V_1\to V_2$ is said to be an* isometry *if*

$$\tau_1(x,y)=\tau_2(Tx,Ty).$$

Let W_1 be a subspace of V_1. If there exists a bijective isometry from V_1 to V_2 and an isometry $T_{W_1}:W_1\to V_2$, then there exists an isometry $T_{V_1}:V_1\to V_2$ such that the restriction of T_{V_1} to W_1 is equal to T_{W_1}. The same result also holds when τ_1,τ_2 are Hermitian forms.

Proof: See Sec. 20 of Ref. 31. ■

Lemma 9: For $M\in E-\{\pm I\}$, let $A_n(M)=\{C\in A_n : f(M)\in C^{\perp}\backslash C\}$. We have

$$\sharp A_n(M)\leqslant(1/2^{n-\lfloor Rn\rfloor})\frac{1-2^{-2\lfloor Rn\rfloor}}{1-2^{-2n}}\sharp A_n<\sharp A_n/2^{n-\lfloor Rn\rfloor}.$$

Proof: Let $\mathrm{Sp}_n(\mathbf{F}_2)$ be the group of bijective linear maps on $\mathbf{F}_2^{2n}$ preserving the symplectic form (4). For every pair of spaces C_1, $C_2\in A_n$, every bijective linear map from C_1 to C_2 is an isometry. Consequently, there exists $\sigma\in\mathrm{Sp}_n(\mathbf{F}_2)$ such that $\sigma C_1=C_2$ by the Witt theorem. A similar argument shows that there exists $\sigma'\in\mathrm{Sp}_n(\mathbf{F}_2)$ such that $\sigma'(\vec{a}|\vec{b})=(\vec{a}'|\vec{b}')$ for every pair of nonzero vectors $(\vec{a}|\vec{b})$, $(\vec{a}'|\vec{b}')\in\mathbf{F}_2^{2n}$.

It follows that

$$\begin{aligned}\sharp A_n(M) &= \sharp\{C \in A_n : f(M) \in C^{\perp}\backslash C\} \\ &= \sharp\{\alpha C_1 : f(M) \in (\alpha C_1)^{\perp}\backslash \alpha C_1, \alpha \in \mathrm{Sp}_n(\mathbf{F}_2)\} \\ &= \sharp\{\alpha C_1 : \beta(f(M)) \in (\alpha C_1)^{\perp}\backslash \alpha C_1, \alpha \in \mathrm{Sp}_n(\mathbf{F}_2)\},\end{aligned}$$

where C_1 (resp. β) is an arbitrary fixed element in A_n [resp. $\mathrm{Sp}_n(\mathbf{F}_2)$]. Therefore $\sharp A_n(M)$ is the same among every nonzero $f(M)$.

Since $\sharp(C^{\perp}\backslash C) = 2^{n+\lfloor Rn\rfloor} - 2^{n-\lfloor Rn\rfloor}$, there are $(2^{n+\lfloor Rn\rfloor} - 2^{n-\lfloor Rn\rfloor})\sharp A_n$ pairs of $((\vec{a}|\vec{b}), C)$ such that $(\vec{a}|\vec{b}) \in C^{\perp}\backslash C$ and $C \in A_n$. Thus if $M \neq \pm I$, then

$$\sharp A_n(M) \leqslant \frac{2^{n+\lfloor Rn\rfloor} - 2^{n-\lfloor Rn\rfloor}}{2^{2n}-1}\sharp A_n = (1/2^{n-\lfloor Rn\rfloor})\frac{1-2^{-2\lfloor Rn\rfloor}}{1-2^{-2n}}\sharp A_n < \sharp A_n/2^{n-\lfloor Rn\rfloor}.$$

■

Remark 10: From Lemma 9 we can improve the quantum Gilbert–Varshamov bound slightly. There exists an $[[n,k,d]]$ *stabilizer code if*

$$\frac{1-2^{-2k}}{1-2^{-2n}} \cdot \frac{1}{2^{n-k}} \sum_{i=1}^{d-1} 3^i \binom{n}{i} < 1. \tag{12}$$

The proof is as follows: For each error $M \in \mathcal{E}$, $A_n(M)$ *is equal to the set of stabilizer codes unable to detect* M *as an error. Therefore, by replacing* $\lfloor Rn\rfloor$ *with* k *in Lemma 9, we see that if Eq. (12) holds, then there is at least one stabilizer code* C *is able to detect all the errors* M *with* $w(M) < d$, *which means that the minimum distance of* C *is at least* d. *The idea behind this proof already appeared in the original proof of the quantum Gilbert–Varshamov bound for stabilizer codes.*[4] *Observe that our bound is slightly better than the quantum Gilbert–Varshamov bound for general codes,*[20] *which implies that an* $[[n,k,d]]$ *quantum code exists if*

$$\frac{1}{2^{n-k}} \sum_{i=0}^{d-1} 3^i \binom{n}{i} < 1.$$

By Eq. (2), $M \in \mathcal{E}$ belongs to $\mathcal{E}_{\mathrm{unc}}(C)$ only if there exists $M' \in \mathcal{E}$ such that $w(M') \leqslant w(M)$, $Mf^{-1}(C^{\perp}) = M'f^{-1}(C^{\perp})$, and $Mf^{-1}(C) \neq M'f^{-1}(C)$. A space $C \in A_n$ belongs to $B_n(M)$ only if there exists $M' \in \mathcal{E}$ such that $w(M') \leqslant w(M)$ and $M^{-1}M' \in f^{-1}(C^{\perp}\backslash C)$. The last condition is equivalent to $C \in A_n(M^{-1}M')$. Since there are

$$\sum_{j=0}^{w(M)} \binom{n}{j} 3^j$$

operators $M' \in \mathcal{E}$ such that $w(M') \leqslant w(M)$, it follows that

$$\begin{aligned}\sharp B_n(M) &\leqslant \sum_{\substack{M' \in \mathcal{E} \\ w(M') \leqslant w(M)}} \sharp A_n(M^{-1}M') \\ &\leqslant \sum_{\substack{M' \in \mathcal{E} \\ w(M') \leqslant w(M)}} \frac{\sharp A_n}{2^{n-[Rn]}} \leqslant \frac{\sharp A_n}{2^{n-[Rn]}} \sum_{j=0}^{w(M)} \binom{n}{j} 3^j.\end{aligned} \tag{13}$$

An upper bound for Eq. (11) is derived as follows:

$$\frac{1}{\sharp A_n}\sum_{\substack{M\in\mathcal{E}\\ 1\leqslant w(M)\leqslant\lfloor\delta n\rfloor}}\sharp B_n(M)\|L_M|0_{\mathrm{env}}\rangle\|^2$$
$$\leqslant\frac{1}{\sharp A_n}\sum_{\substack{M\in\mathcal{E}\\ 1\leqslant w(M)\leqslant\lfloor\delta n\rfloor}}\frac{\sharp A_n}{2^{n-[Rn]}}\sum_{j=0}^{w(M)}\binom{n}{j}3^j\|L_M|0_{\mathrm{env}}\rangle\|^2$$
$$=\frac{1}{2^{n-[Rn]}}\sum_{\substack{M\in\mathcal{E}\\ 1\leqslant w(M)\leqslant\lfloor\delta n\rfloor}}\sum_{j=0}^{w(M)}\binom{n}{j}3^j\|L_M|0_{\mathrm{env}}\rangle\|^2. \tag{14}$$

For an integer $0\leqslant i\leqslant n$, by the same argument as Ref. 22, one can show that

$$\sum_{\substack{M\in\mathcal{E}\\ w(M)=i}}\|L_M|0_{\mathrm{env}}\rangle\|^2=\binom{n}{i}p(\Gamma)^i q(\Gamma)^{n-i}.$$

Therefore Eq. (14) is equal to

$$\frac{1}{2^{n-[Rn]}}\sum_{i=1}^{\lfloor\delta n\rfloor}\binom{n}{i}p(\Gamma)^i q(\Gamma)^{n-i}\sum_{j=0}^{i}\binom{n}{j}3^j,$$

which converges to 0 as $n\to\infty$ by the condition (9).

C. Achievable rate by general stabilizer codes

In the previous subsection, we have shown that if the rate R satisfies Eq. (9), then there exists at least one sequence of subcodes of stabilizer codes of the rate R such that the average of fidelity converges to 1. In this subsection we shall simplify Eqs. (8) and (9) with which we can easily compute a lower bound on the capacity of the channel Γ.

We shall deduce a sufficient condition for δ to satisfy Eq. (8). By Appendix A of Ref. 36, for $0\leqslant\epsilon<\lambda\leqslant 1$ we have

$$\sum_{i=\lambda n}^{n}\binom{n}{i}\epsilon^i(1-\epsilon)^{n-i}\leqslant 2^{-nD(\lambda\|\epsilon)},$$

where $D(\lambda\|\epsilon)$ is the classical relative entropy defined by

$$\lambda\log_2\frac{\lambda}{\epsilon}+(1-\lambda)\log_2\frac{1-\lambda}{1-\epsilon}.$$

Since $p(\Gamma)+q(\Gamma)=1$ by Corollary 6, the condition (8) holds if

$$\delta>p(\Gamma). \tag{15}$$

The term inside of $\log_2$ in Eq. (9) can be bounded as follows:

$$\sum_{i=1}^{\lfloor \delta n \rfloor} \binom{n}{i} p(\Gamma)^i q(\Gamma)^{n-i} \sum_{j=0}^{i} \binom{n}{j} 3^j \leq \sum_{i=0}^{n} \binom{n}{i} p(\Gamma)^i q(\Gamma)^{n-i} \sum_{j=0}^{\lfloor \delta n \rfloor} \binom{n}{j} 3^j$$

$$= [p(\Gamma)+q(\Gamma)]^n \sum_{j=0}^{\lfloor \delta n \rfloor} \binom{n}{j} 3^j = \sum_{j=0}^{\lfloor \delta n \rfloor} \binom{n}{j} 3^j \quad \text{(by Corollary 6)}$$

$$\leq (\delta n+1) \binom{n}{\lfloor \delta n \rfloor} 3^{\delta n}$$

$$\leq (\delta n+1) \exp_2[nH_e(\delta)] 3^{\delta n} \quad \text{(by Appendix B of Ref. 36)}$$

$$= (\delta n+1) \exp_2\{n[H_e(\delta)+\delta \log_2 3]\},$$

where H_e is the binary entropy function.

From Proposition 7, Eq. (15), and the observations above, we see that the capacity of the channel Γ is at least

$$1-\{H_e[p(\Gamma)]+p(\Gamma)\log_2 3\}. \tag{16}$$

Note that the same lower bound on the capacity can also be obtained by the method of Bennett *et al.*,[2] though they stated their result only for the depolarizing channel. However, Bennett *et al.*[2] did not address the achievability of the bound (16) with stabilizer codes, which is the main focus of this article.

We shall compare our bound on the capacity [Eq. (16)] with the conventional bound for a general memoryless channel derived from the quantum Gilbert–Varshamov bound[4,20] and the fidelity bounds for t-error-correcting codes.[21,22] Suppose that we have a sequence of $\lfloor \delta n_i \rfloor$-error-correcting quantum codes of length n_i with $\lim_{i\to\infty} n_i = \infty$. The condition (15) is sufficient in order that the fidelity of error correction by $\lfloor \delta n_i \rfloor$-error-correcting codes converges to 1 as $i \to \infty$. By the quantum Gilbert–Varshamov bound the derived lower bound on the capacity is

$$1-\{H_e[2p(\Gamma)]+2p(\Gamma)\log_2 3\},$$

which is always smaller than Eq. (16).

When the channel Γ is the depolarizing channel of the fidelity parameter f, $p(\Gamma)=1-f$ and $q(\Gamma)=f$. The proposed lower bound [Eq. (16)] for the capacity is

$$1-[H_e(1-f)+(1-f)\log_2 3],$$

which coincides with the lower bound given in Ref. 2. It is not clear to the authors whether our lower bound can be improved by the method in Ref. 7.

Our analysis for the quantum capacity can be generalized to the capacity of an l-adic channel using the l-adic stabilizer codes[37,38] in a straightforward manner when l is prime. The quantum Gilbert–Varshamov bound for l-adic stabilizer codes can also be proved by Lemma 9.

D. Achievable rate by linear stabilizer codes

In this subsection we shall show that the achievable rate (16) by subcodes of general stabilizer codes can also be achieved by those of linear stabilizer codes, which shows the asymptotic optimality of linear stabilizer codes among general ones. As a byproduct we establish an analog of Gilbert–Varshamov bound for linear stabilizer codes.

Let

$$A_n' = \{C \subset \mathbf{F}_4^n : C \text{ is } \mathbf{F}_4\text{-linear}, \ \dim_{\mathbf{F}_4} C = \lfloor (n-Rn)/2 \rfloor, \quad C \subseteq C^{\perp}\}.$$

Recall that we can construct an $[[n,n-2\lfloor(n-Rn)/2\rfloor]]$ linear stabilizer code from every $C \in A'_n$. Note that A'_n is not empty because there exists a self-orthogonal subspace of dimension $\lfloor n/2 \rfloor$ in $\mathbf{F}_4^n$ (see Proposition 2.3.2 in Ref. 39). For $M \in \mathcal{E}$, define

$$A'_n(M)=\{C \in A'_n : g(M) \in C^{\perp} \backslash C\},$$

$$B'_n(M)=\{C \in A'_n : M \text{ is uncorrectable by } C\}.$$

By these definitions of $A'_n(M)$ and $B'_n(M)$, all the arguments except Lemma 9 in the previous subsections can be used for showing that the rate (16) is achieved by subcodes of linear stabilizer codes. In this subsection we prove an upper bound (Lemma 11) for $\sharp A'_n(M)$ that can be used as a substitute for Lemma 9.

Lemma 11: Define τ by Eq. (6). The number of nonzero vectors $\vec{x} \in \mathbf{F}_4^n$ such that $\tau(\vec{x},\vec{x})=0$ is $2^{2n-1}+(-1)^n 2^{n-1}-1$.

Proof: See the proof of Proposition 2.3.3 in Ref. 39. ■

Lemma 12: Let $u=\lfloor(n-Rn)/2\rfloor$. For $M \in E\backslash\{\pm I\}$

$$\sharp A'_n(M) \leqslant \frac{4^{n-u}-4^u}{\min\{2^{2n-1}+(-1)^n 2^{n-1}-1, 2^{2n-1}-(-1)^n 2^{n-1}\}} \sharp A'_n \leqslant \frac{4^{n-u}-4^u}{2^{2n-1}-2^{n-1}-1} \sharp A'_n .$$

Proof: Let $\mathrm{GU}_n(\mathbf{F}_4)$ be the group of bijective linear maps on $\mathbf{F}_4^n$ that preserve the value of the Hermitian form τ. For every pair of spaces $C_1, C_2 \in A'_n$, every bijective linear map from C_1 to C_2 is an isometry. Thus there exists $\sigma \in \mathrm{GU}_n(\mathbf{F}_4)$ such that $\sigma C_1 = C_2$ by the Witt theorem. For a pair of nonzero vectors $\vec{x},\vec{y} \in \mathbf{F}_4^n$ with $\tau(\vec{x},\vec{x})=\tau(\vec{y},\vec{y})=0$, a similar argument shows that there exists $\sigma \in \mathrm{GU}_n(\mathbf{F}_4)$ such that $\sigma\vec{x}=\vec{y}$.

We want to show that for a pair of vectors $\vec{x},\vec{y} \in \mathbf{F}_4^n$ with $\tau(\vec{x},\vec{x}) \neq 0$ and $\tau(\vec{y},\vec{y}) \neq 0$, there exists $\sigma \in \mathrm{GU}_n(\mathbf{F}_4)$ such that $\sigma\vec{x}=\vec{y}$. Since τ is a Hermitian form, $\tau(\vec{x},\vec{x}) \in \mathbf{F}_2$. Therefore $\tau(\vec{x},\vec{x})=\tau(\vec{y},\vec{y})=1$, and there exists $\sigma \in \mathrm{GU}_n(\mathbf{F}_4)$ such that $\sigma\vec{x}=\vec{y}$ by the Witt theorem.

A similar argument to the proof of Lemma 9 shows that for $M \in E\backslash\{\pm I\}$ we have

$$\sharp A'_n(M) \leqslant \frac{4^{n-u}-4^u}{2^{2n-1}+(-1)^n 2^{n-1}-1} \sharp A'_n \quad \text{if} \quad \tau(g(M),g(M))=0,$$

$$\sharp A'_n(M) \leqslant \frac{4^{n-u}-4^u}{2^{2n-1}-(-1)^n 2^{n-1}} \sharp A'_n \quad \text{if} \quad \tau(g(M),g(M)) \neq 0.$$

■

Remark 13: From Lemma 11 we can show that there exists an $[[n,k,d]]$ linear stabilizer code if k is even and

$$\frac{2(1-2^{-2k})}{1-2^{-n}-2^{-2n+1}} \cdot \frac{1}{2^{n-k}} \sum_{i=1}^{d-1} 3^i \binom{n}{i} < 1,$$

which is asymptotically the same as the quantum Gilbert–Varshamov bound for general quantum codes.[20]

Remark 14: The connection between stabilizer codes and classical codes over $\mathbf{F}_4$ was generalized to nonbinary case in Refs. 32–34. The argument in this subsection can be extended to linear l-adic stabilizer codes for a prime l with the following exception: In the proof of Lemma 11, there does not always exist $\sigma \in \mathrm{GU}_n(\mathbf{F}_{l^2})$ such that $\sigma\vec{x}=\vec{y}$ for a pair of vectors $\vec{x},\vec{y} \in \mathbf{F}_{l^2}^n$ with $\tau(\vec{x},\vec{x}) \neq 0$ and $\tau(\vec{y},\vec{y}) \neq 0$. However, there always exists $\sigma \in \mathcal{U}$ such that $\sigma\vec{x}=\vec{y}$, where $\mathcal{U}$ is the group generated by $\mathrm{GU}_n(\mathbf{F}_{l^2})$ and nonzero scalar multiples of the identity map on $\mathbf{F}_{l^2}^n$.

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Trading quantum for classical resources in quantum data compression

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We study the visible compression of a source $\mathcal{E}=\{|\varphi_i\rangle,p_i\}$ of pure quantum signal states or, more formally, the minimal resources per signal required to represent arbitrarily long strings of signals with arbitrarily high fidelity, when the compressor is given the identity of the input state sequence as classical information. According to the quantum source coding theorem, the optimal quantum rate is the von Neumann entropy $S(\mathcal{E})$ qubits per signal. We develop a refinement of this theorem in order to analyze the situation in which the states are coded into classical and quantum bits that are quantified separately. This leads to a trade-off curve $Q^*(R)$, where $Q^*(R)$ qubits per signal is the optimal quantum rate for a given classical rate of R bits per signal. Our main result is an explicit characterization of this trade-off function by a simple formula in terms of only single-signal, perfect fidelity encodings of the source. We give a thorough discussion of many further mathematical properties of our formula, including an analysis of its behavior for group covariant sources and a generalization to sources with continuously parametrized states. We also show that our result leads to a number of corollaries characterizing the trade-off between information gain and state disturbance for quantum sources. In addition, we indicate how our techniques also provide a solution to the so-called remote state preparation problem. Finally, we develop a probability-free version of our main result which may be interpreted as an answer to the question: ''How many classical bits does a qubit cost?'' This theorem provides a type of dual to Holevo's theorem, insofar as the latter characterizes the cost of coding classical bits into qubits. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1497184]

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I. INTRODUCTION

When the term ''quantum information'' was first coined, it would have been hard to predict how thorough and fruitful the analogy between quantum mechanics and classical information theory would ultimately prove to be. The general approach, characterized by the treatment of quantum states as resources to be manipulated, has yielded a promising collection of applications, ranging from unconditionally secure cryptographic protocols[1–3] to quantum algorithms.[4–6] Moreover, the analogy, which was initially unavoidably vague, has gradually been filled in by a diverse variety of rigorous theorems describing achievable limits to the manipulation of quantum states, such as the characterization of the classical information capacity of quantum sources,[7,8] the identification of optimal strategies for entanglement concentration and dilution[9] and many more. One of the pivotal results of the emerging theory is the quantum source coding theorem,[10–12] demonstrating that for the task of compressing quantum states, the von Neumann entropy plays a role directly analogous to the Shannon entropy of classical information theory. Indeed, the quantum theorem subsumes the classical one as the special case in which all the quantum states to be compressed are mutually orthogonal.

A quantum source (or ensemble) $\mathcal{E}=\{|\varphi_i\rangle,p_i\}$ is defined by a set of pure quantum signal (or ''letter'') states $|\varphi_i\rangle$ with given prior probabilities p_i (cf. below for precise definitions of these and other terms used in the Introduction). In this article we will study the so-called *visible* compression of $\mathcal{E}$. More specifically, we wish to characterize the minimal resources per signal that are necessary and sufficient to represent arbitrarily long strings of signals with arbitrarily high fidelity, when the compressor is given the identity of the input state sequence as *classical* information (as the sequence of labels $i_1,\ldots,i_n$ rather than the quantum states $|\varphi_{i_1}\rangle,\ldots,|\varphi_{i_n}\rangle$ themselves, for example). According to the quantum source coding theorem the optimal *quantum* rate in this scenario is the von Neumann entropy $S(\mathcal{E})$ qubits per signal. We will develop a refinement of this theorem in which the states are coded into classical and quantum bits which are quantified *separately*. This leads to a trade-off curve $Q^*(R)$ where $Q^*(R)$ qubits per signal is the optimal quantum rate that suffices for a given classical rate R bits per signal. The quantum source coding theorem implies that $Q^*(0)=S(\mathcal{E})$ and evidently we also have $Q^*(H(p))=0$ where $H(p)$ is the Shannon entropy of the prior distribution of the source. [By standard classical compression, the compressor can represent the full information of the input sequence in $H(p)$ classical bits per signal.] Thus the trade-off curve extends between the limits $0\leqslant R\leqslant H(p)$.

There are various reasons why we might wish to maintain a separation between classical and quantum resources in an encoding.[13] On a purely practical level it seems to be far easier to manufacture classical storage and communication devices than it is to make quantum ones. But

perhaps the primary reason is conceptual: classical and quantum information have quite different fundamental characters, with classical information exhibiting special properties not shared by quantum information in general. For example, classical information is robust compared to quantum information—it may be readily stabilized and corrected by repeated measurement that would destroy quantum information. Also, unlike quantum information, it may be cloned or copied. These and other singular properties indicate that for many purposes it may be useful to regard classical information as a separate resource, distinct from quantum information. Classical information is sometimes formally regarded as a special case of quantum information *viz.* the quantum information of a fixed set of orthogonal states. While this characterization is useful for formal analyses, it is unsatisfactory conceptually because it relies on the essentially nonphysical infinite precision of orthogonality. It is, therefore, desirable to view classical information as a separate resource.

Exploring the trade-off possibilities between the two resources will lead to a better understanding of the interrelation of these concepts and the nature of quantum information itself. If bits can always be represented as qubits (and indeed, by Holevo's information bound,[14] one qubit per bit is necessary and sufficient), what are the limitations on representing qubits as bits? Under what conditions is it possible at all? If there is a penalty to be paid, how large is it? In this article we will give answers to these questions.

Our main result is a simple characterization of the trade-off function $Q^*(R)$ which may be paraphrased as follows. Given the ensemble $\mathcal{E}=\{|\varphi_i\rangle,p_i\}$ comprising m states $|\varphi_i\rangle$ we consider decompositions of $\mathcal{E}$ into at most $(m+1)$ ensembles $\mathcal{E}_j$ with associated probabilities q_j, i.e., the ensembles $\mathcal{E}_j=\{|\varphi_i\rangle,q(i|j)\}$ have the same states as $\mathcal{E}$ and their union $\cup_j q_j\mathcal{E}_j$ reproduces $\mathcal{E}$. This is equivalent to the condition

$$p_i=\sum_j q(i|j)q_j \tag{1}$$

on the chosen probabilities q_j and $q(i|j)$ defining the decomposition. Let $\overline{S}=\Sigma_j q_j S(\mathcal{E}_j)$ be the average von Neumann entropy of any such decomposition and let $H(i:j)$ be the classical mutual information of the joint distribution $q(i,j)$. For any R let $\overline{S}_{\min}(R)$ be the least average von Neumann entropy over all decompositions that have $H(i:j)=R$. Then we will prove that the trade-off function is given by $Q^*(R)=\overline{S}_{\min}(R)$.

The prescription of a decomposition $\mathcal{E}=\cup_j q_j\mathcal{E}_j$ may be equivalently given in terms of a visible encoding map E of the states of $\mathcal{E}$:

$$E(i)=|\varphi_i\rangle\langle\varphi_i|\otimes\sum_j p(j|i)|j\rangle\langle j|. \tag{2}$$

Here $p(j|i)$ are chosen freely subject only to the condition that $H(i:j)=R$ and the previous probability distributions are constructed as $q_j=\Sigma_i p(j|i)p_i$ and $q(i|j)=p(j|i)p_i/q_j$. Under this map, i is encoded into a quantum register, simply containing the state $|\varphi_i\rangle$ itself, and a classical register, containing a classical mixture of j values. Note that this is a *single* signal encoding with *perfect* fidelity since the state $|\varphi_i\rangle$ may be regained perfectly from the encoded version by simply discarding the classical register. Hence our result characterizes optimal classical and quantum resources in compression, in terms of very simple single-signal perfect-fidelity encodings, despite the fact that compression is defined asymptotically in terms of arbitrarily long signal strings and fidelities merely *tending* to 1. This is a remarkable and unexpected simplification—even in classical information theory it is by no means the rule that coding problems have solutions that do *not* involve asymptotics (despite a few well-known examples such as Shannon's source and channel coding theorems[15]). The situation is even more tenuous in quantum information theory, which seems to be plagued by further nonadditivity (or unresolved additivity questions) for some of its basic quantities so that, at the present stage, many basic constructions require a limit over optimization problems of exponentially growing size.

Using our formula we will give a thorough discussion of further properties of the trade-off curve including a generalization to group covariant sources and to sources with infinitely many (continuously parametrized) states. We show that our result also leads to a number of corollaries characterizing the trade-off between information gain and state disturbance for quantum sources (yielding the results of Ref. 13 on blind compression as a corollary), and we indicate how our techniques for characterizing $Q^*(R)$ provide a solution to the so-called remote state preparation problem as well. Finally, we develop a probability-free version of our main result which may be interpreted as an answer to the intuitive question: ''How many classical bits does a qubit cost?'' This may also be interpreted as a kind of dual to Holevo's theorem, insofar as the latter characterizes the qubit cost of coding classical information into qubits.

The presentation of these results is organized as follows. At the top level, the article is divided broadly into two parts. The first part, Secs. II–VIII, sets up a precise formulation of the basic definitions and the trade-off problem and gives the proof of the main theorem characterizing $Q^*(R)$, as well as a discussion of some of its important basic properties. The second part, Secs. IX and X, then goes on to provide some further generalizations of the main result. In more detail, the contents of the various sections are as follows.

In Sec. II, we will define the notions of blind and visible compression, the essential difference being that in the blind setting the encoder is given the actual quantum states, while in the visible setting the encoder is given the names of the quantum states as classical data. We then extend these definitions to quantum-classical trade-off coding and introduce the trade-off function $Q^*(R)$.

In Sec. III we will prove a lower bound to the trade-off curve in terms of the simple single-letter formula of the ensemble decomposition construction paraphrased above. In Sec. IV we will, in turn, show that the lower bound is achievable so that the trade-off curve is identical to the single-letter formula. This is our main result, Theorem 4.4.

In Sec. V we use our characterization of the trade-off curve to evaluate $Q^*(R)$ numerically for a selection of particular ensembles, chosen to illustrate various important properties of the trade-off function. In Sec. VI we extend our results to a different asymptotic setting, known as the arbitrarily varying source (AVS), in which there is no (or only limited) knowledge of the prior probability distribution of the states to be compressed. This provides a probability-free generalization of our main result. In Sec. VII we show that our main result can be reinterpreted to provide statements about the trade-off between information gain and state disturbance for blind sources of quantum states (in particular entailing a new proof of the main result of Ref. 13). Finally, in Sec. VIII we indicate how our techniques—developed to study $Q^*(R)$–can also be used to characterize the trade-off curve for the coding problem of remote state preparation posed in Refs. 16 and 17.

Sections IX and X treats two significant further issues. In Sec. IX we show how to apply our results in the setting of group covariant ensembles, which leads to considerable further elegant simplifications. Section X is devoted to the technicalities of generalizing our main result to sources with infinitely many (continuously parametrized) states. Finally, in the Appendix, we collect proofs of various auxiliary propositions that have been quoted in the body of the article.

II. BLIND AND VISIBLE COMPRESSION

We begin by introducing a number of definitions that are required to give a precise statement of the variations of quantum source coding that we will be considering in this article. We will denote an ensemble of quantum states φ_i with prior probabilities p_i as $\mathcal{E}=\{\varphi_i,p_i\}$. In turn, we will write $S(\mathcal{E})=S(\Sigma_i p_i\varphi_i)$ for the von Neumann entropy of the average state of the ensemble: $S(\rho)=-\mathrm{Tr}\rho\log\rho$. (Throughout this article log and exp will denote the logarithm and exponential functions *to base* 2.) Starting from an ensemble $\mathcal{E}$, we can consider the quantum source producing quantum states that are sequentially drawn independently from $\mathcal{E}$. Such a source corresponds to a sequence of ensembles $\mathcal{E}^{\otimes n}=\{\varphi_I,p_I\}$, where

$$I:=i_1\cdots i_n, \tag{3}$$

$$\varphi_I := \varphi_{i_1} \otimes \cdots \otimes \varphi_{i_n}, \tag{4}$$

$$p_I := p_{i_1} \cdots p_{i_n}. \tag{5}$$

This sequence will be referred to as an independent identically distributed (i.i.d.) source and the states of $\mathcal{E}^{\otimes n}$ are called blocks of length n from $\mathcal{E}$. In this article we will focus on sources of pure quantum states $|\varphi_i\rangle$, often making use of the notation $\varphi_i = |\varphi_i\rangle\langle\varphi_i|$. The measure that we will use to determine whether two quantum states are close is the fidelity F. For two mixed states ρ and ω, F is given by the formula

$$F(\rho,\omega) := (\mathrm{Tr}\sqrt{\omega^{1/2}\rho\omega^{1/2}})^2. \tag{6}$$

(Note that some authors use the name ''fidelity'' to refer to the square-root of this quantity.) If $\omega = |\omega\rangle\langle\omega|$ is a pure state, then the fidelity has a particularly simple form:

$$F(\rho,\omega) = \langle\omega|\rho|\omega\rangle = \mathrm{Tr}(\rho\omega). \tag{7}$$

Finally, we will use the notation $\mathcal{H}_d$ to denote the Hilbert space of dimension d and $\mathcal{B}_d$ to denote the set of all mixed states on $\mathcal{H}_d$. Likewise, $\mathcal{H}_d^{\otimes n}$ will refer to the n-fold tensor product of $\mathcal{H}_d$ and, in a slight abuse of notation, $\mathcal{B}_d^{\otimes n}$ will refer to the set of density operators on $\mathcal{H}_d^{\otimes n}$. We are now ready to introduce the definition of *blind* quantum compression.

Definition 2.1: A blind coding scheme *for blocks of length n, to R qubits per signal and fidelity $1-\epsilon$, comprises the following ingredients:*

(1) a completely positive, trace-preserving (CPTP) encoding map $E_n : \mathcal{B}_d^{\otimes n} \to \mathcal{B}_2^{\otimes nR}$, and

(2) a CPTP decoding map $D_n : \mathcal{B}_2^{\otimes nR} \to \mathcal{B}_d^{\otimes n}$,

such that average fidelity

$$\sum_I p_I \langle\varphi_I|D_n(E_n(\varphi_I))|\varphi_I\rangle \geqslant 1-\epsilon. \tag{8}$$

We say that an i.i.d. source $\mathcal{E}$ can be blindly compressed to R qubits per signal if for all $\delta,\epsilon > 0$ and sufficiently large n there exists a blind coding scheme to $R+\delta$ qubits per signal with fidelity at least $1-\epsilon$.

The definition of visible compression is the same except that the (CPTP) restrictions on the encoding map E_n are relaxed; for visible compression E_n can be an arbitrary association of input states to output states. Equivalently, E_n is a mapping from the *names* of the input states to output states. Thus, we write $E_n(I) \in \mathcal{B}_2^{\otimes nR}$. Note that blind and visible compression schemes differ only in the set of encoding maps that are permitted. For blind (respectively visible) compression, the input states are given as quantum (respectively classical) information. In both cases the decoding must be CPTP. In this language, the central result on the compression of quantum information can be expressed as follows.

Theorem 2.2 (Quantum source coding theorem[10–12]): *A source $\mathcal{E}$ of pure quantum states can be compressed to α qubits per signal if and only if $\alpha \geqslant S(\mathcal{E})$. The result holds for both blind and visible compression.*

It is interesting to study a refinement of quantum source coding in which the states are coded into classical and quantum resources which are quantified separately. Because of restrictions on the manipulation of quantum states such as the no-cloning theorem,[18] blind compression is typically weaker than visible. In Refs. 13 and 19, for example, it was shown that in blind compression it is typically impossible to make use of classical storage. The same is not true in the visible setting, where it is possible to trade classical storage for quantum. In this article we study this trade-off for *visible* compression but, before we begin, we need to recall some basic definitions introduced in Ref. 13.

Consider an encoding operation E_n which maps a signal state $|\varphi_I\rangle$ into a joint state on a quantum register B and a classical register C. If $\{|j\rangle\}$ is the classical orthonormal basis of C, then the most general classical state on C is a probability distribution over j values, implying that the most general form of the encoded state can be written as

$$E_n(I)=\sum_j p(j|I)\omega_{I,j}^B\otimes|j\rangle\langle j|^C. \tag{9}$$

The quantum and classical storage requirements (i.e., resources) of the encoding map are simply the sizes of the registers B and C, respectively.

Definition 2.3: The quantum rate *of the encoding map E_n is defined to be*

$$\mathrm{qsupp}(E_n,\mathcal{E}^{\otimes n})=\frac{1}{n}\log\dim\mathcal{H}_B,$$

while the classical rate *of the encoding is defined to be*

$$\mathrm{csupp}(E_n,\mathcal{E}^{\otimes n})=\frac{1}{n}\log\dim\mathcal{H}_C.$$

With these definitions in place, we can make precise the notion of compression with a quantum and a classical part.

Definition 2.4: A source $\mathcal{E}$ can be compressed to R classical bits per signal plus Q qubits per signal if for all $\epsilon,\delta>0$ there exists an $N>0$ such that for all $n>N$ there exists an encoding-decoding scheme (E_n,D_n) with fidelity $1-\epsilon$ satisfying the inequalities

$$\mathrm{csupp}(E_n,\mathcal{E}^{\otimes n})\leqslant R+\delta, \tag{10}$$

$$\mathrm{qsupp}(E_n,\mathcal{E}^{\otimes n})\leqslant Q+\delta. \tag{11}$$

The main result of this article will be a complete characterization of the curve describing the trade-off between R and Q. As mentioned above, for blind encodings there is usually no trade-off to be made: generically, $Q\geqslant S(\mathcal{E})$, regardless of the size of R. The reason is essentially that making effective use of the classical register amounts to extracting classical information from a quantum system in a reversible fashion, which is impossible unless the quantum states of interest obey some orthogonality condition. The more interesting case, therefore, is to study the structure of the trade-off curve for visible encodings. As it turns out, our technique will yield the older results for blind compression as a corollary.

Definition 2.5: For a given source $\mathcal{E}=\{|\varphi_i\rangle,p_i\}$, define the function $Q^*(R)$ to be the infimum over all values of Q for which the source can be visibly compressed to R classical bits per signal and Q quantum bits per signal.

Some properties of the curve $Q^*(R)$ are immediate. For example, the endpoints of the curve are easily found. If $R=0$, then the compression must be fully quantum mechanical and the quantum source coding Theorem 2.2 applies: $Q^*(0)=S(\mathcal{E})$. More generally, the theorem implies that $Q^*(R)+R\geqslant S(\mathcal{E})$ for all R. Similarly, for $R=H(p)$ we have $Q^*(R)=0$, by Shannon's classical source coding theorem. Moreover, for intermediate values of R, the curve is necessarily convex because one method of compressing with classical rate $\lambda_1R_1+\lambda_2R_2$ is simply to timeshare between the optimal protocols for R_1 and R_2 individually, resulting in quantum rate of $\lambda_1Q^*(R_1)+\lambda_2Q^*(R_2)$.

Example (Parametrized BB84 ensemble): Let us consider in more detail the example of a parametrized version of the BB84 ensemble in order to see what sorts of protocols are possible beyond simple timesharing. For $0<\theta\leqslant\pi/4$, let $\mathcal{E}_{BB}(\theta)$ be the ensemble consisting of the states

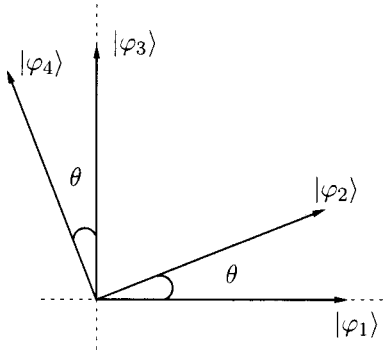

FIG. 1. Parametrized BB84 ensemble $\mathcal{E}_{BB}(\theta)$.

$$|\varphi_1\rangle = |0\rangle, \tag{12}$$

$$|\varphi_2\rangle = \cos\theta|0\rangle + \sin\theta|1\rangle, \tag{13}$$

$$|\varphi_3\rangle = |1\rangle, \tag{14}$$

$$|\varphi_4\rangle = -\sin\theta|0\rangle + \cos\theta|1\rangle, \tag{15}$$

as illustrated in Fig. 1, each occurring with probability $p_i = 1/4$. We then have $S(\mathcal{E}) = 1$ and $H(p) = 2$. From the argument above, we therefore already know two points on the $(R, Q^*(R))$ curve, namely (0,1) and (2,0). To get a better upper bound than the straight line joining these two points, suppose we were to partition the four states into two subsets, $\mathcal{X}_1 = \{|\varphi_1\rangle, |\varphi_2\rangle\}$ and $\mathcal{X}_2 = \{|\varphi_3\rangle, |\varphi_4\rangle\}$. For a given input string $I = i_1 i_2 \cdots i_n$, the classical register could be used to encode, for each k, whether $|\varphi_{i_k}\rangle \in \mathcal{X}_1$ or $|\varphi_{i_k}\rangle \in \mathcal{X}_2$. The classical rate required to do so would be 1 classical bit per signal. Independent of the value of the classical register, the quantum resource required to compress the subensembles is then just the quantum resource required to compress a pair of equiprobable quantum states subtended by the angle θ. Therefore,

$$Q^*(1) \leqslant S(\tfrac{1}{2}|\varphi_1\rangle\langle\varphi_1| + \tfrac{1}{2}|\varphi_2\rangle\langle\varphi_2|) = H_2(\tfrac{1}{2}(1+\cos\theta)). \tag{16}$$

By timesharing between the point corresponding to this protocol and the two endpoints of the curve that we already calculated, we get a piecewise linear upper bound on Q^*. As we will see later, however, the true curve is strictly below this upper bound. (The impatient reader is allowed to peek at Fig. 5 in Sec. V.)

With this example in mind, let us move on to our analysis of the general case.

III. SINGLE-LETTER LOWER BOUND ON $Q^*(R)$

In this section we will prove a lower bound on the quantum-classical trade-off curve by reducing the asymptotic problem to a single-copy problem. Because compression is only possible asymptotically, however, we need to shift the emphasis away from the quantum and classical resources towards quantum and classical mutual information quantities. In the next section we will then prove that nothing was lost by making this shift—we will show that the resulting lower bound to $Q^*(R)$ is actually achievable.

A. Mutual information and additivity

The information quantities in question will be the mutual information between the name of the state being compressed and the quantum and classical registers containing the output of the encoding map E_n. Thus, we define the state

$$\rho^{ABC} := \sum_{I,j} p_I |I\rangle\langle I|^A \otimes p(j|I)\omega_{I,j}^B \otimes |j\rangle\langle j|^C. \tag{17}$$

The names I are stored in orthogonal states on system A while the quantum and classical encoding registers are labeled B and C, respectively. We can then make the following definitions:

$$S(A:C) := S(A) + S(C) - S(AC), \tag{18}$$

$$S(A:B|C) := S(AC) + S(BC) - S(ABC) - S(C), \tag{19}$$

where, for any subsystem X, $S(X)$ denotes the von Neumann entropy of the reduced state of X. Note that $S(A:C)$ is just the classical mutual information $H(I:j)$ between I and j. To interpret $S(A:B|C)$, observe that for a given classical output j, we can write down a conditional ensemble

$$\mathcal{E}_j = \{\omega_{I,j}, q(I|j)\}, \tag{20}$$

where $q(I|j)$ is calculated using Bayes' rule to be $q(I|j) = p(j|I)p_I/q_j$, with $q_j = \Sigma_I p(j|I)p_I$. The conditional quantum mutual information $S(A:B|C)$ is just the average Holevo information χ of the conditional ensembles $\mathcal{E}_j$:

$$S(A:B|C) = \sum_j q_j \chi(\mathcal{E}_j), \tag{21}$$

where χ is defined, for an ensemble $\mathcal{E} = \{\rho_k, p_k\}$, as[14]

$$\chi(\mathcal{E}) := S\left(\sum_k p_k \rho_k\right) - \sum_k p_k S(\rho_k). \tag{22}$$

Because $\mathcal{E}_j$ is an ensemble supported on system B, $\chi(\mathcal{E}_j) \leqslant n\text{qsupp}$, which implies that

$$n\text{qsupp} \geqslant S(A:B|C). \tag{23}$$

Therefore, roughly speaking, we will derive a lower bound on $Q^*(R)$ by minimizing $S(A:B|C)$ subject to the constraint $S(A:C) \leqslant nR$ and developing further properties of that minimum. To that end, define $T_\epsilon(\mathcal{E}^{\otimes n}, nR)$ to be the set of all encoding maps E for which $S(A:C) \leqslant nR$ and there exists a decoding map D satisfying

$$\sum_I p(I) F(\varphi_I, (D \circ E)\varphi_I) \geqslant 1 - \epsilon. \tag{24}$$

Next define $M_\epsilon(\mathcal{E}^{\otimes n}, nR)$ to be the infimum of $S(A:B|C)$ over all $E \in T_\epsilon(\mathcal{E}^{\otimes n}, nR)$. We begin by noting the following basic properties of $M_\epsilon(\mathcal{E}, R)$.

Lemma 3.1: $M_\epsilon(\mathcal{E}, R)$ is a monotonically decreasing function of R. Moreoever, it is jointly convex in ϵ and R, in the sense that, for any set of $\epsilon_k > 0$ and $R_k \geqslant 0$ as well as probabilities $\Sigma_k \lambda_k = 1$,

$$M_\epsilon(\mathcal{E}, R) \leqslant \sum_k \lambda_k M_{\epsilon_k}(\mathcal{E}, R_k), \tag{25}$$

where $\epsilon = \Sigma_k \lambda_k \epsilon_k$ and $R = \Sigma_k \lambda_k R_k$.

Proof: Monotonicity follows immediately from the definitions. If $R_1 \leqslant R_2$ and $S(A:C) \leqslant R_1$, then $S(A:C) \leqslant R_2$. Thus the set $T_\epsilon(\mathcal{E}, R_1)$ is contained in $T_\epsilon(\mathcal{E}, R_2)$ and $M_\epsilon(\mathcal{E}, R_1) \geqslant M_\epsilon(\mathcal{E}, R_2)$.

To prove joint convexity, let ϵ_k, R_k and λ_k be as in the statement of the lemma and assume that $E_k \in T_{\epsilon_k}(\mathcal{E}, R_k)$. Furthermore, suppose that the encoding maps E_k map into orthogonal sectors

C_k of the classical register C. We construct an encoding map with information rate $R \leqslant \Sigma_k \lambda_k R_k$ and fidelity $\epsilon \leqslant \Sigma_k \lambda_k \epsilon_k$ by applying the map E_k with probability λ_k. The first inequality follows from the fact that the sectors C_k are orthogonal:

$$S(A:C) = \sum_k \lambda_k S(A:C_k) \leqslant R. \tag{26}$$

The decoding map for the new encoding consists of first determining which sector C_k was used and then applying the decoding map corresponding to E_k. The output of the encoding-decoding scheme will, therefore, be the average of the outputs of the individual schemes, yielding $1-\epsilon \geqslant \Sigma_k \lambda_k (1-\epsilon_k)$ by the concavity of the fidelity. Finally, if we define $S_k(A:B|C)$ to be the conditional quantum mutual information for the encoding map E_k, then we can calculate the value for the new scheme,

$$S(A:B|C) = \sum_k \lambda_k S_k(A:B|C). \tag{27}$$

Since $M_\epsilon(\mathcal{E},R) \leqslant S(A:B|C)$ by definition and this inequality must hold for all encoding maps E_k, we can conclude that $M_\epsilon(\mathcal{E},R) \leqslant \Sigma_k \lambda_k M_\epsilon(\mathcal{E},R_k)$. □

The particular usefulness of the M_ϵ function derives from an additivity property with respect to the input ensemble given in the next lemma, a property that can be converted into a single-letter lower bound on $Q^*(R)$.

Lemma 3.2: For any ensemble $\mathcal{E}$, numbers $R, \epsilon \geqslant 0$ and non-negative integer n,

$$M_\epsilon(\mathcal{E}^{\otimes n}, nR) \geqslant n M_\epsilon(\mathcal{E},R). \tag{28}$$

Proof: To begin, recall that $I = i_1 i_2 \cdots i_n$ and decompose A into $A_1 A_2 \cdots A_n$, with $|i_k\rangle$ stored on A_k. We will frequently make use of the notation $A_{<k} = A_1 A_2 \cdots A_{k-1}$ and the analogous $I_{<k} = i_1 i_2 \cdots i_{k-1}$, as well the similar $A_{>k}$ and $I_{>k}$. For a fixed $E \in T_\epsilon(\mathcal{E}^{\otimes n}, nR)$, the chain rule for mutual information (cf. Appendix C of Ref. 13) implies that

$$S(A:B|C) = \sum_{k=1}^{n} S(A_k:B|C,A_{<k}). \tag{29}$$

The bulk of the proof will consist of definitions for the purpose of interpreting the individual summands in the chain rule in terms of single-copy encoding maps. Consider one such term, $S(A_k:B|C,A_{<k})$, which we can express as

$$S(A_k:B|C,A_{<k}) = \sum_{I_{<k},j} p(I_{<k},j) \chi(\mathcal{E}_{I_{<k},j}), \tag{30}$$

where $\mathcal{E}_{I_{<k},j}$ is the ensemble of states

$$\mathcal{E}_{I_{<k},j} = \left\{ \sum_{I_{>k}} p(I_{>k}) \omega_{I,j}, q_{I_{<k}}(i_k|j) \right\}, \tag{31}$$

with

$$q_{I_{<k}}(i_k|j) = \frac{\Sigma_{I_{>k}} p(i_k) p(I_{>k}) p(j|I)}{\Sigma_{I_{\geqslant k}} p(I_{\geqslant k}) p(j|I)}. \tag{32}$$

Now define the encoding map $E_{I_{<k}}$ on the ensemble $\mathcal{E}$ to be

$$E_{I_{<k}}(i_k) := \sum_{I_{>k}} p(I_{>k}) E(I) = \sum_{I_{>k}} \sum_j p(I_{>k}) p(j|I) \omega_{I,j} \otimes |j\rangle\langle j|. \tag{33}$$

The output of $E_{I_{<k}}$ on the quantum register is described by the set of ensembles $\mathcal{E}_{I_{<k},j}$. Next, define the decoding map $D_k = \mathrm{Tr}_{\neq k} \circ D$ and the fidelity

$$F_{I_{<k}} := 1 - \epsilon_{I_{<k}} := \sum_{i_k} p(i_k) F(\rho_{i_k}, (D_k \circ E_{I_{<k}})(i_k)). \tag{34}$$

We can then calculate that

$$\begin{aligned}
\sum_{I_{<k}} p(I_{<k}) F_{I_{<k}} &= \sum_{I_{<k}} p(I_{<k}) \sum_{i_k} p(i_k) F(\rho_{i_k}, (D_k \circ E_{I_{<k}})(i_k)) \\
&= \sum_{I_{\leqslant k}} p(I_{\leqslant k}) F\left(\rho_{i_k}, \mathrm{Tr}_{\neq k} D\left(\sum_{I_{>k}} p(I_{>k}) E(I) \right) \right) \\
&= \sum_{I_{\leqslant k}} p(I_{\leqslant k}) F\left(\sum_{I_{>k}} p(I_{>k}) \rho_{i_k}, \sum_{I_{>k}} p(I_{>k}) (\mathrm{Tr}_{\neq k} \circ D \circ E)(I) \right) \\
&\geqslant \sum_I p(I) F(\mathrm{Tr}_{\neq k} \rho_I, (\mathrm{Tr}_{\neq k} \circ D \circ E)(I)) \\
&\geqslant \sum_I p(I) F(\rho_I, (D \circ E)(I)) \geqslant 1 - \epsilon.
\end{aligned} \tag{35}$$

The first three lines are by definition and using linearity to shuffle the terms. The first inequality comes from the joint concavity of the fidelity, the second from its monotonicity under partial trace, and the last from the fidelity condition on $D \circ E$.

Therefore, if we write $j(E_{I_{<k}})$ for the random variable representing the classical output of the encoding map $E_{I_{<k}}$ and $R_{I_{<k}}$ for the corresponding mutual information, then $E_{I_{<k}} \in T_{\epsilon_{I_{<k}}}(\mathcal{E}, R_{I_{<k}})$. Defining $R_k := \Sigma_{I_{<k}} p(I_{<k}) R_{I_{<k}}$ for the average classical information and applying the joint convexity of M then finally yields

$$S(A_k : B|C, A_{<k}) \geqslant M_\epsilon(\mathcal{E}, R_k). \tag{36}$$

A simple calculation allows us to bound the R_k from above; however,

$$\sum_k R_k = \sum_k \sum_{I_{<k}} p(I_{<k}) H(i_k : j(E_{I_{<k}})) \tag{37}$$

$$= \sum_k S(A_k : C|A_{<k}) \tag{38}$$

$$= S(A : C) \leqslant nR. \tag{39}$$

Combining Eqs. (36) and (39) with the chain rule, and applying the convexity of M one more time gives the simple inequality

$$S(A : B|C) \geqslant \sum_k M_\epsilon(\mathcal{E}, R_k) \geqslant n M_\epsilon(\mathcal{E}, R). \tag{40}$$

Since this lower bound must hold for all encoding maps in $T_\epsilon(\mathcal{E}^{\otimes n},R)$, that concludes the proof of the lemma. □

B. Perfect encodings and their properties

Within the set $T_0(\mathcal{E},R)$ of encoding maps with *perfect* fidelity decodings there is a particularly simple subset, in terms of which we will phrase our final bound on $Q^*(R)$. Let $T(\mathcal{E},R)\subset T_0(\mathcal{E},R)$ be the set of all encoding maps E of the form

$$E(i)=|\varphi_i\rangle\langle\varphi_i|^B\otimes\sum_j p(j|i)|j\rangle\langle j|^C. \tag{41}$$

In other words, $T(\mathcal{E},R)$ consists of the encoding maps in which a perfect copy of the state to be compressed is placed in register B. The decoding map is simply to trace over the register C. While such encodings, which simply reproduce the input, are obviously useless for compression, they turn out to be quite sufficient for minimizing $S(A:B|C)$. Indeed, let us define

$$M(\mathcal{E},R)=\inf\{S(A:B|C):E\in T(\mathcal{E},R)\} \tag{42}$$

$$=\inf_{p(\cdot|\cdot)}\{S(A:B|C):S(A:C)\leqslant R\}. \tag{43}$$

By construction, this optimization is no longer over general CPTP maps but only over different possible conditional probability distributions on register C.

Let us collect a few properties of M for later use: First of all, M inherits the convexity of M_ϵ in the variable R. Also, it is clearly nonincreasing, and $M(\mathcal{E},0)=S(\mathcal{E})$ is immediate from the definition. Furthermore, for any choice of $p(\cdot|\cdot)$, we have

$$S(A:C)+S(A:B|C)=S(A:BC)\geqslant S(A:B)=S(\mathcal{E}), \tag{44}$$

from which we conclude that $R+M(\mathcal{E},R)\geqslant S(\mathcal{E})$. This, together with the convexity, implies continuity in R, and the estimates

$$M(\mathcal{E},R)\geqslant M(\mathcal{E},R+\delta)\geqslant M(\mathcal{E},R)-\delta. \tag{45}$$

In what follows, it will also frequently be helpful to use the following fact:

Proposition 3.3:

$$M(\mathcal{E},R)=\inf_{p(\cdot|\cdot)}\{S(A:B|C):S(A:C)=R\}, \tag{46}$$

with an equality condition in the infimum [rather than the inequality of Eq. (43)].

The proof is given in the Appendix, Sec. 1.

In principle one might envisage a limit with larger and larger classical register C. This would constitute a serious obstacle to calculating $M(\mathcal{E},R)$ and carrying through our larger program of evaluating $Q^*(R)$. Fortunately, the next proposition ensures that the range of j's we need to consider in the definition of $M(\mathcal{E},R)$ is bounded universally. Since the mutual informations involved are continuous, the infimum in the definition of $M(\mathcal{E},R)$ can be replaced by a minimum.

Proposition 3.4: In the definition of $M(\mathcal{E},R)$ given in Eq. (43), it suffices to consider encodings of the form Eq. (41) with at most $(m+1)$ j values, where m is the number of states in $\mathcal{E}$.

The proof is given in the Appendix, Sec. 2.

C. Completing the lower bound

Returning to the main argument, we are now prepared to relate $M(\mathcal{E},R)$ to the trade-off curve:

Theorem 3.5: *If a source $\mathcal{E}$ can be visibly compressed to Q qubits per signal and R classical bits per signal, then $Q \geq M(\mathcal{E},R)$. Equivalently, $Q^*(R) \geq M(\mathcal{E},R)$.*

Proof: By the definition of compression and the previous lemma, we note that, for all $\epsilon, \delta > 0$, the inequality $Q^*(R) \geq M_\epsilon(\mathcal{E}, R+\delta)$ must hold. We will give a proof that M_ϵ is continuous at $\epsilon = 0$, from which the stronger lower bound in terms of $M(\mathcal{E},R)$ will follow.

So, fix ϵ, δ for now and suppose that $E \in T_\epsilon(\mathcal{E}, R+\delta)$. Let D be the decoding map associated to E. As usual,

$$E(i) = \sum_j \omega_{i,j}^B \otimes p(j|i)|j\rangle\langle j|^C. \tag{47}$$

For a given j value, the decoding map will produce the ensemble of states $\{\sigma_{i,j}, p(i|j)\}$ where $\sigma_{i,j} = D(\omega_{i,j}^B \otimes |j\rangle\langle j|^B)$. Therefore, applying Markov's inequality (cf. Lemma 6.3 of Ref. 13) and the fidelity condition in the definition of $T_\epsilon(\mathcal{E},R)$, the probability weight of the j's with

$$\sum_i q(i|j) F(\varphi_i, \sigma_{i,j}) \geq 1 - \sqrt{\epsilon} \tag{48}$$

is at least $1-\sqrt{\epsilon}$. In other words, for these good j values, the output of the decoding map is close to $\mathcal{E}_j$. Therefore, for these same good j values, by the monotonicity and continuity of χ, we must have

$$\chi(\mathcal{E}_j) \geq S\left(\sum_i q(i|j) |\varphi_i\rangle\langle\varphi_i| \right) - f(\epsilon), \tag{49}$$

where we may choose $f(\epsilon) = 4(\sqrt[4]{\epsilon} \log d - \sqrt[4]{\epsilon} \log(2\sqrt[4]{\epsilon}))$ (as shown in Appendix A of Ref. 13). Consequently,

$$S(A:B|C) = \sum_j q_j \chi(\mathcal{E}_j) \geq \sum_j q_j S\left(\sum_i q(i|j) |\varphi_i\rangle\langle\varphi_i| \right) - f(\epsilon). \tag{50}$$

Since $f(\epsilon) \to 0$ as $\epsilon \to 0$ we conclude that $\lim_{\epsilon \downarrow 0} M_\epsilon(\mathcal{E}, R+\delta) = M_0(\mathcal{E}, R+\delta)$ and, moreover, in the limit $\epsilon \to 0$ it suffices to consider encoding maps of the type

$$E(i) = |\varphi_i\rangle\langle\varphi_i|^B \otimes \sum_j p(j|i) |j\rangle\langle j|^C. \tag{51}$$

Thus we obtain $Q^*(R) \geq M(\mathcal{E}, R+\delta)$, for all $\delta > 0$, which, by Eq. (45) above yields our claim.□

Remark: The estimate $f(\epsilon)$ above may also be derived using Fannes' inequality,[20] which states that for density operators ρ and σ on a d-dimensional space,

$$\|\rho - \sigma\|_1 \leq \epsilon \Rightarrow |S(\rho) - S(\sigma)| \leq d\, \eta(\epsilon/d). \tag{52}$$

where

$$\eta(x) = \begin{cases} -x \log x & \text{for } x \leq \frac{1}{4}, \\ \frac{1}{2} & \text{for } x > \frac{1}{4}. \end{cases} \tag{53}$$

We will use this inequality again later. □

D. On alternative definitions

Inspecting the proofs of Lemma 3.2 and Theorem 3.5 reveals that we do not actually need the block-based fidelity condition

$$\langle F\rangle := \sum_I p_I F(\varphi_I, (D\circ E)(I)) \geqslant 1-\epsilon \tag{54}$$

of Eq. (8), but only the weaker mean letterwise fidelity

$$\langle \overline{F}\rangle := \sum_I p_I \overline{F}_I \geqslant 1-\epsilon, \tag{55}$$

where

$$\overline{F}_I := \frac{1}{n}\left[\sum_{k=1}^{n} F(\varphi_{i_k}, (\mathrm{Tr}_{\neq k}\circ D\circ E)(I))\right]. \tag{56}$$

By the monotonicity of the fidelity under partial traces, the latter is directly implied by the former.

The lower bound Eq. (35) is then replaced by $1-\epsilon_k$, with $(1/n)\,\Sigma_k \epsilon_k = \epsilon$, and we conclude, instead of Eq. (36), that

$$S(A_k:B|C,A_{<k}) \geqslant M_{\epsilon_k}(\mathcal{E},R_k). \tag{57}$$

The remaining argument is only altered at Eq. (40):

$$S(A:B|C) \geqslant \sum_{k=1}^{n} M_{\epsilon_k}(\mathcal{E},R_k) \geqslant n M_{\epsilon}(\mathcal{E},R), \tag{58}$$

using joint convexity once more.

Hence, we could define the function $\overline{M}_{\epsilon}(\mathcal{E},R)$ in a fashion analogous to $M_{\epsilon}(\mathcal{E},R)$ but using the fidelity function $\overline{F}$ instead of F and Lemma 3.2 would continue to hold for the new function. In fact, $\overline{M}_{\epsilon}(\mathcal{E},R)$ will be strictly additive, in the sense that

$$\overline{M}_{\epsilon}(\mathcal{E}^{\otimes n}, nR) = n\overline{M}_{\epsilon}(\mathcal{E},R), \tag{59}$$

because any single-letter encoding with fidelity $1-\epsilon$ repeated n times gives rise to an n-block coding with mean letterwise fidelity $1-\epsilon$.

We also note at this stage that we could have opted for a slightly more sophisticated definition of the quantum resource of the encoding. In particular, if we introduce $\mathrm{qsupp}_j = (1/n)\log \mathrm{Rank}\,\mathcal{E}_j$ as the minimal number of qubits per signal required to support the conditional ensemble $\mathcal{E}_j$, then we could have defined the quantum rate of the encoding map as

$$\overline{\mathrm{qsupp}} = \sum_j q_j \mathrm{qsupp}_j\,. \tag{60}$$

In this picture, the quantum resource would be the average over classical j values of the minimal number of qubits per signal required to support the quantum portion of the encoded state $E_n(I)$. Such a definition, by treating the classical and quantum storage requirements differently, allows the possibility of variable-length quantum encodings, where the length is a function of the classical message j. Such encodings could potentially be more powerful than the encodings with fixed-sized quantum supports used to define the original qsupp. However, because $\mathrm{qsupp}_j \geqslant \chi(\mathcal{E}_j)$, the analog of Eq. (23) continues to hold. (For a more detailed investigation of the properties of such variable-length quantum memories, see Ref. 21.) More precisely,

$$n\overline{\mathrm{qsupp}} \geqslant S(A:B|C). \tag{61}$$

Therefore, the lower bound of Theorem 3.5 on the trade-off curve $Q^*(R)$ would apply equally well if we had defined $Q^*(R)$ using $\overline{\text{qsupp}}$ instead of qsupp.

Thus, while replacing either F by $\overline{F}$ or qsupp by $\overline{\text{qsupp}}$ in the definition of compression could potentially have reduced the resource requirements, we find that our lower bounds would apply to the modified definitions. Since we will see later in the article that the lower bounds are achievable using the original, restrictive formulation of compression, we can conclude that no advantage can be gained by relaxing the definitions to use $\overline{F}$ and $\overline{\text{qsupp}}$.

IV. ACHIEVING THE LOWER BOUND $M(\mathcal{E},R)$

Recall that the trade-off function $Q^*(R)$ gives the minimal quantum resource Q^* qubits per letter that is sufficient to encode arbitrarily long strings with arbitrarily high fidelity $1-\epsilon$ for any $\epsilon>0$, given a classical resource of R bits per letter. On the other hand, the lower bound $M(\mathcal{E},R)$ is defined as the minimal quantum resource for a particular kind of *single*-letter *perfect* fidelity (i.e., $\epsilon=0$) encoding given in Eq. (51), subject to the constraint that the classical *mutual information* $S(A:C)$ between i and j is R. Hence in the latter case, the classical resource will generally exceed R bits per letter. Thus by implementing the simple encodings of Eq. (51) we can attain $M(\mathcal{E},R)$ as the quantum resource but not generally with a classical resource bounded by R. We now argue that, nevertheless, the classical resource can be reduced to R while retaining the quantum resource at $M(\mathcal{E},R)$ i.e., that the lower bound $M(\mathcal{E},R)$, to $Q^*(R)$ is attainable, so we must then have $Q^*(R)=M(\mathcal{E},R)$.

Our strategy intuitively is the following. We think of the conditional distribution $p(j|i)$ with mutual information $S(A:C)$ in Eq. (51) as a noisy channel from i to j. Then the reverse Shannon theorem[22] states that this noisy channel can be simulated with a noiseless channel of capacity $S(A:C)$ if the receiver and sender have shared randomness, i.e., in the presence of shared randomness, the classical resource can be reduced to $R=S(A:C)$ bits per letter. Finally, we show that only $O(\log n)$ bits of shared randomness suffice to provide a high fidelity encoding-decoding scheme for blocks of length n. Hence this amount of shared randomness can be included in the classical resource of the encoding with asymptotically vanishing cost per letter.

To make the above intuitions mathematically rigorous, we begin by recalling some basic facts from the theory of typical sequences[23,24] and typical subspaces[12,25] in the following two subsections.

A. Typical sequences

For a sequence $I=i_1\cdots i_n\in\mathcal{I}^n$ define the *type* P_I of I as its empirical distribution of letters, i.e.,

$$P_I(i):=\frac{1}{n}N(i|I):=\frac{1}{n}\left|\{k|i_k=i\}\right|. \tag{62}$$

The number of types of sequences is polynomial in n: it is $\binom{n+|\mathcal{I}|-1}{|\mathcal{I}|-1}\leqslant(n+1)^{|\mathcal{I}|}$.

The *type class* $\mathcal{T}_P$ of P is the set of all sequences with type P:

$$\mathcal{T}_P:=\{I\in\mathcal{I}^n|P_I=P\}. \tag{63}$$

Consider now any probability distribution P on $\mathcal{I}$, and let $\delta>0$. Then the set of *typical sequences* (with respect to the distribution P and δ) is

$$\mathcal{T}_{P,\delta}:=\{I\in\mathcal{I}:\forall i\left|P_I(i)-P(i)\right|\leqslant\delta/\sqrt{n}\}. \tag{64}$$

Note that this set is a union of certain type classes.

The following are standard facts:[23,24]

$$P^{\otimes n}(\mathcal{T}_{P,\delta}) \geqslant 1 - \frac{1}{\delta^2}, \tag{65}$$

$$(n+1)^{-|\mathcal{I}|} \exp(n(H(P))) \leqslant |\mathcal{T}_P|, \tag{66}$$

$$\exp(n(H(P))) \geqslant |\mathcal{T}_P|, \tag{67}$$

$$(n+1)^{-|\mathcal{I}|} \exp(n(H(P) - |\mathcal{I}|\,\eta(\delta/\sqrt{n}))) \leqslant |\mathcal{T}_{P,\delta}|, \tag{68}$$

$$(n+1)^{|\mathcal{I}|} \exp(n(H(P) + |\mathcal{I}|\,\eta(\delta/\sqrt{n}))) \geqslant |\mathcal{T}_{P,\delta}|. \tag{69}$$

Note that the latter two follow from the former two by the following well–known explicit estimate on the difference of two entropies[23] [this being a classical case of the Fannes inequality, Eq. (52)]: if P and Q are probability distributions on a set of k elements, then

$$\|P - Q\|_1 \leqslant \epsilon \Rightarrow |H(P) - H(Q)| \leqslant k\,\eta\left(\frac{\epsilon}{k}\right), \tag{70}$$

where the function η is given in Eq. (53).

For sequences $I \in \mathcal{I}^n$, $J \in \mathcal{J}^n$, the *conditional type* $W_{J|I}$ of J (conditional on I) is defined as the stochastic matrix given by

$$\forall ij \quad P_I(i) W_{J|I}(j|i) = P_{IJ}(ij), \tag{71}$$

where P_{IJ} is the joint type of $IJ = (i_1 j_1, \ldots, i_n j_n)$. It is undetermined if $P_I(i) = 0$.

The *conditional type class* of W given I is defined as

$$\mathcal{T}_W(I) := \{J : W_{J|I} = W\} = \{J : \forall ij \quad P_{IJ}(ij) = P_I(i) W(j|i)\}. \tag{72}$$

Let W be now an arbitrary stochastic matrix and $\delta > 0$. The *set of conditionally typical sequences* of W given I is defined as

$$\mathcal{T}_{W,\delta}(I) := \{J : \forall ij \,|\, W_{J|I}(j|i) - W(j|i)| \leqslant \delta/\sqrt{N(i|I)}\}. \tag{73}$$

Again, there are a couple of standard facts:

$$W_I(\mathcal{T}_{W,\delta}(I)) \geqslant 1 - \frac{|\mathcal{I}|}{\delta^2}, \tag{74}$$

for the product distribution $W_I = W_{i_1} \otimes \cdots \otimes W_{i_n}$, and

$$(n+1)^{-|\mathcal{I}||\mathcal{J}|} \exp(nH(W|P_I)) \leqslant |\mathcal{T}_W(I)|, \tag{75}$$

$$\exp(nH(W|P_I)) \geqslant |\mathcal{T}_W(I)|, \tag{76}$$

$$(n+1)^{-|\mathcal{I}||\mathcal{J}|} \exp(n(H(W|P_I) - |\mathcal{I}||\mathcal{J}|\,\eta(\delta|\mathcal{I}|/\sqrt{n}))) \leqslant |\mathcal{T}_{W,\delta}(I)|, \tag{77}$$

$$(n+1)^{|\mathcal{I}||\mathcal{J}|} \exp(n(H(W|P_I) + |\mathcal{I}||\mathcal{J}|\,\eta(\delta|\mathcal{I}|/\sqrt{n}))) \geqslant |\mathcal{T}_{W,\delta}(I)|, \tag{78}$$

where $H(W|P_I)$ is just the conditional Shannon entropy $\Sigma_i P_I(i) H(W(\cdot|i))$.

B. Typical subspaces

The concepts in the previous subsection translate straightforwardly to their Hilbert space versions via the following recipe:

For a state ρ choose a diagonalization $\rho=\Sigma_{i\in\mathcal{I}}r_i|e_i\rangle\langle e_i|$, with eigenvectors $|e_i\rangle$ and eigenvalues r_i, which define a probability distribution on $\mathcal{I}$. Then we have a diagonalization of $\rho^{\otimes n}$:

$$\rho^{\otimes n}=\sum_{I\in\mathcal{I}} r_I|e_I\rangle\langle e_I|, \tag{79}$$

with

$$|e_I\rangle=|e_{i_1}\rangle\otimes\cdots\otimes|e_{i_n}\rangle, \tag{80}$$

$$r_I=r_{i_1}\cdots r_{i_n}. \tag{81}$$

Now for any subset $\mathcal{A}\subset\mathcal{I}^n$ we can define the subspace spanned by the vectors $\{|e_I\rangle: I\in\mathcal{A}\}$, which is most conveniently described by the subspace projector

$$\Pi_{\mathcal{A}}:=\sum_{I\in\mathcal{A}}|e_I\rangle\langle e_I|. \tag{82}$$

In this way we can define, for any distribution P on $\mathcal{I}$,

$$\Pi_P:=\sum_{i\in\mathcal{T}_P}|e_I\rangle\langle e_I|, \tag{83}$$

(note that this is not uniquely specified by the distribution P alone, but also requires specification of the basis $|e_i\rangle$), and

$$\Pi_{\rho,\delta}:=\sum_{i\in\mathcal{T}_{r,\delta}}|e_I\rangle\langle e_I|. \tag{84}$$

Statements on the cardinality of sets translate into statements on the dimension of the corresponding subspaces (i.e., rank, or equivalently, trace, of the projectors).

Similarly, if we have states W_i with diagonalizations $W_i=\Sigma_j W(j|i)|e_{j|i}\rangle\langle e_{j|i}|$, we can define, for any subset $\mathcal{A}\subset\mathcal{J}^n$ and $I\in\mathcal{I}^n$,

$$\Pi_{\mathcal{A}}(I):=\sum_{J\in\mathcal{A}}|e_{J|I}\rangle\langle e_{J|I}|. \tag{85}$$

This leads to the concept of *conditional typical subspace projector*, for $\delta\geqslant 0$,

$$\Pi_{W,\delta}(I):=\sum_{J\in\mathcal{T}_{W,\delta}}|e_{J|I}\rangle\langle e_{J|I}|, \tag{86}$$

and again probability and cardinality statements about the typical sequences translate into equivalent statements about certain traces.

In particular we shall use the following estimate of the rank of the conditional typical subspace projector:

$$\mathrm{Tr}\Pi_{\rho,\delta}(I)\leqslant(n+1)^{|\mathcal{I}|d}\exp(n(S(\rho|P_I)+|\mathcal{I}|d\,\eta(\delta|\mathcal{I}|/\sqrt{n}))). \tag{87}$$

[Here we make use of the notation $S(\rho|P_I):=\Sigma_i S(W_i)$ in an attempt to match the statements about typical sequences as closely as possible.] We'll also use the important probability estimate

$$\mathrm{Tr}(W_I\mathcal{T}_{W,\delta}(I))\geqslant 1-\frac{|\mathcal{I}|}{\delta^2}. \tag{88}$$

C. Trade-off coding

We will use the coding technique that is summarized in the following proposition. The statement is slightly more technical and the estimates more explicit than we would need to prove our main Theorem 4.4. This is because we will reuse it in Secs. VI and X.

Proposition 4.1: For a probability distribution p on $\mathcal{I}$ and a classical noisy channel $p(\cdot|\cdot):\mathcal{I}\to\mathcal{J}$ consider the tripartite state

$$\rho=\sum_i p_i|i\rangle\langle i|^A\otimes|\varphi_i\rangle\langle\varphi_i|^B\otimes\sum_j p(j|i)|j\rangle\langle j|^C.$$

Then there exists a visible code (E,D) such that

$$\forall I\in\mathcal{T}_{p,\delta}\quad F(|\varphi_I\rangle\langle\varphi_I|,(D\circ E)(I))\geqslant 1-\frac{4|\mathcal{I}||\mathcal{J}|}{\delta^2},$$

and having classical and quantum resources

$$nS(A:C)+nK|\mathcal{I}||\mathcal{J}|\eta(\delta/\sqrt{n})+K'|\mathcal{I}||\mathcal{J}|\log(n+1)\quad classical\ \ bits,$$

$$nS(A:B|C)+n\cdot 3d|\mathcal{I}||\mathcal{J}|\eta(2\delta|\mathcal{I}||\mathcal{J}|/\sqrt{n})+d|\mathcal{J}|\log(n+1)\quad quantum\ \ bits,$$

where K and K' are absolute constants.

Proof: We design an n-block code as follows (typicality conditions throughout are with respect to a previously fixed δ):

(a) Encoding:

(1) Given I generate J according to $p(J|I)$.

(2) Compress (i.e., project) the quantum state $|\varphi_I\rangle\langle\varphi_I|$ to the conditional typical subspace $\Pi_{\tilde{\rho}^{IJ},\delta}(J)$, where $\tilde{\rho}_j^{IJ}=\Sigma_i W_{I|J}(i|j)|\varphi_i\rangle\langle\varphi_i|$.

If I is typical and J is conditionally typical, send J and the joint type of I and J as classical data, and send the projected state on $\Pi_{\tilde{\rho}^{IJ},\delta}(J)$ as quantum data.

(b) Decoding:

Given J, one can isometrically embed the quantum state transmitted back into the ambient Hilbert space.

The fidelity of this scheme is analyzed as follows. (We assume that if, at any point of the above protocol, an "if" is not satisfied, then some fixed failure action is taken. Such would be the case when the POVM involving the above subspace projection yields an orthogonal result, for example.) With probability at least $1-|\mathcal{I}|/\delta^2$, J is conditionally typical, and in this case the projection is successful with probability at least $1-|\mathcal{J}|/\delta^2$ [by virtue of Eq. (88)], leaving a state which (cf. Ref. 12) has fidelity $\geqslant 1-2|\mathcal{J}|/\delta^2$ to $|\varphi_I\rangle\langle\varphi_I|$.

Looking at the classical cost of this procedure, we see that it is dominated by sending J, which requires too many, namely $nS(C)$, classical bits. Here the reverse Shannon theorem[22] is invoked. (For a precise statement, see Theorem 4.2 below.) Using this theorem we can simulate the channel p on the typical sequences I sending $nS(A:C)+o(n)$ classical bits, but at the same time needing an amount of shared randomness. The simulation, in fact, has the property that it endows sender and receiver with a common J, the distribution of which is $|\mathcal{I}||\mathcal{J}|/\delta^2$-close to $p(J|I)$. Taking all these points into account, we see that the fidelity of this protocol is at least $1-3|\mathcal{I}||\mathcal{J}|/\delta^2$ for every individual $|\varphi_I\rangle\langle\varphi_I|$ for which I is typical.

The analysis of the quantum resources needed is equally straightforward. By Eq. (87) the number of qubits needed to transmit the projected state is

$$nS(\tilde{\rho}^{IJ}|P_J)+dn|\mathcal{J}|\eta(\delta/\sqrt{n})+d|\mathcal{J}|\log(n+1). \tag{89}$$

Note that the leading term is a conditional von Neumann entropy of the bipartite state

$$\rho=\sum_j \tilde{\rho}_j^{IJ}\otimes P_J(j)|j\rangle\langle j|, \tag{90}$$

which has trace norm distance at most $2\delta|\mathcal{I}||\mathcal{J}|/\sqrt{n}$ from

$$\omega=\sum_{ij} p(i)|\varphi_i\rangle\langle\varphi_i|\otimes p(j|i)|j\rangle\langle j|. \tag{91}$$

(This follows from the typicality of I and conditional typicality of J.) Next, using the Fannes inequality (52), we can upper bound Eq. (89) by

$$nS(\tilde{\rho}|q)+2dn|\mathcal{J}|\eta(2\delta|\mathcal{I}||\mathcal{J}|/\sqrt{n})+dn|\mathcal{J}|\eta(\delta/\sqrt{n})+d|\mathcal{J}|\log(n+1), \tag{92}$$

with $q_j=\Sigma_i P(i)p(j|i)$ and $\tilde{\rho}_j=q_j^{-1}\Sigma_i P(i)p(j|i)|\varphi_i\rangle\langle\varphi_i|$.

We are left with one remaining feature to address: the protocol uses shared randomness (and to a considerable extent, according to Theorem 4.2). We shall now show that we can reduce this requirement to $O(\log n)$ shared random bits using a technique very much like the derandomization argument in Ref. 26. The proof will then be complete because setting up these bits can be absorbed into the classical communication with asymptotically vanishing cost per letter. (Actually, in order to achieve high average fidelity, no random bits are needed at all, but our goal is to prove that high fidelity can be achieved for every state in the typical subspace, a more stringent requirement that is used later in our study of arbitrarily varying sources.)

Observe that a protocol using shared randomness can be viewed as a probabilistic mixture of ordinary, deterministic protocols. Index these by a variable ν, accompanied by a probability x_ν. For each ν we have a corresponding fidelity $F_I(\nu)$ for each individual I. Our construction shows that for typical I,

$$\sum_\nu x_\nu F_I(\nu)\geqslant 1-\frac{3|\mathcal{I}||\mathcal{J}|}{\delta^2}=:\mu. \tag{93}$$

Note that the left hand side is exactly the expectation of the random variable F_I. We now choose $\nu_1,\ldots,\nu_L$ independently and identically distributed (i.i.d.), according to the probabilities x_ν. For fixed I the $F_I(\nu_l)$, $l=1,\ldots,L$ are i.i.d. as well, and in the interval [0, 1]. Thus we can apply the Chernoff–Hoeffding bound for their arithmetic mean (Lemma 4.3 below):

$$\Pr\left\{\frac{1}{L}\sum_{l=1}^{L} F_I(\nu_l)<(1-\epsilon)\mu\right\}\leqslant\exp\left(-L\frac{\epsilon^2\mu}{2\ln 2}\right). \tag{94}$$

By the union bound we can estimate the probability that the above event occurs for a single typical I to be less than or equal to

$$\exp\left(-L\frac{\epsilon^2\mu}{2\ln 2}\right)|\mathcal{I}|^n. \tag{95}$$

Choosing $\epsilon=|\mathcal{I}||\mathcal{J}|/\delta^2$, this bound is itself less than 1 if

$$L>\frac{2\delta^4\ln 2}{|\mathcal{I}|^2|\mathcal{J}|^2\mu}n\log|\mathcal{I}|, \tag{96}$$

in which case we can conclude that there exist values $\nu_1,\ldots,\nu_L$ such that, for all typical I, we have

$$\frac{1}{L}\sum_{l=1}^{L} F_I(\nu_l)\geqslant 1-\frac{4|\mathcal{I}||\mathcal{J}|}{\delta^2}.$$

Therefore, a shared uniform distribution over the numbers $1,\ldots,L$ is sufficient, where L need only satisfy Eq. (96). This can be accomplished with $O(\log n)$ shared random bits, which is what we wanted. □

Here are the auxiliary results we needed in the proof:

Theorem 4.2 (Reverse Shannon Theorem; see Refs. 22 and 27): *For any channel* $W:\mathcal{I}\to\mathcal{J}$, *distribution* P *on* $\mathcal{I}$, *and* $0<\lambda<1$ *there exist maps*

$$E_\nu:\mathcal{I}^n\to\{1,\ldots,M\},$$

$$D_\nu:\{1,\ldots,M\}\to\mathcal{J}^n,$$

$\nu=1,\ldots,N$, *such that*

$$\forall I\in\mathcal{T}_{P,\delta}\quad \frac{1}{2}\left\| W(I)-\frac{1}{N}\sum_{\nu=1}^{N} D_\nu(E_\nu(I))\right\|_1 \leqslant \frac{|\mathcal{I}||\mathcal{J}|}{\delta^2}.$$

Moreover, with an absolute constant K,

$$\log M\leqslant nH(P:W)+nK|\mathcal{I}||\mathcal{J}|\,\eta(\delta/\sqrt{n})+K|\mathcal{I}||\mathcal{J}|\log(n+1),$$

$$\log N\leqslant nH(W|P)+nK|\mathcal{I}||\mathcal{J}|\,\eta(\delta/\sqrt{n})+K|\mathcal{I}||\mathcal{J}|\log(n+1).$$

□

Lemma 4.3 (Chernoff-Hoeffding bound.[28,29]*) Let* $X_1,\ldots,X_L$ *be independent, identically distributed random variables, taking real values in the interval* $[0,1]$, *and with expectation* $\mathbb{E}X_l\geqslant\mu$. *Then, for* $\epsilon>0$,

$$\Pr\left\{\frac{1}{L}\sum_{l=1}^{L} X_l<(1-\epsilon)\mu\right\}\leqslant\exp\left(-L\,\frac{\epsilon^2\mu}{2\ln 2}\right).$$

□

With this we are ready to state our main result:

Theorem 4.4: $Q^*(R)=M(\mathcal{E},R)$.

Proof: The inequality "$\geqslant$" is theorem 3.5. For the opposite inequality choose a $p(\cdot|\cdot)$ such that $S(A:C)\leqslant R$ and $S(A:B|C)\leqslant M(\mathcal{E},R)+\epsilon$. Then, according to Proposition 4.1, there exist n-block codes (E,D) with classical and quantum rates bounded by $R+o(1)$ and $M(\mathcal{E},R)+\epsilon+o(1)$, respectively, which have fidelity $1-\epsilon$ for all *typical* I. But since these carry almost all the probability weight (say, larger than $1-\epsilon$) of all sequences, the fidelity of the scheme is at least $1-2\epsilon$, regardless of what is done on nontypical sequences. As ϵ was arbitrary, we get $Q^*(R)=M(\mathcal{E},R)$. □

Remark: The proof of Proposition 4.1, as the eventual "derandomization" shows, does not use the full power of the reverse Shannon theorem, but only a consequence that is actually also used in rate-distortion coding: that one can map the typical sequences I onto $\exp(nH(P:W)+o(n))$ many J's such that all the pairs $(I,f(I))$ are jointly typical. □

V. EXPLORING THE TRADE-OFF CURVE

In this section we use our formula for the trade-off curve to evaluate $Q^*(R)$ numerically for a selection of particular ensembles chosen to illustrate further important properties of the trade-off function.

To begin, let us consider the simplest possibility, a pair of nonorthogonal states. Figure 2 plots the trade-off curve for the pair $\{|0\rangle,(1/\sqrt{2})(|0\rangle+|1\rangle)\}$, each occurring with probability $\frac{1}{2}$. At first glance, $Q^*(R)$ appears to coincide with the linear upper bound given by interpolating between $(0,S(\mathcal{E}))$ and $(H_2(\frac{1}{2}),0)$. A more detailed examination, however, reveals that the curve is actually

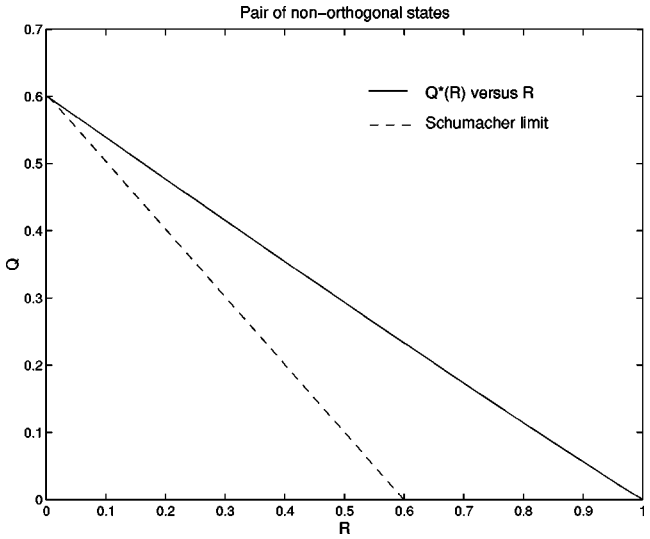

FIG. 2. The trade-off curve for a pair of equiprobable, nonorthogonal states. The dashed line represents the lower bound $Q^*(R)+R \geqslant S(\mathcal{E})$ imposed by the Schumacher limit.

very slightly nonlinear. Therefore, somewhat surprisingly, the simple quantum-classical coding scheme given by timesharing between fully quantum and fully classical coding is nearly optimal but not completely so. As we will see below, this need not always be true.

In general, more complicated ensembles with internal structure will have trade-off curves reflecting that structure. Consider, for example, the three-state ensemble $\mathcal{E}_3$ illustrated in Fig. 3, consisting of the states $|\varphi_1\rangle = |0\rangle$, $|\varphi_2\rangle = (1/\sqrt{2})(|0\rangle + |1\rangle)$ and $|\varphi_3\rangle = |2\rangle$ with equal probabilities. Since the set of states decomposes into two subsets $\mathcal{X}_1 = \{|\varphi_1\rangle, |\varphi_2\rangle\}$ and $\mathcal{X}_2 = \{|\varphi_3\rangle\}$ with mutually orthogonal supports, it is possible to encode whether a given $|\varphi_i\rangle \in \mathcal{X}_1$ or $|\varphi_i\rangle \in \mathcal{X}_2$ efficiently using $H_2(\frac{1}{3})$ classical bits. Indeed, Fig. 4 plots $Q^*(R)$ for this ensemble and we see that the Schumacher limit is achieved for values of $R \leqslant H_2(1/3)$. For values of $R > H_2(\frac{1}{3})$, or once the classical information in the ensemble has been exhausted, the trade-off curve departs from the Schumacher lower bound to meet the point $(H(\frac{1}{3},\frac{1}{3},\frac{1}{3}),0)$.

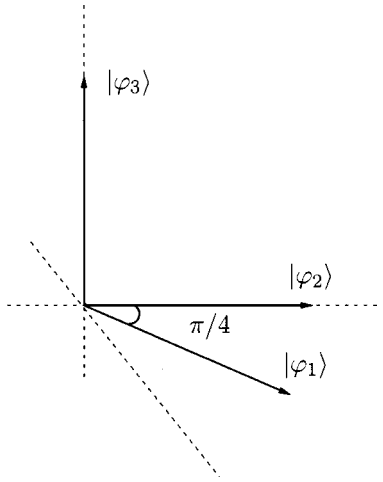

FIG. 3. The three-state ensemble $\mathcal{E}_3$ consists of the states $|\varphi_1\rangle$, $|\varphi_2\rangle$, $|\varphi_3\rangle$ occurring with equal probabilities.

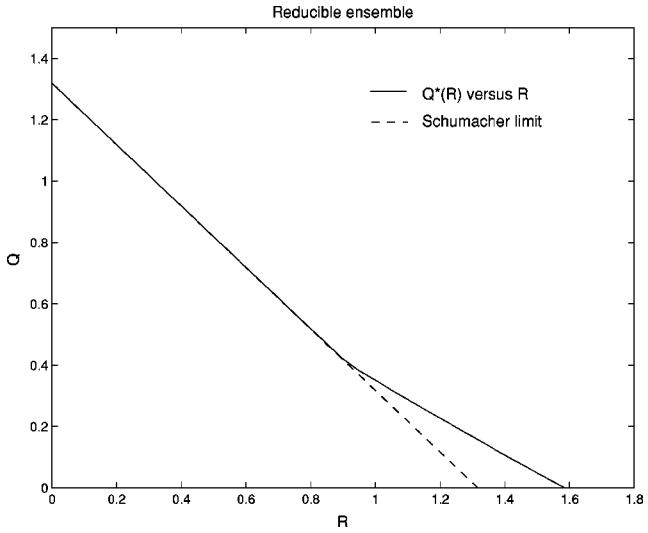

FIG. 4. The trade-off curve for three-state ensemble $\mathcal{E}_3$. The dashed line again represents the Schumacher lower bound, which in this case is achievable for $R \leqslant H(\frac{1}{3})$.

Our third example, the parametrized BB84 ensemble $\mathcal{E}_{BB}(\theta)$ introduced in Sec. II, is an ensemble that, like $\mathcal{E}_3$ above, decomposes naturally into subensembles. On the other hand, unlike for $\mathcal{E}_3$, the subensembles are generally not orthogonal. The trade-off curve for $\theta = \pi/8$ is plotted in Fig. 5. As usual, the dashed lower bound is the Schumacher limit. The dashed-dot line is the piecewise linear upper bound constructed in Sec. II. Squeezed into the intermediate region, we see that $Q^*(R)$ is typically strictly less than the upper bound and, especially in the region $0 < R < 1$, quite strongly curved. The point $(1, H_2(\frac{1}{2}(1+\cos \pi/8))$ provides another surprise: $Q^*(R)$ and the upper bound coincide there. Therefore, the partitioning scheme is optimal if exactly one bit of classical storage is to be consumed per copy but not otherwise.

We now turn to another interesting property of the trade-off curve. Contrary to what one might expect, the function $M(\mathcal{E},R)$ is *not concave in the ensemble*, violating the intuition that it should

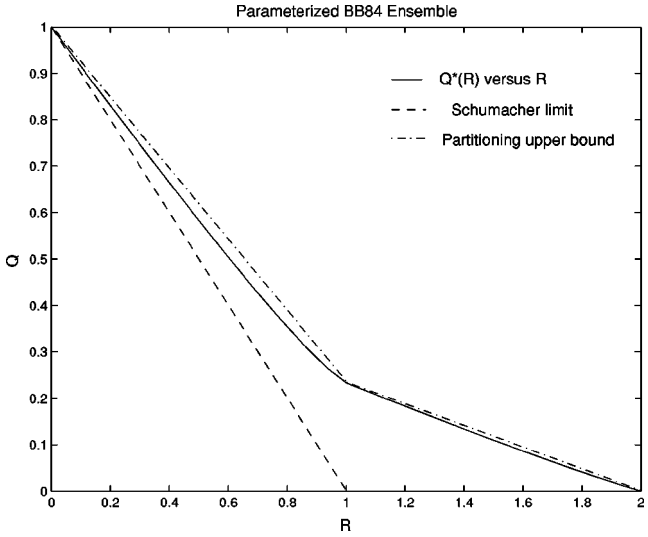

FIG. 5. Trade-off curve for the BB84 ensemble $\mathcal{E}_{BB}(\pi/8)$. The dashed line represents the Schumacher lower bound and the dashed-dot line represents the upper bound from partitioning into the sets $\mathcal{X}_1$ and $\mathcal{X}_2$.

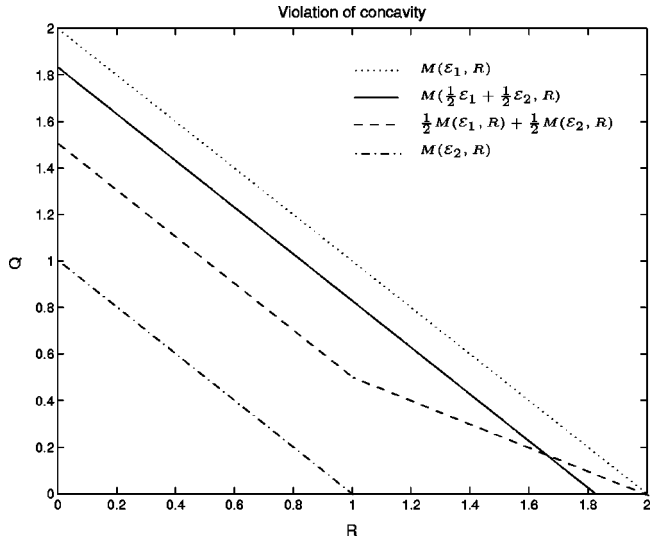

FIG. 6. Violation of concavity in the ensemble. If Q^* were concave in the ensemble, the solid line representing $M(\frac{1}{2}\mathcal{E}_1 + \frac{1}{2}\mathcal{E}_2, R)$ would always exceed the dashed line of $\frac{1}{2}M(\mathcal{E}_1, R) + \frac{1}{2}M(\mathcal{E}_2, R)$. For large values of R we see that is not the case in this example.

be harder to send the mixture of two ensembles than it is to probabilistically send either one. [Note that $M(\mathcal{E},0)$, however, is just the von Neumann entropy $S(\mathcal{E})$ and is, therefore, concave in $\mathcal{E}$.] In fact, counterexamples to concavity can be constructed without even making use of nonorthogonal states. Let $\mathcal{E}_1 = \{|i\rangle, \frac{1}{4}\}_{i=0}^{3}$ be an ensemble consisting of four equiprobable orthonormal states and let $\mathcal{E}_2 = \{|i\rangle, \frac{1}{2}\}_{i=0}^{1}$. We can also consider the mixture of ensembles

$$\mathcal{E} := \tfrac{1}{2}\mathcal{E}_1 + \tfrac{1}{2}\mathcal{E}_2 = \{(|0\rangle, \tfrac{3}{8}), (|1\rangle, \tfrac{3}{8}), (|2\rangle, \tfrac{1}{8}), (|3\rangle, \tfrac{1}{8})\}. \tag{97}$$

Since each of these ensembles is effectively classical, the Schumacher lower bound is attainable and their trade-off curves are just straight lines with slope -1. From there, we can also evaluate $\frac{1}{2}(M(\mathcal{E}_1,R) + M(\mathcal{E}_1,R))$ and compare it to $M(\mathcal{E},R)$. This is done in Fig. 6, revealing a violation of concavity when R comes close to 2.

In the same spirit, note that an analogous construction shows that, while

$$M(\mathcal{E}_1 \otimes \mathcal{E}_2, 2R) \leqslant M(\mathcal{E}_1,R) + M(\mathcal{E}_2,R) \tag{98}$$

always holds, equality (i.e., the natural ''additivity'' property of M under tensor products) may be violated if the ensembles are sufficiently different from each other. More generally we have the following.

Proposition 5.1:

$$M(\mathcal{E}_1 \otimes \mathcal{E}_2, R) = \min\{M(\mathcal{E}_1,R_1) + M(\mathcal{E}_2,R_2) : R_1 + R_2 = R\}.$$

Also, while $M(\mathcal{E},R)$ may not be concave in the ensemble $\mathcal{E}$, it does obey a weaker condition analogous to Schur concavity.

Proposition 5.2: Let $\mathcal{E} = \{|\varphi_i\rangle, p_i\}$ be an ensemble. Let $\{a_k\}$ be a set of probabilities with corresponding unitary operators U_k and $\mathcal{F}$ be the ensemble $\mathcal{F} = \{U_k|\varphi_i\rangle, p_i a_k\}$. Then $M(\mathcal{E},R) \leqslant M(\mathcal{F},R)$.

The proofs of these propositions can be found in Appendix Secs. 3 and 4, respectively.

As our last example, we include the trade-off curve for the uniform (unitarily invariant) ensemble on a single qubit as Fig. 7. Devetak and Berger[30] actually calculated an explicit parametrization of the optimal trade-off curve for a restricted class of encodings. Our lower bound of

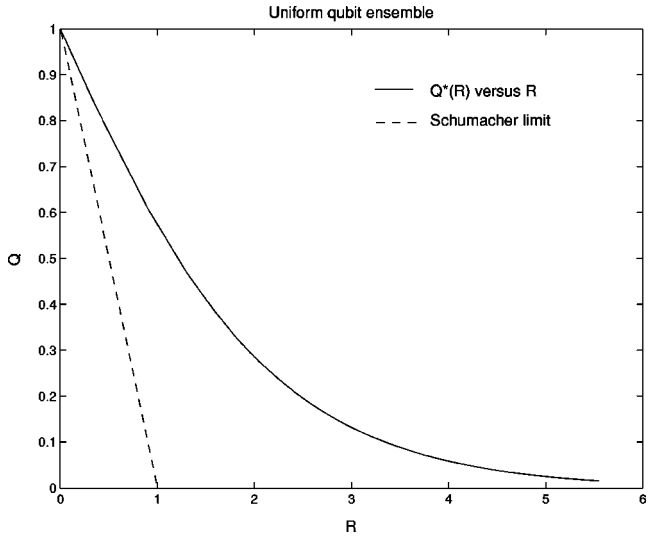

FIG. 7. Trade-off curve for the uniform qubit ensemble. Note that the curve never reaches the $Q=0$ axis, encoding the fact that no finite amount of classical information is sufficient to perfectly transmit an arbitrary qubit state.

Theorem 3.5, or, rather, its infinite source ensemble variant, Theorem 10.1, proves that their construction is optimal within all possible quantum-classical coding strategies. Thus, we can quote their result that, for $\lambda \in (0,\infty)$,

$$R = \frac{\lambda}{\epsilon^{\lambda}-1} - 1 + \log\left(\frac{\lambda e^{\lambda}}{\epsilon^{\lambda}-1}\right), \tag{99}$$

$$Q^*(R) = H_2\left(\frac{1}{\lambda} - \frac{1}{e^{\lambda}-1}\right), \tag{100}$$

gives a parametrization of $Q^*(R)$. This curve will also play an important role when we construct a probability-free version of our main result in Sec. VI. We will find that, in an extremely strong sense, it describes the cost of a qubit in classical bits.

VI. ARBITRARILY VARYING SOURCES

Our main result does not yet say, however, what a qubit costs in bits because it only supplies the trade-off curve $Q^*(R)$ for a given set of quantum states once a set of prior probabilities have been prescribed. Without the probabilities, the curve is undefined and the rate of exchange between bits and qubits cannot be uniquely identified. However, using the theory of *arbitrarily varying sources (AVS)* (see Ref. 31 for an exposition of this concept in classical information theory), we can develop a probability-independent version of our trade-off curve that will eliminate the ambiguity.

Throughout this section, let $\mathcal{E}$ denote not an ensemble, but just a set of states, and let $\mathbf{P} \subset \mathcal{P}_{\mathcal{E}}$ be a subset of probability distributions on $\mathcal{E}$. For each string $I \in \mathcal{I}^n$ of length n we will consider product distributions

$$p^n(I) := p_1(i_1)\cdots p_n(i_n), \tag{101}$$

where each $p_k \in \mathbf{P}$. An *AVS-code of fidelity* $1-\epsilon$ is defined as a visible code, as before (see Definition II), only that now the fidelity condition is required to hold for all probability distributions in $\mathbf{P}$:

$$\forall p^n \in \mathbf{P}^n \quad \sum_I p^n(I) F(\varphi_I, (D \circ E)(I)) \geqslant 1 - \epsilon. \tag{102}$$

The classical and quantum rates are exactly as in Definition 2.3 and, likewise, Definition 2.4 can be used unchanged to characterize attainable rate pairs (R,Q). This leads to the definition of the trade-off function $Q^*(R,\mathbf{P})$ as the minimum Q such that (R,Q) is attainable.

Intuitively, the encoder-decoder pair plays a game against a clairvoyant adversary whose aim is to minimize their average fidelity and who can control the source mechanism so as to create any of the distributions $p^n \in \mathbf{P}^n$. Their goal is to win by keeping the average fidelity above $1-\epsilon$ against arbitrary strategies of the adversary.

A special case is that of $\mathbf{P} = \mathcal{P}_{\mathcal{E}}$, in which case we have no restriction on the source, so that all possible state strings are to maintain high fidelity.

We shall use the notation $M(\mathcal{E},p,R)$ to designate our earlier function M for the ensemble consisting of the states $\mathcal{E}$ and the probabilities p, and define now

$$M(\mathcal{E},\mathbf{P},R) := \sup_{p \in \mathbf{Q}} M(\mathcal{E},p,R), \tag{103}$$

where $\mathbf{Q} := \mathrm{conv}(\mathbf{P})$ is the convex hull of $\mathbf{P}$.

Theorem 6.1: $Q^*(R,\mathbf{P}) = M(\mathcal{E},\mathbf{P},R)$.

Proof: The inequality "$\geqslant$" follows almost directly from Theorem 3.5: only observe that the adversary can simulate any source ensemble $p \in \mathbf{Q}$, and then Theorem 3.5 applies. [More formally, choose a probability distribution s on $\mathbf{P}$ such that $p = \Sigma_k s_k p_k$, and note that averaging Eq. (102) over the measure $s^{\otimes n}$ gives (102) for $p^{\otimes n}$.]

In the other direction, we only need to exhibit a covering of the union of the "probable sets" of the distributions $p^n \in \mathbf{P}^n$ by appropriate sets of typical sequences, and apply Proposition 4.1. This is done as follows:

For $p^n = p_1 \otimes \cdots \otimes p_n \in \mathbf{P}^n$ observe that the set

$$\mathcal{T}_{p^n} := \left\{ I : \forall i \left| N(i|I) - \sum_{k=1}^{n} p_k(i) \right| \leqslant \delta \sqrt{n} \right\} \tag{104}$$

carries (by Chebyshev's inequality) almost all the weight of the distribution:

$$p^n(\mathcal{T}_{p^n}) \geqslant 1 - \delta^{-2}. \tag{105}$$

Since $\mathcal{T}_{p^n}$ is in fact the same as the set of typical sequences $\mathcal{T}_{\overline{p},\delta}$, for $\overline{p} = (1/n)\Sigma_k p_k \in \mathbf{Q}$, the union $\cup_{p^n} \mathcal{T}_{p^n}$ is actually a union of certain type classes, and hence we may choose $\overline{p_1}, \ldots, \overline{p_T}$, $T \leqslant (n+1)^{|\mathcal{I}|}$, such that

$$\mathcal{T} := \bigcup_{p^n \in \mathbf{P}^n} \mathcal{T}_{p^n} = \bigcup_{t=1}^{T} \mathcal{T}_{\overline{p_t},\delta}. \tag{106}$$

The coding is very simple: when $I \in \mathcal{T}$ the encoder chooses t such that $I \in \mathcal{T}_{\overline{p_t},\delta}$. He then communicates t to the decoder, and uses the protocol of Proposition 4.1. (In fact, communication of t is not even necessary, as in the latter protocol the type of I is communicated anyway.) When $I \notin \mathcal{T}$ some fixed default choice is sent.

By construction and by Proposition 4.1, for sufficiently large δ this scheme uses $R+\epsilon$ classical bits and $M(\mathcal{E},\mathbf{P},R)+\epsilon$ qubits per source symbol. For each $p^n \in \mathbf{P}^n$ we obtain high fidelity for all states outside a set of arbitrarily small probability. □

In particular, for the above-mentioned case of no restrictions at all on the probabilities, we get the trade-off function

$$\mathbf{Q}^*(R,\mathcal{P}_{\mathcal{E}}) = \sup_{p\in\mathcal{P}_{\mathcal{E}}} M(\mathcal{E},p,R). \tag{107}$$

which depends only on the states of $\mathcal{E}$. For a finite ensemble it is quite easy to show that $M(\mathcal{E},p,R)$ is continuous in the distribution p. This implies that the suprema in Eqs. (103) and (107) are, in fact, *maxima* (in the former case over the closure of $\mathbf{Q}$).

VII. INFORMATION AND DISTURBANCE

The function $M(\mathcal{E},R)$, in addition to providing the quantum-classical trade-off curve, has a number of other useful interpretations. Recall from Proposition 3.3 that

$$M(\mathcal{E},R) = \inf_{p(\cdot|\cdot)} \{S(A:B|C) : S(A:C) = R\}, \tag{108}$$

with an equality for $S(A:C)$ rather than the inequality we usually use. By the chain rule,

$$S(A:C) + S(A:B|C) = S(A:BC) \tag{109}$$

and $S(A:BC)$ is just the Holevo χ quantity of the ensemble

$$\mathcal{F}^{BC} := \left\{ \varphi_i^B \otimes \sum_j p(j|i)|j\rangle\langle j|^C, p_i \right\}. \tag{110}$$

Therefore, if we define the function $X(\mathcal{E},R) := R + M(\mathcal{E},R)$, then we can rewrite Eq. (108) as

$$X(\mathcal{E},R) = \inf_{p(\cdot|\cdot)} \{\chi(\mathcal{F}^{BC}) : S(A:C) = R\}. \tag{111}$$

The quantity on the right is now perhaps more familiar than the conditional mutual information $S(A:B|C)$: it is a standard measure of the distinguishability present in the ensemble $\mathcal{F}^{BC}$, minimized over all possible ways of including a fixed amount of classical information about the index i in register C. Now suppose that Alice is initially given a state $|\varphi_i\rangle$ from $\mathcal{E}$ (without the name i this time) and, via a CPTP map, manages to extract an amount R of classical information about i without damaging any of the states $|\varphi_i\rangle$. Then her final Holevo χ would necessarily be at least as large as $X(\mathcal{E},R)$, by definition. Typically, however, $X(\mathcal{E},R) > S(\mathcal{E})$ [by the Schumacher lower bound to $Q^*(R) = M(\mathcal{E},R)$], so such an operation will be forbidden by the monotonicity of χ. Therefore, it is impossible for Alice to extract information without disturbing the states.

The simple argument above combined with the additivity of $M_\epsilon(\mathcal{E},R)$ from Sec. III A can be used to prove interesting statements about the trade-off between information gain and state disturbance in an asymptotic and approximate setting. In contrast to the compression problem, however, we can make stronger statements if we use the mean letterwise fidelity measure $\overline{F}$ from Sec. III D instead of the global fidelity measure F. Therefore, we will express our results in terms of the corresponding function $\overline{M}_\epsilon(\mathcal{E}^{\otimes n},nR)$ instead of $M_\epsilon(\mathcal{E}^{\otimes n},nR)$. Recall that these functions are defined identically except that the first uses the mean fidelity function $\overline{F}$ and the second uses the global fidelity F. Likewise, define $\overline{X}_\epsilon(\mathcal{E},R) = R + \overline{M}_\epsilon(\mathcal{E},R)$. Since F and $\overline{F}$ are identical for a single copy, we have $\overline{M}_\epsilon(\mathcal{E},R) = M_\epsilon(\mathcal{E},R)$ and similarly for X and $\overline{X}$. By the discussion in Sec. III D, we know that $\overline{M}_\epsilon(\mathcal{E}^{\otimes n},nR) = n\overline{M}_\epsilon(\mathcal{E},R)$, which in turn implies

$$\overline{X}_\epsilon(\mathcal{E}^{\otimes n},nR) = nX_\epsilon(\mathcal{E},R). \tag{112}$$

Now, generalizing the above single copy argument, suppose that Alice is given a state $|\varphi_I\rangle$ drawn from $\mathcal{E}^{\otimes n}$, which, by a CPTP map Γ, she manages to convert into the state

$$\rho_I = \sum_j \tilde{\varphi}^B_{I,j} \otimes p(j|I)|j\rangle\langle j|^C, \tag{113}$$

with a quantum and classical part such that the mutual information $H(I:j) \geqslant nR$ and the mean letterwise fidelity between Alice's initial states and her final states of system B satisfies

$$\overline{F}(\mathcal{E}^{\otimes n}, \mathrm{Tr}_C \circ \Gamma(\mathcal{E}^{\otimes n})) := \sum_I p_I \frac{1}{n} \sum_{k=1}^{n} F(\varphi_{i_k}, \mathrm{Tr}_{\neq k} \circ \mathrm{Tr}_C(\rho_I)) \geqslant 1 - \epsilon. \tag{114}$$

Writing $\mathcal{F}^{BC} = \{\Gamma(\varphi_I), p_I\}$, the monotonicity of χ guarantees that $nS(\mathcal{E}) \geqslant \chi^{BC}$ and it is easy to see that $\chi^{BC} \geqslant \overline{X}_\epsilon(\mathcal{E}^{\otimes n}, nR)$. By applying Eq. (112), we then find

$$S(\mathcal{E}) \geqslant X_\epsilon(\mathcal{E}, R), \tag{115}$$

in which, conspicuously, all dependence on n has vanished. In other words, in order to maximize her information at a given mean letterwise fidelity, Alice should just repeat the optimal single letter strategy for each position; she need not ever apply any collective operations. Summarizing these observations, we have the following.

Theorem 7.1: *Suppose we have a set of states $|\varphi_I\rangle$ drawn from the ensemble $\mathcal{E}^{\otimes n}$ represented on system B and let Γ be a CPTP map from B to the joint system BC, where C is classical, satisfying the following conditions:*

(1) *$H(I:j) \geqslant nR$, where j is the classical output on system C.*
(2) *The mean letterwise fidelity $\overline{F}(\mathcal{E}^{\otimes n}, \mathrm{Tr}_C \circ \Gamma(\mathcal{E}^{\otimes n})) \geqslant 1 - \epsilon$.*

Then, for each $\epsilon > 0$, the inequality $S(\mathcal{E}) \geqslant X_\epsilon(\mathcal{E}, R)$ holds. Moreover, the Holevo quantity of the ensemble $\mathcal{F}^{BC} = \{\Gamma(\varphi_I), p_I\}$ satisfies the inequality $\chi(\mathcal{F}^{BC}) \geqslant nX_\epsilon(\mathcal{E}, R)$.

□

One application of the theorem is that it provides an alternative method for analyzing the quantum resources required for blind compression, which was the subject of Ref. 13. The idea is simply to think of the map Γ as the composition $D_n \circ E_n$ of the encoding and decoding maps for blocks of size n. (Because classical information can be copied, we can assume without loss of generality that the decoder keeps his classical information around after the decoding stage has been completed.) Now suppose that the scheme has classical mutual information $H(I:j) \geqslant nR$. If it also has mean letterwise fidelity $1 - \epsilon_n$, then, as for the visible case,

$$\mathrm{qsupp} \geqslant \frac{1}{n} \overline{M}_{\epsilon_n}(\mathcal{E}^{\otimes n}, nR) = M_{\epsilon_n}(\mathcal{E}, R). \tag{116}$$

By the previous theorem, however, we must also have the inequality $S(\mathcal{E}) \geqslant X_{\epsilon_n}(\mathcal{E}, R)$. Moreover, if perfect compression is possible asymptotically (using either the block or letterwise fidelity conditions), we get the stronger inequality

$$S(\mathcal{E}) \geqslant \lim_{\epsilon \downarrow 0} X_\epsilon(\mathcal{E}, R) = X_0(\mathcal{E}, R). \tag{117}$$

(The continuity at $\epsilon = 0$ follows from the continuity of M_0, demonstrated earlier.) Because the ensemble $\mathcal{E}$ can always be recovered by tracing over the C register, the monotonicity of χ guarantees that the right hand side is always at least as large as the left, implying $S(\mathcal{E}) = X_0(\mathcal{E}, R)$. We are, therefore, interested in the equality conditions for monotonicity.

Recalling some terminology from Ref. 13, we say an ensemble $\mathcal{E}$ is *reducible* if its states can be partitioned into two nonempty sets with orthogonal supports. An ensemble is said to be irreducible if it is not reducible. Every ensemble, therefore, can be decomposed into orthogonal, irreducible subensembles as

$$\mathcal{E}=\bigcup_{l=1}^{L} a_l\mathcal{E}_l, \tag{118}$$

where a_l is the total probability weight of states in subensemble $\mathcal{E}_l$.

Proposition 7.2: Let $\mathcal{E}=\cup_{l=1}^{L}a_l\mathcal{E}_l$ be a decomposition of the pure-state ensemble $\mathcal{E}$ into irreducible subensembles $\mathcal{E}_l=\{|\varphi_{il}\rangle,p_{i|l}\}$ and let $\mathcal{F}^{BC}=\{\varphi_{il}^B\otimes\omega_{il}^C,a_lp_{i|l}\}$ be a bipartite extension of the ensemble $\mathcal{E}$. Then $S(\mathcal{E})=\chi(\mathcal{F}^{BC})$ if and only if $\omega_{il}=\omega_{jl}$ for all i, j, and l.

A proof is given in the Appendix, Sec. 5. The meaning of the proposition is essentially that the only information that can be stored on register C without increasing χ is the classical information already present on register B, so that ω_{il} must be a function of l alone. Therefore, in order to satisfy Eq. (117) it is necessary that $R\leqslant H(a_1,\ldots,a_L)$. Conversely, provided the inequality holds, it is possible to extract R bits per signal without disturbance at the encoding stage, at which point the encoding scheme we used for visible compression can be used to achieve the quantum rate $S(\mathcal{E})-R$. Putting these observations together, we obtain an alternative demonstration of the main theorem of Ref. 13:

Theorem 7.3: *Let $\mathcal{E}=\cup_{l=1}^{L}a_l\mathcal{E}_l$ be a decomposition of the ensemble $\mathcal{E}$ into orthogonal, irreducible subensembles. Then blind compression of $\mathcal{E}$ to Q qubits per signal plus auxiliary classical storage is possible if and only if*

$$Q\geqslant\sum_l a_lS(\mathcal{E}_l)=S(\mathcal{E})-H(a_1,\ldots,a_L). \tag{119}$$

□

Thus, the techniques we have introduced to analyze the visible compression problem provide a unified framework for analyzing blind compression as well. In fact, we will see in the next section that the trade-off curve for yet another related problem—remote state preparation—can also be calculated using similar methods.

VIII. APPLICATION TO REMOTE STATE PREPARATION

Remote state preparation, introduced in Ref. 17 following a conjecture of Lo's,[16] is very similar to what we have considered here: it is a visible coding problem for quantum states involving classical resources, in the form of communication, and quantum resources, this time in the form of entanglement. Furthermore, these two types of resources can be traded against each other so it is natural to study the optimal trade-off curve.

Without giving formal definitions, let $E^*(R)$ be the minimum rate of entanglement sufficient for a remote state preparation protocol with classical rate R, such that the average fidelity tends to 1 with growing blocklength.

Given that entanglement can be set up using quantum communication at a cost of one qubit per ebit, and that, on the other hand, quantum communication can be accomplished using teleportation[32] at a cost of two cbits and one ebit per qubit, it is clear that coding methods for the one problem immediately yield (possibly suboptimal) procedures for the other. (In fact, by making use of quantum-classical trade-off coding, this resulted in the ''cap-method'' of Ref. 17, which was further refined in Ref. 30.)

In Ref. 33 a method of remote state preparation is developed that works for visible coding of product states and is more efficient than teleportation: we really need only to use *one* cbit and one ebit per qubit, asymptotically.

Theorem 8.1 (See Ref. 33): *Given a finite set $\mathcal{X}$ of states (density operators) on $\mathcal{K}$, there is a probabilistic exact (one-shot) remote state preparation protocol working for all states in $\mathcal{X}$ and with failure probability uniformly ϵ, using a maximally entangled state $|\Phi\rangle$ on $\mathcal{K}\otimes\mathcal{K}$ and classical communication of a message out of*

$$M \leqslant 1 + \frac{2\ln 2}{\epsilon^2} \log(2|\mathcal{X}|\dim\mathcal{K})\dim\mathcal{K}.$$

□

This leads immediately to the following.

Theorem 8.2: *For the source* $\mathcal{E}=\{|\varphi_i\rangle,p_i\}$ *of quantum states, if* $R\geqslant 0$ *and* $Q=Q^*(R)$, *then* $E^*(R+Q)\leqslant Q$.

As a consequence, we obtain

$$E^*(R) \leqslant N(\mathcal{E},R) := \min_{p(\cdot|\cdot)} \{S(A:B|C) : S(A:BC) \leqslant R\},$$

minimization over the same set of tripartite states as in the definition of M.

Proof: We apply Theorem 8.1 to the space $\mathcal{K}$ of *encoded states* of an optimal trade-off coding using R cbits and Q qubits per source symbol, and to the set of all possible encoded states: note that $|\mathcal{X}| \leqslant (|\mathcal{I}||\mathcal{J}|)^n$.

By that result, we need Q ebits to do this, and an additional $Q+o(1)$ cbits to the R cbits from the trade-off coding. □

In fact, in Ref. 33 it is shown, by methods very similar to those in Sec. III, that the above estimate for E^* is in fact an equality, and that our AVS considerations also carry over.

Theorem 8.3: *For the state set* $\mathcal{E}$ *and AVS* $\mathbf{P}$,

$$E^*(R,\mathbf{P}) = \sup_{p\in\mathbf{Q}} N(\mathcal{E},p,R),$$

with $\mathbf{Q}=\mathrm{conv}(\mathbf{P})$. □

For $\mathbf{P}$ the set of all distributions on the pure states (as indeed for any symmetric family of distributions) we can prove symmetry results like those in the upcoming Sec. IX, and arrive at the conclusion that the *absolute trade-off* between cbits and ebits in remote state preparation is given by the curve $N(\mathcal{P}(\mathcal{H}),u)$, where u is the uniform (i.e., unitarily invariant) measure on the set $\mathcal{P}(\mathcal{H})$ of all pure states on $\mathcal{H}$. Devetak and Berger[30] arrived at a slightly different curve as an upper bound to the true trade-off, starting from $M(\mathcal{P}(\mathcal{H}),u)$ as we did, but employing teleporation instead of the newer technique in Theorem 8.1. For this reason their conjecture that their bound is tight is not correct.

IX. SYMMETRY IN THE ENSEMBLE

Our formulas for the trade-off curve, both in the known and arbitrarily varying source case, can be considerably simplified if there is symmetry in the set of states.

Assume that there is a group G acting on the labels i of the states by a projective unitary representation U_g,

$$\forall g\in G, i\in\mathcal{I} \quad |\varphi_{gi}\rangle\langle\varphi_{gi}| = U_g|\varphi_i\rangle\langle\varphi_i|U_g^\dagger. \tag{120}$$

(We will present the following arguments for a finite group, but they also apply to compact groups: in fact, we only need the existence of an invariant measure, see Ref. 34.) The action of G on $\mathcal{I}$ induces an action on the probability distributions on $\mathcal{I}$ in a natural way: if $p\in\mathcal{P}(\mathcal{I})$ is a distribution, then $p^g(i)=p(g^{-1}i)$ defines the translated distribution. Assume now further that the arbitarily varying source $\mathbf{P}$ is stable under this induced action:

$$\forall p\in\mathbf{P} \quad p^g\in\mathbf{P}. \tag{121}$$

[In the "known source" case, $\mathbf{P}=\{p\}$, this simply means that $p(gi)=p(i)$ for all $i\in\mathcal{I}$ and $g\in G$.]

By the formula for the trade-off curve, Eq. (103), we may assume that $\mathbf{P}$ is convex. Letting

$$\mathbf{P}^G := \{p \in \mathbf{P} : \forall g \in G\, p^g = p\}, \tag{122}$$

we can then prove the following.

Theorem 9.1: *For any G-invariant state set and AVS* $\mathbf{P}$,

$$M(\mathcal{E},\mathbf{P},R) = M(\mathcal{E},\mathbf{P}^G,R). \tag{123}$$

Proof: The lhs is by definition greater than or equal than the rhs.

For the opposite inequality we make use of the ''restricted concavity'' given in proposition 5.2. For the rotations U_g applied with equal probabilities to the ensemble $(\mathcal{E},p)$, we get

$$M\left(\bigcup_g U_g \mathcal{E} U_g^\dagger, \frac{1}{|G|}\sum_g p^g, R\right) \geqslant \frac{1}{|G|} M(U_g \mathcal{E} U_g^\dagger, p^g, R) = M(\mathcal{E},p,R). \tag{124}$$

Note that $(1/|G|)\,\Sigma_g p^g \in \mathbf{P}^G$ and, since the state set is G invariant, we have $\cup_g U_g \mathcal{E} U_g^\dagger = \mathcal{E}$, which proves our claim. □

If G acts *transitively*, this leads to a dramatic simplification of the formula for the AVS trade-off curve (Theorem 6.1): in this case the only G-invariant distribution is the uniform distribution, so from Theorem 6.1 we obtain the following.

Corollary 9.2: For an AVS $(\mathcal{E},\mathbf{P})$ *with transitive group action under which* $\mathbf{P}$ *is stable, (e.g., for* $\mathbf{P}=\mathcal{P}_\mathcal{E}$*), we have*

$$Q^*(R,\mathbf{P}) = M(\mathcal{E},u,R),$$

where u is the uniform distribution on $\mathcal{E}$. □

The particular example of $\mathcal{E}$ being the set of all pure states on $\mathcal{H}$ and $\mathbf{P}$ being the set of all distributions on $\mathcal{E}$ is arguably the setting for *the* trade-off between classical and quantum bits: the trade-off coding becomes a statement solely about states, with no mention of prior probabilities. Of course we have not yet justified the application of our results to infinite state sets. The corresponding but more involved treatment of the coding bounds will be given in Sec. X.

Given this generalization to infinite state sets, we conclude that the *absolute trade-off* for pure states on $\mathcal{H}$ is given by $M(\mathcal{P}(\mathcal{H}),u)$, with the uniform (i.e., unitarily invariant) measure u on the set $\mathcal{P}(\mathcal{H})$ of all pure states. The Devetak-Berger curve introduced earlier corresponds to the case $\mathcal{H}=\mathbb{C}^2$.

Remark: From the proof of Theorem 9.1, we see that we may always restrict the classical encodings $p(\cdot|\cdot)$ to be group covariant as well, in the sense that, for each $j \in \mathcal{J}$, the distribution $q(\cdot|j)$ has the property that for each $g \in G$ there exists a j' satisfying $q_{j'} = q_j$ and $q(gi|j) = q(i|j')$ for all $i \in \mathcal{I}$:

Define a new encoding p' by letting

$$p'(j,g|gi) := \frac{1}{|G|} p(j|i). \tag{125}$$

For a G-invariant distribution p on the ensemble states this does not change the values of $S(A:C)$ and $S(A:B|C)$. However, the resulting probabilities $q'_{j,g} = q_j$ and $q'(gi|j,g) = p_i p(j|i)/q'_{j,g}$ have a useful property: there is a group action of G on the indices (j,g) under which the distribution q' is invariant, and the set of conditional distributions $q'(\cdot|j,g)$ is stable. More precisely, h acts on (j,g) by $h\cdot(j,g) = (j,hg)$. Obviously, q' is invariant under this, and

$$q'(gi|h\cdot(j,g)) = q'(gi|j,hg) = q'(h^{-1}hgi|j,gh), \tag{126}$$

saying that $q'(\cdot|h\cdot(j,g)) = (q'(\cdot|j,hg))^h$.

Hence, when discussing optimal codings given by q_j and $q(\cdot|j)$ such that $\Sigma_j q_j q(\cdot|j) = p$, we may always assume that G also acts on the set of j's, and that

$$\forall j \forall g \quad q_{gj} = q_j \text{ and } q(\cdot|gj) = (q(\cdot|j))^g. \tag{127}$$

□

We close this section by giving a bound on the size of the classical register for a finite ensemble with symmetry, which sometimes improves our earlier result in Proposition 3.4:

Proposition 9.3: Let the group G act on the ensemble $\mathcal{E}=\{\varphi_i, p_i\}_{i\in\mathcal{I}}$ in the way described at the beginning of this section, and assume that p is G-invariant. If the group action partitions $\mathcal{I}$ into t G-orbits, then for every R there exists a classical encoding $p(\cdot|\cdot):\mathcal{I}\to\mathcal{J}$ which is covariant in the above sense, and satisfies

$$|\mathcal{J}| \leq |G|(t+1), \quad S(A:C) \leq R, \quad S(A:B|C) = M(\mathcal{E},R).$$

In fact, $\mathcal{J}$ partitions into $t+1$ G-orbits, in the sense described above.

The proof is given in the Appendix, Sec. 6

Example: Let $\mathcal{E}$ consist of any two states: $\mathcal{E}=\{|\varphi_i\rangle\}_{i=1}^2$. By choosing a reflection that swaps $|\varphi_1\rangle$ and $|\varphi_2\rangle$, we get a transitive $\mathbb{Z}_2$ action on the indices i. Therefore, for the AVS $(\mathcal{E},\mathcal{P}_\mathcal{E})$, we have $Q^*(R,\mathbf{P})=M(\mathcal{E},u,R)$, where u is the uniform distribution $p_i=\frac{1}{2}$. This distribution is clearly G-invariant, so Proposition 9.3 ensures that there is an optimal encoding for which $\mathcal{J}$ partitions into at most $t+1=2$ orbits, each of size either 1 or 2. □

Example: For states in the BB84 ensemble $\mathcal{E}_{BB}(\theta)$, the group $\mathbb{Z}_2\times\mathbb{Z}_2$ acts transitively via reflection along the $\theta/2$ axis and rotation by $\pi/2$. Therefore, once again, the unrestricted AVS can be reduced to the uniform ensemble, for which the optimal encoding can be assumed G-covariant, with $\mathcal{J}$ partitioning into at most two orbits of length 1, 2 or 4. □

X. INFINITE SOURCE ENSEMBLES

It should be noted that, even in the technical parts of our proofs, and, indeed, in the very statements of the *coding theorems*, we assumed that the sets of states under consideration were *finite*.

As there are interesting examples of ensembles with infinite state sets, including perhaps most notably the whole manifold of pure states in a Hilbert space, we show here how a certain approximation technique (used in Ref. 25 to deal with coding for nonstationary quantum channels) can be used to transfer our main results quite directly. The procedure, unfortunately, is not entirely painless; we have to go through the proof of Proposition 4.1 again with a modified and more technical version of the typical subspace. That is why we have chosen to treat the infinite source case separately, confining the details to this section.

A. Formulation of information quantities and the lower bound

To be able to consider infinite ensembles and encodings, we have to reformulate our notions from Secs. II and III in terms of general measure spaces (for the background and terminology see any textbooks on probability, such as Ref. 35, and measure theory[34]):

The source ensemble $\mathcal{E}$ is described by a measure space Ω (with probability measure P), and a measurable map $\varphi:\Omega\to\mathcal{P}(\mathcal{H})\subset\mathcal{S}(\mathcal{H})$ from Ω into the set of pure states on the Hilbert space $\mathcal{H}$ (which is still of finite dimension d), mapping $\omega\in\Omega$ to $|\varphi_\omega\rangle\langle\varphi_\omega|$. We can then easily define encoding and decoding (E,D) for blocks of length n:

$$E:\Omega^n\to\mathcal{S}(\mathcal{H}_B)\times\Omega_C, \tag{128}$$

$$D:\mathcal{B}(\mathcal{H}_B)\otimes\mathcal{B}(\ell^2(\Omega_C))\to\mathcal{B}_d^{\otimes n}, \tag{129}$$

where E is a Markov kernel, Ω_C is a *finite set*, and D is CPTP. The quantification of classical and quantum resources we adopt unchanged, and the fidelity condition reads as follows: the combined encoding and decoding gives rise to a Markov kernel

$$D\circ E:\Omega^n\to\mathcal{B}_d^{\otimes n}, \tag{130}$$

and, using the abbreviation

$$(D\circ E)(\omega_1\cdots\omega_n)=\int_{\mathcal{B}(\mathcal{H}_B)}(D\circ E)(\mathrm{d}\sigma|\omega_1\cdots\omega_n)\sigma, \tag{131}$$

we require that

$$F=\int_{\Omega^n}P^{\otimes n}(\mathrm{d}\omega_1\cdots\omega_n)F(\varphi_{\omega_1\cdots\omega_n},(D\circ E)(\omega_1\cdots\omega_n))\geqslant 1-\epsilon. \tag{132}$$

Let us denote by μ the measure induced by P and this Markov kernel on $\Omega\times\mathcal{S}(\mathcal{H}_B)\times\Omega_C$:

$$\mu(F_A\times G_{BC}):=\int_{F_A}P(\mathrm{d}\omega)E(G_{BC}|\omega). \tag{133}$$

We denote its restrictions (marginals) to factors $\Omega_A=\Omega$, $\mathcal{S}(\mathcal{H}_B)$, Ω_C by $P=\mu_A$, μ_B, $q:=\mu_C$, respectively, and analogously μ_{AC}, etc.

With the help of Radon–Nikodym derivatives we can always construct the Bayesian ''inverse'' Markov kernel

$$q:\Omega_C\to\Omega_A\times\mathcal{S}(\mathcal{H}_B) \tag{134}$$

that gives rise to the same joint distribution:

$$\int_{G_C}\mu_C(\mathrm{d}j)q(F_{AB}|j)=\mu(F_{AB}\times G_C). \tag{135}$$

In fact, μ_C-almost everywhere,

$$q(F_{AB}|j)=\frac{\mathrm{d}\mu(F_{AB}\times\{j\})}{\mathrm{d}\mu_C(j)}. \tag{136}$$

To follow the procedure of Sec. III we have to define the relevant information quantities (for their properties, see Refs. 36 and 37):

First, $S(A:C)$ can be expressed as $D(\mu_{AC}\|\mu_A\otimes\mu_C)$, in terms of the relative entropy (or Kullback–Leibler divergence) of two measures

$$D(\mu\|\lambda):=\int\mu(\mathrm{d}x)\log\left(\frac{\mathrm{d}\mu(x)}{\mathrm{d}\lambda(x)}\right), \tag{137}$$

where $\mathrm{d}\mu(x)/\mathrm{d}\lambda(x)$ denotes the Radon–Nikodym derivative. If this does not exist μ-almost everywhere, we define $D(\mu\|\lambda)=\infty$. It is a fact that in Eq. (137) the Radon–Nikodym derivative always exists, and it can be checked that in the finite case the new definition coincides with the old.

Second, $S(A:B|C)=\int_{\Omega_C}q(\mathrm{d}j)S(A:B|C=j)$, with $S(A:B|C=j)$ denoting the quantum mutual information associated to the conditional probability measure $q(\cdot\,|j)$ on $\Omega_A\times\mathcal{S}(\mathcal{H}_B)$: for any such distribution λ, with first marginal λ_A and Markov kernel $L:\Omega_A\to\mathcal{S}(\mathcal{H})$,

$$S_\lambda(A:B)=S\left(\int_{\mathcal{S}(\mathcal{H})}\lambda_B(\mathrm{d}\sigma)\sigma\right)-\int_{\Omega_A}\lambda_A(\mathrm{d}\omega)S\left(\int_{\mathcal{S}(\mathcal{H})}L(\mathrm{d}\sigma|\omega)\sigma\right). \tag{138}$$

Again, it is possible to check that for discrete probability spaces we obtain the same expressions as before.

The proofs of Lemmas 3.1 and 3.2 and of Theorem 3.5 are directly adapted to this language, essentially replacing all sums representing probability averages by integrals. (Note that even the "continuity in ϵ" part in the latter applies as the functions f and g depend only on ϵ and d.) This is possible since the monotonicity and convexity properties we used are still true in the infinite setting.

At the end of the proof we arrive at encodings mapping $\omega\in\Omega$ to $|\varphi_\omega\rangle\langle\varphi_\omega|\otimes\Sigma_j p(j|\omega)|j\rangle\times\langle j|$ (i.e., the corresponding Markov kernel maps i to the point mass at $|\varphi_\omega\rangle\langle\varphi_\omega|$ times a discrete measure on Ω_C). Such encodings we denote "$p:\Omega_A\to\Omega_C$," and we get

$$Q^*(R)\geqslant \inf_{p:\Omega_A\to\Omega_C,|\Omega_C|<\infty}\{S(A:B|C):S(A:C)\leqslant R\}. \tag{139}$$

Dropping the finiteness of Ω_C can only decrease the lower bound, and we arrive at the following general version of Theorem 3.5:

Theorem 10.1: *For the ensemble* $\mathcal{E}=(\Omega,P,\varphi)$,

$$Q^*(R)\geqslant M(\mathcal{E},R):=\inf_{p:\Omega_A\to\Omega_C}\{S(A:B|C):S(A:C)\leqslant R\},$$

with

$$S(A:C)=D(\mu\|P\otimes q),$$

$$S(A:B|C)=\int_{\Omega_C}q(\mathrm{d}j)S\left(\int_{\Omega_A}q(\mathrm{d}\omega|j)|\varphi_\omega\rangle\langle\varphi_\omega|\right),$$

where μ *is the measure on* $\Omega_A\times\Omega_C$ *induced by* P *and the Markov kernel* $p(\cdot|\cdot)$, q *is its marginal on* Ω_C *and* $q(\cdot|\cdot)$ *is the Bayesian Markov kernel* $\Omega_C\to\Omega_A$. □

B. Adaptation of the coding theorem

The obstacles to an application of our coding scheme, Proposition 4.1, are the potentially infinite range of the source register (Ω) and the classical encoding (Ω_C). Of course, when in the previous subsection we allowed the latter to be infinite, we only made M smaller, and at that point it was not clear that this was a good move.

The purpose of the present subsection is to show that it is possible to approximate the effect of an infinite encoding by a strictly finite one: finitely many possible states on $\mathcal{H}$ and finitely many classical symbols. This will inevitably introduce some error, which we will have to counter by a suitably adapted notion of typical subspace.

Lemma 10.2: For $\epsilon>0$ *there exists a partition of* $\mathcal{S}(\mathcal{H})$ *into* $m\leqslant C(d)\epsilon^{-d^2}$ *Borel sets each of which has radius at most* ϵ*: in each part* $\mathcal{S}_i$ *there exists a state* σ_i *such that for all* $\rho\in\mathcal{S}_i$, $\|\rho-\sigma_i\|_1\leqslant\epsilon$. *The constant* $C(d)$ *depends only on* d.

Proof: The set of states on $\mathcal{H}$ is affinely isomorphic to the set of positive complex $d\times d$-matrices with trace 1, which is contained in the set of self-adjoint complex matrices with all d^2 real and imaginary parts of entries in the interval $[-1,1]$: this is a d^2-dimensional hypercube. This can be partitioned into $(2\sqrt{2}d^3)^{d^2}\epsilon^{-d^2}$ many small hypercubes of edge length $\epsilon/(d^3\sqrt{2})$. It is easy to check that for any ρ,σ in the same small cube, $\|\rho-\sigma\|_1\leqslant\epsilon$. □

For a source (Ω,P,φ) such a partition entails a partition $\mathcal{Z}$ of Ω into at most m measurable pieces Z_i, with $\omega_i\in Z_i$ such that $|\varphi_{\omega_i}\rangle\langle\varphi_{\omega_i}|=\sigma_i$. (We need only consider pieces that intersect the image of φ.) A central role will be played by the "contraction" of the infinite ensemble $\mathcal{E}$ to the finite ensemble $\mathcal{E}'=\{\varphi_{\omega_i},\hat{P}(i)=P(Z_i)\}$ which is obtained by identifying all of Z_t to the single state φ_{ω_i}.

We have already defined the set of $\hat{P}$-typical sequences $\mathcal{T}_{\hat{P},\delta}$, and now can define the following typical set for P:

$$\mathcal{T}^{\mathcal{Z}}_{P,\delta} := \bigcup_{I \in \mathcal{T}_{P,\delta}} Z_{i_1} \times \cdots \times Z_{i_n}. \tag{140}$$

It obviously inherits the large probability property of $\mathcal{T}_{p',\delta}$:

$$P^{\otimes n}(\mathcal{T}^{\mathcal{Z}}_{P,\delta}) \geq 1 - \frac{1}{\delta^2}. \tag{141}$$

Before we can describe the coding scheme we have to introduce a variant of the conditional typical sequences and subspaces: for a channel $W:\mathcal{I} \to \mathcal{J}$ and $\delta, \epsilon > 0$ define

$$\mathcal{T}^{(\epsilon)}_{W,\delta}(I) := \{J : \forall ij \, |N(ij|IJ) - N(i|I)W(j|i)| \leq \delta\sqrt{N(i|I)} + \epsilon N(i|I)\}. \tag{142}$$

(Our previous notion is recovered with $\epsilon = 0$, and in the sequel ϵ will be small, compared to δ which we shall choose large.) Observe that this is a union of conditional type classes. Using Eq. (78) it is quite easy to show that

$$\begin{aligned} |\mathcal{T}^{(\epsilon)}_{W,\delta}(I)| &\leq (n+1)^{|\mathcal{I}||\mathcal{J}|} \exp\left(nH(W|P_I) + \sum_i N(i|I)|\mathcal{J}|\, \eta(\epsilon + \delta N(i|I)^{-1/2}) \right) \\ &\leq (n+1)^{|\mathcal{I}||\mathcal{J}|} \exp(nH(W|P_I) + n|\mathcal{J}|\, \eta(\epsilon) + n\, \eta(\delta|\mathcal{I}|/\sqrt{n})), \end{aligned} \tag{143}$$

where we have used the inequality $\eta(x+y) \leq \eta(x) + \eta(y)$ and concavity of η.

Similarly, for a collection of states W_i, which we endow with fixed diagonalizations $W_i = \sum_{j=1}^{d} W(j|i)|e_{j|i}\rangle\langle e_{j|i}|$, we can define the projector

$$\Pi^{(\epsilon)}_{W,\delta}(I) := \sum_{J \in \mathcal{T}^{(\epsilon)}_{W,\delta}(I)} |e_{J|I}\rangle\langle e_{J|I}|, \tag{144}$$

and get from Eq. (143) the estimate

$$\mathrm{Tr}\Pi^{(\epsilon)}_{W,\delta}(I) \leq (n+1)^{d|\mathcal{I}|} \exp(nH(W|P_I) + nd\, \eta(\epsilon) + n\, \eta(\delta|\mathcal{I}|/\sqrt{n})). \tag{145}$$

Its other most important property that we shall use is the following: consider a product state $\sigma = \sigma_1 \otimes \cdots \otimes \sigma_n$ such that, with some $I = i_1 \cdots i_n$,

$$\forall i \quad \left\| \frac{1}{N(i|I)} \sum_{k: i_k = i} \sigma_k - W_i \right\|_1 \leq \epsilon. \tag{146}$$

Then we claim that

$$\mathrm{Tr}(\sigma \Pi^{(\epsilon)}_{W,\delta}(I)) \geq 1 - \frac{|\mathcal{I}|}{\delta^2}. \tag{147}$$

The proof goes as follows: the left hand side above does not change if we replace σ_k by $\sigma'_k := \sum_j |e_{j|i_k}\rangle\langle e_{j|i_k}|\sigma_k|e_{j|i_k}\rangle\langle e_{j|i_k}|$, because the projector is a sum of one-dimensional projectors $|e_{J|I}\rangle\langle e_{J|I}|$. Thus we may assume that σ_k has diagonal form in the chosen eigenbasis of W_{i_k}: $\sigma_k = \sum_j S_k(j)|e_{j|i_k}\rangle\langle e_{j|i_k}|$.

Note that the left hand side of Eq. (147) can be rewritten as $(S_1 \otimes \cdots \otimes S_n)(\mathcal{T}^{(\epsilon)}_{W,\delta}(I))$, a classical probability. Now it is immediate from the definition of the latter set [Eq. (142)] and from the condition (146) on σ that

$$\mathcal{T}^{(\epsilon)}_{W,\delta}(I) \supset \mathcal{T}_{S,\delta}(I), \tag{148}$$

with the channel $\overline{S}(j|i)=[1/N(i|I)]\,\Sigma_{k:i_k=i}S_k(j)$. Hence

$$(S_1\otimes\cdots\otimes S_n)(\mathcal{T}^{(\epsilon)}_{W,\delta}(I))\geqslant(S_1\otimes\cdots\otimes S_n)(\mathcal{T}^{-}_{S,\delta}(I))\geqslant\left(1-\frac{1}{\delta^2}\right)^{|\mathcal{I}|}\geqslant 1-\frac{|\mathcal{I}|}{\delta^2}, \tag{149}$$

the second line by Chebyshev's inequality.

After these preparations we are ready to prove the infinite source version of Proposition 4.1:

Proposition 10.3: Let $\mathcal{E}=(\Omega_a,P,\varphi)$ be a source. For a probability distribution P on Ω and a Markov kernel $p(\cdot|\cdot):\Omega_A\to\Omega_C$, $\epsilon>0$, there exists a partition $\mathcal{Z}$ of Ω_A into $m-1<C(d)\epsilon^{-d^2}$ measurable sets, corresponding to an ϵ-fine partition of the state space, and for $\delta>0$ a visible code (E,D) such that

$$\forall\,\omega=(\omega_1\cdots\omega_n)\in\mathcal{T}^{\mathcal{Z}}_{P,\delta}\quad F(|\varphi_\omega\rangle\langle\varphi_\omega|,(D\circ E)(\omega))\geqslant 1-\frac{4m^2}{\delta^2}.$$

and sending

$$nS(A:C)+nKm^2\eta(\delta/\sqrt{n})+K'm^2\log(n+1)\quad \textit{classical bits},$$

$$nS(A:B|C)+n(3dm^2\eta(2\delta m^2/\sqrt{n})+3d\eta(\epsilon))+dm\log(n+1)\quad \textit{quantum bits}.$$

Proof: We can find the partition by Lemma 10.2 and the discussion thereafter.

Consider now the (measurable) coarse-graining map

$$T:\omega\mapsto i\in\{1,\ldots,m-1\}\text{for}\ \ \omega\in Z_i\,. \tag{150}$$

Applying T to Ω_A [and the identity map to $\mathcal{B}(\mathcal{H}_B)$ and Ω_C] leads to a new distribution μ' on $\Omega_{A'}\times\mathcal{B}(\mathcal{H}_B)\times\Omega_C$, with $\Omega_{A'}=\{1,\ldots,m-1\}$. By the data-processing inequality[23,37] we have

$$S(A':C)\leqslant S(A:C)\ \text{ and }\ S(A':B|C)\leqslant S(A:B|C). \tag{151}$$

Next we change the quantum part of the encoding by collecting all the weight of a piece Z_i into $\varphi_i:=\varphi_{\omega_i}$: we can do this by a similar coarse-graining map

$$\tilde{T}:\sigma\mapsto|\varphi_i\rangle\langle\varphi_i|\ \text{ for }\ \sigma\in Z_i\,. \tag{152}$$

The resulting distribution will be denoted by μ'': it is supported on a finite set $\Omega_{A'}$ and a finite set of states φ_i (in fact, the "contracted" ensemble $\mathcal{E}'$ of the discussion after Lemma 10.2). It is generated by a Markov kernel $\hat{p}:\Omega_{A'}\to\Omega_C$, which in this case is simply a finite collection of (conditional) distributions $\hat{p}(\cdot|i)$ on Ω_C. Note that this is a valid encoding in the sense of the definition of $M(\mathcal{E}',R)$, in the main section. Let us denote the corresponding conditional quantum mutual information by $S(A':B'|C)$.

By definition of $S(A':B|C)$ and the partition $\mathcal{Z}$, we have

$$S(A':B'|C)\leqslant S(A':B|C)+2d\eta(\epsilon/d), \tag{153}$$

using Fannes' inequality (52) twice.

To end this step-by-step discretization, we may change the encoding to a stochastic matrix $p':\Omega_{A'}\to\{1,\ldots,m\}=:\Omega_{C'}$, by the considerations of Sec. III (see also Proposition 9.3), such that

$$S(A':B'|C')\leqslant S(A':B'|C)\ \text{ and }\ S(A':C')=S(A':C). \tag{154}$$

So, finally, we are in a position to apply the coding method of Proposition 4.1, with the sole difference that we use for the quantum encoding the projector $\Pi^{(\epsilon)}_{p',\delta}(I)$ instead of our previous conditional typical projector, and I is such that $\omega_1\cdots\omega_n\in Z_I$.

The fidelity estimate is obtained just like there, only using Eq. (147). The classical rate estimate we copy from Proposition 4.1, and for the quantum rate estimate, we follow its derivation in the proof, using Eq. (145) to estimate the range of the projectors $\Pi^{(\epsilon)}_{p',\delta}(I)$: we have to send

$$nS(A':B'|C')+n(3dm^2\eta(2\delta m^2/\sqrt{n})+d\eta(\epsilon))+dm\log(n+1) \tag{155}$$

quantum bits, which, by Eqs. (151)–(154), yields our desired estimate. □

This immediately leads to the result that we wanted:

Theorem 10.4: *For any ensemble* $\mathcal{E}=(\Omega,P,\varphi)$,

$$Q^*(R)=M(\mathcal{E},R).$$

Proof: That $M(\mathcal{E},R)$ is a lower bound to Q^* is proved by Theorem 10.1. For its achievability choose $\epsilon>0$ and a Markov kernel p such that both $S(A:C)\leqslant R$ and $S(A:B|C)\leqslant M(\mathcal{E},R)+\epsilon$.

Choose now a partition $\mathcal{Z}$ according to Proposition 10.3, fixing m. Now choose δ large enough, so that according to that proposition a code exists which has fidelity $1-\epsilon$ on a state set of probability $1-\epsilon$, i.e., it has average fidelity $1-2\epsilon$ on the ensemble. By the proposition it has cbit rate $S(A:C)+o(1)$ and qubit rate

$$S(A:B|C)+2\eta(\epsilon)+o(1)\leqslant M(\mathcal{E},R)+2\eta(\epsilon)+\epsilon+o(1), \tag{156}$$

as $n\to\infty$. As ϵ was arbitrary, our claim is proved. □

C. On the AVS in the infinite setting

With the help of the above Proposition 10.3 the case of an arbitarily varying source of an *infinite* ensemble is dealt with easily, in much the same way as we did in the finite case (see Sec. VI):

Formally, of course, an arbitrarily varying source is a triple $(\Omega,\mathbf{P},\varphi)$, where Ω and φ are a measurable space and a measurable map into states, as before, and $\mathbf{P}$ is a set of probability distributions on Ω.

With the definitions of encoding and decoding from Sec. X A we require

$$\forall P^n\in\mathbf{P}^n\int_{\Omega^n}P^{\otimes n}(\mathrm{d}\omega_1\cdots\omega_n)F(|\varphi_\omega\rangle\langle\varphi_\omega|,(D\circ E)(\omega))\geqslant 1-\epsilon. \tag{157}$$

Denoting the trade-off function as $Q^*(R,\mathbf{P})$, we obtain the expected result:

Theorem 10.5: $Q^*(R,\mathbf{P})=M(\mathbf{P},R)$, *with*

$$M(\mathbf{P},R)=\sup_{P\in\mathbf{Q}}M(P,R),$$

where $\mathbf{Q}=\mathrm{conv}(\mathbf{P})$ *is the convex hull of* $\mathbf{P}$.

Proof: The inequality "$\geqslant$" is obvious, like in the finite case: the adversary can certainly always mock up an i.i.d. source $P\in\mathbf{Q}$, hence Theorem 10.1 applies.

For the opposite inequality, we start by choosing an $\epsilon>0$ and a partition $\mathcal{Z}$ according to Proposition 10.3. Every distribution P in $\mathbf{P}$ gives rise to a distribution $\hat{P}\in\mathcal{P}_{m-1}$, and we denote

$$\hat{\mathbf{P}}:=\{\hat{P}:P\in\mathbf{P}\}. \tag{158}$$

Note that, because the map $P\mapsto\hat{P}$ is affine linear, we get $\hat{\mathbf{Q}}=\mathrm{conv}(\hat{\mathbf{P}})$.

Now for $\delta>0$ we introduce again the set

$$\mathcal{T}:=\bigcup_{\hat{P}\in\hat{\mathbf{Q}}}\mathcal{T}_{\hat{P},\delta}, \tag{159}$$

and it is easy to see [compare Eq. (141)] that

$$\mathcal{T}^{\mathcal{Z}} := \bigcup_{I \in \mathcal{T}} Z_{i_1} \times \cdots \times Z_{i_n} \tag{160}$$

carries $1-\delta^{-2}$ of the probability of every $P^n \in \mathbf{P}^n$. On the other hand, because $\mathcal{T}$ is a union of type classes, we can find "few" $\hat{P}_1, \ldots, \hat{P}_T$, $T \leqslant (n+1)^m$ such that the corresponding $\mathcal{T}_{\hat{P}_t,\delta}$ cover $\mathcal{T}$. The coding is very simple: on seeing a state $\varphi_{\omega_1 \ldots \omega_n}$ the encoder finds the index I of the piece Z_I in the partition $\mathcal{Z}^n$ such that $\omega_1 \cdots \omega_n \in Z_I$, and the type of I. If $I \in \mathcal{T}$, he looks up t such that $I \in \mathcal{T}_{\hat{P}_t,\delta}$ and uses the coding scheme of Proposition 10.3 for $\hat{P}_t$. (Note that he needs not even send the type of I as that is part of the protocol of Proposition 10.3.) Choosing δ large enough this recipe gives a code with high fidelity for every $P^n \in \mathbf{P}^n$; by construction and Proposition 10.3, it has rates of $R+o(1)$ cbits and $M(\mathbf{P},R)+f(\epsilon)+o(1)$ qubits, with a function $f(\epsilon)$ that tends to 0 as $\epsilon \to 0$. □

To end this discussion, we would like to point out that a similar treatment of remote state preparation can be done: in fact, as we discussed in Sec. VIII, we always use the "1 ebit $+1$ cbit per qubit" technique (Theorem 8.1) on top of an efficient trade-off coding. To do this for an infinite ensemble one only has to understand that the bound of Theorem 8.1 is strong enough to allow approximation of the set of projected (compressed) product states $\varphi_{\omega_1} \otimes \cdots \otimes \varphi_{\omega_n}$, at negligible additional classical cost.

XI. DISCUSSION AND CONCLUSIONS

Our main result is a simple formula for the trade-off between quantum and classical resources in visible compression. The formula expresses the trade-off curve $Q^*(R)$ in terms of a single-letter optimization over conditional probability distributions of bounded size. This unexpectedly simple resolution places optimal trade-off coding into a small but growing class of problems in quantum information theory whose answers are not only known in principle but can be calculated in practice. (Another notable recent addition is the entanglement-assisted capacity of a quantum channel.[22])

At a conceptual level, for any given ensemble $\mathcal{E}$ of quantum states, $Q^*(R)$ can be thought of as a quantitative description of how "classical" the ensemble is. Any deviation from classicality is captured in the trade-off curve in the form of inefficiency of the classical storage. The amount of information that can be extracted from many copies of $\mathcal{E}$ while causing negligible disturbance, for example, can be read directly off the curve by identifying the point at which classical resources begin to become inefficient as compared to quantum. Much more subtle indicators of classicality are also available in $Q^*(R)$, however. We saw, for instance, that for the parametrized BB84 ensemble, $Q^*(R)$ had a kink at the point corresponding to partitioning the ensemble into nearly orthogonal subensembles.

Going beyond the compression of ensembles, we saw that it is possible to formulate a version of our main result in the setting of arbitrarily varying sources, corresponding to the situation in which the encoder and decoder have only partial or even no knowledge of the distribution of input states. Despite this handicap, compression is frequently still possible and we once again find that the trade-off curve can be calculated via a tractable optimization problem. For ensembles with symmetry, the problem can even often be reduced to calculating $Q^*(R)$ for one particular ensemble. Thus, for any given set of pure states, including the whole manifold of states on a given Hilbert space, these tools allow us to calculate the rate of exchange from qubit storage to classical storage. The answer is given, of course, not in terms of a single number but as the trade-off curve. (Like in any market, the going rate depends on supply.)

Our view that $Q^*(R)$ encodes the balance of quantum and classical information in a given ensemble or set of states is further bolstered by the role it was found to play in optimal remote state preparation. In this context, the minimal amount of classical communication required for any given rate of entanglement consumption can, once again, be read directly off the quantum-

classical trade-off curve. That the comparatively exotic process of remote state preparation should reduce, via Theorem 8.1, to visible compression is a tremendous simplification.

Of course, while we have seen that the results of this article resolve some basic questions about trading different types of resources in quantum information, most related questions remain open. To begin, it is possible to trade entanglement, quantum communication and classical communication all together in a generalized type of remote state preparation. Since our results here describe the two extremes when first entanglement and then quantum communication are not permitted, it seems likely that similar techniques could resolve the full trade-off surface. More ambitiously, one could define channel capacities for noisy quantum channels that interpolate between the fully quantum and classical capacities by studying the usefulness of a channel for simultaneously sending quantum and classical information. The problem analogous to the trade-off question studied here would be to determine the achievable *region* of quantum-classical rate pairs. Unfortunately, given that neither the fully classical nor fully quantum extremes are fully understood, it may be a long time before we develop tools capable of analyzing that problem.

Therefore, to end, we offer two related open problems that are perhaps closer to the realm of the tractable. First, it would be useful to have a set of rules for extracting qualitative features of the trade-off curve, such as the location of any kinks and perhaps more detailed differentiability properties, from the structure of the input states (or ensemble). Second, it would be an interesting challenge to apply the observations of Sec. IX on symmetry to the explicit calculation of the trade-off curve for particular examples and, more generally, to find other approaches to simplifying these calculations.

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APPENDIX: PROOFS OF AUXILIARY PROPOSITIONS

1. Proof of Proposition 3.3

Proof: Suppose the classical register C decomposes into parts C_1 and C_2 with corresponding joint density operator

$$\rho^{ABC_1C_2}=\sum_i p_i|i\rangle\langle i|^A\otimes|\varphi_i\rangle\langle\varphi_i|^B\otimes\sum_{j,k} p(i|j,k)|j\rangle\langle j|^{C_1}\otimes|k\rangle\langle k|^{C_2}. \tag{A1}$$

If we define the conditional ensembles $\mathcal{E}_{jk}$ and $\mathcal{E}_j$, then

$$S(A:B|C_1C_2)=\sum_{jk} q_{jk}S(\mathcal{E}_{jk})\leqslant S(A:B|C_1)=\sum_j q_jS(\mathcal{E}_j) \tag{A2}$$

by the concavity of the von Neumann entropy.

Therefore, for any map with $S(A:C_1)<R\leqslant H(p)$, we can always adjoin a second classical register C_2 such that $S(A:C_1C_2)=R$ without increasing the conditional mutual information. □

2. Proof of Proposition 3.4

Proof: W.l.o.g. let $i\in\{1,\ldots,m\}$. The information quantities in the definition of M can be reexpressed as follows:

$$S(A:B|C)=\sum_j q_jS\left(\sum_i q(i|j)|\varphi_i\rangle\langle\varphi_i|\right), \tag{A3}$$

$$S(A:C)=H(p)-\sum_j q_j H(q(\cdot|j)), \tag{A4}$$

with $q_j=\Sigma_i p_i p(j|i)$ and $q_j q(i|j)=p_i p(j|i)$. We read q as a probability distribution on the set $\mathcal{P}_m$ of all probability distributions on $\{1,\ldots,m\}$. Thus the minimization problem in the definition of M can be expressed as finding the infimum of $\Sigma_j q_j S(f(q(\cdot|j)))$ over the set

$$\mathcal{P}(p,R)=\left\{q\text{p.d. on } \mathcal{P}_m : \sum_j q_j q(\cdot|j)=p, \sum_j q_j H(q(\cdot|j))\geqslant H(p)-R\right\},$$

where f is an affine linear function on probability distributions, mapping the distribution p to the quantum state $\Sigma_i p_i|\varphi_i\rangle\langle\varphi_i|$.

Now we argue structurally: the set $\mathcal{P}(p,R)$ is convex (as a subset of an infinite dimensional probability simplex with additional linear inequality constraints), and the aim function is linear. Hence the infimum is an infimum over the extreme points of $\mathcal{P}(p,R)$, which are, by Caratheodory's theorem, distributions q with support at most $m+1$, the number of inequalities that define $\mathcal{P}(p,R)\subset\mathcal{P}(\mathcal{P}_m)$ (see, e.g., Ref. 38). In Sec. IX, Proposition 9.3 and Appendix, Sec. 6, we provide a detailed exposition of a more general form of this result. □

3. Proof of Proposition 5.1

Proof: The "$\leqslant$" inequality follows directly by forming the tensor product of two encodings for $\mathcal{E}_1$ and $\mathcal{E}_2$ with classical rates R_1 and R_2 respectively.

The "$\geqslant$" inequality is shown by choosing an encoding for the tensor product with classical rate R and then using the chain rule several times for subdivisions $A=A_1A_2$ and $B=B_1B_2$ as follows. First observe that

$$R\geqslant S(A_1A_2:C)=S(A_1:C)+S(A_2:C|A_1)=:R_1+R_2 \tag{A5}$$

and then

$$\begin{aligned}
S(A_1A_2:B_1B_2|C)&=S(A_1:B_1B_2|C)+S(A_2:B_1B_2|C,A_1)\\
&\geqslant S(A_1:B_1|C)+S(A_2:B_2|C,A_1)\\
&\geqslant M(\mathcal{E}_1,R_1)+\inf\{S(A_2:B_2|C,A_1):S(A_2:C|A_1)\leqslant R_2\}\\
&\geqslant M(\mathcal{E}_1,R_1)+M(\mathcal{E}_2,R_2)\\
&\geqslant \min\{M(\mathcal{E}_1,R_1)+M(\mathcal{E}_2,R_2):R_1+R_2=R\}.
\end{aligned} \tag{A6}$$

The second last line is seen as follows: in the line above it, the two mutual informations are conditional on A_1, so they both can be written as averages over the values of A_1. Hence the inequality follows by the convexity of M in R. □

4. Proof of Proposition 5.2

Proof: It is sufficient to verify that any encoding operator

$$\rho^{ABC}=\sum_{ik} p_i a_k |i\rangle\langle i|^A\otimes|k\rangle\langle k|^A\otimes U_k|\varphi_i\rangle\langle\varphi_i|U_k^{\dagger B}\otimes\sum_j p(j|i,k)|j\rangle\langle j|^C \tag{A7}$$

for $\mathcal{F}$ gives rise to a valid encoding operator

$$\sigma^{ABC}=\sum_i p_i|i\rangle\langle i|^A\otimes|\varphi_i\rangle\langle\varphi_i|^B\otimes\sum_{jk} p(j|i,k)a_k|j\rangle\langle j|^C\otimes|k\rangle\langle k|^C \tag{A8}$$

for $\mathcal{E}$ satisfying $S_\sigma(A:B|C) \leqslant S_\rho(A:B|C)$ and $S_\sigma(A:C) \leqslant S_\rho(A:C)$. □

5. Proof of Proposition 7.2

Proof: We will first prove the proposition for irreducible $\mathcal{E}$. Using a trick introduced by Holevo,[14] we can reduce the problem further to the case of a two-state ensemble: for an ensemble $\{\rho_i^B \otimes \sigma_i^C, p_i\}$ of states (we assume that all $p_i > 0$) and two specific indices k and l, define a new index

$$j(i) := \begin{cases} i & i \neq k,l, \\ * & i \in \{k,l\}. \end{cases} \tag{A9}$$

(Of course, in the case we have in mind, the ρ_i are the pure states from the ensemble $\mathcal{E}$, and the σ_i are commuting mixed states representing the classical information.) Then consider the multipartite state

$$\Omega = \sum_i p_i |i\rangle\langle i|^{A_1} \otimes |j(i)\rangle\langle j(i)|^{A_2} \otimes \rho_i^B \otimes \sigma_i^C.$$

The definition of $j(i)$ and the familiar chain rule imply

$$S(A_1:BC) = S(A_1A_2:BC) = S(A_2:BC) + S(A_1:BC|A_2). \tag{A10}$$

Note that the second term is an average over the values of $j(i)$ of Holevo quantities for the corresponding reduced ensembles. Therefore, it has only one nonzero contribution, which is

$$S(A_1:BC|A_2) = (p_k + p_l)\chi(\{\rho_i \otimes \sigma_i, p_i/(p_k+p_l)\}_{i=k,l}). \tag{A11}$$

Then, using Eq. (A10) and monotonicity of χ under partial trace repeatedly,

$$\begin{aligned} \chi(\{p_i, \rho_i \otimes \sigma_i\}) = S(A_1:BC) &= S(A_2:BC) + S(A_1:BC|A_2) \\ &\geqslant S(A_2:B) + (p_k+p_l)\chi(\{\rho_i \otimes \sigma_i, p_i/(p_k+p_l)\}_{i=k,l}) \\ &\geqslant S(A_2:B) + (p_k+p_l)\chi(\{\rho_i, p_i/(p_k+p_l)\}_{i=k,l}) \\ &= S(A_2:B) + S(A_1:B|A_2) = S(A_1:B) = \chi(\{\rho_i, p_i\}). \end{aligned}$$

Assuming that the first and the last Holevo quantities have the same value, we must have equality in the third line, implying

$$\chi(\{\rho_i \otimes \sigma_i, q_i\}_{i=k,l}) = \chi(\{\rho_i, q_i\}_{i=k,l}), \tag{A12}$$

with $q_i = p_i/(p_k+p_l)$. Then, applying the general formula

$$\chi(\{\omega_i, p_i\}) = \sum_i p_i D(\omega_i \| \omega) \tag{A13}$$

to Eq. (A12), with $\omega = \Sigma_i p_i \omega_i$ and D the relative entropy function, and using the Lindblad monotonicity once more yields

$$D(\rho_k \otimes \sigma_k \| q_k \rho_k \otimes \sigma_k + q_l \rho_l \otimes \sigma_l) = D(\rho_k \| q_k \rho_k + q_l \rho_l). \tag{A14}$$

(And likewise for l.)

With this we are almost done: invoking a result of Ohya and Petz (see Ref. 37, Theorem 9.12) we conclude that there exists a CPTP map R such that

$$R(\rho_k)=\rho_k\otimes\sigma_k, \tag{A15}$$

$$R(q_k\rho_k+q_l\rho_l)=q_k\rho_k\otimes\sigma_k+q_l\rho_l\otimes\sigma_l, \tag{A16}$$

from which it follows by linearity that

$$R(\rho_l)=\rho_l\otimes\sigma_l. \tag{A17}$$

Since CPTP maps (R and Tr_C) cannot decrease fidelity we thus must have $\rho_k\perp\rho_l$ or $\sigma_k=\sigma_l$.

In the particular case that the initial ensemble is irreducible we conclude that all σ_i must be equal, or else the partial trace over C strictly decreases the Holevo quantity. If the ensemble $\mathcal{E}$ is not irreducible, a simple variation on the previous argument shows that, for each of the irreducible subensembles $\mathcal{E}_l$, $\chi(\mathcal{E}_l)$ must be equal to χ of the corresponding subensemble $\{\varphi_{il}\otimes\sigma_{il},p_{i|l}\}$ of $\mathcal{F}^{BC}$. Applying our conclusions to these subensembles finishes the proof of the proposition. □

6. Proof of Proposition 9.3

Proof: As explained earlier in the proof of Proposition 3.4, any classical encoding map can be viewed as a probability distribution q on the set $\mathcal{P}_\mathcal{I}$ of probability distributions on $\mathcal{I}$ with barycenter p: $p=\Sigma_j q_j q(\cdot|j)$.

Covariance of the encoding means invariance of q under the natural action of G on $\mathcal{P}_\mathcal{I}$, i.e., $g:p\mapsto p^g$. Hence for each distribution p in the support of q we must have all the p^g in the support as well. On the other hand, we need far fewer conditions to obey, as it will turn out:

Assume that the covariant encoding is given by the distributions

$$(q(\cdot|j))^g \text{ with probability } \frac{1}{|G|}q_j,\quad g\in G, j=1,\ldots.$$

Now choose representatives $i_1,\ldots,i_t$ of the orbits, and observe that (by G-invariance)

$$\sum_{j,g}\frac{1}{|G|}q_j(q(\cdot|j))^g=p \tag{A18}$$

if and only if

$$\forall\,\tau=1,\ldots,t\quad \sum_{j,g}\frac{1}{|G|}q_j q(g^{-1}i_\tau|j)=p(i_\tau). \tag{A19}$$

Similarly, $S(A:C)\leqslant R$ if and only if

$$\sum_j q_j H(q(\cdot|j))\geqslant H(p)-R, \tag{A20}$$

and, finally, our aim function reads

$$S(A:B|C)=\sum_{j,g}\frac{1}{|G|}q_j S\left(\sum_i q(i|j)|\varphi_{gi}\rangle\langle\varphi_{gi}|\right). \tag{A21}$$

Now consider the affine linear map from $\mathcal{P}_\mathcal{I}$ to $\mathbb{R}^{t+1}$ defined by

$$A:p\mapsto\left(H(p);\frac{1}{|G|}\sum_g p(g^{-1}i_\tau):\tau=1,\ldots,t\right). \tag{A22}$$

Note that the image of this map is in a certain t-dimensional subspace because, if $t-1$ of the conditions (A19) are satisfied, then the tth is also, automatically. Equations (A19) and (A20) are

really conditions on the q_j-weighted average of the images $A_j = A(q(\cdot|j))$, $A = \Sigma_j q_j A_j$. By Caratheodory's theorem[38] the same average can be obtained by convex combination of $t+1$ of these, i.e., by a distribution q' on the j's with support containing at most $t+1$ points. In fact, q is easily seen to be expressible as a convex combination of such small support distributions, say $q'^{(a)}$ with weights λ_a.

To conclude, we observe that our aim function in Eq. (A21) is *linear* in the distribution q: hence, it is the λ_a–weighted sum of similar such expressions with $q'^{(a)}$ in place of q. For one value of a at least this is smaller than $S(A:B|C)$, the corresponding $q'^{(a)}$ satisfies $\Sigma_j q'^{(a)} A_j = A$, and hence Eqs. (A19) and (A20). As explained in the remark preceding the statement of Proposition 9.3, to obtain a G–covariant encoding we can split up each $q(\cdot|j)$ (with j in the support of $q'^{(a)}$) into the G translated distributions $(q(\cdot|j))^g$, proving the claim. □

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Efficient discrete approximations of quantum gates

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Quantum compiling addresses the problem of approximating an arbitrary quantum gate with a string of gates drawn from a particular finite set. It has been shown that this is possible for almost all choices of base sets and, furthermore, that the number of gates required for precision ϵ is only polynomial in $\log 1/\epsilon$. Here we prove that using certain sets of base gates quantum compiling requires a string length that is linear in $\log 1/\epsilon$, a result which matches the lower bound from counting volume up to constant factor. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Quantum computation generalizes computer science to utilize novel quantum physical resources as elementary building blocks for information processing.[1–4] Quantum algorithms, like their classical analogs, can be written in a number of nearly equivalent ways. While a classical program is typically composed of a series of simple boolean functions, such as NAND and FANOUT, a quantum algorithm is typically written as a product of unitary gates, such as the Hadamard transform H, the controlled-NOT (CNOT), and the $\pi/8$-gate T.[5] For classical computers, a common problem is that of compiling a program, in which one typically wishes to express the program in as few elementary operations as possible. By analogy, we can raise the principal questions of *quantum compiling*: Which sets of gates can be composed to form what sorts of quantum algorithm, how many of them are necessary, and what efficient algorithms can be devised to express quantum programs in terms of a particular set of base gates?

Mathematically, a gate on n quantum bits (qubits) is represented by a unitary transformation on a 2^n-dimensional vector space. We will denote the set of all determinant-one unitary transformations of a d-dimensional vector space by $\mathrm{SU}(d)$. This space is a manifold and is hence parametrized by a *continuum* of real parameters; for example, the 2×2 unitary transforms

$$\begin{pmatrix} e^{i\alpha}\cos\theta & e^{i\beta}\sin\theta \\ -e^{-i\beta}\sin\theta & e^{-i\alpha}\cos\theta \end{pmatrix} \tag{1}$$

parametrized by α, β, θ represent the group SU(2) of valid single qubit gates.

In contrast, digital quantum algorithms compute with only a *finite set* of base gates (such as those mentioned previously: H, T, and CNOT). This is a reasonable restriction in real circuit implementations, since the presence of noise reduces the number of reliably distinguishable gates to a finite subset of the continuous set. Finite gate sets are also intrinsic to fault-tolerant quantum computation, the art of constructing arbitrarily reliable circuits from unreliable parts.[6–9] Thus, in general we do not desire perfect computational universality, but only the ability to approximate any quantum algorithm, preferably without using too many more gates than originally required.

A set of base gates $\mathcal{A}\subset\mathrm{SU}(d)$ is *computationally universal* if given any gate U, we can find a string consisting of gates from $\mathcal{A}$ and their inverses, such that the product of the gates in the

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string approximates U to arbitrary precision. Equivalently, $\mathcal{A}$ must generate a dense subgroup of $\mathrm{SU}(d)$.

Which sets of base gates are computationally universal? It turns out that probabilistically speaking, almost all of them are.[10,11] If base gates are chosen at random, then all but a set of measure zero are computationally universal. The idea is that if the eigenvalues of the base gates have phases that are irrationally related to π (which occurs with probability one), then taking powers of them allows each base gate to approximate a one-parameter subgroup to arbitrary precision, just as integer multiples of a random vector modulo a lattice will almost always fill space. Furthermore, the base gates will almost always lie on different one-parameter subgroups, which will generate all of $\mathrm{SU}(d)$ with probability one.

Given that compiling is generically possible, it is vital to determine *how short a string of base gates is typically required to approximate a given gate to a specified precision*; this is the question we consider in this article. The construction described by Lloyd[10] requires using a number of base gates exponential in $\log 1/\epsilon$ to achieve a precision of ϵ. This is an unreasonable cost for many applications. However, Solovay[12] and Kitaev[13] have independently described an efficient (meaning its running time is polynomial in $\log 1/\epsilon$) algorithm for quantum compiling that produces strings of length only $O(\log^c(1/\epsilon))$, where c is a constant between 3 and 4.[14] The algorithm works by constructing successively finer ϵ-nets; finite sets of gates that can approximate any element of $\mathrm{SU}(d)$ to an accuracy of ϵ.

On the other hand, as we will later discuss, since a ball of radius ϵ in $\mathrm{SU}(d)$ has volume proportional to ϵ^{d^2-1}, it takes $O((1/\epsilon)^{d^2-1})$ different strings of gates to approximate every element of $\mathrm{SU}(d)$ to a precision of ϵ. Therefore, no algorithm will ever be able to reduce c below 1. Furthermore, it is unlikely that the successive approximation method used by the Solovay–Kitaev theorem will be able to do better than $c=2$.[14] This still leaves open the question of whether some other technique could establish an upper bound asymptotically smaller than the one achieved by the Solovay–Kitaev theorem.

Here, our main result is that for at least some universal sets of base gates only $O(\log 1/\epsilon)$ gates are sufficient to approximate any gate to a precision ϵ (i.e., $c=1$). This is within a constant factor of the lower bound obtained from counting arguments. We say that these base gates are not only computationally universal, but also *efficiently universal*, since using them for quantum compiling requires a string length that is optimal up to a constant multiplicative factor.

We present this result as follows. The set of strings from a fixed computationally universal set of base gates covers $\mathrm{SU}(d)$ increasingly densely and uniformly, as the string length grows.[15] First, in Sec. II, we quantify how quickly this occurs by introducing a framework for comparing the distribution of strings with the uniform distribution. We use this formalism in Sec. III to identify a condition on base sets that implies their efficient universality. In Sec. IV we then combine this condition with results from the literature to show that efficiently universal gate sets exist for Hilbert spaces of any finite dimension. In Sec. V we discuss lower bounds for compilation and demonstrates the optimality of the result; we conclude with open questions and further directions.

II. PRELIMINARIES

We begin by developing a metric of how well strings drawn from a finite set of gates approximate arbitrary elements of $\mathrm{SU}(d)$.

Let dg be the Haar measure on $\mathrm{SU}(d)$ normalized so that $\int dg = 1$. Consider the Hilbert space $L^2(\mathrm{SU}(d))$ with norm defined by the usual inner product $\langle \psi, \varphi \rangle \equiv \int \psi(g)^* \varphi(g) dg$. The norm of a linear transformation on $L^2(\mathrm{SU}(d))$ is given by

$$|M| \equiv \sup\{\|Mf\| \,|\, f \in L^2(\mathrm{SU}(d)), \|f\| = 1\}. \tag{2}$$

When M is bounded and Hermitian, the norm is simply the supremum of its spectrum and, as a result, $|M^n| = |M|^n$.

Define a representation $U \mapsto \tilde{U}$ of $\mathrm{SU}(d)$ on $L^2(\mathrm{SU}(d))$ by

$$\tilde{U}f(x)=f(U^{-1}x). \tag{3}$$

Using the right invariance of the Haar measure, we see that $\tilde{U}$ is unitary. For any finite set $\mathcal{A}\subset \mathrm{SU}(d)$, define the mixing operator $T(\mathcal{A})$ by

$$T(\mathcal{A})=\frac{1}{2|\mathcal{A}|}\sum_{A\in\mathcal{A}}\tilde{A}+\tilde{A}^{-1}. \tag{4}$$

All such T's are Hermitian and have norm one. We will often simply write T instead of $T(\mathcal{A})$. These represent averaging the action of the elements of $\mathcal{A}$ and their inverses on a function; when the function is a probability distribution on $\mathrm{SU}(d)$ we can think of T as multiplying by a random element of $\mathcal{A}$.

Applying T^n represents averaging over the action of words of length n. Denote the set of words of length n made up of elements of $\mathcal{A}$ and their inverses by $W_n(\mathcal{A})$, or when the set $\mathcal{A}$ is understood, simply W_n. This set comprises $(2|\mathcal{A}|)^n$ words, though as matrices there are generally some duplicates since substrings such as $AA^{-1}=1$ for all $A\in\mathcal{A}$. For any positive integer n, expanding T^n gives

$$T^n=\sum_{w\in W_n}\frac{\tilde{w}}{(2|\mathcal{A}|)^n}. \tag{5}$$

We want to compare T^n to the integral operator P:

$$Pf(h)=\int f(gh)dg=\int f(g)dg. \tag{6}$$

Note that P is the projection operator onto the set of constant functions on $\mathrm{SU}(d)$, and hence $P=P^\dagger$ and $P^2=P$. It is not hard to show that $TP=P=PT$ and, consequently,

$$(T-P)^n=T^n-P. \tag{7}$$

The metric for comparing $T(\mathcal{A})$ to P is given by

$$\Lambda(\mathcal{A})\equiv|T(\mathcal{A})-P|. \tag{8}$$

From Eq. (7) and the Hermiticity of T and P, it follows that

$$\Lambda(\mathcal{A})^n=|T^n(\mathcal{A})-P|. \tag{9}$$

If one thinks of T^n as a Riemann sum then Λ serves to quantify how quickly T^n converges to the integral. It has been shown[15] that if $\mathcal{A}$ is a computationally universal set, then all the eigenvalues of $T-P$ have absolute value strictly less than one. However, this only implies that $\Lambda(\mathcal{A})\leqslant 1$, since $T-P$ has an infinite number of eigenvalues.

The proof of the main result of our article—that efficiently universal sets of gates exist—is divided in the next two sections. In Sec. III we show that $\Lambda(\mathcal{A})<1$ implies that $\mathcal{A}$ is efficiently universal and in Sec. IV we demonstrate that for any d an efficiently universal set of gates can be found in $\mathrm{SU}(d)$.

III. A CONDITION FOR EFFICIENT UNIVERSALITY

Theorem 1: *For any $\mathcal{A}\subset\mathrm{SU}(d)$ such that $\Lambda(\mathcal{A})<1$, $\mathcal{A}$ is efficiently universal. Specifically, there exists a constant C such that for all $U\in\mathrm{SU}(d)$, $\epsilon>0$, and $n>C\log 1/\epsilon$, there is a $w\in W_n(\mathcal{A})$ such that $|w-U|<\epsilon$.*

Before proving the theorem, we will need to note a fact about the geometry of SU(d). For any d and r_0, if $V(r)$ is the Haar measure of a ball of radius r in SU(d), then there exist constants k_1 and k_2 such that

$$k_1 r^{d^2-1} < V(r) < k_2 r^{d^2-1} \tag{10}$$

for all $r \in (0, r_0)$. This is true because SU(d) is a d^2-1-dimensional manifold and because $V(r)$ does not depend on the center of the ball under the Haar measure.

Now we can proceed with the proof of Theorem 1:

Proof: Define $\chi \in L^2(\mathrm{SU}(d))$ by

$$\chi(g) = \begin{cases} 1 & \text{for } |g-I| < \epsilon/2 \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

Let $V = \|P\chi\| = \|\chi\|^2$ be the measure of the ball around the identity of radius $\epsilon/2$. We will not perform this integration, but recall from Eq. (10) that $V > k_1(\epsilon/2)^{d^2-1}$.

Let $T = T(\mathcal{A})$ and $\Lambda = \Lambda(\mathcal{A})$.

First we use the Cauchy–Schwartz inequality to give

$$|\langle \chi, (T^n - P)\tilde{U}\chi\rangle| \leq \|\chi\| \|(T^n - P)\tilde{U}\chi\| \leq \|\chi\|^2 |(T^n - P)\tilde{U}| < \Lambda^n V. \tag{12}$$

Another way to compute the same inner product is

$$\langle \chi, (T^n - P)\tilde{U}\chi\rangle = \langle \chi, T^n \tilde{U}\chi\rangle - V^2. \tag{13}$$

Combining Eq. (12) and Eq. (13) gives that $|\langle \chi, T^n\tilde{U}\chi\rangle - V^2| < \Lambda^n V$. This means that there exists C which depends only on $\mathcal{A}$ such that if $n > C \log 1/\epsilon$ then $\Lambda^n < V$ and $\langle \chi, T^n\tilde{U}\chi\rangle > 0$. Specifically, it suffices to choose

$$n > \frac{d^2-1}{\log(1/\Lambda)} \log(1/\epsilon) + \frac{\log(2^{d^2-1}/k_1)}{\log(1/\Lambda)}. \tag{14}$$

When this occurs it means that

$$\int \chi(g) \sum_{w \in W_n} \frac{\chi(wU^{-1}g)}{(2|\mathcal{A}|)^n} dg > 0, \tag{15}$$

which implies that $\exists g \in \mathrm{SU}(d)$ and $w \in W_n$ such that $\chi(g) \neq 0$ and $\chi(wU^{-1}g) \neq 0$. Thus $|g-I| < \epsilon/2$ and $|wU^{-1}g - I| < \epsilon/2$, implying that $|w - g^{-1}U| < \epsilon/2$. Combining these and using the triangle inequality gives $|w-U| < \epsilon$. ■

IV. A CLASS OF EFFICIENTLY UNIVERSAL GATE SETS

In this section we show that for each d there exists a set of gates $\mathcal{G}_d$ in SU(d) such that $\Lambda(\mathcal{G}_d) < 1$ (and thus $\mathcal{G}_d$ is efficiently universal). We begin with a result demonstrating this for SU(2) and then extend it to SU(d).

Lemma 2 (Lubotsky, Phillips and Sarnak): Let

$$V_1 = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2i \\ 2i & 1 \end{pmatrix}, \quad V_2 = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2 \\ -2 & 1 \end{pmatrix},$$
$$V_3 = \frac{1}{\sqrt{5}} \begin{pmatrix} 1+2i & 0 \\ 0 & 1-2i \end{pmatrix}. \tag{16}$$

Then $\lambda=\Lambda(\{V_1,V_2,V_3\})=\sqrt{5}/3<1$. *Furthermore, for any* U_1, U_2, $U_3\in \mathrm{SU}(2)$, $\Lambda(\{U_1,U_2,U_3\})\geqslant\lambda$.

The proof of this Lemma is presented in Refs. 16 and 17. Let $\mathcal{G}_2=\{V_1,V_2,V_3\}$, as it is a family of quantum gates from SU(2) for which Λ is strictly less than one. The optimality of Λ for this set is an interesting aside, but has little bearing on what follows.

Extending the result to SU(d) will require slightly more effort. To this end, if I_k denotes the $k\times k$ identity matrix, then, for any $U\in\mathrm{SU}(2)$ and $2\leqslant j\leqslant d$, define $\beta_j^{(d)}(U)$ to be

$$\beta_j^{(d)}(U)=\begin{pmatrix} I_{j-2} & 0 & 0 \\ 0 & U & 0 \\ 0 & 0 & I_{d-j} \end{pmatrix}\in \mathrm{SU}(d). \tag{17}$$

We will typically omit the $^{(d)}$ where it is understood.

Lemma 3 (Diaconis and Shahshahani): Let $\{G_j^i\}$, $1\leqslant i<j\leqslant d$ *be a series of* $\binom{d}{2}$ *independent random matrices in* SU(2) *that are chosen uniformly according to a Haar measure. Then*

$$\prod_{i=1}^{d-1}\prod_{j=i+1}^{d}\beta_j(G_j^i) \tag{18}$$

is uniformly distributed in SU(d).

This Lemma is proved in Ref. 18. It means that if we had access to random elements of SU(2) that were completely uniformly distributed, then we could generate uniformly distributed elements of SU(d). When the elements of SU(2) are only approximately uniform, we can bound the distance to uniformity of the words they form by using what is known as a hybrid argument:[19]

Lemma 4 (Bernstein and Vazirani): If $U_1,\ldots,U_m$, $V_1,\ldots,V_m$ *are linear operators such that* $|U_i|\leqslant 1$, $|V_i|\leqslant 1$ *and* $|U_i-V_i|<\delta$, *then* $|U_m\cdots U_2U_1-V_m\cdots V_2V_1|<m\delta$.

Proof: If we replace a single U_i in the product $U_m\ldots U_1$ with the corresponding V_i, then the entire product will still change by less than δ since $|AB|\leqslant|A|\cdot|B|$ for any operators A, B. Thus we can construct a series of $m+1$ "hybrid" operators, which start with $U_1\cdots U_m$, end with $V_1\cdots V_m$, and are each separated by less than δ. The proof follows from the triangle inequality.■

We now combine all of the other results in this section to demonstrate a set of gates in SU(d) for which Λ is strictly less than one.

Proposition 5: For any $d>2$, *define* $\mathcal{G}_d$ *by*

$$\mathcal{G}_d=\{\beta_j(V)\,|\,1\leqslant j\leqslant(d-1),V\in\mathcal{G}_2\}. \tag{19}$$

Then $\Lambda(\mathcal{G}_d)<1$.

Proof: The approach of our proof will be to approximate the uniform distribution in Lemma 3, and then we show that this forces Λ to be less than one. To this end, let $R_m\subset W_{m\binom{d}{2}}(\mathcal{G}_d)$ be the set of all products of the form

$$\prod_{i=1}^{d-1}\prod_{j=i+1}^{d}\beta_j(G_j^i) \tag{20}$$

such that the G_j^i are selected from $W_m(\mathcal{G}_2)$.

From Lemma 2 we have that $\forall m$, $|T(V_1,V_2,V_3)-P|^m=\lambda^m$ for some $\lambda<1$. There are $\binom{d}{2}$ terms in Eq. (18), each of which is approximated to within an accuracy of λ^m by the appropriate length m substring of R_m. Thus, using the hybrid argument and Lemma 3 gives that

$$\Lambda(R_m)=\left|\sum_{w\in R_m}\frac{\tilde{w}-P}{|R_m|}\right|\leqslant\binom{d}{2}\lambda^m. \tag{21}$$

Now, if we let R_m' denote $W_{m\binom{d}{2}}-R_m$ then

$$\Lambda(W_{m(\binom{d}{2})}) \leqslant \frac{|R'_m|}{|W|}\Lambda(R'_m) + \frac{|R_m|}{|W|}\Lambda(R_m) \leqslant \left(1 - \frac{|R_m|}{|W|}\right) + \frac{|R_m|}{|W|}\Lambda(R_m) = 1 - \frac{|R_m|}{|W|}(1 - \Lambda(R_m)). \tag{22}$$

If we choose m large enough so that $\binom{d}{2}\lambda^m < 1$, then this last expression will be less than one, and $\Lambda(\mathcal{G}_d) < 1$. ■

Thus, efficient quantum compiling is possible for d-dimensional systems, given the appropriate choice of base gate set.

V. LOWER BOUNDS

This proves that sets of base gates exist which can achieve a precision of ϵ in $O(\log 1/\epsilon)$ gates, but can we do any better? An ϵ-ball in SU(d) has measure of order ϵ^{d^2-1}, so if we expect to cover all of SU(d) with strings of length n, then we will require $(2|\mathcal{A}|)^n k_2 \epsilon^{d^2-1} > 1$, or equivalently,

$$n \geqslant \frac{d^2-1}{\log 2|\mathcal{A}|}\log 1/\epsilon - \frac{\log k_2}{\log 2|\mathcal{A}|}. \tag{23}$$

Thus the result is optimal up to a constant factor. This fact is quite general, since it follows from simple counting arguments. However, if the assumptions of the problem are relaxed to allow many gates to act in parallel, then using ancilla qubits it is possible to approximate single-qubit gates with a circuit of *size* poly($\log 1/\epsilon$) but *depth* of only poly($\log\log 1/\epsilon$).[20] This construction, like the one in this article, relies on having access to a specific set of base gates; to date, only the Solovay–Kitaev theorem applies to any computationally universal set.

In our original problem, though, eliminating the constant linear factor turns out to be impossible. Consider any set $\mathcal{A}$ of l base gates that is *not* computationally universal. Let $B(\mathcal{A}, \delta)$ be the set of gates obtained by perturbing each gate in $\mathcal{A}$ by no more than δ. Then $B(\mathcal{A}, \delta)$ has nonzero measure (in SU$(d)^l$), almost all of its elements are computationally universal and from the hybrid argument, any string of length n drawn from gates in $B(\mathcal{A}, \delta)$ will be within $n\delta$ of something in the (nondense) group generated by $\mathcal{A}$. Since we can make δ arbitrarily small, any fixed prefactor in front of $\log 1/\epsilon$ will fail on a computationally universal set of nonzero measure for some values of ϵ.

Note that unlike most results about quantum compiling, this argument also holds if the base gates are parametrized; say, $A_1, \ldots, A_l$ are elements of the algebra $su(d)$ and a single operation now has the form $e^{\pm A_i t}$, for any $t > 0$. The above proof demonstrates that there exist sets with nonzero measure which require arbitrarily many steps, even if the steps are continuous. If we measure cost not in terms of number of steps, but by the total time taken, then we have to modify the argument slightly. For small values of t, $|e^{A_i t} - I|$ is on the order of $t\delta$, but for large t the difference never gets any higher than δ. This means that no matter how many steps we take, in time t, we will stay within $t\delta$ of some nondense subgroup and the same result holds.

These results can be obtained more simply by considering the (nonzero measure) set of gates which are very close to the identity. If every gate does very little, then we will need a large number them in order to accomplish anything. The reason why universal sets that are very close to nonuniversal sets are interesting is because of their frequent appearance in actual physical systems, such as NMR under the weak coupling approximation.[21]

VI. CONCLUSIONS

We have found a condition that implies the efficient universality of a set of gates and demonstrated a family of gate sets in SU(d) that satisfy this condition. This means that given access to such a gate set, arbitrary quantum gates can be approximated to accuracy ϵ using only $O(\log 1/\epsilon)$ gates. Such knowledge will likely be invaluable in crafting future physical implementations of quantum information processing systems.

Many open questions remain, however. For example, determining or bounding Λ (even numerically) for a given set of base gates seems to be very difficult, though it is likely an important step in determining the prefactor C, which measures how effective a set of gates would be for compiling. The method used by Refs. 16 and 17 involves specialized arguments from number theory that do not generalize easily to other sets of gates or to SU(d) for $d>2$. Our proof (like the Solovay–Kitaev algorithm) also requires the ability to perform the inverse of each gate in the base set. This restriction feels unnecessary, yet very little is known in the case where inverses are unavailable.

More broadly, it is also generally unknown which gate sets are efficiently universal and when $\Lambda<1$. Note that $\Lambda(\mathcal{A})<1$ implies that $\mathcal{A}$ is efficiently universal, but the converse is not known to be true. Thus it is possible that the questions of efficient universality and Λ being less than one will be settled separately.

However, if $\Lambda(\mathcal{A})$ were to be a continuous function of $\mathcal{A}$ (for fixed $|\mathcal{A}|$), then the situation would simplify considerably. In this case, it is not hard to show that $\Lambda(\mathcal{A})<1$ if and only if $\mathcal{A}$ is computationally universal, so that computational universality, efficient universality and $\Lambda<1$ would all become equivalent conditions. We suspect that this is the case, but have been unable to prove it.

Finally, the techniques used in our results do not suggest any efficient (i.e., running time polynomial in $\log 1/\epsilon$) algorithms for quantum compiling. The most important, and possibly most difficult, open problem remaining is to find a polynomial time algorithm to approximate any unitary gate by a fixed efficiently universal set of base gates with a string whose length saturates the $O(\log 1/\epsilon)$ bound.

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Topological quantum memory[a)]

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We analyze *surface codes*, the topological quantum error-correcting codes introduced by Kitaev. In these codes, qubits are arranged in a two-dimensional array on a surface of nontrivial topology, and encoded quantum operations are associated with nontrivial homology cycles of the surface. We formulate protocols for error recovery, and study the efficacy of these protocols. An order-disorder phase transition occurs in this system at a nonzero critical value of the error rate; if the error rate is below the critical value (the *accuracy threshold*), encoded information can be protected arbitrarily well in the limit of a large code block. This phase transition can be accurately modeled by a three-dimensional Z_2 lattice gauge theory with quenched disorder. We estimate the accuracy threshold, assuming that all quantum gates are *local*, that qubits can be measured rapidly, and that polynomial-size classical computations can be executed instantaneously. We also devise a robust recovery procedure that does not require measurement or fast classical processing; however, for this procedure the quantum gates are local only if the qubits are arranged in *four* or more spatial dimensions. We discuss procedures for encoding, measurement, and performing fault-tolerant universal quantum computation with surface codes, and argue that these codes provide a promising framework for quantum computing architectures.
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I. INTRODUCTION

The microscopic world is quantum mechanical, but the macroscopic world is classical. This fundamental dichotomy arises because a coherent quantum superposition of two readily distinguishable macroscopic states is highly unstable. The quantum state of a macroscopic system rapidly *decoheres* due to unavoidable interactions between the system and its surroundings.

Decoherence is so pervasive that it might seem to preclude subtle quantum interference phenomena in systems with many degrees of freedom. However, recent advances in the theory of quantum error correction suggest otherwise.[1,2] We have learned that quantum states can be cleverly encoded so that the debilitating effects of decoherence, if not too severe, can be resisted. Furthermore, fault-tolerant protocols have been devised that allow an encoded quantum state to be reliably processed by a quantum computer with imperfect components.[3] In principle, then, very intricate quantum systems can be stabilized and accurately controlled.

The theory of quantum fault tolerance has shown that, even for delicate coherent quantum states, information *processing* can prevent information *loss*. In this article, we will study a particular approach to quantum fault tolerance that has notable advantages: in this approach, based on the *surface codes* introduced in Refs. 4 and 5, the quantum processing needed to control errors has

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especially nice locality properties. For this reason, we think that surface codes suggest a particularly promising approach to quantum computing architecture.

One glittering achievement of the theory of quantum fault tolerance is the *threshold theorem*, which asserts that an arbitrarily long quantum computation can be executed with arbitrarily high reliability, provided that the error rates of the computer's fundamental quantum gates are below a certain critical value, the *accuracy threshold*.[6–10] The numerical value of this accuracy threshold is of great interest for future quantum technologies, as it defines a standard that should be met by designers of quantum hardware. The critical error probability per gate p_c has been estimated as $p_c \gtrsim 10^{-4}$; very roughly speaking, this means that robust quantum computation is possible if the decoherence time of stored qubits is at least 10^4 times longer than the time needed to execute one fundamental quantum gate,[11] assuming that decoherence is the only source of error.

This estimate of the accuracy threshold is obtained by analyzing the efficacy of a *concatenated code*, a hierarchy of codes within codes, and it is based on many assumptions, which we will elaborate in Sec. II. For now, we just emphasize one of these assumptions: that a quantum gate can act on any pair of qubits, with a fidelity that is independent of the spatial separation of the qubits. This assumption is clearly unrealistic; it is made because it greatly simplifies the analysis. Thus this estimate will be reasonable for a practical device only to the extent that the hardware designer is successful in arranging that qubits that must interact are kept close to one another. It is known that the threshold theorem still applies if quantum gates are required to be local,[7,12] but for this realistic case careful estimates of the threshold have not been carried out.

We will perform a quite different estimate of the accuracy threshold, based on surface codes rather than concatenated codes. This estimate applies to a device with strictly local quantum gates, if the device is controlled by a classical computer that is perfectly reliable, and whose clock speed is much faster than the clock speed of the quantum computer. In this approach, some spatial nonlocality in effect is still allowed, but we demand that all the nonlocal processing be classical. Specifically, an error syndrome is extracted by performing local quantum gates and measurements; then a classical computation is executed to infer what quantum gates are needed to recover from error. We will assume that this classical computation, which actually requires a time bounded above by a polynomial in the number of qubits in the quantum computer, can be executed in a constant number of time steps. Under this assumption, the existence of an accuracy threshold can be established and its value can be estimated. If we assume that the classical computation can be completed in a single time step, we estimate that the critical error probability p_c per qubit and per time step satisfies $p_c \geq 1.7 \times 10^{-4}$. This estimate applies to the accuracy threshold for reliable *storage* of quantum information, rather than for reliable processing. The threshold for quantum computation is not as easy to analyze definitively, but we will argue that its numerical value is not likely to be substantially different.

We believe that principles of fault tolerance will dictate the shape of future quantum computing architectures. In Sec. II we compile a list of hardware features that are conducive to fault-tolerant processing, and outline the design of a fault-tolerant quantum computer that incorporates surface coding. We review the properties of surface codes in Sec. III, emphasizing in particular that the qubits in the code block can be arranged in a *planar* sheet,[13,14] and that errors in the syndrome measurement complicate the recovery procedure. The core of the article is Sec. IV, where we relate recovery from errors using surface codes to a statistical-mechanical model with local interactions. In the (unrealistic) case where syndrome measurements are perfect, this model becomes the two-dimensional Ising model with quenched disorder, whose phase diagram has been studied by Monte Carlo simulations. These simulations indicate that if the syndrome information is put to optimal use, error recovery succeeds with a probability that approaches one in the limit of a large code block, if and only if both phase errors and bit-flip errors occur with a probability per qubit less than about 11%. In the more realistic case where syndrome measurements are imperfect, error recovery is modeled by a three-dimensional Z_2 gauge theory with quenched disorder, whose phase diagram (to the best of our knowledge) has not been studied previously. The third dimension that arises can be interpreted as time—since the syndrome information cannot be trusted, we must repeat the measurement many times before we can be confident about the correct

way to recover from the errors. We argue that an order-disorder phase transition of this model corresponds to the accuracy threshold for quantum storage, and, furthermore, that the optimal recovery procedure can be computed efficiently on a classical computer. We proceed in Sec. V to prove a rather crude lower bound on the accuracy threshold, concluding that the error recovery procedure is sure to succeed in the limit of a large code block under suitable conditions: for example, if in each round of syndrome measurement, qubit phase errors, qubit bit-flip errors, and syndrome bit errors all occur with probability below 1.14%. Tighter estimates of the accuracy threshold could be obtained through numerical studies of the quenched gauge theory.

In deriving this accuracy threshold for quantum storage, we assumed that an unlimited amount of syndrome data could be deposited in a classical memory, if necessary. But in Sec. VI we show that this threshold, and a corresponding accuracy threshold for quantum computation, remain intact even if the classical memory is limited to polynomial size. Then in Sec. VII we analyze quantum circuits for syndrome measurement, so that our estimate of the accuracy threshold can be reexpressed as a fidelity requirement for elementary quantum gates. We conclude that our quantum memory can resist decoherence if gates can be executed in parallel, and if the qubit decoherence time is at least 6000 times longer than the time needed to execute a gate. In Sec. VIII we show that encoded qubits can be accurately prepared and reliably measured. We also describe how a surface code with a small block size can be built up gradually to a large block size; this procedure allows us to enter a qubit in an unknown quantum state into our quantum memory with reasonable fidelity, and then to maintain that fidelity for an indefinitely long time. We explain in Sec. IX how a universal set of quantum gates acting on protected quantum information can be executed fault-tolerantly.

Most of the analysis of the accuracy threshold in this article is premised on the assumption that qubits can be measured quickly and that classical computations can be done instantaneously and perfectly. In Sec. X we drop these assumptions. We devise a recovery procedure that does not require measurement or classical computation, and infer a lower bound on the accuracy threshold. Unfortunately, though, the quantum processing in our procedure is not spatially local unless the dimensionality of space is at least four. Section XI contains some concluding remarks.

This article analyzes applications of surface coding to quantum memory and quantum computation that could in principle be realized in any quantum computer that meets the criteria of our computational model, whatever the details of how the local quantum gates are physically implemented. It has also been emphasized[4,5] that surface codes may point the way toward realizations of intrinsically stable quantum memories (*physical* fault tolerance). In that case, protection against decoherence would be achieved without the need for active information processing, and how accurately the protected quantum states can be processed might depend heavily on the details of the implementation.

II. FAULT TOLERANCE AND QUANTUM ARCHITECTURE

To prove that a quantum computer with noisy gates can perform a robust quantum computation, we must make some assumptions about the nature of the noise and about how the computer operates. In fact, similar assumptions are needed to prove that a classical computer with noisy gates is robust.[15] Still, it is useful to list these requirements—they should always be kept in mind when we contemplate proposed schemes for building quantum computing hardware:

(i) *Constant error rate*. We assume that the strength of the noise is independent of the number of qubits in the computer. If the noise increases as we add qubits, then we cannot reduce the error rate to an arbitrarily low value by increasing the size of the code block.

(ii) *Weakly correlated errors*. Errors must not be too strongly correlated, either in space or in time. In particular, fault-tolerant procedures fail if errors act simultaneously on many qubits in the same code block. If possible, the hardware designer should strive to keep qubits in the same block isolated from one another.

(iii) *Parallel operation*. We need to be able to perform many quantum gates in a single time step. Errors occur at a constant rate per unit time, and we are to control these errors through

information processing. We could never keep up with the accumulating errors except by doing processing in different parts of the computer at the same time.

(iv) *Reusable memory*. Errors introduce entropy into the computer, which must be flushed out by the error recovery procedure. Quantum processing transfers the entropy from the qubits that encode the protected data to ''ancilla'' qubits that can be discarded. Thus fresh ancilla qubits must be continually available. The ability to erase (or replace) the ancilla quickly is an essential hardware requirement.[16]

In some estimates of the threshold, additional assumptions are made. While not strictly necessary to ensure the existence of a threshold, these assumptions may be useful, either because they simplify the analysis of the threshold or because they allow us to increase its numerical value. Hence these assumptions, too, should command the attention of the prospective hardware designer:

(i) *Fast measurements*. It is helpful to assume that a qubit can be measured as quickly as a quantum gate can be executed. For some implementations, this may not be a realistic assumption—measurement requires the amplification of a microscopic quantum effect to a macroscopic signal, which may take a while. But by measuring a classical error syndrome for each code block, we can improve the efficiency of error recovery. Furthermore, if we can measure qubits and perform quantum gates conditioned on classical measurement outcomes, then we can erase ancilla qubits by projecting onto the $\{|0\rangle,|1\rangle\}$ basis and flipping the qubit if the outcome is $|1\rangle$.

(ii) *Fast and accurate classical processing*. If classical processing is faster and more accurate than quantum processing, then it is beneficial to substitute classical processing for quantum processing when possible. In particular, if the syndrome is measured, then a classical computation can be executed to determine how recovery should proceed. Ideally, the classical processors that coordinate the control of the quantum computer should be integrated into the quantum hardware.

(iii) *No leakage*. It is typically assumed that, though errors may damage the state of the computer, the qubits themselves remain accessible—they do not ''leak'' out of the device. In fact, at least some types of leakage can be readily detected. If leaked qubits, once detected, can be replaced easily by fresh qubits, then leakage need not badly compromise performance. Hence, a desirable feature of hardware is that leaks are easy to detect and correct.

(iv) *Nonlocal quantum gates*. Higher error rates can be tolerated, and the estimate of the threshold is simplified, if we assume that two-qubit quantum gates can act on any pair of qubits with a fidelity independent of the distance between the qubits. However useful, this assumption is not physically realistic. What the hardware designer can and should do, though, is try to arrange that qubits that will need to interact with one another are kept close to one another. In particular, the ancilla qubits that absorb entropy should be carefully integrated into the design.[12]

If we do insist that all quantum gates are local, then another desirable feature is the following.

(v) *High coordination number*. A threshold theorem applies even if qubits form a one-dimensional array.[7,12] But local gates are more effective if the qubits are arranged in three dimensions, so that each qubit has more neighbors.

Suppose, then, that we are blessed with an implementation of quantum computation that meets all of our desiderata. Qubits are arranged in a three-dimensional lattice, and can be projectively measured quickly. Reasonably accurate quantum gates can be applied in parallel to single qubits or to neighboring pairs of qubits. Fast classical processing is integrated into the qubit array. Under these conditions planar surface codes provide an especially attractive way to operate the quantum computer fault-tolerantly.

We may envision our quantum computer as a stack of planar sheets, with a protected logical qubit encoded in each sheet. Adjacent to each logical sheet is an associated sheet of ancilla qubits that are used to measure the error syndrome of that code block; after each measurement, these ancilla qubits are erased and then immediately reused. Encoded two-qubit gates can be performed between neighboring logical sheets, and any two logical sheets in the stack can be brought into contact by performing swap gates that move the sheets through the intervening layers of logical and ancilla qubits. As a quantum circuit is executed in the stack, error correction is continually applied to each logical sheet to protect against decoherence and other errors. Portions of the stack are designated as ''software factories,'' where special ancilla states are prepared and purified—this software is then consumed during the execution of certain quantum gates that cannot be implemented directly.

A notable feature of this design (or other fault-tolerant designs) is that most of the information processing in the device is devoted to controlling errors, rather than moving the computation forward. How accurately must the fundamental quantum gates be executed for this error control to be effective, so that our machine is computationally powerful? Our goal in this article is to address this question.

III. SURFACE CODES

We will study the family of quantum error-correcting codes introduced in Refs. 4 and 5. These codes are especially well suited for fault-tolerant implementation, because the procedure for measuring the error syndrome is highly local.

A. Toric codes

For the code originally described in Refs. 4 and 5, it is convenient to imagine that the qubits are in one-to-one correspondence with the links of a square lattice drawn on a torus, or, equivalently, drawn on a square with opposite edges identified. Hence we will refer to them as ''toric codes.'' Toric codes can be generalized to a broader class of quantum codes, with each code in the class associated with a tessellation of a two-dimensional surface. Codes in this broader class will be called ''surface codes.''

A surface code is a special type of ''stabilizer code.'' [17,18] A (binary) stabilizer code can be characterized as the simultaneous eigenspace with eigenvalue one of a set of mutually commuting check operators (or ''stabilizer generators''), where each generator is a ''Pauli operator.'' We use the notation

$$I=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \quad X=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \tag{1}$$

$$Y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad Z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \tag{2}$$

for the 2×2 identity and Pauli matrices; a Pauli operator acting on n qubits is one of the 2^{2n} tensor product operators

$$\{I,X,Y,Z\}^{\otimes n}. \tag{3}$$

For the toric code defined by the $L\times L$ square lattice on the torus, there are $2L^2$ links of the lattice, and hence $2L^2$ qubits in the code block. Check operators are associated with each site and with each elementary cell (or ''plaquette'') of the lattice, as shown in Fig. 1. The check operator at site s acts nontrivially on the four links that meet at the site; it is the tensor product

$$X_s=\otimes_{\ell\ni s}X_\ell \tag{4}$$

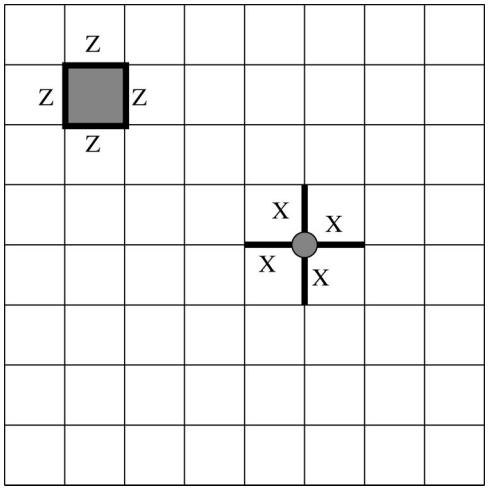

FIG. 1. Check operators of the toric code. Each plaquette operator is a tensor product of Z's acting on the four links contained in the plaquette. Each site operator is a tensor product of X's acting on the four links that meet at the site.

acting on those four qubits, times the identity acting on the remaining qubits. The check operator at plaquette P acts nontrivially on the four links contained in the plaquette, as the tensor product

$$Z_P = \otimes_{\ell \in P} Z_\ell , \tag{5}$$

times the identity on the remaining links.

Although X and Z anticommute, the check operators are mutually commuting. Obviously, site operators commute with site operators, and plaquette operators with plaquette operators. Site operators commute with plaquette operators because a site operator and a plaquette operator act either on disjoint sets of links, or on sets whose intersection contains two links. In the former case, the operators obviously commute, and in the latter case, two canceling minus signs arise when the site operator commutes through the plaquette operator. The check operators generate an Abelian group, the code's stabilizer.

The check operators can be simultaneously diagonalized, and the toric code is the space in which each check operator acts trivially. Because of the periodic boundary conditions, each site or plaquette operator can be expressed as the product of the other L^2-1 such operators; the product of all L^2 site operators or all L^2 plaquette operators is the identity, since each link operator occurs twice in the product, and $X^2=Z^2=I$. There are no further relations among these operators; therefore, there are $2\cdot(L^2-1)$ independent check operators, and hence two encoded qubits (the code subspace is four-dimensional).

A Pauli operator that commutes with all the check operators will preserve the code subspace. What operators have this property? To formulate the answer, it is convenient to recall some standard mathematical terminology. A mapping that assigns an element of $Z_2=\{0,1\}$ to each link of the lattice is called a (Z_2-valued) *one-chain*. In a harmless abuse of language, we will also use the term one-chain (or simply chain) to refer to the set of all links that are assigned the value 1 by such a mapping. The one-chains form a vector space over Z_2—intuitively, the sum $u+v$ of two chains u and v is a disjoint union of the links contained in the two one-chains. Similarly, zero-chains assign elements of Z_2 to lattice sites and two-chains assign elements of Z_2 to lattice plaquettes; these also form vector spaces. A linear boundary operator ∂ can be defined that takes two-chains to one-chains and one-chains to zero-chains: the boundary of a plaquette is the sum of the four links comprising the plaquette, and the boundary of a link is the sum of the two sites at the ends of the link. A chain whose boundary is trivial is called a *cycle*.

Now, any Pauli operator can be expressed as a tensor product of X's (and I's) times a tensor product of Z's (and I's). The tensor product of Z's and I's defines a Z_2-valued one-chain, where

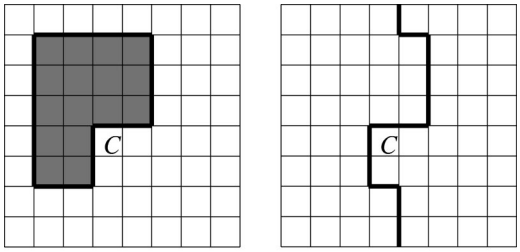

FIG. 2. Cycles on the lattice. (a) A homologically trivial cycle bounds a region that can be tiled by plaquettes. The corresponding tensor product of Z's lies in the stabilizer of the toric code. (b) A homologically nontrivial cycle is not a boundary. The corresponding tensor product of Z's commutes with the stabilizer but is not contained in it. It is a logical operation that acts nontrivially in the code subspace.

links acted on by Z are mapped to 1 and links acted on by I are mapped to 0. This operator trivially commutes with all of the plaquette check operators, but commutes with a site operator if and only if an even number of Z's act on the links adjacent to the site. Thus, the corresponding one-chain must be a cycle. Similarly, the tensor product of X's trivially commutes with the site operators, but commutes with a plaquette operator only if an even number of X's act on the links contained in the plaquette. This condition can be more conveniently expressed if we consider the dual lattice, in which sites and plaquettes are interchanged; the links dual to those on which X acts form a cycle of the dual lattice. In general, then, a Pauli operator that commutes with the stabilizer of the code can be represented as a tensor product of Z's acting on a cycle of the lattice, times a tensor product of X's acting on a cycle of the dual lattice.

Cycles are of two distinct types. A one-cycle is *homologically trivial* if it can be expressed as the boundary of a two-chain [Fig. 2(a)]. Thus, a homologically trivial cycle on our square lattice has an interior that can be "tiled" by plaquettes, and a product of Z's acting on the links of the cycle can be expressed as a product of the enclosed plaquette operators. This operator is therefore a product of the check operators—it is contained in the code stabilizer and acts trivially on the code subspace. Similarly, a product of X's acting on links that comprise a homologically trivial cycle of the dual lattice is also a product of check operators. Furthermore, *any* element of the stabilizer group of the toric code (any product of the generators) can be expressed as a product of Z's acting on a homologically trivial cycle of the lattice times X's acting on a homologically trivial cycle of the dual lattice.

But a cycle could be homologically nontrivial, that is, not the boundary of anything [Fig. 2(b)]. A product of Z's corresponding to a nontrivial cycle commutes with the code stabilizer (because it is a cycle), but is not contained in the stabilizer (because the cycle is nontrivial). Therefore, while this operator preserves the code subspace, it acts nontrivially on encoded quantum information. Associated with the two fundamental nontrivial cycles of the torus, then, are the encoded operations $\overline{Z}_1$ and $\overline{Z}_2$ acting on the two encoded qubits. Associated with the two dual cycles of the dual lattice are the corresponding encoded operations $\overline{X}_1$ and $\overline{X}_2$, as shown in Fig. 3.

A Pauli operator acting on n qubits is said to have *weight* w if the identity I acts on $n-w$ qubits and nontrivial Pauli matrices act on w qubits. The *distance* d of a stabilizer code is the weight of the minimal-weight Pauli operator that preserves the code subspace and acts nontrivially within the code subspace. If an encoded state is damaged by the action of a Pauli operator whose weight is less than half the code distance, then we can recover from the error successfully by applying the minimal weight Pauli operator that returns the damaged state to the code subspace (which can be determined by measuring the check operators). For a toric code, the distance is the number of lattice links contained in the shortest homologically nontrivial cycle on the lattice or dual lattice. Thus in the case of an $L\times L$ square lattice drawn on the torus, the code distance is $d=L$.

The great virtue of the toric code is that the check operators are so simple. Measuring a check

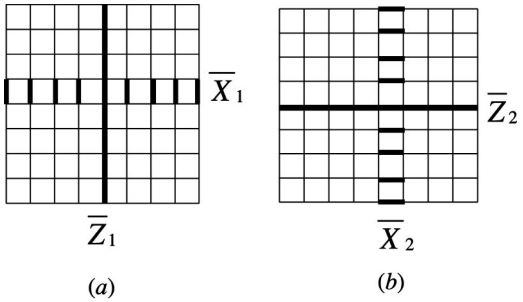

FIG. 3. Basis for the operators that act on the two encoded qubits of the toric code. The logical operators $\overline{Z}_1$ and $\overline{Z}_2$ are tensor products of Z's associated with the fundamental nontrivial cycles of the torus constructed from links of the lattice. The complementary operators $\overline{X}_1$ and $\overline{X}_2$ are tensor products of X's associated with nontrivial cycles constructed from links of the dual lattice.

operator requires a quantum computation, but because each check operator involves just four qubits in the code block, and these qubits are situated near one another, the measurement can be executed by performing just a few quantum gates. Furthermore, the ancilla qubits used in the measurement can be situated where they are needed, so that the gates act on pairs of qubits that are in close proximity.

The observed values of the check operators provide a ''syndrome'' that we may use to diagnose errors. If there are no errors in the code block, then every check operator takes the value 1. Since each check operator is associated with a definite position on the surface, a site of the lattice or the dual lattice, we may describe the syndrome by listing all positions where the check operators take the value -1. It is convenient to regard each such position as the location of a particle, a ''defect'' in the code block.

If errors occur on a particular chain (a set of links of the lattice or dual lattice), then defects occur at the sites on the *boundary* of the chain. Evidently, then, the syndrome is highly ambiguous, as many error chains can share the same boundary, and all generate the same syndrome. For example, the two chains shown in Fig. 4 end on the same two sites. If errors occur on one of these

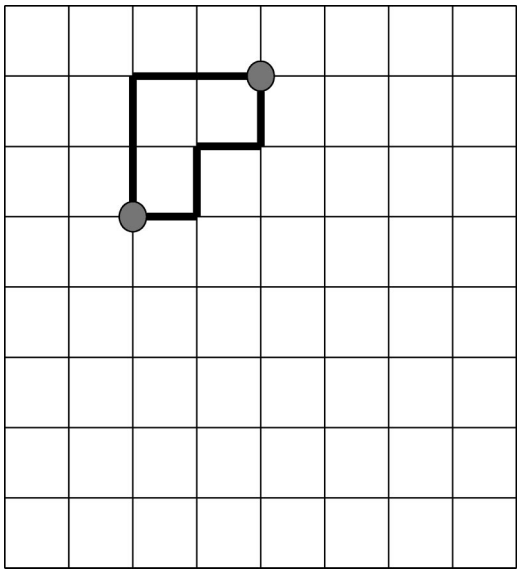

FIG. 4. The highly ambiguous syndrome of the toric code. The two site defects shown could arise from errors on either one of the two chains shown. In general, error chains with the same boundary generate the same syndrome, and error chains that are homologically equivalent act on the code space in the same way.

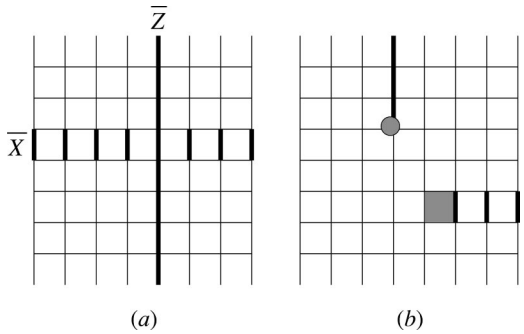

FIG. 5. A planar quantum code. (a) At the top and bottom are the ''plaquette edges'' (or ''rough edges'') where there are three-qubit plaquette operators, and at the left and right are the ''site edges'' (or ''smooth edges'') where there are three-qubit site operators. The logical operation $\overline{Z}$ for the one encoded qubit is a tensor product of Z's acting on a chain running from one rough edge to the other, and the logical operation $\overline{X}$ is a tensor product of X's acting on a chain of the dual lattice running from one smooth edge to the other. For the lattice shown, the code's distance is $L=8$. (b) Site and plaquette defects can appear singly, rather than in pairs. An isolated site defect arises from an error chain that ends at a rough edge, and an isolated plaquette defect arises from a dual error chain that ends at a smooth edge.

chains, we might incorrectly infer that the errors actually occured on the other chain. Fortunately, though, this ambiguity need not cause harm. If Z errors occur on a particular chain, then by applying Z to each link of *any* chain with the same boundary as the actual error chain, we will successfully remove all defects. Furthermore, as long as the chosen chain is *homologically* correct (differs from the actual error chain by the one-dimensional boundary of a two-dimensional region), then the encoded state will be undamaged by the errors. In that event, the product of the actual Z errors and the Z's that we apply is contained in the code stabilizer and therefore acts trivially on the code block.

Heuristically, an error chain can be interpreted as a physical process in which a defect pair nucleates, and the two members of the pair drift apart. To recover from the errors, we lay down a ''recovery chain'' bounded by the two defect positions, which we can think of as a physical process in which the defects are brought together to reannihilate. If the defect world line consisting of both the error chain and the recovery chain is homologically trivial, then the encoded quantum state is undamaged. But if the world line is homologically nontrivial (if the two members of the pair wind around a cycle of the torus before reannihilating), then an error afflicts the encoded quantum state.

B. Planar codes

If all check operators are to be readily measured with local gates, then the qubits of the toric code need to be arranged on a topologically nontrivial surface, the torus, with the ancilla qubits needed for syndrome measurement arranged on an adjacent layer. In practice, the toroidal topology is likely to be inconvenient, especially if we want qubits residing in different tori to interact with one another in the course of a quantum computation. Fortunately, surface codes can be constructed in which all check operators are local and the qubits are arranged on planar sheets.[13,14] The planar topology will be more conducive to realistic quantum computing architectures.

In the planar version of the surface code, there is a distinction between the check operators at the boundary of the surface and the check operators in the interior. Check operators in the interior are four-qubit site or plaquette operators, and those at the boundary are three-qubit operators. Furthermore, the boundary has two different types of edges as shown in Fig. 5. Along a ''plaquette edge'' or ''rough edge,'' each check operator is a three-qubit plaquette operator $Z^{\otimes 3}$. Along a ''site edge'' or ''smooth edge,'' each check operator is a three-qubit site operator $X^{\otimes 3}$.

As before, in order to commute with the code stabilizer, a product of Z's must act on an even number of links adjacent to each site of the lattice. Now, though, the links acted upon by Z's may comprise an *open* path that begins and ends on a rough edge. We may then say that the one-chain

comprised of all links acted upon by Z is a cycle *relative to the rough edges*. Similarly, a product of X's that commutes with the stabilizer acts on a set of links of the dual lattice that comprise a cycle relative to the smooth edges.

Cycles relative to the rough edges come in two varieties. If the chain contains an even number of the free links strung along the rough edge, then it can be tiled by plaquettes (including the boundary plaquettes), and so the corresponding product of Z's is contained in the stabilizer. We say that the relative one-cycle is a relative boundary of a two-chain. However, a chain that stretches from one rough edge to another is not a relative boundary—it is a representative of a nontrivial relative homology class. The corresponding product of Z's commutes with the stabilizer but does not lie in it, and we may take it to be the logical operation $\overline{Z}$ acting on an encoded logical qubit. Similarly, cycles relative to the smooth edges also come in two varieties, and a product of X's associated with the nontrivial relative homology cycle of the dual lattice may be taken to be the logical operation $\overline{X}$ [see Fig. 5(a)].

A code with distance L is obtained from a square lattice, if the shortest paths from rough edge to rough edge, and from smooth edge to smooth edge, both contain L links. The lattice has $L^2+(L-1)^2$ links, $L(L-1)$ plaquettes, and $L(L-1)$ sites. Now all plaquette and site operators are independent, which is another way to see that the number of encoded qubits is $L^2+(L-1)^2-2L(L-1)=1$.

The distinction between a rough edge and a smooth edge can also be characterized by the behavior of the defects at the boundary, as shown in Fig. 5(b). In the toric codes, defects always appear in pairs, because every one-chain has an even number of boundary points. But for planar codes, individual defects can appear, since a one-chain can terminate on a rough edge. Thus a propagating site defect can reach the rough edge and disappear. But if the site defect reaches the smooth edge, it persists at the boundary. Similarly, a plaquette defect can disappear at the smooth edge, but not at the rough edge.

Let us briefly note some generalizations of the toric codes and planar codes that we have described. First, there is no need to restrict attention to lattices that have coordination number 4 at each site and plaquette. Any tessellation of a surface (and its dual tessellation) can be associated with a quantum code. Second, we may consider surfaces of higher genus. For a closed orientable Riemann surface of genus g, $2g$ qubits can be encoded—each time a handle is added to the surface, there are two new homology cycles and hence two new logical $\overline{Z}$'s. The distance of the code is the length of the shortest nontrivial cycle on lattice or dual lattice. For planar codes, we may consider a surface with e distinct rough edges separated by e distinct smooth edges. Then $e-1$ qubits can be encoded, associated with the relative one-cycles that connect one rough edge with any of the others. The distance is the length of the shortest path reaching from one rough edge to another, or from one smooth edge to another on the dual lattice. Alternatively, we can increase the number of encoded qubits stored in a planar sheet by punching holes in the lattice. For example, if the outer boundary of the surface is a smooth edge, and there are h holes, each bounded by a smooth edge, then h qubits are encoded. For each hole, a cycle on the lattice that encloses the hole is associated with the corresponding logical $\overline{Z}$, and a path on the dual lattice from the boundary of the hole to the outer boundary is associated with the logical $\overline{X}$.

If (say) phase errors are more common than bit-flip errors, quantum information can be stored more efficiently with an *asymmetric* planar code, such that the distance from rough edge to rough edge is longer than the distance from smooth edge to smooth edge. However, these asymmetric codes are less convenient for processing of the encoded information.

The surface codes can also be generalized to higher dimensional manifolds, with logical operations again associated with homologically nontrivial cycles. In Sec. X, we will discuss a four-dimensional example.

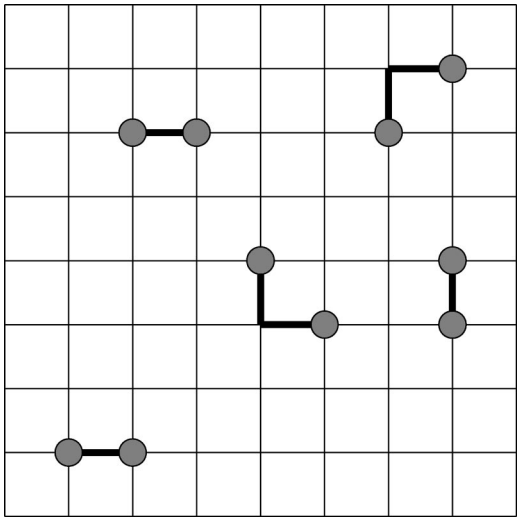

FIG. 6. Pairs of defects. If the error rate is small and errors on distinct links are uncorrelated, then connected error chains are typically short and the positions of defects are highly correlated. It is relatively easy to guess how the defects should be paired up so that each pair is the boundary of a connected chain.

C. Fault-tolerant recovery

A toric code defined on a lattice of linear size L has block size $2L^2$ and distance L. Therefore, if the probability of error per qubit is p, the number of errors expected in a large code block is of order pL^2, and therefore much larger than the code distance.

However, the performance of a toric code is much better than would be guessed naively based on its distance. In principle, $L/2$ errors could suffice to cause damage to the encoded information. But in fact this small number of errors can cause irrevocable damage only if the distribution of the errors is highly atypical.

If the error probability p is small, then links where errors occur (''error links'') are dilute on the lattice. Long connected chains of error links are quite rare, as indicated in Fig. 6. It is relatively easy to guess a way to pair up the observed defects that is homologically equivalent to the actual error chain. Hence we expect that a number of errors that scales *linearly* with the block size can be tolerated. That is, if the error probability p per link is small enough, we expect to be able to recover correctly with a probability that approaches one as the block size increases. We therefore anticipate that there is an accuracy threshold for storage of quantum information using a toric code.

Unfortunately, life is not quite so simple, because the measurement of the syndrome will not be perfect. Occasionally, a faulty measurement will indicate that a defect is present at a site even though no defect is actually there, and sometimes an actual defect will go unobserved. Hence the population of real defects (which have strongly correlated positions) will be obscured by a population of phony ''ghost defects'' and ''missing defects'' (which have randomly distributed positions), as in Fig. 7.

Therefore, we should execute recovery cautiously. It would be dangerous to blithely proceed by flipping qubits on a chain of links bounded by the observed defect positions. Since a ghost defect is typically far from the nearest genuine defect, this procedure would introduce many additional errors—what was formerly a ghost defect would become a real defect connected to another defect by a long error chain. Instead we must repeat the syndrome measurement an adequate number of times to verify its authenticity. It is subtle to formulate a robust recovery procedure that incorporates repeated measurements, since further errors accumulate as the measurements are repeated and the gas of defects continues to evolve.

We know of three general strategies that can be invoked to achieve robust macroscopic control

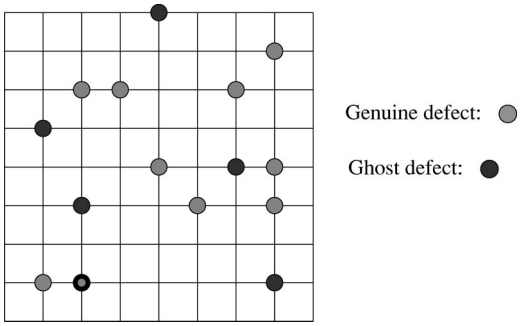

FIG. 7. Ghost defects. Since faults can occur in the measurement of the error syndrome, the measured syndrome includes both genuine defects (lightly shaded) associated with actual errors and phony ''ghost defects'' (darkly shaded) that arise at randomly distributed locations. To perform recovery successfully, we need to be able to distinguish reliably between the genuine defects and the ghost defects. The position that is shaded both lightly and darkly represents a genuine defect that goes unseen due to a measurement error.

of a system that is subjected to microscopic disorder. One method is to introduce a hierarchical organization in such a way that effects of noise get weaker and weaker at higher and higher levels of the hierarchy. This approach is used by Gács[15] in his analysis of robust one-dimensional classical cellular automata, and also in concatenated quantum coding.[6–10] A second method is to introduce more spatial dimensions. A fundamental principle of statistical physics is that local systems with higher spatial dimensionality and hence higher coordination number are more resistant to the disordering effects of fluctuations. In Sec. X we will follow this strategy in devising and analyzing a topological code that has nice locality properties in four dimensions. From the perspective of block coding, the advantage of extra dimensions is that local check operators can be constructed with a higher degree of redundancy, which makes it easier to reject faulty syndrome information.

In the bulk of this article we will address the issue of achieving robustness through a third strategy, namely by introducing a modest amount of nonlocality into our recovery procedure. But we will insist that all quantum processing is strictly local; the nonlocality will be isolated in *classical* processing. Specifically, to decide on the appropriate recovery step, a classical computation will be performed whose input is an error syndrome measured at all the sites of the lattice. We will require that this classical computation can be executed in a time bounded by a polynomial in the number of lattice sites. For the purpose of estimating the accuracy threshold, we will imagine that the classical calculation is instantaneous and perfectly accurate.

Our approach is guided by the expectation that quantum computers will be slow and unreliable while classical computers are fast and accurate. It is advantageous to replace quantum processing by classical processing if the classical processing can accomplish the same task.

D. Surface codes and physical fault tolerance

In this article, we regard the surface codes as block quantum error-correcting codes with properties that make them especially amenable to fault-tolerant quantum storage and computation. But we also remark here that because of the locality of the check operators, these codes admit another tempting interpretation that was emphasized in Refs. 4 and 5.

Consider a model physical system, with qubits arranged in a square lattice, and with a (local) Hamiltonian that can be expressed as minus the sum of the check operators of a surface code. Since the check operators are mutually commuting, we can diagonalize the Hamiltonian by diagonalizing each check operator separately, and its degenerate ground state is the code subspace. Thus, a real system that is described well enough by this model could serve as a robust quantum memory.

The model system has several crucial properties. First of all, it has a mass gap, so that its qualitative properties are stable with respect to generic weak local perturbations. Second, it has

two types of localized quasiparticle excitations, the site defects and plaquette defects. And third, there is an exotic long-range interaction between a site defect and a plaquette defect.

The interaction between the two defects is exactly analogous to the Aharonov–Bohm interaction between a localized magnetic flux Φ and a localized electric charge Q in two-spatial dimensions. When a charge is adiabatically carried around a flux, the wave function of the system is modified by a phase $\exp(iQ\Phi/\hbar c)$ that is independent of the separation between charge and flux. Similarly, if a site defect is transported around a plaquette defect, the wave function of the system is modified by the phase -1 independent of the separation between the defects. Formally, this phase arises because of the anticommutation relation satisfied by X and Z. Physically, it arises because the ground state of the system is very highly entangled and thus is able to support very-long-range quantum correlations. The protected qubits are encoded in the Aharonov–Bohm phases acquired by quasiparticles that travel around the fundamental nontrivial cycles of the surface; these could be measured in principle in a suitable quantum interference experiment.

It is useful to observe that the degeneracy of the ground state of the system is a necessary consequence of the unusual interactions among the quasiparticles.[19,20] A unitary operator $U_{S,1}$ can be constructed that describes a process in which a pair of site defects is created, one member of the pair propagates around a nontrivial cycle C_1 of the surface, and then the pair reannihilates. Similarly a unitary operator $U_{P,2}$ can be constructed associated with a plaquette defect that propagates around a complementary nontrivial cycle C_2 that intersects C_1 once. These operators commute with the Hamiltonian H of the system and can be simultaneously diagonalized with H, but $U_{S,1}$ and $U_{P,2}$ do not commute with one another. Rather, they satisfy (in an infinite system)

$$U_{P,2}{}^{-1}\ U_{S,1}{}^{-1}\ U_{P,2}\ U_{S,1} = -1. \tag{6}$$

The nontrivial commutator arises because the process in which (1) a site defect winds around C_1, (2) a plaquette defect winds around C_2, (3) the site defect winds around C_1 in the reverse direction, and (4) the plaquette defect winds around C_2 in the reverse direction is topologically equivalent to a process in which the site defect winds once around the plaquette defect.

Because $U_{S,1}$ and $U_{P,2}$ do not commute, they cannot be simultaneously diagonalized—indeed applying $U_{P,2}$ to an eigenstate of $U_{S,1}$ flips the sign of the $U_{S,1}$ eigenvalue. Physically, there are two distinct ground states that can be distinguished by the Aharonov–Bohm phase that is acquired when a site defect is carried around C_1; we can change this phase by carrying a plaquette defect around C_2. Similarly, the operator $U_{S,2}$ commutes with $U_{S,1}$ and $U_{P,2}$ but anticommutes with $U_{P,1}$. Therefore there are four distinct ground states, labeled by their $U_{S,1}$ and $U_{S,2}$ eigenvalues.

This reasoning shows that the topological interaction between site defects and plaquette defects implies that the system on an (infinite) torus has a generic four-fold ground-state degeneracy. The argument is easily extended to show that the generic degeneracy on a genus g Riemann surface is 2^{2g}. By a further extension, we see that the generic degeneracy is q^{2g} if the Aharonov–Bohm phase associated with winding one defect around another is

$$\exp(2\pi i p/q), \tag{7}$$

where p and q are integers with no common factor.

The same sort of argument can be applied to planar systems with a mass gap in which single defects can disappear at an edge. For example, consider an annulus in which site defects can disappear at the inner and outer edges. Then states can be classified by the Aharonov–Bohm phase acquired by a plaquette defect that propagates around the annulus, a phase that flips in sign if a site defect propagates from inner edge to outer edge. Hence there is a two-fold degeneracy on the annulus. For a disc with h holes, the degeneracy is 2^h if site defects can disappear at any boundary, or q^h if the Aharonov–Bohm phase of site defect winding about plaquette defect is $\exp(2\pi i p/q)$.

These degeneracies are exact for the unperturbed model system, but will be lifted slightly in a weakly perturbed system of finite size. Loosely speaking, the effect of perturbations will be to

give the defects a finite effective mass, and the lifting of the degeneracy is associated with quantum tunneling processes in which a virtual defect winds around a cycle of the surface. The amplitude A for this process has the form

$$A \sim C \exp(-\sqrt{2}(m^*\Delta)^{1/2}L/\hbar), \tag{8}$$

where L is the physical size of the shortest nontrivial (relative) cycle of the surface, m^* is the defect effective mass, and Δ is the minimal energy cost of creating a defect. The energy splitting is proportional to A, and like A becomes negligible when the system is large compared to the characteristic length $l \equiv \hbar(m^*\Delta)^{-1/2}$.

In this limit, and at sufficiently low temperature, the degenerate ground state provides a reliable quantum memory. If a pair of defects is produced by a thermal fluctuation, and one of the defects wanders around a nontrivial cycle before the pair reannihilates, then the encoded quantum information will be damaged. These fluctuations are suppressed by the Boltzman factor $\exp(-\Delta/kT)$ at low temperature. Even if defect nucleation occurs at a non-negligible rate, we could enhance the performance of the quantum memory by continually monitoring the state of the defect gas. If the winding of defects around nontrivial cycles is detected and carefully recorded, damage to the encoded quantum information can be controlled.

IV. THE STATISTICAL PHYSICS OF ERROR RECOVERY

One of our main objectives in this article is to invoke surface coding to establish an accuracy threshold for quantum computation—how well must quantum hardware perform for quantum storage, or universal quantum computation, to be achievable with arbitrarily small probability of error? In this section, rather than study the efficacy of a particular fault-tolerant protocol for error recovery, we will address whether the syndrome of a surface code is adequate in principle for protecting quantum information from error. Specifically, we will formulate an order parameter that distinguishes two phases of a quantum memory: an ''ordered'' phase in which reliable storage is possible, and a ''disordered phase'' in which errors unavoidably afflict the encoded quantum information. Of course, this phase boundary also provides an upper bound on the accuracy threshold that can be reached by any particular protocol. The toric code and the planar surface code have the same accuracy threshold, so we may study either to learn about the other.

A. The error model

Let us imagine that in a single time step, we will execute a measurement of each stabilizer operator at each site and each plaquette of the lattice. During each time step, new qubit errors might occur. To be concrete and to simplify the discussion, we assume that all qubit errors are stochastic, and so can be assigned probabilities. (For example, errors that arise from decoherence have this property.) We will also assume that the errors acting on different qubits are independent, that bit-flip (X) errors and phase (Z) errors are uncorrelated with one another, and that X and Z errors are equally likely. Thus the error in each time step acting on a qubit with state ρ can be represented by the quantum channel

$$\rho \to (1-p)^2 I\rho I + p(1-p)X\rho X + p(1-p)Z\rho Z + p^2 Y\rho Y, \tag{9}$$

where p denotes the probability of either an X error or a Z error. It is easy to modify our analysis if some of these assumptions are relaxed; in particular, correlations between X and Z errors would not cause much trouble, since we have separate procedures for recovery from the X errors and the Z errors.

Faults can also occur in the syndrome measurement. We assume that these measurement errors are uncorrelated. We will denote by q the probability that the measured syndrome bit is faulty at a given site or plaquette.

Aside from being uncorrelated in space, the qubit and measurement errors are also assumed to be uncorrelated in time. Furthermore, the qubit and measurement errors are not correlated with one another. We assume that p and q are known quantities—our choice of recovery algorithm depends

on their values. In Sec. VII, we will discuss how p and q can be related to more fundamental quantities, namely the fidelities of elementary quantum gates. There we will see that the execution of the syndrome measurement circuit can introduce correlations between errors. Fortunately, these correlations (which we ignore for now) do not have a big impact on the accuracy threshold.

B. Defects in space–time

Because syndrome measurement may be faulty, it is necessary to repeat the measurement to improve our confidence in the outcome. But since new errors may arise during the repeated measurements, it is a subtle matter to formulate an effective procedure for rejecting measurement errors.

Let us suppose, for a toric block of arbitrarily large size, that we measure the error syndrome once per time step, that we monitor the block for an arbitrarily long time, and that we store all of the syndrome information that is collected. We want to address whether this syndrome information enables us to recover from errors with a probability of failure that becomes exponentially small as the size of the toric block increases. The plaquette check operators identify bit flips and the site check operators identify phase errors; therefore we consider bit-flip and phase error recovery separately.

For analyzing how the syndrome information can be used most effectively, it is quite convenient to envision a *three-dimensional* simple cubic lattice, with the third dimension representing an integer-valued *time*. We imagine that the error operation acts at each integer-valued time t, with a syndrome measurement taking place in between each t and $t+1$. Qubits in the code block can now be associated with timelike plaquettes, those lying in the tx and ty planes. A qubit error that occurs at time t is associated with a horizontal (spacelike) link that lies in the time slice labeled by t. The outcome of the measurement of the stabilizer operator $X_s = X^{\otimes 4} = \pm 1$ at site s, performed between time t and time $t+1$, is marked on the vertical (timelike) link connecting site s at time t and site s at time $t+1$. A similar picture applies to the history of the Z_P stabilizer operators at each plaquette, but with the lattice replaced by its dual.

On some of these vertical links, the measured syndrome is erroneous. We will repeat the syndrome measurement T times in succession, and the ''error history'' can be described as a set of marked links on a lattice with altogether T time slices. The error history encompasses both error events that damage the qubits in the code block, and faults in the syndrome measurements. On the initial $(t=0)$ slice are marked all uncorrected qubit errors that are left over from previous rounds of error correction; new qubit errors that arise at a later time t $(t=1,2,\ldots,T-1)$ are marked on horizontal links on slice t. Errors in the syndrome measurement that takes place between time t and $t+1$ are marked on the corresponding vertical links. Errors on horizontal links occur with probability p, and errors on vertical links occur with probability q.

For purposes of visualization, it is helpful to consider the simpler case of a quantum repetition code, which can be used to protect coherent quantum information from bit-flip errors if there are no phase errors (or phase errors if there are no bit-flip errors). In this case we may imagine that qubits reside on sites of a periodically identified one-dimensional lattice (i.e., a circle); at each link the stabilizer generator ZZ acts on the two neighboring sites. Then there is one encoded qubit—the two-dimensional code space is spanned by the state $|000\ldots0\rangle$ with all spins ''up,'' and the state $|111\ldots\rangle$ with all spins ''down.'' In the case where the syndrome measurement is repeated to improve reliability, we may represent the syndrome's history by associating qubits with plaquettes of a two-dimensional lattice, and syndrome bits with the timelike links, as shown in Figs. 8 and 9. Again, bit-flip errors occur on horizontal links with probability p and syndrome measurement errors occur on vertical links with probability q.

Of course, as already noted in Sec. III C, we may also use a two-dimensional lattice to represent the error configuration of the toric code, in the case where the syndrome measurements are perfect. In that case, we can collect reliable information by measuring the syndrome in one shot, and errors occur on links of the two-dimensional lattice with probability p.

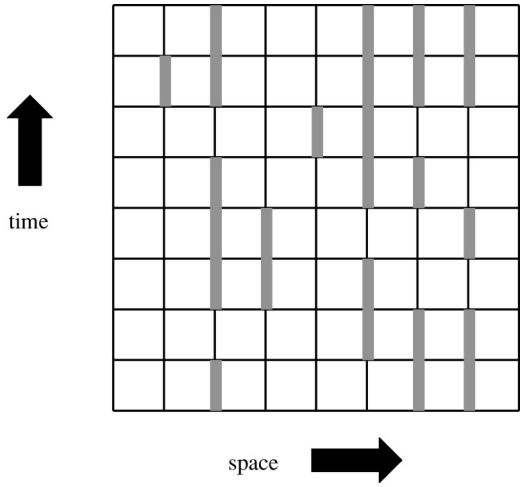

FIG. 8. The two-dimensional lattice depicting a history of the error syndrome for the quantum repetition code, with time running upward. Each row represents the syndrome at a particular time. Qubits reside on plaquettes, and two-qubit check operators are measured at each vertical link. Links where the syndrome is nontrivial are shaded.

C. Error chains, world lines, and magnetic flux tubes

In practice, we will always want to protect quantum information for some finite time. But for the purpose of investigating whether error correction will work effectively in principle, it is convenient to imagine that our repeated rounds of syndrome measurement extend indefinitely into the past and into the future. Qubit errors are continually occurring; as defects are created in pairs, propagate about on the lattice, and annihilate in pairs, the world lines of the defects form closed loops in space–time. Some loops are homologically trivial and some are homologically nontrivial. Error recovery succeeds if we are able to correctly identify the homology class of each closed loop. But if a homologically nontrivial loop arises that we fail to detect, or if we mistakenly believe that a homologically nontrivial loop has been generated when none has been, then error

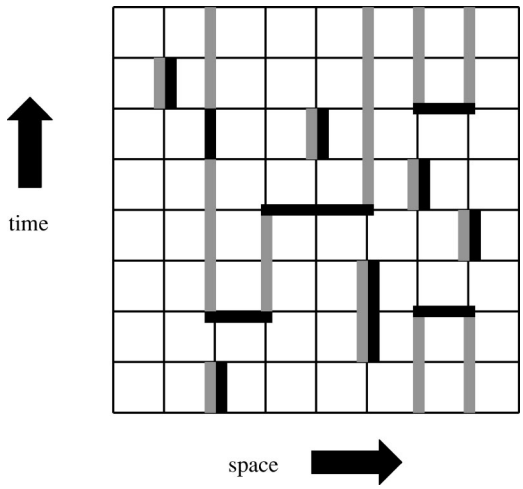

FIG. 9. An error history shown together with the syndrome history that it generates, for the quantum repetition code. Links where errors occurred are darkly shaded, and links where the syndrome is nontrivial are lightly shaded. Errors on horizontal links indicate where a qubit flipped between successive syndrome measurements, and errors on vertical links indicate where the syndrome measurement was wrong. Vertical links that are shaded both lightly and darkly are locations where a nontrivial syndrome was found erroneously. The chain of lightly shaded links (the syndrome) and the chain of darkly shaded links (the errors) both have the same boundary.

recovery will fail. For now, let us consider this scenario in which we continue to measure the syndrome forever—in Sec. VI, we will consider some issues that arise when we perform error correction for a finite time.

So let us imagine a particular history extending over an indefinite number of time slices, with the observed syndrome marked on each vertical link, measurement errors marking selected vertical links, and qubit errors marking selected horizontal links. For this history we may identify several distinct one-chains (sets of links). We denote by S the *syndrome chain* containing all (vertical) links at which the measured syndrome is nontrivial ($X_s=-1$). We denote by E the *error chain* containing all links where errors have occurred, including both qubit errors on horizonal links and measurement errors on vertical links. Consider $S+E$, the disjoint union of S and E ($S+E$ contains the links that are in either S or E, but not both). The chain $S+E$ represents the ''actual'' world lines of the defects generated by qubit errors, as illustrated in Fig. 9. Its vertical links are those on which the syndrome would be nontrivial were it measured without error. Its horizontal links are events where a defect pair is created, a pair annihilates, or an existing defect propagates from one site to a neighboring site. Since the world lines never end, the chain $S+E$ has no boundary, $\partial(S+E)=0$. Equivalently S and E have the same boundary, $\partial S=\partial E$.

Hence, the measured syndrome S reveals the boundary of the error chain E; we may write $E=S+C$, where C is a *cycle* (a chain with no boundary). But any other error chain $E'=S+C'$, where C' is a cycle, has the same boundary as E and therefore could have caused the same syndrome. To recover from error, we will use the syndrome information to make a hypothesis, guessing that the actual error chain was $E'=S+C'$. Now, E' may not be the same chain as E, but, as long as the cycle $E+E'=C+C'$ is homologically trivial (the boundary of a surface), then recovery will be successful. If $C+C'$ is homologically nontrivial, then recovery will fail. We say that C and C' are in the same *homology class* if $C+C'$ is homologically trivial. Therefore, whether we can protect against error hinges on our ability to identify not the cycle C, but rather the homology class of C.

Considering the set of all possible histories, let prob(E') denote the probability of the error chain E' (strictly speaking, we should consider the total elapsed time to be finite for this probability to be defined). Then the probability that the syndrome S was caused by any error chain $E'=S+C'$, such that C' belongs to the homology class h, is

$$\mathrm{prob}(h|S)=\frac{\Sigma_{C'\in h}\mathrm{prob}(S+C')}{\Sigma_{C'}\mathrm{prob}(S+C')}. \tag{10}$$

Clearly, then, given a measured syndrome S, the optimal way to recover is to guess that the homology class h of C is the class with the highest probability according to Eq. (10). Recovery succeeds if C belongs to this class, and fails otherwise.

We say that the probability of error per qubit lies below the accuracy threshold if and only if the recovery procedure fails with a probability that vanishes as the linear size L of the lattice increases to infinity. Therefore, below threshold, the cycle C actually belongs to the class h that maximizes Eq. (10) with a probability that approaches one as $L\to\infty$. It is convenient to restate this criterion in a different way that makes no explicit reference to the syndrome chain S. We may write the relation between the actual error chain E and the hypothetical error chain E' as $E'=E+D$, where D is the cycle that we called $C+C'$ above. Let prob$[(E+D)|E]$ denote the normalized conditional probability for error chains $E'=E+D$ that have the same boundary as E. Then, the probability of error per qubit lies below threshold if and only if, in the limit $L\to\infty$,

$$\sum_E \mathrm{prob}(E)\cdot\sum_{D\ \mathrm{nontrivial}}\mathrm{prob}[(E+D)|E]=0. \tag{11}$$

Equation (11) says that error chains that differ from the actual error chain by a homologically nontrivial cycle have probability zero. Therefore, the observed syndrome S is sure to point to the correct homology class, in the limit of an arbitrarily large code block.

This accuracy threshold achievable with toric codes can be identified with a phase transition in a particular statistical physics model defined on a lattice. In a sense that we will make precise, the error chains are analogous to magnetic flux tubes in a superconductor, and the boundary points of the error chains are magnetic monopoles where these flux tubes terminate. Fixing the syndrome pins down the monopoles, and the ensemble of chains with a specified boundary can be regarded as a thermal ensemble. As the error probability increases, the thermal fluctuations of the flux tubes increase, and at the critical temperature corresponding to the accuracy threshold, the flux tubes condense and the superconductivity is destroyed.

A similar analogy applies to the case where the syndrome is measured perfectly, and a two-dimensional system describes the syndrome on a single time slice. Then the error chains are analogous to domain walls in an Ising ferromagnet, and the boundary points of the error chains are ''Ising vortices'' where domain walls terminate. Fixing the syndrome pins down the vortices, and the ensemble of chains with a specified boundary can be interpreted as a thermal ensemble. As the error probability increases, the domain walls heat up and fluctuate more vigorously. At a critical temperature corresponding to the accuracy threshold, the domain walls condense and the system becomes magnetically disordered. This two-dimensional model also characterizes the accuracy threshold achievable with a quantum repetition code, if the syndrome is imperfect and the qubits are subjected only to bit-flip errors (or only to phase errors).

D. Derivation of the model

Let us establish the precise connection between our error model and the corresponding statistical physics model. In the two-dimensional case, we consider a square lattice with links representing qubits, and assume that errors arise independently on each link with probability p. In the three-dimensional case, we consider a simple cubic lattice. Qubits reside on the timelike plaquettes, and qubit errors arise independently with probability p on spacelike links. Measurement errors occur independently with probability q on timelike links. For now, we will make the simplifying assumption that $q=p$ so that the model is isotropic; the generalization to $q\neq p$ is straightforward.

An error chain E, in either two or three dimensions, can be characterized by a function $n_E(l)$ that takes a link ℓ to $n_E(\ell)\in\{0,1\}$, where $n_E(\ell)=1$ for each link ℓ that is occupied by the chain. Hence the probability that error chain E occurs is

$$\mathrm{prob}(E)=\prod_\ell\,(1-p)^{1-n_E(\ell)}p^{n_E(\ell)}=\left[\prod_\ell\,(1-p)\right]\cdot\prod_\ell\,\left(\frac{p}{1-p}\right)^{n_E(\ell)}, \tag{12}$$

where the product is over all links of the lattice.

Now suppose that the error chain E is fixed, and we are interested in the probability distribution for all chains E' that have the same boundary as E. Note that we may express $E'=E+C$, where C is a cycle (a chain with no boundary) and consider the probability distribution for C. Then if $n_C(\ell)=1$ and $n_E(\ell)=0$, the link ℓ is occupied by E' but not by E, an event whose probability (aside from an overall normalization) is

$$\left(\frac{p}{1-p}\right)^{n_C(\ell)}. \tag{13}$$

But if $n_C(\ell)=1$ and $n_E(\ell)=1$, then the link ℓ is not occupied by E', an event whose probability (aside from an overall normalization) is

$$\left(\frac{1-p}{p}\right)^{n_C(\ell)}. \tag{14}$$

Thus a chain $E'=E+C$ with the same boundary as E occurs with probability

$$\mathrm{prob}(E'|E) \propto \prod_{\ell} \exp(J_\ell u_\ell); \tag{15}$$

here we have defined

$$u_\ell = 1 - 2n_C(\ell) \in \{1,-1\}, \tag{16}$$

and the coupling J_ℓ assigned to link ℓ has the form

$$e^{-2J_\ell} = \begin{cases} p/(1-p), & \text{for } \ell \notin E, \\ (1-p)/p, & \text{for } \ell \in E. \end{cases} \tag{17}$$

Recall that the one-chain $\{\ell | u_l = -1\}$ is required to be a *cycle*—it has no boundary.

It is obvious from this construction that $\mathrm{prob}(E'|E)$ does not depend on how the chain E is chosen—it depends only on the boundary of E. We will verify this explicitly below.

The cycle condition satisfied by the u_l's can be expressed as

$$\prod_{\ell \ni s} u_\ell = 1; \tag{18}$$

at each site s, an even number of links incident on that site have $u_\ell = -1$. It is convenient to *solve* this condition, expressing the u_ℓ's in terms of unconstrained variables. To achieve this in two dimensions, we associate with each link ℓ a link ℓ^* *of the dual lattice*. Under this duality, sites are mapped to plaquettes, and the cycle condition becomes

$$\prod_{\ell^* \in P^*} u_{\ell^*} = 1. \tag{19}$$

To solve the constraint, we introduce variables $\sigma_i \in \{1,-1\}$ associated with each site i of the dual lattice, and write

$$u_{ij} = \sigma_i \sigma_j \tag{20}$$

where i and j are nearest-neighbor sites.

Our solution to the constraint is not quite the most general possible. In the language of differential forms, we have solved the condition $du = 0$ (where u is a discrete version of a one-form, and d denotes the exterior derivative) by writing $u = d\sigma$, where σ is a zero-form. Thus our solution misses the cohomologically nontrivial closed forms, those that are not exact. In the language of homology, our solution includes all and only those cycles that are homologically trivial—that is, cycles that bound a surface.

In three dimensions, links are dual to plaquettes, and sites to cubes. The cycle condition becomes, on the dual lattice,

$$\prod_{P^* \in C^*} u_{P^*} = 1; \tag{21}$$

each dual cube C^* contains an even number of dual plaquettes that are occupied by the cycle. We solve this constraint by introducing variables $\sigma_{\ell^*} \in \{1,-1\}$ on the dual links, and defining

$$u_{P^*} = \prod_{\ell^* \in P^*} \sigma_{\ell^*}. \tag{22}$$

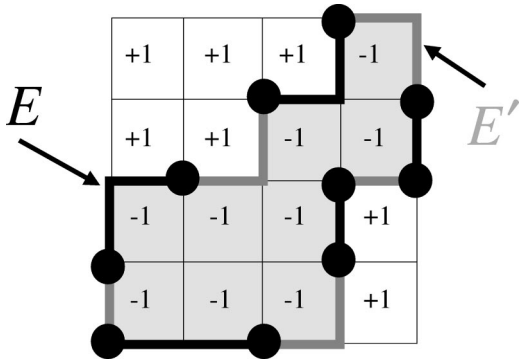

FIG. 10. The "quenched" error chain E and the "fluctuating" error chain E', as represented in the two-dimensional random-bond Ising model. Ising spins taking values in $\{\pm 1\}$ reside on plaquettes, Ising vortices are located on the sites marked by filled circles, and the coupling between neighboring spins is antiferromagnetic along the path E that connects the Ising vortices. The links of E' comprise a domain wall connecting the vortices. The closed path $C=E+E'$ encloses a domain of spins with the value -1.

In this case, we have solved a discrete version of $du=0$, where u is a two-form, by writing $u=d\sigma$, where σ is a one-form. Once again, our solution generates only the cycles that are homologically trivial.

We have now found that, in two dimensions, the "fluctuations" of the error chains E' that share a boundary with the chain E are described by a statistical-mechanical model with partition function

$$Z[J,\eta]=\sum_{\{\sigma_i\}} \exp\left(J\sum_{\langle ij\rangle} \right) \eta_{ij}\sigma_i\sigma_j, \tag{23}$$

where $e^{-2J}=p/(1-p)$. The sum in the exponential is over pairs of nearest neighbors on a square lattice, and $\eta_l \in \{1,-1\}$ is defined by

$$\eta_\ell=\begin{cases} 1, & \text{if } \ell \notin E^*, \\ -1, & \text{if } \ell \in E^*. \end{cases} \tag{24}$$

Furthermore, if the error chains E and E' are generated by sampling the same probability distribution, then the η_ℓ's are chosen at random subject to

$$\eta_\ell=\begin{cases} 1, & \text{with probability } 1-p, \\ -1, & \text{with probability } p. \end{cases} \tag{25}$$

This model is the well-known "random-bond Ising model." Furthermore, the relation $e^{-2J}=p/(1-p)$ between the coupling and the bond probability defines the "Nishimori line" [21] in the phase diagram of the model, which has attracted substantial attention because the model is known to have enhanced symmetry properties on this line. (For a recent discussion, see Ref. 22.)

Perhaps the interpretation of this random-bond Ising model can be grasped better if we picture the original lattice rather than the dual lattice, so that the Ising spins reside on plaquettes as in Fig. 10. The coupling between spins on neighboring plaquettes is antiferromagnetic on the links belonging to the chain E (where $\eta_\ell=-1$), meaning that it is energetically preferred for the spins to antialign at these links. At links not in E (where $\eta=1$), it is energetically preferred for the spins to align. Thus a link ij is excited if $\eta_{ij}\sigma_i\sigma_j=-1$. We say that the excited links constitute "domain walls." In the case where $\eta_\ell=1$ on every link, a wall marks the boundary between two regions in which the spins point in opposite directions. Walls can never end, because the boundary of a boundary is zero.

But if the η configuration is nontrivial, then the ''walls'' can end. Indeed each boundary point of the chain E of links with $\eta_l=-1$ is an endpoint of a wall, what we will call an ''Ising vortex.'' For example, for the configuration shown in Fig. 10, a domain wall occupies the chain E' that terminates on Ising vortices at the marked sites. The figure also illustrates that the model depends only on the boundary of the chain E, and not on other properties of the chain. To see this, imagine performing the change of variables

$$\sigma_i \rightarrow -\sigma_i \tag{26}$$

on the shaded plaquettes of Fig. 10. A mere change of variable cannot alter the locations of the excited links—rather, the effect is to shift the antiferromagnetic couplings from the chain E to a different chain E' with the same boundary.

In three dimensions, the fluctuations of the error chains that share a boundary with the specified chain E are described by a model with partition function

$$Z[J,\eta]=\sum_{\{\sigma_\ell\}} \exp\left(J\sum_P \eta_P u_P \right), \tag{27}$$

where $u_P=\Pi_{\ell\in P}\sigma_\ell$ and

$$\eta_P=\begin{cases} 1, & \text{if } P\notin E^*, \\ -1, & \text{if } P\in E^*. \end{cases} \tag{28}$$

This model is a ''random-plaquette'' Z_2 gauge theory in three dimensions, which, as far as we know, has not been much studied previously. Again, we are interested in the ''Nishimori line'' of this model where $e^{-2J}=p/(1-p)$, and p is the probability that a plaquette has $\eta_P=-1$.

In this three-dimensional model, we say that a plaquette P is excited if $\eta_P u_P=-1$. The excited plaquettes constitute ''magnetic flux tubes''—these form closed loops on the original lattice if $\eta_P=1$ on every plaquette. But at each boundary point of the chain E on the original lattice (each cube on the dual lattice that contains an odd number of plaquettes with $\eta_P=-1$), the flux tubes can end. The sites of the original lattice (or cubes of the dual lattice) that contain endpoints of magnetic flux tubes are said to be ''magnetic monopoles.''

E. Order parameters

As noted, our statistical-mechanical model includes a sum over those and only those chains E' that are *homologically equivalent* to the chain E. To determine whether errors can be corrected reliably, we want to know whether chains E' in a *different* homology class than E have negligible probability in the limit of a large lattice (or code block). The relative likelihood of different homology classes is determined by the free energy difference of the classes; in the ordered phase, we anticipate that the free energy of nontrivial classes exceeds that of the trivial classes by an amount that increases linearly with L, the linear size of the lattice.

But for the purpose of finding the value of the error probability at the accuracy threshold, it suffices to consider the model in an infinite volume (where there is no nontrivial homology). In the ordered phase where errors are correctable, large fluctuations of domain walls or flux tubes are suppressed, while in the disordered phase the walls or tubes ''dissolve'' and cease to be well defined.

Thus, the phase transition corresponding to the accuracy threshold is a singularity, in the infinite-volume limit, in the ''quenched'' free energy, defined as

$$[\beta F(J,\eta)]_p \equiv -\sum_{\{\eta\}} \text{Prob}(\eta)\cdot \ln Z[J,\eta], \tag{29}$$

where

$$\mathrm{Prob}(\eta)=\prod_{\ell}(1-p)^{1-\eta_\ell}p^{\eta_\ell} \tag{30}$$

in two dimensions, or

$$\mathrm{Prob}(\eta)=\prod_{P}(1-p)^{1-\eta_P}p^{\eta_P} \tag{31}$$

in three dimensions. The term ''quenched'' signifies that, although the η chains are generated at random, we consider thermal fluctuations with the positions of the vortices or monopoles pinned down. The inverse temperature β is identical to the coupling J. We use the notation $[\cdot]_p$ to indicate an average with respect to the quenched randomness, and we will denote by $\langle\cdot\rangle_\beta$ an average over thermal fluctuations.

There are various ways to describe the phase transition in this system, and to specify an order parameter. For example, in the two-dimensional Ising system, we may consider a ''disorder parameter'' $\Phi(x)$ that inserts a single Ising vortex at a specified position x. To define this operator, we must consider either an infinite system or a finite system with a boundary; on the torus, Ising vortices can only be inserted in pairs. But for a system with a boundary, we can consider a domain wall with one end at the boundary and one end in the bulk. In the *ferromagnetic* phase, the cost in free energy of introducing an additional vortex at x is proportional to L, the distance from x to the boundary. Correspondingly we find

$$[\langle\Phi(x)\rangle_\beta]_p=0 \tag{32}$$

in the limit $L\to\infty$. The disorder parameter vanishes because we cannot introduce an isolated vortex without creating an infinitely long domain wall. In the disordered phase, an additional vortex can be introduced at finite free energy cost, and hence

$$[\langle\Phi(x)\rangle_\beta]_p\neq 0. \tag{33}$$

On the torus, we may consider an operator that inserts not a semi-infinite domain wall terminating on a vortex, but instead a domain wall that winds about a cycle of the torus. Again, in the ferromagnetically ordered phase, the cost in free energy of inserting the domain wall will be proportional to L, the minimal length of a cycle. Specifically, in our two-dimensional Ising spin model, consider choosing an η-chain and evaluating the corresponding partition function

$$Z[J,\eta]=\exp[-\beta F(J,\eta)]. \tag{34}$$

Now choose a set of links C of the original lattice that constitute a nontrivial cycle wound around the torus, and replace $\eta_l\to-\eta_l$ for the corresponding links of the dual lattice, $l\in C^*$. Evaluate, again, the partition function, obtaining

$$Z_C[J,\eta]=\exp[-\beta F_C(J,\eta)]. \tag{35}$$

Then the free energy cost of the domain wall is given by

$$\beta F_C(J,\eta)-\beta F(J,\eta)=-\ln\left(\frac{Z_C[J,\eta]}{Z[J,\eta]}\right). \tag{36}$$

After averaging over $\{\eta\}$, this free energy cost diverges as $L\to\infty$ in the ordered phase, and converges to a constant in the disordered phase.

There is also a dual order parameter that vanishes in the disordered phase—the spontaneous magnetization of the Ising spin system. Strictly speaking, the defining property of the nonferromagnetic disordered phase is that spin correlations decay with distance, so that

$$\lim_{r\to\infty}[\langle\sigma_0\sigma_r\rangle_\beta]_p=0 \tag{37}$$

in the disordered phase. Correspondingly, the mean squared magnetization per site,

$$m^2\equiv N^{-2}\sum_{i,j}\ [\langle\sigma_i\sigma_j\rangle_\beta]_p\,, \tag{38}$$

where i,j are summed over all spins and N is the total number of spins, approaches a nonzero constant as $N\to\infty$ in the ordered phase, and approaches zero as a positive power of $1/N$ in the disordered phase.

Similarly in our three-dimensional gauge theory, there is a disorder parameter that inserts a single magnetic monopole, which we may think of as the end of a semi-infinite flux tube. Alternatively, we may consider the free energy cost of inserting a flux tube that wraps around the torus, which is proportional to L in the magnetically ordered phase. In the three-dimensional model, the partition function $Z_C[J,\eta]$ in the presence of a flux tube wrapped around the nontrivial cycle C of the original lattice is obtained by replacing $\eta_P\to-\eta_P$ on the plaquettes dual to the links of C. The magnetically ordered phase is called a ''Higgs phase'' or a ''superconducting phase.'' The magnetically disordered phase is called a ''confinement phase'' because in this phase introducing an isolated electric charge has a infinite cost in free energy, and electric charges are confined in pairs by electric flux tubes.

An order parameter for the Higgs-confinement transition is the Wilson loop operator

$$W(C)=\prod_{\ell\in C}\ \sigma_\ell \tag{39}$$

associated with a closed loop C of links on the lattice. This operator can be interpreted as the insertion of a charged particle source whose world line follows the path C. In the confinement phase, this world line becomes the boundary of the world sheet of an electric flux tube, so that the free energy cost of inserting the source is proportional to the minimal area of a surface bounded by C; that is,

$$-\ln[\langle W(C)\rangle_\beta]_p \tag{40}$$

increases like the area enclosed by the loop C in the confinement phase, while in the Higgs phase it increases like the perimeter of C. [A subtle point is that the relevant Wilson loop operator differs from that considered in Sec. 10 of Ref. 23. In that reference, the Wilson loop was modified so that the ''Dirac strings'' connecting the monopoles would be invisible. But in our case, the Dirac strings have a physical meaning (they comprise the chain E) and we are genuinely interested in how far the physical flux tubes (comprising the chain E') fluctuate away from the Dirac strings!]

In the case $q\neq p$, our gauge theory becomes anisotropic—p controls the coupling and the quenched disorder on the timelike plaquettes, while q controls the coupling and the quenched disorder on the spacelike plaquettes. The tubes of flux in $E+E'$ will be stretched in the time direction for $q>p$ and compressed in the time direction for $q<p$. Correspondingly, spacelike and timelike Wilson loops will decay at different rates. Still, one expects that (for $0<q<\frac{1}{2}$) a single phase boundary in the $p-q$ plane separates the region in which both timelike and spacelike Wilson loops decay exponentially with area (confinement phase) from the region in which both timelike and spacelike Wilson loops decay exponentially with perimeter. In the limit $q\to0$, flux on the spacelike plaquettes becomes completely suppressed, and the timelike plaquettes on distinct time slices decouple, each described by the two-dimensional spin model described earlier. Similarly, in the limit $p\to0$, the gauge theory reduces to decoupled one-dimensional spin models extending in the vertical direction, with a critical point at $q=\frac{1}{2}$.

F. Accuracy threshold

What accuracy threshold can be achieved by surface codes? We have found that in the case where the syndrome is measured perfectly ($q=0$), the answer is determined by the value of critical point of the two-dimensional random-bond Ising model on the Nishimori line. This value has been determined by numerically evaluating the domain wall free energy; recent studies by Honecker *et al.*[24] and Merz and Chalker[25] find

$$p_c = 0.1094 \pm 0.0002. \tag{41}$$

A surface code is a Calderbank–Shor–Steane (CSS) code, meaning that each stabilizer generator is either a tensor product of X's or a tensor product of Z's.[26,27] If X errors and Z errors each occur with probability p, then it is known that CSS codes exist with asymptotic rate $R \equiv k/n$ (where n is the block size and k is the number of encoded qubits) such that error recovery will succeed with probability arbitrarily close to one, where

$$R = 1 - 2H_2(p); \tag{42}$$

here $H_2(p) = -p \log_2 p - (1-p)\log_2(1-p)$ is the binary Shannon entropy. This rate hits zero when p has the value

$$p_c = 0.1100, \tag{43}$$

which marginally agrees with Eq. (41) within statistical errors. Thus the critical error probability is (at least approximately) the same regardless of whether we allow arbitrary CSS codes or restrict to those with a locally measurable syndrome. This result is analogous to the property that the classical repetition code achieves reliable recovery from bit-flip errors for any error probability $p < \frac{1}{2}$, the value for which the Shannon capacity hits zero. Note that Eq. (41) can also be interpreted as a threshold for the quantum repetition code, in the case where the bit-flip error rate and the measurement error rate are equal ($p=q$).

If measurement errors are incorporated, then the accuracy threshold achievable with surface codes is determined by the critical point along the Nishimori line of the three-dimensional Z_2 gauge theory with quenched randomness. In that model the measurement error probability q (the error weight for vertical links) and the bit-flip probability p (the error weight for horizontal links) are independent parameters. It seems that numerical studies of this quenched gauge theory have not been done previously, even in the isotropic case; work on this problem is in progress.

Since recovery is more difficult with imperfect syndrome information than with perfect syndrome information, the numerical data on the random-bond Ising model indicate that $p_c < 0.11$ for any $q > 0$. For the case $p=q$, we will derive the lower bound $p_c \geqslant 0.0114$ in Sec. V.

G. Free energy versus energy

In either the two-dimensional model (if $q=0$) or the three-dimensional model (if $q>0$), the critical error probability along the Nishimori line provides a criterion for whether it is possible in principle to perform flawless recovery from errors. In practice, we would have to execute a classical computation, with the measured syndrome as input, to determine how error recovery should proceed. The defects revealed by the syndrome measurement can be brought together to annihilate in several homologically distinct ways; the classical computation determines which of these ''recovery chains'' should be chosen.

We can determine the right homology class by computing the free energy for each homology class, and choosing the one with minimal free energy. In the ordered phase (error probability below threshold) the correct sector will be separated in free energy from other sectors by an amount linear in L, the linear size of the lattice.

The computation of the free energy could be performed by, for example, the Monte Carlo method. It should be possible to identify the homology class that minimizes the free energy in a

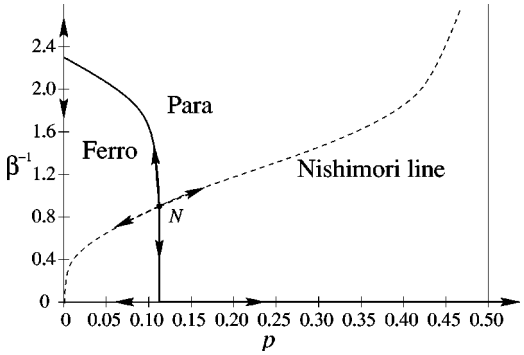

FIG. 11. The phase diagram of the random-bond Ising model, with the temperature β^{-1} on the vertical axis and the probability p of an antiferromagnetic bond on the horizontal axis. The solid line is the boundary between the ferromagnetic (ordered) phase and the paramagnetic (disordered) phase. The dotted line is the Nishimori line $e^{-2\beta}=p/(1-p)$, which crosses the phase boundary at the Nishimori point N. It has been suggested that the phase boundary is *vertical* from the point N to the horizontal axis.

time polynomial in L, unless the equilibration time of the system is exponentially long. Such a long equilibration time would be associated with spin-glass behavior—the existence of a large number of metastable configurations. In the random-bond Ising model, spin glass behavior is not expected in the ferromagnetically ordered phase corresponding to error probability below threshold. Thus, we expect that in the two-dimensional model the correct recovery procedure can be computed efficiently for any $p<p_c$. Similarly, it is also reasonable to expect that, for error probability below threshold, the correct recovery chain can be found efficiently in the three-dimensional model that incorporates measurement errors.

In fact, some folklore concerning the random-bond Ising model suggests that we can recover successfully by finding a recovery chain that minimizes *energy* rather than free energy. Nishimori[28] notes that along the Nishimori line, the free energy $[\beta F(J)]_p$ coincides with the *entropy of frustration*; that is, the *Shannon entropy* of the distribution of Ising vortices. (He considered the isotropic two-dimensional model, but his argument applies just as well to our three-dimensional gauge theory, or to the anisotropic model with $q\neq p$.) Thus, the singularity of the free energy on the Nishimori line can be regarded as a singularity of this Shannon entropy, which is a purely geometrical effect having nothing to do with thermal fluctuations.

On this basis, Nishimori proposed that there is a vertical phase boundary in our model, occurring at a fixed value of p for all temperatures below the critical temperature at the Nishimori point, as indicated in Fig. 11; further support for this conclusion was later offered by Kitatani.[29] If this proposal is correct, then the critical error probability can be computed by analyzing the phase transition at zero temperature, where the thermal entropy of the fluctuating chains can be neglected. In other words, in the ordered phase, the chain of minimal energy with the same boundary as the actual error chain will with probability one be in the same homology class as the error chain, in the infinite-volume limit. Ordinarily, minimizing free energy and energy are quite different procedures that give qualitatively distinct results. What might make this case different is that the quenched disorder (the error chain E) and the thermal fluctuations (the error chain E') are drawn from the same probability distribution.

Minimizing the energy has advantages. For one, the minimum energy configuration is the minimum weight chain with a specified boundary, which we know can be computed in a time polynomial in L using the perfect matching algorithm of Edmonds.[30,31] Kawashima and Rieger[32] computed the energetic cost of introducing a domain wall at zero temperature, and found $p_c \simeq 0.104 \pm 0.001$. It is debatable whether this result is compatible with the value $p_c \simeq 0.1094 \pm 0.0002$ found by Honecker *et al.*[24] and Merz and Chalker[25] at the Nishimori point, but in any case p_c at zero temperature is reasonably close to p_c on the Nishimori line.

Minimizing the energy is easier to analyze than minimizing the free energy, and at the very

least the critical value of p at zero temperature provides a *lower bound* on p_c along the Nishimori line. In Sec. V we will derive a rigorous bound on the accuracy threshold in our error model, by considering the efficacy of the energy minimization procedure in the three-dimensional model.

V. CHAINS OF MINIMAL WEIGHT

A. The most probable world line

As argued in Sec. IV G, an effective way use the error syndrome in our three-dimensional model is to construct an error chain that has the minimal ''energy''—that is, we select from among all error chains that have the same boundary as the syndrome chain S, the single chain $E_{\min}$ that has the highest probability. In this section, we will study the efficacy of this procedure, and so obtain a lower bound on the accuracy threshold for quantum storage.

An error chain E with H horizontal links and V vertical links occurs with probability (aside from an overall normalization)

$$\left(\frac{p}{1-p}\right)^H\left(\frac{q}{1-q}\right)^V, \tag{44}$$

where p is the qubit error probability and q is the measurement error probability. Thus we choose $E_{\min}$ to be the chain with

$$\partial E_{\min}=\partial S \tag{45}$$

that has the *minimal* value of

$$H\cdot\log\left(\frac{1-p}{p}\right)+V\cdot\log\left(\frac{1-q}{q}\right); \tag{46}$$

we minimize the effective length (number of links) of the chain, but with horizontal and vertical links given different linear weights for $p\neq q$. If the minimal chain is not unique, one of the minimal chains is selected randomly.

Given the measured syndrome, and hence its boundary ∂S, the minimal chain $E_{\min}$ can be determined on a classical computer, using standard algorithms, in a time bounded by a polynomial of the number of lattice sites.[30,31] If p and q are small, so that the lattice is sparsely populated by the sites contained in ∂S, this algorithm typically runs quite quickly. We assume this classical computation can be performed instantaneously and flawlessly.

B. A bound on chain probabilities

Recovery succeeds if our hypothesis $E_{\min}$ is homologically equivalent to the actual error chain E that generated the syndrome chain S, and fails otherwise. Hence, we wish to bound the likelihood of homologically nontrivial paths appearing in $E+E_{\min}$.

Consider a particular cycle on our space–time lattice (or in fact any connected path, whether or not the path is closed). Suppose that this path contains H horizontal links and V vertical links. How likely is it that $E+E_{\min}$ contains this particular set of links?

For our particular path with H horizontal links and V vertical links, let H_m, V_m be the number of those links contained in $E_{\min}$, and let H_e, V_e be the number of those links contained in E (cf. Fig. 12). These quantities obey the relations

$$H_m+H_e\geqslant H,\quad V_m+V_e\geqslant V, \tag{47}$$

and so it follows that

$$\left(\frac{p}{1-p}\right)^{H_m}\left(\frac{q}{1-q}\right)^{V_m}\cdot\left(\frac{p}{1-p}\right)^{H_e}\left(\frac{q}{1-q}\right)^{V_e}\leqslant\left(\frac{p}{1-p}\right)^{H}\left(\frac{q}{1-q}\right)^{V}. \tag{48}$$

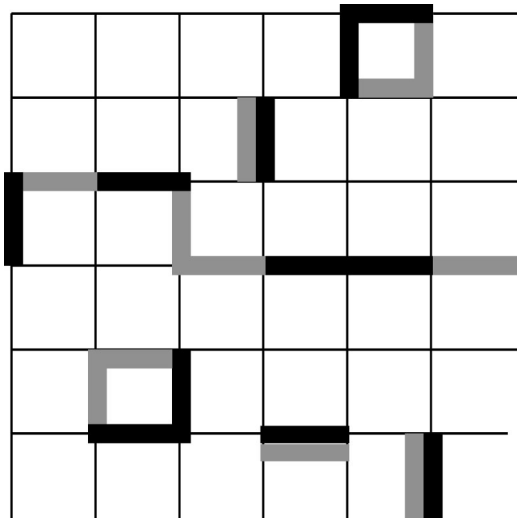

FIG. 12. The error chain E (darkly shaded) and one possible choice for the chain $E_{\min}$ (lightly shaded), illustrated for a 6×6 torus in two dimensions. In this case $E+E_{\min}$ contains a homologically nontrivial cycle of length 8, which contains $H_e=4$ links of E and $H_m=4$ links of $E_{\min}$.

Furthermore, our procedure for constructing $E_{\min}$ ensures that

$$\left(\frac{p}{1-p}\right)^{H_e}\left(\frac{q}{1-q}\right)^{V_e}\leqslant\left(\frac{p}{1-p}\right)^{H_m}\left(\frac{q}{1-q}\right)^{V_m}. \tag{49}$$

This must be so because the e links and the m links share the same boundary; were Eq. (49) not satisfied, we could replace the m links in $E_{\min}$ by the e links and thereby increase the value of $[p/(1-p)]^{H_m}[q/(1-q)]^{V_m}$. Combining the inequalities (48) and (49) we obtain

$$\left(\frac{p}{1-p}\right)^{H_e}\left(\frac{q}{1-q}\right)^{V_e}\leqslant\left[\left(\frac{p}{1-p}\right)^{H}\left(\frac{q}{1-q}\right)^{V}\right]^{1/2}. \tag{50}$$

What can we say about the probability $\mathrm{Prob}(H,V)$ that a particular connected path with (H,V) horizontal and vertical links is contained in $E+E_{\min}$? There are altogether 2^{H+V} ways to distribute errors (links contained in E) at locations on the specified chain—each link either has an error or not. And once the error locations are specified, the probability for errors to occur at those particular locations is

$$p^{H_e}(1-p)^{H-H_e}q^{V_e}(1-q)^{V-V_e}=(1-p)^{H}(1-q)^{V}\left(\frac{p}{1-p}\right)^{H_e}\left(\frac{q}{1-q}\right)^{V_e}. \tag{51}$$

But with those chosen error locations, the cycle can be in $E+E_{\min}$ only if Eq. (50) is satisfied. Combining these observations, we conclude that

$$\mathrm{Prob}(H,V)\leqslant 2^{H+V}(\tilde{p}^{H}\tilde{q}^{V})^{1/2}, \tag{52}$$

where

$$\tilde{p}=p(1-p),\quad \tilde{q}=q(1-q). \tag{53}$$

We can now bound the probability that $E+E_{\min}$ contains any connected path with (H,V) links (whether an open path or a cycle) by counting such paths. We may think of the path as a walk on the lattice (in the case of a cycle we randomly choose a point on the cycle where the walk begins

and ends). Actually, our primary interest is not in how long the walk is (how many links it contains), but rather in how far it wanders—in particular we are interested in whether a closed walk is homologically nontrivial. The walks associated with connected chains of errors visit any given *link* at most once, but it will suffice to restrict the walks further, to be *self-avoiding walks* (SAWs)—those that visit any given *site* at most once (or in the case of a cycle, revisit only the point where the walk starts and ends). This restriction proves adequate for our purposes, because given any open error walk that connects two sites, we can always obtain a SAW by eliminating some closed loops of links from that walk. Similarly, given any homologically nontrivial closed walk, we can obtain a closed SAW (a *self-avoiding polygon*, or SAP) by eliminating some links.

If we wish to consider the probability of an error per unit time in the encoded state, we may confine our attention to SAWs that lie between two time slices separated by the finite time T. [In fact, we will explain in Sec. VI why we can safely assume that $T=O(L)$.] Such a SAW can begin at any one of $L^2\cdot T$ lattice sites of our three-dimensional lattice (and in the case of a SAP, we may arbitrarily select one site that it visits as its "starting point.") If $n_{\mathrm{SAP}}(H,V)$ denotes the number of SAPs with (H,V) links and a specified starting site, then the probability $\mathrm{Prob}_{\mathrm{SAP}}(H,V)$ that $E+E_{\min}$ contains any SAP with (H,V) links satisfies

$$\mathrm{Prob}_{\mathrm{SAP}}(H,V)\leqslant L^2T\cdot n_{\mathrm{SAP}}(H,V)\cdot 2^{H+V}(\tilde{p}^H\tilde{q}^V)^{1/2}. \tag{54}$$

The upper bound Eq. (54) will be the foundation of the results that follow.

The encoded quantum information is damaged if $E+E_{\min}$ contains homologically nontrivial paths. At a minimum, the homologically nontrivial (self-avoiding) path must contain at least L horizontal links. Hence we can bound the failure probability as

$$\mathrm{Prob}_{\mathrm{fail}}\leqslant\sum_V\sum_{H\geqslant L}\mathrm{Prob}_{\mathrm{SAP}}(H,V)\leqslant L^2T\sum_V\sum_{H\geqslant L}n_{\mathrm{SAP}}(H,V)\cdot(4\tilde{p})^{H/2}(4\tilde{q})^{V/2}. \tag{55}$$

C. Counting anisotropic self-avoiding walks

We will obtain bounds on the accuracy threshold for reliable quantum storage with toric codes by establishing conditions under which the upper bound Eq. (55) rapidly approaches zero as L gets large. For this analysis, we will need bounds on the number of self-avoiding polygons with a specified number of horizontal and vertical links.

One such bound is obtained if we ignore the distinction between horizontal and vertical links. The first step of a SAP on a simple (hyper)cubic lattice in d dimensions can be chosen in any of $2d$ directions, and each subsequent step in at most $2d-1$ directions, so for walks containing a total of ℓ links we obtain

$$n^{(d)}_{\mathrm{SAP}}(\ell)\leqslant 2d(2d-1)^{\ell-1},\quad d\ \text{dimensions}. \tag{56}$$

Some tighter bounds are known[33,34] in the cases $d=2,3$:

$$n^{(2)}_{\mathrm{SAP}}(\ell)\leqslant P_2(\ell)(\mu_2)^{\ell},\quad \mu_2\approx 2.638, \tag{57}$$

and

$$n^{(3)}_{\mathrm{SAP}}(\ell)\leqslant P_3(\ell)(\mu_3)^{\ell},\quad \mu_3\approx 4.684, \tag{58}$$

where $P_{2,3}(\ell)$ are polynomials.

Since a SAP with H horizontal and V vertical links has $\ell=H+V$ total links, we may invoke Eq. (58) together with Eq. (55) to obtain

$$\mathrm{Prob}_{\mathrm{fail}}\leqslant L^2T\sum_V\sum_{H\geqslant L}P_3(H+V)\cdot(4\mu_3^2\ \tilde{p})^{H/2}(4\mu_3^2\ \tilde{q})^{V/2}. \tag{59}$$

Provided that

$$\tilde{p}<(4\mu_3^2)^{-1}, \quad \tilde{q}<(4\mu_3^2)^{-1}, \tag{60}$$

we have

$$(4\mu_3^2\ \tilde{p})^{H/2}\cdot(4\mu_3^2\ \tilde{q})^{V/2}\leqslant(4\mu_3^2\ \tilde{p})^{L/2} \tag{61}$$

for every term appearing in the sum. Since there are altogether $2L^2T$ horizontal links and L^2T vertical links on the lattice, the sum over H,V surely can have at most $2L^4T^2$ terms, so that

$$\mathrm{Prob}_{\mathrm{fail}}<Q_3(L,T)\cdot(4\mu_3^2\ \tilde{p})^{L/2}, \tag{62}$$

where $Q_3(L,T)$ is a polynomial. To ensure that quantum information can be stored with arbitrarily good reliability, it will suffice that $\mathrm{Prob}_{\mathrm{fail}}$ becomes arbitrarily small as L gets large (with T increasing no faster than a polynomial of L). Thus Eq. (60) is sufficient for reliable quantum storage. Numerically, the accuracy threshold is surely attained provided that

$$\tilde{p},\tilde{q}<(87.8)^{-1}=0.0113, \tag{63}$$

or

$$p,q<0.0114. \tag{64}$$

Not only does Eq. (62) establish a lower bound on the accuracy threshold, it also shows that, below threshold, the failure probability decreases exponentially with L, the square root of the block size of the surface code.

Equation (64) bounds the accuracy threshold in the case $p=q$, where the sum in Eq. (55) is dominated by isotropic walks with $V\sim H/2$. But for $q<0.0114$, higher values of p can be tolerated, and for $q>0.0114$, there is still a threshold, but the condition on p is more stringent. To obtain stronger results than Eq. (64) from Eq. (55), we need better ways to count anisotropic walks, with a specified ratio of V to H.

One other easy case is the $q\to 0$ limit (perfect syndrome measurement), where the only walks that contribute are two-dimensional SAPs confined to a single time slice. Then we have

$$\mathrm{Prob}_{\mathrm{fail}}<Q_2(L,T)\cdot(4\mu_2^2\ \tilde{p})^{L/2} \tag{65}$$

[where $Q_2(L,T)$ is a polynomial] provided that

$$\tilde{p}=p(1-p)<(4\mu_2^2)^{-1}\approx(27.8)^{-1}=0.0359, \tag{66}$$

or

$$p<0.0373; \tag{67}$$

the threshold value of p can be relaxed to at least 0.0373 in the case where syndrome measurements are always accurate.

This estimate of p_c is considerably smaller than the value $p_c\simeq 0.1094\pm 0.0002$ quoted in Sec. IV F, obtained from the critical behavior of the random-bond Ising model. That discrepancy is not a surprise, considering the crudeness of our arguments in this section. If one accepts the results of the numerical studies of the random-bond Ising model, and Nishimori's argument that the phase boundary of the model is vertical, then apparently constructing the minimum weight chain is a more effective procedure than our bound indicates.

One possible way to treat the case $q\neq p$ would be to exploit an observation due to de Gennes,[35] which relates the counting of SAPs to the partition function of a classical $O(N)$ spin

model in the limit $N \to 0$. This spin model is anisotropic, with nearest-neighbor couplings J_H on horizontal links and J_V on vertical links, and its (suitably rescaled) free energy density has the high-temperature expansion

$$f(J_H, J_V) = \sum_{H,V} n_{\mathrm{SAP}}(H,V)(J_H)^H (J_V)^V. \tag{68}$$

This expansion converges in the disordered phase of the spin system, but diverges in the magnetically ordered phase. Thus, the phase boundary of the spin system in the $J_H - J_V$ plane can be translated into an upper bound on the storage accuracy threshold in the $p-q$ plane, through the relations

$$\tilde{p} = J_H^2/4, \quad \tilde{q} = J_V^2/4, \tag{69}$$

obtained by comparing Eqs. (68) and (55).

To bound the failure probability for a planar code rather than the toric code, we should count the ''relative polygons'' that stretch from one edge of the lattice to the opposite edge. This change has no effect on the estimate of the threshold.

VI. ERROR CORRECTION FOR A FINITE TIME INTERVAL

In estimating the threshold for reliable *storage* of encoded quantum information, we have found it convenient to imagine that we perform error syndrome measurement forever, without any beginning or end. Thus $S+E$ is a cycle (where S is the syndrome chain and E is the error chain) containing the closed world lines of the defects. Though some of these world lines may be homologically nontrivial, resulting in damage to the encoded qubits, we can recover from the damage successfully if the chain $S+E'$ (where E' is our estimated error chain) is homologically equivalent to $S+E$. The analysis is simplified because we need to consider only the errors that have arisen during preceding rounds of syndrome measurement, and need not consider any preexisting errors that were present when the round of error correction began.

However, if we wish to perform a *computation* acting on encoded toric blocks, life will not be so simple. In our analysis of the storage threshold, we have assumed that the complete syndrome history of an encoded block is known. But when two blocks interact with one another in the execution of a quantum gate, the defects in each block may propagate to the other block. Then to assemble a complete history of the defects in any given block, we would need to take into account the measured syndrome of all the blocks in the ''causal past'' of the block in question. In principle this is possible. But in practice, the required classical computation would be far too complex to perform efficiently—in T parallelized time steps, with two-qubit gates acting in each step, it is conceivable that defects from as many as 2^T different blocks could propagate to a given block. Hence, if we wish to compute fault-tolerantly using toric codes, we will need to intervene and perform recovery repeatedly. Since the syndrome measurement is imperfect and the defect positions cannot be precisely determined, errors left over from one round of error correction may cause problems in subsequent rounds.

Intuitively, it should not be necessary to store syndrome information for a very long period to recover successfully, because correlations decay exponentially with time in our statistical-mechanical model. To take advantage of this property, we must modify our recovery procedure.

A. Minimal-weight chains

Consider performing syndrome measurement T times in succession (starting at time $t=0$), generating syndrome chain S and error chain E. Let the error chain E contain any qubit errors that were already present when the syndrome measurements began. Then the chain $S+E$ consisting of all defect world lines contains both closed loops and open paths that end on the final time slice—we say that $S+E$ is closed relative to the final time slice, or $\partial_{\mathrm{rel}}(S+E)=0$. The open connected paths contained in $S+E$ are of two types: pairs of defects created prior to $t=0$ that

have persisted until $t=T$ (if the world line contains links on the initial time slice), and pairs of defects created after $t=0$ that have persisted until $t=T$ (if the world line contains no links on the initial slice).

The syndrome S could have been caused by any error chain E' with the same *relative* boundary as E. To reconstruct the world lines, we should choose an E' that is likely given the observed S. A reasonable procedure is to choose the chain E' with $\partial_{\mathrm{rel}}E'=\partial_{\mathrm{rel}}S$ that minimizes the weight Eq. (46).

The chain $S+E'$ can be projected onto the final time slice—the projected chain $\Pi(S+E')$ contains those and only those horizonal links that are contained in $S+E'$ on an odd number of time slices. Of course, E' has the same projection as $S+E'$; the syndrome chain S contains only vertical links so that its projection is trivial. The projection $\Pi(E')$ is our hypothesis about which links have errors on the final time slice. After $\Pi(E')$ is constructed, we may perform X's or Z's on these links to compensate for the presumed damage. Note that, to construct E', we do not need to store all of S in our (classical) memory—only the relative boundary of S is needed.

Actually, any homologically trivial closed loops in $\Pi(E')$ are harmless and can be safely ignored. Each homologically nontrivial world line modifies the encoded information by the logical operation $\overline{X}$ or $\overline{Z}$. Thus, after the hypothetical closed world lines are reconstructed, we may compensate for the homologically nontrivial closed loops by applying $\overline{X}$ and/or $\overline{Z}$ as needed. Projecting the open world lines in E' onto the final time slice produces a pairing of the presumed positions of surviving defects on the final slice. These defects are removed by performing Z's or X's along a path connecting the pair that is homologically equivalent to the projected chain that connects them. Thus, this recovery step in effect brings the paired defects together to annihilate harmlessly.

Of course, our hypothesis E' will not necessarily agree exactly with the actual error chain E. Thus $E+E'$ contains open chains bounded by the final time slice. Where these open chains meet the final time slice, defects remain that our recovery procedure has failed to remove.

B. Overlapping recovery method

The procedure of constructing the minimal-weight chain E' with the same *relative* boundary as S is not as effective as the procedure in which we continue to measure the syndrome forever. In the latter case, we are in effect blessed with additional information about where monopoles will appear in the future, at times later than T, and that additional information allows us to make a more accurate hypothesis about the defect world lines. However, we can do nearly as well if we use a procedure that stores the syndrome history for only a finite time, if we recognize that the older syndrome is more trustworthy than the more recent syndrome. In our statistical physics model, the fluctuating closed loops in $E+E'$ do not grow indefinitely large in either space or in time. Therefore, we can reconstruct an E' that is homologically equivalent to E *quasilocally in time*—to pair up the monopoles in the vicinity of a given time slice, we do not need to know the error syndrome at times that are much earlier or much later.

So, for example, imagine measuring the syndrome $2T$ times in succession (starting at time $t=0$), and then constructing E' with the same relative boundary as S. The chain E' can be split into two disjoint subchains, as indicated in Fig. 13. The first part consists of all connected chains that terminate on two monopoles, where both monopoles lie in the time interval $0\leqslant t<T$; call this part E'_{old}. The rest of E' we call E'_{keep}. To recover, we flip the links in the projection $\Pi(E'_{\mathrm{old}})$, after which we may erase from memory our record of the monopoles connected by E'_{old}; only E'_{keep} (indeed only the relative boundary of E'_{keep}) will be needed to perform the next recovery step.

In the next step we measure the syndrome another T times in succession, from $t=2T$ to $t=3T-1$. Then we choose our new E' to be the minimal-weight chain whose boundary relative to the new final time slice is the union of the relative boundary of S in the interval $2T\leqslant t<3T$ and the relative boundary of E'_{keep} left over from previous rounds of error correction. We call this procedure the ''overlapping recovery method'' because the minimal-weight chains that are constructed in successive steps occupy overlapping regions of space–time.

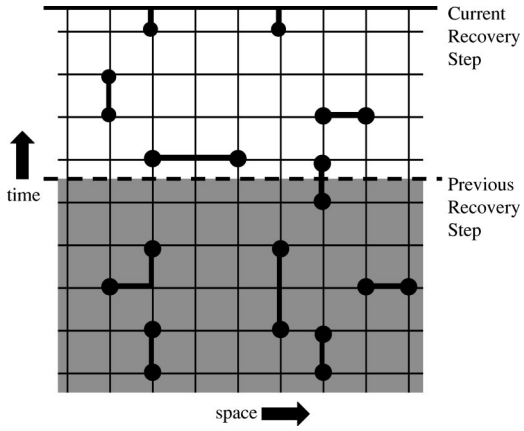

FIG. 13. The "overlapping recovery" method, shown schematically. All monopoles (boundary points of the error syndrome chain) are indicated as filled circles, including both monopoles left over from earlier rounds of error recovery (those in the shaded region below the dotted line) and monopoles generated after the previous round (those in the unshaded region above the dotted line). Also shown is the minimum weight chain E' that connects each monopole to either another monopole or to the current time slice. The chain E' contains E'_{old}, whose boundary lies entirely in the shaded region, and the remainder E'_{keep}. In the current recovery step, errors are corrected on the horizontal links of E'_{old}, and its boundary is then erased from the recorded syndrome history. The boundary of E'_{keep} is retained in the record, to be dealt with in a future recovery step.

If we choose T to be large compared to the characteristic correlation time of our statistical physics model, then only rarely will a monopole survive for more than one round, and the amount of syndrome information we need to store will surely be bounded. Furthermore, for such T, this overlapping recovery method will perform very nearly as well as if an indefinite amount of information were stored.

The time T should be chosen large enough so that connected chains in $E+E'$ are not likely to extend more than a distance T in the time direction. Arguing as in Sec. V C [and recalling that the number $n_{\text{SAW}}(\ell)$ of self-avoiding walks of length ℓ differs from the number $n_{\text{SAP}}(\ell)$ of self-avoiding polygons of length ℓ by a factor polynomial in ℓ], we see that a connected chain containing H horizontal links and V vertical links occurs with a probability

$$\text{Prob}(H,V) \leqslant Q'_3(H,V)(4\mu_3^2\tilde{p})^{H/2}(4\mu_3^2\tilde{q})^{V/2}, \tag{70}$$

where $Q'_3(H,V)$ is a polynomial. Furthermore, a connected chain with temporal extent T must have at least $V=2T$ vertical links if both ends of the chain lie on the final time slice. Therefore the probability $\text{Prob}(H,V)$ is small compared to the failure probability Eq. (62), so that our procedure with finite memory differs in efficacy from the optimal procedure with infinite memory by a negligible amount, provided that

$$T \gg \frac{L}{2} \cdot \frac{\log(4\mu_3^2\tilde{p})^{-1}}{\log(4\mu_3^2\tilde{q})^{-1}}. \tag{71}$$

In particular, if the measurement error and qubit error probabilities are comparable ($q \simeq p$), it suffices to choose $T \gg L$, where L is the linear size of the lattice.

Thus we see that the syndrome history need not be stored indefinitely for our recovery procedure to be robust. The key to fault tolerance is that we should not overreact to syndrome information that is potentially faulty. In particular, if we reconstruct the world lines of the defects and find open world lines that do not extend very far into the past, it might be dangerous to accept the accuracy of these world lines and respond by bringing the defects together to annihilate. But

world lines that persist for a time comparable to L are likely to be trustworthy. In our overlapping recovery scheme, we take action to remove only these long-lived defects, leaving those of more recent vintage to be dealt with in the next recovery step.

C. Computation threshold

Our three-dimensional model describes the history of a single code block; hence its phase transition identifies a threshold for reliable storage of quantum information. Analyzing the threshold for reliable quantum *computation* is more complex, because we need to consider interactions between code blocks.

When two encoded blocks interact through the execution of a gate, errors can propagate from one block to another, or potentially from one qubit in a block to another qubit in the same block. It is important to keep this error propagation under control. We will discuss in Sec. IX how a universal set of fault-tolerant quantum gates can be executed on encoded states. For now let us consider the problem of performing a circuit consisting of CNOT gates acting on pairs of encoded qubits. The encoded CNOT gate with block 1 as its control and block 2 as its target can be implemented *transversally*—that is, by performing CNOT gates in parallel, each acting on a qubit in block 1 and the corresponding qubit in block 2. A CNOT gate propagates bit-flip errors from control to target and phase errors from target to control. Let us first consider the case in which storage errors occur at a constant rate, but errors in the gates themselves can be neglected.

Suppose that a transversal CNOT gate is executed at time $t=0$, propagating bit-flip errors from block 1 to block 2, and imagine that we wish to correct the bit-flip errors in block 2. We suppose that many rounds of syndrome measurement are performed in both blocks before and after $t=0$. Denote by S_1 and S_2 the syndrome chains in the two blocks, and by E_1 and E_2 the error chains. Due to the error propagation, the chain S_2+E_2 in block 2 has a nontrivial boundary at the $t=0$ time slice. Therefore, to diagnose the errors in block 2 we need to modify our procedure.

We may divide each syndrome chain and error chain into two parts, a portion lying in the past of the $t=0$ time slice, and a portion lying in its future. Then the chain

$$S_{1,\text{before}}+S_{2,\text{before}}+S_{2,\text{after}}+E_{1,\text{before}}+E_{2,\text{before}}+E_{2,\text{after}} \tag{72}$$

has a trivial boundary. Therefore, we can estimate $E_{1,\text{before}}+E_{2,\text{before}}+E_{2,\text{after}}$ by constructing the minimal chain with the same boundary as $S_{1,\text{before}}+S_{2,\text{before}}+S_{2,\text{after}}$. Furthermore, because of the error propagation, it is $E_{1,\text{before}}+E_{2,\text{before}}+E_{2,\text{after}}$ whose horizontal projection identifies the damaged links in block 2 after $t=0$.

If in each block the probability of error per qubit and per time step is p, while the probability of a syndrome measurement error is q, then the error chain $E_{1,\text{before}}+E_{2,\text{before}}+E_{2,\text{after}}$ has in effect been selected from a distribution in which the error probabilities are $(2p(1-p),2q(1-q))$ before the gate and (p,q) after the gate. Obviously, these errors are no more damaging than if the error probabilities had been $(2p(1-p),2q(1-q))$ at all times, both before and after $t=0$. Therefore, if (p,q) lies below the accuracy threshold for accurate storage, then error rates $(2p(1-p),2q(1-q))$ will be below the accuracy threshold for a circuit of CNOT gates.

Of course, the transversal CNOT might itself be prone to error, damaging each qubit with probability p_{CNOT}, so that the probability of error is larger on the $t=0$ slice than on earlier or later slices. However, increasing the error probability from p to $p+p_{\text{CNOT}}$ on a single slice is surely no worse than increasing the probability of error to $p+p_{\text{CNOT}}$ on all slices. For a given q, there is a threshold value $p_c(q)$, such that for $p<p_c(q)$ a circuit of CNOTs is robust if the gates are flawless; then the circuit with imperfect gates is robust provided that $p+p_{\text{CNOT}}<p_c(q)$.

By such reasoning, we can infer that the accuracy threshold for quantum computation is comparable to the threshold for reliable storage, differing by factors of order one. Furthermore, below threshold, the probability of error in an encoded gate decreases exponentially with L, the linear size of the lattice. Therefore, to execute a quantum circuit that contains T gates with reasonable fidelity, we should choose $L=O(\log T)$, so that the block size $2L^2$ of the code is $O(\log^2 T)$.

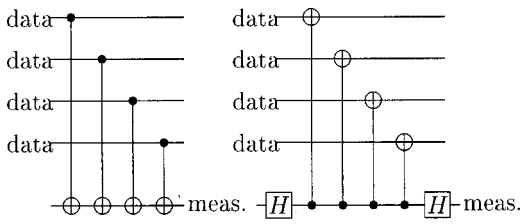

FIG. 14. Circuits for measurement of the plaquette ($Z^{\otimes 4}$) and site ($X^{\otimes 4}$) stabilizer operators.

VII. QUANTUM CIRCUITS FOR SYNDROME MEASUREMENT

In our model with uncorrelated errors, in which qubit errors occur with probability p per time step and measurement errors occur with probability q, we have seen in Sec. IV that it is possible to identify a sharp phase boundary between values of the parameters such that error correction is sure to succeed in the limit of a large code block, and values for which error correction need not succeed. How can we translate this accuracy threshold, expressed as a phase boundary in the $p-q$ plane, into a statement about how well the hardware in our quantum memory must perform in order to protect quantum states effectively? The answer really depends on many details about the kinds of hardware that are potentially at our disposal. For purposes of illustration, we will relate p and q to the error probabilities for the fundamental gates in a particular computational model.

A. Syndrome measurement

Whenever a check operator X_s or Z_P is measured, a quantum circuit is executed in which each of the qubits occurring in the check operator interacts with an ancilla, and then the ancilla is measured to determine the result. Our task is to study this quantum circuit to determine how the faults in the circuit contribute to p and to q. To start we must decide what circuit to study.

For many quantum codes, the design of the syndrome measurement circuit involves subtleties. If the circuit is badly designed, a single error in the ancilla can propagate to many qubits in the code block, compromising the effectiveness of the error correction procedure. To evade this problem, Shor[3] and Steane[36] proposed two different methods for limiting the propagation of error from ancilla to data in the measurement of the check operators of a stabilizer code. In Shor's method, to extract each bit of the error syndrome, an ancilla ''cat state'' is prepared that contains as many qubits as the weight of the check operator. The ancilla interacts with the data code block, and then each qubit of the ancilla is measured; the value of the check operator is the parity of the measurement outcomes. In Steane's method, the ancilla is prepared as an encoded block (containing as many qubits as the length of the code). The ancilla interacts with the data, each qubit in the ancilla is measured, and a classical parity check matrix is applied to the measurement outcomes to extract the syndrome. In either scheme, each ancilla qubit interacts with only a single qubit in the data, so that errors in the ancilla cannot seriously damage the data. The price we pay is the overhead involved in preparing the ancilla states and verifying that the preparation is correct.

We could use the Shor method or the Steane method to measure the stabilizer of a surface code, but it is best not to. We can protect against errors more effectively by using just a single ancilla qubit for the measurement of each check operator, avoiding all the trouble of preparing and verifying ancilla states. The price we pay is modest—a single error in the ancilla might propagate to become two errors in the data, but we will see that these correlated errors in the data are not so damaging.

So, we imagine placing a sheet of ancilla qubits above the qubits of a planar code block. Directly above the site s is the ancilla qubit that will be used to measure X_s, and directly above the center of the plaquette P is the ancilla qubit that will be used to measure Z_P. We suppose that CNOT gates can be executed acting on a data qubit and its neighboring ancilla qubits. The circuits for measuring the plaquette operator $Z^{\otimes 4}$ and the site operator $X^{\otimes 4}$ are shown in Fig. 14.

We have included the Hadamard gates in the circuit for measuring the site operator to signify that the ancilla qubit is initially prepared in the $X=1$ state, and the final measurement is a

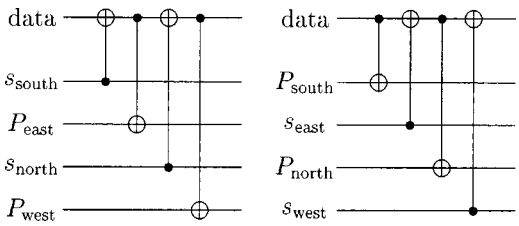

FIG. 15. Gates acting on a given qubit in a complete round of syndrome measurement. Data qubits on links with a north–south orientation participate successively in measurements of check operators at the site to the south, the plaquette to the east, the site to the north, and the plaquette to the west. Qubits on links with an east–west orientation participate successively in measurements of check operators at the plaquette to the south, the site to the east, the plaquette to the north, and the site to the west.

measurement of X, while in the case of the plaquette operator measurement the ancilla is prepared in the $Z=1$ state and Z is measured at the end. But we will suppose that our computer can measure X as easily as it can measure Z; hence in both cases the circuit is executed in six time steps (including preparation and measurement), and there is really no Hadamard gate.

B. Syndrome errors and data errors

We will assume that all errors in the circuit are stochastic (for example, they could be errors caused by decoherence). We will consider both ''storage errors'' and ''gate errors.'' In each time step, the probability that a ''resting'' qubit is damaged will be denoted p_s. For simplicity, we will assume that an error, when it occurs, is one of the Pauli operators X, Y, or Z. (The analysis of the circuit is easily generalized to more general models of stochastic errors.) In our analysis, we will always make a maximally pessimistic assumption about which error occurred at a particular position in the circuit. If a gate acts on a qubit in a particular time step, we will assume that there is still a probability p_s of a storage error in that step, plus an additional probability of error due to the execution of the gate. We denote the probability of an error in the two-qubit CNOT gate by p_{CNOT}; the error is a tensor product of Pauli operators, and again we will always make maximally pessimistic assumptions about which error occurs at a particular position in the circuit. If a storage error and gate error occur in the same time step, we assume that the gate error acts first, followed by the storage error. When a single qubit is measured in the $\{|0\rangle,|1\rangle\}$ basis, p_m is the probability of obtaining the incorrect outcome. (If a storage error occurs during a measurement step, we assume that the error precedes the measurement.) And when a fresh qubit is acquired in the state $|0\rangle$, p_p denotes the probability that its preparation is faulty (it is $|1\rangle$ instead).

In a single cycle of syndrome measurement, each data qubit participates in the measurement of four stabilizer operators: two site operators and two plaquette operators. Each of these measurements requires four time steps (excluding the preparation and measurement steps), as a single ancilla qubit is acted upon by four sequential CNOTs. But to cut down the likelihood of storage errors, we can execute the four measurement circuits in parallel, so that every data qubit participates in a CNOT gate in every step. For example, for each plaquette and each site, we may execute CNOT gates that act on the four edges of the plaquette or the four links meeting at the site in the counterclockwise order north–west–south–east. The CNOT gates that act on a given data qubit, then, alternate between CNOTs with the data qubit as control and CNOTs with the data qubit as target, as indicated in Fig. 15.

For either a site check operator or a plaquette check operator, the probability that the measurement is faulty is

$$q_{\text{single}}=p_p+4p_{\text{CNOT}}+6p_s+p_m+\text{h. o.}, \tag{73}$$

where ''+h. o.'' denotes terms of higher than linear order in the fundamental error probabilities. The measurement can fail if any one of the CNOT gates has an error, if a storage error occurs during any of the six time steps needed to execute the circuit (including the preparation and

measurement step), or because of a fault in the initial preparation or final measurement of the ancilla qubit. By omitting the higher order terms we are actually *overestimating* q. For example, p_s is the probability that a storage error occurs in the first time step, disregarding whether or not additional errors occur in the circuit.

We have used the notation q_{single} in Eq. (73) to emphasize that this is an estimate of the probability of an isolated error on a vertical (timelike) link. More troublesome are syndrome measurement errors that are correlated with qubit errors. These arise if, say, a qubit suffers a Z error that is duly recorded in the syndrome measurement of one of the two adjoining sites but not the other. In our space–time picture, then, there is a timelike plaquette with an error on one of its horizontal links and one of its vertical links. We will refer to this type of correlated error as a ''vertical hook''—hook because the two links with errors meet at a 90° angle, and vertical because one of the links is vertical (and to contrast with the case of a horizontal hook which we will discuss later).

We can estimate the probability of a vertical hook on a specified timelike plaquette by considering the circuits in Fig. 15. The qubit in question participates in the measurement of two site check operators, through the two CNOT gates in the circuit in which the data qubit is the target of the CNOT. A vertical hook can arise due to a fault that occurs in either of these CNOT gates or at a time in between the execution of these gates. Hence the probability of a vertical hook is

$$q_{\text{hook}} = 3p_{\text{CNOT}} + 2p_s + \text{h. o.}; \tag{74}$$

faults in any of three different CNOT gates, or storage errors in either of two time steps, can generate the hook. Note that the hook on the specified plaquette has a unique orientation; the first of the two site operator measurements that the data qubit participated in is the one that fails to detect the error. Of course, the same formula for q_{hook} applies if we are considering the measurement of the plaquette operators rather than the site operators.

A CNOT gate propagates X errors from control qubit to target qubit, and Z errors from target to control. Thus we do not have to worry about a vertical hook that arises from an error in an ancilla bit that propagates to the data. For example, if we are measuring a plaquette operator, then X errors in the ancilla damage the syndrome bit while Z errors in the ancilla propagate to the data; the result is a vertical error in the X-error syndrome that is correlated with a horizontal Z-error in the data. This correlation is not problematic because we deal with X errors and Z errors separately. However, propagation of error from ancilla to data also generates correlated horizontal errors that we need to worry about. In the measurement of, say, the plaquette operator $Z_P = Z^{\otimes 4}$, Z errors (but not X errors) can feed back from the ancilla to the data. Feeding back four Z's means no error at all, because $Z^{\otimes 4}$ is in the code stabilizer, and feeding back three Z's generates the error $IZZZ$, which is equivalent to the single Z error $ZIII$. Therefore, the only way to get a double qubit error from a single fault in the circuit is through an error in the second or third CNOT, or through an ancilla storage error in between the second and third CNOT. (The second CNOT might apply Z to the ancilla but not to the data, and that Z error in the ancilla can then feed back to two data qubits, or the third CNOT could apply Z to both ancilla and data, and the Z error in the ancilla can then feed back to one other data qubit.) Because of the order we have chosen for the execution of the CNOTs, this double error, when it occurs, afflicts the southeast corner of the plaquette (or equivalently the northwest corner, which has the same boundary). We will refer to this two-qubit error as a ''horizontal hook,'' because the two horizontal errors meet at a 90° angle. Similarly, error propagation during the measurement of the site operator X_s can produce X errors on the north and west links meeting at that site. One should emphasize that the only correlated XX or ZZ errors that occur with a probability linear in the fundamental error probabilities are these hooks. This is a blessing—correlated errors affecting two collinear links would be more damaging.

Feedback from the measurement of a plaquette operator can produce ZZ hooks but not XX hooks, and feedback from the measurement of a site operator can produce XX hooks but not ZZ hooks. Thus, in each round of syndrome measurement, the probability of a ZZ hook at a plaquette or an XX hook at a site is

$$p_{\text{hook}} = 2p_{\text{CNOT}} + p_s + \text{h. o.} \tag{75}$$

(Remember that a ''hook'' means two Z's or two X's; in addition, an error in a single CNOT gate could induce, say, an X error in the data and a Z error in the ancilla that subsequently feeds back, but correlated X and Z errors will not cause us any trouble.)

Now we need to count the ways in which a single error can occur in the data during a round of syndrome measurement. First suppose that we measure a single plaquette operator Z_P, and consider the scenarios that lead to a single Z error in the data. The Z error can arise either because a gate or storage error damages the data qubit directly, or because an error in the ancilla feeds back to the data. Actually, single errors occur with slightly different probabilities for different data qubits acted on by the circuit. The worst case occurs for the first and last qubit acted on by the circuit; the probability that the circuit produces a single error that acts on the first (or last) qubit is

$$p_{\text{single,Z}}^{Z_P,1} = p_{\text{single,Z}}^{Z_P,4} = p_{\text{CNOT}} + 6p_s + p_{\text{CNOT}} + p_s + \text{h. o.} \tag{76}$$

The first two terms arise from gate errors and storage errors that damage the data qubit directly. For the first qubit, the last two terms arise from the case in which a Z error in the ancilla is fed back to the data by each of the last three CNOTs—the resulting $IZZZ$ error is equivalent to a $ZIII$ error because $ZZZZ$ is in the code stabilizer. For the fourth qubit, the last two terms arise from an error fed back by the last CNOT gate in the circuit. On the other hand, for the second and third qubit acted on by the circuit, it is not possible for just a single error to feed back; e.g., if the error feeds back to the third qubit, it will feed back to the fourth as well, and the result will be a hook instead of a single error. Hence, the probability of a single error acting on the second or third qubit is

$$p_{\text{single,Z}}^{Z_P,2} = p_{\text{single,Z}}^{Z_P,3} = p_{\text{CNOT}} + 6p_s + \text{h. o.}; \tag{77}$$

there is no feedback term. If we are measuring a site operator X_s, then X errors might feed back from the ancilla to the data, but Z errors will not. Therefore, for each of the four qubits acted on by the circuit, the probability that a single Z error results from the execution of the circuit, acting on that particular qubit, is

$$p_{\text{single,Z}}^{X_s} = p_{\text{CNOT}} + 6p_s + \text{h. o.}; \tag{78}$$

again there is no feedback term.

In a single round of syndrome measurement, each qubit participates in the measurement of four check operators, two site operators and two plaquette operators. For the plaquette operator measurements, depending on the orientation of the link where the qubit resides, the qubit will be either the first qubit in one measurement and the third in the other, or the second in one and the fourth in the other. Either way, the total probability of a single Z error arising that afflicts that qubit is

$$p_{\text{single}} = 4p_{\text{CNOT}} + 6p_s + p_{\text{CNOT}} + p_s + \text{h. o.} = 5p_{\text{CNOT}} + 7p_s + \text{h. o.}, \tag{79}$$

with the $4p_{\text{CNOT}} + 6p_s$ arising from direct damage to the qubit and the $p_{\text{CNOT}} + p_s$ from feedback due to one of the four check operator measurements. The same equation applies to the probability of a single X error arising at a given qubit in a single round of syndrome measurement.

C. Error-chain combinatorics

With both single errors and hooks to contend with, it is more complicated to estimate the failure probability, but we can still obtain useful upper bounds. In fact, the hooks do not modify the estimate of the accuracy threshold as much as might have been naively expected. Encoded information is damaged if $E + E_{\min}$ contains a homologically nontrivial (relative) cycle, which can

wrap around the code block with either a north–south or east–west orientation. Either way, the cycle contains at least L links all with the *same* orientation, where L is the linear size of the lattice. A horizontal hook introduces two errors with *different* orientations, which is not as bad as two errors with the same orientation. Similarly, a vertical hook contains only one horizontal error.

There are two other reasons why the hooks do not badly compromise the effectiveness of error correction. While single errors can occur with any orientation, horizontal hooks can appear only on the northwest corner of a plaquette (hooks on southeast corners are equivalent to hooks on northwest corners and should not be counted separately), and vertical hooks on timelike plaquettes have a unique orientation, too. Therefore, hooks have lower ''orientational entropy'' than the single errors, which means that placing hooks on self-avoiding walks reduces the number of walks of a specified length. And, finally, p_{hook} is smaller than p_{single}, and q_{hook} is smaller than q_{single}, which further reduces the incentive to include hooks in $E+E_{\min}$.

We will suppose that $E_{\min}$ is constructed by the same procedure as before, by minimizing the weight

$$H \log p_{\text{single}}^{-1} + V \log q_{\text{single}}^{-1}. \tag{80}$$

To simplify later expressions, we have replaced $p/(1-p)$ by p here, which will weaken our upper bound on the failure probability by an insignificant amount. Note that our procedure finds the most probable chain under the assumption that only single errors occur (no hooks). If p_{hook} and q_{hook} are assumed to be known, then in principle we could retool our recovery procedure by taking these correlated errors into account in the construction of $E_{\min}$. To keep things simple we will not attempt to do that. Then, as before, for any connected subchain of $E+E_{\min}$ with H horizontal links and V vertical links, the numbers H_e and V_e of horizontal and vertical links of the subchain that are contained in E must satisfy

$$p_{\text{single}}^{H_e} q_{\text{single}}^{V_e} \leqslant p_{\text{single}}^{H/2} q_{\text{single}}^{V/2}. \tag{81}$$

To bound the failure probability, we wish to count the number of ways in which a connected chain with a specified number of horizontal links can occur in $E+E_{\min}$, keeping in mind that the error chain E could contain hooks as well as single errors. Notice that a hook might contribute only a single link to $E+E_{\min}$, if one of the links contained in the hook is also in $E_{\min}$. But since $p_{\text{hook}} < p_{\text{single}}$ and $q_{\text{hook}} < q_{\text{single}}$, we will obtain an upper bound on the failure probability if we pessimistically assume that all of the errors in $E+E_{\min}$ are either two-link hooks occurring with probabilities $p_{\text{hook}}, q_{\text{hook}}$ or single errors occuring with probabilities $p_{\text{single}}, q_{\text{single}}$. If the H_e horizontal errors on a connected chain include H_{hook} horizontal hooks and V_{hook} vertical hooks, then there are $H_e - 2H_{\text{hook}} - V_{\text{hook}}$ single horizontal errors and $V_e - V_{\text{hook}}$ single vertical errors; once the locations of the hooks and the single errors are specified, the probability that errors occur at those locations is no larger than

$$\begin{aligned} &(p_{\text{single}})^{H_e - 2H_{\text{hook}} - V_{\text{hook}}} (p_{\text{hook}})^{H_{\text{hook}}} \cdot (q_{\text{single}})^{V_e - V_{\text{hook}}} (q_{\text{hook}})^{V_{\text{hook}}} \\ &< p_{\text{single}}^{H/2} \left(\frac{p_{\text{hook}}}{p_{\text{single}}^2} \right)^{H_{\text{hook}}} q_{\text{single}}^{V/2} \left(\frac{q_{\text{hook}}}{p_{\text{single}} q_{\text{single}}} \right)^{V_{\text{hook}}}. \end{aligned} \tag{82}$$

Because a horizontal hook contains two errors with different orientations, it will be convenient to distinguish between links oriented east–west and links oriented north–south. We denote by H_1 the number of horizontal links in the connected chain with east–west orientation and by H_2 the number of horizontal links with north–south orientation; then clearly

$$H_{\text{hook}} \leqslant H_1, \quad H_{\text{hook}} \leqslant H_2. \tag{83}$$

To estimate the threshold, we will bound the probability that our connected chain has $H_1 \geqslant L$; of course, the same expression bounds the probability that $H_2 \geqslant L$.

For a specified connected chain, suppose that altogether H_e of the horizontal links and V_e of the vertical links have errors, and that there are H_{hook} horizontal hooks and V_{hook} vertical hooks, so that there are $H_e - 2H_{\text{hook}} - V_{\text{hook}}$ single horizontal errors and $V_e - V_{\text{hook}}$ single vertical errors. In how many ways can we distribute the hooks and single errors along the path? Since each horizontal hook contains a link with north-south orientation, there are no more than $\binom{H_2}{H_{\text{hook}}}$ ways to choose the locations of the horizontal hooks; similarly there are no more than $\binom{V}{V_{\text{hook}}}$ ways to choose the locations of the vertical hooks. (Actually, we have given short shrift here to a slight subtlety. Once we have decided that a vertical hook will cover a particular vertical link, there may be two ways to place the hook—it might cover either one of two adjacent horizontal links. However, for the hook to be free to occupy either position, the orientation of the second horizontal link must be chosen in one of only two possible ways. Thus the freedom to place the hook in two ways is more than compensated by the reduction in the orientational freedom of the other horizontal link by a factor of $\frac{2}{5}$, and can be ignored. A similar remark applies to horizontal hooks.) Then there are no more than $2^{H_1+H_2-2H_{\text{hook}}-V_{\text{hook}}}$ ways to place the single horizontal errors among the remaining horizontal links, and no more than $2^{V-V_{\text{hook}}}$ ways to place the single vertical errors among remaining $V - V_{\text{hook}}$ vertical links on the chain. Now consider counting the self-avoiding paths starting at a specified site, where the path is constructed from hooks, single errors, and the links of $E_{\min}$. Whenever we add a horizontal hook to the path there are at most two choices for the orientation of the hook, and whenever we add a vertical hook there are at most four choices; hence there are no more than $2^{H_{\text{hook}}} 4^{V_{\text{hook}}}$ ways to choose the orientations of the hooks. For the remaining $H_1 + H_2 - 2H_{\text{hook}} + V - 2V_{\text{hook}}$ links of the path, the orientation can be chosen in no more than five ways. Hence, the total number of paths with a specified number of horizontal links, horizontal hooks, vertical links, and vertical hooks is no more than

$$\binom{H_2}{H_{\text{hook}}}\binom{V}{V_{\text{hook}}} \cdot 2^{H_1+H_2-2H_{\text{hook}}-V_{\text{hook}}} 2^{V-V_{\text{hook}}} \cdot 2^{H_{\text{hook}}} 4^{V_{\text{hook}}} \cdot 5^{H_1+H_2-2H_{\text{hook}}+V-2V_{\text{hook}}}. \quad (84)$$

Combining this counting of paths with the bound Eq. (82) on the probability of each path, we conclude that the probability that $E + E_{\min}$ contains a connected path with specified starting site, containing H_1 links with east–west orientation, H_2 links with north–south orientation, V vertical links, H_{hook} horizontal hooks, and V_{hook} vertical hooks, is bounded above by

$$\binom{H_2}{H_{\text{hook}}}\left(\frac{p_{\text{hook}}}{50p_{\text{single}}^2}\right)^{H_{\text{hook}}} (100p_{\text{single}})^{(H_1+H_2)/2} \cdot \binom{V}{V_{\text{hook}}}\left(\frac{q_{\text{hook}}}{25p_{\text{single}}q_{\text{single}}}\right)^{V_{\text{hook}}} \cdot (100q_{\text{single}})^{V/2}. \quad (85)$$

Here H_{hook} can take any value from zero to H_2, and V_{hook} can take any value from zero to V. We can sum over H_{hook} and V_{hook}, to obtain an upper bound on the probability of a chain with an unspecified number of hooks:

$$(100p_{\text{single}})^{(H_1+H_2)/2}\left(1+\frac{p_{\text{hook}}}{50p_{\text{single}}^2}\right)^{H_2} \cdot (100q_{\text{single}})^{V/2}\left(1+\frac{q_{\text{hook}}}{25p_{\text{single}}q_{\text{single}}}\right)^{V}. \quad (86)$$

Finally, since a path can begin at any of L^2T sites, and since there are two types of homologically nontrivial cycles, the probability of failure $\text{Prob}_{\text{fail}}$ satisfies the bound

$$\text{Prob}_{\text{fail}} < 2L^2T \sum_{H_1 \geq L} (100p_{\text{single}})^{H_1/2} \cdot \sum_{H_2 \geq 0}\left[100p_{\text{single}}\left(1+\frac{p_{\text{hook}}}{50p_{\text{single}}^2}\right)^2\right]^{H_2/2} \cdot \sum_{V \geq 0}\left[100q_{\text{single}}\left(1+\frac{q_{\text{hook}}}{25p_{\text{single}}q_{\text{single}}}\right)^2\right]^{V/2}. \quad (87)$$

This sum will be exponentially small for large L provided that

$$p_{\text{single}} < \frac{1}{100}, \quad q < \frac{1}{100},$$

$$p_{\text{hook}} < 5 \; p_{\text{single}}^2 \left(\frac{1}{\sqrt{p_{\text{single}}}} - 10 \right), \tag{88}$$

$$q_{\text{hook}} < \frac{5}{2} p_{\text{single}} q_{\text{single}} \left(\frac{1}{\sqrt{q_{\text{single}}}} - 10 \right).$$

Of course, making p_{single} and q_{single} smaller can only make things better. Our conditions on p_{hook} and q_{hook} in Eq. (88) are not smart enough to know this—for p_{single} sufficiently small, we find that making it still smaller gives us a *more* stringent condition on p_{hook}, and similarly for q_{hook}. Clearly, this behavior is an artifact of our approximations. Thus, for a given p_{single} and q_{single}, we are free to choose any smaller values of p_{single} and q_{single} in order to obtain more liberal conditions on p_{hook} and q_{hook} from Eq. (88). Our expression that bounds p_{hook} achieves its maximum for $p_{\text{single}} = (\frac{3}{40})^2$, and for fixed p_{single}, our expression that bounds q_{hook} achieves its maximum for $q_{\text{single}} = (\frac{1}{20})^2$. We therefore conclude that for recovery to succeed with a probability that approaches one as the block size increases, it suffices that

$$p_{\text{single}} < \tfrac{9}{1600}, \quad q_{\text{single}} < \tfrac{1}{400},$$

$$p_{\text{hook}} < \tfrac{3}{32} \cdot \tfrac{9}{1600}, \quad q_{\text{hook}} < \tfrac{1}{16} \cdot \tfrac{9}{1600}. \tag{89}$$

Comparing to our expressions for q_{single}, p_{single}, and p_{hook}, we see that, unless q_{single} is dominated by preparation or measurement errors, these conditions are all satisfied provided that

$$q_{\text{hook}} = 3p_{\text{CNOT}} + 2p_s < 3.5 \times 10^{-4}. \tag{90}$$

If the probability of a CNOT error is negligible, then we obtain a lower bound on the critical error probability for storage errors,

$$(p_s)_c > 1.7 \times 10^{-4}. \tag{91}$$

In view of the crudeness of our combinatorics, we believe that this estimate is rather conservative, if one accepts the assumptions of our computational model.

VIII. MEASUREMENT AND ENCODING

A. Measurement

At the conclusion of a quantum computation, we need to measure some qubits. If the computation is being executed fault tolerantly, this means measuring an encoded block. How can we perform this measurement fault tolerantly?

Suppose we want to measure the logical operator $\overline{Z}$, that is, measure the encoded block in the basis $\{|\overline{0}\rangle, |\overline{1}\rangle\}$. If we are willing to destroy the encoded block, we first measure Z for each qubit in the block, projecting each onto the basis $\{|0\rangle, |1\rangle\}$. Were there no errors in the code block at the time of the measurement, and were all measurements of the individual qubits performed flawlessly, then we could choose any homologically nontrivial path on the lattice and evaluate the parity of the outcomes for the links along that path. Even parity indicates that the encoded block is in the state $|\overline{0}\rangle$, odd parity the state $|\overline{1}\rangle$.

But the code block *will* contain some errors (not too many, we hope), and some of the measurements of the individual qubits *will* be faulty. Since a single bit flip along the path could

alter the parity of the measurement outcomes, we need to devise a fault-tolerant procedure for translating the observed values of the individual qubits into a value of the encoded qubit.

One such procedure is to evaluate the parity $Z^{\otimes 4}$ of the measurement outcomes at each plaquette of the lattice, determining the locations of all plaquette defects. These defects can arise either because defects were already present in the code block before the measurement, or they could be introduced by the measurement itself. It is useful and important to recognize that the defects introduced by the measurement do not pose any grave difficulties. An isolated measurement error at a single link will produce two neighboring defects on the plaquettes that contain that link. Widely separated defects can arise from the measurement only if there are many correlated measurement errors.

Therefore we can apply a suitable classical algorithm to remove the defects—for example, by choosing a chain of minimal total length that is bounded by the defect locations, which can be found in a polynomial-time classical computation. Flipping the bits on this chain corrects the errors in the measurement outcomes, so that we can then proceed to evaluate the parity along a nontrivial cycle. Assuming sufficiently small rates for the qubit and measurement errors, the encoded qubit will be evaluated correctly, with a probability of error that is exponentially small for large block size.

We can measure $\overline{X}$ by the same procedure, by measuring X for each qubit, and evaluating all site operators $X^{\otimes 4}$ from the outcomes. After removal of the site defects by flipping bits appropriately, $\overline{X}$ is the parity along a nontrivial cycle of the dual lattice.

To measure $\overline{Z}$ of a code block without destroying the encoded state, we can prepare an ancilla block in the encoded state $|\overline{0}\rangle$, and perform a bitwise CNOT from the block to be measured into the ancilla. Then we can measure the ancilla by the destructive procedure just described. A nondestructive measurement of $\overline{X}$ is executed similarly.

B. Encoding of known states

At the beginning of a quantum computation, we need to prepare encoded qubits in eigenstates of the encoded operations, for example the state $|\overline{0}\rangle$ of the planar code, a $\overline{Z}=1$ eigenstate. If syndrome measurement were perfectly reliable, the state $|\overline{0}\rangle$ could be prepared quickly by the following method: Start with the state $|0\rangle^{\otimes n}$ where n is the block size of the code. This is the simultaneous eigenstate with eigenvalue 1 of all plaquette stabilizer operators $Z_P=Z^{\otimes 4}$ and of the logical operator $\overline{Z}$, but not of the site stabilizer operators $X_s=X^{\otimes 4}$. Then measure all the site operators. Since the site operators commute with the plaquette operators and the logical operators, this measurement does not disturb their values. About half of the site measurements have outcome $X_s=1$ and about half have outcome $X_s=-1$; to obtain the state $|\overline{0}\rangle$, we must remove all of the site defects (sites where $X_s=-1$). Thus we select an arbitrary one-chain whose boundary consists of the positions of all site defects, and we apply Z to each link of this chain, thereby imposing $X_s=1$ at each site. In carrying out this procedure, we might apply $\overline{Z}$ to the code block by applying Z to a homologically nontrivial path, but this has no effect since the state is a $\overline{Z}=1$ eigenstate.

Unfortunately, syndrome measurement is not perfectly reliable; therefore this procedure could generate long *open* chains of Z errors in the code block. To keep the open chains under control, we need to repeat the measurement of both the X and Z syndromes of order L times (where L is the linear size of the lattice), and use our global recovery method. Then the initial configuration of the defects will be ''forgotten'' and the error chains in the code block will relax to the equilibrium configuration in which long open chains are highly unlikely. The probability of an $\overline{X}$ error that causes a flip of the encoded state will be exponentially small in L. We can prepare the encoded state with $\overline{X}=1$ by the dual procedure, starting with the state $[(1/\sqrt{2})(|0\rangle+|1\rangle)]^{\otimes n}$.

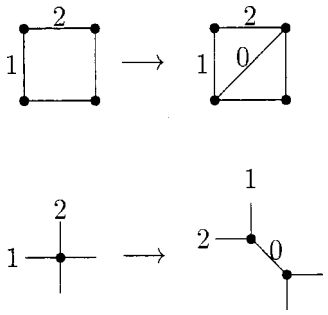

FIG. 16. Two basic moves that modify the triangulation of a surface by adding a link: splitting a plaquette, and splitting a vertex.

C. Encoding of unknown states

Quantum error-correcting codes can protect *unknown* coherent quantum states. This feature is crucial in applications to quantum computation—the operator of a quantum computer need not ''monitor'' the encoded quantum state to keep the computation on track. But to operate a quantum computer, we do not typically need to *encode* unknown quantum states. It is sufficient to initialize the computer by encoding known states, and then execute a known quantum circuit.

Still, a truly robust ''quantum memory'' should be able to receive an unknown quantum state and store it indefinitely. But given any nonzero rate of decoherence, to store an unknown state for an indefinitely long time we need to encode it using a code of indefinitely long block size. How, then, can we expect to encode the state before it decoheres?

The key is to encode the state quickly, providing some measure of protection, while continuing to build up toward larger code blocks. Concatenated codes provide one means of achieving this. We can encode, perform error correction, then encode again at the next level of concatenation. If the error rates are small enough, encoding can outpace the errors so that we can store the unknown state in a large code block with reasonable fidelity.

The surface codes, too, allow us to build larger codes from smaller codes and so to protect unknown states effectively. The key to enlarging the code block is that a code corresponding to one triangulation of a surface can be transformed into a code corresponding to another triangulation.

For example, we can transform one surface code to another using local moves shown in Fig. 16.

Links can be added to (or removed from) the triangulation in either of two ways—one way adds a new plaquette, the other adds a new site. Either way, the new triangulation corresponds to a new code with an additional qubit in the code block and an additional stabilizer generator.

When a new plaquette is added, the new code stabilizer is obtained from the old one by adding the new plaquette operator

$$Z_1 Z_2 Z_0 \tag{92}$$

and by modifying the site operators with the replacements

$$X_1 \to X_1 X_0, \quad X_2 \to X_2 X_0. \tag{93}$$

When a new site is added, the stabilizer is modified similarly, but with X's and Z's interchanged:

$$X_1 X_2 X_0 \tag{94}$$

is a new stabilizer generator, and the existing plaquette operators are modified as

$$Z_1 \to Z_1 Z_0, \quad Z_2 \to Z_2 Z_0. \tag{95}$$

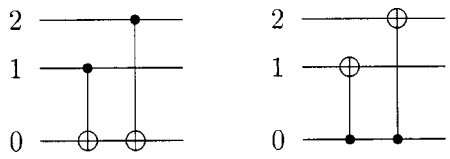

FIG. 17. Circuits that implement the two basic moves of Fig. 16. The circuit with qubit 0 as the target of the CNOTs adds a plaquette; the circuit with qubit 0 as the control of the CNOTs adds a site.

To add a plaquette or a site to a stabilizer code, we prepare the additional qubit in a $Z_0=1$ or $X_0=1$ eigenstate, and then execute the circuit shown in Fig. 17. We recall that, acting by conjugation, a CNOT gate changes a tensor product of Pauli operators acting on its control and target according to

$$IZ\leftrightarrow ZZ, \quad XI\leftrightarrow XX; \tag{96}$$

that is, the CNOT transforms an IZ eigenstate to a ZZ eigenstate and an XI eigenstate to an XX eigenstate, while leaving ZI and IX eigenstates invariant. The circuit in Fig. 17 with qubit 0 as target, then, transforms the site operators as in Eq. (93) while also implementing

$$Z_0\rightarrow Z_1Z_2Z_0\,. \tag{97}$$

The initial $Z_0=1$ eigenstate is transformed into a state that satisfies the plaquette parity checks of the new triangulation. Similarly, the circuit in Fig. 17 with qubit 0 as control implements Eq. (95) as well as

$$X_0\rightarrow X_1X_2X_0\,; \tag{98}$$

the circuit transforms the $X_0=1$ eigenstate into a state that satisfies the new site parity checks.

Of course, these circuits are reversible; they can be used to extricate qubits from a stabilizer code instead of adding them.

If planar codes are used, we can lay out the qubits in a planar array. Starting with a small encoded planar block in the center, we can gradually add new qubits to the boundary using the moves shown in Fig. 18.

These moves add a new three-qubit plaquette or site operator, and can also be implemented by the circuits of Fig. (17).

A procedure that transforms a distance-L planar code to a distance-$(L+1)$ code is shown in Fig. 19. By adding a new row of plaquette operators, we transform what was formerly a smooth edge into a rough edge, and by adding a new row of site operators we transform a rough edge to a smooth edge. We start the row of plaquettes by adding a two-qubit plaquette operator to the corner via the transformations

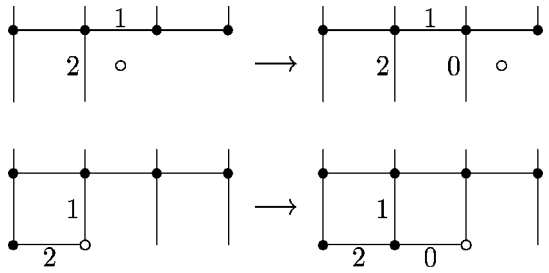

FIG. 18. The same circuits as in Fig. 17 can also be used to build up a planar code by adding a link at the boundary. Sites or plaquettes marked by open circles do not correspond to stabilizer operators.

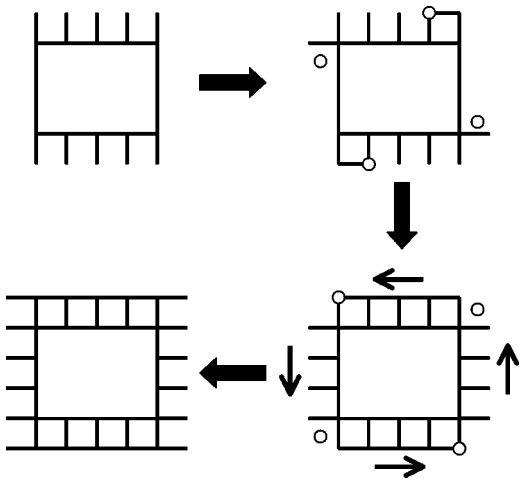

FIG. 19. Building a distance-$(L+1)$ planar code by adding qubits to a distance-L planar code. (Here, $L=5$.) In the first step, new two-qubit stabilizer operators are added in the corners with single CNOTs; in subsequent steps, three-qubit stabilizer operators are added with double CNOTs. The last step promotes the corner operators to three-qubit operators.

$$Z_0 \to Z_1 Z_0, \quad X_1 \to X_1 X_0, \tag{99}$$

which can be implemented by a single CNOT; similarly, we start a row of sites by adding a two-qubit site operator with

$$X_0 \to X_1 X_0, \quad Z_1 \to Z_1 Z_0. \tag{100}$$

Then a new row of boundary stabilizer operators can be ''zipped'' into place.

As is typical of encoding circuits, this procedure can propagate errors badly; a single faulty CNOT can produce a long row of qubit errors (a widely separated pair of defects) along the edge of the block. To ensure fault tolerance, we must measure the boundary stabilizer operators frequently during the procedure. Examining the syndrome record, we can periodically identify the persistent errors and remove them before proceeding to add further qubits.

IX. FAULT-TOLERANT QUANTUM COMPUTATION

We will now consider how information protected by planar surface codes can be processed fault-tolerantly. Our objective is to show that a universal set of fault-tolerant encoded quantum gates can be realized using only local quantum gates among the fundamental qubits and with only polynomial overhead. We will describe one gate set with this property.[4,8] This construction suffices to show that there is an accuracy threshold for quantum computation using surface codes: each gate in our set can be implemented acting on encoded states with arbitrarily good fidelity, in the limit of a large code block. We have not analyzed the numerical value of this computation threshold in detail. Better implementations of fault-tolerant quantum computation can probably be found, requiring less overhead and yielding a better threshold.

We choose the basis introduced by Shor,[3] consisting of four gates. Three of these generate the ''symplectic'' or ''normalizer'' group, the finite subgroup of the unitary group that, acting by conjugation, takes tensor products of Pauli operators to tensor products of Pauli operators. Of these three, two are single-qubit gates: the Hadamard gate

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{101}$$

which acts by conjugation on Pauli operators according to

$$H{:}X\leftrightarrow Z, \tag{102}$$

and the phase gate

$$P\equiv\Lambda(i)=\begin{pmatrix}1 & 0\\ 0 & i\end{pmatrix}, \tag{103}$$

which acts by conjugation on Pauli operators according to

$$P{:}X\rightarrow Y, \quad Z\rightarrow Z. \tag{104}$$

The third generator of the normalizer group is the two-qubit CNOT$=\Lambda(X)$ gates, which acts by conjugation on Pauli operators according to

$$\begin{gathered}\text{CNOT:}\ \ XI\rightarrow XX, \quad IX\rightarrow IX,\\ ZI\rightarrow ZI, \quad IZ\rightarrow ZZ.\end{gathered} \tag{105}$$

Quantum computation in the normalizer group is no more powerful than classical computation.[37] To realize the full power of quantum computing we need to complete the basis with a gate outside the normalizer group. This gate can be chosen to be the three-qubit Toffoli gate $T\equiv\Lambda^2(X)$, which acts on the standard three-qubit orthonormal basis $\{|a,b,c\rangle\}$ as

$$T{:}|a,b,c\rangle\rightarrow|a,b,c\oplus ab\rangle. \tag{106}$$

A. Normalizer gates for surface codes

1. CNOT gate

Implementing normalizer computation on planar codes is relatively simple. First of all, a planar surface code is a Calderbank–Shor–Steane[26,27] (CSS) code, and as for any CSS code with a single encoded qubit, an encoded CNOT can be performed *transversally*—in other words, if simultaneous CNOTs are executed from each qubit in one block to the corresponding qubit in the other block, the effect is to execute the encoded CNOT.[38] To see this, we first need to verify that the transversal CNOT preserves the code space, i.e., that its action by conjugation preserves the code's stabilizer. This follows immediately from Eq. (105), since each stabilizer generator is either a tensor product of X's or a tensor product of Z's. Next we need to check that CNOT$^{\otimes n}$ acts on the encoded operations $\overline{X}$ and $\overline{Z}$ as in Eq. (105), which also follows immediately since $\overline{Z}$ is a tensor product of Z's and $\overline{X}$ is a tensor product of X's.

2. Hadamard gate

What about the Hadamard gate? In fact, applying the bitwise operation $H^{\otimes n}$ does not preserve the code space; rather it maps the code space of one planar code to that of another, different, planar code. If the stabilizer generators of the initial code are site operators X_s and plaquette operators Z_P, then the action of the bitwise Hadamard is

$$H^{\otimes n}{:}X_s\rightarrow Z_s, \quad Z_P\rightarrow X_P. \tag{107}$$

Compared to the initial code, the stabilizer of the new code has sites and plaquettes interchanged. We may reinterpret the new code as a code with X_s and Z_P check operators, but defined on a lattice dual to the lattice of the original code. If the original lattice has its ''rough'' edges at the north and south, then the new lattice has its rough edges at the east and west. We will refer to the two codes as the ''north–south'' (NS) code and the ''east–west'' (EW) code. As indicated in Fig. 20, the action of $H^{\otimes n}$ on the encoded operations $\overline{X}$ and $\overline{Z}$ of the NS code is

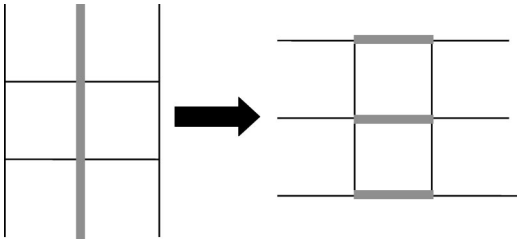

FIG. 20. Action of the bitwise Hadamard gate on the planar code. If Hadamard gates are applied simultaneously to all the qubits in the block, an "NS code" with rough edges at the north and south is transformed to an "EW code" with rough edges at the east and west; the encoded operation $\overline{Z}_{\mathrm{NS}}$ of the NS code is transformed to $\overline{X}_{\mathrm{EW}}$ of the EW code, and $\overline{X}_{\mathrm{NS}}$ is transformed to $\overline{Z}_{\mathrm{EW}}$.

$$H^{\otimes n}\colon \overline{X}_{\mathrm{NS}} \to \overline{Z}_{\mathrm{EW}}, \quad \overline{Z}_{\mathrm{NS}} \to \overline{X}_{\mathrm{EW}}. \tag{108}$$

If we rigidly rotate the lattice by 90°, the EW code is transformed back to the NS code. Hence, the overall effect of a bitwise Hadamard and a 90° rotation is an encoded Hadamard $\overline{H}$.

Of course, a physical rotation of the lattice might be inconvenient in practice! Instead, we will suppose that "peripheral" qubits are available at the edge of the code block, and that we have the option of incorporating these qubits into the block or ejecting them from the block using the method described in Sec. VIII C. After applying the bitwise Hadamard, transforming the $L \times L$ NS code to the EW code, we add $L-1$ plaquettes to the northern edge and $L-1$ sites to the western edge, while removing $L-1$ plaquettes on the east and $L-1$ sites on the south. This procedure transforms the block back to the NS code, but with the qubits shifted by half a lattice spacing to the north and west—we will call this shifted code the NS′ code. Furthermore, this modification of the boundary transforms the logical operations $\overline{Z}_{\mathrm{EW}}$ and $\overline{X}_{\mathrm{EW}}$ of the EW code to the operations $\overline{Z}_{\mathrm{NS}'}$ and $\overline{X}_{\mathrm{NS}'}$ of the NS′ code. The overall effect, then, of the bitwise Hadamard followed by the boundary modification is the operation

$$\overline{X}_{\mathrm{NS}} \to \overline{Z}_{\mathrm{NS}'}, \quad \overline{Z}_{\mathrm{NS}} \to \overline{X}_{\mathrm{NS}'}. \tag{109}$$

In principle, we could complete the encoded Hadamard gate by physically shifting the qubits half a lattice spacing to the south and east, transforming the NS′ code back to the NS code. One way to execute this shift might be to swap the qubits of the NS′ with qubits located at the corresponding sites of the NS lattice. If we prefer to avoid the additional quantum processing required by the swaps, then what we can do instead is associate a classical flag bit with each code block, recording whether the number of Hadamard gates that have been applied in our circuit to that logical qubit is even or odd, and hence whether the logical qubit is encoded in the NS code or the NS′ code. This classical bit is consulted whenever the circuit calls for a Hadamard or CNOT acting on the block. If we perform a Hadamard on a qubit that is initially encoded with the NS′ code, we add qubits on the south and east while removing them from the north and west, returning to the NS code. The CNOT gates are performed transversally between blocks that are both in the NS code or both in the NS′ code; that is, each qubit in one layer interacts with the corresponding qubit directly below it in the next layer. But if one block is in the NS code and the other is in the NS′ code, then each qubit in one layer interacts with the qubit in the next layer that is half a lattice spacing to north and west. Note that the modification of the boundary requires a number of computation steps that is linear in L.

3. Phase gate

For implementation of the phase gate P, note that if we can execute CNOT and H then we can also construct the "controlled-(iY)" gate

$$\Lambda(iY)=\Lambda(ZX)=(IH)\cdot\Lambda(X)\cdot(IH)\cdot\Lambda(X). \tag{110}$$

Hence it suffices to be able to prepare an eigenstate $|+\rangle$ or $|-\rangle$ of Y,

$$Y|\pm\rangle=\pm|\pm\rangle; \tag{111}$$

if we prepare an ancilla in the state $|+\rangle$, and apply a CNOT with the data as its control and the ancilla as its target, the effect on the data is the same as $\Lambda(i)=P$. If the ancilla is the state $|-\rangle$, then we apply $\Lambda(-i)=P^{-1}$ to the data instead.

Now, it is not obvious how to prepare a large toric block in an eigenstate of the encoded Y with good fidelity. Fortunately, we can nevertheless use a CNOT and an ancilla to implement P, thanks to a trick that works because P is the only gate in our set that is not real. Consider a circuit that applies the unitary transformation U to the data if the ancilla has actually been prepared in the state $|+\rangle$. Then if $|+\rangle$ were replaced by $|-\rangle$, this same circuit would apply the complex conjugate unitary U^*, since each P in the circuit would be replaced by P^*.

Instead of a Y eigenstate, suppose we prepare the ancilla in any encoded state we please, for example, $|\overline{0}\rangle$. And then we use this same ancilla block, and a CNOT, every time a P is to be executed. The state of the ancilla can be expressed as a linear combination $a|+\rangle+b|-\rangle$ of the Y eigenstates, and our circuit, acting on the initial state $|\psi\rangle$ of the data, yields

$$a|+\rangle\otimes U|\psi\rangle+b|-\rangle\otimes U^*|\psi\rangle. \tag{112}$$

Now, at the very end of a quantum computation, we will need to make a measurement to read out the final result. Let A denote the observable that we measure. The expectation value of A will be

$$\langle A\rangle=|a|^2\langle\psi|U^\dagger AU|\psi\rangle+|b|^2\langle\psi|U^\dagger A^T U|\psi\rangle, \tag{113}$$

where A^T denotes the transpose of A. Without losing any computational power, we may assume that the observable A is real ($A=A^T$)—for example, it could be $1/2\,(I-Z)$ acting on one of our encoded blocks. Then we get the same answer for the expectation value of A as if the ancilla had been prepared as $|+\rangle$ (or $|-\rangle$); hence our fault-tolerant procedure successfully simulates the desired quantum circuit.

Since there is just one ancilla block that must be used each time the P gate is executed, this block has to be swapped into the position where it is needed, a slowdown that is linear in the width of the quantum circuit that is being simulated.

Thus we have described a way to perform fault-tolerant normalizer computation for planar surface codes. We envision, then, a quantum computer consisting of a stack of planar sheets, with a logical qubit residing in each sheet. Each logical sheet has associated with it an adjacent sheet of ancilla qubits that are used to measure the check operators of the surface code; after each measurement, these ancilla qubits are refreshed in place and then reused. The quantum information in one sheet can be swapped with that in the neighboring sheet through the action of local gates. To perform a logical CNOT between two different logical qubits in the stack, we first use swap gates to pass the qubits through the intervening sheets of logical and ancilla qubits and bring them into contact, then execute the transversal CNOT between the two layers, and then use swap gates to return the logical qubits to their original positions. By inserting a round of error correction after each swap or logical operation, we can execute a normalizer circuit reliably.

B. State purification and universal quantum computation

Now we need to consider how to complete our universal gate set by adding the Toffoli gate. As Shor observed,[3] implementation of the gate can be reduced to the problem of preparing a particular three-qubit state, which may be chosen to be

$$|\psi\rangle_{\text{anc}}=2^{-3/2}\sum_{a,b,c\in\{0,1\}}(-1)^{abc}|a\rangle_1|b\rangle_2|c\rangle_3; \tag{114}$$

this state is the simultaneous eigenstate of three commuting symplectic operators: $\Lambda(Z)_{1,2}X_3$ and its two cyclic permutations, where $\Lambda(Z)$ is the two-qubit conditional phase gate

$$\Lambda(Z):|a,b\rangle\rightarrow(-1)^{ab}|a,b\rangle. \tag{115}$$

Shor's method for constructing this state involved the preparation and measurement of an unprotected n-qubit cat state, where n is the block size of the code. But this method cannot be used for a toric code on a large lattice, because the cat state is too highly vulnerable to error.

Fortunately, there is an alternative procedure for constructing the needed encoded state with high fidelity—*state purification*. Suppose that we have a supply of noisy copies of the state $|\psi\rangle_{\rm anc}$. We can carry out a purification protocol to distill from our initial supply of noisy states a smaller number of states with much better fidelity.[39,40] In this protocol, normalizer gates are applied to a pair of noisy copies, and then one member of the pair is measured. Based on the outcome of the measurement, the other state is either kept or discarded. If the initial ensemble of states approximates the $|\psi\rangle_{\rm anc}$ with adequate fidelity, then, as purification proceeds, the fidelity of the remaining ensemble converges rapidly toward one.

For this procedure to work, it is important that our initial states are not *too* noisy—there is a purification threshold. Therefore, to apply the purification method to toric codes, we will need to build up the size of the toric block gradually, as in the procedure for encoding unknown states described in Sec. VIII C. We start out by encoding $|\psi\rangle_{\rm anc}$ on a small planar sheet of qubits, with a fidelity below the purification threshold. Then we purify for a while to improve the fidelity, and build on the lattice to increase the size of the code block. By building and purifying as many times as necessary, we can construct a copy of the ancilla state that can be used to execute the Toffoli gate with high fidelity.

The time needed to build up the encoded blocks is quadratic in L, and the number of rounds of purification needed is linear in L, if we wish to reach a fidelity that is exponentially small in L. Thus the overhead incurred in our implementation of the Toffoli gate is polynomial in the block size.

We have now assembled all the elements of a fault-tolerant universal quantum computer based on planar surface codes. The computer is a stack of logical qubits, and it contains ''software factories'' where the ancilla states needed for execution of the Toffoli gate are prepared. Once prepared, these states can be transported through swapping to the position in the stack where the Toffoli gate is to be performed.

X. A LOCAL ALGORITHM IN FOUR DIMENSIONS

In our recovery procedure, we have distinguished between quantum and classical computation. Measurements are performed to collect syndrome information about errors that have accumulated in the code block, and then a fast and reliable classical computer processes the measured data to infer what recovery step is likely to remove most of the errors. Our procedures are fault tolerant because the quantum computation needed to measure the syndrome is highly local. But the classical computation is not so local—our algorithm for constructing the chain of minimal weight requires as input the syndrome history of the entire code block.

It would be preferable to replace this procedure by one in which measurements and classical processing are eliminated, and all of the processing is local quantum processing. Can we devise a stable quantum memory based on topological coding such that rapid measurements of the syndrome are not necessary?

Heuristically, errors create pairs of defects in the code block, and trouble may arise if these defects diffuse apart and annihilate other defects, eventually generating homologically nontrivial defect world lines. In principle, we could protect the encoded quantum information effectively if there is a strong attractive interaction between defects that prevents them from wandering apart. A recovery procedure that simulates such interactions was discussed in Ref. 40. For that procedure, an accuracy threshold can be established, but only if the interactions have arbitrarily long range, in

which case the order-disorder transition in the code block is analogous to the Kosterlitz–Thouless transition in a two-dimensional Coulomb gas. But to simulate these infinite-range interactions, nonlocal processing is still required.

A similar problem confronts the proposal[5,41,42] to encode quantum information in a configuration of widely separated nonabelian anyons. Errors create anyons in pairs, and the encoded information is endangered if these ''thermal anyons'' diffuse among the anyons that encode the protected quantum state. In principle, a long-range attractive interaction among anyons might control the diffusion, but this interaction might also interfere with the exchanges of anyons needed to process the encoded state. In any case, a simulation of the long-range dynamics involves nonlocal processing.

We will now describe a procedure for recovery that, at least mathematically, requires no such nonlocal processing of quantum or classical information. With this procedure, based on ''locally available'' quantum information, we can infer a recovery step that is more likely to remove errors than add new ones. Because the procedure is local we can dispense with measurement without degrading its performance very much—measurements followed by quantum gates conditioned on measurement outcomes can be replaced by unitary transformations acting on the data qubits and on nearby ancilla qubits. But since we will still need a reservoir where we can dispose the entropy introduced by random errors, we will continue to assume as usual that the ancilla qubits can be regularly refreshed as needed.

Unfortunately, while our procedure is local in the mathematical sense that recovery operations are conditioned on the state of a small number of ''nearby'' qubits, we do not know how to make it *physically* local in a space of fewer than four dimensions.

A. Repetition code in two dimensions

The principle underlying our local recovery procedure can be understood if we first consider the simpler case of a repetition code. We can imagine that the code block is a periodically identified one-dimensional lattice of binary spins, with two codewords corresponding to the configurations with all spins up or all spins down. To diagnose errors, we can perform a local syndrome measurement by detecting whether each pair of neighboring spins is aligned or anti-aligned, thus finding the locations of defects where the spin orientation flips.

To recover we need to bring these defects together in pairs to annihilate. One way to do this is to track the history of the defects for a while, assembling a record S of the measured syndrome, and then find a minimum-weight chain E' with the same boundary, in order to reconstruct hypothetical world lines of the defects. But in that case the processing required to construct E' is nonlocal.

The way to attain a local recovery procedure is to increase the dimensionality of the lattice. In two dimensions, errors will generate droplets of flipped spins (as in Fig. 21), and the local syndrome measurement will detect the boundary of the droplet. Thus the defects now form one-dimensional closed loops, and our recovery step should be designed to reduce the total length of such defects. Local dynamical rules can easily be devised that are more likely to shrink a loop than stretch it, just as it is possible to endow strings with local dynamics (tension and dissipation) that allow the strings to relax. Thus, in equilibrium, very long loops will be quite rare. If the error rate is small enough, then the droplets of flipped spins will typically remain small, and the encoded information will be well protected.

That the two-dimensional version of the repetition code is more robust than the one-dimensional version illustrates a central principle of statistical mechanics—that order is more resistant to fluctuations in higher dimensions. The code block is described by an Ising spin model, and while the one-dimensional Ising model is disordered at any nonzero temperature, the two-dimensional Ising model remains ordered up to a nonvanishing critical temperature. From the perspective of coding theory, the advantage of the two-dimensional version is that the syndrome is highly redundant. If we check each pair of nearest-neighbor spins to see if they are aligned or anti-aligned, we are collecting more information than is really needed to diagnose all the errors in the block. Hence there is a constraint that must be satisfied by a valid syndrome, namely that the

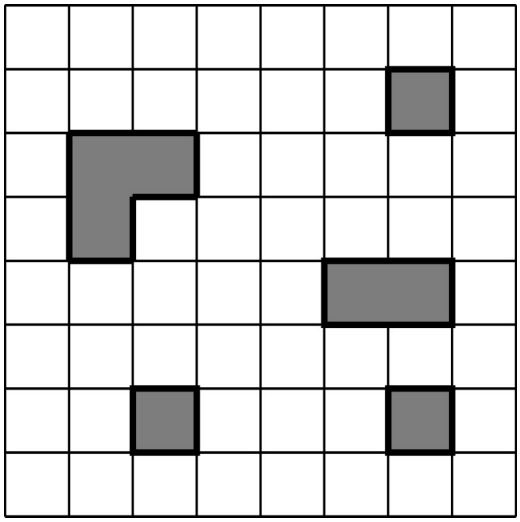

FIG. 21. Droplets of flipped qubits in the two-dimensional quantum repetition code. Qubits reside on plaquettes, and the qubits that have been flipped are shaded. Thick links are locations of ''defects'' where the error syndrome is nontrivial because neighboring qubits are anti-aligned. The defects form closed loops that enclose the droplets.

boundary of a droplet can never end; therefore errors in the syndrome can be detected. Of course, physically, the stability of the ordered state of the Ising model in more than one dimension is the reason that magnetic memories are robust in Nature.

B. Toric code in four dimensions

The defects detected by the measurement of the stabilizer operators of a two-dimensional toric code are also pointlike objects, and error recovery is achieved by bringing the defects together to annihilate. We can promote the annihilation by introducing an effective long-range interaction between defects, but a more local alternative procedure is to increase the dimensionality of the lattice.

So consider a *four-dimensional* toric code. Qubits are associated with each plaquette. With each link is associated the six-qubit stabilizer operator $X_l = X^{\otimes 6}$ acting on the six plaquettes that contain the link, and with each cube is associated the six-qubit stabilizer operator $Z_C = Z^{\otimes 6}$ acting on the six plaquettes contained in the cube. Thus the four-dimensional code maintains the duality between phase and flip errors that we saw in two dimensions. The encoded $\overline{Z}$ or $\overline{X}$ operation is constructed from Z's or X's acting on a homologically nontrivial surface of the lattice or dual lattice, respectively. Z errors on a connected open surface generate a closed loop of defects on the boundary of the surface, and X errors on a connected open surface of the dual lattice generate defects on a set of cubes that form a closed loop on the dual lattice. As in the two-dimensional case, there is a ''hyperplanar'' version of the code that can be defined on a four-dimensional region with a boundary.

Now we want to devise a recovery procedure that will encourage the defect loops to shrink and disappear. Assuming that syndrome measurements are employed, a possible procedure for controlling phase errors can be described as follows: First, the stabilizer operator X_l is measured at each link, and a record is stored of the outcome. We say that each link with $X_l = -1$ is occupied by a string, and each link with $X_l = 1$ is unoccupied. We choose a set of nonoverlapping plaquettes (with no link shared by two plaquettes in the set), and based on the syndrome for the links of that plaquette, decide whether or not to flip the plaquette (by applying a Z). If three or four of the plaquette's links are occupied by string, we always flip the plaquette. If zero or one link is occupied, we never flip it. And if two links are occupied, we flip the plaquette with probability

$\frac{1}{2}$. Then in the next time step, we again measure the syndrome, and decide whether to flip another nonoverlapping set of plaquettes. And so on.

Naturally, we also measure the bit-flip syndrome—Z_C on every cube—in each time step. The procedure for correcting the bit-flip errors is identical, with the lattice replaced by the dual lattice, and X replaced by Z.

Of course the measurement is not essential. A simple reversible computation can imprint the number of string bits bounding a plaquette on ancilla qubits, and subsequent unitary gates controlled by the ancilla can ''decide'' whether to flip the plaquette. Note that a CNOT that is applied with probability $\frac{1}{2}$, needed in the event that the plaquette has two string bits on its boundary, can be realized by a Toffoli gate, where one of the control qubits is a member of a Bell pair so that the control takes the value 1 with probability $\frac{1}{2}$.

This recovery procedure has the property that, if it is perfectly executed and no further errors occur during its execution, it will never increase the total length of string on the lattice, but it will sometimes reduce the length. Indeed, if it is applied repeatedly while no further errors occur, it will eventually eliminate every string. We have chosen to make the procedure nondeterministic in the case where there are two string bits on a plaquette, because otherwise the procedure would have closed orbits—some string configurations would oscillate indefinitely rather than continuing to shrink and annihilate. With the nondeterministic procedure, a steady state can be attained only when all the strings have disappeared.

Actually, following the ideas of Toom,[43] it is possible to devise *anisotropic deterministic* procedures that also are guaranteed to remove all strings. These procedures, in fact, remove the strings more efficiently than our nondeterministic one, but are a little more difficult to analyze.

Of course, the recovery procedure will not really be executed flawlessly, and further errors will continue to accumulate. Still, as error recovery is performed many times, an equilibrium will eventually be attained in which string length is being removed by recovery as often as it is being created by new errors. If the error rates are small enough, the equilibrium population of long string loops will be highly suppressed, so that the encoded quantum information will be well protected.

Eventually, say at the conclusion of a computation, we will want to measure encoded qubits. This measurement procedure does have a nonlocal component (as the encoded information is topological), and for this purpose only we will assume that a reliable classical computer is available to help with the interpretation of the measured data. To measure the logical operator $\overline{Z}$, say, we first measure every qubit in the code block. Then we apply a classical parity check, evaluating Z_C for each cube of the lattice, thereby generating a configuration of closed defect loops on the dual lattice. To complete the measurement, we first eliminate the defects by applying flips to a set of plaquettes bounded by each loop. Then we can evaluate the product of Z's associated with a homologically nontrivial surface to find the value of $\overline{Z}$.

Of course, when we eliminate the defects, we need to make sure that we choose correctly among the homologically inequivalent surfaces bounded by the observed strings. One way to do so, which is unlikely to fail when qubit and measurement error probabilities are small, is to invoke the relaxation algorithm formulated above to the classical measurement outcome. Since our classical computer is reliable, the algorithm eventually removes all strings, and then the value of $\overline{Z}$ can be determined.

C. Accuracy threshold

To evaluate the efficacy of the local recovery method, we need to find the equilibrium distribution of defects. This equilibrium configuration is not so easily characterized, but it will suffice to analyze a less effective algorithm that does attain a simple steady state—the heat bath algorithm. To formulate the heat bath algorithm, suppose that strings carry an energy per lattice unit length that we may normalize to one, and suppose that each plaquette is in contact with a thermal reservoir at inverse temperature β. In each time step, plaquettes are updated, with the change in the string length bounding a plaquette governed by the Boltzmann probability distribution. Thus survival or creation of a length-4 loop is suppressed by the factor

$$\frac{\text{Prob}(0\to 4)}{\text{Prob}(0\to 0)}=\frac{\text{Prob}(4\to 4)}{\text{Prob}(4\to 0)}=e^{-4\beta}. \tag{116}$$

Similarly, the probability of a plaquette flip when the length of bounding string is 3 or 1 satisfies

$$\frac{\text{Prob}(1\to 3)}{\text{Prob}(1\to 1)}=\frac{\text{Prob}(3\to 3)}{\text{Prob}(3\to 1)}=e^{-2\beta}. \tag{117}$$

In the case of a plaquette with two occupied links, we again perform the flip with probability $\frac{1}{2}$. As before, this ensures ergodicity—any initial configuration has some nonvanishing probability of reaching any final configuration.

Damage to encoded information arises from string ''world sheets'' that are homologically nontrivial. At low temperature, string loops are dilute and failure is unlikely, but at a critical temperature the strings ''condense,'' and the encoded data are no longer well protected. The critical temperature is determined by a balance between Boltzmann factor $e^{-\beta l}$ suppressing a string of length l and the string entropy. The abundance of self-avoiding closed loops of length l behaves like,[34]

$$n_{\text{SAW}}^{(4)}(l)\sim P_4(l)(\mu_4)^l, \quad \mu_4\approx 6.77, \tag{118}$$

in $d=4$ dimensions, where $P_4(l)$ is a polynomial. Thus, large loops are rare when the sum

$$\sum_l n_{\text{SAW}}^{(4)}(l)e^{-\beta l}\sim\sum_l P_4(l)(\mu_4 e^{-\beta})^l \tag{119}$$

converges, and the system is surely ordered for $e^{-\beta}<\mu_4^{-1}$. Thus the critical inverse temperature β_c satisfies

$$e^{-\beta_c}\geqslant(\mu_4)^{-1}. \tag{120}$$

Now, our local recovery procedure will not be precisely a heat bath algorithm. But like the heat bath algorithm it is more likely to destroy string than create it, and we can bound its performance by assigning to it an effective temperature. For example, if no new errors arise and the algorithm is perfectly executed, it will with probability one remove a length-4 string loop bounding a plaquette. In practice, though, the plaquette may not flip when the recovery computation is performed, either because of a fault during its execution, or because other neighboring plaquettes have flipped in the meantime. Let us denote by q_4 the probability that a plaquette, occupied by four string bits at the end of the last recovery step, does not in fact flip during the current step. Similarly, let q_3 denote the probability that a plaquette with three string bits fails to flip, and let q_1, q_0 denote the probabilities that plaquettes containing one or zero string bits *do* flip. These quantities can all be calculated, given the quantum circuit for recovery and a stochastic error model.

Now we can find a positive quantity q such that

$$q_0,q_4\leqslant q/(1+q),$$

$$q_1,q_3\leqslant\sqrt{q}/(1+\sqrt{q}). \tag{121}$$

Comparing to Eqs. (116) and (117), we see that our recovery algorithm is at least as effective as a heat bath algorithm with the equivalent temperature

$$e^{-4\beta}=q; \tag{122}$$

in equilibrium strings of length l are therefore suppressed by a factor no larger than $e^{-\beta l}=q^{l/4}$. From our estimate of the critical temperature Eq. (120), we then obtain a lower bound on the critical value of q:

$$q_c \geqslant (\mu_4)^{-4} \approx 4.8\times 10^{-4}. \tag{123}$$

This quantum system with local interactions has an accuracy threshold.

A local procedure that controls the errors in a quantum memory is welcome, but it is disheartening that four spatial dimensions are required. Of course, the four-dimensional code block can be projected to $d<4$ dimensions, but then interactions among four-dimensional neighbors become interactions between qubits that are distance $L^{(4-d)/d}$ apart, where L is the linear size of the lattice. In a three-dimensional version of the toric code, we can place qubits on plaquettes, and associate check operators with links and cubes. Thus, phase error defects are strings and bit-flip error defects are point particles, or vice versa. Then we can recover locally (without measurement or classical computation) from either the phase errors or the bit-flip errors, but not both.

In fewer than four spatial dimensions, how might we devise an intrinsically stable quantum memory, analogous to a magnetic domain with long-range order that encodes a robust classical bit? Perhaps we can build a two-dimensional material with a topologically degenerate ground state, such that errors create point defects that have infinite-range attractive interactions. That system's quasi-long-range order at nonzero temperature could stabilize an arbitrary coherent superposition of ground states.

XI. CONCLUSIONS

In foreseeable quantum computers, the quantum gates that can be executed with good fidelity are likely to be *local* gates—only interactions between qubits that are close to one another will be accurately controllable. Therefore, it is important to contemplate the capabilities of large-scale quantum computers in which all gates are local in three-dimensional space. It is also reasonable to imagine that future quantum computers will include some kind of integrated classical processors, and that the classical processors will be much more accurate and much faster than the quantum processors.

Such considerations have led us to investigate the efficacy of quantum error correction in a computational model in which all quantum gates are local, and in which classical computations of polynomial size can be done instantaneously and with perfect accuracy. We have also assumed that the measurement of a qubit can be done as quickly as the execution of a quantum gate.

These conditions are ideally suited for the use of topological quantum error-correcting codes, such that all quantum computations needed to extract an error syndrome have excellent locality properties. Indeed, we have shown that if the two-dimensional surface codes introduced in Refs. 4 and 5 are used, then an accuracy threshold for quantum storage can be established, and we have estimated its numerical value. This accuracy threshold can be interpreted as a critical point of a three-dimensional lattice gauge theory with quenched randomness, where the third dimension represents time. There is also an accuracy threshold for universal quantum computation, but we have not calculated it carefully.

Topological codes provide a compelling framework for controlling errors in a quantum system via local quantum processing; for this reason, we expect these codes to figure prominently in the future evolution of quantum technologies. In any case, our analysis amply illustrates that principles from statistical physics and topology can be fruitfully applied to the daunting task of accurately manipulating intricate quantum states.

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Qubits as parafermions

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Qubits are neither fermions nor bosons. A Fock space description of qubits leads to a mapping from qubits to parafermions: particles with a hybrid boson-fermion quantum statistics. We study this mapping in detail, and use it to provide a classification of the algebras of operators acting on qubits. These algebras in turn classify the universality of different classes of physically relevant qubit-qubit interaction Hamiltonians. The mapping is further used to elucidate the connections between qubits, bosons, and fermions. These connections allow us to share universality results between the different particle types. Finally, we use the mapping to study the quantum computational power of certain anisotropic exchange Hamiltonians. In particular, we prove that the XY model with nearest-neighbor interactions only is *not* computationally universal. We also generalize previous results about universal quantum computation with encoded qubits to codes with higher rates. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1499208]

I. INTRODUCTION

It is an experimental fact that there are only two types of *fundamental* particles in nature: bosons and fermions. Bosons are particles whose wavefunction is unchanged under permutation of two identical particles. The wavefunction of fermions is multiplied by -1 under the same operation. An equivalent statement is that bosons transform according to the one-dimensional, symmetric, irreducible representation (irrep) of the permutation group, while fermions belong to the one-dimensional antisymmetric irrep. The permutation group has only these two one-dimensional irreps. What about particles transforming according to higher-dimensional irreps of the symmetric group? Much research went into studying this possibility, in the early days of the quark model, before the concept of ''colored'' quarks gained widespread acceptance.[1,2] However, there are now good reasons to believe that particles obeying such ''parastatistics'' do not exist (Ref. 3, p. 137). Nevertheless, as we will show below, the traditional definition of a Hilbert space of qubits is inconsistent with the properties of either bosons or fermions.

The description of bosons and fermions in terms of their properties under particle permutations uses the language of first quantization. A useful alternative description is the second-quantized formalism of Fock space.[3,4] A basis state in the boson or fermion Hilbert–Fock space can be written as $|n_1^\alpha, n_2^\alpha, \ldots\rangle$, where n_i^α counts how many bosons ($\alpha = b$) or fermions ($\alpha = f$) occupy a given mode, or site i. Note that the total number of modes does not need to be specified in the Fock-basis. Ignoring normalization, raising, $\alpha_i^\dagger$ (lowering, α_i) operators increase (decrease) n_i^α by 1. A consequence of the permutation properties of bosons and fermions is that their corresponding raising and lowering operators satisfy commutation and anticommutation relations:

$$[b_i^\dagger, b_j^\dagger] = 0, \quad [b_i, b_j^\dagger] = \delta_{ij} \quad \text{bosons},$$

$$\{f_i^\dagger, f_j^\dagger\} = 0, \quad \{f_i, f_j^\dagger\} = \delta_{ij} \quad \text{fermions}.$$

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From this follow a number of well-known facts.[3,4] Let $\hat{n}_i^\alpha = \alpha_i^\dagger \alpha_i$; this is the number operator, which is diagonal in the Fock-basis $|n_1^\alpha, n_2^\alpha, \dots\rangle$, and has eigenvalues n_i^α. Then we have the following.

(i) $[b_i^\dagger, b_j^\dagger] = 0 \Rightarrow$ an arbitrary number of bosons n_i^α can occupy a given mode i. On the other hand, $\{f_i^\dagger, f_j^\dagger\} = 0 \Rightarrow$ only $n_i^f = 0,1$ is possible for fermions.

(ii) $[b_i, b_j^\dagger] = \delta_{ij} \Rightarrow$ the Hilbert space of bosons has a natural tensor product structure, i.e., $|n_1^b, n_2^b, \dots\rangle = |n_1^b\rangle \otimes |n_2^b\rangle \otimes \cdots$. More specifically, it is possible to *independently* operate on each factor of the Hilbert space. However,

$$\{f_i, f_j^\dagger\} = \delta_{ij} \Rightarrow f_j |n_1^f, \dots, n_{j-1}^f, 1, n_{j+1}^f, \dots\rangle = (-1)^{\sum_{k=1}^{j-1} n_k^f} |n_1^f, \dots, n_{j-1}^f, 0, n_{j+1}^f, \dots\rangle,$$

which means that the outcome of operating on a mode of a multi-fermion state depends on all previous modes (the order of modes is actually arbitrary). This nonlocal property means that the fermionic Fock space does not have a natural tensor product structure, although it can be mapped onto one that does using the Jordan–Wigner transformation[5] (see Ref. 6 for a more detailed discussion).

What about qubits? The standard notion of what a qubit is, is the following:[7]

Qubit:

(i) A qubit is a vector in a two-dimensional Hilbert space $\mathcal{H}_i = \mathrm{span}\{|0\rangle_i, |1\rangle_i\}$ (like a fermion).

(ii) An N-qubit Hilbert space has a tensor product structure: $\mathcal{H} = \otimes_{i=1}^N \mathcal{H}_i$ (like bosons).

It appears that a qubit is a hybrid fermion-boson particle! We conclude that *qubits do not exist as fundamental particles*. This motivates us to consider an intermediate statistics of ''parafermions'' in order to have a Fock space description of a qubit. We define the parafermionic commutation relations by[8,9]

$$\begin{aligned} \{a_i, a_i^\dagger\} &= 1, \\ [a_i, a_j^\dagger] &= 0 \quad \text{if} \quad i \neq j. \end{aligned} \tag{1}$$

Here i,j are different modes, or different qubits. The relation $[a_i, a_j^\dagger] = 0$ for $i \neq j$ immediately implies a tensor product structure, while $\{a_i, a_i^\dagger\} = 1$, which together with $a_i|0\rangle = 0$ ($|0\rangle$ is the vacuum state) implies

$$a_i a_i = a_i^\dagger a_i^\dagger = 0 \tag{2}$$

in the standard (irreducible) two-dimensional representation. Therefore a double-occupation state cannot be realized, i.e., the single-particle Hilbert space is two-dimensional. These are exactly the requirements for a qubit.

In fact, the notion of particles with ''intermediate'' statistics such as parafermions is well known and established in condensed matter physics, e.g., hard-core bosons, excitons, or the Cooper pairs of superconductivity[10] (see also Sec. VI). Such particles are always *composite*, i.e., they are not fundamental. Another way of obtaining a particle that is neither a boson nor a fermion is to simply ignore one or more degrees of freedom. This is by and large the approach taken in current proposals for the physical implementation of quantum computers. For example, a single spin-$\frac{1}{2}$, without the orbital component of its wavefunction, behaves exactly like a qubit. This is the case of the electron-spin qubit in quantum dots.[11] Related to this, a truncated multi-level atom can also approximate a qubit, as in the ion-trap proposal.[12] What are the implications of this for quantum computing (QC)? In a nutshell, ''ideal'' qubits are hard to come by. If a qubit is to exist as an approximate two-level system, or as a composite particle, or as a partial description of an object with additional degrees of freedom, this means that some robustness is lost and the door is

opened to decoherence. For example, the additional levels in a multi-level Hilbert space can cause ''leakage,'' the orbital degrees of freedom act as a bath coupled to the spin-qubit, and a composite particle may decay (e.g., the exciton-qubit[13]).

The advantages of the parafermionic formalism for qubits, however, are not necessarily in understanding these sources of decoherence, because this formalism ''accepts'' qubits as particles. Instead, the parafermionic formalism allows us to naturally establish mappings between qubits, fermions, and bosons. This mapping serves to transport well-known results about one type of particle to another, which, as we show below, clarifies questions regarding the ability of sets of one type of particle to act as universal simulators[14] of sets of another type of particle. It also helps in connecting the Hamiltonians of condensed matter physics to standard tools of quantum computation.

The structure of the article is as follows. In the next section we formally introduce the second quantization of qubits. We then classify the algebraic structure of parafemionic operators in Sec. III. This classification, into subalgebras with different conservation properties, is very useful for establishing which subsets of qubit operators are universal, either on the full Hilbert space, or only on a subspace. This is taken up in the next two sections, where we establish the connection between parafermions and fermions (Sec. IV) and bosons (Sec. V). The connection to fermions and bosons also works in the opposite direction: we are able to classify which fermionic and bosonic operator sets are universal. This has implications, e.g., for the linear optics quantum computing proposals.[15,16] Section VI shows how to construct parafermions out of paired fermions and bosons, emphasizing the compound-particle aspect of qubits. With the connections between fermions, bosons, and parafermions clarified, we explain in Sec. VII a remarkable difference between parafermions and the other particle types: bilinear parafermionic Hamiltonians are sufficient for universal quantum computation, whereas fermionic and bosonic Hamiltonians are not. In Sec. VIII we briefly use the mapping to fermions to derive the thermal fluctuations of noninteracting parafermions at finite temperature. In Sec. IX we apply the classification of the various parafermionic operator subalgebras to the problem of establishing universality of typical Hamiltonians encountered in solid state physics. We generalize a number of our previous results.[17,18] In particular, we establish that the XY model is not universal with nearest-neighbor interactions only; and, we prove universality of the XXZ model for codes with arbitrarily high rates. We conclude in Sec. X.

II. SECOND QUANTIZATION OF QUBITS

As in the cases of bosons and fermions, a parafermion number operator in mode i can be defined as

$$\hat{n}_i = a_i^\dagger a_i ,$$

with eigenvalues $n_i = 0,1$. The total number operator is $\hat{n} = \Sigma_i \hat{n}_i$. A normalized basis state in the parafermionic Fock space is

$$|\cdots n_i \cdots\rangle = \prod_i \, (a_i^\dagger)^{n_i} |0\rangle,$$

which we think of as representing a state with the ith qubit in the ''up'' (''down'') state if the ith parafermion is present (absent), i.e., $n_i = 1$ (0). *Qubit computational basis states are thus mapped to parafermionic Fock states*. Equivalently, consider the following mapping from qubits to parafermions:

$$|0_1 \cdots 0_{i-1} 0_i 0_{i+1} \cdots\rangle \to |0\rangle,$$

$$|0_1 \cdots 0_{i-1} 1_i 0_{i+1} \cdots\rangle \to a_i^\dagger |0\rangle,$$

where on the left 0 and 1 represent the standard (first-quantized) logical states of a qubit. *Qubits can thus be identified with parafermionic operators*.

The mapping of qubits to parafermions is completed by mapping the Pauli matrices σ_i^α to parafermionic operators:

$$\sigma_i^+ \to a_i^\dagger, \quad \sigma_i^- \to a_i, \quad \sigma_i^z \to 2n_i - 1. \tag{3}$$

It is then straightforward to check that the standard sl(2) commutation relations of the Pauli matrices,

$$[\sigma_i^+, \sigma_j^-] = \delta_{ij}\sigma_i^z,$$

$$[\sigma_i^z, \sigma_j^\pm] = \pm \delta_{ij}\sigma_i^\pm,$$

are preserved, so that we have a faithful second-quantized representation of the qubit system Hilbert space and algebra. [Of course we could also have mapped su(2)$=\{\sigma^x, \sigma^y, \sigma^z\}$ to the parafermionic operators, by appropriate linear combinations.] To illustrate the multi-qubit Hilbert–Fock space representation, consider the case of two modes, i.e., $i,j=1,2$. The space splits into a vacuum state $|00\rangle = |0\rangle$, single-particle states $|01\rangle = a_1^\dagger|0\rangle$ and $|10\rangle = a_2^\dagger|0\rangle$, and a two-particle state $|11\rangle = a_1^\dagger a_2^\dagger|0\rangle$. It is important to emphasize that the parafermionic formalism is mathematically equivalent to the standard Pauli matrix formalism. We will be using both in the sections that follow, starting with the parafermionic, as it makes particularly transparent the translation of known results about fermions to qubits.

III. GENERAL PROPERTIES OF PARAFERMIONIC OPERATORS

N-qubit operators in QC are elements of the group U(2^N). We will begin our discussion by identifying a set of infinitesimal parafermionic generators for U(2^N). Recall that with any r-parameter Lie group there are associated r infinitesimal generators,[19] e.g., in the case of su(2) these are, in the two-dimensional irreducible representation, the Pauli matrices $\{\sigma_x, \sigma_y, \sigma_z\}$. Now, let $\alpha=\{\alpha_i\}, \beta=\{\beta_j\}$, where α_i, β_j can be 0 or 1. In terms of parafermionic operations, any element of U(2^N) can be written as $\mathrm{U}(b) = \exp(-i\Sigma_{\alpha,\beta} b^{\alpha\beta} Q_{\alpha,\beta}(N))$, where $b^{\alpha\beta}$ are continuous parameters (generalized Euler angles) and the $2^N \times 2^N$ *infinitesimal group generators* $Q_{\alpha,\beta}(N)$ are defined as follows: Let $N_\alpha = \Sigma_{i=1}^N \alpha_i$, and

$$q_\alpha^\dagger(N_\alpha) = (a_N^\dagger)^{\alpha_N} \cdots (a_1^\dagger)^{\alpha_1}, \quad q_\beta(N - N_\alpha) = a_N^{\beta_N} \cdots a_1^{\beta_1}. \tag{4}$$

Then,

$$Q_{\alpha,\beta}(N) = q_\alpha^\dagger(N_\alpha) q_\beta(N - N_\alpha). \tag{5}$$

The $Q_{\alpha,\beta}(N)$ will be recognized as all possible transformations between N-qubit computational basis states, e.g., for $N=2$ the set of 16 operators is

$$\{I, a_1^\dagger, a_2^\dagger, a_1, a_2, a_2^\dagger a_1^\dagger, a_1 a_2, a_1^\dagger a_1, a_1^\dagger a_2, a_2^\dagger a_1, a_2^\dagger a_2, a_2^\dagger a_1^\dagger a_1, a_2^\dagger a_1^\dagger a_2, a_1^\dagger a_1 a_2, a_2^\dagger a_2 a_1, a_2^\dagger a_1^\dagger a_2 a_1\},$$

where I is the identity operator. The set $Q_{\alpha,0}(N)$ generates all possible basis states from the vacuum state. Hermitian forms are $Q + Q^\dagger$ and $i(Q - Q^\dagger)$. We will turn to the Hermitian set of generators in the discussion of applications, in Sec. IX.

Note that infinitesimal generators are not the generators one usually considers in QC. Rather, in QC, a gate operation is obtained by the unitary evolution generated through the turning on/off of a set of physically available *Hamiltonians* $\{H_\mu\}$, which are generally a small subset of the $2^N \times 2^N$ infinitesimal generators $Q_{\alpha,\beta}(N)$. "Generated" here has the usual meaning of allowing linear combinations and commutation of Hamiltonians. We will say that *a set of Hamiltonians* $\{H_\mu\}$ *is universal with respect to a Lie group* $\mathcal{G}$ if it generates the Lie algebra of that group. The

question of the dimension of the universal set of Hamiltonians with respect to $\mathrm{U}(2^N)$ is somewhat subtle, since it is context dependent. Lloyd showed that given two noncommuting operators A, B, represented by $n\times n$ matrices, one can almost always generate $\mathrm{U}(n)$.[20] However, it is not necessarily clear how this result is related to *physically available* Hamiltonians, since in practice one may have only limited control over terms in a Hamiltonian, e.g., the standard Hamiltonian generators for SU(4) (two qubits) is the five-element set $\{\sigma_1^z,\sigma_2^z,\sigma_1^x,\sigma_2^x,\sigma_1^z\sigma_2^z\}$. However, the four-element set $\{\sigma_1^z,\sigma_2^z,\sigma_1^z\sigma_2^x-\sigma_1^x\sigma_2^z,\vec{\sigma}_1\cdot\vec{\sigma}_2\}$ also generates SU(4), and may be physically available.[17] Another example are the following sets of, respectively, five, four, and three generators: $\{\sigma_1^x,\sigma_2^x,\sigma_1^z,\sigma_2^z,\sigma_1^z\sigma_2^z\}$, $\{\sigma_1^x,\sigma_2^x,c_1\sigma_1^z+c_2\sigma_2^z,\sigma_1^z\sigma_2^z\}$, and $\{\sigma_1^x,\sigma_2^x,c_1\sigma_1^z+c_2\sigma_2^z+c_3\sigma_1^z\sigma_2^z\}$ (where c_i are constants). Which set of generators is physically available (i.e., directly controllable) depends on the specific system used to implement the quantum computer. As we will show later in this work, it is sometimes the case that a given, physically available, set of Hamiltonians is universal with respect to a *subgroup* of $\mathrm{U}(2^N)$, which may be quite useful, provided the subgroup is sufficiently large (typically, still exponential in N). This notion of universality with respect to a subgroup is what gives rise to the idea of *encoded universality*:[17,18,21–24,52] one encodes a logical qubit into two or more physical qubits, and studies the universality of the subgroup-generating Hamiltonians with respect to these encoded/logical qubits.

The infinitesimal parafermionic generators $Q_{\alpha,\beta}(N)$ can be rearranged into certain subsets of operators with clear physical meaning, which we now detail.

(1) Local subalgebras: The tensor product structure of qubits is naturally enforced by $[a_i,a_j^\dagger]=0$ for $i\neq j$. This induces a tensor product structure $\otimes_{i=1}^N \mathrm{sl}_i(2)$ on the subalgebras formed by the grouping $\mathrm{sl}_i(2)=\{a_i,a_i^\dagger,1-2n_i\}$. Each $\mathrm{sl}_i(2)$ can only change states within the same mode.

(2) SAp—Subalgebra with *conserved parity*: Define a *parity* operator as

$$\hat{p}=(-1)^{\hat{n}}.$$

It has eigenvalues 1 (-1) for even (odd) total particle number. The operators that commute with the parity operator form a subalgebra, which we denote by SAp. Let k (l) be the number of $a_i^\dagger$ (a_i) factors in $Q_{\alpha,\beta}(N)$, i.e.,

$$k=\sum\ \alpha_i,\quad l=\sum\ \beta_i.$$

SAp consists of those operators having $k-l$ even, so its dimension (i.e., number of generators) is $2^{2N}/2$. To see this, let Q_I be in SAp, and consider its action on a state with an even number of particles $|n\rangle$. Since $k-l$ is even, $Q_I|n\rangle=|n'\rangle$ where n' is also even. Now, $\hat{p}Q_I|n\rangle=\hat{p}|n'\rangle=+|n'\rangle$, but also $Q_I\hat{p}|n\rangle=Q_I(+|n\rangle)=|n'\rangle$ so $[\hat{p},Q]=0$. For example, for $N=2$ SAp consists of $\{I,a_2^\dagger a_1^\dagger,a_1a_2,a_1^\dagger a_1,a_1^\dagger a_2,a_2^\dagger a_1,a_2^\dagger a_2,a_2^\dagger a_1^\dagger a_2a_1\}$.

(3) SAn—subalgebra with *conserved particle number*. This subalgebra, which we denote SAn, is formed by all operators commuting with the number operator $\hat{n}$. These are the operators for which $k=l$, so its dimension is $\Sigma_{k=0}^N\ (\binom{N}{k})^2=(2N)!/N!N!$. To see this, let Q_{II} be in SAn, and consider its action on a state $|n\rangle$ with n particles. Q_{II} cannot change this number since $k=l$, but it can transform $|n\rangle$: $\hat{n}Q_{II}|n\rangle=\hat{n}|n\rangle'=n|n\rangle'$. However, $Q_{II}\hat{n}|n\rangle=nQ_{II}|n\rangle=n|n\rangle'$, so $[Q_{II},\hat{n}]=0$. For example, for $N=2$ SAn consists of $\{I,a_1^\dagger a_1,a_1^\dagger a_2,a_2^\dagger a_1,a_2^\dagger a_2,a_2^\dagger a_1^\dagger a_2a_1\}$. Clearly, SA$n\subset$SA$p$.

(4) Subsets of bilinear operators: There are two types of bilinear operators for $i\neq j$: $a_i^\dagger a_j$ (which conserve the particle number) and $a_ia_j,a_i^\dagger a_j^\dagger$ (which conserve parity). Let $\mu=(ij)$. Then first

$$\begin{aligned} T_\mu^x&=a_j^\dagger a_i+a_i^\dagger a_j,\\ T_\mu^z&=n_i-n_j, \end{aligned}\tag{6}$$

and $T_\mu^y=i[T_\mu^x,T_\mu^z]$ form an su(2) subalgebra, that we denote $\mathrm{su}_\mu^t(2)$. Clearly, $\mathrm{su}_\mu^t(2)\in\mathrm{SA}n$. Second,

$$R^x_\mu = a_i a_j + a_i^\dagger a_j^\dagger ,$$
$$R^z_\mu = n_i + n_j - 1, \tag{7}$$

and R^y_μ form another su(2) subalgebra, that we denote $\mathrm{su}^r_\mu(2) \in \mathrm{SA}p$. Note that $[\mathrm{su}^t_\mu(2), \mathrm{su}^r_\mu(2)] = 0$ since any product of raising/lowering operators from these algebras contains a factor of $a_i a_i$ or $a_i^\dagger a_i^\dagger$. Consider as an example the case of $N=2$ modes. Whereas the direct product group $\mathrm{SU}_1(2) \otimes \mathrm{SU}_2(2)$ yields all product states, the group $\mathrm{SU}^t(2) \oplus \mathrm{SU}^r(2)$ can transform between states with equal particle number and states differing by two particle numbers.

(5) Generators of SA$n(N)$: The set of Hamiltonians $\{a_i^\dagger a_j\}_{i,j=1}^{N+1}$ generates SA$n(N)$, i.e., the subalgebra of conserved particle number on N modes (qubits). Proof: this set maps to the XY model (see Sec. IX B). The rest follows using the method of Ref. 18. Note that $\{a_i^\dagger a_j\}_{i,j=1}^{N+1}$ does *not* generate SA$n(N+1)$, since this set cannot generate $\hat{n}_1 \hat{n}_2 \cdots \hat{n}_N$.

(6) Generators of SA$p(N)$: The set of Hamiltonians $\{a_i^\dagger a_j, a_i a_j + a_i^\dagger a_j^\dagger, i(a_i a_j - a_i^\dagger a_j^\dagger)\}_{i,j=1}^{N}$ yields all states with even particle number on N modes from the vacuum state. (Proof is trivial.)

(7) Generators of SU(2^N): In order to transform between states differing by an odd number of particles it is necessary to include the operators $\{a_i, a_i^\dagger\}$ as well. The corresponding set $\{a_i^\dagger a_j, a_i a_j, a_i^\dagger a_j^\dagger, a_i, a_i^\dagger\}_{i,j=1}^{N}$ generates a set of universal gates (proof is trivial), and then by standard universality results[25,26] the entire SU(2^N).

Additional structure emerges from a mapping between fermions and parafermions. This structure helps both in simulating fermionic system using qubits, and in understanding the universality of qubit systems.

IV. FERMIONS AND PARAFERMIONS

A general fermionic Fock state is

$$|n_1, n_2, \cdots\rangle_F , \tag{8}$$

where $n_i = 0,1$ is the occupation number of mode i. As is well known,[27] the fermionic ("supergroup" [19]) U(2^N) has infinitesimal generators

$$\tilde{Q}^f_{\alpha,\beta}(N) = (f_N^\dagger)^{\alpha_N} \cdots (f_1^\dagger)^{\alpha_1} A f_N^{\beta_N} \cdots f_1^{\beta_1},$$

where

$$A = \bigotimes_{i=1}^{N} (1 - n_i).$$

This basis is equivalent by a linear transformation to the more familiar set

$$Q^f_{\alpha,\beta}(N) = (f_N^\dagger)^{\alpha_N} \cdots (f_1^\dagger)^{\alpha_1} f_N^{\beta_N} \cdots f_1^{\beta_1},$$

which transforms between all possible fermionic Fock states ("fermionic computational basis state"). There is a group chain of this group,

$$\mathrm{U}(2^N) \supset \mathrm{SO}(2N+1) \supset \mathrm{SO}(2N) \supset \mathrm{U}(N) \tag{9}$$

and the generators of the subgroups are known.[19]

The Jordan–Wigner (JW) transformation,[5] recently generalized in Ref. 28, allows one to establish an isomorphism between fermions and parafermions. Defining

$$S_i^f \equiv \bigotimes_{k=1}^{i-1} (1 - 2n_k^f), \quad S_i \equiv \bigotimes_{k=1}^{i-1} (1 - 2n_k), \tag{10}$$

TABLE I. Infinitesimal generators (h.c.=Hermitian conjugate).

Group	Fermions	Parafermions
$U(2^N)$	$Q^f_{\alpha,\beta}(N)$	$Q_{\alpha,\beta}(N)$
$SO(2N+1)$	$f_i^\dagger f_j, f_i f_j, f_i$, h.c.	$a_i^\dagger S_i S_j a_j, a_i S_i S_j a_j, a_i S_i$, h.c.
$SO(2N)$	$f_i^\dagger f_j, f_i f_j$, h.c.	$a_i^\dagger S_i S_j a_j, a_i S_i S_j a_j$, h.c.
$U(N)$	$f_i^\dagger f_j$	$a_i^\dagger S_i S_j a_j$

the mapping is

$$n_i^f \to n_i,$$
$$f_i \to a_i S_i, \tag{11}$$
$$f_i^\dagger \to a_i^\dagger S_i.$$

The action of the fermionic operators on the state (8) is equivalent to that of the corresponding parafermionic operators on the state $|n_1,n_2,\ldots\rangle$. To see this, note that $[a_i,S_i]=0$. Therefore the effect of the JW transformation is quite simple: by commuting all S_i to the left when mapping a fermionic infinitesimal generator to a parafermionic one, we see that (i) the parafermionic $a_i, a_i^\dagger$ operators will yield a state with the same parafermionic occupation numbers as the corresponding fermionic state and (ii) the action of the product of S_i's is to produce a phase ± 1. (This may become a relative phase when acting on a state that is a superposition of computational basis states.) This allows us to study algebraic properties of one set of particles in terms of the other.

Using the JW transformation we find that the same subgroup chain (9) holds for parafermions, and we can immediately write down also the infinitesimal generators for the corresponding parafermionic subgroups. The result is given in Table I.

The significance of these subgroups for QC is in the classification of the universality properties of fermionic and parafermionic Hamiltonians. For example, a Hamiltonian of noninteracting fermions, i.e., one including only bilinear terms $\{f_i^\dagger f_j, f_i f_j, f_j^\dagger f_i^\dagger\}$, is not by itself universal since it merely generates $SO(2N)$. Recent work has clarified what needs to be added to such a Hamiltonian in order to establish universality.[6,29,30] Regarding $SO(2N+1)$, note that one must carefully discuss the Hermitian terms $f_i+f_i^\dagger$ and $i(f_i-f_i^\dagger)$ if one wants to consider them as Hamiltonians, since it is unclear which physical process can be described by such Hamiltonians (a single fermion creation/annihilation operator can turn an isolated fermion into a boson, a process that does not seem to occur in nature).

A more powerful classification, from the QC viewpoint, is in terms of physically available Hamiltonian generators of the subgroups. An interesting restriction of the set of infinitesimal generators to a physically reasonable set of Hamiltonians is to consider only nearest-neighbor interactions, where possible. The results known to us in this case are presented in Table II.

A couple of comments are in order regarding Table II: First, note the group $SO(2N+1)$ may be unphysical not just for fermions since its generators must contain terms like $f_i+f_i^\dagger$ in its Hamiltonian, but also for parafermions: it requires a nonlocal Hamiltonian due to the S_i term. Second, the corresponding fermionic generators for $U(2^N)$ given here is unphysical because it

TABLE II. Hamiltonian generators.

Group	Fermions	Parafermions
$U(2^N)$	$f_i S_i^f, f_i^\dagger f_{i+1}$, h.c.	$a_i, a_i^\dagger a_{i+1}$, h.c.
$SO(2N+1)$	f_i, h.c.	$a_i S_i$, h.c.
$SO(2N)$	$f_i^\dagger f_{i+1}, f_i f_{i+1}$, h.c.	$a_i^\dagger a_{i+1}, a_i a_{i+1}$, h.c.
$SU(N)$	$f_i^\dagger f_{i+1}$, h.c.	$a_i^\dagger a_{i+1}$, h.c.

includes terms that are linear in f_i and furthermore nonlocal. A physically acceptable set is $\{f_i^\dagger f_{i+1}, f_i f_{i+1}, f_i^\dagger f_{i+1}^\dagger f_i f_{i+1}$, h.c.$\}$, but this set is not universal over the full 2^N-dimensional Hilbert space (since it conserves parity). This means that a qubit needs to be encoded into two fermions in this case, a situation we explore further in Sec. VI. Now let us verify the claims of Table II. Our strategy is to show that in each case, we can use the Hamiltonians for generating all infinitesimal generators of the corresponding subgroup in Table I.

Consider first the subgroup SU(N): In the fermionic case, we claim that this subgroup has nearest-neighbor Hamiltonian generators $f_i^\dagger f_{i+1}$ and their Hermitian conjugates. For example, for $N=3$, if we have the four operators $f_1^\dagger f_2$, $f_2^\dagger f_3$ and h.c., then we can generate $f_1^\dagger f_3 = [f_1^\dagger f_2, f_2^\dagger f_3]$ and h.c., as well as $\hat{n}_i^f - \hat{n}_j^f = [f_i^\dagger f_j, f_j^\dagger f_i]$. This yields a total of nine operators, eight of which are linearly independent, that generate SU(3). As for parafermions, we can use the JW transformation to get $f_{i+1}^\dagger f_i \to a_{i+1}^\dagger S_{i+1} a_i S_i = a_{i+1}^\dagger (1-2\hat{n}_i) a_i = a_{i+1}^\dagger a_i$ (where we have used $[a_i, S_i]=0$ and $\hat{n}_i a_i = a_i^\dagger a_i a_i = 0$). This establishes an isomorphism between the fermionic and parafermionic generators for SU(N). Hence the parafermionic subgroup SU(N) is generated by $a_i^\dagger a_{i+1}$ and h.c.

Now consider SO($2N$): In the fermionic case we have $f_1^\dagger f_2^\dagger$, and using the result for U(N) we also have $f_4^\dagger f_1$; therefore we have $[f_4^\dagger f_1, f_1^\dagger f_2^\dagger] = f_4^\dagger f_2^\dagger$. Clearly, the interaction range can be extended to cover all generators. For the parafermionic case, using the JW transformation we find $f_{i+1}^\dagger f_i^\dagger \to a_{i+1}^\dagger S_{i+1} a_i^\dagger S_i = a_{i+1}^\dagger (1-2\hat{n}_i) a_i^\dagger = a_{i+1}^\dagger a_i^\dagger$, so that we again have an isomorphism with the fermionic case.

Next consider the (unphysical) subgroup SO($2N+1$): In the fermionic case it suffices to note that $\frac{1}{2}[f_i, f_j] = f_i f_j$ and $\frac{1}{2}[f_i^\dagger, f_j] = f_i^\dagger f_j$, $i \leqslant j$ so that we can generate all infinitesimal generators by the linear terms f_i and $f_i^\dagger$. The parafermionic case follows by the JW transformation.

Finally, in the U(2^N) case the universality of the parafermionic set $\{a_i, a_i^\dagger a_{i+1}$, h.c.$\}$ follows from that of the set of all single qubit operations together with the Hamiltonian of the nearest-neighbor XY model [Eq. (17) below], proved in Ref. 31. The fermionic case follows by the JW transformation.

Let us recapitulate the meaning of the results presented in this section: we have shown how to classify subalgebras of fermionic/parafermionic operators in terms of the groups they generate. This therefore classifies their universality properties with respect to these groups. This is particularly important in the context of a given set of physically available Hamiltonians. Our method employed a mapping between fermions and parafermions, which allowed us to easily transport known results about one type of particle to the other.

V. BOSONS FROM PARAFERMIONS

A linear combination of different-mode parafermions can approximately form a boson. Define

$$B = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} a_i .$$

Then using Eq. (1) we have

$$[B, B^\dagger] = \frac{1}{N} \sum_{i=1}^{N} 1 - 2\hat{n}_i = 1 - \frac{2\hat{n}}{N}.$$

If the parafermion number is much smaller than the available number of sites/modes, i.e., when $n \ll N$, then $[B, B^\dagger] \approx 1$, which is an approximate single-mode boson commutation relation.

To get K boson modes, we can divide N into K approximately equal parts. Each part has $N_\alpha = N/K$ qubits and approximately represents a boson. The kth boson is $B_\alpha = (1/\sqrt{N_\alpha}) \sum_{i=1}^{N_\alpha} a_i$. Then

$$[B_\alpha, B_\beta^\dagger] = \delta_{\alpha\beta} \left(1 - \frac{2\hat{n}_\alpha}{N_\alpha}\right)^{n_\alpha \ll N_\alpha} \approx \delta_{\alpha\beta} .$$

Physically, this means that a low-energy qubit system (with most qubits in their ground state) can macroscopically behave like a boson, or a collection of bosons. If the Hamiltonian is of the bilinear form $H=-B^\dagger B=-(1/N)(\hat{n}+\Sigma_{i\neq j}^N a_i^\dagger a_j)$, the ground state with $n\ll N$ parafermions is $(B^\dagger)^n|0\rangle$, i.e., $\hat{n}[(B^\dagger)^n|0\rangle]\approx n[(B^\dagger)^n|0\rangle]$.

A separate conclusion that follows from this result is that a low-energy noninteracting qubit system can *naturally simulate the dynamics of bosons*.

VI. PARAFERMIONS FROM FERMIONS AND BOSONS

As stated in the Introduction, qubits do not exist as fundamental particles. This means that they are either approximate descriptions (e.g., a spin in the absence of its spatial degrees of freedom) or have to be prepared by appropriately combining bosons or fermions, i.e., a qubit can be *encoded* in terms of bosons or fermions under certain conditions (see also Ref. 32). We consider bosonic or fermionic systems with $2N$ single-particle states. Let $k=1,2,\ldots,N$ denote all relevant quantum numbers (including spin, if necessary). The following three cases yield parafermions.

Case 1: Fermionic particle-particle pairs—Under the condition $n_{2k-1}^f=n_{2k}^f$ it can be shown that $\{f_{2k}f_{2k-1},f_{2k-1}^\dagger f_{2k}^\dagger\}=1$ and $[f_{2k-1}f_{2k},f_{2l-1}^\dagger f_{2l}^\dagger]=0$ for $k\neq l$. Furthermore, the set $\{f_{2k-1},f_{2k-1}^\dagger f_{2k}^\dagger,n_{2k-1}^f+n_{2k}^f-1\}$ satisfies the commutation relations of sl(2). Therefore the mapping $a_k\Leftrightarrow f_{2k}f_{2k-1}$, $a_k^\dagger\Leftrightarrow f_{2k-1}^\dagger f_{2k}^\dagger$ and $2n_k\Leftrightarrow n_{2k-1}^f+n_{2k}^f$ is a mapping to parafermions. The vacuum state of parafermions in this case corresponds to the vacuum state $|0\rangle_f$ of fermions. An example is Cooper pairs.

Case 2: Fermionic particle-hole pairs—Under the condition $n_{2k-1}^f+n_{2k}^f=1$ it can be shown as in case 1 that $a_k\Leftrightarrow f_{2k}^\dagger f_{2k-1}$, $a_k^\dagger\Leftrightarrow f_{2k-1}^\dagger f_{2k}$ and $2n_k-1\Leftrightarrow n_{2k-1}^f-n_{2k}^f$ is a mapping to parafermions. However, in this case the vacuum state of parafermions is $|0\rangle=f_{2N}^\dagger\cdots f_4^\dagger f_2^\dagger|0\rangle_f$, because then $a_k|0\rangle=0$ for all k. This vacuum state plays the role of a Fermi level. An example is excitons. In fact, all quantum computer proposals that use electrons, e.g., quantum dots,[11] and electrons on Helium,[33,34] are equivalent to this case. For example, $f_2^\dagger f_1$ and $f_1^\dagger f_2$ can represent the transition operators between two spin states in the quantum dot proposal.

Case 3: Bosonic "particle-hole" pairs—Under the condition $n_{2k-1}^b+n_{2k}^b=1$ it can be shown as in case 1 that $a_k\Leftrightarrow b_{2k}^\dagger b_{2k-1}$, $a_k^\dagger\Leftrightarrow b_{2k-1}^\dagger b_{2k}$ and $2n_k-1\Leftrightarrow n_{2k-1}^b-n_{2k}^b$ is a mapping to parafermions. However, in this case the vacuum state of parafermions is $|0\rangle=b_{2N}^\dagger\cdots b_{2k}^\dagger\cdots b_4^\dagger b_2^\dagger|0\rangle_b$, again because then $a_k|0\rangle=0$ for all k. An example is dual-rail photons in the optical quantum computer proposal.[15]

This classification illustrates the by-necessity compound nature of a qubit, and puts into a unified context the many different proposals for constructing qubits in physical systems. Note that it is possible to use more than two fermions or bosons to construct a parafermion. Further implications, especially as related to the simulation of models of superconductivity (Case 1) on a quantum computer, have been explored in Ref. 35.

VII. PARAFERMIONIC BILINEAR HAMILTONIANS ARE UNIVERSAL BUT FERMIONIC AND BOSONIC ARE NOT

In this section we discuss a rather striking difference between the universality of bilinear Hamiltonians acting on fermions and bosons, as compared to parafermions. Let us consider the set of particle-number-conserving bilinear operators of bosons, fermions and parafermions:

$$b_i^\dagger b_j,\quad f_i^\dagger f_j,\quad a_i^\dagger a_j.$$

As noted in Table I, in the fermionic case these operators generate the group U(N) where N is the number of particles. The same is true for bosons.[19] Clearly, therefore, fermionic and bosonic Hamiltonians containing only these operators are not universal with respect to an interesting (i.e., exponentially large) SU(2^N) subgroup. On the other hand, as discussed in the previous section, these fermionic and bosonic operators can be used to define parafermionic operators $a_i^\dagger a_j$ in

two-to-one correspondence. As mentioned in Sec. III, the set $\{a_i^\dagger a_j\}_{i,j=1}^{N+1}$ generates the subalgebra SA$n(N)$, with dimension $(2N)!/N!N!$ $(>2^N)$ [recall that the total number of $Q_{\alpha,\beta}(N)$ operators is 2^{2N}]. The corresponding Lie group appears to be large enough to be interesting for universal quantum computation. This expectation is borne out, since one can construct an XY model, Eq. (17), using the set $\{a_i^\dagger a_j\}$. As shown in Ref. 23, the XY model is by itself universal provided one uses three physical qubits per *encoded qutrit*, together with nearest-neighbor and next-nearest-neighbor interactions (see also Sec. IX D 1). We discuss the XY model in detail in Sec. IX B. First, however, let us argue qualitatively where the difference between parafermions (qubits) and fermions and bosons originates from. An example will illuminate this. For the case of bosons and fermions, $[b_1^\dagger b_2, b_2^\dagger b_3]=b_1^\dagger b_3$ and $[f_1^\dagger f_2, f_2^\dagger f_3]=f_1^\dagger f_3$. But for parafermions, $[a_1^\dagger a_2, a_2^\dagger a_3]=a_1^\dagger a_3(1-2\hat{n}_2)$. (An easy way to check this, without explicitly calculating the commutator, is to use the mapping to fermions: $f_i^\dagger f_{i+1} \leftrightarrow a_i^\dagger a_{i+1}$ and the Jordan–Wigner transformation $f_i \rightarrow a_i S_i$.) Thus the difference is that *bosons and fermions preserve locality, but parafermions do not*.

Similarly, we can consider additional bilinear operators. For fermions, if we also have $f_i f_j$ and $f_j^\dagger f_i^\dagger$, the group is SO$(2N)$, which is too small to be interesting for QC. In fact this is a model of noninteracting fermions: there exists a canonical transformation to a sum of quadratic terms each of which acts only on a single mode (see also Refs. 6, 29, 30, 32, and 36). For bosons, if we include $b_i b_j$ and $b_j^\dagger b_i^\dagger$, the group generated is the $N(2N+1)$-parameter symplectic group Sp$(2N,R)$ which is noncompact, implying that it has no finite dimensional irreps.[19] If we further include the set of annihilation and creation operators $b_i, b_i^\dagger$ together with the identity operator I, the set $\{I, b_i, b_i^\dagger, b_i b_j, b_j^\dagger b_i^\dagger, b_j^\dagger b_i\}$ generates the semidirect-product group $N(N) \otimes \mathrm{Sp}(2N,R)$, where $N(N)$ is the Heisenberg group, with $(N+1)(2N+1)$ generators (Ref. 19, Chap. 20). This is therefore still too small to be interesting for universal QC. In fact, *this is exactly the reason why linear optics by itself is insufficient for universal QC*. The situation does not change even after introduction of the displacement operators $D_i(\alpha)=\exp(\alpha b_i^\dagger - \alpha^* b_i)$,[16] since $D_i(\alpha) \in N(N) \otimes \mathrm{Sp}(2N,R)$.

The way to universality [with respect to SU(2^N)] is to introduce nonlinear operations such as a Kerr nonlinearity,[37] self-interaction,[38] or conditional measurements.[15,16] A Kerr nonlinearity is a two-qubit interaction of the form $n_i^b n_j^b$ (where i and j are different modes), which directly provides a CPHASE gate. To see this, consider a dual-rail encoding:[37] Suppose that one qubit is encoded into $|0\rangle = b_1^\dagger|0\rangle$, $|1\rangle = b_2^\dagger|0\rangle$, while a second qubit is encoded into $|0\rangle = b_3^\dagger|0\rangle$, $|1\rangle = b_4^\dagger|0\rangle$ ($|0\rangle$ is the vacuum state). The two-qubit states are

$$|00\rangle = b_3^\dagger b_1^\dagger|0\rangle, \quad |01\rangle = b_3^\dagger b_2^\dagger|0\rangle,$$

$$|10\rangle = b_4^\dagger b_1^\dagger|0\rangle, \quad |11\rangle = b_4^\dagger b_2^\dagger|0\rangle.$$

(This is related to case 3 of Sec. VI, where we showed how to make qubits from bosons.) It is then simple to verify that $\exp(-i\pi n_2^b n_4^b)$ acts exactly as a CPHASE gate, i.e., it is represented by the matrix diag(1,1,1,−1) in this two-qubit basis. Here we wish to point out that a recently introduced alternative to a Kerr nonlinearity,[38] namely the self-interaction $(n_i^b)^2$, is in fact closely related to the Kerr nonlinearity. Thus methods developed to use one of these nonlinear interactions can be transported to the other. Let us demonstrate this point by giving a simple circuit to show how one interaction simulates the other. We start with the operator identity

$$\exp(\phi(a^\dagger b - b^\dagger a)) b^\dagger \exp(-\phi(a^\dagger b - b^\dagger a)) = \cos\phi b^\dagger + \sin\phi a^\dagger,$$

which can be proved directly from the Baker–Hausdorff formula

$$e^{-\alpha A} B e^{\alpha A} = B - \alpha[A,B] + \frac{\alpha^2}{2!}[A,[A,B]] - \frac{\alpha^3}{3!}[A,[A,[A,B]]] + \cdots. \tag{12}$$

Using the latter identity it is then simple to verify the following identity, *which holds on the two-qubit subspace above*,

$$\exp(-i\pi n_2^b n_4^b)=\exp\left(-\frac{\pi}{4}(b_2^\dagger b_4-b_4^\dagger b_2)\right)\exp\left(-i\pi\frac{(n_2^b)^2+(n_4^b)^2-n_2^b-n_4^b}{2}\right)$$
$$\times\exp\left(\frac{\pi}{4}(b_2^\dagger b_4-b_4^\dagger b_2)\right).$$

This is an exact three-gate simulation of the Kerr CPHASE gate in terms of the self-interaction. The simulation uses the linear bosonic operators $b_i^\dagger b_j$ and the local energies n_i^b in order to unitarily rotate the self-interaction terms $(n_2^b)^2+(n_4^b)^2$ to a Kerr interaction.

VIII. FLUCTUATIONS IN PARAFERMION NUMBER AT FINITE TEMPERATURE

So far we have not really made use of the full power of the Fock space representation, which allows to consider the case of fluctuating particle number. The quantum statistics of parafermions is determined by their commutation relations, like fermions (Fermi–Dirac statistics) and bosons (Bose–Einstein statistics). A simple case to consider is that of noninteracting parafermions. The Fermi–Dirac distribution for an ideal Fermi gas is derived using only the restriction that no more than a single fermion can occupy a given mode.[39] Hence the statistics of noninteracting parafermions is clearly the same as that of noninteracting fermions.

Fluctuations in particle number will be a result of interaction of the system with an external bath, which imposes a chemical potential μ (essentially the gradient of the particle flow). As a simple example, consider the following system-bath interaction Hamiltonian:

$$H_I=\sum_{i=1}^{N}\sigma_i^z\otimes B_i^z\rightarrow\sum_{i=1}^{N}(2\hat{n}_i-1)\otimes B_i^z, \tag{13}$$

where B_i^z are bath operators. To further simplify things assume the bath is treated classically, i.e., B_i^z are positive c-numbers. With this Hamiltonian, one can study the fluctuations of parafermions under finite temperature T. Mapping from the well-know result for a noninteracting Fermi gas,[39] it then follows that the average occupation for the ith qubit site is

$$\langle n_i\rangle=\frac{1}{e^{(2B_i^z-\mu)/kT}+1},$$

where k is Boltzman's constant. This is the average value of the qubit-''spin'' (whether it is $|0\rangle$ or $|1\rangle$). Keeping the chemical potential μ fixed, in the limit of $T\rightarrow 0$ we find that $\langle n_i\rangle\rightarrow 1$ if $B_i^z<\mu$, but $\langle n_i\rangle\rightarrow 0$ if $B_i^z>\mu$. Thus, as expected, it is essential to keep the interaction with the bath weak (compared to μ) to prevent fluctuations in qubit ''orientation'' at low temperatures. At finite T we find $\langle n_i\rangle<1$, meaning that some fluctuation is unpreventable. Of course, our model is very naive, and the picture is modified when qubit interactions are taken into account. However, it should be clear that a Fock space description of qubits, i.e., in terms of parafermions, could be valuable in studying qubit statistics at finite temperatures.

IX. UNIVERSALITY OF EXCHANGE-TYPE HAMILTONIANS

In this final section we conclude with an application of the formalism we developed earlier to the study of the universality power of Hamiltonians. We have considered this question in detail before for general exchange-type Hamiltonians (isotropic and anisotropic).[17,18] We first briefly review the universality classification of various physically relevant bilinear Hamiltonians. It will be seen that while in certain cases the Hamiltonian is not sufficiently powerful to be universal with respect to $\mathrm{U}(2^N)$, it is universal with respect to a subgroup. As mentioned in Sec. III, this result requires the use of *encoding of physical qubits into logical qubits*.[21–24,52] We then consider in detail the representative example of the XY model, where we give a new proof about universality (in fact, the lack thereof) in the case of nearest-neighbor-only interactions. We then present new

results about codes with higher rates than considered in Refs. 17 and 18. For simplicity we revert when convenient to the Pauli matrix notation in this section, which is more familiar to practitioners of QC.

A. Classification of bilinear Hamiltonians

The most general bilinear Hamiltonian for a qubit system is

$$H(t)\equiv H_0+V+F=\sum_i \frac{1}{2}\varepsilon_i\sigma_i^z+\sum_{i<j} V_{ij}+F, \tag{14}$$

where H_0 is the qubit energy term, the interaction between qubits i and j is

$$V_{ij}=\sum_{\alpha,\beta=x,y,z} J_{ij}^{\alpha\beta}(t)\sigma_i^\alpha\sigma_j^\beta,$$

and the external single-qubit operations are

$$F=\sum_i f_i^x(t)\sigma_i^x+f_i^y(t)\sigma_i^y.$$

Recall the ''standard'' result about universal quantum computation: The group $\mathrm{U}(2^N)$ on N qubits can be generated using arbitrary single qubit gates and a nontrivial two-qubit entangling gate such as CNOT.[25] The general Hamiltonian $H(t)$ can generate such a universal gate set, e.g., as follows: Suppose there are controllable σ_i^z and σ_i^x terms. Then σ_i^y can be generated using Euler angles:

$$\sigma_i^y=\exp(-i\pi\sigma_i^z/4)\sigma_i^x\exp(i\pi\sigma_i^z/4).$$

This is an instance of a simple but extremely useful result: let A and B be anticommuting Hermitian operators where $A^2=I$ (I is the identity matrix). Then, using $Ue^VU^\dagger=e^{UVU^\dagger}$ (U is unitary, V is arbitrary),

$$C_A^\varphi\circ\exp(i\theta B)\equiv\exp(-iA\varphi)\exp(i\theta B)\exp(iA\varphi)=\begin{cases}\exp(-i\theta B) & \text{if } \varphi=\pi/2,\\ \exp[i\theta(iAB)] & \text{if } \varphi=\pi/4.\end{cases} \tag{15}$$

One can also derive these relations for su(2) angular momentum operators, without assuming that $\{A,B\}=0$ and $A^2=I$. Let J_x and J_z be generators of su(2). Then, using the Baker–Hausdorff relation Eq. (12), and $[J_z,J_x]=iJ_y$,

$$\exp(-i\varphi J_z)J_x\exp(i\varphi J_z)=J_x\cos\varphi+J_y\sin\varphi.$$

From here follows, using $Ue^VU^\dagger=e^{UVU^\dagger}$ again,

$$C_{J_z}^\varphi\circ\exp(i\theta J_x)=\exp(i\theta(J_x\cos\varphi+J_y\sin\varphi)),$$

and Eq. (15) can be verified, with $\varphi\to 2\varphi$, and $AB\to[A,B]$.

Different QC proposals usually have different two-qubit interactions. Typical types include $\sigma_i^z\sigma_{i+1}^z,\sigma_i^y\sigma_{i+1}^y$ (or $\sigma_i^x\sigma_{i+1}^x$), $\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y$ (XY model), and $\vec{\sigma}_i\cdot\vec{\sigma}_j$ (Heisenberg model). It is simple to show that they can all be transformed into a common canonical form $\sigma_i^z\sigma_{i+1}^z$, using a few unitary transformation. The term $\sigma_i^z\sigma_{i+1}^z$ can be used to generate CPHASE and, from there, CNOT.[7] For example, the XY term can first be transformed into $\sigma_i^x\sigma_{i+1}^x$ using Euler angle rotations about σ_i^x, which flips the sign of the $\sigma_i^y\sigma_{i+1}^y$ term:

$$\exp\left[\frac{i\theta}{2}(\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y)\right]\left(C_{\sigma_i^x}^{\pi/2}\circ\exp\left[\frac{i\theta}{2}(\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y)\right]\right)=\exp(i\theta\sigma_i^x\sigma_{i+1}^x),$$

which can subsequently be transformed into the canonical form using another Euler angle rotation,

$$C_{\sigma_i^y+\sigma_{i+1}^y}^{\pi/4}\circ\sigma_i^x\sigma_{i+1}^x=\sigma_i^z\sigma_{i+1}^z,$$

where using $[\sigma_i^y,\sigma_{i+1}^y]=0$ we have abbreviated $C_{\sigma_{i+1}^y}^{\pi/4}\circ C_{\sigma_i^y}^{\pi/4}$ as $C_{\sigma_i^y+\sigma_{i+1}^y}^{\pi/4}$. The method of Euler angle rotations as applied here is also known as "selective recoupling" in the NMR literature.[40]

Not all QC proposals have an interaction Hamiltonian that appears to be of the form V_{ij}, e.g., the ion-trap proposal[12] looks quite different since it involves interactions between ions mediated by a phonon. The interaction between the ith ion and the phonon has the form $\sigma_i^- b^\dagger+\sigma_i^+ b$. This is nevertheless equivalent to an XY model, since

$$\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y=C_{\sigma_i^z-\sigma_{i+1}^z}^{\pi/4}\circ 2i[\sigma_i^- b^\dagger+\sigma_i^+ b,\sigma_{i+1}^- b^\dagger+\sigma_{i+1}^+ b].$$

Therefore, in many cases it suffices to study the interaction $\sigma_i^z\sigma_{i+1}^z$.

Let us now consider a number of more restricted models.

1. No external single-qubit operations

If $F=0$, then the *nearest-neighbor* set $\{\sigma_i^z,\sigma_i^z\sigma_{i+1}^z,\sigma_i^x\sigma_{i+1}^z,\sigma_{i+1}^x\sigma_i^z\}$ is still universal, since

$$\sigma_i^y=C_{\sigma_{i+1}^z\sigma_i^z}^{\pi/4}\circ\sigma_{i+1}^z\sigma_i^x.$$

This is the case when H_0 is controllable. More physically, the set $\{\sigma_i^z,\vec{\sigma}_i\cdot\vec{\sigma}_{i+1},(\vec{\sigma}_i\times\vec{\sigma}_{i+1})_y=\sigma_i^z\sigma_{i+1}^x-\sigma_{i+1}^z\sigma_i^x\}$ is also universal, where $\vec{\sigma}=(\sigma^x,\sigma^y,\sigma^z)$. The term $\vec{\sigma}_i\times\vec{\sigma}_{i+1}$ is an anisotropic (Dzyaloshinskii–Moriya) interaction which arises, e.g., in quantum dots in the presence of spin-orbit coupling.[17,41–44]

2. No external single-qubit operations and H_0 uncontrollable

If $F=0$ and H_0 is not controllable, then the nearest-neighbor set $\{\sigma_i^z\sigma_{i+1}^z,\sigma_i^x\sigma_{i+1}^z,\sigma_i^z\sigma_{i+1}^x,\sigma_i^y\sigma_{i+1}^z,\sigma_i^z\sigma_{i+1}^y\}$ is universal, meaning that the interaction term V by itself is universal. One way to see this is to map the set to parafermionic operators and note that it overlaps with the set that generates the parafermionic U(2^N) (Table II).

3. Scalar anisotropic exchange-type interactions

Consider the case $J_{ij}^{\alpha\beta}=J_{ij}^{\alpha}\delta_{\alpha\beta}$ (denoting V by V'), which amounts to limiting the Hamiltonian to scalar anisotropic exchange-type interactions. Using Eq. (3) we then arrive at the second-quantized form

$$H_0=\sum_i\ \eta_i n_i,$$

$$F=\sum_i\ (f_i^* a_i+f_i a_i^\dagger), \tag{16}$$

$$V'=\sum_{i<j}\Delta_{ij}(a_i a_j+a_i^\dagger a_j^\dagger)+J_{ij}(a_i^\dagger a_j+a_j^\dagger a_i)+4J_{ij}^z n_i n_j,$$

where

$$\eta_i=\varepsilon_i+\left(\sum_j J^z_{ij}+J^z_{ji}\right), \quad f_i=(f^x_i-if^y_i),$$

$$\Delta_{ij}=J^x_{ij}-J^y_{ij}, \quad J_{ij}=J^x_{ij}+J^y_{ij},$$

and we dropped a constant energy term.

V' is the so-called XYZ model of solid state physics. Considering the structure of V' and the classification of operator algebras we carried out in Secs. III and IV, it should be clear that some immediate conclusions can be drawn about the universality power of this Hamiltonian. The full Hamiltonian $H_0+V'+F$ contains the generators of the parafermionic $U(2^N)$ (Table II), so it is universal. On the other hand, without external single qubit operations ($F=0$), we have $[H_0+V',\hat{p}]=0$, so $H_0+V'\in \mathrm{SA}p$, i.e., preserves parity. This immediately implies that the XYZ model (even with H_0) is by itself not universal. However, it can be made universal by *encoding* logical qubits into several (two are in fact sufficient) physical qubits.[17] The elimination of single-qubit operations ($F=0$) can be quite useful, since typically single- and two-qubit operations involve very different constraints. In some cases single-qubit operations can be very difficult to implement (see Refs. 17, 18, and 22 and references therein for extensive discussions of this point).

B. XY model

Consider now the XY model, which is defined by

$$V_{XY}=\sum_{i<j} J_{ij}(a^\dagger_i a_j+a^\dagger_j a_i). \tag{17}$$

It is relevant to a number of proposals for quantum computing, including quantum Hall systems,[45,46] quantum dots in microcavities,[32] quantum dots coupled by exciton exchange,[47] and atoms in microcavities.[48] Let us summarize what is currently known about quantum computational universality of this model.

(i) In Ref. 31 it was shown that the XY model with nearest-neighbor interactions only, together with single-qubit operations, is universal.

(ii) In Ref. 23 it was argued that the XY model is universal without single-qubit operations, provided these gates can be applied between nearest-neighbor and next-nearest-neighbor pairs of qubits. This involved encoding a logical qutrit into three physical qubits: $|0_L\rangle=|001\rangle$, $|1_L\rangle=|010\rangle$, $|2_L\rangle=|100\rangle$. We reconsider this in Sec. IX D in the context of the XXZ model (but using the methods of Ref. 18, the results are valid also for the XY model).

(iii) In Ref. 18 we showed that the XY model is universal using only nearest- and next-nearest-neighbor ($J_{i,i+2}$) interactions, together with single-qubit σ_z terms. This too involved an encoding of a logical qubit into two physical qubits: $|0_L\rangle=|01\rangle$, $|1_L\rangle=|10\rangle$. Two comments are in order about this result: first, next-nearest-neighbor interactions can be nearest neighbor in 2D (e.g., in an hexagonal array); second, unlike Ref. 31, we did not assume the σ_z terms to be controllable, i.e., there is no individual control over ε_i [Eq. (14)]. A similar model is treated in Sec. IX C.

The question now arises: *Is the XY model universal with nearest-neighbor interactions only?* We prove that it is not.

The nearest-neighbor XY model in its parafermionic form is

$$H=\sum_i^N \epsilon_i n_i+\sum_i^N J_{i,i+1}(a^\dagger_i a_{i+1}+a^\dagger_{i+1}a_i).$$

Consulting Table II, we see that H can only generate SU(N), which is clearly too small even for encoded quantum computation.

C. Antisymmetric XY model

To illustrate the idea of encoding for universality, let us briefly consider the ''antisymmetric XY model:''

$$V_{aXY}=\sum_{i<j} J_{ij}^{xy}\sigma_i^x\sigma_j^y+J_{ij}^{yx}\sigma_i^y\sigma_j^x. \tag{18}$$

Here J_{ij}^{xy} and J_{ij}^{yx} are real. We encode a logical qubit into pairs of nearest-neighbor physical qubits. Letting

$$\tilde{\Delta}_{ij}=J_{ij}^{xy}-J_{ij}^{yx},\quad \tilde{J}_{ij}\equiv J_{ij}^{xy}+J_{ij}^{yx},\quad \epsilon_m^{\pm}\equiv\varepsilon_{2m-1}-\varepsilon_{2m}, \tag{19}$$

using the compact notation $\cdot_m\equiv\cdot_{2m-1,2m}$, and assuming that interactions are on only inside pairs of qubits encoding one qubit, we find for the Hamiltonian $H=H_0+V_{aXY}$

$$H_{aXY}=\sum_{m=1}^{N/2}(\tilde{J}_m R_m^y+\epsilon_m^+ R_m^z)+(\tilde{\Delta}_m T_m^y+\epsilon_m^- T_m^z), \tag{20}$$

where the T and R operators were defined in Eqs. (6) and (7). Since the T and R operators form commuting sl(2) algebras, the Hilbert space splits into two independent computational subspaces. The R operators conserve parity, so that an appropriate encoding in the axially symmetric case ($\tilde{\Delta}_m=0$), using standard qubit notation, is $|0_L\rangle=|00\rangle$ and $|1_L\rangle=|11\rangle$. On the other hand, the T operators preserve particle number, so that if $\tilde{J}_m=0$ (axially antisymmetric case), the encoding is $|0_L\rangle=|01\rangle$, $|1_L\rangle=|10\rangle$. In both cases control over the pair of parameters $\{\tilde{J}_m,\epsilon_m^+\}$ (or $\{\tilde{\Delta}_m,\epsilon_m^-\}$) is sufficient for the implementation of the single-encoded-qubit $\mathrm{SU}_m(2)$ group (the subscript m refers to the mth logical/encoded qubit).

Logic operations between encoded qubits require the ''encoded selective recoupling'' method introduced in Ref. 18. Consider the ''axially antisymmetric qubit'' $|0_L\rangle=|01\rangle$, $|1_L\rangle=|10\rangle$. First, note that, using Eq. (15),

$$C_{T_{12}^x}^{\pi/2}\circ T_{23}^x=i\sigma_1^z\sigma_2^z T_{13}^x. \tag{21}$$

Now assume we can control $\tilde{\Delta}_{13}$. Then,

$$C_{T_{13}^x}^{\pi/4}\circ(C_{T_{12}^x}\circ T_{23}^x)=\sigma_2^z(\sigma_3^z-\sigma_1^z)/2. \tag{22}$$

Since $\sigma_1^z\sigma_2^z$ is constant on the code subspace it can be ignored. On the other hand, $\sigma_2^z\sigma_3^z$ acts as $-T_1^zT_2^z$:

$$|0_L\rangle_1|0_L\rangle_2=|01\rangle_{12}|01\rangle_{34}\overset{\sigma_2^z\sigma_3^z}{\rightarrow}-|01\rangle_{12}|01\rangle_{34}=-|0_L\rangle_1|0_L\rangle_2, \tag{23}$$

and similarly for the other three combinations: $|0_L\rangle|1_L\rangle\rightarrow|0_L\rangle|1_L\rangle$, $|1_L\rangle|0_L\rangle\rightarrow|1_L\rangle|0_L\rangle$, $|1_L\rangle|1_L\rangle\rightarrow-|1_L\rangle|1_L\rangle$, i.e., $\sigma_2^z\sigma_3^z$ acts as an encoded $\sigma^z\otimes\sigma^z$. This establishes universal encoded computation in the antisymmetric XY model.

D. Codes with higher rates

The encoding of one logical qubit into two physical qubits is not very efficient. Can we do better? That is, can we perform encoded universal QC on codes with a rate (no. of logical qubit to no. of physical qubits) that is greater than $\frac{1}{2}$? We will show how in the case of the XXZ model, defined as $H=H_0+H_{XXZ}$, where

$$H_{XXZ}=\sum_{i<j} J_{ij}^{x}(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)+J_{ij}^{z}\sigma_i^z\sigma_j^z.$$

When surface and interface effects are taken into account, the XY examples of QC proposals,[31,45–48] as well as the Heisenberg examples,[11,49,50] are better described by the axially symmetric XXZ model. Additional sources of nonzero J_{ij}^{z} in the XY examples can be second-order effects (e.g., virtual cavity-photon generation without spin-flips[31]). A natural XXZ example is that of electrons on helium.[33,34]

First, note that the code used in the XY model, $|0_L\rangle=|01\rangle$, $|1_L\rangle=|10\rangle$, is applicable here as well: $T_{ij}^{x}=\frac{1}{2}(\sigma_i^x\sigma_j^x+\sigma_i^y\sigma_j^y)$ preserves particle number, and serves as an encoded σ^x; σ_i^z terms from H_0 serve as encoded σ^z, and $\sigma_i^z\sigma_{i+1}^z$ applied to physical qubits belonging to different encoded qubits acts as encoded $\sigma^z\otimes\sigma^z$.

In the general encoding case we consider a block of N qubits where codewords are computational basis states (bitstrings of 0's and 1's): $\{q_\alpha^\dagger(N_\alpha)|0\rangle\}_\alpha$, where $\alpha=\{\alpha_i\}$ and α_i can be 0 or 1, while $N_\alpha=0,\ldots,N$. A code-subspace $\mathcal{C}(N,n)$ will be defined by having a fixed number n of 1's (i.e., of parafermions). Thus there are

$$d_{N,n}\equiv\dim[\mathcal{C}(N,n)]=\binom{N}{n}$$

codewords in a subspace. Examples are considered below. Note that these subspaces are decoherence-free under the process of collective dephasing,[51] and have been analyzed extensively in this context in Ref. 52. Figure 1 in Ref. 52 provides a nice graphical illustration of the $\mathcal{C}(N,n)$ subspaces. Since the decoherence-avoidance properties of the codes we consider here have been extensively discussed before,[51,52] and even implemented experimentally,[53,54] we do not address this issue here. We further note that Ref. 52 provided an in-principle proof that universal encoded QC is possible on all subspaces $\mathcal{C}(N,n)$ independently. However, this proof had several shortcomings: (i) it used a short-time approximation, (ii) it did not make explicit contact with physically realizable Hamiltonians, and (iii) it proceeded by induction, and thus did not explicitly provide an *efficient* algorithm for universal QC. We remedy all these shortcomings here, i.e., we (i) use only finite-time operations, (ii) use only the XXZ Hamiltonian, and (iii) provide an efficient algorithm that scales polynomially in N.

We need a measure that captures how efficient a $\mathcal{C}(N,n)$ code is. If there are d codewords, supported over N p-dimensional objects ($p=2$ is the case of bits), and information is measured in units of q, then we define the rate of the code as

$$r(d,p,q)=\frac{\log_q d}{\log_q p^N}.$$

The traditional definition for qubits is recovered by setting $p=q=2$, i.e., the rate of a code is the ratio of the number of logical qubits $\log_2 d$ to the number of physical qubits N, which in our case becomes

$$r=\frac{\log_2 d_{N,n}}{N}\overset{N\gg 1}{\longrightarrow}S(\epsilon),\tag{24}$$

where $\epsilon\equiv k/N$,

$$S(\epsilon)=-\epsilon\log_2\epsilon-(1-\epsilon)\log_2(1-\epsilon)$$

is the Shannon entropy, and we have used the Stirling formula $\log x!\approx x\log x-x$. Since $S(\frac{1}{2})=1$ the code has a rate that is asymptotically unity for the ''symmetric subspace'' $\mathcal{C}(N,N/2)$, where the number of 1's equals the number of 0's in each computational basis state. However, we will not in

fact attempt to encode $\log_2 d_{N,n}$ logical qubits in the subspace $\mathcal{C}(N,n)$, since the subspace does not have a natural tensor product structure. Instead we will consider $\mathcal{C}(N,n)$ as a subspace encoding a qu$d$it, where $d=d_{N,n}$. Using the generalized definition of a rate above, and measuring information in units of d so that each subspace encodes one unit of information, the rate of such a code is $r=(\log_d d)/(\log_d 2^N)$. This, however, exactly coincides with r of Eq. (24). Therefore we see that the advantage of working with the symmetric subspace $\mathcal{C}(N,N/2)$ in the limit of large N is that its rate approaches unity.

Before embarking on the general analysis, let us note that for an encoding of one logical qubit into N physical qubits, there is a simple construction in terms of parafermionic operators: $Q_{\alpha,\beta}(N)$, $Q^\dagger_{\alpha,\beta}(N)$, and $[Q^\dagger_{\alpha,\beta}(N), Q_{\alpha,\beta}(N)]$ (which is a function of parafermion number) form an su(2) algebra in the basis $|0_L\rangle=q^\dagger_\alpha(N_\alpha)|\mathtt{0}\rangle$ and $|1_L\rangle=q^\dagger_\beta(N-N_\alpha)|\mathtt{0}\rangle$, e.g., for $N=2$ there are two cases: the sets $\{a_1a_2, a_2^\dagger a_1^\dagger, \hat{n}_1+\hat{n}_2-1\}$ and $\{a_1^\dagger a_2, a_2^\dagger a_1, \hat{n}_1-\hat{n}_2\}$, with corresponding bases $|0_L\rangle=|\mathtt{0}\rangle$, $|1_L\rangle=a_1^\dagger a_2^\dagger|\mathtt{0}\rangle$ and $|0_L\rangle=a_1^\dagger|\mathtt{0}\rangle$, $|1_L\rangle=a_2^\dagger|\mathtt{0}\rangle$. These two encodings are universal (in the sense of blocks of N physical qubits) when only H_0 and V' are controllable [Eq. (16)].

Let us now move on to the general subspace case, starting with an example.

1. Encoded operations: Example

Consider $\mathcal{C}(3,1)=\mathrm{Span}\{|0\rangle\equiv|001\rangle, |1\rangle\equiv|010\rangle, |2\rangle\equiv|100\rangle\}$, i.e., an encoding of a logical qutrit into three physical qubits, as in Ref. 23. Let us count qubits as $i=0,\ldots,N-1$. Our first task is to show how to generate su(3) on this subspace. It is simple to check that $T^x_{01}|001\rangle=0$, $T^x_{01}|010\rangle=|100\rangle$, $T^x_{01}|100\rangle=|010\rangle$, and in total

$$T^x_{01}=\begin{pmatrix}0&0&0\\0&0&1\\0&1&0\end{pmatrix}=|1\rangle\langle 2|+|2\rangle\langle 1|\equiv X_{12},$$

where the notation X_{12} denotes a σ^x operation between states $|1\rangle\equiv|010\rangle$ and $|2\rangle\equiv|100\rangle$. Similarly, it is simple to check that $T^x_{12}=X_{01}$ and $T^x_{02}=X_{02}$. Further, using $T^z_{ij}\equiv\frac{1}{2}(\sigma^z_i-\sigma^z_j)$, we have $T^z_{01}=Z_{12}$, $T^z_{12}=Z_{01}$, and $T^z_{02}=Z_{02}$, where Z_{12} denotes a σ^z operation between states $|1\rangle$ and $|2\rangle$, etc. Therefore each pair $\{T^x_{ij}, T^z_{ij}\}$ generates an encoded su(2). But in the sense of generating, su(N) is a sum of overlapping su(2)'s,[55] so using just the nearest-neighbor interactions $\{T^x_{01}, T^z_{01}, T^x_{12}, T^x_{12}\}$ we can generate all of su(3) on $\mathcal{C}(3,1)$. Note that $[X_{01}, X_{12}]=iY_{02}$, so that su(2) between states $|0\rangle, |2\rangle$ can in fact be generated using T^x_{ij}'s alone, without T^z_{ij}'s. This conclusion clearly holds for the generation of all of su(3) on $\mathcal{C}(3,1)$, as first pointed out in Ref. 23.

Next, we need to show how to implement encoded logical operations between two $\mathcal{C}(3,1)$ code subspaces. Let us number the qubits as $i=0,1,2$ for the first block and $i=3,4,5$ for the second block. Consider the effect of turning on J^z_{23}, i.e., consider the action of $\sigma^z_2\sigma^z_3$ on the tensor product space $\mathcal{C}(3,1)\otimes\mathcal{C}(3,1)$. The operator $\sigma^z_2\sigma^z_3$ is represented by a nine-dimensional diagonal matrix on this space, which is easily found to have the following form in the ordered basis $\{|0\rangle\otimes|0\rangle, |0\rangle\otimes|1\rangle, \ldots, |2\rangle\otimes|2\rangle\}$:

$$\sigma^z_2\sigma^z_3=\mathrm{diag}(-1,1,1,-1,1,1,1,-1,-1)=\mathrm{diag}(-1,1,1)\otimes\mathrm{diag}(1,1,-1),$$

e.g., $\sigma^z_2\sigma^z_3|2\rangle\otimes|2\rangle=\sigma^z_2\sigma^z_3|100\rangle\otimes|100\rangle=(+|100\rangle)\otimes(-|100\rangle)=-|2\rangle\otimes|2\rangle$, which explains the -1 in the ninth position in the diagonal matrix above. The important point is that $\sigma^z_2\sigma^z_3$ acts as a tensor product operator on $\mathcal{C}(3,1)\otimes\mathcal{C}(3,1)$, which *puts a relative phase* between the basis states of each $\mathcal{C}(3,1)$ factor. This means that $\sigma^z_2\sigma^z_3$ acts as an "su(3)-like" $\sigma^z\otimes\sigma^z$ on $\mathcal{C}(3,1)\otimes\mathcal{C}(3,1)$. [It is an "su(3)-like" $\sigma^z\otimes\sigma^z$ since for su(2) $\sigma^z=\mathrm{diag}(1,-1)$ and here we have instead diag($-1,1,1$) and diag($1,1,-1$).] It is well known[7] that the CPHASE gate can be generated from the Hamiltonian $\sigma^z\otimes\sigma^z$. The same holds here, so that we can generate a CPHASE gate between two $\mathcal{C}(3,1)$ subspaces by simply turning on a nearest-neighbor interaction between the last qubit in the first block and the first qubit in the second block.

With this example in mind we can move on to the general case.

2. Encoded operations: General subspace case

Let us now consider the case of a general subspace $\mathcal{C}(N,n)$. We can enumerate the codewords as $\{|0\rangle,\ldots,|d_{N,n}\rangle\}$ where $|0\rangle=|0,\ldots,01,\ldots,1\rangle$, etc., to $|d_{N,n}\rangle=|1,\ldots,10,\ldots,0\rangle$, where there are N qubits in total and n 1's in each codeword. Consider a fixed nearest-neighbor pair of qubits at positions $i,i+1$, and the action of $T^x_{i,i+1},T^z_{i,i+1}$. The four possibilities for qubit values at these positions are {00,01,10,11}. Now consider a pair of codewords $|t\rangle$, $|t'\rangle$ such that $|t\rangle$ has 01 in the $i,i+1$ positions while $|t'\rangle$ has 10 in the $i,i+1$ positions, and they are identical everywhere else. We can always find such a pair by definition of $\mathcal{C}(N,n)$. The action of $T^x_{i,i+1},T^z_{i,i+1}$ on $|t\rangle$, $|t'\rangle$ is to generate su(2) between them, just as shown in the case of $\mathcal{C}(3,1)$ above. On the other hand, the action of $T^x_{i,i+1},T^z_{i,i+1}$ in the case of 00 or 11 in the $i,i+1$ positions is to annihilate all corresponding codewords [which are anyhow outside of the given $\mathcal{C}(N,n)$ subspace]. This null action means that, when exponentiated, $T^x_{i,i+1},T^z_{i,i+1}$ act as identity on these codewords. Therefore the action of $T^x_{i,i+1},T^z_{i,i+1}$ is precisely to generate su(2) between $|t\rangle$, $|t'\rangle$, and nothing more. Denote this by $\mathrm{su}(2)^{(1)}_{i,i+1}$. Let us now keep the 01 and 10 at positions $i,i+1$ fixed, and vary all other $N-2$ positions in $|t\rangle$, $|t'\rangle$, subject to the constraint of n 1's, and in the same manner in both $|t\rangle$, $|t'\rangle$. We then run over $K=\binom{N-2}{n-1}$ codewords, and $T^x_{i,i+1},T^z_{i,i+1}$ generate su(2) between each pair of new $|t\rangle$, $|t'\rangle$. Denote these by $\mathrm{su}(2)^{(k)}_{i,i+1}$, $k=1,...,K$. By further letting $i=0,...,N-2$ we generate $N-1$ *overlapping* su(2)'s. These su(2)'s can be connected by swaps so that we can generate all $\mathrm{su}(2)^{(k)}_{i,j}$, $k=1,...,K$, $i<j$. We thus have a total of $\binom{N-2}{n-1}$ $\binom{N}{2}$ su(2)'s. To generate the entire $\mathrm{su}(d_{N,n})$ we need no more than $d_{N,n}=\binom{N}{n}$ overlapping su(2)'s. Since $\binom{N-2}{n-1}$ $\binom{N}{2}/\binom{N}{n}=\frac{1}{2}n(N-n)>1$, we have more than enough overlapping su(2)'s, and $\mathrm{su}(d_{N,n})$ can be generated.

What is left is to show that we can perform a controlled operation between two $\mathcal{C}(N,n)$ subspaces. To do so we again use the nearest-neighbor interaction $\sigma^z_{N-1}\sigma^z_N$, where the first factor (σ^z_{N-1}) acts on the last qubit $(N-1)$ of the first $\mathcal{C}(N,n)$ subspace, and the second factor (σ^z_N) acts on the first qubit (N) of the second $\mathcal{C}(N,n)$ subspace. Now let us sort the codewords in the two subspaces in an identical manner, e.g., by increasing binary value. Then consider the action of $\sigma^z_{N-1}\sigma^z_N$ on the resulting ordered basis $\{|0\rangle\otimes|0\rangle,|0\rangle\otimes|1\rangle,\ldots,|d_{N,n}\rangle\otimes|d_{N,n}\rangle\}$. This action generates a representation of $\sigma^z_{N-1}\sigma^z_N$ by a $d_{N,n}\times d_{N,n}$ diagonal matrix. As in the $\mathcal{C}(3,1)$ case considered earlier, this matrix is actually a tensor product of an "$\mathrm{su}(d_{N,n})$-like" $\sigma^z\otimes\sigma^z$ on $\mathcal{C}(N,n)\otimes\mathcal{C}(N,n)$. It is simple to determine the form of these two (different) σ^z's. For the codewords belonging to the left $\mathcal{C}(N,n)$ factor, write down a $+1$ (-1) for each 0 (1) in the Nth position. These numbers are the diagonal entries of the left "$\mathrm{su}(d_{N,n})$-like" σ^z factor. Similarly, for the codewords belonging to the right $\mathcal{C}(N,n)$ factor, write down a $+1$ (-1) for each 0 (1) in the $(N+1)$th position. These numbers are the diagonal entries of the right "$\mathrm{su}(d_{N,n})$-like" σ^z factor. Since each such "$\mathrm{su}(d_{N,n})$-like" σ^z puts relative phases between the basis states of $\mathcal{C}(N,n)$, the action of $\sigma^z_{N-1}\sigma^z_N$ is that of a generalized CPHASE between the two code subspaces. This is sufficient together with $\mathrm{su}(d_{N,n})$ on each block to perform universal quantum computation.[56]

X. CONCLUSIONS

The standard quantum information-theoretic approach to qubits and operations on qubits emphasizes qubits as *vectors* in a Hilbert space and operations as *transformations* of these vectors.[7] This is the point of view of the first-quantized formulation of quantum mechanics. An alternative, mathematically equivalent, point of view is the Fock space, second-quantized formulation of quantum mechanics, which emphasizes the particlelike nature of quantum states. Qubit up/down states are replaced by qubit presence/absence, while rotations are replaced by operators that count or change particle occupation numbers. The mapping of qubits to parafermions discussed in this article is a mapping between these first- and second-quantized formulations. It proved to be a useful tool in studying the connection between qubits, bosons, and fermions, in analyzing the algebraic structure of qubit Hamiltonians, and in studying related quantum computational universality questions. In particular, it allowed us to classify subalgebras of fermion, boson, and qubit operators and decide their power for quantum computational universality. These results are relevant for physical implementation of quantum computers: a physical N-qubit system

comes equipped with a given Hamiltonian, which generates a subalgebra of su(2^N). It is important to know whether this Hamiltonian is by itself universal or needs to be supplemented with additional operations, or whether one needs to encode physical qubits into logical qubits in order to attain universality. Our classification settles this question for many subalgebras of physical interest.

Another potential advantage of the parafermionic approach, as a second-quantized formalism for qubits, lies in its ability to naturally deal with a ''qubit-field,'' i.e., situations where the qubit number is not a conserved quantity. This is certainly a concern for optical and various solid-state quantum computer implementations. We leave the study of a qubit field theory as an open area for future explorations.

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[8] The mapping from qubits to parafermions was first pointed out in L.-A. Wu and D. A. Lidar, quant-ph/0103039v1. Our definition of a parafermion is inspired by Green[1] and Greenberg,[9] but differs somewhat. Like these authors we start from $\{a_i, a_i^\dagger\}=1$ and $[a_i, a_j^\dagger]=0$ for $i\neq j$. Green was the first to introduce these commutation relations, but did not name the corresponding particles. Greenberg did not name them either, but called ''parafermion'' a particle defined by $a^\dagger = \sum_{j=1}^N a_j^\dagger$. The commutation relation we use to define parafermions is therefore different from Greenberg's. Nevertheless we prefer to call a particle satisfying these relations a ''parafermion,'' since they emphasize the two-dimensional Hilbert–Fock space of an individual particle (like fermions). The opposite choice of commutation relations, $[a_i, a_i^\dagger]=1$ and $\{a_i, a_j^\dagger\}=0$ for $i\neq j$, can be used to define ''parabosons:'' particles with unlimited occupation number per mode, but without a natural tensor product structure. Finally, we note that the particle we are referring to as a parafermion is also known sometimes as a ''hardcore boson,'' e.g., K. Bernardet *et al.*, Phys. Rev. B **65**, 104519 (2002).
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Secrecy capacity in the four-state protocol of quantum key distribution

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The process of key distillation from the quantum transmission in quantum key distribution is reviewed, with the objective of calculating the secrecy capacity of the four-state protocol in the presence of an individual attack in which the eavesdropping probe is entangled with the signal states, and states of the probe become correlated with the states measured by the legitimate receiver. Emphasis is placed on information leakage to the eavesdropping probe. The calculation generalizes earlier work to include an arbitrary angle between the signal bases.
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I. INTRODUCTION

One effective implementation of the four-state quantum-key-distribution protocol (BB84)[1] uses single photons linearly polarized along one of the four basis vectors of two sets of coplanar orthogonal bases oriented at an angle of $\pi/4$ relative to each other. The polarization measurement operators in one basis do not commute with those in the other, since they correspond to nonorthogonal polarization states. At a fundamental level, the potential security of the key rests on the fact that nonorthogonal photon polarization measurement operators do not commute, and this gives rise to quantum uncertainty in the measurement of those states by an eavesdropper. Before transmission of each photon, the transmitter and receiver each independently and randomly select one of the two bases. The transmitter sends a single photon with polarization chosen at random along one of the orthogonal basis vectors in the chosen basis. The receiver makes a polarization measurement in its chosen basis. Next, the transmitter and the receiver openly compare their choices of basis, without disclosing the polarization states transmitted or received. Events in which the transmitter and the receiver choose different bases are ignored, while the remaining events ideally have completely correlated polarization states. The two orthogonal states in each of the two bases encode binary numbers 0 and 1, and thus a sequence of photons transmitted in this way establishes a random binary sequence shared by both the transmitter and the receiver and can serve as the secret key, following error correction and privacy amplification. The key can then be used to encode a message, using the Vernam cipher, and the message can then be securely transmitted over an open communication line and then decoded, using the shared secret key at the receiver end.

Privacy amplification is, of course necessary, because of the possibility of an eavesdropping attack.[2–4] It is important to note at this point that the present article is not a comprehensive review, but primarily discusses the work of the author and that of Slutsky *et al.*[5–11] In the individual attack,[5–9,12] the most general possible eavesdropping probe consistent with unitarity is assumed, in which each individual transmitted bit is made to interact with the probe so that the carrier and the probe are left in an entangled state, and measurement by the probe, made subsequent to measurement by the legitimate receiver, yields information about the carrier state.

To proceed first with a review of key distillation, let m bits of raw data be received by the legitimate receiver in the four-state quantum-key-distribution protocol, and suppose n bits of sifted data remain following removal of $(m-n)$ inconclusive bits, and suppose there are e_T bits of

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erroneous data, leaving $(n-e_T)$ bits of corrected data. Corrected data includes data remaining after discarding inconclusive results and also erroneous data as determined by block checksums and bisective search. Privacy amplification is the procedure for obtaining a more secure, but shorter, key. This is achieved by removing from the $(n-e_T)$ bits of corrected data a number s of bits (the privacy amplification compression level) that is the sum of the possible contributions to information leakage. There then remain $(n-e_T-s)$ bits, and this is the size of the final key. The privacy amplification compression level s is given by[10,11]

$$s=t(n,e_T)+q+\nu+g, \tag{1}$$

where q is the estimated information leakage during error correction, ν is the estimated leakage from any multi-photon bits, g is an extra safety margin, and $t(n,e_T)$ is the defense function. The defense function, in general, depends on the size n of the sifted data, and on the number e_T of errors, and is chosen appropriately by the legitimate users, in order to effectively defend against an eavesdropping attack. The defense function $t(n,e_T)$ is the estimated upper bound on possible information leakage through eavesdropping on the quantum channel. Quantitatively it is determined by the maximum total Renyi information gain I_T^R by the eavesdropping probe. (It is proved in Ref. 5 that the optimum individual attack maximizes both the Renyi and Shannon information gain by the eavesdropping probe.) The maximum Renyi information gain by the eavesdropper is based on minimizing the overlap of the measured probe states correlated with the disturbed signal states of the legitimate receiver, conditional on fixed induced error rate. The compression level s must be chosen so that the probability is small that $I_T^R>t(n,e_T)$. An attack is successful if it introduces e_T errors on the n bits of sifted data, and yields a Renyi information $I_T^R>t(n,e_T)$ on the $(n-e_T)$ bits of corrected data. The probability of a successful attack must be negligible. In the presence of noise and channel losses, it is not sufficient, for the security of a quantum key distribution system, to detect eavesdropping. It must be insured that the shared data is sufficiently secure.

It is well to recall the privacy amplification theorem.[4] First, however, recall the definition of the Renyi information $I^R(l)$ on an l bit string X having probability distribution $P_X(X)$, namely,

$$I^R(l)=l+\log_2\langle P_X(X)\rangle=l+\log_2\sum_X P_X^2(X), \tag{2}$$

where the bracket denotes the expectation value. [$P_X^2(X)$ is often referred to as the collision probability.] The privacy amplification theorem states that if the eavesdropper's Renyi information gain $I^R(l)$ on an l bit data string is less than some quantity r, namely,

$$I^R(l)\leqslant r, \tag{3}$$

then the eavesdropper's Shannon information $I^H(l-s)$ on the reduced $(l-s)$ bit string, averaged over the choice of privacy amplification hash function, is bounded above, namely,

$$\langle I^H(l-s)\rangle\leqslant\frac{1}{\ln 2}2^{r-s}, \tag{4}$$

where here the brackets denote the average. By choosing the compression level s sufficiently large, the exponent on the right-hand side of Eq. (4) becomes sufficiently negative that the average Shannon information can be made arbitrarily small. Thus, given an upper bound on the eavesdropper's Renyi information gain, the corrected data can be subjected to the reduction procedure of privacy amplification to yield an even shorter string on which the eavesdropper's Shannon information is arbitrarily low. The secrecy of the final key is recovered (but reduced in size) if an upper bound can be determined on the maximum Renyi information gain by the eavesdropper on corrected data.

The average secrecy capacity C_s' of a quantum cryptosystem is the number of secret bits produced per bit from the transmitter, and is given by

$$C_s' = \operatorname*{Lim}_{m\to\infty}\left\langle \frac{n-e_T-s}{m}\right\rangle. \tag{5}$$

Here the limit of a very long transmission is understood in which m, the number of bits of raw data, is very large.

II. CALCULATING SECRECY CAPACITY

The numerator of Eq. (5), $(n-e_T-s)$, is the size of the final key, where n is the number of bits of sifted data with the inconclusive bits removed, e_T is the number of bits of erroneous discarded data due to error correction, and s is the privacy amplification compression level. The average secrecy capacity, Eq. (5), converges in distribution to[10]

$$C_s' = \left\langle \frac{n}{m}\right\rangle\left(1-\left\langle \frac{e_T}{n}\right\rangle - \frac{t_F}{n}\bigg|_{e_T/n=\langle e_T/n\rangle} - \operatorname*{Lim}_{m\to\infty}\left\langle \frac{q}{n}\right\rangle\right). \tag{6}$$

The factor $\langle n/m\rangle$ in Eq. (6) is the conclusive rate. Since the inconclusive rate $R_?$ is $\frac{1}{2}$ for the BB84 protocol,[5,10,11] and remains unchanged in the presence of the individual attack, the conclusive rate must also be $\frac{1}{2}$, namely,

$$\left\langle \frac{n}{m}\right\rangle = (1-R_?) = \left(1-\frac{1}{2}\right) = \frac{1}{2}. \tag{7}$$

Also in Eq. (6), $\langle e_T/n\rangle$ is the average intrinsic error rate, and $\langle q/n\rangle$ is the average information leakage during error correction. Since the present work focuses on the information leakage through eavesdropping [represented by the third term in Eq. (6)], possible additional terms, $(-\langle \nu/n\rangle)$ and $(-\langle g/n\rangle)$, are dropped in Eq. (6). [See Eq. (1)]. In the third term of Eq. (6), $(t_F/n)\,|_{e_T/n=\langle e_T/n\rangle}$ is the average defense frontier t_F evaluated at the average intrinsic error rate. In the individual attack, each signal is attacked individually and in the same way, and it is assumed that the signal states, errors, and measurement outcomes of the probe and the legitimate receiver are all independently and identically distributed.[10] Multiple eavesdropping strategies are considered with different induced error rates, but the attack is restricted to the set of strategies yielding the greatest attainable expected Renyi information gain for a given expected error rate. The defense frontier t_F is, for all possible eavesdropping strategies, the upper bound on the information leakage through eavesdropping, based on an optimal eavesdropper in the limit of a long transmission. The defense frontier t_F is chosen to minimize the chance of any successful eavesdropping strategy, and, for the individual attack, it is given by[10]

$$t_F(n,e_T) = \max_{e\leqslant e_T}\left\{ n\left(1-\frac{e}{n}\right) I^R_{\rm opt}\left(\frac{e}{n}+\xi\right) + \xi\left[n^2\left(1-\frac{e}{n}\right)\right]^{1/2}\right\}, \tag{8}$$

where $I^R_{\rm opt}(E)$ is the maximum Renyi information gain on corrected data by the eavesdropping probe, and conditional on fixed error rate $E=(e/n)$; and ξ is defined by

$$\xi = \frac{1}{(2n)^{1/2}}\,{\rm erf}^{-1}(1-p), \tag{9}$$

where ${\rm erf}^{-1}$ denotes the inverse standard error function. The standard error function ${\rm erf}(z)$ is defined by

$$\mathrm{erf}(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{-y^2}dy. \tag{10}$$

Also in Eq. (9), p is the probability for successful eavesdropping $[I_R^T>t(n,e_T)]$ on $(n-e_T)$ bits of corrected data and producing e_T errors; and p can be made arbitrarily small. The defense frontier, Eq. (8), was determined by Slutsky, Rao, Sun, Tancevski, and Fainman[10] by clever use of the central limit theorem of probability theory, and is constructed to minimize the chance of successful eavesdropping. Using Eqs. (6)–(8), the asymptotic secrecy capacity, in the limit of long transmission with $m\to\infty$, $n\to\infty$, and $\xi\to 0$, and for $q=0$, becomes[10]

$$C_s'|_{q=0,n\to\infty,\xi\to 0}=\tfrac{1}{2}(1-E-\max_{E'\leqslant E}(1-E')I_{\mathrm{opt}}^R(E')), \tag{11}$$

where E is the error rate, and $(\max_{x'\leqslant x}f(x'))$ denotes the maximum value of a function $f(x')$ for $x'\leqslant x$. Also in Eq. (11), $I_{\mathrm{opt}}^R(E')$ is the maximum Renyi information gain on corrected data by the eavesdropping probe, conditional on fixed error rate E'. The asymptotic secrecy capacity, Eq. (11), is based on the definition of average secrecy capacity, Eq. (5), as given in the literature,[10] however it is important to emphasize that the condition of maximum Renyi information gain by the eavesdropper may be overly conservative. (See Sec. VI of Ref. 4.)

For the four-state protocol, the maximum Renyi information gain I_{opt}^R on corrected data by the probe, conditional on fixed error rate E, for the individual attack is given by[5–9]

$$I_{\mathrm{opt}}^R=\log_2(2-Q^2). \tag{12}$$

Here Q is the minimum overlap of the probe states correlated with the signal states, and, for an arbitrary angle between the signal bases, it is given by[9]

$$Q=\begin{cases}\dfrac{1+(1-2\csc^2 2\alpha)E}{1-E}, & \alpha\leqslant\pi/8,\\[2ex] \dfrac{1+(1-2\sec^2 2\alpha)E}{1-E}, & \alpha\geqslant\pi/8,\end{cases} \tag{13}$$

with

$$\alpha=\frac{1}{2}\left(\frac{\pi}{2}-\hat{\theta}\right), \tag{14}$$

where $\hat{\theta}$ is the angle between the nonorthogonal linear polarization states of the signal. The optimization given by Eqs. (12)–(14) is over the set of probe parameters which define the general eavesdropping probe used in the individual attack.[5–9,12] For $\alpha=\pi/8$, corresponding to the standard BB84 protocol with $\hat{\theta}=\pi/4$, Eqs. (12) and (13) agree with Ref. 5. Substituting Eqs. (12) and (13) in Eq. (11), one obtains for the asymptotic secrecy capacity:

$$C_s'|_{q=0,n\to\infty,\xi\to 0}=\begin{cases}\dfrac{1}{2}\left(1-E-\max\limits_{E'\leqslant E}(1-E')\log_2\left[2-\left(\dfrac{1+(1-2\csc^2 2\alpha)E'}{1-E'}\right)^2\right]\right), & \alpha\leqslant\dfrac{\pi}{8}\\[2ex] \dfrac{1}{2}\left(1-E-\max\limits_{E'\leqslant E}(1-E')\log_2\left[2-\left(\dfrac{1+(1-2\sec^2 2\alpha)E'}{1-E'}\right)^2\right]\right), & \alpha\geqslant\dfrac{\pi}{8}.\end{cases} \tag{15}$$

For $\alpha=\pi/8$, Eq. (15) also agrees with Ref. 10. It is evident from Eqs. (12)–(15) that as a function of α, for fixed error rate, the overlap of correlated probe states is greatest, the Renyi information gain by the probe is least, and the secrecy capacity is greatest for $\alpha=\pi/8$, which corresponds to the standard BB84 protocol[1] with $\hat{\theta}=\pi/4$.

III. SUMMARY

Following a review of the process of key distillation from the quantum transmission in quantum key distribution, the asymptotic secrecy capacity, Eq. (15), of the four-state protocol has been calculated for the case of an individual attack in which the eavesdropping probe is entangled with the signal states, and states of the probe become correlated with the states measured by the legitimate receiver. The calculation generalizes earlier work to include an arbitrary angle between the signal bases.

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Hiding messages in quantum data

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A method is proposed to hide messages in arbitrary quantum data files. The messages may act as ''watermarks,'' to secure the authenticity and/or integrity of the data. With the help of classical secret keys, they can be made unreadable by other parties and to reveal whether thay have been tampered with. The basic idea is to encode the data using a quantum error-correcting code and hide the message as (correctible) errors, deliberately inserted, which can be read out from the error syndrome. Also discussed briefly is a ''reverse encoding,'' which would involve putting the actual data in the error syndrome, and letting the encoded qubit itself carry the message. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Steganography is a branch of cryptography concerned with embedding ''invisible'' messages in data files. The message, which is revealed by some appropriate decoding operation, may contain information regarding the owner of the file or its date of creation, for instance. Such techniques have become of particular interest in recent years because of the proliferation of means available to copy, legally or illegally, all sorts of data, such as images, audio, or video files.[1]

Although quantum information processing is still, in practice, a long way from the day where sizable files of ''quantum data'' will be moved from one location to another, it may already be of interest to begin to explore the possibilities inherent in a quantum sort of steganography, and the ways in which this would differ from its classical counterpart. This article is intended to serve as a (small) first step in this direction.

It should be clear from the outset, of course, that copyright protection in its most literal sense could never be an issue for quantum information, since, by the celebrated no-cloning theorem, it is inherently impossible to copy. Nonetheless, there are other useful purposes that could be served by a hidden message embedded in a quantum data file. It could function as a ''watermark,'' for instance, allowing one to identify the file's owner or creator, either as protection against theft or reassurance to the party receiving the data that they come, in fact, from the right source. Also, as will be shown below, the watermark could be embedded in such a way as to provide the receiving party with information that the file has been corrupted, either by errors upon transmission or by tampering by a third party. Another potential use might be in a distributed quantum computing environment, where packets of information are processed at some location and then sent to other processors: a message could be embedded in the data to tell the receiving processor what it is supposed to do with it. Again, corruption of the data could be detected at the receiving end by these means.

A large component of all of the above is, clearly, the question of data authentication, in the broadest sense of making sure both that the data have come from the right source and that they have not been tampered with or otherwise corrupted. A number of ideas have recently been put forth regarding this general issue. Buhrman *et al.*[2] have studied ways to associate a quantum fingerprint with a classical data string; a variation on this idea, due to Gottesman and Chuang,[3] would allow one to attach a quantum signature to a classical message, which would serve to

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certify its authenticity. The general question of authenticating a single classical bit using a single qubit has been studied by Curty and Santos.[4] Moving on to the problem of authenticating *quantum* data, Curty *et al.*[5] have shown that it is impossible to authenticate a qubit with a one-bit (or one-qubit) key (in all authentication schemes, the sender and receiver must share a key in advance, in order to read out the authentication information). Nonetheless, if longer keys are allowed, schemes to authenticate arbitrary quantum data exist; for instance, in Ref. 6, Leung has proposed a scheme to authenticate n qubits given an authenticated two-way classical channel, $2r$ bits of classical key, and an extra $2r$ qubits of quantum communication. In this scheme, forging succeeds with probability no better than 2^{-r} and the fidelity of an accepted message with respect to the original is of the order of $1-O(2^{-r})$. Finally, Barnum *et al.*[7] have also recently reported on a powerful general method of quantum data authentication, whose details should soon be made widely available.

In Leung's scheme, the $2r$ extra qubits are simply appended to the message, as a sort of authentication tag. The tag is uniquely related to the message, so that a would-be forger cannot simply remove it and attach it to a false message to make it pass for an authentic one. Nonetheless, the tag could still be simply removed, leaving the adversary in possession of the data, with no indication as to its provenance. In this respect this scheme differs from a classical steganography situation, where (part of) the idea is that the identification tag could not be deleted without damaging the data.

In what follows I wish to present a simple authentication scheme which accomplishes this last purpose, and has other potential advantages (such as the fact that it is based on a conventional quantum error correction code, and so, under some circumstances, it may function as such, thus helping to protect the integrity of the data). Perhaps it should be acknowledged from the outset that, even though the starting point draws some inspiration from classical steganography, the final result may not look much like it. The main guiding principle has been to arrange for the data and the message (or ''tag'') to be inextricably linked, in such a way that somebody who does not have the key could not alter the one without altering the other.

The approach is heuristic throughout; no attempt has been made to provide formal proofs of security or optimize the resources needed. Nonetheless, it is interesting that this simple-minded approach leads in a natural way to a construction which ends up having some similarities to the much more formal approach of Ref. 7. Hence, it is hoped that the present work may provide some insight into some of the issues involved in quantum data authentication.

II. EMBEDDING A MESSAGE IN A QUANTUM DATA FILE ENCODED WITH AN ERROR-CORRECTING CODE

A. Basic concept

One conventional approach in clasical steganography is to write the hidden message in the data file by replacing some of the original data's bits, according to a certain pattern or key. Such an approach, however, could not work, in general, with quantum data, which are often in coherent superpositions for which the actual state of an individual qubit may simply not be defined, due to entanglement with other qubits. Arbitrarily setting the state of a random qubit to a specific value would not only destroy that qubit's entanglement, it would also collapse the state of any other qubits entangled with it.

This means that one needs to add qubits to the original file, perhaps interspersing them among the original data qubits, and write the message in them. Then one may observe that a systematic method to add qubits to a quantum data file, in such a way that one could, at the same time, introduce ''errors'' in it harmlessly, is provided by QECCs.[8] Hence the simplest approach to ''quantum steganography'' might be as follows: encode the original data file using a suitable QECC; hide the message as ''errors'' in the encoded qubits; and read it out in the *error syndrome*.

As an example of this approach, consider the following simple three-qubit code, which protects one logical qubit against a single bit flip error (of any of the three physical qubits):

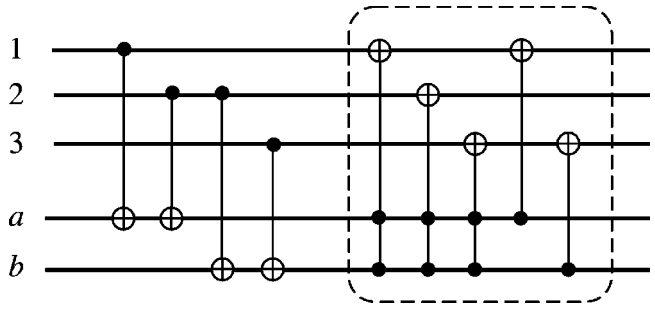

FIG. 1. A circuit to read out the error syndrome for the 3-qubit repetition code. The dashed box shows how the error can be corrected without actually having to measure the state of the ancilla qubits.

$$|0_L\rangle = |000\rangle,$$
$$|1_L\rangle = |111\rangle. \tag{1}$$

The state $|\psi\rangle$ of any of the original data qubits could be encoded as $|\psi\rangle = \alpha|0_L\rangle + \beta|1_L\rangle$. Then, for each such logical qubit, a message of up to four classical bits could be encoded "in parallel," so to speak, on the same three physical qubits, by acting on $|\psi\rangle$ with either the identity or one of the three Pauli operators σ_{ix} (with $i=1, 2, 3$). This message could be read off, for instance, by the error-diagnosing circuit shown on the left half of Fig. 1, which employs two ancillary qubits, a and b. If the state of these ancillary qubits is read out after the four CNOT operations have been carried out, it is easily checked that each of the four possible operations on $|\psi\rangle$ maps to a different joint state of a and b, as follows:

$$1 \rightarrow |00\rangle_{ab},$$
$$\sigma_{1x} \rightarrow |10\rangle_{ab},$$
$$\sigma_{2x} \rightarrow |11\rangle_{ab},$$
$$\sigma_{3x} \rightarrow |01\rangle_{ab}. \tag{2}$$

Thus, all four possible bit values of the two-bit classical mesage can be read and identified, without actually changing the logical qubit's state in any way.

Of course, one problem that arises immediately is that an adversary who knew that the underlying code is the three-qubit, repetition code (1), and wanted to erase the message, could easily do so simply by applying error correction to the encoded qubit! There is, however, a simple way to prevent this from happening, namely, to change the code randomly, from one logical qubit to the next, according to a secret key (shared by the sender and the receiver). For practical purposes, it would be sufficient, for example, to stay with a three-qubit code but encode the message alternatively in bit-flip errors and phase errors. Protection against phase errors is provided by a code like

$$|\overline{0}_L\rangle = H^{\otimes 3}|0_L\rangle = \frac{1}{2^{3/2}}(|0\rangle+|1\rangle)(|0\rangle+|1\rangle)(|0\rangle+|1\rangle),$$
$$|\overline{1}_L\rangle = H^{\otimes 3}|1_L\rangle = \frac{1}{2^{3/2}}(|0\rangle-|1\rangle)(|0\rangle-|1\rangle)(|0\rangle-|1\rangle). \tag{3}$$

(Here, H denotes a Hadamard transform.) Now, a "0" in the classical key could mean that the original qubit is to be encoded as $|\psi\rangle = \alpha|0_L\rangle + \beta|1_L\rangle$, with $|0_L\rangle$ and $|1_L\rangle$ given by (1), and the

message hidden in the error syndrome as any of the four operators identity+one of the σ_{ix}; whereas a "1" in the classical key would mean that the encoding for the original qubit uses the basis $|\overline{0_L}\rangle$ and $|\overline{1_L}\rangle$ given by (3) above, and the error syndrome is encoded using the σ_{iz} operators.

If the eavesdropper does not realize that the message is now encoded as a phase error, he not only cannot read it, but, moreover, he also cannot erase it properly. Suppose that bit-flip error correction is applied to a qubit $\alpha|\overline{0_L}\rangle+\beta|\overline{1_L}\rangle$ originally encoded in the basis (3). The result will be a superposition of the basis states (1); specifically, $\frac{1}{4}$ of the time it will be $\alpha|0_L\rangle+\beta|1_L\rangle$, and $\frac{3}{4}$ of the time it will be $\alpha|1_L\rangle+\beta|0_L\rangle$.[9] Thus, attempts to erase (or, in general, alter) the message result in changes to the data. Needless to say, the message (in the $|\overline{0_L}\rangle,|\overline{1_L}\rangle$ basis) also is changed as a result of this intervention, so if the file is eventually inspected by somebody who knows both the key and the message, he should be able to tell that it has been tampered with.

It is interesting to note that for such a user, who knows both the key and the message, the "errors" deliberately introduced in the encoded qubits do not affect the ability of the code to function as a QECC and protect the data against accidental (additional) errors of the type naturally corrected by the code [e.g., bit errors for the code (1), phase flips for the code (3)]. This can be formally seen as follows: suppose the original (encoded) state is $|\psi\rangle$, and we put an error $\sigma_{i\alpha}$ on it (where i is the qubit index and $\alpha=x,y$ or z). Then suppose another (unknown) error $\sigma_{j\beta}$ occurs; the resulting state is therefore $\sigma_{j\beta}\sigma_{i\alpha}|\psi\rangle$. Then, in order to diagnose properly the error $\sigma_{j\beta}$, all we need to do is apply $\sigma_{i\alpha}$ again to the state, followed by ordinary error correction, since $\sigma_{i\alpha}\sigma_{j\beta}\sigma_{i\alpha}|\psi\rangle=\pm\sigma_{j\beta}|\psi\rangle$. The minus sign only occurs if $i=j$, $\alpha\neq\beta$, and, as an overall sign, it is irrelevant. Therefore, any error that the code could initially diagnose can still be diagnosed correctly. This property alone may make this scheme attractive: if the data are going to be encoded for protection against errors anyway, one might as well take advantage of this to hide a signature in the error syndrome, essentially at no extra cost.

If larger codes are used (to correct for more errors), one can still use essentially the same strategy to protect the message, namely, encode the logical qubits in either the original $|0_L\rangle,|1_L\rangle$, or the conjugate, $|\overline{0_L}\rangle,|\overline{1_L}\rangle$, basis (connected by a Hadamard transform) according to the value of a secret key. Atempts to do error correction on the encoded qubit by somebody who does not know the key will result in the state being projected onto the wrong basis half of the time.

From an authentication perspective, however, one may have to wonder about the reverse possibility: could somebody who does not know the key change the data without changing the message? It turns out that this is, indeed, possible if the message is classical, as will be shown in the next subsection.

B. Inserting a quantum message

Consider again the example (1), as illustrated in Fig. 1. Since the encoding and decoding are linear operations, a coherent superposition of errors acting on the encoded data qubit $|\psi\rangle$ will, in fact, yield a coherent superposition of the ancilla qubits; so the "message" does not have to be classical information, it could be quantum information as well. In other words, the operation

$$(\gamma+\delta\sigma_{1x}+\eta\sigma_{2x}+\epsilon\sigma_{3x})(\alpha|0_L\rangle+\beta|1_L\rangle) \tag{4}$$

actually encodes three qubits worth of information in three physical qubits. The one-qubit state $\alpha|0\rangle+\beta|1\rangle$ is in the "data" that one recovers after error correction, whereas the two-qubit state

$$\gamma|00\rangle+\delta|10\rangle+\eta|11\rangle+\epsilon|01\rangle \tag{5}$$

is the state of the ancilla qubits when the error syndrome is extracted as in Fig. 1. Note that the ancilla qubits will only be in a coherent superposition after error correction has been applied to qubits 1, 2, and 3 (otherwise they are still entangled with them), and only if this is done coherently, i.e., without measurements; this can always be achieved, as indicated, e.g., by the circuit in the

dashed box in Fig. 1. Incidentally, since CNOT gates are their own inverses, the dashed box in Fig. 1 also shows how the encoding (4) could be applied to the qubits 1, 2, 3, if one starts with the qubits a and b in the state (5).

Now consider the possibility mentioned at the end of the previous subsection, that an adversary might attempt to change the data while leaving the message intact. For instance, suppose that he attempts to flip an encoded qubit, by applying the operator $\sigma_{1x}\sigma_{2x}\sigma_{3x}$ to it. If the qubit is encoded in the basis (1), as in Eq. (4), this will indeed change it to $\alpha|1_L\rangle+\beta|0_L\rangle$, while leaving the error syndrome intact, since all the σ_{ix} commute with each other. On the other hand, if the qubit is initially encoded in the conjugate basis $|\overline{0_L}\rangle,|\overline{1_L}\rangle$ as $|\psi\rangle=(\gamma+\delta\sigma_{1z}+\eta\sigma_{2z}+\epsilon\sigma_{3z})\times(\alpha|\overline{0_L}\rangle+\beta|\overline{1_L}\rangle)$, one finds

$$\sigma_{1x}\sigma_{2x}\sigma_{3x}|\psi\rangle=(\gamma-\delta\sigma_{1z}-\eta\sigma_{2z}-\epsilon\sigma_{3z})(\alpha|\overline{0_L}\rangle-\beta|\overline{1_L}\rangle). \tag{6}$$

So, in this basis, the data qubit is also changed (it acquires a ''phase flip''), but now also the syndrome is changed, provided γ and at least one of δ, γ or ϵ are nonzero. That is, in order to provide protection against this type of attack, the ''message'' encoded in the error syndrome must be a quantum superposition state: it must be quantum, not classical, information.

C. Reversing the "data" and "message" roles

The construction in the previous subsection suggests the possibility of reversing the roles of ''data'' and ''message:'' with the scheme in Fig. 1, one could encode two qubits' worth of actual quantum data in the ''error syndrome,'' and a one-bit (or one-qubit) message in the ''logical qubit'' part of Eq. (4) (that is, the part involving α and β). What one gains with this scheme is efficiency, in the sense of a greater data-to-message information ratio. This can be made even greater by going to larger codes: for instance, any $[n,1]$ stabilizer code (encoding 1 logical qubit into n physical qubits) has $n-1$ generators, and measuring them determines the error syndrome; so the error syndrome can be extracted in $n-1$ qubits. With this ''reverse encoding'' approach, therefore, one could ''pack'' $n-1$ qubits worth of data in the error syndrome of every encoded logical qubit, and one qubit worth of ''message'' in the actual logical qubit.

As before, security would be provided by a secret key specifying on what basis each block is to be encoded. Since each block carries only one qubit of message, the key only has to be as long as the message itself; the ratio of length of key to length of data file (in bits, or qubits) is $1/(n-1)$, which could be made very small by using sufficiently large codes. If the total number of packages sent is t, the total number of possible different keys is 2^t, which suggests that the probability of successful tampering with or reading of the message is of the order of $1/2^t$. Clearly, though, this suggestion does not amount to a formal proof of security, and the scheme is only mentioned to give an indication of possibilities—in particular, for greater efficiency—beyond the ''straightforward'' scheme of the previous two subsections.

III. DISCUSSION AND CONCLUSIONS

The ideas proposed here provide some potentially useful ways to hide messages in quantum data for a variety of applications. In all cases, the data and the message are combined so that any change in one is likely to result in a change in the other. The method of Sec. II A is most useful when one is already considering using a QECC to protect the data against accidental errors, and the message to be sent (a sort of ''watermark'') is previously known to all the authorized parties; then the message can ''ride along'' in the error syndrome without compromising the efficacy of the code to correct errors. Note that, for data authentication purposes, the ''watermark'' should be quantum data, in order to provide protection against certain types of attacks.

As emphasized in the Introduction, the presentation here has been heuristic; I have not attempted to study the security features of the proposed schemes, for any specific application, in detail, nor to improve their efficiency beyond the suggestion, in Sec. II C, that smaller ratios of key to data file length might be possible. Nonetheless, as also mentioned in the Introduction, it is

interesting that the result exhibits a number of similarities to the more formal methodology for data authentication studied by Barnum *et al.*;[7] in particular, the use of QECCs (which under some circumstances could be used to provide additional protection for the data, as also remarked in Ref. 7) and the idea of hiding some secret ''key'' information in the error syndrome. It appears as if a careful study of the similarities and differences between the two schemes could be an enlightening and worthwhile task, but at present this must remain beyond the scope of the present manuscript.

In closing, to return, for a moment, to what constituted the original motivation for the present work namely, the idea of exploring the feasiblity of a sort of ''quantum steganography,'' these results do indicate how it may be possible, in principle, to combine a given set of quantum data and a quantum message in an inextricable way. It could be argued, however, that the final result does not look much like classical steganography, since we have ended up encrypting both the message and the data, whereas in classical steganography, instead, the ''data'' are, for the most part, openly visible (although subtly altered), and only the message is hidden. Yet, as I have mentioned above, it is not obvious to me how one could only ''slightly'' alter quantum information in order to accomplish this goal. In fact, it is one of the most interesting results proved in Ref. 7 that (unlike for classical data, where authentication and encryption are two different tasks) in order to authenticate quantum data one must, as it turns out, encrypt them ''almost perfectly.''

ACKNOWLEDGMENTS

I am grateful to Howard Barnum for very useful comments, and to the authors of Ref. 7 for sharing with me a preprint of their work. This research has been supported by the Army Research Office and the National Science Foundation.

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[9] This particular ratio is obtained only if the message is classical (see the following subsection for how to embed a quantum message).

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Unknown quantum states: The quantum de Finetti representation

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We present an elementary proof of the *quantum de Finetti representation theorem*, a quantum analog of de Finetti's classical theorem on exchangeable probability assignments. This contrasts with the original proof of Hudson and Moody [Z. Wahrschein. verw. Geb. **33**, 343 (1976)], which relies on advanced mathematics and does not share the same potential for generalization. The classical de Finetti theorem provides an operational definition of the concept of an unknown probability in Bayesian probability theory, where probabilities are taken to be degrees of belief instead of objective states of nature. The quantum de Finetti theorem, in a closely analogous fashion, deals with exchangeable density-operator assignments and provides an operational definition of the concept of an ''unknown quantum state'' in quantum-state tomography. This result is especially important for information-based interpretations of quantum mechanics, where quantum states, like probabilities, are taken to be states of knowledge rather than states of nature. We further demonstrate that the theorem fails for real Hilbert spaces and discuss the significance of this point. © *2002 American Institute of Physics.*
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I. INTRODUCTION

What is a quantum state? Since the earliest days of quantum theory, the predominant answer has been that the quantum state is a representation of the observer's knowledge of a system.[1] In and of itself, the quantum state has no objective reality.[2] The authors hold this information-based view quite firmly.[3,4] Despite its association with the founders of quantum theory, however, holding this view does not require a concomitant belief that there is nothing left to learn in quantum foundations. It is quite the opposite in fact: Only by pursuing a promising but incomplete program can one hope to learn something of lasting value. Challenges to the information-based view arise regularly, and dealing with these challenges builds an understanding and a problem-solving agility that reading and rereading the founders can never engender.[5] With each challenge successfully resolved, one walks away with a deeper sense of the physical content of quantum theory and a growing confidence for tackling questions of its interpretation and applicability. Questions as fundamental and distinct as ''Will a nonlinear extension of quantum mechanics be needed to quantize gravity?'' [6,7] and ''Which physical resources actually make quantum computation efficient?'' [8,9] start to feel tractable (and even connected) from this perspective.

In this article, we tackle an understanding-building exercise very much in the spirit of these

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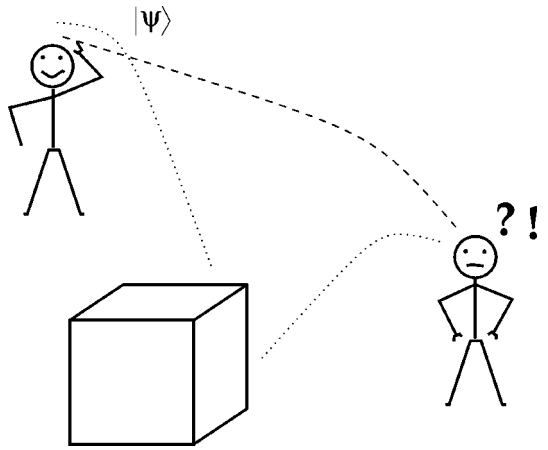

FIG. 1. What can the term ''unknown state'' mean if quantum states are taken exclusively to be states of knowledge rather than states of nature? When we say that a system has an unknown state, must we always imagine a further observer whose state of knowledge is symbolized by some $|\psi\rangle$, and it is the identity of the symbol that we are ignorant of?

remarks. It is motivated by an apparent conundrum arising from quantum information theory. The issue is that of the *unknown* quantum state.

There is hardly a paper in the field of quantum information that does not make use of the idea of an ''unknown quantum state.'' Unknown quantum states are teleported,[10,11] protected with quantum error correcting codes,[12,13] and used to check for quantum eavesdropping.[14,15] The list of uses, already long, grows longer each day. Yet what can the term ''unknown quantum state'' mean? In an information-based interpretation of quantum mechanics, the term is an oxymoron: If quantum states, by their very definition, are states of knowledge and not states of nature,[16] then the state is *known* by someone—at the very least, by the describer himself.

This message is the main point of our article. Faced with a procedure that uses the idea of an unknown quantum state in its description, a consistent information-based interpretation of quantum mechanics offers only two alternatives (see also Fig. 1):

(i) The owner of the unknown state—a further decision-making agent or observer—must be explicitly identified. In this case, the unknown state is merely a stand-in for the unknown *state of knowledge* of an essential player who went unrecognized in the original formulation.

(ii) If there is clearly no further decision-making agent or observer on the scene, then a way must be found to reexpress the procedure with the term ''unknown state'' banished from the formulation. In this case, the end-product of the effort is a single quantum state used for describing the entire procedure—namely, the state that captures the describer's state of knowledge.

Of course, those inclined to an objectivist interpretation of quantum mechanics[17]—that is, an interpretation where quantum states are more like states of nature than states of knowledge—might be tempted to believe that the scarcity of existing analyses of this kind is a hint that quantum states do indeed have some sort of objective status. Why would such currency be made of the unknown-state concept were it not absolutely necessary? As a rejoinder, we advise caution to the objectivist: Tempting though it is to grant objective status to all the mathematical objects in a physical theory, there is much to be gained by a careful delineation of the subjective and objective parts. A case in point is provided by E. T. Jaynes'[18–20] insistence that entropy is a subjective quantity, a measure of ignorance about a physical system. One of the many fruits of this point of view can be found in the definitive solution[21] to the long-standing Maxwell demon problem,[22] where it was realized that the information collected by a demon and used by it to extract work from heat has a thermodynamic cost at least as large as the work extracted.[23]

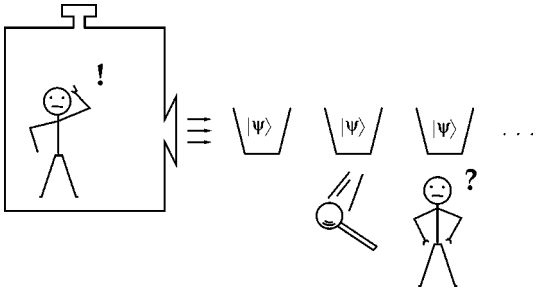

FIG. 2. To make sense of quantum tomography, must we go to the extreme of imagining a ''man in the box'' who has a better description of the systems than we do? How contrived our usage would be if that were so!

The example analyzed in detail in this article provides another case. Along the way, it brings to light a new and distinct point about why quantum mechanics makes use of complex Hilbert spaces rather than real or quaternionic ones.[24–27] Furthermore, the method we use to prove our main theorem employs a novel measurement technique that might be of use in the laboratory.

We analyze in depth a particular use of unknown states, which comes from the measurement technique known as *quantum-state tomography*.[28–30] The usual description of tomography is this. A device of some sort, say a nonlinear optical medium driven by a laser, repeatedly prepares many instances of a quantum system, say many temporally distinct modes of the electromagnetic field, in a fixed quantum state ρ, pure or mixed. An experimentalist who wishes to characterize the operation of the device or to calibrate it for future use might be able to perform measurements on the systems it prepares even if he cannot get at the device itself. This can be useful if the experimenter has some prior knowledge of the device's operation that can be translated into a probability distribution over states. Then learning about the state will also be learning about the device. Most importantly, though, this description of tomography assumes that the precise state ρ is unknown. The goal of the experimenter is to perform enough measurements, and enough kinds of measurements (on a large enough sample), to estimate the identity of ρ.

This is clearly an example where there is no further player on whom to pin the unknown state as a state of knowledge. Any attempt to find a player for the pin is entirely artificial: Where would the player be placed? On the inside of the device the tomographer is trying to characterize?[31] The only available course for an information-based interpretation of quantum-state tomography is the second strategy listed above—to banish completely the idea of the unknown state from the formulation of tomography (see Fig. 2).

To do this, we take a cue from the field of Bayesian probability theory,[32–34] prompted by the realization that Bayesian probability is to probability theory in general what an information-based interpretation is to quantum mechanics.[3,35] In Bayesian theory, probabilities are not objective states of nature, but rather are taken explicitly to be measures of credible belief, reflecting one's state of knowledge. The overarching Bayesian theme is to identify the conditions under which a set of decision-making agents can come to a common belief or probability assignment for a random variable even though their initial beliefs differ.[34] Following that theme is the key to understanding tomography from the informational point of view.

The offending classical concept is an ''unknown probability,'' an oxymoron for the same reason as an unknown quantum state. The procedure analogous to quantum-state tomography is the estimation of an unknown probability from the results of repeated trials on ''identically prepared systems,'' all of which are said to be described by the same, but unknown probability. The way to eliminate unknown probabilities from the discussion, introduced by Bruno de Finetti in the early 1930s,[36,37] is to focus on the equivalence of repeated trials, which means that the systems are indistinguishable as far as probabilistic predictions are concerned and thus that a probability assignment for multiple trials should be symmetric under permutation of the systems. With his *classical representation theorem*, de Finetti[36] showed that a multi-trial probability assignment that is permutation-symmetric for an arbitrarily large number of trials—de Finetti called such multi-

trial probabilities *exchangeable*—is equivalent to a probability for the ''unknown probabilities.'' Thus the unsatisfactory concept of an unknown probability vanishes from the description in favor of the fundamental idea of assigning an exchangeable probability distribution to multiple trials.

This cue in hand, it is easy to see how to reword the description of quantum-state tomography to meet our goals. What is relevant is simply a judgment on the part of the experimenter—notice the essential subjective character of this ''judgment''—that there is no distinction between the systems the device is preparing. In operational terms, this is the judgment that *all the systems are and will be the same as far as observational predictions are concerned*. At first glance this statement might seem to be contentless, but the important point is this: To make this statement, one need never use the notion of an unknown state—a completely operational description is good enough. Putting it into technical terms, the statement is that if the experimenter judges a collection of N of the device's outputs to have an overall quantum state $\rho^{(N)}$, he will also judge any permutation of those outputs to have the same quantum state $\rho^{(N)}$. Moreover, he will do this no matter how large the number N is. This, complemented only by the consistency condition that for any N the state $\rho^{(N)}$ be derivable from $\rho^{(N+1)}$, makes for the complete story.

The words ''quantum state'' appear in this formulation, just as in the original formulation of tomography, but there is no longer any mention of *unknown* quantum states. The state $\rho^{(N)}$ is known by the experimenter (if no one else), for it represents his state of knowledge. More importantly, the experimenter is in a position to make an unambiguous statement about the structure of the whole sequence of states $\rho^{(N)}$: Each of the states $\rho^{(N)}$ has a kind of permutation invariance over its factors. The content of the *quantum de Finetti representation theorem*[38,39]—a new proof of which is the main technical result of this article—is that a sequence of states $\rho^{(N)}$ can have these properties, which are said to make it an *exchangeable* sequence, if and only if each term in it can also be written in the form

$$\rho^{(N)}=\int P(\rho)\,\rho^{\otimes N}\,d\rho, \tag{1.1}$$

where

$$\rho^{\otimes N}=\underbrace{\rho\otimes\rho\otimes\cdots\otimes\rho}_{\substack{N\text{-fold tensor}\\ \text{product}}} \tag{1.2}$$

and $P(\rho)$ is a fixed probability distribution over the density operators.

The interpretive import of this theorem is paramount. It alone gives a mandate to the term unknown state in the usual description of tomography. It says that the experimenter can act *as if* his state of knowledge $\rho^{(N)}$ comes about because he knows there is a ''man in the box,'' hidden from view, repeatedly preparing the same state ρ. He does not know which such state, and the best he can say about the unknown state is captured in the probability distribution $P(\rho)$.

The quantum de Finetti theorem furthermore makes a connection to the overarching theme of Bayesianism stressed above. It guarantees for two independent observers—as long as they have a rather minimal agreement in their initial beliefs—that the outcomes of a sufficiently informative set of measurements will force a convergence in their state assignments for the remaining systems.[40] This ''minimal'' agreement is characterized by a judgment on the part of both parties that the sequence of systems is exchangeable, as described above, and a promise that the observers are not absolutely inflexible in their opinions. Quantitatively, the latter means that though $P(\rho)$ might be arbitrarily close to zero, it can never vanish.

This coming to agreement works because an exchangeable density operator sequence can be updated to reflect information gathered from measurements by a quantum version of Bayes's rule for updating probabilities. Specifically, if measurements on K systems yield results D_K, then the state of additional systems is constructed as in Eq. (1.1), but using an updated probability on density operators given by

$$P(\rho|D_K)=\frac{P(D_K|\rho)P(\rho)}{P(D_K)}. \tag{1.3}$$

Here $P(D_K|\rho)$ is the probability to obtain the measurement results D_K, given the state $\rho^{\otimes K}$ for the K measured systems, and

$$P(D_K)=\int P(D_K|\rho)\,P(\rho)\,d\rho \tag{1.4}$$

is the unconditional probability for the measurement results. Equation (1.3) is a kind of *quantum Bayes rule*.[40] For a sufficiently informative set of measurements, as K becomes large, the updated probability $P(\rho|D_K)$ becomes highly peaked on a particular state ρ_{D_K} dictated by the measurement results, regardless of the prior probability $P(\rho)$, as long as $P(\rho)$ is nonzero in a neighborhood of ρ_{D_K}. Suppose the two observers have different initial beliefs, encapsulated in different priors $P_i(\rho)$, $i=1,2$. The measurement results force them to a common state of knowledge in which any number N of additional systems are assigned the product state $\rho_{D_K}^{\otimes N}$, i.e.,

$$\int P_i(\rho|D_K)\rho^{\otimes N}\,d\rho\rightarrow\rho_{D_K}^{\otimes N}, \tag{1.5}$$

independent of i, for K sufficiently large.

This shifts the perspective on the purpose of quantum-state tomography: It is not about uncovering some ''unknown state of nature,'' but rather about the various observers' coming to agreement over future probabilistic predictions.[41] In this connection, it is interesting to note that the quantum de Finetti theorem and the conclusions just drawn from it work only within the framework of complex vector-space quantum mechanics. For quantum mechanics based on real and quaternionic Hilbert spaces,[24,25] the connection between exchangeable density operators and unknown quantum states does not hold.

The plan of the remainder of the article is as follows. In Sec. II we discuss the classical de Finetti representation theorem[36,42] in the context of Bayesian probability theory. It was our familiarity with the classical theorem[43,44] that motivated our reconsideration of quantum-state tomography. In Sec. III we introduce the information-based formulation of tomography in terms of exchangeable multi-system density operators, accompanied by a critical discussion of the objectivist formulation of tomography, and we state the quantum de Finetti representation theorem. Section IV presents an elementary proof of the quantum de Finetti theorem. There, also, we introduce a novel measurement technique for tomography based upon generalized quantum measurements. Finally, in Sec. V we return to the issue of number fields in quantum mechanics and mention possible extensions of the main theorem.

II. THE CLASSICAL DE FINETTI THEOREM

As a preliminary to the quantum problem, we turn our attention to classical probability theory. In doing so we follow a maxim of the late E. T. Jaynes:[45]

> We think it unlikely that the role of probability in quantum theory will be understood until it is generally understood in classical theory ... . Indeed, our [seventy-five-year-old] bemusement over the notion of state reduction in [quantum theory] need not surprise us when we note that today, in all applications of probability theory, basically the same controversy rages over whether our probabilities represent real situations, or only incomplete human knowledge.

As Jaynes makes clear, the tension between the objectivist and informational points of view is not new with quantum mechanics. It arises already in classical probability theory in the form of the war between ''objective'' and ''subjective'' interpretations.[46] According to the subjective or Bayesian interpretation, probabilities are measures of credible belief, reflecting an agent's poten-

tial states of knowledge. On the other hand, the objective interpretations—in all their varied forms, from frequency interpretations to propensity interpretations—attempt to view probabilities as real states of affairs or "states of nature." Following our discussion in Sec. I, it will come as no surprise to the reader that the authors wholeheartedly adopt the Bayesian approach. For us, the ultimate reason is simply our own experience with this question, part of which is an appreciation that objective interpretations inevitably run into insurmountable difficulties. We will not dwell upon these difficulties here; instead, the reader can find a sampling of criticisms in Refs. 20, 32–34, and 47.

We will note briefly, however, that the game of roulette provides an illuminating example. In the European version of the game, the possible outcomes are the numbers 0,1,...,36. For a player without any privileged information, all 37 outcomes have the same probability $p=\frac{1}{37}$. But suppose that shortly after the ball is launched by the croupier, another player obtains information about the ball's position and velocity relative to the wheel. Using the information obtained, this other player can make more accurate predictions than the first.[48] His probability is peaked around some group of numbers. The probabilities are thus different for two players with different states of knowledge.

Whose probability is the true probability? From the Bayesian viewpoint, this question is meaningless: There is no such thing as a true probability. All probability assignments are subjective assignments based specifically upon one's prior information.

For sufficiently precise data—including precise initial data on positions and velocities and probably also including other details such as surface properties of the wheel—Newtonian mechanics assures us that the outcome can be predicted with certainty. This is an important point: The determinism of classical physics provides a strong reason for adopting the subjectivist view of probabilities.[49] If the conditions of a trial are exactly specified, the outcomes are predictable with certainty, and all probabilities are 0 or 1. In a deterministic theory, all probabilities strictly greater than 0 and less than 1 arise as a consequence of incomplete information and depend upon their assigner's state of knowledge.

Of course, we should keep in mind that our ultimate goal is to consider the status of quantum states and, by way of them, quantum probabilities. One can ask, "Does this not change the flavor of these considerations?" Since quantum mechanics is avowedly *not* a theory of one's ignorance of a set of hidden variables,[50,51] how can the probabilities be subjective? In Sec. III we argue that despite the intrinsic indeterminism of quantum mechanics, the essence of the point above carries over to the quantum setting intact. Furthermore, there are specifically quantum-motivated arguments for a Bayesian interpretation of quantum probabilities.

For the present, though, let us consider in some detail the general problem of a repeated experiment—spinning a roulette wheel N times is an example. As discussed briefly in Sec. I, this allows us to make a conceptual connection to quantum-state tomography. Here the individual trials are described by discrete random variables $x_n \in \{1,2,\ldots,k\}$, $n=1,\ldots,N$; that is to say, there are N random variables, each of which can assume k discrete values. In an objectivist theory, such an experiment has a standard formulation in which the probability in the multi-trial hypothesis space is given by an independent, identically distributed (i.i.d.) distribution

$$p(x_1,x_2,\ldots,x_N)=p_{x_1}p_{x_2}\cdots p_{x_N}=p_1^{n_1}p_2^{n_2}\cdots p_k^{n_k}. \tag{2.1}$$

The number p_j $(j=1,\ldots,k)$ describes the objective, "true" probability that the result of a single experiment will be j $(j=1,\ldots,k)$. The variable n_j, on the other hand, is the number of times outcome j is listed in the outcome vector $(x_1,x_2,\ldots,x_N)$. This simple description—for the objectivist—only describes the situation from a kind of "God's eye" point of view. To the experimentalist, the "true" probabilities $p_1,\ldots,p_k$ will very often be *unknown* at the outset. Thus, his burden is to estimate the unknown probabilities by a statistical analysis of the experiment's outcomes.

In the Bayesian approach, it does not make sense to talk about estimating a true probability. Instead, a Bayesian assigns a prior probability distribution $p(x_1,x_2,\ldots,x_N)$ on the multi-trial hypothesis space, which is generally not an i.i.d., and then uses Bayes's theorem to update the

distribution in the light of measurement results. A common criticism from the objectivist camp is that the choice of distribution $p(x_1,x_2,\ldots,x_N)$ with which to start the process seems overly arbitrary to them. On what can it be grounded, they would ask? From the Bayesian viewpoint, the subjectivity of the prior is a strength rather than a weakness, because assigning a prior amounts to laying bare the necessarily subjective assumptions behind *any* probabilistic argument, be it Bayesian or objectivist. Choosing a prior among all possible distributions on the multi-trial hypothesis space is, however, a daunting task. As we will now see, the de Finetti representation theorem makes this task tractable.

It is very often the case that one or more features of a problem stand out so clearly that there is no question about how to incorporate them into an initial assignment. In the present case, the key feature is contained in the assumption that an arbitrary number of repeated trials are equivalent. This means that one has no reason to believe there will be a difference between one trial and the next. In this case, the prior distribution is judged to have the sort of permutation symmetry discussed briefly in Sec. I, which de Finetti[37] called *exchangeability*. The rigorous definition of exchangeability proceeds in two stages.

A probability distribution $p(x_1,x_2,\ldots,x_N)$ is said to be *symmetric* (or finitely exchangeable) if it is invariant under permutations of its arguments, i.e., if

$$p(x_{\pi(1)},x_{\pi(2)},\ldots,x_{\pi(N)})=p(x_1,x_2,\ldots,x_N) \tag{2.2}$$

for any permutation π of the set $\{1,\ldots,N\}$. The distribution $p(x_1,x_2,\ldots,x_N)$ is called *exchangeable* (or infinitely exchangeable) if it is symmetric and if for any integer $M>0$, there is a symmetric distribution $p_{N+M}(x_1,x_2,\ldots,x_{N+M})$ such that

$$p(x_1,x_2,\ldots,x_N)=\sum_{x_{N+1},\ldots,x_{N+M}} p_{N+M}(x_1,\ldots,x_N,x_{N+1},\ldots,x_{N+M}). \tag{2.3}$$

This last statement means the distribution p can be extended to a symmetric distribution of arbitrarily many random variables. Expressed informally, an exchangeable distribution can be thought of as arising from an infinite sequence of random variables whose order is irrelevant.

We now come to the main statement of this section: If a probability distribution $p(x_1,x_2,\ldots,x_N)$ is exchangeable, then it can be written uniquely in the form

$$p(x_1,x_2,\ldots,x_N)=\int_{\mathcal{S}_k} P(\mathbf{p})p_{x_1}p_{x_2}\cdots p_{x_N}\,d\mathbf{p}=\int_{\mathcal{S}_k} P(\mathbf{p})p_1^{n_1}p_2^{n_2}\cdots p_k^{n_k}\,d\mathbf{p}, \tag{2.4}$$

where $\mathbf{p}=(p_1,p_2,\ldots,p_k)$, and the integral is taken over the probability simplex

$$\mathcal{S}_k=\left\{\mathbf{p}\colon p_j\geqslant 0 \ \text{ for all } \ j \ \text{ and } \ \sum_{j=1}^{k} p_j=1\right\}. \tag{2.5}$$

Furthermore, the function $P(\mathbf{p})\geqslant 0$ is required to be a probability density function on the simplex:

$$\int_{\mathcal{S}_k} P(\mathbf{p})d\mathbf{p}=1. \tag{2.6}$$

Equation (2.4) comprises the classical de Finetti representation theorem for discrete random variables. For completeness and because it deserves to be more widely familiar in the physics and mathematical physics communities, we give a simple proof (due to Heath and Sudderth[42]) of the representation theorem for the binary random-variable case in the Appendix.

Let us reiterate the importance of this result for the present considerations. It says that an agent, making solely the judgment of exchangeability for a sequence of random variables x_j, can proceed *as if* his state of knowledge had instead come about through ignorance of an *unknown*, but

objectively existent set of probabilities **p**. His precise ignorance of **p** is captured by the ''probability on probabilities'' $P(\mathbf{p})$. This is in direct analogy to what we desire of a solution to the problem of the unknown quantum state in quantum-state tomography.

As a final note before finally addressing the quantum problem in Sec. III, we point out that both conditions in the definition of exchangeability are crucial for the proof of the de Finetti theorem. In particular, there are probability distributions $p(x_1,x_2,\ldots,x_N)$ that are symmetric, but not exchangeable. A simple example is the distribution $p(x_1,x_2)$ of two binary random variables $x_1,x_2\in\{0,1\}$,

$$p(0,0)=p(1,1)=0, \tag{2.7}$$

$$p(0,1)=p(1,0)=\tfrac{1}{2}. \tag{2.8}$$

One can easily check that $p(x_1,x_2)$ cannot be written as the marginal of a symmetric distribution of three variables, as in Eq. (2.3). Therefore it can have no representation along the lines of Eq. (2.4). (For an extended discussion of this, see Ref. 52.) Indeed, Eqs. (2.7) and (2.8) characterize a perfect ''anticorrelation'' of the two variables, in contrast to the positive correlation implied by distributions of de Finetti form. The content of this point is that both conditions in the definition of exchangeability (symmetry under interchange and infinite extendibility) are required to ensure, in colloquial terms, ''that the future will appear much as the past,'' [53] rather than, say, the opposite of the past.

III. THE QUANTUM DE FINETTI REPRESENTATION

Let us now return to the problem of quantum-state tomography described in Sec. I. We consider the general situation, where there may be no further agent (or ''man in the box'') whose (unknown) state of knowledge we are trying to determine.

In the objectivist formulation of the problem, a device repeatedly prepares copies of a system in the same quantum state ρ. This is generally a mixed-state density operator on a Hilbert space $\mathcal{H}_d$ of d dimensions; we denote the space of all such density operators by $\mathcal{D}_d$. The joint quantum state of the N systems prepared by the device is then given by

$$\rho^{\otimes N}=\rho\otimes\rho\otimes\cdots\rho, \tag{3.1}$$

the N-fold tensor product of ρ with itself. This, of course, is a very restricted example of a density operator on the tensor-product Hilbert space $\mathcal{H}_d^{\otimes N}\equiv\mathcal{H}_d\otimes\cdots\otimes\mathcal{H}_d$. The experimenter who performs quantum-state tomography tries to determine ρ as precisely as possible; ρ is interpreted as the ''true'' state of each of the systems.

We have already articulated our dissatisfaction with this way of stating the problem, but we give here a further sense of why the interpretation above is untenable. In this discussion it is useful to consider separately the cases of mixed and pure states ρ. The arguments against regarding mixed states as objective properties of a quantum system are essentially the same as those against regarding probabilities as objective. In analogy to the roulette example given in the previous section, we can say that, whenever an observer assigns a mixed state to a physical system, one can think of another observer who assigns a different state based on privileged information.

The quantum argument becomes yet more compelling if the apparently nonlocal nature of quantum states is taken into consideration. Consider two parties, A and B, who are far apart in space, say several light years apart. Each party possesses a spin-$\frac{1}{2}$ particle. Initially the joint state of the two particles is the maximally entangled pure state $(|0\rangle|0\rangle+|1\rangle|1\rangle)/\sqrt{2}$. Consequently, A assigns the totally mixed state $(|0\rangle\langle 0|+|1\rangle\langle 1|)/2$ to her own particle. Now B makes a measurement on his particle, finds the result 0, and assigns to A's particle the pure state $|0\rangle$. Is this now the ''true,'' objective state of A's particle? At what precise time does the objective state of A's particle change from totally mixed to pure? If the answer is ''simultaneously with B's measurement,'' then what frame of reference should be used to determine simultaneity? These questions

and potential paradoxes are avoided if states are interpreted as states of knowledge. In our example, A and B have different states of knowledge and therefore assign different states. For a detailed analysis of this example, see Ref. 54; for an experimental investigation see Ref. 55.

If one admits that mixed states cannot be objective properties, because another observer, possessing privileged information, can know which pure state underlies the mixed state, then it becomes very tempting to regard the pure states as giving the ''true'' state of a system. Probabilities that come from pure states would then be regarded as objective, and the probabilities for pure states within an ensemble decomposition of a mixed state would be regarded as subjective, expressing our ignorance of which pure state is the ''true'' state of the system. An immediate and, in our view, irremediable problem with this idea is that a mixed state has infinitely many ensemble decompositions into pure states,[19,56,57] so the distinction between subjective and objective becomes hopelessly blurred.

This problem can be made concrete by the example of a spin-$\frac{1}{2}$ particle. Any pure state of the particle can be written in terms of the Pauli matrices,

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \tag{3.2}$$

as

$$|\mathbf{n}\rangle\langle\mathbf{n}|=\tfrac{1}{2}(I+\mathbf{n}\cdot\boldsymbol{\sigma})=\tfrac{1}{2}(I+n_1\sigma_1+n_2\sigma_2+n_3\sigma_3), \tag{3.3}$$

where the unit vector $\mathbf{n}=n_1\mathbf{e}_1+n_2\mathbf{e}_2+n_3\mathbf{e}_3$ labels the pure state, and I denotes the unit operator. An arbitrary state ρ, mixed or pure, of the particle can be expressed as

$$\rho=\tfrac{1}{2}(I+\mathbf{S}\cdot\boldsymbol{\sigma}), \tag{3.4}$$

where $0\leqslant|\mathbf{S}|\leqslant 1$. This representation of the states of a spin-$\frac{1}{2}$ particle is called the *Bloch-sphere representation*. If $|\mathbf{S}|<1$, there is an infinite number of ways in which $\mathbf{S}$ can be written in the form $\mathbf{S}=\Sigma_j p_j\mathbf{n}_j$, $|\mathbf{n}_j|=1$, with the numbers p_j comprising a probability distribution, and hence an infinite number of ensemble decompositions of ρ:

$$\rho=\sum_j\, p_j\frac{1}{2}(I+\mathbf{n}_j\cdot\boldsymbol{\sigma})=\sum_j\, p_j|\mathbf{n}_j\rangle\langle\mathbf{n}_j|. \tag{3.5}$$

Suppose for specificity that the particle's state is a mixed state with $\mathbf{S}=\frac{1}{2}\mathbf{e}_3$. Writing $\mathbf{S}=\frac{3}{4}\mathbf{e}_3+\frac{1}{4}(-\mathbf{e}_3)$ gives the eigendecomposition,

$$\rho=\tfrac{3}{4}|\mathbf{e}_3\rangle\langle\mathbf{e}_3|+\tfrac{1}{4}|-\mathbf{e}_3\rangle\langle-\mathbf{e}_3|, \tag{3.6}$$

where we are to regard the probabilities $\frac{3}{4}$ and $\frac{1}{4}$ as subjective expressions of ignorance about which eigenstate is the ''true'' state of the particle. Writing $\mathbf{S}=\frac{1}{2}\mathbf{n}_+ +\frac{1}{2}\mathbf{n}_-$, where $\mathbf{n}_\pm=\frac{1}{2}\mathbf{e}_3\pm\sqrt{3/4}\mathbf{e}_1$, gives another ensemble decomposition,

$$\rho=\tfrac{1}{2}|\mathbf{n}_+\rangle\langle\mathbf{n}_+|+\tfrac{1}{2}|\mathbf{n}_-\rangle\langle\mathbf{n}_-|, \tag{3.7}$$

where we are now to regard the two probabilities of $\frac{1}{2}$ as expressing ignorance of whether the ''true'' state is $|\mathbf{n}_+\rangle$ or $|\mathbf{n}_-\rangle$.

The problem becomes acute when we ask for the probability that a measurement of the z component of spin yields spin up; this probability is given by $\langle\mathbf{e}_3|\rho|\mathbf{e}_3\rangle=\frac{1}{2}(1+\frac{1}{2}\langle\mathbf{e}_3|\sigma_3|\mathbf{e}_3\rangle)=\frac{3}{4}$. The eigendecomposition gets this probability by the route

$$\langle \mathbf{e}_3|\rho|\mathbf{e}_3\rangle = \frac{3}{4}\underbrace{|\langle \mathbf{e}_3|\mathbf{e}_3\rangle|^2}_{1} + \frac{1}{4}\underbrace{|\langle \mathbf{e}_3|-\mathbf{e}_3\rangle|^2}_{0}. \tag{3.8}$$

Here the "objective" quantum probabilities, calculated from the eigenstates, report that the particle definitely has spin up or definitely has spin down; the overall probability of $\frac{3}{4}$ comes from mixing these objective probabilities with the subjective probabilities for the eigenstates. The decomposition (3.7) gets the same overall probability by a different route,

$$\langle \mathbf{e}_3|\rho|\mathbf{e}_3\rangle = \frac{1}{2}\underbrace{|\langle \mathbf{e}_3|\mathbf{n}_+\rangle|^2}_{3/4} + \frac{1}{2}\underbrace{|\langle \mathbf{e}_3|\mathbf{n}_-\rangle|^2}_{3/4}. \tag{3.9}$$

Now the quantum probabilities tell us that the "objective" probability for the particle to have spin up is $\frac{3}{4}$. This simple example illustrates the folly of trying to have two kinds of probabilities in quantum mechanics. The lesson is that if a density operator is even partially a reflection of one's state of knowledge, the multiplicity of ensemble decomposition means that a pure state must also be a state of knowledge.

These problems do not arise in an information-based interpretation, according to which all quantum states, pure or mixed, are states of knowledge. In analogy to the classical case, the quantum de Finetti representation provides an operational definition for the idea of an unknown quantum state in this case.

Let us therefore turn to the information-based formulation of the quantum-state tomography problem. Before the tomographic measurements, the Bayesian experimenter assigns a prior quantum state to the joint system composed of the N systems, reflecting his prior state of knowledge. Just as in the classical case, this is a daunting task unless the assumption of exchangeability is justified.

The definition of the quantum version of exchangeability is closely analogous to the classical definition. Again, the definition proceeds in two stages. First, a joint state $\rho^{(N)}$ of N systems is said to be *symmetric* (or finitely exchangeable) if it is invariant under any permutation of the systems. To see what this means formally, first write out $\rho^{(N)}$ with respect to any orthonormal tensor-product basis on $\mathcal{H}_d^{\otimes N}$, say $|i_1\rangle|i_2\rangle\cdots|i_N\rangle$, where $i_k \in \{1,2,\ldots,d\}$ for all k. The joint state takes the form

$$\rho^{(N)} = \sum_{i_1,\ldots,i_N;j_1,\ldots,j_N} R^{(N)}_{i_1,\ldots,i_N;j_1,\ldots,j_N} |i_1\rangle\cdots|i_N\rangle\langle j_1|\cdots\langle j_N|, \tag{3.10}$$

where $R^{(N)}_{i_1,\ldots,i_N;j_1,\ldots,j_N}$ is the density matrix in this representation. What we demand is that for any permutation π of the set $\{1,\ldots,N\}$,

$$\begin{aligned}\rho^{(N)} &= \sum_{i_1,\ldots,i_N;j_1,\ldots,j_N} R^{(N)}_{i_1,\ldots,i_N;j_1,\ldots,j_N} |i_{\pi^{-1}(1)}\rangle\cdots|i_{\pi^{-1}(N)}\rangle\langle j_{\pi^{-1}(1)}|\cdots\langle j_{\pi^{-1}(N)}| \\ &= \sum_{i_1,\ldots,i_N;j_1,\ldots,j_N} R^{(N)}_{i_{\pi(1)},\ldots,i_{\pi(N)};j_{\pi(1)},\ldots,j_{\pi(N)}} |i_1\rangle\cdots|i_N\rangle\langle j_1|\cdots\langle j_N|,\end{aligned} \tag{3.11}$$

which is equivalent to

$$R^{(N)}_{i_{\pi(1)},\ldots,i_{\pi(N)};j_{\pi(1)},\ldots,j_{\pi(N)}} = R^{(N)}_{i_1,\ldots,i_N;j_1,\ldots,j_N}. \tag{3.12}$$

The state $\rho^{(N)}$ is said to be *exchangeable* (or infinitely exchangeable) if it is symmetric and if, for any $M>0$, there is a symmetric state $\rho^{(N+M)}$ of $N+M$ systems such that the marginal density operator for N systems is $\rho^{(N)}$, i.e.,

$$\rho^{(N)} = \mathrm{tr}_M \rho^{(N+M)}, \tag{3.13}$$

where the trace is taken over the additional M systems. In explicit basis-dependent notation, this requirement is

$$\rho^{(N)} = \sum_{i_1,\ldots,i_N;j_1,\ldots,j_N} \left(\sum_{i_{N+1},\ldots,i_{N+M}} R^{(N+M)}_{i_1,\ldots,i_N,i_{N+1},\ldots,i_{N+M};j_1,\ldots,j_N,i_{N+1},\ldots,i_{N+M}} \right) \times |i_1\rangle\cdots|i_N\rangle\langle j_1|\cdots\langle j_N|. \tag{3.14}$$

In analogy to the classical case, an exchangeable density operator can be thought of informally as the description of a subsystem of an infinite sequence of systems whose order is irrelevant.

The precise statement of the quantum de Finetti representation theorem[38,58] is that any exchangeable state of N systems can be written uniquely in the form

$$\rho^{(N)} = \int_{\mathcal{D}_d} P(\rho)\, \rho^{\otimes N}\, d\rho. \tag{3.15}$$

Here $P(\rho) \geqslant 0$ is normalized by

$$\int_{\mathcal{D}_d} P(\rho)\, d\rho = 1, \tag{3.16}$$

with $d\rho$ being a suitable measure on density operator space $\mathcal{D}_d$ [e.g., for a spin-$\frac{1}{2}$ particle, one could choose the standard flat measure $d\rho = S^2 dS\, d\Omega$ in the parametrization (3.4)]. The upshot of the theorem, as already advertised, is that it makes it possible to think of an exchangeable quantum-state assignment *as if* it were a probabilistic mixture characterized by a probability density $P(\rho)$ for the product states $\rho^{\otimes N}$.

Just as in the classical case, both components of the definition of exchangeability are crucial for arriving at the representation theorem of Eq. (3.15). The reason now, however, is much more interesting than it was previously. In the classical case, extendibility served to exclude symmetric, but anticorrelated probability distributions. Here extendibility has the additional role of excluding the possibility of Bell inequality violations for measurements on the separate systems. This is because the assumption of symmetry alone for an N-party quantum system does not exclude the possibility of quantum entanglement, yet all states that can be written as a mixture of product states—Eq. (3.15) being an example—have no entanglement.[59]

A very simple example of this is the Greenberger–Horne–Zeilinger state of three spin-$\frac{1}{2}$ particles,[60]

$$|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|0\rangle|0\rangle|0\rangle + |1\rangle|1\rangle|1\rangle), \tag{3.17}$$

which is symmetric, but is not extendible to a symmetric state on four systems. This follows because the only states of four particles that marginalize to a three-particle pure state, like the GHZ state, are product states of the form $|\mathrm{GHZ}\rangle\langle\mathrm{GHZ}| \otimes \rho$, where ρ is the state of the fourth particle; such states clearly cannot be symmetric. These considerations show that in order for the proposed theorem to be valid, it must be the case that as M increases in Eq. (3.13), the possibilities for entanglement in the separate systems compensatingly decrease.[61]

The exclusion of entangled states from the set of exchangeable states is essential if we are to substitute exchangeable state assignments for the offending notion of an unknown quantum state. For if an exchangeable density operator could be entangled, it would be impossible even to talk about the separate systems as having states of their own, unknown or otherwise. We stress, however, that this exclusion does not mean that the information-based view of quantum states as states of knowledge is incapable of dealing with entangled states, since the systems in the de

Finetti representation could each be made up of parts that are entangled. In this case the de Finetti representation integral (3.15) would include entangled density operators from the space of single-system, but many-part, density operators, and the unknown quantum state could be entangled. What is excluded by exchangeability is entanglement among the systems that are deemed to be exchangeable.

IV. PROOF OF THE QUANTUM DE FINETTI THEOREM

To prove the quantum version of the de Finetti theorem, we rely on the classical theorem as much as possible. We start from an exchangeable density operator $\rho^{(N)}$ defined on N copies of a system. We bring the classical theorem to our aid by imagining a sequence of identical quantum measurements on the separate systems and considering the outcome probabilities they would produce. Because $\rho^{(N)}$ is assumed exchangeable, such identical measurements give rise to an exchangeable probability distribution for the outcomes. The trick is to recover enough information from the exchangeable statistics of these measurements to characterize the exchangeable density operators.

With this in mind, the proof is expedited by making use of the theory of generalized quantum measurements or positive operator-valued measures (POVMs).[62,63] We give a brief introduction to that theory. The common textbook notion of a measurement—that is, a von Neumann measurement—is that any laboratory procedure counting as an observation can be identified with a Hermitian operator O on the Hilbert space $\mathcal{H}_d$ of the system. Depending upon the presentation, the measurement outcomes are identified either with the eigenvalues μ_i or with a complete set of normalized eigenvectors $|i\rangle$ for O. When the quantum state is ρ, the probabilities for the various outcomes are computed from the eigenprojectors $\Pi_i=|i\rangle\langle i|$ via the standard Born rule,

$$p_i=\mathrm{tr}(\rho\Pi_i)=\langle i|\rho|i\rangle. \tag{4.1}$$

This rule gives a consistent probability assignment because the eigenprojectors Π_i are positive-semidefinite operators, which makes the p_i non-negative, and because the projectors form a resolution of the identity operator I,

$$\sum_{i=1}^{d}\Pi_i=I, \tag{4.2}$$

which guarantees that $\Sigma_i p_i=1$.

POVMs generalize the textbook notion of measurement by distilling the essential properties that make the Born rule work. The generalized notion of measurement is this: *Any* set $\mathcal{E}=\{E_\alpha\}$ of positive-semidefinite operators on $\mathcal{H}_d$ that forms a resolution of the identity, i.e., that satisfies

$$\langle\psi|E_\alpha|\psi\rangle\geqslant 0 \quad \text{for all } |\psi\rangle\in\mathcal{H}_d \tag{4.3}$$

and

$$\sum_\alpha E_\alpha=I, \tag{4.4}$$

corresponds to at least one laboratory procedure counting as a measurement. The condition (4.3) for positive-semidefiniteness is equivalent to requiring that E_α be Hermitian with nonnegative eigenvalues. The outcomes of the measurement are identified with the indices α, and the probabilities of those outcomes are computed according to the generalized Born rule,

$$p_\alpha=\mathrm{tr}(\rho E_\alpha). \tag{4.5}$$

The set $\mathcal{E}$ is called a POVM, and the operators E_α are called POVM elements. Unlike von Neumann measurements, there is no limitation on the number of values α can take, the operators

E_α need not be rank-1, and there is no requirement that the E_α be mutually orthogonal. This definition has important content because the older notion of measurement is simply too restrictive: There are laboratory procedures that clearly should be called ''measurements,'' but that cannot be expressed in terms of the von Neumann measurement process alone.

One might wonder whether the existence of POVMs contradicts everything taught about standard measurements in the traditional graduate textbooks[64] and the well-known classics.[65] Fortunately it does not. The reason is that any POVM can be represented formally as a standard measurement on an ancillary system that has interacted in the past with the system of main interest. Thus, in a certain sense, von Neumann measurements capture everything that can be said about quantum measurements.[63] A way to think about this is that by learning something about the ancillary system through a standard measurement, one in turn learns something about the system of real interest. Indirect though this might seem, it can be a very powerful technique, sometimes revealing information that could not have been revealed otherwise.[66]

For instance, by considering POVMs, one can consider measurements with an outcome cardinality that exceeds the dimensionality of the Hilbert space. What this means is that whereas the statistics of a von Neumann measurement can only reveal information about the d diagonal elements of a density operator ρ, through the probabilities $\mathrm{tr}(\rho\Pi_i)$, the statistics of a POVM generally can reveal things about the off-diagonal elements, too. It is precisely this property that we take advantage of in our proof of the quantum de Finetti theorem.

Our problem hinges on finding a special kind of POVM, one for which any set of outcome probabilities specifies a unique operator. This boils down to a problem in pure linear algebra. The space of operators on $\mathcal{H}_d$ is itself a linear vector space of dimension d^2. The quantity $\mathrm{tr}(A^\dagger B)$ serves as an inner product on that space. If the POVM elements E_α span the space of operators—there must be at least d^2 POVM elements in the set—the measurement probabilities $p_\alpha = \mathrm{tr}(\rho E_\alpha)$—now thought of as *projections* in the directions E_α—are sufficient to specify a unique operator ρ. Two distinct density operators ρ and σ must give rise to different measurement statistics. Such measurements, which might be called *informationally complete*, have been studied for some time.[67]

For our proof we need a slightly refined notion—that of a *minimal* informationally complete measurement. If an informationally complete POVM has more than d^2 operators E_α, these operators form an overcomplete set. This means that given a set of outcome probabilities p_α, there is generally *no* operator A that generates them according to $p_\alpha = \mathrm{tr}(AE_\alpha)$. Our proof requires the existence of such an operator, so we need a POVM that has precisely d^2 linearly independent POVM elements E_α. Such a POVM has the minimal number of POVM elements to be informationally complete. Given a set of outcome probabilities p_α, there is a unique operator A such that $p_\alpha = \mathrm{tr}(AE_\alpha)$, even though, as we discuss below, A is not guaranteed to be a density operator.

Do minimal informationally complete POVMs exist? The answer is yes. We give here a simple way to produce one, though there are surely more elegant ways with greater symmetry. Start with a complete orthonormal basis $|e_j\rangle$ on $\mathcal{H}_d$, and let $\Gamma_{jk} = |e_j\rangle\langle e_k|$. It is easy to check that the following d^2 rank-1 projectors Π_α form a linearly independent set.

(1) For $\alpha = 1,\ldots,d$, let

$$\Pi_\alpha \equiv \Gamma_{jj}, \tag{4.6}$$

where j, too, runs over the values $1,\ldots,d$.

(2) For $\alpha = d+1,\ldots,\frac{1}{2}d(d+1)$, let

$$\Pi_\alpha \equiv \Gamma^{(1)}_{jk} = \tfrac{1}{2}(|e_j\rangle + |e_k\rangle)(\langle e_j| + \langle e_k|) = \tfrac{1}{2}(\Gamma_{jj} + \Gamma_{kk} + \Gamma_{jk} + \Gamma_{kj}), \tag{4.7}$$

where $j < k$.

(3) Finally, for $\alpha = \frac{1}{2}d(d+1)+1,\ldots,d^2$, let

$$\Pi_\alpha \equiv \Gamma^{(2)}_{jk} = \tfrac{1}{2}(|e_j\rangle + i|e_k\rangle)(\langle e_j| - i\langle e_k|) = \tfrac{1}{2}(\Gamma_{jj} + \Gamma_{kk} - i\Gamma_{jk} + i\Gamma_{kj}), \tag{4.8}$$

where again $j<k$.

All that remains is to transform these (positive-semidefinite) linearly independent operators Π_α into a proper POVM. This can be done by considering the positive semidefinite operator G defined by

$$G = \sum_{\alpha=1}^{d^2} \Pi_\alpha . \tag{4.9}$$

It is straightforward to show that $\langle\psi|G|\psi\rangle > 0$ for all $|\psi\rangle \neq 0$, thus establishing that G is positive definite (i.e., Hermitian with positive eigenvalues) and hence invertible. Applying the (invertible) linear transformation $X \to G^{-1/2} X G^{-1/2}$ to Eq. (4.9), we find a valid decomposition of the identity,

$$I = \sum_{\alpha=1}^{d^2} G^{-1/2} \Pi_\alpha G^{-1/2}. \tag{4.10}$$

The operators

$$E_\alpha = G^{-1/2} \Pi_\alpha G^{-1/2} \tag{4.11}$$

satisfy the conditions of a POVM, Eqs. (4.3) and (4.4), and, moreover, they retain the rank and linear independence of the original Π_α.

With this generalized measurement (or any other one like it), we can return to the main line of proof. Recall we assumed that we captured our state of knowledge by an exchangeable density operator $\rho^{(N)}$. Consequently, repeated application of the (imagined) measurement $\mathcal{E}$ must give rise to an exchangeable probability distribution over the N random variables $\alpha_n \in \{1,2,\ldots,d^2\}$, $n = 1,\ldots,N$. We now analyze these probabilities.

Quantum mechanically, it is valid to think of the N repeated measurements of $\mathcal{E}$ as a single measurement on the Hilbert space $\mathcal{H}_d^{\otimes N} \equiv \mathcal{H}_d \otimes \cdots \otimes \mathcal{H}_d$. This measurement, which we denote $\mathcal{E}^{\otimes N}$, consists of d^{2N} POVM elements of the form $E_{\alpha_1} \otimes \cdots \otimes E_{\alpha_N}$. The probability of any particular outcome sequence of length N, namely $\boldsymbol{\alpha} \equiv (\alpha_1,\ldots,\alpha_N)$, is given by the standard quantum rule,

$$p^{(N)}(\boldsymbol{\alpha}) = \mathrm{tr}(\rho^{(N)} E_{\alpha_1} \otimes \cdots \otimes E_{\alpha_N}). \tag{4.12}$$

Because the distribution $p^{(N)}(\boldsymbol{\alpha})$ is exchangeable, we have by the classical de Finetti theorem [see Eq. (2.4)] that there exists a unique probability density $P(\mathbf{p})$ on $\mathcal{S}_{d^2}$ such that

$$p^{(N)}(\boldsymbol{\alpha}) = \int_{\mathcal{S}_{d^2}} P(\mathbf{p}) p_{\alpha_1} p_{\alpha_2} \cdots p_{\alpha_N} \, d\mathbf{p}, \tag{4.13}$$

where the integral runs over the probability simplex for d^2 outcomes.

It should now begin to be apparent why we chose to imagine a measurement $\mathcal{E}$ consisting of precisely d^2 linearly independent elements. This allows us to assert the existence of a *unique* operator $A_{\mathbf{p}}$ on $\mathcal{H}_d$ corresponding to each point $\mathbf{p}$ in the domain of the integral. The ultimate goal here is to turn Eqs. (4.12) and (4.13) into a single operator equation.

With that in mind, let us define $A_{\mathbf{p}}$ as the unique operator satisfying the following d^2 linear equations:

$$\mathrm{tr}(A_{\mathbf{p}} E_\alpha) = p_\alpha , \quad \alpha = 1,\ldots,d^2. \tag{4.14}$$

Inserting this definition into Eq. (4.13) and manipulating it according to the algebraic rules of tensor products—namely $(A\otimes B)(C\otimes D)=AC\otimes BD$ and $\mathrm{tr}(A\otimes B)=(\mathrm{tr}A)(\mathrm{tr}B)$—we see that

$$p^{(N)}(\boldsymbol{\alpha})=\int_{\mathcal{S}_{d^2}} P(\mathbf{p})\mathrm{tr}(A_{\mathbf{p}}E_{\alpha_1})\cdots\mathrm{tr}(A_{\mathbf{p}}E_{\alpha_N})d\mathbf{p}$$
$$=\int_{\mathcal{S}_{d^2}} P(\mathbf{p})\mathrm{tr}(A_{\mathbf{p}}E_{\alpha_1}\otimes\cdots\otimes A_{\mathbf{p}}E_{\alpha_N})d\mathbf{p}=\int_{\mathcal{S}_{d^2}} P(\mathbf{p})\mathrm{tr}[A_{\mathbf{p}}^{\otimes N}(E_{\alpha_1}\otimes\cdots\otimes E_{\alpha_N})]\,d\mathbf{p}. \tag{4.15}$$

If we further use the linearity of the trace, we can write the same expression as

$$p^{(N)}(\boldsymbol{\alpha})=\mathrm{tr}\left[\left(\int_{\mathcal{S}_{d^2}} P(\mathbf{p})A_{\mathbf{p}}^{\otimes n}\,d\mathbf{p}\right)E_{\alpha_1}\otimes\cdots\otimes E_{\alpha_N}\right]. \tag{4.16}$$

The identity between Eqs. (4.12) and (4.16) must hold for all sequences $\boldsymbol{\alpha}$. It follows that

$$\rho^{(N)}=\int_{\mathcal{S}_{d^2}} P(\mathbf{p})A_{\mathbf{p}}^{\otimes N}\,d\mathbf{p}. \tag{4.17}$$

This is because the operators $E_{\alpha_1}\otimes\cdots\otimes E_{\alpha_N}$ form a complete basis for the vector space of operators on $\mathcal{H}_d^{\otimes N}$.

Equation (4.17) already looks very much like our sought after goal, but we are not there quite yet. At this stage one has no right to assert that the $A_{\mathbf{p}}$ are density operators, i.e., Hermitian operators with non-negative eigenvalues that sum to one. Indeed they generally are not: The integral (4.13) ranges over some points $\mathbf{p}$ in $\mathcal{S}_{d^2}$ that cannot be generated by applying the measurement $\mathcal{E}$ to *any* quantum state. Hence some of the $A_{\mathbf{p}}$ in the integral representation are ostensibly nonphysical. An example might be helpful. Consider any four spin-$\frac{1}{2}$ pure states $|\mathbf{n}_\alpha\rangle$ on $\mathcal{H}_2$ for which the vectors $\mathbf{n}_\alpha$ in the Bloch-sphere representation (3.3) are the vertices of a regular tetrahedron. One can check that the elements $E_\alpha=\frac{1}{2}|\mathbf{n}_\alpha\rangle\langle\mathbf{n}_\alpha|$ comprise a minimal informationally complete POVM. For this POVM, because of the factor $\frac{1}{2}$ in front of each projector, it is always the case that $p_\alpha=\mathrm{tr}(\rho E_\alpha)\leqslant\frac{1}{2}$. Therefore, this measurement simply cannot generate a probability distribution like $\mathbf{p}=(\frac{3}{4},\frac{1}{8},\frac{1}{16},\frac{1}{16})$ from a valid density operator. Nevertheless, such probability distributions are in the domain of the integral in Eq. (4.13), and the corresponding $A_{\mathbf{p}}$ are not valid density operators.

The solution to this conundrum is provided by the overall requirement that $\rho^{(N)}$ be a valid density operator. This requirement places a significantly more stringent constraint on the distribution $P(\mathbf{p})$ than was the case in the classical representation theorem. In particular, it must be the case that $P(\mathbf{p})$ vanishes whenever the corresponding $A_{\mathbf{p}}$ is not a proper density operator. Let us move toward showing that.

We first need to delineate two properties of the operators $A_{\mathbf{p}}$. One is that they are Hermitian and thus have real eigenvalues. The argument is simply

$$\mathrm{tr}(E_\alpha A_{\mathbf{p}}^\dagger)=\mathrm{tr}[(A_{\mathbf{p}}E_\alpha)^\dagger]=[\mathrm{tr}(A_{\mathbf{p}}E_\alpha)]^*=\mathrm{tr}(A_{\mathbf{p}}E_\alpha), \tag{4.18}$$

where the last step follows from Eq. (4.14). Because the E_α are a complete set of linearly independent operators, it follows that $A_{\mathbf{p}}^\dagger=A_{\mathbf{p}}$. The second property tells us something further about the eigenvalues of $A_{\mathbf{p}}$:

$$1=\sum_\alpha p_\alpha=\mathrm{tr}\left(A_{\mathbf{p}}\sum_\alpha E_\alpha\right)=\mathrm{tr}A_{\mathbf{p}}. \tag{4.19}$$

In other words the (real) eigenvalues of $A_{\mathbf{p}}$ must sum to unity. These two properties tell us that if $A_{\mathbf{p}}$ is not a valid density operator, then it must have at least one negative eigenvalue.

We now show that these two facts go together to imply that if there are any nonphysical $A_{\mathbf{p}}$ with positive weight $P(\mathbf{p})$ in Eq. (4.17), then one can find a measurement for which $\rho^{(N)}$ produces illegal "probabilities" for sufficiently large N. For instance, take a particular $A_{\mathbf{q}}$ in Eq. (4.17) that has at least one negative eigenvalue $-\lambda<0$. Let $|\psi\rangle$ be a normalized eigenvector corresponding to that eigenvalue and consider the binary-valued POVM consisting of the elements $\widetilde{\Pi}=|\psi\rangle\langle\psi|$ and $\Pi=I-\widetilde{\Pi}$. Since $\mathrm{tr}(A_{\mathbf{q}}\widetilde{\Pi})=-\lambda<0$, it is true by Eq. (4.19) that $\mathrm{tr}(A_{\mathbf{q}}\Pi)=1+\lambda>1$. Consider repeating this measurement over and over. In particular, let us tabulate the probability of getting outcome Π for every single trial to the exclusion of all other outcomes.

The gist of the contradiction is most easily seen by *imagining* that Eq. (4.17) is really a discrete sum:

$$\rho^{(N)}=P(\mathbf{q})A_{\mathbf{q}}^{\otimes N}+\sum_{\mathbf{p}\neq\mathbf{q}}P(\mathbf{p})A_{\mathbf{p}}^{\otimes N}. \tag{4.20}$$

The probability of N occurrences of the outcome Π is thus

$$\begin{aligned}\mathrm{tr}(\rho^{(N)}\Pi^{\otimes N})&=P(\mathbf{q})\mathrm{tr}(A_{\mathbf{q}}^{\otimes N}\Pi^{\otimes N})+\sum_{\mathbf{p}\neq\mathbf{q}}P(\mathbf{p})\mathrm{tr}(A_{\mathbf{p}}^{\otimes N}\Pi^{\otimes N})\\&=P(\mathbf{q})[\mathrm{tr}(A_{\mathbf{q}}\Pi)]^N+\sum_{\mathbf{p}\neq\mathbf{q}}P(\mathbf{p})[\mathrm{tr}(A_{\mathbf{p}}\Pi)]^N\\&=P(\mathbf{q})(1+\lambda)^N+\sum_{\mathbf{p}\neq\mathbf{q}}P(\mathbf{p})[\mathrm{tr}(A_{\mathbf{p}}\Pi)]^N.\end{aligned} \tag{4.21}$$

There are no assurances in general that the rightmost term in Eq. (4.21) is positive, but if N is an even number, it must be. It follows that if $P(\mathbf{q})\geqslant 0$, for sufficiently large *even* N,

$$\mathrm{tr}(\rho^{(N)}\Pi^{\otimes N})>1, \tag{4.22}$$

contradicting the assumption that it should always be a probability.

All we need to do now is transcribe the argument leading to Eq. (4.22) to the general integral case of Eq. (4.17). Note that by Eq. (4.14), the quantity $\mathrm{tr}(A_{\mathbf{p}}\Pi)$ is a (linear) continuous function of the parameter $\mathbf{p}$. Therefore, for any $\epsilon>0$, there exists a $\delta>0$ such that $|\mathrm{tr}(A_{\mathbf{p}}\Pi)-\mathrm{tr}(A_{\mathbf{q}}\Pi)|\leqslant\epsilon$ whenever $|\mathbf{p}-\mathbf{q}|\leqslant\delta$, i.e., whenever $\mathbf{p}$ is contained within an open ball $B_\delta(\mathbf{q})$ centered at $\mathbf{q}$. Choose $\epsilon<\lambda$, and define $\overline{B}_\delta$ to be the intersection of $B_\delta(\mathbf{q})$ with the probability simplex. For $\mathbf{p}\in\overline{B}_\delta$, it follows that

$$\mathrm{tr}(A_{\mathbf{p}}\Pi)\geqslant 1+\lambda-\epsilon>1. \tag{4.23}$$

If we consider an N that is even, $[\mathrm{tr}(A_{\mathbf{p}}\Pi)]^N$ is nonnegative in all of $\mathcal{S}_{d^2}$, and we have that the probability of the outcome $\Pi^{\otimes N}$ satisfies

$$\begin{aligned}\mathrm{tr}(\rho^{(N)}\Pi^{\otimes N})&=\int_{\mathcal{S}_{d^2}}P(\mathbf{p})[\mathrm{tr}(A_{\mathbf{p}}\Pi)]^N\,d\mathbf{p}=\int_{\mathcal{S}_{d^2}-\overline{B}_\delta}P(\mathbf{p})[\mathrm{tr}(A_{\mathbf{p}}\Pi)]^N\,d\mathbf{p}+\int_{\overline{B}_\delta}P(\mathbf{p})[\mathrm{tr}(A_{\mathbf{p}}\Pi)]^N\,d\mathbf{p}\\&\geqslant\int_{\overline{B}_\delta}P(\mathbf{p})[\mathrm{tr}(A_{\mathbf{p}}\Pi)]^N\,d\mathbf{p}\geqslant(1+\lambda-\epsilon)^N\int_{\overline{B}_\delta}P(\mathbf{p})\,d\mathbf{p}.\end{aligned} \tag{4.24}$$

Unless

$$\int_{\overline{B}_\delta} P(\mathbf{p})d\mathbf{p}=0, \tag{4.25}$$

the lower bound (4.24) for the probability of the outcome $\Pi^{\otimes N}$ becomes arbitrarily large as $N \rightarrow \infty$. Thus we conclude that the requirement that $\rho^{(N)}$ be a proper density operator constrains $P(\mathbf{p})$ to vanish almost everywhere in $\overline{B}_\delta$ and, consequently, to vanish almost everywhere that $A_\mathbf{p}$ is not a physical state.

Using Eq. (4.14), we can trivially transform the integral representation (4.17) to one directly over the convex set of density operators $\mathcal{D}_d$ and be left with the following statement. Under the sole assumption that the density operator $\rho^{(N)}$ is exchangeable, there exists a unique probability density $P(\rho)$ such that

$$\rho^{(N)}=\int_{\mathcal{D}_d} P(\rho)\rho^{\otimes N}d\rho. \tag{4.26}$$

This concludes the proof of the quantum de Finetti representation theorem.

V. OUTLOOK

Since the analysis in the previous sections concerned *only* the case of quantum-state tomography, we certainly have not written the last word on unknown quantum states in the sense advocated in Sec. I. There are clearly other examples that need separate analyses. For instance, the use of unknown states in quantum teleportation[10]—where a *single* realization of an unknown state is ''teleported'' with the aid of previously distributed quantum entanglement and a classical side channel—has not been touched upon. The quantum de Finetti theorem, therefore, is not the end of the road for detailing implications of an information-based interpretation of quantum mechanics. What is important, we believe, is that taking the time to think carefully about the referents of various states in a problem can lead to insights into the structure of quantum mechanics that cannot be found by other means.

For instance, one might ask, ''Was this theorem not inevitable?'' After all, is it not already well established that quantum theory is, in some sense, just a noncommutative generalization of probability theory? Should not all the main theorems in classical probability theory carry over to the quantum case?[68,69] One can be skeptical in this way, of course, but then one will miss a large part of the point. There are any number of noncommutative generalizations to probability theory that one can concoct.[70] The deeper issue is, what is it in the natural world that forces quantum theory to the particular noncommutative structure it actually has?[71] It is not a foregone conclusion, for instance, that every theory has a de Finetti representation theorem within it.

Some insight in this regard can be gained by considering very simple modifications of quantum theory. To give a concrete example, let us take the case of real-Hilbert-space quantum mechanics. This theory is the same as ordinary quantum mechanics in all aspects *except* that the Hilbert spaces are defined over the field of real numbers rather than the complex numbers. It turns out that this is a case where the quantum de Finetti theorem fails. Let us start to explain why by first describing how the particular proof technique used above loses validity in the new context.

In order to specify uniquely a Hermitian operator $\rho^{(N)}$ in going from Eq. (4.16) to (4.17), the proof made central use of the fact that a complete basis $\{E_1,\ldots,E_{d^2}\}$ for the vector space of operators on $\mathcal{H}_d$ can be used to generate a complete basis for the operators on $\mathcal{H}_d^{\otimes N}$—one just need take the d^{2N} operators of the form $E_{\alpha_1}\otimes\cdots\otimes E_{\alpha_N}$, $1\leqslant\alpha_j\leqslant d^2$. (All we actually needed was that a basis for the real vector space of Hermitian operators on $\mathcal{H}_d$ can be used to generate a basis for the real vector space of Hermitian operators on $\mathcal{H}_d^{\otimes N}$, but since the vector space of all operators is the complexification of the real vector space of Hermitian operators, this seemingly weaker requirement is, in fact, no different.) This technique works because the dimension of the space of $d^N\times d^N$ matrices is $(d^2)^N$, the Nth power of the dimension of the space of $d\times d$ matrices.

This technique does not carry over to real Hilbert spaces. In a real Hilbert space, states and POVM elements are represented by real symmetric matrices. The dimension of the vector space of real symmetric matrices acting on a d-dimensional real Hilbert space is $\frac{1}{2}d(d+1)$, this then being the number of elements in a minimal informationally complete POVM. The task in going from Eq. (4.16) to (4.17) would be to specify the real matrix $\rho^{(N)}$. When $N\geqslant 2$, however, the dimension of the space of $d^N\times d^N$ real symmetric matrices is strictly greater than the Nth power of the dimension of the space of $d\times d$ real symmetric matrices, i.e.,

$$\tfrac{1}{2}d^N(d^N+1)>(\tfrac{1}{2}d(d+1))^N. \tag{5.1}$$

Hence, specifying Eq. (4.16) for all outcome sequences $\boldsymbol{\alpha}=(\alpha_1,\ldots,\alpha_N)$ is not sufficient to specify a single operator $\rho^{(N)}$. This line of reasoning indicates that the particular *proof* of the quantum de Finetti theorem presented in Sec. IV fails for real Hilbert spaces, but it does not establish that the theorem itself fails. The main point of this discussion is that it draws attention to the crucial difference between real-Hilbert-space and complex-Hilbert-space quantum mechanics—a fact emphasized previously by Araki[26] and Wootters.[27]

To show that the theorem fails, we need a counterexample. One such example is provided by the N-system state

$$\rho^{(N)}=\tfrac{1}{2}\rho_+^{\otimes N}+\tfrac{1}{2}\rho_-^{\otimes N}, \tag{5.2}$$

where

$$\rho_+=\tfrac{1}{2}(I+\sigma_2) \quad \text{and} \quad \rho_-=\tfrac{1}{2}(I-\sigma_2), \tag{5.3}$$

and where σ_2 was defined in Eq. (3.2). In complex-Hilbert-space quantum mechanics, this is clearly a valid density operator: It corresponds to an equally weighted mixture of N spin-up particles and N spin-down particles in the y direction. The state $\rho^{(N)}$ is clearly exchangeable, and the decomposition in Eq. (5.2) is unique according to the quantum de Finetti theorem.

Now consider $\rho^{(N)}$ as an operator in real-Hilbert-space quantum mechanics. Despite the apparent use of the imaginary number i in the σ_2 operator, $\rho^{(N)}$ remains a valid quantum state. This is because, upon expanding the right-hand side of Eq. (5.2), all the terms with an odd number of σ_2 operators cancel away. Yet, even though it is an exchangeable density operator, it cannot be written in de Finetti form of Eq. (3.15) using only real symmetric operators. This follows because Eq. (5.2), the unique de Finetti form, contains σ_2, which is an antisymmetric operator and cannot be written in terms of symmetric operators. Hence the de Finetti representation theorem does not hold in real-Hilbert-space quantum mechanics.

Similar considerations show that in quaternionic quantum mechanics (a theory again precisely the same as ordinary quantum mechanics except that it uses Hilbert spaces over the quaternionic field[25]), the connection between exchangeable density operators and decompositions of the de Finetti form (3.15) breaks down. The failure mode is, however, even more disturbing than for real Hilbert spaces. In quaternionic quantum mechanics, most operators of the de Finetti form (3.15) do not correspond to valid quaternionic quantum states, even though the states ρ in the integral are valid quaternionic states. The reason is that tensor products of quaternionic Hermitian operators are not necessarily Hermitian.

In classical probability theory, exchangeability characterizes those situations where the only data relevant for updating a probability distribution are frequency data, i.e., the numbers n_j in Eq. (2.4) which tell how often the result j occurred. The quantum de Finetti representation shows that the same is true in quantum mechanics: Frequency data (with respect to a sufficiently robust measurement) are sufficient for updating an exchangeable state to the point where nothing more can be learned from sequential measurements; that is, one obtains a convergence of the form (1.5), so that ultimately any further measurements on the individual systems are statistically independent. That there is no quantum de Finetti theorem in real Hilbert space means that there are fundamental differences between real and complex Hilbert spaces with respect to learning from

measurement results. The ultimate reason for this is that in ordinary, complex-Hilbert-space quantum mechanics, exchangeability implies separability, i.e., the absence of entanglement among the component systems. This follows directly from the quantum de Finetti theorem, because states of the form Eq. (3.15) are not entangled. This implication does not carry over to real Hilbert spaces. By the same reasoning used to show that the de Finetti theorem itself fails, the state in Eq. (5.2) cannot be written as *any* mixture of real product states. Interpreted as a state in real Hilbert space, the state in Eq. (5.2) is thus not separable, but rather has entanglement among the component systems.[72] In a real Hilbert space, exchangeable states can be entangled, and local measurements cannot reveal that.

Beyond these conceptual points, we also believe that the technical methods exhibited here might be of interest in the practical arena. Recently there has been a large literature on which classes of measurements have various advantages for tomographic purposes.[73,74] To our knowledge, the present work is the only one to consider tomographic reconstruction based upon minimal informationally complete POVMs. One can imagine several advantages to this approach via the fact that such POVMs with rank-one elements are automatically extreme points in the convex set of all measurements.[75]

Furthermore, the classical de Finetti theorem is only the tip of an iceberg with respect to general questions in statistics to do with exchangeability and various generalizations of the concept.[76] One should expect no less of quantum exchangeability studies. In particular here, we are thinking of things like the question of representation theorems for finitely exchangeable distributions.[52,77] Just as our method for proving the quantum de Finetti theorem was able to rely heavily on the classical theorem, so one might expect similar benefits from the classical results in the case of quantum finite exchangeability—although there will certainly be new aspects to the quantum case due to the possibility of entanglement in finite exchangeable states. A practical application of such representation theorems could be their potential to contribute to the solution of some outstanding problems in constructing security proofs for various quantum key distribution schemes.[78]

In general, our effort in the present article forms part of a larger program to promote a consistent information-based interpretation of quantum mechanics and to delineate its consequences. We find it encouraging that the fruits of this effort might not be restricted solely to an improved understanding of quantum mechanics, but might also possess the potential to contribute to practical applications.

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APPENDIX: PROOF OF THE CLASSICAL DE FINETTI THEOREM

In this Appendix we reprise the admirably simple proof of the classical de Finetti representation theorem given by Heath and Sudderth[42] for the case of binary variables.

Suppose we have an exchangeable probability assignment for M binary random variables, $x_1,x_2,\ldots,x_M$, taking on the values 0 and 1. Let $p(n,N)$, $N\leqslant M$, be the probability for n 1s in N trials. Exchangeability guarantees that

$$p(n,N)=\binom{N}{n}p(x_1=1,\ldots,x_n=1,x_{n+1}=0,\ldots,x_N=0). \tag{A1}$$

We can condition the probability on the right on the occurrence of m 1's in all M trials:

$$p(n,N)=\binom{N}{n}\sum_{m=0}^{M} p(x_1=1,\ldots,x_n=1,x_{n+1}=0,\ldots,x_N=0|m,M)p(m,M). \tag{A2}$$

Given m 1's in M trials, exchangeability guarantees that the $\binom{M}{m}$ sequences are equally likely. Thus the situation is identical to drawing from an urn with m 1's on M balls, and we have that

$$p(x_1=1,\ldots,x_n=1,x_{n+1}=0,\ldots,x_N=0|m,M) = \frac{m}{M}\,\frac{m-1}{M-1}\cdots\frac{m-(n-1)}{M-(n-1)}\,\frac{M-m}{M-n}\,\frac{M-m-1}{M-n-1}\cdots\frac{M-m-(N-n-1)}{M-(N-1)}=\frac{(m)_n(M-m)_{N-n}}{(M)_N}, \tag{A3}$$

where

$$(r)_q\equiv\prod_{j=0}^{q-1}(r-j)=r(r-1)\cdots(r-q+1)=\frac{r!}{(r-q)!}. \tag{A4}$$

The result is that

$$p(n,N)=\binom{N}{n}\sum_{m=0}^{M}\frac{(m)_n(M-m)_{N-n}}{(M)_N}p(m,M). \tag{A5}$$

What remains is to take the limit $M\to\infty$, which we can do because of the extendibility property of exchangeable probabilities. We can write $p(n,N)$ as an integral,

$$p(n,N)=\binom{N}{n}\int_0^1\frac{(zM)_n((1-z)M)_{N-n}}{(M)_N}P_M(z)\,dz, \tag{A6}$$

where

$$P_M(z)=\sum_{m=0}^{M}p(zM,M)\,\delta(z-m/M) \tag{A7}$$

is a distribution concentrated at the M-trial frequencies m/M. In the limit $M\to\infty$, $P_M(z)$ converges to a continuous distribution $P_\infty(z)$, and the other terms in the integrand go to $z^n(1-z)^{N-n}$, giving

$$p(n,N)=\binom{N}{n}\int_0^1 z^n(1-z)^{N-n}P_\infty(z)\,dz. \tag{A8}$$

Thus, if $p(n,N)$ is part of an infinite exchangeable sequence, it has a de Finetti representation in terms of a ''probability on probabilities'' $P_\infty(z)$.

To demonstrate the uniqueness of $P_\infty(z)$, recall that the binomial factor in Eq. (A8),

$$\binom{N}{Ny}z^{Ny}(1-z)^{N(1-y)}, \tag{A9}$$

becomes a multiple of $\delta(z-y)$ as N goes to infinity. The constant is determined by a beta function integral,

$$\int_0^1 z^n(1-z)^{N-n}\,dz=\frac{n!(N-n)!}{(N+1)!}, \tag{A10}$$

thus implying that

$$(N+1)\binom{N}{Ny}z^{Ny}(1-z)^{N(1-y)}\to\delta(y-z) \tag{A11}$$

as N goes to infinity. The result is that as N goes to infinity,

$$\frac{p(yN,N)}{1/N}\to P_\infty(y). \tag{A12}$$

What this means is that, in accordance with the first part of the proof, $P_\infty(z)\,dz$ is uniquely determined to be the probability that the frequency of 1's will lie between z and $z+dz$ in an infinite number of trials.

We have demonstrated the classical de Finetti representation theorem for binary variables: If $p(n,N)$ is part of an infinite exchangeable sequence, then it has a unique de Finetti representation in terms of a "probability on probabilities" $P_\infty(z)$. The proof can readily be extended to nonbinary variables.

[1] See, for instance, Bohr's Como lecture, N. Bohr, "The Quantum Postulate and the Recent Development of Atomic Theory," in *Atti del Congresso Internazionale dei Fisici 11–20 Settembre 1927, Como-Pavia-Roma, Volume Secondo* (Nicola Zanichelli, Bologna, 1928), p. 565. This along with several iterations of the manuscript are reprinted in *Niels Bohr: Collected Works, Volume 6, Foundations of Quantum Physics I (1926–1932)*, edited by J. Kalckar (North-Holland, Amsterdam, 1985).

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> The state of a classical system is an objective property of the system and therefore changes only by dynamical laws. A quantum-mechanical state, being a summary of the observers' information about an individual physical system, changes both by dynamical laws and whenever the observer acquires new information about the system through the process of measurement. The existence of two laws for the evolution of the state vector by the Schrödinger equation on the one hand and by the process of measurement (sometimes described as the "reduction of the wave packet") on the other, is a classic subject for discussion in the quantum theory of measurement. The situation becomes problematical only if it is believed that the state vector is an objective property

of the system. Then, the state vector must be required to change only by dynamical law, and the problem must be faced of justifying the second mode of evolution from the first. If, however, the state of a system is defined as a list of [*experimental*] propositions together with their [*probabilities of occurrence*], it is not surprising that after a measurement the state must be changed to be in accord with the new information ... . The ''reduction of the wave packet'' does take place in the consciousness of the observer, not because of any unique physical process which takes place there, but only because the state is a construct of the observer and not an objective property of the physical system.

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There was a young man who said, ''God
Must think it exceedingly odd
If he finds that this tree
Continues to be
When there's no one about in the Quad.''
REPLY
Dear Sir:
Your astonishment's odd:
I am always about in the Quad.
And that's why the tree
Will continue to be,
Since observed by
Yours faithfully,
God.

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Compatibility of state assignments

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Rudolf Peierls raised the question of when different density matrices can characterize the knowledge available to different people about one and the same physical system. I describe counterexamples to the condition he imposed on such state assignments, and suggest what the correct condition ought to be. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1495897]

According to Rudolph Peierls[1] the answer to the question of what the quantum mechanical formalism represents is ''that the wavefunction or, more generally, the density matrix represents our *knowledge* of the system we are trying to describe.'' Heisenberg took the same position and one can argue that Bohr did, too, though I am unaware of an explicit statement to this effect in his writings. But only Peierls raised and offered an answer to the next question: ''*Whose* knowledge?''

Peierls noted that density matrices describing a system ''may differ, as the nature and amount of knowledge may differ. People may have observed the system by different methods, with more or less accuracy; they may have seen part of the results of another physicist. However, there are limitations to the extent to which their knowledge may differ.... This limitation can be compactly and conveniently expressed by the condition that the density matrices used by the two observers must commute with each other.'' To this he added a second requirement that ''the two observers should not contradict each other. This means the product of the two density matrices should not be zero.'' [2]

So, according to Peierls, if Alice and Bob use density matrices ρ_a and ρ_b to encapsulate what each of them knows about one and the same physical system, then their density matrices must satisfy

$$[\rho_a, \rho_b] = 0 \tag{1}$$

and

$$\rho_a \rho_b \neq 0. \tag{2}$$

While requirement (2) seems fairly straightforward, given (1), I worried about (1) for several years. It had a nice feel to it, but I couldn't see why it had to hold, except in very special cases. There was a time when I went around asking people why the density matrices different people might use to describe the same system had to commute. Nobody could tell me why or even seemed particularly interested in the question, until I put it to Christopher Fuchs. He said he'd think about it. After I kept pestering him by e-mail, he finally wrote that the reason I couldn't understand the condition was that it wasn't true,[3] and he gave me a simple counterexample: Bob knows the system is in one of two nonorthogonal states, but doesn't know which; Alice does know which. For a while I kept inventing objections that Peierls might have raised to this counterexample, but in the end I was able to cast it in a form I feel fairly sure Peierls would have acknowledged to be valid.

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Before examining my Peierls-proof version of Fuchs's counterexample, first consider a case where Peierls' criterion (1) does hold. Suppose Alice and Bob start off both knowing that two qubits are in the entangled but not maximally entangled pure state

$$|\Psi\rangle = \cos\theta|0\rangle|0\rangle + \sin\theta|1\rangle|1\rangle, \quad 0 < \theta < \pi/4. \tag{3}$$

Both will use the same reduced density matrix for the qubit on the left:

$$\rho_a = \rho_b = \mathrm{Tr}_r|\Psi\rangle\langle\Psi| = \cos^2\theta\,|0\rangle\langle 0| + \sin^2\theta|1\rangle\langle 1|. \tag{4}$$

If Alice now measures the qubit on the right in the computational basis $\{|0\rangle,|1\rangle\}$, then, depending on the outcome, she can update her knowledge of the qubit on the left to

$$\rho_a' = |0\rangle\langle 0| \quad \text{or} \quad \rho_a' = |1\rangle\langle 1|. \tag{5}$$

If she tells Bob nothing about the result of her measurement, or even whether she made a measurement at all, then his density matrix for the qubit on the left must remain ρ_b. In either of the cases (5) we have $[\rho_a', \rho_b] = 0$. Peierls' condition (1) holds.

But now suppose that before she measures the qubit on the right Alice applies to it a unitary (Hadamard) transformation changing the state (3) of the two-qubit system into

$$\begin{aligned} |\Psi\rangle' &= \cos\theta|0\rangle\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) + \sin\theta|1\rangle\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \\ &= \frac{1}{\sqrt{2}}(\cos\theta\,|0\rangle + \sin\theta|1\rangle)|0\rangle + \frac{1}{\sqrt{2}}(\cos\theta\,|0\rangle - \sin\theta|1\rangle)|1\rangle. \end{aligned} \tag{6}$$

This by itself leaves both their reduced density matrices ρ_b and ρ_a for the qubit on the left unchanged. But if Alice now measures the qubit on the right in the computational basis, depending on the outcome, she can update her knowledge of the qubit on the left to

$$\rho_a' = (\cos\theta|0\rangle \pm \sin\theta|1\rangle)(\cos\theta\langle 0| \pm \sin\theta\langle 1|) = \rho_b \pm \cos\theta\sin\theta(|0\rangle\langle 1| + |1\rangle\langle 0|). \tag{7}$$

Either outcome violates Peierls' condition (1):

$$[\rho_b, \rho_a'] = \pm\tfrac{1}{4}\sin 4\theta(|0\rangle\langle 1| - |1\rangle\langle 0|) \neq 0. \tag{8}$$

I believe Peierls would have accepted this as a valid counterexample because all of Alice's actions are applied only to the qubit on the right and Bob knows nothing about those actions and their outcomes, or even whether there were any actions at all. So unless one takes a very literal view of ''quantum nonlocality'' (as Peierls did not), insisting that Alice's actions on the right have disrupted the qubit on the left, thereby rendering Bob's knowledge of it obsolete, one must acknowledge that Alice did nothing to affect the validity of Bob's knowledge of the qubit on the left. She merely took advantage of an opportunity to refine her own knowledge of that qubit in an entirely noninvasive way, by acting only on the qubit on the right. Since Bob is ignorant of what Alice did to the qubit on the right or even whether she did anything at all to it, he has acquired no new information to refine his knowledge of the qubit on the left. Since nothing has been done to that qubit, he must therefore continue to describe it with the same density matrix, ρ_b.

But although Peierls' first requirement (1) is overly restrictive, his second requirement (2) remains valid even in the absence of his first, in that it is equivalent to requiring that there should be no measurement that Alice knows *must* have a certain outcome while Bob knows that it *cannot* have that same outcome.

To see this, note first that if (2) fails to hold, so that $\rho_a\rho_b = 0$, then since density matrices are Hermitian we also have $\rho_b\rho_a = 0$, so ρ_a and ρ_b do indeed commute, and there is a basis of joint

eigenstates. The vanishing of $\rho_a\rho_b$ requires at least one of ρ_a and ρ_b to have zero eigenvalue for each eigenstate, so we can resolve the identity (not necessarily uniquely) into the sum of two projections, $1=P_a+P_b$ where P_a and P_b project onto subspaces of eigenstates of ρ_a and ρ_b with eigenvalue zero. The outcomes of any measurement that discriminates between these two orthogonal subspaces will be assigned probabilities 1 or 0 by Alice, and 0 or 1 by Bob. Whatever outcome Alice knows must happen Bob knows cannot happen, and vice versa.

Conversely, and somewhat less trivially, suppose there is some measurement with some outcome that Alice gives probability 0 and Bob gives probability 1. This means there is some Hermitian operator M with eigenvalues m in the range[4]

$$0\leqslant m\leqslant 1 \tag{9}$$

with

$$\mathrm{Tr}\rho_a M=0, \quad \mathrm{Tr}\rho_b M=1. \tag{10}$$

If the eigenstates of M are $|\phi_j\rangle$ with eigenvalues m_j, then expanding (10) in the basis of those eigenstates gives

$$\sum_j \langle\phi_j|\rho_a|\phi_j\rangle m_j=0, \tag{11}$$

and

$$\sum_j \langle\phi_j|\rho_b|\phi_j\rangle m_j=1, \tag{12}$$

or, since $\mathrm{Tr}\rho_b=1$,

$$\sum_j \langle\phi_j|\rho_b|\phi_j\rangle(1-m_j)=0. \tag{13}$$

Since the diagonal matrix elements of ρ_a and ρ_b are non-negative and since the m_j satisfy (9), we conclude from (11) and (13) that

$$\langle\phi_j|\rho_a|\phi_j\rangle=0, \quad m_j\neq 0, \tag{14}$$

$$\langle\phi_j|\rho_b|\phi_j\rangle=0, \quad m_j\neq 1. \tag{15}$$

But if $\langle\phi|\rho|\phi\rangle=0$ for a positive operator ρ, then $\rho|\phi\rangle=0$, so (14) and (15) require every eigenstate $|\phi_k\rangle$ of M to be an eigenstate with zero eigenvalue of either ρ_a or ρ_b. It follows that

$$\langle\phi_i|\rho_a\rho_b|\phi_j\rangle=\sum_k \langle\phi_i|\rho_a|\phi_k\rangle\langle\phi_j|\rho_b|\phi_k\rangle^* \tag{16}$$

must be zero for arbitrary i and j. Since the $|\phi_i\rangle$ are a complete set, we then have $\rho_a\rho_b=0$.

So the existence of at least one measurement with at least one outcome that Alice's density matrix forbids and Bob's requires (or vice versa) means that the product of their density matrices must vanish. Peierls's second requirement (2) is valid even in the absence of his first requirement (1), as a direct expression of the condition that Alice and Bob should not uncover a logical contradiction when they compare what their knowledge implies about the outcomes of measurements made on one and the same system $\mathcal{S}$.

Is (2) the only constraint implied by the requirement that their knowledge not be contradictory?[5] This might appear plausible, since outright contradictions only involve probabilities 0 or 1: if Alice assigns probability 0 to an outcome that Bob assigns any probability less than

1, the failure of the outcome to occur contradicts neither assignment. But the logical structure of quantum mechanics leads to a broader set of restrictions than (2), provided we impose the following compatiblity condition on what different people know about the same system $\mathcal{S}$.[6]

Let us say that the knowledge Alice, Bob, Carol, Dick,... have about one and the same system $\mathcal{S}$ is *compatible* if there is some density matrix ρ that combines all their judgments about impossible outcomes, assigning zero probability to any outcome of any measurement that any one of them assigns zero probability. In particular, under this definition the knowledge of Alice and Bob is incompatible if Alice knows that an outcome of a measurement has probability 0 while Bob knows that the same outcome of that same measurement has probability 1. For Bob then also knows that all the other possible outcomes have probability 0. So any density matrix ρ assigning zero probability to all the outcomes that either one of them assigns zero probability would have to assign zero probability to all possible outcomes, which violates the requirement that $\mathrm{Tr}\rho=1$.

But these are not the only conditions under which there is no density matrix that incorporates all their judgments of impossible outcomes. To formulate the broader condition, let us say that a given pure state is the outcome of a measurement if the projection operator on that state is measured and the result is 1.[7] A state $|\phi\rangle$ is forbidden by a density matrix ρ to be the outcome of a measurement if $\langle\phi|\rho|\phi\rangle=0$. Because ρ is a positive operator any such forbidden state is an eigenstate of ρ with zero eigenvalue, so the set $N(\rho)$ of all forbidden states is a subspace of the state space, called the *null space* of ρ. The orthogonal complement of $N(\rho)$, the subspace $S(\rho)$ spanned by all the eigenvectors of ρ with nonzero eigenvalues, is called the *support* of ρ.

If a group of density matrices ρ_a, ρ_b, ρ_c,... describe compatible knowledge of a system $\mathcal{S}$, then there must be some density matrix ρ whose null space $N(\rho)$ contains all the null spaces $N(\rho_a),N(\rho_b),N(\rho_c),\ldots$. Since $\mathrm{Tr}\rho\neq 0$, its support $S(\rho)$ cannot be empty. Any vector $|\phi\rangle$ in $S(\rho)$ must be orthogonal to any vector in $N(\rho)$ and therefore orthogonal to any vector in $N(\rho_a),N(\rho_b),N(\rho_c),\ldots$. It must therefore be in all the supports $S(\rho_a),S(\rho_b),S(\rho_c),\ldots$. We conclude that *for a set of density matrices to be compatible, their supports must all have at least one state in common.*

What about a converse proposition? If a set of density matrices is compatible in this sense, can there be circumstances under which they actually do represent the knowledge available to Alice, Bob, Carol,... about one and the same physical system? If the state space is finite dimensional, then, if all their supports do have a state in common, such circumstances can indeed arise. To see this we first note the following.[8]

Consider an expansion of a density matrix ρ in orthonormal projections onto its eigenvectors with nonzero eigenvalue:

$$\rho=\sum_i r_i|\psi_i\rangle\langle\psi_i|. \tag{17}$$

If the dimension of the support $S(\rho)$ is finite, then the positive r_i appearing in (17) are all bounded away from 0 by some $r_0>0$, and we can define a positive s_i by

$$s_i=r_i-r_0, \tag{18}$$

in terms of which

$$\rho=\sum_i s_i|\psi_i\rangle\langle\psi_i|+r_0P, \tag{19}$$

where P is the projection operator onto $S(\rho)$. If $|\phi\rangle$ is any unit vector in $S(\rho)$, then one can find an orthonormal basis $|\eta_i\rangle$ for $S(\rho)$ with $|\eta_0\rangle=|\phi\rangle$. Since

$$P=\sum_i |\eta_i\rangle\langle\eta_i|, \tag{20}$$

it follows that ρ has an expansion (not necessarily unique, in not necessarily orthogonal states) in which $|\phi\rangle$ appears with nonzero weight:

$$\rho = p|\phi\rangle\langle\phi| + \sum p_i|\phi_i\rangle\langle\phi_i|, \quad p>0, \ p_i \geqslant 0. \tag{21}$$

So if the supports of ρ_a and ρ_b share a common state $|\phi\rangle$, then Alice and Bob's density matrices have expansions of the form (21),

$$\rho_a = p_a|\phi\rangle\langle\phi| + \sum_{i\geqslant 1} p_{ai}|\phi_{ai}\rangle\langle\phi_{ai}|,$$

$$\rho_b = p_b|\phi\rangle\langle\phi| + \sum_{i\geqslant 1} p_{bi}|\phi_{bi}\rangle\langle\phi_{bi}|, \tag{22}$$

$$p_a, p_b, p_{ai}, p_{bi} > 0,$$

which share a common state $|\phi\rangle$. These density matrices can indeed represent the knowledge Alice and Bob have of one and the same system $\mathcal{S}$ under the following circumstances.[9]

Let there be two more systems, $\mathcal{S}_a$ and $\mathcal{S}_b$, with both Alice and Bob's knowledge of $\mathcal{S}_a + \mathcal{S}_b + \mathcal{S}$ initially described by the pure state

$$|\Psi\rangle \propto |a_0\rangle|b_0\rangle|\phi\rangle + \sum_{i\geqslant 1} \sqrt{p_{ai}/p_a}|a_0\rangle|b_i\rangle|\phi_{ai}\rangle + \sum_{i\geqslant 1} \sqrt{p_{bi}/p_b}|a_i\rangle|b_0\rangle|\phi_{bi}\rangle, \tag{23}$$

where $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$ are orthonormal bases for $\mathcal{S}_a$ and $\mathcal{S}_b$. Alice has access only to $\mathcal{S}_a$ and Bob only to $\mathcal{S}_b$. Each of them knows that nobody has access to $\mathcal{S}$.

Suppose Alice measures on $\mathcal{S}_a$ the nondegenerate observable A with eigenstates $|a_0\rangle, |a_1\rangle, |a_2\rangle, \ldots$, and finds the result associated with $|a_0\rangle$, while Bob measures an analogous observable, B, on $\mathcal{S}_b$ and finds the result associated with $|b_0\rangle$, neither knowing what, if anything, the other did.

Alice will then assign to $\mathcal{S}_b + \mathcal{S}$ the state

$$|\Psi_a\rangle \propto |b_0\rangle|\phi\rangle + \sum \sqrt{\frac{p_{ai}}{p_a}}|b_i\rangle|\phi_{ai}\rangle, \tag{24}$$

leading to the reduced density matrix for $\mathcal{S}$,

$$p_a|\phi\rangle\langle\phi| + \sum p_{ai}|\phi_{ai}\rangle\langle\phi_{ai}| = \rho_a, \tag{25}$$

while Bob will assign to $\mathcal{S}_a + \mathcal{S}$ the state

$$|\Psi_b\rangle \propto |a_0\rangle|\phi\rangle + \sum \sqrt{\frac{p_{bi}}{p_b}}|a_i\rangle|\phi_{bi}\rangle, \tag{26}$$

leading to the reduced density matrix for $\mathcal{S}$,

$$p_b|\phi\rangle\langle\phi| + \sum p_{bi}|\phi_{bi}\rangle\langle\phi_{bi}| = \rho_b. \tag{27}$$

In order for their reduced density matrices for $\mathcal{S}$ to have these desired forms, Alice and Bob must find the appropriate outcomes for their measurements of $\mathcal{S}_a$ and $\mathcal{S}_b$. This is not under anybody's control, but the probability of it happening is nonzero, if p_a and p_b in (21) are both

nonzero. So there can be circumstances under which Alice and Bob will end up assigning the density matrices ρ_a and ρ_b to $\mathcal{S}$. The probability of such circumstances arising under this protocol will, of course, be very small if one or the other member of all possible pairs of common states in all possible expansions (21) of ρ_a and ρ_b has a very small weight.

This construction generalizes to any number of observers. For Alice, Bob, and Carol, for example, we can take $\mathcal{S}_a+\mathcal{S}_b+\mathcal{S}_c+\mathcal{S}$ to be initially in the state

$$|\Psi\rangle\propto|a_0\rangle|b_0\rangle|c_0\rangle|\phi\rangle+\sum_{i\geqslant 1}\sqrt{p_{ai}/p_a}|a_0\rangle|b_i\rangle|c_i\rangle|\phi_{ai}\rangle+\sum_{i\geqslant 1}\sqrt{p_{bi}/p_b}|a_i\rangle|b_0\rangle|c_i\rangle|\phi_{bi}\rangle$$

$$+\sum_{i\geqslant 1}\sqrt{p_{ci}/p_c}|a_i\rangle|b_i\rangle|c_0\rangle|\phi_{ci}\rangle, \tag{28}$$

and then follow the obvious generalization of the Alice–Bob protocol.

We conclude that if the supports of a group of density matrices share a common state, then there can be circumstances under which each density matrix describes the knowledge available to a particular observer of one and the same physical system. But if there is no pure state common to all the supports, then there can be no density matrix that assigns zero probability to every measurement outcome that any one of the observers assigns zero probability; the combined knowledge of the individual observers cannot be reconciled with any quantum-mechanically consistent description of the system.

As a special case of this conclusion, note that since the support of a pure-state density matrix is the one-dimensional subspace spanned by that state, two pure-state density matrices are compatible in this sense only if they are identical: pure state assignments (and only pure state assignments) are unique. If one takes the view that pure states are objective physical properties of the system they describe, this conclusion has very little content. But if, following Peierls, Heisenberg, and perhaps Bohr, one takes the view that a quantum state characterizes the knowledge of the system available to a particular observer, then whether pure-state assignments must be unique becomes a nontrivial question. From the perspective described above their uniqueness follows from the fact that if some body of knowledge about a system leads to the pure state $|\psi\rangle$, then no state orthogonal to $|\psi\rangle$ can be the outcome of a measurement on the system. If a different subset of all the available knowledge of the system leads to the assignment of a different pure state $|\psi'\rangle$, then no state orthogonal to $|\psi'\rangle$ can occur as the outcome of a measurement. But the laws of quantum mechanics require that any superposition of zero-probability outcomes must also have zero probability. Since the states orthogonal to two distinct states span the entire state space, if different subsets of the available knowledge justified two different pure-state assignments, no state whatever could occur as the outcome of a measurement.

One might argue that nobody can ever know with certainty that any outcome of any measurement is strictly impossible. The support of any realistic density matrix would then be the entire Hilbert space, and all these conditions would be vacuous—any set of density matrices would be mutually compatible, though the probability of measurement outcomes leading to such state assignments could be minuscule. But although the quantum theory is inherently probabilistic, the theory is also capable of deterministic assertions, which strictly prohibit certain measurement outcomes under ideal conditions. It is surely a significant feature of that theory that consideration of impossible outcomes leads, without any invocation of ''the uncertainty principle'' or ''maximal information,'' to the uniqueness of pure-state assignments, as well as the more general constraint on mixed-state assignments.

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[1] R. E. Peierls, Phys. World **January**, 19–21 (1991).
[2] Rudolf Peierls, *More Surprises in Theoretical Physics* (Princeton University Press, Princeton, NJ, 1991), p. 11.
[3] C. Fuchs, private communication to N. David Mermin, reproduced in quant-ph/0105039, p. 235.
[4] For an ordinary von Neumann measurement M is just a projection operator. By allowing the eigenvalues of M to be in the interior as well as the end points of the interval $[0,1]$ we can cover the case where the problematic measurement is of a more general kind (a POVM).
[5] I raised this question in N. David Mermin, "Whose Knowledge?" in *Quantum (Un)speakables: Essays in Commemoration of John S. Bell*, edited by R. Bertlmann and A. Zeilinger (Springer Verlag, New York, 2002); quant-ph/0107051.
[6] Almost immediately after Ref. 5 appeared on the ePrint Archive, I received apparently different answers to the question from Todd Brun and Jerry Finkelstein. Those answers and a proof of their equivalence were given in T. A. Brun, J. Finkelstein, and N. D. Mermin, Phys. Rev. A **65**, 032315 (2002); quant-ph/0109041. The derivation that follows is essentially that of Ref. 6, though I have modified the formulation of that derivation in response to criticisms raised by C. Caves, C. Fuchs, and R. Schack (private communication).
[7] This does not, of course, imply anything about the state of the system prior to the measurement.
[8] This was first schown by E. Schrödinger, Proc. Cambridge Philos. Soc. **32**, 446 (1936). Schrödinger does not explicitly require the state space to be finite dimensional, but some such condition is required to validate his assumption that any density matrix has an inverse when restricted to its support.
[9] In general, such a pair of density matrices will not commute, so this construction provides a large class of counterexamples to Peierls-first condition (1).

Behavior of the survival probability in some one-dimensional problems

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We study the behavior of the survival probability $P_\varphi(t)$ in potential barrier problems on the half-line. We consider two cases: when the initial state φ is a truncated outgoing solution corresponding to a scattering frequency and when it is an approximate bound state. Using techniques and methods from Spectral Theory, Fourier Analysis, and from Ordinary Differential Equations, we obtain approximate exponential decay in both cases. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In the usual mathematical formalism in Quantum Mechanics, the *Survival Probability*,

$$P_\varphi(t)=|\langle \varphi, e^{-iHt}\varphi\rangle|^2, \tag{1.1}$$

represents the probability that, at time t, the system is in its initial state φ. Here, H is a self-adjoint operator on a Hilbert space $\mathcal{H}$ and φ is a state, that is, a unit vector in $\mathcal{H}$.

If the operator H is absolutely continuous then, by the Riemann–Lebesgue Lemma, $P_\varphi(t)$ tends to 0 when $|t|$ approaches ∞. The rate of decay of this quantity is relevant from a physical point of view.

Here, we study the behavior of $P_\varphi(t)$ in potential barrier problems in the half-line. First we consider an outgoing solution corresponding to a scattering frequency near the real axis. We show that if φ is a truncated resonant solution, then $P_\varphi(t)$ has an approximate exponential behavior. This result, in this sense of the L^∞-norm appears in Ref. 6. In Sec. III we establish estimates in terms of the L^2-norm, while in Sec. II we prove a formula for computing the spectral measure, for a general potential with compact support.

In the last section, we study the following related problem. Suppose that H is Hamiltonian in the half-line, for a nonnegative potential with compact support. When the potential has a barrier with a long width, H will be close, in a large interval, to a Hamiltonian H^∞ having a bound state φ. We prove that in this case $P_\varphi(t)$ also behaves almost exponentially.

For the sake of completeness we recall some results for general self-adjoint operators. If H is an absolutely continuous self-adjoint operator on a Hilbert space $\mathcal{H}$, then its spectral measure E_λ can be represented as

$$p_\varphi(\lambda)\equiv\frac{d\langle \varphi, E_\lambda\varphi\rangle}{d\lambda}=\frac{1}{\pi}\lim_{\delta\to 0+}\ \mathrm{Im}\langle \varphi,(H-\lambda-i\delta)^{-1}\varphi\rangle, \tag{1.2}$$

for any unit vector φ in a dense subspace of $\mathcal{H}$. The Fourier transform of this expression is precisely,

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$$\langle \varphi, e^{-iHt}\varphi\rangle = \frac{1}{\pi}\int_{-\infty}^{\infty} e^{-i\lambda t}\,\mathrm{Im}\langle \varphi,(H-\lambda-i0)^{-1}\varphi\rangle d\lambda, \tag{1.3}$$

where we have used the notation,

$$\mathrm{Im}\langle \varphi,(H-\lambda-i0)^{-1}\varphi\rangle = \lim_{\delta\to 0+}\ \mathrm{Im}\langle \varphi,(H-\lambda-i\delta)^{-1}\varphi\rangle.$$

Our goal is to prove that in the resonant case, the probability $P(t)=|\langle \varphi, e^{-iHt}\varphi\rangle|^2$ has an almost exponential behavior. More explicitly, we shall estimate,

$$\int_{-\infty}^{\infty} \left|\langle \varphi, e^{-iHt}\varphi\rangle - e^{-i\lambda_0 t}e^{-\epsilon|t|}\right|^2 dt,$$

for adequate φ, λ_0, and ϵ.

Our approach follows the ideas of Lavine,[6] who proved that when φ is a normalized truncated resonant state (see Sec. III), then, for all time t,

$$\left|\langle \varphi, e^{-iHt}\varphi\rangle - e^{-i\lambda_0 t}e^{-\epsilon|t|}\right| \leqslant c\,\epsilon\left|\ln \epsilon\right|,$$

where $\lambda_0 - i\epsilon$ is the corresponding resonance.

The almost exponential behavior, in the sense of the L^2-norm, turns out to give also an explicit estimate on the size of the sojourn time $\tau(\varphi)$, in terms of the imaginary part of the resonance.

Lavine's approach is time-independent and it is based on (1.3), which establishes the fact that the unitary group e^{-iHt} is the Fourier transform of limiting values of the resolvent $R(z)$, as z approaches the real axis.

On the other hand,

$$\begin{aligned} e^{-i\lambda_0 t}e^{-\epsilon|t|} &= \frac{1}{\pi}\int_{-\infty}^{\infty} e^{-i\lambda t}\,\mathrm{Im}(\lambda-\lambda_0-i\epsilon)d\lambda \\ &= \frac{1}{\pi}\int_{-\infty}^{\infty} e^{-i\lambda t}\frac{\epsilon}{(\lambda-\lambda_0)^2+\epsilon^2}d\lambda. \end{aligned}$$

By Plancherel's Theorem, we then have that

$$\begin{aligned} &\int_{-\infty}^{\infty} \left|\langle \varphi, e^{-iHt}\varphi\rangle - e^{-i\lambda_0 t}e^{-\epsilon|t|}\right|^2 dt \\ &\quad = \left(\frac{1}{\pi}\right)^2 \int_{-\infty}^{\infty} \left|\mathrm{Im}\langle \varphi,(H-\lambda-i0)^{-1}\varphi\rangle - \frac{\epsilon}{(\lambda-\lambda_0)^2+\epsilon^2}\right|^2 d\lambda. \end{aligned}$$

It is sufficient then to estimate the L^2-norm of the difference between the imaginary part of the resolvent in the real axis and the Lorentzian $\epsilon/[(\lambda-\lambda_0)^2+\epsilon^2]$, for adequate values of ϵ.

As indicated by Lavine in Ref. 10, the integrand is singular in $\lambda=0$. In Ref. 9 he estimates the L^1-norm of this difference and in Ref. 10 he proposes to truncate the state in energy away from the origin in order to handle the L^2-norm. Here we manage to estimate it for all energy λ.

We mention Refs. 3, 7, 8, and 11–13 for results on decay in presence of a resonant state. Also, Refs. 4–6 for a different characterization of the resonance phenomena.

II. THE SPECTRAL MEASURE

Let H_0 be the (negative) Laplace operator on the half-line $[0, \infty)$, with the Dirichlet boundary condition at the origin. Then, H_0 is a self-adjoint operator on $L^2[0,\infty)$, with domain $\mathcal{H}^2\cap\mathcal{H}_0^1$. We consider a perturbation $H=H_0+V(x)$, where $V(x)$ is a non-negative bounded potential with compact support. This operator is the total Hamiltonian for a quantum mechanical particle in the half-line, moving under the influence of the potential $V(x)$.

If we prescribe the Dirichlet boundary condition at the origin, then H is also a self-adjoint operator on L^2. Moreover, H is positive and absolutely continuous, with spectrum $[0, \infty]$.

We first study the resolvent of the operator H. To this end, given a complex number $z=\lambda+i\delta$ with $\delta\geqslant 0$ and $\lambda>0$, we consider two solutions $\psi_1(x,z)$ and $\psi_2(x,z)$ of the homogeneus equation,

$$-\psi''+V(x)\psi-z\psi=0, \quad x\geqslant 0 \tag{2.1}$$

satisfying the initial conditions,

$$\psi_1(0,z)=0, \psi_1'(0,z)=1,$$

and

$$\psi_2(x,z)=ce^{i\sqrt{z}x} \quad \text{for } x\geqslant R,$$

where c is chosen such that $\psi_2(0,z)=1$.

Here, R is such that the support of V is contained in the interval $[0,R)$. Also, we are choosing the square root in such a way that $\operatorname{Im}\sqrt{z}>0$, for $\delta>0$.

Lemma 2.1: Suppose that $\delta>0$. Given $\varphi\in L^2$, the function,

$$\psi(x,z)=-\left\{\psi_1(x,z)\int_x^\infty \psi_2(y,z)\varphi(y)dy+\psi_2(x,z)\int_0^x \psi_1(y,z)\varphi(y)dy\right\} \tag{2.2}$$

is the solution of the problem,

$$-\psi''+V(x)\psi-z\psi=\varphi, \quad x\geqslant 0, \tag{2.3}$$

$$\psi(0)=0, \tag{2.4}$$

$$\psi\in L^2. \tag{2.5}$$

In other words, ψ is precisely the resolvent $(H-z)^{-1}\varphi$.

Proof: It follows immediately from variation of parameters. □

Lemma 2.2: Suppose that $z=\lambda>0$. Given $\varphi\in L^1\cap L^2$, the function,

$$\psi(x,\lambda)=-\left\{\psi_1(x,\lambda)\int_x^\infty \psi_2(y,\lambda)\varphi(y)dy+\psi_2(x,\lambda)\int_0^x \psi_1(y,\lambda)\varphi(y)dy\right\} \tag{2.6}$$

is a solution of the problem,

$$-\psi''+V(x)\psi-\lambda\psi=\varphi, \quad x\geqslant 0, \tag{2.7}$$

$$\psi(0)=0, \tag{2.8}$$

$$\psi\in L^\infty. \tag{2.9}$$

Moreover, $\langle\varphi,\psi(\cdot,\lambda+i\delta)\rangle$ converges to $\langle\varphi,\psi(\cdot,\lambda)\rangle$, when δ approaches 0.

Proof: The function $\psi(x,\lambda)$ clearly satisfies the differential equation and the initial condition. Moreover, for real λ all the solutions are bounded. The last assertion follows from the Dominated Convergence Theorem. □

The following result is straightforward:

Lemma 2.3: Suppose that $0\leqslant a<b$ and let $V_1(x)$ be a function in $L^\infty(a,b)$. Assume that φ is a solution of

$$-\varphi''+V_1(x)\varphi=z_1\varphi, \quad \text{for } x\in(a,b).$$

Then

$$W(\psi_i(\cdot,\lambda),\varphi)\Big|_a^b=\int_a^b (V(x)-V_1(x)+z_1-\lambda)\psi_i(x,\lambda)\varphi(x))dx. \tag{2.10}$$

Lemma 2.4: Given $\varphi\in L^1[0,\infty]\cap Ł^2[0,\infty]$, *the spectral measure of the operator H satisfies*

$$\frac{d\langle\varphi,E_\lambda\varphi\rangle}{d\lambda}=\frac{1}{\pi}\mathrm{Im}\langle\varphi,\psi(\cdot,\lambda)\rangle, \tag{2.11}$$

where $\psi(\cdot,\lambda)$ *is given by Lemma 2.2.*

Proof: It follows from (1.3) and Lemma 2.2. □

The above result is an explicit formula for the Radon Nikodym derivative of the spectral measure that works on a dense subset of the Hilbert space. For an explicit potential $V(x)$, the integral that appears in this formula will be computed with the aid of Lemma 2.3.

III. ESTIMATES FOR RESONANT SOLUTIONS

Let k be a *scattering frequency* for $-(d^2/dx^2)+V(x)$ and let $z=k^2=\lambda_0-i\epsilon$.
This means that ψ is a nontrivial outgoing [i.e. $\psi(x)=ce^{ikx}$, for $x\geqslant R$] solution of

$$-\frac{d^2}{dx^2}\psi+V(x)\psi=z\psi,\quad 0<x, \tag{3.1}$$

$$\psi(0)=0. \tag{3.2}$$

We choose the constant c in such a way that $\varphi=\chi_{[0,R]}\psi$ satisfies

$$\int_0^R|\varphi(x)|^2dx=1.$$

Lemma 3.1: The spectral measure of the operator $H=(-d^2/dx^2)+V(x)$ *at the state* φ *satisfies*

$$\pi\frac{d\langle\varphi,E_\lambda\varphi\rangle}{d\lambda}-\frac{\epsilon}{(\lambda-\lambda_0)^2+\epsilon^2}=\frac{1}{|z-\lambda|^2}\mathrm{Im}\,W(\psi_2,\varphi)W(\psi_1,\overline{\varphi})(R). \tag{3.3}$$

Proof: By Lemma 2.4, we have that

$$\pi\frac{d}{d\lambda}\langle\varphi,E_\lambda\varphi\rangle=-\mathrm{Im}\Bigg[\int_0^\infty\overline{\varphi}(x)\psi_1(x)\int_x^\infty\psi_2(y)\varphi(y)dydx + \int_0^\infty\overline{\varphi}(x)\psi_2(x)\int_0^x\psi_1(y)\varphi(y)dydx\Bigg].$$

We call I_1 and I_2 the two expressions inside the square brackets. Since $\varphi\equiv 0$ for $x>R$, it follows that

$$I_1=\int_0^R\overline{\varphi}(x)\psi_1(x)\int_x^R\psi_2(y)\varphi(y)dydx,$$

$$I_2=\int_0^R\overline{\varphi}(x)\psi_2(x)\int_0^x\psi_1(y)\varphi(y)dydx.$$

By Lemma 2.3, we obtain

$$\int_x^R \psi_2(y)\varphi(y)dy = \frac{1}{\lambda - z} W(\psi_2, \varphi)|_x^R,$$

$$\int_0^x \psi_1(y)\varphi(y)dy = \frac{1}{\lambda - z} W(\psi_1, \varphi)|_R^x,$$

and substituting these expressions we obtain

$$I_1 + I_2 = \frac{1}{\lambda - z} \int_0^R \overline{\varphi}(x)\{\psi_1(x) W(\psi_2, \varphi)|_x^R + \psi_2(x) W(\psi_1, \varphi)|_0^x\} dx.$$

If we call $B(x)$ the expression in brackets, then

$$B(x) = \psi_1(x) W(\psi_2, \varphi)(R) - \psi_1(x)(\psi_2(x)\varphi'(x) - \psi_2'(x)\varphi(x)) + \psi_2(x)(\psi_1(x)\varphi'(x) - \psi_1'(x)\varphi(x)),$$

since $W(\psi_1, \varphi)(0) = 0$. After some cancellations we get,

$$B(x) = \psi_1(x) W(\psi_2, \varphi)(R) + W(\psi_1, \psi_2)(x)\varphi(x).$$

But the Wronskian of ψ_1, ψ_2 is constant,

$$W(\psi_1, \psi_2)(x) = W(\psi_1, \psi_2)(0) = -1.$$

Hence,

$$B(x) = \psi_1(x) W(\psi_2, \varphi)(R) - \varphi(x)$$

and

$$I_1 + I_2 = \frac{W(\psi_2, \varphi)(R)}{\lambda - z} \int_0^R \overline{\varphi}(x)\psi_1(x)dx - \frac{1}{\lambda - z},$$

since $\int_0^R |\varphi(x)|^2 dx = 1$;

We use Lemma 2.3 again to obtain that

$$\int_0^R \overline{\varphi(x)}\psi_1(x)dx = \frac{1}{\overline{z} - \lambda} W(\psi_1, \overline{\varphi})(R). \tag{3.4}$$

Hence,

$$I_1 + I_2 = -\frac{1}{|z - \lambda|^2} W(\psi_2, \varphi) W(\psi_1, \overline{\varphi})(R) - \frac{1}{\lambda - z}. \tag{3.5}$$

Finally, we compute the imaginary part and obtain the desired result.

□

We again use the fact that the Wronskian $W(\psi_1, \psi_2)$ is constant to obtain that

$$W(\psi_2,\varphi)W(\psi,\overline{\varphi})(R)=\frac{(\psi_2\varphi'-\psi_2'\varphi)(\psi_1\overline{\varphi}'-\psi_1'\overline{\varphi})}{\psi_1\psi_2'-\psi_1'\psi_2}(R)$$

$$=|\varphi(R)|^2\frac{\left(\frac{\varphi'}{\varphi}-\frac{\psi_2'}{\psi_2}\right)\left(\frac{\overline{\varphi}'}{\overline{\varphi}}-\frac{\psi_1'}{\psi_1}\right)}{\frac{\psi_2'}{\psi_2}-\frac{\psi_1'}{\psi_1}}(R). \tag{3.6}$$

Let us introduce the notation,

$$\beta=\frac{\varphi'(R)}{\varphi(R)}$$

and

$$\beta_1=\beta_1(\lambda)=\frac{\psi_1'(R)}{\psi_1(R)}.$$

Also, ψ_2 is known explicitly, for $R\leqslant x$, therefore,

$$W(\psi_2,\varphi)W(\psi_1\overline{\varphi})(R)=|\varphi(R)|^2\frac{(\beta-i\sqrt{\lambda})(\overline{\beta}-\beta_1)}{i\sqrt{\lambda}-\beta_1}$$

$$=|\varphi(R)|^2\frac{(\beta-i\sqrt{\lambda})(\overline{\beta}-i\sqrt{\lambda}+i\sqrt{\lambda}-\beta_1)}{i\sqrt{\lambda}-\beta_1}$$

$$=|\varphi(R)|^2\frac{(\beta-i\sqrt{\lambda})(-\beta_1-i\sqrt{\lambda})}{i\sqrt{\lambda}-\beta_1}+\frac{|\beta-i\sqrt{\lambda}|^2}{i\sqrt{\lambda}-\beta_1}. \tag{3.7}$$

Theorem 3.1: *Suppose that k is a scattering frequency for* $-(d^2/dx^2)+V(x)$. *Then,*

$$\int_{-\infty}^{\infty}\left|\langle\varphi,e^{-iHt}\varphi\rangle-e^{-i\lambda_0 t}e^{-\epsilon|t|}\right|^2dt\leqslant c\,\epsilon.$$

Proof: Consider the function,

$$f(\lambda)=\mathrm{Im}\langle\varphi,(H-\lambda-i0)^{-1}\varphi\rangle-\frac{\epsilon}{(\lambda-\lambda_0)^2+\epsilon^2}.$$

We note that for λ negative,

$$f(\lambda)=\frac{\epsilon}{(\lambda-\lambda_0)^2+\epsilon^2}.$$

Our starting point is the following pointwise estimate, which is a direct consequence of Lemma 3.1 and the identity (3.7)

$$|f(\lambda)| \leqslant \left\{ |i\sqrt{\lambda} - \beta(R)| + \frac{|i\sqrt{\lambda} - \beta(R)|^2}{(\beta_1(R)^2 + \lambda)^{1/2}} \right\} \frac{|\varphi(R)|^2}{(\lambda - \lambda_0)^2 + \epsilon^2},$$

for positive λ.

Also, given $\lambda \geqslant 0$, $\psi_1 = \psi_1(x,\lambda)$ is a nontrivial real-valued solution of the eigenvalue equation,

$$-\frac{d^2}{dx^2}\psi + V(x)\psi = \lambda\psi, \quad 0 < x,$$

with $\psi(0) = 0$.

In this particular case the potential is supported on the interval $[0,R]$, hence $\beta = i\sqrt{\lambda_0 - i\epsilon}$.

Moreover, since,

$$(\operatorname{Im} \overline{\varphi}\varphi')' = \operatorname{Im} \overline{\varphi}(V - k^2)\varphi = \epsilon|\varphi|^2,$$

we obtain, by integrating over $[0, R]$,

$$|\varphi(R)|^2 = \frac{\epsilon}{\operatorname{Im} \beta(R)} = \frac{\epsilon}{\operatorname{Re} \sqrt{\lambda_0 - i\epsilon}}.$$

Using this, we can estimate the L^2-norm of $f(\lambda)$, by separating the integral with respect to λ in four pieces: $(-\infty, 0)$, $(0,\lambda_0/2)$, $(\lambda_0/2,3\lambda_0/2)$, $(3\lambda_0/2,\infty)$.

For $\lambda < 0$,

$$\int_{-\infty}^{0} |f(\lambda)|^2 d\lambda \leqslant \frac{\epsilon^2}{3\lambda_0^3}.$$

On the interval $(3\lambda_0/2,\infty)$, we use $\operatorname{Re} \sqrt{\lambda_0 - i\epsilon} > \sqrt{\lambda_0/2}$ and $|\sqrt{\lambda} - \sqrt{\lambda_0 - i\epsilon}| < \sqrt{[(\lambda - \lambda_0)^2 + \epsilon^2]/\lambda}$. Also neglect the term β_1^2, and get

$$|f(\lambda)| \leqslant \frac{\epsilon\sqrt{2}}{\sqrt{\lambda\lambda_0}} \left(\frac{1}{\sqrt{(\lambda - \lambda_0)^2 + \epsilon^2}} + \frac{1}{\lambda} \right).$$

Thus,

$$\int_{3\lambda_0/2}^{\infty} |f(\lambda)|^2 d\lambda \leqslant C(\lambda_0)\epsilon^2.$$

For $\lambda \in (\lambda_0/2,3\lambda_0/2)$,

$$|f(\lambda)| \leqslant \frac{2\epsilon}{\lambda_0} \left(\frac{1}{\sqrt{(\lambda - \lambda_0)^2 + \epsilon^2}} + \frac{2}{\lambda_0} \right).$$

This gives,

$$\int_{\lambda_0/2}^{3\lambda_0/2} |f(\lambda)|^2 d\lambda \leqslant C_1(\lambda_0)\epsilon + C_2(\lambda_0)\epsilon^2.$$

When working on the interval $[0,\lambda_0/2]$, we cannot neglect the term involving β_1, because the integrand does not belong to L^2 (it does converge in L^1). We then need a lower bound for it. This is given by Lemma 3.2, which after some manipulations, gives

$$|f(\lambda)| \leqslant C \frac{\epsilon}{(\lambda-\lambda_0)^2+\epsilon^2}.$$

Then,

$$\int_0^{\lambda_0/2} |f(\lambda)|^2 d\lambda \leqslant C \int_0^{\lambda_0/2} \left(\frac{\epsilon}{(\lambda-\lambda_0)^2+\epsilon^2} \right)^2 d\lambda \leqslant c\epsilon^2.$$

By combining these four estimates, we obtain the desired result. □

Lemma 3.2: If $0<\lambda<\pi^2/16R^2$, *then,* $\beta_1(R) \geqslant C/R$, *where* $C=M^{-1}$ *and* $M=\max_{[0,\pi/4]}(\tan x/x)=4/\pi$.

Proof: The variable $u=\psi_1/\psi_1'$ is a solution of

$$u' = 1+(\lambda-V)u^2 \leqslant 1+\lambda u^2. \tag{3.8}$$

Moreover, u is real and satisfies $u(0)=0$ and $u'(0)=1$.
The result follows by integration. □

IV. POTENTIAL BARRIERS

We now consider a sequence of barriers of finite height and whose supports are increasing to ∞. Here, we shall establish some explicit estimates concerning the approximate exponential behavior in the resonant case, and, for simplicity, we only consider barriers which are step functions. Explicitly, let us consider $V_n(x)=h\chi_{[a,a+n]}(x)$, $V_\infty(x)=h\chi_{[a,\infty)}(x)$, $H_n=H_0+V_n$, and $H_\infty=H_0+V_\infty$.

The spectrum of H_∞ consists of a finite number of eigenvalues $\lambda_1<\lambda_2\cdots<h$ and an absolutely continuous part $[h, \infty)$. On the other hand, each H_n is absolutely continuous with spectrum $[0, \infty)$.

We consider the first eigenvalue λ_1 of H_∞ with corresponding eigenvector φ. For large n, φ is "almost" an eigenvector of H_n, indeed, one can explicitly estimate $\|(H_n-\lambda_1)\varphi)\|$ and prove that this quantity is small since φ is exponentially decreasing at infinity. By the energy-time uncertainty principle (see Ref. 9), we have that the sojourn time $\tau(\varphi)=\int|\langle\varphi,e^{-iH_nt}\varphi\rangle|^2dt$ satisfies $\tau(H)\|(H_n-\lambda_1)\varphi\| \geqslant 1$, hence, $\tau(\varphi)$ is large. Physically, this means that φ is a resonant state.

According to this fact, one expects that $\langle\varphi,e^{-iH_nt}\varphi\rangle$ has an approximate exponential behavior. Here we prove that there exists a translation in energy by $b\in\mathbb{R}$ and a time rescaling function Γ_n, with $\lim_{n\to\infty}\Gamma_n=0$, such that

$$\lim_{n\to\infty} |\langle\varphi,e^{-i(H_n-\lambda_1-b)(\tau/\Gamma_n)}\varphi\rangle|^2 = e^{-\tau}, \quad \tau>0.$$

We mention Refs. 1 and 2 for similar results.

Since the function φ is exponentially decaying at infinity we can use the formulas of Sec. II to compute the Radon Nikodym derivative $P_n(\lambda)=d/d\lambda\langle\varphi,E_\lambda^n\varphi\rangle$.

To this end, we again consider $\psi_i=\psi_{i,n}(x;\lambda)$, $i=1, 2$, the solutions of

$$-\psi''+V_n\psi=\lambda\psi, \quad x>0,$$

satisfying the boundary conditions,

$$\psi_1(0)=0, \psi_1'(0)=1,$$

and

$$\psi_2(0)=1, \psi_2(x)=c_2(\lambda)e^{i\sqrt{\lambda}x}, \text{ for } x\geqslant a+n.$$

Clearly, the Wronskian $W(\psi_1,\psi_2)=-1$ and ψ_1 is real.

Lemma 4.1: The boundary values of the resolvent satisfy

$$\langle\varphi,(H_n-\lambda-i0)^{-1}\varphi\rangle=\int_0^\infty\overline{\varphi}(x)\psi(x)dx,$$

where

$$\psi(x)=\psi_1(x,\lambda)\int_x^\infty\psi_2\varphi+\psi_2(x,\lambda)\int_0^x\psi_1\varphi.$$

As in the previous section, we can also prove

Lemma 4.2:

$$W(\psi_i,\varphi)|_a^b=\int_a^b(V_\infty-V_n+\lambda-\lambda_1)\varphi\psi_i\,.$$

This can be used to compute $\int_a^b\psi_i\varphi$, for different intervals (a, b), which allows us to obtain the following formula for $\langle\varphi,(H_n-\lambda-i0)^{-1}\varphi\rangle$:

Lemma 4.3: Let $s=\lambda-\lambda_1$. Then,

$$\langle\varphi,(H-\lambda-i0)^{-1}\varphi\rangle=-\frac{1}{s}\int_0^{a+n}|\varphi|^2-\frac{1}{s+h}\int_{a+n}^\infty|\varphi|^2+\frac{h^2}{s^2(s+h)^2}W(\psi_1,\varphi)W(\psi_2,\varphi)(a+n).$$

Proof: This is a straightforward application of Lemmas 4.1 and 4.2. □

We now introduce the logarithmic derivative of ψ_1,

$$\beta(\lambda)\equiv\beta_n(\lambda)=\frac{\psi_1'(a+n,\lambda)}{\psi_1(a+n,\lambda)}.\tag{4.1}$$

Lemma 4.4: The spectral measure,

$$P_n(\lambda)=\frac{1}{\pi}\mathrm{Im}\langle\varphi,(H-\lambda-i0)^{-1}\varphi\rangle\tag{4.2}$$

satisfies

$$\pi P_n(\lambda)=\frac{2\sqrt{\lambda}\lambda_1 h}{(\lambda-\lambda_1)^2(\lambda-\lambda_1+h)^2}\cdot\frac{\sqrt{h-\lambda_1}}{a\sqrt{h-\lambda_1}+1}e^{-2\sqrt{h-\lambda_1}n}\cdot\frac{(\beta(\lambda)+\sqrt{h-\lambda_1})^2}{(\beta^2(\lambda)+\lambda)}.$$

Proof: We know explicitly ψ_1. Also, $W(\psi_1,\psi_2)=-1$. From these facts, it follows that

$$W(\psi_1,\varphi)W(\psi_2,\varphi)(a+n)=\frac{(\varphi'-\beta(\lambda)\varphi)(\varphi'-\beta(\lambda)\varphi)}{\beta(\lambda)-i\sqrt{\lambda}}+(\varphi'-\beta(\lambda)\varphi).$$

Hence,

$$\mathrm{Im}\langle\varphi,(H_n-\lambda-i0)^{-1}\varphi\rangle=\frac{h^2}{(\lambda-\lambda_1)^2(\lambda-\lambda_1+h)^2}\cdot\frac{\sqrt{\lambda}(\varphi'-\beta(\lambda)\varphi)^2(a+n)}{\beta^2(\lambda)+\lambda}.$$

The proof follows by substituting the values of the eigenfunction φ, which are explicitly known for large x. □

One can easily obtain the following formula for the function $\beta=\beta_n$:

$$\beta_n(\lambda)=2\sqrt{h-\lambda}\frac{t(\lambda)}{t(\lambda)+t_1(\lambda)e^{-2\sqrt{h-\lambda}_n}}-\sqrt{h-\lambda},$$

where $t(\lambda)=\tan(a\sqrt{\lambda})+\sqrt{\lambda/(h-\lambda)}$ and $t_1(\lambda)=\tan(a\sqrt{\lambda})-\sqrt{\lambda/(h-\lambda)}$.

By substituting in the expression for the resolvent, we obtain,

$$\Gamma_n\,\mathrm{Im}\langle\varphi,(H_n-\lambda_1-\Gamma_n\lambda-i0)^{-1}\varphi\rangle=F_n(\lambda)G_n(\lambda)(H_n(\lambda))^2,$$

where

$$F_n(\lambda)=\frac{2\lambda_1 h\sqrt{\lambda_1+\Gamma_n\lambda}\sqrt{h-\lambda_1}}{(\Gamma_n\lambda+h)^2(a\sqrt{h-\lambda_1}+1)},$$

$$G_n(\lambda)=(\beta_n^2(\lambda_1+\Gamma_n\lambda)+\lambda_1+\Gamma_n\lambda)^{-1},$$

$$H_n(\lambda)=2\sqrt{h-\lambda_1-\Gamma_n\lambda}\frac{t(\lambda_1+\Gamma_n\lambda)}{\Gamma_n\lambda}R_n(\lambda)+\frac{\sqrt{\Gamma_n}e^{-\sqrt{h-\lambda_1}n}}{\sqrt{h-\lambda_1-\Gamma_n\lambda}+\sqrt{h-\lambda_1}},$$

and

$$R_n(\lambda)=\frac{\sqrt{\Gamma_n}e^{-\sqrt{h-\lambda_1}n}}{t(\lambda_1+\Gamma_n\lambda)+t_1(\lambda_1+\Gamma_n\lambda)e^{-2\sqrt{h-\lambda_1-\Gamma_n\lambda_n}n}}.$$

Assuming that $\Gamma_n\to 0$, we can compute the limit of some of these terms. In order to handle all of them, we choose $\Gamma_n=re^{-2\sqrt{h-\lambda_1}n}$.

With this choice, we have that

(i) $F_n(\lambda)\to 2\lambda_1^{3/2}\sqrt{h-\lambda_1}/h(a\sqrt{h-\lambda_1}+1)$;
(ii) $\beta_n(\lambda)\to\sqrt{h-\lambda_1}\lambda rt'(\lambda_1)-t_1(\lambda_1)/\lambda rt'(\lambda_1)+t_1(\lambda_1)$;
(iii) $G_n(\lambda)\to((h-\lambda_1)(\lambda rt'(\lambda_1)-t_1(\lambda_1)/\lambda rt'(\lambda_1)+t_1(\lambda_1))^2+\lambda_1)^{-1}$;
(iv) $H_n(\lambda)\to 2\sqrt{h-\lambda_1}t'(\lambda_1)\cdot\sqrt{r}/t'(\lambda_1)r\lambda+t_1(\lambda_1)$.

But, $t'(\lambda_1)$ and $t_1(\lambda_1)$ can be explicitly computed. Finally, with the proper choice of r we obtain

Theorem 4.1: *For* $\Gamma_n=re^{-2\sqrt{h-\lambda_1}n}$, *where*

$$r=\frac{8(\lambda_1(h-\lambda_1))^{3/2}}{h^2(a\sqrt{h-\lambda_1}+1)},$$

we have

$$\lim_{n\to\infty} \Gamma_n \operatorname{Im}\langle \varphi, (H_n - \lambda_1 - \lambda\Gamma_n - i0)^{-1}\varphi\rangle = \frac{1}{(\lambda - b)^2 + 1},$$

where

$$b = \frac{h - 2\lambda_1}{2\sqrt{\lambda_1(h - \lambda_1)}}.$$

The convergence is uniform for λ *in compact sets.*

Remark 4.1: Uniform convergence on compact sets implies convergence in L', since the function in question are probability distributions (up to a factor) and this implies uniform convergence of the Fourier transform. Hence,

Corollary 4.1: For all positive τ,

$$\lim_{n\to\infty} \langle \varphi, e^{-i(H_n - \lambda_1 - b)\tau/\Gamma_n}\varphi\rangle = e^{-\tau}.$$

Clearly, upon reintroducing the unscaled time $t = \tau/\Gamma_n$, one obtains that the survival probability $|\langle \varphi, e^{-iH_n t}\varphi\rangle|^2$ behaves asymptotically as $e^{-2\Gamma_n t}$, for all t.

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Reduction of the Hilbert space in strongly correlated systems

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Defining commutation relations between symmetry operators and fundamental operators, we set up the symmetry group for a many-particle Hamiltonian. Using the irreducible representations of the symmetry group, we decompose the Hilbert space. We discuss the advantage of this approach to find the dimensions of reduced Hilbert spaces in numerical exact diagonalization. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1506956]

I. INTRODUCTION

Strongly correlated systems such as the Hubbard model and the Heisenberg model have attracted renewed interest. One method to study strongly correlated systems would be exact diagonalization with the Lanczös algorithm. In relation with high T_c superconductor, an exact diagonalization approach to the $t-J$ model has been used intensively by many authors.[1,2] As a strongly correlated system, the Hall effect has also been studied by the numerical method of exact diagonalization.[3,4]

Nowadays, exact diagonalization has become more popular due to the case of access to a tremendous amount of memory in computers. However, the size of Hilbert space still grows exponentially. The remedy for the exponentially growing problem is to use symmetries that the system has. The symmetries help in reducing the numerical factor in front of the exponential of the Hilbert space dimension. In fact, representation theory[5] makes it possible to find the exact dimension of the reduced Hilbert space. It will be an advantage if one can compare the dimensions of reduced Hilbert spaces obtained analytically with the results found numerically.

In this paper, in order to find the dimension of the reduced Hilbert space, we first define commutation relations between fundamental operators and symmetry operators, and then use representation theory. To the authors' knowledge, no symmetry group representation can be found for any many-particle interacting system.

We can describe general processes of analytical works to find the dimensions of reduced Hilbert spaces. In order to reduce the Hilbert space by using group representation theory, we carry out the following program.

(1) Set up a Hamiltonian, commutation relations between fundamental operators, and an orthonormal basis of the corresponding Hilbert space.
(2) Define relationships between the symmetry operators and the fundamental operators. Then, prove that the symmetry operators commute with the Hamiltonian, and also preserve the commutation relations of fundamental operators.
(3) Find how the symmetry operators commute with themselves in the Hilbert space, and construct the corresponding symmetry group.
(4) Find irreducible representations of the group.

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(5) Calculate the reducible representation of the group with the basis of the Hilbert space.
(6) Decompose the Hilbert space into the irreducible components. The multiplicities in this decomposition are the dimensions of reduced Hilbert spaces.

The purpose of this paper is to emphasize this general procedure as analytical works in exact diagonalization. In doing so, we treat a toy Hamiltonian, which is originated from the second quantized Hamiltonian introduced by Yoshioka, Halperin, and Lee (YHL)[6] to explain the fractional quantum Hall effect.[7,8] The above-mentioned procedure with the YHL Hamiltonian has been done in Ref. 9. Here we take the same procedure with the toy Hamiltonian. Before presenting the toy model, we briefly review the YHL Hamiltonian according to the above-mentioned six steps.

(1) The YHL Hamiltonian is written as

$$H=\sum_{a,b=0}^{N-1} W(a,b)\sum_{k=0}^{N-1} c_{k+a}^{\dagger}c_{k+b}^{\dagger}c_{k+a+b}c_{k}, \tag{1}$$

where the degeneracy of the Landau level is denoted by N, and $c_k^{\dagger}c_l+c_lc_k^{\dagger}=\delta_{kl}$, and $c_{k+N}^{\dagger}=c_k^{\dagger}$. The couplings satisfy $W(a,b)=W(\pm a\pm N,b)=W(a,\pm b\pm N)$. For a system of M electrons, a typical basis of the Hilbert space $\mathcal{H}(N,M)$ is expressed by creation operators:

$$\{c_{i_1}^{\dagger}\cdots c_{i_M}^{\dagger}|0\rangle|0\leqslant i_1<\cdots<i_M\leqslant N-1\}. \tag{2}$$

The dimension of $\mathcal{H}(N,M)$ is given by ${}_NC_M$. Using the symmetries of Hamiltonian H, we study the structure of the Hilbert space $\mathcal{H}(N,M)$.

(2) We define two operators S and T, which act on the Hilbert space in such a way:

$$Sc_k^{\dagger}=\exp\left(i\frac{2\pi}{N}k\right)c_k^{\dagger}S,\quad Sc_k=\exp\left(-i\frac{2\pi}{N}k\right)c_kS,\quad S|0\rangle=|0\rangle, \tag{3}$$

$$Tc_k^{\dagger}=c_{k+1}^{\dagger}T,\quad Tc_k=c_{k+1}T,\quad T|0\rangle=|0\rangle. \tag{4}$$

We find that $SH=HS$, and $TH=HT$, and that S and T are consistent with $c_k^{\dagger}c_l+c_lc_k^{\dagger}=\delta_{kl}$.

(3) When p and q are coprime and $M/N=pG/qG=p/q$ with a greatest common divisor G, the commutation relation between S and T in the Hilbert space $\mathcal{H}(qG,pG)$ is given by

$$ST=\exp\left(i2\pi\frac{p}{q}\right)TS\ \text{ with }\ \xi\equiv\exp\left(i2\pi\frac{p}{q}\right). \tag{5}$$

Note that $S^N=T^N=S^{\dagger}S=T^{\dagger}T=1$. We now consider the symmetry group:

$$G_{\text{core}}=\{\xi^lT^aS^b|l=0,\ldots,q-1;\ a,b=0,\ldots,qG-1\}, \tag{6}$$

where $ST=\xi TS$, and $\xi T=T\xi$, $\xi S=S\xi$.

(4) The irreducible representations, $\Psi_{xts}(\xi^lT^aS^b)$, of the group, G_{core}, are found in Ref. 5.

(5) It is straightforward to calculate the reducible representation:

$$\chi(\xi^lT^aS^b)=\sum_{i_1,\ldots,i_M}\langle 0|c_{i_M}\cdots c_{i_1}\xi^lT^aS^bc_{i_1}^{\dagger}\cdots c_{i_M}^{\dagger}|0\rangle. \tag{7}$$

(6) Using the irreducible representations and the reducible representation, we decompose the Hilbert space $\mathcal{H}(qG,pG)$ as

$$\mathcal{H}(qG,pG)=\bigoplus_{t,s=0}^{G-1}(\mathcal{H}_{pts})^{\oplus d_{ts}}, \tag{8}$$

where $\mathcal{H}_{pts}$ is q-dimensional, and the multiplicity, d_{ts}, is the dimension of the reduced Hilbert space. It is remarkable that the symmetries S and T always exist for any $W(a,b)$. Thus, this structure of the Hilbert space does not depend upon detailed forms of interactions.

A detailed review on $\mathcal{H}_{pts}$ is as follows. A basis of a typical q-dimensional Hilbert space $\mathcal{H}_{pts}$ is given by

$$\{|t,s;n\rangle, T|t,s;n\rangle, \ldots, T^{q-1}|t,s;n\rangle\}, \tag{9}$$

where the quantum number n, which runs from 0 to $d_{ts}-1$, is related with energy spectrum as $H|t,s;n\rangle = E_n|t,s;n\rangle$. The reference state $|t,s;n\rangle$ is actually a linear combination of M creation operators acting on the vacuum state $|0\rangle$. The operators T^a and S^b act on $|t,s;n\rangle$ such that

$$T^{mq+x}|t,s;n\rangle = \exp\left(i\frac{2\pi}{G}mt\right)T^x|t,s;n\rangle, \tag{10}$$

$$S^{lq+y}|t,s;n\rangle = \exp\left(i\frac{2\pi}{G}ls\right)|t,s;n\rangle, \tag{11}$$

where m and l are integers, and $0 \leqslant x,\ y \leqslant q-1$.

It is well known that the ground state of the YHL Hamiltonian always belongs to the $t=s=0$ sector of $\mathcal{H}_{p00}$. Hence, we denote the q-fold ground state as

$$\{|0,0;0\rangle, T|0,0;0\rangle, \ldots, T^{q-1}|0,0;0\rangle\}. \tag{12}$$

The operators, S and T, are actually magnetic translational symmetries, which have been studied for a long time.[10–15] Using magnetic translational symmetries, Haldane[16] showed that many-particle states should have the q-fold degeneracy at rational Landau-level filling p/q in the fractional quantum Hall system. Our work to find the multiplicities in Ref. 9 was beyond Haldane's analysis.

In this paper, we apply this procedure to a toy system, in order to find multiplicities in its energy spectrum. The toy system is described by the unperturbed Hamiltonian, $H_0 = \Sigma_{m=0}^{D-1} H^{(m)}$, and the perturbing Hamiltonian, H_1, where the mth subsystem of $H^{(m)}$ is exactly the quantum Hall system. In the case where some symmetries are broken by H_1, we study the spectrum of low energy states.

Contents are summarized as follows. In Sec. II, we present the unperturbed Hamiltonian in relation with the YHL Hamiltonian. Then, we discuss the symmetries of the unperturbed Hamiltonian. In Sec. III, we construct the symmetry group in the case of lowering symmetries with the perturbing Hamiltonian. Using representations of the group, we find the structure of energy spectrum. We propose future works, and conclude in Sec. IV.

II. DEFORMED YHL HAMILTONIAN AND SYMMETRIES

We now attempt to introduce our unperturbed Hamiltonian H_0 from the YHL Hamiltonian. The first manipulation is to deform the couplings $W(a,b)$. In fact, we write the deformed YHL Hamiltonian from Eq. (1) as

$$\tilde{H} = \sum_{a,b=0}^{qG-1} \sum_{\alpha,\beta=0}^{D-1} W(Da,Db) \sum_{k=0}^{qG-1} \sum_{\kappa=0}^{D-1} c^{\dagger}_{D(k+a)+\kappa+\alpha} c^{\dagger}_{D(k+b)+\kappa+\beta} c_{D(k+a+b)+\kappa+\alpha+\beta} c_{Dk+\kappa}, \tag{13}$$

where we trivially rewrite the indices in a D-times bigger system, $\tilde{N} = qGD$, and deform $W(Da+\alpha, Db+\beta)$ to $W(Da,Db)$. We notice that $\tilde{H}$ still has the symmetries S and T. The next deformation is to transform the operators in $\tilde{H}$. Finally, we present the Hamiltonian H_0, which is rewritten in terms of the new operators as

$$H_0=\sum_{m=0}^{D-1} D \sum_{a,b=0}^{qG-1} W(Da,Db) \sum_{k=0}^{qG-1} a^{\dagger}_{D(k+a)+m} a^{\dagger}_{D(k+b)+m} a_{D(k+a+b)+m} a_{Dk+m}. \tag{14}$$

It should be emphasized that replacing $a^{\dagger}_{Da+m}$ in H_0 by $(1/\sqrt{D})\,\Sigma_{\alpha=0}^{D-1}\exp(-i(2\pi/D)\alpha m)c^{\dagger}_{Da+\alpha}$ does not show $H_0=\tilde{H}$. Furthermore, after this replacement, it turns out that H_0 does not commute with S and T. At this point, H_0 has lost connection to $\tilde{H}$. From now on, we should treat H_0 as a starting point in the following discussion.

We adopt the periodic boundary condition for the operators: $a^{\dagger}_{N+k}=a^{\dagger}_k$, and $a^{\dagger}_k a_l + a_l a^{\dagger}_k = \delta_{kl}$. Denoting $H_0=\Sigma_{m=0}^{D-1} H^{(m)}$, we find that the Hamiltonian $H^{(m)}$ for the mth subsystem has the same structure as that of the original YHL Hamiltonian of Eq. (1). This similarity is reminiscent of scaling. Note that the Hilbert space of H_0 is simply a direct product of the Hilbert space of $H^{(m)}$.

We define the following operators acting on the Hilbert space of the Hamiltonian H_0:

$$S_m a^{\dagger}_{Dk+m}=\exp\left(i\frac{2\pi}{qG}k\right)a^{\dagger}_{Dk+m}S_m, \tag{15}$$

$$S_m a_{Dk+m}=\exp\left(-i\frac{2\pi}{qG}k\right)a_{Dk+m}S_m, \tag{16}$$

$$S_m a^{\dagger}_{Dk+l}=a^{\dagger}_{Dk+l}S_m \quad \text{for } m\neq l, \tag{17}$$

$$S_m a_{Dk+l}=a_{Dk+l}S_m \quad \text{for } m\neq l, \tag{18}$$

$$T_m a^{\dagger}_{Dk+m}=a^{\dagger}_{D(k+1)+m}T_m, \tag{19}$$

$$T_m a_{Dk+m}=a_{D(k+1)+m}T_m, \tag{20}$$

$$T_m a^{\dagger}_{Dk+l}=a^{\dagger}_{Dk+l}T_m \quad \text{for } m\neq l, \tag{21}$$

$$T_m a_{Dk+l}=a_{Dk+l}T_m \quad \text{for } m\neq l, \tag{22}$$

$$Q a^{\dagger}_{Dj+m}=a^{\dagger}_{Dj+m+1}Q, \tag{23}$$

$$Q a_{Dj+m}=a_{Dj+m+1}Q, \tag{24}$$

$$P a^{\dagger}_{Dj+m}=a^{\dagger}_{D(qG-1-j)+D-m}P, \tag{25}$$

$$P a_{Dj+m}=a_{D(qG-1-j)+D-m}P, \tag{26}$$

$$|0\rangle=S_m|0\rangle=T_m|0\rangle=Q|0\rangle=P|0\rangle. \tag{27}$$

We find that $S_m H_0=H_0 S_m$, $T_m H_0=H_0 T_m$, $QH_0=H_0 Q$, and $PH_0=H_0 P$.

We now focus on low energy states of H_0 with $\tilde{M}=pGD$ particles. Note that the ground state of the Hamiltonian H_0 is in the special Hilbert space characterized by equal partition, that is,

$$\bigotimes_{m=0}^{D-1}\mathcal{H}^{(m)}(qG,pG), \tag{28}$$

where the Hilbert space $\mathcal{H}^{(m)}(qG,pG)$ corresponds to the mth subsystem of qG states with pG particles. Since there is no difference between $H^{(m)}$'s except for the dummy index m, the ground state of each Hamiltonian $H^{(m)}$ lives in the subspace characterized by the values $t=s=0$, regardless of m. As a result, the ground state of H_0 lives in

$$\bigotimes_{m=0}^{D-1} \mathcal{H}_{p00}^{(m)} \equiv \mathcal{H}_{\mathrm{g}}. \tag{29}$$

We observe that the degeneracy of ground state for H_0 is given by q^D. The operators S_m and T_m acting on the Hilbert space of $\mathcal{H}_{p00}^{(m)}$ satisfy $S_m^q = T_m^q = 1$ as seen in Eqs. (10) and (11). Like Eq. (12), a basis of the corresponding q^D-dimensional Hilbert space of $\mathcal{H}_{\mathrm{g}}$ is given by

$$\{|\psi_A\rangle = T_0^{i_0} T_1^{i_1} \cdots T_{D-1}^{i_{D-1}} |\psi_0\rangle | 0 \leqslant i_0, \ldots, i_{D-1} \leqslant q-1\}, \tag{30}$$

$$|\psi_0\rangle \equiv |0,0;0\rangle^{(0)} \otimes \cdots \otimes |0,0;0\rangle^{(D-1)}, \tag{31}$$

where the index A runs from 0 to q^D-1, and the reference state $|0,0;0\rangle^{(m)}$ for the mth subsystem is a linear combination of Slater determinants written in terms of the fundamental operators $a_{Dk+m}^{\dagger}$:

$$|0,0;0\rangle^{(m)} = \sum_{k_1,\ldots,k_{pG}=0}^{qG-1} C(k_1,\ldots,k_{pG}) a_{Dk_1+m}^{\dagger} \cdots a_{Dk_{pG}+m}^{\dagger} |0\rangle. \tag{32}$$

III. PERTURBATION WITH LOWERED SYMMETRIES

Symmetries play an important role in studying an energy spectrum of a Hamiltonian. The power of symmetry becomes apparent, when we attempt to analyze a perturbation. Here, the perturbing Hamiltonian, H_1, breaks some symmetries. As a result, degenerated states split in the presence of H_1. Our aim here is to decompose $\mathcal{H}_{\mathrm{g}}$ in the presence of H_1.

The unperturbed Hamiltonian in Sec. II, H_0, certainly has more symmetries than the above-given description. However, when a perturbing Hamiltonian, H_1, is involved, we need to consider only symmetries of the total Hamiltonian, H_0+H_1. We assume that the perturbing Hamiltonian, H_1, has the symmetries Q, P, and $\tilde{S}$, $\tilde{T}$, which are defined as

$$\tilde{S} \equiv \prod_{m=0}^{D-1} S_m, \qquad \tilde{T} \equiv \prod_{m=0}^{D-1} T_m. \tag{33}$$

Although we do not need to present the explicit form of H_1 in the following discussion, a possible form of H_1 would be

$$H_1 = \sum_{n,m=0}^{D-1} \sum_{a,b=0}^{q-1} J(n-m;a,b) T_n^{-b} S_n^{-a} S_m^a T_m^b, \tag{34}$$

which can commute with $\tilde{S}$, $\tilde{T}$, Q, and P with properly chosen couplings $J(n-m;a,b)$. Note that H_1 does not commute with S_m and T_m anymore. For this form of H_1, the operators S_m and T_m effectively play the role of fundamental operators. Their commutation relations in $\mathcal{H}_{\mathrm{g}}$ are given by

$$S_m T_m = \xi T_m S_m \quad \text{with} \quad \xi \equiv \exp\left(i 2\pi \frac{p}{q}\right), \tag{35}$$

$$S_m T_l = T_l S_m \quad \text{for} \quad m \neq l. \tag{36}$$

We calculate commutation relations between the symmetry operators and the fundamental operators. In the space of $\mathcal{H}_{\mathrm{g}}$, the operators satisfy

$$\tilde{S}S_m = S_m\tilde{S}, \tag{37}$$

$$\tilde{S}T_m = \xi T_m\tilde{S}, \tag{38}$$

$$\tilde{T}S_m = \xi^{-1}S_m\tilde{T}, \tag{39}$$

$$\tilde{T}T_m = T_m\tilde{T}, \tag{40}$$

$$QS_m = S_{m+1}Q, \qquad S_D \equiv \xi^{-1}S_0, \tag{41}$$

$$QT_m = T_{m+1}Q, \qquad T_D \equiv T_0, \tag{42}$$

$$PS_m = \xi^{-1}S_{D-m}^{-1}P, \tag{43}$$

$$PT_m = T_{D-m}^{-1}P, \tag{44}$$

$$\tilde{S}|\psi_0\rangle = |\psi_0\rangle, \tag{45}$$

$$\tilde{T}|\psi_0\rangle = \prod_{m=0}^{D-1} T_m|\psi_0\rangle, \tag{46}$$

$$Q|\psi_0\rangle = T_0|\psi_0\rangle, \tag{47}$$

$$P|\psi_0\rangle = \prod_{m=1}^{D-1} T_m^{-1}|\psi_0\rangle. \tag{48}$$

These commutation relations are verified when the operators act on a typical state of Eq. (30). For Eqs. (47) and (48), we have used the definition of Eqs. (23), (25), and (31), and the fact that the coefficients $C(k_1,\cdots,k_{pG})$ in Eq. (32) are independent of m.

We calculate commutation relations between the four symmetry operators in $\mathcal{H}_{\mathrm{g}}$. In order to simplify the commutation relation of $\tilde{S}Q = \xi Q\tilde{S}$, we introduce

$$\tilde{Q} \equiv T^{\alpha}Q, \tag{49}$$

where α is determined for $\tilde{Q}$ to commute with $\tilde{S}$, in fact, as a solution of $\alpha D + 1 \equiv 0 \mod q$. The commutation relations in $\mathcal{H}_{\mathrm{g}}$ between the four operators are given by

$$\tilde{S}\tilde{T} = \xi^D\tilde{T}\tilde{S}, \quad \tilde{S}\tilde{Q} = \tilde{Q}\tilde{S}, \quad \tilde{S}P = \xi^{1-D}P\tilde{S}^{-1}, \tag{50}$$

$$\tilde{T}\tilde{Q} = \tilde{Q}\tilde{T}, \quad \tilde{T}P = P\tilde{T}^{-1}, \quad \tilde{Q}P = P\tilde{Q}^{-1}. \tag{51}$$

The orders of the symmetry operators in $\mathcal{H}_{\mathrm{g}}$ are given by

$$\xi^q = \tilde{S}^q = \tilde{T}^q = \tilde{Q}^{qD} = P^2 = 1, \tag{52}$$

where Eqs. (37)–(48) have been used.

For simplicity, we impose that q and D are coprime. We now consider the symmetry group:

$$G_D^q = \{\xi^l P^n \tilde{Q}^d \tilde{T}^a \tilde{S}^b | l,a,b = 0,\ldots,q-1;\ \ n = 0,1;\ \ d = 0,\ldots,qD-1\}. \tag{53}$$

Representations of G_D^q are essential to decompose the Hilbert space of $\mathcal{H}_g$.

Taking the same approach given in Ref. 9, we find that every irreducible character of G_D^q is a component of Ψ_{xkts}:

$$\Psi_{xkts}(\xi^l P^n \tilde{Q}^d \tilde{T}^a \tilde{S}^b) = \begin{cases} q_x \zeta_q^{xl} (\zeta_{qD}^{kd} \zeta_q^{ta+sb} + \zeta_{qD}^{-kd} \zeta_q^{-ta-sb}) & \text{if } n=0, q_x | a,b, \\ 0 \quad \text{otherwise,} \end{cases} \tag{54}$$

where $0 \leqslant x \leqslant q-1$, $0 \leqslant k \leqslant qD-1$, $0 \leqslant t$, $s \leqslant \gcd(q,x)-1$, $q_x = q/\gcd(q,x)$, and $\zeta_y \equiv \exp(i2\pi/y)$. In order to avoid double counting, we should note that $\Psi_{xkts} = \Psi_{x(qD-k)(q/q_x-t)(q/q_x-s)}$.

It is found that all Ψ_{xkts} are irreducible characters except for $\Psi_{x(\alpha qD/2)(\beta q/2q_x)(\gamma q/2q_x)}$, where $\alpha,\beta,\gamma = 0,1$. Of course, the cases containing $qD/2$ or $q/2q_x$ are meaningful only when they are integers. We decompose the characters, and find the irreducible components,

$$\Psi_{x(\alpha qD/2)(\beta q/2q_x)(\gamma q/2q_x)} = \chi^+_{x\alpha\beta\gamma} + \chi^-_{x\alpha\beta\gamma}. \tag{55}$$

For mathematical completeness, we show the components for $x=0$,

$$\chi^{\pm}_{0\alpha\beta\gamma}(\xi^l P^n \tilde{Q}^d \tilde{T}^a \tilde{S}^b) = (\pm 1)^n (-1)^{\alpha d + \beta a + \gamma b}. \tag{56}$$

For $x \neq 0$, we obtain that

$$\begin{aligned} &\chi^{\pm}_{x\alpha 0\gamma}(\xi^l P^n \tilde{Q}^d \tilde{T}^a \tilde{S}^{q_x m+b}) \\ &\quad = \zeta_q^{xl} (-1)^{\alpha d + \gamma m} \\ &\qquad \times \begin{cases} q_{x,} \quad n=0, \quad q_x | a,b \\ \pm \zeta_q^{xb[(q_x-1)/2][(a+1)D-1]}, \quad n=1, \quad q_x \equiv 1 \mod 2, \ \left(\dfrac{q_x-1}{2}\right) b \in I^+ \\ \pm (-1)^{\gamma} \zeta_q^{xb[(q_x-1)/2][(a+1)D-1]}, \quad n=1, \quad q_x \equiv 1 \mod 2, \ \left(\dfrac{q_x-1}{2}\right) b \in I^- \\ \pm \zeta_q^{-(xb/2)[(a+1)D-1]} (1+(-1)^{x_q[1+(a-1)D]+\gamma}), \quad n=1, \quad q_x \equiv b \equiv 0 \mod 2, \\ 0 \quad \text{otherwise,} \end{cases} \end{aligned} \tag{57}$$

where

$$x_q = x/\gcd(q,x), \quad I^+ = \left\{ \frac{q_x+1}{2}, \ldots, q_x-1, 0 \right\}, \quad \text{and} \quad I^- = \left\{ 1,2,\ldots, \frac{q_x-1}{2} \right\}.$$

We omit presenting $\chi^{\pm}_{x\alpha 1\gamma}$, which is not necessary in the decomposition process.

In summary, the irreducible characters of G_D^q are given by

$$\Psi_{xkts} \quad \text{with } 0 \leqslant x \leqslant q-1, \quad 0 < k < \frac{qD}{2}, \quad 0 < t,s < \frac{q}{2q_x}, \tag{58}$$

$$\chi^+_{x\alpha\beta\gamma}, \ \chi^-_{x\alpha\beta\gamma} \quad \text{with } \alpha,\beta,\gamma = 0,1. \tag{59}$$

The reducible character of the symmetry group for the Hilbert space of $\mathcal{H}_g$ is calculated by using Eqs. (30) and (37)–(48). We find the reducible character of $\mathcal{H}_g$:

$$\chi(\xi^l P^n \tilde{Q}^d \tilde{T}^a \tilde{S}^b) = \sum_{i=0}^{q^D-1} \langle \psi_i | \xi^l P^n \tilde{Q}^d \tilde{T}^a \tilde{S}^b | \psi_i \rangle = \zeta_q^{pl} \times \begin{cases} q^{\gcd(D,d)}, & n=0, \quad q|a,b \\ \zeta^{(pb/2)(q-1)[(a+1)D-1]} q^{(D-1)/2}, & n=1, \quad q\equiv 1, D\equiv 1 \mod 2 \\ \zeta^{(pb/2)(q-1)[(a+1)D-1]} q^{(D/2)-1} & \\ \quad [1+\frac{1}{2}(q-1)(1-(-1)^d)], & n=1, \quad q\equiv 1, D\equiv 0 \mod 2 \\ \zeta^{-(pb/2)[(a+1)D-1]} q^{(D-1)/2} 2, & n=1, \quad q\equiv a\equiv b\equiv 0 \mod 2 \\ 0, \quad \text{otherwise.} & \end{cases} \tag{60}$$

Using the irreducible characters Ψ_{xkts}, $\chi^{\pm}_{x\alpha\beta\gamma}$, and the reducible character χ, we decompose the Hilbert space $\mathcal{H}_g$. Note that (Ψ_{xkts},χ) becomes nonzero only for $x=p$. Furthermore, since $0\leqslant t,\ s\leqslant \gcd(q,p)-1=0$, the case of $t=s=0$ is only possible. Fixing the indices as $x=p$ and $t=s=0$, we calculate the inner product, which is a multiplicity:

$$(\Psi_{pk00},\chi) = \begin{cases} \dfrac{1}{qD} \displaystyle\sum_{d=0}^{D-1} q^{\gcd(D,d)} \cos\left(\frac{2\pi}{qD} kd\right) & k\equiv 0 \mod q \\ 0 \quad \text{otherwise.} \end{cases} \tag{61}$$

Since the multiplicity is nonzero only for $k\equiv 0 \bmod q$, we let $k=ql$ with integer l.

The Hilbert space $\mathcal{H}_g$ is decomposed as

$$\mathcal{H}_g = \bigoplus_{0\leqslant l\leqslant D/2} (\mathcal{H}_l)^{\oplus m_l}, \tag{62}$$

where $m_l=(\Psi_{pql00},\chi)$.

The sectors $(\mathcal{H}_0)^{\oplus m_0}$ and $(\mathcal{H}_{D/2})^{\oplus m_{D/2}}$ are decomposed more as

$$(\mathcal{H}_0)^{\oplus m_0} = (\mathcal{H}_0^+)^{\oplus m_0^+} \bigoplus (\mathcal{H}_0^-)^{\oplus m_0^-}, \tag{63}$$

$$(\mathcal{H}_{D/2})^{\oplus m_{D/2}} = (\mathcal{H}_{D/2}^+)^{\oplus m_{D/2}^+} \bigoplus (\mathcal{H}_{D/2}^-)^{\oplus m_{D/2}^-}, \tag{64}$$

where the multiplicities are given by

$$m_0^{\pm} = (\chi^{\pm}_{p000},\chi) = \frac{1}{2qD} \sum_{d=0}^{D-1} q^{\gcd(D,d)} \pm \begin{cases} \frac{1}{2} q^{(D-1)/2} & D\equiv 1 \mod 2 \\ \dfrac{q+1}{4} q^{(D/2)-1} & D\equiv 0 \mod 2 \end{cases}, \tag{65}$$

and

$$m_{D/2}^{\pm} = (\chi^{\pm}_{p100},\chi) = \frac{1}{2qD} \sum_{d=0}^{D-1} (-1)^d q^{\gcd(D,d)} \pm \frac{1-q}{4} q^{(D/2)-1} \quad \text{for } D\equiv 0 \mod 2. \tag{66}$$

One comment for $m_{D/2}^{\pm}$ is that an integer $D/2$ requires $D\equiv 0 \bmod 2$, and $q\equiv 1 \bmod 2$ because of coprime q and D.

In consequence, with coprime q and D, the Hilbert space $\mathcal{H}_g$ is decomposed as

$$\mathcal{H}_g=(\mathcal{H}_0^+)^{\oplus m_0^+}\bigoplus(\mathcal{H}_0^-)^{\oplus m_0^-}\bigoplus_{1\leqslant l\leqslant(D-1)/2}(\mathcal{H}_l)^{\oplus m_l}\quad\text{for } D\equiv 1 \mod 2, \tag{67}$$

$$\mathcal{H}_g=(\mathcal{H}_0^+)^{\oplus m_0^+}\bigoplus(\mathcal{H}_0^-)^{\oplus m_0^-}\bigoplus_{1\leqslant l\leqslant(D-2)/2}(\mathcal{H}_l)^{\oplus m_l}\bigoplus(\mathcal{H}_{D/2}^+)^{\oplus m_{D/2}^+}\bigoplus(\mathcal{H}_{D/2}^-)^{\oplus m_{D/2}^-}$$

$$\text{for } D\equiv 0 \mod 2. \tag{68}$$

This decomposition is useful in numerical calculations, especially in the Lanczös method. While $q^D=4\,782\,969$ with $q=3$ and $D=14$, we note that $m_0^+=57\,696$.

IV. CONCLUSION

In summary, emphasizing the usefulness of group representation theory, we have considered a model Hamiltonian originated from the YHL Hamiltonian. We consider the symmetries, and construct the symmetry group. Using the representations of the group, we decompose the q^D-fold states into the irreducible components. The main point of this paper is not the model, but the method to find the dimension of the reduced Hilbert space. This method will be useful for exact diagonalization in finite strongly correlated systems.

Future works are proposed as follows. We can consider the reduction of the Hilbert space for a general system that has the symmetry group, $G_t^{(n)}\otimes G_p$, where $G_t^{(n)}$ is an n-dimensional translational group and G_p is a point group. The symmetries of $G_t^{(n)}\otimes G_p$ is not new, but the corresponding representations are not known.

For instance, the Hubbard model in the two-dimensional $N\times N$ square lattice may have the symmetry group $G_t^{(2)}\otimes C_{4v}$, where $G_t^{(2)}$ has two generators, T_x and T_y, and where C_{4v} is one of the Schoenflies symbols. The fundamental operators with two indices satisfy $c_{ij}^\dagger=c_{i+Nj}^\dagger=c_{ij+N}^\dagger$. It is crucial to define commutation relations between symmetry operators and fundamental operators. The generators of the symmetry group are defined as

$$T_x c_{ij}^\dagger=c_{i+1\,j}^\dagger T_x, \tag{69}$$

$$T_y c_{ij}^\dagger=c_{ij+1}^\dagger T_y, \tag{70}$$

$$C_4 c_{ij}^\dagger=c_{-ji}^\dagger C_4, \tag{71}$$

$$\sigma_x c_{ij}^\dagger=c_{i-j}^\dagger \sigma_x, \tag{72}$$

$$\sigma_y c_{ij}^\dagger=c_{-ij}^\dagger \sigma_y, \tag{73}$$

$$\sigma_d c_{ij}^\dagger=c_{ji}^\dagger \sigma_d, \tag{74}$$

$$\sigma_d' c_{ij}^\dagger=c_{-j-i}^\dagger \sigma_d', \tag{75}$$

$$|0\rangle=T_x|0\rangle=T_y|0\rangle=C_4|0\rangle=\sigma_x|0\rangle=\sigma_y|0\rangle=\sigma_d|0\rangle=\sigma_d'|0\rangle. \tag{76}$$

This will be the starting point for the discussion on the reduction of the Hilbert space. Progress in the discussion with all crystallographic point symmetry groups is anticipated.

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Hall effect in noncommutative coordinates

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We consider electrons in uniform external magnetic and electric fields which move on a plane whose coordinates are noncommuting. Spectrum and eigenfunctions of the related Hamiltonian are obtained. We derive the electric current whose expectation value gives the Hall effect in terms of an effective magnetic field. We present a receipt to find the action which can be utilized in path integrals for noncommuting coordinates. In terms of this action we calculate the related Aharonov–Bohm phase and show that it also yields the same effective magnetic field. When magnetic field is strong enough this phase becomes independent of magnetic field. Measurement of it may give some hints on spatial noncommutativity. The noncommutativity parameter θ can be tuned such that electrons moving in noncommutative coordinates are interpreted as either leading to the fractional quantum Hall effect or composite fermions in the usual coordinates. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1504484]

I. INTRODUCTION

To clarify the role which noncommutative coordinates may play in physics a better understanding of quantum mechanics in noncommutative spaces would be useful. Obviously, the simplest case is to consider particles moving in two-dimensional noncommutative spaces. Actually, there exist some realistic physical systems like electrons in a uniform external magnetic field which are effectively moving in a two-dimensional space which is perpendicular to magnetic field. These electrons are investigated in noncommuting coordinates[1] and interesting phenomena like nonextensive statistics[2] and orbital magnetism[3] are resulted. We would like to consider electrons moving in two-dimensional noncommutative space when both uniform external magnetic and electric fields are present. In the usual case this system leads to Hall effect. Indeed, we will show that in noncommuting coordinates one obtains Hall effect in terms of an effective magnetic field.

Once noncommutativity is imposed coordinates behave as operators. However, we can bring in noncommutativity by keeping coordinates as commuting but requiring that composition of their functions is given by star product. After canonical quantization is performed we deal with ordinary coordinates but replace ordinary product with star product. This procedure leads to an ordinary quantum mechanics problem in terms of an effective Hamiltonian depending on the noncommutativity parameter θ. As far as operator description of quantum mechanics is concerned this procedure suits well. However, if one deals with path integrals the suitable action should be given in terms of c-number phase space variables. One of the possibilities is to find an effective action which leads to the Green functions which are calculated in terms of operators.[4] We will adopt another method: The effective action which we use in path integrals is found by replacing deriva-

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tives appearing in Hamiltonian with c-number momentum variables. A similar approach is given in Ref. 5 and a different one in Ref. 6. We will use the action obtained in this manner in path integrals to calculate the related Aharonov–Bohm phase after generalizing the action obtained in symmetric gauge to embrace the other vector potentials at the first order in θ.

In Sec. II we recall how one can find energy eigenvalues and eigenfunctions of an electron moving on plane in uniform external magnetic and electric fields. This serves as a guide in Sec. III when we deal with the same system in noncommuting coordinates. In Sec. IV we present an approach to derive the electric current in noncommutative coordinates. Then, we calculate its expectation value utilizing eigenfunctions derived in Sec. III, yielding the Hall effect in noncommuting coordinates. This can be envisaged as the usual Hall effect in terms of an effective magnetic field. Section V is devoted to calculate Aharonov–Bohm phase in noncommuting coordinates after presenting our receipt to obtain the action suitable to be used in path integrals. This phase is used to define an effective magnetic field in terms of commuting coordinates. We observe that effective magnetic fields obtained in Sec. IV and in Sec. V are the same. In the last section by tuning the parameter θ and utilizing the effective magnetic field we offer two different interpretations of electrons moving in noncommutative space as either leading to the fractional quantum Hall effect[7] or composite fermions[8] in the usual space. Moreover, we propose to measure the Aharonov–Bohm phase for large magnetic fields which may give some hints on the existence of spatial noncommutativity.

II. ELECTRON MOVING ON PLANE

An electron moving on the plane (x,y) in the uniform external electric field $\vec{E}=-\vec{\nabla}\phi$ and the uniform external magnetic field B which is perpendicular to the plane is described by the Hamiltonian

$$H=\frac{1}{2m}\left(\vec{p}+\frac{e}{c}\vec{A}\right)^2-e\phi. \tag{1}$$

We neglect the spin, because taking it into account does not affect our results.

Let us adopt the symmetric gauge

$$\vec{A}=\left(-\frac{B}{2}y,\frac{B}{2}x\right). \tag{2}$$

During the related experiments the electric field $\vec{E}$ is taken in one of the two possible directions. Thus let the scalar potential be

$$\phi=-Ex. \tag{3}$$

Making use of (2) and (3) in (1) leads to the Hamiltonian function

$$H(\vec{p},\vec{r})=\frac{1}{2m}\left[\left(p_x-\frac{eB}{2c}y\right)^2+\left(p_y+\frac{eB}{2c}x\right)^2\right]+eEx. \tag{4}$$

As usual canonical quantization of this system is achieved by introducing the coordinate and momentum operators $\hat{r}_i$, $\hat{p}_i$ satisfying

$$[\hat{r}_i,\hat{p}_j]=i\hbar\delta_{ij} \tag{5}$$

and dealing with the Hamiltonian operator $\hat{H}$ obtained from (4) as $\hat{H}=H(\hat{\vec{p}},\hat{\vec{r}})$.

To discuss the eigenvalue problem

$$\hat{H}\Psi=E\Psi, \tag{6}$$

it is convenient to perform the change of variables

$$\hat{z}=\hat{x}+i\hat{y}, \quad \hat{p}_z=\tfrac{1}{2}(\hat{p}_x-i\hat{p}_y)$$

and introduce two sets of creation and annihilation operators:

$$b^\dagger=-2i\hat{p}_{\bar{z}}+\frac{eB}{2c}\hat{z}+\lambda, \quad b=2i\hat{p}_z+\frac{eB}{2c}\hat{\bar{z}}+\lambda, \tag{7}$$

and

$$d=2i\hat{p}_z-\frac{eB}{2c}\hat{\bar{z}}, \quad d^\dagger=-2i\hat{p}_{\bar{z}}-\frac{eB}{2c}\hat{z}, \tag{8}$$

where $\lambda=mcE/B$. These two sets commute with each other and satisfy the commutation relations

$$[b,b^\dagger]=2m\hbar\omega, \quad [d^\dagger,d]=2m\hbar\omega, \tag{9}$$

where $\omega=eB/mc$ is the cyclotron frequency. Now, the Hamiltonian $\hat{H}$ can be written as

$$\hat{H}=\frac{1}{4m}(b^\dagger b+bb^\dagger)-\frac{\lambda}{2m}(d^\dagger+d)-\frac{\lambda^2}{2m}. \tag{10}$$

To calculate the eigenvalues E and the eigenfunctions Ψ we separate (10) into two mutually commuting parts:

$$\hat{H}=\hat{H}_{\text{osc}}-\hat{T},$$

where $\hat{H}_{\text{osc}}$ denotes the harmonic oscillator part

$$\hat{H}_{\text{osc}}=\frac{1}{4m}(b^\dagger b+bb^\dagger) \tag{11}$$

and the part linear in d and $d^\dagger$ is given by

$$\hat{T}=\frac{\lambda}{2m}(d^\dagger+d)+\frac{\lambda^2}{2m}. \tag{12}$$

The harmonic oscillator eigenvalue equation $\hat{H}_{\text{osc}}\Phi_n=E_n^{\text{osc}}\Phi_n$ is easily solved:

$$\begin{aligned}\Phi_n&=\frac{1}{\sqrt{(2m\hbar\omega)^n n!}}(b^\dagger)^n|0\rangle,\\ E_n^{\text{osc}}&=\frac{\hbar\omega}{2}(2n+1), \quad n=0,1,2,\ldots\end{aligned} \tag{13}$$

leading to a discrete spectrum. However, the eigenvalue equation $\hat{T}\phi=E\phi$ can be analyzed in terms of the eigenvalues of the operators $\hat{r}_i$ denoted by r_i as

$$\begin{aligned}\phi_\alpha&=\exp\left(i(\alpha y+i\frac{m\omega}{2\hbar}xy)\right),\\ E_\alpha&=\frac{\hbar\lambda}{m}\alpha+\frac{\lambda^2}{2m}, \quad \alpha\in\mathbb{R},\end{aligned} \tag{14}$$

yielding a continuous spectrum labeled by α.

Therefore, the eigenfunctions and the energy spectrum of the Hamiltonian $\hat{H}$ are

$$\Psi_{(n,\alpha)}=\Phi_n\otimes\phi_\alpha\equiv|n,\alpha\rangle,$$
$$E_{(n,\alpha)}=\frac{\hbar\omega}{2}(2n+1)-\frac{\hbar\lambda}{m}\alpha-\frac{\lambda^2}{2m},\quad n=0,1,2,\ldots,\quad \alpha\in\mathbb{R}, \tag{15}$$

where $\otimes$ denotes the direct product.

III. ELECTRON MOVING ON NONCOMMUTATIVE PLANE

Let the coordinates of the plane be noncommuting:

$$[\mathbf{x},\mathbf{y}]=i\theta. \tag{16}$$

The parameter θ is a real constant. Noncommutativity can be imposed by treating the coordinates as commuting but requiring that composition of their functions is given in terms of the star product

$$\star\equiv\exp\frac{i\theta}{2}(\overleftarrow{\partial}_x\overrightarrow{\partial}_y-\overleftarrow{\partial}_y\overrightarrow{\partial}_x). \tag{17}$$

Now, we deal with the commutative coordinates x and y but replace the ordinary products with the star product (17). For example, instead of the commutator (16) one defines

$$x\star y-y\star x=i\theta. \tag{18}$$

We would like to study the Hamiltonian (4) in terms of the noncommutative coordinates (16). First we quantize this system by establishing the commutation relations (5). Then, the noncommutativity of the coordinates is taken into account by defining a new operator as

$$\hat{H}\star\Psi(\vec{r})\equiv\hat{H}_{\mathrm{nc}}\Psi(\vec{r}). \tag{19}$$

This definition yields the Hamiltonian operator $\hat{H}_{\mathrm{nc}}$,

$$\hat{H}_{\mathrm{nc}}=\frac{1}{2m}\left[\left((1-\kappa)\hat{p}_x-\frac{eB}{2c}\hat{y}\right)^2+\left((1-\kappa)\hat{p}_y+\frac{eB}{2c}\hat{x}\right)^2\right]+eE\left(\hat{x}-\frac{\theta}{2\hbar}\hat{p}_y\right), \tag{20}$$

when the coordinate representation of momentum $\hat{p}_i=-i\hbar\partial_i$ is used and $\kappa=e\theta B/4\hbar c$.

The eigenvalue problem

$$\hat{H}_{\mathrm{nc}}\Psi^{\mathrm{nc}}=E^{\mathrm{nc}}\Psi^{\mathrm{nc}} \tag{21}$$

is as in ordinary quantum mechanics in spite of the fact that electron moves on noncommutative plane. The solutions of this problem can be worked out in a manner similar to the one used in Sec. II although here there exists a term linear in momentum which was not present in $\hat{H}$. Then, let us introduce two sets of operators

$$\tilde{b}^\dagger=-2i\hat{\bar{p}}_z+\frac{eB}{2c}\hat{z}+\lambda_-,\quad \tilde{b}=2i\hat{\bar{p}}_z+\frac{eB}{2c}\hat{\bar{z}}+\lambda_-, \tag{22}$$

and

$$\tilde{d}=2i\hat{\bar{p}}_z-\frac{eB}{2c}\hat{\bar{z}},\quad \tilde{d}^\dagger=-2i\hat{\bar{p}}_{\bar{z}}-\frac{eB}{2c}\hat{z}, \tag{23}$$

where $\hat{\tilde{p}}_z=\gamma\hat{p}_z$; $\gamma=1-\kappa$. The real parameter λ_- will be fixed later. The sets of operators $(\tilde{b},\tilde{b}^\dagger)$ and $(\tilde{d},\tilde{d}^\dagger)$ commute with each other. Moreover, they satisfy the commutation relations

$$[\tilde{b},\tilde{b}^\dagger]=2m\hbar\tilde{\omega},\quad [\tilde{d}^\dagger,\tilde{d}]=2m\hbar\tilde{\omega}, \tag{24}$$

where $\tilde{\omega}=\gamma\omega$. The Hamiltonian $\hat{H}_{\rm nc}$ can be written as

$$\hat{H}_{\rm nc}=\frac{1}{4m}(\tilde{b}^\dagger\tilde{b}+\tilde{b}\tilde{b}^\dagger)-\frac{\lambda_+}{2m}(\tilde{d}^\dagger+\tilde{d})-\frac{\lambda_-^2}{2m}, \tag{25}$$

where the parameters $\lambda_\pm$ are fixed to be

$$\lambda_\pm=\lambda\pm\frac{emE\theta}{4\gamma\hbar}. \tag{26}$$

We take into account only the values of the noncommutativity parameter $\theta\neq 4\hbar c/eB$. Otherwise, $\lambda_\pm$ diverge. We will give a brief discussion of this fact in the last section.

Observing the similarity between the Hamiltonians (10) and (25) the solutions of the eigenvalue problem (21) can be read from (15) as

$$\begin{aligned}\Psi^{\rm nc}_{(n,\alpha,\theta)}\equiv|n,\alpha,\theta\rangle&=\frac{1}{\sqrt{(2m\hbar\tilde{\omega})^n n!}}\exp\left(i(\alpha y+\frac{m\tilde{\omega}}{2\hbar}xy)\right)(\tilde{b}^\dagger)^n|0\rangle,\\ E^{\rm nc}_{(n,\alpha,\theta)}&=\frac{\hbar\tilde{\omega}}{2}(2n+1)-\frac{\hbar\gamma\lambda_+}{m}\alpha-\frac{m}{2}\lambda_-^2,\quad n=0,1,2,\ldots,\quad \alpha\in\mathbb{R}.\end{aligned} \tag{27}$$

We would like to emphasize that the results of Sec. II are recovered if the noncommutativity parameter θ is switched off.

IV. HALL CONDUCTIVITY ON NONCOMMUTATIVE PLANE

We would like to find conductivity resulting from the Hamiltonian $\hat{H}_{\rm nc}$. The first step in this direction is to define the related current. Although the identification of derivatives with momentum operators $\partial_i=(i/\hbar)\hat{p}_i$ is only valid in coordinate representation, we will use this definition in defining the current operator $\hat{\vec{J}}$ on noncommutative plane as

$$\hat{\vec{J}}=\frac{ie\rho}{\hbar}[\hat{H}_{\rm nc},\hat{\vec{r}}]=\frac{e\gamma\rho}{m}\left(\gamma\hat{\vec{p}}+\frac{e}{c}\vec{A}+\vec{a}\right), \tag{28}$$

where $\vec{a}=(0,-meE\theta/2\hbar\gamma)$ and ρ denotes electron density.

Now, the expectation value of the current operator $\langle\hat{\vec{J}}\rangle$ can be calculated with respect to the eigenstates $|n,\alpha,\theta\rangle$ (27) leading to

$$\begin{aligned}\langle\hat{J}_x\rangle&=0,\\ \langle\hat{J}_y\rangle&=-\gamma\left(\frac{\rho ec}{B}\right)E.\end{aligned} \tag{29}$$

Therefore, the Hall conductivity on noncommutative plane, denoted by $\sigma_H^{\rm nc}$, is

$$\sigma_H^{\rm nc}=-\gamma\left(\frac{\rho ec}{B}\right). \tag{30}$$

Recall that in the ordinary case the Hall conductivity σ_H and the filling factor ν are given as

$$\sigma_H=\frac{e^2}{h}\nu, \quad \nu=\frac{\Phi_0\rho}{B}, \tag{31}$$

where $\Phi_0=hc/e$. Comparison of (30) with (10) suggests that one can interpret the noncommutative case as a theory of Hall effect on commuting plane with an effective magnetic field

$$B_{\text{eff}}=\frac{B}{1-\dfrac{e\theta B}{4\hbar c}}. \tag{32}$$

Moreover, the effective filling factor

$$\nu_{\text{eff}}=\frac{\Phi_0\rho}{B}\left(1-\frac{e\theta B}{4\hbar c}\right), \tag{33}$$

can also be defined.

V. THE AHARONOV–BOHM EFFECT

We would like to calculate the Aharonov–Bohm effect on noncommutative plane by examining the action appearing in the related path integral. When we deal with quantum mechanics in the usual spaces it is the related classical action. However, it is not clear what should be the definition of action appropriate for path integrals when noncommutativity is taken into account. Because, we define Hamiltonian operators in terms of the receipt used in (19) where we identify $\partial_i\equiv(i/\hbar)\hat{p}_i$. We propose to define the path integral in noncommutative space as

$$Z=\int d^2p\,d^2r\,\exp\left(\frac{i}{\hbar}\int \mathrm{d}t[\vec{p}\cdot\dot{\vec{r}}-H_{\text{eff}}(\vec{r},\vec{p})]\right), \tag{34}$$

where $(\vec{r},\vec{p})$ define the commuting phase space and $H_{\text{eff}}(\vec{r},\vec{p})$ will be obtained from the related Hamiltonian operator in noncommutative space by replacing the operators $\hat{\vec{p}}$, $\hat{\vec{r}}$ with c-number variables $\vec{p}$, $\vec{r}$.

Let us deal with the Hamiltonian operator on noncommutive plane in the constant external electric field $\vec{E}=(E_x,E_y)$ and the constant magnetic field B in the symmetric gauge (2):

$$\hat{H}'_{\text{nc}}=\frac{1}{2m}\left[\left(\gamma\hat{p}_x-\frac{eB}{2c}\hat{y}\right)^2+\left(\gamma\hat{p}_y+\frac{eB}{2c}\hat{x}\right)^2\right]+eE_x\left(\hat{x}-\frac{\theta}{2\hbar}\hat{p}_y\right)+eE_y\left(\hat{y}+\frac{\theta}{2\hbar}\hat{p}_x\right). \tag{35}$$

Although the Hamiltonian operator

$$\hat{H}_\theta\equiv\frac{\gamma^2}{2m}\hat{\vec{p}}^2+\frac{e^2}{2mc^2}\vec{A}^2+\frac{e\gamma}{2mc}(\hat{\vec{p}}\cdot\vec{A}+\vec{A}\cdot\hat{\vec{p}})+\hat{\vec{p}}\cdot\vec{K}+e\vec{E}\cdot\hat{\vec{r}}, \tag{36}$$

where $\vec{K}=(e\theta/2\hbar)(-E_y,E_x)$, is equivalent to (35) only when the vector potential $\vec{A}$ is as given in (2), we assume that at least at the first order in θ it is valid for any gauge potential.

The c-number effective Hamiltonian corresponding to (36) is

$$H_{\text{eff}}=\frac{\gamma^2}{2m}\vec{p}^2+\frac{e^2}{2mc^2}\vec{A}^2+\vec{p}\cdot\left(\frac{e\gamma}{mc}\vec{A}+\vec{K}\right)+e\vec{E}\cdot\vec{r}. \tag{37}$$

Thus, the partition function can be written as

$$Z_{\rm nc}=N\int d^2pd^2r\,\exp\left(\frac{i}{\hbar}\int_{t_1}^{t_2}{\rm d}t\left[\vec{p}\cdot\left(\dot{\vec{r}}-\frac{e\gamma}{mc}\vec{A}-\vec{K}\right)-\frac{\gamma^2}{2m}\vec{p}^{\,2}-\frac{e^2}{2mc^2}\vec{A}^2-e\vec{E}\cdot\vec{r}\right]\right), \tag{38}$$

where N is a normalization constant. Now, we can integrate over the momenta $\vec{p}$ to obtain

$$Z_{\rm nc}=\frac{2m}{\gamma^2}N\int d^2r\,\exp\left(\frac{i}{\hbar}\int_{t_1}^{t_2}{\rm d}t\left[\frac{m}{2\gamma^2}\dot{\vec{r}}^{\,2}-\frac{m}{\gamma^2}\dot{\vec{r}}\cdot\left(\frac{e\gamma}{mc}\vec{A}+\vec{K}\right)+\frac{e}{c\gamma}\vec{A}\cdot\vec{K}+\frac{m}{2\gamma^2}\vec{K}^2-e\vec{E}\cdot\vec{r}\right]\right). \tag{39}$$

The constant K^2 term is irrelevant. In terms of a new normalization constant N' we can write

$$Z_{\rm nc}=N'\int d^2r\,\exp\left(\frac{i}{\hbar}S_0-\frac{im}{\hbar\gamma^2}\int_{t_1}^{t_2}{\rm d}t\,\dot{\vec{r}}\cdot\left(\frac{e\gamma}{mc}\vec{A}+\vec{K}\right)\right), \tag{40}$$

where we defined

$$S_0=\int_{t_1}^{t_2}{\rm d}t\left[\frac{m}{2\gamma^2}\dot{\vec{r}}^{\,2}-e\vec{E}\cdot\vec{r}+\frac{e}{c\gamma}\vec{A}\cdot\vec{K}\right]. \tag{41}$$

The last term in the exponent of (40) can be written as

$$i\delta=-\frac{im}{\gamma^2\hbar}\int_{\vec{r}(t_1)}^{\vec{r}(t_2)}{\rm d}\vec{r}\cdot\left(\frac{e\gamma}{mc}\vec{A}+\vec{K}\right). \tag{42}$$

To investigate the Aharonov–Bohm effect for noncommuting coordinates, let $\vec{A}=\vec{\nabla}f(\vec{r})$. Then

$$\delta=-\frac{m}{\gamma^2\hbar}\int_{\vec{r}(t_1)}^{\vec{r}(t_2)}{\rm d}\vec{r}\cdot\left(\frac{e\gamma}{mc}\vec{\nabla}f(\vec{r})+\vec{K}\right) \tag{43}$$

depends only on the points $\vec{r}(t_1)$, $\vec{r}(t_2)$ which are kept fixed in path integrals. Therefore, it is a phase factor. i.e., propagation with the action S_0 is changed up to the phase factor (43).

The Aharonov–Bohm effect can now be calculated as the integral of the phase factor (43) along a loop enclosing a magnetic flux. $\vec{K}$ is a constant vector so that, it does not contribute to the Aharonov–Bohm phase:

$$\oint{\rm d}\vec{r}\cdot\vec{K}=0. \tag{44}$$

As in the ordinary case the unique contribution is due to the gauge potential

$$\Phi_{\rm AB}^{\rm nc}=-2\pi\frac{BS}{\gamma\Phi_0}, \tag{45}$$

where S denotes the surface enclosed. Obviously, when $\theta=0$ the usual Aharonov–Bohm phase results

$$\Phi_{\rm AB}=-2\pi\frac{BS}{\Phi_0}. \tag{46}$$

Thus we can envisage the noncommutative case as a theory in commuting coordinates with an effective magnetic field

$$B_{\text{eff}}=\frac{B}{1-\dfrac{e\theta B}{4\hbar c}}, \tag{47}$$

which is the one obtained previously (32).

VI. DISCUSSIONS

Electrons moving on a noncommutative plane when uniform external magnetic and electric fields are present can be envisaged as the usual motion of electrons experiencing an effective magnetic field (32). This is one of our main results. It followed by considering either Hall effect or Aharonov–Bohm phase in noncommuting coordinates. By tuning the value of the noncommutativity parameter θ we can offer two different interpretations of this fact.

The fractional quantum Hall effect is one of the most interesting features of low dimensional systems.[7] For electrons moving on a plane in a magnetic field which is perpendicular to the plane and a uniform external electric field which is in the plane, the observed Hall conductivity is

$$\sigma_H=f\frac{e^2}{h},$$

where $f=1/3,2/3,1/5,\ldots$, denoting the fractional quantized values of the filling factor ν. We would like to interpret this phenomena, which is known as the fractional quantum Hall effect, in terms of the Hall effect on noncommutative plane. More precisely we identify the effective filling factor (33) with the observed value f by fixing the value of θ to be θ_H:

$$\nu_{\text{eff}}\big|_{\theta=\theta_H}=f. \tag{48}$$

In fact, this can be solved as

$$\theta_H=\frac{2\Phi_0}{\pi B}\left(1-f\frac{B}{\Phi_0\rho}\right). \tag{49}$$

Therefore, when θ is fixed to be θ_H one can envisage the Hall effect on noncommutative plane as the usual fractional quantum Hall effect.

Composite fermions are a new kind of particles appearing in condensed matter physics to provide an explanation of the behavior of electrons moving on plane when a strong magnetic field B is present.[8] Electrons possessing $2p$; $p=1,2,\ldots$, flux quanta (vortices) can be thought of as being composite fermions. One of the most important features of them is they feel effectively the magnetic field

$$B^*=B-2p\Phi_0\rho, \tag{50}$$

where ρ is the electron density. To interpret electrons moving on noncommutative space in the magnetic field B as the usual composite fermions we should tune θ such that

$$B_{\text{eff}}\big|_{\theta=\theta_c}=B^*, \tag{51}$$

where B_{eff} is given in (32). We solve this to obtain

$$\theta_c=\frac{2\Phi_0}{\pi B}\left[1-\left(1-2p\frac{\rho\Phi_0}{B}\right)^{-1}\right], \tag{52}$$

which in the limit of strong magnetic field leads to

$$\theta_c \approx 4p\frac{\rho}{\pi}\left(\frac{\Phi_0}{B}\right)^2. \tag{53}$$

Thus, composite fermions can be envisaged as electrons moving in noncommutative plane in the magnetic field B and the electric field E when we fix $\theta=\theta_c$.

The Aharonov–Bohm phase $\Phi_{\mathrm{AB}}^{\mathrm{nc}}$ possesses a very interesting limit. Let us deal with $\theta\neq 0$ and the magnetic field satisfying the condition

$$B \gg \frac{4c\hbar}{e\theta}. \tag{54}$$

For these values of magnetic field the Aharonov–Bohm phase $\Phi_{\mathrm{AB}}^{\mathrm{nc}}$ (45) becomes

$$\Phi_{\mathrm{AB}}^{\mathrm{nc}} \approx \frac{4c\hbar S}{e\theta\Phi_0}, \tag{55}$$

which is independent of B. For $\vec{E}=0$ the action S_0 reads

$$\tilde{S}_0 \equiv S_0|_{\vec{E}=0} = \frac{m}{2\gamma^2}\int \mathrm{d}t\, \dot{\vec{r}}^2,$$

which depends on the magnetic field as B^{-2} when (54) is satisfied. If the phase $\Phi_{\mathrm{AB}}^{\mathrm{nc}}$ can be measured for the particle propagating with the action $\tilde{S}_0$ when B satisfies (54) and observed that it is independent of B after a certain value of B, it may be evidence for spatial noncommutativity. Obviously, this conclusion is valid only for small values of θ. Because we assume it when we write the action (36). In Ref. 9 the Aharonov–Bohm effect in noncommutative coordinates was studied in terms of a field theoretical approach where an experiment to detect spatial noncomutativity was proposed.

Critical value of θ defined as

$$\theta^* = \frac{4\hbar c}{eB} \tag{56}$$

is avoided through this work. At this value of θ all of our analysis fails, because $\gamma=1-eB\theta/4\hbar c$ cannot be inverted, thus $\lambda_{\pm}$ (26) are not well defined. Indeed, when $\theta=\theta^*$ the Hamiltonian in noncommutative coordinates (20) becomes

$$\hat{H}_{\mathrm{nc}}(\theta=\theta^*) = \frac{m\omega^2}{8}(\hat{x}^2+\hat{y}^2) + eE\left(\hat{x}-\frac{\theta^*}{2\hbar}\hat{p}_y\right). \tag{57}$$

i.e., the terms quadratic in momenta disappear, however a term linear in momenta survives. Obviously, this system should be studied separately.

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Wigner functions with boundaries

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We consider the general Wigner function for a particle confined to a finite interval and subject to Dirichlet boundary conditions. We derive the boundary corrections to the ''stargenvalue'' equation and to the time evolution equation. These corrections can be cast in the form of a boundary potential contributing to the total Hamiltonian which together with a subsidiary boundary condition is responsible for the discretization of the energy levels. We show that a completely analogous formulation (in terms of boundary potentials) is also possible in standard operator quantum mechanics and that the Wigner and the operator formulations are also in one-to-one correspondence in the confined case. In particular, we extend Baker's converse construction to bounded systems. Finally, we elaborate on the applications of the formalism to the subject of Wigner trajectories, namely in the context of collision processes and quantum systems displaying chaotic behavior in the classical limit. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1504885]

I. INTRODUCTION

The Moyal–Wigner–Weyl quantization constitutes a phase space quantization method alternative to canonical or path integral quantizations.[1–13] Instead of wave functions and operators one deals with quasidistribution (Wigner) functions and ordinary c-functions in phase space. The Weyl symbol associated with a general operator $\hat{A}(\hat{x},\hat{p})$ is given by[1,4,12]

$$A^W(x,p)\equiv\frac{\hbar}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\xi\int_{-\infty}^{+\infty}\mathrm{d}\eta\,\mathrm{Tr}\{\hat{A}(\hat{x},\hat{p})e^{i\xi\hat{x}+i\eta\hat{p}}\}e^{-i\xi x-i\eta p}. \tag{1}$$

In this framework the average of $\hat{A}(\hat{x},\hat{p};t)$ is evaluated according to the formula: $\langle\psi|\hat{A}(\hat{x},\hat{p};t)|\psi\rangle=\int_{-\infty}^{+\infty}\mathrm{d}x\int_{-\infty}^{+\infty}\mathrm{d}p\,A^W(x,p;0)F^W(x,p;t)$, where $F^W(x,p;t)$ is proportional to the Weyl symbol of the quantum density matrix, $\hat{\rho}$, and is known as the Wigner function of the system.[2] For a pure state, $\hat{\rho}=|\psi\rangle\langle\psi|$, the Wigner function can be shown to be of the form:

$$F^W(x,p;t)\equiv\frac{1}{\pi\hbar}\int_{-\infty}^{+\infty}\mathrm{d}y e^{-2ipy/\hbar}\psi^*(x-y;t)\psi(x+y;t), \tag{2}$$

where $\psi(x;t)$ is the solution of Schrödinger's equation: $i\hbar\,(\partial\psi/\partial t)\,(x;t)=\hat{H}\psi(x;t)$. The Weyl ''transform'' establishes a biunivocal correspondence between the quantum algebra $\hat{\mathcal{A}}$ of observables with standard operator product $\cdot$ and quantum commutator $[,]$, on the one hand, and the ''classical'' algebra $\mathcal{A}$ defined over the classical phase space T^*M with a ''star-product'' $*$ and a Moyal sine-bracket $[,]_M$, on the other hand. The two latter operations are given by[3,14]

$$A^W(x,p)*B^W(x,p)=A^W(x,p)e^{(i\hbar/2)\overleftrightarrow{\mathcal{J}}}B^W(x,p)=A^W\left(x,p-\frac{i\hbar}{2}\overrightarrow{\partial}_x\right)B^W\left(x,p+\frac{i\hbar}{2}\overleftarrow{\partial}_x\right), \tag{3}$$

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$$[A^W(x,p),B^W(x,p)]_M=\frac{1}{i\hbar}(A^W*B^W-B^W*A^W)=\frac{2}{\hbar}A^W(x,p)\sin\left(\frac{\hbar}{2}\overleftrightarrow{\mathcal{J}}\right)B^W(x,p), \tag{4}$$

where

$$\overleftrightarrow{\mathcal{J}}\equiv\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\vec{\partial}}{\partial p}-\frac{\overleftarrow{\partial}}{\partial p}\frac{\vec{\partial}}{\partial x}\right).$$

One realizes immediately that in the limit $\hbar\to 0$, the star product and the Moyal bracket become the ordinary product of c-numbers and the Poisson bracket, respectively. It is also easy to check that the dynamics of the Wigner function is governed by the Moyal bracket (4):

$$\frac{\partial F^W}{\partial t}(x,p;t)=[H^W(x,p),F^W(x,p;t)]_M, \tag{5}$$

where $H^W(x,p)$ is the Weyl symbol of the quantum Hamiltonian, $\hat{H}(\hat{x},\hat{p})$.

If the time-independent wave function happens to be an energy eigenstate with eigenvalue E, i.e., $\hat{H}\psi(x)=E\psi(x)$, then[15–18] the Wigner function $F_E^W(x,p)$ satisfies an equivalent $*$-genvalue equation with identical $*$-genvalue:

$$H^W(x,p)*F_E^W(x,p)=F_E^W(x,p)*H^W(x,p)=EF_E^W(x,p). \tag{6}$$

More generally, to every eigenstate $|a\rangle$ with eigenvalue a of some operator $\hat{A}$, there is one and only one associated stargenfunction $F_a^W(x,p)$, which is a solution of the stargenvalue equation: $A^W(x,p)*F_a^W(x,p)=aF_a^W(x,p)$.[6,15,18] This stargenfunction allows for the evaluation of the probability of measuring the eigenvalue a:

$$\mathcal{P}(A=a)=\int \mathrm{d}x\int \mathrm{d}p\, F^W(x,p)F_a^W(x,p). \tag{7}$$

It is important to emphasize that, in most cases, the advantage in the Wigner approach does not reside in solving specific problems. Rather, it should be regarded as a means to grasp certain conceptual aspects of quantum mechanics and its connection with classical mechanics. Nevertheless, in some situations it could be a better starting point for finding solutions to specific problems. The Wigner formulation is a useful tool to derive kinetic equations in particular regimes (dilute gas, weakly interacting particles). In nonequilibrium statistical mechanics this is a familiar approach.[19] In collision processes the Wigner methods are also a useful tool.[4,9] Contrary to the standard operator approach they display the important advantage of making possible the use of approximation methods similar to the ones used in the full classical treatment. Furthermore the related subject of Wigner trajectories[4,5,20,21] provides a pictorial and practical tool to study collision process and it is of similar importance in the context of quantum chaotic systems.[4,13,22–24]

Boundary value problems, on the other hand, are one of the cornerstones of quantum mechanics. These are much more realistic models and moreover they entail a discretization of observables' spectra, which is one of the main features of quantum mechanics. They appear in virtually all branches of physics, ranging from quantum mechanics to general relativity, open strings and D-branes, where the noncommutative *-product and the Moyal bracket also find several applications.[16,25,26] In standard operator quantum mechanics some famous examples of boundary value problems include the Kondo problem,[27] quantum Hall liquids with constriction,[28] and the Callan–Rubakov model.[29] Furthermore one of the simplest collision processes is the collision against an impenetrable boundary and some standard examples of quantum chaotic systems are bounded.[4,24]

In spite of the importance of boundary value problems in general and of these models in particular, Wigner quantum mechanics does not provide a self-contained and consistent formula-

tion of confined systems. The aim of this paper is thus to provide such formulation. More precisely our aim is to generalize the two key equations of Wigner quantum mechanics [Eqs. (5) and (6)] to the case when the original wave function is confined to an interval and satisfies Dirichlet boundary conditions.

Let us then consider a general confined system. In standard operator quantum mechanics, we first solve the Schrödinger equation in the bulk (with Hamiltonian $\hat{H}$), subsequently impose the boundary conditions that pin down the physical solutions, and finally impose the wave function to be zero beyond the bulk. Alternatively, we may be able to provide a boundary potential $\hat{V}_D$ that confines the wave function and then solve the unconstrained system, with extended Hamiltonian $\hat{H}_D=\hat{H}+\hat{V}_D$ and the original conditions at the boundaries.

To obtain the solution of the problem in terms of Wigner functions, we just have to insert the solution obtained in the Schrödinger formulation into the definition of the Wigner function. This was the method followed in Ref. 5. But the question that remains is: how do we solve the problem within the Wigner–Weyl formulation?

The first approach cannot be easily translated into the Wigner framework because the highly nonlocal character of the Wigner function produces nontrivial effects of the boundary on the bulk part of the Wigner function, so that the stargenvalue equation has to be altered, as we shall see [Secs. II–IV].

The second procedure seems to be the natural starting point to derive, through the Weyl map, the Wigner formulation for the bounded system. However this is not an easy task, mainly because the formulation of confined systems in terms of boundary potentials is already problematic at the standard operator level. In Sec. VI we will consider this approach and (a) consistently solve the problem at the standard operator level and (b) use the Weyl map to recover the bounded stargenvalue equation derived in Sec. III.

This paper is organized as follows. In Sec. II, we discuss some aspects of the boundary conditions satisfied by the Wigner function. In Secs. III–V we evaluate the boundary corrections to the $*$-genvalue equation (6) and the time evolution equation (5) directly from the general formula of the confined wave function. Furthermore, we (a) extend Baker's converse construction to bounded systems and (b) argue that the results obtained are compatible with the preservation of the Wigner function's normalization under time evolution. In Sec. VI we develop the boundary potential approach for standard operator quantum mechanics and show that through the Weyl map this formulation yields the proper Wigner formulation of confined systems. In Sec. VII we discuss some practical applications of the formalism: the computation of Wigner trajectories for confined chaotic systems and for collision processes. Finally, in Sec. VIII we present our conclusions.

II. WIGNER FUNCTION IN A FINITE INTERVAL

Let us assume that the domain of the wave function is the finite interval $a<x<b$ with $a<b$, so that the wave function vanishes outside this interval. As we now argue, quantum confined systems cannot be treated, in the Wigner formalism, through the standard procedure of solving a differential equation and imposing the boundary conditions thereafter. In particular, the energy stargenfunctions for these systems do not satisfy the stargenvalue equation (6) with the Hamiltonian of the bulk.

As an example, consider the free particle in the infinite well, with $a=-b=-L/2$. The stargenvalue equation would be of the form:

$$\frac{p^2}{2m}*F^W(x,p)=EF^W(x,p).$$

If we solve the corresponding Schrödinger equation with Dirichlet boundary conditions we get for the fundamental state:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)=E\psi(x)\Rightarrow\psi_1(x)=\sqrt{\frac{2}{L}}\cos\left(\frac{\pi}{L}x\right).$$

If we now determine the associated Wigner function using (2) we get[5] that $F^W(x,p)$ is given by Eqs. (39) and (40). We can easily check that $F^W(x,p)$ does not satisfy the previous stargenvalue equation and thus the only possible conclusion is that this equation has to be altered. Similarly, we can check that the time evolution of the system does not satisfy the Moyal equation with bulk Hamiltonian.

Let us start by studying the general properties of the Wigner function for a confined system. Since the wave function vanishes outside the interval $]a,b[$, it satisfies the condition:

$$\psi^*(x-y)\psi(x+y)=0 \quad \text{unless} \quad a<x-y<b \quad \text{and} \quad a<x+y<b.$$

This means that: (1) for $a<x\leqslant x_0=(a+b)/2$, we have

$$\psi^*(x-y)\psi(x+y)=0 \quad \text{unless} \quad a-x<y<x-a,$$

similary, (2) for $x_0<x<b$:

$$\psi^*(x-y)\psi(x+y)=0 \quad \text{unless} \quad x-b<y<b-x,$$

and finally, (3) for $x\leqslant a$ or $x\geqslant b$:

$$\psi^*(x-y)\psi(x+y)=0, \quad \forall y.$$

We conclude that the Wigner function (2) for the bounded system can be written as

$$F^W(x,p)=\frac{1}{\pi\hbar}\int_{-\infty}^{+\infty}\mathrm{d}y\, e^{-2ipy/\hbar}\psi^*(x-y)\psi(x+y)=\Theta_1(x)F_1^W(x,p)+\Theta_2(x)F_2^W(x,p), \quad (8)$$

where

$$\begin{aligned}\Theta_1(x)&=\theta(x-a)-\theta(x-x_0)=\begin{cases}1, & \text{if } a<x\leqslant x_0\\ 0, & \text{otherwise,}\end{cases}\\ \Theta_2(x)&=\theta(x-x_0)+\theta(b-x)-1=\begin{cases}1, & \text{if } x_0<x<b\\ 0, & \text{otherwise.}\end{cases}\end{aligned} \quad (9)$$

$\theta(x)$ is the Heaviside's step function: $\theta(x)=1$ iff $x>0$ and $\theta(x)=0$ otherwise, and finally:

$$\begin{cases}F_1^W(x,p)=\dfrac{1}{\pi\hbar}\displaystyle\int_{a-x}^{x-a}\mathrm{d}y\, e^{-2ipy/\hbar}\psi^*(x-y)\psi(x+y),\\ F_2^W(x,p)=\dfrac{1}{\pi\hbar}\displaystyle\int_{x-b}^{b-x}\mathrm{d}y\, e^{-2ipy/\hbar}\psi^*(x-y)\psi(x+y).\end{cases} \quad (10)$$

Since the wave function or its derivatives are possibly discontinuous at $x=a$ and $x=b$, and to avoid possible misinterpretations in our future calculations, the previous integrals are defined as improper: $\int_{a-x}^{x-a}$ stands for $\lim_{c\to a^+}\int_{c-x}^{x-c}$ and likewise $\int_{x-b}^{b-x}$ stands for $\lim_{c\to b^-}\int_{x-c}^{c-x}$. Notice that this is fully compatible with our previous results identifying the domain where $\psi^*(x-y)\psi(x+y)$ is not identically zero.

As a second remark let us point out that the boundary conditions on $\psi(x)$ are imposed on the bulk side of the boundary. For instance, the Dirichlet boundary conditions would be of the form: $\lim_{\epsilon\to 0^+}\psi(a+\epsilon)=\lim_{\epsilon\to 0^+}\psi(b-\epsilon)=0$, which is not the same as requiring $\psi(a)=\psi(b)=0$, since these are valid independently of the boundary conditions satisfied by $\psi(x)$. This is so

because $\psi(x)$ is confined to the open interval $]a,b[$. It is important to realize that we could equally choose to defined "confined" as "confined to the close interval $[a,b]$" and in fact for Dirichlet boundary conditions the two prescriptions yield exactly the same wave function. However, the confinement to an open interval makes some of the future steps more natural (though occasionally more involved) and this is why we choose to work with this prescription.

Finally, and to make our future expressions more compact, we introduce the notation: $f(c^{\pm})=\lim_{\epsilon\to 0^+} f(c\pm\epsilon)$, which will be used whenever there is no risk of misunderstanding.

Let us then study the boundary conditions that are satisfied by the Wigner function of a confined system. From (8)–(10), one realizes immediately that:

$$\begin{cases} F^W(a^+,p)=F_1^W(a^+,p)=F_2^W(b^-,p)=F^W(b^-,p)=0, \\ F^W(x_0^-,p)=F_1^W(x_0,p)=F_2^W(x_0,p)=F^W(x_0^+,p), \end{cases} \tag{11}$$

where, accordingly to the previous notation, $F^W(a^+,p)$ stands for the limit $\lim_{\epsilon\to 0^+} F^W(a+\epsilon,p)$ and likewise for the other expressions. Since $F^W(x,p)$ is defined as an improper integral it already requires the evaluation of a limit. This limit will always be calculated before the limit $\lim_{x\to a^+} F^W(x,p)$, i.e., first we evaluate the Wigner function for all x and only then do we compute whatever limits of the Wigner function. Let us proceed: Eq. (11) means that $F^W(x,p)$ is continuous at x_0 and obeys Dirichlet boundary conditions irrespective of the particular boundary conditions satisfied by the associated wave function ψ. The boundary conditions obeyed by the confined wave function act only on the derivatives of the Wigner function. For $a<x\leqslant x_0$ a straightforward computation leads to:

$$\frac{\partial F_1^W}{\partial x}(x,p)=\frac{1}{\pi\hbar}\Bigg\{ e^{-(2ip/\hbar)(x-a)}\psi^*(a^+)\psi(2x-a^+)+e^{-(2ip/\hbar)(a-x)}\psi^*(2x-a^+)\psi(a^+) + \int_{a-x}^{x-a} dy\, e^{-2ipy/\hbar}[\psi'^*(x-y)\psi(x+y)+\psi^*(x-y)\psi'(x+y)]\Bigg\}, \tag{12}$$

where the prime denotes the derivative with respect to the argument. Consequently,

$$\frac{\partial F^W}{\partial x}(a^+,p)=\lim_{x\to a^+}\frac{\partial F_1^W}{\partial x}(x,p)=\frac{2}{\pi\hbar}|\psi(a^+)|^2,$$

$$\frac{\partial F^W}{\partial x}(x_0^-,p)=\frac{\partial F_1^W}{\partial x}(x_0,p)=\frac{1}{\pi\hbar}[e^{-(ip/\hbar)(b-a)}\psi^*(a^+)\psi(b^-)+e^{-(ip/\hbar)(a-b)}\psi^*(b^-)\psi(a^+)] + \frac{1}{\pi\hbar}\lim_{\epsilon\to 0^+}\int_{((a-b)/2)+\epsilon}^{((b-a)/2)-\epsilon} dy\, e^{-2ipy/\hbar}[\psi'^*(x_0-y)\psi(x_0+y) + \psi^*(x_0-y)\psi'(x_0+y)]. \tag{13}$$

Similarly, from F_2^W we get

$$\frac{\partial F^W}{\partial x}(b^-,p)=\lim_{x\to b^-}\frac{\partial F_2^W}{\partial x}(x,p)=-\frac{2}{\pi\hbar}|\psi(b^-)|^2,$$

$$\frac{\partial F^W}{\partial x}(x_0^+,p)=\frac{\partial F_2^W}{\partial x}(x_0,p)$$

$$=-\frac{1}{\pi\hbar}[e^{-(ip/\hbar)(b-a)}\psi^*(a^+)\psi(b^-)+e^{-(ip/\hbar)(a-b)}\psi^*(b^-)\psi(a^+)]$$

$$+\frac{1}{\pi\hbar}\lim_{\epsilon\to 0^+}\int_{((a-b)/2)+\epsilon}^{((b-a)/2)-\epsilon}dy\, e^{-2ipy/\hbar}[\psi'^*(x_0-y)\psi(x_0+y)$$

$$+\psi^*(x_0-y)\psi'(x_0+y)]. \tag{14}$$

We conclude that in general $(\partial F^W/\partial x)(x_0^-,p)\neq(\partial F^W/\partial x)(x_0^+,p)$, except for Dirichlet boundary conditions [i.e., $\psi(a^+)=\psi^*(a^+)=\psi(b^-)=\psi^*(b^-)=0$], in which case the Wigner function also obeys Neumann boundary conditions: $(\partial F^W/\partial x)(a^+,p)=(\partial F^W/\partial x)(b^-,p)=0$. We can carry on with this process and compute the second and third derivatives. The results concerning the boundary conditions can then be summarized as follows. All Wigner functions for bounded systems satisfy Eq. (11). These are consistency conditions and, given their general character, cannot give countenance to the discretization of the energy spectrum. The boundary conditions satisfied by the confined wave function yield subsidiary conditions on the Wigner function:

Dirichlet: $\psi(a^+)=\psi^*(a^+)=\psi(b^-)=\psi^*(b^-)=0$,

$$\frac{\partial F^W}{\partial x}(a^+,p)=\frac{\partial F^W}{\partial x}(b^-,p)=0. \tag{15}$$

If a Wigner function satisfies these Neumann conditions, then it *automatically* verifies:

$$\begin{cases}\dfrac{\partial F^W}{\partial x}(x_0^-,p)=\dfrac{\partial F^W}{\partial x}(x_0^+,p),\\[2ex] \dfrac{\partial^2 F^W}{\partial x^2}(a^+,p)=\dfrac{\partial^2 F^W}{\partial x^2}(b^-,p)=0,\\[2ex] \dfrac{\partial^2 F^W}{\partial x^2}(x_0^-,p)=\dfrac{\partial^2 F^W}{\partial x^2}(x_0^+,p)\,.\end{cases} \tag{16}$$

Obviously, this pattern does not continue indefinitely. For instance, $(\partial^3 F^W/\partial x^3)(a^+,p)=(8/\pi\hbar)\,|\psi'(a^+)|^2\neq 0$. It is also important to emphasize that contrary to Eq. (15), the additional set of equations (16), being just a consequence of Eq. (15), do not constrain F^W any further.

Neumann: $\psi'(a^+)=\psi'^*(a^+)=\psi'(b^-)=\psi'^*(b^-)=0$,

$$\begin{cases}\dfrac{\partial F^W}{\partial x}(a^+,p)\neq 0, & \dfrac{\partial F^W}{\partial x}(b^-,p)\neq 0,\\[2ex] \dfrac{\partial F^W}{\partial x}(x_0^-,p)\neq\dfrac{\partial F^W}{\partial x}(x_0^+,p),\\[2ex] \dfrac{\partial^2 F^W}{\partial x^2}(a^+,p)=\dfrac{\partial^2 F^W}{\partial x^2}(b^-,p)=0,\\[2ex] \dfrac{\partial^2 F^W}{\partial x^2}(x_0^-,p)=\dfrac{\partial^2 F^W}{\partial x^2}(x_0^+,p).\end{cases} \tag{17}$$

We also have: $(\partial^3 F^W/\partial x^3)(a^+,p)\neq 0$.

The former results show that the confinement of the system and the boundary conditions satisfied by the wave function influence the Wigner function in a very nontrivial way. Furthermore, conditions (11), (15), and (16) will play an important part in the derivation of the new $*$-genvalue equation for bounded systems.

However, one should realize that the previous results also display some less interesting features: let us focus on the case in which the wave function satisfies Dirichlet boundary conditions. If the system is also confined then the Wigner function will satisfy the set of conditions (11), (15), (16). The problem is that the converse result is not valid, i.e., conditions (11), (15), (16) do not imply the confinement of the system and it is also not clear if, in general, they imply that the original wave function satisfy Dirichlet boundary conditions. Hence, (11), (15), (16) will not completely pin down the Wigner transform of the confined wave function satisfying Dirichlet boundary conditions and thus Eqs. (11), (15), (16) fail to provide the proper translation (into the Wigner language) of the Dirichlet boundary conditions on the wave function.

We now introduce a new set of boundary conditions for the Wigner function, which are fully equivalent to Dirichlet boundary conditions on the original wave function, both for the confined as well as for the unconfined case. We call these conditions *integral Dirichlet boundary conditions* and they can be derived as follows: if the wave function satisfies Dirichlet boundary conditions then $\lim_{\epsilon\to 0^+}\mathcal{P}(a+\epsilon)=\lim_{\epsilon\to 0^+}|\psi(a+\epsilon)|^2=0$ and similarly $\lim_{\epsilon\to 0^+}\mathcal{P}(b-\epsilon)=\lim_{\epsilon\to 0^+}|\psi(b-\epsilon)|^2=0$ where $\mathcal{P}(x)$ stands for the probability distribution. These equations can be written in the Wigner context quite straightforwardly:

$$\begin{cases} \lim\limits_{\epsilon\to 0^+}\displaystyle\int_{-\infty}^{+\infty} dp F^W(a+\epsilon,p)=0, \\ \lim\limits_{\epsilon\to 0^+}\displaystyle\int_{-\infty}^{+\infty} dp F^W(b-\epsilon,p)=0. \end{cases} \tag{18}$$

Notice that the use of the limits is valid (though unnecessary) in the unconfined case (where the wave function and its derivatives are continuous) but it is necessary if the system is confined.

From the two sets of boundary conditions satisfied by the Wigner function [Eqs. (11), (15), (16) and Eq. (18)], the Dirichlet integral ones are the most appealing both from the physical and the mathematical points of view: first, because they represent a physically meaningful imposition that the probability of finding the particle at the boundary is zero. Second, because they are fully equivalent to the Dirichlet boundary conditions on the wave function. From Eqs. (7) and (18), we get

$$\lim_{\epsilon\to 0^+}\int_{-\infty}^{+\infty} dp\, F^W(a+\epsilon,p)=0 \Rightarrow \lim_{\epsilon\to 0^+}|\psi(a+\epsilon)|^2=0 \Rightarrow \lim_{\epsilon\to 0^+}\psi(a+\epsilon)=0, \tag{19}$$

and similarly for the b-boundary. Finally, and to avoid a possible misinterpretation let us point out that Eq. (11) does not imply the satisfaction of conditions (18) given the fact that, in general, it is not possible to interchange the order in which one evaluates the limit and the integral in (18). For instance, if a confined wave function satisfies Neumann conditions then the Wigner function will satisfy (11) but not (18).

III. BOUNDARY STARGENVALUE EQUATION

Let us henceforth assume that the wave function satisfies Dirichlet boundary conditions, so that Eqs. (11), (15), (16), and (18) are valid. Furthermore, we assume that $\psi(x)$ is an energy-eigenstate for a Hamiltonian of the form: $\hat{H}(\hat{x},\hat{p})=(\hat{p}^2/2m)+V(\hat{x})$. If we substitute F^W (8) on the left-hand side of Eq. (6), we get

$$H^W * F^W = H^W * \{\Theta_1 F_1^W + \Theta_2 F_2^W\} = \left\{\frac{p^2}{2m} + V(x)\right\} * (\Theta_1 F_1^W) + \left\{\frac{p^2}{2m} + V(x)\right\} * (\Theta_2 F_2^W). \quad (20)$$

A straightforward calculation leads to

$$H^W * (\Theta_1 F_1^W) = \Theta_1 (H^W * F_1^W) - \frac{i\hbar p}{2m}[\delta(x-a) - \delta(x-x_0)] F_1^W + \frac{\hbar^2}{8m}[\delta'(x-x_0) - \delta'(x-a)] F_1^W + \frac{\hbar^2}{4m}[\delta(x-x_0) - \delta(x-a)] \frac{\partial F_1^W}{\partial x}. \quad (21)$$

Taking into account the boundary conditions at $x=a$, we get

$$H^W * (\Theta_1 F_1^W) = \Theta_1 (H^W * F_1^W) + \frac{i\hbar p}{2m}\delta(x-x_0) F_1^W(x_0,p) + \frac{\hbar^2}{4m}\delta(x-x_0)\frac{\partial F_1^W}{\partial x}(x_0,p) + \frac{\hbar^2}{8m}\delta'(x-x_0) F_1^W(x,p). \quad (22)$$

Similarly, we also have

$$H^W * (\Theta_2 F_2^W) = \Theta_2 (H^W * F_2^W) - \frac{i\hbar p}{2m}\delta(x-x_0) F_2^W(x_0,p) - \frac{\hbar^2}{4m}\delta(x-x_0)\frac{\partial F_2^W}{\partial x}(x_0,p) - \frac{\hbar^2}{8m}\delta'(x-x_0)\, F_2^W(x,p). \quad (23)$$

Adding up all contributions and taking into account the fusing conditions (11) and (16), we obtain

$$H^W * F^W = \Theta_1 (H^W * F_1^W) + \Theta_2 (H^W * F_2^W). \quad (24)$$

Let us then calculate the term $H^W * F_1^W$ for $a < x \leqslant x_0$ and the term $H^W * F_2^W$ for $x_0 < x < b$. The following theorem will do this.

Theorem: Let F_1^W and F_2^W be given by Eq. (10) where $\psi(x)$ is an energy eigenstate satisfying Dirichlet boundary conditions at a and b. Let $H^W = (p^2/2m) + V(x)$. We then have

$$\begin{cases} H^W * F_1^W(x,p) = E F_1^W(x,p) + \dfrac{\hbar^2}{2m}\delta'(x-a) * F_1^W(x^+,p) \quad \text{for } a < x \leqslant x_0, \\ H^W * F_2^W(x,p) = E F_2^W(x,p) - \dfrac{\hbar^2}{2m}\delta'(x-b) * F_2^W(x^-,p) \quad \text{for } x_0 < x < b. \end{cases} \quad (25)$$

Proof: Let us consider the product $H^W * F_1^W$. Following the method described in Ref. 15, we get

$$H^W * F_1^W = \frac{1}{\pi\hbar}\left[\frac{1}{2m}\left(p - \frac{i\hbar}{2}\vec{\partial}_x\right)^2 + V(x)\right]\int_{a-x}^{x-a} dy\, e^{-(2iy/\hbar)(p + (i\hbar/2)\vec{\partial}_x)}\psi^*(x-y)\psi(x+y)$$
$$= \frac{1}{\pi\hbar}\int_{a-x}^{x-a} dy\, e^{-2iyp/\hbar} V(x+y)\psi^*(x-y)\psi(x+y) + \frac{1}{2m\pi\hbar}\left[p^2 - i\hbar p\vec{\partial}_x - \frac{\hbar^2}{4}\vec{\partial}_x^2\right]\int_{a-x}^{x-a} dy\, e^{-(2iyp/\hbar)}\psi^*(x-y)\psi(x+y), \quad (26)$$

where $\vec{\partial}_x$ acts on F_1^W and $\overleftarrow{\partial}_x$ acts on H^W. Taking into account that $pe^{-2iyp/\hbar}=(i\hbar/2)\times(\partial/\partial y)\,e^{-2iyp/\hbar}$ and that $\psi(x)$ is an energy eigenstate, we get after a few integrations by parts:

$$H^W(x,p)*F_1^W(x,p)=EF_1^W(x,p)+\mathcal{B}_1(x,p). \tag{27}$$

The extra term $\mathcal{B}_1(x,p)$ is a boundary correction given by

$$\mathcal{B}_1(x,p)=-\frac{\hbar}{2\pi m}e^{-(2ip/\hbar)(a-x)}\left\{\frac{2ip}{\hbar}\psi^*(2x-a^-)\psi(a^+)+\psi'^*(2x-a^-)\psi(a^+)\right.$$
$$\left.+\psi^*(2x-a^-)\psi'(a^+)\right\}. \tag{28}$$

For Dirichlet boundary conditions, we get

$$\mathcal{B}_1^D(x,p)=-\frac{\hbar}{2\pi m}e^{-(2ip/\hbar)(a-x)}\psi^*(2x-a^-)\psi'(a^+). \tag{29}$$

Let us now attempt to express $\mathcal{B}_1^D(x,p)$ in terms of the Wigner function $F_1^W(x,p)$. Consider the following integral (where $\epsilon>0$):

$$\Lambda_\epsilon\equiv\int_{-\infty}^{+\infty}\mathrm{d}k\,e^{ik(x-a)}kF_1^W\left(x+\epsilon,p-\frac{\hbar}{2}k\right)$$
$$=\frac{1}{\pi\hbar}\int_{-\infty}^{+\infty}\mathrm{d}k\int_{a-x-\epsilon}^{x-a+\epsilon}\mathrm{d}y\,e^{ik(x-a+y)}ke^{-2ipy/\hbar}\psi^*(x+\epsilon-y)\psi(x+\epsilon+y)$$
$$=\frac{2}{i\hbar}\int_{a-x-\epsilon}^{x-a+\epsilon}\mathrm{d}y\left[\frac{\partial}{\partial y}\delta(x-a+y)\right]e^{-2ipy/\hbar}\psi^*(x+\epsilon-y)\psi(x+\epsilon+y)$$
$$=-\frac{2}{i\hbar}\int_{a-x-\epsilon}^{x-a+\epsilon}\mathrm{d}y\,\delta(x-a+y)e^{-2ipy/\hbar}\left\{-\frac{2ip}{\hbar}\psi^*(x+\epsilon-y)\psi(x+\epsilon+y)\right.$$
$$\left.-\psi'^*(x+\epsilon-y)\psi(x+\epsilon+y)+\psi^*(x+\epsilon-y)\psi'(x+\epsilon+y)\right\}$$
$$=\frac{2i}{\hbar}\exp^{-(2ip/\hbar)(a-x)}\left\{-\frac{2ip}{\hbar}\psi^*(2x-a+\epsilon)\psi(a+\epsilon)-\psi'^*(2x-a+\epsilon)\psi(a+\epsilon)\right.$$
$$\left.+\psi^*(2x-a+\epsilon)\psi'(a+\epsilon)\right\}. \tag{30}$$

In particular for a wave function satisfying a Dirichlet boundary condition, we conclude that $\lim_{\epsilon\to0^+}\Lambda_\epsilon^D(x,p;a)=(2i/\hbar)\,e^{-(2ip/\hbar)(a-x)}\psi^*(2x-a^-)\psi'(a^+)$. It is straightforward to obtain from Eq. (29): $\mathcal{B}_1^D(x,p)=\lim_{\epsilon\to0^+}(i\hbar^2/4\pi m)\,\Lambda_\epsilon^D(x,p;a)$. Let us now try to cast this expression in terms of *-products:

$$\Lambda_\epsilon(x,p)=\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{\hbar}{2}\right)^n\frac{\partial^nF_1^W(x+\epsilon,p)}{\partial p^n}\int_{-\infty}^{+\infty}\mathrm{d}k\,e^{ik(x-a)}k^{n+1}$$
$$=-2i\pi\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\hbar}{2}\right)^n\delta^{(n+1)}(x-a)\frac{\partial^nF_1^W}{\partial p^n}(x+\epsilon,p)$$
$$=-2i\pi[\,\delta'(x-a)*F_1^W(x+\epsilon,p)]. \tag{31}$$

Taking the limit $\epsilon\to 0^+$ of the previous expression and substituting it in (29) and (27) yields the first equation of (25) directly. As a final remark we notice that $\delta'(x-a)*F_1^W(x^+,p)=\lim_{\epsilon\to 0}\{\delta'(x-a)*F_1^W(x+\epsilon,p)\}$ is not identical to $\delta'(x-a)*\{\lim_{\epsilon\to 0}F_1^W(x+\epsilon,p)\}=\delta'(x-a)*F_1^W(x,p)$. This last expression is not even well defined [cf. (30)] since the Dirac delta function is evaluated at a point where $\psi'(x)$ is not continuous. Hence, we should keep in mind that in general, we cannot interchange the order in which the star product and the limit $\epsilon\to 0$ are evaluated.

Finally, we perform the analogous procedure for F_2^W and get the second equation of (25), which concludes the proof.

Let us then return to Eq. (24). Using Eq. (25) we get

$$H^W(x,p)*F^W(x,p)=\Theta_1(x)\left\{EF_1^W(x,p)+\frac{\hbar^2}{2m}\delta'(x-a)*F_1^W(x^+,p)\right\}$$
$$+\Theta_2(x)\left\{EF_2^W(x,p)-\frac{\hbar^2}{2m}\delta'(x-b)*F_2^W(x^-,p)\right\}. \tag{32}$$

Let us try to find the corresponding compact version for $F^W(x,p)$ [Eq. (8)]. We notice the following.

(1) $\Theta_1 EF_1^W+\Theta_2 EF_2^W=E\{\Theta_1 F_1^W+\Theta_2 F_2^W\}=EF^W$.

$$(2)\Theta_1(x)\{\delta'(x-a)*F_1^W(x^+,p)\}=\Theta_1(x)\left\{-\frac{1}{\pi\hbar}e^{-(2ip/\hbar)(a-x)}\psi^*(2x-a^-)\psi'(a^+)\right\}$$
$$=\Theta_1(x^+)\left\{-\frac{1}{\pi\hbar}e^{-(2ip/\hbar)(a-x)}\psi^*(2x-a^-)\psi'(a^+)\right\}$$
$$=\delta'(x-a)*\{\Theta_1(x^+)F_1^W(x^+,p)\}, \tag{33}$$

where in the first step we used Eqs. (29) and (31); in the second step the fact that $\Theta_1(x)=\lim_{\epsilon\to 0^+}\Theta_1(x+\epsilon),\forall x\neq a,x_0$ and that $\psi^*(2x-a^-)$ vanishes for $x=a$ and $x=x_0$; and finally in the last step that $\Theta_1(x^+)$ is p-independent.

(3) Similarly, we have $\Theta_2(x)\{\delta'(x-b)*F_2^W(x^-,p)\}=\delta'(x-b)*\{\Theta_2(x^-)F_2^W(x^-,p)\}$.

(4) Finally, we also have

$$\delta'(x-b)*\{\Theta_1(x^+)F_1^W(x^+,p)\}$$
$$=\Theta_1(x^+)\{\delta'(x-b)*F_1^W(x^+,p)\}$$
$$=\frac{i}{2\pi}\Theta_1(x^+)\int_{-\infty}^{+\infty}\mathrm{d}k\,e^{ik(x-b)}kF_1^W\left(x^+,p-\frac{\hbar}{2}k\right)$$
$$=-\frac{1}{\pi\hbar}\Theta_1(x^+)\theta(x^+-x_0)e^{-(2ip/\hbar)(b-x)}$$
$$\times\left\{-\frac{2ip}{\hbar}\psi^*(2x-b^-)\psi(b^+)-\psi'^*(2x-b^-)\psi(b^+)+\psi^*(2x-b^-)\psi'(b^+)\right\}$$
$$=0, \tag{34}$$

where in the third step we made the same calculation as in Eq. (30) and in the last step we used the fact that $\psi(b^+)=\psi'(b^+)=0$, or else that $\Theta_1(x^+)=0,\forall x\geqslant x_0$ and $\theta(x^+-x_0)=0,\forall x<x_0$.

(5) Similarly,

$$\delta'(x-a)*(\Theta_2(x^-)F_2^W(x^-,p))=0. \tag{35}$$

Using these results we can rewrite Eq. (32) as

$$H^W * F^W = EF^W + \frac{\hbar^2}{2m}\delta'(x-a) * \{\Theta_1(x^+)F_1^W(x^+,p) + \Theta_2(x^-)F_2^W(x^-,p)\}$$
$$- \frac{\hbar^2}{2m}\delta'(x-b) * \{\Theta_1(x^+)F_1^W(x^+,p) + \Theta_2(x^-)F_2^W(x^-,p)\}, \tag{36}$$

from where it immediately follows:

$$\left(\frac{p^2}{2m} + V(x)\right) * F^W(x,p) - \frac{\hbar^2}{2m}\delta'(x-a) * F^W(x^+,p) + \frac{\hbar^2}{2m}\delta'(x-b) * F^W(x^-,p) = EF^W(x,p). \tag{37}$$

Following the same procedure, one would also obtain

$$F^W(x,p) * \left(\frac{p^2}{2m} + V(x)\right) - \frac{\hbar^2}{2m}F^W(x^+,p) * \delta'(x-a) + \frac{\hbar^2}{2m}F^W(x^-,p) * \delta'(x-b) = EF^W(x,p). \tag{38}$$

We conclude that, if the eigenfunction satisfies Dirichlet boundary conditions, then the corresponding Wigner function does not satisfy the standard $*$-genvalue equation (6), but rather a modified equation given by (37) and (38). Furthermore, the source of discretization of the energy spectrum are not the Dirichlet conditions on the Wigner function but instead the subsidiary boundary conditions (15) or (18).

As a simple example let us consider the free particle in the infinite potential well. We choose as ansatz:

$$F^W(x,p) = -\frac{\alpha^2}{2\pi p}\cos[2(\beta - k|x|)] \cdot \sin\left[\frac{2p}{\hbar}\left(\frac{L}{2} - |x|\right)\right] + \frac{\alpha^2}{4\pi(p+\hbar k)}\sin\left[\frac{2}{\hbar}(p+\hbar k)\left(\frac{L}{2} - |x|\right)\right]$$
$$+ \frac{\alpha^2}{4\pi(p-\hbar k)}\sin\left[\frac{2}{\hbar}(p-\hbar k)\left(\frac{L}{2} - |x|\right)\right], \tag{39}$$

corresponding to the wave function $\psi(x) = \alpha \sin(kx+\beta)$. This function is continuous at $x_0 = 0$ and satisfies Dirichlet's condition at $x = \pm L/2$, in accordance with (11). If we impose the constraints (15) and substitute this expression in the $*$-genvalue equation (37) and (38), using the integral form Λ [Eq. (30)], we obtain

$$k_n = \frac{n\pi}{L}, \quad \beta_n = \frac{n\pi}{2}, \quad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2\pi^2}{2mL^2}n^2 \quad (n = 1,2,\ldots). \tag{40}$$

Finally, if we impose the normalization $\int_a^b dx \int_{-\infty}^{+\infty} dp\, F^W(x,p) = 1$, we obtain $\alpha = \sqrt{2/L}$. This result is in perfect agreement with Ref. 5.

IV. BAKER'S CONVERSE CONSTRUCTION

In Sec. III we proved that if the wave function is confined to the interval $]a,b[$, satisfies the operator eigenvalue equation and Dirichlet boundary conditions at a^+ and b^- then the corresponding Wigner function satisfies a modified $*$-genvalue equation together with integral Dirichlet boundary conditions at a^+ and b^-. In this section we want to prove the converse result. In the unconfined case this result is known as Baker's converse construction.[6,15] Hence, in this section we want to extend Baker's converse construction to the confined case, thus proving the full equivalence of the Wigner and operator formulations of quantum mechanics when boundaries are present.

Let us then consider some real function $F^W(x,p)$ satisfying the following conditions:
(i) it is a continuous function of x and p;

(ii) it has an infinite number of derivatives with respect to p and is twice differentiable with respect to x;
(iii) F^W obeys integral Dirichlet boundary conditions at $x=a^+$ and $x=b^-$, Eq. (18);
(iv) it obeys the left- and right-boundary stargenvalue equations (37) and (38) when $\epsilon\to 0^+$:

$$\left(\frac{p^2}{2m}+V(x)\right)*F^W(x,p)-\frac{\hbar^2}{2m}\delta'(x-a)*F^W(x+\epsilon,p)+\frac{\hbar^2}{2m}\delta'(x-b)*F^W(x-\epsilon,p)$$
$$=F^W(x,p)*\left(\frac{p^2}{2m}+V(x)\right)-\frac{\hbar^2}{2m}F^W(x+\epsilon,p)*\delta'(x-a)+\frac{\hbar^2}{2m}F^W(x-\epsilon,p)*\delta'(x-b)$$
$$=EF^W(x,p). \tag{41}$$

We will now prove that under these assumptions, there is a unique (up to a global phase factor) normalized complex and continuous function ψ, related to F^W according to (2), which obeys Dirichlet boundary conditions at $x=a^+$ and $x=b^-$ and is a solution of Schrödinger's equation.

It will prove useful to consider the Fourier transform of F^W:

$$F^W(x,p)=\frac{1}{\pi\hbar}\int_{-\infty}^{+\infty}\mathrm{d}y\, e^{-2ipy/\hbar}\tilde{F}(x,y). \tag{42}$$

Substituting this expression in the left- and right-stargenvalue equations (41), and following the same steps as in Eq. (26), we obtain

$$\frac{1}{\pi\hbar}\int_{-\infty}^{+\infty}\mathrm{d}y\, e^{-2ipy/\hbar}\left\{\left[-\frac{\hbar^2}{2m}\left(\frac{\partial_x\pm\partial_y}{2}\right)^2+V(x\pm y)-E\right]\tilde{F}(x,y)-\frac{\hbar^2}{2m}\delta'(x\pm y-a)\tilde{F}(x+\epsilon,y)\right.$$
$$\left.+\frac{\hbar^2}{2m}\delta'(x\pm y-b)\tilde{F}(x-\epsilon,y)\right\}=0. \tag{43}$$

This means that $\tilde{F}(x,y)$ satisfies the equations:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial_x\pm\partial_y}{2}\right)^2+V(x\pm y)\right]\tilde{F}(x,y)-\frac{\hbar^2}{2m}\delta'(x\pm y-a)\tilde{F}(x+\epsilon,y)+\frac{\hbar^2}{2m}\delta'(x\pm y-b)\tilde{F}(x-\epsilon,y)$$
$$=E\tilde{F}(x,y). \tag{44}$$

From now on we will follow the steps of the standard Baker converse construction for unconfined systems.[6] Introducing the function F such that $F(x-y,x+y)=\tilde{F}(x,y)$ and performing the change of variables $u=x-y$ and $v=x+y$, we get

$$\begin{cases}\left[-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial v^2}+V(v)\right]F(u,v)-\dfrac{\hbar^2}{2m}\delta'(v-a)F(u+\epsilon,v+\epsilon)+\dfrac{\hbar^2}{2m}\delta'(v-b)F(u-\epsilon,v-\epsilon)\\ \quad=EF(u,v),\\ \left[-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial u^2}+V(u)\right]F(u,v)-\dfrac{\hbar^2}{2m}\delta'(u-a)F(u+\epsilon,v+\epsilon)+\dfrac{\hbar^2}{2m}\delta'(u-b)F(u-\epsilon,v-\epsilon)\\ \quad=EF(u,v),\end{cases} \tag{45}$$

from where it follows that $F(u,v)=\xi(u)\psi(v)$ and so $\tilde{F}(x,y)=\xi(x-y)\psi(x+y)$. Furthermore, since $F^W(x,p)$ is real, Eq. (42) implies that $\xi=\psi^*$ and so $\tilde{F}(x,y)=\psi^*(x-y)\psi(x+y)$, where the complex function ψ obeys

$$-\frac{\hbar^2}{2m}\psi''(x)+V(x)\psi(x)-\frac{\hbar^2}{2m}\delta'(x-a)\psi(x^+)+\frac{\hbar^2}{2m}\delta'(x-b)\psi(x^-)=E\psi(x), \tag{46}$$

where we performed the limit $\epsilon\to 0^+$. Finally, if $F^W(x,p)$ satisfies integral Dirichlet conditions at $x=a^+$ and $x=b^-$ then the corresponding wave function satisfies $\psi(a^+)=\psi(b^-)=0$, Eq. (19).

In summary, we have shown that if F^W satisfies the above-mentioned conditions (i)–(iv) then F^W is the Wigner transform (2) of a complex function ψ which (1) is a solution of the Schrödinger equation (46) and (2) obeys Dirichlet boundary condition at $x=a^+$ and $x=b^-$. In Sec. VI we will show how to solve this equation and prove that its unique (up to a global phase factor) solution is the standard solution of the corresponding eigenvalue problem in operator quantum mechanics.

V. BOUNDARY DYNAMICS

Let us now consider the time evolution:

$$\frac{\partial F^W}{\partial t}=\Theta_1\frac{\partial F_1^W}{\partial t}+\Theta_2\frac{\partial F_2^W}{\partial t}, \tag{47}$$

and focus on the time derivative $\partial F_1^W/\partial t$:

$$\begin{aligned}\frac{\partial F_1^W}{\partial t}&=\frac{1}{\pi\hbar}\int_{a-x}^{x-a}\mathrm{d}y\, e^{-2ipy/\hbar}\left[\frac{\partial\psi^*}{\partial t}(x-y)\psi(x+y)+\psi^*(x-y)\frac{\partial\psi}{\partial t}(x+y)\right]\\&=\frac{1}{i\pi\hbar^2}\int_{a-x}^{x-a}\mathrm{d}y\, e^{-2ipy/\hbar}\left\{\frac{\hbar^2}{2m}[\psi''^*(x-y)\psi(x+y)-\psi^*(x-y)\psi''(x+y)]+[V(x+y)\right.\\&\quad\left.-V(x-y)]\psi^*(x-y)\psi(x+y)\right\},\end{aligned} \tag{48}$$

where we used the Schrödinger equation. Consider the first term. After a few integrations by parts and by keeping track of the boundary contributions and Dirichlet's condition, we obtain

$$\begin{aligned}&\frac{1}{2im\pi}\int_{a-x}^{x-a}\mathrm{d}y\, e^{-2ipy/\hbar}\psi''^*(x-y)\psi(x+y)\\&\quad=\frac{i}{2m\pi}\{e^{-(2ip/\hbar)(x-a)}\psi'^*(a^+)\psi(2x-a^-)-e^{-(2ip/\hbar)(a-x)}\psi^*(2x-a^-)\psi'(a^+)\}\\&\qquad+\frac{1}{2im\pi}\int_{a-x}^{x-a}\mathrm{d}y\, e^{-2ipy/\hbar}\psi^*(x-y)\psi''(x+y)-\frac{p}{m}\frac{\partial F_1^W}{\partial x}.\end{aligned} \tag{49}$$

The penultimate term exactly cancels the second term on the right-hand side of Eq. (48). The first two terms in Eq. (49) can be written as

$$\begin{aligned}&-\frac{\hbar}{4m\pi}\int_{-\infty}^{+\infty}\mathrm{d}k[e^{ik(a-x)}+e^{ik(x-a)}]kF_1^W\left(x^+,p-\frac{\hbar}{2}k\right)\\&\quad=-\frac{i\hbar}{2m}[F_1^W(x^+,p)*\delta'(x-a)-\delta'(x-a)*F_1^W(x^+,p)]\\&\quad=-\frac{\hbar^2}{2m}[\delta'(x-a),F_1^W(x^+,p)]_M.\end{aligned} \tag{50}$$

The terms involving the potential $V(x)$ are familiar in Wigner quantum mechanics. They yield the contribution $[V(x),F_1^W(x,p)]_M$. After assembling all the results, we get

$$\frac{\partial F_1^W}{\partial t}(x,p;t)=\left[\frac{p^2}{2m}+V(x),F_1^W(x,p;t)\right]_M-\frac{\hbar^2}{2m}[\delta'(x-a),F_1^W(x^+,p;t)]_M. \tag{51}$$

A similar calculation leads to

$$\frac{\partial F_2^W}{\partial t}(x,p;t)=\left[\frac{p^2}{2m}+V(x),F_2^W(x,p;t)\right]_M+\frac{\hbar^2}{2m}[\delta'(x-b),F_2^W(x^-,p;t)]_M. \tag{52}$$

From these results we get for $F^W(x,p;t)=\Theta_1(x)F_1^W(x,p;t)+\Theta_2(x)F_2^W(x,p;t)$:

$$\frac{\partial F^W}{\partial t}(x,p;t)=\left[\frac{p^2}{2m}+V(x),F^W(x,p;t)\right]_M-\frac{\hbar^2}{2m}[\delta'(x-a),F^W(x^+,p;t)]_M+\frac{\hbar^2}{2m}[\delta'(x-b),F^W(x^-,p;t)]_M, \tag{53}$$

where we used the set of relations given by Eqs. (33)–(36).

A straightforward consequence is that probability is conserved (as expected):

$$\frac{\partial}{\partial t}\int_a^b dx\int_{-\infty}^{+\infty}dp\,F^W(x,p;t)=\frac{\partial}{\partial t}\int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dp[\Theta_1(x)F_1^W(x,p;t)+\Theta_2(x)F_2^W(x,p;t)]=0. \tag{54}$$

VI. WEYL TRANSFORM OF THE STANDARD QUANTUM DESCRIPTION

The standard approach to derive the Wigner formulation of the eigenvalue problem for confined systems would amount to applying the Weyl transform, W, Eq. (1), to both the eigenvalue equation and to the boundary conditions. However, we saw in Sec. II, that this procedure does not yield the correct results. As we shall see, this is linked to the way operator quantum mechanics handles confined dynamical systems. The standard procedure is to (1) solve the eigenvalue equation for the unconfined wave function $\phi(x)$ and (2) impose the wave function to be zero outside the bulk and produce the confined state $\psi(x)=\phi(x)\,\theta(x-a)\,\theta(b-x)$. The problem in the Wigner formulation is that $W(|\psi\rangle\langle\psi|)\neq W(|\phi\rangle\langle\phi|)\,\theta(x-a)\,\theta(b-x)$ and thus we cannot solve the unconfined stargenvalue equation and manipulate its solution to obtain the confined Wigner function.

The reason for this apparent contradiction between the standard operator and Wigner formulations of quantum mechanics resides in the fact that ψ is not a globally valid solution of the operator eigenvalue equation. Globally, ψ satisfies a different eigenvalue equation which includes boundary potentials. Given the intrinsically nonlocal character of the Wigner function this fact is crucial to derive the correct Wigner description of the bounded system.

In Secs. VI A, VI B, and VI C we will (a) derive a globally valid eigenvalue equation for confined systems satisfying Dirichlet boundary conditions, (b) show that the only solution of this equation is the confined wave function, and (c) briefly discuss the numerical implementation of the new eigenvalue equation. It will then be trivial to realize that the Weyl transform of the new eigenvalue equation is the bounded stargenvalue equation (37) and (38), thus recovering the usual correspondence between standard operator and Wigner quantum mechanics.

A. Bounded eigenvalue equation

Let ϕ be the unconfined solution of the eigenvalue equation satisfying Dirichlet boundary conditions at $x=a$ and $x=b$:

$$\hat{H}\phi = E\phi, \quad \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}), \quad \phi(a) = \phi(b) = 0. \tag{55}$$

Notice that $\phi(x)$ is the solution of Eq. (55) everywhere, i.e., for all $x \in \mathcal{R}$. To obtain the confined wave function (for instance, for a particle in a box) the standard procedure is to cut off ϕ outside the box and produce the new wave function: $\psi(x) = \phi(x)\,\theta(x-a)\,\theta(b-x)$. Notice that ψ satisfies Eq. (55) inside the box, it also satisfies it outside the box, but it does not satisfy it at the boundaries. Hence, ψ is not a global solution of (55). Due to nonlocal effects the Weyl transform of ψ does not satisfy the stargenvalue equation (6), even in the bulk.

It seems quite natural to expect that if we are able to provide the global eigenvalue equation for ψ then the correct stargenvalue equation would just be its Weyl transform. The aim of this section is to derive this global equation. The first step is to introduce a twice differentiable version of the Heaviside step function and of the confined wave function ψ:

$$\theta_\epsilon(x): \begin{cases} \in C^2(\mathcal{R}) \quad \text{and is nondecreasing} \\ = 0, \ x < -\epsilon, \\ = 1, \ x > \epsilon, \quad 0 < \epsilon \ll 1. \end{cases} \qquad \psi_\epsilon(x) = \phi(x)\,\theta_\epsilon(x-a)\,\theta_\epsilon(b-x) \tag{56}$$

The definition of $\theta_\epsilon(x)$ is fully compatible with the distribution $\theta(x)$ we used previously: $\lim_{\epsilon\to 0^+} \theta_\epsilon(x) = 0$ if $x<0$, $\lim_{\epsilon\to 0^+} \theta_\epsilon(x) = 1$ if $x>0$ and $\lim_{\epsilon\to 0^+} \theta_\epsilon(0)$ remains unspecified (it might be any number between 0 and 1 or it may not be defined at all). The results of this section are not dependent on the particular function $\theta_\epsilon(x)$ but only of the general properties given in (56). From (56) the smooth versions of $\delta(x)$ and $\delta'(x)$ follow immediately: $\delta_\epsilon(x) = \theta'_\epsilon(x)$ and $\delta'_\epsilon(x) = \theta''_\epsilon(x)$. It is also clear that $\lim_{\epsilon\to 0^+}(\delta_\epsilon(x), \delta'_\epsilon(x), \psi_\epsilon(x)) = (\delta(x), \delta'(x), \psi(x))$. Let us then apply $\hat{H}$ to $\psi_\epsilon(x)$:

$$\begin{aligned} \hat{H}\psi_\epsilon(x) &= \left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \right\} \psi_\epsilon(x) \\ &= \left\{ -\frac{\hbar^2}{2m}\phi''(x) + V(x)\phi(x) \right\} \theta_\epsilon(x-a)\,\theta_\epsilon(b-x) \\ &\quad - \frac{\hbar^2}{2m}\{2\phi'(x)\,\delta_\epsilon(x-a) - 2\phi'(x)\,\delta_\epsilon(b-x) + \phi(x)\,\delta'_\epsilon(x-a) + \phi(x)\,\delta'_\epsilon(b-x)\} \\ &= E\psi_\epsilon(x) + \frac{\hbar^2}{2m}\{\phi(x)\,\delta'_\epsilon(x-a) - \phi(x)\,\delta'_\epsilon(x-b)\}, \end{aligned} \tag{57}$$

where in the last step we use the fact that $\phi(x)$ satisfies the eigenvalue equation (55) and that the Dirichlet boundary conditions on $\phi(x)$ imply for sufficiently small ϵ: $\phi'(x)\,\delta_\epsilon(x-a) = -\phi(x)\,\delta'_\epsilon(x-a)$ and likewise $\phi'(x)\,\delta_\epsilon(b-x) = -\phi(x)\,\delta'_\epsilon(x-b)$. The former equation is not yet a closed eigenvalue equation for $\psi_\epsilon(x)$ since it also evolves the wave function $\phi(x)$.

In what follows and to simplify the discussion we will consider the case of just one boundary placed at $a=0$. The derivation of the two-boundary eigenvalue equation follows exactly the same steps and will be written explicitly at the end. In the one boundary case Eq. (57) reduces to

$$\hat{H}\psi_\epsilon(x) = E\psi_\epsilon(x) + \frac{\hbar^2}{2m}\delta'_\epsilon(x)\phi(x), \tag{58}$$

where $\phi(x)$ satisfies Eq. (55) with Dirichlet boundary conditions at $x=0$. The former equation follows from applying $\hat{H}$ to the state $\psi_\epsilon(x) = \phi(x)\,\theta_\epsilon(x)$.

To proceed we notice that for $x > \epsilon$ the two equations (55) and (58)—for $\phi(x)$ and for $\psi_\epsilon(x)$, respectively, are identical. If we supply identical boundary conditions, for instance, at $x = 2\epsilon$ we

will get identical solutions for $x>\epsilon$, i.e., if $\phi(2\epsilon)=\psi_\epsilon(2\epsilon)$ and $\phi'(2\epsilon)=\psi'_\epsilon(2\epsilon)$ then $\phi(x)=\psi_\epsilon(x)$ for all $x>\epsilon$. Furthermore, and since $\phi(x)$ is analytical, we also have

$$\phi(x)=\phi(x+2\epsilon)+\sum_{n=1}^{\infty}\frac{(-2\epsilon)^n}{n!}\frac{\partial^n\phi}{\partial x^n}(x+2\epsilon), \tag{59}$$

and for $x>-\epsilon$ we have $\phi(x+2\epsilon)=\psi_\epsilon(x+2\epsilon)$ and equally $(\partial^n\phi/\partial x^n)(x+2\epsilon)=(\partial^n\psi_\epsilon/\partial x^n)(x+2\epsilon)$, $\forall n\in\mathcal{N}$. Hence,

$$\phi(x)=\psi_\epsilon(x+2\epsilon)+\sum_{n=1}^{\infty}\frac{(-2\epsilon)^n}{n!}\frac{\partial^n\psi_\epsilon}{\partial x^n}(x+2\epsilon),\quad \forall x>-\epsilon. \tag{60}$$

The trick here is that while $\phi(x)$ is analytical $\psi_\epsilon(x)$ is not [cf. (56)] and thus the Taylor expansion (60) yields $\phi(x)$ instead of $\psi_\epsilon(x)$. Substituting the former expansion in Eq. (58) we get

$$\hat{H}\psi_\epsilon(x)=E\psi_\epsilon(x)+\frac{\hbar^2}{2m}\delta'_\epsilon(x)\left\{\psi_\epsilon(x+2\epsilon)+\sum_{n=1}^{\infty}\frac{(-2\epsilon)^n}{n!}\frac{\partial^n\psi_\epsilon}{\partial x^n}(x+2\epsilon)\right\}. \tag{61}$$

Notice that Eq. (61) is valid for all $x\in\mathcal{R}$ because $\delta'_\epsilon(x)=0$ if $x<-\epsilon$. Finally by taking the limit $\epsilon\to 0^+$ we obtain

$$\hat{H}\psi(x)=E\psi(x)+\frac{\hbar^2}{2m}\delta'(x)\psi(x^+), \tag{62}$$

where we used the notation x^+ to make it explicit that in the product of δ' by ψ the two factors are evaluated at different points. This is crucial because Eq. (61) is valid for all $x\in\mathcal{R}$ only in this case, i.e., in the limit $\epsilon\to 0^+$ but not for $\epsilon=0$. Equation (62) is the new eigenvalue equation for $\psi(x)$. Following exactly the same procedure we can easily generalize it to the case of a double boundary placed at $x=a$ and $x=b$, $(a<b)$. We get

$$\hat{H}\psi(x)=E\psi(x)+\frac{\hbar^2}{2m}\{\delta'(x-a)\psi(x^+)-\delta'(x-b)\psi(x^-)\}, \tag{63}$$

which together with the boundary conditions $\psi(a^+)=\psi(b^-)=0$ provide the operator formulation of the confined eigenvalue problem for Dirichlet boundary conditions. To finish let us point out that: (1) Eq. (63) was obtained in Sec. IV from the stargenvalue equations (37) and (38), and (2) conversely, the Weyl transform of Eq. (63) immediately yields the stargenvalue equations (37) and (38).

B. Solving the new eigenvalue equation

Our next step is to solve the modified eigenvalue equation (63) and show that the confined wave function $\psi(x)$ is its only solution. To make it simple let us consider again the one boundary example Eq. (62).

For $x>0$, $\delta(x)=0$ and Eq. (62) reduces to the unconfined equation (55). The boundary conditions $\psi(0^+)=0$ and $\psi'(0^+)=\phi'(0^+)$ impose $\psi(x)=\phi(x)$ for all $x>0$.

For $-\sigma\leqslant x\leqslant\sigma$ and $\sigma\ll 1$ we have

$$\int_{-\sigma}^{x}\hat{H}\psi(x')\mathrm{d}x'=\int_{-\sigma}^{x}E\psi(x')\mathrm{d}x'+\frac{\hbar^2}{2m}\int_{-\sigma}^{x}\delta'(x')\psi(x'+0^+)\mathrm{d}x'$$

$$\Rightarrow-\frac{\hbar^2}{2m}\{\psi'(x)-\psi'(-\sigma)\}+\mathcal{O}(x+\sigma)=E\mathcal{O}(x+\sigma)$$

$$+\frac{\hbar^2}{2m}\left\{[\delta(x')\psi(x'+0^+)]_{-\sigma}^{x}-\int_{-\sigma}^{x}\delta(x')\psi'(x'+0^+)\mathrm{d}x'\right\}$$

$$\Rightarrow\psi'(x)-\psi'(-\sigma)=\psi'(0^+)\theta(x)+\mathcal{O}(x+\sigma),\tag{64}$$

where in the first step we introduced the notation $\mathcal{O}(y)$ to designate an arbitrary continuous function such that $\lim_{y\to0}\mathcal{O}(y)=0$, and in the third step we used the fact that $\psi(0^+)=0$. Taking the limits $\sigma\to0^+$ and $x\to0^+$ we get

$$\psi'(0^+)-\psi'(0^-)=\psi'(0^+)\Rightarrow\psi'(0^-)=0.\tag{65}$$

The second integration of the eigenvalue equation yields

$$\int_{-\sigma}^{\sigma}\psi'(x)\mathrm{d}x-\int_{-\sigma}^{\sigma}\psi'(-\sigma)\mathrm{d}x=\int_{-\sigma}^{\sigma}\psi'(0^+)\theta(x)\mathrm{d}x+\int_{-\sigma}^{\sigma}\mathcal{O}(x+\sigma)\mathrm{d}x$$

$$\Rightarrow\psi(\sigma)-\psi(-\sigma)$$

$$=\sigma\{2\psi'(-\sigma)+\psi'(0^+)\}+\mathcal{O}(\sigma^2),\tag{66}$$

and in the limit $\sigma\to0^+$ we have $\psi(0^+)-\psi(0^-)=0$, which together with the original Dirichlet boundary conditions at $x=0^+$ imply $\psi(0^-)=0$.

We conclude that for $x<0$, $\psi(x)$ satisfies Eq. (55) with boundary conditions $\psi(0^-)=\psi'(0^-)=0$ and thus $\psi(x)=0$, $\forall x<0$. Hence, we are left with the original bounded wave function: $\psi(x)=\phi(x)\theta(x)$. The generalization for a system with two boundaries is straightforward. Following exactly the same procedure we solve Eq. (63) and get $\psi(x)=\phi(x)\theta(x-a)\theta(b-x)$, as we should. This result concludes the proof of Baker's converse construction initiated in Sec. IV.

C. The free particle bounded eigenvalue equation: Numerical solution of a simple example

As a simple example let us consider the case of a free particle confined to the interval $]-1,1[$ and subject to Dirichlet boundary conditions.

The unconfined Hamiltonian in the position representation is given by $\hat{H}=-(\hbar^2/2m)\times(\partial^2/\partial x^2)$ and the unconfined fundamental state [solution of Eq. (55)] is: $\phi_1(x)=\cos((\pi/2)x)$ with $E=E_1=\hbar^2\pi^2/8m$. Figure 1 displays the unconfined wave function for $\hbar=m=1$.

We now consider a first possible approximation to the confined eigenvalue equation (63). We make $\epsilon=0.25$ and use a Gaussian approximation to the Dirac delta function: $\tilde{\delta}_\epsilon(x)=1/(\pi^{1/2}\epsilon')\exp\{-(x/\epsilon')^2\}$ where ϵ' substitutes ϵ for the following reason: the function $\tilde{\delta}_\epsilon(x)$ is not identically zero for $x>\epsilon$ or for $x<-\epsilon$ and thus there is no function $\theta_\epsilon(x)$ satisfying conditions (56) and such that $\tilde{\delta}_\epsilon(x)=\theta_\epsilon'(x)$. However, if we define $\tilde{\delta}_\epsilon(x)$ using a sufficiently small spread ϵ' (when compared with ϵ) then, for our numerical purposes $\tilde{\delta}_\epsilon(x)$ will provide a good enough approximation to $\theta_\epsilon'(x)$. In all future applications we will make: $\epsilon'=0.8\epsilon$. Furthermore, and to simplify the notation we will refer to $\tilde{\delta}_\epsilon(x)$ as just $\delta_\epsilon(x)$. Finally, taking into account the considerable large value of ϵ we have to consider the contribution of higher order terms in the

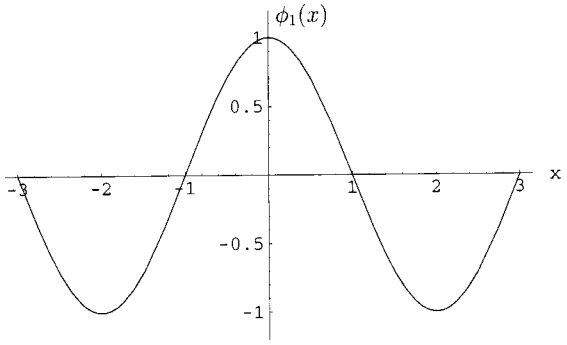

FIG. 1. Unconfined fundamental solution of the free particle eigenvalue equation satisfying Dirichlet boundary conditions at $x=\pm 1$ and for $\hbar=m=1$.

expansion (60), and thus we will use the two boundaries generalization of Eq. (61) as our starting point and truncate the series at the third term. Hence, the equation we want to solve is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_\epsilon(x)=E\psi_\epsilon(x)+\frac{\hbar^2}{2m}\delta'_\epsilon(x+1)\{\psi_\epsilon(x+2\epsilon)-2\epsilon\psi'_\epsilon(x+2\epsilon)+2\epsilon^2\psi''_\epsilon(x+2\epsilon)\}$$
$$-\frac{\hbar^2}{2m}\delta'_\epsilon(x-1)\{\psi_\epsilon(x-2\epsilon)+2\epsilon\psi'_\epsilon(x-2\epsilon)+2\epsilon^2\psi''_\epsilon(x-2\epsilon)\}. \tag{67}$$

Figure 2 displays the numerical solution of the former equation for the boundary conditions $\psi_\epsilon(a+2\epsilon=-0.5)=\psi_\epsilon(b-2\epsilon=0.5)=\phi(0.5)=0.707$ and for $E=E_1=\pi^2/8$, $\hbar=m=1$. Notice that the wave function is not completely confined, which follows from the fact that we are not using the true Dirac delta but a (poor) Gaussian approximation of it. If we decrease the value of ϵ the confinement will increase greatly.

Let us then consider a second approximation to the confined eigenvalue equation by making $\epsilon=0.0025$. Given the considerably small value of ϵ we can now truncate the series in the two boundaries generalization of Eq. (61) to zero order and numerically solve the finite version of Eq. (63):

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_\epsilon(x)=E\psi_\epsilon(x)+\frac{\hbar^2}{2m}\{\delta'_\epsilon(x+1)\psi_\epsilon(x+2\epsilon)-\delta'_\epsilon(x-1)\psi_\epsilon(x-2\epsilon)\}. \tag{68}$$

Figure 3 displays the numerical solution of Eq. (68) for the boundary conditions $\psi_\epsilon(a+2\epsilon=-0.995)=\psi_\epsilon(b-2\epsilon=0.995)=\phi(0.995)=0.008$ and $\hbar=m=1$, $E=E_1=\pi^2/8$.

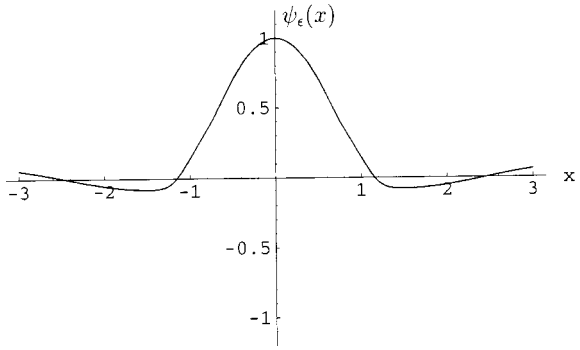

FIG. 2. Numerical solution of the first approximation [Eq. (67)] to the confined eigenvalue equation: $\epsilon=0.25$, $\hbar=m=1$, and $E=\pi^2/8$.

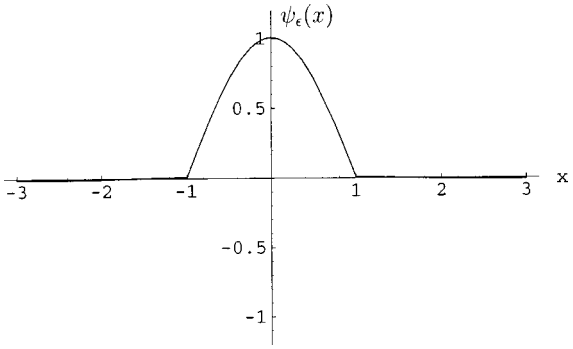

FIG. 3. Numerical solution of the second approximation [Eq. (68)] to the confined eigenvalue equation: $\epsilon=0.0025$, $\hbar=m=1$, and $E=\pi^2/8$.

We will see in Sec. VII that the part of the wave function that escapes from the box corresponds to quantum trajectories with energies much higher than the fundamental state. By making $\epsilon\rightarrow 0^+$ we completely confine the wave function.

VII. WIGNER TRAJECTORIES IN CONFINED SYSTEMS

In the following we briefly review the topic of Wigner trajectories,[4,5,20,21] where the previous work may find some interesting applications. There are two well-known instances where this concept plays an important role: collision processes[4,9] and the study of quantum systems that exhibit chaotic behavior in the classical limit.[4,13,22–24]

The Schrödinger and Wigner formulations of a collision process are obviously equivalent. This notwithstanding, there are important practical differences between the two approaches. In most cases, where an exact solution to the problem is unknown, one has to devise some approximative scheme. If certain conditions hold (concerning the interaction potential), the Moyal equation (5) can be truncated to a good degree of accuracy. Since it does not contain any operator, it is often easier to develop approximations on it than on the Schrödinger equation. Having computed the Wigner function that solves this truncated version of the Moyal equation, one can subsequently evaluate quantum corrections to the classical phase space trajectories. In addition to the benefit of this pictorial and intuitive description in terms of trajectories there is another advantage in this approach: collision cross sections can be computed by applying the same numerical techniques used in classical collision processes.

Another situation where the Wigner trajectories play an important role is that of nonlinear systems exhibiting classical chaotic behavior. In these systems the classical phase space trajectories are of random nature while the Wigner trajectories are smooth paths thus showing that the chaotic behavior disappears upon quantization. A topic of current interest is that of understanding the transition from classical to quantum dynamics. Since the Wigner trajectories might be computed as an $\hbar$ order by order correction to the classical trajectories they provide a powerful, pictorial tool to study this transition.

In following we will (a) briefly review the subject of Wigner trajectories for unconfined systems, (b) discuss the main difficulties in extending the formalism to bounded systems and show that our previous results provide a new approach in this context, and (c) illustrate these results using the simple example of a free particle confined to an infinite square well. The reader should be advised that our aim is not to provide a fully developed and precise formulation of these topics but only to outline (and hopefully motivate) some possible lines of research.

A. Wigner trajectories

Let us then consider the Moyal equation of motion (5) associated with $H=(p^2/2m)+V(x)$:

$$\frac{\partial F^W}{\partial t}(x,p,t) = -\frac{p}{m}\frac{\partial F^W}{\partial x} + \frac{\partial V}{\partial x}\frac{\partial F^W}{\partial p} + \frac{(\hbar/2i)^2}{3!}\frac{\partial^3 V}{\partial x^3}\frac{\partial^3 F^W}{\partial p^3} + \cdots . \tag{69}$$

Alternatively, we can write this equation as

$$\frac{\partial F^W}{\partial t}(x,p,t) = -\frac{p}{m}\frac{\partial F^W}{\partial x} + \int_{-\infty}^{+\infty} \mathrm{d}p'\, J(x,p') F^W(x,p+p',t), \tag{70}$$

where

$$J(x,p) = \frac{i}{\pi\hbar^2}\int_{-\infty}^{+\infty} \mathrm{d}y [V(x+y) - V(x-y)] e^{-2ipy/\hbar}. \tag{71}$$

In the absence of a boundary and if the potential V is at most quadratic in x, then the Moyal equation (69) reduces to the Liouville equation:

$$\frac{\partial F^W}{\partial t}(x,p,t) = -\frac{p}{m}\frac{\partial F^W}{\partial x} + \frac{\partial V}{\partial x}\frac{\partial F^W}{\partial p}. \tag{72}$$

Equation (72) means that the solution $F^W(x,p,t)$ evolves along the classical trajectories, i.e.,

$$\begin{cases} F^W(x,p,t) = F^W(x(-t),p(-t),0), \\ \dot{x} = \dfrac{p}{m}, \quad \dot{p} = -\dfrac{\partial V}{\partial x}. \end{cases} \tag{73}$$

This motivates the concept of Wigner trajectories. If we define an effective quantum potential $V_{\mathrm{eff}}(x,p,t)$ according to

$$\frac{\partial V_{\mathrm{eff}}}{\partial x}\frac{\partial F^W}{\partial p} = \int_{-\infty}^{+\infty} \mathrm{d}p'\, F^W(x,p+p',t) J(x,p'), \tag{74}$$

then we can express the Moyal equation in the form

$$\frac{\partial F^W}{\partial t} = -\frac{p}{m}\frac{F^W}{\partial x} + \frac{\partial V_{\mathrm{eff}}}{\partial x}\frac{\partial F^W}{\partial p}, \tag{75}$$

which can be interpreted in analogy with (72), by stating that the Wigner function evolves along the Wigner trajectories given by

$$\dot{x} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial V_{\mathrm{eff}}}{\partial x}. \tag{76}$$

If an exact solution for F^W is known, then we can, in principle, calculate the effective potential from (74) and subsequently solve (76) to obtain the Wigner trajectories. However, in general, such is not the case. If the potential $V(x)$ does not deviate appreciably from a quadratic potential then we can address the problem by iteratively evaluating order by order the quantum corrections to the classical trajectories.[4,20,21] The zero-order approximation (i.e., the classical solution), satisfies the Liouville equation:

$$\frac{\partial F_0^W}{\partial t} = -\frac{p}{m}\frac{\partial F_0^W}{\partial x} + \frac{\partial V}{\partial x}\frac{\partial F_0^W}{\partial p}. \tag{77}$$

The order zero trajectories correspond to the classical Hamilton equations. The order one equation is given by

$$\frac{\partial F_1^W}{\partial t} = -\frac{p}{m}\frac{\partial F_1^W}{\partial x} + \frac{\partial V}{\partial x}\frac{\partial F_1^W}{\partial p} + \frac{(\hbar/2i)^2}{3!}\frac{\partial^3 V}{\partial x^3}\frac{\partial^3 F_0^W}{\partial p^3}. \tag{78}$$

If we solve this equation for F_1^W and substitute in (75) and (76), we obtain the first-order trajectories:

$$\begin{cases} \dot{x} = \dfrac{p}{m}, \\ \dot{p} = -\dfrac{\partial V}{\partial x} + \dfrac{1}{3!}\left(\dfrac{\hbar}{2i}\right)^2 \dfrac{\partial^3 V}{\partial x^3}\dfrac{\partial^3 F_0^W}{\partial p^3} \Big/ \dfrac{\partial F_1^W}{\partial p}. \end{cases} \tag{79}$$

The second-order approximation is

$$\frac{\partial F_2^W}{\partial t} = -\frac{p}{m}\frac{\partial F_2^W}{\partial x} + \frac{\partial V}{\partial x}\frac{\partial F_2^W}{\partial p} + \frac{(\hbar/2i)^2}{3!}\frac{\partial^3 V}{\partial x^3}\frac{\partial^3 F_1^W}{\partial p^3} + \frac{(\hbar/2i)^4}{5!}\frac{\partial^5 V}{\partial x^5}\frac{\partial^5 F_0^W}{\partial p^5}, \tag{80}$$

and yields the second-order correction to the classical trajectories:

$$\begin{cases} \dot{x} = \dfrac{p}{m}, \\ \dot{p} = -\dfrac{\partial V}{\partial x} + \dfrac{1}{3!}\left(\dfrac{\hbar}{2i}\right)^2 \dfrac{\partial^3 V}{\partial x^3}\dfrac{\partial^3 F_1^W}{\partial p^3} \Big/ \dfrac{\partial F_2^W}{\partial p} + \dfrac{1}{5!}\left(\dfrac{\hbar}{2i}\right)^4 \dfrac{\partial^5 V}{\partial x^5}\dfrac{\partial^5 F_0^W}{\partial p^5} \Big/ \dfrac{\partial F_2^W}{\partial p}. \end{cases} \tag{81}$$

This procedure can be carried on to any order in $\hbar$. Its main advantage is that it transforms the problem of solving an infinite order partial differential equation (the Moyal equation) into the problem of solving a sequence of first-order partial differential equations. It also displays the advantage of casting the transition from classical to quantum dynamics as an order-by-order correction (in $\hbar$) to classical mechanics. There are, however, some weak points in the procedure, the most significant being perhaps that it is not always clear what is the degree of precision of an approximation to a given order or if the entire scheme will converge.

B. Wigner trajectories in bounded systems

If a system has a boundary, then the former approximative scheme will obviously break down, because the boundary contribution was thus far unknown. As we have seen in the previous sections the boundary interaction has a nonlocal nature and will thus affect the Wigner trajectories well inside the bulk part of the system. It therefore must equally contribute to the quantum corrections of the trajectories.

In this case one was left with a single possible approach: to solve the Schrödinger equation for the confined wave function and compute the Wigner function from it. In some cases where an exact solution of the Schrödinger equation is known this method can be taken to completion. Take for instance the simple example of a free particle confined to the interval $]-1,1[$ and subject to Dirichlet boundary conditions.[5] The fundamental state is $\phi_1(x) = \cos((\pi/2)\,x)$ from which we can compute the Wigner function equations (2), (39), and (40). Since the particle is in an energy eigenstate we have

$$\frac{\partial F^W}{\partial t} = [H, F^W]_M = 0 \Rightarrow F^W(q(-t), p(-t), 0) = F^W(q,p,t) = F^W(q,p,0), \tag{82}$$

and thus the Wigner function evolves along the paths where it displays a constant value, i.e., the Wigner trajectories $(q(-t), p(-t))$ are the equi-Wigner curves. Figure 4 displays the Wigner trajectories for this simple system.

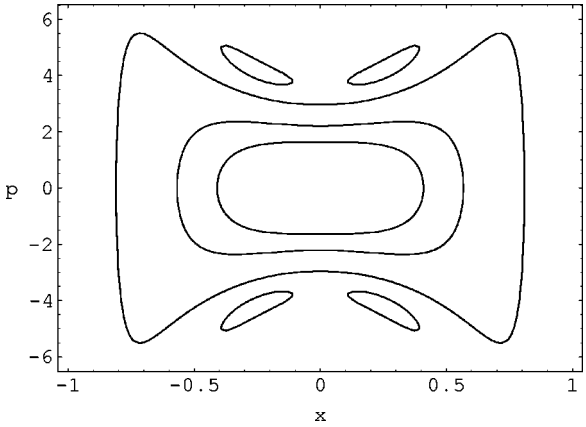

FIG. 4. Exact Wigner trajectories for a particle in the fundamental state and confined to the interval]-1,1[.

For more elaborate examples we are forced to use Eq. (74) or Eq. (75) to calculate the effective potential from the Wigner function and then Eq. (76) to calculate the Wigner trajectories. For instance in Refs. 4 and 24 a system in a symmetric box with Dirichlet boundary conditions and an external driving force was considered. The force, which is of the form $F(t)=F_0\cos(\omega t)$, induces classically the appearance of resonance. Since the system has a boundary, quantum mechanically, the authors were compelled to work in the context of the Schrödinger equation but since an exact, analytic solution is not known the Wigner function and subsequently the Wigner trajectories could not be obtained exactly.

In general, the wave-function-based approach suffers from two major drawbacks: first, in some situations (as in the previous example) it is impossible to obtain an exact solution of the Schrödinger equation, which makes it difficult to infer the degree of precision of the resulting Wigner function. Second, even if an exact solution of the Schrödinger equation is known, this method only provides the exact Wigner trajectories and in some situations it is desirable that the quantum corrections to the classical trajectories might be computed order by order in $\hbar$.

The results of this paper provide a new approach to determine the Wigner trajectories for bounded systems (satisfying Dirichlet boundary conditions) from an exclusive phase space (or c-number) point of view. In fact most of the formalism for the unconfined case can now be applied to the bounded case as well. This is certainly true for Eqs. (69)–(71) and (74)–(76) where one just has to take into account that: (1) $V(x)$ is no longer the bulk potential but it also encompasses a boundary contribution $V_D(x)$ which is associated with the Dirichlet boundary conditions and given in Eq. (53): $V_D(x)=(\hbar^2/2m)\{\delta'(x-b)-\delta'(x-a)\}$, (2) in the boundary corrections to Eqs. (69), (70), and (74) the Wigner function should be evaluated at x^+ and x^- (in the left and right boundary correction, respectively).

It is not so clear if the approximative scheme [Eqs. (77)–(81)] can be also extended to the bounded case. This is because the boundary potential deviates strongly from the harmonic oscillator potential and yields contributions to the Moyal equation to all orders in $\hbar$. We thus have to worry about the magnitude of these contributions and find a suitable criterion to determine the validity of the approximation. These issues are also a problem in the general unconfined case and are certainly not the subject of this paper. Our point here is just that the boundary potential approach is, thus far, the unique exact formulation of confined systems that only appeals to phase space objects and it thus seems to be the proper framework from which the former or other, more suitable, approximative scheme may be devised.

C. Wigner trajectories of a particle in an infinite potential well

In the following we ignore the issues of validity and convergence of the approximative scheme given by Eqs. (77)–(81) and use it to compute the order by order quantum corrections to

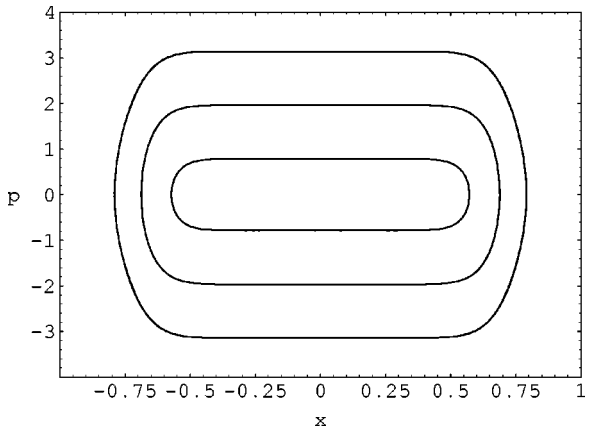

FIG. 5. Zero-order or classical approximation to the Wigner quantum trajectories: $\epsilon=0.25$ and $\hbar=m=1$.

the classical trajectories of a free particle confined to the interval $]-1,1[$. Quite remarkably, we will see that this (in this context, very poor) approximation procedure is already able to reproduce most of the qualitative behavior of the exact quantum trajectories.

The exact Wigner trajectories for a particle in the fundamental state are solutions of Eq. (76) with the effective potential satisfying (74) and (75) and were displayed in Fig. 4. The zero-order approximation to the Moyal equation (53) is given by

$$\frac{\partial F_0^W}{\partial t}(x,p,t)=-\frac{p}{m}\frac{\partial F_0^W}{\partial x}+\frac{\hbar^2}{2m}\left\{\frac{\partial V_R}{\partial x}\frac{\partial F_0^W}{\partial p}(x-\epsilon,p,t)-\frac{\partial V_L}{\partial x}\frac{\partial F_0^W}{\partial p}(x+\epsilon,p,t)\right\}, \tag{83}$$

where $V_R(x)=\delta'_\epsilon(x-1)$ and $V_L(x)=\delta'_\epsilon(x+1)$. To simplify the discussion we assume that for sufficient small ϵ we have

$$\frac{\partial F_0^W/\partial p(x-\epsilon,p,t)}{\partial F_0^W/\partial p(x,p,t)}=\frac{\partial F_0^W/\partial p(x+\epsilon,p,t)}{\partial F_0^W/\partial p(x,p,t)}=1,$$

and use these identities to transform Eq. (83) into the Liouville equation (77) with $V=(\hbar^2/2m)(V_R-V_L)$. The zero-order approximation to the exact quantum trajectories are thus the solutions of Eq. (73). They are displayed in Fig. 5, where we used the Gaussian approximation to the Dirac delta function: $\delta_\epsilon(x)=e^{x^2/\epsilon'^2}/\epsilon'\sqrt{\pi}$, $\epsilon'=0.8\epsilon$ and made $\epsilon=0.25$ (notice that this approximation was used in Sec. VI to compute the numerical solution of the bounded eigenvalue equation, Fig. 2) and $m=\hbar=1$. For sufficiently small ϵ these would be just the classical trajectories.

We now compute the first-order corrections [Eq. (79)]. These are the solutions of

$$\begin{cases}\dot{x}=\dfrac{p}{m},\\ \dot{p}=\dfrac{\hbar^2}{2m}\{\delta''_\epsilon(x+1)-\delta''_\epsilon(x-1)\}+\dfrac{\hbar^2}{48m}\{\delta^{(4)}_\epsilon(x+1)-\delta^{(4)}_\epsilon(x-1)\},\end{cases} \tag{84}$$

where we again ignored the contribution of the factors that involve the (approximate) Wigner function. We get the trajectories displayed in Fig. 6.

Finally, we compute the second-order corrections [Eq. (81)]:

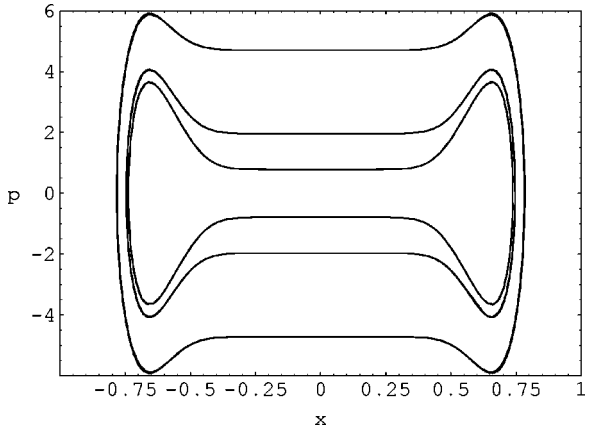

FIG. 6. First-order approximation to the Wigner quantum trajectories: numerical solution of Eq. (84) with $\epsilon=0.25$ and $\hbar=m=1$.

$$\begin{cases} \dot{x}=\dfrac{p}{m}, \\ \dot{p}=\dfrac{\hbar^2}{2m}\{\delta_\epsilon''(x+1)-\delta_\epsilon''(x-1)\}+\dfrac{\hbar^2}{48m}\{\delta_\epsilon^{(4)}(x+1)-\delta_\epsilon^{(4)}(x-1)\} \\ \qquad -\dfrac{\hbar^4}{3840m}\{\delta_\epsilon^{(6)}(x+1)-\delta_\epsilon^{(6)}(x-1)\}, \end{cases} \tag{85}$$

and get the trajectories displayed in Fig. 7.

Several remarks are now in order.

(a) We see that the first-order approximation already displays the deflection of the quantum trajectories toward regions of higher momentum as the particle approaches the boundaries.

(b) In the second approximation the ''islands'' appear. They are not confined, as in the exact case, to regions of positive or negative momentum, but they are already confined to positive or negative positions. Furthermore, the deflection to regions of high momentum is now an exclusive feature (as in the exact case) of the higher momentum trajectories. The slower ones are essentially classical.

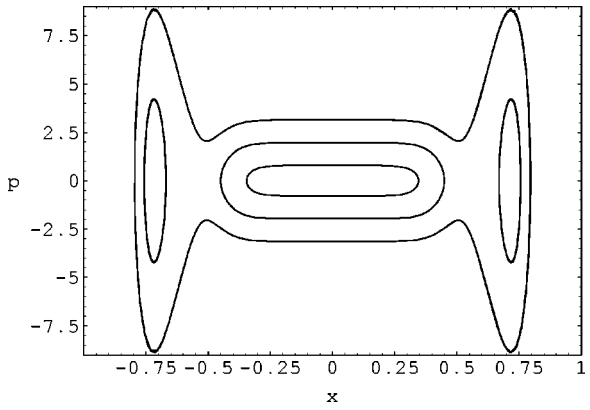

FIG. 7. Second-order approximation to the Wigner quantum trajectories: numerical solution of Eq. (85) with $\epsilon=0.25$ and $\hbar=m=1$.

(c) Not all Wigner trajectories will be confined. For sufficiently high momentum they will escape from the box. This is because we are not using the true Dirac delta but a Gaussian approximation to it. The free Wigner trajectories correspond to the part of the wave function that is outside of the box in Fig. 2.

(d) The former approximative scheme can be refined at least in three different directions: first by taking into account the contributions of the factors that are proportional to the Wigner function. Our rather simple approximative scheme is, in fact, state independent and so could not possibly reproduce the exact Wigner trajectories. This step will be more demanding from the numerical point of view since one will be asked to solve the partial differential equation for the approximate Wigner function before computing each order correction to the classical trajectories. Second, by increasing the degree of approximation to the Dirac delta function, i.e., by decreasing the spread ϵ. This is mandatory if one is interested in the behavior of the quantum trajectories of higher momentum. Finally, and quite obviously, by computing higher order corrections in $\hbar$.

VIII. CONCLUSIONS

In this paper we studied the Wigner–Weyl formulation of a particle confined to a finite interval and subject to Dirichlet boundary conditions. We found that: (1) the standard procedure of solving the unconstrained system and then imposing the boundary conditions does not work out in the Wigner–Weyl formulation; (2) the boundary conditions and the confinement of the wave function determine a boundary correction to the $*$-genvalue equation and to the Moyal equation; (3) Dirichlet boundary conditions on the confined wave function imply both Dirichlet and Neumann boundary conditions on the corresponding confined Wigner function.

Our main task was then the evaluation of the contributions of the boundaries to the $*$-genvalue equation (6) and to the time evolution equation (5) for a wave function satisfying Dirichlet boundary conditions. These contributions were shown to have the form of boundary potentials added to the Hamiltonian, and the same potentials were obtained in the operator formulation of quantum mechanics, when we derived the Schrödinger eigenvalue equation for the confined wave function $\psi(x)=\phi(x)\,\theta(x-a)\,\theta(b-x)$. Together with the boundary conditions they are responsible, both in the Wigner and in the Schrödinger formulations, for the confinement of the system and the consequent discretization of the energy levels. Finally, we extended Baker's converse construction to the bounded case, proving the full equivalence between the operator-Schrödinger and the Wigner formulation of the confined eigenvalue problem.

Finally, we used our previous results to approach the problem of evaluating the Wigner trajectories of bounded systems and ventured the possibility of applying these methods to nonlinear systems displaying classical chaotic behavior.

The procedure described in this work can be generalized to higher-dimensional multiparticle systems and also to any $*$-genvalue equation of the form $A^W(x,p)*F_a^W(x,p)=aF_a^W(x,p)$, associated with the eigenvalue equation: $\hat{A}(\hat{x},\hat{p})\,\psi_a(x)=a\,\psi_a(x)$. From a more general point of view the results of this paper provide a first approach to the problem of solving star-equations with boundaries. This is a difficult but important problem as such equations are known to play a key part in several fields of research ranging from standard topics in quantum mechanics to some important developments in M-theory.[26]

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The dynamical elliptic quantum Gaudin models and their solutions

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In this paper, we construct the Hamiltonians of both periodic and open elliptic quantum Gaudin models and show their relations with the elliptic quantum group, and the boundary elliptic quantum group, respectively. We define the eigenstates of these two models to be the Bethe vectors with $\eta=0$ of the elliptic quantum group and the boundary elliptic quantum group, respectively. Then, the Hamiltonians are exactly diagonalized by using the algebraic Bethe ansatz method. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1505665]

I. INTRODUCTION

The Gaudin model associated with the su(2) Lie algebra was first proposed by Gaudin in 1973.[1–3] It is a new kind of integrable quantum models with the long range interaction. Babujian and Flume generalized it into the general Lie algebra g case, and constructed the corresponding Hamiltonian.[4] They also set up the off-shell Bethe ansatz equation (OSBAE) and gave an explicit proof for su(3). However, they did not give the Bethe ansatz equations. In Ref. 5, Feigin, Frenkel, and Reshetikhin suggested a new method based on the Wakimoto realization of some affine algebra at critical lever, and solved exactly the Gaudin models related to the Lie algebra g. They also obtained the eigenvalues and the corresponding Bethe ansatz equations.

On the other hand, we can simply consider the Gaudin model as the limit of some integrable quantum chains. Sklyanin proposed that the spectrum and eigenfunctions of the spin-1/2 Gaudin models with rational and trigonometric interaction could be derived from those of the XXX and XXZ chains.[6] Then in the Refs. 7–9, Sklyanin and Takebe obtained the arbitrary spin XYZ Gaudin model as a quasiclassical limit of the inhomogeneous higher spin generalization of the XYZ model. Hikami has applied Sklyanin's method into the open Gaudin model by taking quasiclassical limit of the transfer matrix for the inhomogeneous open spin-1/2 XXZ chain.[10] Under the same limit, he has also obtained the eigenvalue and the Bethe ansatz equations.

Recently, the Gaudin models are studied in many integrable systems, such as the supersymmetric Gaudin models[11,12] and the elliptic Gaudin models.[13] In the present paper, we propose the dynamical elliptic quantum Gaudin (DEQG) model with both periodic and open boundary conditions. We obtain the eigenvalues of the Hamiltonians and the Bethe ansatz equations.

The framework of this paper is arranged as follows: In Sec. II we review some basic facts of the elliptic quantum group $E_{\tau,\eta}(\mathrm{sl}_2)$ needed in our paper. In Sec. III we construct the DEQG model under periodic boundary condition, and obtain the eigenvalues of Hamiltonians and the corresponding Bethe ansatz equation in Sec. IV. In Sec. V we construct the open DEQG model and give solutions. In the last section, we give some brief conclusions.

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II. THE ELLIPTIC QUANTUM GROUP

The first part of this paper will contribute in the DEQG model with periodic boundary condition. This model is closely associated with the elliptic quantum group $E_{\tau,\eta}(\mathrm{sl}_2)$ (Refs. 14 and 15) which is an algebraic structure underlying the elliptic solutions of the Yang–Baxter relation in the statistical mechanics, and connected with the Knizhnik–Zamolodchikov–Bernard equation on torus. So, we first recall some basic concepts of the elliptic quantum group $E_{\tau,\eta}(\mathrm{sl}_2)$.

Let h be the generator of a one-dimensional commutative Lie algebra h, and $a(\lambda,w)$, $b(\lambda,w)$, $c(\lambda,w)$, $d(\lambda,w)$ be the elements of a matrix $L(\lambda,w)$. The elliptic quantum group $E_{\tau,\eta}(\mathrm{sl}_2)$ is generated by meromorphic functions of the variable h and the elements of $L(\lambda,w)$ with noncommutative entries, subjects to the dynamical Yang–Baxter relations (DYBR)

$$\begin{aligned} &R^{(12)}(\lambda-2\eta h,w_{12})L^{(1)}(\lambda,w_1)L^{(2)}(\lambda-2\eta h^{(1)},w_2)\\ &\quad=L^{(2)}(\lambda,w_2)L^{(1)}(\lambda-2\eta h^{(2)},w_1)R^{(12)}(\lambda,w_{12}), \end{aligned} \tag{1}$$

with $L^{(1)}(\lambda,w_1)=L(\lambda,w_1)\otimes 1$ and $L^{(2)}(\lambda,w_2)=1\otimes L(\lambda,w_2)$. The $L(\lambda,w)$ is a 2×2 matrix whose elements are quamtum operator and $h^{(j)}$ stands for diagonal matrix $\mathrm{Diag}(1,-1)$ in jth matrix space. For the sake of simplicity, we call the matrix space auxillary space and quantum Hilbert space the quantum space. Here $R^{(12)}(\lambda-2\eta h,w_{12})$ is a 4×4 matrix and $w_{ij}=w_i-w_j$. Note that the h in R is a quantum operator acting on the same quantum Hilbert space as L operator acts on. It is the reason that Eq. (1) is called the dynamical Yang–Baxter relation. The explicit expression of R matrix is given by

$$\begin{aligned} R(\lambda,z)=&E_{1,1}\otimes E_{1,1}+E_{-1,-1}\otimes E_{-1,-1}\\ &+\alpha(\lambda,z)E_{1,1}\otimes E_{-1,-1}+\alpha(-\lambda,z)E_{-1,-1}\otimes E_{1,1}\\ &+\beta(\lambda,z)E_{1,-1}\otimes E_{-1,1}+\beta(-\lambda,z)E_{-1,1}\otimes E_{1,-1} \end{aligned} \tag{2}$$

with

$$\alpha(\lambda,z)=\frac{\theta(z)\,\theta(\lambda+2\eta)}{\theta(z-2\eta)\,\theta(\lambda)},$$

$$\beta(\lambda,z)=-\frac{\theta(\lambda+z)\,\theta(2\eta)}{\theta(z-2\eta)\,\theta(\lambda)},$$

$$\theta(\lambda,\tau)=-\sum_{j=-\infty}^{\infty} e^{\pi i(j+\frac{1}{2})^2\tau+2\pi i(j+\frac{1}{2})(\lambda+\frac{1}{2})}.$$

All commutation relations of the elements of L can be found in Ref. 14. Here we only list some of them to be used frequently later,

$$\begin{aligned} &f(\lambda,h)g(\lambda,h)=g(\lambda,h)f(\lambda,h),\\ &f(\lambda-2\eta,h)\tilde{a}(w)=\tilde{a}(w)f(\lambda,h),\\ &f(\lambda+2\eta,h)\tilde{d}(w)=\tilde{d}(w)f(\lambda,h),\\ &f(\lambda+2\eta,h+2)\tilde{b}(w)=\tilde{b}(w)f(\lambda,h),\\ &f(\lambda-2\eta,h-2)\tilde{c}(w)=\tilde{c}(w)f(\lambda,h), \end{aligned} \tag{3}$$

where we have used the notation $\tilde{a}(w)\equiv a(\lambda,w)$ for convenience. And the others are similar.

For complex numbers Λ and z, one can define an infinite dimensional complex vector space $V_\Lambda(z)$ of $E_{\tau,\eta}(\mathrm{sl}_2)$ (evaluation Verma module).[14] Let e_k, $k\in Z_{\geqslant 0}$ be the basis of $V_\Lambda(z)$, the action of generators of $E_{\tau,\eta}(\mathrm{sl}_2)$ are defined by

$$\begin{aligned} f(h)e_k &= f(\Lambda-2k)e_k, \\ a(\lambda,w)e_k &= g(a,\lambda,w,k)e_k, \\ b(\lambda,w)e_k &= g(b,\lambda,w,k)e_{k+1}, \\ c(\lambda,w)e_k &= g(c,\lambda,w,k)e_{k-1}, \\ d(\lambda,w)e_k &= g(d,\lambda,w,k)e_k, \end{aligned} \tag{4}$$

with

$$\begin{aligned} g(a,\lambda,w,k) &= \frac{\theta(z-w+(\Lambda+1-2k)\eta)\,\theta(\lambda+2k\eta)}{\theta(z-w+(\Lambda+1)\eta)\,\theta(\lambda)}, \\ g(b,\lambda,w,k) &= \frac{\theta(-\lambda+z-w+(\Lambda-1-2k)\eta)\,\theta(2\eta)}{\theta(z-w+(\Lambda+1)\eta)\,\theta(\lambda)}, \\ g(c,\lambda,w,k) &= \frac{\theta(-\lambda-z+w+(\Lambda+1-2k)\eta)\,\theta(2(\Lambda+1-k)\eta)\,\theta(2k\eta)}{\theta(z-w+(\Lambda+1)\eta)\,\theta(\lambda)\,\theta(2\eta)}, \\ g(d,\lambda,w,k) &= \frac{\theta(z-w+(-\Lambda+1+2k)\eta)\,\theta(\lambda-2(\Lambda-k)\eta)}{\theta(z-w+(\Lambda+1)\eta)\,\theta(\lambda)}. \end{aligned} \tag{5}$$

The theorem (3) in Ref. 14 ensures the above definition to be an evaluation representation of elliptic quantum $E_{\tau,\eta}(\mathrm{sl}_2)$. If $\Lambda=n+(m+l)/(2\eta)$, where n,m,l are integer, $n\geqslant 0$, then one can obtain a $n+1$-dimensional vector space from $V_\Lambda(z)$. The e_k can be identified with the eigenvectors of the h. This is similar with the $n+1$-dimensional representation of sl(2).

For any space $W=V_\Lambda$ over $E_{\tau,\eta}(\mathrm{sl}_2)$, the transfer matrix can be defined by

$$t(w)=\tilde{a}(w)+\tilde{d}(w), \tag{6}$$

which preserves the space $H=\mathrm{Fun}(W)[0]$ of functions with the value in the zero weight, and commute pairwise on H, $t(w)t(u)=t(u)t(w)$ on H.

Let $W=V_{\Lambda_1}(z_1)\otimes\cdots\otimes V_{\Lambda_n}(z_n)$ be a tensor product of evaluation spaces, and let $\Lambda=\Lambda_1+\cdots+\Lambda_n$. Then, we can obtain a T operator as the tensor product of L operators. The precise form of the T operator can be defined by

$$\begin{aligned} T(\lambda,w) = L_1\Big(\lambda-\sum_{j=2}^{n}2\eta h_j,w\Big)L_2\Big(\lambda-\sum_{j=3}^{n}2\eta h_j,w\Big)\cdots \\ \times L_{n-1}(\lambda-2\eta h_n,w)L_n(\lambda,w). \end{aligned} \tag{7}$$

By using the relation[14]

$$[h^{(1)}+h,T(\lambda,w)]=0 \tag{8}$$

with $h=\sum_{j=1}^{n}h_j$, we can easily prove that the T operator also satisfies the DYBR Eq. (1). Writing the elements of the T operator $\hat{\mathcal{A}},\hat{\mathcal{B}},\hat{\mathcal{C}}$, and $\hat{\mathcal{D}}$, we can rewrite the transfer matrix as

$$t(w)=\hat{\mathcal{A}}(w)+\hat{\mathcal{D}}(w). \tag{9}$$

Then, the highest weight state of the space H, $W[\Lambda]=Cv_0$, obeys the following highest weight condition: for every w,

$$\begin{aligned}&\hat{\mathcal{C}}(w)v_0=0,\quad \hat{\mathcal{A}}(w)v_0=v_0,\\ &\hat{\mathcal{D}}(w)v_0=\frac{\theta(\lambda-2\eta\Lambda)}{\theta(\lambda)}\prod_{j=1}^{n}\frac{\theta(w-z_j-(-\Lambda_j+1)\eta)}{\theta(w-z_j-(\Lambda_j+1)\eta)}v_0.\end{aligned} \tag{10}$$

The quantum determinant of the elliptic quantum algebra is given by[14]

$$\begin{aligned}\tilde{\Delta}(w)&=\frac{\theta(\lambda)}{\theta(\lambda-2\eta h)}(\hat{\mathcal{D}}(w+2\eta)\hat{\mathcal{A}}(w)-\hat{\mathcal{B}}(w+2\eta)\hat{\mathcal{C}}(w))\\ &=\frac{\theta(\lambda)}{\theta(\lambda-2\eta h)}(\hat{\mathcal{A}}(w+2\eta)\hat{\mathcal{D}}(w)-\hat{\mathcal{C}}(w+2\eta)\hat{\mathcal{B}}(w)).\end{aligned} \tag{11}$$

III. THE DEQG MODEL WITH PERIODIC BOUNDARY CONDITION

The Gaudin model was proposed as a new class of integrable quantum systems by Gaudin. In this section, we propose a periodic DEQG model. For the space $H=\mathrm{Fun}(W)[0]$ with $W=V_{\Lambda_1}\otimes\cdots\otimes V_{\Lambda_n}$, the Hamiltonian of the model is

$$\begin{aligned}\hat{\tau}(\lambda,w)&=2(\mathcal{A}^2+\mathcal{H}^2)-4n\Lambda(\partial_\lambda\varphi(\lambda))-8n\Lambda\varphi(\lambda)\partial_\lambda-8n\mathcal{A}'\partial_\lambda+2[(\mathcal{A}')^2+(\mathcal{H}')^2]\\ &\quad-4(\mathcal{A}\mathcal{A}'+\mathcal{H}\mathcal{H}')+8n^2\partial_\lambda^2+\sum_{j,k=1}^{n}W_1(\lambda,w,z_j)W_2(\lambda,w,z_k)[E_j^+E_k^-+E_j^-E_k^+],\end{aligned} \tag{12}$$

where $\mathcal{A}=\Lambda\varphi(\lambda),\mathcal{A}'=\Sigma_j\Lambda_j\varphi(z_j-w),\mathcal{H}=\Sigma_j h_j\varphi(\lambda)$, and $\mathcal{H}'=\Sigma_j h_j\varphi(z_j-w)$ with

$$\varphi(\lambda)=\frac{\theta'(\lambda)}{\theta(\lambda)},$$

$$W_1\equiv 2\frac{\theta'(0)}{\theta(\lambda)}\frac{\theta(-\lambda+z-w)}{\theta(z-w)}$$

and

$$W_2\equiv 2\frac{\theta'(0)}{\theta(\lambda)}\frac{\theta(-\lambda-z+w)}{\theta(z-w)}.$$

Here the operators h_j and $E_j^{\pm}$, which act on the jth infinite-dimensional complex vector space V_{Λ_j}, satisfy

$$[h_i,E_j^{\pm}]=\pm\delta_{i,j}2E_j^{\pm},\quad [E_i^+,E_j^-]=\delta_{i,j}h_j, \tag{13}$$

$$h_je_k=(\Lambda_j-2k)e_k, \tag{14}$$

$$E_j^-e_k=e_{k+1},\quad E_j^+e_k=k(\Lambda_j+1-k)e_{k-1}. \tag{15}$$

In order to find the eigenvalue of $\hat{\tau}(\lambda,w)$, we have to guess the form of the eigenstates. In principle, one may follow Gaudin's method. But it is very difficult. Thanks to Sklyanin's approach,[6,7] this Hamiltonian can be related to the transfer matrix and the quantum determinant of the periodic elliptic quantum group. We will try to find such relations.

Now, let us examine the asymptotic behavior of the operators in the preceding section when η approaches 0. The results are as follows:

$$R(\lambda,w)=1+2\,\eta r(\lambda,w)+O(\eta^2), \tag{16}$$

$$L(\lambda,w)=1+2\,\eta L'(\lambda,w)+O(\eta^2), \tag{17}$$

where $r(\lambda,w)$ is the so-called classical r matrix,

$$\begin{aligned} r(\lambda,w)=&\{\varphi(\lambda)+\varphi(w)\}E_{1,1}\otimes E_{-1,-1}-\{\varphi(\lambda)-\varphi(w)\}E_{-1,-1}\otimes E_{1,1}\\ &-\frac{\theta(\lambda+z)\theta'(0)}{\theta(\lambda)\theta(z)}E_{1,-1}\otimes E_{-1,1}-\frac{\theta(\lambda-z)\theta'(0)}{\theta(\lambda)\theta(z)}E_{-1,1}\otimes E_{1,-1}, \end{aligned} \tag{18}$$

and the elements of L operator are tended as

$$a(\lambda,w)=1+\eta a'(\lambda,w)+O(\eta^2), \tag{19}$$

$$d(\lambda,w)=1+\eta d'(\lambda,w)+O(\eta^2), \tag{20}$$

$$b(\lambda,w)=\eta b'(\lambda,w)+O(\eta^2), \tag{21}$$

$$c(\lambda,w)=\eta c'(\lambda,w)+O(\eta^2), \tag{22}$$

$$\tag{23}$$

and we call the operators $a'(\lambda,w)$, $b'(\lambda,w)$, $c'(\lambda,w)$, and $d'(\lambda,w)$ generating operators of the DEQG model, which are defined by

$$a'(\lambda,w)=(\Lambda-h)[\varphi(\lambda)-\varphi(z-w)]-2\partial_\lambda, \tag{24}$$

$$d'(\lambda,w)=-(\Lambda+h)[\varphi(\lambda)+\varphi(z-w)]+2\partial_\lambda, \tag{25}$$

$$b'(\lambda,w)=W_1(\lambda,w,z)E^+, \tag{26}$$

$$c'(\lambda,w)=W_2(\lambda,w,z)E^-. \tag{27}$$

For the space $H=\mathrm{Fun}(W)[0]$ with $W=V_{\Lambda_1}\otimes\cdots\otimes V_{\Lambda_n}$, the generating operators of the Gaudin model can be defined by $\hat{a}(\lambda,w)$, $\hat{b}(\lambda,w)$, $\hat{c}(\lambda,w)$, $\hat{d}(\lambda,w)$. The concrete forms of them are as follows:

$$\begin{aligned} \hat{a}(\lambda,w)\equiv&\,\eta^{-1}(\hat{\mathcal{A}}(\lambda,w)-1)\\ =&\sum_{j=1}^{n}(\Lambda_j-h_j)[\varphi(\lambda)-\varphi(z_j-w)]-2n\partial_\lambda+O(\eta), \end{aligned} \tag{28}$$

$$\begin{aligned} \hat{d}(\lambda,w)\equiv&\,\eta^{-1}(\hat{\mathcal{D}}(\lambda,w)-1)\\ =&-\sum_{j=1}^{n}(\Lambda_j+h_j)[\varphi(\lambda)+\varphi(z_j-w)]+2n\partial_\lambda+O(\eta), \end{aligned} \tag{29}$$

$$\hat{b}(\lambda,w)\equiv\eta^{-1}\hat{\mathcal{B}}(\lambda,w)$$
$$=\sum_{j=1}^{n} W_1(\lambda,w,z_j)E_j^{+}+O(\eta), \tag{30}$$

$$\hat{c}(\lambda,w)\equiv\eta^{-1}\hat{\mathcal{C}}(\lambda,w)$$
$$=\sum_{j=1}^{n} W_2(\lambda,w,z_j)E_j^{-}+O(\eta). \tag{31}$$

Taking $\eta\to 0$ for Eq. (7), we have

$$T(\lambda,w)=1+\eta\mathcal{T}(\lambda,w)+O(\eta^2). \tag{32}$$

Substituting Eqs. (28)–(31) into the transfer matrix $t(\lambda,w)$ and the quantum determinant element $\tilde{\Delta}(\lambda,w)$, we can obtain

$$t(\lambda,w)=2+\eta\mathrm{tr}\mathcal{T}(\lambda,w)+O(\eta^2), \tag{33}$$

$$\begin{aligned}\tilde{\Delta}(\lambda,w)=&1+2\eta[\mathrm{tr}\mathcal{T}(\lambda,w)+2h\varphi(\lambda)]\\&+\eta^2[-2h^2\varphi^{(2)}(\lambda)+4\mathrm{tr}\mathcal{T}^2(\lambda,w)\\&+\mathrm{tr}(\partial_w\mathcal{T}(\lambda,w)-\partial_\lambda\mathcal{T}(\lambda,w))\\&+2h\varphi(\lambda)\mathrm{tr}\mathcal{T}(\lambda,w)]+O(\eta^2).\end{aligned} \tag{34}$$

One can easily check that $\mathrm{tr}\,\mathcal{T}^2(\lambda,w)$ in the quantum determinant element $\tilde{\Delta}(\lambda,w)$ is equal to the Hamiltonian $\hat{\tau}(\lambda,w)$. Since the quantum determinant is the center of the elliptic quantum group, and $t(\lambda,w)$'s are a commutative family under zero weight condition, $\hat{\tau}(\lambda,w)$'s for different parameters w are also commutative family. Therefore, the DEQG model is integrable. Taking into account the zero weight condition, we can define the Hamiltonian of the periodic DEQG model by the linear combination of $t(\lambda,w)$, and $\tilde{\Delta}(\lambda,w)$,

$$\hat{\tau}(\lambda,w)\equiv\mathrm{tr}\,\mathcal{T}^2(\lambda,w)$$
$$=\frac{1}{4\eta^2}\{\tilde{\Delta}(\lambda,w)-t(\lambda,w)+1-\eta^2(\partial_w-\partial_\lambda)\mathrm{tr}\,\mathcal{T}(\lambda,w)\}. \tag{35}$$

Substituting Eqs. (7) and (11) into Eq. (35), one can check that the Hamiltonian of the model is proven to be Eq. (12).

Expanding the commutation relations of the operators of the elliptic quantum group by $\eta\to 0$, we can obtain

$$\begin{gathered}[h,\hat{a}(\lambda,w)]=0,\quad[\hat{b}(\lambda,w),h]=2\hat{b}(\lambda,w),\\ \hat{a}(\lambda,w)f(\lambda)=F_1(\lambda)\hat{a}(\lambda,w)+F_2(\lambda),\\ \hat{d}(\lambda,w)f(\lambda)=\mathcal{F}_1(\lambda)\hat{d}(\lambda,w)+\mathcal{F}_2(\lambda),\\ \hat{b}(\lambda,w)f(\lambda)=f(\lambda)\hat{b}(\lambda,w)+2\eta f'(\lambda)\hat{b}(\lambda,w),\end{gathered} \tag{36}$$

where

$$F_1(\lambda)=f(\lambda)-2\eta f'(\lambda),\quad F_2(\lambda)=-2f'(\lambda)+2\eta f''(\lambda),$$
$$\mathcal{F}_1(\lambda)=f(\lambda)+2\eta f'(\lambda),\quad \mathcal{F}_2(\lambda)=2f'(\lambda)+2\eta f''(\lambda). \tag{37}$$

Applying the generating operators of the Gaudin model on the highest weight state v_0, we have

$$\hat{a}(\lambda,w)v_0=0,\quad \hat{c}(\lambda,w)v_0=0,$$
$$\hat{d}(\lambda,w)v_0=\left[-2\eta\varphi(\lambda)+2\Lambda\sum_{j=1}^{n}\varphi(w-z_j)\right]v_0. \tag{38}$$

IV. THE ALGEBRAIC BETHE ANSATZ FOR THE PERIODIC DEQG MODEL

In this section, we try our best to find the eigenvalues of the Hamiltonian $\hat{\tau}(\lambda,w)$ of the periodic DEQG model and the Bethe ansatz equations. To construct the algebraic Bethe ansatz for the present model, as usual, we define first the vacuum state as the highest weight state v_0. And we define the Bethe state Ω_s as

$$\Omega_s=\hat{b}(\lambda,t_1)\hat{b}(\lambda,t_2)\cdots\hat{b}(\lambda,t_s)g(\lambda)v_0,\quad g(\lambda)\neq 0. \tag{39}$$

Here we assume Λ to be an integer $2s\geqslant 0$ in this section to ensure the zero-weight space $W[0]$ is nontrivial.

From Ref. 14, we can find the following commutation relations between $\hat{a}(w)$, $\hat{d}(w)$, and $\hat{b}(w)$ [here we abbreviate $\hat{a}(\lambda,w)$ as $\hat{a}(w)$ for convenience, and the other operators are the same]:

$$\hat{b}(w)\hat{b}(t)=\hat{b}(t)\hat{b}(w), \tag{40}$$

$$\begin{aligned}\hat{a}(w)\hat{b}(t)=&\hat{r}(t-w,\lambda)\hat{b}(t)+\hat{b}(t)\hat{a}(w)+\eta\hat{r}(t-w,\lambda)\hat{b}(t)\hat{a}(w)+\hat{s}(t-w,\lambda)\hat{b}(w)\\&+\eta\hat{s}(t-w,\lambda)\hat{b}(w)\hat{a}(t),\\ \hat{d}(w)\hat{b}(t)=&\hat{r}(w-t,\lambda-2\eta)\hat{b}(t)+\hat{b}(t)\hat{d}(w)+\eta\hat{r}(w-t,\lambda-2\eta)\hat{b}(t)\hat{d}(w)\\&-\hat{s}(t-w,\lambda)\hat{b}(w)-\eta\hat{s}(t-w,\lambda)\hat{b}(w)\hat{d}(t)\end{aligned} \tag{41}$$

with

$$\hat{s}(t,\lambda)=\frac{\theta(t+\lambda)\theta'(0)}{\theta(\lambda)\theta(t)}+O(\eta),$$
$$\hat{r}(t,\lambda)=\varphi(\lambda)-\varphi(t)+2\eta\left\{\frac{\theta''(t)}{\theta(t)}-\frac{\theta''(\lambda)}{\theta(\lambda)}+2(\varphi(\lambda))^2-\varphi(\lambda)\varphi(t)\right\}+O(\eta^2).$$

Moving $\hat{a}$ and $\hat{d}$ from the left-hand side to the right-hand side of $\hat{b}$ by using the commutation relations, we obtain

$$\begin{aligned}\hat{a}(w)\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_s)=&A_0(w,\{t_i\})\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_s)\\&+A_1(w,\{t_i\})\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_s)\hat{a}(w)+A_u,\end{aligned} \tag{42}$$

$$\begin{aligned}\hat{d}(w)\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_s)=&D_0(w,\{t_i\})\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_s)\\&+D_1(w,\{t_i\})\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_s)\hat{d}(w)+D_u,\end{aligned} \tag{43}$$

where A_0, A_1, A_0, and D_1 are the wanted terms and A_u and D_u are the unwanted terms with

$$A_0=\sum_{j=1}^{s}\hat{r}(t_j-w,\lambda)+2\eta\sum_{j=2}^{s}(j-1)\partial_\lambda\hat{r}(t_j-w,\lambda)+\eta\sum_{j=2}^{s}(j-1)\sum_{k=1}^{j-1}\hat{r}(t_k-w,\lambda)\hat{r}(t_j-w,\lambda)+O(\eta^2), \tag{44}$$

$$A_1=1+\eta\sum_{j=1}^{s}\hat{r}(t_j-w,\lambda)+O(\eta^2), \tag{45}$$

$$A_u=\sum_{k=1}^{s}\left\{\hat{s}(t_k-w,\lambda)+\eta\hat{s}(t_k-w,\lambda)\sum_{j\neq k}^{s}\hat{r}(t_j-w,\lambda)\right\}\times\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_{k-1})\hat{b}(w)\hat{b}(t_{k+1})\cdots\hat{b}(t_s)+\sum_{k=1}^{s}\eta\hat{s}(t_k-w,\lambda)\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_{k-1})\hat{b}(w)\hat{b}(t_{k+1})\cdots\hat{b}(t_s)\hat{a}(t_k)+O(\eta^2),$$

$$j=1,2,3,\ldots,s, \tag{46}$$

$$D_0=\sum_{j=1}^{s}\hat{r}(w-t_j,\lambda-2\eta)-2\eta\sum_{j=1}^{s}(j-1)\partial_\lambda\hat{r}(w-t_j,\lambda-2\eta)+\eta\sum_{j=2}^{s}(j-1)\sum_{k=1}^{j-1}\hat{r}(w-t_k,\lambda)\hat{r}(w-t_j,\lambda-2\eta)+O(\eta^2), \tag{47}$$

$$D_1=1+\eta\sum_{j=1}^{s}\hat{r}(w-t_j,\lambda)+O(\eta^2), \tag{48}$$

$$D_u=\sum_{k=1}^{s}\left\{-\hat{s}(t_k-w,\lambda)-\eta\hat{s}(t_k-w,\lambda)\sum_{j\neq k}^{s}\hat{r}(t_j+w,\lambda)\right\}\times\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_{k-1})\hat{b}(w)\hat{b}(t_{k+1})\cdots\hat{b}(t_s)-\sum_{k=1}^{s}\eta\hat{s}(t_k-w,\lambda)\hat{b}(t_1)\hat{b}(t_2)\cdots\hat{b}(t_{k-1})\hat{b}(w)\hat{b}(t_{k+1})\cdots\hat{b}(t_s)\hat{d}(t_1)+O(\eta^2),$$

$$j=1,2,\ldots,s. \tag{49}$$

In the framework of algebraic Bethe ansatz, when the transfer matrix Eq. (33) acts on the Bethe state Ω_s Eq. (39), the unwanted terms should cancel each other. Thus we can obtain the Bethe ansatz equations

$$\sum_{j\neq k}^{s}\varphi(t_j-t_k)+\sum_{i=1}^{n}\varphi(t_k-z_i)=c, \tag{50}$$

with $g(\lambda)=\theta^s(\lambda)e^{-\lambda c}$, and c is a constant.

With the above restrictions of the Bethe ansatz equations, we can obtain the eigenvalues $\Lambda(\lambda,w)$ of the transfer matrix

$$\Lambda(\lambda,w)=2+\eta\Lambda^{(1)}(\lambda,w)+\eta^2\Lambda^{(2)}(\lambda,w)+O(\eta^3), \tag{51}$$

where

$$\Lambda^{(1)}(\lambda,w)=2\sum_{k=1}^{n}\Lambda\varphi(w-z_k),$$

$$\begin{aligned}\Lambda^{(2)}(\lambda,w)=&4c^2+4\sum_{j\neq k=1}^{s}\varphi(t_j-w)\varphi(t_k-w)+\sum_{j=1}^{s}\left\{\frac{\theta''(t_j-w)}{\theta(t_j-w)}+8c\varphi(t_j-w)\right\}\\&+4c\sum_{k=1}^{n}\Lambda\varphi(w-z_k)+4\sum_{j=1}^{s}\sum_{k=1}^{n}\Lambda_k\varphi(t_j-w)\varphi(w-z_k)\\&+2\sum_{k\neq j=1}^{n}\Lambda_k\Lambda_j\varphi(t_j-w)\varphi(w-z_k)\\&+\sum_{k=1}^{n}\left\{2\Lambda_k(\Lambda_k+1)(\varphi\theta(w-z_k))^2-(\Lambda_k^2+1)\frac{\theta''(w-z_k)}{\theta(w-z_k)}\right\}.\end{aligned}$$

For the quantum determinant commutations with all elements of the generating operators of the DEQG model, the quantum determinant takes the same eigenvalues on both highest weight states v_0 and the Bethe state Ω_s,

$$\begin{aligned}\tilde{\Delta}(w,\lambda)=&1+2\eta\sum_{k=1}^{n}\Lambda_k\varphi(w-z_k)+\eta^2\left\{\sum_{k=1}^{n}4\Lambda_k\frac{\theta''(w-z_k)\theta(w-z_k)-(\theta'(w-z_k))^2}{\theta^2(w-z_k)}\right.\\&+2\Lambda^2\frac{\theta''(\lambda)}{\theta(\lambda)}+2\sum_{j=1}^{s}\sum_{k\neq j=1}^{n}\Lambda_k\Lambda_j\varphi(w-z_j)\varphi(w-z_k)\\&+\sum_{k=1}^{n}\left(2\Lambda_k(\Lambda_k+1)(\varphi(w-z_k))^2-(\Lambda_k^2+1)\frac{\theta''(w-z_k)}{\theta(w-z_k)}\right)\\&\left.-4\Lambda\varphi(\lambda)\sum_{k=1}^{n}\Lambda_k\varphi(w-z_k)+2\Lambda^2\frac{2(\theta'(\lambda))^2-\theta''(\lambda)}{\theta^2(\lambda)}\right\}+O(\eta^3).\end{aligned} \tag{52}$$

From Eq. (51), we know that

$$\mathrm{tr}\,\mathcal{T}(\lambda,w)=\Lambda^{(1)}(\lambda,w)=2\sum_{k=1}^{n}\Lambda_k\frac{\theta'(w-z_k)}{\theta(w-z_k)}.$$

So we have

$$(\partial_w-\partial_\lambda)\mathrm{tr}\,\mathcal{T}(\lambda,w)=2\sum_{k=1}^{n}\Lambda_k\frac{\theta''(w-z_k)\theta(w-z_k)-(\theta'(w-z_k))^2}{\theta^2(w-z_k)}. \tag{53}$$

Thus, applying the $\hat{\tau}(\lambda,w)$ on the Ω_s and taking into account Eqs. (51)–(53), we can obtain the final eigenvalue

$$\hat{\tau}(\lambda,w)\Omega_s=\left\{\partial_w\left[\frac{1}{2}\sum_{k=1}^{n}\Lambda_k\varphi(w-z_k)-\sum_{j=1}^{s}\varphi(w-t_j)\right]-\left[c-\sum_{j=1}^{s}\varphi(w-t_j)\right]^2\right.$$
$$\left.+\left[\sum_{j=1}^{s}\varphi(w-t_j)-c\right]\sum_{k=1}^{n}\Lambda_k\varphi(w-z_k)-\Lambda\varphi(\lambda)\sum_{k=1}^{n}\Lambda_k\varphi(w-z_k)\right\}\Omega_s. \quad (54)$$

In this section, we have derived the eigenvalue and the Bethe ansatz equations of the DEQG model by using generating operators of the model. Calculating the residues of the Hamiltonian Eq. (12) and its eigenvalue Eq. (54) at $w=z_j$, one can get the jth Hamiltonian and the corresponding energy spectrum on Ω_s. In Ref. 14, Felder *et al.* have given the eigenvalue and the Bethe ansatz equations of the elliptic quantum group. The Bethe state in their paper is defined by $\tilde{b}(t_1)\tilde{b}(t_2)\cdots\tilde{b}(t_s)g(\lambda)v_0$. If we apply $t(\lambda,w)$ and $\tilde{\Delta}(\lambda,w)$ on that state, then we take the $\eta\to 0$, we can also obtain the same results as Eq. (54) and the Bethe ansatz equation (50).

V. OPEN DEQG MODEL AND ITS SOLUTION

For the space $W=V_{\Lambda_1}\otimes\cdots\otimes V_{\Lambda_n}$ and the parameter $\Lambda=\Lambda_1+\cdots+\Lambda_n$, we define the Hamiltonian of the open DEQG model as

$$H_j(\lambda,w)=\delta(\lambda,z_j,\xi)(1-h_j)+\sum_{k=1}^{N}\left\{\frac{1}{\Lambda_j+1}\left[\frac{\theta(z_i+\xi)\,\theta(z_j+\lambda-\xi)}{\theta(z_i-\xi)\,\theta(z_j-\lambda+\xi)}W_1^+E_k^-E_j^+\right.\right.$$
$$+\frac{\theta(z_i-\xi)\,\theta(z_j-\lambda+\xi)}{\theta(z_i+\xi)\,\theta(z_j+\lambda-\xi)}W_2^+E_k^+E_j^--\varphi(z_k+z_j)(h_kh_j-\Lambda_k)+\varphi(\lambda)(2\Lambda_k-h_k$$
$$\left.\left.-\Lambda_kh_j)\right]\right\}+\sum_{k=1,\neq j}^{N}\left\{\frac{1}{\Lambda_j+1}[W_1^-E_k^-E_j^++W_2^-E_k^+E_j^-+\varphi(z_k-z_j)(h_kh_j-\Lambda_k)\right.$$
$$\left.-\varphi(\lambda)(h_k-\Lambda_kh_j)]\right\}, \quad (55)$$

where

$$\delta(\lambda,z_j,\xi)=-\frac{1}{\Lambda_j+1}\{[2+\varphi(z_j-\xi)+\varphi(z_j+\xi)]+[\varphi(z_j+\lambda-\xi)+\varphi(z_j-\lambda+\xi)](h+1)\},$$

$$W_1^{\pm}=\mp\frac{\theta(-\lambda+z_k\pm z_j)\,\theta'(0)}{\theta(z_k\pm z_j)\,\theta(\lambda)}.$$

To obtain the eigenvalues of this Hamiltonian, we have to find a proper ansatz for eigenvectors. But it is so hard that we cannot solve the present Hamiltonian directly. Fortunately, according to Hikami,[10] the Hamiltonian of the open DEQG model can also be derived from the transfer matrix $t(w)$ of the boundary elliptic quantum group.

The boundary elliptic quantum group is constructed by[16]

$$R_{21}(\lambda,w_1-w_2)\mathcal{L}_1(\lambda-2\,\eta h^{(2)},w_1)R_{12}(\lambda,w_1+w_2)\mathcal{L}_2(\lambda-2\,\eta h^{(1)},w_2)$$
$$=\mathcal{L}_2(\lambda-2\,\eta h^{(1)},w_2)R_{21}(\lambda,w_1+w_2)\mathcal{L}_1(\lambda-2\,\eta h^{(2)},w_1)R_{12}(\lambda,w_1-w_2), \quad (56)$$

where $\mathcal{L}(\lambda,w)=T^{-1}(\lambda,-w)K(\lambda-2\,\eta h,w)T(\lambda,w)$, and $K(\lambda,w)$ is defined by a diagonal matrix

$$K(\lambda,w)_{1,1}=1,\quad K(\lambda,w)_{2,2}=\frac{\theta(w+\xi)\,\theta(w+\lambda-\xi)}{\theta(w-\xi)\,\theta(w-\lambda+\xi)}, \quad (57)$$

where ξ is an arbitrary parameter. Then, the transfer matrix of the open elliptic quantum group takes the form

$$t(w)=\mathrm{tr}(\widetilde{K}(\lambda,w)\mathcal{L}(\lambda,w)). \tag{58}$$

The diagonal matrix $\widetilde{K}$ reads

$$\widetilde{K}_{11}=1, \quad \widetilde{K}_{22}=\frac{\theta(\lambda-2\eta)}{\theta(\lambda+2\eta)}\frac{\theta(w-2\eta-\tilde{\xi})\theta(w-2\eta-\lambda+\tilde{\xi})}{\theta(w-2\eta+\tilde{\xi})\theta(w-2\eta+\lambda-\tilde{\xi})}. \tag{59}$$

Let $\xi=\tilde{\xi}$ and take the quasiclassical limit $\eta\to 0$ in the transfer matrix of the boundary elliptic quantum group, we have obtained

$$t(\lambda,w=z_j)=2\left(\frac{1}{\Lambda_j+1}+H_j+O(\eta^2)\right). \tag{60}$$

Here the H_j is exactly equal to the Hamiltonian of the open DEQG model defined by Eq. (55). It is also easy to prove $[H_j,H_k]=0$ since the first term of Eq. (55) is only an integer. Therefore, this open DEQG model is a well-defined integrable model.

Since the Hamiltonian of the open DEQG model can be obtained from the transfer matrix of the boundary elliptic quantum group by taking the quasiclassical limit, we can also get the eigenvalue of the Hamiltonian by same procedure. In Ref. 16, the eigenstates of $t(w)$ are defined by applying $B(t_1)\cdots B(t_m)v_0$ on the highest weight state v_0 and the eigenvalue is

$$\begin{aligned}\epsilon(w)=&\prod_{i=1}^{m}\frac{\theta(w+t_i)\theta(w-t_i+2\eta)}{\theta(w-t_i)\theta(w+t_i-2\eta)}+\left\{\prod_{i=1}^{m}\frac{\theta(w+t_i-4\eta)\theta(w-t_i-2\eta)}{\theta(w-t_i)\theta(w+t_i-2\eta)}\right\}\\ &\times\frac{\theta(w-2\eta-\tilde{\xi})\theta(w-2\eta-\lambda+\tilde{\xi})}{\theta(w+\tilde{\xi})\theta(w+\lambda-\tilde{\xi})}\frac{\theta(2w)\theta(w-\xi+\lambda-2(\Lambda+1)\eta)\theta(w+\xi-2\eta)}{\theta(2w-4\eta)\theta(w+\xi-\lambda+2\Lambda\eta)\theta(w-\xi)}\\ &\times\left\{\prod_{j=1}^{n}\frac{\theta(z_j+w+(\Lambda_j-1)\eta)\theta(z_j-w-(\Lambda_j-1)\eta)}{\theta(z_j+w-(\Lambda_j+1)\eta)\theta(z_j-w+(\Lambda_j+1)\eta)}\right\}.\end{aligned} \tag{61}$$

The parameters t_j are governed by the Bethe ansatz equations

$$\begin{aligned}1=&\prod_{i=1}^{m}\frac{\theta(t_k-t_i-2\eta)\theta(t_k+t_i-4\eta)}{\theta(t_k+t_i)\theta(t_k-t_i+2\eta)}\frac{\theta(t_k-2\eta-\tilde{\xi})\theta(t_k-2\eta-\lambda+\tilde{\xi})}{\theta(t_k-\lambda-\tilde{\xi})\theta(t_k+\tilde{\xi})}\\ &\times\frac{\theta(t_k-\xi+\lambda-2(\Lambda+1)\eta)\theta(t_k+\xi-2\eta)}{\theta(t_k-\xi)\theta(t_k+\xi-\lambda+2\Lambda\eta)}\\ &\times\prod_{j=1}^{n}\left\{\frac{\theta(z_j+t_k+(\Lambda_j-1)\eta)\theta(z_j-t_k-(\Lambda_j-1)\eta)}{\theta(z_j+t_k-(\Lambda_j+1)\eta)\theta(z_j-t_k+(\Lambda_j+1)\eta)}\right\}, \quad k=1,2,\ldots,m.\end{aligned} \tag{62}$$

Taking the quasiclassical limit of Eqs. (61) and (62), we can obtain the eigenvalues of the open DEQG model

$$\epsilon(\lambda,w=z_j)=2\left(\frac{1}{\Lambda_j+1}+\hat{\epsilon}(z_j)+O(\eta^2)\right), \tag{63}$$

where

$$\hat{\epsilon}(z_j)=\frac{2\Lambda_j}{1+\Lambda_j}\sum_{i=1}^{m}[\varphi(z_j+t_i)+\varphi(z_j-t_i)]+\frac{1-\Lambda_j}{1+\Lambda_j}\Bigg\{\sum_{l=1}^{n}\Lambda_l\varphi(z_l+z_j)-\sum_{l\pm 1}^{n}\Lambda_l\varphi(z_l-z_j)$$
$$-(\Lambda+1)\varphi(z_j+\lambda-\xi)-(\Lambda+1)\varphi(z_j-\lambda+\xi)+2\varphi(2z_j)-\varphi(z_j-\xi)-\varphi(z_j+\xi)\Bigg\} \tag{64}$$

and the Bethe ansatz equations change into

$$-2\sum_{i=1,\neq k}^{m}[\varphi(t_k-t_i)+\varphi(t_k+t_i)]+\sum_{j=1}^{n}\Lambda_j[\varphi(z_j+t_k)-\varphi(z_j-t_k)]$$
$$=\varphi(t_k-\xi)+\varphi(t_k+\xi)+(\Lambda+1)[\varphi(t_k-\xi+\lambda)+\varphi(t_k+\xi-\lambda)]. \tag{65}$$

We have also investigated carefully the eigenstates of the open DEQG model. They can be written as the rescaled Bethe vectors through the quasiclassical limit

$$\phi\equiv\prod_{\alpha=1}^{m}\left.\frac{dB(t_\alpha)}{d\eta}\right|_{\eta=0}v_0. \tag{66}$$

In fact, when deriving the eigenvalue Eq. (64) and the Bethe ansatz equations (65), we have applied the $t(w)$ on ϕ and found

$$t(w)\phi=\epsilon(w)\phi+\hat{u}\phi, \tag{67}$$

where $\hat{u}$ is the unwanted terms. The vanishing condition of the unwanted terms gives out the Bethe ansatz equations (65) which can be considered as the quasiclassical limit of Eq. (62)

VI. SUMMARY

In this paper, we have defined integrable periodic and open DEQG models. We proved that for the periodic case, the Hamiltonian can also be obtained from the transfer matrix and the quantum determinant of the elliptic quantum group. Expanding the transfer matrix of the boundary elliptic quantum group around $\eta=0$, we can also obtain the Hamiltonian of open DEQG model. For periodic DEQG model, we defined the Bethe vector by setting the generating operator of the DEQG model on the highest weight vector. Then, we obtain eigenvalues of the Hamiltonian and the Bethe ansatz equations. For the open DEQG model, we obtained the eigenvalues of Hamiltonian by taking quasiclassical limit $\eta\to 0$ in the eigenvalues of the boundary elliptic quantum group. We can also define the Bethe vectors of open DEQG model by rescaling the Bethe vectors of the boundary quantum group around $\eta=0$. With the rescaled Bethe vectors we obtained the eigenvalues of the Hamiltonian of open DEQG model and the Bethe ansatz equations.

The DEQG models defined in present paper is related to su(2). One interesting problem is how to generalize it to the su(n) case and how to find the solution of the generalized models. One may apply the same approach in this paper. But, it is not the unique method for solving the Gaudin model. With the Wakimoto construction,[5] the rational Gaudin model based on Lie algebra g was solved. In this method, one can avoid using quasiclassical limit. We expect that the DEQG models given in present paper can be treated in terms of the Wakimoto construction. In fact, we have succeeded in constructing general DEQG models related to the Lie algebra g and finding their solutions,[17] which will appear in another paper. Furthermore, it is well known that the Knizhnik–Zamolodchikov–Bernard equation also play an important role in the integrable system.[18–20] It has been shown that the solutions of integrable Knizhnik–Zamolodchikov–Bernard equations can be constructed by using the results of Gaudin models.[10,21] So, in our forthcoming paper,[22] we will study them for our present models.

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Additivity for unital qubit channels

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Additivity of the Holevo capacity is proved for product channels, under the condition that one of the channels is a unital qubit channel, with the other completely arbitrary. As a byproduct this proves that the Holevo bound is the classical information capacity of such qubit channels, and provides an explicit formula for this classical capacity. Additivity of minimal entropy and multiplicativity of p-norms are also proved under the same assumptions. The proof relies on a new bound for the p-norm of an output state from the half-noisy phase-damping channel. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1500791]

I. INTRODUCTION AND STATEMENT OF RESULTS

There are several outstanding conjectures concerning product channels. These all involve the question of finding the ''best'' state or set of states to transmit through a product channel, using some measure of performance at the output to determine ''best.'' In this article we will consider three well-known measures of performance: the Holevo quantity χ^*, which measures the channel's capacity to transmit classical information; the minimal entropy of an output state; and the maximal p-norm of an output state (this was introduced by Amosov, Holevo, and Werner,[2] who called it the ''maximal output purity'' of the channel). An obvious candidate for the ''best'' set of states in each case is constructed by taking the product of the corresponding best states for the individual channels. For the first two performance measures described above, the outstanding conjecture is that this procedure indeed produces the optimal state. That is, the ''best'' states to send through the channel are always product states—there is no advantage in using entangled states. As a consequence, it would follow that the minimal entropy and the Holevo quantity are additive for product channels. Until recently it was conjectured that the maximal p-norm is also multiplicative for product channels; however, Werner recently discovered counterexamples for $p \geqslant 5$, in dimension three and higher.[17] The multiplicative conjecture for the maximal p-norms is still open for small values of p, in particular for values between 1 and 2. At this time, it seems fair to say that there is no good understanding of why these conjectures should be true.

The conjectures have been verified numerically for products of low dimensional channels. However, numerical testing becomes difficult when the dimensions of the state spaces are large. In part, this is because the allowed input states for the product channel include all entangled states in addition to the product states. So it seems to be necessary to develop an analytical method to investigate the conjectures, and that is the overall goal of the work reported in this article.

Recall that a channel Φ on a Hilbert space $\mathcal{H}$ is a completely positive, trace-preserving map on the algebra of observables on $\mathcal{H}$. When $\mathcal{H}=\mathbf{C}^2$ we will call Φ a *qubit channel*. Qubit channels play an important role in quantum information theory, because many applications involve the manipulation and entanglement of qubit states. If the channel satisfies $\Phi(I)=I$, so that it maps the identity to itself, then Φ is a *unital* channel. Examples of unital qubit channels are the depolarizing channel, the phase-damping channel, and the two-Pauli channel of Bennett, Fuchs, and Smolin.[3] The unital qubit channels provide a very useful laboratory for testing analytical approaches to the conjectures. This is because they are parametrized by three real numbers (up to unitary equivalence), and the geometry of this set of parameters is well understood. In this article we will use

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detailed properties of this class of channels to derive some new bounds which lead to proofs of the conjectures for unital qubit channels. Hopefully these results will provide clues about how to proceed in the general case.

The results in this article concern product channels $\Omega\otimes\Phi$ where Φ is a *unital qubit channel*, and Ω is *completely arbitrary*. For such channels we are able to establish the conjectures described above, namely that the three performance measures are optimized on product states of the channel. The main ingredient in the proof is a new inequality for the p-norm of an output state from the half-noisy channel $I\otimes\Phi$. The proof of this bound uses details of the classification of unital qubit channels,[11] and does not obviously extend to other classes of channels. In essence, it uses convexity and symmetry arguments to reduce the bound to the case of the *phase-damping channel*. The phase-damping channel [defined later in (20)] is a one-parameter family of unital channels which has been used as a model for decoherence in a two-state system. The inequality for the phase-damping channel can be proved using the method of Lieb and Ruskai which appears in Ref. 10, although in this article we prove it using a result of Epstein[5] concerning concavity of a certain trace function.

Before stating precisely our results we review the three performance measures for a channel that are used here. First, for any $p\geqslant 1$ the maximal p-norm of the channel Φ is defined to be

$$\nu_p(\Phi)=\sup_{\rho}\|\Phi(\rho)\|_p, \tag{1}$$

where the sup runs over states and where the p-norm of a positive matrix A is defined by

$$\|A\|_p=(\mathrm{Tr}A^p)^{1/p}. \tag{2}$$

Second, the minimal entropy of the channel Φ is defined by

$$S_{\min}(\Phi)=\inf_{\rho} S(\Phi(\rho)), \tag{3}$$

where $S(\rho)=-\mathrm{Tr}\rho\log\rho$ is the von Neumann entropy of the state ρ.

Third, the Holevo capacity of Φ is defined by

$$\chi^*(\Phi)=\sup_{\pi_i,\rho_i}\left[S\left(\sum\ \pi_i\Phi(\rho_i)\right)-\sum\ \pi_i S(\Phi(\rho_i))\right], \tag{4}$$

where the sup runs over all probability distributions $\{\pi_i\}$ and collections of states $\{\rho_i\}$ on $\mathcal{H}$.

Theorem 1: *Let Φ be a unital qubit channel. Then for any channel Ω,*

$$\nu_p(\Omega\otimes\Phi)=\nu_p(\Omega)\ \nu_p(\Phi),\quad \textit{for any}\ \ p\geqslant 1, \tag{5}$$

$$S_{\min}(\Omega\otimes\Phi)=S_{\min}(\Omega)+S_{\min}(\Phi), \tag{6}$$

$$\chi^*(\Omega\otimes\Phi)=\chi^*(\Omega)+\chi^*(\Phi). \tag{7}$$

Results related to Theorem 1 have been proven before. Several authors have proven the results for the half-noisy channel $\Omega\otimes I$.[2,6,15] Holevo proved (7) when both Ω and Φ are QC or CQ channels.[9] In Ref. 10, (5)–(7) were proven for any channel Ω, when Φ is either a QC or CQ channel. Bruss *et al.* proved (7) when both Ω and Φ are depolarizing qubit channels.[4] Amosov and Holevo proved (5) for integer values of p when both Ω and Φ are products of depolarizing channels.[1] King and Ruskai presented strong evidence for (7) when both Ω and Φ are unital qubit channels.[11] In Ref. 10 it was shown that (5) holds for any Ω when p is integer and Φ is a unital qubit map, or when $p=2$ and Φ is any qubit map. Recently Shor has proven (6) and (7) for any channel Ω when Φ is an entanglement breaking channel.[16]

It turns out that for a unital qubit channel all of the performance measures are determined by one number, the maximal output norm, which we define now.

Definition 2: Let Φ *be a unital qubit channel. The maximal output norm of* Φ *is defined to be*

$$M_\Phi = \sup_\rho \|\Phi(\rho)\| = \sup_{\rho,\tau} \mathrm{Tr}(\Phi(\rho)\tau). \tag{8}$$

A qubit channel Φ can be viewed as a map on the Bloch sphere, and the image is an ellipsoid which lies inside the Bloch sphere. For a unital map, this image ellipsoid is centered at the origin, and the number M_Φ is its semi-major axis. Define the functions

$$m_p(x) = [x^p + (1-x)^p]^{1/p} \tag{9}$$

and

$$h(x) = -x \log x - (1-x)\log(1-x). \tag{10}$$

Then it is easy to see that for a unital qubit channel Φ,

$$\begin{aligned} \nu_p(\Phi) &= m_p(M_\Phi), \\ S_{\min}(\Phi) &= h(M_\Phi), \\ \chi^*(\Phi) &= \log 2 - h(M_\Phi). \end{aligned} \tag{11}$$

The third line in (11) follows because the sup in (4) is attained with $\pi_1 = \pi_2 = \frac{1}{2}$, and with both ρ_1 and ρ_2 states of minimal entropy which map to opposite ends of the major axis of the ellipsoid, so that $\rho = \Sigma \pi_i \rho_i = I/2$.

The well-known Holevo–Schumacher–Westmoreland theorem[8,14] shows that $\chi^*(\Phi)$ is the best rate for transmission of classical information through the channel Φ when product states are used at the input (and possibly entangled measurements are used at the output). As a consequence, the ultimate capacity of a quantum channel Φ for faithful transmission of classical information (without prior entanglement between sender and receiver, and without a back-channel from receiver to sender) is given by

$$C_{\mathrm{ult}}(\Phi) = \lim_{n\to\infty} \frac{1}{n} \chi^*(\Phi^{\otimes n}). \tag{12}$$

By taking $\Omega = \Phi^{\otimes(n-1)}$ in (7) and using induction on n we deduce that

$$\chi^*(\Phi^{\otimes n}) = n\chi^*(\Phi). \tag{13}$$

This allows us to compute the limit in (12) and we now state this result as a separate theorem.

Theorem 3: *Let* Φ *be a unital qubit channel. Then the classical capacity of the channel is*

$$C_{\mathrm{ult}}(\Phi) = \chi^*(\Phi) = \log\ 2 - h(M_\Phi). \tag{14}$$

The article is organized as follows. Sections II and III contain the proof of Theorem 1 for two special channels. Section II covers the case of the depolarizing channel. All the main estimates are introduced in this section, and the reader should be able to grasp the essential ideas without the additional complications that arise for a general unital qubit channel. Section III does the same for the two-Pauli channel introduced by Bennett, Fuchs and Smolin. Section IV completes the proof for the general case, by reducing it to the two special cases covered in Secs. II and III. Section V contains the proof of the main estimate used, which bounds the p-norm of an output state from the half-noisy phase-damping channel.

II. PROOF FOR THE DEPOLARIZING CHANNEL

The depolarizing channel Δ_λ is defined by

$$\Delta_\lambda(\rho)=\lambda\rho+\frac{(1-\lambda)}{2}\mathrm{Tr}(\rho)I, \tag{15}$$

where $-\frac{1}{3}\leqslant\lambda\leqslant 1$ and I is the 2×2 identity matrix (the asymmetric bounds on the range of λ are required for the map to be completely positive[11]). The image of the Bloch sphere under this map is the sphere with radius $|\lambda|$ centered at the origin. It follows that the maximal output norm [defined in (2)] is given by

$$M_{\Delta_\lambda}=\frac{1+|\lambda|}{2}, \tag{16}$$

and hence the maximal output purity and the minimal entropy are respectively

$$\nu_p(\Delta_\lambda)=m_p\left(\frac{1+\lambda}{2}\right),\quad S_{\min}(\Delta_\lambda)=h\left(\frac{1+\lambda}{2}\right), \tag{17}$$

and the Holevo quantity is

$$\chi^*(\Delta_\lambda)=\log 2-h\left(\frac{1+\lambda}{2}\right). \tag{18}$$

One special feature of the depolarizing channel is its invariance under unitary conjugation, that is,

$$\Delta_\lambda(U\rho U^*)=U\Delta_\lambda(\rho)U^* \tag{19}$$

for all 2×2 unitary matrices U, and all states ρ. This symmetry property will play a crucial role in the argument.

The proof of additivity for the depolarizing channel proceeds by writing it as a convex combination of a special class of unital channels called the phase-damping channels. These channels are defined by

$$\Psi_\lambda^{(i)}(\rho)=\frac{(1+\lambda)}{2}\rho+\frac{(1-\lambda)}{2}\sigma_i\rho\sigma_i, \tag{20}$$

where $i=1,2,3$, where σ_i are the Pauli matrices, and where $-1\leqslant\lambda\leqslant 1$. The term ''phase-damping channel'' usually refers only to the case $i=3$, but we use it here for $i=1,2$ also.

The depolarizing channel can be rewritten in Kraus form as

$$\Delta_\lambda(\rho)=\frac{1+3\lambda}{4}\rho+\frac{1-\lambda}{4}\sum_{i=1}^{3}\sigma_i\rho\sigma_i. \tag{21}$$

It follows by straightforward calculation that

$$\Delta_\lambda=\frac{1+3\lambda}{4+4\lambda}[\Psi_\lambda^{(1)}+\Psi_\lambda^{(2)}]+\frac{1-\lambda}{4+4\lambda}[\sigma_3\Psi_\lambda^{(1)}\sigma_3+\sigma_3\Psi_\lambda^{(2)}\sigma_3]. \tag{22}$$

The convex decomposition (22) can be checked directly by substitution from (21) and (20). However, it can be derived much more easily using the geometric representation of unital qubit channels which will be explained in Sec. IV.

The main technical result behind the proof of Theorem 1 is the next estimate for the p-norm of an output state from the half-noisy phase-damping channel. In order to state this bound, let ρ be a state on $\mathbf{C}^K\otimes\mathbf{C}^2$ for some K. Then ρ can be written in the form

$$\rho = X\otimes I + \sum_{i=1}^{3} Y_i\otimes\sigma_i = \begin{pmatrix} X+Y_3 & Y_1-iY_2 \\ Y_1+iY_2 & X-Y_3 \end{pmatrix}, \tag{23}$$

where X, Y_i are $K\times K$ Hermitian matrices, with $\mathrm{Tr}X=\frac{1}{2}$. Also the positivity of ρ implies that

$$X\pm Y_i \geqslant 0, \quad i=1,2,3. \tag{24}$$

Theorem 4: *Let ρ be a state on $\mathbf{C}^K\otimes\mathbf{C}^2$ for some $K\geqslant 1$, written in the form* (23). *Then for all $p\geqslant 1$, and for $i=1,2,3$,*

$$\|(I\otimes\Psi_\lambda^{(i)})(\rho)\|_p \leqslant 2\, m_p\left(\frac{1+\lambda}{2}\right)\left[\frac{1}{2}\mathrm{Tr}(X+Y_i)^p+\frac{1}{2}\mathrm{Tr}(X-Y_i)^p\right]^{1/p}. \tag{25}$$

The estimate (25) will be derived in Sec. V, using a result from convex analysis due to Epstein.[5] By taking its derivative at $p=1$, we can obtain a lower bound for the entropy of any output state from the half-noisy channel $(I\otimes\Psi_\lambda^{(i)})$, namely,

$$S((I\otimes\Psi_\lambda^{(i)})(\rho)) \geqslant h\left(\frac{1+\lambda}{2}\right)+h(a_i)-\log 2+a_i S(\alpha_i)+(1-a_i)S(\beta_i), \tag{26}$$

where $a_i=\mathrm{Tr}(X+Y_i)$, $1-a_i=\mathrm{Tr}(X-Y_i)$ and $\alpha_i=(X+Y_i)/a_i$, $\beta_i=(X-Y_i)/(1-a_i)$. The author does not know any way to derive this useful entropy bound directly, without first deriving the p-norm bound (25).

The proof of (5) for the depolarizing channel follows by combining the symmetry property (19) with the convex decomposition (22), and using the bound (25). Indeed, by (17) it is sufficient to prove that for any bipartite state ρ_{12}

$$\|(\Omega\otimes\Delta_\lambda)(\rho_{12})\|_p \leqslant \nu_p(\Omega)\, m_p\left(\frac{1+\lambda}{2}\right), \tag{27}$$

since equality can be achieved with product states. Furthermore, using the symmetry property (19) we may assume that the reduced density matrix $\rho_2=\mathrm{Tr}_1\rho_{12}$ is diagonal. This is because we may replace ρ_{12} by $(I\otimes U)\rho_{12}(I\otimes U^*)$, where U is any 2×2 unitary matrix, without changing the left side of (27), and U may be chosen so that ρ_2 is diagonal. When the state ρ_{12} is written in the form (23), this means that

$$\mathrm{Tr}Y_1=\mathrm{Tr}Y_2=0. \tag{28}$$

Furthermore, applying $\Omega\otimes I$ to ρ_{12} and using (23) gives

$$(\Omega\otimes I)(\rho_{12})=\begin{pmatrix} \Omega(X+Y_3) & \Omega(Y_1-iY_2) \\ \Omega(Y_1+iY_2) & \Omega(X-Y_3) \end{pmatrix}. \tag{29}$$

Now we return to the convex decomposition (22). This implies a corresponding decomposition for $(\Omega\otimes\Delta_\lambda)(\rho_{12})$, in terms of $(\Omega\otimes\Psi_\lambda^{(1)})(\rho_{12})$, $(\Omega\otimes\Psi_\lambda^{(2)})(\rho_{12})$, etc. Therefore, it is sufficient to prove the bound for each term in this decomposition, namely,

$$\|(\Omega\otimes\Psi_\lambda^{(i)})(\rho_{12})\|_p \leqslant \nu_p(\Omega)\, m_p\left(\frac{1+\lambda}{2}\right), \tag{30}$$

where $i=1,2$ and where ρ_2 is assumed to be diagonal.

Now we apply (25) and (29) to deduce

$$\|(\Omega\otimes\Psi_\lambda^{(i)})(\rho_{12})\|_p \leq 2\, m_p\left(\frac{1+\lambda}{2}\right)\left[\frac{1}{2}\mathrm{Tr}(\Omega(X+Y_i))^p+\frac{1}{2}\mathrm{Tr}(\Omega(X-Y_i))^p\right]^{1/p}. \tag{31}$$

Using (28) and the definition of $\nu_p(\Omega)$ it follows that

$$\mathrm{Tr}(\Omega(X\pm Y_i))^p \leq \nu_p(\Omega)^p\,(\mathrm{Tr}(X\pm Y_i))^p=\nu_p(\Omega)^p\,(\mathrm{Tr}X)^p \tag{32}$$

for $i=1,2$. Since ρ_{12} is a state it follows that $\mathrm{Tr}\,X=\frac{1}{2}$ and hence the bound (32) becomes

$$\mathrm{Tr}(\Omega(X\pm Y_i))^p \leq 2^{-p}\nu_p(\Omega)^p. \tag{33}$$

Substituting (33) into (31) gives

$$\|(\Omega\otimes\Psi_\lambda^{(i)})(\rho_{12})\|_p \leq 2\, m_p\left(\frac{1+\lambda}{2}\right)\left(\frac{1}{2}\,\nu_p(\Omega)\right)=\nu_p(\Omega)\, m_p\left(\frac{1+\lambda}{2}\right), \tag{34}$$

which is exactly the desired bound (30). So this proves the result (5) for the depolarizing channel.

Turning now to the minimal entropy equality (6), this follows immediately from (5) by taking the derivative at $p=1$, since from the easily established relation

$$\frac{d}{dp}(\|\rho\|_p)_{p=1}=-S(\rho) \tag{35}$$

it follows that for any channel Ω

$$\frac{d}{dp}(\nu_p(\Omega))_{p=1}=-S_{\min}(\Omega). \tag{36}$$

Next we turn to the additivity of the Holevo capacity (7). To establish this we use the representation of Ohya, Petz and Watanabe[13] and Schumacher–Westmoreland (OPWSW),[15] and follow the method described in Ref. 10. Denote the relative entropy of states ω and ρ by

$$H(\omega,\rho)=\mathrm{Tr}\omega(\log\omega-\log\rho). \tag{37}$$

Then the OPWSW representation is

$$\chi^*(\Omega)=\inf_\rho \sup_\omega H(\Omega(\omega),\Omega(\rho)). \tag{38}$$

The state that achieves the infimum in (38) is the optimal average output state from the channel Ω, and we denote this by ρ_Ω. For any unital qubit channel, and in particular for the depolarizing channel Δ_λ, the optimal average output state is the noisiest state $I/2$. Evaluating (38) for the depolarizing channel Δ_λ with optimal output state $I/2$ gives (18).

Our goal is to show that

$$\chi^*(\Omega\otimes\Delta_\lambda)\leq\chi^*(\Omega)+\chi^*(\Delta_\lambda)=\chi^*(\Omega)+\log 2-h\left(\frac{1+\lambda}{2}\right), \tag{39}$$

since the inequality in the other direction is easy. Since $\rho_\Omega\otimes I/2$ is a valid output state from the channel $\Omega\otimes\Delta_\lambda$, it follows from (38) that

$$\chi^*(\Omega\otimes\Delta_\lambda)\leq\sup_{\tau_{12}} H((\Omega\otimes\Delta_\lambda)(\tau_{12}),\rho_\Omega\otimes I/2), \tag{40}$$

and hence to prove (39) it is sufficient to prove that for any entangled state τ_{12},

$$H((\Omega\otimes\Delta_\lambda)(\tau_{12}),\rho_\Omega\otimes I/2)\leqslant\chi^*(\Omega)+\chi^*(\Delta_\lambda). \tag{41}$$

Denote the reduced density matrix of τ_{12} by

$$\tau_1=\mathrm{Tr}_2(\tau_{12}), \tag{42}$$

where Tr_2 is the trace over the second factor. From (37) it follows that

$$H((\Omega\otimes\Delta_\lambda)(\tau_{12}),\rho_\Omega\otimes I/2)=-S((\Omega\otimes\Delta_\lambda)(\tau_{12}))-\mathrm{Tr}\Omega(\tau_1)\log\rho_\Omega+\log 2. \tag{43}$$

Using (18) and (43) reduces (41) to the inequality

$$S((\Omega\otimes\Delta_\lambda)(\tau_{12}))\geqslant h\left(\frac{1+\lambda}{2}\right)-\mathrm{Tr}\,\Omega(\tau_1)\log(\rho_\Omega)-\chi^*(\Omega). \tag{44}$$

Using again the convex decomposition (22) and the symmetry property (19), it follows that it is sufficient to prove the bound

$$S((\Omega\otimes\Psi_\lambda^{(i)})(\tau_{12}))\geqslant h\left(\frac{1+\lambda}{2}\right)-\mathrm{Tr}\,\Omega(\tau_1)\log(\rho_\Omega)-\chi^*(\Omega) \tag{45}$$

for $i=1,2$ under the assumption that τ_1 is diagonal. Referring to (26) the condition that τ_1 is diagonal means that $a_i=\frac{1}{2}$ for $i=1,2$, and hence the bound (26) becomes

$$S((\Omega\otimes\Psi_\lambda^{(i)})(\tau_{12}))\geqslant h\left(\frac{1+\lambda}{2}\right)+\frac{1}{2}S(2\Omega(X+Y_i))+\frac{1}{2}S(2\Omega(X-Y_i)). \tag{46}$$

Furthermore, we can write $\tau_1=2X$ in the form

$$\tau_1=\tfrac{1}{2}[(2X+2Y_i)+(2X-2Y_i)], \tag{47}$$

and so it follows that

$$\begin{aligned}&-\tfrac{1}{2}S(2\Omega(X+Y_i))-\tfrac{1}{2}S(2\Omega(X-Y_i))-\mathrm{Tr}\Omega(\tau_1)\log(\rho_\Omega)\\&\quad=\tfrac{1}{2}H(\Omega(2X+2Y_i),\rho_\Omega)+\tfrac{1}{2}H(\Omega(2X-2Y_i),\rho_\Omega).\end{aligned} \tag{48}$$

Now since ρ_Ω is the optimal average output state for the channel Ω, it is also the state which achieves the infimum in the OPWSW representation (38). Hence (38) implies

$$H(\Omega(2X\pm 2Y_i),\rho_\Omega)\leqslant\chi^*(\Omega), \tag{49}$$

and therefore from (48)

$$\tfrac{1}{2}S(2\Omega(X+Y_i))+\tfrac{1}{2}S(2\Omega(X-Y_i))+\mathrm{Tr}\Omega(\tau_1)\log(\rho_\Omega) \tag{50}$$

$$\geqslant-\chi^*(\Omega). \tag{51}$$

Combining (46) and (50) yields the required bound (45), and this proves additivity for the depolarizing channel.

III. PROOF FOR THE TWO-PAULI CHANNEL

The two-Pauli channel was introduced by Bennett, Fuchs, and Smolin[3] who presented it as an example of a channel which benefits from the use of entangled inputs, in the sense of minimizing

measurement errors over two uses of the channel. For this reason it is particularly interesting to prove the additivity result for this channel, as it implies a significant difference between the role of entanglement in the channel capacity and the error–minimization problems.

The two-Pauli channel is a one-parameter unital qubit channel Θ_λ, defined by

$$\Theta_\lambda(\rho)=\lambda\rho+\frac{1-\lambda}{2}\sigma_1\rho\sigma_1+\frac{1-\lambda}{2}\sigma_2\rho\sigma_2, \tag{52}$$

where $0\leqslant\lambda\leqslant 1$. The maximal output purity $\nu_p(\Theta_\lambda)$ is attained on the input state $(I+\sigma_1)/2$ for $\lambda\geqslant\frac{1}{3}$, and on the state $(I+\sigma_3)/2$ for $0\leqslant\lambda\leqslant\frac{1}{3}$, and so is given by

$$\nu_p(\Theta_\lambda)=\begin{cases} m_p((1+\lambda)/2) & \text{for } \frac{1}{3}\leqslant\lambda\leqslant 1, \\ m_p(1-\lambda) & \text{for } 0\leqslant\lambda\leqslant\frac{1}{3}. \end{cases} \tag{53}$$

When $\lambda=\frac{1}{3}$ the channel is unitarily equivalent to the depolarizing channel $\Delta_{1/3}$. We will prove additivity here only for the range of parameters $\frac{1}{3}\leqslant\lambda\leqslant 1$. The rest of the parameter range will be covered in the following section on the general unital qubit channel.

It will be necessary to consider two related two-Pauli channels, which are defined using the other choices of Pauli matrices in (52). So, for convenience, we will rename the channel defined in (52) as $\Theta_\lambda^{(3)}$, and define the three channels together by

$$\begin{aligned} \Theta_\lambda^{(1)}(\rho)&=\lambda\rho+\frac{1-\lambda}{2}\sigma_2\rho\sigma_2+\frac{1-\lambda}{2}\sigma_3\rho\sigma_3, \\ \Theta_\lambda^{(2)}(\rho)&=\lambda\rho+\frac{1-\lambda}{2}\sigma_3\rho\sigma_3+\frac{1-\lambda}{2}\sigma_1\rho\sigma_1, \\ \Theta_\lambda^{(3)}(\rho)&=\lambda\rho+\frac{1-\lambda}{2}\sigma_1\rho\sigma_1+\frac{1-\lambda}{2}\sigma_2\rho\sigma_2. \end{aligned} \tag{54}$$

The key result in the proof for the depolarizing channel was the fact that for any channel Ω and for any entangled state ρ_{12}, there was a convex decomposition of the form

$$(\Omega\otimes\Delta_\lambda)(\rho_{12})=\sum_k c_k(\Omega\otimes U_k\Psi_\lambda^{(i_k)}U_k^*)(\rho'_{12}), \tag{55}$$

where $\Sigma c_k=1$, and $i_k=1,2$. The 2×2 matrices U_k are unitary, and we write $U\Psi U^*$ to denote the channel that acts on a state ρ by

$$U\,\Psi\,U^*(\rho)=U\,\Psi(\rho)\,U^*, \tag{56}$$

that is, the matrix U conjugates the state *after* Ψ acts. The state ρ'_{12} is unitarily equivalent to ρ_{12}, and has the property that $\rho'_2=\mathrm{Tr}_1(\rho'_{12})$ is diagonal. The decomposition (55) allowed the bound (25) to be used and this in turn led to the additivity result. In order for this to work, it was crucial that the phase-damping channel on the right side of (55) produced the factor $m_p((1+\lambda)/2)$, which was the correct bound for the channel Δ_λ.

The strategy of proof for the two-Pauli channel is similar, that is, we will produce a convex decomposition of the same form as (55), involving phase-damping channels with the same parameter λ. This decomposition is stated next as Theorem 5. This allows us to use the bound (25), and so produce the factor $m_p((1+\lambda)/2)\nu_p(\Omega)$ again. By (53) this equals $\nu_p(\Theta_\lambda^{(i)})\,\nu_p(\Omega)$ for $\frac{1}{3}\leqslant\lambda\leqslant 1$, and hence the result will be proved for this range of values. Again the crucial part is that the matrices $X\pm Y_i$ appearing on the right side of the bound (25), must satisfy $\mathrm{Tr}(X\pm Y_i)=\frac{1}{2}$, and this

must be arranged before applying the convex decomposition, by using symmetry properties of the channel to rotate the state ρ_{12}. Once this has been done, the rest of the additivity proof proceeds verbatim, and does not need to be repeated.

Theorem 5: *Let ρ_{12} be a state on $\mathbf{C}^K \otimes \mathbf{C}^2$ for some $K \geqslant 1$, written in the form (23), and let Ω be any channel acting on $\mathbf{C}^K$. Then for $i=1,2,3$*

$$(\Omega \otimes \Theta_\lambda^{(i)})(\rho_{12}) = \sum_k c_k \, (\Omega \otimes U_k \Psi_\lambda^{(i_k)} U_k^*)(\rho_{12}^{(k)}), \tag{57}$$

where $\Sigma c_k = 1$, the matrices U_k are unitary, and $i_k = 1,2,3$. Furthermore, if $\rho_{12}^{(k)}$ is written in the block form (23), then $TrY_{i_k} = 0$.

Notice that the same index i_k appears in $\Psi_\lambda^{(i_k)}$ and in the condition $\mathrm{Tr} Y_{i_k} = 0$ on the state $\rho_{12}^{(k)}$. This means that all the arguments of Sec. II can be repeated using the decomposition (57) in place of (55), and the additivity results follow. So the proof for the two-Pauli channel reduces to establishing (57).

The crucial ingredient in getting this decomposition is the following symmetry property of the channel: for any *diagonal* unitary matrix U and any state ρ we have

$$\Theta_\lambda^{(3)}(U\rho U^*) = U\Theta_\lambda^{(3)}(\rho)U^*. \tag{58}$$

The identity (58) follows easily from the Kraus representation (52) using the Pauli matrix relations $\sigma_i \sigma_3 = -\sigma_3 \sigma_i$ for $i=1,2$. This is because any diagonal unitary matrix can be written in the form $U = \alpha I + \beta \sigma_3$ with $|\alpha \pm \beta|^2 = 1$, and such matrices clearly commute with the action of $\Theta_\lambda^{(3)}$. Similar identities hold for $\Theta_\lambda^{(1)}$ and $\Theta_\lambda^{(2)}$, which commute respectively with matrices of the form $\alpha I + \beta \sigma_1$ and $\alpha I + \beta \sigma_2$.

We now prove Theorem 5 for $i=3$, that is for the case $(\Omega \otimes \Theta_\lambda^{(3)})(\rho_{12})$. The proofs for the cases $i=1,2$ are identical. We use a two-step construction to reach the result. First, we have the following convex decomposition:

$$\Theta_\lambda^{(3)} = \frac{3\lambda - 1}{2\lambda} \Psi_\lambda^{(2)} + \frac{1-\lambda}{2\lambda} \sigma_1 \Theta_\lambda^{(2)} \sigma_1 . \tag{59}$$

It is elementary to check that this relation holds, and the geometrical picture of Sec. IV will make it easy to derive. However, before applying the decomposition (59) to an entangled state $(\Omega \otimes \Theta_\lambda^{(3)})(\rho_{12})$, we will use the symmetry property (58) to rotate the reduced density matrix $\rho_2 = 1/2(I + w_1\sigma_1 + w_2\sigma_2 + w_3\sigma_3)$ into the form $\rho_2' = 1/2(I + w_1'\sigma_1 + w_3'\sigma_3)$. That is, we conjugate by a diagonal unitary matrix which removes the component in the direction of σ_2—equivalently, the density matrix is made real by conjugation with a diagonal unitary matrix. When the rotated state ρ_{12}' is written in the 2×2 block form (23), this means that

$$\mathrm{Tr}\ Y_2' = 0. \tag{60}$$

So the first step is to write

$$(\Omega \otimes \Theta_\lambda^{(3)})(\rho_{12}) = (\Omega \otimes U\Theta_\lambda^{(3)} U^*)(\rho_{12}'), \tag{61}$$

where U is the diagonal unitary matrix that produces the rotation. Now (59) is used. The first term on the right side of (59) produces $(\Omega \otimes U\Psi_\lambda^{(2)}U^*)(\rho_{12}')$ where the reduced density matrix ρ_2' is real, and this has exactly the form required in Theorem 5.

We now continue to the second step, and use another convex decomposition for the second term on the right side of (59), namely

$$\Theta_\lambda^{(2)} = \frac{2\lambda}{1+\lambda} \Psi_\lambda^{(3)} + \frac{1-\lambda}{1+\lambda} \sigma_1 \Psi_\lambda^{(2)} \sigma_1 . \tag{62}$$

Before applying (62), we use the symmetry of the channel $\Theta_\lambda^{(2)}$ to rotate the state ρ'_{12} by a unitary matrix of the form $I\otimes V$ where $V=\alpha I+\beta\sigma_2$, and obtain the rotated state ρ''_{12}. Since the reduced density matrix $\rho'_2=1/2(I+w'_1\sigma_1+w'_3\sigma_3)$ has no component in the σ_2 direction, the matrix V may be chosen so that after the second rotation the reduced matrix $\rho''_2=1/2(I+w''_1\sigma_1)$ has no components in either the σ_2 or the σ_3 directions. As a result, the second term on the right side of (59) is transformed as follows:

$$(\Omega\otimes U\sigma_1\Theta_\lambda^{(2)}\sigma_1 U^*)(\rho'_{12})=(\Omega\otimes W\Theta_\lambda^{(2)}W^*)(\rho''_{12}) \tag{63}$$

where $W=U\sigma_1 V$. Having done this rotation, the decomposition (62) can be applied, yielding a convex combination of $(\Omega\otimes W\Psi_\lambda^{(2)}W^*)(\rho''_{12})$ and $(\Omega\otimes W\Psi_\lambda^{(3)}W^*)(\rho''_{12})$, and both of these have the form required on the right side of (57). So this completes the proof for the two-Pauli channels.

IV. THE GENERAL CASE

The basic idea is that any unital qubit channel Φ is unitarily equivalent to a convex combination of depolarizing channels and two-Pauli channels, which all share the same values of ν_p and $S_{\min}$. Additivity in the general case then follows from additivity for the depolarizing and two-Pauli channels, combined with the convexity of the p-norm, and the concavity of the entropy.

We first review the classification of unital qubit maps which was developed in Ref. 11. Any unital qubit map Φ can be represented by a real 3×3 matrix with respect to the basis $\sigma_1,\sigma_2,\sigma_3$. In Ref. 11 it was explained that by using independent unitary transformations in its domain and range, this matrix can be put into the following diagonal form:

$$\Phi=\begin{pmatrix}\lambda_1 & 0 & 0\\ 0 & \lambda_2 & 0\\ 0 & 0 & \lambda_3\end{pmatrix}. \tag{64}$$

The diagonal entries satisfy $|\lambda_i|\leqslant 1$, as well as other conditions implied by complete positivity. These conditions were analyzed in Ref. 11 (and also in Ref. 7), and it was shown that the allowed diagonal entries of Φ in (64) comprise the tetrahedron with corners at the points

$$(1,1,1),\ (1,-1,-1),\ (-1,-1,1),\ (-1,1,-1). \tag{65}$$

The corner (1,1,1) corresponds to the identity channel. The corner $(1,-1,-1)$ corresponds to conjugation by σ_1, and so is unitarily equivalent to the identity channel, and similarly for the corners $(-1,-1,1)$ and $(-1,1,-1)$. The top edge of the tetrahedron $(\lambda,\lambda,1)$ is the phase-damping channel $\Psi_\lambda^{(3)}$. The bottom edge $(\lambda,-\lambda,-1)$ is the channel $\sigma_1\Psi_\lambda^{(3)}\sigma_1$. The other edges are obtained by permutation of the coordinates and conjugation with the Pauli matrices, and correspond to the channels $\Psi_\lambda^{(1)}$ and $\Psi_\lambda^{(2)}$.

The depolarizing channels $(\lambda,\lambda,\lambda)$ correspond to an interior line of the tetrahedron, drawn from a corner to the middle of the opposite side. The point $(-\frac{1}{3},-\frac{1}{3},-\frac{1}{3})$ lies on the face of the tetrahedron, so $\lambda=-\frac{1}{3}$ is the smallest allowed value in (15).

Finally, the two-Pauli channels $\Theta_\lambda^{(3)}$ correspond to the points $(\lambda,\lambda,2\lambda-1)$. These points lie on a face of the tetrahedron, on a line connecting a corner to the middle of the opposite side.

The maximal output norm of the channel (64) [as defined in (8)] is

$$M_\Phi=\tfrac{1}{2}(\max\{|\lambda_1|,|\lambda_2|,|\lambda_3|\}+1). \tag{66}$$

Furthermore, the signs of any two of the parameters $\lambda_1,\lambda_2,\lambda_3$ can be simultaneously flipped with a unitary transformation in the domain of Φ (for example, conjugation by σ_1 in the domain of Φ switches the signs of λ_2 and λ_3 without any other changes). Also, the coordinates can be cyclically permuted using unitary transformations. So without loss of generality, we will assume henceforth that the parameters satisfy

$$1 \geqslant \lambda_3 \geqslant \max(|\lambda_1|,|\lambda_2|), \quad M_\Phi = \frac{1+\lambda_3}{2}. \tag{67}$$

We will say that Φ is in *standard form* if it is diagonal in the basis $\sigma_1,\sigma_2,\sigma_3$ and its diagonal entries satisfy (67).

Now assume that Φ is in standard form, and let

$$\lambda = \lambda_3 = \max(|\lambda_i|). \tag{68}$$

Then the quantities ν_p, $S_{\min}$ and χ^* are determined by M_Φ according to (11), and their values are unchanged by unitary transformations in the domain and the range. Hence, using (68) we get

$$\nu_p(\Phi) = m_p\left(\frac{1+\lambda}{2}\right),$$

$$S_{\min}(\Phi) = h\left(\frac{1+\lambda}{2}\right),$$

$$\chi^*(\Phi) = \log 2 - h\left(\frac{1+\lambda}{2}\right).$$

Armed with the geometric picture of the unital qubit channels, it is quite easy to derive relations like (22), (59), and (62). For example, we get (22) by taking a horizontal slice through the tetrahedron at height λ. This cross-section of the tetrahedron is a rectangle with corners at the four points

$$(1,\lambda,\lambda),\ (\lambda,1,\lambda),\ (-1,-\lambda,\lambda),\ (-\lambda,-1,\lambda). \tag{69}$$

Furthermore, each of the maps corresponding to these corners is a phase-damping channel, either $\Psi_\lambda^{(i)}$ or $\sigma_3\Psi_\lambda^{(i)}\sigma_3$, with $i=1,2$. The depolarizing channel sits at $(\lambda,\lambda,\lambda)$, and clearly there are many ways to write it as a convex combination of the four corners. The relation (22) is one such choice.

Now suppose that Φ is a general unital qubit channel in standard form, so that $\lambda_3=\lambda>0$. Then Φ corresponds to a point in the cross-section of the tetrahedron with corners at (69). Furthermore, the condition (67), namely $\lambda=\lambda_3=\max(|\lambda_i|)$, selects a convex subset of this cross-section. For $\frac{1}{3}\leqslant\lambda\leqslant 1$ this subset is the convex hull of the six points

$$\begin{gathered}(\lambda,\lambda,\lambda), \quad (2\lambda-1,\lambda,\lambda), \quad (\lambda,2\lambda-1,\lambda),\\ (-\lambda,-\lambda,\lambda), \quad (1-2\lambda,-\lambda,\lambda), \quad (-\lambda,1-2\lambda,\lambda),\end{gathered} \tag{70}$$

and for $0\leqslant\lambda\leqslant\frac{1}{3}$ this subset is the convex hull of the four points

$$(\lambda,\lambda,\lambda), \quad (-\lambda,\lambda,\lambda), \quad (\lambda,-\lambda,\lambda), \quad (-\lambda,-\lambda,\lambda). \tag{71}$$

It is important to note that every map in the convex hull of (70) has the *same* values for ν_p and $S_{\min}$, since these are determined only by the maximal output norm, and this has the same value $(1+\lambda)/2$ for each of these channels and similarly for all the channels in the convex hull of (71). Therefore, by convexity, it is sufficient to prove the additivity and multiplicativity results (5)–(7) for these corner maps, since this will imply the same bounds for all the maps in the convex hull. However, we recognize that the corner maps in (70) are unitarily equivalent to either depolarizing channels or two-Pauli channels with the same parameter λ. Hence the results of Secs. II and III imply the bounds for these corner maps, and hence for all maps in the convex hull. Notice that the

results of Sec. III for the two-Pauli channel in the range $\frac{1}{3} \leqslant \lambda \leqslant 1$ are sufficient to get the result for the channels (70). Similarly the maps arising in (71) are unitarily equivalent to depolarizing channels, and so Sec. II can be again applied to deduce the result.

V. PROOF OF THEOREM 4

This theorem is a variant of the bound obtained by Lieb and Ruskai, which appeared as an Appendix in Ref. 10, and it can be proved by the same method. That method uses the Lieb–Thirring bound,[12] which in turn was proved using one of Epstein's concavity results.[5] Since Theorem 3 can be obtained directly from Epstein's result, we present that argument here.

Let ρ be a matrix of the form (23). The condition that ρ be positive means that $Y_1 - iY_2 = \sqrt{X+Y_3} R \sqrt{X-Y_3}$ where R is a contraction. Every contraction is a convex combination of unitaries, so it is sufficient to assume that

$$Y_1 - iY_2 = \sqrt{X+Y_3}\, V \sqrt{X-Y_3}, \quad VV^* = I. \tag{72}$$

We have the factorization

$$(I \otimes \Psi_\lambda)(\rho) = F^{1/2} G F^{1/2}, \tag{73}$$

where

$$F = \begin{pmatrix} X+Y_3 & 0 \\ 0 & X-Y_3 \end{pmatrix}, \quad G = \begin{pmatrix} I & \lambda V \\ \lambda V^* & I \end{pmatrix}. \tag{74}$$

From the identity

$$\begin{pmatrix} I & \lambda V \\ \lambda V^* & I \end{pmatrix} = U \begin{pmatrix} (1+\lambda)I & 0 \\ 0 & (1-\lambda)I \end{pmatrix} U^*, \tag{75}$$

where

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} I & V \\ V^* & -I \end{pmatrix}, \quad UU^* = I, \tag{76}$$

it follows that for all $p \geqslant 1$

$$G^p = \begin{pmatrix} \alpha I & \beta V \\ \beta V^* & \alpha I \end{pmatrix} \tag{77}$$

with

$$\alpha = \tfrac{1}{2}[(1+\lambda)^p + (1-\lambda)^p], \quad \beta = \tfrac{1}{2}[(1+\lambda)^p - (1-\lambda)^p]. \tag{78}$$

We can write

$$\mathrm{Tr}((I \otimes \Psi_\lambda)(\rho))^p = \mathrm{Tr}(F^{1/2} (G^p)^{1/p} F^{1/2})^p. \tag{79}$$

Now we use Epstein's concavity result,[5] which states that for any positive matrix B and any $p \geqslant 1$, the map

$$A \to \mathrm{Tr}(B\,(A)^{1/p}\,B)^p \tag{80}$$

is concave on the set of positive matrices. (In fact Epstein states the result only for integer values of p, but his proof applies to all real values $p \geqslant 1$.) The left side of (79) is an even function of λ, and therefore the right side is unchanged if β is replaced by $-\beta$ in (77). Also note that

$$\tfrac{1}{2}\begin{pmatrix} \alpha I & \beta V \\ \beta V^* & \alpha I \end{pmatrix} + \tfrac{1}{2}\begin{pmatrix} \alpha I & -\beta V \\ -\beta V^* & \alpha I \end{pmatrix} = \begin{pmatrix} \alpha I & 0 \\ 0 & \alpha I \end{pmatrix}. \tag{81}$$

Therefore the concavity result (80) implies that the right side of (79) is bounded above by its value when β is set equal to zero in (77). Furthermore, when $\beta = 0$, the right side of (79) becomes

$$\mathrm{Tr}(F^{1/2}(\alpha I)^{1/p}F^{1/2})^p = \alpha \mathrm{Tr}F^p = 2\alpha[\tfrac{1}{2}\mathrm{Tr}(X+Y_3)^p + \tfrac{1}{2}\mathrm{Tr}(X-Y_3)^p]. \tag{82}$$

Comparing with (9) we see that $2\alpha = 2^p m_p((1+\lambda)/2)^p$, and this proves the theorem.

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Method of solving the homogeneous Bloch equation

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A method of solving the Bloch equation with infinite relaxation times is given. Applying this method we have found unknown analytic solutions as well as the well-known solutions. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Since the Bloch equation[1] was proposed in 1946, various workers have tried to solve it analytically and only a few analytic solutions are well known. Among the various attempts, the spinor approaches by spinorizing the Bloch equation in nuclear magnetic resonance[2] were paid attention to. The reason is due to the fact that there exists a 2×2 unitary evolution matrix. By this unitary transformation the length of the spinor is conserved. The equivalence between vectors and spinors is also well known.[3] Keeping this point in mind, we develop our approach to solving the vector Bloch equation in this paper.

We give a method of solving the homogeneous Bloch equation in Sec. II. Then in Sec. III we apply this method to finding analytic solutions. In Sec. IV we state conclusions.

II. SCENARIO

The homogeneous Bloch equation for magnetization with infinite relaxation times is given by

$$\dot{\vec{M}}+\gamma\vec{B}\times\vec{M}=0, \tag{1}$$

where a dot means differentiation with respect to time. Here γ is the gyromagnetic ratio and $\vec{B}$ is the applied magnetic field.

Taking the scalar product of $\vec{M}$ with Eq. (1) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}(\vec{M}\cdot\vec{M})=0. \tag{2}$$

This turns out to be the magnitude of the magnetic vector being independent of time. This suggests that rotations play a fundamental role. We introduce a time-dependent linear transformation of the magnetic vector as

$$\vec{M}'=A\vec{M}. \tag{3}$$

By using components of Eq. (3), we have

$$M_i'=a_{ij}M_j, \quad (i=1,2,3), \tag{4}$$

with

$$(A)_{ij}=a_{ij}, \quad (i,j=1,2,3). \tag{5}$$

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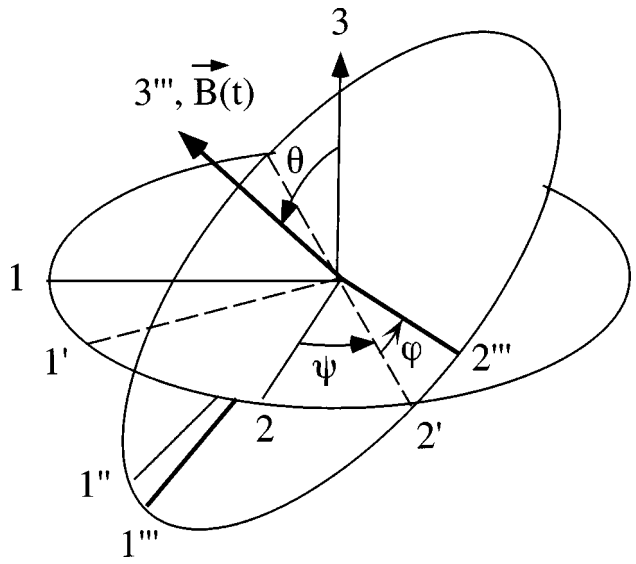

FIG. 1. Definition of the Eulerian angles.

Here the repeated indices mean summation over the index running from 1 to 3. Under the transformation (3), we require

$$\vec{M}'\cdot\vec{M}'=\vec{M}\cdot\vec{M}. \tag{6}$$

Thus the transformation is restricted such that

$$a_{ik}a_{jk}=\delta_{ij}. \tag{7}$$

In the matrix form we have

$$AA^T=A^TA=1, \tag{8}$$

with

$$\det A=\pm 1. \tag{9}$$

This transformation is called the orthogonal transformation. Here we choose proper orthogonal transformations, i.e., rotations in the three-dimensional Euclidean space,

$$\det A=+1. \tag{10}$$

In general a rotation can be expressed in terms of the Eulerian angles (φ,θ,ψ) displayed in Fig. 1 as

$$A=e^{i\varphi T_3}e^{i\theta T_2}e^{i\psi T_3}, \tag{11}$$

where $T_i(i=1,2,3)$ is the generator of rotation around the i axis and given by

$$(T_i)_{kl}=-i\epsilon_{kli}. \tag{12}$$

A straightforward calculation using Eq. (12) shows that an orthogonal evolution matrix becomes

$$A=\begin{pmatrix} \cos\varphi\cos\theta\cos\psi-\sin\varphi\sin\psi & \cos\varphi\cos\theta\sin\psi+\sin\varphi\cos\psi & -\cos\varphi\sin\theta \\ -\sin\varphi\cos\theta\cos\psi-\cos\varphi\sin\psi & -\sin\varphi\cos\theta\sin\psi+\cos\varphi\cos\psi & \sin\varphi\sin\theta \\ \sin\theta\cos\psi & \sin\theta\sin\psi & \cos\theta \end{pmatrix}. \tag{13}$$

By differentiating Eq. (8) with respect to time we have

$$(\dot{A}A^T)_{ij}=-(\dot{A}A^T)_{ji}. \tag{14}$$

Thus we can write $\vec{\omega}$ by

$$(\dot{A}A^T)_{ij}=\epsilon_{ijk}\omega_k. \tag{15}$$

A tedious but straightforward calculation yields

$$\omega_1=\dot{\theta}\sin\varphi-\dot{\psi}\sin\theta\cos\varphi, \tag{16}$$

$$\omega_2=\dot{\theta}\cos\varphi+\dot{\psi}\sin\theta\sin\varphi, \tag{17}$$

and

$$\omega_3=\dot{\varphi}+\dot{\psi}\cos\theta, \tag{18}$$

where ω_i is the angular velocity around the i-axis.

The Bloch equation in the rotated system turns out to be

$$\dot{\vec{M}}'+\gamma\vec{B}'\times\vec{M}'=0, \tag{19}$$

where

$$\vec{B}'=A\vec{B}+\frac{1}{\gamma}\vec{\omega}. \tag{20}$$

Here use has been made of the relationship;

$$a_{ij}\epsilon_{jkl}B_kM_l=\epsilon_{ijn}a_{jk}a_{nl}B_kM_l, \tag{21}$$

which is derived from the definition of $\det A$, i.e.,

$$a_{li}a_{mj}a_{nk}\epsilon_{lmn}=\epsilon_{ijk}\det A. \tag{22}$$

A method of solving the Bloch equation (1) is given as follows.

First we solve the rotated Bloch equation (19) for $\vec{M}'$ by rotating the coordinate system into one with the 3-axis being the direction of the applied magnetic field. Thus we find

$$A\vec{B}=(0,\ 0,\ |\vec{B}|), \tag{23}$$

where

$$\vec{B}=(|\vec{B}|\sin\theta\cos\psi,|\vec{B}|\sin\theta\sin\psi,\ \ |\vec{B}|\cos\theta). \tag{24}$$

Second we try to solve Eq. (19) by choosing

$$\dot{\varphi}=-\gamma|\vec{B}|. \tag{25}$$

This choice has limitations from the beginning. The case of $\dot{\varphi}=0$ is excluded. This case will be discussed later. This allows us a case of having the magnitude of the magnetic vector being time dependent. From this choice $\vec{B}'$ reduces to

$$\vec{B}'=\frac{1}{\gamma}(\omega_1,\ \omega_2,\ \omega_3'), \tag{26}$$

where

$$\omega_3'=\dot{\psi}\cos\theta. \tag{27}$$

By solving Eqs. (16) and (17) for $\dot{\theta}$ and $\dot{\psi}\sin\theta$, we have

$$\dot{\theta}=\omega_1\sin\varphi+\omega_2\cos\varphi=\sqrt{\omega_1^2+\omega_2^2}\sin(\varphi+\delta), \tag{28}$$

and

$$\dot{\psi}\sin\theta=-\omega_1\cos\varphi+\omega_2\sin\varphi=-\sqrt{\omega_1^2+\omega_2^2}\cos(\varphi+\delta), \tag{29}$$

where

$$\delta=\cos^{-1}\frac{\omega_1}{\sqrt{\omega_1^2+\omega_2^2}}=\sin^{-1}\frac{\omega_2}{\sqrt{\omega_1^2+\omega_2^2}}=\tan^{-1}\frac{\omega_2}{\omega_1}. \tag{30}$$

Winding up Eqs. (27), (28), and (29), we find

$$(\dot{\theta})^2+(\dot{\psi})^2=(\omega')^2, \tag{31}$$

$$(\dot{\psi})^2=(\omega')^2-\omega_0^2\sin^2(\varphi+\delta), \tag{32}$$

and

$$\tan\theta=-\frac{\omega_0}{\omega_3'}\cos(\varphi+\delta), \tag{33}$$

where

$$\omega'=\sqrt{\omega_1^2+\omega_2^2+(\omega_3')^2}, \tag{34}$$

and

$$\omega_o=\sqrt{\omega_1^2+\omega_2^2}. \tag{35}$$

Third we look for analytic solutions by combining Eq. (26) with Eqs. (27)–(29). We find a solution such that

$$\vec{M}'=Q\vec{M}_0', \tag{36}$$

where $\vec{M}_0'$ is an initial value of $\vec{M}'$. Moreover we have

$$\vec{M}_0'=A_0\vec{M}_0, \tag{37}$$

where A_0 and $\vec{M}_0$ are initial values of A and $\vec{M}$, respectively. Thus we find a solution:

$$\vec{M}=(A^TA_0)(A_0^TQA_0)\vec{M}_0. \tag{38}$$

Notice that Q is a solution of the rotated Bloch equation (19) with Eq. (26) in the matrix form.

III. EXAMPLES OF ANALYTIC SOLUTIONS

Using the senario developed in Sec. II, we study two cases in the following.

A. $\omega_1=\omega_2=0$

Equations (28) and (29) yield

$$\dot{\theta}=\dot{\psi}\sin\theta=0. \tag{39}$$

1. $\theta=0$

From Eq. (27) we have

$$\omega_3'=\dot{\psi}. \tag{40}$$

The exact solution is obtained by choosing the constant of integration as

$$\int_0^t\omega_3'\,\mathrm{d}t=\psi-\psi(0)+\delta_\psi, \tag{41}$$

with

$$\delta_\psi=\psi(0)=0. \tag{42}$$

Thus we find

$$Q=\begin{pmatrix}\cos\psi & \sin\psi & 0\\ -\sin\psi & \cos\psi & 0\\ 0 & 0 & 1\end{pmatrix}, \tag{43}$$

and

$$A_0=\mathbb{1}. \tag{44}$$

Here we have chosen

$$\varphi(0)=0. \tag{45}$$

The solution is

$$A^TQ=\begin{pmatrix}\cos\varphi & -\sin\varphi & 0\\ \sin\varphi & \cos\varphi & 0\\ 0 & 0 & 1\end{pmatrix}, \tag{46}$$

with

$$\varphi=-\gamma\int_0^t|\vec{B}|\mathrm{d}t. \tag{47}$$

This is the well-known solution.

2. $\dot{\theta}=\dot{\psi}=0$

In this case we have from Eq. (27)

$$\omega_3'=0. \tag{48}$$

Thus we find

$$Q=\mathbb{1}. \tag{49}$$

This case corresponds to the applied magnetic field having a fixed direction.

To get a compact expression of solution we use $\hat{e}$ defined by

$$\hat{e}=\left(\frac{B_1}{|\vec{B}|},\ \frac{B_2}{|\vec{B}|},\ \frac{B_3}{|\vec{B}|}\right)=(\sin\theta\cos\psi,\ \sin\theta\sin\psi,\ \cos\theta), \tag{50}$$

with

$$\hat{e}_3=\cos\theta,\quad \sin\theta=\hat{e}_0=\sqrt{\hat{e}_1^2+\hat{e}_2^2}, \tag{51}$$

and

$$\frac{\hat{e}_1}{\hat{e}_0}=\cos\psi,\quad \sin\psi=\frac{\hat{e}_2}{\hat{e}_0}. \tag{52}$$

The rotation matrix (13) is given by

$$A=\begin{pmatrix} \dfrac{\hat{e}_3\hat{e}_1}{\hat{e}_0}\cos\varphi-\dfrac{\hat{e}_2}{\hat{e}_0}\sin\varphi & \dfrac{\hat{e}_2\hat{e}_3}{\hat{e}_0}\cos\varphi+\dfrac{\hat{e}_1}{\hat{e}_0}\sin\varphi & -\hat{e}_0\cos\varphi \\ -\dfrac{\hat{e}_3\hat{e}_1}{\hat{e}_0}\sin\varphi-\dfrac{\hat{e}_2}{\hat{e}_0}\cos\varphi & -\dfrac{\hat{e}_2\hat{e}_3}{\hat{e}_0}\sin\varphi+\dfrac{\hat{e}_1}{\hat{e}_0}\cos\varphi & \hat{e}_0\sin\varphi \\ \hat{e}_1 & \hat{e}_2 & \hat{e}_3 \end{pmatrix}. \tag{53}$$

Thus we find

$$A_0=\begin{pmatrix} \dfrac{\hat{e}_3\hat{e}_1}{\hat{e}_0} & \dfrac{\hat{e}_2\hat{e}_3}{\hat{e}_0} & -\hat{e}_0 \\ -\dfrac{\hat{e}_2}{\hat{e}_0} & \dfrac{\hat{e}_1}{\hat{e}_0} & 0 \\ \hat{e}_1 & \hat{e}_2 & \hat{e}_3 \end{pmatrix}, \tag{54}$$

and

$$(A^TA_0)_{ij}=\cos\varphi\,\delta_{ij}+(1-\cos\varphi)\hat{e}_i\hat{e}_j+\sin\varphi\,\epsilon_{ikj}\hat{e}_k, \tag{55}$$

where

$$\varphi=-\gamma\int_0^t|\vec{B}|\,\mathrm{d}t. \tag{56}$$

B. $\dot{\omega}_1=\dot{\omega}_2=\dot{\omega}'_3=0$

By differentiating Eq. (33) with respect to time we find the key relationship:

$$\dot{\theta}\left[\dot{\varphi}-\frac{1}{\omega'_3}(\dot{\psi})^2\right]=0. \tag{57}$$

Here we have used Eqs. (27) and (28).

1. $\dot{\theta}=0$

Winding up Eqs. (27), (28), and (29), we find

$$\omega_1=\omega_2=0, \tag{58}$$

$$\theta=0, \tag{59}$$

and

$$\psi=\omega'_3 t. \tag{60}$$

Thus this case is included in Sec. III A 1.

2. $\dot{\varphi}=\frac{1}{\omega'_3}(\dot{\psi})^2$

Using Eq. (32), we have

$$\dot{\varphi}=-\gamma|\vec{B}|=\frac{\omega'}{e_3}[1-e_0^2\sin^2(\varphi+\delta)], \tag{61}$$

where we have defined $\vec{e}$ by

$$\vec{e}=\left(\frac{\omega_1}{\omega'},\frac{\omega_2}{\omega'},\frac{\omega'_3}{\omega'}\right), \tag{62}$$

and

$$e_0=\sqrt{e_1^2+e_2^2}=\frac{\omega_0}{\omega'}. \tag{63}$$

a. $\ddot{\varphi}=0$. Before going into details we comment on the case of $|\vec{B}|$ being independent of time. In this case Eq. (61) yields

$$\omega_1=\omega_2=0, \tag{64}$$

$$\omega'_3=-\gamma|\vec{B}|=\dot{\psi}, \tag{65}$$

and

$$\theta=0. \tag{66}$$

Here we have made the combined use of Eqs. (27) and (32). Thus this case is also included in Sec. III A 1.

b. $\ddot{\varphi}\neq 0$. Solving the differential equation of first order (61) for φ, we find

$$\varphi=-\delta+\tan^{-1}\left[\frac{1}{e_3}\tan(\omega' t+\delta_C)\right], \tag{67}$$

where δ_C is the constant of integration. The magnitude of the applied magnetic field is obtained by differentiating Eq. (67) with respect to time,

$$-\gamma|\vec{B}|=\frac{\omega' e_3}{1-e_0^2\cos^2(\omega' t+\delta_C)} \quad (e_3<0). \tag{68}$$

Again using Eq. (61) we find

$$\dot{\psi}=\frac{\omega' e_3}{\sqrt{1-e_0^2\cos^2(\omega' t+\delta_C)}}. \tag{69}$$

By substituting Eq. (69) back into Eq. (31), we have

$$\dot{\theta}=-\frac{\omega' e_0\sin(\omega' t+\delta_C)}{\sqrt{1-e_0^2\cos^2(\omega' t+\delta_C)}}. \tag{70}$$

Equation (69) yields

$$\psi=e_3F(\tau,\ e_0)+\delta_\psi, \tag{71}$$

with

$$\tau=\sin^{-1}\left[\frac{\sin(\omega' t+\delta_C)}{\sqrt{1-e_0^2\cos^2(\omega' t+\delta_C)}}\right], \tag{72}$$

where $F(x,p)$ is the elliptic integral of the first kind and given by

$$F(x,p)=\int_{x_0}^{x}\frac{\mathrm{d}x}{\sqrt{1-p^2\sin^2 x}} \quad (p^2<1). \tag{73}$$

Also Eq. (70) yields

$$\theta=\sin^{-1}[e_0\cos(\omega' t+\delta_C)]+\delta_\theta. \tag{74}$$

Here δ_ψ and δ_θ are the constants of integration.

Having chosen the constants of integration as

$$\delta_C=\tan^{-1}(e_3\tan\delta), \tag{75}$$

$$\delta_\psi=-e_3F(\tau_0,\ e_0)=0, \tag{76}$$

with

$$\tau_0=\sin^{-1}\left(\frac{\sin\delta_C}{\sqrt{1-e_0^2\cos^2\delta_C}}\right)=-\delta, \tag{77}$$

and

$$\delta_\theta=0, \tag{78}$$

we find

$$\varphi(0)=\psi(0)=0, \tag{79}$$

and

$$\theta_0=\theta(0)=\sin^{-1}(e_0\cos\delta_C)=\sin^{-1}\left(\frac{e_0\cos\delta}{\sqrt{1-e_0^2\sin^2\delta}}\right). \tag{80}$$

In this case the solution of the rotated Bloch equation is well known and given by

$$(Q)_{ij}=\cos(\omega' t)\,\delta_{ij}+[1-\cos(\omega' t)]e_i e_j-\sin(\omega' t)\,\epsilon_{ikj}\,e_k, \tag{81}$$

and

$$A_0=\begin{pmatrix}\cos\theta_0 & 0 & -\sin\theta_0\\ 0 & 1 & 0\\ \sin\theta_0 & 0 & \cos\theta_0\end{pmatrix}=\frac{1}{\sqrt{1-e_2^2}}\begin{pmatrix}-e_3 & 0 & -e_1\\ 0 & \sqrt{1-e_2^2} & 0\\ e_1 & 0 & -e_3\end{pmatrix}. \tag{82}$$

Here we have used Eqs. (79) and (80).

Let us introduce the matrices E_i, $(i=1,2)$ given by

$$(E_1)_{ij}=e_i e_j, \tag{83}$$

and

$$(E_2)_{ij}=-\epsilon_{ikj}e_k, \tag{84}$$

we find

$$A_0^T Q A_0=\cos(\omega' t)\mathbb{1}+[1-\cos(\omega' t)]Q_1+\sin(\omega' t)Q_2, \tag{85}$$

where

$$Q_1=A_0^T E_1 A_0=\begin{pmatrix}0 & 0 & 0\\ 0 & e_2^2 & -e_2\sqrt{1-e_2^2}\\ 0 & -e_2\sqrt{1-e_2^2} & 1-e_2^2\end{pmatrix}, \tag{86}$$

and

$$Q_2=A_0^T E_2 A_0=\begin{pmatrix}0 & -\sqrt{1-e_2^2} & -e_2\\ \sqrt{1-e_2^2} & 0 & 0\\ e_2 & 0 & 0\end{pmatrix}. \tag{87}$$

Thus we find

$$(A^T A_0)(A_0^T Q A_0)=\cos(\omega' t)A^T A_0+[1-\cos(\omega' t)]A^T A_0 Q_1+\sin(\omega' t)A^T A_0 Q_2. \tag{88}$$

Having written Eq. (88) out, we list here in components of $A^T A_0$, $A^T A_0 Q_1$, and $A^T A_0 Q_2$:

$$(A^T A_0)_{ij}=(A^T)_{ik}(A_0)_{kj}=(A)_{ki}(A_0)_{kj}, \tag{89}$$

where

$$(A^TA_0)_{11}=\frac{1}{\sqrt{1-e_2^2}}[-e_3(\cos\varphi\cos\theta\cos\psi-\sin\varphi\sin\psi)+e_1\sin\theta\cos\psi],$$

$$(A^TA_0)_{12}=-\sin\varphi\cos\theta\cos\psi-\cos\varphi\sin\psi,$$

$$(A^TA_0)_{13}=\frac{1}{\sqrt{1-e_2^2}}[-e_1(\cos\varphi\cos\theta\cos\psi-\sin\varphi\sin\psi)-e_3\sin\theta\cos\psi],$$

$$(A^TA_0)_{21}=\frac{1}{\sqrt{1-e_2^2}}[-e_3(\cos\varphi\cos\theta\sin\psi+\sin\varphi\cos\psi)+e_1\sin\theta\sin\psi],$$

$$(A^TA_0)_{22}=-\sin\varphi\cos\theta\sin\psi+\cos\varphi\cos\psi,$$

$$(A^TA_0)_{23}=\frac{1}{\sqrt{1-e_2^2}}[-e_1(\cos\varphi\cos\theta\sin\psi+\sin\varphi\cos\psi)-e_3\sin\theta\sin\psi],$$

$$(A^TA_0)_{31}=\frac{1}{\sqrt{1-e_2^2}}(e_3\cos\varphi\sin\theta+e_1\cos\theta),$$

$$(A^TA_0)_{32}=\sin\varphi\sin\theta,$$

and

$$(A^TA_0)_{33}=\frac{1}{\sqrt{1-e_2^2}}(e_1\cos\varphi\sin\theta-e_3\cos\theta),$$

$$(A^TA_0Q_1)_{ij}=(A^TA_0)_{ik}(Q_1)_{kj}, \tag{90}$$

where

$$(A^TA_0Q_1)_{12}=e_2[(e_1\cos\varphi-e_2\sin\varphi)\cos\theta\cos\psi-(e_2\cos\varphi+e_1\sin\varphi)\sin\psi+e_3\sin\theta\cos\psi],$$

$$(A^TA_0Q_1)_{13}=-\sqrt{1-e_2^2}[(e_1\cos\varphi-e_2\sin\varphi)\cos\theta\cos\psi-(e_2\cos\varphi+e_1\sin\varphi)\sin\psi+e_3\sin\theta\cos\psi],$$

$$(A^TA_0Q_1)_{22}=e_2[(e_1\cos\varphi-e_2\sin\varphi)\cos\theta\sin\psi+(e_2\cos\varphi+e_1\sin\varphi)\cos\psi+e_3\sin\theta\sin\psi],$$

$$(A^TA_0Q_1)_{23}=-\sqrt{1-e_2^2}[(e_1\cos\varphi-e_2\cos\varphi)\cos\theta\sin\psi+(e_2\cos\varphi+e_1\sin\varphi)\cos\psi+e_3\sin\theta\sin\psi],$$

$$(A^TA_0Q_1)_{32}=-e_2[(e_1\cos\varphi-e_2\sin\varphi)\sin\theta-e_3\cos\theta],$$

$$(A^TA_0Q_1)_{33}=\sqrt{1-e_2^2}[(e_1\cos\varphi-e_2\sin\varphi)\sin\theta-e_3\cos\theta],$$

and

$$(A^T A_0 Q_1)_{i1}=0, \quad (i=1,2,3),$$
$$(A^T A_0 Q_2)_{ij}=(A^T A_0)_{ik}(Q_2)_{kj}, \tag{91}$$

where

$$(A^T A_0 Q_2)_{11}=-\frac{1}{\sqrt{1-e_2^2}}\{[e_1e_2\cos\varphi+(1-e_2^2)\sin\varphi]\cos\theta\cos\psi$$
$$+[(1-e_2^2)\cos\varphi-e_1e_2\sin\varphi]\sin\psi+e_2e_3\sin\theta\cos\psi\},$$
$$(A^T A_0 Q_2)_{12}=e_3(\cos\varphi\cos\theta\cos\psi-\sin\varphi\sin\psi)-e_1\sin\theta\cos\psi,$$
$$(A^T A_0 Q_2)_{13}=\frac{e_2}{\sqrt{1-e_2^2}}[e_3(\cos\varphi\cos\theta\cos\psi-\sin\varphi\sin\psi)-e_1\sin\theta\cos\psi],$$
$$(A^T A_0 Q_2)_{21}=-\frac{1}{\sqrt{1-e_2^2}}\{[e_1e_2\cos\varphi+(1-e_2^2)\sin\varphi]\cos\theta\sin\psi$$
$$-[(1-e_2^2)\cos\varphi-e_1e_2\sin\varphi]\cos\psi+e_2e_3\sin\theta\sin\psi\},$$
$$(A^T A_0 Q_2)_{22}=e_3(\cos\varphi\cos\theta\sin\psi+\sin\varphi\cos\psi)-e_1\sin\theta\sin\psi,$$
$$(A^T A_0 Q_2)_{23}=\frac{e_2}{\sqrt{1-e_2^2}}[e_3(\cos\varphi\cos\theta\sin\psi+\sin\varphi\cos\psi)-e_1\sin\theta\sin\psi],$$
$$(A^T A_0 Q_2)_{31}=\frac{1}{\sqrt{1-e_2^2}}\{[e_1e_2\cos\varphi+(1-e_2^2)\sin\varphi]\sin\theta-e_2e_3\cos\theta\},$$
$$(A^T A_0 Q_2)_{32}=-(e_3\cos\varphi\sin\theta+e_1\cos\theta),$$

and

$$(A^T A_0 Q_2)_{33}=-\frac{e_2}{\sqrt{1-e_2^2}}(e_3\cos\varphi\sin\theta+e_1\cos\theta).$$

The Eulerian angles (φ,θ,ψ) are given by

$$\varphi+\delta=\tan^{-1}\left[\frac{1}{e_3}\tan(\omega' t+\delta_C)\right]=\cos^{-1}\left[-\frac{e_3\cos(\omega' t+\delta_C)}{\sqrt{1-e_0^2\cos^2(\omega' t+\delta_C)}}\right]$$
$$=\sin^{-1}\left[-\frac{\sin(\omega' t+\delta_C)}{\sqrt{1-e_0^2\cos^2(\omega' t+\delta_C)}}\right], \tag{92}$$
$$\theta=\sin^{-1}[e_0\cos(\omega' t+\delta_C)]=\cos^{-1}[\sqrt{1-e_0^2\cos^2(\omega' t+\delta_C)}], \tag{93}$$

and

$$\psi=e_3F(\tau,e_0), \quad \tau=\sin^{-1}\left[\frac{\sin(\omega' t+\delta_C)}{\sqrt{1-e_0^2\cos^2(\omega' t+\delta_C)}}\right], \tag{94}$$

with

$$\delta=\cos^{-1}\frac{e_1}{e_0}=\sin^{-1}\frac{e_2}{e_0}=\tan^{-1}\frac{e_2}{e_1}, \tag{95}$$

and

$$\delta_C=\tan^{-1}(e_3\tan\delta)=\cos^{-1}\left(\frac{\cos\delta}{\sqrt{1-e_0^2\sin^2\delta}}\right)=\sin^{-1}\left(\frac{e_3\sin\delta}{\sqrt{1-e_0^2\sin^2\delta}}\right). \tag{96}$$

This solution is a general solution under the condition that the modified angular velocities $(\omega_1,\omega_2,\omega_3')$ are independent of time. The rotated coordinate system moves according to Eqs. (92)–(94) together with Eq. (68).

3. $\dot{\varphi}=0$

As was mentioned before, the choice of Eq. (25) does not make sense for the case of $\dot{\varphi}=0$. Instead of the choice (25) we can impose on φ being independent of time such that

$$\varphi=-\delta, \tag{97}$$

where δ is given by Eq. (30). From this choice Eqs. (27)–(29) together with Eqs. (32) and (33) yield

$$\psi=\omega' t, \tag{98}$$

and

$$\theta=\tan^{-1}\left(-\frac{\omega_0}{\omega_3'}\right)=\cos^{-1}\left(\frac{\omega_3'}{\omega'}\right)=\sin^{-1}\left(-\frac{\omega_0}{\omega'}\right). \tag{99}$$

We can solve the rotated Bloch equation (19) under the condition

$$\dot{|\vec{B}|}=0. \tag{100}$$

Then we have to redefine $\vec{e}$ by

$$\vec{e}=\frac{1}{\omega}(\omega_1,\omega_2,\gamma|\vec{B}|+\omega_3'), \tag{101}$$

with

$$\omega=\sqrt{\omega_0^2+(\gamma|\vec{B}|+\omega_3')^2}, \tag{102}$$

$$\omega_0=\sqrt{\omega_1^2+\omega_2^2}=\omega e_0. \tag{103}$$

Note that

$$\vec{B}=[|\vec{B}|\sin\theta\cos(\omega' t),|\vec{B}|\sin\theta\sin(\omega' t),|\vec{B}|\cos\theta]. \tag{104}$$

The solution is given by

$$(Q)_{ij}=\cos(\omega t)\delta_{ij}+[1-\cos(\omega t)]e_ie_j-\sin(\omega t)\epsilon_{ikj}e_k, \tag{105}$$

where we have used Eq. (101), and

$$A_0=\begin{pmatrix} \cos\delta\cos\theta & -\sin\delta & -\cos\delta\sin\theta \\ \sin\delta\cos\theta & \cos\delta & -\sin\delta\sin\theta \\ \sin\theta & 0 & \cos\theta \end{pmatrix}. \tag{106}$$

Here we have used A as

$$A=\begin{pmatrix} \cos\delta\cos\theta\cos(\omega' t)+\sin\delta\sin(\omega' t) & \cos\delta\cos\theta\sin(\omega' t)-\sin\delta\cos(\omega' t) & -\cos\delta\sin\theta \\ \sin\delta\cos\theta\cos(\omega' t)-\cos\delta\sin(\omega' t) & \sin\delta\cos\theta\sin(\omega' t)+\cos\delta\cos(\omega' t) & -\sin\delta\sin\theta \\ \sin\theta\cos(\omega' t) & \sin\theta\sin(\omega' t) & \cos\theta \end{pmatrix}. \tag{107}$$

Thus we find

$$A^T A_0=\begin{pmatrix} \cos(\omega' t) & -\sin(\omega' t) & 0 \\ \sin(\omega' t) & \cos(\omega' t) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{108}$$

and

$$A_0^T Q A_0=\cos(\omega t)\mathbb{1}+[1-\cos(\omega t)]Q_1+\sin(\omega t)Q_2, \tag{109}$$

where

$$\begin{aligned} Q_1&=A_0^T E_1 A_0 \\ &=\begin{pmatrix} (e_0\cos\theta+e_3\sin\theta)^2 & 0 & (e_0\cos\theta+e_3\sin\theta)(e_3\cos\theta-e_0\sin\theta) \\ 0 & 0 & 0 \\ (e_0\cos\theta+e_3\sin\theta)(e_3\cos\theta-e_0\sin\theta) & 0 & (e_3\cos\theta-e_0\sin\theta)^2 \end{pmatrix}, \end{aligned} \tag{110}$$

and

$$Q_2=A_0^T E_2 A_0=\begin{pmatrix} 0 & e_3\cos\theta-e_0\sin\theta & 0 \\ -(e_3\cos\theta-e_0\sin\theta) & 0 & e_0\cos\theta+e_3\sin\theta \\ 0 & -(e_0\cos\theta+e_3\sin\theta) & 0 \end{pmatrix}, \tag{111}$$

with

$$e_0\cos\theta+e_3\sin\theta=-\frac{1}{\omega}\gamma|\vec{B}|\frac{\omega_0}{\omega'}, \tag{112}$$

and

$$e_3\cos\theta-e_0\sin\theta=\frac{1}{\omega}\left(\omega'+\gamma|\vec{B}|\frac{\omega_3'}{\omega'}\right). \tag{113}$$

Here E_1 and E_2 are given by Eqs. (83) and (84), respectively. Thus we find

$$(A^T A_0)(A_0^T Q A_0)=\cos(\omega t)(A^T A_0)+[1-\cos(\omega t)](A^T A_0)Q_1+\sin(\omega t)(A^T A_0)Q_2, \tag{114}$$

where Eq. (108) yields $A^T A_0$ being the rotation matrix around the 3-axis.

This example is well known as a circularly polarized rf field. Resonance occurrs when $\omega_3' = -\gamma|\vec{B}|$.

IV. CONCLUSIONS

We have found an unknown solution for the case in Sec. III B 2 b in which the applied magnetic vector behaves as the bounded oscillation in time. All the well-known solutions have been contained in our approach. And even in the well-known case of Sec. III A 2, we allow the case of having the magnitude of the magnetic vector being time dependent.

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Semiclassical generalization of the Darboux–Christoffel formula

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The Darboux–Christoffel formula is a closed-form expression for the kernel of the operator that projects onto the first N of a system of one-dimensional polynomials, orthonormal with respect to some weighting function. It is a key element in the theory of Gaussian integration and in the theory of discrete variable representation or Lagrangian mesh methods for diagonalizing quantum Hamiltonians of a few degrees of freedom. The one-dimensional Darboux–Christoffel formula turns out to have a generalization that is valid in a semiclassical or asymptotic sense for a wider class of orthonormal functions than orthonormal polynomials. This class consists of the bound eigenfunctions of one-dimensional Hamiltonians with time-reversal invariance, such as kinetic-plus-potential Hamiltonians. It also has certain generalizations involving the unbound eigenfunctions of such Hamiltonians. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1489071]

I. INTRODUCTION

This paper concerns the Darboux–Christoffel formula, a standard result in the theory of one-dimensional orthonormal polynomials.[1,2] The formula is the following. Let $\{q_n(x),n=0,1,\ldots\}$ be a set of real polynomials, where $q_n(x)$ is of degree n. Let the polynomials be orthonormal on an interval $[a,b]$ with respect to weighting function $\rho(x)>0$, so that $\int_a^b \mathrm{d}x\,\rho(x)q_n(x)q_m(x)=\delta_{nm}$. Let $\phi_n(x)=\sqrt{\rho(x)}q_n(x)$, so that the functions $\{\phi_n(x)\}$ are orthonormal with respect to the measure $\mathrm{d}x$. Then the Darboux–Christoffel formula is

$$\sum_{n=0}^{N-1}\phi_n(x)\phi_n(y)=\langle x|P_N|y\rangle=a_N\frac{\phi_N(x)\phi_{N-1}(y)-\phi_{N-1}(x)\phi_N(y)}{x-y}, \tag{1.1}$$

where P_N is the projection operator onto the first N eigenfunctions,

$$P_N=\sum_{n=0}^{N-1}|\phi_n\rangle\langle\phi_n|, \tag{1.2}$$

and where

$$a_N=\langle\phi_N|x|\phi_{N-1}\rangle=\int_a^b \mathrm{d}x\;\phi_N(x)x\phi_{N-1}(x). \tag{1.3}$$

Here and in the following we use Dirac notation, with $|\phi_n\rangle$ representing $\phi_n(x)$. The Darboux–Christoffel formula has a generalization to systems of orthogonal polynomials in more than one variable,[3] which we shall discuss in the following, but most of this paper is concerned with the one-dimensional case.

This paper presents a semiclassical generalization of the Darboux–Christoffel formula, that is, a generalization that applies to systems of orthogonal functions that are not necessarily orthogonal

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polynomials, but one that is valid only in a semiclassical or asymptotic sense. Our interest in the Darboux–Christoffel formula is an outgrowth of our recent attempts[4–8] to construct multidimensional generalizations of ''Lagrangian mesh'' or ''discrete variable representation'' (LM/DVR) basis functions, which are localized functions useful for diagonalizing Hamiltonians of few degrees of freedom. In the remainder of this section we shall explain what LM/DVR functions are, what their relation to the Darboux–Christoffel formula is, and the reasoning that led us to consider a semiclassical generalization of that formula. In subsequent sections we shall present our derivation of that generalization and a discussion of the result.

The following is a bare outline of one approach to LM/DVR functions. Standard references include Harris *et al.*,[9] Dickinson and Certain,[10] and Baye and Heenan.[11] A review of the application of these functions in chemical physics has recently been given by Light and Carrington,[12] and we have presented our own approach in Ref. 4. A sampling of articles showing the development and the history of the applications of these functions includes Refs. 13–34. These references may be consulted for more details.

Let M be a manifold (possibly multidimensonal) with a metric, let $\mathcal{S}$ be a subspace of $L^2(M)$ of dimension N (possibly infinite), and let P be the orthogonal projector onto $\mathcal{S}$. Let $\{x_\alpha, \alpha = 0,\ldots,N-1\}$ be a collection of N distinct ''grid points'' in M. Let $\Delta_\alpha(x) = P[\,\delta(x-x_\alpha)]$ be the δ function at grid point x_α, projected onto $\mathcal{S}$. This will be written in Dirac notation as $|\Delta_\alpha\rangle = P|x_\alpha\rangle$. Then a simple theorem states that $\langle\Delta_\alpha|\Delta_\beta\rangle = \Delta_\beta(x_\alpha) = \Delta_\alpha(x_\beta)^*$. Finally, we define a *LM/DVR set* as the combination of P plus $\{x_\alpha\}$ such that

$$\Delta_\alpha(x_\beta) = K_\alpha \delta_{\alpha\beta} \tag{1.4}$$

with $K_\alpha > 0$. In view of the theorem just quoted, this implies that the projected δ-functions are orthogonal. In this case, we shall write $F_\alpha(x) = (1/\sqrt{K_\alpha})\Delta_\alpha(x)$ for the orthonormalized versions of these functions. In the case of finite N, the LM/DVR functions $\{F_\alpha(x)\}$ are linearly independent and form an orthonormal basis in $\mathcal{S}$; the same is normally true in the infinite-dimensional case as well.

The LM/DVR functions $\Delta_\alpha(x)$ or $F_\alpha(x)$ are typically localized about their associated grid point x_α, with diffraction-like oscillations that decay slowly as one moves away from the grid point. See Ref. 4 for some plots of these functions. Their virtues in applications to quantum mechanics follow from their orthonormality and the fact that they diagonalize the problem of interpolating on the space $\mathcal{S}$ relative to the grid points $\{x_\alpha\}$ [that is, the matrix $\Delta_\alpha(x_\beta)$ diagonal]. The theory of LM/DVR functions is closely related to that of Gaussian quadratures. The practical advantages of LM/DVR basis functions are the following. First, a simple diagonal approximation is available for the matrix elements of the potential energy in a LM/DVR basis, namely,

$$\langle F_\alpha|V|F_\beta\rangle = V(x_\alpha)\,\delta_{\alpha\beta}\,. \tag{1.5}$$

As it stands, this approximation is not very accurate, but (somewhat paradoxically) its use leads to errors in the computed, low-lying eigenvalues and eigenfunctions of a Hamiltonian that are exponentially small in the size of the matrix, that is, much smaller than the errors in the matrix elements themselves.[4] Second, in applications of LM/DVR functions the basis functions associated with grid points where the wave function is known to be small (for example, deep in a classically forbidden region) can be thrown away, thereby effecting a reduction (or contraction) in the size of the basis. Third, in multidimensional problems with bases that are tensor products of one-dimensional LM/DVR bases, the matrix for the Hamiltonian is sparse, and suitable for iterative algorithms that require the repetitive multiplication of the Hamiltonian matrix times a vector. Fourth, the method of ''sequential diagonalization and truncation,'' in which one diagonalizes a Hamiltonian on sections of increasing dimensionality before finally diagonalizing the full Hamiltonian in the full configuration space, is particularly simple when the basis functions in the last coordinate is a LM/DVR basis.[12]

An important class of LM/DVR functions is associated with real orthonormal polynomials in one dimension. A LM/DVR set requires a projection operator and a set of grid points. Let the

projection operator be P_N of Eq. (1.2), and let the grid points $\{x_\alpha\}$ be the (necessarily simple) zeroes of $\phi_N(x)$, the first polynomial omitted from the sum (1.2). Then by the Darboux–Christoffel formula (1.1), the projected δ-functions are

$$\Delta_\alpha(x) = a_N \phi_{N-1}(x_\alpha) \frac{\phi_N(x)}{x - x_\alpha}. \tag{1.6}$$

These clearly vanish at each other's grid points but not at their own, that is, they satisfy Eq. (1.4) with

$$K_\alpha = a_N \phi_{N-1}(x_\alpha) \phi_N'(x_\alpha), \tag{1.7}$$

and therefore form a LM/DVR set. Note that there is actually a different LM/DVR set for each value of N; in practice, one increases the value of N (the size of the basis) to obtain convergence in a quantum calculation.

On the other hand, a LM/DVR set does not exist on most subspaces $\mathcal{S}$ of functions, that is, given $\mathcal{S}$ (or equivalently, the projection operator P that projects onto $\mathcal{S}$) there does not exist, in general, any set of grid points such that the LM/DVR conditions (1.4) are satisfied. This point is discussed more fully in Refs. 5 and 8, but the basic idea is that given $\mathcal{S}$, Eq. (1.4) can be regarded as a set of $N(N-1)/2$ equations in Nd unknowns, where the unknowns are the coordinates of the N grid points and d is the dimensionality of M. Thus, except possibly for small N the number of equations exceeds the number of unknowns, and, unless the equations are dependent, it is not likely that a solution exists. In fact, in the case of subspaces spanned by orthogonal polynomials, the equations are dependent, since the product of two polynomials is another polynomial. In one dimension, this reduces the number of independent equations below the number of unknowns, and a solution in fact exists, as shown explicitly in the previous paragraph with the aid of the Darboux–Christoffel formula. The same logic does not work, however, for orthogonal polynomials in more than one dimension (see Ref. 8 and the following comments).

Thus there arises the question of what is the most general subspace $\mathcal{S}$ of functions such that grid points exist such that Eq. (1.4) is satisfied. We do not know the answer, but certainly the easiest case is that of one-dimensional, orthogonal polynomials. There also exist certain infinite dimensional subspaces of functions in one dimension that are limiting cases of orthogonal polynomials, with their associated LM/DVR basis functions. These include one-dimensional sinc functions[4] and related functions of the Bessel[6] and Airy[7] types. There are also systematic classes of LM/DVR functions in $\mathbb{R}^n$ that are not obviously limiting cases of orthogonal polynomials;[5] these are generalizations of sinc functions in one dimension. There are also other examples of LM/DVR sets on manifolds such as S^2,[8] but these seem to be isolated cases, not members of systematic families.

The case of multidimensional orthogonal polynomials is one about which much can be said. To be specific, consider two-dimensional polynomials in (x,y), defined over some region of the plane and orthogonal with respect to some weighting function, and let P_N be the projector onto the subspace spanned by all the orthogonal polynomials of degree less than N. This subspace has dimension $N(N+1)/2$. Unlike the case of one-dimensional orthogonal polynomials, the existence of a LM/DVR set on this subspace is not automatic; it only follows when there exists a ''Gaussian cubature formula,'' in the terminolgy of Dunkl and Xu[3] (that is, it only holds for special regions and weighting functions). Those authors give several equivalent conditions for the existence of a Gaussian cubature formula; one is that the $N+1$ polynomials of degree N have $N(N+1)/2$ common roots, and another is that the projected coordinate operators, $P_N x P_N$ and $P_N y P_N$, commute. These facts follow from the multidimensional version of the Darboux–Christoffel formula. There are not many examples known in which these conditions are satisfied, and those examples do not seem useful for quantum mechanical applications.

Thus, while LM/DVR sets could be useful in applications, especially on multidimensional spaces, it does not seem to be easy to find them (the case of one-dimensional orthogonal polyno-

mials being an exception). This is the reason for our interest in the Darboux–Christoffel formula, since generalizations could be useful in finding larger classes of LM/DVR sets. The following considerations led us to consider semiclassical generalizations.

In the case of one-dimensional orthogonal polynomials, the orthogonal polynomials themselves (times the square root of the weighting function) $\{\phi_n(x)\}$ form an orthonormal basis on $\mathcal{S}$, while another orthonormal basis is afforded by the LM/DVR functions $\{F_\alpha(x)\}$. The projection operator P_N corresponds semiclassically to a region of phase space,[35] and the two orthonormal bases correspond to a division of this region into Planck cells of area $2\pi\hbar$ in two different ways (these are two different "polarizations," in the language of geometric quantization[36]). In particular, as argued in Ref. 4, the LM/DVR basis corresponds semiclassically to dividing the region of phase space corresponding to P_N into vertical strips of constant area (see Fig. 5 of Ref. 4 for the case of Hermite polynomials). These strips are centered on the grid points, which are otherwise the roots of $\phi_N(x)$. The grid points are not uniformly spaced, in general, since the height of the strips (the momentum cutoff determined by the region of phase space) depends on x. Indeed, to leading order in $1/N$, the spacing of the roots of $\phi_N(x)$ is precisely that needed to obtain vertical strips in phase space of constant area. This in a sense "explains" the spacing rule for the grid points of the LM/DVR set.

On the other hand, there is nothing in this constant area rule that requires that the projection operator and the region of phase space associated with it should be spanned by orthogonal polynomial functions. Thus, the suggestion arises that something like the Darboux–Christoffel formula might be valid, at least in a semiclassical sense, for more general classes of functions than the orthogonal polynomial functions $\phi_n(x)$ introduced previously. This turns out to be true, as we shall now show.

II. DERIVATION OF THE SEMICLASSICAL DARBOUX–CHRISTOFFEL FORMULA

Consider a one-dimensional Hamiltonian, $H=p^2/2m+V(x)$, with eigenfunctions $\psi_n(x)$ and eigenvalues E_n, $H\psi_n=E_n\psi_n$. The Hamiltonian is invariant under time reversal, so we may choose the eigenfunctions to be real. It is possible to treat more general Hamiltonians (for example, those with fourth powers of the momentum), but time-reversal invariance seems to be necessary for the following derivation. We do not assume that the eigenfunctions $\psi_n(x)$ have any necessary relationship to orthogonal polynomials, although in some special cases (for example, the harmonic oscillator) they may. We shall assume that the classical energy level sets $H(x,p)=E$ are topological circles in phase space, at least in some energy range of interest, or, if the level sets consist of more than one disconnected topological circle, that tunneling between the disconnected pieces can be neglected. For example, a single potential well such as $V(x)=x^4$ satisifes these assumptions.

The projector onto the first N eigenstates is $P_N=\Sigma_{n=0}^{N-1}|\psi_n\rangle\langle\psi_n|$, with kernel

$$\langle x|P_N|y\rangle=\sum_{n=0}^{N-1}\psi_n(x)\psi_n(y). \tag{2.1}$$

We would like to find a semiclassical expression for this sum, analogous to the Darboux–Christoffel formula (1.1). Rather than using the semiclassical expressions for the eigenfunctions ψ_n directly, it will be advantageous to work with the Green's function $G(x,y,E)$, since this is defined for all energies E (not just energy eigenvalues), and at a certain point we shall want to replace the sum in Eq. (2.1) with an integral. Our treatment of the Green's function and its asymptotics follows techniques used by Gutzwiller in his periodic orbit theory,[37–40] but is simpler because we are only dealing with the one-dimensional case. We have also called on techniques demonstrated by Berry and Tabor[41–43] in their classic studies of integrable systems.

The Green's operator $G(z)=1/(z-H)$ is a function of the complexified energy variable $z=E+i\epsilon$. The corresponding kernel is the Green's function, $G(x,y,z)=\langle x|G(z)|y\rangle$. The Green's operator satisfies

$$\delta(E-H)=\frac{i}{2\pi}\lim_{\epsilon\to 0}[G(E+i\epsilon)-G(E-i\epsilon)], \tag{2.2}$$

or, in terms of kernels,

$$\begin{aligned}\langle x|\,\delta(E-H)|y\rangle &= \sum_{n=0}^{\infty}\psi_n(x)\psi_n(y)\,\delta(E-E_n)\\ &= \frac{i}{2\pi}\lim_{\epsilon\to 0}[G(x,y,E+i\epsilon)-G(x,y,E-i\epsilon)]\\ &= -\frac{1}{\pi}\lim_{\epsilon\to 0}\operatorname{Im}G(x,y,E+i\epsilon),\end{aligned} \tag{2.3}$$

where we have used the time-reversal invariance of H in the last step to replace $G(x,y,E-i\epsilon)$ by $G(x,y,E+i\epsilon)^*$. Now let E be some energy such that $E_{N-1}<E<E_N$, so that

$$\int_{-\infty}^{E}\mathrm{d}E'\langle x|\,\delta(E'-H)|y\rangle=\sum_{n=0}^{N-1}\psi_n(x)\psi_n(y). \tag{2.4}$$

Our stategy will be to use the semiclassical expression for the Green's function in Eq. (2.3) to obtain the kernel of $\delta(E-H)$, which we shall then substitute into Eq. (2.4) to obtain the kernel of the projection operator.

The Green's function satisfies an inhomogeneous Schrödinger equation in the variable x,

$$\left[E+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}-V(x)\right]G(x,y,E)=\delta(x-y). \tag{2.5}$$

This equation is valid as it stands for real E when E does not belong to the spectrum (continuous or discrete) of H, and otherwise E should be given a small imaginary part. Since G satisfies a homogeneous Schrödinger equation both for $x<y$ and $x>y$, we can use ordinary semiclassical theory[44] in these regions. To be specific, suppose E lies between two discrete eigenvalues of H, so that E is an an energy at which a classical orbit (a topological circle in phase space, symmetric about the x-axis) exists. Then there are two classical turning points x_0 (left) and x_1 (right). Suppose also that $x_0<x,y<x_1$ (x and y are in the classically allowed region). Then the semiclassical solutions to Eq. (2.5) in the two regions are

$$G(x,y,E)=\frac{1}{\sqrt{p(x)}}\times\begin{cases}A\cos[S(x_0,x,I)/\hbar-\pi/4], & x<y\\ B\cos[S(x_1,x,I)/\hbar+\pi/4], & x>y,\end{cases} \tag{2.6}$$

where $I=(1/2\pi)\oint p\,\mathrm{d}x$ is the classical action of an orbit of energy E, $S(a,b,I)=\int_a^b p\,\mathrm{d}x$ is the action integral along orbit of action I, $p=p(x)=\sqrt{2m[E-V(x)]}$ is the positive branch of the local momentum, and A and B are constants. The connection between the two branches of the semiclassical solution at the left or right turning points has been made in such a way that the wave function is decaying exponentially in the classically forbidden region. Equation (2.6) is valid only to leading order in $\hbar$.

The constants A and B are determined by matching the two solutions at $x=y$. At this point the Green's function is continuous, but its first derivative is discontinuous, as we find by integrating Eq. (2.5) between $y-\eta$ and $y+\eta$. This gives

$$\lim_{\eta\to 0}\frac{\hbar^2}{2m}\left[\left(\frac{\partial G}{\partial x}\right)_{x=y+\eta}-\left(\frac{\partial G}{\partial x}\right)_{x=y-\eta}\right]=1. \tag{2.7}$$

The conditions on G and $\partial G/\partial x$ at $x=y$ give two equations that can be solved for A and B. In computing $\partial G/\partial x$ from Eq. (2.6), we only retain terms of leading order in $\hbar$. Solving for A and B and substituting into Eq. (2.6), we find finally

$$G(x,y,E)=-\frac{2m}{\hbar\sqrt{p(x)p(y)}}\frac{1}{\cos(\pi I/\hbar)} \times\begin{cases}\cos[S(x_0,x,I)/\hbar-\pi/4]\cos[S(x_1,y,I)/\hbar+\pi/4], & x<y\\ \cos[S(x_0,y,I)/\hbar-\pi/4]\cos[S(x_1,x,I)/\hbar+\pi/4], & x>y.\end{cases} \tag{2.8}$$

This is the semiclassical solution for the Green's function, valid under the stated conditions on E, x, and y. If either x or y or both lie in a classically forbidden region, or if E is less than the classical energy at the bottom of the well (in which case there is no classically allowed region), then other semiclassical expressions apply, involving exponentially decaying solutions. We shall not write these down. If E coincides with a semiclassical eigenvalue E_n, that is, when $I=I_n=(n+1/2)\hbar$, then the denominator $\cos(\pi I/\hbar)$ vanishes, giving the expected pole in the Green's function. In this case we may replace E by $E+i\epsilon$ to obtain a finite result, in which case the action $I=I_n$ is replaced by $I_n+i\epsilon/\omega$, where $\omega=\partial E/\partial I$ is the frequency of the classical motion at action I_n.

In the case of kinetic-plus-potential Hamiltonians, $\partial^2 S(x_i,x,I)/\partial x\partial I=\partial p(x)/\partial I=m\omega/p(x)$, where $x_i=x_0$ or x_1, so the prefactor in Eq. (2.8) can be replaced by

$$-\frac{2m}{\hbar\sqrt{p(x)p(y)}}=-\frac{2}{\hbar\omega}\left[\frac{\partial^2 S(x_0,x,I)}{\partial x\partial I}\frac{\partial^2 S(x_1,y,I)}{\partial y\partial I}\right]^{1/2}=-\frac{\pi}{\hbar\omega}A(x,I)A(y,I), \tag{2.9}$$

where the final expression serves to define the amplitude factors $A(x,I)$, $A(y,I)$. With this substitution (that is, with the ampltitudes expressed in terms of the actions), Eq. (2.8) is actually valid for any one-dimensional, time-reversal invariant Hamiltonian satisfying the stated assumptions on the topology of the orbits in phase space. Moreover, when we extract the residue of (2.8) at the pole $E=E_n$, we find the expected semiclassical eigenfunctions,

$$\psi_n(x)=A(x,I_n)\cos[S(x_0,x,I_n)-\pi/4]. \tag{2.10}$$

This expression for the eigenfunctions may be analytically continued to values of I or E other than the quantized values, but the result does not decay exponentially in the classically forbidden region. It is for this reason that we do not simply use these semiclassical eigenfunctions in Eq. (2.1). In contrast, the Green's function decays exponentially outside the classically allowed regions for all values of E.

Now we replace E by $E+i\epsilon$ in Eq. (2.8) and take the imaginary part, as in Eq. (2.3). Only the factor $1/\cos(\pi I/\hbar)$ gives a nonzero contribution, according to the formula, $\lim_{y\to 0}\mathrm{Im}[1/(x+iy)]=-\pi\delta(x)$. Summing the contributions from the poles, we have

$$-\frac{1}{\pi}\lim_{\epsilon\to 0}\mathrm{Im}\frac{1}{\cos[\pi I(E+i\epsilon)/\hbar]}=-\sum_{n=0}^{\infty}(-1)^n\frac{\hbar\omega}{\pi}\delta(E-E_n)=-\frac{\hbar}{\pi}\sum_{n=0}^{\infty}(-1)^n\delta(I-I_n), \tag{2.11}$$

and

$$\langle x|\,\delta(E-H)\,|y\rangle=\frac{1}{\omega}A(x,I)A(y,I)\sum_{n=0}^{\infty}(-1)^n\delta(I-I_n)F_0(y,I)F_1(x,I), \tag{2.12}$$

where for now we consider only the case $x>y$ and where

$$F_0(y,I)=\cos[S(x_0,y,I)/\hbar-\pi/4]=\cos[S(y,I)/\hbar-\pi/4],$$
$$F_1(x,I)=\cos[S(x_1,x,I)/\hbar+\pi/4]=\cos[S(x,I)/\hbar-\pi I/\hbar+\pi/4]. \tag{2.13}$$

Here and henceforth we write simply $S(x,I)$ for $S(x_0,x,I)$, that is, the left turning point is taken as the origin of the action unless otherwise specified. We have also used $S(x_0,x_1,I)=\pi I$. We recall that we have assumed that x and y are in the classically allowed region for the classical orbit of action I. The δ-functions in Eq. (2.12) suggest that we replace I in F_0 and F_1 in that equation by I_n, but we must worry that the given x and y will not be in the classically allowed regions for all values of I_n. In particular, since the orbits shrink as I decreases, we may in general expect x and y to lie outside the classically allowed region for some values of I_n less than I. We fix this worry by regarding Eq. (2.13) as the definitions of F_0, F_1 only when x and y are in the classically allowed regions for the given I; otherwise they are to be replaced by the corresponding exponentially decaying semiclassical formulas (which we do not write down). With this understanding, I can be freely exchanged with I_n in F_0 and F_1 in Eq. (2.12).

Next we argue that the sum in Eq. (2.12) can be extended downward to $n=-\infty$, since the corresponding actions represent complex classical orbits of energy less that the energy at the bottom of the well. These are all in the classically forbidden region (in energy), and the corresponding semiclassical wave functions are exponentially small. With this change we may use a version of the Poisson sum formula to write

$$\sum_{n\in\mathbb{Z}}(-1)^n\delta(I-I_n)=\frac{1}{\hbar}\sum_{n\in\mathbb{Z}}(-1)^n\delta(\nu-n)=\frac{1}{\hbar}\sum_{k\in\mathbb{Z}}e^{i\pi\nu(2k+1)}, \tag{2.14}$$

where we have written

$$I=(\nu+1/2)\hbar, \tag{2.15}$$

effectively making ν a continuous version of the quantum number n.

The use of the Poisson sum formula converts expression (2.12) into an orbit sum, much as in Gutzwiller's work,[37–40] that is, the sum can be reorganized into a sum over classical orbits of energy E that connect initial point y and final point x in positive time. The orbits are not periodic orbits, as in Gutzwiller's work, because we are not taking the trace, but they are composed of four distinct finite orbits connecting y to x, to which an arbitrary number of periodic orbits are glued. Indeed, we could have derived the resulting expression from Gutzwiller's theory rather than working through the semiclassical expressions for the Green's function directly. We preferred the latter procedure, however, because in parallel studies we are interested in tunneling processes, for which the periodic orbit approach is more difficult.

We now carry out the integral on Eq. (2.12) as in Eq. (2.4), where the upper limit E satisfies $E_{N-1}<E<E_N$, that is, $I_{N-1}<I<I_N$ or $N-1<\nu<N$. We also change the variable of integration to ν, using

$$\int_{-\infty}^{E}\frac{dE'}{\hbar\omega}=\int_{-\infty}^{\nu}d\nu'. \tag{2.16}$$

The product of the two cosine factors gives four terms when written in terms of complex exponentials, which we express in terms of ν. For example, one of these four terms is

$$T_1=\frac{1}{4}\sum_{k\in\mathbb{Z}}\int_{-\infty}^{\nu}d\nu'\,A(x,I')A(y,I')e^{i[2\pi k\nu'+S(y,I')/\hbar+S(x,I')/\hbar-\pi/2]}. \tag{2.17}$$

By integrating the exponential by parts, an asymptotic series in $\hbar$ is generated, of which we keep just the first term. The integrand is considered to vanish at the lower limit of integration, which is deep in the classically forbidden region. For example, for the first term this gives

$$T_1 = -\frac{1}{4} A(x,I)A(y,I) e^{i[S(x,I)+S(y,I)]/\hbar} \sum_{k\in\mathbb{Z}} \frac{e^{2\pi i k\nu}}{\theta(x,I)+\theta(y,I)+2\pi k}, \tag{2.18}$$

where $\theta = \partial S/\partial I$ is the classical angle variable, here measured with respect to the left turning point. Next, the Fourier series in this expression can be summed,

$$\sum_{k\in\mathbb{Z}} \frac{e^{2\pi i k\nu}}{\theta(x,I)+\theta(y,I)+2\pi k} = i \frac{e^{-i(\theta_x+\theta_y)\,\mathrm{frac}\,\nu}}{1-e^{-i(\theta_x+\theta_y)}}, \tag{2.19}$$

where $\theta_x = \theta(x,I)$, $\theta_y = \theta(y,I)$, and then exponents may be combined according to

$$\frac{S(x,I)}{\hbar} - \theta(x,I)\,\mathrm{frac}\,\nu = \frac{S(x,I_{N-1})}{\hbar} + O(\hbar), \tag{2.20}$$

where we use Eq. (2.15) and $\nu = N-1+\mathrm{frac}\,\nu$. Thus we obtain

$$T_1 = -\frac{i}{4} A(x,I)A(y,I) \frac{e^{i[S_{N-1}(x)+S_{N-1}(y)]/\hbar}}{1-e^{-i(\theta_x+\theta_y)}}, \tag{2.21}$$

where $S_{N-1}(x) = S(x,I_{N-1})$, etc. The actions I in the amplitude factors or in the denominator can be replaced by either I_{N-1} or I_N with only $O(\hbar)$ errors (which we are neglecting).

Treating the other three terms similarly, we obtain

$$\sum_{n=0}^{N-1} \psi_n(x)\psi_n(y) = \frac{1}{4} A(x,I)A(y,I) \times \left\{ \frac{e^{i[S_{N-1}(x)+S_{N-1}(y)]/\hbar - i\pi/2}}{1-e^{-i(\theta_x+\theta_y)}} + \frac{e^{i[S_{N-1}(y)-S_{N-1}(x)]/\hbar}}{1-e^{-i(\theta_y-\theta_x)}} + \text{c.c.} \right\}. \tag{2.22}$$

By combining denominators this can be transformed into

$$\frac{A(x,I)A(y,I)}{8[\cos\theta(y,I)-\cos\theta(x,I)]} \{ e^{i[S_{N-1}(x)+S_N(y)]/\hbar - i\pi/2} - e^{i[S_N(x)+S_{N-1}(y)]/\hbar - i\pi/2} + e^{i[S_N(y)-S_{N-1}(x)]/\hbar} - e^{i[S_{N-1}(y)-S_N(x)]/\hbar} + \text{c.c} \}, \tag{2.23}$$

where we have used $S_{N-1}(x)/\hbar + \theta(x,I) = S_N(x)/\hbar + O(\hbar)$, etc. This in turn can be written as

$$\frac{A(x)A(y)}{2[\cos\theta(x,I)-\cos\theta(y,I)]} \{ \cos[S_N(x)/\hbar - \pi/4]\cos[S_{N-1}(y)/\hbar - \pi/4] - \cos[S_{N-1}(x)/\hbar - \pi/4]\cos[S_N(y)/\hbar - \pi/4] \}. \tag{2.24}$$

Finally, using Eq. (2.10), we find

$$\sum_{n=0}^{N-1} \psi_n(x)\psi_n(y) = \frac{1}{2} \frac{\psi_N(x)\psi_{N-1}(y) - \psi_{N-1}(x)\psi_N(y)}{\cos\theta(x,I)-\cos\theta(y,I)}. \tag{2.25}$$

This is the semiclassical Darboux–Christoffel formula, and it is one of the main results of this paper. The derivation was carried out for the case $x>y$, but the case $x<y$ gives the same result. The formula has corrections of order $\hbar$, or, equivalently, $1/N$. Within corrections of this order, the action I in the denominator can be replaced by I_{N-1} or I_N or anything in between. This semiclassical approximation may be compared to its (exact) counterpart, Eq. (1.1), for the case of orthogonal polynomials.

III. DISCUSSION AND LIMITING CASES

A simple limit of Eq. (2.25) is $y \to x$, which produces the total particle density of a system of N fermions at zero temeprature. To leading order in $\hbar$, this turns out to be

$$\sum_{n=0}^{N-1} |\psi_n(x)|^2 = \frac{p(x,I_N)}{\pi\hbar}. \tag{3.1}$$

To leading order in $\hbar$, this is the classical result, since a uniform distrubition of N particles in phase space out to orbit I_N produces a particle density in configuration space that is $N_p(x,I_N)/(\pi I_N)$, and since $I_N = (N+1/2)\hbar$. The 1/2 is not accounted for in this calculation, since it is lost in the higher order terms in Eq. (2.25) that we have not computed.

Equation (2.25) can also be used to construct approximate LM/DVR functions in the same way as the exact Darboux–Christoffel formula. That is, let the subspace $\mathcal{S}$ be defined by the first N eigenfunctions $\{\psi_n(x), n=0,\ldots,N-1\}$ of H, let P_N be the projector onto $\mathcal{S}$, and let the grid points $\{x_\alpha\}$ be the zeroes of $\psi_N(x)$. Then, to within errors of order $\hbar$, the projected δ-functions are

$$\Delta_\alpha(x) = \frac{1}{2}\,\frac{\psi_N(x)\psi_{N-1}(x_\alpha)}{\cos\theta(x,I) - \cos\theta_\alpha}, \tag{3.2}$$

where $\theta_\alpha = \theta(x_\alpha, I)$. These functions vanish at each others' grid points but not at their own, that is, they satisfy Eq. (1.4), to within errors of order $\hbar$. In the semiclassical approximation, the roots of $\psi_N(x)$ occur at

$$S(x_\alpha, I_N) = (\alpha + 3/4)\,\pi\hbar. \tag{3.3}$$

By taking the limit $x \to x_\alpha$ in Eq. (3.2) and using Eq. (2.10) we obtain the normalization,

$$K_\alpha = \frac{p(x_\alpha, I_N)}{\pi\hbar}, \tag{3.4}$$

where $p = \partial S/\partial x$. Notice that $1/K_\alpha$ is approximately the spacing between zeros of $\psi_N(x)$ at $x = x_\alpha$. Finally, we obtain the normalized (and approximately orthonormal) LM/DVR functions,

$$F_\alpha(x) = (-1)^\alpha \sin\theta_\alpha \sqrt{\frac{\hbar}{2p_\alpha}\,\frac{\partial^2 S(x_\alpha, I_N)}{\partial x\,\partial I}}\,\frac{\psi_N(x)}{\cos\theta(x,I_N) - \cos\theta_\alpha}. \tag{3.5}$$

The function $F_\alpha(x)$ has a main lobe centered on the grid point x_α, with a height of order $\hbar^{-1/2}$. Near this grid point, the function behaves like a sinc function, as we see if we write $x = x_\alpha + \xi$ in Eq. (3.5) and expand to first order in ξ. This gives

$$F_\alpha(x_\alpha + \xi) = \frac{\sqrt{a}}{\pi}\,\frac{\sin(\pi\xi/a)}{\xi}, \tag{3.6}$$

where $a = \pi\hbar/p_\alpha$ is the local distance between the roots of $\psi_N(x)$. Sinc functions are a standard example of one-dimensional LM/DVR functions.[4,5]

The semiclassical Darboux–Christoffel formula, Eq. (2.25), may be tested in some cases for which the answer is exactly known. For example, in the case of the harmonic oscillator $H = p^2/2 + x^2/2$ we have $x = -\sqrt{2I}\cos\theta$ and $a_N = (N/2)^{1/2}$ (in units where $m = \hbar = \omega = 1$), so if the denominator in Eq. (2.25) is evaluated at $I = I_N = N + 1/2$, then the semiclassical and exact Darboux–Christoffel formulas do agree to order $1/N$. In fact, if the denominator is evaluated at $I = N$ instead of $I = N + 1/2$, the correct value of a_N comes out exactly. This amounts to using an

orbit half-way between the $(N-1)$st and Nth quantizing orbits for evaluating the denominator (the average of the two numbers which appear in the numerator). This may be the best choice for evaluating the denominator in all cases.

The semiclassical Darboux–Christoffel formula, Eq. (2.25), can be generalized to the case of the continuous spectrum. Let us hold the energy E and the left turning point x_0 fixed, but otherwise deform the potential well so that the right turning point recedes to infinity. The bottom of the potential well may flatten out at some finite value of energy below E, or it may drop down to $-\infty$. In any case, the spectrum becomes continuous in this limit, and the eigenstates become scattering states that come in from the right and bounce off the left wall of the potential. Then it is easy to take the corresponding limit in Eq. (2.25). If we denote the continuum eigenstates by $\psi(x,E) = \langle x|E\rangle$ and normalize them according to $\langle E|E'\rangle = \delta(E-E')$, then the semiclassical Darboux–Christoffel formula turns out to be

$$\langle x|P|y\rangle = \hbar^2 \frac{\psi(x,E)[\partial\psi(y,E)/\partial E] - [\partial\psi(x,E)/\partial E]\psi(y,E)}{T(x,E)^2 - T(y,E)^2}, \tag{3.7}$$

where $T(x,E)$ is the time required for a classical particle with energy E to go from the (left) turning point to position x, and where the projection operator is defined by

$$P = \int_{E_0}^{E} \mathrm{d}E' |E'\rangle\langle E'|. \tag{3.8}$$

Here E_0 is the energy at the bottom of the well.

Equation (3.7) is exact in the case of Bessel and Airy functions, if the wave functions in the numerator are interpreted as the exact wave functions and not their semiclassical approximations. Bessel functions of integer order are free particle solutions in the plane of a definite angular momentum, projected onto the radial half-line. The LM/DVR functions associated with Bessel functions have been explored in Ref. 6. The radial Hamiltonian has the form,

$$H = \frac{p_r^2}{2M} + \frac{m^2\hbar^2 - 1/4}{2Mr^2}, \tag{3.9}$$

where M is the mass and m the angular momentum quantum number, and where (r,p_r) play the role of (x,p) in the above-presented discussion. For $E>0$, the potential (actually only the centrifugal potential) has one (left) turning point, exactly as described in the limit leading to Eq. (3.7). The quantity $T(r,E)$ is the time required for a classical particle of energy E to travel from the turning point r_0 to point r. Computing this is a problem in classical mechanics that is most easily solved by viewing the (free) particle motion in the plane. The radial turning point r_0 is the minimum radius for the straight line orbit, and the distance r from the origin at later time t is $\sqrt{r_0^2 + v^2t^2}$, where v is the velocity. Thus $T(r,E) = \sqrt{r^2 - r_0^2}/v$, and the denominator in Eq. (3.7) is

$$T(r,E)^2 - T(r',E)^2 = (r^2 - r'^2)/v^2. \tag{3.10}$$

In fact, Bessel functions satisfy the identity

$$\int_0^K k\,\mathrm{d}k\, J_\nu(kr)J_\nu(kr') = \frac{K}{r^2 - r'^2}[r'J_\nu(Kr)J'_\nu(Kr') - rJ_\nu(Kr')J'_\nu(Kr)], \tag{3.11}$$

where K is the wave number corresponding to energy $E = \hbar^2K^2/2M$. When details such as the continuum normalization are worked out, Eq. (3.11) is seen to agree precisely with Eq. (3.7). In this case the potential well flattens out at $E=0$, hence the lower limit on the integral.

Similarly, in the case of the Airy functions the Hamiltonian (in dimensionless units) is $H = p^2 + x$, so that the potential has only one turning point and all energy eigenfunctions are in the continuum. The LM/DVR functions associated with Airy functions were studied in Ref. 6. Here it

suffices to take $E=0$ due to the translational invariance of the problem, and the energy at the bottom of the well is $E=-\infty$. The turning point (in this case, the right one) is at $x=0$, and the time required to reach position $-x$ under the classical motion is proportional to $\sqrt{-x}$ (this is motion in a uniform gravitational field). Thus we expect the denominator in the Darboux–Christoffel formula to be proportional to $x-y$. In fact, Airy functions satisfy the identity

$$\int_{-\infty}^{0} \mathrm{d}E\ \mathrm{Ai}(x-E)\mathrm{Ai}(y-E)=\frac{\mathrm{Ai}(x)\mathrm{Ai}'(y)-\mathrm{Ai}'(x)\mathrm{Ai}(y)}{x-y}, \tag{3.12}$$

which is proved in Ref. 6. Once again, when details such as the normalization and the fact that we are working with a right turning point are taken into account, this identity is seen to be an exact version of Eq. (3.7).

Finally, we report on a numerical test of the semiclassical Darboux–Christoffel formula (2.25). We used the potential $V(x)=x^4$, for which the eigenfunctions cannot be expressed in terms of orthogonal polynomials. We computed numerically the eigenfunctions $\psi_n(x)$ in this potential for different values of $\hbar$, carrying the calculation out to the first eigenfunction $n=N$ whose energy E_N exceeds 10. We then computed the projected δ-functions, $\Delta_\alpha(x)=\langle x|P_N|x_\alpha\rangle$, using the numerically computed roots x_α of the $\psi_N(x)$ and the exact expression (2.1) for the projection operator (not the semiclassical approximation). Then we computed the exact norms of these functions using $K_\alpha=\Delta_\alpha(x_\alpha)$ [not the semiclassical approximation (3.4)], and from these the functions $F_\alpha(x)=\Delta_\alpha(x)/\sqrt{K_\alpha}$. Thus, the overlap matrix of the functions $\{F_\alpha(x)\}$ is given by

$$\langle F_\alpha|F_\beta\rangle=\frac{\Delta_\beta(x_\alpha)}{\sqrt{K_\alpha K_\beta}}, \tag{3.13}$$

and $\langle F_\alpha|F_\alpha\rangle=1$ exactly. As for the off-diagonal elements, the semiclassical Darboux–Christoffel formula, Eq. (2.25), predicts that $\Delta_\alpha(x_\beta)=O(\hbar)$, and Eq. (3.4) predicts that $K_\alpha=O(1/\hbar)$. Thus, if the semiclassical expressions we have derived are correct, we expect

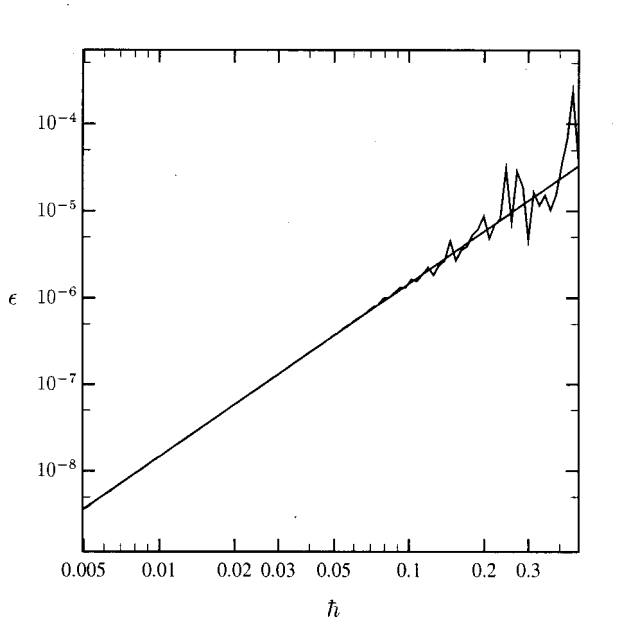

FIG. 1. The rms off-diagonal element in one column of the matrix $\langle F_\alpha|F_\beta\rangle$ is plotted as a function of $\hbar$. The column chosen was the one for which the root x_α was closest to $x=0$. Also plotted is a straight line of slope 2, passing through the data point at the smallest value of $\hbar$. The theory predicts a slope of 2, which is well verified by the data.

$$\langle F_\alpha | F_\beta \rangle = \begin{cases} 1, & \alpha = \beta \\ O(\hbar^2), & \alpha \neq \beta. \end{cases} \tag{3.14}$$

We tested these predictions for the off-diagonal elements by computing the matrix $\langle F_\alpha | F_\beta \rangle$ for various values of $\hbar$. We found that the off-diagonal elements were all approximately of the same order of magnitude, and all much less than the diagonal elements (which are exactly unity) when $\hbar$ is small. Figure 1 contains a log–log plot of the rms value of the off-diagonal elements of this matrix in a central column (near $x=0$), as a function of $\hbar$. According to Eq. (3.14), this value should scale as $\hbar^2$, that is, the curve should be a straight line with a slope of 2 on the plot. Also shown in Fig. 1 is a straight line passing through the point at the smallest value of $\hbar$ with a slope of exactly 2. It will be seen that this straight line provides a good fit to the data, confirming the predicted dependence of the off-diagonal elements of the matix on $\hbar$.

There is the question of whether the approximate LM/DVR functions that are constructed by the methods we have described can be useful in practice. In this regard we point out the work of Lado,[45] Johnson,[46] and Lemoine,[26] in which approximate LM/DVR functions are constructed from the radial eigenfunctions of a particle in a spherical box. These eigenfunctions are not orthogonal polynomials (times the square root of any weighting function), so LM/DVR functions in the usual sense do not exist. But these authors note that a certain matrix, which in the language of this paper is $U_{n\alpha} = \langle \psi_n | F_\alpha \rangle$, is approximately orthogonal, a fact that is equivalent to the approximate orthonormality of the functions $F_\alpha(x)$ as indicated by Eq. (3.14). The functions $F_\alpha(x)$ then turn out to be useful in an approximately unitary, discretized version of the Hankel transform.

IV. CONCLUSIONS

In summary, we have explained the importance of the Darboux–Christoffel formula for the theory of ''Lagrangian mesh'' or ''discrete variable representation'' (LM/DVR) basis sets and we have outlined a semiclassical area rule that suggests that a semiclassical generalization of the Darboux–Christoffel formula should exist. We have then used Green's functions and semiclassical techniques to derive that generalization, which involves the eigenfunctions of one-dimensional, time-reversal invariant systems for which tunneling can be ignored. The result differs in part from the exact Darboux–Christoffel formula by replacing the $x-y$ denominator by $\cos\theta(x) - \cos\theta(y)$, in which θ is the classical angle variable, measured with respect to the left turning point. We have shown how semiclassical approximations to LM/DVR basis functions can be created. We have also taken the continuum limit of the semiclassical Darboux–Christoffel formula, and outlined how it is equivalent to certain exact relations that hold for Bessel and Airy functions. Finally, we have carried out numerical calculations that confirm the expected $\hbar$ dependence of certain quantities (the off-diagonal elements of the overlap matrix of the approximate LM/DVR functions).

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The two-dimensional hydrogen atom revisited

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The bound-state energy eigenvalues for the two-dimensional Kepler problem are found to be degenerate. This ''accidental'' degeneracy is due to the existence of a two-dimensional analog of the quantum-mechanical Runge–Lenz vector. Reformulating the problem in momentum space leads to an integral form of the Schrödinger equation. This equation is solved by projecting the two-dimensional momentum space onto the surface of a three-dimensional sphere. The eigenfunctions are then expanded in terms of spherical harmonics, and this leads to an integral relation in terms of special functions which has not previously been tabulated. The dynamical symmetry of the problem is also considered, and it is shown that the two components of the Runge–Lenz vector in real space correspond to the generators of infinitesimal rotations about the respective coordinate axes in momentum space.
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I. INTRODUCTION

A semiconductor quantum well under illumination is a quasi-two-dimensional system, in which photoexcited electrons and holes are essentially confined to a plane. The mutual Coulomb interaction leads to electron–hole bound states known as excitons, which are extremely important for the optical properties of the quantum well. The relative in-plane motion of the electron and hole can be described by a two-dimensional Schrödinger equation for a single particle with a reduced mass. This is a physical realization of the two-dimensional hydrogenic problem, which originated as a purely theoretical construction.[1] An important similarity with the three-dimensional hydrogen atom is the ''accidental'' degeneracy of the bound-state energy levels. This degeneracy is due to the existence of the quantum-mechanical Runge–Lenz vector, first introduced by Pauli[2] in three dimensions, and indicates the presence of a dynamical symmetry of the system.

The most important study relating to the hidden symmetry of the hydrogen atom was that by Fock in 1935.[3] He considered the Schrödinger equation in momentum space, which led to an integral equation. Considering negative-energy (bound-state) solutions, he projected the three-dimensional momentum space onto the surface of a four-dimensional hypersphere. After a suitable transformation of the wavefunction, the resulting integral equation was seen to be invariant under rotations in four-dimensional momentum space. Fock deduced that the dynamical symmetry of the hydrogen atom is described by the four-dimensional rotation group SO(4), which contains the geometrical symmetry SO(3) as a subgroup. He related this hidden symmetry to the observed degeneracy of the energy eigenvalues.

Shortly afterwards, Bargmann[4] made the connection between Pauli's quantum mechanical Runge–Lenz vector and Fock's discovery of invariance under rotations in four-dimensional momentum space. Fock's method was also extended by Alliluev[5] to the case of d dimensions ($d \geqslant 2$). A comprehensive review concerning the symmetry of the hydrogen atom was later given by Bander and Itzykson,[6,7] including a detailed group-theoretical treatment and extension to scattering states.

Improvements in semiconductor growth techniques over the subsequent decades, which enabled the manufacture of effectively two-dimensional structures, led to a resurgence of interest in

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the two-dimensional hydrogen atom. The Runge–Lenz vector for this case was defined for the first time,[8] and real-space solutions of the Schrödinger equation were applied to problems of atomic physics in two dimensions.[9]

Recent studies have focused on diverse aspects of the hydrogenic problem. The *d*-dimensional case has been reconsidered, leading to a generalized Runge–Lenz vector (see Ref. 10 and references therein). The algebraic basis of the dynamical symmetry has also been given a thorough mathematical treatment.[11,12]

In the present work we return to the two-dimensional problem, and use the method of Fock to obtain a new integral relation in terms of special functions. The dynamical symmetry of the system is also considered, and a new interpretation of the two-dimensional Runge–Lenz vector is presented.

II. PROBLEM FORMULATION

A. Preliminaries

The relative in-plane motion of an electron and hole, with effective masses m_e and m_h, respectively, may be treated as that of a single particle with reduced mass $\mu = m_e m_h/(m_e+m_h)$ and energy E, moving in a Coulomb potential $V(\rho)$. The wavefunction of the particle satisfies the stationary Schrödinger equation

$$\hat{H}\Psi(\boldsymbol{\rho}) = \left[-\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} + V(\rho)\right]\Psi(\boldsymbol{\rho}) = E\Psi(\boldsymbol{\rho}), \tag{1}$$

where (ρ,ϕ) are plane polar coordinates. Note that excitonic Rydberg units are used throughout this article, which leads to a potential of the form $V(\rho) = -2/\rho$.

The eigenfunctions of Eq. (1) are derived in Appendix A. It is well known that the bound-state energy levels are of the form[1]

$$E = -\frac{1}{(n+\frac{1}{2})^2}, \quad n = 0,1,2,..., \tag{2}$$

where n is the principal quantum number. Notably, Eq. (2) does not contain explicitly the azimuthal quantum number m, which enters the radial equation [see Appendix A, Eq. (A4)]. Each energy level is $(2n+1)$-fold degenerate, the so-called accidental degeneracy.

It is convenient to introduce a vector operator corresponding to the z-projection of the angular momentum, $\hat{\mathbf{L}}_z = \mathbf{e}_z\hat{L}_z$, where $\mathbf{e}_z$ is a unit vector normal to the plane of motion of the electron and hole. We now introduce the two-dimensional analog of the quantum-mechanical Runge–Lenz vector as the dimensionless operator

$$\hat{\mathbf{A}} = (\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z - \hat{\mathbf{L}}_z\times\hat{\mathbf{q}}) - \frac{2}{\rho}\boldsymbol{\rho}, \tag{3}$$

where $\hat{\mathbf{q}} = -i\nabla$ is the momentum operator. Note that $\hat{\mathbf{A}}$ lies in the plane and has Cartesian components $\hat{A}_x$ and $\hat{A}_y$.

$\hat{L}_z$, $\hat{A}_x$, and $\hat{A}_y$ represent conserved quantities and therefore commute with the Hamiltonian:

$$[\hat{H},\hat{L}_z] = [\hat{H},\hat{A}_x] = [\hat{H},\hat{A}_y] = 0. \tag{4}$$

They also satisfy the following commutation relations:

$$[\hat{L}_z,\hat{A}_x] = i\hat{A}_y, \tag{5}$$

$$[\hat{L}_z,\hat{A}_y] = -i\hat{A}_x, \tag{6}$$

$$[\hat{A}_x,\hat{A}_y]=-4i\hat{L}_z\hat{H}. \tag{7}$$

B. Derivation of energy eigenvalues from $\hat{A}$

The existence of the noncommuting operators $\hat{A}_x$ and $\hat{A}_y$, representing conserved physical quantities, implies that the Runge–Lenz vector is related to the accidental degeneracy of the energy levels in two dimensions.[13] We now present a simple interpretation of the hidden symmetry underlying this degeneracy.

For eigenfunctions of the Hamiltonian we can replace $\hat{H}$ by the energy E, and defining

$$\hat{\mathbf{A}}'=\frac{\hat{\mathbf{A}}}{2\sqrt{-E}}, \tag{8}$$

we obtain the new commutation relations:

$$[\hat{L}_z,\hat{A}'_x]=i\hat{A}'_y, \tag{9}$$

$$[\hat{L}_z,\hat{A}'_y]=-i\hat{A}'_x, \tag{10}$$

$$[\hat{A}'_x,\hat{A}'_y]=i\hat{L}_z. \tag{11}$$

If we now construct a three-dimensional vector operator

$$\hat{\mathbf{J}}=\hat{\mathbf{A}}'+\hat{\mathbf{L}}_z, \tag{12}$$

then the components of $\hat{\mathbf{J}}$ satisfy the commutation rules of ordinary angular momentum:

$$[\hat{J}_j,\hat{J}_k]=i\epsilon_{jkl}\hat{J}_l, \tag{13}$$

where ϵ_{jkl} is the Levi-Civita symbol.

Noting that $\hat{\mathbf{A}}'\cdot\hat{\mathbf{L}}_z=\hat{\mathbf{L}}_z\cdot\hat{\mathbf{A}}'=0$, we have

$$\hat{\mathbf{J}}^2=(\hat{\mathbf{A}}'+\hat{\mathbf{L}}_z)^2=\hat{\mathbf{A}}'^2+\hat{\mathbf{L}}_z^2, \tag{14}$$

where the operator $\hat{\mathbf{J}}^2$ has eigenvalues $j(j+1)$ and commutes with the Hamiltonian.

We now make use of a special expression relating $\hat{\mathbf{A}}^2$ and $\hat{\mathbf{L}}_z^2$, the derivation of which is given in Appendix B:

$$\hat{\mathbf{A}}^2=\hat{H}(4\hat{\mathbf{L}}_z^2+1)+4. \tag{15}$$

Substituting in Eq. (14) and again replacing $\hat{H}$ with E, we obtain

$$\hat{\mathbf{J}}^2=-\frac{1}{4E}[E(4\hat{\mathbf{L}}_z^2+1)+4]+\hat{\mathbf{L}}_z^2. \tag{16}$$

Because $[\hat{H},\hat{\mathbf{J}}^2]=0$, an eigenfunction of the Hamiltonian will also be an eigenfunction of $\hat{\mathbf{J}}^2$. Operating with both sides of Eq. (16) on an eigenfunction of the Hamiltonian, we obtain for the eigenvalues of $\hat{\mathbf{J}}^2$:

$$j(j+1)=-\left(\frac{1}{4}+\frac{1}{E}\right). \tag{17}$$

Rearranging, and identifying j with the principal quantum number n, we obtain the correct expression for the energy eigenvalues:

$$E=-\frac{1}{(n+\frac{1}{2})^2}, \quad n=0,1,2,\ldots. \tag{18}$$

Note that the z-component of $\hat{\mathbf{J}}$ is simply $\hat{L}_z$. Recalling that the eigenvalues of $\hat{L}_z$ are denoted by m, there are $(2j+1)$ values of m for a given j. However, as $j=n$, we see that there are $(2n+1)$ values of m for a given energy, which corresponds to the observed $(2n+1)$-fold degeneracy.

III. FOCK'S METHOD IN TWO DIMENSIONS

A. Stereographic projection

The method of Fock,[3] in which a three-dimensional momentum space is projected onto the surface of a four-dimensional hypersphere, may be applied to our two-dimensional problem. We begin by defining a pair of two-dimensional Fourier transforms between real space and momentum space:

$$\Phi(\mathbf{q})=\int \Psi(\boldsymbol{\rho})e^{i\mathbf{q}\cdot\boldsymbol{\rho}}\,d\boldsymbol{\rho}, \tag{19}$$

$$\Psi(\boldsymbol{\rho})=\frac{1}{(2\pi)^2}\int \Phi(\mathbf{q})e^{-i\mathbf{q}\cdot\boldsymbol{\rho}}\,d\mathbf{q}. \tag{20}$$

We shall restrict our interest to bound states, and hence the energy $E=-q_0^2$ will be negative.

Substitution of Eq. (20) in Eq. (1) yields the following integral equation for $\Phi(\mathbf{q})$:

$$(q^2+q_0^2)\Phi(\mathbf{q})=\frac{1}{\pi}\int \frac{\Phi(\mathbf{q}')\,d\mathbf{q}'}{|\mathbf{q}-\mathbf{q}'|}. \tag{21}$$

The two-dimensional momentum space is now projected onto the surface of a three-dimensional unit sphere centered at the origin, and so it is natural to scale the in-plane momentum by q_0. Each point on a unit sphere is completely defined by two polar angles, θ and ϕ, and the Cartesian coordinates of a point on the unit sphere are given by

$$u_x=\sin\theta\cos\phi=\frac{2q_0q_x}{q^2+q_0^2}, \tag{22}$$

$$u_y=\sin\theta\sin\phi=\frac{2q_0q_y}{q^2+q_0^2}, \tag{23}$$

$$u_z=\cos\theta=\frac{q^2-q_0^2}{q^2+q_0^2}. \tag{24}$$

An element of surface area on the unit sphere is given by

$$d\Omega=\sin\theta\;d\theta\;d\phi=\left(\frac{2q_0}{q^2+q_0^2}\right)^2 d\mathbf{q}, \tag{25}$$

and the distance between two points transforms as

$$|\mathbf{u}-\mathbf{u}'|=\frac{2q_0}{(q^2+q_0^2)^{1/2}(q'^2+q_0^2)^{1/2}}|\mathbf{q}-\mathbf{q}'|. \tag{26}$$

If the wavefunction on the sphere is expressed as

$$\chi(\mathbf{u})=\frac{1}{\sqrt{q_0}}\left(\frac{q^2+q_0^2}{2q_0}\right)^{3/2}\Phi(\mathbf{q}), \tag{27}$$

then Eq. (21) reduces to the simple form

$$\chi(\mathbf{u})=\frac{1}{2\pi q_0}\int\frac{\chi(\mathbf{u}')\,d\Omega'}{|\mathbf{u}-\mathbf{u}'|}. \tag{28}$$

B. Expansion in spherical harmonics

Any function on a sphere can be expressed in terms of spherical harmonics, so for $\chi(\mathbf{u})$ we have

$$\chi(\mathbf{u})=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}A_{lm}Y_l^m(\theta,\phi), \tag{29}$$

where $Y_l^m(\theta,\phi)$ are basically defined as in Ref. 14:

$$Y_l^m(\theta,\phi)=c_{lm}\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}P_l^{|m|}(\cos\theta)e^{im\phi}, \tag{30}$$

where $P_n^{|m|}(\cos\theta)$ is an associated Legendre function as defined in Ref. 15. The constant c_{lm} is an arbitrary "phase factor." As long as $|c_{lm}|^2=1$ we are free to choose c_{lm}, and for reasons which will become clear we set

$$c_{lm}=(-i)^{|m|}. \tag{31}$$

The kernel of the integral in Eq. (28) can also be expanded in this basis as[16]

$$\frac{1}{|\mathbf{u}-\mathbf{u}'|}=\sum_{\lambda=0}^{\infty}\sum_{\mu=-\lambda}^{\lambda}\frac{4\pi}{2\lambda+1}Y_\lambda^\mu(\theta,\phi)Y_\lambda^{\mu*}(\theta',\phi'). \tag{32}$$

Substituting Eqs. (29) and (32) into Eq. (28) we have

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}A_{lm}Y_l^m(\theta,\phi)=\frac{2}{q_0}\sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}\sum_{m_1=-l_1}^{l_1}\sum_{m_2=-l_2}^{l_2}\int\frac{1}{2l_2+1}A_{l_1m_1}Y_{l_1}^{m_1}(\theta',\phi')\times Y_{l_2}^{m_2}(\theta,\phi)Y_{l_2}^{m_2*}(\theta',\phi')\,d\Omega'. \tag{33}$$

We now make use of the orthogonality property of spherical harmonics to reduce Eq. (33) to the following:

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}A_{lm}Y_l^m(\theta,\phi)=\frac{2}{q_0}\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1}\frac{1}{2l_1+1}A_{l_1m_1}Y_{l_1}^{m_1}(\theta,\phi). \tag{34}$$

Multiplying both sides of Eq. (34) by $Y_n^{m'*}(\theta,\phi)$ and integrating over $d\Omega$ gives

$$A_{nm'}=\frac{2}{q_0(2n+1)}A_{nm'}, \tag{35}$$

where we have again used the orthogonality relation for spherical harmonics. The final step is to rearrange for q_0 and identify the index n with the principal quantum number. This enables us to find an expression for the energy in excitonic Rydbergs:

$$E=-q_0^2=-\frac{1}{(n+\frac{1}{2})^2},\quad n=0,1,2,\ldots. \tag{36}$$

This is seen to be identical to Eq. (2).

For a particular value of n, the general solution of Eq. (28) can be expressed as

$$\chi_n(\mathbf{u})=\sum_{m=-n}^{n} A_{nm}Y_n^m(\theta,\phi). \tag{37}$$

Each of the functions entering the sum in Eq. (37) satisfies Eq. (28) separately. So, for each value of n we have $(2n+1)$ linearly independent solutions, and this explains the observed $(2n+1)$-fold degeneracy.

We are free to choose any linear combination of spherical harmonics for our eigenfunctions, but for convenience we simply choose

$$\chi_{nm}(\mathbf{u})=A_{nm}Y_n^m(\theta,\phi). \tag{38}$$

If we also require our eigenfunctions to be normalized as follows:

$$\frac{1}{(2\pi)^2}\int |\chi(\mathbf{u})|^2\,d\Omega=\frac{1}{(2\pi)^2}\int \frac{q^2+q_0^2}{2q_0^2}|\Phi(\mathbf{q})|^2\,d\mathbf{q}=\int |\Psi(\boldsymbol{\rho})|^2\,d\boldsymbol{\rho}=1, \tag{39}$$

then Eq. (38) reduces to

$$\chi_{nm}(\mathbf{u})=2\pi Y_n^m(\theta,\phi). \tag{40}$$

Applying the transformation in Eq. (27), we can obtain an explicit expression for the orthonormal eigenfunctions of Eq. (21):

$$\Phi_{nm}(\mathbf{q})=c_{nm}\sqrt{2\pi\frac{(n-|m|)!}{(n+|m|)!}}\left(\frac{2q_0}{q^2+q_0^2}\right)^{3/2}P_n^{|m|}(\cos\theta)e^{im\phi}, \tag{41}$$

where we have used the fact that $q_0=(n+\frac{1}{2})^{-1}$, and θ and ϕ are defined by Eqs. (22)–(24).

C. New integral relations

To obtain the real-space eigenfunctions $\Psi(\boldsymbol{\rho})$ we make an inverse Fourier transform:

$$\Psi(\boldsymbol{\rho})=\frac{1}{(2\pi)^2}\int \Phi(\mathbf{q})e^{-i\mathbf{q}\cdot\boldsymbol{\rho}}\,d\mathbf{q}=\frac{1}{(2\pi)^2}\int_0^{2\pi}\int_0^{\infty}\Phi(\mathbf{q})e^{-iq\rho\cos\phi'}q\,dq\,d\phi', \tag{42}$$

where ϕ' is the azimuthal angle between the vectors $\boldsymbol{\rho}$ and $\mathbf{q}$. However, if we now substitute Eq. (41) into this expression, we have to be careful with our notation. The angle labeled ϕ in Eq. (41) is actually related to ϕ' via

$$\phi=\phi'+\phi_\rho, \tag{43}$$

where ϕ_ρ is the azimuthal angle of the vector $\boldsymbol{\rho}$, which can be treated as constant for the purposes of our integration.

Taking this into account, the substitution of Eq. (41) into Eq. (42) yields

$$\Psi(\boldsymbol{\rho})=\frac{c_{nm}}{(2\pi)^{3/2}}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}e^{im\phi_\rho}\int_0^{2\pi}\int_0^{\infty}\left(\frac{2q_0}{q^2+q_0^2}\right)^{3/2}P_n^{|m|}(\cos\theta)e^{i(m\phi'-q\rho\cos\phi')}q\,dq\,d\phi'. \tag{44}$$

From Eq. (24) we obtain

$$P_n^{|m|}(\cos\theta)=P_n^{|m|}\left(\frac{q^2-q_0^2}{q^2+q_0^2}\right), \tag{45}$$

and we use the following form of Bessel's integral:[16]

$$\int_0^{2\pi} e^{i(m\phi'-q\rho\cos\phi')}\,d\phi'=2\pi(-i)^m J_m(q\rho), \tag{46}$$

where $J_m(q\rho)$ is a Bessel function of the first kind of order m. Substituting Eqs. (45) and (46) into Eq. (44) leads to

$$\Psi(\boldsymbol{\rho})=\frac{c_{nm}(-i)^m}{\sqrt{2\pi}}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}e^{im\phi_\rho}\int_0^\infty\left(\frac{2q_0}{q^2+q_0^2}\right)^{3/2}P_n^{|m|}\left(\frac{q^2-q_0^2}{q^2+q_0^2}\right)J_m(q\rho)q\,dq. \tag{47}$$

We now make a change of variables, $x=q_0\rho$ and $y=q^2/q_0^2$, so that Eq. (47) becomes

$$\Psi(\boldsymbol{\rho})=c_{nm}(-1)^{n+m}(-i)^m\sqrt{\frac{q_0(n-|m|)!}{\pi(n+|m|)!}}e^{im\phi_\rho}\int_0^\infty P_n^{|m|}\left(\frac{1-y}{1+y}\right)\frac{J_m(x\sqrt{y})}{(1+y)^{3/2}}dy, \tag{48}$$

where we have used the fact that[16]

$$P_n^{|m|}\left(\frac{y-1}{y+1}\right)=(-1)^{n+m}P_n^{|m|}\left(\frac{1-y}{1+y}\right). \tag{49}$$

If we now equate the expression for $\Psi(\boldsymbol{\rho})$ in Eq. (48) with that derived in Appendix A, we obtain the following:

$$c_{nm}(-1)^{n+m}(-i)^m\int_0^\infty P_n^{|m|}\left(\frac{1-y}{1+y}\right)\frac{J_m(x\sqrt{y})}{(1+y)^{3/2}}dy=\frac{(2x)^{|m|}e^{-x}}{n+1/2}L_{n-|m|}^{2|m|}(2x). \tag{50}$$

The value of c_{nm} chosen earlier in Eq. (31) ensures that both sides of Eq. (50) are numerically equal. If we restrict our interest to $m\geqslant 0$, then the relation simplifies to

$$\int_0^\infty P_n^m\left(\frac{1-y}{1+y}\right)\frac{J_m(x\sqrt{y})}{(1+y)^{3/2}}dy=\frac{(-1)^n(2x)^m e^{-x}}{n+1/2}L_{n-m}^{2m}(2x),\quad n,m=0,1,2,\ldots;\ \ m\leqslant n. \tag{51}$$

As far as we can ascertain, this integral relation between special functions has not previously been tabulated. For $n,m=0$ we recover the known integral relation[15]

$$\int_0^\infty\frac{J_0(x\sqrt{y})}{(1+y)^{3/2}}dy=2e^{-x}. \tag{52}$$

IV. DYNAMICAL SYMMETRY

A. Infinitesimal generators

Consider now a vector $\mathbf{u}$ from the origin to a point on the three-dimensional unit sphere defined in Sec. III A. If this vector is rotated through an infinitesimal angle α in the $(u_x u_z)$ plane, we have a new vector

$$\mathbf{u}'=\mathbf{u}+\delta\mathbf{u}, \tag{53}$$

where the components of **u** are given in Eqs. (22)–(24), and

$$\delta\mathbf{u}=\alpha\mathbf{e}_y\times\mathbf{u}. \tag{54}$$

This rotation on the sphere corresponds to a change in the two-dimensional momentum from **q** to **q**′. The Cartesian components of Eq. (53) are then found to be

$$u_x'=\frac{2q_0q_x'}{q'^2+q_0^2}=\frac{2q_0q_x}{q^2+q_0^2}+\alpha\frac{q^2-q_0^2}{q^2+q_0^2}, \tag{55}$$

$$u_y'=\frac{2q_0q_y'}{q'^2+q_0^2}=\frac{2q_0q_y}{q^2+q_0^2}, \tag{56}$$

$$u_z'=\frac{q'^2-q_0^2}{q'^2+q_0^2}=\frac{q^2-q_0^2}{q^2+q_0^2}-\alpha\frac{2q_0q_x}{q^2+q_0^2}, \tag{57}$$

where $q^2=q_x^2+q_y^2$.

After some manipulation we can also find the components of $\delta\mathbf{q}=\mathbf{q}'-\mathbf{q}$:

$$\delta q_x=\alpha\frac{q^2-q_0^2-2q_x^2}{2q_0}, \tag{58}$$

$$\delta q_y=-\alpha\frac{q_xq_y}{q_0}. \tag{59}$$

The corresponding change in $\Phi(\mathbf{q})$ is given by

$$\delta\Phi(\mathbf{q})=\frac{\alpha}{(q^2+q_0^2)^{3/2}}\left(\frac{q^2-q_0^2-2q_x^2}{2q_0}\frac{\partial}{\partial q_x}-\frac{q_xq_y}{q_0}\frac{\partial}{\partial q_y}\right)[(q^2+q_0^2)^{3/2}\Phi(\mathbf{q})]. \tag{60}$$

We can write this as

$$\delta\Phi(\mathbf{q})=-\frac{i}{2q_0}\alpha\hat{\mathcal{A}}_x\Phi(\mathbf{q}), \tag{61}$$

where the infinitesimal generator is given by

$$\hat{\mathcal{A}}_x=\frac{i}{(q^2+q_0^2)^{3/2}}\left[(q^2-q_0^2-2q_x^2)\frac{\partial}{\partial q_x}-2q_xq_y\frac{\partial}{\partial q_y}\right](q^2+q_0^2)^{3/2}. \tag{62}$$

We now make use of the following operator expression in the momentum representation:

$$\hat{\boldsymbol{\rho}}=\mathbf{e}_x\hat{x}+\mathbf{e}_y\hat{y}=i\nabla_q, \tag{63}$$

and the commutation relation

$$[\hat{\boldsymbol{\rho}},f(\mathbf{q})]=i\nabla_q f, \tag{64}$$

to derive a more compact expression for $\hat{\mathcal{A}}_x$:

$$\hat{\mathcal{A}}_x=(q^2-q_0^2)\hat{x}-2q_x(\mathbf{q}\cdot\hat{\boldsymbol{\rho}})-3iq_x. \tag{65}$$

By considering an infinitesimal rotation in the (u_yu_z) plane we can obtain a similar expression for $\hat{\mathcal{A}}_y$:

$$\hat{\mathcal{A}}_y=(q^2-q_0^2)\hat{y}-2q_y(\mathbf{q}\cdot\hat{\boldsymbol{\rho}})-3iq_y. \tag{66}$$

These expressions operate on a particular energy eigenfunction with eigenvalue $-q_0^2$. If we move the constant $-q_0^2$ to the right and replace it with the Hamiltonian in momentum space, $\hat{\mathcal{H}}$,

$$\hat{\mathcal{A}}_x=q^2\hat{x}+\hat{x}\hat{\mathcal{H}}-2q_x(\mathbf{q}\cdot\hat{\boldsymbol{\rho}})-3iq_x, \tag{67}$$

$$\hat{\mathcal{A}}_y=q^2\hat{y}+\hat{y}\hat{\mathcal{H}}-2q_y(\mathbf{q}\cdot\hat{\boldsymbol{\rho}})-3iq_y, \tag{68}$$

then $\hat{\mathcal{A}}_x$ and $\hat{\mathcal{A}}_y$ can operate on any linear combination of eigenfunctions.

B. Relation to Runge–Lenz vector

Recall the definition of the two-dimensional Runge–Lenz vector in real space:

$$\hat{\mathbf{A}}=(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z-\hat{\mathbf{L}}_z\times\hat{\mathbf{q}})-\frac{2}{\rho}\boldsymbol{\rho}. \tag{69}$$

Using $\hat{\mathbf{L}}_z=\boldsymbol{\rho}\times\hat{\mathbf{q}}$, and the following identity for the triple product of three vectors:

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c})=(\mathbf{a}\cdot\mathbf{c})\mathbf{b}-(\mathbf{a}\cdot\mathbf{b})\mathbf{c}, \tag{70}$$

we can apply the commutation relation $[\boldsymbol{\rho},\hat{\mathbf{q}}]=i$ to rewrite Eq. (69) in the form:

$$\hat{\mathbf{A}}=\hat{\mathbf{q}}^2\boldsymbol{\rho}+\boldsymbol{\rho}\left(\hat{\mathbf{q}}^2-\frac{2}{\rho}\right)-2\hat{\mathbf{q}}(\hat{\mathbf{q}}\cdot\boldsymbol{\rho})-3i\hat{\mathbf{q}}. \tag{71}$$

If we now return to the expression for the real-space Hamiltonian in Eq. (1), it is apparent that we may substitute

$$\hat{\mathbf{q}}^2-\frac{2}{\rho}=\hat{H} \tag{72}$$

in Eq. (71) to yield

$$\hat{\mathbf{A}}=\hat{\mathbf{q}}^2\boldsymbol{\rho}+\boldsymbol{\rho}\hat{H}-2\hat{\mathbf{q}}(\hat{\mathbf{q}}\cdot\boldsymbol{\rho})-3i\hat{\mathbf{q}}. \tag{73}$$

Comparing this with Eqs. (67) and (68), it is evident that the two components of the Runge–Lenz vector in real space correspond to the generators of infinitesimal rotations in the (u_xu_z) and (u_yu_z) planes.

V. CONCLUSION

We have shown that the accidental degeneracy in the energy eigenvalues of the two-dimensional Kepler problem may be explained by the existence of a planar analog of the familiar three-dimensional Runge–Lenz vector. By moving into momentum space and making a stereographic projection onto a three-dimensional sphere, a new integral relation in terms of special functions has been obtained, which to our knowledge has not previously been tabulated. We have also demonstrated explicitly that the components of the two-dimensional Runge–Lenz vector in real space are intimately related to infinitesimal rotations in three-dimensional momentum space.

APPENDIX A: SOLUTION OF REAL-SPACE SCHRÖDINGER EQUATION

We apply the method of separation of variables to Eq. (1), making the substitution

$$\Psi(\boldsymbol{\rho})=R(\rho)\Phi(\phi). \tag{A1}$$

Introducing a separation constant m^2, we can obtain the angular equation

$$\frac{d^2\Phi}{d\phi^2}+m^2\Phi=0, \tag{A2}$$

with the solution

$$\Phi(\phi)=\frac{1}{\sqrt{2\pi}}e^{im\phi}. \tag{A3}$$

The corresponding radial equation (with $E=-q_0^2$) is

$$\frac{d^2R}{d\rho^2}+\frac{1}{\rho}\frac{dR}{d\rho}+\left(\frac{2}{\rho}-q_0^2-\frac{m^2}{\rho^2}\right)R=0. \tag{A4}$$

We make the substitution

$$R(\rho)=C\rho^{|m|}e^{-q_0\rho}w(\rho), \tag{A5}$$

where C is a normalization constant. This leads to the equation

$$\rho\frac{d^2w}{d\rho^2}+(2|m|+1-2q_0\rho)\frac{dw}{d\rho}+(2-2|m|q_0-q_0)w=0. \tag{A6}$$

Making a final change of variables $\beta=2q_0\rho$, we obtain

$$\beta\frac{d^2w}{d\beta^2}+(2|m|+1-\beta)\frac{dw}{d\beta}+\left(\frac{1}{q_0}-|m|-\frac{1}{2}\right)w=0. \tag{A7}$$

This is the confluent hypergeometric equation,[15] which has two linearly independent solutions. If we choose the solution which is regular at the origin, then this becomes a polynomial of finite degree if $q_0=(n+\frac{1}{2})^{-1}$ with $n=0,1,2,\ldots$. Equation (A7) then becomes the associated Laguerre equation,[16] the solutions of which are the associated Laguerre polynomials:

$$w=L_{n-|m|}^{2|m|}(\beta)=L_{n-|m|}^{2|m|}(2q_0\rho). \tag{A8}$$

We can now write the real-space wavefunction in the form

$$\Psi_{nm}(\boldsymbol{\rho})=\frac{C}{2\pi}\rho^{|m|}e^{-q_0\rho}L_{n-|m|}^{2|m|}(2q_0\rho)e^{im\phi_\rho}, \tag{A9}$$

where the reason for the subscript on ϕ is explained in Sec. III C.

To normalize this wavefunction we need to make use of the integral[16]

$$\int_0^\infty e^{-2q_0\rho}(2q_0\rho)^{2|m|+1}L_{n-|m|}^{2|m|}(2q_0\rho)L_{n-|m|}^{2|m|}(2q_0\rho)\,d(2q_0\rho)=\frac{(n+|m|)!}{(n-|m|)!}(2n+1). \tag{A10}$$

The normalized wavefunctions are therefore

$$\Psi_{nm}(\boldsymbol{\rho})=\sqrt{\frac{q_0^3(n-|m|)!}{\pi(n+|m|)!}}(2q_0\rho)^{|m|}e^{-q_0\rho}L_{n-|m|}^{2|m|}(2q_0\rho)e^{im\phi_\rho}, \tag{A11}$$

satisfying the following orthogonality condition:

$$\int \Psi^*_{n_1 m_1}(\boldsymbol{\rho})\Psi_{n_2 m_2}(\boldsymbol{\rho})\, d\boldsymbol{\rho} = \delta_{n_1 n_2}\delta_{m_1 m_2}. \tag{A12}$$

APPENDIX B: DERIVATION OF EQ. (15)

From Eq. (3) we have

$$\hat{\mathbf{A}}^2 = \left[(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z - \hat{\mathbf{L}}_z\times\hat{\mathbf{q}}) - \frac{2}{\rho}\boldsymbol{\rho} \right]^2 = [2(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z) - i\hat{\mathbf{q}}]^2 - \frac{2}{\rho}\boldsymbol{\rho}\cdot[2(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z) - i\hat{\mathbf{q}}] - \frac{2}{\rho}[2(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z) - i\hat{\mathbf{q}}]\cdot\boldsymbol{\rho} + 4. \tag{B1}$$

We further expand as follows:

$$\begin{aligned}[2(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z) - i\hat{\mathbf{q}}]^2 &= 4(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z)^2 - 2i\hat{\mathbf{q}}\cdot(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z) - 2i(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z)\cdot\hat{\mathbf{q}} - \hat{\mathbf{q}}^2 \\ &= 4\hat{\mathbf{q}}^2\hat{\mathbf{L}}_z^2 + 2\hat{\mathbf{q}}^2 - \hat{\mathbf{q}}^2 = \hat{\mathbf{q}}^2(4\hat{\mathbf{L}}_z^2 + 1),\end{aligned} \tag{B2}$$

and

$$-\frac{2}{\rho}\boldsymbol{\rho}\cdot[2(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z) - i\hat{\mathbf{q}}] - \frac{2}{\rho}[2(\hat{\mathbf{q}}\times\hat{\mathbf{L}}_z) - i\hat{\mathbf{q}}]\cdot\boldsymbol{\rho} = -\frac{2}{\rho}(4\hat{\mathbf{L}}_z^2 + 1). \tag{B3}$$

Substituting Eqs. (B2) and (B3) into Eq. (B1) gives

$$\hat{\mathbf{A}}^2 = \hat{\mathbf{q}}^2(4\hat{\mathbf{L}}_z^2 + 1) - \frac{2}{\rho}(4\hat{\mathbf{L}}_z^2 + 1) + 4, \tag{B4}$$

which, from Eq. (72), is just

$$\hat{\mathbf{A}}^2 = \hat{H}(4\hat{\mathbf{L}}_z^2 + 1) + 4. \tag{B5}$$

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Unification of the Jaynes–Cummings model and Planck's radiation law

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By combining iterative methods with Laplace transformation, we construct the solution of a dissipative Jaynes–Cummings model. The dissipative part of the model is based on the standard Markovian master equation for a harmonic oscillator that is coupled to a heat bath of nonzero temperature. Besides photon loss, we also take into account frequency detuning between atom and field. Before commencing the iteration, we subject the matrix elements of the density operator to a transformation that depends on temperature. As a result, the pole structure of all Laplace transformed matrix elements is improved. It becomes manifest which poles do not contribute to the asymptotic behavior of the density operator. In proving that our iterative process yields convergent results, we assume upper bounds on: the matrix elements of the density operator, the matrix elements of the initial density operator, the damping parameter of the heat bath, and the temperature of the heat bath. All of these bounds are physically acceptable. The photon field may start from a coherent state or a number state. For experiments in a microwave cavity, temperatures of the order of 0.1 [K] are allowed. As an application, the evolution of the atomic density matrix is studied. We propose a limit for which this matrix converges to the state of maximum von Neumann entropy. The time, the cubed initial energy density, and the inverse of the damping parameter must tend to infinity equally fast. The photon field is assumed to be in a number state at time zero, whereas the initial state of the atom can be chosen freely. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1504503]

I. INTRODUCTION

A. Motivation

Some 20 years ago, the field of quantum optics witnessed fast developments. Owing to the arrival of new laser sources, atomic states of high quantum number became experimentally accessible.[1] Transitions between these Rydberg states are accompanied by large electric dipole moments, so couplings to the electromagnetic radiation field are quite strong. Being also long-lived, the Rydberg states could be successfully exploited to perform experimental tests on the Jaynes–Cummings model.[2]

Proposed back in 1963,[3] this analytically solvable model describes the interaction between a two-level atom and a single privileged mode of the quantized electromagnetic radiation field. The model relies on various simplifications, for instance, the electric-dipole and rotating-wave approximations. Its dynamics[4] exhibits such challenging features as collapse and revival of Rabi oscillations.[5] In various disciplines, especially quantum statistical mechanics[6,7] and quantum computing,[8] the model is a prime reference.

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In an experimental setup the mode selector is a microwave cavity of high quality. Eventually, all of the initial energy leaks away from the cavity. Hence, the Jaynes–Cummings interaction cannot be observed for an unlimited amount of time. To deal properly with the damping phenomena, further theoretical efforts are indispensable. Such efforts were indeed made,[9] although exact extensions of the Jaynes–Cummings model became available only after some delay.[10,11] The cavity temperature was always set equal to zero. The attempt[12] to capture the effects of finite temperature on the basis of matrix continued fractions has a strictly formal character.

In this paper we intend to solve an extended version of the Jaynes–Cummings model that respects Planck's law for large times. Use is made of a Markovian master equation, which emanates from a weak-coupling procedure.[13] As the temperature of the cavity is nonzero, one may expect good agreement with experiment for all evolutionary stages. We allow for frequency detuning of atom and field, but ignore the possibility that the atom may spontaneously emit a photon into electromagnetic modes other than the privileged one.

A sound mathematical treatment of the temperature effects requires considerable vigilance. If one plainly mimicks techniques from the zero-temperature case, then one quickly runs into unpleasant surprises. For example, the evolution of the photon field toward the thermal state must be safeguarded from the very outset. Before constructing any solutions, one should perform a temperature transformation of the master equation. Omission of this preparatory step confronts us with summations that do not converge uniformly in time. Their asymptotic behavior cannot be found by making the time infinitely large behind a summation sign.

The temperature transformation ensures that our solution converges uniformly in time. As we shall prove, all summations are dominated by a geometric series. The latter is convergent if the average number of thermal photons inside the cavity is sufficiently small. Consequently, we must set a bound on the temperature. In a strict sense, this paper is silent about the case of arbitrarily high temperature.

In Sec. I B we review the Jaynes–Cummings model with cavity damping, whereas in Sec. I C we introduce some handy notations. A summary can be found in Sec. II. It serves the reader who wishes to get a good impression of this paper through a modest effort. We present our four assumptions (i)–(iv), as well as the two limits that will be proved. All material can be easily understood by anyone having some experience in iterative techniques.

In Sec. III we construct our solution. We only perform a finite number of iterations. Hence, the ensuing identities are equivalent to our point of departure, the master equation for the density operator. The issue of convergence turns up in Sec. IV, as the order of iteration is taken to infinity. Sections IV A, IV B, IV C, and IV D each contain one building block of the convergence proof. Use is made of basic linear algebra and function theory.

As an application of the newly established solution, we propose in Sec. V a limit for which the atom reaches the state of maximum entropy. A similar limit was already presented for the zero-temperature case.[11] In contrast to Secs. III and IV, we do not pursue mathematical rigor in Sec. V. Our conclusions appear in Sec. VI. Finally, this paper includes four appendices. In each of the Appendices B, C, and D we prove a result, which is needed in the main text. Appendix A does not include any proofs, but describes a possible approach for extending our mathematical framework to the case of weak damping.

B. The model

The Jaynes–Cummings interaction between a two-level atom A and a single privileged mode of the quantized electromagnetic radiation field F is described by the Hamiltonian $H_0+\hbar g H_1$. The constituents H_0 and H_1, which act on the product Hilbert space $\mathsf{C}^2\otimes\mathcal{H}_F$, are given by

$$H_0=\hbar\omega_F[\tfrac{1}{2}(i_+-i_-)\otimes\mathbf{1}+\mathbf{1}_2\otimes a^\dagger a],$$

$$H_1=\Delta(i_+-i_-)\otimes\mathbf{1}+\sigma_+\otimes a+\sigma_-\otimes a^\dagger.$$

The excited state $\hat{\mathbf{b}}_1=(1,0)^T$ of energy ϵ_2 and the ground state $\hat{\mathbf{b}}_2=(0,1)^T$ of energy ϵ_1 span the atomic Hilbert space C^2. Hence, all atomic operators linearly depend on the matrices

$$i_+=\begin{pmatrix}1&0\\0&0\end{pmatrix},\quad i_-=\begin{pmatrix}0&0\\0&1\end{pmatrix},\quad \sigma_+=\begin{pmatrix}0&1\\0&0\end{pmatrix},\quad \sigma_-=\begin{pmatrix}0&0\\1&0\end{pmatrix}.$$

The privileged mode of frequency ω_F has ladder operators a and $a^\dagger$, the commutator $[a,a^\dagger]$ being equal to unity. They act on the Hilbert space $\mathcal{H}_F$, which is spanned by the orthonormal photon-number states $\{|n\rangle\}_{n=0}^{\infty}$, with $|n\rangle=(n!)^{-1/2}(a^\dagger)^n|0\rangle$ and $a|0\rangle$ identical to the zero element. The detuning parameter $\Delta=(\epsilon_2-\epsilon_1-\hbar\omega_F)/(2\hbar g)$ measures the difference between the atomic and field frequencies in units of the interaction strength g.

To account for photon loss, we couple the field mode to a thermal reservoir of inverse temperature β. Then the evolution of the density operator $\rho(t)$ for atom and field is governed by the master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t)=-i[H_1,\rho(t)]+\frac{\kappa}{1+\bar{n}}\mathcal{L}[\rho(t)]. \tag{1}$$

We have moved to the interaction picture, and divided by g, so the time t and the damping constant κ are dimensionless. Although general expressions for the damping operator $\mathcal{L}$ are available,[14] we assume that the damping process is driven by a quantum dynamical semigroup. The standard[13] weak-coupling procedure leads to

$$\begin{aligned}\mathcal{L}[\rho]=&2(\mathbf{1}_2\otimes a)\rho(\mathbf{1}_2\otimes a^\dagger)-(\mathbf{1}_2\otimes a^\dagger a)\rho-\rho(\mathbf{1}_2\otimes a^\dagger a)+2\bar{n}[(\mathbf{1}_2\otimes a^\dagger)\rho(\mathbf{1}_2\otimes a)\\&+(\mathbf{1}_2\otimes a)\rho(\mathbf{1}_2\otimes a^\dagger)-(\mathbf{1}_2\otimes a^\dagger a)\rho-\rho(\mathbf{1}_2\otimes aa^\dagger)],\end{aligned} \tag{2}$$

where $\bar{n}$ stands for the average number of thermal photons in the privileged mode. Trace, self-adjointness, and positivity of the density operator are conserved.

As t becomes large, the density operator is expected to converge to a thermal state

$$\lim_{t\to\infty}\|\rho(t)-\exp(-\beta H_0)/\mathrm{Tr}[\exp(-\beta H_0)]\|=0, \tag{3}$$

in trace norm. This state is a fixed point of the dynamics (1) if the condition

$$\exp(-\beta\hbar\omega_F)=\frac{\bar{n}}{1+\bar{n}}\equiv\lambda$$

is satisfied. Simply stated, Planck's radiation law must be valid. Finally, note that (3) is invariant under backtransformation to the Schrödinger picture.

C. Notation

The direct product $\otimes$ of two matrices, sometimes called the right Kronecker product, is defined as usual.[15] To avoid heavily burdened formulas, we introduce for any integer n the theta symbol

$$\theta_n=\begin{cases}0 & \text{if } n\leqslant -1\\ 1 & \text{if } n\geqslant 0,\end{cases}$$

and for any integer $k\geqslant -1$ the matrix product

$$\left\{\prod_{s=0}^{k}M(s)\right\}=M(0)M(1)\cdots M(k),\quad \left\{\prod_{s=0}^{-1}M(s)\right\}=\mathbf{1}.$$

We shall stick to the use of curly braces. Our Laplace transform reads

$$\tilde{f}(z) = -i \int_0^\infty \mathrm{d}t\, e^{izt} f(t),$$

with $\mathrm{Im}\, z$ positive. In the sequel, we shall work for n integer with the function

$$\psi(a,b;n) = a^n + (b/n)^n,$$

where a and b are positive. We shall also need the matrices

$$I(n) = \begin{pmatrix} \theta_n & 0 \\ 0 & \theta_{n+1} \end{pmatrix}, \quad W(n) = \begin{pmatrix} n^{1/2}\theta_{n-1} & 0 \\ 0 & (n+1)^{1/2}\theta_n \end{pmatrix},$$

$$B(n) = \begin{pmatrix} (-\kappa n - \kappa\lambda n - \kappa\lambda)\,\theta_n & -i(n+1)^{1/2}\theta_n \\ -i(n+1)^{1/2}\theta_n & (-\kappa n - \kappa - \kappa\lambda n - 2\kappa\lambda + 2i\Delta)\,\theta_{n+1} \end{pmatrix}.$$

The eigenvalues and normalized eigenvectors of the matrix $B(n;\lambda=0)$ are found as

$$\mu_\eta(n) = [-\kappa(n+1/2) + i\Delta - i\,\eta u(n)]\,\theta_n + 2i\Delta\,\delta_{n,-1},$$

$$\hat{\mathbf{q}}_\eta(n) = \nu_\eta^{-1}(n) \begin{pmatrix} (n+1)^{1/2} \\ \eta u(n) - i\kappa/2 - \Delta \end{pmatrix} \theta_n + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \delta_{n,-1}.$$

We have abbreviated

$$\nu_\eta(n) = [n+1+|\eta u(n) - i\kappa/2 - \Delta|^2]^{1/2},$$

$$u(n) = (n+1+\Delta^2 - \kappa^2/4 + i\kappa\Delta)^{1/2}\theta_n,$$

with $\eta = \pm 1$. We shall derive bounds on matrices and vectors by making use of the sup norm and the Euclidean norm, respectively. The dyadic product $\hat{\mathbf{e}}_i\hat{\mathbf{e}}_j$ represents the (4×4) matrix, the ij element of which equals unity; all other matrix elements equal zero. The set $\{\hat{\mathbf{e}}_j\}_{j=1}^4$ contains the Cartesian unit vectors in four dimensions.

II. SOLUTION IN SHORT

In Sec. III we get the iterative process going, but keep the order of iteration finite. Section IV is devoted to our convergence proofs.

Section III A shows in three steps how the primal master equation (1) can be converted to an algebraic c-number equation in four dimensions. As a first step, we take matrix elements of $\rho(t)$ with the help of the product states $\{|\hat{\mathbf{b}}_1\otimes n\rangle, |\hat{\mathbf{b}}_2\otimes n\rangle\}_{n=0}^\infty$, and group these in the following way:

$$\mathbf{v}'(t;m,n) = [\langle\hat{\mathbf{b}}_1\otimes m|\rho(t)|\hat{\mathbf{b}}_1\otimes n\rangle,\ \langle\hat{\mathbf{b}}_2\otimes(m+1)|\rho(t)|\hat{\mathbf{b}}_1\otimes n\rangle,$$
$$\langle\hat{\mathbf{b}}_1\otimes m|\rho(t)|\hat{\mathbf{b}}_2\otimes(n+1)\rangle,\ \langle\hat{\mathbf{b}}_2\otimes(m+1)|\rho(t)|\hat{\mathbf{b}}_2\otimes(n+1)\rangle]^T, \tag{4}$$

with $m,n = -1,0,1,2,\ldots$. We use the convention that a matrix element $\langle\hat{\mathbf{b}}_i\otimes m|\rho(t)|\hat{\mathbf{b}}_j\otimes n\rangle$ be identical to zero for negative photon number m or n. The choice (4) ensures that in the c-number equation for $\mathbf{v}'$ the photon numbers (m,n) only couple to their neighbors $(m+1,n+1)$ and $(m-1,n-1)$.

The second step is made up by the transformation

$$\begin{aligned} \mathbf{v}(t;m,n) &= \mathbf{v}'(t;m,n), \\ \mathbf{v}(t;n,n) &= (\theta_n Q_1 + \delta_{n,-1}Q_2)\mathbf{v}'(t;n,n) - \lambda\,\theta_n Q_2 \mathbf{v}'(t;n-1,n-1), \end{aligned} \tag{5}$$

with $m,n\geqslant -1$ and $m\neq n$. The matrices Q_1 and Q_2 are chosen such that, in case limit (3) holds true, the new vector $\mathbf{v}(t;n,n)$ vanishes for $n\geqslant 0$ and $t\to\infty$. Consequently, the fixed point in (3) is mapped to its zero-temperature counterpart.

A further constraint on Q_1 and Q_2 is that no new couplings between photon numbers be introduced. One then arrives at the equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}(t;m,n)=A(m,n)\mathbf{v}(t;m,n)+2\kappa S(m,n)\mathbf{v}(t;m+1,n+1)+2\kappa\lambda T(m,n)\mathbf{v}(t;m-1,n-1), \tag{6}$$

with $m,n\geqslant -1$. The matrices A, S, and T are defined in Sec. III A. We emphasize the equivalence between the master equation (1) and the differential equation (6).

Laplace transformation of (6) constitutes the third and final step of the conversion. The transformed vector $\tilde{\mathbf{v}}(z;m,n)$ satisfies an algebraic equation. By carrying out a matrix inversion, we arrive at a recursion relation of second order in the photon numbers (m,n).

In Sec. III B the Nth-order iterative solution of (6) is constructed. Upon iterating our recursion relation N times and performing inverse Laplace transformation, we obtain

$$\mathbf{v}(t;m,n)=\mathbf{v}(t;N;m,n)+\mathbf{r}(t;N;m,n), \tag{7}$$

$$\mathbf{v}(t;N;m,n)=\sum_{p=0}^{N-1}\sum_{k=-\min(m,n)-1}^{N-p-1}\lambda^p K(t;k,p;m,n)\mathbf{v}(t=0;m+k,n+k) \tag{8}$$

for $m,n\geqslant -1$ and $N\geqslant 1$. The term $\mathbf{r}(t;N;m,n)$ is a remainder, which still depends on $\mathbf{v}(t;m,n)$. The kernel $K(t;k,p;m,n)$ is a (4×4) matrix, which possesses the properties

$$\begin{aligned} K(t=0;k,p;m,n)&=I(n)\otimes I(m)\,\delta_{k,0}\delta_{p,0},\\ K(t=0;k,p;-1,-1)&=\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2\delta_{k,0}\delta_{p,0}, \end{aligned} \tag{9}$$

with $m,n\geqslant -1$, and the choice $m=n=-1$ forbidden. We have taken care to arrange the iteration such that the temperature makes its appearance through a power series in λ.

In Sec. IV we investigate what happens to identity (7) if the order of iteration N is taken to infinity. The treatment rests on the following four assumptions.

(i) For all non-negative times one may employ the inequalities

$$\begin{aligned} \|\mathbf{v}(t;m,n)\|&\leqslant c_1 e^{-c_2\kappa t}(m/2+n/2+2)^3\psi(c_3\lambda/\kappa,c_4;m/2+n/2+1),\\ \|\mathbf{v}(t;-1,-1)-(1-\lambda)(1+\lambda)^{-1}\hat{\mathbf{e}}_2\|&\leqslant c_1 e^{-c_2\kappa t}. \end{aligned} \tag{10}$$

In the upper line the choice $m=n=-1$ is forbidden. The function ψ is defined in Sec. I C. The positive constants $\{c_i\}$ are specified in Sec. IV.

As $\mathbf{v}(t;m,n)$ is composed of matrix elements of $\rho(t)$, the inequalities (10) determine the class of density operators to which we confine ourselves. This class does not include density operators that do not comply with the thermal limit (3).

(ii) The initial density operator $\rho(t=0)$ is chosen such that for all m and n the inequality

$$\|\mathbf{v}(t=0;m,n)\|\leqslant c_5\left[\frac{(m+2)(n+2)}{(m+1)!(n+1)!}\right]^{1/2}c_6^{m+n+2}\theta_{m+1}\theta_{n+1} \tag{11}$$

holds true. The constants c_5 and c_6 are positive. Note that for $t=0$ and $\lambda>0$ the constraint (10) is weaker than (11).

The bound (11) is physically acceptable, because it is possible to make two familiar choices for the initial density operator, namely

$$\rho(t=0)=\rho_A\otimes|\alpha\rangle\langle\alpha|, \quad \rho(t=0)=\rho_A\otimes|q\rangle\langle q|, \tag{12}$$

where ρ_A denotes any density operator in two dimensions, $|\alpha\rangle=\exp(-|\alpha|^2/2+\alpha a^\dagger)|0\rangle$ stands for a coherent state, with α complex, and $|q\rangle$ stands for a photon-number state, with q a non-negative integer. The constant c_6 must be set equal to $\max(1,|\alpha|)$ if one works with the coherent state.

(iii) On the damping parameter the restriction

$$0<\kappa<2$$

is imposed. Earlier findings for a reservoir of zero temperature[7] tell us that the overdamped case $\kappa\geqslant 2$ is of no physical interest at all. The same goes for the choice $\kappa=0$, which decouples the reservoir from the Jaynes–Cummings interaction.

(iv) The inequality

$$0\leqslant\lambda<\lambda_0<1$$

is indispensable. The temperature of the reservoir is assumed to stay below a certain level, prescribed by the constant λ_0. In Sec. VI we calculate what order of magnitude the temperature may have for experiments in a microwave cavity.

Making use of assumptions (ii)–(iv), we prove in Sec. IV the existence of a vector $\mathbf{v}(t;\infty;m,n)$ such that

$$\lim_{N\to\infty}\ \sup_{0\leqslant t<\infty}\|\mathbf{v}(t;\infty;m,n)-\mathbf{v}(t;N;m,n)\|=0 \tag{13}$$

for $m,n\geqslant -1$. The properties (9) guarantee that for small t the new vector $\mathbf{v}(t;\infty;m,n)$ converges to the initial vector $\mathbf{v}(t=0;m,n)$.

The proof of (13) consists of three steps. In Sec. IV A we derive bounds on the matrices from which the kernel K is built up. This task being accomplished, we can derive in Sec. IV B a bound on K itself. Last, by invoking the Cauchy theorem on the existence of a limit, we prove in Sec. IV C the statement (13). We also check that the limiting vector $\mathbf{v}(t;\infty;m,n)$ fulfills the conditions (10). It thus respects the thermal limit (3).

Assumptions (i)–(iv), with the bound λ_0 replaced by $\lambda_0'<\lambda_0$, allow us to prove in Sec. IV D the limit

$$\lim_{N\to\infty}\ \sup_{0\leqslant t<\infty}\|\mathbf{v}(t;m,n)-\mathbf{v}(t;N;m,n)\|=0 \tag{14}$$

for $m,n\geqslant -1$. The proof starts by employing (7) on the left-hand side of (14). To cope with the dependence of the remainder $\mathbf{r}(t;N;m,n)$ on the vector $\mathbf{v}(t;m,n)$, we must estimate the norm of the latter. At this point assumption (i) comes in.

By means of a triangle inequality we deduce from (13) and (14) the identity

$$\mathbf{v}(t;m,n)=\mathbf{v}(t;\infty;m,n), \tag{15}$$

with $m,n\geqslant -1$. Therefore, the limiting vector $\mathbf{v}(t;\infty;m,n)$ may be viewed as the solution of the dissipative Jaynes–Cummings model. In principle, λ must remain smaller than λ_0'. However, we can exchange the bound λ_0' for λ_0 by applying analytic continuation in λ to the limiting vector.

In Sec. V we utilize our solution to examine the evolution of $\rho_A(t)$, the density matrix describing the two-level atom. We argue that, besides the thermal state, the state of maximum entropy may also be operative as an attractor in atomic phase space. This observation is based on the limit

$$\lim_{t\to\infty,\kappa\to 0,q\to\infty}\rho_A(t)=\tfrac{1}{2}\mathbf{1}_2. \tag{16}$$

The tilde denotes that the products κt and κq^3 must be kept constant. The full density operator starts from the state $\rho(0)=\rho_A\otimes|q\rangle\langle q|$, with ρ_A free and $|q\rangle$ a photon-number state. The temperature may have any fixed value within its interval of convergence. A completely rigorous proof of (16) falls outside the scope of our treatment, because it forces us to tighten the bound (10) on the limiting vector $\mathbf{v}(t;\infty;m,n)$. The factor of κ^{-1} should be removed from the first argument of ψ. In Appendix A we outline a possible method to achieve this.

III. CONSTRUCTION OF THE SOLUTION

We now take on the job of devising the iterative process that generates the solution of the dissipative Jaynes–Cummings model. Convergence proofs are not yet required, because the order of iteration is kept finite. In Sec. III A we replace the master equation (1) by a c-number recursion relation in four dimensions. In Sec. III B we construct the Nth-order iterative solution of this recursion relation.

A. Toward an algebraic equation

We employ the product states $\{|\hat{\mathbf{b}}_1\otimes n\rangle,|\hat{\mathbf{b}}_2\otimes n\rangle\}_{n=0}^{\infty}$ to cast the master equation (1) into c-number shape. For negative photon number m or n the matrix element $\langle\hat{\mathbf{b}}_i\otimes m|\rho(t)|\hat{\mathbf{b}}_j\otimes n\rangle$ vanishes by definition. In terms of vector (4) the c-number equation can be represented as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}'(t;m,n)=A'(m,n)\mathbf{v}'(t;m,n)+2\kappa S'(m,n)\mathbf{v}'(t;m+1,n+1)$$
$$+2\kappa\lambda T'(m,n)\mathbf{v}'(t;m-1,n-1), \tag{17}$$

with $m,n\geqslant -1$. For the matrices we find

$$A'(m,n)=I(n)\otimes B(m)+B(n)^{\dagger}\otimes I(m),$$

$$S'(m,n)=T'(m+1,n+1),\quad T'(m,n)=W(n)\otimes W(m),$$

where we refer to the notation of Sec. I C.

According to (3), the vector (4) is expected to behave for large times as

$$\lim_{t\to\infty}\mathbf{v}'(t;m,n)=\delta_{m,n}(1-\lambda)(1+\lambda)^{-1}\lambda^{n+1}(\hat{\mathbf{e}}_1\theta_n+\hat{\mathbf{e}}_4\theta_{n+1}).$$

We want to set up a one-to-one transformation that maps the limiting vector on the right-hand side to zero, for $m=n$ non-negative. Moreover, the transformed equation (17) should not contain any additional couplings between photon numbers. A transformation meeting these constraints is given by (5), with the matrices

$$Q_1=\begin{pmatrix}1&0&0&-1\\0&0&0&1\\0&1&-1&0\\0&1&1&0\end{pmatrix},\quad Q_2=\hat{\mathbf{e}}_2\hat{\mathbf{e}}_4.$$

The inverse reads

$$\mathbf{v}'(t;n,n)=[\theta_nQ_1^{-1}+\delta_{n,-1}\hat{\mathbf{e}}_4\hat{\mathbf{e}}_2]\mathbf{v}(t;n,n)+\theta_n\sum_{k=1}^{n+1}\lambda^kQ_1^{-1}Q_2Q_1^{-1}\mathbf{v}(t;n-k,n-k).$$

Transformation of (17) brings us to (6). The transformed matrices come out as

$$A(n,n)=Q_1A'(n,n)Q_1^{-1}+2\kappa\lambda(-\hat{\mathbf{e}}_1\hat{\mathbf{e}}_2+\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2),$$

$$S(n,n)=Q_1S'(n,n)Q_1^{-1},$$

$$T(n,n)=Q_1T'(n,n)Q_1^{-1}+\hat{\mathbf{e}}_1\hat{\mathbf{e}}_2-\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2-in^{1/2}(2\kappa)^{-1}\hat{\mathbf{e}}_2\hat{\mathbf{e}}_3,$$

$$A(-1,-1)=T(-1,-1)=0,\quad S(-1,-1)=\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2,$$

with n non-negative. Note that $T(0,0)$ equals zero. Of course, for $m\neq n$ the transformed matrices are identical to their primed counterparts.

To stay in complete control of temperature dependencies, we head for a power series in the parameter λ. We make the split

$$A(m,n)=A_0(m,n)+2\kappa\lambda A_1(m,n),$$

with

$$A_0(n,n)=Q_1A'(n,n;\lambda=0)Q_1^{-1}\theta_n,\quad A_0(m,n)=A'(m,n;\lambda=0) \tag{18}$$

for $m\neq n$, and

$$A_1(m,n)=-\tfrac{1}{2}[I(n)\otimes W^2(m+1)+W^2(n+1)\otimes I(m)]+\hat{\mathbf{e}}_4\hat{\mathbf{e}}_4\delta_{m,-1}\delta_{n,-1}+\tfrac{1}{2}(\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2+\hat{\mathbf{e}}_4\hat{\mathbf{e}}_4)\delta_{m,n}\theta_n,$$

for all $m,n\geqslant -1$. The matrix $A_1(-1,-1)$ equals zero.

Laplace transformation of (6) yields

$$\begin{aligned}\tilde{\mathbf{v}}(z;m,n)=R(z;m,n)[&\mathbf{v}(t=0;m,n)+2i\kappa S(m,n)\tilde{\mathbf{v}}(z;m+1,n+1)\\&+2i\kappa\lambda T(m,n)\tilde{\mathbf{v}}(z;m-1,n-1)+2i\kappa\lambda A_1(m,n)\tilde{\mathbf{v}}(z;m,n)],\end{aligned} \tag{19}$$

with $m,n\geqslant -1$. The resolvents are given by

$$R(z;-1,-1)=\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2/z,\quad R(z;n,n)=[z\mathbf{1}_4-iA_0(n,n)]^{-1},$$

for $n\geqslant 0$, and

$$R(z;m,n)=I(n)\otimes I(m)[z\mathbf{1}_4-iA_0(m,n)]^{-1}I(n)\otimes I(m),$$

for $m,n\geqslant -1$ and $m=n$ forbidden. The projector $I(n)\otimes I(m)$ comes in because of the property

$$I(n)\otimes I(m)\mathbf{v}'(t;m,n)=\mathbf{v}'(t;m,n).$$

It reflects the convention that matrix elements of the density operator disappear if a photon number becomes negative.

The simple pole $z=0$ of $R(z;-1,-1)$ determines the asymptotic behavior of our solution, because the poles of all other resolvents lie below the real axis of the complex z plane. Their location can be deduced from the eigenvalue equation

$$A'(m,n;\lambda=0)\hat{\mathbf{q}}^*_{\eta_2}(n)\otimes\hat{\mathbf{q}}_{\eta_1}(m)=[\mu_{\eta_1}(m)+\mu^*_{\eta_2}(n)]\hat{\mathbf{q}}^*_{\eta_2}(n)\otimes\hat{\mathbf{q}}_{\eta_1}(m), \tag{20}$$

with $\eta_1,\eta_2=\pm 1$. Definitions of eigenvectors and eigenvalues appear in Sec. I C. Note that for either $m=-1$, $n\geqslant 0$ or $m\geqslant 0$, $n=-1$ the resolvent $R(z;m,n)$ has two instead of four poles.

B. Iteration

The recursion (19) is solved in two steps. First, we iterate in the parameter κ, and subsequently, in the parameter $\kappa\lambda$. This route leads to a power series in λ, as planned.

The outcome of the first iteration can be expressed as

$$\tilde{\mathbf{v}}(z;m,n)=R(z;m,n)\sum_{k=0}^{N-1}(2i\kappa)^k D_1(z;k;m,n)\mathbf{v}(t=0;m+k,n+k)$$
$$+\lambda R(z;m,n)\sum_{k=0}^{N}(2i\kappa)^k D_2(z;N;k;m,n)\tilde{\mathbf{v}}(z;m+k-1,n+k-1)+\tilde{\mathbf{r}}_1(z;N;m,n), \tag{21}$$

with $N\geqslant 1$ and the remainder

$$\tilde{\mathbf{r}}_1(z;N;m,n)=(2i\kappa)^N R(z;m,n)D_1(z;N-1;m,n)S(m+N-1,n+N-1)\tilde{\mathbf{v}}(z;m+N,n+N).$$

We have introduced the matrices

$$D_1(z;k;m,n)=\left\{\prod_{s=0}^{k-1}S(m+s,n+s)R(z;m+s+1,n+s+1)\right\},$$

$$D_2(z;N;k;m,n)=\theta_{N-k-1}2i\kappa D_1(z;k;m,n)T(m+k,n+k)$$
$$+\theta_{k-1}D_1(z;k-1;m,n)A_1(m+k-1,n+k-1),$$

where for D_1 the notation of Sec. I C has been employed.

Next, we iterate (21) to arrive at the following schematic result:

$$\tilde{\mathbf{v}}(z;m,n)=\sum_{p=0}^{N-1}\sum_{k=-\min(m,n)-1}^{N-p-1}\lambda^p\tilde{K}(z;k,p;m,n)\mathbf{v}(t=0;m+k,n+k)+\sum_{j=1}^{4}\tilde{\mathbf{r}}_j(z;N;m,n), \tag{22}$$

with $m,n\geqslant -1$ and $N\geqslant 1$. The kernel can be written as

$$\tilde{K}(z;k,p;m,n)=\theta_{k+p}(2i\kappa)^{k+p}\sum_{l_0=0}^{k+p-1}\sum_{l_1=l_0-1}^{k+p-2}\cdots\sum_{l_p=l_{p-1}-1}^{k}R(z;m,n)$$
$$\times\left\{\prod_{s=1}^{p}D_2(z;\infty;l_s-l_{s-1}+1;m+l_{s-1},n+l_{s-1})R(z;m+l_s,n+l_s)\right\}$$
$$\times D_1(z;k-l_p;m+l_p,n+l_p).$$

It is essential to be aware of the condition

$$l_s\geqslant -\min(m,n)-1+\delta_{m,n} \tag{23}$$

for $1\leqslant s\leqslant p$. It is imposed on the summand of $\tilde{K}$ by the matrices A_1 and T figuring in D_2. Note that the above-given summation over l_0 consists of one term only, for which l_0 equals zero.

The remainders in (22) are byproducts of the iteration process. As shown in Sec. IV D, they can be made small by making N large. We thus need the precise expressions for the second remainder

$$\tilde{\mathbf{r}}_2(z;N;m,n)=\sum_{p=1}^{N-1}\sum_{l_0=0}^{N+l_0-1}\sum_{l_1=l_0-1}^{N+l_1-1}\sum_{l_2=l_1-1}^{N+l_{p-1}-1}\cdots\sum_{l_p=l_{p-1}-1}^{N+l_{p-1}-1}\lambda^p(2i\kappa)^{l_p+p}R(z;m,n)$$
$$\times\left\{\prod_{s=1}^{p-1}D_2(z;N;l_s-l_{s-1}+1;m+l_{s-1},n+l_{s-1})R(z;m+l_s,n+l_s)\right\}$$
$$\times D_2(z;N;l_p-l_{p-1}+1;m+l_{p-1},n+l_{p-1})\tilde{\mathbf{r}}_1(z;N;m+l_p,n+l_p),$$

the third remainder

$$\tilde{\mathbf{r}}_3(z;N;m,n)=\sum_{l_0=0}^{N+l_0-1}\sum_{l_1=l_0-1}^{N+l_1-1}\sum_{l_2=l_1-1}^{}\cdots\sum_{l_N=l_{N-1}-1}^{N+l_{N-1}-1}\lambda^N(2i\kappa)^{l_N+N}R(z;m,n)$$
$$\times\left\{\prod_{s=1}^{N-1}D_2(z;N;l_s-l_{s-1}+1;m+l_{s-1},n+l_{s-1})R(z;m+l_s,n+l_s)\right\}$$
$$\times D_2(z;N;l_N-l_{N-1}+1;m+l_{N-1},n+l_{N-1})\tilde{\mathbf{v}}(z;m+l_N,n+l_N),$$

and, finally, the fourth remainder,

$$\tilde{\mathbf{r}}_4(z;N;m,n)=\sum_{p=1}^{N-1}\sum_{k=N-p}^{(p+1)(N-1)}\sum_{l_0=0}^{}\sum_{l_1=l_0-1}^{k+p-1}\sum_{l_2=l_1-1}^{k+p-2}\cdots\sum_{l_p=l_{p-1}-1}^{k}\lambda^p(2i\kappa)^{k+p}R(z;m,n)$$
$$\times\left\{\prod_{s=1}^{p}D_2(z;N;l_s-l_{s-1}+1;m+l_{s-1},n+l_{s-1})R(z;m+l_s,n+l_s)\right\}$$
$$\times D_1(z;k-l_p;m+l_p,n+l_p)\mathbf{v}(t=0;m+k,n+k)$$
$$\times\prod_{s=1}^{p}\theta_{N+l_{s-1}-l_s-1}\theta_{l_s-k+(N-1)(p-s+1)}.$$

With these expressions in hand, we can readily verify that the identity (22) is equivalent to the recursion (19).

Inverse Laplace transformation of (22) confirms Eqs. (7) and (8). Moreover, it gives rise to the following correspondences:

$$K(t;k,p;m,n)=\oint\frac{\mathrm{d}z}{2\pi i}e^{-izt}\tilde{K}(z;k,p;m,n),\tag{24}$$

$$\mathbf{r}(t;N;m,n)=i\sum_{j=1}^{4}\int_C\frac{dz}{2\pi}e^{-izt}\,\tilde{\mathbf{r}}_j(z;N;m,n).\tag{25}$$

The kernel $\tilde{K}$ is meromorphic in z, so in (24) the contour has been closed on account of Jordan's lemma. It encircles all poles of the integrand counterclockwise. In (25) the contour C is a straight line with $\mathrm{Im}\,z$ fixed and positive, and $\mathrm{Re}\,z$ running from $-\infty$ to $+\infty$.

The initial conditions (9) directly relate to the structure of (24), as can be demonstrated with the help of a standard technique.[16] For $t=0$ the contour (24) can be deformed into a circle $|z|=R$. The radius R is chosen sufficiently large, so that each resolvent may be expanded into a Neumann series. Since these uniformly converge on the deformed contour, one may integrate term by term, and hence, invoke the identity

$$\oint\frac{\mathrm{d}z}{2\pi i}z^{-n}=\delta_{n,1},\tag{26}$$

for any integer n. One immediately recovers the right-hand sides of (9).

IV. CONVERGENCE OF THE SOLUTION

We set out to prove statements (13) and (14). Making use of assumption (iii), we derive in Sec. IV A bounds on the matrices that generate the kernel K. In Sec. IV B we prove the inequality (40), which provides us with a bound on the kernel itself. The proof of (13) is presented in Sec. IV C. The bound (40) is needed, as well as assumptions (ii) and (iv). In Sec. IV D we turn to the

proof of the key result (14). We appeal to all assumptions (i)–(iv), with λ_0 replaced by $\lambda_0' < \lambda_0$. In view of the possibility of analytic continuation, we do not bother about the precise value of λ_0'.

A. Basic bounds

Consider a complex $(d\times d)$ matrix M and assume that it satisfies the eigenvalue equation $M\hat{\mathbf{v}}^{(j)}=\lambda_j\hat{\mathbf{v}}^{(j)}$, where the right eigenvectors $\{\hat{\mathbf{v}}^{(j)}\}_{j=1}^d$ are normalized and linearly independent. The set of eigenvalues $\{\lambda_j\}_{j=1}^d$ may contain degeneracies. An arbitrary vector $\mathbf{v}$ can be decomposed as $\mathbf{v}=\Sigma_{j=1}^d c_j(\mathbf{v})\hat{\mathbf{v}}^{(j)}$, where the objects $\{c_j(\mathbf{v})\}_{j=1}^d$ are complex coefficients. They can be expressed as $c_j(\mathbf{v})=\Sigma_{k=1}^d c_j(\hat{\mathbf{w}}^{(k)})\hat{\mathbf{w}}^{(k)}\cdot\mathbf{v}$, if the set $\{\hat{\mathbf{w}}^{(j)}\}_{j=1}^d$ is orthonormal. Hence, we have the inequality $|c_j(\mathbf{v})|\leqslant\|\mathbf{v}\|[\Sigma_{k=1}^d|c_j(\hat{\mathbf{w}}^{(k)})|^2]^{1/2}$ at our disposal. For the sup norm of M we can put forth the bound

$$\|M\|\leqslant\sum_{j=1}^d|\lambda_j|\left(\sum_{k=1}^d|c_j(\hat{\mathbf{w}}^{(k)})|^2\right)^{1/2}. \tag{27}$$

The coefficients on the right-hand side can be evaluated by means of matrix inversion

$$\hat{\mathbf{w}}^{(j)}\cdot\hat{\mathbf{v}}^{(k)}\equiv D_{jk},\quad c_k(\hat{\mathbf{w}}^{(j)})=D_{kj}^{-1}, \tag{28}$$

with $j,k=1,2,3,\ldots,d$.

We apply (27) to our resolvents. The eigenvalues and eigenvectors $\{\lambda_j,\hat{\mathbf{v}}^{(j)}\}_{j=1}^4$ are those of Eq. (20). As orthonormal basis $\{\hat{\mathbf{w}}^{(j)}\}_{j=1}^4$ we take

$$\{\hat{\mathbf{q}}_{\eta_2}^*(n;\kappa=0)\otimes\hat{\mathbf{q}}_{\eta_1}(m;\kappa=0)\}_{\eta_1,\eta_2=\pm1}.$$

Solution of (28) comes down to inversion of a direct product of (2×2) matrices for $m,n\geqslant0$, and a single (2×2) matrix otherwise. The root in (27) can be elaborated with the help of the identity

$$\nu_+^2(n)\nu_-^2(n)=(n+1)[\nu_+^2(n)+\nu_-^2(n)].$$

The result is smaller than the constant

$$\xi=\|Q_1\|\|Q_1^{-1}\|(1-\kappa^2/4)^{-1}.$$

We thus obtain the estimate

$$\|R(z;m,n)\|\leqslant\xi\sum_{\eta_1,\eta_2=\pm1}|z-i\mu_{\eta_1}(m)-i\mu_{\eta_2}^*(n)|^{-1}, \tag{29}$$

for $m,n\geqslant-1$. By assumption (iii), the right-hand side is positive and finite.

For the other matrices figuring in the kernel one derives the bounds

$$\begin{aligned}\|S(m,n)\|&\leqslant2(m+2)^{1/2}(n+2)^{1/2}\theta_{m+1}\theta_{n+1},\\ \|T(m,n)\|&\leqslant5\kappa^{-1}[(m+1)^{1/2}(n+1)^{1/2}-\delta_{m,0}\delta_{n,0}]\theta_m\theta_n,\\ \|A_1(m,n)\|&\leqslant2(m+n+4-2\delta_{m,-1}\delta_{n,-1})\theta_{m+1}\theta_{n+1}.\end{aligned} \tag{30}$$

The factor of κ^{-1}, contained in the bound for T, is due to transformation (5). This factor lives on all the way to the first argument of ψ in the estimate (10) for the limiting vector. No problems arise as long as κ is kept fixed and finite. In Appendix A we sketch what measures must be taken in order to create estimates that do not blow up for small damping parameter.

B. Bound on the kernel

We are now in a position to construct a bound on the kernel. Let us start by fixing the contour on the right-hand side of (24). From the auxiliary inequalities

$$c_2 \equiv \tfrac{1}{4}[1-|\Delta|/|\mathrm{Re}\,u(0)|]>0, \quad |\mathrm{Re}\,u(m)|>|\mathrm{Re}\,u(n)|, \tag{31}$$

valid for $m>n\geqslant 0$, one learns that the poles of the integrand of (24) are contained within the following rectangle:

$$-|\mathrm{Re}\,u(m+k+p)|-|\mathrm{Re}\,u(n+k+p)|-|\Delta|\leqslant \mathrm{Re}\,z\leqslant |\mathrm{Re}\,u(m+k+p)|+|\mathrm{Re}\,u(n+k+p)|+|\Delta|,$$

$$-\kappa(m+n+2k+2p+2)\leqslant \mathrm{Im}\,z\leqslant -2\kappa c_2,$$

the pole at $z=0$ excepted. The latter pertains to the case $m=n=-1$, which will be handled later on.

The contour of our choice is specified by

$$\begin{gathered} z=\kappa w-i\kappa c_2, \\ w=x, \quad -\rho\leqslant x\leqslant \rho \quad (C_1), \\ w=\rho\exp(i\phi), \quad -\pi\leqslant\phi\leqslant 0 \quad (C_2). \end{gathered} \tag{32}$$

If the radius of the closing arc C_2 is taken as $\rho(m/2+n/2+k+p)$, with the definition

$$\rho(l)=12\kappa^{-1}(l+2+|\Delta|+\Delta^2),$$

then surely all of the poles are covered.

Having fixed the contour (32), we can refine the bounds on resolvents. From (29) and (31) we infer the inequalities

$$\begin{gathered} \|R(\kappa w-i\kappa y;m,n)\|\leqslant 4\xi\kappa^{-1}(m\theta_m+n\theta_n+c_2)^{-1}, \\ \|R(\kappa w-i\kappa y;m,n)\|\leqslant \xi\kappa^{-1}\sum_{\eta_1,\eta_2=\pm 1}|x+\mathrm{Im}[\mu_{\eta_1}(m)-\mu_{\eta_2}(n)]/\kappa+ic_2|^{-1}, \end{gathered} \tag{33}$$

with $w\in C_1$, and

$$\|R(\kappa w-i\kappa y;m+s,n+s)\|\leqslant 8\xi[\kappa\rho(m/2+n/2+k+p)]^{-1}, \tag{34}$$

with $w\in C_2$. The conditions $y\leqslant c_2$ and $-\min(m,n)-1\leqslant s\leqslant k+p$ must be satisfied, whereas the choice $m=n=-1$ is forbidden. Combination of (30) with (33) and (34) brings us for $-\min(m,n)-1\leqslant s\leqslant k+p-1$ and $y\leqslant c_2$ to the comfortable estimate

$$\|S(m+s,n+s)\|\|R(\kappa w-i\kappa y;m+s+1,n+s+1)\|\leqslant 8\xi(\kappa c_2)^{-1}, \tag{35}$$

which is valid for $w\in C_1\cup C_2$. Use has been made of the fact that the geometric mean $(mn)^{1/2}$ is smaller than the arithmetic mean $(m+n)/2$.

Special attention must be paid to the zero-temperature case $p=0$, because one must distinguish between the choices $k=0$ and $k\geqslant 1$. For $k=0$ the kernel has one resolvent only. The inequality

$$\left\| \oint \frac{\mathrm{d}z}{2\pi i} e^{-izt}R(z;m,n)\right\|\leqslant 4\xi e^{-c_2\kappa t},$$

can be applied. For the proof, one evaluates all residues on the left-hand side. The result can be estimated with the help of (29).

The choice $k \geqslant 1$ allows for employment of (32), because one meets two resolvents at least. For the contours C_1 and C_2 we control the two resolvents with photon numbers (m,n) and $(m+1,n+1)$ through (33) and (34), respectively. The other $k-1$ resolvents are estimated with the help of (35). Upon extending the boundaries of the integral over x to infinity, we arrive at

$$\|K(t;k,p=0;m,n)\| \leqslant 4\xi e^{-c_2\kappa t}\delta_{k,0} + \xi^2 (16\xi/c_2)^{k-1} e^{-c_2\kappa t} \|S(m,n)\| \times \left[\left(\sum_{\eta_1,\eta_2,\eta_3,\eta_4=\pm 1} \mathcal{J}(a,b)/\pi \right) + 64[\rho(m/2+n/2+k)]^{-1} \right] \theta_{k-1},$$

where the integral

$$\mathcal{J}(a,b) = \int_{-\infty}^{\infty} \mathrm{d}x |x+a+ic_2|^{-1} |x+b+ic_2|^{-1} < 10/c_2$$

appears. The inequality is valid for all real a and b. These parameters must be taken as $\mathrm{Im}[\mu_{\eta_1}(m) - \mu_{\eta_2}(n)]/\kappa$ and $\mathrm{Im}[\mu_{\eta_3}(m+1) - \mu_{\eta_4}(n+1)]/\kappa$, respectively.

Insertion of the bound on $\mathcal{J}$ gives $160/(\pi c_2)$, which is larger than the form containing ρ, at least, if $\kappa < 2$. Therefore, by adding an overall factor of 2, we can drop the latter term. We use (30) to finalize the bound as follows:

$$\|K(t;k,p=0;m,n)\| \leqslant 16\xi (16\xi/c_2)^k (m+2)^{1/2} (n+2)^{1/2} e^{-c_2\kappa t} \theta_k, \tag{36}$$

where the choice $m=n=-1$ is forbidden.

Next, we consider the kernel for $p \geqslant 1$, making use of (32) for all k. From the resolvents with photon numbers (m,n) and $(m+l_p, n+l_p)$ we create an integral $\mathcal{J}$ in the same vein as previously. Owing to condition (23) on the summation indices $\{l_s\}$, the inequality (35) can furnish bounds on the D_1 matrices. Processing the resolvents that are left with the aid of (33) and (34), we find

$$\begin{aligned} \|K(t;k,p;m,n)\| \leqslant{}& \frac{1}{2} (2\kappa)^k (8\xi)^{p+1} e^{-c_2\kappa t} \theta_{k+p} \\ & \times \sum_{l_0=0} \sum_{l_1=l_0-1}^{k+p-1} \sum_{l_2=l_1-1}^{k+p-2} \cdots \sum_{l_p=l_{p-1}-1}^{k} \left[\left(\sum_{\eta_1,\eta_2,\eta_3,\eta_4=\pm 1} \mathcal{J}(a,b)/(32\pi) \right) \right. \\ & \left. \times \prod_{s=1}^{p-1} [(m+l_s)\theta_{m+l_s} + (n+l_s)\theta_{n+l_s} + c_2]^{-1} + [\rho(m/2+n/2+k+p)/2]^{-p} \right] \\ & \times \prod_{s=1}^{p} [\|T(m+l_s+1,n+l_s+1)\| + \|A_1(m+l_s,n+l_s)\|] \left(\frac{8\xi}{\kappa c_2} \right)^{k-l_p} \\ & \times \prod_{s=1}^{p} \left[2\kappa \left(\frac{8\xi}{\kappa c_2} \right)^{l_s - l_{s-1}+1} + \theta_{l_s-l_{s-1}} \left(\frac{8\xi}{\kappa c_2} \right)^{l_s-l_{s-1}} \right], \end{aligned}$$

with $p \geqslant 1$. The parameter a need not be modified, but b must be chosen now as $\mathrm{Im}[\mu_{\eta_3}(m+l_p) - \mu_{\eta_4}(n+l_p)]/\kappa$.

Again, we replace $\mathcal{J}$ by its upper bound, and omit the term containing ρ in exchange for an overall factor of 2. This enables us to appeal to the inequality

$$\frac{\|T(m+1,n+1)\| + \|A_1(m,n)\|}{m\theta_m + n\theta_n + c_2} \leqslant 2c_2^{-1}(4+5/\kappa), \tag{37}$$

which follows from (30). For $s=p$ the denominator of (37) lacks, so that another inequality must be employed, namely

$$\|T(m+l_p+1,n+l_p+1)\|+\|A_1(m+l_p,n+l_p)\|\leqslant(4+5/\kappa)(m/2+n/2+l_p+2), \tag{38}$$

where l_p is put equal to its maximum value of k.

Having disposed of all dependencies on the dummies $\{l_s\}$, we can perform the corresponding summations by the rule

$$\sum_{l_1=0}^{p}\sum_{l_2=l_1}^{p}\sum_{l_3=l_2}^{p}\cdots\sum_{l_q=l_{q-1}}^{p}=\binom{p+q}{q}, \tag{39}$$

with $p\geqslant 0$ and $q\geqslant 1$. In final form, the bound on the kernel reads

$$\|K(t;k,p;m,n)\|\leqslant 16\xi\left(\frac{16\xi}{c_2}\right)^{k+p}\left(1+\frac{16\xi}{c_2}\right)^{p}\left(4+\frac{5}{\kappa}\right)^{p}\binom{2p+k}{p}(m/2+n/2+k+2)e^{-c_2\kappa t}\theta_{k+p}, \tag{40}$$

with $m,n\geqslant -1$, the choice $m=n=-1$ forbidden, and $p\geqslant 0$; note that for $p=0$ the above-mentioned bound exceeds (36). As pointed out already, the factor of κ^{-1} stems from (30). In Appendix A we discuss how this factor can be suppressed.

C. Taking the order of iteration to infinity

Assumption (ii) and Eq. (40) supply us with bounds on the components generating the solution vector. Hence, we are ready to examine the distance $\|\mathbf{v}(t;N;m,n)-\mathbf{v}(t;N';m,n)\|$ for large iteration orders. The involved sums can be rearranged as

$$\begin{aligned}\sum_{p=0}^{N-1}\sum_{k=-\min(m,n)-1}^{N-p-1}-\sum_{p=0}^{N'-1}\sum_{k=-\min(m,n)-1}^{N'-p-1}&=\sum_{p=0}^{N-1}\sum_{k=N'-p}^{N-p-1}\theta_{\min(m,n)+N'-p}\\&+\sum_{p=N'}^{N-1}\sum_{k=-\min(m,n)-1}^{N'-p-1}\theta_{\min(m,n)+N'-p}\\&+\sum_{p=0}^{N-1}\sum_{k=-\min(m,n)-1}^{N-p-1}\theta_{p-\min(m,n)-N'-1},\end{aligned}$$

with $N\geqslant N'\geqslant 1$. We shift $k\to k-p$, and interchange the sums over k and p.

Next, we use assumption (ii) and Eq. (40), as well as the inequalities

$$\frac{(k+p)!}{k!}\leqslant(k+p_{\max})^p,\quad \frac{([m/2+n/2+1])!}{[(m+1)!(n+1)!]^{1/2}}\leqslant 1,$$

where $m,n\geqslant -1$ and $p_{\max}$ denotes the maximum of p in a given sum. By (11), we may set $p_{\max}$ equal to $k+\min(m,n)+1$. This paves the way for applying the binomial theorem. One encounters the factors

$$\left[1+\frac{2\lambda}{c_6^2}\left(1+\frac{16\xi}{c_2}\right)\left(4+\frac{5}{\kappa}\right)[k+\min(m,n)+1]\right]^{k+m/2+n/2+1},$$

and $1/([m/2+n/2+1]+k)!$, the entire function $[\cdots]$ rendering the argument of the factorial integer. To modify these factors, we let us be guided by the inequalities $(a+b)^k\leqslant(2a)^k+(2b)^k$ and $1/k!\leqslant\exp(k+1)/(k+1)^k$. We then obtain the result

$$\|\mathbf{v}(t;N;m,n)-\mathbf{v}(t;N';m,n)\|\leqslant c_1(N,N')e^{-c_2\kappa t}(m/2+n/2+2)^3\psi(c_3\lambda/\kappa,c_4;m/2+n/2+1), \tag{41}$$

with $N\geqslant N'\geqslant \min(m,n)+2$ and the choice $m=n=-1$ forbidden. The constants are found as

$$c_1(N,N')=256e\xi c_5\sum_{k=N'-\min(m,n)-1}^{N-1}\theta_{k-1}k^3\left(\frac{16\xi}{c_2}\right)^k\psi(c_3\lambda/\kappa,c_4;k),$$

$$c_3=4e(4\kappa+5)(1+16\xi/c_2),\quad c_4=2ec_6^2.$$

The constants c_2, c_5, and c_6 appear in (11) and (31).

From (41) we conclude that $\mathbf{v}(t;N;m,n)$ may be regarded as a Cauchy sequence in N. Consequently, a vector $\mathbf{v}(t;\infty;m,n)$ exists such that (13) is true. The upper bound belonging to assumption (iv) comes out as

$$0\leqslant\lambda<\lambda_0=\frac{c_2\kappa}{16\xi c_3}. \tag{42}$$

Repetition of the foregoing proof for $N'=0$ shows that for $c_1=c_1(\infty,0)$ the limiting vector $\mathbf{v}(t;\infty,m,n)$ satisfies the inequality (10). Note that the choice $m=n=-1$ is still forbidden.

Hence, the proof must be repeated for the case $m=n=-1$ as well. By severing the pole at $z=0$ from the contour (24), we can cast (8) into the form

$$\mathbf{v}(t;N;-1,-1)=\mathbf{v}_{\rm ss}(N)+e^{-c_2\kappa t}\mathbf{v}_{\rm fl}(t;N).$$

The steady-state (ss) term and fluctuating (fl) term are given by

$$\mathbf{v}_{\rm ss}(N)=\sum_{p=0}^{N-1}\sum_{k=0}^{N-p-1}\lambda^p\lim_{z\to0}z\tilde{K}(z;k,p;-1,-1)\mathbf{v}(t=0;k-1,k-1),$$

$$\mathbf{v}_{\rm fl}(t;N)=\kappa\sum_{p=0}^{N-1}\sum_{k=0}^{N-p-1}\lambda^p\oint\frac{dw}{2\pi i}e^{-i\kappa tw}\tilde{K}(\kappa w-i\kappa c_2;k,p;-1,-1)\mathbf{v}(t=0;k-1,k-1).$$

In the lower line one may work with contour (32), so for $k=p=0$ the result is vanishing. The radius of C_2 is taken as $\rho(k+p)$.

For the fluctuating term we can establish a counterpart of (41) along the same lines as before. The factor of $|x-ic_2|^{-1}$ pertaining to C_1 is included in the integral $\mathcal{J}$. Owing to condition (23), employment of (33)–(35) is permitted. One is led to the assertion

$$\|\mathbf{v}_{\rm fl}(t;N)-\mathbf{v}_{\rm fl}(t;N')\|\leqslant 8ec_5\sum_{k=N'}^{N-1}k^2\left(\frac{16\xi}{c_2}\right)^k\psi(c_3\lambda/\kappa,c_4;k), \tag{43}$$

for $N\geqslant N'\geqslant 1$.

To deal with the steady-state term, one should recognize that the matrix

$$K_0(k,p)=\lim_{z\to0}z\tilde{K}(z;k,p;-1,-1)$$

obeys the recursion

$$K_0(k+1,p+1)=-2\kappa[K_0(k,p+1)S(k-1,k-1)+K_0(k+2,p)T(k+1,k+1)$$
$$+K_0(k+1,p)A_1(k,k)]A_0^{-1}(k,k),$$

with $k \geqslant 0$, $p \geqslant -1$, and $K_0(k,-1)=0$ by definition. The initial condition $K_0(0,p)=\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2\delta_{p,0}$ gives the solution

$$K_0(k,p)=\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2\delta_{k,0}\delta_{p,0}-\hat{\mathbf{e}}_2\hat{\mathbf{e}}_1\theta_{k-1}\delta_{p,0}+2(-1)^p(\hat{\mathbf{e}}_2\hat{\mathbf{e}}_1+\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2)\theta_{k-1}.$$

The constraint $\mathrm{Tr}\,\rho(t=0)=1$ is equivalent to

$$\sum_{k=-1}^{\infty}\left(\theta_k,\frac{2}{1-\lambda}-\delta_{k,-1},0,0\right)\cdot\mathbf{v}(t=0;k,k)=1.$$

Combination of the last two results yields

$$\|\mathbf{v}_{\mathrm{ss}}(N)-(1-\lambda)(1+\lambda)^{-1}\hat{\mathbf{e}}_2\|\leqslant 14c_5\sum_{k=N-2}^{\infty}\frac{c_6^{2k+2}}{k!}+8c_5\sum_{k=0}^{N-3}\lambda^{N-k-1}\frac{c_6^{2k+2}}{k!}.$$

Together with (43), this statement completes the proof of (13) and shows that the limiting vector $\mathbf{v}(t;\infty;-1,-1)$ satisfies the inequality (10).

D. Controlling the remainders

We aim at proving that all of our remainders tend to zero for large iteration order. Again, the case $m=n=-1$ asks for a separate effort. The argument makes use of assumption (i). Hence, the Laplace transform of the unknown vector $\mathbf{v}(t;m,n)$ can be estimated as

$$\|\tilde{\mathbf{v}}(z;m,n)\|\leqslant\frac{c_1(m/2+n/2+2)^3}{\mathrm{Im}\,z+c_2\kappa}\psi(c_3\lambda/\kappa,c_4;m/2+n/2+1),$$

with $\mathrm{Im}\,z>-c_2\kappa$ and the choice $m=n=-1$ forbidden. The inequality fixes the half space on which the Laplace transform is analytic.

For the first remainder of (25) we may shift the contour downward to the level $\mathrm{Im}\,z=-c_2\kappa/2$. Next, we call upon the inequalities (33) and (35), with y set equal to $c_2/2$. By copying previously explained techniques, we reach the result

$$\left\|\int_C \mathrm{d}z\, e^{-izt}\,\tilde{\mathbf{r}}_1(z;N;m,n)\right\|\leqslant c_1(10N)^4(16\xi/c_2)^N(m/2+n/2+1)^5\times\psi(c_3\lambda/\kappa,c_4;m/2+n/2+N+1).$$

By assumption (iv), the right-hand side tends to zero for large N.

As they do not differ much, the second and third remainders can be treated on a par. The contour is laid out as above. In building integral $\mathcal{J}$, we select the resolvents with photon numbers $(m,n),(m+l_p,n+l_p)$ and $(m,n),(m+l_{N-1},n+l_{N-1})$ for the second and third remainder, respectively. We employ (30) for the matrix $S(m+N+l_p-1,n+N+l_p-1)$ of the second remainder. We also make use of (38); for the second remainder as it stands, for the third one with the replacements $p\to N$ and $p\to N-1$ made. All other matrix norms are taken care of by (35) and (37). We now arrive at the intermediate inequalities

$$\left\| \int_C \mathrm{d}z\, e^{-izt}\, \tilde{\mathbf{r}}_2(z;N;m,n) \right\| \leqslant 20 c_1 \sum_{p=1}^{N-1} \sum_{l_0=0} \sum_{l_1=l_0-1}^{N+l_0-1} \sum_{l_2=l_1-1}^{N+l_1-1} \cdots \sum_{l_p=l_{p-1}-1}^{N+l_{p-1}-1} \left(\frac{16\xi}{c_2}\right)^{N+l_p+p} \left(\frac{c_3\lambda}{4e\kappa}\right)^p$$
$$\times (m/2+n/2+N+l_p+2)^5 \psi(c_3\lambda/\kappa, c_4; m/2+n/2+N+l_p+1)$$
$$\times \prod_{s=1}^{p} \theta_{l_s+\min(m,n)+1},$$

and

$$\left\| \int_C \mathrm{d}z\, e^{-izt} \tilde{\mathbf{r}}_3(z;N;m,n) \right\| \leqslant 10 c_1 \sum_{l_0=0} \sum_{l_1=l_0-1}^{N+l_0-1} \sum_{l_2=l_1-1}^{N+l_1-1} \cdots \sum_{l_N=l_{N-1}-1}^{N+l_{N-1}-1} \left(\frac{16\xi}{c_2}\right)^{N+l_N} \left(\frac{c_3\lambda}{4e\kappa}\right)^N$$
$$\times (m/2+n/2+l_N+3)^5 \psi(c_3\lambda/\kappa, c_4; m/2+n/2+l_N+1)$$
$$\times \prod_{s=1}^{N} \theta_{l_s+\min(m,n)+1}.$$

As for (23), the conditions on the dummies $\{l_s\}$ originate from (30).

In elaborating the bound on the second remainder, we take N such that $c_4/N \leqslant c_3\lambda/\kappa$; consequently, the c_4 term in ψ can be dropped at the cost of a factor of 2. In treating the factor $(m/2+n/2+N+l_p+1)^5$, the inequality $l_p \leqslant N^2$ is helpful. Upon omitting the conditions on $\{l_s\}$, transforming these dummies as $l_s - l_{s-1} + 1 \to l_s$, and extending their upper boundaries to infinity, we meet a product of p identical sums. Problems with convergence do not occur as long as λ stays sufficiently small.

In elaborating the bound on the third remainder, we once more use the inequality $l_N \leqslant N^2$, and subsequently extend the upper boundaries of all sums to infinity. We then must face the following form:

$$\chi(x_1,x_2;p,q) = \sum_{l_0=p} \sum_{l_1=l_0-1}^{\infty} \sum_{l_2=l_1-1}^{\infty} \cdots \sum_{l_q=l_{q-1}-1}^{\infty} \left(x_1^{l_q} + \frac{x_2^{l_q}}{l_q!}\right) \prod_{s=1}^{q} \theta_{l_s},$$

with $x_1 = 16\xi c_3\lambda/(\kappa c_2) < 1$, $x_2 = 16\xi c_4/c_2$, $p = \min(m,n)+1$, and $q = N$. In Appendix B it is demonstrated that

$$\chi(x_1,x_2;p,q) \leqslant [4/(1-x_1)]^q + 4^q \exp[x_2(p+q)], \tag{44}$$

for $0 \leqslant x_1 < 1$, $x_2 \geqslant 0$, and $p,q \geqslant 0$. We can finish the treatment of the second and third remainders through the estimate

$$\sum_{j=2,3} \left\| \int_C \mathrm{d}z\, e^{-izt}\, \tilde{\mathbf{r}}_j(z;N;m,n) \right\| \leqslant c_1 (m/2+n/2+2)^5 c_7^{m/2+n/2+1} (10N)^{11} \left(\frac{16\xi c_3\lambda}{c_2\kappa}\right)^N$$
$$\times \left[\left(1 - \frac{16\xi c_3\lambda}{c_2\kappa}\right)^{-N} + \exp\left(\frac{16\xi c_4 N}{c_2}\right) \right],$$

where constant c_7 need not be specified.

The right-hand side of the above-given inequality tends to zero for $N \to \infty$ and $\lambda < \lambda_0'$, with λ_0' sufficiently small. The new condition on λ does not have any physical significance. The replacement of λ_0 by λ_0', necessary for eliminating the remainders, can be annulled. For the solution vector one should perform analytic continuation in λ.

The fourth remainder does not pose any new difficulties. The integral $\mathcal{J}$ is constructed on the basis of the resolvents with photon numbers (m,n) and $(m+l_p, n+l_p)$. All matrix norms can be dealt with through use of (33), (35), (37), and (38). Of course, for the initial vector the bound (11)

must be substituted. Rule (39) can be applied to the $\{l_s\}$ sums. Upon performing the shift $k \to k - p$, and computing the sum over p by the binomial theorem, we end up with

$$\left\| \int_C \mathrm{d}z\, e^{-izt}\, \tilde{\mathbf{r}}_4(z;N;m,n) \right\| \leqslant 10^4 c_5 \xi (m/2+n/2+2)^3 c_7^{m/2+n/2+1} \times \sum_{k=N}^{\infty} k^3 (16\xi/c_2)^k \psi(c_3 \lambda/\kappa, c_4; k).$$

Again, the right-hand side does not survive the limit $N \to \infty$.

With the above-noted material available, it is straightforward to prove that also for the case $m=n=-1$ one can get rid of the remainders by making the iteration order large. As before, the pole at $z=0$ must be severed from the contour. The ensuing residues must be handled separately. Altogether, we reach the satisfactory conclusion that the important limit (14) holds true.

V. A LIMIT OF MAXIMUM ENTROPY

From here onwards, we adopt as the initial density operator the factorized form (12), with the field in a photon-number state $|q\rangle$, and q positive. We are going to take a closer look at the evolution of the (2×2) density matrix $\rho_A(t) = \mathrm{Tr}_F[\rho(t)]$ describing the atom. A limit will be proposed, for which this matrix converges to the so-called central state $\mathbf{1}_2/2$. Then the von Neumann entropy of the atom, which is proportional to the trace $-\mathrm{Tr}(\rho_A \log \rho_A)$, attains its maximum value.

For the given initial condition the atomic density matrix can be computed from

$$\rho_A(t)_{22} = 1 - \rho_A(t)_{11} = \mathbf{d}(t;q)\cdot(\hat{\mathbf{e}}_1 \rho_{A,11} - \hat{\mathbf{e}}_2 \lambda \rho_{A,22}) + \mathbf{d}(t;q-1)\cdot(\hat{\mathbf{e}}_2 - \hat{\mathbf{e}}_1)\rho_{A,22},$$

$$\rho_A(t)_{12} = \rho_A(t)^*_{21} = \sum_{p=0}^{\infty} \sum_{n=0}^{q+p} \lambda^p \hat{\mathbf{e}}_3 \cdot K(t;q-n,p;n,n-1)\cdot \hat{\mathbf{e}}_3 \rho_{A,12}, \tag{45}$$

$$\mathbf{d}(t;q) = (1-\lambda)^{-1} \sum_{p=0}^{\infty} \sum_{n=-1}^{p+q} \lambda^p \hat{\mathbf{e}}_2 \cdot K(t;q-n,p;n,n)\cdot(\hat{\mathbf{e}}_1 \hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_2 \hat{\mathbf{e}}_2), \tag{46}$$

where the notations $\rho_A(t)_{ij} = \hat{\mathbf{b}}_i \cdot \rho_A(t) \cdot \hat{\mathbf{b}}_j$ and $\rho_A = \rho_A(t=0)$ appear.

In contrast to Sec. IV, we do not conduct the argument in a completely rigorous manner. While working out (45) and (46) for small κ, we operate directly in the summands, without investigating whether the interchange of limit and sum is allowed. Unfortunately, completion of this job is far from immediate, because it necessitates us to strengthen the bounds (10) on the limiting vector $\mathbf{v}(t;\infty,m,n)$. In the first argument of ψ the factor of κ^{-1} must be removed. Appendix A presents a possible strategy. Still, in Appendix D we carry out an important consistency check. We make sure that for large times the weak-damping version of $\rho_A(t)$ neatly converges to the thermal state. Other behavior would be physically unacceptable.

Let us set the detuning Δ equal to zero, and investigate the atomic density matrix in the limit of $\kappa \to 0$, $t \to \infty$, $q \to \infty$, under the constraint that κt and κq^3 be constant. Thus the time scales of the Jaynes–Cummings interaction and the process of photon loss become separated. On top of that, during the time lag of κ^{-1} that photon losses are modest, the field can maximally fuel the atom. Indeed, for the undamped Jaynes–Cummings model one already observes that a field of high energy drives the atom toward the central state.[7] But perpetual oscillations of $\rho_A(t)$ inhibit convergence.

We examine the behavior of (24) for $m=n$ positive. The kernel falls apart into two terms: one pertaining to the poles of order κ, and another to those of order unity. If z remains finite, a resolvent $R(z;n,n)$ cannot diverge, so the latter term is of order κ^{k+p} for κ small. Consequently, only the case $k+p=0$ contributes. Condition (23) causes the closed contour of K to be confined

to the half space $\mathrm{Im}\, z<-\kappa(2n-2p+1)\theta_{n-p}$. Hence, in each residue a factor of $\exp[-\kappa t(2n-2p+1)\theta_{n-p}]$ is contained. It explicitly appears if the transformation $z=y-i\kappa(2n-2p+1)\theta_{n-p}$ is made.

Altogether, for small κ and $n\geqslant 0$ we can write

$$K(t;k,p;n,n)=K_1(t;k,p;n,n)+K_2(t;k,p;n,n),$$

$$K_1(t;k,p;n,n)=\oint\frac{\mathrm{d}y}{2\pi}e^{\kappa t y}\kappa\tilde{K}(i\kappa y;k,p;n,n),$$

$$K_2(t;k,p;n,n)=\delta_{k+p,0}e^{-\kappa t(2n-2p+1)}\oint\frac{\mathrm{d}y}{2\pi i}e^{-iyt}\tilde{K}(y-i\kappa(2n-2p+1);k,p;n,n). \quad (47)$$

In K_1 we have transformed $z=i\kappa y$, so that for small κ all poles are of order unity. One can further simplify the term K_2 by recognizing that for $p\geqslant 2$ and y finite, the product

$$\left\{\prod_{s=1}^{p}2i\kappa T(n-s+1,n-s+1)R(y;n-s,n-s)\right\}$$

is of order κ at least. Therefore, K_2 makes a contribution to (46) that decays as $\exp(-2\kappa tq)$ for q large.

In working out K_1, we must realize that now factors of κ^{-1} are generated by the resolvents. For all $k+p\geqslant 0$ finite contributions occur. On the other hand, we still may neglect terms of order κ against terms of order unity. This offers us the possibility to replace matrices as

$$2i\kappa R(i\kappa y;n,n)=(\hat{\mathbf{e}}_2\hat{\mathbf{e}}_1+2\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2+2\hat{\mathbf{e}}_4\hat{\mathbf{e}}_4)(y+2n+1)^{-1},$$

$$\begin{aligned}2i\kappa T(n+1,n+1)R(i\kappa y;n,n)=&[-y\hat{\mathbf{e}}_2\hat{\mathbf{e}}_1/2+\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2(2n+1)](y+2n+1)^{-1}\\&+2\hat{\mathbf{e}}_4\hat{\mathbf{e}}_4(n+1)^{1/2}(n+2)^{1/2}(y+2n+1)^{-1},\end{aligned}$$

for κ small, $n\geqslant 0$, and y finite. From inspection of the left-hand sides one sees that contributions of order $\kappa n^{5/2}$ have been dropped. Surely n can become of order q, so as soon as q tends to infinity the constraint $\kappa q^3=$constant becomes important. Note that the product with T has the structure

$$(\kappa^{-1}T_0+T_1)(R_0+\kappa R_1)=T_1R_0+T_0R_1+\cdots,$$

where T_0R_0 vanishes. Generally speaking, if the leading term of a matrix expansion is noninvertible, then the next-to-leading term may contribute to the final result. In the present case T_1 indeed does so.

In view of (46), the above-given replacements, and the blocked shape of $A_1(n,n)$ and $S(n,n)$, we can retreat to the subspace spanned by $(1,0)^T$ and $(0,1)^T$. Accordingly, for each (4×4) matrix we only retain the upper left block by carrying out the substitution

$$M\rightarrow\begin{pmatrix}M_{11}&M_{12}\\M_{21}&M_{22}\end{pmatrix}. \quad (48)$$

This gives rise for example to the identity

$$\left\{\prod_{s=0}^{m} S(n+s,n+s)\begin{pmatrix}0 & 0\\ 1 & 2\end{pmatrix}\right\}=(2n+3)^{-1}\prod_{s=1}^{m+1}(2n+2s+1)$$
$$\times\left[\begin{pmatrix}2(n+2) & 2\\ -(n+2) & -1\end{pmatrix}\delta_{m,-1}+\begin{pmatrix}-1 & -2\\ n+2 & 2(n+2)\end{pmatrix}\right],$$

with $m\geqslant -1$ and $n\geqslant 0$. In the sequel, the correction term with the Kronecker delta plays an important role.

The foregoing material safely guides us through the evaluation of the K_1 kernel for weak damping. The final expression reads

$$K_1(t;k,p;n,n)=\theta_{k+p}\oint\frac{\mathrm{d}y}{4\pi i(2n+1)(2n+3)}e^{\kappa t y}\prod_{s=0}^{k+n}\frac{2s+1}{y+2s+1}\prod_{s=0}^{n-1}\frac{y+2s+1}{2s+1}$$
$$\times\begin{pmatrix}0 & 0\\ 1 & 2\end{pmatrix}D_3(y;k+n,p;n). \tag{49}$$

We have imposed $n\geqslant 0$, $p\geqslant 0$, κ small, and κt constant. We have defined the matrix

$$D_3(y;q,p;n)=\sum_{l_0=n}\sum_{l_1=l_0-1}^{q+p-1}\sum_{l_2=l_1-1}^{q+p-2}\cdots\sum_{l_p=l_{p-1}-1}^{q}\prod_{s=1}^{p}\theta_{l_s}\prod_{s=1}^{p}[(y+2l_s+1)(y+2l_s+3)(2l_s+3)]^{-1}$$
$$\times\left\{\prod_{s=1}^{p}V(y;l_s,l_{s-1})\right\}\left[\begin{pmatrix}2(q+2) & 2\\ -(q+2) & -1\end{pmatrix}\delta_{l_p,q}+\begin{pmatrix}-1 & -2\\ l_p+2 & 2(l_p+2)\end{pmatrix}\theta_{q-l_p}\right],$$

where V stands for

$$V(y;k,l)=(2k+3)(2k+5)\begin{pmatrix}0 & 0\\ -y/2 & 2k+1\end{pmatrix}\delta_{k,l-1}-(k+1)(y+2k+3)\begin{pmatrix}2 & 4\\ -1 & -2\end{pmatrix}\delta_{k,l}$$
$$-2\begin{pmatrix}-1 & -1\\ l+2 & l+2\end{pmatrix}\begin{pmatrix}0 & 0\\ y(4k+5)/2+(2k+3)(k+1) & 2y(k+1)+2k+3\end{pmatrix}\theta_{k-l}.$$

One should remember that (48) has been practiced, so K_1 is indeed a (2×2) matrix.

For a full computation of (46) the kernel must be specified for $n=-1$ as well. The K_2 part disappears, because for $k=p=0$ there are no finite poles. In elaborating the K_1 part, the identity $R(z;-1,-1)=\hat{\mathbf{e}}_2\hat{\mathbf{e}}_2/z$ must be employed. For small κ one ends up with

$$K_1(t;k,p;-1,-1)=\oint\frac{\mathrm{d}y}{2\pi i}\frac{e^{\kappa t y}}{y}\prod_{s=0}^{k-1}\frac{2s+1}{y+2s+1}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}D_3(y;k-1,p;-1), \tag{50}$$

where $k\geqslant 1$ and $p\geqslant 0$ must be respected.

We are ready to calculate (46) for κ small, κt constant, and κq^3 constant. As pointed out, the K_2 term may be completely ignored. In K_1 the power series $\Sigma_{j=0}^{\infty}(\kappa t y)^j/j!$ is inserted for the exponential factor. By invoking (26), we can readily find out how the $j=0$ term contributes to (46). In Appendix C we show that the terms with $1\leqslant j\leqslant p+q$ do not produce anything at all. These findings bring us to the relation

$$\mathbf{d}(t;q)-\frac{1}{2}\left(1,\frac{2}{1-\lambda}\right)=\frac{1}{1-\lambda}\sum_{p=0}^{\infty}\lambda^p\oint\frac{dy}{2\pi i}\sum_{j=p+q+1}^{\infty}\frac{(\kappa t y)^j}{j!}\prod_{s=0}^{q}\frac{2s+1}{y+2s+1}$$
$$\times\left[\frac{1}{2}\sum_{n=0}^{p+q}\prod_{s=0}^{n-1}\frac{y+2s+1}{2s+1}\frac{(1,2)\cdot D_3(y;q,p;n)}{(2n+1)(2n+3)}\right.$$
$$\left.+y^{-1}(0,1)\cdot D_3(y;q,p;-1)\right], \tag{51}$$

with κ small, κt constant, and $q\geqslant 1$. For large q the product κq^3 must remain constant.

The only task left consists of investigating how (51) behaves as q tends to infinity. To that end, the contour $y=4(p+q+1)\exp(i\phi)$, with $0\leqslant\phi\leqslant 2\pi$, is employed. Combination of the estimate

$$\|V(y;k,l)\|\leqslant 16(2k+3)(l+3)(|y|+k+1)$$

with (39) leads to

$$\|D_3(y;q,p;n)\|\leqslant 6(n+3)40^p\binom{q+2p-n}{p},$$

for $n\geqslant -1$. In setting a bound on (51), the term containing y^{-1} may be dropped in exchange for an overall factor of 2.

Next, we can profit from the assertions

$$\prod_{s=n}^{p+q}\left|\frac{2s+1}{y+2s+1}\right|\leqslant 1,\quad \prod_{s=q+1}^{p+q}\left|\frac{y+2s+1}{2s+1}\right|\leqslant\frac{3^p(p+q+1)^p q!}{(p+q)!},$$

and substitute for the sum over n the largest term, which is the one with $n=0$, multiplied by the number of terms, which amounts to $p+q+1$. We can finalize the bound on (51) with the help of the results

$$\frac{(2p+q)!q!}{[(p+q)!]^2}\leqslant 4^p,\quad \sum_{j=n}^{\infty}\frac{(\alpha n)^j}{j!}\leqslant\frac{\exp[n(1+\log\alpha)]}{1-\alpha},$$

where $0\leqslant\alpha<1$ must be valid. The desired inequality reads

$$\left\|\mathbf{d}(t;q)-\frac{1}{2}\left(1,\frac{2}{1-\lambda}\right)\right\|\leqslant c_8 q^2\exp\{[1+960\lambda+\log(4\kappa t)]q\}, \tag{52}$$

where c_8 does not depend on q. For $\lambda<1/(960e)$ the constant c_8 is finite. Moreover, if we take $\kappa t<[4\exp(1+1/e)]^{-1}$, then for large q the right-hand side falls off exponentially.

To learn what becomes of the matrix element $\rho_A(t)_{12}$, one has to analyze the kernel $K(t;k,p;n,n-1)$ for κ small. All poles turn out to be of order unity. Hence, only for $k+p=0$ nonzero contributions occur. As the matrix $T(n,n-1)$ is regular for small κ, the choice $p=0$ is also necessary. The contour is confined to the half space $\mathrm{Im}\,z<-2\kappa n$, so in each residue a factor of $\exp(-2\kappa tn)$ is contained. It causes exponential decay for large q, because in (45) only the $q=n$ term differs from zero. Together with (52), this recognition directly implies the validity of the limit (16).

VI. CONCLUSION

The Jaynes–Cummings model owes much of its popularity to the experimental progress in quantum optics that dates back to the early 1980s.[1,2] Remarkable predictions, such as collapse and revival of Rabi oscillations,[5] were experimentally confirmed.[2] Nevertheless, the predictive power

of the Jaynes–Cummings model is limited. For sufficiently large times one is confronted with a departure from experimental reality. Due to contact with the outside world, the photon field evolves to a thermal state, slowly but irreversibly. Planck's radiation law gains control over the dynamics.

In this paper we solve an extended Jaynes–Cummings model, for which the photon field is coupled to a large thermal reservoir. This modification secures the validity of Planck's law for large times. Although the Hilbert space is of infinite dimension, the mathematical problem at hand can be posed in terms of a four-dimensional vector. The composition of this solution vector reflects the fact that energy is conserved in absence of the reservoir.

Our method for evaluating the solution vector is based on Laplace transformation, followed by iteration. To settle the question of convergence, we make use of four assumptions. They are discussed in Sec. II. Assumptions (i) and (ii) impose confinement to a certain class of density operators. Besides this standard measure, there is a second and more subtle point to pay attention to.

For the extended Jaynes–Cummings model, the thermal state $\exp(-\beta H_0)/\mathrm{Tr}[\exp(-\beta H_0)]$ is a fixed point of the dynamics. A transformation can be devised that maps the thermal state to its zero-temperature counterpart. If the solution vector is subjected to the same transformation, then the analytical properties of its Laplace transform change in an advantageous manner. Before transformation, all of the poles generate damped residues. Ambiguity arises if it comes to selecting the poles that describe the evolution to the thermal state. After transformation, one simple pole emerges at the origin. The corresponding residue, which of course does not depend on time, produces the transformed thermal state, as desired.

In spite of the above-noted precautions, the temperature keeps causing problems. The solution vector is constructed as a perturbative series in the Boltzmann factor that determines the average number of thermal photons inside the microwave cavity. In proving convergence, we are forced to set the bound (42) on this factor. It is uncertain whether assumption (iv) can be eliminated by means of analytic continuation of the solution.

If our method of solution is applied to the case of a cold resonator, i.e., no atom present, then a temperature constraint is also necessary. However, it has no physical meaning; by starting from a partial differential equation for a characteristic function, one can represent the solution as a finite sum.[17] Unfortunately, ordering problems for matrices make it improbable that the same can be achieved for the present model.

In Appendix A our bounds on vectors and matrices are judged to be rather crude. At the same time, assumption (iv) is physically acceptable. Let us take $\kappa=0.1$ and $\Delta=0$. For higher values of κ the Rabi oscillations scarcely exhibit any revivals.[7] With the help of the identity $\|Q_1\|\|Q_1^{-1}\| = (3+5^{1/2})/2$,[16] one finds that the bound λ_0 amounts to 6×10^{-8}. One may set the Boltzmann factor $\exp(-\beta\hbar\omega_F)$ equal to this number. In experiments, the atomic transition has a wavelength of the order of 1 [cm].[2] We thus arrive at a cavity temperature of the order of 0.1 [K], which is feasible.

The unification of the Jaynes–Cummings model and Planck's radiation law has one important drawback: the mathematical structure of the solution becomes much less transparent. An in-depth exploration of the dynamics surely demands a numerical effort. For the case of zero temperature such an effort was already made.[7] In preparation for the numerical work, all contour integrals were expressed as sums of residues. If one chooses the same approach for finite temperature, then one should carefully handle the poles of higher order. One may employ the identity

$$\prod_{j=1}^{M}[z+a(n_j)]^{-1}=\prod_{s=\min_j n_j}^{\max_j n_j}[z+a(s)]^{-\nu(s)},$$

where the integer

$$\nu(s)=\sum_{j=1}^{M}\delta_{s,n_j}$$

has been defined.

Owing to the numerical work for zero temperature, the central state $\mathbf{1}_2/2$ can be identified as an attractor in atomic phase space.[7] For weak damping, preferably κ smaller than 10^{-3}, and high average photon number, initially not less than 25, all trajectories in atomic phase space convene at the central state. There they stay for a time of at least 10^3 $[g^{-1}]$, whereafter they all take the Markovian path to i_-, the atomic ground state. If κ is increased, the central state abandons its special role; the trajectories meet each other at the ground state. This course of events was analytically confirmed by a limit of maximum entropy,[11] still for zero temperature.

For the standard configuration of an atom in contact with a heat bath, the thermal state is the attractor in phase space. This immediately follows from the principle of maximum entropy.[18] The von Neumann entropy is maximized under the conditions that $\mathrm{Tr}\,\rho_A$ and $\mathrm{Tr}\,\rho_A H_A$ be constant, where H_A denotes the atomic Hamiltonian. Apparently, for the present configuration we can deactivate the latter condition by making suitable parameter choices. In other words, the extended Jaynes–Cummings model allows us to manipulate the conditions accompanying the principle of maximum entropy. The thermal state can be exchanged for the central state.

The foregoing interpretation supposes that the limit of maximum entropy, proposed in Ref. 11, is not a zero-temperature artifact. The limit should persist as the temperature becomes finite. In Sec. V we utilize our solution of the extended Jaynes–Cummings model to argue that this indeed happens. To evade a great amount of technical work, we assume that the field starts from a photon-number state. For the same reason, we do not present a rigorous proof. The extended limit is given in (16), where the conditions $\kappa t<[4\exp(1+1/e)]^{-1}$ and $\lambda<1/(960e)$ have been omitted. The first one is not violated for the times that are of interest. The second condition is weaker than (42), because κ takes on low values.

The main message of this paper can be phrased as follows: the dissipative Jaynes–Cummings model displays an unexpectedly rich dynamics, which is worthy of further examination. For instance, one may wonder what the consequences are of modifying the damping mechanism, or assuming entanglement of atom and field at time zero. These questions will be addressed in a forthcoming publication.

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APPENDIX A: BOUNDS FOR WEAK DAMPING

For small κ the bound (10) on the limiting vector $\mathbf{v}(t;\infty;m,n)$ diverges. This can be ascribed to the fact that in the 23 element of $T(n,n)$ a factor of κ^{-1} figures. Our rescuing move is inspired by the material of Sec. V, where all divergencies were mastered. One should recognize that in products such as $T(n+1,n+1)R(z;n,n)$, the divergency of T ceases to exist. In reconsidering (24), we concentrate on the C_1 part of the contour. The C_2 part causes no problems for small κ; the radius $\rho(l)$ includes a factor of κ^{-1}, which compensates the divergency in T.

Explicit evaluation of the third row of the resolvent cannot be avoided. One has

$$\hat{\mathbf{e}}_3\cdot R(\kappa x-i\kappa c_2;n,n)=\kappa^2\prod_{\eta_1,\eta_2=\pm 1}[\kappa x-i\kappa c_2-i\mu_{\eta_1}(n)-i\mu^*_{\eta_2}(n)]^{-1}(2(n+1)^{1/2}[x+ia(n)]$$
$$\times[x+ia(n)+i],\ 4i(n+1)^{1/2}[x+ia(n)],$$
$$\kappa[x+ia(n)]^3+\kappa[x+ia(n)],\ -2\Delta[x+ia(n)]^2-2\Delta),$$

with $n\geqslant 0$ and $a(n)=2n+1-c_2$. Employment of the inequalities

$$(n+1)^{1/2}|\mathrm{Re}\,u(n)|^{-1}\leqslant(1-\kappa^2/4)^{-1/2},\quad |\Delta|<|\mathrm{Re}\,u(n)|,$$

and

$$\prod_{\eta_1,\eta_2=\pm 1} |\kappa x - i\kappa c_2 - i\mu_{\eta_1}(n) - i\mu^*_{\eta_2}(n)|^{-1} \leqslant \kappa^{-2} |2\,\mathrm{Re}\,u(n)|^{-1} |x + ia(n)|^{-1} |x + ia(n) + i(4c_2 - 1)|^{-1} |\kappa|x| + 2|\mathrm{Re}\,u(n)| + i\kappa a(n)|^{-1} \times \left[1 + \left|\frac{x}{|x| - 2|\mathrm{Re}\,u(n)|/\kappa + ia(n)}\right|\right],$$

leads to the proposition

$$\|T(n+1,n+1)R(\kappa x - i\kappa c_2; n,n)\| \leqslant \frac{10\xi}{\kappa c_2}\left[1 + \left|\frac{x}{|x| - 2|\mathrm{Re}\,u(n)|/\kappa + ia(n)}\right|\right], \tag{A1}$$

with $n \geqslant 0$. The right-hand side is of order κ^{-1}, but compensation is available in the kernel. Therefore, we can lift the singularity in (10) at the cost of a space-dependent factor. It is well-behaved under extension of the contour to the interval $-\infty < x < \infty$. After replacement of $T(n+1,n+1)$ by $A_1(n,n)$, the result (A1) may still be employed.

In (24) we utilize (33) for controlling the resolvents with photon numbers (n,n) and (h,h). The integer h will not be specified. In principle, h depends on all summation dummies, so that its bounds are merely given by $1 \leqslant h \leqslant k+n+p$. The accompanying matrix $S(h-1,h-1)$ is dominated by $2(k+n+p+1)$. Use of (35) and (A1) now gives

$$\|K(t;k,p;n,n)\| \leqslant \frac{c_2\xi}{8\pi} e^{-c_2\kappa t}(k+n+p+1)(16\xi/c_2)^k (20\xi/c_2)^p (1+16\xi/c_2)^p \times \theta_{k+p} \sum_{l_0=n}^{k+n+p-1} \sum_{l_1=l_0-1}^{k+n+p-2} \cdots \sum_{l_p=l_{p-1}-1}^{k+n} \prod_{s=1}^{p} \theta_{l_s}\, \mathcal{I}(n,p;\{l_s\},h) + B_2,$$

with the integral

$$\mathcal{I}(n,p;\{l_s\},h) = \int_{-\infty}^{\infty} dx \sum_{\eta_1,\eta_2,\eta_3,\eta_4=\pm 1} |x + \mathrm{Im}\,\mu_{\eta_1}(n)/\kappa - \mathrm{Im}\,\mu_{\eta_2}(n)/\kappa + ic_2|^{-1} |x + \mathrm{Im}\,\mu_{\eta_3}(h)/\kappa - \mathrm{Im}\,\mu_{\eta_4}(h)/\kappa + ic_2|^{-1} \prod_{s=1}^{p} \left[1 + \left|\frac{x}{|x| - 2|\mathrm{Re}\,u(l_s)|/\kappa + ia(l_s)}\right|\right].$$

We have assumed that both $k+n$ and p are greater than zero. We remark once more that the behavior of B_2, which denotes the contribution from the arc C_2, is regular for κ small.

It is possible to establish for integral $\mathcal{I}$ a bound that does not depend on κ. The integration axis must be divided into intervals, which are centered around the singular points. These are determined by setting the real parts of all denominators equal to zero. However, one cannot circumvent the restriction that all of the dummies $\{l_s\}$ must differ from each other. To treat the terms that remain, one is obliged to extend (A1) to larger matrix products. The new bounds must furnish additional factors of κ, so as to cancel the higher-order singularities that are brought about by the coincidences among the dummies $\{l_s\}$. Inevitably, the derivation of an improved bound (10) on the limiting vector $\mathbf{v}(t;\infty;m,n)$ degenerates into a rather technical affair.

APPENDIX B: CONTROLLING THE SUM χ

We set out to prove inequality (44) for the sum $\chi(x_1,x_2;p,q)$, with $0 \leqslant x_1 < 1$, $x_2 \geqslant 0$, and p,q non-negative. The proof relies on the following auxiliary result:

$$\chi(x_1,x_2;p,q)\leqslant\sum_{l=0}^{q-1}\alpha(l,q)\left[\frac{x_1^{\max(p-q+l,0)}}{(1-x_1)^{l+1}}+\frac{e^{x_2(l+1)}x_2^{\max(p-q+l,0)}}{\max(p-q+l,0)!}\right], \tag{B1}$$

where the choice of the coefficients $\alpha(l,q)$ is postponed. Verification of the inequality happens by applying induction in q to the recursion relation

$$\chi(x_1,x_2;p,q+1)=\sum_{k=\max(p-1,0)}^{\infty}\chi(x_1,x_2;k,q).$$

On the right we employ the induction assumption (B1). The sum over k can be done on the basis of the results

$$\sum_{k=\max(p-1,0)}^{\infty}x_1^{\max(k+l-q,0)}=\sum_{k=l}^{q-1}x_1^{\max(k+p-q-1,0)}+\frac{x_1^{\max(p-1,0)}}{1-x_1},$$

$$\sum_{k=\max(p-1,0)}^{\infty}\frac{x_2^{\max(k+l-q,0)}}{\max(k+l-q,0)!}\leqslant\sum_{k=l}^{q-1}\frac{x_2^{\max(k+p-q-1,0)}}{\max(k+p-q-1,0)!}+\frac{e^{x_2}x_2^{\max(p-1,0)}}{\max(p-1,0)!},$$

with $q\geqslant l\geqslant 0$. We interchange summations, and reproduce the induction assumption for $q+1$ by operating with the inequalities $(1-x_1)^{-1}\geqslant 1$ and $\exp(x_2)\geqslant 1$ in a suitable manner. It turns out that the coefficients $\alpha(l,q)$ are determined by the recursion

$$\alpha(l,q+1)=\sum_{k=0}^{l}\alpha(k,q)\,\theta_{q-k-1},$$

for $0\leqslant l\leqslant q$. The initial condition is given by $\alpha(l,q=1)=1$.

From our auxiliary result we deduce

$$\chi(x_1,x_2;p,q)\leqslant[(1-x_1)^{-q}+e^{x_2(p+q)}]\sum_{l=0}^{q-1}\alpha(l,q),$$

whereas from an identity similar to (39) we infer

$$\sum_{l=0}^{q-1}\alpha(l,q)\leqslant\binom{2q-1}{q}\leqslant 4^q.$$

This completes the proof.

APPENDIX C: CUT-OFF FOR THE κt EXPANSION

In deriving representation (51) for vector $\mathbf{d}(t;q)$, we expanded the exponential factor $\exp(\kappa t y)$ into a power series. The expansion yields a sum over j running from zero to infinity. For $j=0$ the summand can be evaluated on the basis of (26). The answer is given by the time-independent vector on the left-hand side of (51). We intend to show that for $1\leqslant j\leqslant p+q$ the summand is identical to zero. As far as the term including $D_3(y;q,p;-1)$ is concerned, this claim is an immediate consequence of (26). We thus focus on the term including $D_3(y;q,p;n)$.

Upon exploiting the identities

$$(1,\ 2)M\begin{pmatrix}2\alpha & 2\\ -\alpha & -1\end{pmatrix}=(1,\ 2)\cdot M\cdot\begin{pmatrix}2\\ -1\end{pmatrix}(\alpha,\ 1),$$

$$(1,\ 2)M\begin{pmatrix} -1 & -2 \\ \beta & 2\beta \end{pmatrix} = (1,\ 2)\cdot M \cdot \begin{pmatrix} -1 \\ \beta \end{pmatrix}(1,\ 2),$$

with M any (2×2) matrix, we see that the jth expansion coefficient is proportional to the form

$$\frac{1}{j!}\left[\mathbf{f}(j,p,q)\cdot\begin{pmatrix} 2 \\ -1 \end{pmatrix}(q+2,\ 1)+g(j,p,q)(1,\ 2)\right].$$

We have defined the vector

$$\begin{aligned}\mathbf{f}(j,p,q)=&\sum_{n=0}^{q+p}\sum_{l_0=n}\sum_{l_1=l_0-1}^{q+p-1}\sum_{l_2=l_1-1}^{q+p-2}\cdots\sum_{l_p=l_{p-1}-1}^{q}\prod_{s=1}^{p}\theta_{l_s}\oint\frac{\mathrm{d}y}{2\pi i}\frac{y^j}{(2n+1)(2n+3)}\\ &\times\prod_{s=0}^{q}\frac{2s+1}{y+2s+1}\prod_{s=0}^{n-1}\frac{y+2s+1}{2s+1}\prod_{s=1}^{p}\left[(y+2l_s+1)(y+2l_s+3)(2l_s+3)\right]^{-1}\\ &\times(1,2)\cdot\left\{\prod_{s=1}^{p}V(y;l_s,l_{s-1})\right\}\delta_{l_p,q},\end{aligned}$$

and the scalar

$$\begin{aligned}g(j,p,q)=&\sum_{n=0}^{q+p}\sum_{l_0=n}\sum_{l_1=l_0-1}^{q+p-1}\sum_{l_2=l_1-1}^{q+p-2}\cdots\sum_{l_p=l_{p-1}-1}^{q}\prod_{s=1}^{p}\theta_{l_s}\oint\frac{\mathrm{d}y}{2\pi i}\frac{y^j}{(2n+1)(2n+3)}\\ &\times\prod_{s=0}^{q}\frac{2s+1}{y+2s+1}\prod_{s=0}^{n-1}\frac{y+2s+1}{2s+1}\prod_{s=1}^{p}\left[(y+2l_s+1)(y+2l_s+3)(2l_s+3)\right]^{-1}\\ &\times(1,2)\cdot\left\{\prod_{s=1}^{p}V(y;l_s,l_{s-1})\right\}\cdot\begin{pmatrix} -1 \\ l_p+2 \end{pmatrix}\theta_{q-l_p},\end{aligned}$$

for j, p, and q non-negative.

The following recursion relations will be of service to us

$$g(j+1,p,q)=(2q+1)\left[g(j,p,q-1)\,\theta_{q-1}-g(j,p,q)+\mathbf{f}(j,p,q)\cdot\begin{pmatrix} -1 \\ q+2 \end{pmatrix}\right]+\mathbf{f}(j+1,p,q)\cdot\begin{pmatrix} -1 \\ q+2 \end{pmatrix},$$

$$\begin{aligned}&(2q+3)[\mathbf{f}(j+1,p+1,q)+(2q+1)\mathbf{f}(j,p+1,q)]\\ &\quad=(2q+1)(2q+5)\mathbf{f}(j,p,q+1)\cdot\begin{pmatrix} 0 \\ 1 \end{pmatrix}(0,1)-\frac{1}{2}(2q+5)\mathbf{f}(j+1,p,q+1)\\ &\qquad\cdot\begin{pmatrix} 0 \\ 1 \end{pmatrix}(1,0)-(q+1)\mathbf{f}(j,p,q)\cdot\begin{pmatrix} 2 \\ -1 \end{pmatrix}(1,2)-(2q+3)^{-1}g(j+1,p,q+1)(4q+5,4q+4)\\ &\qquad-2g(j,p,q+1)(q+1,1)+(2q+3)^{-1}\mathbf{f}(j+1,p,q+1)\cdot\begin{pmatrix} -1 \\ q+3 \end{pmatrix}(4q+5,4q+4)\\ &\qquad+2\mathbf{f}(j,p,q+1)\cdot\begin{pmatrix} -1 \\ q+3 \end{pmatrix}(q+1,1),\end{aligned}$$

with j, p, and q non-negative again. To check the first recursion, one should perform for $g(j+1,p,q)$ the reduction $j+1\to j$ by writing $y=y+2q+1-(2q+1)$. The cases $l_p=q$ and $l_p\leqslant q-1$ must be processed separately. To check the second recursion, one should perform for $\mathbf{f}(j+1,p+1,q)+(2q+1)\mathbf{f}(j,p+1,q)$ the reduction $p+1\to p$ by substituting for $V(y;q,l_p)$ the rep-

resentation out of Sec. V. In the second contribution of V the Kronecker delta δ_{q,l_p} is contained. It causes the upper boundaries of all sums to decrease by one, and hence, generates the reduction $q+1\to q$. To reshape the third contribution of V, the above-mentioned identities for matrix M should be employed. The sum over l_p must be extended to $l_p=q+1$; the ensuing correction term can be converted to two vectors of type **f**.

We first solve the above-mentioned recursions for $p=0$. From (26) we learn that $\mathbf{f}(j=0,p=0,q)=(2q+3)^{-1}(1,2)$ and $g(j=0,p=0,q)=1$ make up the initial conditions. Furthermore, one has $\mathbf{f}(j+1,p=0,q)+(2q+1)\mathbf{f}(j,p=0,q)=0$, because the left-hand side gives rise to an analytic integrand. From the first recursion we now infer

$$\mathbf{f}(j,p=0,q)=(-1)^j(2q+3)^{-1}(2q+1)^j(1,2),\quad g(j,p=0,q)=\delta_{j,0}.$$

On the result for g the constraint $0\leqslant j\leqslant q$ must be imposed. For $p=0$ and $1\leqslant j\leqslant q$ the jth coefficient of the κt expansion is indeed identical to zero.

Moving on to the case $p\geqslant 1$, we deduce from the representation of V and (26)

$$\mathbf{f}(j=0,p,q)=-\delta_{p,1}(2q+3)^{-1}(1,0),\quad g(j=0,p,q)=\delta_{p,1}(2q+3)^{-1},$$

with $p\geqslant 1$ and $q\geqslant 0$. Let us make in the first and second recursion the choice $p=1$ and $p=0$, respectively. With the help of the findings for the case $p=0$ the solutions come out as

$$\mathbf{f}(j,p=1,q)=(-1)^j(2q+3)^{-1}(2q+1)^{j-1}(1,2),\quad g(j,p=1,q)=0,$$

where the inequality $1\leqslant j\leqslant q+1$ must be respected. Also for $p=1$ our truncation of the κt expansion is permitted.

Next, we set in the first and second recursion $p=2$ and $p=1$, respectively. The above-mentioned results for the case $p=1$ provide us with the following solutions:

$$\mathbf{f}(j,p=2,q)=g(j,p=2,q)=0,$$

with q non-negative and the condition $0\leqslant j\leqslant q+2$ to be fulfilled. Induction in p shows that the last statement is true for all $p\geqslant 2$ and $0\leqslant j\leqslant p+q$. This completes our proof.

APPENDIX D: CONVERGENCE TO THE THERMAL STATE FOR WEAK DAMPING

We are going to carry out the consistency check that was announced in the main text. The idea is to demonstrate that the interchange of limit and sum, as practiced in Sec. V, does not harm the limit (3). The atomic density operator still converges to the thermal state for large times.

It is sufficient to prove that

$$\lim_{t\to\infty}K(t;q-n,p;n,n)=\left[\begin{pmatrix}0&0\\1&2\end{pmatrix}\delta_{p,0}+2(-1)^p\begin{pmatrix}0&0\\1&1\end{pmatrix}\theta_{p-1}\right]\delta_{n,-1},$$

with $q\geqslant 0$, $p\geqslant 0$, $n\geqslant -1$, and $p+q\geqslant n$. Owing to (48), we can work in two dimensions. For the kernel on the left-hand side the weak-damping expression of Sec. V must be substituted.

For n positive the foregoing statement is a consequence of (47) and (49), whereas for $n=-1$ it reduces to

$$\mathbf{f}'(p,q)\cdot\begin{pmatrix}2\\-1\end{pmatrix}(q+2,1)+g'(p,q)(1,2)=\left(\frac{1}{2},1\right)\delta_{p,0}+(1,1)\,\theta_{p-1},\tag{D1}$$

where p and q are non-negative, and (50) has been used. We have introduced a vector

$$\mathbf{f}'(p,q)=\frac{1}{2}\sum_{l_0=-1}\sum_{l_1=l_0-1}^{q+p-1}\sum_{l_2=l_1-1}^{q+p-2}\cdots\sum_{l_p=l_{p-1}-1}^{q}\prod_{s=1}^{p}\theta_{l_s}\delta_{l_p,q}(0,\ 1)\cdot\left\{\prod_{s=1}^{p}V'(l_s,l_{s-1})\right\},$$

a scalar

$$g'(p,q)=\frac{1}{2}\sum_{l_0=-1}\sum_{l_1=l_0-1}^{q+p-1}\sum_{l_2=l_1-1}^{q+p-2}\cdots\sum_{l_p=l_{p-1}-1}^{q}\prod_{s=1}^{p}\theta_{l_s}(0,1)\cdot\left\{\prod_{s=1}^{p}V'(l_s,l_{s-1})\right\}\cdot\begin{pmatrix}-1\\ l_p+2\end{pmatrix},$$

and a matrix

$$V'(k,l)=(2k+1)^{-1}(2k+3)^{-1}\left[-(2k+1)(2k+5)\begin{pmatrix}0&0\\0&1\end{pmatrix}\delta_{k,l-1}\right.$$
$$\left.+(k+1)\begin{pmatrix}2&4\\-1&-2\end{pmatrix}\delta_{k,l}+2\begin{pmatrix}-1&-1\\l+2&l+2\end{pmatrix}\begin{pmatrix}0&0\\k+1&1\end{pmatrix}\theta_{k-l}\right].$$

From these expressions we see that for $p=0$ the condition (D1) is trivial.

To cope with the case $p\geqslant 1$, one should exploit the recursions

$$\mathbf{f}'(p+1,q)=-\frac{2q+5}{2q+3}\mathbf{f}'(p,q+1)\cdot\begin{pmatrix}0\\1\end{pmatrix}(0,1)+\frac{q+1}{(2q+1)(2q+3)}\mathbf{f}'(p.q)\cdot\begin{pmatrix}2\\-1\end{pmatrix}(1,2)$$
$$+\frac{2g'(p,q)}{(2q+1)(2q+3)}(q+1,1),$$

$$g'(p+1,q)=-\frac{(q+2)(2q+5)}{(2q+3)}\mathbf{f}'(p,q+1)\cdot\begin{pmatrix}0\\1\end{pmatrix}+3\mathbf{f}'(p,0)\cdot\begin{pmatrix}0\\1\end{pmatrix}-\frac{2(q+2)}{2q+3}g'(p,q),$$

with $p\geqslant 1$ and $q\geqslant 0$. In deriving these, one must use the identity

$$\sum_{l=1}^{m}(2l-1)^{-1}(2l+1)^{-1}=m(2m+1)^{-1},$$

with m non-negative. For $p=1$ the solution for $\mathbf{f}'$ and g' can be calculated from the defining expressions. For $p\geqslant 2$ the above-given recursions come into play. One is led to

$$\mathbf{f}'(p,q)=\frac{(q+1,1)}{(2q+1)(2q+3)},\quad g'(p,q)=\frac{q+1}{2q+3},$$

for $p\geqslant 1$. Constraint (D1) turns out to be true, so our consistency check is successful.

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On the invariance of residues of Feynman graphs

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We use simple iterated one-loop graphs in massless Yukawa theory and QED to pose the following question: what are the symmetries of the residues of a graph under a permutation of places to insert subdivergences. The investigation confirms partial invariance of the residue under such permutations: the highest weight transcendental is invariant under such a permutation. For QED this result is gauge invariant, i.e., the permutation invariance holds for any gauge. Computations are done making use of the Hopf algebra structure of graphs and employing GiNaC to automate the calculations. © *2002 American Institute of Physics.*
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I. INTRODUCTION

This paper serves three purposes: (i) it employs GiNaC[1] in Feynman diagram calculations and provides algorithms which automate the renormalization process, very much in the spirit of Ref. 2; (ii) it investigates symmetries of short distance singularities under permutations of places where to insert subdivergences in a graph; (iii) it once more confirms the presence or absence of transcendental coefficients of short-distance singularity in accordance with the topology of a graph.

Our laboratory of investigation are simple one-loop Feynman graphs in massless Yukawa theory or QED, inserted into each other in tree-like hierarchies. Thus, the combinatorics of renormalization boils down to the Hopf algebra of decorated rooted trees with only a small number of decorations and the analytical challenge posed by those decorations reduces to expansions of Γ-functions near unit argument. The question we can ask is for the distribution of the Riemann ζ-function over the various poles in the Laurent series of graphs of that form.

In contrast to Ref. 2 and subsequent papers,[3] where the renormalization problem was automated in a similar context optimized for speed and efficiency, we have developed algorithms which allow for nontrivial spin-structures and an easy generalization to arbitrary decorations: the primitive decorations can be inserted as arguments so that the algorithm can handle arbitrary primitive graphs when their analytic structure becomes known.

We work in the context of dimensional regularization, so that any Feynman graph becomes a Laurent series in $\epsilon=(4-D)/2$, the deviation of the dimension from its integer value four, and the pole terms reflect the short distance singularities in the theory. The first-order pole is denoted as the residue of a graph. Its significance lies in the fact that higher pole terms can be reduced to polynomials in residues,[4] and in the fact that the residue of a primitive graph is an invariant under diffeomorphisms of external parameters of the graph (diffeomorphisms of external momenta and masses) as well as an invariant under variations of renormalization schemes. Such a residue is a motivic number then in some modern mathematic parlance. The question as to which class of such numbers is sufficient to describe the residues of a given quantum field theory is open and fascinating.[5]

We only study two much more basic questions, motivated by previous and ongoing investi-

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FIG. 1. "Swiss cheese" and "ladder" master topology. (a) "Swiss cheese" topology, (b) "ladder" topology.

gations into the analytic structure of pole terms and residues in particular.

The first is the independence of the appearance of transcendentals under variations of the quantum field theory which realizes a graph with a given topology. To specify the topology of a one-particle irreducible Feynman graph Γ, let us consider the adjacency matrix $M(\Gamma)$ of Γ. If Γ has n vertices, this matrix is an $n\times n$ matrix. We take for its nonzero entries pairs (`propagator type, powercounting weight`), i.e., each nonzero entry $M(\Gamma)_{ij}$ specifies that vertex i is connected to vertex j by a propagator of some type, which has a certain powercounting weight. In the cases studied here, the possible entries are

$$(\texttt{fermion,1}),\ (\texttt{photon,2}),\ (\texttt{scalar boson,2}).$$

The listing of the powercounting weight is redundant, as it is determined by the type of the propagator. We list it just for easy reference. Additionally, we can state the types of the vertices in the diagonal entries of the matrix (no vertex is connected to itself by a propagator).

The graphs of QED and Yukawa theory which we will compare always have adjacency matrices which agree in all their zero entries,

$$M(\Gamma_{\mathrm{QED}})_{ij}=0\Leftrightarrow M(\Gamma_{\mathrm{Yuk}})_{ij}=0$$

and agree for each nonzero entry in the powercounting degree of the corresponding edge. It is only the nature of the edges which changes from the spin one vector boson propagator—the QED photon—to the spin zero scalar boson propagator in Yukawa theory. Note that the structure of short distance singularity then remains fixed in the transition of one theory to the other. We then expect and confirm that rational numbers can vary in the transition from one theory to the other, while the transcendentals we see remain invariant and specific for the chosen topology. Here, a topology is uniquely described by considering in such an adjacency matrix all nonzero entries as equal. So it just gives information about how vertices are connected, but forgets about the nature of the propagators establishing that connection. To find nonrational numbers, we have to go up to four loops at least in the simple class of Feynman graphs which we consider. There it is the swiss cheese topology of Fig. 1(a) in which we expect to see a residue $\sim\zeta(3)$, while the ladder topology of Fig. 1(b) is known to have only rational residues.[6]

The second question is of different nature: for a log-divergent vertex graph which is primitive under the coproduct, it is evident that its residue has the above-mentioned invariances. The Hopf algebra structure immediately allows one to prove that in a vertex graph which is not primitive under the coproduct such that the graph contains divergent subgraphs, the coefficient of the highest order pole still has these symmetries and is given by an easy calculable product of residues with a combinatorial factor, determined by the scattering type formula of Ref. 4, which incorporates the 't Hooft relations between higher pole terms in graphs.

What we call here the 't Hooft relations in accordance with Ref. 4 is the simple fact that higher order poles in a graph Γ with UV-divergent subgraphs γ can be calculated from products of lower order poles of these subgraphs γ and their complements Γ/γ. This is well known and a necessary requirement to make the renormalization group work: the Z-factor for a given physical quantity is an invertible (it starts with 1) formal series over counterterms of graphs such that its logarithmic derivative with respect to the variation of the renormalization scale ν, $\mathrm{d}\log(Z)/\mathrm{d}\nu^2$, is finite. This finiteness establishes relations between pole terms which, for the case of dimensional

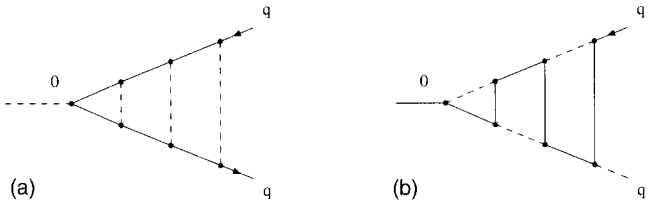


FIG. 2. The two types of vertex corrections. (a) Vertex correction of type one. (b) Vertex correction of type two.

regularization, were, it seems, first explored by 't Hooft. These relations are a direct consequence of the mathematical structure of the Hopf algebra underlying renormalization, and its one-parameter group of automorphisms.[4]

Let us now consider the residue of such a graph which does have divergent subgraphs. Typically, this residue will be a number which can be decomposed in terms of transcendental weight: it will contain contributions ranging from rational numbers to monomials in $\zeta(j)$ of up to transcendental weight $\ell-1$, where ℓ is the bidegree of the graph, calculated from its coproduct.[7] For all graphs considered here, this bidegree simply agrees with the number of loops in Yukawa theory, or can be shifted in the case of QED as explained later in the text. We cannot expect the whole residue to be invariant under the above-mentioned symmetries, as rational numbers can and will vary freely. But here we report a remarkable partial symmetry observed in our rather restricted lab of iterated one-loop graphs: the highest weight transcendental in the residue is invariant under permutations of external momentum as described in the following. We confirm this by empirical calculation to high loop orders. We finally prove the result in the context of the simple iterated one-loop graphs considered here. One has an almost elementary proof in this context and we will discuss the difficulties which arise in the general case. The nature of this result fits nicely with a structural investigation of Dyson–Schwinger equations.[8] Note again that changing the momentum flow but maintaining the topology corresponds to alterations of the type of nonzero entries in a suitable adjacency matrix, as Fig. 2 clearly exhibits. Again, the degree of powercounting and hence the structure of short distance singularities, as well as the topology, remain unchanged.

To understand the type of symmetry we want to investigate, let us consider the one-loop vertex function. If $\Gamma(p_1,p_2,p_3)$ is a vertex correction with momentum p_1 for the external boson, p_2 for the incoming fermion, and $p_3=p_1+p_2$ for the outgoing fermion, then we will compare $\Gamma^1:=\Gamma(0,p,p)$ with $\Gamma^2:=\Gamma(p,p,0)$ at the one-loop level. It is a single permutation of the flow of an external momentum for a vertex function at zero momentum transfer, which distinguishes the two one-loop functions. Locality of counterterms ensures that the counterterm for a vertex correction graph is invariant under this permutation for any graph. So nothing exciting can be learned from just changing the momentum flow in a given vertex graph. Now let us start with such one-loop vertex corrections and let us insert more one-loop vertex corrections always at the vertex of zero momentum transfer (zmt), which indeed changes under the above-mentioned permutation. This gives the topological equivalent Feynman graphs Γ^1, Γ^2, with permuted types of propagators, of Fig. 2. They indeed have adjacency matrices such that again

$$M(\Gamma^1)_{ij}=0\Leftrightarrow M(\Gamma^2)_{ij}=0.$$

Note that it is the requirement to maintain the same topology which forces us to consider quite different looking graphs. For them, the usual field theoretic requirements only demand that the coefficients of the highest order poles are identical. All nonleading pole terms in ϵ do not have to and indeed do not agree.

But a closer investigation will establish a remaining partial symmetry between those graphs, such that the highest weight transcendental in the residue is invariant. Such symmetries are of great interest. Feynman graphs with subdivergences can be built by using the pre-Lie structure of graphs, which results from underlying insertion operads.[5] The question to what extent the permutation group acts trivially under such insertions is a natural question in operad theory which needs

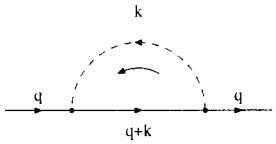
to be answered to understand these operads. It directly leads to the questions studied here in a simplified context. We regard the results reported here as a first step in a detailed analysis of actions of the permutation group in this context.

With regard to the first question, we remind the reader that for a massless Yukawa theory represented as a Laurent-series in ϵ, it was already shown in Ref. 9 that graphs with the swiss cheese topology of Fig. 1(a) possess a $\zeta(n)$ in their counterterm, whereas graphs with a ladder topology like in Fig. 1(b) just evaluate to rational coefficients. Similar results were obtained in QED and other theories for vertex functions of type $\Gamma(0,p,p)$ and self-energies, in Refs. 2, 3, and 6.

Our first aim is now to find out if this remains true in massless QED for both types of momentum flow and if there are any symmetries in the coefficients of the ζ-functions in both theories, under the permutation between the two types of vertex functions Γ^1 and Γ^2. Therefore we will rebuild the scheme given in Ref. 9 for the massless Yukawa theory with an extension to vertex corrections that carry a different flow of momentum in the above-described sense, and similarly for QED using the matrix calculus of Ref. 10. The resulting algorithm is implemented using the GiNaC library and will be described in Sec. V. With the help of this program, we will calculate the antipode of graphs that represent the different topologies given previously and compare them.

II. CALCULATIONS

Consider a one-loop contribution to the fermionic propagator:



$$\equiv \quad \Sigma_{[0,0]}(q^2) = \int d^D k \, \frac{1}{(\not{q}+\not{k})} \frac{1}{k^2}$$

where the subscript "[0, 0]" will soon serve to give the number of one-loop subdivergences to be inserted inside the diagram at the fermionic or bosonic line. All integrals considered in this paper can be reduced to integrals $F_{a,b}$ (Ref. 11) in D-dimensional Euclidean space:

$$\begin{aligned} I(q;a,b) &\equiv \frac{1}{(\nu^2)^{-\varepsilon}} \int d^D k \, \frac{1}{[k^2]^a [(q-k)^2]^b} \\ &=: \frac{1}{(\nu^2)^{-\varepsilon}} [q^2]^{(2-(a+b)-\varepsilon)} F_{a,b} \end{aligned} \tag{1}$$

with

$$F_{a,b} \equiv F_{b,a} := \frac{\Gamma(2-a-\varepsilon)\Gamma(2-b-\varepsilon)\Gamma(a+b-2+\varepsilon)}{\Gamma(a)\Gamma(b)\Gamma(4-a-b-2\varepsilon)}, \tag{2}$$

and $D=4-2\varepsilon$. ν is the renormalization scale that we set equal to "1" in the following. We typically need these integrals for $a=n_1+n_2\varepsilon$, $b=m_1+m_2\varepsilon$, for integers n_1, n_2, m_1, m_2. Note that

$$F_{a,-n} = F_{-n,b} = 0, \quad n \in \mathbb{N}^0. \tag{3}$$

Accordingly, in our conventions

$$\Sigma_{[0,0]}(q^2) = [q^2]^{-\varepsilon} \tfrac{1}{2} F_{1,1} \not{q} =: [q^2]^{-\varepsilon} \Sigma_{0,0} \not{q}. \tag{4}$$

This reduces the identification of nonrationals (transcendentals, we dare say in the following) to an expansion of the Γ-function near unit argument, as promised, given by the formula:

$$\Gamma(1+\varepsilon)=\exp(-\gamma\varepsilon)\exp\left(\sum_{n=2}^{\infty}\frac{\zeta(n)}{n}(-\varepsilon)^n\right),\quad |\varepsilon|<1.$$

Internally, GiNaC follows a different approach. It computes the derivatives $\Gamma'(x)=\Gamma(x)\psi(x)$ and $(\mathrm{d}^n/\mathrm{d}x^n)\psi(x)=\psi_n(x)$ in terms of polygamma functions $\psi_m(x)$ and "knows" how to evaluate polygamma functions at integer arguments, e.g., $\psi(1)=-\gamma$ and $\psi_n(1)=(-)^{n+1}n!\zeta(n+1)$.

A. Yukawa theory

The study of iterated one-loop integrals reduces to the study of the following elementary functions, which we will call *characterizing functions*: The one-loop fermion self-energy with insertions at its two internal propagators demands knowledge of

$$\Sigma_{i,j}:=\tfrac{1}{2}[F_{i\varepsilon,1+j\varepsilon}+F_{1+i\varepsilon,1+j\varepsilon}-F_{1+i\varepsilon,j\varepsilon}]. \tag{5}$$

The one-loop boson self-energy with insertions at its two internal edges is given by $\Pi_{i,j}$ and the two one-loop vertex functions at zero momentum transfer with insertions at either the zero momentum vertex, or internal lines, need knowledge of functions $\Gamma_{i,j}$ for the vertex corrections,

$$\Pi_{i,j}/[\mathrm{tr}(\mathbb{1})]:=-\tfrac{1}{2}[F_{i\varepsilon,1+j\varepsilon}-F_{1+i\varepsilon,1+j\varepsilon}+F_{1+i\varepsilon,j\varepsilon}], \tag{6}$$

$$\Gamma^1_{i,j}:=F_{1+i\varepsilon,1+j\varepsilon}, \tag{7}$$

$$\Gamma^2_{i,j}:=\tfrac{1}{2}[F_{2+i\varepsilon,j\varepsilon}-F_{2+i\varepsilon,1+j\varepsilon}+F_{1+i\varepsilon,1+j\varepsilon}]. \tag{8}$$

Here, we have divided the boson self-energy by the trace of the unit matrix $\mathrm{tr}(\mathbb{1})$ (trace over spinorial indices) for easier comparison of insertions of subgraphs into boson and fermion lines.

The functions Γ^1 and Γ^2 represent the two types of vertex corrections shown in Fig. 2.

The indices i and j give the number of subdivergences at different lines:

$\Sigma_{i,j}$: i = number of subdivergences at the fermion line,
j = number of subdivergences at the boson line.

$\Pi_{i,j}$: i = number of subdivergences at the lower fermion line,
j = number of subdivergences at the upper fermion line.

$\Gamma^1_{i,j}$: i = number of fermion self-energies and vertex corrections plugged into the zmt vertex and the internal edges connected to it,
j = number of subdivergences at the boson line not connected to this vertex.

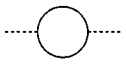
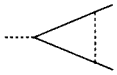
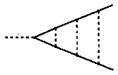
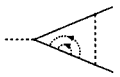
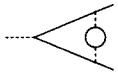
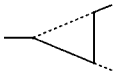
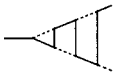
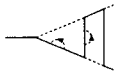
$\Gamma^2_{i,j}$: i = number of fermion or boson self-energies and vertex corrections plugged into the zmt vertex and the internal edges connected to it,
j = number of fermion self-energies at the fermion line not connected to the vertex of zmt.

To denote complete graphs, we introduce additional functions $\Sigma_{[i,j]}$, $\Pi_{[i,j]}$, and $\Gamma_{[i,j,k]}$ which state the different kinds of subdivergences [cf. $\Sigma_{[0,0]}$ in (4)]. The indices count for $\Sigma_{[i,j]}$ and $\Pi_{[i,j]}$ as the indices in their corresponding characterizing functions given earlier. For vertex corrections of type one and two, the notation $\Gamma_{[i,j,k]}$ denotes the three types of insertions in the following way: i insertions of self-energies at the edges connected to the zero momentum vertex, j insertions of self-energies at the edge not connected to that vertex, and k insertions of vertex corrections at the zmt vertex. Table I gives examples.

B. QED

The main difference stems from the presence of a gauge parameter ξ in the photon propagator and from the $-ie\gamma_\mu$ vertex which make the calculations more difficult. In fact, as we will see, we

TABLE I. Some examples how self-energy and vacuum polarization graphs are built up in Yukawa theory.

	$\Sigma_{[0,0]}(q^2) = (-ig)^2\,\Sigma_{0,0}[q^2]^{-\epsilon}\not{q}$
	$\Sigma_{[1,0]}(q^2) = (-ig)^4\Sigma_{1,0}\Sigma_{0,0}[q^2]^{-2\epsilon}\not{q}$
	$\Sigma_{[2,1]}(q^2) = (-ig)^8\,\Sigma_{2,1}\Pi_{0,0}(\Sigma_{0,0})^2[q^2]^{-4\epsilon}\not{q}$
	$\Pi_{[0,0]}(q^2) = (-ig)^2\,\Pi_{0,0}[q^2]^{-\epsilon}q^2$
	$\Pi_{[2,1]}(q^2) = (-ig)^8\,\Pi_{2,1}\Sigma_{1,0}(\Sigma_{0,0})^2[q^2]^{-4\epsilon}q^2$
	$\Gamma^1_{[0,0,0]}(q^2) = (-ig)^3\,\Gamma^1_{0,0}[q^2]^{-\epsilon}$
	$\Gamma^1_{[0,0,2]}(q^2) = (-ig)^7\,\Gamma^1_{2,0}\Gamma^1_{1,0}\Gamma^1_{0,0}[q^2]^{-3\epsilon}$
	$\Gamma^1_{[2,0,0]}(q^2) = (-ig)^7\,\Gamma^1_{2,0}\Sigma_{1,0}\Sigma_{0,0}[q^2]^{-3\epsilon}$
	$\Gamma^1_{[0,1,0]}(q^2) = (-ig)^5\,\Gamma^1_{0,1}\Pi_{0,0}[q^2]^{-2\epsilon}$
	$\Gamma^2_{[0,0,0]}(q^2) = (-ig)^3\,\Gamma^2_{0,0}[q^2]^{-\epsilon}$
	$\Gamma^2_{[0,0,2]}(q^2) = (-ig)^7\,\Gamma^2_{2,0}\Gamma^2_{1,0}\Gamma^2_{0,0}[q^2]^{-3\epsilon}$
	$\Gamma^2_{[1,1,1]}(q^2) = (-ig)^9\Gamma^2_{3,0}\Gamma^2_{1,1}(\Sigma_{0,0})^2[q^2]^{-4\epsilon}$

will have to deal with matrices for the vertex corrections.[10] Nevertheless, the structure for the translation of a graph to an analytical result will be similar to what we had in Yukawa theory. Hence we will mainly give the results and just list the relevant changes.

1. Vacuum polarization

We will only consider one-loop photon self-energies, vacuum polarizations, as in our restricted class of Feynman graphs we cannot construct a gauge invariant set of vacuum polarizations at higher loop orders.

2. Fermion self-energy

The fermionic propagator in QED with insertions at the fermionic and photonic lines demands $\widetilde{\Sigma}$:

$$\begin{aligned}\widetilde{\Sigma}_{i,j} = \tfrac{1}{2}[&(2-D)F_{1+i\varepsilon,j\varepsilon} - (3-D)F_{i\varepsilon,1+j\varepsilon} - (3-D)F_{1+i\varepsilon,1+j\varepsilon}\\ &+ F_{-1+i\varepsilon,2+j\varepsilon} - 2F_{i\varepsilon,2+j\varepsilon} + F_{1+i\varepsilon,2+j\varepsilon}](1-\delta_{0,j})\\ &+ [(2-D)\Sigma_{i,0} + \xi\Sigma'_{i,0}]\delta_{0,j}\,, \end{aligned} \tag{9}$$

with

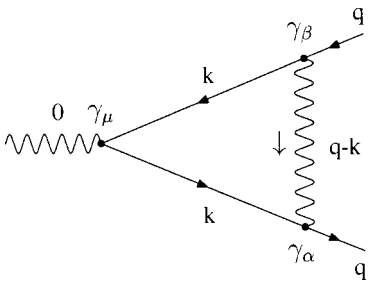


FIG. 3. One-loop contribution to the vertex correction.

$$\Sigma_{i,0}=\tfrac{1}{2}[F_{1+i\varepsilon,1}+F_{i\varepsilon,1}], \tag{10}$$

$$\Sigma'_{i,0}=\tfrac{1}{2}[F_{-1+i\varepsilon,2}-2F_{i\varepsilon,2}-F_{i\varepsilon,1}+F_{1+i\varepsilon,2}-F_{1+i\varepsilon,1}]. \tag{11}$$

The appearance of the Kronecker $\delta_{0,j}$ is obvious from the fact that the presence of one-loop vacuum polarizations in the internal photon line forces transversality of that propagation.

3. Vertex corrections

The most important difference to the Yukawa theory occurs in this part of the calculation. Consider the one-loop vertex correction in QED for vertex graphs as shown in Fig. 3.

The external structure of the vertex consists of two form factors: One for γ_μ and one for $q_\mu \not{q}/q^2$, as $\Gamma_\mu(0,q,q)=F_1(q^2)\gamma_\mu+F_2(q^2)(q_\mu \not{q}/q^2)$. In the previous calculations, every subdivergence just caused a change in the exponent of various momenta in denominators of the integrals, resulting in nonintegral exponents in Eq. (1). Now the result has two form factors F_1, F_2 that emerge through the evaluation of a subgraph in a ''bigger'' graph. We will administer the two form factors in a matrix notation in accordance with Ref. 10. We will need two-by-two matrices. The four entries determine four functions $\Delta^{(i,j)}_{a,b}$. Here, a, $b\in\{1,2\}$ and (i, j) count the number of internal insertions as before. The case $b=1$ corresponds to an internal vertex γ_μ, the case $b=2$ corresponds to an internal vertex $q_\mu \not{q}/q^2$ (where q, say, is the momentum flowing through this zero-momentum transfer vertex), while the index a enumerates the two possible form factors in the result. The result for the one-loop graph of Fig. 3 is then

$$\left[\Delta^{(0,0)}_{1,1}\gamma_\mu+\Delta^{(0,0)}_{2,1}\frac{q_\mu \not{q}}{q^2}\right][q^2]^{-\varepsilon}.$$

For the two-loop graph shown in Fig. 4 we find

$$\Gamma_{[0,0,1]}=\left[(\Delta^{(0,0)}_{11}\Delta^{(1,0)}_{11}+\Delta^{(0,0)}_{21}\Delta^{(1,0)}_{12})\gamma_\mu+(\Delta^{(0,0)}_{11}\Delta^{(1,0)}_{21}+\Delta^{(0,0)}_{21}\Delta^{(1,0)}_{22})\frac{q_\mu \not{q}}{q^2}\right][q^2]^{-2\varepsilon}. \tag{12}$$

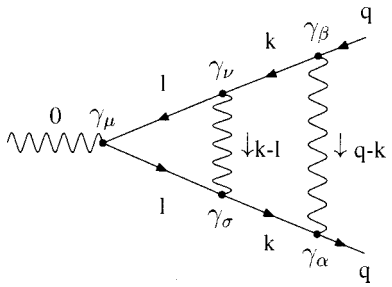


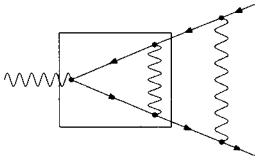
FIG. 4. Two-loop contribution to the vertex correction.

The multiplication of the $\Delta_{kl}^{(i,j)}$ can be reformulated as a matrix multiplication. We define the general matrix (the upper index refers to the two cases of vertex corrections which we consider, we omit that index for simplicity in the matrix entries):

$$M_{i,j}^{1} := \begin{pmatrix} \Delta_{11}^{(i,j)} & \Delta_{12}^{(i,j)} \\ \Delta_{21}^{(i,j)} & \Delta_{22}^{(i,j)} \end{pmatrix}.$$

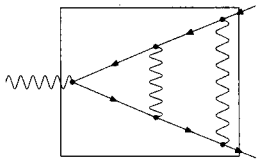
To each part of a graph which has the form of a vertex correction we assign a matrix. In this case of vertex corrections of type one, as in Fig. 2(a), the index i is the total number of subdivergences at the fermionic line (with no difference if it is of the form Σ or Γ) and j the number of subdivergences at the photon line, as in Yukawa theory. One multiplies the matrices for the different divergent parts of a graph, starting from the innermost vertex correction which contains the vertex of zmt, and the corresponding matrix has zero entries in the second column obviously.

Let us make this clear with the help of our example of the two-loop vertex correction again. For the graph of Fig. 4 this means that we begin with the inner vertex correction marked with a box:



$$\equiv M_{0,0}^{1} = \begin{pmatrix} \Delta_{11}^{(0,0)} & 0 \\ \Delta_{21}^{(0,0)} & 0 \end{pmatrix}$$

and then multiply this with the matrix for the outer vertex correction, which has one vertex correction as a subdivergence:



$$\equiv M_{1,0}^{1} = \begin{pmatrix} \Delta_{11}^{(1,0)} & \Delta_{12}^{(1,0)} \\ \Delta_{21}^{(1,0)} & \Delta_{22}^{(1,0)} \end{pmatrix}$$

$$\Rightarrow \quad \begin{pmatrix} \Delta_{11}^{(1,0)} & \Delta_{12}^{(1,0)} \\ \Delta_{21}^{(1,0)} & \Delta_{22}^{(1,0)} \end{pmatrix} \begin{pmatrix} \Delta_{11}^{(0,0)} & 0 \\ \Delta_{21}^{(0,0)} & 0 \end{pmatrix} = \begin{pmatrix} \Delta_{11}^{(1,0)}\Delta_{11}^{(0,0)} + \Delta_{12}^{(1,0)}\Delta_{21}^{(0,0)} & 0 \\ \Delta_{21}^{(1,0)}\Delta_{11}^{(0,0)} + \Delta_{22}^{(1,0)}\Delta_{21}^{(0,0)} & 0 \end{pmatrix}. \tag{13}$$

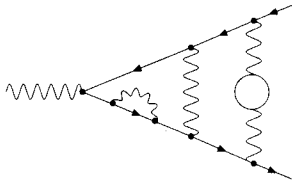
Multiplying (13) with $(1,0)^T[q^2]^{-2\epsilon}$, we get the result as the column vector

$$\begin{pmatrix} (\Delta_{11}^{(1,0)}\Delta_{11}^{(0,0)} + \Delta_{12}^{(1,0)}\Delta_{21}^{(0,0)})[q^2]^{-2\epsilon} \\ (\Delta_{21}^{(1,0)}\Delta_{11}^{(0,0)} + \Delta_{22}^{(1,0)}\Delta_{21}^{(0,0)})[q^2]^{-2\epsilon} \end{pmatrix},$$

where in general the ''upper'' entry of this vector is the form factor $F_1(q^2)$ belonging to γ_μ and the ''lower'' one the form factor $F_2(q^2)$ belonging to $q^\mu \not{q}/q^2$.

Subdivergences that are *not* vertex corrections given by $\Sigma_{i,j}$ and $\Pi_{i,j}$ are multiplied with a unit matrix and inserted in the string of matrices in front of the matrix of the vertex correction which they are part of. They increase subscripts *i,j* accordingly in that matrix.

As an example we get for the following graph:



$$\equiv \begin{pmatrix} \Delta_{11}^{(2,1)} & \Delta_{12}^{(2,1)} \\ \Delta_{21}^{(2,1)} & \Delta_{22}^{(2,1)} \end{pmatrix} \begin{pmatrix} \Pi_{0,0} & 0 \\ 0 & \Pi_{0,0} \end{pmatrix} \begin{pmatrix} \Delta_{11}^{(1,0)} & \Delta_{12}^{(1,0)} \\ \Delta_{21}^{(1,0)} & \Delta_{22}^{(1,0)} \end{pmatrix} \begin{pmatrix} \tilde{\Sigma}_{0,0} & 0 \\ 0 & \tilde{\Sigma}_{0,0} \end{pmatrix}$$

$$\equiv M_{2,1}^{1} \Pi_{0,0} M_{1,0}^{1} \tilde{\Sigma}_{0,0}.$$

As already mentioned, the indices i and j count for QED vertex corrections of type one, $\Gamma^{1}_{[i,j,k]}$, analogous to the ones defined for Yukawa vertex corrections of this type. Similarly, the indices for the type two vertex corrections $\Gamma^{2}_{[i,j,k]}$ in QED count as in Yukawa type two. And the above-described matrix multiplication stays the same apart from different entries for the matrices, which can be readily calculated in terms of functions $F_{a,b}$. We do not list the two sets of four functions $\Delta_{a,b}^{(i,j)}$ in terms of $F_{c,d}$ functions explicitly, but the interested reader can find them from our publicly available programs.[12] Table II shows some examples of how graphs are built in QED.

III. RENORMALIZATION

Renormalization employs a simple principle of multiplicative subtraction, making use of the underlying Hopf algebra structure of Feynman graphs:[14,4] the coproduct

$$\Delta(\Gamma) = \Gamma \otimes 1 + 1 \otimes \Gamma + \sum_{\gamma \subset \Gamma} \gamma \otimes \Gamma / \gamma$$

and antipode

$$S(\Gamma) = -\Gamma - \sum_{\gamma \subset \Gamma} \gamma \Gamma / \gamma$$

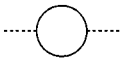
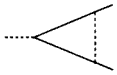
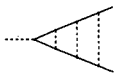
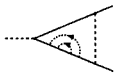
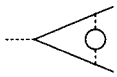
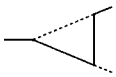
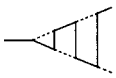
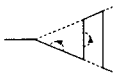
are the structure maps which allow the construction of counterterms and renormalized quantities. One employs Feynman rules $\phi: H \to V$ as an element in the group of characters of the Hopf algebra H, with target space V (a suitable ring or algebra) and makes the target space into a Baxter algebra (V,R) by choosing a renormalization map R such that $R(ab)+R(a)R(b)=R(aR(b))+R(R(a)b)$. One then has the counterterm

$$S_R^{\phi}(\Gamma) = -R\left[\phi(\Gamma) + \sum_{\gamma \subset \Gamma} S_R^{\phi}(\gamma) \phi(\Gamma/\gamma) \right]$$

and a further recursion delivers the renormalized result

$$S_R^{\phi} \star \phi(\Gamma) = S_R^{\phi}(\Gamma) + \phi(\Gamma) + \sum_{\gamma \subset \Gamma} S_R^{\phi}(\gamma) \phi(\Gamma/\gamma).$$

TABLE II. Some examples of how self-energy and vacuum polarization graphs are built up in QED.

	$\Sigma_{[0,0]}(q^2) = (-ig)^2\,\Sigma_{0,0}[q^2]^{-\epsilon}\not{q}$
	$\Sigma_{[1,0]}(q^2) = (-ig)^4\Sigma_{1,0}\Sigma_{0,0}[q^2]^{-2\epsilon}\not{q}$
	$\Sigma_{[2,1]}(q^2) = (-ig)^8\,\Sigma_{2,1}\Pi_{0,0}(\Sigma_{0,0})^2[q^2]^{-4\epsilon}\not{q}$
	$\Pi_{[0,0]}(q^2) = (-ig)^2\,\Pi_{0,0}[q^2]^{-\epsilon}q^2$
	$\Pi_{[2,1]}(q^2) = (-ig)^8\,\Pi_{2,1}\Sigma_{1,0}(\Sigma_{0,0})^2[q^2]^{-4\epsilon}q^2$
	$\Gamma^1_{[0,0,0]}(q^2) = (-ig)^3\,\Gamma^1_{0,0}[q^2]^{-\epsilon}$
	$\Gamma^1_{[0,0,2]}(q^2) = (-ig)^7\,\Gamma^1_{2,0}\Gamma^1_{1,0}\Gamma^1_{0,0}[q^2]^{-3\epsilon}$
	$\Gamma^1_{[2,0,0]}(q^2) = (-ig)^7\,\Gamma^1_{2,0}\Sigma_{1,0}\Sigma_{0,0}[q^2]^{-3\epsilon}$
	$\Gamma^1_{[0,1,0]}(q^2) = (-ig)^5\,\Gamma^1_{0,1}\Pi_{0,0}[q^2]^{-2\epsilon}$
	$\Gamma^2_{[0,0,0]}(q^2) = (-ig)^3\,\Gamma^2_{0,0}[q^2]^{-\epsilon}$
	$\Gamma^2_{[0,0,2]}(q^2) = (-ig)^7\,\Gamma^2_{2,0}\Gamma^2_{1,0}\Gamma^2_{0,0}[q^2]^{-3\epsilon}$
	$\Gamma^2_{[1,1,1]}(q^2) = (-ig)^9\Gamma^2_{3,0}\Gamma^2_{1,1}(\Sigma_{0,0})^2[q^2]^{-4\epsilon}$

The counterterm S_R^ϕ is in the image of R, while $\phi(\Gamma)+\Sigma_{\gamma\subset\Gamma}S_R^\phi(\gamma)\phi(\Gamma/\gamma)$ is the result of Bogoliubov's famous $\overline{R}(\Gamma)$ operation on Γ which eliminates subdivergences in Γ.[13]

Under suitable conditions on the behavior of R, in this ratio of characters short distance singularities drop out.[14,15]

Before we comment on the renormalization scheme chosen for our calculations, let us introduce the bidegree of a Feynman graph. This standard notion can be introduced for any Hopf algebra which is reduced to scalars[7,4] by the counit $\overline{e}$ with

$$\overline{e}(q1)=q,\quad \overline{e}(X)=0,\quad \text{else.}$$

If we decompose $H=H_0\oplus H_{\text{aug}}$, with H_{aug} being the augmentation ideal as the kernel of $\overline{e}$ we can investigate, for any positive integer k and Hopf algebra element X,

$$X_k := \Delta^{k-1}(X)\cap H_{\text{aug}}^{\otimes k}.$$

For sufficiently large k this will necessarily vanish. We define the bidegree bid(X) as the largest k such that $X_k \neq 0$. Elements in H_0 have bidegree zero. Note that Hopf algebra elements of unit bidegree are precisely the primitive elements $X \in H_{\text{aug}}$ in the Hopf algebra, with

$$\Delta(X) = X \otimes 1 + 1 \otimes X \notin H_{\text{aug}} \otimes H_{\text{aug}}.$$

Having introduced this standard notion we introduce the renormalization scheme for which we choose minimal subtraction (MS). Each application of the scheme is given by a projection onto the pole-part of the considered Laurent series and is symbolized with brackets "$\langle\,\rangle$:"

$$\left\langle \sum_{j=-r}^{+\infty} c_j \epsilon^j \right\rangle = \sum_{j=-r}^{-1} c_j \epsilon^j.$$

The reader should convince him/herself that this map makes the ring of Laurent series with poles of finite order into a Baxter algebra,

$$\langle ab \rangle + \langle a \rangle \langle b \rangle = \langle a \langle b \rangle \rangle + \langle \langle a \rangle b \rangle.$$

Note that the degree r of the pole terms in a Laurent series assigned to a graph by the Feynman rules in dimensional regularization is in general majorized by the bidegree $r \leqslant \text{bid}(\Gamma)$ and equals the bidegree in our simple applications.

We expect to encounter $\zeta(n)$ inside the coefficients of the Laurent series in the regularization parameter ϵ emerging from a series expansion of the functions $F_{a,b}$.

In QED we have to take our matrix-calculus into account. The renormalization of such matrix expressions is now given by inserting a diagonal matrix R, which consists of the renormalization map as entries:

$$R := \begin{pmatrix} R_{\text{MS}} & 0 \\ 0 & R_{\text{MS}} \end{pmatrix}.$$

Inside a string of matrices, this matrix has to be inserted wherever the renormalization map is applied. It acts on expressions on the right.

IV. ROOTED TREES

Before we build up graphs and calculate their counterterms, i.e., their antipodes, let us first mention that in our simplified context, the Hopf algebra of Feynman graphs is isomorphic to a Hopf algebra of rooted trees with a very small set of decorations given by our one-loop graphs.

In the class of graphs to which we have restricted ourselves one-particle irreducible subgraphs are either nested in each other, or disjoint. They hence form tree-like hierarchies, and one easily translates graphs in rooted trees,[15] with a one-to-one correspondence between one-particle irreducible subgraphs and vertices in the rooted tree (the map from graphs to rooted trees is one-to-many for overlapping divergent graphs, and can be systematically constructed):[16]

The translation from a Feynman diagram to a rooted tree has to be done in the following way: *Set a box around the subdivergences of a Feynman graph* Γ *and mark the upper horizontal line with a dot (≃ vertex). Dots of nested boxes, that is boxes where one of them is contained inside the other, are connected with a line (≃ edge) (see Fig. 5).*

Each vertex of a tree then represents a divergent subgraph of the diagram. The antipode of such a tree is a sum over all *full cuts* or, recursively, iterates over admissible cuts using the coproduct. This easy-to-implement[2] coproduct

$$\Delta(T) = T \otimes 1 + 1 \otimes T + \sum_{\text{admissible cuts } c} P^c(T) \otimes R^c(T)$$

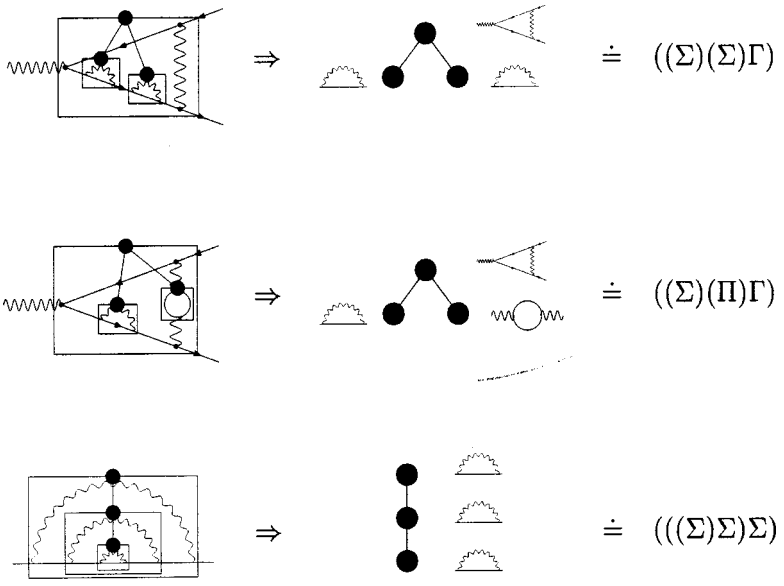


FIG. 5. Translation of Feynman diagrams into rooted trees. Here we are dealing with decorated rooted trees, where the subdivergences are written next to the vertex to which they belong. In the last column one can see another way to encode the structure of the trees in the form of nested lists (Ref. 14): The entries are again the divergent parts of a Feynman diagram and the formation of the parentheses gives the structure of the tree, beginning with the vertices ''at the end'' of a tree up to the root.

is by now a standard combinatorial tool (see, e.g., Ref. 15). Using it, the counterterm is a recursive construct

$$S_{\mathrm{MS}}(T) = -\left\langle T(\Gamma) + \sum_{\text{admissible cuts } c} S_{\mathrm{MS}}(P^c(T)) R^c(T) \right\rangle,$$

where an evaluation of the graph corresponding to the tree using the Feynman rules is understood before applying the projection $\langle\,\rangle$ for minimal subtraction (MS), in accordance with the general formula given for graphs.

V. IMPLEMENTATION

We briefly describe an implementation of our scheme in a computer program. This implementation is not entirely self-contained in the sense that given a Feynman diagram, it would compute the antipode. Instead, its input is a decorated rooted tree in list notation such as $(\Gamma(\Pi)(\Sigma))$. The actual construction of that rooted tree from the diagram, as described in Sec. IV, is left to the user (see also Fig. 5).

Our implementation uses the GiNaC system for symbolic computation in the C++ programming language.[1] GiNaC provides efficient implementations for handling Laurent series as needed in dimensional regularization. From C++, all the linguistic instruments for object-oriented programming are borrowed and available to us. We follow a traditional approach for representation of our rooted trees where there exists a container class called `node` that may or may not have several children of the same class. In addition, each vertex in an object of class `node` contains an object of the abstract and polymorphic class `decoration`. From the abstract `decoration` class a number of concrete classes like `Sigma`, `Gamma` and `Vacuum` are derived, corresponding to primitive Feynman diagrams Σ, Γ, and Π, as well as some additional classes that allow us to distinguish between the position of a subgraph inside its supergraph.

The trees under consideration are not ordered with respect to their children, i.e., the trees $(\Gamma(\Sigma)(\Pi))$ and $(\Gamma(\Pi)(\Sigma))$ are equivalent. Therefore the children form a multiset where only the multiplicity of occurrences is relevant.

A template class `multiset` is part of the C++ Standard Template Library (STL). It has the additional advantage that the elements are always automatically sorted with respect to some specified ordering. This turns out to be useful for convenient identification of equivalent nodes and also to establish an order relation on them. The state of the edges leading to the children of a node (either ''cut'' or ''uncut'') needs to be taken into account as well, so the multiset is really one of pairs of nodes and boolean variables. We chose to delegate methods from class `node` to the corresponding class derived from `decoration` using dynamic type-dispatch. Hence, the decoration must be stored as a pointer, calling for some hand-made memory management in class `node`. A completely realistic layout of our class `node` is then:

```
1 class node {
2 public:
3  // constructors, destructors, delegators,
4  // etc...
5 private:
6 decoration *deco;
7 multiset< pair< node, bool > > children;
8 };
```

Note that a `node` can be either the entire tree, or a subtree or a single (atomic) leaf. The layout of class `decoration` holds a pair of indices and in the case of QED a GiNaC expression (class `ex`) for the gauge. An object of class `ex` is entirely sufficient, since it may contain either a numerical value (integer or fractional) or a symbol (like ξ) (or even more complex expressions, if need should arise).

Knowledge of how to manipulate the indices i and j, depending on the type of decoration and on the state of the edges, is built into the classes of type `decoration`. They are automatically adjusted when the tree is constructed. Furthermore, the state of the edges is also irrelevant for the user of the program since we need all possible combinations of cuts. If there are n vertices inside a tree, then there are $n-1$ edges and we have to construct all possible 2^{n-1} combinations.

Once all the trees have been created we call a method called `evaluate` in each of them that traverses the tree in a top-down fashion: In each node, the expression in terms of $F_{a+i\varepsilon,b+j\varepsilon}$ is dispatched and expanded as a series in the regularization parameter ε before `evaluate` is called on the multiset of children. The resulting 2^{n-1} Laurent series are then added together and the coefficients are expanded. This procedure yields the antipode.

Here is an example how the programs are used in practice:

```
1 $ ./qed1 "(((Sigma[0])(Sigma[xi])Gamma[-1])Gamma[xi])"
2 After decoration the tree has these indices:
3 (Gamma[3,0][xi](Gamma[2,0][-1](Sigma[0,0] [0])(Sigma[0,0][xi])))
4  - - -+- - -#- - -+- - -#- - -+- - -#- - -+- - -#- - -+- - -#- - -
   +- - -#
5 The antipode of this tree is:
6
7 (-1/4-1/4*xi^2-1/2*xi)*x^(-3)
8 +(7/24+1/24*xi^2+1/3*xi)*x^(-2)
9 +(-5/16-13/48*xi^2-7/12*xi)*x^(-1)
```

The graph to be computed is passed in tree form as a string on the command line, together with the gauge parameter. Note how the indices i and j are then set up automatically in line 3. The next line is a simple progress bar, useful when computations become longer. The result is then printed as a power series in the regularization parameter, called `x` instead of ε in order to please the computer.

Computationally, the results are always quite small (cf. Sec. VI) but there is a huge swell of intermediate expressions. After all, the Laurent series arise from expanding products and sums of

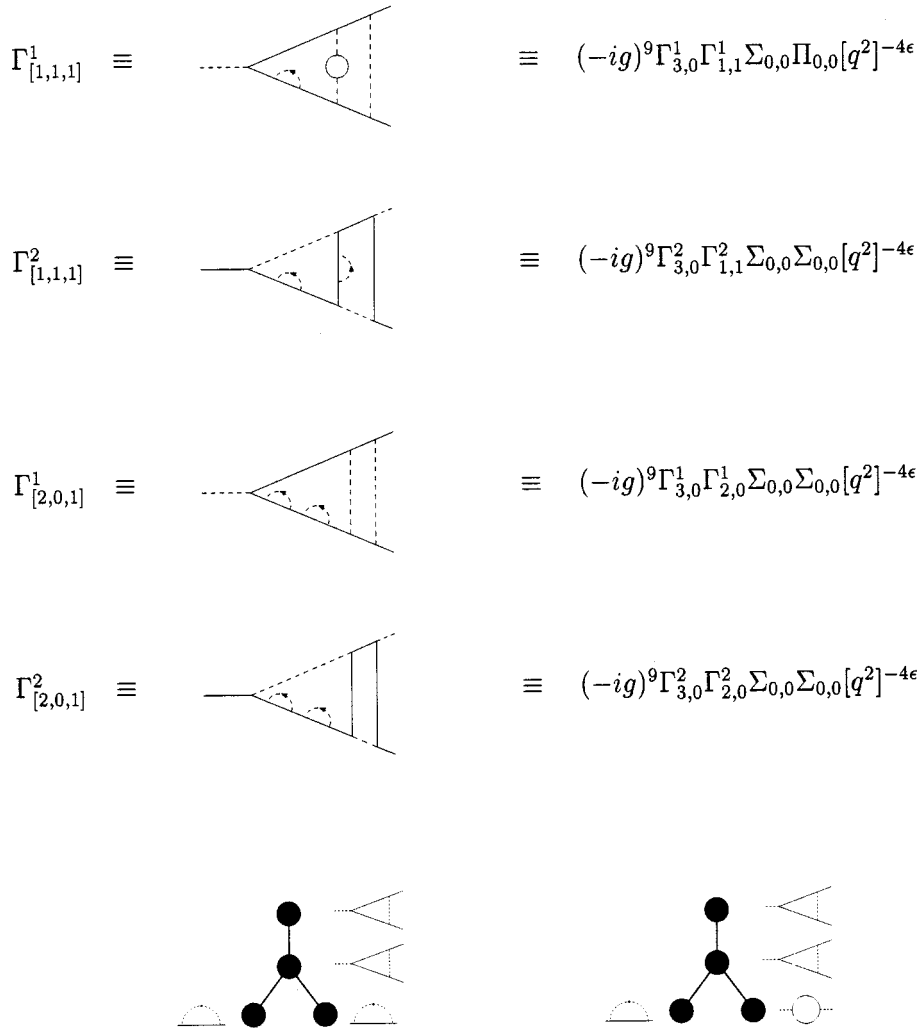


FIG. 6. Graphs in Yukawa theory and their decorated rooted trees.

lots of Γ-functions and so carry Euler–Mascheroni constants. But these have to vanish by cancellations, a fact that is conveniently used as a consistency check for the result. In practice, antipodes of nine-loop graphs in massless QED are still computationally feasible but may require several hours and hundreds of megabytes memory. This emphasizes the drastic loss of efficiency in comparison with Refs. 2 and 3, which is compensated by a gain in flexibility to handle different decorations at any step in the recursion.

The programs developed herein are written in plain ISO C++ (Ref. 17) and will run on any system where the GiNaC library has been ported to. Note that porting to a new platform will require porting CLN[18] to that platform first, since GiNaC depends on CLN for its arbitrary precision arithmetic.

VI. COMPUTATIONAL RESULTS

In a first step, to examine the appearance of ζ-functions, we will now calculate the antipode of different graphs given in Figs. 6 and 7 that represent the two topologies of Fig. 1. In Yukawa theory the graphs $\Gamma^1_{[1,1,1]}$ and $\Gamma^2_{[1,1,1]}$ of Fig. 6 are representations of the ladder topology of Fig. 1(b), the graphs $\Gamma^1_{[2,0,1]}$ and $\Gamma^2_{[2,0,1]}$ of the swiss cheese topology in Fig. 1(a). The same holds for QED with [1,1,1] replaced by [1,1,2] and [2,0,1] by [2,0,2].

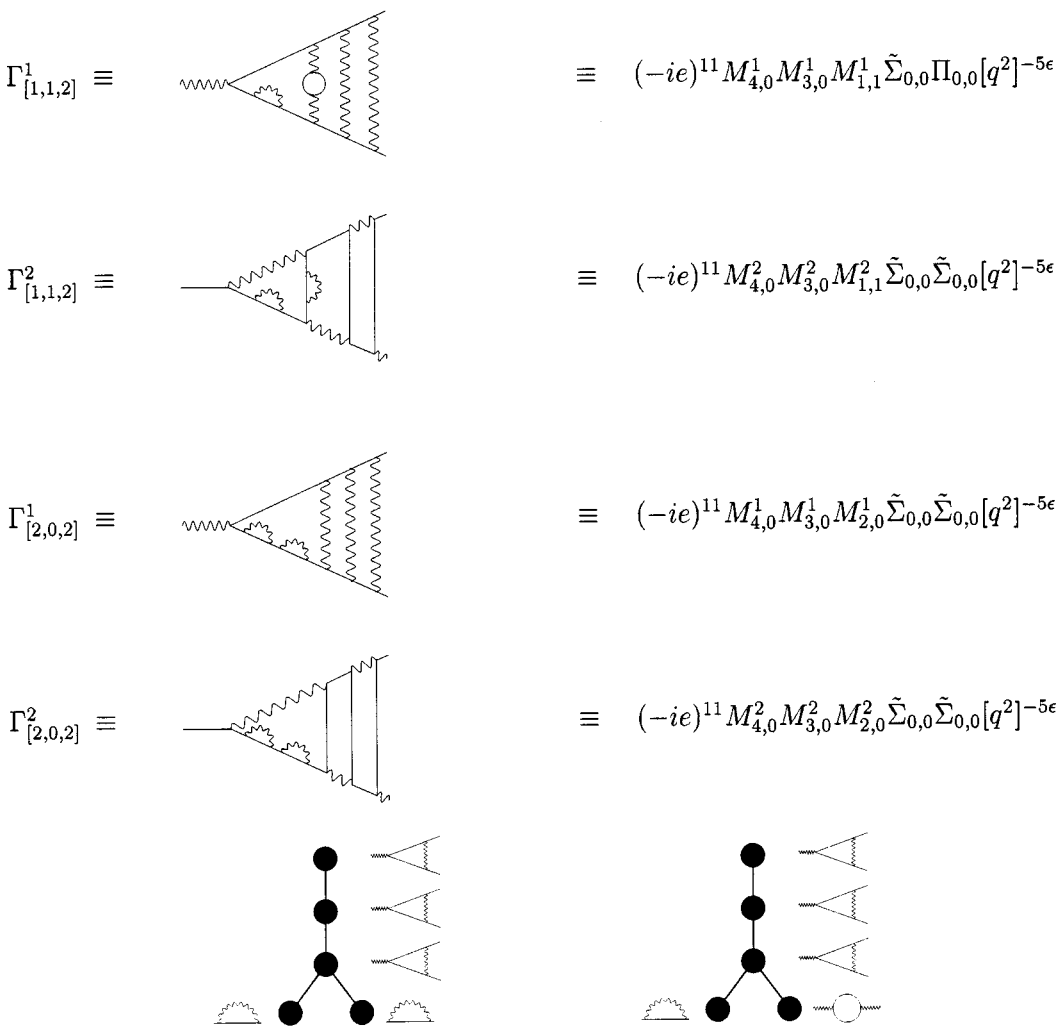


FIG. 7. Graphs in QED and their decorated rooted trees.

The graphs for the Yukawa theory, together with their expressions in characterizing functions, are given in Fig. 6. Figure 6 also contains the decorated rooted trees we get from them to calculate the antipode. One can see that except for the decorations they all belong to the same rooted tree, and hence have the same structure as far as their short distance singularities go, as advertised in Sec. I.

In QED, the considered graphs in Fig. 7 possess one more vertex correction compared to the graphs in Yukawa theory. This additional photon line is necessary because the short distance singularity structure is actually determined by the bidegree, i.e., the number of subdivergent graphs. It so happens in QED that the one-loop fermion self-energy and one-loop vertex corrections (with divergent subgraphs) are overall finite if the internal photon is transversal. In our case, we thus find that the insertion of a one-loop vacuum polarization into the internal photon line in a vertex results in a convergent vertex correction. We have to plug the whole function into one more vertex corrections to get to the next level in the bidegree. And indeed, we need an additional vertex correction, compared to Yukawa theory, to obtain the $\zeta(3)$ in the pole-terms: gauge symmetry delays the appearance of transcendentals.[19] Also let us mention that we can easily compare graphs which have an internal vacuum polarization with graphs which have an internal fermion

self-energy by using the before-mentioned elimination of the trace in the vacuum polarization, using

$$\Pi_{0,0}=\mathrm{tr}(\mathbb{1})\tfrac{1}{2}F_{1,1}=\mathrm{tr}(\mathbb{1})\Sigma_{0,0}.$$

Furthermore, $\Gamma^2_{[1,1,2]}$ and $\Gamma^2_{[2,0,2]}$ in QED do not have this extra shift between loop number and bidegree by themselves, as there the desire to maintain the same topology never forces us to use a vacuum polarization as a subgraph: all one-loop subdivergences are fermion self-energies and vertex corrections. However, we use the same gauges in these graphs as in the graphs $\Gamma^1_{[1,1,2]}$ and $\Gamma^1_{[2,0,2]}$ to compare the results directly (see the following), and therefore obtain the same difference between loop-number and bidegree.

Finally, in our results, we are only interested in residues of counterterms, poles of first order. All interesting relations between transcendental degree and topology will appear there. The scattering type formula[4] will make sure that parts of these relations will then resurface in the poles of higher order in the counterterm, but they contain no new information. So in the following we solely exhibit the residues of the counterterms for our selected class of graphs. We denote by res(Γ) this coefficient of the pole of first order in the MS counterterm in dimensional regularization of a graph Γ. Assorted results for these residues are as follows.

Yukawa theory:

$$\mathrm{res}(\Gamma^1_{[1,1,1]})=\tfrac{5}{48},$$

$$\mathrm{res}(\Gamma^2_{[1,1,1]})=\tfrac{1}{24},$$

$$\mathrm{res}(\Gamma^1_{[2,0,1]})=(\tfrac{5}{48}-\tfrac{1}{8}\zeta(3)),$$

$$\mathrm{res}(\Gamma^2_{[2,0,1]})=(\tfrac{1}{12}-\tfrac{1}{8}\zeta(3)).$$

QED:

$$\mathrm{res}(\Gamma^1_{[1,1,2]})=-(\tfrac{1}{480}(301+143\xi-170\xi^2),)$$

$$\mathrm{res}(\Gamma^2_{[1,1,2]})=-(\tfrac{1}{960}(584+659\xi+59\xi^2)),$$

$$\mathrm{res}(\Gamma^1_{[2,0,2]})=-(\tfrac{1}{480}(521+309\xi-236\xi^2)+\tfrac{3}{10}\zeta(3)(1+\xi)^2),$$

$$\mathrm{res}(\Gamma^2_{[2,0,2]})=-(\tfrac{1}{960}(832+879\xi+31\xi^2)+\tfrac{3}{10}\zeta(3)(1+\xi)^2).$$

We see that in Yukawa theory the graphs $\Gamma^1_{[2,0,1]}$ and $\Gamma^2_{[2,0,1]}$ with the swiss cheese topology have a residue involving $\zeta(3)$, while $\Gamma^1_{[1,1,1]}$ and $\Gamma^2_{[1,1,1]}$ realizing the ladder topology just have a rational residue, as expected. A similar result holds in QED: the graphs $\Gamma^1_{[2,0,2]}$ and $\Gamma^2_{[2,0,2]}$ with the swiss cheese topology again have a residue involving $\zeta(3)$, while $\Gamma^1_{[1,1,2]}$ and $\Gamma^2_{[1,1,2]}$ realizing the ladder topology just have a rational residue.

Those residues are in general a linear combination of terms of varying transcendental weight. This weight vanishes for a rational number, and in accordance with standard practice in the study of multiple zeta values the transcendental weight w of a monomial $\Pi_i\zeta(j_i)$ is

$$w\left(\prod_i \zeta(j_i)\right)=\sum_i j_i.$$

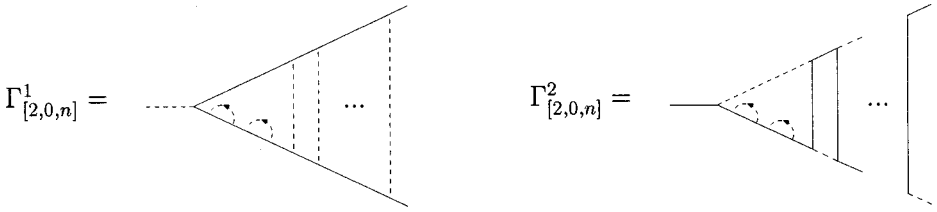


FIG. 8. Iterated vertex corrections.

Then, the above-given results confirm that the coefficient of the highest weight transcendental in the transition from $\mathrm{res}(\Gamma^1_{[2,0,1]})$ to $\mathrm{res}(\Gamma^2_{[2,0,1]})$ ($\mathrm{res}(\Gamma^1_{[2,0,2]})$ to $\mathrm{res}(\Gamma^2_{[2,0,2]})$ for QED) is invariant. This is the partial symmetry announced in Sec. I. It holds for any gauge in the QED case and holds in general, if we increase the loop number as for example in Fig. 8.

In Yukawa theory we get:

$$\mathrm{res}(\Gamma^1_{[2,0,1]})=(\tfrac{5}{48}-\tfrac{1}{8}\zeta(3)),$$

$$\mathrm{res}(\Gamma^2_{[2,0,1]})=(\tfrac{1}{12}-\tfrac{1}{8}\zeta(3)),$$

$$\mathrm{res}(\Gamma^1_{[2,0,2]})=(\tfrac{1}{20}-\tfrac{9}{40}\zeta(3)-\tfrac{3}{80}\zeta(4)),$$

$$\mathrm{res}(\Gamma^2_{[2,0,2]})=(\tfrac{1}{240}-\tfrac{1}{20}\zeta(3)-\tfrac{3}{80}\zeta(4)),$$

$$\mathrm{res}(\Gamma^1_{[2,0,3]})=-(\tfrac{23}{90}+\tfrac{9}{20}\zeta(3)+\tfrac{7}{80}\zeta(3)+\tfrac{7}{240}\zeta(5)),$$

$$\mathrm{res}(\Gamma^2_{[2,0,3]})=-(-\tfrac{1}{240}+\tfrac{1}{6}\zeta(3)+\tfrac{1}{80}\zeta(4)+\tfrac{7}{240}\zeta(5)),$$

$$\mathrm{res}(\Gamma^1_{[2,0,4]})=-(\tfrac{919}{630}+\tfrac{71}{70}\zeta(3)+\tfrac{111}{560}\zeta(4)+\tfrac{1}{12}\zeta(5)+\tfrac{1}{560}\zeta(3)^2+\tfrac{1}{112}\zeta(6)),$$

$$\mathrm{res}(\Gamma^2_{[2,0,4]})=-(\tfrac{65}{224}+\tfrac{11}{140}\zeta(3)+\tfrac{1}{16}\zeta(4)+\tfrac{1}{120}\zeta(5)+\tfrac{1}{560}\zeta(3)^2+\tfrac{1}{112}\zeta(6)),$$

$$\begin{aligned}\mathrm{res}(\Gamma^1_{[2,0,5]})=-(&\tfrac{6481}{1120}+\tfrac{33\,613}{13\,440}\zeta(3)+\tfrac{2133}{4480}\zeta(4)+\tfrac{101}{480}\zeta(5)\\&+\tfrac{27}{4480}\zeta(3)^2+\tfrac{27}{896}\zeta(6)+\tfrac{3}{4480}\zeta(3)\zeta(4)+\tfrac{7}{1920}\zeta(7)),\end{aligned}$$

$$\begin{aligned}\mathrm{res}(\Gamma^2_{[2,0,5]})=-(&\tfrac{863}{3360}+\tfrac{61}{160}\zeta(3)+\tfrac{27}{1120}\zeta(4)+\tfrac{7}{120}\zeta(5)+\tfrac{1}{2240}\zeta(3)^2\\&+\tfrac{1}{448}\zeta(6)+\tfrac{3}{4480}\zeta(3)\zeta(4)+\tfrac{7}{1920}\zeta(7)).\end{aligned}$$

Similarly, for QED we find:

$$\mathrm{res}(\Gamma^1_{[2,0,2]})=-\tfrac{1}{480}(521+309\xi-236\xi^2)-\tfrac{3}{10}(1+\xi)^2\zeta(3),$$

$$\mathrm{res}(\Gamma^2_{[2,0,2]})=-\tfrac{1}{960}(832+879+31\xi^2)-\tfrac{3}{10}(1+\xi)^2\zeta(3),$$

$$\begin{aligned}\mathrm{res}(\Gamma^1_{[2,0,3]})=&-\tfrac{1}{5760}(13\,377+16\,773\xi+12\,091\xi^2+9463\xi^3)\\&+\tfrac{1}{30}(1+\xi)^2(-38+7\xi)\zeta(3)-\tfrac{3}{40}(1+\xi)^3\zeta(4),\end{aligned}$$

$$\begin{aligned}\mathrm{res}(\Gamma^2_{[2,0,3]})=&-\tfrac{1}{5760}(13\,327+32\,578\xi+26\,038\xi^2+6811\xi^3)\\&-\tfrac{1}{60}(1+\xi)^2(31+4\xi)\zeta(3)-\tfrac{3}{40}(1+\xi)^3\zeta(4),\end{aligned}$$

$$\begin{aligned}\mathrm{res}(\Gamma^1_{[2,0,4]}) = &-\tfrac{1}{40\,320}(427\,681+1\,048\,812\xi+889\,375\xi^2+130\,774\xi^3-145\,630\xi^4)\\ &-\tfrac{1}{840}(1+\xi)^2(2551+425\xi+736\xi^2)\zeta(3)\\ &+\tfrac{1}{280}(1+\xi)^3(-121+23\xi)\zeta(4)-\tfrac{1}{20}(1+\xi)^4\zeta(5),\end{aligned}$$

$$\begin{aligned}\mathrm{res}(\Gamma^2_{[2,0,4]}) = &-\tfrac{1}{161\,280}(1\,357\,764+4\,016\,396\xi+4\,028\,301\xi^2+1\,438\,370\xi^3+68\,749\xi^4)\\ &-\tfrac{1}{1680}(1+\xi)^2(1448+2365\xi+836\xi^2)\zeta(3)\\ &-\tfrac{1}{140}(1+\xi)^3(29+2\xi)\zeta(4)-\tfrac{1}{20}(1+\xi)^4\zeta(5),\end{aligned}$$

$$\begin{aligned}\mathrm{res}(\Gamma^1_{[2,0,5]}) = &\tfrac{1}{430\,295\,040}(-19\,150\,607\,852-5\,5087\,254\,529\xi-55\,376\,777\,218\xi^2\\ &-24\,306\,202\,368\xi^3-10\,014\,576\,786\xi^4-5\,440\,770\,359\xi^5)\\ &+\tfrac{1}{4480}(1+\xi)^2(-39\,057-40\,975\xi-19\,389\xi^2+6061\xi^3)\zeta(3)\\ &-\tfrac{3}{4480}(1+\xi)^3(2031+11\xi+446\xi^2)\zeta(4)+\tfrac{1}{960}(1+\xi)^4(-347+67\xi)\zeta(5)\\ &-\tfrac{3}{1120}(1+\xi)^5\zeta(3)^2-\tfrac{3}{224}(1+\xi)^5\zeta(6),\end{aligned}$$

$$\begin{aligned}\mathrm{res}(\Gamma^2_{[2,0,5]}) = &-\tfrac{1}{1290240}(29\,658\,556+111\,493\,999\xi+161\,539\,373\xi^2+112\,812\,993\xi^3\\ &+38\,688\,379\xi^4+5\,579\,364\xi^5)-\tfrac{1}{26\,880}(1+\xi)^2(80\,770+155\,550\xi+79\,521\xi^2\\ &+3472\xi^3)\zeta(3)-\tfrac{1}{8960}(1+\xi)^3(3254+3919\xi+1340\xi^2)\zeta(4)-\tfrac{1}{960}(1+\xi)^4(179\\ &+8\xi)\zeta(5)-\tfrac{3}{1120}(1+\xi)^5\zeta(3)^2-\tfrac{3}{224}(1+\xi)^5\zeta(6).\end{aligned}$$

The reader will note that in QED our residues are polynomials in the gauge parameter of a degree reduced by two steps from what one might expect, to enable comparison between configurations with insertions of self-energies into photon or fermion lines. The corresponding fermion self-energy was for that purpose evaluated in the Feynman gauge, and in the Landau gauge for the affected photon propagator. If one only compares cases with self-energy insertions at fermionic lines, one can abandon these restrictions and we did confirm that the reported invariance holds as expected with coefficients which are polynomials in the gauge parameter of degree equal to the number of photon lines.

VII. DISCUSSION AND PROOF

Actually, results of the form reported in the previous sections can be derived from the analytic structure of the functions $F_{a,b}$ and some basic field theoretic arguments.

Let us reconsider the situation. The simplicity of Feynman graphs considered here manifests itself computationally by the fact that they factorize in a unique manner. Each divergent subgraph γ depends only on a single external momentum q say (that is the reason why we only consider vertex subgraphs at zmt), such that its evaluation in dimensional regularization gives a result of the form

$$\phi(\gamma)(\varepsilon)=[q^2]^{-n(\gamma)\varepsilon}\sum_i F_i(\varepsilon)c_i(q).$$

Here, $n(\gamma)$ is the number of loops in γ, and $F_i(\varepsilon)$ are q-independent form factors, and the dimensionless $c_i(q)$ are

$c_1(q)=\gamma_\mu$, $c_2(q)=q_\mu \not{q}/q^2$ for the QED vertex (the only case here in which the sum has more than one term),
$c_1(q)=1$ for the vertex correction in Yukawa theory,
$c_1(q)=\not{q}$ for any fermion self-energy,
$c_1(q)=(g_{\mu\nu}-q_\mu q_\nu/q^2)\cdot q^2$ for the photon,
$c_1(q)=q^2$ for the scalar boson.

Insertions of such graphs γ in another graph Γ only raises powers of the scalar part of some propagator of Γ:

$$\frac{1}{q^2}\rightarrow\frac{1}{[q^2]^{1+n(\gamma)\varepsilon}}.$$

We can keep track of this by notating these loop numbers $n(\gamma)$ in the entries $M(\Gamma)_{ij}$ for the corresponding propagator in the adjacency matrix $M(\Gamma)$.

Let us now assume that Γ is some primitive vertex correction, i.e., free of divergent subgraphs, and let us write as before Γ^1 and Γ^2 for two distinct choices of zmt.

Consider a bunch of 1PI graphs $X=\Pi_{i=1}^k \gamma_i$ each dependent on a sole external momentum as described previously. Let $k=\mathrm{bid}(X)$ be the bidegree of X, so that X has a highest pole in ε of degree k with coefficient c_k^X. Let now G_X be chosen gluing data such that $\Gamma_X:=\Gamma\star_{G_X} X$ is obtained from inserting X at specified vertices and propagators into Γ, with $\mathrm{bid}(\Gamma)=1$ without loss of generality. (Any 1PI graph can be written in the form $\Gamma\star_{G_X} X$ for such appropriate Γ, X,[14,16,4] in generalization of the closed Hochschild one cocycle B_+ of undecorated rooted trees). Further, each X allows for an expansion

$$\phi(X)=\frac{c_k^X}{\varepsilon^k}(1+T(X)(\varepsilon))$$

and similarly, let

$$\phi(\Gamma)=\frac{\mathrm{res}(\Gamma)}{\varepsilon}(1+T(\Gamma)(\varepsilon)).$$

Now assume that the Taylor series $[1+T(X)(\varepsilon)][1+T(\Gamma)(\varepsilon)]=1+\Sigma_{j=1}^\infty c_j\varepsilon^j$ is such that the transcendental weight $w(c_j)$ of c_j increases with j:

$$w(c_j)<w(c_{j+1}),$$

$\forall j\geqslant k-1$. Here, we define the transcendental weight of an expression which is a sum of terms as the highest transcendental weight appearing in its terms. The question as to how to define the transcendental weight in a context which exceeds the Riemann ζ-functions or MZVs[19] we do not have to answer here. Also, the attentive reader might have noticed that we set the transcendental weight of the gauge parameter to be zero for the QED results, treating it as an independent variable.

Proposition 1: The counterterm is the same for Γ_X^1 and Γ_X^2, and hence their residues are equal.

Proof: Elementary, as $\Gamma^1-\Gamma^2$ is UV convergent, and hence Γ_X^1 and Γ_X^2 generate the same counterterm. □

In particular, we also note that in the above, $\Gamma_X^1-\Gamma_X^2$, when inserted into another graph, produces a result with a bidegree reduced by one unit compared to the insertion of either Γ_X^1 or Γ_X^2 alone.

This is not yet the desired result, as in our case we have to compare $\Gamma^1_{X_1}$ with $\Gamma^2_{X_2}$, where X_1 is a collection of subgraphs in which all vertex subgraphs are of type Γ^1, and X_2 is the same collection of subgraphs apart from the replacement $\Gamma^1 \to \Gamma^2$ for all vertex subgraphs.

Any graph of type $\Gamma^1_{X_1}$ or $\Gamma^2_{X_2}$, which itself can contain subgraphs X_i of these varying types of vertex corrections plus self-energy subgraphs, can now be expressed in terms of the other. Similarly, this holds for these vertex subgraphs of either type, at the expense of generating extra terms of reduced bidegree

$$\mathrm{bid}(\Gamma^1_{X_1} - \Gamma^2_{X_2}) < \mathrm{bid}(\Gamma^1_{X_1}) = \mathrm{bid}(\Gamma^2_{X_2}),$$

which involve differences $\Gamma^1_{X_i} - \Gamma^2_{X_i}$ for appropriate X_i. Hence, under the above-noted assumption of monotonic increase of the transcendental weight with the bidegree, we get upon iterating such insertions

Proposition 2: The coefficient of the term of maximal transcendental weight is the same for $\mathrm{res}(\Gamma^1_{X_1})$ *and* $\mathrm{res}(\Gamma^2_{X_2})$.

Here, X_1, X_2 are related, as above.

This immediately explains our results as a look at the functions $F_{a,b}$, and hence the corresponding evaluations of our subdivergent graphs show that they fulfill the required assumptions of monotonic increase of transcendental weight, which was completely determined from the appearance of the Riemann ζ-function in our simple examples. Note that the factorizations into two-point functions and the absence of all other primitive graphs apart from one-loop functions were the two main simplifications which enabled us to satisfy the assumption.

The study to what extent a sensible transcendental weight can be established in general will be a topic of future work. Any sensible answer we will expect to deliver the same permutation invariance of the residue as reported here.

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Chronon corrections to the Dirac equation

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The Dirac equation is not semisimple. We therefore regard it as a contraction of a simpler decontracted theory. The decontracted theory is necessarily purely algebraic and nonlocal. In one simple model the algebra is a Clifford algebra with $6N$ generators. The quantum imaginary $\hbar i$ is the contraction of a dynamical variable whose backreaction provides the Dirac mass. The simplified Dirac equation is exactly Lorentz invariant but its symmetry group is SO(3, 3), a decontraction of the Poincaré group, and it has a slight but fundamental nonlocality beyond that of the usual Dirac equation. On operational grounds the nonlocality is $\sim 10^{-25}$ s in size and the associated mass is about the Higgs mass. There is a nonstandard small but unique spin–orbit coupling $\sim 1/N$, whose observation would be some evidence for the simpler theory. All the fields of the standard model call for similar nonlocal simplification. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1505666]

I. INTRODUCTION

We begin with basic concepts.

A *simple* theory is one with simple (irreducible) dynamical and symmetry groups. What is not simple or semisimple we call *compound*. A *contraction* of a theory is a deformation of the theory in which some physical scale parameter, called the *simplifier*, approaches a singular limit, taken to be 0 with no loss of generality. The contraction of a simple theory is in general compound.[1–3] By *simplification* we mean the more creative, nonunique inverse process, finding a simple theory that contracts to a given compound theory and agrees better with experiment. The main revolutions in physics of the 20th century were simplifications with simplifiers c, G, $\hbar$.

One sign of a compound theory is a breakdown of reciprocity, the principle that every coupling works both ways. The classic example is Galilean relativity. There reciprocity between space and time breaks down; boosts couple time into space and there is no reciprocal coupling. Special relativity established reciprocity by replacing the compound Galilean bundle of space fibers over the time base by the simple Minkowski space–time. Had Galileo insisted on simplicity and reciprocity he could have formulated special relativity in the 17th century [unless he were to choose SO(4) instead of SO(1, 3)]. Every bundle theory violates reciprocity as much as Galileo's. The bundle group couples the base to the fiber but not conversely. Every bundle theory cries out for simplification.

This now requires us to establish reciprocity between space–time (base coordinates) x^μ and energy-momenta (fiber coordinates) p_μ. (Segal[1] postulated $x \leftrightarrow p$ symmetry exactly on grounds of algebraic simplicity; his work stimulated that of Inönü and Wigner, and ours. Born[4] postulated $x \leftrightarrow p$ reciprocity, on the grounds that it is impossible in principle to measure the usual four-dimensional interval of two events within an atom. We see no law against measuring space–time coordinates and intervals at that gross scale. We use his term ''reciprocity'' in a broader sense that includes his.)

Einstein's gravity theory and the standard model of the other forces are bundle theories, with field space as fiber and space–time as base. Therefore these theories are ripe for simplification.[5] Here we simplify a spinor theory, guided by criteria of experimental adequacy, operationality, causality, and finity.

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Classical field theory is but a singular limit of quantum field theory; it suffices to simplify the quantum field theory. Quantum field theory in turn we regard as many-quantum theory. Its field variables all arise from spin variables of single quanta. By *quantification* we mean the transition from the one-body to the many-body theory, converting yes-or-no predicates about an individual into how-many predicates about an aggregate of isomorphic individuals; as distinct from quantization. For example, a spinor field theory arises by quantifying the theory of a single quantum of spin 1/2.

To unify field with space–time in quantum field theory, it suffices to unify spin with space–time in the one-quantum theory, and to quantify the resulting theory. We unify in this paper and quantify in a sequel.

Some unification programs concern themselves with simplifying just the internal symmetry group of the elementary particles, ignoring the fracture between the internal and external variables. They attempt to unify (say) the hypercharge, isospin and color variables, separate from the space–time variables. Here we close the greatest wound first, expecting that the internal variables will unite with each other when they unite with the external variables; as uniting space with time incidentally unified the electric and magnetic fields. We represent space–time variables x^μ and p_μ as approximate descriptions of many spin variables, in one quantum-spin-space–time structure described in a higher-dimensional spin algebra. This relativizes the split between field and space–time, as Einstein relativized the split between space and time.

The resulting quantum atomistic space–time consists of many small exactly Lorentz-invariant isomorphic quantum bits, qubits which we call *chronons*. [Feynman, Penrose, and Weizsäcker attempted to atomize space or space–time into quantum spins. Feynman wrote a space–time vector as the sum of a great many Dirac spin-operator vectors,[6] $x^\mu \sim \Sigma_n\ \gamma^\mu(n)$, Penrose dissected the sphere S^2 into a spin network;[7] his work inspired this program. Weizsäcker[8] attempted a cosmology of spin-1/2 urs. The respective groups are Feynman's SO(3, 1), Penrose's SO(3), Weizsäckers SU(2), and our SO($3N$,$3N$) ($N \gg 1$).]

Simplifying a physical theory generally detaches us from a supporting condensate. (For Galileo and Kepler, the condensate was the Earth's crust, and to detach from it they moved in thought to a ship or the moon, respectively.[9,10]) In the present situation of physics the prime condensate is the ambient vacuum. Atomizing space–time enables us to present the vacuum as a condensate of a simple system, and to detach from it in thought by a phase transition, a space–time melt-down.

Chronons carry a fundamental time-unit χ, one of our simplifiers. We have argued that χ is much greater than the Planck time and is on the order of the Higgs time $\hbar/M_H c^2$. (In an earlier effort to dissect space–time, assuming multiple Fermi–Dirac statistics for the elements.[11,12] This false start led us eventually to the Clifford–Wilczek statistics;[13–17] an example of Clifford–Wilczek statistics is unwittingly developed in chap. 16 of Ref. 12.) We now replace the classical Maxwell–Boltzmann statistics of space–time events with the simple Clifford–Wilczek statistics appropriate for distinguishable isomorphic units. This enormously reduces the problem of forming a theory.

We single out two main quantifications in field theories like gravitation and the standard model:

A classical quantification assembles a space–time from individual space–time points.

A separate quantification constructs a many-quantum theory or quantum field theory from a one-quantum theory on that space-time.

In the standard physics the space–time quantification tacitly assumes Maxwell–Boltzmann statistics for the elements of space–time, and the field quantification uses Fermi–Dirac or Bose–Einstein statistics. The simplified theory we propose uses one Clifford quantification for all of these purposes.

In this paper we work only with one-quantum processes of $N \gg 1$ chronons. To describe several quanta and their interactions, getting closer to field theory and experiment, will require no further quantification, but only additional internal combinatory structure that is readily accommodated within the one Clifford–Wilczek quantification.

Each physical theory defines at least three algebras that should be simple: the associative

operator algebra of the system,[12,18] the kinematical Lie algebra consisting of possible Hamiltonians, and the symmetry Lie algebra of one preferred Hamiltonian.

There is no second quantization. But there is a second simplification; and a third, and so on, all of different kinds with different simplifiers. Each of the historic revolutions that guide us now introduced a simplifier, small on the scale of previous experience and therefore long overlooked, into the multiplication table and basis elements of one or more of these algebras, and so deformed a compound algebra into a simpler algebra that works better. Among these simplifiers are c, G, and $\hbar$.

Here we simplify the free Dirac equation and its underlying *Dirac–Heisenberg* (real unital associative) algebra

$$A_{\mathrm{DH}}=A_D\otimes A_H, \tag{1}$$

the tensor product of the Dirac and the relativistic Heisenberg algebras, in turn defined as follows.

Relativistic Heisenberg algebra. $A_H=A[i,\hat{p},\hat{x}]$ is generated by the imaginary unit i and the space–time and energy–momentum translation generators $\hat{p}_\nu:=ip_\nu\equiv-\hbar\partial/\partial x^\nu$ and $\hat{x}^\mu:=ix^\mu$, subject to the relations

$$\begin{gathered}[\hat{p}^\mu,\hat{x}^\nu]=-i\hbar g^{\mu\nu},\\ [\hat{p}^\mu,\hat{p}^\nu]=0,\\ [\hat{x}^\mu,\hat{x}^\nu]=0,\\ [i,\hat{p}^\mu]=0,\\ [i,\hat{x}^\mu]=0,\\ i^2=-1.\end{gathered} \tag{2}$$

Here $g^{\mu\nu}$ is the Minkowski metric, held fixed in this paper. The carets (on $\hat{p}$, for example) indicate that a factor i has been absorbed to make the operator anti-Hermitian.[19] The algebra A_H has both the usual associative product and the Lie commutator product. As a real Lie algebra A_H is compound, Segal emphasized, containing the nontrivial ideal generated by the unit i.

The orbital Lorentz-group generators are

$$\hat{\mathcal{O}}^{\mu\nu}:=i\mathcal{O}^{\mu\nu}=-i(\hat{x}^\mu\hat{p}^\nu-\hat{x}^\nu\hat{p}^\mu). \tag{3}$$

These automatically obey the usual relations

$$\begin{gathered}[\hat{\mathcal{O}}^{\mu\nu},\hat{\mathcal{O}}^{\lambda\kappa}]=\hbar(g^{\mu\lambda}\hat{\mathcal{O}}^{\nu\kappa}-g^{\nu\lambda}\hat{\mathcal{O}}^{\mu\kappa}-g^{\mu\kappa}\hat{\mathcal{O}}^{\nu\lambda}+g^{\nu\kappa}\hat{\mathcal{O}}^{\mu\lambda}),\\ [\hat{x}^\mu,\hat{\mathcal{O}}^{\nu\lambda}]=\hbar(g^{\mu\nu}\hat{x}^\lambda-g^{\mu\lambda}\hat{x}^\nu),\\ [\hat{p}^\mu,\hat{\mathcal{O}}^{\nu\lambda}]=\hbar(g^{\mu\nu}\hat{p}^\lambda-g^{\mu\lambda}\hat{p}^\nu),\\ [i,\hat{\mathcal{O}}^{\mu\nu}]=0.\end{gathered} \tag{4}$$

Dirac algebra. $A_D=A[\gamma_\mu]$ is generated by Dirac–Clifford units γ_μ subject to the familiar relations

$$\{\gamma_\nu,\gamma_\mu\}=2g_{\nu\mu}. \tag{5}$$

As usual we write $\gamma_{\mu\nu\cdots}$ for the antisymmetric part of the tensor $\gamma_\mu\gamma_\nu\cdots$.

Statistics. One may define the *statistics* of an (actual, not virtual) aggregate by defining how the aggregate transforms under permutations of its units. That is, to describe N units with given unit mode space V_1 (Refs. 12 and 18) we give, first, the mode space V_N of the aggregate quantum system and, second, a simple representation $R_N : S_N \to \mathrm{End}\, V_N$ of the permutation group S_N on the given N units by linear operators on V_N. This also defines the quantification that converts yes-or-no questions about the individual into how-many questions about a crowd.

In *Clifford statistics* $\mathrm{End}\, V_N$ is a Clifford algebra $C = \mathrm{Cliff}(V_1)$, and so V_N is a spinor space for that Clifford algebra, with $C = \mathrm{End}\, V_N$. We write C_1 for the first-degree subspace of C. A Clifford statistics is defined by a projective (double-valued) representation $R_C : S_N \to C_1 \subset C$ of the permutation group S_N by first-grade Clifford elements over the unit mode space V_1.[17] To define R_C we associate with the nth unit (for all $n = 1,...,N$) a Clifford unit γ_n, and we represent every swap (transposition or two-cycle) (mn) of two distinct units by the difference $\pm(\gamma_n - \gamma_m) \in C_1$ of the associated Clifford units.

For a free Clifford statistics the units γ_n are independent and the metric g_{mn} is Euclidean. This representation has dimension $2^{N/2}$ and is reducible. The irreducible representations have dimension[20]

$$2^{[N-1/2]} = 1,1,2,2,4,4,8,8,16,...$$

$$\text{for } \mathrm{Dim}\, V_1 = N = 0,1,2,3,4,5,6,7,8,.... \tag{6}$$

Some useful terms:

A *cliffordon* is a quantum with Clifford statistics.

A *squadron* is a quantum aggregate of cliffordons.

A *sib* is a quantum aggregate of bosons.

A *set* of quanta is an aggregate of fermions.

A *sequence* of quanta is an aggregate of Maxwell–Boltzmann quanta with a given sequential order.[11]

R_C can be extended to a spinor representation of $\mathrm{SO}(N) \supset \mathrm{S}_N$ on the same spinor space $\Sigma(N)$.

The symmetry group G_U of the quantum kinematics for a universe U of N_U chronons is an orthogonal group

$$G_U = \mathrm{SO}(N_{U+}, N_{U-}),$$
$$N_U = N_{U+} + N_{U-}. \tag{7}$$

The algebra of observables of U is the simple finite-dimensional real Clifford algebra

$$C_U = \mathrm{Cliff}(V_1) = \mathrm{Cliff}[1, \gamma(1), \ldots, \gamma(N_U)] \tag{8}$$

generated by the N_U Clifford units $\gamma(n)$, $n = 1,...,N_U$ representing exchanges. The Clifford units $\gamma(n)$ span a vector space $V_1 \cong C_1$ of first-grade elements of C_U.

Within C_U we shall construct a simplified Dirac–Heisenberg algebra

$$\check{A}_{\mathrm{DH}} = A[\check{i}, \check{p}, \check{x}, \tilde{\gamma}] \subset C(V_1) \tag{9}$$

whose commutator Lie algebra is simple and which contracts to the usual Dirac–Heisenberg algebra A_{DH} in the continuum limit. We factor $\check{A}_{\mathrm{DH}}$ into the Clifford product

$$\check{A}_{\mathrm{DH}} = \mathrm{Cliff}(N\mathbf{6_0}) = \mathrm{Cliff}((N-1)\mathbf{6_0}) \amalg \mathrm{Cliff}(\mathbf{6_0}) \tag{10}$$

of two Clifford algebras, an ''internal'' algebra from the last hexad and an ''external'' algebra from all the others.

We designate our proposed simplifications of γ and i, $\hat{p}$, $\hat{x}$, and $\hat{O}$ by $\tilde{\gamma}$ and $\breve{i}$, $\breve{p}$, $\breve{x}$, and $\breve{O}$. In the limit $\chi\to 0$ the tildes ($\tilde{}$) disappear and the breves ($\breve{}$) become hats ($\hat{}$).

We use the following quadratic spaces:

$N\mathbb{R}:=\mathbb{R}\oplus\ldots\oplus\mathbb{R}$ (with N terms) $=\oplus_1^N\mathbb{R}$ is the positive-definite N-dimensional real quantum-mode space.

$-N\mathbb{R}$ is the corresponding negative-definite space.

$\mathbb{M}$ is Minkowski space with signature $1-3$.

$-\mathbb{M}$ is the same space with the opposite signature $3-1$.

Also,

$$\begin{gathered} X\Theta Y:=X\oplus(-Y),\\ \mathbf{1}:=\mathbb{R},\\ -\mathbf{1}:=-\mathbb{R},\\ \mathbf{3}:=3\mathbb{R},\\ -\mathbf{3}:=-3\mathbb{R},\\ \mathbb{M}:=\mathbf{1}\Theta\mathbf{3},\\ -\mathbb{M}:=\mathbf{3}\Theta\mathbf{1},\\ \mathbf{6_0}:=\mathbf{3}\Theta\mathbf{3}. \end{gathered} \tag{11}$$

$\mathbb{M}$ and $-\mathbb{M}$ are tangent spaces to Minkowski space–times and support natural representations of the Lorentz group.

II. SIMPLIFICATION OF THE RELATIVISTIC HEISENBERG ALGEBRA

As already mentioned, field theory employs a compound field-space–time bundle with space–time for base and field space for fiber; just as Galilean space–time is a four-dimensional bundle with $\mathbb{R}^3$ for base and $\mathbb{R}^1$ for fiber. The prototype is the covector field, where the fiber is the cotangent space to space–time, with coordinates that we designate by p_μ.

We assume that in experiments of sufficiently high resolution the space–time tangent bundle (or the Dirac–Heisenberg algebra) manifests itself as a simple quantum-field-space–time synthesis. The space–time variables x^μ and the tangent space variables p_μ unite into one simple construct, as space and time have already united. Now, however, the simplification requires an atomization, because the field variable actually derives from an atomic spin.

We first split the space–time tangent bundle into quantum cells. The minimum number of elements in a cell for our simplification is six: four for space–time and two for a complex or symplectic plane. We provisionally adopt the hexadic cell. Earlier work, done before our present stringent simplicity standard, assumed a pentadic cell.[16] This provided no natural correspondent for the energy–momentum operators.

N hexads define a unit mode space $V_1=N\mathbf{6_0}$. Each term $\mathbf{6_0}$ has a Clifford algebra Cliff(3, 3) whose spinors have eight real components, forming an $\mathbf{8}_0$. [Eight-component spinors have also been used in physics by Penrose,[7] Robson and Staudte,[21] and Lunsford;[22] though not to unify spin with space–time.] The spinors of V form the spinor space

$$\bigotimes_1^N \mathbf{8}_0=\mathbf{8}_0^N.$$

We do not deal with empty space–time. We explore space–time with one relativistic quantum spin-$\frac{1}{2}$ probe of rest mass $m\sim 1/\chi$. We express the usual spin operators γ^μ, space–time position operators x^μ, and energy–momentum operators p_μ of this probe as contractions of operators in the Clifford algebra Cliff$(3N,3N)$.

We write the dynamics of the usual contracted, compound Dirac theory in manifestly covariant form, with a Poincaré-scalar Dirac operator

$$D=\gamma^\mu p_\mu - mc. \tag{12}$$

D belongs to the algebra of operators on spinor-valued functions $\psi(x^\mu)$ on space–time. Any physical spinor $\psi(x^\mu)$ is to obey the dynamical equation

$$D\psi=0. \tag{13}$$

We simplify the dynamical operator D, preserving the form of the dynamical equation (13).

The compound symmetry group for the Dirac equation is the covering group of the Poincaré group ISO($\mathbb{M}$). We represent this as the contraction of a simple group SO(3, 3) acting on the spinor pseudo-Hilbert (ket) space of $6N$ Clifford generators $\gamma^\omega(n)$ ($\omega=0,...,5$; $n=1,...,N$) of the orthogonal group SO$(3N,3N)$. The size of the experiment fixes the parameter N.

We first simplify the anti-Hermitian space–time and energy–momentum translation generators $\hat{p}_\mu$ and $\hat{x}^\nu$, not the associated Hermitian observables p_μ, x^ν. Then we simplify the Hermitian operators by multiplying the anti-Hermitian ones by a suitably simplified i and symmetrizing the product.

As in Dirac one-electron theory, we use the spinor representation Spin($\mathbb{M}$) of SO($\mathbb{M}$) to describe the contracted generators $\hat{S}^{\mu\nu}$ of rotations and boosts. The spin generators are represented by second-degree elements

$$\hat{S}^{\mu\nu}:=\frac{\hbar}{4}[\gamma^\mu,\gamma^\nu]\equiv\frac{\hbar}{2}\gamma^{\mu\nu},\quad \mu,\nu=0,...,3 \tag{14}$$

of the Clifford algebra Cliff(1, 3).

We simplify ISO($\mathbb{M}$) within Spin($N\mathbf{6_0}$) by representing the simplified space–time symmetry generators of the probe by second degree elements of Cliff V_1. We associate the position and momentum axes with the γ^4 and γ^5 elements of the hexad, respectively, so that an infinitesimal orthogonal transformation in the 45-plane couples momentum into position. This accounts for the symplectic symmetry of classical mechanics and the i of quantum mechanics.

We therefore define the simplified $\breve{i}$, $\breve{x}^\mu$, and $\breve{p}^\nu$ of the probe by

$$\begin{aligned}
\breve{i}&\equiv\frac{1}{N-1}\sum_{n=1}^{N-1}\breve{i}(n):=\frac{1}{N-1}\sum_{n=1}^{N-1}\gamma^{45}(n),\\
\breve{x}^\mu&\equiv\sum_{n=1}^{N-1}\breve{x}^\mu(n):=-\chi\sum_{n=1}^{N-1}\gamma^{\mu 4}(n),\\
\breve{p}^\nu&\equiv\sum_{n=1}^{N-1}\breve{p}^\nu(n):=\phi\sum_{n=1}^{N-1}\gamma^{\nu 5}(n),
\end{aligned} \tag{15}$$

where χ, ϕ, and N are simplifiers of our theory, and

$$\gamma^{\rho\sigma}(n):=\tfrac{1}{2}[\gamma^\rho(n),\gamma^\sigma(n)]. \tag{16}$$

To support this choice for the expanded generators we form the following commutation relations among them (cf. Refs. 23, 1, and 24):

$$
\begin{aligned}
[\check{p}^{\mu},\check{x}^{\nu}] &= -2\phi\chi(N-1)g^{\mu\nu}\check{i},\\
[\check{p}^{\mu},\check{p}^{\nu}] &= -\frac{4\phi^{2}}{\hbar}\check{L}^{\mu\nu},\\
[\check{x},\check{x}^{\nu}] &= -\frac{4\chi^{2}}{\hbar}\check{L}^{\mu\nu},\\
[\check{i},\check{p}^{\mu}] &= -\frac{2\phi}{\chi(N-1)}\check{x}^{\nu},\\
[\check{i},\check{x}^{\mu}] &= +\frac{2\chi}{\phi(N-1)}\check{p}^{\mu}.
\end{aligned}
\tag{17}
$$

In (17),

$$
\begin{aligned}
\check{L}^{\mu\nu} &:= \frac{\hbar}{2}\sum_{n=1}^{N-1}\gamma^{\mu\nu}(n),\\
\check{J}^{\mu\nu} &:= \frac{\hbar}{2}\sum_{n=1}^{N}\gamma^{\mu\nu}(n) \equiv L^{\mu\nu}+S^{\mu\nu}.
\end{aligned}
\tag{18}
$$

where $\check{S}^{\mu\nu}$ is the Dirac spin operator [cf. (29)].

Equation (17) incorporates two decontractions: one leading to finite commutators between coordinates of the Snyder type, and one leading to finite commutators between $\hbar i$ and the coordinates and momenta of the Segal type. Both are necessary for simplicity.

The Snyder decontraction makes the theory more nonlocal than the Dirac equation. In the contracted theory, the coordinates *x,y,z* commute. This means that in principle one can produce the single quantum at a definite place and register it at a definite place. To be sure, to do so will mix positive and negative energy levels. In the more physical many-quantum theory, a pair will be created in these processes. Nevertheless, in the standard interpretation of the quantum theory it is still possible in principle to precisely determine the operators *x,y,z* with arbitrary precision at one instant, before the pair separates.

In the decontracted theory, any one of the operators *x,y,z* can be determined with arbitrary precision, say *z*. Its spectrum will then be discrete. The operators *x,y* will then have fundamental indeterminacies, depending on the magnitude of L_z and the constant χ. Thus the single quantum can no longer be localized in principle. This nonlocality is intrinsic to the space–time–momentum–energy–spin unification that makes the theory simpler.

$J^{\mu\nu}$ obeys the Lorentz-group commutation relations:

$$
[\check{J}^{\mu\nu},\check{J}^{\lambda\kappa}] = \hbar(g^{\mu\lambda}\check{J}^{\nu\kappa}-g^{\nu\lambda}\check{J}^{\mu\kappa}-g^{\mu\kappa}\check{J}^{\nu\lambda}+g^{\nu\kappa}\check{J}^{\mu\lambda}),
\tag{19}
$$

and generates a total Lorentz transformation of the variables x^{μ}, p_{μ}, i and $S^{\mu\nu}$:

$$
\begin{aligned}
[\check{x}^{\mu},\check{J}^{\nu\lambda}] &= \hbar(g^{\mu\nu}\check{x}^{\lambda}-g^{\mu\lambda}\check{x}^{\nu}),\\
[\check{p}^{\mu},\check{J}^{\nu\lambda}] &= \hbar(g^{\mu\nu}\check{p}^{\lambda}-g^{\mu\lambda}\check{p}^{\nu}),\\
[\check{i},\check{J}^{\mu\nu}] &= 0,\\
[\check{S}^{\mu\nu},\check{J}^{\lambda\kappa}] &= 0.
\end{aligned}
\tag{20}
$$

There is a mock orbital angular momentum generator of familiar appearance,

$$\check{O}^{\mu\nu} := -\check{i}(\check{x}^{\mu}\check{p}^{\nu} - \check{x}^{\nu}\check{p}^{\mu}). \tag{21}$$

$\check{O}$ too obeys the Lorent group commutation relations. We relate $\check{L}^{\mu\nu}$ and $\check{O}^{\mu\nu}$ in Sec. III.

Since the usual complex unit i is central and the simplified $\check{i}$ is not, we suppose that the contraction process includes a projection that restricts the probe to one of the two-dimensional invariant subspaces of $\check{i}$, associated with the maximum negative eigenvalue -1 of $\check{i}^2$. This represents a condensation that aligns all the mutually commuting hexad spins $\gamma^{45}(n)$ with each other, so that

$$\gamma^{45}(n)\,\gamma^{45}(n') \to -1 \tag{22}$$

for any n and n'. We call this the condensation of i.

Projection onto a sharp value of i kills i-changing variables like x^{μ} and p_{μ}. Only SO(2)-invariant combinations like $\chi^2 p^2 + \phi^2 x^2$ should survive. Nonetheless one observes position and momentum separately. This is a spontaneous symmetry-breaking by the vacuum condensate, analogous to the fact that a crystal in its ground state, with spherically symmetric Hamiltonian, can have a nonzero internal magnetization.

Under Wigner time-reversal, $t \to -t$ and $i \to -i$. Since the variable t is chosen by the experimenter, not the system, we must suppose that i too is mainly fixed by the experimenter, not the system. But since the boundary between system and experimenter is somewhat arbitrary, we must therefore suppose that the entire universe contributes uniformly to i; it is simply that the system is much smaller than the experimenter, and influences i less. This fits with an earlier theory of i as a Stückelberg–Higgs variable that imparts mass to some otherwise massless gauge vector bosons.[25–28]

Then the momentum variables p_{μ} that we usually attribute to the system, for example, are actually i-invariant bilinear combinations $P^{\rho\sigma}_{[\mu]} J_{\rho\sigma}$ of experimenter standards $P^{\rho\sigma}_{[\mu]}$ and the system tensor $J_{\rho\sigma}$. As creatures of the space–time condensate we do not experience the symmetry of the dynamics that produced it, but only its residual symmetries. The spontaneously broken symmetries reappear when the condensate melts down.

To recover the canonical commutation relations for $\check{x}^{\mu}$ and $\check{p}_{\mu}$ we must impose

$$\chi\phi(N-1) \equiv \frac{\hbar}{2} \tag{23}$$

and assume that

$$\begin{aligned} \chi &\to 0, \\ \phi &\to 0, \\ N &\to \infty. \end{aligned} \tag{24}$$

Then the relations (17) reduce to the commutation relations (2) of the relativistic Heisenberg algebra A_H as required.

The three parameters χ, ϕ, $1/N$ are subject to one constraint $\chi\phi(N-1) = \hbar/2$ leaving two independent simplifiers. N is not a physical constant like $\hbar$ and c, but depends on the scope of the experiment, and is under the experimenter's control. N-dependent effects might appear as curious boundary effects. We set a cosmological limit $N \lesssim N_{\mathrm{Max}}$ in the following.

This leaves one N-independent physical constant with the dimensions of time. We can consider two contractions, $\chi \to 0$ with N constant, and $N \to \infty$ with χ constant. They combine into the continuum limit $\chi \to 0$, $N \to \infty$. We fix one simplifier χ in Sec. IV by supposing that the mass of a probe approaches a finite limit as $N \to \infty$.

III. ORBITAL, SPIN, AND TOTAL ANGULAR MOMENTUM

As was shown in Sec. II, three sets of operators obeying Lorentz-group commutation relations appear in our theory. $\check{L}^{\mu\nu}$ represents the simplified *orbital angular momentum* generators, $\check{S}^{\mu\nu}$ represents the *spin* angular momentum, and $\check{J}^{\mu\nu}$ represents the simplified *total angular momentum* generators. There is a mock orbital angular momentum $\check{O}^{\mu\nu}$ (21).

In this section we show that $\hat{O}\to\hat{L}$ in the contraction limit.

Consider $\check{O}^{\mu\nu}$. By definition,

$$
\begin{aligned}
\check{O}^{\mu\nu} &= -(\check{x}^{\mu}\check{p}^{\nu}-\check{x}^{\nu}\check{p}^{\mu})\check{i} \\
&= +\frac{\chi\phi}{N-1}\left(\sum_{n=1}^{N-1}\gamma^{\mu 4}(n)\sum_{n'=1}^{N-1}\gamma^{\mu 5}(n')-\sum_{n=1}^{N-1}\gamma^{\nu 4}(n)\sum_{n'=1}^{N-1}\gamma^{\mu 5}(n')\right)\sum_{m=1}^{N-1}\gamma^{45}(m) \\
&= +\frac{\chi\phi}{N-1}\sum_{n}\left(\gamma^{\mu 4}(n)\gamma^{\nu 5}(n)-\gamma^{\nu 4}(n)\gamma^{\mu 5}(n)\right)\sum_{m}\gamma^{45}(m) \\
&\quad +\frac{\chi\phi}{N-1}\sum_{n\neq n'}\left(\gamma^{\mu 4}(n)\gamma^{\nu 5}(n')-\gamma^{\nu 4}(n)\gamma^{\mu 5}(n')\right. \\
&\quad \left.+\gamma^{\mu 4}(n')\gamma^{\nu 5}(n)-\gamma^{\nu 4}(n')\gamma^{\mu 5}(n)\right)\left(\gamma^{45}(n)+\gamma^{45}(n')\right) \\
&\quad +\frac{\chi\phi}{N-1}\sum_{n\neq n'}\left(\gamma^{\mu 4}(n)\gamma^{\nu 5}(n')-\gamma^{\nu 4}(n)\gamma^{\mu 5}(n')+\gamma^{\mu 4}(n')\gamma^{\nu 5}(n)\right. \\
&\quad \left.-\gamma^{\nu 4}(n')\gamma^{\mu 5}(n)\right)\sum_{m\neq n,m\neq n'}\gamma^{45}(m) \\
&= -\frac{2\chi\phi}{N-1}\sum_{n}\gamma^{\mu\nu}(n)\gamma^{45}(n)\sum_{m}\gamma^{45}(m) \\
&\quad +\frac{\chi\phi}{N-1}\sum_{n\neq n'}\left(\gamma^{\mu 4}(n)\gamma^{\nu 5}(n')-\gamma^{\nu 4}(n)\gamma^{\mu 5}(n')\right. \\
&\quad \left.+\gamma^{\mu 4}(n')\gamma^{\nu 5}(n)-\gamma^{\nu 4}(n')\gamma^{\mu 5}(n)\right)\sum_{m\neq n,m\neq n'}\gamma^{45}(m). \qquad (25)
\end{aligned}
$$

Thus, in the contraction limit (22)–(24) when condensation singles out the eigenspace of $\gamma^{45}(n)\gamma^{45}(n')$ with eigenvalue -1,

$$\hat{O}^{\mu\nu}\to\hat{J}^{\mu\nu}-\hat{S}^{\mu\nu}\equiv\hat{L}^{\mu\nu}, \qquad (26)$$

as asserted.

IV. SIMPLIFIED DIRAC DYNAMICS

Dirac's *one-body* theory in real (Majorana) form uses the operator algebra A_{DH} acting on a vector space

$$V_1 := \Sigma^{-\mathbb{M}} \qquad (27)$$

of spinor-valued wave functions, mapping the space–time to the spinor space $\Sigma=\Sigma(-\mathbb{M})$ over the Minkowski space–time $-\mathbb{M}$. This exhibits part of the compound structure we must simplify by

decontraction, the split between spin space Σ and space–time $\mathbb{M}$. We construct the new space entirely from spins, replacing the infinite-dimensional function space V_1 by a spinor space of high but finite dimensionality.

To simplify Dirac's spin-$\frac{1}{2}$ dynamics, we regard the position of the probe as the resultant of N quantum steps, each represented by one hexad of chronons. We identify the spin variables of the probe with those of the last hexad in (10), the growing tip of the world line of the probe.

We thereby simplify the Dirac–Heisenberg algebra A_{DH} to $\check{A}_{\mathrm{DH}} := \mathrm{Cliff}(N\mathbf{6_0})$, the Clifford algebra of a large squadron of cliffordons.

To construct the contraction from $\check{A}_{\mathrm{DH}}$ to A_{DH}, we group the generators of Cliff($3N$,$3N$) into N hexads $\gamma^{\omega}(n)$ ($\omega=0,...,5$; $n=1,...,N$). Each hexad algebra acts on eight-component real spinors in $\mathbf{8}_0$. Hexad N will be used for the spin of the quantum. The remaining $N-1$ hexads provide the space–time variables.

We identify the usual Dirac gammas γ^{μ} for $\mu=0,...,3$ of Cliff($-\mathbb{M}$) with second-degree elements of the last hexad:

$$\gamma^{\mu} \cong \tilde{\gamma}^{\mu} := \gamma^{\mu 5}(N). \tag{28}$$

Dirac's spin generators $\hat{S}^{\mu\nu}$ (14) simplify to the corresponding 16 components of the tensor

$$\check{S}^{\omega\rho} := \frac{\hbar}{2}\gamma^{\omega\rho}(N), \tag{29}$$

where ω, $\rho=0,...,5$ and μ, $\nu=0,...,3$.

It is now straightforward to simplify the Dirac equation $D\psi=0$ of (13). The internal degrees of freedom will be seen to contribute a rest mass term $m_{\chi}=\hbar/2\chi c$, and for simplicity we take this to be the entire rest mass of the Dirac equation, omitting any bare mass term in $\tilde{D}$. We simplify $D\rightarrow\tilde{D}$ and extend the internal symmetry group from SO(1, 3) to the group SO(3, 3) of a hexad by setting

$$\tilde{D} := \frac{2\phi}{\hbar^2}\check{S}^{\omega\rho}\check{L}_{\omega\rho}, \tag{30}$$

where [cf. (18)]

$$\check{L}_{\omega\rho} := \frac{\hbar}{2}\sum_{n=1}^{N-1}\gamma_{\omega\rho}(n). \tag{31}$$

Our proposed dynamical operator is invariant under a conformal group SO(3, 3) whose contraction includes the Poincaré group. [Our symmetry group SO(3, 3) incorporates and extends the SO(3, 2) symmetry possessed by Dirac's dynamics for an electron in de-Sitter space–time.[29] That dynamics has the form

$$D' = \frac{1}{\hbar R}\hat{S}^{\omega\rho}\hat{O}_{\omega\rho} - mc,$$

where $\hat{S}^{\omega\rho}$ and $\hat{O}_{\omega\rho}$ are the five-dimensional spinorial and orbital angular momentum generators and R is the radius of the de-Sitter universe. Its group is still compound, not simple, unifying translations, rotations, and boosts, but not symplectic transformations.]

A complete set of commuting generators for the Poincaré group ISO(1, 3) consists of the time translation generator $\hat{p}_0$, the rotation generator $\hat{L}_{12}$, and the boost generator $\hat{L}_{03}$. In the present context, we adjoin the imaginary unit i. In the proposed simplification ISO(1, 3)$\times$SO(2) $\leftarrow$SO(3, 3) these simplify according to $\hat{p}_0\leftarrow\check{L}_{04}$, $\hat{L}_{12}\leftarrow\check{L}_{12}$, $\hat{L}_{03}\leftarrow\check{L}_{03}$, $i\leftarrow\check{L}_{45}$. A commuting set

cannot contain both $\check{L}_{04}$ and $\check{L}_{45}$. Since varying energy is more familiar than varying i, in a first treatment we hold $\check{L}_{45}$ constant and couple different masses in one representation.

V. REDUCTION TO THE POINCARÉ GROUP

We now assume a condensation that reduces SO(3, 3) to its subgroup $\mathrm{SO}(1,3)\times\mathrm{SO}(2)$. Relative to this reduction, the $\tilde{D}$ of (30) breaks up into

$$\tilde{D}=\frac{\phi}{2}\gamma^{\omega\rho}(N)\sum_n\ \gamma_{\omega\rho}(n)\quad(\omega,\rho=0,1,...,5)$$

$$=\phi\gamma^{\mu 5}(N)\sum_n\ \gamma_{\mu 5}(n)+\phi\gamma^{\mu 4}(N)\sum_n\ \gamma_{\mu 4}(n)+\phi\gamma^{\mu\nu}(N)\sum_n\ \gamma_{\mu\nu}(n)+\phi\gamma^{45}(N)\sum_n\ \gamma_{45}(n)$$

$$=\gamma^{\mu 5}\check{p}_\mu-\frac{\phi}{\chi}\gamma^{\mu 4}\check{x}_\mu+\frac{2\phi}{\hbar}\gamma^{\mu\nu}\check{L}_{\mu\nu}+(N-1)\phi\gamma^{45}\check{i}. \tag{32}$$

In the condensate all the operators $\gamma^{45}(n)\gamma_{45}(n')$ attain their minimum eigenvalue -1. Then

$$(N-1)\phi\gamma^{45}\check{i}\to-\frac{\hbar}{2\chi} \tag{33}$$

and the dynamics becomes

$$\tilde{D}=\gamma^{\mu 5}\check{p}_\mu-\frac{\phi}{\chi}\gamma^{\mu 4}\check{x}_\mu+\frac{2\phi}{\hbar}\gamma^{\mu\nu}\check{L}_{\mu\nu}-m_\chi c, \tag{34}$$

with rest mass

$$m_\chi=\frac{\hbar}{2\chi c}. \tag{35}$$

For sufficiently large N this reduces to the usual Dirac dynamics.

We identify the mass m_χ with the N-independent mass m of the Dirac equation for the most massive individual quanta that the condensate can propagate without melt-down, on the order of the top quark or Higgs masses:

$$m_\chi\sim 10^2\ \mathrm{GeV},\quad \chi\sim 10^{-25}\ \mathrm{s}. \tag{36}$$

The universe is $\sim 10^{10}$ years old. This leads to an upper bound

$$N_{\max}\sim 10^{41}. \tag{37}$$

This implies that χ is independent of N as $N\to\infty$ and that $\phi\sim 1/N\to 0$ as $N\to\infty$ even for finite χ. In experiments near the Higgs energy, $p\sim\hbar/\chi$. If we also determine N by setting $x\sim N\chi$ then all four terms in (34) are of the same order of magnitude.

To estimate experimental effects, however, we must take gauge transformations into account. These transform the second term away in the continuum limit. This refinement of the theory is still in progress.

VI. CONCLUSIONS

Like classical Newtonian mechanics, the Dirac equation has a compound (nonsemisimple) invariance group. Its variables break up into three mutually commuting sets: the space–time–energy–momentum variables (x^μ,p_μ), the spin variables γ^μ, and the imaginary unit i.

To unify them we replace the space–time continuum by an aggregate of $M<\infty$ finite elements, chronons, described by spinors with $\sim 2^{M/2}$ components. Chronons have Clifford–Wilczek statistics, whose simple operator algebra is generated by units γ^m, $m=1,...,M$. We express all the variables x^μ, p_μ, γ^μ and i as polynomials in the γ^m. We group the $M=6N$ chronons into N hexads for this purpose, corresponding to tangent spaces; the hexad is the least cell that suffices for this simplification. There are three simplifiers χ, ϕ, $1/N$, all approaching 0 in the continuum limit, subject to the constraint $\chi\phi(N-1)=\hbar/2$ for all N.

In the continuum limit the Dirac mass becomes infinite. In our theory, the finite Dirac masses in nature are consequences of a finite atomistic quantum space–time structure with $\chi>0$.

The theory predicts a certain spin–orbit coupling $\gamma^{\mu\nu}L_{\mu\nu}$ not found in the standard model, and vanishing only in the continuum limit. The experimental observation of this spin–orbit coupling would further indicate the existence of a chronon.

In this theory, the spin we see in nature is a manifestation of the (Clifford) statistics of atomic elements of space-time, as Brownian motion is of the atomic elements of matter. As we improve our theory we will interpret better other indications of chronon structure that we already have, and as we improve our measuring techniques we shall meet more such signs.

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Complex velocity transformations and the Bisognano–Wichmann theorem for quantum fields acting on Krein spaces

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It is proven that in indefinite metric quantum field theory there exists a dense set of analytic vectors for the generator of the one parameter group of x^0-x^1 velocity transformations. This makes it possible to define complex velocity transformations also for the indefinite metric case. In combination with the results of Bros, Epstein, and Moschella [Commun. Math. Phys. **196**, 535–570 (1998)], proving Bisognano–Wichmann (BW) analyticity within the linear program, one then obtains a suitable generalization of the BW theorem for local, relativistic quantum fields acting on Krein spaces (''quantum fields with indefinite metric''). © *2002 American Institute of Physics.* [DOI: 10.1063/1.1503151]

I. INTRODUCTION

The connection of the Unruh effect[39] describing the Hawking radiation seen by a uniformly accelerated observer in local quantum field theory (QFT) with the Tomita–Takesaki modular theory[11,38] of v. Neumann algebras has been one of the most fascinating achievements in the study of the general structure of QFT, cf. Refs. 10 and 18 for an overview. In the Wightmanian formulation of QFT this connection is given by the Bisognano–Wichmann theorem[6] which, under a few additional assumptions, can then be extended to localized v. Neumann algebras associated with the algebras of unbounded Wightman fields, see, e.g., Refs. 5, 6, and 24.

The present work attempts to adapt the Bisognano–Wichmann theorem[6] to the case of quantum fields with indefinite metric in the framework of Morchio and Strocchi.[26,34,36] That this should in fact be possible was proven by J. Bros, H. Epstein and U. Moschella in Ref. 12. In this reference the authors show that the KMS condition for the algebra localized in the right wedge $\mathcal{W}_R=\{x\in\mathbb{R}^d: x^1>|x^0|\}$ w.r.t. the one parameter group of Lorentz boosts in the x^0-x^1 direction follows from the analyticity properties of Wightman functions from solely the linear program, i.e., without using positivity. In contrast to this, the original proof of Ref. 6 uses functional calculus for the generators of the Lorentz boosts, and thus positivity, to establish that property.

Quantum fields with indefinite metric have been introduced in the Wightmanian formulation of QFT in order to deal also with gauge fields in local and covariant gauges. Such fields can not be fields with positive metric.[35–37] Quantum fields with indefinite metric surely have to be considered to be artificial and ''nonphysical'' (at least as long as the related physical Hilbert space with positive metric and the algebra of gauge invariant fields acting on that space have not been constructed), but still some motivation can be found to consider the BW theorem also in this framework:

(i) QFT with indefinite metric is close to perturbation theory where local and covariant gauges are needed for technical reasons (see Refs. 32 and 36).
(ii) There are nontrivial examples in arbitrary space–time dimension.[1–3,29,30,31,32]

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(iii) The BW theorem might be important to develop a bounded operator approach for quantum fields with indefinite metric defining wedge algebras as weak commutants in the style of Refs. 6 and 24.
(iv) The BW theorem can be seen as a first step towards studying the influence of constraints (gauge) to wedge-duality.
(v) It is an interesting technical exercise to develop a suitable substitute for functional calculus in the case of quantum fields with indefinite metric.

This article is organized as follows: In Sec. II we collect the basic tools for the formulation of QFT with indefinite metric.

In Sec. III we prove a crucial continuity property for GNS-like representations on maximal inner product spaces (Krein spaces[4,7]) and we recall basic properties of the field algebra as the Reeh–Schlieder property. As the vacuum plays a special role in modular theory, we clarify the status of the vacuum as the only translation invariant state for QFTs with indefinite metric and a mass gap—this then also implies the irreducibility of the field algebra (see also Ref. 26). In particular we show that the occurrence of theta-vacua, in the description of G. Morchio and F. Strocchi,[26] and reducibility of the field algebra due to classical long range fluctuations[13] are strictly linked to mass zero phenomena, as of course suggested by these references.

In Sec. IV we define the complex velocity transformations for the case of quantum fields with indefinite metric using the continuity properties established in Sec. III in connection with functional calculus on the Borchers algebra. Rather than using functional calculus for η-symmetric operators, see, e.g., Refs. 4 and 19 and references therein, we follow a ''pedestian's approach'' and prove the existence of a dense set of entire analytic vectors for the generator of the Lorentz boosts.

In Sect. V we recall the result of Bisognano–Wichmann (BW) analyticity within the linear program as proven by Bros–Epstein–Moschella[12] and derive a version of the BW theorem for quantum fields with indefinite metric. In particular, we identify the ''modular objects:'' The antiunitary implementation of the reflection $\Theta_{0,1}:(x^0,x^1,x^2,\ldots,x^{d-1})\to(-x^0,-x^1,x^2,\ldots,x^{d-1})$ is the ''modular conjugation'' and velocity transformations at imaginary boost parameter $i\pi$ are Tomita's modular operator $\Delta^{1/2}$. For space–time dimension $d=4$ the modular conjugation thus coincides with the rotation around $e_1=(0,1,0,\ldots,0)$ by an angle π times the PCT-operator $\Theta:x\to -x$, which is the description given in Ref. 6. Here, of course, no answer is given to what extent Tomita–Takesaki theory can be generalized to η- v.Neumann algebras acting on Krein spaces and thus to what extent the ''modular objects'' defined here really can be related to some extension of Tomita–Takesaki theory. This might, however, be an interesting question for the future. At least Tomita–Takesaki theory on the Pontryagin space Π_1 has been established in Ref. 25.

II. QFT WITH INDEFINITE METRIC

Here some notation is introduced and basic results on the GNS construction on maximal inner product spaces (Krein spaces) are recalled (see, however, Refs. 21, 26 and 40 for more details). We only consider Bosonic, scalar and chargeless QFTs over a d-dimensional Minkowski space–time $(\mathbb{R}^d,\cdot)$. Generalization to arbitrary spin, charge and statistics is straightforward. The associated Borchers algebra[8,9] is the free, unital, involutive, topological tensor algebra over $\mathcal{S}_1=\mathcal{S}(\mathbb{R}^d,\mathbb{C})$, the space of complex Schwartz test functions over $\mathbb{R}^d$. In more explicit terms, we set

$$\underline{\mathcal{S}}=\oplus_{n=0}^{\infty}\mathcal{S}_n,\quad \mathcal{S}_n=\mathcal{S}(\mathbb{R}^{dn},\mathbb{C}),\quad \mathcal{S}_0=\mathbb{C}, \tag{1}$$

with $\underline{f}+\underline{h}=(f_0+h_0,f_1+h_1,\ldots)$, $\underline{f}\otimes\underline{h}$ given by $(\underline{f}\otimes\underline{h})_n=\Sigma_{j+l=n}^{\infty,l=0}f_j\otimes h_l\ \forall n\in\mathbb{N}_0$, $\mathbf{1}=(1,0,\ldots)$ and $\underline{f}^*=(f_0^*,\ldots,f_n^*,0\ldots)$ with $f_l^*(x_1,\ldots,x_l)=\overline{f_l(x_l,\ldots,x_1)}$. Here the bar denotes complex conjugation and the product always exists as for $\underline{f}\in\underline{\mathcal{S}}$ only finitely many $f_l\in\mathcal{S}_l$ are different from zero.

The canonic action $\alpha:P_+^{\uparrow}\to\mathrm{Aut}(\mathcal{S}_l)$ of the orthochronous, proper Poincaré group on $\mathcal{S}_l$, $l\in\mathbb{N}$, induces a representation $\underline{\alpha}:P_+^{\uparrow}\to\mathrm{Aut}(\underline{\mathcal{S}})$ by continuous $*$-algebra homomorphisms on $\underline{\mathcal{S}}$.

The spectral ideal $I_{\mathrm{sp}}\subset\underline{\mathcal{S}}$ is the left-ideal generated by elements of the form

$$\underline{g}=\underline{g}(\underline{f},h)=\int_{\mathbb{R}^d}\underline{\alpha}_{\{1,a\}}(\underline{f})h(a)da\in\underline{\mathcal{S}} \tag{2}$$

for supp $\hat{h}\cap\overline{V}_0^+=\varnothing$ where $h\in\mathcal{S}_1$, $\hat{h}(k)=\int_{\mathbb{R}^d}e^{ik\cdot a}h(a)da$ and $\overline{V}_0^+=\{k\in\mathbb{R}^d,k^0\geqslant 0,k\cdot k\geqslant 0\}$ is the closed forward light cone. The related left-ideal I_{sp}^m where in the definition of I_{sp} $\overline{V}_0^+$ is replaced by $\{0\}\cup\overline{V}_m^+=\{0\}\cup\{k\in\mathbb{R}^d,k^0\geqslant 0,k\cdot k\geqslant m^2\}$, $m>0$, is called spectral ideal with mass-gap m.

A further useful ideal in $\underline{\mathcal{S}}$ is the two-sided ideal generated by $(0,0,[f_1,h_1],0,\ldots)$ with $f_1,h_1\in\mathcal{S}_1$ and supp f_1, supp h_1 space-like separated, i.e., $(x-y)\cdot(x-y)<0\ \forall x\in\text{supp } f_1, y\in\text{supp } h_1$. It is called the ideal of locality.

We recall that $\underline{\mathcal{S}}$ is endowed with the strongest topology, such that the relative topology of $\mathcal{S}_n$ in $\underline{\mathcal{S}}$ is the Schwartz topology (direct sum topology). Let $\underline{\mathcal{S}}'=\underline{\mathcal{S}}'(\mathbb{R}^d,\mathbb{C})$ be the topological dual space of $\underline{\mathcal{S}}$. Then $\underline{R}\in\underline{\mathcal{S}}'$ is of the form $\underline{R}=(R_0,R_1,R_2,\ldots)$ with $R_0\in\mathbb{C},R_n\in\mathcal{S}_n',n\in\mathbb{N}$. Furthermore, any such sequence defines uniquely an element of $\underline{\mathcal{S}}'$. An element $\underline{W}\in\underline{\mathcal{S}}'$ is called a Wightman functional if it fulfills the following set of conditions, which are also called the modified Wightman axioms, cf. Refs. 26 and 40:

Axioms 2.1: (A1) Temperedness and normalization: $\underline{W}\in\underline{\mathcal{S}}'$ and $W_0=1$.

(A2) Poincaré invariance: $\underline{W}(\underline{\alpha}_{\{\Lambda,a\}}(\underline{f}))=\underline{W}(\underline{f})\ \forall\{\Lambda,a\}\in\tilde{P}_+^{\uparrow}$, $\underline{f}\in\underline{\mathcal{S}}$.

(A3) Spectral property: Let I_{sp} be the spectral (left) ideal in $\underline{\mathcal{S}}$. Then $I_{\mathrm{sp}}\subseteq$kernel $\underline{W}$.

(A4) Locality: Let I_{loc} be the (two-sided) ideal of locality in $\underline{\mathcal{S}}$. Then $I_{\mathrm{loc}}\subseteq$kernel $\underline{W}$.

(A5) Hilbert space structure condition (HSSC): There exists a Hilbert seminorm $\underline{p}$ on $\underline{\mathcal{S}}$ s.t. $|\underline{W}(\underline{f}^*\otimes\underline{g})|\leqslant\underline{p}(\underline{f})\underline{p}(\underline{g})\forall\underline{f},\underline{g}\in\underline{\mathcal{S}}$.

(A6) Cluster property: $\lim_{t\to\infty}\underline{W}(\underline{f}\otimes\underline{\alpha}_{\{1,ta\}}(\underline{g}))=\underline{W}(\underline{f})\ \underline{W}(\underline{h})\ \forall\underline{f},\underline{g}\in\underline{\mathcal{S}},a\in\mathbb{R}^d$ space like.

(A7) Hermiticity: $\underline{W}(\underline{f}^*)=\overline{\underline{W}(\underline{f})}\ \forall\underline{f}\in\underline{\mathcal{S}}$.

We say that the Hilbert seminorm $\underline{p}$ in (A5) is of Sobolev type, if

$$\underline{p}(\underline{f})=\sum_{l=0}^{\infty}p_n(f_n)\forall\underline{f}\in\underline{\mathcal{S}} \tag{3}$$

s.t. p_n defined on $\mathcal{S}_n$ up to multiplication with a positive constant is given by a Hilbert norm of Sobolev type,[17]

$$p_n(f_n)^2=c^2\int_{\mathbb{R}^{dn}}\left|\prod_{l=1}^{n}(1+|x_l|^2)^{N/2}(1-\Delta_{x_l})^{L/2}f_n(x_1,\ldots,x_n)\right|^2dx_1\cdots dx_n, \tag{4}$$

for some possibly n-dependent $L,N\in\mathbb{N}_0$ and $c>0$ with $\Delta_{x_l}=\Sigma_{l=1}^n\partial^2/(\partial x_l)^2$. $\underline{p}$ is called Sobolev dominated, if there exists a Hilbert norm $\underline{p}'$ of Sobolev type s.t. $\underline{p}\leqslant\underline{p}'$ or, in other words, if $\underline{p}$ is continuous with respect to (w.r.t.) the $\underline{\mathcal{S}}$-topology.

If I_{sp} in (A3) can be replaced with some bigger I_{sp}^m, $m>0$, then we say that $\underline{W}$ fulfills the strong spectral condition. One can show by explicit calculations that the axioms (A1)–(A4), (A6) and (A7) are equivalent to the usual Wightman axioms,[33] whereas positivity has been replaced by the weaker assumption (A5). Nevertheless, (A5) is enough to get an analog of the Wightman reconstruction theorem on maximal, non degenerate inner product spaces as follows:

A metric operator $\eta:\mathcal{H}\to\mathcal{H}$ by definition is a self-adjoint operator on a complex separable Hilbert space $(\mathcal{H},(.,.))$ with $\eta^2=1$. η induces a second, in general indefinite, inner product on $\mathcal{H}$ via $\langle .,.\rangle=(.,\eta.)$ and η then gives a fundamental decomposition of $\mathcal{H}$ into intrinsically complete subspaces $\mathcal{H}=\mathcal{H}^+\oplus\mathcal{H}^-$ s.t. $\langle .,.\rangle$ restricted to $\mathcal{H}^{\pm}$ is positive/negative definite. Hence $(\mathcal{H},\langle .,.\rangle)$ is a Krein space.[4,7] It should be mentioned that $(.,.)$, η and the fundamental decomposition $\mathcal{H}^{\pm}$ are not unique given $(\mathcal{H},\langle .,.\rangle)$; η, for example, can be replaced by $\eta_C=\mathrm{sign}(|C|^{-2}\eta)$ for a bounded, continuously invertible operator on $\mathcal{H}$ leading to an in general different, but topologically equivalent, $(.,.)_C=(.,|C|^2||C|^{-2}\eta|.)$ and also a new fundamental decomposition according to η_C.

Let $\mathcal{D}$ be a dense and linear subspace of $\mathcal{H}$. The set of (possibly unbounded) Hilbert space operators $\mathsf{L}:\mathcal{D}\to\mathcal{D}$ with (restricted) η-adjoint $\mathsf{L}^{[*]}=\eta\mathsf{L}^*\eta|_{\mathcal{D}}:\mathcal{D}\to\mathcal{D}$ is denoted with $\mathsf{O}_\eta(\mathcal{D})$. Clearly, $\mathsf{O}_\eta(\mathcal{D})$ is an unital algebra with involution $[*]$. The canonical topology on $\mathsf{O}_\eta(\mathcal{D})$ is generated by the seminorms $\mathsf{L}\to|\langle\Psi_1,\mathsf{L}\Psi_2\rangle|$, $\Psi_1,\Psi_2\in\mathcal{D}$. We then have the following theorem:

Theorem 2.2: *Let $\underline{W}\in\underline{\mathcal{S}}$ be a Wightman functional which fulfills Axioms 2.1. Then we have the following.*

(i) *There is a Hilbert space $(\mathcal{H},(.,.))$ with a distinguished normalized vector $\Omega\in\mathcal{H}$ called the vacuum, a metric operator η with $\eta\Omega=\Omega$ inducing a nondegenerate inner product $\langle.,.\rangle=(.,\eta.)$ and a continuous $*$-algebra representation $\phi:\underline{\mathcal{S}}\to\mathsf{O}_\eta(\mathcal{D})$ with $\mathcal{D}=\phi(\underline{\mathcal{S}})\Omega$ which is connected to the Wightman functional $\underline{W}$ via $\underline{W}(\underline{f})=\langle\Omega,\phi(\underline{f})\Omega\rangle\forall\underline{f}\in\underline{\mathcal{S}}$.*

(ii) *There is a η-unitary continuous representation $\mathsf{U}:\widetilde{P}^\uparrow_+\to\mathsf{O}_\eta(\mathcal{D})$ $(\mathsf{U}^{[*]}=\mathsf{U}^{-1})$ such that $\mathsf{U}(\Lambda,a)\phi(\underline{f})\mathsf{U}(\Lambda,a)^{-1}=\phi(\underline{\alpha}_{\{\Lambda,a\}}(\underline{f}))\forall\underline{f}\in\underline{\mathcal{S}},\{\Lambda,a\}\in\widetilde{P}^\uparrow_+$ and Ω is invariant under the action of U.*

(iii) *ϕ fulfills the spectral condition $\phi(I_{\mathrm{sp}})\Omega=0$.*

(iv) *ϕ is a local representation in the sense that $I_{\mathrm{loc}}\subseteq\mathrm{kernel}\ \phi$.*

(v) *For $\Psi_1,\Psi_2\in\mathcal{D}$ and $a\in\mathbb{R}^d$ space like, we get $\lim_{t\to\infty}\langle\Psi_1,\mathsf{U}(1,ta)\Psi_2\rangle=\langle\Psi_1,\Omega\rangle\langle\Omega,\Psi_2\rangle$.*

A quadruple $((\mathcal{H},\langle.,.\rangle,\Omega),\eta,\mathsf{U},\phi)$ is called a local relativistic QFT in indefinite metric.

Conversely, let $((\mathcal{H},\langle.,.\rangle,\Omega),\eta,\mathsf{U},\phi)$ be a local relativistic QFT in indefinite metric. Then $\underline{W}(\underline{f})=\langle\Omega,\phi(\underline{f})\Omega\rangle\ \forall\ \underline{f}\in\underline{\mathcal{S}}$ defines a Wightman functional $\underline{W}\in\underline{\mathcal{S}}'$ which fulfills Axioms 2.1.

As we will come back to some details of the proof of Theorem 2.2 in the next section, we recall these points here while for the rest of the proof we refer to Refs. 26, 40 and 21.

Sketch of Proof: Without loss of generality one can assume that $\underline{p}$ is a Hilbert norm. If $\underline{p}$ is only a Hilbert seminorm we can replace it by the Hilbert norm $\underline{p}'=\sqrt{\underline{p}^2+\underline{p}_1^2}$ where $\underline{p}_1$ is a Hilbert norm on $\underline{\mathcal{S}}$ which not necessarily dominates $\underline{W}$. Such $\underline{p}_1$ can, e.g., be chosen as a direct sum of Sobolev norms on $\mathcal{S}_n$.

Then, $\mathcal{H}_1=\overline{\underline{\mathcal{S}}}^{\underline{p}}$ defines the Hilbert space completion of $\mathcal{D}_1=\underline{\mathcal{S}}$ w.r.t. $\underline{p}$. The Hermitian inner product $\langle\underline{f},\underline{g}\rangle=\underline{W}(\underline{f}^*\otimes\underline{g})$ defined for $\underline{f},\underline{g}\in\mathcal{D}_1$ is continuous and thus extends uniquely to $\mathcal{H}_1$. By the Riesz representation theorem there exists a self-adjoint operator η_1 bounded by one s.t. $\langle.,.\rangle=(.,\eta_1.)_1$. The algebra $\underline{\mathcal{S}}$ acts via the identical representation ϕ_1 by multiplication from the left on $\mathcal{D}_1\subseteq\mathcal{H}_1$. Likewise, a η_1-unitary continuous representation $\mathsf{U}_1:P^\uparrow_+\to\mathsf{O}_{\eta_1}(\mathcal{D}_1)$ is defined by the action of $\underline{\alpha}$ on $\mathcal{D}_1$.

Let $\mathcal{K}_0=\{v\in\mathcal{H}_1:\langle w,v\rangle=0\forall w\in\mathcal{H}_1\}$ and $\underline{\mathcal{S}}_0=\{\underline{f}:\underline{W}(\underline{g}\otimes\underline{f})=0\forall\underline{g}\in\underline{\mathcal{S}}\}$. Then, $\mathcal{K}_0$ is a closed subspace of $\mathcal{H}_1$. Let $\mathcal{H}_2=\mathcal{H}_1/\mathcal{K}_0$ be quotient Hilbert space of $\mathcal{H}_1$ and $\mathcal{K}_0$ with scalar product $(.,.)_2$. By Hermiticity, linearity and definition of $\mathcal{K}_0$, $\langle.,.\rangle$ is also defined on the quotient space $\mathcal{H}_2$. Let $\pi:\mathcal{H}_1\to\mathcal{H}_2$ be the quotient map. Then, by the definition of $\mathcal{K}_0$, $(\pi(\underline{f}),\pi(\underline{g}))_2$ still dominates $\langle.,.\rangle$. Thus, there exists a self-adjoint operator η_2 bounded by one s.t. $\langle.,.\rangle=(.,\eta_2.)_2$. Furthermore, we set $\mathcal{D}=\pi(\mathcal{D}_1)\cong\underline{\mathcal{S}}/\underline{\mathcal{S}}_0$ as $\mathcal{D}_1\cap\mathcal{K}_0=\phi_1(\underline{\mathcal{S}}_0)$. As $\underline{\mathcal{S}}_0$ is a left ideal and is taken into itself by the action of $\underline{\alpha}$, $\phi=\pi\circ\phi_1$ and $\mathsf{U}=\pi\circ\mathsf{U}_1$ define a left-representation of $\underline{\mathcal{S}}$ and $\widetilde{P}^\uparrow_+$, respectively, in $\mathsf{O}_{\eta_2}(\mathcal{D})$.

Let $(.,.)=(.,|\eta_2|.)_2$. Then, the metric operator η defined by $\langle.,.\rangle=(.,\eta.)$ is $\eta=\mathrm{sign}(\eta_2)$. Thus, also $(.,.)$ dominates $\langle.,.\rangle$ and obviously $\|.\|\leqslant\|.\|_2$. We can now set $\mathcal{H}$ to be the completion of $\mathcal{D}$ w.r.t. $\|.\|$, and extend η and $\langle.,.\rangle$ to $\mathcal{H}$ in order to obtain a Krein space representation, as described by the assertion of the theorem. The representations ϕ and U in $\mathsf{O}_\eta(\mathcal{D})$ then fulfill the requirements $(i)-(v)$, as proven in Refs. 26, 21, 33, 40 (see also Ref. 16). For the fact that η can be chosen s.t. $\eta\Omega=\Omega$, $\Omega=\pi(1,0,\ldots)$, cf. Ref. 21. ∎

Let $\Theta_{0,1}$ be the antilinear PCT-like transformation given by the action $\alpha_{\{\Theta_{0,1},0\}}(f_n)\times(x_1,\ldots,x_n)=\overline{f_n(\Theta_{0,1}x_1,\ldots,\Theta_{0,1}x_n)}$ for $f_n\in\mathcal{S}_n$, $\Theta_{0,1}x$ as in the Introduction, and $\underline{\alpha}_{\{\Theta_{0,1},0\}}$ the related action on $\underline{\mathcal{S}}$. From the proof of Theorem 2.2 one immediately (cf. Ref. 36) obtains the following.

Corollary 2.3: Let $\underline{p}$ in (A5) be such that $\underline{p}(\underline{\alpha}_{\{\Lambda,0\}}(\underline{f}))=\underline{p}(\underline{f})\ \forall\underline{f}\in\underline{\mathcal{S}}$ and $\Lambda\in G\subseteq L$, with G

generated by rotations (in a given frame of reference) and the PCT-like transformation $\Theta_{0,1}$. *Then,* U *extends to all* G *and* $\mathsf{U}(G)$ *commutes with the metric operator* η *constructed in the Proof of Theorem 2.2. In particular,* $\mathsf{U}(G)$ *is represented by (anti-) unitary, and hence bounded, operators on* $\mathcal{H}$.

Proof: By the PCT-theorem in d space–time dimensions, which does not require positivity (here we assumed the standard connection of spin and statistics, which is required for the PCT theorem—in theories with indefinite metric where also ghost fields are included, the results of this article on the BW theorem do not apply), $\underline{W}$ is invariant under the antilinear PCT-like transformation $\Theta_{0,1}$,[12,33] and thus $\mathsf{U}(G)$ is (anti-)η-unitarily represented. As $\underline{p}$ is invariant under the action of G, η_1 commutes with $\mathsf{U}_1(G)$. Since the construction of $\mathcal{H}$ consists of twice changing the operators η_1 and η_2 by functions of these operators, $\mathsf{U}(G)$ also commutes with η. (Anti-) unitarity of $\mathsf{U}(G)$ now follows from $\eta^2=1$. ■

It is demonstrated in Ref. 28, Theorem 3.1, that Sobolev dominated Hilbert norms which do not fulfill the condition of Corollary 2.3 can be replaced by equivalent norms which fulfill that condition. It is automatically fulfilled by Hilbert norms of Sobolev type.

To close this section we would like to address two points concerning the usefulness of Theorem 2.2 to describe the physics of quantum fields with indefinite metric. The first point is that the construction of $\mathcal{H}$ depends not only on $\underline{W}$ but possibly depends also on the auxilary Hilbert seminorm $\underline{p}$. In fact, unless the fundamental decomposition $\mathcal{H}^{\pm}$ of $\mathcal{H}$ given by η has either $\mathcal{H}^{+}$ or $\mathcal{H}^{-}$ intrinsically complete, i.e., complete w.r.t. the topology generated by the restriction of $\langle .,. \rangle$ to $\mathcal{H}^{\pm}$, recent results prove that there are infinitely many topologically inequivalent maximal Hilbert space structures.[15,22,23] In the generic situation in QFT the fundamental decomposition $\mathcal{H}^{\pm}$ can not be expected to have an intrinsically complete component. On the other hand it is argued in Refs. 27 and 28 that exactly this nonuniqueness can be exploited for the construction of charged states in certain infrared representations (depending on the space–time splitting) and thus is a necessary feature of gauge QFT. Another application involving an adequate choice of the closure of local states is, e.g., bosonization in low-dimensional QFT, cf. Ref. 36. The present article deals with this issue in the way that we prove our results for *all* such maximal Hilbert space structures which originate from Sobolev dominated $\underline{p}$.

The second point, which has recently been expressed by O. Steinmann, is that maximal Hilbert topologies on the space(s) $\mathcal{H}$ might have little to do with the topology on the space of physical states, as in the case of quantum electrodynamics it is not possible to construct charged states for the Maxwell (Gauss) charge in a physical Hilbert space constructed from $\mathcal{H}$ with the help of an abstract Gupta–Bleuler formalism in the spirit of Ref. 26, cf. Theorem 7.3 of Ref. 32. Instead, Steinmann proposes to work with the inner product space $\mathcal{D}=\underline{\mathcal{S}}/\underline{\mathcal{S}}_0$ and to avoid a (possibly nonunique) maximal Hilbert closure. Endowing $\mathcal{D}$ with a suitable quotient topology, the arguments of the present article can also be formulated without reference to maximal Hilbert space closures of $\mathcal{D}$. This will in fact be the main strategy of this article. As the results which take reference to Hilbert space structures are mathematically slightly stronger and it might be of interest to compare them with results on functional calculus on Krein spaces,[4,19] here we use the language of Krein spaces and do not restrict the analysis to $\mathcal{D}$.

Remark 2.4: Section 5 of Ref. 27 states that charged, physical states *can be* constructed in a closure of the local states. Theorem 7.3 of Ref. 32 is just the opposite of this statement. As far as I can see, this contradiction can be traced back to different assumptions in Refs. 27 and 32. In Ref. 32 it is assumed that the local states are in the domain of definition of the Maxwell charge Q. This assumption leaves open a kind of loophole as Q resulting from a closure of the Maxwell charge defined on states of the type of Eq. (86) of Ref. 27 might not contain all local states in its domain.

On the other hand, the construction of the metric operator in Ref. 27 according to conditions $\mathbf{A}_2$) for the ''in''-field and Eq. (70), leading to the construction of charged physical states, could also be problematic: The vacuum expectation values of local and ''in''-fields, which can be calculated from the local theory, partially fix the action of the metric operator on the ''in''-fields, as, e.g., sequences of states converging in the ''in''-space must have finite inner product with the local states. In a hypothetic, nonperturbative QED $\mathbf{A}_2$) and Eq. (70) of Ref. 27 might not match

with this *a priori* requirement on the metric operator. In a related situation (again not exactly the same as in Ref. 27), Steinmann gives evidence from perturbation theory that there could in fact be a problem, cf. Chap. 12.4 of Ref. 32. But the Hilbert space of an interacting theory usually is singular to the Hilbert space of the free theory, on which perturbation theory is carried out, thus perturbative arguments on the states of the interacting theory are not fully conclusive. ■

III. SOME PROPERTIES OF THE FIELD ALGEBRA

The reason why we went through the well-known construction in the proof of Theorem 2.2 is that the continuity $\phi:\underline{\mathcal{S}}\to\mathsf{O}_\eta(\mathcal{D})$ for most applications is insufficient, as the topology on $\mathsf{O}_\eta(\mathcal{D})$ is very weak. From the above construction we get, however, that

$$\|\phi(\underline{f})\Omega\|\leqslant \underline{p}(\underline{f})-\forall\,\underline{f}\in\underline{\mathcal{S}}, \tag{5}$$

and we thus get the following lemma, which gives sufficient continuity properties of the representation ϕ to effectively control certain constructions on $\mathcal{H}$.

Lemma 3.1: Suppose $\underline{W}$ fulfills the HSSC (A5) with $\underline{p}$ Sobolev dominated. Then, ϕ is strongly continuous in the sense $\underline{f}_n\to\underline{f}$ in $\underline{\mathcal{S}}\Rightarrow\phi(\underline{f}_n)\Omega\to\phi(\underline{f})\Omega$ strongly in $\mathcal{H}$.

Proof: As $\underline{\mathcal{S}}$ carries the direct sum topology, $\underline{f}_n\to\underline{f}$ implies the convergence of any component in $\mathcal{S}_n$ and the existence of a maximal N s.t. the components of $\underline{f}_n$ in $\mathcal{S}_l$, $l>N$, are equal to zero $\forall n\in\mathbb{N}$. As the topology on $\mathcal{S}_n$ is generated by Sobolev dominated norms and convergence in $\mathcal{S}_n$ thus implies the convergence in any specific Sobolev norm, we get $0\leqslant\underline{p}(\underline{f}_n-\underline{f})\leqslant\underline{p}'(\underline{f}_n-\underline{f})\to 0$, as $n\to\infty$, for $\underline{p}'$ a seminorm of Sobolev type dominating $\underline{p}$. Together with (5) this gives $\|\phi(\underline{f}_n)\Omega-\phi(\underline{f})\Omega\|=\|\phi(\underline{f}_n-\underline{f})\Omega\|\to 0$. ■

From now on we assume that the maximal Hilbert space $\mathcal{H}$ with metric operator η has been constructed from a Sobolev dominated Hilbert norm $\underline{p}$. That such a $\underline{p}$ exists can be checked explicitly using the following sufficient condition, which has been verified in Refs. 1 and 3 for models of QFT with indefinite metric and nontrivial scattering matrix. It should be no major problem to verify the condition of Theorem 3.2 also for the truncated Wightman functions of nth order perturbation theory of Refs. 30–32 and the conformally invariant Wightman functions as classified by Nikolov and Todorov.[29]

Theorem 3.2: *Let $\|.\|$ be a Schwartz norm on $\mathcal{S}_1$. If the truncated Wightman functions W_n^T associated with $\underline{W}$ [cf. (8) below] are continuous w.r.t. $\|.\|^{\otimes n}$ $\forall n\in\mathbb{N}$, then $\underline{W}$ fulfills the HSSC with respect to a Hilbert norm $\underline{p}$ of Sobolev type. (As $\mathcal{S}_1$ is a nuclear space, the tensor product of norms exists, cf. e.g., Ref. 20.)*

For the proof see Refs. 3 and 20. Here we only recall that the Schwarz norms $\|.\|=\|.\|_{L,N}$, $L,N\in\mathbb{N}_0$, on $\mathcal{S}_1$ are given by

$$\|f\|_{L,N}=\sup_{x\in\mathbb{R}^d,|\beta|\leqslant L}|(1+|x|^2)^{N/2}\partial^\beta f(x)|, \tag{6}$$

where β is a multiindex and $\partial^\beta=\Pi_{l=0}^{d-1}\partial^{|\beta^l|}/(\partial x^l)^{\beta_l}$. The topology generated by the family of Schwartz norms is equivalent to the topology generated by the Sobolev norms, which also generate the Schwartz topology. For concrete estimates it is often more convenient to work with Schwartz norms, therefore Theorem 3.2 is formulated for such norms.

For $\mathcal{A}\subseteq\mathsf{O}_\eta(\mathcal{D})$ the weak commutant of $\mathcal{A}$ is given by

$$\mathcal{A}'=\{C\in\mathcal{B}(\mathcal{H}):\langle\Psi_1,C\mathsf{L}\Psi_2\rangle=\langle\mathsf{L}^{[*]}\Psi_1,C\Psi_2\rangle\ \ \forall\Psi_1,\Psi_2\in\mathcal{D},\mathsf{L}\in\mathcal{A}\}. \tag{7}$$

Here $\mathcal{B}(\mathcal{H})$ is the set of bounded operators on $\mathcal{H}$. $\mathcal{A}$ is called irreducible if $\mathcal{A}'=\mathbb{C}1_{\mathcal{H}}$.

For $\mathcal{O}\subseteq\mathbb{R}^d$ we define $\underline{\mathcal{S}}(\mathcal{O})$ to be the unital*-algebra of those $\underline{f}\in\underline{\mathcal{S}}$ which have components f_n, $\mathrm{supp}f_n\subseteq\mathcal{O}^{\times n}$. We set $\mathcal{P}(\mathcal{O})=\phi(\underline{\mathcal{S}}(\mathcal{O}))$ and we call this set the polynomial field algebra localized in $\mathcal{O}$. Furthermore, we let $\mathsf{E}_0=(\Omega,.)\Omega\in\mathsf{O}_\eta(\mathcal{D})$ be the projection operator onto the vacuum. One then gets the Reeh–Schlieder property of the field in analogy to the positive metric case (the proof essentially is due to Refs. 26 and 34):

Theorem 3.3:

(i) For $\mathcal{O}\subseteq\mathbb{R}^d$ *open and not empty,* Ω *is cyclic w.r.t.* $\mathcal{P}(\mathcal{O})$
(ii) For $\mathcal{O}$ *as in (i), the set of operators* $\{\mathcal{P}(\mathcal{O}),\mathsf{E}_0\}$ *is irreducible.*
(iii) For $\mathcal{O}$ *as in* (i) *s.t.* $\mathcal{O}'=\{x\in\mathbb{R}^d,(x-y)\cdot(x-y)<0\,\forall y\in\mathcal{O}\}$ *has nonempty open interior,* Ω *is standard (i.e., cyclic and separating) for* $\mathcal{P}(\mathcal{O})$.

Proof: (i) By Lemma 3.1, $\underline{\mathcal{S}}\ni\underline{f}\to\langle\Psi_1,\phi(\underline{f})\Omega\rangle$ defines a functional in $\underline{\mathcal{S}}'$ for arbitrary $\Psi_1\in\mathcal{H}$. This step has been used also in Refs. 34 and 26 without being explicitly mentioned. For the standard Wightman axioms it follows from positivity, cf. Ref. 33. As in Ref. 33 we may now conclude that the n-point functions associated to such Wightman functionals are boundary values of analytic functions and thus vanish everywhere, if they vanish in $\mathcal{O}$. Now suppose that Ψ is perpendicular (w.r.t. $(.,.)$) to $\mathcal{P}(\mathcal{O})\Omega$. This implies for $\Psi_1=\eta\Psi$, using the above argument, that $\langle\Psi_1,\phi(\underline{f})\Omega\rangle=0\,\forall\underline{f}\in\underline{\mathcal{S}}$. Thus $\Psi_1=0$ and $\Psi=\eta\Psi_1=0$.

(ii) We have to show that for any $C\in\mathcal{B}(\mathcal{H})$

$$\langle\Psi_1,C\phi(\underline{f})\Psi_2\rangle=\langle\phi(\underline{f}^*)\Psi_1,C\Psi_2\rangle\quad\forall\underline{f}\in\underline{\mathcal{S}}(\mathcal{O}),\quad\Psi_1,\Psi_2\in\mathcal{D},$$

and $C\mathsf{E}_0=\mathsf{E}_0C$ implies $C=c1_{\mathcal{H}}$ for some $c\in\mathbb{C}$. Let $\Psi_1\in\mathcal{D}$ and $\Psi_2\in\mathcal{P}(\mathcal{O})\Omega$, i.e., $\Psi_2=\phi(\underline{f})\Omega$ for some $\underline{f}\in\underline{\mathcal{S}}(\mathcal{O})$. We get in analogy to Eqs. (4–16) of Ref. 33:

$$\langle\Psi_1,C\Psi_2\rangle=\langle\phi(\underline{f}^*)\Psi_1,C\Omega\rangle=\langle\phi(\underline{f}^*)\Psi_1,C\mathsf{E}_0\Omega\rangle=(\phi(\underline{f}^*)\Psi_1,\eta\mathsf{E}_0C\Omega)=(\phi(\underline{f}^*)\Psi_1,\eta\Omega)$$
$$\times(\Omega,C\Omega)=\langle\phi(\underline{f}^*)\Psi_1,\Omega\rangle(\Omega,C\Omega)=\langle\Psi_1,\Psi_2\rangle(\Omega,C\Omega).$$

Since $\mathcal{P}(\mathcal{O})\Omega$ is dense in $\mathcal{H}$ by (i), this implies $C=(\Omega,C\Omega)1_{\mathcal{H}}$.

(iii) Follows from property (i) for $\mathcal{P}(\mathcal{O})$ and $\mathcal{P}(\mathcal{O}')$ since locality implies that these algebras commute and thus cyclicity of Ω for $\mathcal{P}(\mathcal{O}')$ implies separability of Ω for $\mathcal{P}(\mathcal{O})$. ■

We want to adapt further results of positive metric QFT to the case of indefinite metric QFT, namely the irreducibility of the field algebra and the uniqueness of the vacuum. The proofs in the positive metric case use the spectral resolution of the translation group—something which is not at disposal in ''indefinite metric.'' Instead we use a smooth cut-off function to separate the vacuum from the remaining states and we have to restrict ourselves to the case of QFTs with a mass-gap $m>0$.

Since U is only densely defined, one calls $\tilde{\Omega}\in\mathcal{H}$ invariant under the action of the translation group $\mathsf{U}(1,a)$ if $\langle\tilde{\Omega},\mathsf{U}(1,a)\Psi_1\rangle=\langle\tilde{\Omega},\Psi_1\rangle\forall a\in\mathbb{R}^d,\Psi_1\in\mathcal{D}$, cf. Ref. 36.

Theorem 3.4: *Suppose that* $\underline{W}$ *fulfills the strong spectral condition with mass gap* $m>0$. *Then*

(i) $\mathcal{P}(\mathbb{R}^d)$ *is irreducible, and*
(ii) the vacuum Ω *is the unique translation invariant state in* $\mathcal{H}$ *(up to multiplication with a constant).*

Related results have been proven by Morchio and Strocchi:[26] (ii) has been verified for nonmaximal Hilbert spaces of Sobolev type and (i) has been deduced from the assumption of (essential) uniqueness of the vacuum. Here we extend these results also to maximal Hilbert closures originating from a Sobolev dominated HSSC and we prove that such closures do not contain any theta-vacua,[26] provided the strong spectral condition holds. That this statement can not be obtained in the mass-zero case is proven in Ref. 26 by explicit examples. These examples, however, do not fulfill the cluster property, which in Ref. 26 is not included in the modified Wightman axioms. Such a statement fits nicely into the picture that there is a connection of symmetry breaking and the presence of massless fields.[14] Also, (i) shows that a potential reducibility of the algebra of local fields can occur in the mass-zero case only. For massless gauge theories reducibility of the representation can be expected resulting from classical long range fluctuations, see Ref. 13 for the example of QED. For nontrivial examples of massive theories, see Ref. 1.

The proof of Theorem 3.4 starts with some technical preparations: Let $\underline{f}\in\underline{\mathcal{S}}$ and $h\in\mathcal{S}_1$ and $\underline{g}=\underline{g}(\underline{f},h)$ be defined as in (2). We assume that supp $\hat{f}_n$ is compact $\forall n\in\mathbb{N}$ with $\hat{f}_n$ the Fourier

transform of f_n in all arguments, supp $\hat{h} \subseteq (m/3,\infty) \times \mathbb{R}^{d-1}$ and $\hat{h}=1$ on the set $\{k=k_1+\cdots+k_n : (k_1,\ldots,k_n) \in \text{supp } \hat{f}_n, n \in \mathbb{N}\} \cap \overline{V}^+_{m/2}$. We denote the vector space of all such $\underline{g}$ which are obtained in this way by $\underline{\mathcal{S}}^+$.

Let $\lambda_l=(\lambda_l^1,\ldots,\lambda_l^j) \subseteq (1,\ldots,n)$ where the inclusion means that λ_l is a subset of $\{1,\ldots,n\}$ and the natural order of $(1,\ldots,n)$ is preserved. Let $\mathcal{P}(1,\ldots,n)$ denote the collection of all partitions of $(1,\ldots,n)$ into disjoint sets λ_l, i.e., for $\lambda \in \mathcal{P}(1,\ldots,n)$ we have $\lambda=\{\lambda_1,\ldots,\lambda_r\}$ for some r where $\lambda_l \subseteq (1,\ldots,n)$, $\lambda_l \cap \lambda_{l'}=\emptyset$ for $l \neq l'$ and $\cup_{l=1}^r \lambda_l=\{1,\ldots,n\}$. Given a Wightman functional $\underline{W} \in \underline{\mathcal{S}}'$ and $\lambda_l=(\lambda_l^1,\ldots,\lambda_l^j)$, we set $W(\lambda_l)=W_j(x_{\lambda_l^1},\ldots,x_{\lambda_l^j})$.

With this definition at hand we can recursively define the truncated Wightman functional $\underline{W}^T \in \underline{\mathcal{S}}'$ associated to $\underline{W} \in \underline{\mathcal{S}}'$ via $W_0^T=0$ and

$$W(1,\ldots,n)=\sum_{\lambda \in \mathcal{P}(1,\ldots,n)} \prod_{l=1}^{|\lambda|} W^T(\lambda_l), n \in \mathbb{N}, \tag{8}$$

where $|\lambda|$ is the number of sets λ_l in λ. We also recall that the translation invariance of $\underline{W}$, clustering and the strong spectral property imply supp $\hat{W}_n^T(k_1,\ldots,k_n) \subseteq \{(k_1,\ldots,k_n) \in \mathbb{R}^{dn} : \Sigma_{l=1}^n k_l=0, \Sigma_{l=j}^n k_l \in \overline{V}_m^+, j=2,\ldots,n\}$.

Lemma 3.5: In a QFT with indefinite metric which fulfills the strong spectral condition, $\phi(\underline{\mathcal{S}}^+)\Omega$ is orthogonal [w.r.t. $(.,.)$] to Ω and is dense in the orthogonal complement of Ω.

Proof: We consider the following equation for $\underline{g} \in \underline{\mathcal{S}}^+$ with $\underline{f}$ and h as above:

$$0=\hat{h}(0)\langle \Omega, \phi(\underline{f})\Omega\rangle=\int_{\mathbb{R}^d} \langle \Omega, \phi(\underline{\alpha}_{\{1,a\}}(\underline{f}))\Omega\rangle h(a)da=\langle \Omega, \phi(\underline{g})\Omega\rangle=(\Omega, \eta\phi(\underline{g})\Omega). \tag{9}$$

Thus, $\eta\phi(\underline{g})\Omega$ is perpendicular to Ω w.r.t. $(.,.)$. Since $\eta\Omega=\Omega$ and η is self adjoint, the same applies to $\eta^2\phi(\underline{g})\Omega=\phi(\underline{g})\Omega$.

It remains to show that vectors of the form $\phi(\underline{g})\Omega$ are dense in the orthogonal complement [w.r.t. $(.,.)$] of Ω in $\mathcal{H}$. By Lemma 3.1, the span of states of the form $(1-\mathsf{E}_0)\phi(\underline{f})\Omega$ with $\underline{f}=(0,0,\ldots,f_r,0\ldots)$, with supp $\hat{f}_r$ compact, is dense in the orthogonal complement of Ω. We want to show that for such states

$$(1-\mathsf{E}_0)\phi(\underline{f})\Omega=\phi(\underline{g})\Omega \tag{10}$$

for some $\underline{g}=\underline{g}(\underline{f},h) \in \underline{\mathcal{S}}^+$, h as above. To prove this, it is sufficient to show that the expectation values (w.r.t. $\langle .,. \rangle$) of both sides coincide for a set of vectors which span a dense set in $\mathcal{H}$, namely $\phi(\underline{q})\Omega$ with $\underline{q}=(0,0,\ldots,q_j,0,\ldots)$. Taking this expectation value for the left hand side of (10) we get

$$\langle \phi(\underline{q})\Omega, (1-\mathsf{E}_0)\phi(\underline{f})\Omega\rangle=\langle \Omega, \phi(\underline{q}^* \otimes \underline{f})\Omega\rangle-\langle \Omega, \phi(\underline{q}^*)\Omega\rangle\langle \Omega, \phi(\underline{f})\Omega\rangle,$$

where we used that $\eta\Omega=\Omega$. Expanding the right hand side into truncated Wightman functions according to Eq. (8) and Fourier transforming we get for $n=r+j$

$$\ldots=(2\pi)^{-dn}\int_{\mathbb{R}^{dn}} \sum_{\lambda \in \mathcal{P}(1,\ldots,n)}{}' \prod_{l=1}^{|\lambda|} \hat{W}^T_{|\lambda_l|}(k_{\lambda_l^1},\ldots,k_{\lambda_l^{|\lambda_l|}}) \hat{q}^*(k_1,\ldots,k_j)\hat{f}(k_{j+1},\ldots,k_n)dk_1\cdots dk_n,$$

where the reduced sum Σ' runs over all partitions λ s.t. there is at least one set $\lambda_l \in \lambda$ with $\lambda_l \cap (1,\ldots,j) \neq \emptyset$ and $\lambda_l \cap (j+1,\ldots,n) \neq \emptyset$.

For $(k_1,\ldots,k_n) \in \text{supp } \Pi_{l=1}^{|\lambda|} \hat{W}^T(\lambda_l)$ with λ in the range of the sum, we obtain that $k=k_{j+1}+\cdots+k_n \in \overline{V}_m^+$ by the strong spectral condition fulfilled by $\hat{W}^T_{|\lambda|}$. [In fact, k is a sum of zero vectors and vectors from $\overline{V}_m^+$. Since λ is in the range of the reduced sum, there must be at least one vector from $\overline{V}_m^+$ due to the support properties of $\hat{W}^T(\lambda_l)$.] Thus, we can replace

$\hat{f}_r(k_{j+1},\ldots,k_n)$ by $\hat{h}(k)\hat{f}_r(k_{j+1},\ldots,k_n)$ which does not change $\hat{f}_r$ on the support of $\Pi_{l=1}^{|\lambda|}\hat{W}^T(\lambda_l)$. Furthermore, we can then drop the restriction of the sum and sum up over all partitions, since the terms which do not belong to the restricted sum give zero contribution if evaluated on $\hat{q}^*(k_1,\ldots,k_j)\hat{h}(k)\hat{f}(k_{j+1},\ldots,k_n)$ (on the support of such terms we have $k=0$).

If we now Fourier transform back, we get the $\langle .,. \rangle$-inner product of $\phi(q)\Omega$ with right hand side of Eq. (10). ■

Proof of Theorem 3.4: (i) We have to make sure that for $C \in \mathcal{B}(\mathcal{H})$

$$\langle \Psi_1, C\phi(\underline{f})\Psi_2 \rangle = \langle \phi(\underline{f}^*)\Psi_1, C\Psi_2 \rangle \forall \underline{f} \in \mathcal{S}, \Psi_1, \Psi_2 \in \mathcal{D}$$

implies $C = c1_{\mathcal{H}}$. Applying the above equation to $\underline{g}^*$ where $\underline{g} \in \mathcal{S}^+$ and $\Psi_1 = \Psi_2 = \Omega$ we get that

$$\langle \phi(\underline{g})\Omega, C\Omega \rangle = \langle \Omega, C\phi(\underline{g}^*)\Omega \rangle = 0$$

since $\underline{g}^* = \int_{\mathbb{R}^d} \underline{\alpha}_{\{1,a\}}(\underline{f}^*)\overline{h}(a)da \in I_{\text{sp}}$ by the support properties of $\hat{h}$.

Since $\phi(\mathcal{S}^+)\Omega$ is dense in the orthogonal complement of Ω, we have thus obtained $C\Omega = c\Omega$. For $\Psi_1, \Psi_2 \in \mathcal{D}, \Psi_2 = \phi(\underline{f})\Omega$ for some $\underline{f} \in \mathcal{S}$ we obtain

$$\langle \Psi_1, C\Psi_2 \rangle = \langle \phi(\underline{f}^*)\Psi_1, C\Omega \rangle = c\langle \Psi_1, \Psi_2 \rangle$$

and thus $C = c1_{\mathcal{H}}$.

(ii) Suppose $\tilde{\Omega}$ is translation invariant. We note that in Eq. (9) we can replace the vector Ω in the first argument of $\langle .,. \rangle$ and $(.,.)$ respectively by $\tilde{\Omega}$ without changing the rest of the calculation. Thus, $\tilde{\Omega}$ is perpendicular [w.r.t. $(.,.)$] to $\eta\phi(\mathcal{S}^+)\Omega$. By Lemma 3.5 $\phi(\mathcal{S}^+)\Omega$ is dense in the orthogonal complement of Ω. Since η self-adjoint and $\eta\Omega = \Omega$, this is also true for $\eta\phi(\mathcal{S}^+)\Omega$. Thus $\tilde{\Omega} = c\Omega$. ■

IV. COMPLEX VELOCITY TRANSFORMATIONS FOR THE INDEFINITE METRIC CASE

In this section we prove the existence of a dense set of entire analytic vectors for the generator of the velocity transformations (Lorentz boosts) in $x^0 - x^1$ direction. This will then allow us to define the complex velocity transformations, which are needed in the BW theorem to express the ''modular operator,'' on this domain. In this way we avoid the use of functional calculus which in general is not available on Krein spaces. The strategy is as follows: One first defines ''Gaussian spectral cut-offs'' for the Lorentz boosts on the Borchers algebra and thereby obtains an analytic action of the velocity transformations on a dense sub-*-algebra $\mathcal{S}^{\text{anal}}$ of the Borchers algebra. Then one uses Lemma 3.1 to derive the existence of a dense set of analytic vectors $\mathcal{D}^{\text{anal}} \supseteq \phi(\mathcal{S}^{\text{anal}})\Omega$.

We start with the definition of Gaussian mollifiers and their complex extension. Let, for $z \in \mathbb{C}$,

$$c_\epsilon(z) = (\sqrt{2\pi\epsilon})^{-1} e^{-z^2/2\epsilon}, \quad \epsilon > 0, \tag{11}$$

such that $c_\epsilon(t)$ for $t \in \mathbb{R}$ is the centered Gaussian bell curve with (variation) parameter $\epsilon > 0$. We also note that $c_\epsilon * c_{\epsilon'}(t) = c_{\epsilon+\epsilon'}(t)$ where $*$ means convolution in t, i.e., the c_ϵ form a convolution semigroup. As $\epsilon \downarrow 0$, $c_\epsilon(t) \to \delta(t)$ in the following sense:

Lemma 4.1: Let $F(t)$ be a continuous and exponentially bounded function, i.e., $\exists\ C, M > 0$ s.t. $|F(t)| \leq Ce^{M|t|}\ \forall t \in \mathbb{R}$. Then $\int_{\mathbb{R}} F(t)c_\epsilon(t)dt \to F(0)$ as $\epsilon \downarrow 0$.

Proof: If F is continuous and has compact support, the statement is well-known. Using a partition of unity we can represent $F = F_1 + F_2$ as a sum of a function F_1 with compact support and a function F_2 which is zero on $[-1,1]$, thus $F(0) = F_1(0)$. It remains to show that the integral $\int_{\mathbb{R}} F_2(t)c_\epsilon(t)dt$ vanishes as $\epsilon \downarrow 0$. This is true by the theorem of dominated convergence as $F_2(t)c_\epsilon(t)$ converge to zero pointwisely $\forall t \in \mathbb{R}$ and this function, for $\epsilon < 1$, is dominated by the integrable function $|F_2(t)|c_1(t)$. ■

Let $\alpha_t = \alpha_{\{\Lambda(t),0\}}$ with

$$\Lambda(t)=\Lambda_{0,1}(t)=\begin{pmatrix}\cosh t & \sinh t & 0 & \cdots & 0\\ \sinh t & \cosh t & 0 & \cdots & 0\\ 0 & 0 & 1 & \ddots & \vdots\\ \vdots & & \ddots & \ddots & 0\\ 0 & \cdots & & 0 & 1\end{pmatrix}, \tag{12}$$

the velocity transformation in x^0-x^1 direction. By $|\Lambda(t)|$ we denote the maximum norm of the matrix $\Lambda(t)$ and we note that this is an exponentially bounded function.

For $f\in\mathcal{S}_1$ and $\epsilon>0$ we set

$$f_\epsilon=\int_{\mathbb{R}}\alpha_t(f)c_\epsilon(t)dt \tag{13}$$

and we obtain the following lemma:

Lemma 4.2: Let $f\in S_1$. Then

(i) $f_\epsilon\in\mathcal{S}_1\ \forall\epsilon>0$, *and*
(ii) $f_\epsilon\to f$ *in* $\mathcal{S}_1$ *as* $\epsilon\downarrow 0$.

Proof: (i) Recall that $\mathcal{S}_1$ is the projective limit $\cap_{L,N\geqslant 0}\mathcal{S}_{L,N}$ of L-time continuously differentiable functions on $\mathbb{R}^d$ with finite Schwartz norm $\|.\|_{L,N}$. It is thus sufficient to prove that f_ϵ for all $\epsilon>0$ and $L,N\geqslant 0$ has finite $\|.\|_{L,N}$ norm:

$$\|f_\epsilon\|_{L,N}\leqslant\int_{\mathbb{R}}\|\alpha_t(f)\|_{L,N}c_\epsilon(t)dt\leqslant\int_{\mathbb{R}}(1+|\Lambda(t)|^2)^{(N+L)/2}c_\epsilon(t)dt\|f\|_{L,N}, \tag{14}$$

and we note that the integral on the right hand side is finite due to the Gaussian decay of $c_\epsilon(t)$ and the only exponential increase of $|\Lambda(t)|$. Here we used the estimate

$$\|\alpha_t(f)\|_{L,N}\leqslant\sup_{x\in\mathbb{R}^d,|\beta|<L}|(1+|\Lambda(-t)x|^2)^{N/2}|\Lambda(t)|^{|\beta|}\partial^\beta f(x)|\leqslant(1+|\Lambda(t)|^2)^{(L+N)/2}\|f\|_{L,N}. \tag{15}$$

(ii) As $\int_{\mathbb{R}}c_\epsilon(t)dt=1$,

$$\|f_\epsilon-f\|_{L,N}\leqslant\int_{\mathbb{R}}\|\alpha_t(f)-f\|_{L,N}c_\epsilon(t)dt.$$

Note that by (15) $F(t)=\|\alpha_t(f)-f\|_{L,N}$ is exponentially bounded in t. $F(t)$ is also continuous. Thus, by Lemma 4.1, we get for arbitrary $L,N\in\mathbb{N}_0$ that the right hand side of the above estimate converges to $F(0)=0$ for $\epsilon\downarrow 0$. As the family of Schwartz norms $\{\|.\|_{L,N}\}_{L,N\in\mathbb{N}_0}$ generates the Schwartz topology, the statement follows. ■

Remark 4.3: If we do not deal with a scalar theory, Lemma 4.2 and all other constructions of this work can be generalized to representations $\alpha_{\{\Lambda,0\}}$ where Λ acts on the spin components via a finite-dimensional linear representation τ s.t. the matrix elements of $\tau(\Lambda(t))$ are exponentially bounded. This follows from $\tau(\Lambda(t))$ being additive and continuous in $t\in\mathbb{R}$. ■

Clearly, (13) can be interpreted as a Gaussian cut-off $\hat{c}_\epsilon(q)=e^{-\epsilon|q|^2}$ of the spectrum of the generator of the velocity transformations on $\mathcal{S}_1\subseteq L^2(\mathbb{R}^d,\mathbb{C})$. Lemma 4.2 then proves that such cut-offs (in contrast to a simple L^2-projection to a compact spectral set) take $\mathcal{S}_1$ to itself and can also be removed without leaving $\mathcal{S}_1$. We next show that such cut-offs give the required analyticity on $\mathcal{S}_1$:

Proposition 4.4: Let $f\in\mathcal{S}_1$ and $\epsilon>0$. The function $\alpha_t(f_\epsilon)$ from $\mathbb{R}$ to $\mathcal{S}_1$ has an entire analytic continuation $\alpha_z(f_\epsilon)$ from $\mathbb{C}$ to $\mathcal{S}_1$.

Proof: We first note that for $f\in\mathcal{S}_1$, $\epsilon>0$, $\alpha_t(f_\epsilon)=\int_{\mathbb{R}}\alpha_s(f)c_\epsilon(s-t)ds$ and thus the natural extention of α_t, $t\in\mathbb{R}$, to complex parameters is given by

$$\alpha_z(f_\epsilon)=\int_{\mathbb{R}}\alpha_s(f)c_\epsilon(s-z)ds,\quad z\in\mathbb{C}. \tag{16}$$

Since $c_\epsilon(z-s)=e^{-(z^2-2sz)/2\epsilon}c_\epsilon(s)$ and $e^{-(z^2-2sz)/2\epsilon}$ for $z\in\mathbb{C}$ fixed is exponentially bounded in s, one can show that $\alpha_z(f_\epsilon)\in\mathcal{S}_1$ $\forall z\in\mathbb{C}$ in analogy to the proof of Lemma 4.2 (i).

Next we have to prove that $\alpha_z(f_\epsilon)$ is entire analytic in z, hence $\alpha_z(f_\epsilon)=\Sigma_{l=0}^{\infty}z^l f_l$ for $z\in\mathbb{C}$. Complex differentiability of $\alpha_z(f_\epsilon)$ then holds automatically and we get $f_l=(1/l!)d^l\alpha_z(f_\epsilon)/dz^l|_{z=0}$. For notational convenience we prove this statement for $\tilde{\alpha}_z(f_\epsilon)=e^{z^2/2\epsilon}\alpha_z(f_\epsilon)$ which is equivalent. Note that by an argument as in the proof of Lemma 4.2 (i) $\int_{\mathbb{R}}\alpha_s(f)c_\epsilon(s)s^l ds\in\mathcal{S}_1$. What we have to show is thus that for $L,N\in\mathbb{N}_0$

$$\left\|\tilde{\alpha}_z(f_\epsilon)-\sum_{l=0}^{n}\frac{(z/\epsilon)^l}{l!}\int_{\mathbb{R}}\alpha_s(f)c_\epsilon(s)s^l ds\right\|_{L,N}\leqslant\sum_{l=n+1}^{\infty}\frac{(|z|/\epsilon)^l}{l!}\int_{\mathbb{R}}\|\alpha_s(f)\|_{L,N}c_\epsilon(s)|s|^l ds$$
$$\to 0\ \text{ as }\ n\to\infty. \tag{17}$$

We also note that by a calculation as (15) for l even

$$\int_{\mathbb{R}}\|\alpha_s(f)\|_{L,N}c_\epsilon(s)|s|^l ds\leqslant\int_{\mathbb{R}}c_\epsilon(s)|s|^l(1+|\Lambda(s)|^2)^{(N+L)/2}ds\|f\|_{L,N}.$$

Let $0<\epsilon<\epsilon'$. Then there exists a constant $C>0$ depending on L,N and ϵ,ϵ' such that the integral on the right hand side of the above estimate is smaller than $C\int_{\mathbb{R}}c_{\epsilon'}(s)|s|^l ds$. Since

$$\sum_{l=0}^{\infty}\frac{R^l}{l!}\int_{\mathbb{R}}c_{\epsilon'}(s)|s|^l ds=\int_{\mathbb{R}}c_{\epsilon'}(s)e^{R|s|}ds<\infty$$

for all $R>0$, (17) follows. ■

We now define $\mathcal{S}_1^{\text{anal}}$ to be the $\mathbb{C}$-linear span of $\{\alpha_z(f_\epsilon): f\in\mathcal{S}_1,\epsilon>0,z\in\mathbb{C}\}$. Some properties of this space are listed in the following lemma:

Lemma 4.5:

(i) $\mathcal{S}_1^{\text{anal}}$ *is a vector space which is closed under taking the complex conjugate.*
(ii) $\mathcal{S}_1^{\text{anal}}\subseteq\mathcal{S}_1$ *is dense in* $\mathcal{S}_1$.
(iii) The mapping $\alpha_z:\mathcal{S}_1^{\text{anal}}\to\mathcal{S}_1^{\text{anal}}$ *is well-defined for* $z\in\mathbb{C}$.
(iv) $\mathbb{C}\ni z\to\alpha_z(f)\in\mathcal{S}_1^{\text{anal}}$, $f\in\mathcal{S}_1^{\text{anal}}$, *is additive in* z, *i.e.,* $\alpha_{z_1}(\alpha_{z_2}(f))=\alpha_{z_1+z_2}(f)$ $\forall z_1,z_2\in\mathbb{C}$, *and* $\alpha_z(f)^*=\alpha_{\bar{z}}(f^*)$.
(v) The mapping $\mathbb{C}\ni z\to\alpha_z(f)\in\mathcal{S}_1^{\text{anal}}$ *for* $f\in\mathcal{S}_1^{\text{anal}}$ *is entire analytic [here we admit the coefficients for the expansion of* $\alpha_z(f)$, $f\in\mathcal{S}_1^{\text{anal}}$, *in* z *to be in* $\mathcal{S}_1$, *not necessarily in* $\mathcal{S}_1^{\text{anal}}$*] in* z.

Proof:

(i) Closedness under taking the complex conjugation is obvious, cf. (13).
(ii) This follows from Lemma 4.2 *(i)* and *(ii).*
(iii) We first have to show that for $g\in\mathcal{S}_1^{\text{anal}}$, $g=\alpha_{z_1}(f_{\epsilon_1})=\alpha_{z_2}(h_{\epsilon_2})$, $f,h\in\mathcal{S}_1$, $\epsilon_1,\epsilon_2>0$, $z_1,z_2\in\mathbb{C}$, $\alpha_z(g)=\alpha_z(\alpha_{z_1}(f_{\epsilon_1}))=\alpha_{z+z_1}(f_{\epsilon_1})=\alpha_{z+z_2}(h_{\epsilon_2})=\alpha_z(\alpha_{z_2}(h_{\epsilon_2}))$ is not ambiguous. Note that this holds for real z. By entire analyticity in z, cf. Proposition 4.4, $\alpha_z(\alpha_{z_2}(f_{\epsilon_1}))=\alpha_z(\alpha_{z_2}(h_{\epsilon_2}))$ then extends to all $z\in\mathbb{C}$.
(iv) That α_z is additive in z and $\alpha_z(f)^*=\alpha_{\bar{z}}(f^*)$ follows from Eq. (16).
(v) is an immediate consequence of (iii) and Proposition 4.4. ■

Let $\underline{\mathcal{S}}^{\mathrm{anal}}$ be the free, unital,*-algebra generated by $\mathcal{S}_1^{\mathrm{anal}}$, i.e.,

$$\underline{\mathcal{S}}^{\mathrm{anal}}=\oplus_{n=1}^{\infty}\mathcal{S}_n^{\mathrm{anal}},\ \ \mathcal{S}_n^{\mathrm{anal}}=\mathcal{S}_1^{\mathrm{anal}\otimes n},\ \ n\geqslant 1,\ \ \mathcal{S}_0^{\mathrm{anal}}=\mathbb{C}. \tag{18}$$

By Lemma 4.5 (i) this is well defined. Then $\mathcal{S}_1^{\mathrm{anal}}$ is a dense, unital sub-*-algebra of $\underline{\mathcal{S}}$, cf. Lemma 4.5 (ii).

Proposition 4.6:

(i) $\underline{\alpha}_z:\underline{\mathcal{S}}^{\mathrm{anal}}\to\underline{\mathcal{S}}^{\mathrm{anal}}$ *is a well defined unital algebra automorphism for* $z\in\mathbb{C}$. *It behaves under taking the involution as* $\underline{\alpha}_z(\underline{f})^*=\underline{\alpha}_{\overline{z}}(\underline{f}^*)$ *and is entire analytic and additive in* $z\in\mathbb{C}$.

(ii) Let $\underline{W}\in\underline{\mathcal{S}}'$ *be Poincaré invariant [cf. (A2)] and* $\underline{\mathcal{S}}_0^{\mathrm{anal}}=\{\underline{f}\in\underline{\mathcal{S}}^{\mathrm{anal}}:\underline{W}(\underline{g}\otimes\underline{f})=0\ \forall\,\underline{g}\in\underline{\mathcal{S}}\}$. *Then* $\underline{\alpha}_z(\underline{\mathcal{S}}_0^{\mathrm{anal}})\subseteq\underline{\mathcal{S}}_0^{\mathrm{anal}}$.

Proof: (i) It is sufficient to prove this for the restriction of $\underline{\alpha}_z$ to $\mathcal{S}_n^{\mathrm{anal}}$. By Lemma 4.5, the statement holds for elements $\alpha_{z_1}(f_1)\otimes\cdots\otimes\alpha_{z_n}(f_n)$, $f_l\in\mathcal{S}_1^{\mathrm{anal}}$, $z_l\in\mathbb{C}$, $l=1,\ldots,n$ in each of the components $\alpha_{z_l}(f_l)$. The claim now follows from going to the diagonal $z=z_1=\cdots=z_n$.

(ii) Let $\underline{f}\in\underline{\mathcal{S}}_0^{\mathrm{anal}}$. Then $\underline{W}(\underline{g}\otimes\underline{\alpha}_z(\underline{f}))=0$ for all real z. By (i) and $\underline{W}\in\underline{\mathcal{S}}'$, $\underline{W}(\underline{g}\otimes\underline{\alpha}_z(\underline{f}))$ is an analytic function in z and thus vanishes identically. ■

We now want to use Lemma 3.1 in order to show that the results of Proposition 4.6 carry over to the Krein space representation on $\mathcal{H}$. We first give some definitions:

Definition 4.7: Let $(\mathcal{H},\eta)$ *be a Krein space with fundamental decomposition* η *and let* $\mathsf{U}:\mathbb{R}\to\mathsf{O}_\eta(\mathcal{D})$ *be a one parameter group of* η*-unitary operators* $\mathsf{U}(t):\mathcal{D}\to\mathcal{D}$.

(i) *Let*

$$\mathcal{D}(\mathsf{A})=\left\{\Psi\in\mathcal{D}:\ \lim_{t\to 0,t\neq 0}\frac{\mathsf{U}(t)-1}{it}\Psi\ \text{ converges strongly in }\ \mathcal{H}\right\}.$$

Then $\mathsf{A}=(\mathsf{A},\mathcal{D}(\mathsf{A}))$, $\mathsf{A}\Psi=\lim_{t\to 0,t\neq 0}(it)^{-1}(\mathsf{U}(t)-1)\Psi$, $\Psi\in\mathcal{D}(\mathsf{A})$, is called the generator of $\{\mathsf{U}(t)\}_{t\in\mathbb{R}}$.

(ii) A vector $\Psi\in\mathcal{D}(\mathsf{A})$ is called analytic for A if $\forall n\in\mathbb{N}\ \mathsf{A}^n\Psi\in\mathcal{D}(\mathsf{A})$ and $\exists R>0$ such that $\forall z\in\mathbb{C}$, $|z|<R$, $\Sigma_{n=0}^{\infty}(z^n/n!)\mathsf{A}^n\Psi$ converges strongly in $\mathcal{H}$. If this holds for all $R>0$, Ψ is called entire analytic.

(iii) By $\mathcal{D}^{\mathrm{anal}}=\mathcal{D}^{\mathrm{anal}}(\mathsf{A})$ we denote the set of all entire analytic vectors of A. ■

By standard methods one shows that A is η-symmetric on $\mathcal{D}(\mathsf{A})$. By these very definitions we get $\mathsf{U}(z)=\Sigma_{n=0}^{\infty}((iz)^n/n!)\mathsf{A}^n:\mathcal{D}^{\mathrm{anal}}\to\mathcal{H}$ is well-defined and additive for $z\in\mathbb{C}$ and $\mathsf{U}(z)\Psi$, $\Psi\in\mathcal{D}^{\mathrm{anal}}$, is entire analytic in $z\in\mathbb{C}$ in the strong topology on $\mathcal{H}$.

We now get as the main theorem of this section:

Theorem 4.8: *Let* $\underline{W}\in\underline{\mathcal{S}}'$ *fulfill the Axioms 2.1 with Sobolev dominated Hilbert seminorm* $\underline{p}$ *and let* $((\mathcal{H},\langle .,.\rangle,\Omega),\eta,\mathsf{U},\phi)$ *be the associated QFT with indefinite metric, cf. Theorem 2.2. Let, furthermore,* $\mathsf{U}(t)=\mathsf{U}(\{\Lambda(t),0\})$, $t\in\mathbb{R}$ *and* A *be the generator of the one parameter* η*-unitary group* $\{\mathsf{U}(t)\}_{t\in\mathbb{R}}$.

Then A *has a dense domain* $\mathcal{D}^{\mathrm{anal}}$ *of entire analytic vectors. In particular,* $\{\mathsf{U}(t)\}_{t\in\mathbb{R}}$ on $\mathcal{D}^{\mathrm{anal}}$ *has a well-defined additive extension to* $\mathsf{U}(z)$, $z\in\mathbb{C}$, *given by* $\mathsf{U}(z)=\Sigma_{n=0}^{\infty}((iz)^n/n!)\mathsf{A}^n$ *and* $\mathsf{U}(z)^{[*]}=\mathsf{U}(-\overline{z})$ *holds on this domain.*

Proof: As $\underline{\mathcal{S}}^{\mathrm{anal}}$ is dense in $\underline{\mathcal{S}}$, it follows from Lemma 3.1 and the fact that $\phi(\underline{\mathcal{S}})\Omega$ is dense in $\mathcal{H}$ that also $\phi(\underline{\mathcal{S}}^{\mathrm{anal}})\Omega$ is dense in $\mathcal{H}$.

It therefore suffices to show that $\phi(\underline{\mathcal{S}}^{\mathrm{anal}})\Omega\subseteq\mathcal{D}^{\mathrm{anal}}$. Let $\Psi\in\phi(\underline{\mathcal{S}}^{\mathrm{anal}})\Omega$, $\Psi=\phi(\underline{f})\Omega$, $\underline{f}\in\underline{\mathcal{S}}^{\mathrm{anal}}$. By Proposition 4.6 (ii), $\mathsf{U}(z)\Psi=\phi(\underline{\alpha}_z(\underline{f}))\Omega$ is well-defined. Furthermore, by Proposition 4.6 $\exists\ \underline{f}_n\in\underline{\mathcal{S}}$ such that $\underline{\alpha}_z(\underline{f})=\Sigma_{l=0}^{\infty}((iz)^n/n!)\underline{f}_n$. Hence, $\lim_{t\to 0,t\neq 0}(it)^{-1}(\underline{\alpha}_t(\underline{f})-\underline{f})=\underline{f}_1$ in $\underline{\mathcal{S}}$. By Lemma 3.1 this implies

$$\phi(\underline{f}_1)\Omega=\phi\left(\lim_{t\to 0,t\neq 0}\frac{\underline{\alpha}_t(\underline{f})-\underline{f}}{it}\right)\Omega=\lim_{t\to 0,t\neq 0}\frac{\mathsf{U}(t)-1}{it}\Psi.$$

Thus $\Psi \in \mathcal{D}(\mathsf{A})$ and $\mathsf{A}\Psi = \phi(\underline{f}_1)\Omega$. Repeating this argument n times we get that $\mathsf{A}^{n-1}\Psi \in \mathcal{D}(\mathsf{A})$ and $\mathsf{A}^n\Psi = \phi(\underline{f}_n)\Omega$. Again by Lemma 3.1 we get that the following chain of equation holds:

$$\mathsf{U}(z)\Psi = \phi(\underline{\alpha}_z(\underline{f}))\Omega = \phi\left(\lim_{N\to\infty}\sum_{n=0}^{N}\frac{(iz)^n}{n!}\underline{f}_n\right)\Omega = \lim_{N\to\infty}\phi\left(\sum_{n=0}^{N}\frac{(iz)^n}{n!}\underline{f}_n\right)\Omega = \lim_{N\to\infty}\sum_{n=0}^{N}\frac{(iz)^n}{n!}\mathsf{A}^n\Psi,$$

where the convergence is strong convergence in $\mathcal{H}$ and $z \in \mathbb{C}$ is arbitrary. This, by definition of $\mathcal{D}^{\text{anal}}$, just means that $\Psi \in \mathcal{D}^{\text{anal}}$. ■

Let us briefly discuss the relation of Therorem 4.8 with functional calculus on Krein spaces: Setting $\mathcal{C} = \{\xi: \mathbb{C} \to \mathbb{C}, \xi(z) = \Sigma_{l=1}^{\infty} a_l z^l \ a_l \in \mathbb{C} \text{ s.t. } \exists R > 0, C > 0, |a_l| < CR^l/l! \forall l \in \mathbb{N}\}$, we get by the same methods as in the proof of Proposition 4.4 and Theorem 4.8 that $(F(\mathsf{A}), \phi(\underline{\mathcal{S}}^{\text{anal}})\Omega)$ is well-defined for all F in the algebra $\mathcal{C}$. This defines a restricted functional calculus for A. But this algebra of entire analytic functions of course does not contain any characteristic sets (''spectral projections'').

If one would try to use the approach of this article to define spectral projections, one essentially has to continuously extend the Wightman functional $\underline{W}$ to a bigger algebra generated by elements

$$\int_{\mathbb{R}} \alpha_t(f) c_{[a,b]}(t)\,dt, \quad f \in \mathcal{S}_1, \tag{19}$$

where $c_{[a,b]}$ is the inverse Fourier transform of the characteristic function of the set $[a,b]$. While it is easy to show that this defines a function on $\mathbb{R}^d - \{x \in \mathbb{R}^d : |x^0| = |x^1|\}$, the estimates of the proof of Lemma 4.2 obviously fail as $c_{[a,b]}(t)$ falls to zero no faster than $1/t$ as $t \to \infty$. One thus would have to restrict to Wightman functionals $\underline{W}$ with Wightman functions being rather functions of sufficiently fast decay than just distributions. This, however, is not a physical assumption, as, e.g., the two-point function of a scalar field in the physical space–time $d=4$ has singularities on the light cone $\sim 1/x^2$ and thus is not a locally integrable function and due to Lorentz invariance is constant along the orbits of the Lorentz group. This forced us in (13) to work with the Gaussian cut-offs giving a less sharp localization of the spectrum. Of course, spectral projections in some cases could be defined using different methods.

Remark 4.9: On an informal level, spectral calculus can also be defined using Gaussian localization of the spectrum $\hat{c}_{a,\epsilon}(\mathsf{A}) = \sqrt{\epsilon/\pi}\, e^{-\epsilon|a-\mathsf{A}|^2}$, $a \in \mathbb{R}, \epsilon > 0$. Informally, $\lim_{\epsilon\uparrow\infty}\hat{c}_{a,\epsilon}(\mathsf{A}) = d\mathsf{E}_{(-\infty,a]}/da$ where $\mathsf{E}_{(-\infty,a]} = \hat{c}_{(-\infty,a]}(\mathsf{A})$ is the spectral projection of A on $(-\infty, a]$. Thus one gets the following heuristic formula,

$$F(\mathsf{A}) = ''\int_{\mathbb{R}} F(a)\,d\mathsf{E}_{(-\infty,a]}'' = \lim_{\epsilon\uparrow\infty}\int_{\mathbb{R}} F(a)\hat{c}_{a,\epsilon}(\mathsf{A})\,da, \tag{20}$$

and one could study the existence of this limit depending on the choice of F and suitable domains in order to extend the choice of admissible F beyond $\mathcal{C}$. ■

V. ON THE BW THEOREM FOR QFTs WITH INDEFINITE METRIC

In this section we combine the existence of complex velocity transformations established in the previous section with a theorem of J. Bros, H. Epstein, and U. Moschella which shows that Bisognano–Wichmann analyticity (in particular, the KMS condition) does not depend on positivity. We first recall this result, which is the crucial step towards the BW theorem for QFT with indefinite metric. Here $\mathcal{W}_R = \{x \in \mathbb{R}^d : x^1 > |x^0|\}$, $\mathcal{W}_L = -\mathcal{W}_R$. We also note that $\underline{\alpha}_t$ takes the $*$-algebras $\underline{\mathcal{S}}(\mathcal{W}_{R/L})$ into themselves. We only formulate our statements for the right wedge—the related statement for the left wedge can be derived analogously.

Theorem 5.1:[12] *Let $\underline{W} \in \underline{\mathcal{S}}'$ fulfill temperedness, locality and the spectral condition [cf. (A1), (A3) and (A4) of Axioms 2.1]. Then we have the following.*

(i) The "dynamical system" $(\underline{\mathcal{S}}(\mathcal{W}_R), \underline{\alpha}_t, \underline{W})$ fulfills the KMS condition with temperature $1/2\pi$, i.e., $\forall \underline{f}, \underline{g} \in \underline{\mathcal{S}}(\mathcal{W}_R)$ $\exists$ a holomorphic function $F(z)$ on the strip $\mathbb{R}+i(0,2\pi)$ which continuously extends to $\mathbb{R}+i[0,2\pi]$ such that

$$F(t) = \underline{W}(\underline{f} \otimes \underline{\alpha}_t(\underline{g})), \quad \text{and} \quad F(t+i2\pi) = \underline{W}(\underline{\alpha}_t(\underline{g}) \otimes \underline{f}), \quad t \in \mathbb{R}.$$

(ii) For *F as in (i), the Bisognano–Wichmann relation is fulfilled:*

$$F(i\pi) = \underline{W}(\underline{f} \otimes \underline{\alpha}_{\{\Theta_{0,1},0\}}(\underline{g}^*)).$$

Remark 5.2: The proof for this theorem, based on analytic completion along the orbits of the group of complex Lorentz boosts, has been formulated for the case of de Sitter space–time, but the same proof also holds for Minkowski space–time, cf. Ref. 12. Here, up to different notation, *(i)* corresponds to Eq. (45) of Ref. 12 and (ii) is the special case $\lambda = -1$ of Eq. (46) of that reference where $\lambda = e^z$, z being the argument of F.

It should also be remarked that the statement of Ref. 12 has been formulated for the case of test functions with compact support. Nevertheless, the proof of the crucial Lemma 2 of that reference is based on the estimate (67) which guarantees in (69) of Ref. 12 boundary values in $\mathcal{S}'$, see Theorem 2-10 of Ref. 33. But in the Minkowski case, (67) follows automatically from the assumption of temperedness Theorem 2-10 of Ref. 33 [see also (17) of Ref. 12]. Hence the statement of Theorem 5.1 also holds for Schwartz test functions. ■

If we re-write (ii) of Theorem 5.1 for a Wightman functional $\underline{W}$ associated to some quantum field theory with indefinite metric, cf. Theorem 2.2, we find

$$\langle \phi(\underline{f}^*)\Omega, \mathsf{U}(i\pi)\phi(\underline{g})\Omega \rangle = \langle \phi(\underline{f}^*)\Omega, \mathsf{J}\phi(\underline{g}^*)\Omega \rangle, \quad \mathsf{J} = \mathsf{U}(\{\Theta_{0,1},0\}), \tag{21}$$

where $\underline{f}, \underline{g} \in \underline{\mathcal{S}}(\mathcal{W}_R)$. J is a η-antiunitary and antiunitary (cf. Corollary 2.3) operator and $\mathsf{J}^2 = 1$. Equation (21) is, however, only symbolic as it is not clear whether one can make sense out of the expression $\mathsf{U}(i\pi)\phi(\underline{g})\Omega$ for all $\underline{g} \in \underline{\mathcal{S}}(\mathcal{W}_R)$. We therefore have to consider a wedge algebra which is smaller than $\mathcal{P}_R = \phi(\underline{\mathcal{S}}(\mathcal{W}_R))$ and maps Ω to $\mathcal{D}^{\text{anal}}$. At the same time, such a smaller wedge algebra must not be too small as important properties, e.g., the Reeh–Schlieder property, have to be preserved and the weak commutant should coincide with the wedge algebra. Here we suggest the following solution:

Let $\underline{\mathcal{S}}^{\text{anal}}(\mathcal{W}_{R/L}) = \underline{\mathcal{S}}^{\text{anal}} \cap \underline{\mathcal{S}}(\mathcal{W}_{R/L})$ and $\mathcal{P}^{\text{anal}}_{R/L} = \phi(\underline{\mathcal{S}}^{\text{anal}}(\mathcal{W}_{R/L}))$. By definition $\mathcal{P}^{\text{anal}}_{R/L} \subseteq \mathsf{O}_\eta(\mathcal{D})$ and $\mathcal{P}^{\text{anal}}_{R/L}\Omega \subseteq \mathcal{D}^{\text{anal}}$.

The following properties of $\mathcal{P}^{\text{anal}}_{R/L}$ show that these algebras can be seen as legitimate substitutes for the wedge algebras $\mathcal{P}_{R/L}$:

Proposition 5.3: Let $\mathcal{P}^{\text{anal}}_{L/R}$ be defined as above. Then,

(i) Ω is standard (cyclic and separating) for $\mathcal{P}^{\text{anal}}_{R/L}$;

(ii) $\mathcal{P}^{\text{anal}}_{R/L}$ is dense in $\mathcal{P}_{R/L}$ w.r.t. the separating norm $\mathcal{P}_{R/L} \ni \mathsf{L} \to \|\mathsf{L}\Omega\|$; and

(iii) the weak commutants of $\mathcal{P}_{R/L}$ and $\mathcal{P}^{\text{anal}}_{R/L}$ coincide.

Proof:

(i) By Theorem 3.3 Ω is cyclic and separating for $\mathcal{P}_{R/L}$. As $\mathcal{P}^{\text{anal}}_{R/L} \subseteq \mathcal{P}_{R/L}$, Ω is separating for $\mathcal{P}^{\text{anal}}_{R/L}$. It remains to show that Ω is also cyclic. Note that $\mathcal{S}_1(\mathcal{W}_{L/R})$ is mapped into itself by the action of α_t. Thus, as in Lemma 4.2 (ii), one can show that $\mathcal{S}_1^{\text{anal}}(\mathcal{W}_{R/L}) = \mathcal{S}_1^{\text{anal}} \cap \mathcal{S}_1(\mathcal{W}_{R/L})$ is dense in $\mathcal{S}_1(\mathcal{W}_{R/L})$. Thus, $\underline{\mathcal{S}}^{\text{anal}}(\mathcal{W}_{R/L})$ is dense in $\underline{\mathcal{S}}(\mathcal{W}_{R/L})$. Consequently, by Lemma 3.1, any vector $\Psi = \phi(\underline{f})\Omega$, $\underline{f} \in \underline{\mathcal{S}}(\mathcal{W}_{R/L})$, can be approximated in the strong sense by a sequence of vectors $\Psi_n = \phi(\underline{f}_n)\Omega$, $\underline{f}_n \in \underline{\mathcal{S}}^{\text{anal}}(\mathcal{W}_{R/L})$.

(ii) As we only have to show that any vector $\Psi = \mathsf{L}\Omega$, $\mathsf{L} \in \mathcal{P}_{R/L}$, can be approximated in the strong topology by vectors in $\{\mathsf{L}\Omega : \mathsf{L} \in \mathcal{P}^{\text{anal}}_{R/L}\}$, the same argument as in (i) can be used.

(iii) Obviously $\mathcal{P}'_{R/L} \subseteq \mathcal{P}_{R/L}^{\text{anal}\,\prime}$. We have to show the opposite inclusion. Let $C \in \mathcal{P}_{R/L}^{\text{anal}\,\prime}$. Then, by Lemma 3.1, we get for $\Psi_1, \Psi_2 \in \mathcal{D}$, $\Psi_1 = \phi(\underline{f})\Omega$, $\Psi_2 = \phi(\underline{h})\Omega$, $\underline{f}, \underline{h} \in \underline{\mathcal{S}}$ and $\mathsf{L} \in \mathcal{P}_{R/L}$, $\mathsf{L} = \phi(\underline{g})$, $\underline{g} \in \underline{\mathcal{S}}(\mathcal{W}_{R/L})$,

$$\langle \Psi_1, C\mathsf{L}\Psi_2 \rangle = \langle \phi(\underline{f})\Omega, C\phi(\underline{g})\phi(\underline{h})\Omega \rangle = \langle \phi(\underline{f})\Omega, C\phi(\underline{g} \otimes \underline{h})\Omega \rangle = \lim_{n\to\infty} \langle \phi(\underline{f})\Omega, C\phi(\underline{g}_n \otimes \underline{h})\Omega \rangle$$

$$= \lim_{n\to\infty} \langle \Psi_1, C\mathsf{L}_n\Psi_2 \rangle = \lim_{n\to\infty} \langle \mathsf{L}_n^{[*]}\Psi_1, C\Psi_2 \rangle = \langle \mathsf{L}^{[*]}\Psi_1, C\Psi_2 \rangle,$$

where in the last step one has to repeat the argument of the first four steps in reverse order to see that the equality follows from Lemma 3.1. Here we used that there exists a sequence $\underline{g}_n \in \underline{\mathcal{S}}^{\text{anal}}(\mathcal{W}_{R/L})$ such that $\underline{g}_n \to \underline{g}$ in $\underline{\mathcal{S}}$ as $n \to \infty$ [cf. the proof of (i)] and $\mathsf{L}_n = \phi(\underline{g}_n) \in \mathcal{P}_{R/L}^{\text{anal}}$. ■

We define the domain $\mathcal{D}_R^{\text{anal}} = \mathcal{P}_R^{\text{anal}}\Omega$. By Proposition 5.3, $\mathcal{D}_R^{\text{anal}}$ is dense in $\mathcal{H}$ and

$$\mathsf{S}_R : \mathcal{D}_R^{\text{anal}} \to \mathcal{D}_R^{\text{anal}} \subseteq \mathcal{H}, \quad \mathsf{S}_R : \mathsf{L}\Omega \mapsto \mathsf{L}^{[*]}\Omega, \quad \mathsf{L} \in \mathcal{P}_R^{\text{anal}} \tag{22}$$

densely defines an antilinear operator S_R. Note that Ω is separating for $\mathcal{P}_R^{\text{anal}}$, hence (22) is not ambiguous. Also, $(\mathsf{S}_R^{[*]}, \mathcal{D}_R^{\text{anal}[*]}) \supseteq (\mathsf{S}_L, \mathcal{D}_L^{\text{anal}})$, with S_L defined in analogy to (22) for the right wedge replaced by the left wedge. This implies that S_R is closable.

We can now collect the pieces and formulate a version of the Bisognano–Wichmann theorem for quantum fields acting on Krein spaces:

Theorem 5.4: *Let $\mathcal{P}_{R/L}^{\text{anal}}$ be the analytic right/left wedge algebras associated with some quantum field theory with indefinite metric and let J and S_R be defined as in Eqs.* (21) *and* (22). *Then,*

(i) $[\mathcal{P}_R^{\text{anal}}, \mathcal{P}_L^{\text{anal}}] = 0$ *on* $\mathcal{D}$;
(ii) $\mathsf{J}\mathcal{P}_R^{\text{anal}}\mathsf{J} = \mathcal{P}_L^{\text{anal}}$ *and* $\mathsf{J}\mathcal{P}_L^{\text{anal}}\mathsf{J} = \mathcal{P}_R^{\text{anal}}$;
(iii) $\mathsf{U}(t)\mathcal{P}_{R/L}^{\text{anal}}\mathsf{U}(t)^{-1} = \mathcal{P}_{R/L}^{\text{anal}}$;
(iv) $\mathsf{S}_R = \mathsf{J}\mathsf{U}(i\pi)|_{\mathcal{D}_R^{\text{anal}}}$;
(v) $(\mathcal{P}_R^{\text{anal}}, \mathsf{U}(t), \Omega)$ *fulfill the KMS condition (w.r.t.* $\langle .,. \rangle$).

Proof: (i) holds by locality. (ii) This is a simple consequence of

$$\underline{\alpha}_{\{\Theta_{0,1},0\}}(\underline{\mathcal{S}}^{\text{anal}}) = \underline{\mathcal{S}}^{\text{anal}} \quad \text{and} \quad \underline{\alpha}_{\{\Theta_{0,1},0\}}(\underline{\mathcal{S}}(\mathcal{W}_{R/L})) = \underline{\mathcal{S}}(\mathcal{W}_{L/R}).$$

(iii) Similar as in *(ii)*, this point follows from

$$\underline{\alpha}_t(\underline{\mathcal{S}}^{\text{anal}}) = \underline{\mathcal{S}}^{\text{anal}} \quad \text{and} \quad \underline{\alpha}_t(\underline{\mathcal{S}}(\mathcal{W}_{R/L})) = \underline{\mathcal{S}}(\mathcal{W}_{R/L}).$$

(iv) We note that for $\underline{f}, \underline{g} \in \underline{\mathcal{S}}^{\text{anal}}(\mathcal{W}_R)$, $\tilde{F}(z) = \langle \phi(\underline{f}^*)\Omega, \mathsf{U}(z)\phi(\underline{g})\Omega \rangle$ defines an entire analytic function in z, cf. Theorem 4.8. This function $\tilde{F}(z)$ coincides for real z with the continuation of the analytic function $F(z)$ of Theorem 5.1 (i). By the edge of the wedge theorem, $\tilde{F}(z)$ is thus an analytic continuation of $F(z)$ to all $\mathbb{C}$. We identify these two functions. For $z = i\pi$ we then get by Theorem 5.1 (ii) that (21) holds rigorously. Thus,

$$\langle \Psi_1, \mathsf{U}(i\pi)\mathsf{L}\Omega \rangle = \langle \Psi_1, \mathsf{J}\mathsf{L}^{[*]}\Omega \rangle, \quad \forall \Psi_1 \in \mathcal{D}_R^{\text{anal}}, \ \mathsf{L} \in \mathcal{P}_R^{\text{anal}}.$$

Ω is cyclic for $\mathcal{P}_R^{\text{anal}}$, cf. Proposition 5.3 (i), hence $\mathcal{D}_R^{\text{anal}}$ is dense in $\mathcal{H}$ and one gets from the above equation that $\mathsf{U}(i\pi)\Psi = \mathsf{J}\mathsf{S}_R\Psi \ \forall \Psi \in \mathcal{D}_R^{\text{anal}}$. The assertion now follows by multiplication of both sides with J using $\mathsf{J}^2 = 1$.

(v) Like in (iv) one shows that the function $F(z)$ for suitable choice of $\underline{f}, \underline{g} \in \underline{\mathcal{S}}^{\text{anal}}(\mathcal{W}_R)$ coincides with $\langle \Omega, \mathsf{L}_1\mathsf{U}(z)\mathsf{L}_2\Omega \rangle$, $\mathsf{L}_1, \mathsf{L}_2 \in \mathcal{P}_R^{\text{anal}}$ and one then gets the KMS condition

$$\langle \Omega, \mathsf{L}_1\mathsf{U}(t + i2\pi)\mathsf{L}_2\Omega \rangle = \langle \Omega, \mathsf{L}_2\mathsf{U}(-t)\mathsf{L}_1\Omega \rangle$$

from Theorem 5.1 (i). ■

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Twistor representation of null two-surfaces

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We present a twistor description for null two-surfaces (null strings) in four-dimensional Minkowski space–time. The Lagrangian density for a variational principle is taken as a surface-forming null bivector. The proposed formulation is reparametrization invariant and free of any algebraic and differential constraints. The spinor formalism of Cartan–Penrose allows us to derive a nonlinear evolution equation for the world-sheet coordinate $x^a(\tau,\sigma)$. An example of null two-surface given by the two-dimensional self-intersection (caustic) of a null hypersurface is studied. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1501166]

I. INTRODUCTION

The study of massless (null) objects in four-dimensional (4D) Minkowski and curved space–times has drawn considerable attention in recent years.[1–8] These investigations are concerned not only with physical implications stemming from the theory of massless particles and string theory but also with the geometrical entities which found a convenient representation as extended null objects. The research is mainly confined to one-dimensional null objects (massless particles and superparticles)[1,9–12] and to the null hypersurfaces because of their relevance in relativity.[8,13–16] It is surprising that a study of generic null two-dimensional surfaces is quite rare (see, however, Refs. 17 and 18). This situation is rather unfortunate because a generic null two-surface corresponds to the notion of a tensionless string, which plays an important role in the current research on the string theory.[5,6,19,20] Besides, null two-surfaces can naturally arise as two-dimensional caustics of null hypersurfaces and the availability of such a description could provide additional insights into the geometry of the latter ones. Finally, our understanding of the geometry of the null submanifolds in space–times of special and general relativity is certainly incomplete without a satisfactory description of the null two-surfaces.

Initially, the notion of a null two-surface was put forward by Schild[21] in the form of a geodesic null string, i.e., a two-dimensional degenerate submanifold of 4D Minkowski or curved space–time ruled by null geodesics. The degenerate property of the induced metric can be written in the form

$$\dot{x}^2 x'^2 - (\dot{x}x')^2 = 0. \tag{1.1}$$

Here $x^a(\tau,\sigma)$ is the world-sheet coordinate, $\dot{x}x'$ stands for $\dot{x}^a x'_a$, etc. The dots and primes denote differentiation with respect to τ and σ, respectively. It is worth noting that the degenerate property (1.1) is manifestly reparametrization invariant while the Schild's variational principle does not possess this feature.

In Ref. 3 Bandos and Zheltukhin proposed a spinor version of the null string action functional. A study of null string dynamics in external fields in three-dimensional and 4D Minkowski space–times was undertaken in Refs. 22–25. In Refs. 23 and 24 Ilyenko and Zheltukhin showed that interaction with antisymmetric tensor gauge field may lead to the violation of the geodesic property of the resulting null two-dimensional submanifold of the 4D Minkowski space–time.

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A different approach was employed in Refs. 5 and 26. The idea was to use an algebraically special differential two-form obeying certain integrability conditions. In Ref. 26 Stächel took a null bivector field $p_{ab}(x)$ ($p_{ab}=-p_{ba}$, $p_{ab}{}^*p^{ab}=0$, $p_{ab}p^{ab}=0$ and $p_{a[b}\nabla_c p_{de]}=0$; the asterisk denotes dualization) as the Lagrangian density and showed that Schild's null string could be treated in this way. Recently, Gusev and Zheltukhin[5] have used a fundamental result of spinor calculus on the representation of a real null bivector in 4D Minkowski space–time to cast the variational principle in the form

$$S=\int (\bar{\pi}_A\bar{\pi}_B\epsilon_{A'B'}+\pi_{A'}\pi_{B'}\epsilon_{AB})dx^{AA'}\wedge dx^{BB'}.$$

They proved the degenerate property of the resulting two-dimensional manifold and treated the case of geodesic null string.

In the present article we show that the above-mentioned variational principle admits a natural twistor form. The corresponding Euler–Lagrange equations possess solutions not only in the form of ruled null two-surfaces (geodesic null strings) but also generic (i.e., nongeodesic, cf. Ref. 24) null strings. A nonlinear counterpart of the geodesic evolution equation for a generic null string is derived.

An outline of the paper is as follows. In Sec. II we propose a twistor variational principle for null two-surfaces in 4D Minkowski space–time. Section III is devoted to a study of the corresponding equations of motion. An evolution equation for a generic nongeodesic null two-surface is derived in Sec. IV. Section V contains an example of nongeodesic null two-surface as a two-dimensional caustic of a wave front. Discussion and outlook are presented in Sec. VI.

The conventions are those of Penrose–Rindler.[13]

II. VARIATIONAL PRINCIPLE

We begin with the Stächel's variational principle. By definition, a bivector $p_{ab}(x)=-p_{ba}(x)$ is simple if the condition $\det(p_{ab})=0$ holds. In 4D Minkowski space–time one can show that $\det(p_{ab})=(1/16)(p_{ab}{}^*p^{ab})^2$ [see Ref. 13, Vol. 1], where ${}^*p^{ab}=(1/2!)\varepsilon^{abcd}p_{cd}$ ($\varepsilon_{0123}=-\varepsilon^{0123}=1$) is the dual of p_{ab}. This means that there exists a pair of vector fields $u_a(x)$ and $v_b(x)$ which obey the identity $p_{ab}=u_{[a}v_{b]}$. The null property $p_{ab}p^{ab}=0$ gives

$$u_a u^a=0,\quad v_a v^a<0$$

and without loss of generality we will assume that they are normalized by the conditions

$$u_a v^a=0,\quad v_a v^a=-2. \tag{2.1}$$

Let the spinors $\bar{\pi}^A$ and $\bar{\eta}^A$ constitute a normalized Newman–Penrose dyad (spin-frame) and spinor $\bar{\pi}^A$ be chosen so as to represent the coincident principal null directions of the null bivector p_{ab}. Then, one can write the following representation for u_a and v_b:

$$u_a=\bar{\pi}_A\pi_{A'},\quad v_b=\bar{\pi}_B\eta_{B'}+\pi_{B'}\bar{\eta}_B. \tag{2.2}$$

Introducing a null twistor $Z^\alpha=^{\text{def}}(\bar{\omega}^A,\pi_{A'})$ and its complex conjugate $\bar{Z}_\alpha=(\bar{\pi}_A,\omega^{A'})$, where $\bar{\omega}^A$ is given by the usual definition $\bar{\omega}^A=ix^{AA'}\pi_{A'}$, we obtain

$$iu_a\,dx^a=i\bar{\pi}_A\pi_{A'}dx^{AA'}=\bar{Z}_\alpha dZ^\alpha.$$

The null property of the twistor Z^α corresponds to the Hermitian property of $x^{AA'}$ and reflects the reality condition imposed on the points of 4D Minkowski space–time.

Next we consider another one-form

$$iv_b\mathrm{d}x^b = i(\overline{\pi}_B\eta_{B'} + \pi_{B'}\overline{\eta}_B)\mathrm{d}x^{BB'} = \frac{i}{2}[(\overline{\pi}_B + \overline{\eta}_B)(\pi_{B'} + \eta_{B'}) - (\overline{\pi}_B - \overline{\eta}_B)(\pi_{B'} - \eta_{B'})]\mathrm{d}x^{BB'} \tag{2.3}$$

and introduce a second null twistor $W^\beta = {}^{\mathrm{def}}(\overline{\xi}^B, \eta_{B'})$ and its complex conjugate $\overline{W}_\beta = (\overline{\eta}_B, \xi^{B'})$. Calculating $\mathrm{d}(\overline{\xi}^B \pm \overline{\omega}^B) = i(\pi_{B'} \pm \eta_{B'})\mathrm{d}x^{BB'} + ix^{BB'}\mathrm{d}(\pi_{B'} \pm \eta_{B'})$, we find

$$i(\overline{\pi}_B + \overline{\eta}_B)(\pi_{B'} + \eta_{B'})\mathrm{d}x^{BB'} = (\overline{\pi}_B + \overline{\eta}_B)d(\overline{\xi}^B + \overline{\omega}^B) + (\xi^{B'} + \omega^{B'})d(\pi_{B'} + \eta_{B'}),$$

$$i(\overline{\pi}_B - \overline{\eta}_B)(\pi_{B'} - \eta_{B'})\mathrm{d}x^{BB'} = -(\overline{\pi}_B - \overline{\eta}_B)d(\overline{\xi}^B - \overline{\omega}^B) - (\xi^{B'} - \omega^{B'})\mathrm{d}(\pi_{B'} - \eta_{B'}).$$

Subtracting these two equations and using (2.3) we obtain

$$iv_b\mathrm{d}x^b = \overline{Z}_\beta\mathrm{d}W^\beta + \overline{W}_\beta\mathrm{d}Z^\beta.$$

Since

$$p_{ab}\mathrm{d}x^a \wedge \mathrm{d}x^b = u_{[a}v_{b]}\mathrm{d}x^a \wedge \mathrm{d}x^b = u_a\mathrm{d}x^a \wedge v_b\mathrm{d}x^b, \tag{2.4}$$

we can take the following expression:

$$S = \int \overline{Z}_\alpha\mathrm{d}Z^\alpha \wedge (\overline{Z}_\beta\mathrm{d}W^\beta + \overline{W}_\beta\mathrm{d}Z^\beta) \tag{2.5}$$

as a twistor variational principle for the null two-surfaces. The two-form in (2.5) is understood to be restricted to a two-dimensional submanifold of 4D Minkowski space–time parametrized by τ and σ. The null property of the twistors Z^α and W^α leads to the following identities:

$$\overline{Z}_\alpha Z^\alpha = \overline{W}_\alpha W^\alpha = \overline{Z}_\alpha W^\alpha = \overline{W}_\alpha Z^\alpha = 0.$$

The Lagrangian density of the twistor action functional (2.5) is multiplied by the factor q^2 under the gauge transformations of the form

$$Z^\alpha \to qZ^\alpha, \quad W^\alpha \to q^{-1}W^\alpha + pZ^\alpha.$$

Here $q(\tau,\sigma)$ is a nowhere-vanishing real-valued function and $p(\tau,\sigma)$ is an arbitrary complex-valued function. This is an admissible freedom for a differential form representing a surface.[27] It gives rise to the invariance of the Euler–Lagrange equations under the above-mentioned transformations. The invariance corresponds to the possibility of rescaling with real multiples of the extent of the null direction tangent to the null two-surface and to addition of any real multiple of the null direction to the space-like tangent direction

$$\overline{\pi}^A \to q\overline{\pi}^A, \quad \overline{\eta}^A \to q^{-1}\overline{\eta}^A + p\overline{\pi}^A. \tag{2.6}$$

These transformations comprise the null-rotations and boost-rotations (cf. Ref. 28).

III. EQUATIONS OF MOTION

A. Euler–Lagrange equations

The Lagrangian of the twistor variational principle derived in Sec. II has the form

$$\mathcal{L} = \varepsilon^{\mu\nu}\partial_\mu Z^\alpha \overline{Z}_\alpha(\overline{Z}_\beta\partial_\nu W^\beta + \overline{W}_\beta\partial_\nu Z^\beta), \tag{3.1}$$

where the indices μ,ν run over τ, σ and $\varepsilon^{\tau\sigma}=-\varepsilon^{\sigma\tau}=1$. We also write $\partial_\mu=\partial/\partial\xi^\mu=(\partial/\partial\tau,\partial/\partial\sigma)$ and extensively use the shorthand notations $`````=\partial_\tau$ and $```'''=\partial_\sigma$. The Euler–Lagrange equations are

$$\frac{\partial\mathcal{L}}{\partial\Upsilon^u}-\frac{\partial}{\partial\xi^\mu}\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\Upsilon^u)}\right]=0.$$

Here $\Upsilon^u=\{Z^\alpha,W^\alpha,\overline{Z}_\alpha,\overline{W}_\alpha\}$ are the dynamical quantities. The substitution of the Lagrangian density (3.1) into the equations yields

$$\begin{aligned}&\varepsilon^{\mu\nu}(\overline{Z}_\alpha\partial_\mu\overline{Z}_\beta\partial_\nu W^\beta+\partial_\mu\overline{Z}_\alpha\overline{Z}_\beta\partial_\nu W^\beta+\overline{Z}_\alpha\partial_\mu\overline{W}_\beta\partial_\nu Z^\beta+\partial_\mu\overline{Z}_\alpha\overline{W}_\beta\partial_\nu Z^\beta-\overline{W}_\alpha\partial_\mu\overline{Z}_\beta\partial_\nu Z^\beta\\&\quad-\partial_\mu\overline{W}_\alpha\overline{Z}_\beta\partial_\nu Z^\beta)=0,\\&\varepsilon^{\mu\nu}(\partial_\mu Z^\alpha\overline{Z}_\beta\partial_\nu W^\beta+\partial_\mu Z^\alpha\overline{W}_\beta\partial_\nu Z^\beta-\partial_\mu W^\alpha\overline{Z}_\beta\partial_\nu Z^\beta)=0,\\&\varepsilon^{\mu\nu}(\overline{Z}_\alpha\partial_\mu\overline{Z}_\beta+\partial_\mu\overline{Z}_\alpha\overline{Z}_\beta)\partial_\nu Z^\beta=0,\quad\varepsilon^{\mu\nu}\partial_\mu Z^\alpha\overline{Z}_\beta\partial_\nu Z^\beta=0.\end{aligned}\tag{3.2}$$

We can rewrite these equations in terms of the spinor fields $\overline{\pi}^A$ and $\overline{\eta}^A$ and the world-sheet derivatives of $x^{AA'}$ employing the definitions of the null twistors Z^α and W^α. In what follows it will be also convenient to take advantage of the identities

$$\begin{aligned}&\overline{\pi}^A\pi^{A'}\overline{\eta}^B-(\overline{\pi}^A\eta^{A'}+\pi^{A'}\overline{\eta}^A)\overline{\pi}^B=\pi^{A'}\epsilon^{AB}-\eta^{A'}\overline{\pi}^A\overline{\pi}^B,\\&\dot{x}^{AA'}\acute{x}^{BB'}-\acute{x}^{AA'}\dot{x}^{BB'}=\phi^{AB}\epsilon^{A'B'}+\overline{\phi}^{A'B'}\epsilon^{AB}.\end{aligned}\tag{3.3}$$

Here we use the normalization condition

$$\varepsilon_{AB}=\overline{\pi}_A\overline{\eta}_B-\overline{\eta}_A\overline{\pi}_B\tag{3.4}$$

and the symmetric spin-tensor ϕ^{AB} is given by the expression $\phi^{AB}=\dot{x}^{(A}{}_{C'}\acute{x}^{B)C'}$.

Let us consider the first equation in the system (3.2). Utilizing the above-presented formulas, we obtain that this equation is equivalent to the following system:

$$\begin{aligned}&\dot{x}^{BB'}[x^{AA'}(\pi_{B'}\epsilon_{AB}+\eta_{B'}\overline{\pi}_A\overline{\pi}_B)]'-\acute{x}^{BB'}[x^{AA'}(\pi_{B'}\epsilon_{AB}+\eta_{B'}\overline{\pi}_A\overline{\pi}_B)]^{\cdot}=0,\\&\dot{x}^{BB'}(\pi_{B'}\epsilon_{AB}+\eta_{B'}\overline{\pi}_A\overline{\pi}_B)'-\acute{x}(\pi_{B'}\epsilon_{AB}+\eta_{B'}\overline{\pi}_A\overline{\pi}_B)^{\cdot}=0.\end{aligned}\tag{3.5}$$

Substituting the second equation in (3.5) into the first one and using the second identity in (3.3), we can represent the first equation in (3.2) in the form

$$\begin{aligned}&\dot{x}^{BB'}[\overline{\eta}_A\overline{\pi}_B\pi_{B'}-\overline{\pi}_A(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})]'-\acute{x}^{BB'}[\overline{\eta}_A\overline{\pi}_B\pi_{B'}-\overline{\pi}_A(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})]^{\cdot}=0,\\&2\overline{\phi}^{A'B'}\pi_{B'}+\eta^{A'}(\phi^{AB}\overline{\pi}_A\overline{\pi}_B)=0.\end{aligned}\tag{3.6}$$

The second equation in the system (3.2) yields

$$\begin{aligned}&\dot{x}^{BB'}[(x^{AA'}\eta_{A'})'\overline{\pi}_B\pi_{B'}-(x^{AA'}\pi_{A'})'(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})]-\acute{x}^{BB'}[(x^{AA'}\eta_{A'})^{\cdot}\overline{\pi}_B\pi_{B'}\\&\quad-(x^{AA'}\pi_{A'})^{\cdot}(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})]=0,\\&\dot{x}^{BB'}[\acute{\eta}_{A'}\overline{\pi}_B\pi_{B'}-\acute{\pi}_{A'}(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})]-\acute{x}^{BB'}[\dot{\eta}_{A'}\overline{\pi}_B\pi_{B'}-\dot{\pi}_{A'}(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})]=0.\end{aligned}$$

Substituting the second equation in this system into the first and using (3.3) again, we find that the second equation in (3.2) results in

$$\dot{x}^{BB'}[\acute{\eta}_{A'}\overline{\pi}_B\pi_{B'}-\acute{\pi}_{A'}(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})]-\acute{x}^{BB'}[\dot{\eta}_{A'}\overline{\pi}_B\pi_{B'}-\dot{\pi}_{A'}(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})]=0,$$
$$2\phi^{AB}\overline{\pi}_B+\overline{\eta}^A(\overline{\phi}^{A'B'}\pi_{A'}\pi_{B'})=0. \tag{3.7}$$

We incidentally observe that the second equations in the systems (3.6) and (3.7) are complex conjugates of one another. We next consider the third equation of the system (3.2). It can be represented as follows:

$$\dot{x}^{BB'}(x^{AA'}\overline{\pi}_A\overline{\pi}_B\pi_{B'})'-\acute{x}^{BB'}(x^{AA'}\overline{\pi}_A\overline{\pi}_B\pi_{B'})^{\cdot}=0,$$
$$\dot{x}^{BB'}(\overline{\pi}_A\overline{\pi}_B\pi_{B'})'-\acute{x}^{BB'}(\overline{\pi}_A\overline{\pi}_B\pi_{B'})^{\cdot}=0.$$

The substitution of the second equation above into the first and the use of (3.3) allow us to write this pair of equations in the form

$$\dot{x}^{BB'}(\overline{\pi}_A\overline{\pi}_B\pi_{B'})'-\acute{x}^{BB'}(\overline{\pi}_A\overline{\pi}_B\pi_{B'})^{\cdot}=0,$$
$$\phi^{AB}\overline{\pi}_A\overline{\pi}_B=0. \tag{3.8}$$

The fourth equation in (3.2) gives

$$[\dot{x}^{BB'}(x^{AA'}\pi_{A'})'-\acute{x}^{BB'}(x^{AA'}\pi_{A'})^{\cdot}]\overline{\pi}_B\pi_{B'}=0,$$
$$(\dot{x}^{BB'}\acute{\pi}_{A'}-\acute{x}^{BB'}\dot{\pi}_{A'})\overline{\pi}_B\pi_{B'}=0. \tag{3.9}$$

The second equation in (3.9) can be used to rewrite the two equations (3.8) as follows:

$$(\dot{x}^{BB'}\acute{\pi}_{A'}-\acute{x}^{BB'}\dot{\pi}_{A'})\overline{\pi}_B\pi_{B'}=0,$$
$$\overline{\phi}^{A'B'}\pi_{A'}\pi_{B'}=0. \tag{3.10}$$

We also find that the second equation in (3.8) is a complex conjugate of the second equation in (3.10).

Let us use the first equation in (3.7) to simplify the first equation in the system (3.6). The calculation gives

$$[\dot{x}^{BB'}(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})'-\acute{x}^{BB'}(\overline{\pi}_B\eta_{B'}+\overline{\eta}_B\pi_{B'})^{\cdot}]\overline{\pi}_A-[\dot{x}^{BB'}(\overline{\pi}_B\pi_{B'})'-\acute{x}^{BB'}(\overline{\pi}_B\pi_{B'})^{\cdot}]\overline{\eta}_A=0. \tag{3.11}$$

Since $\overline{\pi}^A$ and $\overline{\eta}^A$ constitute a normalized basis for the two-dimensional vector space $\mathbb{C}^2$, Eq. (3.11) is equivalent to the following pair:

$$\dot{x}^{AA'}(\overline{\pi}_A\eta_{A'}+\overline{\eta}_A\pi_{A'})'-\acute{x}^{AA'}(\overline{\pi}_A\eta_{A'}+\overline{\eta}_A\pi_{A'})^{\cdot}=0,$$
$$\dot{x}^{AA'}(\overline{\pi}_A\pi_{A'})'-\acute{x}^{AA'}(\overline{\pi}_A\pi_{A'})^{\cdot}=0. \tag{3.12}$$

Performing the same procedure with the first equations in (3.8) and (3.10), we derive

$$\dot{x}^{AA'}(\overline{\pi}_A\pi_{A'})'-\acute{x}^{AA'}(\overline{\pi}_A\pi_{A'})^{\cdot}=0.$$

It coincides with the second equation in the system (3.12).

Finally, for the purposes of the future analysis, we divide the independent Euler–Lagrange equations in the following three pairs:

$$(\dot{x}^{AA'}\overleftarrow{\overline{\pi}}_B-\acute{x}^{AA'}\dot{\overline{\pi}}_B)(\overline{\pi}_A\eta_{A'}+\pi_{A'}\overline{\eta}_A)-(\dot{x}^{AA'}\overleftarrow{\overline{\eta}}_B-\acute{x}^{AA'}\dot{\overline{\eta}}_B)\overline{\pi}_A\pi_{A'}=0,$$
$$\dot{x}^{AA'}(\overline{\pi}_A\eta_{A'}+\pi_{A'}\overline{\eta}_A)'-\acute{x}^{AA'}(\overline{\pi}_A\eta_{A'}+\pi_{A'}\overline{\eta}_A)^{\cdot}=0; \tag{3.13}$$

$$\dot{x}^{AA'}(\overline{\pi}_A\pi_{A'})'-\acute{x}^{AA'}(\overline{\pi}_A\pi_{A'})^{\cdot}=0,$$
$$(\dot{x}^{AA'}\overleftarrow{\overline{\pi}}_B-\acute{x}^{AA'}\dot{\overline{\pi}}_B)\overline{\pi}_A\pi_{A'}=0; \tag{3.14}$$

$$2\overline{\phi}^{A'B'}\pi_{A'}+(\phi^{AB}\overline{\pi}_A\overline{\pi}_B)\eta^{B'}=0,$$
$$\phi^{AB}\overline{\pi}_A\overline{\pi}_B=0. \tag{3.15}$$

Here we made substitutions of dummy indices, where appropriate, and presented complex conjugate versions of some equations.

B. Preliminary analysis

Now we will establish a few auxiliary results.

The third pair of the equations of motion (3.15) gives $\phi^{AB}\overline{\pi}_B=0$, which means that

$$2\phi^{AB}=v\,\overline{\pi}^A\overline{\pi}^B \tag{3.16}$$

for some complex-valued function $v(\tau,\sigma)$.

Let us substitute the representation (3.16) into the second equation of (3.3),

$$2(\dot{x}^{AA'}\acute{x}^{BB'}-\acute{x}^{AA'}\dot{x}^{BB'})=v\,\overline{\pi}^A\overline{\pi}^B\epsilon^{A'B'}+\overline{v}\,\overline{\pi}^{A'}\pi^{B'}\epsilon^{AB}.$$

Multiplying both sides of this equation by $\dot{x}_{BB'}$ we obtain

$$2[\dot{x}^2\acute{x}^{AA'}-(\dot{x}\acute{x})\dot{x}^{AA'}]=v\,\overline{\pi}^A\overline{\pi}_B\dot{x}^{BA'}+\overline{v}\,\overline{\pi}^{A'}\pi_{B'}\dot{x}^{AB'}. \tag{3.17}$$

Following Ref. 5 we calculate

$$2\dot{x}^A{}_{C'}\acute{x}^{BC'}=2\dot{x}^{(A}{}_{C'}\acute{x}^{B)C'}+2\dot{x}^{[A}{}_{C'}\acute{x}^{B]C'}=2\phi^{AB}+(\dot{x}\acute{x})\epsilon^{AB}=v\,\overline{\pi}^A\overline{\pi}^B+(\dot{x}\acute{x})\epsilon^{AB}.$$

Using this result one obtains

$$2\dot{x}^A{}_{C'}\acute{x}^{BC'}\dot{x}_{AD'}\acute{x}_B{}^{D'}=(\dot{x}\acute{x})^2. \tag{3.18}$$

On the other hand,

$$\dot{x}^A{}_{D'}\acute{x}^{BC'}\dot{x}_{AC'}\acute{x}_B{}^{D'}=-\dot{x}^A{}_{C'}\dot{x}_{AD'}\acute{x}^{BC'}\acute{x}_B{}^{D'}$$

and this fact can be used to show that the left-hand side of Eq. (3.18) is also given by

$$2\dot{x}^A{}_{C'}\acute{x}^{BC'}\dot{x}_{AD'}\acute{x}_B{}^{D'}=(\dot{x}^A{}_{C'}\dot{x}_{AD'}-\dot{x}^A{}_{D'}\dot{x}_{AC'})\acute{x}^{BC'}\acute{x}_B{}^{D'}=2\dot{x}^A{}_{[C'}\dot{x}_{|A|D']}\acute{x}^{BC'}\acute{x}_B{}^{D'}=\dot{x}^2\acute{x}^2. \tag{3.19}$$

Equations (3.18) and (3.19) result in identity (1.1). The left-hand side of (1.1) is the determinant of the induced metric on the null string world-sheet, or equivalently, on a two-dimensional real

null submanifold of 4D Minkowski space–time, and this equation shows that it vanishes identically. The vanishing property of the determinant of the induced metric is invariant under the group of nondegenerate diffeomorphisms of the null string world-sheet

$$\tau \to f(\tau,\sigma), \quad \sigma \to \varphi(\tau,\sigma). \tag{3.20}$$

According to the second Noether theorem,[29,30] the reparametrization invariance (3.20) of the twistor action functional implies that the equations of motion contain two arbitrary real-valued functions. Then, without loss of generality, we can choose one of them in such a way as to ensure that $\dot{x}^2=0$. Taking into account (1.1), this entails

$$\dot{x}^2=0, \quad \dot{x}\acute{x}=0. \tag{3.21}$$

Having fixed the orthogonal gauge (3.21), we restrict the group of diffeomorphisms of the null string world-sheet to the following subgroup of transformations:

$$\tau \to f(\tau,\sigma), \quad \sigma \to \varphi(\sigma). \tag{3.22}$$

It, therefore, follows from (3.17) and (3.21) that

$$v\,\overline{\pi}^A \dot{x}^{BA'}\,\overline{\pi}_B + \overline{v}\,\overline{\pi}_{B'}\dot{x}^{AB'}\pi^{A'}=0,$$

and projection of this equation on the elements of the spin-tensor basis $\overline{\pi}_A\pi_{A'}$, $\overline{\pi}_A\eta_{A'}$, $\pi_{A'}\overline{\eta}_{A'}$ and $\overline{\eta}_A\eta_{A'}$ yields

$$\begin{gathered} v\dot{x}^{AA'}\overline{\pi}_A\eta_{A'} + \overline{v}\dot{x}^{AA'}\overline{\eta}_A\pi_{A'}=0, \\ \dot{x}^{AA'}\overline{\pi}_A\pi_{A'}=0. \end{gathered} \tag{3.23}$$

The second equation in the system (3.23), together with the null property (3.21) of the vector field $\dot{x}^a$, gives rise to the representation for this vector field in the form

$$\dot{x}^{AA'} = r\,\overline{\pi}^A\pi^{A'}, \tag{3.24}$$

where $r(\tau,\sigma)$ is a real-valued function. This representation for one of the two vector fields tangent to the null string world-sheet automatically solves the first equation of the system (3.23). The result (3.24) and the second equation in (3.21) imply

$$\acute{x}^{AA'}\overline{\pi}_A\pi_{A'}=0.$$

Now $\acute{x}^{AA'}$ can be written as

$$\acute{x}^{AA'} = \overline{\zeta}\,\overline{\pi}^A\eta^{A'} + \zeta\,\overline{\eta}^A\pi^{A'} + g\,\overline{\pi}^A\pi^{A'},$$

where $\zeta(\tau,\sigma)$ and $g(\tau,\sigma)$ are complex- and real-valued functions, respectively. Therefore, the representation for two linearly independent vector fields tangent to the null string world-sheet which obey constraints (3.21) is

$$\dot{x}^{AA'} = r\,\overline{\pi}^A\pi^{A'}, \quad \acute{x}^{AA'} = \overline{\zeta}\,\overline{\pi}^A\eta^{A'} + \zeta\,\overline{\eta}^A\pi^{A'} + g\,\overline{\pi}^A\pi^{A'}. \tag{3.25}$$

The substitution of the representation (3.25) into the first equation of the system (3.13) gives

$$\dot{\overline{\pi}}^A(\zeta+\overline{\zeta})=0. \tag{3.26}$$

The situation in which $\dot{\bar{\pi}}^A$ vanishes corresponds to the geodesic property of the null string world-sheets and it has been considered in Ref. 5. Unfortunately, the authors of that article had overlooked the other possibility, given by the vanishing of the expression in parentheses in Eq. (3.26), and had not paid any attention to nongeodesic null strings. The remainder of this paper will be devoted to the analysis of the nongeodesic case, which corresponds, as we will see, to the situation where the function $\zeta(\tau,\sigma)$ is purely imaginary.

It is convenient to redefine the function ζ to be a real-valued function in the null string motion equations and in the representations for the vector fields $\dot{x}^{AA'}$ and $\acute{x}^{AA'}$ by means of the substitution $\zeta \to -i\zeta$. Taking into account (3.25), we can reduce the remainder of the motion equations (3.13)–(3.14) to the system

$$r(\bar{\pi}^A \overleftarrow{\bar{\pi}}_A + \pi^{A'} \acute{\pi}_{A'}) = 2i\zeta(\pi^{A'} \dot{\eta}_{A'} - \bar{\pi}^A \dot{\bar{\eta}}_A) + g(\bar{\pi}^A \dot{\bar{\pi}}_A + \pi^{A'} \dot{\pi}_{A'}),$$

$$\bar{\pi}^A \dot{\bar{\pi}}_A - \pi^{A'} \dot{\pi}_{A'} = 0.$$

Finally, we obtain the motion equations of the null string in the form

$$\begin{gathered} \dot{x}^{AA'} = r\bar{\pi}^A \pi^{A'}, \quad \acute{x}^{AA'} = i\zeta(\bar{\pi}^A \eta^{A'} - \bar{\eta}^A \pi^{A'}) + g\bar{\pi}^A \pi^{A'}, \quad \bar{\pi}^A \dot{\bar{\pi}}_A - \pi^{A'} \dot{\pi}_{A'} = 0, \\ r(\bar{\pi}^A \overleftarrow{\bar{\pi}}_A + \pi^{A'} \acute{\pi}_{A'}) = 2i\zeta(\pi^{A'} \dot{\eta}_{A'} - \bar{\pi}^A \dot{\bar{\eta}}_A) + g(\bar{\pi}^A \dot{\bar{\pi}}_A + \pi^{A'} \dot{\pi}_{A'}), \end{gathered} \tag{3.27}$$

where $r(\tau,\sigma)$ and $\zeta(\tau,\sigma)$ are arbitrary real-valued functions.

Let us briefly explore the effects of the gauge transformations (2.6) and the null string world-sheet reparametrizations (3.22) on the equations of motion. The gauge transformations (2.6) leave the null string motion equations (3.27) invariant and result in simple redefinitions of the functions r and g,

$$r \to q^2 r, \quad g \to q^2 g - iq(p - \bar{p})\zeta.$$

Under the world-sheet reparametrizations (3.22)

$$\dot{x}^a \to \dot{f}^{-1} \dot{x}^a, \quad \acute{x}^a \to \acute{\varphi}^{-1} \acute{x}^a - (\acute{\varphi}\dot{f})^{-1} \acute{f} \dot{x}^a.$$

We then observe that the reparametrizations (3.22) preserve the form of the null string motion equations (3.27) while leading to the following redifinitions of the functions r, g, and ζ:

$$r \to \dot{f}^{-1} r, \quad g \to \acute{\varphi}^{-1} g - (\acute{\varphi}\dot{f})^{-1} \acute{f} r, \quad \zeta \to \acute{\varphi}^{-1} \zeta.$$

One can make sure that the null property of the vector field $\dot{x}^a$ and the orthogonal character of the vector fields $\dot{x}^a$ and $\acute{x}^a$ are preserved with respect to both transformations.

The invariant property of the twistor action functional with respect to either of those transformations can be used in order to eliminate the null component, $g\bar{\pi}^A \pi^{A'}$, of the space-like vector field $\acute{x}^{AA'}$ from the null string equations of motion (3.27). This can be achieved by performing the transformations (2.6) with the parameters

$$q = 1, \quad i(p - \bar{p}) = \zeta^{-1} g,$$

where the real part of the function p may remain arbitrary. Then, the null string equations of motion take the reduced form

$$\begin{gathered} \dot{x}^{AA'} = r\bar{\pi}^A \pi^{A'}, \quad \acute{x}^{AA'} = i\zeta(\bar{\pi}^A \eta^{A'} - \bar{\eta}^A \pi^{A'}), \quad \bar{\pi}^A \dot{\bar{\pi}}_A - \pi^{A'} \dot{\pi}_{A'} = 0, \\ r(\bar{\pi}^A \overleftarrow{\bar{\pi}}_A + \pi^{A'} \acute{\pi}_{A'}) = 2i\zeta(\pi^{A'} \dot{\eta}_{A'} - \bar{\pi}^A \dot{\bar{\eta}}_A). \end{gathered} \tag{3.28}$$

They are invariant under the gauge transformations (2.6) with real functions $p(\tau,\sigma)$. These restricted gauge transformations result in trivial rescaling of the function $r(\tau,\sigma)$ in the null string motion equations (3.28),

$$r \to q^2 r,$$

and reflect the freedom inherent in the choice of the extent of the null direction represented by the vector field $\dot{x}^a$. This restriction of the admissible gauge transformations to those with real p's further reduces the reparametrization freedom of the null string world-sheet. The invariance of the null string equations of motion in the form (3.28) requires that the function f entering the reparametrization transformations (3.22) is a function of τ alone, thereby restricting the reparametrization freedom to the following transformations:

$$\tau \to f(\tau), \quad \sigma \to \varphi(\sigma). \tag{3.29}$$

In the above-given equations the function r defines the extent of the flagpole direction $l^a \equiv \overline{\pi}^A \pi^{A'}$ tangent to the null string world-sheet. We also note that unrestricted gauge transformations (2.6) preserve the associated flag plane represented by the space-like vector field $\mu^a \equiv \overline{\pi}^A \eta^{A'} + \pi^{A'} \overline{\eta}^A$. This vector is orthogonal to the space-like vector field $q^a \equiv i(\overline{\pi}^A \eta^{A'} - \overline{\eta}^A \pi^{A'})$ tangent to the null string world-sheet. The vector fields l^a, μ^a, and q^a together with the second null vector field $n^a \equiv \overline{\eta}^A \eta^{A'}$ define a (non-normalized) Newman–Penrose tetrad for 4D Minkowski space–time. Here the vector fields μ^a and q^a can be expressed in terms of the usual complex elements of the tetrad as follows:

$$\mu^a = m^a + \overline{m}^a, \quad q^a = i(m^a - \overline{m}^a).$$

C. Integrability conditions

The representations for $\dot{x}^{AA'}$ and $\acute{x}^{AA'}$ in (3.28) must satisfy the compatibility conditions

$$(\dot{x}^{AA'})' = (\acute{x}^{AA'})^{\cdot}. \tag{3.30}$$

In turn, this leads to some compatibility conditions on the τ- and σ-derivatives of the basis spinor fields $\overline{\pi}^A$ and $\overline{\eta}^A$. It will have proven to be interesting to explore the geometrical significance of the compatibility conditions (3.30).

Using the definitions of the vector fields l^a and q^a we find

$$\begin{aligned} \frac{\partial}{\partial \tau} &= \frac{\partial x^a}{\partial \tau} \frac{\partial}{\partial x^a} \equiv \dot{x}^a \nabla_a = r l^a \nabla_a, \\ \frac{\partial}{\partial \sigma} &= \frac{\partial x^a}{\partial \sigma} \frac{\partial}{\partial x^a} \equiv \acute{x}^a \nabla_a = \zeta q^a \nabla_a. \end{aligned} \tag{3.31}$$

We next calculate the Lie derivative of the vector field ∂_σ along ∂_τ,

$$\pounds_{rl}(\zeta q^a) = \tilde{a} l^a + \tilde{b} q^a + r\zeta \pounds_l \eta^a,$$

where we have defined $\tilde{a} = -\zeta q^a \nabla_a r$ and $\tilde{b} = r l^a \nabla_a \zeta$. In the derivation we have used the fact that in 4D Minkowski space–time the derivatives ∇_a commute. Now, the geometrical meaning of the condition (3.30) becomes apparent, it requires the Lie derivative of the connecting vector field q^a along the vector field l^a to be contained in the subspace spanned by those vector fields

$$\pounds_l \eta^a = a l^a + b q^a. \tag{3.32}$$

Here $a=-r^{-1}q^a\nabla_a r$ and $b=\zeta^{-1}l^a\nabla_a\zeta$ are some real-valued functions of τ and σ. This equation can be recognized as the Frobenius integrability condition applied to the vector fields l^a and q^a. We note in passing that the vector field ζq^a plays the role of the Jacobi field along the null congruence given by the vector field rl^a and, therefore, is simply a Lie-dragged vector field. This condition can be phrased in a yet another form by observing that (3.32) entails that the projections of the vector field $\pounds_l\eta^a$ on the elements l^a and μ^a of the Newman–Penrose tetrad must vanish

$$l_a\pounds_l q^a=0, \quad \mu_a\pounds_l q^a=0. \tag{3.33}$$

Having established the geometrical meaning of the compatibility conditions (3.30), or equivalently (3.33), we can proceed with their analysis. The first equation in (3.33) gives

$$l^a l^b\nabla_b q_a - l^a q^b\nabla_b l_a=0.$$

Noting that the second term on the left-hand side vanishes identically and using the orthogonal property of the vector fields l^a and q^a we obtain

$$q^a l^b\nabla_b l_a=0 \tag{3.34}$$

as the first integrability condition. The second equation in (3.33) yields

$$\mu^a q^b\nabla_b l_a - \mu^a l^b\nabla_b q_a=0. \tag{3.35}$$

Summarizing, the Frobenius integrability conditions for the two-dimensional submanifold of 4D Minkowski space–time representing the null string world-sheet are given by the formulas (3.34) and (3.35). A straightforward calculation shows that these equations are invariant under the restricted to real q's and p's gauge transformations of the form (2.6).

At this point we can compare the different forms of the integrability conditions, namely, the differential condition for the null bivector $p_{ab}(x)$ stated in Sec. I and (3.32). For this purpose, we note that the null bivector can be written in the form

$$2p_{ab}=\overline{\pi}_A\overline{\pi}_B\epsilon_{A'B'}+\pi_{A'}\pi_{B'}\epsilon_{AB}. \tag{3.36}$$

Here we have used the definitions (2.4) and (2.2) for the null bivector and the vector fields u^a and v^a, the normalization conditions (2.1) and identity (3.4). The above-mentioned integrability condition is equivalent to

$$p_{ab}\nabla_c p_{de}\boldsymbol{\epsilon}^{bcde}=0, \tag{3.37}$$

where the totally antisymmetric tensor density $\boldsymbol{\epsilon}^{bcde}$ is given by the expression[13] (Vol. 1),

$$\boldsymbol{\epsilon}^{bcde}=i(\boldsymbol{\epsilon}^{BD}\boldsymbol{\epsilon}^{CE}\boldsymbol{\epsilon}^{B'E'}\boldsymbol{\epsilon}^{C'D'}-\boldsymbol{\epsilon}^{BE}\boldsymbol{\epsilon}^{CD}\boldsymbol{\epsilon}^{B'D'}\boldsymbol{\epsilon}^{C'E'}).$$

First, we write

$$2\nabla_c p_{de}=\overline{\pi}_E\epsilon_{D'E'}\nabla_{CC'}\overline{\pi}_D+\overline{\pi}_D\epsilon_{D'E'}\nabla_{CC'}\overline{\pi}_E+\pi_{E'}\epsilon_{DE}\nabla_{CC'}\pi_{D'}+\pi_{D'}\epsilon_{DE}\nabla_{CC'}\pi_{E'}.$$

Second, we calculate

$$\boldsymbol{\epsilon}^{bcde}\nabla_c p_{de}=i(\overline{\pi}^B\nabla^{CB'}\overline{\pi}_C-\pi^{B'}\nabla^{BC'}\pi_{C'}+\overline{\pi}_C\nabla^{CB'}\overline{\pi}^B-\pi_{C'}\nabla^{BC'}\pi^{B'}).$$

Finally, we obtain

$$\begin{aligned}2p_{ab}\nabla_c p_{de}\boldsymbol{\epsilon}^{bcde}=i[&\overline{\pi}_A\overline{\pi}^B\pi^{B'}\nabla_{BB'}\pi_{A'}-\pi_{A'}\overline{\pi}^B\pi^{B'}\nabla_{BB'}\overline{\pi}_A+\pi_{A'}\pi^{B'}\pi^{C'}\nabla_{AC'}\pi_{B'}\\&-\overline{\pi}_A\overline{\pi}^B\overline{\pi}^C\nabla_{CA'}\overline{\pi}_B+\overline{\pi}_A\pi_{A'}(\overline{\pi}^B\nabla_{BB'}\pi^{B'}-\pi^{B'}\nabla_{BB'}\overline{\pi}_B)].\end{aligned} \tag{3.38}$$

Then, the desired result follows from equating the right-hand side of the formula (3.38) to zero. Since Eq. (3.37) is equivalent to its projections on the spin-tensor basis elements $\bar{\pi}^A\pi^{A'}$, $\bar{\pi}^A\eta^{A'}$, $\bar{\eta}^A\pi^{A'}$, and $\bar{\eta}^A\eta^{A'}$, we derive the results which are presented in the following. First, the projection of Eq. (3.37) on $\bar{\pi}^A\pi^{A'}$ vanishes identically. Second, its projections on the spin–tensor basis elements $\bar{\pi}^A\eta^{A'}$ and $\bar{\eta}^A\pi^{A'}$ are the complex conjugates of one another and can be represented in the form

$$\bar{\pi}^A\bar{\pi}^B\pi^{B'}\nabla_{BB'}\bar{\pi}_A-\pi^{A'}\bar{\pi}^B\pi^{B'}\nabla_{BB'}\pi_{A'}=0. \tag{3.39}$$

Finally, the projection of (3.37) on the remaining element of the spin-tensor basis, $\bar{\eta}^A\eta^{A'}$, is given by

$$\begin{aligned}2(\bar{\pi}^A\bar{\pi}^B\pi^{B'}\nabla_{BB'}\bar{\eta}_A-\pi^{A'}\bar{\pi}^B\pi^{B'}\nabla_{BB'}\eta_{A'})+\pi^{A'}\bar{\pi}^B\eta^{B'}\nabla_{BB'}\pi_{A'}-\pi^{A'}\bar{\eta}^B\pi^{B'}\nabla_{BB'}\pi_{A'}\\ -\bar{\pi}^A\bar{\eta}^B\pi^{B'}\nabla_{BB'}\bar{\pi}_A+\bar{\pi}^A\bar{\pi}^B\eta^{B'}\nabla_{BB'}\bar{\pi}_A=0.\end{aligned} \tag{3.40}$$

The substitution of the definitions for the vector fields l^a, q^a and μ^a through the spinors $\bar{\pi}^A$ and $\bar{\eta}^A$ into (3.39) and (3.40) reduces those equations to the system (3.34) and (3.35). This concludes our demonstration of the equivalence of the integrability conditions (3.37) and (3.32).

Using (3.31) we can rewrite formulas (3.39) and (3.40) as

$$\begin{gathered}r(\bar{\pi}^A\overleftarrow{\bar{\pi}}_A+\pi^{A'}\acute{\pi}_{A'})=2i\zeta(\pi^{A'}\dot{\eta}_{A'}-\bar{\pi}^A\dot{\bar{\eta}}_A),\\ \bar{\pi}^A\dot{\bar{\pi}}_A-\pi^{A'}\dot{\pi}_{A'}=0.\end{gathered} \tag{3.41}$$

We find that the integrability conditions (3.41) coincide with the null string equations of motion in the system (3.28).

The conclusion of the subsection is that the integrability conditions do not contribute additional constraints to the null string equations of motion (3.28). Moreover, the complete system of the null string equations of motion consists of the spinor representations for $\dot{x}^a$ and $\acute{x}^a$ in (3.28) together with their compatibility conditions (3.30).

It is easy to show that nongeodesic null string equations of motion derived in Ref. 24 can be cast into the form (3.28). This proves that the two variational formulations are equivalent on the classical level. All the results on the properties of those equations also hold in our case. For more details we refer an interested reader to that paper. It is also remarkable that the present formulation is free of the pair of artificial auxiliary world-sheet quantities, ρ^μ, in the action principle, which was proposed by Bandos and Zheltukhin in Ref. 3 and studied by Zheltukhin and Ilyenko in Refs. 22–25. The action principle of Ref. 24 contains eight arbitrary functions of τ and σ, namely, two ρ^μ's and six components of the external antisymmetric gauge field $B_{ab}(x)$. Nevertheless, as we showed there, only two gauge invariant combinations of the field strength components of $B_{ab}(x)$ enter the equations of motion. This means that only four functions define generic null string dynamics in 4D Minkowski space–time, as is the case with the present formulation.

To summarize, in this section we have shown that the twistor action functional (2.5) describes a two-dimensional submanifold of 4D Minkowski space–time with a degenerate induced metric. The twistor action also gives the equations of motion for a generic null string in 4D Minkowski space–time.

IV. EVOLUTION EQUATION

A. Preliminary results

The invariance of the null string equations of motion under the restricted gauge transformations of the form (2.6) with real functions q and p enables us to impose one more gauge condition

on the functions entering the complete equations of motion of a null string. It will prove convenient in the nongeodesic case to fix the extents of the null directions tangent to the null string world-sheet by imposing the so-called natural parametrization

$$\dot{\bar{\pi}}_A \bar{\pi}^A = 1. \tag{4.1}$$

This amounts to taking $r = \kappa^{-1}$, where κ is the spin-coefficient, whose nonvanishing property shows that a null congruence is non-geodesic [cf. Ref. 13 (Vol. 2)]. The resulting equations are invariant under the residual gauge transformations

$$\bar{\pi}^A \to \bar{\pi}^A, \quad \bar{\eta}^A \to \bar{\eta}^A + p\,\bar{\pi}^A. \tag{4.2}$$

Here p is a real-valued function of τ and σ. The gauge transformations of the form (4.2) correspond to the freedom inherent in the definition of the flag planes, which are associated with the flagpole directions l^a tangent to the null string world-sheet. The condition (4.1) fixes natural parameter, τ, along the integral curves of the vector field l^a, thus restricting the reparametrization invariance (3.29) to trivial transformations

$$\tau \to \tau, \quad \sigma \to \varphi(\sigma).$$

Under these transformations the flagpole extent, κ^{-1}, remains invariant, whereas ζ changes to $\acute{\varphi}^{-1}\zeta$.

The condition for the natural parametrization (4.1) leads to the identity

$$\ddot{\bar{\pi}}_A \bar{\pi}^A = 0.$$

It follows that $\ddot{\bar{\pi}}^A$ is proportional to $\bar{\pi}^A$. Using the definition of the spin-coefficients κ, ε, and τ' and noting that $D \equiv l^a \nabla_a$, we obtain

$$\ddot{\bar{\pi}}^A = [\kappa^{-1} D(\varepsilon \kappa^{-1}) + \kappa^{-2}(\varepsilon^2 + \kappa\tau')]\,\bar{\pi}^A. \tag{4.3}$$

In what follows, we will denote the expression in square brackets in Eq. (4.3) as U. The natural parametrization (4.1) also gives that

$$\bar{\eta}^A = -\dot{\bar{\pi}}^A \tag{4.4}$$

up to addition of real multiples of $\bar{\pi}^A$.

B. Derivation of equation

We use the spinor representations in (3.28) for the vector fields $\dot{x}^a$ and $\acute{x}^a$ to find a nonlinear evolution equation satisfied by the coordinate, $x^a(\tau, \sigma)$, of the null string world-sheet. Since the analysis here is applicable only to the nongeodesic case, we will restrict our derivation to the situation in which the natural parametrization is applied.

Let us substitute (4.4) and $r = \kappa^{-1}$ into the definitions of $\dot{x}^a$ and $\acute{x}^a$ in (3.28), the result reads

$$\dot{x}^a = \kappa^{-1}\bar{\pi}^A \pi^{A'}, \quad \acute{x}^a = i\zeta(\dot{\bar{\pi}}^A \pi^{A'} - \bar{\pi}^A \dot{\bar{\pi}}^{A'}). \tag{4.5}$$

First, taking the τ-derivative of $\acute{x}^a$, we calculate with the aid of (4.3):

$$\dot{x}'^a = i\dot{\zeta}(\dot{\bar{\pi}}^A \pi^{A'} - \bar{\pi}^A \dot{\bar{\pi}}^{A'}) + i\zeta(U - \bar{U})\,\bar{\pi}^A \pi^{A'}. \tag{4.6}$$

Second, taking the τ-derivative of $\dot{x}^a$, we obtain

$$\ddot{x}^a = -\kappa^{-2}\dot{\kappa}\bar{\pi}^A \pi^{A'} + \kappa^{-1}(\dot{\bar{\pi}}^A \pi^{A'} + \bar{\pi}^A \dot{\bar{\pi}}^{A'}), \quad \ddot{x}^2 = -2\kappa^{-2}. \tag{4.7}$$

One can also find that

$$\acute{x}^2=-2\zeta^2,\quad \acute{x}\dot{x}'=-2\zeta\dot{\zeta},\quad \ddot{x}\ddot{x}'=2\kappa^{-3}\acute{\kappa}. \tag{4.8}$$

Here we have made use of the identity $(\ddot{x}^2)'=2\ddot{x}\ddot{x}'$. In order to obtain the σ derivative of κ we can employ the compatibility conditions of Sec. III C with the necessary substitution $\overline{\eta}^A\mapsto -\dot{\bar{\pi}}^A$. Taking the σ-derivative of $\dot{x}^a$ and using (4.5), we derive

$$\dot{x}'^A=-\kappa^{-2}\acute{\kappa}\overline{\pi}^A\pi^{A'}+\kappa^{-1}(\acute{\overline{\pi}}^A\pi^{A'}+\overline{\pi}^A\acute{\pi}^{A'}).$$

Since $(\dot{x}^a)'$ equals to $(\acute{x}^a)^{\cdot}$, we must also have $\dot{\bar{\pi}}_A\dot{\pi}_{A'}(\acute{x}^{AA'})^{\cdot}=\dot{\bar{\pi}}_A\dot{\pi}_{A'}(\dot{x}^{AA'})'$. This entails

$$-\kappa^{-2}\acute{\kappa}+\kappa^{-1}(\dot{\bar{\pi}}_A\acute{\overline{\pi}}^A+\dot{\pi}_{A'}\acute{\pi}^{A'})=i\zeta(U-\overline{U}), \tag{4.9}$$

where we used the normalization condition (4.1). Employing the same normalization condition again we find

$$\dot{\bar{\pi}}_A\acute{\overline{\pi}}^A-\overline{\pi}_A\dot{\overline{\pi}}'^A=0. \tag{4.10}$$

On the other hand, taking into account (4.3), the first motion equation in (3.28) gives

$$\overline{\pi}_A\acute{\overline{\pi}}^A+\pi_{A'}\acute{\pi}^{A'}=0.$$

Differentiating this equation with respect to τ and making the use of (4.10) we obtain

$$2(\dot{\bar{\pi}}_A\acute{\overline{\pi}}^A+\dot{\pi}_{A'}\acute{\pi}^{A'})=(\overline{\pi}_A\acute{\overline{\pi}}^A+\pi_{A'}\acute{\pi}^{A'})^{\cdot}=0.$$

The substitution of this result into Eq. (4.9) finally yields

$$\acute{\kappa}=-i\kappa^2\zeta(U-\overline{U}). \tag{4.11}$$

In a generic situation of a nongeodesic case neither κ nor ζ are equal to zero. Let us then multiply Eq. (4.6) by $\kappa^{-2}\zeta^2$; the results (4.5), (4.7), (4.8), and (4.11) can be used to show that the evolution equation has the form

$$\ddot{x}^2[\acute{x}^2\dot{x}'^a-(\acute{x}\dot{x}')\acute{x}^a]-\acute{x}^2(\ddot{x}\ddot{x}')\dot{x}^a=0. \tag{4.12}$$

This equation is accompanied by the two constraints (3.21). A straightforward but tedious calculation shows that the evolution equation and the constraints are invariant under the world-sheet reparametrizations of the form (3.29).

The evolution equation (4.12), satisfied by the coordinate $x^a(\tau,\sigma)$ of the nongeodesic null string world-sheet, is a nonlinear counterpart of the free (geodesic) null string evolution equation

$$\ddot{x}^a=0.$$

V. WAVE-FRONT CAUSTIC

Here we present an example of a nongeodesic null two-surface and explore its connections with the null string interpretation of such surfaces in 4D Minkowski space–time and the evolution equation derived for the nongeodesic null two-surfaces in Sec. IV. We will construct this example as a two-dimensional caustic of a suitable null hypersurface in 4D Minkowski space–time.

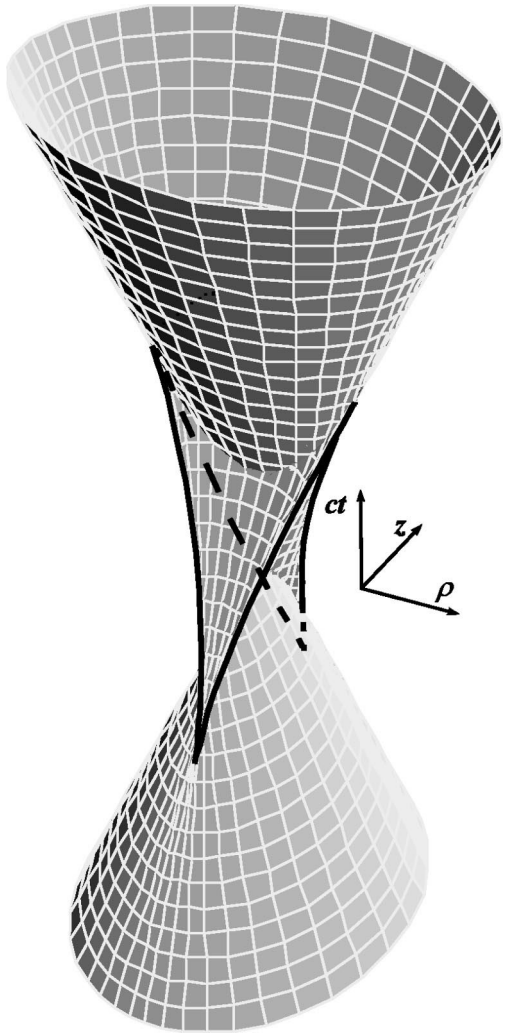

FIG. 1. The null hypersurface (5.1). One dimension is suppressed. The dark solid and dashed lines show its two-dimensional null caustic surface.

A. Null hypersurface

Let us start with considering the hypersurface given parametrically:

$$x^a(u,v,w)=\frac{a}{4}\begin{bmatrix} u \\ (1+2\sin^2 v+u)\cos v\cos w \\ (1+2\sin^2 v+u)\cos v\sin w \\ (3-2\sin^2 v-u)\sin v \end{bmatrix}. \tag{5.1}$$

Here a is a constant with the dimension of length. Taking advantage of an axial symmetry present in our example, we schematically draw the hypersurface using coordinates $(\rho=\sqrt{x^2+y^2},z,ct)$ in Fig. 1. Denoting $x^a_u=\partial x^a/\partial u$, $x^a_v=\partial x^a/\partial v$, and $x^a_w=\partial x^a/\partial w$, we can calculate the vector fields spanning the tangent space to this hypersurface. The result reads

$$x^a_u=\frac{a}{4}[1,\cos v\cos w,\cos v\sin w,-\sin v],$$

$$x^a_v=\frac{a}{4}(3\cos 2v-u)[0,\sin v\cos w,\sin v\sin w,\cos v], \tag{5.2}$$

$$x^a_w=\frac{a}{4}(u+2-\cos 2v)\cos v[0,-\sin w,\cos w,0].$$

For the Lorentz norms of the vector fields we have

$$x^2_u=0,\quad x^2_v=-\frac{a^2}{16}(u-3\cos 2v)^2,\quad x^2_w=-\frac{a^2}{16}\cos^2 v(u+2-\cos 2v)^2.$$

One can also check the orthogonal property of these vector fields in the Lorentz norm $x_u x_v=x_u x_w=x_v x_w=0$. The above-mentioned equations show that the hypersurface (5.1) is null. We can also write the necessarily degenerate induced metric, $G_{\mu\nu}$. Here the subscript indices μ and ν run over u, v, and w. By definition, it is given by $G_{\mu\nu}=\partial_\mu x^a\partial_\nu x_a$. Writing $G_{\mu\nu}$ as a three by three matrix we obtain

$$G_{\mu\nu}=-\frac{a^2}{16}\mathrm{diag}[0,(u-3\cos 2v)^2,\cos^2 v(u+2-\cos 2v)^2].$$

This matrix has the rank of two everywhere with the exception of the following parameter values:

$$u=3\cos 2v,\quad \cos v=0\ \text{ or }\ u=\cos 2v-2. \tag{5.3}$$

It is of rank one matrix there excluding two points $x^a=(-3a/4,0,0,\pm a)$, where the induced metric is of zero rank. One can show that parameter values $\cos v=0$ determine two null straight lines

$$ct=\frac{a}{4}\pm z,\quad x=y=0$$

and the parameter values given by the last equality in (5.3) correspond to the segment $|z|\leqslant a$ contained by the null plain curve

$$ct=-\frac{1}{4a}(2z^2+a^2).$$

On the contrary, the first equality in (5.3) defines a two-dimensional surface. Substituting $u=3\cos 2v$ into (5.1), we find for the space–time points belonging to it:

$$\tilde{x}^a=a[\tfrac{3}{4}\cos 2v,\cos^3 v\cos w,\cos^3 v\sin w,\sin^3 v]. \tag{5.4}$$

By construction, this is a caustic two-surface for the null hypersurface (5.1) and the tangent plains to the two-surface span the null hypersurface. Accounting to the axial symmetry of our example, the caustic null two-surface is shown by thick solid and dashed lines in Fig. 1.

The new tangent fields at the two-surface are

$$\tilde{x}^a_v=-\tfrac{3}{2}a\sin 2v[1,\cos v\cos w,\cos v\sin w,-\sin v],\quad \tilde{x}^a_w=a\cos^3 v[0,-\sin w,\cos w,0].$$

The latter new tangent field coincides with the field obtained as a result of substitution $u=3\cos 2v$ in the expression for x^a_w in (5.2), while the former one is only a multiple of the null vector field x^a_u in (5.2). For this reason and to simplify subsequent calculations, we can equally use the null vector field x^a_u in order to find the spinor corresponding to the null direction tangent to the two-surface. Since the first tangent vector field $\tilde{x}^a_v$ has a zero Lorentz norm and the second tangent

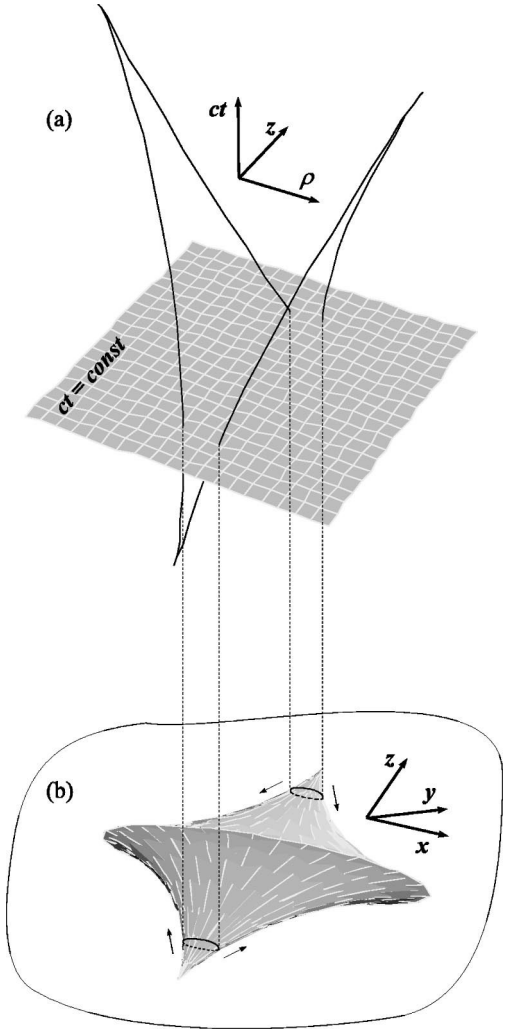

FIG. 2. Null string interpretation of the two-dimensional caustic surface. (a) A section of the two-surface by a hyperplane of constant time (one space dimension is not shown). (b) The space picture of the null strings dynamics.

vector field $\tilde{x}^a_w$ is space-like at the points given by Eq. (5.4), we infer that the two-surface is a null two-surface in 4D Minkowski space–time. The parametric representation (5.4) also provides a representation for this surface as an intersection of two hypersurfaces:

$$x^2+y^2+z^2=\frac{a^2}{4}\left[1+3\left(\frac{4ct}{3a}\right)^2\right], \quad x^2+y^2-z^2=\frac{a^2}{4}\left(\frac{4ct}{3a}\right)\left[3+\left(\frac{4ct}{3a}\right)^2\right]. \tag{5.5}$$

Here $|4ct/3a|\leqslant 1$. Eliminating $4ct/3a$ from the equations in (5.5), we observe that in a particular reference frame the projection of this null two-surface in a hyperplane of constant time is an astroid of revolution with the parameter a given by

$$[x^2+y^2+z^2-a^2]^3+27a^2[x^2+y^2]z^2=0$$

(see Fig. 2).

As is well known, a compact space-like two-surface in 4D Minkowski space–time can be represented as an intersection of two null hypersurfaces. Somewhat analogous to that situation, two-dimensional self-intersections (caustics) of null hypersurfaces provide examples of nongeodesic null two-surfaces in 4D Minkowski space–time.

In order to make a connection with the description of the previous sections, we need the spin-tensor expressions of various vector field quantities. As mentioned previously, the null vector field x_u^a can be employed to obtain the spinor field describing the null directions tangent to the null two-surface. First, we explicitly calculate

$$x_u^{AA'} = x_u^a (\sigma_a)^{AA'} = \frac{a}{4\sqrt{2}} \begin{bmatrix} 1-\sin v & \cos v\, e^{iw} \\ \cos v\, e^{-iw} & 1+\sin v \end{bmatrix}. \tag{5.6}$$

Here $(\sigma_a)^{AA'}$ are the Pauli matrices. Since the vector field x_u^a is real-valued and null, the determinant of the matrix in (5.6) vanishes and we must have $x_u^{AA'} \propto \overline{\pi}^A \pi^{A'}$. The components of the spinor $\overline{\pi}_A$ can be taken as follows:

$$\overline{\pi}_A = -i\sqrt{2} \begin{bmatrix} \cos\left(\frac{v}{2}-\frac{\pi}{4}\right) e^{-iw/2} \\ \sin\left(\frac{v}{2}-\frac{\pi}{4}\right) e^{iw/2} \end{bmatrix}. \tag{5.7}$$

B. Nongeodesic null string

Now we are in a position to explore connections between the example null two-surface and a nongeodesic null string world-sheet in 4D Minkowski space–time.[24] Changing the parameters (v,w) to (τ, σ) we can rewrite the parametric representation (5.4) for the null two-surface as $x^a = a[(3/4)\cos 2\tau, \cos^3\tau\cos\sigma, \cos^3\tau\sin\sigma, \sin^3\tau]$. The range of the parameters is $\tau \in [\pi/2, \pi]$ and $\sigma \in [0, 2\pi]$. This corresponds to a closed null string with the parameter τ playing the role of a time variable. The results (5.6) and (5.7) allow us to write

$$\dot{x}^{AA'} = \frac{3a}{2\sqrt{2}} \sin 2\tau\, \overline{\pi}^A \pi^{A'}. \tag{5.8}$$

Here $\overline{\pi}_A$ is given by formula (5.7) with the necessary change of (v,w) to (τ, σ). Next, we introduce a second spinor field $\overline{\eta}^A$:

$$\overline{\eta}^A = \frac{i}{\sqrt{2}} \begin{bmatrix} \cos\left(\frac{\tau}{2}-\frac{\pi}{4}\right) e^{i\sigma/2} \\ \sin\left(\frac{\tau}{2}-\frac{\pi}{4}\right) e^{-i\sigma/2} \end{bmatrix}. \tag{5.9}$$

which, together with $\overline{\pi}_A$, constitutes a normalized Newman–Penrose dyad (spin-frame) for all admissible values of the parameters τ and σ. Making use of (5.7) and (5.9) we obtain

$$\acute{x}^{AA'} = -i\frac{a}{\sqrt{2}} \cos^3\tau\, (\overline{\pi}^A \eta^{A'} - \overline{\eta}^A \pi^{A'}). \tag{5.10}$$

The vector fields $\dot{x}^a$ and $\acute{x}^a$ tangent to the null two-surface vanish at two space–time points

$$ct = -\frac{3a}{4}, \quad x = y = 0, \quad z = \pm a \tag{5.11}$$

and, in addition, the vector field $\dot{x}^a$ vanishes on the circle

$$ct=\frac{3a}{4},\quad x^2+y^2=a^2,\quad z=0. \tag{5.12}$$

Comparing the results (5.8) and (5.10) with the first two equations in the system (3.28), we can identify the functions r and ζ as follows:

$$r=\frac{3a}{2\sqrt{2}}\sin 2\tau,\quad \zeta=-\frac{a}{\sqrt{2}}\cos^3\tau.$$

The expressions for $\overline{\pi}^A$ and $\overline{\eta}^A$ can be used to obtain the functions $(\omega-\ln|\zeta|)^{\cdot}$ and ψ of the Ref. 24 directly. The result reads:

$$(\omega-\ln|\zeta|)^{\cdot}=0,\quad \psi=\frac{a}{4\sqrt{2}}. \tag{5.13}$$

This knowledge is important for relating $\mathrm{Re}\,\dot{\omega}$ and ψ with the quantities which represent the field strength of the gauge field $B_{ab}(x)$ of Ref. 24 Thus, we obtain

$$\begin{gathered}\psi=-\tfrac{3}{4}\text{æ}a^2\sin 2\tau\cos^3\tau(\rho^{\tau})^{-1}\phi,\\ 2\,\mathrm{Re}\,\dot{\omega}=-\tfrac{3}{2}\text{æ}a^2\sin 2\tau\cos^3\tau(\rho^{\tau})^{-1}\,\mathrm{Re}\,\nu+(\ln|\cos^6\tau(\rho^{\tau})^{-1}|)^{\cdot}.\end{gathered} \tag{5.14}$$

Substituting the result (5.13) in these equations we have

$$\phi=-\rho^{\tau}[3\sqrt{2}\text{æ}a\sin 2\tau\cos^3\tau]^{-1},\quad \mathrm{Re}\,\nu=-\rho^{\tau}[\tfrac{3}{2}\text{æ}a^2\sin 2\tau\cos^3\tau]^{-1}(\ln|\cos^6\tau(\rho^{\tau})^{-1}|)^{\cdot}.$$

The above-mentioned formulas show that the quantity ϕ, which represents the only physical degree of freedom of the field strength, diverges at the space–time points (5.11) and on the circle (5.12).

Therefore, in a particular reference frame, Fig. 2, one can interpret the null two-surface of this section as a pair of circular null strings which appear with zero radius at $t=-3a/4c$ at spatial points $(x,y,z)=(0,0,\pm a)$. They then expand until the time $t=3a/4c$, when they disappear having the circumference of $2\pi a$. The null strings are the sections of the caustic two-surface in Fig. 1 by the hyperplanes of constant time. Projection of the world-sheets of the null strings into a particular reference frame constitutes the astroid of revolution described earlier in this section.

C. Evolution equation

It is also interesting to make connections of this example with the evolution equation for nongeodesic null strings derived in the previous section. The parametric expressions for $\overline{\pi}^A$ and $\overline{\eta}^A$, together with the results (5.8) and (5.10), can be utilized to verify the equality (4.4). Noting that $\kappa=r^{-1}$, we find

$$\acute{\kappa}=0,\quad \dot{\zeta}=\frac{3a}{2\sqrt{2}}\sin 2\tau\cos\tau,\quad \text{and}\quad U-\overline{U}=0.$$

Then, we have $\dot{x}'^a=\zeta^{-1}\dot{\zeta}\acute{x}^a$. Next, the formulas (4.7) and (4.8) yield

$$\acute{x}^2=-a^2\cos^6\tau,\quad \ddot{x}\ddot{x}'=0,$$

$$\acute{x}\dot{x}'=\tfrac{3}{2}a^2\sin 2\tau\cos^4\tau,\quad \ddot{x}^2=-\tfrac{9}{4}a^2\sin^2 2\tau.$$

Finally, with the aid of the above-obtained results, we observe that the evolution equation (4.12) holds.

VI. DISCUSSION AND OUTLOOK

First, the method employed in this paper to obtain a variational principle, (2.5), for a null two-surface can be, in principle, used to design a twistor variational principle for time-like two-surfaces (conventional strings) and space-like two-surfaces. The idea is to take a simple bivector field $p_{ab}(x)$ and impose one of the algebraic conditions $p_{ab}p^{ab}=1$ or $p_{ab}p^{ab}=-1$. The latter condition would single out the string (compare with the last part of Ref. 5), while the former would correspond to a space-like two-surface. It is easy to see that such a procedure uniquely fixes the symmetric second rank spin-tensor field $\phi_{AB}(x)$ in the standard decomposition of an antisymmetric 4D Minkowski space–time tensor field $p_{ab}(x)=\phi_{AB}(x)\varepsilon_{A'B'}+\overline{\phi}_{A'B'}(x)\varepsilon_{AB}$. Then, the variational principle

$$S=\frac{1}{2!}\int [\phi_{AB}(x)\varepsilon_{A'B'}+\overline{\phi}_{A'B'}(x)\varepsilon_{AB}]\mathrm{d}x^{AA'}\wedge\mathrm{d}x^{BB'}$$

would define a two-surface subject to the differential constraint stated in Sec. I [see Eq. (3.36)]. It is hoped that the use of spinor decomposition for $p_{ab}(x)$, consistent with either of the formulated algebraic constraints, would provide equations of motion, which automatically incorporate the differential constraints formulated in Sec. I. Such an assertion is supported by the success of this procedure for the null two-surfaces (null strings) presented in the current contribution. It may well be possible to derive the analogs of the evolution equation (4.12) for generic (interacting) strings in 4D Minkowski space–time and curved space–times of general relativity, where exist explicit spinor and twistor constructions [cf. Ref. 31—Eq. (16) and Ref. 32—Eqs. (3.6)–(3.11)]. In the same way it should be possible to build twistor action functionals in the both cases for generic time-like and space-like two-surfaces of 4D Minkowski space–time.

Second, if one employs Feber's definition of a $\mathrm{SU}(2,2|N)$ supertwistor,[33] (s)he could construct a description of null strings with spin in the physical dimensions of space-time. Its analysis presumably would follow the standard pass outlined in the works of Shirafuji[10] and Bengtsson *et al.*[34]

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The peculiarity of a negative coordinate axis in dyonic solutions of noncommutative $\mathcal{N}=4$ super Yang–Mills

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We show that in the neighborhood of a negative coordinate axis, the U(1) sector of the static dyonic solutions to the noncommutative U(4) $\mathcal{N}=4$ super Yang–Mills (SYM) can be consistently decoupled from the SU(4) to *all orders in the noncommutativity parameter*. We show the above decoupling in two ways. First, we show the noncommutative dyon being the same as the commutative dyon, is a consistent solution to noncommutative equations of motion in the abovementioned region of noncommutative space. Second, as an example of decoupling of a non-null U(1) sector, we also obtain a family of solutions with nontrivial U(1) components for all components of the gauge field in the same region of noncommutative space. In both cases, the SU(4) and U(1) components separately satisfy the equations of motion. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1500773]

I. INTRODUCTION

Nonperturbative solutions in super Yang–Mills (SYM) theories have been an important area of work. More recently, static dyonic solutions in SU(N), $N\geqslant 3$, 4 $\mathcal{N}=4$ SYM corresponding to planar and nonplanar (respectively) string junctions have been obtained in Refs. 1 and 2 (see also references therein). Also, solitonic solutions in noncommutative SYM have been considered by others before (see Refs. 3, 4, and references therein). Now, the gauge group SU(N), in general is not allowed in noncommutative gauge theories.[5] [See Ref. 6 though, where the gauge parameter in noncommutative gauge tranformations is allowed to depend on the usual SU(N) gauge paramater and gauge fields. The explicit form of the map to all orders in the noncommutativity parameter (which is what we are interested in, in this paper) is quite involved and has not been worked out.] One of the questions that we address in this work is whether it is possible to construct solutions to the equations of motion of a noncommutative supersymmetric gauge theory in which one can decouple the U(1) components from the SU components of the fields at least in some region of the noncommutative space, *to all orders in the noncommutativity parameter*. There are the following two additional motivations for this work. The equality of the angular momentum and (null) quadrupole moment of the commutative and noncommutative monopoles of (S)U(2) $N=2$ SYM up to O(θ^2) was shown in Ref. 13 and in all of space. This makes it natural to pose the following question: Is it possible to construct solutions of a noncommutative supersymmetric gauge theory that are characterized by quantities that receive no noncommutativity corrections *to all orders in the noncommutativity parameter*? Finally, it is of obvious interest to construct solutions that are valid up to all orders in the noncommutativity paramater.

In this paper, we show that for noncommutative U(4) $\mathcal{N}=4$ SYM, the static dyonic solutions in the neighborhood of a negative coordinate axis of the noncommutative space, are such that one can decouple the U(1) from the SU(4), and construct a 6-parameter family of noncommutative dyonic solutions [for a non-null U(1) decoupling]. Even though, the decoupling has been shown for a very limited region of the noncommutative space, the reason the solutions are of interest is because they have the same electric and magnetic charges as and energy differing infinitesimally from the commutative dyonic solutions of Ref. 1, *to all orders in the noncommutativity parameter*.

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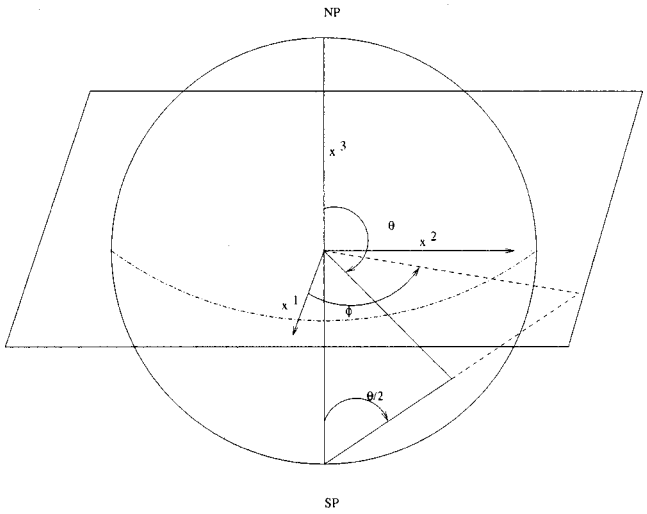

FIG. 1. The stereographic coordinate system.

This points to the peculiar nature of the negative x^3 axis when constructing dyonic solutions to noncommutative $\mathcal{N}=4$ SYM, which requires further investigation.

The paper is organized as follows: In Sec. II, we discuss the basics needed for getting static dyonic solutions in commutative $\mathcal{N}=4$ super Yang–Mills (SYM). In Sec. III, we discuss the modifications in the techniques of Sec. II to get static dyonic solutions of noncommutative $\mathcal{N}=4$ SYM. It has two subsections: (a short) 3.1 on decoupling of a null U(1) from the SU(4), and 3.2 on decoupling of a non-null U(1) from the SU(4). In Sec. IV, we give a summary of and a discussion on the results obtained in the paper, and indicate possible future directions for work.

II. BASICS

In this section, we give a brief review of the techniques given in Ref. 1 to obtain dyonic solutions in commutative SU(4) $\mathcal{N}=4$ SYM.

It is advisable to write the equations of motion as if one were working in curved space–time. The reason is that for solutions of the equations of motion, it is convenient to go to the stereographic coordinate system (see Fig. 1, $z=e^{i\phi}\tan\theta/2$) in which the metric is not constant. The equations of motion for commutative SU(4) $\mathcal{N}=4$ SYM are given by

$$D_i(\sqrt{g}g^{ii_1}g^{jj_1}F_{i_1j_1})=i\sqrt{g}\sum_J [D^j\Phi^J,\Phi^J],$$

$$D_i(\sqrt{g}g^{ij}D_j\Phi^J)=\sqrt{g}[\Phi^I,[\Phi^I,\Phi^J]]. \tag{1}$$

The component-form of the above equations is given in Ref. 1 which we will not be repeating here. Following the close parallel with Skyrme models,[7] one uses the harmonic-map anzatz to solve the equations of motion; the Higgs and gauge fields are assumed to have the following form:

$$\begin{aligned} A_z=A_z^aT^a=&-(1+c_1-c_2-c_0)(r)(\partial P_0)P_0\\ &+(c_2-c_1)(r)[P_1,\partial P_1]+(1-c_2(r))[P_2,\partial P_2], \quad A_r=0,\\ \Phi^I=\Phi^{I,a}T^a=&(b_2^I+b_0^I+b_1^I)(r)(P_0-\tfrac{1}{4}\mathbf{1}_4)\\ &+(b_2^I+b_1^I)(r)(P_1-\tfrac{1}{4}\mathbf{1}_4)+b_2^I(r)(P_2-\tfrac{1}{4}\mathbf{1}_4), \end{aligned} \tag{2}$$

T^a being the generators of SU(4), I indexing the number of scalars that are turned on, and for this paper taking values 1, 2, and 3, $c_{0,1,2}(r)$ and $b^I_{0,1,2}(r)$ being the "profile functions" of the gauge field and Higgs, respectively, and P_i the orthogonal set of $\mathbf{CP}^3$ sigma model projectors defined as

$$P_0=\frac{ff^\dagger}{f^\dagger f},$$

$$P_j=\frac{(\Delta^j f)(\Delta^j f)^\dagger}{|\Delta^j f|^2},\quad j=1,2, \tag{3}$$

where

$$\Delta f\equiv\partial f-f\frac{f^\dagger\partial f}{|f|^2},$$

$$f\equiv(1,\sqrt{3}z,\sqrt{3}z^2,z^3)^t, \tag{4}$$

and $\Delta^2 f=\Delta(\Delta f)$. They can be thought of as Hermitian maps from S^2 to $\mathbf{CP}^3$. The explicit forms of the projectors P_is can be worked out using Mathematica or Maple.

The substitution of the harmonic map anzatz into the equations of motion (written in components) either results in an equation of motion being identically satisfied, or a system of nonlinear second-order coupled differential equations involving the Higgs and gauge field profile functions that can be solved using techniques referred to in Ref. 1. The solutions corresponding to (non-)planar string networks (for nonplanar, assuming an infinitesimal nonplanarity corresponding to an infinitesimal deformation from the BPS nature of the planar solution) were then obtained in Ref. 1.

III. NONCOMMUTATIVE DYONIC SOLUTIONS

In this section we derive a class of static noncommutative dyonic solutions assuming $r-z$ and $r-\overline{z}$ noncommutativity only. Thus, the star product of two functions $f(r,z,\overline{z})$ and $h(r,z,\overline{z})$ will be

$$\begin{aligned}&f(r,z,\overline{z})*h(r,z,\overline{z})\\&\quad=e^{(i/2)[\Theta^{rz}(\partial_r^1\partial^2-\partial_r^2\partial^1)+\Theta^{r\overline{z}}(\partial_r^1\overline{\partial^2}-\partial_r^2\overline{\partial^1})]}f(r_1,z_1,\overline{z_1})h(r_2,z_2,\overline{z_2})\big|_{1=2}.\end{aligned} \tag{5}$$

We show that using stereogrpahic coordinates, in the neighborhood of the South Pole, or equivalently the neighborhood of the negative x^3 axis, one can consistently decouple in the equations of motion, the U(1) from the SU(4) components of the Higgs and the gauge fields.

The noncommutative equations of motion are given by

$$\hat{D}_i*(\sqrt{g}*g^{ii_1}*g^{jj_1}*\hat{F}_{i_1j_1})=i\sqrt{g}*\sum_J[\hat{D}^j*\hat{\Phi}^J,\hat{\Phi}^J]_*,$$

$$\hat{D}_i*(\sqrt{g}*g^{ij}*\hat{D}_j*\hat{\Phi}^J)=\sqrt{g}*[\hat{\Phi}^I,[\hat{\Phi}^I,\hat{\Phi}^J]_*]_*. \tag{6}$$

As we are considering only $r-z,r-\overline{z}$-noncommutativity, the projectors of Ref. 1 are still valid here. We assume the following anzatz for the gauge field $\hat{A}_z$, $\hat{A}_r$, and the Higgs field $\hat{\Phi}^I$,

$$\hat{A}_z=\hat{A}_z^aT^a+i\epsilon F_z(\Theta)g_z(r)\hat{\mathcal{A}}_z^0\mathbf{1}_4,$$

$$\hat{A}_r=i\epsilon F_r(\Theta)g_r(r)\hat{\mathcal{A}}_r^0\mathbf{1}_4,$$

$$\hat{\Phi}^I=\hat{\Phi}^{I,a}T^a+i\epsilon F_\Phi(\Theta)g^I_\Phi(r)\hat{\phi}^0\mathbf{1}_4, \tag{7}$$

where $F_{z,r,\Phi}(\Theta)$ are functions of the noncommutativity parameter Θ which vanish as Θ is set to zero and are bounded as $\Theta\to\infty$, and

$$\hat{A}_z^a T^a = -(1+c_1-c_2-c_0)(r)*(\partial P_0)P_0 + (c_2-c_1)(r)*[P_1,\partial P_1]+(1-c_2(r))*[P_2,\partial P_2],$$

$$\hat{\Phi}^{I,a}T^a=(b_2^I+b_0^I+b_1^I)(r)*(P_0-\tfrac{1}{4}\mathbf{1}_4)+(b_2^I+b_1^I)(r)*(P_1-\tfrac{1}{4}\mathbf{1}_4)+b_2^I(r)*(P_2-\tfrac{1}{4}\mathbf{1}_4), \quad (8)$$

$c_{0,1,2}(r)$ and $b^I_{0,1,2}(r)$ being the ''profile functions'' of the gauge field and Higgs, respectively, as in (2). We have thus taken an anzatz in which the U(4) fields have infinitesimal U(1) components. We will work up to $O(\epsilon)$. Hence, the noncommutative U(1) field strengths are the same as the commutative U(1) field strengths. There is no star product in the anzatz (7) in the U(1) components of the fields because as argued below, the star products can be dropped in the neighborhood of the South Pole in the SU(4)-components of the fields, and we assume similar behavior for the U(1) and SU(4) components. The anzatz for the U(1) components that we choose in (10) below, is such that if one were to put in a star product between the radial and angular functions, then it (the star product) cannot be dropped in the neighborhood of the South Pole.

As *expanding the star product in (8) will involve taking derivatives of* $(\partial)P_i$, using the explicit forms of the projectors that can be worked out using Mathematica or Maple, one sees that *one can drop* $(\partial)\partial P_i$ *relative to* $(\partial)P_i$ *as one approaches the neighborhood of the South Pole*, as the former is suppressed relative to the latter by terms of $O(1/|z|^m), m>0$ that vanish as $|z|\to\infty$ (i.e., in the neighborhood of the South Pole). *One thus has for the SU part of* $\hat{A}_z,\hat{\Phi}$ *the same expression as in Ref. 1*. One can argue similarly that the $*$ products in (6) can also be dropped (in the neighborhood of the South Pole). We now discuss the decoupling from SU(4), of a null U(1) in Sec. III A and non-null U(1) in Sec. III B.

A. Decoupling of null U(1)

Using (7), for null U(1) components, one can require consistently that the SU(4) and U(1) components, separately, satisfy the equations of motion, and one can show there is no mixing between the SU(4) and U(1) sectors. Hence, one can consistently set the U(1) components to zero. The entire analysis of Ref. 1 to show the connection between (non-)planar stable (non-)BPS string junctions and dyon solutions, then goes through even in the neighborhood of the South Pole of the abovementioned noncommutative space if one notices and uses the following transformation that takes one from the North Pole to the South Pole [and is also a symmetry of the equations of motion of the SU(4) part of the solutions, as given in Ref. 2 of Ref. 1],

$$c_0\leftrightarrow c_2;\ \ b_0^I\leftrightarrow b_2^I. \quad (9)$$

One also uses the fact that if $\hat{\Phi}$ is a solution then $-\hat{\Phi}$ is also a solution to the equations of motion.

B. Decoupling of non-null U(1)

Here we discuss in detail, the decoupling of non-null U(1) components of the Higgs and the gauge fields from their SU(4) components in the neighborhood of the South Pole of the noncommutative space. To show the decoupling of a non-null U(1) from SU(4), we choose the following anzatz for the U(1) components (of the Higgs and gauge fields):

$$\hat{\phi}^0,\hat{\mathcal{A}}_z^0=\det[(P_0-a_{\Phi,z}\mathbf{1}_4)(P_1-M_{\Phi,z})(P_2-M_{\Phi,z})]+\text{c.c.},$$

$$\hat{A}_r^0=z\det[(P_0-a_r\mathbf{1}_4)(P_1-M_r)(P_2-M_r)]+\text{c.c.}, \quad (10)$$

where

$$M_i=\begin{pmatrix} 0 & b_i & 0 & 0 \\ c_i & 0 & 0 & 0 \\ 0 & 0 & 0 & e_i \\ 0 & 0 & f_i & 0 \end{pmatrix}, \tag{11}$$

where $i\equiv r,z,\Phi$, and the parameters a_i,b_i,c_i,e_i, and f_i have been introduced to get nonzero determinants using the projectors and some constant matrices; the parameters get constrained later. We now assume that one approaches the South Pole along any path very close to ϕ ($\equiv$azimuthal angle)$=\pi/2$. This implies that $\mathrm{Re}\, z$ is finite, but $\mathrm{Im}\, z$ approaches infinity. Hence, one sees that $\partial\overline{\partial}\hat{\mathcal{A}}_r^0$ [as shown in (A5)] and $(\partial-\overline{\partial})(\hat{\phi}^0,\hat{\mathcal{A}}_z^0)$ [as shown in (A8)] are real. If

$$b_i=f_i,\ \ c_i=e_i, \tag{12}$$

then $\partial((1+|z|^2)^2(\partial+\overline{\partial})(\hat{\phi}^0,\hat{\mathcal{A}}_z^0))$ [as shown in (A9)] will be finite and real as $\mathrm{Im}\, z\to\infty$. These considerations become useful when one solves the equations of motion for the U(1) components as done in (19) and (20) in the neighborhood of the South Pole.

From power (of $|z|$ or $\mathrm{Im}\, z$) counting arguments using expressions given in the Appendix, one can require consistently that the SU(4) and U(1) components, separately, satisfy the equations of motion, and one can show there is no mixing between the SU(4) and U(1) sectors. As the decoupling for non-null U(1) is nontrivial, to illustrate the point, we consider the example of $\hat{F}_{rz}$. We see that up to $\mathrm{O}(\epsilon)$,

$$\hat{F}_{rz}^{\mathrm{U}(4)}=\hat{F}_{rz}^{\mathrm{SU}(4)}+\hat{F}_{rz}^{\mathrm{U}(1)}-i[\hat{A}_r^{\mathrm{U}(1)},\hat{A}_z^{\mathrm{SU}(4)}]_*. \tag{13}$$

Now,

$$\begin{aligned}[\hat{A}_r^{\mathrm{U}(1)},\hat{A}_z^{\mathrm{SU}(4)}]_*=&\,i\Theta^{rz}(\partial_r\hat{A}_r^{\mathrm{U}(1)}\partial\hat{A}_z^{\mathrm{SU}(4)}-\partial\hat{A}_r^{\mathrm{U}(1)}\partial_r\hat{A}_z^{\mathrm{SU}(4)})+i\Theta^{r\overline{z}}(\partial_r\hat{A}_r^{\mathrm{U}(1)}\overline{\partial}\hat{A}_z^{\mathrm{SU}(4)}\\ &-\overline{\partial}\hat{A}_r^{\mathrm{U}(1)}\partial_r\hat{A}_z^{\mathrm{SU}(4)})+\mathrm{O}(\Theta^2).\end{aligned} \tag{14}$$

Using expressions in the Appendix, one sees that

$$\begin{gathered}\partial_r\hat{A}_r^{\mathrm{U}(1)}\equiv\mathrm{O}(1),\ \ \partial\hat{A}_r^{\mathrm{U}(1)},\overline{\partial}\hat{A}_r^{\mathrm{U}(1)}\equiv\mathrm{O}(1),\\ \partial\hat{A}_z^{\mathrm{SU}(4)}\equiv\mathrm{O}\left(\frac{1}{|z|^3}\right)\times M,\ \ \overline{\partial}\hat{A}_z^{\mathrm{SU}(4)}\equiv\mathrm{O}\left(\frac{1}{|z|^4}\right)\times\mathbf{1}_4,\\ \partial_r\hat{A}_z^{\mathrm{SU}(4)}\equiv\mathrm{O}\left(\frac{1}{|z|^2}\right)\times M,\\ \partial_r\hat{A}_z^{\mathrm{U}(1)}\equiv\mathrm{O}(1),\ \ \partial\hat{A}_z^{\mathrm{U}(1)},\\ \overline{\partial}\hat{A}_z^{\mathrm{U}(1)}\equiv\mathrm{O}\left(\frac{1}{|z|^2}\right)\{\text{relevant for } [\hat{A}_r^{\mathrm{U}(1)},\hat{A}_z^{\mathrm{U}(1)}]_*\},\end{gathered} \tag{15}$$

where

$$M\equiv\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{16}$$

TABLE I. Consequences of power counting done in (15).

Term that can be dropped	Relative to
$\partial_r \hat{A}_r^{\mathrm{U}(1)} \partial \hat{A}_z^{\mathrm{SU}(4)}$	$\hat{F}_{rz}^{\mathrm{SU}(4)}$
$\partial \hat{A}_r^{\mathrm{U}(1)} \partial_r \hat{A}_z^{\mathrm{SU}(4)}$	$\hat{F}_{rz}^{\mathrm{SU}(4)}$
$\partial_r \hat{A}_r^{\mathrm{U}(1)} \bar{\partial} \hat{A}_z^{\mathrm{SU}(4)}$	$\hat{F}_{rz}^{\mathrm{U}(1)}$
$\bar{\partial} \hat{A}_r^{\mathrm{U}(1)} \partial_r \hat{A}_z^{\mathrm{SU}(4)}$	$\hat{F}_{rz}^{\mathrm{SU}(4)}$

Thus

$$\hat{F}_{rz}^{\mathrm{U}(1)} \equiv \mathrm{O}(1); \quad \hat{F}_{rz}^{\mathrm{SU}(4)} \equiv \mathrm{O}\left(\frac{1}{|z|^2}\right) \times M, \tag{17}$$

and in Table I, we show which terms can be dropped relative to which terms as $\mathrm{Im}\, z \to \infty$. Similar reasoning can be used to argue that terms of higher order in Θ, can also be dropped relative to the commutative counterparts. Hence, as $\mathrm{Im}\, z \to \infty$,

$$\hat{F}_{rz}^{\mathrm{U}(4)} \sim \hat{F}_{rz}^{\mathrm{SU}(4)} + \hat{F}_{rz}^{\mathrm{U}(1)}, \tag{18}$$

showing the stated decoupling.

By requiring that the SU components of the Higgs and gauge fields still satisfy the commutative equations of motion (having dropped the star product at the South pole), the U(1) components should satisfy these equations,

$$\frac{dg_z}{dr}(\partial - \bar{\partial}) \hat{\mathcal{A}}_z^0 - 2 g_r \partial \bar{\partial} \hat{\mathcal{A}}_r^0 = 0,$$

$$\frac{d^2 g_z}{dr^2} \hat{\mathcal{A}}_z^0 - g_r \partial \hat{\mathcal{A}}_r^0 + \frac{g_z}{2r^2} \partial ((1+|z|^2)^2 (\partial + \bar{\partial}) \hat{A}_z) = 0,$$

$$\frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{dg_\Phi^I}{dr} \right) \hat{\phi}^0 + \frac{(1+|z|^2)^2}{r^2} g_\Phi^I \partial \bar{\partial} \hat{\phi}^0 = 0. \tag{19}$$

The $*$ product has been dropped as it will generate $\mathrm{O}(1/|z|^m)$-corrections [relative to O(1)], which can be dropped in the neighborhood of the South Pole. We now discuss a family of dyonic solutions to (19).

One gets (setting $c_r = e_r$ and $b_r = f_r$ for convenience),

$$\frac{dg_z}{dr} + 2 g_r \frac{[(b_r c_r)^3 (2c_r - b_r)]}{(b_z c_z)^3 (c_z - b_z)} = 0,$$

$$2 \frac{d^2 g_z}{dr^2} (-1 + a_z) a_z^3 (b_z c_z)^4 - g_r (-1 + a_r) a_r^3 (b_r c_r)^4$$

$$+ \frac{g_z}{r^2} (3(-1 + a_z) a_z^3 b_z^2 c_z^2 (b_z - c_z)^2) = 0,$$

$$2 \frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{dg_\Phi^I}{dr} \right) (-1 + a_\Phi) a_\Phi^3 (b_\Phi c_\Phi)^4,$$

$$- \frac{6}{r^2} |z|^2 g_\Phi^I (-1 + a_{\Phi,z}) a_\Phi^3 (c_\Phi^4 b_\Phi^2 + b_\Phi^4 c_\Phi^2) = 0. \tag{20}$$

By eliminating $\hat{\mathcal{A}}_r^0$ from the first two equations, one gets the following differential equation for g_z:

$$\frac{d^2g_z}{dr^2}+\frac{dg_r}{dr}\frac{(-1+a_r)a_r^3(b_rc_r)^4\sqrt{3}(-1+a_z)a_z^3[(b_zc_z)^3(c_z-b_z)]}{4(-1+a_z)^2a_z^6(b_zc_z)^4[b_r^3c_r^3\sqrt{3}(2c_r-b_r)]}$$
$$+\frac{g_z}{r^2}\left(3(-1+a_z)a_z^3\frac{(b_z-c_z)^2}{2b_z^2c_z^2}\right)=0. \tag{21}$$

Equation (21) is of the form,

$$r^2y''(r)+\alpha r^2y'(r)+\beta y(r)=0, \tag{22}$$

the solution to which (using maple) is given by

$$y(r)=C_1\sqrt{r}I_{1/2\sqrt{1-4\beta}}(\tfrac{1}{2}\alpha r)e^{-(1/2)\alpha r}+C_2\sqrt{r}I_{-1/2\sqrt{1-4\beta}}(\tfrac{1}{2}\alpha r)e^{-(1/2)\alpha r}, \tag{23}$$

for $\frac{1}{2}\sqrt{1-4\beta}\notin\mathbf{Z}$ and

$$y(r)=C_1'\sqrt{r}I_{1/2\sqrt{1-4\beta}}(\tfrac{1}{2}\alpha r)e^{-(1/2)\alpha r}+C_2'\sqrt{r}K_{1/2\sqrt{1-4\beta}}(\tfrac{1}{2}\alpha r)e^{-(1/2)\alpha r}, \tag{24}$$

for $\frac{1}{2}\sqrt{1-4\beta}\in\mathbf{Z}$. Let us consider the two cases separately.

For the former, to make sure that the solution goes to zero as $r\to\infty$, one sets

$$C_1=-C_2. \tag{25}$$

Even though this is a singular solution (at $r=0$), as we shall see, it is a finite energy solution.

The derivative of the solution involving $I_{\pm\nu}(\alpha r)$ is given by

$$\frac{d}{dr}\left(e^{-\alpha r/2}\sqrt{r}\left(I_{1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)-I_{-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)\right)\right)$$
$$=\frac{e^{(-\alpha r/2)}}{4\sqrt{r}}\left(\alpha rI_{-1+1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)+\alpha rI_{1+1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)\right.$$
$$+2(-1+\alpha r)I_{-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)$$
$$\left.-\alpha rI_{-1-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)-\alpha rI_{1-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)-2(-1+\alpha r)I_{1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)\right). \tag{26}$$

For the purpose of getting finite energy, as we will very shortly see, one is required to impose that $r^2(dy(r)/dr)^2\to0$ as $r\to\infty$, and that it is finite at $r=0$. Using the series expansions around $r=0$ and the asymptotic expansions for $I_\nu(r)$, the former is satisfied identically, and the latter is satisfied if one imposes

$$\sqrt{1-4\beta}<1\Leftrightarrow0<\beta<\tfrac{1}{4}. \tag{27}$$

The solution for $g_\Phi^I(r)$ that one gets is

$$g_\Phi^I(r)=0. \tag{28}$$

Hence, the final result for the U(1) components of the Higgs and gauge fields, in the neighborhood of the South Pole (approaching it along ϕ close to $\pi/2$) are

$$\hat{A}_z^0(r,z)=i\epsilon f_z(\Theta)\sqrt{r}e^{-(1/2)\,\alpha r}(I_{1/2\sqrt{1-4\beta}}(\tfrac{1}{2}\alpha r)-I_{-1/2\sqrt{1-4\beta}}(\tfrac{1}{2}\alpha r))$$
$$\times\det[(P_0-a_z\mathbf{1}_4)(P_1-M_r)(P_2-M_r)]+\text{c.c.});$$

$$\hat{A}_r^0=i\epsilon f_r(\Theta)\frac{e^{(-\alpha r/2)}}{4\sqrt{r}}\Bigg(\alpha r I_{-1+1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)+\alpha r I_{1+1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)$$
$$+2(-1+\alpha r)I_{-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)-\alpha r I_{-1-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)-\alpha r I_{1-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)$$
$$-2(-1+\alpha r)I_{1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)\Bigg)(z\,\det[(P_0-a_z\mathbf{1}_4)(P_1-M_r)(P_2-M_r)]+\text{c.c.});$$

$$\hat{\Phi}^0=0, \tag{29}$$

where

$$\beta\equiv\left(3(-1+a_z)a_z^3\frac{(b_z-c_z)^2}{2b_z^2c_z^2}\right)<0;$$

$$\alpha\equiv\frac{(-1+a_r)a_r^3(b_rc_r)^4\sqrt{3}(-1+a_z)a_z^3[(b_ze_z)^3(c_z-b_z)]}{4(-1+a_z)^2a_z^6(b_zc_z)^4[b_r^3c_r^3\sqrt{3}(2c_r-b_r)]};$$

$$0<a_z<1;\quad c_{z,r}=e_{z,r};\quad b_{z,r}=f_{z,r}. \tag{30}$$

Let us consider the energy of the above solution. It is given by (we follow the conventions of Ref. 1),

$$E=-\frac{1}{4\pi}\int r^2dr\frac{dzd\bar{z}}{(1+|z|^2)^2}\text{Tr}\left[(\hat{D}_i*\hat{\Phi})^2+\frac{1}{2}(\hat{F}_{ij})^2{}_*\right]=E_{\text{SU}(4)}+E_{\text{U}(1)}. \tag{31}$$

But, in the neighborhood of the South Pole, where one can drop the $*$ product,

$$E_{\text{U}(1)}=-\int r^2dr\frac{dzd\bar{z}}{(1+|z|^2)^2}[(\partial_r\hat{\mathcal{A}}_z^0-\partial\hat{\mathcal{A}}_r^0)^2+(\partial_r\hat{\mathcal{A}}_z^0+\bar{\partial}\hat{\mathcal{A}}_r^0)^2+((\partial+\bar{\partial})\hat{\mathcal{A}}_z^0)^2]\geqslant 0. \tag{32}$$

Hence, in the neighborhood of the South Pole, even though one is dealing with non-BPS solutions, one gets the following inequality:

$$E_{\text{U}(4)}\geqslant E_{\text{SU}(4)}, \tag{33}$$

with saturation of the inequality occuring for the null U(1) component. Substituting (29) in the $\text{Im}\,z\to\infty$ limit into (32), and integrating in the neighborhood of the South Pole as described earlier, i.e., around $\phi=\pi/2$ and $\theta\in[\pi-\epsilon,\pi]$, $\lim_{\epsilon\to 0}$, one gets an infinitesimal result, provided one gets a finite result from the r integration. The r-integral should converge to get a finite-energy solution. One sees that one has to evaluate

$$E_{\mathrm{U}(1)}\sim\int_0^\infty dr r^2\frac{e^{-\alpha r}}{16r}\Bigg(\alpha r I_{-1+1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)+\alpha r I_{1+1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)$$
$$+2(-1+\alpha r)I_{-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)-\alpha r I_{-1-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)-\alpha r I_{1-1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)$$
$$-2(-1+\alpha r)I_{1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)\Bigg)^2. \tag{34}$$

We have not been able to evaluate the above integral. But the integrand for $0<\beta<\frac{1}{4}$ is analytic for all values of $r\in[0,\infty)$, and it vanishes at $r=0$ and $r\to\infty$. We hence assume that it is convergent corresponding to a finite energy solution. We have verified the same numerically using Mathematica for several values of $\beta<\frac{1}{4}$.

Let us now consider the case $\frac{1}{2}\sqrt{1-4\beta}\in\mathbf{Z}$. In that case in order to get a solution that vanishes as $r\to\infty$, one sets $C_1'=0$ in (24).

One then requires

$$E_{\mathrm{U}(1)}\sim\int_0^\infty dr r^2\frac{e^{-\alpha r}}{16r}\Bigg(-\alpha r K_{-1+1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)$$
$$-2(-1+\alpha r)K_{1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)-\alpha r K_{1+1/2\sqrt{1-4\beta}}\left(\frac{\alpha r}{2}\right)\Bigg)^2$$
$$<\infty. \tag{35}$$

By using the series expansion of $K_\nu(x)$ about $x=0$ (see Ref. 8), one sees that one cannot find a β: $\frac{1}{2}\sqrt{1-4\beta}\in\mathbf{Z}$ that will satisfy (35) because of the singular nature of the integrand at $r=0$.

Now, let us turn to calculating the commutative Higgs and gauge field: $\Phi^I, A_{r,z,\bar{z}}$. As we have thus far continued working to all orders in the noncommutativity parameter Θ, one hence requires an all-order (in Θ) Seiberg–Witten map.[9–11] There is a conjecture for that as given in Ref. 10. We will not explicitly construct the SW map, but conjecture that in the neighborhood of the negative x^3 axis (or the neighborhood of the South Pole of the Riemann Sphere, approaching it the way described in the paper), the noncommutative hatted fields are the same as the commutative unhatted fields. Noting that as $\mathrm{Im}\,z\to\infty$, $\hat{A}^{\mathrm{SU}(4)}_{z,\bar{z}},\partial,\bar{\partial}\hat{\Phi}^{\mathrm{SU}(4)},\partial\hat{A}^{\mathrm{U}(1)}_z$, $\partial^2\hat{A}^{\mathrm{U}(1)}_r\to 0$, and dropping terms of $\mathrm{O}(\epsilon^2)$ in $\hat{A}^{\mathrm{U}(1)}_{r,\bar{z}}$ in Eqs. (3.3), (3.4), and (3.7) for the Higgs and Eqs. (A3), (A6), and (A8) for the gauge field of Ref. 12, the conjecture can be explicitly verified to $\mathrm{O}(\Theta^2)$. Hence, in the neighborhood of the South Pole, approaching it along an azimuthal angle close to $\pi/2$,

$$\hat{\Phi}=\hat{\Phi}^a T^a=\Phi^a T^a;$$

$$\hat{A}_i=\hat{A}^a_i T^a+\hat{A}^0_i\mathbf{1}_4=A^a_i T^a+A^0_i\mathbf{1}_4. \tag{36}$$

The electric charge is then the same as that given in Ref. 1. The magnetic charge will receive a U(1) contribution proportional to $(\partial+\bar{\partial})A_z(z,\bar{z},r\to\infty)$, which using (29), vanishes. Hence, the noncommutative dyon in the neighborhood of the South Pole, carries the same electric and magnetic charges as the commutative dyon of Ref. 1. Their energy will be more than that of the commutative dyons in the neighborhood of the South Pole, though by an infinitesimal amount. As the equality of the commutative and noncommutative electric and magnetic charges is valid only in the neighborhood of the South Pole, these noncommutative dyonic solutions are likely to be stable.

IV. SUMMARY AND DISCUSSION

To summarize, we have shown that noncommutative (with $r-z$ and $r-\overline{z}$ noncommutativity) U(4) SYM possesses static dyonic solutions in the neighborhood of the South Pole of the Riemann sphere or equivalently the negative x^3 axis, that either are the same as the static commutative SU(4) dyonic solutions of Ref. 1 [corresponding to *decoupling of a null U(1) from the SU(4)*] or, have the same electric and magnetic charges as the commutative dyons and differ infinitesimally in their energy [corresponding to *decoupling of a non-null U(1) from the SU(4)*], to *all orders in the noncommutativity parameter*. We have thus shown the decoupling of the U(1) sector, both for null and infinitesimal U(1) components in the neighborhood of the negative x^3 axis. This decoupling to $O(\Theta)$ for the whole of space, was also seen in the context of noncommutative monopole solutions in SYM in Ref. 3. The noncommutative hatted fields are the same as the commutative unhatted fields [we conjecture to all orders in the noncommutativity parameter and show explicitly up to $O(\Theta^2)$]. Thus, we see that the neighborhood of the negative x^3 axis, acts as "denoncommutatifier." It will be interesting to study the same problem using noncommutative ADHMN construction (see Ref. 14 and references therein), and to be able to establish the existence of such solutions using techniques of Ref. 15 using Morse theory. Also, finding similar solutions with $z-\overline{z}$ noncommutativity will be nice.

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APPENDIX

In this Appendix, we summarize the asymptotic (w.r.t. to z) expressions for $A^{\mathrm{U}(1)}_{r,z}$ and some expressions involving them necessary to obtain the U(1) components of the gauge field and Higgs. We have used mathematica for arriving at the expressions given in this Appendix.

Using (10), one can explicity write out the expressions for $\hat{\phi}^0$, $\hat{A}^0_z = \det[(P_0 - a_{\Phi,z}\mathbf{1}_4)(P_1 - M_{\Phi,z})\cdot(P_2 - M_{\Phi,z})] + \text{c.c.}$ and $\hat{A}^0_r = z\det[(P_0 - a_r\mathbf{1}_4)(P_1 - M_r)\cdot(P_2 - M_r)] + \text{c.c.}$, using Mathematica, but because of the length of the expressions, we will give only their asymptotic forms.

One gets as $\mathrm{Im}\, z \to \infty$,

$$\hat{\phi}^0, \hat{A}^0_z \sim 2(-1 + a_{\Phi,z}) a^3_{\Phi,z} (b_{\Phi,z} c_{\Phi,z} e_{\Phi,z} f_{\Phi,z})^2. \tag{A1}$$

Simlarly, as $z \to \infty$, one gets

$$\hat{A}^0_r \sim 2(-1 + a_r) a^3_r (b_r c_r e_r f_r)^2 \,\mathrm{Re}\, z. \tag{A2}$$

Hence, we see that if $z \to \infty$ as $z = (\mathrm{Re}\, z)_0 + i\infty$, where $(\mathrm{Re}\, z)_0$ is finite, then $\hat{A}_r$ is nonsingular, else it is singular.

One sees that as $z \to \infty$,

$$\partial \hat{\mathcal{A}}^0_r \sim (-1 + a_r) a^3_r (b_r e_r c_r f_r)^2. \tag{A3}$$

For the purpose of calculation of energy and imposing it to be finite, one requires to calculate $\overline{\partial}\hat{\mathcal{A}}^0_r$, and its asymptotic expression is given by

$$\overline{\partial}\hat{\mathcal{A}}^0_r \sim (-1 + a_r) a^3_r b^2_r c^2_r e^2_r f^2_r. \tag{A4}$$

One also needs to evaluate $\partial\overline{\partial}\hat{\mathcal{A}}^0_r$ as $z \to \infty$, and is given by

$$\partial\overline{\partial}\hat{\mathcal{A}}^0_r \sim (-1 + a_r) a^3_r \frac{b^2_r c_r e^2_r f_r (\sqrt{3} c_r - \sqrt{3} f_r)\overline{z}^2 + \sqrt{3}(b_r e_r c_r)^2 f_r z^2}{|z|^4}. \tag{A5}$$

Also, one one sees that

$$\partial\overline{\partial}(\hat{\phi}^0,A_z^{\hat{0}})\sim -6(-1+a_{\Phi,z})a_{\Phi,z}^3 \times\frac{((c_{\Phi,z}e_{\Phi,z})^2b_{\Phi,z}f_{\Phi,z}+(b_{\Phi,z}f_{\Phi,z})^2c_{\Phi,z}e_{\Phi,z})}{|z|^2}. \tag{A6}$$

For the purpose of solving for the U(1) components of the gauge field, and for getting the magnetic charge of the dyon, one needs to evaluate $(\partial+\overline{\partial})\mathcal{A}_z^0$, and as $z\to\infty$, one gets

$$(\partial+\overline{\partial})\hat{\mathcal{A}}_z^0\sim\frac{b_zc_z^2e_zf_z^2(\sqrt{3}b_z-\sqrt{3}e_z)\overline{z}^2+(c_zf_zb_z^2(-e_zf_z\sqrt{3}e_z+c_ze_z\sqrt{3}e_z)-3c_zf_zb_ze_zc_ze_z)z^2}{|z|^4}. \tag{A7}$$

Two other quantities that one needs to calculate are $(\partial-\overline{\partial})(\hat{\Phi},\hat{A}_z)$ and $\partial((1+|z|^2)^2(\partial+\overline{\partial})\times(\hat{\Phi},\hat{A}_z))$. The former as $z\to\infty$, is given by

$$(\partial-\overline{\partial})(\hat{\phi}^0,\hat{\mathcal{A}}_z^0) \sim\frac{\sqrt{3}(-1+a_i)a_i^3[(b_ie_i)^2c_if_i(c_i-f_i)\overline{z}+(-b_ic_i^2e_i^2f_i(f_i-b_i)+e_ib_i^2c_if_i^2(c_i-e_i))z](z-\overline{z})}{|z|^4}, \tag{A8}$$

The latter as $z\to\infty$ is given by

$$\begin{aligned}\partial((1+|z|^2)^2(\partial+\overline{\partial})(\hat{\phi}^0,\hat{\mathcal{A}}_z^0))&\\ \sim -2(-1+a_i)a_i^3\Bigg(&\sqrt{3}[c_i^2e_i^2b_if_i(-f_i+b_i)+b_i^2f_i^2c_ie_i(c_i-e_i)]z\\ &-(3b_if_i(c_ie_i)^2+3c_ie_i(b_if_i)^2)+\frac{3b_ic_ie_if_i(b_ie_i+c_if_i)\overline{z}^4}{|z|^4}\Bigg).\end{aligned} \tag{A9}$$

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Becchi–Rouet–Stora–Tyutin quantization of histories electrodynamics

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This article is a continuation of earlier work where a classical history theory of pure electrodynamics was developed in which the history fields have *five* components. The extra component is associated with an extra constraint, thus enlarging the gauge group of histories electrodynamics. In this article we quantize the classical theory developed previously by two methods. First we quantize the reduced classical history space to obtain a reduced quantum history theory. Second we quantize the classical BRST-extended history space, and use the Becchi–Rouet–Stora–Tyutin charge to define a ''cohomological'' quantum history theory. Finally, we show that the reduced history theory is isomorphic (as a history theory) to the cohomological history theory. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The history projection operator (HPO) approach to consistent histories was inspired by Isham,[1] and developed by Isham and collaborators.[2,3] An HPO theory is concerned with projection operators on the quantum history Hilbert space $\mathcal{E}$ which represent propositions about the entire *history* of the system under consideration. This should be contrasted with standard quantum logic which is concerned with propositions about the system at a particular instant of time. The quantum history theories with which this article will be concerned are described by a pair $(P(\mathcal{E}),\mathcal{D})$ where $P(\mathcal{E})$ is the lattice of projection operators on the Hilbert space $\mathcal{E}$, and $\mathcal{D}$ is the space of decoherence functionals. A decoherence functional is a map $d:P(\mathcal{E})\times P(\mathcal{E})\rightarrow\mathbb{C}$ that satisfies the following conditions:

(1) *Hermiticity:* $d(\alpha,\beta)=d(\beta,\alpha)^*$ for all $\alpha,\beta\in P(\mathcal{E})$.
(2) *Positivity:* $d(\alpha,\alpha)\geqslant 0$ for all $\alpha\in P(\mathcal{E})$.
(3) *Null triviality:* $d(0,\alpha)=0$ for all $\alpha\in P(\mathcal{E})$.
(4) *Additivity:* if $\alpha\perp\beta$, then $d(\alpha\oplus\beta,\gamma)=d(\alpha,\gamma)+d(\beta,\gamma)$, for all $\gamma\in P(\mathcal{E})$.
(5) *Normalization:* $d(1,1)=1$.

The off-diagonal components of the decoherence functional represent the ''quantum interference'' between histories, while the diagonal components are interpreted as the probability that a particular history ''occurs.''

In this article we construct a quantum history theory of pure electrodynamics by two methods. In Sec. II we quantize the reduced classical history space to obtain a reduced history theory $(P(\mathcal{E}^{red}),d^{red})$. In Sec. III we augment the history fields with ghost fields and quantize the extended theory to obtain a representation of the extended algebra on the Becchi–Rouet–Stora–Tyutin- (BRST) extended history space $\mathcal{E}$. We then define $H^*(\Omega)$, the projection operator cohomology, and show that it has a natural lattice structure. In Sec. IV we define $\mathcal{D}_{gf}$, the space of gauge-fixed decoherence functionals, and show that each gauge-fixed decoherence functional in-

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duces a functional $\tilde{d}$ on $H^*(\Omega)$. Our main result is to show that the cohomological history theory $(H^*(\Omega),\tilde{d})$ is isomorphic (as a history theory) to the reduced history theory $(P(\mathcal{E}^{red}),d^{red})$.

II. RADIATION GAUGE QUANTIZATION

A. Preliminaries

The quantum history space arises as the representation space of a certain Lie group, the *history group*, and the associated Lie algebra is the histories analog of the canonical commutation relations. In the histories approach to scalar field theory proposed by Savvidou,[4] there is an inequivalent representation of the history group for each Lorentzian foliation of space–time. By a Lorentzian foliation of space–time we mean a foliation in which each leaf is a spacelike hyperplane. The *Schrödinger* picture fields satisfy the *covariant* history algebra

$$[\hat{\phi}_n(X),\hat{\phi}_n(X')]=0, \tag{1}$$

$$[\hat{\pi}_n(X),\hat{\pi}_n(X')]=0, \tag{2}$$

$$[\hat{\phi}_n(X),\hat{\pi}_n(X')]=i\hbar\,\delta^{(4)}(X-X'), \tag{3}$$

where n is a future pointing timelike unit vector labeling a particular Lorentzian foliation. The fields are genuine space–time fields under the action of a representation of the Poincare group.[4] This Poincare group acts as

$$\hat{\phi}_n(X)\mapsto\hat{\phi}_{\Lambda n}(\Lambda X) \tag{4}$$

and generates changes in the space–time foliation. Heisenberg picture fields can be defined using the time-averaged Hamiltonian which is also foliation dependent. These Heisenberg picture fields are of the form $\hat{\phi}_n(X,s)$, and there is a second representation of the Poincare group in which the boosts act in the ''internal'' time direction s, and leave the foliation fixed.

In a previous paper[5] we considered the extension of the classical analog of the above theory to the case of electrodynamics. It was argued that in order to preserve the two representations of the Poincare group, the history fields should have *five* components as opposed to the usual four. The extra component is associated with the internal time direction. It is important to note that the theory is not covariant under the action of the SO(3,2) isometry group of the space–time manifold $\mathcal{M}\times\mathbb{R}$, but only under the internal and external SO(3,1) subgroups. It was also shown in Ref. 5 how the extra component leads to an extra constraint, and thus to an enlarged gauge group.

The theory in Ref. 5 is concerned with history configuration fields $A^n_M(X)$, and their canonical momenta $E^M_n(X)$. The index M runs from 0 to 4, X is a four-vector and n is a future-pointing timelike unit vector which labels a particular foliation of space–time. These fields can be considered as vectors tangent to the space of embeddings of $\mathcal{M}$ into $\mathcal{N}\simeq\mathcal{M}\times\mathbb{R}$. The history fields satisfy the Poisson algebra

$$\{A^n_M(X),A^n_N(Y)\}=0, \tag{5}$$

$$\{E^M_n(X),E^N_n(Y)\}=0, \tag{6}$$

$$\{A^n_M(X),E^N_n(Y)\}=\delta^N_M\delta^{(4)}(X-Y). \tag{7}$$

The four-vector n can be embedded in $\mathcal{N}$, resulting in a five-vector $\tilde{n}^M$ given in coordinates by $(n,0)$. We also have the five-vector $\tilde{e}^M$ given by (0,1), and we use these vectors to decompose the fields into their temporal components

$$A^n_t(X):=\tilde{n}^MA^n_M(X),\quad A^n_s(X):=\tilde{e}^MA^n_M(X), \tag{8}$$

and similarly for the momentum field. The n-spatial projection tensor is defined as

$$ {}^{n}P^{M}_{N} = \delta^{M}_{N} - \tilde{e}^{M}\tilde{e}_{N} - \tilde{n}^{M}\tilde{n}_{N}, \tag{9} $$

and can be used to decompose fields on the five-dimensional space-time into their "n-spatial" components

$$ {}^{n}A_{M}(X) := {}^{n}P^{N}_{M}A^{n}_{N}(X). \tag{10} $$

We define "n-spatial tensors" in a similar way, e.g.,

$$ {}^{n}F_{MN}(X) := {}^{n}P^{R}_{M}\,{}^{n}P^{S}_{N}F^{n}_{RS}(X). \tag{11} $$

The first-class constraints can now be written as

$$ E^{s}_{n}(X) \approx 0, \tag{12} $$

$$ E^{t}_{n}(X) \approx 0, \tag{13} $$

$$ {}^{n}E^{M}_{\parallel}(X) \approx 0, \tag{14} $$

where the longitudinal component of the electric field is defined by

$$ {}^{n}E_{\parallel}(X) := {}^{n}\partial_{M}\,{}^{n}E^{M}(X). \tag{15} $$

B. Reduced state space

We now augment the constraints with the histories radiation gauge conditions:

$$ A^{n}_{s}(X) = 0, \tag{16} $$

$$ A^{n}_{t}(X) = 0, \tag{17} $$

$$ {}^{n}A_{\parallel}(X) = 0, \tag{18} $$

where

$$ {}^{n}A_{\parallel}(X) := \frac{{}^{n}\partial^{M}\,{}^{n}A_{M}(X)}{\Delta_{n}} \tag{19} $$

and $\Delta_{n} = {}^{n}\partial_{M}\,{}^{n}\partial^{M}$. The six equations (12)–(14) and (16)–(18) form a second class set of constraints and we can follow the usual procedure to find the Dirac brackets of the reduced history space $\mathcal{C}_{n}$. In terms of the transverse fields

$$ {}^{n}A^{\perp}_{M}(X) := {}^{n}A_{M}(X) - {}^{n}\partial_{M}\,{}^{n}A^{\parallel}(X), \tag{20} $$

$$ {}^{n}E^{M}_{\perp}(X) := {}^{n}E^{M}(X) - {}^{n}\partial^{M}\frac{{}^{n}E_{\parallel}(X)}{\Delta_{n}}, \tag{21} $$

they turn out to be

$$ \{{}^{n}A^{\perp}_{M}(X), {}^{n}A^{\perp}_{N}(Y)\}_{D} = 0, \tag{22} $$

$$ \{{}^{n}E^{M}_{\perp}(X), {}^{n}E^{N}_{\perp}(Y)\}_{D} = 0, \tag{23} $$

$$ \{{}^{n}A^{\perp}_{M}(X), {}^{n}E^{N}_{\perp}(Y)\}_{D} = ({}^{n}P^{N}_{M} - \Delta_{n}^{-1}\,{}^{n}\partial_{M}\,{}^{n}\partial^{N})\,\delta^{(4)}(X-Y). \tag{24} $$

The right hand side of this algebra has become explicitly foliation dependent with the non-covariant gauge choice. In the radiation gauge the time-averaged Hamiltonian is

$$H_n^0 = \int d^4X \left(\frac{1}{2} {}^nE_M^\perp \, {}^nE_\perp^M + \frac{1}{4} {}^nF_{MN} \, {}^nF^{MN} \right), \tag{25}$$

where $F_{MN}^n = 2\partial_{[M} A_{N]}^n$ and ${}^nF_{MN}$ is the corresponding n-spatial tensor [cf. Eq. (11)].

C. Quantization

We wish to find an irreducible representation of the commutator algebra

$$[{}^n\hat{A}_M^\perp(X), {}^n\hat{A}_N^\perp(Y)] = 0, \tag{26}$$

$$[{}^n\hat{E}_\perp^M(X), {}^n\hat{E}_\perp^N(Y)] = 0, \tag{27}$$

$$[{}^n\hat{A}_M^\perp(X), {}^n\hat{E}_\perp^N(Y)] = i\hbar ({}^nP_M^N - \Delta_n^{-1} \, {}^n\partial_M \, {}^n\partial^N) \delta^{(4)}(X-Y) \tag{28}$$

on a Hilbert space such that the radiation gauge quantum Hamiltonian is represented by a *self-adjoint* operator. The self-adjointness condition is required to select one of the infinitely many unitarily inequivalent representations of the infinite dimensional algebra (26)–(28). Such a representation exists on the bosonic Fock space $\mathcal{E}^{red} := \mathcal{F}_B[L^2(\mathbb{R}^4)] \otimes \mathcal{F}_B[L^2(\mathbb{R}^4)]$. This space is associated with annihilation and creation operators which obey the following algebra

$$[\hat{a}_a(X), \hat{a}_b(X')] = 0, \tag{29}$$

$$[\hat{a}_a(X), \hat{a}_b^\dagger(X')] = \hbar \, \delta_{ab} \delta^{(4)}(X-X'), \tag{30}$$

for $a = 1,2$. Using the Fourier transformed operators

$$\hat{a}_a^\dagger(K) = \frac{1}{(2\pi)^2} \int d^4X \hat{a}_a^\dagger(X) e^{iK\cdot X}, \tag{31}$$

$$\hat{a}_a(K) = \frac{1}{(2\pi)^2} \int d^4X \hat{a}_a(X) e^{-iK\cdot X}, \tag{32}$$

we define field operators satisfying the algebra (26)–(28) in the following way:

$${}^n\hat{A}_M^\perp(X) = \frac{1}{(2\pi)^2} \sum_{a=1}^2 \int \frac{d^4K}{\sqrt{2\omega_n(K)}} \, {}^n\epsilon_M^a(K) [\hat{a}_a(K) e^{-iK\cdot X} + \hat{a}_a^\dagger(K) e^{iK\cdot X}], \tag{33}$$

$${}^n\hat{E}_\perp^M(X) = \frac{1}{i(2\pi)^2} \sum_{a=1}^2 \int d^4K \sqrt{\frac{\omega_n(K)}{2}} \, {}^n\epsilon_a^M(K) [\hat{a}_a(K) e^{-iK\cdot X} - \hat{a}_a^\dagger(K) e^{iK\cdot X}]. \tag{34}$$

In the above expressions, K is a four-vector representing the four-momentum of a photon and $\omega_n(K)$ is the modulus of the n-spatial four vector $(\delta_\nu^\mu - n^\mu n_\nu) K^\nu$ with respect to the Minkowski metric. For each K, we define the five-vector $\tilde{K}$ to be the embedding of K into the five-dimensional space–time $\mathcal{N}$. In coordinates (X,s) the vector $\tilde{K}$ can be written as $(K,0)$. The five-vectors ${}^n\epsilon_a^M(K)$ are a pair of mutually orthogonal, n-spatial unit vectors which are in addition orthogonal to the vector ${}^n\tilde{K}^M = {}^nP_N^M \tilde{K}^N$. These vectors satisfy the following completeness relation:

$$\sum_{a=1}^2 {}^n\epsilon_M^a(K) \, {}^n\epsilon_a^N(K) = {}^nP_M^N - \frac{{}^n\tilde{K}_M \, {}^n\tilde{K}^N}{\omega_n(K)^2}. \tag{35}$$

This property ensures that the algebra defined by Eqs. (26)–(28) is satisfied. Using the fact that the polarization vectors are orthonormal,

$$ {}^{n}\epsilon_a^M(K)\,{}^{n}\epsilon_M^b(K)=\delta_a^b, \tag{36}$$

the normal-ordered time-averaged Hamiltonian can be written

$$\hat{H}_n^0=\sum_{a=1}^{2}\int d^4K\,\omega_n(K)\hat{a}_a^\dagger(K)\hat{a}_a(K). \tag{37}$$

This Hamiltonian generates translations in internal time, and it is easy to see that

$$e^{-is\hat{H}_n^0/\hbar}\hat{a}_a(K)e^{is\hat{H}_n^0/\hbar}=e^{is\omega_n(K)}\hat{a}_a(K). \tag{38}$$

Following the argument in Ref. 3, these transformations are unitarily implementable and we conclude that $\hat{H}_n^R$ exists as a self-adjoint operator in this representation. Therefore, for each n, there exists a unitarily inequivalent representation of the radiation gauge history algebra on the Fock space $\mathcal{E}^{red}$.

D. The decoherence functional

In the case when history propositions are realized as the lattice of projection operators on a Hilbert space $\mathcal{V}$, every decoherence functional d can be written in the form[6]

$$d(\alpha,\beta)=Tr_{\mathcal{V}\otimes\mathcal{V}}(\alpha\otimes\beta\Theta_d), \tag{39}$$

where Θ_d is an operator on $\mathcal{V}\otimes\mathcal{V}$. In fact Θ_d must satisfy certain conditions for d to be a decoherence functional.[6] In the case of the scalar field, the operator Θ is dependent on the foliation, and can be written[4,12]

$$\Theta_n=\langle 0|\rho_{-\infty}|0\rangle(\mathcal{SU})_n^\dagger\otimes(\mathcal{SU})_n. \tag{40}$$

The quantum history space for the scalar field is the bosonic Fock space $\mathcal{F}_B[L^2(\mathbb{R}^4)]$. To each operator O, on the base space $L^2(\mathbb{R}^4)$, there is an associated operator on $\mathcal{F}_B[L^2(\mathbb{R}^4)]$ defined by

$$\Gamma(O)=O\oplus(O\otimes O)\oplus\cdots. \tag{41}$$

Using this construction, the operator $(\mathcal{SU})_n$ can be written

$$(\mathcal{SU})_n=\Gamma(1+i\sigma_n), \tag{42}$$

where $\sigma_n=n^\mu\partial_\mu+(-\Delta_n+m^2)^{1/2}$ is an operator on the base Hilbert space $L^2(\mathbb{R}^4)$. The operator σ_n is related to the canonical history action S_n in the following simple way:[4]

$$e^{isS_n}=\Gamma(e^{is\sigma_n}). \tag{43}$$

Equation (43) can be used to *define* the decoherence functional corresponding to a given action operator S on a Fock space $\mathcal{F}=\mathcal{F}_B[\mathcal{H}]$. First S defines σ, the "generator" of the decoherence functional, which is the operator on $\mathcal{H}$ given by

$$e^{isS}=\Gamma(e^{is\sigma}). \tag{44}$$

Now the decoherence functional is defined by the operator on $\mathcal{F}\otimes\mathcal{F}$ given by

$$\Theta_S=\langle 0|\rho_{-\infty}|0\rangle\Gamma(1+i\sigma)^\dagger\otimes\Gamma(1+i\sigma). \tag{45}$$

The reduced canonical history action of electrodynamics in the radiation gauge is

$$S_n^{red} = \int d^4X ({}^n\hat{E}_\perp^M \partial_n^t {}^n\hat{A}_M^\perp - \hat{H}_n^0), \tag{46}$$

where $\partial_n^t := \tilde{n}^M \partial_M$. The corresponding generator of the decoherence functional is the operator σ_n^{red}, defined on vectors of the form $f \otimes g$ in the base Hilbert space $\mathcal{H}^{red} = L^2(\mathbb{R}^4) \otimes L^2(\mathbb{R}^4)$ by

$$\sigma_n^{red}(f \otimes g) = (n^\mu \partial_\mu - \Delta_n^{1/2}) f \otimes (n^\mu \partial_\mu - \Delta_n^{1/2}) g, \tag{47}$$

and extended to an operator on $\mathcal{H}^{red}$ by linearity. The associated decoherence functional is denoted d_n^{red}. The pair $(P(\mathcal{E}^{red}), d_n^{red})$ is the reduced history theory of pure quantum electrodynamics with respect to the foliation n.

III. BRST COHOMOLOGY

As shown in the previous section, electrodynamics can be quantized starting from the reduced state space. This is because the reduced state space has a simple structure, in particular it is a linear space. This is not the case for other constrained field theories such as Yang–Mills theory and gravity. For such theories another, more general, approach is needed. The BRST formalism[7] is a powerful approach to the quantization of constrained systems, and can be formulated using rigorous operator methods. Motivated by these considerations we develop the BRST approach to the quantum theory of histories electrodynamics. In this section we follow closely the notation of Ref. 7.

A. Classical BRST cohomology

The central idea in the BRST formalism is to extend the state space by including fermionic ''ghost'' fields. The extended state space maintains manifest covariance and locality, unlike the reduced state space approach. The BRST charge is constructed from the ghost fields and the constraints and, in the classical case, is a functional on the extended state space. The BRST charge generates *nilpotent* canonical transformations on the extended state space. The physical degrees of freedom are identified with the corresponding set of cohomology classes. The idea is that the ghost fields cancel out the gauge fields in the cohomology.

We begin by briefly recalling the BRST approach to the standard classical theory of electrodynamics as given in Chap. 19 of Ref. 7. We have fields $E^\mu(\underline{x})$ and $A_\mu(\underline{x})$ satisfying the algebra

$$\{A_\mu(\underline{x}), E^\nu(\underline{x}')\} = \delta_\mu^\nu \delta^{(3)}(\underline{x} - \underline{x}'), \tag{48}$$

and a pair of constraints $E^0(\underline{x}) \approx 0$ and $\partial_i E^i(\underline{x}) \approx 0$. Corresponding to the first constraint we add a ghost pair $\eta(\underline{x}), \mathcal{P}(\underline{x})$ with

$$\{\mathcal{P}(\underline{x}), \eta(\underline{x}')\} = -\delta^{(3)}(\underline{x} - \underline{x}'), \tag{49}$$

where the bracket is *symmetric* representing the fact that the ghost fields are fermionic. The Lagrange multiplier field $A_0(\underline{x})$ and its conjugate momentum are associated with an antighost field $\overline{C}(\underline{x})$ and conjugate momentum $\rho(\underline{x})$ satisfying

$$\{\rho(\underline{x}), \overline{C}(\underline{x}')\} = -\delta^{(3)}(\underline{x} - \underline{x}'). \tag{50}$$

The BRST charge is

$$\Omega = \int d^3\underline{x} [-i\rho E^0 + \eta \partial_i E^i], \tag{51}$$

and Ω generates *nilpotent* canonical transformations which are explicitly given in Ref. 7, and we denote by τ, that is $\tau(F) := \{\Omega, F\}$. A functional F is said to be BRST-closed if and only if

$$\tau(F)=0, \tag{52}$$

and a functional G is said to be BRST-exact if and only if

$$G=\tau(G'), \tag{53}$$

for some functional G'. By the nilpotency of τ closed functionals are exact, but the converse is not necessarily true, and the set of functionals which are closed but not exact is isomorphic to the set of functionals on the reduced state space. In addition,[7] there is a natural Poisson algebra defined on the set of cohomology classes which is a Poisson subalgebra of the extended Poisson algebra, and is isomorphic to the Poisson algebra of the reduced classical history space.

This analysis is easy to extend to the classical history theory of electrodynamics. Corresponding to the constraint ${}^nE_{\|}(X)\approx 0$ we introduce a pair of fermionic, scalar ghost history fields $\eta_n^1(X)$ and $\mathcal{P}_n^1(X)$ which satisfy the algebra

$$\{\mathcal{P}_n^1(X),\eta_n^1(X')\}=-\delta^{(4)}(X-X'). \tag{54}$$

In addition we have two Lagrange multipliers in the history theory so we add two antighost fields $C_a^n(X)$ $(a\in\{1,2\})$, along with their conjugate momenta $\rho_n^a(X)$. These fields satisfy

$$\{\rho_n^a(X),C_b^n(X')\}=-\delta_b^a\delta^{(4)}(X-X'). \tag{55}$$

In this way the ring of functions on the extended classical history space is given the structure of a graded Lie algebra. The history BRST charge Ω_n' is defined as

$$\Omega_n'=\int d^4X[-i\rho_n^1E_n^t-i\rho_n^2E_n^s+\eta_n^1\,{}^nE_{\|}], \tag{56}$$

and generates canonical transformations denoted by τ^n. The transformations are

$$\tau^n({}^nA^{\|})=\eta_n^1,\quad \tau^n(\eta_n^1)=0,\quad \tau^n(\mathcal{P}_n^1)={}^nE^{\|},\quad \tau^n({}^nE^{\|})=0, \tag{57}$$

$$\tau^n(A_s^n)=-i\rho_n^1,\quad \tau^n(A_t^n)=-i\rho_n^2,\quad \tau^n(\rho_n^1)=0,\quad \tau^n(\rho_n^2)=0, \tag{58}$$

$$\tau^n(C_n^1)=iE_n^s,\quad \tau^n(C_n^2)=iE_n^t,\quad \tau^n(E_n^s)=0,\quad \tau^n(E_n^t)=0, \tag{59}$$

$$\tau^n({}^nA^{\perp})=0,\quad \tau^n({}^nE_{\perp})=0. \tag{60}$$

From these transformations it is clear that τ^n is nilpotent, and thus defines a cohomology on the space of functionals on the BRST-extended classical history space. The classical history BRST cohomology, $H_{cl}^*(\Omega_n')$, is defined to be the space of equivalence classes of BRST-closed functionals modulo BRST-exact ones. The only fields which are closed but not exact are ${}^nA^{\perp}$ and ${}^nE_{\perp}$, and so the cohomology classes are in bijective correspondence with functionals of the transverse fields. Thus $H_{cl}^*(\Omega_n')$ is isomorphic to the space of functionals on the reduced classical history space.

B. Operator quantization

The BRST operator quantization of standard electrodynamics proceeds by expanding the quantum fields in terms of operators which satisfy the algebra of creation and annihilation operators, thus defining a representation of the field algebra on a Fock space. Then, using the quantum BRST charge $\hat{\Omega}$, which is the operator corresponding to the functional in Eq. (51), a cohomology can be defined on operators on the quantum Hilbert space as follows. An operator $\hat{O}$ is defined to be *BRST-closed* if and only if

$$[\hat{\Omega},\hat{O}]=0, \tag{61}$$

and an operator $\hat{Q}$ is *BRST-exact* if and only if

$$\hat{Q}=[\hat{\Omega},\hat{W}] \tag{62}$$

for some operator $\hat{W}$. Because $\hat{\Omega}$ generates nilpotent transformations and the commutator satisfies the graded Jacobi identity, a BRST-exact operator is necessarily BRST-closed. However, the converse is not true and two BRST-closed operators $\hat{O}$ and $\hat{O}'$ are defined to be BRST-equivalent if $\hat{O}'=\hat{O}+\hat{Q}$ for some BRST-exact operator $\hat{Q}$. The *operator cohomology* of $\hat{\Omega}$, $H^{*}_{op}(\hat{\Omega})$, is defined to be the set of equivalence classes of closed operators modulo this equivalence relation. The expansion of the fields in terms of creation and annihilation operators is given in Ref. 7, and it follows that the quantum BRST charge can be written in the form

$$\hat{\Omega}=\int d^3\underline{k}[\hat{c}^{\dagger}(\underline{k})\hat{a}(\underline{k})+\hat{a}^{\dagger}(\underline{k})\hat{c}(\underline{k})]. \tag{63}$$

Now the nonphysical field modes ''cancel out'' the ghost modes in the cohomology or, more precisely, the operator cohomology is isomorphic to the set of operators on the reduced quantum Hilbert space. This is a consequence of a general result known as the ''quartet mechanism'' [7] which applies to any quantum theory in which the BRST operator is the sum of terms of the form (63).

C. Quantum history theory in quartet form

For the Fock space quantization of a BRST-extended theory it is necessary that the constraints come in pairs allowing the definition of creation and annihilation operators as complex linear combinations of pairs of fields. In the history theory there are three constraints which cannot be grouped in pairs for the Fock space quantization. To proceed we include an extra Lagrange multiplier along with the associated momenta and ghosts. More precisely, we introduce a bosonic scalar field $\hat{\lambda}_n(X)$, the Lagrange multiplier corresponding to the constraint $\hat{E}^s_n(X)\approx 0$. Its canonical momentum is denoted $\hat{B}_n(X)$ and is constrained to vanish

$$\hat{B}_n(X)\approx 0. \tag{64}$$

The associated ghost pair is $(\hat{\eta}^2_n,\hat{\mathcal{P}}^2_n)$. Now the fields do form ''quartets,'' and the results of Ref. 7 can be applied. The detailed transformations of the fields into the ''quartet'' form have been relegated to the Appendix. The important result is that the bosonic fields can be defined in terms of six pairs of bosonic creation and annihilation operators:

$$[\hat{a}_a(K),\hat{b}^{\dagger}_b(K')]=-\hbar\,\delta_{ab}\delta^{(4)}(K-K'), \tag{65}$$

$$[\hat{b}_a(K),\hat{a}^{\dagger}_b(K')]=-\hbar\,\delta_{ab}\delta^{(4)}(K-K'), \tag{66}$$

$$[{}^{\perp}\hat{a}_a(K),{}^{\perp}\hat{a}^{\dagger}_b(K')]=\hbar\,\delta_{ab}\delta^{(4)}(K-K'), \tag{67}$$

for $a,b\in\{1,2\}$. So we have a representation of the bosonic part of the BRST-extended history algebra on the Fock space $\mathcal{E}^B$ which is defined as the tensor product of six copies of the bosonic Fock space $\mathcal{F}_B[L^2(\mathbb{R}^4)]$. Similarly, the fermionic fields can be expanded in terms of four pairs of fermionic creation and annihilation operators, which satisfy the anti-commutators

$$[\hat{c}_a(K),\hat{e}^{\dagger}_b(K')]=-\hbar\,\delta_{ab}\delta^{(4)}(K-K'), \tag{68}$$

$$[\hat{e}_a(K),\hat{c}^{\dagger}_b(K')]=-\hbar\,\delta_{ab}\delta^{(4)}(K-K'), \tag{69}$$

where $a,b\in\{1,2\}$. In this way we have a representation of the fermionic part of the BRST-extended history algebra on the Fock space $\mathcal{E}^F$, which is defined as the tensor product of four copies of the fermionic Fock space $\mathcal{F}_F[L^2(\mathbb{R}^4)]$. The whole algebra is represented on the space $\mathcal{E}=\mathcal{E}^B\otimes\mathcal{E}^F$, which we call the BRST-extended quantum history space.

D. Quantum operator cohomology

The extended BRST charge is

$$\hat{\Omega}_n=\int d^4X[-i\hat{\rho}^1_n\hat{E}^s_n+\hat{\eta}^1_n\,{}^n\hat{E}_\parallel-i\hat{\rho}^2_n\hat{E}^t_n+\hat{\eta}^2_n\hat{B}_n], \tag{70}$$

and in terms of oscillators it takes the n-independent form

$$\hat{\Omega}=\sum_{a=1}^{2}\int d^4K[\hat{c}^\dagger_a(K)\hat{a}_a(K)+\hat{a}^\dagger_a(K)\hat{c}_a(K)]. \tag{71}$$

The anti-Hermitian ghost number operator $\hat{\mathcal{G}}$ is defined in terms of oscillators as

$$\hat{\mathcal{G}}=\sum_a\int d^4K(\hat{c}^\dagger_a(K)\hat{e}_a(K)-\hat{e}_a(K)^\dagger\hat{c}_a(K)). \tag{72}$$

Any operator $\hat{O}$ on $\mathcal{E}$ can be decomposed in components of definite ghost number

$$\hat{O}=\sum_g\hat{O}_g,\quad [\hat{\mathcal{G}},\hat{O}_g]=g\hat{O}_g,\quad g\in\mathbb{Z}. \tag{73}$$

It follows from these definitions that all bosonic fields are of ghost number zero, the fields $\hat{\eta}^a$ and $\hat{\rho}^a$ are of ghost number $+1$, and $\hat{\mathcal{P}}^a$ and $\hat{C}^a$ are of ghost number -1. Vectors in the nonzero eigenspaces of $\hat{\mathcal{G}}$ have an ill-defined scalar product, therefore a ghost number zero condition is often imposed on the physical states. However, in the Fock space quantization the ghost number zero condition is automatically satisfied in the cohomology classes.

From Eq. (70) it is clear that for the case of histories electrodynamics the operators $\hat{\eta}^a_n,\hat{\rho}^a_n,{}^n\hat{E}_\parallel,\hat{E}^s_n,\hat{E}^t_n,\hat{B}_n,{}^n\hat{A}^\perp,{}^n\hat{E}_\perp$ are closed. Similarly, the operators $\hat{\eta}^a_n,\hat{\rho}^a_n,{}^n\hat{E}_\parallel,\hat{E}^s_n,\hat{E}^t_n,\hat{B}_n$ are exact; for example, the smeared ghost field can be written

$$\hat{\eta}^1_n(f)=[\hat{\Omega},\hat{A}^\parallel_n(f)]. \tag{74}$$

The transverse field operators are closed but not exact.

E. Projection operator cohomology

In a history theory it is projection operators that appear in the decoherence functional, and operators which are not projectors lack a direct physical interpretation. In the equivalence classes of $H^*_{op}(\hat{\Omega})$, projection operators are identified with operators which are not projection operators. This identification is unnatural from the histories perspective, so in this subsection we define an equivalence relation directly on the lattice of projectors. We then use this equivalence relation to define $H^*(\hat{\Omega})$, the *projection operator cohomology* associated with $\hat{\Omega}$. Finally we show that $H^*(\hat{\Omega})$ can be given the structure of a lattice, and that this lattice is isomorphic to the lattice of projection operators on the reduced quantum history space.

Definition 3.5.1: Given two closed projectors α and β, we say that "α is an exact fine-graining of β," written $\alpha\preccurlyeq\beta$, if and only if $\beta=\alpha+\gamma$ for some projection operator γ which is exact (i.e., $\gamma=[\hat{\Omega},\hat{Q}]$ for some operator $\hat{Q}$) and disjoint to α.

The relation $\preccurlyeq$ is a partial order. The *primitive* part of α is denoted α_0 and is defined as the limit of exact fine-grainings of α. A unique α_0 exists for each closed α because $\preccurlyeq$ is a partial order. If α is exact, then α_0 is the zero projector. If α is closed but not exact, then α_0 projects onto the spectrum of a closed but not exact field operator. For histories electrodynamics we have seen that the closed but not exact field operators are the transverse field operators, and so closed primitive projectors are in bijective correspondence with elements of $P(\mathcal{E}^{red})$.

Definition 3.5.2: Two BRST-closed projection operators α and β are said to be BRST-equivalent *if and only if $\alpha_0=\beta_0$.*

The projection operator cohomology $H^*(\hat{\Omega})$ is defined as the space of closed projection operators modulo this equivalence relation, and elements of $H^*(\hat{\Omega})$ are identified with *physical* propositions. Given a primitive projection operator α_0, the equivalence class containing α_0 is the collection of all exact coarse-grainings of α_0. The statement "α is an *exact fine-graining* of β" is equivalent to the statement "β is an *exact coarse-graining* of α." Let $[\alpha]$ denote the equivalence class containing the closed projector α. The map $\pi:[\alpha]\mapsto\alpha_0$ is well-defined on $H^*(\hat{\Omega})$, and is in fact an isomorphism between $H^*(\hat{\Omega})$ and $P(\mathcal{E}^{red})$; the inverse is given by $\pi^{-1}:\alpha_0\mapsto[\alpha_0]$. In order to give $H^*(\hat{\Omega})$ the structure of a lattice, we need to examine the geometry of the linear subspaces associated to closed and exact projection operators.

Definition 3.5.3: A BRST-closed subspace $L\subset\mathcal{E}$ is a topologically closed linear subspace of $Ker(\hat{\Omega})$.

Proposition 3.5.4: BRST-closed projection operators are in bijective correspondence with BRST-closed subspaces of $\mathcal{E}$.

Proof: Each projection operator α is associated with a topologically closed linear subspace $L_\alpha\subset\mathcal{E}$. If α is a BRST-closed projection operator, i.e., $[\hat{\Omega},\alpha]=0$, then by writing α in Dirac notation as

$$\alpha=\sum_i |l_i\rangle\langle l_i|, \tag{75}$$

where $|l_i\rangle$ is a basis of L_α, it follows from the independence of the basis vectors and the Hermiticity of $\hat{\Omega}$ that $\hat{\Omega}|l\rangle=0$ for all $|l\rangle\in L_\alpha$. Therefore $L_\alpha\subset\mathrm{Ker}(\hat{\Omega})$.

Conversely, each BRST-closed subspace is associated with a BRST-closed projection operator because $\hat{\Omega}$ is self-adjoint. □

In the case of histories electrodynamics BRST-closed subspaces are spanned by vectors created by the operators ${}^{\perp}\hat{a}_a^\dagger,\hat{a}_a^\dagger,\hat{c}_a^\dagger$ acting on the cyclic vacuum state.

Definition 3.5.5: A BRST-exact subspace $M\subset\mathcal{E}$ is a topologically closed linear subspace of $\mathrm{Im}(\hat{\Omega})$.

Proposition 3.5.6: BRST-exact projection operators are in bijective correspondence with BRST-exact subspaces of $\mathcal{E}$.

Proof: A BRST-exact projection operator can be written in the form $\gamma=[\hat{\Omega},\hat{Q}]$ for some operator $\hat{Q}$. γ is closed, and so is associated with a BRST-closed subspace $M_\gamma\subset\mathcal{E}$. Now

$$\gamma|m\rangle=[\hat{\Omega},\hat{Q}]|m\rangle=\hat{\Omega}(\hat{Q}|m\rangle)\quad\forall|m\rangle\in M_\gamma \tag{76}$$

because $\hat{\Omega}|m\rangle=0$. However, $\gamma|m\rangle=|m\rangle$ for any $|m\rangle\in M_\gamma$ so

$$|m\rangle=\hat{\Omega}(\hat{Q}|m\rangle)\quad\forall|m\rangle\in M_\gamma, \tag{77}$$

and hence $M_\gamma\subset\mathrm{Im}(\hat{\Omega})$.

Conversely, each BRST-exact subspace M with basis $|m_i\rangle$ is associated with an exact projection operator γ,

$$\gamma=\sum_i |m_i\rangle\langle m_i|=\left[\hat{\Omega},\sum_i |u_{m_i}\rangle\langle m_i|\right], \tag{78}$$

where $|u_{m_i}\rangle$ is any vector such that $\hat{\Omega}|u_{m_i}\rangle=|m_i\rangle$. □

In the case of histories electrodynamics BRST-exact subspaces are spanned by vectors created by the operators $\hat{a}_a^\dagger,\hat{c}_a^\dagger$ on the vacuum state.

Definition 3.5.7: A primitive subspace $R\subset\mathcal{E}$ is a BRST-closed subspace with no BRST-exact proper subspaces. The closure of the union of all primitive subspaces is denoted $\mathcal{E}_0$.

Proposition 3.5.8: Primitive projection operators are in bijective correspondence with primitive subspaces of $\mathcal{E}$.

Proof: Let α_0 be a primitive projector. Then the only exact fine graining of α_0 is α_0 itself. This implies that the linear subspace associated with α_0 has no BRST-exact proper subspaces.

Conversely, because a primitive subspace has no BRST-exact proper subspaces it follows that the corresponding projection operator must be a limit of exact fine-grainings, and thus primitive.□

In the case of histories electrodynamics primitive subspaces are spanned by vectors created by the action of the transverse creation operators ${}^\perp\hat{a}_a^\dagger$ on the vacuum state.

From the above discussion it follows that $\mathcal{E}_0$ and $\mathrm{Im}(\hat{\Omega})$ are disjoint, and that the closure of $\mathcal{E}_0\cup\mathrm{Im}(\hat{\Omega})$ is $\mathrm{Ker}(\hat{\Omega})$. Therefore every exact projector is disjoint to every primitive projector, and $\mathrm{id}_0+\mathrm{id}_{\mathrm{Im}}=\mathrm{id}_{Ker}$, where $\mathrm{id}_0,\mathrm{id}_{\mathrm{Im}}$ and id_{Ker} are the identity operators on $\mathcal{E}_0,\mathrm{Im}(\hat{\Omega})$ and $\mathrm{Ker}(\hat{\Omega})$, respectively. These results can be used to prove the following theorem.

Theorem 3.5.9: *(i) The lattice $P(Ker(\hat{\Omega}))$ induces a lattice structure on $H^*(\hat{\Omega})$ by*

$$[\alpha]\wedge[\beta]:=[\alpha\wedge\beta], \tag{79}$$

$$[\alpha]\vee[\beta]:=[\alpha\vee\beta], \tag{80}$$

$$\neg[\alpha]:=[\neg\alpha]. \tag{81}$$

(ii) The map π is a lattice isomorphism of $H^*(\hat{\Omega})$ and $P(\mathcal{E}^{red})$.

Proof:

(i) We have to show that the definitions give the same results when evaluated on different members of an equivalence class. We define the maximal exact part of α to be the unique exact projector γ_α such that $\alpha=\alpha_0+\gamma_\alpha$. Every exact subspace is orthogonal to every primitive subspace so $\alpha\wedge\beta=\alpha_0\wedge\beta_0+\gamma_\alpha\wedge\gamma_\beta$. The intersection of two exact subspaces is exact so $\gamma_\alpha\wedge\gamma_\beta$ is exact, and $[\alpha\wedge\beta]=[\alpha_0\wedge\beta_0]$. In a similar way we have $[\alpha\vee\beta]=[\alpha_0\vee\beta_0]$. Finally, consider $\neg\alpha=\mathrm{id}_{Ker}-(\alpha_0+\gamma_\alpha)$ which can be written $\neg\alpha=(\mathrm{id}_0-\alpha_0)+(\mathrm{id}_{\mathrm{Im}}-\gamma_\alpha)$. Now $\mathrm{id}_{\mathrm{Im}}-\gamma_\alpha$ is exact, so $[\neg\alpha]=[\mathrm{id}_0-\alpha_0]$. Similarly we have $\neg\alpha_0=(\mathrm{id}_0-\alpha_0)+\mathrm{id}_{\mathrm{Im}}$ so $[\neg\alpha_0]=[\mathrm{id}_0-\alpha_0]=[\neg\alpha]$.

(ii) It is straightforward to check that
(a) $\pi([\alpha]\wedge[\beta])=\pi[\alpha]\wedge\pi[\beta]$,
(b) $\pi([\alpha]\vee[\beta])=\pi[\alpha]\vee\pi[\beta]$, and
(c) $\pi(\neg[\alpha])=\neg\pi[\alpha]$,
where the lattice operations on the right hand side of the above equations are defined in $P(\mathcal{E}^{red})$. □

Thus the projection operator cohomology is isomorphic to the lattice of projection operators on the reduced history space. In order to show that the corresponding history theories are ''the same'' we first investigate the space of decoherence functionals on the BRST-extended quantum history space.

IV. GAUGE-FIXED DECOHERENCE FUNCTIONALS

To each gauge-fixed action operator on $\mathcal{E}$, there corresponds a gauge-fixed decoherence functional. The gauge-fixed decoherence functionals assign nontrivial values to propositions regarding the gauge and ghost fields. However, as we shall see, each gauge-fixed decoherence functional induces a well-defined functional on $H^*(\hat{\Omega})$ in such a way that the resulting history theory is equivalent to the reduced quantum history theory.

A. Radiation and Feynman gauges

We begin by giving two explicit examples of gauge-fixed decoherence functionals. The radiation gauge corresponds to the following canonical action

$$\hat{S}_n^R = \hat{V}_n - \hat{H}_n^0, \tag{82}$$

where the Louiville operator is the sum of three parts:

(1) a gauge-invariant part $\hat{V}_n^0$,

$$\hat{V}_n^0 = \int d^4X \, {}^n\hat{E}_\perp^M \partial_n^t \, {}^n\hat{A}_M^\perp, \tag{83}$$

(2) a ghost part

$$\hat{V}_n^{gh} = \int d^4X \sum_{a=1}^{2} (\hat{\mathcal{P}}_n^a \partial_n^t \hat{\eta}_n^a + \hat{\rho}_n^a \partial_n^t \hat{C}_n^a), \tag{84}$$

(3) a gauge part

$$\hat{V}_n^{ga} = \int d^4X (\hat{E}_n^t \partial_n^t \hat{A}_t^n + \hat{E}_n^s \partial_n^t \hat{A}_s^n + {}^n\hat{E}_\parallel^M \partial_n^t \, {}^n\hat{A}_M^\parallel + \hat{B}_n \partial_n^t \hat{\lambda}_n). \tag{85}$$

The gauge-invariant Hamiltonian $\hat{H}_n^0$ is given by

$$\hat{H}_n^0 = \int d^4X \left(\frac{1}{2} \, {}^n\hat{E}_M^\perp \, {}^n\hat{E}_\perp^M + \frac{1}{4} \, {}^n\hat{F}_{MN} \, {}^n\hat{F}^{MN} \right). \tag{86}$$

Using an argument similar to that in Sec. II, it follows that the normal ordered Hamiltonian exists as a self-adjoint operator on $\mathcal{E}$. The Louiville operator also exists, and therefore so does the radiation gauge action $\hat{S}_n^R$. If the gauge and ghost fields vanish initially, then they vanish identically on the extrema of this action. However, note that the extrema of this action satisfy the constraints if and only if the constraints are satisfied initially.

Let $\mathcal{H}_0 \simeq L^2(\mathbb{R}^4) \otimes L^2(\mathbb{R}^4)$ denote the base Hilbert space of the primitive Fock space $\mathcal{E}_0$, i.e., $\mathcal{E}_0 = \mathcal{F}_B[\mathcal{H}_0]$. Then the generator of the decoherence functional associated with the radiation gauge action acts on vectors $f \otimes g \in \mathcal{H}_0$ as

$$\sigma_n^R(f \otimes g) = \left(n^\mu \partial_\mu - \Delta_n^{1/2} \right) f \otimes \left(n^\mu \partial_\mu - \Delta_n^{1/2} \right) g, \tag{87}$$

and is extended to an operator on $\mathcal{H}_0$ by linearity. The radiation gauge Hamiltonian commutes with the gauge and ghost fields. Therefore, as argued in Ref. 9, projectors onto the gauge and ghost fields form a canonical consistent set and the probabilities assigned to these projectors are just the probability in the initial state. This implies that if either ϵ or κ is a projector onto subspaces of the orthogonal complement of $\mathcal{E}_0$, and the initial density matrix contains no gauge or ghost modes, then

$$d^R(\epsilon, \kappa) = 0. \tag{88}$$

This completes the definition of d^R.

In the "Feynman gauge" all fields satisfy the wave equation internally. Let $\mathcal{H}$ denote the base Hilbert space of the BRST-extended quantum history space $\mathcal{E}$. A vector in $\mathcal{H}$ is a linear combination of homogeneous vectors of the form

$$v = \otimes_{i=1}^{10} v_i, \tag{89}$$

where $v_i \in L^2(\mathbb{R}^4)$. The generator of the Feynman gauge decoherence functional is defined on homogeneous vectors by

$$\sigma_n^F v = \otimes_{i=1}^{10} (n^\mu \partial_\mu - \Delta_n^{1/2}) v_i, \tag{90}$$

and is extended to an operator on $\mathcal{H}$ by linearity.

B. Gauge transformations

In this subsection we investigate gauge transformations. For simplicity we consider the constraint $\hat{E}_n^t \approx 0$, but analogous remarks apply to the other three constraints.

In the operator cohomology, the constraint $\hat{E}_n^t \approx 0$ is identified with operators of the form

$$\hat{D}_n^t = \hat{E}_n^t + [\hat{\Omega}, \hat{Q}]. \tag{91}$$

The operator $\hat{D}_n^t$ generates gauge transformations in the gauge field $\hat{A}_t^n$, and also in the ghost fields. We require that the the ghost number zero eigenspace of $\hat{\mathcal{G}}$ is mapped into itself under gauge transformations, which implies that $[\hat{\mathcal{G}}, \hat{D}_n^t] = 0$. As $\hat{\Omega}$ is a ghost number 1 operator, the operator $\hat{Q}$ must be of ghost number -1. In addition we choose $\hat{Q}$ to be self-adjoint, so that $\hat{D}_n^t$ generates unitary transformations.

$\hat{D}_n^t$ is exact, and can be written as $[\hat{\Omega}, \hat{G}_n]$ where $\hat{G}_n = \hat{C}_n^1 + \hat{Q}$. It follows from the Jacobi identity that

$$[\hat{D}_n^t, \hat{O}] = [[\hat{\Omega}, \hat{G}_n], \hat{O}] = [[\hat{G}_n, \hat{O}], \hat{\Omega}], \tag{92}$$

if $\hat{O}$ is a closed operator. Thus closed operators are mapped into exact operators by infinitesimal gauge transformations. Under finite gauge transformations, closed operators transform as

$$\hat{O} \mapsto \hat{U} \hat{O} \hat{U}^\dagger = \hat{O} + [\hat{\Omega}, \hat{W}], \tag{93}$$

where $\hat{W}$ is a ghost number -1 operator. Therefore, gauge transformations act trivially on the equivalence classes of the operator cohomology.

As the gauge transformations are unitary, they map projection operators onto projection operators and, because $\mathcal{E}_0$ and $\mathrm{Im}(\hat{\Omega})$ are disjoint, exact self-adjoint operators commute with primitive projectors. Therefore, the action of a gauge transformation on a BRST-closed projector, $\alpha = \alpha_0 + \gamma_\alpha$, is

$$\alpha \mapsto \hat{U} \alpha \hat{U}^\dagger = \alpha_0 + \hat{U} \gamma_\alpha \hat{U}^\dagger. \tag{94}$$

This shows that the gauge group acts trivially on $H^*(\hat{\Omega})$, and that primitive projectors are *gauge invariant*.

There is also a natural unitary action of the gauge transformations on the space of decoherence functionals. The decoherence functional d is associated with an operator on $\mathcal{E} \otimes \mathcal{E}$, denoted Θ_d. Gauge transformations act on Θ_d as $\Theta_d \mapsto \Theta_{d'}$ where $\Theta_{d'} = U \otimes U \Theta_d U^\dagger \otimes U^\dagger$. As shown in Ref. 8, the operator $\Theta_{d'}$ is indeed associated with a *bone fide* decoherence functional d'. We say that the decoherence functionals d and d' are *related by the gauge transformation* U.

Definition 4.2.1: The collection of all decoherence functionals related to the radiation gauge decoherence functional, d^R, by a gauge transformation is denoted $\mathcal{D}_{gf}$ and called the space of gauge-fixed decoherence functionals.

V. GAUGE INVARIANCE

We now fix a particular foliation, drop the n-label, and use coordinates adapted to the foliation. Let $\mathcal{D}$ denote the space of decoherence functionals associated with the quantum history space $\mathcal{E}$. A physical symmetry of a *history* quantum theory (PSHQT) realized on the Hilbert space $\mathcal{E}$ is defined in Ref. 8 as an affine one-to-one map

$$P(\mathcal{E})\otimes P(\mathcal{E})\times\mathcal{D}\rightarrow P(\mathcal{E})\otimes P(\mathcal{E})\times\mathcal{D}, \tag{95}$$

$$([\alpha\otimes\beta],\Theta)\mapsto([\alpha\otimes\beta]',\Theta'), \tag{96}$$

that preserves the pairing between history propositions and operators associated with decoherence functionals, i.e.,

$$tr_{\mathcal{E}\otimes\mathcal{E}}([\alpha\otimes\beta]\Theta)=tr_{\mathcal{E}\otimes\mathcal{E}}([\alpha\otimes\beta]'\Theta'). \tag{97}$$

Schreckenberg[8] proved the following histories analogue of Wigners theorem:

Theorem 5.0.1: *Every PSHQT can be induced by a unitary or antiunitary operator $\hat{U}$ on $\mathcal{E}$ in the sense that each PSHQT can be written as*

$$[\alpha\otimes\beta]\mapsto\hat{U}\otimes\hat{U}[\alpha\otimes\beta]\hat{U}^\dagger\otimes\hat{U}^\dagger, \tag{98}$$

$$\Theta\mapsto\hat{U}\otimes\hat{U}\Theta\hat{U}^\dagger\otimes\hat{U}^\dagger, \tag{99}$$

for some unitary or antiunitary operator $\hat{U}$. Conversely, every transformation of the form (98) and (99) for unitary or antiunitary $\hat{U}$ induces a PSHQT.

We have seen that gauge transformations act unitarily on projection operators and on the space of decoherence functionals. Therefore gauge transformations induce a PSHQT and we can use the histories analog of Wigner's theorem. The following is an immediate consequence:

Proposition 5.0.2.: For any gauge-fixed decoherence functional $d\in\mathcal{D}_{gf}$, and any two primitive projectors $\alpha_0,\beta_0\in P(\mathcal{E}_0)$,

$$d(\alpha_0,\beta_0)=d^{red}(\alpha_0,\beta_0). \tag{100}$$

Proof: Since $d\in\mathcal{D}_{gf}$, it is related to d^R by a gauge transformation. We denote the unitary operator associated with this gauge transformation by $\hat{U}_d$. The primitive projectors α_0 and β_0 satisfy $\hat{U}_d\alpha_0\hat{U}_d^\dagger=\alpha_0$ and $\hat{U}_d\beta_0\hat{U}_d^\dagger=\beta_0$. Now Eq. (97) implies $d(\alpha_0,\beta_0)=d^R(\alpha_0,\beta_0)$. Finally, from the definition of d^R it follows that $d^R(\alpha_0,\beta_0)=d^{red}(\alpha_0,\beta_0)$. □

This shows that gauge-fixed decoherence functionals ensure the following.

(i) The *probabilities* assigned to gauge-invariant propositions are gauge invariant.
(ii) The *quantum interference* between gauge-invariant propositions is gauge invariant.

We have the following lemma:

Lemma 5.0.3: For any gauge-fixed decoherence functional $d\in\mathcal{D}_{gf}$, any projector $\alpha\in P(\mathcal{E})$, and any exact projector γ,

$$d(\alpha,\gamma)=0. \tag{101}$$

Proof: We act on $d(\alpha,\gamma)$ with $\hat{U}_d$, the gauge transformation that maps d into d^R. Under the action of $\hat{U}_d$, α and γ transform to $\alpha_d:=\hat{U}_d\alpha\hat{U}_d^\dagger$ and $\gamma_d:=\hat{U}_d\gamma\hat{U}_d^\dagger$. Now using Eq. (97) we have

$$d(\alpha,\gamma)=d^R(\alpha_d,\gamma_d), \tag{102}$$

which is equal to zero by Eq. (88) because γ_d is exact. □

Corollary 5.0.4: Let γ and δ be exact propositions. Then $d(\gamma,\delta)=0$ for any gauge-fixed decoherence functional $d\in\mathcal{D}_{gf}$.

Proof: Immediate. □

This implies that there is no interference between exact projectors, and that exact propositions are assigned a probability of zero by any gauge-fixed decoherence functional. Projectors onto the spectrum of the constraint fields are exact, so a special case of this result is that any gauge-fixed decoherence functional assigns a probability of zero to any propositions that are not compatible with the constraints.

Theorem 5.0.5: *Any gauge-fixed decoherence functional $d\in\mathcal{D}_{gf}$ reduces to a well-defined functional $\tilde{d}:H^*(\hat{\Omega})\times H^*(\hat{\Omega})\to\mathbb{C}$ defined by*

$$\tilde{d}([\alpha],[\beta]):=d(\alpha,\beta). \tag{103}$$

In addition,

$$\tilde{d}([\alpha],[\beta])=d^{red}(\alpha_0,\beta_0), \tag{104}$$

for all $[\alpha],[\beta]\in H^*(\hat{\Omega})$, where α_0 and β_0 are the primitive parts of α and β, respectively.

Proof: We use the additivity axiom of the space of decoherence functionals,

$$d(\alpha,\beta)=d(\alpha_0+\gamma_\alpha,\beta)=d(\alpha_0,\beta)+d(\gamma_\alpha,\beta), \tag{105}$$

because α_0 and γ_α are disjoint. Now because γ_α is exact, Lemma (5.0.3) along with the Hermiticity of d implies that $d(\gamma_\alpha,\beta)=0$. This means that

$$d(\alpha,\beta)=d(\alpha_0,\beta). \tag{106}$$

Repeating this for the other argument of d, we have

$$d(\alpha,\beta)=d(\alpha_0,\beta_0), \tag{107}$$

for any gauge-fixed decoherence functional d. This shows that every gauge-fixed decoherence functional reduces to a well-defined functional $\tilde{d}:H^*(\hat{\Omega})\times H^*(\hat{\Omega})\to\mathbb{C}$ defined by $\tilde{d}([\alpha],[\beta]):=d(\alpha,\beta)$. Now Proposition (5.0.2) proves the theorem. □

Theorem (5.0.5) shows that the cohomological history theory $(H^*(\hat{\Omega}),\tilde{d})$ is "the same" as the reduced history theory $(P(\mathcal{E}^{red}),d^{red})$. More precisely, we have the following.

Definition 5.0.6: Two quantum history theories $(P_1,\mathcal{D}_1)$ and $(P_2,\mathcal{D}_2)$ are defined to be isomorphic *if there exists (i) an isomorphism of lattices $\lambda:P_1\to P_2$, and (ii) a bijective map $\vartheta:\mathcal{D}_1\to\mathcal{D}_2$, such that*

$$d(\alpha,\beta)=\vartheta(d)(\lambda(\alpha),\lambda(\beta)), \tag{108}$$

for all $\alpha,\beta\in P_1$ and all $d\in\mathcal{D}_1$.

Proposition 5.0.7: $(H^*(\hat{\Omega}),\tilde{d})$ is isomorphic to $(P(\mathcal{E}^{red}),d^{red})$.

Proof: The map $\pi:[\alpha]\mapsto\alpha_0$ provides the required lattice isomorphism between $H^*(\hat{\Omega})$ and $P(\mathcal{E}^{red})$. Now define ϑ by $\vartheta(\tilde{d})=d^{red}$, and Eq. (104) states precisely that the two history theories are isomorphic. □

VI. CONCLUSION

We have constructed two concrete models of history quantum electrodynamics on Fock space. First, we quantized the classical reduced history space by finding an inequivalent representation of

the reduced history algebra on $\mathcal{E}^{red}$ for each foliation. We then defined the decoherence functional using the canonical history action on the reduced history space. This results in the reduced history theory $(P(\mathcal{E}^{red}),d^{red})$.

Second, we extended the history algebra by including ghost fields, and found representations of the extended history algebra on the extended quantum history space $\mathcal{E}$. Using the BRST charge Ω, we defined $H^*(\Omega)$, the projection operator cohomology of Ω, and showed that $H^*(\Omega)$ is isomorphic (as a lattice) to $P(\mathcal{E}^{red})$. Finally, we defined the space of gauge-fixed decoherence functionals and showed that, for each gauge-fixed decoherence functional d, $(H^*(\Omega),\tilde{d})$ is isomorphic to $(P(\mathcal{E}^{red}),d^{red})$.

Although the construction of quantum history electrodynamics is interesting in itself, it is hoped that the results obtained here will be useful in a wider context. Given a general BRST-extended quantum history space and a nilpotent BRST charge, Sec. III provides a definition of the corresponding projection operator cohomology, and shows that it is isomorphic to the lattice of projection operators on the reduced history space. In addition, the discussion of the space of gauge-fixed decoherence functionals is relevant to any gauge theory. It would be interesting to apply the histories BRST formalism developed here to mini-superspace models, or to topological quantum field theory. These examples are of particular importance in light of the recent interest in diffeomorphism invariance in history theories.[10,11]

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APPENDIX

First, we consider the bosonic part of the BRST-extended commutator algebra:

$$[\hat{\lambda}_n(X),\hat{B}_n(X')]=i\hbar\,\delta^{(4)}(X-X'), \tag{A1}$$

$$[\hat{A}^n_M(X),\hat{E}^N_n(X')]=i\hbar\,\delta^N_M\delta^{(4)}(X-X'), \tag{A2}$$

where all unwritten commutators vanish. We expand the configuration fields as

$$\hat{\lambda}_n(X)=\frac{1}{(2\pi)^2}\int\frac{d^4K}{\sqrt{2\omega_n(K)}}[\hat{d}(K)e^{iK\cdot X}+\hat{d}^\dagger(K)e^{-iK\cdot X}], \tag{A3}$$

$$\hat{A}^n_s(X)=\frac{1}{(2\pi)^2}\int\frac{d^4K}{\sqrt{2\omega_n(K)}}[\hat{d}_s(K)e^{iK\cdot X}+\hat{d}^\dagger_s(K)e^{-iK\cdot X}], \tag{A4}$$

$$\hat{A}^n_t(X)=\frac{1}{(2\pi)^2}\int\frac{d^4K}{\sqrt{2\omega_n(K)}}[\hat{d}_t(K)e^{iK\cdot X}+\hat{d}^\dagger_t(K)e^{-iK\cdot X}], \tag{A5}$$

$${}^n\hat{A}_M(X)=\frac{1}{(2\pi)^2}\sum_{i=1}^{3}\int\frac{d^4K}{\sqrt{2\omega_n(K)}}, \tag{A6}$$

$$[\hat{d}_i(K){}^n\epsilon^i_M(K)e^{iK\cdot X}+\hat{d}^\dagger_i(K){}^n\epsilon^i_M(K)e^{-iK\cdot X}]. \tag{A7}$$

The five-vectors ${}^n\epsilon^a_M(K)$ for $a=1,2$ are defined as in Sec. II, and ${}^n\epsilon^3_M(K)$ is the unit vector pointing in the direction of ${}^n\tilde{K}$. Now the momentum fields are expanded as

$$\hat{B}_n(X)=\frac{1}{i(2\pi)^2}\int d^4K\sqrt{\frac{\omega_n(K)}{2}} \tag{A8}$$

$$[(\hat{d}(K)+\hat{d}_s(K))e^{iK\cdot X}-(\hat{d}^\dagger(K)+\hat{d}_s^\dagger(K))e^{-iK\cdot X}], \tag{A9}$$

$$\hat{E}_n^s(X)=\frac{1}{i(2\pi)^2}\int d^4K\sqrt{\frac{\omega_n(K)}{2}}[(\hat{d}_s(K)+\hat{d}(K))e^{iK\cdot X} \tag{A10}$$

$$-(\hat{d}_s^\dagger(K)+\hat{d}^\dagger(K))e^{-iK\cdot X}], \tag{A11}$$

$$\hat{E}_n^t(X)=\frac{1}{i(2\pi)^2}\int d^4K\sqrt{\frac{\omega_n(K)}{2}}[(\hat{d}_t(K)+\hat{d}_3(K))e^{iK\cdot X} \tag{A12}$$

$$-(\hat{d}_t^\dagger(K)+\hat{d}_3^\dagger(K))e^{-iK\cdot X}], \tag{A13}$$

$${}^n\hat{E}^M(X)=\frac{1}{i(2\pi)^2}\sum_{i=1}^{3}\int d^4K\sqrt{\frac{\omega_n(K)}{2}} \tag{A14}$$

$$[(\hat{d}_i(K){}^n\epsilon_M^i(K)+\hat{d}_t(K){}^n\epsilon_3^M(K))e^{iK\cdot X} \tag{A15}$$

$$-(\hat{d}_i^\dagger(K){}^n\epsilon_i^M(K)+\hat{d}_t^\dagger(K){}^n\epsilon_3^M(K))e^{-iK\cdot X}]. \tag{A16}$$

Defining

$$\hat{a}_1(K)=\frac{1}{\sqrt{2}}(\hat{d}_t(K)+\hat{d}_3(K)), \tag{A17}$$

$$\hat{b}_1(K)=\frac{1}{\sqrt{2}}(\hat{d}_t(K)-\hat{d}_3(K)), \tag{A18}$$

$$\hat{a}_2(K)=\frac{1}{\sqrt{2}}(\hat{d}_s(K)+\hat{d}(K)), \tag{A19}$$

$$\hat{b}_2(K)=\frac{1}{\sqrt{2}}(\hat{d}_s(K)-\hat{d}(K)), \tag{A20}$$

we obtain the commutators (65)–(67) in which $\hat{d}_a$ has been written ${}^\perp\hat{a}_a$ for $a\in\{1,2\}$.

The fermionic part of the BRST-extended quantum history algebra is

$$[\hat{\eta}_n^a(X),\hat{\mathcal{P}}_n^b(X')]=\hbar\,\delta^{ab}\delta^{(4)}(X-X'), \tag{A21}$$

$$[\overline{C}_n^a(X),\hat{\rho}_n^b(X')]=\hbar\,\delta^{ab}\delta^{(4)}(X-X'), \tag{A22}$$

where on fermionic fields square brackets represent anti-commutators. We write the ghost fields as

$$\hat{\eta}_n^1(X)=-\frac{1}{(2\pi)^2}\int\frac{d^4K}{2\,\omega_n(K)^{3/2}}[c_1(K)e^{iK\cdot X}+c_1^\dagger(K)e^{-iK\cdot X}], \tag{A23}$$

$$\hat{\mathcal{P}}_n^1(X) = \frac{i}{(2\pi)^2}\int d^4K\,\omega_n(K)^{3/2}[\overline{c_1}(K)e^{iK\cdot X} + \overline{c}_1^{\dagger}(K)e^{-iK\cdot X}], \tag{A24}$$

$$\hat{\rho}_n^1(X) = -\frac{1}{(2\pi)^2}\int \frac{d^4K}{2\omega_n(K)^{1/2}}[c_1(K)e^{iK\cdot X} - c_1^{\dagger}(K)e^{-iK\cdot X}], \tag{A25}$$

$$\overline{C_n^1}(X) = \frac{1}{i(2\pi)^2}\int d^4K\,\omega_n(K)^{1/2}[\overline{c_1}(K)e^{iK\cdot X} + \overline{c}_1^{\dagger}(K)e^{-iK\cdot X}], \tag{A26}$$

$$\hat{\eta}_n^2(X) = -\frac{1}{(2\pi)^2}\int \frac{d^4K}{2\omega_n(K)^{1/2}}[c_2(K)e^{iK\cdot X} + c_2^{\dagger}(K)e^{-iK\cdot X}], \tag{A27}$$

$$\hat{\mathcal{P}}_n^2(X) = \frac{i}{(2\pi)^2}\int d^4K\,\omega_n(K)^{1/2}[\overline{c_2}(K)e^{iK\cdot X} + \overline{c}_2^{\dagger}(K)e^{-iK\cdot X}], \tag{A28}$$

$$\hat{\rho}_n^2(X) = -\frac{1}{(2\pi)^2}\int \frac{d^4K}{2\omega_n(K)^{1/2}}[c_2(K)e^{iK\cdot X} - c_2^{\dagger}(K)e^{-iK\cdot X}], \tag{A29}$$

$$\overline{C_n^2}(X) = \frac{1}{i(2\pi)^2}\int d^4K\,\omega_n(K)^{1/2}[\overline{c_2}(K)e^{iK\cdot X} + \overline{c}_2^{\dagger}(K)e^{-iK\cdot X}], \tag{A30}$$

and the algebra (A21) and (A22) implies the anti-commutators in Eqs. (68) and (69).

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Chiral superconducting strings and Nambu–Goto strings in arbitrary dimensions

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We present general solutions to the equations of motion for a superconducting relativistic chiral string that satisfy the unit magnitude constraint in terms of products of rotations. From this result we show how to construct a general family of odd harmonic superconducting chiral loops. We further generalize the product of rotations to an arbitrary number of dimensions. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1501169]

I. PRELIMINARIES

Particle physics models where symmetry breaking is involved predict, in many cases, the existence of topological defects, which are formed when the topology of the vacuum manifold of the low energy theory is nontrivial.[1] Cosmic strings, in particular, are linelike objects that are formed when the the vacuum manifold contains unshrinkable loops. For a review, see Ref. 2.

In Ref. 3 it was shown that cosmic strings can be superconducting. In the case when the charge carriers on the string are not coupled to a gauge field, the action for the string and the current can be taken to be

$$S=\int d^2\xi\sqrt{-\gamma}\left(-\mu+\frac{1}{2}\gamma^{ab}\phi_{,a}\phi_{,b}\right), \tag{1}$$

where μ is the mass per unit length of the string, γ^{ab} is the induced metric on the string worldsheet and ϕ is the field of the charge carriers living on the string. These strings were shown in Refs. 4 and 5 to have solutions in the case when $\gamma^{ab}\phi_{,a}\phi_{,b}=0$ of the form

$$\mathbf{x}=\tfrac{1}{2}[\mathbf{a}(u)+\mathbf{b}(v)] \tag{2}$$

for the string position and

$$\phi=\tfrac{1}{2}f(v) \tag{3}$$

for the field living on the string with the constraints

$$\mathbf{a}'^2=1 \tag{4}$$

and

$$\mathbf{b}'^2+f'^2=1, \tag{5}$$

where $u=\sigma-\tau$ and $v=\sigma+\tau$ and σ and τ are spacelike and timelike parameters, respectively, that parametrize the string world-sheet. These strings are called chiral because the current only moves in one direction on the string.

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Comparing this to the usual Nambu–Goto case, one can see that $f(v)$ acts like a fourth component of the three-vector $\mathbf{b}(v)$, making chiral superconducting strings behave like Nambu–Goto ones with chiral excitations in an extra fifth dimension. Indeed, this property was used in Ref. 6 in an investigation of the properties of superconducting cosmic string cusps.

The right- and left-moving excitations, $\mathbf{a}'$ and $\mathbf{b}'$, on a regular Nambu–Goto string in Minkowski space–time are arbitrary functions that satisfy the unit magnitude constraint, $|\mathbf{a}'| = |\mathbf{b}'| = 1$. Expressions for these functions are often given as Fourier sums and the unit magnitude constraint generally gives a nonlinear set of equations involving the vector coefficients of the Fourier expansion. As a result, parametrizing strings beyond the first few harmonics proves to be a difficult task. Fortunately, in that case, there exists a method to generate strings involving products of rotation matrices[7] that act on a starting unit vector so that the unit magnitude constraint is satisfied trivially.

In a recent study of the properties of chiral cosmic strings[8] it was assumed that the current is constant. The work in Ref. 9 assumed that the current takes a very simple nonconstant form. As was pointed out in the latter work, one could expect to have loops with varying currents if the loops are formed by intersections involving different strings or if different segments of the loop or string were at some point in causally disconnected regions. For long strings this is always the case and we therefore expect varying chiral currents to be generic.

The purpose of this work is to generalize the work in Ref. 7 for generating three-dimensional unit vectors to four-dimensional ones that include the current as a fourth component of $\mathbf{b}(\sigma + \tau)$. We start by casting the method somewhat differently and generalize it to four dimensions. From this result we construct a family of chiral superconducting odd-harmonic loops. We further generalize the product of rotations to an arbitrary number of dimensions.

In Sec. II we show how to construct an arbitrary N harmonic unit vector in four and three dimensions. In Sec. III we use these results to construct arbitrary chiral current carrying superconducting odd harmonic loops. In Sec. IV we generalize the arguments in Sec. II to an arbitrary number of dimensions and we conclude in Sec. V.

II. SOLUTION TO THE UNIT MAGNITUDE CONSTRAINT IN TERMS OF PRODUCTS OF ROTATIONS

We can think of the Euclidean four-vector

$$\tilde{\mathbf{b}}' = \begin{pmatrix} b'_w \\ b'_x \\ b'_y \\ b'_z \end{pmatrix} \tag{6}$$

as having unit magnitude according to (5) with $b_w = f$. Consider the vector $\tilde{\mathbf{b}}'_N$, which can be constructed from a finite sum of Fourier components,

$$\tilde{\mathbf{b}}'_N(v) = \mathbf{Z} + \sum_{n=1}^{N} \{\mathbf{A}_n \cos nv + \mathbf{B}_n \sin nv\}. \tag{7}$$

The Fourier coefficients satisfy the set of $4N+1$ nonlinear relations derived in Ref. 7,

$$\sum_{n=m-N}^{N} (\alpha_n \cdot \alpha_{m-n} - \beta_n \cdot \beta_{m-n}) = 4\delta_{m0} \tag{8}$$

with $m = 0,1,\ldots,2N$,

$$\sum_{n=m-N}^{N} (\alpha_n \cdot \beta_{m-n} - \beta_n \cdot \alpha_{m-n}) = 0 \tag{9}$$

with $m=1,\ldots,2N$,

$$\alpha_n=\alpha_{-n}=\mathbf{A}_n, \quad \beta_n=-\beta_{-n}=\mathbf{B}_n, \quad n\neq 0, \tag{10}$$

and

$$\alpha_0=2\mathbf{Z}, \quad \beta_0=0. \tag{11}$$

These equations can be obtained from the constraint equation (5). The total number of degrees of freedom in the coefficients in (7) is $8N+4$, so the remaining number of degrees of freedom after satisfying the constraint is $4N+3$. Below we show how to construct (7) from a product of rotation matrices by generalizing a modified version of the three-dimensional method presented in Ref. 7 to four dimensions.

The constraint equations (8) and (9) for $m=2N$ and $m=2N-1$ are

$$\mathbf{A}_N^2=\mathbf{B}_N^2, \quad \mathbf{A}_N\cdot\mathbf{B}_N=0, \tag{12}$$

and

$$\begin{aligned}\mathbf{A}_N\cdot\mathbf{A}_{N-1}-\mathbf{B}_N\cdot\mathbf{B}_{N-1}&=0,\\ \mathbf{A}_N\cdot\mathbf{B}_{N-1}+\mathbf{B}_N\cdot\mathbf{A}_{N-1}&=0,\end{aligned} \tag{13}$$

respectively. It follows from (12) that the highest harmonic is a circle that lives on some arbitrary plane. Clearly, we can introduce coordinates such that $\mathbf{A}_N$ and $\mathbf{B}_N$ lie on the w and x axes,

$$\mathbf{A}_N=a\hat{w}, \quad \mathbf{B}_N=a\hat{x}, \tag{14}$$

making the highest harmonic a circle of radius a on the w-x plane. This puts the vector $\tilde{\mathbf{b}}_N'$ into the so-called standard form.[7] Let $R_{wx}(\theta)$ be a matrix that rotates the w-x plane by an angle θ. Acting on $\tilde{\mathbf{b}}_N'$ with $R_{wx}(-v)$ in these coordinates lowers the highest harmonic term of (7),

$$R_{wx}(-v)\begin{pmatrix} a\cos Nv\\ a\sin Nv\\ 0\\ 0\end{pmatrix}=\begin{pmatrix} a\cos(N-1)v\\ a\sin(N-1)v\\ 0\\ 0\end{pmatrix}. \tag{15}$$

This is not sufficient to verify that the overall harmonic content has been lowered because the $N-1$ terms of (7) could still give us an N harmonic through trigonometric identities. We now show, however, that this is not the case.

The constraint equations for $m=2N-1$ in (13) give us, using (14), the conditions on the coefficients,

$$(\mathbf{A}_{N-1})_w=(\mathbf{B}_{N-1})_x, \quad (\mathbf{A}_{N-1})_x=-(\mathbf{B}_{N-1})_w. \tag{16}$$

It is not too difficult to see that using the conditions (16) when acting with $R_{wx}(-v)$ on the $N-1$ terms of (7) does not lead to the creation of N harmonic terms,

$$\begin{aligned}&R_{wx}(-v)[\mathbf{A}_{N-1}\cos(N-1)v+\mathbf{B}_{N-1}\sin(N-1)v]\\ &=\begin{pmatrix}(\mathbf{A}_{N-1})_w\cos(N-2)v-(\mathbf{A}_{N-1})_x\sin(N-2)v\\ (\mathbf{A}_{N-1})_x\cos(N-2)v+(\mathbf{A}_{N-1})_w\sin(N-2)v\\ (\mathbf{A}_{N-1})_y\cos(N-1)v+(\mathbf{B}_{N-1})_y\sin(N-1)v\\ (\mathbf{A}_{N-1})_z\cos(N-1)v+(\mathbf{B}_{N-1})_z\sin(N-1)v\end{pmatrix}.\end{aligned} \tag{17}$$

Clearly, the $N-2$ terms will not yield an N harmonic term when acted on by $R_{wx}(-v)$.

We now have a string in the form of (7) with $N \to N-1$. Its highest harmonic is therefore also a circle of some other radius living on some other arbitrary plane. Armed with this knowledge, we can see that the unit magnitude constraints are such that, in general, we can write

$$\tilde{\mathbf{b}}'_N = R_{P_N}(v)\tilde{\mathbf{b}}'_{N-1}, \tag{18}$$

where $R_{P_N}(v)$ is a rotation by an angle v on the plane P_N where the highest harmonic lives. By induction it must be that

$$\tilde{\mathbf{b}}'_N = \prod_{i=N}^{1} R_{P_i}(v)\tilde{\mathbf{b}}'_0, \tag{19}$$

where the $R_{P_i}(v)$ are rotations by an angle v on arbitrary planes P_i and $\tilde{\mathbf{b}}'_0$ is an arbitrary constant unit vector in four dimensions.

To specify a plane in four dimensions one needs to specify a direction on the plane (three angles), a linearly independent direction (two angles), but now the plane is overspecified by internal rotations (-1 angle), giving a total of four degrees of freedom for the matrices $R_{P_i}(v)$. For an N harmonic vector, one therefore has $4N$ parameters in the rotators and three parameters in the constant unit vector $\tilde{\mathbf{b}}'_0$ giving a total of $4N+3$ parameters which checks perfectly with $8N+4$ vector coefficients in (7) minus the $4N+1$ constraints (8) and (9).

The form of the $R_{P_i}(v)$ matrices is quite simple. Generally, if we want to transform, say, a rotation by an angle v on the w-x plane to one on an arbitrary plane, we will need to perform a transformation of the type

$$R_{P_i}(v) = E_i R_{wx}(v) E_i^T. \tag{20}$$

For the purpose of finding the form of the rotators E_i it is easiest to envision the inverse process to the one we are seeking, namely the rotation of an arbitrary oriented plane to lie on the w-x plane. Let us consider first the projection of the four-dimensional arbitrary plane onto the (x,y,z) subspace. We can perform a rotation by some angle α about the z axis $[R_{xy}(\alpha)]$ until the vector perpendicular to the projected plane lies on the y-z plane and perform a further rotation by an angle β about the x axis $[R_{yz}(\beta)]$ until that vector lies on the z axis. At this stage the projected plane lies wholly on the x-y plane. The ranges of both α and β from 0 to π are sufficient to perform these transformations. After performing these two rotations, our original four dimensional plane lies entirely in the (w,x,y) subspace and we can repeat an analogous process to the one above to rotate it into the w-x plane. A rotation by an angle γ about the y axis $[R_{wx}(\gamma)]$ puts the vector perpendicular to the plane on the x-y plane and a rotation by an angle δ about w $[R_{xy}(\delta)]$ makes that vector parallel with the y axis. For the first of these rotations a range of γ from 0 to π is sufficient, for the second rotation, however, matters are slightly different. If the plane we were trying to rotate was featureless, it would be enough for the range of δ to be from 0 to π. In fact, this is not the case. The plane contains a circle in v which can be oriented clockwise or counterclockwise on the w-x plane and therefore the final rotation on the x-y plane in general requires an angle that ranges from 0 to 2π.

Keeping in mind these considerations, we can quite generally write

$$E_i = R_{xy}(\alpha_i)R_{yz}(\beta_i)R_{wx}(\gamma_i)R_{xy}(\delta_i), \tag{21}$$

where α_i, β_i, γ_i range from 0 to π and δ_i ranges from 0 to 2π. Then

$$\tilde{\mathbf{b}}'_N(v) = \prod_{i=N}^{1} E_i R_{wx}(v) E_i^T \tilde{\mathbf{b}}'_0. \tag{22}$$

In order to construct the entire chiral string, we also need to find the form of $\mathbf{a}(u)$ in (2). The constraints (4) can be satisfied using a product of rotations that can be found from analogous arguments to the ones in the preceding section. For M harmonics this yields

$$\mathbf{a}'_M(u)=\prod_{i=M}^{1} D_i R_{xy}(u) D_i^T \mathbf{a}'_0 \tag{23}$$

with the rotator

$$D_i=R_{xy}(\phi_i)R_{yz}(\theta_i) \tag{24}$$

where the angles θ_i range from 0 to π, the angles ϕ_i from 0 to 2π and R are the three dimensional rotation matrices.

III. AN APPLICATION: A FAMILY OF ODD HARMONIC SUPERCONDUCTING CHIRAL LOOPS

A. Overall orientation freedom

Both expressions for the oppositely moving excitations on the string (22) and (23) include overall orientation freedom. In some applications, for instance self-intersection or gravitational radiation analyses, only the shape of a loop, and not its orientation, is important. In this case the inclusion of overall orientation freedom of the right- and left-moving excitations separately is unnecessary: All that matters is the relative orientation between $\mathbf{a}'$ and the spatial part of $\tilde{\mathbf{b}}'$.

Overall orientation freedom of the loop is set by an Euler matrix Q that acts only on $\mathbf{a}'$ and the spatial components of $\tilde{\mathbf{b}}'$ and contains three angles. We can use this freedom to standardize the vectors in some way. We will choose the plane of the last rotation in $\mathbf{a}'$ and $\tilde{\mathbf{b}}'$ to contain some coordinate axis (this will enable us in the following subsection to use the arbitrariness in the origin of u and v to eliminate more parameters).

The four-dimensional circle that constitutes the highest harmonic of $\tilde{\mathbf{b}}'$ projected onto three-dimensional space typically looks like an ellipse. We can perform ordinary three-dimensional rotations on it to put it in some convenient form. In particular, we can rotate the ellipse on the x-y plane until its major axis, say, lies on the y-z plane and further rotate on the y-z plane until it lies entirely on the z axis. We still have one more rotation left in Q which we choose to be a rotation on the x-y plane. This leaves the major axis of the ellipse on the z-axis but orients the circle of the highest harmonic in $\mathbf{a}'$ such that it contains the x-axis.

We now construct a four-dimensional planar rotator that contains the z-axis but is otherwise arbitrary. Starting with $R_{wz}(v)$, we see that we can perform an arbitrary planar rotation on it in the (w,x,y) subspace that preserves the z-axis. This requires only two rotations. Therefore, to rotate about a plane that contains the z-axis but is otherwise arbitrary we can use

$$R_{xy}(\gamma)R_{wx}(\delta)R_{wz}(v)R_{wx}(-\delta)R_{xy}(-\gamma) \tag{25}$$

where δ ranges from 0 to π and γ from 0 to 2π. This procedure eliminates two of the parameters in the last planar rotation of $\tilde{\mathbf{b}}'$.

In three dimensions, to rotate by an angle u on a plane that contains the x-axis, but is otherwise arbitrary, we may use

$$R_{yz}(\theta)R_{xy}(u)R_{yz}(-\theta) \tag{26}$$

where θ ranges from 0 to 2π. This procedure eliminates one of the parameters in the last planar rotation of $\mathbf{a}'$.

This leaves $\mathbf{a}'$ and $\tilde{\mathbf{b}}'$ in the form

$$\tilde{\mathbf{b}}'_N(v)=\tilde{R}^b_{P_N}(v)\prod_{i=N-1}^{1}E_iR_{wx}(v)E_i^T\tilde{\mathbf{b}}'_0 \tag{27}$$

with

$$\tilde{R}^b_{P_N}(v)=R_{wx}(\gamma)R_{xy}(\delta)R_{wz}(v)R_{xy}(-\delta)R_{wx}(-\gamma) \tag{28}$$

and

$$\mathbf{a}'_M(u)=\tilde{R}^a_{P_M}(u)\prod_{i=M-1}^{1}D_iR_{xy}(u)D_i^T\mathbf{a}'_0 \tag{29}$$

with

$$\tilde{R}^a_{P_M}(u)=R_{yz}(\theta)R_{xy}(u)R_{yz}(-\theta). \tag{30}$$

B. The origin of *u* and *v*

The conditions on the coefficients of the highest harmonics (12) only specify the planar rotation up to a phase so that generally we can take $\tilde{R}^b_N(v+\beta)$ and $\tilde{R}^a_M(u+\alpha)$ in (27) and (29).

We consider the action of this extra planar rotation matrix on $\tilde{\mathbf{b}}'_N(v)$. It can be verified to be

$$\tilde{\mathbf{b}}'_N(v)=\tilde{R}^b_{P_N}(v)\prod_{i=N-1}^{1}R_{P'_i}(v)\tilde{R}^b_{P_N}(\beta)\tilde{\mathbf{b}}'_0, \tag{31}$$

where

$$R_{P'_i}(v)=\tilde{R}^b_{P_N}(\beta)R_{P_i}(v)\tilde{R}^b_{P_N}(-\beta) \tag{32}$$

with analogous expressions for $\mathbf{a}'_M(u)$. It is important to note that the effect of replacing $R_{P_i}(v)$ with $R_{P'_i}(v)$ is to make the same transformation on each of the planes of rotation, in other words, to rotate on some other set of planes. Since we can express any rotation on a plane using (21), however, the effect of the matrices $\tilde{R}^b_{P_N}(\beta)$ and $\tilde{R}^a_{P_M}(\alpha)$ on the rotators can be ignored.

Since the planar rotations $\tilde{R}^b_{P_N}$ and $\tilde{R}^a_{P_M}$ both contain one of the coordinate axes we can choose β and α so that the z component of $\tilde{\mathbf{b}}'_0$ and the x component $\mathbf{a}'_0$ vanish. This leaves them in the form

$$\tilde{R}^b_{P_N}(\beta)\tilde{\mathbf{b}}'_0=\begin{pmatrix}\cos\theta_b\\ \cos\phi_b\sin\theta_b\\ \sin\phi_b\sin\theta_b\\ 0\end{pmatrix}=R_{xy}(\phi_b)R_{wx}(\theta_b)\hat{w} \tag{33}$$

and

$$\tilde{R}^a_{P_M}(\alpha)\mathbf{a}'_0=\begin{pmatrix}0\\ \cos\theta_a\\ \sin\theta_a\end{pmatrix}=R_{yz}(\theta_a)\hat{y}, \tag{34}$$

where ϕ_b and θ_a range from 0 to 2π and θ_b ranges from 0 to π. This means we can write $\mathbf{a}'$ and $\tilde{\mathbf{b}}'$ as

$$\mathbf{a}'_M(u)=\tilde{R}^a_{P_M}(u)\prod_{i=M-1}^{1}R_{P_i}(u)R_{yz}(\theta_a)\hat{y} \tag{35}$$

and

$$\tilde{\mathbf{b}}'_N(v)=\tilde{R}^b_{P_N}(v)\prod_{i=N-1}^{1}R_{P_i}(v)R_{xy}(\phi_b)R_{wx}(\theta_b)\hat{w}. \tag{36}$$

C. The center of mass constraint

In order to construct string loops, apart from solving the unit magnitude constraint, we need to satisfy the center of mass constraint, namely that the loop should be closed and that we want to work in the rest frame of the loop. These constraints imply that the center of mass term must vanish, $\mathbf{Z}=0$ in (7), for both $\mathbf{a}'$ and $\tilde{\mathbf{b}}'$. In general this is an intractable problem because the center of mass term $\mathbf{Z}$ is a nonlinear function of the angles in the rotation matrices. We can, however, solve this problem in an analogous way to that introduced in Ref. 10. The guiding principle behind such a construction is to set the starting center of mass terms to zero, and to apply further rotation matrices in such a way as to ensure that trigonometric identities never lead to the production of a zero harmonic. In practice this was done by using odd harmonics only and choosing some parameters so that the starting center of mass term is zero. Here we will proceed along similar lines.

Generally, if the starting unit vector lies somewhere on the plane of the first rotation, $i=1$ in (35) and (36), no center of mass term will be generated. Since our starting unit vectors are given by (33) and (34) we need to choose the first planes of rotation appropriately.

Earlier we established that if we want a rotation by an angle u on a plane that contains the x-axis, we can use (26). If we want an arbitrary rotation that contains the y-axis, instead we may use

$$R_{xz}(\phi)R_{xy}(u)R_{xz}(-\phi). \tag{37}$$

If we now decide we want a rotation by u on a plane that contains a vector lying somewhere on the y-z plane, it is sufficient rotate this last matrix (37) on the y-z plane by whatever angle the vector makes with the y-axis. This is precisely the situation in (34). We therefore write the first rotation, $i=1$ in (35), as

$$R_{P_1}(u)=R_{yz}(\theta_a)R_{xz}(\phi_1)R_{xy}(u)R_{xz}(-\phi_1)R_{yz}(-\theta_a) \tag{38}$$

where ϕ_1 ranges from 0 to 2π.

To find the first rotator in (35) we proceed analogously. We want to find a rotation by an angle v on a plane that contains a vector lying somewhere in the (w,x,y) subspace, but is otherwise arbitrary, because this is the situation of (33). If we start with a rotator that contains the w-axis but is otherwise arbitrary, taking say,

$$R_{yz}(\gamma_1)R_{xy}(\delta_1)R_{wx}(v)R_{xy}(-\delta_1)R_{yz}(-\gamma_1), \tag{39}$$

where δ_1 ranges from 0 to π and γ_1 ranges from 0 to 2π, it is not hard to see that the first rotator in (35) must be

$$R_{P_1}(v)=R_{xy}(\theta_b)R_{wx}(\phi_b)R_{yz}(\gamma_1)R_{xy}(\delta_1)R_{wx}(v)R_{xy}(-\delta_1)R_{yz}(-\gamma_1)R_{wx}(-\phi_b)R_{xy}(-\theta_b). \tag{40}$$

Further rotations should be by $2u$ and $2v$ to avoid the production of center of mass terms through trigonometric identities. These considerations yield

$$\tilde{\mathbf{b}}'_{2N-1}(v)=\tilde{R}^{b}_{P_N}(2v)\prod_{i=N-1}^{2}E_iR_{wx}(2v)E_i^TR_{xy}(\theta_b)R_{wx}(\phi_b)R_{xz}(\gamma_1)R_{xy}(\delta_1)R_{wx}(v)\hat{w} \quad (41)$$

and

$$\mathbf{a}'_{2M-1}(u)=\tilde{R}^{a}_{P_M}(2u)\prod_{i=M}^{2}D_iR_{xy}(2u)D_i^TR_{xy}(\theta_a)R_{yz}(\phi_1)R_{xy}(u)\hat{y}. \quad (42)$$

IV. GENERALIZATION TO HIGHER DIMENSIONS

Here we show the straightforward generalization of our four-dimensional argument in Sec. II to a unit vector living in arbitrary dimensions. The constraint equations (8) and (9) as well as the argument leading to (19) and (20) are independent of the number of dimensions the vector lives in. The only thing that changes with the number of dimensions is the parametrization of E, the rotator that takes an arbitrary oriented plane to the plane of the first two coordinates. In the following, we label our spatial coordinates by the numbers 1 through d.

If we consider the projection of the plane onto the subspace given by the last three coordinates $(d-2,d-1,d)$, one can see that a rotation by α_d about the d axis $[R_{d-2,d-1}(\alpha_d)]$ until the vector perpendicular to the projected plane lies in the d-$d-1$ plane followed by a rotation by an angle β_d about the $d-2$ axis $[R_{d-1,d}(\beta_d)]$ is sufficient to rotate the projected plane out of the d axis. To perform these transformations it is sufficient for the angles to range from 0 to π. We can repeat this procedure by moving up $d-2$ times in the coordinates until the plane lies entirely in the 1-2 plane as desired, ensuring that the range of the angle in the very last rotation $R_{2,3}(\beta_3)$ is from 0 to 2π to account for the fact that we are dealing with an oriented plane. We can then write the rotator as

$$E=R_{d-2,d-1}(\alpha_d)R_{d-1,d}(\beta_d)\cdots R_{1,2}(\alpha_3)R_{2,3}(\beta_3). \quad (43)$$

The number of parameters introduced by such a product is $2(d-2)$ per harmonic plus $(d-1)$ parameters to specify the initial unit vector, giving a total of $2N(d-2)+d-1$ which checks with $d(2N+1)$ degrees of freedom in the vector coefficients of the Fourier series minus $4N+1$ constraints.

In the case of Nambu–Goto strings in an arbitrary number of dimensions d one would span both right- and left-moving excitations according to

$$\mathbf{a}'_N(u)=\prod_{i=N}^{1}E_iR_{1,2}(u)E_i^T\mathbf{a}'_0 \quad (44)$$

and

$$\mathbf{b}'_N(v)=\prod_{i=N}^{1}E_iR_{1,2}(v)E_i^T\mathbf{b}'_0 \quad (45)$$

with the E_i given by the choice of (43) appropriate to the desired number of dimensions.

V. CONCLUSIONS

We have generalized the solution to the unit magnitude constraint presented in Ref. 7 from three to four dimensions, casting it somewhat differently, in an effort to arrive at a general parametrization of chiral superconducting strings with a finite number of harmonics. We have further shown how to construct loop solutions that satisfy the center of mass constraint and exclude overall orientation freedom. This result is useful because in studies of the properties of chiral loops, such as self-intersection and gravitational radiation properties, overall orientation of the loop is unimportant.

Studies of chiral cosmic string loops with constant currents[8] and simple varying currents[9] have been performed. Generally, however, we expect the current to be arbitrarily varying when loops are formed by intersections involving different strings or if different segments of the loop or string were at some point in causally disconnected regions. This is a fairly generic situation and a study of the properties of more general chiral loops should account for these variations.

Along the way, we have found that our modification of the method lends itself readily to a generalization to arbitrary dimensions. We use such a generalization to present solutions that could be useful in the investigation of classical relativistic strings in higher dimensions as well as strings in $3+1$ Minkowski space with currents and charges induced by Kaluza–Klein compactification[11] when the back-reaction from the gauge fields can be considered negligible.

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On three-dimensional coupled bosons

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In this work we study two complex scalar fields coupled through a quadratic interaction in $2+1$ dimensions using the method of bilinears as suggested by Rajeev [Int. J. Mod. Phys. A **9**, 5583 (1994)]. The resulting theory can be formulated as a classical theory. We study the linear approximation, and show that there is a possible bound state in a range of coupling constants. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1501167]

I. INTRODUCTION

Quantum field theory has been an essential tool for the modeling of various physical phenomena. One of the major problems in field theory is the understanding of relativistic bound states. The standard way to look at field theories is via perturbation theory around the free theory, and bound state problems are difficult to formulate in this approach. The most common way is to use a Bethe–Salpeter approach for the four-point function (for two particle bound states) and find a self-consistency condition for the bound state solution. Typically this requires various approximations which may break down in the highly relativistic cases.

One of the most successful applications of this approach is within the large-N_c approximation: In his classic paper, 't Hooft obtained a bound state equation for mesons in two dimensions in the large-N_c where N_c refers to the color for the non-Abelian SU(N_c) gauge theory.[1] This leads to a singular integral equation for the possible masses of the mesonic excitations. This equation is expressed in terms of the wave function of the meson given as a function of the fractional light-cone momentum. The analysis of this integral equation in Ref. 2 shows that there are only bound states corresponding to positive eigenvalues with finite multiplicity, and these eigenvalues tend to infinity. The scalar version of this model is worked out in Ref. 3 using the original approach of 't Hooft and in Ref. 4 via a Hamiltonian approach to the large-N_c limit. These relativistic equations behave in a very similar way to the standard 't Hooft equation. In two dimensions we can generalize the Yang–Mills Lagrangian, since the gauge fields are not dynamical, by means of a nondynamical scalar field. The large-N_c limit meson bound state equation of these models have some other interesting features.[5] In Ref. 6, Aoki has generalized these bound state equations for bosons and fermions coupled via SU(N_c) gauge theory. A good presentation of many two-dimensional models using the bilocal fields in the path integral formalism within the large-N_c limit is given in Ref. 7. In this article several interesting bound state equations are derived, and further references are given.

In Ref. 8 Rajeev has formulated the large-N_c model as a classical field theory using color invariant bilinears, and he has shown that the phase space of the theory is the restricted Grassmannian. The knowledge of the phase space allows one to make a variational ansatz for the baryons in this theory, which correspond to the large fluctuations of the field (see Ref. 9). Further details of this approach are given in Ref. 10. Toprak and the author of this paper have extended this work to SO(N_c) gauge theory of bosons and fermions and obtained variants of the 't Hooft equation for these cases.[11,12] The adjoint matter fields in the large-N_c limit yields again singular integral equations for possible mesonic strings, they exhibit a very similar bound state structure as

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the original model, but these equations are more complicated due to the fact that mesons are now color invariant strings of operators.[13–16]

The two-dimensional Yukawa model is analyzed within the light-cone method in Refs. 17–19. These models are more complicated due to nonlocal renormalization effects; it is possible to get an integral equation for bound states using some further approximations. A four-dimensional extension of these ideas is given in Ref. 20. The common feature of all these bound state equations is that they are singular integral equations. In the gauge theory cases these singular integral equations are rather restrictive in that they only allow for a discrete spectrum. In the other cases this is not necessarily true. There is usually a finite number (typically one) bound state. There are investigations in three dimensional QCD for the bound state equations of mesons (see the recent article—Ref. 21). Four-dimensional realistic theories are very complicated since one has to deal with renormalization. The author is not knowledgeable enough about these realistic bound state equations, however some information can be found in Ref. 22 (see also Ref. 23 for a review of renormalization in the light-front point of view and some nonperturbative applications in this formalism).

In this article we will apply a certain kind of mean field theory, which is a large-N_f limit to two coupled complex bosons (we call it flavor symmetry to emphasize that it is not gauged). This theory is simple since it does not require coupling constant and wave function renormalization in the perturbation theory. Defining the scalar field around the free field theory may not be so interesting from a physical point of view, but we regard this as an interesting toy model. The linear approximation yields a bound state for the composite of two bosons. We will apply the methods of Rajeev[10] and formulate it as a classical field theory of bilinears. In this case (unlike the gauge theory case) this is only an approximation since the theory does not have to be restricted to this flavor invariant sector. To avoid repetitions we sometimes refer to our work on complex bosons in Ref. 24. There is an interesting Bethe–Salpeter treatment of bound states in the broken phase of ϕ^4 theory in Ref. 25, in some sense this is similar to the model we work with.

II. THE MODEL IN THE LIGHT-CONE AND LARGE-N_f LIMIT

We write down a $U(N_f)$ invariant action for two complex scalars ϕ_a and ϕ_b,

$$S=\int \mathrm{d}^3x\Big(\partial^\mu\phi_a^\dagger\partial_\mu\phi_a+\partial^\mu\phi_b^\dagger\partial_\mu\phi_b-m_a^2\phi_a^\dagger\phi_a-m_b^2\phi_b^\dagger\phi_b$$
$$-\frac{\lambda}{4}[(\phi_a^\dagger\phi_a)^2+(\phi_b^\dagger\phi_b)^2-2(\phi_a^\dagger\phi_b)(\phi_b^\dagger\phi_a)]\Big). \tag{1}$$

We introduced a common coupling λ, for the two complex fields $\phi_{a\alpha}$ and $\phi_{b\alpha}$. We assume that the internal index α takes the values 1,...,N_f. If we do not have the last term which couples the two fields the action would have a $U(N_f)\times U(N_f)$ symmetry, and the interaction term explicitly breaks this. The interaction may look discomforting, but it is easy to see that it is always positive. The classical ground state of the massive theory is when both fields are set to zero. This means that we can quantize the theory around its classical minimum by introducing creation–annihilation operators for the Fourier modes, as we will see in the following. Note that this theory in three dimensions is super-renormalizable from a perturbative point of view, so we do not expect any multiplicative renormalizations (when $\lambda<0$ the theory is unstable, it can be defined by a perturbation theory analysis, but we restrict ourselves to positive values).

Perturbatively, there is only one type of divergence after normal ordering which we will comment on later.[26] To apply the methods developed by Rajeev, we will use the light-cone coordinates, introduce $x^+=(1/\sqrt{2})(x^0+x^2)$ and $x^-=(1/\sqrt{2})(x^0-x^2)$, and x^1 remains as the transverse coordinate. We choose x^+ as time (that is our evolution variable). A good review of light-front methods is given in Ref. 27; a good discussion of the scalar field in the light-front is also given in Refs. 28 and 29. The three-dimensional scalar field theory has been investigated from different points of view in Refs. 26, 30–32.

We basically use the same conventions as in our previous work,[24,33]

$$S=\int \mathrm{d}x^+\,\mathrm{d}x^-\mathrm{d}x^1\Big(\frac{1}{2}\phi_a^\dagger(-2\partial_-)\partial_+\phi_a+\frac{1}{2}\phi_b^\dagger(-2\partial_-)\partial_+\phi_b-\phi_a^\dagger(m_a^2-\partial_1^2)\phi_a-\phi_b^\dagger(m_b^2-\partial_1^2)\phi_b$$
$$-\frac{\lambda}{4}[(\phi_a^\dagger\phi_a)^2+(\phi_b^\dagger\phi_b)^2-2(\phi_a^\dagger\phi_b)(\phi_b^\dagger\phi_a)]\Big).$$

The action is first order in time x^+, which means that we are already in the Hamiltonian formalism. The Hamiltonian can be read off directly,

$$H=\int \mathrm{d}x^-\,\mathrm{d}x^1\Big(\phi_a^\dagger(-\partial_1^2+m_a^2)\phi_a+\phi_b^\dagger(-\partial_1^2+m_b^2)\phi_b$$
$$+\frac{\lambda}{4}[(\phi_a^\dagger\phi_a)^2+(\phi_b^\dagger\phi_b)^2-2(\phi_a^\dagger\phi_b)(\phi_b^\dagger\phi_a)]\Big). \tag{2}$$

The quantization at equal time following Dirac gives

$$[\hat{\phi}_a^{\alpha\dagger}(x^-,x^1),\hat{\phi}_{a\beta}(y^-,y^1)]=-\frac{i}{4}\delta_\beta^\alpha\,\mathrm{sgn}(x^--y^-)\,\delta(x^1-y^1), \tag{3}$$

and the same rule applies for ϕ_b. We recall that the field can be expanded in terms of creation–annihilation operators at initial light-front time (since the classical minimum is the zero configuration for the fields),

$$\hat{\phi}_{a\alpha}(x^-,x^1)=\int\frac{[\mathrm{d}p_-\,\mathrm{d}p_1]}{\sqrt{2|p_-|}}a_\alpha(p_-,p_1)e^{-ip_-x^--p_1x^1},$$

$$\hat{\phi}_{b\alpha}(x^-,x^1)=\int\frac{[\mathrm{d}p_-\,\mathrm{d}p_1]}{\sqrt{2|p_-|}}b_\alpha(p_-,p_1)e^{-ip_-x^--p_1x^1},$$

where we use $[\mathrm{d}p]=\mathrm{d}p/2\pi$. (To properly define everything we should assume that this expansion is given for $(-\infty,-\epsilon_0]\cup[\epsilon_0,\infty)$ at the end we take $\epsilon_0\to 0$ limit.)

The creation and annihilation operators now satisfy

$$[a_\alpha(p_-,p_1),a^{\beta\dagger}(q_-,q_1)]=\mathrm{sgn}(p_-)\,\delta_\alpha^\beta\delta[p_--q_-]\delta[p_1-q_1],$$

$$[b_\alpha(p_-,p_1),b^{\beta\dagger}(q_-,q_1)]=\mathrm{sgn}(p_-)\,\delta_\alpha^\beta\delta[p_--q_-]\delta[p_1-q_1].$$

Since the fields are complex valued, annihilation and creation operators are not related. We introduce a vacuum state $|0\rangle$ for the Fock space construction,

$$a_\alpha(p_-,p_1)|0\rangle=0\quad\text{for } p_->0,\quad a^{\alpha\dagger}(p_-,p_1)|0\rangle=0\quad\text{for } p_-<0,$$

$$b_\alpha(p_-,p_1)|0\rangle=0\quad\text{for } p_->0,\quad b^{\alpha\dagger}(p_-,p_1)|0\rangle=0\quad\text{for } p_-<0.$$

It is important to keep in mind that the operator $a_\alpha(p_-,p_1)$ for $p_-<0$, *creates an antiparticle of momentum* $(-p_-,-p_1)$ and similarly for b_α (which one can see by rewriting the above-given expansions in a more conventional way, by separating particle and antiparticle operators). We define normal ordering rules with respect to this vacuum as usual and denote it by a colon $:\phi_a\ldots\phi_a:$, for the computations we will use the following relation:

$$:a^{\alpha\dagger}(p_-,p_1)a_\beta(q_-,q_1):=a^{\alpha\dagger}(p_-,p_1)a_\beta(q_-,q_1)-\frac{\delta^\alpha_\beta}{2}(1-\mathrm{sgn}(p_-))\,\delta[p_--q_-]\,\delta[p_1-q_1], \tag{4}$$

and exactly the same for b quanta.

We have the following Hamiltonian in the quantized theory:

$$\hat{H}=\int \mathrm{d}x^1\,\mathrm{d}x^-\Big(:\hat{\phi}_a^\dagger(m_a^2-\partial_1^2)\hat{\phi}_a:+:\hat{\phi}_b^\dagger(m_b^2-\partial_1^2)\hat{\phi}_b:$$
$$+\frac{\lambda}{4}[:(\hat{\phi}_a^\dagger\hat{\phi}_a)^2:+:(\hat{\phi}_b^\dagger\hat{\phi}_b)^2:-2:(\hat{\phi}_a^\dagger\hat{\phi}_b)(\hat{\phi}_b^\dagger\hat{\phi}_a):]\Big).$$

As it stands the Hamiltonian would not be a well-defined operator for finite N_f theory. We need to introduce mass renormalization terms which correspond in the diagramatic language to the setting-sun diagrams.[26,30,31] When we take the large-N_f limit these counterterms become of smaller order, therefore the Hamiltonian as written will have a well-defined limit.

We now define as an approximation a large-N_f limit and restrict the theory to the flavor invariant sector. This is to be taken as an approximation to the full quantum theory. We introduce a set of flavor invariant operators, which are directly written in the momentum representation, and to simplify notation we write p to denote p_-,p_1 collectively, and $\delta[p-q]=\delta[p_--q_-]\times\delta[p_1-q_1]$,

$$\hat{N}_a(p,q)=\frac{2}{N_f}:a^{\alpha\dagger}(p_-,p_1)a_\alpha(q_-,q_1):,$$

$$\hat{N}_b(p,q)=\frac{2}{N_f}:b^{\alpha\dagger}(p_-,p_1)b_\alpha(q_-,q_1):,$$

$$\hat{C}(p,q)=\frac{2}{N_f}a^{\alpha\dagger}(p_-,p_1)b_\alpha(q_-,q_1),$$

$$\hat{\bar{C}}(p,q)=\frac{2}{N_f}b^{\alpha\dagger}(p_-,p_1)a_\alpha(q_-,q_1). \tag{5}$$

Note that $\hat{C}$ and $\hat{\bar{C}}$ are just Hermitian conjugates of each other.

The idea behind Refs. 8 and 10 is that when we take the large-N_f limit the flavor invariant operators have smaller and smaller fluctuations, and if we compute their commutator, for example, for N_a with itself, we get

$$[\hat{N}_a(p,q),\hat{N}_a(s,t)]=\frac{2}{N_f}(\hat{N}_a(p,s)\mathrm{sgn}(p_-)\,\delta[q-r]-\hat{N}_a(r,q)\mathrm{sgn}(p_-)\,\delta[p-s]-(\mathrm{sgn}(p_-)$$
$$-\mathrm{sgn}(q_-))\,\delta[p-s]\,\delta[q-r]).$$

We assume that when we let $N_f\to\infty$ there are proper large-N_f limits for these bilinears restricted to the flavor invariant states. As a result the theory becomes classical, and the expectation values of flavor invariant operators factorize as $N_f\to\infty$.[10,34] Thus we may postulate a set of Poisson brackets for these *classical* variables:

$$\{N_a(p,q),N_a(s,t)\}=-2i(N_a(p,s)\mathrm{sgn}(p_-)\,\delta[q-r]-N_a(r,q)\mathrm{sgn}(p_-)\,\delta[p-s]-(\mathrm{sgn}(p_-)$$
$$-\mathrm{sgn}(q_-))\,\delta[p-s]\,\delta[q-r]),$$

$$\{N_b(p,q),N_b(s,t)\}=-2i(N_b(p,s)\mathrm{sgn}(p_-)\delta[q-r]-N_b(r,q)\mathrm{sgn}(p_-)\delta[p-s]$$
$$-(\mathrm{sgn}(p_-)-\mathrm{sgn}(q_-))\delta[p-s]\delta[q-r]),$$

$$\{C(p,q),\overline{C}(s,t)\}=-2i(N_a(p,t)\mathrm{sgn}(q_-)\delta[q-s]-N_b(s,q)\mathrm{sgn}(t_-)\delta[p-t]$$
$$-(\mathrm{sgn}(p_-)-\mathrm{sgn}(q_-))\delta[p-t]\delta[q-s]),$$

$$\{N_a(p,q),C(s,t)\}=-2i\,\mathrm{sgn}(q_-)\delta[q-s]C(p,t),$$

$$\{N_b(p,q),C(s,t)\}=2i\,\mathrm{sgn}(q_-)\delta[p-t]C(s,q),$$

$$\{N_a(p,q),\overline{C}(s,t)\}=2i\,\mathrm{sgn}(p_-)\delta[p-t]\overline{C}(s,q),$$

$$\{N_b(p,q),\overline{C}(s,t)\}=-2i\,\mathrm{sgn}(q_-)\delta[q-s]\overline{C}(p,t),$$

all other Poisson brackets being zero.

There are constraints coming from the $U(N_f)$ invariance, if we restrict the theory to the flavor invariant sector. They are very similar to the ones found in Ref. 24,

$$(\epsilon N_a+\epsilon)^2+\epsilon C\epsilon C^\dagger=1,$$

$$(\epsilon N_b+\epsilon)^2+\epsilon C^\dagger\epsilon C=1,$$

$$N_a\epsilon C+C\epsilon N_b+\epsilon C+C\epsilon=0,$$

and the Hermitian conjugate of the last equation. These conditions are derived using techniques similar to Refs. 33 and 24. Here we are using $\epsilon(p,q)=\mathrm{sgn}(p_-)\delta[p_--q_-]\delta[p_1-q_1]$, $1(p,q)=\delta[p-q]$, and a shorthand for the operator products, for example, N_aC means

$$(N_aC)(p,s)=\int[\mathrm{d}q_-\mathrm{d}q_1]N_a(p_-,p_1;q_-,q_1)C(q_-,q_1;s_-,s_1), \tag{6}$$

and similarly for the others.

We will have further convergence conditions coming from the super-renormalizability. These should be regarded as sufficiently restrictive conditions to keep the system's evolution in phase space. The Hamiltonian puts more stringent conditions on the admissible class of observables—we believe its domain should be dense inside the phase space. Correct normalization should then be found using the Hamiltonian as a quadratic form on the space of these variables and demanding this form to be finite for all physical states. To state our conditions we recall that the one-particle Hilbert spaces of bosons are divided into positive and negative energy subspaces according to $\mathrm{sgn}(p_-)$. We assume that the operators which act between positive and negative energy subspaces will be Hilbert–Schmidt, whereas the operators acting between the same subspaces will be trace class.[35] We write explicitly the one for C: $C(u_-,u_1;v_-,v_1)$ is trace class for $u_-v_->0$, and Hilbert–Schmidt for $u_-v_-<0$, and the same for the other variables. Note that these are consistent with the constraints on the system, which defines the geometry of the phase space. The constraints and the convergence conditions can be cast into a coherent geometric picture: it defines a homogeneous manifold of $U_1((\mathcal{H}_a\oplus\mathcal{H}_b)_+,(\mathcal{H}_a\oplus\mathcal{H}_b)_-)$, but we will not use it in this work.

We can rewrite the large-N_f Hamiltonian in terms of these variables,

$$H=\frac{1}{4}\int [\mathrm{d}p]\frac{m_a^2+p_1^2}{|p_-|}N_a(p,p)+\frac{1}{4}\int [\mathrm{d}p]\frac{m_b^2+p_1^2}{|p_-|}N_b(p,p)$$
$$+\frac{\lambda}{64}\int [\mathrm{d}p\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t]\frac{\delta[p-q+s-t]}{\sqrt{|p_-q_-s_-t_-|}}[N_a(p,q)N_a(s,t)+N_b(p,q)N_b(s,t)$$
$$-2C(p,q)\overline{C}(s,t)].$$

This defines our large-N_f approximation, and in principle we can calculate the equations of motion of the basic observables by

$$\frac{\partial O(u,v)}{\partial x^+}=\{O(u,v),H\}, \tag{7}$$

where O refers to any one of N_a, N_b, C, $\overline{C}$. The resulting equations are nonlinear integral equations and we also have the constraint to satisfy. It would be interesting to study this system using a variational ansatz. We will leave the analysis of the full system to a future work and look at a linearized version.

III. LINEARIZATION AND A POSSIBLE BOUND STATE

To get a better feeling about the system we can start with a linear approximation. This means we should linearize the constraint as well as the equations of motion. The linearization of the constraint gives us, for our basic variables,

$$(1+\mathrm{sgn}(u_-)\mathrm{sgn}(v_-))N_a(u_-,u_1;v_-,v_1)=0,\quad (1+\mathrm{sgn}(u_-)\mathrm{sgn}(v_-))N_b(u_-,u_1;v_-,v_1)=0,$$
$$(\mathrm{sgn}(u_-)+\mathrm{sgn}(v_-))C(u_-,u_1,v_-,v_1)=0. \tag{8}$$

We will be using the last one in our computations, it says that the light-cone momenta should be opposite to each other: $C(u_-,u_1;v_-,v_1)=0$ if $u_-v_->0$, and nonzero if $u_-v_-<0$. The same conditions hold for N_a and N_b as well. In the linear approximation we will search for a possible bound state of a and b particles. In principle we can compute the linearized equations for all the other variables, but they will not lead to a solution for the bound state or a solution for a resonance: they only have scattering states. Therefore we work only with the composite $C(u,v)$, let us choose $u_->0$, $v_-<0$. The equations of motion of $C(u,v)$ for $u_->0$, $v_-<0$, in the linear approximation become

$$\frac{\partial C(u,v)}{\partial x^+}=\{C(u,v),H\}$$
$$=\frac{i}{2}\left[\frac{m_a^2+u_1^2}{u_-}-\frac{m_b^2+v_1^2}{v_-}\right]C(u,v)$$
$$-i\frac{\lambda}{8\pi}\int\frac{[\mathrm{d}p\,\mathrm{d}q]}{\sqrt{|p_-q_-u_-v_-|}}\delta[p_--q_-+v_--u_-]\delta[p_1-q_1+v_1-u_1]C(u,v).$$

Let us make an ansatz, in the light-front direction we make a 't Hooft-like choice with respect to the relative momentum variable $\zeta=u_-/(u_--v_-)$. This variable now satisfies $0<\zeta<1$, and we set $C(u_-,u_1;v_-,v_1)=\tilde{f}(\zeta;u_1,v_1)e^{iP_+x^+}$. Notice that $P_-=u_--v_->0$, and we introduce a relativistically invariant mass variable $\mu^2=2P_+|u_--v_-|-(u_1+(-v_1))^2$, which will be the mass of the bound state [recall that the momentum v_1 denotes an antiparticle with momentum

$-v_1$, thus $u_1+(-v_1)$ is the total transversal momentum of the two particle state]. After some manipulations, similar to the ones in Refs. 8 and 11, this gives us an eigenvalue equation for the invariant mass:

$$\mu^2\tilde{f}(\zeta;u_1,v_1)=\left[\frac{m_a^2+(u_1-\zeta(u_1+(-v_1)))^2}{\zeta}+\frac{m_b^2+(v_1-(1-\zeta)(u_1+(-v_1)))^2}{1-\zeta}\right]\tilde{f}(\zeta;u_1,v_1)$$
$$-\frac{\lambda}{8\pi}\int_0^1 d\eta\int_{-\infty}^{\infty}\frac{[dp_1dq_1]\tilde{f}(\eta;p_1,q_1)}{\sqrt{\eta(1-\eta)\zeta(1-\zeta)}}\delta[p_1-q_1-(u_1+(-v_1))].$$

(Note that this form reduces to $\mu=m_a+m_b$ if we set $\lambda=0$, and choose the function $\tilde{f}$ properly.) We may equivalently use a new set of variables, $R=u_1-\zeta(u_1+(-v_1))$ and $u_1+(-v_1)$, relative transversal light-front momentum and transversal total momentum, respectively, instead of the above-mentioned variables. If we write everything in terms of these new set of variables we get

$$\mu^2\tilde{f}(\zeta;R,u_1+(-v_1))=\left[\frac{m_a^2+R^2}{\zeta}+\frac{m_b^2+(-R)^2}{1-\zeta}\right]\tilde{f}(\zeta;R,u_1+(-v_1))$$
$$-\frac{\lambda}{8\pi}\int_0^1 d\eta\int_{-\infty}^{\infty}\frac{[dQ][d(p_1-q_1)]\tilde{f}(\eta;Q,p_1+(-q_1))}{\sqrt{\eta(1-\eta)\zeta(1-\zeta)}}$$
$$\times\delta[p_1-q_1-(u_1+(-v_1))].$$

(The Jacobian of this transformation in the integral is one.) The total momentum integral can be done due to the delta function and we end up with

$$\mu^2\tilde{f}(\zeta;R,u_1+(-v_1))=\left[\frac{m_a^2+R^2}{\zeta}+\frac{m_b^2+(-R)^2}{1-\zeta}\right]\tilde{f}(\zeta;R,u_1+(-v_1))$$
$$-\frac{\lambda}{8\pi}\int_0^1 d\eta\int_{-\infty}^{\infty}\frac{[dQ]\tilde{f}(\eta;Q,u_1+(-v_1))}{\sqrt{\eta(1-\eta)\zeta(1-\zeta)}}.$$

We see that the total momentum $u_1+(-v_1)$ is conserved, thus we can factor out the transversal center of mass motion by assuming $\tilde{f}(\zeta;u_1,v_1)=f(\zeta,R)g(u_1+(-v_1))$:

$$\mu^2 f(\zeta,R)=\left[\frac{m_a^2+R^2}{\zeta}+\frac{m_b^2+R^2}{1-\zeta}\right]f(\zeta,R)-\frac{\lambda}{16\pi^2}\int_{-\infty}^{\infty}dQ\int_0^1 d\eta\frac{f(\eta,Q)}{\sqrt{\eta(1-\eta)\zeta(1-\zeta)}}. \tag{9}$$

We can reduce this again to a functional equation for the unknown eigenvalue, by using the standard techniques,

$$\frac{\lambda}{16\pi^2}\int_{-\infty}^{\infty}\int_0^1\frac{d\eta\,dQ}{Q^2+m_a^2+\mu^2\eta^2+(m_b^2-m_a^2-\mu^2)\eta}=1. \tag{10}$$

The integrand will have no poles if the quadratic expression involving η has no real roots, or if it has a double root. This is the case if we can assume that $|m_a-m_b|\leqslant\mu\leqslant m_a+m_b$. The last inequality is clear, the bound state mass cannot be bigger than the sum of its constituent's masses. The other inequality says that the fundamental quanta should be stable against decay if, for example, $m_a>m_b$, then it would be favorable to have m_a decaying into μ and m_b. Then we can evaluate the integral in any way we want. First we take the Q integral, this gives us

$$\int_0^1 \frac{d\eta}{\sqrt{\mu^2\eta^2+(m_b^2-m_a^2-\mu^2)\eta+m_a^2}}=\frac{16\pi}{\lambda}. \tag{11}$$

The next integral can be done and simplified into

$$\frac{1}{\mu}\ln\left[\frac{m_a+m_b+\mu}{m_a+m_b-\mu}\right]=\frac{16\pi}{\lambda}, \tag{12}$$

which is valid when $|m_a-m_b|\leqslant\mu\leqslant m_a+m_b$. We may study the small coupling limit of this expression. In this case we expect that the bound state mass becomes very close to the two mass treshold, then we can write

$$\frac{m_a+m_b-\mu}{m_a+m_b+\mu}\approx e^{-16\pi(m_a+m_b)/\lambda}, \quad \mu\approx(m_a+m_b)(1-2e^{-16\pi(m_a+m_b)/\lambda}), \tag{13}$$

which is consistent if we take $\lambda/(m_a+m_b)\ll 1$. The other extreme is interesting as well, $\mu\approx m_a-m_b$ (assuming a is the heavier particle). This implies a critical coupling λ_c beyond which our methods break down, due to the appearance of a tachyon,

$$\frac{16\pi}{\lambda_c}=\frac{1}{m_a-m_b}\ln\left[\frac{m_a}{m_b}\right]$$

or

$$\lambda_c=\frac{16\pi}{\ln\left[\frac{m_a}{m_b}\right]}(m_a-m_b). \tag{14}$$

This critical coupling is pushed to higher and higher values if b becomes lighter and lighter with respect to the a particle. For any given value of the coupling constant in the interval $(0,\lambda_c]$, there is a solution for the bound state energy. Hence we see that there is a composite bound state for these values of the coupling constants. It is not clear what happens beyond this value. It is possible that the linear approximation breaks down. It is also possible that the large-N_f limit is not a good approximation beyond a certain value. The other possibility is that the naive vacuum is not a true vacuum of the quantum theory and we should redefine the vacuum of the system. We are not able to analyze these possiblities at the moment.

Let us compare this with the results we would have found if we looked at a $1+1$-dimensional version of the same model. Then the bound state equation could be written in terms of the fractional light-cone momentum ζ only. There is no transversal component and we have only one integral to compute. As a result we find the equation that should be satisfied by the eigenvalue μ (with the condition $|m_a-m_b|\leqslant\mu\leqslant m_a+m_b$),

$$\frac{1}{\sqrt{4m_a^2m_b^2-z^2}}\left[\arctan\left(\frac{2m_b^2+z}{\sqrt{4m_a^2m_b^2-z^2}}\right)+\arctan\left(\frac{2m_a^2+z}{\sqrt{4m_a^2m_b^2-z^2}}\right)\right]=\frac{8\pi}{\lambda^2}, \tag{15}$$

where $\mu^2=m_a^2+m_b^2+z$ and we wrote λ^2 for the coupling constant since it has dimensions mass-squared. To analyze the behavior it is more natural to define the dimensionless variables, $\tilde{z}=z/2m_am_b$, and $\sigma=m_a/m_b$, and rescale the coupling $\tilde{\lambda}^2=\lambda^2/m_am_b$,

$$\frac{1}{\sqrt{1-\tilde{z}^2}}\left[\arctan\left(\frac{\sigma+\tilde{z}}{\sqrt{1-\tilde{z}^2}}\right)+\arctan\left(\frac{1/\sigma+\tilde{z}}{\sqrt{1-\tilde{z}^2}}\right)\right]=\frac{16\pi}{\tilde{\lambda}^2}. \tag{16}$$

Note that now $\tilde{z}$ satisfies $-1<\tilde{z}<1$. If we take the limit $\tilde{z}\to -1^{+}$, this corresponds to $\mu\to|m_a-m_b|^{+}$ and the other limit $\tilde{z}\to 1^{-}$ corresponds to $\mu\to(m_a+m_b)^{-}$. If we assume $\tilde{z}\approx 1^{-}$ we see that the bound states satisfy the relation

$$\tilde{z}\approx 1-\frac{\tilde{\lambda}^4}{128}$$

or

$$\mu\approx(m_a+m_b)\left[1-\frac{\lambda^4}{128m_am_b(m_a+m_b)^2}\right], \tag{17}$$

and if we take $\tilde{\lambda}$ sufficiently small this is consistent. Notice that in $2+1$ dimensions we have an exponential behavior in the inverse coupling, which is nonanalytic in the coupling constant (around zero), as opposed to this power law change. If we look at the other extreme we see that there is a finite limit for $\tilde{z}\to -1^{+}$, in fact it is equal to 1. This implies a critical coupling again, beyond which our methods predict a tachyonic state,

$$\tilde{\lambda}_c^2=16\pi$$

or

$$\lambda_c^2=16\pi m_am_b\,. \tag{18}$$

This is to be compared with the result in Eq. (14), which is sensitive to the mass difference.

Let us comment on the convergence conditions in this context. Since we are looking for a normalizable solution it looks natural to demand

$$\int_0^1 d\zeta\int_{-\infty}^{\infty}[dR]|f(\zeta,R)|^2<\infty. \tag{19}$$

In fact this is right, and we could see this from our Hilbert–Schmidt condition,

$$\int_{u_-v_-<0}[du_-dv_-][du_1dv_1]|C(u_-,u_1;v_-,v_1)|^2<\infty. \tag{20}$$

If we now make the above change of variables by calling $u_--v_-=P_-$ we have

$$\frac{1}{\pi}\int_0^1 d\zeta\int_{0^+}^{\infty}P_-[dP_-]\int[d(u_1+(-v_1))dR]|C(P_-,\zeta;R,(u_1+(-v_1)))|^2<\infty. \tag{21}$$

In our case we are restricting P_- to the surface $2P_-P_+=\mu^2+(u_1+(-v_1))^2$ (for fixed μ,P_+), this means we should reinterpret the above-mentioned normalization as

$$\int_0^1 d\zeta\int[dR]|f(\zeta,R)|^2\int\frac{\mu^2+(u_1+(-v_1))^2}{2P_+}|g(u_1+(-v_1))|^2[d(u_1+(-v_1))]<\infty \tag{22}$$

(notice that P_+ is not allowed to be zero), which means two separate conditions,

$$\int_0^1 d\zeta\int[dR]|f(\zeta,R)|^2<\infty\quad\int\frac{\mu^2+(u_1+(-v_1))^2}{2P_+}|g(u_1+(-v_1))|^2[d(u_1+(-v_1))]<\infty. \tag{23}$$

The second one simply is a Sobolev-type condition, which states that the energy of the transversal center of momentum component should also be finite. We see that our solution actually satisfies a stronger condition for equations of motion to make sense.

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1/*r*-potential without charge

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In order to get geodesically complete Reißner–Nordstrøm space–times, it is necessary to identify pairs of singular points. This can be done in such a way that ''wormholes'' are created which generate electric field lines without any charge. Finally, it is shown that it is possible to glue this space–time not in the singularities $r=0$, but at some $r>0$. The surface energy generated by this gluing is exotic, but tends to zero in the limit $r\to 0$. © *2002 American Institute of Physics.*
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I. INTRODUCTION

More than 40 years ago, Archibald Wheeler realized[1,2] that nontrivial electric fields can be generated whose field lines do not end in electric charges. Instead some domain of the space is cut out, in which the charge would be expected. To this ''hole,'' a channel (''wormhole'') is attached, through which the field lines pass to some other place such that the divergence of the field lines vanishes. So no charges are needed—they are replaced by special topological structures.

For the realization of this idea, one starts from the Reißner–Nordstrøm solution[3,4] to Einstein's equations. It contains an electric field proportional to $1/r^2$. Visser has cut out the regions $r<\epsilon$ from two Reißner–Nordstrøm space–times and has glued together the remaining parts along the subspaces $r=\epsilon$.[5,6] He wanted to obtain a ''transversable'' wormhole. Therefore he chose ϵ larger than the outer horizon r_+. But this causes some problems.

The geodesics passing through the subspace $r=\epsilon$ are not C^2. (Trivially, they can be made continuously differentiable everywhere.) This means that freely falling particles get a δ-like kick at $r=\epsilon$. Second, the Ricci tensor contains a singularity proportional to $\delta(r-\epsilon)$. Therefore the energy-momentum tensor T has surface terms. They violate the ''average null energy condition'' [6,7]

$$g_{ij}\dot{\gamma}^i(\tau)\dot{\gamma}^j(\tau)=0\Rightarrow\int T_{ij}\dot{\gamma}^i(\tau)\dot{\gamma}^j(\tau)d\tau\geqslant 0, \qquad (1)$$

τ: generalized affine parameter

for some curves $\tau\to\gamma(\tau)$, i.e., the surface matter is ''exotic.'' This is true for all spherically symmetric transversable wormholes, whatever the specific assumptions are. A good survey of the literature on this subject is given in Ref. 6.

In the present work, we want to develop a model for the topological generation of charge via wormholes. This is done for the specific example of electric charge, but, of course, the idea applies to all kinds of charge. For this purpose, it is not necessary to have transversable wormholes: We do not need information from the ''other part of the world.'' In addition, we cannot even expect to get transversable wormholes, because in the Reißner–Nordstrøm solution with $M^2>Q^2$, the mass and charge are hidden by two horizons. So it would be very surprising, if one could avoid all horizons by introducing wormholes and leave the rest of physics unchanged.

The most natural way to reach our goal is to identify singularities $r=0$ in the maximal analytic extension of the Reißner–Nordstrøm solution. Then in the case $M^2>Q^2$, no changes of

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space–time outside the horizons are needed. By this identification, the topology becomes nontrivial—a fact which is to be expected: Einstein's equations determine only the local geometry, but in most cases give little information about the global structure of space–time. It has to be determined by other requirements.

In order that this identification makes sense, one needs a precise definition of singularities. This is still an open problem. But here, we are not interested in the most general situation. Instead, one can start from the maximal analytical extension and use some theory defining the necessary geometric quantities in the singularity. The details of such a theory are irrelevant in this connection, because all functions are uniquely determined by their behavior near the singularity. In the present work, the Reißner–Nordstrøm solution together with its singularities is considered as a d-space.[8,9] This is almost identical to the differential space of Refs. 10 and 11. For the discussion of differential equations on these spaces, the results of Ref. 12 are used. But as remarked above, most other generalizations of differential manifolds will lead to the same results. This is true in particular for the differential spaces described in Refs. 10 and 11.

In addition, gluing of two Reißner–Nordstrøm solutions at some $r=\epsilon>0$ will be discussed. Here, exotic surface matter appears. But the energy of the electromagnetic field rises as $1/r$, whereas the contribution of the surface matter tends to zero for $\epsilon\to 0$. Therefore, by an appropriate choice of ϵ, the ratio of the surface energy to the electric energy can be made arbitrarily small.

Gluing at $r=0$ has the advantage that all geodesics are everywhere C^3. On the other hand, gluing at some $\epsilon>0$ avoids the singularities in the metric and the electric field, but entails surface matter.

II. THE GLOBAL STRUCTURE OF THE REIßNER–NORDSTRØM SOLUTION

The Reißner–Nordstrøm solution[3,4] to Einstein's equations

$$R_{ik}-\frac{1}{2}Rg_{ik}=\frac{8\pi G}{c^2}T_{ik}, \quad G\text{: Newton's gravitational constant,}$$

describes a static spherically symmetric object with electric and magnetic fields. It is given by the metric

$$ds^2=\frac{\Delta}{r^2}dt^2-\frac{r^2}{\Delta}dr^2-r^2d\Omega^2 \tag{2}$$

with the abbreviations

$$\Delta=r^2-2Mr+Q^2$$

and

$$d\Omega^2=d\vartheta^2+\sin^2\vartheta\, d\varphi^2.$$

Here M and Q are constants determined by the mass m, the electric charge q and the magnetic charge q_m, respectively, of the object:

$$M=\frac{2Gm}{c^2}; \quad Q^2=\frac{G}{4\pi\epsilon_0 c^4}(q^2+q_m^2).$$

So, the Reißner–Nordstrøm solution may also contain a magnetic monopole. But in the following, we will set $q_m=0$, unless the contrary is stated explicitly.

We shall restrict ourselves to the case $M^2>Q^2$. For elementary particles, this condition is violated by many orders of magnitude. On the other hand, all ''elementary'' objects, i.e., quarks and leptons, have spin. Therefore the Reißner–Nordstrøm solution does not apply to them, no matter whether $M^2>Q^2$ or $M^2<Q^2$.

The construction of the maximal analytic extention starts from the three regions

$$A:\ 0<r<r_-,$$

$$B:\ r_-<r<r_+,$$

$$C:\ r_+<r<\infty.$$

Here r_+ and r_- are the zeros of Δ:

$$r_+ := M+\sqrt{M^2-Q^2}, \tag{3}$$

$$r_- := M-\sqrt{M^2-Q^2}. \tag{4}$$

It is convenient to introduce new coordinates u,v by

$$A \text{ and } C: \quad u := t-r_*, \quad v := t+r_*, \tag{5}$$

$$B: \quad u := t+r_*, \quad v := r_*-t, \tag{6}$$

with the abbreviation

$$r_* := \int \frac{r^2}{\Delta}\,dr = r+\frac{r_+^2}{r_+-r_-}\ln|r-r_+|-\frac{r_-^2}{r_+-r_-}\ln|r-r_-|. \tag{7}$$

Next, one constructs the new regions A', B' and C' from A, B and C, respectively, by replacing $u\mapsto -u$; $u\mapsto -v$ in (5) and (6). These six regions are composed to a periodic ''ladder'' according to Fig. 1 (see, e.g., Refs. 7 and 13). The transformations

$$A_n: U := \operatorname{arctg}(-e^{-\alpha u})+(n+1)\pi,$$

$$V := \operatorname{arctg}(e^{\alpha v})+n\pi,$$

$$B_n: U := \operatorname{arctg}(e^{\alpha u})+n\pi,$$

$$V := \operatorname{arctg}(e^{\alpha v})+n\pi,$$

$$C_n: U := \operatorname{arctg}(-e^{-\alpha u})+n\pi,$$

$$V := \operatorname{arctg}(e^{\alpha v})+n\pi,$$

$$A'_n: U := \operatorname{arctg}(-e^{-\alpha u})+(n-\tfrac{1}{2})\pi,$$

$$V := \operatorname{arctg}(e^{\alpha v})+(n-\tfrac{1}{2})\pi,$$

$$B'_n: U := \operatorname{arctg}(e^{\alpha u})+(n-\tfrac{1}{2})\pi,$$

$$V := \operatorname{arctg}(e^{\alpha v})+(n-\tfrac{1}{2})\pi,$$

$$C'_n: U := \operatorname{arctg}(-e^{-\alpha u})+(n+\tfrac{1}{2})\pi,$$

$$V := \operatorname{arctg}(e^{\alpha v})+(n-\tfrac{1}{2})\pi,$$

$$\alpha := (r_+-r_-)/(2r_+^2) \tag{8}$$

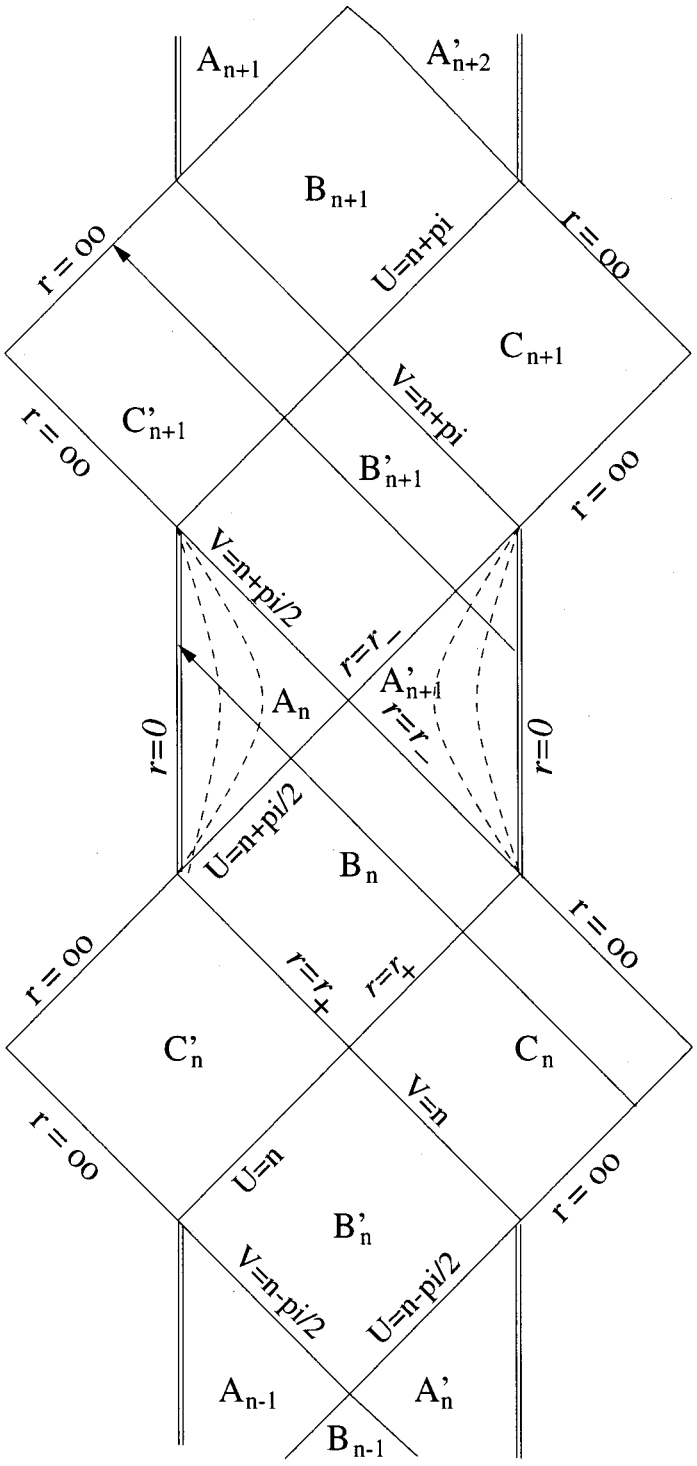

FIG. 1. Maximal analytic extension of the Reißner–Nordstrøm space–time. Dashed lines: $r=\text{const}$. The solid line with arrows shows a photon starting in C_n and passing to C'_{n+1} through a singularity.

define global parameters (U,V,ϑ,φ). Here $U+V$ may be interpreted as ''time,'' and $U-V$ as ''radius.'' With these coordinates, the line element (2) becomes

$$ds^2=-\frac{4}{\alpha^2 r^2}\frac{|r-r_+||r-r_-|}{\sin(2U)\sin(2V)}dUdV-r^2d\Omega^2. \tag{9}$$

It can be seen from Fig. 1 that this maximal analytic extension is not geodesically complete, because all radial spacelike and lightlike geodesics end in the singularities. This suggests to identify the singularities in A_n with those in A'_m for suitable pairs *m, n*. But, of course, the metric (9) and its derivatives are not defined in $r=0$. So it is not possible to apply here the usual rules[14,15] for gluing spaces in general relativity, i.e., to require that the metric (9) is at least C^2 in the tangential directions and C^1 in the normal direction. Instead, one considers the geodesics passing through the singularities. By definition, they need to be C^2-functions of their parameters. And in order to define ''geodesic'' coordinates, it is necessary,[16] that their limits for $r\to 0$ are at least C^3 in $A_n\cup A'_m$. But in general it is not possible to work with affine parameters, as the metric is singular at $r=0$.

The first step is to generalize differential manifolds in such a way that the singularities can be included. For this, the d-spaces of Refs. 8 and 9 will be used, which have been very useful in the discussion of Schwarzschild's metric, the radiation filled Friedmann universe and some more exotic space–times.[17,18] The basic idea is to replace the coordinate functions in the definition of differential manifolds by a more general set *C* of functions. In particular, no compatibility conditions between different charts are needed. The only requirement is that one can add, substract and multiply the functions in *C*. This leads to the following definition:

Let *M* be a topological space. The pair (*M, C*) is called d-space, if *C* is a sheaf of continuous real-valued functions on *M* which form an algebra w.r.t. pointwise operation.

For these d-spaces, it is simple to construct the tangent vectors as ''directional derivatives:''

Let (*M, C*) be a d-space and C_x the stalk at $x\in M$. A map

$$V:C_x\to\mathbb{R}$$

is called tangent vector to (*M, C*) in *x*, if for all $n\in\mathbb{N}$, all $f_1,\ldots,f_n\in C_x$, and all germs α of $C^1(\mathbb{R}^n,\mathbb{R})$ at $y:=(f_1(x),\ldots,f_n(x))\in\mathbb{R}^n$, the equation

$$V(\alpha\circ(f_1(x),\ldots,f_n(x)))=\sum_{i=1}^{n}(\partial_i\alpha)\cdot V(f_i)$$

holds, provided $\alpha\circ(f_1,\ldots,f_n)\in C_x$. Here $\partial_i\alpha$ denotes the partial derivative of α w.r.t. the *i*th argument.

For the construction of geodesics, it is necessary to have some theory of differential equations. In general, such a theory does not exist. But in the case under discussion, the regular points are dense in the d-space. Here the results of Ref. 12 guarantee existence and uniqueness of the solutions.

In such a theory it is possible to glue the singular points in A_n to those in A'_m. It is natural to require $m=n+1$ and to identify points with equal ''local times'' *t* or with equal ''global times'' $U+V$. We choose the latter possibility: If the points $(r=0,\,t)\in A_n$ are identified with the points $(r=0,\,t)\in A'_{n+1}$, there exist causal geodesics, which come arbitrarily close to themselves. To see this, regard the lines in Fig. 1 with $U=n+\pi/2$ or $V=n+\pi/2$. A lightlike geodesic just below such a line would be continued to a geodesic just above that line.

Gluing points with $r=0$ and equal values of $U+V$ entails a time reflexion, i.e., an identification of the points $(r=0,\,t)$ in A_n with the points $(r=0,\,-t)$ in A'_{n+1}.

III. THE GEODESICS IN $r=0$

The geodesics are most easily computed in the local coordinates (r,ϑ,φ,t). The method is similar to that used for Schwarzschild's solution: Because of spherical symmetry, it is possible to put $\vartheta=\pi/2=\text{const}$. In this way, the equations are considerably simplified, and the first integrals are easily obtained. The results for spacelike geodesics are[13]

$$\frac{d\varphi}{d\tau}=\frac{L}{r^2}, \tag{10}$$

$$\frac{dt}{d\tau}=E\frac{r^2}{\Delta}, \tag{11}$$

$$\left(\frac{dr}{d\tau}\right)^2=E^2+\frac{\Delta}{r^2}\left(1-\frac{L^2}{r^2}\right). \tag{12}$$

Here E and L are constants of integration. It can be seen from (12) that spacelike geodesics in A_n and in A'_m reach the value $r=0$, if and only if $L=0$ (radial geodesics). In the limit $r\to 0$, Eqs. (10)–(12) yield for $L=0$

$$\frac{d}{d\tau}(r(\tau),\vartheta(\tau),\varphi(\tau),t(\tau))\to\left(\pm\frac{Q}{r},0,0,E\frac{r^2}{Q^2}\right) \tag{13}$$

or

$$(r(\tau),\vartheta(\tau),\varphi(\tau),t(\tau))\to\left(\pm\sqrt{2|Q\tau|},\frac{\pi}{2},\varphi_0,\text{sign}(\tau)\frac{E}{|Q|}\tau^2+t_0\right). \tag{14}$$

These equations show that the radial spacelike geodesics can be continued through the singularities such that they are (at least) C^3 in the sense of d-spaces. This includes the fact that they are three times continuously differentiable on $A_n\cup A'_{n+1}-\{(r=0,\ t)|t\in\mathbb{R}\}$. But this is only true, if suitable curve parameters σ (not the arc length τ, but, e.g., $\sigma:=\tau/r$) and appropriate constants of integration are chosen [positive sign in (14) and positive (resp. negative) sign in (13) for $Q\tau>0$ (resp. <0); E and t_0 change their sign in $\tau=0$]. Notice that in $\sigma=0$ both $dr/d\sigma$ and $t(\sigma)$ have to change sign. Otherwise, the geodesics are not C^3. A general discussion of the gluing conditions can be found in Ref. 16.

Of course, the arc length τ is not a good parameter near $r=0$, because the metric is singular and τ is not well defined. If the tangent points in the r-direction, i.e., if $E=0$, Eq. (12) yields

$$\frac{dr}{d\tau}=\pm\sqrt{\frac{\Delta}{r^2}} \tag{15}$$

with the solution (remember that $\Delta\geqslant 0$ holds in A and A')

$$\sqrt{\Delta}+M\ln(M-r-\sqrt{\Delta})=\pm\tau+\tau_0.$$

Here τ_0 is a constant of integration. This implicit equation for $r(\tau)$ shows that the r-lines are geodesics which can be continued through the singularities.

In addition to the spacelike geodesics, also the radial lightlike geodesics reach the singulatity. Their equations can be derived as in the spacelike case.[13] With an affine parameter τ they read

$$\frac{dr}{d\tau}=\pm E,$$

$$\frac{dt}{d\tau}=\frac{Er^2}{\Delta}, \tag{16}$$

$$\frac{d\vartheta}{d\tau}=\frac{d\varphi}{d\tau}=0.$$

This yields

$$\frac{dr}{dt}=\pm\frac{\Delta}{r^2}$$

with the solution

$$t=\pm r_*+\text{const}$$

[cf. (7)]. It is convenient to choose the parameter τ such that $r(0)=0$ holds. If in addition the constant E changes sign in $r=0$, then these geodesics are of class C^∞ in $r=0$ [in the local coordinates U and V modulo $\pi/2$; cf. (8) and Ref. 19].

IV. THE CHARGE IN THE REIßNER–NORDSTRØM SOLUTION

The electromagnetic field tensor of the Reißner–Nordstrøm solution is[6]

$$F=\frac{1}{4\pi\epsilon_0}\left(\frac{q}{r^2}\frac{\partial}{\partial t}\wedge\frac{\partial}{\partial r}+\frac{q_m}{r^4\sin\vartheta}\frac{\partial}{\partial\vartheta}\wedge\frac{\partial}{\partial\varphi}\right). \tag{17}$$

From this, the components j^i of the four current can be computed:

$$j^i=F^{ik}_{;k}. \tag{18}$$

Here the semicolon denotes the covariant derivative. For $r>0$, it follows immediately from (20) that the components j^1 and j^2 vanish. The other components are

$$j^3=\frac{-1}{4\pi\epsilon_0}\left[\frac{d}{d\vartheta}\left(\frac{q_m}{r^4\sin\vartheta}\right)+\frac{q_m}{r^4\sin\vartheta}\cot\vartheta\right]=0$$

and

$$j^4=\frac{q}{4\pi\epsilon_0}\left(\frac{2}{r^3}-\frac{2}{r^3}\right)=0.$$

At $r=0$, Eq. (18) cannot be used, as F diverges. But it is possible to compute the exterior derivative by Gauß's theorem. This means to discuss the electric field lines near $r=0$. In our coordinates, these are the r-lines. It has been shown in the last section that they pass through the singularities. Therefore the divergence of the electric field vanishes: After gluing the space–time, the ϵ-neighborhood V of the points $r=0$ consists of two balls with center at $r=0$: one in A_n, and one in A'_{n+1}. Consider

$$\int_V J=\int_V dF^*=\int_V d(\epsilon_{ijkl}F^{kl}dx^i\wedge dx^j)=\int_{\partial V}\epsilon_{ijkl}F^{kl}dx^i\wedge dx^j \tag{19}$$

with $q_m=0$. Then only the components $(k,l)=(1,4)$ contribute. As the field lines crossing the sphere in A_n pass it from outside to inside, while they pass the sphere in A'_{n+1} in the opposite direction, the total surface integral over ∂V vanishes. This is even true, if $q_m\neq 0$: The term F^{23} in

(19) is present only in integrals in the x^1- and x^4-directions. But in the x^1-integration, the contribution from A_n cancels that from A'_{n+1}. So also this integral vanishes, and we finally get

$$\int_V J = 0.$$

V. ENERGY AND MOMENTUM

In this section, we glue the space–time not in the singularity $r=0$, but at finite values of r. For this, we choose some ϵ satisfying $0<\epsilon<r_-$ [see (4)] and delete all points with $r<\epsilon$. Then we identify the points $(r=\epsilon,\ t)$ in A_n with the points $(r=\epsilon,\ -t)$ in A'_{n+1} in a similar way as we did before. The stability of such surfaces $r=\epsilon$ between two parts of Reißner–Nordstrøm space–times has been discussed by Visser.[5,6]

The r-lines are geodesics perpendicular to the boundary $r=\epsilon$. If one follows such a line, the r-values first decrease, until the boundary $r=\epsilon$ is reached. Then they increase again. But, of course, at the boundary $dr/d\tau \neq 0$ [cf. (15)]. Therefore the derivatives of the metric in the direction of τ are discontinuous and the Einstein tensor gets additional terms proportional to $\delta(r-\epsilon)$.[14,15] The existence of such terms can also be seen from a simple consideration: If they would be absent, the radial lightlike geodesics would go on to the singularity $r=0$. But at $r=\epsilon$, they have to change their direction towards increasing r-values. Therefore some interaction is needed which forces them to do this.

In the coordinates (r,ϑ,φ,t), the only nonvanishing Christoffel symbols are

$$\Gamma^1_{11} = \frac{1}{2}\,\frac{-2M/r^2+2Q^2/r^3}{1-2M/r+Q^2/r^2},$$

$$\Gamma^1_{22} = -\left(1-\frac{2M}{r}+\frac{Q^2}{r^2}\right)\cdot r,$$

$$\Gamma^1_{33} = -\left(1-\frac{2M}{r}+\frac{Q^2}{r^2}\right)\cdot r\sin^2\vartheta,$$

$$\Gamma^1_{44} = -\frac{1}{2}\left(1-\frac{2M}{r}+\frac{Q^2}{r^2}\right)\left(-\frac{2M}{r^2}+\frac{2Q^2}{r^3}\right),$$

$$\Gamma^2_{12} = \Gamma^2_{21} = \frac{1}{r}, \tag{20}$$

$$\Gamma^2_{33} = -\sin\vartheta\cos\vartheta,$$

$$\Gamma^3_{13} = \Gamma^3_{31} = \frac{1}{r},$$

$$\Gamma^3_{23} = \Gamma^3_{32} = \cot\vartheta,$$

$$\Gamma^4_{14} = \Gamma^4_{41} = -\frac{1}{2}\,\frac{-2M/r^2+2Q^2/r^3}{1-2M/r+Q^2/r^2}.$$

The normal to the boundary, pointing away from the region A, resp. A', has the components

$$(n_i) = \left(\frac{-1}{\sqrt{1-2M/\epsilon+Q^2/\epsilon^2}},0,0,0\right);\quad n^i n_i = -1. \tag{21}$$

The second fundamental form K of the boundary is defined by

$$K_{ij}=-\tfrac{1}{2}((\nabla_i\, n)_j+(\nabla_j\, n)_i);\quad i,j=2,3,4.$$

Together with (20), this yields in the limit $r\to\epsilon,\ r<\epsilon$,

$$K_{22}=\epsilon\sqrt{1-2M/\epsilon+Q^2/\epsilon^2},$$

$$K_{33}=\epsilon\sin^2\vartheta\sqrt{1-2M/\epsilon+Q^2/\epsilon^2}, \tag{22}$$

$$K_{44}=-(M/\epsilon^2-Q^2/\epsilon^3)\sqrt{1-2M/\epsilon+Q^2/\epsilon^2}.$$

All other components of K vanish. Therefore the energy-momentum tensor T gets the additional terms from the boundary[6]

$$Z_{ij}=\frac{c^2}{4\pi G}\,\delta(r-\epsilon)(-K_{ij}+K^r_r g_{ij});\quad i,j,r=2,3,4.$$

For K^r_r, (22) yields

$$K^r_r=\frac{-2+3M/\epsilon-Q^2/\epsilon^2}{\epsilon\sqrt{1-2M/\epsilon+Q^2/\epsilon^2}}.$$

In the limit $\epsilon\to 0$, the leading terms in K^r_r are $-|Q|/\epsilon^2$. So one obtains

$$Z_{44}\to\frac{-c^2\delta(r-\epsilon)}{4\pi G}\,\frac{2|Q|^3}{\epsilon^4}. \tag{23}$$

The additional energy due to the gluing is

$$E=\frac{1}{6}\int u^r Z^i_r\epsilon_{ijkl}dx^j dx^k dx^l,$$

where ϵ_{ijkl} is defined as

$$\epsilon_{ijkl}=\sqrt{|\det g|}\begin{cases}+1\\0\\-1\end{cases}$$

and u is the four-velocity of an observer at rest:

$$(u^r)=\left(0,0,0,\frac{1}{\sqrt{1-2M/\epsilon+Q^2/\epsilon^2}}\right).$$

Equation (23) shows that the additional energy E is negative and tends to zero, if ϵ goes to zero. Therefore there is exotic matter (i.e., matter violating the average null energy condition) on the surface $r=\epsilon$, but its contribution to the total energy can be made arbitrarily small: Remember that the components $T^{(em)i}_j$ of the electromagnetic energy-momentum tensor are proportional to $1/\epsilon^4$ [see (17)]. So we obtain the well-known result that the electromagnetic energy E' is proportional to $1/\epsilon$, i.e., the ratio between the electromagnetic energy and the surface energy becomes arbitrarily large. Therefore also the stability of the system is completely determined by the electromagnetic self-energy.

To sum up, we have the following results: Gluing the two parts of the Reißner–Nordstrøm solution at some small $r=\epsilon>0$ avoids the infinite self-energy of a point charge and the singu-

larities in the metric. Furthermore, although there exists exotic surface matter, its contribution to the total energy can be made arbitrarily small, if ϵ tends to zero. On the other hand, if the two parts of the Reißner–Nordstrøm solution are glued together in the singularity $r=0$, there is no surface energy.

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Inhomogeneous M-theory cosmologies

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We study a class of inhomogeneous and anisotropic G_2 string cosmological models. In the case of separable G_2 models we show that the governing equations reduce to a system of ordinary differential equations. We focus on a class of separable G_2 M-theory cosmological models, and study their qualitative behavior (a class of models with time-reversed dynamics is also possible). We find that generically these inhomogeneous M-theory cosmologies evolve from a spatially inhomogeneous and negatively curved model with a nontrivial form field toward spatially flat and spatially homogeneous dilaton-moduli-vacuum solutions with trivial form fields. The late time behavior is the same as that of spatially homogeneous models previously studied. However, the inhomogeneities are not dynamically insignificant at early times in these models. © *2002 American Institute of Physics.*
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I. STRING COSMOLOGY

Nonperturbative M-theory encompasses and unifies all five anomaly free, perturbative superstring theories[1] and corresponds to eleven-dimensional supergravity in the low-energy limit.[2] In particular, the compactification of M-theory on a circle, S^1, leads to the type IIA superstring. A study of the qualitative cosmological effects that can arise in M-theory is therefore of considerable importance. To lowest order (in the inverse string tension), the tree-level effective action for massless fields contains a dilaton, a form field (which in four-dimensions is dynamically dual to pseudoscalar axion field) and (a) stringy cosmological constant(s). Even in this approximation the one-loop string equations of motion for inhomogeneous backgrounds are very difficult to solve, and it is a useful first step to consider models in which the homogeneity is broken only in one spatial direction. Metrics that admit two commuting (orthogonally transitive) space-like Killing vectors are referred to as G_2 space–times.

String models admitting an Abelian group, G_2, of isometries have a number of important physical applications. The spatially homogeneous Bianchi types I–VII$_h$ and locally rotationally symmetric (LRS) types VIII and IX admit a G_2 group of isometries[3] and so the G_2 cosmologies can be considered as inhomogeneous generalizations of these Bianchi models. Nonlinear inhomogeneities in the dilaton and axion fields can be investigated and, in principle, this allows density perturbations in string-inspired inflationary models such as the pre-big bang scenario to be studied.[4,5] Given the potential importance of this scenario it is important to study its generality with respect to inhomogeneities as well with respect to anisotropies. The general effects of small inhomogeneities and anisotropies have been studied by Veneziano.[4]

In general relativity (GR) the generic singularity is neither spatially homogeneous nor isotropic. Hence it is of interest to study more general models. In particular, it has been conjectured that G_2 metrics represent a first approximation to the general solution of Einstein gravity in the vicinity

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of a curvature singularity.[6–9] The high curvature regime is precisely the regime where stringy deviations from GR are expected to be significant. The G_2 models studied here may therefore provide insight into the generic behavior of cosmologies at very early times.

A number of exact inhomogeneous and anisotropic G_2 string cosmologies have been found. Barrow and Kunze studied an inhomogeneous generalization of the Bianchi type I string cosmology[10] and Feinstein, Lazkoz, and Vazquez-Mozo derived a closed, inhomogeneous model by applying duality transformations on the LRS Bianchi type IX cosmology.[11] Clancy *et al.* have found inhomogeneous generalizations of the Bianchi type VI_h universe and have studied their asymptotic behavior.[12]

In general, the field equations reduce to a system of coupled, partial differential equations in two variables when spatial homogeneity is broken along a single direction. Unfortunately, these equations are still very complicated. However, solutions can be found due to the noncompact global symmetries of the string effective action. When the metric admits two commuting spacelike Killing vectors, there exists an infinite-dimensional symmetry on the space of solutions that may be identified infinitesimally with the O(2,2) current algebra.[13–15] This symmetry reduces to the Geroch group, corresponding to the SL(2,R) current algebra, when the dilaton and two-form potential are trivial,[16] and includes the global SL(2,R) S-duality of the action.

New inhomogeneous G_2 string cosmologies containing a nontrivial two-form potential may be generated by an application of both the S- and T-duality symmetries from simpler (dilaton-vacuum) seed solutions. Lidsey *et al.*[17] discuss the noncompact, global symmetries of the string effective action in a variety of settings and review various methods for solving the Einstein-scalar field equations utilizing generating techniques (from solutions with a minimally coupled, massless scalar field from a vacuum, G_2 cosmology). In particular, Feinstein, Lazkoz, and Vázquez-Mozo[11] present an algorithm which permits the construction of inhomogeneous string solutions by employing a Buscher transformation, inverse scattering techniques,[7,8] followed by the generating technique of Wainwright, Ince, and Marshman.[18] Feinstein *et al.* employ this algorithm to generate a closed, inhomogeneous string cosmology with S^3 topology from a LRS Bianchi type IX solution.[11,19] However, this algorithm involves a number of nontrivial operations, and an alternative and more straightforward approach is to apply an O(2,2) transformation directly to the seed cosmology.[17]

In this paper we shall consider a class of separable string cosmological models whose governing equations reduce to ordinary differential equations (ODE) which can be studied by qualitative methods. In particular, we shall focus on a class of M-theory cosmological models.

II. STRING ACTION

We consider the general string action in the form[20]

$$S=\int \mathrm{d}^4x\sqrt{-g}\left\{e^{-\Phi}\left[R+(\nabla\Phi)^2-6(\nabla\beta)^2-\frac{1}{2}e^{2\Phi}(\nabla\sigma)^2-2\Lambda\right]-\frac{1}{2}Q^2e^{-6\beta}-\Lambda_M\right\}, \quad (2.1)$$

in terms of the pseudoscalar axion field, σ, the four-dimensional dilaton field Φ, and the modulus field β, where Λ and Λ_M represent cosmological constant terms and Q^2 may be interpreted as a zero-form field strength. This is a phenomenological action representing the bosonic sector of the effective supergravity action for the low-energy limit of M-theory and encompasses other string theories.[20] We are particularly interested in the class of four-dimensional cosmologies derived from the type IIA string and M-theory effective actions and which include a nontrivial Ramond–Ramond (RR) sector.[21] In these models a specific compactification from eleven to four dimensions was considered, where the topology of the internal dimensions was assumed to be a product space consisting of a circle and an isotropic six-torus;[21] this is dynamically equivalent to compactifications on a Calabi–Yau threefold.[22] The FRW models in this class of cosmologies was studied in Ref. 21.

Defining

$$\mathcal{L}_M=-3e^{-\Phi}(\nabla\beta)^2-\frac{1}{4}e^{\Phi}(\nabla\sigma)^2-\Lambda e^{-\Phi}-\frac{1}{4}Q^2e^{-6\beta}-\frac{1}{2}\Lambda_M;\quad T_{\alpha\beta}\equiv g_{\alpha\beta}\mathcal{L}_M-2\frac{\partial\mathcal{L}_M}{\partial g^{\alpha\beta}},$$

the Euler–Lagrange equations then lead to the field equations (FE)[23]

$$G_{\mu\nu}=-\nabla_\mu\nabla_\nu\Phi+6\nabla_\mu\beta\nabla_\nu\beta+\tfrac{1}{2}e^{2\Phi}\nabla_\mu\sigma\nabla_\nu\sigma-\tfrac{1}{2}g_{\mu\nu}[(\nabla\Phi)^2+6(\nabla\beta)^2+\tfrac{1}{2}e^{2\Phi}(\nabla\sigma)^2+2\Lambda$$
$$+\tfrac{1}{2}Q^2e^{\Phi-6\beta}+\Lambda_Me^{\Phi}-2\Box\Phi],\tag{2.2a}$$

$$\Box\Phi=\tfrac{1}{2}(\nabla\Phi)^2+3(\nabla\beta)^2-\tfrac{1}{4}e^{2\Phi}(\nabla\sigma)^2+\Lambda-\tfrac{1}{2}R,\tag{2.2b}$$

$$\Box\beta=\nabla_\mu\Phi\nabla^\mu\beta-\tfrac{1}{4}Q^2e^{\Phi-6\beta},\tag{2.2c}$$

$$\Box\sigma=-\nabla_\mu\Phi\nabla^\mu\sigma.\tag{2.2d}$$

In Eqs. (2.2a)–(2.2d), greek indices take on values 0, 1, 2, 3, and units are chosen so that $16\pi\hat{G}=1$.

III. G_2 COSMOLOGIES

Let us examine (2.2) within the context of G_2 cosmological models described by the line element

$$ds^2=e^{2F}(-dt^2+dz^2)+e^{G}(e^{q}\,dx^2+e^{-q}\,dy^2),\tag{3.1}$$

where the metric functions $\{F,G,q\}$ and the string functions $\{\Phi,\beta,\sigma\}$ are all functions of t and z only. For any $q(t,z)$, we define $\dot{q}\equiv\partial q/\partial t$, $q'\equiv\partial q/\partial z$, and $\Delta^2q\equiv\ddot{q}-q''$. The local behavior of these models is determined by the gradient $B_\mu\equiv\partial_\mu G$, and cosmological solutions arise if B_μ is globally time-like.

Also, the Ricci scalar is given by

$$R=\tfrac{1}{2}e^{-2F}[4\Delta^2G+4\Delta^2F+3(\dot{G}^2-G'^2)+(\dot{q}^2-q'^2)].\tag{3.2}$$

Using these expressions, and defining the modified dilaton field,

$$\varphi\equiv\Phi-F-G,\tag{3.3}$$

the field equations become

$$\Delta^2\varphi=\tfrac{1}{2}[(\dot{\varphi}+\dot{F})^2-(\varphi'+F')^2]+\tfrac{1}{4}(\dot{G}^2-G'^2)+\tfrac{1}{4}(\dot{q}^2-q'^2)+3(\dot{\beta}^2-\beta'^2)$$
$$-\tfrac{1}{4}e^{2\varphi+2F+2G}(\dot{\sigma}^2-\sigma'^2)-\Lambda e^{2F},\tag{3.4a}$$

$$\Delta^2\beta=[(\dot{\varphi}+\dot{F})\dot{\beta}-(\varphi'+F')\beta']+\tfrac{1}{4}Q^2e^{\varphi+3F+G-6\beta},\tag{3.4b}$$

$$\Delta^2\sigma=-[(\dot{\varphi}+\dot{F}+2\dot{G})\dot{\sigma}-(\varphi'+F'+2G')\sigma'],\tag{3.4c}$$

$$\Delta^2q=[(\dot{\varphi}+\dot{F})\dot{q}-(\varphi'+F')q'],\tag{3.4d}$$

$$\Delta^2F=\tfrac{1}{2}(\dot{\varphi}+\dot{F})^2-\tfrac{1}{2}(\varphi'+F')^2-\tfrac{1}{4}(\dot{G}^2-G'^2)-\tfrac{1}{4}(\dot{q}^2-q'^2)-3(\dot{\beta}^2-\beta'^2)$$
$$+\tfrac{1}{4}e^{2\varphi+2F+2G}(\dot{\sigma}^2-\sigma'^2)-\Lambda e^{2F}-\tfrac{1}{2}Q^2e^{\varphi+3F+G-6\beta}-\Lambda_Me^{\varphi+3F+G},\tag{3.4e}$$

$$\Delta^2 G=[(\dot{\varphi}+\dot{F})\dot{G}-(\varphi'+F')G']+(\dot{\sigma}^2-\sigma'^2)e^{2\varphi+2F+2G}-\tfrac{1}{2}Q^2e^{\varphi+3F+G-6\beta}-\Lambda_M e^{\varphi+3F+G}, \tag{3.4f}$$

$$(\dot{\varphi}+\dot{F})^{\cdot}+(\varphi'+F')'=2(\dot{\varphi}+\dot{F})\dot{F}+2(\varphi'+F')F'+\tfrac{1}{2}(\dot{G}^2+G'^2)+\tfrac{1}{2}(\dot{q}^2+q'^2)+6(\dot{\beta}^2+\beta'^2)$$
$$+\tfrac{1}{2}(\dot{\sigma}^2+\sigma'^2)e^{2\varphi+2F+2G}, \tag{3.4g}$$

$$(\dot{\varphi}+\dot{F})'=\tfrac{1}{2}\dot{G}G'+\tfrac{1}{2}\dot{q}q'+6\dot{\beta}\beta'+F'(\dot{\varphi}+\dot{F})+\dot{F}(\varphi'+F')+\tfrac{1}{2}e^{2\varphi+2F+2G}\dot{\sigma}\sigma'. \tag{3.4h}$$

These equations reduce to those in Refs. 20 and 21 in the appropriate limits.

IV. SEPARABLE G_2 STRING COSMOLOGIES

A. General case

Let us assume separability of the metric functions of the form

$$F(t,z)\equiv F(t)+f(z),\quad G(t,z)\equiv G(t)+g(z),\quad q(t,z)\equiv q(t)+\nu(z),$$

and appropriate separability conditions on the matter fields $\Phi(t,z)$, $\beta(t,z)$, $\sigma(t,z)$. Then the Ricci scalar is given by

$$R=\tfrac{1}{2}e^{-2F-2f}[4\ddot{G}+4\ddot{F}+3\dot{G}^2+\dot{q}^2-(4g''+4f''+3g'^2+\nu'^2)].$$

If

$$4g''+4f''+3g'^2+\nu'^2=C, \tag{4.1}$$

where C is a constant, then we obtain a condition which constrains the spatial dependence of the metric. The Ricci scalar is then given by

$$R=\tfrac{1}{2}e^{-2F-2f}[4\ddot{G}+4\ddot{F}+3\dot{G}^2+\dot{q}^2-C].$$

Putting this expression for the Ricci scalar into the action (2.1), the spatial dependence of the geometrical terms can be eliminated (by integration over the spatial coordinates in the action). After applying any further separability conditions (on the matter fields), the resulting FE will be a system of ODEs. Note that the effect of the spatial dependence is to add a further contribution (C) to the cosmological constant Λ in the action.

B. Specific example: Linear dependence in z

In an attempt to remove the z dependence, let us assume separability of the form

$$F(t,z)\equiv F(t)+\tfrac{1}{2}cz,\quad G(t,z)\equiv G(t),\quad q(t,z)\equiv q(t)+az,$$

$$\Phi(t,z)\equiv\Phi(t)+mz,\quad \beta(t,z)\equiv\beta(t)+nz,$$

$$\sigma(t,z)\equiv\sigma(t)+lz,$$

where a, c, l, m, n are constants [a^2 is equivalent to the constant C in Eq. (4.1)], and therefore

$$\varphi(t,z)=\Phi(t)-F(t)-G(t)+(m-\tfrac{1}{2}c)z\equiv\varphi(t)+(m-\tfrac{1}{2}c)z.$$

With the above-given assumptions, the metric becomes an extension of the inhomogeneous scalar-field G_2 solutions found by Feinstein and Ibanez[24] to M-theoretical models. In addition, for particular values of the parameters, the metric reduces to spatially homogeneous Bianchi I, III, and VI_0 models. Hence,

$$\ddot{\varphi}=\tfrac{1}{2}(\dot{\varphi}+\dot{F})^2+\tfrac{1}{4}\dot{G}^2+\tfrac{1}{4}\dot{q}^2+3\dot{\beta}^2-\tfrac{1}{4}e^{2\varphi+2F+2G+2mz}(\dot{\sigma}^2-l^2)-\Lambda e^{2F+cz}-\tfrac{1}{4}(a^2+2m^2+12n^2), \tag{4.2a}$$

$$\ddot{\beta}=(\dot{\varphi}+\dot{F})\dot{\beta}+\tfrac{1}{4}Q^2e^{[\varphi+3F+G-6\beta+(c+m-6n)z]}-mn, \tag{4.2b}$$

$$\ddot{\sigma}=-(\dot{\varphi}+\dot{F}+2\dot{G})\dot{\sigma}+ml, \tag{4.2c}$$

$$\ddot{q}=(\dot{\varphi}+\dot{F})\dot{q}-ma, \tag{4.2d}$$

$$\ddot{F}=\tfrac{1}{2}(\dot{\varphi}+\dot{F})^2-\tfrac{1}{4}\dot{G}^2-\tfrac{1}{4}\dot{q}^2-3\dot{\beta}^2+\tfrac{1}{4}e^{2\varphi+2F+2G+2mz}(\dot{\sigma}^2-l)-\Lambda e^{2F+cz}$$
$$-\tfrac{1}{2}Q^2e^{[\varphi+3F+G-6\beta+(c+m-6n)z]}-\Lambda_M e^{\varphi+3F+G+(c+m)z}+\tfrac{1}{4}(a^2-2m^2+12n^2), \tag{4.2e}$$

$$\ddot{G}=(\dot{\varphi}+\dot{F})\dot{G}+(\dot{\sigma}^2-l^2)e^{2\varphi+2F+2G+2mz}-\tfrac{1}{2}Q^2e^{[\varphi+3F+G-6\beta+(c+m-6n)z]}-\Lambda_M e^{\varphi+3F+G+(c+m)z}, \tag{4.2f}$$

$$(\ddot{F}+\ddot{\varphi})=2(\dot{F}+\dot{\varphi}+m)(\dot{F}+\tfrac{1}{2}c)+\tfrac{1}{2}\dot{G}^2+\tfrac{1}{2}(\dot{q}+a)^2+6(\dot{\beta}+n)^2+\tfrac{1}{2}(\dot{\sigma}+l)^2e^{2\varphi+2F+2G+2mz}. \tag{4.2g}$$

Note that the constraint equation can be rewritten as

$$0=(\dot{F}+m)^2-\dot{\varphi}^2+c(\dot{F}+\dot{\varphi}+m)+\tfrac{1}{2}\dot{G}^2+\tfrac{1}{2}(\dot{q}+a)^2+6(\dot{\beta}+n)^2+\tfrac{1}{2}(\dot{\sigma}+l)^2e^{2\varphi+2F+2G+2mz}$$
$$+\Lambda e^{2F+cz}+\tfrac{1}{2}Q^2e^{[\varphi+3F+G-6\beta+(c+m-6n)z]}+\Lambda_M e^{\varphi+3F+G+(c+m)z}. \tag{4.3}$$

In order for the FE to be independent of z, it is necessary that $m=0$ and that either $c=0$ or $c=6n$. Furthermore if $c=0$ then we have that either $n=0$ or $Q=0$. In the $c=6n$ case, we have that $\Lambda=\Lambda_M=0$. It is the latter case that is of interest to us here. From here forth we shall assume that $c=6n$ and that $\Lambda=\Lambda_M=0$. This particular subcase, which is of relevence in M-theory cosmology, is of special physical interest. (The resulting FE in the remaining cases are displayed in Ref. 23.)

V. INHOMOGENEOUS M-THEORY COSMOLOGICAL MODELS

Substituting $c=6n$, $m=0$, $\Lambda=0$, $\Lambda_M=0$ into (3.4), (4.3) (and taking the linear combination [(4.2g)–(4.2e)–(4.2a)]) we obtain the following system of ODE with two constraints:

$$\ddot{\varphi}=\tfrac{1}{4}(\dot{q}^2+\dot{G}^2-a^2+2(\dot{\varphi}+\dot{F})^2+12\dot{\beta}^2-12n^2+e^{2\varphi+2F+2G}(l^2-\dot{\sigma}^2)), \tag{5.1a}$$

$$\ddot{\beta}=\dot{\beta}(\dot{\varphi}+\dot{F})+\tfrac{1}{4}Q^2e^{-6\beta+\varphi+3F+G}, \tag{5.1b}$$

$$\ddot{\sigma}=-\dot{\sigma}(\dot{\varphi}+\dot{F}+2\dot{G}), \tag{5.1c}$$

$$\ddot{q}=\dot{q}(\dot{\varphi}+\dot{F}), \tag{5.1d}$$

$$\ddot{F}=\tfrac{1}{4}(3a^2+\dot{q}^2+\dot{G}^2+36n^2+12\dot{\beta}^2+e^{2\varphi+2F+2G}(l^2+3\dot{\sigma}^2)-2(\dot{\varphi}-\dot{F})^2+8\dot{F}^2), \tag{5.1e}$$

$$\ddot{G}=\dot{G}(\dot{\varphi}+\dot{F})-e^{2\varphi+2F+2G}(l^2-\dot{\sigma}^2)-\tfrac{1}{2}Q^2e^{-6\beta+\varphi+3F+G}, \tag{5.1f}$$

$$0=2\dot{\varphi}^2-\dot{G}^2-\dot{q}^2-12\dot{\beta}^2-2\dot{F}^2-12n^2-a^2-e^{2\varphi+2F+2G}(l^2+\dot{\sigma}^2)-Q^2e^{-6\beta+\varphi+3F+G}, \tag{5.1g}$$

$$0=a\dot{q}+le^{2\varphi+2F+2G}\dot{\sigma}+6n(\dot{\varphi}+\dot{F}+2\dot{\beta}). \tag{5.1h}$$

From Eq. (5.1g) we are able solve for and make a global substitution for the quantity $Q^2e^{-6\beta+\varphi+3F+G}$. Making this substitution we have the following system of ODEs:

$$\ddot{\varphi}=\tfrac{1}{4}(\dot{q}^2+\dot{G}^2-a^2+2(\dot{\varphi}+\dot{F})^2+12\dot{\beta}^2-12n^2+e^{2\varphi+2F+2G}(l^2-\dot{\sigma}^2)), \tag{5.2a}$$

$$\ddot{\beta}=\tfrac{1}{4}(2\dot{\varphi}^2-\dot{G}^2-\dot{q}^2-12\dot{\beta}^2-2\dot{F}^2-12n^2-a^2-e^{2\varphi+2F+2G}(l^2+\dot{\sigma}^2))+\dot{\beta}(\dot{\varphi}+\dot{F}), \tag{5.2b}$$

$$\ddot{\sigma}=-\dot{\sigma}(\dot{\varphi}+\dot{F}+2\dot{G}), \tag{5.2c}$$

$$\ddot{q}=\dot{q}(\dot{\varphi}+\dot{F}), \tag{5.2d}$$

$$\ddot{F}=\tfrac{1}{4}(3a^2+\dot{q}^2+\dot{G}^2+36n^2+12\dot{\beta}^2+e^{2\varphi+2F+2G}(l^2+3\dot{\sigma}^2)-2(\dot{\varphi}-\dot{F})^2+8\dot{F}^2), \tag{5.2e}$$

$$\ddot{G}=\dot{G}(\dot{\varphi}+\dot{F})-e^{2\varphi+2F+2G}(l^2-\dot{\sigma}^2)-\tfrac{1}{2}(2\dot{\varphi}^2-\dot{G}^2-\dot{q}^2-12\dot{\beta}^2-2\dot{F}^2-12n^2-a^2 -e^{2\varphi+2F+2G}(l^2+\dot{\sigma}^2)), \tag{5.2f}$$

$$0=a\dot{q}+le^{2\varphi+2F+2G}\dot{\sigma}+6n(\dot{\varphi}+\dot{F}+2\dot{\beta}). \tag{5.2g}$$

From the constraint (5.1g) we see that if $\dot{\varphi}=0$, then all of the other state variables must be simultaneously zero, which can only occur at an equilibrium point of the system. Hence $\dot{\varphi}$ must be positive (or negative) throughout the physical phase space. Here we shall assume $\dot{\varphi}>0$ (the case $\dot{\varphi}<0$ can be obtained by a time reversal—see the following).

We define new variables of the form

$$\tilde{F}=\frac{\dot{F}}{\dot{\varphi}},\quad \tilde{G}=\frac{1}{\sqrt{2}}\frac{\dot{G}}{\dot{\varphi}},\quad \tilde{q}=\frac{1}{\sqrt{2}}\frac{\dot{q}}{\dot{\varphi}},\quad \tilde{\sigma}=\frac{1}{\sqrt{2}}e^{\varphi+F+G}\frac{\dot{\sigma}}{\dot{\varphi}},$$

$$\tilde{\beta}=\sqrt{6}\,\frac{\dot{\beta}}{\dot{\varphi}},\quad \tilde{\Psi}_1=\sqrt{\frac{a^2+12n^2}{2}}\frac{1}{\dot{\varphi}},\quad \tilde{\Psi}_2=\frac{1}{\sqrt{2}}e^{\varphi+F+G}\frac{l}{\dot{\varphi}}$$

and a new time variable

$$\frac{\mathrm{d}t}{\mathrm{d}\tau}=\frac{1}{\dot{\varphi}}. \tag{5.3}$$

The variables are chosen so that the transformed dynamical system has a compactified phase space. This property comes from the fact that $Q^2e^{-6\beta+\varphi+3F+G}\geqslant 0$ which implies that Eq. (5.1g) yields

$$1\geqslant\tilde{F}^2+\tilde{G}^2+\tilde{q}^2+\tilde{\sigma}^2+\tilde{\beta}^2+\tilde{\Psi}_1^2+\tilde{\Psi}_2^2. \tag{5.4}$$

The dynamical system (5.2) becomes

$$\frac{\mathrm{d}\tilde{F}}{d\tau}=\tilde{F}(2\tilde{F}-\tilde{r})+\frac{1}{2}(\tilde{q}^2+\tilde{G}^2+\tilde{\beta}^2+3\tilde{\sigma}^2+3\tilde{\Psi}_1^2+\tilde{\Psi}_2^2-(1-\tilde{F})^2), \tag{5.5a}$$

$$\frac{d\tilde{G}}{d\tau}=\tilde{G}(1+\tilde{F}-\tilde{r})-\frac{1}{\sqrt{2}}(1-\tilde{F}^2-\tilde{G}^2-\tilde{q}^2-3\tilde{\sigma}^2-\tilde{\beta}^2-\tilde{\Psi}_1^2+\tilde{\Psi}_2^2), \tag{5.5b}$$

$$\frac{d\tilde{q}}{d\tau}=\tilde{q}(1+\tilde{F}-\tilde{r}), \tag{5.5c}$$

$$\frac{d\tilde{\sigma}}{d\tau}=-\tilde{\sigma}(\sqrt{2}\tilde{G}+\tilde{r}), \tag{5.5d}$$

$$\frac{d\tilde{\beta}}{d\tau}=\tilde{\beta}(1+\tilde{F}-\tilde{r})+\frac{\sqrt{6}}{2}(1-\tilde{F}^2-\tilde{G}^2-\tilde{q}^2-\tilde{\sigma}^2-\tilde{\beta}^2-\tilde{\Psi}_1^2-\tilde{\Psi}_2^2), \tag{5.5e}$$

$$\frac{d\tilde{\Psi}_1}{d\tau}=-\tilde{\Psi}_1\tilde{r}, \tag{5.5f}$$

$$\frac{d\tilde{\Psi}_2}{d\tau}=\tilde{\Psi}_2(1+\tilde{F}+\sqrt{2}\tilde{G}-\tilde{r}), \tag{5.5g}$$

and

$$\tilde{r}=\tfrac{1}{2}[(1+\tilde{F})^2+\tilde{G}^2+\tilde{q}^2+\tilde{\beta}^2+\tilde{\Psi}_2^2-\tilde{\Psi}_1^2-\tilde{\sigma}^2],$$

where the constraint equation becomes

$$0=\sqrt{\frac{2}{a^2+12n^2}}\tilde{\Psi}_1\left[\sqrt{2}a\tilde{q}+6n\left(1+\tilde{F}+\frac{2}{\sqrt{6}}\tilde{\beta}\right)\right]+2\tilde{\Psi}_2\tilde{\sigma}. \tag{5.6}$$

There exists a first integral in the physical phase space $(\tilde{q}\neq 0,\tilde{\Psi}_1\neq 0)$ for this system. The function

$$M=\frac{\tilde{\sigma}\tilde{\Psi}_2}{\tilde{q}\tilde{\Psi}_1}$$

is constant, i.e., $M'=0$. This implies a first integral for the original system of ordinary differential equations (5.2)

$$\dot{q}=C\dot{\sigma}e^{2\varphi+2F+2G},$$

where C is a constant.

A. Invariant sets, monotonic functions

We first recall that the phase space for this dynamical system is the interior and boundary of the compact set given by

$$1\geqslant\tilde{F}^2+\tilde{G}^2+\tilde{q}^2+\tilde{\sigma}^2+\tilde{\beta}^2+\tilde{\Psi}_1^2+\tilde{\Psi}_2^2. \tag{5.7}$$

Various hyperplanes divide the phase space into a number of different regions, they are $\tilde{q}=0$, $\tilde{\sigma}=0$, $\tilde{\Psi}_1=0$, and $\tilde{\Psi}_2=0$ hyperplanes. We note that $\tilde{\Psi}_1=0$ divides the phase space into two distinct regions $\tilde{\Psi}_1<0$ and $\tilde{\Psi}_1>0$. The dynamics in the invariant set $\tilde{\Psi}_1<0$ is the time reversal of the dynamics in the invariant set $\tilde{\Psi}_1>0$ [see (5.3)].

Consider the function

$$M_1=\frac{\tilde{\sigma}^2\tilde{\Psi}_2^2}{\tilde{q}^4}$$

and its derivative

$$\frac{dM_1}{d\tau}=-2M_1(1+\tilde{F}).$$

We easily see that this function is monotonically decreasing in the invariant set $\tilde{q}\neq 0,\tilde{\sigma}\neq 0$, $\tilde{\Psi}_2\neq 0$. Therefore, we can conclude that there are no closed or periodic orbits in the seven-dimensional phase space, except possibly on the lower dimensional boundaries of this seven-dimensional invariant set.

We restrict ourselves now to the invariant set $\tilde{\sigma}=0$. Consider the function

$$M_2=\frac{\tilde{\Psi}_1^2}{\tilde{q}^2}$$

and its derivative

$$\frac{dM_2}{d\tau}=-2M_2(1+\tilde{F}).$$

We easily see that this function is monotonically decreasing in the invariant set $\tilde{q}\neq 0,\tilde{\Psi}_1\neq 0$. Therefore, we can conclude that there are no closed or periodic orbits in this six-dimensional phase space, except possibly on the lower dimensional boundaries of this six-dimensional invariant set.

In the six-dimensional invariant set $\tilde{\Psi}_2=0$, the function

$$M_3=\frac{\tilde{\Psi}_1^2}{\tilde{q}^2}$$

has the derivative

$$\frac{dM_3}{d\tau}=-2M_3(1+\tilde{F})$$

which is monotonically decreasing in the set $\tilde{\Psi}_2=0,\tilde{q}\neq 0,\tilde{\Psi}_1\neq 0$. Therefore we conclude that there are no closed or periodic orbits in this six-dimensional invariant set.

In the six-dimensional invariant set $\tilde{q}=0$, the function

$$M_4=\frac{\tilde{\sigma}^2\tilde{\Psi}_2^2}{\tilde{\Psi}_1^4}$$

has the derivative

$$\frac{dM_4}{d\tau}=2M_4(1+\tilde{F}),$$

which is monotonically increasing in the set $\tilde{q}=0,\tilde{\sigma}\neq 0,\tilde{\Psi}_2\neq 0$. Therefore we can conclude that there are no closed or periodic orbits in this six-dimensional set.

With the existence of these monotonic functions M_1, M_2, M_3, and M_4, we can conclude that there are no closed or periodic orbits in the physical six-dimensional phase space [except possibly on lower dimensional (less than 5) invariant sets].

The zero-curvature spatially homogeneous and isotropic space–times are contained in the set $\tilde{q}=\tilde{\Psi}_1=\tilde{\Psi}_2=\tilde{G}-\sqrt{2}\tilde{F}=0$ union $\tilde{q}=\tilde{\Psi}_1=\tilde{\sigma}=\widetilde{G-\sqrt{2}F}=0$.

The matter fields in (2.1) satisfy various energy conditions. For example, the positivity of the kinetic energy of the pseudoaxion scalar field, σ, demands that $\dot{\sigma}^2-l^2\geqslant 0$ (i.e., $\tilde{\sigma}^2-\tilde{\Psi}_2^2\geqslant 0$). However, we note that $\tilde{\sigma}^2-\tilde{\Psi}_2^2=0$ is not an invariant set.

B. Equilibrium points and exact solutions

There are two equilibrium points and one three-dimensional equilibrium set.

The three-dimensional equilibrium set is given by

$$\{\tilde{F}^2+\tilde{G}^2+\tilde{q}^2+\tilde{\beta}^2=1,\tilde{\sigma}=0,\tilde{\Psi}_1=0,\tilde{\Psi}_2=0\}.$$

Note that since both $\tilde{\Psi}_1=0$ and $\tilde{\Psi}_2=0$ we necessarily have that $a=n=l=0$. At this point the value of $\tilde{r}=1+\tilde{F}_0$. The exact solution is then

$$\varphi(t)=h_1-\frac{1}{\tilde{r}}\ln(\tilde{r}t+h_0),$$

$$F(t)=F_0\left(h_1-\frac{1}{\tilde{r}}\ln(\tilde{r}t+h_0)\right)+F_1,$$

$$G(t)=\sqrt{2}G_0\left(h_1-\frac{1}{\tilde{r}}\ln(\tilde{r}t+h_0)\right)+G_1,$$

$$q(t)=\sqrt{2}q_0\left(h_1-\frac{1}{\tilde{r}}\ln(\tilde{r}t+h_0)\right)+q_1,$$

$$\sigma(t)=\sigma_1,$$

$$\beta(t)=\frac{1}{\sqrt{6}}\beta_0\left(h_1-\frac{1}{\tilde{r}}\ln(\tilde{r}t+h_0)\right)+\beta_1,$$

where $F_0^2+G_0^2+q_0^2+\beta_0^2=1$ and where F_1, G_1, q_1, σ_1, β_1, h_1, and h_0 are integration constants.

Since $a=n=l=0$, this metric is spatially homogeneous (and flat). Since $\tilde{\sigma}=0$ and $Q=0$ (which follows from the other conditions), this equilibrium set represents spatially flat solutions where the form-fields (the axion field and the four-form field strength) are trivial and only the dilaton and moduli fields are dynamically important. These solutions are known as the ''dilaton-moduli-vacuum'' solutions (and their analytical form is given in Ref. 25).

Recall that the dynamics of these models is restricted by the constraint given by Eq. (5.6). At these equilibrium points we are able to locally solve for the value of $\tilde{\Psi}_1$ and substitute into the remaining equations. The eigenvalues in the six-dimensional constraint surface are

$$0,0,0,\sqrt{2}\tilde{G},-\sqrt{2}\tilde{G}-1-\tilde{F},-1+\tilde{F}+\sqrt{2}\tilde{G}-\sqrt{6}\tilde{\beta}.$$

The three zero eigenvalues correspond to the fact that this equilibrium set is three-dimensional. It is clear that a subset of this equilibrium set will act as saddles of varying degree of stability, while

another subset will act as sinks. Consequently, a subset of these dilaton-moduli-vacuum solutions with trivial form fields are sinks in the physical phase space, even in the presence of (negative) spatial curvature, and are thus generic attracting solutions.

A second equilibrium point is

$$\left\{\tilde{F}=-\frac{2}{3},\tilde{G}=0,\tilde{q}=0,\tilde{\beta}=-\frac{1}{\sqrt{6}},\tilde{\sigma}=\pm\frac{\sqrt{2}}{6},\tilde{\Psi}_1=\frac{\sqrt{2}}{3},\tilde{\Psi}_2=0\right\}.$$

Note that since $\tilde{\Psi}_2=0$ we necessarily have that $l=0$. At this point the value of $\tilde{r}=0$. [Note, since the dynamical system (5.5) is invariant under the transformation $(\tilde{\Psi}_1,\tilde{\Psi}_2)\rightarrow(-\tilde{\Psi}_1,-\tilde{\Psi}_2)$ there exists a corresponding equilibrium point with a $\tilde{\Psi}_1=-\sqrt{2}/3$.] The exact solution is then

$$\varphi(t)=h_0t+h_1,\quad F(t)=-\tfrac{2}{3}(h_0t+h_1)+F_1,\quad G(t)=G_1,$$

$$q(t)=q_1,\quad \sigma(t)=\mp e^{-1/3(h_0t+h_1)-(F_1+G_1)}+\sigma_1,\quad \beta(t)=-\tfrac{1}{6}(h_0t+h_1)+\beta_1,$$

where $h_0=\frac{3}{2}\sqrt{a^2+12n^2}$, $Q^2=\frac{1}{2}(a^2+12n^2)e^{6\beta_1-3F_1-G_1}$, and F_1, G_1, q_1, σ_1, β_1, h_1 are all constants. In this situation the variable $\tilde{q}$ can be eliminated. The eigenvalues restricted to the constraint surface are

$$\tfrac{1}{3},\tfrac{1}{3},\tfrac{1}{6}(1\pm\sqrt{15+8\sqrt{2}i}),\tfrac{1}{6}(1\pm\sqrt{15-8\sqrt{2}i}).$$

This point represents a past attractor or a source. This corresponds to a spatially nonvacuum inhomogeneous model with a diagonal Einstein tensor, having negative curvature.

The line element corresponding to this solution (after a few coordinate redefinitions) is

$$ds^2=C^2e^{-2\sqrt{a^2+12n^2}t+6nz}(-dt^2+dz^2)+(e^{az}dx^2+e^{-az}dy^2). \tag{5.8}$$

The third equilibrium point is

$$\left\{\tilde{F}=-\frac{5}{7},\tilde{G}=\frac{\sqrt{2}}{7},\tilde{q}=0,\tilde{\beta}=-\frac{\sqrt{6}}{7},\tilde{\sigma}=0,\tilde{\Psi}_1=\frac{2\sqrt{3}}{7},\tilde{\Psi}_2=0\right\}.$$

Note that since $\tilde{\Psi}_2=0$ we necessarily have that $l=0$. At this point the value of $\tilde{r}=0$. [Note, since the dynamical system (5.5) is invariant under the transformation $(\tilde{\Psi}_1,\tilde{\Psi}_2)\rightarrow(-\tilde{\Psi}_1,-\tilde{\Psi}_2)$ there exists a corresponding equilibrium point with a $\tilde{\Psi}_1=-2\sqrt{3}/7$.] The exact solution is then

$$\varphi(t)=h_0t+h_1,\quad F(t)=-\tfrac{5}{7}(h_0t+h_1)+F_1,\quad G(t)=\tfrac{2}{7}(h_0t+h_1)+G_1,$$

$$q(t)=q_1,\quad \sigma(t)=\sigma_1,\quad \beta(t)=-\tfrac{1}{2}(h_0t+h_1)+\beta_1,$$

where $h_0=(7/2\sqrt{3})\sqrt{a^2+12n^2}$, $Q^2=\frac{1}{3}(a^2+12n^2)e^{6\beta_1-3F_1-G_1}$, and F_1, G_1, q_1, σ_1, β_1, h_1 are all constants. This solution is a curved inhomogeneous model with a trivial axion field. In this situation the variable $\tilde{q}$ can be eliminated. The eigenvalues restricted to the constraint surface are

$$\tfrac{2}{7},\tfrac{2}{7},\tfrac{4}{7},-\tfrac{2}{7},\tfrac{1}{7}(1\pm\sqrt{23}i).$$

This point is always a saddle.

VI. DISCUSSION

We have studied several classes of inhomogeneous string models whose governing equations reduce to ODE. In particular, we have found that generically solutions of the class of separable G_2

inhomogeneous M-theory cosmologies studied evolve from a spatially inhomogeneous and negatively curved model with a nontrivial form fields toward (a subset) of spatially flat and spatially homogeneous dilaton-moduli-vacuum solutions where the form-fields (the axion field and the four-form field strength) are trivial and only the dilaton and moduli fields are dynamically important. This late time behavior is the same as that of the spatially homogeneous models studied previously. However, in these models the inhomogeneities are not dynamically insignificant at early times, and the models asymptote (in the past) toward a new class of inhomogeneous cosmological models.

As noted earlier, the time-reversed dynamics of the $\dot{\varphi}>0$ models we have considered thus far is equivalent to the dynamics of the case where $\dot{\varphi}<0$. This follows by redefining the time variable according to $dt/d\tau = -1/\dot{\varphi}$ and appropriate definitions of the other state variables. The evolution equations will have an ''overall'' change in sign, and hence the equilibrium points are identical in both cases, but the eigenvalues have opposite signs. Consequently, the dynamics of the $\dot{\varphi}<0$ models is the time reversal of the $\dot{\varphi}>0$ models and the time-reversed dynamics of the above class of models is deduced by interchanging the sources and sinks and reinterpreting expanding solutions in terms of contracting ones, and vice versa.

Although at late times (in the $\dot{\varphi}>0$ models) the inhomogeneities decay, the inhomogeneities are important at intermediate times and, in particular, at early times. Thus the qualitative features of the models are quite different to those of spatially homogeneous models studied previously. For example, in a study of FRW models[21] it was found that all negatively curved FRW models evolve from the solution corresponding to a global source in which the curvature is (negative and) dynamically important (but with a trivial axion field) toward the dilaton-moduli-vacuum solutions,[25] even in the presence of spatial curvature. The physical interpretation of these models, where both the NS–NS two-form potential and RR three-form potential are dynamically significant, was discussed in Ref. 21, with particular emphasis on the fact that the RR field causes the universe to collapse, but the NS–NS field has the opposite effect, whereby the interplay between these two fields leads to the models undergoing bounces. In the models under investigation here, orbits in the full phase space (with $\dot{\varphi}$ monotone) approach the dilaton-moduli-vacuum solution on the zero-curvature boundary (at late times) and again exhibit a ''bouncing'' behavior; this bouncing behavior is the result of the orbits shadowing orbits in the boundary that are constantly being redirected to saddle points of the same or higher stability until it reaches a stable equilibrium.

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A topological method for geodesic connectedness of space–times: Outer Kerr space–time

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The geodesic connectedness of outer Kerr space–time is proven by using a topological method. The proof is based on arguments about Brouwer's degree for the solutions of functional equations. The applicability of these topological arguments for dealing with geodesics in space–times is stressed. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1506403]

I. INTRODUCTION

For a space–time, the question whether two causally related points can be joined by means of a causal geodesic has a clear physical meaning. More geometrically, geodesic connectedness (the possibility of joining any two points by a geodesic of any causal type) is a basic property. Some techniques introduced to study geodesic connectedness are appliable to related problems of physical interest, such as the gravitational lensing effect, or the connectedness of two submanifolds by a causal geodesic (see, e.g., Refs. 1–5).

Different tools have been introduced to study geodesic connectedness of Lorentzian manifolds. The first nontrivial examples were spaceforms, which become specially relevant from the geometrical viewpoint.[6] A complete positive Lorentzian spaceform is geodesically connected if and only if it is not time-orientable. In particular, de Sitter space–time S_1^n is not geodesically connected; this happens in spite of the fact that it is globally hyperbolic and, thus, each two causally related points in S_1^n can be joined by a causal geodesic.[7,8] The results about geodesic connectedness of manifolds endowed with an affine connection[9] (see also Refs. 10–12) are potentially appliable to any manifold endowed with a nondegenerate metric. Geodesics of Lorentzian tori provide interesting examples related to connectedness.[13–15]

But the systematic study of the geodesic connectedness of physically relevant space–times was carried out after the introduction of some variational methods in Lorentzian geometry.[16] These methods permit one to prove the geodesic connectedness of stationary and splitting type manifolds under reasonable conditions (see the book—Ref. 17 or the survey—Ref. 18). Moreover, with different improvements, they ensure the connectedness of outer Schwarzschild space–time,[19] intermediate Reissner–Nordström,[20] Gödel type,[21] and other space–times. Recently, the authors have obtained the necessary and sufficient condition for the connectedness of generalized Robertson–Walker space–times.[22] Moreover, topological arguments have been developed which prove the connectedness of multiwarped space–times, under sufficient conditions which are close to necessary conditions[23] (see also Refs. 24 and 25). In particular, not only space–times as Schwarzschild black hole are shown to be geodesically connected,[23] but also new proofs of the geodesic connectedness of space–times such as intermediate Reissner–Nördstrom[23] and outer Schwarzschild[26] are obtained.

Significantly, geodesic connectedness of outer Kerr space–time has not been studied yet.[27] It is not difficult to prove that the stationary part of Kerr space–time is not geodesically connected; moreover, fast rotating Kerr space–time (i.e., Kerr space–time with parameters $a^2 > m^2$) is not geodesically connected.[26] On the other hand, for values of the parameter a close to 0, the hyper-

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surface between the stationary part and the ergosphere has some good properties from a variational viewpoint (it is time and light-*convex*, essentially). This ensures some properties of causal geodesics, such as the multiplicity of connecting timelike or lightlike geodesics for big time-separation (Ref. 17, Theorem 7.2.4).

Nevertheless, the inexistence of a privileged time function or timelike Killing vector field on the ergosphere introduces difficulties for its study. In fact, the following result holds.[26] *Let r_+ be the outer radius which determines the first event horizon of Kerr space–time. For any $\nu>0$ the region $r>r_+ + \nu$ is not geodesically connected*. In this article, we show that the topological arguments introduced by the authors in Ref. 23 are applicable to study geodesic connectedness of Kerr space–time, and prove that the whole region $r>r_+$ is geodesically connected. Even though our study is restricted to Kerr space–time for simplicity, the method would work for some different generalizations of this space–time.

This article is organized as follows.

In Sec. II Kerr space–time is briefly recalled. In Sec. III we give a general overview of our proof, which may serve as a guide for the following sections. The importance of the topological arguments first introduced in Ref. 23 (for the rather different class of multiwarped space–times) is stressed. In Sec. IV general properties of the geodesics of Kerr space–time are recalled, and those geodesics relevant under our approach are selected. Then, we reduce the problem of geodesic connectedness to an analytic problem (Lemma 4.3), among other technical results.

In Secs. V and VI geodesic connectedness is proven for the slow rotating Kerr $a^2<m^2$. In Sec. V the case when one of the two points to be connected lies in the symmetry axis z, is solved. Otherwise, the problem is technically more complicated, and solved in Sec. VI. Some concluding remarks are given in Sec. VII.[28]

II. KERR SPACE–TIME

Kerr space–time is the standard relativistic model of the gravitational field of a rotating massive object. The simplest description of the Kerr metric tensor is in terms of the time coordinate t on $\mathbb{R}$ and spherical coordinates r, θ, φ on $\mathbb{R}^3$ (θ denotes colatitude and φ longitude), which are called Boyer–Lindquist coordinates. Following Ref. 31, Sec. 1.1 we treat the coordinate φ as circular, so the coordinate system θ, φ covers all of the sphere except its north and south poles $(0,0,\pm 1)$. The coordinate function φ is undefined at the poles, but its coordinate vector field ∂_φ is well-defined and smooth on the entire sphere and is zero at the poles. Defining $\theta(0,0,+1)=0$ and $\theta(0,0,-1)=\pi$ extends the function θ to the entire sphere with $0\leqslant\theta\leqslant\pi$. At the poles, θ is only continuous, but $\cos\theta$ and $\sin\theta$ are smooth (indeed, analytic) everywhere.

Let $m>0$ and a be two constants, such that m represents the mass of the object and ma the angular momentum as measured from infinity. In previous coordinates, Kerr metric takes the form

$$\mathrm{d}s^2 = g_{t,t}\mathrm{d}t^2 + g_{r,r}\mathrm{d}r^2 + g_{\theta,\theta}\mathrm{d}\theta^2 + g_{\varphi,\varphi}\mathrm{d}\varphi^2 + 2g_{\varphi,t}\mathrm{d}\varphi\,\mathrm{d}t \tag{2.1}$$

with

$$g_{r,r}=\frac{\lambda(r,\theta)}{\Delta(r)},\quad g_{\varphi,\varphi}=\left[r^2+a^2+\frac{2mra^2\sin^2\theta}{\lambda(r,\theta)}\right]\sin^2\theta,\quad g_{t,t}=-1+\frac{2mr}{\lambda(r,\theta)},$$

$$g_{\theta,\theta}=\lambda(r,\theta),\quad g_{\varphi,t}=-\frac{2mra\sin^2\theta}{\lambda(r,\theta)}$$

and using

$$\lambda(r,\theta)=r^2+a^2\cos^2\theta,\quad \Delta(r)=r^2-2mr+a^2.$$

Halting the rotation by setting $a=0$, Kerr space–time becomes Schwarzschild space–time; if, then, the mass is removed ($m=0$) only (empty) Minkowski space–time remains.

In this article we only consider the case $0<a^2<m^2$, we mean, *slow rotating Kerr space–time*. Fast Kerr space–time is simpler; its (non)geodesic connectedness is studied in Ref. 26. Note that the above-given formulas show that Kerr metric fails when either $\lambda(r,\theta)=0$ or $\Delta(r)=0$. The function $\Delta(r)$ has the zeroes $r_+=m+\sqrt{m^2-a^2}$ and $r_-=m-\sqrt{m^2-a^2}$ and

$$\Delta(r)=(r-r_-)(r-r_+). \tag{2.2}$$

So the hypersurfaces $\mathbb{R}\times\{x\in\mathbb{R}^3: r=r_+\}$ and $\mathbb{R}\times\{x\in\mathbb{R}^3: r=r_-\}$ are singular for (2.1) and are *event horizons*. From now on, we will consider the *exterior Kerr space–time* $\mathbb{K}$, we mean the region without singularities in the metric tensor defined by imposing $r>r_+$. Recall that the region between the two event horizons has a strange physical behavior: matter might disappear in finite proper time, or suddenly appear from nowhere. Beyond the second event horizon, the ring singularity appears with its associated time machine.

III. OVERVIEW

The relation between geodesic connectedness and our topological arguments can be seen intuitively as follows. Consider two points $p_0\neq p_1$ of a Lorentzian manifold M, and fix a topological sphere of the tangent space to p_0, $S\subset T_{p_0}M$, such that the vector 0 is included in the interior of S. Consider now the subset $\exp_{p_0}sS, s\in\mathbb{R}$, yielded by the geodesics emanating at p_0 ($\exp_{p_0}$ is the exponential map at p_0). Initially, for small s, p_1 is outside $\exp_{p_0}sS$, but for some bigger s, p_1 may lie inside $\exp_{p_0}sS$. This topological change (from being outside to being inside the exponential of a sphere) reflects that p_0 and p_1 can be connected by a geodesic.

In order to be more precise mathematically, let us see a variation of this idea. Assume that M is an open subset of $\mathbb{R}^k$, and consider the function

$$F:\mathcal{D}\subset T_{p_0}M\equiv\mathbb{R}^k\to\mathbb{R}^k,\quad F(v)=\gamma_v(1)-p_1, \tag{3.1}$$

where γ_v is the unique geodesic starting at p_0 satisfying $\gamma_v'(0)=v$, for any $v\in T_{p_0}M$, and γ_v is defined at 1 for all v in the domain $\mathcal{D}$. Now, the zeroes of the function F correspond with geodesics connecting p_0 and p_1. If F satisfies certain conditions at the boundary of $\mathcal{D}$ then topological arguments may imply the existence of a zero. In dimension $k=1$ these conditions will be quite trivial: if $[a,b]\subset\mathcal{D}$ and $F(a)\cdot F(b)<0$ then F will have a zero. For $k=2$, and, say, $[a,b]\times[a',b']\subset\mathcal{D}$, $F=(F^1(x,y),F^2(x,y))$, if $F^1(a,y)\cdot F^1(b,y)<0,\forall y\in[a',b']$, $F^2(x,a')\cdot F^2(x,b')<0,\forall x\in[a,b]$, then the degree of F will be $\neq 0$, and F will have a zero; natural extensions of these conditions will be needed for $k\geqslant 3$. More exactly, we will need a variation of this argument. We will consider a sequence of increasing intervals $[a_n,b_n]$, $[a_n',b_n']$. Under the condition for F^1, $F^1(a_n,y)\cdot F^1(b_n,y)<0,\forall y\in[a_n',b_n']$, a connected set $\mathcal{C}_n$ of zeroes of F^1 which joins the horizontal lines $y=a_n', y=b_n'$ can be found. Then, we will look for a zero of F^2 in $\mathcal{C}_n$ for n big enough.

Clearly, a crucial step in this procedure is to ensure the boundary conditions on F. Thus, it is important to have a partial integration of the geodesic equations, as in most classical space–times.

For Kerr space–time $\mathbb{K}$, the geodesic equations admit four independent first integrals [see (4.1)]. But the problem is still complicated, and previous arguments will be used by including some subtleties and technical computations. Our approach can be summarized in the following steps.

(1) In order to connect two given points $p_0=(t_0,r_0,\theta_0,\varphi_0), p_1=(t_1,r_1,\theta_1,\varphi_1)$, we will consider all the geodesics emanating from p_0. Each geodesic $\gamma(s)$ is determined by its initial velocity $\gamma'(s_0)$. In Kerr space–time, this initial velocity is essentially characterized by *the constants of motion* q,K,L,E (see Sec. IV). More precisely, $\gamma'(s_0)$ yields naturally q,K,L,E, and fixing the values of q,K,L,E, one obtains $t'(s_0), r'(s_0)^2, \theta'(s_0)^2, \varphi'(s_0)$ [see Eq. (4.1)]. The sign

of $r'(s_0), \theta'(s_0)$ will be canonically fixed ($r'(s_0) \leqslant 0, \theta'(s_0) \geqslant 0$) for the geodesics which are relevant under our approach. Recall that there are restrictions for the possible values of q, K, L, E because $r'(s_0)^2, \theta'(s_0)^2$ calculated from (4.1) cannot be negative.

Geodesics with $L=0, E=0$ will be used to connect points in the simple case $t_0=t_1$ and either p_0 or p_1 lying in the z axis. In what follows we will consider geodesics with $E^2+L^2>0$. Moreover, we will also assume for simplicity $r_0 \leqslant r_1$, $t_0 \leqslant t_1$ (see Remark 4.5). Among geodesics with $L \neq 0$ those normalized with $L=1$ will always be chosen; if $L=0$ the chosen normalization will be $E=1$. These last geodesics will be useful when at least one of the points p_0, p_1 lies in the z axis; otherwise, geodesics with $L=1$ will be enough.

Summing up, we have *three degrees of freedom* for geodesics starting at p_0, corresponding to the set of directions in the tangent space to p_0, which will be described either by parameters $(q, K, L=1, E)$ or by $(q, K, L=0, E=1)$.

(2) The dimension of the manifold is four and, thus, there are four geodesic equations; nevertheless, the reparametrization of the geodesics is not relevant for geodesic connectedness and *one of the equations will be dropped*.

Concretely, we will prove that p_0, p_1 can be geodesically connected by using geodesics with $r'(s) \neq 0$ for all s in the domain of γ except at a point s^* such that $r^*=r(s^*)$ satisfies $r_+ < r^* < r_0$. Thus, taking into account this singular point r^*, any such geodesic $\gamma(s) = (t(s), r(s), \theta(s), \varphi(s))$ [characterized by its initial conditions as explained in step (1)] *will be reparametrized with* r, that is, as $\gamma(r) \equiv \gamma(s(r)) = (t(r), r, \theta(r), \varphi(r))$ for $r > r^*$.

The other two steps depend on if at least one of the points p_0, p_1 lies in the z axis or not. The first case is simpler; assume that, say, p_1 lies in the z axis.

(3^A) Because of the importance of the returning point r^* *the initial parameters* q, K ($L=0, E=1$) *will be changed by other parameters*, (r^*, S) in a domain $\hat{\mathcal{D}} \equiv (r_+, r_0) \times (0, \infty)$ [parameter S will also be related with properties of r^*, see formula (5.2)].

Given a value $(r^*, S) \in \hat{\mathcal{D}}$ we can recover the values of q and K [Eq. (5.3)]. Nevertheless, the domain $\hat{\mathcal{D}}$ will be restricted to a subset $\mathcal{D} = (r_+, r_L^*] \times (0, \infty) \subset \hat{\mathcal{D}}$. The value of $r_L^* (\in (r_+, r_0))$, which characterizes $\mathcal{D}$, is calculated to ensure the following properties:

($3^A I$) As commented in step (1), the values of q, K have some restrictions to characterize $\gamma'(s_0)$. When (r^*, S) belongs to $\mathcal{D}$, these restrictions are satisfied for the corresponding q, K. [In fact, $h(r_0)$ in Eq. (5.1) will be positive, and Eq. (5.6) will hold; thus, from (4.1) we will be able to choose $r'(s_0) < 0$, $\theta'(s_0) > 0$].

($3^A II$) As commented in step (2), the behavior of $r(s)$ for the relevant geodesics will be: first $r(s_0)=r_0$ then $r(s)$ decreases until $r=r^*$ and finally $r(s)$ increases until r_1. This behavior is ensured in $\mathcal{D}$ by the characterization of r_L^* in (5.4). [This can be checked because Eq. (4.10) with (5.1) will be satisfied when $r^* \in (r_+, r_L^*]$.]

($3^A III$) The component $\theta(s)$ of any geodesic γ in $\mathcal{D}$ will satisfy $\theta'(s) \neq 0$ out of the z-axis (see (4.1), (5.6)); in particular, from (1), $\theta'(s) > 0$ initially.

Only geodesics with $(r^*, S) \in \mathcal{D}$ will be used for connectedness.

(4^A) Now, for each $(r^*, S) \in \mathcal{D}$ we have a reparametrized geodesic $\gamma(r)$ with the parameter r going from r_0 to r^* and, finally, to r_1. When this parameter arrives at r_1, the coordinates t, θ, and φ will have increments $\Delta t, \Delta\theta$, and $\Delta\varphi$ on γ. The increment $\Delta\varphi$ will not be relevant in this case, because p_1 lies in the z axis. But, in order to connect p_0 and p_1, we have to find one of such geodesics with $\Delta t = t_1 - t_0$ and $\Delta\theta = \theta_1 - \theta_0$. Moreover, for the increment of θ the following trick will be useful. Let $\Delta|\theta|$ be the increment in the coordinate θ where it is regarded as a "circular coordinate," that is, as if θ increased even after crossing the z axis. Then, it is enough for θ: $\Delta|\theta| = \theta_1 - \theta_0 + 2n\pi$, for some integer $n \geqslant 0$.

Topological arguments will be relevant now. If we study how Δt varies with parameter S, we will find that (5.7) holds (see Fig. 1). Thus, applications of Brouwer's topological degree yield connected sets $\mathcal{C}_m$, $m \in \mathbb{N}$ of values of the parameters (r^*, S) such that:

(i) for all $(r^*, S) \in \mathcal{C}_m$, $\Delta t = t_1 - t_0$, and

(ii) the projection of the points in $\mathcal{C}_m$ on the r^* axis [that is, the image of the map (r^*, S)

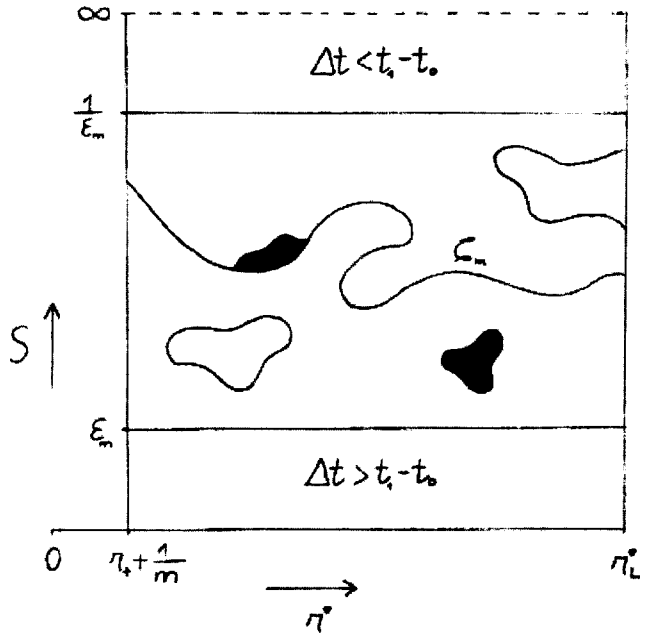

FIG. 1. When the behavior of $\Delta t(r^*,S)$ is as in formulas (5.7) then a connected set $\mathcal{C}_m$ of zeros of $\Delta t - t_1 + t_0$ which connect $r^* = r_+ + 1/m$ and $r^* = r_L^*$ can be found.

$\to r^*$ for $(r^*,S) \in \mathcal{C}_m$] is equal to the whole interval $[r_+ + 1/m, r_L^*]$. Now, the behavior of $\Delta|\theta|$ on $\mathcal{C}_m$ can be studied, finding: (a) the value of $\Delta|\theta|$ on the points of $\mathcal{C}_m$ in the line $r^* = r_L^*$ admit an upper bound independent of m, and (b) the value of $\Delta|\theta|$ on the points of $\mathcal{C}_m$ in the line $r^* = r_+ + 1/m$ becomes arbitrarily big. Thus, obviously, there exists at least one point in some $\mathcal{C}_m$ such that $\Delta|\theta| = \theta_1 - \theta_0 + 2n\pi$, for some integer $n \geqslant 0$ [in addition to $\Delta t = t_1 - t_0$, satisfied by (i)]. So, the required geodesic is found.

Let us see what happens if neither p_0 nor p_1 belongs to the z axis. Now, we will consider always geodesics with $L = 1$ (in particular, they do not cross the z axis).

(3^B) Analogously to case (3^A), *parameters* (q,K,E) *will be changed by parameters* $(r^*,S,E) \in \hat{\mathcal{D}} \equiv (r_+, r_0) \times (0,\infty)^2$, more closely related to the "returning point" of the geodesic. Analogously, the domain $\hat{\mathcal{D}}$ of (r^*,S,E) will be restricted to a subset $\mathcal{D}$ to solve the following similar problems to ($3^A I$), ($3^A II$), ($3^A III$):

($3^B I$) The values of q,K,E have some restrictions to characterize $\gamma'(s_0)$. Given (r^*,S,E), parameters q,K,E are directly computed [formula (6.1)], but perhaps the restrictions are not satisfied and, thus, they are not associated with any geodesic.

($3^B II$) Again, the behavior of $r(s)$ must be as in ($3^A II$). First, $r(s_0) = r_0$ then $r(s)$ decrease until $r = r^*$ and finally $r(s)$ increase until r_1. To achieve this, Eq. (4.10) [with (4.5)] must be satisfied.

($3^B III$) In ($3^A III$) the found connecting geodesic might cross the z axis many times [because of (5.6)]. But now, we are considering geodesics which do not cross the z axis. In fact, for any geodesic with $L = 1$, an angle $\theta_L \in (0, \pi/2]$ will exist such that if $\theta_L \leqslant \theta_0 \leqslant \pi - \theta_L$ then the component $\theta(s)$ of the geodesic varies between θ_L and $\pi - \theta_L$. Thus, θ_L can be regarded as a limit angle for $\theta(s)$ (see Definition 4.1 and Remark 4.2). Recall that, if also $\theta_L \leqslant \theta_1 \leqslant \pi - \theta_L$, $\theta(s)$ will find no obstruction to cross θ_0 and θ_1.

($3^B IV$) Technical conditions [Eq. (6.4), Remark 6.4] will be required for $\mathcal{D}$ in order to apply topological arguments.

In case 3^A a value of r_L^* is found such that the corresponding problems $3^A I$–$3^A III$ for the parameters (r^*,S) are solved if $r^* \in (r_+, r_L^*]$. Unfortunately, this is not sufficient now. The best

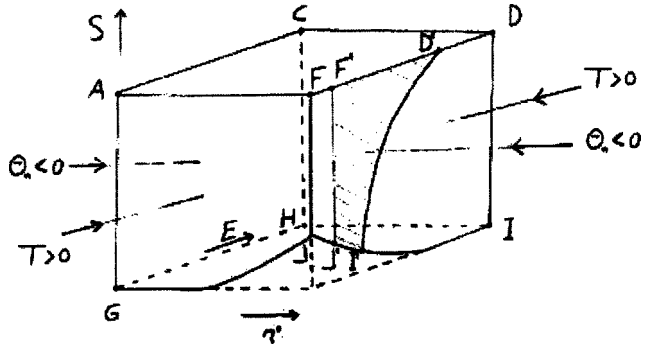

FIG. 2. Domain $\mathcal{D}_n$ in (6.32): $A=(r_+ + \epsilon_n, \overline{S}_n, \delta_n)$, $C=(r_+ + \epsilon_n, \overline{S}_n, 1/\delta_n)$, $D=(r_L^*, \overline{S}_n, 1/\delta_n)$, $G=(r_+ + \epsilon_n, S(r_+ + \epsilon_n, \delta_n), \delta_n)$, Behavior of T, Θ_n from Lemma 6.3 and (6.34) in Proposition 6.7: $T<0$ on $(AFJG)\cup(FF'J'J)$; $T>0$ on $(CHID)\cup(D'DII')$; $\Theta_n>0$ on $(ACHG)$; $\Theta_n<0$ on $(F'D'I'J')$. Lower face: graph of $S=S(r^*,E)(\geq 0)$.

we can find is some domain $\mathcal{D}$, with restrictions not only for r^* but also for S, such that restrictions $3^B I - 3^B IV$ are satisfied when $(r^*,S,E)\in\mathcal{D}$ (see Lemma 6.2 and Remark 6.4). More precisely, fixed $\overline{\theta}>0$ let $S(r^*,E)\geqslant 0$ be the minimum non-negative number such that $\theta_L(r^*,S,E)\leqslant\overline{\theta}$ if $S>S(r^*,E)$ (see Definition 4.1 and Lemma 6.3). $S(r^*,E)$ is a continuous function with finite supremum $\mathcal{S}$, but it will vanish for some (r^*,E) (this must be taken into account noticing that $S>0$ for the elements of $\hat{\mathcal{D}}$). Then there exist $r_L^*\in(r_+,r_0)$ and $\overline{\theta}\in(0,\pi/2)$ such that $\mathcal{D}\equiv\{(r^*,S,E)\in\hat{\mathcal{D}}: r^*\in(r_+,r_L^*], E\in(0,\infty), S\in[S(r^*,E),\infty)\}$ is the required domain.

(4^B) Now, for each $(r^*,S,E)\in\mathcal{D}$ we have a reparametrized geodesic $\gamma(r)$ with the parameter r going from r_0 to r^* and, finally, to r_1. As in case (4^A), when this parameter arrives at r_1, the coordinates t,θ, and φ will have increments $\Delta t,\Delta\theta$, and $\Delta\varphi$ on γ, but now the increment $\Delta\varphi$ is also relevant. In order to connect p_0 and p_1, it is sufficient to find one of such geodesics with $\Delta t=t_1-t_0$, $\Delta\theta=\theta_1-\theta_0$, and $\Delta\varphi=\varphi_1-\varphi_0$. Moreover, we will denote by $\Delta|\theta|$ the increment in the coordinate θ computed as if it were positive beyond any rebound of $\theta(s)$ at θ_L or $\pi-\theta_L$; for example, if $\theta(s)$ increases from $\theta(s_0)$ to $\pi-\theta_L$ and then decreases to $\theta(s_1)$ we define $\Delta|\theta| = |(\pi-\theta_L)-\theta(s_0)|+|(\pi-\theta_L)-\theta(s_1)|$. Thus, it is sufficient for θ: $\Delta|\theta|=\theta_1-\theta_0+2n(\pi-2\theta_L)$, for some integer $n\geqslant 0$. Finally, as φ will be regarded as a circular coordinate it is enough $\Delta\varphi=\varphi_1-\varphi_0+2n'\pi$, for some integer $n'\geqslant 0$. The *topological arguments* are now subtler.

First we will find connected sets $\mathcal{C}_n$ of parameters such that the associated geodesics have exactly $\Delta t=t_1-t_0$, $\Delta|\theta|=\theta_1-\theta_0+2n(\pi-2\theta_L)$.

$(4^B I)$ Consider the functions $T=\Delta t-(t_1-t_0)$ and $\Theta_n=\Delta|\theta|-(\theta_1-\theta_0)-2n(\pi-2\theta_L)$ with domain $\mathcal{D}$, for some integer $n\geqslant 0$. Given $\{\overline{S}_n\}_n$ diverging, there exist $\{\epsilon_n\}_n$, $\epsilon_n>0$, $\epsilon_n\searrow 0$, and $\{\delta_n\}_n$, $\delta_n>0$, $\delta_n\searrow 0$ such that functions T and Θ_n satisfy the boundary conditions (6.34) in a domain $\mathcal{D}_n$ (Fig. 2), for n big enough (Proposition 6.7).

$(4^B II)$ Taking into account that in some points $S(r^*,E)$ vanishes, a natural compact subset $\mathcal{D}_n^m\subset\mathcal{D}$ can be defined [see (6.35)] where connected sets $\mathcal{C}_n^m$ of simultaneous zeroes of T and Θ_n will be found. In order to obtain $\mathcal{C}_n^m$, recall that a homeomorphism z_n^m maps $\mathcal{D}_n^m$ to a cube as in Fig. 3. Thus, topological arguments imply the existence of a connected set $z_n^m(\mathcal{C}_n^m)$ of zeroes of the two functions $T\circ(z_n^m)^{-1}$, $\Theta_n\circ(z_n^m)^{-1}$ connecting the upper and the lower faces of the cube (Lemma 6.9).

$(4^B III)$ Using Whyburn arguments on the sets $\mathcal{C}_n^m$ we construct a new connected set $\mathcal{C}_n\subset\overline{\mathcal{D}}_n$ (depicted in Fig. 4). We will prove:

(i) $\mathcal{C}_n\subset\mathcal{D}_n$ and thus, points in $\mathcal{C}_n$ are zeroes of T and Θ_n, and

(ii) each $\mathcal{C}_n$ has a point with $S=\overline{S}_n$ and a point with $S=S(r^*,E)>0$ (and, thus $\theta_L=\overline{\theta}$) for all n (Lemma 6.10 and comments above).

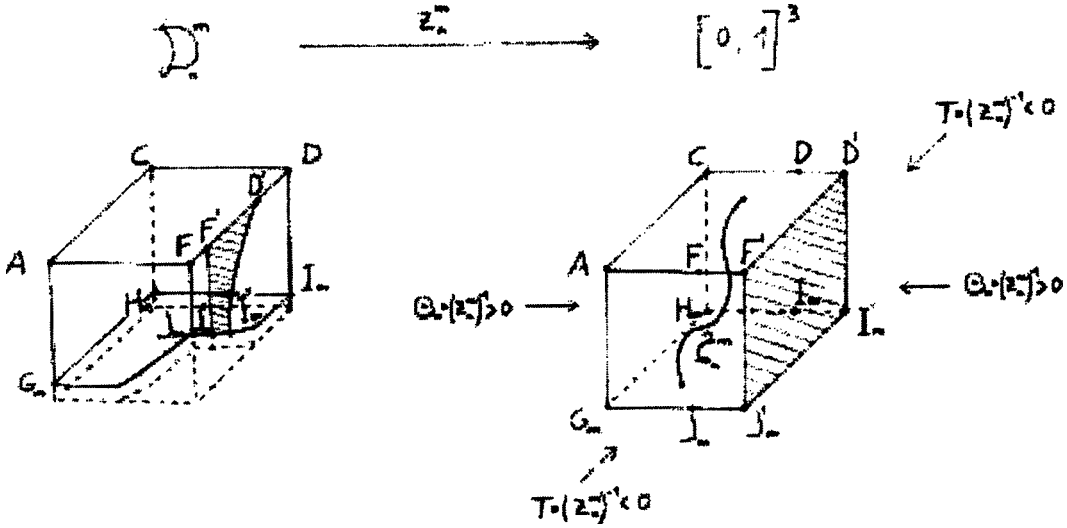

FIG. 3. (1) Homeomorphism z_n^m between $\mathcal{D}_n^m$ in (6.35) and the cube $[0,1]^3$. The dashed region ($F'D'I'_mJ'_m$) corresponds by the homeomorphism. (2) Brouwer's topological degree applied to $T\circ(z_n^m)^{-1}$ and $\Theta\circ(z_n^m)^{-1}$ yields a simultaneous connected set of zeroes $\hat{\mathcal{C}}_n^m = z_n^m(\mathcal{C}_n^m)$ joining the upper and lower faces of the cube $[0,1]^3$.

Now, geodesics associated to each $(r^*,S,E)\in\mathcal{C}_n$ have the required value of Δt, $\Delta|\theta|$, but we have not controlled the value of $\Delta\varphi$ yet. Our aim will be to find two points in a connected set $\mathcal{C}_n$ for some (big) n, whose difference in $\Delta\varphi$ is greater than 2π. Thus, some point in $\mathcal{C}_n$ will satisfy $\Delta\varphi=\varphi_1-\varphi_0+2\pi n'$, $n'\geqslant 0$, which concludes the proof. In fact, we prove the existence of a

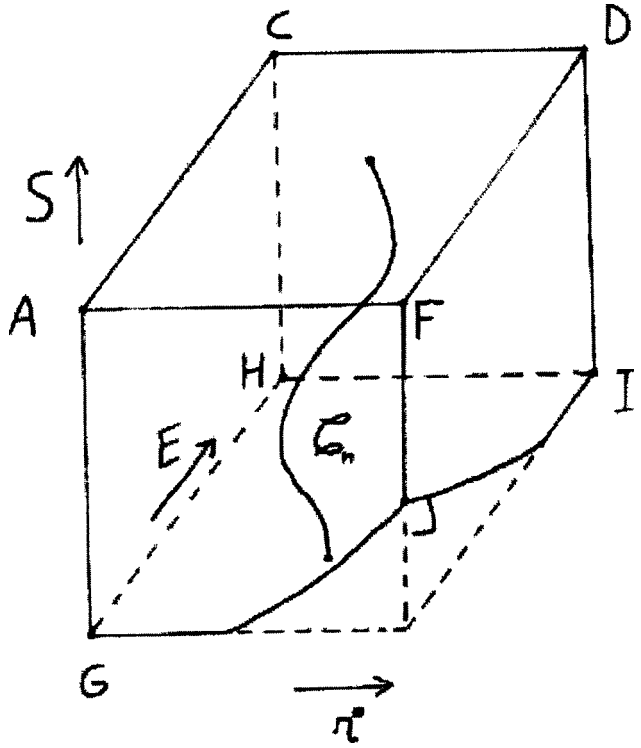

FIG. 4. Taking $\limsup_m$ on $\mathcal{C}_n^m$ a connected set $\mathcal{C}_n$ is obtained, satisfying: (a) all the points in $\mathcal{D}_n\cap\mathcal{C}_n$ are zeroes of T and Θ_n, (b) $\mathcal{C}_n$ touches the upper and the lower faces, the latter in a point with $S>0$ (Lemma 6.10; in particular, $\mathcal{C}_n\subset\mathcal{D}_n$), and (c) for big n, function $\Delta\varphi|_{\mathcal{C}_n}$ covers an interval of length greater than 2π (Lemmas 6.11 and 6.12).

choice of $\{\overline{S_n}\}_n$ such that points $(r_n^*,\overline{S_n},E_n)\in\mathcal{C}_n$ obtained in (ii) satisfy:

$$2n\pi-(\Delta\varphi)(r_n^*,\overline{S_n},E_n)<n\cdot\epsilon \tag{3.2}$$

for every $\epsilon>0$ and n big enough (Lemma 6.11). On the other hand, again from (ii) we can take a sequence of points $(r_n^{*\prime},S_n',E_n')\in\mathcal{C}_n$ with $\theta_L(r_n^{*\prime},S_n',E_n')=\overline{\theta}>0$ for all n which, from Lemma 6.12, implies

$$2n\pi-(\Delta\varphi)(r_n^{*\prime},S_n',E_n')>n\cdot\epsilon_0 \tag{3.3}$$

for some $\epsilon_0>0$. The result follows then from (3.2) and (3.3).

IV. GENERAL BEHAVIOR OF THE GEODESICS

Let $\gamma:\mathcal{J}\to\mathbb{R}^4$, $\gamma(s)=(t(s),r(s),\theta(s),\varphi(s))$ be a (smooth) curve on the interval $\mathcal{J}$. The first integrals of the geodesics equations of Kerr space–time are

$$\begin{aligned}
\lambda(r,\theta)t' &= a\mathbb{D}(\theta)+(r^2+a^2)\frac{\mathbb{P}(r)}{\Delta(r)},\\
\lambda(r,\theta)^2r'^2 &= \Delta(r)(qr^2-K)+\mathbb{P}^2(r),\\
\lambda(r,\theta)^2\theta'^2 &= K+qa^2\cos^2\theta-\frac{\mathbb{D}^2(\theta)}{\sin^2\theta},\\
\lambda(r,\theta)\varphi' &= \frac{\mathbb{D}(\theta)}{\sin^2\theta}+a\frac{\mathbb{P}(r)}{\Delta(r)},
\end{aligned} \tag{4.1}$$

where

$$\begin{aligned}
\mathbb{D}(\theta) &= L-Ea\sin^2\theta,\\
\mathbb{P}(r) &= (r^2+a^2)E-La
\end{aligned} \tag{4.2}$$

and q (normalization of the geodesic; rest mass), K (Carter constant), L (angular momentum), and E (energy measured by observers in ∂_t) are constants; we follow essentially the notation in Ref. 31, Chap. 4. So, if we assume $r'(s_0)\leqslant 0$, $\theta'(s_0)\geqslant 0$ every geodesic is fixed by an initial point p_0 [i.e., $\gamma(s_0)=p_0$] and the constants q, K, L, and E. Moreover, from the third equation in (4.1), if γ reaches the z axis then, necessarily $L=0$; recall that when $L\neq 0$ we can normalize $L=1$.

Let $s(r)$ be the inverse function (where it exists) of $r(s)$ in (4.1); using r as the parameter in the other three equations in (4.1):

$$\begin{aligned}
\frac{dt}{dr} &= \epsilon\frac{a\mathbb{D}(\theta)+(r^2+a^2)\dfrac{\mathbb{P}(r)}{\Delta(r)}}{\sqrt{\Delta(r)(qr^2-K)+\mathbb{P}^2(r)}},\\
\frac{d\theta}{dr} &= \epsilon'\frac{\sqrt{K+qa^2\cos^2\theta-\dfrac{\mathbb{D}^2(\theta)}{\sin^2\theta}}}{\sqrt{\Delta(r)(qr^2-K)+\mathbb{P}^2(r)}},\\
\frac{d\varphi}{dr} &= \epsilon\frac{\dfrac{\mathbb{D}(\theta)}{\sin^2\theta}+a\dfrac{\mathbb{P}(r)}{\Delta(r)}}{\sqrt{\Delta(r)(qr^2-K)+\mathbb{P}^2(r)}}
\end{aligned} \tag{4.3}$$

on a certain domain, being $\epsilon,\epsilon' \in \{\pm 1\}$. Equation (4.3) will be used to prove the geodesic connectedness of outer Kerr space–time $\mathbb{K}$. But, previously, we need the following definition related to the expression of θ'.

Definition 4.1: For any $(q,K,L,E) \in \mathbb{R}^4$ *we define* $\theta_L \equiv \theta_L(q,K,L,E)$ *as the smaller angle in* $[0,\pi/2]$ *satisfying*

$$K + qa^2 \cos^2\theta - \frac{\mathbb{D}^2(\theta)}{\sin^2\theta} > 0, \quad \forall\, \theta \in \left(\theta_L, \frac{\pi}{2}\right], \tag{4.4}$$

with $\mathbb{D}(\theta) \equiv \mathbb{D}(\theta,L,E)$ *given in (4.2).*

[Recall that if for some (q,K,L,E) the left-hand side of inequality (4.4) is nonpositive at $\theta = \pi/2$ then $\theta_L = \pi/2$].

Remark 4.2: Assume that (q,K,L,E) corresponds to a geodesic with $\gamma(s_0) = p_0 \equiv (t_0, r_0, \theta_0, \varphi_0)$ and $\theta_L \leqslant \theta_0 \leqslant \pi - \theta_L$. If $L = 1$ then θ_L can be seen as a limit angle for $\theta(s)$ as explained in $(3^{B}III)$; in fact, it is clear from (4.1) that $\theta(s)$ takes values in $[\theta_L, \pi - \theta_L]$ being $\theta'(s) = 0$ only when $\theta(s) \in \{\theta_L, \pi - \theta_L\}$.

If one consider geodesics with $r' \neq 0$ at any point, then the geodesic can be reparametrized by[29] r and the increments Δt, $\Delta\theta$, and $\Delta\varphi$ can be calculated integrating in (4.3). Nevertheless, in this article we are going to see that two arbitrary points $p_0 = (t_0, r_0, \theta_0, \varphi_0)$, $p_1 = (t_1, r_1, \theta_1, \varphi_1)$ in $\mathbb{K}$ with $r_0 \leqslant r_1$ can be always joined with a geodesic such that $r'(s)$ vanishes exactly at one point s^*, and $r^* = r(s^*)$ satisfies $r_+ < r^* < r_0$. Recall that, for these geodesics the denominator in formula (4.3), that is

$$h(r) = \Delta(r)(qr^2 - K) + \mathbb{P}^2(r), \tag{4.5}$$

will vanish at r^*. As $r(s)$ will go from r_0 to r^* then necessarily $h'(r^*) > 0$; in fact, this implies $|s(r^*) - s(r_0)| < \infty$ (see Ref. 29). As later on $r(s)$ will go from r^* to r_1, then $h(r) > 0$ if $r^* < r < r_1$; we will consider geodesics with $h(r_1) > 0$ too. Thus, the increment in the variable t will be

$$\Delta t = \int_{r^*}^{r_0} \frac{a\mathbb{D}(\theta) + (r^2 + a^2)\dfrac{\mathbb{P}(r)}{\Delta(r)}}{\sqrt{h(r)}}\,\mathrm{d}r + \int_{r^*}^{r_1} \frac{a\mathbb{D}(\theta) + (r^2 + a^2)\dfrac{\mathbb{P}(r)}{\Delta(r)}}{\sqrt{h(r)}}\,\mathrm{d}r. \tag{4.6}$$

For the coordinate θ, if $L = 1$ we will assume that $\theta(s)$ will go from θ_0 to θ_1 with $\theta'(s)$ only vanishing at an even number of points s_i, $i = 1,\ldots,2n$, such that $\theta(s_i)$ is equal either to the limit angle θ_L or to $\pi - \theta_L$, Remark 4.2. If $L = 0$, we will choose always geodesics such that q, K, E make the left-hand side of (4.4) positive for all θ and thus, $\theta_L = 0$; that is, $\theta'(s) \neq 0$ always except at the points s_i, $i = 1,\ldots,2n$, where γ reaches the z axis [at these points $\theta(s)$ is not differentiable and the sign of $\theta'(s)$ changes]. In particular,

$$\begin{gathered} \theta_L \leqslant \theta_0, \quad \theta_1 \leqslant \pi - \theta_L \ \text{ if } \ L = 1, \\ \theta_L = 0 \quad \text{and} \quad (4.4) \ \text{holds strictly at} \ \theta_L \ \text{if} \ L = 0. \end{gathered} \tag{4.7}$$

As explained in (4^{A}) and (4^{B}) we will define $\Delta|\theta|$ considering the increments as positive beyond the points s_i. That is, we define

$$\Delta|\theta| = \int_{r^*}^{r_0} \frac{\sqrt{K + qa^2\cos^2\theta - \dfrac{\mathbb{D}^2(\theta)}{\sin^2\theta}}}{\sqrt{h(r)}}\,\mathrm{d}r + \int_{r^*}^{r_1} \frac{\sqrt{K + qa^2\cos^2\theta - \dfrac{\mathbb{D}^2(\theta)}{\sin^2\theta}}}{\sqrt{h(r)}}\,\mathrm{d}r. \tag{4.8}$$

Finally, the circular coordinate φ will have an increment

$$\Delta\varphi=\int_{r^*}^{r_0}\frac{\frac{\mathbb{D}(\theta)}{\sin^2\theta}+a\frac{\mathbb{P}(r)}{\Delta(r)}}{\sqrt{h(r)}}\mathrm{d}r+\int_{r^*}^{r_1}\frac{\frac{\mathbb{D}(\theta)}{\sin^2\theta}+a\frac{\mathbb{P}(r)}{\Delta(r)}}{\sqrt{h(r)}}\mathrm{d}r. \tag{4.9}$$

Recall that this increment also represents a certain number n' of turns around the z axis (if $2n'\pi\leqslant\Delta\varphi<2(n'+1)\pi$). Summing up:

Lemma 4.3: Let $p_0=(t_0,r_0,\theta_0,\varphi_0)$, $p_1=(t_1,r_1,\theta_1,\varphi_1)$ be two points in $\mathbb{K}$ with $r_0\leqslant r_1$, such that $\sin\theta_0\neq 0\neq\sin\theta_1$ (*respectively, one or both points in the z axis*). *Assume that there exist q, K, and E as well as $r^*\in(r_+,r_0)$ such that (4.7) and the following relations (4.10) and (4.11) hold with $L=1$ (respectively, $L=0$):*

$$h(r^*)=0,\quad h'(r^*)>0,\quad h(r)>0\quad on\quad (r^*,r_1]; \tag{4.10}$$

$$\begin{cases}\Delta t=t_1-t_0,\\ \Delta|\theta|=\theta_1-\theta_0+2n(\pi-2\theta_L),\\ \Delta\varphi=\varphi_1-\varphi_0+2\pi n'\end{cases} \tag{4.11}$$

for some integers $n,n'\geqslant 0$ [for the case $L=0$, without the restriction on $\Delta\varphi$ in (4.11)]. Then, there exists $s_1>s_0$ such that the geodesic $\gamma:[s_0,s_1]\to\mathbb{K}$, $\gamma(s_0)=p_0$ with constants $L=1$ (respectively, $L=0$), q, K and E, satisfies $\gamma(s_1)=p_1$.

Remark 4.4: Recall that the restriction on $\Delta\varphi$ in (4.11) is not imposed when $L=0$ because if $\sin\theta_1=0$ (as we assumed in the overview) then the coordinate φ becomes irrelevant. If $\sin\theta_0=0\neq\sin\theta_1$ then Lemma 4.3 yields a geodesic $\gamma(s)=(t(s),r(s),\theta(s),\varphi(s))$ with the appropiate values of Δt, $\Delta|\theta|$. Then $\overline{\gamma}(s)=(t(s),r(s),\theta(s),\varphi(s)+\overline{\varphi})$ with $\overline{\varphi}=\varphi_1-\varphi(s_1)$ is the required geodesic.

Remark 4.5: In order to prove the connectedness of two arbitrary points $p_0=(t_0,r_0,\theta_0,\varphi_0)$, $p_1=(t_1,r_1,\theta_1,\varphi_1)$ we will assume $t_0\leqslant t_1$ and $r_0\leqslant r_1$. In fact, if this last inequality does not hold, Lemma 4.3 can be obviously modified taking $r^*\in(r_+,r_1)$.

The following simple technical result will be useful in the following sections (see Ref. 26 for a detailed proof):

Lemma 4.6: Let $\{f_n(x)\}_n$ be a sequence of continuous functions on $[a_n,b_n]\subset\mathbb{R}$, $a_n\to a$, $b_n\to b$, $a<b$ satisfying $0<c\leqslant f_n(x)\leqslant C$ for all n, and let $\{p_n(x)\}_n$ be a sequence of polynomials with degree bounded in n satisfying for all n: $p_n(a_n)=0$, $p_n'(a_n)=R_n>0$ and $p_n^{(k)}(a_n)\geqslant 0$ for $k\geqslant 2$.

(i) If $R_n\to\infty$, then

$$\int_{a_n}^{b_n}\frac{f_n(x)}{\sqrt{p_n(x)}}\mathrm{d}x\to 0.$$

(ii) If $R_n\to 0$ and $p_n^{(k)}(a_n)$ admits an upper bound for $k\geqslant 2$ and for all n, then

$$\int_{a_n}^{b_n}\frac{f_n(x)}{\sqrt{p_n(x)}}\mathrm{d}x\to\infty.$$

V. GEODESIC CONNECTEDNESS WITH THE *z* AXIS

In this section we prove that there exists a geodesic joining two arbitrary points when, at least, one of them lies in the z axis. From Remark 4.5, it suffices:

Theorem 5.1: *Given two points $p_0=(t_0,r_0,\theta_0,\varphi_0)$, $p_1=(t_1,r_1,\theta_1,\varphi_1)$ in $\mathbb{K}$, at least one of them in the z axis, with $r_0\leqslant r_1$, $t_0\leqslant t_1$, there exists a geodesic $\gamma:[s_0,s_1]\to\mathbb{K}$ such that $\gamma(s_0)=p_0$, $\gamma(s_1)=p_1$.*

Proof: Taking into account Lemma 4.3 it is sufficient to prove that there exist constants q, K, and E as well as $r^*\in(r_+,r_0)$ satisfying (4.7), (4.10), and (4.11) for $L=0$.

First, consider the case $t_0<t_1$ and choose $E=1$; so (4.5) becomes

$$h(r)=(r-r_-)(r-r_+)(qr^2-K)+(r^2+a^2)^2. \tag{5.1}$$

If we look for r^* such that

$$h(r^*)=0, \quad h'(r^*)=S>0 \tag{5.2}$$

then the following two relations for the constants q and K are obtained:

$$\begin{aligned} qr^{*2}-K&=-\frac{(r^{*2}+a^2)^2}{(r^*-r_-)(r^*-r_+)},\\ q&=\frac{(r^{*2}+a^2)^2}{2r^*(r^*-r_-)^2(r^*-r_+)}+\frac{(r^{*2}+a^2)^2}{2r^*(r^*-r_-)(r^*-r_+)^2}\\ &\quad-\frac{2(r^{*2}+a^2)}{(r^*-r_-)(r^*-r_+)}+\frac{S}{2r^*(r^*-r_-)(r^*-r_+)}. \end{aligned} \tag{5.3}$$

Taking into account the dependencies of q on (r^*-r_+) in the second equation in (5.3), there exists $r_L^*\in(r_+,r_0)$ near enough to r_+ such that if $r^*\in(r_+,r_L^*]$ then

$$r_+^2 q(r^*,S)>a^2, \quad \forall S>0 \quad (\Rightarrow K(r^*,S)>a^2, \quad \forall S>0). \tag{5.4}$$

Moreover, derivating in (5.1) in order to apply Lemma 4.6,

$$\begin{aligned} h^{(2)}(r^*)&=4qr^*(r^*-r_+)+4qr^*(r^*-r_-)+2(qr^{*2}-K)+2q(r^*-r_-)(r^*-r_+)+12r^{*2}+4a^2,\\ h^{(3)}(r^*)&=6q(r^*-r_+)+6q(r^*-r_-)+(12q+24)r^*,\\ h^{(4)}(r^*)&=24q+24. \end{aligned} \tag{5.5}$$

Clearly $h^{(3)}(r^*)$, $h^{(4)}(r^*)>0$. Moreover, r_L^* can be chosen such that the sum of the second plus third terms in the expression of q in (5.3) is positive and thus, $h^{(2)}(r^*)>0$. In particular, $h(r)>0$ if $r>r^*$. On the other hand, from (5.4)

$$K+qa^2\cos^2\theta-\frac{\mathbb{D}^2(\theta)}{\sin^2\theta}=K+(qa^2+a^2)\cos^2\theta-a^2>0 \tag{5.6}$$

for all θ [in particular, (4.7) is satisfied with $L=0$]. Summing up, because of Lemma 4.3 it is sufficient to find an element of $\mathcal{D}\equiv\{(r^*,S):r^*\in(r_+,r_L^*],S\in(0,\infty)\}$ such that the corresponding (q,K) given from (5.3) and the function $h(r)\equiv h(r,q,K)$ in (5.1) satisfy the first two equalities (4.11) with Δt, $\Delta|\theta|$ as in (4.6) and (4.8) (and $L=0$, $E=1$).

Fix sequences $\{S_n\}_n\to\infty$, $\{r_n^*\}_n\to r^*\in(r_+,r_L^*]$, and put

$$f_n(r)\equiv a\mathbb{D}(\theta_n(r))+(r^2+a^2)\frac{\mathbb{P}(r)}{\Delta(r)}, \quad p_n(r)\equiv h_n(r)$$

with $h_n(r)\equiv h(r,q(r_n^*,S_n),K(r_n^*,S_n))$ and $\theta_n(r)$ computed with (r_n^*,S_n) from the second equation in (4.3) [recall (5.6)]. Using (5.2) and the positiveness of (5.5), hypotheses of Lemma 4.6 (i) clearly hold on the interval $[a_n,b_n]=[r_n^*,r_1]$. Therefore,

$$(\Delta t)_n=\int_{r_n^*}^{r_0}\frac{f_n(r)}{\sqrt{p_n(r)}}\mathrm{d}r+\int_{r_n^*}^{r_1}\frac{f_n(r)}{\sqrt{p_n(r)}}\mathrm{d}r\to 0.$$

Analogously, if we consider $\{S_n\}_n \to 0$ then, from (5.5) and (5.3), $h_n^{(k)}(r_n^*)$ admits an upper bound for $k \geqslant 2$ and all n thus, from Lemma 4.6(ii), $(\Delta t)_n \to \infty$. In conclusion, there exists $\{\epsilon_m\}_m$, $\epsilon_m > 0$, $\epsilon_m \searrow 0$, such that

$$\Delta t(r^*,S) < t_1 - t_0 \quad \text{when} \quad (r^*,S) \in \left[r_+ + \frac{1}{m}, r_L^* \right] \times \left[\frac{1}{\epsilon_m}, \infty \right),$$
$$\Delta t(r^*,S) > t_1 - t_0 \quad \text{when} \quad (r^*,S) \in \left[r_+ + \frac{1}{m}, r_L^* \right] \times (0, \epsilon_m] \tag{5.7}$$

(see Fig. 1). This is a typical situation where Brouwer's topological degree ensures, for each m, the existence of a connected set $\mathcal{C}_m$ of zeroes of $\Delta t - t_1 + t_0$ connecting the extreme vertical lines. More precisely,

Lemma 5.2: There exists a connected subset $\mathcal{C}_m$ of zeroes of $T(r^*,S) = \Delta t - t_1 + t_0$ such that

$$\mathcal{C}_m \cap \left(\left\{ r_+ + \frac{1}{m} \right\} \times \left(\epsilon_m, \frac{1}{\epsilon_m} \right) \right) \neq \varnothing \quad \textit{and} \quad \mathcal{C}_m \cap \left(\{ r_L^* \} \times \left(\epsilon_m, \frac{1}{\epsilon_m} \right) \right) \neq \varnothing$$

for every $m \in \mathbb{N}$.

(For a detailed proof, see Ref. 26 Lemma 2.) Therefore, for these subsets (i) and (ii) in (4^A) holds. So, we only need to prove that among the found zeroes of T there is a $(r^*,S) \in \mathcal{D}$ such that $\Delta|\theta|$ satisfies (4.11), for some n.

Let $(r_m^*, S_m) \in \mathcal{C}_m$ be with $r_m^* = r_+ + 1/m$, and take in Lemma 4.6(ii)

$$f_m(r) \equiv \frac{\sqrt{K_m + q_m a^2 \cos^2 \theta_m(r) - a^2 \sin^2 \theta_m(r)}}{\sqrt{q_m}} \quad \text{and} \quad p_m(r) \equiv \frac{h_m(r)}{q_m}$$

with K_m, q_m obtained from (5.3), $\theta_m(r)$ from (4.3). From (5.3), q_m will grow at least as m^2 and, from (5.4) and (5.5) one checks that the hypotheses of this lemma hold on the intervals $[a_m, b_m] = [r_m^*, r_1]$, obtaining

$$(\Delta|\theta|)_m = \int_{r_m^*}^{r_0} \frac{f_m(r)}{\sqrt{p_m(r)}} \mathrm{d}r + \int_{r_m^*}^{r_1} \frac{f_m(r)}{\sqrt{p_m(r)}} \mathrm{d}r \to \infty. \tag{5.8}$$

On the other hand, from (5.7) the points in $\mathcal{C}_m$ with $r^* = r_L^*$ have $S \in (\epsilon_1, 1/\epsilon_1)$, thus q, K is upper bounded for these points and all m [see (5.3)] and so is $\Delta|\theta|$. This fact, (5.8) and the connectedness of each $\mathcal{C}_m$ imply for some big m the existence of $(r^*,S) \in \mathcal{C}_m$ such that the second equality (4.11) also holds, as required.

Finally, consider the case $t_0 = t_1$. Choose $E = 0$ and, thus, $T = 0$ automatically. Now (4.5) becomes

$$h(r) \equiv (r - r_-)(r - r_+)(qr^2 - K).$$

By imposing $h(r^*) = 0$ and $h'(r^*) = 1$ we obtain the following values for the constants q and K:

$$qr^{*2}-K=0,$$
$$q=\frac{1}{2r^*(r^*-r_-)(r^*-r_+)}. \tag{5.9}$$

If we take $\{r_m^*\}_m\to r_+$, (5.9) and formulas analogous to (5.5) imply that Lemma 4.6(ii) can be applied to the functions

$$f_m(r)\equiv\frac{\sqrt{K_m+q_m a^2\cos^2\theta_m(r)}}{\sqrt{q_m}},\quad p_m(r)\equiv\frac{h_m(r)}{q_m},$$

on the intervals $[a_m,b_m]=[r_m^*,r_1]$. Thus, we obtain (5.8) and, so, $(\Delta|\theta|)_m\equiv\Delta|\theta|(r_m^*)\to\infty$. Therefore, a required value for r^* can be found in $[r_m^*,r_L^*]$ for some big m. □

VI. GEODESIC CONNECTEDNESS BETWEEN POINTS OUT OF THE *z* AXIS

In this section we conclude the proof of the geodesic connectedness of $\mathbb{K}$ by proving that there exists a geodesic joining two arbitrary points out of the z axis. Recalling again Remark 4.5, we will prove:

Theorem 6.1: *Given two points* $p_0=(t_0,r_0,\theta_0,\varphi_0)$, $p_1=(t_1,r_1,\theta_1,\varphi_1)$ *in* $\mathbb{K}$, $\sin\theta_0\neq 0\neq\sin\theta_1$, $r_0\leqslant r_1$, $t_0\leqslant t_1$, *there exists a geodesic* $\gamma:[s_0,s_1]\to\mathbb{K}$ *such that* $\gamma(s_0)=p_0$, $\gamma(s_1)=p_1$.

Taking into account Lemma 4.3, it is sufficient to prove that there exist constants q, K, and E as well as $r^*\in(r_+,r_0)$ satisfying (4.7), (4.10), and (4.11) with $L=1$.

We will again use r^* such that (5.2) holds. Then the following two relations for the constants q and K are obtained from (4.5):

$$qr^{*2}-K=-\frac{[(r^{*2}+a^2)E-a]^2}{(r^*-r_-)(r^*-r_+)},$$
$$q=\frac{[(r^{*2}+a^2)E-a]^2}{2r^*(r^*-r_-)^2(r^*-r_+)}+\frac{[(r^{*2}+a^2)E-a]^2}{2r^*(r^*-r_-)(r^*-r_+)^2}$$
$$-\frac{2[(r^{*2}+a^2)E-a]E}{(r^*-r_-)(r^*-r_+)}+\frac{S}{2r^*(r^*-r_-)(r^*-r_+)}. \tag{6.1}$$

Moreover,

$$h^{(2)}(r^*)=4qr^*(r^*-r_+)+4qr^*(r^*-r_-)+2(qr^{*2}-K)$$
$$+2q(r^*-r_-)(r^*-r_+)+4E[(r^{*2}+a^2)E-a]+8r^{*2}E^2,$$
$$h^{(3)}(r^*)=12qr^*+6q(r^*-r_+)+6q(r^*-r_-)+24E^2r^*, \tag{6.2}$$
$$h^{(4)}(r^*)=24q+24E^2.$$

From (6.1), given $(r^*,S,E)\in\hat{\mathcal{D}}\equiv(r_+,r_0)\times(0,\infty)^2$ we obtain $(q(r^*,S,E),K(r^*,S,E),E)$. So, we can define $\theta_L\equiv\theta_L(r^*,S,E)(\equiv\theta_L(q,K,E))$, Definition 4.1, and write the following result:

Lemma 6.2: There exist $r_L^*\in(r_+,r_0)$ *close to* r_+ *and* $\overline{\theta}\in(0,\pi/2)$ *close to 0 with* $\overline{\theta}<\theta_0,\theta_1<\pi-\overline{\theta}$ *such that for all* (r^*,S,E) *with* $r_+<r^*\leqslant r_L^*$ *and* $\theta_L(r^*,S,E)\leqslant\overline{\theta}$ *we have*:

(i)

$$q\geqslant\mu_1>0\quad \textit{for some}\ \ \mu_1, \tag{6.3}$$

(ii) derivatives in (6.2) are greater than 0 [*in particular,* $h(r)>0$ *if* $r>r^*$], *and*

(iii)

$$\int_{\theta_L}^{\pi/2} \frac{1}{\sqrt{\dfrac{K}{q}+a^2\cos^2\theta-\dfrac{\mathbb{D}^2(\theta)}{q\sin^2\theta}}}\,d\theta \tag{6.4}$$

is upper bounded.

Proof of Lemma 6.2: From Definition 4.1 and formula (4.2),

$$\frac{1}{\sin^2\theta_L}=K+2Ea-E^2a^2+(qa^2+E^2a^2)\cos^2\theta_L\leqslant K+2Ea+qa^2\cos^2\theta_L\,; \tag{6.5}$$

thus taking into account the different terms in (6.1), there exist $a_i,b_i,c_i>0$, $i=1,\ldots,4$ and $\nu>0$ such that:

$$\frac{1}{\sin^2\theta_L}<\left[a_1\frac{((r^{*2}+a^2)E-a)^2}{(r^*-r_+)^2}-a_2\frac{|(r^{*2}+a^2)E-a|E}{(r^*-r_+)}\right]+a_3\frac{S}{(r^*-r_+)}+a_4, \tag{6.6}$$

$$\begin{aligned}\nu q&>4qr^*(r^*-r_-)>4qr^*(r^*-r_-)+2(qr^{*2}-K)\\&>\left[b_1\frac{((r^{*2}+a^2)E-a)^2}{(r^*-r_+)^2}-b_2\frac{|(r^{*2}+a^2)E-a|E}{(r^*-r_+)}\right]+b_3\frac{S}{(r^*-r_+)},\end{aligned} \tag{6.7}$$

$$\frac{K}{2}-E^2a^2>\left[c_1\frac{((r^{*2}+a^2)E-a)^2}{(r^*-r_+)^2}-c_2\frac{|(r^{*2}+a^2)E-a|E}{(r^*-r_+)}\right]+c_3\frac{S}{(r^*-r_+)}-c_4 \tag{6.8}$$

for any $(r^*,S,E)\in\hat{\mathcal{D}}$.

Now, we claim that for some $r_L^*\in(r_+,r_0)$ and $\overline{\theta}>0$ small, if $r^*\in(r_+,r_L^*]$ and $\theta_L(r^*,S,E)\leqslant\overline{\theta}$ then

$$4qr^*(r^*-r_-)+2(qr^{*2}-K)>\mu_0, \tag{6.9}$$

$$\frac{K}{2}-E^2a^2>0 \tag{6.10}$$

for some $\mu_0>0$; in particular, from (6.7) and (6.9), we obtain (i) with $\mu_1=\mu_0/\nu$. In fact, if $E>1/a$ then for some $r_L^*>r_+$ if $r^*\in(r_+,r_L^*]$:

$$\frac{(r^{*2}+a^2)E-a}{(r^*-r_+)}>d\cdot E,\quad d=\max\left\{\frac{a_2}{a_1},\frac{b_2}{b_1},\frac{c_2}{c_1}\right\}+1. \tag{6.11}$$

Therefore, the square brackets in (6.6), (6.7), and (6.8) are positive. Thus, from (6.6) if $\overline{\theta}$ is small, then either $[(r^{*2}+a^2)E-a]/(r^*-r_+)$ or $S/(r^*-r_+)$ are big, and (6.9), (6.10) are a consequence of (6.7), (6.8), respectively. If $E\leqslant 1/a$, some square brackets in (6.6), (6.7), (6.8) might be negative. But if this happens, then instead of (6.11) one has

$$\frac{|(r^{*2}+a^2)E-a|}{(r^*-r_+)}\leqslant\frac{d}{a}. \tag{6.12}$$

As a consequence, if $\overline{\theta}$ is chosen small enough then, from (6.6), $S/(r^*-r_+)$ is big. Thus, (6.9) and (6.10) are again a consequence of (6.7) and (6.8). Moreover, we can also prove:

$$\forall M>0 \quad \exists \overline{\theta}>0: \quad q(r^*,S,E)>M \ \text{ if } \ \theta_L(r^*,S,E)\leqslant\overline{\theta}, \quad r^*\in(r_+,r_L^*]. \tag{6.13}$$

From (6.3), $h^{(3)}(r^*),h^{(4)}(r^*)>0$ and, from (6.9), $h^{(2)}(r^*)>0$ too and, thus, (ii) is obtained. In order to prove (iii), put

$$\Lambda_{q,K,E}(\theta)=\frac{K}{q}+a^2\cos^2\theta-\frac{\mathbb{D}^2(\theta)}{q\sin^2\theta}, \quad \theta\in\left[\theta_L,\frac{\pi}{2}\right]. \tag{6.14}$$

When the integral (6.4) is carried out, $\Lambda_{q,K,E}(\theta)$ vanishes just in θ_L. It is sufficient to prove that, when $\Lambda_{q,K,E}(\theta)$ is smaller than, say, $r_+^2/4$ the contribution to the integral (6.4) is bounded. So, we need just to find $\overline{\theta}$ such that, for the corresponding q,K,E with $\theta_L\leqslant\overline{\theta}$:

$$\text{if} \quad \Lambda_{q,K,E}(\theta)\leqslant\frac{r_+^2}{4} \ \text{ with } \ \theta\in\left[\theta_L,\frac{\pi}{2}\right] \quad \text{then} \quad \frac{\mathrm{d}}{\mathrm{d}\theta}\Lambda_{q,K,E}(\theta)\geqslant 1. \tag{6.15}$$

Using (6.3) and (6.10) it is easy to check:

$$\Lambda_{q,K,E}(\theta)>\frac{K}{2q}-\frac{1}{q\sin^2\theta}. \tag{6.16}$$

Therefore, as $K/q>r_+^2$ [from the first Eq. (6.1)], we have

$$\text{if} \quad \Lambda_{q,K,E}(\theta)\leqslant\frac{r_+^2}{4} \quad \text{then} \quad \frac{1}{q\sin^2\theta}>\frac{K}{4q} \tag{6.17}$$

and, again using (6.10), we obtain

$$\frac{1}{q\sin^2\theta}>\mathcal{M}(E,q):=\max\left\{\frac{r_+^2}{4},\frac{E^2a^2}{2q}\right\}. \tag{6.18}$$

On the other hand, from (6.14)

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\Lambda_{q,K,E}(\theta)=-\left(1+\frac{E^2}{q}\right)a^2\sin 2\theta+\frac{2\cos\theta}{q\sin^3\theta} \tag{6.19}$$

which, from (6.18), imply

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\Lambda_{q,K,E}(\theta)>-a^2\sin 2\theta+2\mathcal{M}(E,q)\left(-\sin 2\theta+\frac{\cos\theta}{\sin\theta}\right). \tag{6.20}$$

In conclusion, from (6.13) if $\overline{\theta}$ is small the angles θ satisfying (6.18) are small too and, thus, the right-hand side in (6.20) is greater than 1. □

From (6.1), $\lim_{S\to\infty}q(r^*,S,E)=\lim_{S\to\infty}K(r^*,S,E)=\infty$ and, thus, using (6.5): $\lim_{S\to\infty}\theta_L(r^*,S,E)=0$. So, fixed $\overline{\theta}$ and r_L^* in Lemma 6.2 we can define $S(r^*,E)=\mathrm{Inf}\{S>0:\theta_L(r^*,\overline{S},E)\leqslant\overline{\theta},\forall\overline{S}>S\}\geqslant 0$ for all $(r^*,E)\in(r_+,r_L^*]\times(0,\infty)$. Recall that $\theta_L(r^*,S,E)$ is differentiable [use $(\mathrm{d}/\mathrm{d}\theta)\,\Lambda_{q,K,E}(\theta_L)\neq 0$ because of (6.15) and, thus $\theta_L(q,K,E)$ is differentiable]; moreover, $S(r^*,E)$ is continuous [when $\theta_L(r^*,S,E)=\overline{\theta}$ from (6.5) and (6.1) $\partial\theta_L/\partial S>0$]. Recall also that $S(r^*,E)$ has a finite supremum $\mathcal{S}$. In fact, from (6.11) and (6.12) the square brackets in (6.8) are lower bounded. So, for some big value S_0 of S, the expression $K/2-E^2a^2$ can be made arbitrarily big. Thus, from (6.5) and (6.3), $\theta_L(r^*,S,E)$ will be less than $\overline{\theta}$, independently of (r^*,E), and $S(r^*,E)<S_0$ as required. Define now:

$$\mathcal{D}=\{(r^*,S,E)\in\hat{\mathcal{D}}:r^*\in(r_+,r_L^*],S\in[S(r^*,E),\infty),E\in(0,\infty)\}. \tag{6.21}$$

Lemma 6.3: Consider the continuous function $T(r^*,S,E)=\Delta t-(t_1-t_0)$ *defined on* $\mathcal{D}$. *There exist positive constants* $M_1(r^*)$, $M_2(r^*)$ *and* $m(r^*)$ *such that*

$$\begin{gathered} E\leqslant m(r^*)\Rightarrow T(r^*,S,E)<0,\\ M_1(r^*)\cdot\sqrt{S}+M_2(r^*)\leqslant E\Rightarrow T(r^*,S,E)>0. \end{gathered} \tag{6.22}$$

Moreover, these constants can be chosen such that if either $m(r_n^*)\to 0$ *or* $M_1(r_n^*)\to\infty$ *or* $M_2(r_n^*)\to\infty$ *for some sequence* $\{r_n^*\}_n$ *then, necessarily,* $r_n^*\to r_+$.

Proof of Lemma 6.3: Fix $(r^*,S,E)\in\mathcal{D}$, recalling the expression of Δt in (4.6) put:

$$a\mathbb{D}(\theta(r))+(r^2+a^2)\frac{\mathbb{P}(r)}{\Delta(r)}=\left[\frac{(r^2+a^2)^2}{(r-r_-)(r-r_+)}-a^2\sin^2\theta(r)\right]E-\left[\frac{a(r^2+a^2)}{(r-r_-)(r-r_+)}-a\right] \tag{6.23}$$

being $\theta(r)$ computed from the second equation in (4.3) with constants $(q(r^*,S,E),K(r^*,S,E),E)$. But each term on the right-hand side of (6.23) will be bounded, say:

$$0<r_+^2<\frac{(r^2+a^2)^2}{(r-r_-)(r-r_+)}-a^2\sin^2\theta(r)<\frac{(r_1^2+a^2)^2}{(r^*-r_+)^2},\quad r\in[r^*,r_1], \tag{6.24}$$

and

$$0<\frac{a^3}{r_1^2}<\frac{a(r^2+a^2)}{(r-r_-)(r-r_+)}-a<\frac{a(r_1^2+a^2)}{(r^*-r_+)^2},\quad r\in[r^*,r_1]. \tag{6.25}$$

Now, put:

$$m(r^*)=\frac{1}{2}\cdot\frac{a^3(r^*-r_+)^2}{r_1^2(r_1^2+a^2)^2}. \tag{6.26}$$

Thus, if $E\leqslant m(r^*)$ then (6.23) is less than 0 and $(\Delta t)(r^*,S,E)<0\leqslant t_1-t_0$, thus $T(r^*,S,E)<0$ [see (4.6)]. Let

$$M_1(r^*)=\sup_{\mathcal{D}}\left\{\frac{E}{\sqrt{S}}:T(r^*,S,E)\leqslant 0,S\geqslant 1\right\},$$

$$M_2(r^*)=\sup_{\mathcal{D}}\{E:T(r^*,S,E)\leqslant 0,S(r^*,E)\leqslant S<1\}+1.$$

To prove (6.22) it is sufficient to prove $M_1(r^*)<\infty$, $M_2(r^*)<\infty$. But, if some of these inequalities do not hold then there exists a sequence of points $\{(r^*,S_n,E_n)\}_n\subset\mathcal{D}$ satisfying hypotheses of Lemma 4.6(ii) for the functions

$$f_n(r)=\frac{1}{E_n}\left[a\mathbb{D}_n(\theta_n(r))+(r^2+a^2)\frac{\mathbb{P}_n(r)}{\Delta(r)}\right],\quad p_n(r)=\frac{h_n(r)}{E_n^2} \tag{6.27}$$

with $h_n(r)\equiv h(r,q(r^*,S_n,E_n),K(r^*,S_n,E_n),E_n)$ in $[r^*,r_1]$ and thus $R_n=S_n/E_n^2$ [see (6.24), (6.25), (6.1), and (6.2)]. Thus, the conclusion of Lemma 4.6(ii) contradicts $T(r^*,S_n,E_n)\leqslant 0$ for all n [see (4.6)].

For the last assertion, it is clear that $m(r_n^*)\to 0$ implies $r_n^*\to r_+$ [see (6.26)]. Even more, if either $M_1(r_n^*)$ or $M_2(r_n^*)$ go to ∞ and, up to a subsequence, $r_n^*\geqslant r_++\epsilon_0$, $\epsilon_0>0$ then there exists a sequence of points $\{(r_n^*,S_n,E_n)\}_n\subset\mathcal{D}$ with $T(r_n^*,S_n,E_n)\leqslant 0$ and either $S_n/E_n^2\to 0$ and $S_n\geqslant 1$ or $1/E_n^2\to 0$ and $S(r_n^*,E_n)\leqslant S_n\leqslant 1$. Then, by applying Lemma 4.6(ii) to (6.27) as before but, now, with the sequence $\{(r_n^*,S_n,E_n)\}_n\subset\mathcal{D}$ we obtain a contradiction again. □

Remark 6.4: Notice that we can choose $\overline{\theta}$ in Lemma 6.2 small enough such that $\mathcal{D}$ in (6.21) satisfies, additionally:

(i) the component S of the points $(r^*,S,E)\in\mathcal{D}$ with $r^*=r_L^*$ and $m(r_L^*)\leqslant E\leqslant M_1(r_L^*)+M_2(r_L^*)$ admits a positive lower bound [from (6.5) if θ_L is small then either q or K is big and, from (6.1) S will be big too], and

(ii) if $(r^*,S,E)\in\mathcal{D}$ and $S/(r^*-r_+)\leqslant 1$ then

$$\left|\frac{(r^{*2}+a^2)E-a}{(r^*-r_-)(r^*-r_+)}\right|>\frac{2a}{r_+^2+a^2}$$

[use (6.6)].

From now on we will assume that $\mathcal{D}$ is the domain fixed by this new value of $\overline{\theta}$, and Lemma 6.2 with Remark 6.4 will ensure that none of the problems 3^BI–3^BIV explained in Sec. III. Summing up, it is sufficient to find an element of $\mathcal{D}$ such that the corresponding (q,K,E) given from (6.1) and the function $h(r)\equiv h(r,q,K,E)$ in (4.5) satisfy the equalities (4.11) with Δt, $\Delta|\theta|$ and $\Delta\varphi$ as in (4.6), (4.8), and (4.9), and with $L=1$. For this aim, we establish the next two technical Lemmas. First, taking into account Lemma 6.3 define the subset

$$B=\{(r_L^*,S,E)\in\mathcal{D}:0<m(r_L^*)\leqslant E\leqslant M_1(r_L^*)\cdot\sqrt{S}+M_2(r_L^*)\}. \tag{6.28}$$

Lemma 6.5: (*i*) *For* $(r^*,S,E)\in\mathcal{D}$ *then* $((r^{*2}+a^2)E-a)^2/q$ *and* E^2/q *are upper bounded.* (*ii*) *If also* $(r_L^*,S,E)\in B$ *then*

$$(\Delta|\theta|)(r_L^*,S,E)=\int_{r_L^*}^{r_0}\frac{\sqrt{\Lambda_{q,K,E}(\theta(r))}}{\sqrt{\dfrac{h(r)}{q}}}\mathrm{d}r+\int_{r_L^*}^{r_1}\frac{\sqrt{\Lambda_{q,K,E}(\theta(r))}}{\sqrt{\dfrac{h(r)}{q}}}\mathrm{d}r$$

is upper bounded too.

Proof of Lemma 6.5: (i) If $E\leqslant 1/a$ these terms are obviously bounded from (6.3); otherwise, first use (6.7) and (6.11) to prove

$$\nu q>b_1\frac{E((r^{*2}+a^2)E-a)}{(r^*-r_+)}.$$

(ii) From Remark 6.4(i) the component S of the points in B admits a positive lower bound (see points J', I' in Fig. 2). Then, there exists $L_0>0$ such that

$$\frac{h'(r_L^*)}{q}=\frac{S}{q}>L_0 \tag{6.29}$$

for all $(r_L^*,S,E)\in B$ [see (6.1)]. But taking into account (6.1), (6.14) and (i) there exists $C_0>0$ such that

$$\sqrt{\Lambda_{q,K,E}(\theta(s))}<C_0 \tag{6.30}$$

along the geodesic $\gamma(s)$ corresponding to each $(r_L^*,S,E)\in B$. Summing up, inequalities (6.29), (6.30) joined with $h^{(k)}(r_L^*)/q\geqslant 0$ for $k\geqslant 2$ (see Lemma 6.2) imply that

$$(\Delta|\theta|)(r_L^*,S,E)=\int_{r_L^*}^{r_0}\frac{\sqrt{\Lambda_{q,K,E}(\theta(r))}}{\sqrt{\frac{h(r)}{q}}}\mathrm{d}r+\int_{r_L^*}^{r_1}\frac{\sqrt{\Lambda_{q,K,E}(\theta(r))}}{\sqrt{\frac{h(r)}{q}}}\mathrm{d}r$$

is upper bounded on B. □

Lemma 6.6: For any sequence $\{(r_n^*,S_n,E_n)\}_n\subset\mathcal{D}$ *satisfying either* $r_n^*\searrow r_+$ *or* $S_n\searrow 0$ *then* $(\Delta|\theta|)(r_n^*,S_n,E_n)\to\infty$.

Proof of Lemma 6.6: This result is a consequence of the following two steps:

Step 1. For any such sequence $\{(r_n^*,S_n,E_n)\}_n\subset\mathcal{D}$, the polynomials $p_n(r)=h_n(r)/q_n$ satisfy hypotheses in Lemma 4.6(ii) in $[r_n^*,r_1]$. In fact, $p_n'(r_n^*)=S_n/q_n\to 0$ [use that the square brackets in (6.7) is lower bounded and (6.3)] and, from (6.2) and Lemma 6.5(i), derivatives $p_n^{(k)}(r_n^*)$ $(\geqslant 0)$ admit an upper bound for $k\geqslant 2$.

Step 2. For any sequence $\{(r_n^*,S_n,E_n)\}_n\subset\mathcal{D}$ such that the polynomials $p_n(r)=h_n(r)/q_n$ satisfy hypotheses in Lemma 4.6(ii) in $[r_n^*,r_1]$ then $(\Delta|\theta|)(r_n^*,S_n,E_n)\to\infty$. Otherwise, $(\Delta|\theta|)$ (r_n^*,S_n,E_n) is bounded up to a subsequence. Using (6.14) and (4.5), the second equation in (4.3) is rewritten as

$$\epsilon'\frac{\sqrt{q_n}\mathrm{d}r}{\sqrt{h_n(r)}}=\frac{\mathrm{d}\theta}{\sqrt{\Lambda_{q_n,K_n,E_n}(\theta)}},$$

and using that $(\Delta|\theta|)(r_n^*,S_n,E_n)$ is bounded:

$$\int_{r_n^*}^{r_0}\frac{\sqrt{q_n}}{\sqrt{h_n(r)}}\mathrm{d}r+\int_{r_n^*}^{r_1}\frac{\sqrt{q_n}}{\sqrt{h_n(r)}}\mathrm{d}r\leqslant\int_{\theta_0}^{\theta_1}\frac{1}{\sqrt{\Lambda_{q_n,K_n,E_n}(\theta)}}\mathrm{d}\theta+2n_0\int_{\theta_{L,n}}^{\pi-\theta_{L,n}}\frac{1}{\sqrt{\Lambda_{q_n,K_n,E_n}(\theta)}}\mathrm{d}\theta \tag{6.31}$$

for some integer $n_0>0$. As $\{(r_n^*,S_n,E_n)\}_n\subset\mathcal{D}$ for all n, Lemma 6.2 implies that the second member of (6.31) is upper bounded. This contradicts Lemma 4.6(ii) applied to the functions $f_n(r)\equiv 1$ and $p_n(r)=h_n(r)/q_n$ in $[r_n^*,r_1]$. □

Next, consider the continuous functions on $\mathcal{D}$, $\Theta_n=\Delta|\theta|-(\theta_1-\theta_0)-2n(\pi-2\theta_L)$, $n\geqslant 0$. Then, the following result on boundary conditions of T and Θ_n on $\mathcal{D}$ holds.

Proposition 6.7: Let $\{\overline{S_n}\}_n$ *be a sequence with* $\overline{S_n}>\mathcal{S}(\equiv\mathrm{Sup}\{S(r^*,E):(r^*,E)\in(r_+,r_0)\times(0,\infty)\})$ *for all* n. *There exists* $\{\epsilon_n\}_n$, $\epsilon_n>0$, $\epsilon_n\searrow 0$ *and* $\{\delta_n\}_n$, $\delta_n>0$, $\delta_n\searrow 0$, *such that if*

$$\mathcal{D}_n=\left\{(r^*,S,E)\in\hat{\mathcal{D}}:r^*\in[r_+\!+\epsilon_n,r_L^*],S\in[S(r^*,E),\overline{S_n}],E\in\left[\delta_n,\frac{1}{\delta_n}\right]\right\} \tag{6.32}$$

then

$$B\cap\{(r^*,S,E)\in\mathcal{D}_n:r^*=r_L^*\}\subseteq\left\{(r^*,S,E)\in\mathcal{D}_n:r^*=r_L^*,E\in\left(\delta_n,\frac{1}{\delta_n}\right)\right\} \tag{6.33}$$

[*for B in* (6.28)], *and*

$$\begin{gathered}T>0\quad on\quad\left(r^*,S,\frac{1}{\delta_n}\right)\in\mathcal{D}_n,\\ T<0\quad on\quad(r^*,S,\delta_n)\in\mathcal{D}_n,\\ \Theta_n>0\quad on\quad(r_+\!+\epsilon_n,S,E)\in\mathcal{D}_n,\end{gathered} \tag{6.34}$$

$$\Theta_n<0 \quad on \quad (r^*,S,E)\in B\cap\{(r^*,S,E)\in\mathcal{D}_n : r^*=r_L^*\}$$

for n big enough (see Fig. 2).

Proof of Proposition 6.7: From Lemma 6.5(ii), $\Delta|\theta|$ is upper bounded on B and, thus, $\Theta_n<0$ on B for n big enough.

On the other hand, there exists a sequence $\{\epsilon_n\}_n$, $\epsilon_n>0$, $\epsilon_n\searrow 0$ such that $\Theta_n>0$ when $r^*=r_+ +\epsilon_n$. In fact, otherwise we obtain a sequence of points $\{(r_l^*,S_l,E_l)\}_l\subset\mathcal{D}$, $r_l^*<r_+ +1/l$ with $\Theta_n(r_l^*,S_l,E_l)\leqslant 0$ for all l. But these last inequalities contradict the conclusion of Lemma 6.6.

Finally, the sequence $\{\delta_n\}_n$ is obtained from Lemma 6.3 applied to $r^*\in[r_+ +\epsilon_n,r_L^*]$. □

Remark 6.8: The choice of $\{\epsilon_n\}_n$ in Proposition 6.7 does not depend on the sequence $\{\overline{S_n}\}_n$. Nevertheless, $\{\delta_n\}_n$ does depend on $\{\epsilon_n\}_n$ and $\{\overline{S_n}\}_n$.

Following step $(4^B II)$ (Sec. III), if we define the sequence of homeomorphisms $\{z_n^m\}_m$, $z_n^m:\mathcal{D}_n^m\to[0,1]^3$ with

$$\mathcal{D}_n^m=\left\{(r^*,S,E)\in\mathcal{D}_n : S\geqslant S(r^*,E)+\frac{1}{m}\right\} \tag{6.35}$$

as depicted in Fig. 3 then, from (6.34) and Lemma 6.3, the functions $T\circ(z_n^m)^{-1}$, $\Theta_n\circ(z_n^m)^{-1}$ satisfy

$$\begin{aligned}
&T\circ(z_n^m)^{-1}>0 \quad on \quad (r^*,S,E)\in[0,1]^2\times\{1\},\\
&T\circ(z_n^m)^{-1}<0 \quad on \quad (r^*,S,E)\in[0,1]^2\times\{0\},\\
&\Theta_n\circ(z_n^m)^{-1}>0 \quad on \quad (r^*,S,E)\in\{0\}\times[0,1]^2,\\
&\Theta_n\circ(z_n^m)^{-1}<0 \quad on \quad (r^*,S,E)\in\{1\}\times[0,1]^2.
\end{aligned} \tag{6.36}$$

Now, we are in conditions to apply topological arguments based on Brouwer's degree. In fact,

Lemma 6.9: There exists a connected subset $z_n^m(\mathcal{C}_n^m)$ of zeroes of $T\circ(z_n^m)^{-1}$ and $\Theta_n\circ(z_n^m)^{-1}$ such that

$$z_n^m(\mathcal{C}_n^m)\cap([0,1]\times\{0\}\times[0,1])\neq\varnothing \quad and \quad z_n^m(\mathcal{C}_n^m)\cap([0,1]\times\{1\}\times[0,1])\neq\varnothing$$

for every $m\in\mathbb{N}$.

Proof of Lemma 6.9: Consider the function

$$\mathcal{F}_n^m: \quad (0,1)\times[0,1]\times(0,1)\to X\equiv\mathbb{R}^2,$$

$$(r^*,S,E)\mapsto(\Theta_n\circ(z_n^m)^{-1}(r^*,S,E),T\circ(z_n^m)^{-1}(r^*,S,E))+(r^*,E)$$

and put $\mathcal{F}_{n,0}^m(r^*,E)=\mathcal{F}_n^m(r^*,0,E)$, $G=(0,1)^2$. By Ref. 32, Lemma 3.4 it is sufficient to prove that, because of (6.36):

$$\deg(\mathrm{Id}-\mathcal{F}_{n,0}^m,G,0)\neq 0,$$

where $\deg(Id-\mathcal{F}_{n,0}^m,G,0)$ is the degree of the function $\mathrm{Id}-\mathcal{F}_{n,0}^m$ in the open subset G with respect to the value 0.[30] But the affine map

$$\hat{\mathcal{F}}^m: \quad (0,1)^2\to\mathbb{R}^2,$$

$$(r^*,E)\mapsto(1-2r^*,-1+2E)+(r^*,E)$$

has obviously $\deg(\mathrm{Id}-\hat{\mathcal{F}}^m,G,0)\neq 0$, and $\deg(\mathrm{Id}-\mathcal{F}^m_{n,0},G,0)=\deg(\mathrm{Id}-\hat{\mathcal{F}}^m,G,0)$ [the map $\lambda\mapsto \mathrm{Id}-\mathcal{F}^m_{n,0}+\lambda(\mathcal{F}^m_{n,0}-\hat{\mathcal{F}}^m)$, $\lambda\in[0,1]$ is a homotopy from $\mathrm{Id}-\mathcal{F}^m_{n,0}$ to $\mathrm{Id}-\hat{\mathcal{F}}^m$ without zeroes on the boundary from (6.36)] which concludes the proof. □

Up to a subsequence, $\lim_m f_m\mathcal{C}^m_n\neq\varnothing$ and, thus, $\mathcal{C}_n=\limsup_m\mathcal{C}^m_n\subset\overline{\mathcal{D}}_n$ is connected (see Ref. 33 Chap. I, Theorem 9.1). By continuity $T=\Theta_n=0$ in $\mathcal{C}_n\cap\mathcal{D}_n$ and

$$\mathcal{C}_n\cap\{(r^*,S,E)\in\overline{\mathcal{D}}_n : S=S(r^*,E)\}\neq\varnothing \quad\text{and}\quad \mathcal{C}_n\cap\{(r^*,S,E)\in\mathcal{D}_n : S=\overline{S}_n\}\neq\varnothing.$$

(see Fig. 4). This joined with the following result implies (i) and (ii) in ($4^B III$):

Lemma 6.10: If $(r^*,S,E)\in\mathcal{C}_n$ *then* $S>0$ (*in particular,* $\mathcal{C}_n\subset\mathcal{D}_n$).

Proof of Lemma 6.10: Otherwise, there exists a sequence $\{(r^*_l,S_l,E_l)\}_l\subset\mathcal{D}_n\subset\mathcal{D}$ in $\mathcal{C}_n$ such that $S_l\to 0$. Then, from Lemma 6.6, we obtain a contradiction with $\Theta_n=0$ in $\mathcal{C}_n\cap\mathcal{D}_n$. □

Finally, as Δt and $\Delta|\theta|$ satisfy (4.11) for geodesics in each $\mathcal{C}_n$ we only have to prove that one of such geodesics satisfies the required value for $\Delta\varphi$. This will be straightforward from the following two lemmas:

Lemma 6.11: *There exists a choice of the sequence* $\{\overline{S}_n\}_n$ *in Proposition 6.7 such that for any* $\epsilon>0$ *points* $(r^*_n,\overline{S}_n,E_n)\in\mathcal{C}_n$ *satisfy*:

$$2n\pi-(\Delta\varphi)(r^*_n,\overline{S}_n,E_n)<n\cdot\epsilon \tag{6.37}$$

for n big enough.

Proof of Lemma 6.11: First, we will prove that for any sequence $\{\overline{S}_n\}_n$ diverging fast enough there exists a constant $\delta>0$ such that

$$(\Delta\varphi)(r^*_n,\overline{S}_n,E_n)+\delta>\int_{r^*_n}^{r_0}\frac{1}{\sqrt{\sin^2\theta_n(r)}}\frac{1}{\sqrt{h_n(r)}}\mathrm{d}r+\int_{r^*_n}^{r_1}\frac{1}{\sqrt{\sin^2\theta_n(r)}}\frac{1}{\sqrt{h_n(r)}}\mathrm{d}r. \tag{6.38}$$

Thus, the right-hand side in (6.38) can replace $(\Delta\varphi)(r^*_n,\overline{S}_n,E_n)$ in order to prove (6.37). To prove (6.38) note, taking into account (4.9):

$$\mathcal{P}_n(r)\equiv\frac{\mathbb{D}_n(\theta_n(r))}{\sin^2\theta_n(r)}+a\,\frac{\mathbb{P}_n(r)}{\Delta(r)}-\frac{1}{\sin^2\theta_n(r)}=E_n\left(\frac{a(r^2+a^2)}{(r-r_-)(r-r_+)}-a\right)-\frac{a^2}{(r-r_-)(r-r_+)}. \tag{6.39}$$

If $E_n>1/a$ then (6.39) is positive. In the case $E_n\leqslant 1/a$ note first that, from Remark 6.8, points $(r^*_n,\overline{S}_n,E_n)\in\mathcal{C}_n$ satisfy $r^*_n>r_++\epsilon_n$, independently of $\overline{S}_n$. Thus, for every n there exists $\overline{S}_n$ big enough such that

$$\int_{r^*_n}^{r_0}\frac{\mathcal{P}_n(r)}{\sqrt{h_n(r)}}\mathrm{d}r+\int_{r^*_n}^{r_1}\frac{\mathcal{P}_n(r)}{\sqrt{h_n(r)}}\mathrm{d}r>-\delta,$$

and (6.38) is obtained.

Using the second equation in (4.3), the variable of integration r in (6.38) can be substituted by θ. Then, as $(\Delta|\theta|)_n=\theta_1-\theta_0+2n(\pi-2\theta_{L,n})$, (6.38) can be written

$$(\Delta\varphi)_n+\delta>\int_{\theta_0}^{\theta_1}\Omega_n(\theta)\mathrm{d}\theta+2n\cdot\int_{\theta_{L,n}}^{\pi-\theta_{L,n}}\Omega_n(\theta)\mathrm{d}\theta, \tag{6.40}$$

where

$$\Omega_n(\theta)=\frac{\dfrac{1}{\sin^2\theta}}{\sqrt{K_n+q_n a^2\cos^2\theta-\dfrac{\mathbb{D}_n^2(\theta)}{\sin^2\theta}}}. \tag{6.41}$$

Therefore, from (6.40) and the symmetry of the integrals

$$\int_{\theta_{L,n}}^{\pi/2}\Omega_n(\theta)\mathrm{d}\theta,\quad \int_{\pi/2}^{\pi-\Theta_{L,n}}\Omega_n(\theta)\mathrm{d}\theta$$

it is sufficient to prove

$$\lim\ \inf_{n\to\infty}\int_{\theta_{L,n}}^{\pi/2}\Omega_n(\theta)\mathrm{d}\theta\geqslant\frac{\pi}{2}. \tag{6.42}$$

In fact, from an elemental integration:

$$\int_{\theta_{L,n}}^{\pi/2}\frac{\dfrac{1}{\sin^2\theta}}{\sqrt{\dfrac{1}{\sin^2\theta_{L,n}}-\dfrac{1}{\sin^2\theta}}}\mathrm{d}\theta=\frac{\pi}{2}, \tag{6.43}$$

for all n. But from the equality in (6.5)

$$\begin{aligned}\frac{1}{\sin^2\theta_{L,n}}&=K_n+2E_n a-E_n^2a^2+(q_na^2+E_n^2a^2)\cos^2\theta_{L,n}\\&\geqslant K_n+2E_n a-E_n^2a^2+(q_na^2+E_n^2a^2)\cos^2\theta\\&=\frac{1}{\sin^2\theta}+K_n+q_na^2\cos^2\theta-\frac{\mathbb{D}_n^2(\theta)}{\sin^2\theta}\end{aligned} \tag{6.44}$$

if $\theta\in[\theta_{L,n},\pi/2]$. Thus (6.42) is a consequence of (6.43) and (6.44). □

As explained in ($4^B III$), each $\mathcal{C}_n$ contains a point with $\theta_L=\overline{\theta}$. Thus, the following result will be appliable:

Lemma 6.12: Let $\{(r_n^{*\prime},S_n',E_n')\}_n$ *be a sequence of points, each one in the corresponding* $\mathcal{C}_n$ *with* $\theta_{L,n}=\theta_L(r_n^{*\prime},S_n',E_n')=\overline{\theta}>0$. *Then, there exists* $\epsilon_0>0$ *such that*

$$2n\pi-(\Delta\varphi)(r_n^{*\prime},S_n',E_n')>n\cdot\epsilon_0 \tag{6.45}$$

for n big enough.

Proof of Lemma 6.12: First, we will prove

$$h_n'(r_n^{*\prime})=S_n'\to 0 \tag{6.46}$$

and then the limits:

$$r_n^{*\prime}\to r_+,\quad E_n'\to\frac{a}{r_+^2+a^2},\quad q_n'\to q',\quad K_n'\to q'r_+^2, \tag{6.47}$$

where

$$q' = \frac{r_+^2 + a^2 \cos^2 \overline{\theta}}{(r_+^2 + a^2)^2 \sin^2 \overline{\theta}}.$$

In order to prove (6.46) and taking into account that $\Theta_n = 0$ on $\mathcal{C}_n$ we have that

$$(\Delta|\theta|)(r_n^{*\prime}, S_n', E_n') = \theta_1 - \theta_0 + 2n(\pi - 2\overline{\theta}) \to \infty \quad \text{when} \quad n \to \infty. \tag{6.48}$$

By using (6.44) with $\theta_{L,n} \equiv \overline{\theta}$ the numerator in (4.8) is upper bounded by $1/\sin \overline{\theta}$ in our sequence, thus from (6.48)

$$\int_{r_n^{*\prime}}^{r_0} \frac{1}{\sqrt{h_n(r)}} \mathrm{d}r + \int_{r_n^{*\prime}}^{r_1} \frac{1}{\sqrt{h_n(r)}} \mathrm{d}r \to \infty, \tag{6.49}$$

which implies (6.46) (recall that from Lemma 6.2 the remainder of the derivatives of h_n are positive). Notice that we also obtain $E_n' \leqslant 1/a$ for big n. In fact, otherwise computing directly from (4.2):

$$a\mathbb{D}_n(\theta_n(r)) + (r^2 + a^2)\frac{\mathbb{P}_n(r)}{\Delta(r)} \geqslant a + \frac{r_+^2}{a} > 0,$$

thus, from (4.6) and (6.49) we have $(\Delta t)_n \to \infty > t_1 - t_0$, in contradiction with $(r_n^{*\prime}, S_n', E_n') \in \mathcal{C}_n$. In order to prove the first limit in (6.47) assume, by contradiction, $r_n^{*\prime} \geqslant r_+ + \delta_0$ for some $\delta_0 > 0$ up to a subsequence. Then, from (6.46) we have

$$\frac{S_n'}{(r_n^{*\prime} - r_+)} \to 0.$$

This joined with Remark 6.4(ii) allows us to assume

$$\left| \frac{(r_n^{*\prime 2} + a^2)E_n' - a}{(r_n^{*\prime} - r_-)(r_n^{*\prime} - r_+)} \right| > \frac{2a}{r_+^2 + a^2} \tag{6.50}$$

for n big enough. Even more, we can extend the lower bound in (6.50) through $r_n^{*\prime}$. More precisely, for $E_n' \in (0, 1/a]$ and $r \in [r_+ + \delta_0, r_0]$ function

$$r \mapsto \frac{(r^2 + a^2)E_n' - a}{(r - r_-)(r - r_+)}$$

has a derivative which admits a bound independent of E_n'. Thus, there exists $\overline{\delta_0} > 0$ such that

$$\left| \frac{(r^2 + a^2)E_n' - a}{(r - r_-)(r - r_+)} \right| > \frac{3a}{2(r_+^2 + a^2)}, \quad \forall r \in [r_n^{*\prime}, r_n^{*\prime} + \overline{\delta_0}];$$

therefore

$$\left| a\mathbb{D}_n(\theta_n(r)) + (r^2 + a^2)\frac{\mathbb{P}_n(r)}{\Delta(r)} \right| \geqslant \frac{a}{2}, \quad \forall r \in [r_n^{*\prime}, r_n^{*\prime} + \overline{\delta_0}]. \tag{6.51}$$

We will prove that (6.51) implies the contradiction $|(\Delta t)_n| \to \infty > |t_1 - t_0|$ and, thus, $r_n^{*\prime} \to r_+$. In fact, assuming $\overline{\delta_0} < r_0 - r_L^*$ Lemma 4.6(ii) is applicable to the expression of $|\Delta t(r_n^{*\prime}, S_n', E_n')|$ in (4.6) when the integrals are carried out in $[r_n^{*\prime}, r_n^{*\prime} + \overline{\delta_0}]$ [use (6.51), (6.46), and the facts that

$E_n' \leqslant 1/a$ and $r_n^{*\prime} \geqslant r_+ + \delta_0$, with (6.2), (6.1)]. As the integrals of the expression of $\Delta t(r_n^{*\prime}, S_n', E_n')$ in $[r_n^{*\prime}+\delta_0, r_0]$ and $[r_n^{*\prime}+\delta_0, r_1]$ are bounded [the numerator is bounded and the derivatives $h^{(k)}(r_n^{*\prime})$ are positive with $h^{(4)}(r_n^{*\prime}) > 24\mu_1 > 0$], the contradiction is obtained, and $r_n^{*\prime} \to r_+$.

For the convergence of E_n' in (6.47), recall that

$$\left| \frac{(r_n^{*\prime 2} + a^2)E_n' - a}{(r_n^{*\prime} - r_+)} \right| \tag{6.52}$$

is bounded. In fact, otherwise q_n' and $K_n'/2 - E_n'^2 a^2$ go to ∞, up to a subsequence [see (6.7) and (6.8)]; this and (6.5) contradict that $\theta_{L,n} = \overline{\theta}$ for all n. Therefore, as $r_n^{*\prime} \to r_+$, the second limit in (6.47) is obtained. Finally, for the other two limits, the boundedness of (6.52) and the convergence of E_n' imply that $q_n' r_n^{*\prime 2} - K_n' \to 0$ [see the first equation in (6.1)] which, joined to the fact that $\theta_{L,n} = \overline{\theta}$ for all n, implies the two required limits [use the equality in (6.5)].

In order to prove (6.45) notice that the second limit in (6.47) implies

$$\int_{r_n^{*\prime}}^{r_0} \frac{1 - E_n' a \sin^2 \theta_n(r)}{\sqrt{h_n(r)}} \mathrm{d}r + \int_{r_n^{*\prime}}^{r_1} \frac{1 - E_n' a \sin^2 \theta_n(r)}{\sqrt{h_n(r)}} \mathrm{d}r$$
$$\geqslant \frac{r_+^2}{2(r_+^2 + a^2)} \left(\int_{r_n^{*\prime}}^{r_0} \frac{1}{\sqrt{h_n(r)}} \mathrm{d}r + \int_{r_n^{*\prime}}^{r_1} \frac{1}{\sqrt{h_n(r)}} \mathrm{d}r \right), \tag{6.53}$$

which goes to ∞ by (6.49). But $(\Delta t)_n = t_1 - t_0$ for all n, thus from (6.53), (4.6) and the expression of $\mathbb{D}(\theta)$ [formula (4.2) with $L = 1$]

$$\int_{r_n^{*\prime}}^{r_0} \frac{(r^2 + a^2) \dfrac{\mathbb{P}_n(r)}{\Delta(r)}}{\sqrt{h_n(r)}} \mathrm{d}r + \int_{r_n^{*\prime}}^{r_1} \frac{(r^2 + a^2) \dfrac{\mathbb{P}_n(r)}{\Delta(r)}}{\sqrt{h_n(r)}} \mathrm{d}r \to -\infty. \tag{6.54}$$

Obviously, from (6.54) and (4.9)

$$(\Delta\varphi)_n < \int_{r_n^{*\prime}}^{r_0} \frac{\dfrac{1 - E_n' a \sin^2 \theta_n(r)}{\sin^2 \theta_n(r)}}{\sqrt{h_n(r)}} \mathrm{d}r + \int_{r_n^{*\prime}}^{r_1} \frac{\dfrac{1 - E_n' a \sin^2 \theta_n(r)}{\sin^2 \theta_n(r)}}{\sqrt{h_n(r)}} \mathrm{d}r. \tag{6.55}$$

If the variable of integration r in (6.55) is changed by θ (as in Lemma 6.11) and taking into account that now $(\Delta|\theta|)_n = \theta_1 - \theta_0 + 2n(\pi - 2\overline{\theta})$, (6.55) can be written

$$(\Delta\varphi)_n < \int_{\theta_0}^{\theta_1} W_n(\theta) \mathrm{d}\theta + 2n \cdot \int_{\overline{\theta}}^{\pi - \overline{\theta}} W_n(\theta) \mathrm{d}\theta, \tag{6.56}$$

where

$$W_n(\theta) = \frac{\dfrac{1}{\sin^2 \theta}}{\sqrt{\dfrac{K_n' + q_n' a^2 \cos^2 \theta}{(1 - E_n' a \sin^2 \theta)^2} - \dfrac{1}{\sin^2 \theta}}}.$$

Then, taking the limit $W(\theta)$ of $\{W_n(\theta)\}_n$ we have from (6.47):

$$W(\theta)=\lim_{n\to\infty} W_n(\theta)=\frac{\dfrac{1}{\sin^2\theta}}{\sqrt{q'\dfrac{(r_+^2+a^2)^2}{r_+^2+a^2\cos^2\theta}-\dfrac{1}{\sin^2\theta}}}. \tag{6.57}$$

Notice that

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\frac{(r_+^2+a^2)^2}{r_+^2+a^2\cos^2\theta}=\frac{a^2(r_+^2+a^2)^2\sin 2\theta}{(r_+^2+a^2\cos^2\theta)^2}\begin{cases}\geqslant 0, & \theta\in\left(0,\dfrac{\pi}{2}\right]\\ \leqslant 0, & \theta\in\left[\dfrac{\pi}{2},\pi\right).\end{cases} \tag{6.58}$$

and the denominator of (6.57) vanishes just in $\overline{\theta}$, $\pi-\overline{\theta}$. As $\{W_n\}_n$ is a sequence of dominated functions, $\lim_n\int_{\overline{\theta}}^{\pi-\overline{\theta}} W_n(\theta)d\theta=\int_{\overline{\theta}}^{\pi-\overline{\theta}}W(\theta)\mathrm{d}\theta$, and from (6.56):

$$(\Delta\varphi)_n<(2n+1)\int_{\overline{\theta}}^{\pi-\overline{\theta}}W(\theta)\mathrm{d}\theta, \tag{6.59}$$

for n big enough. But from (6.58), if $\cos\theta$ is replaced by $\cos\overline{\theta}$ in (6.57):

$$\int_{\overline{\theta}}^{\pi-\overline{\theta}}W(\theta)\mathrm{d}\theta<\int_{\overline{\theta}}^{\pi-\overline{\theta}}\frac{\dfrac{1}{\sin^2\theta}}{\sqrt{q'\dfrac{(r_+^2+a^2)^2}{r_+^2+a^2\cos^2\overline{\theta}}-\dfrac{1}{\sin^2\theta}}}\mathrm{d}\theta=\pi.$$

Thus, the proof concludes putting $\int_{\overline{\theta}}^{\pi-\overline{\theta}}W(\theta)\mathrm{d}\theta=\pi-\epsilon_0$ in (6.59). □

From Lemmas 6.11 and 6.12, there exist two points in a $\mathcal{C}_n$ for some (big) n whose difference in $\Delta\varphi$ is greater than 2π, which implies the existence of $(r^*,S,E)\in\mathcal{C}_n$ such that (4.11) holds, as required.

VII. CONCLUSION

We have proven a relevant geometric property of outer Kerr space–time $\mathbb{K}$ ($a^2<m^2$), the geodesic connectedness. The proof uses essentially topological arguments. These arguments are appliable to most of the classical relativistic space–times (Schwarzschild, Robertson–Walker, Reissner–Nordström, etc.).

The difficulty to study $\mathbb{K}$ seems to arise from the following facts:

(1) No Killing vector field of $\mathbb{K}$ is timelike; otherwise, the problem would be reducible to a ''Riemannian'' problem, where variational methods yields very precise results.

(2) $\mathbb{K}$ can be seen as a splitting type manifold such as those studied by using variational methods and Rabinowitz's saddle point theorem in Ref. 34. These results are especially appropiate to study globally hyperbolic space–times under a splitting with complete Cauchy hypersurfaces $t=$constant. But no clear choice of the time function t seems to be natural to apply such techniques for $\mathbb{K}$.

(3) At any case, the role of the event horizon $r=r_+$ seems to be unavoidable (recall that, under our approach, geodesics approaching the event horizon play an essential role). It is known that the convexity of the boundary of a semi-Riemannian manifold sometimes yields the geodesic connectedness of the manifold, especially in the Riemannian case.[18] The boundary $r=r_+$ of $\mathbb{K}$ is singular, and the approaching hypersurfaces $r=r_++\nu, \nu>0$, are not convex (regions $r>r_++\nu$

are not geodesically connected). In the Riemannian case, there are techniques to measure if the lack of convexity goes to zero, when $\nu \to 0$, yielding geodesic connectedness.[35] In the static case, some of these techniques are translatable,[36] and geodesic connectedness of some space–times with singular boundary, including outer Schwarzschild, have been proven.[19] But none of these techniques seem applicable to a nonstationary situation.

Thus, our method circumvents previous difficulties.

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[27] We point out that there is a recent book (Ref. 31) devoted systematically to the geometric study of Kerr space–time, which we refer as a basic reference.
[28] If M is not included in $\mathbb{R}^n$, assume that suitable coordinates can be chosen. Even though Kerr space–time $\mathbb{K}$ is an open subset of $\mathbb{R}^4$, arbitrary values for coordinates θ, ϕ will be permitted for convenience; thus, an extension of the idea underlying in (3.1) is used.
[29] Recall that $|s(r)-s(r')|<\infty$ for all r, r' and thus r is a valid new parameter.
[30] Recall that when $f\in C^1(a,b)\cap C[a,b]$, $f(a)\neq 0\neq f(b)$ and $f'(x)\neq 0$ if $f(x)=0$ then $\deg(f,(a,b),0)=\Sigma_{x\in f^{-1}(0)}\mathrm{sign} f'(x)$. In the standard notation of Ref. 32, $\deg(\mathrm{Id}-\mathcal{F}^m_{n,0},G,0)$ is written $i_\chi(\mathcal{F}^m_{n,0},G)$.
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Embedding of the brane into six dimensions

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Embedding of the brane metric into Euclidean $(2+4)$-space is found. Brane geometry can be visualized as the surface of the hypersphere in six dimensions which ''radius'' is governed by the cosmological constant. Minkowski space in this picture is placed on the intersection of this surface with the plane formed by the extra space-like and time-like coordinates. © *2002 American Institute of Physics.*
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There has been great interest in recent years in models with extended extra dimensions. Ordinary gravity can be recovered if the observable universe is represented by a brane embedded in a higher-dimensional space with a nonfactorizable geometry.[1]

A useful method to study brane models can be the embedding theory.[2] It is well known that n-dimensional space–time can be embedded into N-dimensional pseudo-Euclidean space with $n \leqslant N \leqslant n(n+1)/2$.[2,3] Thus, no more than ten dimensions are required to embed any four-dimensional solution of Einstein's equations with arbitrary energy–momentum tensor. There also exists Campbell's theorem,[4] which implies that any solution of n-dimensional Einstein's equations can be embedded, at least locally, in a space–time that is itself a solution of $(n+1)$-dimensional, vacuum Einstein's equations.[5] Several authors tried to interpret the embedding as producing an effective stress–energy tensor in low dimensions.[6]

The embedding procedure is also interesting from a purely mathematical point of view. It allows invariant classification of known solutions of Einstein's equations to be made.[7] Furthermore, the embedding method may lead to new solutions. For example, the maximal analytic extension of Schwarzschild's solution was independently found in this way.[8]

Embedding of the space–time with the coordinates x^α and metric $g_{\alpha\nu}$ into pseudo-Euclidean space with the coordinates X^A and with the flat metric η_{AB} is given by

$$ds^2 = g_{\alpha\nu} dx^\alpha dx^\nu = \eta_{AB} \partial_\alpha X^A \partial_\nu X^B dx^\alpha dx^\nu = \eta_{AB} dX^A dX^B. \tag{1}$$

For example, it is well known[9] that the Schwarzschild metric

$$ds^2 = \left(1 - \frac{2m}{r}\right) dt^2 - \frac{dr^2}{(1-2m/r)} - r^2 d\Omega^2 \tag{2}$$

admits isometric embedding of class 2 into Euclidean $(2+4)$-space. Embedding functions in this case are

$$\begin{gathered} X^1 = \sqrt{1 - \frac{2m}{r}} \cos t, \quad X^2 = \sqrt{1 - \frac{2m}{r}} \sin t, \quad X^3 = f(r), \\ X^4 = r \sin\theta \cos\varphi, \quad X^5 = r \sin\theta \sin\varphi, \quad X^6 = r \cos\theta, \end{gathered} \tag{3}$$

where $f(r)$ is solution of

$$f'^2 = (m^2/r^4 + 2m/r)/(1-2m/r). \tag{4}$$

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In this paper we consider embedding of the brane metric (which was introduced in Ref. 1) into six-dimensional pseudo-Euclidean space with the same signature $(2+4)$ as for the Schwarzschild case. The necessity of two time directions for embedding of P- and M-branes was shown in Ref. 10.

We are looking for the functions X^A which fulfill the relation

$$ds^2 = e^{2a\xi} dl^2 - d\xi^2 = dX_0^2 - dX_1^2 - dX_2^2 - dX_3^2 + dX_\tau^2 - dX_\kappa^2. \tag{5}$$

Here

$$l = \sqrt{t^2 - x^2 - y^2 - z^2} \tag{6}$$

is the length in four-dimensional Minkowski space–time, ξ is the fifth coordinate orthogonal to the brane, and a is the parameter connected with the five-dimensional cosmological constant $\pm\Lambda$. For simplicity on the brane we consider the Minkowski metric. The Ricci tensor of the five-dimensional space–time where the cosmological constant Λ appears is not zero,[1] while we assume bulk $(2+4)$-space to be pseudo-Euclidean again. This can be interpreted as a kind of geometrical introduction of the cosmological constant.

It can be checked that the embedding (5) is done by the functions

$$X_\alpha = e^{a\xi} x_\alpha, \quad X_\tau = \left(l^2 - \frac{1}{4} \right) e^{a\xi} - \frac{1}{a^2} e^{-a\xi}, \quad X_\kappa = \left(l^2 + \frac{1}{4} \right) e^{a\xi} - \frac{1}{a^2} e^{-a\xi}, \tag{7}$$

where x^α are coordinates of Minkowski space–time and the index α runs over 0, 1, 2, 3.

The inverse expression of five-dimensional coordinates by the embedding functions has the form

$$x_\alpha = \frac{X_\alpha}{2(X_\kappa - X_\tau)}, \quad \xi = \frac{1}{a} \ln[2(X_\kappa - X_\tau)]. \tag{8}$$

The geometry of the five-dimensional metric (5) can be visualized as the surface of the hypersphere in six dimensions, since

$$X_0^2 - X_1^2 - X_2^2 - X_3^2 + X_\tau^2 - X_\kappa^2 = \frac{1}{a^2}. \tag{9}$$

The radius of this ''sphere'' is $1/|a|$ and thus governed by the value of the five-dimensional cosmological constant $\pm\Lambda$. In this picture four-dimensional Minkowski space–time is the intersection of this hypersphere with the plane

$$X_\kappa - X_\tau = \tfrac{1}{2}, \tag{10}$$

where X_κ and X_τ are, respectively, extra space-like and time-like coordinates of the six-dimensional space–time.

Possibly here we have correlations with the situation of the linearization of conformal group, the symmetry group of the main equations of physics in zero-mass limit. A long time ago it was discovered that the nonlinear 15-parameter conformal transformations can be written as a linear Lorentz-type transformation in a $(2+4)$-space. For this case the intersection of the null six-cone with the null five-plane formed by the extra time-like and space-like coordinates has induced metric of the Minkowski form (for these subjects see, e.g., Ref. 11) and formulas of this embedding are similar to (8)–(10) we have in the branes case.

At the end of the paper we want to note that $(2+4)$-space is the object of interest for Kaluza–Klein models. For compact extra dimensions this space was studied in Ref. 12 and in the context of brane models with nonfactorizable geometry in Ref. 13.

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Anisotropic geodesic fluid spheres in general relativity

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It is shown that unlike the perfect fluid case, anisotropic fluids (principal stresses unequal) may be geodesic, without this implying the vanishing of (spatial) pressure gradients. Then the condition of vanishing four acceleration is integrated in noncomoving coordinates. The resulting models are necessarily dynamic, and the mass function is expressed in terms of the fluid velocity as measured by a locally Minkowskian observer. An explicit example is worked out. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1505985]

I. INTRODUCTION

As is well known, the vanishing of four acceleration (geodesic condition) implies for a perfect fluid that pressure gradients vanish. In the case of spherical bounded (nondissipative) configuration, the vanishing of pressure at the boundary surface implies in turn the vanishing of pressure everywhere within the distribution (dust).

Indeed, for a perfect fluid the equation of motion reads

$$(\rho+p)a^{\alpha}=h^{\alpha\nu}p_{,\nu} \tag{1}$$

with

$$h^{\alpha}_{\mu}\equiv\delta^{\alpha}_{\mu}-u^{\alpha}u_{\mu}, \tag{2}$$

$$a^{\mu}=u^{\nu}u^{\mu}_{;\nu}, \tag{3}$$

where the colon and semicolon denote partial and covariant derivatives, and as usual a^{μ}, u^{μ}, ρ, and p stand for the four acceleration, the four velocity, the energy density, and the pressure, respectively.

From the above it becomes evident that the geodesic condition implies the vanishing of pressure gradients. From purely physics considerations this conclusion is also obvious: the vanishing of four-acceleration means that only gravitational forces are acting on any fluid element, thereby implying that pressure gradients (the only hydrodynamic force in a perfect fluid) vanish. However in the case of anisotropic fluids, an additional force term appears besides the pressure gradient (see Sec. II). Therefore it is in principle possible to have a fluid distribution, such that both terms cancel each other, leading to a geodesic fluid with nonvanishing pressure gradients.

Since the original Lemaitre paper[1] and particularly since the work of Bowers and Liang[2] anisotropic fluids have attracted the attention of many researchers in relativity and relativistic astrophysics (see Ref. 3, and references therein), due to the conspicuous role played by local anisotropy of pressure in the structure and evolution of self–gravitating objects. It is the purpose

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of this work to present further models of anisotropic spheres, based on the geodesic condition. Besides the natural interest of such models in general relativity, the presented models are interesting because they represent the generalization of Tolman–Bondi[4] models to anisotropic fluids, in noncomoving coordinates. Incidentally, it is worth noticing that in the classical paper by Oppenheimer and Snyder on dust collapse,[5] they start their study, using the same kind of coordinates we use here, and then switch to comoving ones, in order to integrate the field equations.

The plan of the paper is as follows. In Sec. II we define the conventions and give the field equations and expressions for the kinematic variables we shall need, in noncomoving coordinates. The geodesic condition is explicitly integrated in Sec. III. In Sec. IV we work out an example. Finally a discussion of results is presented in Sec. V.

II. RELEVANT EQUATIONS AND CONVENTIONS

We consider spherically symmetric distributions of collapsing anisotropic fluid, which we assume to evolve adiabatically (without dissipation), bounded by a spherical surface Σ. The line element is given in Schwarzschild-type coordinates by

$$ds^2 = e^{\nu}dt^2 - e^{\lambda}dr^2 - r^2(d\theta^2 + \sin^2\theta\, d\phi^2), \tag{4}$$

where $\nu(t,r)$ and $\lambda(t,r)$ are functions of their arguments. We number the coordinates: $x^0 = t$; $x^1 = r$; $x^2 = \theta$; $x^3 = \phi$.

The metric (4) has to satisfy Einstein field equations

$$G^{\nu}_{\mu} = -8\pi T^{\nu}_{\mu}, \tag{5}$$

which in our case read:[6]

$$-8\pi T^0_0 = -\frac{1}{r^2} + e^{-\lambda}\left(\frac{1}{r^2} - \frac{\lambda'}{r}\right), \tag{6}$$

$$-8\pi T^1_1 = -\frac{1}{r^2} + e^{-\lambda}\left(\frac{1}{r^2} + \frac{\nu'}{r}\right), \tag{7}$$

$$-8\pi T^2_2 = -8\pi T^3_3 = -\frac{e^{-\nu}}{4}(2\ddot{\lambda} + \dot{\lambda}(\dot{\lambda} - \dot{\nu})) + \frac{e^{-\lambda}}{4}\left(2\nu'' + \nu'^2 - \lambda'\nu' + 2\frac{\nu' - \lambda'}{r}\right), \tag{8}$$

$$-8\pi T_{01} = -\frac{\dot{\lambda}}{r}, \tag{9}$$

where dots and primes stand for partial differentiation with respect to t and r, respectively.

In order to give physical significance to the T^{μ}_{ν} components we apply the Bondi approach.[6]

Thus, following Bondi, let us introduce purely locally Minkowski coordinates (τ,x,y,z) (alternatively one may introduce a tetrad field associated with locally Minkowskian observers):

$$d\tau = e^{\nu/2}dt, \quad dx = e^{\lambda/2}dr, \quad dy = r\,d\theta, \quad dz = r\sin\theta\, d\phi.$$

Then, denoting the Minkowski components of the energy tensor by a bar, we have

$$\overline{T^0_0} = T^0_0, \quad \overline{T^1_1} = T^1_1, \quad \overline{T^2_2} = T^2_2, \quad \overline{T^3_3} = T^3_3, \quad \overline{T_{01}} = e^{-(\nu+\lambda)/2}T_{01}.$$

Next, we suppose that when viewed by an observer moving relative to these coordinates with proper velocity $\omega(t,r)$ in the radial direction, the physical content of space consists of an anisotropic fluid of energy density ρ, radial pressure P_r, and tangential pressure $P_{\perp}$. Thus, when viewed by this moving observer the covariant tensor in Minkowski coordinates is

$$\begin{pmatrix} \rho & 0 & 0 & 0 \\ 0 & P_r & 0 & 0 \\ 0 & 0 & P_\perp & 0 \\ 0 & 0 & 0 & P_\perp \end{pmatrix}.$$

Then a Lorentz transformation readily shows that

$$T_0^0 = \overline{T}_0^0 = \frac{\rho + P_r\omega^2}{1-\omega^2}, \tag{10}$$

$$T_1^1 = \overline{T}_1^1 = -\frac{P_r + \rho\omega^2}{1-\omega^2}, \tag{11}$$

$$T_2^2 = T_3^3 = \overline{T}_2^2 = \overline{T}_3^3 = -P_\perp, \tag{12}$$

$$T_{01} = e^{(\nu+\lambda)/2}\overline{T}_{01} = -\frac{(\rho + P_r)\omega e^{(\nu+\lambda)/2}}{1-\omega^2}. \tag{13}$$

Note that the coordinate velocity in the (t, r, θ, ϕ) system, $\mathrm{d}r/\mathrm{d}t$, is related to ω by

$$\omega(t,r) = \frac{\mathrm{d}r}{\mathrm{d}t} e^{(\lambda-\nu)/2}. \tag{14}$$

Feeding back (10)–(13) into (6)–(9), we get the field equations in the form

$$\frac{\rho + P_r\omega^2}{1-\omega^2} = -\frac{1}{8\pi}\left\{ -\frac{1}{r^2} + e^{-\lambda}\left(\frac{1}{r^2} - \frac{\lambda'}{r}\right)\right\}, \tag{15}$$

$$\frac{P_r + \rho\omega^2}{1-\omega^2} = -\frac{1}{8\pi}\left\{ \frac{1}{r^2} - e^{-\lambda}\left(\frac{1}{r^2} + \frac{\nu'}{r}\right)\right\}, \tag{16}$$

$$P_\perp = -\frac{1}{8\pi}\left\{ \frac{e^{-\nu}}{4}(2\ddot{\lambda} + \dot{\lambda}(\dot{\lambda} - \dot{\nu})) - \frac{e^{-\lambda}}{4}\left(2\nu'' + \nu'^2 - \lambda'\nu' + 2\frac{\nu' - \lambda'}{r}\right)\right\}, \tag{17}$$

$$\frac{(\rho + P_r)\omega e^{(\nu+\lambda)/2}}{1-\omega^2} = -\frac{\dot{\lambda}}{8\pi r}. \tag{18}$$

At the outside of the fluid distribution, the space–time is that of Schwarzschild, given by

$$\mathrm{d}s^2 = \left(1 - \frac{2M}{r}\right)\mathrm{d}t^2 - \left(1 - \frac{2M}{r}\right)^{-1}\mathrm{d}r^2 - r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2), \tag{19}$$

As is well known, in order to match smoothly the two metrics above on the boundary surface $r = r_\Sigma(t)$, we must require the continuity of the first and the second fundamental form across that surface. In our notation this implies

$$e^{\nu_\Sigma} = 1 - \frac{2M}{r_\Sigma}, \tag{20}$$

$$e^{-\lambda_\Sigma} = 1 - \frac{2M}{r_\Sigma}. \tag{21}$$

and

$$[P_r]_\Sigma = 0, \tag{22}$$

where, from now on, subscript Σ indicates that the quantity is evaluated at the boundary surface Σ.

Equations (20)–(22) are the necessary and sufficient conditions for a smooth matching of the two metrics (4) and (19) on Σ.

Next, let us write the energy momentum tensor in the form

$$T_{\mu\nu} = (\rho + P_\perp)u_\mu u_\nu - P_\perp g_{\mu\nu} + (P_r - P_\perp)s_\mu s_\nu \tag{23}$$

with

$$u^\mu = \left(\frac{e^{-\nu/2}}{(1-\omega^2)^{1/2}}, \frac{\omega e^{-\lambda/2}}{(1-\omega^2)^{1/2}}, 0, 0 \right), \tag{24}$$

$$s^\mu = \left(\frac{\omega e^{-\nu/2}}{(1-\omega^2)^{1/2}}, \frac{e^{-\lambda/2}}{(1-\omega^2)^{1/2}}, 0, 0 \right), \tag{25}$$

where u^μ denotes the four velocity of the fluid and s^μ is a radially directed space-like vector orthogonal to u^μ. Then the radial component of the conservation law

$$T^\mu_{\nu;\mu} = 0 \tag{26}$$

may be written as

$$(-8\pi T_1^1)' = \frac{16\pi}{r}(T_1^1 - T_2^2) + 4\pi\nu'(T_1^1 - T_0^0) + \frac{e^{-\nu}}{r}\left(\ddot{\lambda} + \frac{\dot{\lambda}^2}{2} - \frac{\dot{\lambda}\dot{\nu}}{2} \right), \tag{27}$$

which in the static case becomes

$$P_r' = -\frac{\nu'}{2}(\rho + P_r) + \frac{2(P_\perp - P_r)}{r}, \tag{28}$$

representing the generalization of the Tolman–Oppenheimer–Volkof equation for anisotropic fluids.[2] Thus, as mentioned before, local anisotropy introduces an extra term in this ''force'' equation, besides the usual pressure gradient term.

Finally, for the two nonvanishing components of the four acceleration, we easily find

$$a_0 = \frac{1}{1-\omega^2}\left[\left(\frac{\omega\dot{\omega}}{1-\omega^2} + \frac{\omega^2\dot{\lambda}}{2} \right) + e^{\nu/2}e^{-\lambda/2}\left(\frac{\omega\nu'}{2} + \frac{\omega^2\omega'}{1-\omega^2} \right) \right], \tag{29}$$

$$a_1 = -\frac{1}{1-\omega^2}\left[\left(\frac{\omega\omega'}{1-\omega^2} + \frac{\nu'}{2} \right) + e^{-\nu/2}e^{\lambda/2}\left(\frac{\omega\dot{\lambda}}{2} + \frac{\dot{\omega}}{1-\omega^2} \right) \right]. \tag{30}$$

III. INTEGRATING THE GEODESIC CONDITION

Let us now integrate the geodesic condition. First, observe that from the field equations (15), (16), and (18), one obtains after simple manipulations

$$\omega e^{(\nu-\lambda)/2}(\lambda' + \nu') + (1+\omega^2)\dot{\lambda} = 0. \tag{31}$$

Next, it follows at once from (29) and (30) that

$$\omega a_1 = -a_0 e^{(\lambda-\nu)/2}. \tag{32}$$

Therefore the vanishing four-acceleration condition amounts to

$$\left(\frac{\omega\omega'}{1-\omega^2}+\frac{\nu'}{2}\right)+e^{-\nu/2}e^{\lambda/2}\left(\frac{\omega\dot{\lambda}}{2}+\frac{\dot{\omega}}{1-\omega^2}\right)=0. \tag{33}$$

Then, replacing ν' by its expression from (31), into (33), this last equation becomes

$$\omega e^{(\nu-\lambda)/2}\left(\lambda'-\frac{2\omega\omega'}{1-\omega^2}\right)+\dot{\lambda}-\frac{2\omega\dot{\omega}}{1-\omega^2}=0, \tag{34}$$

or, using (14)

$$\dot{\phi}\,\mathrm{d}t+\phi'\,\mathrm{d}r=0, \tag{35}$$

whose solution is

$$\phi=\ln(1-\omega^2)+\lambda=\text{constant}. \tag{36}$$

Finally, from the fact that $\omega(t,0)=0$ we obtain

$$e^{-\lambda}=1-\omega^2. \tag{37}$$

Introducing the mass function as usual,

$$e^{-\lambda}=1-\frac{2m}{r}, \tag{38}$$

we have

$$m=\frac{\omega^2 r}{2}. \tag{39}$$

In all the above we have assumed $\omega\neq 0$, since from simple physical considerations we should not expect static solutions to exist.

Indeed, if we assume staticity ($\omega=0$) then the geodesic condition implies $\nu'=0$, which in turn, using (16) and (38), leads to

$$8\pi P_r=-\frac{2m}{r^3}. \tag{40}$$

Then junction condition (22) would lead to $m_\Sigma=M=0$.

There is however one possible case of static geodesic solution, which appears if we relax the condition of continuity of the second fundamental form (implying the continuity of radial pressure) across the boundary surface, and assume the existence of a surface layer.[7]

In this specific case, it follows from (40), the geodesic condition and field equations (15) and (17) that

$$\rho+P_r+2P_\perp=0, \tag{41}$$

implying that the active gravitational mass (Tolman[8]) defined for any $r<r_\Sigma$ as

$$m_T=4\pi\int_0^r r^2 e^{(\nu+\lambda)/2}(T_0^0-T_1^1-2T_2^2)\mathrm{d}r, \tag{42}$$

vanishes inside the sphere.

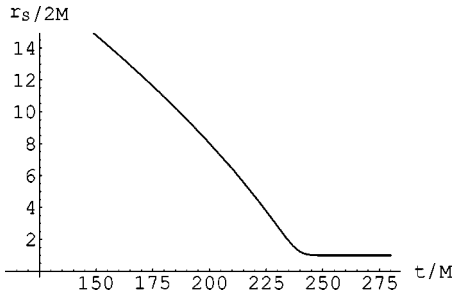

FIG. 1. $y=r_\Sigma/2M$ as function of t/M for the inital value $y(0)=30$.

We shall not consider here these kinds of solutions and accordingly all our models will be dynamic ($\omega\neq 0$) and satisfy all junction conditions.

Now, from (14) evaluated at the boundary surface, and (20) and (21), we obtain

$$\omega_\Sigma=\frac{\dot r_\Sigma}{1-2M/r_\Sigma}. \tag{43}$$

On the other hand, from (39) evaluated at the boundary surface, we have

$$\omega_\Sigma=\pm\sqrt{\frac{2M}{r_\Sigma}}, \tag{44}$$

where the $+$ $(-)$ refers to the expansion (contraction) of the surface (from now on we shall only consider the contracting case). Feeding back (44) into (43), we get

$$\omega_\Sigma=\frac{\dot r_\Sigma}{1-\omega_\Sigma^2}. \tag{45}$$

Then equating (45) and (44) we have

$$\dot r_\Sigma=\left(\frac{2M}{r_\Sigma}\right)^{3/2}-\left(\frac{2M}{r_\Sigma}\right)^{1/2}. \tag{46}$$

This equation may be integrated to give

$$\frac{t}{2M}=2\tanh^{-1}\sqrt{\frac{2M}{r_\Sigma}}-\frac{2[1+6M/r_\Sigma]}{3(2M/r_\Sigma)^{3/2}} \tag{47}$$

giving the evolution of the boundary surface. Unfortunately Eq. (47) cannot be inverted (at least we were unable to do that) to obtain the explicit form $r=r_\Sigma(t)$. Accordingly we have also integrated (46) numerically, in order to exhibit the evolution of r_Σ, see Fig. 1.

So far we have found all consequences derived from the geodesic condition which, obviously, are valid in the pure dust case as well as in the anisotropic case. In Sec. IV we shall work out an explicit example by imposing an ''equation of state'' for the physical variables.

IV. A MODEL

The purpose of this section is not to model any specific physical system, but just to illustrate the consequences derived from the geodesic condition. Thus, somehow inspired by the incompressible fluid model, let us assume

$$T_0^0=f(t). \tag{48}$$

Then from (39) and the fact that

$$m' = 4\pi r^2 T_0^0 \tag{49}$$

one obtains

$$\omega = -r\sqrt{\frac{8\pi}{3} f(t)}, \tag{50}$$

where

$$f(t) = \frac{3M}{4\pi r_\Sigma^3}. \tag{51}$$

Observe from (50) that the evolution in this model is homologous.

Next, introducing the dimensionless variables

$$x \equiv \frac{r}{r_\Sigma}, \quad y \equiv \frac{r_\Sigma}{2M}, \tag{52}$$

we have

$$e^{-\lambda} = 1 - \frac{x^2}{y}, \tag{53}$$

$$\omega = -\frac{x}{\sqrt{y}}. \tag{54}$$

Finally, from the field equations the following relations follow:

$$\rho y + P_r x^2 = \frac{3(y - x^2)}{32\pi M^2 y^3}, \tag{55}$$

$$P_r y + \rho x^2 = \frac{(y - x^2)}{8\pi}\left[\left(1 - \frac{x^2}{y}\right)\left(\frac{1}{4M^2x^2y^2} + \frac{\partial \nu}{\partial x}\frac{1}{4M^2xy^2}\right) - \frac{1}{4M^2x^2y^2}\right], \tag{56}$$

$$\rho + P_r = -\frac{3\dot{y}(y - x^2)^{1/2} e^{-\nu/2}}{8\pi(2My^3)}. \tag{57}$$

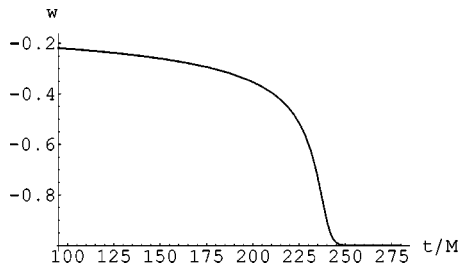

FIG. 2. ω_Σ as function of t/M for the same initial data as in Fig. 1.

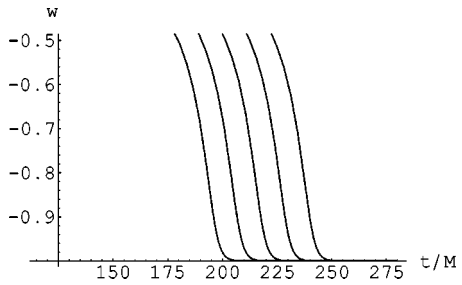

FIG. 3. ω_Σ as function of t/M for $y(0)=30,29,28,27,26$ curves from right to left, respectively.

Then from (55) and (56) we obtain $\rho+P_r$ as function of $\partial\nu/\partial x$, x and y. Feeding back this expression into (57), this equation may be solved for ν, which in turn allows one to express all physical variables (ρ, P_r, and $P_\perp$) in terms of x and y which are given by (47) or alternatively by the numerical solution of (46).

V. CONCLUSIONS

We have seen that the geodesic condition, which for anisotropic fluids is compatible with the presence of pressure gradients, can be integrated, giving the explicit form of the evolution of the boundary surface. Resulting models may be regarded as generalizations of Tolman–Bondi solutions, to anisotropic fluids. In order to obtain the evolution of all physical variables for different pieces of matter, additional information has to be given. In the above-presented model we have assumed condition (48), which in turn leads to the homology condition (50). Parenthetically, this last condition is widely used by astrophysicists in their modeling of stellar structure and evolution.[9]

Figures 1 and 2 display the behavior of the radius and the evolution of ω_Σ in the contracting case. As expected, as the boundary surface approaches the horizon, its coordinate velocity ($\dot{r}_\Sigma$) stalls, whereas the velocity ω_Σ measured by the locally Minkowskian observer, tends to light velocity. Figure 3 shows the sensitivity of the pattern evolution with respect to the compactness of the initial configuration. As expected more compact configurations collapse faster. The good behavior of ρ and p_r is easily deduced from (55) to (57).

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Schwinger terms in gravitation in two dimensions as a consequence of the gravitational anomaly

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We compute the Schwinger term in the gravitational constraints in two dimensions, starting from the path integral in Hamiltonian form and the Einstein anomaly. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1505127]

I. INTRODUCTION

A Yang–Mills theory with a non-Abelian anomaly (gauge anomaly) leads to Schwinger terms (central charges) in the constraint algebra (the Gauss law operators) as well as in the algebra of currents (see, e.g., Refs. 1 and 2). Theories of gravitation and matter that have a gravitational anomaly (Einstein or Lorentz) also lead to Schwinger terms in the constraints and currents (energy-momentum tensors). As we will see later, in the tensor theory of Einstein in two dimensions, the gravitational constraints reduce to the energy-momentum tensor and therefore the two Schwinger terms are equivalent. This case has been considered in Refs. 3–6. The Schwinger terms in the constraints of a scalar-tensor theory are discussed in Refs. 7–10.

In Ref. 11, Faddeev *et al.* found the following method to compute the Schwinger term in the algebra of the Gauss law operators in a Yang–Mills theory: starting with the path integral in Hamiltonian form, they make a gauge transformation and include the non-Abelian anomaly. From the Ward identity in second order in the gauge parameter, one can then extract the Schwinger term by acting with a suitable operator. Our goal is to generalize this to gravitation.

II. GRAVITATION AS A CONSTRAINED HAMILTONIAN SYSTEM

We start with Einstein's theory of gravitation and a massless chiral fermion, which are described by the action [we have either $P_+\psi=0$ or $P_-\psi=0$ with $P_\pm=\frac{1}{2}(1\pm\gamma_5)$]

$$S=\int dx\ \ e\left[R+\frac{i}{2}e^{a\mu}\overline{\psi}\gamma_a\overleftrightarrow{\nabla}_\mu\psi\right]. \tag{1}$$

This action can also be written as a constrained Hamiltonian system (see, e.g., Refs. 12–14) (in d-dimensions i runs from 1 to $d-1$):

$$S=\int dx\left[\pi_a^i\dot{e}_i^a+i^{(3)}g^{1/2}\overline{\psi}\Gamma^\perp\dot{\psi}-N\tilde{\mathcal{H}}_\perp-N^i\tilde{\mathcal{H}}_i-\frac{1}{2}\omega_0^{ab}J_{ab}\right], \tag{2}$$

where ${}^{(3)}g^{ij}$ is the induced metric and π_a^i is the canonical momentum to e_i^a defined by $p^{ij}=\frac{1}{4}(\pi_a^i\ {}^{(3)}e^{aj}+\pi_a^j\ {}^{(3)}e^{ai})$, where the canonical momentum to g_{ij} is expressed in terms of the extrinsic curvature K_{ij},

$$p^{ij}={}^{(3)}g^{1/2}(K^{ij}-K^{(3)}g^{ij}). \tag{3}$$

The Lagrangian multipliers are the lapse N, the shift N_i, $N^i={}^{(3)}g^{ij}N_j$, and the 0-component of the spin connection ω_0^{ab}. The constraints are

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$$\tilde{\mathcal{H}}_\perp = \mathcal{H}_\perp + \partial_k J^{\perp k} - i^{(3)}g^{1/2}\overline{\psi}\Gamma^i D_i\psi, \tag{4}$$

$$\tilde{\mathcal{H}}_i = \mathcal{H}_i + \tfrac{1}{2}g_{ij}\partial_k J^{kj} + K_{ik}J^{\perp k} + i[{}^{(3)}g^{1/2}\overline{\psi}\Gamma^\perp D_i\psi - \tfrac{1}{4}\partial_k({}^{(3)}g^{1/2}\overline{\psi}[\Gamma_i,\Gamma^k]\Gamma^\perp\psi)], \tag{5}$$

$$J_{ab} = \pi^i_a e_{bi} - \pi^i_b e_{ai} - \frac{i}{4}{}^{(3)}g^{1/2}\overline{\psi}(\Gamma^\perp\gamma_a\Gamma^i - \Gamma^i\gamma_a\Gamma^\perp)e_{bi} + \frac{i}{4}{}^{(3)}g^{1/2}\overline{\psi}(\Gamma^\perp\gamma_b\Gamma^i - \Gamma^i\gamma_b\Gamma^\perp)e_{ai}, \tag{6}$$

$$\Gamma^i = {}^{(3)}g^{ij}e^a_j\gamma_a = {}^{(3)}e^{ai}\gamma_a, \quad \Gamma^\perp = -n^a\gamma_a. \tag{7}$$

Remember that the gravitational Hamiltonian is vanishing.

III. THE GRAVITATIONAL PATH INTEGRAL

The general coordinate transformations are the gauge transformations of gravitation. To define a well behaved path integral, we choose the gauge fixing $e^a_0 = \delta^a_0$ and introduce the coordinate ghosts using the Faddeev–Popov method. Under infinitesimal active coordinate transformations (Einstein transformations) the vielbein transforms as

$$\delta^c_\xi e^a_\mu(x) = e'^a_\mu(x) - e^a_\mu(x) = \xi^\nu\partial_\nu e^a_\mu(x) + e^a_\nu(x)\partial_\mu\xi^\nu. \tag{8}$$

This leads to the ghost action

$$\begin{aligned} S_{GH} &= \int dxdy e(x)\overline{v}^\nu(x)e_{a\nu}(x)\left.\frac{\delta^c_\xi(e^a_0 - \delta^a_0)}{\delta\xi_\mu(y)}\right|_{\xi=0} v_\mu(y) \\ &= \int dx e(x)\overline{v}_\nu(x)(e^\nu_a(x)\partial_\mu e^a_0(x)v^\mu(x) + \partial_0 v^\nu(x)). \end{aligned} \tag{9}$$

We find the path integral in Hamiltonian form for gravitation and a chiral fermion:

$$\begin{aligned} Z = \frac{1}{N}\int d\pi^i_a de^a_i de^a_0 d\overline{\psi}d\psi d\overline{v}_\alpha dv^\alpha \delta(e^a_0 - \delta^a_0) \\ \times\exp\left\{ i\int dx\left[\pi^i_a\dot{e}^a_i + i^{(3)}g^{1/2}\overline{\psi}\Gamma^\perp\dot{\psi} - N^\mu\tilde{\mathcal{H}}_\mu - \frac{1}{2}\omega^{ab}_0 J_{ab} + e\overline{v}_\nu(e^\nu_a\partial_\mu e^a_0 v^\mu + \partial_0 v^\nu)\right]\right\}. \end{aligned} \tag{10}$$

The inclusion of powers of e as weights in the fermionic measure, as it is explained in Refs. 15 and 16, would be no problem but we will not need it.

IV. SCHWINGER TERMS IN GRAVITATION IN TWO DIMENSIONS

In two dimensions the Einstein–Hilbert action is proportional to the Euler number of the two-dimensional manifold (see, e.g., Ref 17). We choose a manifold where the Euler number vanishes. So in two dimensions there are no dynamical degrees of freedom for gravity in Einstein's theory. From (3) we see that the conjugate momenta π^1_a identically vanish. Using $e^a_1 e^b_1[\gamma_a,\gamma_b] = 0$ and $\gamma_b\gamma_0\gamma_a - \gamma_a\gamma_0\gamma_b = 0$ the constraints reduce to

$$\tilde{\mathcal{H}}_\perp = -i^{(1)}g^{1/2}\overline{\psi}\Gamma^1\partial_1\psi, \tag{11}$$

$$\tilde{\mathcal{H}}_1 = i^{(1)}g^{1/2}\overline{\psi}\Gamma^\perp\partial_1\psi, \tag{12}$$

$$J_{ab} = 0. \tag{13}$$

We have

$$\Gamma^1 = {}^{(1)}e^{a1}\gamma_a = (g_{11})^{-1}e_1^a\gamma_a = e^{a1}\gamma_a - \frac{N^1}{N}n^a\gamma_a, \tag{14}$$

$$\Gamma^\perp = N^\perp e^{a0}\gamma_a = -n^a\gamma_a, \tag{15}$$

$$e = |g|^{1/2} = {}^{(1)}g^{1/2}N, \tag{16}$$

so that

$$N^\mu\mathcal{H}_\mu = -ie\,\overline{\psi}e^{a1}\gamma_a\partial_1\psi. \tag{17}$$

The path integral (10) reduces to

$$Z = \frac{1}{N}\int d\pi_a^1 de_1^a de_0^a d\overline{\psi}d\psi d\overline{v}_\alpha dv^\alpha \delta(e_0^a - \delta_0^a) \times \exp\left\{ i\int dx[\pi_a^1\dot{e}_1^a + ie\,\overline{\psi}e^{a0}\gamma_a\partial_0\psi + ie\,\overline{\psi}e^{a1}\gamma_a\partial_1\psi + e\overline{v}_\nu(e_a^\nu\partial_\mu e_0^a v^\mu + \partial_0 v^\nu)]\right\}. \tag{18}$$

We relabel all fields, $e_\mu^a(x)\to e'^a_\mu(x)$, as for the other fields. We interpret this as an active coordinate transformation and use the invariance of the classical action and the bosonic measure under coordinate transformations. The fermionic measure gives us the Einstein anomaly $G[\Lambda,\Gamma]$, and we are left with

$$Z = \frac{1}{N}\int d\pi_a^1 de_1^a de'^a_0 d\overline{\psi}d\psi d\overline{v}_\alpha dv^\alpha \delta(e'^a_0 - \delta_0^a) \times \exp\left\{ i\int dx[\pi_a^1\dot{e}_1^a + ie\,\overline{\psi}e^{a0}\gamma_a\partial_0\psi + ie\,\overline{\psi}e^{a1}\gamma_a\partial_1\psi + e\overline{v}_\nu(e_a^\nu\partial_\mu e_0^a v^\mu + \partial_0 v^\nu)]\right\} G[\Lambda,\Gamma] \tag{19}$$

with the explicit expression (see, e.g., Ref. 18)

$$G[\Lambda,\Gamma] = \exp\left\{ \pm\frac{i}{96\pi}\left[\frac{1}{3}\int_{\Gamma^+}\mathrm{tr}(d\Lambda\Lambda^{-1})^3 + \int_{M_2}\mathrm{tr}(d\Lambda\Lambda^{-1}\Gamma)\right]\right\}, \tag{20}$$

where Γ_b^a is the Christoffel connexion one-form, Λ_b^a is the "gauge" element and $\partial\Gamma^+ = M_2$. For a general coordinate transformation $x' = x'(x)$ we define the "gauge" parameter ξ by

$$x'^\alpha = x^\alpha - \xi^\alpha(x), \tag{21}$$

$$(\Lambda^{-1})_\beta^\alpha = \frac{\partial x'^\alpha}{\partial x^\beta} = \delta_\beta^\alpha - \partial_\beta\xi^\alpha(x), \tag{22}$$

so that, in second order in ξ, we have

$$x^\alpha = x'^\alpha + \xi^\alpha(x') + \xi^\lambda\partial_\lambda\xi^\alpha(x') + O(\xi^3), \tag{23}$$

$$\Lambda_\beta^\alpha = \frac{\partial x^\alpha}{\partial x'^\beta} = \delta_\beta^\alpha + \partial_\beta\xi^\alpha(x) + \partial_\beta\xi^\lambda\partial_\lambda\xi^\alpha(x) + O(\xi^3). \tag{24}$$

The zweibein transforms under passive coordinate transformations as

$$e'^a_\mu(x') = \Lambda_\mu^\nu e_\nu^a(x) = e_\mu^a(x) + \partial_\mu\xi^\nu e_\nu^a(x) + \partial_\mu\xi^\lambda\partial_\lambda\xi^\nu e_\nu^a(x) + O(\xi^3) \tag{25}$$

and under active coordinate tranformations (Einstein transformations) as

$$e'^{a}_{\mu}(x)=e^{a}_{\mu}(x)+\partial_\mu\xi^\nu e^{a}_{\nu}(x)+\xi^\alpha\partial_\alpha e^{a}_{\mu}(x)+\partial_\mu\xi^\lambda\partial_\lambda\xi^\nu e^{a}_{\nu}(x)+\xi^\alpha\partial_\alpha\partial_\mu\xi^\nu e^{a}_{\nu}(x)$$
$$+\xi^\alpha\partial_\mu\xi^\nu\partial_\alpha e^{a}_{\nu}(x)+\xi^\alpha\partial_\alpha\xi^\beta\partial_\beta e^{a}_{\mu}(x)+\tfrac{1}{2}\xi^\alpha\xi^\beta\partial_\alpha\partial_\beta e^{a}_{\mu}(x)+O(\xi^3). \tag{26}$$

The gauge fixing $e'^{a}_{0}(x)=\delta^a_0$ leads to a second order differential equation for e^a_0. If we are in two dimensions and choose $\xi^1=0$, then we find

$$\delta^a_0=[1+\partial_0\xi^0+\xi^0\partial_0+\partial_0\xi^0\partial_0\xi^0+\xi^0\partial_0\partial_0\xi^0+2\xi^0\partial_0\xi^0\partial_0+\tfrac{1}{2}\xi^0\xi^0\partial_0\partial_0]e^a_0. \tag{27}$$

Its solution is

$$e^a_0=(1-\partial_0\xi^0)\,\delta^a_0+O(\xi^3). \tag{28}$$

Using (28) we express everything up to second order in ξ, in terms of e^0_1 and e^1_1. For the Einstein anomaly (20) we find

$$G[\xi,\Gamma]=\exp\left\{\pm\frac{i}{48\pi}\int dx[\partial_0\partial_0\xi^0\partial_1\partial_0\xi^0(e^0_1)^2(e^1_1)^{-2}+\partial_1\partial_0\xi^0\partial_1\partial_1\xi^0(e^1_1)^{-2}\right.$$
$$-2\partial_1\partial_0\xi^0\partial_1\partial_0\xi^0e^0_1(e^1_1)^{-2}+[(\partial_0\partial_0\xi^0+2\partial_0\partial_0\xi^0\partial_0\xi^0)(e^0_1)^2(e^1_1)^{-2}-2(\partial_1\partial_0\xi^0$$
$$+\partial_1\partial_0\xi^0\partial_0\xi^0)e^0_1(e^1_1)^{-2}+\partial_1\partial_1\xi^0(e^1_1)^{-2}]\partial_0e^0_1+[-(\partial_0\partial_0\xi^0+2\partial_0\partial_0\xi^0\partial_0\xi^0)e^0_1(e^1_1)^{-1}$$
$$\left.+(\partial_1\partial_0\xi^0+\partial_1\partial_0\xi^0\partial_0\xi^0)(e^1_1)^{-1}]\partial_0e^1_1]\right\}+O(\xi^3), \tag{29}$$

where we use the convention $\varepsilon^{01}=1$. As can be seen from (19), the momentum π^1_a is no longer conjugate to e^a_1, since there are terms in (29) proportional to $\partial_0e^0_1$ and $\partial_0e^1_1$. Therefore we make a shift in π^1_a to absorb these terms. The functional determinant is simply 1 and its effect is to kill all terms proportional to $\partial_0e^0_1$ and $\partial_0e^1_1$ in (29). Using

$$\mathcal{L}_{GH}=e\overline{v}_\nu(e^\nu_a\partial_\mu e^a_0v^\mu+\partial_0v^\nu)=e\overline{v}_\nu\partial_0v^\nu+e^1_1\partial_\mu e^0_0\overline{v}_0v^\mu, \tag{30}$$

$$ee^{a0}\gamma_a=-(e^1_1\gamma_0+e^0_1\gamma_1),\quad ee^{a1}\gamma_a=e(e^1_1)^{-1}\gamma_1, \tag{31}$$

we find the generating functional in second order in the gauge parameter

$$Z=\frac{1}{N}\int d\pi^1_ade^a_1d\overline{\psi}d\psi d\overline{v}_\alpha dv^\alpha\exp\left\{i\int dx\left[\pi^1_a\dot{e}^a_1-i\overline{\psi}(e^1_1\gamma_0+e^0_1\gamma_1)\partial_0\psi+(1-\partial_0\xi^0)i\overline{\psi}\gamma_1\partial_1\psi\right.\right.$$
$$+(1-\partial_0\xi^0)e^1_1\overline{v}_\nu\partial_0v^\nu-\partial_\mu\partial_0\xi^0e^1_1\overline{v}_0v^\mu\pm\frac{1}{48\pi}[\partial_0\partial_0\xi^0\partial_1\partial_0\xi^0(e^0_1)^2(e^1_1)^{-2}$$
$$\left.\left.-2\partial_1\partial_0\xi^0\partial_1\partial_0\xi^0e^0_1(e^1_1)^{-2}+\partial_1\partial_0\xi^0\partial_1\partial_1\xi^0(e^1_1)^{-2}]\right]\right\}+O(\xi^3). \tag{32}$$

In $O((\xi^0)^2)$ we find the following Ward identity:

$$0=\left\langle\pm\frac{i}{48\pi}\int dx[\partial_0\partial_0\xi^0\partial_1\partial_0\xi^0(e^0_1)^2(e^1_1)^{-2}-2\partial_1\partial_0\xi^0\partial_1\partial_0\xi^0e^0_1(e^1_1)^{-2}+\partial_1\partial_0\xi^0\partial_1\partial_1\xi^0(e^1_1)^{-2}]\right.$$
$$\left.+\frac{1}{2}\left[\int dx[\partial_0\xi^0\overline{\psi}\gamma_1\partial_1\psi-i\partial_0\xi^0e^1_1v_\nu\partial_0v^\nu-i\partial_\mu\partial_0\xi^0e^1_1\overline{v}_0v^\mu]\right]^2\right\rangle. \tag{33}$$

Acting with $\delta^2/\delta\xi^0(x)\,\delta\xi^0(y)$ on (33) we arrive at

$$0=\Big\langle \pm\frac{i}{48\pi}[(2\partial_1^y\partial_0^y\partial_0^y\partial_0^y\delta(x-y)+3\partial_1^y\partial_0^y\partial_0^y\delta(x-y)\partial_0^y+\partial_0^y\partial_0^y\partial_0^y\delta(x-y)\partial_1^y+\partial_0^y\partial_0^y\delta(x-y)\partial_1^y\partial_0^y$$
$$+\partial_1^y\partial_0^y\delta(x-y)\partial_0^y\partial_0^y)((e_1^0)^2(e_1^1)^{-2})-4(\partial_1^y\partial_1^y\partial_0^y\partial_0^y\delta(x-y)+\partial_1^y\partial_1^y\partial_0^y\delta(x-y)\partial_0^y$$
$$+\partial_1^y\partial_0^y\partial_0^y\delta(x-y)\partial_1^y+\partial_1^y\partial_0^y\delta(x-y)\partial_1^y\partial_0^y)(e_1^0(e_1^1)^{-2})+(2\partial_1^y\partial_1^y\partial_1^y\partial_0^y\delta(x-y)+\partial_1^y\partial_1^y\partial_1^y\delta(x-y)\partial_0^y$$
$$+3\partial_1^y\partial_1^y\partial_0^y\delta(x-y)\partial_1^y+\partial_1^y\partial_1^y\delta(x-y)\partial_1^y\partial_0^y+\partial_1^y\partial_0^y\delta(x-y)\partial_1^y\partial_1^y)(e_1^1)^{-2}]\rangle+\partial_0^x\partial_0^y\langle(-\overline{\psi}\gamma_1\partial_1\psi(x)$$
$$+ie_1^1\overline{v}_\nu\partial_0 v^\nu(x)+i\partial_\mu^x(e_1^1\overline{v}_0 v^\mu(x)))\times(-\overline{\psi}\gamma_1\partial_1\psi(y)+ie_1^1\overline{v}_\nu\partial_0 v^\nu(y)+i\partial_\mu^y(e_1^1\overline{v}_0 v^\mu(y)))\Big\rangle. \tag{34}$$

The last two lines give the commutator times $\partial_0^y\delta(x^0-y^0)$:

$$\partial_0^y\delta(x-y)[\overline{\psi}\gamma_1\partial_1\psi(x),\overline{\psi}\gamma_1\partial_1\psi(y)], \tag{35}$$

plus terms that are proportional to $\delta(x^0-y^0)$ or regular as $y^0\to x^0$. Next we apply

$$\lim_{(p_0-q_0)\to\infty}\frac{p_0-q_0}{p_0q_0^3}\int dx^0dy^0e^{ip_0x^0+iq_0y^0} \tag{36}$$

on (34) to project onto terms proportional to $\partial_0^y\partial_0^y\partial_0^y\delta(x-y)$ and we find

$$0=\pm\frac{i}{48\pi}\langle(2\partial_1^y\delta(x^1-y^1)+\delta(x^1-y^1)\partial_1^y)((e_1^0)^2(e_1^1)^{-2})\rangle. \tag{37}$$

Using this, we apply

$$\lim_{(p_0-q_0)\to\infty}\frac{p_0-q_0}{p_0q_0^2}\int dx^0dy^0e^{ip_0x^0+iq_0y^0} \tag{38}$$

on (34) to project onto terms proportional to $\partial_0^y\partial_0^y\delta(x-y)$. We obtain

$$0=\Big\langle \pm\frac{i}{48\pi}[\partial_1^y\delta(x^1-y^1)\partial_0^y((e_1^0)^2(e_1^1)^{-2})-4(\partial_1^y\partial_1^y\delta(x^1-y^1)+\partial_1^y\delta(x^1-y^1)\partial_1^y)(e_1^0(e_1^1)^{-2})]\Big\rangle. \tag{39}$$

Using this and finally applying

$$\lim_{(p_0-q_0)\to\infty}\frac{p_0-q_0}{p_0q_0}\int dx^0dy^0e^{ip_0x^0+iq_0y^0} \tag{40}$$

on (34) to project onto terms proportional to $\partial_0^y\delta(x-y)$, we arrive at

$$\langle[-i\overline{\psi}\gamma_1\partial_1\psi(x),-i\overline{\psi}\gamma_1\partial_1\psi(y)]\rangle$$
$$=\pm\frac{i}{48\pi}\langle[2\partial_1^y\partial_1^y\partial_1^y\delta(x^1-y^1)+3\partial_1^y\partial_1^y\delta(x^1-y^1)\partial_1^y+\partial_1^y\delta(x^1-y^1)\partial_1^y\partial_1^y](e_1^1)^{-2}\rangle. \tag{41}$$

From the fermionic part of the action (1) we find the energy-momentum tensor

$$T_{\mu\nu} = -\frac{i}{4}[\bar{\psi}\gamma_\mu \overleftrightarrow{\nabla}_\nu \psi + \bar{\psi}\gamma_\nu \overleftrightarrow{\nabla}_\mu \psi] + g_{\mu\nu}\frac{i}{2}\bar{\psi}\gamma^\lambda \overleftrightarrow{\nabla}_\lambda \psi. \tag{42}$$

For flat space, we have $e_1^0 = 0, e_1^1 = 1$, and we find the Schwinger term in the energy–momentum tensor

$$\langle [T_{00}(x), T_{00}(y)]_{ET} \rangle = \pm \frac{i}{24\pi} \partial_1^y \partial_1^y \partial_1^y \delta(x^1 - y^1). \tag{43}$$

This indeed agrees with Refs. 3–6.

V. CONCLUSION

From (17) we see that we found an elegant way to compute the Schwinger term in the gravitational constraints in two dimensions, which emphasizes its relation to the gravitational anomaly. The gravitational anomaly contributes in $4k+2 = 2,6,10,\ldots$ dimensions, and we expect that this method could be generalized to these higher dimensions. However, the calculation will become more complicated there.

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Time-dependent solution for a star immersed in a background radiation

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We study a time-dependent and spherically symmetric solution with a starlike source. We show that this solution can be interpreted as an exterior solution of a contracting star which has a decreasing temperature and is immersed in a homogenous and isotropic background radiation. Distribution of the temperature in the fields and close-to-Schwarzschild approximation of the solution are studied. By identifying the radiation with the cosmic background one, we find that the close-to-Schwarzschild approximate solution is valid in a wide range in our solar system. Possible experimental tests of the solution are discussed briefly. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1503147]

I. INTRODUCTION

It is well known that spherically symmetric sources such as stars can be modeled in the simplest way by the interior and exterior Schwarzschild solutions. But to include the radiation outside a star, more complicated solutions are required.[1] These include the Vaidya metric which uses a retarded time coordinate to describe a radiating atmosphere,[2] the metrics of Herrera and co-workers wherein spheres of matter are matched to exterior space–times,[3–5] and the metrics of Glass and Krisch which extend the Vaidya solution to include both a radiation field and a string fluid.[6] Recently, Liu and Wesson presented a new kind of solution in which the metric is time-dependent (but not of the Vaidya form) and the energy-momentum tensor is of the form of a perfect fluid for radiation plus a radial heat flow.[7] Clearly, this solution describes sources which are time-dependent and spherically symmetric. However, we wish to know specifically what kind of sources the solution represents. In this article we will show that it can describe **exterior** fields of a contracting (or expanding) star immersed in a homogenous and isotropic background radiation.

II. 4D SOLUTION DERIVED FROM 5D SOLUTIONS

Campbell's theorem says that any 4D Einstein solution with a source can be locally embedded in a 5D manifold *without* sources whose field equations in terms of the Ricci tensor are $R_{AB}=0$.[8] (Here and elsewhere lower case Greek letter run 0,123 and uppercase Latin letters run 0, 123, 4, and we use units $c=1$.) A major application of Campbell's theorem is to study embeddings of known 4D Einstein solutions in 5D Ricci flat manifolds.[9] Another application of the theorem is to generate new 4D solutions from known 5D Ricci flat solutions.[7,10] In the following we will show briefly how a new 4D solution is generated in Ref. 7. For the purpose of convenience, some of the equations and notations in Ref. 7 will be reexpressed.

In Ref. 7, Liu and Wesson presented a class of 5D solutions. This class of solutions is time-dependent in 5D and spherically symmetric in 3D with the 5D metric being

$$dS^2=B(r)dt^2-(1-\lambda t)^2[A(r)dr^2+r^2(d\theta^2+\sin^2\theta d\varphi^2)]-(1-\lambda t)^{-4}dy^2, \tag{1}$$

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where λ is a constant and the two functions B and A are determined by

$$\frac{B'}{B}=3\lambda^2 r\frac{A}{B}+\frac{A-1}{r}, \tag{2}$$

$$\frac{A'}{A}=3\lambda^2 r\frac{A}{B}-\frac{A-1}{r}, \tag{3}$$

where a prime denotes derivative with respect to r. Clearly, (2) and (3) can be solved, at least numerically, by imposing boundary conditions on $B(r)$ and $A(r)$. This 5D solution satisfies the 5D equations $R_{AB}=0$ and therefore is 5D empty. However, the 4D part of the 5D metric (1), together with the two equations (2) and (3), defines a 4D solution as shown in the following:[7]

$$ds^2=B(r)dt^2-(1-\lambda t)^2[A(r)dr^2+r^2(d\theta^2+\sin^2\theta d\varphi^2)] \quad , \tag{4}$$

$$\frac{B'}{B}=3\lambda^2 r\frac{A}{B}+\frac{A-1}{r}, \tag{5}$$

$$\frac{A'}{A}=3\lambda^2 r\frac{A}{B}-\frac{A-1}{r}, \tag{6}$$

$$8\pi G T_{\alpha\beta}\equiv G_{\alpha\beta}, \tag{7}$$

where $T_{\alpha\beta}$ is an effective or induced energy-momentum tensor with

$$8\pi G T_0^0=\frac{6\lambda^2}{B(1-\lambda t)^2}, \tag{8}$$

$$8\pi G T_1^1=8\pi G T_2^2=8\pi G T_3^3=-\frac{2\lambda^2}{B(1-\lambda t)^2}, \tag{9}$$

$$8\pi G T_0^1=\frac{\lambda B'}{AB(1-\lambda t)^3}. \tag{10}$$

It was also shown in Ref. 7 that this $T_{\alpha\beta}$ can be modeled as a perfect fluid plus a radial heat flow,

$$T_{\alpha\beta}=(\rho+p)u_\alpha u_\beta-pg_{\alpha\beta}+q_\alpha u_\beta+u_\alpha q_\beta, \tag{11}$$

where ρ is the mass density, p is the pressure, $u^\alpha=(u^0,0,0,0)$ is the four-velocity, $q^\alpha=(0,q^1,0,0)$ is the heat-flux vector, and u_α and q_α obey the orthogonality condition $q_\alpha u^\alpha=0$. Then Eqs. (8)–(10) yield

$$\rho=3p=\frac{3\lambda^2}{4\pi GB(1-\lambda t)^2}, \tag{12}$$

$$q^1=\frac{\lambda B'}{8\pi GAB^{3/2}(1-\lambda t)^3}. \tag{13}$$

Equations (4)–(13) constitute a complete set of the 4D solution, from which we see that the equation of state of the 4D fluid is $\rho=3p$, so it represents a radiation or extra-relativistic particles accompanied by a radial heat flow.

III. HEAT FLOW AND TEMPERATURE OF THE FIELDS

The induced 4D energy-momentum tensor (11) describes a thermodynamical system in which the radial heat current q_α implies a radial temperature gradient. Now we wish to calculate this temperature distribution over the fields. The generalized relativistic relation between heat current and temperature gradient can be found in Refs. 11 and 12 with

$$q^\alpha = -\kappa(T_{,\mu} - \dot{u}_\mu T)h^{\alpha\mu}, \quad \dot{u}_\mu \equiv u_{\mu;\nu}u^\nu, \tag{14}$$

where κ is the coefficient of the thermal conductivity and $h^{\alpha\mu}$ is the projection tensor,

$$h^{\alpha\beta} = u^\alpha u^\beta - g^{\alpha\beta}. \tag{15}$$

To calculate Eqs. (14), we calculate $\dot{u}_\mu$ first. With use of (4), we find the only nonvanishing $\dot{u}_\mu$ being $\dot{u}_1 = -B'/(2B)$. Furthermore, we assume $T = T(t,r)$. Then Eqs. (14) reduce to $q^0 = q^2 = q^3 = 0$ and

$$q^1 = -\frac{\kappa}{A(1-\lambda t)^2}\left(T_{,1} + \frac{B'}{2B}T\right). \tag{16}$$

Combining (13) and (16), we get

$$-\kappa\left(T_{,1} + \frac{B'}{2B}T\right) = \frac{\lambda B'}{8\pi G(1-\lambda t)B^{3/2}}. \tag{17}$$

We find that this equation can be integrated, giving an exact solution

$$\sqrt{B(r)}T(t,r) = \sqrt{B_R}T_R(t) + \frac{\lambda}{8\pi G\kappa(1-\lambda t)}\ln\frac{B_R}{B(r)}, \tag{18}$$

where R is a constant radius, and B_R and $T_R(t)$ are values of $B(r)$ and $T(t,r)$ at $r = R$, respectively. From (13) we see that $\lambda = 0$ corresponds to thermal equilibrium $q^\alpha = 0$. Then, from (18), if $\lambda = 0$, we get $\sqrt{B}T = \text{const}$. Thus we recover the conclusion that thermal equilibrium corresponds not to constant temperature, but to the redshifted temperature distribution $\sqrt{g_{00}}T = \text{const}$.[11] Generally we have $\lambda \neq 0$ and the exact solution (18) determines both the space distribution and the time variation of the temperature T over the fields.

IV. CLOSE-TO-SCHWARZSCHILD APPROXIMATION

The close-to-Schwarzschild approximation of the solution (4) was given in Ref. 7. We find that it can be reexpressed in the following form:

$$ds^2 = B(r)dt^2 - (1-\lambda t)^2[A(r)dr^2 + r^2(d\theta^2 + \sin^2\theta d\varphi^2)], \tag{19}$$

$$B = 1 - \frac{2GM}{r} + 2\lambda^2 r^2 + O(\varepsilon^3), \tag{20}$$

$$A^{-1} = 1 - \frac{2GM}{r} - \lambda^2 r^2 + O(\varepsilon^3). \tag{21}$$

Here ε is a small quantity of the order of the Newtonian potential GM/r, $O(\varepsilon^3)$ are terms of the order of ε^3 or higher, and we have assumed, for practical usage, that λr is also a small quantity of the order ε, i.e.,

$$|\lambda|r \sim GM/r \sim \varepsilon \ll 1. \tag{22}$$

To verify the accuracy of this solution, one can calculate B'/B and A'/A first, and then substitute them into the two equations (2) and (3). Thus the approximate solutions (19)–(21) are correct in the range (22), or, equivalently, in

$$GM \ll r \ll |\lambda|^{-1}. \tag{23}$$

We also conclude that (19)–(21) are accurate up to the second order of ε and give back to the Schwarzschild solution if $\lambda = 0$. So generally we can interpret the solution as an exterior solution of a starlike source. We will show, in the next section, that in a wide range in our solar system the condition (22), or, equivalently, (23), is satisfied.

Consider now the equation (12), which, by (20), reduces to

$$\rho = 3p = \frac{3\lambda^2}{4\pi G(1-\lambda t)^2}\left[1 + \frac{2GM}{r} + O(\varepsilon^2)\right]. \tag{24}$$

Here ρ and p constitute a perfect fluid with the equation of state $\rho = 3p$, implying a property for radiation or ultra-relativistic particles. From (24) we see that neglecting higher-order terms in the square bracket on the rhs of (24), the densities ρ and p are homogenous and isotropic. Thus we find that one can not interpret the fluid as a radiating atmosphere of a star such as in the Vaidya metric.[2] Apparently, we can interpret it as to describe a star immersed in a homogenous and isotropic background radiation.

The existence of the heat flow term in the energy-momentum tensor (11) implies that there must be a temperature gradient in the field and a heat interchanges between the star and the background radiation. Using (20) and (21) in (18) gives

$$\sqrt{B(r)}T(t,r) - \sqrt{B_R}T_R(t) = \frac{\lambda M}{4\pi\kappa(1-\lambda t)}\left\langle \frac{1}{r} - \frac{1}{R}\right\rangle [1 + O(\varepsilon)]. \tag{25}$$

If we choose R as the radius of the star, then in the exterior $r > R$, Eq. (25) implies that if $\lambda > 0$, then $\sqrt{B(r)}T(t,r) < \sqrt{B_R}T_R(t)$. Be aware that the thermal equilibrium corresponds to $\sqrt{B(r)}T(t,r) = \sqrt{B_R}T_R(t)$ for which there is no heat flow.[11] So we conclude that the heat flows outwards if $\lambda > 0$ and inwards if $\lambda < 0$. This agrees with the original relation (13) in which $q^1 > 0$ for $\lambda > 0$ and $q^1 < 0$ for $\lambda < 0$ since $B' > 0$ according to (20). Meanwhile, from the metric (19) and the result (24) we also see that if $\lambda > 0$, then as the time t increases, the 3D space contracts and the energy density of the outside fluid increases. All these properties are physically reasonable.

V. DISCUSSION

We have concluded in Sec. IV that the 4D solution discussed in this article can be interpreted as an exterior solution of a spherical source such as a star which has a nonzero temperature and is immersed in a homogenous and isotropic background radiation. A natural candidate for this kind of radiation is the cosmic background radiation, for which the temperature is about $T_0 \approx 2.7$ K at present days with an energy density around $\rho_b \approx 4.0 \times 10^{-13}$ erg cm^{-3}. Thus, by using (12), we determine the constant λ as

$$|\lambda|^{-1} \approx \sqrt{\frac{3c^4}{4\pi G\rho_b}} \approx 2.7 \times 10^{30} \text{ cm} \approx 1.8 \times 10^{17} \text{ AU}. \tag{26}$$

So, λ is of the order of the Hubble constant. Now we wish to know if the close-to-Schwarzschild solution given in (19)–(21) can describe our solar system. That is, we need to calculate and compare orders of the two terms GM/r and $\lambda^2 r^2$ appearing in (20) and (21). The average distance between the Sun and the nearest planet Mercury is about 0.387 AU. So, we have

$$\frac{GM_\odot}{R_{\rm Merc}c^2}\approx 2.55\times 10^{-8},\quad |\lambda|R_{\rm Merc}\approx 2\times 10^{-18}. \tag{27}$$

The average distance between the Sun and the Pluto is about 39.53 AU. So,

$$\frac{GM_\odot}{R_{\rm Pluto}c^2}\approx 2.5\times 10^{-10},\quad |\lambda|R_{\rm Pluto}\approx 2\times 10^{-16}. \tag{28}$$

Therefore, we conclude that in a wide range in our solar system, we have $|\lambda|r\ll GM/r$. So, $\lambda^2 r^2$ is of an order higher than the post-Newtonian order. This implies that the contributions of the cosmic background radiation to all of the known solar system experiments[13] are negligible. However, there may be other ways to detect possible new effects of the solution. For example, according to the time-dependent metric (19) and the value of λ in (26), the radius of the central star should be contracting or expanding, depending on whether λ is positive or negative, with a relative rate at present time being

$$\left(\frac{\dot R}{R}\right)_0 = -\lambda c\approx -3.5\times 10^{-13}\ \ {\rm yer}^{-1}\quad \text{for}\ \ \lambda>0. \tag{29}$$

It is worthwhile to study whether this kind of effect is observable.

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Separation of variables and exact solution of the Klein–Gordon and Dirac equations in an open universe

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We solve the Klein–Gordon and Dirac equations in an open cosmological universe with a partially horn topology in the presence of a time dependent magnetic field. Since the exact solution cannot be obtained explicitly for arbitrary time dependence of the field, we discuss the asymptotic behavior of the solutions with the help of the relativistic Hamilton–Jacobi equation. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1501445]

I. INTRODUCTION

During the last years a large amount of observational data has been reported showing that our universe is almost isotropic and homogeneous. The study of the structure of the cosmic microwave radiation leads us to conclude that the ratio of the total density to the critical density of the universe Ω_0 is likely to be close to one,[1–3] favoring a spatially flat Robertson–Walker metric over other topologies.

It is well known that general relativity is a local metrical theory and, therefore, the corresponding Einstein field equations do not fix the global topology of space–time and, consequently, the universe may have compact spatial sections with a nontrivial topology.[4,5] Then the observational data does not rule out the possibility that our universe possesses a hyperbolic topology.[4,6–8]

The study of cosmological models with nonstandard topologies is not new and goes back to the works by Zelmanov,[9,10] showing that, upon different coordinate transformations, spatially closed or flat sections can be transformed into hyperbolic sections and vice versa.

The line element associated with a spatially open Friedman universe has the form

$$ds^2 = a^2(\eta)[-d\eta^2 + dr^2 + \sinh^2(d\theta^2 + \sin^2\theta d\phi^2)]. \tag{1}$$

Making the coordinate transformation[5]

$$e^{-z} = \cosh r - \sinh r \cos\theta, \quad e^{-z}x = \sin\theta\cos\phi\sinh r, \quad e^{-z}y = \sin\theta\sin\phi\sinh r, \tag{2}$$

the metric (1) becomes

$$a^{-2}(\eta)ds^2 = -d\eta^2 + dz^2 + e^{-2z}(dx^2 + dy^2). \tag{3}$$

The topology is induced by identifying points periodically along x and y by $(x,y) = (x+b, y+h)$, where b and h are constant, to create a two dimensional torus. The torus is stretched by the factor e^{-2z} along the z axis to create a toroidal horn. The comoving proper area of the torus is $e^{-2z}bh$ and depends on location along the z axis. The global topology induces global inhomogeneity as well as global anisotropy.[4]

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The study of quantum effects in cosmological universes with a nontrivial topology allows us a deeper understanding of the properties of different scenarios and which of them can describe our universe. In this direction the metric (3) represents a very interesting scenario in order to discuss particle production and propagation of perturbations in cosmology.

After the publication of the pioneering article by Schrödinger,[11] discussing particle production in a deSitter universe, many articles have been published on the problem of quantum effects in cosmological scenarios,[12–14] most of them dealing with a Robertson–Walker line element with spatially flat topology. This particularly simple line element, which is the most used in inflationary models, permits one to compute the Green function as well as to solve the relativistic wave equations.[15–17]

In order to study quantum processes in curved space–times one has to fulfill a preliminary step which consists in having a description of the single-mode solution of the relativistic particles or perturbations in those background fields, i.e., exact solution of the relativistic scalar and spinor wave equations. In the literature we have at our disposal different methods for solving relativistic wave equations in curved spaces and in curvilinear coordinates; among them, the method of separation of variables is one of the most widely used.[18–21]

It is the purpose of the present article to solve the Klein–Gordon and Dirac equations in the Friedman universe associated with the metric (3) in the presence of a time dependent magnetic field. In order to solve the Dirac equation we apply the algebraic method of separation of variables.[20–24] We compare the solutions with those of obtained after solving the relativistic Hamilton Jacobi equation. The article is structured as follows: In Sec. II we solve the relativistic Hamilton–Jacobi equation in an open cosmological universe with a horn topology. In Sec. III we separate variables and solve the Klein–Gordon equation. In Sec IV, using the algebraic method of separation of variables, we reduce the Dirac equation to a system of first order coupled differential equations that we solve in terms of special functions. Finally, in Sec. V we briefly discuss the results reported in this article.

II. SOLUTION OF THE HAMILTON–JACOBI EQUATION

The covariant generalization of the Hamilton–Jacobi equation has the form[25]

$$g^{\alpha\beta}\left(\frac{\partial S}{\partial x^{\alpha}}-eA_{\alpha}\right)\left(\frac{\partial S}{\partial x^{\beta}}-eA_{\beta}\right)+M^{2}=0, \tag{4}$$

where $g^{\alpha\beta}$ is the contravariant metric, A_{α} is the vector potential and M is the mass of the particle. Here and elsewhere we adopt the convention $c=\hbar=1$.

Let us introduce an electromagnetic field associated with the vector potential

$$A^{\mu}=A_{1}(y)\,\delta_{1}^{\mu}, \tag{5}$$

where the index $\mu=0$ is associated with the evolution parameter η and $\mu=1,2,3$ correspond to the space coordinates x,y,z, respectively. Looking at the relativistic invariants

$$\frac{1}{2}F^{\mu\nu}F_{\mu\nu}=B^{2}-E^{2}=\frac{e^{4z}}{\alpha(\eta)^{4}}\left(\frac{dA_{1}(y)}{dy}\right)^{2}, \tag{6}$$

$$F^{\mu\nu}F^{*}_{\mu\nu}=0, \tag{7}$$

and taking into account that only F_{23} is different from zero, we notice that (5) corresponds to a nonconstant magnetic field B, directed along the z axis, with strength

$$B=\frac{e^{2z}}{\alpha(\eta)^{2}}\left|\frac{dA_{1}(y)}{dy}\right|, \tag{8}$$

whose value is inversely proportional to the expansion factor $\alpha(\eta)^2$.

The line element (3) is a Stäckel space,[26] and the Hamilton–Jacobi equation (4) is completely separable in (3) in the presence of the vector potential (5), therefore we can look for a solution in the form

$$S=k_x+S_y(y)+S_z(z)+S_\eta(\eta). \tag{9}$$

Substituting (9) into Eq. (4) we obtain

$$\frac{(k_x-A_1(y))^2}{e^{-2z}}+\frac{1}{e^{-2z}}\left(\frac{dS_y}{dy}\right)^2+\left(\frac{dS_z}{dz}\right)^2-\left(\frac{dS_\eta}{d\eta}\right)^2-M^2\alpha(\eta)^2=0. \tag{10}$$

Equation (10) reduces to the following system of differential equations:

$$\left(\frac{dS_z}{dz}\right)^2+k_{xy}^2e^{2z}=k_z^2, \tag{11}$$

$$\left(\frac{dS_\eta}{d\eta}\right)^2+M^2\alpha(\eta)^2=k_z^2, \tag{12}$$

$$(k_x-A_1(y))^2+\left(\frac{dS_y}{dy}\right)^2=k_{xy}^2, \tag{13}$$

where k_{xy}^2 and k_z^2 are separation constants.

In the absence of electromagnetic interaction, we have that $A_1(y)=0$ and the solution of Eq. (13) takes the form

$$S_y=\pm\sqrt{k_{xy}^2-k_x^2}y=\pm k_y y, \tag{14}$$

where we have introduced the constant k_y. Equation (14) can also be derived looking at the symmetry between the torus coordinates x and y in the line element (3) and Eq. (10) when $A_1(y)=0$.

When the vector potential has the simple form $A_1(y)=A_1y$, the magnetic field reads $B=[e^{2z}/\alpha(\eta)^2]|A_1|$ and the function $S_y(y)$ is

$$S_y(y)=-\frac{k_x-A_1y}{2A_1}\sqrt{k_{xy}^2-(k_x-A_1y)^2}+\frac{k_{xy}^2}{2A_1}\arctan\frac{A_yy-k_x}{\sqrt{k_{xy}^2-(k_x-A_1y)^2}}. \tag{15}$$

The solution of Eq. (11) can be expressed in terms of elementary functions as follows:

$$S_z=\sqrt{k_z^2-k_{xy}^2\exp(2z)}-k_z\tanh^{-1}\sqrt{\frac{k_z^2-k_{xy}^2\exp(2z)}{k_z^2}}. \tag{16}$$

The solution of Eq. (12) can be written as

$$S_\eta=\pm\int\sqrt{k_z^2-M^2\alpha(\eta)^2}d\eta, \tag{17}$$

whose explicit form in terms of elementary functions will depend on a particular choice of the expansion function $\alpha(\eta)$.

Since we have been able to solve the Hamilton–Jacobi equation in the Stäckel space given by (4), we can construct the quasiclassical modes of the relativistic wave equations through the identification

$$\Phi \to e^{iS} = e^{\pm i\int \sqrt{k_z^2 - M^2\alpha(\eta)^2}\, d\eta} e^{ik_x x} e^{iS_y} e^{iS_z}, \tag{18}$$

where S_z and S_y take the following values at the asymptotes:

$$S_{z(\infty)} \to ik_{xy}e^z, \quad S_{z(-\infty)} \to k_z z, \tag{19}$$

$$S_{y(\infty)} \to \mp i \frac{(k_x - A_1 y)^2}{2A_1}. \tag{20}$$

When the electromagnetic interaction is not present we have that $S_y = \exp(ik_y y)$.

III. SOLUTION OF THE KLEIN–GORDON EQUATION

The covariant generalization of the Klein–Gordon equation in curved space–time has the form[12]

$$g^{\alpha\beta}(\nabla_\alpha - ieA_\alpha)(\nabla_\beta - ieA_\beta)\Phi - (M^2 + \xi R)\Phi = 0, \tag{21}$$

where ∇_α is the covariant derivative, R is the curvature scalar and ξ is a scalar dimensionless coupling constant which takes the value $\xi = \frac{1}{6}$ in the conformal case and $\xi = 0$ when a minimal coupling is considered. The value of the R for the metric (3) is

$$R = 6\frac{-a(\eta) + (d^2a(\eta)/d\eta^2)}{a(\eta)^3}. \tag{22}$$

Substituting the metric associated with the line element (3) into the Klein–Gordon equation (21) one obtains

$$e^{2z}\frac{\partial^2\Phi}{\partial x^2} + e^{2z}\frac{\partial^2\Phi}{\partial y^2} - 2\frac{\partial\Phi}{\partial z} + \frac{\partial^2\Phi}{\partial z^2} - 2\frac{\partial\Phi}{\partial\eta}\frac{d\alpha}{d\eta}\frac{1}{\alpha^3} - e^{2z}A_1(y)^2\Phi - 2ie^{2z}\frac{\partial\Phi}{\partial x}A_1(y) - M^2\alpha^2\Phi = 0, \tag{23}$$

where we have chosen to work with a minimal coupling $\xi = 0$. The Klein–Gordon equation (21) is completely separable in (3), therefore we look for its solution in the form

$$\Phi = H(\eta)Z(z)Y(y)e^{ik_x x}. \tag{24}$$

Substituting (24) into Eq. (21) we reduce the problem of solving the Klein–Gordon equation to that of finding solutions of the following set of ordinary differential equations

$$\frac{d^2Y}{dy^2} - ((k_x - A_1(y))^2 - k^2)Y = 0, \tag{25}$$

$$\frac{d^2Z}{dz^2} - 2\frac{dZ}{dz} - (\lambda^2 + k^2e^{2z})Z = 0, \tag{26}$$

$$\frac{d^2H}{d\eta^2} + 2\frac{dH}{d\eta}\frac{d\alpha}{d\eta} + (\alpha^2(\eta)M^2 - \lambda^2)H = 0, \tag{27}$$

with λ^2 and k^2 as separation constants. For $A(y) = A_1 y$ the solution of Eq. (25) can be expressed in terms of Whittaker functions[27] as follows:

$$Y = C_1 v^{-1/2} M_{k^2/4A_1,\,1/4}(v^2) + C_2 v^{-1/2} W_{k^2/4A_1,\,1/4}(v^2), \tag{28}$$

where

$$v=\frac{A_1 y-k_x}{\sqrt{A_1}}, \tag{29}$$

and C_1 and C_2 are arbitrary constants. In the absence of electromagnetic field the solution of Eq. (25) reduces to

$$Y=C_1 e^{\pm i\sqrt{k^2-k_x^2}y}=C_1 e^{\pm ik_y y}. \tag{30}$$

The solution of Eq. (26) is[28]

$$Z=C_3 e^z H^{(1)}_{\sqrt{1+\lambda^2}}(ike^z)+C_4 e^z H^{(2)}_{\sqrt{1+\lambda^2}}(ike^z), \tag{31}$$

where $H^{(1)}_\nu(z)$ and $H^{(2)}_\nu(z)$ are the Hankel functions and C_3 and C_4 are arbitrary constants. We can also express the solution of (26) in terms of Bessel functions $J_\nu(z)$ as

$$Z=D_3 e^z J_{\sqrt{1+\lambda^2}}(ike^z)+D_4 e^z J_{-\sqrt{1+\lambda^2}}(ike^z), \tag{32}$$

where D_3 and D_4 are arbitrary constants.

After introducing the function $h(\eta)$,

$$H(\eta)=\frac{h(\eta)}{\alpha(\eta)}, \tag{33}$$

Eq. (27) reduces to

$$\frac{d^2h}{d\eta^2}+\left(\alpha^2(\eta)M^2-\lambda^2-\frac{d^2\alpha(\eta)}{d\eta^2}\right)h=0. \tag{34}$$

In order to analyze the asymptotic behavior of the solutions of the Klein–Gordon equation (21) we make use of the asymptotic behavior of the Hankel functions,[27]

$$H^{(1)}_\nu(z)\to\left(\frac{2}{\pi z}\right)^{1/2}e^{i(z-\pi\nu/2-\pi/4)},\quad H^{(2)}_\nu(z)\to\left(\frac{2}{\pi z}\right)^{1/2}e^{-i(z-\pi\nu/2-\pi/4)}, \tag{35}$$

as $z\to\infty$, and the behavior of $J_\nu(z)$ as $z\to 0$ (Ref. 28),

$$J_\nu(z)\to\frac{\left(\frac{z}{2}\right)^\nu}{\Gamma(1+\nu)} \tag{36}$$

The asymptotic behavior of the Whittaker function $W_{k,\mu}(z)$ for large values of z is[28]

$$W_{k,\mu}(z)\to e^{-z/2}z^k, \tag{37}$$

and the function $M_{k,\mu}(z)$ has the following asymptotic behavior as $z\to 0$:

$$M_{k,\mu}(z)\to e^{-z/2}z^{\mu+(1/2)}. \tag{38}$$

An approximate solution of Eq. (34) can be obtained provided that the expansion parameter $\alpha(\eta)$ satisfies the conditions of validity of the adiabatic approximation. In this case one has that $h(\eta)$ has the form[29–31]

$$h(\eta)=\frac{1}{\sqrt{2W(\eta)}}\exp\left(\pm i\int^\eta W(\eta')d\eta'\right), \tag{39}$$

with

$$W(\eta)^2=\omega(\eta)^2[1+\delta_2(\eta)\omega^{-2}+\cdots], \tag{40}$$

where the function $\omega(\eta)$ has the form

$$\omega(\eta)^2=\alpha^2(\eta)M^2-\lambda^2-\frac{d^2\alpha(\eta)}{d\eta^2}, \tag{41}$$

$\delta_n(\eta)$ is a function of $\omega(\eta)$ and its derivatives at η up through $\omega^{(n)}(\eta)$ and $\delta_n(\eta)$ is bounded as $\omega\to\infty$. The solution of the Klein–Gordon equation (21) can be written as

$$\Phi=\frac{\exp(\pm i\int\sqrt{\alpha^2(\eta)M^2-\lambda^2-(d^2\alpha(\eta)/d\eta^2)}\,d\eta}{\sqrt{2}a(\eta)^{3/2}}Z(z)Y(y)e^{ik_xx}. \tag{42}$$

Let us analyze the asymptotic behavior of (42) as $y\to\infty$ and $z\to-\infty$. Using (19) and (36) we obtain that, when the electromagnetic interaction is switched off, the mode solutions of Eq. (21) take the asymptotic form

$$\Phi\to\frac{\exp(\pm i\int\sqrt{\alpha^2(\eta)M^2-\lambda^2-(d^2\alpha(\eta)/d\eta^2)}\,d\eta}{\sqrt{2}a(\eta)^{3/2}}e^{\mp ik_yy}e^{ik_xx}e^{(\mp\sqrt{1+\lambda^2}+1)z}. \tag{43}$$

Analogously, we have that in the presence of the electromagnetic potential the mode solutions of Eq. (21) take the following asymptotic form:

$$\Phi\to\frac{\exp(\pm i\int\sqrt{\alpha^2(\eta)M^2-\lambda^2-(d^2\alpha(\eta)/d\eta^2)}\,d\eta}{\sqrt{2}a(\eta)^{3/2}}e^{(\pm\sqrt{1+\lambda^2}+1)z}\nu^{k^2/2A_1}e^{-\nu^2/2}e^{ik_xx}. \tag{44}$$

For large positive values of z we have that the asymptotic behavior of Φ is

$$\Phi\to\frac{\exp(\pm i\int\sqrt{\alpha^2(\eta)M^2-\lambda^2-(d^2\alpha(\eta)/d\eta^2)}\,d\eta}{\sqrt{2}a(\eta)^{3/2}}e^{\mp e^{-ke^z}}e^{z/2}\nu^{k^2/2A_1}e^{-\nu^2/2}e^{ik_xx}. \tag{45}$$

From Eq. (44) we can identify the quasiclassical modes as $y\to\infty$ and $z\to-\infty$ as

$$\Phi_{\text{class}(z\to-\infty)}=\frac{h(\eta)}{\alpha(\eta)}e^zJ_{\pm\sqrt{1+\lambda^2}}(ike^z)v^{-1/2}W_{k^2/4A_1,\,1/4}(v^2)e^{ik_xx}. \tag{46}$$

Analogously, from Eq. (45) we have that the quasiclassical modes as $y\to\infty$ and $z\to\infty$ are

$$\Phi_{\text{class}(z\to\infty)}=\frac{h(\eta)}{\alpha(\eta)}e^zH^{(1,2)}_{\pm\sqrt{1+\lambda^2}}(ike^z)v^{-1/2}W_{k^2/4A_1,\,1/4}(v^2)e^{ik_xx}. \tag{47}$$

IV. SOLUTION OF THE DIRAC EQUATION

The Dirac equation is a system of coupled partial differential equations which is separable in a very restricted set of metrics. Among the space–times where the separability of the Klein–Gordon and Dirac equations has been studied one can mention the Stäckel spaces,[26] which are those metrics where the Hamilton–Jacobi equation is separable. Nevertheless, recently it has been shown that this condition is neither necessary nor sufficient in order to guarantee a complete separability of variables in the Dirac equation (see Ref. 32 and references therein). A systematic

classification of the gravitational backgrounds where the Dirac equation is separable with the help of the algebraic method is presented in Ref. 20 The line element (3) belongs to this family and, consequently, one can apply the algebraic method of separation.

The covariant generalization of the Dirac equation in curved space–time is[12,33]

$$\tilde{\gamma}^{\alpha}(\partial_{\alpha}-\Gamma_{\alpha}-ieA_{\alpha})\tilde{\Psi}+M\tilde{\Psi}=0, \tag{48}$$

where the curved Dirac matrices $\tilde{\gamma}^{\alpha}$ satisfy the commutation relation

$$\{\tilde{\gamma}^{\alpha},\tilde{\gamma}^{\beta}\}=2g^{\alpha\beta}, \tag{49}$$

and Γ_{α} are the spin connections[33]

$$\Gamma_{\alpha}=\frac{1}{4}g_{\mu\lambda}\left[\left(\frac{\partial b_{\nu}^{\beta}}{\partial x^{\alpha}}\right)a_{\beta}^{\lambda}-\Gamma_{\nu\alpha}^{\lambda}\right]s^{\mu\nu}, \tag{50}$$

where

$$s^{\mu\nu}=\tfrac{1}{2}(\tilde{\gamma}^{\mu}\tilde{\gamma}^{\nu}-\tilde{\gamma}^{\nu}\tilde{\gamma}^{\mu}), \tag{51}$$

and the matrices b_{μ}^{α}, a_{β}^{μ} establish the connection between the Dirac matrices $\tilde{\gamma}^{\mu}$ on a curved space–time and the flat Dirac matrices γ^{μ} as follows:

$$\tilde{\gamma}_{\mu}=b_{\mu}^{\alpha}\gamma_{\alpha}, \quad \tilde{\gamma}^{\mu}=a_{\beta}^{\mu}\gamma^{\beta}. \tag{52}$$

Since the line element (3) is associated with a diagonal metric, we can work in the diagonal tetrad gauge for $\tilde{\gamma}^{\mu}$:

$$\tilde{\gamma}^{0}=\frac{\gamma^{0}}{a(\eta)}, \quad \tilde{\gamma}^{1}=\frac{\gamma^{1}}{a(\eta)e^{-z}}, \quad \tilde{\gamma}^{2}=\frac{\gamma^{2}}{a(\eta)e^{-z}}, \quad \tilde{\gamma}^{3}=\frac{\gamma^{0}}{a(\eta)}. \tag{53}$$

Substituting (53) into (50) we obtain that the spinor connections are

$$\Gamma_{1}=-\frac{1}{2}\frac{e^{-z}}{\alpha(\eta)}\left\{-\alpha(\eta)\gamma^{1}\gamma^{3}+\frac{d\alpha(\eta)}{d\eta}\gamma^{1}\gamma^{4}\right\}, \tag{54}$$

$$\Gamma_{2}=-\frac{1}{2}\frac{e^{-z}}{\alpha(\eta)}\left\{-\alpha(\eta)\gamma^{2}\gamma^{3}+\frac{d\alpha(\eta)}{d\eta}\gamma^{2}\gamma^{4}\right\}, \tag{55}$$

$$\Gamma_{3}=-\frac{1}{2}\frac{d\alpha(\eta)}{d\eta}\frac{1}{\alpha(\eta)}\gamma^{3}\gamma^{4}, \quad \Gamma_{4}=0. \tag{56}$$

Substituting (53)–(56) into (48) we find that the Dirac equation takes the simple form

$$\left\{\gamma^{0}\frac{\partial}{\partial\eta}+\gamma^{1}e^{z}\left(\frac{\partial}{\partial x}-A_{1}(y)\right)+\gamma^{2}e^{z}\frac{\partial}{\partial y}+\gamma^{3}\frac{\partial}{\partial z}+M\alpha(\eta)\right\}\Psi=0, \tag{57}$$

where we have introduced the spinor Ψ,

$$\tilde{\Psi}=a(\eta)^{-3/2}e^{z}\Psi. \tag{58}$$

Regarding Eq. (57), we should mention that it does exhibit a nonfactorizable structure.[22,34] In order to solve Eq. (57) we apply the algebraic method of separation of variables.[20–24] The method consists in rewriting the Dirac equation (57) as a sum of two first order differential operators $\hat{K}_{1}$, $\hat{K}_{2}$ satisfying the relation

$$[\hat{K}_1,\hat{K}_2]_-=0, \quad \{\hat{K}_1+\hat{K}_2\}\Phi=0, \tag{59}$$

with

$$\gamma^3\gamma^0\Psi=\Phi \tag{60}$$

and

$$\hat{K}_1(x,y)\Phi=\left\{\gamma^2\frac{\partial}{\partial y}+\gamma^1\left(\frac{\partial}{\partial x}-iA_1(y)\right)\right\}\gamma^3\gamma^0\Phi=ik\Phi, \tag{61}$$

$$\hat{K}_2(z,\eta)\Phi=e^z\left\{\gamma^0\frac{\partial}{\partial\eta}+\gamma^3\frac{\partial}{\partial z}+M\alpha(\eta)\right\}\gamma^3\gamma^0\Phi=-ik\Phi. \tag{62}$$

It should be noticed that, using the pairwise scheme of separation, one has been able to reduce the problem of solving the Dirac equation to finding solutions of the decoupled system of Eqs. (61) and (62). A further problem arises when we try to separate variables in Eq. (62). Here it is not possible to reduce the problem to a set of two commuting first order differential operators. In order to separate variables in Eq. (62), we rewrite it in the following form:[22,35]

$$(\hat{L}_1\gamma^3\gamma^0+\hat{L}_2)\Phi=0, \tag{63}$$

where $\hat{L}_1$ and $\hat{L}_2$ are two commuting differential operators given by the expressions

$$\hat{L}_1=\gamma^0\frac{\partial}{\partial\eta}+M\alpha(\eta), \tag{64}$$

$$\hat{L}_2=\gamma^0\frac{\partial}{\partial z}+ike^z. \tag{65}$$

In order to separate variables in Eq. (63), we introduce the auxiliary spinor $\mathcal{Y}$,

$$(\hat{L}_1\gamma^3\gamma^0+\tilde{L}_2)\mathcal{Y}=\Phi, \tag{66}$$

where the differential operator $\tilde{L}_2$ is given by the expression

$$\tilde{L}_2=\gamma^0\frac{\partial}{\partial z}-ike^z. \tag{67}$$

Substituting (66) into (63) we obtain that $\mathcal{Y}$ satisfies the following equation:

$$\{\hat{M}_1+\hat{M}_2\}\mathcal{Y}=0, \tag{68}$$

with $[\hat{M}_1,\hat{M}_2]=0$, and

$$(\hat{M}_1+\tilde{\lambda})\mathcal{Y}=\left(-\frac{\partial^2}{\partial z^2}-i\gamma^0ke^z+k^2e^{2z}+\tilde{\lambda}\right)\mathcal{Y}=0, \tag{69}$$

$$(\hat{M}_2-\tilde{\lambda})\mathcal{Y}=\left(\frac{\partial^2}{\partial\eta^2}+\gamma^0M\frac{d\alpha(\eta)}{d\eta}+M^2\alpha^2(\eta)-\tilde{\lambda}\right)\mathcal{Y}=0, \tag{70}$$

where $\tilde{\lambda}$ is a separation constant. Introducing the new variable $u=2ke^z$, we have that Eq. (69) can be written as

$$\left(\frac{\partial^2}{\partial u^2}+\frac{i}{2u}\gamma^0-\frac{1}{4}+\left(\frac{1}{4}-\lambda\right)\frac{1}{u^2}\right)\mathcal{S}=0, \tag{71}$$

where

$$u^{-1/2}\mathcal{S}=\mathcal{Y}. \tag{72}$$

Choosing the following representation of the Dirac matrices,[36]

$$\gamma^0=\begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix},\quad \gamma^j=\begin{pmatrix}0 & \sigma^j\\ \sigma^j & 0\end{pmatrix},\quad 1\leqslant j\leqslant 3, \tag{73}$$

we readily obtain that the spinor Φ has the following structure:

$$\left[\sigma_1\frac{\partial}{\partial y}-i\sigma_2(k_x-A_1(y))\right]\Phi_1=ik\Phi_2, \tag{74}$$

$$\left[-\sigma_1\frac{\partial}{\partial y}+i\sigma_2(k_x-A_1(y))\right]\Phi_2=ik\Phi_1, \tag{75}$$

$$\Phi=\begin{pmatrix}\Phi_1\\ \Phi_2\end{pmatrix}=\begin{pmatrix}\phi(y)\\ F\sigma^3\phi(y)\end{pmatrix}\exp(ik_x x), \tag{76}$$

where

$$\phi(y)=\begin{pmatrix}A(y)\\ B(y)\end{pmatrix}. \tag{77}$$

Using the representation (73) we obtain that the solution of Eq. (71) can be written in terms of Whittaker functions

$$S_{1,2}=D_1W_{-1/2,\sqrt{\lambda}}(u)+D_2M_{-1/2,\sqrt{\lambda}}(u),\quad S_{3,4}=D_3W_{1/2,\sqrt{\lambda}}(u)+D_4M_{1/2,\sqrt{\lambda}}(u), \tag{78}$$

where D_1, D_2, D_3, D_4 do not depend on the variable u. Looking at (70) and (71), we have that, for regular solutions at $u=0$, the spinor $\mathcal{Y}$ has the following structure:

$$\mathcal{Y}=\begin{pmatrix}a(y)c_1(\eta)u^{-1/2}M_{+1/2,\sqrt{\lambda}}(u)\\ b(y)c_1(\eta)u^{-1/2}M_{+1/2,\sqrt{\lambda}}(u)\\ c(y)c_2(\eta)u^{-1/2}M_{-1/2,\sqrt{\lambda}}(u)\\ d(y)c_2(\eta)u^{-1/2}M_{-1/2,\sqrt{\lambda}}(u)\end{pmatrix}\exp(ik_x x). \tag{79}$$

Substituting (79) into (66) and noticing that Eq. (70) is equivalent to the following system of equations,

$$\left(\frac{\partial}{\partial\eta}-iM\alpha(\eta)\right)c_1(\eta)=\sqrt{\tilde{\lambda}}c_2(\eta), \tag{80}$$

$$\left(\frac{\partial}{\partial\eta}+iM\alpha(\eta)\right)c_2(\eta)=\sqrt{\tilde{\lambda}}c_1(\eta), \tag{81}$$

we obtain that the spinor Φ has the following structure

$$\Phi=\begin{pmatrix} A(v)c_1(\eta)e^{-z/2}M_{-1/2,\sqrt{\tilde{\lambda}}}(2ke^z) \\ B(v)c_1(\eta)e^{-z/2}M_{-1/2,\sqrt{\tilde{\lambda}}}(2ke^z) \\ iA(v)c_2(\eta)e^{-z/2}M_{1/2,\sqrt{\tilde{\lambda}}}(2ke^z) \\ -iB(v)c_2(\eta)e^{-z/2}M_{1/2,\sqrt{\tilde{\lambda}}}(2ke^z) \end{pmatrix}\exp(ik_x x), \tag{82}$$

where $A(v)$ and $B(v)$ satisfy the system coupled system of equations

$$\left(\frac{d}{dy}-(k_x-A_1(y))\right)B=ikA, \tag{83}$$

$$\left(\frac{d}{dy}+(k_x-A_1(y))\right)A=ikB, \tag{84}$$

where v was defined in Eq. (29).

The corresponding solution of Eq. (59) in terms of the Whittaker functions $W_{k,\mu}(z)$ has the form

$$\Phi=\begin{pmatrix} \sqrt{\tilde{\lambda}}iA(v)c_1(\eta)e^{-z/2}W_{-1/2,\sqrt{\tilde{\lambda}}}(2ke^z) \\ -i\sqrt{\tilde{\lambda}}B(v)c_1(\eta)e^{-z/2}W_{-1/2,\sqrt{\tilde{\lambda}}}(2ke^z) \\ A(v)c_2(\eta)e^{-z/2}W_{1/2,\sqrt{\tilde{\lambda}}}(2ke^z) \\ B(v)c_2(\eta)e^{-z/2}W_{1/2,\sqrt{\tilde{\lambda}}}(2ke^z) \end{pmatrix}\exp(ik_x x). \tag{85}$$

Let us look for solutions of the system (83) and (84) when the electromagnetic potential has the simple functional dependence $A_1(y)=A_1 y$. In this case one can obtain exact solutions for $A(v)$ and $B(v)$ in terms of hypergeometric functions. After making the change of variable (29) and using the recurrence relations[27]

$$(b-1)M(a,b-1,z)=(b-1)M(a,b,z)+z\frac{dM(a,b,z)}{dz}, \tag{86}$$

$$\frac{1}{a}\frac{dM(a,b,z)}{dz}+M(a,b,z)=M(a+1,b,z), \tag{87}$$

$$\frac{dU(a,b,z)}{dz}-U(a,b,z)=-U(a,b+1,z), \tag{88}$$

we find that the general solution of the system of equations (83) and (84) reads

$$A=\frac{\sqrt{2A_1}}{ik}e^{-(1/2)v^2}\left(C_1M\left(-\frac{k^2}{4A_1}+\frac{1}{2},\frac{1}{2},v^2\right)+C_2U\left(-\frac{k^2}{4A_1}+\frac{1}{2},\frac{1}{2},v^2\right)\right), \tag{89}$$

$$B=e^{-(1/2)v^2}v\left(C_1M\left(-\frac{k^2}{4A_1}+\frac{1}{2},\frac{3}{2},v^2\right)-C_2U\left(-\frac{k^2}{4A_1}+\frac{1}{2},\frac{3}{2},v^2\right)\right). \tag{90}$$

The exact solution of the system of equations (83) and (84) in the absence of electromagnetic interaction has the form

$$A=C_1e^{i\sqrt{k^2-k_x^2}y}+C_2e^{-i\sqrt{k^2-k_x^2}y}, \tag{91}$$

$$B=\frac{\sqrt{k^2-k_x^2}-ik_x}{k}C_1e^{i\sqrt{k^2-k_x^2}y}-\frac{\sqrt{k^2-k_x^2}+ik_x}{k}C_2e^{-i\sqrt{k^2-k_x^2}y}, \tag{92}$$

where C_1 and C_2 are arbitrary constants. The solutions of the Dirac equations (82) and (85) exhibit an asymptotic behavior which can be identified with the quasiclassical solutions of the Hamilton–Jacobi equation (4). With the help of the asymptotic expressions (38), we find that the Dirac spinor Φ as $z\to-\infty$, and $y\to\infty$ takes the form

$$\Phi_{z\to-\infty}=\begin{pmatrix} \frac{\sqrt{2A_1}}{ik}c_1(\eta) \\ -vc_1(\eta) \\ -\frac{\sqrt{2A_1}}{k}c_2(\eta) \\ ivc_2(\eta) \end{pmatrix} e^{-ke^z}e^{\sqrt{\tilde{\lambda}}z}e^{-v^2/2}v^{(k^2/2A_1)-1}\exp(ik_x x), \tag{93}$$

where the functions $c_1(\eta)$ and $c_2(\eta)$ satisfy the system of equations (80) and (81). For asymptotically large values of z we have that the spinor Φ takes the form

$$\Phi_{z\to\infty}=\begin{pmatrix} \sqrt{\tilde{\lambda}}\frac{\sqrt{2A_1}}{k}c_1(\eta)e^{-z} \\ i\sqrt{\tilde{\lambda}}vc_1(\eta)e^{-z} \\ -i2\sqrt{2A_1}c_2(\eta) \\ -2kvc_2(\eta) \end{pmatrix} e^{-ke^z}e^{-v^2/2}v^{k^2/2A_1}\exp(ik_x x). \tag{94}$$

Looking at the solution of the Hamilton–Jacobi equation, we can identify (82) and (85) as the corresponding quasiclassical modes as $z\to-\infty$ and $z\to\infty$, respectively. An approximate expression for the time dependence of the spinor Φ can be obtained with the help of the WKB approximation. In this case we obtain

$$c_2(\eta)\sim c_{10}\exp(i\omega(\eta)), \tag{95}$$

$$c_1(\eta)\sim -i\frac{c_{10}}{\omega(\eta)+M\alpha(\eta)}\exp(i\omega(\eta)), \tag{96}$$

where c_{10} is a normalization constant and $\omega(\eta)=\sqrt{iM(d\alpha/d\eta)+M^2\alpha^2-\tilde{\lambda}}$. Looking at (95), (96) and (93) we readily see that, for large values of η we obtain $c_1(\eta)\to -i[c_{10}/2M\alpha(\eta)]\exp(i\omega(\eta))$. Analytic solutions of the system of equations (95) and (96) can be obtained for some particular expansion parameter $\alpha(\eta)$.[22,35]

V. CONCLUDING REMARKS

In this article, we have solved the Klein–Gordon and Dirac equations in an open cosmological universe with partially horn topology. The solutions of the relativistic wave equations are expressed in terms of special functions. In Sec. IV we have shown that the algebraic method of separation[22–24,35] permits one a complete separation of variables of the Dirac equation in the line element associated with a horn topology. The identification of the quasiclassical modes with the help of the relativistic Hamilton–Jacobi equation shows that this method is a very useful tool in the study of quantum effects in curved spaces.

As a final remark, we should mention that the introduction of nonstandard topologies in order to describe the large scale structure of the space–time also opens new possibilities to discuss quantum effects in globally inhomogeneous and anisotropic backgrounds in the presence of nontrivial electromagnetic interactions.

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A bidirectional Kaup–Kupershmidt equation and directionally dependent solitons

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Exact multisoliton solutions are obtained for the bidirectional Kaup–Kupershmidt equation that was reported in a recent paper [J. Math. Phys. **42**, 2567 (2001)]—this fills the gap that was left in the prior study. These solutions are found to possess the same remarkable, and unusual, property as the solitary-wave solution; namely, *their wave profiles are directionally dependent*. In particular, solitons are presented which describe multiple ''head-on'' collisions between *single*- and *double*-humped solitary waves. Explicit expressions are given for the first few multisoliton solutions and a procedure is described for constucting the general N-soliton by iteration on the solitons of lower order. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In a recent paper,[1] we constructed two fifth-order nonlinear evolution equations (NEEs) of ''Boussinesq''-type which govern wave propagation in two opposite directions. The first of these equations can be written in the nonlocal form

$$5\partial_x^{-1}u_{tt}+5u_{xxt}-15uu_t-15u_x\partial_x^{-1}u_t-45u^2u_x+\frac{75}{2}u_xu_{xx}+15uu_{3x}-u_{5x}=0, \tag{1}$$

and may be considered a *bidirectional* version of the well-known Kaup–Kupershmidt (KK) equation[2,3]

$$u_t+45u^2u_x-\frac{75}{2}u_xu_{xx}-15uu_{3x}+u_{5x}=0. \tag{2}$$

In Ref. 1, we designated Eq. (1) the *bidirectional Kaup–Kupershmidt* (or bKK) equation—it is the main interest of the present study.

The second equation studied in Ref. 1—and of equal relevance here—is

$$5\partial_x^{-1}u_{tt}+5u_{xxt}-15uu_t-15u_x\partial_x^{-1}u_t-45u^2u_x+15u_xu_{xx}+15uu_{3x}-u_{5x}=0; \tag{3}$$

it was formulated there as a bidirectional generalization of the Sawada–Kotera (SK) equation[4,5]

$$u_t+45u^2u_x-15u_xu_{xx}-15uu_{3x}+u_{5x}=0. \tag{4}$$

By constructing its bilinear form,[1] we were able to identify the *bidirectional Sawada–Kotera* (bSK) equation (3) with the well-known Ramani equation[6] [Eq. (9)]. In this study, we shall refer to Eq. (3) as the ''bSK-Ramani'' equation so as to emphasize its *bi*directional character and genealogy with the SK equation (4) while, at the same time, signaling its equivalence to Ramani's bilinear equation (9).

The KK and SK equations (2) and (4) have been studied extensively in the literature and their complete integrability is now firmly established (see, e.g., Refs. 2 and 6–11 and Refs. 2, 4, 5, 12,

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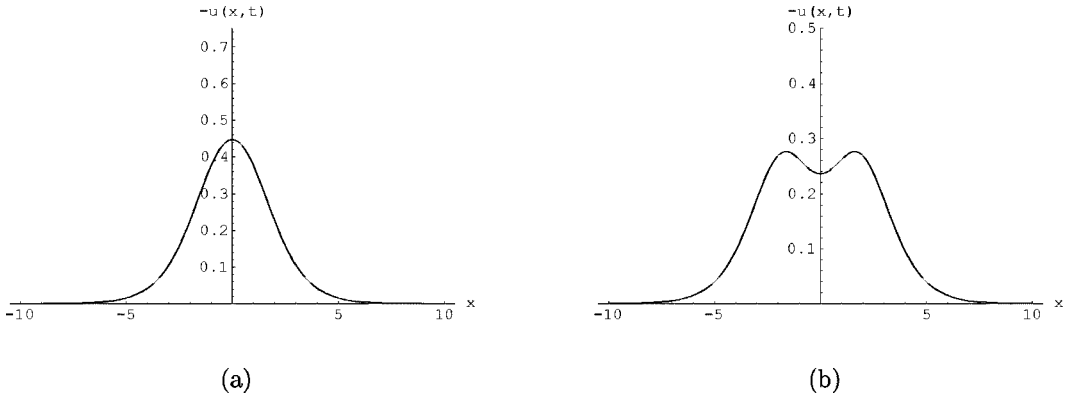

FIG. 1. Solitary-wave solutions of the bKK equation: (a) a right-traveling single-humped wave, (b) a left-traveling double-humped pulse.

and 13, respectively). Further, the intimate connection between these two *uni*directional NEEs has long been known;[2,10–12,14,15] nevertheless, Eqs. (2) and (4) are fundamentally different.[14] Indeed, the equations belong to quite distinct integrable hierarchies;[7,16] the KK Eq. (2) appears as a reduction in the so-called CKP system (KP hierarchy of C-type), while the SK Eq. (4) can be found in the BKP hierarchy.

The bSK-Ramani equation, Eq. (3), has likewise received considerable attention over the last two decades,[6,17–19] though it should be said, primarily in the guise of the bilinear form Eq. (9). However, we recently pointed to its bidirectional nature and relation to the SK Eq. (4) through the normal form (3).[1] The mathematical properties that assure the complete integrability of the bSK-Ramani equation have largely been established.[6,7,16–19] In Ref. 1 we were able to construct a Lax pair directly, along with an infinite number of conserved densities; we remark that the former associates Eq. (3) with a *fifth*-order scattering problem. In view of its connection with the SK equation, we might anticipate that the bSK-Ramani equation will also belong to the BKP hierarchy. This is indeed the case; yet, the equation appears in Ref. 16 neither in its normal form (3) nor in the form of Ramani's Eq. (9), but, rather, as the coupled bilinear form (8).

In contrast to the bSK-Ramani equation, it appears that very little of detail is known about the bKK Eq. (1). In Ref. 1 we formulated this NEE specifically as a bidirectional counterpart of the KK Eq. (2). Not surprisingly, then, the bKK equation is listed in Ref. 16 as a reduction of the CKP hierarchy and is given there in the normal form (1). The Lax pair reported by us in Ref. 1—together with an infinity of conservation laws—would seem to confirm its integrable status and, moreover, associates the bKK equation with a *fifth*-order spectral operator. Yet, arguably, the chief distinguishing property of any completely integrable equation is the existence of an infinite sequence of soliton solutions which describe the ''elastic'' interaction of multiple solitary waves.[20–23] In the previous study[1] we were able to derive the solitary wave of the bKK Eq. (1), but no further soliton solutions. This ''anomalous'' solitary wave possesses a remarkable property; namely, *its profile is dependent on the direction of travel* (see Fig. 1). This type of soliton behavior would seem to be quite unusual and, to our knowledge, had not been reported before then.

The aim of the present article is to obtain explicit multisoliton solutions of the bidirectional Kaup–Kupershmidt equation (1), and so fill the gap that was left in Ref. 1. To do so, we shall build on the results of our prior work;[1] we showed there that the ''anomalous'' character of these solitons arises quite naturally within Hirota's bilinear formalism.[24,25] Consequently, we were able to predict the structure—though not the precise analytical form—of the N-soliton solution of the bKK Eq. (1). In this regard, we will follow the strategy pursued by one of us (AP) to obtain the soliton solutions of its unidirectional cousin, the KK Eq. (2).[11] However, the current problem differs from that for the KK equation in one important respect—for the bKK equation we must additionally take account of its bidirectionality. Thus, in the case of the KK Eq. (2), one is able to

take advantage of its unidirectional character; this endows the solitons with a large measure of symmetry that facilitates the analysis greatly.[11] But, as we shall see, the soliton solutions of the bKK equation inherit the property of *directional dependence* from their constituent ''solitary'' waves. As a result, much, though by no means all, of the symmetry possessed by their unidirectional counterparts of the KK equation is lost. This makes the results for the bKK equation that much more complicated, though, by the same token, that much more interesting. This scenario differs markedly from that for its near relative, the bSK-Ramani Eq. (3). It too admits solitons which describe counter-propagating solitary waves, but its purely left- and right-traveling solitons are simply mirror images of one another! In short—and to the best of our knowledge—the directional dependence of the multisoliton solutions presented here distinguishes the bKK Eq. (1) from other bidirectional NEEs and makes it worthy of study.

Notwithstanding our comments above regarding the extra complications encountered here, the parallels with the solution procedure adopted in Ref. 11 for deriving soliton solutions of the KK equation are evident and illuminating. For example, we shall find that the analytic description of the N-soliton of the bKK equation requires the introduction of a ''new'' parameter at each order N; computing this parameter may be considered the central problem of the present work. This is quite unlike the bSK-Ramani equation whose N-soliton solution is given by Hirota's well-known *ansatz* [24] and is described by essentially a single parameter [see Eq. (10)]. We will also exploit the duality between the bKK and bSK-Ramani equations that is evident from Eqs. (1) and (3). This mirrors the deep connection between their unidirectional cousins, the KK and SK Eqs. (2) and (4), which was used to good effect in Ref. 11. We formulate the first three multisolitons of the bKK equation explicitly, and describe an iterative procedure for generating its soliton solutions to any order.

II. BILINEAR FORMS AND DIRECTIONALLY DEPENDENT SOLITARY WAVES

In the earlier study,[1] we introduced the change of dependent variable

$$u(x,t)=\alpha\partial_x^2 \ln f(x,t), \tag{5}$$

where α is a constant (and ∂_x^n denoted the nth partial derivative with respect to x). Then, following Hirota's direct method,[24,25] we showed that, under the transformation (5), the bKK Eq. (1) admits *two* possible bilinear forms:[1] with $\alpha=-1$, we obtain

$$(80\mathrm{D}_t^2+20\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6)f\cdot f-120\mathrm{D}_x\mathrm{D}_t f\cdot g+30\mathrm{D}_x^2 f\cdot h=0, \tag{6a}$$

$$\mathrm{D}_x^2 f\cdot f+2\,f\cdot g=0, \tag{6b}$$

$$\mathrm{D}_x^4 f\cdot f+2\,f\cdot h=0, \tag{6c}$$

where the Hirota derivatives $\mathrm{D}_x,\mathrm{D}_t$ are defined by[25]

$$\mathrm{D}_x\mathrm{D}_t a(x,t)\cdot b(x,t)=(\partial_x-\partial_{x'})(\partial_t-\partial_{t'})a(x,t)b(x',t')\big|_{x'=x,\ t'=t}.$$

The second bilinear form has $\alpha=-2$ and reads

$$\begin{aligned}&4(5\mathrm{D}_t^2+5\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6)f\cdot f-15\mathrm{D}_x^4 f\cdot g+15\mathrm{D}_x^2 f\cdot h=0,\\ &\mathrm{D}_x^2 f\cdot f+2\,f\cdot g=0,\\ &\mathrm{D}_x^4 f\cdot f+2\,f\cdot h=0.\end{aligned} \tag{7}$$

The derivations of Eqs. (6) and (7), in which $g(x,t)$ and $h(x,t)$ are auxiliary functions, can be found in Ref. 1.

Similarly, with u and f related by Eq. (5), the bSK-Ramani Eq. (3) has precisely two bilinear representations:[1] with $\alpha=-1$, we get

$$(80\mathrm{D}_t^2+20\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6)f\cdot f+30(4\mathrm{D}_x\mathrm{D}_t-\mathrm{D}_x^4)f\cdot g=0, \tag{8a}$$

$$\mathrm{D}_x^2 f\cdot f-2\,f\cdot g=0, \tag{8b}$$

where $g(x,t)$ is again some auxiliary function. On the other hand, when $\alpha=-2$ we obtain the single bilinear equation

$$(5\mathrm{D}_t^2+5\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6)f\cdot f=0, \tag{9}$$

which identifies the bidirectional Sawada–Kotera Eq. (3) with the eponymous Ramani equation.[6] A cursory comparison of the bilinear forms (6) and (8) (with $u=-\partial_x^2\ln f$), and, more particularly, Eqs. (7) and (9) (for which $u=-2\partial_x^2\ln f$), underlines the duality of the bKK and bSK-Ramani equations that is apparent from Eqs. (1) and (3), and will be of some importance to the analysis that follows. [We remark that the choice of transformation (5) and the admissible values $\alpha=-1$ or -2 are no accident, but derive from the deeper structural form of the solutions to Eqs. (1) and (3); see the Appendix and the further comments at the end of this section.]

Obtaining multisoliton solutions of the bSK-Ramani equation is relatively straightforward since we can choose to solve the single (Ramani) bilinear form (9), rather than the coupled system (8a) and (8b). The N-soliton solution of Eq. (9) is given by Hirota's celebrated formula[24]

$$f(x,t)=\sum_{\mu=0,1}\exp\left[\sum_{i=1}^{N}\mu_i\theta_i+\sum_{1\leqslant i<j\leqslant N}\mu_i\mu_j\ln A_{ij}\right], \tag{10}$$

where $\theta_i=p_ix+\omega_it+\eta_i$ $(i=1,\ldots,N)$ and p_i, ω_i, η_i are constant (possibly complex) parameters. In the remainder of this article we will refer to the generic expression (10) as simply the *regular* N-soliton. Significantly, it is described by essentially a single interaction coefficient, A_{ij}, that measures the mutual phase shift following the collision of the ith and jth "solitary" waves. For the bSK-Ramani equation, one easily shows that

$$A_{ij}=-\frac{5(\omega_i-\omega_j)^2+5(\omega_i-\omega_j)(p_i-p_j)^3-(p_i-p_j)^6}{5(\omega_i+\omega_j)^2+5(\omega_i+\omega_j)(p_i+p_j)^3-(p_i+p_j)^6},\quad 1\leqslant i<j\leqslant N, \tag{11}$$

where $\omega_i(p_i)$ is given by the quadratic dispersion law

$$5\omega_i^2+5\omega_ip_i^3-p_i^6=0,\quad i=1,\ldots,N. \tag{12}$$

The explicit N-soliton solution $u(x,t)$ of the bSK-Ramani Eq. (3) is then obtained from (10) and the relation $u=-2\partial_x^2\ln f$: we will say more about this solution later. For now, we note that the solitary wave is given by setting $N=1$ in Eq. (10) and leads to the familiar sech^2 pulse[1]

$$u(x,t)=-\frac{1}{2}\,p^2\,\mathrm{sech}^2\frac{1}{2}(px+\omega t+\eta). \tag{13}$$

For our part, the important feature of this solitary wave is that it propagates either to the left or right with the *same* bell-shaped profile.

For the bKK equation, however, things are not quite so simple. Neither of the two alternative bilinear forms (6) and (7) can be reduced to a single bilinear equation of the type $F(\mathrm{D}_x,\mathrm{D}_t)f\cdot f=0$, akin to Ramani's Eq. (9). We therefore have to solve one or the other of the *coupled* bilinear systems (6) or (7) for which no prescribed solution is available analagous to the Hirota ansatz (10)! In fact, we will later formulate and work with a simpler version of the bilinear form (6); but, for now, we pursue the argument set down in Ref. 1. There we were able to exploit the close connection between the bKK and bSK-Ramani equations and argued as follows: Because the

bilinear forms (8) and (9) of the bSK-Ramani equation are equivalent under the mapping $f^2 \leftrightarrow f$,[1] we can immediately infer that the N-soliton solution of the coupled system (8a) and (8b) is given by *squaring* the regular N-soliton (10). But, then, the duality of the bilinear forms (6) and (8) strongly suggests that the N-soliton solution of the bKK equation will mimic its bSK-Ramani counterpart. Applying this argument to the regular solitary wave [set $N=1$ in (10)], we find that[1]

$$f(x,t)=1+\mathrm{e}^{\theta}+\tfrac{1}{16}a^2\mathrm{e}^{2\theta}, \quad \theta=px+\omega t+\eta, \tag{14}$$

solves Eq. (6) if

$$a^2=\frac{4\omega-p^3}{\omega-p^3} \quad (a>0) \tag{15}$$

and $\omega(p)$ satisfies the (bSK-Ramani) dispersion law [Eq. (12)]

$$5\omega^2+5\omega p^3-p^6=0. \tag{16}$$

Then, using $u=-\partial_x^2 \ln f$, we obtain the ''anomalous'' solitary wave of the bKK Eq. (1),

$$u(x,t)=-ap^2\frac{a+2\cosh\theta}{(a\cosh\theta+2)^2}; \tag{17}$$

this solution was first reported by us in Ref. 1. (The detailed computations, along with the expressions for the auxiliary functions g and h, are given in Ref. 1.) The most compelling feature of the bKK solitary wave (17) is that *its profile depends on the direction of propagation*. The right-traveling solitary wave is a single-humped pulse shown in Fig. 1(a), while the left-going solitary wave has the symmetrical double-humped shape in Fig. 1(b). The left $(-)$ and right $(+)$ running waves are distinguished by solving the dispersion relation (16) for its two (real) roots

$$\omega=-\Omega_{\pm}p^3, \quad \Omega_{\pm}=\frac{1}{2}\left(1\pm\frac{3}{\sqrt{5}}\right), \tag{18}$$

which, in turn, give $a(\Omega_{\pm})=\frac{1}{2}(\sqrt{5}\pm 1)$.

Extending this reasoning to the N-soliton of the bKK Eq. (6), we postulate that it has the structure—though not the exact analytical form—of a *squared* regular soliton (10). We shall exploit this duality argument—which was formulated in Ref. 1 , but used there only to derive the solitary wave (17)—to obtain higher-order soliton solutions of the bKK equation. In short, we elect to solve the coupled bilinear form (6) rather than the alternative Eq. (7). This makes good sense for, as we show in the Appendix, the Hirota ansatz f of Eq. (6) is an *entire* function, whereas that for Eq. (7) is *not* entire.

Before proceeding, there is a further preliminary consideration which will assist our analysis. Were we to employ the bKK bilinear form (6) as it stands—as we did in the previous study[1]—the calculations very soon become prohibitively complex and unwieldy (as the order of the N-soliton increases). The reason for this is simple: just as for the solitary wave,[1] the auxiliary functions g and h in Eqs. (6b) and (6c) turn out to be irreducible quotients [and this makes the subsequent solution of the third bilinear Eq. (6a) extremely difficult, even for lower-order solitons]. More precisely, Eq. (6) is not a ''good'' bilinear form in the sense that g and h are *not* in general entire functions, notwithstanding that the ansatz f is entire (see the Appendix). This suggests that we should first recast the bilinear form (6) so that any auxiliary function is also entire. To this end, we first substitute for g and h from Eqs. (6b) and (6c) into Eq. (6a) to obtain

$$(80\mathrm{D}_t^2+20\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6)f\cdot f+15\mathrm{D}_x^2\left[f\cdot\frac{(4\mathrm{D}_x\mathrm{D}_t-\mathrm{D}_x^4)f\cdot f}{f}\right]=0.$$

We now introduce a ''new'' auxiliary variable $\tilde{g}(x,t)$ so as to obtain the coupled equations

$$(80\mathrm{D}_t^2+20\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6)f\cdot f+30\mathrm{D}_x^2 f\cdot\tilde{g}=0, \tag{19a}$$

$$(4\mathrm{D}_x\mathrm{D}_t-\mathrm{D}_x^4)f\cdot f-2\,f\cdot\tilde{g}=0. \tag{19b}$$

A singularity analysis of the solutions to the bKK Eq. (1) shows that the auxiliary function $\tilde{g}$ in the simplified bilinear form (19) *is* entire. (A brief outline of this Painlevé analysis is presented in the Appendix). Henceforth, we will use this ''good'' bilinear form of the bKK equation in preference to Eq. (6) as it justifies expanding $\tilde{g}$ in terms of exponentials [Eq. (27)] and leads to considerable computational simplification. The similarity of the bilinear forms (8) and (19) is striking, and provides further evidence of the duality between the bSK-Ramani and bKK equations.

III. TWO-SOLITON SOLUTION OF THE BIDIRECTIONAL KAUP–KUPERSHMIDT EQUATION

To generate the regular two-soliton solution of the bSK-Ramani equation, Eq. (9), we set $N=2$ in Eqs. (10)–(12): this gives

$$f(x,t)=1+\mathrm{e}^{\theta_1}+\mathrm{e}^{\theta_2}+A_{12}\mathrm{e}^{\theta_1+\theta_2},\quad \theta_i=p_ix+\omega_it+\eta_i,\quad i=1,2, \tag{20}$$

with ω_i satisfying the the dispersion law (12) and

$$A_{12}=-\frac{5(\omega_1-\omega_2)^2+5(\omega_1-\omega_2)(p_1-p_2)^3-(p_1-p_2)^6}{5(\omega_1+\omega_2)^2+5(\omega_1+\omega_2)(p_1+p_2)^3-(p_1+p_2)^6}. \tag{21}$$

The two-soliton solution of the bSK-Ramani Eq. (3) is then obtained via the relation $u=-2\partial_x^2\ln f$. Now, following our argument in Sec. II, the two-soliton solution of the bKK Eq. (19) mimics the structure of f^2. Accordingly, we seek a two-soliton solution of the bilinear equations (19a) and (19b) in the form

$$f(x,t)=1+\mathrm{e}^{\theta_1}+\mathrm{e}^{\theta_2}+\alpha_1\mathrm{e}^{2\theta_1}+\alpha_2\mathrm{e}^{2\theta_2}+b_{12}\mathrm{e}^{\theta_1+\theta_2}+c_1\mathrm{e}^{2\theta_1+\theta_2}+c_2\mathrm{e}^{\theta_1+2\theta_2}+B\mathrm{e}^{2(\theta_1+\theta_2)}, \tag{22}$$

where $\theta_i=p_ix+\omega_it+\eta_i$, $i=1,2$, and α_1, α_2, b_{12}, c_1, c_2 and B are constants. The expression (22) warrants further comment: to begin with, it has been *normalized* by setting the coefficients of the terms e^{θ_1} and e^{θ_2} to unity (which is always possible since η_1, η_2 are arbitrary). Further, f must be a symmetrical function of the two phase variables θ_1 and θ_2. This means that, in effect, there are just four unknown coefficients which are either symmetrical (b_{12},B) or invertible (α_i,c_i) under the transformation $(p_1,\omega_1)\leftrightarrow(p_2,\omega_2)$.

Although we could proceed to solve Eqs. (19a) and (19b) with f given by (22), some further simplification is possible. Since the bKK Eq. (1) is deemed to be completely integrable,[1] its soliton solutions should exhibit the characteristic ''elastic'' interaction property of colliding solitary waves.[21,22] If we apply this principle to (22)—which (asymptotically) separates into a pair of ''solitary'' waves—and compare the results to the bKK solitary wave (14), we find that

$$f(x,t)=1+\mathrm{e}^{\theta_1}+\mathrm{e}^{\theta_2}+\frac{1}{16}a_1^2\mathrm{e}^{2\theta_1}+\frac{1}{16}a_2^2\mathrm{e}^{2\theta_2}+b_{12}\mathrm{e}^{\theta_1+\theta_2}+\frac{A}{16}(a_1^2\mathrm{e}^{2\theta_1+\theta_2}+a_2^2\mathrm{e}^{\theta_1+2\theta_2})$$
$$+\left(\frac{A}{16}\right)^2 a_1^2a_2^2\mathrm{e}^{2(\theta_1+\theta_2)}, \tag{23}$$

where [cf. Eq. (15)]

$$a_i^2=\frac{4\omega_i-p_i^3}{\omega_i-p_i^3},\quad i=1,2, \tag{24}$$

and ω_i satisfies the (bSK-Ramani) dispersion law (12). The parameter "A" in Eq. (23) arises quite naturally in the asymptotic analysis as a measure of the post-interaction phase shifts. It therefore plays the same role in the putative bKK two-soliton (23) as the interaction coefficient "A_{12}" in the bSK-Ramani two-soliton (20). Thus, it only remains to determine the unknown parameters b_{12} and A in Eq. (23).

To proceed, we shall make use of the fundamental result[25]

$$F(\mathrm{D}_x,\mathrm{D}_t)\mathrm{e}^{\theta_1}\cdot\mathrm{e}^{\theta_2}=F(\mathbf{p}_1-\mathbf{p}_2)\mathrm{e}^{\theta_1+\theta_2},\quad \theta_i=p_ix+\omega_it+\eta_i,\quad i=1,2, \tag{25}$$

where $F(\mathrm{D}_x,\mathrm{D}_t)$is a general bilinear operator, and we write $F(\mathbf{p})=F(p,\omega)$. Then, with f given by Eq. (23), it is straightforward to show that

$$\begin{aligned}
F(\mathrm{D}_x,\mathrm{D}_t)f\cdot f=2\Bigg\{&F(\mathbf{p}_1)\mathrm{e}^{\theta_1}+F(\mathbf{p}_2)\mathrm{e}^{\theta_2}+\frac{1}{16}a_1^2F(2\mathbf{p}_1)\mathrm{e}^{2\theta_1}+\frac{1}{16}a_2^2F(2\mathbf{p}_2)\mathrm{e}^{2\theta_2}+[b_{12}F(\mathbf{p}_1+\mathbf{p}_2)\\
&+F(\mathbf{p}_1-\mathbf{p}_2)]\mathrm{e}^{\theta_1+\theta_2}+\left[\frac{1}{16}a_1^2[AF(2\mathbf{p}_1+\mathbf{p}_2)+F(2\mathbf{p}_1-\mathbf{p}_2)]+b_{12}F(\mathbf{p}_2)\right]\mathrm{e}^{2\theta_1+\theta_2}\\
&+\left[\frac{1}{16}a_2^2[AF(\mathbf{p}_1+2\mathbf{p}_2)+F(\mathbf{p}_1-2\mathbf{p}_2)]+b_{12}F(\mathbf{p}_1)\right]\mathrm{e}^{\theta_1+2\theta_2}+\frac{1}{16}a_1^2F(\mathbf{p}_1)\mathrm{e}^{3\theta_1}\\
&+\frac{1}{16}a_2^2F(\mathbf{p}_2)\mathrm{e}^{3\theta_2}+\left[\frac{1}{16}A[a_1^2F(2\mathbf{p}_1)+a_2^2F(2\mathbf{p}_2)]+\frac{1}{16^2}a_1^2a_2^2[A^2F(2\mathbf{p}_1+2\mathbf{p}_2)\right.\\
&\left.+F(2\mathbf{p}_1-2\mathbf{p}_2)]\right]\mathrm{e}^{2(\theta_1+\theta_2)}+\frac{1}{16}[AF(\mathbf{p}_1+\mathbf{p}_2)+b_{12}F(\mathbf{p}_1-\mathbf{p}_2)]\\
&\times(a_1^2\mathrm{e}^{3\theta_1+\theta_2}+a_2^2\mathrm{e}^{\theta_1+3\theta_2})+\frac{1}{16^2}a_1^4AF(\mathbf{p}_2)\mathrm{e}^{4\theta_1+\theta_2}+\frac{1}{16^2}a_2^4AF(\mathbf{p}_1)\mathrm{e}^{\theta_1+4\theta_2}\\
&+\frac{1}{16}a_1^2A\left[\frac{1}{16}a_2^2[AF(\mathbf{p}_1+2\mathbf{p}_2)+F(\mathbf{p}_1-2\mathbf{p}_2)]+b_{12}F(\mathbf{p}_1)\right]\mathrm{e}^{3\theta_1+2\theta_2}\\
&+\frac{1}{16}a_2^2A\left[\frac{1}{16}a_1^2[AF(2\mathbf{p}_1+\mathbf{p}_2)+F(2\mathbf{p}_1-\mathbf{p}_2)]+b_{12}F(\mathbf{p}_2)\right]\mathrm{e}^{2\theta_1+3\theta_2}\\
&+\frac{1}{16^3}a_1^2a_2^2A^2[a_1^2F(2\mathbf{p}_2)\mathrm{e}^{4\theta_1+2\theta_2}+a_2^2F(2\mathbf{p}_1)\mathrm{e}^{2\theta_1+4\theta_2}]\\
&+\frac{1}{16^2}a_1^2a_2^2A^2[b_{12}F(\mathbf{p}_1+\mathbf{p}_2)+F(\mathbf{p}_1-\mathbf{p}_2)]\mathrm{e}^{3(\theta_1+\theta_2)}\\
&+\frac{1}{16^3}a_1^2a_2^2A^3[a_1^2F(\mathbf{p}_2)\mathrm{e}^{4\theta_1+3\theta_2}+a_2^2F(\mathbf{p}_1)\mathrm{e}^{3\theta_1+4\theta_2}]\Bigg\}
\end{aligned} \tag{26}$$

whenever the bilinear operator F is even and $F(\mathbf{0})=0$. With the aid of (26), we are now in a position to solve the bKK bilinear form (19).

We begin by rewriting Eq. (19b) as $F_2f\cdot f=2\,f\tilde{g}$, with $F_2(\mathrm{D}_x,\mathrm{D}_t)=4\mathrm{D}_x\mathrm{D}_t-\mathrm{D}_x^4$. Now, in view of (23) and (26)—and recalling that $\tilde{g}$ is *entire*—the left and right sides of this equation will be consistent if the auxiliary function $\tilde{g}$ has the form

$$\tilde{g}=\beta_1\mathrm{e}^{\theta_1}+\beta_2\,\mathrm{e}^{\theta_2}+\mu\,\mathrm{e}^{\theta_1+\theta_2}+\nu_1\mathrm{e}^{2\theta_1+\theta_2}+\nu_2\,\mathrm{e}^{\theta_1+2\theta_2} \tag{27}$$

for some constants β_1, β_2, μ, ν_1, ν_2 [with the implied symmetry in $\mathbf{p}_1=(p_1,\omega_1)$ and $\mathbf{p}_2=(p_2,\omega_2)$]. Substituting (23), (26) (with $F\to F_2$) and (27) into Eq. (19b), and equating terms on both sides, we obtain

$$\beta_i=F_2(\mathbf{p}_i)=p_i(4\omega_i-p_i^3), \tag{28a}$$

$$\nu_1=\frac{1}{16}\,a_1^2\beta_2 A, \tag{28b}$$

$$\nu_2=\frac{1}{16}\,a_2^2\beta_1 A, \tag{28c}$$

and

$$\mu+\beta_1+\beta_2=b_{12}F_2(\mathbf{p}_1+\mathbf{p}_2)+F_2(\mathbf{p}_1-\mathbf{p}_2), \tag{29a}$$

$$\mu+A(\beta_1+\beta_2)=A\,F_2(\mathbf{p}_1+\mathbf{p}_2)+b_{12}F_2(\mathbf{p}_1-\mathbf{p}_2), \tag{29b}$$

$$\mu+\frac{1}{16}\,a_1^2\beta_2(A+1)=\frac{1}{16}\,a_1^2[AF_2(2\mathbf{p}_1+\mathbf{p}_2)+F_2(2\mathbf{p}_1-\mathbf{p}_2)]-b_{12}(\beta_1-\beta_2), \tag{29c}$$

$$\mu+\frac{1}{16}\,a_2^2\beta_1(A+1)=\frac{1}{16}\,a_2^2[AF_2(\mathbf{p}_1+2\mathbf{p}_2)+F_2(\mathbf{p}_1-2\mathbf{p}_2)]+b_{12}(\beta_1-\beta_2), \tag{29d}$$

$$\mu b_{12}+\frac{1}{8}\,A(a_1^2\beta_2+a_2^2\beta_1)=\frac{1}{16^2}\,a_1^2a_2^2[A^2F_2(2\mathbf{p}_1+2\mathbf{p}_2)+F_2(2\mathbf{p}_1-2\mathbf{p}_2)]+A(\beta_1+\beta_2), \tag{29e}$$

where a_i^2, $i=1,2$, is given in Eq. (24). Equations (29a)–(29e) are an overdetermining set of equations for the unknowns A, b_{12}, and μ which bear comparison with the corresponding set of equations obtained in[11] for the KK Eq. (2). However, rather than solve these equations directly and, at the same time, ensure their compatibility—which was the path taken in Ref. 11—we will follow a different route here and consider next the bilinear equation (19a).

We substitute for f and $\tilde{g}$, Eqs. (23) and (27), into (19a) and once again use the basic results (25) (with $F=\mathrm{D}_x^2$) and (26) with $F\to F_1=80\mathrm{D}_t^2+20\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6$. This yields the further set of equations [the routine calculations—which additionally make use of the dispersion relations (12)—are omitted]

$$b_{12}F_1(\mathbf{p}_1+\mathbf{p}_2)+F_1(\mathbf{p}_1-\mathbf{p}_2)+15[\mu(p_1+p_2)^2+(\beta_1+\beta_2)(p_1-p_2)^2]=0, \tag{30a}$$

$$AF_1(\mathbf{p}_1+\mathbf{p}_2)+b_{12}F_1(\mathbf{p}_1-\mathbf{p}_2)+15[\mu(p_1-p_2)^2+A(\beta_1+\beta_2)(p_1+p_2)^2]=0, \tag{30b}$$

$$\begin{aligned}&\frac{1}{16}\,a_1^2[AF_1(2\mathbf{p}_1+\mathbf{p}_2)+F_1(2\mathbf{p}_1-\mathbf{p}_2)]+15b_{12}p_2^2(\beta_1-\beta_2)\\&\quad+15\left[\mu p_2^2+\frac{1}{16}\,a_1^2\beta_2[A(2p_1+p_2)^2+(2p_1-p_2)^2]\right]=0,\end{aligned} \tag{30c}$$

$$\begin{aligned}&\frac{1}{16}\,a_2^2[AF_1(\mathbf{p}_1+2\mathbf{p}_2)+F_1(\mathbf{p}_1-2\mathbf{p}_2)]-15b_{12}p_1^2(\beta_1-\beta_2)\\&\quad+15\left[\mu p_1^2+\frac{1}{16}\,a_2^2\beta_1[A(p_1+2p_2)^2+(p_1-2p_2)^2]\right]=0,\end{aligned} \tag{30d}$$

$$\frac{1}{16^2}a_1^2a_2^2[A^2F_1(2\mathbf{p}_1+2\mathbf{p}_2)+F_1(2\mathbf{p}_1-2\mathbf{p}_2)]+\frac{15}{2}A(a_1^2\beta_2p_1^2+a_2^2\beta_1p_2^2)=0. \tag{30e}$$

We notice that these last equations bear more than a passing resemblance to Eqs. (29a)–(29e). Ostensibly, we have ten equations for just three unknowns—they should therefore conceal a large measure of redundancy. For example, it is evident that Eqs. (29c) and (29d)—and, similarly, Eqs. (30c) and (30d)—are essentially the same equation under the symmetry requirement $\mathbf{p}_1\leftrightarrow\mathbf{p}_2$. To make further progress, we need some additional notation and results.

The key to solving the bKK equation is its duality with the bSK-Ramani equation: this intimacy is already apparent through the shared dispersion law (12) (both for the solitary wave[1] and now the two-soliton solution). To reinforce this connection, we introduce the bSK-Ramani (strictly Ramani) bilinear operator [see Eq. (9)]

$$F_{\mathrm{R}}(\mathrm{D}_x,\mathrm{D}_t)=5\mathrm{D}_t^2+5\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6, \tag{31}$$

so that the dispersion law (12) reads $F_{\mathrm{R}}(\mathbf{p}_i)=0$. The equally important interaction coefficient A_{ij}, Eq. (11), can now be written as

$$A_{ij}=-\frac{F_{\mathrm{R}}(\mathbf{p}_i-\mathbf{p}_j)}{F_{\mathrm{R}}(\mathbf{p}_i+\mathbf{p}_j)}=-\frac{D_{ij}^-}{D_{ij}},\quad 1\leqslant i<j\leqslant N, \tag{32}$$

where $D_{ij}^-(\mathbf{p}_i,\mathbf{p}_j)=D_{ij}(\mathbf{p}_i,-\mathbf{p}_j)$ and

$$D_{ij}(\mathbf{p}_i,\mathbf{p}_j)=F_{\mathrm{R}}(\mathbf{p}_i+\mathbf{p}_j)=5(\omega_i+\omega_j)^2+5(\omega_i+\omega_j)(p_i+p_j)^3-(p_i+p_j)^6. \tag{33}$$

However, with the help of the dispersion law (12), we may recast D_{ij} as

$$\begin{aligned}D_{ij}=&10\omega_i\omega_j+5\omega_ip_j(3p_i^2+3p_ip_j+p_j^2)+5\omega_jp_i(p_i^2+3p_ip_j+3p_j^2)-p_ip_j(6p_i^4+15p_i^3p_j\\&+20p_i^2p_j^2+15p_ip_j^3+6p_j^4).\end{aligned} \tag{34}$$

The dispersion relation (12)—which here effects the replacement of the terms ω_i^2 in (33)—will become indispensable to our development as it will be used repeatedly to remove powers of ω_i.

Now, since the wave numbers $p_i(i=1,2)$are entirely arbitrary—and bearing in mind the dispersion formula (18)—all our equations must remain valid under the parity transformation $\mathbf{p}_i\rightarrow-\mathbf{p}_i$. But, if we let $\mathbf{p}_2\rightarrow-\mathbf{p}_2$ in Eqs. (29a) and (30a), and combine the resulting equations with (29b) and (30b), then we readily deduce the following useful transformations:

$$\left.\begin{aligned}A&\rightarrow\frac{1}{A},&(35a)\\ b_{12}&\rightarrow\frac{1}{A}b_{12},&(35b)\\ \mu&\rightarrow\frac{1}{A}\mu,&(35c)\end{aligned}\right\}\quad\text{if}\quad\mathbf{p}_2\rightarrow-\mathbf{p}_2.$$

One immediate consequence of these results is to show that Eqs. (29a) and (29b), and also (30a) and (30b), are equivalent. This means that we have effectively reduced each of the systems (29a)–(29e) and (30a)–(30e) to three equations. We could, of course, elect to solve one of these two sets of equations for A, b_{12} and μ, and then ensure the compatibility of the other set (the approach, incidentally, adopted in Ref. 11). However, as our intention is to solve these equations as efficiently as posssible, we will solve Eqs. (29) and (30) simultaneously. Before doing so, we wish to emphasize our use of the vector argument $(\mathbf{p}_1,\mathbf{p}_2)$ for all parameters: this is essential if we are to capture the bidirectionality of the solutions that stems from the choice of ω in Eq. (18).

Eliminating μ between Eqs. (29a) and (30a), we get

$$b_{12}=\frac{60p_1p_2(\beta_1+\beta_2)-[F_1(\mathbf{p}_1-\mathbf{p}_2)+15(p_1+p_2)^2F_2(\mathbf{p}_1-\mathbf{p}_2)]}{[F_1(\mathbf{p}_1+\mathbf{p}_2)+15(p_1+p_2)^2F_2(\mathbf{p}_1+\mathbf{p}_2)]}.$$

But, if we substitute for β_i from (28a)—and note the identity $F_1(\mathbf{p})+15p^2F_2(\mathbf{p})=16F_{\mathrm{R}}(\mathbf{p})$—then we obtain the compact result

$$b_{12}=\frac{\Delta_{12}}{2D_{12}}, \tag{36}$$

where

$$\Delta_{12}=20\omega_1\omega_2+10\omega_1p_2(3p_1^2+p_2^2)+10\omega_2p_1(p_1^2+3p_2^2)-p_1p_2(12p_1^4-5p_1^2p_2^2+12p_2^4) \tag{37}$$

and D_{12} is defined in Eq. (33). The similarity between Δ_{12} and D_{12}, Eq. (34), is striking. Both are homogeneous polynomials in p_1,p_2 of total degree six [since $\omega_i\propto p_i^3$; see Eq. (18)], which implies that b_{12} is a parameter of, effectively, degree zero. The key difference is that the numerator Δ_{12} is of *odd* degree in each of the wave numbers p_i, so that $\Delta_{12}(\mathbf{p}_1,-\mathbf{p}_2)=-\Delta_{12}(\mathbf{p}_1,\mathbf{p}_2)$. Combining this with the parity transformation for b_{12}, Eq. (35b), and Eq. (36), yields [by way of Eq. (32)]

$$A=\frac{b_{12}(\mathbf{p}_1,\mathbf{p}_2)}{b_{12}(\mathbf{p}_1,-\mathbf{p}_2)}=-\frac{D_{12}^-}{D_{12}}=A_{12}. \tag{38}$$

Although it is not needed to compute f, Eq. (23), for completeness, we easily calculate the remaining unknown quantity μ: using Eqs. (28a), (29a) and (36), we find that

$$\mu=\frac{C_{12}}{2D_{12}},\quad C_{12}=\Delta_{12}F_2(\mathbf{p}_1+\mathbf{p}_2)+2D_{12}[F_2(\mathbf{p}_1-\mathbf{p}_2)-F_2(\mathbf{p}_1)-F_2(\mathbf{p}_2)]. \tag{39}$$

The numerator C_{12} is readily expanded in terms of p_1, p_2 and is (homogeneous) of total degree ten (so that μ has net degree four). Bearing in mind our earlier comments, it only remains to check that Eqs. (29c), (29e), (30c) and (30e) are satisfied identically. This is a routine exercise, although, in view of the lengthy expressions involved, it is best carried out using a symbolic manipulation program (we used Mathematica).

Combining these results with Eq. (23), we finally obtain the solution of the bKK bilinear form (19a) and (19b),

$$f(x,t)=1+\mathrm{e}^{\theta_1}+\mathrm{e}^{\theta_2}+\frac{1}{16}a_1^2\mathrm{e}^{2\theta_1}+\frac{1}{16}a_2^2\mathrm{e}^{2\theta_2}+b_{12}\mathrm{e}^{\theta_1+\theta_2}+\frac{A_{12}}{16}(a_1^2\mathrm{e}^{2\theta_1+\theta_2}+a_2^2\mathrm{e}^{\theta_1+2\theta_2})$$
$$+\left(\frac{A_{12}}{16}\right)^2a_1^2a_2^2\mathrm{e}^{2(\theta_1+\theta_2)}, \tag{40}$$

with the auxiliary function $\tilde{g}$ given by inserting (28a)–(28c), (38) and (39) into (27). The explicit two-soliton solution $u(x,t)$ of the bKK Eq. (1) follows immediately from (40) and the relation $u=-\partial_x^2\ln f$ [Eq. (5) with $\alpha=-1$]. Figures 2–4 illustrate various two-soliton interactions [where here, and in all subsequent figures, we graph the physical wave $-u(x,t)$]. Figure 2 pictures a two-soliton comprising a pair of double-humped ''solitary'' waves propagating to the left: typically, it shows the taller, faster pulse catching and then colliding with the shorter, slower solitary wave, only for each wave to emerge unscathed from the interaction (except for a phase shift). Figure 3 shows perhaps the most interesting of the bKK two-soliton interactions, the head-on collision of a pair of counter-propagating ''solitary'' waves. Here, we illustrate the case in which the right-going single-peaked pulse is taller than the left-running twin-peaked wave. Figure 4 is a perspective view (in time) of the same two-soliton solutions in which the phase shifts are clearly visible.

It is important to emphasize the difference between the two-soliton solutions of the bKK and bSK-Ramani equations. The bKK two-soliton is *directionally dependent*, a property that it inherits from the solitary wave (17). This means that there are *three* quite distinct versions of this two-

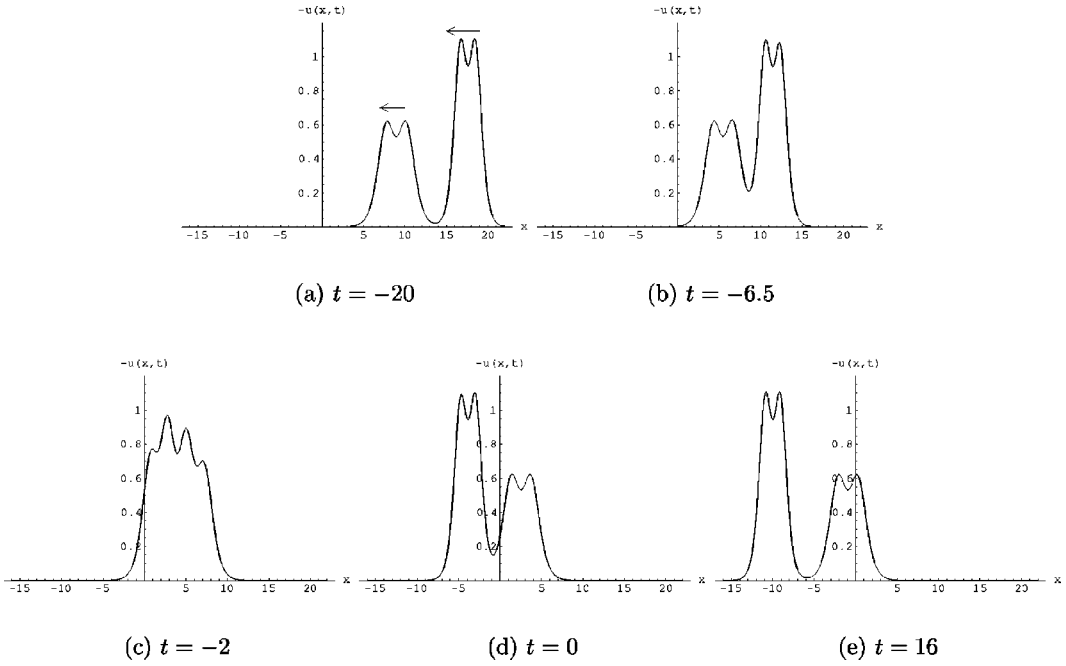

FIG. 2. A two-soliton solution of the bKK equation comprising two left-traveling double-humped solitary waves: $p_1=1.5$, $p_2=2.0$.

soliton interaction. On the other hand, the bSK-Ramani solitary wave (13) has the same sech^2 profile irrespective of its direction of travel. Consequently, the bSK-Ramani equation admits only *two* variants of the two-soliton solution because those comprised of two left-running or two right-running solitary waves are essentially mirror images of one another. To our knowledge, the

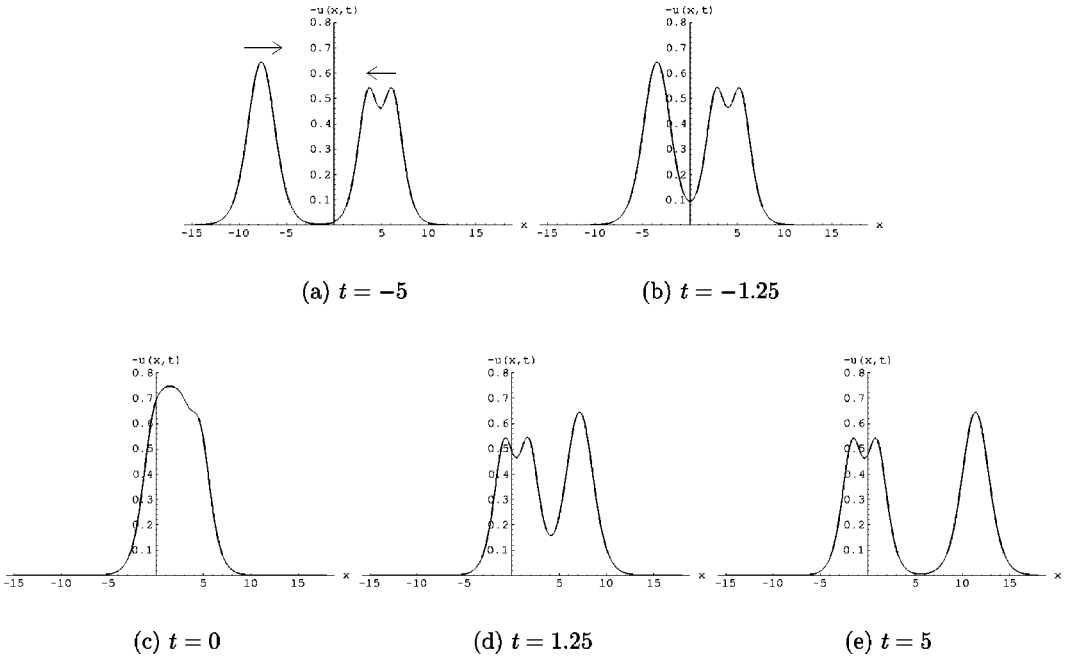

FIG. 3. A bKK two-soliton solution showing the head-on collision of a right-going single-peaked solitary wave ($p_1=1.2$) and a left-running double-peaked pulse ($p_2=1.4$).

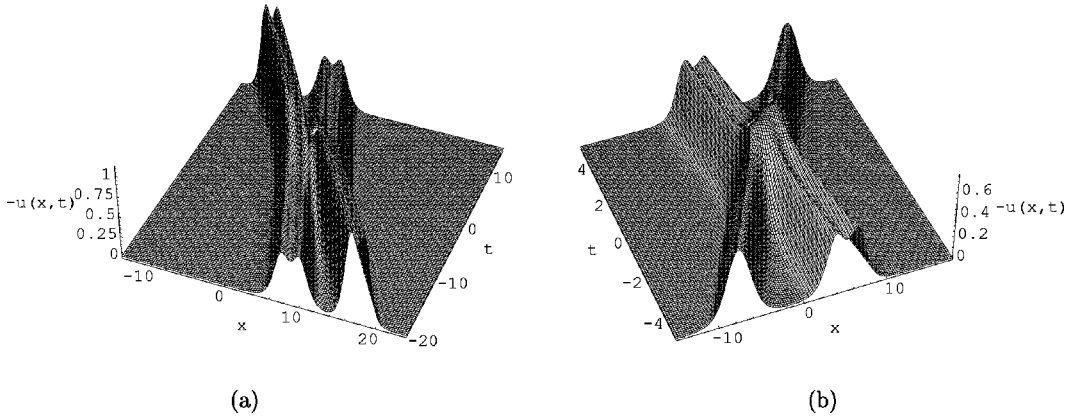

FIG. 4. Perspective views of the bKK two-soliton: (a) the interaction of two left-traveling twin-peaked solitary waves ($p_1=1.5,\ p_2=2.0$), (b) the head-on collision of a single-humped ($p_2=1.2$) and double-humped pulse ($p_2=1.4$).

directional dependence that is exhibited here by the bKK two-soliton solution has not been observed before now, and sets it apart from previously known multisoliton interactions.

The expression for f, Eq. (40), deserves further scrutiny. Equation (38) shows that the bKK and bSK-Ramani two-solitons have a common interaction coefficient, A_{12}, which underlines the duality between the equations. Thus, in spite of appearances, the solutions (20) and (40) share the same wave dynamics; in particular, their colliding solitary waves undergo identical phase shifts after separation that are completely determined by A_{12}, Eq. (21). Another notable feature of (40) is the additional parameter b_{12}, Eq. (36), that is required to formulate f explicitly (although, unlike A_{12}, it would appear to have no obvious dynamical interpretation). We stress that b_{12} is a "new" parameter in the sense that it cannot be expressed solely in terms of A_{12} [cf. the bSK-Ramani two-soliton solution (20)]. Furthermore, b_{12} is given in Eq. (36) in its simplest possible form; even so, this expression is far more complicated than its counterpart for the two-soliton of the unidirectional KK Eq. (2) (see Ref. 11). Finally, if one uses Eqs. (35a) and (35b) (with $A \to A_{12}$), it is easy to show that the two-soliton solution $u(x,t)$ is invariant under the parity transformation $\mathbf{p}_i \to -\mathbf{p}_i$ $(i=1,2)$. It follows that, without loss of generality, we need only consider wave numbers $p_i>0$.

Before we continue, it is instructive to examine the key parameter b_{12} a little more carefully. In view of the duality argument that led to the putative bKK two-soliton (22), we might conjecture that b_{12} will mimic the corresponding coefficient (of $e^{\theta_1+\theta_2}$) in the squared regular two-soliton solution of the bSK-Ramani equation. This is, in fact, the case: squaring f in Eq. (20), and normalizing, leads to

$$b_{12}^{\mathrm{R}}=\frac{1}{2}(A_{12}+1)=\frac{\Delta_{12}^{\mathrm{R}}}{2D_{12}},$$

with

$$\Delta_{12}^{\mathrm{R}}=20\omega_1\omega_2+10\omega_1 p_2(3p_1^2+p_2^2)+10\omega_2 p_1(p_1^2+3p_2^2)-p_1p_2(12p_1^4+40p_1^2p_2^2+12p_2^4).$$

Hence, the parameter b_{12} differs from b_{12}^{R} in just the $p_1^3p_2^3$ term of its numerator Δ_{12}, Eq. (37). With hindsight, we may extend the duality argument—which at present provides only the general structure of the bKK solitons—to include a more precise formulation of this key coefficient. This further insight will prove helpful when we seek bKK solitons of higher order.

IV. FURTHER SOLITON SOLUTIONS OF THE BIDIRECTIONAL KAUP–KUPERSHMIDT EQUATION

It is apparent from the results of the preceding section that we cannot write down the explicit three-soliton solution of the bKK equation—much less any higher-order solitons—based on prior knowledge of the two-soliton (40). For, unlike the (regular) N-soliton solution of the bSK-Ramani equation—which depends on a single generic parameter and is entirely predictable [Eqs. (10)–(12)]—we can expect its bKK counterpart to include an additional parameter (akin to b_{12}) at every order N. [Coincidentally, this is analogous to the structure that was found for the N-soliton solution of the related KK Eq. (2).[11]] The remainder of this study is bound up with computing this extra parameter.

A. The three-soliton solution

Our starting point is the regular three-soliton [put $N=3$ in Eq. (10)] which, after squaring and normalizing, yields the putative three-soliton solution of the bKK equation

$$\begin{aligned} f(x,t) = 1 &+ e^{\theta_1} + e^{\theta_2} + e^{\theta_3} + \frac{1}{16}(a_1^2 e^{2\theta_1} + a_2^2 e^{2\theta_2} + a_3^2 e^{2\theta_3}) + b_1 e^{\theta_1+\theta_2} + b_2 e^{\theta_1+\theta_3} + b_3 e^{\theta_2+\theta_3} \\ &+ c_1 e^{2\theta_1+\theta_2} + c_2 e^{\theta_1+2\theta_2} + c_3 e^{2\theta_1+\theta_3} + c_4 e^{\theta_1+2\theta_3} + c_5 e^{2\theta_2+\theta_3} + c_6 e^{\theta_2+2\theta_3} + b_{123} e^{\theta_1+\theta_2+\theta_3} \\ &+ d_1 e^{2(\theta_1+\theta_2)} + d_2 e^{2(\theta_1+\theta_3)} + d_3 e^{2(\theta_2+\theta_3)} + k_1 e^{2\theta_1+\theta_2+\theta_3} + k_2 e^{\theta_1+2\theta_2+\theta_3} + k_3 e^{\theta_1+\theta_2+2\theta_3} \\ &+ m_1 e^{2(\theta_1+\theta_2)+\theta_3} + m_2 e^{2\theta_1+\theta_2+2\theta_3} + m_3 e^{\theta_1+2(\theta_2+\theta_3)} + K e^{2(\theta_1+\theta_2+\theta_3)}, \end{aligned} \tag{41}$$

in which the undetermined coefficients are consonant with the symmetry in the phase variables $\theta_i = p_i x + \omega_i t + \eta_i$, $i=1, 2, 3$. Once again, we have used the requirement that (41) separates (asymptotically) into three "solitary" waves to fix the coefficients of the terms $e^{2\theta_i}$ and the dispersion laws $\omega_i(p_i)$, Eq. (12).

There are two ways we can proceed. We could attempt to solve the coupled bilinear form (19a) and (19b) for the auxiliary variable $\tilde{g}$ and the unknown coefficients in (41), just as we did for the two-soliton solution in the previous section. But this avenue will more than likely involve some extremely lengthy, possibly intractable, algebraic computation (and almost certainly prove impossible for higher-order solitons); moreover, we do not need $\tilde{g}$ in order to compute $u(x,t)$. Instead, we adopt the alternative route which proceeds by iteration on the solitons of lower order [a technique that was first presented in Ref. 11 to solve the related KK Eq. (2)]. Thus, after reducing f to a two-soliton solution—which arises (asymptotically as $t \to \pm\infty$) when the third solitary wave is well-separated from the remaining two—and comparing the results to the bKK two-soliton (40), the three-soliton (41) becomes

$$\begin{aligned} f = 1 &+ \sum_{i=1}^{3} e^{\theta_i} + \frac{1}{16}\sum_{i=1}^{3} a_i^2 e^{2\theta_i} + \sum_{1\leqslant i<j\leqslant 3} b_{ij} e^{\theta_i+\theta_j} + \frac{1}{16}\sum_{1\leqslant i<j\leqslant 3} A_{ij}(a_i^2 e^{2\theta_i+\theta_j} + a_j^2 e^{\theta_i+2\theta_j}) \\ &+ b_{123} e^{\theta_1+\theta_2+\theta_3} + \frac{1}{16^2}\sum_{1\leqslant i<j\leqslant 3} a_i^2 a_j^2 A_{ij}^2 e^{2(\theta_i+\theta_j)} + \frac{1}{16}[a_1^2 b_{23} A_{12} A_{13} e^{2\theta_1+\theta_2+\theta_3} \\ &+ a_2^2 b_{13} A_{12} A_{23} e^{\theta_1+2\theta_2+\theta_3} + a_3^2 b_{12} A_{13} A_{23} e^{\theta_1+\theta_2+2\theta_3}] + \frac{1}{16^2} A_{12} A_{13} A_{23}[a_1^2 a_2^2 A_{12} e^{2(\theta_1+\theta_2)+\theta_3} \\ &+ a_1^2 a_3^2 A_{13} e^{2\theta_1+\theta_2+2\theta_3} + a_2^2 a_3^2 A_{23} e^{\theta_1+2(\theta_2+\theta_3)}] + \frac{1}{16^3} a_1^2 a_2^2 a_3^2 A_{12}^2 A_{13}^2 A_{23}^2 e^{2(\theta_1+\theta_2+\theta_3)}, \end{aligned} \tag{42}$$

in which all but one of the coefficients have been determined [and b_{13}, b_{23} generalize b_{12}, Eq. (36), in the obvious way]. The remaining unknown coefficient b_{123} is a "new" parameter that cannot be found by reducing f to a lower-order soliton. Nevertheless, we are still able to deduce three useful reductions of b_{123} in this way:

$$b_{123}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{0})=b_{12}(\mathbf{p}_1,\mathbf{p}_2), \tag{43a}$$

$$b_{123}(\mathbf{p}_1,\mathbf{0},\mathbf{0})=b_{23}(\mathbf{0},\mathbf{0}), \tag{43b}$$

$$b_{123}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_2)=\frac{1}{18}a_2^2A_{12}. \tag{43c}$$

Some care is required when using the first two reductions which must be interpreted in the limiting sense $\mathbf{p}_i=(p_i,\omega_i)\to\mathbf{0}$.

We now invoke the further premise that the parameter b_{123} will mimic its counterpart b_{123}^{R} in the three-soliton solution of the bSK-Ramani equation. After squaring and normalizing the regular three-soliton, Eq. (10), and extracting the coefficient of $\mathrm{e}^{\theta_1+\theta_2+\theta_3}$, we discover that

$$b_{123}^{\mathrm{R}}=\frac{1}{4}(A_{12}A_{13}A_{23}+A_{12}+A_{13}+A_{23})=\frac{\Delta_{123}^{\mathrm{R}}}{4D_{12}D_{13}D_{23}} \tag{44}$$

with

$$\begin{aligned}\Delta_{123}^{\mathrm{R}}=&-108[18\langle\langle p_i^{10}p_j^6p_k^2\rangle\rangle+60\langle\langle p_i^{10}p_j^4p_k^4\rangle\rangle+30\langle\langle p_i^8p_j^8p_k^2\rangle\rangle-20\langle\langle p_i^8p_j^6p_k^4\rangle\rangle+72\,p_1^6p_2^6p_3^6\\&-90\langle\langle\omega_ip_i^7p_j^6p_k^2\rangle\rangle-75\langle\langle\omega_ip_i^5p_j^8p_k^2\rangle\rangle-45\langle\langle\omega_ip_i^3p_j^{10}p_k^2\rangle\rangle-300\langle\langle\omega_ip_i^7p_j^4p_k^4\rangle\rangle-10\langle\langle\omega_ip_i^5p_j^6p_k^4\rangle\rangle\\&+50\langle\langle\omega_ip_i^3p_j^8p_k^4\rangle\rangle+60\langle\langle\omega_ip_i^3p_j^6p_k^6\rangle\rangle-15\langle\langle\omega_ip_ip_j^{10}p_k^4\rangle\rangle-25\langle\langle\omega_ip_ip_j^8p_k^6\rangle\rangle+225\langle\langle\omega_i\omega_jp_i^7p_j^3p_k^2\rangle\rangle\\&+75\langle\langle\omega_i\omega_jp_i^7p_jp_k^4\rangle\rangle+120\langle\langle\omega_i\omega_jp_i^5p_j^5p_k^2\rangle\rangle-200\langle\langle\omega_i\omega_jp_i^5p_j^3p_k^4\rangle\rangle+55\langle\langle\omega_i\omega_jp_i^5p_jp_k^6\rangle\rangle\\&-300\langle\langle\omega_i\omega_jp_i^3p_j^3p_k^6\rangle\rangle-50\langle\langle\omega_i\omega_jp_i^3p_jp_k^8\rangle\rangle-30\langle\langle\omega_i\omega_jp_ip_jp_k^{10}\rangle\rangle+150\langle\langle\omega_i\omega_j\omega_kp_i^7p_jp_k\rangle\rangle\\&+200\langle\langle\omega_i\omega_j\omega_kp_i^5p_j^3p_k\rangle\rangle].\end{aligned} \tag{45}$$

The symbol $\langle\langle\ \rangle\rangle$ in (45) denotes the sum over all distinct permutations of (1,2,3) assigned to the subscripts (i,j,k) of the enclosed product. The expression (45) has been simplified by using the dispersion laws (12) to remove any powers of ω_i; this is essential if we are to use b_{123}^{R} as a template for the parameter b_{123}. The derivation of $\Delta_{123}^{\mathrm{R}}$ from Eq. (44)—and its subsequent simplification—requires some lengthy (albeit routine) algebraic manipulation that is best carried out using symbolic computation. (Henceforth, we shall make use of Mathematica to perform algebraic computations whenever it is necessary or convenient, and without further mention.) We observe that [modulo the dispersion relations $\omega_i\propto p_i^3$, Eq. (18)] $\Delta_{123}^{\mathrm{R}}$ is homogeneous of total degree 18 and *even* in each of the wave numbers $p_i(i=1,2,3)$.

We therefore write

$$b_{123}=\frac{\Delta_{123}}{4D_{123}},\quad D_{123}=\prod_{1\leqslant i<j\leqslant 3}D_{ij}, \tag{46}$$

analogous to Eq. (44), and take

$$\Delta_{123}=18\langle\langle p_i^2p_j^2p_k^2(5\omega_i-2p_i^3)(5\omega_j-2p_j^3)\Delta_{ij}\rangle\rangle+H_{123}, \tag{47}$$

where

$$\begin{aligned}H_{123}=&\alpha_1\langle\langle p_i^{10}p_j^4p_k^4\rangle\rangle+\alpha_2\langle\langle p_i^8p_j^6p_k^4\rangle\rangle+\alpha_3p_1^6p_2^6p_3^6+\beta_1\langle\langle\omega_ip_i^7p_j^4p_k^4\rangle\rangle+\beta_2\langle\langle\omega_ip_i^5p_j^6p_k^4\rangle\rangle\\&+\beta_3\langle\langle\omega_ip_i^3p_j^8p_k^4\rangle\rangle+\beta_4\langle\langle\omega_ip_i^3p_j^6p_k^6\rangle\rangle+\beta_5\langle\langle\omega_ip_ip_j^{10}p_k^4\rangle\rangle+\beta_6\langle\langle\omega_ip_ip_j^8p_k^6\rangle\rangle+\gamma_1\langle\langle\omega_i\omega_jp_i^7p_jp_k^4\rangle\rangle\\&+\gamma_2\langle\langle\omega_i\omega_jp_i^5p_j^3p_k^4\rangle\rangle+\gamma_3\langle\langle\omega_i\omega_jp_i^5p_jp_k^6\rangle\rangle+\gamma_4\langle\langle\omega_i\omega_jp_i^3p_j^3p_k^6\rangle\rangle+\gamma_5\langle\langle\omega_i\omega_jp_i^3p_jp_k^8\rangle\rangle\end{aligned}$$

$$+\gamma_6\langle\!\langle \omega_i\omega_j p_i p_j p_k^{10}\rangle\!\rangle+\delta_1\langle\!\langle \omega_i\omega_j\omega_k p_i^7 p_j p_k\rangle\!\rangle+\delta_2\langle\!\langle \omega_i\omega_j\omega_k p_i^5 p_j^3 p_k\rangle\!\rangle+\delta_3\omega_1\omega_2\omega_3 p_1^3 p_2^3 p_3^3 \tag{48}$$

and Δ_{13}, Δ_{23} generalize Δ_{12}, Eq. (37). The formulation of Δ_{123} requires some further explanation. Like its counterpart $\Delta_{123}^{\mathrm{R}}$, every term in the expression (47) is *even* in each p_i and is of (total) degree 18 (recall that Δ_{ij} is odd and of degree six). This means that, just like a_i^2, A_{ij} and b_{ij}, the parameter b_{123} has effectively degree *zero*. The coefficients in the first term of Eq. (47) are fixed by virtue of the reduction (43a) (and symmetry). To see this, we let $\mathbf{p}_3\to\mathbf{0}$ in Eq. (46) and substitute the result into Eq. (43a): this shows that

$$\Delta_{123}=18p_1^2p_2^2p_3^2(5\omega_1-p_1^3)(5\omega_2-p_2^3)\Delta_{12}+O(p_3^4)\quad \text{as}\quad p_3\to 0\,, \tag{49}$$

(where we use $\omega_3\propto p_3^3$). In other words, the $\langle\!\langle\ \rangle\!\rangle$ term in (47) contains the leading order terms as $p_i\to 0$ $(i=1,2,3)$—these correspond to the terms in $\Delta_{123}^{\mathrm{R}}$, Eq. (45), of lowest degree (p_i^2) in any one of the wave numbers. [Of course, it now makes no sense to remove the ω_i^2 terms from this sum, as we did in (45).] The remaining terms in H_{123}, Eq. (48), follow directly: each term is even and of minimum degree four in each wave number, and of (total) degree 18. However, we must be sure to include in H_{123} *all* possible combinations of such product terms; these have been conveniently grouped according to type by the four sets of coefficients (α_i), (β_j), (γ_k) and (δ_m). Significantly, these terms do not duplicate exactly the terms in $\Delta_{123}^{\mathrm{R}}$ of the same type—observe that the final symmetrical term in (48) is absent from (45)! Hence, notwithstanding that we have used $\Delta_{123}^{\mathrm{R}}$ as a template, we cannot rely on it to provide all the terms that are needed to construct Δ_{123}. We shall return to the formulation of the parameter Δ_{123} later.

To determine the 18 unknown constants in (48), we proceed as follows. We first let $\mathbf{p}_2$, $\mathbf{p}_3\to\mathbf{0}$ in b_{123} and b_{23}, and make use of the second reduction (43b): to leading order, this yields

$$\alpha_1=810,\ \ \beta_1=-4050,\ \ \beta_5=1620,\ \ \gamma_1=-8100,\ \ \gamma_6=3240,\ \ \delta_1=-16200. \tag{50}$$

We now substitute the constants (50) into (47) and set $\mathbf{p}_3=\mathbf{p}_2$ in b_{123}, Eq. (46). Then, inserting the result in the final reduction (43c)—taking care to remove any powers of ω_i via the dispersion relation (12)—we obtain just ten independent equations for the remaining 12 coefficients. These can be solved in terms of two of the coefficients (we chose γ_5 and δ_3) to give

$$\begin{gathered}\alpha_2=-\frac{1}{5}\,\gamma_5,\quad \alpha_3=\frac{6}{5}\,\gamma_5+324,\quad \beta_2=\frac{1}{30}\,\delta_3+3105,\quad \beta_3=\gamma_5-\frac{1}{30}\,\delta_3-2700,\\ \beta_4=-2\,\gamma_5-\frac{1}{15}\,\delta_3-7830,\quad \beta_6=\frac{1}{30}\,\delta_3+2700,\quad \gamma_2=\gamma_5-4050,\\ \gamma_3=-\gamma_5-\frac{1}{6}\,\delta_3-12\,690,\quad \gamma_4=-2\,\gamma_5+\frac{1}{3}\,\delta_3+43\,200,\quad \delta_2=-\frac{1}{6}\,\delta_3-21\,600.\end{gathered} \tag{51}$$

Unfortunately, the reductions (43a)–(43c) are insufficient to fix all the coefficients in Δ_{123}. This scenario differs markedly from that for the sister KK Eq. (2). There, the soliton solutions possess a greater degree of symmetry so that just two reductions [comparable to Eqs. (43a) and (43c)] are needed to compute the equivalent KK parameter.[11] But for the bKK Eq. (1), much of this symmetry is lost because of the bidirectional nature of its solitons. We are therefore obliged to introduce a larger number of unknown coefficients in Δ_{123} to allow for the directional dependence of the constituent ''solitary'' waves. Regrettably, the additional unknowns cannot be matched by further soliton reductions that capture the *head-on* collisions of solitary waves. Put another way, information is wanting because we are unable to reduce a bKK soliton to one of lower order by coalescing a single-humped pulse with a double-humped solitary wave (because the latter wave profile is immutable [1]).

To complete the derivation of the three-soliton, we revert back to the bilinear form of the bKK equation, Eqs. (19a) and (19b). Fortunately, for this final step we need only take a truncated form of the ansatz (42),

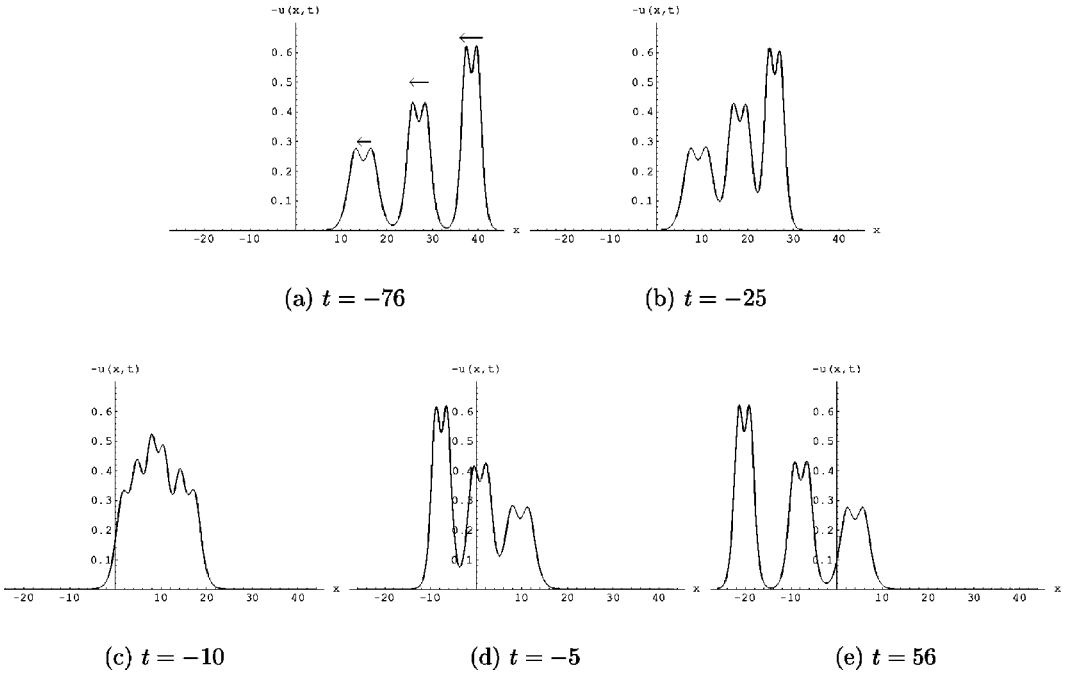

FIG. 5. A bKK three-soliton solution comprised of three left-traveling double-humped solitary waves: $p_1=1.0$, $p_2=1.25$, $p_3=1.5$.

$$\hat{f}=1+\sum_{i=1}^{3} e^{\theta_i}+\sum_{1\leqslant i<j\leqslant 3} b_{ij}e^{\theta_i+\theta_j}+b_{123}e^{\theta_1+\theta_2+\theta_3}, \tag{52}$$

since no other terms of f contribute to the $e^{\theta_1+\theta_2+\theta_3}$ terms in which the desired parameter b_{123} first appears. We substitute $\hat{f}$, and a similarly truncated expansion for $\tilde{g}$ [cf. Eq. (27)],

$$\hat{g}=\sum_{i=1}^{3} \rho_i e^{\theta_i}+\sum_{1\leqslant i<j\leqslant 3} \mu_{ij}e^{\theta_i+\theta_j}+\lambda e^{\theta_1+\theta_2+\theta_3}, \tag{53}$$

into the bilinear equations (19a) and (19b) (retaining terms only as far as $e^{\theta_1+\theta_2+\theta_3}$). The resulting equations (omitted here) are solved for b_{123} which is then equated with (46). This leads to an equation for Δ_{123} which, after substituting the expression (47) along with the known coefficients (50) and (51), is satisfied identically if

$$\gamma_5=0, \quad \delta_3=-81\,000. \tag{54}$$

Then, using Eq. (51), we get

$$\begin{gathered}\alpha_2=0, \quad \alpha_3=324, \quad \beta_2=405, \quad \beta_3=0, \quad \beta_4=-2430,\\ \beta_6=0, \quad \gamma_2=-4050, \quad \gamma_3=810, \quad \gamma_4=16\,200, \quad \delta_2=-8100,\end{gathered} \tag{55}$$

so that Δ_{123}, and hence b_{123}, is fully determined.

The derivation of f, Eq. (42), is now complete: the explicit three-soliton solution of the bKK Eq. (1) is given by $u=-\partial_x^2 \ln f$. The additional parameter b_{123} in Eq. (42) is essential to the formulation of the three-soliton solution, but it cannot be expressed solely in terms of the interaction parameters A_{12}, A_{13}, A_{23} that characterize the pairwise collisions between the three constituent ''solitary'' waves. Figures 5–7 illustrate two of the *four* possible versions of the three-

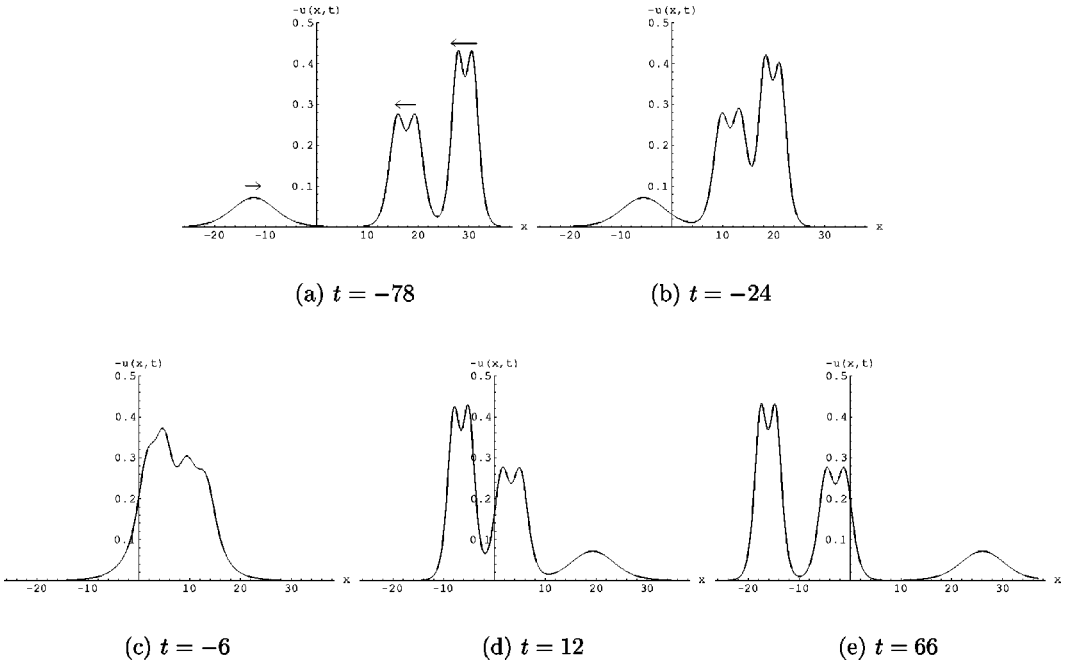

FIG. 6. A bKK three-soliton showing the head-on collision of a right-going single-peaked solitary wave ($p_1=0.4$) with a pair of left-running double-humped pulses ($p_2=1.0,\ p_3=1.25$).

soliton in both transverse and perspective views (this compares with just *two* for the bSK-Ramani equation). Figure 5 pictures a typical bKK three-soliton that consists of a triplet of double-humped ''solitary'' waves all propagating to the left. Figure 6 shows a three-soliton solution depicting the head-on interaction of a right-traveling single-peaked soliton with a counter-propagating pair of twin-peaked pulses. Figure 7 shows these same two three-solitons in perspective view—they exhibit the familiar ''elastic'' interaction property whereby the three individual solitons retain their identities, save for a cumulative phase shift.

Before we move on, let us return to the formulation of the key parameter Δ_{123}. We recall that Δ_{123} is of even degree in each $p_i\,(i=1,2,3)$, whereas Δ_{12} is odd: this is no coincidence. If we let $\mathbf{p}_3\rightarrow-\mathbf{p}_3$ in Eq. (46), and use Eq. (32), then we obtain the parity transformation

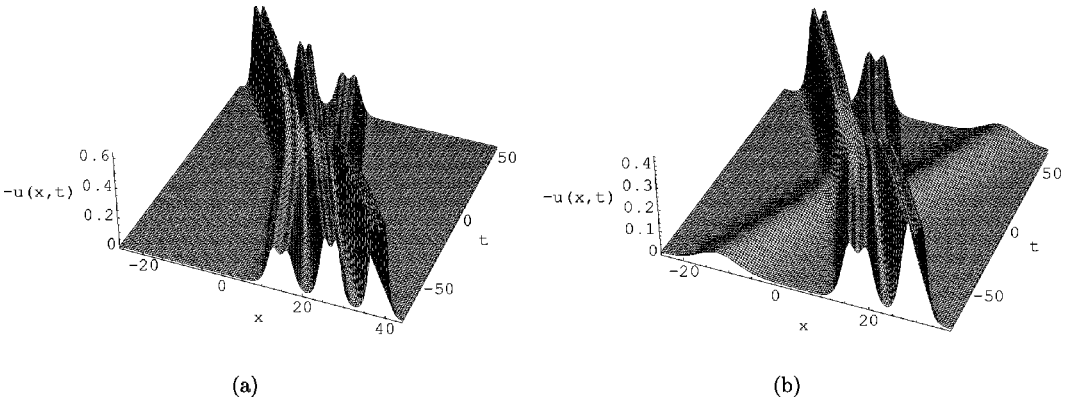

FIG. 7. Perspective views of the bKK three-soliton: (a) three left-travelling twin-peaked pulses ($p_1=1.0,\ p_2=1.25,\ p_3=1.5$), (b) the head-on interaction of a right-running single-peaked wave ($p_1=0.4$) with a pair of counter-propagating double-humped pulses ($p_2=1.0,\ p_3=1.25$).

$$b_{123}\to\frac{1}{A_{13}A_{23}}b_{123}\quad\text{if }\mathbf{p}_3\to-\mathbf{p}_3,\tag{56}$$

which should be compared with Eq. (35b) (with $A\to A_{12}$). This result ensures that, like the lower-order solitons (14) and (40), the bKK three-soliton solution $u(x,t)$ is invariant under the parity transformation $\mathbf{p}_i\to-\mathbf{p}_i(i=1,2,3)$ and we may assume that $p_i>0$, without loss of generality. But the even parity of Δ_{123} has yet a further important consequence. Barring the first (and quantifiable) term of Δ_{123}, Eq. (47), it is evident that the key term is $\langle\langle p_i^{10}p_j^4p_k^4\rangle\rangle$ in the expression for H_{123}, Eq. (48): it can be fixed by the degree and parity property of Δ_{123}. Once this *principal term* is known, the remaining terms of H_{123} follow immediately by cascading down the (even) powers of p_i and successively replacing $p_i^3\to\omega_i$ [according to the dispersion relation (18)]. It follows that we may formulate Δ_{123} without relying on its bSK-Ramani counterpart $\Delta_{123}^{\mathrm{R}}$: these observations will assist us when we seek solitons of higher order.

B. The four-soliton solution

We follow the solution strategy of the preceding section, except that now we iterate on the first three bKK solitons. Starting with a squared regular four-soliton [set $N=4$ in (10)], and applying the soliton reduction procedure (we omit the routine details), we arrive at the bKK four-soliton solution

$$\begin{aligned}
f(x,t)=1&+\sum_{i=1}^{4}\mathrm{e}^{\theta_i}+\frac{1}{16}\sum_{i=1}^{4}a_i^2\mathrm{e}^{2\theta_i}+\sum_{1\leqslant i<j\leqslant 4}b_{ij}\mathrm{e}^{\theta_i+\theta_j}+\frac{1}{16}\sum_{1\leqslant i<j\leqslant 4}A_{ij}[a_i^2\mathrm{e}^{2\theta_i+\theta_j}+a_j^2\mathrm{e}^{\theta_i+2\theta_j}]\\
&+\sum_{1\leqslant i<j<k\leqslant 4}b_{ijk}\mathrm{e}^{\theta_i+\theta_j+\theta_k}+\frac{1}{16^2}\sum_{1\leqslant i<j\leqslant 4}a_i^2a_j^2A_{ij}^2\mathrm{e}^{2(\theta_i+\theta_j)}+b_{1234}\mathrm{e}^{\theta_1+\theta_2+\theta_3+\theta_4}\\
&+\frac{1}{16}\sum_{1\leqslant i<j<k\leqslant 4}[a_i^2b_{jk}A_{ij}A_{ik}\mathrm{e}^{2\theta_i+\theta_j+\theta_k}+a_j^2b_{ik}A_{ij}A_{jk}\mathrm{e}^{\theta_i+2\theta_j+\theta_k}\\
&+a_k^2b_{ij}A_{ik}A_{jk}\mathrm{e}^{\theta_i+\theta_j+2\theta_k}]+\frac{1}{16}[a_1^2b_{234}A_{12}A_{13}A_{14}\mathrm{e}^{2\theta_1+\theta_2+\theta_3+\theta_4}\\
&+a_2^2b_{134}A_{12}A_{23}A_{24}\mathrm{e}^{\theta_1+2\theta_2+\theta_3+\theta_4}+a_3^2b_{124}A_{13}A_{23}A_{34}\mathrm{e}^{\theta_1+\theta_2+2\theta_3+\theta_4}\\
&+a_4^2b_{123}A_{14}A_{24}A_{34}\mathrm{e}^{\theta_1+\theta_2+\theta_3+2\theta_4}]+\frac{1}{16^2}\sum_{1\leqslant i<j<k\leqslant 4}A_{ij}A_{ik}A_{jk}[a_i^2a_j^2A_{ij}\mathrm{e}^{2(\theta_i+\theta_j)+\theta_k}\\
&+a_i^2a_k^2A_{ik}\mathrm{e}^{2\theta_i+\theta_j+2\theta_k}+a_j^2a_k^2A_{jk}\mathrm{e}^{\theta_i+2(\theta_j+\theta_k)}]\\
&+\frac{1}{16^2}[a_1^2a_2^2b_{34}A_{12}^2A_{13}A_{14}A_{23}A_{24}\mathrm{e}^{2(\theta_1+\theta_2)+\theta_3+\theta_4}\\
&+a_1^2a_3^2b_{24}A_{12}A_{13}^2A_{14}A_{23}A_{34}\mathrm{e}^{2\theta_1+\theta_2+2\theta_3+\theta_4}+a_1^2a_4^2b_{23}A_{12}A_{13}A_{14}^2A_{24}A_{34}\mathrm{e}^{2\theta_1+\theta_2+\theta_3+2\theta_4}\\
&+a_2^2a_3^2b_{14}A_{12}A_{13}A_{23}^2A_{24}A_{34}\mathrm{e}^{\theta_1+2(\theta_2+\theta_3)+\theta_4}+a_2^2a_4^2b_{13}A_{12}A_{14}A_{23}A_{24}^2A_{34}\mathrm{e}^{\theta_1+2\theta_2+\theta_3+2\theta_4}\\
&+a_3^2a_4^2b_{12}A_{13}A_{14}A_{23}A_{24}A_{34}^2\mathrm{e}^{\theta_1+\theta_2+2(\theta_3+\theta_4)}]\\
&+\frac{1}{16^3}\sum_{1\leqslant i<j<k\leqslant 4}a_i^2a_j^2a_k^2A_{ij}^2A_{ik}^2A_{jk}^2\mathrm{e}^{2(\theta_i+\theta_j+\theta_k)}+\frac{1}{16^3}A_{12}A_{13}A_{14}A_{23}A_{24}A_{34}\\
&\times[a_1^2a_2^2a_3^2A_{12}A_{13}A_{23}\mathrm{e}^{2(\theta_1+\theta_2+\theta_3)+\theta_4}+a_1^2a_2^2a_4^2A_{12}A_{14}A_{24}\mathrm{e}^{2(\theta_1+\theta_2)+\theta_3+2\theta_4}\\
&+a_1^2a_3^2a_4^2A_{13}A_{14}A_{34}\mathrm{e}^{2\theta_1+\theta_2+2(\theta_3+\theta_4)}+a_2^2a_3^2a_4^2A_{23}A_{24}A_{34}\mathrm{e}^{\theta_1+2(\theta_2+\theta_3+\theta_4)}]\\
&+\frac{1}{16^4}a_1^2a_2^2a_3^2a_4^2A_{12}^2A_{13}^2A_{14}^2A_{23}^2A_{24}^2A_{34}^2\mathrm{e}^{2(\theta_1+\theta_2+\theta_3+\theta_4)},
\end{aligned}\tag{57}$$

where $\theta_i = p_i x + \omega_i t + \eta_i$, $i=1,2,3,4$, and $\omega_i(p_i)$ are the usual (bSK-Ramani) dispersion laws, Eq. (12). The parameters b_{124}, b_{134}, b_{234} in (57) generalize b_{123}, Eq. (46), in the obvious manner. All but one of the coefficients in (57) have been obtained by reducing f to a three-soliton solution of the form (42)—the only remaining unknown is the "new" parameter b_{1234}. Although b_{1234} cannot be determined completely by further reducing (57) to solitons of lower order, we do obtain the reductions

$$b_{1234}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{0}) = b_{123}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3), \tag{58a}$$

$$b_{1234}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{0},\mathbf{0}) = b_{12}(\mathbf{p}_1,\mathbf{p}_2)\,b_{34}(\mathbf{0},\mathbf{0}), \tag{58b}$$

$$b_{1234}(\mathbf{p}_1,\mathbf{0},\mathbf{0},\mathbf{0}) = b_{234}(\mathbf{0},\mathbf{0},\mathbf{0}), \tag{58c}$$

$$b_{1234}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_3) = \frac{1}{8}\,a_3^2 b_{12} A_{13} A_{23}; \tag{58d}$$

once again, the reductions (58a)–(58c) must be treated as limits ($\mathbf{p}_i \to \mathbf{0}$). In addition, we have the parity transformation [cf. Eq. (56)]

$$b_{1234} \to \frac{1}{A_{14}A_{24}A_{34}}\, b_{1234} \quad \text{if } \mathbf{p}_4 \to -\mathbf{p}_4, \tag{59}$$

which follows by virtue of the fact that p_i is arbitrary in (57) and by noting the gauge invariance of the solution $u = -\partial_x^2 \ln f$. As before, this last result ensures that the four-soliton u is parity invariant under $\mathbf{p}_i \to -\mathbf{p}_i$.

Following our observations in Sec. IV A, we can now formulate b_{1234} *without* reference to the bSK-Ramani equation. Thus, Eqs. (36) and (46) generalize to

$$b_{1234} = \frac{\Delta_{1234}}{8 D_{1234}}, \quad D_{1234} = \prod_{1 \le i < j \le 4} D_{ij}, \tag{60}$$

with D_{ij} defined in Eq. (34). It only remains to find the numerator Δ_{1234} which is homogeneous in p_i [modulo $\omega_i \propto p_i^3$, Eq. (18)] of total degree 36 (equal to that of the denominator D_{1234}). But, if we make use of the parity transformation (59), one easily shows that Δ_{1234} is of *odd* degree in each of the wave numbers p_i (as expected). From this we immediately infer that

$$\Delta_{1234} = 54 \langle\!\langle p_i^2 p_j^2 p_k^2 p_l^3 (5\omega_i - 2p_i^3)(5\omega_j - 2p_j^3)(5\omega_k - 2p_k^3)\Delta_{ijk} \rangle\!\rangle + H_{1234} \tag{61}$$

with

$$\begin{aligned}
H_{1234} = {} & \alpha_1 \langle\!\langle p_i^{15} p_j^{11} p_k^5 p_l^5 \rangle\!\rangle + \alpha_2 \langle\!\langle p_i^{15} p_j^9 p_k^7 p_l^5 \rangle\!\rangle + \alpha_3 \langle\!\langle p_i^{15} p_j^7 p_k^7 p_l^7 \rangle\!\rangle + \alpha_4 \langle\!\langle p_i^{13} p_j^{13} p_k^5 p_l^5 \rangle\!\rangle \\
& + \alpha_5 \langle\!\langle p_i^{13} p_j^{11} p_k^7 p_l^5 \rangle\!\rangle + \alpha_6 \langle\!\langle p_i^{13} p_j^9 p_k^9 p_l^5 \rangle\!\rangle + \alpha_7 \langle\!\langle p_i^{13} p_j^9 p_k^7 p_l^7 \rangle\!\rangle + \alpha_8 \langle\!\langle p_i^{11} p_j^{11} p_k^9 p_l^5 \rangle\!\rangle \\
& + \alpha_9 \langle\!\langle p_i^{11} p_j^{11} p_k^7 p_l^7 \rangle\!\rangle + \alpha_{10} \langle\!\langle p_i^{11} p_j^9 p_k^9 p_l^7 \rangle\!\rangle + \alpha_{11} p_1^9 p_2^9 p_3^9 p_4^9 + \beta_1 \langle\!\langle \omega_i p_i^{12} p_j^{11} p_k^5 p_l^5 \rangle\!\rangle \\
& + \beta_2 \langle\!\langle \omega_i p_i^{12} p_j^9 p_k^7 p_l^5 \rangle\!\rangle + \beta_3 \langle\!\langle \omega_i p_i^{12} p_j^7 p_k^7 p_l^7 \rangle\!\rangle + \beta_4 \langle\!\langle \omega_i p_i^{10} p_j^{13} p_k^5 p_l^5 \rangle\!\rangle + \beta_5 \langle\!\langle \omega_i p_i^{10} p_j^{11} p_k^7 p_l^5 \rangle\!\rangle \\
& + \beta_6 \langle\!\langle \omega_i p_i^{10} p_j^9 p_k^9 p_l^5 \rangle\!\rangle + \beta_7 \langle\!\langle \omega_i p_i^{10} p_j^9 p_k^7 p_l^7 \rangle\!\rangle + \beta_8 \langle\!\langle \omega_i p_i^8 p_j^{15} p_k^5 p_l^5 \rangle\!\rangle + \beta_9 \langle\!\langle \omega_i p_i^8 p_j^{13} p_k^7 p_l^5 \rangle\!\rangle \\
& + \beta_{10} \langle\!\langle \omega_i p_i^8 p_j^{11} p_k^9 p_l^5 \rangle\!\rangle + \beta_{11} \langle\!\langle \omega_i p_i^8 p_j^{11} p_k^7 p_l^7 \rangle\!\rangle + \beta_{12} \langle\!\langle \omega_i p_i^8 p_j^9 p_k^9 p_l^7 \rangle\!\rangle + \beta_{13} \langle\!\langle \omega_i p_i^6 p_j^{15} p_k^7 p_l^5 \rangle\!\rangle \\
& + \beta_{14} \langle\!\langle \omega_i p_i^6 p_j^{13} p_k^9 p_l^5 \rangle\!\rangle + \beta_{15} \langle\!\langle \omega_i p_i^6 p_j^{13} p_k^7 p_l^7 \rangle\!\rangle + \beta_{16} \langle\!\langle \omega_i p_i^6 p_j^{11} p_k^{11} p_l^5 \rangle\!\rangle + \beta_{17} \langle\!\langle \omega_i p_i^6 p_j^{11} p_k^9 p_l^7 \rangle\!\rangle
\end{aligned}$$

$$
\begin{aligned}
&+\beta_{18}\langle\langle\omega_i p_i^6 p_j^9 p_k^9 p_l^9\rangle\rangle+\beta_{19}\langle\langle\omega_i p_i^4 p_j^{15} p_k^9 p_l^5\rangle\rangle+\beta_{20}\langle\langle\omega_i p_i^4 p_j^{15} p_k^7 p_l^7\rangle\rangle+\beta_{21}\langle\langle\omega_i p_i^4 p_j^{13} p_k^{11} p_l^5\rangle\rangle\\
&+\beta_{22}\langle\langle\omega_i p_i^4 p_j^{13} p_k^9 p_l^7\rangle\rangle+\beta_{23}\langle\langle\omega_i p_i^4 p_j^{11} p_k^{11} p_l^7\rangle\rangle+\beta_{24}\langle\langle\omega_i p_i^4 p_j^{11} p_k^9 p_l^9\rangle\rangle+\beta_{25}\langle\langle\omega_i p_i^2 p_j^{15} p_k^{11} p_l^5\rangle\rangle\\
&+\beta_{26}\langle\langle\omega_i p_i^2 p_j^{15} p_k^9 p_l^7\rangle\rangle+\beta_{27}\langle\langle\omega_i p_i^2 p_j^{13} p_k^{13} p_l^5\rangle\rangle+\beta_{28}\langle\langle\omega_i p_i^2 p_j^{13} p_k^{11} p_l^7\rangle\rangle+\beta_{29}\langle\langle\omega_i p_i^2 p_j^{13} p_k^9 p_l^9\rangle\rangle\\
&+\beta_{30}\langle\langle\omega_i p_i^2 p_j^{11} p_k^{11} p_l^9\rangle\rangle+\gamma_1\langle\langle\omega_i\omega_j p_i^{12} p_j^8 p_k^5 p_l^5\rangle\rangle+\gamma_2\langle\langle\omega_i\omega_j p_i^{12} p_j^6 p_k^7 p_l^5\rangle\rangle\\
&+\gamma_3\langle\langle\omega_i\omega_j p_i^{12} p_j^4 p_k^9 p_l^5\rangle\rangle+\gamma_4\langle\langle\omega_i\omega_j p_i^{12} p_j^4 p_k^7 p_l^7\rangle\rangle+\gamma_5\langle\langle\omega_i\omega_j p_i^{12} p_j^2 p_k^{11} p_l^5\rangle\rangle\\
&+\gamma_6\langle\langle\omega_i\omega_j p_i^{12} p_j^2 p_k^9 p_l^7\rangle\rangle+\gamma_7\langle\langle\omega_i\omega_j p_i^{10} p_j^{10} p_k^5 p_l^5\rangle\rangle+\gamma_8\langle\langle\omega_i\omega_j p_i^{10} p_j^8 p_k^7 p_l^5\rangle\rangle\\
&+\gamma_9\langle\langle\omega_i\omega_j p_i^{10} p_j^6 p_k^9 p_l^5\rangle\rangle+\gamma_{10}\langle\langle\omega_i\omega_j p_i^{10} p_j^6 p_k^7 p_l^7\rangle\rangle+\gamma_{11}\langle\langle\omega_i\omega_j p_i^{10} p_j^4 p_k^{11} p_l^5\rangle\rangle\\
&+\gamma_{12}\langle\langle\omega_i\omega_j p_i^{10} p_j^4 p_k^9 p_l^7\rangle\rangle+\gamma_{13}\langle\langle\omega_i\omega_j p_i^{10} p_j^2 p_k^{13} p_l^5\rangle\rangle+\gamma_{14}\langle\langle\omega_i\omega_j p_i^{10} p_j^2 p_k^{11} p_l^7\rangle\rangle\\
&+\gamma_{15}\langle\langle\omega_i\omega_j p_i^{10} p_j^2 p_k^9 p_l^9\rangle\rangle+\gamma_{16}\langle\langle\omega_i\omega_j p_i^8 p_j^8 p_k^9 p_l^5\rangle\rangle+\gamma_{17}\langle\langle\omega_i\omega_j p_i^8 p_j^8 p_k^7 p_l^7\rangle\rangle\\
&+\gamma_{18}\langle\langle\omega_i\omega_j p_i^8 p_j^6 p_k^{11} p_l^5\rangle\rangle+\gamma_{19}\langle\langle\omega_i\omega_j p_i^8 p_j^6 p_k^9 p_l^7\rangle\rangle+\gamma_{20}\langle\langle\omega_i\omega_j p_i^8 p_j^4 p_k^{13} p_l^5\rangle\rangle\\
&+\gamma_{21}\langle\langle\omega_i\omega_j p_i^8 p_j^4 p_k^{11} p_l^7\rangle\rangle+\gamma_{22}\langle\langle\omega_i\omega_j p_i^8 p_j^4 p_k^9 p_l^9\rangle\rangle+\gamma_{23}\langle\langle\omega_i\omega_j p_i^8 p_j^2 p_k^{15} p_l^5\rangle\rangle\\
&+\gamma_{24}\langle\langle\omega_i\omega_j p_i^8 p_j^2 p_k^{13} p_l^7\rangle\rangle+\gamma_{25}\langle\langle\omega_i\omega_j p_i^8 p_j^2 p_k^{11} p_l^9\rangle\rangle+\gamma_{26}\langle\langle\omega_i\omega_j p_i^6 p_j^6 p_k^{13} p_l^5\rangle\rangle\\
&+\gamma_{27}\langle\langle\omega_i\omega_j p_i^6 p_j^6 p_k^{11} p_l^7\rangle\rangle+\gamma_{28}\langle\langle\omega_i\omega_j p_i^6 p_j^6 p_k^9 p_l^9\rangle\rangle+\gamma_{29}\langle\langle\omega_i\omega_j p_i^6 p_j^4 p_k^{15} p_l^5\rangle\rangle\\
&+\gamma_{30}\langle\langle\omega_i\omega_j p_i^6 p_j^4 p_k^{13} p_l^7\rangle\rangle+\gamma_{31}\langle\langle\omega_i\omega_j p_i^6 p_j^4 p_k^{11} p_l^9\rangle\rangle+\gamma_{32}\langle\langle\omega_i\omega_j p_i^6 p_j^2 p_k^{15} p_l^7\rangle\rangle\\
&+\gamma_{33}\langle\langle\omega_i\omega_j p_i^6 p_j^2 p_k^{13} p_l^9\rangle\rangle+\gamma_{34}\langle\langle\omega_i\omega_j p_i^6 p_j^2 p_k^{11} p_l^{11}\rangle\rangle+\gamma_{35}\langle\langle\omega_i\omega_j p_i^4 p_j^4 p_k^{15} p_l^7\rangle\rangle\\
&+\gamma_{36}\langle\langle\omega_i\omega_j p_i^4 p_j^4 p_k^{13} p_l^9\rangle\rangle+\gamma_{37}\langle\langle\omega_i\omega_j p_i^4 p_j^4 p_k^{11} p_l^{11}\rangle\rangle+\gamma_{38}\langle\langle\omega_i\omega_j p_i^4 p_j^2 p_k^{15} p_l^9\rangle\rangle\\
&+\gamma_{39}\langle\langle\omega_i\omega_j p_i^4 p_j^2 p_k^{13} p_l^{11}\rangle\rangle+\ \gamma_{40}\langle\langle\omega_i\omega_j p_i^2 p_j^2 p_k^{15} p_l^{11}\rangle\rangle+\gamma_{41}\langle\langle\omega_i\omega_j p_i^2 p_j^2 p_k^{13} p_l^{13}\rangle\rangle\\
&+\delta_1\langle\langle\omega_i\omega_j\omega_k p_i^{12} p_j^8 p_k^2 p_l^5\rangle\rangle+\delta_2\langle\langle\omega_i\omega_j\omega_k p_i^{12} p_j^6 p_k^4 p_l^5\rangle\rangle+\delta_3\langle\langle\omega_i\omega_j\omega_k p_i^{12} p_j^6 p_k^2 p_l^7\rangle\rangle\\
&+\delta_4\langle\langle\omega_i\omega_j\omega_k p_i^{12} p_j^4 p_k^4 p_l^7\rangle\rangle+\delta_5\langle\langle\omega_i\omega_j\omega_k p_i^{12} p_j^4 p_k^2 p_l^9\rangle\rangle+\delta_6\langle\langle\omega_i\omega_j\omega_k p_i^{12} p_j^2 p_k^2 p_l^{11}\rangle\rangle\\
&+\delta_7\langle\langle\omega_i\omega_j\omega_k p_i^{10} p_j^{10} p_k^2 p_l^5\rangle\rangle+\ \delta_8\langle\langle\omega_i\omega_j\omega_k p_i^{10} p_j^8 p_k^4 p_l^5\rangle\rangle+\delta_9\langle\langle\omega_i\omega_j\omega_k p_i^{10} p_j^8 p_k^2 p_l^7\rangle\rangle\\
&+\delta_{10}\langle\langle\omega_i\omega_j\omega_k p_i^{10} p_j^6 p_k^6 p_l^5\rangle\rangle+\delta_{11}\langle\langle\omega_i\omega_j\omega_k p_i^{10} p_j^6 p_k^4 p_l^7\rangle\rangle+\delta_{12}\langle\langle\omega_i\omega_j\omega_k p_i^{10} p_j^6 p_k^2 p_l^9\rangle\rangle\\
&+\delta_{13}\langle\langle\omega_i\omega_j\omega_k p_i^{10} p_j^4 p_k^4 p_l^9\rangle\rangle+\delta_{14}\langle\langle\omega_i\omega_j\omega_k p_i^{10} p_j^4 p_k^2 p_l^{11}\rangle\rangle+\delta_{15}\langle\langle\omega_i\omega_j\omega_k p_i^{10} p_j^2 p_k^2 p_l^{13}\rangle\rangle\\
&+\delta_{16}\langle\langle\omega_i\omega_j\omega_k p_i^8 p_j^8 p_k^6 p_l^5\rangle\rangle+\delta_{17}\langle\langle\omega_i\omega_j\omega_k p_i^8 p_j^8 p_k^4 p_l^7\rangle\rangle+\delta_{18}\langle\langle\omega_i\omega_j\omega_k p_i^8 p_j^8 p_k^2 p_l^9\rangle\rangle\\
&+\delta_{19}\langle\langle\omega_i\omega_j\omega_k p_i^8 p_j^6 p_k^6 p_l^7\rangle\rangle+\delta_{20}\langle\langle\omega_i\omega_j\omega_k p_i^8 p_j^6 p_k^4 p_l^9\rangle\rangle+\delta_{21}\langle\langle\omega_i\omega_j\omega_k p_i^8 p_j^6 p_k^2 p_l^{11}\rangle\rangle\\
&+\delta_{22}\langle\langle\omega_i\omega_j\omega_k p_i^8 p_j^4 p_k^4 p_l^{11}\rangle\rangle+\delta_{23}\langle\langle\omega_i\omega_j\omega_k p_i^8 p_j^4 p_k^2 p_l^{13}\rangle\rangle+\delta_{24}\langle\langle\omega_i\omega_j\omega_k p_i^8 p_j^2 p_k^2 p_l^{15}\rangle\rangle\\
&+\delta_{25}\langle\langle\omega_i\omega_j\omega_k p_i^6 p_j^6 p_k^6 p_l^9\rangle\rangle+\delta_{26}\langle\langle\omega_i\omega_j\omega_k p_i^6 p_j^6 p_k^4 p_l^{11}\rangle\rangle+\delta_{27}\langle\langle\omega_i\omega_j\omega_k p_i^6 p_j^6 p_k^2 p_l^{13}\rangle\rangle\\
&+\delta_{28}\langle\langle\omega_i\omega_j\omega_k p_i^6 p_j^4 p_k^4 p_l^{13}\rangle\rangle+\delta_{29}\langle\langle\omega_i\omega_j\omega_k p_i^6 p_j^4 p_k^2 p_l^{15}\rangle\rangle+\delta_{30}\langle\langle\omega_i\omega_j\omega_k p_i^4 p_j^4 p_k^4 p_l^{15}\rangle\rangle\\
&+\epsilon_1\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^{12} p_j^8 p_k^2 p_l^2\rangle\rangle+\epsilon_2\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^{12} p_j^6 p_k^4 p_l^2\rangle\rangle+\epsilon_3\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^{12} p_j^4 p_k^4 p_l^4\rangle\rangle\\
&+\epsilon_4\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^{10} p_j^{10} p_k^2 p_l^2\rangle\rangle+\epsilon_5\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^{10} p_j^8 p_k^4 p_l^2\rangle\rangle+\epsilon_6\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^{10} p_j^6 p_k^6 p_l^2\rangle\rangle\\
&+\epsilon_7\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^{10} p_j^6 p_k^4 p_l^4\rangle\rangle+\epsilon_8\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^8 p_j^8 p_k^6 p_l^2\rangle\rangle+\epsilon_9\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^8 p_j^8 p_k^4 p_l^4\rangle\rangle\\
&+\epsilon_{10}\langle\langle\omega_i\omega_j\omega_k\omega_l p_i^8 p_j^6 p_k^6 p_l^4\rangle\rangle+\epsilon_{11}\omega_1\omega_2\omega_3\omega_4 p_1^6 p_2^6 p_3^6 p_4^6, \qquad (62)
\end{aligned}
$$

where the symbol $\langle\langle\ \rangle\rangle$ now denotes the sum over all distinct permutations of (1,2,3,4). The increased complexity in stepping from $N=3$ to $N=4$ is evident: the expression H_{1234} contains 123 unknown coefficients and a total of 2000 terms (whereas H_{123} has just 18 and 80, respectively). The first term of Δ_{1234}, Eq. (61), is fixed by the reduction (58a) and symmetry [in just the same way as for the three-soliton; cf. Eq. (49)]. It contains the leading order terms p_l^3 as $p_l \to 0$ ($l=1,2,3,4$); this implies that H_{1234} is comprised of products of *at least* degree five in each of the wave numbers. To determine the principal term of H_{1234} we argue as follows: Setting $\mathbf{p}_4=\mathbf{p}_3$ in Eq. (60), and using the reduction (58d), we find that

$$\Delta_{1234}\big|_{\mathbf{p}_4=\mathbf{p}_3} = 30\,p_3^3(4\omega_3 - p_3^3)\Delta_{12}D_{13}D_{23}D_{13}^{-}D_{23}^{-}. \tag{63}$$

We see that the right-hand side of Eq. (63) has a maximum degree of 15 in p_1 [refer to Eqs. (34) and (37), and recall that $D_{ij}^{-}=D_{ij}(\mathbf{p}_i,-\mathbf{p}_j)$]. But since this reduction leaves the wave number p_1 untouched, it follows that the maximum degree of *any* one of the wave numbers p_i in Δ_{1234}, and hence in H_{1234}, must also be 15. Combining this with the total degree of 36—and a minimum degree of five in each p_i—yields the principal term $\langle\langle p_i^{15}p_j^{11}p_k^5p_l^5\rangle\rangle$ (and not $\langle\langle p_i^{21}p_j^5p_k^5p_l^5\rangle\rangle$!). The remaining terms in (62) are then obtained by systematically reducing the (odd) powers of p_i and successively replacing $p_i^3 \to \omega_i$ [via the dispersion relation (18)] to accommodate the bidirectionality.

Now, letting $\mathbf{p}_3$, $\mathbf{p}_4 \to \mathbf{0}$ in b_{1234} and making use of the reduction (58b), we obtain (to leading order) the 21 coefficients

$$\begin{gathered}
\alpha_1=-2\,755\,620,\quad \alpha_4=328\,050,\quad \beta_1=15\,746\,400,\quad \beta_4=-2\,296\,350,\\
\beta_8=13\,778\,100,\quad \beta_{25}=-5\,511\,240,\quad \beta_{27}=656\,100,\quad \gamma_1=-78\,732\,000,\\
\gamma_5=31\,492\,800,\quad \gamma_7=16\,074\,450,\quad \gamma_{13}=-4\,592\,700,\quad \gamma_{23}=27\,556\,200,\\
\gamma_{40}=-11\,022\,480,\quad \gamma_{41}=1\,312\,200,\quad \delta_1=-157\,464\,000,\quad \delta_6=62\,985\,600,\\
\delta_7=32\,148\,900,\quad \delta_{15}=-9\,185\,400,\quad \delta_{24}=55\,112\,400,\\
\epsilon_1=-314\,928\,000,\quad \epsilon_4=64\,297\,800.
\end{gathered} \tag{64}$$

Next, we invoke the reduction (58c): balancing the leading order terms as p_2, p_3, $p_4 \to 0$ leads to the further 24 coefficients:

$$\begin{gathered}
\alpha_2=0,\quad \alpha_3=-1\,102\,248,\quad \beta_2=0,\quad \beta_3=6\,298\,560,\quad \beta_{13}=-1\,377\,810,\\
\beta_{19}=0,\quad \beta_{20}=8\,266\,860,\quad \beta_{26}=0,\quad \gamma_2=7\,873\,200,\quad \gamma_3=0,\\
\gamma_4=-47\,239\,200,\quad \gamma_6=0,\quad \gamma_{29}=13\,778\,100,\quad \gamma_{32}=-2\,755\,620,\\
\gamma_{35}=-55\,112\,400,\quad \gamma_{38}=0,\quad \delta_2=-78\,732\,000,\quad \delta_3=15\,746\,400,\\
\delta_4=314\,928\,000,\quad \delta_5=0,\quad \delta_{29}=27\,556\,200,\quad \delta_{30}=275\,562\,000,\\
\epsilon_2=-157\,464\,000,\quad \epsilon_3=-1\,574\,640\,000.
\end{gathered} \tag{65}$$

To obtain the remaining coefficients in H_{1234}, we first use the reduction (58d). After substituting the constants (64) and (65) into Δ_{1234}, Eq. (61), and setting $\mathbf{p}_4=\mathbf{p}_3$, we insert the result into Eq. (63) (being sure to remove any powers of ω_i as usual). This gives 69 equations (we do not list them here) which may be solved in terms of any nine of the remaining 78 unknown coefficients

(we chose β_6, β_7, β_9, β_{18}, β_{24}, β_{29}, β_{30}, γ_9 and ϵ_8). As anticipated, the reductions (58a)–(58d) are not sufficient to fix all the coefficients in H_{1234} and we therefore return to the bilinear form (19) to complete the derivation of the bKK four-soliton.

We substitute truncated expansions for f and $\tilde{g}$ [cf. Eqs. (52) and (53)]—consistent with extracting just the terms in $e^{\theta_1+\theta_2+\theta_3+\theta_4}$—into the bilinear equations (19a) and (19b). Solving for b_{1234} and equating with Eq. (60), we obtain an equation for Δ_{1234} which, after inserting (61) along with all the coefficients so far determined, is satisfied identically if

$$
\begin{gathered}
\alpha_5=131\,220,\quad \alpha_6=0,\quad \alpha_7=262\,440,\quad \alpha_8=-1\,574\,640,\\
\alpha_9=209\,952,\quad \alpha_{10}=-787\,320,\quad \alpha_{11}=0,\quad \beta_5=-918\,540,\quad \beta_6=0,\\
\beta_7=-1\,837\,080,\quad \beta_9=-820\,125,\quad \beta_{10}=8\,857\,350,\quad \beta_{11}=-1\,312\,200,\\
\beta_{12}=3\,936\,600,\quad \beta_{14}=492\,075,\quad \beta_{15}=-1\,837\,080,\quad \beta_{16}=11\,022\,480,\\
\beta_{17}=5\,117\,580,\quad \beta_{18}=0,\quad \beta_{21}=-1\,312\,200,\quad \beta_{22}=-1\,640\,250,\\
\beta_{23}=-2\,099\,520,\quad \beta_{24}=1\,968\,300,\quad \beta_{28}=262\,440,\quad \beta_{29}=0,\\
\beta_{30}=-3\,149\,280,\quad \gamma_8=5\,740\,875,\quad \gamma_9=-3\,444\,525,\quad \gamma_{10}=12\,859\,560,\\
\gamma_{11}=9\,185\,400,\quad \gamma_{12}=11\,481\,750,\quad \gamma_{14}=-1\,837\,080,\quad \gamma_{15}=0,\\
\gamma_{16}=-49\,207\,500,\quad \gamma_{17}=8\,201\,250,\quad \gamma_{18}=-62\,001\,450,\quad \gamma_{19}=-25\,095\,825,\\
\gamma_{20}=8\,201\,250,\quad \gamma_{21}=13\,122\,000,\quad \gamma_{22}=-9\,841\,500,\quad \gamma_{24}=-1\,640\,250,\\
\gamma_{25}=17\,714\,700,\quad \gamma_{26}=-6\,889\,050,\quad \gamma_{27}=-33\,067\,440,\quad \gamma_{28}=2\,952\,450,\\
\gamma_{30}=11\,481\,750,\quad \gamma_{31}=-9\,841\,500,\quad \gamma_{33}=984\,150,\quad \gamma_{34}=22\,044\,960,\\
\gamma_{36}=6\,561\,000,\quad \gamma_{37}=20\,995\,200,\quad \gamma_{39}=-2\,624\,400,\quad \delta_8=-57\,408\,750,\\
\delta_9=11\,481\,750,\quad \delta_{10}=48\,223\,350,\quad \delta_{11}=-80\,372\,250,\quad \delta_{12}=-6\,889\,050,\\
\delta_{13}=-45\,927\,000,\quad \delta_{14}=18\,370\,800,\quad \delta_{16}=344\,452\,500,\quad \delta_{17}=-82\,012\,500,\\
\delta_{18}=-98\,415\,000,\quad \delta_{19}=158\,448\,150,\quad \delta_{20}=44\,286\,750,\quad \delta_{21}=-124\,002\,900,\\
\delta_{22}=-131\,220\,000,\quad \delta_{23}=16\,402\,500,\quad \delta_{25}=-62\,001\,450,\quad \delta_{26}=41\,334\,300,\\
\delta_{27}=-13\,778\,100,\quad \delta_{28}=-45\,927\,000,\quad \epsilon_5=-114\,817\,500,\quad \epsilon_6=96\,446\,700,\\
\epsilon_7=321\,489\,000,\quad \epsilon_8=688\,905\,000,\quad \epsilon_9=820\,125\,000,\\
\epsilon_{10}=-137\,781\,000,\quad \epsilon_{11}=868\,020\,300.
\end{gathered}
\tag{66}
$$

We reiterate that the routine (but lengthy) algebra needed to extract these coefficients has been performed with the assistance of Mathematica.

With the formulation of b_{1234}, and hence f, now complete, the four-soliton solution $u(x,t)$ of the bKK Eq. (1) follows directly from Eq. (57) and $u=-\partial_x^2 \ln f$. There are *five* variants of the four-soliton interaction, dependent on the direction of propagation of the constituent solitary waves (compared with just *three* for the bSK-Ramani equation). Several of these are illustrated in Figs. 8–11; in each case, we see that the four solitons emerge from the mutual collisions in

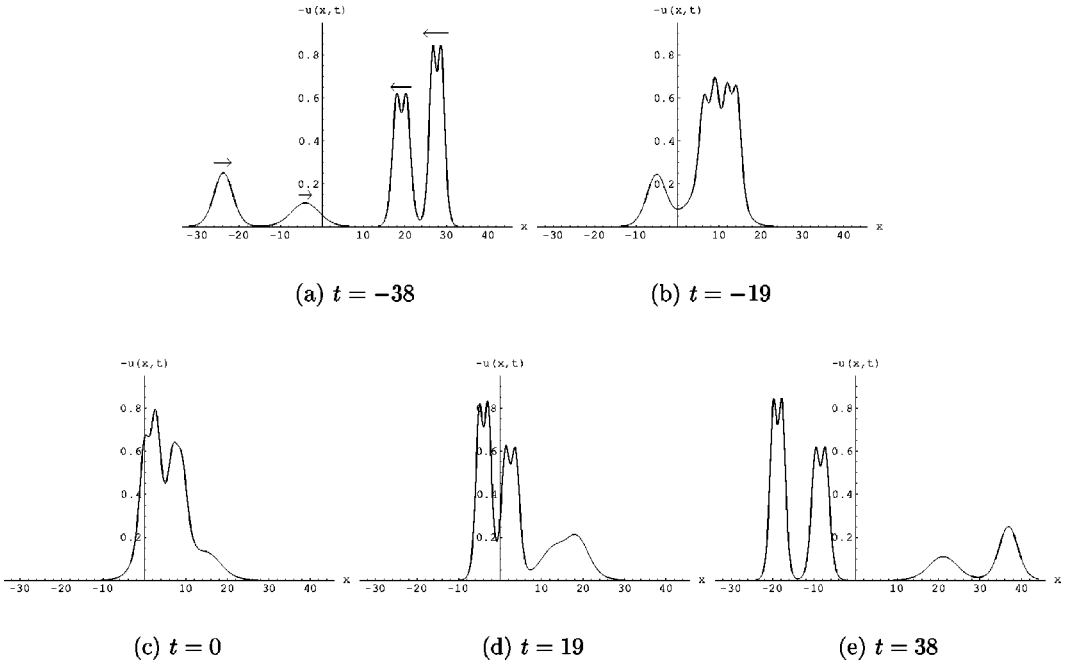

FIG. 8. A four-soliton solution of the bKK equation comprised of two right-running single-humped solitary waves ($p_1=0.5$, $p_2=0.75$) and a pair of left-going double-humped pulses ($p_3=1.5$, $p_4=1.75$).

characteristic fashion with their profiles unchanged. [Note that, because of the scaling, in Fig. 9(a) the incoming single-peaked soliton lies far to the left and so is absent; similarly in Fig. 9(e) where it is now far to the right.] Particularly noteworthy are the unusually large, almost resonantlike amplitude spikes that can be seen in Figs. 9(c) and 10(c) when at least three left-traveling double-

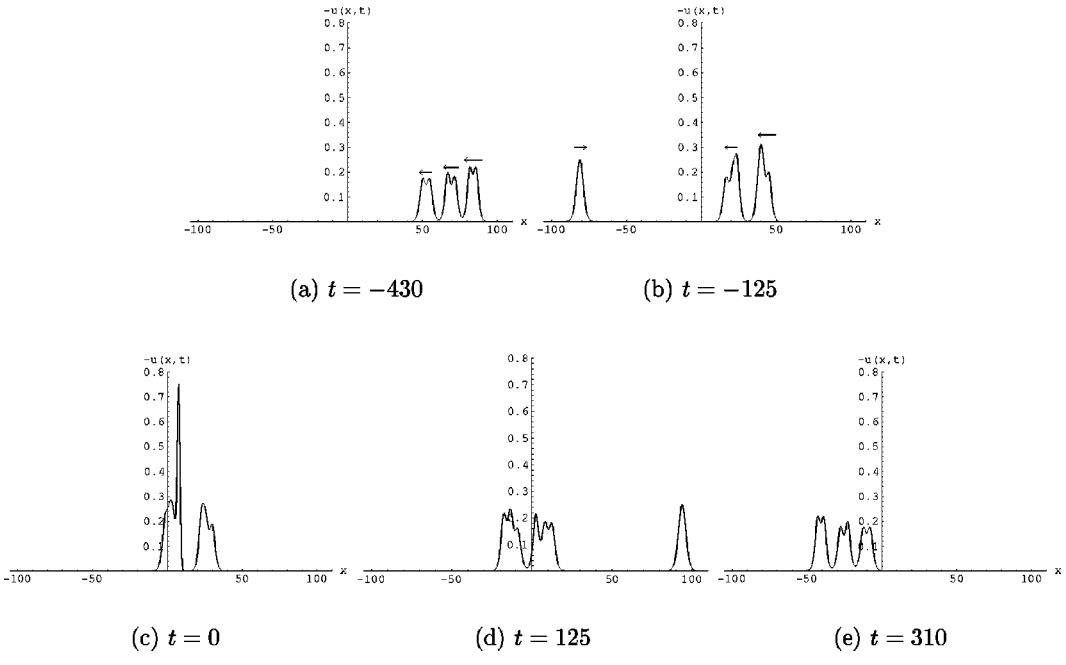

FIG. 9. A bKK four-soliton showing the head-on collision of a right-moving single-peaked pulse ($p_1=0.75$) with a triplet of left-traveling twin-peaked pulses ($p_2=0.8$, $p_3=0.85$, $p_4=0.9$).

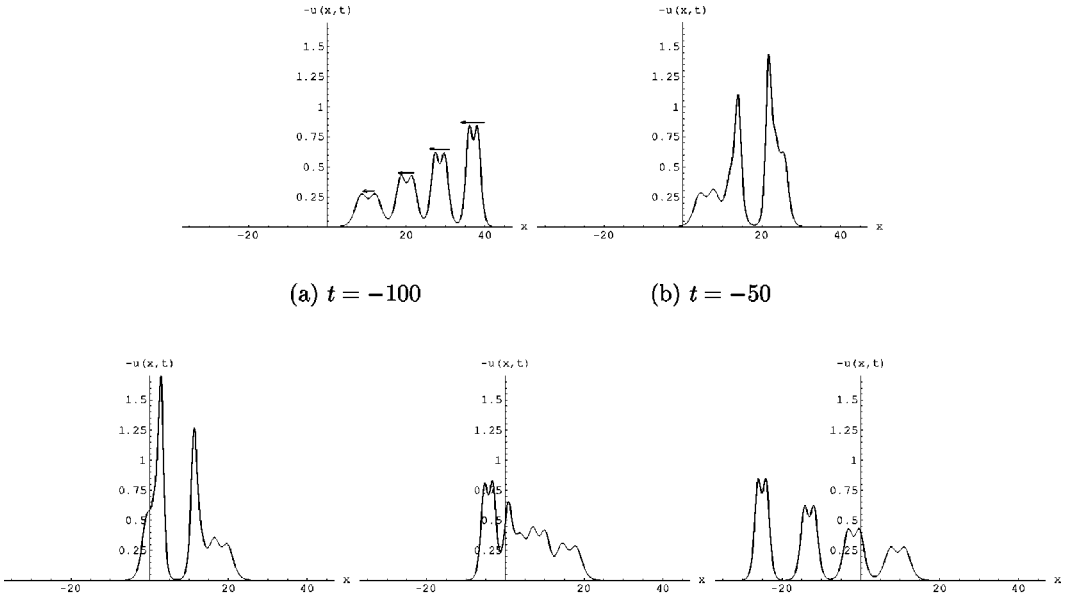

FIG. 10. A bKK four-soliton interaction comprised of four leftward propagating double-peaked solitary waves ($p_1=1.0$, $p_2=1.25$, $p_3=1.5$, $p_4=1.75$).

peaked ''solitary'' waves are present. Here we content ourselves with just two perspective views of the bKK four-soliton, Figs. 11(a) and 11(b). Bearing in mind the length and complexity of the expressions for f, Eq. (57), and its coefficients—particularly that of b_{1234}—it is clear that the computational demands of plotting these last two figures are considerable.

C. An iteration procedure for higher-order solitons

We are now in a position to outline an iterative method for constructing—at least in principle—the general N-soliton solution of the bKK equation by generalising the procedure of the preceding section for the four-soliton. Following our now well-rehearsed argument, we begin by writing down the general form of the solution. Accordingly, we square and normalize the regular

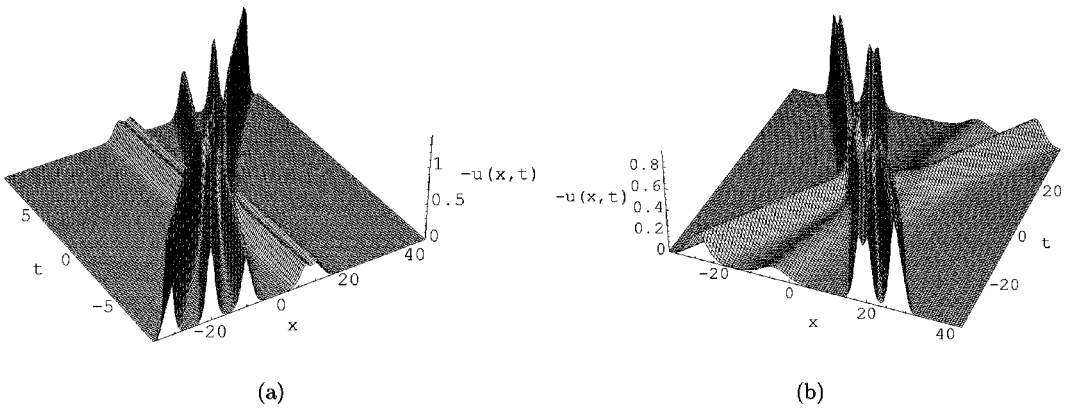

FIG. 11. Perspective views of the bKK four-soliton: (a) three single-peaked pulses ($p_1=1.25$, $p_2=1.5$, $p_3=1.75$) colliding head-on with a double-humped solitary wave ($p_4=1.0$), (b) head-on collision of a pair of single-humped ($p_1=0.5$, $p_2=0.75$) and a doublet of twin-peaked ($p_3=1.5$, $p_4=1.75$) pulses.

N-soliton (10), introducing arbitrary coefficients consonant with the symmetry in the phase variables $\theta_i = p_i x + \omega_i t + \eta_i$, $i = 1, \ldots, N$. This gives the putative N-soliton solution $f(x,t)$ of the bKK bilinear form (19a) and (19b).

We now use the soliton reduction procedure,[11] to reduce $f(x,t)$ to a soliton of order $N-1$ (in the limits $t \to \pm\infty$). Then comparison with the *known* bKK $(N-1)$-soliton fixes the dispersion relations $\omega_i(p_i)$, Eq. (12), and all but one of the coefficients in the expression for f. The only unknown is the coefficient $b_{12\ldots N}$ of the term $e^{\theta_1+\theta_2+\cdots+\theta_N}$, a "new" parameter that cannot be determined by reducing f to lower order. Nevertheless, we can deduce reductions of $b_{12\ldots N}$ of the type (58) in this way: this gives N conditions of which we note the two key results (for $N \geqslant 4$)

$$b_{12\ldots N}(\mathbf{p}_1, \ldots, \mathbf{p}_{N-1}, \mathbf{0}) = b_{12\ldots N-1}(\mathbf{p}_1, \ldots, \mathbf{p}_{N-1}); \tag{67}$$

$$b_{12\ldots N}(\mathbf{p}_1, \ldots, \mathbf{p}_{N-1}, \mathbf{p}_{N-1}) = \frac{1}{8} a_{N-1}^2 b_{12\ldots N-2} \prod_{i=1}^{N-2} A_{i,N-1}. \tag{68}$$

Now, generalizing the expressions (36), (46) and (60), we have

$$b_{12\ldots N} = \frac{1}{2^{N-1}} \frac{\Delta_{12\ldots N}}{D_{12\ldots N}}, \quad D_{12\ldots N} = \prod_{1 \leqslant i < j \leqslant N} D_{ij}, \tag{69}$$

with D_{ij} given in Eq. (34). It only remains to determine the numerator $\Delta_{12\ldots N}$ in Eq. (69) which is a homogeneous polynomial in p_i [modulo the dispersion relations $\omega_i \propto p_i^3$, Eq. (18)] of total degree $3N(N-1)$, equal to that of $D_{12\ldots N}$. Further, one easily verifies the parity transformation

$$b_{12\ldots N}(\mathbf{p}_1, \ldots, \mathbf{p}_{N-1}, -\mathbf{p}_N) = \frac{b_{12\ldots N}(\mathbf{p}_1, \ldots, \mathbf{p}_N)}{A_{1N} A_{2N} \cdots A_{N-1,N}},$$

which implies that $\Delta_{12\ldots N}$ is of even/odd degree in each of the wave numbers if N is odd/even.

To deduce the functional form of $\Delta_{12\ldots N}$, we first make use of the reduction (67) which shows that

$$\Delta_{12\ldots N} \sim 2.3^{N-1} p_1^2 p_2^2 \cdots p_{N-1}^2 p_N^{N-1} \Delta_{12\ldots N-1} \prod_{i=1}^{N-1} (5\omega_i - 2p_i^3) \quad \text{as} \quad p_N \to 0.$$

Allowing for symmetry, we may therefore write [cf. Eqs. (47) and (61)]

$$\Delta_{12\ldots N} = 2.3^{N-1} \left\langle\!\!\left\langle p_{i_1}^2 p_{i_2}^2 \cdots p_{i_{N-1}}^2 p_{i_N}^{N-1} \Delta_{i_1 i_2 \ldots i_{N-1}} \prod_{k=1}^{N-1} (5\omega_{i_k} - 2p_{i_k}^3) \right\rangle\!\!\right\rangle + H_{12\ldots N}, \tag{70}$$

where $\langle\!\langle\ \rangle\!\rangle$ denotes the sum over all distinct permutations of $(1,2,\ldots,N)$ assigned to the subscripts $(i_1, i_2, \ldots, i_N)$ of the enclosed product. Thus, the $\langle\!\langle\ \rangle\!\rangle$ term in (70) contains the terms of lowest degree p_i^{N-1} in any of the wave numbers; but then the even/odd parity of $\Delta_{12\ldots N}$ implies that $H_{12\ldots N}$ is comprised of terms having minimum degree $N+1$ in each wave number. To obtain the *principal term* of $H_{12\ldots N}$ we use the reduction (68) and maximum degree argument. Putting $\mathbf{p}_N = \mathbf{p}_{N-1}$ in Eq. (69) and equating with (68), we find that [cf. Eq. (63)]

$$\Delta_{12\ldots N}\big|_{\mathbf{p}_N = \mathbf{p}_{N-1}} = (-1)^{N-2} 30 p_{N-1}^3 (4\omega_{N-1} - p_{N-1}^3) \Delta_{12\ldots N-2} \prod_{i=1}^{N-2} D_{i,N-1} D_{i,N-1}^{-}. \tag{71}$$

We note that the right-hand side of Eq. (71) has maximum degree $T_N = T_{N-2} + 10$ in p_1 with $T_2 = 5$ and $T_3 = 10$, whereupon $T_N = 5(N-1)$, $N \geqslant 2$. But since this reduction leaves p_1 untouched,

the maximum degree of *any* p_i in $\Delta_{12\ldots N}$, and hence in $H_{12\ldots N}$, must also be $5(N-1)$. If we combine this result with the total degree $3N(N-1)$, and minimum degree $N+1$ in each p_i, we are able to formulate the principal term of $H_{12\ldots N}$ as

$$\langle\!\langle p_{i_1}^{5(N-1)} p_{i_2}^{5(N-1)} \cdots p_{i_k}^{5(N-1)} \cdots p_{i_{N-l+1}}^{N+1} \cdots p_{i_{N-1}}^{N+1} p_{i_N}^{N+1} \rangle\!\rangle.$$

The precise number k and l of terms with maximum and minimum degree, respectively—and the consequent intermediary terms of decreasing degree—will depend on N [cf. Eqs. (48) and (62)]. The remaining terms that make up $H_{12\ldots N}$ follow by systematically cascading the powers of p_i and successively replacing $p_i^3 \to \omega_i$ [via the dispersion relation (18)], just as we did in Eq. (62) for $N=4$. We can now formulate $H_{12\ldots N}$ as a linear combination of these terms, fixing as many of the coefficients as possible by using the other $N-2$ reductions of the type (67), $b_{12\ldots N}(\mathbf{p}_1,\ldots,\mathbf{p}_k,\mathbf{0},\ldots,\mathbf{0})$, $1 \leqslant k \leqslant N-2$, and the reduction (68). However, these reductions will not be sufficient to determine all the coefficients in $H_{12\ldots N}$ and we return to bilinear form (19) to complete the derivation of the N-soliton. We substitute *truncated* versions of f and $\tilde{g}$ [cf. Eqs. (52) and (53)]—consistent with extracting only the terms in $e^{\theta_1+\theta_2+\cdots+\theta_N}$—into the bilinear equations (19a) and (19b). This yields an equation for $\Delta_{12\ldots N}$ which is equated with (70) to find the remaining unknown coefficients in $H_{12\ldots N}$. With $\Delta_{12\ldots N}$, and hence $b_{12\ldots N}$ and $f(x,t)$, now completely determined, we obtain the explicit N-soliton solution of the bKK Eq. (1) using $u=-\partial_x^2 \ln f$.

V. DISCUSSION

In this sequel to a recent study,[1] we have presented a direct method for obtaining explicit multisoliton solutions of the bidirectional Kaup–Kupershmidt equation (1). Not surprisingly, these solitons possess the remarkable property that their wave profiles are *directionally dependent*, a property that is inherited from the constituent solitary waves.[1] To our knowledge, this type of soliton interaction is quite unusual and is reported here for the first time. In particular, soliton solutions are presented that describe multiple head-on collisions of *single*- and *double*-humped "solitary" waves.

The "anomalous" character of the bKK solitons arises quite naturally within Hirota's bilinear formalism[24,25] in the guise of a *squared* regular N-soliton.[1] This canonical form, which derives from the duality of the bKK and bSK-Ramani equations, provides the basis for the iterative procedure that we have developed to obtain higher-order solitons. Significantly, the expression for the bKK N-soliton—like its unidirectional counterpart for the sister KK Eq. (2)[11]—requires the introduction of a new parameter $b_{12\ldots N}$, Eq. (69), at every order N; we therefore cannot write down an explicit formula for this solution akin to Hirota's generic form (10). This is in marked contrast to the bSK–Ramani equation whose N-soliton solution (10) is described by the single parameter A_{ij}, Eq. (11). Nevertheless, our formulation of the bKK solitons—couched in terms of the common interaction parameter A_{ij} and shared dispersion laws (12)—would seem to be a natural one, for it makes explicit the dynamical duality of the soliton solutions of the bKK and bSK-Ramani equations and points to the deep connection between these two fundamentally different integrable bidirectional equations. This mirrors the intimacy between their better known unidirectional cousins, the KK Eq. (2) and SK Eq. (4), respectively.[2,11,14]

Although we have sought to describe the iterative procedure in some detail (Sec. IV C), a few salutary remarks are in order. Compared with the iteration method that was used to obtain the multisoliton solutions of the sister KK Eq. (2),[11] the procedure given here for the bKK equation is less definitive. The reason for this is clear. The unidirectional KK solitons possess a high degree of symmetry which permits a precise description of the iterative steps.[11] For the bKK equation, much, though by no means all, of this symmetry is lost due to the need to account for the bidirectionality. In particular, there is insufficient *a priori* information available to completely determine the "new" parameter $b_{12\ldots N}$ that is pivotal to formulating the bKK N-soliton [whereas just two reductions, comparable to Eqs. (67) and (68), were required to compute the equivalent KK parameter]. This lack of information stems from the fact that a bKK soliton cannot be reduced

to one of lower order by coalescing a single- and a double-humped solitary wave (the reason for this is given in Ref. 11). Consequently, it is necessary to revert to the bilinear form of the bKK equation to complete the derivation of $b_{12\ldots N}$ and, thereby, the N-soliton solution. Notwithstanding this ''extra'' step, we stress that the above iteration procedure yields the key parameter $b_{12\ldots N}$ in its simplest possible form since the quotient expression (69) is irreducible. Indeed, it is this simple and repetitive structure that makes an iterative approach viable. Were we to attempt to obtain this parameter by solving the bilinear equations directly, the algebraic demands would soon become intractable (as the order N increases) and lie beyond the competence of symbolic software (even with the necessary computational resources). To give a measure of the complexity one faces, even for $N=4$, direct substitution into the bilinear form yields a coefficient of $e^{\theta_1+\theta_2+\theta_3+\theta_4}$ with in excess of *half a million* terms. Moreover, it is extremely unlikely that the compact expression (69) could be obtained in this way. In part, this is because of the immense difficulty in identifying the ''correct'' factors that are needed to effect the simplification. But here the task is compounded by the option of using the dispersion relations (12) which enable us to recast an expression by removing (or inserting) powers of ω_i (a facility that has been been crucial to our analysis).

The simplification that derives from our direct approach—and from the structured procedure described in Sec. IV C—makes the computations manageable and should not be underestimated. Nevertheless, at some point, the length and complexity of the algebraic expressions involved will still be such that they will almost certainly breach the limit of available computational resource (though not the competence of algebraic software such as Mathematica). That said, the synergy between mathematical analysis and the power of symbolic computation to manage lengthy, but otherwise routine, algebraic manipulation is evident in this study. We have been able to exploit this synergy to elicit—and display—multisoliton solutions of the bKK equation which might otherwise be inaccessible. Naturally, it is interesting to speculate whether there are other bidirectional nonlinear evolution equations that possess directionally dependent solitons: to date, they appear to be unique to the bKK Eq. (1).

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APPENDIX: SINGULARITY ANALYSIS FOR THE BKK EQUATION

We briefly describe a singularity analysis for solutions of the bidirectional Kaup–Kupershmidt (bKK) equation (1). The results show that the bKK equation passes the Painlevé test for partial differential equations due to Weiss, Tabor and Carnevale (WTC).[26] [The full analysis for both this equation and the bSK-Ramani Eq. (3) will be presented elsewhere.] Using the results of the WTC analysis, we then examine the singularity properties of the functions that appear in the various bilinear forms of the bKK equation given in Sec. II. Judged from this perspective, we conclude that the coupled system (19) is a ''good'' Hirota bilinear form whereas the alternative bilinear equations (6) and (7) are not.

1. Painlevé analysis

To proceed with the singularity analysis, it is convenient to write the bKK Eq. (1) in its conservative form with $u=v_x$:

$$5v_{tt}+5v_{xxxt}-15v_xv_{xt}-15v_{xx}v_t-45v_x^2v_{xx}+\frac{75}{2}v_{xx}v_{3x}+15v_xv_{4x}-v_{6x}=0. \tag{A1}$$

Following the WTC method,[26] we seek a Laurent expansion

$$v(x,t)=\phi^{-\rho}\sum_{k=0}^{\infty}v_k(x,t)\phi^k \quad (v_0\not\equiv 0), \tag{A2}$$

where $\phi(x,t)$, $v_k(x,t)$ are analytic functions in the neighborhood of an arbitrary (noncharacteristic) singular manifold $\phi(x,t)=0$ (ϕ_x, $\phi_t\neq 0$). Substituting the series (A2) into (A1), the balance of leading order terms in ϕ^{-7} yields $\rho=1$ and the two choices

$$v_0=-\phi_x, \quad v_0=-8\phi_x. \tag{A3}$$

Inserting the series (A2) with $\rho=1$ into (A1), and collecting terms in ϕ^{k-7}, we obtain a recurrence relation for v_k ($k\geqslant 1$):

$$(k-1)(k-6)\phi_x^4[(k-2)(k-3)(k-4)(k-5)\phi_x^2+15(k^2-8k+18)\phi_x v_0+45v_0^2]v_k=F_k, \tag{A4}$$

with $F_k=F_k(v_0,v_1,\ldots,v_{k-1};\phi_x,\phi_t,\ldots)$. The choices (A3) lead to the resonance families

$$k=-1, 1, 3, 5, 6, 7; \tag{A5}$$

$$k=-7,-1, 1, 6, 10, 12, \tag{A6}$$

respectively. To simplify the succeeding analysis, we introduce the Kruskal manifold ansatz[27]

$$\phi(x,t)=x-x_0(t), \tag{A7}$$

where $x_0(t)$ and $v_k(t)$ are analytic functions of t only. It can be shown that all compatibility conditions are satisfied for both resonant sets (A5) and (A6). It follows that Eq. (A1), and hence the bKK Eq. (1), has the Painlevé property.[26,28]

We observe that only the first family (A5) has a full complement of positive resonances and, for our purposes, we need consider only this principal branch. In this case, the Laurent series (A2) provides a local representation of the general solution of Eq. (A1) in which x_0, v_1, v_3, v_5, v_6, v_7 are arbitrary functions of t. Using the recurrence relation (A4) with $v_0=-\phi_x=-1$, one finds that

$$v(x,t)=-\frac{1}{x-x_0}+v_1+\frac{1}{3}x_0'(x-x_0)+v_3(x-x_0)^2+\frac{1}{9}(2x_0'^2-3v_1')(x-x_0)^3+\cdots, \tag{A8}$$

where a prime denotes the derivative with respect to t. Hence, $v(x,t)$ has a simple pole on the movable singular manifold path $x=x_0(t)$. The Laurent expansion for $u=v_x$ follows directly from (A8) as

$$u(x,t)=\frac{1}{(x-x_0)^2}+\frac{1}{3}x_0'+2v_3(x-x_0)+\frac{1}{3}(2x_0'^2-3v_1')(x-x_0)^2+\cdots. \tag{A9}$$

Thus, solutions of the bKK Eq. (1) have, at worst, a polelike behavior of order 2 in the neighborhood of the singular manifold $x=x_0(t)$.

2. Hirota bilinear transform

We consider the consequences of the Painlevé analysis for the bilinearization of the bKK equation. From Eq. (5) we have $v=\alpha\partial_x \ln f$: after equating this with (A8) and integrating with respect to x, we have

$$f(x,t)=(x-x_0)^{-1/\alpha}\exp\left\{\frac{1}{\alpha}\left[c+v_1(x-x_0)+\frac{1}{6}x_0'(x-x_0)^2+\frac{1}{3}v_3(x-x_0)^3+\cdots\right]\right\}, \tag{A10}$$

where $c=c(t)$ is an arbitrary function. Equation (A10) shows that, for the bKK Eq. (1), the appropriate choice is $\alpha=-1$ since it leads to an Hirota function $f(x,t)$ which is *entire*. This accords with our choice of dependent variable transformation $u=-\partial_x^2 \ln f$ and justifies expanding

f as a finite polynomial of exponentials. We note that the alternative choice $\alpha=-2$ in (A10) yields an ansatz f in the bilinear form (7) having a square-root branch singularity—it does not therefore lead to a "good" Hirota form. [Incidentally, a similar Painlevé analysis for the bSK-Ramnai Eq. (3) shows that the choice $\alpha=-2$ in (5) leads to entire f in the Ramani bilinear form (9) as expected.]

We are left to consider the two possible bilinear forms (6) and (19) of the bKK equation corresponding to $\alpha=-1$ (with f entire). Then (A10) shows that $f\sim(x-x_0)$ near a pole singularity of $v(x,t)$. Now, substituting the Laurent expansion (A8) into Eq. (6b), one readily obtains

$$g(x,t)=\frac{1}{x-x_0}+O(x-x_0),$$

while Eq. (6c) gives

$$h(x,t)=-\frac{4x_0'}{x-x_0}+O(1),$$

near $x_0(t)$. Hence, the auxiliary functions g and h in the bilinear form (6) are *not* entire since each has a simple pole singularity in the vicinity of a zero of f. On the other hand, from (19b) we deduce that

$$\tilde{g}(x,t)=-24v_3+6(v_1'-x_0'^2)(x-x_0)+O(x-x_0)^2,$$

which shows that $\tilde{g}$ *is* an entire function. We conclude that (19) is a "good" Hirota bilinear form and should therefore be used instead of the alternate bilinear system (6) which is not.

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A nonconfocal involutive system and constrained flows associated with the MKdV_ equation

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By symmetry constraints, new finite-dimensional integrable systems are deduced from a Lax representation of the MKdV_ equation, whose two terms containing spatial derivatives have the same sign. Lax representations are presented for the resulting finite-dimensional integrable systems and an r-matrix formulation is established for the corresponding Lax operator. From the Lax operator, a nonconfocal involutive system of functionally independent polynomial functions is constructed. Solutions of the MKdV_ can be obtained by the method of separation of variables. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1506202]

I. INTRODUCTION

The technique of symmetry constraints of soliton equations is a powerful tool to generate $1+1$ dimensional soliton equations from $2+1$ dimensional soliton equations[1,2] and finite-dimensional integrable systems (FDISs) from $1+1$ dimensional soliton equations.[3] Various FDISs have been presented starting from the Lax representations (or zero curvature equation representations) of $1+1$ dimensional soliton equations,[3–13] by using that symmetry constraint technique (or direct nonlinearization of Lax systems[4–8]). The resulting FDISs have many nice mathematical properties. For example, they possess Lax representations and their Lax operators satisfy r-matrix relations. Following a procedure of Sklyanin,[15] one can define separated variables for most of the resulting FDISs, which serve for constructing the Jacobi inversion problems.

In recent years, the study of separation of variables of soliton equations in $1+1$ dimensions (or $2+1$ dimensions) has attracted an increasing attention.[15–20] It has been shown that soliton equations in $1+1$ dimensions possessing Lax representations can be separated into two commuting FDISs (x-part and t-part of constrained flows) by symmetry constraints. Then, one can get solutions of soliton equations by solving the corresponding x-part and t-part of constrained flows. This process together with separating variables for the constrained flows constitutes separation of variables for soliton equations.[18]

The method of separation of variables has been used to construct solutions of soliton equations associated with the ZS-AKNS spectral problem.[18,21] It is well known that from the ZS-AKNS spectral problem, under the potential reductions $r=+q$ and $r=-q$, one obtains the MKdV equations

$$q_t-q_{xxx}+6q^2q_x=0$$

and

$$q_t+q_{xxx}+6q^2q_x=0,$$

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respectively. They are called the MKdV_+ and MKdV_- equations, respectively. The MKdV_+ equation has different signs but the MKdV_- equation has the same sign for the two terms containing spatial derivatives of the dependent variable q. Starting from other two specific spectral problems, the FDISs associated with the MKdV_+ equation have been obtained by symmetry constraints (Bargmann type),[22–25] and the associated r-matrices are different from the r-matrix in the case of the ZS-AKNS spectral problem.[24,25] However, there is no result on symmetry constraints of the MKdV_- equation, although there exists some analysis on symmetry constraints of the MKdV_+ equation.[23,24]

In this paper, we would like to start from a new, convenient spectral problem to derive the MKdV_- hierarchy and consider the corresponding problem of symmetry constraints for the MKdV_- equation. It is known that all important 2×2 matrix spectral problems associated with soliton equations are exhausted. However, the classification task of constrained flows always presents problems. To our surprise, the resulting r-matrices in the case of the MKdV_- equation are very different from the existing r-matrices in the case of the MKdV_+ equation,[24,25] and the type of the Lie algebra generated from the Lax operator associated with the resulting constrained flows has not been seen so far in the study of constrained flows. More importantly, an involutive system being nonconfocal can be presented. It is absolutely not easy to get nonconfocal involutive systems of polynomial functions, starting from 2×2 matrix spectral problems. Almost all examples established in the theory of constrained flows are confocal. Moreover, through the difference between two Lie algebras associated with two Lax operators, we will see different solution types for the MKdV_+ equations and the MKdV_- equation.

The paper is organized as follows. In Sec. II, starting from a new, specific spectral problem, we derive a soliton hierarchy of the MKdV_- equations. In Sec. III, we construct the constrained flows of the MKdV_- equation by the Bargmann symmetry constraints and decompose the MKdV_- equation into two FDISs, the x-part and t-part of the constrained flows. In Sec. IV, we deduce the r-matrix formulation, present a nonconfocal involutive system of functionally independent polynomial functions and show the Liouville integrability of the constrained flows. In Sec. V, we construct action-angle variables and the Jacobi inversion problems for the resulting constrained flows of the MKdV_- equation. Some concluding remarks are given in Sec. VI. Finally, in the Appendix, we show that the different spectral problems appearing in the literature associated with the MKdV_+ equation and the MKdV_- equation are gauge equivalent to each other, respectively.

II. MKdV_- SOLITON HIERARCHY

Let us consider a specific spectral problem

$$\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}_x = U(q,\lambda)\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}, \quad U(q,\lambda)=\begin{pmatrix}0 & \lambda+q\\ \lambda-q & 0\end{pmatrix}, \tag{1}$$

where λ is a spectral parameter and $q=q(x,t)$ is the potential. We solve the adjoint equation

$$V_x=[U,V]\equiv UV-VU, \tag{2}$$

by assuming

$$V=\begin{pmatrix}A & B\\ C & -A\end{pmatrix}=\sum_{j=0}^{\infty}\begin{pmatrix}a_j & b_j\\ c_j & -a_j\end{pmatrix}\lambda^{-j}. \tag{3}$$

The components of the adjoint equation (2) read as

$$A_x=(\lambda+q)C-B(\lambda-q), \quad B_x=-2A(\lambda+q), \quad C_x=2A(\lambda-q). \tag{4}$$

Upon introducing

$$E=B+C, \quad F=C-B, \quad \text{or} \quad C=\frac{E+F}{2}, \quad B=\frac{E-F}{2}, \tag{5}$$

the conditions (4) can be written as follows:

$$A_x=\lambda F+qE, \quad E_x=-4Aq, \quad F_x=4\lambda A.$$

It is direct to obtain the recursion relation

$$LF=\lambda^2 F, \quad L=\frac{1}{4}\partial_x^2+q\partial_x^{-1}q\partial_x, \quad \partial_x=\frac{\partial}{\partial x}. \tag{6}$$

Assuming that

$$E=\sum_{j=0}^{\infty} e_j\lambda^{-j}, \quad F=\sum_{j=0}^{\infty} f_j\lambda^{-j}, \tag{7}$$

if we take $a_0=f_0=a_1=0$, $e_0=-1$, then we find

$$f_{2n}=a_{2n+1}=e_{2n+1}=0, \quad n=1,2,\ldots$$

and

$$f_1=q, \quad f_{2n+1}=Lf_{2n-1}, \quad a_{2n}=\tfrac{1}{4}f_{2n-1,x}, \quad e_{2n}=-\partial_x^{-1}q\partial_x f_{2n-1}, \quad n=1,2,\ldots. \tag{8}$$

The first few of the above functions read as

$$f_3=\tfrac{1}{4}q_{xx}+\tfrac{1}{2}q^3, \quad a_2=\tfrac{1}{4}q_x, \quad e_2=-\tfrac{1}{2}q^2;$$

$$f_5=\tfrac{1}{16}q_{xxxx}+\tfrac{5}{8}q^2q_{xx}+\tfrac{5}{8}qq_x^2+\tfrac{3}{8}q^5, \quad a_4=\tfrac{1}{8}q_{xxx}+\tfrac{3}{4}q^2q_x, \quad e_4=-\tfrac{1}{4}q^2q_{xx}+\tfrac{1}{8}qq_x^2-\tfrac{3}{8}q^5.$$

Let us associate the spectral problem (1) with the auxiliary spectral problem

$$\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}_{t_n}=V^{(n)}(q,\lambda)\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}=V^{(n)}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}, \tag{9}$$

with $V^{(n)}$ being chosen as

$$V^{(n)}=V^{(n)}(q,\lambda)=(\lambda^{2n-1}V)_+, \quad n\geqslant 0, \tag{10}$$

where the plus symbol $_+$ denotes taking the terms of non-negative powers of λ. The zero curvature equations

$$U_{t_n}-V_x^{(n)}+[U,V^{(n)}]=0, \quad n\geqslant 1, \tag{11}$$

lead to the following soliton hierarchy of MKdV$_-$ equations

$$q_{t_n}+\tfrac{1}{2}\partial_x f_{2n-1}=0, \quad n=1,2,\ldots, \tag{12}$$

which when $n=2$, gives the MKdV$_-$ equation

$$q_{t_2}+\tfrac{1}{8}q_{xxx}+\tfrac{3}{4}q^2q_x=0, \tag{13}$$

where the constants can be rescaled to the previous one in the introduction.

III. CONSTRAINED MKdV_ FLOWS

It is direct to find that for the spectral problem (1), we have

$$\int_{-\infty}^{\infty}[\lambda'[K](\phi_1^2-\phi_2^2)-K(\phi_1^2+\phi_2^2)]dx=0,$$

and thus we obtain the variatial derivative of the spectral parameter λ (up to a constant factor)

$$\frac{\delta\lambda}{\delta q}=\phi_1^2+\phi_2^2. \tag{14}$$

There are also the following relations for the spectral problem (1):

$$(\phi_1^2+\phi_2^2)_x=4\lambda\phi_1\phi_2,\ \ (\phi_1^2+\phi_2^2)_{xx}=4\lambda(\phi_2^2+\phi_1^2)+4\lambda(\phi_2^2-\phi_1^2),\ \ (\phi_2^2-\phi_1^2)_x=-4\phi_1\phi_2 q, \tag{15}$$

and thus under zero boundary conditions of ϕ_1 and ϕ_2, we can show that

$$L\frac{\delta\lambda}{\delta q}=\lambda^2\frac{\delta\lambda}{\delta q}, \tag{16}$$

which implies that the operator L has an eigenvalue λ^2.

We take N copies of the spectral problem (1) with N distinct λ_j

$$\begin{pmatrix}\phi_{1j}\\ \phi_{2j}\end{pmatrix}_x=U(q,\lambda_j)\begin{pmatrix}\phi_{1j}\\ \phi_{2j}\end{pmatrix},\quad j=1,2,\ldots,N. \tag{17}$$

From (14), we have (up to a constant factor)

$$\frac{\delta\lambda_j}{\delta q}=\phi_{1j}^2+\phi_{2j}^2,\quad j=1,2,\ldots,N.$$

Now, we take the Bargmann symmetry constraint[3]

$$a_2=\sum_{j=1}^{N}\frac{1}{4}\partial_x\frac{\delta\lambda_j}{\delta q},\quad \text{i.e.,}\quad q=\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle, \tag{18}$$

where $\langle .,. \rangle$ denotes the standard inner product in $\mathbb{R}^N$ and

$$\Phi_j=(\phi_{j1},\ldots,\phi_{jN})^T,\quad j=1,2. \tag{19}$$

From (8), (15), and (16), we have

$$\begin{aligned}&\tilde{f}_1=\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle,\quad \tilde{f}_{2n+1}=\langle\Lambda^{2n}\Phi_1,\Phi_1\rangle+\langle\Lambda^{2n}\Phi_2,\Phi_2\rangle,\\ &\tilde{a}_{2n}=\langle\Lambda^{2n-1}\Phi_1,\Phi_2\rangle,\quad \tilde{e}_{2n}=\langle\Lambda^{2n-1}\Phi_2,\Phi_2\rangle-\langle\Lambda^{2n-1}\Phi_1,\Phi_1\rangle,\end{aligned} \tag{20}$$

where $\tilde{a}_i$, $\tilde{e}_i$, and $\tilde{f}_i$ denote the constrained expressions under the constraint (18) and zero boundary conditions of ϕ_{ij}, and the matrix Λ is defined by

$$\Lambda=\mathrm{diag}(\lambda_1,\ldots,\lambda_N). \tag{21}$$

Under the symmetry constraint (18), the N copies of the spectral problem (1) are nonlinearized into a system of ordinary differential equations

$$\Phi_{1x}=(\Lambda+\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle)\Phi_2,\quad \Phi_{2x}=(\Lambda-\langle\Phi_1,\Phi_1\rangle-\langle\Phi_2,\Phi_2\rangle)\Phi_1, \tag{22}$$

which can be transformed into a Hamiltonian system in the symplectic space $(R^{2n}, d\Phi_2 \wedge d\Phi_1)$

$$\Phi_{1x} = \frac{\partial H_1}{\partial \Phi_2}, \quad \Phi_{2x} = -\frac{\partial H_1}{\partial \Phi_1}, \tag{23}$$

with the Hamiltonian H_1 being defined by

$$H_1 = \tfrac{1}{4}(\langle \Phi_1, \Phi_1 \rangle + \langle \Phi_2, \Phi_2 \rangle)^2 + \tfrac{1}{2}\langle \Lambda \Phi_2, \Phi_2 \rangle - \tfrac{1}{2}\langle \Lambda \Phi_1, \Phi_1 \rangle.$$

From (5) and (20), we have

$$A(\lambda) = \sum_{j=1}^{N} \frac{\lambda_j \phi_{1j} \phi_{2j}}{\lambda^2 - \lambda_j^2}, \quad F(\lambda) = \sum_{j=1}^{N} \frac{\lambda(\phi_{1j}^2 + \phi_{2j}^2)}{\lambda^2 - \lambda_j^2}, \quad E(\lambda) = -1 + \sum_{j=1}^{N} \frac{\lambda_j(\phi_{2j}^2 - \phi_{1j}^2)}{\lambda^2 - \lambda_j^2}, \tag{24}$$

and then we define a Lax operator as

$$\begin{aligned} L(\lambda) &\equiv \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & -A(\lambda) \end{pmatrix} \\ &\equiv \begin{pmatrix} A(\lambda) & \dfrac{E(\lambda) - F(\lambda)}{2} \\ \dfrac{E(\lambda) + F(\lambda)}{2} & -A(\lambda) \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} + \frac{1}{2}\sum_{j=1}^{N} \begin{pmatrix} \dfrac{2\lambda_j \phi_{1j} \phi_{2j}}{\lambda^2 - \lambda_j^2} & \dfrac{\lambda_j(\phi_{2j}^2 - \phi_{1j}^2) - \lambda(\phi_{1j}^2 + \phi_{2j}^2)}{\lambda^2 - \lambda_j^2} \\ \dfrac{\lambda_j(\phi_{2j}^2 - \phi_{1j}^2) + \lambda(\phi_{1j}^2 + \phi_{2j}^2)}{\lambda^2 - \lambda_j^2} & \dfrac{-2\lambda_j \phi_{1j} \phi_{2j}}{\lambda^2 - \lambda_j^2} \end{pmatrix}. \end{aligned} \tag{25}$$

Now, by a direct computation, we have the following theorem.

Theorem 1. *The spectral constrained MKdV$_-$ flow (23) admits the Lax representation*

$$(L(\lambda))_x = [\tilde{U}, L(\lambda)], \tag{26}$$

where $\tilde{U}$ is given by

$$\tilde{U} = \begin{pmatrix} 0 & \lambda + \langle \Phi_1, \Phi_1 \rangle + \langle \Phi_2, \Phi_2 \rangle \\ \lambda - \langle \Phi_1, \Phi_1 \rangle - \langle \Phi_2, \Phi_2 \rangle & 0 \end{pmatrix}. \tag{27}$$

Under the symmetry constraint (18) and the control of the x-constrained flow (22), the t_2-constrained flow obtained from N copies of the temporal spectral problem (9) and (10) for N distinct λ_j reads as follows:

$$\begin{aligned} \Phi_{1j,t_2} &= \lambda_j \overline{A} \phi_{1j} + \tfrac{1}{2}(-\lambda_j^3 - \overline{B}\lambda_j^2 + \overline{C}\lambda_j - \overline{D})\phi_{2j}, \\ \phi_{2j,t_2} &= \tfrac{1}{2}(-\lambda_j^3 + \overline{B}\lambda_j^2 + \overline{C}\lambda_j + \overline{D})\phi_{1j} - \lambda_j \overline{A} \phi_{2j}, \end{aligned} \tag{28}$$

where $j = 1, 2, \ldots, N$, and

$$\begin{aligned}&\overline{A}=\langle\Lambda\Phi_1,\Phi_2\rangle,\ \ \overline{B}=\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle,\ \ \overline{C}=-\tfrac{1}{2}(\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle)^2,\\&\overline{D}=\langle\Lambda^2\Phi_1,\Phi_1\rangle+\langle\Lambda^2\Phi_2,\Phi_2\rangle+(\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle)(\langle\Lambda\Phi_2,\Phi_2\rangle-\langle\Lambda\Phi_1,\Phi_1\rangle)\\&\quad+\tfrac{1}{2}(\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle)^3.\end{aligned}\tag{29}$$

By a direct computation, this system can be rewritten in Hamiltonian form

$$\Phi_{1,t_2}=\frac{\partial H_2}{\partial\Phi_2},\quad \Phi_{2,t_2}=-\frac{\partial H_2}{\partial\Phi_1},\tag{30}$$

with H_2 being defined by

$$\begin{aligned}H_2=&\tfrac{1}{2}\langle\Lambda\Phi_1,\Phi_2\rangle^2-\tfrac{1}{4}(\langle\Lambda^3\Phi_2,\Phi_2\rangle-\langle\Lambda^3\Phi_1,\Phi_1\rangle)-\tfrac{1}{4}(\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle)(\langle\Lambda^2\Phi_1,\Phi_1\rangle\\&+\langle\Lambda^2\Phi_2,\Phi_2\rangle)-\tfrac{1}{8}(\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle)^2(\langle\Lambda\Phi_2,\Phi_2\rangle-\langle\Lambda\Phi_1,\Phi_1\rangle)\\&-\tfrac{1}{16}(\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle)^4.\end{aligned}$$

Therefore, we have the following theorem.

Theorem 2. *The temporal constrained MKdV$_-$ flow (30) admits the Lax representation*

$$L_{t_2}=[\tilde{V}^{(2)},L],\tag{31}$$

where $\tilde{V}^{(2)}$ is given by

$$\tilde{V}^{(2)}=\frac{1}{2}\begin{pmatrix}2\overline{A}\lambda & -\lambda^3-\overline{B}\lambda^2+\overline{C}\lambda-\overline{D}\\ -\lambda^3+\overline{B}\lambda^2+\overline{C}\lambda+\overline{D} & -2\overline{A}\lambda\end{pmatrix},\tag{32}$$

with $\overline{A}$, $\overline{B}$, $\overline{C}$, and $\overline{D}$ being defined by (29).

Proof. By using (26), the zero curvature equation and the Jacobi identity,

$$\tilde{U}_{t_n}-\tilde{V}^{(2)}_x+[\tilde{U},\tilde{V}^{(2)}]=0,$$

$$[[\tilde{V}^{(2)},\tilde{U}],L]+[[L,\tilde{V}^{(2)}],\tilde{U}]+[[\tilde{U},L],\tilde{V}^{(2)}]=0,$$

we can prove $\tilde{V}_x=[\tilde{U},\tilde{V}]$, where $\tilde{V}=L_{t_2}-[\tilde{V}^{(2)},L]$. Note that $\tilde{V}|_{\phi_{ij}=0}=0$ ($i=1,2$, $j=1,\ldots,N$). It follows from $\tilde{V}_x=[\tilde{U},\tilde{V}]$ that $\tilde{V}\equiv 0$. Thus we have the Lax representation (31). The Theorem is proved.

IV. A NONCONFOCAL INVOLUTIVE SYSTEM AND COMPLETE INTEGRABILITY OF THE CONSTRAINED FLOWS

In this section, we use the r-matrix theory to prove that the constrained MKdV$_-$ flows (23) and (30) are completely integrable Hamiltonian systems in the sense of Liouville.[14]

Under the standard Poisson bracket in $\mathbb{R}^{2n}$

$$\{f,g\}=\sum_{j=1}^{N}\left(\frac{\partial f}{\partial\phi_{1j}}\frac{\partial g}{\partial\phi_{2j}}-\frac{\partial f}{\partial\phi_{2j}}\frac{\partial g}{\partial\phi_{1j}}\right),\tag{33}$$

a direct computation can give rise to

$$\begin{aligned}
&\{A(\lambda),A(\mu)\}=\{E(\lambda),E(\mu)\}=\{F(\lambda),F(\mu)\}=0,\\
&\{A(\lambda),E(\mu)\}=\frac{2(\lambda F(\lambda)-\mu F(\mu))}{\mu^2-\lambda^2},\\
&\{A(\lambda),F(\mu)\}=\frac{2\mu(E(\lambda)-E(\mu))}{\mu^2-\lambda^2},\\
&\{E(\lambda),F(\mu)\}=\frac{-8\mu(A(\lambda)-A(\mu))}{\mu^2-\lambda^2}.
\end{aligned} \tag{34}$$

Therefore, we can obtain an important Lie algebra

$$\begin{aligned}
&\{A(\lambda),A(\mu)\}=0,\\
&\{B(\lambda),B(\mu)\}=\frac{2}{\lambda+\mu}(A(\lambda)-A(\mu)),\\
&\{C(\lambda),C(\mu)\}=\frac{2}{\lambda+\mu}(A(\lambda)-A(\mu)),\\
&\{A(\lambda),B(\mu)\}=\frac{1}{\lambda-\mu}B(\lambda)-\frac{1}{\lambda+\mu}C(\lambda)-\frac{2\mu}{\lambda^2-\mu^2}B(\mu),\\
&\{A(\lambda),C(\mu)\}=\frac{1}{\lambda+\mu}B(\lambda)-\frac{1}{\lambda-\mu}C(\lambda)+\frac{2\mu}{\lambda^2-\mu^2}C(\mu),\\
&\{B(\lambda),C(\mu)\}=\frac{2}{\lambda-\mu}(A(\lambda)-A(\mu)).
\end{aligned} \tag{35}$$

These commutator relations show us a specific characteristic for the resulting MKdV$_-$ hierarchy. Usually, $\{A(\lambda),B(\mu)\}$ is a linear combination of A and B, and $\{A(\lambda),C(\mu)\}$ is a linear combination of A and C. But in (35), the situation is different. The commutator relations (35) are of new type among examples of Lax operators appearing in the study of constrained flows.

Now as usual, assume that

$$L_1(\lambda)=L(\lambda)\otimes I,\quad L_2(\mu)=I\otimes L(\mu), \tag{36}$$

and $\{L_1(\lambda)\overset{\otimes}{,}L_2(\mu)\}$ is the fundamental Poisson bracket. A tactful search can present the following r-matrix formulation for the Lax operator $L(\lambda)$.

Theorem 3. *Let $L(\lambda)$ be defined by (25). Then we have the r-matrix formulation*

$$\{L_1(\lambda)\overset{\otimes}{,}L_2(\mu)\}=[L_1(\lambda),r_{12}(\lambda,\mu)]+[r_{21}(\lambda,\mu),L_2(\mu)], \tag{37}$$

where the r matrices are given by

$$r_{12}(\lambda,\mu)=\begin{pmatrix}
\frac{\lambda}{\lambda^2-\mu^2} & 0 & 0 & \frac{1}{\lambda+\mu}\\
0 & \frac{\lambda}{\mu^2-\lambda^2} & \frac{1}{\lambda-\mu} & 0\\
0 & \frac{1}{\lambda-\mu} & \frac{\lambda}{\mu^2-\lambda^2} & 0\\
\frac{1}{\lambda+\mu} & 0 & 0 & \frac{\lambda}{\lambda^2-\mu^2}
\end{pmatrix},\quad r_{21}(\lambda,\mu)=r_{12}(\mu,\lambda). \tag{38}$$

The integrals of motion of two constrained flows can be obtained from expanding $\frac{1}{2}trL^2(\lambda) = -\det L(\lambda)$. We observe that

$$-\det L(\lambda)=A^2(\lambda)+B(\lambda)C(\lambda)=A^2(\lambda)+\frac{1}{4}(E^2(\lambda)-F^2(\lambda))=\frac{1}{4}+\sum_{j=1}^{N}\frac{\lambda_j I_j}{\lambda^2-\lambda_j^2},$$

where the I_j are defined by

$$I_j=-\frac{1}{2}(\phi_{2j}^2-\phi_{1j}^2)-\frac{1}{4\lambda_j}(\phi_{2j}^2+\phi_{1j}^2)^2+\sum_{k\neq j,k=1}^{N}\frac{\lambda_k B_{jk}-\lambda_j A_{jk}}{\lambda_j^2-\lambda_k^2}, \tag{39}$$

with A_{ij} and B_{ij} being defined by

$$A_{ij}=A_{ji}=(\phi_{2j}^2+\phi_{1j}^2)(\phi_{2i}^2+\phi_{1i}^2), \quad B_{ij}=B_{ji}=(\phi_{1i}\phi_{1j}+\phi_{2i}\phi_{2j})^2-(\phi_{1i}\phi_{2j}-\phi_{1j}\phi_{2i})^2.$$

Alternatively, expanding $-\det(A)$ in powers of λ^{-2}, based on (20) and (24), we have

$$\begin{aligned}\sum_{n=0}^{\infty}F_n\lambda^{-2n}:=A^2+\frac{1}{4}(E^2-F^2)&=\left(\sum_{j=1}^{\infty}\frac{\tilde{a}_{2j}}{\lambda^{2j}}\right)^2+\frac{1}{4}\left[\left(-1+\sum_{j=1}^{\infty}\frac{\tilde{e}_{2j}}{\lambda^{2j}}\right)^2-\left(\sum_{j=1}^{\infty}\frac{\tilde{f}_{2j-1}}{\lambda^{2j-1}}\right)^2\right]\\&=\frac{1}{4}+\left(-\frac{1}{2}\tilde{e}_2+\frac{1}{4}\tilde{f}_1^2\right)\frac{1}{\lambda^2}+\sum_{n=2}^{\infty}\left(\sum_{k+l=n}\tilde{a}_{2l}\tilde{a}_{2n}-\frac{1}{2}\tilde{e}_{2n}\right.\\&\quad\left.+\frac{1}{4}\sum_{k+l=n}\tilde{e}_{2k}\tilde{e}_{2l}-\frac{1}{4}\sum_{l+k=n-1}\tilde{f}_{2l+1}\tilde{f}_{2k+1}\right)\frac{1}{\lambda^{2n}}.\end{aligned}$$

Therefore, the integrals of motion F_n read as

$$F_0=\frac{1}{4},\quad F_1=-\frac{1}{2}\tilde{e}_2-\frac{1}{4}\tilde{f}_1^2=-H_1,$$

$$F_n=\sum_{k+l=n}\tilde{a}_{2l}\tilde{a}_{2n}-\frac{1}{2}\tilde{e}_{2n}+\frac{1}{4}\sum_{k+l=n}\tilde{e}_{2k}\tilde{e}_{2l}-\frac{1}{4}\sum_{k+l=n-1}\tilde{f}_{2l+1}\tilde{f}_{2k+1},\quad n\geqslant 2. \tag{40}$$

From the r-matrix formulation (37) or a direct computation of

$$\{A^2(\lambda)+B(\lambda)C(\lambda),A^2(\mu)+B(\mu)C(\mu)\}=0,$$

it follows that:

$$\{I_i(\lambda),I_j(\mu)\}=0 \ \text{ or } \ \{F_i(\lambda),F_j(\mu)\}=0. \tag{41}$$

This means that the integrals of motion are involution in pair. The involutive system of the polynomial functions I_j, $j=1,2,\ldots,N$, is completely different from the confocal system,[7] and actually it is nonconfocal.

To show the complete integrability of the constrained flows (23) and (30) we need only to prove that the integrals of motion F_n, $n=1,2,\ldots,N$, are functionally independent over some open subset of $\mathbb{R}^{2N}$.

To the end, we use the ϵ-technique proposed in Ref. 26. Let $p_0=(\phi_{11},\ldots,\phi_{1N},\phi_{21},\ldots,\phi_{2N})$ be a point of $\mathbb{R}^{2N}$ satisfying $\phi_{jl}=\epsilon$, $j=1,2$, $l=1,2,\ldots,N$, where ϵ is a small parameter. From the expressions of F_n defined by (40) and (20), it follows that:

$$\left.\frac{\partial F_n}{\partial\phi_{jl}}\right|_{p_0}=-(-1)^j\lambda_l^{2n-1}\epsilon+O(\epsilon^3).$$

Therefore,

$$\left.\begin{pmatrix} \frac{\partial F_1}{\partial \phi_{11}} & \frac{\partial F_2}{\partial \phi_{11}} & \cdots & \frac{\partial F_N}{\partial \phi_{11}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial F_1}{\partial \phi_{1N}} & \frac{\partial F_2}{\partial \phi_{1N}} & \cdots & \frac{\partial F_N}{\partial \phi_{1N}} \end{pmatrix}\right|_{p_0} = \begin{pmatrix} \lambda_1 & \lambda_1^3 & \cdots & \lambda_1^{2N-1} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_N & \lambda_N^3 & \cdots & \lambda_N^{2N-1} \end{pmatrix} \epsilon^N + O(\epsilon^{3N})$$

$$= \epsilon^N \prod_{j=1}^{N} \lambda_j \prod_{1 \leqslant i < j \leqslant N} (\lambda_j^2 - \lambda_i^2) + O(\epsilon^{3N}).$$

This implies that when

$$\lambda_j \neq 0, \quad j = 1,2,\ldots,N, \quad \lambda_i^2 - \lambda_j^2 \neq 0, \quad 1 \leqslant i \neq j \leqslant N, \tag{42}$$

the functions F_n, $n=1,2,\ldots,N$, are functionally independent over some dense open subset of $\mathbb{R}^{2N}$ and so are the functions I_j, $j=1,2,\ldots,N$.

Theorem 4. *Assume that (42) holds. Then the Hamiltonian systems (23) and (30) have N functionally independent integrals of motion F_n, $n=1,2,\ldots,N$, which are in involution in pair, and thus the systems (23) and (30) are completely integrable systems in the sense of Liouville.*

V. ACTION-ANGLE VARIABLES AND THE JACOB INVERSION PROBLEMS

We present action-angle variables for the finite-dimensional integrable systems (23) and (30). Let us introduce

$$\tilde{A}(\lambda) = \frac{iF(\lambda)}{2}, \quad \tilde{B}(\lambda) = A(\lambda) + \frac{iE(\lambda)}{2}, \quad \tilde{C}(\lambda) = A(\lambda) - \frac{iE(\lambda)}{2}. \tag{43}$$

By using the relations (34), we have

$$\begin{gathered} \{\tilde{A}(\lambda), \tilde{A}(\mu)\} = 0, \ \{\tilde{B}(\lambda), \tilde{B}(\mu)\} = 0, \ \{\tilde{C}(\lambda), \tilde{C}(\mu)\} = 0, \\ \{\tilde{A}(\lambda), \tilde{B}(\mu)\} = \frac{\lambda}{\mu^2 - \lambda^2}(\tilde{B}(\mu) - \tilde{B}(\lambda)), \\ \{\tilde{A}(\lambda), \tilde{C}(\mu)\} = \frac{\lambda}{\mu^2 - \lambda^2}(\tilde{C}(\lambda) - \tilde{C}(\mu)), \\ \{\tilde{B}(\lambda), \tilde{C}(\mu)\} = \frac{2}{\mu^2 - \lambda^2}(\mu\tilde{A}(\mu) - \lambda\tilde{A}(\lambda)). \end{gathered} \tag{44}$$

These relations are just the same as the relations (33) in Ref. 25, and thus we can use the same process as that in Ref. 25 to present action-angle variables as follows. Note that if u_k is a zero point of $\tilde{B}(\lambda)$, then so is $-u_k$, and thus we have

$$\tilde{B}(\pm u_k) = 0, \quad k = 1,2,\ldots,N. \tag{45}$$

We assume that the choice of $\lambda_1,\ldots,\lambda_N$, makes all zero points of $B(\lambda)$ simple. But note that not all these zero points are real, since $\tilde{B}(\lambda)$ is complex. In the case of the MKdV$_+$ equation, $\tilde{B}(\lambda)$ is real.

The other N variables are chosen to be

$$v_k=\tilde{A}(u_k)=\sum_{j=1}^{N}\frac{u_k(i\phi_{1j}^2+i\phi_{2j}^2)}{u_k^2-\lambda_j^2},\quad k=1,2,\ldots,N. \tag{46}$$

A similar deduction as in Ref. 25 yields that u_k and v_k, $k=1,2,\ldots,N$, are canonically conjugated variables, i.e.,

$$\{u_i,u_j\}=\{v_i,v_j\}=0,\quad \{u_i,v_j\}=\delta_{ij},\quad i,j=1,2,\ldots,N. \tag{47}$$

We denote

$$\det L(\lambda)=\frac{P(\lambda)}{K(\lambda)},\quad K(\lambda)=\prod_{j=1}^{N}(\lambda^2-\lambda_j^2), \tag{48}$$

and $P(\lambda)$ is a $2N$th-order polynomial of λ:

$$P(\lambda)=P_N\lambda^{2N}+P_{N-1}\lambda^{2N-2}+\cdots+P_0=\sum_{j=0}^{N}P_j\lambda^{2j},$$

$$P_N=\tfrac{1}{4},\quad P_{N-1}=-H_1-\tfrac{1}{4}\alpha_1,\quad P_{N-2}=2H_2+\alpha_1(-P_{N-1}-\tfrac{1}{4}\alpha_1)+\tfrac{1}{4}\alpha_2, \tag{49}$$

$$\alpha_1=\sum_{j=1}^{N}\lambda_j^2,\quad \alpha_2=\sum_{1\leqslant j<l\leqslant N}\lambda_j^2\lambda_l^2.$$

All P_j can be expressed by $I_1,\ldots,I_N$ or $F_1,\ldots,F_N$, and thus the P_i's are integrals of motion of (23) and (30), and we have

$$\{P_i,P_j\}=0,\quad i,j=1,2,\ldots,N. \tag{50}$$

We observe that

$$\det L(u_k)=-\tfrac{1}{4}F^2(u_k)=\tilde{A}^2(u_k)=v_k^2,$$

which leads to

$$P(u_k)=K(u_k)v_k^2,\quad k=1,2,\ldots,N. \tag{51}$$

Therefore, u_k and v_k, $k=1,2,\ldots,N$, constitute a set of separated variables for (23) and (30). To obtain the Hamilton–Jacobi equation, we replace the canonical momentum components v_k in (51) by the partial derivatives $v_k=\partial S/\partial u_k$. The function S can be separated as $S(u_1,\ldots,u_N)=\Sigma_{k=1}^{N}S_k(u_k)$, where

$$\left[\frac{\partial S_k(u_k)}{\partial u_k}\right]^2=\frac{P(u_k)}{K(u_k)},\quad k=1,2,\ldots,N. \tag{52}$$

Therefore, we have

$$S(u_1,\ldots,u_N)=\sum_{k=1}^{N}\int^{u_k}\frac{P(\lambda)}{\sqrt{P(\lambda)K(\lambda)}}d\lambda,$$

which gives rise to the linearization coordinates

$$Q_k=\frac{\partial S}{\partial P_k}=\frac{1}{2}\sum_{k=1}^{N}\int^{u_k}\frac{\lambda^{2k}d\lambda}{\sqrt{P(\lambda)K(\lambda)}},\quad k=0,\ldots,N-1. \tag{53}$$

These angle variables Q_k, $k=1,2,\ldots,N$, constitute the whole set of action-angle variables together with the action variables P_k, $k=1,2\ldots,N$.

Now based on (49), the linear flow defined by (23) is then given by

$$Q_i=c_i+\frac{\partial H_1}{\partial P_i}x=c_i-x\delta_{i,N-1}, \quad i=0,1,\ldots,N-1, \tag{54}$$

where the c_i's are independent of t_2, and the linear flow defined by (30) is then given by

$$Q_i=\overline{c}_i+\frac{\partial H_2}{\partial P_i}t_2=\overline{c}_i+\frac{1}{2}(\delta_{i,N-2}+\alpha_i\delta_{i,N-1})t_2, \quad i=0,1,\ldots,N-1, \tag{55}$$

where the $\overline{c}_i$'s are independent of x. These two linear flows together with (53) yield the Jacobi inversion problems for (23) and (30)

$$\frac{1}{2}\sum_{k=1}^{N}\int^{u_k}\frac{\lambda^{2k}d\lambda}{\sqrt{P(\lambda)K(\lambda)}}=c_i-x\delta_{i,N-1}, \quad k=0,\ldots,N-1,$$

$$\frac{1}{2}\sum_{k=1}^{N}\int^{u_k}\frac{\lambda^{2k}d\lambda}{\sqrt{P(\lambda)K(\lambda)}}=\overline{c}_i+\frac{1}{2}(\delta_{i,N-2}+\alpha_i\delta_{i,N-1})t_2, \quad k=0,\ldots,N-1,$$

respectively. Then by using the Jacobi inversion technique, one can find solutions of the MKdV$_-$ equation (13) in terms of Riemann theta functions.

VI. CONCLUSIONS AND REMARKS

By the Bargmann symmetry constraints, two commuting finite-dimensional integrable Hamiltonian systems were presented from the constrained flows of a specific spectral problem for the MKdV$_-$ equation. The Lax pairs of those two finite-dimensional systems were given, and the r-matrix formulation was established for the corresponding common Lax operator. We point up that the resulting r-matrices are of new type and the Lax operator leads to a nonconfocal involutive system of polynomial functions, which is a good supplement to the existing theory of symmetry constraints.

Moreover, we presented action-angle variables and the Jacobi inversion problems for those two finite-dimensional integrable systems. Then the solutions of the MKdV$_-$ equation can be obtained by the method of separation of variables and solving the resulting Jacobi inversion problems. The difference from the deduction in the case of the MKdV$_+$ equation[25] is that not all the separated variables are real. Therefore, the MKdV$_+$ equation and the MKdV$_-$ equation have different type solutions. This is also reflected by a Bäcklund transformation $q_+(ix,it)=q_-(x,t)$, where $q_\pm$ are solutions of the MKdV$_+$ equation and the MKdV$_-$ equation, respectively.

Finally in the Appendix, we show that a couple of different spectral problems appearing in the literature associated with the MKdV$_+$ equation and the MKdV$_-$ equation are gauge equivalent to each other, respectively.

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APPENDIX A

By the reductions $r=\pm q$, the ZS-AKNS spectral problem (1) becomes

$$\mathrm{MKdV}_+: \quad \Psi_x=\begin{pmatrix} -\lambda & q \\ q & \lambda \end{pmatrix}\Psi \equiv U_+\Psi, \tag{A1}$$

$$\mathrm{MKdV}_-: \quad \Psi_x=\begin{pmatrix} -\lambda & q \\ -q & \lambda \end{pmatrix}\Psi \equiv U_-\Psi, \tag{A2}$$

which generate the MKdV_+ and MKdV_- hierarchies, respectively. The MKdV_+ equation also can be associated with the spectral problem[22]

$$\bar{\Phi}_x=\begin{pmatrix} -q & \lambda^2 \\ 1 & q \end{pmatrix}\bar{\Phi} \equiv \bar{M}\bar{\Phi}, \tag{A3}$$

and the spectral problem[22,25]

$$\Phi_x=\begin{pmatrix} -q & \lambda \\ \lambda & q \end{pmatrix}\Phi \equiv M\Phi. \tag{A4}$$

By using the gauge transformations

$$\bar{\Phi}=T_1\Phi, \quad T_1=\begin{pmatrix} \lambda & 0 \\ 0 & 1 \end{pmatrix},$$

we have

$$\bar{M}=T_1MT_1^{-1}.$$

By using the gauge transformation

$$\Phi=T_3\Psi, \quad T_3=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix},$$

and noting

$$T_3^{-1}=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix},$$

we have

$$M=T_3U_+T_3^{-1}$$

and

$$U=T_3U_-T_3^{-1},$$

where U is defined by (1). Therefore, for the MKdV_+ equation, the spectral problems (A1), (A3) and (A4) are gauge equivalent to each other, and for the MKdV_- equation, the spectral problem (1) is gauge equivalent to the spectral problem (A2).

The MKdV_+ equation discussed here is also related to the spectral problem[23,24]

$$\hat{\Phi}_x = \begin{pmatrix} q & \lambda^2 \\ -1 & -q \end{pmatrix} \hat{\Phi} = \hat{M}\hat{\Phi}. \tag{A5}$$

We take $i\lambda$ to replace λ, then $\hat{M}$ is transformed into

$$\begin{pmatrix} q & -\lambda^2 \\ -1 & -q \end{pmatrix} = -\overline{M}.$$

The zero curvature equation associated with (A3) reads as

$$\overline{M}_{t_n} - V_x + \overline{M}V - V\overline{M} = 0, \tag{A6}$$

and the zero curvature equation associated with (A5)

$$-\overline{M}_{t_n} - W_x - \overline{M}W + W\overline{M} = 0. \tag{A7}$$

Interestingly, if we take $-x$ to replace x, then (A6) and (A7) are transformed into each other. Therefore, the MKdV$_+$ equation obtained in Refs. 23 and 24 is equivalent to the MKdV$_+$ equation discussed in this paper.

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Hamiltonian flow associated with a two-dimensional map

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For a given differentiable map $(x,y)\to(X(x,y),Y(x,y))$, which has an inverse, we show that there exists a Hamiltonian flow in which x plays the role of the time variable while y is fixed. © *2002 American Institute of Physics.*
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Let us consider a differentiable map

$$(x,y)\to(X(x,y),Y(x,y)), \tag{1}$$

and assume that it has an inverse

$$(X,Y)\to(x,y). \tag{2}$$

A small change of (x,y) causes a variation of (X,Y). They are governed by

$$\begin{pmatrix}\partial_x\\ \partial_y\end{pmatrix}=J\begin{pmatrix}\partial_X\\ \partial_Y\end{pmatrix},\quad J:=\begin{pmatrix}J_{xX} & J_{xY}\\ J_{yX} & J_{yY}\end{pmatrix}, \tag{3}$$

where $\partial_x:=\partial/\partial x$, $J_{xX}:=\partial X/\partial x$, etc., or

$$\begin{pmatrix}\partial_X\\ \partial_Y\end{pmatrix}=J^{-1}\begin{pmatrix}\partial_x\\ \partial_y\end{pmatrix}. \tag{4}$$

To be specific we consider the case in which y is fixed while x is changed. We introduce the notation

$$Q(x):=X(x,y),\quad P(x):=Y(x,y).$$

Then from (3) the variations of (Q,P) are given by

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$$\frac{dQ}{dx}=J_{xX},\quad \frac{dP}{dx}=J_{xY}. \tag{5}$$

We can prove the following:

Proposition 1: Let H be a function of (Q,P) which is given by

$$H(Q,P)=\int^{y(Q,P)}(\det J)dy, \tag{6}$$

and satisfies

$$\frac{\partial H}{\partial x}=0.$$

Then the following system of Hamilton's equations holds:

$$\frac{dQ}{dx}=\frac{\partial H}{\partial P},\quad \frac{dP}{dx}=-\frac{\partial H}{\partial Q}. \tag{7}$$

Conversely, if $H(Q,P)$ satisfies Hamilton's equations, then it must be of the above form.

Note that the value x plays the role of time variable of this system. The proof is straightforward. Applying (4) to H yields

$$\begin{pmatrix}\partial_Q H\\ \partial_P H\end{pmatrix}=J^{-1}\begin{pmatrix}\partial_x H\\ \partial_y H\end{pmatrix}. \tag{8}$$

If we impose the condition that H satisfies

$$J^{-1}\begin{pmatrix}\partial_x H\\ \partial_y H\end{pmatrix}=\begin{pmatrix}-J_{xY}\\ J_{xX}\end{pmatrix}, \tag{9}$$

and compare with (5), the Hamilton equations (7) follow. To solve (9) for H, we multiply J from the left and obtain

$$\begin{pmatrix}\partial_x H\\ \partial_y H\end{pmatrix}=J\begin{pmatrix}-J_{xY}\\ J_{xX}\end{pmatrix}=\begin{pmatrix}0\\ \dfrac{\partial X}{\partial x}\dfrac{\partial Y}{\partial y}-\dfrac{\partial X}{\partial y}\dfrac{\partial Y}{\partial x}\end{pmatrix},$$

hence

$$\partial_x H=0,\quad \partial_y H=\frac{\partial X}{\partial x}\frac{\partial Y}{\partial y}-\frac{\partial X}{\partial y}\frac{\partial Y}{\partial x}=\det J.$$

Therefore (6) is obtained. (*QED*)

This article is motivated by an observation found by one of the authors (AS) during the study of the quantized Hénon map,[1] and generalizes the result to a wide class of maps. Before closing let us present the case of the Hénon map, which is defined by

$$\begin{pmatrix}X\\ Y\end{pmatrix}=\begin{pmatrix}x^2-y+c\\ x\end{pmatrix},\quad \begin{pmatrix}x\\ y\end{pmatrix}=\begin{pmatrix}Y\\ Y^2-X+c\end{pmatrix},\quad J=\begin{pmatrix}2x & 1\\ -1 & 0\end{pmatrix}. \tag{10}$$

Since $\det J=1$, we have simply $H=y+\text{const}$, hence

$$H(Q,P)=P^2-Q+c. \tag{11}$$

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Hamiltonian structures on foliations

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We discuss Hamiltonian structures of the Gelfand–Dorfman complex of projectable vector fields and differential forms on a foliated manifold. Such a structure defines a Poisson structure on the algebra of foliated functions, and embeds the given foliation into a larger, generalized foliation with presymplectic leaves. In a so-called tame case, the structure is induced by a Poisson structure of the manifold. Cohomology spaces and classes relevant to geometric quantization are also considered. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1502928]

I. PRELIMINARIES

Let $\mathcal{S}$ be a moving body with supplementary physical characteristics, expressed by scalar parameters, which have no impact on the motion but depend on the latter. For instance, the temperature of a rigid body which moves with high friction.

The mathematical model of such a system will consist of a *configuration space* which is an s-dimensional differentiable manifold N endowed with a p-dimensional foliation $\mathcal{G}$ such that the supplementary parameters are the coordinates along the leaves of $\mathcal{G}$, and the position coordinates are constant along these leaves. Then, the *phase space* of $\mathcal{S}$ will be the total space M of the annihilator bundle $\nu^*\mathcal{G}\subseteq T^*N$ of the tangent bundle $T\mathcal{G}$, and M is endowed with the natural lift $\mathcal{F}$ of $\mathcal{G}$, which is such that the leaves of $\mathcal{F}$ are covering spaces of the leaves of $\mathcal{G}$ (see, e.g., see Ref. 7).

Since the motion does not depend on the supplementary parameters, the Hamiltonian function H of the system will be an *$\mathcal{F}$-foliated function* on M, i.e., a function which is constant along the leaves of $\mathcal{F}$. On the other hand, since we want the motion to determine the time evolution of the supplementary parameters, we should be able to define the Hamiltonian vector field of H as a foliated vector field on the phase space of $\mathcal{S}$.

Therefore, $(M,\mathcal{F})$ should be endowed with a *generalized Hamiltonian structure* that prescribes foliated Hamiltonian vector fields to foliated functions. The aim of this paper is to initiate the study of such Hamiltonian structures.

The generalized Hamiltonian structures we need may be defined within the general Gelfand–Dorfman scheme of Hamiltonian structures on complexes over a Lie algebra.[1,2] For convenience, we refer to such complexes as *Gelfand–Dorfman complexes*,[13] and recall their definition in the following.

Definition 1.1: A *Gelfand–Dorfman complex* consists of:
(i) a real Lie algebra $(\chi,[\ ,\ ])$;
(ii) a cochain complex of real vector spaces

$$\mathcal{C}=\left(\bigoplus_{k=0}^{\infty}\Omega^k,\ \ d:\Omega^k\to\Omega^{k+1},\ \ d^2=0\right);$$

(iii) mappings $X\mapsto i(X)\in L_{\mathbf{R}}(\Omega^k,\Omega^{k-1})$, $(\Omega^{-1}:=0;\ :=$ denotes a definition), defined for all X

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$\in\chi$ and $k=0,1,2,\ldots$, such that
(a) if $\alpha\in\Omega^1$ and $i(X)\alpha=0$ for all $X\in\chi$ then $\alpha=0$;
(b) if $L_X:=di(X)+i(X)d$ then

$$i(X)i(Y)+i(Y)i(X)=0,\ \ i([X,Y])=L_Xi(Y)-i(Y)L_X. \tag{1}$$

Usually, one says that $\mathcal{C}$ is a *complex over* χ, and the mapping $X\mapsto i(X)$ encountered in Definition 1.1 may be seen as a *representation of* χ *on* $\mathcal{C}$. This mapping also defines a pairing

$$\langle\alpha,X\rangle=\langle X,\alpha\rangle:=i(X)\alpha,\quad X\in\chi,\alpha\in\Omega^1,$$

and, in particular, one denotes $Xf:=\langle \mathrm{d}f,X\rangle,\ f\in\Omega^0,X\in\chi$.

A linear mapping $H\in L_{\mathbf{R}}(\Omega^1,\chi)$ is said to be *skew symmetric* if

$$\langle\alpha,H\beta\rangle=-\langle\beta,H\alpha\rangle,\quad \forall\alpha,\beta\in\Omega^1. \tag{2}$$

The Hamiltonian structures of a Gelfand–Dorfman complex are defined by generalizing the notion of a Poisson bivector (e.g., Ref. 11). For this purpose, one notices that the formula[1,2]

$$[H,K](\alpha,\beta,\gamma):=\sum_{\mathrm{Cycl}(\alpha,\beta,\gamma)}\{\langle KL_{H\alpha}\beta,\gamma\rangle+\langle HL_{K\alpha}\beta,\gamma\rangle\}, \tag{3}$$

where $H,\ K\in L_{\mathbf{R}}(\Omega^1,\chi)$ are skew symmetric and $\alpha,\ \beta,\ \gamma\in\Omega^1$, may be seen as defining a bracket

$$[H,K]\in L_{\mathrm{alt},\mathbf{R}}((\Omega^1)^3,\Omega^0),$$

which is a generalization of the Schouten–Nijenhuis bracket of bivector fields on manifolds. We call bracket (3) the *Gelfand–Dorfman bracket*. Then, one defines

Definition 1.2: A skew-symmetric homomorphism $H\in L_{\mathbf{R}}(\Omega^1,\chi)$ which satisfies the *Poisson condition* $[H,H]=0$ is called a *Hamiltonian structure* on the Gelfand–Dorfman complex $(\chi,\mathcal{C})$.

For a Hamiltonian structure one defines the following generalizations of classical notions:
(i) $\forall f\in\Omega^0,\ X_f:=H(\mathrm{d}f)\in\chi$ is the *Hamiltonian vector* of f;
(ii) $\forall f,g\in\Omega^0,\ \{f,g\}:=X_fg$ is the *Poisson bracket*; this bracket is skew-symmetric because of (2), and it satisfies the Jacobi identity because (3) yields

$$[H,H](\mathrm{d}f,\mathrm{d}g,\mathrm{d}h)=2\sum_{\mathrm{Cycl}(f,g,h)}\{\{f,g\},h\};$$

(iii) $\forall\alpha,\beta\in\Omega^1$, one has a Ω^1-*bracket*

$$\{\alpha,\beta\}:=L_{H\alpha}\beta-L_{H\beta}\alpha-d\langle H\alpha,\beta\rangle, \tag{4}$$

with the particular case

$$\{\mathrm{d}f,\mathrm{d}g\}=\mathrm{d}\{f,g\}. \tag{5}$$

The Ω^1-bracket (4) may be defined for any skew-symmetric mapping $H\in L_{\mathbf{R}}(\Omega^1,\chi)$, and it satisfies the following fundamental identities:[4,12]

$$\langle\gamma,H\{\alpha,\beta\}\rangle=\langle\gamma,[H\alpha,H\beta]\rangle+\tfrac{1}{2}[H,H](\alpha,\beta,\gamma), \tag{6}$$

$$\sum_{\mathrm{Cycl}(\alpha,\beta,\gamma)}\langle\{\{\alpha,\beta\},\gamma\},X\rangle=[H,L_XH](\alpha,\beta,\gamma)+\frac{1}{2}\sum_{\mathrm{Cycl}(\alpha,\beta,\gamma)}[H,H](\alpha,\beta,d\langle\gamma,X\rangle), \tag{7}$$

where $\alpha,\ \beta,\ \gamma\in\Omega^1,\ X\in\chi$, and

$$L_X H(\alpha) := [X, H\alpha] - H(L_X \alpha). \tag{8}$$

In the Hamiltonian case $[H,H]=0$, it follows from (7) that the Ω^1-bracket is a Lie algebra bracket. Furthermore, under the supplementary *regularity hypothesis*: if $\forall\, \alpha \in \Omega^1\ \langle \alpha, X\rangle = 0$ then $X=0$ $(X \in \chi)$, H is a homomorphism of Lie algebras, i.e.,

$$H\{\alpha,\beta\} = [H\alpha, H\beta]. \tag{9}$$

On the other hand, even without the regularity hypothesis, (6) shows that if we ask $H \in L_{\mathbf{R}}(\Omega^1, \chi)$ to be skew symmetric and satisfy (9), H is a Hamiltonian structure.

II. HAMILTONIAN STRUCTURES OF FOLIATIONS

With the motivation of Sec. I in mind, let us consider an arbitrary n-dimensional differentiable manifold M (in the present paper "everything" is of differentiability class C^∞) endowed with a p-dimensional foliation $\mathcal{F}$. An object of M that projects to the space of the leaves of $\mathcal{F}$ is called either *projectable* or *foliated*. We refer the reader to Ref. 7 for all the notions of foliation theory which we are going to use.

The Lie algebra $\chi_{\mathcal{F}}$ of the $\mathcal{F}$-foliated vector fields and the complex of projectable differential forms $\Omega_{\mathcal{F}} = \oplus_{k=1}^{q} \Omega^k_{\mathcal{F}}$ $(q := n-p)$, with the usual exterior differential and contraction operators $i(X)$, $X \in \chi_{\mathcal{F}}$, define a Gelfand–Dorfman complex associated with the pair $(M,\mathcal{F})$. One might consider general Hamiltonian structures on this complex, but, such a structure may have a nonlocal character. We avoid nonlocality by

Definition 2.1: A *Hamiltonian structure* on (or of) the foliation $\mathcal{F}$ is a vector bundle morphism $h: \nu^*\mathcal{F} \to TM$ ($\nu\mathcal{F} = TM/T\mathcal{F}$ is the transversal bundle of $\mathcal{F}$) such that the induced map of cross sections $H: \Omega^1_{\mathcal{F}} \to \chi(M)$ [$\chi(M)$ is the space of all the tangent vector fields of M] is a Hamiltonian structure of the Gelfand–Dorfman complex of $(M,\mathcal{F})$.

In particular, Definition 2.1 implies that the morphism h is skew symmetric [i.e., it satisfies (2) pointwisely], and that the values of the mapping H are in $\chi_{\mathcal{F}}$.

Example 2.1: Any skew symmetric $h \in L_{\mathbf{R}}(\nu^*\mathcal{F}, T\mathcal{F})$ may be seen as a trivial Hamiltonian structure of the foliation $\mathcal{F}$. Indeed, formula (3) shows that $[H,H]=0$ if the values of H are vector fields tangent to $\mathcal{F}$

Example 2.2: Let P be a Poisson bivector field on the foliated manifold $(M,\mathcal{F})$, such that for any foliated function $f \in \Omega^0_{\mathcal{F}}$ the Hamiltonian vector field X^P_f is a foliated vector field. Define $\sharp_P : T^*M \to TM$ by $\langle \sharp_P \alpha, \beta\rangle := P(\alpha,\beta)$. Then, $h := \sharp_P|_{\nu^*\mathcal{F}}$ defines a Hamiltonian structure of the foliation $\mathcal{F}$.

Example 2.3: A bivector field P is called a *transversal Poisson structure* of $\mathcal{F}$ if the bracket

$$\{f,g\} := P(\mathrm{d}f, \mathrm{d}g) \quad (f,g \in C^\infty(M))$$

makes $\Omega^0_{\mathcal{F}}$ a Poisson algebra.[6] In this case, again, $h := \sharp_P|_{\nu^*\mathcal{F}}$ is a Hamiltonian structure of $\mathcal{F}$. Moreover, for any Hamiltonian structure h of $\mathcal{F}$ and any choice of a decomposition $TM = E \oplus T\mathcal{F}$, the bivector field P defined by

$$\sharp_P|_{E^* \approx \nu^*\mathcal{F}} = h, \quad \sharp_P|_{T^*\mathcal{F}} = 0$$

is a transversal Poisson structure of $\mathcal{F}$.

We also show how to express Hamiltonian structures of a foliation $\mathcal{F}$ by means of *adapted local coordinates* (x^a, y^u), where $a = 1,\ldots,q$; $u = q+1,\ldots,n$, and $x^a = \text{const}$ are the local equations of $\mathcal{F}$. In order to get an expression by tensors, we fix a decomposition $TM = E \oplus T\mathcal{F}$ where[8]

$$E = \mathrm{span}\left\{ X_a := \frac{\partial}{\partial x^a} - t^u_a \frac{\partial}{\partial y^u} \right\}, \quad T\mathcal{F} = \mathrm{span}\left\{ \frac{\partial}{\partial y^u} \right\}, \tag{10}$$

for some local coefficients t_a^u and with the Einstein summation convention. The local bases of TM defined by (10) have the dual co-bases

$$dx^a, \quad \theta^u := dy^u + t_a^u\, dx^a, \tag{11}$$

and $\nu^*\mathcal{F} = \mathrm{span}\{dx^a\}$.

Then, a skew-symmetric morphism $h: \nu^*\mathcal{F} \to TM$ has local equations

$$h(dx^a) = h^{ab} X_b + k^{au} \frac{\partial}{\partial y^u}. \tag{12}$$

The components h^{ab} define a global cross section W of $\wedge^2 E$, therefore, a global cross section of $\wedge^2 \nu\mathcal{F}$, which is independent of the choice of E, and the components k^{au} define a global cross section of $E \otimes T\mathcal{F}$. The following assertion is obvious.

Proposition 2.1: The morphism h defined by (12) is a Hamiltonian structure of $\mathcal{F}$ iff the cross section W with local components h^{ab} is foliated and defines a structure of Poisson algebra on $\Omega^0_{\mathcal{F}}$.

The Poisson bracket defined by W on $\Omega^0_{\mathcal{F}}$ is of the local type, and it has the following interpretation. Let U be an open neighborhood of M such that the manifold N of the slices of $\mathcal{F}$ in U exists, and let $p: U \to N$ be the natural projection (constant along the slices of $\mathcal{F}$ in U). Then $h_N(p(x)) := p_*(x) \circ (h|_U(x)) \circ p^*(p(x))$, $x \in U$, is the morphism $\sharp_{P_N}$ of a well-defined Poisson bivector field P_N on N, which defines the same local Poisson brackets as W. (h_N is well defined since the values of the mapping H defined by h are foliated vector fields.)

Furthermore, any Poisson algebra structure of local type on $\Omega^0_{\mathcal{F}}$ is defined by a family of Hamiltonian structures on $\mathcal{F}$. Indeed, the required structure is equivalent to a foliated section W of $\wedge^2 \nu(\mathcal{F})$, which satisfies the Poisson condition $[W,W] = 0$. Choose a decomposition $TM = E \oplus T\mathcal{F}$, and, $\forall \alpha \in \nu^*\mathcal{F}$, define $h(\alpha)$ to be the unique vector of E with projection $\sharp_W \alpha$ on $\nu\mathcal{F}$. Since by (3)

$$[H,H](\alpha,\beta,\gamma) = [W,W](\alpha,\beta,\gamma) \quad (\alpha,\beta,\gamma \in \Omega^1_{\mathcal{F}}),$$

h is a Hamiltonian structure of $\mathcal{F}$, and h induces W.

More exactly, if h_0 is one of the Hamiltonian structures which define W, the whole family which defines W is $h_0 + k$, where $k \in L_{\mathbf{R}}(\nu^*\mathcal{F}, T\mathcal{F})$ is skew symmetric. This holds since for any Hamiltonian structure h of $\mathcal{F}$ and any skew symmetric $k \in L_{\mathbf{R}}(\nu^*\mathcal{F}, T\mathcal{F})$, the corresponding morphisms H, K of global cross sections satisfy the relation $[H,K] = 0$ [see (3)].

Proposition 2.2: For any Hamiltonian structure h on a foliation $\mathcal{F}$, the generalized distribution $\mathcal{H} := T\mathcal{F} + \mathcal{H}_0$ ($\mathcal{H}_0 :=$ im h) is a projectable, completely integrable distribution, and its leaves are presymplectic manifolds with kernel $T\mathcal{F}$. Furthermore, $h(\mathrm{ann}\,\mathcal{H}) = \mathcal{H}_0 \cap T\mathcal{F}$ (ann *denotes the annihilator of a vector space or bundle*).

Proof: We continue to use the previous notation. Let $x_0 \in U \subseteq M$ where U is a neighborhood such that $\mathcal{F}|_U$ has a q-dimensional, transversal submanifold N. Since the projection p is a submersion, if $L_{p(x_0)}$ is the symplectic leaf of the Poisson structure P_N through $p(x_0) \in N$, $\tilde{L}_{x_0} := p^{-1}(L_{x_0})$ is an integral submanifold of $\mathcal{H}$ through x_0. The existence of these integral submanifolds shows the complete integrability of $\mathcal{H}$. Projectability follows from the fact that $\mathcal{H}_0$ is spanned by the projectable vector fields $H(\alpha)$, $\alpha \in \Omega^1_{\mathcal{F}}$, and $\mathcal{H}$ projects onto the symplectic distribution of P_N. The lift of the symplectic form of $L_{p(x_0)}$ by p^* yields the required presymplectic form of the corresponding leaf of $\mathcal{H}$. Finally, notice that $\alpha \in \mathrm{ann}\,\mathcal{H}$ iff $\alpha = p^*(\lambda)$ for some $\lambda \in \ker \sharp_{P_N}$, and then $p_* h(\alpha) = 0$. This implies $h(\mathrm{ann}\,\mathcal{H}) \subseteq \mathcal{H}_0 \cap T\mathcal{F}$. On the other hand, if $h(\alpha) \in T\mathcal{F}$, we must have $\alpha = p^*(\lambda)$ where $\lambda \in \ker \sharp_{P_N}$, and this justifies the converse inclusion. (All these also follow immediately from the local equations (12) of h.) Q.E.D.

The distribution $\mathcal{H}$ will be called the *characteristic distribution* of the Hamiltonian structure h, and its leaves constitute the *presymplectic foliation*. The Hamiltonian structure h of the foliation $\mathcal{F}$ on M will be called *transitive* if the characteristic distribution is $\mathcal{H} = TM$. In this case,

Proposition 2.2 tells us that M is a presymplectic manifold with the kernel foliation $\mathcal{F}$, and that $TM=\mathcal{H}_0\oplus T\mathcal{F}$. The latter equality also shows that the corresponding local Poisson structures P_N are the symplectic reduction of the presymplectic form of M. Conversely, if M is a presymplectic manifold with the presymplectic two-form σ, and if E is a complementary distribution of the kernel foliation $\mathcal{F}$ of σ, there exists a well-defined, transitive, Hamiltonian structure h of $\mathcal{F}$ such that $\mathcal{H}_0=E$ and the local Poisson structures P_N are the symplectic reductions of σ.

Example 2.4: Let $\mathcal{H}$ be a coisotropic foliation of dimension $n+k(k\leqslant n)$ of a symplectic manifold M of dimension $2n$, with the symplectic form ω. It is well known that the ω-orthogonal distribution of $\mathcal{H}$ is tangent to a foliation $\mathcal{F}$, and that, $\forall x\in M$, there exist local coordinates (x^a,x^u,y^i) around x such that $a=1,\ldots,p:=n-k$, $u=p+1,\ldots,n$, $i=1,\ldots,n$, $x^a=\text{const}$ are the local equations of $\mathcal{H}$, and the symplectic form has the canonical expression

$$\omega=\sum_{a=1}^{p}\mathrm{d}x^a\wedge\mathrm{d}y^a+\sum_{u=p+1}^{n}\mathrm{d}x^u\wedge\mathrm{d}y^u. \tag{13}$$

(This result is a theorem due to Lie.[5]) The local equations of the foliation $\mathcal{F}$ are $x^a=\text{const}$, $x^u=\text{const}$, $y^u=\text{const}$, and the computation of the Hamiltonian vector field X_f^ω of an $\mathcal{F}$-foliated function [via (13)] shows that X_f^ω is an $\mathcal{F}$-foliated vector field tangent to the leaves of $\mathcal{H}$. Therefore, $h:=-\flat_\omega^{-1}|_{\nu^*\mathcal{F}}$ is a Hamiltonian structure of the foliation $\mathcal{F}$ with the presymplectic foliation $\mathcal{H}$. Moreover, in this case we have $T\mathcal{F}\subseteq\mathcal{H}_0$.

Example 2.5: Example 2.4 can be generalized as follows. Let (M,ω) be an almost symplectic manifold (i.e., we ask ω to be nondegenerate but not necessarily closed), and let $\mathcal{H}$ be a coisotropic foliation such that the pullback of ω to every leaf of $\mathcal{H}$ is closed on the leaf. Then formula (13) is to be replaced by

$$\omega=\sum_{a=1}^{p}\mathrm{d}x^a\wedge\varpi^a+\sum_{u=p+1}^{n}\mathrm{d}x^u\wedge\mathrm{d}y^u, \tag{14}$$

where ϖ^a are linearly independent, local, one-forms which contain only the differentials $\mathrm{d}y^a$. Now, we obtain the foliation $\mathcal{F}$ and its Hamiltonian structure h in the same way as in the symplectic case.

We finish this section with a remark about the chosen definition of the notion of a Hamiltonian structure on a foliation.

If we start with the physical motivation of Sec. I, and do not think of Gelfand–Dorfman complexes *a priori*, the natural definition of a generalized Hamiltonian structure (ghs) that suites the problem is that of an **R**-linear morphism of sheaves

$$\Phi:\underline{\Omega^0_{\mathcal{F}}}\to\underline{\chi},\quad f\mapsto X_f, \tag{15}$$

(underlining means passing to germs of the corresponding type of objects), such that the bracket defined by

$$\{f,g\}=X_fg,\quad f,g\in\underline{\Omega^0_{\mathcal{F}}}, \tag{16}$$

makes $\Omega^0_{\mathcal{F}}$ a Poisson algebra sheaf.

In particular, the action of a Hamiltonian vector field X_f on foliated functions $g\in\Omega^0_{\mathcal{F}}$ depends only on the first jet j^1f. This is not enough to ensure that the ghs has local type. A natural condition for the latter property is to ask $X_f=0$ for all $f\in\Omega^0_{\mathcal{F}}$ such that $j^1_xf=0$ at each point $x\in M$. If the ghs structure Φ satisfies this locality condition, Φ is completely defined by local vector fields

$$X_{x^a}=h^{ab}X_b+k^{au}\frac{\partial}{\partial y^u}, \tag{17}$$

that satisfy the conditions of Proposition 2.1.

Therefore, the generalized Hamiltonian structures of local type are exactly the Hamiltonian structures of foliations which we defined earlier.

III. TAME HAMILTONIAN STRUCTURES

The Gelfand–Dorfman complex of a foliation does not satisfy the regularity hypothesis formulated at the end of Sec. I. The equality $\langle \alpha, X\rangle = 0$, $\forall \alpha \in \Omega^1_{\mathcal{F}}$, only implies $X \in \Gamma T\mathcal{F}$ (Γ denotes the space of global cross sections). Therefore, (9), or the equivalent property

$$X_{\{f,g\}} = [X_f, X_g], \quad \forall f, g \in \Omega^0_{\mathcal{F}}, \tag{18}$$

obtained by taking $\alpha = \mathrm{d}f$, $\beta = \mathrm{d}g$, f, $g \in \Omega^0_{\mathcal{F}}$ in (9), may not hold, and we shall define

Definition 3.1: A skew symmetric morphism $h: \nu^*\mathcal{F} \to TM$ which satisfies condition (18) is a *strong Hamiltonian structure* on $\mathcal{F}$.

Remark 3.1: If h is a strong Hamiltonian structure, the sheaf $\nu^*\mathcal{F}$ has a natural structure of a sheaf of twisted Lie algebras[3] over $(\mathbf{R}, \underline{\Omega^0_{\mathcal{F}}})$, with the action of $\underline{\text{germs}}$ $\alpha \in \underline{\nu^*\mathcal{F}}$ defined as the action of $H(\alpha)$.

Formula (6) shows that a strong Hamiltonian structure is Hamiltonian. The Hamiltonian structures indicated in Examples 2.2 and 2.4 are strong but this is not necessarily true for Examples 2.3 and 2.5. If h is a strong Hamiltonian structure, the generalized distribution $\mathcal{H}_0 = \mathrm{im}\, h$ is involutive. Conversely, if $\mathcal{H}_0$ is involutive and if $\mathcal{H}_0 \cap T\mathcal{F} = 0$, h is a strong Hamiltonian structure [use (6)]. These facts suggest

Definition 3.2: A Hamiltonian structure h of a foliation $\mathcal{F}$ is *transversal* (to $\mathcal{F}$) if there exists a differentiable complementary distribution E of $T\mathcal{F}$ ($E \oplus T\mathcal{F} = TM$) such that $\mathcal{H}_0 \subseteq E$. The distribution E will be called an *image extension* of h. (It is possible to have more than one image extension.) A transversal Hamiltonian structure of $\mathcal{F}$ is a *tame* structure if all the brackets of differentiable vector fields that belong to $\mathcal{H}_0$ are contained in an image extension E. (In the tame case, only such image extensions will be used.)

A tame Hamiltonian structure is strong [see (6)], and a transversal, strong Hamiltonian structure is tame. The condition $\mathcal{H}_0 \cap T\mathcal{F} = 0$, which is implicit in the definition of transversality, is equivalent to $h(\mathrm{ann}\,\mathcal{H}) = 0$ and also to the fact that the rank of the morphism h is equal to the rank of the Poisson structures induced by h on the manifolds of local slices of $\mathcal{F}$. [See Proposition 2.2 and formula (12)] This condition is not enough for transversality. Indeed, there always exists a smallest regular distribution $\overline{\mathcal{H}_0}$ which contains the generalized distribution $\mathcal{H}_0$ but, we may have $\overline{\mathcal{H}_0} \cap T\mathcal{F} \neq 0$.

Example 3.1: Let $TM = F \oplus F'$ be a locally product structure on the manifold M, and $\mathcal{F}$ the foliation tangent to F. Assume that one has a Poisson algebra structure of the local type on $\Omega^0_{\mathcal{F}}$. Then, the Hamiltonian structure h which induces the former and has its Hamiltonian vector field in F' is tame. Indeed, F' is an image extension of h of the kind required for tame structures. Notice also that a transitive, tame, Hamiltonian structure must be of the locally product type shown in the example.

Proposition 3.1: Let h be a transversal Hamiltonian structure of the foliation $\mathcal{F}$ with image extension E. Then h is tame with image extension E iff the Nijenhuis tensor N_E of the projection $p_E: TM \to TM$ of $TM = E \oplus T\mathcal{F}$ onto E satisfies the condition

$$N_E(h\alpha, h\beta) = 0, \quad \forall \alpha, \beta \in \nu^*_x\mathcal{F}, \quad \forall x \in M. \tag{19}$$

Proof: Following the general definition of a Nijenhuis tensor, e.g., Refs. 4 and 13 and since $p_E^2 = p_E$, for $X, Y \in \Gamma TM$, one has

$$N_E(X,Y) = [p_E X, p_E Y] - p_E[p_E X, Y] - p_E[X, p_E Y] + p_E[X,Y]. \tag{20}$$

Consider the local equations (12) of h using an image extension E, which implies that $k^{au}=0$. Then, h is tame iff

$$H(\mathrm{d}h^{ab})=[H(\mathrm{d}x^a),H(\mathrm{d}x^b)],$$

which is equivalent to

$$h^{ac}h^{be}\tau^u_{ce}=0,\quad \tau^u_{ce}:=\frac{\partial t^u_c}{\partial x^e}-\frac{\partial t^u_e}{\partial x^c}+t^v_c\frac{\partial t^u_e}{\partial y^v}-t^v_e\frac{\partial t^u_c}{\partial y^v}. \tag{21}$$

The invariant meaning of (21) is exactly (19). Q.e.d.

In the case of a transversal Hamiltonian structure h on a foliated manifold $(M,\mathcal{F})$ it is possible to extend the Hamiltonian formalism in a way similar to what was done for presymplectic manifolds in Ref. 9.

Let us recall that, if $(M,\mathcal{F})$ is a foliated manifold and if E is a complementary distribution of $T\mathcal{F}$, the use of the local bases (10), (11) yields a bigrading of tensor fields and differential forms, with the convention that the first degree is the E-degree and the second is the $T\mathcal{F}$-degree.[8] For instance, a differential k-form is of bidegree (s,t) if its local expressions contain s forms $\mathrm{d}x^a$ and t forms θ^u $(s+t=k)$. Then, one has a decomposition

$$d=d'_{(1,0)}+d''_{(0,1)}+\partial_{(2,-1)}, \tag{22}$$

and $d^2=0$ is equivalent to

$$\begin{gathered} d''^2=0,\quad \partial^2=0,\quad d'^2+d''\partial+\partial d''=0,\\ d'd''+d''d'=0,\quad \partial d'+d'\partial=0. \end{gathered} \tag{23}$$

Now, we return to the transversal Hamiltonian structure h of $\mathcal{F}$, and fix an image extension E of h. Then the corresponding section mapping H is well defined for any differential form $\alpha\in\Omega^{(1,0)}(M)$ of bidegree (1,0), and $H\alpha\in\Gamma E$. For any differentiable function $f\in C^\infty(M)$, we can define the Hamiltonian vector field $X'_f\in\Gamma E$ by

$$X'_f=H(d'f) \tag{24}$$

and $\forall f,g\in C^\infty(M)$ we get an *extended Poisson bracket*

$$\{f,g\}':=X'_fg=\langle Hd'f,dg\rangle=\langle Hd'f,d'g\rangle=-\{g,f\}'. \tag{25}$$

Furthermore, if $X\in\Gamma E$ and $\alpha\in\Omega^{(1,0)}(M)$, (22) leads to

$$L_X\alpha=L'_X\alpha+L''_X\alpha, \tag{26}$$

where

$$L'_X=i(X)d'+d'i(X),\quad L''_X=i(X)d''+d''i(X). \tag{27}$$

Accordingly, it is possible to extend the Gelfand–Dorfman bracket (3) to arbitrary (1,0)-forms α,β,γ by

$$[H,K]'(\alpha,\beta,\gamma):=\sum_{\mathrm{Cycl}(\alpha,\beta,\gamma)}\{\langle KL'_{H\alpha}\beta,\gamma\rangle+\langle HL'_{K\alpha}\beta,\gamma\rangle\}, \tag{28}$$

where H,K are defined by skew symmetric morphisms $h,k:\nu^*\mathcal{F}\to E$. A straightforward computation shows that the extended bracket is trilinear over $C^\infty(M)$, and for a Hamiltonian structure h we have $[H,H]'(\alpha,\beta,\gamma)=0$ for any $\alpha,\beta,\gamma\in\Omega^{(1,0)}(M)$.

In particular, using (25) and (27), one gets

$$[H,H]'(d'f,d'g,d'k)=2\sum_{\mathrm{Cycl}(f,g,k)}[\{\{f,g\}',k\}'+d'^2f(X'_g,X'_k)]=0. \tag{29}$$

Proposition 3.2: If h is a tame Hamiltonian structure on $(M,\mathcal{F})$ the Poisson bracket $\{,\}'$ defines a Poisson structure on the manifold M.

Proof: For any foliation and any choice of a complementary distribution E one gets

$$d'^2f(X,Y)=\langle d''f,N_E(X,Y)\rangle,\quad \forall f\in C^\infty(M),\ \forall X,Y\in\Gamma E, \tag{30}$$

where N_E is the Nijenhuis tensor (20). Indeed, if $X,Y\in\Gamma E$, (20) yields

$$N_E(X,Y)=p_{T\mathcal{F}}[X,Y], \tag{31}$$

where $p_{T\mathcal{F}}$ denotes the projection onto the second term of the decomposition $TM=E\oplus T\mathcal{F}$. On the other hand,

$$\begin{aligned}d'^2f(X,Y)&=d(d'f)(X,Y)=XYf-YXf-\langle d'f,[X,Y]\rangle=[X,Y]f-(p_E[X,Y])f\\&=\langle df,p_{T\mathcal{F}}[X,Y]\rangle=\langle d''f,p_{T\mathcal{F}}[X,Y]\rangle.\end{aligned}$$

Thus, (30) is justified, and the conclusion follows from the characterization (19) of the tame Hamiltonian structures and formula (29). Q.E.D.

Proposition 3.2 tells us that a tame Hamiltonian structure h is defined by a usual Poisson structure P on the foliated manifold $(M,\mathcal{F})$. The Hamiltonian vector fields of foliated functions with respect to h coincide with those with respect to P, $\sharp_P|_{E^*}=h$ and $\sharp_P|_{T^*\mathcal{F}}=0$. Thus, the tame Hamiltonian structures are included in Example 2.2. But, not all the structures of Example 2.2 are tame.

Similarly, it is possible to extend the bracket (4) of foliated one-forms to any $\alpha,\beta\in\Omega^{(1,0)}(M)$ by

$$\{\alpha,\beta\}':=L'_{H\alpha}\beta-L'_{H\beta}\alpha-d'\langle H\alpha,\beta\rangle. \tag{32}$$

From (32), it follows that $\forall f,g\in C^\infty(M)$ one has

$$\{f\alpha,g\beta\}'=fg\{\alpha,\beta\}'+f(H(\alpha)g)\beta-g(H(\beta)f)\alpha. \tag{33}$$

In particular, we see that the bracket (32) is skew symmetric because it is such for foliated one-forms, where it reduces to (4).

Let us also evaluate the bracket (32) on an argument $X\in\Gamma E$. First we define $L'_XH\in L_{\mathbf{R}}(\Omega^{(1,0)}(M),\Gamma E)$ by

$$L'_XH(\alpha):=p_E[X,H(\alpha)]-H(L'_X\alpha). \tag{34}$$

Taking the derivative of (2) in direction X, and with the decomposition (26), we see that L'_XH is skew symmetric. Then, if the derivatives L' of (32) are replaced by $L-L''$ one gets

$$\{\alpha,\beta\}'(X)=H(\alpha)i(X)\beta-H(\beta)i(X)\alpha-\langle\alpha,L'_XH(\beta)\rangle. \tag{35}$$

In particular, if $\alpha=d'f$, $\beta=d'g$, (35) yields

$$\{d'f,d'g\}'=d'\{f,g\}'+L_{X'_g}d''f-L_{X'_f}d''g. \tag{36}$$

The result follows by an easy computation which takes into account the fact that the space of (1,0)-forms is the annihilator of E.

We will say that $f\in C^\infty(M)$ is a *distinguished function*[9] if (a) $d'f$ is a foliated one-form, and (b) $\mathcal{H}\subseteq\ker d'^2 f$, and we will denote by Ω^0_d the space of distinguished functions. Any foliated function is distinguished, but not conversely. Formula (29) shows that the extended Poisson bracket of distinguished functions satisfies the Jacobi identity, and (a) implies that $\{f,g\}'\in\Omega^0_{\mathcal{F}}$, $\forall f,\ g\in\Omega^0_d$. Therefore, Ω^0_d is a Poisson algebra and $\Omega^0_{\mathcal{F}}$ is an ideal of the former. Furthermore, if $f,g\in\Omega^0_{\mathcal{F}}$, one gets $L_{X'_g}d''f=0$, and (36) implies

$$\{d'f,d'g\}'=d'\{f,g\}',\quad \forall f,g\in\Omega^0_d. \tag{37}$$

Then, if we take $f,g\in\Omega^0_d, k\in C^\infty(M)$ in (29) and use (31), we get

$$X'_{\{f,g\}'}=p_E[X'_f,X'_g],\quad f,g\in\Omega^0_d. \tag{38}$$

Proposition 3.3: Let h be a tame Hamiltonian structure of the foliation $\mathcal{F}$, E an image extension of h, and P the Poisson structure defined by the brackets $\{,\}'$. Then, the triple $(\nu^*\mathcal{F},\{,\}',h)$, with the bracket (32)*, is a Lie subalgebroid of the cotangent Lie algebroid $(T^*M,\{,\}_P,\sharp_P)$.*

Proof: The bracket $\{,\}_P$ is given by (4) with H replaced by $\sharp_P$, and, since $\sharp_P|_{E^*}=h$, we have $\forall\alpha,\beta\in\Omega^1_{\mathcal{F}}$,

$$\{\alpha,\beta\}_P=\{\alpha,\beta\}=\{\alpha,\beta\}'.$$

Then, (33) implies

$$\{f\alpha,g\beta\}_P=\{f\alpha,g\beta\}',\quad \forall f,g\in C^\infty(M),\forall\alpha,\beta\in\Omega^1_{\mathcal{F}}.$$

Q.E.D.

Now, let us notice that there exist an inclusion and a splitting morphism of Lie algebroids

$$\iota:\nu^*\mathcal{F}\hookrightarrow T^*M,\pi=p_{E^*}:T^*M\to\nu^*\mathcal{F}\quad(\pi\circ\iota=id), \tag{39}$$

where p_{E^*} is the projection onto E^* in the decomposition $T^*M=E^*\oplus T^*\mathcal{F}$.

Proposition 3.4: Under the hypotheses of Proposition 3.3, the projection π induces an injection π^* of the de Rham cohomology of the Lie subalgebroid $\nu^*\mathcal{F}$ into the Lichnerowicz–Poisson cohomology of (M,P). For any complex vector bundle S over M, the Lichnerowicz–Poisson Chern classes $c_k^{LP}(S)$ belong to the image of the injection π^*.

Proof: For the definition of the de Rham cohomology of Lie algebroids, see Ref. 4; the Lichnerowicz–Poisson cohomology is the de Rham cohomology of the cotangent Lie algebroid T^*M of the Poisson manifold (M,P) (e.g., Ref. 11). These definitions show the existence of homomorphisms

$$H^*_{\text{de Rham}}(M)\xrightarrow{j_1^*}H^*_{\text{LP}}(M,P)\xrightarrow{\iota^*}H^*(\nu^*\mathcal{F}),$$

$$H^*_{\text{de Rham}}(M)\xrightarrow{j_2^*}H^*(\nu^*\mathcal{F})\xrightarrow{\pi^*}H^*_{\text{LP}}(M,P),$$

where the morphisms are naturally induced by $j_1=\sharp_P, j_2=h,\iota,\pi$. [For instance, at the level of cochains we define

$$(j_2^*\lambda)(\alpha_1,\ldots,\alpha_k)=\lambda(H\alpha_1,\ldots,H\alpha_k),(\lambda\in\Omega^k(M),\alpha_1,\ldots,\alpha_k\in\Gamma E^*),$$

etc.] The following relations are obvious: $\iota^*\circ j_1^*=j_2^*$, $\pi^*\circ j_2^*=j_1^*$, $\iota^*\circ\pi^*=id$. The last one shows that π^* is injective; the others were mentioned for a later utilization.

Now, we recall that the Lichnerowicz–Poisson Chern classes are the j_1^*-image of the real Chern classes. Representatives of $c_k^{\text{LP}}(S)$ are obtained by evaluating Chern–Weil polynomials on

the curvature of an arbitrary contravariant derivative ${}^{P}D$ on S (i.e., a connection of the Lie algebroid T^*M on S) like in the usual Chern–Weil theory.[11] In particular, if ${}^{h}D$ is a connection of the Lie algebroid $\nu^*\mathcal{F}$ on S then

$$ {}^{P}D_{\alpha}s = {}^{h}D_{\pi\alpha}s \tag{40}$$

is a contravariant derivative on S, and, if C denotes curvatures, one has

$$ C_{P_D} = \pi^* C_{h_D}, \tag{41}$$

where π^* is used at the level of cochains. Now, the same procedure of evaluating Chern–Weil polynomials on curvature applied to C_{h_D} yields Chern classes $c_k^h(S) \in H^{2k}(\nu^*\mathcal{F})$, which are the j_2^*-images of the real Chern classes. Furthermore, (41) shows that $c_k^{\mathrm{LP}}(S) = \pi^* c_k^h(S)$. Q.E.D.

Corollary 3.1: Let h be a tame Hamiltonian structure and let P be the bivector field of the Poisson brackets $\{,\}'$. Then, there exists a prequantization bundle of the h-Poisson bracket iff $\iota^*[P] \in j_2^*(H^2(M,\mathbf{Z}))$.

Proof: $[P] \in H^2_{\mathrm{LP}}(M,P)$ is the cohomology class defined by the cocycle P. We refer the reader to Ref. 11 for the geometric quantization theory involved in the corollary. Since P defines the same Poisson brackets as h, the existence of a prequantization bundle implies $[P] = j_1^*(\zeta)$ for some $\zeta \in H^2(M,\mathbf{Z})$, which implies $\iota^*[P] = j_2^*(\zeta)$. Conversely, if this condition is satisfied, and if [as a consequence of (40)] we see the Kostant–Souriau prequantization formula as

$$ \hat{f}(s) = {}^{h}D_{d'f}s + 2\pi\sqrt{-1}fs, \quad s \in \Gamma K, \tag{42}$$

where K is the required prequantization bundle, the Dirac quantization principle implies that $c_1^h(K) = \iota^*[P]$. Since we assumed that $\iota^*[P]$ is an integral cohomology class, K exists. Q.e.d.

Now, let us consider the case of a transversal Hamiltonian structure h on $(M,\mathcal{F})$, and fix an image extension E. In this case, we may still see the cross sections of $\wedge^k E$ as a kind of generalized cochains with a coboundary $\delta^{(k)} = \delta$ defined by

$$\begin{aligned}(\delta Q)(\alpha_0,\ldots,\alpha_k) = &\sum_{i=0}^{k} (-1)^i H(\alpha_i)(Q(\alpha_0,\ldots,\hat{\alpha}_i,\ldots,\alpha_k)) \\ &+ \sum_{i<j=1}^{k} (-1)^{i+j} Q(\{\alpha_i,\alpha_j\}',\alpha_0,\ldots,\hat{\alpha}_i,\ldots,\hat{\alpha}_j,\ldots,\alpha_k),\end{aligned} \tag{43}$$

where $Q \in \wedge^k E$, $\alpha_i \in \Gamma E^*$ $(i = 0,\ldots,k)$, and the caret denotes the absence of the corresponding argument.

If we denote $\delta^2 = \delta^{(k+1)} \circ \delta^{(k)}$, a straightforward computation yields

$$\begin{aligned}&(\delta^2 Q)(\alpha_0,\ldots,\alpha_{k+1}) \\ &= \sum_{i<j=1}^{k+1} (-1)^{i+j} \Delta_h(\alpha_i,\alpha_j)(Q(\alpha_0,\ldots,\hat{\alpha}_i,\ldots,\hat{\alpha}_j,\ldots,\alpha_{k+1})) \\ &\quad + \sum_{i<j<k=2}^{k+1} (-1)^{i+j+k} Q\left(\sum_{\mathrm{Cycl}(i,j,k)} \{\alpha_k,\{\alpha_i,\alpha_j\}'\}',\alpha_0,\ldots,\hat{\alpha}_i,\ldots,\hat{\alpha}_j,\ldots,\hat{\alpha}_k,\ldots,\alpha_{k+1}\right),\end{aligned} \tag{44}$$

where

$$ \Delta_h(\alpha_i,\alpha_j) := H(\{\alpha_i,\alpha_j\}') - [H(\alpha_i),H(\alpha_j)]. \tag{45}$$

Since $\delta^2 \neq 0$, we can only define the *twisted cohomology spaces* (e.g., Ref. 10)

$$H^k_{tw}(h) := \frac{\ker \delta^{(k)}}{\mathrm{Im}\, \delta^{(k-1)} \cap \ker \delta^{(k)}}. \tag{46}$$

For instance, by straightforward computations one gets

$$H^0_{tw}(h) = \{f \in C^\infty(M)/X'_f = 0\}, \quad H^1_{tw}(h) = \frac{\{Q \in \Gamma E/L'_Q H = 0\}}{\{X'_f/f \in C^\infty(M), L'_{X'_f} = 0\}}.$$

But, if we define $W' \in \Gamma \wedge^2 E$ by $W'(d'f, d'g) = \{f,g\}'$, we do not get a cocycle since

$$(\delta W')(d'f, d'g, d'k) = -2 \sum_{\mathrm{Cycl}(i,j,k)} \{\{f,g\}', k\}',$$

and the Jacobi identity may not hold.

Several interpretations of twisted cohomology as a usual cohomology exist (e.g., Ref. 10). For instance, the subspaces $\tilde{\mathcal{C}}^k(h) = \ker(\delta^{(k+1)} \circ \delta^{(k)})$ with the coboundary δ constitute a usual cochain complex $\tilde{\mathcal{C}}(h)$, and $H^k_{tw}(h)$ are the usual cohomology spaces of $\tilde{\mathcal{C}}(h)$.

On the other hand, since the Poisson bracket $\{,\}'$ defines a representation of the Lie–Poisson algebra Ω^0_d of distinguished functions on the space $\Omega^0_{\mathcal{F}}$ of foliated functions, we get corresponding cohomology spaces $H^*_d(h) := H^*(\Omega^0_d, \Omega^0_{\mathcal{F}})$. Then, the cochains

$$c(f_1, \ldots, f_k) = Q(d'f_1, \ldots, d'f_k), \quad Q \in \Gamma \wedge^k E, \quad f_1, \ldots, f_k \in \Omega^0_{\mathcal{F}},$$

with values in $\Omega^0_{\mathcal{F}}$ and the coboundary (43) define the cochain complex of projectable cross sections of $\wedge E$ with the Lichnerowicz-like coboundary (see Ref. 11) $\delta Q = -p_{\Gamma \wedge^{k+1} E}[W, Q]$ (p denotes the projection), where W defines the h-Poisson bracket of foliated functions, and $[,]$ is the Schouten–Nijenhuis bracket. We may say that the cohomology spaces, say $H^*_{\mathrm{LPb}}(h)$, of this complex are the *basic Lichnerowicz–Poisson cohomology spaces* of h. The restriction of the cochain W' to distinguished functions is W, and we have a *fundamental class* $[W] \in H^2_{\mathrm{LPb}}(h)$.

Now, remember that a foliated manifold also has *basic de Rham cohomology spaces* $H^*_b(M, \mathcal{F})$,[7] defined as the cohomology spaces of the complex $(\Omega^*_{\mathcal{F}}, d)$, and there exist natural homomorphisms

$$\varphi : H^*_b(M, \mathcal{F}) \to H^*_{\mathrm{de\ Rham}}(M), \psi : H^*_b(M, \mathcal{F}) \to H^*_{\mathrm{LPb}}(h),$$

induced by inclusion and h, respectively.

These facts have the following consequences for geometric quantization. Assume that $[W] = \psi[\Phi]$ where $\varphi[\Phi]$ is an integral de Rham cohomology class. Then $\Phi \in \Omega^2_{\mathcal{F}}$ is a closed two-form with integral periods, such that

$$\{f,g\}' = \Phi(X'_f, X'_g), \quad \forall f, g \in \Omega^0_d. \tag{47}$$

Accordingly, there exists a Hermitian line bundle K over M with a connection ∇ of curvature $2\pi\sqrt{-1}\Phi$, and the Kostant–Souriau formula

$$\hat{f}s = \nabla_{X'_f} s + 2\pi\sqrt{-1} f s \tag{48}$$

provides a prequantization such that the Dirac principle holds for distinguished functions but, generally, not for arbitrary functions [use (47)]. The transitive case, i.e., presymplectic manifolds, was discussed in Ref. 9.

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A family of new integrable couplings with two arbitrary functions of TC hierarchy

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Seeking new integrable couplings of the known integrable hierarchies of evolution equations is a quite new interesting aspect and is of great significance in soliton theory. In this paper, a loop algebra $\tilde{P}$ and its basis are first presented. Second, a new isospectral problem with four potentials in the loop algebra $\tilde{P}$ is considered to construct integrable couplings of the well-known TC hierarchy by the zero-curvature equation such that a family of new integrable couplings including two arbitrary functions are obtained. In particular, when we set two arbitrary functions to be zero, a special integrable couplings of the generalized Korteweg–de Vries equation is also given. © *2002 American Institute of Physics.*
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I. INTRODUCTION

It is of important significance in the field of soliton theory and dynamical integrable system to find more new hierarchies evolution equations and to further consider their algebraic properties and geometrical structures, such as Hamiltonian structure, conserved density, symmetry, and Liouville integrable property.[1–7] In 1989, Tu[5] presented a so-called loop algebra scheme to generate a hierarchy of Lax integrable evolution equations and used a trace identity to construct their Hamiltonian structures from an eigenvalue problem. This approach has been applied to find many new important nonlinear evolution equations hierarchies (AKNS, TA, TB, TC, BTP, Kaup-Newell, WKI, etc.) and the corresponding Hamiltonian structures.

A natural problem is how to extend these known integrable systems from small to large and from simple to complicated. Recently, Fuchssteiner[8] presented the notion of ''integrable couplings.'' It originates from an investigation on centerless Virasoro symmetry algebras of integrable systems or soliton equations. Some papers about integrable couplings have been published.[8–13]

Mathematically, a system of integrable coupling means that it is a nontrivial system of evolution equations which is still integrable and includes the known integrable system of evolution equations $u_t=F(u)$ as a subsystem. Simply, for a given integrable system of evolution equations

$$u_t=F(u)=F(u,u_x,u_{xx},\ldots) \tag{1}$$

if we can find the following new bigger integrable system of evolution equations:

$$\begin{aligned} u_t&=F(u),\\ w_t&=C(u,w), \end{aligned} \tag{2}$$

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with the condition $\partial C/\partial[u]\neq 0$, then system (2) is called the system of integrable couplings of system (1), where $[u]$ denotes a vector consisting of all derivatives of u with respect to a space variable.[13]

The symmetry approach,[8] the perturbation system method,[9–11] and a direct method[12] have been used to construct integrable couplings of evolution equations. Recently, Ma[13] presented the general theory by perturbations and was used to study the problems of integrable couplings of the Korteweg–de Vries (KdV) hierarchy, but the approach is complex to calculate. Finding a more powerful approach to construct integrable couplings of evolution equations is still an important subject.

In this paper, based on the idea in Ref. 12, we would like to present a loop algebra $\tilde{P}$ and construct its basis $\{h_1(n),h_2(n),h_3(n),h_4(n),h_5(n)\}$ such that by using the zero-curvature equation a new isospectral problem in loop algebra $\tilde{P}$ is used to construct integrable couplings of the known TC hierarchy,[5,14]

$$u_{t_n}=\begin{pmatrix} q \\ r \end{pmatrix}_{t_n}=JL^{n-1}\begin{pmatrix} 0 \\ \frac{1}{2}\beta r \end{pmatrix}, \quad J=\begin{pmatrix} \partial & \partial\frac{q}{r} \\ \frac{q}{r}\partial & \partial \end{pmatrix}, \quad L=-\frac{1}{4}\begin{pmatrix} 2\partial^{-1}q\partial & 2\partial^{-1}r\partial \\ 2r-\partial\frac{q}{r}\partial & 2q-\partial^2 \end{pmatrix}, \tag{3}$$

whose associated isospectral problem is

$$\phi_x=U\phi, \quad U=\begin{pmatrix} 0 & 1+\frac{q+r}{2\lambda} \\ \lambda+\frac{q-r}{2} & 0 \end{pmatrix}, \quad \phi=\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad u=\begin{pmatrix} q \\ r \end{pmatrix}, \tag{4}$$

where q and r are two scalar potentials, λ being a constant spectral parameter.

This paper is organized as follows. In Sec. II, we give a simply general approach to construct integrable couplings by use of a loop algebra and some properties of its basis. In Sec. III, we first give a loop algebra $\tilde{P}$ and its new basis $\{h_i(n)|i=1,2,3,4,5\}$. And then the TC hierarchy is chosen to illustrate the general theory determined by the loop algebra $\tilde{P}$ by using a new isopsectral problem such that a new integrable coupling with two arbitrary functions of TC hierarchy is obtained. In addition, a special integrable coupling of the generalized KdV equation is also given. Finally, some summaries and conclusions are given in Sec. IV.

II. A SIMPLY GENERAL THEORY TO CONSTRUCT INTEGRABLE COUPLINGS

For the given isospectral problem (4), taking a basis of loop algebra $\tilde{A}_1$ as

$$h(n)=\begin{pmatrix} \frac{1}{2}\lambda^n & 0 \\ 0 & -\frac{1}{2}\lambda^n \end{pmatrix}, \quad e_+(n)=\begin{pmatrix} 0 & \frac{1}{2}\lambda^{n-1}, \\ \frac{1}{2}\lambda^n & 0 \end{pmatrix}, \quad e_-(n)=\begin{pmatrix} 0 & \frac{1}{2}\lambda^{n-1} \\ -\frac{1}{2}\lambda^n & 0 \end{pmatrix},$$

$$\deg e_\pm(n)=2n-1, \quad \deg h(n)=2n, \tag{5}$$

which has the relations

$$[h(m),e_\pm(n)]=e_\mp(m+n), \quad [e_-(m),e_+(n)]=h(m+n-1), \tag{6}$$

Eq. (1) becomes

$$\phi_x=U\phi, \quad U=2e_+(1)+qe_+(0)+re_-(0). \tag{7}$$

In order to deduce TC hierarchy of evolution equations from (1), we consider the auxiliary problem of (1), namely

$$\phi_{t_n}=V^{(n)}\phi=V^{(n)}(\lambda,u)\phi, \tag{8}$$

$$V^{(n)}=(\lambda^n V)_+ +\Delta_n=\sum_{i=0}^{n}(a_i h(n-i)+b_i e_+(n-i)+c_i e_-(n-i))+\left[\frac{q}{r}c_n-b_n\right]e_+(0).$$

Therefore it is easy to prove that the compatibility condition $\phi_{xt}=\phi_{tx}$ of (7) and (8) generates the zero curvature equation $U_{t_n}-V_x^{(n)}+[U,V^{(n)}]=0$, namely,

$$u_t=\begin{pmatrix} q_{t_n} \\ r_{t_n}\end{pmatrix}=J_0\begin{pmatrix} -b_n \\ c_n\end{pmatrix}=J_0 L_0^{n-1}\begin{pmatrix} 0 \\ \frac{1}{2}\beta r\end{pmatrix} \tag{9}$$

with β as a constant and

$$J_0=\begin{pmatrix} \partial & \partial\frac{q}{r} \\ \frac{q}{r}\partial & \partial\end{pmatrix},\quad L_0=-\frac{1}{4}\begin{pmatrix} 2\partial^{-1}q\partial & 2\partial^{-1}r\partial \\ 2r-\partial\frac{q}{r}\partial & 2q-\partial^2\end{pmatrix}. \tag{10}$$

In order to use the zero curvature equation to consider the integrable couplings of TC hierarchy (9), we need to seek a bigger loop algebra $\tilde{P}$ and to construct its basis $\{h_i(n)(i=1,2,..,m)\}$.[12]

If $\tilde{P}_1=\{h_1(n),h_2(n),h_3(n)\}$ and $\tilde{P}_2=\{h_4(n),h_5(n),\ldots,h_m(n)\}$ satisfy

$$[\tilde{P}_1,\tilde{P}_1]\subset\tilde{P}_1,\quad [\tilde{P}_1,\tilde{P}_2]\subset\tilde{P}_2,\quad [\tilde{P}_2,\tilde{P}_2]\subset\tilde{P}_2 \tag{11}$$

and $\tilde{P}_1$ is isomorphic to $\tilde{A}_1$, then for the isospectral problem

$$\phi_x=U\phi,\quad U=2h_2(1)+qh_2(0)+rh_3(0)+\sum_{i=3}^{m-1}u_i h_{i+1}(0)$$

and its properly chosen auxiliary problem

$$\phi_{t_n}=V^{(n)}\phi=V^{(n)}(\lambda,u)\phi,\quad V^{(n)}\in\tilde{P}.$$

It is easy to prove that the compatibility condition $\phi_{xt}=\phi_{tx}$ of the above two equations, i.e.,

$$\phi_{xt}=U_t\phi+U\phi_t=U_t\phi+UV^{(n)}\phi=\phi_{tx}=V_x^{(n)}\phi+V^{(n)}\phi_x=V_x^{(n)}\phi+V^{(n)}U\phi_x,$$

gives rise to the zero curvature equation

$$U_{t_n}-V_x^{(n)}+[U,V^{(n)}]=0,$$

which will be the integrable couplings of TC hierarchy we would like to obtain.

III. APPLICATIONS AND INTEGRABLE COUPLINGS OF TC HIERARCHY

According to the above-mentioned simply general theory, in order to deduce integrable couplings of TC hierarchy (9), we need introduce a new loop algebra $\tilde{P}$ and its basis.

We easily know that when $m=3$ only trivial integrable couplings of TC hierarchy are obtained. More recently we find that when $m=4$, we can also obtain some nontrivial integrable couplings of TC hierarchy.[15] But the obtained integrable couplings of TC hierarchy are simpler than the integrable couplings (25) obtained under the case $m=5$. We guess that when $m>5$, we may find some more complex integrable couplings of TC hierarchy. In what follows we choose a more complex case, i.e., $m=5$, to illustrate the theory. We take its basis, say, $\{h_1(n),h_2(n),h_3(n),h_4(n),h_5(n)\}$, which is different from the one in Ref. 12 and satisfies the commutative relation

$$\begin{gathered}
[h_1(m),h_2(n)]=h_3(m+n), \quad [h_1(m),h_3(n)]=h_2(m+n),\\
[h_1(m),h_4(n)]=0, \quad [h_1(m),h_5(n)]=0,\\
[h_2(m),h_3(n)]=-h_1(m+n-1), \quad [h_2(m),h_4(n)]=h_5(m+n),\\
[h_2(m),h_5(n)]=h_4(m+n), \quad [h_3(m),h_4(n)]=h_5(m+n),\\
[h_3(m),h_5(n)]=h_4(m+n), \quad [h_4(m),h_5(n)]=0,\\
\deg h_1(n)=2n, \quad \deg h_2(n)=\deg h_3(n)=\deg h_4(n)=\deg h_5(n)=2n-1
\end{gathered} \tag{12}$$

and set

$$\tilde{P}_1=\{h_1(n),h_2(n),h_3(n)\}, \quad \tilde{P}_2=\{h_4(n),h_5(n)\}, \tag{13}$$

and we easily know that $\tilde{P}_1$ is isomorphic to $\tilde{A}_1$ and $[\tilde{P},\tilde{P}_2]\subset\tilde{P}_2$.

Remark 1: For a give basis of a loop algebra $\tilde{P}$ with $m=5$, the corresponding commutative relation can be determined, which is similar to the loop algebra $\tilde{A}_1$ used by Tu.[5] To seek integrable couplings of TC hierarchy (9), we choose one of all possible bases of $\tilde{P}$ with $m=5$ and its corresponding commutative relation (12) here. Of course we can also choose other bases and the corresponding commutation relation. But one key condition is that the basis must satisfy (11), (13) and $\tilde{P}_1$ is isomorphic to $\tilde{A}_1$.

In what follows, we would like to choose an isospectral problem in the loop algebra $\tilde{P}$ with $m=5$ in order to construct integrable couplings of TC hierarchy (9).

Choose the following proper isospectral problem ($\lambda_t=0$):

$$\phi_x=U\phi, \quad U=2h_2(1)+u_1h_2(0)+u_2h_3(0)+u_3h_4(0)+u_4h_5(0). \tag{14}$$

It is clear that the adjoint equation of (14) can be written as

$$V_x=[U,V]\equiv UV-VU, \tag{15}$$

where

$$V=V(\lambda,u)=\sum_{m=0}^{\infty}[a_mh_1(-m)+b_mh_2(-m)+c_mh_3(-m)+d_mh_4(-m)+e_mh_5(-m),$$

where a_m, b_m, c_m, d_m, $e_m(m=0,1,2,\dots)$ are all functions of $u_i(i=1,2,3,4,5)$ to be determined later. Equation (15) leads to

$$\begin{aligned} a_{m,x}&=-u_1c_{m-1}+u_2b_{m-1}-2c_m,\\ b_{m,x}&=-u_2a_m,\\ c_{m,x}&=-u_1a_m-2a_{m+1},\\ d_{m,x}&=2e_{m+1}+(u_1+u_2)e_m-u_4(b_m+c_m),\\ e_{m,x}&=2d_{m+1}+(u_1+u_2)d_m-u_3(b_m+c_m). \end{aligned} \tag{16}$$

The following recursion formulas are obtained from (16):

$$\begin{pmatrix} -b_{n+1}\\ c_{n+1}\\ d_{n+1}\\ e_{n+1} \end{pmatrix}=L\begin{pmatrix} -b_n\\ c_n\\ d_n\\ e_n \end{pmatrix}, \tag{17}$$

$$L=\begin{pmatrix} -\frac{1}{2}\partial^{-1}u_1\partial & -\frac{1}{2}\partial^{-1}u_2\partial & 0 & 0\\ -\frac{1}{2}u_2+\frac{1}{4}\partial\dfrac{u_1}{u_2}\partial & -\frac{1}{2}u_1+\frac{1}{4}\partial^2 & 0 & 0\\ -\frac{1}{2}u_3 & \frac{1}{2}u_3 & -\frac{1}{2}(u_1+u_2) & \frac{1}{2}\partial\\ -\frac{1}{2}u_4 & \frac{1}{2}u_4 & \frac{1}{2}\partial & -\frac{1}{2}(u_1+u_2) \end{pmatrix}, \tag{18}$$

where $\partial=\partial/\partial x$, $\partial\partial^{-1}=\partial^{-1}\partial=1$. If we take the initial values $a_0=0$, $b_0=\beta=\text{const}$, $c_0=d_0=e_0=0$. Then, (17) and (18) imply the following results:

$$a_1=0,\quad b_1=0,\quad c_1=\tfrac{1}{2}\beta u_2,\quad d_1=\tfrac{1}{2}\beta u_3,\quad e_1=\tfrac{1}{2}\beta u_4,$$

$$a_2=-\tfrac{1}{4}\beta u_{2x},\quad b_2=\tfrac{1}{8}\beta u_2^2,\quad c_2=\tfrac{1}{8}(u_{2,xx}-2u_1u_2),$$

$$d_2=\tfrac{1}{4}\beta u_{4x}-\tfrac{1}{4}\beta u_1u_3,\quad e_2=\tfrac{1}{4}\beta u_{3x}-\tfrac{1}{4}\beta u_1u_4,\cdots.$$

Set

$$\begin{aligned} (\lambda^nV)_+&=\sum_{m=0}^{n}[a_mh_1(n-m)+b_mh_2(n-m)+c_mh_3(n-m)+d_mh_4(n-m)+e_mh_5(n-m),\\ (\lambda^nV)_-&=\lambda^nV-(\lambda^nV)_+. \end{aligned} \tag{19}$$

Therefore we from (15) and (19) have

$$-(\lambda^nV)_{+,x}+[U,(\lambda^nV)_+]=(\lambda^nV)_{-,x}-[U,(\lambda^nV)_-]. \tag{20}$$

It is clear to know that the terms on the left-hand side of (20) are of degree $\leqslant -2$, while the terms on the right-hand side of (20) are of degree $\geqslant -1$. Therefore both sides of (20) are of degree -1 and -2, that is

$$\begin{aligned} -(\lambda^nV)_{+,x}+[U,(\lambda^nV)_+]&=(u_2b_n-u_1c_n)h_1(-1)-(b_{n,x}+u_2a_n)h_2(0)-(c_{nx}+u_1a_n)h_3(0)\\ &\quad+[-d_{nx}+u_1e_n+u_2e_n-u_4(b_n+c_n)]h_4(0)\\ &\quad+[-e_{nx}+u_1d_n+u_2d_n-u_3(b_n+c_n)]h_5(0). \end{aligned} \tag{21}$$

In order to cancel the term $(u_2b_n-u_1c_n)h_1(-1)$, we introduce the term

$$\Delta_n=\left[\frac{u_1}{u_2}c_n-b_n\right]h_2(0)+\delta_{1n}h_4(0)+\delta_{2n}h_5(0), \tag{22}$$

where δ_{1n} and δ_{2n} are arbitrary functions of $u_i(i=1,2,3,4,5)$ Thus it is clear to know that if we set

$$V^{(n)}=(\lambda^nV)_+ +\Delta_n, \tag{23}$$

then we get

$$\begin{aligned}-(\lambda^nV)_{+,x}+[U,(\lambda^nV)_+]=&\left(b_n-\frac{u_1}{u_2}c_n\right)_x h_2(0)-\left(c_{nx}-\frac{u_1}{u_2}b_{nx}\right)h_3(0)\\&+\left[-d_{nx}-\delta_{1nx}+(u_1+u_2)(e_n+\delta_{2n})-u_4\left(1+\frac{u_1}{u_2}\right)c_n\right]h_4(0)\\&+\left[-e_{nx}-\delta_{2nx}+(u_1+u_2)(d_n+\delta_{1n})-u_3\left(1+\frac{u_1}{u_2}\right)c_n\right]h_5(0).\end{aligned} \tag{24}$$

Therefore according to the zero curvature equation, we have the following Lax integrable hierarchy of evolution equations with two arbitrary functions:

$$u_{t_n}=\begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix}_{t_n}=-\begin{pmatrix}\left(b_n-\frac{u_1}{u_2}c_n\right)_x\\-\left(c_{nx}-\frac{u_1}{u_2}b_{nx}\right)\\-d_{nx}-\delta_{1nx}+(u_1+u_2)(e_n+\delta_{2n})-u_4\left(1+\frac{u_1}{u_2}\right)c_n\\-e_{nx}-\delta_{2nx}+(u_1+u_2)(d_n+\delta_{1n})-u_3\left(1+\frac{u_1}{u_2}\right)c_n\end{pmatrix}, \tag{25}$$

which has the Lax pair

$$\phi_x=U\phi,\quad \phi_{t_n}=V^{(n)}\phi, \tag{26}$$

where U and $V^{(n)}$ satisfy (14) and (23), respectively.

Remark 2: In particular, when taking $\delta_{1n}=\delta_{2n}=0$, from (17) and (25), we have

$$u_{t_n}=\begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix}_{t_n}=-\begin{pmatrix}\left(b_n-\dfrac{u_1}{u_2}c_n\right)_x\\-\left(c_{nx}-\dfrac{u_1}{u_2}b_{nx}\right)\\-d_{nx}+(u_1+u_2)e_n-u_4\left(1+\dfrac{u_1}{u_2}\right)c_n\\-e_{nx}+(u_1+u_2)d_n-u_3\left(1+\dfrac{u_1}{u_2}\right)c_n\end{pmatrix}$$

$$=\begin{pmatrix}\partial & \partial\dfrac{u_1}{u_2} & 0 & 0\\ \dfrac{u_1}{u_2}\partial & \partial & 0 & 0\\ 0 & u_4+\dfrac{u_1u_4}{u_2} & \partial & -(u_1+u_2)\\ 0 & u_3+\dfrac{u_1u_3}{u_2} & -(u_1+u_2) & \partial\end{pmatrix}\begin{pmatrix}-b_n\\c_n\\d_n\\e_n\end{pmatrix}$$

$$=J\begin{pmatrix}-b_n\\c_n\\d_n\\e_n\end{pmatrix}=JL^{n-1}\begin{pmatrix}-b_1\\c_1\\d_n\\e_1\end{pmatrix}=JL^{n-1}\begin{pmatrix}0\\\frac{1}{2}\beta u_2\\\frac{1}{2}\beta u_3\\\frac{1}{2}\beta u_4\end{pmatrix}. \tag{27}$$

Set

$$w_{t_n}=\begin{pmatrix}u_1\\u_2\end{pmatrix}_{t_n},\quad v_{t_n}=\begin{pmatrix}u_3\\u_4\end{pmatrix}_{t_n}.$$

Then the hierarchy of evolution equations (27) can be rewritten as

$$w_{t_n}=\begin{pmatrix}u_1\\u_2\end{pmatrix}_{t_n}=F_n(w)=\begin{pmatrix}\partial & \partial\dfrac{u_1}{u_2} & 0 & 0\\ \dfrac{u_1}{u_2}\partial & \partial & 0 & 0\end{pmatrix}\begin{pmatrix}-b_n\\c_n\\d_n\\e_n\end{pmatrix}$$

$$=J_0\begin{pmatrix}-b_n\\c_n\end{pmatrix}=J_0L_0^{n-1}\begin{pmatrix}0\\\frac{1}{2}\beta u_2\end{pmatrix}, \tag{28}$$

$$v_{t_n}=\begin{pmatrix}u_3\\u_4\end{pmatrix}_{t_n}=C_n(w,v)=\begin{pmatrix}0 & u_4+\dfrac{u_1u_4}{u_2} & \partial & -(u_1+u_2)\\ 0 & u_3+\dfrac{u_1u_3}{u_2} & -(u_1+u_2) & \partial\end{pmatrix}\begin{pmatrix}-b_n\\c_n\\d_n\\e_n\end{pmatrix}.$$

If we set $u_1=q$, $u_2=r$, then it is clear to see that the first one of system (28) is just the TC hierarchy (9).

Remark 3: In particular, when $n=2$, $\beta=8$, system (28) becomes

$$w_{t_2}=\begin{pmatrix}u_1\\u_2\end{pmatrix}_{t_2}=F_2(w)=\begin{pmatrix}\left(\dfrac{u_1}{u_2}u_{2,xx}-2u_1^2-u_2^2\right)_x\\ u_{2,xxx}-2u_{1x}u_2-4u_1u_{2x}\end{pmatrix},$$

$$v_{t_2}=\begin{pmatrix}u_3\\u_4\end{pmatrix}_{t_2}=C_2(w,v) \tag{29}$$

$$=\begin{pmatrix}2u_{4,xx}-2u_{1x}u_3-2u_2u_{3x}+u_4\left(1+\dfrac{u_1}{u_2}\right)(u_{2xx}-2u_1u_2)+u_1u_4(u_1+u_2)\\ 2u_{3,xx}-2u_{1x}u_4-2u_2u_{4x}+u_3\left(1+\dfrac{u_1}{u_2}\right)(u_{2,xx}-2u_1u_2)+u_1u_3(u_1+u_2)\end{pmatrix}.$$

If we set $u_1=q$, $u_2=r$, then the first system of (29) is just (20) in Ref. 5. When $q=\pm r$, the system of equations reduces to the celebrated KdV equation. It is clear to know that $\partial C_2(w,v)/\partial[w]\neq 0$. In addition because the hierarchy (28) possesses Lax pair, it is Lax integrable. Therefore according to the notion of integrable couplings,[8] we know that the hierarchy of evolution equations (28) is the integrable couplings of TC hierarchy (9).

IV. SUMMARY AND CONCLUSIONS

In summary, we have obtained integrable couplings of the well-known TC hierarchy by considering a new isospectral problem in a new loop algebra $\tilde{P}$. This denotes that the approach is powerful to obtain new integrable couplings. The obtained integrable couplings contain two arbitrary functions of old potentials (u_1,u_2) and new potentials (u_3,u_4) which are different from the results which do not contain arbitrary functions.[8–13] In the loop algebra $\tilde{P}$, other new isopsectral problems may be used to construct many integrable couplings of other many known hierarchies of evolution equations. As is well known, there exist two integrable forms: (1) Lax integrable; (2) Liouville integrable. In this paper, we use the zero curvature equation (Lax pair) to construct integrable couplings. It is clear to see that TC hierarchy is both Lax integrable and Liouville integrable. Recently many authors have devoted efforts to seeking symplectic structures of some Lax pair systems(seem Ref. 16, and references therein).

Therefore some natural open problems are as follows: (1) whether the integrable couplings (28) are shown also to be Liouville integrable according to the methods used in Ref. 16 and therein? (2) Can Backlund transformation of the hierarchy (28) be obtained? (3) Can the hierarchy (28) pass the Painleve test?, etc. These need to be further studied.

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Exponential factors and Darbouxian first integrals of the Lorenz system

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In this article we characterize all the exponential factors and the Darbouxian first integrals for the Lorenz system $\dot{x}=s(y-x)$, $\dot{y}=rx-y-xz$, $\dot{z}=-bz+xy$. In the proofs, we use the weight homogeneous polynomials and the method of characteristic curves for solving linear partial differential equations. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1503152]

I. INTRODUCTION AND DEFINITIONS

We consider the Lorenz system

$$\begin{aligned}\dot{x}&=s(y-x)=\xi(x,y,z),\\ \dot{y}&=rx-y-xz=\eta(x,y,z),\\ \dot{z}&=-bz+xy=\zeta(x,y,z),\end{aligned}\tag{1}$$

where x,y and z are real variables, and s,r and b are real parameters. This system is a famous dynamic model [see, for instance, Lorenz (1963) and Sparrow (1982)]. From the point of view of integrability, it was intensively studied using different theory of integrability (for example, Cairó and Hua, 1993; Giacomini *et al.*, 1991, 1997; Gupta, 1993; Kús, 1983; Segur, 1982; Strelcyn and Wojciechowski, 1988). Recently, using the weight homogeneous polynomials and the method of characteristic curves, Llibre and Zhang (2002) characterized all the irreducible invariant algebraic surfaces, the invariants, the rational first integrals and the algebraic integrability for the Lorenz system. In this article, applying the method given in Llibre and Zhang (2002) to the Lorenz system, we obtain all the exponential factors and provide the necessary and sufficient conditions for the Lorenz system to have a Darbouxian first integral.

The Darboux theory of integrability is classical. It mainly received contributions from Darboux (1878), who gave a link between the algebraic geometry and the search of first integrals, and showed how to construct the first integral of a planar polynomial vector field having sufficient number of Darboux polynomials. Poincaré (1891) noticed the difficulty in obtaining an algorithm to compute Darboux polynomials. Singer (1992) proved that a polynomial differential system has a Liouvillian first integral if and only if it has a Darbouxian integrating factor (see also Camacho and Scárdua, 2001). For three dimensional dynamic systems, Labrunie (1996) and Moulin Ollagnier (1997) characterized independently all the polynomial first integrals of the (a,b,c) Lotka-Volterra systems, and Moulin Ollagnier (1999) investigated its rational first integrals. Llibre and Zhang (2000) obtained all the Darboux polynomials, the polynomial first integrals, the rational first integrals and the algebraic integrability for the Rikitake system.

For presenting our main results, we first recall some definitions.

A polynomial $f(x,y,z)\in\mathbb{C}[x,y,z]$ is called a *Darboux polynomial* of the Lorenz system if

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$$\xi(x,y,z)\frac{\partial f}{\partial x}+\eta(x,y,z)\frac{\partial f}{\partial y}+\zeta(x,y,z)\frac{\partial f}{\partial z}=k(x,y,z)f, \tag{2}$$

for some polynomial $k(x,y,z)\in\mathbb{C}[x,y,z]$, which is called a *cofactor* of f. As usual, $\mathbb{C}[x,y,z]$ denotes the ring of polynomials with complex coefficients in the variables x,y and z.

An *exponential factor* $F(x,y,z)$ of the Lorenz system is an exponential function of the form $\exp(g/h)$ with $g,h\in\mathbb{C}[x,y,z]$ coprime, denoted by $(g,h)=1$, and satisfying

$$\xi(x,y,z)\frac{\partial F}{\partial x}+\eta(x,y,z)\frac{\partial F}{\partial y}+\zeta(x,y,z)\frac{\partial F}{\partial z}=l(x,y,z)F, \tag{3}$$

for some $l(x,y,z)\in\mathbb{C}[x,y,z]$ a polynomial of degree at most one. The polynomial l is called a *cofactor* of F.

We say that a real function $H(x,y,z,t):\mathbb{R}^3\times\mathbb{R}\to\mathbb{R}$, is a *first integral* of the Lorenz system, if $H(x(t),y(t),z(t),t)\equiv$const for all values of t for which the solution $(x(t),y(t),z(t))$ of the Lorenz system is defined. A first integral H of the Lorenz system is called *Darbouxian* if it has the form

$$H=f_1^{\lambda_1}\cdots f_p^{\lambda_p}\left(\exp\left(\frac{h_1}{g_1^{n_1}}\right)\right)^{\mu_1}\cdots\left(\exp\left(\frac{h_q}{g_q^{n_q}}\right)\right)^{\mu_q},$$

where f_i, g_j and h_j are polynomials in $\mathbb{C}[x,y,z]$, f_i and g_j are irreducible, the polynomials g_j and h_j are coprime, and λ_i and μ_j are real or complex numbers appearing together with their conjugates. Obviously, polynomial first integrals and rational first integrals are Darboux first integrals.

A polynomial $g(x,y,z)$ is said to be *weight homogeneous* if there exist $\mathbf{s}=(s_1,s_2,s_3)$ with s_i natural numbers for $i=1,2,3$, and $m\in\mathbb{N}$ such that for all $\alpha\in\mathbb{R}\backslash\{0\}$ we have

$$g(\alpha^{s_1}x,\alpha^{s_2}y,\alpha^{s_3}z)=\alpha^m g(x,y,z),$$

where $\mathbb{N}$ is the set of natural numbers. We shall refer to $\mathbf{s}$ as the *weight* of g, and m as the *weight degree*.

This article is organized as follows. In Sec. II we state our main result. Its proof is given in Sec. III.

II. STATEMENT OF THE MAIN RESULT

Theorem 1: For *the Lorenz system, if* $s\neq 0$, *then the following statements hold*.

(a) *The generator of exponential factors of the Lorenz system is* $F=\exp(x/s)$ *with the cofactor* $l=y-x$.

(b) *The Lorenz system has a Darbouxian first integral if and only if* $b=1$, $s=\frac{1}{2}$ *and* $r=0$. *In this case the first integral is* $(y^2+z^2)/(x^2-z)^2$.

We remark that when $s=0$, the Lorenz system has always the Darbouxian first integral $H=x$, and then on each plane $x=$const the system becomes linear.

For proving this theorem, we need the following two results. The first one is given in Llibre and Zhang (2002).

Theorem 2: *When* $s\neq 0$, *a set of generators for the set of all Darboux polynomials of the Lorenz system consists of the following six ones:*

Darboux polynomial	Cofactor	Parameters
x^2-2sz	$-2s$	$b=2s$
$x^4+\frac{4}{3}x^2z-\frac{4}{9}y^2-\frac{8}{9}xy+\frac{4}{3}rx^2$	$-\frac{4}{3}$	$b=0,\ s=\frac{1}{3}$
y^2+z^2	-2	$b=1,\ r=0$
$x^4-4x^2z-4y^2+8xy-4rx^2-16(1-r)z$	-4	$b=4,\ s=1$
$y^2+z^2-rx^2$	-2	$b=1,\ s=1$
$x^4-4sx^2z-4s^2y^2+4s(4s-2)xy-(4s-2)^2x^2$	$-4s$	$b=6s-2,\ r=2s-1$

The next result is related to the Darboux theory of integrability (see for instance, Darboux, 1878; Joualonou, 1979; Chavarriga *et al.*, 1997, Christopher and Llibre, 1999, 2000).

Theorem 3: *(Darboux theory of integrability) Suppose that a polynomial vector field X defined in $\mathbb{R}^n$ admits p Darboux polynomials f_i with cofactors K_i for $i=1,\ldots,p$, and q exponential factors $F_j=\exp(g_j/h_j)$ with cofactors L_j for $j=1,\ldots,q$. If there exist $\lambda_i,\mu_j\in\mathbb{C}$ not all zero such that*

$$\sum_{i=1}^{p}\lambda_i K_i+\sum_{j=1}^{q}\mu_j L_j=0, \tag{4}$$

then the following real (multi-valued) function of Darbouxian type

$$f_1^{\lambda_1}\cdots f_p^{\lambda_p}F_1^{\mu_1}\cdots F_q^{\mu_q}, \tag{5}$$

substituting $f_i^{\lambda_i}$ by $|f_i|^{\lambda_i}$ if $\lambda_i\in\mathbb{R}$, is a first integral of the vector field $\mathcal{X}$.

It is clear that condition (4) is also necessary for function (5) to be a Darbouxian first integral of the vector field $\mathcal{X}$.

In Theorem 3 we said that function (5) is real. It follows from the following fact. Since the vector field $\mathcal{X}$ is real, it is well known that if a complex Darboux polynomial or exponential factor appears, then its conjugate must appear simultaneously. If among the Darboux polynomials of $\mathcal{X}$ a complex conjugate pair f and $\overline{f}$ occur, the first integral (5) has a real factor of the form $f^{\lambda}\overline{f}^{\overline{\lambda}}$, which is the multi-valued real function

$$[(\mathrm{Re}\,f)^2+(\mathrm{Im}\,f)^2]^{\mathrm{Re}\,\lambda}\exp\left(-2\,\mathrm{Im}\,\lambda\arctan\left(\frac{\mathrm{Im}\,f}{\mathrm{Re}\,f}\right)\right),$$

if $\mathrm{Im}\,\lambda\,\mathrm{Im}\,f\not\equiv 0$. If among the exponential factors of $\mathcal{X}$ a complex conjugate pair $F=\exp(h/g)$ and $\overline{F}=\exp(\overline{h}/\overline{g})$ occur, the first integral (5) has a real factor of the form

$$\left(\exp\left(\frac{h}{g}\right)\right)^{\mu}\left(\exp\left(\frac{\overline{h}}{\overline{g}}\right)\right)^{\overline{\mu}}=\exp\left(2\,\mathrm{Re}\left(\mu\frac{h}{g}\right)\right).$$

III. PROOF OF THEOREM I

Proof of statement (a): Let $F=\exp(g/h)$ be an exponential factor of the Lorenz system with a cofactor l, where $g,\ h\in\mathbb{C}[x,y,z]$ with $(g,h)=1$. Then from the definition of the exponential factor we get that

$$h\left(\xi\frac{\partial g}{\partial x}+\eta\frac{\partial g}{\partial y}+\zeta\frac{\partial g}{\partial z}\right)-g\left(\xi\frac{\partial h}{\partial x}+\eta\frac{\partial h}{\partial y}+\zeta\frac{\partial h}{\partial z}\right)=lh^2. \tag{6}$$

If $h\equiv\mathrm{const}$, without loss of generality we set $h=1$. Then Eq. (6) becomes

$$\xi(x,y,z)\frac{\partial g}{\partial x}+\eta(x,y,z)\frac{\partial g}{\partial y}+\zeta(x,y,z)\frac{\partial g}{\partial z}=l(x,y,z). \tag{7}$$

If $h\not\equiv$const, since $(g,h)=1$, there exists a polynomial $k\in\mathbb{C}[x,y,z]$ such that

$$\xi(x,y,z)\frac{\partial h}{\partial x}+\eta(x,y,z)\frac{\partial h}{\partial y}+\zeta(x,y,z)\frac{\partial h}{\partial z}=kh, \tag{8}$$

i.e., h is a Darboux polynomial with the cofactor k. Then Eq. (6) becomes

$$\xi(x,y,z)\frac{\partial g}{\partial x}+\eta(x,y,z)\frac{\partial g}{\partial y}+\zeta(x,y,z)\frac{\partial g}{\partial z}=kg+lh. \tag{9}$$

In order to simplify the computations we introduce the weight change of the variables

$$x=\alpha^{-1}X,\quad y=\alpha^{-2}Y,\quad z=\alpha^{-2}Z,\quad t=\alpha T. \tag{10}$$

The Lorenz system is transformed to

$$\begin{aligned} X'&=s(Y-\alpha X)=P(X,Y,Z),\\ Y'&=-XZ-\alpha Y+\alpha^2 rX=Q(X,Y,Z),\\ Z'&=XY-\alpha bZ=R(X,Y,Z), \end{aligned} \tag{11}$$

where the prime denotes the derivative of the dependent variables with respect to T. Set

$$l(x,y,z)=l_0+l_1x+l_2y+l_3z,$$

$$G(X,Y,Z)=\alpha^m g(\alpha^{-1}X,\alpha^{-2}Y,\alpha^{-2}Z)=G_0(X,Y,Z)+\alpha G_1(X,Y,Z)+\cdots+\alpha^m G_m(X,Y,Z),$$

where m is the highest weight degree in the weight homogeneous components of g associated with the weight $\mathbf{s}=(1,2,2)$, and G_i has the weight degree $m-i$. Obviously, we have $g=G|_{\alpha=1}$.

Depending on whether h is constant or not, we separate the following proofs into two parts.

A. *g* satisfies Eq. (7)

Since an exponential factor multiplicative with a constant is also an exponential factor, without loss of generality, we assume that $G_m=0$. Using the weight change (10), we get from (7) and (11) that G satisfies

$$P(X,Y,Z)\frac{\partial G}{\partial X}+Q(X,Y,Z)\frac{\partial G}{\partial Y}+R(X,Y,Z)\frac{\partial G}{\partial Z}=\alpha^{m+1}l(x,y,z).$$

It can be written as

$$\begin{aligned} &(sy-\alpha sx)\sum_{i=0}^{m-1}\alpha^i\frac{\partial G_i}{\partial x}+(-xz-\alpha y+\alpha^2 rx)\sum_{i=0}^{m-1}\alpha^i\frac{\partial G_i}{\partial y}+(xy-\alpha bz)\sum_{i=0}^{m-1}\alpha^i\frac{\partial G_i}{\partial z}\\ &\quad=\alpha^{m-1}(l_2y+l_3z)+\alpha^m l_1x+\alpha^{m+1}l_0, \end{aligned} \tag{12}$$

where we use x,y,z to denote X,Y,Z.

Case 1: $m=1$. Then we can assume that $G=G_0=ax$. An easy computation shows that $l_0=l_3=0$, $l_2+l_1=0$ and $a=l_2/s$. So, we have $g=(l_2/s)x$ and $l=l_2(y-x)$. This verifies that the Lorenz system has always the exponential factor $F=\exp((l_2/s)x)$ with the cofactor $l=l_2(y-x)$, where l_2 is an arbitrary nonzero constant.

Case 2: $m=2$. Comparing the terms with the same degree in α of (12), we get that

$$\begin{aligned} L[G_0]&=0,\\ L[G_1]&=sx\frac{\partial G_0}{\partial x}+y\frac{\partial G_0}{\partial y}+bz\frac{\partial G_0}{\partial z}+l_2y+l_3z, \end{aligned} \tag{13}$$

where L is the linear partial differential operator

$$L=sy\frac{\partial}{\partial x}-xz\frac{\partial}{\partial y}+xy\frac{\partial}{\partial z}.$$

We now use the method of characteristic curves for solving linear partial differential equations to solve Eqs. (13) (see for instance, Bleecker and Csordas, 1992). The characteristic equation associated with the linear operator L is

$$\frac{dx}{dz}=\frac{sy}{xy},\quad \frac{dy}{dz}=-\frac{xz}{xy}.$$

It has general solutions

$$x^2-2sz=d_1,\quad y^2+z^2=d_2,$$

where d_1 and d_2 are arbitrary constants. We make the change of the variables

$$u=x^2-2sz,\quad v=y^2+z^2,\quad w=z. \tag{14}$$

Its inverse change is

$$x=\pm\sqrt{u+2sw},\quad y=\pm\sqrt{v-w^2},\quad z=w. \tag{15}$$

In the following we only consider the positive case. The negative one can be proved similarly.

From the last two transformations, and applying the method of characteristic curves to the first equation of (13), we obtain the following ordinary differential equation (for fixed u and v).

$$\frac{d\overline{G}_0}{dw}=0.$$

Here and after, we always use $\overline{A}(u,v,w)$ to denote $A(x,y,z)$ written in terms of u,v and w. The above equation has a general solution $\overline{G}_0(u,v,w)=G_0^*(u,v)$, where G_0^* is an arbitrary function in u and v. Since G_0 is a weight homogeneous polynomial of weight degree 2, we should have $G_0(x,y,z)=G_0^*(u,v)=a_0(x^2-2sz)$ with $a_0\in\mathbb{C}$.

Substituting G_0 into the second equation of (13) and using the changes (14) and (15), we obtain the following ordinary differential equation:

$$\sqrt{u+2sw}\sqrt{v-w^2}\frac{d\overline{G}_1}{dw}=2su+l_2\sqrt{v-w^2}+(4s^2-2sb+l_3)w.$$

It has a general solution

$$\overline{G}_1=\frac{l_2}{s}\sqrt{u+2sw}+2su\int\frac{dw}{\sqrt{u+2sw}\sqrt{v-w^2}}+(4s^2-2sb+l_3)\int\frac{wdw}{\sqrt{u+2sw}\sqrt{v-w^2}}.$$

From integrating formulas (A1) to (A3) of the Appendix, in order that $G_1(x,y,z)=\overline{G}_1(u,v,w)$ is a polynomial, we should have $s=0$. It is in contradiction with the assumption $s\neq 0$. So, the Lorenz system does not have exponential factors of the given form.

Case 3: $m\geqslant 3$. Then from (12) we get that $L[G_0]=0$ and

$$L[G_1]=sx\frac{\partial G_0}{\partial x}+y\frac{\partial G_0}{\partial y}+bz\frac{\partial G_0}{\partial z}. \tag{16}$$

Working in a similar way to the proof of case 2, we can prove that $G_0(x,y,z)=\overline{G}_1(u,v,w)=G_0^*(u,v)=G_0^*(x^2-2sz,y^2+z^2)$. Since G_0 is a weight homogeneous polynomial with the weight degree m, we must have $m=4n$ or $m=4n-2$ for $n\in\mathbb{N}$. Hence, G_0 has the form

$$G_0=\sum_{i=0}^{n} a_i(x^2-2sz)^{2i}(y^2+z^2)^{n-i},\quad m=4n, \tag{17}$$

or

$$G_0=\sum_{i=1}^{n} a_i(x^2-2sz)^{2i-1}(y^2+z^2)^{n-i},\quad m=4n-2. \tag{18}$$

If G_0 has form (17), then from Eq. (16) and using the method of characteristic curves, we can prove that

$$\begin{aligned}\overline{G}_1(u,v,w)=&\sum_{i=0}^{n}\frac{1}{s}[4si+2(n-i)]a_iu^{2i}v^{n-i-1}\sqrt{u+2sw}\sqrt{v-w^2}\\&+\sum_{i=0}^{n-1}\left\{\frac{1}{s}[4si+2(n-i)]a_i+4s(2s-b)(i+1)a_{i+1}\right\}\\&\times u^{2i+1}v^{n-i-1}\int\frac{wdw}{\sqrt{u+2sw}\sqrt{v-w^2}}+4na_nu^{2n+1}v^{-1}\\&+\sum_{i=0}^{n-1}[12si+2(b+2)(n-i)]a_iu^{2i}v^{n-i-1}\int\frac{w^2dw}{\sqrt{u+2sw}\sqrt{v-w^2}}.\end{aligned}$$

Using formulas (A2) and (A3) of the Appendix and the fact that G_1 is a polynomial, we get that $na_n=0$, and

$$[4si+2(n-i)]a_i+4s^2(2s-b)(i+1)a_{i+1}=0,$$

$$[6si+(b+2)(n-i)]a_i=0,$$

for $i=0,1,\ldots,n-1$. It implies that $a_i=0$ for $i=0,1,\ldots,n$. So, we have $G_0(x,y,z)\equiv 0$.

If G_0 has form (18), we can prove that

$$\overline{G}_1(u,v,w)=\sum_{i=1}^{n}\frac{1}{s}[2(2i-1)s+2(n-i)]a_i u^{2i-1}v^{n-i-1}\sqrt{u+2sw}\sqrt{v-w^2}$$
$$+\sum_{i=0}^{n}\left\{\frac{1}{s}[2(2i-1)s+2(n-i)]a_i+(4s^2-2sb)(2i+1)a_{i+1}\right\}$$
$$\times u^{2i}v^{n-i-1}\int\frac{wdw}{\sqrt{u+2sw}\sqrt{v-w^2}}$$
$$+\sum_{i=1}^{n}[6(2i-1)s+(2b+4)(n-i)]a_i u^{2i-1}v^{n-i-1}\int\frac{w^2dw}{\sqrt{u+2sw}\sqrt{v-w^2}}.$$

Hence, we have

$$(2s^2-sb)(2i+1)a_{i+1}+\frac{1}{s}[(2i-1)s+(n-i)]a_i=0,\quad i=0,1,\ldots,n,$$

$$[3(2i-1)s+(b+2)(n-i)]a_i=0,\quad i=1,\ldots,n.$$

This verifies that $a_i=0$ for $i=1,\cdots,n$. So, we also have $G_0(x,y,z)\equiv 0$.

This proves that the Lorenz system does not have the exponential factors of the given form.

B. *g* satisfies Eq. (9)

Using the weight change (10), we get from (11) that G satisfies

$$P(X,Y,Z)\frac{\partial G}{\partial X}+Q(X,Y,Z)\frac{\partial G}{\partial Y}+R(X,Y,Z)\frac{\partial G}{\partial Z}=\alpha kG+\alpha^{m+1}l(x,y,z)h(x,y,z),$$

i.e.,

$$(sY-\alpha sX)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial X}+(-XZ-\alpha Y+\alpha^2 rX)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial Y}+(XY-\alpha bZ)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial Z}$$
$$=\alpha k\sum_{i=0}^{m}\alpha^i G_i+\alpha^{m-1}(l_2Y+l_3Z+\alpha l_1X+\alpha^2 l_0)h(x,y,z). \tag{19}$$

In what follows we need the following result [for a proof, see, for instance Christopher and Llibre (2000)].

Lemma 4: Assume that f is a polynomial and that $f=f_1^{m_1}\cdots f_l^{m_l}$ is the irreducible factorization with $(f_i,f_j)=1$ for $i\neq j$. Then f is a Darboux polynomial of a polynomial vector filed $\mathcal{X}$ with a cofactor k if and only if $f_1,\ldots,f_l$ are Darboux polynomials of the vector filed $\mathcal{X}$ with cofactors $k_1,\ldots,k_l$. Moreover, we have $k=m_1k_1+\cdots+m_lk_l$.

Since h is a Darboux polynomial, by Theorem 2, depending on the different conditions for the Lorenz system to have a Darboux polynomial, we separate the following proofs into five cases.

Case 1. $b=2s$. Then $f=x^2-2sz$ is the generator of Darboux polynomials of the Lorenz system. The corresponding cofactor is $-2s$. From Lemma 4 we assume that $h=(x^2-2sz)^\mu$ with the cofactor $k=-2s\mu$, where $\mu\in\mathbb{N}$. Now Eq. (19) becomes

$$(sy-\alpha sx)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial x}+(-xz-\alpha y+\alpha^2 rx)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial y}+(xy-\alpha bz)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial z}$$
$$=\alpha(-2s\mu)\sum_{i=0}^{m}\alpha^i G_i+\alpha^{m-1-2\mu}(l_2y++l_3z+\alpha l_1x+\alpha^2 l_0)(x^2-2sz)^\mu, \tag{20}$$

where we first use the weight change (10), and then use x,y,z to denote X,Y,Z.

We claim that $m \geqslant 2\mu+1$. Otherwise, in what follows we can prove that $l=0$. So g is a Darboux polynomial with the cofactor $-2s\mu$. From the proof of Llibre and Zhang (2002), we obtain that $g=a(x^2-2sz)^\mu$, where a is an arbitrary constant. Hence, we have $(g,h)=(x^2-2sz)^\mu$. It is in contradiction with the assumption $(g,h)=1$.

We now prove the claim. If $m-1-2\mu<-2$, from (20) it is easy to check that $l_2=l_3=l_1=l_0=0$. Hence we have $l=0$.

If $m-1-2\mu=-2$, Eq. (20) shows that $l_2=l_3=l_1=0$ and

$$L[G_0]=l_0(x^2-2sz)^\mu.$$

Applying the method of characteristic curves to this equation, we obtain that

$$G_0(x,y,z)=\overline{G}_0(u,v,w)=l_0u^\mu\int\frac{dw}{\sqrt{u+2sw}\sqrt{v-w^2}}.$$

Since G_0 is a polynomial, from integrating formulas (A1)–(A3) of the Appendix we should have $l_0=0$. This verifies that $l=0$.

If $m-1-2\mu=-1$, then from (20) we get that $l_2=l_3=0$, and

$$\begin{aligned} L[G_0]&=l_1x(x^2-2sz)^\mu,\\ L[G_1]&=D_1[G_0]+l_0(x^2-2sz)^\mu, \end{aligned} \tag{21}$$

where D_1 is the linear partial differential operator

$$D_1=sx\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}+bz\frac{\partial}{\partial z}-2s\mu.$$

Since the operators L and D_1 are linear, we separate G_i into $G_i=G_i^{(0)}+G_i^{(1)}$ for $i=0,1$. Then Eq. (21) can be written as

$$L[G_0^{(0)}]=0,\quad L[G_0^{(1)}]=l_1x(x^2-2sz)^\mu, \tag{22}$$

$$L[G_1^{(0)}]=D_1[G_0^{(0)}],\quad L[G_1^{(1)}]=D_1[G_0^{(1)}]+l_0(x^2-2sz)^\mu, \tag{23}$$

where we require that in the process to solve the above equations, $G_i^{(1)}$, for $i=0,1$, do not contain integrating constants.

From the proof of Llibre and Zhang (2002) we get that $L[G_0^{(0)}]=0$ and $L[G_1^{(0)}]=D_1[G_0^{(0)}]$ always have polynomial solutions. The second equation of (22) has the solution

$$G_0^{(1)}(x,y,z)=\overline{G}_0^{(1)}(u,v,w)=l_1u^\mu\arcsin\frac{w}{\sqrt{v}}.$$

So we must have $l_1=0$, and hence $G_0^{(1)}=0$. Solving the second equation of (23) we get that

$$G_1^{(1)}(x,y,z)=\overline{G}_1^{(1)}(u,v,w)=l_0u^\mu\int\frac{dw}{\sqrt{u+2sw}\sqrt{v-w^2}}.$$

This verifies that $l_0=0$, and so we have $l=0$. This proves the claim.

We assume that $m=2\mu+1+\nu$ for some $\nu\in\mathbb{N}\cup\{0\}$. Then from (20) we obtain that

$$L[G_{\nu-i}]=D_1[G_{\nu-i-1}]-rx\frac{\partial G_{\nu-i-2}}{\partial y},\quad i=1,\ldots,\nu,$$

$$L[G_{\nu}]=D_1[G_{\nu-1}]-rx\frac{\partial G_{\nu-2}}{\partial y}+(l_2y+l_3z)(x^2-2sz)^{\mu},$$

$$L[G_{\nu+1}]=D_1[G_{\nu}]-rx\frac{\partial G_{\nu-1}}{\partial y}+l_1x(x^2-2sz)^{\mu},\tag{24}$$

$$L[G_{\nu+2}]=D_1[G_{\nu+1}]-rx\frac{\partial G_{\nu}}{\partial y}+l_0(x^2-2sz)^{\mu},$$

$$L[G_j]=D_1[G_{j-1}]-rx\frac{\partial G_{j-2}}{\partial y},\quad j=\nu+3,\ldots,2\mu+\nu+3,$$

where $G_i=0$ for $i<0$ or $i>2\mu+1+\nu$.

We write $G_i=G_i^{(0)}+G_i^{(1)}$ such that

$$L[G_i^{(0)}]=D_1[G_{i-1}^{(0)}]-rx\frac{\partial G_{i-2}^{(0)}}{\partial y},\quad i=0,1,\ldots,2\mu+\nu+3,\tag{25}$$

$$L[G_{\nu-i}^{(1)}]=0,\quad i=1,\ldots,\nu,\tag{26}$$

$$L[G_{\nu}^{(1)}]=(l_2y+l_3z)(x^2-2sz)^{\mu},\tag{27}$$

$$L[G_{\nu+1}^{(1)}]=D_1[G_{\nu}^{(1)}]-rx\frac{\partial G_{\nu-1}^{(1)}}{\partial y}+l_1x(x^2-2sz)^{\mu},\tag{28}$$

$$L[G_{\nu+2}^{(1)}]=D_1[G_{\nu+1}^{(1)}]-rx\frac{\partial G_{\nu}^{(1)}}{\partial y}+l_0(x^2-2sz)^{\mu},\tag{29}$$

$$L[G_j^{(1)}]=D_1[G_{j-1}^{(1)}]-rx\frac{\partial G_{j-2}^{(1)}}{\partial y},\quad j=\nu+3,\ldots,2\mu+\nu+3.\tag{30}$$

Moreover, we require that in the process to solve $G_i^{(l)}$ for $i=0,1,\ldots,m$ and $l=0,1$, the polynomials $G_i^{(1)}$ do not contain integrating constants. Set $G^{(0)}=\Sigma_{i=0}^{m}\alpha^iG_i^{(0)}$ and $G^{(1)}=\Sigma_{i=0}^{m}\alpha^iG_i^{(1)}$. Then we have $G=G^{(0)}+G^{(1)}$.

From (25) and working in a similar way to the proof of Llibre and Zhang (2002), we obtain that $g^{(0)}=G^{(0)}|_{\alpha=1}=\Sigma_{i=0}^{m}G_i^{(0)}$ is a Darboux polynomial of the Lorenz system with the cofactor $-2s\mu$. So, we should have $g^{(0)}=a(x^2-2sz)^{\mu}$, where a is an arbitrary constant.

Under the assumptions on $G_i^{(1)}$, we obtain that Eqs. (26) have the unique solutions $G_{\nu-i}^{(1)}=0$ for $i=1,\ldots,\nu$. From Eq. (27) we get that

$$G_{\nu}^{(1)}(x,y,z)=\overline{G}_{\nu}^{(1)}(u,v,w)=\frac{l_2}{s}u^{\mu}\sqrt{u+2sw}+l_3u^{\mu}\int\frac{wdw}{\sqrt{u+2sw}\sqrt{v-w^2}}.$$

Since $G_{\nu}^{(1)}$ is a polynomial, using formula (A2) we obtain that $l_3=0$ and

$$G_{\nu}^{(1)}=\frac{l_2}{s}x(x^2-2sz)^{\mu}.$$

This implies that $m=2\mu+1$, i.e., $\nu=0$.

Substituting $G_\nu^{(1)}$ into Eq. (28), we can prove that

$$G_{\nu+1}^{(1)}(x,y,z)=\overline{G}_{\nu+1}^{(1)}(u,v,w)=(l_1+l_2)u^\mu \arcsin\frac{w}{\sqrt{v}}.$$

Hence, we should have $l_1+l_2=0$ and $G_{\nu+1}^{(1)}=0$.

Introducing $G_\nu^{(1)}$ and $G_{\nu+1}^{(1)}$ into (29) and in a similar way to the proof of the case $m-2\mu=-1$, we get that $l_0=0$ and $G_{\nu+2}^{(1)}=0$. Furthermore, using the assumptions on $G_i^{(1)}$ we can prove that Eqs. (30) have only the solutions $G_j^{(1)}=0$ for $j=\nu+3,\ldots,m$. This proves that

$$g=(G^{(0)}+G^{(1)})|_{\alpha=1}=\frac{l_2}{s}x(x^2-2sz)^\mu+a(x^2-2sz)^\mu,$$

with $l=l_2(y-x)$. But $(g,h)=(x^2-2sz)^\mu$. It is in contradiction with the assumption $(g,h)=1$.

Case 2. $b=1$ and $r=0$. The Darboux polynomial is $h=(y^2+z^2)^\mu$ with the cofactor $k=-2\mu$, where $\mu\in\mathbb{N}$. Working in a similar way to the proof of case 1, we can prove that

$$g=\frac{l_2}{s}x(y^2+z^2)^\mu+a(y^2+z^2)^\mu,$$

with $l=l_2(y-x)$.

Case 3. $b=1$ and $s=1$. Then the Darboux polynomial is $h=(y^2+z^2-rx^2)^\mu$ with the cofactor $k=-2\mu$. Equation (19) becomes

$$\begin{aligned}&(y-\alpha x)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial x}+(-xz-\alpha y+\alpha^2 rx)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial y}+(xy-\alpha z)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial z}\\&\quad=-2\alpha\mu\sum_{i=0}^{m}\alpha^i G_i+\alpha^{m-1-4\mu}(l_2y+l_3z+\alpha l_1x+\alpha^2 l_0)(y^2+z^2-\alpha^2 rx)^\mu,\end{aligned}\tag{31}$$

where we first use the weight change (10), and then use x,y,z to denote X,Y,Z. Similar to the proof of case 1, we can assume that $m=4\mu+1+\nu$ for some $\nu\in\mathbb{N}\cup\{0\}$.

Consider the following equations:

$$L[G_i^{(0)}]=D_2[G_{i-1}^{(0)}]-rx\frac{\partial G_{i-2}^{(0)}}{\partial y},\quad i=0,1,\ldots,m+2,\tag{32}$$

$$L[G_{\nu-i}^{(1)}]=0,\quad i=1,\ldots,\nu\tag{33}$$

$$\begin{aligned}L[G_{\nu+2k}^{(1)}]&=D_2[G_{\nu+2k-1}^{(1)}]-rx\frac{\partial G_{\nu+2k-2}^{(1)}}{\partial y}+(l_2y+l_3z)\binom{\mu}{k}(y^2+z^2)^{\mu-k}(-rx^2)^k\\&\quad+l_0\binom{\mu}{k-1}(y^2+z^2)^{\mu-k+1}(-rx^2)^{k-1},\quad k=0,\ldots,\mu+1,\end{aligned}\tag{34}$$

$$L[G_{\nu+2k+1}^{(1)}]=D_2[G_{\nu+2k}^{(1)}]-rx\frac{\partial G_{\nu+2k-1}^{(1)}}{\partial y}+l_1x\binom{\mu}{k}(y^2+z^2)^{\mu-k}(-rx^2)^k,\quad k=0,\ldots,\mu,\tag{35}$$

$$L[G_{\nu+j}^{(1)}]=D_2[G_{\nu+j-1}^{(1)}]-rx\frac{\partial G_{\nu+j-2}^{(1)}}{\partial y},\quad j=2\mu+3,\ldots,4\mu+1,\tag{36}$$

where $G_i^{(l)}=0$ with $l=0,1$ for $i<0$ or $i>m$, $\binom{\mu}{k}=0$ for $k<0$ or $k>\mu$, and

$$D_2=x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}+z\frac{\partial}{\partial z}-2\mu.$$

We can prove that $G=\Sigma_{i=0}^{m}\alpha^i G_i$ satisfies (31) if and only if there exists a decomposition of G_i into $G_i=G_i^{(0)}+G_i^{(1)}$ such that $G_i^{(0)}$ and $G_i^{(1)}$ are weight homogeneous polynomials of the weight degrees same as those of G_i, and that $G_i^{(0)}$ satisfy (32), and $G_i^{(1)}$ satisfy (33)–(36). As before, we require that in the process to solve $G_i^{(1)}$, the integration constants are always equal to zero.

From Eqs. (32) and using the method given in Llibre and Zhang (2002), we can prove that $g^{(0)}=G^{(0)}|_{\alpha=1}=\Sigma_{i=0}^{m}G_i^{(0)}=a(y^2+z^2-rx^2)^{\mu}$, where a is an arbitrary constant. Using the assumptions on $G_i^{(1)}$, we obtain that Eqs. (33) have only the solutions $G_{\nu-i}^{(1)}=0$ for $i=1,\ldots,\nu$. Then Eq. (34) with $k=0$ becomes

$$L[G_\nu^{(1)}]=(l_2y+l_3z)(y^2+z^2)^{\mu}.$$

Working in a similar way to solve (27) we can prove that $l_3=0$ and

$$G_\nu^{(1)}=l_2x(y^2+z^2)^{\mu}.$$

Moreover, from Eq. (35) with $k=0$, we get that $l_2+l_1=0$ and $G_{\nu+1}^{(1)}=0$.

Now, Eq. (34) with $k=1$ becomes

$$L[G_{\nu+2}^{(1)}]=l_0(y^2+z^2)^{\mu}-3rl_2\mu x^2y(y^2+z^2)^{\mu-1}.$$

Solving this equation gives $l_0=0$ and

$$G_{\nu+2}^{(1)}=l_2x\binom{\mu}{1}(y^2+z^2)^{\mu-1}(-rx^2).$$

Introducing $G_{\nu+1}^{(1)}$ and $G_{\nu+2}^{(1)}$ into (35) with $k=1$, we obtain that $L[G_{\nu+3}^{(1)}]=0$. So, we have $G_{\nu+3}^{(1)}=0$.

By induction we assume that

$$G_{\nu+2k-1}^{(1)}=0,\quad G_{\nu+2k}^{(1)}=l_2x\binom{\mu}{k}(y^2+z^2)^{\mu-k}(-rx^2)^k.$$

Then, Eq. (35) can be simplified to

$$L[G_{\nu+2k+1}^{(1)}]=(l_2+l_1)x\binom{\mu}{k}(y^2+z^2)^{\mu-k}(-rx^2)^k=0.$$

Hence, we have $G_{\nu+2k+1}^{(1)}=0$. Now Eq. (34) becomes

$$L[G_{\nu+2k+2}^{(1)}]=(-r)^{k+1}l_2\binom{\mu}{k+1}(2k+3)(y^2+z^2)^{\mu-k-1}x^{2k+2}y.$$

Applying the method of characteristic curves to this equation, we obtain that

$$G_{\nu+2k+2}^{(1)}=l_2x\binom{\mu}{k+1}(y^2+z^2)^{\mu-k-1}(-rx^2)^{k+1}.$$

Therefore, we have

$$g^{(1)}=G^{(1)}|_{\alpha=1}=\sum_{i=0}^{m} G_i^{(1)}=l_2x\sum_{i=0}^{\mu}\binom{\mu}{i}(y^2+z^2)^{\mu-i}(-rx^2)^i=l_2x(y^2+z^2-rx^2)^{\mu}.$$

Moreover, from the above proof we get that $m=4\mu+1$, and

$$g=g^{(0)}+g^{(1)}=l_2x(y^2+z^2-rx^2)^{\mu}+a(y^2+z^2-rx^2)^{\mu}.$$

It is in contradiction with the assumption $(g,h)=1$.

Case 4. $b=6s-2$ and $r=2s-1$. The Darboux polynomial is $h=[x^4-4sx^2z-4s^2y^2+4s(4s-2)xy-(4s-2)^2x^2]^{\mu}$ with the cofactor $k=-4s\mu$. Equation (19) becomes

$$\begin{aligned}&(sy-\alpha sx)\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial x}+[-xz-\alpha y+\alpha^2(2s-1)x)]\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial y}+[xy-\alpha(6s-2)z]\sum_{i=0}^{m}\alpha^i\frac{\partial G_i}{\partial z}\\&=-4\alpha s\mu\sum_{i=0}^{m}\alpha^iG_i+\alpha^{m-1-4\mu}(l_2y+l_3z+\alpha l_1x+\alpha^2l_0)\\&\quad\times[x^4-4sx^2z-4s^2y^2+4\alpha s(4s-2)xy-\alpha^2(4s-2)^2x^2]^{\mu}.\end{aligned}\tag{37}$$

Working in a similar way to the proof of cases 1 and 3, we can prove that $m=4\mu+1$ and $G=G^{(0)}+G^{(1)}$ with $G^{(0)}|_{\alpha=1}=ah(x,y,z)$, and $G^{(1)}=\Sigma_{i=0}^{m}\alpha^iG_i^{(1)}$, where $G_i^{(1)}$ satisfy

$$L[G_0^{(1)}]=(l_2y+l_3z)(x^4-4sx^2z-4s^2y^2)^{\mu},\tag{38}$$

$$\begin{aligned}L[G_1^{(1)}]=&sx\frac{\partial G_0^{(1)}}{\partial x}+y\frac{\partial G_0^{(1)}}{\partial y}+(6s-2)z\frac{\partial G_0^{(1)}}{\partial z}-4s\mu G_0+(l_2y+l_3z)\binom{\mu}{1}\\&\times(x^4-4sx^2z-4s^2y^2)^{\mu-1}4s(4s-2)xy+l_1x(x^4-4sx^2z-4s^2y^2)^{\mu}.\end{aligned}\tag{39}$$

We still assume that the solutions $G_0^{(1)}$ and $G_1^{(1)}$ of (38) and (39) do not contain integrating constants.

Solving Eq. (38), we obtain that $l_3=0$ and

$$G_0^{(1)}=\frac{l_2}{s}x(x^4-4sx^2z-4s^2y^2)^{\mu}.$$

Then Eq. (39) becomes

$$\begin{aligned}L[G_1^{(1)}]=&(l_2+l_1)x(x^4-4sx^2z-4s^2y^2)^{\mu}+\mu l_2x(x^4-4sx^2z-4s^2y^2)^{\mu-1}\\&\times[-4(4s-2)(x^2-2sz)z-16s(4s-2)z^2+8s(4s-2)(y^2+z^2)].\end{aligned}$$

Applying the method of characteristic curves to this equation, we obtain that

$$\begin{aligned}G_1^{(1)}=\bar{G}_1^{(1)}=&(l_2+l_1)(u^2-4s^2v)^{\mu}\arcsin\frac{w}{\sqrt{v}}+\mu l_2(u^2-4s^2v)^{\mu-1}\\&\times\left[4(4s-2)u\sqrt{v-w^2}+16s(4s-2)\int\sqrt{v-w^2}dw-8s(4s-2)v\arcsin\frac{w}{\sqrt{v}}\right].\end{aligned}$$

If $s\neq\frac{1}{2}$, we must have $l_2+l_1=0$ and $l_2=0$. So, we get that $G_0^{(1)}=G_0^{(2)}=0$. Moreover, we have

$$L[G_2^{(1)}]=l_0(x^4-4sx^2z-4s^2y^2)^{\mu}.$$

Solving this equation yields $l_0=0$ and $G_2^{(1)}=0$. This proves that $l=0$. Hence, we have $g=g^{(0)}=ah(x,y,z)$. This means that the Lorenz system does not have exponential factors of the given form.

If $s=\frac{1}{2}$, then $b=1$ and $r=0$. The function $H=(x^2-z)^2/(y^2+z^2)$ is a rational first integral of the Lorenz system. The Darboux polynomial of the Lorenz system has a general form

$$h(x,y,z)=\prod_{i=1}^{m_1} f_i^{\mu_i}\prod_{j=1}^{m_2} g_j^{\nu_j},$$

where $f_i=(x^2-z)^2-c_i^{(1)}(y^2+z^2)$ and $g_j=(y^2+z^2)-c_j^{(2)}(x^2-z)^2$, with $c_i^{(1)}$ and $c_j^{(2)}$ arbitrary constants, are Darboux polynomials. The polynomial h has the weight degree $4(\Sigma_{i=1}^{m_1}\mu_i+\Sigma_{j=1}^{m_2}\nu_j)$. Working in a similar way to the proof of case 1 of this section, we can prove that $g=((l_2/s)x+a)h(x,y,z)$, where a is an arbitrary constant. It is also in contradiction with the assumption $(g,h)=1$.

Case 5. $b=0$, $s=\frac{1}{3}$; or $b=4$, $s=1$. The Darboux polynomial of the Lorenz system is $h=(x^4-\frac{4}{3}x^2z-\frac{4}{9}y^2-\frac{8}{9}xy+\frac{4}{3}rx^2)^\mu$ with the cofactor $k=-\frac{4}{3}\mu$, or $h=[x^4-4x^2z-4y^2+8xy-4rx^2-16(1-r)z]^\mu$ with the cofactor $k=-4\mu$, where $\mu\in\mathbb{N}$. Doing some similar computations as those in case 4, we may obtain that $g=ah(x,y,z)$, where a is an arbitrary constant. So, the Lorenz system does not have the exponential factor of the given form.

Summing up the above five cases, we have proved that the Lorenz system does not have exponential factors of the form $\exp(g(x,y,z)/h(x,y,z))$ with $(g,h)=1$. This proves statement (a).

Proof of statement (b): From Theorem 3 the Lorenz system has a Darbouxian first integral if and only if there exist $\mu_i,\nu_j\in\mathbb{C}$ not all zero such that

$$\sum_{i=1}^{m_1}\mu_i k_i+\sum_{j=1}^{m_2}\nu_j l_j=0, \tag{40}$$

where m_1 and m_2 are the numbers of Darboux polynomials and exponential factors, respectively; and k_i and l_j are the cofactors of Darboux polynomials and exponential factors, respectively. Theorem 2 shows that the cofactors of Darboux polynomials are constants. Statement (a) of Theorem 1 gives that the cofactors of exponential factors are of the form $l_j=c_j(y-x)$, where c_j are constants. So, Eq. (40) is equivalent to $\Sigma_{i=1}^{m_1}\mu_i k_i=0$ and $\Sigma_{j=1}^{m_2}\nu_j l_j=0$. This last equation is equivalent to $\Sigma_{j=1}^{m_2}\nu_j c_j=0$. Corresponding to the cofactor l_j, the exponential factor is $F_j=\exp((c_j/s)x)$. Hence, we have $\Pi_{j=1}^{m_2}F_j^{\nu_j}=\exp(\Sigma_{j=1}^{m_2}(\nu_j c_j/s)x)=1$. Thus, from Theorem 3 we obtain that the Lorenz system has a Darbouxian first integral H if and only if $H(x,y,z)=\Pi_{i=1}^{m_1}f_i^{\mu_i}$ with

$$\sum_{i=1}^{m_1}\mu_i k_i=0, \tag{41}$$

where $\mu_i\in\mathbb{C}$ are not all equal to zero, and each f_i is a Darboux polynomial with the cofactor k_i.

From Theorem 2 we get that the Lorenz system has Darboux polynomials such that their cofactors k_i satisfy (41) if and only if $b=1$, $r=0$ and $s=\frac{1}{2}$. Under these conditions the Lorenz system has the two independent Darboux polynomials $f_1=x^2-z$ and $f_2=y^2+z^2$ with the cofactors $k_1=-1$ and $k_2=-2$, respectively. Hence, the Lorenz system has a Darbouxian first integral

$$H=(x^2-z)^{-2\mu}(y^2+z^2)^\mu.$$

Of course, the Lorenz system may have other forms of Darbouxian first integrals, but they are dependent on H. This proves statement (b).

We have finished the proof of the theorem.

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APPENDIX

The following formulas are used in the proof of Theorem 1.

$$\int \frac{dw}{\sqrt{u+2sw}\sqrt{v-w^2}} = \frac{1}{sv}\sqrt{u+2sw}\sqrt{v-w^2} + \frac{u}{sv}\int \frac{wdw}{\sqrt{u+2sw}\sqrt{v-w^2}} + \frac{3}{v}\int \frac{w^2dw}{\sqrt{u+2sw}\sqrt{v-w^2}}. \tag{A1}$$

The following two integrating formulas are obtained by using the change $w=\sqrt{v}\sin\theta$ for $\theta \in [-\pi/2,\pi/2)$ and Formulas 2.571.2 and 2.571.3 of Gradshteyn and Ryzhik (1980).

$$\int \frac{wdw}{\sqrt{u+2sw}\sqrt{v-w^2}} = \int \frac{\sqrt{v}\sin\theta}{\sqrt{u+2s\sqrt{v}\sin\theta}}d\theta = \begin{cases} \dfrac{u}{s\sqrt{u+2s\sqrt{v}}}W(\delta,\gamma) - \dfrac{\sqrt{u+2s\sqrt{v}}}{s}E(\delta,\gamma), \\ \qquad \text{for } u>2s\sqrt{v}>0, -\dfrac{\pi}{2}\leqslant\theta<\dfrac{\pi}{2}, \\ \sqrt{v}\sqrt{\dfrac{1}{s\sqrt{v}}}\left[W\left(\beta,\dfrac{1}{\gamma}\right) - 2E\left(\beta,\dfrac{1}{\gamma}\right)\right], \\ \qquad \text{for } 0<|u|<2s\sqrt{v}, -\arcsin\dfrac{u}{2s\sqrt{v}}<\theta<\dfrac{\pi}{2}, \end{cases} \tag{A2}$$

$$\int \frac{w^2dw}{\sqrt{u+2sw}\sqrt{v-w^2}} = v\int \frac{\sin^2\theta}{\sqrt{u+2s\sqrt{v}\sin\theta}}d\theta = \begin{cases} \dfrac{u\sqrt{u+2s\sqrt{v}}}{3s^2}E(\delta,\gamma) - \dfrac{u^2+2s^2v}{3s^2\sqrt{u+2s\sqrt{v}}}W(\delta,\gamma) \\ \qquad -\dfrac{1}{3s}\sqrt{v-w^2}\sqrt{u+2sw}, \\ \qquad \text{for } u>2s\sqrt{v}>0, -\dfrac{\pi}{2}\leqslant\theta<\dfrac{\pi}{2}, \\ \sqrt{\dfrac{1}{s\sqrt{v}}}\left[\dfrac{2u\sqrt{v}}{3s}E\left(\beta,\dfrac{1}{\gamma}\right) - \dfrac{\sqrt{v}(u+s\sqrt{v})}{3s}W\left(\beta,\dfrac{1}{\gamma}\right)\right] \\ \qquad -\dfrac{1}{3s}\sqrt{v-w^2}\sqrt{u+2sw}, \\ \qquad \text{for } 0<|u|<2s\sqrt{v}, -\arcsin\dfrac{u}{2s\sqrt{v}}<\theta<\dfrac{\pi}{2} \end{cases} \tag{A3}$$

where

$$\beta=\arcsin\sqrt{\frac{2s\sqrt{v}(1-\sin\theta)}{u+2s\sqrt{v}}}=\arcsin\sqrt{\frac{2s(\sqrt{v}-w)}{u+2s\sqrt{v}}},$$

$$\gamma=\sqrt{\frac{4s\sqrt{v}}{u+2s\sqrt{v}}},\quad \delta=\arcsin\sqrt{\frac{1-\sin\theta}{2}}=\arcsin\sqrt{\frac{\sqrt{v}-w}{2\sqrt{v}}},$$

and

$$W(\phi,k)=\int_0^{\phi}\frac{d\zeta}{\sqrt{1-k^2\sin^2\zeta}}=\int_0^{\sin\phi}\frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}},$$

$$E(\phi,k)=\int_0^{\phi}\sqrt{1-k^2\sin^2\zeta}\,d\zeta=\int_0^{\sin\phi}\frac{\sqrt{1-k^2x^2}}{\sqrt{1-x^2}}dx$$

are elliptic integrals of the first and second kind in the Legendre normal form [see, for instance, Formulas 8.111.2 and 8.111.3 of Gradshteyn and Ryzhik (1980)].

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Liouville integrability of the finite dimensional Hamiltonian systems derived from principal chiral field

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For finite dimensional Hamiltonian systems derived from $1+1$ dimensional integrable systems, if they have Lax representations, then the Lax operator creates a set of conserved integrals. When these conserved integrals are in involution, it is believed quite popularly that there will be enough functionally independent ones among them to guarantee the Liouville integrability of the Hamiltonian systems, at least for those derived from physical problems. In this article, we give a counterexample based on the $U(2)$ principal chiral field. It is proved that the finite dimensional Hamiltonian systems derived from the $U(2)$ principal chiral field are Liouville integrable. Moreover, their Lax operator gives a set of involutive conserved integrals, but they are not enough to guarantee the integrability of the Hamiltonian systems. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1501446]

I. INTRODUCTION

For many $1+1$ dimensional integrable systems, the nonlinearization method can be applied to get finite dimensional ($1+0$ dimensional) Hamiltonian systems.[1] Usually these Hamiltonian systems have Lax representations so that the involutive conserved integrals can be obtained. In this way the original nonlinear partial differential equations are changed to systems of nonlinear ordinary differential equations.[2–8] Many interesting exact solutions, especially quasi-periodic solutions, were obtained in this way.

For a finite dimensional Hamiltonian system, if it can be written in the Lax form as

$$\frac{\mathrm{d}}{\mathrm{d}t}L(\lambda)=[M(\lambda),L(\lambda)], \tag{1.1}$$

then the conserved integrals are easily derived from the coefficients of $\mathrm{tr}(L^k(\lambda))$'s ($k\geqslant 1$) when they are expanded as Laurent series of λ. Usually the number of these coefficients is infinite. It is believed quite popularly that when these conserved integrals are in involution, there will be enough functionally independent ones among them to guarantee the Liouville integrability of the Hamiltonian systems. Indeed, this is the case for most known physically interesting systems, such as the equations in the AKNS system, Kaup–Newell system and many other examples including those derived from $2+1$ dimensional integrable systems.[3,4,7,9–11]

However, we will give a counterexample in this article to show that this is not always true.

This counterexample is based on a well-known physical model–the $U(n)$ principal chiral field [or, mathematically, the harmonic map from $\mathbf{R}^{1,1}$ to $U(n)$].[12–16] In this article, the equation of $U(n)$ principal chiral field can be first reduced to a set of Hamiltonian systems by the standard procedure of the nonlinearization method. This will be done in Secs. II and III. Then, in Sec. IV, we show that there are not enough conserved integrals in those given by $\mathrm{tr}(L^k(\lambda))$'s to guarantee the Liouville integrability of the systems. In Sec. V, it is proved that these Hamiltonian systems are actually Liouville integrable for $n=2$. That is, they still have a full set of involutive and independent conserved integrals. These conserved integrals are obtained from $\mathrm{tr}L^k(\lambda)$ and other obvious

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conserved integrals. When $n>2$, it is still open whether one can find enough involutive and independent conserved integrals by adding some obvious ones to $\mathrm{tr}L^k(\lambda)$'s. Therefore, at least for $n=2$, the Hamiltonian systems derived from the $U(2)$ principal chiral field are Liouville integrable, but their conserved integrals for Liouville integrability can not be fully obtained from $\mathrm{tr}L^k(\lambda)$.

II. HAMILTONIAN SYSTEMS DERIVED FROM $U(n)$ PRINCIPAL CHIRAL FIELD

The equation for the $U(n)$ principal chiral field is

$$(g_x g^{-1})_t+(g_t g^{-1})_x=0, \tag{2.1}$$

where the field $g(x,t)\in U(n)$. Write

$$P=g_x g^{-1}, \quad Q=g_t g^{-1}. \tag{2.2}$$

Then $P,Q\in u(n)$ (i.e., $P^*+P=0$, $Q^*+Q=0$) and (2.1) becomes

$$P_t+Q_x=0, \quad P_t-Q_x+[P,Q]=0. \tag{2.3}$$

Here the second equation is the integrability condition of (2.2).

It is known that (2.3) has a Lax pair

$$\Phi_x=\frac{1}{1-\lambda}P\Phi, \quad \Phi_t=\frac{1}{1+\lambda}Q\Phi, \tag{2.4}$$

where λ is a complex spectral parameter.

Now we write down the corresponding finite dimensional Hamiltonian systems and their Lax operators.

Let $\lambda_1,\ldots,\lambda_N$ be N distinct real constants with $\lambda_j\neq\pm1$ $(j=1,\ldots,N)$, and let $(\phi_{1\alpha},\ldots,\phi_{n\alpha})^T$ be an arbitrary solution of the Lax pair (2.4) with $\lambda=\lambda_\alpha$, $\Lambda=\mathrm{diag}(\lambda_1,\ldots,\lambda_N)$, $\Phi_j=(\phi_{j1},\ldots,\phi_{jN})^T$. Let

$$L=\sum_{\alpha=1}^{N}\frac{1}{\lambda-\lambda_\alpha}\begin{pmatrix}\bar{\phi}_{1\alpha}\phi_{1\alpha} & \bar{\phi}_{2\alpha}\phi_{1\alpha} & \cdots & \bar{\phi}_{n\alpha}\phi_{1\alpha}\\ \vdots & \vdots & \ddots & \vdots\\ \bar{\phi}_{1\alpha}\phi_{n\alpha} & \bar{\phi}_{2\alpha}\phi_{n\alpha} & \cdots & \bar{\phi}_{n\alpha}\phi_{n\alpha}\end{pmatrix}. \tag{2.5}$$

Expand L to power series of $1-\lambda$ and $1+\lambda$, respectively:

$$\begin{aligned}L=L^{(1)}&=\sum_{k=1}^{\infty}(1-\lambda)^{k-1}\begin{pmatrix}\langle\Phi_1,(1-\Lambda)^{-k}\Phi_1\rangle & \cdots & \langle\Phi_n,(1-\Lambda)^{-k}\Phi_1\rangle\\ \vdots & \ddots & \vdots\\ \langle\Phi_1,(1-\Lambda)^{-k}\Phi_n\rangle & \cdots & \langle\Phi_n,(1-\Lambda)^{-k}\Phi_n\rangle\end{pmatrix},\\ L=L^{(2)}&=-\sum_{k=1}^{\infty}(1+\lambda)^{k-1}\begin{pmatrix}\langle\Phi_1,(1+\Lambda)^{-k}\Phi_1\rangle & \cdots & \langle\Phi_n,(1+\Lambda)^{-k}\Phi_1\rangle\\ \vdots & \ddots & \vdots\\ \langle\Phi_1,(1+\Lambda)^{-k}\Phi_n\rangle & \cdots & \langle\Phi_n,(1+\Lambda)^{-k}\Phi_n\rangle\end{pmatrix},\end{aligned} \tag{2.6}$$

where the inner product $\langle V_1,V_2\rangle$ of two vectors is defined as $V_1^*V_2$. The first series converges when $|\lambda-1|<\min_{1\leq\alpha\leq N}|\lambda_\alpha-1|$ and the second one converges when $|\lambda+1|<\min_{1\leq\alpha\leq N}|\lambda_\alpha+1|$.

Lemma 1: If

$$P_{jk}=\mathrm{i}\langle\Phi_k,(1-\Lambda)^{-1}\Phi_j\rangle, \quad Q_{jk}=\mathrm{i}\langle\Phi_k,(1+\Lambda)^{-1}\Phi_j\rangle, \tag{2.7}$$

then

$$L_x=\frac{1}{1-\lambda}[P,L],\quad L_t=\frac{1}{1+\lambda}[Q,L], \tag{2.8}$$

and (P,Q) *gives a solution of (2.3).*

Proof: Let $\phi_\alpha=(\phi_{1\alpha},\ldots,\phi_{n\alpha})^T$. Then

$$L=\sum_{\alpha=1}^{N}\frac{1}{\lambda-\lambda_\alpha}\phi_\alpha\phi_\alpha^*. \tag{2.9}$$

Since $P^*=-P$ and λ_α's are real,

$$\begin{aligned}L_x&=\sum_{\alpha=1}^{N}\frac{1}{\lambda-\lambda_\alpha}\left(\phi_\alpha\frac{1}{1-\lambda_\alpha}\phi_\alpha^*P^*+\frac{1}{1-\lambda_\alpha}P\phi_\alpha\phi_\alpha^*\right)\\&=\sum_{\alpha=1}^{N}\frac{1}{\lambda-\lambda_\alpha}\frac{1}{1-\lambda_\alpha}[P,\phi_\alpha\phi_\alpha^*]\\&=\sum_{\alpha=1}^{N}\left(\frac{1}{\lambda-\lambda_\alpha}\frac{1}{1-\lambda}-\frac{1}{1-\lambda_\alpha}\frac{1}{1-\lambda}\right)[P,\phi_\alpha\phi_\alpha^*]=\frac{1}{1-\lambda}[P,L].\end{aligned} \tag{2.10}$$

The last equality holds due to (2.7). The equation for L_t in (2.8) is derived similarly. Finally, by computing the integrability condition $L_{xt}=L_{tx}$ from (2.8) or substituting (2.7) into (2.3) directly, we know that (P,Q) satisfies (2.3). The lemma is proved.

Now we always suppose (2.7) holds for the $U(n)$ principal chiral field, which gives the nonlinear constraints. Substituting (2.7) into (2.4), we get a system of partial differential equations

$$\begin{aligned}\Phi_{j,x}&=\mathrm{i}(1-\Lambda)^{-1}\sum_{k=1}^{n}\langle\Phi_k,(1-\Lambda)^{-1}\Phi_j\rangle\Phi_k,\\\Phi_{j,t}&=\mathrm{i}(1+\Lambda)^{-1}\sum_{k=1}^{n}\langle\Phi_k,(1+\Lambda)^{-1}\Phi_j\rangle\Phi_k,\end{aligned} \tag{2.11}$$

which can be studied as two systems of ordinary differential equations when t and x are considered as constants, respectively.

Now $\phi_{11},\phi_{12},\ldots,\phi_{1N},\ldots,\phi_{n1},\phi_{n2},\ldots,\phi_{nN}$ and their complex conjugations form the complex coordinates of $\mathbf{R}^{2nN}$. In this $\mathbf{R}^{2nN}$, let ω be the standard symplectic form

$$\omega=2\sum_{j=1}^{n}\sum_{\alpha=1}^{N}\mathrm{d}\,\mathrm{Im}(\phi_{j\alpha})\wedge\mathrm{d}\,\mathrm{Re}(\phi_{j\alpha})=\mathrm{i}\sum_{j=1}^{n}\sum_{\alpha=1}^{N}\mathrm{d}\bar{\phi}_{j\alpha}\wedge\mathrm{d}\phi_{j\alpha}. \tag{2.12}$$

Then the corresponding Poisson bracket for two functions f and g is

$$\{f,g\}=\frac{1}{\mathrm{i}}\sum_{j=1}^{n}\sum_{\alpha=1}^{N}\left(\frac{\partial f}{\partial\phi_{j\alpha}}\frac{\partial g}{\partial\bar{\phi}_{j\alpha}}-\frac{\partial g}{\partial\phi_{j\alpha}}\frac{\partial f}{\partial\bar{\phi}_{j\alpha}}\right). \tag{2.13}$$

From (2.8), the coefficients of $(1-\lambda)^j$ $(j=0,1,2,\ldots)$ in $\mathrm{tr}(L^{(1)})^k$ $(k=1,2,\ldots)$ and the coefficients of $(1+\lambda)^j$ $(j=0,1,2,\ldots)$ in $\mathrm{tr}(L^{(2)})^k$ $(k=1,2,\ldots)$ are all conserved. Suppose

$$\mathrm{tr}(L^{(1)})^m=\sum_{k=1}^{\infty}(1-\lambda)^{k-1}\mathcal{E}_{mk}^{(1)},\quad \mathrm{tr}(L^{(2)})^m=(-1)^m\sum_{k=1}^{\infty}(1+\lambda)^{k-1}\mathcal{E}_{mk}^{(2)}. \tag{2.14}$$

Since $\mathrm{tr}P=\mathrm{i}\mathcal{E}_{11}^{(1)}$ and $\mathrm{tr}Q=\mathrm{i}\mathcal{E}_{11}^{(2)}$, both $\mathrm{tr}P$ and $\mathrm{tr}Q$ are conserved. On the other hand, the Hamiltonians for Eqs. (2.11) are given by $\mathcal{E}_{21}^{(1)}$ and $\mathcal{E}_{21}^{(2)}$ according to the following lemma.

Moreover, direct computation shows that they commute with each other under the Poisson bracket (2.13) (this can also be derived directly from Lemma 3 in Sec. III).

Lemma 2: The Hamiltonians for the x-equation and the t-equation of (2.11) are given by

$$H^x=-\tfrac{1}{2}\mathcal{E}_{21}^{(1)}=-\tfrac{1}{2}\sum_{j,k=1}^{n}\langle\Phi_k,(1-\Lambda)^{-1}\Phi_j\rangle\langle\Phi_j,(1-\Lambda)^{-1}\Phi_k\rangle,$$
$$H^t=-\tfrac{1}{2}\mathcal{E}_{21}^{(2)}=-\tfrac{1}{2}\sum_{j,k=1}^{n}\langle\Phi_k,(1+\Lambda)^{-1}\Phi_j\rangle\langle\Phi_j,(1+\Lambda)^{-1}\Phi_k\rangle, \tag{2.15}$$

respectively. That is, (2.11) is equivalent to the Hamiltonian equations

$$\mathrm{i}\phi_{j\alpha,x}=\frac{\partial H^x}{\partial\bar{\phi}_{j\alpha}},\quad -\mathrm{i}\bar{\phi}_{j\alpha,x}=\frac{\partial H^x}{\partial\phi_{j\alpha}},\quad \mathrm{i}\phi_{j\alpha,t}=\frac{\partial H^t}{\partial\bar{\phi}_{j\alpha}},\quad -\mathrm{i}\bar{\phi}_{j\alpha,t}=\frac{\partial H^t}{\partial\phi_{j\alpha}}. \tag{2.16}$$

Moreover, $\{H^x,H^t\}=0$.

Remark 1: The above procedure can also be used for the harmonic map from $\mathbf{R}^2$ *to* $U(n)$. *In this case, the equation is*

$$(g_zg^{-1})_{\bar{z}}+(g_{\bar{z}}g^{-1})_z=0, \tag{2.17}$$

where z *is the complex coordinate of* $\mathbf{R}^2$, $g(z,\bar{z})\in U(n)$. *The Lax pair is*

$$\Phi_z=\frac{1}{1-\mathrm{i}\lambda}g_zg^{-1}\Phi,\quad \Phi_{\bar{z}}=\frac{1}{1+\mathrm{i}\lambda}g_{\bar{z}}g^{-1}\Phi, \tag{2.18}$$

where λ *is a complex spectral parameter. Using the same method in this section, we can also get finite dimensional Hamiltonian systems whose Lax operator is completely the same as (2.5).*

III. CONSERVED INTEGRALS

Lemma 3: With the Poisson bracket (2.13), the following two conclusions hold.
(1) For any two complex numbers λ, μ *and two positive integers* k, l,

$$\{\mathrm{tr}L^k(\lambda),\mathrm{tr}L^l(\mu)\}=0. \tag{3.1}$$

(2) For any complex number λ *and integers* j, k, l *with* $1\leqslant j,k\leqslant n$,

$$\{\langle\Phi_j,\Phi_k\rangle,\mathrm{tr}L^l(\lambda)\}=0. \tag{3.2}$$

This can be verified by direct computation of the Poisson brackets and was given in Ref. 11. Suppose the eigenvalues of $L(\lambda)$ are $\nu_1(\lambda)$, $\nu_2(\lambda),\ldots,\nu_n(\lambda)$. Then

$$\mathrm{tr}L^k(\lambda)=\nu_1^k(\lambda)+\cdots+\nu_n^k(\lambda),\quad (k=1,2,\ldots),$$
$$\det(\mu-L(\lambda))=\mu^n-p_1(\lambda)\mu^{n-1}+\cdots+(-1)^np_n(\lambda), \tag{3.3}$$

for any complex number μ where

$$p_k(\lambda)=\sum_{1\leqslant j_1<\cdots<j_k\leqslant n}\nu_{j_1}(\lambda)\cdots\nu_{j_k}(\lambda) \tag{3.4}$$

is the sum of all the determinants of the principal submatrices of $L(\lambda)$ of order k. Hence $\mathrm{tr}L^k(\lambda)$ $(k=1,2,\ldots)$ are uniquely determined by $p_k(\lambda)$ $(k=1,2,\ldots,n)$ and vise versa. Moreover, $\mathrm{tr}(L^{(1)})^k$ and $\mathrm{tr}(L^{(2)})^k$ in (2.14) can all be uniquely determined by $p_k(\lambda)$ $(k=1,2,\ldots,n)$.

Each $p_k(\lambda)$ is a holomorphic function of λ near $\lambda=\infty$. Let

$$p_m(\lambda)=\sum_{k=0}^{\infty} E_k^{(m)}\lambda^{-k-m}. \tag{3.5}$$

Then

$$\begin{aligned} E_k^{(m)} &= \sum_{1\leqslant i_1<\cdots<i_m\leqslant n}\ \sum_{\substack{r_1+\cdots+r_m=k\\ r_1,\cdots,r_m\geqslant 0}} \begin{vmatrix} \langle\Phi_{i_1},\Lambda^{r_1}\Phi_{i_1}\rangle & \langle\Phi_{i_2},\Lambda^{r_2}\Phi_{i_1}\rangle & \cdots & \langle\Phi_{i_m},\Lambda^{r_m}\Phi_{i_1}\rangle \\ \langle\Phi_{i_1},\Lambda^{r_1}\Phi_{i_2}\rangle & \langle\Phi_{i_2},\Lambda^{r_2}\Phi_{i_2}\rangle & \cdots & \langle\Phi_{i_m},\Lambda^{r_m}\Phi_{i_2}\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\Phi_{i_1},\Lambda^{r_1}\Phi_{i_m}\rangle & \langle\Phi_{i_2},\Lambda^{r_2}\Phi_{i_m}\rangle & \cdots & \langle\Phi_{i_m},\Lambda^{r_m}\Phi_{i_m}\rangle \end{vmatrix} \\ &= \sum_{1\leqslant i_1<\cdots<i_m\leqslant n}\ \sum_{\substack{r_1+\cdots+r_m=k\\ r_1,\cdots,r_m\geqslant 0}}\ \sum_{\substack{\alpha_1,\cdots,\alpha_m=1\\ \alpha_a\neq\alpha_b \text{ for } a\neq b}}^{N} \lambda_{\alpha_1}^{r_1}\cdots\lambda_{\alpha_m}^{r_m} \\ &\quad\times \begin{vmatrix} \overline{\phi}_{i_1\alpha_1}\phi_{i_1\alpha_1} & \overline{\phi}_{i_2\alpha_2}\phi_{i_1\alpha_2} & \cdots & \overline{\phi}_{i_m\alpha_m}\phi_{i_1\alpha_m} \\ \overline{\phi}_{i_1\alpha_1}\phi_{i_2\alpha_1} & \overline{\phi}_{i_2\alpha_2}\phi_{i_2\alpha_2} & \cdots & \overline{\phi}_{i_m\alpha_m}\phi_{i_2\alpha_m} \\ \vdots & \vdots & \ddots & \vdots \\ \overline{\phi}_{i_1\alpha_1}\phi_{i_m\alpha_1} & \overline{\phi}_{i_2\alpha_2}\phi_{i_m\alpha_2} & \cdots & \overline{\phi}_{i_m\alpha_m}\phi_{i_m\alpha_m} \end{vmatrix}. \end{aligned} \tag{3.6}$$

In the last summation, the condition "$\alpha_a\neq\alpha_b$ for $a\neq b$" is added since the determinants with $\alpha_a=\alpha_b$ $(a\neq b)$ are all zero.

Remark 2: When $m\geqslant N+1$, the last summation in (3.6) for "$1\leqslant\alpha_1,\ldots,\alpha_m\leqslant N$ with $\alpha_a\neq\alpha_b$ for $a\neq b$" is empty. This means that $E_k^{(m)}\equiv 0$ for $m\geqslant N+1$.

According to (2.8), all $E_k^{(m)}$'s are conserved.

From the first part of Lemma 3, all $E_k^{(m)}$'s are in involution. The second part of Lemma 3 implies that all $\langle\Phi_j,\Phi_k\rangle$'s commute with $E_k^{(m)}$'s. However, these $\langle\Phi_j,\Phi_k\rangle$'s may not commute with each other.

Remark 3: For the Heisenberg ferromagnetic equation, the x-equation of its Lax pair is similar to that of the $U(2)$ principal chiral field. The nonlinearization for this equation was dealt with in Ref. 2 and a set of involutive conserved integrals was obtained there.

Remark 4: Since tr$P$, tr$Q$ *are conserved, if (P,Q) is a solution of (2.3) in $u(n)$, then*

$$P'=P-\frac{1}{n}\mathrm{tr}P,\quad Q'=Q-\frac{1}{n}\mathrm{tr}Q \tag{3.7}$$

gives a solution of the same equation (2.3) in $su(n)$.

IV. DEPENDENCE OF CONSERVED INTEGRALS

In order to consider the integrability of the Hamiltonian systems, we should find a full set of involutive and independent conserved integrals. Unlike many other cases, here we cannot get a full set of independent conserved integrals simply from tr$L^k(\lambda)$'s.

For further discussion, we need the following lemma.

Lemma 4: Suppose k, m are two integers with $k\geqslant 0$ and $m\geqslant 2$, and $\mu_1,\ldots,\mu_m$ are distinct complex numbers. Then

$$\sum_{j=1}^{m} \mu_j^k \prod_{\substack{r=1 \\ r\neq j}}^{m} (\mu_j-\mu_r)^{-1} = \begin{cases} 0 & \text{if } k<m-1, \\ \displaystyle\sum_{\substack{p_1+\cdots+p_m=k-m+1 \\ p_1,\cdots,p_m\geqslant 0}} \mu_1^{p_1}\cdots\mu_m^{p_m} & \text{if } k\geqslant m-1. \end{cases} \tag{4.1}$$

Proof: Let

$$f(\zeta)=\zeta^k \prod_{r=1}^{m} (\zeta-\mu_r)^{-1}. \tag{4.2}$$

Then $f(\zeta)$ is a meromorphic function of ζ with poles $\mu_1,\ldots,\mu_m$. Let C_R be a circle with radius R, center 0 and positive orientation. Then, when $R>\max_{1\leqslant j\leqslant m}|\mu_j|$,

$$\frac{1}{2\pi \mathrm{i}} \int_{C_R} f(\zeta)\mathrm{d}\zeta = \sum_{j=1}^{m} \operatorname*{Res}_{\zeta=\mu_j} f(\zeta) = \sum_{j=1}^{m} \mu_j^k \prod_{\substack{r=1 \\ r\neq j}}^{m} (\mu_j-\mu_r)^{-1}. \tag{4.3}$$

On the other hand, let $\xi=\zeta^{-1}$. Then

$$\begin{aligned} \frac{1}{2\pi \mathrm{i}} \int_{C_R} f(\zeta)\mathrm{d}\zeta &= \lim_{R\to\infty} \frac{1}{2\pi \mathrm{i}} \int_{C_{1/R}} \xi^{m-k-2} \prod_{r=1}^{m} (1-\mu_r\xi)^{-1}\mathrm{d}\xi \\ &= \begin{cases} 0 & \text{if } k-m+1<0, \\ \displaystyle\sum_{\substack{p_1+\cdots+p_m=k-m+1 \\ p_1,\cdots,p_m\geqslant 0}} \mu_1^{p_1}\cdots\mu_m^{p_m} & \text{if } k-m+1\geqslant 0 \end{cases} \end{aligned} \tag{4.4}$$

by expanding all the terms $(1-\mu_j\xi)^{-1}$ at $\xi=0$. The lemma is proved.

Theorem 1: *For* $1\leqslant m\leqslant n$, *there are at most* $\max(0,N-m+1)$ *linearly independent functions in* $E_k^{(m)}$ $(k=0,1,2,\ldots)$. *Therefore, the number of linearly independent functions in* $E_k^{(m)}$ $(m=1,2,\ldots,n;\ k=0,1,2,\ldots)$ *cannot exceed* $nN-\frac{1}{2}n(n-1)$ *if* $N\geqslant n$ *or* $\frac{1}{2}N(N+1)$ *if* $N<n$.

Proof: According to Remark 2, $E_k^{(m)}\equiv 0$ for $m\geqslant N+1$. Hence we always suppose $m\leqslant N$.

By definition, $\Lambda=\mathrm{diag}(\lambda_1,\ldots,\lambda_N)$, $\lambda_j\neq\lambda_k$ $(j\neq k)$. Clearly, for any non-negative integers $(k_1,\ldots,k_l)$ with $k_i\neq k_j$ $(i\neq j)$ and $l\geqslant N+1$, $E_{k_1}^{(1)},\ldots,E_{k_l}^{(1)}$ are linearly dependent. On the other hand, since the Van de Monde determinant of $\lambda_1,\ldots,\lambda_N$ is not zero, there are exactly N independent functions in $E_k^{(1)}$ $(k=0,1,2,\ldots)$.

For $m\geqslant 2$, we show that there are at most $N-m+1$ independent functions in $E_k^{(m)}$ $(k=0,1,2,\ldots)$ for fixed m.

Let $k_1,\ldots,k_N$ be N arbitrary distinct non-negative integers. For fixed s with $0\leqslant s\leqslant m-2$, let $(\gamma_1^{(s)},\ldots,\gamma_N^{(s)})$ be a solution of the linear algebraic system

$$\sum_{j=1}^{N} \lambda_\alpha^{k_j+m-1}\gamma_j^{(s)}=\lambda_\alpha^s \quad (\alpha=1,2,\ldots,N). \tag{4.5}$$

Since the coefficient matrix in (4.5) is $(\lambda_\alpha^{k_j+m+1})_{\alpha,j=1,\ldots,N}$ which is invertible, $(\gamma_1^{(s)},\ldots,\gamma_N^{(s)})$ exists uniquely.

Let

$$F_s^{(m)}=\sum_{j=1}^{N} \gamma_j^{(s)} E_{k_j}^{(m)} \quad (s=0,1,\ldots,m-2). \tag{4.6}$$

Then

$$F_s^{(m)}=\sum_{j=1}^{N}\sum_{1\leqslant i_1<\cdots<i_m\leqslant n}\ \sum_{\substack{r_1+\cdots+r_m=k_j\\ r_1,\cdots,r_m\geqslant 0}}\ \sum_{\substack{\alpha_1,\cdots,\alpha_m=1\\ \alpha_a\neq\alpha_b \text{ for } a\neq b}}^{N}\gamma_j^{(s)}\lambda_{\alpha_1}^{r_1}\cdots\lambda_{\alpha_m}^{r_m}$$
$$\times\begin{vmatrix}\overline{\phi}_{i_1\alpha_1}\phi_{i_1\alpha_1} & \overline{\phi}_{i_2\alpha_2}\phi_{i_1\alpha_2} & \cdots & \overline{\phi}_{i_m\alpha_m}\phi_{i_1\alpha_m}\\ \overline{\phi}_{i_1\alpha_1}\phi_{i_2\alpha_1} & \overline{\phi}_{i_2\alpha_2}\phi_{i_2\alpha_2} & \cdots & \overline{\phi}_{i_m\alpha_m}\phi_{i_2\alpha_m}\\ \vdots & \vdots & \ddots & \vdots\\ \overline{\phi}_{i_1\alpha_1}\phi_{i_m\alpha_1} & \overline{\phi}_{i_2\alpha_2}\phi_{i_m\alpha_2} & \cdots & \overline{\phi}_{i_m\alpha_m}\phi_{i_m\alpha_m}\end{vmatrix}. \tag{4.7}$$

For fixed $i_1,\ldots,i_m$, $\alpha_1,\ldots,\alpha_m$ and s with $0\leqslant s\leqslant m-2$, let

$$\Delta=\sum_{j=1}^{N}\sum_{\substack{r_1+\ldots+r_m=k_j\\ r_1,\ldots,r_m\geqslant 0}}\gamma_j^{(s)}\lambda_{\alpha_1}^{r_1}\cdots\lambda_{\alpha_m}^{r_m}. \tag{4.8}$$

Then

$$\Delta=\sum_{j=1}^{N}\gamma_j^{(s)}\sum_{a=1}^{m}\lambda_{\alpha_a}^{k_j+m-1}\prod_{\substack{r=1\\ r\neq a}}^{m}(\lambda_{\alpha_a}-\lambda_{\alpha_r})^{-1} \tag{4.9}$$

by Lemma 4. The relations (4.5) imply

$$\Delta=\sum_{a=1}^{m}\lambda_{\alpha_a}^{s}\prod_{\substack{r=1\\ r\neq a}}^{m}(\lambda_{\alpha_a}-\lambda_{\alpha_r})^{-1}. \tag{4.10}$$

Using Lemma 4 again, we get $\Delta=0$ for $s=0,1,2,\ldots,m-2$. Hence

$$F_0^{(m)}=F_1^{(m)}=\cdots=F_{m-2}^{(m)}=0. \tag{4.11}$$

By (4.5), the matrix $(\gamma_j^{(s)})_{1\leqslant j\leqslant N;\ 0\leqslant s\leqslant m-2}$ has rank $m-1$. Hence $E_{k_j}^{(m)}$ $(j=1,2,\ldots,N)$ satisfy $m-1$ independent linear relations for fixed m. This means that there are at most $N-m+1$ independent functions in N functions $E_{k_j}^{(m)}$ for fixed m.

Since $k_1,\ldots,k_N$ are arbitrary, there are at most $N-m+1$ independent functions in $E_k^{(m)}$ $(k=0,1,2,\ldots)$.

The total number of possible linearly independent functions in $E_k^{(m)}$ $(m=1,2,\ldots,n;\ k=0,1,2,\ldots)$ is

$$\sum_{m=1}^{n}(N-m+1)=nN-\tfrac{1}{2}n(n-1) \tag{4.12}$$

for $N\geqslant n$ and

$$\sum_{m=1}^{N}(N-m+1)=\tfrac{1}{2}N(N+1) \tag{4.13}$$

for $N<n$. The theorem is proved.

A completely integrable Hamiltonian system in $\mathbf{R}^{2nN}$ needs nN independent involutive conserved integrals. Hence the above theorem shows that it is not possible to find enough conserved integrals only from $E_k^{(m)}$'s for Liouville integrability.

V. LIOUVILLE INTEGRABILITY OF THE HAMILTONIAN SYSTEMS

In general, we have not been able to determine whether the Hamiltonian systems for the $U(n)$ principal chiral field are Liouville integrable or not. However, when $n=2$, the answer is positive.

Hereafter, we suppose $n=2$. Therefore, we want to find $2N$ independent conserved integrals for the Hamiltonian systems in $\mathbf{R}^{4N}$.

If $N=1$, let

$$\begin{aligned}\tilde{E}_0^{(1)}&=E_0^{(1)}=\langle\Phi_1,\Phi_1\rangle+\langle\Phi_2,\Phi_2\rangle,\\ \tilde{E}_0^{(2)}&=\langle\Phi_1,\Phi_2\rangle+\langle\Phi_2,\Phi_1\rangle.\end{aligned}\tag{5.1}$$

If $N\geqslant 2$, let

$$\begin{aligned}\tilde{E}_k^{(1)}&=E_k^{(1)}=\langle\Phi_1,\Lambda^k\Phi_1\rangle+\langle\Phi_2,\Lambda^k\Phi_2\rangle \quad (k=0,1,\ldots,N-1),\\ \tilde{E}_k^{(2)}&=E_k^{(2)}=\sum_{j=0}^{k}\begin{vmatrix}\langle\Phi_1,\Lambda^j\Phi_1\rangle & \langle\Phi_2,\Lambda^{k-j}\Phi_1\rangle\\ \langle\Phi_1,\Lambda^j\Phi_2\rangle & \langle\Phi_2,\Lambda^{k-j}\Phi_2\rangle\end{vmatrix} \quad (k=0,1,\ldots,N-2),\\ \tilde{E}_{N-1}^{(2)}&=\langle\Phi_1,\Phi_2\rangle+\langle\Phi_2,\Phi_1\rangle.\end{aligned}\tag{5.2}$$

Here the last one is chosen to be $\langle\Phi_1,\Phi_2\rangle+\langle\Phi_2,\Phi_1\rangle$ because all the conserved integrals should take real value.

Theorem 2: *When $n=2$, $\tilde{E}_k^{(m)}$ $(m=1,2;\ k=0,1,\ldots,N-1)$ are in involution and are functionally independent in a dense open subset of $\mathbf{R}^{4N}$.*

Proof: By Lemma 3, $\tilde{E}_k^{(m)}$ $(m=1,2;\ k=0,1,\ldots,N-1)$ are in involution.

It is obvious that they are independent for $N=1$. Hence we suppose $N\geqslant 2$. Let $a_{1\alpha}$ $(\alpha=1,2,\ldots,N)$ be N nonzero real numbers,

$$a_{2\alpha}=a_{1\alpha}^{-1}\prod_{\substack{\beta=1\\ \beta\neq\alpha}}^{N}(\lambda_\alpha-\lambda_\beta)^{-1} \quad (\alpha=1,2,\ldots,N).\tag{5.3}$$

Then Lemma 4 implies

$$\begin{aligned}\sum_{\beta=1}^{N}\lambda_\beta^k\overline{a}_{2\beta}a_{1\beta}&=0 \quad (k=0,1,\ldots,N-2),\\ \sum_{\beta=1}^{N}\lambda_\beta^{N-1}\overline{a}_{2\beta}a_{1\beta}&=1.\end{aligned}\tag{5.4}$$

Let $P_0\in\mathbf{R}^{4N}$ be given by $\phi_{1\beta}=a_{1\beta}$, $\phi_{2\beta}=\epsilon a_{2\beta}$ $(\beta=1,2,\ldots,N)$. Here ϵ is a nonzero small real constant to be determined. Then, at P_0,

$$\begin{aligned}&\frac{\partial\tilde{E}_k^{(1)}}{\partial\overline{\phi}_{1\alpha}}=\lambda_\alpha^k\phi_{1\alpha}, \quad \frac{\partial\tilde{E}_k^{(1)}}{\partial\overline{\phi}_{2\alpha}}=\lambda_\alpha^k\phi_{2\alpha} \quad (k=0,1,\ldots,N-1),\\ &\frac{\partial\tilde{E}_k^{(2)}}{\partial\overline{\phi}_{1\alpha}}=\sum_{j=0}^{k}\begin{vmatrix}\lambda_\alpha^j\phi_{1\alpha} & \displaystyle\sum_{\beta=1}^{N}\lambda_\beta^{k-j}\overline{\phi}_{2\beta}\phi_{1\beta}\\ \lambda_\alpha^j\phi_{2\alpha} & \displaystyle\sum_{\beta=1}^{N}\lambda_\beta^{k-j}|\phi_{2\beta}|^2\end{vmatrix}=\sum_{j=0}^{k}r_{2,k-j}\lambda_\alpha^j\phi_{1\alpha},\end{aligned}\tag{5.5}$$

$$\frac{\partial \tilde{E}_k^{(2)}}{\partial \overline{\phi}_{2\alpha}} = \sum_{j=0}^{k} \begin{vmatrix} \sum_{\beta=1}^{N} \lambda_\beta^{k-j} |\phi_{1\beta}|^2 & \lambda_\alpha^j \phi_{1\alpha} \\ \sum_{\beta=1}^{N} \lambda_\beta^{k-j} \overline{\phi}_{1\beta} \phi_{2\beta} & \lambda_\alpha^j \phi_{2\alpha} \end{vmatrix} = \sum_{j=0}^{k} r_{1,k-j} \lambda_\alpha^j \phi_{2\alpha} \qquad (k=0,1,\ldots,N-2),$$

$$\frac{\partial \tilde{E}_{N-1}^{(2)}}{\partial \overline{\phi}_{1\alpha}} = \phi_{2\alpha}, \quad \frac{\partial \tilde{E}_{N-1}^{(2)}}{\partial \overline{\phi}_{2\alpha}} = \phi_{1\alpha}$$

by using (5.4) where

$$r_{jk} = \sum_{\beta=1}^{N} \lambda_\beta^k |\phi_{j\beta}|^2. \tag{5.6}$$

Let J be the Jacobian matrix

$$J = \left. \frac{\partial(\tilde{E}_0^{(1)},\ldots,\tilde{E}_{N-1}^{(1)},\tilde{E}_0^{(2)},\ldots,\tilde{E}_{N-1}^{(2)})}{\partial(\overline{\phi}_{11},\ldots,\overline{\phi}_{1N},\overline{\phi}_{21},\ldots,\overline{\phi}_{2N})} \right|_{P_0}. \tag{5.7}$$

Denote ROW_j to be the jth row of J. Take the elementary transformations for the rows of J as follows:

(1) k from 1 to $N-1$:

$$\mathrm{ROW}_{N+k} - \sum_{j=0}^{k-1} r_{2,k-1-j} \mathrm{ROW}_{j+1} \to \mathrm{ROW}_{N+k},$$

(2) k from 2 to $N-1$:

$$\mathrm{ROW}_{N+k} - \sum_{j=1}^{k-1} \frac{r_{1j}-r_{2j}}{r_{10}-r_{20}} \mathrm{ROW}_{N+k-j} \to \mathrm{ROW}_{N+k}, \tag{5.8}$$

(3) k from 1 to $N-1$:

$$(r_{10}-r_{20})^{-1} \mathrm{ROW}_{N+k} \to \mathrm{ROW}_{N+k},$$

(4) k from 1 to $N-1$:

$$\mathrm{ROW}_k - \mathrm{ROW}_{N+k} \to \mathrm{ROW}_k.$$

Then J is transformed to

$$\tilde{J}=\begin{pmatrix} \phi_{11} & \phi_{12} & \cdots & \phi_{1N} & 0 & 0 & \cdots & 0 \\ \lambda_1\phi_{11} & \lambda_2\phi_{12} & \cdots & \lambda_N\phi_{1N} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \lambda_1^{N-2}\phi_{11} & \lambda_2^{N-2}\phi_{12} & \cdots & \lambda_N^{N-2}\phi_{1N} & 0 & 0 & \cdots & 0 \\ \lambda_1^{N-1}\phi_{11} & \lambda_2^{N-1}\phi_{12} & \cdots & \lambda_N^{N-1}\phi_{1N} & \lambda_1^{N-1}\phi_{21} & \lambda_2^{N-1}\phi_{22} & \cdots & \lambda_N^{N-1}\phi_{2N} \\ 0 & 0 & \cdots & 0 & \phi_{21} & \phi_{22} & \cdots & \phi_{2N} \\ 0 & 0 & \cdots & 0 & \lambda_1\phi_{21} & \lambda_2\phi_{22} & \cdots & \lambda_N\phi_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & \lambda_1^{N-2}\phi_{21} & \lambda_2^{N-2}\phi_{22} & \cdots & \lambda_N^{N-2}\phi_{2N} \\ \phi_{21} & \phi_{22} & \cdots & \phi_{2N} & \phi_{11} & \phi_{12} & \cdots & \phi_{1N} \end{pmatrix}. \tag{5.9}$$

Let

$$T=\begin{pmatrix} T_2 & \\ & T_1 \end{pmatrix}, \tag{5.10}$$

where

$$T_j=\begin{pmatrix} \lambda_1^{N-1}\overline{\phi}_{j1} & \lambda_1^{N-2}\overline{\phi}_{j1} & \cdots & \overline{\phi}_{j1} \\ \lambda_2^{N-1}\overline{\phi}_{j2} & \lambda_2^{N-2}\overline{\phi}_{j2} & \cdots & \overline{\phi}_{j2} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_N^{N-1}\overline{\phi}_{jN} & \lambda_N^{N-2}\overline{\phi}_{jN} & \cdots & \overline{\phi}_{jN} \end{pmatrix}\Bigg|_{P_0} \qquad (j=1,2). \tag{5.11}$$

Then

$$\det T=\prod_{1\leqslant\alpha<\beta\leqslant N}(\lambda_\alpha-\lambda_\beta)^2\prod_{\gamma=1}^{N}\overline{\phi}_{1\gamma}\overline{\phi}_{2\gamma}|_{P_0}\neq 0. \tag{5.12}$$

Using the relations (5.4), we have, at P_0,

$$\tilde{J}T=\begin{pmatrix} \rho & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ * & \rho & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ * & * & \cdots & \rho & 0 & 0 & 0 & \cdots & 0 & 0 \\ * & * & \cdots & * & \rho & * & * & \cdots & * & \overline{\rho} \\ 0 & 0 & \cdots & 0 & 0 & \rho & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & * & \rho & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & * & * & \cdots & \rho & 0 \\ * & * & \cdots & * & \sum_{j=1}^{N}|\phi_{2j}|^2 & * & * & \cdots & * & \sum_{j=1}^{N}|\phi_{1j}|^2 \end{pmatrix}, \tag{5.13}$$

where

$$\rho=\sum_{\beta=1}^{N}\lambda_{\beta}^{N-1}\overline{\phi}_{2\beta}\phi_{1\beta}\Big|_{P_0}=\epsilon\neq 0 \tag{5.14}$$

and $*$ represents the entries which may not be zero.

Hence, at P_0,

$$\begin{aligned}(r_{10}-r_{20})^{-N+1}\det(JT)=\det(\tilde{J}T)&=\rho^{2N-2}\left(\rho\sum_{j=1}^{N}|\phi_{1j}|^2-\overline{\rho}\sum_{j=1}^{N}|\phi_{2j}|^2\right)\\&=\epsilon^{2N-1}\left(\sum_{j=1}^{N}a_{1j}^2-\epsilon^2\sum_{j=1}^{N}a_{2j}^2\right).\end{aligned} \tag{5.15}$$

It is not zero when ϵ is small enough. Since $\det J$ is a real analytical function on $\mathbf{R}^{4N}$, $\det J$ is not zero in a dense open subset of $\mathbf{R}^{4N}$. The theorem is proved.

Remark 5: Although the constraint here is of Bargmann type, the proof of the independence of the conserved integrals is not so simple as in the AKNS system. In that case, P_0 is simply chosen as a point near 0. *However, here $L(\lambda)$ is homogeneous to all Φ_j's so the choice of P_0 near* 0 *does not have any effect on the simplification of the computation on J.*

The Liouville integrability of the $U(2)$ principal chiral field follows from Lemma 2 and Theorem 2. It is given by the following theorem.

Theorem 3: *When $n=2$, the Hamiltonian systems given by* (2.15) *are completely integrable in the Liouville sense. Each solution of the Hamiltonian systems* (2.15) *gives a solution (P,Q) of* (2.3), *the equation of the $U(2)$ principal chiral field, and $(P-\frac{1}{2}\mathrm{tr}P, Q-\frac{1}{2}\mathrm{tr}Q)$ is a solution of the $SU(2)$ principal chiral field.*

Remark 6: Theorem 1 implies that one needs at least $n(n+1)/2$ extra conserved integrals together with $E_k^{(m)}$'s to form a full set of conserved integrals for the complete integrability of the Hamiltonian systems. According to Lemma 3, all $\langle\Phi_k,\Phi_j\rangle$'s commute with $E_k^{(m)}$. However, two elements in $\{\langle\Phi_k,\Phi_j\rangle\}$ may not commute with each other. Therefore, it is not obvious how to add at least $n(n+1)/2$ extra conserved integrals to $E_k^{(m)}$ in general.

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Geometric quantization of time-dependent completely integrable Hamiltonian systems

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A time-dependent completely integrable Hamiltonian system is quantized with respect to time-dependent action-angle variables near an instantly compact regular invariant manifold. Its Hamiltonian depends only on action variables, and has a time-independent countable energy spectrum. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1502927]

I. INTRODUCTION

A time-dependent Hamiltonian system of m degrees of freedom is called a completely integrable system (CIS) if it admits m independent first integrals in involution. Choosing appropriate dynamic variables, one may hope to quantize a time-dependent CIS so that its quantum Hamiltonian and first integral operators possess time-independent spectra.[1] The time-dependent action-angle variables introduced in the following are of this type. Written relative to these variables, a Hamiltonian of a time-dependent CIS is a function only of the action coordinates. It follows that, if time-dependent action-angle coordinates hold fixed, a time-dependent CIS can be quantized just as an autonomous one, and its energy spectrum is time-independent.

In order to introduce time-dependent action-angle variables, we use the fact that a time-dependent CIS of m degrees of freedom can be extended to an autonomous one of $m+1$ degrees of freedom where the time is regarded as a dynamic variable.[2–4] By virtue of the classical Arnold–Liouville theorem,[5,6] an autonomous CIS admits the action-angle coordinates around a regular connected compact invariant manifold. The problem is that invariant manifolds of a time-dependent CIS are not compact because of the time axis. Therefore, we first generalize the above-mentioned theorem to noncompact invariant manifolds. Then we show that, if a regular connected invariant manifold N of a time-dependent CIS is compact at each instant, it admits an open neighborhood in the ambient momentum phase space which is isomorphic to the product

$$W=\mathbb{R}\times T^m\times V \tag{1}$$

of the time axis $\mathbb{R}$, an m-dimensional torus T^m, and an open domain $V\subset\mathbb{R}^m$. This product is equipped with the coordinates

$$(t,\phi^i,I_i), \quad i=1,\ldots,m, \tag{2}$$

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where t is the Cartesian coordinate on $\mathbb{R}$ and ϕ^i are cyclic coordinates on T^m. Written with respect to these coordinates, a Hamiltonian and first integrals of a time-dependent CIS are functions only of action coordinates I_i. The corresponding Hamilton equation on W reads

$$\dot{I}_i = 0, \quad \dot{\phi}^i = \partial^i \mathcal{H}(I_j).$$

A glance at this equation shows that, given action-angle coordinates (2), a time-dependent CIS can be seen as an autonomous CIS on the symplectic annulus

$$P = V \times T^m, \tag{3}$$

equipped with the action-angle coordinates (ϕ^i, I_i) and provided with the symplectic form

$$\Omega_P = \mathrm{d}I_i \wedge \mathrm{d}\phi^i. \tag{4}$$

Therefore, we can quantize a time-dependent CIS with respect to action-angle variables similarly to that of an autonomous CIS. Of course, the choice of time-dependent action-angle coordinates by no means is unique. They are changed by canonical transformations. Therefore, we employ the geometric quantization technique[7–9] which remains equivalent under such kind transformations. At the same time, geometric quantization essentially depends on the choice of polarization.[10,11]

Geometric quantization of an autonomous CIS has been studied with respect to polarization spanned by Hamiltonian vector fields of first integrals.[12] In fact, the Simms quantization of the harmonic oscillator[9] is also of this type. The problem is that the associated quantum algebra includes functions which are not defined on the whole momentum phase space, and elements of the carrier space fail to be smooth sections of the quantum bundle. Indeed, written with respect to the action-angle variables, this quantum algebra consists of functions which are affine in angle coordinates.

We choose a different polarization spanned by almost-Hamiltonian vector fields ∂^k of angle variables. The associated quantum algebra $\mathcal{A}$ consists of smooth functions which are affine in action variables. Note that this quantization of the symplectic annulus P (3) is equivalent to geometric quantization of the cotangent bundle T^*T^m of the torus T^m with respect to the familiar vertical polarization. As is well known, the vertical polarization of a cotangent bundle leads to its Schrödinger quantization. We show that $\mathcal{A}$ possesses a set of nonequivalent representations in the separable pre-Hilbert space $\mathbb{C}^\infty(T^m)$ of smooth complex functions on T^m. In particular, the action operators read

$$\hat{I}_k = -i\partial_k - \lambda_k, \tag{5}$$

where λ_k are real numbers which specify different representations of $\mathcal{A}$. By virtue of the multidimensional Fourier theorem, an orthonormal basis for $\mathbb{C}^\infty(T^m)$ consists of functions

$$\psi_{(n_r)} = \exp[i(n_r\phi^r)], \quad (n_r) = (n_1, \ldots, n_m) \in \mathbb{Z}^m. \tag{6}$$

With respect to this basis, the action operators (5) are countable diagonal matrices

$$\hat{I}_k \psi_{(n_r)} = (n_k - \lambda_k)\psi_{(n_r)}. \tag{7}$$

Given the representation (5), any polynomial Hamiltonian $\mathcal{H}(I_k)$ of a CIS is uniquely quantized as a Hermitian element $\hat{\mathcal{H}}(I_k) = \mathcal{H}(\hat{I}_k)$ of the enveloping algebra $\overline{\mathcal{A}}$ of $\mathcal{A}$. It has the countable time-independent spectrum

$$\hat{\mathcal{H}}(I_k)\psi_{(n_r)} = E_{(n_r)}\psi_{(n_r)}, \quad E_{(n_r)} = \mathcal{H}(n_k - \lambda_k), \quad n_k \in (n_r). \tag{8}$$

Similarly, polynomial first integrals are quantized. Since $\hat{I}_k$ are diagonal, one can also quantize Hamiltonians $\mathcal{H}(I_j)$ and first integrals $F(I_j)$ which are analytic functions on $\mathbb{R}^m$.

Note that, because geometric quantization is equivalent under canonical transformations, quantization of a time-dependent CIS with respect to action-angle variables induces its quantization with respect to initial variables near an invariant manifold in the ambient momentum phase space. However, its Hamiltonian need not be represented in terms of first integrals and need not belong to the quantum algebra $\overline{\mathcal{A}}$ because it fails to be a scalar under time-dependent transformations. Moreover, this induced quantization cannot be in general extended to the whole momentum phase space because of the topological obstructions to the existence of global action-angle coordinates.[13,14]

For instance, one usually mentions a harmonic oscillator as the simplest CIS whose quantization in the action-angle variables looks notoriously difficult.[15] However, a harmonic oscillator written relative to action-angle coordinates (ϕ,I) is located in the momentum phase space $\mathbb{R}^2\backslash\{0\}$, but it is not the standard oscillator on $\mathbb{R}^2$. Namely, there is a monomorphism, but not an isomorphism of the Poisson algebra of smooth complex functions on $\mathbb{R}^2$ to that on $\mathbb{R}^2\backslash\{0\}$. In particular, the angle polarization on $\mathbb{R}^2\backslash\{0\}$ is not extended to $\mathbb{R}^2$. As a consequence, the quantum algebra associated with this polarization is not extended to $\mathbb{R}^2$, and so is its carrier space $\mathbb{C}^\infty(T^m)$.

In conclusion, let us remark that, since Hamiltonians depend only on action variables and possess time-independent countable spectra, quantum CISs look especially promising for holonomic quantum computation, based on driving degenerate eigenstates of a Hamiltonian over a parameter space.[16–18] We will construct the corresponding quantum control operator.

II. CLASSICAL COMPLETELY INTEGRABLE SYSTEMS

Recall that the configuration space of time-dependent mechanics is a fiber bundle $Q\to\mathbb{R}$ over the time axis $\mathbb{R}$ equipped with the bundle coordinates (t,q^k), $k=1,\ldots,m$. The corresponding momentum phase space is the vertical cotangent bundle V^*Q of $Q\to\mathbb{R}$ endowed with holonomic coordinates (t,q^k,p_k).[19,20] The cotangent bundle T^*Q, coordinated by $(q^\lambda,p_\lambda)=(t,q^k,p_0,p_k)$, plays a role of the homogeneous momentum phase space. It is provided with the canonical Liouville form $\Xi=p_\lambda dq^\lambda$, the symplectic form $\Omega=d\Xi$, and the corresponding Poisson bracket

$$\{f,f'\}_T=\partial^\lambda f\partial_\lambda f'-\partial_\lambda f\partial^\lambda f', \quad f,f'\in C^\infty(T^*Q). \tag{9}$$

There is the one-dimensional trivial affine bundle

$$\zeta: T^*Q\to V^*Q. \tag{10}$$

Given its global section h, one can equip T^*Q with the global bundle coordinate $r=p_0-h$.

The fiber bundle (10) provides the vertical cotangent bundle V^*Q with the canonical Poisson structure $\{,\}_V$ such that

$$\zeta^*\{f,f'\}_V=\{\zeta^*f,\zeta^*f'\}_T, \quad \forall f,f'\in C^\infty(V^*Q), \tag{11}$$

$$\{f,f'\}_V=\partial^k f\partial_k f'-\partial_k f\partial^k f'. \tag{12}$$

Its characteristic symplectic foliation coincides with the fibration $V^*Q\to\mathbb{R}$. However, the Poisson structure (12) fails to set any dynamic equation on the momentum phase space V^*Q because Hamiltonian vector fields

$$\vartheta_f=\partial^k f\partial_k-\partial_k f\partial^k, \quad \vartheta_f\rfloor df'=\{f,f'\}_V, \quad f,f'\in C^\infty(V^*Q),$$

of functions on V^*Q are vertical.

A Hamiltonian of time-dependent mechanics is defined as a global section

$$h: V^*Q\to T^*Q, \quad p_0\circ h=-\mathcal{H}(t,q^j,p_j),$$

of the affine bundle ζ (10).[19,20] It yields the pull-back Hamiltonian form

$$H = h^*\Xi = p_k \mathrm{d}q^k - \mathcal{H}\,\mathrm{d}t \tag{13}$$

on V^*Q. Then there exists a unique vector field γ_H on V^*Q such that

$$\begin{gathered} \gamma_H \rfloor \mathrm{d}t = 1, \quad \gamma_H \rfloor \mathrm{d}H = 0, \\ \gamma_H = \partial_t + \partial^k \mathcal{H} \partial_k - \partial_k \mathcal{H} \partial^k. \end{gathered} \tag{14}$$

Its trajectories obey the Hamilton equation

$$\dot{q}^k = \partial^k \mathcal{H}, \quad \dot{p}_k = -\partial_k \mathcal{H}. \tag{15}$$

A first integral of the Hamilton equation (15) is a smooth real function F on V^*Q whose Lie derivative

$$L_{\gamma_H} F = \gamma_H \rfloor \mathrm{d}F = \partial_t F + \{\mathcal{H}, F\}_V$$

along the vector field γ_H (14) vanishes, i.e., F is constant on trajectories of γ_H. A time-dependent Hamiltonian system (V^*Q, H) is said to be completely integrable if the Hamilton equation (15) admits m first integrals F_k which are in involution with respect to the Poisson bracket $\{,\}_V$ (12) and whose differentials $\mathrm{d}F_k$ are linearly independent almost everywhere, i.e., the set of points where this condition fails is nowhere dense in V^*Q. One can associate to this system an autonomous CIS on T^*Q as follows.

Let us consider the pull-back $\zeta^* H$ of the Hamiltonian form H (13) onto the cotangent bundle T^*Q. It is readily observed that

$$\mathcal{H}^* = \partial_t \rfloor (\Xi - \zeta^* h^* \Xi) = p_0 + \mathcal{H} \tag{16}$$

is a function on T^*Q. Let us regard $\mathcal{H}^*$ as a Hamiltonian of an autonomous Hamiltonian system on the symplectic manifold (T^*Q, Ω). Its Hamiltonian vector field

$$\gamma_T = \partial_t - \partial_t \mathcal{H} \partial^0 + \partial^k \mathcal{H} \partial_k - \partial_k \mathcal{H} \partial^k \tag{17}$$

is projected onto the vector field γ_H (14) on V^*Q so that

$$\zeta^*(L_{\gamma_H} f) = \{\mathcal{H}^*, \zeta^* f\}_T, \quad \forall f \in C^\infty(V^*Q).$$

An immediate consequence of this relation is the following:

Proposition 1: (i) Given a time-dependent CIS $(V^*Q, H; F_k)$ on V^*Q, the Hamiltonian system $(T^*Q; \mathcal{H}^*, \zeta^* F_k)$ on T^*Q is completely integrable. (ii) Let N be a connected regular invariant manifold of $(V^*Q, H; F_k)$. Then $h(N) \subset T^*Q$ is a connected regular invariant manifold of the autonomous CIS $(T^*Q; \mathcal{H}^*, \zeta^* F_k)$.

Hereafter, the vector field γ_H (14) is assumed to be complete. In this case, the Hamilton equation (15) admits a unique global solution through each point of the momentum phase space V^*Q, and trajectories of γ_H define a trivial bundle $V^*Q \to V_t^*Q$ over any fiber V_t^*Q of $V^*Q \to \mathbb{R}$. Without loss of generality, one can choose the fiber $i_0 : V_0^*Q \to V^*Q$ at $t = 0$. Since N is an invariant manifold, the fibration

$$\xi : V^*Q \to V_0^*Q \tag{18}$$

also yields the fibration of N onto $N_0 = N \cap V_0^*Q$ such that $N \cong \mathbb{R} \times N_0$ is a trivial bundle.

III. TIME-DEPENDENT ACTION-ANGLE COORDINATES

Let us introduce the action-angle coordinates around an invariant manifold N of a time-dependent CIS on V^*Q by use of the action-angle coordinates around the invariant manifold $h(N)$ of the autonomous CIS on T^*Q in Proposition 1. Since N and, consequently, $h(N)$ are noncompact, we first prove the following:

Proposition 2: Let M be a connected invariant manifold of an autonomous CIS $\{F_\lambda\}$, $\lambda=1,\ldots,n$, on a symplectic manifold (Z,Ω_Z), and let the Hamiltonian vector fields of the first integrals F_α on M be complete. Let U be a neighborhood of M such that $\{F_\lambda\}$ have no critical points in U and the submersion $\times F_\lambda: U\to\mathbb{R}^n$ is a trivial bundle of Lagrangian invariant manifolds over a domain $V'\subset\mathbb{R}^n$. Then U is isomorphic to the symplectic annulus

$$W'=\mathbb{R}^{n-m}\times T^m\times V' \tag{19}$$

provided with the generalized action-angle coordinates

$$(x^1,\ldots,x^{n-m},\phi^{n-m+1},\ldots,\phi^n,I_1,\ldots,I_n) \tag{20}$$

such that the symplectic form on W' reads

$$\Omega_Z=\mathrm{d}I_a\wedge\mathrm{d}x^a+\mathrm{d}I_k\wedge\mathrm{d}\phi^k,$$

and the first integrals F_λ depend only on the action coordinates (I_α).

Proof: In accordance with the well-known theorem,[5,21] the invariant manifold M is diffeomorphic to the product $\mathbb{R}^{n-m}\times T^m$, provided with coordinates $(y^\lambda)=(s^a,\varphi^i)$, where φ^i are linear functions of parameters s^λ along the integral curves of Hamiltonian vector fields of first integrals F_λ on M. Let (J_λ) be coordinates on V' which are values of first integrals F_λ. Since $W'\to V'$ is a trivial bundle, (y^λ,J_λ) are bundle coordinates on the annulus W' (19). It should be emphasized that, since group parameters are given up to a shift, the coordinates y^λ on W' are determined up to a shift by functions of coordinates J_λ. Written relative to these coordinates, the symplectic form Ω_Z on W' reads

$$\Omega_Z=\Omega^{\alpha\beta}\mathrm{d}J_\alpha\wedge\mathrm{d}J_\beta+\Omega^\alpha_\beta\mathrm{d}J_\alpha\wedge\mathrm{d}y^\beta. \tag{21}$$

By the definition of coordinates (y^λ), the Hamiltonian vector fields ϑ_λ of first integrals take the coordinate form $\vartheta_\lambda=\vartheta^\alpha_\lambda(J_\mu)\partial_\alpha$ where

$$\vartheta_a=\partial_a+\vartheta^i_a(J_\lambda)\partial_i,\quad \vartheta_i=\vartheta^k_i(J_\lambda)\partial_k, \tag{22}$$

and they obey the relations

$$\vartheta_\lambda\rfloor\Omega_Z=-\mathrm{d}J_\lambda,\quad \Omega^\alpha_\beta\vartheta^\beta_\lambda=\delta^\alpha_\lambda. \tag{23}$$

It follows that Ω^α_β is a nondegenerate matrix and $\vartheta^\alpha_\lambda=(\Omega^{-1})^\alpha_\lambda$, i.e., the matrix functions Ω^α_β depend only on coordinates J_λ. In Appendix A, we obtain the desired coordinates

$$x^a=s^a,\quad \phi^a(s^b,\varphi^i,J_\lambda),\quad I_a=J_a,\quad I_i(J_k). \tag{24}$$

Note that, if M is a compact invariant manifold, the conditions of Proposition 2 always hold.[6]

Of course, the generalized action-angle coordinates (20) by no means are unique. For instance, let $\mathcal{F}_a$, $a=1,\ldots,n-m$ be an arbitrary smooth function on $\mathbb{R}^m$. Let us consider the canonical coordinate transformation

$$x'^a=x^a,\quad \phi'^i=\phi^i+x^a\partial^i\mathcal{F}_a(I_j),\quad I'_a=I_a-\mathcal{F}_a(I_j),\quad I'_k=I_k. \tag{25}$$

Then (x'^a,ϕ'^k,I'_a,I'_k) also generalized action-angle coordinates on the symplectic annulus which differs from W' (19) in another trivialization.

Now, we apply Proposition 2 to the CISs in Proposition 1.

Proposition 3: Let N be a connected regular invariant manifold of a time-dependent CIS $(V^*Q,H;F_k)$, and let the image N_0 of its projection ξ (18) be compact. Then the invariant manifold $h(N)$ of the autonomous CIS $(T^*Q;\mathcal{H}^*,\zeta^*F_k)$ has an open neighborhood U obeying the condition of Proposition 2.

The proof is in Appendix B. In accordance with Proposition 2, the open neighborhood U of the invariant manifold $h(N)$ in Proposition 3 is isomorphic to the symplectic annulus

$$W'=\mathbb{R}\times T^m\times V', \tag{26}$$

provided with the generalized action-angle coordinates $(t,\phi^1,\ldots,\phi^m,I_0,\ldots,I_m)$ such that the symplectic form on W' reads

$$\Omega'=\mathrm{d}I_0\wedge\mathrm{d}t+\mathrm{d}I_k\wedge\mathrm{d}\phi^k.$$

A glance at the Hamiltonian vector field $\vartheta_0=\gamma_T$ (17) and relations (23) and (24) shows that $I_0=J_0=\mathcal{H}^*$ and the corresponding generalized angle coordinate is $x^0=t$, while the first integrals $J_k=\zeta^*F_k$ depend only on the action coordinates I_i.

Since the action coordinates I_i are independent of the coordinate J_0, the symplectic annulus W' (26) inherits the fibration (10) which reads

$$\zeta: W'\ni(t,\phi^i,I_0,I_i)\to(t,\phi^i,I_i)\in W=\mathbb{R}\times T^m\times V.$$

By the relation similar to (11), the product W is provided with the Poisson structure

$$\{f,f'\}_W=\partial^i f\partial_i f'-\partial_i f\partial^i f',\quad f,f'\in C^\infty(W). \tag{27}$$

Therefore, one can regard W with coordinates (t,ϕ^i,I_i) as the momentum phase space of the time-dependent CIS in question around its invariant manifold N.

It is readily observed that the Hamiltonian vector field γ_T of the autonomous Hamiltonian $\mathcal{H}^*=I_0$ is $\gamma_T=\partial_t$, and so is its projection γ_H (14) on W. Consequently, the Hamilton equation (15) with respect to the action-angle coordinates takes the form $\dot I_i=0$, $\dot\phi^i=0$. Hence, (t,ϕ^i,I_i) are the initial date coordinates. One can introduce such coordinates as follows. Given the fibration ξ (18), let us provide $N_0\times V\subset V_0^*Q$ in Proposition 3 with action-angle coordinates $(\overline{\phi^i},\overline{I_i})$ for the CIS $\{i_0^*F_k\}$ on the symplectic leaf V_0^*Q. Then, it is readily observed that $(t,\overline{\phi^i},\overline{I_i})$ are time-dependent action-angle coordinates on W (1) such that the Hamiltonian $\mathcal{H}(\overline{I_j})$ of a time-dependent CIS relative to these coordinates vanishes, i.e., $\mathcal{H}^*=\overline{I_0}$. Using the canonical transformations (25), one can consider time-dependent action-angle coordinates besides the initial date ones. Given a smooth function $\mathcal{H}$ on $\mathbb{R}^m$, let us further provide W with the action-angle coordinates

$$\phi^i=\overline{\phi^i}+t\partial^i\mathcal{H}(\overline{I_j}),\quad I_0=\overline{I_0}-\mathcal{H}(\overline{I_j}),\quad I_i=\overline{I_i}$$

such that $\mathcal{H}(I_i)$ is the Hamiltonian.

Thus, action-angle coordinates for a time-dependent CIS provide a particular solution of the problem of a representation of its Hamiltonian in terms of first integrals.[22,23] However, this representation need not hold with respect to the initial bundle coordinates on V^*Q because a Hamiltonian fails to be a scalar under time-dependent transformations.

IV. QUANTUM COMPLETELY INTEGRABLE SYSTEMS

In order to quantize a time-dependent CIS on the Poisson manifold $(W,\{,\}_W)$, one may follow the general procedure of instantwise geometric quantization of time-dependent Hamiltonian sys-

tems in Ref. 24. As was mentioned previously, it however can be quantized as an autonomous CIS on the symplectic annulus (P,Ω_P) (3) with respect to fixed time-dependent action-angle coordinates.

In accordance with the standard geometric quantization procedure,[7,8] since the symplectic form Ω_P (4) is exact, the prequantum bundle is defined as a trivial complex line bundle C over P. Since the action-angle coordinates are canonical for the symplectic form (4), the prequantum bundle C needs no metaplectic correction. Let its trivialization

$$C\cong P\times\mathbb{C} \tag{28}$$

hold fixed. Any other trivialization leads to equivalent quantization of P. Given the associated bundle coordinates (ϕ^k,I_k,c), $c\in\mathbb{C}$, on C (28), one can treat its sections as smooth complex functions on P.

The Konstant–Souriau prequantization formula associates to each smooth real function $f\in C^\infty(P)$ on P the first-order differential operator

$$\hat{f}=-i\nabla_{\vartheta_f}+f \tag{29}$$

on sections of C, where $\vartheta_f=\partial^k f\partial_k-\partial_k f\partial^k$ is the Hamiltonian vector field of f and ∇ is the covariant differential with respect to a suitable $U(1)$-principal connection on C. This connection preserves the Hermitian metric $g(c,c')=c\overline{c'}$ on C, and its curvature form obeys the prequantization condition $R=i\Omega_P$. It reads

$$A=A_0+icI_k d\phi^k\otimes\partial_c, \tag{30}$$

where A_0 is a flat $U(1)$-principal connection on $C\to P$. The equivalence classes of flat principal connections on C are indexed by the set $\mathbb{R}^m/\mathbb{Z}^m$ of homomorphisms of the de Rham cohomology group

$$H^1(P)=H^1(T^m)=\mathbb{R}^m$$

of P to the cycle group $U(1)$.[9] We choose their representatives of the form

$$A_0[(\lambda_k)]=\mathrm{d}I_k\otimes\partial^k+\mathrm{d}\phi^k\otimes(\partial_k+i\lambda_k c\partial_c),\quad \lambda_k\in[0,1).$$

Then the connection (30) up to gauge transformations reads

$$A[(\lambda_k)]=\mathrm{d}I_k\otimes\partial^k+\mathrm{d}\phi^k\otimes(\partial_k+i(I_k+\lambda_k)c\partial_c). \tag{31}$$

For the sake of simplicity, we will assume that the numbers λ_k in expression (31) belong to $\mathbb{R}$, but will bear in mind that connections $A[(\lambda_k)]$ and $A[(\lambda'_k)]$ with $\lambda_k-\lambda'_k\in\mathbb{Z}$ are gauge conjugated. Given a connection (31), the prequantization operators (29) read

$$\hat{f}=-i\vartheta_f+(f-(I_k+\lambda_k)\partial^k f). \tag{32}$$

Let us choose the above-mentioned angle polarization $V\pi$ which is the vertical tangent bundle of the fibration $\pi:P\to T^m$, and is spanned by the vectors ∂^k. It is readily observed that the corresponding quantum algebra $\mathcal{A}\subset C^\infty(P)$ consists of affine functions

$$f=a^k(\phi^j)I_k+b(\phi^j) \tag{33}$$

of action coordinates I_k. The carrier space of its representation by operators (32) is defined as the space E of sections ρ of the prequantum bundle C of compact support which obey the condition $\nabla_\vartheta\rho=0$ for any Hamiltonian vector field ϑ subordinate to the distribution $V\pi$. This condition reads

$$\partial_k f \partial^k \rho = 0, \quad \forall f \in C^\infty(T^m).$$

It follows that elements of E are independent of action variables and, consequently, fail to be of compact support, unless $\rho = 0$. This well-known problem of Schrödinger geometric quantization is solved as follows:[24,25]

Fix a slice $i_T : T^m \to T^m \times V$. Let $C_T = i_T^* C$ be the pull-back of the prequantum bundle C (28) over the torus T^m. It is a trivial complex line bundle $C_T = T^m \times \mathbb{C}$ provided with the pull-back Hermitian metric $g(c,c') = c\overline{c'}$. Its sections are smooth complex functions on T^m. Let

$$\overline{A} = i_T^* A = \mathrm{d}\phi^k \otimes (\partial_k + i(I_k + \lambda_k) c \partial_c)$$

be the pull-back of the connection A (31) onto C_T. Let $\mathcal{D}$ be a metalinear bundle of complex half-forms on the torus T^m. It admits the canonical lift of any vector field τ on T^m, and the corresponding Lie derivative of its sections reads

$$\mathbf{L}_\tau = \tau^k \partial_k + \tfrac{1}{2} \partial_k \tau^k.$$

Let us consider the tensor product

$$Y = C_T \otimes \mathcal{D} \to T^m. \tag{34}$$

Since the Hamiltonian vector fields

$$\vartheta_f = a^k \partial_k - (I_r \partial_k a^r + \partial_k b) \partial^k$$

of functions f (33) are projectable onto T^m, one can associate to each element f of the quantum algebra $\mathcal{A}$ the first-order differential operator

$$\hat{f} = (-i\overline{\nabla}_{\pi\vartheta_f} + f) \otimes \mathrm{Id} + \mathrm{Id} \otimes \mathbf{L}_{\pi\vartheta_f} = -ia^k \partial_k - \frac{i}{2} \partial_k a^k - a^k \lambda_k + b \tag{35}$$

on sections of Y. A direct computation shows that the operators (35) obey the Dirac condition

$$[\hat{f}, \hat{f}'] = -i\widehat{\{f, f'\}}.$$

Sections ρ_T of the quantum bundle $Y \to T^m$ (34) constitute a pre-Hilbert space E_T with respect to the nondegenerate Hermitian form

$$\langle \rho_T | \rho_T' \rangle = \left(\frac{1}{2\pi} \right)^m \int_{T^m} \rho_T \overline{\rho_T'}, \quad \rho_T, \rho_T' \in E_T.$$

Then it is readily observed that $\hat{f}$ (35) are Hermitian operators in E_T. In particular, the action operators take the form (5).

Of course, the above-noted quantization depends on the choice of a connection $A[(\lambda_k)]$ (31) and a metalinear bundle $\mathcal{D}$. The latter need not be trivial. If $\mathcal{D}$ is trivial, sections of the quantum bundle $Y \to T^m$ (34) obey the transformation rule

$$\rho_T(\phi^k + 2\pi) = \rho_T(\phi^k)$$

for all indices k. They are naturally complex smooth functions on T^m. In this case, E_T is the above-mentioned pre-Hilbert space $\mathcal{C}^\infty(T^m)$ of complex smooth functions on T^m whose basis consists of functions (6). The action operators $\hat{I}$ (5) with respect to this basis are represented by countable diagonal matrices (7), while functions $a(\phi)$ are decomposed into the pull-back functions $\psi_{(n_r)}$ which act on $\mathbb{C}^\infty(T^m)$ by multiplications

$$\psi_{(n_r)}\psi_{(n'_r)}=\psi_{(n_r)}\psi_{(n'_r)}=\psi_{(n_r+n'_r)}. \tag{36}$$

If $\mathcal{D}$ is a nontrivial metalinear bundle, sections of the quantum bundle $Y\to T^m$ (34) obey the transformation rule

$$\rho_T(\phi^j+2\pi)=-\rho_T(\phi^j) \tag{37}$$

for some indices j. In this case, the orthonormal basis of the pre-Hilbert space E_T can be represented by double-valued complex functions

$$\psi_{(n_i,n_j)}=\exp[i(n_i\phi^i+(n_j+\tfrac{1}{2})\phi^j)] \tag{38}$$

on T^m. They are eigenvectors

$$\hat{I}_i\psi_{(n_i,n_j)}=(n_i-\lambda_i)\psi_{(n_i,n_j)}, \quad \hat{I}_j\psi_{(n_i,n_j)}=(n_j-\lambda_j+\tfrac{1}{2})\psi_{(n_i,n_j)}$$

of the operators $\hat{I}_k$ (5), and the functions $a(\phi)$ act on the basis (38) by the above-given law (36). It follows that the representation of $\mathcal{A}$ determined by the connection $A[(\lambda_k)]$ (31) in the space of sections (37) of a nontrivial quantum bundle Y (34) is equivalent to its representation determined by the connection $A[(\lambda_i,\lambda_j-\frac{1}{2})]$ in the space $\mathbb{C}^\infty(T^m)$ of smooth complex functions on T^m.

Therefore, one can restrict the study of representations of the quantum algebra $\mathcal{A}$ to its representations in $\mathbb{C}^\infty(\mathbb{T}^m)$ associated to different connections (31). These representations are nonequivalent, unless $\lambda_k-\lambda'_k\in\mathbb{Z}$ for all indices k.

Now, in order to quantize the Poisson manifold $(W,\{,\}_W)$, one can simply replace functions on T^m with those on $\mathbb{R}\times T^m$.[7,24] Let us choose the angle polarization of W spanned by the vectors ∂^k. The corresponding quantum algebra $\mathcal{A}_W\subset C^\infty(W)$ consists of affine functions

$$f=a^k(t,\phi^j)I_k+b(t,\phi^j) \tag{39}$$

of action coordinates I_k, represented by the operators (35) in the space $\mathbb{C}^\infty(\mathbb{R}\times T^m)$ of smooth complex functions on $\mathbb{R}\times T^m$. This space is provided with the structure of the pre-Hilbert $\mathbb{C}^\infty(\mathbb{R})$-module with respect to the nondegenerate $\mathbb{C}^\infty(\mathbb{R})$-bilinear form

$$\langle\psi|\psi'\rangle=\left(\frac{1}{2\pi}\right)^m\int_{T^m}\psi\overline{\psi'}, \quad \psi,\psi'\in\mathbb{C}^\infty(\mathbb{R}\times T^m).$$

Its basis consists of the pull-backs onto $\mathbb{R}\times T^m$ of the functions $\psi_{(n_r)}$ (6).

Since the Poisson structure (27) defines no dynamics on the momentum phase space W (1), we should quantize the homogeneous momentum phase space W' (26) in order to describe evolution of a quantum time-dependent CIS. Following the general scheme in Refs. 25 and 26, one can provide the relevant geometric quantization of the symplectic annulus (W',Ω'). The corresponding quantum algebra $\mathcal{A}_{W'}\subset C^\infty(W')$ consists of affine functions

$$f=a^\lambda(t,\phi^j)I_\lambda+b(t,\phi^j)$$

of action coordinates I_λ. It suffices to consider its subalgebra consisting of the elements f and I_0+f for all $f\in\mathcal{A}_W$ (39). They are represented by the operators $\hat{f}$ (35) and $I_0=-i\partial_t$ in the pre-Hilbert module $\mathbb{C}^\infty(\mathbb{R}\times T^m)$. If a Hamiltonian $\mathcal{H}(I_j)$ of the time-dependent CIS is a polynomial (or analytic) function in action variables, the Hamiltonian $\mathcal{H}^*$ of the associated autonomous CIS is quantized as

$$\hat{\mathcal{H}}^*=-i\partial_t+\mathcal{H}(\hat{I}_j).$$

Then we obtain the Schrödinger equation

$$\hat{\mathcal{H}}^*\psi = -i\partial_t\psi + \mathcal{H}(-i\partial_k - \lambda_k)\psi = 0, \quad \psi \in \mathbf{C}^\infty(\mathbb{R}\times T^m).$$

Its solutions are the series

$$\psi = \sum_{(n_r)} B_{(n_r)} \exp[-iE_{(n_r)}t]\psi_{(n_r)}, \quad B_{(n_r)} \in \mathbb{C},$$

where $E_{(n_r)}$ are the eigenvalues (8) of the Hamiltonian $\hat{\mathcal{H}}$.

In conclusion, bearing in mind applications to holonomic quantum computation, let us choose action-angle coordinates such that a Hamiltonian $\mathcal{H}$ of a CIS is independent of action variables I_a $(a,b,c=1,\ldots,l)$. Then its eigenvalues are countably degenerate. Let us consider the perturbed Hamiltonian

$$\mathcal{H}' = \Delta(s^\mu, \phi^b, I_a) + \mathcal{H}(I_j),$$

where the perturbation term Δ depends on the action-angle coordinates with the above-mentioned indices $a,b,c,\ldots$ and on some time-dependent parameters $s^\mu(t)$ by the law

$$\Delta = \Lambda^a_\beta(s^\mu, \phi^b)\partial_t s^\beta I_a. \tag{40}$$

The Hamiltonian $\mathcal{H}'$ characterizes a CIS with time-dependent parameters.[20,26,27] Being affine in action variables, the perturbation term Δ (40) is represented by the operator

$$\hat{\Delta} = -\left(i\Lambda^a_\beta\partial_a + \frac{i}{2}\partial_a\Lambda^a_\beta + \lambda_a\Lambda^a_\beta\right)\partial_t s^\beta.$$

Since the operators $\hat{\Delta}$ and $\hat{\mathcal{H}}$ mutually commute, the total quantum evolution operator falls into the product

$$T\exp\left[-i\int_0^t \hat{\mathcal{H}}'\,dt'\right] = T\exp\left[-i\int_0^t \hat{\mathcal{H}}\,dt'\right]\circ T\exp\left[-i\int_0^t \hat{\Delta}\,dt'\right].$$

The first factor in this product is the dynamic evolution operator of the quantum CIS. The second one acts in the eigenspaces of the dynamic Hamiltonian $\hat{\mathcal{H}}$ and reads

$$T\exp\left[\int_0^t \{-\Lambda^a_\beta(\phi^b, s^\mu(t'))\partial_a - \tfrac{1}{2}\partial_a\Lambda^a_\beta(\phi^b, s^\mu(t')) + i\lambda_a\Lambda^a_\beta(\phi^b, s^\mu(t'))\}\partial_t s^\beta\,dt'\right]$$
$$= T\exp\left[\int_{s([0,t])} \{-\Lambda^a_\beta(\phi^b, \sigma^\mu)\partial_a - \tfrac{1}{2}\partial_a\Lambda^a_\beta(\phi^b, \sigma^\mu) + i\lambda_a\Lambda^a_\beta(\phi^b, \sigma^\mu)\}d\sigma^\beta\right]. \tag{41}$$

It is readily observed that this operator depends on the curve $s([0,1])\subset S$ in the parameter space S. One can treat it as an operator of parallel displacement along the curve s.[26–28] For instance, if $s([0,1])$ is a loop in S, the operator (41) is the geometric Berry factor, and it can be treated as a holonomy control operator.[26,29]

APPENDIX A

In order to complete the proof of Proposition 2, let us first apply relation (23) to the Hamiltonian vector fields ϑ_a and ϑ_i (22). We obtain

$$\Omega^a_b = \delta^a_b, \quad \vartheta^\lambda_a\Omega^i_\lambda = 0, \tag{A1}$$

$$\vartheta^k_i\Omega^j_k = \delta^j_i, \quad \vartheta^k_i\Omega^a_k = 0. \tag{A2}$$

The first of the equalities (A2) shows that the matrix Ω^j_k is nondegenerate, and so is ϑ^k_i. Then the second one results in $\Omega^a_k=0$.

Using the well-known Künneth formula for the de Rham cohomology of a product, one can easily justify that the closed form Ω_Z on W' (19) is exact. Moreover, $\Omega_Z=\mathrm{d}\Xi$ where Ξ takes the form

$$\Xi=\Xi^\alpha(J_\lambda,y^\lambda)\mathrm{d}J_\alpha+\Xi_i(J_\lambda)\mathrm{d}\varphi^i.$$

Of course, Ξ is determined up to an exact form. Using the fact that components of $\mathrm{d}\Xi=\Omega_Z$ are independent of y^λ and obey equalities (A1) and (A2), we obtain the following.

(i) $\Omega^a_i=-\partial_i\Xi^a+\partial^a\Xi_i=0$. It follows that $\partial_i\Xi^a$ is independent of φ, i.e., Ξ^a is affine in φ and, consequently, is independent of φ since φ is a cyclic coordinate. Hence, $\partial^a\Xi_i=0$, i.e., Ξ_i is a function only of coordinates J_j.

(ii) $\Omega^k_i=-\partial_i\Xi^k+\partial^k\Xi_i$. Similarly, one shows that Ξ^k is independent of φ and $\Omega^k_i=\partial^k\Xi_i$, i.e., $\partial^k\Xi_i$ is a nondegenerate matrix.

(iii) $\Omega^a_b=-\partial_b\Xi^a=\delta^a_b$. Hence, $\Xi^a=D^a(J_\lambda)+s^a$.

(iv) $\Omega^i_b=-\partial_b\Xi^i$, i.e., Ξ^i is affine in s^a.

In view of items (i)–(iv), the Liouville form Ξ reads

$$\Xi=x^a\,\mathrm{d}J_a+[D^i(J_\lambda)+B^i_a(J_\lambda)s^a]\mathrm{d}J_i+\Xi_i(J_j)\mathrm{d}\varphi^i,$$

where $x^a=s^a+D^a(J_\lambda)$. Since the matrix $\partial^k\Xi_i$ is nondegenerate, one can introduce new coordinates $I_i=\Xi_i(J_j)$, $I_a=J_a$. We obtain

$$\Xi=x^a\,\mathrm{d}I_a+[D'^i(I_\lambda)+B'^i_a(I_\lambda)s^a]\mathrm{d}I_i+I_i\mathrm{d}\varphi^i.$$

Finally, put

$$\phi^i=\varphi^i-[D'^i(I_\lambda)+B'^i_a(I_\lambda)s^a]$$

in order to obtain the desired coordinates (24).

APPENDIX B

In order to prove Proposition 3, we first show that functions $i_0^*F_k$ make up a CIS on the symplectic leaf (V_0^*Q,Ω_0) and N_0 is its invariant manifold without critical points. Clearly, the functions $i_0^*F_k$ are in involution, and N_0 is their connected invariant manifold. Let us show that the set of critical points of $\{i_0^*F_k\}$ is nowhere dense in V_0^*Q and N_0 has none of these points. Let V_0^*Q be equipped with some coordinates $(\overline{q}^k,\overline{p}_k)$. Then the trivial bundle ξ (18) is provided with the bundle coordinates $(t,\overline{q}^k,\overline{p}_k)$ which play a role of the initial date coordinates on the momentum phase space V^*Q. Written with respect to these coordinates, the first integrals F_k become time-independent. It follows that

$$\mathrm{d}F_k(y)=\mathrm{d}i_0^*F_k(\xi(y)) \tag{B1}$$

for any point $y\in V^*Q$. In particular, if $y_0\in V_0^*Q$ is a critical point of $\{i_0^*F_k\}$, then the trajectory $\xi^{-1}(y_0)$ is a critical set for the first integrals $\{F_k\}$. The desired statement at once follows from this result.

Since N_0 is compact and regular, there is an open neighborhood of N_0 in V_0^*Q isomorphic to $N_0\times V$ where $V\subset\mathbb{R}^m$ is a domain, and $N_0\times\{v\}$, $v\in V$, are also invariant manifolds in V_0^*Q.[6] Then

$$W''=\xi^{-1}(N_0\times V)\cong N\times V \tag{B2}$$

is an open neighborhood in V^*Q of the invariant manifold N foliated by invariant manifolds $\xi^{-1}(N_0\times\{v\})$, $v\in V$, of the time-dependent CIS on V^*Q. By virtue of the equality (B1), the first integrals $\{F_k\}$ have no critical points in W''. For any real number $r\in(-\varepsilon,\varepsilon)$, let us consider a section

$$h_r: V^*Q\to T^*Q, \quad p_0\circ h_r=-\mathcal{H}(t,q^j,p_j)+r,$$

of the affine bundle ζ (10). Then the images $h_r(W'')$ of W'' (B2) make up an open neighborhood U of $h(N)$ in T^*Q. Because $\zeta(U)=W''$, the pull-backs ζ^*F_k of first integrals F_k are free from critical points in U, and so is the function $\mathcal{H}^*$ (16). Since the coordinate $r=p_0-h$ provides a trivialization of the affine bundle ζ, the open neighborhood U of $h(N)$ is diffeomorphic to the product

$$h(W'')\times(-\varepsilon,\varepsilon)\cong h(N)\times V\times(-\varepsilon,\varepsilon),$$

which is a trivialization of the fibration

$$\mathcal{H}^*\times(\times\zeta^*F_k): U\to V\times(-\varepsilon,\varepsilon).$$

It remains to prove that the Hamiltonian vector fields of $\mathcal{H}^*$ and ζ^*F_k on U are complete. It is readily observed that the Hamiltonian vector field γ_T (17) of $\mathcal{H}^*$ is tangent to the manifolds $h_r(W'')$, and is the image $\gamma_T=Th_r\circ\gamma_H\circ\zeta$ of the vector field γ_H (14). The latter is complete on W'', and so is γ_T on U. Similarly, the Hamiltonian vector field

$$\gamma_k=-\partial_t F_k\partial^0+\partial^i F_k\partial_i-\partial_i F_k\partial^i$$

of the function ζ^*F_k on T^*Q with respect to the Poisson bracket $\{,\}_T$ (9) is tangent to the manifolds $h_r(W'')$, and is the image $\gamma_k=Th_r\circ\vartheta_k\circ\zeta$ of the Hamiltonian vector field ϑ_k of the first integral F_k on W'' with respect to the Poisson bracket $\{,\}_V$ (12). The vector fields ϑ_k on W'' are vertical relative to the fibration $W''\to\mathbb{R}$, and are tangent to compact manifolds. Therefore, they are complete, and so are the vector fields γ_k on U. Thus, U is the desired open neighborhood of the invariant manifold $h(N)$.

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A family of solutions with radiation reaction and retarded interactions for two charges in classical electrodynamics

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A family of solutions of the Lorentz–Dirac equation is constructed. It consists in the motion of two charges e_1 and e_2 of masses m_1 and m_2 in two coplanar and concentric circles of radii a and b. The charges rotate with constant angular velocity, and have an angular separation ψ. The radiation reaction forces and the retarded interactions between the charges are taken into account. The external electromagnetic field that allows the motion consists of a tangential time-independent electric field that takes a fixed value on each orbit, and a homogeneous time-independent magnetic field perpendicular to the plane of the motion. For all the solutions energy conservation is rigorously demonstrated by evaluating the energy radiated, with independence of the equation of motion, through the calculation of the instantaneous energy flux across a sphere of an infinitely large radius. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1500792]

I. INTRODUCTION

Classical electrodynamics is one of the most fundamental and successful frameworks of physics. However, one of its most fundamental aspects, namely, the equation of motion of a point charge that takes into account the effect of radiation reaction, still remains in an unsatisfactory state. The equation of motion, derived by Dirac[1] in 1938 and known as the Lorentz–Dirac equation, has been objected because it presents some inconsistencies such as runaway solutions and violation of causality.

Although electromagnetic phenomena are properly described by quantum theory, classical electrodynamics is of interest not only because of its wide range of applicability and the large variety of physical phenomena it successfully describes, but also because both theories have common basic problems, not completely understood yet, as for instance the electron mass renormalization. The mass renormalization procedure was introduced by Dirac[1] in his derivation of the equation of motion in order to deal with the infinite self-energy associated to the electromagnetic field of a point electron. In spite of the fact that the derivation of the Lorentz–Dirac equation is based on the conservation equation of the energy-momentum tensor, the manipulation of the infinite self-energy of the electron makes obscure the conservation of the energy in the equation of motion. The existence of runaway solutions, where the electron accelerates even in the absence of an external field, is a clear illustration of this aspect.

The energy radiated away by a system of charges plays a fundamental role in the study of the consistency of the equation of motion with the energy conservation law. This problem is completely solved, in the case of only one charge, by Rohrlich's radiation criterion,[2] since with its help it is easy to identify the term in the Lorentz–Dirac equation that describes the radiation that escapes to infinity. Unfortunately, in the case of more than one charge it is in general impossible, mainly due to the complications introduced by the retarded effects, to identify the rate of radiation that escapes to infinity starting from the equations of motion of the charges. In this context let us

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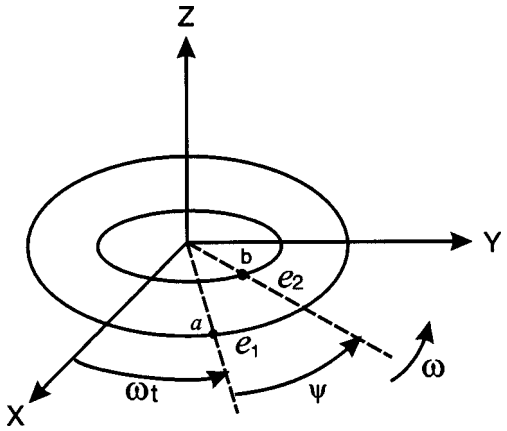

FIG. 1. The positions at time t of charges e_1 and e_2 moving with constant angular velocity ω in concentric circles of radius a and b, respectively.

recall that in Dirac's derivation of the equations of motion the retarded field includes both the near and the far fields, whereas the energy radiated that escapes to infinity is determined exclusively by the far fields. Therefore the connection between these two ways of describing the radiation is by no means immediate, a point that was first emphasized by Comay.[3]

The construction of exact solutions of the equation of motion for more than one charge is of interest both from a mathematical and from a physical point of view. In fact, the equations of motion for several charges have a rich mathematical structure, since they constitute a set of nonlinear third order differential equations that are coupled by means of the retarded interactions between the different charges. On the other hand, the construction of exact solutions constitutes a powerful tool in order to clarify the description of the radiation by the equations of motion and the consistence of them with the conservation of the energy.

Recently, the first exact solution of the Lorentz–Dirac equation for more than one charge[4] was constructed. It corresponds to the motion of two identical charges that rotate at constant angular velocity at opposite ends of a diameter. The external fields that make possible this motion consist of a static homogeneous magnetic field perpendicular to the plane of the motion and a time-independent electric field of fixed magnitude over the orbit and tangent to it. In this case it was demonstrated that the Lorentz–Dirac equation satisfies energy conservation, since the energy supplied by the external electric field to the two charges turns out to be exactly equal to the energy that escapes to infinity. In this article a family of solutions of the Lorentz–Dirac equations with the same external fields is constructed in the case of two electrical charges e_1 and e_2 of masses m_1 and m_2 that move in a plane in two concentric circumferences of radii a and b with constant angular velocity, and where the angular separation of charge e_2 with respect to charge e_1 is ψ, as shown in Fig. 1. The Lorentz–Dirac equation imposes, of course, restrictions in the values of the different parameters that make possible the motion, that is, the charges, masses, radii, angular velocity and angular separation ψ; but in general continuous ranges are admissible for the variation of those parameters. The exact solution of Ref. 4 constitutes a very special case within the family of solutions that we present in this article.

The simple mathematical structure of the external fields plays a determinant role in the construction of the analytical solution of the Lorentz–Dirac equation given below. However, in order to obtain an external field that is an exact analytical solution of Maxwell's equations and that also has a simple mathematical structure it is necessary to use idealized sources. The case of a flat, unbounded sheet in which a current flows with constant density and direction everywhere, and which gives rise to an homogeneous magnetic field, is a well-known example.[5] Our source for the electric field is also an idealized one, and consists of an infinitely long solenoid fed with a density of current that increases linearly with time. Of course, from a practical point of view, an idealized source like this can be implemented only in an approximate way; but this work is focused on the

study of the solutions of the Lorentz–Dirac equation from a fundamental point of view, and practical or experimental aspects are out of the scope of this article.

The radiation that escapes to infinity is studied independently of the equation of motion, by calculating explicitly the energy flux across the surface of a sphere of infinite radius that encloses the charges' orbit. The result splits into the Larmor formulas for the radiation rate of each charge and an interference rate of radiation that mixes the fields of the particles. The calculation is somewhat elaborate due to the complications that the retardation condition introduces. Fortunately, the equation that defines the retarded times is formally equal to the one that appears in Kepler's problem, and therefore the formalism developed by Bessel and Watson for Kepler's problem can be applied here. This technique conducts to a Fourier series in angle ψ for the interference rate of radiation, series that turns out to be identical to the one that is obtained from the solution of the Lorentz–Dirac equation, where the fields appear evaluated not at infinity, but at the retarded positions of the charges.

The family of solutions found here expands considerably the set of solutions of the Lorentz–Dirac equation and corroborates its consistency with the basic principle of energy conservation.

II. THE SOLUTIONS

Figure 1 shows the motion under consideration, which consists in charges e_1 and e_2 moving in the x-y plane with constant angular velocity ω in concentric circular orbits of radii a and b, respectively. The angular separation of charge e_2 with respect to e_1, measured in the direction of the motion, is denoted by ψ. The charges move in the electric field generated by an infinitely long solenoid whose axis is the z-axis and whose radius is $\rho_0<b$. The current density that flows around the solenoid is given, for any time t, by

$$\mathbf{J}=-\alpha t\,\delta(\rho-\rho_0)\,\hat{\boldsymbol{\varphi}}, \tag{1}$$

where α is a positive number, δ is the usual Dirac delta function, ρ is the radial cylindrical coordinate and $\hat{\boldsymbol{\varphi}}$ is the unit vector associated with the cylindrical coordinate φ. The current density (1), together with a charge density that vanishes everywhere, gives rise to the following electric and magnetic fields, expressed in terms of their Cartesian coordinates:

$$\begin{aligned} E_x&=-(2\pi\alpha\rho_0^2/c^2)\,\frac{y}{x^2+y^2},\\ E_y&=+(2\pi\alpha\rho_0^2/c^2)\,\frac{x}{x^2+y^2},\\ E_z&=0,\\ B_x&=B_y=B_z=0 \end{aligned} \tag{2}$$

outside the solenoid, and

$$\begin{aligned} E_x&=-(2\pi\alpha/c^2)y,\\ E_y&=+(2\pi\alpha/c^2)x,\\ E_z&=0,\\ B_x&=B_y=0,\quad B_z=-4\pi\alpha t/c \end{aligned} \tag{3}$$

inside it. The fields (2) and (3) satisfy the source-free Maxwell equations, and since they also satisfy the corresponding boundary conditions at the solenoid's surface, they are indeed an exact solution of Maxwell's equations. We will need these fields only in the region $\rho>\rho_0$, where their values in cylindrical coordinates are given by

$$\mathbf{E}=\frac{2\pi\alpha\rho_0^2}{c^2}\,\frac{1}{\rho}\,\hat{\boldsymbol{\varphi}}, \tag{4}$$

$$\mathbf{B}=0. \tag{5}$$

The magnitude of the electric field (4) can be adjusted by choosing an appropriate value of the parameter α. In order for the motion of Fig. 1 to be a solution of the Lorentz–Dirac equation, an external homogeneous time-independent magnetic field $\mathbf{B}^{\text{ext}}$ will be also necessary.

The Lorentz–Dirac equation for particle 1 is

$$m_1 a_1^\mu=(e_1/c)F_{\text{ext}}^{\mu\alpha}v_{1\alpha}+(e_1/c)(F_{2\text{ret}}^{\mu\alpha})v_{1\alpha}+(2e_1^2/3c^3)(\dot{a}_1^\mu-(1/c^2)a_1^\lambda a_\lambda^1 v_1^\mu), \tag{6}$$

where v_1^μ and a_1^μ denote the four-velocity and four-acceleration of charge e_1, respectively, c is the velocity of light and $\dot{a}_1^\mu$ is the proper time derivative of a_1^μ. Greek indices range from 0 to 3 and the diagonal metric of Minkowski space is $(-1,+1,+1,+1)$. The equation for particle 2 can be obtained from Eq. (6) by interchanging the indices 1 and 2.

The tensor $F_{\text{ext}}^{\mu\alpha}$ in the first term of Eq. (6) contains the external fields in which particle 1 moves, and gives rise to the associated Lorentz-force term. In a similar way, the tensor $F_{2\text{ret}}^{\mu\alpha}$ contains the retarded fields exerted by particle 2 at the position of particle 1, and gives rise to the retarded Lorentz force. Finally, the last term in Eq. (6) arises from the self-field of the charge and is known as the Abraham four-vector. For the circular motion under consideration, it gives rise to a radiation reaction force that is tangential to the particle's orbit.

As it is usually done, we will study the solutions of Eq. (6) in a specific Lorentz frame, namely the ''laboratory frame,'' where the infinitely long solenoid is at rest. Because of the relativistic invariance of both the Maxwell equations and the Lorentz–Dirac equation, the solutions of Eq. (6) in any Lorentz frame can be obtained by simply carrying out the corresponding Lorentz transformation.

We will study solutions of the equations of motion for the external fields

$$\begin{aligned}\mathbf{E}^{\text{ext}}&=E_t^{\text{ext}}\hat{\boldsymbol{\varphi}}=\frac{D}{\rho}\hat{\boldsymbol{\varphi}},\\ \mathbf{B}^{\text{ext}}&=-B_{\text{ext}}\hat{\mathbf{z}}.\end{aligned} \tag{7}$$

The orientation of the coordinate axes will be chosen such that particle 1 is on the x-axis at $t=0$. Thus, the trajectory of particle 1 is given by $x_1=a\cos(\omega t)$, $y_1=a\sin(\omega t)$, $z_1=0$, and similar equations hold for the trajectory of particle 2. From these equations it follows that the components with $\mu=3$ of the equations of motion of both particles are identically satisfied by the external fields (7). On the other hand, the equations with $\mu=1$ and $\mu=2$ can be combined into one tangential and one radial equation for each particle. These equations can be simultaneously satisfied only for certain range of values of the parameters of the system. It is convenient to introduce the following ones:

$$\begin{aligned}\chi&=b/a<1,\\ \beta_1&=\omega a/c<1,\\ \beta_2&=\omega b/c=\chi\beta_1,\\ \lambda&=e_2/e_1,\\ \sigma&=m_2/m_1,\end{aligned} \tag{8}$$

which make it possible to obtain the orbit's radius, speed, charge and mass of particle 2 if the corresponding values of particle 1 are known.

The retarded fields that appear in the equations of motion can be computed by using the Liénard–Wiechert formula[6]

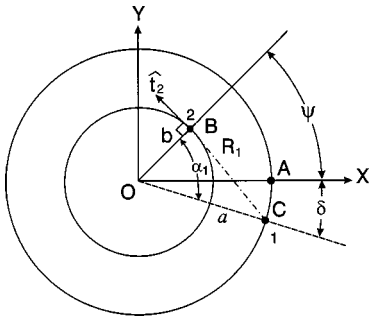

FIG. 2. The locations at time $t=0$ of charges e_1 (position A) and e_2 (position B) and the retarded position of charge e_1 (position C) associated to the actual position of charge e_2. We also show the retarded angle α_1, the retarded distance R_1, the tangential unit vector $\hat{\mathbf{t}}_2$ at the actual position of charge e_2 and the angle δ that particle 1 travels from its retarded time to the actual time.

$$\mathbf{E}(\mathbf{x},t)=e\left[\frac{(\hat{\mathbf{n}}-\boldsymbol{\beta})(1-\beta^2)}{\kappa^3R^2}\right]+\frac{e}{c}\left[\frac{\hat{\mathbf{n}}\times\{(\hat{\mathbf{n}}-\boldsymbol{\beta})\times\dot{\boldsymbol{\beta}}\}}{\kappa^3R}\right],$$
$$\mathbf{B}(\mathbf{x},t)=\hat{\mathbf{n}}\times\mathbf{E}(\mathbf{x},t), \tag{9}$$

where $\hat{\mathbf{n}}$ is the unit vector that points from the retarded position $\mathbf{r}(t')$ of the charge that produces the field to the point $\mathbf{x}$ where the field is being considered at time t; R is the distance from the retarded position of the charge to point $\mathbf{x}$, that is, $R=|\mathbf{x}-\mathbf{r}(t')|$; $\boldsymbol{\beta}$ and $\dot{\boldsymbol{\beta}}$ are defined by $(1/c)\times(d\mathbf{r}(t')/dt')$ and $d\boldsymbol{\beta}/dt'$, respectively, and are both evaluated at the retarded time t', which is implicitly defined by $t-t'=|\mathbf{x}-\mathbf{r}(t')|/c$; and κ is the positive number

$$\kappa=1-\boldsymbol{\beta}\cdot\hat{\mathbf{n}}. \tag{10}$$

In these formulas the observation point $\mathbf{x}$ will be the position at time t of one of the charges. Then, the retarded electromagnetic fields produced by particle k ($k=1,2$) result to be a function of the retarded angle α_k, which is defined as the angle between the retarded position of the particle that generates the field and the actual position of the particle that experiences the retarded force. The retarded angle is measured starting from the retarded position of particle k in the sense of motion in the case $k=1$, and opposite to the sense of motion in the case $k=2$. In Fig. 2 we show the actual position of particle 2 and the retarded position of particle 1. We also show the retarded distance R_1 between those positions, the tangential unit vector $\hat{\mathbf{t}}_2$ at the actual position of particle 2 and the angle δ that particle 1 travels from its retarded time to the laboratory time.

These quantities are related by

$$\alpha_1=\psi+\delta,$$
$$R_1=a\{1+\chi^2-2\chi\cos\alpha_1\}^{1/2}, \tag{11}$$

and therefore the retardation condition $R_1/c=\delta/\omega$ is

$$\alpha_1-\beta_1\{1+\chi^2-2\chi\cos\alpha_1\}^{1/2}=\psi. \tag{12}$$

By using Eq. (9) the following result for the tangential component of the retarded electric field exerted by particle 1 on particle 2 is obtained:

$$E_{12t}=\mathbf{E}_{12}\cdot\hat{\mathbf{t}}_2=\frac{e_1}{\kappa_1^3R_1^2}\left\{(1-\beta_1^2)\left(\frac{\sin\alpha_1}{\{1+\chi^2-2\chi\cos\alpha_1\}^{1/2}}-\beta_1\cos\alpha_1\right)+\beta_1^2(\cos\alpha_1-\chi)\right.$$
$$\left.\times\left(\frac{\chi\sin\alpha_1}{\{1+\chi^2-2\chi\cos\alpha_1\}^{1/2}}-\beta_1\right)\right\}, \tag{13}$$

where, according to Eq. (10), κ_1 is given by

$$\kappa_1=1-\frac{\beta_1\chi\sin\alpha_1}{\{1+\chi^2-2\chi\cos\alpha_1\}^{1/2}}. \tag{14}$$

In the same way, in the case of the field exerted by particle 2 on particle 1, we have

$$R_2=a\{1+\chi^2-2\chi\cos\alpha_2\}^{1/2}, \tag{15}$$

and angle α_2 satisfies now the retardation condition

$$\alpha_2+\beta_1\{1+\chi^2-2\chi\cos\alpha_2\}^{1/2}=\psi. \tag{16}$$

The factor κ_2 is given by

$$\kappa_2=1+\frac{\beta_2\sin\alpha_2}{\{1+\chi^2-2\chi\cos\alpha_2\}^{1/2}}, \tag{17}$$

and the tangential component of the retarded electric field exerted by particle 2 on particle 1 is

$$E_{21t}=\frac{e_2}{\kappa_2^3R_2^2}\left\{-(1-\beta_2^2)\left(\frac{\chi\sin\alpha_2}{\{1+\chi^2-2\chi\cos\alpha_2\}^{1/2}}+\beta_2\cos\alpha_2\right)+\frac{\beta_2^2}{\chi}(1-\chi\cos\alpha_2)\right.$$
$$\left.\times\left(\frac{\sin\alpha_2}{\{1+\chi^2-2\chi\cos\alpha_2\}^{1/2}}+\beta_2\right)\right\}. \tag{18}$$

The tangential equations of motion for particles 1 and 2 obtained from the Lorentz–Dirac equation are given by

$$\begin{aligned} e_1E_t^{\mathrm{ext}}(\rho=a)+e_1E_{21t}&=\frac{2e_1^2\beta_1^3\gamma_1^4}{3a^2},\\ e_2E_t^{\mathrm{ext}}(\rho=b)+e_2E_{12t}&=\frac{2e_2^2\beta_2^3\gamma_2^4}{3b^2}, \end{aligned} \tag{19}$$

where γ is the usual relativistic parameter $\gamma=(1-\beta^2)^{-1/2}$. These equations can be simultaneously solved for the constant D in the external electric field of Eq. (7) and for the parameter $\lambda=e_2/e_1$. The following results are obtained:

$$\lambda=\frac{2\beta_1^3\gamma_1^4/3+\chi(a^2/e_1)E_{12t}}{2\chi^2\beta_1^3\gamma_2^4/3+(a^2/e_2)E_{21t}}, \tag{20}$$

$$D=\rho E_t^{\mathrm{ext}}=\left(\frac{e_1}{a}\right)\left\{\frac{4\chi^2\beta_1^6\gamma_1^4\gamma_2^4/9-\chi(a^2/e_1)(a^2/e_2)E_{12t}E_{21t}}{2\chi^2\beta_1^3\gamma_2^4/3+(a^2/e_2)E_{21t}}\right\}. \tag{21}$$

Thus, for a given value of the charge e_1, Eq. (20) determines the value of the charge e_2 for which it is possible to simultaneously balance the radiation reaction and retarded interactions acting on each charge, while Eq. (21) fixes the magnitude of the external electric field that makes

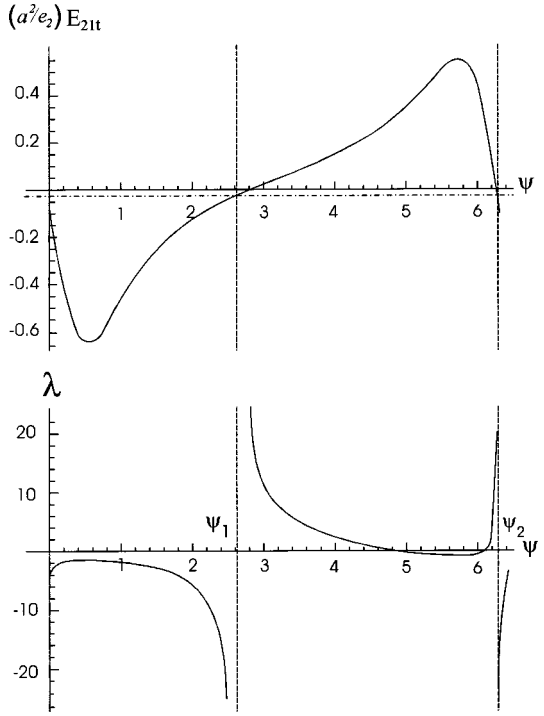

FIG. 3. The dimensionless quantity $(a^2/e_2)E_{21t}$ and the ratio of charges $\lambda = e_2/e_1$ as a function of the angle ψ in the case $\beta_1 = 0.6$ and $\chi = 0.4$. The dot-dashed line in the first graph corresponds to the value $-2\chi^2\beta_1^3\gamma_2^4/3$ for which the denominator of Eq. (20) vanishes.

this possible. From Eqs. (11), (13), (15) and (18) it follows that $(a^2/e_1)E_{12t}$ and $(a^2/e_2)E_{21t}$ are independent of the orbit's radius a for given values of β_1 and χ, and therefore λ is also independent of a. On the other hand, the constant D does depend on a, and therefore a given value of a fixes the value of the parameter α in Eq. (4).

Equations (20) and (21) depend implicitly on the angular separation ψ, since from the retardation conditions (12) and (16) we obtain $\partial\alpha_1/\partial\psi = 1/\kappa_1 > 0$ and $\partial\alpha_2/\partial\psi = 1/\kappa_2 > 0$, and therefore for fixed values of β_1 and χ the retarded angles α_1 and α_2 are uniquely determined as functions of ψ. In Fig. 3 we illustrate the dependence on ψ of the dimensionless combination $(a^2/e_2)E_{21t}$ and of λ, in the case $\beta_1 = 0.6$ and $\chi = 0.4$.

The dimensionless quantity $(a^2/e_2)E_{21t}$, associated to the retarded field exerted by particle 2 on particle 1, depends qualitatively on ψ as one expects. Note in particular that $(a^2/e_2)E_{21t}$ takes positive and negative values in two ranges of values of ψ which correspond roughly to $\pi < \psi < 2\pi$ and $0 < \psi < \pi$, with one maximum absolute value in each zone.

The behavior of $(a^2/e_1)E_{12t}$ is similar to the one sketched above, and since $2\beta_1^3\gamma_1^4/3$ is usually smaller than the maximum absolute value of $\chi(a^2/e_1)E_{12t}$, due to the factor β_1^3, there exist two values of ψ for which the numerator in Eq. (20) vanishes. In this case we have $e_2 = 0$ and the only solution of the Lorentz–Dirac equation corresponds to the one-particle solution in which particle 1 moves in a circular orbit of radius a with velocity β_1. Similarly, there exist two values of ψ, which we will denote by ψ_1 and ψ_2, located near $\psi = \pi$ and $\psi = 2\pi$, for which the denominator of Eq. (20) vanishes. Since the equations of motion only determine the ratio of charges λ, this is the same situation as above and it means that for a given value of e_2 the only solution of the Lorentz–Dirac equations when $\psi = \psi_1$ or $\psi = \psi_2$ is the one-particle solution in which particle 2 moves in a circular orbit of radius $b = \chi a$ and velocity $\beta_2 = \chi\beta_1$. Finally, from Eq. (20) it follows that for any given value of χ there exists a threshold value β_0 such that λ does not vanish if $\beta_1 > \beta_0$.

Of course, the details of the general behavior that we have sketched above depend on the

specific values of β_1 and χ chosen. Thus, the value ψ_1, which is a little less than π for $\beta_1 \to 0$, shifts to lower values with increasing β_1 for a fixed χ. For instance, for the case $\chi = 0.4$, ψ_1 is approximately 1.4 for $\beta_1 \to 1$. On the other hand, ψ_2 is a little less than 2π for $\beta_1 \to 0$ and shifts only very slightly to lower values when $\beta_1 \to 1$ for any fixed value of χ.

The above discussion shows that for any given values of β_1 and χ it is always possible (with exception of at most four values of ψ for which one of the charges vanishes) to adjust the external electric field in Eq. (7) and the charge of particle 2 so that the tangential equations of motion of both particles are satisfied. We will see below that the radial equations of motion obtained from the Lorentz–Dirac equation determine the mass of particle 2 in a more restrictive way. They are given by

$$\begin{aligned} -m_1\beta_1^2 c^2 \gamma_1 / a &= e_1 E_{21r} + e_1 \beta_1 B_{21z} - e_1 \beta_1 B_{\text{ext}}, \\ -m_2\beta_2^2 c^2 \gamma_2 / b &= e_2 E_{12r} + e_2 \beta_2 B_{12z} - e_2 \beta_2 B_{\text{ext}}, \end{aligned} \tag{22}$$

where E_{ijr} denotes the radial component of the retarded electric field exerted by particle i on particle j, and B_{ijz} denotes the z component of the retarded magnetic field exerted by particle i on particle j. By using Eq. (9) the following expressions follow:

$$\begin{aligned} E_{12r} = \frac{e_1}{\kappa_1^3 R_1^2} \Bigg\{ (1-\beta_1^2) \Bigg(\frac{\chi - \cos\alpha_1}{\{1+\chi^2 - 2\chi\cos\alpha_1\}^{1/2}} - \beta_1 \sin\alpha_1 \Bigg) \\ + \beta_1^2 \sin\alpha_1 \Bigg(\frac{\chi \sin\alpha_1}{\{1+\chi^2 - 2\chi\cos\alpha_1\}^{1/2}} - \beta_1 \Bigg) \Bigg\}, \end{aligned} \tag{23}$$

$$\begin{aligned} E_{21r} = \frac{e_2}{\kappa_2^3 R_2^2} \Bigg\{ (1-\beta_2^2) \Bigg(\frac{1 - \chi\cos\alpha_2}{\{1+\chi^2 - 2\chi\cos\alpha_2\}^{1/2}} + \beta_2 \sin\alpha_2 \Bigg) \\ + \beta_2^2 \sin\alpha_2 \Bigg(\frac{\sin\alpha_2}{\{1+\chi^2 - 2\chi\cos\alpha_2\}^{1/2}} + \beta_2 \Bigg) \Bigg\}, \end{aligned} \tag{24}$$

$$B_{12z} = \frac{\chi - \cos\alpha_1}{\{1+\chi^2 - 2\chi\cos\alpha_1\}^{1/2}} E_{12t} - \frac{\sin\alpha_1}{\{1+\chi^2 - 2\chi\cos\alpha_1\}^{1/2}} E_{12r}, \tag{25}$$

$$B_{21z} = \frac{1 - \chi\cos\alpha_2}{\{1+\chi^2 - 2\chi\cos\alpha_2\}^{1/2}} E_{21t} + \frac{\chi \sin\alpha_2}{\{1+\chi^2 - 2\chi\cos\alpha_2\}^{1/2}} E_{21r}. \tag{26}$$

Equations (22) can be simultaneously solved for the ratio of masses $\sigma = m_2/m_1$ and for the external magnetic field B_{ext} in Eq. (7). We obtain

$$\sigma = \frac{\lambda}{\gamma_2} \Bigg\{ \gamma_1 + \frac{(r_1/a)F}{\beta_1} \Bigg\} := \frac{\lambda}{\gamma_2} \sigma_r, \tag{27}$$

$$B_{\text{ext}} = \Bigg(\frac{e_1 \beta_1 \gamma_1}{r_1 a} \Bigg) + \frac{1 - \chi\cos\alpha_2}{\{1+\chi^2 - 2\chi\cos\alpha_2\}^{1/2}} E_{21t} + \Bigg(\frac{1}{\beta_1} + \frac{\chi \sin\alpha_2}{\{1+\chi^2 - 2\chi\cos\alpha_2\}^{1/2}} \Bigg) E_{21r}, \tag{28}$$

where r_1 is the classical radius of particle 1, $r_1 = e_1^2/(m_1 c^2)$, and F is the combination of retarded fields:

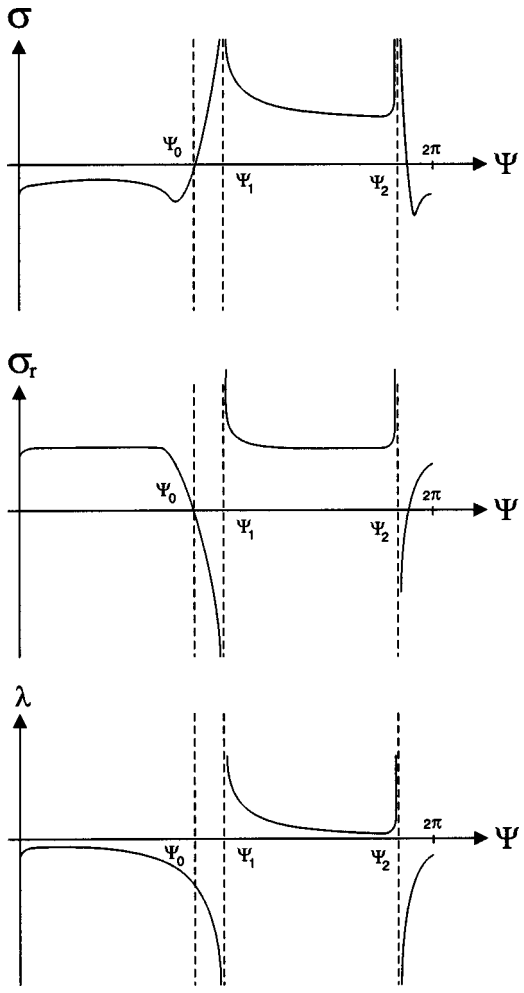

FIG. 4. Schematic behavior of the ratio of masses $\sigma=m_2/m_1$ as a function of angular separation ψ. We also show the behavior of σ_r defined in Eq. (27) and of the ratio of charges λ.

$$F=\lambda\left\{\frac{(1-\chi\cos\alpha_2)(a^2/e_2)E_{21t}}{\{1+\chi^2-2\chi\cos\alpha_2\}^{1/2}}+\left(\frac{1}{\beta_1}+\frac{\chi\sin\alpha_2}{\{1+\chi^2-2\chi\cos\alpha_2\}^{1/2}}\right)(a^2/e_2)E_{21r}\right\}$$
$$-\frac{(\chi-\cos\alpha_1)(a^2/e_1)E_{12t}}{\{1+\chi^2-2\chi\cos\alpha_1\}^{1/2}}-\left(\frac{1}{\beta_2}-\frac{\sin\alpha_1}{\{1+\chi^2-2\chi\cos\alpha_1\}^{1/2}}\right)(a^2/e_1)E_{12r}. \tag{29}$$

The first terms on the right hand sides of Eqs. (27) and (28) correspond to the results that would have been obtained if there were no retarded interactions between the charges. The term that depends on the retarded fields in Eq. (27) is proportional to the dimensionless number r_1/a, which is usually a very small number. However, it will be shown below that this term has qualitative implications.

The physical solutions of the Lorentz–Dirac equations are those with $\sigma>0$. The behavior of σ as a function of ψ arises from the behavior of both λ and the quantity in curly brackets in Eq. (27), which we have called σ_r. The typical behavior of these quantities is sketched in Fig. 4, where for simplicity we have chosen the case in which λ does not become zero for any value of ψ.

The behavior of σ_r in Fig. 4 follows from Eq. (27), since the smallness of r_1/a implies that σ_r does not differ appreciably from γ_1 for most values of ψ. However, Eq. (29) shows that the first

two terms of F are proportional to λ, and therefore σ_r is singular at points $\psi=\psi_1$ and $\psi=\psi_2$. A detailed analysis shows that the expression inside the curly brackets in Eq. (29) is positive for any β and χ, and therefore $\sigma_r\to\pm\infty$ when $\lambda\to\pm\infty$. Therefore, since σ_r has the same sign that λ near $\psi=\psi_1$ and $\psi=\psi_2$, σ in Eq. (27) is positive at both sides of those points. Besides, σ_r must take the value zero for some $\psi=\psi_0<\psi_1$ as it goes down towards $-\infty$, thus making $\sigma=0$ at that point. Therefore the physical solutions around $\psi=\psi_1$ consist of a narrow interval $\psi_0<\psi<\psi_1$ for which $\lambda<0$, followed by a range of solutions with $\lambda>0$ which extends up to $\psi=\psi_2$ in Fig. 4. The pattern of solutions around $\psi=\psi_2$ is similar.

The features sketched in Fig. 4 are valid in general, except of course when β_1 is very small, of the order of r_1/a, case in which the behavior of F as a function of ψ is relevant. A similar analysis can be performed in this case and it shows that again ranges of solutions exist around $\psi=\psi_1$ and $\psi=\psi_2$ with both $\lambda>0$ and $\lambda<0$, but this time the solutions that exist in a small angular interval are the ones with $\lambda>0$.

III. STUDY OF ENERGY CONSERVATION

For all the solutions that we have built it is possible to obtain an energy balance equation starting directly from the tangential equations of motion. By multiplying the first equation in (19) by $v_1=\beta_1 c$ and the second one by $v_2=\beta_2 c$ and adding the results, it follows that

$$e_1\mathbf{E}^{\mathbf{ext}}\cdot\mathbf{v_1}+e_2\mathbf{E}^{\mathbf{ext}}\cdot\mathbf{v_2}=\frac{2e_1^2c}{3a^2}\beta_1^4\gamma_1^4+\frac{2e_2^2c}{3b^2}\beta_2^4\gamma_2^4-e_1\mathbf{E_{21}}\cdot\mathbf{v_1}-e_2\mathbf{E_{12}}\cdot\mathbf{v_2}. \tag{30}$$

The left hand side of Eq. (30) corresponds to the energy provided by the external field to the charges. Since the kinetic energy of the charges and the total energy stored in the fields are time-independent, consistency with energy conservation demands the right hand side of Eq. (30) to be equal to the energy that escapes to infinity. Thus, in order to have a conclusive proof of energy conservation, it is necessary to calculate with independence of the equations of motion the energy that escapes to infinity, using only the far fields of the charges. To this end the total power of radiation at time t will be evaluated by computing the surface integral

$$\frac{c}{4\pi}\int_{\Sigma_r}(\mathbf{E}\times\mathbf{B})\cdot d\boldsymbol{\Sigma}, \tag{31}$$

where Σ_r is the surface of a sphere of very large radius, centered at the orbit's center, and $\mathbf{E}$, $\mathbf{B}$ are the retarded electric and magnetic fields generated by the charges, which are evaluated over Σ_r at time t.

The fields in (31) correspond to the superposition of the retarded electric fields $\mathbf{E}_1$ and $\mathbf{E}_2$ and retarded magnetic fields $\mathbf{B}_1$ and $\mathbf{B}_2$ generated by charges e_1 and e_2, respectively. Therefore the integral in (31) splits into three parts:

$$\frac{c}{4\pi}\int_{\Sigma_r}(\mathbf{E}_1\times\mathbf{B}_1)\cdot d\boldsymbol{\Sigma}+\frac{c}{4\pi}\int_{\Sigma_r}(\mathbf{E}_2\times\mathbf{B}_2)\cdot d\boldsymbol{\Sigma}+\frac{c}{4\pi}\int_{\Sigma_r}(\mathbf{E}_1\times\mathbf{B}_2+\mathbf{E}_2\times\mathbf{B}_1)\cdot d\boldsymbol{\Sigma}. \tag{32}$$

Each of the first two integrals in (32) deals with the fields of only one of the charges, and its evaluation gives the total power of radiation of a monoenergetic electron in circular motion, namely[7] $(\frac{2}{3})(e_1^2c/a^2)\beta_1^4\gamma_1^4$ for charge e_1 and $(\frac{2}{3})(e_2^2c/b^2)\beta_2^4\gamma_2^4$ for charge e_2. Therefore, from the comparison of (32) and the right hand side of (30) it is seen that energy conservation requires the equality of the last term in (32) and the negative of the retarded interaction power W, defined by

$$W=e_1E_{21t}\beta_1c+e_2E_{12t}\beta_2c, \tag{33}$$

where E_{21t} and E_{12t} are given by Eqs. (13) and (18), respectively.

The last integral in (32) represents the radiation rate associated with the interference of the fields of the two charges, and involves only the far fields of both charges. This situation contrasts with the definition of W in Eq. (33), where the exact fields are involved, that is, both the far and the near fields. In what follows the explicit calculation of the interference rate of radiation and of W will be performed.

A. The interference rate of radiation

If we denote by (θ,φ) the usual spherical angles, the last integral in Eq. (32) can be performed by considering first the contribution of the ribbon parallel to the orbit plane defined between the angles θ and $\theta+d\theta$. Even though the electric and magnetic fields at a fixed point of the ribbon are changing with time, the instantaneous energy flux across the ribbon is time-independent. This is so because of the symmetry of the charge's motion, which makes different positions of the system of charges to appear as completely equivalent for the ribbon as a whole. This property of time-independence of the instantaneous energy flux across the ribbon is of course valid for any ribbon of Σ_r, and therefore the instantaneous energy flux over Σ_r is time-independent.

The surface element on the sphere Σ_r is $d\boldsymbol{\Sigma}=r^2\sin\theta d\theta d\varphi\hat{\mathbf{r}}$, where the unit normal to the sphere, $\hat{\mathbf{r}}$, is given by $\hat{\mathbf{r}}=\sin\theta\cos\varphi\hat{\mathbf{x}}+\sin\theta\sin\varphi\hat{\mathbf{y}}+\cos\theta\hat{\mathbf{z}}$. The detection point $\mathbf{x}$ on the surface of the sphere is $\mathbf{x}=r\sin\theta\cos\varphi\hat{\mathbf{x}}+r\sin\theta\sin\varphi\hat{\mathbf{y}}+r\cos\theta\hat{\mathbf{z}}$, and therefore the retarded times t_1' and t_2' of charges e_1 and e_2 associated to the point $\mathbf{x}$ at time t satisfy

$$t-t_1'=\frac{1}{c}\{r^2+a^2-2ar\sin\theta\cos(\varphi-\omega t_1')\}^{1/2}, \tag{34}$$

$$t-t_2'=\frac{1}{c}\{r^2+b^2-2br\sin\theta\cos(\varphi-\omega t_2'-\psi)\}^{1/2}. \tag{35}$$

It turns out convenient to introduce the variables x and y defined by

$$x=\varphi-\omega t_1', \tag{36}$$

$$y=\varphi-\omega t_2'-\psi, \tag{37}$$

which, according to Eqs. (34) and (35), are linked by

$$y-x+\psi=\frac{\omega r}{c}[\{1+(a/r)^2-2(a/r)\sin\theta\cos x\}^{1/2}-\{1+(b/r)^2-2(b/r)\sin\theta\cos y\}^{1/2}]. \tag{38}$$

This equation defines a one-to-one correspondence between variables x and y for any ribbon on the sphere of radius r. In fact, from Eq. (38) it follows that

$$\frac{dy}{dx}=\frac{\kappa_1}{\kappa_2}>0, \tag{39}$$

where, according to (10), we have

$$\kappa_1=1-\frac{\beta_1\sin\theta\sin x}{\{1+(a/r)^2-2(a/r)\sin\theta\cos x\}^{1/2}}, \tag{40}$$

$$\kappa_2=1-\frac{\beta_2\sin\theta\sin y}{\{1+(b/r)^2-2(b/r)\sin\theta\cos y\}^{1/2}}. \tag{41}$$

In a similar way, Eq. (34) determines t_1' as a function of the angle φ over the ribbon and therefore variable x defined by Eq. (36) has a unique value for each φ in the interval $0<\varphi \leqslant 2\pi$. In fact, taking the derivative with respect to φ of Eqs. (34) and (36) and combining them we obtain

$$\frac{d\varphi}{dx}=\kappa_1>0,$$

and therefore the surface integral over the ribbon

$$\frac{c}{4\pi}\int_0^{2\pi}(\mathbf{E}_1\times\mathbf{B}_2+\mathbf{E}_2\times\mathbf{B}_1)\cdot\hat{\mathbf{r}}d\varphi \tag{42}$$

can be written as an integral over variable x,

$$\frac{c}{4\pi}\int_\alpha^{2\pi+\alpha}(\mathbf{E}_1\times\mathbf{B}_2+\mathbf{E}_2\times\mathbf{B}_1)\cdot\hat{\mathbf{r}}\kappa_1 dx, \tag{43}$$

where variable y is determined as a function of x through Eq. (38), and where parameter α is given by $\alpha=-\omega t_2'(\varphi=0)=-\omega t_2'(\varphi=2\pi)$. When we explicitly evaluate the integrand of (43), it turns out that it depends on x and y only through the functions $\cos x$, $\cos y$, $\sin x$ and $\sin y$. Moreover, from Eq. (38) it follows that y is a periodic function of x of period 2π, and therefore the integrand of (43) is a periodic function of x, of period 2π. Thus, (43) does not depend on the value of α and we can set $\alpha=0$. The instantaneous energy flux over the sphere Σ_r is therefore

$$P=\frac{c}{4\pi}r^2\int_0^{\pi}\sin\theta d\theta\int_0^{2\pi}(\mathbf{E}_1\times\mathbf{B}_2+\mathbf{E}_2\times\mathbf{B}_1)\cdot\hat{\mathbf{r}}\kappa_1 dx. \tag{44}$$

In the limit when the radius of the sphere r tends to infinity we obtain the following explicit expression,

$$P=\frac{e_1e_2c\beta_1^2\beta_2^2}{2\pi ab}\int_0^{\pi}\sin\theta d\theta\int\frac{\{\}}{\kappa_1^2\kappa_2^3}dx, \tag{45}$$

where

$$\{\}=\cos^2\theta\cos x\cos y+\sin x\sin y-\beta_1\sin\theta\sin y-\beta_2\sin\theta\sin x+\beta_1\beta_2\sin^2\theta, \tag{46}$$

and where Eqs. (40) and (41) simplify to

$$\kappa_1=1-\beta_1\sin\theta\sin x, \tag{47}$$

$$\kappa_2=1-\beta_2\sin\theta\sin y. \tag{48}$$

Similarly, the retardation condition (38) becomes

$$y-x+\psi=\sin\theta\{\beta_1\cos x-\beta_2\cos y\}. \tag{49}$$

The expression (45) is an exact formula for the part of the radiation rate associated with the interference between the charge's fields.

The retardation condition (49) is a functional relation similar to that studied by Watson in his well known book,[8] and it makes it possible to perform the x-integration. To this end it is useful to shift the x and y variables to

$$\overline{x}=x-\pi/2,$$

$$\overline{y}=y-\pi/2$$

to write $\varepsilon_1=\beta_1\sin\theta$, $\varepsilon_2=\beta_2\sin\theta$ and to introduce the combination

$$u=\overline{x}-\varepsilon_1\sin\overline{x}-\psi, \tag{50}$$

in terms of which Eq. (49) becomes

$$\overline{y}-\varepsilon_2\sin\overline{y}=u, \tag{51}$$

which is essentially the same relation studied by Watson. Equations (50) and (51) determine $\overline{x}$ and $\overline{y}$ respectively as functions of the independent variables u,ψ,ε_1 and ε_2. For fixed values of ψ,ε_1 and ε_2, both $\overline{x}$ and $\overline{y}$ are uniquely determined by u, since $d\overline{x}/du=1/(1-\varepsilon_1\cos\overline{x})>0$ and $d\overline{y}/du=1/(1-\varepsilon_2\cos\overline{y})>0$. Besides, if $\overline{x}\to\overline{x}+2\pi$ in Eq. (50) or $\overline{y}\to\overline{y}+2\pi$ in Eq. (51), we have $u\to u+2\pi$, and therefore $\overline{x}$ and $\overline{y}$ are periodic functions of u of period 2π. Also, it can be seen that $\overline{y}$ is an odd function of u.

In terms of the new variables, (45) can be written

$$P=\frac{e_1e_2c\beta_1^2\beta_2^2}{2\pi ab}\int_0^{\pi}\sin\theta d\theta\int_0^{2\pi}\frac{\cos^2\theta\sin\overline{x}\sin\overline{y}+(\cos\overline{x}-\varepsilon_1)(\cos\overline{y}-\varepsilon_2)}{(1-\varepsilon_1\cos\overline{x})^3(1-\varepsilon_2\cos\overline{y})^3}du. \tag{52}$$

The integrand of (52) can be rewritten by using the following identities,

$$\begin{aligned}
\frac{\sin\overline{x}}{(1-\varepsilon_1\cos\overline{x})^3}&=-\frac{1}{\varepsilon_1}\frac{\partial}{\partial u}\left(\frac{1}{\kappa_1}\right),\\
\frac{\sin\overline{y}}{(1-\varepsilon_2\cos\overline{y})^3}&=-\frac{1}{\varepsilon_2}\frac{\partial}{\partial u}\left(\frac{1}{\kappa_2}\right),\\
\frac{(\cos\overline{x}-\varepsilon_1)}{(1-\varepsilon_1\cos\overline{x})^3}&=\frac{\partial}{\partial\varepsilon_1}\left(\frac{1}{\kappa_1}\right),\\
\frac{\cos\overline{y}-\varepsilon_2}{(1-\varepsilon_2\cos\overline{y})^3}&=\frac{\partial}{\partial\varepsilon_2}\left(\frac{1}{\kappa_2}\right),
\end{aligned} \tag{53}$$

where $1/\kappa_1$ and $1/\kappa_2$ are periodic functions of u, and therefore can be expanded in Fourier series by using the techniques developed by Watson.[8] The results are

$$\begin{aligned}
\frac{1}{\kappa_1}&=\frac{1}{1-\varepsilon_1\cos\overline{x}}=1+2\sum_{n=1}\{-\sin(n\psi)J_n(n\varepsilon_1)\sin(nu)+\cos(n\psi)J_n(n\varepsilon_1)\cos(nu)\},\\
\frac{1}{\kappa_2}&=\frac{1}{1-\varepsilon_2\cos\overline{y}}=1+2\sum_{n=1}J_n(n\varepsilon_2)\cdot\cos(nu).
\end{aligned} \tag{54}$$

Replacing Eqs. (53) and (54) in (52) and performing the u-integration, which now is trivial, (52) becomes

$$P=\frac{e_1e_2c\beta_1^2\beta_2^2}{2ab}\int_0^{\pi}\sin\theta\sum_{n=1}^{\infty}\cos(n\psi)\left\{\frac{n^2\cos^2\theta J_n(n\varepsilon_1)J_n(n\varepsilon_2)}{\varepsilon_1\varepsilon_2}+n^2J_n'(n\varepsilon_1)J_n'(n\varepsilon_2)\right\}d\theta. \tag{55}$$

The angular integration in (55) is performed by using the series representation of the Bessel function

$$J_n(z)=\sum_{p=0}^{\infty}\frac{(-1)^p z^{n+2p}}{2^{n+2p}p!(n+p)!}$$

and its derivative, evaluated at $z_1=n\varepsilon_1=n\beta_1\sin\theta$ and $z_2=n\varepsilon_2=n\beta_2\sin\theta$, and by using the result

$$\int_0^{\pi}(\sin\theta)^{2j-1}d\theta=\frac{\pi^{1/2}\Gamma(j)}{\Gamma(j+\frac{1}{2})},$$

where $\Gamma(z)$ is the Gamma function. Then, the interference rate of radiation can be written as

$$P=\frac{2e_1e_2c\beta_1^2}{a^2}\sum_{n=1}^{\infty}\cos(n\psi)(n^2\beta_1\beta_2)^n\sum_{p,q=0}^{\infty}\frac{(-1)^{p+q}n^{2p+2q}(n+p+q)!(n+p+q-1)!}{p!q!(n+p)!(n+q)!(2n+2p+2q)!}$$
$$\times\left\{\frac{n^2}{(2n+2p+2q+1)}+(n+2p)(n+2q)\right\}\beta_1^{2p}\beta_2^{2q}. \tag{56}$$

According to the discussion after Eq. (32), Eq. (56) for the interference rate of radiation should equal the negative of the rate of work W defined in Eq. (33). In order to compare P and $-W$, in what follows we will explicitly calculate the right hand side of (33), expressing it as a double series in β_1 and β_2.

B. The rate of work

The retardation conditions (12) and (16) determine implicitly α_1 and α_2 as functions of β_1,χ and ψ, which will be chosen as independent parameters. For fixed χ and β_1, α_1 and α_2 are uniquely determined as functions of ψ, since

$$\partial\alpha_1/\partial\psi=1/\kappa_1>0, \tag{57}$$

$$\partial\alpha_2/\partial\psi=1/\kappa_2>0, \tag{58}$$

where κ_1 and κ_2 are given by Eqs. (14) and (17). Besides, if $\alpha_1\to\alpha_1+2\pi$ in Eq. (12) or $\alpha_2\to\alpha_2+2\pi$ in Eq. (16), we have $\psi\to\psi+2\pi$, and therefore α_1 and α_2 are periodic functions of ψ of period 2π.

From Eqs. (12) and (16) it follows that

$$\frac{\partial\alpha_1}{\partial\beta_1}=\frac{\{1+\chi^2-2\chi\cos\alpha_1\}^{1/2}}{\kappa_1}>0,$$
$$\frac{\partial\alpha_2}{\partial\beta_1}=-\frac{\{1+\chi^2-2\chi\cos\alpha_2\}^{1/2}}{\kappa_2}<0. \tag{59}$$

By using these results it is easily verified that expressions (13) and (18) for the tangential components of the retarded electric fields can be written as

$$E_{12t}/e_1=-\frac{1}{\chi}\left(1-\frac{\beta_1^2}{2}-\frac{\beta_1^2\chi^2}{2}\right)\frac{\partial}{\partial\beta_1}\left(\frac{1}{\kappa_1R_1^2}\right)-\frac{\beta_1^2}{2a^2\chi}\frac{\partial}{\partial\beta_1}\left(\frac{1}{\kappa_1}\right),$$
$$E_{21t}/e_2=\left(-1+\frac{\beta_1^2}{2}+\frac{\beta_1^2\chi^2}{2}\right)\frac{\partial}{\partial\beta_1}\left(\frac{1}{\kappa_2R_2^2}\right)-\frac{\beta_1^2}{2a^2}\frac{\partial}{\partial\beta_1}\left(\frac{1}{\kappa_2}\right), \tag{60}$$

and therefore the retarded interaction power W in Eq. (33) can be expressed as

$$W=e_1e_2c\left\{\left(-1+\frac{\beta_1^2}{2}+\frac{\beta_1^2\chi^2}{2}\right)\beta_1\frac{\partial}{\partial\beta_1}\left(\frac{1}{\kappa_1R_1^2}+\frac{1}{\kappa_2R_2^2}\right)-\frac{\beta_1^3}{2a^2}\frac{\partial}{\partial\beta_1}\left(\frac{1}{\kappa_1}+\frac{1}{\kappa_2}\right)\right\}. \tag{61}$$

W will be now expanded as a Fourier series in angle ψ, by doing the corresponding expansions of the factors containing κ_1 and κ_2 in Eq. (61). These factors are even functions of ψ, as can be seen from the following symmetry of the retardation conditions, Eqs. (12) and (16). If α_2 satisfies Eq. (16) for the angle ψ, then $\alpha_1=-\alpha_2$ satisfies Eq. (12) for the angle $-\psi$. Also, if α_1 satisfies Eq. (12) for the angle ψ, then $\alpha_2=-\alpha_1$ satisfies Eq. (16) for the angle $-\psi$. That is, when $\psi\rightarrow-\psi$, $\alpha_1\rightarrow-\alpha_2$ and $\alpha_2\rightarrow-\alpha_1$, which in turn implies that $\kappa_1\rightarrow\kappa_2$, $\kappa_2\rightarrow\kappa_1$, $R_1\rightarrow R_2$ and $R_2\rightarrow R_1$. Therefore, $1/\kappa_1+1/\kappa_2$ and $1/(\kappa_1R_1^2)+1/(\kappa_2R_2^2)$ remain unchanged when $\psi\rightarrow-\psi$. Thus, it follows

$$\frac{1}{\kappa_1}+\frac{1}{\kappa_2}=\sum_n A_n\cos n\psi,$$

where

$$A_n=\frac{1}{\pi}\int_{-\pi}^{\pi}\frac{\cos n\psi}{\kappa_1}d\psi+\frac{1}{\pi}\int_{-\pi}^{\pi}\frac{\cos n\psi}{\kappa_2}d\psi. \tag{62}$$

Using Eqs. (57) and (58) to change the variable of integration, we have

$$A_n=\frac{1}{\pi}\int_{-\pi}^{\pi}\cos(n\alpha_1-n\beta_1\{1+\chi^2-2\chi\cos\alpha_1\}^{1/2})d\alpha_1+\frac{1}{\pi}\int_{-\pi}^{\pi}\cos(n\alpha_2+n\beta_1\{1+\chi^2$$

$$-2\chi\cos\alpha_2\}^{1/2})d\alpha_2=\frac{4}{\pi}\int_0^{\pi}\cos(n\alpha)\cos(n\beta_1\{1+\chi^2-2\chi\cos\alpha\}^{1/2})d\alpha. \tag{63}$$

In the same way we obtain

$$\frac{1}{\kappa_1R_1^2}+\frac{1}{\kappa_2R_2^2}=\frac{1}{a^2}\sum_n B_n\cos n\psi, \tag{64}$$

where

$$B_n=\frac{4}{\pi}\int_0^{\pi}\frac{\cos(n\alpha)\cos(n\beta_1\{1+\chi^2-2\chi\cos\alpha\}^{1/2})}{1+\chi^2-2\chi\cos\alpha}d\alpha. \tag{65}$$

Replacing Eqs. (62)–(65) in Eq. (61), we obtain

$$W=-\frac{e_1e_2c\beta_1}{2a^2}\sum_n\cos n\psi\left\{(2-\beta_1^2-\chi^2\beta_1^2)\frac{\partial B_n}{\partial\beta_1}+\beta_1^2\frac{\partial A_n}{\partial\beta_1}\right\}. \tag{66}$$

The coefficients A_n and B_n can be expressed as power series in β_1 by expanding the factor $\cos(n\beta_1\{1+\chi^2-2\chi\cos\alpha\}^{1/2})$ in Eqs. (63) and (65). For instance,

$$A_n=\frac{4}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^m(n\beta_1)^{2m}}{(2m)!}\int_0^{\pi}\cos(n\alpha)(1+\chi^2-2\chi\cos\alpha)^m d\alpha. \tag{67}$$

Writing $1+\chi^2-2\chi\cos\alpha=c-d\cos\alpha$, with parameters c and d given by

$$\begin{aligned}c&=1+\chi^2,\\ d&=2\chi,\end{aligned} \tag{68}$$

and using the binomial theorem, Eq. (67) becomes

$$A_n=\frac{4}{\pi}\sum_{m=0}^{\infty}\frac{(-1)^m(n\beta_1)^{2m}}{(2m)!}\sum_{k=0}^{m}\binom{m}{k}(-1)^k c^{m-k}d^k\int_0^{\pi}\cos(n\alpha)(\cos\alpha)^k d\alpha. \tag{69}$$

The result of the integration is[9]

$$\int_0^{\pi}\cos n\alpha(\cos\alpha)^k d\alpha=\begin{cases}0 & \text{if } k<n \quad \text{or} \quad k=n+2i-1, \quad i>0,\\ \dfrac{\pi}{2^k}\binom{k}{i} & \text{if } k=n+2i, \quad i>0.\end{cases} \tag{70}$$

Therefore, the terms with $m<n$ on the right hand side of Eq. (69) vanish. Putting $m=n+j$, and since only $k=n+2i$ gives a nonvanishing result, Eq. (69) becomes

$$\begin{aligned}A_n&=4\sum_{j=0}^{\infty}\frac{(-1)^{n+j}(n\beta_1)^{2n+2j}}{(2n+2j)!}\sum_{k=n}^{n+j}\binom{n+j}{k}\binom{k}{i}(-1)^k\frac{c^{n+j-k}d^k}{2^k}\\ &=4\sum_{j=0}^{\infty}\frac{(-1)^{n+j}(n\beta_1)^{2n+2j}}{(2n+2j)!}\sum_{i=0}^{[j/2]}\binom{n+j}{n+2i}\binom{n+2i}{i}(-1)^{n+2i}\frac{c^{j-2i}d^{n+2i}}{2^{n+2i}},\end{aligned} \tag{71}$$

where $[x]$ represents the integer part of x. From Eq. (71) it is immediate that

$$\frac{\partial A_n}{\partial\beta_1}=4\sum_{j=0}^{\infty}(-1)^j\frac{n^{2n+2j}\beta_1^{2n+2j-1}}{(2n+2j-1)!}\sum_{i=0}^{[j/2]}\binom{n+j}{n+2i}\binom{n+2i}{i}\frac{c^{j-2i}d^{n+2i}}{2^{n+2i}}. \tag{72}$$

The dependence of Eq. (72) on χ and β_1 can be changed to a dependence on $\beta_2=\chi\beta_1$ and β_1 by using Eq. (68) and by regrouping factors as follows:

$$\frac{d^{n+2i}}{2^{n+2i}}\beta_1^{n+2i}=(\beta_1^2\chi)^{n+2i}=(\beta_1\beta_2)^{n+2i},$$

$$c^{j-2i}\beta_1^{2j-4i}=(\beta_1^2(1+\chi^2))^{j-2i}=(\beta_1^2+\beta_2^2)^{j-2i}=\sum_{\ell=0}^{j-2i}\binom{j-2i}{\ell}\beta_1^{2j-4i-2\ell}\beta_2^{2\ell},$$

which, when replaced in Eq. (72), give

$$\frac{\partial A_n}{\partial\beta_1}=4\sum_{j=0}^{\infty}\frac{(-1)^j n^{2j+2n}(\beta_1\beta_2)^n\beta_1^{-1}}{(2n+2j-1)!}\times\sum_{i=0}^{[j/2]}\sum_{\ell=0}^{j-2i}\binom{n+j}{n+2i}\binom{n+2i}{i}\binom{j-2i}{\ell}\beta_1^{2j-2i-2\ell}\beta_2^{2i+2\ell}. \tag{73}$$

In the same way, it is readily obtained that

$$\frac{\partial B_n}{\partial\beta_1}=4\sum_{j=0}^{\infty}\frac{(-1)^{j+1}n^{2n+2j+2}(\beta_1\beta_2)^n\beta_1}{(2n+2j+1)!}\times\sum_{i=0}^{[j/2]}\sum_{\ell=0}^{j-2i}\binom{n+j}{n+2i}\binom{n+2i}{i}\binom{j-2i}{\ell}\beta_1^{2j-2i-2\ell}\beta_2^{2i+2\ell}. \tag{74}$$

Replacing Eqs. (73) and (74) in Eq. (66) we obtain

$$\begin{aligned}W=&-\frac{2e_1e_2c\beta_1^2}{a^2}\sum_{n=0}^{\infty}\cos(n\psi)(n^2\beta_1\beta_2)^n\sum_{j=0}^{\infty}\frac{n^{2j}(-1)^{j+1}}{(2n+2j+1)!}\times\{n^2(2-\beta_1^2-\beta_2^2)\\ &-(2n+2j)(2n+2j+1)\}S(n,j),\end{aligned} \tag{75}$$

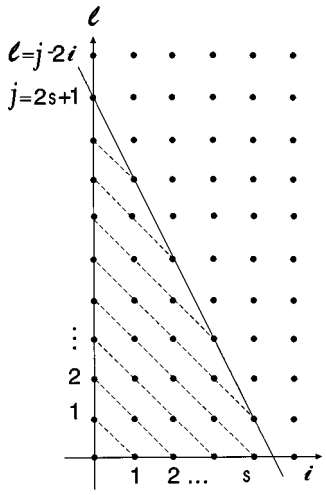

FIG. 5. The values of ℓ and i that occur in the double sum S are located inside the triangular region delimited by the straight line $\ell=j-2i$ and the coordinate axes. The points located on the segmented lines have a constant value of $q=\ell+i$.

where

$$S(n,j)=\sum_{i=0}^{[j/2]}\sum_{\ell=0}^{j-2i}\binom{n+j}{n+2i}\binom{n+2i}{i}\binom{j-2i}{\ell}\beta_1^{2j-2i-2\ell}\beta_2^{2i+2\ell}. \tag{76}$$

Equation (75) would have the same structure as the retarded interference rate P in Eq. (56) if one of the sums in Eq. (76) could be performed. To this end, it turns out convenient to collect terms in (76) with a fixed value of $\ell+i:=q$. In order to see more clearly how to arrange the terms of the double sum in Eq. (76) according to the new variables q and i, it is useful to plot in the $\ell-i$ plane the values that ℓ and i take in Eq. (76).

In Fig. 5 we assume for simplicity that j is odd, that is, $j=2s+1$. From Eq. (76) it follows that the possible values of i and ℓ are located inside the triangular region delimited by the positive coordinate axes and the slope -2 straight line $\ell=j-2i$. In this plot the combinations of values of ℓ and i that have a constant value of $q=\ell+i$ are located on straight lines of slope -1. Therefore, q takes values in the range $0\rightarrow j$. From Fig. 5 we see that the values taken by i for a given value of q depend on whether $q\leqslant s$ or $q>s$. If $q\leqslant s$, then the straight line $i+\ell=q$ joins both catets of the triangular allowed region, and therefore i takes values $0,1,\ldots,q$. On the other hand, if $q>s$, the straight line $i+\ell=q$ joins the $i=0$ axis with the straight line $\ell=j-2i$. In this case the maximum value that i takes is the one corresponding to the intersection point of both straight lines, that is, $i=j-q$. Therefore, the value of S in the case $j=2s+1$ is

$$\begin{aligned}S(n,j)=&\sum_{q=0}^{s}\sum_{i=0}^{q}\binom{n+j}{n+2i}\binom{n+2i}{i}\binom{j-2i}{q-i}\beta_1^{2j-2q}\beta_2^{2q}+\sum_{q=s+1}^{j}\sum_{i=0}^{j-q}\binom{n+j}{n+2i}\binom{n+2i}{i}\\&\times\binom{j-2i}{q-i}\beta_1^{2j-2q}\beta_2^{2q}.\end{aligned} \tag{77}$$

Making the change of dummy index $q=j-v$ in the second term of Eq. (77), and using the symmetry of the binomial coefficient

$$\binom{j-2i}{j-v-i}=\binom{j-2i}{v-i},$$

Eq. (77) can be rewritten as

$$S(n,j)=\sum_{q=0}^{s}\sum_{i=0}^{q}\binom{n+j}{n+2i}\binom{n+2i}{i}\binom{j-2i}{q-i}(\beta_1^{2j-2q}\beta_2^{2q}+\beta_1^{2q}\beta_2^{2j-2q}). \tag{78}$$

The sum over the index i in Eq. (78) can be carried out by noting that it corresponds to a hypergeometric series. In effect, the ratio of consecutive terms of the sum is

$$\frac{a_{i+1}}{a_i}=\frac{(i-q)(i-(j-q))}{(i+n+1)(i+1)},$$

and, therefore, from the definition of the hypergeometric series we have

$$A(n,j,q):=\sum_{i=0}^{q}\binom{n+j}{n+2i}\binom{n+2i}{i}\binom{j-2i}{q-i}=\frac{(j+n)!}{n!q!(j-q)!}\,{}_2F_1(-q,-(j-q),n+1;1). \tag{79}$$

Using the well known relation

$${}_2F_1(a,b,c;1)=\frac{\Gamma(c-a-b)\Gamma(c)}{\Gamma(c-a)\Gamma(c-b)},$$

it follows that

$$A(n,j,q)=\frac{[(j+n)!]^2}{q!(j-q)!(j+n-q)!(q+n)!}, \tag{80}$$

a result that is invariant under the interchange of q and $j-q$.

The analysis can be repeated for the case of even j, that is, for $j=2s$, and the final result is exactly the same. Thus, for any j we have

$$S(n,j)=\sum_{q=0}^{j}A(n,j,q)\beta_1^{2j-2q}\beta_2^{2q}, \tag{81}$$

where $A(n,j,q)$ is given by Eq. (80). Replacing Eqs. (81) and (80) in Eq. (75), changing the index j in the sums for the new dummy index $p=j-q$, and using the identity for absolutely convergent series

$$\sum_{j=0}^{\infty}\sum_{q=0}^{j}a_{q,j}=\sum_{q=0}^{\infty}\sum_{p=0}^{\infty}a_{q,p+q}, \tag{82}$$

the following expression for W is obtained:

$$W=\frac{2e_1e_2c\beta_1^2}{a^2}\sum_{n=0}^{\infty}\cos(n\psi)(n^2\beta_1\beta_2)^n\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\{a_{p,q}(2-\beta_1^2-\beta_2^2)-b_{p,q}\}\beta_1^{2p}\beta_2^{2q}, \tag{83}$$

where the coefficients $a_{p,q}$ and $b_{p,q}$ are given by

$$\begin{aligned}a_{p,q}&=\frac{(-1)^{p+q}n^{2p+2q+2}[(n+p+q)!]^2}{(2n+2p+2q+1)!p!q!(n+p)!(n+q)!},\\ b_{p,q}&=\frac{(-1)^{p+q}n^{2p+2q}(2n+2p+2q)(2n+2p+2q+1)[(n+p+q)!]^2}{(2n+2p+2q+1)!p!q!(n+p)!(n+q)!}.\end{aligned} \tag{84}$$

Note that Eq. (56) for the interference rate of radiation P can be written in terms of the coefficient $a_{p,q}$ in (84). The resulting expression is

$$P=\frac{2e_1e_2c\beta_1^2}{a^2}\sum_{n=0}^{\infty}\cos(n\psi)(n^2\beta_1\beta_2)^n\sum_{p,q=0}^{\infty}\frac{a_{p,q}}{n^2(n+p+q)}$$
$$\times\{n^2+(2n+2p+2q+1)(n+2p)(n+2q)\}\beta_1^{2p}\beta_2^{2q}. \tag{85}$$

On the other hand, Eq. (83) for the rate of retarded work W is not still in its final form as a double power series in β_1 and β_2, due to the factor $(2-\beta_1^2-\beta_2^2)$ in the numerator. Equation (83) can be rewritten in the form

$$W=\frac{2e_1e_2c\beta_1^2}{a^2}\sum_{n=0}^{\infty}\cos(n\psi)(n^2\beta_1\beta_2)^n\sum_{p,q=0}^{\infty}\{2a_{p,q}-b_{p,q}-a_{p-1,q}-a_{p,q-1}\}\beta_1^{2p}\beta_2^{2q}, \tag{86}$$

where the coefficients $a_{p=-1,q}$ and $a_{p,q=-1}$ are defined to be zero. Introducing in (86) the following relations between the different coefficients,

$$b_{p,q}=\frac{(2n+2p+2q)(2n+2p+2q+1)}{n^2}a_{p,q},$$
$$a_{p-1,q}=-\frac{2p(n+p)(2n+2p+2q+1)}{n^2(n+p+q)}a_{p,q}, \tag{87}$$
$$a_{p,q-1}=-\frac{2q(n+q)(2n+2p+2q+1)}{n^2(n+p+q)}a_{p,q},$$

and comparing with Eq. (85) it is readily seen that $-W$ reduces to the interference rate of radiation P, thus showing the consistency of the Lorentz–Dirac equation with energy conservation.

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Wave front layer stripping approach to inverse scattering for the wave equation

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The inverse problem involving a point pulse source exterior to a scattering medium, where the velocity $c(x)$ is continuous, is considered. The layer stripping approach is applied to thin curvilinear layers whose surfaces are the primary wave fronts [with $c(x)$ continuous, the reflected wave fronts will be secondary, i.e., of lower order singularity]. It is shown that the layer stripping approach can be used in the time-domain inverse problem without employing the added complexity of having to perform wave splitting. Furthermore the procedure to determine the normal derivative of c from the asymptotic short time behavior of the field quantities on an adjacent wave front surface has been simplified compared to earlier wave splitting methods. Uniqueness results are given. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1504502]

I. INTRODUCTION

Wave splitting in the time domain for one-dimensional inverse problems involving the wave equation was employed by Corones and Kreuger[1,2] and subsequently extended to more complicated one-dimensional equations, like viscoelastic equations, Karlsson,[3] etc. In three dimensions, Fishman,[4,5] used the pseudodifferential operator resulting from the planar splitting to obtain one-way propagation in the frequency domain. Planar wave splitting was formulated for the three-dimensional wave equation in the time domain by Weston,[6,7] and applied to the inverse problem for the telegraph equation by Weston and He.[8] Working in a sector of the complex Laplace transform plane of the wave equation, de Hoop[9,10] was able to get rigorous results for planar wave splitting and the resulting Bremmer series, etc. A comprehensive review and bibliography of time-domain wave splitting for the wave equation and Maxwells equation is given in the book by He, Ström, and Weston.[11]

Nonplanar wave splitting in time-domain was introduced by Weston[12] for the three-dimensional wave equation. This formulation proved useful in obtaining the appropriate absorbing boundary condition for the wave equation. Here the procedure of the layer stripping process on curved surfaces is given for the case when the curved surfaces are the wave fronts associated with a particular scattering problem.

An alternative approach to inverse scattering in an inhomogeneous medium is to use the Bremmer series. In this connection, some very fast algorithms have been developed for the calculation of the Bremmer series. They are the Generalized Screen method[13] and the rational approximation method.[14]

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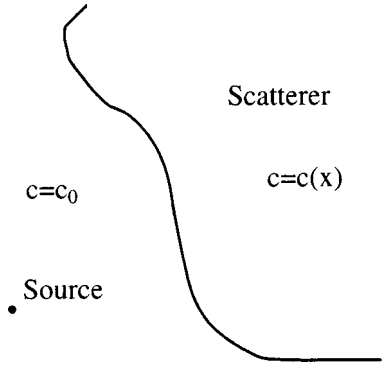

FIG. 1. Scattering geometry.

II. OVERVIEW OF THE WAVE FRONT CONNECTION TO THE INVERSE PROBLEM

Consider the scattering problem where there is a point impulse source at x^0, which is exterior to a scatterer whose domain is characterized by the support of $(c(x)-c_0)$ where c_0 is the free space value of the velocity $c(x)$ (see Fig. 1). The total field $u(x,t)$ satisfies the wave equation

$$\frac{1}{c^2(x)}\frac{\partial^2 u}{\partial t^2}-\Delta u=\delta(x-x^0)H(t), \quad x^0,x\in\mathbb{R}^3, \tag{1}$$

where, initially, it will be assumed that $c(x)$ is a continuous function of x.

The incident field portion, $u^i(x,t)$, in free space, of $u(x,t)$ will have the form

$$u^i(x,t)=\frac{1}{4\pi R}H\left(t-\frac{R}{c_0}\right), \quad R=|x-x^0|. \tag{2}$$

Let $\tau(x,x^0)$ be the travel time from the source point x^0 to the observation point x, then the wave front surface at time t is given by

$$\tau(x,x^0)=t, \tag{3}$$

with $\tau(x,x^0)$ satisfying the Eikonal equation

$$|\nabla\tau|^2=\frac{1}{|c(x)|^2}. \tag{4}$$

The rays (the trajectories orthogonal to the wave front surfaces) emanating from the source point in the direction of the unit vector

$$\nu=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta), \tag{5}$$

can be represented in terms of the two parameter family of curves

$$x_j=X_j(\tau,\theta,\phi), \quad 0\leqslant\theta\leqslant\pi, \quad 0\leqslant\phi<2\pi, \quad 0\leqslant\tau, \quad j=1,2,3, \tag{6}$$

with the parameters θ and ϕ being the angles associated with a local spherical coordinate system centered at the source point x^0. The rays satisfy the following differential equation.[15]

$$\frac{\partial}{\partial\tau}\left(\frac{1}{c^2}\frac{\partial X}{\partial\tau}\right)=c\nabla\left(\frac{1}{c}\right). \tag{7}$$

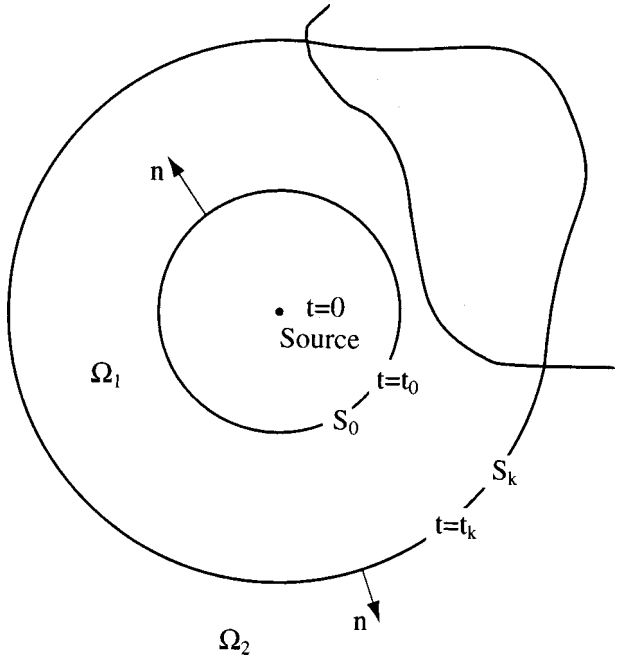

FIG. 2. Wave front geometry.

Note that the ray coordinate system (τ,θ,ϕ), is an orthogonal system which maps, in an 1:1 fashion, the domain $0\leqslant\tau\leqslant\tau^*$, $0\leqslant\theta\leqslant\pi$, $0\leqslant\phi<2\pi$ into a simply connected domain containing the source point x^0, provided that τ^* is restricted so that no caustics appear.

Let the time $t=t_0>0$ be such that the incident wave front has not impinged on the scatterer, and let S_0 be the wave front surface at that time. S_0 will then be a spherical surface with a radius c_0t_0 and centered at x^0; see Fig. 2. At a later time $t_k<T$, when the incident wave has impinged on the scatterer, let the corresponding wave front surface be S_k where

$$S_k=\{x\in\mathbb{R}^3:\tau(x,x^0)=t_k\}. \tag{8}$$

Let the open domain between the two surfaces S_0 and S_k be denoted Ω_1, and the region exterior to S_k be denoted Ω_2; see Fig. 2. Then it follows that the total field satisfies the following initial conditions in the domains Ω_1 and Ω_2, respectively:

$$u=u_t=0, \quad x\in\Omega_1, \quad t=t_0, \tag{9}$$

$$u=u_t=0, \quad x\in\Omega_2, \quad t=t_k. \tag{10}$$

The inverse problem can now be stated. Assume that the total field u and its normal derivative $\partial_n u$ are known on S_0, for $0\leqslant t\leqslant T$, either through direct measurements or through indirect measurements and calculations. For the latter case if the incident field is known and the scattered field u^r (which vanishes on S_0 for $t<t_0$) is measured on S_0 for times $0\leqslant t\leqslant T$, one can compute the normal component of each, especially that of the scattered wave component by using the ingoing and outgoing wave conditions on the spherical surface S_0,[12] and identifying the outgoing and incoming wave components, respectively, with u^i and u^r.

In the layer stripping process as applied to wave front surfaces, one has a set of nested (wave front) surfaces $S_0\subset S_1\subset S_2\subset\cdots\subset S_k$, each corresponding to the wave fronts at times $t_0,t_1,t_2,\ldots,t_k$, where $t_k=t_0+k\Delta_t$, and where Δ_t is a very small time interval.

When the initial wave front surface S_0 is known, one can compute in succession each wave front surface $\{S_n\}_{n=0}^k$, using the ray equation (7). If $x_k=X_k(\tau,\theta_0,\phi_0)$ is a point on the surface S_k

associated with the ray (θ_0,ϕ_0) then, upon integrating Eq. (7), one can show that the point x_{k+1}, on the wave front surface S_{k+1} associated with the same ray (θ_0,ϕ_0), is given by

$$x_{k+1}=x_k+\Delta_t c_k n_k+(\Delta_t)^2(-\tfrac{1}{2}c_k(\nabla c)_k+c_k(n\cdot\nabla c)_k n_k)+\cdots, \tag{11}$$

where n_k is the unit normal to the wave front surface S_k at the point x_k and c_k, $(\nabla c)_k$ are evaluated at the point x_k. Thus to determine the wave front surface S_{k+1} from the wave front surface S_k to order $(\Delta_t)^2$, one needs only the values of c and its normal derivative $\partial_n c$ on S_k.

On the surface S_0, as mentioned previously, u and $\partial_n u$ are known for $0\leqslant t\leqslant T$ as well as c and $\partial_n c$ ($c=c_0$ and $\partial_n c=0$). From knowledge of c and $\partial_n c$ on S_0, one can find the wave front surface S_1 by using expression (11) and also obtain an estimate for the value of c on S_1. Using this value of c in the first layer and knowledge of u and $\partial_n u$ on S_0 one wants to obtain the values of u and $\partial_n u$ on S_0 for $0\leqslant t\leqslant T$. This is discussed in Sec. III. Then from the asymptotic (leading time) behavior of u and $\partial_n u$ on S_1, one wants to obtain $\partial_n c$ on S_k. This is investigated in Sec. IV. Finally these steps are repeated, layer by layer. The above-mentioned analysis holds for a time period where there are no caustics. The effect of caustics is discussed in Sec. V.

To investigate the mathematics behind the layer stripping process, the kth step will be considered starting with the knowledge or estimate of $c(x)$ in the kth layer bounded by S_{k-1} and S_k, but instead of working with the knowledge of u and $\partial_n u$ on S_{k-1} for $0\leqslant t\leqslant T$, and working in the kth layer, the domain Ω_1 bounded by the surfaces S_0 and S_k will be used together with the knowledge of u and $\partial_n u$ on S_0. This will then shed light on the influence of the *data* u and $\partial_n u$ on S_0 upon the determination of u and $\partial_n u$ on S_k.

Note that although $c(x)$ is assumed to be continuous throughout, its derivatives may or may not be continuous. In the typical numerical procedure for layer stripping, $c(x)$ and its first derivatives are continuous in each layer, but the normal derivative may have a jump discontinuity across each surface of the layer.

III. DETERMINATION OF u AND $\partial_n u$ ON S_k FROM KNOWLEDGE OF u AND $\partial_n u$ ON S_0

Given, the continuous velocity, $c(x)$, in $\overline{\Omega}_1$, the problem is to determine u and $\partial_n u$ on S_k for an appropriate time interval (to be determined) from knowledge of u and $\partial_n u$ on S_0 for $0\leqslant t\leqslant T$. Both quantities vanish on S_0 for $0\leqslant t\leqslant t_0$.

The problem of determining $u(x,t)$ in Ω_1 for $0\leqslant t\leqslant t_k$, from knowledge of either $u(x,t)$ or $\partial_n u(x,t)$ on S_0, is well-posed, and can be found in many ways. This fact will be used to first determine the leading (short time) term for $u(x,t)$ and $\partial_n u(x,t)$ on S_k as follows. Since the data on S_0 [the surface $|x-x^0|=c_0 t_0$, where c_0 is the free space value of $c(x)$] have the leading asymptotic terms

$$u(x,t)=\frac{1}{4\pi|x-x^0|}H\left(t-\frac{|x-x^0|}{c_0}\right)+\cdots,\quad x\in S_0, \tag{12}$$

$$\frac{\partial u(x,t)}{\partial n}=-\frac{1}{4\pi c_0|x-x^0|}\delta\left(t-\frac{|x-x^0|}{c_0}\right)+\ldots,\quad x\in S_0, \tag{13}$$

the leading term of $u(x,t)$ in $\overline{\Omega}_1$ for $0\leqslant t\leqslant t_k$ is given by

$$u(x,t)=U_0(x)H(t-\tau(x,x^0))+\cdots. \tag{14}$$

The surfaces S_0 and S_k are given by the wave front surfaces $\tau(x,x^0)=|x-x^0|/c_0=t_0$ and $\tau(x,x^0)=t_k$, respectively. Thus, since the problem is well-posed for $0\leqslant t\leqslant t_k$, and $c(x)$ is continuous, the value of $U_0(x)$ on the surface can be determined. Since the normal to the wave front is in the direction of the gradient of $\tau(x,x^0)$, it follows that the leading form $V_0(x)$ to $\partial_n u$ on S_k as given in the following:

$$\frac{\partial u(x,t)}{\partial n} = V_0(x)\,\delta(t-t_k)+\cdots, \quad t_k=\tau(x,x^0) \tag{15}$$

is given in terms of $U_0(x)$ by

$$V_0(x) = -\frac{\partial \tau}{\partial n} U_0(x) = -\frac{1}{c(x)} U_0(x). \tag{16}$$

Hence the leading term $V_0(x)$ can be found.

The problem now is to determine the remaining portion of $u(x,t)$ and $\partial_n u(x,t)$ on S_k for a time interval (to be specified).

The fundamental solution (or Green's function) $\mathcal{E}(x,y,t)$ of the wave equation will be introduced. It satisfies the system for fixed x,

$$\frac{1}{c^2(y)}\frac{\partial^2 \mathcal{E}}{\partial t^2} - \Delta \mathcal{E} = \delta(x-y)\,\delta(t), \quad x,y\in\mathbb{R}^3, \tag{17}$$

$$\mathcal{E}(x,y,t)=0 \quad \text{for } t<0. \tag{18}$$

Since $c(x)$ is continuous, the fundamental solution will have the leading asymptotic behavior

$$\mathcal{E}(x,y,t)\sim \frac{1}{\rho(x,y)}\,\delta(t-\tau(x,y))+\cdots, \tag{19}$$

where $\tau(x,y)$ is the travel time from point x to point y and vice verse. If $c(x)$ is differentiable, the amplitude factor $\rho(x,y)$ can be found by solving the transport equation. Further details are given in Sec. IV, but are not needed here, other than that $\rho(x,y)$ has the asymptotic value $\rho(x,y)\sim 4\pi|x-y|$ as $y\to x$.

Let $\mathcal{E}_{\mathcal{N}}(x,y,t)$ be the Neumann Green's function for the domain Ω_1, satisfying the Neumann boundary conditions

$$\frac{\partial \mathcal{E}_{\mathcal{N}}(x,y,t)}{\partial n_y}=0, \quad \text{for } x\in\Omega_1 \quad \text{and } y\in S_0\cup S_k. \tag{20}$$

Using this Green's function one can write down the solution $u(x,t)$ to the scattering problem, which satisfies initial conditions $u(x,0)=u_t(x,0)=0$ in $\overline{\Omega}_1$, and Neumann data on S_0 and S_k. We have

$$u(x,t)=\int_0^t \mathrm{d}s\int_{S_k}\mathrm{d}\sigma_y \mathcal{E}_{\mathcal{N}}(x,y,t-s)\frac{\partial u(y,s)}{\partial n_y} - \int_0^t \mathrm{d}s\int_{S_0}\mathrm{d}\sigma_y \mathcal{E}_{\mathcal{N}}(x,y,t-s)\frac{\partial u(y,s)}{\partial n_y}, \quad x\in\Omega_1, \tag{21}$$

where the normal derivative on both surfaces is taken in the direction of wave front propagation, see Fig. 2. Note that $\partial_n u$ on S_0 vanishes for $0\leqslant t<t_0$, and on S_k for $0\leqslant t<t_k$.

An alternative to expression (21) can be obtained by the usual approach for solving a homogeneous partial differential equation with nonhomogeneous boundary conditions, and that is to replace the solution $u(x,t)$ by the sum $w(x,t)+q(x,t)$ where $q(x,t)$ is a known function that satisfies the initial conditions $q(x,0)=q_t(x,0)=0$, and nonhomogeneous Neumann boundary conditions $\partial_n u=\partial_n q$ on S_0 and S_k. Then $w(x,t)$ satisfies homogeneous boundary and initial conditions and the nonhomogeneous equation

$$\frac{1}{c^2(x)}\frac{\partial^2 w}{\partial t^2} - \nabla^2 w = \nabla^2 q - \frac{1}{c^2(x)}\frac{\partial^2 q}{\partial t^2} = F(x,t). \tag{22}$$

The solution[16] for $w(x,t)$ can then be found in terms of the orthonormal set of eigenfunctions $\{\phi_m\}_{m=0}^{\infty}$ satisfying

$$-c^2(x)\nabla^2\phi_m = w_m^2\phi_m, \quad x\in\Omega_1,$$
$$\frac{\partial\phi_m}{\partial n}=0, \quad x\in S_0 \text{ and } S_k, \tag{23}$$

where w_0 is the zero eigenvalue, and the inner product is given by

$$(\phi_n,\phi_m)=\int_{\Omega_1}\frac{\phi_n(x)\phi_m(y)}{c^2(x)}\,dx. \tag{24}$$

Using this approach, one can show that the resulting solution can be expressed in the form given by Eq. (21) with

$$\mathcal{E}_{\mathcal{N}}(x,y,t)=\sum_{m=0}^{\infty}\frac{\sin(w_m t)}{w_m}\phi_m(x)\phi_m(y), \tag{25}$$

where the convergence of the series (25) is in the sense of distributions. The eigenfunction representation is useful when $\partial_n u$ is known. For the present case $\partial_n u$ on S_k is unknown. To obtain an equation to determine $\partial_n u$ on S_k (apart from the leading term which is already determined), let the $x\in\Omega_1$ in expression (21) approach a point on the surface S_0. One obtains the following integral equation of the first kind for $\partial_n u$ on S_k:

$$u(x,t)=\int_0^t ds\int_{S_k} d\sigma_y\,\mathcal{E}_{\mathcal{N}}(x,y,t-s)\frac{\partial u(y,s)}{\partial n_y}-\int_0^t ds\int_{S_0} d\sigma_y\,\mathcal{E}_{\mathcal{N}}(x,y,t-s)\frac{\partial u(y,s)}{\partial n_y},$$
$$x\in S_0, \quad 2t_k-t_0\leqslant x\leqslant T. \tag{26}$$

In taking the limit of the second integral on the right-hand side of Eq. (26), one uses the local behavior of $\mathcal{E}_{\mathcal{N}}(x,y,t)$,

$$\mathcal{E}_{\mathcal{N}}(x,y,t)\sim\frac{\delta(t-|x-y|/c(x))}{2\pi|x-y|}, \tag{27}$$

for y on the smooth surface S_0 and x on S_0, very close to y.

From Eq. (26) it is seen that the values of the measured data $u(x,t)$ where $x\in S_0$, $2t_k-t_0\leqslant t\leqslant T$ and $\partial_n u(x,t)$, $x\in S_0$ for $t_0\leqslant t\leqslant T$, can be used to obtain the values of $\partial_n u$ (apart from the leading term which is already known) on S_k for $t_k<t\leqslant T-t_k-t_0$. This implies that when $t_k>(T-t_0)/2$, the nonzero values of $\partial_n u$ cannot be deduced, hence in the inverse problem one cannot obtain the value of $c(x)$ in the region beyond the surface $\tau(x,x_0)=(T-t_0)/2$.

The problem of obtaining $\partial_n u$ on S_k, for $t_k<t\leqslant T-t_k-t_0$, from Eq. (26) is not well-posed. It will require some regularization method or an optimization approach. This will not be pursued here. The question of uniqueness will be examined next.

Let $\mathcal{M}$ be the class of functions $w(y,t)$, $y\in S_k$, $0\leqslant t\leqslant T-t_k-t_0$, such that

(i) $w(y,0)=0$, $0\leqslant t<t_k$;

and if K is the operator

$$u(x,t)=Kw=\int_0^t\int_{S_k}\mathcal{E}_{\mathcal{N}}(x,y,t-s)w(y,s)\,d\sigma_y\,ds, \tag{28}$$

then:

(ii) $u(x,t)\in C(\overline{\Omega}_1)$;

(iii) $u(x,t)$ is a generalized solution of the system

$$\frac{1}{c^2(x)}\frac{\partial^2 u}{\partial t^2}-\nabla^2 u=0, \quad x\in\Omega_1, \quad 0<t,$$
$$u(x,t)=0, \quad x\in\overline{\Omega}_1, \quad 0\leqslant t<t_k. \tag{29}$$

(iv) If n_1 is the unit normal (pointing into Ω_1) at $x^1\in S_k$, the normal derivative of u at x^1 is given by

$$\frac{\partial u(x^1,t)}{\partial n_1}=\lim_{x\in\Omega_1\to x^1} n_1\cdot\nabla_x Kw$$
$$=w(x^1,t)+\int_0^t\int_{S_k}\frac{\partial\mathcal{E}_{\mathcal{N}}}{\partial n_1}(x^1,y,t-s)w(y,s)\,d\sigma_y ds=w(x^1,t), \quad x^1\in S_k, \tag{30}$$

where use is made of the fact that the normal derivative of the Green's function vanishes on the surface.

(v) If n_1 is the unit normal to (pointing into Ω_1) at a point x^1, on S_0, then

$$\frac{\partial u(x^1,t)}{\partial n_1}=\lim_{x\in\Omega_1\to x^1} n_1\cdot\nabla_x u=0, \quad x^1\in S_0. \tag{31}$$

Remark: For condition (30) to hold the surface S_k must be sufficiently smooth and $w(y,t)$ must be at least Hölder continuous. [A similar result involving the Green's function $\mathcal{E}(x,y,t)$ is examined in detail in Sec. IV, where sharper results are required.]

One can now examine the uniqueness of the solution to Eq. (26). If $\partial_n u^1$ and $\partial_n u^2$ are two solutions, let $v(y,t)$ be their difference. It follows from Eq. (26) that

$$Kv=0, \quad x\in S_0, \quad 0\leqslant t\leqslant T. \tag{32}$$

Hence if $v(y,t)$ belongs to class $\mathcal{M}$, then it follows that $u=Kv$ satisfies system (iv), and boundary conditions

$$u+Kv=0, \quad \frac{\partial u}{\partial n}=v, \quad x\in S_k, \quad 0\leqslant t\leqslant T-t_k-t_0, \tag{33}$$

$$u=0, \quad \frac{\partial u}{\partial n}=0, \quad x\in S_0, \quad 0\leqslant t\leqslant T. \tag{34}$$

Conditions (33) imply that $v(y,t)$ generates an incoming wave across the surface S_k (produced by sources in Ω_2). Conditions (34) imply that the surface S_0 is both a hard and soft surface, which in general are incompatible, unless $v\equiv 0$. This suggests that Eq. (26) is unique in the class of functions $\mathcal{M}$.

Once $\partial_n u$ is known on S_k, then $u(x,t)$ for $x\in S_k$ and $0\leqslant t\leqslant T-t_k-t_0$ can be obtained from the following:

$$u(x,t)=\int_0^t ds\int_{S_k} d\sigma_y\,\mathcal{E}_{\mathcal{N}}(x,y,t-s)\frac{\partial u(y,s)}{\partial n_y}-\int_0^t\int_{S_0} d\sigma_y\,\mathcal{E}_{\mathcal{N}}(x,y,t-s)\frac{\partial u(y,s)}{\partial n_y},$$
$$x\in S_k, \quad t_k\leqslant t\leqslant T-t_k-t_0, \tag{35}$$

which is derived from Eq. (21) by letting $x\in\Omega_1$ approach the surface S_k. As a result, $u(x,t)$ and $\partial_n u(x,t)$ on the surface S_k can be found from Eqs. (26) and (35).

IV. OUTGOING WAVE CONDITION AND DETERMINATION OF $\partial_n c$ ON S_k

Once the values of u and $\partial_n u$ (or at least the leading asymptotic short-time behavior) are known on S_k, the next step is to develop a condition that utilizes this information on S_k, to infer values of $c(x)$, in particular $\partial_n c$.

The leading asymptotic terms for u and $\partial_n u$ on S_k will be given as follows:

$$u(x,t)=H(t-t_k)[U_0(x)+(t-t_k)U_1(x)+\cdots], \quad x\in S_k, \tag{36}$$

$$\frac{\partial u(x,t)}{\partial n}=\delta(t-t_k)V_0(x)+H(t-t_k)[V_1(x)+\cdots], \quad x\in S_k, \tag{37}$$

where, as will be seen, $U_0(x)$ and $V_0(x)$ are not independent, since S_k is the wave front at time $t=t_k$. For the present purposes it will be assumed that $U_0(x)$, $U_1(x)$ and $V_1(x)$ are at least Hölder continuous, and $V_0(x)$ is a Hölder differentiable function of x on S_k.

It will be assumed that the surface is C^2. In particular, if x^1 is a point on the surface and (y_1,y_2,y_3) is a local Cartesian coordinate system centered at x^1 so that $x^1=(0,0,0)$, with the y_3 pointing into the domain Ω_2 in a direction normal to the surface at x^1, then the surface will be described locally by

$$y_3=a_1y_1^2+a_3y_2^2+\cdots, \tag{38}$$

where the y_1 and y_2 axes are along the directions of principal curvature.

Let $\mathcal{E}(x,y,t)$ be the fundamental solution of the wave equation for points $x,y\in\overline{\Omega}_2$. Hence if $x\in\Omega_2$, the solution $u(x,t)$ of the wave equation in Ω_2, which satisfies the initial condition $u(x,0)=u_t(x,0)=0$ in Ω_2, can be expressed in terms of the Dirichlet and Neumann data on S_k by the relation

$$u(x,t)=-\int_0^t\int_{S_k}\mathcal{E}(x,y,t-s)\frac{\partial u(y,s)}{\partial n_y}\mathrm{d}\sigma_y\,\mathrm{d}s+\int_0^t\int_{S_k}\frac{\partial\mathcal{E}(x,y,t-s)}{\partial n_y}u(y,s)\mathrm{d}\sigma_y\,\mathrm{d}s, \tag{39}$$

where the normal to S_k points into Ω_2.

Next, the resulting equation obtained from (39) when $x\in\Omega_2$ approaches a point x (say x^1) on S_k will be sought. Then, this will be used to obtain the relationship between the coefficients of the short-time behavior of u and $\partial_n u$ as expressed by Eqs. (36) and (37). This means that the short-time behavior of $\mathcal{E}(x,y,t)$ for a point x in Ω_2 close to or on S_k, and point a y on S_k close to x will be needed.

Since in the derivation of Eq. (39) only the domain Ω_2 (but not Ω_1) is involved, the value of $c(x)$ in Ω_1 is not specified and is free to be chosen. With this in mind, it will be assumed that in order to get the short-time behavior of $\mathcal{E}(x,y,t)$ with x close to $y\in S_k$, that $c(x)$ is defined to be locally extended into Ω_1 as a C^2 function.

The Green's function will take the form

$$\mathcal{E}(x,y,t)=\frac{\delta(t-\tau(x,y))}{\rho(x,y)}+p(x,y,t), \tag{40}$$

where $\tau(x,y)$ satisfies the Eikonal equation

$$|\nabla\tau(x,y)|^2=1/|c(x)|^2. \tag{41}$$

It can be shown that it has the form for small (x,y),

$$\tau(x,y)=\frac{|x-y|}{\sqrt{c(x)c(y)}}[1-q(x,y)+O(|x-y|)^3], \tag{42}$$

$$q(x,y)=-\frac{|x-y|^2}{12}\left(\frac{|\nabla c(x)|}{c(x)}\right)^2+\frac{1}{6}\sum_{j=k=1}^{3}(y_j-x_j)(y_k-x_k)\left(\frac{1}{c}\frac{\partial^2 c}{\partial x_j \partial x_k}\right). \tag{43}$$

The amplitude factor $(1/\rho)$ satisfies the transport equation

$$2\nabla\tau\cdot\nabla\rho-\rho\nabla^2\tau=0, \tag{44}$$

and is given for small $|x-y|$, by

$$\rho(x,y)=4\pi|x-y|[1+Q|x-y|^2+\cdots], \tag{45}$$

where Q, the term of order $|x-y|^2$ in expression (45), depends upon the first and second partial derivatives of $c(x)$, as well as the direction cosines of the vector $y-x$.

The second term in expression (40) satisfies the system

$$\frac{1}{c^2(y)}\frac{\partial^2 p}{\partial t^2}-\nabla^2 p=\delta(t-\tau(x,y))\nabla^2\left(\frac{1}{\rho}-\frac{1}{4\pi|x-y|}\right), \tag{46}$$

$$p(x,y,t)=0, \quad t<0. \tag{47}$$

Since the term in the Laplacian on the right-hand side of (46) behaves like

$$\left(\frac{1}{\rho}-\frac{1}{4\pi|x-y|}\right)\sim-\frac{1}{4\pi}Q|x-y|+\cdots, \tag{48}$$

for $|x-y|$ small, the Laplacian of this quantity has at most a singularity of order $|x-y|^{-1}$ as $y\to x$. From this it can be deduced that, besides vanishing for $t>\tau(x,y)$, $p(x,y,t)$ is bounded as y approaches x.

For y a point on S_k, it follows from (40) that

$$\frac{\partial\mathcal{E}(x,y,t)}{\partial n_y}=-\frac{\delta'(t-\tau(x,y))}{\rho(x,y)}\frac{\partial\tau(x,y)}{\partial n_y}-\frac{\delta(t-\tau(x,y))}{[\rho(x,y)]^2}\frac{\partial\rho(x,y)}{\partial n_y}+\frac{\partial p(x,y,t)}{\partial n_y}. \tag{49}$$

In terms of local coordinates centered at $x^1=(0,0,0)$ on S_k and with $x=(0,0,x_3)$ and $y=(y_1,y_2,y_3)$ a point on S_k where y_3 is given by Eq. (38), it can be shown that

$$\frac{1}{\rho(x,y)}\frac{\partial\tau(x,y)}{\partial n_y}\mathrm{d}\sigma_y=-\frac{\left[\Sigma_{j=1}^2 y_j^2\left(a_j+\frac{1}{2}\alpha_3\right)+x_3\left(1-\frac{1}{2}\Sigma_{j=1}^2\alpha_j y_j+\alpha_3 x_3\right)\right]}{4\pi c(x)[y_1^2+y_2^2+(x_3-a_1y_1^2-a_2y_2^2)^2]}\mathrm{d}y_1\mathrm{d}y_2, \tag{50}$$

where cubic and higher order terms are neglected in the numerator, and

$$\alpha_j=\frac{1}{c(x)}\frac{\partial c(x)}{\partial x_j}, \quad j=1,2,3. \tag{51}$$

Similarly it can be shown to the same order that

$$\frac{1}{[\rho(x,y)]^2}\frac{\partial\rho(x,y)}{\partial n_y}\mathrm{d}\sigma_y=-\frac{[a_1y_1^2+a_2y_2^2+x_3]\mathrm{d}y_1\mathrm{d}y_2}{4\pi[y_1^2+y_2^2+(x_3-a_1y_1^2-a_2y_2^2)^2]^{3/2}}. \tag{52}$$

One is now in a position to let x_3 approach zero, and thus obtain the equation corresponding to (39), when x is now on S_k. The approach that is employed is the usual procedure that is used

for a double layer potential.[16] Because of this, the only modification that is needed is due to the leading step function behavior of $u(x,t)$ when t approaches t_k, as is indicated by Eq. (36). The critical term in Eq. (39) is the integral

$$-\int_{S_k}\frac{u(x,t-\tau(x,y))}{[\rho(x,y)]^2}\frac{\partial\rho(x,y)}{\partial n_y}\mathrm{d}\sigma_y, \tag{53}$$

which arises when expression (49) is inserted into (39). In particular, the portion of $\partial_{n_y}\rho$ that is critical is the component in Eq. (52) involving x_3 in the numerator. One first integrates this portion over a small disk of radius ϵ and centered at (0,0) in the (y_1,y_2) plane, and then lets x_3 approach zero (through positive values). Finally the limit $\epsilon\to 0$ is taken. The integral under consideration is thus

$$x_3\int_0^{2\pi}\int_0^{\epsilon}\frac{H(t-t_k-\tau(x,y))U_0(y)}{4\pi(r^2+x_3^2)^{3/2}}r\,\mathrm{d}r\,\mathrm{d}\theta, \tag{54}$$

where the leading term of $u(y,t)$ is taken, and polar coordinates (r,θ)

$$y_1=r\cos\theta,\quad y_2=r\sin\theta, \tag{55}$$

are introduced. One needs to consider the integral (54) in the time interval $0<c(x)(t-t_k)\leqslant\epsilon$. With $\tau(x,y)$ given approximately by $\sqrt{r^2+x_3^2}/c(x)$, $U_0(y)H(t-t_k-\tau(x,y))$ is expanded about the point $x^1=(0,0,0)$ as follows:

$$[H(t-t_k-\tau(x,y))-H(t-t_k)]U_0(x^1)+H(t-t_k-\tau(x,y))[U_0(y)-U_0(x^1)]+H(t-t_k)U_0(x^1). \tag{56}$$

Since $U_0(y)$ is differentiable $|U_0(y)-U_0(x^1)|\leqslant$ constant $\cdot r$, so that the second term in (56) poses no problem. The last term in (56) inserted into (54) yields, on letting $x_3\to 0$,

$$\int_0^{2\pi}\int_0^{\epsilon}\frac{x_3H(t-t_k)U_0(x^1)}{4\pi(r^2+x_3^2)^{3/2}}r\,\mathrm{d}r\,\mathrm{d}\theta=\frac{H(t-t_k)U_0(x^1)}{2}\left[1-\frac{x_3}{\sqrt{\epsilon^2+x_3^2}}\right]\to\frac{1}{2}H(t-t_k)U_0(x^1), \tag{57}$$

as is expected. Insertion of the first term of (56) into (54) yields the limit, as $x_3\to 0$,

$$-\frac{1}{4\pi}\int_0^{2\pi}\int_{r_0}^{\epsilon}\frac{x_3U_0(x^1)}{(r^2+x_3^2)^{3/2}}r\,\mathrm{d}r\,\mathrm{d}\theta\to 0,\quad 0<c(x)(t-t_k)\leqslant\epsilon, \tag{58}$$

where $r_0^2+x_3^2=(t-t_k)^2c^2(x)$ and the approximation $\tau(x,y)=(r^2+x_3^2)^{1/2}/c(x)$ is used.

Thus one obtains the usual result as $x\in\Omega_2\to x^1$ on S_k, namely that the limit of expression (53) as $x\to x^1$ is given by

$$\frac{1}{2}u(x^1,t)-\int_{S_k}\frac{u(y,t-\tau(x^1,y))}{[\rho(x^1,y)]^2}\frac{\partial\rho(x^1,y)}{\partial n_y}\mathrm{d}y,\quad t>t_k. \tag{59}$$

Henceforth the superscript one for x on S_k will be dropped. The resulting equation corresponding to Eq. (39) when $x\in S_k$ is

$$u(x,t)=-2\int_0^t\int_{S_k}\mathcal{E}(x,y,t-s)\frac{\partial u(y,s)}{\partial n_y}\mathrm{d}\sigma_y\,\mathrm{d}s+2\int_0^t\int_{S_k}\frac{\partial\mathcal{E}(x,y,t-s)}{\partial n_y}u(y,s)\mathrm{d}\sigma_y\,\mathrm{d}s \tag{60}$$

for $t>t_k$. When $t<t_k$, both sides are zero. When both $u(x,t)$ and $\partial_n u(x,t)$ are known on S_k for $t_k \leqslant t \leqslant T-t_k-t_0$, Eq. (60) constitutes a nonlinear equation to determine $c(x)$ in Ω_2. A numerical method could be used to solve this nonlinear equation for $c(x)$.

As an example of how Eq. (60) can be used to determine the normal derivative of $c(x)$, we will use an asymptotic expansion approach here. We assume that $c(x)$ has sufficient smoothness in a small neighborhood of the boundary, such that the asymptotic expansion of the Green's function in the form (40) is valid. We notice that Eq. (60) only uses the exterior values of the Green's function, and hence is independent of the velocity in the interior region Ω_1, and hence we can assume that $c(x)$ is sufficiently smooth over the boundary. We assume that only the leading coefficients, U_0, U_1, V_0, and V_1 of $u(x,t)$ and $\partial_n u(x,t)$ [as given by Eqs. (36) and (37)] are known.

Let x be the point $(0,0,0)$ on S_k and y the point $(r\cos\theta, r\sin\theta, r^2(a_1\cos^2\theta + a_2\cos^2\theta)+\cdots)$ on S_k, where the polar coordinates Eq. (55) are used. It then follows from Eqs. (42), (45), (50), and (51) with $x_3=0$, that

$$c(x)\tau(x,y) = r\left[1 - \frac{r}{2}(\alpha_1\cos\theta + \alpha_2\sin\theta)+\cdots\right], \tag{61}$$

$$\frac{1}{\rho(x,y)}\,d\sigma_y = \frac{1}{4\pi}[1+O(r^2)]\,dr\,d\theta, \tag{62}$$

$$\frac{1}{\left(\dfrac{\partial\tau}{\partial\rho}\right)} = c(x)[1 + r(\alpha_1\cos\theta + \alpha_2\sin\theta)+\cdots], \tag{63}$$

$$\frac{1}{\rho(x,y)}\,\frac{\partial\tau(x,y)}{\partial n_y}\,d\sigma_y = -\frac{[(a_1+\frac{1}{2}\alpha_3)\cos^2\theta + (a_2+\frac{1}{2}\alpha_3)\sin^2\theta]r\,dr\,d\theta}{4\pi c(x)}, \tag{64}$$

$$\frac{1}{[\rho(x,y)]^2}\,\frac{\partial\rho(x,y)}{\partial n_y}\,d\sigma_y = -\frac{1}{4\pi}(a_1\cos^2\theta + a_2\sin^2\theta)\,dr\,d\theta\,. \tag{65}$$

To obtain the asymptotic results the following result,

$$\begin{aligned}\int_0^\infty \delta(t-\tau(x,y))r^n dr &= H(t)\left(r^n\left(\frac{\partial\tau}{\partial r}\right)^{-1}_{\tau=t}\right)\\ &= c(x)H(t)[c(x)t]^n\left[1+\left(\frac{n}{2}+1\right)c(x)t(\alpha_1\cos\theta+\alpha_2\sin\theta)+O(t^2)\right],\end{aligned} \tag{66}$$

will be used.

The leading asymptotic form (for small $t-t_k$) of the integral

$$-2\int_0^t\int_{S_k}\mathcal{E}(x,y,t-s)\,\frac{\partial u(y,s)}{\partial n_y}\,d\sigma_y\,ds \tag{67}$$

is obtained by replacing $\partial_n u$ in Eq. (67) by the asymptotic expression (for small $s-t_k$)

$$\frac{\partial u(y,s)}{\partial n_y} = \delta(s-t_k)\left[V_0(x) + r\left(\frac{\partial V_0}{\partial x_1}\cos\theta + \frac{\partial V_0}{\partial x_2}\sin\theta\right)+O(r^2)\right] + H(s-t_k)[V_1(x)+\cdots, \tag{68}$$

and neglecting the contribution to $\mathcal{E}(x,y,t-s)$ of $p(x,y,t-s)$ which, since it is bounded and vanishes for $t-s<\tau(x,y)$, produces a term of $O(t-t_k)^2$ in the resulting expression for the integral (67). Thus the leading terms of the integral (67) is given by

$$-\frac{1}{2\pi}\int_0^t\int_0^{2\pi}\int_0^\infty \delta(t-s-\tau(x,y))\,\delta(s-t_k)\left[V_0(x)+r\left(\frac{\partial V_0}{\partial x_1}\cos\theta+\frac{\partial V_0}{\partial x_2}\cos\theta\right)+\cdots\right] r\,dr\,d\theta\,ds$$

$$-\frac{1}{2\pi}\int_0^t\int_0^{2\pi}\int_0^\infty \delta(t-s-\tau(x,y))H(s-t_k)[V_1(x)+\cdots]\,dr\,d\theta\,ds. \tag{69}$$

This can be evaluated using (66), to give

$$-c(x)H(t-t_k)[V_0(x)+(t-t_k)V_1(x)+O(t-t_k)^2]. \tag{70}$$

The second integral on the right-hand side of Eq. (60) [on using Eq. (49)] has the explicit form

$$-2\frac{\partial}{\partial t}\int_0^t\int_{S_k}\frac{\delta(t-s-\tau(x,y)}{\rho(x,y)}\frac{\partial\tau}{\partial n_y}(x,y)u(y,s)\,d\sigma_y\,ds$$

$$-2\int_0^t\int_{S_k}\left\{\frac{\delta(t-s-\tau(x,y))}{[\rho(x,y)]^2}\frac{\partial\rho(x,y)}{\partial n_y}-\frac{\partial p(x,y,t-s)}{\partial n_y}\right\}u(y,s)\,d\sigma_y\,ds\,. \tag{71}$$

Replacing $u(y,s)$ by $H(s-t_k)[U_0(x)+O(s-t_k)]$ the leading terms of expression (71) are given by

$$\frac{1}{2\pi c(x)}\frac{\partial}{\partial t}\int_{t_k}^t\int_0^{2\pi}\int_0^\infty \delta(t-s-\tau(x,y))\left[\left(a_1+\frac{1}{2}\alpha_3\right)\cos^2\theta+\left(a_2+\frac{1}{2}\alpha_3\right)\sin^2\theta\right]U_0(x)r\,dr\,d\theta\,ds$$

$$+\frac{1}{2\pi}\int_{t_k}^t\int_0^{2\pi}\int_0^\infty \delta(t-s-\tau(x,y))[a_1\cos^2\theta+a_2\sin^2\theta]U_0(x)\,dr\,d\theta\,ds$$

which, on using relation (66), reduces to

$$\frac{c(x)}{4}\frac{\partial}{\partial t}\{H(t-t_k)(t-t_k)^2[U_0(x)(a_1+a_2+\alpha_3)+O(t-t_k)^3]\}$$

$$+\frac{1}{2}c(x)H(t-t_k)[(t-t_k)U_0(x)(a_1+a_2)+O(t-t_k)^2]$$

$$=H(t-t_k)\left[(t-t_k)c(x)\left(a_1+a_2+\frac{1}{2}\alpha_3\right)U_0(x)+O(t-t_k)^2\right]. \tag{72}$$

Thus inserting the results of Eqs. (70) and (72) into the right-hand side of Eq. (60) and Eq. (36) into the left-hand side of Eq. (60), one has the following asymptotic result:

$$H(t-t_k)[U_0(x)+(t-t_k)U_1(x)+\cdots]=-H(t-t_k)[c(x)V_0(x)+(t-t_k)c(x)(V_1(x)$$

$$-(a_1+a_2+\tfrac{1}{2}\alpha_3)U_0(x))]. \tag{73}$$

Equating coefficients of $t-t_k$, one obtains

$$U_0(x)=-c(x)V_0(x), \tag{74}$$

which is to be expected since S_k is a wave front at $t=t_k$. Equating the coefficients of $(t-t_k)H(t-t_k)$ one obtains

$$U_1(x) = -c(x)[V_1(x) - (a_1 + a_2 + \tfrac{1}{2}\alpha_3)U_0(x)], \tag{75}$$

where $U_1(x)$, $U_0(x)$, $V_1(x)$, $c(x)$, a_1, and a_2 are known at the point x on S_k. Since

$$\alpha_3 = \lim_{x \in \Omega_2 \to x \in S_k} \frac{1}{c(x)} \frac{\partial c}{\partial x_3}, \tag{76}$$

it follows that from Eq. (75) one can determine

$$\lim_{x \in \Omega_2 \to x \in S_k} \frac{\partial c}{\partial n}, \tag{77}$$

at the point x on S_k. In the practical use of layer stripping one assumes that $c(x)$, $\partial_n c$ are known at the bottom of each layer and using a model of $c(x)$ which is linear in the direction normal to the bottom surface, one uses the results of condition (75) to determine $\partial_n c$ at the bottom of the next layer [i.e., $c(x)$ is piecewise differentiable in the direction normal to the wave front].

The process is strongly dependent on good estimates of the wave front surfaces S_k, $k = 1,2,\ldots$, which depend upon the value of c, $\partial_n c$ on each surface S_{k-1}. However one can use an iterative Newton process to improve the value of c, $\partial_n c$ on S_k by using both the values of c, $\partial_n c$ on S_{k-1} and the derived values of c, $\partial_n c$ on S_k.

V. EFFECT OF CAUSTICS

The procedure developed in the previous sections has to be modified considerably when caustics appear. The approach in these sections stresses the formulation of the problem primarily in terms of wave fronts at the expense of the rays. However when rays intersect to form caustics, the rays must be emphazised instead of the wave fronts. Thus one has to use the Hamilton–Jacobi system for the bicharacteristics [the rays being the projection onto $x = (x_1, x_2, x_3)$] given as follows:

$$\frac{\partial x_j}{\partial s} = p_j, \quad \frac{\partial p_j}{\partial s} = \frac{1}{c} \frac{\partial c^{-1}}{\partial x_j}, \quad j = 1,2,3, \tag{78}$$

where the ray parameter s is related to the travel time parameter τ by the relation

$$c^2 \, \mathrm{d}\tau = \mathrm{d}s. \tag{79}$$

Even though global ray coordinates (s, θ, ϕ) can be used to specify points on the rays, also at caustics and beyond, the local coordinates (x_1, x_2, x_3) cannot be used to specify the rays at caustics and instead one must use one of the sets (x_i, x_j, p_k), (x_i, p_j, p_k), or (p_1, p_2, p_3), where i, j, k are distinct numbers belonging to the set 1,2,3, choosing the set of local coordinates that yield a unique point for the rays. This choice depends upon the local structure of the caustics. Thus, at a caustic and beyond, one cannot use the asymptotic formulation (36) of the wave equation that was used in Sec. IV. In addition, once the initial wave front has passed through the caustic one may end up with multiple wave fronts. This means that the simple formulation of global nested wave front layers cannot be used at caustics and beyond and has to be modified.

Because the procedure in Sec. IV involves local analysis in time and space, the basic idea behind the method used in Sec. IV to determine the value of the normal derivative of c, namely $\partial_n c$, on a local portion of an adjacent wave front surface, can still be employed. A possible approach is to use the Maslov Lagrangian formulation,[17,18] to determine the asymptotic nature of the field in a neighborhood of the caustic. To get the short-time behavior of the field, one could take the Fourier transform with respect to the time variable, (mapping the t-line into the ω-line) and on setting

$$k=\omega/c_0, \quad \frac{\omega^2}{c^2}=k^2\epsilon(x), \tag{80}$$

reducing the wave equation to the form

$$\nabla^2 u+k^2\epsilon(x)u=0. \tag{81}$$

Then one can look for asymptotic solutions of Eq. (81) for large ω or k, using the Maslov precanonical operator K. In the neighborhood of a caustic point, taken as origin, the asymptotic form of the solution $u(x,k)$ of Eq. (81) will have the various forms

$$u(x,k)=\int_{\mathbb{R}}\phi(x_2,x_3,p_1)e^{ik(\pm p_1^3-x_1p_1)}\mathrm{d}p_1,$$

$$u(x,k)=\int_{\mathbb{R}}\phi(x_2,x_3,p_1)e^{ik(\pm p_1^4+x_2p_1^2-x_1p_1)}\mathrm{d}p_1,$$

$$u(x,k)=\int_{\mathbb{R}}\phi(x_2,x_3,p_1)e^{ik(\pm p_1^5+x_3p_1^3+x_2p_1^2-x_1p_1)}\mathrm{d}p_1,$$

$$u(x,k)=\int_{\mathbb{R}^2}\phi(x_3,p_1,p_2)e^{ik(\pm p_1^2p_2\pm p_2^3+x_3p_2^2-x_2p_2-x_1p_1)}\mathrm{d}p_1\,\mathrm{d}p_2,$$

the choice of which depends upon which local coordinate system that can be used to specify the rays in the neighborhood of the caustic. By Fourier transforming back to the time domain and using the result that the near wave front time behavior t can be obtained from the asymptotic behavior for large ω or k, one can obtain the proper local small time asymptotic behavior of the wave field $u(x,t)$ that can be used in Eq. (60) of Sec. IV. As can be seen there will be a considerable amount of analysis to estimate the integrals in these expressions. The details and hard analysis will be pursued in future work.

VI. SUMMARY

It has been demonstrated in the inverse problem that one can do layer stripping following the wave front until caustics appear, without resorting to wave splitting. The procedure for obtaining the values of u and $\partial_n u$ on the surface S_k (wave front at time $t=t_k$) from knowledge of the corresponding values on the surface S_{k-1} (wave front at time $t=t_{k-1}$), has been examined from a theoretical viewpoint in Sec. III, in order to determine what limitations there are. In order to investigate how far into the interior of the scattering object one can determine $c(x)$ when the initial data were measured on the surface S_0 for a restricted time T, the actual analysis was performed for the region S_0 and S_k instead of the curvilinear slab between S_{k-1} and S_k. By using the value of c and $\partial_n c$ on the bottom surface S_{k-1} of the curvilinear slab, one can obtain an estimate for the value of $c(x)$ for the top surface S_k of the curvilinear slab. Then the results of Sec. IV can be used to obtain the value of $\partial_n c$ on the top surface S_k.

In Sec. V an approach is briefly outlined as how to extend the method to the region in and beyond a neighborhood of a caustic. This will require future work to pursue.

One of the advantages of wave-front layer stripping as opposed to planar wave stripping is that it is a more natural numerical procedure in that rays are used to follow the propagation of singularities (the wave front). Also the procedure to determine the normal derivative of c from the asymptotic short-time behavior of the field quantities on an adjacent wave front surface is much simpler.

The procedure to determine u and $\partial_n u$ on the top surface S_k from the data on the bottom surfaces S_{k-1} of the curvilinear slabs needs to be examined further to develop a better numerical

approach to the problem. First, Eqs. (26) and (25) must be modified by taking as the spatial domain of the second integrals, the surface S_{k-1} (instead of S_0) and by replacing t_0 by t_{k-1} in the corresponding time intervals. In addition x in Eq. (26) must lie on S_{k-1} (instead of S_0). The normal derivative of the Green's function $\partial_n \mathcal{E}$ vanishes on S_k and S_{k-1}. [Note that the latter condition can be relaxed by requiring that the normal derivative only vanishes on S_k. In this case, Eqs. (26) and (25) would have to be modified accordingly.] Since the equation corresponding to Eq. (26) is an integral equation of the first kind for the unknown $\partial_n u$, it should be replaced by a regularized version for numerical stability.

As a first step in determining u and $\partial_n u$ on the surface S_k from knowledge of their values on the surface S_{k-1}, together with knowledge of $c(x)$ between the two surfaces S_k and S_{k-1}, it should be noted that their leading terms U_0 and V_0 in expansions (36) and (37) are immediately obtained through ray theory.

In order to determine the remaining portions of the unknowns u and $\partial_n u$ on S_k, it should be noted that the layer between the surfaces S_k and S_{k-1} is very thin, and this allows some approximations to be made to simplify the calculations. For a short-time interval beginning with time t_k (the time the wave front inpinges on the surface S_k), a local parallel plane approximation to the domain between the two surfaces, and hence, a local expansion for the Green's function can be used. (An even simpler representation is achieved if one uses the formulation where the normal derivative of the Green's function vanishes on S_k only, as mentioned previously). It may be possible to extend the results for a longer time interval by including the local curvature of the surfaces.

Even for times much greater than t_k the local approximation may give a good approximation to u and $\partial_n u$ at a point x on S_k, provided that the values of the data u and $\partial_n u$ on S_{k-1} are not too small in a small neighborhood of x, and at the same time their values outside the neighborhood are not too large. All this has to be quantized by the appropiate analysis. For cases where this approach is invalid, other methods have to be investigated and employed.

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Direct calculation of thermodynamic quantities for the Heisenberg model

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The XXX Heisenberg model is studied at finite temperature. The free energy is derived without recourse to thermal Bethe ansatz method and quantum transfer matrix method. The result perfectly agrees with the free energy derived by thermal Bethe ansatz method. An explicit expression of the cluster expansion coefficient in arbitrary order is presented for the first time. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1501444]

I. INTRODUCTION

In a pioneer work,[1] Bethe solved the XXX Heisenberg model. The Hamiltonian of the model is written as

$$H(J,h)=-J\sum_{j=1}^{N}(S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+S_j^zS_{j+1}^z)+2h\sum_{j=1}^{N}S_j^x+\text{constant}, \tag{1.1}$$

where J is the coupling constant and h is the external field. The energy of the system is given by

$$E_M=2hM+\sum_{j=1}^{M}\frac{2J}{x_j^2+1}, \tag{1.2}$$

where M is the number of up-spins and the variables x_j are required to satisfy the Bethe ansatz (BA) equation,

$$\left(\frac{x_j+i}{x_j-i}\right)^N=\prod_{j'\neq j}\frac{x_j-x_{j'}+2i}{x_j-x_{j'}-2i}. \tag{1.3}$$

It was shown[1] that every eigenstate of this model corresponds to a solution of this simultaneous equation.

The XXX Heisenberg model is the quantum integrable system. The thermal Bethe ansatz method (TBA)[2] and quantum transfer matrix method (QTM)[3–7] are the well-known methods to derive thermodynamic quantities for quantum integrable systems. TBA was originated by Yang and Yang,[2] who derived the thermodynamics of repulsive δ-function Bose gas system. Then, on the assumption of the so-called string hypothesis, Takahashi[8] applied TBA to the Heisenberg model. Recently, some analytical results of thermodynamic quantities using QTM were presented by Klümper.[9,10] Many pieces of the concept with respect to QTM had been introduced before then. The equivalence of the results using TBA and QTM was proved by several researchers.[9,11–13]

Our purpose is to derive the free energy of this system independent of TBA and QTM. In this paper, we use a method which we call a direct method. We start from the string hypothesis. There are no other mathematical assumptions except for the string hypothesis. In other words, using the

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direct method, a problem based on the string hypothesis is solved. On the other hand, TBA is a method to solve the problem using a definition of nonequilibrium state entropy. As a main result of this paper, the direct method justifies TBA.

The direct method was used for the δ-function Bose system.[14–17] We apply the method to the Heisenberg model here. We define z and β as $z \equiv e^{-2\beta h}$ and $\beta \equiv 1/k_B T$. The direct method enables us to express the cluster expansion coefficients b_n in arbitrary order explicitly,

$$\log[z^{N/2}\mathrm{Tr}\, e^{-\beta H(J,h)}] \equiv \sum_{n=1}^{\infty} b_n z^n, \tag{1.4}$$

and, the free energy,

$$\frac{1}{N}\log[\mathrm{Tr}\, e^{-\beta H(J,h)}], \tag{1.5}$$

by use of a function which is a solution of a nonlinear integral equation. Thus, we can show that the expression of the free energy perfectly agrees with the results of TBA.[11]

The outline of this paper is the following. In Sec. II, we derive an explicit expression of cluster expansion coefficients in all orders. In Sec. III, we prove that the free energy can be expressed in terms of a solution of a nonlinear integral equation. Section IV is devoted to the concluding remarks. Technical details of calculations are summarized in Appendices A–H.

II. THE CLUSTER EXPANSION

The string hypothesis is formulated as follows. In the thermodynamic limit, the energy of the Heisenberg model (1.1) can be written as

$$E_M(J,h) = 2hM + \sum_{n,\alpha} \frac{2Jn}{(x_\alpha^n)^2 + n^2}. \tag{2.1}$$

Here, the variables x_α^n are determined by

$$\left(\frac{x_\alpha^n + ni}{x_\alpha^n - ni}\right)^N = \prod_{(m,\beta)\neq(n,\alpha)} E_{nm}(x_\alpha^n - x_\beta^m), \tag{2.2}$$

where

$$E_{nm}(x) = \frac{(x-(n+m)i)(x-|n-m|i)}{(x+(n+m)i)(x+|n-m|i)} \prod_{l=0}^{\min(n,m)} \left(\frac{x+(n+m-2l)i}{x-(n+m-2l)i}\right)^2. \tag{2.3}$$

Equation (2.2) is referred to as string center equation. Every eigenstate corresponds to a solution of these simultaneous equations. Taking a logarithm of both sides of (2.2), we obtain

$$2N\tan^{-1}\left(\frac{x_\alpha^n}{n}\right) = 2\pi I_\alpha^n + \sum_{(m,\beta)\neq(n,\alpha)} \Delta_{n,m}(x_\alpha^n - x_\beta^m), \tag{2.4}$$

where

$$\Delta_{n,m}(x) = -2\tan^{-1}\left(\frac{x}{n+m}\right) - 2(1+\delta_{nm})\tan^{-1}\left(\frac{x}{|n-m|}\right) + \sum_{l=0}^{\min(n,m)} 4\tan^{-1}\left(\frac{x}{n+m-2l}\right). \tag{2.5}$$

From now on, we call (2.4) modified Bethe ansatz (mBA) equation.

The string hypothesis indicates that the partition function is a sum of the Boltzmann weights with respect to integers (or half integers) $\{I_\alpha^n\}$ which define the energy of the system,

$$z^{N/2}\mathrm{Tr}\, e^{-\beta H(J,h)}=\sum_M \sum_{\{I_\alpha^n\}} e^{-\beta E_M(J,h)}. \tag{2.6}$$

When we take the thermodynamic limit, we can replace the summations over discrete variables by integral,

$$\sum_M \int e^{-\beta E_M(J,h)} \prod dI_\alpha^n. \tag{2.7}$$

There are some points which we have to consider carefully. The Fermi statistics must be taken into account in this integral. In this case, the exclusion property leads to the conditions that $x_\alpha^n \neq x_\beta^n$ and that a state specified by $\{x_\alpha^n\}$ and a state specified by $\{x_\alpha'^n\}$ which satisfies $x_\alpha'^n = x_{p(\alpha)}^n$ are the same, where p is a permutation.

To express a concrete form of (2.7), we prepare three symbols.

Definition 1: N_A denotes the number of elements in a set A.

Definition 2: $\Theta(A)$ denotes all the patterns of division of a set A. A pattern of division is represented as a set having elements each of which is a cluster. The cluster is one of the pieces into which a set A is divided, and the cluster is regarded as a set. For example, for $A=\{a,b,c\}$, $\Theta(A)$ means

$$\Theta(\{a,b,c\})=\{\{a\},\{b\},\{c\}\},\{\{a\},\{b,c\}\},$$
$$\{\{b\},\{c,a\}\},\{\{c\},\{a,b\}\},\{\{a,b,c\}\}. \tag{2.8}$$

On condition that the domain of $\Theta(n)$ is the natural number, $n\in\mathbb{N}$, $\Theta(n)$ is interpreted as $\Theta(\{1,2,...,n\})$.

Definition 3: $\overline{\Theta}(B)$ denotes all the patterns of division of a set B, when each element of B is a set and each pattern of division satisfies the following condition—all the sets which are included in each cluster have the same number of elements. For example, we can show for $\sigma_1=\{a,b\}$, $\sigma_2=\{c\}$, $\sigma_3=\{d\}$,

$$\overline{\Theta}(\{\sigma_1,\sigma_2,\sigma_3\})=\{\{\sigma_1\},\{\sigma_2\},\{\sigma_3\}\},\{\{\sigma_1\},\{\sigma_2,\sigma_3\}\}. \tag{2.9}$$

Using the above given symbols, the integral (2.7) can be written explicitly in the following form:

$$z^{N/2}\mathrm{Tr}\, e^{-\beta H(J,h)}=1+\sum_{n=1}^{\infty}\frac{z^n}{n!}\sum_{\theta\in\Theta(n)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\overline{\Theta}(\theta)}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}(N_{\theta'}-1)!\right]$$
$$\times\int\left|\frac{\partial I}{\partial x}\right|_{N,\zeta} e^{-\beta E(\zeta)}\prod_{\theta'\in\zeta}\mathrm{d}x_{\theta'}. \tag{2.10}$$

We explain functions, $|\partial I/\partial x|_{N,\zeta}$ and $E(\zeta)$ used in this equation, where $\zeta\in\overline{\Theta}(\theta)$ and $\theta\in\Theta(n)$. The Jacobian $|\partial I/\partial x|_{N,\zeta}$ is constructed as follows. First, we consider θ uniquely determined by the condition $\zeta\in\overline{\Theta}(\theta)$. Second, we make correspondence between each element σ of θ and two suffixes (n,α) for the variables I_α^n and x_α^n introduced in the string hypothesis. In this case, the condition $N_\sigma=n$ is required. Third, we consider the mBA equation for the variables $\{I_\alpha^n\}$, $\{x_\alpha^n\}$, which are constructed out of θ. Fourth, we introduce $x_{\theta'}$, $I_{\theta'}$, where θ' is an element of ζ. Here, we have constraining conditions; $x_{\theta'}=x_\alpha^n$ and $I_{\theta'}=I_\alpha^n$, where (n,α) corresponds to $\sigma\in\theta'$. Finally, $|\partial I/\partial x|_{N,\zeta}$ is the Jacobian between $\{x_{\theta'}\}$ and $\{I_{\theta'}\}$ which satisfy, respectively, the mBA

equation made from θ and the constraining conditions made from ζ. Explicit expression of such Jacobian matrix is given in Eq. (A1). We show the above-given procedure by an example. For the case,

$$\zeta=\{\theta_1,\theta_2\},\quad \theta_1=\{\{1,2\}\},\quad \theta_2=\{\{3\},\{4\}\},\tag{2.11}$$

we have

$$\theta=\{\{1,2\},\{3\},\{4\}\},\quad \zeta\in\overline{\Theta}(\theta),$$

$$2N\tan^{-1}\left(\frac{x_{\theta_1}}{2}\right)=2\pi I_{\theta_1}+2\Delta_{2,1}(x_{\theta_1}-x_{\theta_2}),$$

$$2N\tan^{-1}(x_{\theta_2})=2\pi I_{\theta_2}+\Delta_{1,2}(x_{\theta_2}-x_{\theta_1}),$$

$$\begin{aligned}(2\pi)^2\left|\frac{\partial I}{\partial x}\right|_{N,\zeta}=&\frac{4N}{x_{\theta_1}^2+4}\,\frac{2N}{x_{\theta_2}^2+1}-\frac{4N}{x_{\theta_1}^2+4}\left(\frac{2}{(x_{\theta_1}-x_{\theta_2})^2+1}+\frac{6}{(x_{\theta_1}-x_{\theta_2})^2+9}\right)\\&-2\,\frac{2N}{x_{\theta_2}^2+1}\left(\frac{2}{(x_{\theta_2}-x_{\theta_1})^2+1}+\frac{6}{(x_{\theta_2}-x_{\theta_1})^2+9}\right).\end{aligned}\tag{2.12}$$

The energy $E(\zeta)$ is expressed in terms of $\{x_\alpha^n\}$ made from θ,

$$E(\zeta)=\sum_{n,\alpha}\frac{2Jn}{(x_\alpha^n)^2+n^2}.\tag{2.13}$$

For the case (2.11), $E(\zeta)$ is given by

$$E(\zeta)=\frac{2J\times 2}{x_{\theta_1}^2+4}+2\,\frac{2J}{x_{\theta_2}^2+1}.\tag{2.14}$$

Note that the constraining conditions made from ζ have been used.

Now, we show how (2.10) is derived. We notice two important facts. One is that we must exclude unphysical states from the sum, when the sum is represented as the integral in (2.7). The unphysical state means the state corresponding to $\{x_\alpha^n\}$ where some two elements of $\{x_\alpha^n\}$ coincide, $x_\alpha^n=x_\beta^n$. Those states should be excluded because the norm of the state constructed out of $\{x_\alpha^n\}$ satisfying such a condition is zero. In Eq. (2.10),

$$\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}(N_{\theta'}-1)!\tag{2.15}$$

are factors which exclude the unphysical states. In expression (2.10), we add unphysical states in some terms of series and subtract them in some other terms. Then, the sum of positive terms and negative terms is zero with respect to unphysical states. This mathematical manipulation enables us to write the free energy explicitly like (2.10). Let us explain this manipulation for the case of ζ in (2.11) in detail. The states corresponding to ζ in (2.11) are unphysical states. We define $\zeta'=\{\{1,2\}\},\{\{3\}\},\{\{4\}\}$. ζ' corresponds to the results of a string center equation (2.2) which defines one two-string $x_{1,2}$ and two one-strings x_3 x_4. On the other hand, $\zeta=\{\{1,2\}\},\{\{3\},\{4\}\}$ in (2.11) corresponds to the results of the string center equation which satisfy $x_3=x_4$. Therefore, the results corresponding to ζ are part of the results corresponding to ζ'. Here, in the sum with respect to elements in $\overline{\Theta}$ (2.10), both ζ and ζ' are summed up. And, the sum of coordinates (2.15) of terms corresponding to both ζ and ζ' is zero. Therefore, unphysical states corresponding to ζ do not affect the sum in (2.10). The other important fact is that we must divide the sum by the number of

the symmetry. Here, the symmetry means that when $\{x_\alpha^n\}$ is a solution of the mBA equation, $\{x_\alpha'^n\}$ which satisfies the relation $x_\alpha'^n = x_{p(\alpha)}^n$ is also a solution of the mBA equation. In this case, it is necessary to divide the sum by the number of the symmetry because $\{x_\alpha^n\}$ and $\{x_\alpha'^n\}$ correspond to the same state. In Eq. (2.10),

$$\left[\prod_{\sigma\in\theta} N_\sigma!\right] \Big/ n! \tag{2.16}$$

is a factor for the correction of the sum which takes such symmetry into account.

We have met similar correction factors in the analysis of the δ-function Bose gas system. The reason for the appearance of the correction factors is common. A detailed proof for the δ-function bose gas system case is given in Sec. 3.1 of Ref. 15.

In order to express the Jacobian $|\partial I/\partial x|_{N,\zeta}$ explicitly, we further define three symbols.

Definition 4: M_B denotes a number of elements in one of the sets. Here, all the elements of a set B are sets, and all sets in B have the same number of elements. Then, M_B is defined as the number of elements in one of the sets,

$$M_\theta = N_\sigma, \tag{2.17}$$

where $\sigma\in\theta\in\zeta\in\overline{\Theta}(\theta')$ and $\theta'\in\Theta(n)$.

Definition 5: $\Lambda(A)$ denotes all the patterns of connection of a set A. Here, what we call a pattern of connection satisfies the following two conditions. (1) Any two elements of A are connected or not. In other words, there is no multiple connection. (2) There is no closed path in the connections. Then, a pattern of connection is represented as a set of elements each of which corresponds to a connection. Here, an element corresponding to a connection is a set which consists of two elements connected by the connection. For example, we have

$$\begin{aligned}\Lambda(\{a,b,c\}) = \varnothing, &\{\{b,c\}\},\{\{c,a\}\},\{\{a,b\}\},\\ &\{\{a,b\},\{a,c\}\},\{\{b,a\},\{b,c\}\},\{\{c,a\},\{c,b\}\}.\end{aligned} \tag{2.18}$$

Definition 6: $G([\lambda,A])$ is an element of $\Theta(A)$, where $\lambda\in\Lambda(A)$. In other words, $G([\lambda,A])$ is a pattern of division of A. The pattern of division θ satisfies the following conditions; (1) any two connected elements are in the same set in θ, and (2) elements of θ are larger in number than elements of any other $\theta'\in\Theta(A)$ satisfying (1). For example, we can show that

$$G([\{\{a,b\}\},\{a,b,c\}]) = \{\{a,b\},\{c\}\}. \tag{2.19}$$

By use of the above three symbols, the Jacobian can be expressed as

$$\begin{aligned}(2\pi)^{N_\zeta}\left|\frac{\partial I}{\partial x}\right|_{N,\zeta} = &\left[\prod_{\theta\in\zeta} N_\theta\right]^{-1} \sum_{\lambda\in\Lambda(\zeta)} \left[\prod_{\{\theta,\theta'\}\in\lambda} -N_\theta N_{\theta'} K_{M_\theta,M_{\theta'}}(x_\theta - x_{\theta'})\right]\\ &\times \prod_{\zeta'\in G([\lambda,\zeta])} \left[\sum_{\theta\in\zeta'} \frac{2N_\theta M_\theta N}{M_\theta^2 + x_\theta^2}\right],\end{aligned} \tag{2.20}$$

where $K_{n,m}(x) \equiv \mathrm{d}\Delta_{n,m}(x)/\mathrm{d}x$. A proof of Eq. (2.20) is given in Appendix A.

At last, we show the explicit expression of the cluster expansion. Taking a logarithm of both sides of (2.10) and rewriting the right-hand side, we get

$$\log[z^{N/2}\mathrm{Tr}\,e^{-\beta H(J,h)}]=\sum_{n=1}^{\infty}\frac{z^n}{n!}\sum_{\theta\in\Theta(n)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\Theta(\theta)}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}(N_{\theta'}-1)!\right]$$
$$\times\int\left|\frac{\partial I}{\partial x}\right|_{cN,\zeta}e^{-\beta E(\zeta)}\prod_{\theta'\in\zeta}\mathrm{d}x_{\theta'}. \tag{2.21}$$

A proof is given in Appendix B. Here, $|\partial I/\partial x|_{cN,\zeta}$ is the first-order term of $|\partial I/\partial x|_{N,\zeta}$ regarded as a polynomial with respect to the number of spins, N. From expression (2.21), the cluster expansion coefficient b_n is given by

$$b_n=\frac{1}{n!}\sum_{\theta\in\Theta(n)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\Theta(\theta)}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}(N_{\theta'}-1)!\right]\int\left|\frac{\partial I}{\partial x}\right|_{cN,\zeta}e^{-\beta E(\zeta)}\prod_{\theta'\in\zeta}\mathrm{d}x_{\theta'}, \tag{2.22}$$

where the explicit form of $|\partial I/\partial x|_{cN,\zeta}$ is

$$(2\pi)^{N_\zeta}\left|\frac{\partial I}{\partial x}\right|_{cN,\zeta}=\left[\prod_{\theta\in\zeta}N_\theta\right]^{-1}\sum_{\lambda\in\Lambda_c(\zeta)}\left[\prod_{\{\theta,\theta'\}\in\lambda}-N_\theta N_{\theta'}K_{M_\theta,M_{\theta'}}(x_\theta-x_{\theta'})\right]\sum_{\theta\in\zeta}\frac{2N_\theta M_\theta N}{M_\theta^2+x_\theta^2}. \tag{2.23}$$

The symbol $\Lambda_c(A)$ is defined as follows.

Definition 7: $\Lambda_c(A)$ is a subset of $\Lambda(A)$, where any element $\lambda\in\Lambda_c(A)$ satisfies the condition $N_{G[\lambda,A]}=1$. For example, we can show that

$$\Lambda_c(\{a,b,c\})=\{\{a,b\},\{a,c\}\},\{\{b,a\},\{b,c\}\},\{\{c,a\},\{c,b\}\}. \tag{2.24}$$

A derivation of the expression $|\partial I/\partial x|_{cN,\zeta}$ in (2.23) is given in Appendix C.

III. THE FREE ENERGY

From Eqs. (2.10) and (2.21), we can easily show that

$$z^{1/2}[\mathrm{Tr}\,e^{-\beta H(J,h)}]^{1/N}=1+\sum_{n=1}^{\infty}\frac{z^n}{n!}\sum_{\theta\in\Theta(n)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\Theta(\theta)}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}(N_{\theta'}-1)!\right]$$
$$\times\int\left|\frac{\partial I}{\partial x}\right|_{1,\zeta}e^{-\beta E(\zeta)}\prod_{\theta'\in\zeta}\mathrm{d}x_{\theta'}, \tag{3.1}$$

where $|\partial I/\partial x|_{1,\zeta}$ means $|\partial I/\partial x|_{N,\zeta}$ in which N is replaced with 1.

Now, we introduce a function $u(x)$,

$$u(x)\equiv 1+\sum_{n=1}^{\infty}z^n u_n(x), \tag{3.2}$$

where $u_n(x)$ is given by

$$u_n(x)\equiv\frac{1}{n!}\sum_{\theta\in\Theta(n)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\Theta(\theta)}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}(N_{\theta'}-1)!\right]$$
$$\times\int\left|\frac{\partial I}{\partial x}\right|_{1,\zeta}(x)e^{-\beta E(\zeta)}\prod_{\theta'\in\zeta}\mathrm{d}x_{\theta'} \tag{3.3}$$

with the modified Jacobian $|\partial I/\partial x|_{1,\zeta}(y)$ defined as

$$(2\pi)^{N_\zeta}\left|\frac{\partial I}{\partial x}\right|_{1,\zeta}(y)\equiv\left[\prod_{\theta\in\zeta}N_\theta\right]^{-1}\sum_{\lambda\in\Lambda(\zeta)}\left[\prod_{\{\theta,\theta'\}\in\lambda}-N_\theta N_{\theta'}K_{M_\theta,M_{\theta'}}(x_\theta-x_{\theta'})\right]$$
$$\times\prod_{\zeta'\in G([\lambda,\zeta])}\left[\sum_{\theta\in\zeta'}\frac{2N_\theta M_\theta}{M_\theta^2+(x_\theta-y)^2}\right]. \tag{3.4}$$

Comparing this definition with (2.20), it is readily seen that $|\partial I/\partial x|_{1,\zeta}=|\partial I/\partial x|_{1,\zeta}(0)$. Then, it is clear that we can get a relation

$$[\mathrm{Tr}\,e^{-\beta H(J,h)}]^{1/N}=u(0)z^{-1/2}. \tag{3.5}$$

It can be shown (see Appendix D for a proof) that the function $u_n(x)$ satisfies the following recursion relation;

$$u_{n+1}(x)=\oint_{0+}\left[\frac{\exp\left(-\frac{2J\beta}{(y+i)^2+1}\right)}{x-y-2i}+\frac{\exp\left(-\frac{2J\beta}{(y-i)^2+1}\right)}{x-y+2i}\right]$$
$$\times\sum_{\theta\in\Theta(n)}\frac{N_\theta!}{n!}\left[\prod_{\sigma\in\theta}-N_\sigma!u_{N_\sigma}(y)\right]\frac{dy}{2\pi i}, \tag{3.6}$$

$$u_1(x)=1+\oint_{0+}\left[\frac{\exp\left(-\frac{2J\beta}{(y+i)^2+1}\right)}{x-y-2i}+\frac{\exp\left(-\frac{2J\beta}{(y-i)^2+1}\right)}{x-y+2i}\right]\frac{dy}{2\pi i}, \tag{3.7}$$

where n is the natural number. Using this recursion relation we obtain a relation

$$u(x)=z+1+\oint_{0+}\left[\frac{\exp\left(-\frac{2J\beta}{(y+i)^2+1}\right)}{x-y-2i}+\frac{\exp\left(-\frac{2J\beta}{(y-i)^2+1}\right)}{x-y+2i}\right]\frac{z}{u(y)}\frac{dy}{2\pi i}. \tag{3.8}$$

These results, (3.5) and (3.8), are the same as those of Ref. 11 in the XXX Heisenberg model limit.

IV. CONCLUSION

We have shown a method, which we call the direct method, to derive the free energy of the XXX Heisenberg model using the BA equation. The cluster expansion coefficient in arbitrary order is given for the first time. The expression of the free energy perfectly agrees with that by TBA. It is remarkable that the free energy is obtained without recourse to TBA and QTM. On the other hand, there remains a problem. We have started from the string hypothesis in this paper. Therefore, it is still a challenging problem to derive each cluster expansion coefficient only from the BA equation. This problem is under investigation.

We think, however, that these results have theoretical significance. What we have done here is calculate a certain summation using combinatorial argument with mathematical justification. The summation may contain a problem which comes from the string hypothesis. On the contrary, TBA solves this problem as follows. We define a nonequilibrium entropy, and minimize the free energy using such entropy. Then, the condition of minimization gives the summation. In other words, TBA entirely relies on the physical definition of the entropy. In this paper, it is proved that the two results by TBA and by the direct method are the same. Therefore, in addition to the δ-function Bose gas, for the XXX Heisenberg model, the direct method gives the mathematical justification of TBA. To summarize, it is suggested that TBA can be systematically proved for many other integrable systems using the combinatorial argument presented here.

APPENDIX A: EXPLICIT FORM OF JACOBIAN $|\partial I/\partial x|_{N,\zeta}$

In this appendix, we prove (2.20). Recall that $|\partial I/\partial x|_{N,\zeta}$ is the Jacobian defined for $\zeta \in \overline{\Theta}(\theta)$, where $\theta \in \Theta(n)$. The Jacobian matrix can be rewritten as follows: the Jacobian matrix has the order $N_\zeta \times N_\zeta$, and each element of the matrix is

$$2\pi \frac{\partial I_{\theta'}}{\partial x_\theta} = \begin{cases} \dfrac{2M_\theta N}{M_\theta^2 + x_\theta^2} - \displaystyle\sum_{\theta'' \neq \theta} N_{\theta''} K_{M_\theta, M_{\theta''}}(x_\theta - x_{\theta''}) & \text{if } \theta = \theta' \\ N_\theta K_{M_\theta M_{\theta'}}(x_\theta - x_{\theta'}) & \text{if } \theta \neq \theta', \end{cases} \tag{A1}$$

where θ, θ', $\theta'' \in \zeta$ and $K_{n,m}(x) \equiv \mathrm{d}\Delta_{n,m}(x)/\mathrm{d}x$.

Here, we generalize the setting of the problem. We define $N \times N$ matrix

$$A_{n,m} = \begin{cases} e_n - \displaystyle\sum_{k \neq n} c_k a_{n,k} & \text{if } n = m \\ c_n a_{n,m} & \text{if } n \neq m, \end{cases} \tag{A2}$$

where $\{a_{n,m}\}$, $\{c_n\}$, and $\{e_n\}$ are arbitrary series and $a_{n,m}$ is symmetric, $a_{n,m} = a_{m,n}$. This matrix is a generalized form of the Jacobian matrix (A1). Therefore, what we have to prove becomes that the determinant of $A_{n,m}$ is

$$|A_{n,m}| = \left[\prod_{n=1}^{N} c_n\right]^{-1} \sum_{\lambda \in \Lambda(\{1,\ldots,N\})} \left[\prod_{\{n,m\} \in \lambda} -c_n c_m a_{n,m}\right] \prod_{\sigma \in G([\lambda, \{1,\ldots,N\}])} \left[\sum_{n \in \sigma} c_n e_n\right]. \tag{A3}$$

First, we prove that each term of the determinant $|A_{n,m}|$ can be considered as a pattern of connection $\lambda \in \Lambda(\{1,\ldots,N\})$. When we regard the determinant as a multi-variable polynomial with respect to $\{a_{n,m}\}$ and regard $a_{n,m}$ as a connection between n and m, we can consider each term of the polynomial as a pattern of connection λ. In other words, we can prove the following two facts. First, there is no multiple connection. That is to say, there is no $a_{n,m}$ to the power of 2 or more in any term of the polynomial. Second, there is no closed path made from connections. That is to say, there is no product $a_{p(1),p(2)} a_{p(2),p(3)} \cdots a_{p(M-1),p(M)} a_{p(M),p(1)}$ in any term, where p is a permutation.

To prove these two facts, we use the method of false position. We assume there is a term that has at least one closed path through M connections. Without loss of generality, the above-mentioned assumption can be rewritten that there is a product $a_{1,2} a_{2,3} \cdots a_{M-1,M} a_{M,1}$ in any term. Then, we introduce a matrix $A'_{n,m}$ such that

$$A'_{n,m} = \begin{cases} -\displaystyle\sum_{k \neq n} c_k a_{n,k} & \text{if } n = m \leqslant M \\ e_n - \displaystyle\sum_{k \neq n} c_k a_{n,k} & \text{if } n = m > M \\ 0 & \text{if } n \leqslant M < m \text{ or } m \leqslant M < n \\ c_n a_{n,m} & \text{other.} \end{cases} \tag{A4}$$

Now, we regard $|A'_{n,m}|$ as a multi-variable polynomial with respect to $\{a_{n,m}\}$. From the definition of determinant, it is easily shown that the term with a product $a_{1,2} a_{2,3} \cdots a_{M-1,M} a_{M,1}$ in $|A_{n,m}|$ has the same coefficient as a term with such product in $|A'_{n,m}|$. However, $|A'_{n,m}|$ is identically 0 because the matrix $A'_{n,m}$ is linearly dependent. Therefore, there is no term containing a product $a_{1,2} a_{2,3} \cdots a_{M-1,M} a_{M,1}$. Substituting 2 for M, we can prove that there is no $a_{n,m}$ to the power of 2 or more in any term of the polynomial. Then, we can consider each term of the matrix $|A_{n,m}|$ as a pattern of connection λ.

Second, we find where a term considered as a pattern of connection is formed. From the definition, we can write the determinant $|A_{n,m}|$ as

$$|A_{n,m}| = \sum_{p \in P_N} \operatorname{sgn} p \cdot \prod_{n=1}^{N} A_{n,p(n)}, \tag{A5}$$

where P_N is a permutation group with respect to $\{1,...,N\}$. It can be shown that any term considered as a pattern of connection is in an expansion of a product only in the case where p is the identity permutation. The following is a proof of the fact by the method of false position. If there is such term in the case where p is not the identity permutation, there exist n_0 and l_0 which satisfy $p^{l_0}(n_0)=n_0$, $p^{l}(n_0)\neq n_0$ and $l_0 \neq 0$, where $l_0 > l$ and $p^m(n)$ means that p operates on n for m times, $p(p(\cdots p(n)\cdots))$. Therefore, we can rewrite $\Pi_{n=1}^{N} A_{n,p(n)}$ as

$$\left[\prod_{l=0}^{l_0-1} c_{p^l(n_0)} a_{p^l(n_0),p^{l+1}(n_0)} \right] \prod_{n \neq p^l(n_0)} A_{n,p(n)}. \tag{A6}$$

This term clearly has a closed path, and conflict with the definition of the p.

Finally, we can rewrite $|A_{n,m}|$ as follows. We expand

$$\prod_{n=1}^{N} A_{n,n}, \tag{A7}$$

and regard it as a multivariable polynomial with respect to $\{a_{n,m}\}$. $|A_{n,m}|$ is a sum of terms which are in this polynomial and can be considered as a pattern of connection. This means that the term has no multiple connection and no closed path. This sum means the right-hand side of (A3).

APPENDIX B: A PROOF OF (2.21)

In this appendix, we prove (2.21) from (2.10).

We define Z_n by

$$z^{N/2} \operatorname{Tr} e^{-\beta H(J,h)} \equiv 1 + \sum_{n=1}^{\infty} Z_n z^n. \tag{B1}$$

From (2.10) we get

$$Z_n = \frac{1}{n!} \sum_{\theta \in \Theta(n)} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \Theta(\theta)} \left[\prod_{\theta' \in \zeta} (-1)^{N_{\theta'}-1} (N_{\theta'}-1)! \right] \int \left| \frac{\partial I}{\partial x} \right|_{N,\zeta} e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} \mathrm{d}x_{\theta'}, \tag{B2}$$

where $|\partial I/\partial x|_{N,\zeta}$ is the Jacobian defined for ζ. It is convenient to introduce $f(\zeta)$ as

$$f(\zeta) \equiv \int \left| \frac{\partial I}{\partial x} \right|_{cN,\zeta} e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} \mathrm{d}x_{\theta'}. \tag{B3}$$

Using this function and relation (C1) proved in Appendix C, we can rewrite Z_n as

$$Z_n = \frac{1}{n!} \sum_{\theta \in \Theta(n)} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \Theta(\theta)} \left[\prod_{\theta' \in \zeta} (-1)^{N_{\theta'}-1} (N_{\theta'}-1)! \right] \sum_{\xi \in \Theta(\zeta)} \prod_{\zeta' \in \xi} f(\zeta'). \tag{B4}$$

We also define b_n by

$$\log\left[1+\sum_{n=1}^{\infty} Z_n z^n\right] \equiv \sum_{n=1}^{\infty} b_n z^n. \tag{B5}$$

We can easily show the following relation between b_n and Z_n:

$$b_n = \frac{1}{n!} \sum_{\theta \in \Theta(n)} (N_\theta - 1)!(-1)^{N_\theta - 1} \sum_{\sigma \in \theta} N_\sigma! Z_{N_\sigma}. \tag{B6}$$

Substituting (B4) for Z_n in (B6), we get

$$\begin{aligned} b_n &= \frac{1}{n!} \sum_{\theta \in \Theta(n)} (N_\theta - 1)!(-1)^{N_\theta - 1} \prod_{\sigma \in \theta} \left[\sum_{\theta' \in \Theta(\sigma)} \left[\prod_{\sigma' \in \theta'} N_{\sigma'}! \right] \right. \\ &\quad \left. \times \sum_{\zeta \in \Theta(\theta')} \left[\prod_{\theta'' \in \zeta} (-1)^{N_{\theta''} - 1} (N_{\theta''} - 1)! \right] \sum_{\xi \in \Theta(\zeta)} \prod_{\zeta' \in \xi} f(\zeta') \right] \\ &= \frac{1}{n!} \sum_{\theta \in \Theta(n)} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \Theta(\theta)} \left[\prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} (N_{\theta'} - 1)! \right] \\ &\quad \times \sum_{\xi \in \Theta(\zeta)} \left[\prod_{\zeta' \in \xi} f(\zeta') \right] \sum_{\eta \in \Theta(\xi)} (N_\eta - 1)!(-1)^{N_\eta - 1} \\ &= \frac{1}{n!} \sum_{\theta \in \Theta(n)} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \Theta(\theta)} \left[\prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} (N_{\theta'} - 1)! \right] f(\zeta). \end{aligned} \tag{B7}$$

In the first equality, we have only performed the substitution. In the second equality, we have done the following manipulation. We regard each side of the equality as the sum with respect to elements in a set which satisfies some conditions. Therefore, we may change the order of the sums. Here, we show a simple example of ''change of order,''

$$\sum_{n=1}^{N} \sum_{m=1}^{n} f(\{n,m\}) = \sum_{m=1}^{N} \sum_{n=m}^{N} f(\{n,m\}). \tag{B8}$$

Similar to this example, both sides of the second equality are the sum of the same function with respect to elements in the same set. In the third equality, we have simplified the last term of the left-hand side using a relation,

$$\sum_{\theta \in \Theta(\sigma)} (N_\theta - 1)!(-1)^{N_\theta - 1} = \delta_{N_\sigma, 1}. \tag{B9}$$

Finally, combining (B1), (B3), (B5), and (B7) we arrive at Eq. (2.21).

APPENDIX C: THE STRUCTURE OF THE JACOBIAN $|\partial I/\partial x|_{N,\zeta}$

In this appendix, we prove

$$\left|\frac{\partial I}{\partial x}\right|_{N,\zeta} = \sum_{\xi \in \Theta(\zeta)} \prod_{\zeta' \in \xi} \left|\frac{\partial I}{\partial x}\right|_{cN,\zeta'} \tag{C1}$$

and Eq. (2.23) from Eq. (2.20). We here repeat that $|\partial I/\partial x|_{cN,\zeta}$ is the first-order term of $|\partial I/\partial x|_{N,\zeta}$ with respect to N.

Equation (2.20) can be rewritten as

$$(2\pi)^{N_\zeta}\left|\frac{\partial I}{\partial x}\right|_{N,\zeta}=\sum_{\xi\in\Theta(\zeta)}\prod_{\zeta'\in\xi}\left[\left[\prod_{\theta\in\zeta'}N_\theta\right]^{-1}\right.$$
$$\left.\times\sum_{\lambda\in\Lambda_c(\zeta')}\left[\prod_{\{\theta,\theta'\}\in\lambda}-N_\theta N_{\theta'}K_{M_\theta,M_{\theta'}}(x_\theta-x_{\theta'})\right]\sum_{\theta\in\zeta' N}\frac{2N_\theta M_\theta}{M_\theta^2+x_\theta^2}\right]. \quad \text{(C2)}$$

In this equality, we have changed the order of the sums. We can easily show the relation (2.23) from this expression. Then, Eqs. (C2) and (2.23) prove (C1).

APPENDIX D: A PROOF OF (3.6) AND (3.7)

In this appendix, using the mathematical induction we prove the relations with respect to $u_n(x)$, (3.6) and (3.7). The definition of $u_n(x)$ is given in Eq. (3.3).

We can change the right-hand side of (3.7) into

$$\int\frac{2}{1+(x-y)^2}\exp\left(-\frac{2J\beta}{y^2+1}\right)\frac{dy}{2\pi i}. \quad \text{(D1)}$$

This is the same as the definition of $u_1(x)$. Thus, we have shown the relation (3.7).

We suppose (3.6) and (3.7) hold for $1\leqslant n<n_0$, where n_0 is a natural number. For simplicity, n_0 is merely written as n in what follows. Then, the function $u_m(x)$ has poles only at $x=\pm 2i$, and satisfies $\lim_{|x|\to\infty}u_m(x)=\delta_{m,1}$, where $1\leqslant m\leqslant n$. By use of these two properties, the right-hand side of (3.6) becomes

$$\oint_{0+}\left[\frac{\exp\left(-\frac{2J\beta}{(y+i)^2+1}\right)}{x-y-2i}+\frac{\exp\left(-\frac{2J\beta}{(y-i)^2+1}\right)}{x-y+2i}\right]\sum_{\theta\in\Theta(n)}\frac{N_\theta!}{n!}\left[\prod_{\sigma\in\theta}-N_\sigma!u_{N_\sigma}(y)\right]\frac{dy}{2\pi i}$$
$$=\sum_{\theta\in\Theta(n)}\frac{N_\theta!}{n!}\int_{-\infty}^{\infty}\left[\frac{\Pi_{\sigma\in\theta}-N_\sigma!u_{N_\sigma}(y-i)}{x-y-i}-\frac{\Pi_{\sigma\in\theta}-N_\sigma!u_{N_\sigma}(y+i)}{x-y+i}\right]\exp\left(-\frac{2J\beta}{y^2+1}\right)\frac{dy}{2\pi i}$$
$$-\sum_{\theta\in\Theta(n)}\frac{N_\theta!}{n!}\int_{C_+}\frac{\Pi_{\sigma\in\theta}-N_\sigma!u_{N_\sigma}(y)}{x-y-2i}\exp\left(-\frac{2J\beta}{(y+i)^2+1}\right)\frac{dy}{2\pi i}$$
$$+\sum_{\theta\in\Theta(n)}\frac{N_\theta!}{n!}\int_{C_-}\frac{\Pi_{\sigma\in\theta}-N_\sigma!u_{N_\sigma}(y)}{x-y+2i}\exp\left(-\frac{2J\beta}{(y-i)^2+1}\right)\frac{dy}{2\pi i}. \quad \text{(D2)}$$

In this equality we have changed the path of integration. Both C_+ and C_- are the paths of integration which counterclockwise surround the region $\Im y>0$. When these paths are in the neighborhood of real axis, C_+ passes above the real axis and C_- passes below the real axis. We separate (D2) into two parts, and calculate them separately.

First, we consider the first term of (D2) which is rewritten as

$$\sum_{\theta\in\Theta(n)}\frac{N_\theta!}{n!}\int_{-\infty}^{\infty}\sum_{s=\pm 1}\frac{s\Pi_{\sigma\in\theta}-N_\sigma!u_{N_\sigma}(y-si)}{s-(y-x)i}\exp\left(-\frac{2J\beta}{y^2+1}\right)\frac{dy}{2\pi}. \quad \text{(D3)}$$

The integral diverges in cases that we do not sum up with respect to s. However, the sum turns out not to play an important role in the following calculation. Hence, to shorten the expression, the symbol $\Sigma_{s=\pm 1}$ is omitted for a while. Now, by use of relation (E1) proved in Appendix E, Eq. (D3) is rewritten as

$$\frac{1}{n!}\int_{-\infty+s\delta i}^{\infty+s\delta i}\frac{dy}{2\pi}\sum_{\theta\in\Theta(n)}\prod_{\sigma\in\theta}\left[-\sum_{\theta'\in\Theta(\sigma)}\left[\prod_{\sigma'\in\theta'}N_{\sigma'}!\right]\sum_{\zeta\in\Theta(\theta')}\left[\prod_{\theta''\in\zeta}(-1)^{N_{\theta''}-1}\frac{(N_{\theta''}-1)!}{N_{\theta''}}\right]\right.$$
$$\times\left[\prod_{\theta''\in\zeta}\int_{-\infty}^{\infty}\frac{dx_{\theta''}}{2\pi}\right]\sum_{\lambda\in\Lambda_c(\zeta)}\left[\prod_{\{\theta'',\theta'''\}\in\lambda}-N_{\theta''}N_{\theta'''}K_{M_{\theta''},M_{\theta'''}}(x_{\theta''}-x_{\theta'''})\right]$$
$$\left.\times\sum_{\theta''\in\zeta}\frac{2N_{\theta''}M_{\theta''}}{M_{\theta''}^2+(x_{\theta''}-y+si)^2}\frac{s\exp\left(-\beta\left(\frac{2J}{y^2+1}+E(\zeta)\right)\right)}{s-(y-x)i}\right]. \tag{D4}$$

On condition that we take a limit $\delta\to 0$ and $M_\theta=1$, $1/(M_\theta^2+(x_\theta-y+si)^2)$ yields a pole on the real axis with respect to the variable y. To detour the pole on the real axis and symmetrize the integral paths, we use the relation (F1) proved in Appendix F. Then, (D4) becomes

$$\frac{1}{n!}\sum_{\theta\in\Theta(n)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\bar{\Theta}(\theta+\{n+1\})}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}\frac{(N_{\theta'}-1)!}{N_{\theta'}}\right]\frac{N_{\theta_{n+1}}}{(N_{\theta_{n+1}}-1)!}$$
$$\times\left[\sum_{\zeta'\in\Theta(N_{\theta_{n+1}}-1)}B_{N_{\zeta'}}\prod_{\theta'\in\zeta'}(N_{\theta'}-1)!\right]\int_{\mathrm{sym}}\left[\prod_{\theta'\in\zeta}\frac{dx_{\theta'}}{2\pi}\right]\sum_{\lambda\in\Lambda_c(\zeta)}\frac{se^{-\beta E(\zeta)}}{s-(x_{\theta_{n+1}}-x)i}$$
$$\times\left[\prod_{\{\theta',\theta''\}\in\lambda,\ \theta',\theta''\neq\theta_{n+1}}C(\theta',\theta'')\right]\left[\prod_{\{\theta_{n+1},\theta'\}\in\lambda}E(\theta_{n+1},\theta')\right]. \tag{D5}$$

Here, we assume the relation $\{n+1\}\in\sigma_{n+1}\in\theta_{n+1}\in\zeta$. We also use this symbol in the same sense as in (D12), (D19), and (D20). The constant B_n in (D5) is known as the Bernoulli number and is determined by

$$\sum_{n=0}^{\infty}\frac{B_n}{n!}x^n\equiv\frac{x}{1-e^{-x}}. \tag{D6}$$

For example, the first few B_n's are

$$B_0=1,\quad B_1=\tfrac{1}{2},\quad B_2=\tfrac{1}{6},\quad B_3=0,\quad B_4=-\tfrac{1}{30},\quad \cdots. \tag{D7}$$

The symbol $\int_{\mathrm{sym}}$ in (D5) indicates that each path of integration symmetrically avoids poles on the real axis. Because all the poles on the real axis have the form $1/(x_\theta-x_{\theta'})$, we can explicitly write $\int_{\mathrm{sym}}$ as

$$\int_{\mathrm{sym}}\prod_{n=1}^{N}dx_n\equiv\frac{1}{N!}\sum_{\{p\in P_N\}}\prod_{n=1}^{N}\left[\int_{-\infty+n\delta i}^{\infty+n\delta i}dx_{p(n)}\right]. \tag{D8}$$

The functions $C(\theta,\theta')$ and $E(\theta,\theta')$ are defined by

$$C(\theta,\theta')\equiv -N_\theta,N_{\theta'}K_{M_\theta,M_{\theta'}}(x_\theta-x_{\theta'}), \tag{D9}$$

$$E(\theta,\theta')\equiv-(N_\theta-1)N_{\theta'}K_{M_\theta,M_{\theta'}}(x_\theta-x_{\theta'})-N_{\theta'}K_{M_\theta-1,M_{\theta'}}(x_\theta-x_{\theta'}-si)$$
$$-\frac{2N_{\theta'}M_{\theta'}}{M_{\theta'}^2+(x_\theta-x_{\theta'}+s(M_\theta-2)i)^2}. \tag{D10}$$

Note here that the second term of (D10) is 0 for $E(\theta,\theta')$ used in (D5) because of the relation $M_{\theta_{n+1}}=1$. Then, by use of the relation

$$\sum_{\theta\in\Theta(n)} B_{N_\theta}\prod_{\sigma\in\theta}(N_\sigma-1)!=\frac{n!}{n+1}, \tag{D11}$$

which is easily shown, (D5) becomes

$$\frac{1}{n!}\sum_{\theta\in\Theta(n)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\overline{\Theta}(\theta+\{n+1\})}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}\frac{(N_{\theta'}-1)!}{N_{\theta'}}\right]\frac{1}{N_{\theta_{n+1}}}\int_{\mathrm{sym}}\left[\prod_{\theta'\in\zeta}\frac{dx_{\theta'}}{2\pi}\right]$$
$$\times\sum_{\lambda\in\Lambda_c(\zeta)}\frac{sN_{\theta_{n+1}}e^{-\beta E(\zeta)}}{s-(x_{\theta_{n+1}}-x)i}\left[\prod_{\{\theta',\theta''\}\in\lambda,\theta',\theta''\neq\theta_{n+1}}C(\theta',\theta'')\right]\left[\prod_{\{\theta_{n+1},\theta'\}\in\lambda}E(\theta_{n+1},\theta')\right]. \tag{D12}$$

Changing the order of the sums, this expression becomes

$$\frac{1}{(n+1)!}\sum_{\theta\in\Theta(n+1)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\Theta(\theta)}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}\frac{(N_{\theta'}-1)!}{N_{\theta'}}\right]\int_{\mathrm{sym}}\left[\prod_{\theta'\in\zeta}\frac{dx_{\theta'}}{2\pi}\right]$$
$$\times\sum_{\lambda\in\Lambda_c(\zeta)}\sum_{\theta_0\in\zeta,M_{\theta_0}=1}\frac{sN_{\theta_0}e^{-\beta E(\zeta)}}{s-(x_{\theta_0}-x)i}\left[\prod_{\{\theta',\theta''\}\in\lambda,\theta',\theta''\neq\theta_0}C(\theta',\theta'')\right]\left[\prod_{\{\theta_0,\theta'\}\in\lambda}E(\theta_0,\theta')\right]. \tag{D13}$$

Thus, using the above-given relations we have shown that (D3) is expressed as (D13).

Second, we write the sum of the second and third terms of (D2),

$$-\sum_{s=\pm1}s\sum_{\theta\in\Theta(n)}\frac{N_\theta!}{n!}\int_{C_s}\frac{\Pi_{\sigma\in\theta}-N_\sigma!u_{N_\sigma}(y)}{2s-(y-x)i}\exp\left(-\frac{2J\beta}{(y+si)^2+1}\right)\frac{dy}{2\pi}, \tag{D14}$$

where $C_{\pm1}$ means $C_\pm$. In the following change of the expressions, the sum with respect to s does not play an important role. This situation is similar to the one for (D3). Then, the symbol $\Sigma_{s=\pm1}$ will be also omitted for a while. Using relation (E1), we have from (D14),

$$-\frac{1}{n!}\int_{C_s}\frac{dy}{2\pi}\sum_{\theta\in\Theta(n)}\prod_{\sigma\in\theta}\left[-\sum_{\theta'\in\Theta(\sigma)}\left[\prod_{\sigma\in\theta'}N_{\sigma'}!\right]\sum_{\zeta\in\overline{\Theta}(\theta)'}\left[\prod_{\theta''\in\zeta}(-1)^{N_{\theta''}-1}\frac{(N_{\theta''}-1)!}{N_{\theta''}}\right]\right.$$
$$\times\left[\prod_{\theta''\in\zeta}\int_{-\infty}^{\infty}\frac{dx_{\theta''}}{2\pi}\right]\sum_{\lambda\in\Lambda_c(\zeta)}\left[\prod_{\{\theta'',\theta'''\}\in\lambda}-N_{\theta''}N_{\theta'''}K_{M_{\theta''},M_{\theta'''}}(x_{\theta''}-x_{\theta'''})\right]$$
$$\left.\times\sum_{\theta''\in\zeta}\frac{2N_{\theta''}M_{\theta''}}{M_{\theta''}^2+(x_{\theta''}-y)^2}\frac{s\exp\left(-\beta\left(\frac{2J}{(y+si)^2+1}+E(\zeta)\right)\right)}{2s-(y-x)i}\right]. \tag{D15}$$

We use a relation,

$$\int_{C_s} dy\, f(y) \prod_{\sigma\in\theta}\left[\int_{-\infty}^{\infty}\frac{dx_\sigma}{2\pi}\frac{2N_\sigma f_\sigma(x_\sigma)}{N_\sigma^2+(y-x_\sigma)^2}\right]$$
$$= \int_{C_s} dy\, f(y+msi)\prod_{\sigma\in\theta}\left[\int_{-\infty}^{\infty}\frac{dx_\sigma}{2\pi}\frac{2N_\sigma f_\sigma(x_\sigma)}{N_\sigma^2+(y-x_\sigma+msi)^2}\right]+\sum_{n=1}^{m-1}\int_{C_s} dy\, f(y+nsi)$$
$$\times\left[\prod_{\sigma\in\theta}\int_{-\infty}^{\infty}\frac{dx_\sigma}{2\pi}\frac{f_\sigma(x_\sigma)}{N_\sigma^2+(y-x_\sigma+nsi)^2}-\prod_{\sigma\in\theta}\left[\int_{-\infty}^{\infty}\frac{dx_\sigma}{2\pi}\frac{2N_\sigma f_\sigma(x_\sigma)}{N_\sigma^2+(y-x_\sigma+nsi)^2}\right.\right.$$
$$\left.\left.-\delta(n+1,N_\sigma)f_\sigma(y-si)\right]\right], \tag{D16}$$

where $f_\sigma(x)$ and $f(x)$ are analytic functions in the regions $-1<\Im x\leqslant 0$ and $0<\Im x\leqslant m$ in case of $s=1$ ($0\leqslant\Im x<1$ and $-m\leqslant\Im x<0$ in case of $s=-1$) respectively, and $\max_{\sigma\in\theta}N_\sigma=m$. Then, (D15) becomes

$$\frac{1}{n!}\sum_{\theta\in\Theta(n)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\zeta\in\bar{\Theta}(\theta)}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}\frac{(N_{\theta'}-1)!}{N'_\theta}\right]\sum_{\theta'\in\zeta}\frac{N_{\theta'}(-1)^{N_{\theta'}-1}}{(N_{\theta'}-1)!}$$
$$\times\left[\sum_{\theta''\in\Theta(N_{\theta'})}\prod_{\sigma''\in\theta''}(-1)^{N_{\sigma''}-1}(N_{\sigma''}-1)!\right]\int_{C_s}\frac{dx_{\theta'}}{2\pi}\left[\prod_{\theta''\in\zeta,\theta''\neq\theta'}\int_{-\infty}^{\infty}\frac{dx_{\theta''}}{2\pi}\right]$$
$$\times\sum_{\lambda\in\Lambda_c(\zeta)}\frac{s\exp\left[-\beta\left(E(\zeta)+\frac{2J}{(x_{\theta'}+sM_{\theta'}i)^2+1}+\frac{2JM_{\theta'}}{(x_{\theta'}-si)^2+M_{\theta'}^2}-\frac{2JM_{\theta'}}{x_{\theta'}^2+M_{\theta'}^2}\right)\right]}{(M_{\theta'}+1)s-(x_{\theta'}-x)i}$$
$$\times\left[\prod_{\{\theta'',\theta'''\}\in\lambda,\theta'',\theta'''\neq\theta'}C(\theta'',\theta''')\right]\prod_{\{\theta',\theta''\}\in\lambda}\left[-N_{\theta'}N_{\theta''}K_{M_{\theta'},M_{\theta''}}(x_{\theta'}-x_{\theta''}-si)\right.$$
$$\left.-\frac{2N_{\theta''}M_{\theta''}}{M_{\theta''}^2+(x_{\theta'}-x_{\theta''}+s(M_{\theta'}-1)i)^2}\right]. \tag{D17}$$

We point out that in this case the first term of the right-hand side in (D16) is 0 because there is no pole inside (outside) the path of integration C_+ (C_-) with respect to y including the point $|y|=\infty$. Then, using a simple relation $\Sigma_{\theta\in\Theta_n}\Pi_{\sigma\in\theta}(-)^{N_\sigma-1}(N_\sigma-1)!=\delta_{n,1}$, we get from (D17),

$$\frac{1}{n!}\sum_{\theta\in\Theta(n)}\left[\prod_{\sigma\in\theta}N_\sigma!\right]\sum_{\sigma_0\in\theta}\sum_{\zeta\in\bar{\Theta}(\theta-\sigma_0)}\left[\prod_{\theta'\in\zeta}(-1)^{N_{\theta'}-1}\frac{(N_{\theta'}-1)!}{N_{\theta'}}\right]\int_{-\infty+s\delta i}^{\infty+s\delta i}\frac{dx_{\theta_0}}{2\pi}$$
$$\times\left[\prod_{\theta'\in\zeta}\int_{-\infty}^{\infty}\frac{dx_{\theta'}}{2\pi}\right]\sum_{\lambda\in\Lambda_c(\zeta+\theta_0)}+\frac{s\exp\left[-\beta\left(E(\zeta)+\frac{2J(M_{\theta_0}+1)}{x_{\sigma_0}^2+(M_{\theta_0}+1)^2}-\frac{2JM_{\theta_0}}{x_{\sigma_0}^2+M_{\theta_0}^2}\right)\right]}{(M_{\theta_0}+1)s-(x_{\sigma_0}-x)i}$$
$$\times\left[\prod_{\{\theta',\theta''\}\in\lambda,\theta',\theta''\neq\theta_0}C(\theta',\theta'')\right]$$
$$\times\prod_{\{\theta_0,\theta'\}\in\lambda}\left[-N_{\theta'}K_{M_{\theta_0},M_{\theta'}}(x_{\theta_0}-x_{\theta'}-si)-\frac{2N_{\theta'}M_{\theta'}}{M_{\theta'}^2+(x_{\theta_0}-x_{\theta'}+s(M_{\theta_0}-1)i)^2}\right]. \tag{D18}$$

where $\theta_0 \equiv \{\sigma_0\}$. Here, we have changed the path of integration from C_s to $-\infty + s\delta i \to \infty + s\delta i$, because there is no pole at $|x_{\theta_0}| \to \infty$. In Eq. (D18), when we take a limit $\delta \to 0$ and $M_\theta = M_{\theta_0} + 1$, the last term contains a pole on the real axis with respect to x_θ. Symmetrizing by use of (F1) the integral paths which avoid the pole on the real axis, we obtain from (D18),

$$\frac{1}{n!} \sum_{\theta \in \Theta(n+1), N_{\sigma_{n+1}} \neq 1} \left[\prod_{\sigma \in \sigma} N_\sigma! \right] \sum_{\zeta \in \Theta(\theta)} \left[\prod_{\theta' \in \zeta} (-1)^{N_{\theta'}-1} \frac{(N_{\theta'}-1)!}{N_{\theta'}} \right] \frac{N_{\theta_{n+1}}}{N_{\sigma_{n+1}} (N_{\theta_{n+1}}-1)!}$$
$$\times \left[\sum_{\theta' \in \Theta(N_{\theta_{n+1}}-1)} B_{N_{\theta'}} \prod_{\sigma' \in \theta'} (N_{\sigma'}-1)! \right] \int_{\mathrm{sym}} \left[\prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \right] \sum_{\lambda \in \Lambda_c(\zeta)} \frac{s e^{E(\zeta)}}{M_{\theta_{n+1}} s - (x_{\theta_{n+1}} - x) i}$$
$$\times \left[\prod_{\{\theta', \theta''\} \in \lambda, \ \theta', \theta'' \neq \theta_{n+1}} C(\theta', \theta'') \right] \left[\prod_{\{\theta_{n+1}, \theta'\} \in \lambda} E(\theta_{n+1}, \theta') \right]. \tag{D19}$$

By use of (D11), (D19) is written as

$$\frac{1}{n!} \sum_{\theta \in \Theta(n+1), N_{\sigma_{n+1}} \neq 1} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \Theta(\theta)} \left[\prod_{\theta' \in \zeta} (-1)^{N_{\theta'}-1} \frac{(N_{\theta'}-1)!}{N_{\theta'}} \right] \frac{1}{N_{\sigma_{n+1}} N_{\theta_{n+1}}}$$
$$\times \int_{\mathrm{sym}} \left[\prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \right] \sum_{\lambda \in \Lambda_c(\zeta)} \frac{s N_{\theta_{n+1}} e^{E(\zeta)}}{M_{\theta_{n+1}} s - (x_{\theta_{n+1}} - x) i}$$
$$\times \left[\prod_{\{\theta', \theta''\} \in \lambda, \theta', \theta'' \neq \theta_{n+1}} C(\theta', \theta'') \right] \left[\prod_{\{\theta_{n+1}, \theta'\} \in \lambda} E(\theta_{n+1}, \theta') \right]. \tag{D20}$$

Changing the order of the summations, this expression becomes

$$\frac{1}{(n+1)!} \sum_{\theta \in \Theta(n+1)} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \Theta(\theta)} \left[\prod_{\theta' \in \zeta} (-1)^{N_{\theta'}-1} \frac{(N_{\theta'}-1)!}{N_{\theta'}} \right] \int_{\mathrm{sym}} \left[\prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \right]$$
$$\times \sum_{\lambda \in \Lambda_c(\zeta)} \sum_{\theta_0 \in \zeta, M_{\theta_0} \neq 1} \frac{s N_{\theta_0} e^{E(\zeta)}}{M_{\theta_0} s - (x_{\theta_0} - x) i} \left[\prod_{\{\theta', \theta''\} \in \lambda, \theta', \theta'' \neq \theta_0} C(\theta', \theta'') \right] \left[\prod_{\{\theta_0 \theta'\} \in \lambda} E(\theta_0, \theta') \right]. \tag{D21}$$

From the above-mentioned relations we see that (D14) is equal to (D21).

Both parts of the right-hand side of (D2) are replaced with (D12) and (D21). Then, the right-hand side of (D2) is expressed as

$$\frac{1}{(n+1)!} \sum_{\theta \in \Theta(n+1)} \left[\prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\zeta \in \Theta(\theta)} \left[\prod_{\theta' \in \zeta} (-1)^{N_{\theta'}-1} \frac{(N_{\theta'}-1)!}{N_{\theta'}} \right] \int_{\mathrm{sym}} \left[\prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \right]$$
$$\times \sum_{\lambda \in \Lambda_c(\zeta)} \sum_{\theta_0 \in \zeta} \sum_{s = \pm 1} \frac{s N_{\theta_0} e^{E(\zeta)}}{M_{\theta_0} s - (x_{\theta_0} - x) i} \left[\prod_{\{\theta' \theta''\} \in \lambda, \theta', \theta'' \neq \theta_0} C(\theta', \theta'') \right] \left[\prod_{\{\theta_0 \theta'\} \in \lambda} E(\theta_0, \theta') \right]. \tag{D22}$$

Using Eq. (G1) proved in Appendix G, we can confirm the definition of $u_{n+1}(x)$, which is the right-hand side of (3.6).

APPENDIX E: AN EXPRESSION OF $u_n(x)$

In this appendix, we prove the following expression of $u_n(x)$,

$$\sum_{\theta\in\Theta(n)}\frac{N_\theta!}{n!}\prod_{\sigma\in\theta}-N_\sigma!u_{N_\sigma}(y)$$
$$=\frac{1}{n!}\sum_{\theta\in\Theta(n)}\prod_{\sigma\in\theta}\left[-\sum_{\theta'\in\Theta(\sigma)}\left[\prod_{\sigma'\in\theta'}N_{\sigma'}!\right]\sum_{\zeta\in\Theta(\theta')}\left[\prod_{\theta''\in\zeta}(-1)^{N_{\theta''}-1}(N_{\theta''}-1)!\right]\right.$$
$$\left.\times\int\left|\frac{\partial I}{\partial x}\right|_{c1,\zeta}(y)e^{-\beta E(\zeta)}\prod_{\theta'\in\zeta}\mathrm{d}x_{\theta'}\right]. \tag{E1}$$

Here, the definition of $u_n(x)$ is (3.3), and the definition of $|\partial I/\partial x|_{c1,\zeta}(y)$ is

$$(2\pi)^{N_\zeta}\left|\frac{\partial I}{\partial x}\right|_{c1,\zeta}(y)\equiv\left[\prod_{\theta\in\zeta}N_\theta\right]^{-1}\sum_{\lambda\in\Lambda_c(\zeta)}\left[\prod_{\{\theta,\theta'\}\in\lambda}-N_\theta N_{\theta'}K_{M_\theta,M_{\theta'}}(x_\theta-x_{\theta'})\right]$$
$$\times\sum_{\theta\in\zeta}\frac{2N_\theta M_\theta}{M_\theta^2+(x_\theta-y)^2}. \tag{E2}$$

Substituting (3.3) for $u_{N\sigma}(y)$ on the left-hand side of (E1) and using a relation

$$\left|\frac{\partial I}{\partial x}\right|_{1,\zeta}(y)=\sum_{\xi\in\Theta(\zeta)}\prod_{\zeta'\in\xi}\left|\frac{\partial I}{\partial x}\right|_{c1,\zeta'}(y), \tag{E3}$$

which is proved in the same way as (C1), we can show that the left-hand side of (E1) is calculated as

$$\sum_{\theta\in\Theta(n)}\frac{N_\theta!}{n!}\prod_{\sigma\in\theta}\left[-\sum_{\theta'\in\Theta(\sigma)}\left[\prod_{\sigma'\in\theta'}N_{\sigma'}!\right]\sum_{\zeta\in\Theta(\theta')}\left[\prod_{\theta''\in\zeta}(-1)^{N_{\theta''}-1}(N_{\sigma''}-1)!\right]\right.$$
$$\left.\times\sum_{\xi\in\Theta(\zeta)}\left[\prod_{\zeta'\in\xi}\int\left|\frac{\partial I}{\partial x}\right|_{c1,\zeta'}(y)e^{-\beta E(\zeta')}\prod_{\theta'\in\zeta}\mathrm{d}x_{\theta'}\right]\right]$$
$$=\frac{1}{n!}\sum_{\theta\in\Theta(n)}\left[\sum_{\theta'\in\Theta(N_\theta)}N_{\theta'}!(-1)^{N_{\theta'}}\right]\prod_{\sigma\in\theta}\left[\sum_{\theta'\in\Theta(\sigma)}\left[\prod_{\sigma'\in\theta'}N_{\sigma'}!\right]\right.$$
$$\left.\times\sum_{\zeta\in\Theta(\theta')}\left[\prod_{\theta''\in\zeta}(-1)^{N_{\theta''}-1}(N_{\theta''}-1)!\right]\int\left|\frac{\partial I}{\partial x}\right|_{c1,\zeta}(y)e^{-\beta E(\zeta)}\prod_{\theta'\in\zeta}\mathrm{d}x_{\theta'}\right]. \tag{E4}$$

In this equality, we have changed the order of the sums. Using a relation

$$\sum_{\theta\in\Theta(n)}N_\theta!(-1)^{N_\theta}=(-1)^n \tag{E5}$$

for simplification of the first term of (E4), we obtain the right-hand side of (E1).

APPENDIX F: SYMMETRIZATION OF THE PATHS OF INTEGRALS

In this appendix, we prove a relation,

$$\int_{-\infty+\delta i}^{\infty+\delta i} dx\, f_0(x) \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \frac{dy_n}{2\pi i} \frac{1}{y_n - x} f_n(y_n) \right]$$
$$= \sum_{\sigma \subseteq \{1,\ldots,N\}} B_{N_\sigma} \int_{\mathrm{sym}} f_0(x) \left[\prod_{n \in \sigma} f_n(x) \right] \left[\prod_{n \in \{1,\ldots,N\}-\sigma} \frac{1}{y_n - x} f_n(y_n) \frac{dy_n}{2\pi i} \right] dx. \quad \text{(F1)}$$

Here, the definitions of B_n and $\int_{\mathrm{sym}}$ are in (D6) and (D8), respectively, and we assume that $f_n(x)$ is an analytic function on the real axis.

The paths of integrations on the right-hand side of (F1) are changed into ones on the left-hand side of (F1). In other words, symmetrical paths of integrations are changed into ones which keep the relation $\Im y_n < \Im x$. Then, the right-hand side of (F1) becomes

$$\sum_{\sigma \subseteq \{1,\ldots,N\}} \left[\sum_{m=0}^{N_\sigma} (-1)^{N_\sigma - m} \frac{N_\sigma!}{(N_\sigma - m)!\, m!} \left[\sum_{l=0}^{N-N_\sigma} \frac{(l + N_\sigma - m)!}{l!} \frac{(N - N_\sigma)!}{(N - m + 1)!} \right] B_m \right]$$
$$\times \int_{-\infty+\delta i}^{\infty+\delta i} dx\, f_0(x) \left[\prod_{n \in \sigma} f_n(x) \right] \prod_{n \in \{1,\ldots,N\}-\sigma} \left[\int_{-\infty}^{\infty} \frac{dy_n}{2\pi i} \frac{1}{y_n - x} f_n(y_n) \right]. \quad \text{(F2)}$$

Using the following two relations which are easily shown,

$$\sum_{l=0}^{n} \frac{(l+m)!}{l!} = \frac{(n+m+1)!}{n!(m+1)}, \quad \text{(F3)}$$

$$\sum_{m=0}^{n} (-1)^{n-m} \frac{n!}{(n-m+1)!\, m!} B_m = \delta_{n,0} \quad \text{(F4)}$$

for (F2), we obtain the the left-hand side of (F1).

APPENDIX G: ALTERNATIVE REPRESENTATION OF THE MODIFIED JACOBIAN

In this appendix, we show that

$$(2\pi)^{N_\zeta} \left| \frac{\partial I}{\partial x} \right|_{1,\zeta} (y) = \left[\prod_{\theta \in \zeta} N_\theta \right]^{-1} \sum_{\lambda \in \Lambda_c(\zeta)} \sum_{\theta \in \zeta} \sum_{s=1,-1} \frac{s N_\theta}{s M_\theta - (x_\theta - y) i}$$
$$\times \left[\prod_{\{\theta', \theta''\} \in \lambda} \prod_{\theta', \theta'' \neq \theta} C(\theta', \theta'') \right] \left[\prod_{\{\theta, \theta'\} \in \lambda} E(\theta, \theta') \right] \quad \text{(G1)}$$

is an alternative representation of the modified Jacobian (3.4). Here, $C(\theta, \theta')$ and $E(\theta, \theta')$ are defined in (D9) and (D10), respectively.

We can rewrite (3.4) as

$$(2\pi)^{N_\xi}\left|\frac{\partial I}{\partial x}\right|_{1,\zeta}(y)=\left[\prod_{\theta\in\zeta}N_\theta\right]^{-1}\sum_{\lambda\in\Lambda_c(\zeta)}\sum_{\theta\in\zeta}\left[\prod_{\{\theta',\theta''\}\in\lambda}\prod_{\theta',\theta''\neq\theta}C(\theta',\theta'')\right]\frac{2N_\theta M_\theta}{M_\theta^2+(x_\theta-y)^2}$$
$$\times\sum_{\zeta'\subseteq\{\theta'|\{\theta,\theta'\}\in\lambda\}}\frac{1}{N_{\zeta'}+1}\left[\prod_{\theta'\in\{\theta'|\{\theta,\theta'\}\in\lambda\}-\zeta'}C(\theta,\theta')\right]$$
$$\times\left[\prod_{\theta'\in\zeta'}\frac{2N_{\theta'}M_{\theta'}}{M_{\theta'}^2+(x_{\theta'}-y)^2}\right]$$
$$=\left[\prod_{\theta\in\zeta}N_\theta\right]^{-1}\sum_{\lambda\in\Lambda_c(\zeta)}\sum_{\theta\in\zeta}\sum_{s=1,-1}\frac{sN_\theta}{sM_\theta-(x_\theta-y)i}\left[\prod_{\{\theta',\theta''\}\in\lambda}\prod_{\theta',\theta''\neq 0}C(\theta',\theta'')\right]$$
$$\times\prod_{\{\theta,\theta'\}\in\lambda}\left[C(\theta,\theta')+\frac{2N_{\theta'}M_{\theta'}}{M_{\theta'}^2+(x_{\theta'}-x_\theta-sM_\theta)^2}\right]. \tag{G2}$$

In the first equality, we have changed the order of the sums. In the second equality, we have used the relation (H1) proved in Appendix H. Applying a relation

$$K_{M_\theta,M_{\theta'}}(x_\theta-x_{\theta'})-\frac{2M_{\theta'}}{M_{\theta'}^2+(x_{\theta'}-x_\theta-sM_\theta i)^2}=K_{M_\theta-1,M_{\theta'}}(x_\theta-x_{\theta'}-si)$$
$$+\frac{2M_{\theta'}}{M_{\theta'}^2+(x_\theta-x_{\theta'}+s(M_\theta-2)i)^2} \tag{G3}$$

to (G2), we obtain the right-hand-side of (G1). In relation (G3), it is supposed that s is ±1.

APPENDIX H: A PROOF OF A FRACTIONAL RELATION

In this appendix, we prove

$$\sum_{n=1}^{N}\sum_{\sigma\subseteq\{1,\ldots,N\}-\{n\}}\frac{1}{N-N_\sigma}\left[\prod_{m\in\sigma}c_m\right]\left[\prod_{m\in\{1,\ldots,N\}-\sigma}\frac{2a_md_m}{a_m^2+(y-x_m)^2}\right]$$
$$=\sum_{s=\pm1}\sum_{n=1}^{N}\frac{sd_n}{sa_n-(x_n-y)i}\prod_{m\neq n}\left[c_m+\frac{2a_md_m}{a_m^2+(x_m-x_n-sa_ni)^2}\right], \tag{H1}$$

where a_n, c_n, d_n, x_n, and y are arbitrary numbers.

We first prove a relation

$$1=\sum_{n=1}^{N}\prod_{m\neq n}\frac{s_ma_m-(x_m-y)i}{(s_ma_m-s_na_n)-(x_m-x_n)i}. \tag{H2}$$

We regard the right-hand side as a polynomial of degree $N-1$ with respect to y. It is clear that this relation holds on the N points $y=x_n+s_na_ni$. Therefore, this equation is nothing but an identical equation. Dividing both sides of this identical equation by $\Pi_n[a_n-s_n(x_n-y)i]d_n^{-1}$, we get

$$\prod_n\frac{s_nd_n}{s_na_n-(x_n-y)i}=\sum_{n=1}^{N}\frac{s_nd_n}{s_na_n-(x_n-y)i}\prod_{m\neq n}\frac{s_md_m}{(s_ma_m-s_na_n)-(x_m-x_n)i}. \tag{H3}$$

Here, we restrict that s_n is ±1. The sum of each side of this equation with respect to $\{s_n\}$ gives

$$\prod_n \frac{2a_n d_n}{a_n^2+(y-x_n)^2} = \sum_{s=\pm 1} \sum_{n=1}^{N} \frac{2d_n}{sa_n-(x_n-y)i} \prod_{m\neq n} \frac{2a_m d_m}{a_m^2+(x_m-x_n-sa_n i)^2}. \tag{H4}$$

We are in a position to prove the main issue of this appendix. Using (H4) for the left-hand side of (H1), we get

$$\sum_{s=\pm 1} \sum_{n=1}^{N} \frac{sd_n}{sa_n-(x_n-y)i} \sum_{\sigma\subseteq\{1,\ldots,N\}-\{n\}} \left[\prod_{m\in\sigma} c_m\right] \left[\prod_{m\subseteq\{1,\ldots,N\}-\{n\}-\sigma} \frac{2a_m d_m}{a_m^2+(x_m-x_n-sa_n i)^2}\right]. \tag{H5}$$

Expanding the right-hand side of (H1), we also get (H5). This completes a proof of (H1).

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Extensive form of equilibrium nonextensive statistics

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It is argued that, in nonextensive statistical mechanics with Tsallis entropy, the factorization of compound probability over subsystems is a consequence of the existence of thermodynamic equilibrium in the composite system and should be respected by all exact calculations concerning equilibrium subsystems. Using nonadditive energy satisfying this factorization, we propose an additive formalism of nonextensive statistical mechanics with additive q-deformed physical quantities and exponential distributions. This formalism leads to exact quantum gas distributions different from those given by factorization approximation with additive energy. The fermion distribution of the present work shows similar characteristics to the distribution of strongly correlated electrons given by numerical analysis with the Kondo t-J model. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In this paper we will discuss some problems of nonextensive statistical mechanics (NSM) relevant to the factorization of compound probability into the product of single body probability

$$\rho=\prod_{n=1}^{N}\rho_n, \tag{1}$$

where N is the number of subsystems in the system of interest, ρ is the q-exponential distribution (QED): $\rho\propto[1-(1-q)\beta H]^{1/(1-q)}$ ($[.]\geqslant 0$), as given by the maximization of Tsallis entropy $S_q=-\mathrm{Tr}(\rho-\rho^q)/(1-q)$ (Boltzmann constant $k_B=1$ and $q>0$) under some constraints.[1–3] This factorization Eq. (1) has been viewed as a result of the independence of noninteracting subsystems having additive energy, just as in Boltzmann–Gibbs statistics (BGS) supposing short-range interactions, and caused confusion in some theoretical studies of NSM and its applications to many-body problems. On the basis of a new idea relating Eq. (1) to thermodynamic equilibrium, we will argue that the confusion can be avoided if we introduce suitable nonadditive thermodynamic variables satisfying Eq. (1). Some theoretical consequences for quantum distributions of this ''equilibrium version'' of NSM will be studied.

Due to the necessity of defining additive average value of some extensive q-deformed thermodynamic variables, the discussions will be made within the formalism of incomplete statistics (IS) with $\mathrm{Tr}\,\rho^q=1$ and normalized average $\overline{x}=\mathrm{Tr}\,\rho^q x$.[3] The reader will find that the quantum distributions of IS indeed show some particular properties already noticed with strongly correlated electrons.

II. ABOUT INCOMPLETE NORMALIZATION

IS as an alternative version of NSM was originally motivated by some theoretical peculiarities in the last Tsallis version of NSM based on the conventional normalization and unnormalized expectations.[3]

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The basic assumption of IS is that our knowledge about physical systems is in general incomplete due to unknown space–time correlations or the effects of known interactions which cannot be exactly described. In this case, probability distributions are incomplete, i.e., $\mathrm{Tr}\,\rho = Q \neq 1$[4] (or $\Sigma_{i=1}^{w} p_i = Q$ where w is only the number of accessible states in phase space). One can only write $\mathrm{Tr}\,F(\rho) = 1$ where F is a certain function of ρ. In the case of complete or approximately complete distribution (such as in BGS), F is an identity function. Recently, in order to overcome some of the theoretical difficulties of NSM in keeping the framework prescribed by Tsallis entropy, we proposed[3] $F(\rho) = \rho^q$ so that

$$\mathrm{Tr}\,\rho^q = 1, \tag{2}$$

where q is incompleteness index.[3] Since $\rho < 1$, we have to set $q \in [0,\infty]$. $q = 0$ should be avoided because it leads to $\rho = 0$ for all states. We note that Eq. (2) has been successfully employed to deduce some power laws based on Rényi's entropy.[5] This kind of *incomplete normalization* is possible whenever the phase space is partially known or accessible. With a fractal or chaotic phase space, e.g., a complete calculation of probability becomes, in general, impossible. In this sense, a plausible justification of Eq. (2) may be inspired by a work of Tsallis[6] discussing nonadditive energy and probability distributions on fractal supports, although at that stage the work was not connected to anomalous normalization like Eq. (2). In that work, considering some simple self-similar fractal structures (e.g., Cantor set), one can obtain

$$\sum_{i=1}^{W} \left[\frac{V_i(k)}{V(0)} \right]^{d_f/d} = 1, \tag{3}$$

where $V_i(k)$ may be seen as the segments of the fractal structure at a given iteration of order k, $V(0)$ a characteristic volume of the fractal structure embedded in a d-dimension Euclidean space, $d_f = \ln n / \ln m$ is the fractal dimension, n the number of segments replacing a segment of the precedent iteration, m the scale factor of the iterations, and $W = n^k$ the total number of segments at the kth iteration. If we suppose that the fractal structure with $k \to \infty$ is a phase space containing homogeneously distributed points, the *exact microcanonical probability distribution* of the kth iteration can be defined as

$$p_i = \frac{V_i(k)}{V} = \frac{V_i(k)}{\Sigma_i^W V_i(k)}$$

where V is the total volume of the phase space. This distribution obviously sums to one. The problem is that V is an indefinite volume as $k \to \infty$ and impertinent for exact probability definition. In addition, V is not differentiable and contains inaccessible points. Thus exact summation in V would be impossible. Now if we define $p_i = V_i(k)/V_0$ as a physical or effective distribution, then we have $\Sigma_{i=1}^{W} p_i^{d_f/d} [V_0/V(0)]^{d_f/d} = 1$, where V_0 is *a completely accessible and infinitely differentiable support* on which the calculation of p_i is possible. If we choose $V_0 = V(0)$, we can write Eq. (2) with $q = d_f/d$. The conventional normalization $\Sigma_{i=1}^{W} p_i = 1$ can be recovered when $d_f = d$.

The above-given example is only a case of equiprobable distribution on simple fractal structure, but it illustrates very well the possibility that, in complex cases, a physical probability may not sum to one and may sum to unity only through a kind of power normalization, which, pertinent and useful for incomplete distributions, is consistent with the discussions of Ref. 6 on the mass calculation and the information consideration in porous structures.

III. FACTORIZATION OF COMPOUND PROBABILITY AND THERMODYNAMIC EQUILIBRIUM

In NSM, there are two major problems connected tightly to the factorization of compound probability. The first concerns the application of NSM to many-body systems via one-body distribution. NSM is originally intended to describe complex systems with long-range interactions or

fractal structure of space–time showing nonextensive phenomena. So from the beginning of this theory, Eq. (1) is supposed for composite systems containing N *statistically* independent subsystems in order to elicit the nonextensive character by the following relation:

$$\ln[1+(1-q)S_q]=\sum_{n=1}^{N}\ln[1+(1-q)S_q(n)]. \tag{4}$$

For $N=2$, $S_q=S_q(1)+S_q(2)+(1-q)S_q(1)S_q(2)$ as one often finds in the literature. Due to this *independence*, it has been believed by many that exact calculations within NSM should use the additive Hamiltonian $H_0=\Sigma_{n=1}^{N}H_n$, where H_n is the Hamiltonian of nth subsystem.[2,7–11] However, this Hamiltonian is not compatible with either Eq. (1) or Eq. (4) since these equations applied to QED mean:[1,12,13]

$$H=\sum_{n=1}^{N}H_n+\sum_{k=2}^{N}[(q-1)\beta]^{k-1}\sum_{n_1<n_2<\cdots<n_k}^{N}\prod_{j=1}^{k}H_{n_j}=H_0+H_c, \tag{5}$$

where β is the inverse temperature. In order to reconcile H_0 and Eq. (1), a so-called *factorization approximation* is proposed[14] by neglecting the second term on the right-hand side of Eq. (5). This approximation has been, explicitly or not, employed in most of the applications of NSM[13–18] via one-body QED. These applications certainly show the usefulness of one-body QED, but the approximation neglecting the correlation energy by supposing sometimes weak interacting dilute particles[19] is not a reassuring basis. Indeed, some recent works show that the correlation energy (H_c) given by the second term of Eq. (5) is in general not negligible[12] and that the partition function given by using additive energy is completely different from that given by using Eq. (5) when N is large.[11] So a doubt arises about the connection between independence of subsystems and additive energy. Recently, an interesting idea is forwarded to define a ''quasi-independence'' according to nonadditive energy Eq. (5) in order to apply NSM to turbulence flow problems.[19] As a matter of fact, this proposal implies rejection of classical independence for Eq. (1).

The second problem connected with probability factorization is the establishment of zeroth law and the definition of temperature for NSM. It was believed that the zeroth law of thermodynamics was absent within NSM[20] due to the paradox between Eq. (1) and the additive energy. Recently, a series of works have been published on this issue[21] claiming the establishment of zeroth law and the definition of a generalized temperature on the basis of additive Hamiltonian H_0 and Eq. (4) by neglecting H_c. It is evident that the above-mentioned paradox persists behind this approximate zeroth law.

The central question is as follows. Equation (1) certainly implies independence of noninteracting systems for BGS, but does it mean the same thing for NSM? Very recently, Abe[22] proposed a general pseudoadditivity for entropy required by the existence of thermal equilibrium in composite nonextensive systems. For a system containing N subsystems, the pseudoadditivity is

$$\ln[1+\lambda_S f(S)]=\sum_{n=1}^{N}\ln[1+\lambda_S f(S_n)], \tag{6}$$

where f is certain differentiable function satisfying $f(0)=0$ and λ_S a constant depending on the nature of the system of interest. On the other hand, Eq. (6) applied to Tsallis entropy means $f(S)=S$ and $\lambda_S=1-q$,[22] which directly leads to $\ln \mathrm{Tr}\,\rho^q=\Sigma_{i=1}^{N}\ln \mathrm{Tr}\,\rho_i^q$ or Eq. (1) (i.e., with classical probability p_i of the state i, $(p_ip_j)^q=p_{ij}^q$ means $p_ip_j=p_{ij}$). So Eq. (1) *has nothing to do with statistical independence of subsystems. It is a consequence of the existence of thermodynamic equilibrium* and must be rigorously respected by all exact calculations. Equilibrium energy has been proved[23] to satisfy the same kind of pseudoadditivity as Eq. (6) (S is replaced by H). If we choose $f(H)=H$ and $\lambda_H=(q-1)\beta$, we get

$$\ln[1+(q-1)\beta H]=\sum_{n=1}^{N}\ln[1+(q-1)\beta H_n], \tag{7}$$

which is just Eq. (5) satisfying Eq. (1). In this way, the zeroth law becomes evident and a temperature can be straightforwardly defined at maximum entropy and minimum energy.[3,12]

IV. ADDITIVE FORMALISM OF NSM

A. Information measure

The g-logarithmic information measure

$$I_\nu=\frac{(1/\rho)^\nu-1}{\nu} \tag{8}$$

is a nonadditive generalization of Hartley formula $I=\ln(1/\rho)$ and can be employed to deduce Tsallis entropy.[1,3,24] I_g or I is the information needed to specify at which state the system is localized. ν equals $1-q$ or $q-1$, depending on the normalization procedures of ρ.[25] Using Eq. (1), we get

$$\ln(1+\nu I_\nu)=\sum_{n=1}^{N}\ln(1+\nu I_\nu^{(n)}), \tag{9}$$

where $I_\nu^{(n)}$ is the information needed to specify the nth subsystem. This pseudoadditivity is evident if we recast the generalized Hartley formula, Eq. (8), as follows

$$I_\nu=\frac{e^{-\nu\ln\rho}-1}{\nu}=\frac{e^{\nu I}-1}{\nu}, \tag{10}$$

where

$$I=\ln\frac{1}{\rho}=\frac{\ln(1+\nu I_\nu)}{\nu} \tag{11}$$

can be referred to as q-deformed information measure and is additive supposed Eq. (1). It is noteworthy that this I is not the quantity of Hartley information if ρ is a nonextensive distribution for $\nu\neq 0$.

B. Canonical ensemble

Now let us define an additive entropy S as follows:

$$S=\mathrm{Tr}\,\rho^q\ln\frac{1}{\rho} \tag{12}$$

and an additive q-deformed ''Hamiltonian''

$$h=\frac{\ln[1+(q-1)\beta H]}{(q-1)\beta}. \tag{13}$$

So Eq. (7) becomes

$$h=\sum_{n=1}^{N}h_n. \tag{14}$$

This means the following transformations:

$$H=\frac{e^{(q-1)\beta h}-1}{(q-1)\beta}, \quad H_n=\frac{e^{(q-1)\beta h_n}-1}{(q-1)\beta} \tag{15}$$

and

$$\rho=\frac{1}{Z}[1+(q-1)\beta H]^{1/(1-q)}=\frac{1}{Z}e^{-\beta h}, \tag{16}$$

where $Z^q=\mathrm{Tr}\, e^{-q\beta h}$.[3] It should be noticed that, when addressing a system of N particles, we have to write $H_n=p_n^2/2m+V_n$ for a single particle so that

$$h_n=\frac{\ln\left[1+(q-1)\beta\left(\frac{p_n^2}{2m}+V_n\right)\right]}{(q-1)\beta}$$

where $p_n^2/2m$ is the classical kinetic energy and V_n is the potential energy. It is clear that H_n, instead of h_n, is the physical energy. When $q=1$ ($H_c=0$), we recover $H_n=h_n$ and $H=h=\Sigma_{n=1}^{N} p_n^2/2m$. The q-deformed internal energy u is defined as follows:

$$u=\mathrm{Tr}\,\rho^q h. \tag{17}$$

We can easily show that the distribution Eq. (16) can be yielded by the maximum of the additive "entropy" S (which surely exists due to the monotonic relation between I and I_ν) under the constraints of Eq. (17) and incomplete normalization $\mathrm{Tr}\,\rho^q=1$. It is easy to verify that $S=\ln Z+\beta u$ and, via the zeroth law, $\partial S/\partial u=\beta=1/T$. The "first law" is given by $\mathrm{d}u=T\,dS-p\mathrm{d}V$ where p is q-deformed pressure and V the volume of the system which is chosen to be additive here. The q-deformed Helmholtz free energy f is defined as $f=u-TS=-T\ln Z$ and can be connected to the nonadditive one

$$F_q=-T\frac{Z^{1-q}-1}{1-q}$$

(Refs. 1 and 3) as follows:

$$f=\frac{\ln[1+(q-1)\beta F_q]}{(q-1)\beta}. \tag{18}$$

So $p=-(\partial f/\partial V)_T=P/Z^{1-q}$ where $P=-(\partial F_q/\partial V)_T$ is the real pressure. In this scenario, the thermodynamic equilibrium of a system C containing two equilibrium systems A and B satisfying $V(C)=V(A)+V(B)$ corresponds to $\beta(A)=\beta(B)$ and $p(A)=p(B)$. This implies that $P(A)\neq P(B)$ if $Z(A)\neq Z(B)$. This is because we have supposed nonadditive energy and additive volume. As a matter of fact, in this formalism, if we want $P(A)=P(B)$ at equilibrium, we must accept nonadditive volume and additive q-deformed volume v with which the first law becomes $\mathrm{d}u=T\,\mathrm{d}S-P\,\mathrm{d}v$. This means: $P=-(\partial F_q/\partial V)_T=-(\partial f/\partial v)_T$. This relation can help to deduce the $v-V$ relation. We also have $v=(\partial g/\partial P)_T$ where the q-deformed Gibbs energy is given by $g=f+Pv$. Since v is additive, V will be nonadditive if v is not a linear function of V. We will come back to this issue later in this paper.

C. Grand canonical ensemble

It is known that the grand canonical ensemble QED has been given by[1,9,14]

$$\rho\propto[1-(1-q)\beta(H-\mu N)]^{1/(1-q)} \tag{19}$$

for N identical particle systems, where μ is chemical potential. This distribution has been widely used for quantum particle systems.[14–16,26] But the zeroth law has never been rigorously established for this ensemble. In a previous work,[26] one of the authors of present paper (Q.A.W.) deduced exact quantum distributions on the basis of Eq. (19) and the following relation suggested by Eq. (1):

$$\rho \propto [1-(1-q)\beta(H_n-\mu)]^{N/(1-q)}. \tag{20}$$

In the framework of IS,[3,26] the exact distributions are given by

$$\overline{n_k}=\frac{1}{[1+(q-1)\beta(e_k-\mu)]^{q/(q-1)}\pm 1}, \tag{21}$$

where e_k is the energy of the one-particle state k and "+" and "−" correspond to fermions and bosons, respectively. Now we show that this distribution can be written in exponential form just as for conventional noninteracting quantum gases and that the zeroth law can be rigorously verified.

Let us suppose $\beta=\beta'/[1+(q-1)\beta'\mu]=\beta'[1-(q-1)\beta'\mu']$ (or $\beta'=\beta/[1-(q-1)\beta\mu]$) and $\mu=\mu'/[1+(1-q)\beta'\mu']$ (or $\mu'=\mu/[1+(q-1)\beta'\mu]=\mu[1-(q-1)\beta\mu]$) which imply $\beta'\mu'=\beta\mu$. Equation (20) can be recast as

$$\rho=\frac{1}{Z}[1-(1-q)\beta' H_n]^{N/(1-q)}[1+(1-q)\beta'\mu']^{N/(1-q)}=\frac{1}{Z}e^{-N\beta(h_n-\omega)}, \tag{22}$$

where

$$\omega=\frac{\ln[1+(1-q)\beta'\mu']}{(1-q)\beta'}, \quad h_n=\frac{\ln[1+(q-1)\beta' H_n]}{(q-1)\beta'}.$$

$Z^q=\mathrm{Tr}[1-(1-q)\beta(H-\mu N)]^{q/(1-q)}=\{\mathrm{Tr}[1-(1-q)\beta' H_n]^{q/(1-q)}[1+(1-q)\beta'\mu']^{q/(1-q)}\}^N$ $=(\mathrm{Tr}\, e^{-q\beta(h_n-\omega)})^N=z^N$ and where z is one-particle partition function. Just as for the canonical ensemble, this exponential distribution can be shown to be the result of the maximization of S under the constraint $\overline{N}=\mathrm{Tr}\,\rho^q N$ in addition to Eq. (17) and incomplete normalization. Now Eq. (21) can be written as

$$\overline{n_k}=\mathrm{Tr}\,\rho^q n_k=\frac{1}{e^{q\beta'(\epsilon_k-\omega)}\pm 1}=\frac{1}{[1+(q-1)\beta' e_k]^{q/(q-1)}[1-(q-1)\beta'\mu']^{q/(q-1)}\pm 1}, \tag{23}$$

where ϵ_k is the eigenvalue of h_n. From Eq. (21), we see that, for free particles (*in the sense that we do not write the energy of interaction between particles in the Hamiltonian and let it be "absorbed" in the nonextensive part of energy H_c and related to q different from unity*), we have to set $q<1$ to ensure positive $[1+(q-1)\beta(H_n-\mu)]$ for fermions when $T\to 0$. This means that, at low temperatures, there will be few fermions beyond Fermi energy. For bosons with $\mu<0$, we have to put $q>1$.

It is straightforward to write $S=\ln Z+\beta' u+\beta'\omega\overline{N}$ and, with the method employed in Refs. 3 and 12 to show that, for a system C containing two equilibrium systems A and B satisfying $\overline{N}(C)=\overline{N}(A)+\overline{N}(B)$, $\beta'(A)=\beta'(B)$, and $\omega(A)=\omega(B)$ thus $\mu'(A)=\mu'(B)$, $\mu(A)=\mu(B)$ and $\beta(A)=\beta(B)$ or $T(A)=T(B)$. The zeroth law is verified. One may ask why we identify β, instead of β', to real temperature. The possible reasons are the following: (1) β is the Lagrange multiplier of the constraint on real energy in entropy maximization; (2) if β' is inverse temperature, then μ' must be chemical potential, which makes it impossible to get distribution Eq. (22) by real entropy maximization with the constraint on $\overline{N}$; (3) e_f would be different from the chemical potential μ' and equal to $\mu'/[1+(1-q)\beta'\mu']$ which inevitably drops to zero when $T\to 0$.

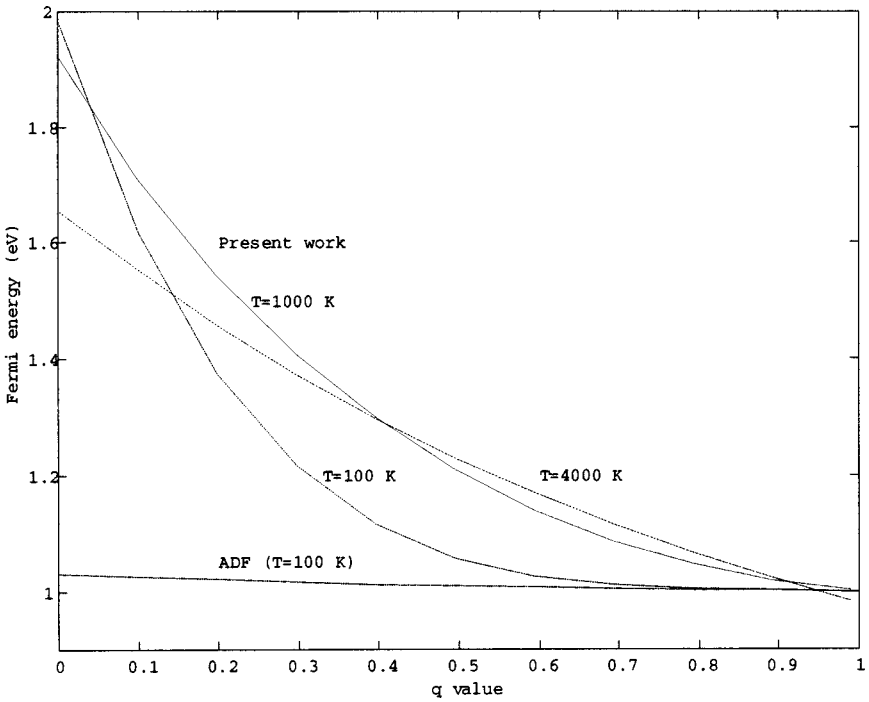

FIG. 1. q-dependence of Fermi energy e_f of IS quantum distribution in the present work and of ADF given by the factorization approximation with additive energy. The fermion density σ is chosen to give $e_f^0=1$ eV for CFD distribution at $T=0$. IS e_f shows strong increase with decreasing q up to two times e_{f_0}. But ADF e_f depends only slightly on q. We also notice that the T-dependence of IS e_f is not monotonic as shown in Fig. 2.

Now we will focus the discussion on two-dimensional fermion distribution. According to Eq. (21) the Fermi energy e_{f_0} at $T=0$ is given by $e_{f_0}=2\pi\hbar^2\sigma/m$ where σ is the particle density and $\hbar$ Planck constant.

When $T>0$, the summation $\overline{N}=\Sigma_k \overline{n_k}$ cannot be calculated for arbitrary q to give an explicit expression of e_f. So we have recourse to numerical calculation of q-dependence of e_f for given temperatures (Fig. 1) and T dependence for given q values (Fig. 2). We see that, for the approximate distributions functions (ADF) $n_k=1/\{[1+(q-1)\beta(e_k-\mu)]^{1/(q-1)}+1\}$ deduced from Eq. (19) with factorization approximation and additive energy,[14] e_f depends only slightly on q. On the other hand, the e_f of IS in the present work shows a strong increase with decreasing q up to two times e_{f_0} of conventional Fermi–Dirac distribution (CFD). This e_f increase has indeed been noticed through numerical calculations for strongly correlated heavy electrons on the basis of a tight-binding Kondo lattice model.[27,28] In Fig. 2, we show that e_f of IS does not monotonically decrease with increasing temperature, in contrast with the e_f behavior of CFD. This kind of nonmonotonic temperature evolution of e_f was also seen through numerical work for correlated electrons in the two-dimensional $t-J$ model.[29]

The IS distribution given by Eq. (21) is plotted in Fig. 3 for $T=100$ K. The particle density σ is chosen to give $e_{f_0}=1$ eV. As expected, the distribution changes drastically with q. When q decreases, we notice a flattening of the distribution always with a sharp drop of occupation number n at e_f which increases. This flattening is also noticed in numerical calculations for strong coupling electrons.[27,28]

The grand canonical partition function Z can be calculated to give the q-deformed grand potential $\overline{\omega}=-T'\ln Z=(T'/q)\Sigma_k \ln(1-\overline{n_k})$ as usual, where $T'=1/\beta'=T+(1-q)\mu$. The grand potential is given by

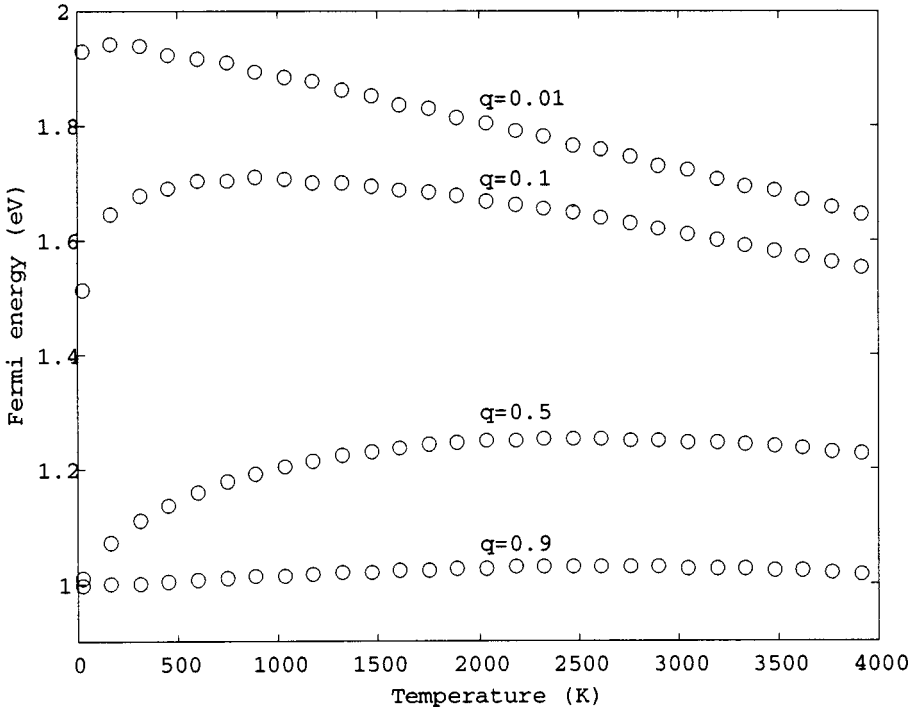

FIG. 2. T-dependence of Fermi energy e_f of IS quantum distribution in present work. The fermion density σ is chosen to give $e_f^0=1$ eV for CFD distribution at $T=0$. The T-dependence of e_f is in general not monotonic, in contrast with the classical decreasing behavior of e_f with increasing temperature. We notice that, at low temperature, e_f shows an increase with increasing T.

$$\Omega=\frac{e^{(q-1)\beta'\overline{\omega}}-1}{(q-1)\beta}=T\frac{\Pi_k(1-\overline{n_k})^{(q-1)/q}-1}{(q-1)}. \tag{24}$$

In this q-deformed extensive formalism, Euler theorem applies just as in BGS. So we have $g=\omega\overline{N}=u+pV-T'S$. Compare this with $S=\ln Z+\beta' u-\beta'\omega\overline{N}$ to obtain the following equations of state:

$$pV=T'\ln Z=\frac{T'}{q}\sum_k \ln(1-\overline{n_k}). \tag{25}$$

V. DISCUSSION AND CONCLUSION

The formalism of NSM presented here is required by the existence of thermodynamic equilibrium or by Eq. (1) for nonextensive systems described by Tsallis entropy. Theoretically the formalism is self-consistent. Experimental or numerical evidence is needed to verify the thermodynamic relations. In this framework, all the successful applications of NSM conforming with Eq. (1) are still valid. But the approximate applications carried out for many-body systems using additive energy as exact Hamiltonian (not consistent with the existence of thermodynamic equilibrium) should be carefully reviewed.

As mentioned previously, we have noticed similar properties between the IS fermion distribution and that of strongly correlated electrons.[27,28] This similarity shows the merit of NSM in describing strong interacting systems. On the other hand, we noticed that a flattening of n drop at e_f with increasing correlation, observed experimentally and numerically with weakly correlated

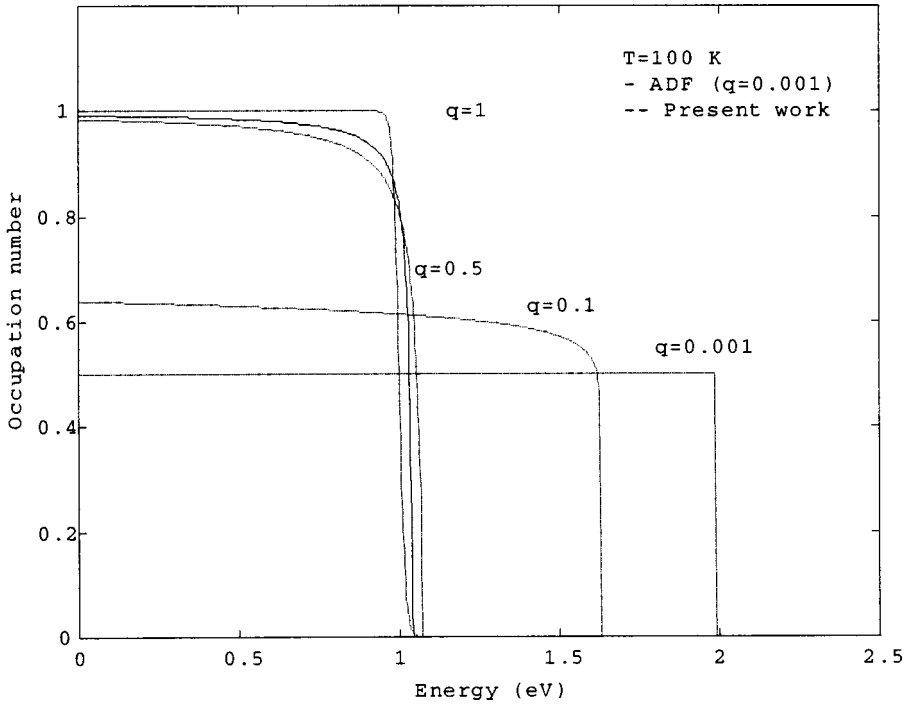

FIG. 3. Fermion distributions of ADF and of IS in the present work. ADF distribution is only slightly different from that at $q=1$ (CFD one) even with q very different from unity. The IS distribution of the present work changes drastically with decreasing q. As $q\to 0$, the occupation number tends to 1/2 for all states below e_f which increases up to 2 times e_{f_0}.

electrons,[27,28,30–32] is absent within NSM fermion distributions which always show very sharp n drop at e_f at low temperatures. A detailed study of this problem will be presented in another paper of ours.

It is worth mentioning that, in the present work, energy is nonadditive to satisfy the requirement of thermodynamic equilibrium. Nonadditive energy can happen if interaction is no longer of short-range and not localized only between the containing walls of subsystems. But in the literature, there are rarely explicit expressions of nonadditive energy. One of explicit examples is the long-range Ising model[33] where the internal energy $U(N,T)$ may be proportional to N^c (c is a constant), instead of N, the number of spins in the system. This energy can be shown to satisfy Abe's pseudoadditivity for energy[23] if we choose $f(U)$ to be proportional, e.g., to N (with $\lambda_H=0$) or to e^N-1 (with $\lambda_H=1$).

Indeed, theoretically, nonadditive physical quantities (energy, volume, ...) are not evident within the statistics with complete distributions because all possible states (all points in phase space) are counted and summed here. But from the viewpoint of incomplete statistics, nonadditivity may be interpreted as a consequence of incomplete summation of state points in phase space due to the incompleteness of our knowledge about the physical systems.[3]

Nevertheless, the fact that the correlation energy H_c of NSM depends on temperature, as shown in Eq. (5) or Eq. (7), is not an easy aspect to be understood. A possible interpretation is that these nonadditive equations are required or prescribed by thermal equilibrium with Tsallis entropy and so naturally change with temperature. This implies that the effect of correlations may depend on temperature.

Summing up, within the framework of *incomplete statistics*, it is argued that the nonextensive thermostatistics should be based on the factorization of compound probability suggested, not by ''independence'' of noninteracting systems, but by *existence of thermodynamic equilibrium in interacting systems having Tsallis entropy*. So this factorization must be viewed as a fundamental hypothesis of NSM and rigorously satisfied by all exact calculations relative to equilibrium sys-

tems. On this basis, we have elaborated an additive formalism of NSM based on the maximization of an additive deformed entropy subject to constraints on additive particle number and additive q-deformed energy. The IS quantum distributions of this formalism are compared with the distributions previously obtained by using complete probability and additive energy in factorization approximation and also with numerical results for strongly correlated electrons. It is shown that some effects of strong correlations—the flattening of the fermion distribution and the sharp cutoff of occupation number at e_f which shows strong increase with increasing interaction—can be observed in IS fermion distribution with decreasing q value.

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d-dimensional Lévy flights: Exact and asymptotic

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The analytic and asymptotic properties of the spherically symmetric d-dimensional Lévy stable probability density function, $p_\alpha^d(r)$, are discussed in detail. These isotropic stable probability density functions (pdfs) are analogous to the one-dimensional symmetric Lévy stable pdfs previously studied by the present authors [J. Math. Phys. **43**, 2670 (2002)]. We construct a hypergeometric representation of $p_\alpha^d(r)$ when α is rational, and find a number of new representations of $p_\alpha^d(r)$ in terms of special functions for various values of d and α. A recursion relation is found between $p_\alpha^d(r)$ and $p_\alpha^{d+2}(r)$, which, in particular, implies there exists a simple map between $p_\alpha^1(r)$ and $p_\alpha^3(r)$. As in our previous paper, we discuss the properties of $p_\alpha^d(r)$ for both the cases $\alpha \leqslant 2$ and $\alpha > 2$. We demonstrate the existence of intricate exponentially small series in the large r asymptotics of $p_\alpha^d(r)$ when α is an integer, which are dominant when α is even. We explicitly construct this beyond all orders expansion of $p_\alpha^d(r)$ for arbitrary integral α and d. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1500423]

I. INTRODUCTION

Applications of the Lévy stable probability density function (pdf) abound, in disciplines as diverse as physics, biology, and finance, as a mechanism for constructing stochastic models which possess no characteristic scale.[1] In d spatial dimensions, isotropic Lévy stable pdfs, denoted $p_\alpha^d(r)$, display large r asymptotic behavior of the form $p_\alpha^d(r) \to r^{-d-\alpha}$, where the parameter $0 < \alpha \leqslant 2$ is referred to as the order of the given pdf.[2] This asymptotic power law behavior leads to the divergence of all moments $\langle |\mathbf{r}|^n \rangle$ for $n > \alpha$. Random flights whose steps are chosen via an isotropic pdf displaying $r^{-d-\alpha}$ large r behavior have been used to model widely varied phenomena from the paths followed by animals searching for food,[3] to classical problems in statistical mechanics, e.g., Ref. 4. It has recently been argued[5,6] that the drip paintings of Jackson Pollock involve paint trajectories displaying $r^{-d-\alpha}$ behavior. The Lévy walk[1,7] model, which is a continuous time random walk whose step pdf is asymptotic to $r^{-d-\alpha}$, and its generalizations,[8] are popular methods for modeling systems displaying anomalous diffusion.[9–11]

A number of interesting mathematical questions concerning d-dimensional random flights whose steps are chosen via isotropic Lévy stable pdfs have been addressed recently, e.g., Refs. 12 and 13. However, the mathematical treatises on the analytic properties of the Lévy stable pdf are largely restricted to one dimension.[14,15] We recently demonstrated that the one-dimensional symmetric Lévy stable pdfs of rational order can be expressed in terms of hypergeometric functions, and listed a number of new representations for various values of α in terms of special functions.[16] We also discussed the utility of the symmetric stable densities when the order is larger than two. In such cases $p_\alpha^1(r)$ fails to satisfy the non-negativity condition required of a pdf despite being stable in every sense, but does however display remarkably intricate and interesting exponential asymptotic behavior when α is an even integer. A link between $p_4^1(r)$ and Pearcey's integral was demonstrated. In this work we investigate in detail the analytic and asymptotic properties of $p_\alpha^d(r)$. These functions are the natural generalization to higher dimensions of the symmetric one-dimensional Lévy stable pdfs studied in Ref. 16, and it is found that analogs of virtually all

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results obtained in that work can be carried through to the d-dimensional case.

The isotropic d-dimensional Lévy stable pdf can be defined in an identical way to the one-dimensional case. Let X_1 and X_2 be independent random d vectors with the same pdf $p_\alpha^d(r)$, then $p_\alpha^d(r)$ is defined to be Lévy stable[17,18] if it is a solution to the following, for all positive c_1 and c_2:

$$c_1X_1+c_2X_2=cX, \tag{1.1}$$

where X has the same pdf as X_1 and X_2.

The isotropic solutions of this equation have characteristic functions of the form[17,18]

$$\tilde{p}_\alpha^d(q)=\exp(-|\mathbf{q}|^\alpha), \tag{1.2}$$

which is identical to the characteristic function of the one-dimensional symmetric Lévy stable pdfs (with the domain considered as $\mathbb{R}_{\geqslant 0}$ rather than $\mathbb{R}^d$). It is interesting to note that pdfs with characteristic functions of the form (1.2) are stable for all positive α, including $\alpha>2$, as stressed by Bouchaud.[1] Due to the form of (1.2), the only d dependence appears via the inverse Fourier transform that yields the pdf. The isotropy of $\tilde{p}_\alpha^d(q)$ implies that its d-dimensional Fourier transform decomposes into one integral over the radial variable,

$$p_\alpha^d(r)=\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} d^dq e^{-i\mathbf{r}\cdot\mathbf{q}}\exp(-|\mathbf{q}|^\alpha), \tag{1.3}$$

$$p_\alpha^d(r)=\frac{r}{(2\pi r)^{d/2}}\int_0^\infty \mathrm{d}q\, J_{(d/2)-1}(qr)q^{d/2}e^{-q^\alpha}, \tag{1.4}$$

$J_{(d/2)-1}(qr)$ is a Bessel function.

An interesting property of (1.4) that we will make use of later is the following recursion relation linking $p_\alpha^d(r)$ to $p_\alpha^{d+2}(r)$:

$$\frac{-1}{2\pi r}\frac{\partial}{\partial r}p_\alpha^d(r)=p_\alpha^{d+2}(r). \tag{1.5}$$

The proof of this relation is straightforward, and relies only on the identity $(-\mathrm{d}/\mathrm{d}z)[z^{-\nu}J_\nu(z)]=z^{-\nu-1}J_{\nu+1}(z)$.[19] As such, (1.5) is just a special case of a general relation that holds between the d-dimensional and $d+2$-dimensional Fourier transforms of any isotropic function $f(\mathbf{q})=f(q)$. An important consequence of (1.5) is that it allows us to construct the three-dimensional analog of all the one-dimensional results in Ref. 16, in particular the analogs of the special function representations of $p_\alpha^1(r)$ for various α.

It is the analytic and asymptotic properties of (1.4) that we shall study in detail in this work, both when $0<\alpha\leqslant 2$ and $p_\alpha^d(r)$ defines a pdf, and also when $\alpha>2$. We begin by displaying a number of special functions representations of $p_\alpha^d(r)$ for various α in both two and three dimensions, using the dimensional recursion relation (1.5). The large and small r power series of $p_\alpha^d(r)$ are constructed using standard Mellin transform techniques, and we then utilize these representations to construct hypergeometric representations of $p_\alpha^d(r)$ when α is rational. The similarities and differences between this and the one-dimensional result[16] are discussed. We go on to demonstrate that as in the one-dimensional case $p_\alpha^d(r)$ displays intricate exponential asymptotic behavior when $\alpha\in\mathbb{Z}_{\geqslant 3}$, which deserves attention for its own intrinsic interest despite the fact that $p_\alpha^d(r)$ does not define a pdf when $\alpha>2$. We obtain the complete asymptotic expansion of $p_\alpha^d(r)$ for general d, and arbitrary $\alpha\in\mathbb{Z}_{\geqslant 3}$. This not only generalizes the asymptotic results in Ref. 16 from one dimension to d dimensions, but it also generalizes from the specific cases of α considered in Ref. 16 to arbitrary integral $\alpha\geqslant 3$. Finally, we calculate the absolute moments for $p_\alpha^d(r)$, whose convergence or divergence is intimately linked to the question of whether the dominant behavior of the large r asymptotics is exponential or algebraic.

II. ISOTROPIC STABLE PDFS vs LÉVY FLIGHTS

Before beginning our investigation of (1.4), we think it useful to clarify a distinction between $p_\alpha^d(r)$ and a related pdf which is often referred to in the literature.

Any isotropic pdf $p(\mathbf{r})$ can be written in the form[17]

$$p(\mathbf{r}) = \frac{1}{S_d|\mathbf{r}|^{d-1}} w(r), \tag{2.1}$$

where S_d is the surface area of the unit d-sphere, and we refer to $w(r)$ as the *step length* pdf. Recasting $p_\alpha^d(r)$ into this form we obtain

$$p_\alpha^d(r) = \frac{1}{S_d|\mathbf{r}|^{d-1}} w_\alpha^d(r), \tag{2.2}$$

$$w_\alpha^d(r) = \frac{2}{\Gamma\left(\frac{d}{2}\right)} \int_0^\infty dq \left(\sqrt{\frac{qr}{2}}\right)^d J_{(d/2)-1}(qr) e^{-q^\alpha}. \tag{2.3}$$

In physical applications[3,4,9,10,13,20] the pdf underlying $r^{-d-\alpha}$ asymptotic behavior appears to be generally regarded as an isotropic pdf with a stable *step length* pdf. Such a pdf, which we denote $m_\alpha^d(\mathbf{r})$, has the form

$$m_\alpha^d(\mathbf{r}) = \frac{1}{S_d|\mathbf{r}|^{d-1}} 2p_\alpha^1(|\mathbf{r}|) = \frac{1}{S_d|\mathbf{r}|^{d-1}} w_\alpha^1(r). \tag{2.4}$$

Despite being constructed from a stable pdf, $m_\alpha^d(\mathbf{r})$ itself is not stable (except trivially when $d=1$). This is easily observed by taking its Fourier transform and noting that one does not obtain (1.2). The difference between $m_\alpha^d(\mathbf{r})$ and $p_\alpha^d(r)$ is clearly that the *step length* pdf of $p_\alpha^d(r)$ is highly d dependent, which is how it manages to satisfy stability for arbitrary d, whereas the *step length* pdf for $m_\alpha^d(\mathbf{r})$ is independent of d. There appears to be no advantage in taking $m_\alpha^d(\mathbf{r})$ as the ansatz for pdfs displaying $r^{-d-\alpha}$ asymptotic behavior. As we demonstrate, $p_\alpha^d(r)$ is no more complicated to handle than $p_\alpha^1(r)$. Stability is especially useful in the simple case of an n step random flight, because by definition stability of the step pdf implies that the pdf for the position of the walker after n steps is simply the step pdf rescaled.

III. SOME SPECIAL FUNCTION REPRESENTATIONS

A number of special function representations for the case of $d=1$ are listed in Ref. 16. We find here the three-dimensional analogs of these results, by utilizing the dimensional recursion relation, (1.5), or via more direct methods where appropriate. The case of $d=2$ is more complicated since we cannot generate any of the two-dimensional results from the known one-dimensional results. We will construct however a hitherto unknown representation of $p_{1/2}^2(r)$ in terms of Bessel functions. We begin this section by listing the simple known cases of $p_2^d(r)$ and $p_1^d(r)$, which correspond to the d-dimensional Gaussian and Cauchy pdfs, respectively. These are the only known cases where (1.4) can be simplified for arbitrary d.

Starting with (1.3) it is trivial to obtain

$$p_2^d(r) = \frac{e^{-r^2/4}}{(\sqrt{4\pi})^d}. \tag{3.1}$$

The Cauchy result can be recovered from (1.4), since when $\alpha=1$ this is a known integral[21]

$$p_1^d(r)=\frac{\Gamma\left(\frac{d+1}{2}\right)}{\pi^{(d+1)/2}}\frac{1}{(1+r^2)^{(d+1)/2}}. \tag{3.2}$$

A. Three dimensions

Representations of $p_\alpha^3(r)$ in the cases of $\alpha=3$, $\frac{1}{3}$, and $\frac{2}{3}$ can all be generated in a straightforward fashion from the results in Ref. 16 via (1.5), and we find that

$$p_{2/3}^3(r)=\frac{5}{2^{4/3}3^{5/2}\pi^{3/2}}r^{-8/3}\Psi\left(\frac{5}{6},\frac{2}{3};\frac{4}{27r^2}\right)-\frac{5}{2^{1/3}3^{11/2}\pi^{3/2}}r^{-14/3}\Psi\left(\frac{11}{6},\frac{5}{3};\frac{4}{27r^2}\right), \tag{3.3}$$

$$\begin{aligned}p_{1/3}^3(r)=&\frac{5e^{-(\pi/4)i}}{18\sqrt{3}\pi^2}S_{0,1/3}\left(\frac{2e^{(\pi/4)i}}{3\sqrt{3r}}\right)+\frac{5e^{(\pi/4)i}}{18\sqrt{3}\pi^2}S_{0,1/3}\left(\frac{2e^{-(\pi/4)i}}{3\sqrt{3r}}\right)\\&-\frac{2}{81\pi^2r^4}S_{-1,4/3}\left(\frac{2e^{(\pi/4)i}}{3\sqrt{3r}}\right)-\frac{2}{81\pi^2r^4}S_{-1,4/3}\left(\frac{2e^{-(\pi/4)i}}{3\sqrt{3r}}\right),\end{aligned} \tag{3.4}$$

$$\begin{aligned}p_3^3(r)=&\frac{e^{-(3\pi/4)i}}{6\sqrt{3}\pi^2r^{3/2}}S_{0,1/3}\left[2e^{(3\pi/4)i}\left(\frac{r}{3}\right)^{3/2}\right]+\frac{e^{(3\pi/4)i}}{6\sqrt{3}\pi^2r^{3/2}}S_{0,1/3}\left[2e^{-(3\pi/4)i}\left(\frac{r}{3}\right)^{3/2}\right]\\&-\frac{2}{27\pi^2}S_{-1,4/3}\left[2e^{(3\pi/4)i}\left(\frac{r}{3}\right)^{3/2}\right]-\frac{2}{27\pi^2}S_{-1,4/3}\left[2e^{-(3\pi/4)i}\left(\frac{r}{3}\right)^{3/2}\right],\end{aligned} \tag{3.5}$$

where $\Psi(z)$ is the Tricomi confluent hypergeometric function,[22] and $S_{\mu,\nu}(z)$ is a Lommel function.[22]

Recalling that $J_{1/2}(z)=(2/\pi z)\sin(z)$, the integral representation of $p_{1/2}^3(r)$ can be found directly in Ref. 23 in terms of a sum of parabolic cylinder functions, $D_{-4}(z)$,

$$p_{1/2}^3(r)=\frac{1}{2r\pi^2}\int_0^\infty \mathrm{d}t\, e^{-\sqrt{t}}t\sin(rt) \tag{3.6}$$

$$=\frac{3}{4\pi^2r^3}\left[\exp\left(\frac{i}{2}\left[\pi+\frac{1}{4r}\right]\right)D_{-4}\left(\frac{e^{i(\pi/4)}}{\sqrt{2r}}\right)+\exp\left(-\frac{i}{2}\left[\pi+\frac{1}{4r}\right]\right)D_{-4}\left(\frac{e^{-i(\pi/4)}}{\sqrt{2r}}\right)\right]. \tag{3.7}$$

B. Two dimensions

Finding special function representations for $p_\alpha^2(r)$ is more time consuming than the three-dimensional case since we do not have a stock pile of zero-dimensional results with which to apply the dimensional recursion relation (1.5). We note however that in general $p_\alpha^0(r)$, defined via (1.4), is a simpler object than $p_\alpha^2(r)$, and in fact $p_{1/2}^0(r)$ is listed in Ref. 22 in terms of parabolic cylinder functions. Hence the dimensional recursion relation leads to

$$p_{1/2}^2(r)=-\frac{1}{2\pi r}\frac{\partial}{\partial r}\frac{1}{\sqrt{2r}}D_{-1/2}\left(\frac{e^{(\pi/4)i}}{\sqrt{2r}}\right)D_{-1/2}\left(\frac{e^{-(\pi/4)i}}{\sqrt{2r}}\right), \tag{3.8}$$

$$p_{1/2}^2(r) = -\frac{1}{2\pi r}\frac{\partial}{\partial r}\frac{\pi^3}{16r}\left[J_{1/4}^2\left(\frac{1}{8r}\right)+Y_{1/4}^2\left(\frac{1}{8r}\right)\right], \tag{3.9}$$

where $Y_{1/4}(1/8r)$ is a Neumann function. In obtaining this last step we have used the fact that $D_{-1/2}(z)=\sqrt{(\pi z/2)}K_{1/4}(z^2/4)$, where $K_{1/4}(z^2/4)$ is a modified Bessel function of the third kind.[22–24]

IV. POWER SERIES REPRESENTATIONS FOR $p_\alpha^d(r)$

We now construct the convergent series, and asymptotic power series representations of $p_\alpha^d(r)$, since we shall have need to employ these expansions in later discussions. This process is a straightforward generalization of that employed in the construction of the series representations of $p_\alpha^1(r)$.[16,17] One can easily construct the Mellin–Barnes integral representation of $p_\alpha^d(r)$ by simply calculating its Mellin transform and then using the inverse Mellin transform formula. The Mellin transform of $p_\alpha^d(r)$ is listed in Ref. 23,

$$p_\alpha^d(r) = \frac{1}{\alpha(2\sqrt{\pi})^d}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} ds\left(\frac{r}{2}\right)^{-s}\frac{\Gamma\left(\frac{s}{2}\right)\Gamma\left(\frac{d-s}{\alpha}\right)}{\Gamma\left(\frac{d-s}{2}\right)} \tag{4.1}$$

$$= \frac{1}{\alpha(2\sqrt{\pi})^d}H_{1,2}^{1,1}\left[\frac{r}{2}\middle|\begin{matrix}\left(1-\frac{d}{\alpha},\frac{1}{\alpha}\right)\\ \left(0,\frac{1}{2}\right);\left(1-\frac{d}{2},\frac{1}{2}\right)\end{matrix}\right], \tag{4.2}$$

where $0<c<\min((d+1)/2,d)$, and we have observed that (4.1) defines a Fox H function[23] for all values of d and α. We also mention here that if α is rational the ratio of gamma functions in (4.1) can be so massaged that each gamma function has the form $\Gamma(\pm s+\text{stuff})$, and we can hence identify this result with a Meijer G-function. We shall return to this point in Sec. V when we obtain the hypergeometric representation of $p_{p/q}^d(r)$ via a slightly different, yet equivalent route using the small r power series representation of $p_\alpha^d(r)$. This expansion is found from (4.1) by simply closing the contour to the left,

$$p_\alpha^d(r) = \frac{1}{2^{d-1}\alpha\pi^{d/2}}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\frac{\Gamma\left(\frac{2k+d}{\alpha}\right)}{\Gamma\left(k+\frac{d}{2}\right)}\left(\frac{r}{2}\right)^{2k}, \quad \forall r, \quad \alpha>1,$$

$$p_\alpha^d(r) \sim \frac{1}{2^{d-1}\alpha\pi^{d/2}}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\frac{\Gamma\left(\frac{2k+d}{\alpha}\right)}{\Gamma\left(k+\frac{d}{2}\right)}\left(\frac{r}{2}\right)^{2k}, \quad r\to 0, \quad \alpha<1. \tag{4.3}$$

Applying the ratio test it can be shown that (4.3) is absolutely convergent for all r when $\alpha>1$. The gamma function structure of (4.3) should be compared to that of the $d=1$ result discussed in Ref. 16, which we list here for ease of comparison,

$$p_\alpha^1(r)=\frac{1}{\alpha\sqrt{\pi}}\sum_{k=0}^{\infty}\frac{(-1)^k\Gamma\left[\dfrac{2k+1}{\alpha}\right]}{\sqrt{\pi}\Gamma[2k+1]}r^{2k},\quad \forall r,\quad \alpha>1. \tag{4.4}$$

Note in particular that (4.4) contains only one gamma function in the denominator, whereas (4.3) contains two. Via the duplication formula we see that (4.3) with $d=1$ is equivalent to (4.4) since $2^{2k}\Gamma(k+1)\Gamma(k+\frac{1}{2})=\sqrt{\pi}\Gamma(2k+1)$. For general d however, $k!\Gamma(k+d/2)$ cannot be reduced to a single gamma function. The essence of the difference is that the duplication formula provides us a relation of the form $\Gamma(z)\Gamma(z+\frac{1}{2})\propto\Gamma(2z)$, but the objects that we see for general d are of the form $\Gamma(z)\Gamma(z+d/2)$, for which no similar simplification is known. This observation will be important when we identify (4.3) as a sum of hypergeometric functions in Sec. V. Similar behavior is again present in the large r power series for general d, which we construct by closing the contour to the right,

$$p_\alpha^d(r)=\frac{1}{\pi(\sqrt{\pi}r)^d}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k!}\sin\left(\frac{k\alpha\pi}{2}\right)\Gamma\left(\frac{k\alpha}{2}+1\right)\Gamma\left(\frac{k\alpha}{2}+\frac{d}{2}\right)\left(\frac{2}{r}\right)^{\alpha k},\quad r>0,\quad \alpha<1,$$

$$p_\alpha^d(r)\sim\frac{1}{\pi(\sqrt{\pi}r)^d}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k!}\sin\left(\frac{k\alpha\pi}{2}\right)\Gamma\left(\frac{k\alpha}{2}+1\right)\Gamma\left(\frac{k\alpha}{2}+\frac{d}{2}\right)\left(\frac{2}{r}\right)^{\alpha k},\quad r\to\infty,\quad \alpha>1. \tag{4.5}$$

It is readily verified that (4.5) is absolutely convergent when $\alpha<1$. For $\alpha>1$ (4.5) provides the asymptotic power series for $p_\alpha^d(r)$, but as we shall show later there exist interesting cases in which this expansion is not complete, precisely as was found when $d=1$.[16] For $\alpha=3,4,5,6,7$ we found in Ref. 16 that there exist series of exponentially small terms lying beyond all orders of the large r asymptotic power series of $p_\alpha^1(r)$. We will show that this same behavior arises for general d, $\forall\,\alpha\in\mathbb{Z}_{\geqslant 3}$. It was also noted in Ref. 16 that when α is an even integer that the large r power series expansion of $p_\alpha^1(r)$ vanishes identically, and from (4.5) we see that this is true also for general d. In the case of $\alpha=2$ in which $p_\alpha^d(r)$ simplifies to the d-dimensional Gaussian, $(4\pi)^{-d/2}e^{-|\mathbf{r}|^2/4}$, this simply expresses the fact that the large r asymptotic behavior of a Gaussian is smaller than any power. When $\alpha>2$ and an even integer we see that these exponentially small series occurring in the large r expansions of $p_\alpha^d(r)$ again become dominant precisely as they did for $p_\alpha^1(r)$. The explicit construction of these exponentially small series will be studied in detail, but first we will show how to obtain hypergeometric representations for $p_{p/q}^d(r)$. These representations are interesting in their own right, and will be the starting point for our asymptotic work.

V. HYPERGEOMETRIC REPRESENTATION OF $p_\alpha^d(r)$

We demonstrated in Ref. 16 that with p,q integers, $p_{p/q}^1(r)$ can be identified with a finite sum of generalized hypergeometric functions, or Meijer G-functions. We now show that essentially the same procedure can be utilized to make a similar identification for $p_{p/q}^d(r)$. We begin with (4.3) which, as mentioned previously, is convergent for $\alpha>1$. As discussed in Refs. 16 and 25, we can still identify $p_{p/q}^d(r)$ with (4.3) for $p/q<1$, and utilize Borel summation[26] where necessary.

The series representation for the generalized hypergeometric function is

$${}_aF_b\left(\begin{matrix}\alpha_1,\alpha_2,\ldots,\alpha_a\\ \beta_1,\beta_2,\ldots,\beta_b\end{matrix}\middle|z\right)=\sum_{m=0}^{\infty}\frac{z^m}{m!}\frac{\Pi_{h=1}^a(\alpha_h)_m}{\Pi_{h=1}^b(\beta_h)_m}, \tag{5.1}$$

where $(a)_m$ is Pochhammer's symbol,

$$(a)_m=\frac{\Gamma(a+m)}{\Gamma(a)}. \tag{5.2}$$

As in the $d=1$ case[16] we begin by making the change of summation index $k=mp+l$ in (4.3), with the goal of transforming the ratio of gamma functions into the form required by (5.1) and (5.2). We obtain

$$p^d_{p/q}(r)=\frac{q}{2^{d-1}\pi^{d/2}p}\sum_{l=0}^{p-1}(-1)^l\left(\frac{r}{2}\right)^{2l}\sum_{m=0}^{\infty}\left[(-1)^p\left(\frac{r}{2}\right)^{2p}\right]^m\frac{\Gamma\left[2qm+\frac{2ql}{p}+\frac{dq}{p}\right]}{\Gamma[pm+l+1]\Gamma\left[pm+l+\frac{d}{2}\right]}. \tag{5.3}$$

We now apply Gauss' multiplication formula,

$$\Gamma(mz)\propto\Pi_{h=0}^{m-1}\Gamma\left(z+\frac{h}{m}\right),$$

to the gamma functions in (5.3),

$$\begin{aligned}\frac{\Gamma\left[2mq+\frac{2ql}{p}+\frac{dq}{p}\right]}{\Gamma[pm+l+1]\Gamma\left[pm+l+\frac{d}{2}\right]}=&\left(\frac{(2\pi)^{p-q-1/2}(2q)^{qd/p-1/2}}{p^{d/2}}\right)\\&\times\left(\left[\frac{(2q)^{2q}}{p^{2p}}\right]^{l/p}\frac{\Pi_{h=1}^{2q-1}\Gamma\left[\frac{l+\frac{d}{2}}{p}+\frac{h}{2q}\right]}{\Pi_{h=1}^{p-1}\Gamma\left[\frac{l+\frac{d}{2}+h}{p}\right]\Pi_{h=1}^{p}\Gamma\left[\frac{l+h}{p}\right]}\right)\\&\times\left(\left[\frac{(2q)^{2q}}{p^{2p}}\right]^{m}\frac{\Pi_{h=1}^{2q-1}\left(\frac{l+\frac{d}{2}}{p}+\frac{h}{2q}\right)_m}{\Pi_{h=1}^{p-1}\left(\frac{l+\frac{d}{2}+h}{p}\right)_m\Pi_{h=1}^{p}\left(\frac{l+h}{p}\right)_m}\right).\end{aligned} \tag{5.4}$$

Inserting (5.4) into (5.3), and comparing with (5.1) we can immediately make the following identification:

$$p^d_{p/q}(r)=\frac{(2q)^{dq/p+1/2}}{p^{d/2+1}2^{d/2}(2\pi)^{(d+1)/2+q-p}}\sum_{l=0}^{p-1}(-1)^l\left[\frac{(2q)^{2q}r^{2p}}{(2p)^{2p}}\right]^{l/p}$$
$$\times\frac{\Pi_{h=1}^{2q-1}\Gamma\left(\dfrac{l+\dfrac{d}{2}}{p}+\dfrac{h}{2q}\right)}{\Pi_{h=1}^{p-1}\Gamma\left(\dfrac{l+\dfrac{d}{2}+h}{p}\right)\Pi_{h=1}^{p}\Gamma\left(\dfrac{l+h}{p}\right)}$$
$$\times{}_{2q}F_{2p-1}\left(\left.\begin{matrix}1,\dfrac{l+\frac{d}{2}}{p}+\dfrac{1}{2q},\dfrac{l+\frac{d}{2}}{p}+\dfrac{2}{2q},\ldots,\dfrac{l+\frac{d}{2}}{p}+\dfrac{2q-1}{2q}\\ \dfrac{l+\frac{d}{2}+1}{p},\dfrac{l+\frac{d}{2}+2}{p},\ldots,\dfrac{l+\frac{d}{2}+p-1}{p},\dfrac{l+1}{p},\dfrac{l+2}{p},\ldots,\dfrac{l+p}{p}\end{matrix}\right|(-1)^p\frac{(2q)^{2q}r^{2p}}{(2p)^{2p}}\right). \tag{5.5}$$

We can also use the relationship between the generalized hypergeometric function and the Meijer G-function[27] to exhibit (5.5) in the following form:

$$p^d_{p/q}(r)=\frac{(2q)^{dq/p+1/2}}{p^{d/2+1}2^{d/2}(2\pi)^{(d+1)/2+q-p}}\sum_{l=0}^{p-1}\left[\frac{(2q)^{2q}r^{2p}}{(2p)^{2p}}\right]^{l/p}$$
$$\times G^{1,2q}_{2q,2p}\left(\left.(-1)^{p+1}\frac{(2q)^{2q}r^{2p}}{(2p)^{2p}}\right|\begin{matrix}0,\dfrac{1}{2q}-\dfrac{l+\frac{d}{2}}{p},\dfrac{2}{2q}-\dfrac{l+\frac{d}{2}}{p},\ldots,\dfrac{2q-1}{2q}-\dfrac{l+\frac{d}{2}}{p}\\ 0,\dfrac{1-l-\frac{d}{2}}{p},\dfrac{2-l-\frac{d}{2}}{p},\ldots\dfrac{p-1-l-\frac{d}{2}}{p},-\dfrac{l}{p},\dfrac{1-l}{p},\dfrac{2-l}{p},\ldots,\dfrac{p-1-l}{p}\end{matrix}\right). \tag{5.6}$$

As discussed in Sec. IV this result could equivalently have been obtained by performing similar manipulations on the ratio of gamma functions in (4.1) and we could then have obtained the hypergeometric functions from the Meijer G-functions.

Comparing (5.5) to the $d=1$ result given in Ref. 16 we note that in the general d case we have only half as many hypergeometric functions in the sum, but that each one has twice as many parameters as in the $d=1$ case. We shall again make use of the notation used in Ref. 16, $f(\pm z)^+\equiv f(z)+f(-z)$ for some function f, and we refer to $f(\pm z)^+$ as a symmetrized pair. In the $d=1$ case it is possible to express $p^d_{p/q}(r)$ in terms of a sum of symmetrized pairs of generalized hypergeometric functions, since we can utilize the duplication formula to simplify the product of the two gamma functions in the denominator of (4.3). By making such a simplification we are able in the $d=1$ case to make a second change of summation index to (5.3), $s=2m$, before using the multiplication formula. The effect of this is to simultaneously introduce the factor

$$\left[\frac{1+(-1)^s}{2}\right],$$

which accounts for the appearance of the symmetrized pairs, and also to halve the number of both numerator and denominator parameters. Such a process is not possible for general d for all p,q. It is useful to have representations of $p^d_{p/q}(r)$ with the smallest number of parameters possible, and to this end we ask the question "when $d\neq 1$, are there any values of p/q for which we can symmetrize (5.5)?" Observing the form of (5.3) we see that when p is even we can indeed make

the change of summation index $s=2m$ before using Gauss' multiplication formula and therefore halve the number of parameters appearing in (5.5), at the cost of replacing the single hypergeometric functions in the sum by symmetrized pairs,

$$p^d_{p/q}(r)=\frac{(2\pi)^{(p-q-1-d)/2}q^{dq/p\,+\,1/2}}{p^{d/2+1}}\sum_{l=0}^{p-1}(-1)^l\left(\frac{q^q r^p}{p^p}\right)^{2l/p}$$
$$\times\frac{\Pi_{h=1}^{q-1}\Gamma\left(\dfrac{2l+d}{p}+\dfrac{h}{q}\right)}{\Pi_{h=1}^{p/2-1}\Gamma\left(\dfrac{2l+d+2h}{p}\right)\Pi_{h=0}^{p/2-1}\Gamma\left(\dfrac{2l+2+2h}{p}\right)}$$
$$\times{}_qF_{p-1}\left(\left.\begin{matrix}1,\dfrac{2l+d}{p}+\dfrac{1}{q},\dfrac{2l+d}{p}+\dfrac{2}{q},\ldots,\dfrac{2l+d}{p}+\dfrac{q-1}{q}\\ \dfrac{2l+d+2}{p},\dfrac{2l+d+4}{p},\ldots,\dfrac{2l+d+p-2}{p},\dfrac{2l+2}{p},\dfrac{2l+4}{p},\ldots,\dfrac{2l+p}{p}\end{matrix}\right|\pm\frac{q^q r^p}{p^p}\right)^{+},\quad p\in\mathbb{N}_{\text{even}}. \tag{5.7}$$

We see therefore that when p is even the structure of the hypergeometric representation for general d is much closer to the $d=1$ case,[16] with $p^d_{p/q}(r)$ a sum of symmetrized ${}_qF_{p-1}$ functions with d-dependent parameters. Compare this to the odd p case where we have a sum over single ${}_{2q}F_{2p-1}$ functions when $d\neq 1$. Thus for even p, extrapolating from Ref. 1 to $d>1$ essentially just generalizes the parameters, but when p is odd the $d>1$ generalization changes the structure of the hypergeometric representation. It is instructive to observe that the explicit structure of $p^d_{2n}(r)$ can be simplified still further by noticing some drastic cancellations which occur between the $0\leqslant l\leqslant n-1$ terms and the $n\leqslant l\leqslant 2n-1$ terms of (5.7),

$$p^d_{2n}(r)=\frac{2(2\pi)^{(p-2-d)/2}}{p^{d/2+1}}\sum_{l=0}^{n-1}(-1)^l\left(\frac{r^p}{p^p}\right)^{l/n}\frac{1}{\Pi_{h=1}^{n-1}\Gamma\left(\dfrac{\dfrac{d}{2}+l+h}{n}\right)\Pi_{h=1}^{n}\Gamma\left(\dfrac{l+h}{n}\right)}$$
$$\times{}_0F_{p-2}\left(\left\{\frac{d}{2n}+\frac{l+h}{n}\,\middle|\,h\in\{1,\ldots,n-1\}\right\}\cup\left\{\frac{l+h}{n}\,\middle|\,h\in\{1,\ldots,n\}\backslash\{n-l\}\right\}\,\middle|\,(-1)^n\left(\frac{r^p}{p^p}\right)\right). \tag{5.8}$$

From this representation of $p^d_{2n}(r)$ we gain a new perspective on why $p^d_{2n}(r)$ has no algebraic terms in its large r asymptotic expansion, since it is known[27] that generalized hypergeometric functions with no numerator parameters always display purely transcendental asymptotic behavior.

VI. ASYMPTOTICS BEYOND ALL ORDERS

We now turn our attention to the asymptotic properties of $p^d_p(r)$, where $p\geqslant 3$ is an integer. The treatment here is not only a generalization of the results in Ref. 16 to general d, but also to general p; in Ref. 16 we listed the $d=1$ complete asymptotic expansions for $p=3,4,5,6,7$, whereas we now proceed to construct the complete asymptotic expansions for arbitrary values of p and d. We demonstrated in Sec. V that the hypergeometric representation of $p^d_{2n}(r)$ can be written in a much simplified form that is of precisely the same structure as the analogous one-dimensional case. For p an odd integer such a simplification is only possible when $d=1$. As we

shall see however, the structure of the asymptotic expansion of $p_p^d(r)$ is only weakly dependent on d, and for both odd and even p the expansions for general d are surprisingly similar in appearance to the one-dimensional results discussed in Ref. 16.

Our starting point is the following hypergeometric representation for $p_p^d(r)$:

$$p_p^d(r)=\phi_p^d\sum_{l=0}^{p-1}(-)^l z^{l/p}\frac{\Gamma\left(\frac{l}{p}+\frac{d}{2p}+\frac{1}{2}\right)}{\Pi_{h=1}^{p-1}\Gamma\left(\frac{d}{2p}+\frac{l+h}{p}\right)\Pi_{h=1}^{p}\Gamma\left(\frac{l+h}{p}\right)}$$
$$\times{}_1F_{2p-2}\left(\left(\frac{l}{p}+\frac{d}{2p}+\frac{1}{2}\right);\left\{\frac{d}{2p}+\frac{l+h}{p}\,\middle|\,h\in\{1,\ldots,p-1\}\right\}\cup\left\{\frac{l+h}{p}\,\middle|\,h\in\{1,\ldots,p\}\backslash\{p-l\}\right\};(-)^p z\right) \tag{6.1}$$

with

$$z\equiv\frac{2^{2(1-p)}}{p^{2p}}r^{2p}\in\mathbb{R}_{\geqslant 0},\quad \phi_p^d\equiv\frac{2^{d/p+p-d-1}}{p^{d/2+1}\pi^{d/2+3/2-p}}.$$

The complete large r asymptotic expansions of $p_p^d(r)$ will be derived by applying the general results in Ref. 27 for the complete asymptotic expansions of the generalized hypergeometric functions to (6.1).

From Ref. 27 we have in general, when $\beta=b+1-a>3\in\mathbb{Z}_{even}$,

$$\frac{\Pi_{h=1}^{a}\Gamma(\alpha_h)}{\Pi_{h=1}^{b}\Gamma(\rho_h)}{}_aF_b\left(\begin{matrix}\alpha_1,\alpha_2,\ldots,\alpha_a\\ \rho_1,\rho_2,\ldots,\rho_b\end{matrix}\,\middle|\,-z\right)\sim L_{a,b}(z)$$
$$+\sum_{k=0}^{\beta/2-1}\left[\Gamma_{b+1}^{1,a}(k)K_{a,b}(ze^{-i\pi(2k+1)})+\overline{\Gamma}_{b+1}^{1,a}(k)K_{a,b}(ze^{i\pi(2k+1)})\right], \tag{6.2}$$

$$K_{a,b}(z)=\frac{(2\pi)^{(1-\beta)/2}}{\sqrt{\beta}}e^{\beta z^{1/\beta}}z^{\gamma}\sum_{m=0}^{\infty}N_m z^{-m/\beta}, \tag{6.3}$$

$$\gamma=\frac{(\beta-1)}{2\beta}+\frac{1}{\beta}\sum_{h=1}^{a}\alpha_h-\frac{1}{\beta}\sum_{h=1}^{b}\rho_h, \tag{6.4}$$

$$\arg(z)\in[\delta-2\pi,2\pi-\delta],\quad \delta>0. \tag{6.5}$$

$L_{a,b}(z)$ is the power series contribution to the complete asymptotic expansion of ${}_aF_b$, and vanishes identically when $a=0$. This implies that the asymptotic expansions of $p_{2n}^d(r)$ will be purely transcendental. For odd p not all the $L_{a,b}(z)$ will vanish, but their sum merely produces the large r asymptotic power series derived in Sec. IV so we need not focus on them in this section. In what follows it is to be understood that the power series is to be appended to the beyond all orders asymptotic expansions here constructed, in order to yield the complete expansions.

The N_m and $\Gamma_{b+1}^{1,a}$ are found recursively, and their construction is discussed in depth in Ref. 27.

We now apply these general results to (6.1),

$$\beta=2p-2>3,\quad \gamma=-\frac{l}{p}-\frac{(p-2)}{4p(p-1)}d, \tag{6.6}$$

$$p_p^d(r)\sim\phi_p^d\sum_{l=0}^{p-1}(-)^l z^{l/p}\sum_{k=0}^{p-2}\Gamma_{2p-1}^{1,1}(k)K_{1,2p-2}[(-)^{p+1}ze^{-i\pi(2k+1)}]$$
$$+\phi_p^d\sum_{l=0}^{p-1}(-)^l z^{l/p}\sum_{k=0}^{p-2}\overline{\Gamma}_{2p-1}^{1,1}(k)K_{1,2p-2}[(-)^{p+1}ze^{i\pi(2k+1)}], \tag{6.7}$$

$$\Gamma_{2p-1}^{1,1}(2m)=\Gamma_{2p-1}^{1,1}(2m+1)=\sum_{j=0}^{m}\exp\left(-2j\frac{(2l+d)\pi i}{p}\right),\quad m\in\left\{0,1,2,\ldots,\left[\frac{p-1}{2}\right]\right\}, \tag{6.8}$$

where $[n]$ represents the integer part of n. The derivation of the $\Gamma_{2p-1}^{1,1}$ is discussed in an Appendix. To avoid notational clutter we shall drop the subscripts and superscripts on the $\Gamma_{2p-1}^{1,1}$ and $K_{1,2p-2}$ in what follows; since no gamma functions are encountered for the remainder of this section no confusion should arise.

It is straight forward to show using Ref. 27 that the N_m for all choices of l are the same; thus N_m depends only on m, and on p and d. The recursion relation is as follows:

$$N_k=\sum_{s=1}^{2(p-1)}\sum_{r=0}^{2(p-1)-s}\left(\frac{p}{2(p-1)}(r+s-k)-(p-1)+\frac{dp}{4(p-1)}\right)_{p-1}$$
$$\times\left(\frac{p}{2(p-1)}(r+s-k)-(p-1)-\frac{(p-2)d}{4(p-1)}\right)_p\times\frac{(-)^{s+r}[2(p-1)]^{2p-s-2}}{r![2(p-1)-s-r]!p^{2p-1}k}N_{k-s}, \tag{6.9}$$

$$N_s=0,\quad s<0,\quad N_0=1. \tag{6.10}$$

We list the first four values of N_k for $d=1,2,3$ and $\alpha=3,4,5,6$, in Tables I–IV

According to (6.5) we have the following restriction on $\arg[(-)^{p+1}z]$:

$$(-)^{p+1}z=\begin{cases}z & \text{if } p \text{ is odd}\\ e^{\pm i\pi}z & \text{if } p \text{ is even.}\end{cases} \tag{6.11}$$

Thus our choice of phase depends on the parity of p, but we can get around this and treat both odd and even p cases simultaneously by introducing

$$\sigma=\begin{cases}0 & \text{if } p \text{ is odd}\\ 1 & \text{if } p \text{ is even}\end{cases}\qquad (-)^{p+1}z=e^{\sigma\pi i}z. \tag{6.12}$$

Notice that we have chosen $(-)^{p+1}z=e^{i\pi}z$ for the even p case; substituting the choice $(-)^{p+1}z=e^{-i\pi}z$ into (6.7) merely results in the conjugate expression, but since our final result is real this introduces nothing new. Inserting (6.12) into (6.7), and massaging suitably results in

$$p_p^d(r)\sim\phi_p^d\sum_{l=0}^{\infty}(-)^l z^{l/p}\sum_{k=\sigma}^{p-2+\sigma}[\Gamma(k)K(ze^{-i\pi(2k+1-\sigma)})+\overline{\Gamma}(k-\sigma)K(ze^{i\pi(2k+1-\sigma)})]$$
$$+\phi_p^d\sum_{l=0}^{\infty}(-)^l z^{l/p}\delta_{\sigma,1}[K(z)-\Gamma(p-1)K(ze^{-i\pi 2(p-1)})], \tag{6.13}$$

where $\delta_{n,m}$ is the Kronecker delta.

It is convenient to simplify the two terms of (6.13) multiplied by $\delta_{\sigma,1}$ using (6.3) and (6.8) at this stage before proceeding to tackle the remaining piece. First however, we introduce the following convenient notation:

$$\tau = 2p\phi_p^d \frac{(2\pi)^{[1-2(p-1)]/2}}{\sqrt{2(p-1)}} z^{-d[(p-2)]/[4p(p-1)]} = \frac{2}{\sqrt{(p-1)}(\sqrt{2\pi(pr^{(p-2)})^{1/(p-1)}})^d}, \quad (6.14)$$

$$\bigwedge_{m=0}^{\infty} = \tau \sum_{m=0}^{\infty} N_m z^{-m/[2(p-1)]} = \frac{2}{\sqrt{(p-1)}(\sqrt{2\pi(pr^{(p-2)})^{1/(p-1)}})^d} \sum_{m=0}^{\infty} 2^m N_m \left(\frac{p}{r}\right)^{mp/(p-1)}. \quad (6.15)$$

We observe that the $\delta_{\sigma,1}K(z)$ term vanishes identically since

$$\phi_p^d \sum_{l=0}^{p-1} (-)^l z^{l/p} \delta_{\sigma,1} K(z) = \frac{e^{\beta z^{1/\beta}}}{2p} \bigwedge_{m=0}^{\infty} \delta_{\sigma,1} \sum_{l=0}^{p-1} (-)^l = 0 \quad (6.16)$$

and the sum over l vanishes when p is even ($\sigma = 1$).

The last term in (6.13) is only nonzero for certain values of p; by inserting the explicit form of $\Gamma(p-1)$ and massaging this term becomes

$$\frac{e^{-\beta z^{1/\beta}}}{2p} \bigwedge_{m=0}^{\infty} (-)^m \sum_{j=0}^{p/2-1} \exp\left[\frac{2d\pi i}{p}\left(j - \frac{(p-2)}{4}\right)\right] \delta_{\sigma,1} \sum_{l=0}^{p-1} (-)^l \exp\left(-l\frac{[4j-2(p-1)]\pi i}{p}\right). \quad (6.17)$$

For even p this l sum is only nonvanishing when $[4j-2(p-1)]/p$ is an odd integer which is only possible for $j=(p-2)/4$, which in turn is only possible when $p \equiv 2 \pmod 4$. We see then from this analysis of the last two terms in (6.13) that the l sum acts as a powerful selection rule, and that this selection rule introduces a structure into the expansion of $p_p^d(r)$ that depends on a simple arithmetic property of p, namely on the residue of p modulo 4. We now investigate the remaining terms in (6.13) and we shall see shortly that both of these phenomena arise again. In order to substitute the explicit forms of $\Gamma(k)$ and $\overline{\Gamma}(k-\sigma)$ from (6.8) into (6.13) we need to write the k sum in terms of its even and odd terms separately,

$$\begin{aligned} p_p^d(r) \sim{}& \phi_p^d \sum_{l=0}^{p-1} (-)^l z^{l/p} \sum_{k=\sigma}^{[p/2]-1} \sum_{j=0}^{k} \left[\exp\left(\pm\frac{(2l+d)\pi i}{p} 2j\right) K(ze^{\pm i\pi(4k+1-\sigma)})\right]^+ \\ &+ \phi_p^d \sum_{l=0}^{p-1} (-)^l z^{l/p} \sum_{k=0}^{[p/2]-1} \sum_{j=0}^{k} \left[\exp\left(\pm\frac{(2l+d)\pi i}{p} 2j\right) K(ze^{\pm i\pi(4k+3-\sigma)})\right]^+ \\ &- \frac{\delta_{s,2}}{2} \bigwedge_{m=0}^{\infty} (-)^m e^{-\beta z^{1/\beta}} - \delta_{\sigma,1}\phi_p^d \sum_{l=0}^{p-1} (-)^l z^{l/p} \sum_{k=\sigma}^{[p/2]-1} \exp\left(\frac{(2l+d)\pi i}{p} 2k\right) K(ze^{i\pi 4k}). \end{aligned} \quad (6.18)$$

If we insert the explicit form for $K[ze^{i\pi 4k}]$ from (6.3) into the last term of Eq. (6.18) we find that the l sum vanishes for even p and so this term is identically zero. We now need only to simplify the first two terms in (6.18). To do this it is expedient to observe the following result which is a straightforward consequence of (6.3),

$$\begin{aligned} [e^{\pm i\epsilon} K_{p,q}(ye^{\pm m\pi i})]^+ &= e^{i\epsilon} K_{p,q}(ye^{m\pi i}) + e^{-i\epsilon} K_{p,q}(ye^{-m\pi i}) \\ &= 2\frac{(2\pi)^{(1-\beta)/2}}{\sqrt{\beta}} y^{\gamma} \sum_{r=0}^{\infty} N_r y^{-r/\beta} \exp\left(\beta y^{1/\beta} \cos\left[\frac{m\pi}{\beta}\right]\right) \\ &\quad \times \cos\left(\beta y^{1/\beta} \sin\left[\frac{m\pi}{\beta}\right] + \gamma m\pi + \epsilon - \frac{r\pi m}{\beta}\right). \end{aligned} \quad (6.19)$$

We apply this to (6.18),

$$p_p^d(r)\sim \bigwedge_{m=0}^{\infty} \sum_{k=\sigma}^{[p/2]-1} \sum_{j=0}^{k} \exp(\beta\eta_{1-\sigma}z^{1/\beta})\frac{1}{p}\sum_{l=0}^{p-1}\cos\left(\theta_{1-\sigma}(j)-\frac{l\pi}{p}(4k-4j+1-\sigma)\right)$$
$$+\bigwedge_{m=0}^{\infty} \sum_{k=0}^{[p/2]-1} \sum_{j=0}^{k} \exp(\beta\eta_{3-\sigma}z^{1/\beta})\frac{1}{p}\sum_{l=0}^{p-1}\cos\left(\theta_{3-\sigma}(j)-\frac{l\pi}{p}(4k-4j+3-\sigma)\right)$$
$$-\frac{\delta_{s,2}}{2}\bigwedge_{m=0}^{\infty}(-)^m\exp(-\beta z^{1/\beta}), \tag{6.20}$$

$$\theta_t(j)=2(p-1)\sin\left[\frac{(4k+t)\pi}{2(p-1)}\right]z^{1/[2(p-1)]}-\frac{m\pi(4k+t)}{2(p-1)}+\frac{d\pi}{p}\left[2j-\frac{(p-2)}{4(p-1)}(4k+t)\right], \tag{6.21}$$

$$\eta_t=\cos\left[\frac{(4k+t)\pi}{2(p-1)}\right]. \tag{6.22}$$

We now have the first two terms of (6.20) in a form where we can easily utilize the selection rule properties of the l sum. It is a simple matter to verify the following identity:

$$\sum_{l=0}^{n-1}(-)^l\cos\left(\phi+\frac{m\pi l}{n}\right)=\begin{cases}0 & \text{if } \dfrac{m}{n}\notin\mathbb{Z}_{\text{odd}}\\ n\cos(\phi) & \text{if } \dfrac{m}{n}\in\mathbb{Z}_{\text{odd}}\end{cases} \tag{6.23}$$

with m, $n\in\mathbb{Z}$, and providing m and n have the same parity.

From this result we see that the only terms in (6.20) which can survive are those for which $(4k-4j+f-\sigma)/p$ is an odd integer, where $f=1,3$ in the first and second pieces of (6.20), respectively. By analyzing the summation limits on k and j it can be seen that $(4k-4j+f-\sigma)/p$ can only be an odd integer when $(4k-4j+f-\sigma)/p=1$. Hence it is only the $j=k-([p-(f-\sigma)]/4)$ components that result in a nonvanishing contribution. But j is an integer, so it is only those terms for which $p\equiv(f-\sigma)(\mathrm{mod}\,4)$ that can survive. So the $f=1$ term only survives for the specific p values when $p\equiv(1-\sigma)(\mathrm{mod}\,4)$, i.e., when $p\equiv s(\mathrm{mod}\,4)$ with $s=0,1$. Likewise the $f=3$ term only survives when $p\equiv s(\mathrm{mod}\,4)$ with $s=2,3$. So for any choice of p, only one of the first two pieces of (6.20) will be nonzero. Further, since $j\geqslant 0$, only the $k\geqslant[p-(f-\sigma)]/4$ components of the k sum will contribute. Utilizing all these observations we can write the beyond all orders contribution of the complete asymptotic expansion of $p_p^d(r)$ in a rather simple form, which depends in an essential way on the parameter s which is defined as the arithmetic residue of p modulo 4,

$$p_p^d(r)\sim\bigwedge_{m=0}^{\infty}\sum_{k=(p-s)/4}^{[p/2]-1}\exp\left(\beta z^{1/\beta}\eta_s\right)\cos\left[\theta_s\left(k-\frac{(p-s)}{4}\right)\right]$$
$$-\frac{\delta_{s,2}}{2}\bigwedge_{m=0}^{\infty}(-)^m\exp(-2(p-1)z^{1/2(p-1)}), \tag{6.24}$$

$$p_p^d(r)\sim \frac{2}{\sqrt{(p-1)}(\sqrt{2\pi(pr^{(p-2)})^{1/(p-1)}})^d}\sum_{m=0}^{\infty}2^m N_m\left(\frac{p}{r}\right)^{mp/(p-1)}$$
$$\times\sum_{k=(p-s)/4}^{[p/2]-1}\exp\left((p-1)\cos\left[\frac{(4k+s)\pi}{2(p-1)}\right]\left(\frac{r}{p}\right)^{p/(p-1)}\right)$$
$$\times\cos\left((p-1)\sin\left[\frac{(4k+s)\pi}{2(p-1)}\right]\left(\frac{r}{p}\right)^{p/(p-1)}-\frac{m\pi(4k+s)}{2(p-1)}+\frac{dk\pi}{(p-1)}-\frac{[2p-(s+2)]d\pi}{4(p-1)}\right)$$
$$-\frac{\delta_{s,2}}{\sqrt{(p-1)}(\sqrt{2\pi(pr^{(p-2)})^{1/(p-1)}})^d}\sum_{m=0}^{\infty}2^m N_m\left(\frac{p}{r}\right)^{mp/(p-1)}(-)^m\exp\left(-(p-1)\left(\frac{r}{p}\right)^{p/(p-1)}\right). \tag{6.25}$$

This general expression should be compared to the specific results listed in Ref. 16, in particular note the increasing number of different exponentially decaying oscillatory series as p increases, which verifies our conjecture in Ref. 16 that such behavior should be expected. It is also interesting to note that although increasing p increases the number of series in the transcendental expansion, increasing d has no such effect. We see then from this result, and from the asymptotic power series of Sec. IV, that the asymptotics of $p_p^d(r)$ is only weakly dependent on d. The number of exponentially decaying oscillatory series depends only on α, and the power series vanishes only when α is an even integer, regardless of d. The structure of the complete asymptotic expansion of $p_p^d(r)$ is affected by the introduction of general d only in so far as d appears as a factor or and index in certain places.

VII. MOMENTS

Consider any isotropic pdf of a d-dimensional random walker, call it $p(r)$, then if $p(r)$ possess finite absolute moments the characteristic function will possess a power series expansion of the form

$$\tilde{p}(q)=\sum_{k=0}^{\infty}\frac{(-)^k}{k!}\frac{\langle|\mathbf{r}|^{2k}\rangle}{2^{2k}(d/2)_k}q^{2k}, \tag{7.1}$$

where we define the absolute moments of $p(r)$ in the usual way via

$$\langle|\mathbf{r}|^n\rangle=\int_{\mathbb{R}^d}d^d r p(r)|\mathbf{r}|^n \tag{7.2}$$

$$=\frac{2\pi^{d/2}}{\Gamma(d/2)}\int_0^{\infty}d^d r p(r)r^{n+d-1}. \tag{7.3}$$

Thus the analyticity of the characteristic function and the existence of the even absolute moments of the pdf are mutually implicative. From this result we can deduce that since $\tilde{p}_\alpha^d(q)=e^{-q^\alpha}$ is only analytic when α is an even integer, that $p_\alpha^d(r)$ can possess finite absolute moments to all orders only when α is an even integer. This is completely in agreement with what we found in our asymptotic results since it is only when α is even that the algebraic terms in the asymptotic expansion of $p_\alpha^d(r)$ vanish, which implies the existence of a characteristic scale. This characteristic scale is provided by the finite moments when α is even. In this section we list the absolute moments of $p_\alpha^d(r)$ when they exist, or describe how they diverge when they do not, in order to fully elucidate the connections between moments, exponential asymptotics of $p_\alpha^d(r)$, and analyticity of $\tilde{p}_\alpha^d(q)$.

TABLE I. Numerical values of $N_m(\alpha=3,d)$.

m	$N_m(\alpha=3,d=1)$	$N_m(\alpha=3,d=2)$	$N_m(\alpha=3,d=3)$
1	$\frac{5}{288}$	$\frac{1}{144}$	$-\frac{7}{288}$
2	$\frac{385}{165\,888}$	$\frac{1}{41\,472}$	$-\frac{455}{165\,888}$
3	$\frac{85\,085}{143\,327\,232}$	$-\frac{3203}{17\,915\,904}$	$-\frac{95\,095}{143\,327\,232}$
4	$\frac{37\,182\,145}{165\,112\,971\,264}$	$-\frac{1\,412\,495}{10\,319\,560\,704}$	$-\frac{40\,415\,375}{165\,112\,971\,264}$

TABLE II. Numerical values of $N_m(\alpha=4,d)$.

m	$N_m(\alpha=4,d=1)$	$N_m(\alpha=4,d=2)$	$N_m(\alpha=4,d=3)$
1	$\frac{7}{288}$	$\frac{1}{72}$	$-\frac{5}{288}$
2	$\frac{385}{165\,888}$	$\frac{1}{10\,368}$	$-\frac{455}{165\,888}$
3	$\frac{39\,655}{143\,327\,232}$	$-\frac{575}{2\,239\,488}$	$-\frac{85\,085}{143\,327\,232}$
4	$\frac{665\,665}{165\,112\,971\,264}$	$-\frac{86\,975}{644\,972\,544}$	$-\frac{24\,079\,055}{165\,112\,971\,264}$

TABLE III. Numerical values of $N_m(\alpha=5,d)$.

m	$N_m(\alpha=5,d=1)$	$N_m(\alpha=5,d=2)$	$N_m(\alpha=5,d=3)$
1	$\frac{9}{320}$	$\frac{3}{160}$	$-\frac{3}{320}$
2	$\frac{441}{204\,800}$	$\frac{9}{51\,200}$	$-\frac{99}{40\,960}$
3	$\frac{30\,303}{327\,680\,000}$	$-\frac{11\,679}{40\,960\,000}$	$-\frac{172\,557}{327\,680\,000}$
4	$-\frac{25\,162\,137}{419\,430\,400\,000}$	$-\frac{3\,026\,313}{26\,214\,400\,000}$	$-\frac{41\,162\,121}{419\,430\,400\,000}$

TABLE IV. Numerical values of $N_m(\alpha=6,d)$.

m	$N_m(\alpha=6,d=1)$	$N_m(\alpha=6,d=2)$	$N_m(\alpha=6,d=3)$
1	$\frac{11}{360}$	$\frac{1}{45}$	$-\frac{1}{360}$
2	$\frac{517}{259\,200}$	$\frac{1}{4050}$	$-\frac{539}{259\,200}$
3	$-\frac{22\,253}{1\,399\,680\,000}$	$-\frac{407}{1\,366\,875}$	$\frac{673\,673}{1\,399\,680\,000}$
4	$-\frac{158\,440\,051}{2\,015\,539\,200\,000}$	$-\frac{6089}{61\,509\,375}$	$-\frac{147\,758\,611}{2\,015\,539\,200\,000}$

To ascertain the divergence or values of the moments for various α it is convenient to consider a slightly generalized integral, $\langle|\mathbf{r}|^n\rangle_\lambda$, in which we insert the factor $e^{-\lambda r}$ into the integrand, which tends to $\langle|\mathbf{r}|^n\rangle$ as $\lambda\to 0$. The Mellin Barnes representation of $\langle|\mathbf{r}|^n\rangle_\lambda$ is easily shown to be

$$\langle|\mathbf{r}|^n\rangle_\lambda=\frac{-1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}ds\,\frac{2^{s+1}}{\alpha\Gamma(d/2)}\Gamma\left(\frac{-s}{\alpha}\right)\Gamma\left(\frac{d+s}{2}\right)\frac{\Gamma(n-2)}{\Gamma\left(\frac{-s}{2}\right)}\lambda^{s-n}-d<\sigma<-\frac{(d-1)}{2}. \quad (7.4)$$

By inspecting the small λ behavior of this well behaved integral we can determine whether the $2m$th moment diverges for a given α, and if this moment is finite we can calculate its numerical value by taking $\lambda\to 0$. The small λ expansion of $\langle|\mathbf{r}|^n\rangle_\lambda$ is obtained by closing the contour to the right. We find that the pole structure of (7.4) is identical to that of the analogous $d=1$ result examined in Ref. 16. Hence whether $\langle|\mathbf{r}|^n\rangle$ diverges, vanishes, or converges to a finite value depends only on α and not on d. As noted in Ref. 16, the moments may become negative when $\alpha>2$ since then $p_\alpha^d(r)$ can take on negative values. The only effect that leaving d arbitrary has on the calculation is to generalize the finite nonzero moments when α is an even integer. This is to be expected since the existence or otherwise of the asymptotic power series is determined by the form of α alone, as is the analyticity of the characteristic function $\tilde{p}_\alpha^d(q)$. Following the procedure in Ref. 16 we arrive at the following results for the $2m$th absolute moment of $p_\alpha^d(r)$ for general d:

$$\langle|\mathbf{r}|^{2m}\rangle=\begin{cases}(-1)^{m+j}2^{2m}(d/2)_m\dfrac{(m)!}{j!}, & \alpha=2\dfrac{m}{j}\in\{2,4,6,\ldots\}\\ +\infty, & 2m>\alpha\in\cup_{k=0}^{\infty}(4k,4k+2)\\ -\infty, & 2m>\alpha\in\cup_{k=0}^{\infty}(4k+2,4k+4)\\ 0, & \text{otherwise.}\end{cases} \quad (7.5)$$

VIII. DISCUSSION

As Pólya[28] generalized Rayleigh's[29] work on Pearson's original random walk problem, from specific dimensions to arbitrary, so we, humbly, have now generalized our first investigation (Ref. 16) on the properties of the symmetric Lévy stable pdfs. The analytic results for $p_\alpha^d(r)$, i.e., the dimensional recursion relation and the identification of $p_\alpha^d(r)$ with certain special functions for various α and d will no doubt be of use in the diverse applications to random phenomena that $p_\alpha^d(r)$ enjoys when $\alpha\leqslant 2$ and it defines a pdf. Equally as exciting is the intricate exponentially small asymptotic behavior of $p_\alpha^d(r)$ which occurs for integral $\alpha\geqslant 3$, and which is dominant when α is even. By constructing this asymptotic expansion for arbitrary integral α and d we have exhibited a family of functions displaying dominant asymptotics beyond all orders, which provides a detailed case study for the exciting new field of asymptotics beyond all orders. As discussed in Ref. 16 we feel for this reason that $p_\alpha^d(r)$ for $\alpha>2$ will in time find interesting physical applications. A final interesting observation involves a number theoretic series which we referred to in Ref. 16 as the generalized Euler Jacobi series.[25] As discussed therein, there is a direct link between $p_\alpha^1(r)$ and the generalized Euler Jacobi series. As a consequence of the asymptotic analysis undertaken herein the general expression for the asymptotics of this series is now known.

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APPENDIX: CALCULATING $\Gamma^{1,1}_{2p-1}(k)$

Proposition 1:

$$\Gamma^{1,1}_{2p-1}(2m)=\Gamma^{1,1}_{2p-1}(2m+1)=\sum_{j=0}^{m}\exp\left(-2j\frac{(2l+d)\pi i}{p}\right),\quad m\in\left\{0,1,2,\ldots,\left[\frac{p-1}{2}\right]\right\}, \tag{A1}$$

where $[n]$ *represents the integer part of* n.

The proof of Proposition 1 begins with the following two recursion relations which we deduce from the general result 5.11.1(16) on page 197 of Ref. 27.

$$2m\Gamma^{1,1}_{2p-1}(2m)=\sum_{r=0}^{m-1}\left[1+2\exp\left(-\frac{2(r+1)(2l+d)\pi i}{p}\right)\right]\Gamma^{1,1}_{2p-1}[2(m-r-1)]$$
$$+\sum_{r=0}^{m-1}\Gamma^{1,1}_{2p-1}[2(m-r-1)+1]\qquad m\in\left\{1,2,\ldots,\left[\frac{p}{2}\right]\right\}, \tag{A2}$$

$$(2m+1)\Gamma^{1,1}_{2p-1}(2m+1)=\sum_{r=0}^{m-1}\left[1+2\exp\left(-\frac{2(r+1)(2l+d)\pi i}{p}\right)\right]\Gamma^{1,1}_{2p-1}[2(m-r-1)+1]$$
$$+\sum_{r=0}^{m}\Gamma^{1,1}_{2p-1}[2(m-r)],\quad m\in\left\{0,1,2,\ldots,\left[\frac{p-1}{2}\right]\right\}. \tag{A3}$$

Next we observe the validity of the following two lemmas, the second being a consequence of the first

Lemma 1:

$$\sum_{r=0}^{m-1}\sum_{j=0}^{m-r-1}\theta^{2j}+\sum_{r=0}^{m-1}[1+2\theta^{2(r+1)}]\sum_{j=0}^{m-r-1}\theta^{2j}=(2m)\sum_{j=0}^{m}\theta^{2j},\quad \forall m\in\mathbb{Z}_{>0}. \tag{A4}$$

Lemma 2:

$$\sum_{r=0}^{m}\sum_{j=0}^{m-r}\theta^{2j}+\sum_{r=0}^{m-1}[1+2\theta^{2(r+1)}]\sum_{j=0}^{m-r-1}\theta^{2j}=(2m+1)\sum_{j=0}^{m}\theta^{2j},\quad \forall m\in\mathbb{Z}_{\geqslant 0}, \tag{A5}$$

$\Gamma^{1,p}_{q+1}(0)=1$ always, so from (A2) and (A3) we obtain

$$\Gamma^{1,p}_{q+1}(0)=\Gamma^{1,1}_{2p-1}(1)=1,\quad \Gamma^{1,1}_{2p-1}(2)=\Gamma^{1,1}_{2p-1}(3)=1+\exp\left(-2\frac{(2l+d)\pi i}{p}\right), \tag{A6}$$

etc., which suggests the form

$$\Gamma^{1,1}_{2p-1}(2s)=\Gamma^{1,1}_{2p-1}(2s+1)=\sum_{j=0}^{s}\exp\left(-2j\frac{(2l+d)\pi i}{p}\right). \tag{A7}$$

If we assume that all the $\Gamma^{1,p}_{q+1}[2(m-r-1)]$ and $\Gamma^{1,p}_{q+1}[2(m-r-1)+1]$ in (A2) are of the form (A7) then by applying Lemma 1 we induce that

$$\Gamma^{1,1}_{2p-1}(2m)=\sum_{j=0}^{m}\exp\left(-2j\frac{(2l+d)\pi i}{p}\right),\quad m\in\left\{1,2,\ldots,\left[\frac{p}{2}\right]\right\}. \tag{A8}$$

Similarly, applying Lemma 2 to (A3) we induce

$$\Gamma^{1,1}_{2p-1}(2m+1)=\sum_{j=0}^{m}\ \exp\left(-2j\,\frac{(2l+d)\pi i}{p}\right),\quad m\in\left\{0,1,2,\ldots,\left[\frac{p-1}{2}\right]\right\},\tag{A9}$$

which proves Proposition 1.

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A new parametrization and all integral realizations of the Lorentz group

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A simple linear transformation of the biquaternionic parameters α and β of the group SL(2, **C**), which is two-to-one homomorphic to the restricted Lorentz group $\mathcal{L}$, is used to express each element of SL(2, **C**) and $\mathcal{L}$ in terms of the first column of an element of $\mathcal{L}$ and the quaternionic parameters α. This parametrization is shown to bring the determination of the integral realizations of the restricted Lorentz group under the purview of classical Diophantine analysis, involving the expression of a given pair of integers, respectively, as a sum of three squares and a sum of four squares. These solutions are further constrained by the condition that a set of four integers, which is linear in the solution of the three squares problem and in the solution of the four squares problem, have a common factor. These are all classical problems addressed and solved by Euclid, Euler, Fermat, Gauss, Jacobi, and others. The corresponding realizations of SL(2, **C**) fall into three distinct classes: those in which the elements of the matrix are Gaussian integers, Gaussian integers divided by $\sqrt{2}$, and Gaussian half-odd integers. These results apply also to the principal subgroups of SL(2, **C**). [DOI: 10.1063/1.1505124]

I. INTRODUCTION

P. A. M. Dirac[1] pointed out in 1972 the interesting structure possessed by the Gaussian integer and half-odd integer realizations of the group SL(2, **C**), which leads through the two-to-one homomorphism of this group onto the restricted Lorentz group $\mathcal{L}=\mathrm{SO}(3,1)$ to integral realizations of $\mathcal{L}$. He gave a parametrization of SL(2, **C**) in terms of biquaternionic parameters which he suggested was useful for such studies, but did not go very far in determining such integer realizations, nor was he specific about the applications he had in mind. Schild[2] earlier had studied such integer realizations of $\mathcal{L}$ with the purpose of using them to model a discrete space–time viewpoint of the physical world. Lorente[3] has used the Cayley parametrization, which is essentially the same as the biquaternionic parametrization, of the classical groups in a series of papers (see References in Ref. 3), and more recently in collaborations with Kramer,[4–7] and applied integral realizations of the Lorentz group to physical law formulated on a lattice. Balazs *et al.*[8,9] use integer representations of the Lorentz group in their construction of a relativistic lattice dynamics for modeling the dynamics of points of a relativistic fluid.

Lorente and Kramer,[6,7] using a set of generators attributed to Coxeter by Schild (Ref. 2. p. 47) and a result of Kac,[10] give a general expression for all integral representations of $\mathcal{L}$ in terms of these generators (see Remark 2 in Sec. VIII). Knowing a set of generators of a group, while eloquently specifying uniquely the group, is not always the easiest way to characterize the group elements themselves, and we shall proceed differently.

The author,[11] in a paper presenting a unified viewpoint of the role of the quantum mechanical rotation group SU(2) in its action in Euclidean three-space $\mathbf{R}^3$ and in spin space, used the methods of Cartan[12] and Wigner,[13] and the paper of Dirac,[1] to derive the following formula relating the elements $Z \in \mathrm{SL}(2,\mathbf{C})$ to the elements $L \in \mathcal{L}$:

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$$L = A_0^{\dagger}(Z \otimes Z^*)A_0, \tag{1.1}$$

where $\otimes$ denotes the Kronecker product, and A is the numerical unitary matrix given by

$$A_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -i & 0 \\ 0 & 1 & i & 0 \\ 1 & 0 & 0 & -1 \end{pmatrix}. \tag{1.2}$$

The real matrix L is defined so as to leave invariant the quadratic form $x^T G x$, $G = \mathrm{diag}(1,-1,-1,-1)$, $x = \mathrm{col}(x^0,x^1,x^2,x^3)$ (T denotes matrix transposition) under the linear transformation $x \mapsto Lx$. Thus, the matrix $L = (L)_{0 \leqslant \mu,\nu \leqslant 3}$ satisfies $L^T G L = G$, and may be shown also to satisfy $\det L = 1$, $L_{00} \geqslant 1$. Thus, L is an element of the restricted Lorentz group.

Relation (1.1) is not only quite easy to solve for Z in terms of L, but is especially useful for relating the biquaternionic parametrization of SL(2, **C**) to that of $\mathcal{L}$. This relationship can then be used in an obvious manner to parametrize all matrices in $Z \in \mathrm{SL}(2,\mathbf{C})$ and $L \in \mathcal{L}$ in terms of the first column of L and one set of the biquaternionic parameters. This parametrization, in turn, brings the problem of determining all integral realizations of $\mathcal{L}$ within the purview of classical methods in number theory, known and solved since the time of Euclid, Euler, Fermat, Gauss, Jacobi, and others. These methods are all described in the elementary and readable book by Uspensky and Heaslet.[14]

The purpose of this article is to effect the steps described above. A principal feature that emerges is the existence of a 384 element finite group, which acts in the biquaternionic parameter space to effect signed permutations of these parameters, that is, permutations as well as $\pm$ signs on the permuted quantities, and the transfer of this action to that of a second finite group with 48 elements, which acts on the elements of the Lorentz matrix to effect signed permutations of these elements. It is this structure, together with the classical number theory mentioned above, that leads to algorithms for the construction of all integral L, and to the elements of Z that are homomorphic to the integral L. A somewhat unexpected feature is that the matrices in SL(2, **C**) mapping to integral matrices in $\mathcal{L}$ fall into the two classes with elements given by Gaussian integers and Gaussian half-odd integers, as pointed out by Dirac,[1] and a third class with elements given by (Gaussian integers)/$\sqrt{2}$.

The plan of the article is as follows: In the Introduction, we continue with the review of the biquaternionic parametrization of SL(2, **C**), deriving quite easily from Eq. (1.1) a result given by MacFarlane.[15] It is quite tedious to obtain the form given by Eqs. (1.12)–(1.14) from MacFarlane's result, despite its eloquent compactness. In Sec. II, we introduce a finite group with 384 elements, denoted H_4, of signed permutations, which is a finite symmetry group of the Lorentz group, where the action of the group H_4 is defined on the biquaternionic parameters. A second finite group with 48 elements, denoted H_3, of signed permutations is also introduced, and its action defined on the elements of a given Lorentz matrix L. In Sec. III, we establish an eight-to-one homomorphism between the groups H_4 and H_3. In Sec. IV, we give the explicit parametrization of each matrix $L \in \mathcal{L}$ in terms of its first column, as well as the corresponding elements $Z \in \mathrm{SL}(2,\mathbf{C})$. In Sec. V, we apply these results to the four principal subgroups of SL(2, **C**). In Sec. VI, this general parametrization in terms of the first column leads easily to the integral realizations of the Lorentz group $\mathcal{L}$, and the corresponding elements of SL(2, **C**), falling into the three classes mentioned above. Explicit algorithms are given for constructing these three classes using classical number theory for a pair of Diophantine equations expressing a given pair of integers, respectively, as the sum of three squares and the sum four squares, and the Euclidean algorithm for determining the greatest common divisor of a related set of four integers.

We now continue in this Introduction with solving relation (1.1) for the matrix Z in terms of L. We write Eq. (1.1) in the form

$$A_0 L A_0^\dagger = Z \otimes Z^* = \text{Kronecker product of } Z \text{ and } Z^* = \begin{pmatrix} z_{11}Z^* & z_{12}Z^* \\ z_{21}Z^* & z_{22}Z^* \end{pmatrix}. \tag{1.3}$$

We work out the left-hand side of this relation and write it in the 2×2 block form

$$A_0 L A_0^\dagger = \frac{1}{2}\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22}. \end{pmatrix}, \tag{1.4}$$

where

$$\begin{aligned}
M_{11} &= \begin{pmatrix} L_{00}+L_{33}+L_{03}+L_{30} & L_{01}+L_{31}+i(L_{02}+L_{32}) \\ L_{10}+L_{13}-i(L_{20}+L_{23}) & L_{11}+L_{22}+i(L_{12}-L_{21}) \end{pmatrix}, \\
M_{12} &= \begin{pmatrix} L_{01}+L_{31}-i(L_{02}+L_{32}) & L_{00}+L_{33}-L_{03}+L_{30} \\ L_{11}-L_{22}-i(L_{21}+L_{12}) & L_{10}-L_{13}-i(L_{20}-L_{23}) \end{pmatrix}, \\
M_{21} &= \begin{pmatrix} L_{10}+L_{13}+i(L_{20}+L_{23}) & L_{11}-L_{22}+i(L_{21}+L_{12}) \\ L_{00}-L_{33}+L_{03}-L_{30} & L_{01}-L_{31}+i(L_{02}-L_{32}) \end{pmatrix}, \\
M_{22} &= \begin{pmatrix} L_{11}+L_{22}+i(L_{21}-L_{12}) & L_{00}-L_{13}+i(L_{20}-L_{23}) \\ L_{01}-L_{31}-i(L_{02}-L_{32}) & L_{00}+L_{33}-L_{03}-L_{30} \end{pmatrix}.
\end{aligned} \tag{1.5}$$

Here we write L in the following form with elements $L_{\mu\nu}, 0\leqslant \mu,\nu\leqslant 3$:

$$L = \begin{pmatrix} L_{00} & L_{01} & L_{02} & L_{03} \\ L_{10} & L_{11} & L_{12} & L_{13} \\ L_{20} & L_{21} & L_{22} & L_{23} \\ L_{30} & L_{31} & L_{32} & L_{33} \end{pmatrix}. \tag{1.6}$$

We next solve for Z, noting the several other relations that come from the present approach. We first have from Eqs. (1.2) and (1.3) that

$$z_{ij}Z^* = \tfrac{1}{2}M_{ij}, \quad i,j=1,2. \tag{1.7}$$

Moreover, we have from Eq. (1.3) that

$$\operatorname{tr} L = \operatorname{tr} Z \operatorname{tr} Z^* = |\operatorname{tr} Z|^2, \tag{1.8}$$

while from (1.7) we have

$$z_{ij} \operatorname{tr} Z^* = \tfrac{1}{2}\operatorname{tr} M_{ij}, \quad z_{ij}^2 = \tfrac{1}{4}\det M_{ij}. \tag{1.9}$$

If $\operatorname{tr} L \neq 0$, we obtain immediately from these relations and $\det Z = 1$ that

$$Z = \frac{1}{2\operatorname{tr} Z^*}A = \frac{A}{\sqrt{\det A}}, \quad \text{for} \quad \operatorname{tr} L \neq 0, \tag{1.10}$$

where

$$A = \begin{pmatrix} \operatorname{tr} M_{11} & \operatorname{tr} M_{12} \\ \operatorname{tr} M_{21} & \operatorname{tr} M_{22} \end{pmatrix}, \tag{1.11}$$

$$\begin{aligned}
\operatorname{tr} M_{11} &= \operatorname{tr} L + (L_{03}+L_{30}) + i(L_{12}-L_{21}),\\
\operatorname{tr} M_{12} &= (L_{01}+L_{10}) - (L_{13}-L_{31}) + i(-L_{02}-L_{20}+L_{23}-L_{32}),\\
\operatorname{tr} M_{21} &= (L_{01}+L_{10}) + (L_{13}-L_{31}) - i(-L_{02}-L_{20}-L_{23}+L_{32}),\\
\operatorname{tr} M_{22} &= \operatorname{tr} L - (L_{03}+L_{30}) - i(L_{12}-L_{21}).
\end{aligned} \tag{1.12}$$

In general, $\det A$ is complex in Eq. (1.10), and this must be taken into account in extracting the square root. Moreover, if the singular case $\det L=0$ holds, then one appeals directly to the second of Eqs. (1.9) for the solution.

The result given by Eqs. (1.10)–(1.12) is the same as that obtained from MacFarlane's[15] Eq. (69) with $L_{00}=L_0^0$, $L_{0i}=-L_i^0$, $L_{i0}=-L_0^i$, $L_{ij}=L_j^i$, $i,j=1,2,3$. This is accounted for by the fact that MacFarlane's homomorphism of SL(2, **C**) onto $\mathcal{L}$ is related to the one given by relation (1.1) as follows: For $Z' \mapsto L'$ in the MacFarlane homomorphism, then $Z \mapsto L = GL'G$ in the homomorphism (1.1), where $G=\operatorname{diag}(1,-1,-1,-1)$. [See also relation (1.19)].

The parametrization of Z in terms of biquaternionic parameters (see Refs. 1 and 11) is given as follows:

$$\begin{aligned}
Z = Z(\alpha,\beta) &= \begin{pmatrix} \alpha_0 - i\alpha_3 & -i\alpha_1-\alpha_2 \\ -i\alpha_1+\alpha_2 & \alpha_0+i\alpha_3 \end{pmatrix} + i\begin{pmatrix} \beta_0 - i\beta_3 & -i\beta_1-\beta_2 \\ -i\beta_1+\beta_2 & \beta_0+i\beta_3 \end{pmatrix}\\
&= \begin{pmatrix} \alpha_0+\beta_3 - i(\alpha_3-\beta_0) & -\alpha_2+\beta_1 - i(\alpha_1+\beta_2) \\ \alpha_2+\beta_1 - i(\alpha_1-\beta_2) & \alpha_0-\beta_3+i(\alpha_3+\beta_0) \end{pmatrix},
\end{aligned} \tag{1.13}$$

where the condition that $Z \in \mathrm{SL}(2,\mathbf{C})$ is expressed by

$$\alpha^2-\beta^2=1, \quad \alpha\cdot\beta=\alpha_0\beta_0+\alpha_1\beta_1+\alpha_2\beta_2+\alpha_3\beta_3=0,$$

in which

$$\alpha=(\alpha_0,\alpha_1,\alpha_2,\alpha_3), \quad \beta=(\beta_0,\beta_1,\beta_2,\beta_3)$$

are real points. These parameters are given in terms of Z by

$$\begin{aligned}
\alpha_0+i\beta_0 &= \frac{1}{2}(z_{11}+z_{22}), \quad \alpha_1+i\beta_1=\frac{i}{2}(z_{12}+z_{21}),\\
\alpha_2+i\beta_2 &= \frac{-1}{2}(z_{12}-z_{21}), \quad \alpha_3+i\beta_3=\frac{i}{2}(z_{11}-z_{22}),
\end{aligned} \tag{1.14}$$

which show that each $Z \in \mathrm{SL}(2,\mathbf{C})$ defines a unique set of real parameters α and β. These real parameters are also given in terms of L by

$$\begin{aligned}
\alpha_0+i\beta_0 &= \frac{\operatorname{tr} L}{\sqrt{\det A}}, \quad \alpha_1+i\beta_1=\frac{L_{32}-L_{23}+i(L_{01}+L_{10})}{\sqrt{\det A}},\\
\alpha_2+i\beta_2 &= \frac{L_{13}-L_{31}+i(L_{02}+L_{20})}{\sqrt{\det A}}, \quad \alpha_3+i\beta_3=\frac{L_{21}-L_{12}+i(L_{03}+L_{30})}{\sqrt{\det A}}.
\end{aligned} \tag{1.15}$$

Recall that in general $\det A$ is complex, and this must be accounted for in solving these relations for α and β. The biquaternion parameters α and β are related to the Cayley parameters used by Lorente[3] by $\alpha=(m,-q,p,-n), \beta=(-\lambda,-r,s,-t)$.

The expression of the matrix $L \in \mathcal{L}$ in terms of the quaternionic parameters α and β is obtained directly from Eqs. (1.1) and (1.13). For a concise expression of this result, it is convenient to write $L(\alpha,\beta)$ in the form

$$L(\alpha,\beta)=\begin{pmatrix} y_0(\alpha,\beta) & x_1(\alpha,\beta) & x_2(\alpha,\beta) & x_3(\alpha,\beta) \\ y_1(\alpha,\beta) & w_1(\alpha,\beta) & u_3(\alpha,\beta) & v_2(\alpha,\beta) \\ y_2(\alpha,\beta) & v_3(\alpha,\beta) & w_2(\alpha,\beta) & u_1(\alpha,\beta) \\ y_3(\alpha,\beta) & u_2(\alpha,\beta) & v_1(\alpha,\beta) & w_3(\alpha,\beta) \end{pmatrix}, \tag{1.16}$$

where

$$\begin{aligned} y_0(\alpha,\beta)&=\alpha^2+\beta^2=2(\alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2)-1, \\ y_i(\alpha,\beta)&=2(\alpha_0\beta_i-\alpha_i\beta_0+\alpha_j\beta_k-\alpha_k\beta_j), \\ x_i(\alpha,\beta)&=2(\alpha_0\beta_i-\alpha_i\beta_0-\alpha_j\beta_k+\alpha_k\beta_j), \\ u_i(\alpha,\beta)&=2(-\alpha_0\alpha_i+\alpha_j\alpha_k-\beta_0\beta_i+\beta_j\beta_k), \\ v_i(\alpha,\beta)&=2(\alpha_0\alpha_i+\alpha_j\alpha_k+\beta_0\beta_i+\beta_j\beta_k), \\ w_i(\alpha,\beta)&=2(\alpha_0^2+\beta_0^2+\alpha_i^2+\beta_i^2)-(\alpha^2+\beta^2)=2(\alpha_0^2+\alpha_i^2-\beta_j^2-\beta_k^2)-1, \\ &(i,j,k) \text{ is cyclic in } 1,2,3. \end{aligned} \tag{1.17}$$

The two-to-one homomorphism $\mathrm{SL}(2,\mathbf{C})\to\mathcal{L}$ is expressed in terms of the parameters α and β by

$$Z(\alpha,\beta)\mapsto L(\alpha,\beta), \quad Z(-\alpha,-\beta)=-Z(\alpha,\beta)\mapsto L(\alpha,\beta). \tag{1.18}$$

We also note that the MacFarlane homomorphism $\mathrm{SL}(2,\mathbf{C})\to\mathcal{L}$ is given by

$$Z'(\alpha,\beta)=Z(-\alpha_0,\alpha_1,\alpha_2,\alpha_3;-\beta_0,\beta_1,\beta_2,\beta_3). \tag{1.19}$$

Observe that Eqs. (1.17) show explicitly that $L_{00}\geqslant 1$ and also imply the following: *Every Gaussian integer element of* $\mathrm{SL}(2,\mathbf{C})$ *maps to a real integer element of* $\mathcal{L}$.

II. DISCRETE SYMMETRIES IN THE PARAMETERS α AND β

Let S_n denote the group of permutations of the integers $(1,2,...,n)$ with action on an arbitrary sequence $x=(x_1,x_2,\ldots,x_n)$ defined by

$$\pi: x\mapsto \pi(x_1,x_2,\ldots,x_4)=(x_{\pi_1},x_{\pi_2},\ldots,x_{\pi_n}), \quad \text{for } \pi=\begin{pmatrix} 1 & 2 & \ldots & n \\ \pi_1 & \pi_2 & \ldots & \pi_n \end{pmatrix}. \tag{2.1}$$

Thus, the action of the permutation π is a substitution of the subscripts $(1,2,\ldots,n)$ by $(\pi_1,\pi_2,\ldots,\pi_n)$. The parity of a permutation is even or odd if it takes an even or odd number of transpositions to restore the sequence $(\pi_1,\pi_2,\ldots,\pi_n)$ to the order $(1,2,\ldots,n)$.

Let Σ_n denote the set of sequences defined by

$$\Sigma_n=\{\sigma=(\sigma_1,\sigma_2,\ldots,\sigma_n)| \quad \text{each } \sigma_i=\pm 1\}. \tag{2.2}$$

The set Σ_n is an Abelian group under component-wise multiplication of sequences, which is a realization of the direct product group $S_2\times S_2\times\cdots\times S_2$.

The direct product group $H_n=\Sigma_n\times S_n$ is the group of order $2^n n!$ of *signed permutations* with elements given by the ordered pairs (σ,π) with multiplication rule

$$(\sigma'\times\pi')(\sigma\times\pi)=(\sigma'\sigma)\times(\pi'\pi), \tag{2.3}$$

and action on x defined by

$$x\rightarrow(\sigma,\pi)x=(\sigma_1 x_{\pi_1},\sigma_2 x_{\pi_2},\ldots,\sigma_n x_{\pi_n}). \tag{2.4}$$

We define the sequence $\sigma=(\sigma_1,\sigma_2,\ldots,\sigma_n)$ to have *even parity* if $\sigma_1\sigma_2\cdots\sigma_n=1$ and *odd parity* if $\sigma_1\sigma_2\cdots\sigma_n=-1$.

We choose S_4 to be the group of permutations on (0,1,2,3) for application to the pair of sequences $\alpha=(\alpha_0,\alpha_1,\alpha_2,\alpha_3)$ and $\beta=(\beta_0,\beta_1,\beta_2,\beta_3)$. The action of S_4 on the pair (α,β) of sequences is to effect the same permutation on each sequence:

$$\pi:(\alpha,\beta)\mapsto(\pi(\alpha),\pi(\beta)),$$

$$\pi(\alpha)=(\alpha_{\pi_0},\alpha_{\pi_1},\alpha_{\pi_2},\alpha_{\pi_3}),\quad \pi(\beta)=(\beta_{\pi_0},\beta_{\pi_1},\beta_{\pi_2},\beta_{\pi_3}), \tag{2.5}$$

$$\pi=\begin{pmatrix}0&1&2&3\\ \pi_0&\pi_1&\pi_2&\pi_3\end{pmatrix}.$$

For symmetry of notation, we also denote the elements of Σ_4 by $(\sigma_0,\sigma_1,\sigma_2,\sigma_3)$.

The significance of the group $H_4=\Sigma_4\times S_4$ of signed substitutions is that $\det Z(\alpha,\beta)=\alpha^2-\beta^2+2i\alpha\cdot\beta$ is invariant under the simultaneous transformations

$$\begin{aligned}\alpha&\mapsto h(\alpha)=(\sigma_0\alpha_{\pi_0},\sigma_1\alpha_{\pi_1},\sigma_2\alpha_{\pi_2},\sigma_3\alpha_{\pi_3}),\\ \beta&\mapsto h(\beta)=(\sigma_0\beta_{\pi_0},\sigma_1\beta_{\pi_1},\sigma_2\beta_{\pi_2},\sigma_3\beta_{\pi_3}),\end{aligned} \tag{2.6}$$

where the action of $h\in H_4$ on $Z(\alpha,\beta)$ is defined by

$$h:Z(\alpha,\beta)\mapsto Z(h(\alpha),h(\beta)). \tag{2.7}$$

For the group SL(2, **C**), where $\alpha^2-\beta^2=1$ and $\alpha\cdot\beta=0$, the group $H_4=\Sigma_4\times S_4$ can be enlarged by adjoining the two element group $\Sigma_2=\{(1,1),(1,-1)\}$ to form the direct product group

$$H_{2,4}=\Sigma_2\times H_4=\Sigma_2\times(\Sigma_4\times S_4) \tag{2.8}$$

with elements (τ,σ,π) having action on the pair (α,β) given by

$$(\tau,\sigma,\pi):(\alpha,\beta)\rightarrow(\tau,\sigma,\pi)(\alpha,\beta)=(\tau_1 h(\alpha),\tau_2 h(\beta)). \tag{2.9}$$

The group $H_{2,4}$ is a symmetry group of SL(2, **C**) of order 776, that is,

$$Z(h'(\alpha,\beta))\in \mathrm{SL}(2,\mathbf{C}),\quad \text{each}\quad h'\in H_{2,4}. \tag{2.10}$$

Since the extra symmetry

$$Z(-\alpha,\beta)=Z(\alpha,\beta)=-Z(\alpha,\beta) \tag{2.11}$$

originated from the group $H_{2,4}$ is easily taken into account, we restrict our attention to the group H_4, which is a normal subgroup of $H_{2,4}$, and Σ_2 is the factor group $H_{2,4}/H_4$.

Let us note that the mapping $h:\mathrm{SL}(2,\mathbf{C})\rightarrow\mathrm{SL}(2,\mathbf{C})$ is an inner automorphism if and only if one can write

$$Z(h(\alpha,\beta))=A_h Z(\alpha,\beta)A_h^{-1}, A_h\in \mathrm{SL}(2,\mathbf{C}); \tag{2.12}$$

otherwise the mapping is an outer automorphism. We have not determined which elements of H_4 are inner and which are outer automorphisms.

For each $h\in H_4$, we have the mapping of elements of SL(2, **C**) to elements of $\mathcal{L}$ given by

$$Z(h(\alpha,\beta))\mapsto L(h(\alpha,\beta)). \tag{2.13}$$

Thus, in the general case, 384 distinct matrices in SL(2, **C**) map to matrices in $\mathcal{L}$. But, as we shall show, at most 48 distinct matrices in $\mathcal{L}$ can arise, and these correspond to signed permutations of the elements of L. This result is an easy consequence of the explicit results we give below.

No ambiguity will arise if we write the ordered pair of elements in Eq. (2.3) in juxtaposition:

$$h(\sigma,\pi)=(\sigma_0,\sigma_1,\sigma_2,\sigma_3)\begin{pmatrix}0&1&2&3\\ \pi_0&\pi_1&\pi_2&\pi_3\end{pmatrix}. \tag{2.14}$$

Observing the permutational symmetry of the elements in column 1 of $L(\alpha,\beta)$ given by Eq. (1.17), especially the distinguished position of α_0, we are led to enumerate the set of 384 signed permutations in H_4 by the following notation:

$$\begin{aligned}
h^{(0)}_{\sigma_0}(\tau,\rho)&=(\sigma_0,\sigma_0\tau_1,\sigma_0\tau_2,\sigma_0\tau_3)\begin{pmatrix}0&1&2&3\\ 0&\rho_1&\rho_2&\rho_3\end{pmatrix},\\
h^{(1)}_{\sigma_1}(\tau,\rho)&=(-\sigma_1\tau_1,\sigma_1,\sigma_1\tau_3,-\sigma_1\tau_2)\begin{pmatrix}0&1&2&3\\ \rho_1&0&\rho_3&\rho_2\end{pmatrix},\\
h^{(2)}_{\sigma_2}(\tau,\rho)&=(-\sigma_2\tau_2,-\sigma_2\tau_3,\sigma_2,\sigma_2\tau_1)\begin{pmatrix}0&1&2&3\\ \rho_2&\rho_3&0&\rho_1\end{pmatrix},\\
h^{(3)}_{\sigma_3}(\tau,\rho)&=(-\sigma_3\tau_3,\sigma_3\tau_2,-\sigma_3\tau_1,\sigma_3)\begin{pmatrix}0&1&2&3\\ \rho_3&\rho_2&\rho_1&0\end{pmatrix},
\end{aligned} \tag{2.15}$$

where $\tau\in\Sigma_3$ and

$$\begin{pmatrix}1&2&3\\ \rho_1&\rho_2&\rho_3\end{pmatrix}\in S_3.$$

Thus, introducing the notation

$$p(\tau,\rho)=(\tau_1,\tau_2,\tau_3)\begin{pmatrix}1&2&3\\ \rho_1&\rho_2&\rho_3\end{pmatrix} \tag{2.16}$$

for an element of H_3, we have partitioned the group H_4 into 48 subsets $S(\tau,\rho)$, each containing eight elements, and defined by

$$S(\tau,\rho)=\{h^{(k)}_{\sigma_k}(\tau,\rho)\,|\,k=0,1,2,3;\ \text{each}\ \ \sigma_k=\pm 1,\ \ p(\tau,\rho)\in H_3\}. \tag{2.17}$$

The actions of the group elements $h^{(k)}_{\sigma_k}(\tau,\rho)\in H_4$ are implemented directly on the elements of the Lorentz matrix $L(\alpha,\beta)$ by applying

$$h{:}L_{\mu,\nu}(\alpha,\beta)\mapsto L_{\mu,\nu}(h(\alpha),h(\beta)),\ \ \text{each}\ \ h\in H_4. \tag{2.18}$$

The group elements $p(\tau,\rho)\in H_3$ act on the indices of an arbitrary sequence (z_1,z_2,z_3) is to effect the signed permutation $(\tau_1 z_{\rho_1},\tau_2 x_{\rho_2},\tau_3 z_{\rho_3})$. It is the case that action of each $h\in H_4$ effects a signed permutation $p(\tau,\sigma)$ of the elements in $L(\alpha,\beta)$. For a concise description of this latter action, it is notationally convenient to suppress the parameters α and β and write $L(\alpha,\beta)$ in the form

$$L(\alpha,\beta)=\begin{pmatrix} y_0 & x_1 & x_2 & x_3 \\ y_1 & w_1 & u_3 & v_2 \\ y_2 & v_3 & w_2 & u_1 \\ y_3 & u_2 & v_1 & w_3 \end{pmatrix}, \tag{2.19}$$

where $y_0=L_{0,0}$ and

$$\begin{gathered} x_i=L_{0,i}(\alpha,\beta),y_i=L_{i,0}(\alpha,\beta),w_i=L_{i,i}(\alpha,\beta), \quad \text{for } i=1,2,3 \\ u_i=L_{j,k}(\alpha,\beta),v_i=L_{k,j}(\alpha,\beta), \\ (i,j,k) \text{ an even permutation of } (1,2,3). \end{gathered} \tag{2.20}$$

The explicit calculations given in Eqs. (4.14)–(4.17) in Sec. IV show that *the action of the group H_4 is transferred to the action of the group H_3* on the elements (x_1,x_2,x_3), (y_1,y_2,y_3), (u_l,u_2,u_3), (v_1,v_2,v_3), (w_1,w_2,w_3) of $L(\alpha,\beta)$ in accordance with the rule

$$h^{(k)}_{\sigma_k}(\tau,\rho):(z_1,z_2,z_3)\mapsto p(\tau',\rho)(z_1,z_2,z_3), \quad k=0,1,2,3, \quad \sigma_k=\pm 1, \tag{2.21}$$

where the sequence τ' depends only on the index k, and the identification of (z_1,z_2,z_3) with one of (x_1,x_2,x_3), (y_1,y_2,y_3), (u_l,u_2,u_3), (v_1,v_2,v_3), (w_1,w_2,w_3).

The complete set of group actions is given in Eqs. (4.14)–(4.17) in Sec. IV, after we develop the properties of the groups H_4 and H_3.

III. RELATIONSHIP BETWEEN THE GROUPS H_4 AND H_3

We can obtain the relationship between the groups H_4 and H_3 by determining the *little group* (also called the stabilizer) that leaves the column sequence (y_1,y_2,y_3) fixed. This group is found from Eqs. (1.17) and definitions (2.15) to be the group S containing eight elements:

$$S=S((1,1,1),(123))=\{S^{(0)}_{\sigma_0},S^{(1)}_{\sigma_1},S^{(2)}_{\sigma_2},S^{(3)}_{\sigma_3}| \text{ each } \sigma_k=\pm 1\}, \tag{3.1}$$

where

$$\begin{gathered} S^{(0)}_{\sigma_0}=\sigma_0(1,1,1,1)\cdot(0)(1))(2)(3), \quad S^{(1)}_{\sigma_1}=\sigma_1(-1,1,1,-1)\cdot(01)(23), \\ S^{(2)}_{\sigma_2}=\sigma_2(-1,-1,1,1)\cdot(02)(13), \quad S^{(3)}_{\sigma_3}=\sigma_3(-1,1,-1,1)\cdot(03)(12), \end{gathered} \tag{3.2}$$

where the cycle notation for permutations is used, and a $\cdot$ is placed between elements of Σ_4 and elements of S_4 for clarity. The four even elements $\{(0)(1)(2)(3),(01)(23),(02)(13),(03)(12)\}$ constitute a normal subgroup of S_4, and S is a normal subgroup of the direct product group $H_4=\Sigma_4\times S_4$.

The above result establishes an eight-to-one homomorphism between the groups H_4 and H_3 given by

$$S(\tau,\rho)\mapsto(\tau_1,\tau_2,\tau_3)\begin{pmatrix} 1 & 2 & 3 \\ \rho_1 & \rho_2 & \rho_3 \end{pmatrix}=p(\tau,\rho). \tag{3.3}$$

Since S is a normal subgroup of H_4, left cosets and right cosets are equal. Representatives of the 48 cosets, or equivalently of the factor group H_4/S, may be chosen as follows. Define the following elements of S_4, using cycle notation:

$$\begin{aligned} &s_1=(0)(1)(2)(3), \quad s_2=(0)(123), \quad s_3=(1)(023), \quad \text{even elements,} \\ &s_4=(01)(2)(3), \quad s_5=(02)(1)(3), \quad s_6=(03)(1)(2), \quad \text{odd elements.} \end{aligned} \tag{3.4}$$

Define the following representative elements of the factor group H_4/S:

$$f_m(\sigma_1,\sigma_2,\sigma_3)=(1,\sigma_1,\sigma_2,\sigma_3)s_m, \quad m=1,2,\ldots,6; \ \text{each} \ \sigma_i=\pm 1. \tag{3.5}$$

The cosets of S in H_4 are given by

$$\{Sf_m(\sigma_1,\sigma_2,\sigma_3)|m=1,2,\ldots,6; \ \text{each} \ \sigma_i=\pm 1\}. \tag{3.6}$$

The results given in this section are important for enumerating the symmetries of the new parametrization of the restricted Lorentz group given in the next section.

IV. PARAMETRIZATION OF L IN TERMS OF ITS FIRST COLUMN AND THE QUATERNIONIC PARAMETERS α

In this section, we make a transformation of parameters α and β such that every Lorentz matrix $L(\alpha,\beta)$ as given by Eqs. (1.16) and (1.17) is expressed in terms of its first column (y_0,y_1,y_2,y_3) and the parameters α alone. The resulting new Lorentz matrix, which we denote by $(y|\alpha)$, is given explicitly in relations (4.6) and Eqs. (4.11) and (4.12).

Let us first mention some general features of this new parametrization. The elements in the first column of L satisfy

$$y_1^2+y_2^2+y_3^2=y_0^2-1, \tag{4.1}$$

and the parameters $(\alpha_0,\alpha_1,\alpha_2,\alpha_3)$ satisfy

$$\alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2=\frac{y_0+1}{2}. \tag{4.2}$$

We define the sphere $S_n(r)$ of radius r to be the set of real points x as follows:

$$S_n(r)=\{x=(x_1,x_2,\ldots,x_n)|x_1^2+x_2^2+\ldots+x_n^2=r^2)\}. \tag{4.3}$$

Thus, the first column of the Lorentz matrix Z is any point $(y_1,y_2,y_3)\in S_3(r_1)$, $r_1^2=y_0^2-1$, $y_0 \geqslant 1$. The quaternionic parameter sequence $(\alpha_0,\alpha_1,\alpha_2,\alpha_3)$ is any point $\alpha\in S_4(r_2)$, $r_2^2=(1+y_0)/2$. From a given pair of points solving Eqs. (4.1) and (4.2), we obtain a set of new points that are signed partitions of the old ones by applying the group elements of H_3 and H_4, respectively, namely, $p(\tau',\rho')y$ and $h^{(k)}_{\sigma_k}(\tau,\rho)\alpha$.

By adjoining the relation $\alpha\cdot\beta=0$ to the three relations for $L_{10}(\alpha,\beta)$, $L_{20}(\alpha,\beta)$, $L_{30}(\alpha,\beta)$ given by Eqs. (1.17), and writing $\beta=\text{col}(\beta_0,\beta_1,\beta_2,\beta_3)$ and $\hat{y}=\text{col}(y_1,y_2,y_3,0)$, we obtain

$$A^T(\alpha)\beta=\frac{1}{2}\hat{y}, \quad A(\alpha)=A(\alpha_0,\alpha_1,\alpha_2,\alpha_3)=\begin{pmatrix} -\alpha_1 & -\alpha_2 & -\alpha_3 & \alpha_0 \\ \alpha_0 & \alpha_3 & -\alpha_2 & \alpha_1 \\ -\alpha_3 & \alpha_0 & \alpha_1 & \alpha_2 \\ \alpha_2 & -\alpha_1 & \alpha_0 & \alpha_3 \end{pmatrix}. \tag{4.4}$$

Noting that $A(\alpha)A^T(\alpha)=(\alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2)I_4=[(y_0+1)/2]I_4$, we thus obtain

$$\beta=\beta(y,\alpha)=\frac{1}{1+y_0}\gamma(y,\alpha),\quad \gamma(y,\alpha)=A(\alpha)\hat{y}. \tag{4.5}$$

The γ_μ are given by

$$\begin{aligned}&\gamma_0(y,\alpha)=-\alpha_1y_1-\alpha_2y_2-\alpha_3y_3,\quad \gamma_1(y,\alpha)=\alpha_0y_1+\alpha_3y_2-\alpha_2y_3,\\&\gamma_2(y,\alpha)=-\alpha_3y_1+\alpha_0y_2+\alpha_1y_3,\quad \gamma_3(y,\alpha)=\alpha_2y_1-\alpha_1y_2+\alpha_0y_3.\end{aligned} \tag{4.6}$$

One verifies directly that the following relations are satisfied:

$$\beta_0^2+\beta_1^2+\beta_2^2+\beta_3^2=\frac{y_0-1}{2},\quad \alpha^2-\beta^2=1,\quad \alpha\cdot\beta=0. \tag{4.7}$$

We now eliminate the parameters β from $L(\alpha,\beta)$ by using relation (4.5). We denote the corresponding Lorentz matrix by $(y|\alpha)$, suppressing L_{00}, but regaining it through $(y|\alpha)_{00}=L_{00}=y_0$. The elements of this matrix are denoted by $(y|\alpha)_{\mu\nu}$, $0\leqslant\mu,\ \nu\leqslant3$.

We summarize the results for this new parametrization of the Lorentz matrices in $\mathcal{L}$:

For each point $y\in S_3(r_1)\subset\mathbf{R}^3$ *and for each point* $\alpha\in S_4(r_2)\subset\mathbf{R}^4$, *that is,*

$$y_1^2+y_2^2+y_3^2=y_0^2-1,\quad \alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2=\frac{y_0+1}{2}, \tag{4.8}$$

the set of restricted Lorentz matrices $\mathcal{L}$ *is given by*

$$(y|\alpha)=L\left(\alpha,\frac{1}{1+y_0}\gamma(y,\alpha)\right),\quad \gamma(y,\alpha)=A(\alpha)\hat{y}. \tag{4.9}$$

The homomorphism of SL(2, **C**) *onto* $\mathcal{L}$ *is given by*

$$Z(y|\alpha)=Z(\alpha,\beta(y,\alpha))\mapsto(y|\alpha), \tag{4.10}$$

where

$$(y|\alpha)=\begin{pmatrix}y_0 & x_1(y,\alpha) & x_2(y,\alpha) & x_3(y,\alpha)\\ y_1 & w_1(y,\alpha) & u_3(y,\alpha) & v_2(y,\alpha)\\ y_2 & v_3(y,\alpha) & w_2(y,\alpha) & u_1(y,\alpha)\\ y_3 & u_2(y,\alpha) & v_1(y,\alpha) & w_3(y,\alpha)\end{pmatrix}, \tag{4.11}$$

$$x_i(y,\alpha)=(y|\alpha)_{0,i}=\frac{2}{1+y_0}[\alpha_0\gamma_i(y,\alpha)-\alpha_i\gamma_0(y,\alpha)-\alpha_j\gamma_k(y,\alpha)+\alpha_k\gamma_j(y,\alpha)],$$

$$u_i(y,\alpha)=(y|\alpha)_{j,k}=2(-\alpha_0\alpha_i+\alpha_j\alpha_k)+\frac{2}{(1+y_0)^2}[-\gamma_0(y,\alpha)\gamma_i(y,\alpha)+\gamma_j(y,\alpha)\gamma_k(y,\alpha)],$$

$$v_i(y,\alpha)=(y|\alpha)_{k,j}=2(\alpha_0\alpha_i+\alpha_j\alpha_k)+\frac{2}{(1+y_0)^2}[\gamma_0(y,\alpha)\gamma_i(y,\alpha)+\gamma_j(y,\alpha)\gamma_k(y,\alpha)], \tag{4.12}$$

$$w_i(y,\alpha)=2(\alpha_0^2+\alpha_i^2)-1-\frac{2}{(1+y_0)^2}[\gamma_j^2(y,\alpha)+\gamma_k^2(y,\alpha)],$$

(i,j,k) *is a cyclic permutation of* (1,2,3).

The homomorphism of SL(2, **C**) *onto the restricted Lorentz group* $\mathcal{L}$ *is now given by*

$$Z(y|\alpha) =$$

$$\left(\begin{array}{c|c} (\alpha_0 - i\alpha_3)(1+\frac{y_3}{y_0+1}) - \frac{(\alpha_1+i\alpha_2)(iy_1+y_2)}{y_0+1} & -(\alpha_2+i\alpha_1)(1+\frac{y_3}{y_0+1}) + \frac{(\alpha_0+i\alpha_3)(y_1-iy_2)}{y_0+1} \\ \hline (\alpha_2 - i\alpha_1)(1-\frac{y_3}{y_0+1}) + \frac{(\alpha_0-i\alpha_3)(y_1+iy_2)}{y_0+1} & (\alpha_0+i\alpha_3)(1-\frac{y_3}{y_0+1}) - \frac{(i\alpha_1+\alpha_2)(y_1+iy_2)}{y_0+1} \end{array}\right)$$

$$\mapsto (y|\alpha). \tag{4.13}$$

By construction, we have that $\det Z(y|\alpha)=1$ *for all* $y \in S_3(r_1)$ *and all* $\alpha \in S_4(r_2)$. *The property* $Z(y|-\alpha) = -Z(y|\alpha) \mapsto (y|-\alpha) = (y|\alpha)$ *is exhibited directly by the mapping (4.13).*

We now give explicitly the transfer of the action of the group H_4 on the parameters α to the action of the group H_3 on the parameters y,x,u,v,w in terms of the notation in Eq. (4.11) for the Lorentz matrix $(y|\alpha)$:

$$h^{(0)}_{\sigma_0}(\tau,\rho): \quad (y_1,y_2,y_3) \mapsto p(\tau,\rho)(y_1,y_2,y_3),$$

$$(x_1,x_2,x_3) \mapsto p(\tau,\rho)(x_1,x_2,x_3),$$

$$(u_1,u_2,u_3) \mapsto p(\tau,\rho)(u_1,u_2,u_3),$$

$$(v_1,v_2,v_3) \mapsto p(\tau,\rho)(v_1,v_2,v_3),$$

for parity of (τ,ρ) (even,even) or (odd,odd);

$$(y_1,y_2,y_3) \mapsto p(\tau,\rho)(x_1,x_2,x_3), \tag{4.14}$$

$$(x_1,x_2,x_3) \mapsto p(\tau,\rho)(y_1,y_2,y_3),$$

$$(u_1,u_2,u_3) \mapsto p(-\tau,\rho)(v_1,v_2,v_3),$$

$$(v_1,v_2,v_3) \mapsto p(-\tau,\rho)(u_1,u_2,u_3),$$

for parity of (τ,ρ) (even,odd) or (odd,even);

$$(w_1,w_2,w_3) \mapsto p((1,1,1),\rho)(w_1,w_2,w_3).$$

$$h^{(1)}_{\sigma_1}(\tau,\rho): \quad (y_1,y_2,y_3) \mapsto p((\tau_1,\tau_2,\tau_3),\rho)(y_1,y_2,y_3),$$

$$(x_1,x_2,x_3) \mapsto p((\tau_1,-\tau_2,-\tau_3),\rho)(x_1,x_2,x_3),$$

$$(u_1,u_2,u_3) \mapsto p((-\tau_1,\tau_2,-\tau_3),\rho)(u_1,u_2,u_3),$$

$$(v_1,v_2,v_3) \mapsto p((-\tau_1,-\tau_2,\tau_3),\rho)(v_1,v_2,v_3),$$

for parity of (τ,ρ) (even,even) or (odd,odd);

$$(y_1,y_2,y_3)\mapsto p((\tau_1,\tau_2,\tau_3),\rho)(x_1,x_2,x_3), \tag{4.15}$$

$$(x_1,x_2,x_3)\mapsto p((\tau_1,-\tau_2,-\tau_3),\rho)(y_1,y_2,y_3),$$

$$(u_1,u_2,u_3)\mapsto p((\tau_1,-\tau_2,\tau_3),\rho)(v_1,v_2,v_3),$$

$$(v_1,v_2,v_3)\mapsto p((\tau_1,\tau_2,-\tau_3)\rho)(u_1,u_2,u_3),$$

for parity of (τ,ρ) (even,odd) or (odd,even);

$$(w_1,w_2,w_3)\mapsto p((1,-1,-1),\rho)(w_1,w_2,w_3).$$

$h^{(2)}_{\sigma_2}(\tau,\rho)$: $(y_1,y_2,y_3)\mapsto p((\tau_1,\tau_2,\tau_3),\rho)(y_1,y_2,y_3)$,

$$(x_1,x_2,x_3)\mapsto p((-\tau_1,\tau_2,-\tau_3),\rho)(x_1,x_2,x_3),$$

$$(u_1,u_2,u_3)\mapsto p((-\tau_1,-\tau_2,\tau_3),\rho)(u_1,u_2,u_3),$$

$$(v_1,v_2,v_3)\mapsto p((\tau_1,-\tau_2,-\tau_3),\rho)(v_1,v_2,v_3),$$

for parity of (τ,ρ) (even,even) or (odd,odd);

$$(y_1,y_2,y_3)\mapsto p((\tau_1,\tau_2,\tau_3),\rho)(x_1,x_2,x_3), \tag{4.16}$$

$$(x_1,x_2,x_3)\mapsto p((-\tau_1,\tau_2,-\tau_3),\rho)(y_1,y_2,y_3),$$

$$(u_1,u_2,u_3)\mapsto p((\tau_1,\tau_2,-\tau_3),\rho)(v_1,v_2,v_3),$$

$$(v_1,v_2,v_3)\mapsto p((-\tau_1,\tau_2,\tau_3)\rho)(u_1,u_2,u_3),$$

for parity of (τ,ρ) (even,odd) or (odd,even);

$$(w_1,w_2,w_3)\mapsto p(-1,1,-1),\rho)(w_1,w_2,w_3).$$

$h^{(3)}_{\sigma_3}(\tau,\rho)$: $(y_1,y_2,y_3)\mapsto p((\tau_1,\tau_2,\tau_3),\rho)(y_1,y_2,y_3)$,

$$(x_1,x_2,x_3)\mapsto p((-\tau_1,-\tau_2,\tau_3),\rho)(x_1,x_2,x_3),$$

$$(u_1,u_2,u_3)\mapsto p((\tau_1,-\tau_2,-\tau_3),\rho)(u_1,u_2,u_3),$$

$$(v_1,v_2,v_3)\mapsto p((-\tau_1,\tau_2,-\tau_3),\rho)(v_1,v_2,v_3),$$

for parity of (τ,ρ) (even,even) or (odd,odd);

$$(y_1,y_2,y_3)\mapsto p((\tau_1,\tau_2,\tau_3),\rho)(x_1,x_2,x_3), \tag{4.17}$$

$$(x_1,x_2,x_3)\mapsto p((-\tau_1,-\tau_2,\tau_3),\rho)(y_1,y_2,y_3),$$

$$(u_1,u_2,u_3)\mapsto p((-\tau_1,\tau_2,\tau_3),\rho)(v_1,v_2,v_3),$$

$$(v_1,v_2,v_3)\mapsto p((\tau_1,-\tau_2,\tau_3)\rho)(u_1,u_2,u_3),$$

for parity of (τ,ρ) (even,odd) or (odd,even);

$$(w_1,w_2,w_3)\mapsto p(-1,-1,1),\rho)(w_1,w_2,w_3).$$

For the application of the above results to integral realizations in Sec. VI, it is useful to formulate them in a coset presentation. Thus, we first write out the special case of the above transformations for the eight group elements in the normal subgroup S, and then replace α by $h(\alpha), h\in H_4$ to obtain the following relations:

$$Z(y|(S^{(0)}_{\sigma_0}h)(\alpha))\mapsto\begin{pmatrix} y_0 & x_1(y,h(\alpha)) & x_2(y,h(\alpha)) & x_3(y,h(\alpha)) \\ y_1 & w_1(y,h(\alpha)) & u_3(y,h(\alpha)) & v_2(y,h(\alpha)) \\ y_2 & v_3(y,h(\alpha)) & w_2(y,h(\alpha)) & u_1(y,h(\alpha)) \\ y_3 & u_2(y,h(\alpha)) & v_1(y,h(\alpha)) & w_3(y,h(\alpha)) \end{pmatrix},$$

$$Z(y|(S^{(1)}_{\sigma_1}h)(\alpha))\mapsto\begin{pmatrix} y_0 & x_1(y,h(\alpha)) & -x_2(y,h(\alpha)) & -x_3(y,h(\alpha)) \\ y_1 & w_1(y,h(\alpha)) & -u_3(y,h(\alpha)) & -v_2(y,h(\alpha)) \\ y_2 & v_3(y,h(\alpha)) & -w_2(y,h(\alpha)) & -u_1(y,h(\alpha)) \\ y_3 & u_2(y,h(\alpha)) & -v_1(y,h(\alpha)) & -w_3(y,h(\alpha)) \end{pmatrix},$$

$$Z(y|(S^{(2)}_{\sigma_2}h)(\alpha))\mapsto\begin{pmatrix} y_0 & -x_1(y,h(\alpha)) & x_2(y,h(\alpha)) & -x_3(y,h(\alpha)) \\ y_1 & -w_1(y,h(\alpha)) & u_3(y,h(\alpha)) & -v_2(y,h(\alpha)) \\ y_2 & -v_3(y,h(\alpha)) & w_2(y,h(\alpha)) & -u_1(y,h(\alpha)) \\ y_3 & -u_2(y,h(\alpha)) & v_1(y,h(\alpha)) & -w_3(y,h(\alpha)) \end{pmatrix}, \tag{4.18}$$

$$Z(y|(S^{(3)}_{\sigma_3}h)(\alpha))\mapsto\begin{pmatrix} y_0 & -x_1(y,h(\alpha)) & -x_2(y,h(\alpha)) & x_3(y,h(\alpha)) \\ y_1 & -w_1(y,h(\alpha)) & -u_3(y,h(\alpha)) & v_2(y,h(\alpha)) \\ y_2 & -v_3(y,h(\alpha)) & -w_2(y,h(\alpha)) & u_1(y,h(\alpha)) \\ y_3 & -u_2(y,h(\alpha)) & -v_1(y,h(\alpha)) & w_3(y,h(\alpha)) \end{pmatrix}.$$

The cosets of H_4 are enumerated by taking

$$h\in\{Sf_m(\sigma_1,\sigma_2,\sigma_3)|m=1,2,\ldots,6;\ \text{each}\ \ \sigma_i=\pm 1\},$$

where the set of factor group representatives is defined by Eq. (3.6). The elements

$$x(y,h(\alpha)),u(y,h(\alpha)),v(y,h(\alpha)),w(y,h(\alpha)) \tag{4.19}$$

of the Lorentz matrices in Eq. (4.18) are, of course, signed permutations of $x(y,\alpha)$, $u(y,\alpha)$, $v(y,\alpha)$, $w(y,\alpha)$, which may be obtained explicitly from Eqs. (4.14)–(4.17). The forms given by Eqs. (4.18) are needed in Sec. VI. The cosets of S in H_4 partition the set of signed permutations of the parameters α into *orbits* under the action of the normal subgroup S, as given by

$$[h(\alpha)]=\{(sh)(\alpha)|s\in S,h=\text{any coset representative of } H_4/S\}. \tag{4.20}$$

For general sequences α having distinct, nonzero components, the 384 signed permutations of α are partitioned into 48 distinct orbits with eight sequences in each orbit. If, however, one chooses sequences such as $(\alpha_1,\alpha_2,0,0),\alpha_1\neq\alpha_2$, there are only six distinct orbits. In the extreme case of a sequence $(\alpha_1,0,0,0)$, all orbits coincide with $[(\alpha_1,0,0,)]$. One can, of course, enumerate all such degenerate cases.

The results given in this section for the restricted Lorentz group extend to the full Lorentz group (see Ref. 13) by adjoining the operations of space inversion $\Sigma=G$, time inversion $\Theta=-G$, and their product, thus obtaining the full Lorentz group $\{\mathcal{L}I_4,\mathcal{L}\Sigma,\mathcal{L}\Theta,\mathcal{L}\Sigma\Theta\}$ of which $\mathcal{L}$ is a normal subgroup, and $\{I_4,\Sigma,\Theta,\Sigma\Theta\}$ are the elements of the factor group. Thus, writing the

matrix $L=(y|\alpha)\in\mathcal{L}$ given by Eq. (4.11) in terms of its columns, $(y|\alpha)=(L_0(y),L_1(y,\alpha),L_2(y,\alpha),L_3(y,\alpha))$, we obtain the full Lorentz group by adjoining the elements of the cosets, which are, respectively,

$$\begin{aligned} L\Sigma&=(-L_0(y),L_1(y,\alpha),L_2(y,\alpha),L_3(y,\alpha)),\\ L\Theta&=(L_0(y),-L_1(y,\alpha),-L_2(y,\alpha),-L_3(y,\alpha)),\\ L\Sigma\Theta&=(-L_0(y),-L_1(y,\alpha),-L_2(y,\alpha),-L_3(y,\alpha)). \end{aligned} \tag{4.21}$$

V. PRINCIPAL SUBGROUPS

In this section, we given the two-to-one homomorphisms between several subgroups of SL(2, **C**) to subgroups of the restricted Lorentz group in the $(y|\alpha)$ parametrization. The development of the integral realizations of $(y|\alpha)$ given in the next section then applies, as well, to the results given below. In order to give a uniform presentation of the SL(2,**R**), SU(1,1), and K subgroup cases below, it is convenient to introduce the indicated notational changes.

(1) Subgroup $\mathrm{SU}(2)\subset\mathrm{SL}(2,\mathbf{C})$. This is the case $y_0=1$, $y=(0,0,0)$, where the point α belongs to the unit sphere in $\mathbf{R}^4$: $\alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2=1$. The two-to-one correspondence of the group SU(2) onto the special Lorentz matrices $((0,0,0)|\alpha)$ is given by

$$Z((0,0,0)|\alpha)=\begin{pmatrix} \alpha_0-i\alpha_3 & -i\alpha_1-\alpha_2\\ -i\alpha_1+\alpha_2 & \alpha_0+i\alpha_3\end{pmatrix}\mapsto((0,0,0)|\alpha)=\begin{pmatrix} 1&0&0&0\\ 0& & & \\ 0& & R(\alpha)& \\ 0& & & \end{pmatrix}, \tag{5.1}$$

where $R(\alpha)\in\mathrm{SO}(3,\mathbf{R})$ is the proper orthogonal matrix given by

$$R=\begin{pmatrix} 2(\alpha_0^2+\alpha_1^2)-1 & 2(\alpha_1\alpha_2-\alpha_0\alpha_3) & 2(\alpha_1\alpha_3+\alpha_0\alpha_2)\\ 2(\alpha_2\alpha_1+\alpha_0\alpha_3) & 2(\alpha_0^2+\alpha_2^2)-1 & 2(\alpha_2\alpha_3-\alpha_0\alpha_1)\\ 2(\alpha_3\alpha_1-\alpha_0\alpha_2) & 2(\alpha_3\alpha_2+\alpha_0\alpha_1) & 2(\alpha_0^2+\alpha_3^2)-1\end{pmatrix}. \tag{5.2}$$

The β parameters are

$$\beta_0=0,\quad \beta_1=0,\quad \beta_2=0,\quad \beta_3=0. \tag{5.3}$$

(2) Subgroup $\mathrm{SL}(2,\mathbf{R})\subset\mathrm{SL}(2,\mathbf{C})$. Notation: $y_0=\lambda$, $(y_1,y_2,y_3)=(x,0,y)$, $\alpha=(v,0,u,0)$. These parameters then satisfy

$$x^2+y^2=\lambda^2-1,\quad u^2+v^2=\frac{1+\lambda}{2}. \tag{5.4}$$

The two-to-one correspondence of SL(2, **R**) onto the special Lorentz matrices $((x,0,y)|(v,0,u,0))$ is given by

$$\begin{pmatrix} v+\dfrac{ux+vy}{1+\lambda} & -u+\dfrac{vx-uy}{1+\lambda}\\ u+\dfrac{vx-uy}{1+\lambda} & v-\dfrac{ux+vy}{1+\lambda}\end{pmatrix}\mapsto\begin{pmatrix} \lambda & x_1 & 0 & x_3\\ x & w_1 & 0 & v_2\\ 0 & 0 & 1 & 0\\ y & u_2 & 0 & w_3\end{pmatrix}, \tag{5.5}$$

where

$$x_1=x-\frac{4u(ux+vy)}{1+\lambda},\quad x_3=y+\frac{4u(vx-uy)}{1+\lambda},$$

$$w_1=2v^2-1-2\left(\frac{ux+vy}{1+\lambda}\right)^2,\quad v_2=2uv+\frac{2(ux+vy)(vx-uy)}{(1+\lambda)^2},\tag{5.6}$$

$$u_2=-2uv+\frac{2(ux+vy)(vx-uy)}{(1+\lambda)^2},\quad w_3=2v^2-1-2\left(\frac{vx-uy}{1+\lambda}\right)^2.$$

(3) Subgroup SU(1,1)$\subset$SL(2,**C**). Notation: $y_0=\lambda$, $(y_1,y_2,y_3)=(x,y,0))$, $\alpha=(u,0,0,v)$. These parameters then satisfy

$$x^2+y^2=\lambda^2-1,\ u^2+v^2=\frac{1+\lambda}{2}.\tag{5.7}$$

The two-to-one correspondence of SU(1,1) onto the special Lorentz matrices $((x,y,0)|(u,0,0,v))$ is given by

$$\begin{pmatrix} u-iv & \dfrac{(u+iv)(x-iy)}{1+\lambda} \\ \dfrac{(u-iv)(x+iy)}{1+\lambda} & u+iv \end{pmatrix}\mapsto\begin{pmatrix} \lambda & x_1 & x_2 & 0 \\ x & w_1 & u_3 & 0 \\ y & v_3 & w_2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},\tag{5.8}$$

where

$$x_1=-x+\frac{4u(ux+vy)}{1+\lambda},\quad x_2=-y-\frac{4u(vx-uy)}{1+\lambda},$$

$$w_1=2u^2-1-2\left(\frac{vx-uy}{1+\lambda}\right)^2,\quad u_3=-2uv-\frac{2(ux+vy)(vx-uy)}{(1+\lambda)^2},\tag{5.9}$$

$$v_3=2uv-\frac{2(ux+vy)(vx-uy)}{(1+\lambda)^2},\quad w_2=2u^2-1-2\left(\frac{ux+vy}{1+\lambda}\right)^2.$$

(4) Subgroup $K\subset$SL(2,**C**). Notation: $y_0=\lambda$, $(y_1,y_2,y_3)=(0,x,y)$, $\alpha=(u,v,0,0)$. These parameters then satisfy

$$x^2+y^2=\lambda^2-1,\ u^2+v^2=\frac{1+\lambda}{2}.\tag{5.10}$$

The two-to-one correspondence of K onto the special Lorentz matrices $((0,x,y)|(u,v,0,0))$ is given by

$$\begin{pmatrix} u-\dfrac{vx-uy}{1+\lambda} & -i\left(v+\dfrac{ux+vy}{1+\lambda}\right) \\ -i\left(v-\dfrac{ux+vy}{1+\lambda}\right) & u+\dfrac{vx-uy}{1+\lambda} \end{pmatrix}\mapsto\begin{pmatrix} \lambda & 0 & x_2 & x_3 \\ 0 & 1 & 0 & 0 \\ x & 0 & w_2 & u_1 \\ y & 0 & v_1 & w_3 \end{pmatrix},\tag{5.11}$$

where

$$x_2=-x+\frac{4u(ux+vy)}{1+\lambda},\quad x_3=-y-\frac{4u(vx-uy)}{1+\lambda},$$

$$w_2=2u^2-1-2\left(\frac{vx-uy}{1+\lambda}\right)^2, \quad u_1=-2uv-\frac{2(ux+vy)(vx-uy)}{(1+\lambda)^2}, \tag{5.12}$$

$$v_1=2uv-\frac{2(ux+vy)(vx-uy)}{(1+\lambda)^2}, \quad w_3=2u^2-1-2\left(\frac{ux+vy}{1+\lambda}\right)^2.$$

While the subgroups SL(2,**R**), SU(1,1), and K have distinct structures, they are parameterized in a uniform way in that the parameters satisfy the same relations (5.4), (5.7), and (5.10), and the elements of the matrix have the same factors $ux+vy$ and $vx-uy$. This is important in Sec. VII for integral realizations.

VI. ALGORITHMS FOR THE CONSTRUCTION OF ALL INTEGRAL LORENTZ MATRICES

We have given in Sec. IV a parametrization that is not only suitable for obtaining all the integral realizations of the Lorentz group, but which also casts the problem in a form that brings it within the purview of classical number theory, known since the time of Euclid, Fermat, and Gauss. In this section, we apply these results to the determination of all integral realizations of the restricted Lorentz group, which we denote by $I(\mathcal{L})$ with elements $I(y|\alpha)$.

Necessary and sufficient conditions that a matrix $(y|\alpha)\in I(\mathcal{L})$ are that the following set of conditions be true:

Condition I: For $y_0=m\in\{1,2,\ldots\}$, the first column solves, in integers,

$$y_1^2+y_2^2+y_3^2=m^2-1, \tag{6.1}$$

Condition II: The integer $m+1$ divides each of the quantities

$$\begin{aligned}&\gamma_0(y,\alpha)=-\alpha_1y_1-\alpha_2y_2-\alpha_3y_3, \quad \gamma_1(y,\alpha)=\alpha_0y_1+\alpha_3y_2-\alpha_2y_3,\\ &\gamma_2(y,\alpha)=-\alpha_3y_1+\alpha_0y_2+\alpha_1y_3, \quad \gamma_3(y,\alpha)=\alpha_2y_1-\alpha_1y_2+\alpha_0y_3.\end{aligned} \tag{6.2}$$

Condition III: The parameters $\alpha=(\alpha_0,\alpha_1,\alpha_2,\alpha_3)$ satisfy

$$\alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2=\frac{m+1}{2},$$

$$2(\alpha_0^2+\alpha_i^2)=n_i\in\{0,1,\ldots\}, \quad -2\alpha_0\alpha_i+2\alpha_j\alpha_k=\text{ integer}, \tag{6.3}$$

$$2\alpha_0\alpha_i+2\alpha_j\alpha_k=\text{ integer}, \quad (i,j,k)\text{ cyclic in }(1,2,3).$$

It follows from $2(\alpha_0^2+\alpha_i^2)=n_i=$ non-negative integer and $\alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2=(m+1)/2$ that $4\alpha_0^2+m+1=n_1+n_2+n_3$, hence, $4\alpha_0^2=$ non-negative integer. There are three distinct possibilities: $\alpha_0=$integer, $\alpha_0=$(integer)/$\sqrt{2}$, $\alpha_0=$(odd integer)/2. It then follows from $2\alpha_i^2=n_i-2\alpha_0^2$ that the sequence $(\alpha_0,\alpha_1,\alpha_2,\alpha_3)$ is either all integral, all (integer)/$\sqrt{2}$, or all (odd integer)/2. All cases satisfy the criteria in Condition III that the entries in $(y|\alpha)$ be integral.

The three classes of integral matrices $I(y|\alpha)\in I(\mathcal{L})$ are given explicitly as follows:

Class I. $y_0=m=2k+1$, the α_μ are all integers, and $y=(y_1,y_2,y_3)$ and $\alpha=(\alpha_0,\alpha_1,\alpha_2,\alpha_3)$ satisfy

$$\begin{aligned}&y_1^2+y_2^2+y_3^2=4k(k+1),\\ &\alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2=k+1.\end{aligned} \tag{6.4}$$

Class II. $y_0=m=k$, $\alpha_\mu=a_\mu/\sqrt{2}$, where the a_μ are all integers, and $y=(y_1,y_2,y_3)$ and $a=(a_0,a_1,a_2,a_3)$ satisfy

$$\begin{aligned} y_1^2+y_2^2+y_3^2&=k^2-1,\\ a_0^2+a_1^2+a_2^2+a_3^2&=k+1. \end{aligned} \tag{6.5}$$

Class III. $y_0=m=k$, $\alpha_\mu=b_\mu/2$, where the b_μ are all odd integers, and $y=(y_1,y_2,y_3)$ and $b=(b_0,b_1,b_2,b_3)$ satisfy

$$\begin{aligned} y_1^2+y_2^2+y_3^2&=k^2-1,\\ b_0^2+b_1^2+b_2^2+b_3^2&=2k+2,\ \text{each}\ \ b_\mu\ \ \text{odd}. \end{aligned} \tag{6.6}$$

The problems posed in each of these three classes are all classical number theoretic problems, and were considered by Euclid, Euler, Fermat, and Gauss, and others (see Ref. 14). Two relevant results are the following:

(1) Each positive integer, except those of the form $4^s(8N+7), s,N\in\{0,1,2,\ldots\}$, can be expressed as the sum of at most three squares.
(2) Each positive integer can be expressed as the sum of at most four squares.

Note that the condition given in (1) excludes certain k in each of the three classes. For example, there are no integer solutions y of (6.4) for $k=12$, since $(4)(12)(13)=4(156)=(4^2)(39)=4[(8)(4)+7]$, and none for $k=4$ of (6.5) and (6.6), since $4^2-1=15=8(1)+7$.

We mention that methods for solving Diophantine equations of the type occurring in the three classes above are developed in Refs. 16 and 17. Also, Uspensky and Heaslet[14] is a very readable book on number theory that introduces basic concepts and proves statements (1) and (2). The general problem of solving, in non-negative integers, the pair of relations

$$n_1+n_2+\cdots n_k=n,\quad n_1^2+n_2^2+\cdots+n_k^2=m,\quad (n,m)\ \text{positive integers} \tag{6.7}$$

is considered in Refs. 16 and 17, where these relations are treated in the context of the number theoretic degeneracy of the energy levels of an n-dimensional perturbed isotropic quantum harmonic oscillator. The main idea is to transform these relations to ''center-of-mass'' coordinates. In particular for $n=3$, this leads to barycentric or Möbius coordinates familiar from the eightfold way in particle physics. One is then able to classify the solutions in terms of finite multiplets consisting of sets of lattice points lying on cirlces in the Möbius plane. For $n>3$, one loses the elegance of the Möbius plane construction, but nonetheless still has a classification in terms of finite multiplets.[17] There are, of course, no closed forms for the set of all solutions of such Diophantine equations. We refer to these references and Ref. 14 for these procedures, and consider the Diophantine problems for Eqs. (6.4)–(6.6) as solved for the purpose of the discussion that follows.

In each of the three classes, the main problem is to determine the first column sequence $y=(y_1,y_2,y_3)$ and integral parameters $(\alpha_0,\alpha_1,\alpha_2,\alpha_3),(a_0,a_1,a_2,a_3)$, and (b_0,b_1,b_2,b_3), respectively, such that the factor $m+1$ divides the sequence

$$\begin{aligned} \gamma(y,\delta)&=(\gamma_0(y,\delta),\gamma_1(y,\delta),\gamma_2(y,\delta),\gamma_3(y,\delta)),\\ \delta&=\alpha,\quad \delta=\alpha/\sqrt{2}=a,\quad \delta=\alpha/2=b, \end{aligned} \tag{6.8}$$

defined in relation (6.2), where to unify the discussion of the three classes we let the sequence δ run over the three sequences that occur in the three classes.

The determination of a common factor in a sequence of integers is a classic number theoretical problem solved, in principle, by Euclid's algorithm. One can see how the general result goes from

a single example (see Ref. 14 for a proof of the general method): Find the greatest common divisor (gcd) of the integers 19332 and 1368: We perform the successive divisions given by

$$19332=14\cdot 1368+180,\ \ 1368=7\cdot 180+108,\ \ 180=1\cdot 72+36,\ \ 72=2\cdot 36,$$

thus arriving at 36, which is the gcd of the pair (19332, 1368). *Then, every divisor of this pair is a divisor of* 36, *namely*, 1, 2, 3, 4, 6, 9, 12, 18, 36.

The determination of the gcd D of a finite sequence of $n+2,\ n\geqslant 1$, integers $(d_1,d_2,\ldots,d_{n+2})$ is as follows. One calculates successively

$$D_1=\gcd(d_1,d_2),\quad D_2=\gcd(D_1,d_3),\quad D_3=\gcd(D_2,d_4),\quad \ldots,\quad D_{n+1}=\gcd(D_n,d_{n+2}),$$

and finds that

$$D=\gcd(d_1,d_2,\ldots,d_{n+2})=D_{n+1}.$$

Finally, each divisor of the sequence $(d_1,d_2,\ldots,d_{n+2})$ is a divisor of D.

For our problem and the three classes introduced above, we have $n=2$, and $y_0+1=m+1$ must be a factor of $D=\gcd(\gamma(y,\delta))$.

We have found no way to implement Euclid's algorithm such that for each $(y,\delta),\delta=\alpha,a,b$ solving Eqs. (6.4)–(6.6), respectively, one obtains algebraic constraints on the sequence of integers δ such that the sequence $\gamma(y,\delta)$ has divisor $m+1$. There are, however, several properties of the sequence $\gamma(y,\delta)$ that reduce the labor involved in implementing Condition II. Three obvious properties are

$$\gamma(-y,\delta)=-\gamma(y,\delta),\ \ \gamma(y,-\delta)=-\gamma(y,\delta),\gamma(-y,-\delta)=\gamma(y,\delta),\tag{6.9}$$

which are also consequences of the factor group Σ_2 introduced in Eq. (2.8). There is also a simplification originating from the transfer of the action of the group H_4 on the parameters δ [see Eq. (6.8)] to the action of the group H_3 on the parameters y. To describe this, we introduce the little group $H_3(y)\subset H_3$ that leaves y fixed:

$$H_3(y)=\{p(\tau,\rho)|p(\tau,\rho)(y)=y,p(\tau,\rho)\in H_3\}.\tag{6.10}$$

This, in turn, leads us to introduce the *set* $H_4(y)\subset H_4$ defined by

$$H_4(y)=\{h^{(k)}_{\sigma_k}(\tau,\rho)|p(\tau,\rho)\in H_3(y),k\in\{0,1,2,3\},\sigma_k\in\{1,-1\}\}.\tag{6.11}$$

We then have the identity

$$\gamma(y,h_y(\delta))=\gamma(y,\delta),\ \ \text{each}\ \ h_y\in H_4(y).\tag{6.12}$$

We conclude from relations (6.9) and (6.12) that, *if the pair of sequences* (y,δ) *satisfies Condition II given by Eq. (6.2), then so do all the pairs of sequences given by*

$$(-y,\delta),(y,-\delta),(-y,-\delta),\{(y,h_y(\delta))|\ \ each\ \ h_y\in H_4(y)\}.\tag{6.13}$$

The normal subgroup S of H_4 satisfies $S\subset H_4(y)$. It follows then that every $h_y\in H_4(y)$ belongs to a coset of S, that is, $h_y(\delta)$ is in one of the coset orbits of the normal subgroup S. It now follows from Eq. (6.12) that for sequences in the same coset orbit of S, either all or none satisfy Condition II.

We now give the details of the algorithms for constructing all integral Lorentz matrices in $\mathcal{L}$ and the corresponding matrices SL(2, **C**) in three subsections. One easily extends these results to obtain all integral realizations of the full Lorentz group by adjoining the additional signed elements originating from relations (4.21).

A. Class I: Integral Gaussian matrices in SL(2, C) mapping to $I(\mathcal{L})$

It is evident from Eq. (6.4) that we must have

$$(y_1,y_2,y_2)=2(z_1,z_2,z_3). \tag{6.14}$$

The above results for Class I may be summarized in the following algorithm for calculating all integral realizations $I(2z|\alpha)$ of the restricted Lorentz group $\mathcal{L}$ together with the Gaussian integer matrices $\pm Z(2z|\alpha)$ of SL(2, **C**) corresponding to $I(2z|\alpha)$.

Algorithm I.

(1) Fix a solution z of

$$z_1^2+z_2^2+z_3^2=k(k+1). \tag{6.15}$$

(2) Classify all solutions of

$$\alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2=k+1 \tag{6.16}$$

into disjoint coset orbits with respect to the normal subgroup S, defining the orbit $[\alpha]$ *by*

$$\begin{aligned}[\alpha]=S(\alpha)=\{&\pm(\alpha_0,\alpha_1,\alpha_2,\alpha_3),\pm(\alpha_1,-\alpha_0,\alpha_3,-\alpha_2),\\ &\pm(-\alpha_2,-\alpha_3,\alpha_0,\alpha_1),\pm(-\alpha_3,\alpha_2,-\alpha_1,\alpha_0)\}.\end{aligned} \tag{6.17}$$

(3) Select an α-sequence in each of the orbits obtained in (2). If the selected sequence satisfies the conditions that the integer $k+1$ *divides each of the quantities*

$$\begin{aligned}&\gamma_0(z,\alpha)=-\alpha_1z_1-\alpha_2z_2-\alpha_3z_3,\ \gamma_1(z,\alpha)=\alpha_0z_1+\alpha_3z_2-\alpha_2z_3,\\ &\gamma_2(z,\alpha)=-\alpha_3z_1+\alpha_0z_2+\alpha_1z_3,\quad \gamma_3(z,\alpha)=\alpha_2z_1-\alpha_1z_2+\alpha_0z_3,\end{aligned} \tag{6.18}$$

retain all sequences in the orbit, but otherwise reject the orbit, denoting the retained orbits by $[\alpha^{(1)}],[\alpha^{(2)}],\ldots$. *Then, the integer Lorentz matrices with fixed column sequence* $(y_1,y_2,y_3)=(2z_1,2z_2,2z_3)$ *are those in the set*

$$\{I(2z|\alpha)|\alpha\in[\alpha^{(1)}],\ \alpha\in[\alpha^{(2)}],\ldots\}. \tag{6.19}$$

The two-to-one homomorphism from Gaussian integer matrices in SL(2, **C**) *to* $I(\mathcal{L})$ *is given by*

$$\pm Z(2z|\alpha)\mapsto I(2z|\alpha),\quad \alpha\in[\alpha^{(1)}],\ \alpha\in[\alpha^{(2)}],\ldots \tag{6.20}$$

In selecting a solution of Eq. (6.15), in consequence of Eq. (6.17), it is only necessary to consider those solutions y that have parity (even,even) and (even,odd) with respect to H_3. The Lorentz matrices $I(2z|\alpha)$ given by this algorithm are obtained from relations (4.11) and (4.12) or (4.18) for $y_0=2k+1$, $y=(2z_1,2z_2,2z_3)$, where the sequences $h(\alpha)\in[\alpha^{(1)}],h(\alpha)\in[\alpha^{(2)}],\ldots$, and $Z(2z|\alpha)$ is obtained from Eq. (4.13).

An example is useful for illustrating the algorithm. Choose $k=8$, so that we must find solutions, in integers, of the two equations

$$z_1^2+z_2^2+z_3^2=72, \tag{6.21}$$

$$\alpha_0^2+\alpha_1^2+\alpha_2^2+\alpha_3^2=9, \tag{6.22}$$

subject to the condition that the integer 9 must divide each of the four quantities given by Eq. (6.18).

We also fix $|z_1|+|z_2|+|z_3|=12$, and apply the methods of Refs. 14 and 16 for solving Eqs. (6.21) and (6.22) (or by inspection). The solutions of Eq. (6.21) are (6,6,0),(8,2,2), and all signed permutations of these sequences. The solutions of Eq. (6.22) are (3,0,0,0),(2,2,1,0), and all signed permutations of these sequences.

We consider two subcases:

(1) Fix $z=(6,6,0)$. There are eight signed permutations of (3,0,0,0) They must therefore all fall in the normal subgroup orbit $[(3,0,0,0)]$, and all other coset orbits are equal to this one. Conditions (6.18) are satisfied by (3,0,0,0), giving $\gamma=(0,18,18,0)$, hence, by all sequences in the orbit $[(3,0,0,0)]$. Thus, we have the following results from Eq. (4.18):

$$\pm\begin{pmatrix} 3 & 2(1+i) \\ 2(1-i) & 3 \end{pmatrix} \to \begin{pmatrix} 17 & 12 & 12 & 0 \\ 12 & 9 & 8 & 0 \\ 12 & 8 & 9 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\pm\begin{pmatrix} 2(1+i) & 3i \\ 3i & 2(-1+i) \end{pmatrix} \to \begin{pmatrix} 17 & 12 & -12 & 0 \\ 12 & 9 & -8 & 0 \\ 12 & 8 & -9 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\pm\begin{pmatrix} 2(1-i) & -3 \\ 3 & -2(1+i) \end{pmatrix} \to \begin{pmatrix} 17 & -12 & 12 & 0 \\ 12 & -9 & 8 & 0 \\ 12 & -8 & 9 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\pm\begin{pmatrix} -3i & 2(1+i) \\ 2(1-i) & 3i \end{pmatrix} \to \begin{pmatrix} 17 & -12 & -12 & 0 \\ 12 & -9 & -8 & 0 \\ 12 & -8 & -9 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

There are 96 signed permutations of (2,2,1,0). They must, therefore, be distributed into 12 disjoint coset orbits, which may be taken to be the orbit $[(2,2,1,0)]$ and all orbits obtained from the 12 permutations of the integers (2,2,1,0), that is, $[(2,2,0,1)]$,$[(2,1,2,0)]$, etc. From conditions (6.18), we have $\gamma_0=-6(\alpha_1+\alpha_2)$, $\gamma_1=6(\alpha_0+\alpha_3)$. Since $\alpha_0+\alpha_1+\alpha_2+\alpha_3=5$, the integers γ_0 and γ_1 are divisible by 9 if and only if both $\alpha_1+\alpha_2=3$ and $\alpha_0+\alpha_3=3$, which is impossible. We conclude there are no solutions of Eqs. (6.18), (6.21), and (6.22).

(2) Fix $z=(8,2,2)$. As in (1), all signed permutations of (3,0,0,0) fall in the normal subgroup orbit $[(3,0,0,0)]$. But now conditions (6.18) fail for (3,0,0,0), and we obtain no solutions of Eqs.

(6.18), (6.21), and (6.22). There are 96 signed permutations of (2,2,1,0). They must, therefore, be distributed into 12 disjoint coset orbits, just as in case 1. Conditions (6.18) now read:

$$\gamma_0=-8\alpha_1-2\alpha_2-2\alpha_3, \quad \gamma_1=8\alpha_0-2\alpha_2+2\alpha_3,$$

$$\gamma_2=2\alpha_0+2\alpha_1-8\alpha_3, \quad \gamma_3=2\alpha_0-2\alpha_1+8\alpha_2.$$

The form of γ_0 shows that no sequence with $\alpha_1=0$ can occur, and the form of γ_2 shows that no sequence with $\alpha_3=0$ can occur. Checking each of the remaining six candidates in which either $\alpha_0=0$ or $\alpha_2=0$, we find that only the sequence (2,2,0,1) gives a solution, hence, all eight sequences in the orbit

$$[(2,2,0,1)]=\{\pm(2,2,0,1),\pm(-2,2,1,0),\pm(0,-1,2,2),\pm(-1,0,-2,2)\}$$

give solutions of relations (6.18). We have the following results from Eq. (4.18):

$$\pm\begin{pmatrix} 2-3i & 2(1-i) \\ 2(1-i) & 2-i \end{pmatrix}\mapsto\begin{pmatrix} 17 & 16 & -4 & 4 \\ 16 & 15 & -4 & 4 \\ 4 & 4 & -1 & 0 \\ 4 & 4 & 0 & 1 \end{pmatrix},$$

$$\pm\begin{pmatrix} 2(1+i) & 3+2i \\ 1+2i & 2(1+i) \end{pmatrix}\mapsto\begin{pmatrix} 17 & 16 & 4 & -4 \\ 16 & 15 & 4 & -4 \\ 4 & 4 & 1 & 0 \\ 4 & 4 & 0 & -1 \end{pmatrix},$$

$$\pm\begin{pmatrix} 2(1-i) & -2+3i \\ 2-i & -2(1-i) \end{pmatrix}\mapsto\begin{pmatrix} 17 & -16 & -4 & -4 \\ 16 & -15 & -4 & -4 \\ 4 & -4 & -1 & 0 \\ 4 & -4 & 0 & -1 \end{pmatrix},$$

$$\pm\begin{pmatrix} -3-2i & 2(1+i) \\ -2(1+i) & 1+2i \end{pmatrix}\mapsto\begin{pmatrix} 17 & -16 & 4 & 4 \\ 16 & -15 & 4 & 4 \\ 4 & -4 & 1 & 0 \\ 4 & -4 & 0 & 1 \end{pmatrix}.$$

B. Class II: (Integral Gaussian/$\sqrt{2}$) matrices in SL(2, C) mapping to $I(\mathcal{L})$

We have the following results:

$$y_1^2+y_2^2+y_3^2=k^2-1,$$
$$a_0^2+a_1^2+a_2^2+a_3^2=k+1. \tag{6.23}$$

$$\frac{1}{\sqrt{2}}\left(\begin{array}{c|c} (a_0-ia_3)(1+\frac{y_3}{k+1})-\frac{(a_1+ia_2)(iy_1+y_2)}{k+1} & -(a_2+ia_1)(1+\frac{y_3}{k+1})+\frac{(a_0+ia_3)(y_1-iy_2)}{k+1} \\ \hline (a_2-ia_1)(1-\frac{y_3}{k+1})+\frac{(a_0-ia_3)(y_1+iy_2)}{k+1} & (a_0+ia_3)(1-\frac{y_3}{k+1})-\frac{(ia_1+a_2)(y_1+iy_2)}{k+1} \end{array}\right)$$

$$\mapsto (y|a)=\begin{pmatrix} k & x_1(y,a) & x_2(y,a) & x_3(y,a) \\ y_1 & w_1(y,a) & u_3(y,a) & v_2(y,a) \\ y_2 & v_3(y,a) & w_2(y,a) & u_1(y,a) \\ y_3 & u_2(y,a) & v_1(y,a) & w_3(y,a) \end{pmatrix}; \tag{6.24}$$

$$x_i(y,a)=(y|a)_{0,i}=\frac{1}{k+1}[a_0\gamma_i(y,a)-a_i\gamma_0(y,a)-a_j\gamma_k(y,a)+a_k\gamma_j(y,a)],$$

$$u_i(y,a)=(y|a)_{j,k}=-a_0a_i+a_ja_k+\frac{1}{(k+1)^2}[-\gamma_0(y,a)\gamma_i(y,a)+\gamma_j(y,a)\gamma_k(y,a)],$$

$$v_i(y,a)=(y|a)_{k,j}=a_0a_i+a_ja_k+\frac{1}{(k+1)^2}[\gamma_0(y,a)\gamma_i(y,a)+\gamma_j(y,a)\gamma_k(y,a)], \tag{6.25}$$

$$w_i(y,a)=(y|a)_{i,i}=a_0^2+a_i^2-1-\frac{1}{(k+1)^2}[\gamma_j^2(y,a)+\gamma_k^2(y,a)],$$

(i,j,k) is a cyclic permutation of (1,2,3);

$$\gamma_0(y,a)=-a_1y_1-a_2y_2-a_3y_3, \quad \gamma_1(y,a)=a_0y_1+a_3y_2-a_2y_3,$$
$$\gamma_2(y,a)=-a_3y_1+a_0y_2+a_1y_3, \quad \gamma_3(y,a)=a_2y_1-a_1y_2+a_0y_3. \tag{6.26}$$

It is important to note that for general Lorentz matrices, the scaling above gives no new results, since it just changes how one describes the parameter domain. However, for integral realizations, this scaling transformation introduces an entirely new class of integral Lorentz matrices, now corresponding to matrices in SL(2, **C**) that have Gaussian integers divided by $\sqrt{2}$ as elements.

The modification of Algorithm I for Class II solutions is the following.

Algorithm II. In Algorithm I, replace Eqs. (6.15) and (6.16) by Eqs. (6.23), the sequence $2z$ by the sequence y, and the sequence α by the sequence a, using now relations (6.24)–(6.26) to obtain the explicit results for the mapping of (Gaussian integers)/$\sqrt{2}$ in SL(2, **C**) to integral matrices in $I(\mathcal{L})$. [One can also use the obvious modification of Eq. (4.18).]

C. Class III: Gaussian half-odd integral matrices in SL(2, C) mapping to $I(\mathcal{L})$

We have the following results:

$$y_1^2+y_2^2+y_3^2=k^2-1,$$
$$b_0^2+b_1^2+b_2^2+b_3^2=2k+2, \text{ each } b_\mu \text{ odd.} \tag{6.27}$$

$$\frac{1}{2}\left(\begin{array}{c|c} (b_0-ib_3)(1+\frac{y_3}{k+1})-\frac{(b_1+ib_2)(iy_1+y_2)}{k+1} & -(b_2+ib_1)(1+\frac{y_3}{k+1})+\frac{(b_0+ib_3)(y_1-iy_2)}{k+1} \\ \hline (b_2-ib_1)(1-\frac{y_3}{k+1})+\frac{(b_0-ib_3)(y_1+iy_2)}{k+1} & (b_0+ib_3)(1-\frac{y_3}{k+1})-\frac{(ib_1+b_2)(y_1+iy_2)}{k+1} \end{array}\right)$$

$$\mapsto (y|b)=\left(\begin{array}{cccc} k & x_1(y,b) & x_2(y,b) & x_3(y,b) \\ y_1 & w_1(y,b) & u_3(y,b) & v_2(y,b) \\ y_2 & v_3(y,b) & w_2(y,b) & u_1(y,b) \\ y_3 & u_2(y,b) & v_1(y,b) & w_3(y,b) \end{array}\right); \tag{6.28}$$

$$x_i(y,b)=(y|b)_{0,i}=\frac{1}{2(k+1)}[b_0\gamma_i(y,b)-b_i\gamma_0(y,b)-b_j\gamma_k(y,b)+b_k\gamma_j(y,b)],$$

$$u_i(y,b)=(y|b)_{j,k}=\frac{-b_0b_i+b_jb_k}{2}+\frac{1}{2(k+1)^2}[-\gamma_0(y,b)\gamma_i(y,b)+\gamma_j(y,b)\gamma_k(y,b)],$$

$$v_i(y,b)=(y|b)_{k,j}=\frac{b_0b_i+b_jb_k}{2}+\frac{1}{2(k+1)^2}[\gamma_0(y,b)\gamma_i(y,b)+\gamma_j(y,b)\gamma_k(y,b)], \tag{6.29}$$

$$w_i(y,b)=(y|b)_{i,i}=\frac{b_0^2+b_i^2}{2}-1-\frac{1}{2(k+1)^2}[\gamma_j^2(y,b)+\gamma_k^2(y,b)],$$

$$(i,j,k) \text{ is a cyclic permutation of } (1,2,3);$$

$$\gamma_0(y,b)=-b_1y_1-b_2y_2-b_3y_3, \quad \gamma_1(y,b)=b_0y_1+b_3y_2-b_2y_3,$$
$$\gamma_2(y,b)=-b_3y_1+b_0y_2+b_1y_3, \quad \gamma_3(y,b)=b_2y_1-b_1y_2+b_0y_3. \tag{6.30}$$

The modification of Algorithm I for Class III solutions is as follows.

Algorithm III. In Algorithm I, replace Eqs. (6.15) and (6.16) by Eqs. (6.27), the sequence $2z$ by the sequence y, and the sequence α by the sequence b, using now relations (6.28)–(6.30) to obtain the explicit results for the mapping of (Gaussian integers)/2 in SL(2, **C**) to integral matrices in $I(\mathcal{L})$. [One can also use the obvious modification of Eq. (4.18).]

We note that the denominator factor $k+1$ in relations (6.29) is removed because, by construction, $k+1$ divides the factors $\gamma_\mu(y,b)$; the denominator factor 2 is removed by the property that the b_μ are odd integers, which results in only integers appearing in $(y|b)$.

VII. INTEGRAL REALIZATIONS OF THE PRINCIPAL SUBGROUPS

As a by-product of the above construction of the integral realizations of the restricted Lorentz group, we also obtain all the integral realizations of the principal subgroups given in Sec. V.

A. Integral realizations of the orthogonal group SO(3, R)

In this case, we turn the situation around and identify first the integral representations of SO(3, **R**), and then the matrices in SL(2, **C**) corresponding to them. The integral realizations of the proper orthogonal group can only be permutations of the columns of the matrix $(\pm e_1, \pm e_2, \pm e_3)$, where e_i is a unit column vector. Since we must have $\det R=1$, we can have zero or two minus signs and all even column permutations, or one or three minus signs and all odd column permutations, thus obtaining a group of 24 discrete orthogonal matrices with unit determinant. This is the group of rotations that carries the cube with vertices at $(1,1,1)$, $(-1,1,1)$, $(-1,-1,1)$, $(1,-1,1)$, $(1,1,-1)$, $(-1,1,-1)$, $(-1,-1,-1)$, $(1,-1,-1)$ into itself, or, equivalently, the octahedron with vertices at $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(-1,0,0)$, $(0,-1,0)$, $(0,0,-1)$. The corresponding subgroup of SU(2) is the so-called double covering group with 48 elements. An interesting point is that the elements of SU(2) that are Gaussian integers divided by $\sqrt{2}$ already make their appearance. For example, we have

$$\pm\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}\mapsto\begin{pmatrix}0 & 0 & -1\\ 0 & 1 & 0\\ 1 & 0 & 0\end{pmatrix},\quad \pm\frac{i}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\mapsto\begin{pmatrix}0 & 0 & 1\\ 0 & -1 & 0\\ 1 & 0 & 0\end{pmatrix},$$

$$\pm i\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\mapsto\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix},\quad \pm\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\mapsto\begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix},$$

$$\pm i\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\mapsto\begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{pmatrix},\quad \text{etc.}$$

It is interesting to note that the half-odd integral realizations of SL(2, **C**), which are allowed in the general theory, are excluded here because there is no solution, by four odd integers, of the relation $b_0^2+b_1^2+b_2^2+b_3^2=2$.

B. Gaussian integer realizations of SL(2,R), SU(1,1), and K

We have already noted at the end of Sec. V that these subgroups can be parametrized in a uniform manner. For integral realizations this transcribes to the following special cases, respectively, of Algorithms I, II, and III:

Algorithm I′:

(1) Set $x=2s$, $y=2t$. *Select and fix a solution* (s,t) *of*

$$s^2+t^2=k(k+1). \tag{7.1}$$

(2) Select any solution (u,v) *with non-negative components of*

$$u^2+v^2=k+1. \tag{7.2}$$

(3) The mappings given by Eqs. (5.5), (5.8), and (5.11) for the integer pair (u,v), *and by each of the substitutions* $(u,v)\to(-u,-v)$, $(u,v)\to(-v,u)$, $(u,v)\to(v,-u)$, *all give mappings of Gaussian integer realizations of the respective subgroups to the corresponding integral realization of the Lorentz group if and only if* $k+1$ *is a divisor of* $\gcd(us+vt, vs-ut)$. *The mappings given by Eqs. (5.5), (5.8), and (5.11) for the integer pair* (v,u), *and by each of the substitutions*

$(v,u)\to(-v,-u),(v,u)\to(-u,v),(v,u)\to(u,-v)$, *all give mappings of Gaussian integer realizations of the respective subgroups to the corresponding integral realization of the Lorentz group if and only if* $k+1$ *is a divisor of* $\gcd(vs+ut,us-vt)$.

Algorithm II′:

(1) Select and fix a solution (x,y) *of*

$$x^2+y^2=k^2-1. \tag{7.3}$$

(2) Select a non-negative solution (u,v)

$$u^2+v^2=k+1. \tag{7.4}$$

(3) The mappings given by Eqs. (5.5), (5.8), and (5.11) for the integer pair (u,v), *and by each of the substitutions* $(u,v)\to(-u,-v),(u,v)\to(-v,u),(u,v)\to(v,-u)$, *all give mappings of* (Gaussian integer)/$\sqrt{2}$ *realizations of the respective subgroups to the corresponding integral realization of the Lorentz group if and only if* $k+1$ *is a divisor of* $\gcd(ux+vy,vx-uy)$. *The mappings given by Eqs. (5.5), (5.8), and (5.11) for the integer pair* (v,u), *and by each of the substitutions* $(v,u)\to(-v,-u),(v,u)\to(-u,v),(v,u)\to(u,-v)$, *all give mappings of* (Gaussian integer)/$\sqrt{2}$ *realizations of the respective subgroups to the corresponding integral realization of the Lorentz group if and only if* $k+1$ *is a divisor of* $\gcd(vx+uy,ux-vy)$.

Algorithm III′:

(1) Select and fix a solution (x,y) *of*

$$x^2+y^2=k^2-1. \tag{7.5}$$

(2) Select a non-negative solution $(u,v)=(odd,odd)$

$$u^2+v^2=2(k+1). \tag{7.6}$$

(3) The mappings given by Eqs. (5.5), (5.8), and (5.11) for the integer pair (u,v), *and by each of the substitutions* $(u,v)\to(-u,-v),(u,v)\to(-v,u),(u,v)\to(v,-u)$, *all give mappings of* (Gaussian integer)/$\sqrt{2}$ *realizations of the respective subgroups to the corresponding integral realization of the Lorentz group if and only if* $k+1$ *is a divisor of* $\gcd(ux+vy,vx-uy)$. *The mappings given by Eqs. (5.5), (5.8), and (5.11) for the integer pair* (v,u), *and by each of the substitutions* $(v,u)\to(-v,-u),(v,u)\to(-u,v),(v,u)\to(u,-v)$, *all give mappings of (Gaussian odd integer)/2 realizations of the respective subgroups to the corresponding integral realization of the Lorentz group if and only if* $k+1$ *is a divisor of* $\gcd(vx+uy,ux-vy)$.

A comprehensive theory, using Algorithms I′–III′, can now be used to construct all Gaussian integer, (Gaussian integer)/$\sqrt{2}$, and (Gaussian odd integer)/2 realizations of the subgroups SL(2, **R**), SU(1,1), and K from classical results of number theory (see Ref. 14). We close our discussion by noting examples showing interesting aspects of such solutions:

$$\text{Algorithm I}'\text{: Choose } (x,y)=(2au,2av), \text{ where } u^2+v^2=a^2+1.$$

$$\text{Algorithm II}'\text{: Choose } (x,y)=(bu,bv), \text{ where } u^2+v^2=b^2+2.$$

In particular, if $a^2+1=$prime number is of form $4r+1$, or if b^2+2 is of this same form, then the solution (u,v) is unique, up to signed permutations, for each such r, and the integers u and v are relatively prime. On the other hand, if $u=v$, we obtain, respectively, Pell equations, $a^2-2u^2=-1$ and $b^2-2u^2=-2$, which have infinitely many solutions given by

$$\begin{pmatrix} a \\ u \end{pmatrix} = \begin{pmatrix} 3 & 4 \\ 2 & 3 \end{pmatrix}^m \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad m = 0,1,2,\ldots,$$

$$\begin{pmatrix} b \\ u \end{pmatrix} = \begin{pmatrix} 3 & 4 \\ 2 & 3 \end{pmatrix}^m \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad m = 0,1,2,\ldots .$$

Pell's equation has fascinating applications to the determination of zeros of $3j$ and $6j$ coefficients that arise in the theory of angular momentum [the group SU(2)]. An elementary example is given in Ref. 18, and a brief summary of papers on such zeros is given in Ref. 19.

VIII. CONCLUDING REMARKS

(1) Using the biquaternionic parameters (α, β) introduced by Dirac (equivalent to the Cayley parameters) to parametrize the group SL(2, **C**), we have obtained a corresponding parametrization of the restricted Lorentz group $\mathcal{L}$ in terms of the first column of an element of $\mathcal{L}$ and the quaternionic parameters α. It is this parametrization that is used to address the problem of determining all integral realizations of the restricted Lorentz group. This leads to the problem of solving simultaneously three classical Diophantine problems, as follows: One is given a pair (n_1, n_2) of positive integers, the first expressed as a quadractic function of a positive integer k and the second linear in k. One must then express n_1 as a sum of three squares; n_2 as a sum of four squares, and then select from the set of solutions of the three-squares problem and the set of solutions of the four-squares problem those particular pairs of solutions such that four new integers, each linear in the three-squares solution and in the four-squares solution, possess a common factor. It is the interrelations between the solutions of these three classical Diophantine problems that makes the general determination of the integer representations of the restricted Lorentz group difficult. The algorithmic character of the procedure may, however, make computer calculations quite tractable. In any case, the recognition of the underlying classical Diophantine structure of the problem is intriguing and interesting. That there are three classes of SL(2, **C**) matrices, Gaussian integral, half-odd Gaussian integral, and Gaussian integral/$\sqrt{2}$, each class giving integral restricted Lorentz matrices, is a bonus of addressing the problem through the homomorphism between the groups, from which one also obtains corresponding results for the principal subgroups of $\mathcal{L}$.

(2) The method presented here, as summarized in (1), is to be contrasted with the generator method described by Lorente and Kramer,[6,7] and attributed to Coxeter and Kac,[10] which asserts the following. All integral Lorentz transformations L of the point (x_0, x_1, x_2, x_3) that leave the upper half of the light cone invariant are generated by the four transformations

$$S_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad S_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$S_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad S_4 = \begin{pmatrix} 2 & 1 & 1 & 1 \\ -1 & 0 & -1 & -1 \\ -1 & -1 & 0 & -1 \\ -1 & -1 & -1 & 0 \end{pmatrix}.$$

Based on this result, Lorente and Kramer[6,7] give a polynomial form in these four generators for the general integral transformation L. It is a rather unwieldy appearing expression, but the authors use it effectively to present various classes of special matrices. Moreover, in Ref. 7, they also relate their results to matrices in SL(2, **C**).

(3) In consequence of the observations made in (1) and (2), it must be the case that one can transform the results obtained in this article into generator expressions. This poses the interesting question as to how the generator method solves the three interrelated classical Diophantine problems presented here.

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Integration over matrix spaces with unique invariant measures

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We present a method to calculate integrals over monomials of matrix elements with invariant measures in terms of Wick contractions. The method gives exact results for monomials of low order. For higher-order monomials, it leads to an error of order $1/N^{\alpha}$, where N is the dimension of the matrix and where α is independent of the degree of the monomial. We give a lower bound on the integer α and show how α can be increased systematically. The method is particularly suited for symbolic computer calculation. Explicit results are given for O(N), U(N), and for the circular orthogonal ensemble. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The calculation of group integrals of monomials of matrix elements for compact Lie groups has a long tradition going back to Ullah and Porter.[1] Their results were later extended[2] to the space of symmetric unitary matrices endowed with Dyson's invariant measure.[3] The problem was nearly dormant for some years but was recently solved completely for the orthogonal group by recursion.[4] Unfortunately, it seems that there is no easy generalization of this method to other groups. The method proposed in Ref. 2, on the other hand, is quite general but soon becomes rather cumbersome. Moreover, that method is not suited for computer-supported analytical work.

Aside from their immanent group-theoretical significance, group integrals over monomials of matrix elements for compact Lie groups are important in many applications. This is true not only of random-matrix theory which has seen an explosive growth over the last decade and has become an important tool in a great variety of fields in physics, chemistry, and related areas.[5] The statement applies likewise to a number of mathematical fields where integrals of the Itzykson–Zuber-type appear. Such integrals typically extend over the Haar measure of some group. As examples, we mention the Itzykson–Zuber model itself,[6] the Bessel functions associated with Jack polynomials,[7] or multivariate analysis.[8] The wide occurrence of such group integrals then lends further urgency to the evaluation of the above-mentioned group integrals.

In this paper, we present and analyze a novel approach to the problem. We encountered the problem in the study of a random-matrix model for a class of chaotic systems (the semiseparable systems).[9] We found that we could use the invariants of the orthogonal group to construct a weight function. With the help of this function, it was possible to evaluate the group integrals in question by simple Wick contractions. We implemented the scheme on the computer and found that beyond the expected exact results for low-order monomials, monomials of higher order were also calcu-

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lated correctly up to and including the subleading order in $1/N$, where N is the dimension of the matrices under consideration. We conjectured that this statement holds for monomials of any order. It is the purpose of the present paper to extend and prove the conjecture and to explore the scope of its validity beyond the orthogonal group.

The group integrals extend over a compact matrix space with a measure which is uniquely determined by the underlying symmetry group. In order to reduce the computation to Wick contractions, we consider an extended matrix space where all matrix elements are independent Gaussian variables. In this space, all integrations trivially reduce to Wick contractions and can easily be implemented in many programming languages. The constraints due to the group structure are then introduced in an approximate fashion through a weight function w appearing as factor in the integrand. This function is chosen in such a way that the integrals yield the exact values for the lowest-order invariants of the group. It turns out that w is not always positive and, thus, not a measure. This, however, is not a significant obstacle.

Candidates for our spaces are the orthogonal group $\mathrm{O}(N)$, the unitary group $\mathrm{U}(N)=\mathrm{CUE}(N)$, also known as the circular unitary ensemble, the circular orthogonal ensemble of symmetric unitary matrices $\mathrm{COE}(N)$, and the circular symplectic ensemble which is isomorphic to the unitary symplectic group $\mathrm{CSE}(N)=\mathrm{USP}(2N)$. We note that $\mathrm{COE}(N)$ is not a group—for all other cases we can use the Haar measure, while in this case we have to use Dyson's invariant measure.

We first present our arguments for the case of the orthogonal group. In Sec. II we construct the weight function w from the invariants of the orthogonal group. We show that the defining equations for w always have a unique solution. We give explicit expressions for w in the simplest cases. We show that low-order monomials are calculated exactly using Wick contraction. In Sec. III, we show that monomials of higher order are evaluated correctly by Wick contraction, up to an error of order $N^{-\alpha}$. We establish a lower bound for the exponent α. In Sec. IV we extend our arguments to other matrix spaces. We give explicit expressions for the weight functions for $\mathrm{U}(N)$ and for $\mathrm{COE}(N)$. The more involved and less important case of CSE is only touched upon.

II. THE WEIGHT FUNCTION FOR O(N)

As explained in Sec. I, we start with a space of real matrices M. The elements are taken as independent Gaussian-distributed variables with zero mean and identical variances. In other words, our measure $\mathrm{d}\mu_g$ for integration is the product of the differentials of all matrix elements times $\mathcal{N}\exp\{-N\ \mathrm{tr}(MM^T)\}$ where $\mathcal{N}$ is a normalization factor. We recall that N is the dimension of the matrices M. We are interested in values of $N\gg 1$. The measure is invariant under right or left multiplication of M with any orthogonal matrix. To restrict the integration to the orthogonal group, we could think of multiplying $\mathrm{d}\mu_g$ with a set of delta functions expressing all the constraints due to orthonormality. This is clearly impractical. Instead, we modify the measure by multiplying $\mathrm{d}\mu_g$ with a weight function w_κ. This function is chosen in such a way that all orthogonal invariants up to and including order 2κ are exactly reproduced when we use w_κ as a weight function under the integrals over M. We note in passing that our present notation differs from that of Ref. 9. Our index κ equals half of the even index k used there.

To determine w_κ, we consider all invariants $I_j(O)$ up to order 2κ in the matrix elements O of the orthogonal group. Here, j is a running index. We recall that all such invariants are even in the O's. In every invariant $I_j(O)$, we replace O by M to obtain $I_j(M)$. We write w_κ as a linear combination of all the $I_j(M)$'s up to order 2κ in M. The coefficients of the linear combination are determined by the requirement that the average of every $I_j(M)$, calculated by integration over $\mathrm{d}\mu_g$ with weight function w_κ, yields the same result as integration of $I_j(O)$ over the orthogonal group. We recall that with n a positive integer, the invariants of the orthogonal group are given by expressions of the form $\mathrm{tr}\{(OO^T)^n\}$, or by products of such expressions. We accordingly write the quantities $I_j(M)$ in the form

$$I_{\mathbf{k}}^{(k)}(M)=\prod_{k_i}\ \mathrm{tr}\{(MM^T)^{k_i}\}. \tag{1}$$

Here $2k$ denotes the degree of I in M, and $\mathbf{k}=(k_1,k_2,\ldots)$ is a partition of k into positive integers $k_i\geqslant 1$ with $k_1+k_2+\cdots=k$. Without loss of generality we require that $k_1\geqslant k_2\geqslant\cdots$. The weight function w_κ is now written as

$$w_\kappa(M)=a_0^{(\kappa)}+\sum_{k=1}^{\kappa}\ \sum_{\mathbf{k}}\ a_{\mathbf{k}}^{(\kappa)}I_{\mathbf{k}}^{(k)}(M). \tag{2}$$

The sum on the right-hand side of Eq. (2) extends over a complete set of linearly independent invariants up to order 2κ in M.

We determine the coefficients $a_{\mathbf{k}}^{(\kappa)}$ from the conditions of orthonormality. More precisely, we require that the relations

$$\int\ \mathrm{d}\mu_g w_\kappa(M)=1,$$

$$\int\ \mathrm{d}\mu_g w_\kappa(M)(MM^T)_{i_1j_1}=\delta_{i_1,j_1},$$

$$\int\ \mathrm{d}\mu_g w_\kappa(M)(MM^T)_{i_1j_1}(MM^T)_{i_2j_2}=\delta_{i_1,j_1}\delta_{i_2,j_2}, \tag{3}$$

$$\cdots$$

$$\int\ \mathrm{d}\mu_g w_\kappa(M)(MM^T)_{i_1j_1}(MM^T)_{i_2j_2}\cdots(MM^T)_{i_\kappa j_\kappa}=\delta_{i_1,j_1}\delta_{i_2,j_2}\times\cdots\times\delta_{i_\kappa,j_\kappa}$$

be fulfilled identically. Relations of the form (3) hold for any value of κ for the orthogonal group but must be imposed for the integration over the matrices M.

Equation (3) determines the coefficients $a_{\mathbf{k}}^{(\kappa)}$ uniquely. To show this, we take traces over these equations in such a way that the integrals on the left-hand sides take the form $\int \mathrm{d}\mu_g w_\kappa(M)I_{\mathbf{k}}^{(k)}(M)$. The resulting set of equations has the form

$$\int\ \mathrm{d}\mu_g w_\kappa(M)I_{\mathbf{k}}^{(k)}(M)=B_{\mathbf{k}}^{(k)}, \tag{4}$$

where the coefficients $B_{\mathbf{k}}^{(k)}$ are given by powers of N, with N the dimension of the matrices M. Recalling Eq. (2), we see that Eq. (4) constitutes a set of linear equations for the coefficients $a_{\mathbf{k}}^{(\kappa)}$. There are obviously as many equations as there are coefficients $a_{\mathbf{k}}^{(\kappa)}$. We conclude that Eq. (4) possesses a unique solution unless the determinant of the matrix C with elements $C_{\mathbf{k}_1\mathbf{k}_2}^{(k_1k_2)}=\int \mathrm{d}\mu_g I_{\mathbf{k}_1}^{(k_1)}I_{\mathbf{k}_2}^{(k_2)}$ vanishes. But if $\det(C_{\mathbf{k}_1\mathbf{k}_2}^{(k_1k_2)})=0$, there exists a nontrivial solution $b_{\mathbf{k}_2}^{(k_2)}$ of the homogeneous equation $\Sigma_{k_2\mathbf{k}_2}C_{\mathbf{k}_1\mathbf{k}_2}^{(k_1k_2)}b_{\mathbf{k}_2}^{(k_2)}=0$. The existence of this solution implies that we also have $\Sigma_{k_1k_2}\Sigma_{\mathbf{k}_1\mathbf{k}_2}b_{\mathbf{k}_1}^{(k_1)}C_{\mathbf{k}_1\mathbf{k}_2}^{(k_1k_2)}b_{\mathbf{k}_2}^{(k_2)}=0$. Recalling the definition of the matrix C, we observe that the last relation can be written as $\int \mathrm{d}\mu_g|\Sigma_{\mathbf{k}_1\mathbf{k}_1}I_{\mathbf{k}_1}^{(k_1)}b_{\mathbf{k}_1}^{(k_1)}|^2=0$. But the integrand in the last expression is positive semidefinite and does not vanish identically. Therefore, it is not possible that $\det(C_{\mathbf{k}_1\mathbf{k}_2}^{(k_1k_2)})$ vanishes, and the solution of Eq. (4) exists and is unique. This solution also solves Eq. (3). To see this, let us assume the contrary and focus attention on the second equation of (3). [The argument is easily extended to the entire set of equations (3).] Inserting the solution of (4) into the left-hand side of that equation yields on the right-hand side the terms $\delta_{i_1j_1}+A_{i_1j_1}$ where the matrix A is both

traceless and invariant under every orthogonal transformation. This implies $A=0$, in contradiction to the assumption that we did not find a solution of the second equation of (3).

Equation (3) implies that the integrals over all polynomials of degree $n\leqslant 2\kappa$ in M are equal to the corresponding expressions for O(N). To see this, it suffices to consider the integral over an arbitrary monomial of degree n. It is obvious that the integral vanishes unless n is even, $n=2k$. We write the monomial as $\mathcal{M}^{(n)}=M_{i_1j_1}M_{i_2j_2}\cdots M_{i_nj_n}$. The integral over $\mathcal{M}^{(n)}$ is obviously invariant under right or left multiplication with any orthogonal transformation. Therefore, the integral over $\mathcal{M}^{(n)}$ must be a linear combination of invariants multiplied by a suitable set of Kronecker deltas in the indices $i_1,\ldots,i_n$ and $j_1,\ldots,j_n$. By construction the invariants have the same values as in O(N).

Inspection shows that the weight function $w_0=1$ fulfills the second equation of (3) automatically. Thus, $w_1=w_0$ and, therefore, $a_0^{(1)}=1$, $a_1^{(1)}=0$. The first nontrivial condition is, therefore, the one appearing in line 3 of (3). This condition (and all that follow below it) is violated by w_0. We now give the explicit results for the first few weight functions w_κ. These were obtained with the help of the MATHEMATICA program. For $\kappa=2$, we find

$$\begin{aligned} a_0^{(2)}&=1-\frac{N^2}{4},\\ a_1^{(2)}&=\frac{N}{2},\\ a_2^{(2)}&=-\frac{N^3}{4(-1+N)(2+N)},\\ a_{11}^{(2)}&=\frac{N^2}{4(-1+N)(2+N)}. \end{aligned} \tag{5}$$

For $\kappa=3$, we have

$$\begin{aligned} a_0^{(3)}&=1-\frac{7N^2}{12},\\ a_1^{(3)}&=\frac{3N}{2},\\ a_2^{(3)}&=-\frac{5N^3}{4(-1+N)(2+N)},\\ a_{11}^{(3)}&=\frac{5N^2}{4(-1+N)(2+N)},\\ a_3^{(3)}&=\frac{N^5}{3(-2+N)(-1+N)(2+N)(4+N)},\\ a_{21}^{(3)}&=-\frac{N^4}{(-2+N)(-1+N)(2+N)(4+N)},\\ a_{111}^{(3)}&=\frac{2N^3}{3(-2+N)(-1+N)(2+N)(4+N)}. \end{aligned} \tag{6}$$

For $\kappa=4$, we have

$$a_0^{(4)}=1-\frac{23\ N^2}{24}+\frac{N^4}{32},$$

$$a_1^{(4)}=3\ N-\frac{N^3}{8},$$

$$a_2^{(4)}=\frac{-60\ N^3+N^5}{16(-1+N)(2+N)},$$

$$a_{11}^{(4)}=\frac{56\ N^2+2\ N^3+N^4}{16(-1+N)(2+N)},$$

$$a_3^{(4)}=\frac{7\ N^5}{3(-2+N)(-1+N)(2+N)(4+N)},$$

$$a_{21}^{(4)}=\frac{-48\ N^4-2\ N^5-N^6}{8(-2+N)(-1+N)(2+N)(4+N)},$$

$$a_{111}^{(4)}=\frac{88\ N^3+6\ N^4+3\ N^5}{24\ (-2+N)(-1+N)(2+N)(4+N)}, \tag{7}$$

$$a_4^{(4)}=-\frac{N^7\ (6+5\ N)}{8(-3+N)(-2+N)(-1+N)(1+N)(2+N)(4+N)(6+N)},$$

$$a_{31}^{(4)}=\frac{N^6\ (6+5\ N)}{2(-3+N)(-2+N)(-1+N)(1+N)(2+N)(4+N)(6+N)},$$

$$a_{22}^{(4)}=\frac{N^7\ (18+5\ N+N^2)}{32\ (-3+N)(-2+N)(-1+N)(1+N)(2+N)(4+N)(6+N)},$$

$$a_{211}^{(4)}=-\frac{N^5\ (72+78\ N+5\ N^2+N^3)}{16\ (-3+N)\ (-2+N)(-1+N)(1+N)(2+N)(4+N)(6+N)},$$

$$a_{1111}^{(4)}=\frac{N^4\ (72+78\ N+5\ N^2+N^3)}{32\ (-3+N)(-2+N)(-1+N)(1+N)(2+N)(4+N)(6+N).}$$

We note that with increasing κ, the expressions become rather involved. Moreover, the coefficients $a_{\mathbf{k}}^{(\kappa)}$ with the same lower indices $\mathbf{k}$ change with κ.

III. MONOMIALS OF HIGHER ORDER FOR O(N): THE 1/N EXPANSION

We have seen that integrals over all polynomials of degree $n\leqslant 2\kappa$ have the same values as for O(N). What about polynomials of higher order? Again, it suffices to consider monomials $\mathcal{M}^{(2)}$ of even degree $2k$ with $k>\kappa$. We show that the integral over $\mathcal{M}^{(2)}$ coincides with the result for O(N) up to terms of order $N^{-\alpha}$ where the integer exponent α is positive and independent of k. More precisely, we show that for $k>\kappa$, we have

$$N^k\int \mathrm{d}\mu_g w_\kappa(M)\prod_{\nu=1}^{2k} M_{i_\nu j_\nu}=N^k\int \mathrm{d}h_{\mathrm{O}(N)}\prod_{\nu=1}^{2k} O_{i_\nu j_\nu}+\mathcal{O}(1/N^\alpha)\ \text{ where }\ \alpha\geqslant[\kappa/2]+1. \tag{8}$$

Here $[\kappa/2]$ indicates the integer part of $\kappa/2$, and $\mathrm{d}h_{\mathrm{O}(N)}$ denotes the Haar measure for integration over O(N). We note that the factors N^k in front of the integrals normalize the N dependence so

that these terms are (at most) of order 1. Another equivalent form of Eq. (8) is obtained by summing over pairs of indices $j_1=j_2, j_3=j_4, \ldots$. This removes the factors N^k and yields

$$\int \mathrm{d}\mu_g w_\kappa(M) \prod_{\nu=1}^{k} (MM^T)_{i_\nu l_\nu} = \int dh_{\mathrm{O}(N)} \prod_{\nu=1}^{k} (OO^T)_{i_\nu l_\nu} + \mathcal{O}(1/N^\alpha) \quad \text{where} \quad \alpha \geqslant [\kappa/2]+1. \tag{9}$$

The equivalence of Eq. (8) and Eq. (9) follows from the fact the matrix C discussed previously, if defined with respect to properly scaled monomials, does not depend on N. The remainder of this section is devoted to proving Eq. (9).

It is useful to introduce a few auxiliary concepts. We consider Gaussian integrals over monomials of M without the weight function w_κ. We write for brevity

$$\int \mathrm{d}\mu_g \prod_{\nu=1}^{k} (MM^T)_{i_\nu l_\nu} = \langle (MM^T)^k \rangle_g, \tag{10}$$

where the index g indicates the purely Gaussian integration. To define the completely correlated part of this expression, we consider first the case $k=2$. We use Wick contraction and have

$$\langle (MM^T)^2 \rangle_g = \langle (MM^T) \rangle_g \langle (MM^T) \rangle_g + \langle (MM^T)^2 \rangle_{gc}. \tag{11}$$

The last term on the right-hand side of Eq. (11) is the completely correlated term. For the general case of arbitrary order $2k$, we define the correlated part $\langle (MM^T)^k \rangle_{gc}$ as that contribution to $\langle (MM^T)^k \rangle_g$ which cannot be written in the form of products of two or more factors, each of which is a complete Wick contraction of powers of MM^T. It is easy to see that

$$\langle (MM^T)^k \rangle_{gc} = \mathcal{O}(1/N^{k-1}). \tag{12}$$

The linear increase with k in inverse powers of N in Eq. (12) is due to the fact that every Wick contraction which connects two M's appearing in different factors MM^T suppresses one summation index. Therefore, the correlated part $\langle (MM^T)^k \rangle_{gc}$ contributes the highest-order terms in $1/N$ to $\langle (MM^T)^k \rangle_g$.

We now consider integrals involving the weight function w_κ and use the same notation,

$$\int \mathrm{d}\mu_g w_\kappa \prod_{\nu=1}^{k} (MM^T)_{i_\nu l_\nu} = \langle w_\kappa (MM^T)^k \rangle_g. \tag{13}$$

Again using Wick contraction, we define the correlated part $\langle w_\kappa (MM^T)^k \rangle_{gc}$ of this expression as that part which cannot be written as the product of two or more factors, each of which is a complete Wick contraction of powers of MM^T and/or w_κ.

We proceed to show that in the equations relating the integral $\langle w_\kappa (MM^T)^k \rangle_g$ to the integral over the Haar measure, the leading correction term (lowest order in $1/N$) which does not cancel is given by

$$\langle w_\kappa (MM^T)^k \rangle_{gc} = \mathcal{O}(1/N^{[(k+1)/2]}) \quad \text{for } 1 < k \leqslant \kappa. \tag{14}$$

This relation is based upon the assumption that there is no accidental cancellation among the terms contributing to lowest order in $1/N$. Therefore, $[(k+1)]/2$ actually constitutes a lower bound on the exponent of $1/N$.

To prove relation (14), we rewrite the defining equations for w_κ, Eq. (3), as follows. We consider the expression $\langle w_\kappa (MM^T)^k \rangle_g$ with k integer and $k \leqslant \kappa$. We decompose this expression into correlated contributions. These originate from all partitions $\mathbf{k}=(k_1,k_2,\ldots)$ of k with $k_i \geqslant k_{i+1}$ and $\Sigma_i k_i = k$. We denote by i_0 the smallest index for which all k_i with $i > i_0$ are equal to one. Then, we have

$$\langle w_\kappa (MM^T)^k\rangle_g = \sum_{\mathbf{k}} \prod_i \langle (MM^T)^{k_i}\rangle_{gc} + \sum_{\mathbf{k}\neq \mathbf{1}^k} \sum_i^{i_0} \langle w_\kappa (MM^T)^{k_i}\rangle_{gc} \prod_{j\neq i} \langle (MM^T)^{k_j}\rangle_{gc}. \quad (15)$$

In the first term on the right-hand side, we have used that $\langle w_\kappa\rangle_g = 1$. In the second term, we have used that $\langle w_\kappa (MM^T)\rangle_{gc} = 0$. Trivially, the second sum on the right-hand side of Eq. (15) does not extend over the partition $\mathbf{1}^k = (1,1,1,\ldots)$ (k terms unity). According to (3), the expression in Eq. (15) equals $(\langle (MM^T)\rangle_g)^k$. This equals the contribution from the first sum on the right-hand side for the partition $\mathbf{1}^k$. The remaining terms must vanish,

$$\sum_{\mathbf{k}\neq \mathbf{1}^k} \prod_i \langle (MM^T)^{k_i}\rangle_{gc} + \sum_{\mathbf{k}\neq \mathbf{1}^k} \sum_i^{i_0} \langle w_\kappa (MM^T)^{k_i}\rangle_{gc} \prod_{j\neq i} \langle (MM^T)^{k_j}\rangle_{gc} = 0. \quad (16)$$

Equation (16) must hold for all values of k with $k \leqslant \kappa$. To proceed, we observe that the partitions of k can be grouped into classes as follows: Partitions within the same class carry the same number p of k_i's that have value unity. The classes are labeled by p, namely $\mathcal{C}_p$. For instance, for $k=6$, class $\mathcal{C}_2$ contains the partitions (4,1,1) and (2,2,1,1). In Eq. (16), we order the sum over $\mathbf{k}$ by grouping together all partitions which belong to the same class. We show presently that each such contribution must vanish separately. Then, we have for every $p = 0,1,\ldots,k-2$ that

$$\sum_{\mathbf{k}\neq \mathbf{1}^k, \mathbf{k}\in \mathcal{C}_p} \prod \langle (MM^T)^{k_i}\rangle_{gc} + \sum_{\mathbf{k}\in \mathcal{C}_p} \sum_i^{i_0} \langle w_\kappa (MM^T)^{k_i}\rangle_{gc} \prod_{j\neq i} \langle (MM^T)^{k_j}\rangle_{gc} = 0. \quad (17)$$

Equation (17) follows directly from the facts that Eq. (16) holds for all $k \leqslant \kappa$, and that the contributions from class $\mathcal{C}_p$ to a partition of k are the same as the contributions of class $\mathcal{C}_0$ to a partition of $k-p$, except for a string of Kronecker delta's due to the factors $(\langle (MM^T)\rangle_g)^p$.

We are now in the position to prove relation (14). We observe that in (17), the term $\langle w_\kappa (MM^T)^k\rangle_{gc}$ appears only in the class $\mathcal{C}_0$. Therefore, we have

$$\langle w_\kappa (MM^T)^k\rangle_{gc} = -\sum_{\mathbf{k}\in \mathcal{C}_0} \prod_i \langle (MM^T)^{k_i}\rangle_{gc} - \sum_{\mathbf{k}\in \mathcal{C}_0, \mathbf{k}\neq (k)} \sum_i \langle w_\kappa (MM^T)^{k_i}\rangle_{gc} \prod_{j\neq i} \langle (MM^T)^{k_j}\rangle_{gc}. \quad (18)$$

Using complete induction, i.e., assuming that relation (14) holds for all values of k' with $k' < k$, and using Eq. (12), we conclude from Eq. (18) that relation (14) also holds for $k'+1 = k$. The terms of lowest order in $1/N$ originate from partitions which have either the form (2,2,2,...) (for even k) or (3,2,2,2,...) (for odd k). Again, we cannot rule out the occurrence of accidental cancellations which would increase the power $[(k+1)]/2$ in relation (14).

Having established relation (14), we turn to the center piece of this section, Eq. (9). We first consider the case $k = \kappa+1$ and decompose the integral into correlated terms with contributions from all partitions of $\kappa+1$. For these partitions, we write $\mathbf{K+1} = (k_1, k_2, \ldots)$ with $k_1 + k_2 + \cdots = \kappa+1$ and $k_1 \geqslant k_2 \geqslant \cdots$. We use the notation introduced previously. Then,

$$\langle w_\kappa (MM^T)^{\kappa+1}\rangle_g = \sum_p \sum_{(\mathbf{K+1})\in \mathcal{C}_p} \prod_i \langle (MM^T)^{k_i}\rangle_{gc} + \sum_p \sum_{(\mathbf{K+1})\in \mathcal{C}_p} \sum_i^{i_0} \langle w_\kappa (MM^T)^{k_i}\rangle_{gc} \prod_{j\neq i} \langle (MM^T)^{k_j}\rangle_{gc}. \quad (19)$$

Equation (17) implies that all terms with $p \neq 0$ and $p \neq \kappa+1$ vanish, and we are left with

$$\langle w_\kappa (MM^T)^{\kappa+1}\rangle_g = (\langle (MM^T)\rangle_g)^{\kappa+1} + \sum_{(\mathbf{K+1})\in \mathcal{C}_0} \prod_i \langle (MM^T)^{k_i}\rangle_{gc}$$

$$+ \sum_{(\mathbf{K+1})\in \mathcal{C}_0} \sum_i \langle w_\kappa (MM^T)^{k_i}\rangle_{gc} \prod_{j\neq i} \langle (MM^T)^{k_j}\rangle_{gc}. \tag{20}$$

We use the same argument as in the previous paragraph and the result (14) and Eq. (12). We conclude that the contributions of lowest order in $1/N$ result from the partitions (2,2,2,...) or (3,2,2,2,...), respectively, and arrive at Eq. (9). The exponent α has the value $\alpha \geqslant [\kappa/2]+1$. In writing the inequality sign, we again allow for the possibility that an accidental cancellation of contributions from these partitions occurs.

We finally have to consider the case where $k-\kappa=n>1$. Decomposing the expression $\langle w_\kappa (MM^T)^{\kappa+n}\rangle_g$ as in Eq. (19), we easily see that the terms of lowest nonvanishing order in $1/N$ stem from the partitions in class $\mathcal{C}_{n-1}$. But these give exactly the same contributions as those for $k=\kappa+1$ that were estimated in the last paragraph. This completes the proof of Eq. (9).

IV. THE UNITARY GROUP AND OTHER UNITARY ENSEMBLES

In this section, we primarily address integrals over momomials of unitary matrices U with respect to the Haar measure of the unitary group. We start with Gaussian integrals over complex matrices M. The real and imaginary parts of the matrix elements are independent and Gaussian-distributed. The integrals are again worked out using Wick contractions. For the weight function w_κ^u, we write in analogy to Eq. (2)

$$w_\kappa^u(M) = b_0^{(\kappa)} + \sum_{k=1}^{\kappa} \sum_{\mathbf{k}} b_{\mathbf{k}}^{(\kappa)} I_{\mathbf{k}}^{(k)}(M). \tag{21}$$

The invariants are defined as in Eq. (1) with MM^T replaced by $MM^\dagger$ where a dagger stands for Hermitean conjugation. The upper index u refers to the unitary case. The values of the coefficients $b_{\mathbf{k}}^\kappa$ are, of course, not the same as for the orthogonal case. The arguments for the existence and uniqueness of the solutions carry over without change, and again computer programs are available to perform the contractions and calculate the coefficients $b_{\mathbf{k}}^\kappa$. For w_2^u and w_4^u we find

$$\begin{aligned} b_0^2 &= 1 - \frac{N^2}{2}, \\ b_1^2 &= N, \\ b_2^2 &= -\frac{N^3}{2(N-1)(N+1)}, \\ b_{11}^2 &= \frac{N^2}{2(N-1)(N+1)}, \end{aligned} \tag{22}$$

and

$$b_0^4 = \frac{24 - 46\,N^2 + 3\,N^4}{24},$$

$$b_1^4 = \frac{-(N(-12+N^2))}{2},$$

$$b_2^4=\frac{N^3\ (-30+N^2)}{4(-1+N)(1+N)},$$

$$b_{11}^4=\frac{N^2\ (28+N^2)}{4(-1+N)(1+N)},$$

$$b_3^4=\frac{14\ N^5}{3(-2+N)(-1+N)(1+N)(2+N)},$$

$$b_{21}^4=\frac{-N^4\ (24+N^2)}{2(-2+N)(-1+N)(1+N)(2+N)},$$

$$b_{111}^4=\frac{N^3\ (44+3N^2)}{6(-2+N)(-1+N)(1+N)(2+N)},$$

$$b_4^4=\frac{-5N^7}{4(-3+N)(-2+N)(-1+N)(1+N)(2+N)(3+N)},$$

$$b_{31}^4=\frac{5\ N^6}{(-3+N)(-2+N)(-1+N)(1+N)(2+N)(3+N)},$$

$$b_{22}^4=\frac{N^6\ (6+N^2)}{8(-3+N)(-2+N)(-1+N)(1+N)(2+N)(3+N)},$$

$$b_{211}^4=\frac{-N^5\ (36+N^2)}{4(-3+N)(-2+N)(-1+N)(1+N)(2+N)(3+N)},$$

$$b_{1111}^4=\frac{N^4\ (36+N^2)}{8(-3+N)(-2+N)(-1+N)(1+N)(2+N)(3+N)}. \tag{23}$$

The arguments determining the leading contribution to the $1/N$ expansion are the same ones as for the orthogonal group. Thus, we have to increase κ by two to improve the error by one order in $1/N$ in the calculation of monomials of high order. This is the reason for our not giving w_3^u but only w_4^u which yields correct values for the integrals up to order $1/N^2$.

For COE and CSE, the situation is slightly more complicated. The constraints on the matrices are not expressible in a simple way in terms of products as done in (3). It seems, therefore, most convenient to limit the space of independent matrix elements from the outset. In the case of the COE this is fairly simple: The symmetry reduces the number of independent complex matrix elements to $N(N+1)/2$. Therefore, we consider Gaussian averages in the space of complex symmetric matrices $S=S^T$. We accordingly have a contraction rule with two terms,

$$\int \mathrm{d}\mu_g(S)S_{ij}^*S_{kl}=\frac{1}{N}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}). \tag{24}$$

The invariants are now defined in terms of SS^*. Introducing the rule (24) into our program we can again calculate w_κ^c. As an example we compute the coefficients $c_{\mathbf{k}}^2$ for w_2^c,

$$c_0^2=1-\frac{N(N+1)}{4},$$

$$c_1^2=\frac{N+1}{2},$$
$$c_2^2=-\frac{(N+1)^3}{4N(N+3)}, \tag{25}$$
$$c_{11}^2=\frac{(N+1)^2}{4N(N+3)}.$$

In addition, the following subtle point must be considered. In Sec. II we have used the invariance of the Haar measure to justify that contraction with w_κ gives exact results for all polynomials up to order 2κ in the matrix elements. In the present case we have no invariance group and by consequence no Haar measure. On the other hand Dyson's measure with respect to which we integrate is also totally defined by an invariance group albeit a smaller one than that of U(N). The important point is that again the measure is uniquely defined by a linear group of transformations. The orthogonality conditions resulting from the unitarity of the matrices are the same and symmetry is taken into account explicitly in the contractions. Therefore all arguments again go through and indeed inspection of the results obtained by our code with those obtained in Ref. 2 shows agreement.

The case of CSE is simpler because it involves an invariance group, but more complicated because the matrices are symplectic. Two ways seem open to address this case. We might include the symplectic property from the outset in the contraction rules, or we might introduce this property as a constraint in the expression for the weight function. While both ways seem possible it is not clear which one is easier to follow. In view of the fact that CSE is of minor importance for practical applications, we have left this problem open. It is clear, however, that it can be tackled along the same lines.

V. CONCLUSIONS

We have presented a systematic way to calculate integrals over monomials of matrix elements for compact matrix groups and for other matrix ensembles whose measure is defined uniquely by an invariance group, such as the circular orthogonal ensemble of unitary symmetric matrices. This method gives exact results for monomials of low order. For higher-order monomials, it leads to an error of order $1/N^\alpha$ which is independent of the degree of the monomial. We have given a lower bound on the integer α, and we have shown how α can be increased systematically. The method is particularly suited for symbolic computer calculation. Codes are available for O(N), U(N) as well as for the circular orthogonal ensemble in MATHEMATICA and in C from one of the authors (T.P.).

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Finite-dimensional Lie algebras of order *F*

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F-Lie algebras are natural generalizations of Lie algebras ($F=1$) and Lie superalgebras ($F=2$). When $F>2$ not many finite-dimensional examples are known. In this article we construct finite-dimensional F-Lie algebras $F>2$ by an inductive process starting from Lie algebras and Lie superalgebras. Matrix realizations of F-Lie algebras constructed in this way from $\mathfrak{su}(n)$,$\mathfrak{sp}(2n)$ $\mathfrak{so}(n)$ and $\mathfrak{sl}(n|m)$, $\mathfrak{osp}(2|m)$ are given. We obtain nontrivial extensions of the Poincaré algebra by Inönü–Wigner contraction of certain F-Lie algebras with $F>2$. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1503148]

I. INTRODUCTION

The classification of algebraic objects satisfying certain axioms may be considered a fundamental objective on purely mathematical grounds. If, in addition, these objects turn out to to be relevant for the description of the possible symmetries of a physical system, such a classification takes on a whole new meaning. The main question is, of course, what are the mathematical structures which are useful in describing the laws of physics? Simple complex finite-dimensional Lie algebras were classified at the end of the 19th century by W. Killing and E. Cartan well before any physical applications were known. Since then, Lie algebras have become essential for the description of space–time symmetries and fundamental interactions. On the other hand, it was the discovery of supersymmetry in relativistic quantum field theory or as a possible extension of Poincaré invariance[1] which gave rise to the concept of Lie superalgebras and their subsequent classification.[2,3]

It is generally accepted that because of the theorems of Coleman and Mandula[4] and Haag, Lopuszanski, and Sohnius,[5] one cannot go beyond supersymmetry. However, if one weakens the hypotheses of these two theorems, one can imagine symmetries which go beyond supersymmetry,[6–28] the idea being that then the generators of the Poincaré algebra can be obtained as an appropriate product of more than two fundamental additional symmetries. These new generators are in a representation of the Lorentz algebra which is neither bosonic nor fermionic. Two kinds of representations are generally taken: parafermionic representations,[29] or infinite-dimensional representations (Verma module).[30]

Fractional supersymmetry (FSUSY)[9–28] is among the possible extensions of supersymmetry which have been studied in the literature. Basically, in such extensions, the generators of the Poincaré algebra are obtained as F-fold ($F\in\mathbb{N}^\star$) symmetric products of more fundamental generators. A natural generalization of Lie (super)algebras which is relevant for the algebraic description of FSUSY was defined in Ref. 24 and 28 and called an F-Lie algebra. An F-Lie algebra admits a $\mathbb{Z}_F$-gradation, the zero-graded part being a Lie algebra. An F-fold symmetric product (playing the role of the anticommutator in the case $F=2$) expresses the zero-graded part in terms of the non-zero-graded part.

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The purpose of this article is to show how one can construct many examples of finite-dimensional F-Lie algebras by an inductive process starting from Lie algebras and Lie superalgebras. Some preliminary results is this direction were given in Ref. 28. Two types of finite-dimensional F-Lie algebras will be constructed. The first family of examples, which we call trivial, are obtained by taking the direct sum of a Lie (super)algebra with the trivial representation. The second family is more interesting: by an inductive procedure we show how one can give the underlying vector space of any Lie algebra or any classical Lie superalgebra the structure of an F-Lie algebra. This procedure involves Casimir operators in the case of Lie algebras and invariant symmetric forms on the odd part of the algebra in the case of Lie superalgebras.

The article is organized as follows. In Sec. II we recall the definition of an F-Lie algebra and show how one can construct an F-Lie algebra of order F_1+F_2 from an F-Lie algebra of order $F_1\geqslant 2$ and an invariant symmetric form of order F_2 on its non-zero-graded part (c.f. Theorem II.6). In Sec. III we introduce the notion of a graded 1-Lie algebra in order to prove a version of Theorem II.6 when $F_1=1$ (Theorem III.6), and give some explicit examples of F-Lie algebras associated to Lie algebras. In Sec. IV we give explicit examples of F-Lie algebras associated to Lie superalgebras. In Sec. V we obtain FSUSY extensions of the Poincaré algebra by Inönü–Wigner contraction of certain F-Lie algebras constructed in the two previous sections. In Sec. VI we define a notion of simplicity for F-Lie algebras and give examples of simple and non-simple F-Lie algebras. Finally, in Sec. VII we give finite-dimensional matrix realizations of the F-Lie algebras of Sec. IV induced from $\mathfrak{sl}(m|n)$ and $\mathfrak{osp}(2|2n)$ and a quadratic form. Using finite-dimensional matrices, we also show that the underlying vector spaces of the graded 1-Lie algebras $\mathfrak{su}(n)\oplus\mathfrak{su}(n),\mathfrak{so}(n)\oplus\mathfrak{so}(n)$ and $\mathfrak{sp}(2n)\oplus\mathfrak{sp}(2n)$ can be given F-Lie algebra structures which cannot be obtained by our inductive process.

II. *F*-LIE ALGEBRAS

A. Definition of *F*-Lie algebras

In this section, we recall briefly the definition of F-Lie algebras given in Refs. 24 and 28. Let F be a positive integer and let $q=e^{2\pi i/F}$. We consider S a complex vector space and ε an automorphism of S satisfying $\varepsilon^F=1$. We set $\mathcal{A}_k=S_{q^k},1\leqslant k\leqslant F-1$, and $\mathcal{B}=S_1$ (S_{q^k} is the eigenspace corresponding to the eigenvalue q^k of ε). Then we have $S=\mathcal{B}\oplus\sum_{k=1}^{F-1}\mathcal{A}_k$.

Definition II.1: $S=\mathcal{B}\oplus\sum_{k=1}^{F-1}\mathcal{A}_k$ is called a (complex) F-Lie algebra if it is endowed with the following structure:

(1) $\mathcal{B}$ is a (complex) Lie algebra and $\mathcal{A}_k,1\leqslant k\leqslant F-1$, are representations of $\mathcal{B}$. If $[,]$ denotes the bracket on $\mathcal{B}$ and the action of $\mathcal{B}$ on S, it is clear that $\forall b\in\mathcal{B},\forall s\in S,[\varepsilon(b),\varepsilon(s)]=\varepsilon([b,s])$.

(2) There exist multilinear $\mathcal{B}$-equivariant maps $\{,\ldots,\}$: $\mathcal{S}^F(\mathcal{A}_k)\to\mathcal{B}$, where $\mathcal{S}^F(D)$ denotes the F-fold symmetric product of D. It is easy to see that $\{\varepsilon(a_1),\ldots,\varepsilon(a_F)\}=\varepsilon(\{a_1,\ldots,a_F\}),\forall a_1,\ldots,a_F\in\mathcal{A}_k$.

(3) For $b_i\in\mathcal{B}$ and $a_j\in\mathcal{A}_k$ the following "Jacobi identities" hold:

$$[[b_1,b_2],b_3]+[[b_2,b_3],b_1]+[[b_3,b_1],b_2]=0,$$
$$[[b_1,b_2],a_3]+[[b_2,a_3],b_1]+[[a_3,b_1],b_2]=0,$$
$$[b,\{a_1,\ldots,a_F\}]=\{[b,a_1],\ldots,a_F\}+\cdots+\{a_1,\ldots,[b,a_F]\},$$
$$\sum_{i=1}^{F+1}[a_i,\{a_1,\ldots,a_{i-1},a_{i+1},\ldots,a_{F+1}\}]=0. \qquad (J_4)$$

Note that the three first identities are automatic, but the fourth, which we will refer to as J_4, is an extra constraint.

Remark II.2: An F-Lie algebra is more than a Lie algebra $\mathfrak{g}_0$, a representation $\mathfrak{g}_1$ of $\mathfrak{g}_0$ and a $\mathfrak{g}_0$-valued $\mathfrak{g}_0$-equivariant symmetric form on $\mathfrak{g}_1$. Indeed, although the three first Jacobi identities

are manifest in this situation, the fourth is not necessarily true. As an example, consider $\mathfrak{g}_0=\mathfrak{sl}(2,\mathbb{C})$ *and* $\mathfrak{g}_1=\mathcal{S}_{2k+1}$, $k\in\mathbb{N}$ *(the irreducible representation of dimension* $2k+2$*). From the decomposition* $\mathcal{S}^2(\mathcal{S}_{2k+1})=\mathcal{S}_{4k+2}\oplus\mathcal{S}_{4k-2}\oplus\cdots\oplus\mathcal{S}_2$ *one has an* $\mathfrak{sl}(2,\mathbb{C})$*-equivariant mapping from* $\mathcal{S}^2(\mathcal{S}_{2k+1})\to\mathcal{S}_2\to\mathfrak{sl}(2,\mathbb{C})$. *But* $\mathfrak{g}=\mathfrak{sl}(2,\mathbb{C})\oplus\mathcal{S}_{2k+1}$ *is not a Lie superalgebra (the fourth Jacobi identity is not satisfied) except when* $k=0$ *where it reduces to* $\mathfrak{osp}(1|2)$.

Remark II.3: A 1*-Lie algebra is a Lie algebra, and a* 2*-Lie algebra is a Lie superalgebra. We will also refer to these objects as* F*-Lie algebras of order* 1 *and* 2*, respectively.*

Remark II.4: Notice that $\{a_1,\ldots,a_F\}$ *is only defined if the* a_i *are in the same* $\mathcal{A}_k$ *and that* $\forall k=1,\ldots,F-1$*, the spaces* $S_k=\mathcal{B}\oplus\mathcal{A}_k$ *are* F*-Lie algebras.*

From now on, we consider only F**-Lie algebras** $S=\mathcal{B}\oplus\mathcal{A}$ **such that** $\mathcal{A}$ **is an eigenspace of** ε.

Remark II.5: If $\mathfrak{h}\subset\mathcal{B}$ *is a Cartan subalgebra and* $F_{\lambda_1},\ldots,F_{\lambda_F}\in\mathcal{F}$ *are respectively of weight* $\lambda_1,\ldots,\lambda_F$*, then* $\{F_{\lambda_1},\ldots,F_{\lambda_F}\}\in\mathcal{B}$ *is of weight* $\lambda_1+\cdots+\lambda_F$. *In particular, if* $\lambda_1+\cdots+\lambda_F\neq 0$ *is not a root of* $\mathcal{B}$*, this bracket is zero.*

This structure can be seen as a possible generalization of Lie algebras ($F=1$) or Lie superalgebras ($F=2$) and can be compared, in some sense, to the ternary algebras ($F=3$) considered in Ref. 31, and to the n-ary algebras ($F=n$) introduced in Ref. 32 but in a different context. We have shown[24,28] that all examples of FSUSY considered in the literature can be described within the framework of F-Lie algebras.

B. An inductive construction of *F*-Lie algebras

Let $\mathfrak{g}$ be a complex Lie algebra and let $\mathfrak{r},\mathfrak{r}'$ be representations of $\mathfrak{g}$ such that there is a $\mathfrak{g}$-equivariant map $\mu_F:S^F(\mathfrak{r})\to\mathfrak{r}'$. We set

$$S=\mathcal{B}\oplus\mathcal{A}_1=(\mathfrak{g}\oplus\mathfrak{r}')\oplus\mathfrak{r}.$$

Then, $\mathcal{B}=\mathfrak{g}\oplus\mathfrak{r}'$ is a Lie algebra as the semi-direct product of $\mathfrak{g}$ and $\mathfrak{r}'$ (the latter with the trivial bracket). We can extend the action of $\mathfrak{g}$ on $\mathfrak{r}$ to an action of $\mathcal{B}$ on $\mathfrak{r}$ by letting $\mathfrak{r}'$ act trivially on $\mathfrak{r}$. This defines the bracket $[,]$ on S. For the map $\{\cdots\}$ we take μ_F. The first three Jacobi identities are clearly satisfied, and the fourth is also satisfied as each term in the expression on the lhs of J_4 vanishes. Hence S is an F-Lie algebra. There are two essentially opposite ways of giving explicit examples of F-Lie algebras of this type. One can either start from $\mathfrak{g}$ and $\mathfrak{r}'$ and extract an "F-root" of $\mathfrak{r}'$, or one can decompose $\mathcal{S}^F(\mathfrak{r})$ into irreducible summands and project onto one of them.[24] The first approach is the more difficult since, in general, it involves infinite-dimensional representation theory. For example, if one starts with $\mathfrak{r}'=\mathfrak{D}_{\mu_1}$, the vector representation of $\mathfrak{so}(1,d-1)$ of highest weight μ_1, the representation $\mathfrak{r}=\mathfrak{D}_{\mu_1/F}$ of highest weight μ_1/F is not exponentializable (see, e.g., Ref. 33) and does not define a representation of the Lie group $\mathrm{SO}(1,d-1)$, except when $d=3$ where such representations describe relativistic anyons.[34] The second approach, on the other hand, will always give finite-dimensional F-Lie algebras if one starts from finite-dimensional representations.

The following theorem gives an inductive procedure for constructing finite-dimensional F-Lie algebras.

Theorem II.6: *Let* $\mathfrak{g}_0$ *be a Lie algebra and* $\mathfrak{g}_1$ *a representation of* $\mathfrak{g}_0$ *such that*

(i) $S_1=\mathfrak{g}_0\oplus\mathfrak{g}_1$ *is an* F*-Lie algebra of order* $F_1>1$;
(ii) $\mathfrak{g}_1$ *admits a* $\mathfrak{g}_0$*-equivariant symmetric form* μ_2 *of order* $F_2\geqslant 1$.

Then $S=\mathfrak{g}_0\oplus\mathfrak{g}_1$ *admits an* F*-Lie algebra structure of order* F_1+F_2*, which we call the* F*-Lie algebra induced from* S_1 *and* μ_2.

Proof: By hypothesis, there exist $\mathfrak{g}_0$-equivariant maps $\mu_1:\mathcal{S}^{F_1}(\mathfrak{g}_1)\to\mathfrak{g}_0$ and $\mu_2:\mathcal{S}^{F_2}(\mathfrak{g}_1)\to\mathbb{C}$. Now, consider $\mu:\mathcal{S}^{F_1+F_2}(\mathfrak{g}_1)\to\mathfrak{g}_0\otimes\mathbb{C}\cong\mathfrak{g}_0$ defined by

$$\mu(f_1,\ldots,f_{F_1+F_2})=\frac{1}{F_1!}\frac{1}{F_2!}\sum_{\sigma\in S_{F_1+F_2}}\mu_1(f_{\sigma(1)},\ldots,f_{\sigma(f_{F_1})})\otimes\mu_2(f_{\sigma(f_{F_1+1})},\ldots,f_{\sigma(f_{F_1+F_2})}),\tag{2.1}$$

where $f_1,\ldots,f_{F_1+F_2}\in\mathfrak{g}_1$ and $S_{F_1+F_2}$ is the group of permutations on F_1+F_2 elements. By construction, this is a $\mathfrak{g}_0$-equivariant map from $\mathcal{S}^{F_1+F_2}(\mathfrak{g}_1)\to\mathfrak{g}_0$, thus the three first Jacobi identities are satisfied. The last Jacobi identity J_4, is more difficult to check and is a consequence of J_4 for the F-Lie algebra S_1 and a factorization property. Indeed, setting $F=F_1+F_2$, the identity J_4 for the terms in

$$\sum_{i=0}^{F}[f_i,\mu(f_1,\ldots,f_{i-1},f_{i+1},\ldots,f_F)],$$

of the form $\mu_1(f_{\sigma(1)},\ldots,f_{\sigma(f_{F_1})})\otimes\mu_2(f_{\sigma(f_{F_1+1})},\ldots,f_{\sigma(f_{F_1+F_2})}$ with $\sigma\in S_{F_1+F_2+1}$, reduces to

$$\sum_{i=0}^{F_1}[f_{\sigma(i)},\mu_1(f_{\sigma(1)},\ldots,f_{\sigma(i-1)},f_{\sigma(i+1)},\ldots,f_{\sigma(f_{F_1})})]\otimes\mu_2(f_{\sigma(f_{F_1+1})},\ldots,f_{\sigma(f_{F_1+F_2})})=0,$$

using $\mu_2(f_{\sigma(f_{F_1+1})},\ldots,f_{\sigma(f_{F_1+F_2})})\in\mathbb{C}$. But the lhs vanishes by J_4 for the F-Lie algebra S_1. A similar argument works for the other terms and hence J_4 is satisfied and S is an F-Lie algebra of order F_1+F_2. Q.E.D.

Remark II.7: Theorem II.6 is equivalent to the fact that the product of two $\mathfrak{g}_0$-equivariant symmetric forms satisfying J_4 also satisfies J_4 if one of them is scalar-valued.

III. FINITE-DIMENSIONAL *F*-LIE ALGEBRAS ASSOCIATED TO LIE ALGEBRAS

In this section we first introduce the notion of a graded 1-Lie algebra in order to have a version of Theorem II.6 when $F_1=1$.

A. Graded 1-Lie algebras

Definition III.1: A graded 1*-Lie algebra is a $\mathbb{Z}_2$-graded vector space $S=\mathcal{B}\oplus\mathcal{F}$ such that*
(1) *$\mathcal{B}$ is a Lie algebra*;
(2) *$\mathcal{F}$ is a representation of $\mathcal{B}$*;
(3) *there is a $\mathcal{B}$-equivariant map $\mu:\mathcal{F}\to\mathcal{B}$; and*
(4) $[\mu(f_1),f_2]+[\mu(f_2),f_1]=0,\forall f_1,f_2\in\mathcal{F}$.

Example III.2: Let $\mathfrak{g}$ be a Lie algebra. Set $\mathcal{B}=\mathfrak{g}$, $\mathcal{F}=\mathrm{ad}\mathfrak{g}$ and $S=\mathcal{B}\oplus\mathcal{F}$. If $\mu:\mathcal{F}\to\mathcal{B}$ is the identity, then (S,μ) is a graded 1*-Lie algebra.*

Remark III.3: A graded 1*-Lie algebra is not a priori a Lie algebra but it easy to see that, in fact, it has a natural graded Lie algebra structure.*

Remark III.4: $\mathrm{Ker}\mu$ is a $\mathcal{B}$-invariant subspace of $\mathcal{F}$ and $\mathrm{Im}\mu$ is a $\mathcal{B}$-invariant subspace of $\mathcal{B}$. In particular, if $\mathcal{B}$ is simple, $\mathcal{F}$ irreducible, and μ nontrivial, then μ defines a $\mathcal{B}$-equivariant isomorphism between $\mathcal{F}$ and $\mathcal{B}$.

A graded 1-Lie algebra is a graded Lie algebra in the usual sense. In general, however, a graded Lie algebra is not a graded 1-Lie algebra since there is no preferred map from the odd to the even part.

Proposition III.5: Let $\mathfrak{g}=\mathfrak{g}_+\oplus\mathfrak{g}_-$ be a graded Lie algebra, and let $\mu:\mathfrak{g}\to\mathfrak{g}$ be an odd $\mathfrak{g}_+$-equivariant map of $\mathfrak{g}$ such that μ is injective on $[\mathfrak{g}_+,\mathfrak{g}_-]$. Then $(\mathfrak{g},\mu)$ is a graded 1*-Lie algebra.*

Proof: One only has to check Definition III.1(4). One has $\forall f_1,f_2\in\mathfrak{g}_-$, $\mu([\mu(f_1),f_2]+[\mu(f_2),f_1])=[\mu(f_1),\mu(f_2)]+[\mu(f_2),\mu(f_1)]=0$. Since μ is injective on $[\mathfrak{g}_+,\mathfrak{g}_-]$ this implies Definition III.1(4). Q.E.D.

Theorem III.6 (II.6-bis): *Let* $\mathfrak{g}_0$ *be a Lie algebra and* $\mathfrak{g}_1$ *a representation of* $\mathfrak{g}_0$ *such that*

(i) $S_1=\mathfrak{g}_0\oplus\mathfrak{g}_1$ *is a graded* 1*-Lie algebra* and
(ii) $\mathfrak{g}_1$ *admits a* $\mathfrak{g}_0$*-equivariant symmetric* μ_2 *form of order* $F_2\geqslant 1$.

Then $S=\mathfrak{g}_0\oplus\mathfrak{g}_1$ *admits an F-Lie algebra structure of order* $1+F_2$ *which we call the F-Lie algebra induced from* S_1 *and* μ_2.

Proof: Analogous to Theorem II.6. Q.E.D.

B. Trivial and induced *F*-Lie algebras

Consider the graded 1-Lie algebra $S=\mathfrak{g}_0\oplus\mathfrak{g}_1$ where $\mathfrak{g}_0$ is a Lie algebra, $\mathfrak{g}_1$ is the adjoint representation of $\mathfrak{g}_0$ and $\mu:\mathfrak{g}_1\to\mathfrak{g}_0$ is the identity. Let $J_1,\ldots,J_{\dim\mathfrak{g}_0}$ be a basis of $\mathfrak{g}_0$, and $A_1,\ldots,A_{\dim\mathfrak{g}_0}$ be the corresponding basis of $\mathfrak{g}_1$. The graded 1-Lie algebra structure on S is then

$$[J_a,J_b]=f_{ab}{}^cJ_c,\quad [J_a,A_b]=f_{ab}{}^cA_c,\quad \mu(A_a)=J_a, \tag{3.1}$$

where $f_{ab}{}^c$ are the structure constant of $\mathfrak{g}_0$, Two types of F-Lie algebras associated to S will be defined.

The first type of F-Lie algebra associated to S will be called trivial and is constructed as follows:

Theorem III.7: *Let* $\mathfrak{g}_0$ *be a Lie algebra and let* $F\geqslant 1$ *be an integer. Then* $S=\mathfrak{g}_0\oplus(\mathfrak{g}_1\oplus\mathbb{C})$ *can be given the structure of an F-Lie algebra (graded* 1*-Lie algebra if* $F=1$*) where* $\mathfrak{g}_1$ *is the adjoint representation of* $\mathfrak{g}_0$ *and* $\mathbb{C}$ *is the trivial representation.*

Proof: The map $\mu:\mathcal{S}^F(\mathfrak{g}_1\oplus\mathbb{C})\to\mathfrak{g}_0$ is given by projection on $\mathfrak{g}_1$ in the decomposition $\mathcal{S}^F(\mathfrak{g}_1\oplus\mathbb{C})=\mathcal{S}^F(\mathfrak{g}_1)\oplus\mathcal{S}^{F-1}(\mathfrak{g}_1)\oplus\cdots\oplus\mathcal{S}^2(\mathfrak{g}_1)\oplus\mathfrak{g}_1\oplus\mathbb{C}$, followed by the identification of $\mathfrak{g}_1$ with $\mathfrak{g}_0$.

With the notations of (3.1) the brackets are

$$\begin{gathered}\{\lambda,\ldots,\lambda\}=0\\ \{\lambda,\ldots,\lambda,A_a\}=J_a\\ \vdots\\ \{\lambda,\ldots,\lambda,A_{a_1},\ldots,A_{a_k}\}=0,\quad 1<k\leqslant F\\ \vdots\\ \{A_{a_1},\ldots,A_{a_F}\}=0\end{gathered} \tag{3.2}$$

with $A_a,\in\mathfrak{g}_1,\lambda\in\mathbb{C}$, and $J_a\in\mathfrak{g}_0$.

It is easy to check that the four Jacobi identities are satisfied. Q.E.D.

The second type of F-Lie algebras associated to S are those induced from S and Casimir operators of $\mathfrak{g}_0$ (see Theorem III.6). It is well known that the invariant tensors on $\mathfrak{g}_0^\star$ are generated by primitive invariant tensors which are either fully symmetric or fully antisymmetric.[35] By duality, symmetric invariant tensors are related to the Casimir operators of $\mathfrak{g}_0$, and it is well known that for a rank r Lie algebra one can find r independent primitive Casimir operators.

Theorem III.8: *Let* $\mathfrak{g}_0$ *be a simple (complex) Lie algebra and* $\mathfrak{g}_1$ *be the adjoint representation of* $\mathfrak{g}_0$. *Then a Casimir operator of* $\mathfrak{g}_0$ *of order m induces the structure of an F-Lie algebra of order* $m+1$ *on* $S_{m+1}=\mathfrak{g}_0\oplus\mathfrak{g}_1$.

Proof: By Example III.2 $\mathfrak{g}_0\oplus\mathfrak{g}_1$ is a graded 1-Lie algebra and the result follows from Theorem III.6. Q.E.D.

Remark III.9: One can give explicit formulas for the bracket of these F-Lie algebras as follows. Let $J_a,a=1,\ldots,\dim(\mathfrak{g}_0)$ *and let* $A_a,a=1,\ldots,\dim(\mathfrak{g}_0)$ *be bases as at the beginning of this*

section. Let $h_{a_1\cdots a_m}$ *be a Casimir operator of order* m *[for* $m=2$*, the Killing form* $g_{ab}=\mathrm{Tr}(A_aA_b)$ *is a primitive Casimir of order* 2*]. Then, the* F*-bracket of the* F*-Lie algebra is*

$$\{A_{a_1},A_{a_2},\ldots,A_{a_{m+1}}\}=\sum_{\ell=1}^{m+1} h_{a_1\cdots a_{\ell-1}a_{\ell+1}\cdots a_{m+1}}J_{a_\ell}. \tag{3.3}$$

For the Killing form this gives

$$\{A_a,A_b,A_c\}=g_{ab}J_c+g_{ac}J_b+g_{bc}J_a. \tag{3.4}$$

If $\mathfrak{g}_0=\mathfrak{sl}(2)$, the F-Lie algebra of order 3 induced from the Killing form is the F-Lie algebra of Ref. 36.

IV. FINITE-DIMENSIONAL *F*-LIE ALGEBRAS ASSOCIATED TO LIE SUPERALGEBRAS

In this section we will consider some F-Lie algebras which can be associated to Lie superalgebras using Theorem II.6.

A. Lie superalgebras

We first recall some basic results on simple complex Lie superalgebras (for more details, see Ref. 37 and 38). Simple Lie superalgebras can be divided into two types: classical and Cartan type. Classical Lie superalgebras can be further divided into two families: basic and strange. A basic Lie superalgebra $\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$ is said to be respectively of type I or type II depending on whether the $\mathfrak{g}_0$-module $\mathfrak{g}_1$ is respectively reducible or irreducible. Here is the complete list of simple classical Lie superalgebras.[2,3] In the statement of 1(i) the symbol $(\overline{\mathbf{m+1}},\mathbf{n+1})^+\oplus(\mathbf{m+1},\overline{\mathbf{n+1}})^-$ denotes $(\mathbb{C}^{m+1\star}\otimes\mathbb{C}^{n+1}\otimes\mathbb{C})\oplus(\mathbb{C}^{m+1}\otimes\mathbb{C}^{n+1\star}\otimes\mathbb{C}^\star)$, where $\mathbb{C}^{m+1}$ is the fundamental representation of $\mathfrak{sl}(m+1)$, $\mathbb{C}^{m+1\star}$ is its dual representation and $\mathbb{C}$ is the standard one-dimensional representation of $\mathfrak{gl}(1)$. In the rest of the theorem we use analogous notation.

Theorem IV.1: *Let* $\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$ *be a classical simple complex Lie superalgebra. Then* $\mathfrak{g}$ *is isomorphic to one of the following:*

(1) *Basic of type I:*

(i) $A(m,n):m>n\geqslant 0,\mathfrak{g}_0=\mathfrak{sl}(m+1)\oplus\mathfrak{sl}(n+1)\oplus\mathfrak{gl}(1),\mathfrak{g}_1=(\overline{\mathbf{m+1}},\mathbf{n+1})^+\oplus(\mathbf{m+1},\overline{\mathbf{n+1}})^-$.
(ii) $A(n,n):n\geqslant 1,\mathfrak{g}_0=\mathfrak{sl}(n+1)\oplus\mathfrak{sl}(n+1),\mathfrak{g}_1=(\overline{\mathbf{n+1}},\mathbf{n+1})\oplus(\mathbf{n+1},\overline{\mathbf{n+1}})$.
(iii) $C(n+1):n\geqslant 1,\mathfrak{g}_0=\mathfrak{sp}(2n)\oplus\mathfrak{gl}(1),\mathfrak{g}_1=\mathbf{2n}^+\oplus\mathbf{2n}^-$.

(2) *Basic of type II:*

(i) $B(m,n):m\geqslant 0,n\geqslant 1,\mathfrak{g}_0=\mathfrak{so}(2m+1)\oplus\mathfrak{sp}(2n),\mathfrak{g}_1=(\mathbf{2m+1},\mathbf{2n})$.
(ii) $D(m,n):m\geqslant 2,n\geqslant 1,m\neq n+1,\mathfrak{g}_0=\mathfrak{so}(2m)\oplus\mathfrak{sp}(2n),\mathfrak{g}_1=(\mathbf{2m},\mathbf{2n})$.
(iii) $D(n+1,n):\mathfrak{g}_0=\mathfrak{so}(2(n+1))\oplus\mathfrak{sp}(2n),\mathfrak{g}_1=(\mathbf{2(n+1)},\mathbf{2n})$.
(iv) $D(2,1;\alpha):\alpha\in\mathbb{C}-\{0,-1\},\mathfrak{g}_0=\mathfrak{sl}(2)\oplus\mathfrak{sl}(2)\oplus\mathfrak{sl}(2),\mathfrak{g}_1=(\mathbf{2},\mathbf{2},\mathbf{2})$.
(v) $F(4):\mathfrak{g}_0=\mathfrak{sl}(2)\oplus\mathfrak{so}(7),\mathfrak{g}_1=(\mathbf{2},\mathbf{8})$.
(vi) $G(3):\mathfrak{g}_0=\mathfrak{sl}(2)\oplus G_2,\mathfrak{g}_1=(\mathbf{2},\mathbf{7})$.

(3) *(Strange):*

(i) $Q(n):n>1\,\mathfrak{g}_0=\mathfrak{sl}(n),\mathfrak{g}_1=\mathrm{ad}(\mathfrak{sl}(n))$, *with ad the adjoint representation.*
(ii) $P(n):n>1\,\mathfrak{g}_0=\mathfrak{sl}(n),\mathfrak{g}_1=[2]\oplus[1^{n-2}]$, *where* $[2]$ *denotes* $\mathcal{S}^2(\mathbb{C}^n)$ *the twofold symmetric representation and* $[1^{n-2}]$ *denotes* $\Lambda^{n-2}(\mathbb{C}^n)$ *the* $(n-2)$*-fold antisymmetric representation.*

[The superscript in 1(i) and 1(iii) indicates the $\mathfrak{gl}(1)$ *charge.]*

B. Symmetric invariant forms

By Theorem II.6 one can construct an F-Lie algebra from a Lie superalgebra $\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$ and a $\mathfrak{g}_0$-invariant symmetric form on $\mathfrak{g}_1$. In general determining *all* invariant symmetric forms on a given representation of a given Lie algebra is very difficult. However, for the Lie superalgebras given in the above list we will show how one can construct many invariant symmetric forms. The key observation is that for each basic Lie superalgebra in the list, the odd part $\mathfrak{g}_1$ is either a tensor product (type II) or a sum of two dual tensor products (type I) as a representation of $\mathfrak{g}_0$. Thus, to find $\mathfrak{g}_0$-invariant symmetric forms on $\mathfrak{g}_1$, one can use the following well known isomorphisms of representations of $\mathrm{GL}(A)\times\mathrm{GL}(B)$:[39]

$$\mathcal{S}^p(A\oplus B)=\sum_{k=0}^{p}\mathcal{S}^k(A)\otimes\mathcal{S}^{p-k}(B), \tag{4.1}$$

$$\mathcal{S}^p(A\otimes B)=\sum_{\Gamma}\$^{\Gamma}(A)\otimes\$^{\Gamma}(B), \tag{4.2}$$

where the second sum is taken over all Young diagrams Γ of length p and $\$^{\Gamma}(A)$ denotes the irreducible representation of $\mathrm{GL}(A)$ corresponding to the Young symmetrizer of Γ.

1. Type I

We consider the Lie superalgebra $A(m,n)$. The case of the other basic type I Lie superalgebras is similar. Then $\mathfrak{g}_0=\mathfrak{sl}(m+1)\oplus\mathfrak{sl}(n+1)\oplus\mathfrak{gl}(1)$ and $\mathfrak{g}_1=(\mathbb{C}^{m+1\star}\otimes\mathbb{C}^{n+1}\otimes\mathbb{C})\oplus(\mathbb{C}^{m+1\star}\otimes\mathbb{C}^{n+1}\otimes\mathbb{C})^{\star}$. Using the formulas (4.1) and (4.2), one sees that $\mathcal{S}^p(\mathfrak{g}_1)$ is a direct sum of terms of the form

$$\$^{\Gamma}(\mathbb{C}^{m+1\star})\otimes\$^{\Gamma'}(\mathbb{C}^{m+1})\otimes\$^{\Gamma}(\mathbb{C}^{n+1})\otimes\$^{\Gamma'}(\mathbb{C}^{n+1\star})\otimes\mathbb{C}^{|\Gamma|-|\Gamma'|}, \tag{4.3}$$

where $|\Gamma|$ is the length of Γ and $|\Gamma|+|\Gamma'|=p$. If this term contains the trivial representation, then n must be even and $|\Gamma|=|\Gamma'|$. Furthermore, the dimension of the vector space of $\mathfrak{g}_0$ invariants is then

$$I_{\Gamma,\Gamma'}=\dim\ \mathrm{Hom}_{\mathfrak{sl}(m+1)}(\$^{\Gamma'}(\mathbb{C}^{m+1}),\$^{\Gamma}(\mathbb{C}^{m+1}))\times\dim\ \mathrm{Hom}_{\mathfrak{sl}(n+1)}(\$^{\Gamma'}(\mathbb{C}^{n+1}),\$^{\Gamma}(\mathbb{C}^{n+1})), \tag{4.4}$$

where $\mathrm{Hom}_{\mathfrak{sl}(m+1)}$ denotes homomorphisms which are $\mathfrak{sl}(n+1)$ equivariant. One can calculate the dimensions of these spaces using well known results.[39] If $\Gamma=\Gamma'$, then $I_{\Gamma,\Gamma'}\geqslant 1$; if $\Gamma=\Gamma'$ and $|\Gamma|=|\Gamma'|=1$, then $I_{\Gamma,\Gamma'}=1$ and the invariant quadratic form corresponds to the tautological metric on $\mathfrak{g}_1$. In Ref. 28 F-Lie algebras were constructed using this symmetric form.

2. Type II

All basic type II Lie superalgebras except (iv) have $\mathfrak{g}_0=\mathfrak{g}_0'\oplus\mathfrak{g}_0''$ and $\mathfrak{g}_1=\mathcal{D}'\otimes\mathcal{D}''$, where $\mathcal{D}'$ and $\mathcal{D}''$ are irreducible self-dual representations of respectively $\mathfrak{g}_0'$ and $\mathfrak{g}_0''$. Therefore, $\mathcal{S}^p(\mathfrak{g}_1)$ is the direct sum of terms of the form

$$\$^{\Gamma}(\mathcal{D}')\otimes\$^{\Gamma}(\mathcal{D}''), \tag{4.5}$$

where $|\Gamma|=p$. The dimension of the vector space of $\mathfrak{g}_0$ invariants is

$$I_{\Gamma}=\dim\$^{\Gamma}(\mathcal{D}')^{\mathfrak{g}_0'}\times\dim\$^{\Gamma}(\mathcal{D}'')^{\mathfrak{g}_0''}, \tag{4.6}$$

where $\$^{\Gamma}(\mathcal{D}')^{\mathfrak{g}_0'}$ denotes the space of $\mathfrak{g}_0'$ invariant vectors in $\$^{\Gamma}(\mathcal{D}')$. Although the respective factors in the product (4.5) are irreducible for $\mathrm{GL}(\mathcal{D}')$ and $\mathrm{GL}(\mathcal{D}'')$, they may become reducible for $\mathfrak{g}_0'$, $\mathfrak{g}_0''$. For example the representations associated to the Young diagram $\boxplus$ are reducible for both $\mathfrak{g}_0'=\mathfrak{so}(m)$ and $\mathfrak{g}_0''=\mathfrak{sp}(2n)$.

3. The strange superalgebra $Q(n)$

Up to duality $\mathcal{S}^\star(\mathfrak{g}_1)$ (the symmetric algebra on $\mathfrak{g}_1$) is generated by the Casimir operators of $\mathfrak{sl}(n)$ (see Sec. III).

4. The strange superalgebra $P(n)$

In this case $\mathcal{S}^\star(\mathfrak{g}_1)$ is a direct sum of terms of the form

$$\mathcal{S}^k(\mathcal{S}^2(\mathbb{C}^n))\otimes\mathcal{S}^{p-k}(\Lambda^{n-2}(\mathbb{C}^n)). \tag{4.7}$$

This representation is in general reducible, but we do not know of a simple general formula for the dimension of $\mathfrak{sl}(n)$ invariants.

C. Trivial and induced *F*-Lie algebras

In this section F-Lie algebras associated to Lie superalgebras will be constructed explicitly. To fix our notations, consider $\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$ a classical Lie superalgebra. Let $J_a, 1\leqslant a\leqslant \dim\ \mathfrak{g}_0$, be a basis of $\mathfrak{g}_0$ and $F_\alpha, 1\leqslant\alpha\leqslant\dim\ \mathfrak{g}_1$, be a basis of $\mathfrak{g}_1$. The structure constants of $\mathfrak{g}$ are given by

$$\begin{aligned}[J_a,J_b]&=f_{ab}{}^cJ_c,\\ [J_a,F_\alpha]&=(R_a)_\alpha{}^\beta F_\beta,\\ \{F_\alpha,F_\beta\}&=E_{\alpha\beta}=S^a_{\alpha\beta}J_a.\end{aligned} \tag{4.8}$$

The structure constants are given, e.g., in Ref. 38 for particular choices of bases.

The first type of F-Lie algebra associated to $\mathfrak{g}$ will be called trivial and are constructed as follows:

Theorem IV.2: *Let $\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$ be a Lie superalgebra and let $F\geqslant 1$ be an integer. Then $S=\mathfrak{g}_0\oplus(\mathfrak{g}_1\oplus\mathbb{C})$ (with $\mathbb{C}$ the trivial representation of $\mathfrak{g}_0$) can be given the structure of an F-Lie algebra.*

Proof: The proof is analogous to the proof of Theorem III.7. Q.E.D.

The second type of F-Lie algebra associated to $\mathfrak{g}$ are those induced from $\mathfrak{g}$ and symmetric forms on $\mathfrak{g}_1$. Let $\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$ be one of the classical Lie superalgebras in the statement of Theorem IV.1 and let g be a $\mathfrak{g}_0$ invariant symmetric form of order m on $\mathfrak{g}_1$. The bracket of the associated F-Lie algebra of order $m+2$ in the above basis is given by (2.1):

$$\{F_{\alpha_1},\cdots,F_{\alpha_{m+2}}\}=\frac{1}{m!}\sum_{i<j}g_{\alpha_1\cdots\alpha_{i-1}\alpha_{i+1}\cdots\alpha_{j-1}\alpha_{j+1}\cdots\alpha_{m+2}}E_{\alpha_i\alpha_j}. \tag{4.9}$$

Example IV.3: We denote by S the F-Lie algebra of order 4 induced from the Lie superalgebra

$$A(m-1,n-1)=(\mathfrak{sl}(m)\oplus\mathfrak{sl}(n)\oplus\mathfrak{gl}(1))\oplus(\mathbb{C}^m\otimes\mathbb{C}^{n\star}\otimes\mathbb{C})\oplus(\mathbb{C}^m\otimes\mathbb{C}^{n\star}\otimes\mathbb{C})^\star,$$

and the tautological quadratic form on $(\mathbb{C}^m\otimes\mathbb{C}^{n\star}\otimes\mathbb{C})\oplus(\mathbb{C}^m\otimes\mathbb{C}^{n\star}\otimes\mathbb{C})^\star$. Let $\{E_{IJ}\}_{1\leqslant J\leqslant m}^{1\leqslant I\leqslant m}$ and $\{E_{IJ}\}_{m+1\leqslant J\leqslant m+n}^{m+1\leqslant I\leqslant m+n}$ be the standard bases of $\mathfrak{gl}(m)$ and $\mathfrak{gl}(n)$, respectively. Let $\{F_{IJ}\}_{m+1\leqslant J\leqslant m+n}^{1\leqslant I\leqslant m}$ and $\{F_{IJ}\}_{1\leqslant J\leqslant m}^{m+1\leqslant I\leqslant m+n}$ be bases of $(\overline{\mathbf{m}},\mathbf{n})^+$ and $(\mathbf{m},\overline{\mathbf{n}})^-$, respectively.

Then the four brackets of S have the following simple form:

$$\begin{aligned}\{F_{I_1J_1},F_{I_2J_2},F_{I_3J_3},F_{I_4J_4}\}=&\ \delta_{I_1I_2}\delta_{J_1J_2}(\delta_{I_3J_4}E_{J_3I_4}+\delta_{J_3I_4}E_{I_3J_4})+\delta_{I_1I_3}\delta_{J_1J_3}(\delta_{I_2J_4}E_{J_2I_4}+\delta_{J_2I_4}E_{I_2J_4})\\ &+\delta_{I_1I_4}\delta_{J_1J_4}(\delta_{I_2J_3}E_{J_2I_3}+\delta_{J_2I_3}E_{I_2J_3})+\delta_{I_2I_3}\delta_{J_2J_3}(\delta_{I_1J_4}E_{J_1I_4}\\ &+\delta_{J_1I_4}E_{I_1J_4})+\delta_{I_2I_4}\delta_{J_2J_4}(\delta_{I_1J_3}E_{J_1I_3}+\delta_{J_1I_3}E_{I_1J_3})\end{aligned}$$

$$+\delta_{I_3I_4}\delta_{J_3J_4}(\delta_{I_1J_2}E_{J_1I_2}+\delta_{J_1I_2}E_{I_1J_2}). \tag{4.10}$$

The fact that the rhs is in $\mathfrak{sl}(m)\oplus\mathfrak{sl}(n)\oplus\mathfrak{gl}(1)$ *is a consequence of Theorem II.6.*

Example IV.4: We denote by S the F-Lie algebra of order 4 *induced from the Lie superalgebra*

$$\mathfrak{osp}(2|2m)=(\mathfrak{so}(2)\oplus\mathfrak{sp}(2m))\oplus\mathbb{C}^2\otimes\mathbb{C}^{2m},$$

and the quadratic form $g=\varepsilon\otimes\Omega$, *where* ε *is the invariant symplectic form on* $\mathbb{C}^2$ *and* Ω *is the invariant symplectic form on* $\mathbb{C}^{2m}$. *Let* $\{S_{\alpha\beta}=S_{\beta\alpha}\}_{\substack{1\leqslant\alpha\leqslant 2m\\1\leqslant\beta\leqslant 2m}}$ *be a basis of* $\mathfrak{sp}(2m)$ *and* $\{h\}$ *be a basis of* $\mathfrak{so}(2)$. *Let* $\{F_{q\alpha}\}_{\substack{q=\pm 1\\1\leqslant\alpha\leqslant 2m}}$ *be a basis of* $\mathbb{C}^2\otimes\mathbb{C}^{2m}$. *Then the four brackets of S take the following form:*

$$\begin{aligned}\{F_{q_1\alpha_1},F_{q_2\alpha_2},F_{q_3\alpha_3},F_{q_4\alpha_4}\}=&\varepsilon_{q_1q_2}\Omega_{\alpha_1\alpha_2}(\delta_{q_3+q_4}S_{\alpha_3\alpha_4}+\varepsilon_{q_3+q_4}\Omega_{\alpha_3\alpha_4}h)\\&+\varepsilon_{q_1q_3}\Omega_{\alpha_1\alpha_3}(\delta_{q_2+q_4}S_{\alpha_2\alpha_4}+\varepsilon_{q_2+q_4}\Omega_{\alpha_2\alpha_4}h)\\&+\varepsilon_{q_1q_4}\Omega_{\alpha_1\alpha_4}(\delta_{q_2+q_3}S_{\alpha_2\alpha_3}+\varepsilon_{q_2+q_3}\Omega_{\alpha_2\alpha_3}h)\\&+\varepsilon_{q_2q_3}\Omega_{\alpha_2\alpha_3}(\delta_{q_1+q_4}S_{\alpha_1\alpha_4}+\varepsilon_{q_1+q_4}\Omega_{\alpha_1\alpha_4}h)\\&+\varepsilon_{q_2q_4}\Omega_{\alpha_2\alpha_4}(\delta_{q_1+q_3}S_{\alpha_1\alpha_3}+\varepsilon_{q_1+q_3}\Omega_{\alpha_1\alpha_3}h)\\&+\varepsilon_{q_3q_4}\Omega_{\alpha_3\alpha_4}(\delta_{q_1+q_2}S_{\alpha_1\alpha_2}+\varepsilon_{q_1+q_2}\Omega_{\alpha_1\alpha_2}h).\end{aligned} \tag{4.11}$$

Other extensions of Lie superalgebras have been considered in the literature. For instance, extensions of the orthosymplectic superalgebra $\mathfrak{osp}(1|4)$ or the unitary $\mathfrak{sl}(4|1)$ were constructed by means of parafermions and parabosons.[40] The first example of an F-Lie algebra was considered in Refs. 20 and 21 as a possible extension of the Virasoro algebra. In Ref. 36 an example of a ''trivial'' F-Lie algebra, related to the superalgebra $\mathfrak{osp}(1|2)$, was constructed.

Remark IV.5: By repeated application of Theorem II.6 one can construct F-Lie algebras of higher and higher order.

V. FINITE-DIMENSIONAL FSUSY EXTENSIONS OF THE POINCARÉ ALGEBRA

It is well known that supersymmetric extensions of the Poincaré algebra can be obtained by Inönü–Wigner contraction of certain Lie superalgebras. In fact, one can also obtain FSUSY extensions of the Poincaré algebra by Inönü–Wigner contraction of certain F-Lie algebras as we now show with two examples.

For the first example, we let $S_3=\mathfrak{sp}(4)\oplus\mathrm{ad}\mathfrak{sp}(4)$ be the real F-Lie algebra of order 3 (see Remark III.9) induced from the real graded 1-Lie algebra $S_1=\mathfrak{sp}(4)\oplus\mathrm{ad}\mathfrak{sp}(4)$ (see Example III.2) and the Killing form on $\mathrm{ad}\mathfrak{s}p(4)$. Using vector indices of $\mathfrak{so}(1,3)$ coming from the inclusion $\mathfrak{so}(1,3)\subset\mathfrak{so}(2,3)\cong\mathfrak{sp}(4)$, the bosonic part of S_3 is generated by $M_{\mu\nu},M_{\mu 4}$, with $\mu,\nu=0,1,2,3$, and the graded part by $J_{\mu\nu},J_{4\mu}$. Letting $\lambda\to 0$ after the Inönü–Wigner contraction,

$$\begin{aligned}&M_{\mu\nu}\to L_{\mu\nu},\quad M_{\mu 4}\to\frac{1}{\lambda}P_\mu\\&J_{\mu\nu}\to\frac{1}{\sqrt[3]{\lambda}}Q_{\mu\nu},\quad J_{4\mu}\to\frac{1}{\sqrt[3]{\lambda}}Q_\mu,\end{aligned} \tag{5.1}$$

one sees that $L_{\mu\nu}$ and P_μ generate the $(1+3)D$ Poincaré algebra and that $Q_{\mu\nu},Q_\mu$ are the fractional supercharges in respectively the adjoint and vector representations of $\mathfrak{so}(1,3)$. This F-Lie algebra of order 3 is therefore a nontrivial extension of the Poincaré algebra where trans-

lations are cubes of more fundamental generators. The subspace generated by $L_{\mu\nu}, P_\mu, Q_\mu$ is also an F-Lie algebra of order 3 extending the Poincaré algebra in which the trilinear symmetric brackets have the simple form

$$\{Q_\mu, Q_\nu, Q_\rho\} = \eta_{\mu\nu} P_\rho + \eta_{\mu\rho} P_\nu + \eta_{\rho\nu} P_\mu, \tag{5.2}$$

where $\eta_{\mu\nu}$ is the Minkowski metric. This algebra should be compared to the algebra recently obtained in a different context, where a ''trilinear'' extension of the Poincaré algebra involving ''supercharges'' in the vector representation was constructed.[41]

For the second example, we let $S_4 = (\mathfrak{so}(2) \oplus \mathfrak{sp}(4)) \oplus \underline{\mathbf{2}} \otimes \underline{\mathbf{4}}$ be the real F-Lie algebra of order four induced from $\mathfrak{osp}(2|4)$ and the symmetric form $\varepsilon \otimes \Omega$, where Ω is the symplectic form on $\mathbf{4}$ and ε the antisymmetric two-form on $\underline{\mathbf{2}}$. Using spinor indices coming from $\mathfrak{sl}(2,\mathbb{C}) \cong \mathfrak{so}(1,3) \subset \mathfrak{so}(2,3)$ the bosonic part is generated by $E_{\alpha\beta}, E_{\dot\alpha\dot\beta}, E_{\dot\alpha\beta}$ and the fermionic part by $F^{\pm}_{\alpha}, \overline{F}^{\pm}_{\dot\alpha}, \alpha, \beta = 1,2$ and $\dot\alpha, \dot\beta = \dot1, \dot2$. Letting $\lambda \to 0$ after the Inönü–Wigner contraction

$$E_{\alpha\beta} \to L_{\alpha\beta}, \quad E_{\dot\alpha\dot\beta} \to L_{\dot\alpha\dot\beta}, \quad E_{\alpha\dot\alpha} \to \frac{1}{\lambda} P_{\alpha\dot\alpha}, \quad h \to \frac{1}{\lambda} Z, \quad F^{\pm}_{\alpha} \to \frac{1}{\sqrt[4]{\lambda}} Q^{\pm}_{\alpha}, \quad \overline{F}^{\pm}_{\dot\alpha} \to \frac{1}{\sqrt[4]{\lambda}} \overline{Q}^{\pm}_{\dot\alpha}, \tag{5.3}$$

one sees that $L_{\alpha\beta}, L_{\dot\alpha\dot\beta}$ and $P_{\alpha\dot\alpha}$ generate the $(1+3)D$ Poincaré algebra, that Z is central and that $Q^{\pm}_{\alpha}, \overline{Q}^{\pm}_{\dot\alpha}$ are the fractional supercharges in the spinor representations of $\mathfrak{so}(1,3)$. This F-Lie algebra of order 4 is therefore a nontrivial extension of the Poincaré algebra where translations are fourth powers of more fundamental generators. The four bracket can be expressed simply if we introduce the following notation: $\sigma^{\mu}_{\alpha\dot\alpha}, \overline{\sigma}^{\mu\dot\alpha\alpha}$ are the Dirac matrices, and $\sigma^{\mu\nu}_{\alpha\beta}$, $\overline{\sigma}^{\mu\nu}_{\dot\alpha\dot\beta}$ and P_μ are the Poincaré generators (for details, e.g., Ref. 42). One then has

$$\begin{aligned}
\{Q^{q_1}_{\alpha_1}, Q^{q_2}_{\alpha_2}, Q^{q_3}_{\alpha_3}, Q^{q_4}_{\alpha_4}\} &= 2\varepsilon^{q_1q_2}\varepsilon^{q_3q_4}\varepsilon_{\alpha_1\alpha_2}\varepsilon_{\alpha_3\alpha_4} Z + 2\varepsilon^{q_1q_4}\varepsilon^{q_2q_3}\varepsilon_{\alpha_1\alpha_4}\varepsilon_{\alpha_2\alpha_3} Z \\
&\quad + 2\varepsilon^{q_1q_3}\varepsilon^{q_2q_4}\varepsilon_{\alpha_1\alpha_3}\varepsilon_{\alpha_2\alpha_4} Z, \\
\{Q^{q_1}_{\alpha_1}, Q^{q_2}_{\alpha_2}, Q^{q_3}_{\alpha_3}, \overline{Q}^{q_4}_{\dot\alpha_4}\} &= \delta^{q_1+q_4}\varepsilon^{q_2q_3}\varepsilon_{\alpha_2\alpha_3}\sigma^{\mu}_{\alpha_1\dot\alpha_4} P_\mu + \delta^{q_2+q_4}\varepsilon^{q_1q_3}\varepsilon_{\alpha_1\alpha_3}\sigma^{\mu}_{\alpha_2\dot\alpha_4} P_\mu \\
&\quad + \delta^{q_3+q_4}\varepsilon^{q_1q_2}\varepsilon_{\alpha_1\alpha_2}\sigma^{\mu}_{\alpha_3\dot\alpha_4} P_\mu, \\
\{Q^{q_1}_{\alpha_1}, Q^{q_2}_{\alpha_2}, \overline{Q}^{q_3}_{\dot\alpha_3}, \overline{Q}^{q_4}_{\dot\alpha_4}\} &= 0,
\end{aligned} \tag{5.4}$$

together with similar relations involving $\{Q^{q_1}_{\alpha_1}, \overline{Q}^{q_2}_{\dot\alpha_2}, \overline{Q}^{q_3}_{\dot\alpha_3}, \overline{Q}^{q_4}_{\dot\alpha_4}\}$ and $\{\overline{Q}^{q_1}_{\dot\alpha_1}, \overline{Q}^{q_2}_{\dot\alpha_2}, \overline{Q}^{q_3}_{\dot\alpha_3}, \overline{Q}^{q_4}_{\dot\alpha_4}\}$.

Analogous constructions lead to FSUSY extensions of the Poincaré algebra in any space–time dimensions.

VI. SIMPLE *F*-LIE ALGEBRAS

By analogy with the case of Lie (super)algebras we define ideals and the notion of simplicity for F-Lie algebras.

Definition VI.1: Let $S = \mathcal{B} \oplus \mathcal{F}$ be an F-Lie algebra, or a graded 1-Lie algebra. Then $\mathcal{I} = \mathcal{B}' \oplus \mathcal{F}'$ is an ideal of S if and only if

(i) $\forall f'_1 \in \mathcal{F}', \forall f_2, \ldots, f_F \in \mathcal{F}: \{f'_1, f_2, \ldots, f_F\} \in \mathcal{B}'$.
(ii) $\mathcal{B}'$ *is an ideal of* $\mathcal{B}$ $(\forall b' \in \mathcal{B}', \forall b \in \mathcal{B}, [b, b'] \in \mathcal{B}')$.
(iii) $\forall b \in \mathcal{B}, \forall f' \in \mathcal{F}' [b, f'] \in \mathcal{F}'$.
(iv) $\forall b' \in \mathcal{B}', \forall f \in \mathcal{F} [b', f] \in \mathcal{F}'$.

Remark VI.2: For a graded 1*-Lie algebra* $S=\mathcal{B}\oplus\mathcal{F}$*, denoting* μ *the map from* $\mathcal{F}$ *to* $\mathcal{B}$*, the property (i) of Theorem VI.1 becomes* $\mathrm{Im}\,\mu\subset\mathcal{B}'$.

Remark VI.3: By Theorem VI.1, $\mathrm{Im}\,\mu\oplus\mathcal{F}$ *is an ideal of* S *[*μ *denotes the* $\mathcal{B}$*-equivariant map from* $\mathcal{S}^F(\mathcal{F})\to\mathcal{B}$*].*

Remark VI.4: In the case of Lie algebras and Lie superalgebras, this is the usual definition. In the case of a graded 1*-Lie algebra* $S=\mathcal{B}\oplus\mathcal{F}$*,* $S'=\mathcal{B}'\oplus\mathcal{F}'$ *is an ideal if and only if it is a* $\mathbb{Z}_2$*-graded ideal for the natural Lie bracket on* S (*cf. Remark III.3*).

Definition VI.5: An F*-Lie algebra* S *is said to be simple if and only if its only ideals are* S *and* $\{0\}$*, and* $\mu:\mathcal{S}^F(\mathcal{F})\to\mathcal{B}$ *is nonzero.*

Remark VI.6: Let $S=\mathcal{B}\oplus\mathcal{F}$ *be a graded* 1*-Lie algebra such that* $\mu:\mathcal{F}\to\mathcal{B}$ *is nonzero. Then,* S *is simple if and only if* $\mathcal{B}$ *is a simple Lie algebra and* $\mathcal{F}$ *is an irreducible representation of* $\mathcal{B}$*.*

Remark VI.7: If $\mathfrak{g}$ *is a simple Lie algebra, and* $S=\mathfrak{g}\oplus\mathrm{ad}\mathfrak{g}$ *is the graded* 1*-Lie algebra of Example III.2, then* S *is simple as a graded* 1*-Lie algebra but is not simple as a Lie algebra, with respect to the natural Lie bracket III.3.*

Proposition VI.8: Let $S=\mathcal{B}\oplus\mathcal{F}$ *be an* F*-Lie algebra such that (i)* $\mathcal{B}$ *is semi-simple, (ii) the map* $\mu:\mathcal{S}^F(\mathcal{F})\to\mathcal{B}$ *is a surjection and (iii) no nonzero ideal of* $\mathcal{B}$ *has nonzero fixed points in* $\mathcal{F}$*. Then*

(a) S *is simple and*
(b) the F*-Lie algebra of order* $(F+2)$ *induced from a* $\mathcal{B}$*-equivariant nondegenerate quadratic form on* $\mathcal{F}$ *(see II.6–III.6) also satisfies (i) and (ii).*

Proof: Let $\mathfrak{I}=\mathcal{B}'\oplus\mathcal{F}'$ be a nontrivial ideal of S. Then $\mathcal{B}'$ is an ideal of $\mathcal{B}$ and $[\mathcal{B}',\mathcal{F}]\subset\mathcal{F}'$. But if $\mathcal{F}=\mathcal{F}'\oplus\mathcal{F}''$ as $\mathcal{B}'$-modules, then $[\mathcal{B}',\mathcal{F}'']=0$, and, therefore, $\mathcal{F}''=\{0\}$ since by hypothesis $\mathcal{B}'$ does not admit nonzero fixed points. This proves (a).
To prove (b) it is enough to prove that the induced $(F+2)$-bracket is surjective. Since the F-bracket $\mu:\mathcal{S}^F(\mathcal{F})\to\mathcal{B}$ is surjective, by diagonalizing the quadratic form, it is easy to see that the $(F+2)$-bracket (2.1) is also surjective. Q.E.D.

Remark VI.9: If $\mathfrak{g}$ *is a simple Lie algebra, the graded* 1*-Lie algebras* $\mathfrak{g}\oplus\mathrm{ad}\mathfrak{g}$ *satisfies (i), (ii) and (iii) above. As one can check, the Lie superalgebras in the list IV.1 also satisfy (i), (ii) and (iii). Thus the induced* F*-Lie algebras associated to nondegenerate quadratic forms and these graded* 1*-Lie algebras or Lie superalgebras are always simple.*

The trivial F-Lie algebras associated to graded 1-Lie algebras or Lie superalgebras III.7–IV.2 are not simple since in both cases $\mathfrak{g}_0\oplus\mathfrak{g}_1$ is an ideal of S. In particular, when $F=2$, the trivial Lie superalgebras associated to graded 1-Lie algebras are not simple. The direct sum of two simple F-Lie algebras of the same order is clearly not simple. These two kinds of examples of nonsimple F-Lie algebras indicate that probably, as for Lie superalgebras, there are different inequivalent ways to define semi-simple F-Lie algebras.

VII. REPRESENTATIONS

Definition VII.1: A representation of an F*-Lie algebra* S *is a linear map* $\rho:S\to\mathrm{End}(H)$ *and an automorphism* $\hat{\varepsilon}$ *such that* $\hat{\varepsilon}^F=1$ *which satisfy*

$$\rho([x,y])=\rho(x)\rho(y)-\rho(y)\rho(x), \tag{7.1a}$$

$$\rho\{a_1,\ldots,a_F\}=\Sigma_{\sigma\in S_F}\rho(a_{\sigma(1)})\ldots\rho(a_{\sigma(F)}), \tag{7.1b}$$

$$\hat{\varepsilon}\rho(s)\hat{\varepsilon}^{-1}=\rho(\varepsilon(s)) \tag{7.1c}$$

(S_F *being the group of permutations of* F *elements).*

As a consequence of these properties, since the eigenvalues of $\hat{\varepsilon}$ are Fth roots of unity, we have the following decomposition,

$$H=\bigoplus_{k=0}^{F-1} H_k,$$

where $H_k=\{|h\rangle\in H:\hat{\varepsilon}|h\rangle=q^k|h\rangle\}$. The operator $N\in\mathrm{End}(H)$ defined by $N|h\rangle=k|h\rangle$ if $|h\rangle\in H_k$ is the "number operator" (obviously $q^N=\hat{\varepsilon}$). Since $\hat{\varepsilon}\rho(b)=\rho(b)\hat{\varepsilon},\forall b\in\mathcal{B}$ each H_k provides a representation of the Lie algebra $\mathcal{B}$. Furthermore, for $a\in\mathcal{A}_{\not}$, $\hat{\varepsilon}\rho(a)=q^{\not}\rho(a)\hat{\varepsilon}$, and so we have $\rho(a).H_k\subseteq H_{k+\not(\mathrm{mod}\ F)}$.

Example VII.2: Let X,Y,Z be $n\times n$ (resp. $2n\times 2n$) matrices in $\mathfrak{so}(n)$ [resp. $\mathfrak{sp}(2n)$]. Then, it is easy to see that $\{X,Y,Z\}$ is also in $\mathfrak{so}(n)$ [resp. $\mathfrak{sp}(2n)$]. Consequently, $S=\mathfrak{so}(n)\oplus\mathfrak{so}(n)$ [resp. $S=\mathfrak{sp}(2n)\oplus\mathfrak{sp}(2n)$] is an F-Lie algebra of order 3 [the only nontrivial point to be checked is the Jacobi identity (J4) in Definition II.1]. A similar property is true for any odd number of matrices. We will calculate the structure constants in the case of $\mathfrak{so}(n)$, the calculation for $\mathfrak{sp}(2n)$ being analogous. If X_a, $1\leqslant a\leqslant\dim\ \mathfrak{so}(n)$, is a basis of $\mathfrak{so}(n)$, then the three-bracket of S is given by

$$\{X_a,X_b,X_c\}=k_{abc}^{d}X_d. \tag{7.2}$$

Writing $\{X_a,X_b,X_c,X_d\}=(\{X_a,X_b,X_c\}X_d+\{X_a,X_b,X_d\}X_c+\{X_a,X_c,X_d\}X_b+\{X_b,X_c,X_d\}X_a)$ and taking the trace using (7.2), we get $4k_{abc}{}^{d}tr(X_dX_e)=\mathrm{Tr}(\{X_a,X_b,X_c,X_e\})$. Since the trace defines a metric on $\mathfrak{so}(n)$ this gives $k_{abc}{}^{d}=\frac{1}{4}\mathrm{Tr}\{X_a,X_b,X_c,X_d\}g^{de}$.

This F-Lie algebra of order 3 is not induced from the graded 1-Lie algebra $\mathfrak{so}(n)\oplus\mathfrak{so}(n)$ and the Killing form: if this were the case we would have $\{X_a,X_b,X_c\}=\mathrm{Tr}(X_aX_b)X_c+\mathrm{Tr}(X_aX_c)X_b+\mathrm{Tr}(X_bX_c)X_a$, which is clearly false if $a=b=c$. However, by Proposition VI.8, S is simple.

We can construct a representation of S in $\mathbb{C}^n\otimes\mathbb{C}^3$ as follows: define $\rho:S\to\mathrm{End}(\mathbb{C}^n\otimes\mathbb{C}^3)$ by

$$\rho(X)=\begin{cases}X\otimes\mathbf{Id} & \text{if } X \text{ is in the first } \mathfrak{so}(n),\\ X\otimes Q & \text{if } X \text{ is in the second } \mathfrak{so}(n),\end{cases} \tag{7.3}$$

where $Q:\mathbb{C}^3\to\mathbb{C}^3$ is any linear map whose minimal polynomial is λ^3-1 (i.e., $Q^3=\mathbf{Id}$ and Q has three distinct eigenvalues).

Related results were obtained for $\mathfrak{so}(n)$ and $\mathfrak{sp}(2n)$ in Ref. 43.

Example VII.3: Let X,Y,Z be three $n\times n$ matrices in $\mathfrak{u}(n)$. Then, it is easy to see that $\{X,Y,Z\}$ is also in $\mathfrak{u}(n)$. As in the previous example, this simple observation enables us to give $\mathfrak{u}(n)\oplus\mathfrak{u}(n)$ or $\mathfrak{u}(n)\oplus\mathfrak{su}(n)$ the structure of an F-Lie algebra of order 3.

Example VII.4: Let $A(m-1,n-1)$, $n\neq m$, be the Lie superalgebra of $(n+m)\times(n+m)$ matrices,[3,38]

$$M=\begin{pmatrix}E_{mm} & F_{mn}\\ F_{nm} & E_{nn}\end{pmatrix},$$

of supertrace zero (i.e., $\mathrm{sTr}M=\mathrm{tr}E_{mm}-\mathrm{tr}E_{nn}=0$).

If $J_{i_1},\ldots,J_{i_{2F}}$ are arbitrary matrices, then

$$\{J_{i_1},\ldots,J_{i_{2F}}\}=\sum_{\substack{a<b=1\\ a\neq b}}^{F}\{\{J_{i_a},J_{i_b}\},\{\hat{J}_{i_a},\hat{J}_{i_b},J_{i_1},\ldots,J_{i_{2F}}\}\}. \tag{7.4}$$

Applying this formula to $2F$ odd matrices in $A(m-1,n-1)$, one sees by an induction that the supertrace of the $2F$-bracket (7.4) vanishes. Using the $\mathbb{Z}_2$ graduation of $A(m-1,n-1)$ one sees that this bracket belongs to the even part of the algebra and hence defines the structure of an F-Lie algebra of order $2F$ on the underlying vector space of $A(m-1,n-1)$. For $F=4$ this is just the F-Lie algebra of order 4 induced by the tautological quadratic form of Example IV.3. Indeed, let $V=\mathbb{C}^{\star n}\otimes\mathbb{C}^m\otimes\mathbb{C}$ and let $\mathfrak{g}_0=\mathfrak{sl}(n)\oplus\mathfrak{sl}(m)\oplus\mathfrak{gl}(1)$. Then, comparing $\mathfrak{gl}(1)$ charges, we have $\mathrm{Hom}_{\mathfrak{g}_0}(\mathcal{S}^4(V\oplus V^\star),\mathfrak{g}_0)=\mathrm{Hom}_{\mathfrak{g}_0}(\mathcal{S}^2(V)\otimes\mathcal{S}^2(V^\star),\mathfrak{g}_0)$. Since

$$\mathcal{S}^2(V)\otimes\mathcal{S}^2(V^\star)\cong(\mathcal{S}^2(\mathbb{C}^{\star n})\otimes\mathcal{S}^2(\mathbb{C}^m)\oplus\Lambda^2(\mathbb{C}^{\star n})\otimes\Lambda^2(\mathbb{C}^m))\otimes(\mathcal{S}^2(\mathbb{C}^n)\otimes\mathcal{S}^2(\mathbb{C}^{\star m})\oplus\Lambda^2(\mathbb{C}^n)\otimes\Lambda^2(\mathbb{C}^{\star m}))$$

and since the representations **1** *and* $\mathfrak{sl}(n)$ *occur exactly once in* $\mathcal{S}^2(\mathbb{C}^n)\otimes\mathcal{S}^2(\mathbb{C}^{\star n})$ *and not at all in* $\Lambda^2(\mathbb{C}^n)\otimes\Lambda^2(\mathbb{C}^{\star n})$, *we deduce that* $\mathrm{Hom}_{\mathfrak{g}_0}(\mathcal{S}^4(V\oplus V^\star),\mathfrak{g}_0)$ *is of dimension one.*

By definition, the fundamental $(n+m)\times(n+m)$ *matrix representation of the Lie superalgebra* $A(m-1,n-1)$ *is also a representation of the* F*-Lie algebra of order* $2F$ *constructed above. In general, this is not true: for instance, if* $m=2,n=1$, *one can check that the six-dimensional representation of* $A(2,1)$ *is not a representation of the associated* F*-Lie algebra of order* 4.

Example VII.5: Let S *be the set of all matrices of the form*

$$M=\begin{pmatrix} q & 0 & F_+ \\ 0 & -q & F_- \\ -\Omega F_-^t & -i\Omega F_+^t & S \end{pmatrix}, \tag{7.5}$$

where q *is a complex number,* $F_\pm$ *are two* $1\times 2n$ *matrices,* Ω *is the standard* $2n\times 2n$ *symplectic form on* $\mathbb{C}^{2n}$ *and* S *is a* $2n\times 2n$ *matrix in* $\mathfrak{sp}(2n)$, *i.e.,* $S^t=\Omega S\Omega$. *Let*

$$\mathcal{B}=\left\{\begin{pmatrix} q & 0 & 0 \\ 0 & -q & 0 \\ 0 & 0 & S \end{pmatrix}, q\in\mathbb{C}, S\in\mathfrak{sp}(2n)\right\}\cong\mathfrak{so}(2)\oplus\mathfrak{sp}(2n)$$

and let

$$\mathcal{F}=\left\{\begin{pmatrix} 0 & 0 & F_+ \\ 0 & 0 & F_- \\ -\Omega F_-^t & -i\Omega F_+^t & 0 \end{pmatrix}, F_\pm\in\mathcal{M}_{1,2n}(\mathbb{C})\right\}.$$

If one now takes

$$\mathcal{F}_{a+}=\begin{pmatrix} 0 & 0 & F_{a+} \\ 0 & 0 & 0 \\ 0 & -i\Omega F_{a+}^t & 0 \end{pmatrix}, \mathcal{F}_{a-}=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & F_{a-} \\ -\Omega F_{a-}^t & 0 & 0 \end{pmatrix},$$

and $\mathcal{F}_a=\mathcal{F}_{a+}+\mathcal{F}_{a-}$, *we get*

$$\{\mathcal{F}_a,\mathcal{F}_b\}=\begin{pmatrix} \alpha_{ab} & 0 & 0 \\ 0 & -i\alpha_{ab} & 0 \\ 0 & 0 & A_{ab} \end{pmatrix},$$

where $A_{ab}=-\Omega F_{a-}^t F_{b+}-i\Omega F_{a+}^t F_{b-}-\Omega F_{b-}^t F_{a+}-i\Omega F_{b+}^t F_{a-}$ *and where* $\alpha_{ab}=-F_{a+}\Omega F_{b-}^t-F_{b+}\Omega F_{a-}^t$. *This shows that* $\mathcal{B}\oplus\mathcal{F}$ *is not closed under the superbracket. From the formula* $\{\mathcal{F}_{a_1},\mathcal{F}_{a_2},\mathcal{F}_{a_3},\mathcal{F}_{a_4}\}=\{\{\mathcal{F}_{a_1},\mathcal{F}_{a_2}\},\{\mathcal{F}_{a_3},\mathcal{F}_{a_4}\}\}+\{\{\mathcal{F}_{a_1},\mathcal{F}_{a_3}\},\{\mathcal{F}_{a_2},\mathcal{F}_{a_4}\}\}+\{\{\mathcal{F}_{a_1},\mathcal{F}_{a_4}\},\{\mathcal{F}_{a_2},\mathcal{F}_{a_3}\}\}$, *observing that* $\{\mathcal{F}_{a+},\mathcal{F}_{b+}\}=\{\mathcal{F}_{a-},\mathcal{F}_{b-}\}=0$, *the four-bracket* $\{\mathcal{F}_{a_1q_1},\mathcal{F}_{a_2q_2},\mathcal{F}_{a_3q_3},\mathcal{F}_{a_4q_4}\}=0$ *if* $q_1+q_2+q_3+q_4\neq 0$. *We then calculate four-brackets for* $q_1=q_2=-q_3=-q_4=1$ *and obtain*

$$\{\mathcal{F}_{a+},\mathcal{F}_{b+},\mathcal{F}_{c-},\mathcal{F}_{d-}\}=\begin{pmatrix} q & 0 & 0 \\ 0 & -q & 0 \\ 0 & 0 & S \end{pmatrix},$$

$$q=2(F_{a+}\Omega F_{c-}^t)(F_{b+}\Omega F_{d-}^t)+2(F_{a+}\Omega F_{d-}^t)(F_{b+}\Omega F_{c-}^t) \tag{7.6}$$

$$\begin{aligned}S=&F_{a+}\Omega F_{d-}^t(\Omega F_{c-}^t F_{b+}+\Omega F_{b+}^t F_{c-})+F_{a+}\Omega F_{c-}^t(\Omega F_{d-}^t F_{b+}+\Omega F_{b+}^t F_{d-})\\&+F_{b+}\Omega F_{d-}^t(\Omega F_{c-}^t F_{a+}+\Omega F_{a+}^t F_{c-})+F_{b+}\Omega F_{c-}^t(\Omega F_{d-}^t F_{a+}+\Omega F_{a+}^t F_{d-}).\end{aligned}$$

This shows that $\mathcal{B}\oplus\mathcal{F}$ is an F-Lie algebra of order 4 since $S^t=\Omega S\Omega$.

In fact, the matrices of $\mathcal{B}\oplus\mathcal{F}$ define a representation of the F-Lie algebra of order 4 induced from $\mathfrak{osp}(2|2m)$ and $\varepsilon\otimes\Omega$ (see Example IV.4). Indeed, setting

$$\overline{\mathcal{F}}_{a+}=\begin{pmatrix}0&0&F_{a+}\\0&0&0\\0&-\Omega F_{a+}^t&0\end{pmatrix},\overline{\mathcal{F}}_{a-}=\begin{pmatrix}0&0&0\\0&0&F_{a-}\\-\Omega F_{a-}^t&0&0\end{pmatrix},$$

we see that $\mathcal{B}\oplus\overline{\mathcal{F}}\cong\mathfrak{osp}(2|2m)$ and that $\{\mathcal{F}_{a+},\mathcal{F}_{b+},\mathcal{F}_{c-},\mathcal{F}_{d-}\}=\langle\overline{\mathcal{F}}_{a+},\overline{\mathcal{F}}_{c-}\rangle\{\overline{\mathcal{F}}_{b+},\overline{\mathcal{F}}_{d-}\}+\langle\overline{\mathcal{F}}_{b+},\overline{\mathcal{F}}_{d-}\rangle\{\overline{\mathcal{F}}_{a+},\overline{\mathcal{F}}_{c-}\}+\langle\overline{\mathcal{F}}_{a+},\overline{\mathcal{F}}_{d-}\rangle\{\overline{\mathcal{F}}_{b+},\overline{\mathcal{F}}_{c-}\}+\langle\overline{\mathcal{F}}_{b+},\overline{\mathcal{F}}_{c-}\rangle\{\overline{\mathcal{F}}_{a+},\overline{\mathcal{F}}_{d-}\}$ where $\langle\overline{\mathcal{F}}_{a+},\overline{\mathcal{F}}_{c-}\rangle$ denotes the $\varepsilon\otimes\Omega$ invariant form.

Given an F-Lie algebra $S=\mathcal{B}\oplus\mathcal{F}$ one can define the universal enveloping algebra $\mathcal{U}(S)$ by taking the quotient of the tensor algebra $\mathcal{T}(S)$ by the two-sided ideal generated by (see Definition II.1)

$$\begin{gathered}\Sigma_{\sigma\in\Sigma_F}a_{\sigma(1)}\otimes\cdots\otimes a_{\sigma(F)}-\{a_1,\ldots,a_F\},\\b_1\otimes b_2-b_2\otimes b_1-[b_1,b_2],\\b_1\otimes a_2-a_2\otimes b_1-[b_1,a_2],\end{gathered}\tag{7.7}$$

with $a_1,\ldots,a_F\in\mathcal{A}_1,b_1,b_2\in\mathcal{B}$. It is not necessary to impose the Jacobi identity (J4) since it is true in $\mathcal{T}(S)$.

The natural filtration of $\mathcal{T}(S)$ factors to a filtration of $\mathcal{U}(S)$ and, denoting the associated graded algebra by $\mathrm{gr}(\mathcal{U}(S))$, we conjecture the following:

(1) $\mathrm{gr}(\mathcal{U}(S))$ is isomorphic to $\mathcal{T}(S)/\overline{I}$, where $\overline{I}$ is the two-sided ideal generated by

$$\begin{gathered}\Sigma_{\sigma\in\Sigma_F}a_{\sigma(1)}\otimes\cdots\otimes a_{\sigma(F)},\\b_1\otimes b_2-b_2\otimes b_1,\\b_1\otimes a_2-a_2\otimes b_1.\end{gathered}$$

[This would then imply that $\mathrm{gr}(\mathcal{U}(S))\cong S(\mathcal{B})\otimes\Lambda_F(\mathcal{F})$, where $S(\mathcal{B})$ is the symmetric algebra on $\mathcal{B}$ and $\Lambda_F(\mathcal{F})$ is the F-exterior algebra on $\mathcal{F}$.[44]]

(2) The natural map $\pi:\mathcal{U}(S)\to\mathrm{gr}(\mathcal{U}(S))$ is a linear isomorphism. (This would be an analog of the Poincaré–Birkhoff–Witt theorem.)

In the usual way, the representations of S are in bijective correspondence with the representations of the associative algebra $\mathcal{U}(S)$. Consequently, if $\mathcal{I}\subset\mathcal{U}(S)$ is a two-sided ideal, then the quotient $\mathcal{U}(S)/\mathcal{I}$ gives a representation of S. It would be very convenient to have a theory of "Cartan sub-algebras," "roots" and "weights" for S. However, even for simple Lie superalgebras this kind of theory only works well for basic Lie superalgebras.[38] One might expect F-Lie algebras induced from basic Lie superalgebras to be amenable to this approach. This seems not to be the case. Indeed, recall that if S is a basic Lie superalgebra with Borel decomposition $S=\mathfrak{h}\oplus\mathfrak{n}_+\oplus\mathfrak{n}_-$ and $\lambda\in\mathfrak{h}^\star$ is a dominant weight, then $\mathcal{V}_\lambda=\mathcal{U}/\mathcal{I}_\mu$ (where $\mathcal{I}_\lambda$ is the ideal corresponding to λ) is (i) generated by the action of $\mathfrak{n}_+$ on the vacuum and (ii) has a unique quotient $\mathcal{D}_\lambda$ on which the action of $\mathfrak{n}_+$ is nilpotent and which is therefore finite-dimensional. However, if S_g is the F-Lie

algebra induced from S and a symmetric form g, the quotient $\mathcal{V}'_\lambda = \mathcal{U}(S_g)/\mathcal{I}'_\lambda$ is (i) not generated by the action of $\mathfrak{n}_+$ on the vacuum and (ii) the nilpotence of the action of $\mathfrak{n}_+$ in a quotient does not guarantee finite-dimensionality. This means that in finite-dimensional representations of S, as in the examples of Sec. VII, the elements of $\mathfrak{n}_+$ are not only nilpotent but also satisfy additional relations.

VIII. CONCLUSION

The mathematical structure underlying supersymmetry is that of a Lie superalgebra. Given the classification of Lie superalgebras, one can list the possible supersymmetric extensions of the Poincaré algebra. These extensions have had a wide range of applications in physics.

Fractional supersymmetries were first studied in the early 1990s in relation with low dimensional physics ($D \leqslant 3$) where fields which are neither bosonic nor fermionic[34] do exist. It was understood a few years later that FSUSY can be considered in arbitrary dimensions and the definition of an F-Lie algebra, the underlying mathematical structure, was given.[24] However, when $F > 2$, most of the examples of F-Lie algebras which have been found since then are of infinite dimensions. In this article, we show how one can construct many finite-dimensional F-Lie algebras starting from Lie algebras or Lie superalgebras equipped with appropriate symmetric forms. We define a notion of simplicity in this context and show that some of our examples are simple. Furthermore, we construct the first finite-dimensional FSUSY extensions of the Poincaré algebra by Inönü–Wigner contraction of certain F-Lie algebras.

These results can be seen as a first step in classifying F-Lie algebras.

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Hamiltonian Feynman path integrals via the Chernoff formula

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The main aim of the present paper is using a Chernoff theorem (i.e., the Chernoff formula) to formulate and to prove some rigorous results on representations for solutions of Schrödinger equations by the Hamiltonian Feynman path integrals (=Feynman integrals over trajectories in the phase space). The corresponding theorem is related to the original (Feynman) approach to Feynman path integrals over trajectories in the phase space in much the same way as the famous theorem of Nelson is related to the Feynman approach to the Feynman path integral over trajectories in the configuration space. We also give a representation for solutions of some Schrödinger equations by a series which represents an integral with respect to the complex Poisson measure on trajectories in the phase space. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1500422]

I. INTRODUCTION

The Hamiltonian Feynman map (pseudomeasure) is a linear functional (its precise definition in our frame is given in the following) on a vector space of functionals whose common domain is a (vector) space of functions defined on a segment $[0,t]$, $t>0$ and taking values in the phase space $E=Q\times P$ of a classical Hamiltonian system. The value $\Phi(F)$ which the Feynman map Φ takes on a functional F is called the Hamiltonian Feynman path integral, or Feynman integral over trajectories in the phase space, of F; the number $\Phi(F)$ is often denoted by

$$\int F(q(\cdot),p(\cdot))\exp\left(i\int_0^t p(\tau)q'(\tau)\mathrm{d}\tau\right)\prod_0^t \mathrm{d}q(\tau)\mathrm{d}p(\tau)$$

and coincides with (can even be defined as) the limit of a suitable sequence of finite dimensional integrals of functions which are finite dimensional approximations for F. Such a definition can be traced back to Feynman himself;[1,2] there also exist some other definitions (see Refs. 3–8); in particular a definition of the Hamiltonian Feynman map by an analytical continuation of a Gaussian measure, which refutes a claim of Berezin,[9] was suggested in 1985[4,5] (see also Ref. 10).

If H is a classical Hamiltonian (i.e., a number valued function on the phase space) then one can show (under some additional assumptions) that the function

$$(t,z)\mapsto\int \exp\left(-i\int_0^t H(q(\tau)+z,p(\tau))d\tau+i\int_0^t p(\tau)q'(\tau)\mathrm{d}\tau\right)\phi_0(q(0)+z)\prod_0^t \mathrm{d}q(\tau)\mathrm{d}p(\tau)$$

gives a solution (in a proper space) to the Cauchy problem for the Schrödinger equation $i\phi'(t)$

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$=\hat{H}\phi(t)$, where $\hat{H}$ is a pseudodifferential operator (PDO) with the symbol (e.g., in the sense of Weyl) H. If $\hat{H}$ is a self-adjoint operator in a suitable domain then this formula gives an explicit representation of the one parameter unitary group $e^{-it\hat{H}}$, $t\in\mathbb{R}$.

The main aim of the present paper is to formulate and to prove some rigorous versions of these assertions using a Chernoff theorem[11] (i.e., the Chernoff formula). The corresponding Theorem 1 in the following is related to the original (Feynman) approach to Feynman path integrals over trajectories in the phase space in much the same way as the famous theorem from the paper (Ref. 12) of Nelson is related to the Feynman approach to the Feynman path integral over trajectories in the configuration space.

We give also a representation for solutions of some Schrödinger equations by a series which represents an integral with respect to the complex Poisson measure on trajectories in the phase space (Refs. 3–5; see also Refs. 13–16 for the case of configuration space). The corresponding result (in the proof of which we again use the Chernoff formula) is an improvement of a theorem from Ref. 3 (cf. Ref. 17).

Let E be a (real) vector space and for any $x\in E$ and any linear functional g on E let $\phi_g(x)=e^{ig(x)}$. If F_E is a locally convex space (LCS) of some complex valued functions on E, G is a vector space of some linear functionals on E distinguishing elements of E and, for any $g\in G$, $\phi_g\in F_E$ then the Fourier (G-)transform of any element $\eta\in F_E^*$ is the function on G which is denoted by $\tilde{\eta}$ or by $\mathcal{F}\eta$ and is defined by $\tilde{\eta}(g)(\equiv\mathcal{F}\eta(g))=\eta(\phi_g)$. If the set $\{\phi_g:g\in G\}$ is total in F_E (that means that the linear span of $\{\phi_g:g\in G\}$ is dense in F_E) then the element η (which can be called in this respect an F_E-distribution, or a distribution on E) is uniquely defined by its Fourier transform. In the following sometimes we do not define explicitly the space F_E and even drop the symbol F_E.

If b is a quadratic functional on E^*, $a\in E$ and $\alpha\in\mathbb{C}$ then the Feynman α-pseudomeasure on E, with the correlation functional b and mean value a, is the distribution $\Phi_{b,a,\alpha}$ on E whose Fourier transform is defined by

$$\mathcal{F}\Phi_{b,a,\alpha}(g)=\exp\left\{\frac{\alpha b(g)}{2}+ig(a)\right\}.$$

Let $E=Q\times P$, where Q and P are LCS, $Q=P^*$, $P=Q^*$ (as vector spaces); the space $G=P\times Q$ is identified with a space of linear functionals on E [for any $g=(p_g,q_g)\in G$ and $x=(q,p)\in E$ $g(x)=p_g(q)+p(q_g)$]. Then the Hamiltonian (or symplectic) Feynman pseudomeasure on E is any Feynman i-pseudomeasure on E with the correlational functional b defined by $b(p_g,q_g)=2p_g(q_g)$. The Hamiltonian Feynman pseudomeasure which we use in the following is a so-called sequential Feynman pseudomeasure.

The sequential Feynman pseudomeasure on E is defined as follows (now we only define what one can call a sequential Feynman pseudomeasure with the zero mean value but the general case is quite similar). Let $\{E_n:n\in\mathbb{N}\}$ be an increasing sequence of finite dimensional vector subspaces of $E(=Q\times P)$ such that, for any $n\in\mathbb{N}$, $E_n=Q_n\times P_n$, where Q_n and P_n are vector subspaces of Q and P, respectively. Then the value of the sequential Feynman pseudomeasure $\Phi_{\{E_n\}}$, associated with the sequence $\{E_n:n\in\mathbb{N}\}$, on a function $f:E\to\mathbb{C}$ [this value is called a sequential Feynman (path) integral of f] is defined by

$$\Phi_{\{E_n\}}(f)=\lim\left(\int_{E_n}e^{i\langle p,q\rangle}\mathrm{d}q\,\mathrm{d}p\right)^{-1}\int_{E_n}f(q,p)e^{i\langle p,q\rangle}\mathrm{d}q\,\mathrm{d}p$$

[where $\langle p,q\rangle=p(q)$] if this limit exists. So the fact that a function belongs to the domain of $\Phi_{\{E_n\}}$ depends only on its restrictions to E_n. In the preceding formula we used some regularized integrals whose definition is given in the following.

A locally integrable in the sense of Bochner function g on $\mathbb{R}^n$ taking values in a Banach space is called integrable if there exists the limit $\lim_{\epsilon\to 0}\int_{\mathbb{R}^n} g(s)e^{-\epsilon|s|^2}\mathrm{d}s$ $(\epsilon>0)$; then the integral $\int_{\mathbb{R}^n} g(s)\mathrm{d}s$ is defined by $\int_{\mathbb{R}^n} g(s)\mathrm{d}s=\lim_{\epsilon\to 0}\int_{\mathbb{R}^n} g(s)e^{-\epsilon|s|^2}\mathrm{d}s$, $\epsilon>0$.

If $f(\cdot,\cdot):\mathbb{R}^m\times\mathbb{R}^k\to\mathbb{C}$ is a measurable function then we define the integral $\int_{\mathbb{R}^k} f(q,u)\mathrm{d}u$ as follows. We assume that $\int_{\mathbb{R}^k} e^{-\epsilon|u|^2}|f(q,u)|\mathrm{d}u<\infty$ for almost all $q\in\mathbb{R}^m$ and for all $\epsilon>0$. We also assume that the function I_ϵ which is defined by $I_\epsilon(q)=\int_{\mathbb{R}^k} e^{-\epsilon|u|^2}f(q,u)\mathrm{d}u$ belongs to $L^2(\mathbb{R}^m)$ and I_ϵ converges in $L^2(\mathbb{R}^m)$ when $\epsilon\to 0$. Finally we put $\int_{\mathbb{R}^k} f(\cdot,u)\mathrm{d}u=\lim_{\epsilon\to 0} I_\epsilon(\cdot)$, where the limit is taken in $L^2(\mathbb{R}^m)$.

One could also define $\int g(s)\mathrm{d}s$ to be equal to the limit $\lim_{\epsilon\to 0}\int g(s)\phi(\epsilon s)\mathrm{d}s$ where $\phi\in\mathcal{D}(\mathbb{R}^n)$, $\phi(0)=1$ if this limit exists for any such ϕ (then it does not depend on the choice of ϕ). We have chosen the above-formulated more restricted definition for the sake of simplicity.

In what follows the spaces Q and P will be spaces of some functions defined on subsets of the real line and taking values in finite dimensional vector spaces (in applications they are configuration and momentum spaces of some Hamiltonian systems).

Namely for any Banach space T and any $a>0$ let $C_g([0,a],T)$ be the vector space of all functions on $[0,a]$ taking values in T whose distributional derivatives are measures with finite supports and let $C_g^0([0,a],T)$ (respectively, $C_g^1([0,a],T)$) denote the vector space of all right continuous (respectively, left continuous) functions from $C_g([0,a],T)$. For any $\tau\in(0,1)$ let $C_g^\tau([0,a],T)$ be the collection of functions f having the form $f=(1-\tau)g_f^0+\tau g_f^1$, where $g_f^0\in C_g^0([0,a],T)$, $g_f^1\in C_g^1([0,a],T)$ and distributional derivatives of g_f^0 and g_f^1 coincide.

Let $\mathcal{Q}$, $\mathcal{P}$ be finite dimensional Euclidean spaces and for any $t>0$, $\tau\in[0,1]$ let Q_t be the image of $C_g^0([0,t],\mathcal{Q})$ in $L_2([0,t],\mathcal{Q})$, $P_t^\tau=C_p^\tau([0,t],\mathcal{P})$, $E_t^\tau=Q_t\times P_t^\tau$. The spaces Q_t and P_t^τ are taken in duality by the form $(q(\cdot),p(\cdot))\mapsto\int_0^t p(s)q'(s)\mathrm{d}s$ where $q'(s)\mathrm{d}s$ denotes the measure which is the distributional derivative of $q(\cdot)$. We will consider elements of E_t^τ as functions taking values in $\mathcal{Q}\times\mathcal{P}$.

Now we will define a sequence $\{E_n\}$ of subspaces of E_t^τ to which we associate the sequential Feynman pseudomeasure. Let $t_0=0$ and, for any $n\in\mathbb{N}$ and any $k\in\mathbb{N}, k\leqslant 2^n$ let $t_k=k2^{-n}t$. We define E_n to be equal to the collection of functions from E_t^τ the restrictions of which to any interval $((k-1)2^{-n},k2^{-n})(k\in\mathbb{N})$ are constant functions. If f is a function on E_t^τ then the sequential Feynman integral over this space, of f, denoted by

$$\int_{E_t^\tau} f(q(\cdot),p(\cdot))\exp\left(i\int_0^t p(s)q'(s)\mathrm{d}s\right)\prod_0^t \mathrm{d}q(s)\mathrm{d}p(s),$$

is defined to be equal to $\Phi_{\{E_n\}}(f)$ (for the sake of simplicity we assume that $z=0$). One can check immediately that for any $\tau\in[0,1]$ the sequential Feynman integral defines a Hamiltonian Feynman pseudomeasure Φ^τ on E_t^τ: $\Phi^\tau(f)=\int_{E_t^\tau} f(q(\cdot),p(\cdot))\exp(i\int_0^t p(s)q'(s)\mathrm{d}s)\Pi_0^t\mathrm{d}q(s)\mathrm{d}p(s)$.

The main result of the paper, about the representation of solutions to the Schrödinger equation by the Feynman integral over trajectories in the phase space, is based on the observation that if $f(q,p)=\exp(-i\int_0^t H(q(\tau),p(\tau))\mathrm{d}\tau)\phi_0(q(0))$ then the finite dimensional integrals which were used above to define the sequential Feynman pseudomeasure coincide with $[\widehat{(e^{-i(t/n)H})^n}\phi_0](0)$; then one can use the Chernoff theorem according to which

$$e^{-it\hat{H}}\phi=\lim_{n\to\infty}\widehat{(e^{-i(t/n)H})^n}\phi,$$

where the caret means the PDO with the corresponding τ-symbol. It is worth mentioning that just the representation of the latter limit as a Feynman path integral allows are to discover its various connections with stochastic analysis.

Now we would like to mention some related results about Feynman path integrals over trajectories in the phase space. Actually there exists a surprisingly small number of mathematical papers devoted to such Feynman path integrals; even in the very recent book—Ref. 18—there is

actually no information on the subject. Nevertheless one can point out some mathematical texts on the problem. In particular in papers Refs. 19 and 20 the authors proved a convergence of some approximations to Feynman path integrals over trajectories in the phase space using the method of finite differences. A similar convergence was proved in Ref. 21 using some direct calculations. On the other hand in Refs. 4 and 5 (cf. Refs. 8, 22, and 23) an analytical continuation and Parseval equality (i.e., Fourier transform) were suggested to investigate Feynman path integrals over trajectories in the phase space; the latter approach uses a Poisson-type measure on the trajectories in the phase space and can be considered as an extension to the phase space of the approach of Albeverio–Hoegh–Krohn–Maslov–Chebotarev, which was originally applied only to Feynman integrals over trajectories either in the configuration or in the momentum space. Both these approaches—for Hamiltonian Feynman path integrals—were developed in some detail in Ref. 3; in particular using an integration over a Poisson-type measure some decompositions of solutions to Schrödinger equations were obtained (for an approach via analytical continuation to Feynman integrals for the Dirac equation see Ref. 24).

The main novelty in the approach which we use in the present paper is the direct application of the Chernoff formula (see Ref. 17) rather than the Trotter formula; besides we use the same Chernoff formula in order to improve some results from Ref. 3 (cf. Refs. 17 and 25) about representations of solutions of Schrödinger equations by Feynman integrals over Poisson-type measures. In both cases the more direct approach allows us to get representation theorems for new classes of Hamiltonians.

Notations and terminology of Refs. 26 and 27 are usually used without explanations. For any topological space X the symbol $\mathcal{B}(X)$ denotes the σ algebra of its Borel subsets; the symbol δ_x denotes the Dirac measure concentrated at the point $x \in X$; if μ is a measure on $(X,\mathcal{B}(X))$ and h is a $(\mathcal{B}(Y),\mathcal{B}(X))$ measurable mapping of X into a topological space Y then μh^{-1} is the image of μ with respect to this mapping; $v(\mu)$ is the total variation of μ. Besides $\mu \otimes \nu$ is the product of measures μ and ν, $\nu^{\otimes n}$ is the nth product power of the measure ν.

If X and Y are real Banach spaces, then $M(X)$ is the space of all complex-valued σ-additive measures on $(X,\mathcal{B}(X))$; we assume that $M(X)$ is equipped with the norm $v(\cdot)$. For $\mu,\nu \in M(X)$ let $\mu * \nu$ be the convolution of measures μ and ν; ν^{*n}—the nth convolution power of the measure ν, $\nu^{*0} = \delta_0$. For any $p \in X$ let ν_p be the shift of the measure ν with respect to the vector $p \in X$: $\nu_p(A) = \nu(A+p)$, $A \in \mathcal{B}(X)$.

Any measure $\mu \in M(X)$ is considered as an F_X-distribution for a proper F_X; if $\langle \cdot,\cdot \rangle : X \times Y \to \mathbb{R}$ is a duality between X and Y then for the Fourier Y-transform of μ the following identity holds: $\tilde{\mu}(z) (= \mathcal{F}\mu) = \int_X e^{i\langle z,x \rangle} \mu(\mathrm{d}x)$. In a similar way if $\phi \in L^2(\mathbb{R}^n)$ then $\tilde{\phi}(z) = \int_{\mathbb{R}^n} e^{i(z,x)_{\mathbb{R}^n}} \phi(x) \mathrm{d}x$ (the signs under the exponents depend on agreements).

The paper is organized as follows. In Sec. II we formulate a theorem which is an (easy) generalization of the Chernoff theorem; in Sec. III we apply this theorem to obtain some representations of solutions for Schrödinger equations. We call our main formula here a Feynman formula. What is done in Sec. IV can be described as obtaining representations of solutions for Schrödinger equations by integrals over Poisson-type complex measures on trajectories in the phase space. As was already mentioned, we again use the Chernoff theorem in the proof.

II. THE CHERNOFF THEOREM

Let X be a Banach space, $\mathcal{L}(X)$—the space of all bounded linear operators in X equipped, if otherwise not mentioned, with the topology of pointwise convergence (strong operator topology), $\|\cdot\|$—the operator norm on $\mathcal{L}(X)$, I—the identity operator in X. For any linear operator A in X let $D(A)$ be the domain of A.

The (strong) derivative at zero of a function $F:[0,\infty) \to \mathcal{L}(X)$ is a linear operator $F'(0):D(F'(0)) \to X$ defined by $F'(0)\phi = \lim_{h \to 0} h^{-1}(F(h)\phi - F(0)\phi)$, where $D(F'(0))$ is the space of all $\phi \in X$ such that the limit exists.

In this paper the following theorem is called the Chernoff theorem (this theorem is an immediate generalization of the theorem proved in Ref. 11).

Theorem 1: *Let X be a Banach space. Let $F:[0,\infty)\to\mathcal{L}(X)$ be a strongly continuous mapping such that $F(0)=I$, $\|F(t)\|\leqslant\exp(at)$ for some $a\in\mathbb{R}$, D be a linear subspace in $D(F'(0))$ and the restriction of $F'(0)$ to D be a closable operator whose closure we denote by C. If C is the generator of a strongly continuous semigroup $\exp(tC)$, then $F(t/n)^n$ converges to $\exp(tC)$ as $n\to\infty$ in the strong operator topology uniformly with respect to $t\in[0,T]$ for each $T>0$.*

III. THE FEYNMAN FORMULA VIA THE CHERNOFF THEOREM

Let the caret be a mapping from a space of functions on $\mathbb{R}^N\times\mathbb{R}^N$ into the space of linear operators in $L^2(\mathbb{R}^N)$, $\hat{}:H\to\hat{H}$ (then one can say that H is a symbol of $\hat{H}$). We say that the Feynman formula is valid for an operator $\hat{H}|_L$ which is the restriction of $\hat{H}$ to a domain $L\subset D(\hat{H})$ if $D(\widehat{e^{-i(t/n)H}})=L^2(\mathbb{R}^N)$ for any $n\in\mathbb{N}$ and $t\in[0,\infty)$, there exists the closure $\hat{H}^c$ of the operator $\hat{H}|_L$ and $-i\hat{H}^c$ is the generator of a strongly continuous semigroup $\exp(-it\hat{H}^c)$, $t\in[0,\infty)$,

$$e^{-it\hat{H}^c}\phi=\lim_{n\to\infty}\widehat{(e^{-i(t/n)H})}^n\phi, \tag{1}$$

for all $\phi\in L^2(\mathbb{R}^N)$ and $t\in[0,\infty)$. Of course, if $\hat{H}^c$ is self-adjoint, $e^{-it\hat{H}^c}$ is a unitary group.

For a function $\psi:\Omega\to\mathbb{C}$ and $a>0$ define $\overline{\psi}_a:\Omega\to\mathbb{C}$ by $\overline{\psi}_a(\omega)=\psi(\omega)$ if $|\psi(\omega)|\leqslant a$ and $\overline{\psi}_a(\omega)=0$ if $|\psi(\omega)|>a$.

Let $H:\mathbb{R}^N\times\mathbb{R}^N\to\mathbb{C}$ be a measurable function and $\tau\in[0,1]$. We define the operator $\hat{H}:D(\hat{H})\to L^2(\mathbb{R}^N)$ by

$$(\hat{H}\phi)(q)=\lim_{a\to\infty}(2\pi)^{-N}\int_{\mathbb{R}^N}\int_{\mathbb{R}^N}\overline{H}_a((1-\tau)q+\tau q',p)e^{ip(q-q')}\phi(q')\,dq'\,dp, \tag{2}$$

where the limit is taken in $L^2(\mathbb{R}^N)$. We assume that $D(\hat{H})$ is the set of all $\phi\in L^2(\mathbb{R}^N)$ such that $(\hat{H}\phi)(\cdot)$ exists. We say that the function $H(\cdot,\cdot)$ is the τ-symbol of the pseudodifferential operator $\hat{H}$ and the mapping caret is the τ-quantization.

Note that the zero-quantization is the qp-quantization, the one-quantization is the pq-quantization and the one-half-quantization is the Weyl quantization.

Lemma 2: Let $\mu\in M(\mathbb{R}^N\times\mathbb{R}^N)$, $h=\tilde{\mu}$, $F:\mathbb{R}^N\to\mathbb{C}$ be a bounded measurable function, $H(q,p)=h(q,p)F(p)$ and the caret be the τ-quantization ($\tau\in[0,1]$). Then $D(\hat{H})=L^2(\mathbb{R}^N)$,

$$\hat{H}\phi=\mathcal{F}\int_{\mathbb{R}^N\times\mathbb{R}^N}F(\cdot-(1-\tau)y)e^{i(\cdot-(1-\tau)y)x}[\mathcal{F}^{-1}\phi](\cdot-y)\,\mu(dy,dx), \tag{3}$$

for all $\phi\in L^2(\mathbb{R}^N)$ and $\|\hat{H}\|\leqslant\|F\|_\infty v(\mu)$. In particular, $\hat{h}\in\mathcal{L}(L^2(\mathbb{R}^N))$ and $\|\hat{h}\|\leqslant v(\mu)$.

Proof: Let $\phi\in L^2(\mathbb{R}^N)$, $\epsilon>0$ and $(P_\epsilon(H)\phi)(q)=(2\pi)^{-N}\int_{\mathbb{R}^N}\int_{\mathbb{R}^N}\exp(-\epsilon|p|^2-\epsilon|q'|^2)H((1-\tau)q+\tau q',p)e^{ip(q-q')}\phi(q')\,dq'\,dp$. Using the Fubini theorem we get

$$\begin{aligned}(P_\epsilon(H)\phi)(q)&=(2\pi)^{-N}\int_{\mathbb{R}^N\times\mathbb{R}^N}\Bigg(\int_{\mathbb{R}^N}\int_{\mathbb{R}^N}F(p)\\&\quad\times e^{-\epsilon|p|^2-\epsilon|q'|^2}e^{i(1-\tau)qy+i\tau q'y+ipx}e^{ip(q-q')}\phi(q')\,dq'\,dp\Bigg)\mu(dy,dx)\\&=\mathcal{F}\Bigg[\int_{\mathbb{R}^N\times\mathbb{R}^N}f_\epsilon(y,x;\cdot)\,\mu(dy,dx)\Bigg](q),\end{aligned} \tag{4}$$

where $f_\epsilon(y,x;p)=F(p-(1-\tau)y)\chi_\epsilon(p-(1-\tau)y)e^{i(p-(1-\tau)y)x}[\mathcal{F}^{-1}\chi_\epsilon\phi](p-y)$ and $\chi_\epsilon(\cdot)=e^{-\epsilon|\cdot|^2}$.

The latter integral in (4) is the Bochner integral of the function $g_\epsilon:\mathbb{R}^N\times\mathbb{R}^N\to L^2(\mathbb{R}^N)$, $g_\epsilon(y,x)(\cdot)=f_\epsilon(y,x;\cdot)$ with respect to the measure μ. We observe that $\|g_\epsilon(y,x)\|\leqslant\|\mathcal{F}^{-1}\|\|\phi\|_{L^2}\|F\|_\infty$ and that $\lim_{\epsilon\to\infty}g_\epsilon(y,x)=g(y,x)$ in $L^2(\mathbb{R}^N)$, where $g(y,x)=F(\cdot-(1-\tau)y)e^{i(\cdot-(1-\tau)y)x}[\mathcal{F}^{-1}\phi](\cdot-y)$. Applying Lebesgue's dominated convergence theorem to the Bochner integral we see that $P(H)\phi=\lim_{\epsilon\to0}P_\epsilon(H)\phi=\mathcal{F}\int_{\mathbb{R}^N\times\mathbb{R}^N}g(y,x)\mu(\mathrm{d}y,\mathrm{d}x)\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$. Since H is a bounded function we see that $\overline{H_a}=H$ for sufficiently large $a>0$. From this it follows that $\hat{H}\phi$ is defined for all $\phi\in L^2(\mathbb{R}^N)$ and $\hat{H}\phi=P(H)\phi$. Thus (3) is valid. From (3) it follows that $\|\hat{H}\|\leqslant\|F\|_\infty v(\mu)$. The lemma is proved.

Corollary 3: Let $\mu\in M(\mathbb{R}^N\times\mathbb{R}^N)$, $h=\tilde{\mu}$, $b:\mathbb{R}^N\to\mathbb{C}$ be a measurable function such that $\operatorname{Im}b\leqslant C_b$ *for some $C_b\in\mathbb{R}$, $B,H:\mathbb{R}^N\times\mathbb{R}^N\to\mathbb{C}$, $B(q,p)=b(p)$, $H(q,p)=b(p)+h(q,p)$, the caret be a τ-quantization ($\tau\in[0,1]$), $f_t(q,p)=\exp(-itH(q,p))$ and $A(t)=\hat{f}_t$. Then $A(t)\in\mathcal{L}(L^2(\mathbb{R}^N))$ for $t\in[0,\infty)$, $A(0)=I$, $\|A(t)\|\leqslant e^{ta}$ for some $a\in\mathbb{R}$, the function $A:[0,\infty)\to\mathcal{L}(L^2(\mathbb{R}^N))$ is strongly continuous, $A'(0)=-i\hat{B}-i\hat{h}$ and $D(A'(0))=D(\hat{B})$.*

Proof: For $k\in\mathbb{N}$ and $t\in[0,\infty)$ define operator $A_k(t):L^2(\mathbb{R}^N)\to L^2(\mathbb{R}^N)$, $A_k(t)\phi=\mathcal{F}\int_{\mathbb{R}^N\times\mathbb{R}^N}e^{-itb(\cdot-(1-\tau)y)}e^{i(\cdot-(1-\tau)y)x}[\mathcal{F}^{-1}\phi](\cdot-y)\mu^{*k}(\mathrm{d}y,\mathrm{d}x)$. Since $\|e^{-itb}\|_\infty\leqslant e^{tC_b}$ we have $\|A_k(t)\phi\|\leqslant e^{tC_b}\|\phi\|_{L^2}v(\mu)^k$. Therefore $\|A_k(t)\|\leqslant e^{tC_b}v(\mu)^k$.

Since $\exp(-ith)=\tilde{\nu}$ for $\nu=\delta_0+\sum_{k=1}^\infty((-it)^k/k!)\mu^{*k}$ from Lemma 2 it follows that $D(A(t))=L^2(\mathbb{R}^N)$ and we have $A(t)\phi=e^{-it\hat{B}}\phi+\sum_{k=1}^\infty((-it)^k/k!)A_k(t)\phi$ for $\phi\in L^2(\mathbb{R}^N)$. Therefore $\|A(t)\|\leqslant e^{tC_b}+\sum_{k=1}^\infty e^{tC_b}v(\mu)^kt^k/k!=e^{t(C_b+v(\mu))}$. It is clear that $A(0)=I$. Since $A_k(\cdot):[0,\infty)\to\mathcal{L}(L^2(\mathbb{R}^N))$ is strongly continuous we see that $A(\cdot)$ is strongly continuous.

Note that $A_1(0)\phi=\lim_{t\to0}A_1(t)\phi=\hat{h}\phi$ for $\phi\in L^2(\mathbb{R}^N)$ (see Lemma 2). Therefore $\lim_{t\to0}\sum_{k=1}^\infty(-it)^kA_k(t)\phi/k!t=-i\hat{h}\phi+\sum_{k=2}^\infty(-i)^k\lim_{t\to0}t^{k-1}A_k(t)\phi/k!=-i\hat{h}\phi$ for all $\phi\in L^2(\mathbb{R}^N)$. Thus $A'(0)=-i\hat{B}-i\hat{h}$ and $D(A'(0))=D(\hat{B})$. The corollary is proved.

Lemma 4: Let $\mu\in M(\mathbb{R}^N\times\mathbb{R}^N)$, $h=\tilde{\mu}$, the caret be the qp- or pq-quantization, $k\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$ be a real function, $H=h+k$, $g_t(q,p)=\exp(-itH(q,p))$ and $V(t)=\hat{g}_t$, $t\geqslant0$. Then

(a) $\hat{H}\in\mathcal{L}(L^2(\mathbb{R}^N))$ and $\|\hat{H}\|\leqslant v(\mu)+\varkappa\|k\|_{L^2}$ for some $\varkappa>0$,

(b) $V(t)\in\mathcal{L}(L^2(\mathbb{R}^N))$, $V(0)=I$, $\|V(t)\|\leqslant\exp(at)$ for some $a\in\mathbb{R}$, the function $V:[0,\infty)\to\mathcal{L}(L^2(\mathbb{R}^N))$ is strongly continuous and $V'(0)=-i\hat{H}$, $D(V'(0))=L^2(\mathbb{R}^N)$.

(c) Let $F_0,G_0:\mathbb{R}^N\to\mathbb{C}$ be bounded measurable functions and $F:\mathbb{R}^N\times\mathbb{R}^N\to\mathbb{C}$. Let $F(q,p)=F_0(p)$, $G(q,p)=G_0(q)$. If the caret is the qp-quantization then $\widehat{FG}_t=\hat{G}\hat{g}_t\hat{F}$. If the caret is the pq-quantization then $\widehat{FG}_t=\hat{F}\hat{g}_t\hat{G}$.

Proof: We give the proof only in the case when the caret is the qp-quantization. For the pq-quantization the proof is analogous. Let $\sigma\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$. Define operator $U(\sigma):L^2(\mathbb{R}^N)\to L^2(\mathbb{R}^N)$, $[U(\sigma)\phi](q)=\int_{\mathbb{R}^N}\sigma(q,p)e^{ipq}\phi(p)\mathrm{d}p$. Note that $|\int_{\mathbb{R}^N}\sigma(q,p)e^{ipq}\phi(p)\mathrm{d}p|\leqslant(\int_{\mathbb{R}^N}|\sigma(q,p)|^2\mathrm{d}p)^{1/2}\|\phi\|_{L^2}$ for all $\sigma\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$ and $\phi\in L^2(\mathbb{R}^N)$; hence $U(\sigma)\in\mathcal{L}(L^2(\mathbb{R}^N))$ and $\|U(\sigma)\|\leqslant\|\sigma\|_{L^2}$ for all $\sigma\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$.

For $\epsilon,a>0$ let $(P_{\epsilon,a}\phi)(q)=(2\pi)^{-N}\int_{\mathbb{R}^N}\int_{\mathbb{R}^N}e^{-\epsilon|p|^2-\epsilon|q'|^2}\overline{\sigma_a}(q,p)e^{ip(q-q')}\phi(q')\mathrm{d}q'\,\mathrm{d}p$. Then $P_{\epsilon,a}\phi=U(\overline{\sigma_a})C_\epsilon\mathcal{F}^{-1}C_\epsilon\phi$, where C_ϵ is the multiplication operator by the function $e^{-\epsilon|\cdot|^2}$. Hence $P_a\phi=\lim_{\epsilon\to0}P_{\epsilon,a}\phi=U(\overline{\sigma_a})\mathcal{F}^{-1}\phi$. Since $\overline{\sigma_a}\to\sigma$ as $a\to\infty$ in $L^2(\mathbb{R}^N\times\mathbb{R}^N)$ we get $\hat{\sigma}\phi=\lim_{a\to\infty}P_a\phi=U(\sigma)\mathcal{F}^{-1}\phi$. Thus $\hat{\sigma}\in\mathcal{L}(L^2(\mathbb{R}^N))$ and $\|\hat{\sigma}\|\leqslant\|\sigma\|_{L^2}\|\mathcal{F}^{-1}\|$. Since $k\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$ and $H=h+k$, in view of Lemma 2 we get $\hat{H}=\hat{h}+\hat{k}$, $\hat{H}\in\mathcal{L}(L^2(\mathbb{R}^N))$ and $\|\hat{H}\|\leqslant v(\mu)+\varkappa\|k\|_{L^2}$ for some $\varkappa>0$.

Let $f_t(q,p)=e^{-ith(q,p)}$, $A(t)=\hat{f}_t$ and

$$w_t(q,p)=(e^{-itk(q,p)}-1+itk(q,p))e^{-ith(q,p)},\quad u_t(q,p)=-itk(q,p)e^{-ith(q,p)}.$$

For $x\in\mathbb{R}$ we have $|\exp(-ix)-1+ix|=|x|\varepsilon(x)$, where the function $\varepsilon(\cdot)$ is bounded and $\varepsilon(x)\to0$ as $|x|\to0$. Therefore $w_t\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$. Hence $\hat{w}_t\in\mathcal{L}(L^2(\mathbb{R}^N))$ and $\|\hat{w}_t\|\leqslant\varkappa\|w_t\|_{L^2}$

$\leqslant t\varkappa \exp(tM)\|k\varepsilon(tk)\|_{L^2}=t\varepsilon_1(t)$ and $\varepsilon_1(t)\to 0$ as $t\to 0$, where $M=\sup_{q,p}|h(q,p)|$. This implies that if $B(t)=\hat{w}_t$ then $B'(0)=0$. Since $u_t\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$ we have $\hat{u}_t\in\mathcal{L}(L^2(\mathbb{R}^N))$. From Corollary 3 it follows that $\hat{f}_t\in\mathcal{L}(L^2(\mathbb{R}^N))$ and we see that $V(t)=A(t)+\hat{u}_t+\hat{w}_t$. Hence $V(t)\in\mathcal{L}(L^2(\mathbb{R}^N))$. By Corollary 3 we get $A'(0)=-i\hat{h}$ and $D(A'(0))=L^2(\mathbb{R}^N)$. Direct calculations show that if $E(t)=\hat{u}_t$ then $E'(0)=-i\hat{k}$ and $D(E'(0))=L^2(\mathbb{R}^N)$. Thus $V'(0)=-i\hat{h}-i\hat{k}=-i\hat{H}$ and $D(V'(0))=L^2(\mathbb{R}^N)$. Since $\|\hat{u}_t\|\leqslant bt\exp(tM)$ and $\|\hat{w}_t\|\leqslant ct\exp(tM)$ for some $b,c>0$ we obtain $\|V(t)\|\leqslant\exp(t(v(\mu)+b+c+M))$. From the fact that for all $t_0\in[0,\infty)$ $\|u_t-u_{t_0}\|_{L^2}\to 0$ and $\|w_t-w_{t_0}\|_{L^2}\to 0$ as $t\to t_0$ it follows that $\|\hat{u}_t-\hat{u}_{t_0}\|\to 0$ and $\|\hat{w}_t-\hat{w}_{t_0}\|\to 0$ as $t\to t_0$. By virtue of Corollary 3 the mapping $A:[0,\infty)\to\mathcal{L}(L^2(\mathbb{R}^N))$ is strongly continuous. Hence the mapping $V(\cdot)$ is strongly continuous. It is clear that $V(0)=I$.

To prove (c) we note that for all $\sigma\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$ we have $FG\sigma\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$ and $\widehat{FG\sigma}=U(FG\sigma)\mathcal{F}^{-1}=\hat{G}U(\sigma)\mathcal{F}^{-1}\hat{F}=\hat{G}\hat{\sigma}\hat{F}$. If $\sigma=\tilde{\nu}$ for some $\nu\in M(\mathbb{R}^N\times\mathbb{R}^N)$ then it follows from (3) that $\widehat{F\sigma}=\hat{\sigma}\hat{F}$. Since F,G,σ are bounded functions, from (2) it follows that $\widehat{FG\sigma}=\hat{G}\widehat{F\sigma}$. Hence $\widehat{FG\sigma}=\hat{G}\hat{\sigma}\hat{F}$. Thus $\widehat{FGf_t}=\hat{G}\hat{f}_t\hat{F}$. Therefore since $w_t,u_t\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$ and $g_t=f_t+w_t+u_t$ we get $\widehat{FGg_t}=\hat{G}\hat{g}_t\hat{F}$. The lemma is proved.

In the next theorem we assume that measurable functions $f_0,g_0:\mathbb{R}^N\to\mathbb{C}$ satisfy the following conditions. We assume that $\operatorname{Im} f_0\leqslant\tilde{c}$ and $\operatorname{Im} g_0\leqslant\tilde{c}$ for some $\tilde{c}\in\mathbb{R}$. Let $f,g:\mathbb{R}^N\times\mathbb{R}^N\to\mathbb{C}$, $f(q,p)=f_0(p)$, $g(q,p)=g_0(q)$. Suppose that there exists the closure A of the operator $\hat{f}+\hat{g}|_L$ defined on a subspace $L\subset D(\hat{f})\cap D(\hat{g})$. We assume that $-iA$ is the generator of a strongly continuous semigroup. For example in the case of $\mathbb{R}^3$ real functions $f_0(p)=p^2$, $p\in\mathbb{R}^3$ and $g_0\in L^2(\mathbb{R}^3)+L^\infty(\mathbb{R}^3)$ satisfy the introduced condition (see Ref. 28 Chap. X,2, Theorem X.15).

Theorem 5: *Let the caret be the qp- or pq-quantization, $\mu\in M(\mathbb{R}^N\times\mathbb{R}^N)$, $h=\tilde{\mu}$, $k\in L^2(\mathbb{R}^N\times\mathbb{R}^N)$ be a real function, $H(q,p)=f_0(p)+g_0(q)+h(q,p)+k(q,p)$. Then the Feynman formula is valid for the operator $\hat{H}|_L$.*

Proof: We give a proof only when the caret is the qp-quantization. For the case of pq-quantization the proof is analogous. It is sufficient to apply the Chernoff theorem to the function $F(t)=e^{\widehat{-itH}}$ choosing $D=L(\subset D(\hat{f})\cap D(\hat{g}))$. According to Lemma 4(c) we get $F(t)=e^{\widehat{-itg}}e^{\widehat{-it(h+k)}}e^{\widehat{-itf}}=e^{-it\hat{g}}e^{\widehat{-it(h+k)}}e^{-it\hat{f}}$. In view of Lemma 4(b) the restriction $F'(0)|_D$ of the strong derivative $F'(0)$ to $D(=L)$ coincides with $-i(\hat{f}+\hat{g}+\hat{h}+\hat{k})$ on D. Hence $F'(0)|_D=\hat{H}|_L$. By Lemma 4(a) we have $\hat{h}+\hat{k}\in\mathcal{L}(L^2(\mathbb{R}^N))$. Therefore the closure $\hat{H}^c$ of $\hat{H}|_L$ exists and is equal to $-i(A+\hat{h}+\hat{k})$ with $D(\hat{H}^c)=D(A)$. From the theorem on perturbations of generators of semigroups (Ref. 26, Chap. VIII,1, Theorem 19) it follows that $-i\hat{H}^c$ is the generator of a strongly continuous semigroup $\exp(-it\hat{H}^c)$. Using Lemma 4 one can verify the other conditions of Theorem 1. The theorem is proved.

Direct application of Theorem 1 and Corollary 3 gives a proof of Theorem 6.

Theorem 6: *Let the caret be a τ-quantization ($\tau\in[0,1]$), $f:\mathbb{R}^N\to\mathbb{C}$ be a measurable function such that $\operatorname{Im} f\leqslant C_f$ for some $C_f\in\mathbb{R}$, $h=\tilde{\mu}$, where $\mu\in M(\mathbb{R}^N\times\mathbb{R}^N)$, and $H(q,p)=f(p)+h(q,p)$. Then the Feynman formula is valid for $\hat{H}$ defined on $D(\hat{H})$.*

We expect that a similar approach can be used to extend Theorems 5 and 6 to a more general situation. In order to do that it is of course necessary to generalize properly the Chernoff theorem.

The Feynman formula (1) gives a representation of solutions of the Schrödinger equation $i\,\mathrm{d}\phi/\mathrm{d}t=\hat{H}\phi$. One can prove statements similar to Theorems 5 and 6 for the "heat equation" $\mathrm{d}\phi/\mathrm{d}t=\hat{H}\phi$ if one substitutes hypotheses of Theorem 5 by some additional proper conditions. In particular: the operators $\hat{f}$, $\hat{g}$ and the closure C of the operator $(\hat{f}+\hat{g})|_L$ defined on a subspace $L\subset D(\hat{f})\cap D(\hat{g})$ are the generators of strongly continuous semigroups.

IV. THE SERIES REPRESENTATIONS OF SOLUTIONS

Let $D_m(t)=\{(t_1,\ldots,t_m)|0\leqslant t_m\leqslant\cdots\leqslant t_1\leqslant t\}$ for $t\geqslant 0$ and $D_m^0(t)=\{(t_1,\ldots,t_m)|0<t_m<\ldots<t_1<t\}$. Let λ_m be the Lebesgue measure on $\mathbb{R}^m$, $\lambda_{m,n}^t$ be the measure on $D_m(t)$ concentrated on

the set of elements $y \in D_m(t)$ such that $y_j \in T_n$, $T_n = \{(lt/n) \mid l = 1,\ldots,n\}$ and $\lambda^t_{m,n}(\{y\}) = (t/n)^m/k_1!\cdots k_n!$, where $0! = 1$ and k_l is the number of components of y equal to $lt/n, 1 \leqslant l \leqslant n$.

Lemma 7: $\lambda_m(D_m(t)) = v(\lambda^t_{m,n}) = t^m/m!$. *If* $f: D_m(t) \to \mathbb{R}$ *is a bounded function such that the restriction of* f *to* $D^0_m(t)$ *is continuous then* $\int_{D_m(t)} f \, d\lambda^t_{m,n} \to \int_{D_m(t)} f \, d\lambda_m$ *as* $n \to \infty$.

Proof: Fix $t > 0$, $m \in \mathbb{N}$ and for $y = (y_1, \ldots, y_m) \in (T_n)^m \cap D_m(t)$, $n \in \mathbb{N}$ we define the set $C_{n,y} = \{x \in \mathbb{R}^m \mid y_j - 1/n \leqslant x_j \leqslant y_j, j = 1, \ldots, m\} \cap D_m(t)$. The direct calculation shows that $\lambda_m(C_{n,y}) = \lambda^t_{m,n}(\{y\})$, $y \in (T_n)^m \cap D_m(t)$. Thus we get $v(\lambda^t_{m,n}) = \lambda_m(D_m(t))$. Direct calculations show that $\lambda_m(D_m(t)) = t^m/m!$.

Let $R_n(f) = \Sigma f(y) \lambda_m(C_{n,y})$, where the sum is taken over all $y \in (T_n)^m \cap D_m(t)$. Then $R_n(f)$ is a Riemannian sum for the integral $\int_{\mathbb{R}^m} F \, d\lambda_m$, where $F(x) = f(x)$ for $x \in D_m(t)$ and $F(x) = 0$ for $x \notin D_m(t)$. Since the set of points where the function F is discontinuous belongs to the boundary $\partial D_m(t)$ of $D_m(t)$ and $\lambda_m(\partial D_m(t)) = 0$ we get $\lim_{n \to \infty} R_n(f) = \int_{\mathbb{R}^m} F \, d\lambda_m = \int_{D_m(t)} f \, d\lambda_m$. The lemma is proved.

Actually the following theorem is an improvement of the Smolyanov–Shavgulidze formula.[17,25]

Theorem 8: *Let the caret denote the qp-quantization,* $P = Q = \mathbb{R}^N$, $a: P \to \mathbb{C}$ *be a measurable function such that* $\operatorname{Im} a \leqslant C_a$ *for some* $C_a \in \mathbb{R}$, $h: Q \times P \to \mathbb{C}$ *be the Fourier transform of a measure* $\nu \in M(P \times Q)$. *For* $t \in [0, \infty)$, $m = 0,1,\ldots$ *define functions* $U^m_t: \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{C}$, $U^0_t(q,p) = e^{-ita(p)}$ *and*

$$
\begin{aligned}
U^m_t(q,p) = (-i)^m \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{m-1}} dt_m \\
\times \int_{(P \times Q)^m} \exp\left(i \left\langle q, \sum_{l=1}^m p_l \right\rangle - ia\left(p + \sum_{l=1}^m p_l \right)(t - t_1) \right. \\
\left. - i \sum_{k=2}^m a\left(p + \sum_{l=k}^m p_l \right)(t_{k-1} - t_k) - ia(p) t_m \right) \\
\times \exp\left(i \sum_{k=1}^{m-1} \left\langle q_k, p + \sum_{l=k+1}^m p_l \right\rangle + i \langle q_m, p \rangle \right) \nu(dp_1, dq_1) \ldots \nu(dp_m, dq_m). \qquad (5)
\end{aligned}
$$

Then $\Sigma^\infty_{m=0} |U^m_t(q,p)| < \infty$ *and if* $U_t(q,p) = \Sigma^\infty_{m=0} U^m_t(q,p)$ *then* $\hat{U}_t \in \mathcal{L}(L^2(Q))$ *and* $t \mapsto \hat{U}_t$ *is a strongly continuous semigroup in* $L^2(Q)$ *with the generator* $-i\hat{H}$, *where* $H(q,p) = a(p) + h(q,p)$. *Moreover* $\hat{U}^m_t \in \mathcal{L}(L^2(Q))$ *and* $\hat{U}_t = \Sigma^\infty_{m=0} \hat{U}^m_t$, *where the sum converges in the uniform operator topology in* $\mathcal{L}(L^2(Q))$.

Proof: Let $A(q,p) = a(p)$. Note that $\hat{A}$ is the generator of the strongly continuous semigroup $B(t) = \hat{f}_t$, $f_t = \exp(-itA)$. Since $g_t = \exp(-ith) = \widetilde{\varkappa_t}$ for $\varkappa_t = \delta_0 + \Sigma^\infty_{k=1} ((-it)^k/k!) \nu^{*k}$, by Lemma 2 we get $\hat{g}_t = \Sigma^\infty_{k=0} ((-it)^k/k!) \widehat{h^k}$. From this it follows that the function $F(t) = \hat{g}_t \exp(-it\hat{A})$ satisfies the conditions of Theorem 1. In particular $F'(0) = -i(\hat{A} + \hat{h}) = -i\hat{H}$ and $D = D(\hat{A})$. Since by Lemma 2 $\hat{h} \in \mathcal{L}(L^2(\mathbb{R}^N))$, from the theorem on perturbation of generators of strongly continuous semigroups (see Ref. 26, Chap. VIII, 1, Theorem 19), it follows that $-i\hat{H} = -i(\hat{A} + \hat{h})$ is the generator of a semigroup $V_t = \exp(-it\hat{H})$. Thus by Theorem 1 we get

$$
e^{-it\hat{H}}\phi = \lim_{n \to \infty} (\widehat{e^{-i(t/n)h}} \widehat{e^{-i(t/n)A}})^n \phi
$$

for all $\phi \in L^2(Q)$.

Define the measures $\nu_n \in M(P\times Q)$, $\nu_n = \delta_0 + \Sigma_{k=1}^{\infty}((-it)^k/k!n^k)\nu^{*k}$, $n\in\mathbb{N}$. Then $\exp(-ith/n)=\widetilde{\nu}_n$. Denote $V_{n,t}=(\widehat{e^{-i(t/n)h}e^{-i(t/n)A}})^n$. Using Lemma 2 (with $\tau=0$ and $F\equiv 1$) and direct calculations we get

$$V_{n,t}\phi = \mathcal{F}\int_{(P\times Q)^n} \exp(i\Sigma_{k=1}^{n}\langle q_k, \cdot - \Sigma_{m=1}^{k} p_m\rangle)\exp\left(-i\frac{t}{n}\sum_{k=1}^{n} a(\cdot - \Sigma_{m=1}^{k} p_m)\right)$$
$$\times[\mathcal{F}^{-1}\phi](\cdot - p_1 - \cdots - p_n)\,\nu_n(dp_1,dq_1)\cdots\nu_n(dp_n,dq_n).$$

Let $(t_1,\ldots,t_r,(p_1,q_1),\ldots,(p_r,q_r))\in D_r(t)\times(P\times Q)^r$. Let $\overline{r}$ be the number of different elements in the set $\{t_1,\ldots,t_r\}$ and $j_0=0$, $1\leq j_1<\cdots<j_{\overline{r}}=r$ be such that $t_m=t_{j_k}$ for $j_{k-1}<m\leq j_k$ $(m=1,\ldots,r)$ and $t_{j_k}\neq t_{j_l}$ for $k\neq l$. For $1\leq k\leq\overline{r}$ we put $\overline{q_k}=\Sigma_{j_{k-1}<m\leq j_k} q_m$ and $\overline{p_k}=\Sigma_{j_{k-1}<m\leq j_k} p_m$.

Let $A_0=\mathcal{F}[e^{-ita(\cdot)}\mathcal{F}^{-1}\phi]$. Direct calculations show that

$$V_{n,t}\phi = A_0 + \sum_{r=1}^{\infty}(-i)^r\mathcal{F}\int_{D_r(t)}\int_{(P\times Q)^r}\exp(i\Sigma_{k=1}^{\overline{r}}\langle\overline{q_k},\cdot-\Sigma_{m=1}^{k}\overline{p_m}\rangle)\times\exp(-ia(\cdot)(t-t_1)$$
$$-i\Sigma_{k=2}^{r}a(\cdot-\Sigma_{m=1}^{k-1}p_m)(t_{k-1}-t_k)-ia(\cdot-\Sigma_{m=1}^{r}p_m)t_r)[\mathcal{F}^{-1}\phi](\cdot-p_1-\ldots-p_r)d\lambda_{r,n}^{t}$$
$$\otimes\nu^{\otimes r} = A_0 + \sum_{r=1}^{\infty}(-i)^r\mathcal{F}\int_{D_r(t)}\int_{(P\times Q)^r}\zeta_{r,\phi}\,d\lambda_{r,n}^{t}\otimes\nu^{\otimes r}, \tag{6}$$

where $\zeta_{r,\phi}: D_r(t)\times(P\times Q)^r\to L^2(\mathbb{R}^N)$, $\zeta_{r,\phi}(t_1,\ldots,t_r,(p_1,q_1),\ldots,(p_r,q_r))=\exp(i\Sigma_{k=1}^{\overline{r}}\langle\overline{q_k},\cdot-\Sigma_{m=1}^{k}\overline{p_m}\rangle - ia(\cdot)(t-t_1) - i\Sigma_{k=2}^{r}a(\cdot-\Sigma_{m=1}^{k-1}p_m)(t_{k-1}-t_k) - ia(\cdot-\Sigma_{m=1}^{r}p_m)t_r)[\mathcal{F}^{-1}\phi](\cdot-p_1-\ldots-p_r)$. Note that $\|\zeta_{r,\phi}\|_{\infty}\leq e^{tC_a}\|\phi\|_{L^2}\|\mathcal{F}^{-1}\|$.

For $\phi\in L^2(Q)$ let $A_{r,n}\phi=(-i)^r\mathcal{F}\int_{D_r(t)}\int_{(P\times Q)^r}\zeta_{r,\phi}\,d\lambda_{r,n}^{t}\otimes\nu^{\otimes r}$ and $A_r\phi=(-i)^r\mathcal{F}\int_{D_r(t)}\int_{(P\times Q)^r}\zeta_{r,\phi}\,d\lambda_{r,n}^{t}\otimes\nu^{\otimes r}$, $r\in\mathbb{N}$. Let $\eta_{r,n}((p_1,q_1),\ldots,(p_r,q_r))=\int_{D_r(t)}\zeta_{r,\phi}(t_1,\ldots,t_r,(p_1,q_1),\ldots,(p_r,q_r))d\lambda_{r,n}^{t}$ and $\eta_r((p_1,q_1),\ldots,(p_r,q_r))=\int_{D_r(t)}\zeta_{r,\phi}(t_1,\ldots,t_r,(p_1,q_1),\ldots,(p_r,q_r))d\lambda_r$.

Since for all fixed $q_1,\ldots,q_r,p_1,\ldots,p_r$ the function $\zeta_{r,\phi}$ is bounded on the set $D_r(t)$ and continuous on the set $D_r^0(t)$ from Lemma 7 it follows that $\lim_{n\to\infty}\eta_{r,n}((p_1,q_1),\ldots,(p_r,q_r))=\lim_{n\to\infty}\int_{D_r(t)}\zeta_{r,\phi}(t_1,\ldots,t_r,(p_1,q_1),\ldots,(p_r,q_r))d\lambda_{r,n}^{t}=\int_{D_r(t)}\zeta_{r,\phi}(t_1,\ldots,t_r,(p_1,q_1),\ldots,(p_r,q_r))d\lambda_r=\eta_r((p_1,q_1),\ldots,(p_r,q_r))$.

Using Lemma 7 we get $\|\eta_{r,n}\|_{\infty}\leq\|\zeta_{r,\phi}\|_{\infty}v(\lambda_{r,n}^{t})\leq e^{tC_a}t^r\|\phi\|_{L^2}\|\mathcal{F}^{-1}\|/r!$ and $\|\eta_r\|_{\infty}\leq\|\zeta_{r,\phi}\|_{\infty}\lambda_r(D_r(t))=e^{tC_a}t^r\|\phi\|_{L^2}\|\mathcal{F}^{-1}\|/r!$. Thus by the Lebesgue theorem on the dominated convergence we get $\lim_{n\to\infty}A_{r,n}\phi=\lim_{n\to\infty}(-i)^r\mathcal{F}\int_{(P\times Q)^r}\eta_{r,n}((p_1,q_1),\ldots,(p_r,q_r))d\nu^{\otimes r}=(-i)^r\mathcal{F}\int_{(P\times Q)^r}\eta_r((p_1,q_1),\ldots,(p_r,q_r))d\nu^{\otimes r}=A_r\phi$.

Note that $\|A_{r,n}\phi\|_{L^2}\leq\|\eta_{r,n}\|_{\infty}|\nu|^r\|\mathcal{F}\|\leq e^{tC_a}\|\phi\|_{L^2}|\nu|^r t^r/r!$ and $\|A_r\phi\|_{L^2}\leq\|\eta_{r,n}\|_{\infty}|\nu|^r\|\mathcal{F}\|\leq e^{tC_a}|\nu|^r\|\phi\|_{L^2}t^r/r!$. From this it follows that $A_{r,n}$, $A_r\in\mathcal{L}(L^2(Q))$ and that $V_t\phi=\lim_{n\to\infty}V_{n,t}\phi=\lim_{n\to\infty}(A_0\phi+\Sigma_{r=1}^{\infty}A_{r,n}\phi)=A_0\phi+\Sigma_{r=1}^{\infty}\lim_{n\to\infty}A_{r,n}\phi=\Sigma_{r=0}^{\infty}A_r\phi$.

Let $\phi\in L^2(Q)$, $\epsilon>0$ and $\overline{\phi_\epsilon}=\chi_\epsilon\mathcal{F}^{-1}\chi_\epsilon\phi$, where χ_ϵ is the multiplication operator by the function $e^{-\epsilon|\cdot|^2}$. For $r\in\mathbb{N}$ let $(\hat{U}_{t,\epsilon}^{r}\phi)(q)=(2\pi)^{-N}\int_{\mathbb{R}^N}\int_{\mathbb{R}^N}U_t^r(q,p)e^{ip(q-q')}e^{-\epsilon|p|^2-\epsilon|q'|^2}\times\phi(q')dq'dp$. Then $(\hat{U}_{t,\epsilon}^{r}\phi)(q)=\int_{\mathbb{R}^N}U_t^r(q,p)e^{i\langle p,q\rangle}\overline{\phi_\epsilon}(p)dp$ and by Fubini's theorem we get

$$(\hat{U}_{t,\epsilon}^{r}\phi)(q)=(-i)^r\int_{\mathbb{R}^N}dp\int_0^t dt_1\int_0^{t_1}dt_2\cdots\int_0^{t_{r-1}}dt_r\int_{(P\times Q)^r}\exp(i\langle q,\Sigma_{l=1}^{r}p_l\rangle$$
$$-ia(p+\Sigma_{l=1}^{r}p_l)(t-t_1)-i\Sigma_{k=2}^{r}a(p+\Sigma_{l=k}^{r}p_l)(t_{k-1}-t_k)-ia(p)t_r)$$
$$\times\exp(i\Sigma_{k=1}^{r-1}\langle q_k,p+\Sigma_{l=k+1}^{r}p_l\rangle+i\langle q_r,p\rangle)e^{i\langle p,q\rangle}\overline{\phi_\epsilon}(p)\,\nu(dp_1,dq_1)\cdots\nu(dp_r,dq_r).$$

Changing the variable $p \to p - p_1 - \cdots - p_r$ we get

$$(\hat{U}^r_{t,\epsilon}\phi)(q) = (-i)^r \int_{\mathbb{R}^N} dp \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{r-1}} dt_r \int_{(P\times Q)^r} \exp(i\Sigma_{k=1}^r \langle q_k, p - \Sigma_{m=1}^k p_m\rangle)$$
$$\times \exp(-ia(p)(t-t_1) - i\Sigma_{k=2}^r a(p - \Sigma_{m=1}^{k-1} p_m)(t_{k-1} - t_k)$$
$$- ia(p - \Sigma_{m=1}^r p_m)t_r) e^{i\langle p,q\rangle} \times \overline{\phi}_\epsilon(p - p_1 - \ldots - p_r)\, \nu(dp_1, dq_1) \cdots \nu(dp_r, dq_r)$$
$$= A_r \mathcal{F}\overline{\phi}_\epsilon(q).$$

Therefore we get the Bochner integral

$$\hat{U}^r_{t,\epsilon}\phi = (-i)^r \mathcal{F} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{r-1}} dt_r \int_{(P\times Q)^r} \exp(i\Sigma_{k=1}^r \langle q_k, \cdot - \Sigma_{m=1}^k p_m\rangle)$$
$$\times \exp(-ia(\cdot)(t-t_1) - i\Sigma_{k=2}^r a(\cdot - \Sigma_{m=1}^{k-1} p_m)(t_{k-1} - t_k) - ia(\cdot - \Sigma_{m=1}^r p_m)t_r)$$
$$\times \overline{\phi}_\epsilon(\cdot - p_1 - \cdots - p_r)\, \nu(dp_1, dq_1) \cdots \nu(dp_r, dq_r)$$
$$= A_r \mathcal{F}\overline{\phi}_\epsilon.$$

Since $\lim_{\epsilon\to 0} \overline{\phi}_\epsilon = \mathcal{F}^{-1}\phi$ by the Lebesgue theorem on dominated convergence we obtain that $\lim_{\epsilon\to 0} \hat{U}^r_{t,\epsilon}\phi = A_r\phi$. Therefore from the fact that $U^r_t(\cdot,\cdot)$ is a bounded function we get $\hat{U}^r_t\phi = A_r\phi$. From this it follows that $\hat{U}^r_t \in \mathcal{L}(L^2(\mathbb{R}^N))$, $\|\hat{U}^r_t\| = \|A_r\| \le e^{tC_a}|\nu|^r t^r/r!$ and the series $\Sigma_{r=0}^\infty \hat{U}^r_t$ converges in the uniform operator topology. Since $\hat{U}^0_t = A_0$ we see that $V_t = \Sigma_{r=0}^\infty \hat{U}^r_t$.

Note that $|U^r_t(q,p)| \le e^{tC_a}|\nu|^r \lambda_r(D_r(t)) = e^{tC_a}|\nu|^r t^r/r!$. From this it follows that $\Sigma_{m=0}^\infty |U^m_t(q,p)| < \infty$ and $|U_t(q,p)| \le e^{tC_a + |\nu|t}$. For $\epsilon > 0$ let $(\hat{U}_{t,\epsilon}\phi)(q) = (2\pi)^{-N} \int_{\mathbb{R}^N} U_t(q,p) \exp(-\epsilon|p|^2 - \epsilon|q'|^2) e^{ip(q-q')}\phi(q')\, dq'\, dp$. Then $(\hat{U}_{t,\epsilon}\phi)(\cdot) = \mathcal{F}[e^{-ita(\cdot)}\overline{\phi}_\epsilon(\cdot)] + \Sigma_{r=1}^\infty (\hat{U}^r_{t,\epsilon}\phi)(\cdot)$. Since $\hat{U}^r_{t,\epsilon}\phi = A_r\mathcal{F}\overline{\phi}_\epsilon$ we get $\|\hat{U}^r_{t,\epsilon}\phi\|_{L^2} \le \|\phi\|_{L^2}|\nu|^r e^{tC_a} t^r/r!$. Therefore $\lim_{\epsilon\to 0} \hat{U}_{t,\epsilon}\phi = \lim_{\epsilon\to 0}(\mathcal{F}[e^{-ita(\cdot)}\overline{\phi}_\epsilon(\cdot)] + \Sigma_{r=1}^\infty \hat{U}^r_{t,\epsilon}\phi) = \hat{U}^0_t\phi + \Sigma_{r=1}^\infty \lim_{\epsilon\to 0} \hat{U}^r_{t,\epsilon}\phi = \hat{U}^0_t\phi + \Sigma_{r=1}^\infty \hat{U}^r_t\phi$ in $L^2(Q)$. Since $U_t(\cdot,\cdot)$ is bounded we obtain $\hat{U}_t\phi = \hat{U}^0_t\phi + \Sigma_{r=1}^\infty \hat{U}^r_t\phi$. From this it follows that $\hat{U}_t \in \mathcal{L}(L^2(Q))$ and $\hat{U}_t = V_t$.

The theorem is proved.

Let us notice that if the conditions of Theorem 8 are valid then from the representation of the symbol $U_t(q,p)$ of the propagator for the Schrödinger equation $i\,du/dt = \hat{H}u$, where $H(q,p) = a(p) + h(q,p)$, one can get the following identity for representation of a solution for this equation:

$$u(t,z) = \int u_0(q(0)+z) \exp\left(-i\int_0^t a(p(\tau))\,d\tau - i\int_0^t h(q(\tau)+z, p(\tau))\,d\tau\right) \Phi_{a^-}(dq, dp),$$

where the symbol on the right-hand side denotes the functional integral (corresponding to the quadratic form a^-) defined with the help of the Parseval equality (see Ref. 3, Chap. 3, Sec. 2). Therefore as a corollary of Theorem 8 we again get a theorem on the representation of solutions for the Schrödinger equation by the Feynman path integral over trajectories in the phase space.

It is also worth noticing that similar considerations can be also applied to pq, Weyl and other types of symbols. We plan to do this in the next paper.

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Multipole expansion of a plane wave

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The spherical components of the multipole expansion of a plane wave with arbitrary spin are obtained in terms of spin-weighted spherical harmonics. It is shown that the expansion coefficients are essentially spin-weighted spherical harmonics evaluated at the direction of propagation of the wave. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1500425]

I. INTRODUCTION

In the standard treatment of the multipole expansion of nonscalar fields a huge variety of vector, tensor, or spinor fields is employed (see, e.g., Refs. 1–3) with widely variable notations and conventions. A uniform formalism applicable to fields of any spin is based on the use of two-component spinors and spin-weighted spherical harmonics.[4–7] The fact that, in a three-dimensional space, the spinor indices take two values only (as in the case of the two-component spinors employed in general relativity) leads to many simplifications in the algebraic manipulations.

The spin-weighted spherical harmonics appear in the solution by separation of variables in spherical coordinates of linear partial differential equations for nonscalar fields, when the equations are written in terms of quantities with a well-defined spin weight (see, e.g., Refs. 5 and 7). Each spin-weighted spherical harmonic, ${}_sY_{jm}$, is an eigenfunction of the square of the total angular momentum, J^2, and of the z component of the total angular momentum, J_z. As shown in the following, the expansion of a plane wave of any spin in terms of spin-weighted spherical harmonics can be easily obtained and the coefficients of the expansion are essentially spin-weighted spherical harmonics evaluated in the direction of propagation of the wave.

In Sec. II some basic notions about the two-component spinor formalism are summarized and some useful expressions for the spin-weighted spherical harmonics are given which are employed in Sec. III to find the expression of a plane wave in terms of spin-weighted spherical harmonics.

II. SPINORS AND SPIN-WEIGHTED SPHERICAL HARMONICS

The components of a field with arbitrary spin in Euclidean three-dimensional space can be expressed in a unified way using two-component spinors, which are well known from the treatment of electron's spin in nonrelativistic quantum mechanics. The two-component spinor formalism in three-dimensional space is relatively simple because, among other things, a single nonzero one-index spinor gives rise to bases for tensors or spinors of any rank. If ψ^A $(A,B,\ldots=1,2)$ are the components of a spinor field and the mate of ψ^A, denoted by $\hat{\psi}^A$, is defined by

$$\hat{\psi}_A=\overline{\psi^A}$$

or

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$$\hat{\psi}^A = -\overline{\psi_A}, \tag{1}$$

where the bar denotes complex conjugation, then at each point where ψ^A does not vanish, $\{\psi^A, \hat{\psi}^A\}$ is linearly independent and, hence, a basis for the one-index spinors. The spinor indices are raised or lowered following the rules

$$\psi_A = \varepsilon_{AB}\psi^B, \quad \psi^A = -\varepsilon^{AB}\psi_B, \tag{2}$$

where

$$(\varepsilon_{AB}) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = (\varepsilon^{AB}). \tag{3}$$

Therefore, $\psi_A\phi^A = -\psi^A\phi_A$ and $\psi_A\psi^A = 0$.

A symmetric two-index spinor, $v_{AB} = v_{BA}$, corresponds to a (possibly complex) vector v_i $(i,j,\ldots = 1,2,3)$ with Cartesian components

$$v_i = -\frac{1}{\sqrt{2}}\sigma_i{}^{AB}v_{AB}, \tag{4}$$

where the connection symbols σ_{iAB} satisfy

$$\sigma_{iAB} = \sigma_{iBA} \tag{5}$$

and

$$\sigma_{iAB}\sigma_j{}^{AB} = -2\,\delta_{ij}. \tag{6}$$

The connection symbols can be chosen as

$$(\sigma_{1AB}) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (\sigma_{2AB}) = \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix}, \quad (\sigma_{3AB}) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \tag{7}$$

which satisfy the condition

$$\overline{\sigma_{iAB}} = -\sigma_i{}^{AB}. \tag{8}$$

Thus, a symmetric two-index spinor v_{AB} corresponds to a real vector if and only if $\overline{v_{AB}} = -v^{AB}$. [The matrices (7) are the products of (ε_{AB}) by the usual Pauli matrices.]

Making use of the relation

$$\sigma^i{}_{AB}\sigma_{iCD} = -(\varepsilon_{AC}\varepsilon_{BD} + \varepsilon_{AD}\varepsilon_{BC}), \tag{9}$$

which follows from Eq. (6), one finds that Eq. (4) is equivalent to

$$v_{AB} = \frac{1}{\sqrt{2}}\sigma^i{}_{AB}v_i. \tag{10}$$

(The tensor indices are raised or lowered by means of δ^{ij} and δ_{ij}.) More generally, the spinor equivalent of a tensor $t_{ij\cdots k}$ is defined by

$$t_{ABCD\cdots EF} = \frac{1}{\sqrt{2}}\sigma^i{}_{AB}\frac{1}{\sqrt{2}}\sigma^j{}_{CD}\cdots\frac{1}{\sqrt{2}}\sigma^k{}_{EF}t_{ij\cdots k}. \tag{11}$$

Then $t_{ABCD\cdots EF}$ is totally symmetric if and only if $t_{ij\cdots k}$ is symmetric and trace free. A spin-S field ($S=1/2,1,3/2,\ldots$) corresponds to a $2S$-index totally symmetric spinor field (or, as in the case of the Dirac equation, to several $2S$-index totally symmetric spinor fields).

Starting from a one-index spinor field ψ^A one can construct the real vector field

$$R_i=-\sigma_{iAB}\psi^A\hat{\psi}^B \tag{12}$$

and the complex vector field

$$M_i=\sigma_{iAB}\psi^A\psi^B, \tag{13}$$

which, according to Eq. (9), satisfy

$$R_iR^i=-(\varepsilon_{AC}\varepsilon_{BD}+\varepsilon_{AD}\varepsilon_{BC})\psi^A\hat{\psi}^B\psi^C\hat{\psi}^D=(\psi^A\hat{\psi}_A)^2,$$

$$\overline{M_i}M^i=(\varepsilon_{AC}\varepsilon_{BD}+\varepsilon_{AD}\varepsilon_{BC})\hat{\psi}^A\hat{\psi}^B\psi^C\psi^D=2(\psi^A\hat{\psi}_A)^2,$$

and, similarly, $R_iM^i=0$, $M_iM^i=0$; hence, R_i, $\mathrm{Re}\,M_i$, $\mathrm{Im}\,M_i$ are orthogonal to each other and have the magnitude $\psi^A\hat{\psi}_A$. (Note that for any one-index spinor ϕ^A, $\phi^A\hat{\phi}_A=|\phi^1|^2+|\phi^2|^2$, which is always real and non-negative.)

In what follows we will make use of the spinor field o^A, with components

$$\begin{pmatrix} o^1 \\ o^2 \end{pmatrix}=\begin{pmatrix} e^{-i\varphi/2}\cos(\theta/2) \\ e^{i\varphi/2}\sin(\theta/2) \end{pmatrix}, \tag{14}$$

where θ and φ are the usual polar and azimuth angles associated with the spherical coordinates. The spinor field o^A satisfies $o^A\hat{o}_A=1$ and the three mutually orthogonal vectors defined by o^A form the orthonormal basis, $\{\mathbf{e}_r,\mathbf{e}_\theta,\mathbf{e}_\varphi\}$, induced by the spherical coordinates r,θ,φ, i.e.,

$$(\mathbf{e}_r)_j=-\sigma_{jAB}o^A\hat{o}^B, \quad (\mathbf{e}_\theta+i\mathbf{e}_\varphi)_j=\sigma_{jAB}o^Ao^B. \tag{15}$$

In terms of o^A and $\hat{o}^A$ the spherical harmonics are given by

$$Y_{lm}=(-1)^m\frac{(2l)!}{l!}\left[\frac{2l+1}{4\pi}\,\frac{1}{(l+m)!(l-m)!}\right]^{1/2}\overbrace{\underbrace{o^{(1}o^1\cdots o^1}_{l}\underbrace{\hat{o}^1\hat{o}^2\cdots\hat{o}^{2)}}_{l}}^{(l-m)1\text{'s},\,(l+m)2\text{'s}}, \tag{16}$$

where the parentheses denote symmetrization on the indices enclosed. Since the number of o^A's and of $\hat{o}^A$'s appearing in (16) coincide, the spherical harmonics (16) are invariant under the transformation

$$o^A\mapsto e^{i\alpha/2}o^A \tag{17}$$

(which implies that $\hat{o}^A\mapsto e^{-i\alpha/2}\hat{o}^A$). A quantity η has spin weight s if under the transformation (17) transforms according to $\eta\mapsto e^{is\alpha}\eta$.[4] Thus, the ordinary spherical harmonics have spin weight 0.

The spherical components of a totally symmetric $2S$-index spinor field, $\phi_{AB\cdots D}$, are obtained by contracting all its indices with o^A's and $\hat{o}^A$'s. For $s=-S,-S+1,\ldots,S$, the spherical component of $\phi_{AB\cdots D}$,

$${}_s\phi\equiv\phi_{AB\cdots D}\underbrace{o^Ao^B\cdots\hat{o}^D}_{(S+s)o\text{'s},(S-s)\hat{o}\text{'s}} \tag{18}$$

has spin weight s. For instance, the three spherical components of a spin-1 field (which is just a possibly complex vector field) are [see Eqs. (10) and (15)]

$$
{}_1\phi = \phi_{AB} o^A o^B = \frac{1}{\sqrt{2}}\,\boldsymbol{\phi}\cdot(\mathbf{e}_\theta + i\mathbf{e}_\varphi),
$$

$$
{}_0\phi = \phi_{AB} o^A \hat{o}^B = -\frac{1}{\sqrt{2}}\,\boldsymbol{\phi}\cdot\mathbf{e}_r\,, \tag{19}
$$

$$
{}_{-1}\phi = \phi_{AB} \hat{o}^A \hat{o}^B = -\frac{1}{\sqrt{2}}\,\boldsymbol{\phi}\cdot(\mathbf{e}_\theta - i\mathbf{e}_\varphi),
$$

where $\boldsymbol{\phi}$ is the vector field with Cartesian components $\phi_i = -(1/\sqrt{2})\sigma_{iAB}\phi^{AB}$ [see Eq. (4)]. Hence, $\boldsymbol{\phi} = -{}_{-1}\phi\,(1/\sqrt{2})(\mathbf{e}_\theta + i\mathbf{e}_\varphi) + {}_1\phi\,(1/\sqrt{2})(\mathbf{e}_\theta - i\mathbf{e}_\varphi) - {}_0\phi\,\sqrt{2}\mathbf{e}_r$. Similarly, any one-index spinor field, ϕ^A, can be expressed as $\phi^A = (\phi_B o^B)\hat{o}^A - (\phi_B \hat{o}^B) o^A = {}_{1/2}\phi\,\hat{o}^A - {}_{-1/2}\phi\, o^A$.

The spin-weighted spherical harmonics,[4–6] ${}_sY_{jm}$, can also be expressed in terms of o and $\hat{o}$ as[7]

$$
{}_sY_{jm} = (-1)^m \left[\frac{2j+1}{4\pi}\,\frac{(2j)!}{(j+m)!(j-m)!}\,\frac{(2j)!}{(j+s)!(j-s)!}\right]^{1/2} \underbrace{\overbrace{o^{(1} o^1 \cdots o^1}^{j+s}\,\overbrace{\hat{o}^1 \hat{o}^2 \cdots \hat{o}^{2)}}^{j-s}}^{(j-m)1\text{'s},\,(j+m)2\text{'s}}, \tag{20}
$$

with $j = 0, 1/2, 1, \ldots$, $m = -j, -j+1, \ldots, j$, $s = -j, -j+1, \ldots, j$. Thus, $Y_{jm} = {}_0Y_{jm}$ and ${}_sY_{jm}$ has spin weight s. The spin-weighted spherical harmonics are related to the Wigner D functions by[5,7]

$$
\overline{D^l_{m'm}(\varphi,\theta,\chi)} = (-1)^{-m}\sqrt{\frac{4\pi}{2l+1}}\,{}_{-m}Y_{lm'}(\theta,\varphi)e^{im\chi}, \tag{21}
$$

where φ, θ, χ are Euler angles; therefore, from[8,9]

$$
D^j_{ms}(\varphi,\theta,\chi) D^{j'}_{m's'}(\varphi,\theta,\chi) = \sum_{J,M,S} \langle jj';mm'|jj';JM\rangle\ \langle jj';ss'|jj';JS\rangle\ D^J_{MS}(\varphi,\theta,\chi),
$$

where the $\langle jj';mm'|jj';JM\rangle$ denote the Clebsch–Gordan coefficients, it follows that

$$
\begin{aligned}
{}_sY_{jm}(\theta,\varphi)\ {}_{s'}Y_{j'm'}(\theta,\varphi) = \sum_{J,M,S} (-1)^{j+j'-J}\sqrt{\frac{(2j+1)(2j'+1)}{4\pi(2J+1)}}\ \langle jj';mm'|jj';JM\rangle \\
\times \langle jj';ss'|jj';JS\rangle\ {}_SY_{JM}(\theta,\varphi).
\end{aligned} \tag{22}
$$

III. PLANE WAVES

The totally symmetric $2S$-index spinor field

$$
\phi_{AB\cdots D} = \chi_{AB\cdots D} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}, \tag{23}
$$

where $\chi_{AB\cdots D}$ is a *constant* totally symmetric spinor, corresponds to a spin-S plane wave propagating in the direction of the wave vector $\mathbf{k}$. The Cartesian components of $\mathbf{k}$ can be written in terms of the constant one-index spinor

$$
\begin{pmatrix} \kappa^1 \\ \kappa^2 \end{pmatrix} = \begin{pmatrix} e^{-i\varphi'/2}\cos(\theta'/2) \\ e^{i\varphi'/2}\sin(\theta'/2) \end{pmatrix}, \tag{24}
$$

where θ' and φ' are the polar and azimuth angles of the wave vector $\mathbf{k}$ [cf. Eq. (14)], which satisfies $\kappa^A \hat{\kappa}_A = 1$, according to

$$k_i = -|\mathbf{k}|\,\sigma_{iAB}\kappa^A\hat{\kappa}^B \tag{25}$$

[cf. Eq. (12)]. Then the spinor $\chi_{AB\cdots D}$ can be expressed as a linear combination (with constant coefficients) of the $2S+1$ symmetrized products $\kappa_A\kappa_B\cdots\kappa_D$, $\hat{\kappa}_{(A}\kappa_B\cdots\kappa_{D)}$, $\hat{\kappa}_{(A}\hat{\kappa}_B\cdots\kappa_{D)},\ldots,$ $\hat{\kappa}_A\hat{\kappa}_B\cdots\hat{\kappa}_D$; therefore, it suffices to consider plane waves of the form

$$\underbrace{\kappa_{(A}\kappa_B\cdots\hat{\kappa}_{D)}}_{(S+s')\kappa\text{'s},(S-s')\hat{\kappa}\text{'s}}\ \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)},\quad s'=-S,-S+1,\ldots,S. \tag{26}$$

The parameter s' corresponds to the helicity[3] of the wave.

The allowed values of s' depend on the equations satisfied by the field under consideration. For instance, the equations for a massless free field are

$$\sqrt{2}\,\partial^R{}_{(A}\phi_{B\cdots D)R} = \pm\frac{1}{c}\frac{\partial}{\partial t}\phi_{AB\cdots D}, \tag{27}$$

and

$$\partial^{AB}\phi_{AB\cdots D} = 0, \tag{28}$$

where $\partial_{AB} = (1/\sqrt{2})\sigma^i{}_{AB}(\partial/\partial x^i)$, $\phi_{AB\cdots D}$ is a $2S$-index totally symmetric spinor and the sign on the right-hand side of Eq. (27) depends on the helicity of the field. Substituting Eq. (23) into Eqs. (27) and (28), assuming $\omega>0$, one finds that $\chi_{AB\cdots D}$ must be equal to $\kappa_A\kappa_B\cdots\kappa_D$ or to $\hat{\kappa}_A\hat{\kappa}_B\cdots\hat{\kappa}_D$, according to whether the sign on the right-hand side of Eq. (27) is plus or minus, respectively. Thus, s' only takes the values S and $-S$. In the case of the Weyl equation for the (massless) neutrino the only possible value of s' is $-1/2$.

According to Eq. (18), the spherical (or spin-weighted) components of the plane wave (26) are

$${}_s\phi = \underbrace{o^A o^B\cdots\hat{o}^D}_{(S+s)o\text{'s},(S-s)\hat{o}\text{'s}}\ \underbrace{\kappa_{(A}\kappa_B\cdots\hat{\kappa}_{D)}}_{(S+s')\kappa\text{'s},(S-s')\hat{\kappa}\text{'s}}\ \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}. \tag{29}$$

Making use of Eq. (20) one finds that

$$\underbrace{o^A o^B\cdots\hat{o}^D}_{(S+s)o\text{'s},(S-s)\hat{o}\text{'s}}\ \underbrace{\kappa_{(A}\kappa_B\cdots\hat{\kappa}_{D)}}_{(S+s')\kappa\text{'s},(S-s')\hat{\kappa}\text{'s}} = (-1)^{S+s'}\frac{4\pi}{2S+1}\left[\frac{(S+s)!(S-s)!}{(2S)!}\,\frac{(S+s')!(S-s')!}{(2S)!}\right]^{1/2}$$
$$\times\sum_{m=-S}^{S}{}_sY_{Sm}(\theta,\varphi)\ \overline{{}_{-s'}Y_{Sm}(\theta',\varphi')}. \tag{30}$$

From this last relation, taking $\kappa^A = o^A$, one obtains the formula

$$\sum_{m=-S}^{S}{}_sY_{Sm}(\theta,\varphi)\ \overline{{}_{s'}Y_{Sm}(\theta,\varphi)} = \frac{2S+1}{4\pi}\,\delta_{ss'},$$

which also follows from Eq. (21) using the fact that the Wigner functions are the matrix elements of a representation of the rotation group.[7]

Using now Eqs. (22) and (30), the expansion

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l} i^l j_l(kr)Y_{lm}(\theta,\varphi)\ \overline{Y_{lm}(\theta',\varphi')}, \tag{31}$$

and the properties of the Clebsch–Gordan coefficients we find that the component ${}_s\phi$, defined by Eq. (29), has the expansion

$$
{}_s\phi=(-1)^{S+s'}4\pi\left[\frac{(S+s)!(S-s)!}{(2S)!}\,\frac{(S+s')!(S-s')!}{(2S)!}\right]^{1/2}\sum_{J,M}\overline{{}_{-s'}Y_{JM}(\theta',\varphi')}
$$

$$
\times\left[\sum_{l=|J-S|}^{J+S}\frac{2l+1}{2J+1}\langle lS;Js|lS;0s\rangle\ \langle lS;0,-s'|lS;J,-s'\rangle i^l j_l(kr)\right]{}_sY_{JM}(\theta,\varphi)e^{-i\omega t},
\tag{32}
$$

which expresses each spherical component of the helicity-s' plane wave (26) as a superposition of eigenfunctions of the square of the total angular momentum and of the z component of the total angular momentum.

For example, according to Eq. (32), the multipole expansion of the Weyl neutrino field $\phi_A=\hat{\kappa}_A e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$, is given by

$$
\begin{pmatrix}{}_{1/2}\phi\\ {}_{-1/2}\phi\end{pmatrix}=2\pi\sum_{J,M}\overline{{}_{1/2}Y_{JM}(\theta',\varphi')}i^{J-1/2}\begin{pmatrix}(j_{J-1/2}(kr)+ij_{J+1/2}(kr)){}_{1/2}Y_{JM}(\theta,\varphi)\\ (j_{J-1/2}(kr)-ij_{J+1/2}(kr)){}_{-1/2}Y_{JM}(\theta,\varphi)\end{pmatrix}e^{-i\omega t}.
\tag{33}
$$

Similarly, for the spin-3/2 field $\phi_{ABC}=\hat{\kappa}_A\hat{\kappa}_B\hat{\kappa}_C e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ one readily obtains

$$
\begin{pmatrix}{}_{3/2}\phi\\ {}_{1/2}\phi\\ {}_{-1/2}\phi\\ {}_{-3/2}\phi\end{pmatrix}=\frac{\pi}{2}\sum_{J,M}\overline{{}_{3/2}Y_{JM}(\theta',\varphi')}i^{J-3/2}\begin{pmatrix}f_J^+(kr){}_{3/2}Y_{JM}(\theta,\varphi)\\ g_J^+(kr){}_{1/2}Y_{JM}(\theta,\varphi)\\ g_J^-(kr){}_{-1/2}Y_{JM}(\theta,\varphi)\\ f_J^-(kr){}_{-3/2}Y_{JM}(\theta,\varphi)\end{pmatrix}e^{-i\omega t},
\tag{34}
$$

where

$$
f_J^{\pm}(x)\equiv\frac{1}{J(J+1)}\left[(J+1)\left(J+\frac{3}{2}\right)j_{J-3/2}(x)\pm 3iJ\left(J+\frac{3}{2}\right)j_{J-1/2}(x)-3\left(J-\frac{1}{2}\right)(J+1)j_{J+1/2}(x)\right.
$$

$$
\left.\mp iJ\left(J-\frac{1}{2}\right)j_{J+3/2}(x)\right],
$$

$$
g_J^{\pm}(x)\equiv\frac{\sqrt{(J-\frac{1}{2})(J+\frac{3}{2})}}{J(J+1)}[(J+1)j_{J-3/2}(x)\pm iJj_{J-1/2}(x)+(J+1)j_{J+1/2}(x)\mp iJj_{J+3/2}(x)].
$$

It may be remarked that the fields

$$
\begin{pmatrix}{}_{3/2}\phi\\ {}_{1/2}\phi\\ {}_{-1/2}\phi\\ {}_{-3/2}\phi\end{pmatrix}=\begin{pmatrix}f_J^+(kr){}_{3/2}Y_{JM}(\theta,\varphi)\\ g_J^+(kr){}_{1/2}Y_{JM}(\theta,\varphi)\\ g_J^-(kr){}_{-1/2}Y_{JM}(\theta,\varphi)\\ f_J^-(kr){}_{-3/2}Y_{JM}(\theta,\varphi)\end{pmatrix}e^{-i\omega t},
$$

appearing in Eq. (34), are separable solutions in spherical coordinates of Eqs. (27) and (28) with $S=3/2$, $s'=-3/2$, and Eq. (34) is the relation between two different bases of the solutions of these equations, with $\overline{{}_{3/2}Y_{JM}(\theta',\varphi')}$ being essentially the matrix elements of this relation. Similarly, Eqs. (31)–(33) correspond to changes of bases and, in all cases, the matrix elements of these (unitary) transformations are proportional to $\overline{{}_{-s'}Y_{JM}(\theta',\varphi')}$.

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Remarks on the connection between the additive separation of the Hamilton–Jacobi equation and the multiplicative separation of the Schrödinger equation. I. The completeness and Robertson conditions

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The fundamental elements of the variable separation theory are revisited, including the Eisenhart and Robertson theorems, Kalnins–Miller theory, and the intrinsic characterization of the separation of the Hamilton–Jacobi equation, in a unitary and geometrical perspective. The general notion of complete integrability of first-order normal systems of PDEs leads in a natural way to completeness conditions for separated solutions of the Schrödinger equation and to the Robertson condition. Two general types of multiplicative separation for the Schrödinger equation are defined and analyzed: they are called ''free'' and ''reduced'' separation, respectively. In the free separation the coordinates are necessarily orthogonal, while the reduced separation may occur in nonorthogonal coordinates, but only in the presence of symmetries (Killing vectors). © *2002 American Institute of Physics.*
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I. INTRODUCTION

With a smooth real function V (potential energy) on a Riemannian manifold $(Q_n, \mathbf{g})$ (configuration manifold) we associate two differential equations, the time-independent Hamilton–Jacobi equation

$$\tfrac{1}{2}\nabla W \cdot \nabla W + V = E, \tag{1.1}$$

and the corresponding steady-state Schrödinger equation

$$-\frac{\hbar^2}{2}\Delta\psi + (V-E)\psi = 0. \tag{1.2}$$

In these equations, E is a constant parameter (the energy constant), ∇ is the gradient operator

$$(\nabla W)^i = g^{ij}\partial_j W,$$

and Δ is the Laplace–Beltrami operator

$$\Delta\psi = g^{ij}\nabla_i\nabla_j\psi,$$

where ∇_i is the covariant derivative with respect to the Levi-Civita connection. Besides the well-known physical connection between these two equations (we consider here the time-independent case only), there is an interesting mathematical connection due to the phenomenon of the *separation of variables*.

It is well known that, in many interesting cases, these equations admit *local separated solutions* of the form

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$$W(\underline{q},\underline{c})=\sum_{i=1}^{n} W_i(q^i,\underline{c}) \tag{1.3}$$

for the Hamilton–Jacobi equation, and of the form

$$\psi(\underline{q},\underline{c})=\prod_{i=1}^{n} \psi_i(q^i,\underline{c}), \tag{1.4}$$

or

$$\psi(\underline{q},\underline{c})=e^{R(\underline{q})}\prod_{i=1}^{n} \psi_i(q^i,\underline{c}), \tag{1.5}$$

for the Schrödinger equation, where $\underline{q}=(q^i)$ is a suitable coordinate system on Q, and $\underline{c}$ denotes a set of constant parameters, whose number depends on an appropriate definition of *separation*. Note that in (1.5) the function $R(\underline{q})$ does not depend on the constant parameters: this kind of separation is called *R-separation*.

It happens that for solutions of this kind, Eqs. (1.1) and (1.2) become equivalent to a system of ordinary differential *separated equations*, each one involving a single coordinate. The interesting fact is that, in most cases, the separation of variables occurs simultaneously for both equations and in the same coordinate system. Although this fact is easy to illustrate for basic important examples, its general description and motivation is rather difficult and subtle to understand. Let us consider, for instance, the particular case of the orthogonal separation, where $g^{ij}=0$ for $i\neq j$. For this kind of separation we usually refer to three classical theorems of Stäckel, Robertson, and Eisenhart.[1–3]

Theorem 1.1: (Stäckel, 1893) *The Hamilton–Jacobi equation is separable in orthogonal coordinates $\underline{q}$ if and only if the diagonal components g^{ii} of the metric tensor and the potential V have the form*

$$g^{ii}=\varphi^i_{(n)}, \quad V=\phi_i g^{ii}=\phi_i\varphi^i_{(n)}, \tag{1.6}$$

where $\varphi^i_{(n)}$ is the last row of the inverse $[\varphi^i_{(j)}]$ of an $n\times n$ Stäckel matrix $[\varphi^{(j)}_i]$ and ϕ_i are functions of the coordinate corresponding to the index only.

A *Stäckel matrix* is a regular $n\times n$ matrix whose components $\varphi^{(j)}_i(q^i)$ are functions depending on the coordinate corresponding to the lower index only. A function V of the kind (1.6) is then called a *Stäckel multiplier*.

Theorem 1.2: (Robertson, 1927) *The Schrödinger equation is separable in orthogonal coordinates $\underline{q}$ if and only if in these coordinates the Hamilton–Jacobi equation is separable (i.e., the Stäckel requirements are satisfied) and moreover, the following condition is satisfied*

$$\sqrt{\Pi^n_{i=1}g^{ii}}\det(\varphi^{(j)}_i)=\Pi^n_{i=1}f_i(q^i), \tag{1.7}$$

where $f_i(q^i)$ are functions of the corresponding coordinate only.

This additional requirement is called the *Robertson condition*. It has a meaningful geometrical interpretation:

Theorem 1.3: (Eisenhart, 1934) *The Robertson condition is satisfied if and only if the Ricci tensor is diagonal:*

$$R_{ij}=0, \quad i\neq j.$$

However, while it can be easily seen that requirements (1.6) and (1.7) are sufficient for reducing the Schrödinger equation to separated equations, the proof given by Robertson (and

accepted by Eisenhart) that they are also necessary for the separation is not satisfactory. This is due to the fact that for the separability of the Schrödinger equation these authors assumed (apparently) the existence of a single solution of the kind

$$\psi(\underline{q}) = \Pi_{i=1}^{n} \psi_i(q^i),$$

without any reference to the presence and to the role of constant (real or complex) parameters [as is done in analytical mechanics for a complete solution of the Hamilton–Jacobi (HJ) equation]. Indeed, as we shall see in the following, the existence of a single separated solution of the Schrödinger equation does not imply the separation of the HJ equation for the same reason that the existence of a single solution of a first-order differential system does not imply, in general, its complete integrability. In other words, while for the HJ equation one looks for a separated solution (1.3) containing n constant parameters $\underline{c} = (c_i)$ satisfying the *completeness condition*

$$\det\left[\frac{\partial^2 W}{\partial q^i \partial c_j}\right] = \det\left[\frac{\partial p_i}{\partial c_j}\right] \neq 0, \quad p_i = W_i', \tag{1.8}$$

a similar requirement for a separated solution (1.4) of the Schrödinger equation does not appear explicitly either in the celebrated works cited previously or in many other standard reference books.[4,5] In fact, also for the Schrödinger equation we are not interested in a single separated solution, but in a parametrized family of local solutions, in order to build up a global one satisfying suitable boundary or normalization conditions. In conclusion: the statements of Robertson and Eisenhart (Theorems 1.2 and 1.3) are meaningless without a proper definition of *separation* of the Schrödinger equation.

A first ''precise'' definition of separation has been proposed by Koornwinder[6] within a rather general context, and strongly related to the basic properties of the Stäckel matrices. However, the systematic use of these matrices hides many interesting intrinsic features of the separation connected, for instance, with the existence of Killing tensors and of second-order symmetries of the Schrödinger equation. Other definitions of separation have been introduced by Olevsky[7] and more recently by Zhdanov and Zhalij[8] (both for the case $n=3$).

A crucial contribution to this matter is due to Kalnins and Miller.[9,10] Their approach is based on a definition of *regular* additive separation of a generalized Hamilton–Jacobi equation of any order, which is equivalent to the complete integrability of a suitable first-order differential system. In such a way they give an extension of the classical Levi-Civita separability conditions.[11] As a second step, they relate the definition of multiplicative separation of the Schrödinger equation to the additive separation of a suitable second-order Hamilton–Jacobi equation. A similar approach has been followed earlier by Agostinelli.[12] Kalnins and Miller begin their analysis of the separation of the Schrödinger equation by assuming that the coordinates are orthogonal, while in Agostinelli's paper (as well as in that of Koornwinder) it is shown that for the regular separation of the Schrödinger equation (in the sense of Kalnins and Miller) the coordinates are in fact necessarily orthogonal. Furthermore, Agostinelli shows that the nonorthogonal separation occurs when some of the separated factors ψ_i in (1.4) are of a special kind and the corresponding coordinates are ignorable. However, Agostinelli's approach is heavily coordinate dependent and somehow unsatisfactory, since at that time the geometrical theory of the variable separation of the Hamilton–Jacobi equation was not yet developed.

These remarks show that a revisitation and a resetting of all this matter is needed, from the very beginning, in light of the recent developments of the separability theory. The crucial question for a correct definition of separation for the Schrödinger equation is, as we said previously, how many constant parameters should enter a multiplicative separated solution and which conditions should they satisfy; in other words, as well as for the Hamilton–Jacobi equation, we need a *completeness condition* for a solution of the Schrödinger equation.

In the present paper it is shown that a completeness condition follows necessarily and in a ''natural'' way (i.e., without any consideration concerning the particular kind of equation we are

dealing with) from the general theory of the first-order normal differential systems (recalled in Sec. II, from a geometrical view point) applied to the general theory of the additive separation of Kalnins and Miller. The resulting definition of separation is quite different from those previously proposed in Refs. 6–8. First of all because it is not unique. Indeed, following our general approach we are led, again in a ''natural'' way, to consider at least two types of separation for the Schrödinger equation, which we have called *free* and *constrained*, respectively. These terms are motivated by the fact that one can impose ''constraints'' on some of the factors $\psi_i(q^i)$ of a separated solution; in other words, one can assume that some of these factors have a special form or satisfy a special kind of equations. One can, for instance, impose that $n-m$ factors have the form $\psi_\alpha = \exp(c_\alpha q^\alpha)$, for $\alpha = m+1,...,n$, where c_α are arbitrary constants (see Refs. 12 and 13). We call *reduced separation* a constrained separation of this type. The remarkable fact is that, as a consequence of these assumptions, in the free separation the coordinates are necessarily orthogonal and the number of essential parameters entering the completeness condition is $2n$, while the reduced separation may occur in nonorthogonal coordinates and the number of the essential parameters reduces to $m+n<2n$, including (c_α). This is apparently in contrast to a common ''ansatz'' which considers only n parameters in a separated solution.[6,13,14] In fact, as we shall see, up to a transformation of the $2n$ parameters entering the completeness condition for the free separation, half of them are true ''separation constants'' corresponding to constants of motion (first integrals), while the remaining n are integration constants. This is quite reasonable since we are dealing with second-order equations. For a correct definition of ''completeness'' both groups of constant parameters are jointly involved, but in the process of integration by separation of variables all these essential constants automatically find their own place. This explains the curious fact that, in spite of the absence of the notion of ''complete separable solution,'' the method of separation of variables in the Schrödinger equation has been applied with success, at least in the elementary cases. Thus, the content of the present paper is essentially theoretical and propedeutical to a further analysis of remaining topics on the separation: the relationship between first integrals and symmetry operators, the *R*-separation, the extensions to the case in which a vector potential is present, and to the case of a Lorentzian metric. As we shall see, a conspicuous and rich matter is hidden behind the usual approach to the separation of the Schrödinger equation.

II. FIRST-ORDER DIFFERENTIAL SYSTEMS AND THE GENERAL DEFINITION OF SEPARATION

Let us recall some classical basic facts concerning normal systems of first-order partial differential equations, from a geometrical viewpoint and in a way suitable for our purposes.

Let us consider a trivial fibration $\pi: M = Q \times Z \to Q$, where Z is an N-dimensional linear space (over $\mathbb{C}$ or $\mathbb{R}$) with coordinates $\underline{z} = (z_A)$ (capital indices $A,B,...$ will run from 1 to N) and Q is an n-dimensional real differentiable manifold, with local coordinates $\underline{q} = (q^i)$ (latin indices $h,i,j,...$ will run from 1 to n). A *connection* over this fibration is a regular distribution C over the tangent bundle TZ transversal and complementary to the fibers of π. This means that C is a subbundle of TM such that at each point $x \in M$ the set $C_x = C \cap T_x M$ is an n-dimensional subspace transversal to the fiber at the point z. A vector field D over M is *horizontal* if $D(M) \subset C$ i.e., if $D(x) \in C_x$ for each $x \in M$. A vector field V over M is *vertical* if it is tangent to the fibers. The only field which is simultaneously vertical and horizontal is the zero-vector field. If we consider local coordinates $(\underline{q},\underline{z}) = (q^i, z_A)$ of M, then the distribution C is locally spanned by the following n horizontal vector fields (interpreted as derivations):

$$D_i = \frac{\partial}{\partial q^i} + C_{iA}\frac{\partial}{\partial z_A}, \tag{2.1}$$

called *generators* of C. The functions C_{iA} are the *coefficients* of the connection in these coordinates. It can be seen that the Lie brackets of two generators (as well as of any two horizontal vector fields) are vertical. Hence, by the Frobenius theorem, the distribution C is completely integrable (i.e., the connection C is *flat*) if and only if the generators commute,

$$[D_i, D_j] = 0. \tag{2.2}$$

The complete integrability of C means that there exists a foliation of integral manifolds transversal to the fibers and locally represented by equations of the kind

$$z_A = f_A(\underline{q}, \underline{c}), \tag{2.3}$$

where the N functions f_A depend on N constant parameters $\underline{c} = (c_A)$ which must be uniquely determined by assigning at any fixed point $q_0 \in Q$ (belonging to the domain of the coordinates) any arbitrary set of values of $\underline{z}$. This means that the functions (2.3) satisfy the *completeness condition*

$$\det\left[\frac{\partial \underline{z}}{\partial \underline{c}}\right] \neq 0. \tag{2.4}$$

Moreover, since the integral manifolds are tangent to the generators, equations

$$D_i(z_A - f_A(\underline{q}, \underline{c})) = 0$$

must be identically satisfied. Due to (2.1), these equations are equivalent to

$$\partial_i z_A = C_{iA}(\underline{q}, \underline{z}). \tag{2.5}$$

This proves that

Theorem 2.1: *A first-order differential system in the* normal form (2.5) *is* completely integrable, *i.e., it admits a local* complete solution (2.3) *satisfying the completeness condition* (2.4) *if and only if the generators* D_i *commute,* $[D_i, D_j] = 0$.

On the basis of these general considerations, we can reformulate the definition of separation of Kalnins and Miller[9,10] as follows. Let us consider a partial differential equation

$$\mathcal{H}(\underline{q}, u, u_i, u_{ij}, \ldots, u_{ij\cdots h}) = E, \tag{2.6}$$

in the independent variables $\underline{q} = (q^i)$ and in the unknown function $u(\underline{q})$. Here $u_{ij\cdots h}$ denote the partial derivatives of u with respect to these variables, E is a constant parameter, and $\mathcal{H}$ is a smooth real function of the variables $\underline{q}$, u and its partial derivatives up to a degree l. A *separable solution* of this equation is a solution of the form

$$u = \sum_{i=1}^{n} S_i(q^i, E), \tag{2.7}$$

i.e., a sum of functions depending on a single variable. For separable solutions all the mixed partial derivatives (corresponding to distinct indices) vanish identically, so that Eq. (2.6) gets the simpler form

$$\mathcal{H}_s(\underline{q}, u, \underline{u}^{(1)}, \underline{u}^{(2)}, \ldots, \underline{u}^{(l)}) = E, \tag{2.8}$$

where $\underline{u}^{(1)} = (u_i^{(1)}) = (u_i)$, $\underline{u}^{(2)} = (u_i^{(2)}) = (u_{ii})$, etc., and $\mathcal{H}_s$ is the function we get by replacing $u_{i\cdots j} = 0$ in $\mathcal{H}$, for at least two distinct indices. Note that $\mathcal{H}_s$ in (2.8) is in general a function different from $\mathcal{H}$ in (2.6). However, for the sake of simplicity, in the following discussion we shall use the same symbol $\mathcal{H}$. Since for any solution of this equation the left-hand side of (2.8) reduces to a constant, the total derivatives of $\mathcal{H}$ with respect to the coordinates must vanish identically,

$$\frac{\partial \mathcal{H}}{\partial q^i} + \frac{\partial \mathcal{H}}{\partial u} u_i + \frac{\partial \mathcal{H}}{\partial u_i} u_i^{(2)} + \frac{\partial \mathcal{H}}{\partial u_i^{(2)}} u_i^{(3)} + \cdots + \frac{\partial \mathcal{H}}{\partial u_i^{(l)}} u_i^{(l+1)} = 0. \tag{2.9}$$

Hence, for

$$\frac{\partial \mathcal{H}}{\partial u_i^{(l)}} \neq 0$$

we can define the function

$$R_i(\underline{q},u,\underline{u}^{(1)},\underline{u}^{(2)},\ldots,\underline{u}^{(l)}) = -\left(\frac{\partial \mathcal{H}}{\partial u_i^{(l)}}\right)^{-1} \times\left(\frac{\partial \mathcal{H}}{\partial q^i}+\frac{\partial \mathcal{H}}{\partial u}u_i^{(1)}+\frac{\partial \mathcal{H}}{\partial u_i}u_i^{(2)}+\frac{\partial \mathcal{H}}{\partial u_i^{(2)}}u_i^{(3)}+\cdots+\frac{\partial \mathcal{H}}{\partial u_i^{(l-1)}}u_i^{(l)}\right), \tag{2.10}$$

so that Eq. (2.9) becomes

$$u_i^{(l+1)} = R_i(\underline{q},u,\underline{u}^{(1)},\underline{u}^{(2)},\ldots,\underline{u}^{(l)}).$$

Now, let us consider the following first-order differential system where $j \neq i$ and $\partial_i = \frac{\partial}{\partial q i}$:

$$\begin{aligned} &\partial_i u = u_i^{(1)}, \\ &\partial_i u_i^{(1)} = u_i^{(2)}, \quad \partial_i u_j^{(1)} = 0, \\ &\partial_i u_i^{(2)} = u_i^{(3)}, \quad \partial_i u_j^{(2)} = 0, \\ &\cdots \quad \cdots \\ &\partial_i u_i^{(l)} = R_i, \quad \partial_i u_j^{(l)} = 0. \end{aligned} \tag{2.11}$$

This is a normal system of the kind (2.5) in the unknown $N = n \cdot l + 1$ functions

$$\underline{z} = (z_A) = (u,\underline{u}^{(1)},\underline{u}^{(2)},\ldots,\underline{u}^{(l)}).$$

The comparison with (2.1) and (2.5) shows that the corresponding generators are

$$D_i = \partial_i + u_i^{(1)}\frac{\partial}{\partial u} + u_i^{(2)}\frac{\partial}{\partial u_i^{(1)}} + u_i^{(3)}\frac{\partial}{\partial u_i^{(2)}} + \cdots + R_i\frac{\partial}{\partial u_i^{(l)}}. \tag{2.12}$$

We remark that a separable solution (2.7) corresponds to a solution of this system. Due to Theorem 2.1 we can introduce the following

Definition 2.2: We say that Eq. (2.6) is *separable* in the coordinates $\underline{q}$ if it admits a *complete separable* solution, i.e., a solution of the form

$$u = \sum_{i=1}^{n} S_i(q^i,\underline{c}) \tag{2.13}$$

depending on $N = nl + 1$ constant parameters $\underline{c} = (c_A)$ and satisfying the *completeness condition*

$$\det\left[\frac{\partial \underline{z}}{\partial \underline{c}}\right] = \det\left[\frac{\partial u}{\partial c_A}\middle|\frac{\partial u_i}{\partial c_A}\middle|\frac{\partial u_i^{(2)}}{\partial c_A}\middle|\cdots\middle|\frac{\partial u_i^{(l)}}{\partial c_A}\right] \neq 0. \tag{2.14}$$

It follows that

Theorem 2.3: *Equation (2.6) is separable (i.e., it admits a complete separable solution) in the coordinates $\underline{q}$ if and only if the first-order system (2.11) is completely integrable, i.e., if and only if the separability conditions*

$$[D_i, D_j] = 0 \tag{2.15}$$

are identically satisfied for D_i defined by (2.12) and R_i defined by (2.10).

Remark 2.4: In the following applications we shall deal with equations of the kind (2.6) or (2.8) where $\mathcal{H}$ does not depend on u. In this case the dependent variables are

$$\underline{z} = (z_A) = (\underline{u}^{(1)}, \underline{u}^{(2)}, \ldots, \underline{u}^{(l)}),$$

and the first line of system (2.11) disappears, as well as the term $\partial/\partial u$ in the generators (2.12). Moreover, the number of the constants $\underline{c} = (c_A)$ entering a complete solution (2.13) is $n \cdot l$, and the completeness condition (2.14) reduces to

$$\det\left[\frac{\partial \underline{z}}{\partial \underline{c}}\right] = \det\left[\frac{\partial u_i}{\partial c_A} \middle| \frac{\partial u_i^{(2)}}{\partial c_A} \middle| \cdots \middle| \frac{\partial u_i^{(l)}}{\partial c_A}\right] \neq 0. \tag{2.16}$$

Remark 2.5: The case in which the complete integrability conditions (2.15) are identically satisfied corresponds to the case of *regular separation* of Kalnins and Miller.[9] They call *non-regular* a type of separation in which these conditions are nonidentically satisfied and, consequently, separable solutions may exist, but depending on a reduced number of constants. However, the meaning of this non-regular separation is rather obscure. As we shall see (Sec. V), in dealing with the Schrödinger equation we are led to introduce, in natural way, an alternative definition of the regular separation: the reduced separation.

Remark 2.6: Definition 2.2 and Theorem 2.3 are the basic statements for the theory of variable separation (additive, multiplicative, or any other kind) provided the kind of separation we are dealing with can be transformed, by a suitable transformation, into an additive separation. This is in fact the case of the multiplicative separation: the transformation is $u = \ln \psi$.

III. THE LEVI-CIVITA SEPARABILITY CONDITIONS AND THEIR CONSEQUENCES

Let us apply the general theory illustrated in Sec. II to the case of the Hamilton–Jacobi equation corresponding to a Hamiltonian $H: T^*Q \to \mathbb{R}$ over a cotangent bundle T^*Q. In this case we deal with the cotangent fibration $\pi: M = T^*Q \to Q$ of a configuration manifold Q. This is (in general) a nontrivial fibration, but our previous considerations can be applied, since they have a local character.

The differential equation (2.6) is now

$$H(\underline{q}, \underline{u}^{(1)}) = E, \tag{3.1}$$

with $\mathcal{H} = H$ and, according to the standard notation,

$$u = W, \quad \underline{u}^{(1)} = (u_i) = (p_i) = (\partial_i W).$$

Now $l = 1$ and $\underline{z} = (\underline{u}^{(1)}) = (p_i)$. In a complete solution we have exactly n constants $\underline{c} = (c_i)$ and the completeness condition (2.16) takes the form (1.8),

$$\det\left[\frac{\partial p_i}{\partial c_j}\right] \neq 0. \tag{3.2}$$

The differential system (2.11) reads

$$\partial_i p_i = R_i, \quad \partial_i p_j = 0 \quad (j \neq i), \tag{3.3}$$

where the functions R_i (2.10) are

$$R_i = -\frac{\partial_i H}{\partial^i H} \quad \left(\partial_i = \frac{\partial}{\partial q^i}, \partial^i = \frac{\partial}{\partial p_i}\right).$$

Since the generators D_i (2.14) are

$$D_i = \partial_i + R_i \partial^i,$$

the separability conditions $[D_i, D_j] = 0$ (2.15) are equivalent to the well-known *Levi-Civita separability conditions*

$$\partial^i \partial^j H \partial_i H \partial_j H + \partial_i \partial_j H \partial^i H \partial^j H - \partial^i \partial_j H \partial_i H \partial^j H - \partial_i \partial^j H \partial^i H \partial_j H = 0, \quad i \neq j, \ \text{n.s.}, \tag{3.4}$$

where "n.s." means that there is no summation over the repeated indices. As a consequence, Theorem 2.3 reduces to the celebrated *Levi-Civita theorem*,

Theorem 3.1: *The Hamilton–Jacobi equation (3.1) is separable in the coordinates* $\underline{q} = (q^i)$ *i.e., it admits a solution of the kind (2.3) satisfying the completeness condition (3.2), if and only if (3.4) are identically satisfied.*

This theorem holds for any kind of Hamiltonian. We can apply it to a *natural Hamiltonian*

$$H = G + V = \tfrac{1}{2} g^{ij}(\underline{q}) p_i p_j + V(\underline{q}),$$

where G is the geodesic Hamiltonian, $V: Q \to \mathbb{R}$ a potential energy. The corresponding Hamilton–Jacobi equation is now Eq. (1.1), which in any local canonical coordinate system becomes

$$\tfrac{1}{2} g^{ij} \partial_i W \partial_j W + V = E.$$

Moreover, we can consider two special types of coordinates: *orthogonal* and *standard* coordinates (Definition 3.3). It is straightforward to prove that

Proposition 3.2: If the coordinates are orthogonal ($g^{ij} = 0$ *for* $i \neq j$)*, then the Levi-Civita separability conditions are equivalent to*

$$\begin{array}{c} g^{ii} g^{jj} \partial_i \partial_j g^{hh} - g^{ii} \partial_i g^{jj} \partial_j g^{hh} - g^{jj} \partial_j g^{ii} \partial_i g^{hh} = 0, \\ g^{ii} g^{jj} \partial_i \partial_j V - g^{ii} \partial_i g^{jj} \partial_j V - g^{jj} \partial_j g^{ii} \partial_i V = 0, \end{array} \quad i \neq j, \ \text{n.s.} \tag{3.5}$$

These equations do not involve the momenta $\underline{p}$. An equivalent form of these equations were first established by Eisenhart.[3] It can be shown that their general solutions have the Stäckel form (1.6).[15] It follows that the Hamilton–Jacobi equations split into separated equations of the form

$$\tfrac{1}{2} p_i^2 = \varphi_i^{(j)} c_j - \phi_i,$$

where $\underline{c} = (c_j)$ are arbitrary constants satisfying the completeness condition. Equation (3.5) can also be written in the form

$$\begin{array}{c} \partial_i \partial_j g^{hh} - \partial_i \ln g^{jj} \partial_j g^{hh} - \partial_j \ln g^{ii} \partial_i g^{hh} = 0, \\ \partial_i \partial_j V - \partial_i \ln g^{jj} \partial_j V - \partial_j \ln g^{ii} \partial_i V = 0, \end{array} \quad i \neq j, \ \text{n.s.} \tag{3.5$'$}$$

Note that the first equations (3.5′) characterize the orthogonal separation of the pure geodesic Hamiltonian.

Definition 3.3: A *standard coordinate system* is a coordinate system $(q^i) = (q^a, q^\alpha)$ with $a = 1,...,m$ and $\alpha = m+1,...,n$, such that (i) the metric tensor assumes the semidiagonal *standard form*

$$\mathbf{G} = g^{aa} \partial_a \otimes \partial_a + g^{\alpha\beta} \partial_\alpha \otimes \partial_\beta, \tag{3.6}$$

and (ii) the coordinates (q^{α}) are *ignorable*,

$$\partial_{\alpha} g^{ij} = 0, \quad \partial_{\alpha} V = 0. \tag{3.7}$$

We call *essential* the coordinates (q^{a}).
It is straightforward to prove that

Proposition 3.4: In standard coordinates the Levi-Civita separability conditions are equivalent to the following:

$$\begin{gathered} g^{aa} g^{bb} \partial_a \partial_b g^{cc} - g^{aa} \partial_a g^{bb} \partial_b g^{cc} - g^{bb} \partial_b g^{aa} \partial_a g^{cc} = 0, \\ g^{aa} g^{bb} \partial_a \partial_b g^{\alpha\beta} - g^{aa} \partial_a g^{bb} \partial_b g^{\alpha\beta} - g^{bb} \partial_b g^{aa} \partial_a g^{\alpha\beta} = 0, \\ g^{aa} g^{bb} \partial_a \partial_b V - g^{aa} \partial_a g^{bb} \partial_b V - g^{bb} \partial_b g^{aa} \partial_a V = 0, \end{gathered} \tag{3.8}$$

with $a \neq b$ not summed.

These equations can be written in the equivalent form

$$\begin{gathered} \partial_a \partial_b g^{cc} - \partial_a \ln g^{bb} \partial_b g^{cc} - \partial_b \ln g^{aa} \partial_a g^{cc} = 0, \\ \partial_a \partial_b g^{\alpha\beta} - \partial_a \ln g^{bb} \partial_b g^{\alpha\beta} - \partial_b \ln g^{aa} \partial_a g^{\alpha\beta} = 0, \\ \partial_a \partial_b V - \partial_a \ln g^{bb} \partial_b V - \partial_b \ln g^{aa} \partial_a V = 0. \end{gathered} \tag{3.8$'$}$$

Their general solutions are still of Stäckel type, but involving an $m \times m$ Stäckel matrix $[\varphi_a^{(b)}]$ of functions depending on the essential coordinates only,

$$g^{aa} = \varphi^{a}_{(m)}, \quad g^{\alpha\beta} = \phi_a^{\alpha\beta} g^{aa}, \quad V = \phi_a g^{aa}, \tag{3.9}$$

with functions $(\phi_a^{\alpha\beta}, \phi_a)$ depending on the essential coordinate corresponding to the lower index only. Then the Hamilton–Jacobi equation splits into separated equations of the kind

$$p_{\alpha} = c_{\alpha}, \quad \tfrac{1}{2} p_{\alpha}^2 = \varphi_a^{(b)} c_b - \phi_a^{\alpha\beta} c_{\alpha} c_{\beta} - \phi_a,$$

where $c = (c_i) = (c_a, c_{\alpha})$ are n arbitrary constants.

Remark 3.5: The above-given definition of standard coordinates needs some comments. (i) In a given standard coordinate system (q^{i}) the distinction between ''ignorable'' and ''essential'' coordinates is in general not univocal. Indeed, an ignorable coordinate may be orthogonal to the other ones and considered as essential; conversely, an essential coordinate may be ignorable, i.e., it may satisfy (3.7). However, in the process of integration by separation of variables of the Hamilton–Jacobi equation it is useless to consider an ignorable coordinate as ''essential,'' since it corresponds to a linear homogeneous first integral and thus to a trivial separated equation. (ii) The distinction between ignorable and essential coordinates becomes univocal and assumes a full meaning when related to a given separable Killing web,[16,17] that is when related to the geometrical characterization of the separation (see Sec. VII).

Remark 3.6: It is known that there is no loss of generality in considering separable standard coordinates. Indeed, the analysis of the Levi-Civita separability conditions shows that any separable coordinate system admits an equivalent standard system (q^{a}, q^{α}) where the number of essential coordinates is minimalized, i.e., it coincides with the number of second-class coordinates, according to the classification of Levi-Civita. This number is invariant within an equivalence class of separable coordinates. A standard coordinate system in which the essential coordinates (q^{a}) are exactly those of second class has been called *normal*.[17] For our present purposes we do not need to take into account the classification of Levi-Civita and the subtle distinction between ''normal'' and ''standard'' coordinates. We need only to refer to the above-given definition of standard coordinates and to the corresponding separability conditions (3.8) or (3.8$'$).

Definition 3.7: We say that a symmetric two-tensor $\mathbf{K}=(K^{ij})$ has a *standard form* or that it is a *standard tensor* with respect to a standard coordinate system if it assumes the form

$$\mathbf{K}=K^{aa}\partial_a\otimes\partial_a+K^{\alpha\beta}\partial_\alpha\otimes\partial_\beta=\lambda^a g^{aa}\partial_a\otimes\partial_a+K^{\alpha\beta}\partial_\alpha\otimes\partial_\beta, \tag{3.10}$$

where (λ^a) and $K^{\alpha\beta}$ do not depend on the ignorable coordinates (q^α). Then the matrix $[K^{ij}]$ has a form similar to (3.6).

Note that a tensor may be simultaneously in standard form with respect to nonequivalent separable standard coordinate systems.

IV. THE FREE SEPARATION OF THE SCHRÖDINGER EQUATION

In this section we shall show that a convenient and precise ''ansatz'' for the multiplicative separation of the Schrödinger equation (1.2) is given by the following

Definition 4.1: A *complete separated solution* of the Schrödinger equation is a solution of the form $\psi(\underline{q},\underline{c})=\Pi_i^n\ \psi_i(q^i,\underline{c})$, depending on $2n$ parameters $\underline{c}=(c_I)$ satisfying the *completeness condition*

$$\det\left[\begin{array}{c}\dfrac{\partial u_i}{\partial c_I}\\[2ex]\dfrac{\partial v_i}{\partial c_I}\end{array}\right]\neq 0,\quad u_i=\frac{\psi_i'}{\psi_i},\quad v_i=\frac{\psi_i''}{\psi_i}. \tag{4.1}$$

When such a solution exists we say that the Schrödinger equation is *separable* (or *freely separable*) in the coordinates $\underline{q}=(q^i)$.

The completeness condition (4.1) means that the $2n$ constants (c_I) can be uniquely determined by assigning arbitrary values to the $2n$ ratios $(\underline{u},\underline{v})$, at any fixed point. Hence, no restriction is imposed on the values that the functions $(\psi_i,\psi_i',\psi_i'')$ can assume at any given point of the domain of the coordinates, for $\psi\neq 0$. For this reason we call this kind of separation *free*. As we shall see in Sec. V, we can in fact consider another kind of separation in which such a ''freedom'' is lost. As we shall see in the following (Remark 4.8), the $2n$ parameters appearing in a free separated solution have a different role: in the process of integration n of them are related to constants of motion in involution or, equivalently, to second-order commuting symmetries of the Schrödinger operator, so that they can be interpreted as ''separation constants,'' while the remaining n parameters arise as ''integration constants.''

By assuming Definition 4.1 we shall prove

Theorem 4.2: *The Schrödinger equation is freely separable in a coordinate system $\underline{q}$ if and only if: (i) these coordinates are orthogonal, (ii) the corresponding Hamilton–Jacobi equation is separable, (iii) the following conditions are satisfied:*

$$\partial_i\Gamma_j=0\quad (i\neq j), \tag{4.2}$$

where

$$\Gamma_i=g^{hj}\Gamma_{hj,i},\quad \Gamma_{hj,i}=\tfrac{1}{2}(\partial_h g_{ji}+\partial_j g_{ih}-\partial_i g_{hj}). \tag{4.3}$$

Since $\Gamma_{hj,i}$ are the Christoffel symbols of the Levi-Civita connection, we call the functions Γ_i the *contracted Christoffel symbols*, associated with the coordinates $\underline{q}$. From their definition (4.3) it follows that

$$\Gamma_i=\tfrac{1}{2}\partial_i\ln\det[g^{hj}]-g_{ik}\partial_h g^{hk}. \tag{4.4}$$

We call the whole set of equations (4.2) the *Robertson condition for the free separation* of the Schrödinger equation. In this form the Robertson condition means that each contracted Christoffel

symbol Γ_i is a function of the corresponding coordinate q^i only (see Remark 4.7). As we know, an equivalent form of the Robertson condition is the diagonalization of the Ricci tensor. We shall discuss this equivalence in Sec. VI.

In order to justify all the above-given statements, let us start from the local coordinate expression of the Schrödinger equation (1.2),

$$g^{ij}\partial_i\partial_j\psi-\Gamma^k\partial_k\psi+\frac{2}{\hbar^2}(E-V)\psi=0, \quad \Gamma^k=g^{ki}\Gamma_i. \tag{4.5}$$

Since the constant factor $2/\hbar^2$ is inessential for our consideration, from now on we shall replace $(2/\hbar^2)V$ with V and $(2/\hbar^2)E$ by E.

For a separated solution of the kind (1.4) we have

$$\partial_i\psi=\frac{\psi_i'}{\psi_i}\psi, \quad \partial_i\partial_j\psi=\frac{\psi_i'\psi_j'}{\psi_i\psi_j}\psi \quad (i\neq j), \quad \partial_i\partial_i\psi=\frac{\psi_i''}{\psi_i}\psi. \tag{4.6}$$

Here the prime denotes the derivative operator on a function of a single variable. We remark that in these formulas the fraction ψ/ψ_i is the product $\psi_1\cdots\hat{\psi}_i\cdots\psi_n$, without the factor ψ_i. Thus, expressions (4.6) also hold at the points where $\psi_i=0$. If we set $u=\ln\psi$, then

$$u_i=\partial_i u=\frac{\partial_i\psi}{\psi}=\frac{\psi_i'}{\psi_i} \tag{4.7}$$

are functions of the corresponding variable q^i and moreover,

$$\partial_i\psi=\psi u_i,$$

$$\partial_i\partial_j\psi=\psi u_i u_j \quad (i\neq j),$$

$$\partial_i\partial_i\psi=\psi(u_i^2+u_i^{(2)}), \quad u_i^{(2)}=u_{ii}=\partial_i\partial_i u.$$

It follows that for a separated solution Eq. (4.5) assumes the form

$$(g^{ij}u_iu_j+g^{ii}u_i^{(2)}-\Gamma^i u_i+E-V)\psi=0, \tag{4.8}$$

where the sum over the repeated indices is understood. Thus, for $\psi\neq 0$ we get a partial differential equation of the kind (2.8) with $l=2$,

$$\mathcal{S}(\underline{q},\underline{u}^{(1)},\underline{u}^{(2)})=-E,$$

by setting (see Ref. 12)

$$\begin{gathered}\mathcal{S}(\underline{q},\underline{u}^{(1)},\underline{u}^{(2)})=g^{ij}u_iu_j+g^{ii}u_i^{(2)}-\Gamma^i u_i-V,\\ \underline{u}^{(1)}=(u_i), \quad \underline{u}^{(2)}=(u_{ii}).\end{gathered} \tag{4.9}$$

As a consequence, by applying Definition 2.2 to the present case and Theorem 2.3 related to the general equation (2.8), taking into account Remark 2.4, the completeness condition (2.16), and expression (4.7), we are led to the following definition and theorem.

Definition 4.3: A complete separated solution of the Schrödinger equation (4.5) is a solution of the form (1.4) depending on $2n$ constant parameters $\underline{c}=(c_I)$ satisfying the completeness condition

$$\det\begin{bmatrix} \dfrac{\partial u_i}{\partial c_I} \\ \dfrac{\partial u_i^{(2)}}{\partial c_I} \end{bmatrix} \neq 0, \quad u_i = \frac{\psi_i'}{\psi_i}, \quad u_i^{(2)} = u_{ii} = \left(\frac{\psi_i'}{\psi_i}\right)'. \tag{4.10}$$

Theorem 4.4: *The Schrödinger equation (4.5) is separable in the coordinates $\underline{q}$ if and only if the following first-order differential system is completely integrable*

$$\begin{aligned} \partial_i u_i^{(1)} &= u_i^{(2)}, \quad & \partial_i u_j^{(1)} &= 0, \\ \partial_i u_i^{(2)} &= R_i, \quad & \partial_i u_j^{(2)} &= 0, \end{aligned} \quad (i \neq j), \tag{4.11}$$

where

$$R_i(\underline{q}, \underline{u}^{(1)}, \underline{u}^{(2)}) = -\left(\frac{\partial \mathcal{S}}{\partial u_i^{(2)}}\right)^{-1}\left(\frac{\partial \mathcal{S}}{\partial q^i} + \frac{\partial \mathcal{S}}{\partial u_i} u_i^{(2)}\right), \tag{4.12}$$

$\mathcal{S}$ being defined as in (4.9) i.e., if and only if the commutation relations

$$[D_i, D_j] = 0, \tag{4.13}$$

are identically satisfied for

$$D_i = \partial_i + u_i^{(2)} \frac{\partial}{\partial u_i} + R_i \frac{\partial}{\partial u_i^{(2)}}.$$

Remark 4.5: If we replace the $2n$ variables $(\underline{u}^{(1)}, \underline{u}^{(2)})$ with the variables

$$(\underline{u}, \underline{v}) = (u_i, v_i)$$

where

$$v_i = u_i^{(2)} + u_i^2 = \frac{\psi_i''}{\psi_i}, \tag{4.14}$$

then the completeness condition (4.10) becomes equivalent to (4.1), so that Definition 4.3 is equivalent to Definition 4.1.

This transformation of dependent variables turns out to be convenient for the analysis of the integrability (or separability) conditions (4.13). We note first of all that

$$\frac{\partial \mathcal{S}}{\partial u_i^{(2)}} = g^{ii},$$

so that the definition (4.12) becomes

$$R_i(\underline{q}, \underline{u}^{(1)}, \underline{u}^{(2)}) = -(g^{ii})^{-1}\left(\frac{\partial \mathcal{S}}{\partial q^i} + \frac{\partial \mathcal{S}}{\partial u_i} u_i^{(2)}\right).$$

In the new variables we have

$$\mathcal{S}(\underline{q}, \underline{u}, \underline{v}) = g^{ij} u_i u_j + g^{ii}(v_i - u_i^2) - \Gamma^i u_i - V,$$

$$R_i(\underline{q}, \underline{u}, \underline{v}) = -\frac{1}{g^{ii}}\left(\frac{\partial \mathcal{S}}{\partial q^i} + (v_i - u_i^2)\frac{\partial \mathcal{S}}{\partial u_i}\right), \tag{4.15}$$

$$D_i=\partial_i+(v_i-u_i^2)\frac{\partial}{\partial u_i}+R_i\frac{\partial}{\partial v_i},$$

and system (4.11) becomes equivalent to

$$\begin{array}{ll}\partial_i u_i=v_i-u_i^2, & \partial_i u_j=0,\\ \partial_i v_i=R_i, & \partial_i v_j=0,\end{array}\quad (i\neq j). \tag{4.16}$$

Using (4.15), a straightforward calculation shows that

$$[D_i,D_j]=\left((v_i-u_i^2)\frac{\partial R_j}{\partial u_i}+R_i\frac{\partial R_j}{\partial v_i}+\frac{\partial R_j}{\partial q^i}\right)\frac{\partial}{\partial v_j}-\left((v_j-u_j^2)\frac{\partial R_i}{\partial u_j}+R_j\frac{\partial R_i}{\partial v_j}+\frac{\partial R_i}{\partial q^j}\right)\frac{\partial}{\partial v_i}.$$

Hence, the integrability conditions (4.13) become equivalent to

$$(v_i-u_i^2)\frac{\partial R_j}{\partial u_i}+R_i\frac{\partial R_j}{\partial v_i}+\frac{\partial R_j}{\partial q^i}=0\quad (i\neq j). \tag{4.17}$$

Because of (4.15),

$$\frac{\partial R_i}{\partial q^i}=-\frac{1}{g^{jj}}\partial_i g^{jj}R_j-\frac{1}{g^{jj}}\left[\partial_i\partial_j\mathcal{S}+\frac{\partial^2\mathcal{S}}{\partial q^i\partial u_j}(v_j-u_j^2)\right]$$

and, for $i\neq j$,

$$\frac{\partial R_j}{\partial v_i}=-\frac{1}{g^{jj}}\left[\frac{\partial^2\mathcal{S}}{\partial q^j\partial v_i}+\frac{\partial^2\mathcal{S}}{\partial v_i\partial u_j}(v_j-u_j^2)\right]=-\frac{1}{g^{jj}}\partial_j g^{ii}\quad (i\neq j).$$

Moreover,

$$\frac{\partial\mathcal{S}}{\partial u_i}=2g^{ik}u_k-2g^{ii}u_i-\Gamma^i.$$

Thus,

$$\frac{\partial^2\mathcal{S}}{\partial u_i\partial u_j}=2g^{ij}\quad (i\neq j).$$

It follows that

$$\frac{\partial R_j}{\partial u_i}=-\frac{1}{g^{jj}}\left[\frac{\partial^2\mathcal{S}}{\partial u_i\partial q^j}+2g^{ij}(v_j-u_j^2)\right]\quad (i\neq j).$$

Due to these last equations, the integrability conditions (4.17) become equivalent to

$$2g^{ij}(v_i-u_i^2)(v_j-u_j^2)+\frac{\partial^2\mathcal{S}}{\partial q^i\partial u_j}(v_j-u_j^2)+\frac{\partial^2\mathcal{S}}{\partial q^j\partial u_i}(v_i-u_i^2)+\partial_i\partial_j\mathcal{S}+R_i\partial_j g^{ii}+R_j\partial_i g^{jj}=0$$

$$(i\neq j). \tag{4.18}$$

Note that in this form they are symmetric in the distinct indices (i,j). We remark that these are algebraic equations in the variables $(\underline{u},\underline{v})$ and that they must be identically satisfied for all values of these variables, due to the completeness condition. A closer analysis of expressions (4.15) shows that (4.18) are of second degree in $\underline{v}$, and that the corresponding second-degree homogeneous polynomial is given by the first term $g^{ij}v_iv_j$, with $i\neq j$ not summed. This implies

$$g^{ij}=0 \quad (i\neq j) \tag{4.19}$$

and shows that

Proposition 4.6: In the free separation of the Schrödinger equation the coordinates are necessarily orthogonal.

In orthogonal coordinates, Eqs. (4.18) and (4.15) assume the simpler form

$$\frac{\partial^2\mathcal{S}}{\partial q^i\partial u_j}(v_j-u_j^2)+\frac{\partial^2\mathcal{S}}{\partial q^j\partial u_i}(v_i-u_i^2)+\partial_i\partial_j\mathcal{S}+R_i\partial_j g^{ii}+R_j\partial_i g^{jj}=0 \quad (i\neq j) \tag{4.20}$$

and

$$\mathcal{S}=g^{ii}v_i-\Gamma^i u_i-V, \quad R_i=\frac{1}{g^{ii}}[\Gamma^i(v_i-u_i^2)-\partial_i\mathcal{S}]. \tag{4.21}$$

It follows that

$$R_i=\frac{1}{2g^{ii}}[2\Gamma^i(v_i-u_i^2)-\partial_i g^{kk}v_k+\partial_i\Gamma^k u_k+\partial_i V].$$

By inserting this last expression of R_i into (4.20) we conclude that the integrability conditions of system (4.16) are equivalent to the orthogonality conditions (4.19) and to the following:

$$\begin{aligned}&2(u_j^2-v_j)(\partial_i\Gamma^j-\Gamma^j\partial_i\ln g^{jj})+2(u_i^2-v_i)(\partial_j\Gamma^i-\Gamma^i\partial_j\ln g^{ii})\\&\quad+v_k(\partial_i\partial_j g^{kk}-\partial_i\ln g^{jj}\partial_j g^{kk}-\partial_j\ln g^{ii}\partial_i g^{kk})-u_k(\partial_i\partial_j\Gamma^k-\partial_i\ln g^{jj}\partial_j\Gamma^k-\partial_j\ln g^{ii}\partial_i\Gamma^k)\\&\quad-(\partial_i\partial_j V-\partial_i\ln g^{jj}\partial_j V-\partial_j\ln g^{ii}\partial_i V)=0 \quad (i\neq j).\end{aligned} \tag{4.22}$$

Since these last equations are polynomial in the variables $(\underline{u},\underline{v})$, they are identically satisfied if and only if all the coefficients vanish, namely:

$$\begin{gathered}\partial_i\partial_j g^{kk}-\partial_i\ln g^{jj}\partial_j g^{kk}-\partial_j\ln g^{ii}\partial_i g^{kk}=0,\\ \partial_i\partial_j V-\partial_i\ln g^{jj}\partial_j V-\partial_j\ln g^{ii}\partial_i V=0,\\ \partial_j\Gamma^i-\Gamma^i\partial_j\ln g^{ii}=0,\\ \partial_i\partial_j\Gamma^k-\partial_i\ln g^{jj}\partial_j\Gamma^k-\partial_j\ln g^{ii}\partial_i\Gamma^k=0.\end{gathered} \quad (i\neq j) \tag{4.23}$$

These equations are in fact redundant. Indeed, it can be seen that due to the first and third equations, the last equation is identically satisfied. Moreover, the third equation is equivalent to

$$\partial_j\Gamma_i=0 \quad (i\neq j),$$

where, in orthogonal coordinates,

$$\Gamma_i=g_{ii}\Gamma^i=\tfrac{1}{2}\Sigma_{k\neq i}\partial_i\ln g^{kk}-\tfrac{1}{2}\partial_i\ln g^{ii}=\partial_i\ln(g_{ii}\sqrt{\Pi_k g^{kk}}). \tag{4.24}$$

Finally, we recognize in the first two equations of (4.23) the necessary and sufficient conditions (3.5') for the orthogonal separation of the Hamilton–Jacobi equation. Thus, due to Theorem 4.4, Theorem 4.2 is proved.

Remark 4.7: After Theorem 4.2, the integration of the Schrödinger equation by separation of variables is accomplished as follows. Due to the Stäckel form (1.6) of the metric tensor components and of the potential, the Schrödinger equation (4.8) takes the form

$$\varphi^i_{(n)}(u_i'+u_i^2-\Gamma_i u_i-\phi_i)=-E, \quad u_i=\frac{\psi_i'}{\psi_i}.$$

This equation is interpreted as the last one of a system of n equations involving all the remaining rows of the matrix $[\varphi^i_{(j)}]$ and n constants $\underline{a}=(a_i)$,

$$\varphi^i_{(j)}(u_i'+u_i^2-\Gamma_i u_i-\phi_i)=-a_j, \quad a_n=E, \tag{4.25}$$

which is equivalent to the following system of separated equations:

$$u_i'+u_i^2-\Gamma_i u_i-\phi_i+\varphi_i^{(j)}a_j=0. \tag{4.26}$$

These are first-order Riccati equations in the unknown functions $u_i(q^i)$, depending on the n constant parameters $\underline{a}=(a_j)$. Their integration yields functions

$$u_i=u_i(q^i,\underline{a},b_i), \tag{4.27}$$

each one depending on a further constant b_i. The complete separated solution is then given, up to an inessential constant factor, by

$$\psi=\exp\int u_i\,\mathrm{d}q^i. \tag{4.28}$$

We note that (as happens for any Riccati equation) (4.26) are equivalent to the linear second-order equations

$$\psi_i''-\Gamma_i\psi_i'-(\phi_i-\varphi_i^{(j)}a_j)\psi_i=0 \tag{4.29}$$

in the original unknown functions ψ_i.

Remark 4.8: The $2n$ constants $\underline{c}=(c_I)=(\underline{a},\underline{b})=(a_i,b_i)$, appearing in a separated solution (4.28) as a result of the process of integration by separation of variables illustrated previously, play a different role. While $\underline{b}$ arise as integration constants from the integration of the first-order Riccati equations (4.26), or of the second-order linear equations (4.29), the constants $\underline{a}$ have two interpretations. (i) They are the constant values taken by the quadratic first integrals in involution related to the separation of the Hamilton–Jacobi equation (see Theorem 7.14), whose expressions in orthogonal separable coordinates are

$$H_j=\tfrac{1}{2}\varphi^i_{(j)}(p_i^2+2\phi_i). \tag{4.30}$$

(ii) They are the eigenvalues of the second-order symmetry operators of the Schrödinger equation corresponding to H_j,

$$\hat{H}_j\psi=\psi^i_{(j)}(-\partial_i^2\psi+\Gamma_i\partial_i\psi+\phi_i\psi). \tag{4.31}$$

The link between H_j and $\hat{H}_j$ will be discussed in a following paper.[18] If we apply these operators to a separated solution (1.4) then, due to (4.6), (4.7) and (4.14), we get

$$\hat{H}_j\psi=\varphi^i_{(j)}(\Gamma_i u_i-v_i+\phi_i)\psi, \tag{4.32}$$

which shows that the eigenvalues are

$$a_j=\varphi^i_{(j)}(\Gamma_i u_i-v_i+\phi_i). \tag{4.33}$$

Remark 4.9: The values of the constants $\underline{a}$ are determined through (4.25), which are equivalent to (4.33), by the initial values at a point q_0 of (u_i,u_i') i.e., by the initial values of $(\psi_i,\psi_i',\psi_i'')$, for $\psi_i(q_0)\neq 0$. The values of $\underline{b}$ are then determined by reversing (4.27) at the initial point q_0: $u_i(q_0)=u_i(q_0^i,\underline{a},b_i)$. If instead of the first-order equations (4.26) we consider the equivalent second-order equations (4.29), the resulting integration constants are $2n$, but only half

of them are essential, since the functions ψ_i are determined up to a constant factor. Thus, also in this case we reduce to n essential constants (b_i). See Sec. IX for an example.

V. THE REDUCED SEPARATION OF THE SCHRÖDINGER EQUATION

In Sec. IV we have considered a kind of multiplicative separation of the Schrödinger equation involving $2n$ constant parameters $\underline{c}$ which can be uniquely determined by assigning the values, at any chosen point, of the functions $u_i=\psi_i'/\psi_i$ and $v_i=\psi_i''/\psi_i$. This means that we have no restriction on the values that the functions $(\psi_i,\psi_i',\psi_i'')$ can assume at any given point of the domain of the coordinates, for $\psi\neq 0$. As we have seen, this freedom implies the orthogonality of the separable coordinates.

However, we can think of a kind of separation in which *constraints* are "*a priori*" imposed on some of the factors ψ_i.

Although it is not interpreted in this sense, a usual constraint appearing in the literature is represented by the following supplementary conditions (see for instance Refs. 9, 10, and 12):

$$\psi_\alpha'=\kappa_\alpha\psi_\alpha, \quad \alpha=m+1,...,n, \tag{5.1}$$

where (κ_α) are arbitrary (real or complex) constants. This means that, up to an inessential multiplicative constant,

$$\psi_\alpha(q^\alpha)=\exp(\kappa_\alpha q^\alpha). \tag{5.2}$$

In this way we define a kind of *constrained separation*, which we call *reduced separation*. As we shall see, for this separation the coordinates are not necessarily orthogonal and the number of essential constants appearing in a separated solution is $n+m<2n$ (the case $m=n$ corresponds to the free separation). We base our approach on a definition similar to Definition 4.1.

Definition 5.1: A *reduced separated solution* of the Schrödinger equation is a solution (1.4) where the factors ψ_α are of the type (5.2) for $\alpha=m+1,...,n$ and where all factors ψ_α depend on further $2m$ parameters $\underline{c}=(c_A)$ $(A=1,...,2m)$ satisfying the *completeness condition*

$$\det\begin{bmatrix}\dfrac{\partial u_a}{\partial c_A}\\[2ex] \dfrac{\partial v_a}{\partial c_A}\end{bmatrix}\neq 0, \quad u_a=\frac{\psi_a'}{\psi_a}, \quad v_a=\frac{\psi_a''}{\psi_a} \quad (a=1,...,m). \tag{5.3}$$

When such a solution exists we say that the Schrödinger equation is *reductively separable* in the coordinates (q^a,q^α). The coordinates (q^α) and (q^a) are called *constrained* and *free* coordinates, respectively.

The completeness condition (5.3) means that the $2m$ constant parameters (c_A) can be uniquely determined by assigning arbitrary values of the $2m$ ratios (u_a,v_a) at any given point. Hence, we have no restriction on the values that the functions $(\psi_a,\psi_a',\psi_a'')$ can assume at any given point of the domain of the coordinates, for $\psi\neq 0$. Moreover, we remark that the total number of constant parameters in a reduced separated solution is $m+n$. Indeed, besides the $2m$ constants (c_A), also the $n-m$ constants (κ_α) are present, although they are not involved in the completeness condition.

In this section we shall prove the following theorem (analogous to Theorem 4.2).

Theorem 5.2: *The Schrödinger equation is reductively separable in a coordinate system* $\underline{q}=(q^a,q^\alpha)$ *if and only if: (i) the constrained coordinates* (q^α) *are ignorable,*

$$\partial_\alpha g^{ij}=0, \quad \partial_\alpha V=0,$$

(ii) the free coordinates (q^a) *are orthogonal,*

$$g^{ab}=0, \quad a\neq b,$$

(iii) there exists a coordinate transformation leaving the coordinates (q^a) *invariant, preserving the constraints and the separation, in which the metric tensor assumes the standard form (3.6) and such that (iv) the Hamilton–Jacobi equation is separable and (v) the following conditions are satisfied:*

$$\partial_a\Gamma_b=0 \quad (a\neq b), \quad \Gamma_a=g^{ij}\Gamma_{ij,a}. \tag{5.4}$$

We call Eq. (5.4) the *Robertson condition for the reduced separation* of the Schrödinger equation. As will be discussed in Sec. VI, this is in fact equivalent to $R_{ab}=0$ for $a\neq b$.

In order to justify Definition 5.1 and prove Theorem 5.2 we begin by observing that the constraints (5.1) imply that the functions u_i, defined as in (4.7) and labeled with Greek indices (running from $m+1$ to n) are constant

$$u_\alpha=\frac{\psi'_\alpha}{\psi_\alpha}=\kappa_\alpha, \quad u^{(2)}_\alpha=0,$$

so that, for such a separated solution, Eq. (4.8) becomes equivalent (for $\psi\neq 0$) to

$$g^{ab}u_au_b+g^{aa}u^{(2)}_a+2g^{a\alpha}u_a\kappa_\alpha+g^{\alpha\beta}\kappa_\alpha\kappa_\beta-\Gamma^au_a-\Gamma^\alpha\kappa_\alpha-V+E=0,$$

with summation over the repeated indices a, $b=1,\ldots,m$ and α, $\beta=m+1,...,n$. This equation can be written in the form

$$\mathcal{S}(\underline{q},\underline{u}^{(1)},\underline{u}^{(2)},\kappa_\alpha)=-E, \tag{5.5}$$

by setting

$$\begin{gathered}\mathcal{S}(\underline{q},\underline{u}^{(1)},\underline{u}^{(2)},\kappa_\alpha)=g^{ab}u_au_b+g^{aa}u^{(2)}_a+2g^{a\alpha}u_a\kappa_\alpha+g^{\alpha\beta}\kappa_\alpha\kappa_\beta-\Gamma^au_a-\Gamma^\alpha\kappa_\alpha-V,\\ \underline{u}^{(1)}=(u_a), \quad \underline{u}^{(2)}=(u_{aa}).\end{gathered} \tag{5.6}$$

Equation (5.5) is of the type (2.8). The constants (κ_α) play the role of independent constant parameters and the relevant dependent variables are $\underline{z}=(\underline{u}^{(1)},\underline{u}^{(2)})=(u_a,u_{aa})$. Their number is $2m$. By applying the method of Sec. II, we have for a solution of this equation

$$\sum_{a=1}^{m}\left(\frac{\partial\mathcal{S}}{\partial q^i}+\frac{\partial\mathcal{S}}{\partial u^{(1)}_a}\frac{\partial u^{(1)}_a}{\partial q^i}+\frac{\partial\mathcal{S}}{\partial u^{(2)}_a}\frac{\partial u^{(2)}_a}{\partial q^i}\right)=0,$$

thus (no sum over the index a)

$$\frac{\partial\mathcal{S}}{\partial q^a}+\frac{\partial\mathcal{S}}{\partial u^{(1)}_a}\frac{\partial u^{(2)}_a}{\partial q^a}+\frac{\partial\mathcal{S}}{\partial u^{(2)}_a}\frac{\partial u^{(2)}_a}{\partial q^a}=0, \quad \frac{\partial\mathcal{S}}{\partial q^\alpha}=0.$$

As a consequence, by adapting Definition 2.2 to the present case, we are led to the following

Definition 5.3: A *reduced separable solution* of the Schrödinger equation is a solution of the form (1.4)–(5.2), depending on $2m$ parameters $\underline{c}=(c_A)$ $(A=1,...,2m)$ satisfying the completeness condition

$$\det\begin{bmatrix} \dfrac{\partial u_a}{\partial c_A} \\ \dfrac{\partial u_a^{(2)}}{\partial c_A} \end{bmatrix} \neq 0, \quad u_a = \frac{\psi_a'}{\psi_a}, \quad u_a^{(2)} = u_{aa} = \left(\frac{\psi_a'}{\psi_a}\right)'. \tag{5.7}$$

Hence, by applying Theorem 2.3 and recalling (2.5) and (2.2), we get

Proposition 5.4: The Schrödinger equation is reductively separable in the coordinates $\underline{q} = (q^a, q^\alpha)$ *if and only if*

$$\partial_\alpha \mathcal{S} = 0, \tag{5.8}$$

$\mathcal{S}$ *being defined as in (5.6), and the first-order differential system*

$$\begin{aligned} &\partial_a u_a^{(i)} = u_a^{(2)}, \quad \partial_i u_a^{(1)} = 0, \\ &\partial_a u_a^{(2)} = R_a, \quad \partial_i u_a^{(2)} = 0, \end{aligned} \quad (i \neq a) \tag{5.9}$$

is completely integrable for

$$R_a(\underline{q}, \underline{u}^{(1)}, \underline{u}^{(2)}) = -\left(\frac{\partial \mathcal{S}}{\partial u_a^{(2)}}\right)^{-1}\left(\frac{\partial \mathcal{S}}{\partial q^a} + \frac{\partial \mathcal{S}}{\partial u_a} u_a^{(2)}\right).$$

The complete integrability conditions for this system are

$$[D_i, D_j] = 0, \quad \begin{cases} D_a = \partial_a + u_a^{(2)} \dfrac{\partial}{\partial u_a} + R_a \dfrac{\partial}{\partial u_a^{(2)}}, \\ D_\alpha = \partial_\alpha. \end{cases} \tag{5.10}$$

From (5.8) and (5.6) it follows that

$$\partial_\alpha g^{ij} = 0, \quad \partial_\alpha \Gamma^i = 0, \quad \partial_\alpha V = 0,$$

since $\mathcal{S}$ is a polynomial function in the variables $(\underline{u}, \underline{u}^{(2)}, \kappa_\alpha)$ assuming arbitrary values. This proves that

Proposition 5.5: In the reduced separation of the Schrödinger equation the constrained coordinates (q^α) *are ignorable.*

It follows that the significant part of the integrability conditions (5.10) is that related to the free (and nonignorable) coordinates, $[D_a, D_b] = 0$ (for $a \neq b$). For examining these conditions, as in the case of the free separation, it is convenient to deal with the new $2m$ variables

$$(\underline{u}, \underline{v}) = (u_a, v_a), \quad v_a = u_{aa} + u_a^2 = \frac{\psi_\alpha''}{\psi_\alpha}.$$

Remark 5.6: Under such a transformation the completeness condition (5.7) is equivalent to (5.3), so that Definition 5.3 is equivalent to Definition 5.1.

Furthermore, the differential system (5.9) becomes equivalent to

$$\begin{aligned} &\partial_i u_a = 0, \\ &\partial_i v_a = 0, \\ &\partial_a u_a = v_a - u_a^2, \\ &\partial_a v_a = R_a, \end{aligned} \quad (i \neq a = 1, \ldots, m), \tag{5.11}$$

where

$$R_a = -\frac{1}{g^{aa}}\left(\frac{\partial \mathcal{S}}{\partial q^a} + \frac{\partial \mathcal{S}}{\partial u_a}(v_a - u_a^2)\right),$$

$$\mathcal{S}(\underline{q},\underline{u},\underline{v}) = g^{aa}(v_a - u_a^2) + g^{ab}u_a u_b + 2g^{a\alpha}u_a\kappa_\alpha + g^{\alpha\beta}\kappa_\alpha\kappa_\beta - \Gamma^a u_a - \Gamma^\alpha\kappa_\alpha - V,$$

$$D_a = \partial_a + (v_a - u_a^2)\frac{\partial}{\partial u_a} + R_a\frac{\partial}{\partial v_a},$$

$$D_\alpha = \partial_\alpha .$$

The complete integrability conditions $[D_a, D_b] = 0$ of system (5.11) are then equivalent to equations similar to (4.17),

$$(v_a - u_a^2)\frac{\partial R_b}{\partial u_a} + R_a\frac{\partial R_b}{\partial v_a} + \frac{\partial R_b}{\partial q^a} = 0 \quad (a \neq b).$$

A calculation similar to that of Sec. IV shows that

Proposition 5.7: In a reduced separation the free coordinates are orthogonal,

$$g^{ab} = 0, \quad a \neq b,$$

and the integrability conditions of system (5.11) are equivalent to

$$\frac{\partial^2 \mathcal{S}}{\partial q^a \partial u_b}(v_b - u_b^2) + \frac{\partial^2 \mathcal{S}}{\partial q^b \partial u_a}(v_a - u_a^2) + \partial_a\partial_b\mathcal{S} + R_a\partial_b g^{aa} + R_b\partial_a g^{bb} = 0 \quad (a \neq b), \tag{5.12}$$

where

$$\begin{aligned} \mathcal{S} &= g^{aa}v_a + 2g^{a\alpha}u_a\kappa_\alpha + g^{\alpha\beta}\kappa_\alpha\kappa_\beta - \Gamma^a u_a - \Gamma^\alpha\kappa_\alpha - V, \\ R_a &= \frac{1}{g^{aa}}((\Gamma^a - 2g^{a\alpha}\kappa_\alpha)(v_a - u_a^2) - \partial_a S). \end{aligned} \tag{5.13}$$

From these last equations we can derive the following

Proposition 5.8: The reduced separation of the Schrödinger equation always occurs in a standard coordinate system $(q^i) = (q^a, q^\alpha)$*, for which (3.6) and (3.7) hold, and such that the following equations are satisfied for* $a \neq b$:

$$\begin{aligned} &\partial_a\partial_b g^{cc} - \partial_b \ln g^{aa}\partial_a g^{cc} - \partial_a \ln g^{bb}\partial_b g^{cc} = 0, \\ &\partial_a\partial_b g^{\alpha\beta} - \partial_b \ln g^{aa}\partial_a g^{\alpha\beta} - \partial_a \ln g^{bb}\partial_b g^{\alpha\beta} = 0, \\ &\partial_a\partial_b V - \partial_b \ln g^{aa}\partial_a V - \partial_a \ln g^{bb}\partial_b V = 0, \\ &\partial_b\Gamma_a = 0, \end{aligned} \tag{5.14}$$

where

$$\Gamma_a = g_{aa}\Gamma^a = \frac{1}{2}\sum_{c \neq a}\partial_c \ln g^{cc} - \frac{1}{2}\partial_a \ln g^{aa} + \frac{1}{2}\partial_a \ln \det[g^{\alpha\beta}]. \tag{5.15}$$

Proof: By setting

$$\hat{\Gamma}^a = \Gamma^a - 2g^{a\alpha}\kappa_\alpha, \quad \hat{V} = V + \Gamma^\alpha\kappa_\alpha - g^{\alpha\beta}\kappa_\alpha\kappa_\beta,$$

(5.13) assume the form

$$\mathcal{S}=g^{aa}v_a-\hat{\Gamma}^a u_a-\hat{V},\quad R_a=\frac{1}{g^{aa}}((\hat{\Gamma}^a(v_a-u_a^2)-\partial_a\mathcal{S}),\tag{5.16}$$

so that the integrability conditions (5.12) become

$$\begin{aligned}&2(u_b^2-v_b)(\partial_a\hat{\Gamma}^b-\hat{\Gamma}^b\partial_a\ln g^{bb})+2(u_a^2-v_a)(\partial_b\hat{\Gamma}^a-\hat{\Gamma}^a\partial_b\ln g^{aa})+v_c(\partial_a\partial_b g^{cc}-\partial_a\ln g^{bb}\partial_b g^{cc}\\&\quad-\partial_b\ln g^{aa}\partial_a g^{cc})-u_c(\partial_a\partial_b\hat{\Gamma}^c-\partial_a\ln g^{bb}\partial_b\hat{\Gamma}^c-\partial_b\ln g^{aa}\partial_a\hat{\Gamma}^c)\\&\quad-(\partial_a\partial_b\hat{V}-\partial_a\ln g^{bb}\partial_b\hat{V}-\partial_b\ln g^{aa}\partial_a\hat{V})=0.\end{aligned}\tag{5.17}$$

We remark that (5.12) and (5.16) are similar to (4.20) and (4.21), so that (5.17) are similar to (4.22) and, since (u_a,v_a) can assume arbitrary values, we get equations similar to (4.23),

$$\begin{gathered}\partial_a\partial_b g^{cc}-\partial_a\ln g^{bb}\partial_b g^{cc}-\partial_b\ln g^{aa}\partial_a g^{cc}=0,\\\partial_a\partial_b\hat{V}-\partial_a\ln g^{bb}\partial_b\hat{V}-\partial_b\ln g^{aa}\partial_a\hat{V}=0,\\\partial_a\hat{\Gamma}^b-\hat{\Gamma}^b\partial_a\ln g^{bb}=0,\\\partial_a\partial_b\hat{\Gamma}^c-\partial_a\ln g^{bb}\partial_b\hat{\Gamma}^c-\partial_b\ln g^{aa}\partial_a\hat{\Gamma}^c=0.\end{gathered}\tag{5.18}$$

The first equations are just the first equations in (5.14). Since also the constant parameters (κ_α) assume arbitrary values, the fourth equations (5.18) are equivalent to

$$\begin{gathered}\partial_a\partial_b\Gamma^c-\partial_a\ln g^{bb}\partial_b\Gamma^c-\partial_b\ln g^{aa}\partial_a\Gamma^c=0,\\\partial_a\partial_b g^{c\alpha}-\partial_a\ln g^{bb}\partial_b g^{c\alpha}-\partial_b\ln g^{aa}\partial_a g^{c\alpha}=0,\end{gathered}\tag{5.19}$$

while the second equations (5.18) are equivalent to the second and third equations of (5.14) and

$$\partial_a\partial_b\Gamma^\alpha-\partial_a\ln g^{bb}\partial_b\Gamma^\alpha-\partial_b\ln g^{aa}\partial_a\Gamma^\alpha=0.\tag{5.20}$$

Finally, the third equations (5.18) are equivalent to

$$\partial_a\Gamma^b-\Gamma^b\partial_a\ln g^{bb}=0,\quad \partial_a g^{b\alpha}-g^{b\alpha}\partial_a\ln g^{bb}=0,$$

which can be written in the form

$$\partial_a\left(\frac{\Gamma^b}{g^{bb}}\right)=0,\quad \partial_a\left(\frac{g^{b\alpha}}{g^{bb}}\right)=0,\quad a\neq b.\tag{5.21}$$

These last equations show that

$$\Gamma^a=g^{aa}f_a,\quad g^{a\alpha}=g^{aa}f_a^\alpha,\tag{5.22}$$

where (f_a,f_a^α) are functions of the coordinate corresponding to the lower index only. As a consequence, due to the first equations (5.18), (5.19) are identically satisfied and do not add further information. But (5.22) have another important consequence which allows a remarkable simplification of our analysis (a similar argument has been used in Refs. 15, 17 in the discussion of the separation of the HJ equations). Indeed, let us consider a coordinate transformation of the kind

$$\mathrm{d}x^a=\mathrm{d}q^a,\quad \mathrm{d}x^a=\mathrm{d}q^\alpha-f_a^\alpha\,\mathrm{d}q^a.\tag{5.23}$$

For the components $g_x^{ij}=\mathrm{d}x^i\cdot\mathrm{d}x^j$ of the metric tensor in the new coordinates $(x^i)=(x^a,x^\alpha)$ we have $g_x^{ab}=g^{ab}$ and

$$g_x^{a\alpha}=\mathrm{d}x^a\cdot\mathrm{d}x^\alpha=\mathrm{d}q^a\cdot(\mathrm{d}q^\alpha-f_b^\alpha\mathrm{d}q^b)=g^{a\alpha}-f_b^\alpha g^{ab}=g^{a\alpha}-f_a^\alpha g^{aa}=0.$$

This coordinate transformation is compatible with the separation, in the sense that in the new coordinates the solution of the Schrödinger equation is still separable and the constraint equations (5.1) hold (with the same constants κ_α). Indeed, the essential coordinates remain unchanged ($x^a=q^a$ up to inessential additive constants) and moreover,

$$\frac{\mathrm{d}\psi_\alpha}{\mathrm{d}x^\alpha}=\frac{\partial\psi_\alpha\partial q^\beta}{\partial q^\beta\partial x^\alpha}=\frac{\mathrm{d}\psi_\alpha\mathrm{d}q^\alpha}{\mathrm{d}q^\alpha\mathrm{d}x^\alpha}=\frac{\mathrm{d}\psi_\alpha}{\mathrm{d}q^\alpha}.$$

Hence, *without loss of generality* we can assume

$$g^{a\alpha}=0, \tag{5.24}$$

so that the metric tensor takes the standard form (3.6), with ignorable coordinates (q^α). For a metric of this kind,

$$\Gamma_a=g_{ai}\Gamma^i=g_{aa}\Gamma^a=(g^{aa})^{-1}\Gamma^a.$$

Thus, the first equations (5.21) are equivalent to the fourth equations (5.14). Moreover, $\Gamma^\alpha=0$ (see Sec. VI) so that (5.20) are identically satisfied. We conclude that the integrability conditions (5.12) of system (5.11), up to a coordinate transformation preserving the separation and reducing the metric tensor in the standard form, are equivalent to (5.14). ■

We recognize in the first three lines of system (5.14) the necessary and sufficient conditions (3.8′) for the separation of the Hamilton–Jacobi equation in standard coordinates. Hence, we have proved the following

Proposition 5.9: Up to a coordinate transformation of the kind (5.23), the reduced separation of the Schrödinger equation always occurs in standard separable coordinates $\underline{q}=(q^a,q^\alpha)$ $(a=1,...,m,\alpha=m+1,...,n)$ *for which* $\partial_b\Gamma_a=0$ *for* $a\neq b$.

As a conclusion, from Propositions 5.5, 5.7, 5.8, and 5.9, we derive Theorem 5.2.

Remark 5.10: Let us see how the integration by separation of variables is performed when the items in Theorem 5.2 are satisfied (this will give a further proof of the sufficiency of these items for the separation) and how the $m+n$ constants arise in a reduced separated solution. Due to the factorization

$$\psi=\Pi_{a=1}^m\psi_a\cdot\Pi_{\alpha=m+1}^n\psi_\alpha,$$

and to the constraints (5.1), since $\Gamma^\alpha=0$, the Schrödinger equation (4.5) becomes equivalent to the following *reduced Schrödinger equation:*

$$g^{aa}\partial_a^2\tilde{\psi}+\Gamma^a\partial_a\tilde{\psi}+(E-V+g^{\alpha\beta}\kappa_a\kappa_\beta)\tilde{\psi}=0,\quad \tilde{\psi}=\Pi_{a=1}^m\psi_a. \tag{5.25}$$

The additional condition $\partial_b\Gamma_a=0$ for $a\neq b$ means that the contracted Christoffel symbols Γ_a (with indices $a=1,...,m$) are functions of the corresponding coordinate q^a only. By a method similar to that illustrated in Remark 4.7, due to expressions (3.9), the integration of the Schrödinger equation is reduced to the integration of m separated Riccati equations,

$$u_a'+u_a^2-\Gamma_a u_a-\phi_a+\phi_a^{\alpha\beta}\kappa_\alpha\kappa_\beta+\varphi_a^{(b)}\tilde{a}_b=0 \tag{5.26}$$

parametrized by n constants $(\tilde{a}_b,\kappa_\alpha)$, with $\tilde{a}_m=E$. Its solutions $u_a=u_a(q^a;\tilde{a}_b,\kappa_\alpha,\tilde{b}_a)$ give rise, separately, to other m constants $(\tilde{b}_a)$ and generate, by a further integration, the reduced separated solution (summation over the indices)

$$\psi=\exp\left(\kappa_\alpha q^\alpha+\int u_a\,\mathrm{d}q^a\right)=\Pi_{a=1}^m\psi_a\cdot\Pi_{\alpha=m+1}^n\psi_\alpha.$$

Equations (5.26) are equivalent to the m linear second-order equations

$$\psi_a''-\Gamma_a\psi_a'+(\phi_a^{\alpha\beta}\kappa_\alpha\kappa_\beta+\varphi_a^{(b)}\tilde{a}_b-\phi_a)\psi_a=0 \tag{5.27}$$

in the functions ψ_a. In the reduced separation the number of the constants appearing in a complete solution (1.4), as a result of this process of integration, is $m+n<2n$, but only the $2m$ constants $(\tilde{a}_a,\tilde{b}_a)$ are involved in the completeness condition.

Remark 5.11: A coordinate transformation of the kind

$$q^a=\overline{q}^a,\quad q^\alpha=\sum_i F_i^\alpha(\overline{q}^I)=\sum_a F_a^\alpha(q^a)+\sum_\beta F_\beta^\alpha(\overline{q}^\beta),$$

with

$$\det[f_\beta^\alpha]\neq 0,\quad f_\beta^\alpha=(F_\beta^\alpha)',$$

composed by any transformation over single coordinates, is the most general transformation leading to nonstandard separable coordinates $(\overline{q}^a,\overline{q}^\alpha)$ for the Hamilton–Jacobi equation.[15,17] The same transformation applied to standard separable coordinates, in general, does not preserve (5.24), $g^{a\alpha}\neq 0$, and the coordinates $(\overline{q}^\alpha)$ are no longer ignorable. However, this transformation preserves the multiplicative separation of the Schrödinger equation. Indeed, the factors $\psi_a(q^a)$ remain unchanged, while the factors $\psi_\alpha(q^\alpha)$ are transformed as follows:

$$\psi_\alpha(q^\alpha)=\exp(\kappa_\alpha q^\alpha)=\exp(\kappa_\alpha F_\beta^\alpha(\overline{q}^\beta))\cdot\exp(\kappa_\alpha F_a^\alpha(q^a))=\prod_\beta\tilde{\psi}_\beta(\overline{q}^\beta)\cdot\prod_a\tilde{\psi}_a(q^a),$$

where

$$\tilde{\psi}_\beta(\overline{q}^\beta)=\exp(\kappa_\alpha F_\beta^\alpha(\overline{q}^\beta)),\quad \tilde{\psi}_a(q^a)=\exp(\kappa_\alpha F_a^\alpha(q^a)),$$

and we finally get a solution of the kind

$$\psi=\prod_\beta\tilde{\psi}_\beta(\overline{q}^\beta)\prod_a\psi_a(q^a)\tilde{\psi}_a(q^a).$$

We observe that

$$\tilde{\psi}_\beta'=\kappa_\alpha f_\beta^\alpha(\overline{q}^\beta)\tilde{\psi}_\beta,$$

where $f=F'$. This shows that a constraint of the kind (5.1) is still satisfied if and only if $f_\beta^\alpha=\delta_\beta^\alpha c'_\beta$ with arbitrary constants (c'_β). It shows also that a constraint of the kind

$$\psi'_\beta=\kappa_\alpha f_\beta^\alpha(q^\beta)\psi_\beta,\quad \det[f_\beta^\alpha]\neq 0$$

could be considered, but that it is equivalent to (5.1).

Remark 5.12: A remark analogous to Remark 4.8 is in order. The constants $\tilde{a}_b$ have two interpretations: (i) They are the constant values taken by the quadratic first integrals in involution related to the nonorthogonal separation of the Hamilton–Jacobi equation in standard coordinates (cf. Theorem 7.25) whose expressions are

$$H_a=\tfrac{1}{2}\varphi_{(a)}^b(p_b^2+\phi_a^{\alpha\beta}p_\alpha p_\beta+\phi_a). \tag{5.28}$$

(ii) They are the eigenvalues of the second-order symmetry operators corresponding to H_a of the reduced Schrödinger equation (5.25):

$$\hat{H}_b\tilde{\psi}=\varphi^a_{(b)}(-\partial_a^2\tilde{\psi}+\Gamma_a\partial_a\tilde{\psi}+(\phi_a-\phi_a^{\alpha\beta}\kappa_\alpha\kappa_\beta)\psi). \tag{5.29}$$

About the constants κ_α introduced in the constraint equations (5.1), we observe that they correspond to the eigenvalues of the first-order symmetry operators of the Schrödinger equation

$$\hat{H}_\alpha\psi=-i\hbar\partial_\alpha\psi. \tag{5.30}$$

Indeed, from (5.1) it follows that

$$\partial_\alpha\psi=\kappa_\alpha\psi.$$

Thus,

$$\hat{H}_\alpha\psi=-i\hbar\kappa_\alpha\psi. \tag{5.31}$$

As will be shown in Ref. 18, these operators are related to the linear first integrals

$$H_\alpha=p_\alpha \tag{5.32}$$

corresponding to the ignorable coordinates and thus to the Killing vectors characterizing the separation in standard coordinates (see Sec. VII). From (5.31) we observe that κ_α must be pure imaginary, since the operators $\hat{H}_\alpha$ are self-adjoint. This is in agreement with the fact that the choice of the constraint equations (5.2) does not change the state represented by ψ.

VI. THE ROBERTSON CONDITION

In this section we analyze the Robertson condition in a standard separable coordinate system. We shall extend to the reduced separation the analysis on the Robertson condition done by Eisenhart[3] in the case of the orthogonal separation. This extension has already been discussed in Ref. 19; here we give an improved and simplified version.

For a metric tensor in the standard form (3.6), where (q^α) are ignorable, the nonvanishing Christoffel symbols are

$$\begin{gathered}\Gamma_{\alpha\beta a}=-\tfrac{1}{2}\partial_a g_{\alpha\beta},\quad \Gamma^a_{\alpha\beta}=-\tfrac{1}{2}g^{aa}\partial_a\partial_{\alpha\beta},\\ \Gamma_{\alpha a\beta}=\tfrac{1}{2}\partial_a g_{\alpha\beta},\quad \Gamma^\beta_{\alpha a}=\tfrac{1}{2}\sum_\gamma g^{\beta\gamma}\partial_a g_{\alpha\gamma},\\ \Gamma_{aba}=\tfrac{1}{2}\partial_b g_{aa},\quad \Gamma^a_{ac}=\tfrac{1}{2}g^{aa}\partial_c g_{aa},\\ \Gamma_{aab}=-\tfrac{1}{2}\partial_b g_{aa}\quad (a\neq b),\quad \Gamma^b_{aa}=-\tfrac{1}{2}g^{bb}\partial_b g_{aa}\quad (a\neq b).\end{gathered} \tag{6.1}$$

It follows that

$$\Gamma^\alpha=g^{ij}\Gamma^\alpha_{ij}=0,\quad \Gamma^i_{i\alpha}=0, \tag{6.2}$$

and from (4.3),

$$\Gamma_a=g_{aa}\Gamma^a=-\partial_a\ln g^{aa}+\tfrac{1}{2}\partial_a\ln\det[g^{ij}]=-\partial_a\ln g^{aa}+\tfrac{1}{2}\partial_a\ln\det[g^{\alpha\beta}]+\tfrac{1}{2}\sum_{c=1}^{m}\partial_a\ln g^{cc}. \tag{6.3}$$

Moreover,

$$\Gamma^i_{ia}=\Gamma^b_{ba}+\Gamma^\alpha_{a\alpha}=\tfrac{1}{2}g^{bb}\partial_a g_{bb}+\tfrac{1}{2}g^{\alpha\beta}\partial_a g_{\alpha\beta},$$

so that

$$\Gamma^i_{ia}=-\tfrac{1}{2}\partial_a \ln\det[g^{ij}]=-\Gamma_a-\partial_a \ln g^{aa}. \tag{6.4}$$

Let us consider the Riemann tensor and the Ricci tensor defined as follows:

$$R^l_{ijk}=\partial_i\Gamma^l_{jk}-\partial_j\Gamma^l_{ik}+\Gamma^r_{jk}\Gamma^l_{ir}-\Gamma^r_{ik}\Gamma^l_{jr},\quad R_{jk}=R^l_{ljk}.$$

By a straightforward calculation it can be seen that the Riemann tensor components which are needed for the computation of the nondiagonal Ricci tensor components, R_{ab}, $a\neq b$, have the following expressions:

$$R^c_{cab}=\tfrac{3}{4}\partial_a\partial_b \ln g^{cc}-\tfrac{1}{4}g_{cc}(\partial_a\partial_b g^{cc}-\partial_b \ln g^{aa}\partial_a g^{cc}-\partial_a \ln g^{bb}\partial_b g^{cc})\quad (c\neq a,b;c \text{ n.s.}),$$

$$R^a_{aab}=0, \tag{6.5}$$

$$R^\alpha_{\alpha ab}=\tfrac{3}{4}\partial_a(g_{\alpha\beta}\partial_b g^{\alpha\beta})-\tfrac{1}{4}g_{\alpha\beta}(\partial_a\partial_b g^{\alpha\beta}-\partial_b \ln g^{aa}\partial_a g^{\alpha\beta}-\partial_a \ln g^{bb}\partial_b g^{\alpha\beta})\quad (\alpha \text{ n.s.})$$

and that

$$R_{a\alpha}=0. \tag{6.6}$$

A remarkable fact is that, due to the separability conditions (3.8′), expressions (6.5) reduce to

$$R^c_{cab}=\tfrac{3}{4}\partial_a\partial_b \ln g^{cc},\quad R^\alpha_{\alpha ab}=\tfrac{3}{4}\partial_a(g_{\alpha\beta}\partial_b g^{\alpha\beta}),$$

so that

$$R_{ab}=\frac{3}{4}\partial_a\partial_b\left(\sum_{c\neq a,b}\ln g^{cc}+\ln\det[g^{\alpha\beta}]\right)\quad (a\neq b). \tag{6.7}$$

For the case $m=n$ the second term on the right-hand side of (6.7) disappears and we find a formula first stated by Eisenhart[20] and related to the orthogonal separation.

Another remarkable fact is that for $c=a$ the first equation (3.8′) is equivalent to

$$\partial_a\partial_b \ln g^{aa}=\partial_a \ln g^{bb}\partial_b \ln g^{aa}\quad (a\neq b),$$

so that, due to the symmetry in the indices of the right-hand side of this equation, we can write

$$\partial_a\partial_b \ln g^{aa}=\tfrac{1}{2}(\partial_a\partial_b \ln g^{aa}+\partial_a\partial_b \ln g^{bb}),$$

and from (6.3) we get

$$\partial_b\Gamma_a=\frac{1}{2}\partial_a\partial_b\left(\sum_{c\neq a,b}\ln g^{cc}+\ln\det[g^{\alpha\beta}]\right). \tag{6.8}$$

Formula (6.6) and the comparison between (6.8) and (6.7) show that

Theorem 6.1: *(i) In standard separable coordinates* (q^a,q^α),

$$R_{ab}=\tfrac{3}{2}\partial_b\Gamma_a\quad (a\neq b),\quad R_{a\alpha}=0. \tag{6.9}$$

(ii) In orthogonal separable coordinates,

$$R_{ij}=\tfrac{3}{2}\partial_j\Gamma_i, \quad i\neq j. \tag{6.10}$$

This last equation is simply the reduction of (6.9) to the case $m=n$ (no greek indices). Thus,

Theorem 6.2: *The Robertson condition in orthogonal separable coordinates* $\partial_i\Gamma_j=0$ $(i\neq j)$ *is equivalent to*

$$R_{ij}=0 \quad (i\neq j).$$

The Robertson condition in standard separable coordinates $\partial_a\Gamma_b=0$ $(a\neq b)$ *is equivalent to*

$$R_{ab}=0 \quad (a\neq b).$$

Remark 6.3: Theorem 6.2 gives a geometrical meaning of the Robertson condition for the free and the reduced separation. For the reduced separation we take the standard coordinates as required by Proposition 5.8.

Since $R_{a\alpha}=0$, it is proved that

Theorem 6.4: *The Robertson condition in standard coordinates is fulfilled if and only if the Ricci tensor assumes the standard form*.

Remark 6.5: The Robertson condition is identically satisfied, so that there is a simultaneous separation of the Schrödinger and Hamilton–Jacobi equations, for Einstein manifolds, where the Ricci tensor is proportional to the metric tensor, $\mathbf{R}=a\mathbf{G}$ (thus, in particular, for constant curvature manifolds and Ricci-flat manifolds).

VII. THE EISENHART–KILLING EQUATIONS AND THE INTRINSIC CHARACTERIZATION OF THE SEPARATION

As has been illustrated in the preceding sections, the separation of variables is apparently a strictly ''coordinate dependent'' matter. This is perhaps the reason why for long it has not been recognized as a ''modern'' theory. However, as we know today, the existence of separable coordinates for the Hamilton–Jacobi and Schrödinger equations requires the presence on the underlying Riemannian manifold of a rich intrinsic (coordinate independent) structure, described by algebraic or geometrical objects: Killing vectors, Killing tensors, and webs (sets of foliations).

The first fundamental contibution to the intrinsic theory of the variable separation dates back to Levi-Civita.[11] He pointed out first, that the separation of the geodesic Hamiltonian is a necessary condition for the separation of all the associated natural Hamiltonians with scalar and vector potentials.[21] This gives a prominent role to the separation of the geodesic Hamilton–Jacobi equation. Second, he proposed a classification of the separable coordinates into two classes and, by using his methods of ''calcolo differenziale assoluto,'' developed together with Ricci[22] a few years earlier, he proved that when all the coordinates are of first class then the manifold is necessarily locally flat. This result was later extended to the general case by Agostinelli,[23] who proved that the separation associated with r first-class coordinates corresponds to the existence of a foliation of r-dimensional locally flat submanifolds. These pioneering results have recently been incorporated within a general geometrical framework of the geodesic separation, based on the notion of *separable Killing web*.[16] However, a milestone in this way is represented by the contribution of Eisenhart,[3] which we shall revisit in the present section, with suitable modifications and extensions.

We recall that a contravariant symmetric tensor $\mathbf{K}=(K^{i\cdots j})$ is said to be a *Killing tensor* if its components satisfy the *Killing equation*

$$\nabla^{(h}K^{i\cdots j)}=0,$$

where ∇ denotes the covariant derivative with respect to the Levi-Civita connection and the parentheses (...) denote the symmetrization of the indices. There is however an alternative equivalent definition of Killing tensor, which is not related to the covariant derivative but to the canonical

symplectic structure of a cotangent bundle. This definition is based on the one-to-one correspondence between the contravariant symmetric tensors and the homogeneous polynomial functions on T^*Q,

$$P(\mathbf{K}) = P_{\mathbf{K}} = K^{i\cdots j} p_i \cdots p_j .$$

We say that two tensors $\mathbf{K}$ and $\mathbf{K}'$ are *in involution* if the corresponding polynomial functions are in involution, i.e., if their Poisson bracket vanishes identically:

$$\{P(\mathbf{K}), P(\mathbf{K}')\} = 0.$$

Then a tensor $\mathbf{K}$ is a Killing tensor if and only if $P(\mathbf{K})$ is a first integral of the geodesic flow, i.e., it is in involution with the geodesic Hamiltonian $G = \frac{1}{2} P_{\mathbf{G}}$:

$$\{P_{\mathbf{K}}, G\} = 0. \tag{7.1}$$

Also this definition does not depend on the choice of the coordinates. Let us call (7.1) the *Poisson–Killing equation*.

In the theory of the separation of variables a fundamental role is played by Killing vectors, corresponding to linear first integrals and to one-parameter groups of isometries, and by Killing two-tensors, interpreted as symmetric linear operators on one-forms or vector fields. Thus, in the following discussion by ''Killing tensor'' we mean ''Killing two-tensor.''

Remark 7.1: We shall use the following notation. If $\mathbf{K} = (K^{ij})$ is a contravariant two-tensor and $\mathbf{X} = (X^i)$ a vector field, then by $\mathbf{KX}$ we denote the vector field image of $\mathbf{X}$ by $\mathbf{K}$ (as linear operator) whose components are

$$(\mathbf{KX})^i = K^{ij} g_{jh} X^h = K^i_{\cdot j} X^j,$$

and by $\mathbf{K}\varphi$ the one-form image by $\mathbf{K}$ of the one-form $\varphi = \varphi_i \mathrm{d}q^i$ whose components are

$$(\mathbf{K}\varphi)_i = g_{ih} K^{hj} \varphi_j = K_i^{\cdot j} \varphi_j .$$

If $\mathbf{K}$ and $\mathbf{L}$ are two such tensors then by $\mathbf{LK}$ we mean their composition as linear operators. It is a contravariant two-tensor whose components are

$$(\mathbf{LK})^{ij} = L^{ih} g_{hk} K^{kj} = L^{i\cdot}_{\cdot k} K^{kj} = L^{ih} K_h^{\cdot j} .$$

We begin by considering the orthogonal separation. The link between the orthogonal separation and the existence of Killing tensors is based on the following statement due to Eisenhart:[20]

Proposition 7.2: Let $\mathbf{K}$ *be a symmetric tensor on a Riemannian manifold* $(Q, \mathbf{g})$ *which is diagonalized in an orthogonal coordinate system* $\underline{q} = (q^i)$. *Then* $\mathbf{K}$ *is a Killing tensor if and only if its eigenvalues* (λ^i) *satisfy*

$$\partial_i \lambda^j = (\lambda^i - \lambda^j) \partial_i \ln g^{jj}. \tag{7.2}$$

Proof: In the coordinates $\underline{q}$ the components of $\mathbf{K}$ are

$$K^{ii} = \lambda^i g^{ii}, \quad K^{ij} = 0 \quad (i \neq j),$$

so that $P(\mathbf{K}) = \lambda^i g^{ii} p_i^2$. A straightforward calculation shows that (7.1) are equivalent to (7.2). ■

We call (7.2) the *Eisenhart–Killing equations*. These equations can be interpreted as a linear normal first-order differential system in the unknown functions (λ^i), of the kind considered in Sec. II. It is a crucial fact that its complete integrability conditions (as shown by a straightforward calculation) are

$$(\lambda^i - \lambda^j) S^k_{ij} = 0 \quad (i \neq j, \ \text{n.s.}), \tag{7.3}$$

where

$$S_{ij}^{k}=\partial_i\partial_j g^{kk}-\partial_i \ln g^{jj}\partial_j g^{kk}-\partial_j \ln g^{ii}\partial_i g^{kk}$$

are just the left-hand sides of the first separability conditions (3.5).

Remark 7.3: The orthogonal separability theory lies in the following rather surprising circumstance: there are three ''different'' first-order differential systems with the ''same'' complete integrability conditions, $S_{ij}^{k}=0$ $(i\neq j)$. They are: (i) system (3.3), with

$$R_i(\underline{q},\underline{p})=-\frac{\partial_i G}{\partial^i G},\quad G=\frac{1}{2}g^{ii}p_i^2,$$

related to the orthogonal separation of the geodesic Hamilton–Jacobi equation; (ii) system (4.11) with

$$R_i(\underline{q},\underline{u}^{(1)},\underline{u}^{(2)})=-\left(\frac{\partial \mathcal{S}}{\partial u_i^{(2)}}\right)^{-1}\left(\frac{\partial \mathcal{S}}{\partial q^i}+\frac{\partial \mathcal{S}}{\partial u_i}u_i^{(2)}\right),\quad \mathcal{S}(\underline{q},\underline{u}^{(1)},\underline{u}^{(2)})=g^{ij}u_iu_j+g^{ii}u_i^{(2)}-\Gamma^i u_i,$$

related to the free (thus, orthogonal) separation of the geodesic Schrödinger equation $(V=0)$; (iii) system (7.2) related to the existence of Killing tensors diagonalized in orthogonal coordinates. Actually, as we have seen, the complete integrability of the second system requires an additional condition: the Robertson condition $R_{ij}=0$ for $i\neq j$. The same remarkable property holds for a nonconstant potential V.

According to this remark, it is convenient to introduce the following

Definition 7.4: We call *Killing–Stäckel algebra* an n-dimensional linear space $\mathcal{K}$ of Killing tensors which are (i) simultaneously diagonalized in orthogonal coordinates, or equivalently, (ii) with n common normal (i.e., orthogonally integrable or surface forming) eigenvectors.

Item (ii) in this definition is a coordinate-free translation of item (i). Thus, we can affirm that

Theorem 7.5: *The orthogonal separation of the geodesic Hamilton–Jacobi equation is equivalent to the complete integrability of the Eisenhart–Killing equations i.e., to the existence of a Killing–Stäckel algebra.*

This is a synthetic and simplified version of the classical theorem of Eisenhart on ''separable systems of Stäckel.''[3]

Remark 7.6: The submanifolds of codimension 1 orthogonal to the normal eigenvectors of a Killing–Stäckel algebra form an *orthogonal separable web*. A coordinate system $\underline{q}$ is called *adapted* to this web if the corresponding coordinate hypersurfaces belong to the web. Any coordinate system adapted to a separable web is orthogonal and separable. It follows that: *an orthogonal web is separable if and only if its leaves are orthogonal to the eigenvectors of a Killing–Stäckel algebra.*

Remark 7.7: A Killing–Stäckel algebra, as well as a separable orthogonal web, may not be defined on the whole configuration manifold Q. The points of Q where the requirements of Definition 7.4 are not fulfilled (or where the manifolds orthogonal to the normal eigenvectors are not defined) form the *singular set* of the algebra (or of the web).

Due to Theorem 7.5, the analysis of the orthogonal separation is now related to the analysis of the Killing–Stäckel algebras. Going back to Definition 7.4, we observe that: (i) when the Eisenhart–Killing equations are completely integrable, we can always find, locally, a solution such that $\lambda^i\neq\lambda^j$ for $i\neq j$; (ii) as shown by a straightforward calculation, two functions $P(\mathbf{K})$ and $P(\mathbf{K}')$ corresponding to two solutions of system (7.2) are in involution; (iii) $\lambda^i=1$ is a trivial solution. Thus,

Theorem 7.8: *(i) A Killing–Stäckel algebra admits locally a Killing tensor with pointwise distinct eigenvalues. (ii) All Killing tensors in a Killing–Stäckel algebra are in involution. (iii) The metric tensor* $\mathbf{G}$ *belongs to any Killing–Stäckel algebra.*

Furthermore, the presence of the term $\lambda^i-\lambda^j$ in (7.3) implies that if there exists a Killing tensor which is diagonalized in orthogonal coordinates and with pointwise simple eigenvalues,

$\lambda^i \neq \lambda^j$, then all S^k_{ij} $(i \neq j)$ vanish identically (these are functions of the coordinates only), so that the Eisenhart–Killing equations are completely integrable.[24] This proves that

Theorem 7.9: *A Killing–Stäckel algebra is uniquely determined by a Killing tensor with normal eigenvectors and pointwise simple eigenvalues.*

Remark 7.10: The "uniqueness" in this last statement has a local meaning. It means that if $\mathcal{K}$ and $\mathcal{K}'$ are two Killing–Stäckel algebras both containing a Killing tensor **K** with simple eigenvalues, then $\mathcal{K}=\mathcal{K}'$ at least in the domain of definition of **K**. Then we say that **K** is a *characteristic tensor* of the Killing–Stäckel algebra $\mathcal{K}$. Note that it is not uniquely determined in $\mathcal{K}$. We also remark that there are cases in which a Killing–Stäckel algebra does not admit a "global" characteristic Killing tensor. An example is the parabolic translational web in the Euclidean three-space (see Ref. 25 for a description of this web).

Remark 7.11: As a consequence of the preceding remarks and statements, we have at least two ways for characterizing intrinsically the orthogonal separation of a geodesic Hamilton–Jacobi equation: (A) by means of a Killing–Stäckel algebra $\mathcal{K}$, or (B) by means of a characteristic Killing tensor **K**, i.e., a Killing tensor with simple eigenvalues and normal eigenvectors. This second characterization seems to be more effective that the first one, since it involves only one Killing tensor **K**.[24] But difficulties could arise in checking if first, this tensor has simple eigenvalues (via the analysis of the discriminant of the corresponding characteristic equation) and second, if its eigenvectors are normal. Of course, analogous problems arise in dealing with a whole Killing–Stäckel algebra (i.e., with n independent Killing tensors) at least as it is defined in Definition 7.4, item (ii): we still have the algebraic problem of checking if n independent tensors have common eigenvectors, and the differential problem of checking if these eigenvectors are normal. However, these problems can be simultaneously solved by using the following characterization of a Killing–Stäckel algebra:

Theorem 7.12: *An n-dimensional space $\mathcal{K}$ of Killing tensors is a Killing–Stäckel algebra if and only if its elements (i) commute as linear operators,*

$$\mathbf{K}_1\mathbf{K}_2-\mathbf{K}_2\mathbf{K}_1=0, \quad \forall \mathbf{K}_1,\mathbf{K}_2 \in \mathcal{K}, \tag{7.4}$$

and (ii) are in involution,

$$\{P(\mathbf{K}_1),P(\mathbf{K}_2)\}=0, \quad \forall \mathbf{K}_1,\mathbf{K}_2 \in \mathcal{K}. \tag{7.5}$$

We postpone the proof of this theorem to Sec. VIII. What is important in this characterization is that, (i) as first pointed out by Kalnins and Miller,[26] if n independent Killing tensors have n common eigenvectors and are in involution, then the eigenvectors are necessarily normal; (ii) if they commute as linear operators, then they have necessarily the same eigenvectors (this holds, however, only in a positive-definite metric); (iii) both conditions (7.4) and (7.5) require simple calculations, of algebraic and differential character, respectively.

Going back to Remark 7.11, we emphasize the advantage of dealing with a single characteristic tensor in the nongeodesic case, i.e., when a potential V is present. Indeed, it can be proved[24] that

Theorem 7.13: *The Hamilton–Jacobi equation associated with a natural Hamiltonian $H=G+V$ is orthogonally separable if and only if (i) there exists a first integral*

$$H_{\mathbf{K}}=\tfrac{1}{2}P_{\mathbf{K}}+U=\tfrac{1}{2}K^{ij}p_ip_j+U,$$

where **K** *is a tensor with pointwise simple eigenvalues and normal eigenvectors, or equivalently, (ii) if and only if there exists a Killing tensor* **K** *with pointwise simple eigenvalues and normal eigenvectors such that the one-form image of* $\mathrm{d}V$ *by* **K** *is closed:*

$$\mathrm{d}(\mathbf{K}\mathrm{d}V)=0. \tag{7.6}$$

In fact, the equivalence of items (i) and (ii) is only "local." Indeed, a function $H_{\mathbf{K}}$ is in involution with $H=G+V$ if and only if

$$\{G, P_{\mathbf{K}}\} = 0, \quad \mathrm{d}U = \mathbf{K}\,\mathrm{d}V.$$

The first equation is the Poisson–Killing equation, while the second one implies (7.6) and is implied by (7.6) only locally. However, in most of the applications this equivalence turns out to be global (that is, the closed one-form $\mathbf{K}\,\mathrm{d}V$ is exact) at least on the manifold Q deprived of the singular set of the Killing tensor $\mathbf{K}$ (where the eigenvalues are not simple).

Equation (7.6) has been called the *characteristic equation of a separable potential*. Indeed, for checking if a potential V is separable in an orthogonal separable web (thus, in any orthogonal coordinate system adapted to this web) it is sufficient to apply this equation to a single characteristic Killing tensor, and not to all elements of a basis of the corresponding Killing–Stäckel algebra. In fact, it can be proved that[24]

Theorem 7.14: *If the characteristic equation is satisfied by a characteristic Killing tensor* $\mathbf{K}$*, then it is satisfied by all elements of the Killing–Stäckel algebra* $\mathcal{K}$ *generated by* $\mathbf{K}$*, and the functions on* T^*Q*,*

$$H_{\mathbf{K}} = \tfrac{1}{2}P_{\mathbf{K}} + V_{\mathbf{K}}, \quad \mathrm{d}V_{\mathbf{K}} = \mathbf{K}\,\mathrm{d}V, \quad \forall \mathbf{K} \in \mathcal{K}, \tag{7.7}$$

form an n-dimensional space of quadratic first integrals in involution. A basis (H_j) *of this space is expressed in terms of Stäckel matrices by formula (4.30).*

By combining Theorem 7.12 and Theorems 7.13, 7.14, we get a further characterization of the separation, which uses n Killing tensors (the metric tensor $\mathbf{G}$ may be included) but which avoids the use of eigenvectors and their normality conditions:

Theorem 7.15: *The Hamilton–Jacobi equation associated with a natural Hamiltonian* $H = G + V$ *is orthogonally separable if and only if there exist n pointwise independent Killing tensors* $(\mathbf{K}_j)$ *one other (i) commuting as linear operators, (ii) in involution and such that (iii)*

$$\mathrm{d}(\mathbf{K}_j \mathrm{d}V) = 0$$

or equivalently, such that (iii′)

$$\mathrm{d}(\mathbf{K}\mathrm{d}V) = 0$$

for a suitable linear combination $\mathbf{K} = c^j\mathbf{K}_j$, $c^j \in \mathbb{R}$*, with simple eigenvalues.*

After Theorem 7.13, we can give an intrinsic translation of Theorem 4.2 by applying Theorem 6.2:

Theorem 7.16: *The Schrödinger equation is freely separable if and only if there exists a Killing tensor* $\mathbf{K}$ *with simple eigenvalues and normal eigenvectors, satisfying the characteristic equation (7.6) and commuting with the Ricci tensor*

$$\mathbf{KR} - \mathbf{RK} = 0. \tag{7.8}$$

Indeed, since $\mathbf{K}$ has simple eigenvalues, the commutation relation (7.8) means that $\mathbf{R}$ has the same eigenvectors of $\mathbf{K}$.

For a general treatment of the separation (orthogonal or nonorthogonal) we follow a similar way, starting from a suitable extension of the Eisenhart equations, that is from the following extension of Proposition 7.1, which can be easily proved by using the Poisson–Killing equations (7.1):

Theorem 7.17: *Let* $\mathbf{K}$ *be a symmetric tensor on a Riemannian manifold. Assume that in a coordinate system* (q^a, q^α) *both the contravariant metric tensor* $\mathbf{G}$ *and* $\mathbf{K}$ *assume the standard form (3.6) and (3.10), with* (q^α) *ignorable for both tensors, so that*

$$\mathbf{G} = g^{aa}\partial_a \otimes \partial_a + g^{\alpha\beta}\partial_\alpha \otimes \partial_\beta, \quad \mathbf{K} = \lambda^a g^{aa}\partial_a \otimes \partial_a + K^{\alpha\beta}\partial_\alpha \otimes \partial_\beta,$$

where (λ^a) *are the eigenvalues of* $\mathbf{K}$ *corresponding to the eigenforms* $(\mathrm{d}q^a)$*. Then* $\mathbf{K}$ *is a Killing tensor if and only if*

$$\partial_a \lambda^b = (\lambda^a - \lambda^b)\partial_a \ln g^{bb}, \quad \partial_a K^{\alpha\beta} = \lambda^a \partial_a g^{\alpha\beta}. \tag{7.9}$$

These equations can be interpreted as a linear normal first-order differential system in the unknown functions $(\lambda^a, K^{\alpha\beta})$. The complete integrability conditions assume the form

$$(\lambda^a - \lambda^b) S^{cc}_{ab} = 0, \quad (\lambda^a - \lambda^b) S^{\alpha\beta}_{ab} = 0 \quad (a \neq b, \text{ n.s}),$$

where

$$S^{hk}_{ab} = \partial_a \partial_b g^{hk} - \partial_a \ln g^{bb} \partial_b g^{hk} - \partial_b \ln g^{aa} \partial_a g^{hk} \quad (a \neq b, \text{ n.s.})$$

are just the left-hand sides of the first two separability conditions (3.8′).

Thus, remarks and theorems similar to those illustrated for the orthogonal separation are in order. The only difference is that now Eqs. (7.9), when completely integrable, generates a space $\mathcal{K}$ of Killing tensors of dimension $m < n$. The lost dimensions are replaced by a linear space D of Killing vectors. The resulting structure is a pair $(D, \mathcal{K})$ having the properties listed in the following

Definition 7.18: We call *separable Killing algebra* a pair $(D, \mathcal{K})$ where (I) D is an r-dimensional linear space of commuting Killing vectors, (II) $\mathcal{K}$ is a D-invariant $n-r$-dimensional linear space of Killing two-tensors with $m = n - r$ normal eigenvectors in common and orthogonal to D. We call these eigenvectors *essential*.

As has been proved in Ref. 16,

Theorem 7.19: *The separation of the geodesic Hamilton–Jacobi equation is equivalent to the existence of a separable Killing algebra.*

Remark 7.20: The m orthogonal foliations $\mathcal{S}^a$ of the one-codimensional submanifolds orthogonal to the essential eigenvectors of $\mathcal{K}$ (thus tangent to D and containing the orbits of D) form a geometrical structure called *separable Killing web*. A standard coordinate system (q^a, q^α) is related to such a structure in the following way: (i) $(\mathrm{d}q^a)$ are common (local) eigenforms of all elements of $\mathcal{K}$ corresponding to the common essential eigenvectors, or equivalently, their coordinate hypersurfaces belong to the web $\mathcal{S}^a$, (ii) the partial derivatives (∂_α), interpreted as vector fields, are commuting Killing vectors and form a local basis of D.

Furthermore, by a straightforward analysis of system (7.9) we can prove the following two statements:[16]

Theorem 7.21: *In a separable Killing algebra: (i) there are Killing tensors with distinct eigenvalues corresponding to the essential eigenvectors, (ii) all Killing tensors are in involution, (iii) the metric tensor is included, (iv) D is normal (i.e., orthogonally integrable).*

Theorem 7.22: *A separable Killing algebra is uniquely determined by a characteristic Killing pair* $(D, \mathbf{K})$ *where D is an r-dimensional space of Killing vectors in involution and* $\mathbf{K}$ *is a D-invariant Killing tensor with* $m = n - r$ *normal eigenvectors orthogonal to D and corresponding to pointwise distinct eigenvalues.*

Remark 7.23: Also for the general separation we have two equivalent intrinsic characterizations: (A) by means of a separable Killing algebra $(D, \mathcal{K})$ or, (B) by a characteristic Killing pair $(D, \mathbf{K})$, and what has been said in Remark 7.11 can be adapted to this case.

The use of a separable Killing algebra is made more effective by the following theorem analogous to Theorem 7.12 (see Sec. VIII for the proof).

Theorem 7.24: *A pair* $(D, \mathcal{K})$, *where D is an r-dimensional space of Killing vectors in involution and* $\mathcal{K}$ *is an m-dimensional space of D-invariant Killing tensors, is a separable Killing algebra if and only if: (i) the distribution* $\Delta^\perp$ *orthogonal to D is invariant under the elements of* $\mathcal{K}$ *interpreted as linear operators, (ii) the restrictions to* $\Delta^\perp$ *of the elements of* $\mathcal{K}$ *form at each point an m-dimensional space and commute; (iii) the elements of* $\mathcal{K}$ *are in involution.*

Finally, it can be proved[16] that

Theorem 7.25: *The Hamilton–Jacobi equation associated with a natural Hamiltonian* $H = G + V$ *is separable if and only if there exists a characteristic Killing pair* $(D, \mathbf{K})$ *such that V is D-invariant and the characteristic equation (7.6) is satisfied. In this case the functions*

$$H_{\mathbf{K}}=\tfrac{1}{2}P_{\mathbf{K}}+V_{\mathbf{K}}, \quad \mathrm{d}V_{\mathbf{K}}=\mathbf{K}\,\mathrm{d}V, \quad \mathbf{K}\in\mathcal{K},$$

$$\mathcal{H}_{\mathbf{X}}=P_{\mathbf{X}}, \quad \mathbf{X}\in D,$$

form an n-dimensional space of first integrals in involution. A basis (H_a,H_α) *of this space is expressed in terms of Stäckel matrices by formulas (5.28) and (5.32).*

Hence, the corresponding Hamiltonian system is integrable in the Arnold–Liouville sense. This theorem shows that the existence of m quadratic and $n-m$ linear first integrals in involution is a necessary condition for the separation.

Remark 7.26: It is important to remark that the use of a characteristic Killing pair $(D,\mathbf{K})$ provides a finer classification of the orthogonal separation. Indeed, an orthogonal web could admit two (or more) different characteristic Killing pairs, thus two (or more) different classes of separable potentials. This is the case, for instance, of the translational or rotational webs in the Euclidean three-space, as described in Ref. 25, where an orthogonal coordinate system may be interpreted in more than one way as a standard separable coordinate system (see the examples in Ref. 21).

As a consequence of Theorem 7.25, we get the following intrinsic translation of Theorems 5.2 and 6.4 related to the reduced separation of the Schrödinger equation. We observe that, $\mathbf{K}$ and $\mathbf{R}$ being in standard form, the tangent subspaces orthogonal to D are invariant subspaces for both.

Theorem 7.27: *The Schrödinger equation is reductively separable if and only if there exists a characteristic Killing pair* $(D,\mathbf{K})$ *such that: (i) the potential V is D-invariant; (ii) the characteristic equation (7.6) is satisfied; (iii) the spaces orthogonal to D are invariant under the Ricci tensor* $\mathbf{R}$*, interpreted as a linear operator, and the restrictions to these spaces of* $\mathbf{R}$ *and* $\mathbf{K}$ *commute or equivalently, (iii′) the essential eigenvectors are eigenvectors of the Ricci tensor* $\mathbf{R}$ *(i.e., "Ricci principal directions").*

Remark 7.28: Let $\widetilde{Q}$ be the quotient of the manifold Q by the orbits of D (that is the set of the orbits of D). At least locally, it is an m-dimensional *reduced Riemannian manifold*, whose *reduced metric tensor* $\widetilde{\mathbf{G}}=(g^{ab})$ is the result of the projection of $\mathbf{G}$ by the $(n-m)$-dimensional group of isometries associated with D. Due to the D-invariance, the separable Killing algebra $(D,\mathcal{K})$ is projectable onto an m-dimensional *reduced Killing–Stäckel algebra* $\widetilde{\mathcal{K}}$, and a characteristic Killing tensor $\mathbf{K}=(K^{ij})$ onto a *reduced characteristic Killing tensor* $\widetilde{\mathbf{K}}=(K^{ab})$. Then, the *reduced Schrödinger equation* (5.25) is just the Schrödinger equation written on the reduced manifold, but with respect to the *reduced potential*

$$\widetilde{V}=V-g^{\alpha\beta}\kappa_\alpha\kappa_\beta.$$

For this reduced equation we have a free separation.

Remark 7.29: All the preceding discussion and statements hold for pseudo-Riemannian manifolds, by excluding the case of null (or isotropic) coordinates, i.e., under the assumption $g^{ii}\neq 0$ for the free separation and $g^{aa}\neq 0$ for the reduced separation.

VIII. INTEGRABILITY OF FRAMES

As mentioned in Sec. VII, n independent Killing tensors in involution and commuting as linear operators have common and normal eigenvectors. This remarkable fact, discovered by Kalnins and Miller,[27] reduces the number of sufficient conditions for the geodesic separation listed in the original version of the Eisenhart theorem,[3] as well as in the version given by Woodhouse.[28] We illustrate in this section a detailed proof of this property, showing that in fact it lies in basic properties of frames in pure differential manifolds, apart from any Riemannian structure, which plays a role only at the very end.

A *frame* (a "moving frame" in the classical literature) on a differentiable manifold Q_n is a set of n pointwise independent vector fields $(\mathbf{X}_i)$. In general, frames exist only locally. A manifold Q

admits global frames if and only if it is parallelizable, that is $TQ=Q\times\mathbb{R}^n$. Two frames $(\mathbf{X}_i)$ and $(\mathbf{X}'_i)$ are said to be *equivalent* if there are (nowhere vanishing) functions (f_i) such that $\mathbf{X}'_i = f_i\mathbf{X}_i$.

Definition 8.1: A frame is *integrable* if for each index $i=1,...,n$ the distribution $\Delta_{\hat{i}}$ of rank $n-1$ spanned by all vectors of the frame with the exception of $\mathbf{X}_i$ is completely integrable.

Remark 8.2: The integrability is an invariant property within a class of equivalent frames.

We have two equivalent definitions of integrability, illustrated in the two following propositions.

Proposition 8.3: A frame is integrable if and only if there exist local coordinate systems (q^i) *such that the frame is equivalent to* (∂_i),

$$\partial_i = f_i\mathbf{X}_i .$$

Proof: (i) Assume that the frame is integrable. Let us consider the distribution $\Delta_{\hat{1}}$ spanned by $(\mathbf{X}_2,\ldots,\mathbf{X}_n)$. The corresponding foliation can be locally parametrized by a regular function q^1; $\mathrm{d}q^1\neq 0$ is a characteristic one-form, so that $\langle \mathbf{X}_i,\mathrm{d}q^1\rangle = 0$ for $i\neq 1$. Moreover, $\langle \mathbf{X}_1,\mathrm{d}q^1\rangle = g_1\neq 0$, otherwise $\mathrm{d}q^1=0$. Thus, $\langle f_1\mathbf{X}_1,\mathrm{d}q^1\rangle = 1$, with $f_1 = 1/g_1$. By the same procedure applied to all distributions $\Delta_{\hat{i}}$ we get a system of functions (q^i) such that $\langle f_i\mathbf{X}_i,\mathrm{d}q^j\rangle = \delta^j_i$. Hence, (q^i) are independent functions forming a coordinate system such that $\partial_i = f_i\mathbf{X}_i$. (ii). The natural frame (∂_i) associated with coordinates is obviously integrable; hence the equivalent frame $(\mathbf{X}_i)$ is integrable (Remark 8.2). ■

Proposition 8.4: A frame is integrable if and only if for each pair of indices $i\neq j$ *the distribution* Δ_{ij} *spanned by the two vectors* $(\mathbf{X}_i,\mathbf{X}_j)$ *is completely integrable*.

Proof: With each frame $(\mathbf{X}_i)$ we can always associate a *co-frame* (ξ^i) made of independent one-forms such that $\langle \mathbf{X}_i,\xi^j\rangle = \delta^j_i$. Then ξ^i is a characteristic form of the distribution $\Delta_{\hat{i}}$, that is $\langle \Delta_{\hat{i}},\xi^i\rangle = 0$. As we know, this distribution is completely integrable if and only if $\mathrm{d}\xi^i\wedge\xi^i = 0$. Moreover, each distribution Δ_{ij} is characterized by the $n-2$ forms (ξ^a), $a\neq i,j$, and for instance, Δ_{12} is completely integrable if and only if $(\dagger)\,\mathrm{d}\xi^a\wedge\xi^3\wedge\cdots\wedge\xi^n = 0$ for $a=3,...,n$. (i) Assume that the frame $(\mathbf{X}_i)$ is integrable: all $\Delta_{\hat{i}}$ are completely integrable, thus $\mathrm{d}\xi^i\wedge\xi^i = 0$ for all i. Then $(\dagger)$ is satisfied, as well as the similar equations associated with all pairs of distinct indices. (ii) Assume that all Δ_{ij} are completely integrable. Then, by the Frobenius theorem each Lie bracket $[\mathbf{X}_i,\mathbf{X}_j]$ is a linear combination of the same vectors $(\mathbf{X}_i,\mathbf{X}_j)$. This is enough for the complete integrability of any distribution (of any rank) spanned by any choice of the vectors of the frame. ■

Remark 8.5: There is a geometrical (and intuitive) proof of this proposition. (i) If the frame is integrable, let us consider the integral foliations $\mathcal{S}_{\hat{i}}$ of $\Delta_{\hat{i}}$. They are made of submanifolds of codimension 1. Submanifolds belonging to different foliations are transversal. For any choice of $i\neq j$ the foliation given by the intersection of all $\mathcal{S}_{\hat{k}}$ with $k\neq i,j$ is made of submanifolds of dimension 2 which are tangent to $(\mathbf{X}_i,\mathbf{X}_j)$. Hence, Δ_{ij} is integrable. (ii) Conversely, assume that all Δ_{ij} are integrable and let us consider the corresponding foliations $\mathcal{S}_{ij}$ made of submanifolds of dimension 2. For any fixed i, let us consider the foliation $\mathcal{S}_{\hat{i}}$ given by the union of the foliations $\mathcal{S}_{jk}$ with $j,k\neq i$. This is a foliation of submanifolds of codimension 1 tangent to $\Delta_{\hat{i}}$; then this distribution is integrable.

We base our discussion on the following general considerations. As we have seen in Sec. VII, we have a one-to-one correspondence between contravariant symmetric tensors of any order $\mathbf{K}=(K^{i\cdots j})$ on Q and homogeneous polynomial functions $P(\mathbf{K})=K^{i\cdots j}p_i\cdots p_j$ on T^*Q. For a function f (zero-order tensor) on Q, $P(f)$ is by definition the canonical lift to T^*Q (constant along the fibers), which we denote by the same symbol f, so that

$$P(f)=f.$$

By this correspondence we define two operations over symmetric tensors. (i) The symmetric tensor product $\odot$,

$$P(\mathbf{K}\odot\mathbf{L}) = P(\mathbf{K})P(\mathbf{L}).$$

This product is comutative and associative. In particular, for vector fields $\mathbf{X}$ and $\mathbf{Y}$,

$$\mathbf{X}\odot\mathbf{Y}=\tfrac{1}{2}(\mathbf{X}\otimes\mathbf{Y}+\mathbf{Y}\otimes\mathbf{X}).$$

(ii) The Lie–Nijenhuis bracket $[\cdot,\cdot]$,

$$P([\mathbf{K},\mathbf{L}])=\{P(\mathbf{K}),P(\mathbf{L})\},$$

where $\{,\}$ is the canonical Poisson–Lie bracket of functions on T^*Q, defined in local canonical coordinates (q^i,p_i) by

$$\{E,F\}=\partial^i E\,\partial_i F-\partial^i F\,\partial_i E,\quad \partial_i=\frac{\partial}{\partial q^i},\quad \partial^i=\frac{\partial}{\partial p_i}.$$

In particular, for vector fields $\mathbf{X}$ and $\mathbf{Y}$,

$$\{P(\mathbf{X}),P(\mathbf{Y})\}=P([\mathbf{X},\mathbf{Y}]),$$

where $[,]$ is the ordinary Lie bracket, and

$$\{P(\mathbf{X}),P(f)\}=[\mathbf{X},f]=\langle\mathbf{X},\mathrm{d}f\rangle.$$

This bracket is anticommutative, bilinear, and obeys the Jacobi rule. Since the Poisson bracket is a bi-derivation, the Leibnitz rule holds,

$$[\mathbf{K},\mathbf{L}\odot\mathbf{M}]=[\mathbf{K},\mathbf{L}]\odot\mathbf{M}+[\mathbf{K},\mathbf{M}]\odot\mathbf{L}.$$

Moreover, two tensors are said to be in involution if $[\mathbf{K},\mathbf{L}]=0$, i.e., $\{P(\mathbf{K}),P(\mathbf{L})\}=0$.

Let $(\mathbf{X}_i)$ be a frame on Q. Let us set

$$[\mathbf{X}_i,\mathbf{X}_j]=\Omega_{ij}{}^h\mathbf{X}_h,\quad \Omega_{ij}{}^h=-\Omega_{ji}{}^h,$$

and use the notation

$$P(\mathbf{X}_i)=x_i, \tag{8.1}$$

so that

$$\{x_i,f\}=\langle\mathbf{X}_i,\mathrm{d}f\rangle,\quad \{x_i,x_j\}=P([\mathbf{X}_i,\mathbf{X}_j])=\Omega_{ij}{}^h x_h.$$

Let us consider two contravariant symmetric two-tensors $\mathbf{K}$ and $\mathbf{L}$. Suppose that they are diagonalized in the frame, i.e.,

$$\mathbf{K}=K^i\mathbf{X}_i\odot\mathbf{X}_i,\quad \mathbf{L}=L^i\mathbf{X}_i\odot\mathbf{X}_i.$$

By using the previous formulas, it is straightforward to compute the Poisson bracket of the corresponding quadratic functions:

$$\begin{aligned}\{P(\mathbf{K}),P(\mathbf{L})\}&=\{P(K^i\mathbf{X}_i\odot\mathbf{X}_i),P(L^h\mathbf{X}_h\odot\mathbf{X}_h)\}\\&=\{K^i x_i^2,L^h x_h^2\}\\&=K^iL^h\{x_i^2,x_h^2\}+K^i\{x_i^2,L^h\}x_h^2+L^h\{K^i,x_h^2\}x_i^2\\&=4K^iL^h\Omega_{ih}{}^j x_i x_h x_j+2(K^i\langle\mathbf{X}_i,\mathrm{d}L^h\rangle-L^i\langle\mathbf{X}_i,\mathrm{d}K^h\rangle)x_i x_h^2\\&=2(2K^iL^h\Omega_{ih}{}^j+(K^i\langle\mathbf{X}_i,\mathrm{d}L^k\rangle-L^i\langle\mathbf{X}_i,\mathrm{d}K^k\rangle)\,\delta_k^h\delta_k^j)x_i x_h x_j.\end{aligned} \tag{8.2}$$

By using this formula we can prove

Theorem 8.6: *Suppose that n contravariant two-tensors* $(\mathbf{K}_a)$ *are (i) pointwise independent, (ii) in involution, and (iii) simultaneously diagonalized in a frame* $(\mathbf{X}_i)$. *Then the distributions* Δ_{ij} *spanned by pairs of vectors* $(\mathbf{X}_i,\mathbf{X}_j)$ *are completely integrable*.

Proof: By assumption (iii), $\mathbf{K}_a=K_a^i\mathbf{X}_i\odot\mathbf{X}_i$, and the independence of the tensors is equivalent to

$$\det[K_a^i]\neq 0.$$

Due to (8.2), equation $\{P(\mathbf{K}_a),P(\mathbf{K}_b)\}=0$ is equivalent to

$$(2K_a^iK_b^h\Omega_{ih}{}^j+(K_a^i\langle\mathbf{X}_i,\mathrm{d}K_b^k\rangle-K_b^i\langle\mathbf{X}_i,\mathrm{d}K_a^k\rangle)\,\delta_k^h\delta_k^j)x_ix_hx_j=0.$$

This is a homogeneous polynomial equation which must be identically satisfied for all values of the variables (p_k), thus for all values of the variables (x_i), since $x_i=P(\mathbf{X}_i)=X_i^kp_k$, and $\det[X_i^k]\neq 0$. Thus, all coefficients vanish. In particular, the coefficient of $x_1x_2x_3$ (as well as for all possible choice of three distinct indices) gives rise to

$$K_a^1K_b^2\Omega_{12}{}^3+K_a^1K_b^3\Omega_{13}{}^2+K_a^2K_b^3\Omega_{23}{}^1+K_a^2K_b^1\Omega_{21}{}^3+K_a^3K_b^1\Omega_{31}{}^2+K_a^3K_b^2\Omega_{32}{}^1=0,$$

i.e., due to the skew-symmetry of Ω,

$$\Omega_{12}{}^3(K_a^1K_b^2-K_a^2K_b^1)+\Omega_{23}{}^1(K_a^2K_b^3-K_a^3K_b^2)+\Omega_{31}{}^2(K_a^3K_b^1-K_a^1K_b^3)=0.$$

This equation can be represented in the form

$$\det\begin{bmatrix}\Omega_{23}{}^1 & \Omega_{31}{}^2 & \Omega_{12}{}^3\\ K_a^1 & K_a^2 & K_a^3\\ K_b^1 & K_b^2 & K_b^3\end{bmatrix}=0.$$

This means that the three vectors of $\mathbb{R}^3$,

$$\boldsymbol{\omega}=(\Omega_{23}{}^1,\Omega_{31}{}^2,\Omega_{12}{}^3),\quad \boldsymbol{\kappa}_a=(K_a^1,K_a^2,K_a^3),\quad \boldsymbol{\kappa}_b=(K_b^1,K_b^2,K_b^3)$$

are linearly dependent (i.e., coplanar). Assume that $\boldsymbol{\omega}\neq 0$. It follows that all vectors $(\boldsymbol{\kappa}_1,\ldots,\boldsymbol{\kappa}_n)$ belong to a same three-plane (containing $\boldsymbol{\omega}$). This means that, for any choice of three distinct indices (a,b,c), we have

$$\det\begin{bmatrix}K_a^1 & K_a^2 & K_a^3\\ K_b^1 & K_b^2 & K_b^3\\ K_c^1 & K_c^2 & K_c^3\end{bmatrix}=0.$$

As a consequence, by applying the Laplace rule to the lines (1,2,3) of the matrix $[K_a^i]$ for the calculus of its determinant, we get $\det[K_a^i]=0$: absurd. Thus $\boldsymbol{\omega}=0$. This means that $\Omega_{23}{}^1=\Omega_{31}{}^2=\Omega_{12}{}^3=0$. So, we have proved that $\Omega_{ij}{}^h=0$ for any choice of distinct indices. This means that $[\mathbf{X}_i,\mathbf{X}_j]$ is a linear combination of $\mathbf{X}_i$ and $\mathbf{X}_j$ only. Due to Frobenius' theorem, the statement is proved. ■

Due to Propositions 8.3 and 8.4 it follows that

Theorem 8.7: *Under the same assumptions of Theorem 8.6, the frame* $(\mathbf{X}_i)$ *is integrable and there are coordinates* (q^i) *in which all tensors are simultaneously diagonalized:* $K_a^{ij}=0$ *for* $i\neq j$.

We remark that the preceding statements hold in a pure differential framework; they do not involve a metric at all. When a metric tensor **G** is present, we can consider the case in which the frame is orthogonal and made of common eigenvectors of *n* independent symmetric two-tensors (not necessarily Killing tensors) $(\mathbf{K}_a)$. Then we can write

$$\mathbf{K}_a=\lambda_a^i\varepsilon^i\mathbf{X}_i\odot\mathbf{X}_i,\quad \mathbf{X}_i\cdot\mathbf{X}_j=0,\quad i\neq j,$$

where λ_a^i is the eigenvalue of $\mathbf{K}_a$ corresponding to the eigenvector $\mathbf{X}_i$,

$$\mathbf{K}_a\mathbf{X}_i=\lambda_a^i\mathbf{X}_i,$$

and

$$\varepsilon^i=\varepsilon_i^{-1},\quad \varepsilon_i=\mathbf{X}_i\cdot\mathbf{X}_i.$$

Thus, we can assert that

Theorem 8.8: *An orthogonal frame made of common eigenvectors of n independent symmetric two-tensors in involution is integrable and the tensors are simultaneously diagonalzed in an orthogonal coordinate system.*

Note that the metric tensor **G** may be one of the tensors considered in this statement (as it happens in a Killing–Stäckel algebra). Then all the two-tensors are Killing tensors. This proves Theorem 7.12, by remarking that item (i) is equivalent to the existence of common eigenvectors, according to the following

Proposition 8.9: Let $(\mathbf{K}_a)$ *be a set of n pointwise independent symmetric two-tensors on a Riemannian manifold. If they commute as linear operators then they generate locally a unique orthogonal frame (up to an equivalence) made of common eigenvectors.*

This is a pure algebraic property, which follows from the spectral theorem of self-adjoint linear operators (see for instance Ref. 29, Secs. 79, 84). However, for the sake of completeness, here we give direct proof based on the following

Proposition 8.10: Let **K** *and* **L** *be two symmetric linear operators over an n-dimensional real Euclidean vector space* $\mathbb{E}_n$. *If they commute, then they have n common eigenvectors.*

Proof: Let us denote by $\mathbf{u}\cdot\mathbf{v}=\mathbf{g}(\mathbf{u},\mathbf{v})$ the scalar product of vectors of $\mathbb{E}_n$, defined by a positive-definite metric tensor **g**. A linear operator $\mathbf{K}:\mathbb{E}_n\to\mathbb{E}_n$ is, by definition, symmetric if $\mathbf{v}\cdot\mathbf{K}\mathbf{u}=\mathbf{u}\cdot\mathbf{K}\mathbf{v}$ for each pair of vectors. It is well known that, for a metric tensor of any signature, (i) eigenvectors corresponding to distinct eigenvalues are orthogonal:

$$\mathbf{K}\mathbf{u}=\lambda\mathbf{u},\quad \mathbf{K}\mathbf{u}'=\lambda'\mathbf{u}',\quad \lambda\neq\lambda'\Leftrightarrow\mathbf{u}\cdot\mathbf{u}'=0.$$

(ii) An eigenvalue λ determines a maximal invariant linear subspace $S(\lambda)\subseteq\mathbb{E}_n$ of eigenvectors; if λ is complex, then also the conjugate λ^* is an eigenvalue (with the same multiplicity) and the dimension of $S(\lambda)$ is even. (iii) $\mathrm{am}(\lambda)\geqslant\mathrm{gm}(\lambda)$, where $\mathrm{am}(\lambda)$ is the *algebraic multiplicity* of λ as root of the characteristic equation, and $\mathrm{gm}(\lambda)$ is its *geometric multiplicity*, which is the dimension of $S(\lambda)$, if λ is real, or half of this dimension if complex. However, in a positive definite metric the eigenvalues are real and $\mathrm{am}(\lambda)=\mathrm{gm}(\lambda)=\dim S(\lambda)$. It follows that if all the eigenvalues are simple, $\dim S(\lambda)=1$ and the eigenvectors form (up to factors) a canonical basis. Let **L** be a linear operator commuting with **K**. Then

$$\mathbf{v}\in S(\lambda)\Leftrightarrow\mathbf{K}\mathbf{v}=\lambda\mathbf{v}\Rightarrow\mathbf{L}\mathbf{K}\mathbf{v}=\lambda\mathbf{L}\mathbf{v}\Rightarrow\mathbf{K}\mathbf{L}\mathbf{v}=\lambda\mathbf{L}\mathbf{v}\Rightarrow\mathbf{L}\mathbf{v}\in S(\lambda).$$

This means that $S(\lambda)$ is an invariant space of **L**. If λ is a simple root of **K**, then **v** is also an eigenvector of **L**. It follows that the space $\mathbb{E}_n$ is decomposed into a direct sum

$$\mathbb{E}_n=V_1\oplus\cdots\oplus V_k\oplus W_1\oplus\cdots\oplus W_l,$$

of mutually orthogonal subspaces, where $(V_1,\ldots,V_k)$ are one-dimensional subspaces of common eigenvectors generated by simple eigenvalues of **K** and **L**, and $(W_1,\ldots,W_k)$ are subspaces of dimension $\geqslant 2$ made of simultaneous eigevectors of **K** and **L**. By choosing an orthogonal basis on each of these subspaces we find a basis made of orthogonal common eigenvectors. ■

If, instead of two operators, we consider a set of *n* commuting symmetric operators $(\mathbf{K}_a)$ we find again a direct-sum decomposition as previously and an orthogonal basis made of common

eigenvectors. But if these operators are independent, the spaces W are not present and the basis is uniquely determined up to constant factors. Indeed, if $(\mathbf{X}_i)$ is a basis of common eigenvectors, then $\mathbf{K}_a\mathbf{X}_i=\lambda_a^i\mathbf{X}_i$ and the independence of $(\mathbf{K}_a)$ is equivalent to $\det[\lambda_a^i]\neq 0$. It follows that we can always find a linear combination of $(\mathbf{K}_a)$ which has all distinct eigenvalues. This proves Proposition 8.9.

Finally, we prove Theorem 7.24.

Proof: Conditions (i)–(ii)–(iii) are obviously necessary. To prove that they are also sufficient, let us apply Proposition 8.9 to the restrictions $\mathcal{K}^\perp$ of $\mathcal{K}$ to the orthogonal distribution $\Delta^\perp$; it follows that they define, in a unique way up to an equivalence, a *subframe* $(\mathbf{X}_a)$ $(a=1,...,m)$ of eigenvectors of $\mathcal{K}$. Since $\mathcal{K}$ is D-invariant, this subframe can be chosen to be D-invariant. If $(\mathbf{X}_\alpha)$ $(\alpha=m+1,...,n)$ is a (local) basis of D, then $(\mathbf{X}_a,\mathbf{X}_\alpha)$ form a frame such that $[\mathbf{X}_a,\mathbf{X}_\alpha]=0$, and two elements of $\mathcal{K}$ can be written in the form

$$\mathbf{K}=K^a\mathbf{X}_a\odot\mathbf{X}_a+K^{\alpha\beta}\mathbf{X}_\alpha\odot\mathbf{X}_\beta,\quad \mathbf{L}=L^a\mathbf{X}_a\odot\mathbf{X}_a+L^{\alpha\beta}\mathbf{X}_\alpha\odot\mathbf{X}_\beta,$$

where all the components are D-invariant. Recalling notation (8.1) we have

$$\{x_a,x_\alpha\}=0,\quad \{x_\alpha,x_\beta\}=0,\quad \{x_a,x_b\}=\Omega_{ab}^c x_c+\Omega_{ab}^\alpha,x_\alpha,$$

where Ω's are D-invariant. A calculation similar to that in the proof of Theorem 8.6, shows that the involutivity of a basis $(\mathbf{K}_a)$ of $\mathcal{K}$ implies that all Ω's with distinct indices vanish. Then we apply Proposition 8.4. ■

The second part of this proof can be replaced by the following geometrical (and intuitive) reasoning. We can consider (at least locally) the reduced manifold $\tilde{Q}$ (see Remark 7.28). Due to the D-invariance of $\mathcal{K}$, the vector fields $\mathbf{X}_a$ can be chosen (up to factors) to be projectable onto an orthogonal frame $\tilde{\mathbf{X}}_a$ of $\tilde{Q}$ and the orthogonal components of the elements of $\mathcal{K}$ onto the m-dimensional reduced Killing–Stäckel algebra $\tilde{\mathcal{K}}$. Then we can apply to this algebra the above-given results related to Killing–Stäckel algebras, remarking that the involutivity of $\mathcal{K}$ implies the involutivity of $\tilde{\mathcal{K}}$. It follows that the frame $(\tilde{\mathbf{X}}_a)$ is integrable. Pulling back the integral orthogonal manifolds, we get submanifolds of dimension $m-1$ whose unions with the orbits of D are manifolds of dimension $n-1$ orthogonal to the $(\mathbf{X}_a)$. Thus, these vectors are normal.

IX. AN ILLUSTRATIVE EXAMPLE: THE COMPARISON BETWEEN THE FREE AND THE REDUCED SEPARATION

Let us consider in the Euclidean three-space $Q=\mathbb{E}_3$ the Hamilton–Jacobi equation of the Kepler problem, $V=-k/r$,

$$\frac{1}{2}|\mathbf{p}|^2-\frac{k}{r}-E=0,$$

where r is the distance from the origin, and the corresponding Schrödinger equation of the ''hydrogen atom'' (as usual, see Sec. IV, we replace $(2/\hbar^2)V$ and $(2/\hbar^2)E$ with V and E)

$$\Delta\psi+\left(E+\frac{k}{r}\right)\psi=0.$$

It is known that the Kepler problem is separable with respect to four separable webs: spherical, spherical conical, parabolic, all centered at the origin, and prolate spheroidal centered at any point with focus at the origin (see Ref. 30 for a group-theoretical approach and Ref. 31 for a geometrical and tensorial approach). Since $\mathbf{R}=0$, the Schrödinger equation is separable in all possible coordinate systems associated with these webs. In order to analyze the different features between the free and the reduced separation, let us consider the spherical web, which is orthogonal (thus

allowing the free separation) and rotational (thus allowing the reduced separation). This web can be parametrized by the usual spherical coordinates $(q^1,q^2,q^3)=(r,\theta,\varphi)$.

Free separation. The Killing–Stäckel algebra $\mathcal{K}_3$ associated with the spherical web has the following basis:

$$\mathbf{K}_1=\partial_\theta\otimes\partial_\theta+\frac{1}{\sin^2\theta}\partial_\varphi\otimes\partial_\varphi,$$

$$\mathbf{K}_2=\partial_\varphi\otimes\partial_\varphi, \tag{9.1}$$

$$\mathbf{G}=\partial_r\otimes\partial_r+\frac{1}{r^2}\partial_\theta\otimes\partial_\theta+\frac{1}{r^2\sin^2\theta}\partial_\varphi\otimes\partial_\varphi.$$

The (diagonal) components of these tensors form the inverse matrix

$$[\varphi^i_{(j)}]=\begin{bmatrix}0 & 1 & \frac{1}{\sin^2\theta}\\ 0 & 0 & 1\\ 1 & \frac{1}{r^2} & \frac{1}{r^2\sin^2\theta}\end{bmatrix} \tag{9.2}$$

of the Stäckel matrix

$$[\varphi^{(j)}_i]=\begin{bmatrix}-\frac{1}{r^2} & 1 & 0\\ 0 & -\frac{1}{\sin^2\theta} & 1\\ 1 & 0 & 0\end{bmatrix}.$$

The last line of matrix (9.2) represents the diagonal components g^{ii} of the metric tensor. The contracted Christoffel symbols (4.3) are

$$\Gamma_1=-\frac{2}{r},\quad \Gamma_2=-\frac{1}{\tan\theta},\quad \Gamma_3=0. \tag{9.3}$$

Looking at the expression of the Newtonian potential energy, written as a Stäckel multiplier (1.6),

$$V=-\frac{k}{r}=\phi_i g^{ii}=\phi_i\varphi^i_{(3)}=\phi_1(r)+\phi_2(\theta)\frac{1}{r^2}+\phi_3(\varphi)\frac{1}{r^2\sin^2\theta},$$

we get (at least) two solutions,

$$\phi_1=-\frac{k}{r}-\frac{c}{r^2},\quad \phi_2=c\in\mathbb{R},\quad \phi_3=0,$$

or

$$\phi_1=-\frac{k}{r},\quad \phi_2=-\frac{c}{\sin^2\theta},\quad \phi_3=c\in\mathbb{R}.$$

However, for our purposes, there is no loss of generality in choosing $c=0$, so that they coincide:

$$\phi_1 = -\frac{k}{r}, \quad \phi_2 = 0, \quad \phi_3 = 0. \tag{9.4}$$

In the free separation the Killing tensors of the spherical Killing–Stäckel algebra correspond to the constants of motion $a=(a_j)$ entering Eqs. (4.32),

$$\varphi^i_{(j)}\left(\frac{\psi_i''}{\psi_i} - \Gamma_i \frac{\psi_i'}{\psi_i} - \phi_i\right) + a_j = 0.$$

Due to (9.3) and (9.4), these equations are equivalent to the well-known separated ordinary differential equations of the kind (4.29),

$$\psi_1'' + \frac{2}{r}\psi_1' + \left(a_3 - \frac{1}{r^2}a_1 + \frac{k}{r}\right)\psi_1 = 0 \quad (a_3 = E),$$

$$\psi_2'' + \cot\theta\,\psi_2' + \left(a_1 - \frac{1}{\sin^2\theta}a_2\right)\psi_2 = 0, \tag{9.5}$$

$$\psi_3'' + a_2\psi_3 = 0,$$

in the unknown functions $\psi_1(r)$, $\psi_2(\theta)$, $\psi_3(\varphi)$. The general solution of the first equation (9.5) can be written

$$\psi_1 = c_1 F_1 + c_2 F_2$$

where $F_1(a_1,a_3;r)$ and $F_2(a_1,a_3;r)$ are two independent confluent hypergeometric functions[32] and (c_1,c_2) arbitrary constants. Since any ψ_i can be determined up to an inessential multiplicative constant, we can choose the solution

$$\psi_1 = F_1 + b_1 F_2, \quad b_1 \in \mathbb{R}.$$

In a similar way, for the second equation (9.5) we consider the solution

$$\psi_2 = S_1(a_1,a_2;\theta) + b_2 S_2(a_1,a_2;\theta),$$

where S_1 and S_2 are independent spherical harmonics.[32] For the last equation (9.5) we can consider the solution

$$\psi_3 = e^{-\sqrt{-a_2}\varphi} + b_3 e^{\sqrt{-a_2}\varphi}.$$

Thus, the resulting separated solution $\psi = \psi_1\psi_2\psi_3$ depends on $2n=6$ constants (a_i,b_i). However, in order to get solutions $\psi = \psi_1\psi_2\psi_3$ with a physical meaning, the constant parameters (a_1,a_2,a_3), corresponding to the constants of motion, must verify further well known (quantization) conditions, assuring for instance, the summability of ψ_1 and ψ_2, and the periodicity of ψ_3. These are the results of the free separation, as explained in Remarks 4.7, 4.8, and 4.9.

Reduced separation. Since the spherical web is rotational, so that φ is ignorable, we can consider the reduced separation according to Definition 5.1 and Theorem 5.2, by setting (being $\alpha=3$)

$$\psi_3 = e^{\kappa_3\varphi}. \tag{9.6}$$

Now the Stäckel matrix and its inverse are the 2×2 matrices

$$[\varphi_b^{(a)}]=\begin{bmatrix} -\frac{1}{r^2} & 1 \\ 1 & 0 \end{bmatrix}, \quad [\varphi_{(a)}^b]=\begin{bmatrix} 0 & 1 \\ 1 & \frac{1}{r^2} \end{bmatrix},$$

respectively. The other two functions $\psi_1(r)$ and $\psi_2(\theta)$ must satisfy the separated equations (5.27). In the present case, from the general expressions (3.9), where $\alpha=\beta=3$, we derive

$$g^{33}=\frac{1}{r^2\sin^2\theta}=\phi_1^{33}+\phi_2^{33}\frac{1}{r^2},$$

thus,

$$\phi_1^{33}=\frac{c}{r^2}, \quad \phi_2^{33}=\frac{1}{\sin^2\theta}-c, \quad c\in\mathbb{R},$$

and ϕ_1, ϕ_2, Γ_1, and Γ_2 are as above. For $c=0$ (5.27) become

$$\psi_1''+\frac{2}{r}\psi_1'+\left(\tilde{a}_2-\frac{1}{r^2}\tilde{a}_1+\frac{k}{r}\right)\psi_1=0 \quad (\tilde{a}_2=E),$$

$$\psi_2''+\cot\theta\psi_2'+\left(\tilde{a}_1+\frac{1}{\sin^2\theta}\kappa_3^2\right)\psi_2=0.$$

Up to the transformation of the constant parameters,

$$\tilde{a}_1=a_1, \quad \tilde{a}_2=a_3, \quad \kappa_3^2=-a_2,$$

these equations coincide with the first two equations (9.5), and ψ_3 given by the constraint (9.1) is a solution of the third equation (9.5). Finally, we observe that the Killing–Stäckel algebra $\mathcal{K}_3$ associated with the free separation in the spherical web is determined by the Killing tensors $(\mathbf{G},\mathbf{K}_1,\mathbf{K}_2)$ given in (9.1). With the same web we associate the separable Killing algebra $(D_1,\mathcal{K}_2)$, with $\mathcal{K}_2=\text{span}(\mathbf{G},\mathbf{K}_1)$ and $D=\text{span}(\partial_\varphi)$. This geometrical structure can be interpreted in two different ways. (i) We can use ∂_φ for constructing $\mathbf{K}_2=\partial_\varphi\otimes\partial_\varphi$, by interpreting φ as an essential coordinate (this is possible since the web is orthogonal). In this way we reconstruct the Killing–Stäckel algebra $\mathcal{K}_3$, associated with the free separation. (ii) We can associate with D the solution (9.6), by interpreting φ as an ignorable coordinate, and we reduce the problem of the separation to the remaining two essential coordinates: this is the reduced separation.

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Remarks on the connection between the additive separation of the Hamilton–Jacobi equation and the multiplicative separation of the Schrödinger equation. II. First integrals and symmetry operators

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The commutation relations of the first-order and second-order operators associated with the first integrals in involution of a Hamiltonian separable system are examined. It is shown that these operators commute if and only if a ''pre-Robertson condition'' is satisfied. This condition involves the Ricci tensor of the configuration manifold and it is implied by the Robertson condition, which is necessary and sufficient for the separability of the Schrödinger equation. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1506181]

I. INTRODUCTION

The connection between the additive separation of the Hamilton–Jacobi equation and the multiplicative separation of the corresponding Schrödinger equation has been examined in paper 1.[1] Two different kinds of separation have been introduced for the Schrödinger equation, called ''free'' and ''reduced separation,'' respectively, related to two suitable completeness conditions for a separated solution and geometrically characterized in terms of ''Killing–Stäckel algebras'' and of ''separable Killing algebras.'' These are linear spaces of Killing tensors and Killing vectors which generate complete systems of first integrals in involution, and which characterize the separation of the Hamilton–Jacobi equation in orthogonal and in standard coordinates, respectively. The corresponding Schrödinger equation is then separable in the same coordinate system if and only if a ''Robertson condition'' is satisfied. This condition involves the Ricci tensor of the configuration manifold and it is fulfilled in the most common applications of the theory (for instance, on Einstein manifolds).

In the present paper we revisit the matter relating the separation of the Schrödinger equation to the existence of ''symmetry operators,'' [2] i.e., to the existence of linear second-order operators on wave functions which commute with the Schrödinger operator. These operators are in one-to-one correspondence with the quadratic first integrals associated with the separation. We shall show that the ''quantization problem,'' i.e., the problem of defining a correspondence between classical observables and linear operators preserving the commutation relations,[3] is solvable for the involutive algebra of first integrals associated with the separation of the Hamilton–Jacobi equation provided a ''pre-Robertson'' condition is satisfied. This condition is implied by the Robertson condition, so that the quantization problem for a classical natural Hamiltonian system is solvable if the corresponding Schrödinger equation is separable. The main theorems and remarks are stated in Secs. III and VI in the case of the orthogonal and general separation, respectively. The proofs are given in Secs. V and VIII, after general considerations about Killing tensors in orthogonal and standard form illustrated in Secs. IV and VII.

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II. GENERAL COMMUTATION RELATIONS FOR SECOND-ORDER DIFFERENTIAL LINEAR OPERATORS

By the "quantization problem" [3] we mean the problem of defining a correspondence $F \mapsto \hat{F}$ between classical and quantum observables, i.e., between smooth real functions on the cotangent bundle T^*Q (the "phase space") of the configuration manifold of a mechanical system and self-adjoint linear operators on a suitable "state-space" of complex-valued functions (or distributions) on Q. This correspondence is required to be $\mathbb{R}$-linear and preserving the Lie-algebra structure of classical and quantum observables:

$$(F+G)\hat{} = \hat{F}+\hat{G}, \quad (cF)\hat{} = c\hat{F} \quad (c \in \mathbb{R}), \quad \{F,G\}\hat{} = \gamma[\hat{F},\hat{G}].$$

Here, $\{F,G\}$ denotes the canonical Poisson bracket of functions, γ is a universal constant, and

$$[\hat{F},\hat{G}] = \hat{F}\hat{G} - \hat{G}\hat{F}$$

is the commutator of linear operators.

The quantization problem is not solvable on the whole set of observables of a phase space.[4–6] (see Ref. 3 for details, comments, and references). In accordance with Schwinger (Ref. 7, Sec. 2.4) we can say not only that "it is a convenient fiction to assert that every Hermitian operator symbolizes a physical quantity [...]" but also that it is a "convenient fiction" to assert that with every classical observable we can associate an Hermitian operator (i.e., a quantum observable). However, as we shall see, the quantization problem is solvable for the classical observables involved in the separation of variables of a natural Hamiltonian system, which are polynomials of second degree in the momenta (p_i).

We consider as a starting point the following assumptions: (i) The universal constant γ is a positive-imaginary number: $\gamma = i/h$, $\hbar \in \mathbb{R}_+$. (ii) The operator $\hat{f}$ corresponding to a function f on Q, interpreted as a function on T^*Q constant on the fibers, is defined by

$$\hat{f}\psi = f \cdot \psi.$$

As usual, the operator $\hat{f}$ will be simply denoted by f. (iii) The operator $\hat{P}_{\mathbf{X}}$ corresponding to a first-degree homogeneous polynomial

$$P_{\mathbf{X}} = X^i p_i$$

associated with a vector field $\mathbf{X}$ on Q, is defined by

$$\hat{P}_{\mathbf{X}}\psi = \frac{1}{\gamma}\langle \mathbf{X}, \mathrm{d}\psi \rangle = -i\hbar \langle \mathbf{X}, \mathrm{d}\psi \rangle.$$

(iv) The operator $\hat{P}_{\mathbf{K}}$ corresponding to a second-degree homogeneous polynomial

$$P_{\mathbf{K}} = K^{ij} p_i p_j$$

associated with a symmetric contravariant two-tensor $\mathbf{K}$ on Q, is defined by

$$\hat{P}_{\mathbf{K}}\psi = -\hbar^2 \Delta_{\mathbf{K}}\psi = -\hbar^2 \nabla_i (K^{ij} \nabla_j \psi),$$

where $\Delta_{\mathbf{K}}$ is the *pseudo-Laplacian* operator defined by

$$\Delta_{\mathbf{K}}\psi = \nabla_i (K^{ij} \nabla_j \psi) \tag{2.1}$$

(by ∇_i we denote the covariant derivative with respect to the Levi-Civita connection). For $\mathbf{K} = \mathbf{G}$ (the contravariant metric tensor) we find the Laplace–Beltrami operator $\Delta_{\mathbf{G}} = \Delta$,

$$\Delta\psi = g^{ij}\nabla_i\nabla_j\psi.$$

We shall use the *co-differential or divergence operator* δ on contravariant skew-symmetric tensors **A**, defined by

$$(\delta\mathbf{A})^{j\cdots k} = \nabla_i A^{ij\cdots k}.$$

For a function (zero-tensor), $\delta f = 0$. It follows that $\delta^2 = 0$.

According to the notation used in Ref. 1, Remark 7.1, we shall identify a (contravariant) two-tensor $\mathbf{K} = (K^{ij})$ with the corresponding linear endomorphisms on vectors and one-forms, so that we shall denote by $\mathbf{K}\nabla\psi$ the vector field image of the gradient $\nabla\psi$ (whose components are $K^{ij}\partial_j\psi$) and by $\mathbf{K}\,\mathrm{d}\psi$ the one-form image of the differential $\mathrm{d}\psi$ (whose components are $g_{ih}K^{hj}\partial_j\psi$). With this notation, the coordinate independent definition of the pseudo-Laplacian (2.1) is

$$\Delta_{\mathbf{K}}\psi = \delta(\mathbf{K}\nabla\psi).$$

We shall deal with quadratic classical observables of the kind

$$H_{\mathbf{K}} = \tfrac{1}{2}P_{\mathbf{K}} + V_{\mathbf{K}}, \quad V_{\mathbf{K}}: Q \to \mathbb{R},$$

and with the corresponding second-order operators

$$\hat{H}_{\mathbf{K}} = \frac{1}{2}\hat{P}_{\mathbf{K}} + V_{\mathbf{K}} = -\frac{\hbar^2}{2}\Delta_{\mathbf{K}} + V_{\mathbf{K}}. \tag{2.2}$$

For $\mathbf{K} = \mathbf{G}$ we find the *Hamiltonian* and the *Schrödinger operator*,

$$H = H_G = \frac{1}{2}P_{\mathbf{G}} + V, \quad \hat{H} = \frac{1}{2}\hat{P}_{\mathbf{G}} + V = -\frac{\hbar^2}{2}\Delta + V.$$

A classical observable F in involution with H, $\{F,H\} = 0$, is a *first integral* (or *constant of motion*) of the Hamiltonian system generated by H. A linear operator $\hat{F}$ commuting with $\hat{H}$,

$$[\hat{F},\hat{H}] = 0,$$

is called a *symmetry operator* of the Schrödinger equation. The following commutation rules hold for these classical observables,

$$\begin{aligned} \{H_{\mathbf{K}_1}, H_{\mathbf{K}_2}\} &= \{P_{\mathbf{K}_1}, P_{\mathbf{K}_2}\} + P_{\mathbf{K}_1\nabla V_{\mathbf{K}_2}} - P_{\mathbf{K}_2\nabla V_{\mathbf{K}_1}}, \\ \{H_{\mathbf{K}}, H\} &= \{P_{\mathbf{K}}, P_{\mathbf{G}}\} + P_{\mathbf{K}\nabla V} - P_{\nabla V_{\mathbf{K}}}. \end{aligned} \tag{2.3}$$

We recall that a *Killing tensor* is a symmetric tensor (of any order) satisfying one of the following two equivalent conditions:

$$\{P_{\mathbf{K}}, P_G\} = 0 \;\Leftrightarrow\; \nabla^{(i}K^{j\cdots k)} = 0, \tag{2.4}$$

where $P_{\mathbf{K}} = K^{ij\cdots k}p_i p_j \ldots p_k$ and the brackets $(\cdots)$ denote the symmetrization of the indices. The first equation (2.4) means that $P_{\mathbf{K}}$ is a first integral of the godesic flow.

In the second equation (2.3) the term $\{P_{\mathbf{K}}, P_{\mathbf{G}}\}$ is a third-degree homogeneous polynomial in the momenta (p_i), while the remaining term is of first degree. This shows that

Theorem 2.1: *The quadratic function $H_{\mathbf{K}}$ is a first integral of the Hamiltonian flow generated by H if and only if $\mathbf{K}$ is a Killing tensor and $\mathbf{K}\,\mathrm{d}V = \mathrm{d}V_{\mathbf{K}}$ i.e., the following conditions are equivalent*

$$\{H_{\mathbf{K}},H\}=0 \Leftrightarrow \begin{array}{c}\{P_{\mathbf{K}},P_{\mathbf{G}}\}=0 \quad (\mathbf{K} \text{ Killing tensor}),\\ \nabla V_{\mathbf{K}}=\mathbf{K}\nabla V.\end{array} \tag{2.5}$$

For the related operators we have

Theorem 2.2: *The following conditions are equivalent*

$$[\hat{H}_{\mathbf{K}},\hat{H}]=0 \Leftrightarrow \begin{array}{c}\{P_{\mathbf{K}},G_{\mathbf{G}}\}=0 \quad (\mathbf{K} \text{ Killing tensor}),\\ \mathbf{K}\nabla V-\nabla V_{\mathbf{K}}+\dfrac{\hbar^2}{6}\delta\mathbf{C}=0,\end{array} \Leftrightarrow \{H_{\mathbf{K}},H\}=-\frac{\hbar^2}{6}P_{\delta\mathbf{C}}, \tag{2.6}$$

where

$$\mathbf{C}=\mathbf{KR}-\mathbf{RK}, \quad C^{ij}=K^{ih}R^j_h-R^{ih}K^j_h=K^{ih}g_{hk}R^{kj}-R^{ih}g_{hk}K^{kj}, \quad C^{ij}=-C^{ji},$$

and $\mathbf{R}$ *is the Ricci tensor:*

Proof: In accordance with the above-given definitions we have

$$\hat{H}\hat{H}_{\mathbf{K}}\psi=-\frac{\hbar^2}{2}\Delta\left(-\frac{\hbar^2}{2}\Delta_{\mathbf{K}}\psi+V_{\mathbf{K}}\psi\right)+V\left(-\frac{\hbar^2}{2}\Delta_{\mathbf{K}}\psi+V_{\mathbf{K}}\psi\right)$$

$$=\frac{\hbar^4}{4}\Delta\Delta_{\mathbf{K}}\psi-\frac{\hbar^2}{2}(\Delta(V_{\mathbf{K}}\psi)+V\Delta_{\mathbf{K}}\psi)+VV_{\mathbf{K}}\psi,$$

$$\hat{H}_{\mathbf{K}}\hat{H}\psi=\frac{\hbar^4}{4}\Delta_{\mathbf{K}}\Delta\psi-\frac{\hbar^2}{2}(\Delta_{\mathbf{K}}(V\psi)+V_{\mathbf{K}}\Delta\psi)+V_{\mathbf{K}}V\psi,$$

$$\Delta_{\mathbf{K}}(V\psi)=\psi\Delta_{\mathbf{K}}V+2\mathbf{K}(\mathrm{d}V,\mathrm{d}\psi)+V\Delta_{\mathbf{K}}\psi,$$

$$\Delta(V_{\mathbf{K}}\psi)=\psi\Delta V_{\mathbf{K}}+2\mathbf{G}(\mathrm{d}V_{\mathbf{K}},\mathrm{d}\psi)+V_{\mathbf{K}}\Delta\psi.$$

Hence,

$$[\hat{H},\hat{H}_{\mathbf{K}}]\psi=\frac{\hbar^4}{4}[\Delta,\Delta_{\mathbf{K}}]\psi+\frac{\hbar^2}{2}(\psi\Delta_{\mathbf{K}}V+2\mathbf{K}(\mathrm{d}V,\mathrm{d}\psi)-\psi\Delta V_{\mathbf{K}}-2\mathbf{G}(\mathrm{d}V_{\mathbf{K}},\mathrm{d}\psi))$$

$$=\frac{\hbar^4}{4}[\Delta,\Delta_{\mathbf{K}}]\psi+\hbar^2(\mathbf{K}\nabla V-\nabla V_{\mathbf{K}})\cdot\nabla\psi+\frac{\hbar^2}{2}(\Delta_{\mathbf{K}}V-\Delta V_{\mathbf{K}})\psi. \tag{2.7}$$

Now we use a formula due to Carter[8] which gives an explicit expression of the commutator of a pseudo-Laplacian with the ordinary Laplacian,

$$[\Delta,\Delta_{\mathbf{K}}]\psi=2\nabla^hK^{ij}\nabla_{(i}\nabla_j\nabla_{h)}\psi+3\nabla_h\nabla^{(h}K^{ij)}\nabla_{(i}\nabla_{j)}\psi$$
$$+\nabla_j(\tfrac{1}{2}g_{hk}(\nabla^j\nabla^{(i}K^{hk)}-\nabla^i\nabla^{(j}K^{hk)})+\tfrac{4}{3}K^{[j}_hR^{i]h})\nabla_i\psi, \tag{2.8}$$

where the brackets $[\cdots]$ denote the skew-symmetrization of the indices. Gathering together and equating to zero the terms of third, first-, and zero-order derivatives of ψ on the right-hand side of (2.7) we get the following equations, respectively,

$$\nabla^{(h}K^{ij)}=0 \quad (\mathbf{K} \text{ is a Killing tensor}),$$

$$\mathbf{K}\nabla V-\nabla V_{\mathbf{K}}+\frac{\hbar^2}{6}\delta(\mathbf{KR}-\mathbf{RK})=0, \tag{2.9}$$

$$\Delta_{\mathbf{K}}V-\Delta V_{\mathbf{K}}=0.$$

The second-order terms in (2.7) disappear because of the first equation (2.9). The last equation (2.9) can be written $\delta(\mathbf{K}\nabla V-\nabla V_{\mathbf{K}})=0$, so that it becomes a consequence of the second equation, since $\mathbf{C}=\mathbf{KR}-\mathbf{RK}$ is skew-symmetric and $\delta^2=0$. This proves the first equivalence (2.6). The second equivalence follows from the last equation (2.3), since $\{P_{\mathbf{K}},P_{\mathbf{G}}\}$ is a homogeneous polynomial of third degree in (p_i), while $P_{\mathbf{K}\nabla V}-P_{\nabla V_{\mathbf{K}}}$ and $P_{\delta\mathbf{C}}$ are of first degree. ■

The following three propositions are a consequence of Theorem 2.2 and of the *Carter formula* (2.8).

Proposition 2.3: If $\mathbf{K}=(K^{ij})$ *is a symmetric tensor, then* $[\hat{P}_{\mathbf{K}},\hat{P}_{\mathbf{G}}]=0$ *if and only if* $\mathbf{K}$ *is a Killing tensor and*

$$\delta\mathbf{C}=\delta(\mathbf{KR}-\mathbf{RK})=0. \tag{2.10}$$

Proof: This is a special case of the first equivalence (2.6), for $V=0$ and $V_{\mathbf{K}}=0$. ■

We call (2.10) the *Carter condition*. Note that $[\hat{P}_{\mathbf{K}},\hat{P}_{\mathbf{G}}]=0$ is equivalent to $[\Delta_{\mathbf{K}},\Delta]=0$.

Proposition 2.4: If $\mathbf{K}$ *is a Killing tensor, then*

$$\{H,H_{\mathbf{K}}\}=0 \Rightarrow [\hat{H},\hat{H}_{\mathbf{K}}]\psi=\frac{\hbar^4}{6}\,\delta\mathbf{C}\cdot\nabla\psi. \tag{2.11}$$

Proof: For a Killing tensor the Carter formula (2.8) reduces to

$$[\Delta,\Delta_{\mathbf{K}}]\psi=\tfrac{2}{3}\delta\mathbf{C}\cdot\nabla\psi$$

so that (2.7) becomes

$$[\hat{H},\hat{H}_{\mathbf{K}}]\psi=\frac{\hbar^4}{6}\,\delta C\cdot\nabla\psi+\hbar^2(\mathbf{K}\nabla V-\nabla V_{\mathbf{K}})+\frac{\hbar^2}{2}\,\delta(\mathbf{K}\nabla V-\nabla V_{\mathbf{K}}).$$

Because of the equivalence (2.5), we get the second equation (2.11). ■

Proposition 2.5: Let $H_{\mathbf{K}}=\frac{1}{2}P_{\mathbf{K}}+V_{\mathbf{K}}$ *be a quadratic first integral i.e.,* $\{H_{\mathbf{K}},H\}=0$. *Then,* $[\hat{H}_{\mathbf{K}},\hat{H}]=0$ *if and only if the Carter condition (2.10) is satisfied.*

Proof: If (2.10) holds, then $[\hat{H}_{\mathbf{K}},\hat{H}]=0$ because of the implication (2.11). Conversely, the simultaneous conditions $[\hat{H}_{\mathbf{K}},\hat{H}]=0$ and $\{H_{\mathbf{K}},H\}=0$ imply $\delta\mathbf{C}=0$ because of the equivalence (2.6) ■

As a corollary of Theorem 2.2 we have

Theorem 2.6: *If* $\mathbf{R}=\kappa\mathbf{G}$, *then*

$$\{H_{\mathbf{K}},H\}=0 \Leftrightarrow [\hat{H}_{\mathbf{K}},\hat{H}]=0.$$

This shows that on Einstein manifolds (in particular, on manifolds with constant curvature, on flat manifolds, on Ricci-flat manifolds, etc.) a quadratic function $H_{\mathbf{K}}=\frac{1}{2}P_{\mathbf{K}}+V_{\mathbf{K}}$ is a first integral if and only if the corresponding operator $\hat{H}_{\mathbf{K}}$, defined according to (2.1) and (2.2), is a symmetry of the Schrödinger equation.

For a first-order operator $\hat{P}_{\mathbf{X}}$ we have a similar equivalence, but without any condition (like the Carter condition) involving the Ricci tensor:

Theorem 2.7: *The operator* $\hat{P}_{\mathbf{X}}$ *commutes with the Laplacian if and only if* $\mathbf{X}$ *is a Killing vector,*

$$[\hat{P}_{\mathbf{X}},\Delta]=0 \Leftrightarrow \{P_{\mathbf{X}},P_{\mathbf{G}}\}=0.$$

Proof: This follows from three basic facts. (i) A vector field is a Killing vector if and only if its covariant components satisfy equation

$$\nabla_i X_j + \nabla_j X_i = 0. \tag{2.12}$$

This is in accordance with (2.4). (ii) If $\mathbf{X}=(X^i)$ is a Killing vector, then[9]

$$\Delta X^i + R^i_j X^j = 0, \tag{2.13}$$

where R_{ij} is the Ricci tensor. This follows from the general commutation rule

$$\nabla_l \nabla_k X_i - \nabla_k \nabla_l X_i = X_m R^m_{\cdot ikl}, \tag{2.14}$$

where $R^m_{\cdot ikl}$ are the components of the Riemann tensor. Indeed, by setting $g^{il}R^m_{\cdot ikl}=R^m_k$, we get

$$g^{il}(\nabla_l \nabla_k X_i - \nabla_k \nabla_l X_i) = R^m_k X_m .$$

For a Killing vector, $\nabla_k X_i$ is skew-symmetric due to (2.12) thus,

$$-g^{il}\nabla_l \nabla_i X_k = R^m_k X_m ,$$

and this equation is equivalent to (2.13). (iii) For any vector field $\mathbf{X}$, the general commutation relation

$$[\mathbf{X},\Delta]\psi = -(\Delta X^l + X^i R^l_i)\nabla_l \psi - 2\nabla^h X^i \nabla_h \nabla_i \psi, \tag{2.15}$$

holds, where $\mathbf{X}(\psi)=X^i\nabla_i\psi$. Indeed,

$$\begin{aligned}[\mathbf{X},\Delta]\psi &= [X^i\nabla_i, g^{hk}\nabla_h\nabla_k]\psi \\ &= X^i g^{hk}\nabla_i\nabla_h\nabla_k\psi - g^{hk}\nabla_h\nabla_k(X^i\nabla_i\psi) \\ &= g^{hk}(X^i\nabla_i\nabla_h\nabla_k\psi - X^i\nabla_h\nabla_k\nabla_i\psi - \nabla_h\nabla_k X^i\nabla_i\psi - \nabla_k X^i\nabla_h\nabla_i\psi - \nabla_h X^i\nabla_k\nabla_i\psi)\end{aligned} \tag{2.16}$$

However, because of (2.14),

$$\nabla_i\nabla_h\nabla_k\psi = \nabla_h\nabla_i\nabla_k\psi = \nabla_j\psi R^j_{\cdot khi} = \nabla_h\nabla_k\nabla_i\psi + \nabla_j\psi R^j_{\cdot khi},$$

since $\nabla_i\nabla_k\psi$ is symmetric. Thus, the last expression (2.16) becomes

$$[\mathbf{X},\Delta]\psi = g^{hk}X^i R^j_{\cdot khi}\nabla_j\psi - \Delta X^i\nabla_i\psi - 2\nabla^h X^i\nabla_h\nabla_i\psi$$

and (2.15) is proved. Assume that $\mathbf{X}$ is a Killing vector. Then the first term on the right-hand side of (2.15) vanishes because of (2.13), as well as the second term, since $\nabla^h X^i$ is skew-symmetric because of (2.12). Conversely, assume that (2.15) is satisfied for all functions ψ. Then the coefficients of the first and second derivatives of ψ must vanish separately. The coefficients of the second derivatives yield equation $\nabla^h X^i \partial_h \partial_i \psi = 0$, which shows that $\nabla^h X^i$ is skew-symmetric. Thus, $\mathbf{X}$ is a Killing vector according to (2.12), and the first-order terms vanish due to (2.13). ■

From Theorem 2.7 it follows that

Theorem 2.8: *The operator $\hat{P}_{\mathbf{X}}$ commutes with the Schrödinger operator $\hat{H}$ if and only if $\mathbf{X}$ is a Killing vector and $\langle \mathbf{X}, \mathrm{d}V\rangle = 0$ i.e.,*

$$[\hat{P}_{\mathbf{X}}, \hat{H}] = 0 \Leftrightarrow \{P_{\mathbf{X}}, H\} = 0. \tag{2.17}$$

Proof: Since

$$[\hat{P}_{\mathbf{X}}, \tfrac{1}{2}\hat{P}_{\mathbf{G}} + V]\psi = \tfrac{1}{2}[\hat{P}_{\mathbf{X}}, \hat{P}_{\mathbf{G}}]\psi + \hat{P}_{\mathbf{X}}(V\psi) - V\hat{P}_{\mathbf{X}}\psi = \tfrac{1}{2}[\hat{P}_{\mathbf{X}}, \hat{P}_{\mathbf{G}}]\psi + \hat{P}_{\mathbf{X}}(V)\psi,$$

the first commutation relation (2.17) is equivalent to

$$[\hat{P}_{\mathbf{X}},\Delta]=0, \quad \hat{P}_{\mathbf{X}}(V)=0.$$

Moreover,

$$\{P_{\mathbf{X}},\tfrac{1}{2}P_{\mathbf{G}}+V\}=\tfrac{1}{2}\{P_{\mathbf{X}},P_{\mathbf{G}}\}+\{P_{\mathbf{X}},V\}=\tfrac{1}{2}\{P_{\mathbf{X}},P_{\mathbf{G}}\}+\langle\mathbf{X},\mathrm{d}V\rangle,$$

and the second commutation relation (2.17) is equivalent to

$$\{P_{\mathbf{X}},P_{\mathbf{G}}\}=0, \quad \langle\mathbf{X},\mathrm{d}V\rangle=0.$$

Thus, the two commutation relations are equivalent due to Theorem 2.7. ■

III. SYMMETRY OPERATORS ASSOCIATED WITH THE ORTHOGONAL SEPARATION OF THE HAMILTON–JACOBI EQUATION

A *Killing–Stäckel algebra* is an n-dimensional linear space $\mathcal{K}$ of Killing two-tensors with common normal eigenvectors.[1] It can be proved that $\mathbf{G}\in\mathcal{K}$ and that all functions $P_{\mathbf{K}}$, $\mathbf{K}\in\mathcal{K}$, are in involution. The Hamilton–Jacobi equation associated with a natural Hamiltonian

$$H=\tfrac{1}{2}P_{\mathbf{G}}+V=\tfrac{1}{2}g^{ij}(\underline{q})p_ip_j+V(\underline{q})$$

is separable (i.e., integrable by separation of variables) in orthogonal coordinates if and only if there exists a Killing–Stäckel algebra such that equation $\mathrm{d}(\mathbf{K}\,\mathrm{d}V)=0$ is satisfied for all $\mathbf{K}\in\mathcal{K}$, or for a single Killing tensor $\mathbf{K}$ with simple eigenvalues (such a tensor is called a *characteristic tensor* of $\mathcal{K}$). Then: (i) The separation occurs in any coordinate system (q^i) such that $\mathrm{d}q^i$ are (common) eigenforms of the elements of $\mathcal{K}$. In these coordinates all elements of $\mathcal{K}$ are diagonalized,

$$\mathbf{K}=K^{ii}\partial_i\otimes\partial_i=\lambda^i g^{ii}\partial_i\otimes\partial_i, \tag{3.1}$$

λ^i being the eigenvalues of $\mathbf{K}$ (for $\mathbf{K}=\mathbf{G}$ we have $\lambda^i=1$). (ii) There are local functions $V_{\mathbf{K}}$ on Q such that $\mathrm{d}V_{\mathbf{K}}=\mathbf{K}\,\mathrm{d}V$ or

$$\nabla V_{\mathbf{K}}=\mathbf{K}\nabla V \tag{3.2}$$

for all $\mathbf{K}\in\mathcal{K}$. It follows that the functions

$$H_{\mathbf{K}}=\tfrac{1}{2}P_{\mathbf{K}}+V_{\mathbf{K}}, \quad \mathbf{K}\in\mathcal{K},$$

are first integrals in involution,

$$\{H_{\mathbf{K}_1},H_{\mathbf{K}_2}\}=0, \quad \forall\mathbf{K}_1,\mathbf{K}_2\in\mathcal{K}.$$

We denote by

$$\mathcal{H}=(\mathcal{K},V)$$

the n-dimensional space of these first integrals determined by a Killing-Stäckel algebra $\mathcal{K}$ and by a potential V satisfying (3.2).

In general, the linear operators $\hat{H}_{\mathbf{K}}$ (2.2) corresponding to these quadratic first integrals do not commute, as shown by the following

Theorem 3.1: *Let $\mathcal{H}=(\mathcal{K},V)$ be the space of first integrals in involution associated with the orthogonal separation of the Hamilton–Jacobi equation. Then the following conditions are equivalent*

$$\begin{aligned}
&\text{(a)}\quad [\hat{H}_{\mathbf{K}},\hat{H}]=0, \quad \forall \mathbf{K}\in\mathcal{K},\\
&\text{(b)}\quad \delta(\mathbf{KR}-\mathbf{RK})=0, \quad \forall \mathbf{K}\in\mathcal{K},\\
&\text{(c)}\quad \partial_i R_{ij}-\Gamma_i R_{ij}=0, \quad i\neq j,\ \ i \ \text{ n.s.},\\
&\text{(d)}\quad [\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=0, \quad \forall \mathbf{K}_1,\mathbf{K}_2,\in\mathcal{K},\\
&\text{(e)}\quad \delta(\mathbf{K}_1\mathbf{R}\mathbf{K}_2-\mathbf{K}_2\mathbf{R}\mathbf{K}_1)=0, \quad \forall \mathbf{K}_1,\mathbf{K}_2,\in\mathcal{K},
\end{aligned} \tag{3.3}$$

where $\mathbf{R}$ *is the Ricci tensor,* R_{ij} *are its components in any orthogonal separable coordinate system and* Γ_i *are the contracted Christoffel symbols,* $\Gamma_i=g^{hj}\Gamma_{hj,i}$.

The proof will be given in Sec. V. In Sec. VI, a theorem analogous to Theorem 3.1 will be stated for the general nonorthogonal separation of the Hamilton–Jacobi equation, where the Killing tensors involved are in ''standard form.'' For the proofs of these theorems we need preliminary general results about Killing tensors and second-order operators. Indeed, since we do not know how to extend the Carter formula to two arbitrary symmetric tensors, we are able to study the commutator $[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]$ only for Killing tensors in orthogonal form (Secs. IV and V) or in standard form (Secs. VII and VIII).

Remark 3.2: Note that conditions (b), (c), and (e) in (3.3) do not involve the potentials $V_{\mathbf{K}}$.

Remark 3.3: Since $\mathbf{G}\in\mathcal{K}$, equation (3.3a) is an obvious consequence of (3.3d), while (3.3b) is a consequence of (3.3e). Moreover, the equivalence of (3.3a) and (3.3b) follows from Theorems 2.1 and 2.2. We call condition (3.3b),

$$\delta(\mathbf{KR}-\mathbf{RK})=0, \quad \forall \mathbf{K}\in\mathcal{K}$$

the *pre-Robertson condition*. It means that the Carter condition (2.10) is satisfied by all elements of the Killing–Stäckel algebra. Theorem 3.1 shows that Eq. (3.3c),

$$\partial_i R_{ij}-\Gamma_i R_{ij}=0 \quad (i\neq j,\ \ i \ \text{ n.s.})$$

is the coordinate expression of the pre-Robertson condition. The pre-Robertson condition (3.3b) is an obvious consequence of the *Robertson condition*[1]

$$\mathbf{KR}-\mathbf{RK}=0, \quad \forall \mathbf{K}\in\mathcal{K},$$

whose coordinate expression is

$$R_{ij}=0, \quad i\neq j. \tag{3.4}$$

Note that both conditions are fulfilled when $\mathbf{R}=\kappa\mathbf{G}$. We know[1] that in separable orthogonal coordinates

$$\partial_i\Gamma_j=\tfrac{2}{3}R_{ij}, \quad i\neq j, \tag{3.5}$$

and that the Schrödinger equation is freely separable if and only if the Hamilton–Jacobi equation is orthogonally separable and the Robertson condition holds. Hence,

Theorem 3.4: *If the Schrödinger equation associated with an orthogonal separable Hamiltonian system is freely separable, then all the operators* $\hat{H}_{\mathbf{K}}$ *corresponding to the quadratic first integrals in involution* $H_{\mathbf{K}}\in\mathcal{H}$ *commute.*

In particular, they commute with the Schrödinger operator $\hat{H}=\hat{H}_{\mathbf{G}}$. From Theorem 3.1 we derive an extension of Theorem 2.6,

Theorem 3.5: *On Einstein manifolds all operators* $\hat{H}_{\mathbf{K}}$, $\mathbf{K}\in\mathcal{K}$, *associated with the quadratic first integrals of an orthogonal separable system commute.*

Remark 3.6: In orthogonal separable coordinates the components of the Killing tensors and the potential functions assume the *Stäckel form*

$$g^{ii}=\varphi^i_{(n)}, \quad V=\phi_i(q^i)\varphi^i_{(n)}, \quad K^{ii}_j=\varphi^i_{(j)}, \quad V_{\mathbf{K}_j}=\phi_i(q^i)\varphi^i_{(j)},$$

where $(\mathbf{K}_j)$ is a local basis of $\mathcal{K}$, with $\mathbf{K}_n=\mathbf{G}$. Thus, in terms of Stäckel matrices, a local basis of $\mathcal{H}$ is given by

$$H_j=\tfrac{1}{2}\varphi^i_{(j)}(p_i^2+2\phi_i).$$

As it will be shown (Remark 5.2), the corresponding operators assume the form

$$\hat{H}_j\psi=-\frac{\hbar^2}{2}\varphi^i_{(j)}\left(\partial_i^2\psi-\Gamma_i\partial_i\psi-\frac{2}{\hbar^2}\phi_i\psi\right). \tag{3.6}$$

The Robertson condition is equivalent to $\partial_j\Gamma_i=0$ for $i\neq j$. This means that the contracted Christoffel symbols Γ_i are functions of the corresponding coordinate q^i only.

IV. KILLING TENSORS DIAGONALIZED IN ORTHOGONAL COORDINATES

In the next section we shall analyze the commutation relations of the second-order operators assuming that all the tensors **K** involved, including the metric tensor **G**, are simultaneously diagonalized in orthogonal coordinates (q^i), so that they assume the *orthogonal form* (3.1). This is equivalent to assume that all these tensors have common normal eigenvectors (or closed eigenforms). For this purpose we need some preliminary theorems about Killing tensors diagonalized in orthogonal coordinates. For such a Killing tensor the following equations hold:

$$\begin{gathered}\partial_i\lambda^j=(\lambda^i-\lambda^j)\partial_i\ln g^{jj}\\ \partial_i\lambda^i=0\\ \partial_i(\lambda^j g^{jj})=\lambda^i\partial_i g^{jj}\qquad (i,j \text{ n.s.})\\ \partial_i^2(\lambda^j g^{jj})=\lambda^i\partial_i^2 g^{jj}.\end{gathered} \tag{4.1}$$

We call *Eisenhart–Killing equations* the first equations (4.1).[10] They characterize a Killing tensor and imply the remaining equations.

In orthogonal coordinates, the nonvanishing Christoffel symbols are

$$\begin{gathered}\Gamma^j_{ij}=\Gamma^j_{ji}=-\tfrac{1}{2}\partial_i\ln g^{jj}, \quad i \text{ n.s.},\\ \Gamma^i_{jj}=-\tfrac{1}{2}g^{ii}\partial_i g_{jj}, \quad i\neq j.\end{gathered} \tag{4.2}$$

It follows that

$$\Gamma_i=\frac{1}{2}\partial_i\sum_k \ln g^{kk}-\partial_i\ln g^{ii}, \tag{4.3}$$

and

$$\sum_i \Gamma^i_{ih}=-\Gamma_h-\partial_h\ln g^{hh}. \tag{4.4}$$

Proposition 4.1: If (q^i) *are orthogonal coordinates in which a Killing tensor* **K** *is diagonalized, then*

$$(\lambda^i-\lambda^j)(\partial_i\Gamma_j-\partial_j\Gamma_i)=0 \quad (i,j \text{ n.s.}). \tag{4.5}$$

Proof: For $\lambda^i=\lambda^j$ Eq. (4.5) is obviously satisfied. Assume $\lambda^i\neq\lambda^j$. Because of (4.3) and (4.1),

$$\begin{aligned}\partial_i\Gamma_j-\partial_j\Gamma_i&=-\partial_i\partial_j\ln g^{jj}+\partial_j\partial_i\ln g^{ii}\\&=\partial_i\partial_j\ln g^{ii}-\partial_j\partial_i\ln g^{jj}=\partial_i\frac{\partial_j\lambda^i}{\lambda^j-\lambda^i}-\partial_j\frac{\partial_i\lambda^j}{\lambda^i-\lambda^j}\\&=\frac{1}{(\lambda^i-\lambda^j)^2}[\partial_i\partial_j\lambda^i(\lambda^j-\lambda^i)-\partial_j\lambda^i\partial_i(\lambda^j-\lambda^i)-\partial_j\partial_i\lambda^j(\lambda^i-\lambda^j)+\partial_i\lambda^j\partial_j(\lambda^i-\lambda^j)]=0,\end{aligned}$$

since $\partial_i\lambda^i=0$. ■

Proposition 4.2: Let $\mathbf{K}_I$, $I=1, 2$, *be two Killing tensors simultaneously diagonalized in orthogonal coordinates. Then,*

$$(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)(\partial_i\Gamma_j-\partial_j\Gamma_i)=0\quad(i\neq j\ \text{ n.s.}).\tag{4.6}$$

Proof: Because of (4.5),

$$(\lambda_1^i-\lambda_1^j)(\partial_i\Gamma_j-\partial_j\Gamma_i)=0,\quad(\lambda_2^i-\lambda_2^j)(\partial_i\Gamma_j-\partial_j\Gamma_i)=0.\tag{4.7}$$

Assume $\lambda_I^j\neq0$. If we multiply the first equation (4.7) by λ_2^j, the second one by λ_1^j and subtract the two resulting equations, then we get (4.6). If $\lambda_2^j=0$, then the second equation (4.7) becomes $\lambda_2^i(\partial_i\Gamma_j-\partial_j\Gamma_i)=0$ and (4.6) is satisfied. Similarly for $\lambda_1^j=0$. ■

Proposition 4.3: Let $\mathbf{K}_I=(K_I^{ij})$, $I=1, 2$, *be two Killing tensors simultaneously diagonalized in orthogonal coordinates. Let us define*

$$\mathbf{C}=\mathbf{K}_1\mathbf{D}\mathbf{K}_2-\mathbf{K}_2\mathbf{D}\mathbf{K}_1,\quad C^{ij}=K_1^{ih}D_{hk}K_2^{kj}-K_2^{ih}D_{hk}K_1^{kj},\tag{4.8}$$

where $\mathbf{D}=(D_{ij})$ *is a geometrical object. Then,*

$$C^{ij}=g^{ii}g^{jj}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)D_{ij},\quad C_j^i=C^i_{\cdot j}=g^{ii}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)D_{ij}\tag{4.9}$$

and

$$\nabla_iC_j^i=\sum_i\ g^{ii}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)\left(\partial_iD_{ij}-\Gamma_iD_{ij}+\frac{1}{2}\partial_i\ln g^{jj}(D_{ji}-D_{ij})\right).\tag{4.10}$$

Proof: In orthogonal coordinates

$$C^{ij}=K_1^{ii}D_{ij}K_2^{jj}-K_2^{ii}D_{ij}K_1^{jj}$$

and (4.9) follow from $K_I^{ii}=\lambda_I^ig^{ii}$. Moreover, by definition of covariant derivative,

$$\nabla_iC_j^i=\partial_iC_j^i+\Gamma^i_{ih}C_j^h-\Gamma^h_{ij}C_h^i.\tag{4.11}$$

We compute these three terms separately by using Eqs. (4.1). For the first term,

$$\begin{aligned}\partial_iC_j^i&=\partial_ig^{ii}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)D_{ij}+g^{ii}D_{ij}(\lambda_1^i\partial_i\lambda_2^j-\lambda_2^i\partial_i\lambda_1^j)+g^{ii}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)\partial_iD_{ij}\\&=g^{ii}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)(D_{ij}\partial_i\ln g^{ii}+\partial_iD_{ij})+g^{ii}D_{ij}(\lambda_1^i(\lambda_2^i-\lambda_2^j)-\lambda_2^i(\lambda_1^i-\lambda_1^j))\partial_i\ln g^{jj}\\&=g^{ii}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)[(\partial_i\ln g^{ii}-\partial_i\ln g^{jj})D_{ij}+\partial_iD_{ij}].\end{aligned}\tag{4.12}$$

To compute the second term we use formula (4.4),

$$\Gamma^i_{ih}C_j^h=-g^{ii}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)(\Gamma_i+\partial_i\ln g^{ii})D_{ij}.\tag{4.13}$$

To compute the third term we use formulas (4.2),

$$\sum_{i,h}\Gamma^h_{ij}C^i_h=\sum_{h\neq j}\Gamma^h_{jj}C^j_h+\sum_{i\neq j}\sum_h\Gamma^h_{ij}C^i_h=\cdots.$$

Since $C^i_i=0$ (i n.s.),

$$\begin{aligned}\cdots&=\sum_h\Gamma^h_{jj}C^j_h+\sum_{i\neq j}\Gamma^i_{ij}C^i_i+\sum_{i\neq j}\sum_{h\neq i}\Gamma^h_{ij}C^i_h\\&=\sum_i\Gamma^i_{jj}C^j_i+\sum_{i\neq j}\Gamma^j_{ij}C^i_j\\&=-\frac{1}{2}\sum_i g^{ii}(\lambda^i_1\lambda^j_2-\lambda^i_2\lambda^j_1)[-\partial_i g_{jj}g^{jj}D_{ji}+\partial_i\ln g^{jj}D_{ij}]\\&=-\frac{1}{2}\sum_i g^{ii}(\lambda^i_1\lambda^j_2-\lambda^i_2\lambda^j_1)\partial_i\ln g^{jj}(D_{ij}+D_{ji}).\end{aligned}\tag{4.14}$$

Thus, (4.10) follows from (4.12)+(4.13)−(4.14). ■

Remark 4.4: From the first equations (4.9), it follows that: (i) $C^{ii}=0$, (ii) the diagonal components D_{ii} are not involved in the definition (4.8) of **C**, (iii) if **D** is symmetric, $D_{ij}=D_{ji}$, then $C^{ij}+C^{ji}=0$ and **C** is skew-symmetric.

Remark 4.5: For $D_{ij}=\partial_i\Gamma_j$, due to (4.6), Eq. (4.10) becomes

$$\nabla_i C^i_j=\sum_i g^{ii}(\lambda^i_1\lambda^j_2-\lambda^i_2\lambda^j_1)(\partial^2_i\Gamma_j-\Gamma_i\partial_i\Gamma_j),\tag{4.15}$$

and, due to the first equations (4.9), $C^{ij}+C^{ji}=0$. Hence, **C** is skew-symmetric and (4.15) gives the components of $\delta\mathbf{C}$. It follows that

$$\delta\mathbf{C}=0\Leftrightarrow\sum_i g^{ii}(\lambda^i_1\lambda^j_2-\lambda^i_2\lambda^j_1)(\partial^2_i\Gamma_j-\Gamma_i\partial_i\Gamma_j)=0.\tag{4.16}$$

Remark 4.6: For $\mathbf{K}_1=\mathbf{K}$ and $\mathbf{K}_2=\mathbf{G}$, the definition (4.8) and equations (4.9) become

$$\mathbf{C}=\mathbf{KD}-\mathbf{DK},\quad C^{ij}=g^{ii}g^{jj}(\lambda_i-\lambda_j)D_{ij},\quad C^i_j=g^{ii}(\lambda^i-\lambda^j)D_{ij},$$

and (4.10) reduces to

$$\nabla_i C^i_j=\sum_i g^{ii}(\lambda^i-\lambda^j)(\partial_i D_{ij}-\Gamma_i D_{ij}+\tfrac{1}{2}\partial_i\ln g^{jj}(D_{ji}-D_{ij})).$$

For $D_{ij}=\partial_i\Gamma_j$, because of (4.5), we have

$$\nabla_i C^i_j=\sum_i g^{ii}(\lambda^i-\lambda^j)(\partial^2_i\Gamma_j-\Gamma_i\partial_i\Gamma_j).\tag{4.17}$$

C is skew-symmetric and (4.17) gives the components of $\delta\mathbf{C}$. Thus,

$$\delta\mathbf{C}=0\Leftrightarrow\sum_i g^{ii}(\lambda^i-\lambda^j)(\partial^2_i\Gamma_j-\Gamma_i\partial_i\Gamma_j)=0.\tag{4.18}$$

Remark 4.7: If the Killing tensor **K** in Proposition 4.1 has simple eigenvalues, $\lambda^i \neq \lambda^j$ for $i \neq j$, then (4.5) implies

$$\partial_i \Gamma_j = \partial_j \Gamma_i . \tag{4.19}$$

This is the case of a characteristic Killing tensor associated with the orthogonal separation. This proves

Proposition 4.8: Equation (4.19) holds for any separable orthogonal coordinate system.

This property has some interesting consequences. First, from (4.19) and (4.3) it follows that

Proposition 4.9: In any orthogonal separable coordinate system

$$\partial_i \partial_j \ln g^{ii} = \partial_i \partial_j \ln g^{jj}, \quad i \neq j.$$

A second consequence is concerned with the eigenvalues of a characteristic Killing tensor.

Proposition 4.10: For the eigenvalues (λ^i) *of a characteristic Killing tensor of a Killing–Stäckel algebra the following equations hold:*

$$\partial_i \partial_j \ln g^{ii} = -\frac{\partial_j \lambda^i \partial_i \lambda^j}{(\lambda^i - \lambda^j)^2}, \quad i \neq j, \tag{4.20}$$

Proof: For $\lambda^i \neq \lambda^j$, the first equations (4.1) can be written

$$\partial_j \ln g^{ii} = \frac{\partial_j \lambda^i}{\lambda^j - \lambda^i}.$$

If we apply the partial derivative ∂_i to this formula, and use again (4.1), then we get Eq. (4.20).■

A third consequence is concerned with the Robertson and the pre-Roberston conditions.

Proposition 4.11: For any orthogonal separable coordinate system $\underline{q} = (q^i)$ *there are local functions* $F(\underline{q})$ *such that*

$$\Gamma_i = \partial_i F.$$

The Robertson condition (3.3c) is equivalent to

$$\partial_i \partial_j F = 0, \quad i \neq j, \tag{4.21}$$

and the pre-Robertson condition (3.4) is equivalent to

$$\partial_j [\, \partial_i^2 F - \tfrac{1}{2} (\partial_i F)^2] = 0, \quad i \neq j. \tag{4.22}$$

Equation (4.21) means that the function F is a sum of functions depending on a single coordinate i.e., of functions constant on the leaves of the web: $F = \Sigma_i F_i(q^i)$. Equation (4.22) means that each function $\partial_i^2 F - 1/2(\partial_i F)^2$ is a function of the coordinate corresponding to the index only. A further interpretation of the pre-Robertson condition is expressed by the following

Proposition 4.12: The pre-Robertson condition is equivalent to

$$\partial_i Q_{ij} = 0, \quad i \neq j \quad \text{n.s.},$$

where

$$Q_{ij} = e^{-F} R_{ij}. \tag{4.23}$$

Proof: $\partial_i Q_{ij} = e^{-F}(\partial_i R_{ij} - \partial_i F R_{ij})$. ■

Remark 4.13: Let $\underline{q} = (q^i)$ and $\underline{q}' = (q^{i'})$ be two equivalent and equioriented orthogonal separable coordinate systems. Let us set

$$A_i^{i'}=\frac{\partial q^{i'}}{\partial q^i},\quad A_{i'}^{i}=\frac{\partial q^{i}}{\partial q^{i'}},\quad A=\det[A_i^{i'}]=\prod_i A_i^{i'},$$
$$G=\det[g^{ij}]=\prod_i g^{ii},\quad G'=\det[g^{i'j'}]=\prod_{i'} g^{i'i'}. \tag{4.24}$$

Note that $A_i^{j'}=0$ for $i\neq j$ and that $A>0$. The link between functions F and F' corresponding to these coordinates is

$$F'=F-\ln A+\text{const.}$$

i.e.,

$$e^{-F'}=cAe^{-F}. \tag{4.25}$$

Indeed, the relationship between the contracted Christoffel symbols is

$$\Gamma_{i'}=A_{i'}^{i}(\Gamma_i-\partial_i\ln A_i^{i'})=A_{i'}^{i}(\Gamma_i-\partial_i\ln A). \tag{4.26}$$

To prove (4.26) we observe that, since $A_i^{i'}$ is a function of q^i only,

$$\partial_i\ln A=\partial_i\ln\prod_j A_j^{j'}=\partial_i\ln A_i^{i'}.$$

Moreover, since $A>0$, from (4.24) it follows that

$$\sqrt{G'}=A\sqrt{G},$$
$$\partial_{i'}\ln\sqrt{G'}=A_{i'}^{i}(\partial_i\ln A+\partial_i\ln\sqrt{G}), \tag{4.27}$$
$$\partial_{i'}\ln g^{i'i'}=A_{i'}^{i}(2\partial_i\ln A_i^{i'}+\partial_i\ln g^{ii}).$$

By (4.3) and (4.27) we get

$$\begin{aligned}\Gamma_{i'}&=\partial_{i'}\ln\sqrt{G'}-\partial_{i'}\ln g^{i'i'}\\&=A_{i'}^{i}(\partial_i\ln A+\partial_i\ln\sqrt{G}-2\partial_i\ln A_i^{i'}-\partial_i\ln g^{ii})\\&=A_{i'}^{i}(\Gamma_i+\partial_i\ln A-2\partial_i\ln A_i^{i'}),\end{aligned}$$

which implies both equations (4.26). Finally, we observe that the object Q_{ij} is defined by (4.23) up to a multiplicative constant, since F is defined up to an additive constant. From (4.23), (4.25) and the first equation (4.27) it follows that

$$Q_{i'j'}=e^{-F'}R_{i'j'}=cAe^{-F}A_{i'}^{i}A_{j'}^{j}R_{ij}=cAA_{i'}^{i}A_{j'}^{j}Q_{ij}.$$

Thus,

$$\frac{1}{\sqrt{G'}}Q_{i'j'}=\frac{c}{\sqrt{G}}A_{i'}^{i}A_{j'}^{j}Q_{ij}.$$

V. COMMUTATION RELATIONS IN ORTHOGONAL COORDINATES

Proposition 5.1: If a symmetric tensor $\mathbf{K}=(K^{ij})$ *is diagonalized in orthogonal coordinates, then the corresponding pseudo-Laplacian assumes the form*

$$\Delta_{\mathbf{K}}\psi=A^i\partial_i^2\psi+B^i\partial_i\psi, \quad A^i=K^{ii}=\lambda^i g^{ii}, \quad B^i=g^{ii}(\partial_i\lambda^i-\lambda^i\Gamma_i). \tag{5.1}$$

Proof: By definition (2.1) and formula (4.4),

$$\begin{aligned}\Delta_{\mathbf{K}}\psi&=\nabla_i(K^{ij}\partial_j\psi)\\&=\partial_i(K^{ij}\partial_j\psi)+\Gamma^i_{ih}K^{hj}\partial_j\psi\\&=\partial_i(K^{ii}\partial_i\psi)+\Gamma^i_{ih}K^{hh}\partial_h\psi\\&=K^{ii}\partial_i^2\psi+(\partial_hK^{hh}+\Gamma^i_{ih}K^{hh})\partial_h\psi\\&=\lambda^i g^{ii}\partial_i^2\psi+(\partial_h(\lambda^h g^{hh})-\lambda^h g^{hh}(\Gamma_h+\partial_h\ln g^{hh}))\partial_h\psi\\&=\lambda^i g^{ii}\partial_i^2\psi+g^{hh}(\partial_h\lambda^h-\lambda^h\Gamma_h)\partial_h\psi.\end{aligned}$$

■

Remark 5.2: For the ordinary Laplacian, $K^{ii}=g^{ii}$, $\lambda^i=1$, and $B^i=-g^{ii}\Gamma_i$, so that

$$\Delta\psi=g^{ii}[\partial_i^2\psi-\Gamma_i\partial_i\psi].$$

A second-order operator (2.12) assumes the form

$$\hat{H}_{\mathbf{K}}\psi=\frac{\hbar^2}{2}(A^i\partial_i^2\psi+B^i\partial_i\psi)+V_{\mathbf{K}}\psi=\frac{\hbar^2}{2}g^{ii}(\lambda^i\partial_i^2\psi+(\partial_i\lambda^i-\lambda^i\Gamma_i)\partial_i\psi)+V_{\mathbf{K}}\psi. \tag{5.2}$$

For a Killing tensor **K** Eqs. (4.1) hold, so that

$$\Delta_{\mathbf{K}}\psi=g^{ii}\lambda^i[\partial_i^2\psi-\Gamma_i\partial_i\psi].$$

For a basis $(\mathbf{K}_j)$ of a Killing–Stäckel algebra we have $\varphi^i_{(j)}=\lambda^i_j g^{ii}$ (Remark 3.6) and we find expressions (3.6) of the corresponding operators $\hat{H}_j$.

Proposition 5.3: The commutator of two second-order operators of the kind (5.2) has the following expression:

$$\begin{aligned}[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]\psi=&\frac{\hbar^4}{2}(A^i_1\partial_iA^j_2-A^i_2\partial_iA^j_1)\partial_i\partial_j^2\psi+\frac{\hbar^4}{4}(A^i_1\partial_i^2A^j_2-A^i_2\partial_i^2A^j_1+B^i_1\partial_iA^j_2-B^i_2\partial_iA^j_1)\partial_j^2\psi\\&+\frac{\hbar^4}{2}(A^i_1\partial_iB^j_2-A^i_2\partial_iB^j_1)\partial_i\partial_j\psi+\Bigg(\frac{\hbar^4}{4}(A^i_1\partial_i^2B^j_2+B^i_1\partial_iB^j_2-A^i_2\partial_i^2B^j_1-B^i_2\partial_iB^j_1)\\&-\hbar^2(A^j_1\partial_jV_{\mathbf{K}_2}-A^j_2\partial_jV_{\mathbf{K}_1})\Bigg)\partial_j\psi-\frac{\hbar^2}{2}(\Delta_{\mathbf{K}_1}V_{\mathbf{K}_2}-\Delta_{\mathbf{K}_2}V_{\mathbf{K}_1})\psi.\end{aligned} \tag{5.3}$$

Proof: For two second-order operators (2.2),

$$[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=\left[\frac{1}{2}\hat{P}_{\mathbf{K}_1}+V_{\mathbf{K}_1},\frac{1}{2}\hat{P}_{\mathbf{K}_2}+V_{\mathbf{K}_2}\right]$$
$$=\frac{1}{4}[\hat{P}_{\mathbf{K}_1},\hat{P}_{\mathbf{K}_2}]+\frac{1}{2}[\hat{P}_{\mathbf{K}_1},V_{\mathbf{K}_2}]-\frac{1}{2}[\hat{P}_{\mathbf{K}_2},V_{\mathbf{K}_1}]$$
$$=\frac{\hbar^4}{4}[\Delta_{\mathbf{K}_1},\Delta_{\mathbf{K}_2}]-\frac{\hbar^2}{2}[\Delta_{\mathbf{K}_1},V_{\mathbf{K}_2}]+\frac{\hbar^2}{2}[\Delta_{\mathbf{K}_2},V_{\mathbf{K}_1}].$$

Since

$$\delta(f\mathbf{X})=\mathbf{X}\cdot\nabla f+f\delta\mathbf{X},$$

we have

$$[\Delta_{\mathbf{K}},V]\psi=\Delta_{\mathbf{K}}(V\psi)-V\Delta_{\mathbf{K}}\psi$$
$$=\delta(\mathbf{K}\nabla(V\psi))-V\Delta_{\mathbf{K}}\psi$$
$$=\delta((\mathbf{K}\nabla V)\psi+(\mathbf{K}\nabla\psi)V)-V\Delta_{\mathbf{K}}\psi$$
$$=\psi\Delta_{\mathbf{K}}V+2\mathbf{K}(\nabla\psi,\nabla V)$$
$$=\Delta_{\mathbf{K}}V\psi+2A^i\partial_iV\partial_i\psi.$$

Hence,

$$[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]\psi=\frac{\hbar^4}{4}[\Delta_{\mathbf{K}_1},\Delta_{\mathbf{K}_2}]\psi+\frac{\hbar^2}{2}(\Delta_{\mathbf{K}_2}V_{\mathbf{K}_1}-\Delta_{\mathbf{K}_1}V_{\mathbf{K}_2})\psi+\hbar^2(\mathbf{K}_2\nabla V_{\mathbf{K}_1}-\mathbf{K}_1\nabla V_{\mathbf{K}_2})\cdot\nabla\psi, \tag{5.4}$$

Because of (5.1),

$$\Delta_{\mathbf{K}_1}\Delta_{\mathbf{K}_2}\psi=A_1^i\partial_i^2(A_2^j\partial_j^2\psi+B_2^j\partial_j\psi)+B_1^i\partial_i(A_2^j\partial_j^2\psi+B_2^j\partial_j\psi)$$
$$=A_1^i(\partial_i^2A_2^j\partial_j^2\psi+2\partial_iA_2^j\partial_i\partial_j^2\psi+A_2^j\partial_i^2\partial_j^2\psi+\partial_i^2B_2^j\partial_j\psi+2\partial_iB_2^j\partial_i\partial_j\psi+B_2^j\partial_i^2\partial_j\psi)$$
$$+B_1^i(\partial_iA_2^j\partial_j^2\psi+A_2^j\partial_i\partial_j^2\psi+\partial_iB_2^j\partial_j\psi+B_2^j\partial_i\partial_j\psi)$$
$$=A_1^iA_2^j\partial_i^2\partial_j^2\psi+(2A_1^i\partial_iA_2^j+B_1^iA_2^j+A_1^jB_2^i)\partial_i\partial_j^2\psi+(A_1^i\partial_i^2A_2^j+B_1^i\partial_iA_2^j)\partial_j^2\psi$$
$$+(2A_1^i\partial_iB_2^j+B_1^iB_2^j)\partial_i\partial_j\psi+(A_1^i\partial_i^2B_2^j+B_1^i\partial_iB_2^j)\partial_j\psi,$$

so that,

$$[\Delta_{\mathbf{K}_1},\Delta_{\mathbf{K}_2}]\psi=\Delta_{\mathbf{K}_1}\Delta_{\mathbf{K}_2}\psi-\Delta_{\mathbf{K}_2}\Delta_{\mathbf{K}_1}\psi$$
$$=2(A_1^i\partial_iA_2^j-A_2^i\partial_iA_1^j)\partial_i\partial_j^2\psi+(A_1^i\partial_i^2A_2^j-A_2^i\partial_i^2A_1^j+B_1^i\partial_iA_2^j-B_2^i\partial_iA_1^j)\partial_j^2\psi$$
$$+2(A_1^i\partial_iB_2^j-A_2^i\partial_iB_1^j)\partial_i\partial_j\psi+(A_1^i\partial_i^2B_2^j+B_1^i\partial_iB_2^j-A_2^i\partial_i^2B_1^j-B_2^i\partial_iB_1^j)\partial_j\psi.$$

Thus, from (5.4) we derive (5.3). ■

Proposition 5.4: Let $\mathbf{K}_1$ *and* $\mathbf{K}_2$ *be symmetric tensors simultaneously diagonalized in orthogonal coordinates. Then,* $[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=0$ *if and only if*

$$A_1^i\partial_iA_2^j-A_2^i\partial_iA_1^j=0 \quad (i \text{ n.s.}), \tag{5.5a}$$

$$\sum_i \left(A_1^i\partial_i^2 A_2^j - A_2^i\partial_i^2 A_1^j + B_1^i\partial_i A_2^j - B_2^i\partial_i A_1^j\right) + 2\left(A_1^j\partial_j B_2^j - A_2^j\partial_j B_1^j\right) = 0, \tag{5.5b}$$

$$A_1^i\partial_i B_2^j - A_2^i\partial_i B_1^j + A_1^j\partial_j B_2^i - A_2^j\partial_j B_1^j = 0 \quad (i \neq j \text{ n.s.}), \tag{5.5c}$$

$$\frac{\hbar^2}{4}\sum_i \left(A_1^i\partial_i^2 B_2^j + B_1^i\partial_i B_2^j - A_2^i\partial_i^2 B_1^j - B_2^i\partial_i B_1^j\right) - A_1^j\partial_j V_{\mathbf{K}_2} + A_2^j\partial_j V_{\mathbf{K}_1} = 0 \quad (j \text{ n.s.}), \tag{5.5d}$$

$$\Delta_{\mathbf{K}_1} V_{\mathbf{K}_2} - \Delta_{\mathbf{K}_2} V_{\mathbf{K}_1} = 0. \tag{5.5e}$$

Proof: (i) Assume that (5.3) vanishes identically for all functions ψ. For $\psi = 1$ we get (5.5e) and the last term in (5.3) disappears. For $\psi = q^j$ we get (5.5d), so that also the fourth term in (5.3) disappears. As a consequence, for $\psi = (q^j)^2$ we get (5.5b) and we reduce the vanishing of (5.3) to

$$\sum_{i,j} \left(A_1^i\partial_i A_2^j - A_2^i\partial_i A_1^j\right)\partial_i\partial_j^2\psi + \sum_{i,j\neq} \left(A_1^i\partial_i B_2^j - A_2^i\partial_i B_1^j\right)\partial_i\partial_j\psi = 0. \tag{5.6}$$

For $\psi = q^1 q^2$, we have $\partial_i\partial_j\psi = \delta_j^1\delta_i^2 + \delta_i^1\delta_j^2$, thus we get (5.5c) for distinct indices and moreover, (5.6) reduces to

$$\sum_{i,j} \left(A_1^i\partial_i A_2^j - A_2^i\partial_i A_1^j\right)\partial_i\partial_j^2\psi = 0. \tag{5.7}$$

Finally, for $\psi = q^1(q^2)^2$ we have $\partial_j^2\partial_i\psi = \partial_j^2(\delta_i^1(q^2)^2 + 2q^1q^2\delta_i^2) = 2\delta_i^1\delta_j^2 + 4\delta_j^1\delta_j^2\delta_i^2 = 2\delta_i^1\delta_j^2$. Thus, we get (5.5a) for distinct indices (and no summation), so that (5.7) reduces to

$$\sum_j \left(A_1^j\partial_j A_2^j - A_2^j\partial_j A_1^j\right)\partial_j^3\psi = 0.$$

This shows that (5.5a) also holds for $i = j$. (ii) Conversely, assume that (5.5) hold. Then, due to (5.5a,d,e), Eq. (5.3) reduces to

$$[\hat{H}_{\mathbf{K}_1}, \hat{H}_{\mathbf{K}_2}]\psi = \frac{\hbar^4}{4}\left(A_1^i\partial_i^2 A_2^j - A_2^i\partial_i^2 A_1^j + B_1^i\partial_i A_2^j - B_2^i\partial_i A_1^j\right)\partial_j^2\psi + \frac{\hbar^4}{2}\left(A_1^i\partial_i B_2^j - A_2^i\partial_i B_1^j\right)\partial_i\partial_j\psi$$

and, because of (5.5b), we obtain

$$[\hat{H}_{\mathbf{K}_1}, \hat{H}_{\mathbf{K}_2}]\psi = \frac{\hbar^4}{2}\sum_{i,j\neq} \left(A_1^i\partial_i B_2^j - A_2^i\partial_i B_1^j\right)\partial_i\partial_j\psi.$$

But this last expression vanishes identically because of the skew-symmetry of Eq. (5.5c). ■

Remark 5.5: Since

$$\{P_{\mathbf{K}_1}, P_{\mathbf{K}_2}\} = \{A_1^i p_i^2, A_2^j p_j^2\} = 2p_i p_j^2\left(A_1^i\partial_i A_2^j - A_2^i\partial_i A_1^j\right), \tag{5.8}$$

Eq. (5.5a) is equivalent to $\{P_{\mathbf{K}_1}, P_{\mathbf{K}_2}\} = 0$. Thus,

$$[\hat{H}_{\mathbf{K}_1}, \hat{H}_{\mathbf{K}_2}] = 0 \Rightarrow \{P_{\mathbf{K}_1}, P_{\mathbf{K}_2}\} = 0. \tag{5.9}$$

Theorem 5.6: *Let* **K** *be a symmetric tensor diagonalized in orthogonal coordinates. Then the following conditions are equivalent:*

$$[\hat{H}_{\mathbf{K}},\hat{H}]=0 \Leftrightarrow \begin{matrix}\{P_{\mathbf{K}},P_{\mathbf{G}}\}=0 \quad (\mathbf{K}\ \text{Killing tensor})\\ \dfrac{\hbar^2}{4}\delta\mathbf{C}+\mathbf{K}\nabla V-\nabla V_{\mathbf{K}}=0\end{matrix} \Leftrightarrow \{H_{\mathbf{K}},H\}=-\frac{\hbar^2}{4}P_{\delta C}, \tag{5.10}$$

where

$$C=\mathbf{KD}-\mathbf{DK}, \quad \mathbf{D}=(D_{ij})=(\partial_i\Gamma_j).$$

Proof: We use (5.5) of Proposition 5.4 for the case

$$\begin{matrix}\mathbf{K}_1=\mathbf{K}\\ \mathbf{K}_2=\mathbf{G}\end{matrix}\overset{\Leftrightarrow}{}\begin{matrix}\lambda_1^i=\lambda^i\\ \lambda_2^i=1\end{matrix}\overset{\Leftrightarrow}{}\begin{matrix}A_1^i=\lambda^i g^{ii}, & B_1^i=g^{ii}(\partial_i\lambda^i-\lambda^i\Gamma_i)\\ A_2^i=g^{ii}, & B_2^i=-g^{ii}\Gamma_i\end{matrix}.$$

Assume $[\hat{H}_{\mathbf{K}},\hat{H}_{\mathbf{G}}]=0$. From (5.9) it follows that $\mathbf{K}$ is a Killing tensor. Then we use (4.1) and in (5.5) we consider

$$B_1^i=-g^{ii}\lambda^i\Gamma_i, \quad B_2^i=-g^{ii}\Gamma_i, \tag{5.11}$$

and

$$\begin{aligned}&\partial_i A_1^j=\lambda^i\partial_i g^{jj}, \quad \partial_i B_1^j=-\partial_i(g^{jj}\lambda^j\Gamma_j)=-\lambda^i\partial_i g^{jj}\Gamma_j-g^{jj}\lambda^j\partial_i\Gamma_j,\\ &\partial_i A_2^j=\partial_i g^{jj}, \quad \partial_i B_2^j=-\partial_i(g^{jj}\Gamma_j)=-\partial_i g^{jj}\Gamma_j-g^{jj}\partial_i\Gamma_j,\\ &\partial_i^2 A_1^j=\lambda^i\partial_i^2 g^{jj}, \quad \partial_i^2 B_1^j=-\lambda^i\partial_i^2 g^{jj}\Gamma_j-2\lambda^i\partial_i g^{jj}\partial_i\Gamma_j-g^{jj}\lambda^j\partial_i^2\Gamma_j,\\ &\partial_i^2 A_2^j=\partial_i^2 g^{jj}, \quad \partial_i^2 B_2^j=-\partial_i^2 g^{jj}\Gamma_j-2\partial_i g^{jj}\partial_i\Gamma_j-g^{jj}\partial_i^2\Gamma_j,\end{aligned} \tag{5.12}$$

Equations (5.5a) and (5.5b) are then identically satisfied, while the remaining three equations become

$$\begin{aligned}&(\lambda^i-\lambda^j)(\partial_i\Gamma_j-\partial_j\Gamma_i)=0 \quad (i\neq j \ \text{ n.s.}),\\ &\frac{\hbar^2}{4}\sum_i g^{ii}(\lambda^i-\lambda^j)(\partial_i^2\Gamma_j-\Gamma_i\partial_i\Gamma_j)+\lambda^j\partial_j V-\partial_j V_{\mathbf{K}}=0 \quad (j \ \text{ n.s.}),\\ &\delta(\mathbf{K}\nabla V-\nabla V_{\mathbf{K}})=0.\end{aligned} \tag{5.13}$$

Due to (4.5), the first equation is identically satisfied. According to Remark 4.6 and Eq. (4.17), the second equation (5.13) is equivalent to

$$\frac{\hbar^2}{4}\delta\mathbf{C}+\mathbf{K}\nabla V-\nabla V_{\mathbf{K}}=0,$$

where $\mathbf{C}$ is skew-symmetric. Since $\delta^2\mathbf{C}=0$, the last equation (5.13) is a consequence of the second equation (5.13). The above-given reasoning is reversible, and the first equivalence (5.10) is proved. The second equivalence follows from last equation (2.3). ■

Remark 5.7: The comparison between Theorem 2.2, proved by using the Carter formula (2.8) without any special assumption on $\mathbf{K}$, and Theorem 5.6, proved under the assumption that $\mathbf{K}$ is diagonalized in orthogonal coordinates, shows that for such a Killing tensor the following equation holds:

$$\delta(\mathbf{KD}-\mathbf{DK})=\tfrac{2}{3}\delta(\mathbf{KR}-\mathbf{RK}), \tag{5.14}$$

where $\mathbf{D}=(\partial_i\Gamma_j)$. Note that the components D_{ii} are not involved in the definition of $\mathbf{C}=\mathbf{KD}-\mathbf{DK}$ (Remark 4.4). This is in accordance with formula (3.5), which holds in separable orthogonal coordinates.

Now we apply Proposition 5.4 to the case of two Killing tensors.

Theorem 5.8: *Let* $\mathbf{K}_1$ *and* $\mathbf{K}_2$ *be Killing tensors simultaneously diagonalized in orthogonal coordinates. Then* $\{P_{\mathbf{K}_1},P_{\mathbf{K}_2}\}=0$ *and the following conditions are equivalent:*

$$[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=0 \Leftrightarrow \frac{\hbar^2}{4}\delta\mathbf{C}+\mathbf{K}_1\nabla V_{\mathbf{K}_2}-\mathbf{K}_2\nabla V_{\mathbf{K}_1}=0 \Leftrightarrow \{H_{\mathbf{K}_1},H_{\mathbf{K}_2}\}=-\frac{\hbar^2}{4}P_{\delta\mathbf{C}}, \tag{5.15}$$

where

$$\mathbf{C}=\mathbf{K}_1\mathbf{D}\mathbf{K}_2-\mathbf{K}_2\mathbf{D}\mathbf{K}_1, \quad \mathbf{D}=(\partial_i\Gamma_j). \tag{5.16}$$

Proof: The components of $\mathbf{C}$ defined in (5.16) are [recall (4.8) and (4.9)]

$$C^{ij}=g^{ii}g^{jj}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)\partial_i\Gamma_j, \quad C^i_j=C^{i\cdot}_{\cdot j}=g^{ii}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)\partial_i\Gamma_j.$$

The involutivity condition $\{P_{\mathbf{K}_1},P_{\mathbf{K}_2}\}=0$ follows from (5.8), (5.1), and (4.1). We use (5.5). According to (5.1), (5.11), and (5.12), for a Killing tensor $\mathbf{K}_I$ $(I=1,2)$ we have

$$\begin{aligned}
&A_I^i=\lambda_I^i g^{ii}, \quad B_I^i=-A_I^i\Gamma_i,\\
&\partial_i A_I^j=A_I^i\partial_i g^{jj}=\lambda_I^i\partial_i g^{jj},\\
&\partial_i^2 A_I^j=A_I^i\partial_i^2 g^{jj}=\lambda_I^i\partial_i^2 g^{jj}\\
&\partial_i B_I^j=-\partial_i(A_I^j\Gamma_j)=-\partial_i A_I^j\Gamma_j-A_I^j\partial_i\Gamma_j,\\
&\partial_i^2 B_I^j=-\partial_i^2 A_I^j\Gamma_j-2\partial_i A_I^j\partial_i\Gamma_j-A_I^j\partial_i^2\Gamma_j.
\end{aligned} \tag{5.17}$$

Because of the first two equations (5.17), Eq. (5.5a) is identically satisfied and the sum of the first two terms in Eq. (5.5b) vanishes, so that this equation reduces to

$$\sum_i \Gamma_i[A_1^i\partial_i A_2^j-A_2^i\partial_i A_1^j]+2[A_1^j\partial_j(A_2^j\Gamma_j)-A_2^j\partial_j(A_1^j\Gamma_j)]=0.$$

But all the terms in this sum vanish because of (5.5a). Thus, also (5.5b) is identically satisfied. Equation (5.5c) becomes

$$A_1^i\partial_i(A_2^j\Gamma_j)-A_2^i\partial_i(A_1^j\Gamma_j)+A_1^j\partial_j(A_2^i\Gamma_i)-A_2^j\partial_j(A_1^i\Gamma_i)=0.$$

Because of (5.5a) it reduces to

$$(A_1^iA_2^j-A_2^iA_1^j)(\partial_i\Gamma_j-\partial_j\Gamma_i)=0 \quad (i\neq j, \text{ n.s.}),$$

that is (up to a factor $g^{ii}g^{jj}$) to (4.6), which is identically satisfied. Due to the last two equations (5.17), Eq. (5.5d) becomes

$$\frac{\hbar^2}{4}\sum_i [A_1^i\partial_i^2(A_2^j\Gamma_j)-A_1^i\Gamma_i\partial_i(A_2^j\Gamma_j)-A_2^i\partial_i^2(A_1^j\Gamma_j)+A_2^i\Gamma_i\partial_i(A_1^j\Gamma_j)]+A_1^j\partial_j V_{\mathbf{K}_2}-A_2^j\partial_j V_{\mathbf{K}_1}=0,$$

thus,

$$\frac{\hbar^2}{4}\sum_i\,[(A_1^iA_2^j-A_2^iA_1^j)\partial_i^2\Gamma_j]+\frac{\hbar^2}{4}\sum_i\,[A_1^i\Gamma_j\partial_i^2A_2^j-A_2^i\Gamma_j\partial_i^2A_1^j+2A_1^i\partial_iA_2^j\partial_i\Gamma_j-2A_2^i\partial_iA_1^j\partial_i\Gamma_j]$$

$$-\frac{\hbar^2}{4}\sum_i\,\Gamma_i[A_1^i\partial_i(A_2^i\Gamma_j)-A_2^i\partial_i(A_1^j\Gamma_j)]+A_1^j\partial_jV_{\mathbf{K}_2}-A_2^j\partial_jV_{\mathbf{K}_1}=0.$$

Because of the second equation (5.17) and (5.5a), the second sum vanishes identically and this equation reduces to

$$\frac{\hbar^2}{4}\sum_i\,[(A_1^iA_2^j-A_2^iA_1^j)\partial_i^2\Gamma_j]-\frac{\hbar^2}{4}\sum_i\,[\Gamma_i(A_1^iA_2^j-A_2^iA_1^j)\partial_i\Gamma_j]+A_1^j\partial_jV_{\mathbf{K}_2}-A_2^j\partial_jV_{\mathbf{K}_1}=0,$$

which is equivalent to

$$\frac{\hbar^2}{4}\sum_i\,[g^{ii}(\lambda_1^i\lambda_2^j-\lambda_2^i\lambda_1^j)(\partial_i^2\Gamma_j-\Gamma_i\partial_i\Gamma_j)]+\lambda_1^j\partial_jV_{\mathbf{K}_2}-\lambda_2^j\partial_jV_{\mathbf{K}_1}=0. \tag{5.18}$$

Due to (4.15) this equation is equivalent to the second equation in (5.15). So, the first commutation relation (5.15) is equivalent to the second equation (5.15) plus the last equation (5.5). However, **C** is skew-symmetric (Remark 4.5), so that the second equation (5.15) implies equation $\delta(\mathbf{K}_1\nabla V_{\mathbf{K}_2}-\mathbf{K}_2\nabla V_{\mathbf{K}_1})=0$, that is (5.5e). This proves the first equivalence (5.15). The second equivalence follows from the first equation (2.3), which now reads $\{H_{\mathbf{K}_1},H_{\mathbf{K}_2}\}=P(\mathbf{K}_1\nabla V_{\mathbf{K}_2}-\mathbf{K}_2\nabla V_{\mathbf{K}_1})$.

Proposition 5.9: Let $\mathbf{K}_1$ *and* $\mathbf{K}_2$ *be Killing tensors simultaneously diagonalized in orthogonal coordinates. Then*

$$[\hat{H}_{\mathbf{K}_1},\hat{H}]=0,\quad [\hat{H}_{\mathbf{K}_2},\hat{H}]=0\Rightarrow[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=0. \tag{5.19}$$

Proof: Since $\{P_{\mathbf{K}_1},P_{\mathbf{G}}\}=0$, due to Theorem 5.6 the first two conditions (5.19) are equivalent to

$$\frac{\hbar^2}{4}\delta\mathbf{C}+\mathbf{K}_I\nabla V-\nabla V_{\mathbf{K}_I}=0,\quad I=1,2.$$

Because of (4.17), Remark 4.6, these equations are equivalent to

$$\begin{aligned}&\frac{\hbar^2}{4}\sum_i\,g^{ii}(\lambda_1^i-\lambda_1^j)(\partial_i^2\Gamma_j-\Gamma_i\partial_i\Gamma_j)+\lambda_1^j\partial_jV-\partial_jV_{\mathbf{K}_1}=0,\\&\frac{\hbar^2}{4}\sum_i\,g^{ii}(\lambda_2^i-\lambda_2^j)(\partial_i^2\Gamma_j-\Gamma_i\partial_i\Gamma_j)+\lambda_2^j\partial_jV-\partial_jV_{\mathbf{K}_2}=0.\end{aligned} \tag{5.20}$$

As we have done above, if we multiply the first equation by $\lambda_2^j\neq0$, the second one by $\lambda_1^j\neq0$ and subtract the two resulting equations, then we get (5.18), which is equivalent to the first equation (5.15). For $\lambda_2^j=0$, Eq. (5.18) follows from the first equation (5.20) multiplied by $\lambda_1^j\neq0$. For $\lambda_1^j=\lambda_2^j=0$, (5.18) is obviously satisfied. ■

Now we are able to prove Theorem 3.1 by applying the preceding results to the space $\mathcal{H}=(\mathcal{K},V)$ of the first integrals in involution associated with the orthogonal separation of the Hamilton–Jacobi equation (Sec. III). First, we prove the equivalence of the first three conditions (3.3).

Proposition 5.10: Let $\mathcal{H}=(\mathcal{K},V)$ be the space of quadratic first integrals in involution associated with the orthogonal separation of the Hamilton–Jacobi equation. Then the following conditions are equivalent:

$$[\hat{H}_{\mathbf{K}},\hat{H}]=0, \quad \forall \mathbf{K}\in\mathcal{K},$$

$$\delta(\mathbf{KR}-\mathbf{RK})=0, \quad \forall \mathbf{K}\in\mathcal{K}, \tag{5.21}$$

$$\partial_i R_{ij}-\Gamma_i R_{ij}=0, \quad (i\neq j \ \text{ n.s.}).$$

Proof: Let us use Theorem 5.6. Since $\{H_{\mathbf{K}},H\}=0$, the first equation (5.21), coinciding with the first equation (5.10), is equivalent to $\delta\mathbf{C}=0$ for $\mathbf{C}=\mathbf{KD}-\mathbf{DK}$ and $D_{ij}=\partial_i\Gamma_j$. However, since the components D_{ii} are not involved in this definition of $\mathbf{C}$ (Remark 4.4), we can replace $\mathbf{D}$ with $\frac{2}{3}\mathbf{R}$, in agreement with (5.14). This proves the equivalence of the first two conditions (5.21). From the equivalence (4.18) it follows that the coordinate expression of the second equation (5.21) is

$$\sum_i g^{ii}(\lambda^i-\lambda^j)(\partial_i R_{ij}-\Gamma_i R_{ij})=0, \tag{5.22}$$

where only the nondiagonal covariant components of $\mathbf{R}$ are involved. If we introduce the vectors

$$\mathbf{X}_j=(X_j^i)=(g^{ii}(\partial_i R_{ij}-\Gamma_i R_{ij})), \quad \mathbf{Y}_j=(Y_j^i)=(\lambda^i-\lambda^j),$$

then equation (5.22) can be written

$$\mathbf{X}_j\cdot\mathbf{Y}_j=0. \tag{5.23}$$

Let us consider a basis $(\mathbf{K}_a)=(K_a^{ii})=(\lambda_a^i g^{ii})$ of $\mathcal{K}$, $a=1,...,n$, with $\mathbf{K}_n=\mathbf{G}$. We have $\det[\lambda_a^i]\neq 0$ and $\lambda_n^i=1$. Let us chose a value of the index j, say $j=1$. Then the $n-1$ vectors $\mathbf{Y}_{1a}=(\lambda_a^i-\lambda_a^1)$, $a=1,2,...,n-1$, are independent vectors in the $(n-1)$-space Π_1 orthogonal to the vector (1, 0,..., 0). Indeed, the rank of the $n\times(n-1)$ matrix $[\lambda_a^i-\lambda_a^1]$ is maximal. According to the second equation (5.21), Eq. (5.23) must be satisfied by all these vectors:

$$\mathbf{X}_1\cdot\mathbf{Y}_{1a}=0.$$

This means that $\mathbf{X}_1$ is orthogonal to Π_1, i.e., that $X_1^i=0$ for $i\neq 1$. In a similar way we prove that $X_j^i=0$ for $j\neq i$. Thus, the second equation (5.21) implies the third one. The converse is obvious.■

Proposition 5.11: Let $\mathcal{H}=(\mathcal{K},V)$ be the space of quadratic first integrals in involution associated with the orthogonal separation of the Hamilton–Jacobi equation. Then the following conditions are equivalent,

$$[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=0, \quad \forall \mathbf{K}_1,\mathbf{K}_2,\in\mathcal{K},$$

$$\delta(\mathbf{K}_1\mathbf{R}\mathbf{K}_2-\mathbf{K}_2\mathbf{R}\mathbf{K}_1)=0, \quad \forall \mathbf{K}_1,\mathbf{K}_2,\in\mathcal{K}, \tag{5.24}$$

$$\partial_i R_{ij}-\Gamma_i R_{ij}=0, \quad i\neq j.$$

Proof: The first condition is equivalent to $\delta\mathbf{C}=0$, because of the second equivalence (5.15) (Theorem 5.8), with $\mathbf{C}$ defined in (5.16). However, in definition (5.16) $\mathbf{D}$ can be replaced by $\mathbf{R}$, due to (5.14) and Remark 4.4(ii). Thus, the first two conditions (5.24) are equivalent. The second equation (5.24) implies the second equation (5.21), since $\mathbf{G}\in\mathcal{K}$, and the last equation (5.24) because of Proposition 5.10. The last condition (5.24) implies the second condition (5.24) because of (4.16). ■

The last condition (5.24) appears also in (5.21). Thus, all the conditions (5.24) and (5.21) are equivalent. This proves Theorem 3.1.

VI. SYMMETRY OPERATORS ASSOCIATED WITH THE GENERAL SEPARATION OF THE HAMILTON–JACOBI EQUATION

A *separable Killing algebra*[1] is a pair $(D,\mathcal{K})$ where D is an r-dimensional linear space of commuting Killing vectors and $\mathcal{K}$ is a D-invariant $(n-r)$-dimensional linear space of Killing two-tensors with $m=n-r$ normal eigenvectors orthogonal to D. These eigenvectors are called *essential eigenvectors*. The eigenvalues of a $\mathbf{K}\in\mathcal{K}$ corresponding to essential eigenvectors are called *essential eigenvalues*. It can be proved that: (i) D is normal, i.e., the distribution $\Delta^{\perp}$ orthogonal to the vectors of D is completely integrable, (ii) $\mathcal{K}$ contains the metric tensor $\mathbf{G}$ and Killing tensors with distinct essential eigenvalues (called *characteristic Killing tensors*); (iii) all functions $P_{\mathbf{X}}$ and $P_{\mathbf{K}}$, with $\mathbf{X}\in D$ and $\mathbf{K}\in\mathcal{K}$ are in involution; (iv) there exist *standard coordinates* (q^a,q^α) such that $\mathrm{d}q^a$ are eigenforms of $\mathcal{K}$ corresponding to the essential eigenvectors and ∂_α form a local basis of D, so that (q^α) are ignorable; (v) these coordinates are separable for the geodesic flow; (vi) in these coordinates all elements of $\mathcal{K}$ assume the *standard form*

$$\mathbf{K}=K^{aa}\partial_a\otimes\partial_a+K^{\alpha\beta}\partial_\alpha\otimes\partial_\beta=\lambda^a g^{aa}\partial_a\otimes\partial_a+K^{\alpha\beta}\partial_\alpha\otimes\partial_\beta, \tag{6.1}$$

where λ^a are the essential eigenvalues of $\mathbf{K}$ and the coordinates (q^α) are ignorable; (vii) the natural Hamiltonian $H=\frac{1}{2}P_{\mathbf{G}}+V$ is separable if and only if there exists a separable Killing algebra such that $DV=0$ and the *characteristic equation* $\mathrm{d}(\mathbf{K}\mathrm{d}V)=0$ is satisfied for a single characteristic Killing tensor of $\mathcal{K}$. It follows that (viii) the characteristic equation is satisfied for all $\mathbf{K}\in\mathcal{K}$ and that there are local D-invariant functions $V_{\mathbf{K}}$ such that $\mathrm{d}V_{\mathbf{K}}=\mathbf{K}\mathrm{d}V$, i.e.,

$$\nabla V_{\mathbf{K}}=\mathbf{K}\nabla V,\quad DV_{\mathbf{K}}=0;$$

(ix) the functions

$$P_{\mathbf{X}},\quad \mathbf{X}\in D,$$

$$H_{\mathbf{K}}=\tfrac{1}{2}P_{\mathbf{K}}+V_{\mathbf{K}},\quad \mathbf{K}\in\mathcal{K}$$

are first integrals in involution. We denote by

$$\mathcal{H}=(\mathcal{K},V)$$

the m-dimensional linear space of the quadratic first integrals $H_{\mathbf{K}}$.

For the first- and second-order operators corresponding to these first integrals in involution the commutation relations

$$[\hat{P}_{\mathbf{X}_1},\hat{P}_{\mathbf{X}_2}]=0,\quad [\hat{P}_{\mathbf{X}},\hat{H}_{\mathbf{K}}]=0,\quad \forall\mathbf{X}_1,\mathbf{X}_2,\mathbf{X}\in D,\quad \forall\mathbf{K}\in\mathcal{K},$$

hold. This follows from the fact that $\mathbf{X}\in D$ are commuting Killing vectors and the elements of $\mathcal{H}$ are D-invariant. However, in general the operators $\hat{H}_{\mathbf{K}}$ do not commute one other. Indeed, we have a theorem similar to Theorem 3.1,

Theorem 6.1: *Let $\mathcal{H}=(\mathcal{K},V)$ be the space of quadratic first integrals in involution associated with the separation of the Hamilton–Jacobi equation. Then the following conditions are equivalent:*

$$[\hat{H}_{\mathbf{K}},\hat{H}]=0,\quad \forall\mathbf{K}\in\mathcal{K}, \tag{6.2a}$$

$$\delta(\mathbf{KR}-\mathbf{RK})=0,\quad \forall\mathbf{K}\in\mathcal{K}, \tag{6.2b}$$

$$\partial_a R_{ab}-\Gamma_a R_{ab}=0,\quad a\neq b \ \text{ n.s.}, \tag{6.2c}$$

$$[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=0,\quad \forall\mathbf{K}_1,\mathbf{K}_2,\in\mathcal{K}, \tag{6.2d}$$

$$\delta(\mathbf{K}_1\mathbf{R}\mathbf{K}_2-\mathbf{K}_2\mathbf{R}\mathbf{K}_1)=0, \quad \forall \mathbf{K}_1,\mathbf{K}_2, \in \mathcal{K}, \tag{6.2e}$$

where $R_{ab}=\mathbf{R}(\partial_a,\partial_b)$ *are the essential covariant components of the Ricci tensor* $\mathbf{R}$ (*corresponding to essential separable coordinates* (q^a)) *and* $\Gamma_a=g^{ij}\Gamma_{ij,a}$ *are the essential contracted Christoffel symbols*.

The proof of this theorem will be given in Sec. VIII.

Remark 6.2: Formulas (6.2) are formally identical to formulas (3.3) concerning the orthogonal separation, and a remark similar to Remark 3.2 also holds in the present case. The only difference is that now the coordinate expression of the pre-Robertson condition (6.2c) involves only the essential components R_{ab} of the Ricci tensor. In standard separable coordinates the Ricci tensor $\mathbf{R}$ assume the form (cf. Ref. 1, Sec. VI)

$$\mathbf{R}=R^{ab}\partial_a\otimes\partial_b+R^{\alpha\beta}\partial_\alpha\otimes\partial_\beta, \tag{6.3}$$

and moreover,

$$\partial_a\Gamma_b=\tfrac{2}{3}R_{ab}, \quad a\neq b. \tag{6.4}$$

It assumes the standard form, i.e.,

$$R_{ab}=0, \quad a\neq b, \tag{6.5}$$

if and only if the Schrödinger equation is separable in the reduced sense (Robertson condition). The Robertson condition (6.5) obviously implies the pre-Robertson condition (6.3). Hence,

Theorem 6.3: *If the Schrödinger equation associated with a separable Hamiltonian is reductively separable, then all operators* $\hat{P}_{\mathbf{X}}$ *and* $\hat{H}_{\mathbf{K}}$ *corresponding to the linear and quadratic first integrals in involution commute*.

In particular they commute with the Schrödinger operator $\hat{H}=\hat{H}_{\mathbf{G}}$. The Robertson and pre-Robertson conditions are obviously satisfied for $\mathbf{R}=\kappa\mathbf{G}$. Hence,

Theorem 6.4: *On Einstein manifolds all operators* $\hat{P}_{\mathbf{X}}$ *and* $\hat{H}_{\mathbf{K}}$ *corresponding to the first integrals in involution of a separable Hamiltonian system commute*.

Remark 6.5: An algebraic form of the Robertson condition is expressed by the commutability of the Ricci tensor $\mathbf{R}$ with a characteristic tensor (thus, with all the Killing tensors) $\mathbf{K}\in\mathcal{K}$, interpreted as linear operators, when restricted to the distribution $\Delta^\perp$ orthogonal to D,

$$(\mathbf{K}\mathbf{R}-\mathbf{R}\mathbf{K})\big|\Delta^\perp=0, \quad \forall \mathbf{K}\in\mathcal{K}. \tag{6.6}$$

Indeed, this distribution is invariant with respect to these linear operators. If we denote by $\mathbf{R}'$ and $\mathbf{K}'$ the restrictions to $\Delta^\perp$, cf. (7.1), then (6.6) is equivalent to

$$\mathbf{K}'\mathbf{R}-\mathbf{R}\mathbf{K}'=0, \tag{6.7}$$

or to $\mathbf{K}\mathbf{R}'-\mathbf{R}'\mathbf{K}=\mathbf{K}'\mathbf{R}'-\mathbf{R}'\mathbf{K}'=0$. Condition (6.7) obviously implies

$$\delta(\mathbf{K}'\mathbf{R}-\mathbf{R}\mathbf{K}')=0. \tag{6.8}$$

As we shall see in Sec. VIII, the fact that (6.8) is equivalent to (6.2b) is remarkable.

Remark 6.6: In standard separable coordinates the components of the elements of $\mathcal{K}$ and the potential functions assume the form

$$g^{aa}=\varphi^a_{(m)}, \quad g^{\alpha\beta}=\phi_a^{\alpha\beta}(q^a)\varphi^a_{(m)}, \quad V=\phi_a(q^a)\varphi^a_{(m)},$$

$$K_b^{aa}=\varphi^a_{(b)}, \quad K_b^{\alpha\beta}=\phi_a^{\alpha\beta}(q^a)\varphi^a_{(b)}, \quad V_{K_b}=\phi_a(q^a)\varphi^a_{(b)},$$

where $(\mathbf{K}_b)$ is a local basis of $\mathcal{K}$, with $\mathbf{K}_m=\mathbf{G}$. Then, a local basis of $\mathcal{H}$ is

$$H_b = \tfrac{1}{2}\varphi^a_{(b)}(p_a^2 + \phi_a^{\alpha\beta} p_\alpha p_\beta + 2\phi_a).$$

The corresponding operators assume the form (see Remark 8.2 and Ref. 1, Sec. V).

$$\hat{H}_b\tilde{\psi} = -\frac{\hbar^2}{2}\varphi^a_{(b)}\left(\partial_a^2\tilde{\psi} - \Gamma_a\partial_a\tilde{\psi} + \left(\phi_a^{\alpha\beta}\kappa_\alpha\kappa_\beta - \frac{2}{\hbar^2}\phi_a\right)\tilde{\psi}\right),$$

where $\psi = \tilde{\psi}\cdot\Pi_\alpha e^{\kappa_\alpha q^\alpha}$, $\tilde{\psi} = \Pi_a\psi_a(q^a)$. The Robertson condition in standard separable coordinates is equivalent to $\partial_b\Gamma_a = 0$ for $a \neq b$. This means that $\Gamma_a = \Gamma_a(q^a)$.

VII. KILLING TENSORS IN STANDARD FORM

In the next section we shall analyze the commutation relations of the second-order operators assuming that all the tensors **K** involved, including the metric tensor **G**, are simultaneously in standard form (6.1) with respect to a given standard coordinate system $(q^i) = (q^a, q^\alpha)$. We shall use the decomposition

$$\mathbf{K} = \mathbf{K}' + \mathbf{K}'',$$

$$\mathbf{K}' = K^{aa}\partial_a\otimes\partial_a = \lambda^a g^{aa}\partial_a\otimes\partial_a, \tag{7.1}$$

$$\mathbf{K}'' = K^{\alpha\beta}\partial_\alpha\otimes\partial_\beta.$$

In analogy with Sec. IV, in this section we state some general properties concerning Killing tensors. For a Killing tensor in standard form the following equations hold:

$$\begin{aligned}
&\partial_a\lambda^b = (\lambda^a - \lambda^b)\partial_a \ln g^{bb}\\
&\partial_a K^{\alpha\beta} = \lambda^a\partial_a g^{\alpha\beta}\\
&\partial_a\lambda^a = 0\\
&\partial_a(\lambda^b g^{bb}) = \lambda^a\partial_a g^{bb} \qquad (a,b \text{ n.s.}).\\
&\partial_a^2(\lambda^b g^{bb}) = \lambda^a\partial_a^2 g^{bb}\\
&\partial_a^2 K^{\alpha\beta} = \lambda^a\partial_a^2 g^{\alpha\beta}
\end{aligned} \tag{7.2}$$

We call the two first equations (7.2) the *extended Eisenhart–Killing equations*. They characterize the Killing tensors in standard form and imply the remaining equations.

Proposition 7.1: If (q^a, q^α) *are standard coordinates in which a Killing tensor* **K** *assumes the standard form (6.1), then*

$$(\lambda^a - \lambda^b)(\partial_a\Gamma_b - \partial_b\Gamma_a) = 0 \quad (a,b \text{ n.s.}). \tag{7.3}$$

Proof: The proof follows the same pattern of the proof of Proposition 4.1. The only difference is that (4.3) is replaced by (cf. Ref. 1, Sec. VI)

$$\Gamma_a = \tfrac{1}{2}\partial_a\sum_c \ln g^{cc} - \partial_a \ln g^{aa} + \tfrac{1}{2}\partial_a \ln\det[g^{\alpha\beta}],$$

but the last term does not give any contribution to the difference $\partial_a\Gamma_b - \partial_b\Gamma_a$. ■

In a similar way we can prove

Proposition 7.2: Let $\mathbf{K}_I$, $I = 1,2$, *be two Killing tensors in standard form (6.1). Then*

$$(\lambda_1^a\lambda_2^b-\lambda_2^a\lambda_1^b)(\partial_a\Gamma_b-\partial_b\Gamma_a)=0 \quad (a\neq b \ \text{ n.s.}). \tag{7.4}$$

Proposition 7.3: Let $\mathbf{K}_I$, $I=1,2$, *be two Killing tensors in standard form (6.1). If*

$$\mathbf{C}=\mathbf{K}_1'\mathbf{D}\mathbf{K}_2'-\mathbf{K}_2'\mathbf{D}\mathbf{K}_1', \quad C^{ij}=(K_1')^{ih}D_{hk}(K_2')^{kj}-(K_2')^{ih}D_{hk}(K_1')^{kj}, \tag{7.5}$$

where $\mathbf{D}=(D_{ij})$ *is a geometrical object, then*

$$\begin{aligned} &C^{ab}=g^{aa}g^{bb}(\lambda_1^a\lambda_2^b-\lambda_2^a\lambda_1^b)D_{ab}, \quad C^{a\alpha}=C^{\alpha a}=C^{\alpha\beta}=0,\\ &C_b^a=C^a_{\cdot b}=g^{aa}(\lambda_1^a\lambda_2^b-\lambda_2^a\lambda_1^b)D_{ab}, \quad C_\alpha^a=C_a^\alpha=C_\alpha^\beta=0, \end{aligned} \tag{7.6}$$

and

$$\nabla_iC^i_\alpha=0, \quad \nabla_iC^i_b=\sum_a g^{aa}(\lambda_1^a\lambda_2^b-\lambda_2^a\lambda_1^b)(\partial_aD_{ab}-\Gamma_aD_{ab}+\tfrac{1}{2}\partial_a\ln g^{bb}(D_{ba}-D_{ab})). \tag{7.7}$$

Proof: Equations (7.6) are a direct consequence of definitions (7.5) and (7.1). In standard coordinates (cf. Ref. 1, Sec. VI)

$$\Gamma^i_{i\alpha}=0, \quad \Gamma^i_{ia}=-\tfrac{1}{2}\partial_a(\ln\det[g^{ij}])=-\partial_a\ln g^{aa}-\Gamma_a, \tag{7.8}$$

and formula (4.11) reduces to

$$\nabla_iC^i_j=\partial_aC^a_j+\Gamma^i_{ia}C^a_j-\Gamma^h_{ij}C^i_h.$$

It follows that $\nabla_iC^i_\alpha=0$ and

$$\nabla_iC^i_b=\partial_aC^a_b-(\Gamma_a+\partial_a\ln g^{aa})C^a_b-\Gamma^c_{ab}C^a_c.$$

The development of this last expression follows the same pattern of the proof of Proposition 4.3.■

Remark 7.4: From (7.6) it follows that: (i) $C^{ii}=0$, (ii) only the nondiagonal components D_{ab}, $a\neq b$, are involved in the definition (7.5) of $\mathbf{C}$, (iii) if the essential components of D are symmetric, $D_{ab}=D_{ba}$, then $\mathbf{C}$ is skew-symmetric.

Remark 7.5: Let us apply Proposition 7.3 to the cases $D_{ij}=\partial_i\Gamma_j$. In standard coordinates $\Gamma_\alpha=0$ and $\partial_\alpha\Gamma_a=0$. Thus, $D_{\alpha\beta}=D_{a\alpha}=D_{\alpha a}=0$ and $\mathbf{C}$ defined in (7.5) is equal to

$$\mathbf{C}=\mathbf{K}_1\mathbf{D}\mathbf{K}_2-\mathbf{K}_2\mathbf{D}\mathbf{K}_1, \quad \mathbf{D}=(\partial_i\Gamma_j).$$

Equations (7.6) hold with D_{ab} replaced by $\partial_a\Gamma_b$,

$$C^{ab}=g^{aa}g^{bb}(\lambda_1^a\lambda_2^b-\lambda_2^a\lambda_1^b)\partial_a\Gamma_b, \quad C^a_b=g^{aa}(\lambda_1^a\lambda_2^b-\lambda_2^a\lambda_1^b)\partial_a\Gamma_b, \tag{7.9}$$

and, due to (7.4), equations (7.7) become

$$\nabla_iC^i_\alpha=0, \quad \nabla_iC^i_b=\sum_a g^{aa}(\lambda_1^a\lambda_2^b-\lambda_2^a\lambda_1^b)(\partial_a^2\Gamma_b-\Gamma_a\partial_a\Gamma_b). \tag{7.10}$$

From (7.4) and (7.9) it follows that $C^{ij}+C^{ji}=0$. Hence, $\mathbf{C}$ is skew-symmetric and (7.10) give the components of $\delta\mathbf{C}$. Thus,

$$\delta\mathbf{C}=0\Leftrightarrow\sum_a g^{aa}(\lambda_1^a\lambda_2^b-\lambda_2^a\lambda_1^b)(\partial_a^2\Gamma_b-\Gamma_a\partial_a\Gamma_b)=0.$$

Remark 7.6: For $\mathbf{K}_2=\mathbf{G}$ and $\mathbf{K}_1=\mathbf{K}$, definition (7.5) and equations (7.6) become

$$\mathbf{C}=\mathbf{K}'\mathbf{D}-\mathbf{D}\mathbf{K}', \quad C^{ab}=g^{aa}g^{bb}(\lambda^a-\lambda^b)D_{ab}, \quad C^a_b=g^{aa}(\lambda^a-\lambda^b)D_{ab}, \tag{7.11}$$

the remaining components being identically zero. Equations (7.7) become

$$\nabla_i C^i_\alpha=0, \quad \nabla_i C^i_b=\sum_a g^{aa}(\lambda^a-\lambda^b)(\partial_a D_{ab}-\Gamma_a D_{ab}+\tfrac{1}{2}\partial_a \ln g^{bb}(D_{ba}-D_{ab})).$$

For $D_{ij}=\partial_i\Gamma_j$ the definition (7.11) is equivalent to

$$\mathbf{C}=\mathbf{K}\mathbf{D}-\mathbf{D}\mathbf{K}$$

and

$$\nabla_i C^i_\alpha=0, \quad \nabla_i C^i_b=\sum_a g^{aa}(\lambda^a-\lambda^b)(\partial_a^2\Gamma_b-\Gamma_a\partial_a\Gamma_b). \tag{7.12}$$

$\mathbf{C}$ is skew-symmetric and (7.12) give the components of $\delta\mathbf{C}$. Thus,

$$\delta\mathbf{C}=0 \Leftrightarrow \sum_a g^{aa}(\lambda^a-\lambda^b)(\partial_a^2\Gamma_b-\Gamma_a\partial_a\Gamma_b)=0. \tag{7.13}$$

Remarks and propositions similar to Remarks 4.6, 4.7, 4.13, 4.14 and Propositions 4.8–12 hold in the present case, with obvious modifications.

VIII. COMMUTATION RELATIONS IN STANDARD COORDINATES

Proposition 8.1: If $\mathbf{K}$ *is a symmetric tensor in standard form (6.1), then the corresponding pseudo-Laplacian assumes the form*

$$\Delta_{\mathbf{K}}\psi=A^a\partial_a^2\psi+B^a\partial_a\psi+K^{\alpha\beta}\partial_\alpha\partial_\beta\psi,$$

$$A^a=K^{aa}=\lambda^a g^{aa}, \tag{8.1}$$

$$B^a=g^{aa}(\partial_a\lambda^a-\lambda^a\Gamma_a).$$

Proof:

$$\Delta_{\mathbf{K}}\psi=\partial_i(K^{ij}\partial_j\psi)+\Gamma^i_{ih}K^{hj}\partial_j\psi=\partial_iK^{ij}\partial_j\psi+K^{ij}\partial_i\partial_j\psi+\Gamma^i_{ia}K^{aj}\partial_j\psi$$
$$=\partial_aK^{aa}\partial_a\psi+K^{aa}\partial_a^2\psi+K^{\alpha\beta}\partial_\alpha\partial_\beta\psi+\Gamma^i_{ia}K^{aa}\partial_a\psi.$$

Then (8.1) follow from (7.8) and $K^{aa}=\lambda^a g^{aa}$. ■

Remark 8.2: For a pseudo-Laplacian we use the decomposition

$$\Delta_{\mathbf{K}}=\Delta'_{\mathbf{K}}+\Delta''_{\mathbf{K}},$$

$$\Delta'_{\mathbf{K}}\psi=A^a\partial_a^2\psi+B^a\partial_a\psi=g^{aa}(\lambda^a\partial_a^2\psi+(\partial_a\lambda^a-\lambda^a\Gamma_a)\partial_a\psi),$$

$$\Delta''_{\mathbf{K}}\psi=K^{\alpha\beta}\partial_\alpha\partial_\beta\psi.$$

Note that, in accordance with the decomposition (7.1), we have

$$\Delta'_{\mathbf{K}}=\Delta_{\mathbf{K}'}.$$

For a Killing tensor,

$$\Delta'_{\mathbf{K}}=\lambda^a g^{aa}(\partial_a^2\psi-\Gamma_a\partial_a\psi).$$

For a second-order operator (2.12) we use the decomposition

$$\hat{H}_{\mathbf{K}}=\hat{H}'_{\mathbf{K}}+\hat{H}''_{\mathbf{K}},\quad \hat{H}'_{\mathbf{K}}=-\frac{\hbar^2}{2}\Delta'_{\mathbf{K}}+V_{\mathbf{K}},\quad \hat{H}''_{\mathbf{K}}=-\frac{\hbar^2}{2}\Delta''_{\mathbf{K}},$$

so that

$$\begin{aligned}\hat{H}_{\mathbf{K}}\psi&=-\frac{\hbar^2}{2}(\Delta'_{\mathbf{K}}+\Delta''_{\mathbf{K}})\psi+V_{\mathbf{K}}\psi\\&=-\frac{\hbar^2}{2}(A^a\partial_a^2\psi+B^a\partial_a\psi+K^{\alpha\beta}\partial_\alpha\partial_\beta\psi)+V_{\mathbf{K}}\psi\\&=-\frac{\hbar^2}{2}[g^{aa}(\lambda^a\partial_a^2\psi+(\partial_a\lambda^a-\lambda^a\Gamma_a)\partial_a\psi)+K^{\alpha\beta}\partial_\alpha\partial_\beta\psi]+V_{\mathbf{K}}\psi.\end{aligned}\tag{8.2}$$

For a Killing tensor,

$$\hat{H}_{\mathbf{K}}\psi=-\frac{\hbar^2}{2}[\lambda^a g^{aa}(\partial_a^2\psi-\Gamma_a\partial_a\psi)+K^{\alpha\beta}\partial_\alpha\partial_\beta\psi]+V_{\mathbf{K}}\psi.$$

In all the above-given expressions the coordinates (q^α) are ignorable.

Proposition 8.3: The commutator of two second-order operators of the kind (8.2) has the following expression:

$$\begin{aligned}[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]\psi&=[\hat{H}'_{\mathbf{K}_1},\hat{H}'_{\mathbf{K}_2}]\psi+\frac{\hbar^4}{2}(A_1^a\partial_a^2K_2^{\alpha\beta}-A_2^a\partial_a^2K_1^{\alpha\beta}+B_1^a\partial_aK_2^{\alpha\beta}-B_2^a\partial_aK_1^{\alpha\beta})\partial_{\alpha\beta}\psi\\&\quad+\hbar^4(A_1^a\partial_aK_2^{\alpha\beta}-A_2^a\partial_aK_1^{\alpha\beta})\partial_a\partial_\alpha\partial_\beta\psi,\end{aligned}\tag{8.3}$$

where

$$[\hat{H}'_{\mathbf{K}_1},\hat{H}'_{\mathbf{K}_2}]\psi=\frac{\hbar^4}{4}[\Delta'_{\mathbf{K}_1},\Delta'_{\mathbf{K}_2}]\psi-\hbar^2(A_1^a\partial_aV_{\mathbf{K}_2}-A_2^a\partial_aV_{\mathbf{K}_1})\partial_a\psi-\frac{\hbar^2}{2}(\Delta'_{\mathbf{K}_1}V_{\mathbf{K}_2}-\Delta'_{\mathbf{K}_2}V_{\mathbf{K}_1})\psi.\tag{8.4}$$

Proof: Since

$$\begin{aligned}\Delta'_{\mathbf{K}_1}\Delta'_{\mathbf{K}_2}\psi&=A_1^b\partial_b^2(A_2^a\partial_a^2\psi+B_2^a\partial_a\psi)+B_1^b\partial_b(A_2^a\partial_a^2\psi+B_2^a\partial_a\psi)\\&=A_1^bA_2^a\partial_b^2\partial_a^2\psi+A_1^b\partial_b^2A_2^a\partial_a^2\psi+2A_1^b\partial_bA_2^a\partial_b\partial_a^2\psi+A_1^b\partial_b^2B_2^a\partial_a\psi+A_1^bB_2^a\partial_b^2\partial_a\psi\\&\quad+2A_1^b\partial_bB_2^a\partial_a\partial_b\psi+B_1^bA_2^a\partial_b\partial_a^2\psi+B_1^b\partial_bA_2^a\partial_a^2\psi+B_1^bB_2^a\partial_b\partial_a\psi+B_1^b\partial_bB_2^a\partial_a\psi,\end{aligned}$$

we have

$$\begin{aligned}[\Delta'_{\mathbf{K}_1},\Delta'_{\mathbf{K}_2}]&=2(A_1^a\partial_aA_2^b-A_2^a\partial_aA_1^b)\partial_a\partial_b^2\psi+(A_1^a\partial_a^2A_2^b-A_2^a\partial_a^2A_1^b+B_1^a\partial_aA_2^b-B_2^a\partial_aA_1^b)\partial_b^2\psi\\&\quad+2(A_1^a\partial_aB_2^b-A_2^a\partial_aB_1^b)\partial_a\partial_b\psi+(A_1^a\partial_a^2B_2^b+B_1^a\partial_aB_2^b-A_2^a\partial_a^2B_1^b-B_2^a\partial_aB_1^b)\partial_b\psi.\end{aligned}$$

Since

$$\Delta''_{\mathbf{K}_1},\Delta''_{\mathbf{K}_2}\psi=K_1^{\alpha\beta}K_2^{\mu\nu}\partial_{\alpha\beta\mu\nu}\psi,$$

we have

$$[\Delta''_{\mathbf{K}_1},\Delta''_{\mathbf{K}_2}]=0, \quad [\hat{H}''_{\mathbf{K}_1},\hat{H}''_{\mathbf{K}_2}]=0.$$

Thus,

$$[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=[\hat{H}'_{\mathbf{K}_1},\hat{H}'_{\mathbf{K}_2}]+[\hat{H}'_{\mathbf{K}_1},\hat{H}''_{\mathbf{K}_2}]+[\hat{H}''_{\mathbf{K}_1},\hat{H}'_{\mathbf{K}_2}].$$

A straightforward calculation shows that

$$[\hat{H}'_{\mathbf{K}_1},\hat{H}'_{\mathbf{K}_2}]\psi=\frac{\hbar^4}{2}(A_1^a\partial_a^2K_2^{\alpha\beta}+B_1^a\partial_aK_2^{\alpha\beta})\partial_\alpha\partial_\beta\psi+\hbar^4A_1^a\partial_aK_2^{\alpha\beta}\partial_a\partial_\alpha\partial_\beta\psi.$$

These two last equations prove (8.3) and (8.4). ■

Proposition 8.4: Let $\mathbf{K}_1$ *and* $\mathbf{K}_2$ *be symmetric tensors in standard form. Then* $[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=0$ *if and only if*

$$A_1^a\partial_aA_2^b-A_2^a\partial_aA_1^b=0 \quad (a, \text{ n.s.}), \tag{8.5a}$$

$$\sum_a (A_1^a\partial_a^2A_2^b-A_2^a\partial_a^2A_1^b+B_1^a\partial_aA_2^b-B_2^a\partial_aA_1^b)+2(A_1^b\partial_bB_2^b-A_2^b\partial_bB_1^b)=0, \tag{8.5b}$$

$$A_1^a\partial_aB_2^b-A_2^a\partial_aB_1^b+A_1^b\partial_bB_2^a-A_2^b\partial_bB_1^a=0 \quad (a\neq b \text{ n.s.}), \tag{8.5c}$$

$$\frac{\hbar^2}{4}\sum_a (A_1^a\partial_a^2B_2^b+B_1^a\partial_aB_2^b-A_2^a\partial_a^2B_1^b-B_2^a\partial_aB_1^b)-A_1^b\partial_bV_{\mathbf{K}_2}+A_2^b\partial_bV_{\mathbf{K}_1}=0 \quad (b \text{ n.s.}), \tag{8.5d}$$

$$\Delta'_{\mathbf{K}_1}V_{\mathbf{K}_2}-\Delta'_{\mathbf{K}_2}V_{\mathbf{K}_1}=0, \tag{8.5e}$$

and

$$A_1^a\partial_a^2K_2^{\alpha\beta}-A_2^a\partial_a^2K_1^{\alpha\beta}+B_1^a\partial_aK_2^{\alpha\beta}-B_2^a\partial_aK_1^{\alpha\beta}=0, \tag{8.6a}$$

$$A_1^a\partial_aK_2^{\alpha\beta}-A_2^a\partial_aK_1^{\alpha\beta}=0. \tag{8.6b}$$

Proof: Equations (8.6) follow from the second and third term in (8.3) i.e., from the vanishing of the coefficients of $\partial_\alpha\partial_\beta\psi$ and of $\partial_a\partial_\alpha\partial_\beta\psi$. The first term (8.3) involves only the partial derivatives ∂_a and a factor of ψ, and it is similar (with an obvious change of indices) to (5.3). Thus, (8.5) are similar to (5.5).

Remark 8.5: Since,

$$\{P_{\mathbf{K}_1},P_{\mathbf{K}_2}\}=2(A_1^a\partial_1^aA_2^b-A_2^a\partial_aA_1^b)p_ap_b^2+2(A_1^a\partial_aK_2^{\alpha\beta}-A_2^a\partial_aK_1^{\alpha\beta})p_ap_\alpha p_\beta, \tag{8.7}$$

Eqs. (8.5a) and (8.6a) are equivalent to $\{P_{\mathbf{K}_1},P_{\mathbf{K}_2}\}=0$. Thus,

$$[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=0 \Rightarrow \{P_{\mathbf{K}_1},P_{\mathbf{K}_2}\}=0. \tag{8.8}$$

Theorem 8.6: *Let* $\mathbf{K}$ *be a symmetric tensor in standard form. Then the following conditions are equivalent:*

$$\{P_{\mathbf{K}},P_{\mathbf{G}}\}=0 \quad (\mathbf{K} \text{ Killing tensor}),$$
$$[\hat{H}_{\mathbf{K}},\hat{H}]=0 \Leftrightarrow \frac{\hbar^2}{4}\delta\mathbf{C}+\mathbf{K}\nabla V-\nabla V_{\mathbf{K}}=0 \Leftrightarrow \{H_{\mathbf{K}},H\}=-\frac{\hbar^2}{4}P_{\delta\mathbf{C}}, \tag{8.9}$$

where

$$\mathbf{C}=\mathbf{K}\mathbf{D}-\mathbf{D}\mathbf{K}=\mathbf{K}'\mathbf{D}-\mathbf{D}\mathbf{K}', \quad \mathbf{D}=(\partial_i\Gamma_j). \tag{8.10}$$

Proof: The equivalence of the two definitions (8.10) of **C** follows from Remarks 7.5 and 7.6. We use (8.5), Proposition 8.4, for $\mathbf{K}_1=\mathbf{K}$ and $\mathbf{K}_2=\mathbf{G}$. Assume $[\hat{H}_{\mathbf{K}},\hat{H}]=0$. From (8.8) it follows that **K** is a Killing tensor. For a Killing tensor in standard form we have formulas similar to (5.11) and (5.12), with indices (a,b). Equations (8.5a, b) and (8.6b) are then identically satisfied. The remaining equations are similar to (5.13),

$$(\lambda^a-\lambda^b)(\partial_a\Gamma_b-\partial_b\Gamma_a)=0,$$

$$\frac{\hbar^2}{4}\sum_a g^{aa}(\lambda^a-\lambda^b)(\partial_a^2\Gamma_b-\Gamma_a\partial_a\Gamma_b)+\lambda^b\partial_b V-\partial_b V_{\mathbf{K}}=0 \quad (b \text{ n.s.}), \tag{8.11}$$

$$\delta(\mathbf{K}\nabla V-\nabla V_{\mathbf{K}})=0.$$

Due to (7.3), the first equation is identically satisfied. According to Remark 7.6 and Eq. (7.12), the second equation (8.11) is equivalent to

$$\frac{\hbar^2}{4}\delta\mathbf{C}+\mathbf{K}\nabla V-\nabla V_{\mathbf{K}}=0,$$

where **C** is skew-symmetric. Since $\delta^2\mathbf{C}=0$, the last equation (8.11) is a consequence of the second equation (8.11). The above-noted reasoning is reversible, and the first equivalence (8.9) is proved. The second equivalence follows from the last equation (2.3). ■

Theorem 8.7: *Let* $\mathbf{K}_1$ *and* $\mathbf{K}_2$ *be Killing tensors in standard form. Then* $\{P_{\mathbf{K}_1},P_{\mathbf{K}_2}\}=0$, *and the following conditions are equivalent:*

$$[\hat{H}_{\mathbf{K}_1},\hat{H}_{\mathbf{K}_2}]=0 \Leftrightarrow \frac{\hbar^2}{4}\delta\mathbf{C}+\mathbf{K}_1\nabla V_{\mathbf{K}_2}-\mathbf{K}_2\nabla V_{\mathbf{K}_1}=0 \Leftrightarrow \{H_{\mathbf{K}_1},H_{\mathbf{K}_2}\}=-\frac{\hbar^2}{4}P_{\delta\mathbf{C}}, \tag{8.12}$$

where

$$\mathbf{C}=\mathbf{K}_1\mathbf{D}\mathbf{K}_2-\mathbf{K}_2\mathbf{D}\mathbf{K}_1=\mathbf{K}_1'\mathbf{D}\mathbf{K}_2'-\mathbf{K}_2'\mathbf{D}\mathbf{K}_1', \quad \mathbf{D}=(\partial_i\Gamma_j). \tag{8.13}$$

Proof: The equivalence of the two definitions of **C** in (8.13) follows from Remark 7.5. The components of **C** are given in (7.9). The involutivity condition $\{P_{\mathbf{K}_1},P_{\mathbf{K}_2}\}=0$ follow from (8.7), (8.5a), (8.6b), and (7.2). We use Eqs. (8.5) and (8.6). For Killing tensors $\mathbf{K}_I$ $(I=1,2)$ in standard form we have, cf. (8.1) and (7.2),

$$A_1^a=\lambda_I^a g^{aa}, \quad B_I^a=-g^{aa}\lambda_I^a\Gamma_a,$$

$$\partial_a K_I^{\alpha\beta}=\lambda_I^a\partial_a g^{\alpha\beta}, \quad \partial_a^2 K^{\alpha\beta}=\lambda_I^a\partial_a^2 g^{\alpha\beta}.$$

Thus, (8.6) are identically satisfied. Moreover, formulas similar to (5.17) hold with indices (a,b),

$$A_I^a=\lambda_I^a g^{aa},\quad B_I^a=-A_I^a\Gamma_a,$$

$$\partial_a A_I^b=A_I^a\partial_a g^{bb}=\lambda_I^a\partial_a g^{bb},$$

$$\partial_a^2 A_I^b=A_I^a\partial_a^2 g^{bb}=\lambda_I^a\partial_a^2 g^{bb},$$

$$\partial_a B_I^b=-\partial_a(A_I^b\Gamma_b)=-\partial_a A_I^b\Gamma_b-A_I^b\partial_a\Gamma_b,$$

$$\partial_a^2 B_I^b=-\partial_a^2 A_I^b\Gamma_b-2\partial_a A_I^b\partial_a\Gamma_b-A_I^b\partial_a^2\Gamma_b.$$

Since the coordinates q^α are ignorable and no greek index is involved in (8.5) the proof of the first equivalence (8.12) is similar to that of the first equivalence (5.15) in Theorem 5.8. The second equivalence (8.12) follows from the first equation (2.3) (cf. the end of the proof of Theorem 5.8). ■

Proposition 8.8: Let $\mathbf{K}_1$ *and* $\mathbf{K}_2$ *be Killing tensors in standard form. Then*

$$[\hat H_{\mathbf{K}_1},\hat H]=0,\quad [\hat H_{\mathbf{K}_2},\hat H]=0\Rightarrow[\hat H_{\mathbf{K}_1},\hat H_{\mathbf{K}_2}]=0.$$

Proof: This implication is similar to (5.19) of Proposition 5.9. The proof follows the same pattern. ■

Propositions similar to Propositions 5.10 and 5.11 hold.

Proposition 8.9: Let $\mathcal{H}=(\mathcal{K},V)$ *be the space of quadratic first integrals in involution associated with the separation of the Hamilton–Jacobi equation. Then the following conditions are equivalent:*

$$[\hat H_{\mathbf{K}},\hat H]=0,\quad \forall\mathbf{K}\in\mathcal{K},$$

$$\delta(\mathbf{K}'\mathbf{R}-\mathbf{R}\mathbf{K}')=0,\quad \forall\mathbf{K}\in\mathcal{K},\tag{8.14}$$

$$\partial_a R_{ab}-\Gamma_a R_{ab}=0,\quad (a\neq b\ \text{ n.s.}).$$

Proof: We apply the equivalence of the first and last conditions (8.9) in Theorem 8.6. Since $H_{\mathbf{K}}$ are first integrals, the commutation relation $[\hat H_{\mathbf{K}},\hat H]=0$ is equivalent to $\delta\mathbf{C}=0$ with $\mathbf{C}=\mathbf{K}\mathbf{D}-\mathbf{D}\mathbf{K}=\mathbf{K}'\mathbf{D}-\mathbf{D}\mathbf{K}'$ and $\mathbf{D}=(\partial_i\Gamma_j)$. If we consider $\mathbf{C}=\mathbf{K}'\mathbf{D}-\mathbf{D}\mathbf{K}'$ then only the components $D_{ab}=\partial_a\Gamma_b$ with $a\neq b$ are involved and, since the coordinates are separable, we can replace $\mathbf{D}$ by $\frac{2}{3}\mathbf{R}$, because of (8.13) and (6.4). This proves the equivalence of the first two conditions (8.14). On the other hand, due to Remark 7.5 and (6.4), in the equivalence (7.13) we can replace $\partial_a\Gamma_b$ by R_{ab}, since only the indices $a\neq b$ are involved. This proves the equivalence between $\delta\mathbf{C}=0$ and the last condition (8.14). ■

Proposition 8.10: Let $\mathcal{H}=(\mathcal{K},V)$ *be the space of quadratic first integrals in involution associated with the separation of the Hamilton–Jacobi equation. Then the following conditions are equivalent:*

$$[\hat H_{\mathbf{K}_1},\hat H_{\mathbf{K}_2}]=0,\quad \forall\mathbf{K}_1,\mathbf{K}_2,\in\mathcal{K},$$

$$\delta(\mathbf{K}_1'\mathbf{R}\mathbf{K}_2'-\mathbf{K}_2'\mathbf{R}\mathbf{K}_1')=0,\quad \forall\mathbf{K}_1,\mathbf{K}_2,\in\mathcal{K},\tag{8.15}$$

$$\partial_a R_{ab}-\Gamma_a R_{ab}=0,\quad a\neq b.$$

The proof is similar to that of Proposition 5.11. The last condition (8.15) also appears in (8.14). Thus all these conditions are equivalent. For proving Theorem 6.1 it remains to prove that

$$\delta(\mathbf{K}'\mathbf{R}-\mathbf{R}\mathbf{K}')=\delta(\mathbf{K}\mathbf{R}-\mathbf{R}\mathbf{K})\tag{8.16}$$

and

$$\delta(\mathbf{K}_1'\mathbf{R}\mathbf{K}_2'-\mathbf{K}_2'\mathbf{R}\mathbf{K}_1')=\delta(\mathbf{K}_1\mathbf{R}\mathbf{K}_2-\mathbf{K}_2\mathbf{R}\mathbf{K}_1). \tag{8.17}$$

These equalities can be proved by the following general considerations on the tensors in *prestandard form*. We say that a contravariant two-tensor $\mathbf{T}=(T^{ij})$ has a prestandard form with respect to a standard coordinate system $(q^i)=(q^a,q^\alpha)$ if $T^{a\alpha}=T^{\alpha a}=0$ and all the remaining components do not depend on the ignorable coordinates (q^α).

Proposition 8.11: For a tensor in prestandard form $\nabla_i T^{i\alpha}=0$.

Proof: Since (q^α) are ignorable, $\partial_i T^{i\alpha}=\partial_a T^{a\alpha}=0$ and we have

$$\nabla_i T^{i\alpha}=\partial_i T^{i\alpha}+\Gamma^i_{il}T^{l\alpha}+\Gamma^\alpha_{il}T^{il}=\Gamma^i_{i\beta}T^{\beta\alpha}+\Gamma^\alpha_{il}T^{il}.$$

However, in standard coordinates $\Gamma^i_{i\beta}=0$ and Γ^α_{il} are all vanishing except for $(i,l)=(a,\beta)$ or (β,a). ■

Proposition 8.12: If $\mathbf{T}_1$ *and* $\mathbf{T}_2$ *are in prestandard form, then also the commutator* $\mathbf{C}=\mathbf{T}_1\mathbf{T}_2-\mathbf{T}_2\mathbf{T}_1$ *is in prestandard form.*

Proof: By definition of commutator,

$$C^{ij}=T_1^{il}g_{lm}T_2^{mj}-T_2^{il}g_{lm}T_1^{mj}=T_1^{ic}g_{cd}T_2^{dj}+T_1^{i\mu}g_{\mu\nu}T_2^{\nu j}-T_2^{ic}g_{cd}T_1^{dj}-T_2^{i\mu}g_{\mu\nu}T_1^{\nu j},$$

so that

$$C^{ab}=T_1^{ac}g_{cd}T_2^{db}-T_2^{ac}g_{cd}T_1^{db}=T_1^{ac}g_{cc}T_2^{cb}-T_2^{ac}g_{cc}T_1^{cb},$$

$$C^{a\alpha}=C^{\alpha a}=0, \tag{8.18}$$

$$C^{\alpha\beta}=T_1^{\alpha\mu}g_{\mu\nu}T_2^{\nu\beta}-T_2^{\alpha\mu}g_{\mu\nu}T_1^{\nu\beta}.$$

■

For a tensor in a prestandard form let us use the decomposition

$$\mathbf{T}=\mathbf{T}'+\mathbf{T}''=T^{ab}\partial_a\otimes\partial_b+T^{\alpha\beta}\partial_\alpha\otimes\partial_\beta.$$

By setting $T_1^{\alpha\beta}=0$ or $T_2^{\alpha\beta}=0$ in (8.18) we get

$$\mathbf{T}_1'\mathbf{T}_2-\mathbf{T}_2\mathbf{T}_1'=\mathbf{T}_1\mathbf{T}_2'-\mathbf{T}_2'\mathbf{T}_1=\mathbf{T}_1'\mathbf{T}_2'-\mathbf{T}_2'\mathbf{T}_1'=\mathbf{C}'.$$

Proposition 8.13: If $\mathbf{C}$ *is a skew-symmetric tensor in prestandard form then* $\delta\mathbf{C}=\delta\mathbf{C}'$.

Proof: Since also $\mathbf{C}'$ is in prestandard form, due to Proposition 8.11 we have $\nabla_i C^{i\alpha}=\nabla_i C'^{i\alpha}=0$. Moreover, $\nabla_i C^{ia}=\partial_i C^{ia}+\Gamma^i_{il}C^{la}+\Gamma^a_{il}C^{il}=\partial_b C^{ba}+\Gamma^i_{ib}C^{ba}$, since $\Gamma^i_{i\alpha}=0$, $\Gamma^a_{il}=\Gamma^a_{li}$ and $C^{il}=-C^{li}$. In this last expression the components $C^{\alpha\beta}$ are not involved. Thus, $\nabla_i C^{ia}=\nabla_i C'^{ia}$. ■

Proposition 8.14: If $\mathbf{T}_1$ *and* $\mathbf{T}_2$ *are symmetric tensors in prestandard form, then*

$$\delta(\mathbf{T}_1'\mathbf{T}_2-\mathbf{T}_2\mathbf{T}_1')=\delta(\mathbf{T}_1\mathbf{T}_2-\mathbf{T}_2\mathbf{T}_1).$$

Proof: The commutator $\mathbf{C}=\mathbf{T}_1\mathbf{T}_2-\mathbf{T}_2\mathbf{T}_1$ is skew-symmetric and in prestandard form (Proposition 8.12). The same for $\mathbf{T}_1'\mathbf{T}_2-\mathbf{T}_2\mathbf{T}_1'=\mathbf{C}'$. Then we apply Proposition 8.13. ■

For $\mathbf{T}_1=\mathbf{K}$ (which is in standard form) and $\mathbf{T}_2=\mathbf{R}$ (which is in prestandard form) we get (8.16).

Proposition 8.15: If $\mathbf{T}$, $\mathbf{T}_1$, *and* $\mathbf{T}_2$ *are symmetric tensors in prestandard form, then*

$$\delta(\mathbf{T}_1'\mathbf{T}\mathbf{T}_2'-\mathbf{T}_2'\mathbf{T}\mathbf{T}_1')=\delta(\mathbf{T}_1\mathbf{T}\mathbf{T}_2-\mathbf{T}_2\mathbf{T}\mathbf{T}_1).$$

Proof: The components of $\mathbf{C}=\mathbf{T}_1\mathbf{T}\mathbf{T}_2-\mathbf{T}_2\mathbf{T}\mathbf{T}_1$ are

$$C^{ij}=T_1^{il}T_{lm}T_2^{mj}-T_2^{il}T_{lm}T_1^{mj}=T_1^{ic}T_{cd}T_2^{dj}+T_1^{i\mu}T_{\mu\nu}T_2^{\nu j}-T_2^{ic}T_{cd}T_1^{dj}-T_2^{i\mu}T_{\mu\nu}T_1^{\nu j},$$

so that

$$C^{ab}=T_1^{ac}T_{cd}T_2^{db}-T_2^{ac}T_{cd}T_1^{db},$$

$$C^{a\alpha}=C^{\alpha a}=0,$$

$$C^{\alpha\beta}=T_1^{\alpha\mu}T_{\mu\nu}T_2^{\nu\beta}-T_2^{\alpha\mu}T_{\mu\nu}T_1^{\nu\beta}.$$

This shows that $\mathbf{C}$ is skew-symmetric and in prestandard form. By setting $T_1^{\alpha\beta}=T_2^{\alpha\beta}=0$ we get $C^{\alpha\beta}=0$. This shows that $\mathbf{T}_1'\mathbf{T}\mathbf{T}_2'-\mathbf{T}_2'\mathbf{T}\mathbf{T}_1'=\mathbf{C}'$. Then we apply Proposition 8.13. ■

For $\mathbf{T}_1=\mathbf{K}_1$, $\mathbf{T}_2=\mathbf{K}_2$, and $\mathbf{T}=\mathbf{R}$ we get (8.17). This completes the proof of Theorem 6.1.

IX. FINAL REMARKS

In this paper we have considered the symmetry operators corresponding to the separation of the Schrödinger equation, but deeper and wider research on this topic still has to be done. Indeed, we have not included here a revisitation of the *R*-separation, leading to a different development of the separation of variables for both Schrödinger and Hamilton–Jacobi equations. This will be the subject of a future paper. A further topic to be investigated is the link between the commutation relations of second-order polynomial observables $H_{\mathbf{K}}$ and the associated second-order operators $\hat{H}_{\mathbf{K}}$, for generic two-tensors $\mathbf{K}$ on Riemannian manifolds. This matter is concerned mainly with integrability of systems with quadratic first integrals, and the separability appears only as a special case.

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Efficient simulation of quantum state reduction

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The energy-based stochastic extension of the Schrödinger equation is a rather special nonlinear stochastic differential equation on Hilbert space, involving a single free parameter, that has been shown to be very useful for modeling the phenomenon of quantum state reduction. Here we construct a general closed form solution to this equation, for any given initial condition, in terms of a random variable representing the terminal value of the energy and an independent Brownian motion. The solution is essentially algebraic in character, involving no integration, and is thus suitable as a basis for efficient simulation studies of state reduction in complex systems. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1512975]

The standard energy-based stochastic extension of the Schrödinger equation is given by the following stochastic differential equation:

$$\mathrm{d}|\psi_t\rangle = -\mathrm{i}\hat{H}|\psi_t\rangle \mathrm{d}t - \tfrac{1}{8}\sigma^2(\hat{H}-H_t)^2|\psi_t\rangle \mathrm{d}t + \tfrac{1}{2}\sigma(\hat{H}-H_t)|\psi_t\rangle \mathrm{d}W_t, \tag{1}$$

with initial condition $|\psi_0\rangle$. Here $|\psi_t\rangle$ is the state vector at time t, $\hat{H}$ is the Hamiltonian operator, W_t denotes a one-dimensional Brownian motion, and

$$H_t = \frac{\langle\psi_t|\hat{H}|\psi_t\rangle}{\langle\psi_t|\psi_t\rangle} \tag{2}$$

is the expectation of $\hat{H}$ in the state $|\psi_t\rangle$. The parameter σ, which has the units $\sigma \sim [\text{energy}]^{-1}[\text{time}]^{-1/2}$, governs the characteristic timescale τ_R associated with the collapse of the wave function induced by (1). This is given by $\tau_R = 1/\sigma^2 V_0$, where V_0 is the initial value of the squared energy uncertainty, which at time t is

$$V_t = \frac{\langle\psi_t|(\hat{H}-H_t)^2|\psi_t\rangle}{\langle\psi_t|\psi_t\rangle}. \tag{3}$$

The stochastic equation (1) is perhaps the simplest known dynamic model for state reduction in quantum mechanics consistent with both the Born probability rules and the principle of energy conservation. Although the mathematical and phenomenological properties of (1) have been studied extensively,[1–4] it has hitherto been necessary to resort to numerical methods to solve dynamical equations of this type,[5] and exact solutions have been unavailable except in very simple cases. The purpose of this article is to present a general analytic solution for the dynamics of $|\psi_t\rangle$.

We begin with a brief overview of the stochastic framework implicit in the extended Schrödinger dynamics given by Eq. (1), following a line of argument developed in Ref. 4. Specifically,

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we introduce the key notions of filtration, conditional expectation, martingale, and supermartingale, and show how these concepts can be used effectively to characterize the reductive properties of (1). We then proceed to establish, by novel use of a *nonlinear filtering* technique, that the energy expectation process (2) can be expressed as the conditional expectation of a random variable representing the terminal value of the energy. As a consequence, we are led to simple analytic expressions for the energy (20) and the state vector (33) in terms of a pair of independent state variables. These results open up the possibility of efficiently simulating the reduction process for a variety of models. Finally, we illustrate the practical advantages of our method by analyzing the timescale associated with the reduction process in the case of a two-state system.

The dynamics of $|\psi_t\rangle$ are defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with filtration $\{\mathcal{F}_t\}$ $(0 \leqslant t < \infty)$. Here Ω is the sample space over which $\mathcal{F}$ is a σ-field of open sets upon which the probability measure $\mathbb{P}$ is defined.

The filtration determines for each $t \geqslant 0$ the information available at that time. More specifically, the filtration consists of a family $\{\mathcal{F}_t\}$ of σ-subfields of $\mathcal{F}$ such that $s \leqslant t$ implies $\mathcal{F}_s \subset \mathcal{F}_t$. Given a random variable X on $(\Omega, \mathcal{F}, \mathbb{P})$, we write $\mathbb{E}[X|\mathcal{F}_t]$ for the *conditional expectation* of X with respect to the σ-subfield $\mathcal{F}_t \subset \mathcal{F}$. Intuitively, conditioning with respect to $\mathcal{F}_t$ means giving all the information available up to time t. The nesting $\mathcal{F}_s \subset \mathcal{F}_t$ for $s \leqslant t$ thus embodies a notion of causality. For convenience, we use the abbreviation $\mathbb{E}_t[X] = \mathbb{E}[X|\mathcal{F}_t]$, and we note that the conditional expectation satisfies the tower property $\mathbb{E}_s[\mathbb{E}_t[X]] = \mathbb{E}_s[X]$ for $s \leqslant t$. If $\mathbb{E}_t[X] = X$, we say that X is $\mathcal{F}_t$*-measurable*.

The conditional expectation operation allows us to introduce the concept of a martingale, the stochastic analog of a conserved quantity. A process X_t is said to be an $\{\mathcal{F}_t\}$*-martingale* if $\mathbb{E}[|X_t|] < \infty$ and $\mathbb{E}_s[X_t] = X_s$ for all $0 \leqslant s \leqslant t < \infty$. In other words, X_t is an $\{\mathcal{F}_t\}$-martingale if it is integrable and if its conditional expectation, given information up to time s, is the value X_s of the process at that time.

For a concise mathematical representation of the state reduction process, we also require the concept of a supermartingale. A process X_t is an $\{\mathcal{F}_t\}$*-supermartingale* if $\mathbb{E}[|X_t|] < \infty$ and $\mathbb{E}_s[X_t] \leqslant X_s$ for all $0 \leqslant s \leqslant t < \infty$. Intuitively, a supermartingale is on average a nonincreasing process.

The filtration $\{\mathcal{F}_t\}$ with respect to which the state vector $|\psi_t\rangle$ evolves is generated in a standard way by the Wiener process W_t. We signify this by writing $\{\mathcal{F}_t\} = \{\mathcal{F}_t^W\}$. It is straightforward to verify that the energy process H_t is an $\{\mathcal{F}_t^W\}$-martingale, and that the variance process V_t is an $\{\mathcal{F}_t^W\}$-supermartingale. That is to say,

$$\mathbb{E}_s[H_t] = H_s, \tag{4}$$

and

$$\mathbb{E}_s[V_t] \leqslant V_s. \tag{5}$$

These relations can be deduced by applying Ito's lemma to (2) and (3), from which we infer that

$$\mathrm{d}H_t = \sigma V_t \mathrm{d}W_t, \tag{6}$$

and that

$$\mathrm{d}V_t = -\sigma^2 V_t^2 \mathrm{d}t + \sigma \beta_t \mathrm{d}W_t, \tag{7}$$

where

$$\beta_t = \frac{\langle \psi_t | (\hat{H} - H_t)^3 | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle} \tag{8}$$

is the *skewness* of the energy distribution at time t. The fact that (6) has no drift shows that H_t is a martingale, and the fact that the drift in (7) is negative shows that V_t is a supermartingale.

In the case of the ordinary Schrödinger equation with a time-independent Hamiltonian, the energy process (2) is constant. This is usually interpreted as the quantum mechanical expression of an energy conservation law. However, if a system is in an indefinite state of energy, then it is not immediately evident what is meant by energy conservation. The martingale condition $\mathbb{E}_s[H_t] = H_s$ can be interpreted as a *generalized energy conservation law* applicable if a system is in an indefinite state of energy. In particular, it implies that once state reduction has occurred, the probabilistic average of the outcome for the energy must equal the initial expectation.

The supermartingale property satisfied by V_t is the essence of what is meant by a *reduction process*. In fact, it follows from Eq. (7) that the asymptotic behavior of V_t is given by

$$\lim_{t\to\infty} \mathbb{E}[V_t] = 0, \tag{9}$$

which signifies the collapse of the wave function. A positive supermartingale with the property that its expectation vanishes in the limit as t goes to infinity is called a *potential* process. Writing H_∞ for the random terminal value of the energy, one can then prove as a consequence of (6) and (7) that

$$H_t = \mathbb{E}_t[H_\infty] \tag{10}$$

and that

$$V_t = \mathbb{E}_t[(H_\infty - H_t)^2]. \tag{11}$$

That is to say, the processes H_t and V_t are respectively the $\mathcal{F}_t^W$-conditional mean and variance of H_∞.

With these facts in hand, we now present a method for solving the stochastic equation (1). Our approach is based on the theory of nonlinear filtering.[6] Filtering techniques have been shown to be useful in quantum optics in connection with the theory of continuous observations, and in some situations phenomenological equations similar to (1) for the *a posteriori* dynamics of a continuously observed system can be derived.[7] We shall, however, regard the dynamics of $|\psi_t\rangle$ as being given, and use the filtering methodology with a different end in view: namely, to construct the *solution* of (1).

The setup is as follows. We denote by E_i $(i=1,2,...)$ the eigenvalues of the Hamiltonian of a given quantum system, and write

$$\pi_i = \frac{|\langle \psi_0|\psi_i\rangle|^2}{\langle \psi_0|\psi_0\rangle\langle \psi_i|\psi_i\rangle} \tag{12}$$

for the transition probability from the given initial state $|\psi_0\rangle$ to the eigenstate $|\psi_i\rangle$ with energy E_i. If the spectrum of $\hat{H}$ is degenerate, then $|\psi_i\rangle$ denotes the Lüders state, i.e., the projection of $|\psi_0\rangle$ onto the linear subspace of states corresponding to the eigenvalue E_i.

Now let the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ be given, and on it specify a random variable H that takes the values E_i with probabilities π_i. We assume that $(\Omega, \mathcal{F}, \mathbb{P})$ comes equipped with a filtration $\{\mathcal{G}_t\}$ with respect to which a standard Brownian motion B_t is specified, and that H and B_t are *independent*. We assign no *a priori* physical significance to H and B_t, which are introduced here simply as an ansatz for obtaining a solution for (1). Next we define the process

$$\xi_t = \sigma H t + B_t. \tag{13}$$

Intuitively, we can think of ξ_t as giving us a ''noisy'' representation of the information encoded in the random variable H.

We let $\{\mathcal{F}_t^\xi\}$ denote the filtration generated by the process ξ_t, i.e., the information generated by ξ_t as time progresses, and consider the conditional expectation

$$H_t = \mathbb{E}[H|\mathcal{F}_t^{\xi}]. \tag{14}$$

Clearly, $\mathcal{F}_t^{\xi} \subset \mathcal{G}_t$ since knowledge of H together with the path $\{B_s\}_{0\leqslant s\leqslant t}$ implies knowledge of the path $\{\xi_s\}_{0\leqslant s\leqslant t}$, although the converse is not the case.

It follows from the tower property that H_t is an $\{\mathcal{F}_t^{\xi}\}$-martingale. One can think of H_t as representing an estimate for the value of H given the history of the process ξ_s from time 0 up to time t. More precisely, an $\{\mathcal{F}_t^{\xi}\}$-measurable random variable H_t minimizes the expectation of the squared deviation of H from H_t, given the history of ξ_s from time 0 to time t, if and only if (14) holds. This can be seen by varying the expression $\mathbb{E}[(H-H_t)^2|\mathcal{F}_t^{\xi}]$ with respect to H_t.

We shall now establish the remarkable fact that the *process H_t defined by (14) is statistically indistinguishable from the energy process (2) associated with the stochastic extension of the Schrödinger equation (1).*

The argument goes as follows. First, because ξ_t is a Markov process satisfying

$$\lim_{t\to\infty} t^{-1}\xi_t = \sigma H, \tag{15}$$

we can replace (14) with the simpler relation $H_t = \mathbb{E}[H|\xi_t]$. In other words, to determine the conditional expectation of H given the path $\{\xi_s\}_{0\leqslant s\leqslant t}$, it suffices to condition on the value ξ_t of the process at the end of the path.

To calculate $\mathbb{E}[H|\xi_t]$, we require a version of the Bayes formula applicable when we consider the probability of a discrete random variable conditioned on the value of a continuous random variable. This is given by

$$\mathbb{P}(H=E_i|\xi_t) = \frac{\pi_i \rho(\xi_t|H=E_i)}{\Sigma_i \pi_i \rho(\xi_t|H=E_i)}, \tag{16}$$

where

$$\pi_i = \mathbb{P}(H=E_i). \tag{17}$$

Here $\rho(\xi_t|H=E_i)$ denotes the conditional probability density for the continuous random variable ξ_t given that $H=E_i$. Since B_t is a standard Brownian motion, the conditional density for ξ_t is

$$\rho(\xi_t|H=E_i) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{1}{2t}(\xi_t - \sigma E_i t)^2\right). \tag{18}$$

It follows from the Bayes law (16) that the conditional probability for the random variable H is

$$\mathbb{P}(H=E_i|\xi_t) = \frac{\pi_i \exp(\sigma E_i \xi_t - \frac{1}{2}\sigma^2 E_i^2 t)}{\Sigma_i \pi_i \exp(\sigma E_i \xi_t - \frac{1}{2}\sigma^2 E_i^2 t)}. \tag{19}$$

Therefore, multiplying each side of (19) by E_i and summing over i, we deduce that the conditional expectation of the random variable H given ξ_t is

$$H_t = \frac{\Sigma_i \pi_i E_i \exp(\sigma E_i \xi_t - \frac{1}{2}\sigma^2 E_i^2 t)}{\Sigma_i \pi_i \exp(\sigma E_i \xi_t - \frac{1}{2}\sigma^2 E_i^2 t)}. \tag{20}$$

In order to show that H_t is the energy process associated with (1), one further key result is required: namely, that *the process W_t defined by*

$$W_t = \xi_t - \sigma \int_0^t H_s \, \mathrm{d}s \tag{21}$$

is an $\{\mathcal{F}_t^\xi\}$*-Brownian motion*. To verify this, it suffices, by virtue of Lévy's characterization of Brownian motion,[6] to demonstrate (a) that $(\mathrm{d}W_t)^2=\mathrm{d}t$ and (b) that W_t is an $\{\mathcal{F}_t^\xi\}$-martingale. To verify (a) we note that (13) implies

$$\mathrm{d}\xi_t=\sigma H\mathrm{d}t+\mathrm{d}B_t, \tag{22}$$

and thus $(\mathrm{d}\xi_t)^2=\mathrm{d}t$. On the other hand, (21) implies that $\mathrm{d}W_t=\mathrm{d}\xi_t-\sigma H_t\mathrm{d}t$, and hence $(\mathrm{d}W_t)^2=(\mathrm{d}\xi_t)^2$. To establish (b), let (20) define a function $H(\xi,t)$ of two variables such that $H_t=H(\xi_t,t)$:

$$H(\xi,t)=\frac{\Sigma_i\pi_iE_i\exp(\sigma E_i\xi-\frac{1}{2}\sigma^2E_i^2t)}{\Sigma_i\pi_i\exp(\sigma E_i\xi-\frac{1}{2}\sigma^2E_i^2t)}. \tag{23}$$

Then applying Ito's lemma and using the relation $(\mathrm{d}\xi_t)^2=\mathrm{d}t$, we obtain

$$\mathrm{d}H_t=(\partial_tH(\xi_t,t)+\tfrac{1}{2}\partial_\xi^2H(\xi_t,t))\mathrm{d}t+\partial_\xi H(\xi_t,t)\mathrm{d}\xi_t, \tag{24}$$

where $\partial_tH(\xi_t,t)$ denotes $\partial H(\xi,t)/\partial t$ valued at $\xi=\xi_t$, and so on. A calculation making use of (21), (23), and (24) then shows that

$$\mathrm{d}H_t=\sigma V(\xi_t,t)\mathrm{d}W_t, \tag{25}$$

where the function $V(\xi,t)$ is

$$V(\xi,t)=\frac{\Sigma_i\pi_i(E_i-H(\xi,t))^2\exp(\sigma E_i\xi-\frac{1}{2}\sigma^2E_i^2t)}{\Sigma_i\pi_i\exp(\sigma E_i\xi-\frac{1}{2}\sigma^2E_i^2t)}. \tag{26}$$

Because H_t is an $\{\mathcal{F}_t^\xi\}$-martingale, we conclude that W_t is also an $\{\mathcal{F}_t^\xi\}$-martingale, and that establishes (b). We thus deduce that W_t is an $\{\mathcal{F}_t^\xi\}$-Brownian motion, with respect to which ξ_t is a diffusion process satisfying

$$\mathrm{d}\xi_t=\sigma H(\xi_t,t)\mathrm{d}t+\mathrm{d}W_t. \tag{27}$$

Now let $|\psi_0\rangle$ be the initial normalized state vector of the quantum system, and let $\hat{P}_i$ denote for each value of i the projection operator onto the Hilbert subspace corresponding to the energy eigenvalue E_i. We let

$$|\psi_i\rangle=\pi_i^{-1/2}\hat{P}_i|\psi_0\rangle \tag{28}$$

denote the Lüders state corresponding to E_i, and write

$$\Pi_{it}=\mathbb{P}(H=E_i|\xi_t) \tag{29}$$

for the process defined by (19). Then we can establish our main result, that

$$|\psi_t\rangle=\sum_i e^{-\mathrm{i}E_it}\Pi_{it}^{1/2}|\psi_i\rangle \tag{30}$$

satisfies the stochastic extension of the Schrödinger equation (1) with the given initial condition. In particular, by applying Ito's lemma to (19) and using (27) we obtain

$$\mathrm{d}\Pi_{it}=\sigma(E_i-H_t)\Pi_{it}\mathrm{d}W_t. \tag{31}$$

With another application of Ito's lemma we deduce that

$$d\Pi_{it}^{1/2} = -\tfrac{1}{8}\sigma^2(E_i - H_t)^2\Pi_{it}^{1/2}dt + \tfrac{1}{2}\sigma(E_i - H_t)\Pi_{it}^{1/2}dW_t. \tag{32}$$

A short calculation then shows that (30) satisfies the stochastic equation (1), and that the expectation of the operator $\hat{H}$ in the state $|\psi_t\rangle$ is the process (20).

In summary, the stochastic equation (1) can be solved as follows. We let H be a random variable taking the values E_i with the probabilities π_i defined by (12). Letting B_t denote an independent Brownian motion, we define ξ_t as in (13). The solution of (1) is then given by

$$|\psi_t\rangle = \frac{\Sigma_i \sqrt{\pi_i}\exp(-iE_it + \frac{1}{2}\sigma E_i\xi_t - \frac{1}{4}\sigma^2E_i^2t)|\psi_i\rangle}{(\Sigma_i \pi_i \exp(\sigma E_i\xi_t - \frac{1}{2}\sigma^2E_i^2t))^{1/2}}, \tag{33}$$

where the $\{\mathcal{F}_t^\xi\}$-Brownian motion W_t driving $|\psi_t\rangle$ in (1) is given by (21). Expression (20) for H_t follows at once from (33) since $\langle\psi_i|\hat{H}|\psi_j\rangle = E_i\delta_{ij}$, and for the variance of the energy we deduce that $V_t = V(\xi_t, t)$. To obtain a realization of the process $|\psi_t\rangle$, i.e., to carry out a simulation, we simply choose a value for H in accordance with the given probability law, and then let B_t run its course.

The fact that (20) is indeed a reduction process can be verified directly as follows. Suppose, in a particular realization of the process H_t, the random variable H takes the value E_j for some choice of the index j. Writing $\omega_{ij} = E_i - E_j$ and seting $\xi_t = \sigma E_j t + B_t$, we obtain

$$H_t = \frac{\pi_jE_j + \Sigma_{i(\neq j)}\pi_iE_i\exp(\sigma\omega_{ij}B_t - \frac{1}{2}\sigma^2\omega_{ij}^2t)}{\pi_j + \Sigma_{i(\neq j)}\pi_i\exp(\sigma\omega_{ij}B_t - \frac{1}{2}\sigma^2\omega_{ij}^2t)}, \tag{34}$$

for the corresponding realization of H_t. However, the exponential martingale M_{ijt} defined for $i \neq j$ by

$$M_{ijt} = \exp(\sigma\omega_{ij}B_t - \tfrac{1}{2}\sigma^2\omega_{ij}^2t) \tag{35}$$

that appears in expression (34) has the property

$$\lim_{t\to\infty} \mathbb{P}(M_{ijt} > 0) = 0. \tag{36}$$

Given that

$$H_t = \frac{\pi_jE_j + \Sigma_{i(\neq j)}\pi_iE_iM_{ijt}}{\pi_j + \Sigma_{i(\neq j)}\pi_iM_{ijt}}, \tag{37}$$

we see that H_t converges to the value E_j with probability one. A similar argument shows that if $H = E_j$, then for each value of i we have $\lim_{t\to\infty}\Pi_{it} = 0$ unless $i = j$, which allows us to verify that $|\psi_t\rangle$ converges to the Lüders state corresponding to the energy eigenvalue E_j with probability one.[4]

Therefore, we see that the random variable H can be identified with the terminal value H_∞ of the energy process. The fact that H is not $\mathcal{F}_t^W$-measurable for $t < \infty$ indicates that the "true value" of H is "hidden" until the reduction process is complete. On a related point we note that in stochastic models for state reduction it is sometimes assumed that the driving process W_t is in some way "external" to the quantum system. This assumption, however, is unnecessary: the filtrations associated with W_t, ξ_t, H_t, and $|\psi_t\rangle$ all coincide, and it is thus consistent to regard the innovation process W_t as being endogenous.

The advantage of expressions (20) and (33) from a computational point of view is that H_t and $|\psi_t\rangle$ are expressed *algebraically* in terms of the underlying random variable H and the Brownian motion B_t. These quantities can be thought of as representing independent *state variables* for the

reduction dynamics. As a consequence, we are able to investigate properties of the process (1) directly without having to resort to numerical integration. In particular, by use of (33), a numerical simulation of the state reduction of complex systems is feasible, including cases for which the Hamiltonian has a nondiscrete spectrum. It should be emphasized that in our simulation methodology there is no need at any stage for the introduction of a change of probability measure.

In conclusion we present a probabilistic analysis of the timescale associated with the reduction process, in the case of a two-state system with energies E_1 and E_2. The initial state is given by $|\psi_0\rangle$, and the transition probabilities to the energy eigenstates $|E_1\rangle$ and $|E_2\rangle$ are given by π_1 and π_2.

Suppose a measurement of the energy is made, and we condition on the outcome of the measurement being E_1. In that case, according to (37), we have

$$H_t=\frac{\pi_1 E_1+\pi_2 E_2 M_{21t}}{\pi_1+\pi_2 M_{21t}}, \tag{38}$$

where

$$M_{21t}=\exp\left(\sigma\omega_{21}B_t-\tfrac{1}{2}\sigma^2\omega_{21}^2 t\right). \tag{39}$$

Writing $\beta=\frac{1}{4}\sigma^2\omega_{21}^2$ for the parameter that determines the characteristic rate of reduction, we can work out the probability that $M_{21t}<e^{-n}$ for some value of n. Since B_t is normally distributed with zero mean and variance t, we find

$$\mathbb{P}(M_{21t}<e^{-n})=N((\beta t)^{1/2}-\tfrac{1}{2}n(\beta t)^{-1/2}), \tag{40}$$

where $N(x)$ is the standard normal distribution function. Therefore, for example, we see that provided $t>5\tau_R$, we have

$$\mathbb{P}(M_{21t}<e^{-10})>\tfrac{1}{2}, \tag{41}$$

where $\tau_R=1/\beta$. In particular, as H_t draws near E_1 we have the relation

$$H_t-E_1\sim\frac{\pi_2}{\pi_1}(E_2-E_1)M_{21t}. \tag{42}$$

Thus, after only a relatively few multiples of the characteristic reduction timescale, the amount by which H_t differs from E_1 will with high probability be reduced to a tiny fraction of the energy difference E_2-E_1.

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The Schwinger SU(3) construction. I. Multiplicity problem and relation to induced representations

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The Schwinger oscillator operator representation of SU(3) is analyzed with particular reference to the problem of multiplicity of irreducible representations. It is shown that with the use of an $\mathrm{Sp}(2,R)$ unitary representation commuting with the SU(3) representation, the infinity of occurrences of each SU(3) irreducible representation can be handled in complete detail. A natural ''generating representation'' for SU(3), containing each irreducible representation exactly once, is identified within a subspace of the Schwinger construction, and this is shown to be equivalent to an induced representation of SU(3). © *2002 American Institute of Physics.* [DOI: 10.1063/1.1508810]

I. INTRODUCTION

The well known Schwinger representation of the Lie algebra of SU(2),[1] constructed using the annihilation and creation operators of two independent quantum mechanical harmonic oscillators, has played an important role in many widely differing contexts. Within the quantum theory of angular momentum it has made the calculation of various quantities somewhat easier than by other methods. Beyond this, it has been very effectively exploited in the physics of strongly correlated systems,[2] in quantum optics of two mode radiation fields,[3] and in the study of certain classes of partially coherent optical beams,[4] namely to obtain the coherent mode decomposition of anisotropic Gaussian Schell model beams. It arises quite naturally in the context of a classical description of particles with non-Abelian charges[5] and has also been used in a recent investigation of the Pauli spin-statistics theorem.[6]

Bargmann has presented an entire function Hilbert space analog of the Schwinger construction, which is extremely elegant and possesses special merits of its own.[7] This may be viewed as a counterpart to the Fock space description of quantum mechanical oscillator systems.

Certain specially attractive features of the Schwinger SU(2) construction should be mentioned. It leads upon exponentiation to a unitary representation (UR) of SU(2) in which each unitary irreducible representation (UIR), labeled as usual by the spin quantum number j with possible values $0,\frac{1}{2},1,\ldots$, appears exactly once. In other words, it is complete in the sense that no UIR of SU(2) is missed, and also economical in the sense of being multiplicity free. Thus, reflecting these two features, it may be regarded as a ''generating representation'' for SU(2), a concept that has been effectively used in understanding the structures of various kinds of Clebsch–Gordan series for UIRs of the noncompact group SU(1,1).[8] In addition, of course, the use of boson operator methods makes many operator and state vector calculations relatively easy to carry out.

It is of considerable interest to extend the Schwinger construction to other compact Lie groups, the next natural case after SU(2) being SU(3). The aims behind any such attempt would be

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to preserve the simplicity of the boson calculus, to cover all UIRs of the concerned group, and to do it in a multiplicity free manner.

The case of SU(3) has been studied by several authors since the work of Moshinsky.[9] The aim of the present article is somewhat different from previous studies, being motivated by the particular points of view mentioned above. In particular our aim is to see to what extent the attractive features of the SU(2) construction survive when we consider SU(3), and which ones have to be given up.

A brief overview of this article is as follows. In Sec. II we collect together some relevant facts regarding unitary representations of compact Lie groups with special attention to SU(3). In particular, we highlight the fact that the theory of induced representations leads to a unitary representation of SU(3) which has all the properties becoming of a ''generating representation'' of SU(3) in that it contains all the UIRs of SU(3) exactly once each. The Hilbert space carrying this unitary representation turns out to be the Hilbert space of functions on unit sphere in C^3. In Sec. III, we turn to the Schwinger oscillator construction for SU(3) and show that a naive extension of the Schwinger SU(2)-construction making use of six oscillators leads to a very ''fat'' UR of SU(3) containing each UIR of SU(3) infinitely many times. We then show how the group $\mathrm{Sp}(2,R)$ enables us to completely handle this multiplicity and also neatly isolate from this rather large space a subspace carrying a UR of SU(3) of a ''generating representation'' type. At this stage, we have two ''generating representations'' of SU(3), one based on the Hilbert space of functions on a unit sphere in C^3 and the other based on the Fock space of six oscillators, and a natural question to ask is how the two are related. To this end, in Sec. IV, we make use of the Bargmann representation, to transcribe the Fock space description into a description based on a Hilbert space of square integrable functions in six complex variables satisfying certain conditions. This transcription enables us to establish an equivalence map between the Hilbert spaces supporting the two incarnations of the ''generating representation'' for SU(3), details of which are given in Secs. V and VI. Section VII contains concluding remarks and further outlook, and an appendix gives the details of the construction of $\mathrm{SU}(3)\times\mathrm{Sp}(2,R)$ basis states.

II. UNITARY REPRESENTATIONS OF COMPACT LIE GROUPS, THE SU(3) CASE

It is useful to first recall some basic facts concerning the representation theory of any compact simple Lie group G. The basic building blocks are the UIRs of G. Each UIR carries certain identifying labels (eigenvalues of Casimir operators), such as j for SU(2). It is of a characteristic dimension, such as $2j+1$ for SU(2). In addition, we may set up some convenient orthonormal basis in the space of the UIR, as simultaneous eigenvectors of some complete commuting set of Hermitian operators. The eigenvalue sets labeling the basis vectors are generalizations of the single magnetic quantum number m for SU(2).

A general UR of G is reducible into UIRs, each occurring with some multiplicity. Thus the UR as a whole is in principle completely determined upto equivalence by these multiplicities. However, certain URs have special significance, reflecting the way they are constructed, and so deserve special attention. We consider two cases—the regular representation, and representations induced from various Lie subgroups of G.

The Hilbert space carrying the regular representation of G is the space $L^2(G)$ of all complex square integrable functions on G, the integration being with respect to the (left and right) translation invariant volume element on G. On this space there are in fact two (mutually commuting) regular representations of G, the left and the right regular representations. Upon reduction into UIRs each of these contains every UIR of G without exception, the multiplicity of occurrence of a particular UIR is just its dimension. Thus the regular representations possess the completeness property of the Schwinger SU(2) construction, but not its economy.

Next we look at the family of induced URs of G.[10] Let H be some Lie subgroup of G, and let $D(h)$, $h\in H$, be the operators of a UIR of H on some Hilbert space $\mathcal{V}$. Then a certain unique UR of G, with operators $\mathcal{D}_H^{(\mathrm{ind},D)}(g)$ for $g\in G$, can be constructed. As the labels indicate, this UR is induced from the UIR $D(\cdot)$ of H. The Hilbert space $\mathcal{H}_H^{(\mathrm{ind},D)}$ of this UR consists of functions on

G with values in $\mathcal{V}$ obeying a covariance condition and having finite norm:

$$\psi \in \mathcal{H}_H^{(\mathrm{ind},D)}: \quad \psi(g) \in \mathcal{V}, g \in G,$$
$$\psi(gh) = D(h^{-1})\psi(g), h \in H, \tag{2.1}$$
$$\|\psi\|^2 = \int_G dg\,(\psi(g), \psi(g))_{\mathcal{V}} < \infty.$$

Here dg is the (suitably normalized) invariant volume element on G, and the integrand is the squared norm of $\psi(g) \in \mathcal{V}$. The covariance condition means that $\psi(g)$ is essentially a function on the coset space G/H, in the sense that the ''values'' of $\psi(g)$ all over a coset are determined by its ''value'' at any one representative point. Correspondingly, due to unitarity of $D(h)$, $(\psi(g), \psi(g))_{\mathcal{V}}$ is constant over each coset; so, the expression for $\|\psi\|^2$ can be simplified and expressed in terms of a G-invariant volume element on G/H. The action of $\mathcal{D}_H^{(\mathrm{ind},D)}(g)$ on ψ is then given by

$$g \in G: \mathcal{D}_H^{(\mathrm{ind},D)}(g)\psi = \psi',$$
$$\psi'(g') = \psi(g^{-1}g'). \tag{2.2}$$

It is clear that G action preserves the covariance condition, and we have a UR of G on $\mathcal{H}_H^{(\mathrm{ind},D)}$.

Whereas $D(\cdot)$ was assumed to be a UIR of H, $\mathcal{D}_H^{(\mathrm{ind},D)}(\cdot)$ is in general reducible; so it is a direct sum of the various UIRs of G, each occurring with some multiplicity. These multiplicities are determined by the reciprocity theorem:[10] Each UIR $\mathcal{D}(\cdot)$ of G appears in $\mathcal{D}_H^{(\mathrm{ind},D)}(\cdot)$ as often as $\mathcal{D}(\cdot)$ contains $D(\cdot)$ upon restriction from G to H.

With this general background we now take up the specific case of SU(3). The defining representation of this group is

$$\mathrm{SU}(3) = \{A = 3\times 3 \ \text{ complex matrix} | A^\dagger A = I_{3\times 3}, \det A = 1\}, \tag{2.3}$$

with the group operation given by matrix multiplication. In this representation the eight Hermitian generators are $\frac{1}{2}\lambda_\alpha$, $\alpha = 1,2,\ldots,8$, where the matrices λ_α and the structure constants $f_{\alpha\beta\gamma}$ occurring in the commutation relations

$$[\lambda_\alpha, \lambda_\beta] = 2if_{\alpha\beta\gamma}\lambda_\gamma, \quad \alpha,\beta,\gamma = 1,2,\ldots,8, \tag{2.4}$$

are all very well known.[11]

A general UIR of SU(3) is determined by two independent nonnegative integers p and q, so it may be denoted as (p,q). It is of dimension $d(p,q) = \frac{1}{2}(p+1)(q+1)(p+q+2)$. The defining three-dimensional UIR in (2.3) is (1,0), while the inequivalent complex conjugate UIR is (0,1). In general the complex conjugate of (p,q) is (q,p), and the adjoint UIR is (1,1) of dimension eight. Various choices of ''magnetic quantum numbers'' within a UIR may be made. The one corresponding to the canonical subgroup $\mathrm{SU}(2)\times\mathrm{U}(1)/Z_2 = \mathrm{U}(2) \subset \mathrm{SU}(3)$ leads to the three quantum numbers I, M, Y in standard notation. Here I and M are the isospin and magnetic quantum number labels for a general UIR of SU(2), while Y is the eigenvalue of the (suitably normalized) U(1) or hypercharge generator. The subgroups SU(2) and U(1) commute, and for definiteness we take SU(2) to be the one acting on the first two dimensions of the three dimensions in the UIR (1,0). The spectrum of ''$I-Y$'' multiplets present in the UIR (p,q) can be described thus:

$$I = \tfrac{1}{2}(r+s), \quad Y = r - s + \tfrac{2}{3}(q-p), \quad 0 \leqslant r \leqslant p, \quad 0 \leqslant s \leqslant q. \tag{2.5}$$

Thus for each pair of integers (r,s) in the above ranges, we have one $I-Y$ multiplet, with M going over the usual $2I+1$ values $I, I-1, \ldots, -I+1, -I$. Then the orthonormal basis vectors for the UIR (p,q) of SU(3) may be written as $|p,q;IMY\rangle$. This UIR can be realized via suitably

constructed irreducible tensors. A tensor T with p indices belonging to the UIR (1,0) and q indices to the UIR (0,1) is a collection of complex components $T^{j_1\cdots j_p}_{k_1\cdots k_q}$, j and $k=1,2,3$, transforming under $A\in \mathrm{SU}(3)$ by the rule

$$T'^{j_1\cdots j_p}_{k_1\cdots k_q}=A^{j_1}_{l_1}\cdots A^{j_p}_{l_p}A^{k_1*}_{m_1}\cdots A^{k_q*}_{m_q}T^{l_1\cdots l_p}_{m_1\cdots m_q}. \tag{2.6}$$

If in addition T is completely symmetric separately in the superscripts and in the subscripts, and is traceless, i.e., contraction of any upper index with any lower index leads to zero, then all these properties are maintained under SU(3) action and T is an irreducible tensor. It then has precisely $d(p,q)$ independent components (in the complex sense), and the space of all such tensors carries the UIR (p,q). The explicit transition from the tensor components $T^{j_1\cdots j_p}_{k_1\cdots k_q}$ to the canonical components $T^{(p,q)}_{IMY}$ may be found in Ref. 12

The regular representations of SU(3) act on the space $L^2(\mathrm{SU}(3))$, and in each of them the UIR (p,q) appears $d(p,q)$ times. We shall not be concerned with this UR of SU(3) in our work. Instead we give now the UIR contents of some selected induced URs of SU(3). For illustrative purposes we consider the following four subgroups:

$$\mathrm{U}(1)\times\mathrm{U}(1)=\{A=\mathrm{diag}(e^{i(\theta_1+\theta_2)},e^{i(\theta_1-\theta_2)},e^{-2i\theta_1})\,|\,0\leqslant\theta_1,\theta_2\leqslant 2\pi\}; \tag{2.7a}$$

$$\mathrm{SU}(2)=\left\{A=\begin{pmatrix} a & \mathbf{0}\\ \mathbf{0} & 1\end{pmatrix}\,\middle|\, a\in\mathrm{SU}(2)\right\}; \tag{2.7b}$$

$$\mathrm{U}(2)=\left\{A=\begin{pmatrix} u & \mathbf{0}\\ \mathbf{0} & (\det u)^{-1}\end{pmatrix}\,\middle|\, u\in\mathrm{U}(2)\right\}; \tag{2.7c}$$

$$\mathrm{SO}(3)=\{A\in\mathrm{SU}(3)\,|\,A^*=A\}. \tag{2.7d}$$

In each case, we look at the induced UR of SU(3) arising from the trivial one-dimensional UIR of the subgroup. In the first two cases, in order to apply the reciprocity theorem, we can use the information in (2.5) giving the $\mathrm{SU}(2)\times\mathrm{U}(1)/Z_2$ content of the UIR (p,q) of SU(3). Defining by a zero in the superscript the trivial UIR of the relevant subgroup, we have the results:

$$\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{U}(1)\times\mathrm{U}(1)}=\sum_{\substack{p,q=0,1,\cdots\\ p=q\,\mathrm{mod}3}}^{\infty}\oplus n_{p,q}(p,q),\quad n_{p,q}=\min(p+1,q+1); \tag{2.8a}$$

$$\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}=\sum_{p,q=0,1,\cdots}^{\infty}\oplus(p,q); \tag{2.8b}$$

$$\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{U}(2)}=\sum_{p=0,1,\cdots}^{\infty}\oplus(p,p). \tag{2.8c}$$

The real dimensions of the corresponding coset spaces $\mathrm{SU}(3)/\mathrm{U}(1)\times\mathrm{U}(1)$, $\mathrm{SU}(3)/\mathrm{SU}(2)$ and $\mathrm{SU}(3)/\mathrm{U}(2)$ are 6, 5 and 4, respectively. In the case of induction from the trivial UIR of SO(3), we need to use the fact that the UIR (p,q) of SU(3) does not contain an SO(3) invariant state if either p or q or both are odd, while it contains one such state if both p and q are even. Then we arrive at the reduction

$$\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{SO}(3)}=\sum_{r,s=0,1,\cdots}^{\infty}\oplus(2r,2s), \tag{2.9}$$

with $\mathrm{SU}(3)/\mathrm{SO}(3)$ being of real dimension 5.

From the above discussion we see that the induced UR $\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}$ of SU(3) is particularly interesting in that it captures both the completeness and the economy properties of the Schwinger SU(2) construction: each UIR of SU(3) is present, exactly once. Thus we may call this a generating representation of SU(3); it is much leaner than the regular representations.

III. THE MINIMAL SU(3) SCHWINGER OSCILLATOR CONSTRUCTION

An elementary oscillator operator construction of the SU(3) generators is based on three independent pairs of annihilation and creation operators $\hat{a}_j$, $\hat{a}_j^\dagger$ obeying

$$[\hat{a}_j,\hat{a}_k^\dagger]=\delta_{jk}, \quad [\hat{a}_j,\hat{a}_k]=[\hat{a}_j^\dagger,\hat{a}_k^\dagger]=0, \quad j,k=1,2,3. \tag{3.1}$$

We write $\mathcal{H}^{(a)}$ for the Hilbert space on which these operators act irreducibly. The individual and total number operators are

$$\hat{N}_1^{(a)}=\hat{a}_1^\dagger\hat{a}_1, \quad \hat{N}_2^{(a)}=\hat{a}_2^\dagger\hat{a}_2, \quad \hat{N}_3^{(a)}=\hat{a}_3^\dagger\hat{a}_3, \quad \hat{N}^{(a)}=\hat{a}_j^\dagger\hat{a}_j. \tag{3.2}$$

If we now define the bilinear operators

$$Q_\alpha^{(a)}=\tfrac{1}{2}\hat{a}^\dagger\lambda_\alpha\hat{a}, \quad \alpha=1,2,\ldots,8, \tag{3.3}$$

each $Q_\alpha^{(a)}$ is Hermitian, and they obey the SU(3) Lie algebra commutation relations

$$[Q_\alpha^{(a)},Q_\beta^{(a)}]=if_{\alpha\beta\gamma}Q_\gamma^{(a)}. \tag{3.4}$$

In addition they conserve the total number operator:

$$[Q_\alpha^{(a)},\hat{N}^{(a)}]=0. \tag{3.5}$$

Upon exponentiation of these generators we obtain a particular UR, $\mathcal{U}^{(a)}(A)$ say, of SU(3) acting on $\mathcal{H}^{(a)}$, under which the creation (annihilation) operators $\hat{a}_j^\dagger$ ($\hat{a}_j$) transform via the UIR (1,0) ((0,1)):

$$\begin{aligned}\mathcal{U}^{(a)}(A)\hat{a}_j^\dagger\mathcal{U}^{(a)}(A)^{-1}&=A_j^k\hat{a}_k^\dagger,\\ \mathcal{U}^{(a)}(A)\hat{a}_j\mathcal{U}^{(a)}(A)^{-1}&=A_j^{k*}\hat{a}_k.\end{aligned} \tag{3.6}$$

However, upon reduction, $\mathcal{U}^{(a)}(A)$ contains only the "triangular" UIRs $(p,0)$ of SU(3), once each. In that sense this UR may be regarded as the "generating representation" for this subset of UIRs. For any given $p\geqslant 0$, the UIR $(p,0)$ is realized on that subspace $\mathcal{H}^{(p,0)}$ of $\mathcal{H}^{(a)}$ over which the total number operator $\hat{N}^{(a)}$ takes the eigenvalue p; and the connection between the tensor and the Fock space descriptions is given in this manner:

$$\begin{gathered}\{T^{j_1\cdots j_p}\}\rightarrow|T\rangle=T^{j_1\cdots j_p}\hat{a}_{j_1}^\dagger\cdots\hat{a}_{j_p}^\dagger|\underline{0}\rangle\in\mathcal{H}^{(p,0)}\subset\mathcal{H}^{(a)},\\ \hat{a}_j|\underline{0}\rangle=0;\\ \mathcal{U}^{(a)}(A)|T\rangle=|T'\rangle,\\ T'^{j_1\cdots j_p}=A_{l_1}^{j_1}\cdots A_{l_p}^{j_p}T^{l_1\cdots l_p}.\end{gathered} \tag{3.7}$$

Therefore we have the (orthogonal) direct sum decompositions

$$\mathcal{H}^{(a)}=\sum_{p=0,1,\cdots}^{\infty}\oplus\mathcal{H}^{(p,0)},$$

$$\mathcal{H}^{(p,0)}=\mathrm{Sp}\{\hat{a}_{j_1}^{\dagger}\cdots\hat{a}_{j_p}^{\dagger}|\underline{0}\rangle\}, \tag{3.8}$$

$$\mathcal{U}^{(a)}=\sum_{p=0,1,\cdots}^{\infty}\oplus(p,0).$$

To be able to obtain the other UIRs as well, we bring in another independent triplet of oscillator operators $\hat{b}_j$ and $\hat{b}_j^{\dagger}$ obeying the same commutation relations (3.1) and commuting with $\hat{a}$'s and $\hat{a}^{\dagger}$'s:

$$\begin{gathered}[\hat{b}_j,\hat{b}_k^{\dagger}]=\delta_{jk},\quad [\hat{b}_j,\hat{b}_k]=[\hat{b}_j^{\dagger},\hat{b}_k^{\dagger}]=0,\quad j,k=1,2,3,\\ [\hat{a}_j\ \text{or}\ \hat{a}_j^{\dagger},\ \hat{b}_k\ \text{or}\ \hat{b}_k^{\dagger}]=0.\end{gathered} \tag{3.9}$$

The corresponding Hilbert space is $\mathcal{H}^{(b)}$, and the b-type number operators are

$$\hat{N}_1^{(b)}=\hat{b}_1^{\dagger}\hat{b}_1,\quad \hat{N}_2^{(b)}=\hat{b}_2^{\dagger}\hat{b}_2,\quad \hat{N}_3^{(b)}=\hat{b}_3^{\dagger}\hat{b}_3,\quad \hat{N}^{(b)}=\hat{b}_j^{\dagger}\hat{b}_j. \tag{3.10}$$

We define the b-type SU(3) generators as

$$Q_{\alpha}^{(b)}=-\tfrac{1}{2}\hat{b}^{\dagger}\lambda_{\alpha}^{*}\hat{b},\quad \alpha=1,2,\ldots,8, \tag{3.11}$$

and they obey

$$\begin{gathered}[Q_{\alpha}^{(b)},Q_{\beta}^{(b)}]=if_{\alpha\beta\gamma}Q_{\gamma}^{(b)},\\ [Q_{\alpha}^{(b)},\hat{N}^{(b)}]=0.\end{gathered} \tag{3.12}$$

Exponentiation of these generators leads to a UR $\mathcal{U}^{(b)}(A)$ acting on $\mathcal{H}^{(b)}$, under which the creation (annihilation) operators $\hat{b}_j^{\dagger}$ ($\hat{b}_j$) transform via the UIR (0,1) ((1,0)):

$$\begin{gathered}\mathcal{U}^{(b)}(A)\hat{b}_j^{\dagger}\mathcal{U}^{(b)}(A)^{-1}=A_j^{k*}\hat{b}_k^{\dagger},\\ \mathcal{U}^{(b)}(A)\hat{b}_j\mathcal{U}^{(b)}(A)^{-1}=A_j^{k}\hat{b}_k.\end{gathered} \tag{3.13}$$

Now this UR of SU(3) contains each of the triangular UIRs $(0,q)$ for $q\geqslant 0$ once each, so it is a generating representation for this family of UIRs. For each $q\geqslant 0$, the UIR $(0,q)$ is realized on that subspace $\mathcal{H}^{(0,q)}$ of $\mathcal{H}^{(b)}$ over which the total number operator $\hat{N}^{(b)}$ takes the eigenvalue q. Analogous to (3.7), the tensor-Fock space connection is now

$$\begin{gathered}\{T_{k_1\cdots k_q}\}\rightarrow|T\rangle=T_{k_1\cdots k_q}\hat{b}_{k_1}^{\dagger}\cdots\hat{b}_{k_q}^{\dagger}|\underline{0}\rangle\in\mathcal{H}^{(0,q)}\subset\mathcal{H}^{(b)},\\ \hat{b}_k|\underline{0}\rangle=0;\\ \mathcal{U}^{(b)}(A)|T\rangle=|T'\rangle,\\ T'_{k_1\cdots k_q}=A_{m_1}^{k_1*}\cdots A_{m_q}^{k_q*}T_{m_1\cdots m_q}.\end{gathered} \tag{3.14}$$

[The use of a common symbol $|\underline{0}\rangle$ for the Fock ground states in $\mathcal{H}^{(a)}$ and $\mathcal{H}^{(b)}$, and $|T\rangle$ in (3.7) and (3.14), should cause no confusion as the meanings are always clear from the context.] In place of (3.8) we now have

$$\mathcal{H}^{(b)}=\sum_{q=0,1,\cdots}^{\infty}\oplus\mathcal{H}^{(0,q)},$$

$$\mathcal{H}^{(0,q)}=\mathrm{Sp}\{\hat{b}_{k_1}^{\dagger}\cdots\hat{b}_{k_q}^{\dagger}|\underline{0}\rangle\}, \tag{3.15}$$

$$\mathcal{U}^{(b)}=\sum_{q=0,1,\cdots}^{\infty}\oplus(0,q).$$

From these considerations it is clear that if we want to obtain all the UIRs (p,q) of SU(3), missing none, the minimal scheme is to use all six independent oscillators $\hat{a}_j$, $\hat{a}_j^{\dagger}$, $\hat{b}_j$, $\hat{b}_j^{\dagger}$ and define the SU(3) generators[13]

$$Q_\alpha=Q_\alpha^{(a)}+Q_\alpha^{(b)}. \tag{3.16}$$

They act on the product Hilbert space $\mathcal{H}=\mathcal{H}^{(a)}\times\mathcal{H}^{(b)}$, of course obey the SU(3) commutation relations, and upon exponentiation lead to the UR $\mathcal{U}(A)=\mathcal{U}^{(a)}(A)\times\mathcal{U}^{(b)}(A)$. However, as we see in a moment, while each UIR (p,q) is certainly present in $\mathcal{U}(A)$, it occurs infinitely many times. A systematic group theoretic procedure to handle this multiplicity, based on the noncompact group $\mathrm{Sp}(2,R)$, will be set up below. The tensor-Fock space connection is now given as follows. To an irreducible tensor $T_{k_1\cdots k_q}^{j_1\cdots j_p}$ which is symmetric and traceless and so "belongs" to the UIR (p,q) we associate the vector $|T\rangle\in\mathcal{H}$ by

$$|T\rangle=T_{k_1\cdots k_q}^{j_1\cdots j_p}\hat{a}_{j_1}^{\dagger}\cdots\hat{a}_{j_p}^{\dagger}\hat{b}_{k_1}^{\dagger}\cdots\hat{b}_{k_q}^{\dagger}|\underline{0},\underline{0}\rangle\in\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}\subset\mathcal{H},$$

$$\hat{a}_j|\underline{0},\underline{0}\rangle=\hat{b}_j|\underline{0},\underline{0}\rangle=0, \tag{3.17}$$

$$\mathcal{U}(A)|T\rangle=|T'\rangle,$$

the components of T' being given by (2.6). While this vector $|T\rangle$ is certainly a simultaneous eigenvector of the two number operators $\hat{N}^{(a)}$, $\hat{N}^{(b)}$ with eigenvalues p, q, respectively, the tracelessness of the tensor $T_{k_1\cdots k_q}^{j_1\cdots j_p}$ implies that (unless at least one of p and q vanishes) we do not get all such independent vectors in $\mathcal{H}$. This aspect is further clarified below. On the other hand, if we drop the tracelessness condition and retain only symmetry, we do span all of $\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$ via (3.17).

The decomposition of $\mathcal{U}(A)$ into UIRs, and the counting of multiplicities, is accomplished by appealing to the Clebsch–Gordan series for the product of two triangular UIRs $(p,0)$ and $(0,q)$:[14]

$$(p,0)\times(0,q)=(p,q)\oplus(p-1,q-1)\oplus(p-2,q-2)\oplus\ldots\oplus(p-r,q-r),\quad r=\min(p,q). \tag{3.18}$$

Therefore, at the Hilbert space level one has the orthogonal subspace decomposition

$$\mathcal{H}=\mathcal{H}^{(a)}\times\mathcal{H}^{(b)}=\left(\sum_{p=0,1,\cdots}^{\infty}\oplus\mathcal{H}^{(p,0)}\right)\times\left(\sum_{q=0,1,\cdots}^{\infty}\oplus\mathcal{H}^{(0,q)}\right)=\sum_{p,q=0,1,\cdots}^{\infty}\oplus\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}, \tag{3.19}$$

$$\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}=\sum_{\rho=0,1,\cdots}^{r}\oplus\mathcal{H}^{(p-\rho,q-\rho;\rho)},\quad r=\min(p,q).$$

Here $\mathcal{H}^{(p-\rho,q-\rho;\rho)}$ is that unique subspace of $\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$ carrying the UIR $(p-\rho,q-\rho)$ present on the right hand side of (3.18). All vectors in $\mathcal{H}^{(p-\rho,q-\rho;\rho)}$ are eigenvectors of $\hat{N}^{(a)}$ and $\hat{N}^{(b)}$ with eigenvalues p and q, respectively; and if the tensor T in (3.17) is assumed traceless, only vectors in $\mathcal{H}^{(p,q;0)}\subset\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$ are obtained on the right in that equation.

Focusing on a given UIR (p,q), we see that it appears once each in $\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)},\mathcal{H}^{(p+1,0)}\times\mathcal{H}^{(0,q+1)},\ldots$, in the respective irreducible subspaces $\mathcal{H}^{(p,q;0)},\mathcal{H}^{(p,q;1)},\ldots$. Thus it is the leading piece in $\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$, the next to the leading piece in $\mathcal{H}^{(p+1,0)}\times\mathcal{H}^{(0,q+1)}$, and so on. Therefore, the decomposition (3.19) of $\mathcal{H}$ can be presented in the alternative manner

$$\mathcal{H}=\sum_{p,q=0,1.\cdots}^{\infty}\ \oplus\ \sum_{\rho=0,1.\cdots}^{\infty}\oplus\mathcal{H}^{(p,q;\rho)},\mathcal{H}^{(p,q;\rho)}\subset\mathcal{H}^{(p+\rho,0)}\times\mathcal{H}^{(0,q+\rho)}, \tag{3.20}$$

each $\mathcal{H}^{(p,q;\rho)}$ carrying the same UIR (p,q). Thus the index ρ is an (orthogonal) multiplicity label with an infinite number of values. For $\rho\neq\rho'$, $\mathcal{H}^{(p,q;\rho')}$ and $\mathcal{H}^{(p,q;\rho)}$ are mutually orthogonal. This is also evident as $\hat{N}^{(a)}=p+\rho'$, $\hat{N}^{(b)}=q+\rho'$ in the former and $\hat{N}^{(a)}=p+\rho$, $\hat{N}^{(b)}=q+\rho$ in the latter.

We now introduce the group Sp(2,R) to handle in a systematic way the multiplicity index ρ. The Hermitian generators of Sp(2,R) and their commutation relations are[15]

$$\begin{gathered}J_0=\tfrac{1}{2}(\hat{N}^{(a)}+\hat{N}^{(b)}+3),\\ K_1=\tfrac{1}{2}(\hat{a}_j^\dagger\hat{b}_j^\dagger+\hat{a}_j\hat{b}_j),\\ K_2=-\frac{i}{2}(\hat{a}_j^\dagger\hat{b}_j^\dagger-\hat{a}_j\hat{b}_j);\end{gathered}\tag{3.21}$$

$$[J_0,K_1]=iK_2,\quad [J_0,K_2]=-iK_1,\quad [K_1,K_2]=-iJ_0.$$

Using the raising and lowering combinations $K_\pm=K_1\pm iK_2$ we have

$$\begin{gathered}K_+=\hat{a}_j^\dagger\hat{b}_j^\dagger,\quad K_-=K_+^\dagger=\hat{a}_j\hat{b}_j;\\ [J_0,K_\pm]=\pm K_\pm,\quad [K_+,K_-]=-2J_0.\end{gathered}\tag{3.22}$$

The significance of this construction is that the two groups SU(3) and Sp(2,R), both acting unitarily on $\mathcal{H}$, commute with one another:

$$[J_0\ \text{ or }\ K_1\ \text{ or }\ K_2,Q_\alpha]=0. \tag{3.23}$$

It is this that helps us handle the multiplicity of occurrences of each SU(3) UIR (p,q) in $\mathcal{H}$:ρ becoming a ''magnetic quantum number'' within a suitable UIR of Sp(2,R).

The family of (infinite dimensional) UIRs of Sp(2,R) relevant here is the positive discrete family $D_k^{(+)}$, labeled by $k=\frac{1}{2},1,\frac{3}{2},2,2\ldots$. (Actually we encounter only $k\geqslant\frac{3}{2}$.) Within the UIR $D_k^{(+)}$ we have an orthonormal basis $|k,m\rangle$ on which the generators act as follows:[16]

$$\begin{gathered}J_0|k,m\rangle=m|k,m\rangle,\quad m=k,k+1,k+2,\ldots,\\ K_\pm|k,m\rangle=\sqrt{(m\pm k)(m\mp k\pm 1)}\,|k,m\pm 1\rangle.\end{gathered}\tag{3.24}$$

From these follow the useful results

$$K_1^2+K_2^2-J_0^2=k(1-k), \tag{3.25a}$$

$$|k,m\rangle = \sqrt{\frac{(2k-1)!}{(m-k)!(m+k-1)!}} K_+^{m-k}|k,k\rangle, \tag{3.25b}$$

$$K_+^{m-k}K_-^{m-k}|k,m\rangle = \frac{(m-k)!(m+k-1)!}{(2k-1)!}|k,m\rangle. \tag{3.25c}$$

Going back to the generators (3.21) it is clear that on all of $\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$, and so on each $\mathcal{H}^{(p-\rho,q-\rho;\rho)}$, J_0 has the eigenvalue $\frac{1}{2}(p+q+3)$; therefore on $\mathcal{H}^{(p,q;\rho)}$ it has the eigenvalue $\frac{1}{2}(p+q+3)+\rho$. It is also clear that action by $K_\pm$ on $\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$ leads to a subspace of $\mathcal{H}^{(p\pm1,0)}\times\mathcal{H}^{(0,q\pm1)}$. Therefore, because of (3.23), we see that $K_\pm$ acting on $\mathcal{H}^{(p,q;\rho)}$ yield $\mathcal{H}^{(p,q;\rho\pm1)}$. Of course $\mathcal{H}^{(p,q;0)}$ is annihilated by K_-.

Reflecting all this we see that an orthonormal basis for $\mathcal{H}$ can be set up labeled as follows:

$$\begin{gathered}|p,q;IMY;m\rangle : p,q=0,1,2,\ldots;\\ m=k,k+1,k+2,\ldots,\\ k=\tfrac{1}{2}(p+q+3);\\ N^{(a)}=p+m-k,\quad N^{(b)}=q+m-k.\end{gathered} \tag{3.26}$$

Since k is determined in terms of p and q, we do not include it as an additional label in the basis kets above. [The ranges for I, M, Y within the SU(3) UIR (p,q) are given in (2.5).] The SU(3) UIR labels p, q determine k and so the associated UIR $D_k^{(+)}$ of Sp(2,R). For fixed p, q as I, M, Y, m vary we get a set of states carrying the UIR $(p,q)\times D_k^{(+)}$ of SU(3)$\times$Sp(2,R). We can now appreciate the following relationships:

$$\mathcal{H}^{(p,q;\rho)} = \mathrm{Sp}\{|p,q;IMY;k+\rho\rangle | IMY \ \text{ varying}\},$$

$$\rho = 0,1,2,\ldots; \tag{3.27a}$$

$$\mathcal{H}^{(p,q;\rho)} = K_+^\rho \mathcal{H}^{(p,q;0)}; \tag{3.27b}$$

$$K_-\mathcal{H}^{(p,q;0)} = 0. \tag{3.27c}$$

Therefore, the null space of K_- within $\mathcal{H}$ is the subspace

$$\mathcal{H}_0 = \sum_{p,q=0,1,\ldots}^{\infty} \oplus \mathcal{H}^{(p,q;0)} = \mathrm{Sp}\{|p,q;IMY;k\rangle | p,q,IMY \ \text{ varying}\}, \tag{3.28}$$

and we see that the UR $\mathcal{U}(A)$ of SU(3) on $\mathcal{H}$ when restricted to $\mathcal{H}_0$ gives a UR $\mathcal{D}_0$ which is multiplicity free and includes every UIR of SU(3). It is thus identical in structure to the induced representation $\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}$ in (2.8b). We see how the use of Sp(2,R) helps us isolate $\mathcal{H}_0$ in a neat manner.

In addition to the subspaces $\mathcal{H}^{(p,q;\rho)}$, $\mathcal{H}_0$ of $\mathcal{H}$ defined above, it is also useful to define the series of mutually orthogonal infinite dimensional subspaces

$$\mathcal{H}^{(p,q)} = \sum_{\rho=0}^{\infty} \oplus \mathcal{H}^{(p,q;\rho)} = \mathrm{Sp}\{|p,q;IMY;m\rangle | IMYm \ \text{ varying}\},$$

$$p,q = 0,1,2,\ldots. \tag{3.29}$$

Thus the infinity of occurrences of the SU(3) UIR (p,q) are collected together in $\mathcal{H}^{(p,q)}$.

In the Appendix we give explicit formulas for the state vectors $|p,q;IMY;m\rangle$ as functions of the operators $\hat{a}_j^\dagger$, $\hat{b}_j^\dagger$ acting on the Fock vacuum $|\underline{0},\underline{0}\rangle$.

IV. THE BARGMANN REPRESENTATION

For some purposes the use of the Bargmann representation of the canonical commutation relations is more convenient than the Fock space description.[17] We outline the definitions of $\mathcal{H}$ and the SU(3) UR $\mathcal{U}(A)=\mathcal{U}^{(a)}(A)\times\mathcal{U}^{(b)}(A)$ in this language, and then turn to the problem of isolating the subspace $\mathcal{H}_0$ in $\mathcal{H}$.

Vectors in $\mathcal{H}$ correspond to entire functions $f(\underline{z},\underline{w})$ in six independent complex variables $\underline{z}=(z_j)$, $\underline{w}=(w_j)$, $j=1,2,3$, with the squared norm defined as

$$\|f\|^2=\int\prod_{j=1}^{3}\left(\frac{d^2z_j}{\pi}\right)\left(\frac{d^2w_j}{\pi}\right)e^{-z^\dagger z-w^\dagger w}|f(\underline{z},\underline{w})|^2. \tag{4.1}$$

Any such $f(\underline{z},\underline{w})$ has a unique Taylor series expansion

$$f(\underline{z},\underline{w})=\sum_{p,q=0,1,\cdots}^{\infty}f^{j_1\cdots j_p}_{k_1\cdots k_q}z_{j_1}\cdots z_{j_p}w_{k_1}\cdots w_{k_q}, \tag{4.2}$$

involving the tensor components $f^{j_1\cdots j_p}_{k_1\cdots k_q}$ separately symmetric in the superscripts and the subscripts. In terms of these the squared norm is

$$\|f\|^2=\sum_{p,q=0,1,\cdots}^{\infty}p!q!f^{j_1\cdots j_p\,*}_{k_1\cdots k_q}f^{j_1\cdots j_p}_{k_1\cdots k_q}. \tag{4.3}$$

The operators $\hat{a}_j$, $\hat{a}_j^\dagger$, $\hat{b}_j$, $\hat{b}_j^\dagger$ act on $f(\underline{z},\underline{w})$ as follows:

$$\hat{a}_j\to\frac{\partial}{\partial z_j},\quad \hat{a}_j^\dagger\to z_j,\quad \hat{b}_j\to\frac{\partial}{\partial w_j},\quad \hat{b}_j^\dagger\to w_j. \tag{4.4}$$

The UR $\mathcal{U}(A)$ of SU(3) acts very simply via point transformations:

$$(\mathcal{U}(A)f)(\underline{z},\underline{w})=f(A^{-1}\underline{z},A^{-1*}\underline{w}). \tag{4.5}$$

The Sp(2,R) generators are particularly simple:

$$\begin{aligned}J_0&=\frac{1}{2}\left(z_j\frac{\partial}{\partial z_j}+w_j\frac{\partial}{\partial w_j}+3\right),\\ K_+&=z_jw_j\equiv\underline{z}\cdot\underline{w},\\ K_-&=\frac{\partial^2}{\partial z_j\partial w_j}\equiv\frac{\partial}{\partial\underline{z}}\cdot\frac{\partial}{\partial\underline{w}}.\end{aligned} \tag{4.6}$$

We will use these below.

It is clear that the terms in (4.2) and (4.3) for fixed p and q are contributions from $\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$. The action by K_+ obeys

$$f(\underline{z},\underline{w})\in\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}\to K_+f(\underline{z},\underline{w})=\underline{z}\cdot\underline{w}f(\underline{z},\underline{w})\in\mathcal{H}^{(p+1,0)}\times\mathcal{H}^{(0,q+1)}. \tag{4.7}$$

On the other hand, action by K_- is the analytic equivalent of taking the trace: starting with (4.2) we get

$$K_-f(\underline{z},\underline{w})=\sum_{p,q=0,1,\cdots}^{\infty} pq f^{jj_1\cdots j_{p-1}}_{jk_1\cdots k_{q-1}} z_{j_1}\cdots z_{j_{p-1}} w_{k_1}\cdots w_{k_{q-1}}. \tag{4.8}$$

From these and earlier remarks we can see that the correspondences between (symmetric, traceless) tensors, entire functions, and subspaces of $\mathcal{H}$ are

$$\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}\leftrightarrow\{f^{j_1\cdots j_p}_{k_1\cdots k_q}\}\leftrightarrow f(\underline{z},\underline{w}):$$
$$f(\lambda\underline{z},\mu\underline{w})=\lambda^p\mu^q f(\underline{z},\underline{w}); \tag{4.9a}$$

$$f(\underline{z},\underline{w})\in\mathcal{H}^{(p,q;\rho)}\Leftrightarrow f(\underline{z},\underline{w})=(\underline{z}\cdot\underline{w})^\rho f_0(\underline{z},\underline{w}), f_0(\underline{z},\underline{w})\in\mathcal{H}^{(p,q;0)}\subset\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)},$$
$$\frac{\partial}{\partial\underline{z}}\cdot\frac{\partial}{\partial\underline{w}}f_0(\underline{z},\underline{w})=0. \tag{4.9b}$$

Thus traceless symmetric tensors of type (p,q) are in correspondence with entire functions $f_0(\underline{z},\underline{w})$ of degrees of homogeneity p and q, respectively, obeying the partial differential equation (4.9b). Alternatively, given any $f(\underline{z},\underline{w})\in\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$, there is a unique "traceless" part $f_0(\underline{z},\underline{w})$ belonging to the leading subspace $\mathcal{H}^{(p,q;0)}$ and annihilated by K_-. Thus "trace removal" can be accomplished by analytical means. We now give the procedure to pass from $f(\underline{z},\underline{w})$ to $f_0(\underline{z},\underline{w})$.

For any $f(\underline{z},\underline{w})\in\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$ we can easily establish the general formula

$$K_-\{(\underline{z}\cdot\underline{w})^nK_-^nf(\underline{z},\underline{w})\}=n(p+q+2-n)(\underline{z}\cdot\underline{w})^{n-1}K_-^nf(\underline{z},\underline{w})+(\underline{z}\cdot\underline{w})^nK_-^{n+1}f(\underline{z},\underline{w}). \tag{4.10}$$

We try for $f_0(\underline{z},\underline{w})$ the expression

$$f_0(\underline{z},\underline{w})=f(\underline{z},\underline{w})-\sum_{n=1,2,\cdots}\alpha_n(\underline{z}\cdot\underline{w})^nK_-^nf(\underline{z},\underline{w}), \tag{4.11}$$

and get, using (4.10) (and omitting the arguments $\underline{z},\underline{w}$),

$$K_-f_0=K_-f-(p+q+1)\alpha_1K_-f-\sum_{n=1,2,\cdots}\{\alpha_n+(n+1)(p+q+1-n)\alpha_{n+1}\}(\underline{z}\cdot\underline{w})^nK_-^{n+1}f. \tag{4.12}$$

We can therefore attain $K_-f_0=0$ by choosing

$$\alpha_n=(-1)^{n-1}\frac{(p+q+1-n)!}{n!(p+q+1)!},\quad n=1,2,\ldots. \tag{4.13}$$

Therefore, for any (bihomogeneous) polynomial $f(\underline{z},\underline{w})\in\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$ the leading traceless part annihilated by K_- is an element $f_0(\underline{z},\underline{w})$ in $\mathcal{H}^{(p,q;0)}$:

$$f_0(\underline{z},\underline{w})=f(\underline{z},\underline{w})-\sum_{n=1,2,\cdots}(-1)^{n-1}\frac{(p+q+1-n)!}{n!(p+q+1)!}(\underline{z}\cdot\underline{w})^nK_-^nf(\underline{z},\underline{w}). \tag{4.14}$$

This result can be extended and expressed in the Fock space language. Any $|\psi\rangle\in\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}$ has a unique orthogonal decomposition into various parts belonging to various UIRs of SU(3); using (3.25c) this reads

$$|\psi\rangle\in\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}=\mathcal{H}^{(p,q;0)}\bigoplus\mathcal{H}^{(p-1,q-1;1)}\bigoplus\mathcal{H}^{(p-2,q-2;2)}\bigoplus\cdots:$$

$$
\begin{aligned}
&|\psi\rangle = |\psi_0\rangle + |\psi_1\rangle + |\psi_2\rangle + \cdots,\\
&|\psi_0\rangle \in \mathcal{H}^{(p,q;0)},\ \ K_-|\psi_0\rangle = 0;\\
&|\psi_1\rangle = K_+|\phi_1\rangle \in \mathcal{H}^{(p-1,q-1;1)},\\
&|\phi_1\rangle = \frac{(p+q)!}{1!(p+q+1)!} K_-|\psi_1\rangle \in \mathcal{H}^{(p-1,q-1;0)},\\
&K_-^2|\psi_1\rangle = 0;\\
&|\psi_2\rangle = K_+^2|\phi_2\rangle \in \mathcal{H}^{(p-2,q-2;2)},\\
&|\phi_2\rangle = \frac{(p+q-2)!}{2!(p+q)!} K_-^2|\psi_2\rangle \in \mathcal{H}^{(p-2,q-2;0)},\\
&K_-^3|\psi_2\rangle = 0;\cdots.
\end{aligned}
\tag{4.15}
$$

The "leading" piece in $|\psi\rangle$ is thus

$$
\begin{aligned}
&|\psi_0\rangle = |\psi\rangle - |\psi_1\rangle - |\psi_2\rangle - \cdots = |\psi\rangle - \hat{\underline{a}}^\dagger \cdot \hat{\underline{b}}^\dagger |\phi\rangle,\\
&|\phi\rangle = |\phi_1\rangle + \hat{\underline{a}}^\dagger \cdot \hat{\underline{b}}^\dagger |\phi_2\rangle + \cdots \in \mathcal{H}^{(p-1,0)} \times \mathcal{H}^{(0,q-1)}.
\end{aligned}
\tag{4.16}
$$

We can now infer that if to begin with we had $|\psi\rangle = \hat{\underline{a}}^\dagger \cdot \hat{\underline{b}}^\dagger |\phi\rangle$ for some $\phi \in \mathcal{H}^{(p-1,0)} \times \mathcal{H}^{(0,q-1)}$, then $|\psi_0\rangle$ necessarily vanishes:

$$
|\psi\rangle = \hat{\underline{a}}^\dagger \cdot \hat{\underline{b}}^\dagger |\phi\rangle \Leftrightarrow |\psi_0\rangle = 0. \tag{4.17}
$$

In the Bargmann description this means in terms of (4.14)

$$
f(\underline{z},\underline{w}) = \underline{z} \cdot \underline{w} g(\underline{z},\underline{w}) \Leftrightarrow f_0(\underline{z},\underline{w}) = 0, \tag{4.18}
$$

a result which can be directly verified with some effort.

The subspace $\mathcal{H}_0 \subset \mathcal{H}$ identified in (3.28) is describable in the Bargmann language as follows:

$$
\mathcal{H}_0 = \left\{ f(\underline{z},\underline{w}) \in \mathcal{H} \left| \frac{\partial}{\partial \underline{z}} \cdot \frac{\partial}{\partial \underline{w}} f(\underline{z},\underline{w}) = 0 \right. \right\}. \tag{4.19}
$$

In the Taylor series expansion (4.2) for such $f(\underline{z},\underline{w})$, the tensors $f^{j_1 \cdots j_p}_{k_1 \cdots k_q}$ are traceless and vice versa. The squared norm and SU(3) action are given for $\mathcal{H}_0$ by (4.3) and (4.5), respectively.

V. THE UR $\mathcal{D}^{(\mathrm{IND},0)}_{\mathrm{SU}(2)}$ OF SU(3)

The Hilbert space $\mathcal{H}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}$ carrying the UR $\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}$ of SU(3) consists of single component (scalar) complex functions on the coset space SU(3)/SU(2). This coset space is the unit sphere in three-dimensional complex space C^3, with the natural norm and SU(3) action. Temporarily omitting the superscript zero and subscript SU(2) for simplicity, we have

$$
\begin{aligned}
&\mathcal{H}^{(\mathrm{ind})} = \left\{ \psi(\underline{\xi}) \in C, \underline{\xi} \in C^3 \left| \|\psi\|^2 = \int \prod_{j=1}^{3} \left(\frac{d^2\xi_j}{\pi} \right) \delta(\underline{\xi}^\dagger \underline{\xi} - 1) |\psi(\underline{\xi})|^2 \right. \right\},\\
&(\mathcal{D}^{(\mathrm{ind})}(A)\psi)(\underline{\xi}) = \psi(A^{-1}\underline{\xi}).
\end{aligned}
\tag{5.1}
$$

Clearly only the values of $\psi(\underline{\xi})$ for $\xi^\dagger\xi=1$ are relevant. For a general $\psi(\underline{\xi})$ with a Taylor series expansion we write

$$\psi(\underline{\xi})=\sum_{p,q=0,1,\cdots}^{\infty}\psi^{j_1\cdots j_p}_{k_1\cdots k_q}\xi_{j_1}\cdots\xi_{j_p}\xi^*_{k_1}\cdots\xi^*_{k_q}. \tag{5.2}$$

[Strictly speaking, such an expansion holds only for $\psi(\underline{\xi})$ in some dense subset of $\mathcal{H}^{(\mathrm{ind})}$.] We note that here $\psi(\underline{\xi})$ is not an entire function of ξ_j, and since $\xi^\dagger\xi=1$, the tensor components $\psi^{j_1\cdots j_p}_{k_1\cdots k_q}$ may be assumed to be traceless apart from being symmetric. Then they determine $\psi(\underline{\xi})$ uniquely and vice versa.

To express the inner product (ϕ,ψ) for general $\phi,\psi\in\mathcal{H}^{(\mathrm{ind})}$ in terms of their tensor components, we need to evaluate

$$I^{k\cdots l\cdots}_{j\cdots m\cdots}=\int\prod_{j=1}^{3}\left(\frac{d^2\xi_j}{\pi}\right)\delta(\xi^\dagger\xi-1)\xi_{j_1}\cdots\xi_{j_p}(\xi_{k_1}\cdots\xi_{k_q})^*(\xi_{l_1}\cdots\xi_{l_{p'}})^*(\xi_{m_1}\cdots\xi_{m_{q'}}), \tag{5.3}$$

for general p, q, p', q' and indices j, k, l, m. Using SU(3) invariance and symmetry, we see that the result must be expressible in terms of products of Kronecker deltas. Combining this with the tracelessness of the tensor components of ϕ and ψ, we can check first that we need only consider the case $p=p'$, $q=q'$, and next that

$$I^{k\cdots l\cdots}_{j\cdots m\cdots}=\mathcal{N}\sum_{P\in S_p}\sum_{Q\in S_q}\delta^{l_{P(1)}}_{j_1}\cdots\delta^{l_{P(p)}}_{j_p}\delta^{k_1}_{m_{Q(1)}}\cdots\delta^{k_q}_{m_{Q(q)}}+\cdots. \tag{5.4}$$

Here $\mathcal{N}$ is a normalizing factor, and the dots denote terms with factors δ^k_j or δ^m_l or both. Again the latter can be ignored. The factor $\mathcal{N}$ can be computed say by setting all $j=l=1$ and all $k=m=2$:

$$\mathcal{N}=\frac{1}{(p+q+2)!}. \tag{5.5}$$

We then get the result for any $\phi,\psi\in\mathcal{H}^{(\mathrm{ind})}$:

$$(\phi,\psi)=\sum_{p,q=0,1,\cdots}\frac{p!q!}{(p+q+2)!}\phi^{j_1\cdots j_p}{}^*_{k_1\cdots k_q}\psi^{j_1\cdots j_p}_{k_1\cdots k_q}. \tag{5.6}$$

With these results, all details of the induced UR $\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}$ of SU(3) are in hand: the Hilbert space $\mathcal{H}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}$ in (5.1), the expression (5.6) for inner products, and the SU(3) action as in (5.1).

VI. EQUIVALENCE MAP

The full equivalence of the two UR's of SU(3), one on the subspace $\mathcal{H}_0\subset\mathcal{H}$ based on the six oscillator Schwinger construction of Sec. III, and the other the induced representation $\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}$, can now be set up. The tensor component expressions (4.2) and (5.2) for vectors, and (4.3) and (5.6) for inner products, determine the one-to-one map to achieve this in full detail:

$$f(\underline{z},\underline{w})=\{f^{j_1\cdots j_p}_{k_1\cdots k_q}\}\in\mathcal{H}_0\leftrightarrow\psi(\underline{\xi})=\{\psi^{j_1\cdots j_p}_{k_1\cdots k_q}\}\in\mathcal{H}^{(\mathrm{ind})}:$$

$$\psi^{j_1\cdots j_p}_{k_1\cdots k_q}=\sqrt{(p+q+2)!}\,f^{j_1\cdots j_p}_{k_1\cdots k_q},p,q=0,1,\ldots. \tag{6.1}$$

The two inner products then match, and the SU(3) actions given in (4.5) and (5.1) on $f(\underline{z},\underline{w})$ and $\psi(\underline{\xi})$ also match.

It is worth emphasizing here the two different arguments leading to the tracelessness of the symmetric tensors on the two sides of (6.1). In the case of the left hand side, the reason is that the argument of $\psi(\underline{\xi})$ obeys the constraint $\underline{\xi}^\dagger\underline{\xi}=1$. As for the right hand side, it happens because entire functions $f(\underline{z},\underline{w})\in\mathcal{H}_0$ obey the partial differential equation in (4.19). In both cases tracelessness leads to the UR being multiplicity free, apart from being complete in the sense that all SU(3) UIR's do appear.

VII. CONCLUDING REMARKS

To conclude, we have brought out the difficulties one encounters in naively extending the Schwinger SU(2) construction to SU(3) particularly if one wishes to retain the simplicity and economy intrinsic to the SU(2) case. We have shown how these difficulties can be overcome by exploiting the group Sp(2,R) to obtain a ''generating representation'' of SU(3) based on six bosonic oscillators. This UR of SU(3) contains all the representations of SU(3) exactly once. (It has been drawn to our attention by the referee that this result of ours is a special case of more general results available in mathematics literature.[18,19]) Further, we have shown how this ''generating representation'' for SU(3) can also be constructed using the theory of induced representations and have constructively established the equivalence between the two by making use of the Bargmann representation. It is hoped that the construction presented here will have useful applications in various branches of physics much the same way as the SU(2) construction has. Indeed, the work presented here has direct relevance to SU(3) coherent states as will be shown in a succeeding publication.

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APPENDIX: BOSON OPERATOR CONSTRUCTION OF $SU(3)\times$Sp(2,R) BASIS STATES

We give here the explicit construction of the orthonormal basis states $|p,q;IMY;m\rangle$ for $\mathcal{H}$ introduced in Eq. (3.26). We deal first with the states $|p,q;IIY;k\rangle\in\mathcal{H}^{(p,q;0)}\subset\mathcal{H}^{(p,q)}\cap\mathcal{H}_0$ having highest SU(2) weight; then by repeated use of the Sp(2,R) raising operator $K_+=\hat{\underline{a}}^\dagger\cdot\hat{\underline{b}}^\dagger$ with $|p,q;IIY;m\rangle\in\mathcal{H}^{(p,q;m-k)}\subset\mathcal{H}^{(p,q)}$; and finally with the general state $|p,q;IMY;m\rangle$ using the SU(2) lowering operator. At each stage the normalization will be ensured.

As is well known, the boson operators $\hat{a}_j^\dagger$, $\hat{b}_j^\dagger$ carry the following U(2) quantum numbers:[11]

$$\begin{array}{cccc} & I & M & Y \\ \hat{a}_1^\dagger,\hat{a}_2^\dagger & \frac{1}{2} & \pm\frac{1}{2} & \frac{1}{3} \\ \hat{a}_3^\dagger & 0 & 0 & -\frac{2}{3} \\ \hat{b}_2^\dagger,-\hat{b}_1^\dagger & \frac{1}{2} & \pm\frac{1}{2} & -\frac{1}{3} \\ \hat{b}_3^\dagger & 0 & 0 & \frac{2}{3} \end{array}. \tag{A1}$$

Therefore, $\hat{a}_\alpha^\dagger\hat{b}_\alpha^\dagger\equiv\hat{a}_1^\dagger\hat{b}_1^\dagger+\hat{a}_2^\dagger\hat{b}_2^\dagger$, $\hat{a}_3^\dagger$ and $\hat{b}_3^\dagger$ are SU(2) scalars. The I-Y multiplets present in the SU(3) UIR (p,q) are listed in Eq. (2.5), and are parametrized by two integers r, s. The state $|p,q;IIY;k\rangle\in\mathcal{H}_0$ involves p factors $\hat{a}^\dagger$ and q factors $\hat{b}^\dagger$ acting on the Fock vacuum $|\underline{0},\underline{0}\rangle$, and in addition it is annihilated by $K_-=\hat{\underline{a}}\cdot\hat{\underline{b}}$. We therefore start with the expression [guided by (A1)]:

$$|p,q;IIY;k\rangle=(\hat{a}_1^\dagger)^r(\hat{b}_2^\dagger)^s\sum_{n=0,1,\ldots}^{(p-r,q-s)_<}C_n(\hat{a}_\alpha^\dagger\hat{b}_\alpha^\dagger)^n(\hat{a}_3^\dagger)^{p-r-n}(\hat{b}_3^\dagger)^{q-s-n}|\underline{0},\underline{0}\rangle,$$
$$r=I+\frac{Y}{2}+\frac{1}{3}(p-q),\quad s=I-\frac{Y}{2}+\frac{1}{3}(q-p). \tag{A2}$$

The condition

$$K_-|p,q;IIY;k\rangle=0 \tag{A3}$$

gives the recursion relation

$$n(r+s+n+1)C_n=-(p-r-n+1)(q-s-n+1)C_{n-1},\quad n=1,2,\ldots, \tag{A4}$$

with the solution

$$C_n=\frac{(-1)^n}{n!}\frac{(p-r)!(q-s)!(r+s+1)!}{(p-r-n)!(q-s-n)!(r+s+n+1)!}C_0,\quad n=1,2,\ldots. \tag{A5}$$

Using this in Eq. (A2), and after some algebra, the normalized state is found to be

$$|p,q;IIY;k\rangle=\mathcal{N}_{pqIY}\frac{(\hat{a}_1^\dagger)^r}{r!}\frac{(\hat{b}_2^\dagger)^s}{s!}\times\sum_{n=0,1,\ldots}^{(p-r,q-s)_<}\frac{(-1)^n}{(r+s+n+1)!}\frac{(\hat{a}_\alpha^\dagger\hat{b}_\alpha^\dagger)^n}{n!}\frac{(\hat{a}_3^\dagger)^{p-r-n}}{(p-r-n)!}\frac{(\hat{b}_3^\dagger)^{q-s-n}}{(q-s-n)!}|\underline{0},\underline{0}\rangle\in\mathcal{H}^{(p,q;0)},$$
$$\mathcal{N}_{pqIY}=\{r!s!(r+s+1)!(p-r)!(q-s)!(p+s+1)!(q+r+1)!/(p+q+1)!\}^{1/2}. \tag{A6}$$

From Eq. (3.27a) we know that vectors in $\mathcal{H}^{(p,q;m-k)}$ for $m>k$ are obtained from vectors in $\mathcal{H}^{(p,q;0)}$ by applying K_+^{m-k}. Further, the normalization is controlled by Eq. (3.25b). We thus obtain

$$|p,q;IIY;m\rangle=\{(2k-1)!/(m-k)!(m+k-1)!\}^{1/2}(\underline{\hat{a}}^\dagger\cdot\underline{\hat{b}}^\dagger)^{m-k}|p,q;IIY;k\rangle\in\mathcal{H}^{(p,q;m-k)}. \tag{A7}$$

The last step is to reach a general value $M\leqslant I$ for the SU(2) magnetic quantum number. For this we apply the SU(2) lowering operator $J_-=\hat{a}_2^\dagger\hat{a}_1-\hat{b}_1^\dagger\hat{b}_2(I-M)$ times to the state (A7), keeping track of normalization. This leads to the result

$$|p,q;IMY;m\rangle=\{(I+M)!/2I!(I-M)!\}^{1/2}(\hat{a}_2^\dagger\hat{a}_1-\hat{b}_1^\dagger\hat{b}_2)^{I-M}|p,q;IIY;m\rangle. \tag{A8}$$

If we combine Eqs. (A6) to (A8) we get the complete expression

$$|p,q;IMY;m\rangle=\mathcal{N}_{pqIY}\{(2k-1)!(I+M)!(I-M)!/(m-k)!(m+k-1)!2I!\}^{1/2}\times(\underline{\hat{a}}^\dagger\cdot\underline{\hat{b}}^\dagger)^{m-k}\sum_{L=0}^{I-M}\sum_{n=0}^{(p-r,q-s)_<}\frac{(-1)^{n+I-M-L}}{(r+s+n+1)!}\cdot\frac{(\hat{a}_\alpha^\dagger\hat{b}_\alpha^\dagger)^n}{n!}\times\frac{(\hat{a}_3^\dagger)^{p-r-n}}{(p-r-n)!}\frac{(\hat{b}_3^\dagger)^{q-s-n}}{(q-s-n)!}\frac{(\hat{a}_1^\dagger)^{r-L}}{(r-L)!}\frac{(\hat{a}_2^\dagger)^L}{L!}\frac{(\hat{b}_2^\dagger)^{s-I+M+L}}{(s-I+M+L)!}\frac{(\hat{b}_1^\dagger)^{I-M-L}}{(I-M-L)!}|\underline{0},\underline{0}\rangle. \tag{A9}$$

We thus have explicit expressions for all the normalized basis states $|p,q;IMY;m\rangle$ of $\mathcal{H}$.

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The Schwinger SU(3) construction. II. Relations between Heisenberg–Weyl and SU(3) coherent states

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The Schwinger oscillator operator representation of SU(3), studied in a previous paper from the representation theory point of view, is analyzed to discuss the intimate relationships between standard oscillator coherent state systems and systems of SU(3) coherent states. Both SU(3) standard coherent states, based on choice of highest weight vector as fiducial vector, and certain other specific systems of generalized coherent states, are found to be relevant. A complete analysis is presented, covering all the oscillator coherent states without exception, and amounting to SU(3) harmonic analysis of these states. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1508811]

I. INTRODUCTION

In a previous paper[1] we have presented an analysis of the reducible unitary representation(UR) of SU(3) that is obtained by a generalization of the well-known Schwinger oscillator operator construction in the case of SU(2).[2] This construction, based on six independent pairs of oscillator operators, is a minimal one in the sense that all unitary irreducible representations (UIRs) of SU(3) are obtained without exception. However, in contrast to the SU(2) case, there is an unavoidable multiplicity in that each UIR occurs a denumerably infinite number of times. A systematic way to handle this multiplicity, based on the use of the noncompact group $\mathrm{Sp}(2,R)$, has been developed; its salient features are recapitulated in the next section.

The aim of the present article is to extend this study and discuss various properties of coherent states in this framework. The use of oscillator operators automatically brings in the Heisenberg–Weyl (H-W) group with a dimension appropriate to the number of independent oscillators or degrees of freedom. And it is indeed in the context of this group that the standard coherent states in quantum mechanics were originally defined and applied to a very large number of problems.[3] On the other hand, the basic kinematic relations for any system of independent oscillator operators have a well-defined covariance group associated with them—a group of linear inhomogeneous transformations on the oscillator operators which leave their commutation relations invariant. The homogeneous part of this covariance group is the metaplectic group of appropriate dimension, containing a unitary group as its maximal compact subgroup. Thus for n oscillators or n canonical pairs of degrees of freedom, we encounter the groups $\mathrm{Mp}(2n)$, $\mathrm{U}(n)$ and $\mathrm{SU}(n)$, and certain of their URs, in a natural way.[4]

Now the original concept of coherent states has been generalized from the H-W case to a general Lie group, and it consists of the orbit of a chosen fiducial vector under group action in any UIR of the group.[5] The usual coherent states arise by the action of the elements of the H-W group on the Fock vacuum. Given all this, it is natural and to be expected that via the Schwinger type construction we have an intricate interplay between the familiar H-W coherent states, and certain

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systems of coherent states associated with the groups $\mathrm{Mp}(2n)$, $\mathrm{U}(n)$ and $\mathrm{SU}(n)$.

In passing we may also mention that with this generalization, even for the H-W group we have not only the originally defined coherent states, which may be called standard coherent states (SCSs), but other systems of generalized coherent states (GCSs).[6] These are based on choices of states other than the Fock vacuum as the fiducial state. Similarly, for the unitary group $\mathrm{SU}(n)$, within any given UIR the SCSs are obtained when the highest weight state is used as the fiducial state, while for other choices we have systems of GCSs.[7] It is therefore of interest to see how these various systems of coherent states for different groups get interconnected via the Schwinger construction. This is the main aim of the present work, in the particular case of the H-W group for six oscillators, and SU(3).

A brief outline of this work is as follows. Our earlier work[1] has shown how in a natural manner we can identify and isolate a subspace $\mathcal{H}_0$ carrying a complete and multiplicity-free UR of SU(3) [a ''generating representation'' for SU(3)], within the full Schwinger representation characterized by infinite multiplicity. As this decomposition, in which the compact generator J_0 of $\mathrm{Sp}(2,R)$ plays a crucial role, provides the starting point of the present work, to set the notation and to make the article reasonably self-contained, we briefly recapitulate the relevant details of Ref. 1 in Sec. II. In Sec. III, we recall the largely familiar interconnections between H-W and U(1) and SU(2) coherent states, to highlight some special features of the Klauder resolution of the identity and its modifications. This helps set the stage for a unified analysis of the relations between the appropriate H-W SCS and SU(3) SCSs and GCSs carried out in detail in Secs. IV–VI. Section IV contains a detailed classification of the orbits of H-W SCSs, under SU(3) action; we identify both generic orbits of maximal dimension, and nongeneric lower order ones. The rest of Sec. IV carries out the SU(3) harmonic analysis of generic orbits lying in the subspace $\mathcal{H}_0$. In Sec. V we examine the remaining generic orbits, lying in subspaces $\mathcal{H}_\kappa$ which are generalizations of $\mathcal{H}_0$ and are labeled by a complex parameter κ. Some calculational details pertaining to this section are put together in an appendix. Section VI contains an analysis of the SU(3) content of a family of H-W SCSs belonging to a nongeneric orbit under SU(3) action. Some concluding remarks are presented in Sec. VII.

II. REVIEW OF SCHWINGER CONSTRUCTION FOR SU(3)

This construction uses six independent sets of oscillator creation and annihilation operators $\hat{a}_j^\dagger, \hat{b}_j^\dagger, \hat{a}_j, \hat{b}_j, j=1,2,3$, among which the only nonvanishing commutators are

$$[\hat{a}_j, \hat{a}_k^\dagger] = [\hat{b}_j, \hat{b}_k^\dagger] = \delta_{jk}, \quad j,k=1,2,3. \tag{2.1}$$

The Hilbert space $\mathcal{H}$ carrying an irreducible representation of these operators is the tensor product $\mathcal{H}=\mathcal{H}^{(a)}\times\mathcal{H}^{(b)}$, where $\mathcal{H}^{(a)}$ and $\mathcal{H}^{(b)}$ are the individual Hilbert spaces carrying irreducible representations of the independent sets $\hat{a}_j, \hat{a}_j^\dagger$ and $\hat{b}_j, \hat{b}_j^\dagger$, respectively. The Schwinger UR of SU(3) acts on $\mathcal{H}$, and its Hermitian generators are[1]

$$\begin{gathered} Q_\alpha = Q_\alpha^{(a)} + Q_\alpha^{(b)}, \\ Q_\alpha^{(a)} = \tfrac{1}{2}\hat{a}^\dagger \lambda_\alpha \hat{a}, \quad Q_\alpha^{(b)} = -\tfrac{1}{2}\hat{b}^\dagger \lambda_\alpha^* \hat{b}, \quad \alpha = 1,2,\ldots,8. \end{gathered} \tag{2.2}$$

Here $\frac{1}{2}\lambda_\alpha$ are the eight Hermitian traceless 3×3 matrices generating the defining UIR (1,0) of SU(3).[8] [For ease in writing, the UIRs of SU(3) will be denoted by (p,q) where $p,q=0,1,2,\ldots$, independently, instead of the more elaborate notation $D^{(p,q)}$.]

The independent mutually commuting generators $Q_\alpha^{(a)}, Q_\alpha^{(b)}$ lead to specific multiplicity-free URs $\mathcal{U}^{(a)}(A), \mathcal{U}^{(b)}(A)$ of SU(3) on $\mathcal{H}^{(a)}, \mathcal{H}^{(b)}$, respectively. Here A is a general matrix in the UIR (1,0). The UR $\mathcal{U}^{(a)}(A)$ is a direct sum of the ''triangular'' UIRs $(p,0)$ of SU(3), for $p=0,1,2,\ldots$, and similarly $\mathcal{U}^{(b)}(A)$ is a direct sum of the conjugate ''triangular'' UIRs $(0,q)$. We indicate this by

$$\mathcal{U}^{(a)}=\sum_{p=0,1,\ldots}^{\infty}\oplus(p,0),$$

$$\mathcal{U}^{(b)}=\sum_{q=0,1,\ldots}^{\infty}\oplus(0,q). \tag{2.3}$$

The total generators Q_α defined in Eq. (2.2) then generate the product UR $\mathcal{U}(A)=\mathcal{U}^{(a)}(A)\times\mathcal{U}^{(b)}(A)$ on $\mathcal{H}$, and this is the Schwinger UR of SU(3). It does contain every UIR (p,q) of SU(3), but each one occurs an infinite number of times. This can be seen from the Clebsch–Gordan decomposition of the direct product $(p,0)\times(0,q)$ of two triangular UIRs:[9]

$$(p,0)\times(0,q)=\sum_{\rho=0,1,\ldots}^{r}\oplus(p-\rho,q-\rho),\quad r=\min(p,q), \tag{2.4}$$

which is multiplicity-free. Applying this to each pair in the product $\mathcal{U}^{(a)}\times\mathcal{U}^{(b)}$ we easily reach the stated conclusion.

An efficient way to handle this infinite multiplicity is based on the use of the semi-simple noncompact Lie group Sp(2,R), more specifically some of its UIRs belonging to the positive discrete class.[10] In the present context the Hermitian Sp(2,R) generators and their commutation relations are

$$J_0=\tfrac{1}{2}(\hat{a}_j^\dagger\hat{a}_j+\hat{b}_j^\dagger\hat{b}_j+3),$$

$$K_1=\tfrac{1}{2}(\hat{a}_j^\dagger\hat{b}_j^\dagger+\hat{a}_j\hat{b}_j), \tag{2.5a}$$

$$K_2=\frac{-i}{2}(\hat{a}_j^\dagger\hat{b}_j^\dagger-\hat{a}_j\hat{b}_j);$$

$$[J_0,K_1]=i\ K_2,\quad [J_0,K_2]=-i\ K_1,\quad [K_1,K_2]=-i\ J_0. \tag{2.5b}$$

The crucial property is that the SU(3) and the Sp(2,R) generators mutually commute:

$$[J_0\ \text{or}\ K_1\ \text{or}\ K_2,\quad Q_\alpha]=0. \tag{2.6}$$

Thus the two URs commute as well, and Sp(2,R) is just large enough to be able to completely lift the degeneracy or multiplicity of SU(3) UIRs. In other words, the UIRs of the product group SU(3)$\times$Sp(2,R) that occur in $\mathcal{H}$ do so in a multiplicity-free manner. This is reflected at the Hilbert space level in the following manner. We first decompose the individual Hilbert spaces $\mathcal{H}^{(a)},\mathcal{H}^{(b)}$ into mutually orthogonal subspaces reflecting the decompositions (2.3):

$$\mathcal{H}^{(a)}=\sum_{p=0,1,\ldots}^{\infty}\oplus\mathcal{H}^{(p,0)},$$

$$\mathcal{H}^{(b)}=\sum_{q=0,1,\ldots}^{\infty}\oplus\mathcal{H}^{(0,q)}. \tag{2.7}$$

The subspace $\mathcal{H}^{(p,0)}\subset\mathcal{H}^{(a)}$ is of dimension $d(p,0)=\frac{1}{2}(p+1)(p+2)$, consists of all eigenvectors in $\mathcal{H}^{(a)}$ of the total a-type number operator $\hat{a}_j^\dagger\hat{a}_j$ with eigenvalue p, and carries the UIR $(p,0)$ of SU(3). Similarly the subspace $\mathcal{H}^{(0,q)}\subset\mathcal{H}^{(b)}$ is of dimension $d(0,q)=\frac{1}{2}(q+1)(q+2)$, consists of all eigenvectors in $\mathcal{H}^{(b)}$ of the total b-type number operator $\hat{b}_j^\dagger\hat{b}_j$ with eigenvalue q, and carries

the UIR $(0,q)$ of SU(3). After forming the direct product $\mathcal{H}^{(a)}\times\mathcal{H}^{(b)}$, using Eq. (2.7) and the Clebsch–Gordan decomposition (2.4), we arrive at an orthogonal subspace decomposition for $\mathcal{H}=\mathcal{H}^{(a)}\times\mathcal{H}^{(b)}$:

$$\mathcal{H}=\sum_{p,q=0,1,\ldots}^{\infty}\oplus\mathcal{H}^{(p,0)}\times\mathcal{H}^{(0,q)}=\sum_{p,q=0,1,\ldots}^{\infty}\sum_{\rho=0,1,\ldots}^{\infty}\oplus\mathcal{H}^{(p,q;\rho)},$$
$$\mathcal{H}^{(p,q;\rho)}\subset\mathcal{H}^{(p+\rho,0)}\times\mathcal{H}^{(0,q+\rho)}. \tag{2.8}$$

For each $\rho,\mathcal{H}^{(p,q;\rho)}$ is of dimension $d(p,q)=\frac{1}{2}(p+1)(q+1)(p+q+2)$ and carries the ρth occurrence of the UIR (p,q) of SU(3). For $\rho'\neq\rho,\mathcal{H}^{(p,q;\rho')}$ and $\mathcal{H}^{(p,q;\rho)}$ are mutually orthogonal subspaces; and if $p'\neq p$ and/or $q'\neq q$, again $\mathcal{H}^{(p',q';\rho)}$ and $\mathcal{H}^{(p,q;\rho)}$ are mutually orthogonal. An orthonormal basis for $\mathcal{H}$ consists of vectors labeled as follows:

$$|p,q;\ I,M,Y;m\rangle:$$
$$p,q=0,1,2,\ldots,$$
$$m=k,k+1,k+2,\ldots,$$
$$k=\tfrac{1}{2}(p+q+3)=\tfrac{3}{2},2,\tfrac{5}{2},\ldots. \tag{2.9}$$

Here I,M,Y are "magnetic quantum numbers" within the UIR (p,q) of SU(3), with well-known ranges,[11] and m is the eigenvalue of the Sp(2,R) generator J_0. The total numbers of a-type quanta and of b-type quanta in the state displayed in Eq. (2.9) are

$$N_a=\text{eigenvalue of } \hat{a}_j^{\dagger}\hat{a}_j=p+m-k,$$
$$N_b=\text{eigenvalue of } \hat{b}_j^{\dagger}\hat{b}_j=q+m-k. \tag{2.10}$$

For fixed p,q and m, as I,M,Y vary within the UIR (p,q) of SU(3), we obtain an orthonormal basis for $\mathcal{H}^{(p,q;m-k)}$. Switching to $\rho=m-k$ we can say

$$\mathcal{H}^{(p,q;\rho)}=\mathrm{Sp}\{|p,q;I,M,Y;k+\rho\rangle|p,q,\rho \text{ fixed},I,M,Y \text{ varying}\}, \tag{2.11}$$

where Sp$\{\cdot\}$ stands for the linear span of the set of vectors $\{\cdot\}$. On the other hand, if we keep p,q,I,M,Y fixed and let m vary, we get an orthonormal basis for a subspace of $\mathcal{H}$ carrying the infinite dimensional positive discrete class UIR $D_k^{(+)}$ of Sp(2,R).[10] In other words, each of these UIRs $D_k^{(+)}$ of Sp(2,R) occurs $d(2k-3,0)+d(2k-4,1)+\cdots+d(1,2k-4)+d(2k-3)$ times, being the sum of the dimensions of the SU(3) UIRs $(2k-3,0),(2k-4,1),\ldots,(1,2k-4),(0,2k-3)$. (The range of $2k$ is 3,4,5,....) Since our main interest is in URs and UIRs of SU(3), and we wish to use UIRs of Sp(2,R) mainly to keep track of the multiplicities of the former, we do not introduce special notations for the subspaces of $\mathcal{H}$ carrying the various Sp(2,R) UIRs. However, we do note that, as stated earlier, each of the UIRs $(p,q)\times D^{(+)}_{(1/2)(p+q+3)}$ of SU(3)$\times$Sp(2,R) appears just once in $\mathcal{H}$, for $p,q=0,1,2,\ldots$.

At the generator level we can say that when the SU(3) generators Q_α act on $|p,q;I,M,Y;m\rangle$, they alter only the quantum numbers I,M,Y in a manner known from the representation theory of SU(3),[12] while the actions by the Sp(2,R) generators J_0,K_1,K_2 lead only to changes in the quantum number m according to the UIR $D_k^{(+)}$.[10]

It is in this manner that the Sp(2,R) structure helps us handle the multiplicity problem of UIRs of SU(3) which is an unavoidable feature of the Schwinger construction. One can now look for a natural subspace of $\mathcal{H},\mathcal{H}_0$ say, such that it carries every UIR (p,q) of SU(3) exactly once. This can be done if we restrict ourselves to the "ground state" within each Sp(2,R) UIR $D_k^{(+)}$, namely

if we set $m=k$. This amounts to picking up the "first" occurrence of each UIR (p,q) of SU(3) corresponding to $\rho=0$, or to the "leading piece" in the reduction of each tensor product $\mathcal{H}^{(p,0)} \times \mathcal{H}^{(0,q)}$:

$$\mathcal{H}_0 = \sum_{p,q=0,1,\ldots}^{\infty} \oplus \mathcal{H}^{(p,q;0)} = \mathrm{Sp}\{|p,q;I,M,Y;k\rangle | p,q,I,M,Y \ \text{ varying}\}$$

$$= \{|\psi\rangle \in \mathcal{H} | (K_1 - iK_2)|\psi\rangle = 0\}. \tag{2.12}$$

The UR of SU(3) carried by $\mathcal{H}_0$, $\mathcal{D}_0$ say, may be called a generating representation for this group, in the sense that each UIR is present, and exactly once:

$$\mathcal{D}_0 = \sum_{p,q=0,1,\ldots}^{\infty} \oplus (p,q). \tag{2.13}$$

It now turns out that just this property is also present in the UR $\mathcal{D}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}$ of SU(3) induced from the trivial one-dimensional UIR of the canonical SU(2) subgroup.[13] The corresponding Hilbert space is denoted by $\mathcal{H}^{(\mathrm{ind},0)}_{\mathrm{SU}(2)}$. [Hereafter, for simplicity, the superscript zero and the subscript SU(2) will be omitted.] We can set up a one-to-one mapping between $\mathcal{H}_0$ and $\mathcal{H}^{(\mathrm{ind})}$ preserving scalar products and SU(3) actions, thus realizing the equivalence of $\mathcal{D}_0$ and $\mathcal{D}^{(\mathrm{ind})}$. First we describe $\mathcal{H}_0$ and $\mathcal{D}_0$ more explicitly. Denote by $|\underline{0},\underline{0}\rangle$ the Fock vacuum in $\mathcal{H}$ annihilated by $\hat{a}_j$ and $\hat{b}_j$, $j=1,2,3$. Then a general vector in $\mathcal{H}_0$ is a collection of symmetric traceless tensors with respect to SU(3), one for each UIR (p,q):

$$|\psi\rangle \in \mathcal{H}_0 :$$

$$|\psi\rangle = \sum_{p,q=0,1,\ldots}^{\infty} \psi^{j_1 \ldots j_p}_{k_1 \ldots k_q} \hat{a}^{\dagger}_{j_1} \ldots \hat{a}^{\dagger}_{j_p} \hat{b}^{\dagger}_{k_1} \ldots \hat{b}^{\dagger}_{k_q} |\underline{0},\underline{0}\rangle; \tag{2.14a}$$

$$\psi^{j_{P(1)} \ldots j_{P(p)}}_{k_{Q(1)} \ldots k_{Q(q)}} = \psi^{j_1 \ldots j_p}_{k_1 \ldots k_q}, \quad P \in S_p, \quad Q \in S_q; \tag{2.14b}$$

$$\psi^{j \ j_2 \ldots j_p}_{j \ k_2 \ldots k_q} = 0, \tag{2.14c}$$

$$\langle \psi | \psi \rangle = \|\psi\|^2 = \sum_{p,q=0,1,\ldots}^{\infty} p!\,q!\, \psi^{j_1 \ldots j_p}_{k_1 \ldots k_q} * \psi^{j_1 \ldots j_p}_{k_1 \ldots k_q}; \tag{2.14d}$$

$$\mathcal{D}_0(A)|\psi\rangle = |\psi'\rangle,$$

$$\psi'^{j_1 \ldots j_p}_{k_1 \ldots k_q} = A^{j_1}{}_{\ell_1} \ldots A^{j_p}{}_{\ell_p} A^{k_1}{}_{m_1} * \ldots A^{k_q}{}_{m_q} * \ldots \psi^{\ell_1 \ldots \ell_p}_{m_1 \ldots m_q}. \tag{2.14e}$$

Here S_p and S_q are the permutation groups on p and on q objects, respectively. Turning to $\mathcal{H}^{(\mathrm{ind})}$ and $\mathcal{D}^{(\mathrm{ind})}$, the former consists of complex square integrable functions on the coset space SU(3)/SU(2), namely the unit sphere in $\mathcal{C}^3$:[14]

$$\mathcal{H}^{(\mathrm{ind})} = \left\{ \psi(\underline{\xi}) \in \mathcal{C}, \underline{\xi} \in \mathcal{C}^3 \,|\, \|\psi\|^2 = \int \prod_{j=1}^{3} \left(\frac{d^2 \xi_j}{\pi} \right) \delta(\underline{\xi}^{\dagger} \underline{\xi} - 1) |\psi(\underline{\xi})|^2 \right\}. \tag{2.15}$$

The group action is by change of argument:

$$\mathcal{D}^{(\mathrm{ind})}(A)\psi = \psi',$$

$$\psi'(\underline{\xi}) = \psi(A^{-1}\underline{\xi}). \tag{2.16}$$

Then the one-to-one mapping between $\mathcal{H}_0$ and $\mathcal{H}^{(\mathrm{ind})}$ consistent with the two norm definitions (2.14d) and (2.15) and the two group actions (2.14e) and (2.16) is

$$|\psi\rangle = \{\psi^{j_1\ldots j_p}_{k_1\ldots k_q}\} \in \mathcal{H}_0 \leftrightarrow$$

$$\psi(\underline{\xi}) = \sum_{p,q=0,1,\ldots}^{\infty} \sqrt{(p+q+2)!}\,\psi^{j_1\ldots j_p}_{k_1\ldots k_q}\xi_{j_1}\ldots\xi_{j_p}\xi^*_{k_1}\ldots\xi^*_{k_q} \in \mathcal{H}^{(\mathrm{ind})}. \tag{2.17}$$

The fact that $\psi(\underline{\xi}) \in \mathcal{H}^{(\mathrm{ind})}$ is expressible in this way in terms of traceless symmetric tensors is a consequence of the constraint $\underline{\xi}^\dagger\underline{\xi} = 1$.

In this way we see how the Schwinger UR $\mathcal{U}(A)$ of SU(3) contains within it a multiplicity-free UR $\mathcal{D}_0$ including every UIR of SU(3), which is also accessible by the method of induced representations. We will see later that in fact there is a continuously infinite family of subspaces $\mathcal{H}_\kappa \subset \mathcal{H}$, labeled by a complex number κ, such that each $\mathcal{H}_\kappa$ is SU(3) invariant and carries a UR $\mathcal{D}_\kappa$ of SU(3) which, like $\mathcal{D}_0$, is multiplicity-free and contains each UIR (p,q) without exception.

III. INTERPLAY BETWEEN HEISENBERG–WEYL AND UNITARY GROUP COHERENT STATES—ONE AND TWO DEGREES OF FREEDOM

We now turn to an examination of the interconnections between H-W coherent states and unitary group coherent states. In each case there are both standard and generalized coherent state systems. In this section we look at the cases of $n=1$ and $n=2$ degrees of freedom, the relevant unitary groups being U(1) and SU(2) and there being no multiplicity problems. We review briefly some known material, but highlight some special aspects. This material is then used as guidance when we take up in the next section the case $n=6$ and the Schwinger SU(3) construction.

A. One degree of freedom

It is convenient to be able to switch between the use of non-Hermitian creation and annihilation operators $\hat{a}^\dagger$, $\hat{a}$ and their Hermitian position and momentum components $\hat{q}$, $\hat{p}$:

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p}), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{p}). \tag{3.1}$$

For one degree of freedom, the canonical commutation relation,

$$\begin{aligned} [\hat{a},\hat{a}^\dagger] &= 1, \\ [\hat{q},\hat{p}] &= i, \end{aligned} \tag{3.2}$$

is preserved under the linear inhomogeneous transformation

$$\begin{aligned} \begin{pmatrix} \hat{q} \\ \hat{p} \end{pmatrix} \to \begin{pmatrix} \hat{q}' \\ \hat{p}' \end{pmatrix} &= S\begin{pmatrix} \hat{q} \\ \hat{p} \end{pmatrix} + \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}; \\ S = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad ad - bc &= 1; \quad q_0, p_0 \in \mathcal{R}. \end{aligned} \tag{3.3}$$

Here S is an element of $\mathrm{Sp}(2,R) = \mathrm{SL}(2,R)$, and these transformations constitute the semi-direct product of $\mathrm{Sp}(2,R)$ with the two-dimensional Abelian group of phase-space translations. However, as is well known, these transformations are realized on the Hilbert space $\mathcal{H}$, on which $\hat{a}^\dagger$, $\hat{a}$ or $\hat{q}$, $\hat{p}$ act irreducibly, by unitary transformations forming a faithful UIR of a group $G^{(1)}$ which is the semi-direct product of the metaplectic group Mp(2) with the H-W group:[15]

$$G^{(1)} = \mathrm{Mp}(2) \times \{\text{H-W group}\}. \tag{3.4}$$

Each factor here is a three parameter Lie group, so $G^{(1)}$ is a six-parameter Lie group. The H-W group is the invariant subgroup; it is non-Abelian because of the nonzero right hand sides in the commutators (3.2). Its generators are $\hat{q}$, $\hat{p}$ and the unit operator on $\mathcal{H}$. The homogeneous part Mp(2) is a double cover of Sp(2,R); its generators are Hermitian quadratic expressions in $\hat{a}^\dagger$ and $\hat{a}$, or in $\hat{q}$ and $\hat{p}$.[16] In particular, the U(1) generator is $\frac{1}{2}(\hat{a}^\dagger\hat{a}+\frac{1}{2})$, and this is the analog of J_0 in the Sp(2,R) Lie algebra (2.5).

As stated above, $\mathcal{H}$ carries a particular UIR of $G^{(1)}$. Upon restriction to the H-W subgroup, this representation remains irreducible; it is the result of exponentiating the well-known unique Stone–von Neumann representation of the commutation relations (3.2).[17] On the other hand, upon restriction to the Mp(2) subgroup, we get a direct sum of two UIRs of the positive discrete class, namely $D^{(+)}_{1/4}$ and $D^{(+)}_{3/4}$.[18] These act on the subspaces $\mathcal{H}^{(\pm)}$ of $\mathcal{H}$ consisting of even/odd parity states or Schrodinger wave functions. The nontrivial H-W generators $\hat{q}$ and $\hat{p}$ intertwine these two UIRs of Mp(2).

With this background, we collect some remarks regarding various systems of coherent states. As both $G^{(1)}$ and the H-W group are represented irreducibly on $\mathcal{H}$, for any choice of a (normalized) fiducial vector $\psi_0 \in \mathcal{H}$ we can build up a family of $G^{(1)}$—GCSs or a family of H-W GCSs.[5] These are the orbits of ψ_0 under $G^{(1)}$ action and under H-W action, respectively, and the latter orbit is a subset of the former. In the case of Mp(2), we can construct systems of GCS separately in $\mathcal{H}^{(+)}$ and in $\mathcal{H}^{(-)}$, associated with any choices of fiducial vectors in these subspaces. Examples are the single mode squeezed coherent states and their variations.[18]

Now let us limit ourselves to H-W coherent states, and to their behaviors under the maximal compact U(1) subgroup of Mp(2). As mentioned earlier, the generator of this U(1) is $\frac{1}{2}(\hat{a}^\dagger\hat{a}+\frac{1}{2})$. However, for simplicity we shall work with

$$\overline{U}(\alpha)=e^{-i\alpha\hat{a}^\dagger\hat{a}}, \quad 0\leqslant\alpha<2\pi. \tag{3.5}$$

Conjugation by $\overline{U}(\alpha)$ has these effects on $\hat{a}$, $\hat{a}^\dagger$, and the unitary phase space displacement operators $D(z)$ which represent elements of the H-W group:

$$\begin{gathered}\overline{U}(\alpha)\hat{a}\overline{U}(\alpha)^{-1}=e^{i\alpha}\hat{a},\\ \overline{U}(\alpha)\hat{a}^\dagger\overline{U}(\alpha)^{-1}=e^{-i\alpha}\hat{a}^\dagger;\\ D(z)=\exp(z\hat{a}^\dagger-z^*\hat{a}),\\ \overline{U}(\alpha)D(z)\overline{U}(\alpha)^{-1}=D(e^{-i\alpha}z).\end{gathered} \tag{3.6}$$

The H-W SCSs correspond to the choice of the Fock vacuum $|0\rangle$ as the fiducial vector:[3]

$$|z\rangle=D(z)|0\rangle, \quad z\in\mathcal{C}. \tag{3.7}$$

Invariance of $|0\rangle$ under $\overline{U}(\alpha)$ action then leads to the behavior

$$\overline{U}(\alpha)|z\rangle=|e^{-i\alpha}z\rangle. \tag{3.8}$$

These states enjoy the well-known Klauder formula for resolution of the identity operator:

$$\int_{\mathcal{C}}\frac{d^2z}{\pi}|z\rangle\langle z|=1 \text{ on } \mathcal{H}. \tag{3.9}$$

This can be viewed as a consequence of the Schur lemma and the square integrability of the Stone–von Neumann UIR of the H-W group,[19] since the uniform integration measure on the complex plane in (3.9) is essentially the invariant measure on the H-W group.

We now examine two variations of these familiar results. By Eq. (3.8), the left hand side of Eq. (3.9) is explicitly U(1)-invariant. We can consider including some nontrivial function $f(z^*z)$ inside the integral, which would maintain U(1) invariance, and define the operator

$$A(f)=\int_{\mathcal{C}}\frac{d^2z}{\pi}f(z^*z)\ \ |z\rangle\langle z|. \tag{3.10}$$

As long as $f(z^*z)$ is not a constant, the integration measure here is no longer the invariant measure on the H-W group, so the Schur lemma is not available. Formally,

$$f(z^*z)\neq \text{const}\Leftrightarrow D(z)A(f)\neq A(f)D(z), \tag{3.11}$$

so there is no reason to expect $A(f)$ to be a multiple of the identity. However, U(1) invariance,

$$\overline{U}(\alpha)A(f)=A(f)\overline{U}(\alpha), \tag{3.12}$$

implies that $A(f)$ is a linear combination of projections on to the various Fock states, and indeed we find

$$A(f)=\sum_{n=0}^{\infty}\int_0^{\infty}dx f(x)x^n e^{-x}\cdot\frac{|n\rangle\langle n|}{n!}. \tag{3.13}$$

Clearly the only choice of f leading to the Klauder formula (3.9) is $f=1$. On the other hand, if we choose $f(z^*z)=\delta(z^*z-r_0^2)$ for some real positive r_0, we are limiting ourselves to a subset of H-W SCSs lying on a circle in the complex plane. This is essentially the U(1) group manifold; and, if $r_0=1$, we have exactly the manifold S^1, that is, we have a U(1)-worth of H-W SCSs. In this case, we find

$$f(x)=\delta(x-r_0^2):$$

$$\begin{aligned}A(f)&=\int\frac{d^2z}{\pi}\delta(z^*z-r_0^2)|z\rangle\langle z|\\&=\int_0^{2\pi}\frac{d\theta}{2\pi}|r_0e^{i\theta}\rangle\langle r_0e^{i\theta}|\\&=\sum_{n=0}^{\infty}e^{-r_0^2}\frac{r_0^{2n}}{n!}|n\rangle\langle n|\\&=e^{-r_0^2}\cdot r_0^{2\hat{N}}/\hat{N}!,\end{aligned} \tag{3.14}$$

$$\hat{N}=\hat{a}^{\dagger}\hat{a}.$$

This means that even though the subset of H-W SCSs $\{|r_0e^{i\theta}\rangle,0\leqslant\theta<2\pi\}$ lying on a circle in the complex plane is "total," [20] and each Fock state $|n\rangle$ can be projected out of this subset as

$$|n\rangle=e^{r_0^2/2}\cdot\sqrt{n!}r_0^{-n}\cdot\int_0^{2\pi}\frac{d\theta}{2\pi}\cdot e^{-in\theta}\cdot|r_0e^{i\theta}\rangle, \tag{3.15}$$

we cannot obtain a Klauder-type resolution of the identity using them. Thus this U(1)-worth of SCSs does not form a system of GCSs in the Klauder sense.

The next variation we consider is replacing the Fock vacuum $|0\rangle$ by a generic unit vector $|\psi_0\rangle\in\mathcal{H}$ as fiducial vector. We then get a family of H-W GCSs:[21]

$$|z;\psi_0\rangle = D(z)|\psi_0\rangle, \quad z \in \mathcal{C}. \tag{3.16}$$

Once again, the Schur lemma leads to the Klauder resolution of the identity,

$$\int \frac{d^2z}{\pi} |z;\psi_0\rangle\langle z;\psi_0| = c.1, \tag{3.17}$$

for some constant c, and square integrability ensures that c is finite. If in the manner of Eq. (3.10) we next define

$$A(f;\psi_0) = \int \frac{d^2z}{\pi} f(z^*z)|z;\psi_0\rangle\langle z;\psi_0|, \tag{3.18}$$

then, on the one hand, we do not expect $A(f;\psi_0)$ to be a multiple of the unit operator since we lose Schur lemma; and, on the other hand, we do not even expect $A(f;\psi_0)$ to commute with $\overline{U}(\alpha)$. That is, in general $A(f;\psi_0)$ is not a linear combination of the projections $|n\rangle\langle n|$ on to the Fock states. The exceptions are when $|\psi_0\rangle$ is an eigenstate of $\hat{a}^\dagger\hat{a}$, i.e., a Fock state $|n_0\rangle$ for some integer n_0. This possibility arises because U(1) is Abelian, and its UIRs are all one-dimensional. In that case we find[22]

$$\begin{gathered}
|\psi_0\rangle = |n_0\rangle: \\
\overline{U}(\alpha)|z;n_0\rangle = e^{-i\alpha n_0}|e^{-i\alpha}z;n_0\rangle, \\
\overline{U}(\alpha)A(f;n_0) = A(f;n_0)\overline{U}(\alpha); \\
A(f;n_0) = \sum_{n=0}^{\infty} C_{n,n_0}(f)|n\rangle\langle n|,
\end{gathered} \tag{3.19}$$

$$C_{n,n_0}(f) = \frac{n_<!}{n_>!}\int_0^\infty dx f(x) x^{|n-n_0|} e^{-x} (L_{n_<}^{|n-n_0|}(x))^2,$$

$$n_> = \max(n,n_0), n_< = \min(n,n_0).$$

When $n_0 = 0$ we recover Eq. (3.13). If we next choose $f(z^*z) = \delta(z^*z - r_0^2)$, thus limiting ourselves to a U(1)-worth of H-W GCSs, we find, in place of Eq. (3.14),

$$\begin{gathered}
f(x) = \delta(x - r_0^2): \\
A(f;n_0) = \int \frac{d^2z}{\pi} \delta(z^*z - r_0^2)|z;n_0\rangle\langle z;n_0| \\
= \int_0^{2\pi} \frac{d\theta}{2\pi} |r_0 e^{i\theta};n_0\rangle\langle r_0 e^{i\theta};n_0| \\
= \sum_{n=0}^{\infty} e^{-r_0^2} r_0^{2n} (L_{n_<}^{|n-n_0|}(r_0^2))^2 \frac{n_<!}{n_>!} |n\rangle\langle n|.
\end{gathered} \tag{3.20}$$

The main result of these considerations is that with SCSs or GCSs for the H-W group for one degree of freedom, we can get a Klauder-type resolution of the identity only if we use the invariant measure on the group, but understandably not if we limit ourselves to a subset amounting to a U(1)-worth of these states.

B. Two degrees of freedom

Here we are interested in the interplay between coherent state systems for the relevant five-parameter H-W group, and the unitary groups U(2) and SU(2) which were the subject of the original Schwinger construction.

The nonvanishing commutators in non-Hermitian and Hermitian forms are

$$[\hat{a}_r,\hat{a}_s^\dagger]=\delta_{rs},$$
$$[\hat{q}_r,\hat{p}_s]=i\delta_{rs},\quad r,s=1,2. \tag{3.21}$$

There is no cause for confusion if again we write $\mathcal{H}$ for the Hilbert space carrying the irreducible Stone–von Neumann representation of these relations. The largest natural invariance group now acts on the four $\hat{q}$'s and $\hat{p}$'s as follows:

$$\begin{pmatrix}\hat{q}_r\\ \hat{p}_r\end{pmatrix}\to\begin{pmatrix}\hat{q}_r'\\ \hat{p}_r'\end{pmatrix}=S\begin{pmatrix}\hat{q}_r\\ \hat{p}_r\end{pmatrix}+\begin{pmatrix}q_{r,0}\\ p_{r,0}\end{pmatrix}. \tag{3.22}$$

Here $S\in \mathrm{Sp}(4,R)$ is a four-dimensional real symplectic matrix, and $q_{r,0},p_{r,0}$ denote an Abelian phase space translation.[23] These 14 parameter transformations preserve (3.21). They make up the semi-direct product of $\mathrm{Sp}(4,R)$, which is ten-dimensional, with the four-dimensional Abelian translations. On the space $\mathcal{H}$, however, these transformations are realized as a faithful UIR of the fifteen-parameter semi-direct product

$$G^{(2)}=\mathrm{Mp}(4)\times\{\text{H-W group}\}. \tag{3.23}$$

Here the invariant subgroup is the five-parameter non-Abelian H-W group appropriate for two degrees of freedom, while the homogeneous part is the metaplectic group Mp(4), a double cover of $\mathrm{Sp}(4,R)$. The generators of the former are $\hat{q}_r,\hat{p}_r$ and the unit operator, while those of the latter are Hermitian symmetrized quadratics in $\hat{q}_r,\hat{p}_r$.

The Hilbert space $\mathcal{H}$ carries a UIR of $G^{(2)}$, which remains irreducible when restricted to the H-W group. On the other hand, Mp(4) is represented by the direct sum of two UIRs, one each on the subspaces of even and odd parity states in $\mathcal{H}$. The general statements that can be made about GCS with respect to $G^{(2)}$, Mp(4) and the H-W group are similar to those in the one degree of freedom case. Once again, our main interest is in the connections between H-W and SU(2) coherent state systems.

The maximal compact subgroup of Mp(4) is U(2). The SU(2) part of U(2) has the generators and commutation relations (Schwinger construction)

$$J_j=\tfrac{1}{2}\hat{a}^\dagger\sigma_j\hat{a},$$
$$[J_j,J_k]=i\ \epsilon_{jk\not j}J_{\not j},\quad j,k=1,2,3. \tag{3.24}$$

The U(1) part of U(2) has as generator the total number operator

$$\hat{N}=\hat{N}_1+\hat{N}_2,$$
$$\hat{N}_r=\hat{a}_r^\dagger\hat{a}_r, \tag{3.25}$$
$$[J_j,\hat{N}]=0.$$

For general $u\in \mathrm{U}(2)$, we write $\overline{\mathrm{U}}(u)$ for the corresponding unitary operator on $\mathcal{H}$, generated by $J_j,\hat{N}$. Then, in place of Eq. (3.6), we now have

$$\begin{aligned}
&\overline{\mathrm{U}}(u)\hat{a}\overline{\mathrm{U}}(u)^{-1}=u^{-1}\hat{a},\\
&\overline{\mathrm{U}}(u)\hat{a}^{\dagger}\overline{\mathrm{U}}(u)^{-1}=\hat{a}^{\dagger}u;\\
&D(\underline{z})=\exp(\hat{a}^{\dagger}\underline{z}-\underline{z}^{\dagger}\hat{a}),\\
&\overline{\mathrm{U}}(u)D(\underline{z})\overline{\mathrm{U}}(u)^{-1}=D(u\underline{z}).
\end{aligned} \tag{3.26}$$

Here $\underline{z}=(z_1,z_2)^T$ is a complex two-component column vector, while $\hat{a}$ and $\hat{a}^{\dagger}$ are written as column and row vectors, respectively.

The reduction of $\overline{\mathrm{U}}(u)$ into UIRs is accomplished by the break-up of $\mathcal{H}$ into the mutually orthogonal eigenspaces $\mathcal{H}^{(j)}$ of $\hat{N}$ with eigenvalues $2j$, where $j=0,\frac{1}{2},1,\ldots$. The orthonormal Fock basis for $\mathcal{H}$ is made up of the simultaneous eigenvectors of $\hat{N}_1$ and $\hat{N}_2$:

$$\begin{aligned}
&|n_1,n_2\rangle=\frac{(\hat{a}_1^{\dagger})^{n_1}(\hat{a}_2^{\dagger})^{n_2}}{\sqrt{n_1!n_2!}}|0,0\rangle,\\
&\hat{N}_r|n_1,n_2\rangle=n_r|n_1,n_2\rangle,\quad r=1,2.
\end{aligned} \tag{3.27}$$

For the purposes of reduction of $\overline{\mathrm{U}}$, with no danger of confusion we use vectors labeled $|j,m\rangle$ and defined in terms of these Fock states by

$$\begin{aligned}
&|j,m\rangle=|n_1,n_2\rangle,\\
&n_1=\tfrac{1}{2}(j+m),\quad n_2=\tfrac{1}{2}(j-m),\\
&j=0,\tfrac{1}{2},1,\ldots,\quad m=j,j-1,\ldots,-j.
\end{aligned} \tag{3.28}$$

Then the subspaces $\mathcal{H}^{(j)}$ are given by

$$\begin{aligned}
&\mathcal{H}^{(j)}=\mathrm{Sp}\{|j,m\rangle|j\ \text{ fixed},\quad m=j,j-1,\ldots,-j\},\\
&j=0,\tfrac{1}{2},1,\ldots.
\end{aligned} \tag{3.29}$$

The operators $\overline{\mathrm{U}}(u)$ leave each $\mathcal{H}^{(j)}$, of dimension $(2j+1)$, invariant, and reduce thereon to the spin j UIR of SU(2), along with the value $2j$ for the U(1) generator $\hat{N}$. This is the known multiplicity-free reduction of the SU(2) Schwinger construction.[2] The projection operator P_j onto the subspace $\mathcal{H}^{(j)}$, which will be needed later, is

$$P_j=\sum_{m=-j}^{+j}|j,m\rangle\langle j,m|=\delta_{\hat{N},2j}\,. \tag{3.30}$$

The H-W SCSs use the Fock vacuum $|0,0\rangle$ as the fiducial vector:

$$|\underline{z}\rangle=D(\underline{z})|0,0\rangle, \tag{3.31}$$

and, on account of Eq. (3.26), they have the U(2) behavior

$$\overline{\mathrm{U}}(u)|\underline{z}\rangle=|u\underline{z}\rangle. \tag{3.32}$$

This is because $|0,0\rangle$ is invariant under U(2) action; in fact, it is the only such vector in $\mathcal{H}$. Therefore, the general H-W SCS $|\underline{z}\rangle$ is obtainable by suitable U(2) action from a SCS for the first degree of freedom alone:

$$|\underline{z}\rangle = \overline{\mathrm{U}}(u)|\underline{z}^{(0)}\rangle, \quad \text{suitable } u \in \mathrm{U}(2),$$

$$\underline{z}^{(0)} = r\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{3.33}$$

$$r^2 = \underline{z}^\dagger \underline{z}, \quad 0 \leqslant r < \infty.$$

To bring out the connection between these H-W SCSs and SU(2) SCSs (identified below) in the clearest possible manner, we parametrize $\underline{z}$ and define elements $A(\theta,\phi) \in \mathrm{SU}(2)$ in a coordinated manner:

$$\underline{z} = e^{i\alpha} A(\theta,\phi)\underline{z}^{(0)},$$

$$A(\theta,\phi) = e^{(-i/2)\,\phi\sigma_3} e^{(-i/2)\,\theta\sigma_2} \in \mathrm{SU}(2),$$

$$0 \leqslant \theta \leqslant \pi, \quad 0 \leqslant \alpha, \quad \phi \leqslant 2\pi; \tag{3.34}$$

$$z_1 = r\ \ e^{i\alpha} e^{-i\phi/2} \cos\theta/2, \quad z_2 = r\ \ e^{i\alpha} e^{i\phi/2} \sin\theta/2.$$

We view θ, ϕ as spherical polar angles on S^2. Then Eq. (3.33) assumes the more detailed form

$$|\underline{z}\rangle = e^{i\alpha\hat{N}} \overline{\mathrm{U}}(A(\theta,\phi))|\underline{z}^{(0)}\rangle,$$

$$|\underline{z}^{(0)}\rangle = e^{r(\hat{a}_1^\dagger - \hat{a}_1)}|0,0\rangle = e^{-(1/2)r^2} \sum_{j=0,1/2,1,\ldots}^{\infty} \frac{r^{2j}}{\sqrt{2j!}}|j,j\rangle. \tag{3.35}$$

The component of $|\underline{z}^{(0)}\rangle$ within $\mathcal{H}^{(j)}$ is a multiple of $|j,j\rangle$, the highest weight vector in the spin j UIR of SU(2). By definition, the SU(2) SCSs in any UIR are based on the choice of highest weight vector [or any SU(2) transform of it] as fiducial vector.[24] This vector is the eigenvector of J_3 with maximum eigenvalue j, so any SU(2) transform of it is an eigenvector of a suitable combination of J_k with the same (maximum) eigenvalue. These remarks lead to the following notations for SU(2) SCS:

$$\overline{\mathrm{U}}(A(\theta,\phi))|j,j\rangle \equiv |j,\hat{n}(\theta,\phi)\rangle = \sum_{m=-j}^{j} \sqrt{\frac{2j!}{(j+m)!(j-m)!}}\, e^{-im\phi} (\cos\theta/2)^{j+m} (\sin\theta/2)^{j-m} |j,m\rangle,$$

$$\hat{n}(\theta,\phi)\cdot\vec{J}|j,\hat{n}(\theta,\phi)\rangle = j|j,\hat{n}(\theta,\phi)\rangle, \tag{3.36}$$

$$\hat{n}(\theta,\phi) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) = \frac{1}{r^2}\underline{z}^\dagger \underline{\sigma}\underline{z} \in S^2.$$

Thus the family of SU(2) SCSs in the spin j UIR is $\{|j,\hat{n}(\theta,\phi)\rangle\}$, one for each point on S^2 which is the coset space SU(2)/U(1). For these states we have the well-known properties

$$\langle j,\hat{n}(\theta',\phi')|j,\hat{n}(\theta,\phi)\rangle = (\cos\theta'/2\cos\theta/2 e^{i(\phi'-\phi)/2} + \sin\theta'/2\sin\theta/2 e^{i(\phi-\phi')/2})^{2j}, \tag{3.37a}$$

$$A \in \mathrm{SU}(2): \overline{\mathrm{U}}(A)|j,\hat{n}\rangle = e^{i\omega(A;\hat{n})}|j, \quad R(A)\hat{n}\rangle, \tag{3.37b}$$

where $R(A) \in \mathrm{SO}(3)$ is the image of $A \in \mathrm{SU}(2)$ under the $\mathrm{SU}(2) \to \mathrm{SO}(3)$ homomorphism, and $\omega(A;\hat{n})$ is a (Wigner) phase angle.[25] Combining Eqs. (3.35) and (3.36) we get the connection between H-W and SU(2) SCSs:

$$|\underline{z}\rangle = e^{-(1/2)r^2} \sum_{j=0,1/2,1,\ldots}^{\infty} \frac{(r\ e^{i\alpha})^{2j}}{\sqrt{2j!}} |j,\hat{n}(\theta,\phi)\rangle. \tag{3.38}$$

We trace this direct connection to the simple U(2) action (3.32), and the expansion (3.35) of $|\underline{z}^{(0)}\rangle$ in terms of SU(2) highest weight states.

We now look at the Klauder resolution of unity for the H-W SCS, highlighting the SU(2) SCS structure. Using the parametrization (3.34) for $\underline{z}$ we find

$$\begin{aligned}\int \frac{d^2z_1}{\pi}\frac{d^2z_2}{\pi}|\underline{z}\rangle\langle\underline{z}| &= \frac{1}{4\pi^2}\int_0^\infty r^3dr\int_0^{2\pi}d\alpha\int_{S^2}d\Omega(\theta,\phi)|\underline{z}\rangle\langle\underline{z}| \\ &= \frac{1}{4\pi^2}\int r^3drd\alpha d\Omega(\theta,\phi)\sum_{j,j'=0,1/2,1,\ldots}^{\infty} e^{-r^2}r^{2(j+j')}e^{2i\alpha(j-j')} \\ &\quad\times|j,\hat{n}(\theta,\phi)\rangle\langle j',\hat{n}(\theta,\phi)|/\sqrt{2j!2j'!} \\ &= \frac{1}{2\pi}\sum_{j=0,1/2,1,\ldots}^{\infty}\frac{1}{2j!}\int_0^\infty r^3dre^{-r^2}r^{4j}\int_{S^2}d\Omega(\theta,\phi)|j,\hat{n}(\theta,\phi)\rangle\langle j,\hat{n}(\theta,\phi)|.\end{aligned} \tag{3.39}$$

Here $d\Omega(\theta,\phi)$ is the element of solid angle on S^2. Using Eq. (3.37b) we see that the integral over S^2 results in an operator invariant under the spin j UIR of SU(2) appearing on $\mathcal{H}^{(j)}$, therefore by Schur lemma for this UIR we have

$$\int_{S^2}d\Omega(\theta,\phi)|j,\hat{n}(\theta,\phi)\rangle\langle j,\hat{n}(\theta,\phi)| = \frac{4\pi}{2j+1}P_j. \tag{3.40}$$

Substituting this in Eq. (3.39) we get

$$\int \frac{d^2z_1}{\pi}\frac{d^2z_2}{\pi}|\underline{z}\rangle\langle\underline{z}| = 2\sum_{j=0,1/2,1,\ldots}^{\infty}\frac{1}{(2j+1)!}\int_0^\infty r^3dre^{-r^2}\cdot r^{4j}\cdot P_j = \sum_{j=0,1/2,1,\ldots}^{\infty}P_j = 1 \ \text{ on } \ \mathcal{H}. \tag{3.41}$$

This is known and expected on account of the Schur lemma for the H-W UIR, since the integration measure is the invariant one on the H-W group. At the same time we can immediately trace the consequences of modifying the measure in a U(2)-invariant way, when we lose the possibility of using the lemma for the H-W UIR:

$$A(f) = \int \frac{d^2z_1}{\pi}\frac{d^2z_2}{\pi}f(\underline{z}^\dagger\underline{z})|\underline{z}\rangle\langle\underline{z}| = \sum_{j=0,1/2,1,\ldots}^{\infty}\int_0^\infty dxf(x)x^{2j+1}e^{-x}\frac{P_j}{(2j+1)!}, \tag{3.42}$$

$$f \neq \text{const} \Leftrightarrow D(\underline{z})A(f) \neq A(f)D(\underline{z}).$$

With the particular choice $f(x) = \delta(x - r_0^2)$ for real positive r_0, we limit ourselves to an ''SU(2)-worth'' of H-W SCS, and in that case we have

$$f(x)=\delta(x-r_0^2):$$

$$A(f)=\int \frac{d^2z_1}{\pi}\frac{d^2z_2}{\pi}\,\delta(\underline{z}^\dagger\underline{z}-r_0^2)|\underline{z}\rangle\langle\underline{z}|$$

$$=r_0^2\int_0^{2\pi}\frac{d\alpha}{2\pi}\cdot\int_{S^2}\frac{d\Omega(\theta,\phi)}{4\pi}\cdot\left|e^{i\alpha}A(\theta,\phi)\begin{pmatrix}r_0\\0\end{pmatrix}\right\rangle\left\langle e^{i\alpha}A(\theta,\phi)\begin{pmatrix}r_0\\0\end{pmatrix}\right|$$

$$=\sum_{j=0,1/2,1,\ldots}^{\infty}e^{-r_0^2}\cdot\frac{(r_0^2)^{2j+1}}{(2j+1)!}P_j\,. \tag{3.43}$$

The structure of these results (3.42) and (3.43) is as expected since $A(f)$ does commute with $\overline{\mathrm{U}}(u)$.

Lastly we consider briefly some aspects of H-W GCS in the case of two degrees of freedom. These arise by replacing the Fock vacuum $|0,0\rangle$ by some other (normalized) vector $|\psi_0\rangle\in\mathcal{H}$ as fiducial vector:

$$|\underline{z};\psi_0\rangle=D(\underline{z})|\psi_0\rangle. \tag{3.44}$$

The Schur lemma and square integrability of the H-W UIR ensure the Klauder formula

$$\int\frac{d^2z_1}{\pi}\frac{d^2z_2}{\pi}|\underline{z};\psi_0\rangle\langle\underline{z};\psi_0|=c.1, \tag{3.45}$$

for some finite constant c. However, if $|\psi_0\rangle\neq|0,0\rangle$, we never have any simple behavior for these GCSs under U(2) action. This is in contrast to Eq. (3.19) in the case of one degree of freedom. The reason is that the only one-dimensional UIR of SU(2) is the trivial UIR, all others are of dimension two or greater. This can be traced to the non-Abelian nature of SU(2), in contrast to U(1). For this reason we are unable to obtain $|\underline{z};\psi_0\rangle$ for general $\underline{z}$ from some specially chosen and simpler state $|\underline{z}^{(0)};\psi_0\rangle$ via U(2) action; so, the possibility of relating H-W GCS to some sequence of SU(2) GCSs within each subspace $\mathcal{H}^{(j)}$ is also lost. Going one step further, if we consider a modified U(2)-invariant measure in place of the translation invariant one in Eq. (3.45), but for a GCS system, and if we define

$$A(f;\psi_0)=\int\frac{d^2z_1}{\pi}\frac{d^2z_2}{\pi}f(\underline{z}^\dagger\underline{z})|\underline{z};\psi_0\rangle\langle\underline{z};\psi_0|, \tag{3.46}$$

for $|\psi_0\rangle\neq|0,0\rangle$, this will not commute with $\overline{\mathrm{U}}(u)$ and will not reduce to a linear combination of the projections P_j.

IV. RELATION BETWEEN H-W AND SU(3) SCS, RESTRICTION TO $\mathcal{H}_0$

Now that we have explored the relationships between H-W SCS and unitary group SCS for one and two degrees of freedom, we proceed to the SU(3) Schwinger construction recalled in Sec. II, and the corresponding H-W SCS for six oscillators. Here we invert the order of development as compared to the previous section. We recall first the definition of SU(3) SCS within each UIR, then proceed to the H-W system. The specific new feature is the multiplicity problem, to be handled using $\mathrm{Sp}(2,R)$.

A. SU(3) standard coherent states

The familiar orthonormal basis states within the UIR (p,q) of SU(3), corresponding to the canonical subgroup chain $\mathrm{U}(1)\subset\mathrm{U}(2)\subset\mathrm{SU}(3)$, consist of a set of isospin-hypercharge multiplets [cf. Eqs. (2.9) and (2.11)]:[26]

$$
\begin{gathered}
|p,q;IMY\rangle, \\
I=\tfrac{1}{2}(r+s), \quad Y=\tfrac{2}{3}(q-p)+r-s, \\
M=I,I-1,\ldots, \quad -I+1,-I, \\
0\leqslant r\leqslant p, \quad 0\leqslant s\leqslant q.
\end{gathered}
\tag{4.1}
$$

The highest weight state is the one with maximum possible value of M:

$$
|p,q;\tfrac{1}{2}(p+q),\ \tfrac{1}{2}(p+q),\ \tfrac{1}{3}(p-q)\rangle. \tag{4.2}
$$

In terms of the realization of the UIR (p,q) via irreducible tensors $T=\{T^{j_1\cdots j_p}_{k_1\cdots k_q}\}$, this state corresponds to the component

$$
T^{11\ldots1}_{22\ldots2}. \tag{4.3}
$$

From this one can see that the stability group (upto phase factors) of the state (4.2) is a subgroup $H\subset \mathrm{SU}(3)$ dependent on p and q. Disregarding the trivial UIR (0,0), we have

$$
p\geqslant 1, q=0: H=\mathrm{U}(2) \ \text{ on dimensions } \ 2,3; \tag{4.4a}
$$

$$
p=0, q\geqslant 1: H=\mathrm{U}(2) \ \text{ on dimensions } \ 1,3; \tag{4.4b}
$$

$$
p,q\geqslant 1: H=\text{diagonal subgroup of } \mathrm{SU}(3)\,. \tag{4.4c}
$$

[Here the dimensions 1,2,3 refer to the space of the defining UIR (1,0).] In Eq. (4.4a) [Eq. (4.4b)], a U(2) transformation on dimensions 2 and 3 (1 and 3) is to be accompanied by a phase change in dimension 1(2) to preserve unimodularity of the SU(3) transformation. The dimensionalities of these three stability groups are four, four and two, respectively.

The SU(3) SCSs within the UIR (p,q) are the states obtained by acting with all SU(3) elements on the highest weight state (4.2). They may be written as $|p,q;A\rangle$, $A\in \mathrm{SU}(3)$:

$$
|p,q;A\rangle=\overline{\mathrm{U}}(A)|p,q;\tfrac{1}{2}(p+q),\tfrac{1}{2}(p+q),\tfrac{1}{3}(p-q)\rangle. \tag{4.5}
$$

Therefore in the UIRs $(p,0)$ and $(0,q)$, they form four-parameter continuous families of normalized states, while in (p,q) with $p,q\geqslant 1$ we have six-parameter continuous families. Referring to Eq. (4.4) we have

$$
h\in \ H: |p,q;Ah\rangle=e^{i\varphi(h)}|p,q;A\rangle, \tag{4.6}
$$

for some phase $\varphi(h)$.

These SU(3) SCSs have been studied in detail in Ref. 27, individually within each UIR. As we see below, the Schwinger construction helps us generate them collectively and explore some of their properties in an efficient manner, just as in Eq. (3.38) we have a construction of the SU(2) SCS in all its UIRs at one stroke.

If within the UIR (p,q) we choose as fiducial vector some vector other than the highest weight vector (4.2) or any SU(3) transform of it, then we obtain a family of SU(3) GCSs. For the present we consider only SCSs, turning to particular GCSs in subsequent sections.

In the Hilbert space $\mathcal{H}$ of the SU(3) Schwinger construction the ''first'' occurrence of the UIR (p,q) is in the subspace $\mathcal{H}^{(p,q;0)}\subset\mathcal{H}_0$ which is annihilated by K_-. The corresponding highest weight state (4.2), using the complete notation of Eq. (2.9) and recalling Eq. (4.3), is

$$|p,q;\tfrac{1}{2}(p+q),\tfrac{1}{2}(p+q),\tfrac{1}{3}(p-q);\tfrac{1}{2}(p+q+3)\rangle=\frac{(\hat{a}_1^\dagger)^p(\hat{b}_2^\dagger)^q}{\sqrt{p!q!}}|\underline{0},\underline{0}\rangle\in\mathcal{H}^{(p,q;0)}\subset\mathcal{H}_0. \quad (4.7)$$

It follows that all these highest weight states, one for each UIR (p,q), are generated by the special H-W SCS

$$|z_1,0,0;0,w_2,0\rangle=D(z_1,0,0,0,w_2,0)|\underline{0},\underline{0}\rangle\in\mathcal{H}_0,$$

$$D(\underline{z},\underline{w})=\exp(\underline{z}\cdot\hat{\underline{a}}^\dagger-\underline{z}^*\cdot\hat{\underline{a}}+\underline{w}\cdot\hat{\underline{b}}^\dagger-\underline{w}^*\cdot\hat{\underline{b}})=\exp(-\tfrac{1}{2}\underline{z}^\dagger\underline{z}-\tfrac{1}{2}\underline{w}^\dagger\underline{w}+\underline{z}\cdot\hat{\underline{a}}^\dagger+\underline{w}\cdot\hat{\underline{b}}^\dagger). \quad (4.8)$$

Here $\underline{z}$ and $\underline{w}$ are independent complex three-vectors, and $D(\underline{z},\underline{w})$ are the displacement operators for the six-oscillator system of the Schwinger construction. Indeed we have:

$$|z_1,0,0;0,w_2,0\rangle=e^{-(1/2)|z_1|^2-(1/2)|w_2|^2}\sum_{p,q=0}^{\infty}\frac{z_1^p w_2^q}{\sqrt{p!q!}}$$
$$\times|p,q;\tfrac{1}{2}(p+q),\tfrac{1}{2}(p+q),\tfrac{1}{3}(p-q);\tfrac{1}{2}(p+q+3)\rangle, \quad (4.9)$$

which is analogous to the second of Eqs. (3.35). We will use this below.

B. SU(3) analysis of the H-W SCS

For the six-oscillator system used in the Schwinger SU(3) construction the H-W SCSs are labeled by two complex three-dimensional vectors $\underline{z}$ and $\underline{w}$, thus the pair $(\underline{z},\underline{w})$ is a point in $\mathcal{C}^6$. They are obtained by applying the displacement operators $D(\underline{z},\underline{w})$ to the Fock vacuum $|\underline{0},\underline{0}\rangle$ as fiducial vector:

$$|\underline{z},\underline{w}\rangle=D(\underline{z},\underline{w})|\underline{0},\underline{0}\rangle. \quad (4.10)$$

We see from Eq. (2.5) that they are eigenstates of the Sp(2,R) lowering operator $K_-=K_1-iK_2$:

$$\hat{a}_j|\underline{z},\underline{w}\rangle=z_j|\underline{z},\underline{w}\rangle,$$
$$\hat{b}_j|\underline{z},\underline{w}\rangle=w_j|\underline{z},\underline{w}\rangle, \quad (4.11)$$
$$K_-|\underline{z},\underline{w}\rangle=\underline{z}^T\underline{w}|\underline{z},\underline{w}\rangle.$$

Therefore only those SCSs $|\underline{z},\underline{w}\rangle$ for which $\underline{z}^T\underline{w}=0$ belong to $\mathcal{H}_0$. The complete set of SCSs obeys the Klauder resolution of the identity,

$$\int_{\mathcal{C}^6}\prod_{j=1}^{3}\left(\frac{d^2z_j}{\pi}\frac{d^2w_j}{\pi}\right)|\underline{z},\underline{w}\rangle\langle\underline{z},\underline{w}|=1 \ \text{ on } \ \mathcal{H}, \quad (4.12)$$

the integration measure being the invariant one on the H-W group.

We now explore the behavior of these SCSs under SU(3) action. From the manner in which the generators Q_α are constructed in Eq. (2.2) we have

$$A\in\mathrm{SU}(3):\mathcal{U}(A)D(\underline{z},\underline{w})\mathcal{U}(A)^{-1}=D(A\underline{z},A^*\underline{w}), \quad (4.13)$$

from which it follows that

$$\mathcal{U}(A)|\underline{z},\underline{w}\rangle=|A\underline{z},A^*\underline{w}\rangle. \quad (4.14)$$

The independent invariants under this action are $\underline{z}^\dagger\underline{z}$, $\underline{w}^\dagger\underline{w}$ and $\underline{z}^T\underline{w}$, the last being the eigenvalue of K_-. We describe them using four real independent parameters u, v, x, y as

$$\underline{z}^\dagger\underline{z}=u^2,\quad \underline{w}^\dagger\underline{w}=v^2,\quad \underline{z}^T\underline{w}=uv(x+iy),$$
$$u,v\geqslant 0,\quad 0\leqslant x^2+y^2\leqslant 1. \tag{4.15}$$

The upper bound on x^2+y^2 is an expression of the Cauchy–Schwarz inequality. For each set of values of (u,v,x,y), the SCS $|\underline{z},\underline{w}\rangle$ form an orbit under SU(3) action. On each orbit we can choose a convenient representative point $(\underline{z}^{(0)},\underline{w}^{(0)})$, with any other point $(\underline{z},\underline{w})$ on the orbit arising from $(\underline{z}^{(0)},\underline{w}^{(0)})$ via suitable SU(3) action as $(A\underline{z}^{(0)},A^*\underline{w}^{(0)})$. The complete list of orbits, representative points, stability subgroups $H(\underline{z}^{(0)},\underline{w}^{(0)})\subset$SU(3) and orbit dimensions are as follows (with x, y omitted when irrelevant):

$$(a)\quad \vartheta_1=\{u,v|u=v=0\},(\underline{z}^{(0)},\underline{w}^{(0)})=(\underline{0},\underline{0}),H=\mathrm{SU}(3),\text{dimension }0;$$

$$(b)\quad \vartheta_2=\{u,v|u\rangle 0,v=0\},\underline{z}^{(0)}=u(1,0,0)^T,\underline{w}^{(0)}=\underline{0},H=\mathrm{SU}(2),\text{ dimension }5;$$

$$(c)\quad \vartheta_3=\{u,v|u=0,v\rangle 0\},\underline{z}^{(0)}=\underline{0},\underline{w}^{(0)}=v(0,1,0)^T,H=\mathrm{SU}(2),\text{ dimension }5;$$

$$(d)\quad \vartheta_4=\{u,v,x,y|u,v\rangle 0,0\leqslant x^2+y^2<1\}, \tag{4.16}$$

$$\underline{z}^{(0)}=u(1,0,0)^T,\underline{w}^{(0)}=v(x+iy,\sqrt{1-x^2-y^2},0)^T,H=\{e\},\text{ dimension }8;$$

$$(e)\quad \vartheta_5=\{u,v,x,y|u,v\rangle 0,x^2+y^2=1\},$$

$$\underline{z}^{(0)}=u(0,0,1)^T,\underline{w}^{(0)}=v(x+iy)(0,0,1)^T,H=\mathrm{SU}(2),\text{ dimension }5.$$

We add some comments: Class (a) comprises just the Fock vacuum $|\underline{0},\underline{0}\rangle$, invariant under SU(3) and forming a trivial orbit by itself. Classes (b) and (c) form collections of orbits with one of $\underline{z}$ and $\underline{w}$ vanishing identically, so these are simply SCSs for systems of three oscillators. Class (d) is a four-parameter family consisting of generic orbits. Each orbit in this class is eight-dimensional and is essentially the SU(3) group manifold. Class (e) is a limiting form, as $x^2+y^2\to 1$, of class (d); in these orbits, $\underline{w}$ is a complex multiple of $\underline{z}^*$. However, the limit is a singular one, as is evident from the rise in the dimension of H from zero to three, and the drop in orbit dimension from eight to five. This is why we have listed class (e) separately. Moreover, the representative point $(z^{(0)},w^{(0)})$ in this class has been chosen so that the stability group SU(2) acts on dimensions 1 and 2, thus coinciding with the subgroup relevant for the canonical basis (4.21). Disregarding class (a), and recalling that $\mathcal{C}^6$ is of real dimension 12, we see that classes (b), (c), (d), and (e) are nonoverlapping regions in $\mathcal{C}^6$ of real dimensions 6, 6, 12, and 8, respectively. Thus almost all of $\mathcal{C}^6$ is covered by orbits of class (d).

Based on this orbit structure, we now express the Klauder resolution of the identity, Eq. (4.12), in a manner similar to Eq. (3.39), namely as an integration over the SU(3) manifold followed by an integration over the invariants (4.15). [The difference compared to the case of two degrees of freedom is that here we integrate over the whole of SU(3), not just over a coset space such as $\mathrm{SU}(2)/\mathrm{U}(1)=S^2$ in Eq. (3.39).] In this process we can limit ourselves to class (d) orbits which are generic, as long as we do not at any later stage alter the integrand of Eq. (4.12) by inserting a Dirac delta function with support in one of the exceptional orbits in Eq. (4.16). To obtain a general pair $(\underline{z},\underline{w})$ from $(\underline{z}^{(0)},\underline{w}^{(0)})$ in Eq. (4.16) class (d), we need to parametrize (almost all) elements of SU(3) in a convenient manner. Here we use the fact that, except on a set of vanishing measure, each $A\in\mathrm{SU}(3)$ is uniquely determined by a pair $(\hat{\underline{\eta}},\hat{\underline{\xi}})$, where $\hat{\underline{\eta}}$ is a complex three-component unit vector and $\hat{\underline{\xi}}$ is a complex two-component unit vector:[28]

$$\underline{\hat{\eta}}=(\hat{\eta}_1,\hat{\eta}_2,\hat{\eta}_3)^T,\quad \underline{\hat{\xi}}=(\hat{\xi}_2,\hat{\xi}_3)^T,$$
$$\underline{\hat{\eta}}^\dagger\underline{\hat{\eta}}=\underline{\hat{\xi}}^\dagger\underline{\hat{\xi}}=1. \tag{4.17}$$

Then we have

$$A\in \mathrm{SU}(3)\Leftrightarrow A=A(\underline{\hat{\eta}},\underline{\hat{\xi}}=A_3(\underline{\hat{\eta}})A_2(\underline{\hat{\xi}}),$$
$$A_3(\underline{\hat{\eta}})=\begin{pmatrix}\hat{\eta}_1 & \rho_1 & 0\\ \hat{\eta}_2 & -\hat{\eta}_2\hat{\eta}_1^*/\rho_1 & \hat{\eta}_3^*/\rho_1\\ \hat{\eta}_3 & -\hat{\eta}_3\hat{\eta}_1^*/\rho_1 & -\hat{\eta}_2^*/\rho_1\end{pmatrix}\in \mathrm{SU}(3),$$
$$\rho_1=(1-|\hat{\eta}_1|^2)^{1/2}; \tag{4.18}$$
$$A_2(\underline{\hat{\xi}})=\begin{pmatrix}1 & 0 & 0\\ 0 & \hat{\xi}_2 & -\hat{\xi}_3^*\\ 0 & \hat{\xi}_3 & \hat{\xi}_2^*\end{pmatrix}\in \mathrm{SU}(2)\subset \mathrm{SU}(3).$$

For each $\underline{\hat{\eta}}$ (provided $|\hat{\eta}_1|<1$), $A_3(\underline{\hat{\eta}})$ is a particular SU(3) element completely determined by its first column which is $\underline{\hat{\eta}}$; and for each $\underline{\hat{\xi}}$, $A_2(\underline{\hat{\xi}})$ is an element in the SU(2) subgroup leaving $\underline{z}^{(0)}$ invariant. We can picture $\underline{\hat{\eta}}$ and $\underline{\hat{\xi}}$ as representing points on $S^5\subset\mathcal{R}^6$ and $S^3\subset\mathcal{R}^4$, respectively. Then the normalized invariant volume element on SU(3) is a numerical factor times the product of the solid angle elements on S^5 and S^3:

$$dA(\underline{\hat{\eta}},\underline{\hat{\xi}})=(2\pi^5)^{-1}d\Omega_5(\underline{\hat{\eta}})d\Omega_3(\underline{\hat{\xi}}),$$
$$\int_{\mathrm{SU}(3)}dA=1. \tag{4.19}$$

The expressions for $(\underline{z},\underline{w})$ in terms of $A(\underline{\hat{\eta}},\underline{\hat{\xi}})$ and $(\underline{z}^{(0)},\underline{w}^{(0)})$ are

$$\underline{z}=A(\underline{\hat{\eta}},\underline{\hat{\xi}})\underline{z}^{(0)}(u)=u\,\underline{\hat{\eta}},$$
$$\underline{w}=A(\underline{\hat{\eta}},\underline{\hat{\xi}})^*\underline{w}^{(0)}(v,x,y)=vA_3(\underline{\hat{\eta}})^*\begin{pmatrix}x+iy & \\ \sqrt{1-x^2-y^2} & \hat{\xi}_2^*\\ \sqrt{1-x^2-y^2} & \hat{\xi}_3^*\end{pmatrix}. \tag{4.20}$$

These are the generalizations of Eq. (3.34). Straightforward computations of the Jacobians yield

$$\prod_{j=1}^{3}(d^2z_j\ d^2w_j)=u^5v^5(1-x^2-y^2)du\ \ dv\ \ dx\ \ dy\ \ d\Omega_5(\underline{\hat{\eta}})\ \ d\Omega_3(\underline{\hat{\xi}}). \tag{4.21}$$

We can now rewrite the Klauder result (4.12) as

$$\frac{2}{\pi}\int_0^\infty u^5du\int_0^\infty v^5dv\int_{x^2+y^2\leqslant 1}(1-x^2-y^2)dx\ \ dy\int_{\mathrm{SU}(3)}dA\mathcal{U}(A)|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle$$
$$\times\langle\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)|\mathcal{U}(A)^{-1}=1\ \text{ on }\ \mathcal{H}. \tag{4.22}$$

This is the analog of (the initial form of) Eq. (3.39).

In the spirit of Eqs. (3.10) and (3.42) we can now consider modifications of Eq. (4.22) by including in the integrand a function of the SU(3) invariants. Thus we define

$$A(f)=\int\prod_{j=1}^{3}\left(\frac{d^2z_j}{\pi}\frac{d^2w_j}{\pi}\right)f(u,v,x,y)|\underline{z},\underline{w}\rangle\langle\underline{z},\underline{w}|$$

$$=\frac{2}{\pi}\int_0^\infty u^5du\int_0^\infty v^5dv\int_{x^2+y^2\leq 1}(1-x^2-y^2)dx\ \ dy\ \ f(u,v,x,y)$$

$$\times\int_{\mathrm{SU}(3)}dA\mathcal{U}(A)|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle\langle\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)|\mathcal{U}(A)^{-1}. \tag{4.23}$$

Such an operator definitely obeys

$$\mathcal{U}(A)A(f)=A(f)\mathcal{U}(A),\ \ \text{all}\ \ A\in\mathrm{SU}(3). \tag{4.24}$$

However, as long as $f(u,v,x,y)$ is nontrivial, the measure in Eq. (4.23) is not the invariant one on the H-W group, we do not have recourse to the Schur lemma for the UIR of this group, and $A(f)$ is not proportional to the identity operator on $\mathcal{H}$. The presence of (infinite!) multiplicity in the reduction of $\mathcal{U}(A)$ on $\mathcal{H}$ into UIRs of SU(3) means, furthermore, that we do not immediately get for $A(f)$ a simple combination of SU(3)-invariant projections as we did in Eqs. (3.42) and (3.43) with SU(2).

C. The restriction to $\mathcal{H}_0$

Now we limit ourselves to the SCS $|\underline{z},\underline{w}\rangle$ belonging to $\mathcal{H}_0\subset\mathcal{H}$, as in this subspace the multiplicity problem is avoided. As noted following Eq. (4.11), the condition $\underline{z}^T\underline{w}=0$ ensures $|\underline{z},\underline{w}\rangle\in\mathcal{H}_0$. This happens in classes (a)–(c) of Eq. (4.16) in a trivial manner, and in class (d) when $x=y=0$. The former can be disregarded as being sets of vanishing measure.

We deal first with vector level relations in $\mathcal{H}_0$, then look at modifications of $A(f)$ in Eq. (4.23). We begin with Eq. (4.9). For the highest weight states of SU(3) UIRs occurring there, we introduce a simpler notation:

$$|p,q;\tfrac{1}{2}(p+q),\tfrac{1}{2}(p+q);\tfrac{1}{3}(p-q);\tfrac{1}{2}(p+q+3)\rangle$$

$$\equiv|p,q;\tfrac{1}{2}(p+q),\tfrac{1}{2}(p+q);\tfrac{1}{3}(p-q)\rangle_0\in\mathcal{H}^{(p,q;0)}\subset\mathcal{H}_0. \tag{4.25}$$

We have omitted the Sp(2,R) quantum number m as it is superfluous within $\mathcal{H}_0$. Then Eq. (4.9) takes the form

$$\underline{z}^{(0)}(u)=u(1,0,0)^T,\underline{w}^{(0)}(v,0,0)=v(0,1,0)^T:$$

$$|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,0,0)\rangle=e^{-(1/2)(u^2+v^2)}\sum_{p,q=0}^{\infty}\frac{u^pv^q}{\sqrt{p!q!}} \tag{4.26}$$

$$|p,q;\tfrac{1}{2}(p+q),\tfrac{1}{2}(p+q),\tfrac{1}{3}(p-q)\rangle_0\in\mathcal{H}_0.$$

In place of Eq. (4.5), the SU(3) SCS within each UIR (p,q) contained in $\mathcal{H}_0$ can be written as

$$A\in\mathrm{SU}(3):|p,q;A\rangle_0=\mathcal{U}(A)|p,q;\tfrac{1}{2}(p+q),\tfrac{1}{2}(p+q),\tfrac{1}{3}(p-q)\rangle_0\in\mathcal{H}^{(p,q;0)}. \tag{4.27}$$

Applying $\mathcal{U}(A)$ for general $A\in\mathrm{SU}(3)$ to both sides of Eq. (4.26) we get a result linking those H-W SCSs that lie in $\mathcal{H}_0$, and the SU(3) SCS (4.27) within each UIR (p,q) in $\mathcal{H}_0$:

$$A \in \mathrm{SU}(3), \quad \underline{z} = A\underline{z}^{(0)}(u), \quad \underline{w} = A^* \underline{w}^{(0)}(v,0,0):$$

$$|\underline{z},\underline{w}\rangle = e^{-(1/2)(u^2+v^2)} \sum_{p,q=0}^{\infty} \frac{u^p v^q}{\sqrt{p!q!}} |p,q;A\rangle_0 \in \mathcal{H}_0 . \tag{4.28}$$

This is the SU(3) analog to the SU(2) relation (3.38).

Now we turn to the operator $A(f)$ in Eq. (4.23) and make the choice

$$f(u,v,x,y) = f_0(u,v)\,\delta(x)\,\delta(y). \tag{4.29}$$

This leads to

$$A(f_0) = \frac{2}{\pi} \int_0^{\infty} u^5 du \int_0^{\infty} v^5 dv\, f_0(u,v) \int_{\mathrm{SU}(3)} dA \mathcal{U}(A)$$

$$|\underline{z}^{(0)}(u), \underline{w}^{(0)}(v,0,0)\rangle\langle \underline{z}^{(0)}(u), \underline{w}^{(0)}(v,0,0)| \mathcal{U}(A)^{-1}. \tag{4.30}$$

Such an operator obeys the following:

$$\psi \in \mathcal{H}_0^{\perp} : A(f_0)\psi = 0;$$

$$\psi \in \mathcal{H}_0 : A(f_0)\psi \in \mathcal{H}_0; \tag{4.31}$$

$$A \in \mathrm{SU}(3) : \mathcal{U}(A) A(f_0) = A(f_0) \mathcal{U}(A).$$

Therefore $A(f_0)$ must be a linear combination of the projection operators $P^{(p,q;0)}$ onto the subspaces $\mathcal{H}^{(p,q;0)} \subset \mathcal{H}_0$; it is here that we exploit the multiplicity-free reduction of the SU(3) UR $\mathcal{D}_0$ on $\mathcal{H}_0$. To get $A(f_0)$ explicitly, we use the following immediate consequences of the Schur lemma applied to SU(3), the multiplicity-free nature of $\mathcal{D}_0$, and the orthogonality of inequivalent UIRs:

$$\int_{\mathrm{SU}(3)} dA |p,q;A\rangle_{0\,0}\langle p',q';A| = \delta_{p'p}\delta_{q'q} P^{(p,q;0)}/d(p,q). \tag{4.32}$$

Then a combination of Eqs. (4.30), (4.26), (4.27), and (4.32) immediately gives

$$A(f_0) = \sum_{p,q=0}^{\infty} C(f_0;p,q) P^{(p,q;0)},$$

$$C(f_0;p,q) = \{p!q!d(p,q)\}^{-1} \cdot \frac{2}{\pi} \cdot \int_0^{\infty} u^5 du \int_0^{\infty} v^5 dv\, f_0(u,v) u^{2p} v^{2q} e^{-(u^2+v^2)}. \tag{4.33}$$

This is an SU(3) analog of the SU(2) result (3.42), but it is valid only after the restriction to $\mathcal{H}_0$. On account of the freedom still remaining in Eqs. (4.30) and (4.33) in the choice of the function $f_0(u,v)$, we see that the H-W SCSs occurring there are overcomplete in $\mathcal{H}_0$. If we wish to limit ourselves to an exact "SU(3)-worth" of H-W SCSs within $\mathcal{H}_0$, then we have the analogue to Eq. (3.43):

$$f_0(u,v)=\delta(u-u_0)\,\delta(v-v_0):$$
$$A(f_0)=\int\prod_{j=1}^{3}\left(\frac{d^2z_j}{\pi}\,\frac{d^2w_j}{\pi}\right)\delta(u-u_0)\,\delta(v-v_0)\,\delta(x)\,\delta(y)|\underline{z},\underline{w}\rangle\langle\underline{z},\underline{w}| \tag{4.34}$$
$$=e^{-(u_0^2+v_0^2)}.\,\frac{2}{\pi}\sum_{p,q=0}^{\infty}u_0^{2p+5}v_0^{2q+5}P^{(p,q;0)}/p!q!d(p,q).$$

The point to be emphasized is how far this result departs from being the identity operator in $\mathcal{H}_0$, leave alone in $\mathcal{H}$, but understandably so.

D. Description in $\mathcal{H}^{(\mathrm{ind})}$

As recalled in Sec. II, and established in detail in Sec. I, the multiplicity-free UR $\mathcal{D}_0$ of SU(3) on $\mathcal{H}_0$ is equivalent to an induced UR $\mathcal{D}^{(\mathrm{ind})}$ of SU(3), namely the one arising from the trivial representation of an SU(2) subgroup of SU(3). The isomorphism between $\mathcal{H}_0$ and $\mathcal{H}^{(\mathrm{ind})}$ carrying $\mathcal{D}^{(\mathrm{ind})}$, consistent with the two group actions, is given in Eq. (2.17). It is of interest to see what wave functions $\psi(\underline{\xi})\in\mathcal{H}^{(\mathrm{ind})}$ one obtains for the various vectors in $\mathcal{H}_0$ that have played a role earlier in this section. We now give these wave functions and comment briefly on them.

For the highest weight state in the SU(3) UIR (p,q) on $\mathcal{H}^{(p,q;0)}$, and the associated SU(3) SCS, we find the following wavefunctions in $\mathcal{H}^{(\mathrm{ind})}$:

$$|p,q;\tfrac{1}{2}(p+q),\tfrac{1}{2}(p+q),\tfrac{1}{3}(p-q)\rangle_0\rightarrow\sqrt{\frac{(p+q+2)!}{p!q!}}(\xi_1)^p(\xi_2^*)^q;$$
$$|p,q;A\rangle_0=\mathcal{U}(A)|p,q;\tfrac{1}{2}(p+q),\tfrac{1}{2}(p+q),\tfrac{1}{3}(p-q)\rangle_0\rightarrow\sqrt{\frac{(p+q+2)!}{p!q!}}(A_{j1}^*\xi_j)^p(A_{k2}\xi_k^*)^q. \tag{4.35}$$

For the H-W SCS in $\mathcal{H}_0$ generating these states within each UIR we have

$$|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,0,0)\rangle\rightarrow e^{-(1/2)(u^2+v^2)}\sum_{p,q=0}^{\infty}\sqrt{(p+q+2)!}\frac{(u\xi_1)^p}{p!}\,\frac{(v\xi_2^*)^q}{q!};$$
$$|\underline{z},\underline{w}\rangle=\mathcal{U}(A)|\underline{z}^{(0}(u),\underline{w}^{(0)}(v,0,0)\rangle\rightarrow e^{-(1/2)(u^2+v^2)}\sum_{p,q=0}^{\infty}\sqrt{(p+q+2)!}\frac{(uA_{j1}^*\xi_j)^p}{p!}\,\frac{(vA_{k2}\xi_k^*)^q}{q!}. \tag{4.36}$$

The principal comment we may make is that these particular H-W SCS do not have wave functions in $\mathcal{H}^{(\mathrm{ind})}$ in the form of any simple expressions involving exponential functions. The reason for this can be traced to the factorial in Eq. (2.17) as compared to Eq. (2.14a). Another way of understanding this situation is to realize that $\mathcal{H}_0$ (and so $\mathcal{H}^{(\mathrm{ind})}$ as well) is too small to carry a representation of the H-W system used in the Schwinger SU(3) construction; in addition the argument $\underline{\xi}$ in $\psi(\underline{\xi})$ is a complex unit vector in three dimensions rather than a variable in all of $\mathcal{C}^3$.

V. GENERAL EIGENSPACES $\mathcal{H}_\kappa$ OF K_-

The subspace $\mathcal{H}_0\subset\mathcal{H}$ carrying the multiplicity-free UR $\mathcal{D}_0$ of SU(3), the focus of analysis in the preceding section, is spanned by those H-W SCSs $|\underline{z},\underline{w}\rangle$ for which $\underline{z}^T\underline{w}=0$, and belonging to a particular collection of orbits under class (d) of Eq. (4.16):

$$\mathcal{H}_0=\mathrm{Sp}\{|\underline{z},\underline{w}\rangle|\underline{z},\underline{w}\in\mathcal{C}^3,\underline{z}^T\underline{w}=0\}. \tag{5.1}$$

As noted earlier, these SCS are actually overcomplete within $\mathcal{H}_0$. Since, by Eq. (4.11), $\underline{z}^T\underline{w}$ is the eigenvalue of the SU(3) invariant Sp(2,R) lowering operator K_-, this means that $\mathcal{H}_0$ is spanned

by those H-W SCSs that are eigenvectors of K_- with eigenvalue zero. Moreover, Eqs. (4.26) and (4.28) show that these H-W SCSs are directly connected to the SU(3) SCSs within each SU(3) UIR (p,q), carried by $\mathcal{H}^{(p,q;0)}\subset\mathcal{H}_0$.

It now turns out that a somewhat similar situation exists involving eigenvectors of K_- corresponding to nonzero eigenvalues as well, but with one major difference: we encounter certain specific SU(3) GCS systems. This also connects up with a certain class of coherent states within the UIRs $D_k^{(+)}$ of Sp(2,R). We analyze these matters in this section. It turns out that H-W SCSs of both classes (d) and (e) are involved.

We begin by generalizing Eq. (5.1) and defining a subspace $\mathcal{H}_\kappa\subset\mathcal{H}$, for any complex number κ, as consisting of eigenvectors of K_- with eigenvalue κ; equally well it is the span of all those H-W SCSs which obey this condition:

$$\mathcal{H}_\kappa=\{|\psi\rangle\in\mathcal{H}|K_-|\psi\rangle=\kappa|\psi\rangle\}=\mathrm{Sp}\{|\underline{z},\underline{w}\rangle|\underline{z},\underline{w}\in\mathcal{C}^3,\underline{z}^T\underline{w}=\kappa\}\subset\mathcal{H}. \tag{5.2}$$

These H-W SCSs comprise a particular subset of class (d) orbits in Eq. (4.16); for $\kappa=0$ we get back $\mathcal{H}_0$. It is important to remark that even though κ varies over a continuum, each $\mathcal{H}_\kappa$ consists of bona fide (i.e., normalizable) vectors in $\mathcal{H}$; and for $\kappa'\neq\kappa$, $\mathcal{H}_{\kappa'}$ and $\mathcal{H}_\kappa$ are not mutually orthogonal. As in the case of the oscillator annihilation operator, these are consequences of K_- being non-Hermitian. Since K_- is SU(3) invariant, each $\mathcal{H}_\kappa$ is SU(3) invariant as well:

$$A\in\mathrm{SU}(3),|\psi\rangle\in\mathcal{H}_\kappa\Rightarrow\mathcal{U}(A)|\psi\rangle\in\mathcal{H}_\kappa. \tag{5.3}$$

Therefore the UR $\mathcal{U}(A)$ of SU(3) on $\mathcal{H}$, when restricted to $\mathcal{H}_\kappa$, leads to a UR $\mathcal{D}_\kappa$ acting on $\mathcal{H}_\kappa$. We will see that this UR contains each UIR (p,q) exactly once, just like $\mathcal{D}_0$ on $\mathcal{H}_0$. Thus it is also multiplicity-free and complete.

To exhibit these properties, we first recall the construction of eigenvectors of K_- in any discrete class UIR $D_k^{(+)}$ of Sp(2,R).[29] (Though the following results are valid for all real $k>0$, we require only the cases $k=\frac{3}{2},2,\frac{5}{2}\ldots$.) As in Eqs. (I.3.24) and (I.3.25), denote the eigenvectors of J_0 in $D_k^{(+)}$ by $|k,m\rangle$. Then we have the well-known results

$$|k,\kappa\rangle=({}_0F_1(2k;|\kappa|^2))^{-1/2}\sum_{m=k}^{\infty}(\Gamma(2k)/(m-k)!\Gamma(m+k))^{1/2}\kappa^{m-k}|k,m\rangle,$$
$$K_-|k,\kappa\rangle=\kappa|k,\kappa\rangle,\kappa\in\mathcal{C}; \tag{5.4a}$$

$$\langle k,\kappa'|k,\kappa\rangle={}_0F_1(2k;\kappa'^*\kappa)/\{{}_0F_1(2k;|\kappa'|^2)\,{}_0F_1(2k;|\kappa|^2)\}^{1/2}; \tag{5.4b}$$

$$\int_{\mathcal{C}}\frac{d^2\kappa}{\pi}\sigma(|\kappa|^2)|k,\kappa\rangle\langle k,\kappa|=1,$$
$$\sigma(|\kappa|^2)=\frac{2}{\Gamma(2k)}\,{}_0F_1(2k;|\kappa|^2)|\kappa|^{2k-1}K_{1/2-k}(2|\kappa|), \tag{5.4c}$$

where $K_\nu(z)$ denotes modified Bessel function of the third kind. (For simplicity the k-dependence of the weight function σ is omitted.) We note that even though these states $|k,\kappa\rangle$ within $D_k^{(+)}$ do not form an Sp(2,R) orbit, they do furnish a Klauder-type resolution of the identity.

We now exploit this construction in the present context. We begin with two facts: (a) the vectors $|p,q;IMY;m\rangle$, as all labels vary, form an orthonormal basis for the total Hilbert space $\mathcal{H}$; and (b) if we keep p,q,IMY fixed and allow only m to vary, we get an orthonormal basis for a subspace carrying just the UIR $D_k^{(+)}$ of Sp(2,R). Therefore, in view of the construction (5.4), within each such subspace we can define and have

$$|p,q;IMY\rangle_\kappa=\{{}_0F_1(2k;|\kappa|^2)\}^{-1/2}\sum_{m=k}^{\infty}((2k-1)!/(m-k)!(m+k-1)!)^{1/2}\kappa^{m-k}|p,q;IMY;m\rangle,$$

$$K_-|p,q;IMY\rangle_\kappa=\kappa|p,q;IMY\rangle_\kappa; \tag{5.5}$$

$${}_{\kappa'}\langle p',q';I'M'Y'|p,q;IMY\rangle_\kappa=\delta_{p'p}\delta_{q'q}\delta_{I'I}\delta_{M'M}\delta_{Y'Y}\times{}_0F_1(2k;\kappa'^*\kappa)/\{{}_0F_1(2k;|\kappa'|^2){}_0F_1(2k;|\kappa|^2)\}^{1/2}.$$

[For fixed p,q,IMY we also have a resolution of the appropriate identity in the form of Eq. (5.4c), but we omit it.] For $\kappa=0$ we recover the orthonormal basis for $\mathcal{H}_0$. However, for $\kappa\neq0$, these vectors are not eigenvectors of the total a- and b-type number operators $\hat{N}^{(a)},\hat{N}^{(b)}$. It is now evident that if we keep κ fixed, allow $pqIMY$ to vary, and recall that the range $\mathcal{C}$ of κ is k-independent, we get an orthonormal basis for $\mathcal{H}_\kappa$:

$$\mathcal{H}_\kappa=\mathrm{Sp}\{|p,q;IMY\rangle_\kappa|\kappa\ \text{fixed},pqIMY\ \text{varying}\},$$
$${}_\kappa\langle p',q';I'M'Y'|p,q;IMY\rangle_\kappa=\delta_{p'p}\delta_{q'q}\delta_{I'I}\delta_{M'M}\delta_{Y'Y}. \tag{5.6}$$

It is also clear that each UIR (p,q) of SU(3), carried by the $d(p,q)$ vectors $|p,q;IMY\rangle_\kappa\in\mathcal{H}_\kappa$ as IMY alone vary, appears exactly once in $\mathcal{H}_\kappa$. In other words, $\mathcal{D}_\kappa$ is multiplicity-free. In Eqs. (5.2) and (5.6) we have three equally good ways of identifying the subspace $\mathcal{H}_\kappa\subset\mathcal{H}$.

We next relate the orthonormal basis vectors (5.6) for $\mathcal{H}_\kappa$ to the corresponding ones for $\mathcal{H}_0$ in Eq. (2.12), in a compact manner. For this we use Eq. (I.3.25b) valid within each UIR $D_k^{(+)}$ of Sp(2,R), along with $K_+=\hat{\underline{a}}^\dagger\cdot\hat{\underline{b}}^\dagger$:

$$|p,q;IMY;m\rangle=((2k-1)!/(m-k)!(m+k-1)!)^{1/2}(\hat{\underline{a}}^\dagger\cdot\hat{\underline{b}}^\dagger)^{m-k}|p,q;IMY;k\rangle;$$

$$|p,q;IMY\rangle_\kappa=\{{}_0F_1(2k;|\kappa|^2)\}^{-1/2}\sum_{m=k}^{\infty}\frac{(2k-1)!}{(m-k)!(m+k-1)!}(\kappa\hat{\underline{a}}^\dagger\cdot\hat{\underline{b}}^\dagger)^{m-k}|p,q;IMY;k\rangle$$
$$=A^\dagger_{k,\kappa}|p,q;IMY\rangle_0, \tag{5.7}$$

$$A^\dagger_{k,\kappa}=\{{}_0F_1(2k;|\kappa|^2)\}^{-1/2}\sum_{m=k}^{\infty}\frac{(2k-1)!}{(m-k)!(m+k-1)!}(\kappa\hat{\underline{a}}^\dagger\cdot\hat{\underline{b}}^\dagger)^{m-k}$$
$$={}_0F_1(2k;\kappa\hat{\underline{a}}^\dagger\cdot\hat{\underline{b}}^\dagger)/\{{}_0F_1(2k;|\kappa|^2)\}^{1/2}.$$

It is important to notice that there is a dependence on $k=\frac{1}{2}(p+q+3)$ in the operator $A^\dagger_{k,\kappa}$; so the basis vectors $|p,q;IMY\rangle_\kappa$ for $\mathcal{H}_\kappa$ do not arise from the basis vectors $|p,q;IMY\rangle_0$ for $\mathcal{H}_0$ by application of a single operator dependent on κ alone. In spite of this, we will see below the usefulness of the connection (5.7).

We now obtain an expansion of the H-W SCS $|\underline{z},\underline{w}\rangle$ with $\underline{z}^T\underline{w}=\kappa$, in the orthonormal basis (5.6) for $\mathcal{H}_\kappa$. Thus we seek analog to Eqs. (4.26) and (4.28), as well as to Eqs. (4.27) and (4.32), in the case of $\mathcal{H}_0$. Given $|\underline{z},\underline{w}\rangle\in\mathcal{H}_\kappa$, by a suitable SU(3) transformation we can relate it to a standard state $|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle$ on its orbit. We parametrize the latter as in Eq. (4.16) class (d) (assume here for definiteness that $x^2+y^2<1$, the possibility $x^2+y^2=1$ which is of vanishing measure being handled in the next section):

$$\underline{z}^{(0)}(u)=u(1,0,0)^T,$$
$$\underline{w}^{(0)}(v,x,y)=v(x+iy,\sqrt{1-x^2-y^2},0)^T, \tag{5.8}$$
$$uv(x+iy)=\kappa.$$

We develop first the replacement for Eq. (4.26). The point of interest is to see which vector within each UIR (p,q) in $\mathcal{D}_\kappa$ appears, in place of the higher weight vector present in Eq. (4.26). Thanks to Eq. (5.7), the relevant overlap simplifies to a calculation in $\mathcal{H}_0$:

$$\begin{aligned}{}_\kappa\langle p,q;IMY|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle &= {}_0\langle p,q;IMY|A_{k,\kappa}|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle \\ &= \{{}_0F_1(2k;|\kappa|^2)\}^{1/2}\langle p,q;IMY;k|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle.\end{aligned} \tag{5.9}$$

Here the bra vector, in $\mathcal{H}_0$, is an eigenvector of $\hat{N}^{(a)},\hat{N}^{(b)}$ with eigenvalues p,q, respectively. This leads to further simplification:

$$\begin{aligned}\langle p,q;IMY;k|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle = e^{-(1/2)(u^2+v^2)}\frac{u^p}{p!}\frac{v^q}{q!}\langle p,q;IMY;k|(\hat{a}_1^\dagger)^p((x+iy)\hat{b}_1^\dagger \\ +\sqrt{1-x^2-y^2}\hat{b}_2^\dagger)^q|\underline{0},\underline{0}\rangle.\end{aligned} \tag{5.10}$$

The ket vector here has hypercharge $\frac{1}{3}(p-q)$, as does the highest weight state in (p,q), so this overlap is nonzero only if $Y=\frac{1}{3}(p-q)$. This then determines the possible values of I:

$$\begin{aligned}I &= I_0, I_0-1,\ldots,\tfrac{1}{2}|p-q|, \\ I_0 &= \tfrac{1}{2}(p+q).\end{aligned} \tag{5.11}$$

Notice that I_0 is the highest possible value of I in the UIR (p,q). For the bra vector in Eq. (5.10) we have the explicit expression [Eq. (I.A9)]:

$$\begin{aligned}\langle p,q;IMY;k| = \mathcal{N}_{pqIY}((I+M)!(I-M)!/2I!)^{1/2}\sum_{n=0}^{(p-r,q-s)_<}\sum_{L=0}^{I-M}\frac{(-1)^{n+I-M-L}}{(r+s+n+1)!} \\ \times\langle\underline{0},\underline{0}|\frac{(\hat{a}_\alpha\hat{b}_\alpha)^n}{n!}\frac{\hat{a}_1^{r-L}}{(r-L)!}\frac{\hat{a}_2^L}{L!} \\ \times\frac{\hat{b}_1^{I-M-L}}{(I-M-L)!}\frac{\hat{b}_2^{s-I+M+L}}{(s-I+M+L)!}\frac{\hat{a}_3^{p-r-n}}{(p-r-n)!}\frac{\hat{b}_3^{q-s-n}}{(q-s-n)!},\end{aligned}$$

$$\hat{a}_\alpha\hat{b}_\alpha = \hat{a}_1\hat{b}_1+\hat{a}_2\hat{b}_2,$$

$$\mathcal{N}_{pqIY} = \{r!s!(r+s+1)!(p-r)!(q-s)!(p+s+1)!(q+r+1)!/(p+q+1)!\}^{1/2},$$

$$r = I+\frac{Y}{2}+\frac{1}{3}(p-q), S = I-\frac{Y}{2}+\frac{1}{3}(q-p). \tag{5.12}$$

Here, as before, $(p,q)_<$ stands for smaller of the two integers p,q.

Use of this in Eq. (5.10) leads to further simplifications. The condition $Y=\frac{1}{3}(p-q)$ gives

$$\begin{aligned}r &= I+M_0, \quad s = I-M_0, \\ p-r &= q-s = I_0-I, \\ M_0 &= \tfrac{1}{2}(p-q).\end{aligned} \tag{5.13}$$

Then, in the sums over n and L in Eq. (5.12), only the terms $n=p-r=q-s$ and $L=0$ survive. Using all this, the scalar product in Eq. (5.9) can be explicitly computed:

$$
\begin{aligned}
{}_\kappa\langle p,q;IMY|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle &= \{{}_0F_1(2k;|\kappa|^2)\}^{1/2}\cdot e^{-(1/2)(u^2+v^2)}\cdot u^p v^q \\
&\quad\times\delta_{Y,(1/3)(p-q)}\frac{(-1)^{I_0-M}}{(M-M_0)!}\{(2I+1)(I+M)!(I-M_0)!/ \\
&\quad(2I_0+1)!(I-M)!(I+M_0)!\}^{1/2} \\
&\quad\times(x+iy)^{I_0-M}(1-x^2-y^2)^{(1/2)(M-M_0)}, \\
&\quad uv(x+iy)=\kappa.
\end{aligned}
\tag{5.14}
$$

We see that, provided $Y=\frac{1}{3}(p-q)$ and $M\geqslant M_0$, this overlap is nonzero for all values of I in the range (5.11). This shows how far the projection of $|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle$ onto the subspace of $\mathcal{H}_\kappa$ carrying the UIR (p,q) differs from the highest weight state.

We can now obtain the replacement for the previous Eq. (4.26). It is unavoidably somewhat more complicated. Using Eq. (5.14) and with $\kappa=uv(x+iy)$, we have

$$
\begin{aligned}
|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle &= e^{-(1/2)(u^2+v^2)}\sum_{p,q=0}^{\infty}u^p v^q\{{}_0F_1(2k;|\kappa|^2)/(p+q+1)!\}^{1/2} \\
&\quad\times\mathcal{N}'(p,q;|\kappa|/uv)|p,q;\kappa/uv\rangle_\kappa, \\
\mathcal{N}'(p,q;|\kappa|/uv)|p,q;\kappa/uv\rangle_\kappa &= \sum_{I=|M_0|}^{I_0}\sum_{M=M_0}^{I}\frac{(-1)^{I_0-M}}{(M-M_0)!}(\kappa/uv)^{I_0-M} \\
&\quad\times\left(1-\frac{|\kappa|^2}{u^2v^2}\right)^{(1/2)(M-M_0)}\{(2I+1)(I-M_0)!(I+M)!/ \\
&\quad(I+M_0)!(I-M)!\}^{1/2}|p,q;I,M,\tfrac{1}{3}(p-q)\rangle_\kappa, \\
\mathcal{N}'(p,q;|\kappa|/uv) &= \left\{\sum_{I=|M_0|}^{I_0}\sum_{M=M_0}^{I}\frac{(2I+1)(I-M_0)!(I+M)!}{(I+M_0)!(I-M)!(M-M_0)!^2}(|\kappa|/uv)^{2(I_0-M)}\right. \\
&\quad\left.\times\left(1-\frac{|\kappa|^2}{u^2v^2}\right)^{M-M_0}\right\}^{1/2},
\end{aligned}
\tag{5.15}
$$

which, as shown in the Appendix, can be compactly written as

$$
\begin{aligned}
\mathcal{N}'(p,q;|\kappa|/uv) &= \{(I_0-|M_0|+1)(I_0+|M_0|+1)_2F_1(-(I_0-|M_0|),-(I_0+|M_0|),2,1 \\
&\quad-|\kappa|^2/(u^2v^2))\}^{1/2}.
\end{aligned}
\tag{5.16}
$$

The normalization factor $\mathcal{N}'(p,q;|\kappa|/uv)$ has been defined so as to make the vector $|p,q;\kappa/uv\rangle_\kappa$ have unit norm; this vector lies in the subspace of $\mathcal{H}_\kappa$ carrying the (single occurrence of the) UIR (p,q) in $\mathcal{D}_\kappa$. Now we apply $\mathcal{U}(A)$ to both sides of Eq. (5.15) and get the replacements for Eqs. (4.27) and (4.28):

$$
\begin{aligned}
&A\in\mathrm{SU}(3),\underline{z}=A\underline{z}^{(0)}(u),\underline{w}=A^*\underline{w}^{(0)}(v,x,y),\underline{z}^T\underline{w}=\kappa: \\
|\underline{z},\underline{w}\rangle &= e^{-(1/2)(u^2+v^2)}\sum_{p,q=0}^{\infty}u^p v^q\{{}_0F_1(2k;|\kappa|^2)/(p+q+1)!\}^{1/2}\mathcal{N}'(p,q;|\kappa|/uv) \\
&\quad\times|p,q;\kappa/uv;A\rangle_\kappa, \\
&|p,q;\kappa/uv;A\rangle_\kappa=\mathcal{U}(A)|p,q;\kappa/uv\rangle_\kappa.
\end{aligned}
\tag{5.17}
$$

We see that for $(\underline{z},\underline{w})\in\mathcal{C}^6$ with given u,v,κ, corresponding to class (d) in Eq. (4.16), the H-W SCS $|\underline{z},\underline{w}\rangle$ is expressible in terms of a sequence of SU(3) GCS, all contained in $\mathcal{H}_\kappa$. The SU(3) GCSs within the UIR (p,q) use $|p,q;\kappa/uv\rangle_\kappa$ as the fiducial vector, and this is very different from the highest weight vector. For this family of SU(3) GCSs we have in place of Eq. (4.32)

$$\int_{\mathrm{SU(3)}} dA|p,q;\kappa/uv;A\rangle_{\kappa\kappa}\langle p',q';\kappa/uv;A|=\delta_{p'p}\delta_{q'q}\frac{P^{(p,q;\kappa)}}{d(p,q)}, \tag{5.18}$$

where $P^{(p,q;\kappa)}$ is the projection operator onto the subspace of $\mathcal{H}_\kappa$ carrying the UIR (p,q). This follows from the Schur lemma for SU(3) UIRs, and the fact that $\mathcal{D}_\kappa$ is multiplicity-free.

With these replacements for Eqs. (4.26)–(4.28) and (4.32) in hand, we can study the analog of the operator $A(f_0)$ in Eq. (4.30). We begin with the general definition (4.23) of $A(f)$ and choose

$$f(u,v,x,y)=f_0(u,v)\,\delta^{(2)}(x+iy-\kappa/uv)=f_0(u,v)\,\delta(x-\mathrm{Re}\,\kappa/uv)\,\delta/y-\mathrm{Im}\,\kappa/uv). \tag{5.19}$$

This achieves the restriction to $\mathcal{H}_\kappa$. We then define

$$\begin{aligned}A(f_0)&=\int\prod_{j=1}^{3}\left(\frac{d^2z_j}{\pi}\frac{d^2w_j}{\pi}\right)f_0(u,v)\,\delta^{(2)}(x+iy-\kappa/uv)|\underline{z},\underline{w}\rangle\langle\underline{z},\underline{w}|\\&=\frac{2}{\pi}\int_0^\infty u^5du\int_0^\infty v^5dv\,f_0(u,v)\,\theta(uv-|\kappa|)\left(1-\frac{|\kappa|^2}{u^2v^2}\right)\\&\quad\times\int_{\mathrm{SU(3)}}dA\mathcal{U}(A)|\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)\rangle\langle\underline{z}^{(0)}(u),\underline{w}^{(0)}(v,x,y)|\mathcal{U}(A)^{-1},\end{aligned} \tag{5.20}$$

it being understood in the last expression that $x+iy=\kappa/uv$. We can now use Eqs. (5.17) and (5.18) here and get the final result replacing Eq. (4.33):

$$A(f_0)=\sum_{p,q=0}^{\infty}C(f_0;p,q;\kappa)P^{(p,q;\kappa)},$$

$$\begin{aligned}C(f_0;p,q;\kappa)&=\frac{2}{\pi}\{{}_0F_1(2k;|\kappa|^2)/(p+q+1)!\,d(p,q)\}\int_0^\infty u^5du\int_0^\infty v^5dv\,f_0(u,v)\\&\quad\times\theta(uv-|\kappa|)\left(\left|-\frac{|\kappa|^2}{u^2v^2}\right)e^{-(u^2+v^2)}u^{2p}v^{2q}\{\mathcal{N}'(p,q;|\kappa|/uv)\}^2.\end{aligned} \tag{5.21}$$

The freedom remaining in the choice of $f_0(u,v)$ displays the overcompleteness, within $\mathcal{H}_\kappa$, of the H-W SCS belonging to $\mathcal{H}_\kappa$. To limit ourselves to an exact "SU(3)-worth" of these states, we choose $f_0(u,v)$ to be the product of two delta functions. Then we get a generalization of Eq. (4.34):

$$\begin{aligned}&f_0(u,v)=\delta(u-u_0)\,\delta(v-v_0),\quad u_0v_0>|\kappa|:\\&A(f_0)=\int\prod_{j=1}^{3}\left(\frac{d^2z_j}{\pi}\frac{d^2w_j}{\pi}\right)\delta(u-u_0)\,\delta(v-v_0)\,\delta^{(2)}\left(x+iy-\frac{\kappa}{uv}\right)|\underline{z},\underline{w}\rangle\langle\underline{z},\underline{w}|\\&=\frac{2}{\pi}\cdot e^{-(u_0^2+v_0^2)}\sum_{p,q=0}^{\infty}\{{}_0F_1(2k;|\kappa|^2)/(p+q+1)!\,d(p,q)\}\\&\quad\times u_0^{2p+5}v_0^{2q+5}\left(1-\frac{|\kappa|^2}{u_0^2v_0^2}\right)\{\mathcal{N}'(p,q;|\kappa|/u_0v_0)\}^2P^{(p,q;\kappa)}.\end{aligned} \tag{5.22}$$

In this manner all the results found in the preceeding section for the subspace $\mathcal{H}_0 \subset \mathcal{H}$, the null space of K_-, generalize to a general eigenspace $\mathcal{H}_\kappa \subset \mathcal{H}$ of K_-. Here again, limiting oneself to an exact "SU(3)-worth" of H-W SCSs does give us a total set of vectors, but they do not obey the Klauder resolution of the identity within $\mathcal{H}_\kappa$

VI. H-W SCSs OF CLASS (e) AND THEIR SU(3) CONTENT

In the listing of SU(3) orbits of H-W SCSs given in Eq. (4.16), it was pointed out that only classes (d) and (e) involve all six oscillators of the Schwinger SU(3) construction in a nontrivial manner. Furthermore, of these, only the former are generic. As we have seen, class (d) orbits form a four-parameter continuous family, each orbit being of dimension eight. In contrast, class (e) orbits are a three-parameter family, with each orbit of dimension five. Another characteristic is that each H-W SCS $|\underline{z},\underline{w}\rangle$ in class (d) is such that the complex three-vectors $\underline{z}^*$ and $\underline{w}$ are linearly independent; on the other hand, if $|\underline{z},\underline{w}\rangle$ is in class (e), then $\underline{w}$ is a (complex) multiple of $\underline{z}^*$.

In Secs. IV and V we have analyzed in detail the SU(3) structure and representation content of H-W SCSs on all class (d) orbits, for $\underline{z}^T\underline{w}=0$ and $\underline{z}^T\underline{w}=\kappa\neq 0$, respectively. Now we turn to a similar analysis of the class (e) orbits.[30] There is, however, a difficulty in handling this case by starting with the Klauder resolution of the identity, Eq. (4.12), and then modifying the integrand by inserting some function of the SU(3) invariants with the aim of restricting the integration to a chosen subset of orbits. We are unable to use the methods of Secs. IV and V here. The reason is that in terms of the SU(3) invariant parameters u,v,x,y in Eq. (4.15), class (e) corresponds to $x^2+y^2=1$, while in the volume element (4.21) on the H-W group there is an explicit factor $(1-x^2-y^2)$. For this reason, we handle class (e) orbits more directly, guided, however, by the results in class (d).

A convenient representative point on a general class (e) orbit is given by the pair of complex three-vectors

$$\begin{gathered}\underline{z}^{(0)}(u)=u(0,0,1)^T, \quad u>0,\\ \underline{w}^{(0)}(ve^{i\alpha})=ve^{i\alpha}(0,0,1)^T, \quad v>0,\ 0\leqslant\alpha<2\pi,\\ \underline{z}^{(0)}(u)^T\underline{w}^{(0)}(ve^{i\alpha})=uve^{i\alpha}.\end{gathered} \tag{6.1}$$

[As mentioned earlier in Sec. IV, the reason for choosing this configuration is that the corresponding stability group is the SU(2) subgroup acting on dimensions 1 and 2 in the defining representation (1,0), and it is just this subgroup that is involved in the canonical basis vectors $|p,q;IMY\rangle$ in a general SU(3) UIR (p,q).] Acting with a general $A\in \mathrm{SU}(3)$, we reach a general point $(\underline{z},\underline{w})$ on the orbit given by

$$\begin{gathered}\underline{z}=A\underline{z}^{(0)}(u),\\ \underline{w}=A^*\underline{w}^{(0)}(ve^{i\alpha})=\left(\frac{ve^{i\alpha}}{u}\right)\underline{z}^*,\\ \underline{z}^T\underline{w}=uve^{i\alpha}=e^{i\alpha}(\underline{z}^\dagger\underline{z}\underline{w}^\dagger\underline{w})^{1/2}.\end{gathered} \tag{6.2}$$

The H-W SCS $|\underline{z}^{(0)}(u),\underline{w}^{(0)}(ve^{i\alpha})\rangle$ is of course given by

$$|\underline{z}^{(0)}(u),\underline{w}^{(0)}(ve^{i\alpha})\rangle=e^{-(1/2)(u^2+v^2)+u\hat{a}_3^\dagger+ve^{i\alpha}\hat{b}_3^\dagger}|\underline{0},\underline{0}\rangle. \tag{6.3}$$

We can expand this in the orthonormal basis $|p,q;IMY;m\rangle$ for $\mathcal{H}$, recognizing that the only states that appear have $I=M=0, Y=\frac{2}{3}(q-p)$ for various (p,q). We need the results (I.A6) and (I.A7):

$$|p,q;0,0,\tfrac{2}{3}(q-p);k\rangle = p!q!\{(p+1)(q+1)/(p+q+1)!\}^{1/2} \times \sum_{n=0}^{(p,q)_<} \frac{(-1)^n}{(n+1)!}\frac{(\hat{a}_\alpha^\dagger \hat{b}_\alpha^\dagger)^n}{n!}\frac{(\hat{a}_3^\dagger)^{p-n}}{(p-n)!}\frac{(\hat{b}_3^\dagger)^{q-n}}{(q-n)!}|\underline{0},\underline{0}\rangle, \qquad \hat{a}_\alpha^\dagger \hat{b}_\alpha^\dagger = \hat{a}_1^\dagger \hat{b}_1^\dagger + \hat{a}_2^\dagger \hat{b}_2^\dagger; \tag{6.4a}$$

$$|p,q;0,0,\tfrac{2}{3}(q-p);m\rangle = \{(2k-1)!/(m-k)!(m+k-1)!\}^{1/2}\cdot(\hat{\underline{a}}^\dagger\cdot\hat{\underline{b}}^\dagger)^{m-k}|p,q;0,0,\tfrac{2}{3}(q-p);k\rangle. \tag{6.4b}$$

We can now easily compute the desired overlap:

$$\begin{aligned}
&\langle p,q;0,0,\tfrac{2}{3}(q-p);m|\underline{z}^{(0)}(u),\underline{w}^{(0)}(ve^{i\alpha})\rangle \\
&\quad = \{(2k-1)!/(m-k)!(m+k-1)!\}^{1/2}\times(uve^{i\alpha})^{m-k}\langle p,q;0,0,\tfrac{2}{3}(q-p);k|\underline{z}^{(0)}(u),\underline{w}^{(0)}(ve^{i\alpha})\rangle \\
&\quad = \{(2k-1)!/(m-k)!(m+k-1)!\}^{1/2}(uve^{i\alpha})^{m-k}\cdot p!q!\{(p+1)(q+1)/ \\
&\qquad (p+q+1)!\}^{1/2}\langle\underline{0},\underline{0}|\frac{\hat{a}_3^p}{p!}\frac{\hat{b}_3^q}{q!}|\underline{z}^{(0)}(u),\underline{w}^{(0)}(ve^{i\alpha})\rangle \\
&\quad = \{(p+1)(q+1)(2k-1)!/(p+q+1)!(m-k)!(m+k-1)!\}^{1/2}(uve^{i\alpha})^{m-k} \\
&\quad \times e^{-(1/2)(u^2+v^2)}u^p(ve^{i\alpha})^q.
\end{aligned} \tag{6.5}$$

In the second step here, when using the expansion (6.4a), only the term $n=0$ contributes. We therefore have the expansion of the representative class (e) H-W SCS in the SU(3)×Sp(2,*R*) basis:

$$\begin{aligned}
|\underline{z}^{(0)}(u),\underline{w}^{(0)}(ve^{i\alpha})\rangle &= e^{-(1/2)(u^2+v^2)}\sum_{p,q=0}^{\infty}\{(p+1)(q+1)/(p+q+1)!\}^{1/2}u^p(ve^{i\alpha})^q \\
&\quad\times\sum_{m=k}^{\infty}\{(2k-1)!/(m-k)!(m+k-1)!\}^{1/2}(uve^{i\alpha})^{m-k}|p,q;0,0,\tfrac{2}{3}(q-p);m\rangle \\
&= e^{-(1/2)(u^2+v^2)}\sum_{p,q=0}^{\infty}\{(p+1)(q+1/(p+q+1)!\}^{1/2}u^p(ve^{i\alpha})^q \\
&\quad\times\{{}_0F_1(2k;u^2v^2)\}^{1/2}|p,q;0,0,\tfrac{2}{3}(q-p))_{uve^{i\alpha}}.
\end{aligned} \tag{6.6}$$

As we would expect, this expansion involves just the K_- eigenstate defined in Eq. (5.5), namely the $I=M=0$, $Y=2/3(q-p)$ member of the orthonormal basis $\{|p,q;IMY\rangle_{uve^{i\alpha}}\}$ for $\mathcal{H}_{uve^{i\alpha}}$. As in the case of the SU(3) SCS, where the fiducial vector within the UIR (p,q) is the single highest weight vector $|p,q;1/2(p+q),1/2(p+q),1/3(p-q)\rangle$, here too a single vector of the canonical basis appears as fiducial vector, but it is of course not the highest weight state.

Now within each UIR (p,q) contained in the UR $\mathcal{D}_{uve^{i\alpha}}$ on $\mathcal{H}_{uve^{i\alpha}}$, we define the family of SU(3) GCSs:

$$A\in\mathrm{SU}(3):|p,q;0,0,\tfrac{2}{3}(q-p);A\rangle_{uve^{i\alpha}} = \mathcal{U}(A)|p,q;0,0,\tfrac{2}{3}(q-p)\rangle_{uve^{i\alpha}}. \tag{6.7}$$

Then, applying $\mathcal{U}(A)$ to both sides of Eq. (6.6), we have the general connection between class (e) H-W SCS and the SU(3) GCS (6.7):

$$|A\underline{z}^{(0)}(u),\ A^*\underline{w}^{(0)}(ve^{i\alpha})\rangle = e^{-(1/2)(u^2+v^2)} \sum_{p,q=0}^{\infty} \{(p+1)(q+1)/(p+q+1)!\}^{1/2} \times u^p (ve^{i\alpha})^q \{{}_0F_1(2k;u^2v^2)\}^{1/2} |p,q;0,0,\tfrac{2}{3}(q-p);A\rangle_{uve^{i\alpha}}. \tag{6.8}$$

We recognize that Eqs. (6.6)–(6.8) are replacements for Eqs. (4.26)–(4.28) and Eqs. (5.15) and (5.17) of class (d).

Keeping $uve^{i\alpha}$ fixed, the SU(3) GCSs (6.7) all belong to $\mathcal{H}_{uve^{i\alpha}}$, and from the Schur lemma they obey the analogs to Eqs. (4.32) and (5.18):

$$\int_{\mathrm{SU}(3)} dA |p,q;0,0,\tfrac{2}{3}(q-p);A\rangle_{uve^{i\alpha}uve^{i\alpha}} \langle p',q';0,0,\tfrac{2}{3}(q'-p');A| = \delta_{p'p}\delta_{q'q} \frac{P^{(p,q;uve^{i\alpha})}}{d(p,q)}. \tag{6.9}$$

Here, of course, we exploit the multiplicity-free reduction of $\mathcal{D}_{uve^{i\alpha}}$. It follows that for the H-W SCS (6.8) we have

$$\int_{\mathrm{SU}(3)} dA |A\underline{z}^{(0)}(u), A^*\underline{w}^{(0)}(ve^{i\alpha})\rangle\langle A\underline{z}^{(0)}(u), A^*\underline{w}^{(0)}(ve^{i\alpha})| = 2e^{-(u^2+v^2)} \sum_{p,q=0}^{\infty} u^{2p}v^{2q}\, {}_0F_1(2k;u^2v^2) P^{(p,q;uve^{i\alpha})}/(p+q+2)! \tag{6.10}$$

The integration over SU(3) here is in effect only over the five-dimensional coset space SU(3)/SU(2), in contrast to Eqs. (4.32) and (5.18) in class (d).

If we write $\kappa = uve^{i\alpha}$ and allow u and v to vary reciprocally, and also keep α fixed so that κ stays fixed, we never leave the subspace $\mathcal{H}_{uve^{i\alpha}}$ and the projection operators $P^{(p,q;uve^{i\alpha})}$. Therefore we can multiply both sides of Eq. (6.10) by any function

$$f(u,v) = f_0(u)\,\delta(uv - |\kappa|), \tag{6.11}$$

and integrate over both u and v to get results similar to Eqs. (4.33) and (5.21). Here $f_0(u)$ is free. This then shows that for each fixed κ, the class (e) H-W SCSs $|\underline{z},\underline{w}\rangle$ with $\underline{z}^T\underline{w} = \kappa$ are overcomplete in $\mathcal{H}_\kappa$.

VII. CONCLUDING REMARKS

To conclude, we have given a unified analysis of the interconnections between the Heisenberg–Weyl standard coherent states and the standard coherent states as well as certain generalized coherent states of SU(3). The specific family of SU(3) coherent states to be used is dependent on the type of orbit of the H-W SCSs belong to. This situation is describable in detail as follows. In terms of the SU(3) invariant parameters x and y, at $x=y=0$ we have those generic class (d) orbits which lie entirely within the subspace $\mathcal{H}_0$. For these H-W SCSs, the SU(3) harmonic analysis involves precisely the SU(3) SCS within each UIR. For $0<x^2+y^2<1$ we deal with the subspaces $\mathcal{H}_\kappa \subset \mathcal{H}$ which generalize $\mathcal{H}_0$; the corresponding orbits consist of H-W SCS whose SU(3) content brings in the SU(3) GCS studied in Sec. V. The fiducial vectors here are rather complicated, at any rate in the canonical basis for SU(3) UIRs. In the limit $x^2+y^2=1$, we have the class (e) orbits. These H-W SCS involve yet another family of SU(3) GCSs, though now the fiducial vectors are the unique SU(2) scalar states within each SU(3) UIR, and their properties are studied in Sec. VI. In this entire development the group $\mathrm{Sp}(2,R)$ plays a particularly helpful role and so does the Schur lemma wherever it is available. Indeed we have used this lemma for UIRs of the H-W group wherever possible, and, after modifications of the completeness identity,

used it for UIRs of SU(3). This systematic use of the Schur lemma makes several computations much easier than they would otherwise be. It must be emphasized that all the Heisenberg standard coherent states have been included in our study in the spirit of SU(3) harmonic analysis, so that there is a satisfactory completeness in our analysis. The significant property of the discrete series UIRs of Sp(2,R), which we have exploited, is worth mention. It is that while the spectrum of the compact generator J_0 depends on k, hence on the UIR, the "spectrum" of the non-Hermitian lowering operator K_- is the entire complex plane, thus being UIR independent. The calculations in Sec. V clearly show the importance of these facts.

APPENDIX

We outline here the steps involved in going from (5.15) to (5.16). Equation (5.15),

$$\mathcal{N}'(p,q;|\kappa|/uv)=\left\{\sum_{I=|M_0|}^{I_0}\sum_{M=M_0}^{I}\frac{(2I+1)(I-M_0)!(I+M)!}{(I+M_0)!(I-M)!(M-M_0)!^2}\right.$$
$$\left.\times(|\kappa|/uv)^{2(I_0-M)}\left(1-\frac{|\kappa|^2}{u^2v^2}\right)^{M-M_0}\right\}^{1/2}, \tag{A1}$$

can be written in terms of the Jacobi polynomials

$$P_n^{(\alpha,\beta)}(x)\equiv\frac{\Gamma(\alpha+n+1)}{n!\Gamma(\alpha+\beta+n+1)}\sum_{m=0}^{n}\binom{n}{m}\frac{\Gamma(\alpha+\beta+n+m+1)}{2^m\Gamma(\alpha+m+1)}(x-1)^m, \tag{A2}$$

as

$$\mathcal{N}'(p,q;|\kappa|/uv)=\left\{\sum_{I=|M_0|}^{I_0}(2I+1)\left(\frac{|\kappa|}{uv}\right)^{2(I_0-M_0)}P_{I-M_0}^{(0,2M_0)}\left(\frac{2u^2v^2}{|\kappa|^2}-1\right)\right\}^{1/2} \tag{A3}$$

Using the fact that $P_n^{(\alpha,\beta)}$ can also be written as

$$P_n^{(\alpha,\beta)}(x)=\frac{1}{2^n}\sum_{m=0}^{n}\binom{n+\alpha}{m}\binom{n+\beta}{n-m}(x-1)^{n-m}(x+1)^m, \tag{A4}$$

one can show that

$$x^{M_0}P_{I-M_0}^{(0,2M_0)}(2x-1)=x^{-M_0}P_{I+M_0}^{(0,-2M_0)}(2x-1), \tag{A5}$$

which implies that $\mathcal{N}'$ depends on M_0 only through its magnitude $|M_0|$. Replacing M_0 on the rhs of (A1) by $|M_0|$ and rewriting it as a polynomial in $(1-|\kappa|^2/u^2v^2)$, we obtain

$$\mathcal{N}'(p,q;|\kappa|/uv)=\left\{\sum_{k=0}^{I_0-|M_0|}a_k\left(1-\frac{|\kappa|^2}{u^2v^2}\right)^k\right\}^{1/2}, \tag{A6}$$

where

$$a_k=\sum_{M=0}^{k}\sum_{I=M}^{I_0-|M_0|}(2I+2|M_0|+1)\binom{I+2|M_0|+M}{M}\binom{I}{M}\binom{I-|M_0|-M}{k-M}(-1)^{k-M}, \tag{A7}$$

which, after some rearrangement, can be written as

$$a_k=\sum_{M=0}^{k}(-1)^M\binom{I_0-|M_0|+M-k}{M}\cdot\sum_{I=0}^{I_0-|M_0|-k+M}(2I+2k+2|M_0|-2M+1)\binom{I+k-M}{I}\times\binom{I+2k+2|M_0|-2M}{k-M}. \tag{A8}$$

Using the identities

$$\sum_{I=0}^{I_0-|M_0|-k+M}(2I+2k+2|M_0|-2M+1)\binom{I+k-M}{I}\binom{I+2k+2|M_0|-2M}{k-M}=(I_0-|M_0|+1)\binom{I_0+|M_0|+k-M+1}{I_0+|M_0|}\binom{I_0-|M_0|}{k-M} \tag{A9}$$

and

$$\sum_{M=0}^{k}(-1)^M\binom{I_0-|M_0|+M-k}{M}\binom{I_0+|M_0|+k-M+1}{I_0+|M_0|}\binom{I_0-|M_0|}{k-M}=\binom{I_0+|M_0|+1}{k+1}\binom{I_0-|M_0|}{k}, \tag{A10}$$

we obtain

$$a_k=(k+1)\binom{I_0+|M_0|+1}{k+1}\binom{I_0-|M_0|+1}{k+1}. \tag{A11}$$

Substituting this in (A6) we finally obtain the result (5.16).

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New classes of quasi-solvable potentials, their exactly solvable limit, and related orthogonal polynomials

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We have generated, using an sl(2,R) Lie-algebraic formalism, several new classes of quasi-solvable elliptic potentials, which in the appropriate limit go over to the exactly solvable forms. We have obtained exact solutions of the corresponding spectral problem for some real values of the potential parameters. We have also given explicit expressions of the families of associated orthogonal polynomials in the energy variable. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In recent times elliptic potentials have proved to be an important addition[1–3] to the class of solvable[4,5] and quasi-solvable[6–8] potentials in quantum mechanics. In particular, within the sl(2,R) algebra, exact solutions of Lamé and associated Lamé equation have been obtained[9–12] for various ranges of the potential parameters. Indeed a handful of theorems relating to the properties of elliptic potentials are known for a long time[13–16] including the study of the properties of the corresponding wavefunctions.[14] The solutions of associated Lamé equation have also been obtained[17] by using these theorems which, however, do not use the sl(2,R) technique. Note that some new elliptic models based on Weierstrass $\wp$ function have recently been proposed[18] wherein it is shown that the corresponding Hamiltonians possess the so-called energy-reflection symmetry.[19]

By the term quasi-exactly solvable (QES) periodic potentials we mean potentials consisting of finite number of allowed bands and expressible as doubly periodic elliptic functions which are either Jacobian elliptic functions $snx \equiv sn(x,k)$, $cnx \equiv cn(x,k)$, $dnx \equiv dn(x,k)$ of real elliptic modulus parameter $k(0<k^2<1)$ or Weierstrass $\wp$ function. This is in sharp contrast with the ordinary ES periodic potentials with a single period.

There is an intriguing relation between ES and QES class. In fact, an sl(2) based construction with an n-dimensional finite space representation gives $(n+1)$ levels for a Hamiltonian designated as a QES model. It was pointed out in Ref. 8 that if one can construct a Hamiltonian having no explicit dependence on n, then in the limit $n \to \infty$ the ES models are recovered. This provides a sufficient reason to believe that corresponding to every ES model there ought to exist a QES model which in the proper limit goes over to the former.

In this article we show that the elliptic parameter k can be used for passage from QES to ES in the periodic models. We derive three new QES periodic potentials involving Jacobian elliptic functions. The elliptic functions having real and imaginary period reduce to ordinary periodic functions, namely hyperbolic (imaginary period) and trigonometric (real period) functions as the modulus parameter k goes to 1 and 0. We exploit this interesting property of elliptic functions to show that our QES models are connected with some well known ES periodic class. Note that we do not intend to take the limit $n \to \infty$ and as such we cannot expect to recover the whole spectrum for ES models. Rather we show that the limit $k \to 1$ and 0 correctly map the few lower states of the QES and ES periodic potentials.

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The plan of this article is as follows. In Sec. II we briefly review the basics of the sl(2,R) Lie-algebraic formalism and generate type I, II and III models within this framework. The method of construction of the related orthogonal polynomials is also sketched here. Specific examples are constructed in Sec. III for each of them based on some real values of the potential parameters. In Sec. IV we systematically analyze the ES limit of our results to show how this limit can reproduce the ES results. Finally we present our conclusions in Sec. V.

II. NEW QES POTENTIALS FROM sl(2,R) AND RELATED ORTHOGONAL POLYNOMIALS

To start with, let us adopt the following differential realization of the sl(2,R) generators

$$T^+=\xi^2\partial_\xi-n\xi,\quad T^0=\xi\partial_\xi-\tfrac{1}{2}n,\quad T^-=\partial_\xi, \tag{2.1}$$

obeying commutation relations

$$[T^+,T^-]=-2T^0,\quad [T^0,T^\pm]=\pm T^\pm, \tag{2.2}$$

where n is a non-negative integer. The gauged Hamiltonian is taken as the standard homogeneous quadratic combination of sl(2,R) generators along with linear terms:

$$H_G=-C_{++}T^{+^2}-C_{00}T^{0^2}-C_{--}T^{-^2}-C_+T^+-C_0T^0-C_-T^--d, \tag{2.3}$$

where C_{ii}, $C_j(i,j=0,\pm)$ are numerical parameters and d is a suitably chosen constant taken as function of C_j. Note that d plays the role of an overall shift in the energy scale. This pseudo degree of freedom allows us to obtain QES models in the desired form.

Substitution of (2.1) into (2.3) yields

$$\begin{aligned}H_G(\xi)=&-(C_{++}\xi^4+C_{00}\xi^2+C_{--})\partial_\xi^2\\&-[2(1-n)C_{++}\xi^3+C_+\xi^2+\{(1-n)C_{00}+C_0\}\xi+C_-]\partial_\xi\\&-\left[n(n-1)C_{++}\xi^2-nC_+\xi+\frac{n^2}{4}C_{00}-\frac{n}{2}C_0+d\right],\end{aligned} \tag{2.4}$$

which after a coordinate transformation

$$x(\xi)=\int^\xi d\tau/\sqrt{C_{++}\tau^4+C_{00}\tau^2+C_{--}}, \tag{2.5}$$

converts H_G into the form

$$\begin{aligned}H_G(x)=&-\partial_x^2+\frac{2nC_{++}\xi^3(x)-C_+\xi^2(x)+(nC_{00}-C_0)\xi(x)-C_-}{\sqrt{C_{++}\xi^4(x)+C_{00}\xi^2(x)+C_{--}}}\partial_x\\&-\left[n(n-1)C_{++}\xi^2(x)-nC_+\xi(x)+\frac{n^2}{4}C_{00}-\frac{n}{2}C_0+d\right],\end{aligned} \tag{2.6}$$

where $\xi=\xi(x)$ is determined by (2.5).

Let us now consider the Schrödinger equation with the potential $V(x)$

$$H(x)\psi(x)\equiv[-\partial_x^2+V(x)]\psi(x)=E\psi(x). \tag{2.7}$$

Writing $\psi(x)$ in the form

$$\psi(x)=\mu(x)\chi(x), \tag{2.8}$$

we obtain

$$H_G(x)\chi(x)\equiv\left[-\partial_x^2-2\left(\frac{\mu'}{\mu}\right)\partial_x-\left(\frac{\mu'}{\mu}\right)^2-\left(\frac{\mu'}{\mu}\right)'+V\right]\chi(x)=E\chi(x). \tag{2.9}$$

Comparing (2.6) and (2.9) we find for the potential $V(x)$ and the gauge factor $\mu(x)$ the following relationships

$$V(x)=\left(\frac{\mu'}{\mu}\right)^2+\left(\frac{\mu'}{\mu}\right)'-\left[n(n-1)C_{++}\xi^2-nC_+\xi+\frac{n^2}{4}C_{00}-\frac{n}{2}C_0+d\right], \tag{2.10}$$

$$\mu(x)=[C_{++}\xi^4+C_{00}\xi^2+C_{--}]^{-n/4}\exp\left[\int^{\xi}\frac{C_+\tau^2+C_0\tau+C_-}{2(C_{++}\tau^4+C_{00}\tau^2+C_{--})}d\tau\right]. \tag{2.11}$$

Note that the choice of numerical parameters C_{ii} must be such that Eq. (2.5) may be invertible in terms of $\xi=\xi(x)$. For our purpose $\xi(x)$ needs to be expressed in terms of Jacobian elliptic functions. In Ref. 12 we gave an almost exhaustive list of the choice of C_{ii} leading to various new classes of elliptic potentials. Here we consider the following three types of combinations of parameters, namely,

$$\text{type I:}\quad C_{++}=-k^2,\quad C_{00}=2k^2-1,\quad C_{--}=k'^2, \tag{2.12}$$

$$\text{type II:}\quad C_{++}=k^2,\quad C_{00}=-(1+k^2),\quad C_{--}=1, \tag{2.13}$$

$$\text{type III:}\quad C_{++}=k'^2,\quad C_{00}=1+k'^2,\quad C_{--}=1, \tag{2.14}$$

where $k^2\in(0,1)$ and $k'^2=1-k^2$. Each of the above types defines different coordinate transformations through (2.5). These give respectively $\xi=-cnx$, $-cnx/dnx$ and snx/cnx for the three types mentioned above.

In this way we are then led to the following new classes of elliptic potentials:

$$\text{type I:}\quad V(x)=[B^2+A(A+1)]\frac{dn^2x}{sn^2x}-2B\left(A+\frac{1}{2}\right)\frac{cnx}{sn^2x},\quad x\in(0,2K), \tag{2.15}$$

$$\text{type II:}\quad V(x)=B(B+1)\frac{dn^2x}{sn^2x}-A(A+1)dn^2x,\quad x\in(0,2K), \tag{2.16}$$

$$\text{type III:}\quad V(x)=[B^2-A(A+1)]k^2cn^2x+2Bk^2(A+\tfrac{1}{2})snxcnx,\quad x\in(-\infty,\infty), \tag{2.17}$$

where $K=\int_0^{\pi/2}d\alpha/\sqrt{1-k^2\sin^2\alpha}$ is the complete elliptic integral of the first kind. Note that in (2.15)–(2.17) the potential parameters $A,B\in R$ and the choices of C_j and the spin parameter n in (2.10) in terms of A,B are given in Table I. The constant d is chosen as

$$\text{type I:}\quad d=\frac{C_0}{4}\{C_0-4k'^2(n+1)\}+\frac{C_+}{2k^2}(k^2C_--k'^2C_+)+\frac{n(n+2)}{2}k'^2, \tag{2.18}$$

$$\text{type II:}\quad d=\left(\frac{C_+}{2k}\right)^2-\frac{C_0}{2}(n+1)+\frac{n(n+2)}{4}(1+k^2), \tag{2.19}$$

$$\text{type III:}\quad d=\frac{1}{4}\left[\left(\frac{C_+}{k'}\right)^2-n(n+2)(2-k^2)-2C_0(n+1)\right]. \tag{2.20}$$

TABLE I. Different algebraizations for type I–III potentials are given. Last column gives restrictions on potential parameters to keep n to a non-negative integer.

Classification	Solution no.	n	C_+	C_-	C_0	Restrictions on A, B
	1.1	A	$2k^2B$	$2k'^2B$	A	$A\in\mathrm{N}-1$, $B\in\mathrm{R}$
	1.2	$A-1$	$2k^2B$	$2k'^2B$	$A+1$	$A\in\mathrm{N}$, $B\in\mathrm{R}$
Type I	1.3	$B-1$	$2k^2(A+\frac{1}{2})-ikk'$	$2k'^2(A+\frac{1}{2})+ikk'$	B	$A\in\mathrm{R}$, $B\in\mathrm{N}$
	1.4	$A-\frac{1}{2}$	$2k^2B-ikk'$	$2k'^2B+ikk'$	$A+\frac{1}{2}$	$A\in\mathrm{N}-\frac{1}{2}$, $B\in\mathrm{R}$
	1.5	$B-\frac{1}{2}$	$2k^2(A+\frac{1}{2})$	$2k'^2(A+\frac{1}{2})$	$B-\frac{1}{2}$	$A\in\mathrm{R}$, $B\in\mathrm{N}-\frac{1}{2}$
	1.6	$B-\frac{3}{2}$	$2k^2(A+\frac{1}{2})$	$2k'^2(A+\frac{1}{2})$	$B+\frac{1}{2}$	$A\in\mathrm{R}$, $B\in\mathrm{N}+\frac{1}{2}$
Type II	2.1	$A-\frac{1}{2}$	$-2k^2(B+\frac{1}{2})$	$2(B+\frac{1}{2})$	$-k'^2(A+\frac{1}{2})$	$A\in\mathrm{N}-\frac{1}{2}$, $B\in\mathrm{R}$
	2.2	$A-\frac{1}{2}$	$2k^2(B+\frac{1}{2})$	$-2(B+\frac{1}{2})$	$-k'^2(A+\frac{1}{2})$	$A\in\mathrm{N}-\frac{1}{2}$, $B\in\mathrm{R}$
	3.1	A	$-2k'^2B$	$-2B$	$-Ak^2$	$A\in\mathrm{N}-1$,$B\in\mathrm{R}$
Type III	3.2	$A-1$	$-2k'^2B$	$-2B$	$-(A+1)k^2$	$A\in\mathrm{N}$, $B\in\mathrm{R}$
	3.3	$A-\frac{1}{2}$	$-2k'^2B+ik'$	$-2B+ik'$	$-(A+\frac{1}{2})k^2$	$A\in\mathrm{N}-\frac{1}{2}$, $B\in\mathrm{R}$

Note that while the type III potential is defined over the entire x-axis, type I and II potentials are singular at $x=0,2K$ and so defined over an open domain $(0,2K)$. It follows from the oscillation theorem that we need to find the periodic solutions [of period 4K(or 8K)] for 4K-periodic potential of type I and periodic solutions [of period 2K(or 4K)] for 2K-periodic potentials of types II and III at $E=E_j$. The monotonic increasing sequence $\{E_j\}$, where $E_0<E_1\leqslant E_2<E_3\leqslant E_4\ldots$, gives the characteristic values of the energy parameter.

Following the analysis made in Ref. 12 we can find the effective combinations of the potential parameters A,B. We see that the type I and III potentials are invariant under the translation $A,B\to A'$, B' where $A'=-A-1$, $B'=-B$ and type II potential is invariant under $A,B\to A'$, B' where $A'=-A-1$, $B'=-B-1$. Further, due to the periodic relations $sn(x+2K)=-snx$, $cn(x+2K)=-cnx$, $dn(x+2K)=dnx$, it results that the effective regions in the $A-B$ plane for type I-III models are bounded by the constraints $A\geqslant-\frac{1}{2}$, $B\geqslant0$; A, $B\geqslant-\frac{1}{2}$ and $A\geqslant-\frac{1}{2}$,$B\in R$, respectively. It may be pointed out that the eigenstates and spectra of type I potential for $B<0$ can be obtained from those for $B>0$ under the coordinate translation $x\to x+2K$.

Before concluding this section let us briefly describe the method of construction of families of orthogonal polynomials[12,20,21] generated by the eigenstates of a QES Hamiltonian. Let us consider a gauged eigenvalue equation

$$H_G(\xi)\chi(\xi)=E\chi(\xi), \tag{2.21}$$

where we identify $\chi(\xi(x))\equiv\chi(x)$ as given in (2.8). We now expand the gauged eigenfunction $\chi(\xi)$ in the form

$$\chi(\xi)=\left(\frac{\xi_2-\xi}{\xi_1-\xi_2}\right)^n\sum_{j=0}^{\infty}\frac{P_j(E)}{j!}\left(\frac{\xi_1-\xi}{\xi_2-\xi}\right)^j, \tag{2.22}$$

where ξ_1, ξ_2 are two distinct roots of the coeffecient of ∂_ξ^2 in (2.4). Now a suitable choice of ξ_1, ξ_2 (note that ξ_1, ξ_2 can be chosen in six ways) gives us a three-term recursion relation satisfied by $\{P_j(E)\}$,

$$
\begin{aligned}
&-[(2j-n+1)\hat{C}_{0-}+\hat{C}_{-}]P_{j+1}\\
&\quad=\left[E+d_1+\hat{C}_0\left(j-\frac{n}{2}\right)+\hat{C}_{00}\left(j-\frac{n}{2}\right)^2\right]P_j\\
&\qquad+j(j-1-n)[(2j-n-1)\hat{C}_{+0}+\hat{C}_{+}]P_{j-1}, \quad (j\geqslant 0),
\end{aligned}
\tag{2.23}
$$

where $\hat{C}_{ij}$ are determined from the relations

$$
\begin{aligned}
\hat{C}_{+0}&=-\frac{1}{(\xi_1-\xi_2)^2}[2\xi_1\xi_2^3C_{++}+\xi_2(\xi_1+\xi_2)C_{00}+2C_{--}],\\
\hat{C}_{00}&=\frac{1}{(\xi_1-\xi_2)^2}[6\xi_1^2\xi_2^2C_{++}+(\xi_1^2+\xi_2^2+4\xi_1\xi_2)C_{00}+6C_{--}],\\
\hat{C}_{0-}&=-\frac{1}{(\xi_1-\xi_2)^2}[2\xi_1^3\xi_2C_{++}+\xi_1(\xi_1+\xi_2)C_{00}+2C_{--}],
\end{aligned}
\tag{2.24}
$$

and $\hat{C}_j$, d_1 are given by

$$
\begin{aligned}
\hat{C}_{+}&=\frac{1}{\xi_1-\xi_2}[\xi_2^2C_{+}+\xi_2C_0+C_{-}],\\
\hat{C}_0&=-\frac{1}{\xi_1-\xi_2}[2\xi_1\xi_2C_{+}+(\xi_1+\xi_2)C_0+2C_{-}],\\
\hat{C}_{-}&=\frac{1}{\xi_1-\xi_2}[\xi_1^2C_{+}+\xi_1C_0+C_{-}],\\
d_1&=d+\frac{n(n+2)}{12}(C_{00}-\hat{C}_{00}).
\end{aligned}
\tag{2.25}
$$

From Eq. (2.23)–(2.25) it transpires that the eigenstates of type I–III Hamiltonians generate, in general, different orthogonal family of polynomials in the energy variable corresponding to each algebraization of Table I provided

$$
(2j-n+1)\hat{C}_{0-}+\hat{C}_{-}\neq 0, \quad \forall j\geqslant 0. \tag{2.26}
$$

The family $\{P_j(E)\}$ can be expressed in terms of monic polynomials $\{\tilde{P}_j(E)\}$ satisfying the recurrence relation

$$
\tilde{P}_{j+1}=(E-\lambda_j)\tilde{P}_j-\rho_j\tilde{P}_{j-1}, \tag{2.27}
$$

$$
\tilde{P}_j=\omega_jP_j, \quad j\geqslant 0, \tag{2.28}
$$

where $\tilde{P}_{-1}=P_1\equiv 0$ and $\tilde{P}_0=P_0\equiv 1$. It is now straightforward to write down the expression of eigenfunctions from (2.8) and (2.22). It follows from Eq. (2.23) that $\rho_0=0$ and $\rho_{n+1}=0$; so the infinite power series expansion in (2.22) truncates after the $(n+1)$-th term since the coeffecients $P_j(E_i)$ vanishes for $j>n$, where $E_i(i=0,1,...,n)$ are the zeros of the critical polynomial $\tilde{P}_{n+1}(E)$. This points to the fact that type I–III potentials belong to QES class having $(n+1)$ levels for each algebraization. The final expression of the band-edge eigenfunctions may be written in the form

TABLE II. The coeffecients ρ_j, λ_j, ω_j of the recurrence relation (2.26) and (2.27) are given for type I model. The choice of roots ξ_1, ξ_2 and the overall restrictions on potential parameters are also provided for each algebraization.

Solution no.	n	ρ_j	λ_j	ω_j	(ξ_1, ξ_2)	Overall restrictions on A, B
1.1	A	$(\frac{1}{2})^2 j(j-1-A)(2j+2B-1)(2B-2A+2j-1)$	$\frac{1-2k^2}{2}[A(A+1)+(A-2j)(2B-A+2j)]$	$(\frac{1}{2})^j \frac{\Pi_{r=0}^{[B]-A+j}(2B-2A+2j-1-2r)}{\Pi_{r=0}^{[B]-A}(2B-2A-1-2r)}$	$(-1,1)$	$A \in N-1,\ B \in R,$ $B-A \geqslant 0.$
1.2	$A-1$	$(\frac{1}{2})^2 j(j-A)(2j+2B+1)(2B-2A+2j-1)$	$\frac{1-2k^2}{2}[A(A+1)+(A-1-2j)(2B+2j-A+1)]$	,,	,,	$A \in N,\ B \in R,$ $B-A \geqslant 0.$
1.3	$B-1$	$(\frac{1}{2})^2 j(j-B)(2j+1)(2j-2B+1)$	$\frac{1-2k^2}{4}[2B^2-1+2(B-1-2j)(2j-B+2)]$ $+\frac{1}{2}ikk'(2A+1)(2B-2A-4j-3)$	$(\frac{-1}{2})^j \Pi_{r=0}^{j}(2j+1-2r)$	$\left(\frac{ik'}{k}, \frac{-ik'}{k}\right)$	$A \in R,\ B \in N,$ $A-B+1 \geqslant 0.$
1.4	$A-\frac{1}{2}$	$(\frac{1}{2})^2 j(2j-2A-1)(j-A)(2j+1)$	$\frac{1-2k^2}{8}[4A(A+1)-1+(2A-4j-1)(4j-2A+3)]$ $+2Bikk'(A-2j-1)$	,,	,,	$A \in N-\frac{1}{2},\ B \in R,$ $B-A \geqslant 0.$
1.5	$B-\frac{1}{2}$	$(\frac{1}{2})^2 j(j+A)(2j-2B-1)(2A-2B+2j+1)$	$\frac{1-2k^2}{8}[4B^2-1+(2B-4j-1)(4j+4A-2B+3)]$	$(\frac{1}{2})^j \frac{\Pi_{r=0}^{[A-B]+j}(2A-2B+2j-2r+1)}{\Pi_{r=0}^{[A-B]}(2A-2B-2r+1)}$	$(-1,1)$	$A \in R,\ B \in N-\frac{1}{2},$ $A-B+1 \geqslant 0.$
1.6	$B-\frac{3}{2}$	$(\frac{1}{2})^2 j(2j-2B+1)(j+A+1)(2A-2B+2j+1)$	$\frac{1-2k^2}{8}[4B^2-1+(2B-4j-3)(4j+4A-2B+5)]$	,,	,,	$A \in R,\ B \in N+\frac{1}{2},$ $A-B+1 \geqslant 0$

$$\psi_{E_i}(x)=\mu(x)(\xi(x)-\xi_2)^n\sum_{j=0}^{n}\frac{P_j(E_i)}{j!}\left(\frac{\xi(x)-\xi_1}{\xi(x)-\xi_2}\right)^j,\quad (i=0,1,,\ldots,n),\tag{2.29}$$

where $\mu(x)$ is determined from (2.11) for each of the three types given by (2.12)–(2.14) and the band-edge eigenvalues are E_0, $E_1,\ldots,E_n$. Note that n is to be computed for each of the algebraization in Table I.

III. EIGENSTATES AND SPECTRA OF TYPE I–III MODELS FOR SOME REAL VALUES OF THE POTENTIAL PARAMETERS

In this section we construct some examples based upon the general results obtained in the previous section. It may be useful to collect the following identities and differential relations among the Jacobian elliptic functions which will be frequently used:

$$sn^2x+cn^2x=1,\ \ dn^2x+k^2sn^2x=1,$$

$$sn'x=cnxdnx,\quad cn'x=-snxdnx,\quad dn'x=-k^2snxcnx.$$

In the following examples we denote the eigenstates[spectra] by $\phi_r(x)[e_r]$ whenever ordering is possible. Otherwise we denote them by $\psi_{E_i}[E_i]$, and $\psi_{E_i'}[E_i']$, indicating different algebraizations.

A. Type I model [defined on the domain (0,2K)]

We have got six algebraizations (see the solution 1.1–1.6 of Table I) for type I Hamiltonian (2.15). For each of them the corresponding eigenstates generate an orthogonal family of polynomials satisfying the recurrence relation (2.26). The explicit expressions of $\rho_j,\lambda_j,\omega_j$ together with the choice of ξ_1,ξ_2 and the overall restrictions on potential parameters are given in Table II.

It is clear that the algebraic solutions are obtained for the following two cases:

Case 1: $A\in(N-1)\cup(N-\frac{1}{2}),B\in R$

Here B is any real parameter and for each real values of B, A is allowed to take $0,\frac{1}{2},1,\frac{3}{2},\ldots,\Lambda\leqslant B$ (Λ is an integer or half-integer). For integer values of A, from the algebraizations 1.1–1.2 we get $(2A+1)$ band edge eigenstates and eigenvalues. Also for half-integer values of A the algebraization 1.4 gives $(A+\frac{1}{2})$ solutions of the Schrödinger equation.

Case 2: $B\in N\cup N-\frac{1}{2},A\in R$

Here A is any real number and B is allowed to take values $\frac{1}{2},1,\frac{3}{2},\ldots,\Lambda\leqslant A+1$ (Λ is integer or half-integer). It is to be noted that algebraization 1.3 is considered for integer values of B and 1.5–1.6 for half-integer B.

We now consider some specific examples when both of A and B are integer or half-integer.

1. $A=0$, $B=\frac{1}{2}$

$$V(x)=\frac{1}{4}\frac{dn^2x}{sn^2x}-\frac{1}{2}\frac{cnx}{sn^2x},$$
$$\phi_0(x)=\sqrt{\frac{snx}{1+cnx}},\quad e_0=0.\tag{3.1}$$

2. $A=0$, $B=\frac{3}{2}$

$$V(x)=\frac{9}{4}\frac{dn^2x}{sn^2x}-\frac{3}{2}\frac{cnx}{sn^2x},\tag{3.2}$$

$$\phi_0(x)=\left(\frac{snx}{1+cnx}\right)^{3/2}, \quad e_0=0.$$

3. A=½, B=1

$$V(x)=\frac{7}{4}\frac{dn^2x}{sn^2x}-2\frac{cnx}{sn^2x},$$
$$\phi_0(x)=\frac{\sqrt{snxdnx}}{1+cnx}exp\left(-\frac{i}{2}tan^{-1}\frac{kcnx}{k'}\right), \quad e_0=\frac{1-2k^2}{4}-ikk'. \tag{3.3}$$

4. A=½, B=2

$$V(x)=\frac{19}{4}\frac{dn^2x}{sn^2x}-4\frac{cnx}{sn^2x},$$
$$\phi_0(x)=\frac{\sqrt{dnx}sn^{3/2}x}{(1+cnx)^2}\exp\left(-\frac{i}{2}\tan^{-1}\frac{kcnx}{k'}\right), \quad e_0=\frac{1-2k^2}{4}-2ikk'. \tag{3.4}$$

5. A=1, B=3/2

$$V(x)=\frac{17}{4}\frac{dn^2x}{sn^2x}-\frac{9}{2}\frac{cnx}{sn^2x}.$$

For $0<k^2<\frac{1}{2}$,

$$\phi_{0,1}(x)=\frac{\sqrt{snx}}{(1+cnx)^{5/2}}[g_{\mp}(k)cn^2x+4cnx+4-g_{\mp}(k)], \quad e_{0,1}=1-4k^2+\frac{1}{2}g_{\mp}(k), \tag{3.5}$$

$$\phi_2(x)=\frac{dnx\sqrt{snx}}{(1+cnx)^{3/2}}, \quad e_2=1-2k^2, \tag{3.6}$$

where $g_{\pm}(k)=6k^2-1\pm\sqrt{1-36k^2k'^2}$.

For $\frac{1}{2}<k^2<1$, the suffixes 0,1,2 have to be replaced by 1,2,0, respectively.

Proceeding in the same fashion, we can find the eigenstates and spectra for higher values of A and B.

B. Type II model [defined on the domain (0,2K)]

Here two algebraizations are obtained (see the solution 2.1–2.2 of Table I). The related orthogonal polynomials are determined by the entries 2.1–2.2 of Table III. Note that both algebraizations are valid provided A is restricted to positive half-integer values only while the other parameter B is arbitrary.

Some examples are furnished below.

1. A=½

$$V(x)=B(B+1)\frac{dn^2x}{sn^2x}-\frac{3}{4}dn^2x,$$
$$\phi_0(x)=\frac{sn^{B+1}x}{(cnx+dnx)^{B+1/2}}, \quad e_0=-\frac{k'^2}{2}-\frac{k^2}{4}(2B+1)^2. \tag{3.7}$$

For $B\leqslant 0$, the following degenerated state is found:

TABLE III. The coeffecients ρ_j, λ_j, ω_j of the recurrence relation (2.26) and (2.27) together with the choice of ξ_1, ξ_2 and the overall restrictions on potential parameters are provided for type II (first two rows) and type III models.

Solution no.	n	ρ_j	λ_j	ω_j	(ξ_1, ξ_2)	Overall restrictions on A, B
2.1	$A-\frac{1}{2}$	$\left(\frac{k'^2}{2}\right)^2 j(2j-2A-1)(j-A+B)(2j+2B+1)$	$-\frac{k^2}{4}(2B+1)^2-\frac{k'^2}{8}(2A+1)^2+\frac{1+k^2}{8}$ $\times(2A-4j-1)(4B-2A+4j+3)$	$\left(\frac{k'^2}{2}\right)^j \frac{\Pi_{r=0}^{j+[B]}(2j+2B-2r+1)}{\Pi_{r=0}^{[B]}(2B-2r+1)}$	$(-1,1)$	$A \in N-\frac{1}{2},\ B \in R.$
2.2	$A-\frac{1}{2}$	$\left(\frac{k'^2}{2}\right)^2 j(2j-2A-1)(j-A-B-1)(2j-2B-1)$	$-\frac{k^2}{4}(2B+1)^2-\frac{k'^2}{8}(2A+1)^2+\frac{1+k^2}{8}$ $\times(2A-4j-1)(4j-2A-4B-1)$	$\left(\frac{k'^2}{2}\right)^j \frac{\Pi_{r=0}^{j}(2j-2B-2r-1)}{-2B-1}$	$(-1,1)$	$A \in N-\frac{1}{2},\ B \in R,$ $B \leqslant 0.$
3.1	A	$\left(\frac{k^2}{2}\right)^2 j(j-A-1)(2j-1)(2j-2A-1)$	$\frac{2j-A}{2}[(2j-A)(2-k^2)+4Bik']$ $-B^2k'^2-A(A+1)k^2/2$	$\left(\frac{k^2}{2}\right)^j \frac{\Pi_{r=0}^{j}(2j-1-2r)}{(-1)}$	$\left(\frac{i}{k'}, \frac{-i}{k'}\right)$	$A \in N-1,\ B \in R.$
3.2	$A-1$	$\left(\frac{k^2}{2}\right)^2 j(j-A)(2j-2A-1)(2j+1)$	$\frac{2j-A+1}{2}[(2j-A+1)(2-k^2)+4Bik']$ $-B^2k'^2-A(A+1)k^2/2$	$\left(\frac{k^2}{2}\right)^j \Pi_{r=0}^{j}(2j+1-2r)$	,,	$A \in N,\ B \in R.$
3.3	$A-\frac{1}{2}$	,,	$\left(\frac{1+2Bik'}{2}\right)^2-\frac{k^2}{8}(2A+1)^2+\frac{1}{8}(2A-4j-1)$ $\times[(k^2-2)(4j-2A+3)-8Bik']$	,,	,,	$A \in N-\frac{1}{2},\ B \in R.$

$$\psi_0(x)=(cnx+dnx)^{B+1/2}/sn^B x.$$

2. $A=\frac{3}{2}$

$$V(x)=B(B+1)\frac{dn^2x}{sn^2x}-\frac{15}{4}dn^2x,$$

$$\phi_{0,1}(x)=\frac{sn^{B+1}x}{(cnx+dnx)^{B+3/2}}\left[\left\{(1+k^2)\left(B+\frac{3}{2}\right)+\eta_{\mp}(k)\right\}cn^2x\right.$$
$$\left.+2\left(B+\frac{3}{2}\right)cnxdnx+k'^2\left(B+\frac{3}{2}\right)-\eta_{\mp}(k)\right], \tag{3.8}$$

$$e_{0,1}=\frac{6k^2-10-k^2(2B+1)^2}{4}\mp\sqrt{2(1+k^4)\left(B+\frac{1}{2}\right)^2-k'^4},$$

where

$$\eta_{\pm}(k)=-(1+k^2)\left(B+\frac{1}{2}\right)\pm\sqrt{2(1+k^4)\left(B+\frac{1}{2}\right)^2-k'^4}.$$

For $B\leqslant 0$, two other degenerated states are obtained:

$$\psi_{0,1}(x)=\frac{(cnx+dnx)^{B-1/2}}{sn^B x}\left[\left\{(1+k^2)\left(B+\frac{3}{2}\right)+\eta_{\mp}(k)\right\}cn^2x\right.$$
$$\left.+(1-2B)cnxdnx-k'^2\left(B-\frac{1}{2}\right)-(1+k^2)(2B+1)-\eta_{\mp}(k)\right].$$

C. Type III model [defined on the entire real line]

This corresponds to three algebraizations (see the solution 3.1–3.3 of Table I), the first two of which are for an integer A while the third one is for a half-integer A. As before, the eigenstates generate an orthogonal family of polynomials in the energy variable for each algebraization. The recurrence relation (2.26) is determined by the entries 3.1–3.3 of Table III. The other parameter B takes arbitrary values.

We now consider some examples.

1. $A=0$

$$V(x)=B^2k^2cn^2x+Bk^2snxcnx,$$
$$\phi_0(x)=\exp\left(-B\tan^{-1}\frac{snx}{cnx}\right),\quad e_0=-B^2k'^2. \tag{3.9}$$

2. $A=\frac{1}{2}$

$$V(x)=(B^2-\tfrac{3}{4})k^2cn^2x+2Bk^2snxcnx,$$

$$\phi_0(x)=\sqrt{dnx}\exp\left[-B\tan^{-1}\left(\frac{snx}{cnx}\right)+\frac{i}{2}\tan^{-1}\left(\frac{k'snx}{cnx}\right)\right], \tag{3.10}$$

$$e_0=-\frac{k^2}{2}+\left(\frac{1+2Bik'}{2}\right)^2.$$

3. $A=1$

$$V(x)=(B^2-2)k^2cn^2x+3Bk^2snxcnx,$$

$$\phi_0(x)=dnx\exp\left(-B\tan^{-1}\frac{snx}{cnx}\right),\quad e_0=-B^2k'^2-k^2, \tag{3.11}$$

$$\phi_{1,2}^{(i)}(x)=[(k^2\mp\sqrt{k^4-16k'^2B^2})snx+4Bcnx]\exp\left(-B\tan^{-1}\frac{snx}{cnx}\right),$$

$$\phi_{1,2}^{(ii)}(x)=[4Bk'^2snx+(k^2\pm\sqrt{k^4-16k'^2B^2})cnx]\exp\left(-B\tan^{-1}\frac{snx}{cnx}\right),$$

$$e_{1,2}=1-\tfrac{3}{2}k^2-B^2k'^2\mp\tfrac{1}{2}\sqrt{k^4-16k'^2B^2},$$

where the superscripts in the eigenstates indicate their double-degeneracy.

IV. ES LIMIT OF QES MODELS

We have so far constructed three new classes of QES potentials and explicitly obtained their eigenstates and spectra. Our purpose in this section is to show that corresponding to each type there is associated an ES class potential. It is useful to write down the following results of the ES limit:

$$sn(x,k)\underset{k\to0}{\overset{k\to1}{\to}}\begin{cases}\tanh x\\ \sin x\end{cases},\quad cn(x,k)\underset{k\to0}{\overset{k\to1}{\to}}\begin{cases}\operatorname{sech}x\\ \cos x\end{cases},\quad dn(x,k)\underset{k\to0}{\overset{k\to1}{\to}}\begin{cases}\operatorname{sech}x\\ 1\end{cases}. \tag{4.1}$$

Each of the three types of potentials are doubly periodic, one is real and the other imaginary. As $k\to1$ (or 0) we get an ES potential having an imaginary (or real) period.

A. ES classes associated to type I model

We have already shown that the type I model [cf. Eq. (2.15)] belongs to the QES periodic class. The potential has a real period $4K$ and imaginary period $4K'$, where $K'\equiv K(k')$. Using the relation (4.1) and the relation

$$K[K']\underset{k\to0}{\overset{k\to1}{\to}}\begin{cases}\infty & [\pi/2]\\ \pi/2 & [\infty]\end{cases}, \tag{4.2}$$

we see that the QES model is also exactly solvable when the modulus parameter $k\to1$ and 0. The associated ES classes are given by

$$k\to1:V_1(x)=[B^2+A(A+1)]\operatorname{cosech}^2x-2B(A+\tfrac{1}{2})\operatorname{cosech}x\coth x,\quad x\in(0,\infty), \tag{4.3}$$

$$k\to0:V_2(x)=[B^2+A(A+1)]\operatorname{cosec}^2x-2B(A+\tfrac{1}{2})\operatorname{cosec}x\cot x,\quad x\in(0,\pi), \tag{4.4}$$

whose eigenstates and spectra are[4]

$$\begin{aligned}\psi_r^{(1)}(x)&=(\cosh x-1)^{(B-A)/2}(\cosh x+1)^{-(B+A)/2}P_r^{(B-A-1/2,-B-A-1/2)}(\cosh x),\\ \psi_r^{(2)}(x)&=(1-\cos x)^{(B-A)/2}(1+\cos x)^{-(B+A)/2}P_r^{(B-A-1/2,-B-A-1/2)}(\cos x),\end{aligned} \tag{4.5}$$

$$E_r^{(1)}=-(A-r)^2,\quad E_r^{(2)}=(A-r)^2,\quad (r=0,1,2,\ldots), \tag{4.6}$$

where $P_r^{(\alpha,\beta)}(x)$ is the Jacobi polynomial and the superscripts 1 and 2 indicate the potentials $V_1(x)$ and $V_2(x)$, respectively. Note that we have solved the type I spectral problem (see Sec. III A) when at least one of the parameters A,B is an integer or a half-integer. Thus the ES results (4.5) and (4.6) can be reproduced from the associated QES results for this restricted domain of potential parameters only.

We now consider the ES limits of the examples given in Sec. III A [see Eqs. (3.1)–(3.5)]. In the following the superscripts in the eigenstates indicate whether they correspond to the potentials $V_1(x)$ and $V_2(x)$.

1. $A=0$, $B=\frac{1}{2}$

$$V_1(x)=\tfrac{1}{4}\operatorname{cosech}^2 x-\tfrac{1}{2}\operatorname{cosech} x\coth x, \tag{4.7}$$

$$V_2(x)=\tfrac{1}{4}\operatorname{cosec}^2 x-\tfrac{1}{2}\operatorname{cosec} x\cot x, \tag{4.8}$$

$$\phi_0^{(1)}(x)=\sqrt{\tanh\frac{x}{2}},\quad \phi_0^{(2)}(x)=\sqrt{\tan\frac{x}{2}},\quad e_0^{(1)}=e_0^{(2)}=0.$$

From (4.5) and (4.6) it follows that we can reproduce the ground states for the two ES classes.

2. $A=0$, $B=\frac{3}{2}$

$$V_1(x)=\tfrac{9}{4}\operatorname{cosech}^2 x-\tfrac{3}{2}\operatorname{cosech} x\coth x, \tag{4.9}$$

$$V_2(x)=\tfrac{9}{4}\operatorname{cosec}^2 x-\tfrac{3}{2}\operatorname{cosec} x\cot x, \tag{4.10}$$

$$\phi_0^{(1)}(x)=\tanh^{3/2}\frac{x}{2},\quad \phi_0^{(2)}(x)=\tan^{3/2}\frac{x}{2},\quad e_0^{(1)}=e_0^{(2)}=0.$$

Again ground levels for two ES potentials (4.9) and (4.10) are reproduced.

3. $A=\frac{1}{2}$, $B=1$

$$V_1(x)=\tfrac{7}{4}\operatorname{cosech}^2 x-2\operatorname{cosech} x\coth x, \tag{4.11}$$

$$V_2(x)=\tfrac{7}{4}\operatorname{cosec}^2 x-2\operatorname{cosec} x\cot x, \tag{4.12}$$

$$\phi_0^{(1)}(x)=\frac{\sqrt{\operatorname{sech} x\tanh x}}{1+\operatorname{sech} x},\quad \phi_0^{(2)}(x)=\frac{\sqrt{\sin x}}{1+\cos x},\quad e_0^{(1)}=-\frac{1}{4}=-e_0^{(2)}.$$

These are the ground states for the ES classes.

4. $A=\frac{1}{2}$, $B=2$

$$V_1(x)=\tfrac{19}{4}\operatorname{cosech}^2 x-4\operatorname{cosech} x\coth x, \tag{4.13}$$

$$V_2(x)=\tfrac{19}{4}\operatorname{cosec}^2 x-4\operatorname{cosec} x\cot x, \tag{4.14}$$

$$\phi_0^{(1)}(x)=\frac{\sinh^{3/2} x}{(1+\cosh x)^2},\quad \phi_0^{(2)}(x)=\frac{\sin^{3/2} x}{(1+\cos x)^2},\quad e_0^{(1)}=-\frac{1}{4}=-e_0^{(2)}.$$

These are the ground levels for ES potentials.

5. $A=1$, $B=\frac{3}{2}$

$$V_1(x)=\tfrac{17}{4}\operatorname{cosech}^2 x-\tfrac{9}{2}\operatorname{cosech} x\coth x, \tag{4.15}$$

$$V_2(x)=\tfrac{17}{4}\operatorname{cosec}^2 x-\tfrac{9}{2}\operatorname{cosec} x\cot x, \tag{4.16}$$

$$\phi_0^{(1)}(x)=\frac{\sqrt{\sinh x}}{(1+\cosh x)^{3/2}},\quad \phi_1^{(2)}(x)=\frac{\sqrt{\sin x}}{(1+\cos x)^{3/2}},\quad e_0^{(1)}=-1=-e_1^{(2)},$$

$$\phi_1^{(1)}(x)=\frac{\sqrt{\sinh x}(\cosh x-3)}{(1+\cosh x)^{3/2}},\quad \phi_0^{(2)}(x)=\frac{\sqrt{\sin x}(\cos x-3)}{(1+\cos x)^{3/2}},\quad e_1^{(1)}=0=e_0^{(2)}.$$

Here two ES levels are reproduced.

B. ES class associated to type II model

Using as before the relations (4.1) and (4.2), we see that in the limit $k\to 1$ type II potential (2.16) goes over to the following ES class known as the generalized Pöschl–Teller potential:

$$V_3(x)=B(B+1)\operatorname{cosech}^2 x-A(A+1)\operatorname{sech}^2 x, \tag{4.17}$$

its eigenstates and spectra being given by

$$\begin{gathered}\psi_r^{(3)}(x)=(\cosh 2x-1)^{-B/2}(\cosh 2x+1)^{-A/2}P_r^{(-B-1/2,-A-1/2)}(\cosh 2x),\\ E_r^{(3)}=-(A+B-2r)^2\quad (r=0,1,2,\ldots),\end{gathered} \tag{4.18}$$

where the superscripts indicate correspondance with $V_3(x)$.

We recall that the QES levels for the type II model are obtained for half-integer values of A. Let us now take the ES limit of the examples given in Sec III B [see Eqs. (3.6) and (3.7)]. The other parameter B is taken as negative real number.

1. $A=\frac{1}{2}$

$$\begin{gathered}V_3(x)=B(B+1)\operatorname{cosech}^2 x-\tfrac{3}{4}\operatorname{sech}^2 x,\\ \psi_0^{(3)}(x)=\operatorname{cosech}^B x\sqrt{\operatorname{sech} x},\quad e_0^{(3)}=-\frac{(2B+1)^2}{4}.\end{gathered} \tag{4.19}$$

Here $\psi_0^{(3)}$, $e_0^{(3)}$ are ground level for the ES potential $V_3(x)$.

2. $A=\frac{3}{2}$

$$\begin{gathered}V_3(x)=B(B+1)\operatorname{cosech}^2 x-\tfrac{15}{4}\operatorname{sech}^2 x,\\ \psi_0^{(3)}(x)=\sinh^{-B} x\cosh^{-3/2} x,\quad e_0^{(3)}=-(B+\tfrac{3}{2})^2,\\ \psi_1^{(3)}(x)=\frac{\sinh^{-B} x}{\cosh^{3/2} x}[(2B+1)\cosh^2 x-2],\quad e_1^{(3)}=-(B-\tfrac{1}{2})^2.\end{gathered} \tag{4.20}$$

Here $\psi_{0,1}^{(3)}$, $e_{0,1}^{(3)}$ are two levels for the ES potential (4.20).

C. ES class associated to type III model

The type III potential (2.17) is defined on the entire real line. This is a QES periodic potential having a real period $2K$ and an imaginary period $4K'$. The algebraic sector is determined for an integer or a half-integer A, while B is arbitrary real parameter. In the limit $k\to 1$, this potential coincides to the following ES class:

$$V_4(x)=[B^2-A(A+1)]\operatorname{sech}^2 x+2B(A+\tfrac{1}{2})\operatorname{sech} x\tanh x. \tag{4.21}$$

The eigenstates and spectra of the potential (4.21) are

$$\psi_r^{(4)}(x)=\operatorname{sech}^A x\exp[-B\tan^{-1}(\sinh x)]P_r^{(-iB-A-1/2,iB-A-1/2)}(i\sinh x),$$

$$E_r^{(4)}=-(A-r)^2 \quad (r=0,1,2,\ldots). \tag{4.22}$$

We now take the ES limit (here $k\to 1$ only) of the examples given in Sec III C. Note that the limit $k\to 0$ gives a free particle motion.

1. $A=0$

$$\begin{aligned} V_4(x)&=B^2\operatorname{sech}^2 x+B\operatorname{sech} x\tanh x,\\ \phi_0^{(4)}(x)&=\exp(-B\tan^{-1}\sinh x),\quad e_0^{(4)}=0. \end{aligned} \tag{4.23}$$

Clearly, the ground state for (4.23) agrees with the general results (4.22) for $A=0$.

2. $A=\frac{1}{2}$

$$\begin{aligned} V_4(x)&=(B^2-\tfrac{3}{4})\operatorname{sech}^2 x+2B\operatorname{sech} x\tanh x,\\ \phi_0^{(4)}(x)&=\sqrt{\operatorname{sech} x}\exp[-B\tan^{-1}(\sinh x)],\quad e_0^{(4)}=-\tfrac{1}{4}. \end{aligned} \tag{4.24}$$

This is also in agreement with (4.22) for $A=\frac{1}{2}$.

3. $A=1$

$$\begin{aligned} V_4(x)&=(B^2-2)\operatorname{sech}^2 x+3B\operatorname{sech} x\tanh x,\\ \phi_0^{(4)}(x)&=\operatorname{sech} x\exp(-B\tan^{-1}\sinh x)=\phi_1^{(4)}(x),\quad e_0^{(4)}=-1=e_1^{(4)},\\ \phi_2^{(4)}(x)&=\operatorname{sech} x(\sinh x+2B)\exp(-B\tan^{-1}\sinh x),\quad e_2^{(4)}=0. \end{aligned} \tag{4.25}$$

Thus two ES levels are reproduced from the corresponding QES levels.

Hence we have shown that corresponding to three QES models types I, II and III, there is associated some definite ES classes namely V_1, V_2 (for type I),V_3 (for type II) and V_4 (for type III), respectively. In the ES limit we can reproduce some ES levels from the corresponding QES levels as well.

V. CONCLUSION

To conclude, we have constructed three new QES elliptic potentials types I–III using an sl(2,R) Lie-algebraic scheme and obtained their algebraic levels analytically. Further, we have shown that the eigenstates of QES Hamiltonians generate an orthogonal family of polynomials in the energy variable. The interesting point is that the elliptic parameter $k(0<k^2<1)$ in the models

turns out to be responsible for QES class and, when it touches the end-points 0 and 1 of its domain, the ES classes are revealed. We have explicitly shown that some ES levels can be reproduced on a restricted domain of potential parameters.

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Density and current of a dissipative Schrödinger operator

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We regard a current flow through an open one-dimensional quantum system which is determined by a dissipative Schrödinger operator. The imaginary part of the corresponding form originates from Robin boundary conditions with certain complex valued coefficients imposed on Schrödinger's equation. This dissipative Schrödinger operator can be regarded as a pseudo-Hamiltonian of the corresponding open quantum system. The dilation of the dissipative operator provides a (self-adjoint) quasi-Hamiltonian of the system, more precisely, the Hamiltonian of the minimal closed system which contains the open one is used to define physical quantities such as density and current for the open quantum system. The carrier density turns out to be an expression in the generalized eigenstates of the dilation while the current density is related to the characteristic function of the dissipative operator. Finally a rigorous setup of a dissipative Schrödinger–Poisson system is outlined. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1507825]

I. INTRODUCTION

Quantum wells are an important feature of many optoelectronic devices, e.g., semiconductor quantum well lasers. While the drift-diffusion and energy models in general provide an adequate description, see, e.g., Refs. 1 and 2, the optical active zones and their environment require a more refined modeling because genuine quantum effects come to bear.[3]

A comprehensive model reflecting both the necessity of quantum mechanical simulations and their restriction for technical and economic reasons will combine some quantum mechanical model for the optical active zone and a drift-diffusion or energy model elsewhere. The main conceptual problem in matching macroscopic and quantum mechanical quantities, see, e.g., Refs. 4 and 5, is to obtain some form of current continuity all over the device. The main idea is to postulate the continuity of the the normal components of the currents at the model interface. This poses a variety of problems on both sides—the macroscopic model and the quantum mechanical one. In particular many quantum mechanical models for the active zone such as the stationary Kohn–Sham system, see, e.g., Refs. 6 and 7, are closed systems and thus, the flow vanishes identically all over the system. This assumption is not justified in the intended combined model in view of the electric flow through the interface. Hence, one has to pass to open quantum systems; and here the first difficulty consists in defining particle densities and currents at all. The aim of this paper is a rigorous definition of these physical quantities with respect to the dissipative Schrödinger operator related to an open quantum system which might serve as a quantum mechanical model for one-dimensional semiconductor nanostructures, as quantum wells or multi-quantum wells.

Let us first have a look at the case of a closed quantum system situated in a bounded one-dimensional spatial domain $\Omega=[a,b]$. We regard Schrödinger's equation

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$$-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{m(x)}\frac{\mathrm{d}\psi(x)}{\mathrm{d}x}\right)+V(x)\psi(x)=\lambda\psi(x),\quad x\in[a,b] \tag{1.1}$$

with a real valued potential V and a positive function m, which represents the position-dependent effective mass multiplied by $1/\hbar^2$. If we impose homogeneous Neumann or Dirichlet boundary conditions at a and b, then the corresponding operator H on the Hilbert space $L^2([a,b])$ of complex valued, square integrable functions on $[a,b]$ becomes a self-adjoint one. For that case the formalism of quantum mechanics is well developed and one obtains the carrier density in the following way: H is an operator with compact resolvent. Let us denote by $\{\mathcal{E}_l\}_{l=1}^{\infty}$ and $\{\psi_l\}_{l=1}^{\infty}$ the sequence of eigenvalues and eigenfunctions counting multiplicities and let $\hat{\varrho}:=\{\varrho_l\}_{l=1}^{\infty}$ be a sequence of occupation numbers which add up to the total number N of carriers in the system

$$N:=\sum_{l=1}^{\infty}\varrho_l. \tag{1.2}$$

The carrier density is given by

$$u_{\hat{\varrho}}(x)=\sum_{l=1}^{\infty}\varrho_l|\psi_l(x)|^2,\qquad x\in[a,b]. \tag{1.3}$$

Usually, the sequence $\hat{\varrho}$ is expressed in terms of an equilibrium distribution function f which is non-negative and decreasing:

$$\varrho_l:=f(\mathcal{E}_l),\quad l=1,2,\ldots. \tag{1.4}$$

Thus, the operator

$$\varrho:=f(H) \tag{1.5}$$

is self-adjoint and non-negative. If the equilibrium distribution function $f(\lambda)$ tends to zero sufficiently fast as $\lambda\to+\infty$, then ϱ is nuclear. Moreover, there is $N=\mathrm{tr}(\varrho)=\mathrm{tr}(f(H))$. Non-negative, self-adjoint, nuclear operators are density matrices. Since ϱ commutes with H the density matrix ϱ remains unchanged in time, i.e., ϱ is a steady state. If the density matrix is given, then the number of carriers $N_\varrho(\omega)$ in the set $\omega\subseteq[a,b]$ can be expressed by

$$N_\varrho(\omega)=\mathrm{tr}(\varrho\chi_\omega), \tag{1.6}$$

where $\chi_\omega(\cdot)$ is the indicator function of the subset ω. It turns out that (1.6) defines an absolutely continuous measure (with respect to the Lebesgue measure). One verifies that its Radon–Nikodym derivative u_ϱ coincides with the carrier density defined by (1.3), i.e., $u_{\hat{\varrho}}=u_\varrho$.

The system described by H is closed. Hence, there is no interaction with the environment, in particular, no carrier exchange. Consequently, the current density $j_{\hat{\varrho}}(x)$ defined by

$$j_{\hat{\varrho}}(x):=\sum_{l=1}^{\infty}\varrho_l j_l(x),\quad x\in[a,b], \tag{1.7}$$

is identical zero, where in accordance with Ref. 8 the current density $j_l(x)$ of the eigenstate ψ_l is given by

$$j_l(x):=\mathrm{Im}\left(\frac{1}{m(x)}\psi_l'(x)\overline{\psi_l(x)}\right),\quad x\in[a,b],\quad l=1,2,\ldots. \tag{1.8}$$

This consequence is unacceptable, if we want to model a net current flow through the boundary of the system. To that end we devised non-self-adjoint boundary conditions for Schrödinger's equation, see Refs. 6, 7, and 5, i.e., we regard the Schrödinger operator H with the domain

$$\mathrm{dom}(H)=\left\{ g\in W^{1,2}([a,b]):\ \begin{array}{l} \dfrac{1}{m(x)}g'(x)\in W^{1,2}([a,b]),\\ \dfrac{1}{2m(a)}g'(a)=-\kappa_a g(a),\\ \dfrac{1}{2m(b)}g'(b)=\kappa_b g(b) \end{array} \right\}, \tag{1.9}$$

where $\kappa_a,\kappa_b\in\mathbb{C}$. If at least one of the imaginary parts is different from zero, then the operator H is non-self-adjoint. However, this non-self-adjointness implies several complications. In particular, the notion of carrier density becomes unclear.

This situation can be handled if we restrict ourselves to dissipative operators. Let us recall that an operator is called dissipative if the imaginary part of its associated quadratic form is nonpositive. In the present case the operator H is dissipative if $\kappa_a,\kappa_b\in\mathbb{C}_+:=\{z\in\mathbb{C}:\mathrm{Im}(z)>0\}$. Moreover, under this assumption the operator H becomes maximal dissipative, i.e., it admits no proper dissipative extension, see Ref. 5. The main technical tool to overcome the difficulties is the dilation theory for maximal dissipative operators. In Ref. 9 the minimal self-adjoint dilation K of H was explicitly constructed and analyzed in detail. From the physical point of view the minimal self-adjoint dilation plays the role of the Hamiltonian of a larger closed system which contains the original system described by the pseudo-Hamiltonian H, i.e., it acts as a quasi-Hamiltonian of the open system, cf. Ref. 5. Using this fact one defines steady states, carrier densities and current densities of the dissipative quantum system by means of the corresponding quantities derived from the quasi-Hamiltonian K. In this paper we aim at expressing these quantities in terms of the pseudo-Hamiltonian H itself. Indeed, the carrier and current densities are expectation values of the corresponding observables which are composites of H. In particular, the current density observable is related to the characteristic function of the operator H. It turns out that the current density is independent of $x\in[a,b]$ and, in general, different from zero. So we have a constant current through $[a,b]$.

This formal approach to the net current flow problem fits into scattering models, see, e.g., Refs. 10–12 and in particular the concept of transparent boundary conditions, (see e.g., Refs. 13 and 14), which has been extended to the multi dimensional case in Refs. 15 and 16. In these models one replaces the maximal dissipative operator H by a family of maximal dissipative operators $\{H(z)\}_{z\in\overline{\mathbb{C}_+}}$ defined on $L^2([a,b])$. If $a=0$, $b=1$, and $m(x)\equiv 1/2$, then $H(z)$ is given by

$$\begin{aligned} \mathrm{dom}(H(z))&:=\left\{ g\in W^{2,2}([0,1]):\ \begin{array}{l} g'(1)=\kappa_1(z)g(1)\\ g'(0)=-\kappa_0(z)g(0), \end{array} \right\},\\ (H(z)g)(x)&:=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}g(x)+V(x)g(x),\quad g\in\mathrm{dom}(H(z)), \end{aligned} \tag{1.10}$$

with

$$\kappa_1(z):=i\sqrt{z}\quad\text{and}\quad\kappa_0(z):=i\sqrt{z-V_-},\quad z\in\overline{\mathbb{C}_+}, \tag{1.11}$$

see Ref. 10, where the cut of the square root is along $[0,\infty)$ and $\mathrm{Im}(\sqrt{z})\geqslant 0$ for $z\in\mathbb{C}_+$. Let us consider the self-adjoint Schrödinger operator K,

$$\begin{aligned} \mathrm{dom}(K) &:= W^{2,2}(\mathbb{R}), \\ (Kf)(x) &:= -\frac{\mathrm{d}^2}{\mathrm{d}x^2} f(x) + V_{KL}(x) f(x), \quad f \in \mathrm{dom}(K), \end{aligned} \tag{1.12}$$

on the Hilbert space $L^2(\mathbb{R})$ whose potential $V_{KL} \in C(\mathbb{R})$ looks like

$$V_{KL} = \begin{cases} V_- & : \ x \in \mathbb{R}_- \\ V & : \ x \in [0,1] \\ 0 & : \ x \in (1,+\infty) \end{cases}, \tag{1.13}$$

where $V_- > 0$,

$$V(0) = V_- \quad \text{and} \quad V(1) = 0. \tag{1.14}$$

Operators of this type have been investigated in Ref. 17. It turns out that

$$P(K-z)^{-1}\big|_{L^2([0,1])} = (H(z)-z)^{-1}, \quad z \in \mathbb{C}_+, \tag{1.15}$$

where P is the orthogonal projector from $L^2(\mathbb{R})$ onto $L^2([0,1])$. This means that the operator K can be regarded as a self-adjoint dilation of the family $\{H(z)\}_{z \in \overline{\mathbb{C}_+}}$. Moreover,

$$\bigvee_{z \in \mathbb{C} \setminus \mathbb{R}} (K-z)^{-1} L^2([0,1]) = L^2(\mathbb{R}), \tag{1.16}$$

i.e., K is a minimal self-adjoint dilation, hence, uniquely determined up to an isomorphism. Thus, if we want to compute quantities which are related to the subspace $L^2([0,1])$, for instance, carrier densities on the interval $[0,1]$, we can do this using either the self-adjoint operator K or the family $\{H(\lambda)\}_{\lambda \in \mathbb{R}}$ of maximal dissipative operators. Moreover, if we are only interested in quantities with respect to a small energy interval around the energy $\lambda_0 \in \mathbb{R}$ (in the limit only quantities for the energy λ_0), then it suffices to consider the maximal dissipative operator $H(\lambda_0)$ which leads to a model described at the beginning.

The paper is organized as follows. In Sec. II we rigorously define Schrödinger-type operators and briefly recall their properties, see Ref. 5. Moreover, we introduce the important notion of the characteristic function $\Theta_H(z)$ and briefly describe the minimal self-adjoint dilation K of H. Further we state its generalized eigenfunction expansion following Ref. 9. In Sec. III we introduce generalized steady states and define carrier densities. In Sec. IV we define the current density and express it in terms of the characteristic function. In particular, it turns out that if the steady state is given by $\varrho = f(K)$, then the current density is zero. In Sec. V we comment on the results, in particular, we clarify the relation to the Lax–Phillips scattering theory and verify the continuity equation. Finally, we give a rigorous setting of dissipative Schrödinger–Poisson systems which have the advantage that their current densities are different from zero for suitably chosen steady states.

II. SCHRÖDINGER-TYPE OPERATORS

Following the proposal of Ref. 6 we consider the non-self-adjoint Schrödinger-type operator H on the Hilbert space $\mathfrak{h} = L^2([a,b])$ given by the domain (1.9) and

$$(Hg)(x) = (l(g))(x), \quad g \in \mathrm{dom}(H), \tag{2.1}$$

where

$$(l(g))(x) := -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x} g(x) + V(x) g(x), \tag{2.2}$$

and $V\in L^2([a,b])$ is a real potential, the effective mass $m(x)>0$ obeys $m(x)+1/m(x)\in L^\infty([a,b])$ and κ_a, $\kappa_b\in\mathbb{C}_+$. The operator H is maximal dissipative and completely non-self-adjoint, see Ref. 5. The spectrum of H consists of isolated eigenvalues in the lower half-plane with the only accumulation point at infinity. Since the operator H is completely non-self-adjoint there do not exist real eigenvalues. To analyze the operator H it is useful to introduce the elementary solutions $v_a(x,z)$ and $v_b(x,z)$,

$$l(v_a(x,z))-zv_a(x,z)=0,\quad v_a(a,z)=1,\quad \frac{1}{2m(a)}v_a'(a,z)=-\kappa_a, \tag{2.3}$$

$$l(v_b(x,z))-zv_b(x,z)=0,\quad v_b(b,z)=1,\quad \frac{1}{2m(b)}v_b'(b,z)=\kappa_b, \tag{2.4}$$

$x\in[a,b]$, $z\in\mathbb{C}$, which always exist. The Wronskian $W(z)$ of $v_a(x,z)$ and $v_b(x,z)$ is defined by

$$W(z)=v_a(x,z)\frac{1}{2m(x)}v_b'(x,z)-v_b(x,z)\frac{1}{2m(x)}v_a'(x,z). \tag{2.5}$$

We note that the Wronskian does not depend on x. Similarly, the functions $v_{*a}(x,z)$ and $v_{*b}(x,z)$,

$$v_{*a}(x,z):=\overline{v_a(x,\overline{z})}\qquad\text{and}\qquad v_{*b}(x,z):=\overline{v_b(x,\overline{z})},\quad z\in\mathbb{C}, \tag{2.6}$$

$x\in[a,b]$, $z\in\mathbb{C}$, are elementary solutions of

$$l(v_{*a}(x,z))-zv_{*a}(x,z)=0,\quad v_{*a}(a,z)=1,\quad \frac{1}{2m(a)}v_{*a}'(a,z)=-\overline{\kappa_a}, \tag{2.7}$$

$$l(v_{*b}(x,z))-zv_{*b}(x,z)=0,\quad v_{*b}(b,z)=1,\quad \frac{1}{2m(b)}v_{*b}'(b,z)=\overline{\kappa_b}, \tag{2.8}$$

$x\in[a,b]$. The Wronskian of $v_{*a}(x,z)$ and $v_{*b}(x,z)$ is denoted by $W_*(z)$ and is also independent of x. By these elementary solutions one gets for the resolvents the representations

$$((H-z)^{-1}f)(x)=-\frac{v_b(x,z)}{W(z)}\int_a^x dy\, v_a(y,z)f(y)-\frac{v_a(x,z)}{W(z)}\int_x^b dy\, v_b(y,z)f(y), \tag{2.9}$$

for $z\in\varrho(H)$, $f\in L^2([a,b])$ and

$$((H^*-z)^{-1}f)(x)=-\frac{v_{*b}(x,z)}{W_*(z)}\int_a^x dy\, v_{*a}(y,z)f(y)-\frac{v_{*a}(x,z)}{W_*(z)}\int_x^b dy\, v_{*b}(y,z)f(y), \tag{2.10}$$

for $z\in\varrho(H^*)$ and $f\in L^2([a,b])$, see Ref. 9.

Since H is completely non-self-adjoint the maximal dissipative operator H can be completely characterized by its characteristic function $\Theta_H(z)$, $z\in\varrho(H)\cap\varrho(H^*)$, cf. Ref. 18. The definition of the characteristic function relies on the so-called boundary operators $T(z):\mathfrak{h}\to\mathbb{C}^2$, $z\in\varrho(H)$ and $T_*(z):\mathfrak{h}\to\mathbb{C}^2$, $z\in\varrho(H^*)$, which are defined in Ref. 9. Writing

$$\kappa_a=q_a+\frac{i}{2}\alpha_a^2\quad\text{and}\quad\kappa_b=q_b+\frac{i}{2}\alpha_b^2,\quad \alpha_a,\alpha_b>0, \tag{2.11}$$

the boundary operators are defined by

$$T(z)f := \begin{pmatrix} \alpha_b((H-z)^{-1}f)(b) \\ -\alpha_a((H-z)^{-1}f)(a) \end{pmatrix} \tag{2.12}$$

and

$$T_*(z)f := \begin{pmatrix} \alpha_b((H^*-z)^{-1}f)(b) \\ -\alpha_a((H^*-z)^{-1}f)(a) \end{pmatrix}, \tag{2.13}$$

$f \in L^2([a,b])$. Using the resolvent representations (2.9) and (2.10) we obtain

$$T(z)f = \frac{1}{W(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\, v_a(y,z)f(y) \\ \alpha_a \int_a^b dy\, v_b(y,z)f(y) \end{pmatrix} \tag{2.14}$$

and

$$T_*(z)f = \frac{1}{W_*(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\, v_{*a}(y,z)f(y) \\ \alpha_b \int_a^b dy\, v_{*b}(y,z)f(y) \end{pmatrix}, \tag{2.15}$$

$f \in L^2([a,b])$. The adjoint operators are given by

$$(T(z)^*\xi)(x) = \frac{1}{\overline{W(z)}}(-\alpha_b \overline{v_a(x,z)}, \alpha_a \overline{v_b(x,z)})\xi = \frac{1}{W_*(\overline{z})}(-\alpha_b v_{*a}(x,\overline{z}), \alpha_a v_{*b}(x,\overline{z}))\xi, \tag{2.16}$$

and

$$(T_*(z)^*\xi)(x) = \frac{1}{\overline{W_*(z)}}(-\alpha_b \overline{v_{*a}(x,z)}, \alpha_a \overline{v_{*b}(x,z)})\xi = \frac{1}{W(\overline{z})}(-\alpha_b v_a(x,\overline{z}), \alpha_a v_b(x,\overline{z}))\xi, \tag{2.17}$$

where

$$\xi = \begin{pmatrix} \xi^b \\ \xi^a \end{pmatrix} \in \mathbb{C}^2. \tag{2.18}$$

The characteristic function Θ_H of the maximal dissipative operator H is a two-by-two matrix-valued function which satisfies

$$\Theta_H(z)T(z)f = T_*(z)f, \quad z \in \varrho(H) \cap \varrho(H^*), \tag{2.19}$$

$f \in L^2([a,b])$. It depends meromorphically on $z \in \varrho(H) \cap \varrho(H^*)$ and is contractive in $\mathbb{C}_-$, i.e.,

$$\|\Theta_H(z)\| \leqslant 1 \quad \text{for} \quad z \in \mathbb{C}_-. \tag{2.20}$$

Using the elementary solutions the characteristic function Θ_H takes the form

$$\Theta_H(z) = I_{\mathbb{C}^2} + i\frac{1}{W_*(z)} \begin{pmatrix} \alpha_b^2 v_{*a}(b,z) & -\alpha_b\alpha_a \\ -\alpha_b\alpha_a & \alpha_a^2 v_{*b}(a,z) \end{pmatrix}. \tag{2.21}$$

for $z \in \varrho(H) \cap \varrho(H^*)$, cf. Ref. 9.

Since H is a maximal dissipative operator there is a larger Hilbert space $\mathfrak{k} \supseteq \mathfrak{h}$ and a self-adjoint operator K on $\mathfrak{k}$ such that

$$P_{\mathfrak{h}}^{\mathfrak{k}}(K-z)^{-1}|\mathfrak{h} = (H-z)^{-1}, \quad \mathrm{Im}(z) > 0, \tag{2.22}$$

see Ref. 18. The operator K is called a self-adjoint dilation of the maximal dissipative operator H. Obviously, from the condition (2.22) one gets

$$P_{\mathfrak{h}}^{\mathfrak{k}}(K-z)^{-1}|\mathfrak{h} = (H^*-z)^{-1}, \quad \mathrm{Im}(z) < 0. \tag{2.23}$$

K is called a minimal self-adjoint dilation of H if the condition

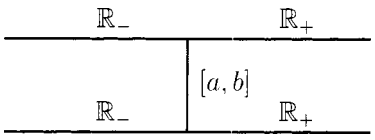
$$\bigvee_{z \in \mathbb{C} \setminus \mathbb{R}} (K-z)^{-1}\mathfrak{h} = \mathfrak{k} \tag{2.24}$$

is satisfied. Minimal self-adjoint dilations of maximal dissipative operators are determined up to a certain isomorphism, in particular, all minimal self-adjoint dilations are unitarily equivalent.

In the present case the minimal self-adjoint dilation of the maximal dissipative operator H can be constructed in an explicit manner. Following Ref. 9 we introduce the larger Hilbert space

$$\mathfrak{k} = \mathcal{D}_- \oplus \mathfrak{h} \oplus \mathcal{D}_+, \tag{2.25}$$

where $\mathcal{D}_\pm := L^2(\mathbb{R}_\pm, \mathbb{C}^2)$. Introducing the graph $\hat{\Omega}$,



one can write the Hilbert space $\mathfrak{k}$ as $L^2(\hat{\Omega})$. Furthermore, we define

$$\vec{g} := g_- \oplus g \oplus g_+, \tag{2.26}$$

where

$$g_-(x) := \begin{pmatrix} g_-^b(x) \\ g_-^a(x) \end{pmatrix} \quad \text{and} \quad g_+(x) := \begin{pmatrix} g_+^b(x) \\ g_+^a(x) \end{pmatrix}, \tag{2.27}$$

for $x \in \mathbb{R}_-$ and $x \in \mathbb{R}_+$, respectively. Let the matrices $K_\pm^a$ and $K_\pm^b$ given by

$$K_-^a := \frac{1}{\alpha_a}\begin{pmatrix} 0 & 0 \\ 1 & \kappa_a \end{pmatrix} \quad \text{and} \quad K_+^a := \frac{1}{\alpha_a}\begin{pmatrix} 0 & 0 \\ 1 & \overline{\kappa_a} \end{pmatrix} \tag{2.28}$$

as well as

$$K_-^b := \frac{1}{\alpha_b}\begin{pmatrix} 1 & -\kappa_b \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad K_+^b := \frac{1}{\alpha_b}\begin{pmatrix} 1 & -\overline{\kappa_b} \\ 0 & 0 \end{pmatrix}. \tag{2.29}$$

Using these notations the self-adjoint dilation K is defined by

$$\mathrm{dom}(K) := \left\{ \vec{g} \in \mathfrak{k}: \begin{array}{l} g_\pm \in W^{1,2}(\mathbb{R}_\pm, \mathbb{C}^2) \\ g, \dfrac{1}{m} g' \in W^{1,2}([a,b]) \\ K_-^a g_a + K_-^b g_b = g_-(0) \\ K_+^a g_a + K_+^b g_b = g_+(0) \end{array} \right\} \tag{2.30}$$

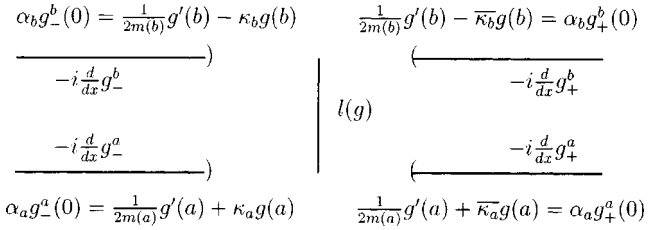
and

$$K\vec{g} := -i\frac{\mathrm{d}}{\mathrm{d}x} g_- \oplus l(g) \oplus -i\frac{\mathrm{d}}{\mathrm{d}x} g_+, \quad \vec{g} \in \mathrm{dom}(K), \tag{2.31}$$

where

$$g_a = \begin{pmatrix} \dfrac{1}{2m(a)} g'(a) \\ g(a) \end{pmatrix} \quad \text{and} \quad g_b = \begin{pmatrix} \dfrac{1}{2m(b)} g'(b) \\ g(b) \end{pmatrix}. \tag{2.32}$$

With respect to a graph picture the operator K looks like



The self-adjoint operator K is absolutely continuous and its spectrum coincides with the real axis, i.e., $\sigma(K) = \mathbb{R}$. The multiplicity of its spectrum is two. The resolvent of K admits the representation

$$\begin{aligned} (K-z)^{-1}(f_- \oplus f \oplus f_+) = {} & i\int_{-\infty}^{x} \mathrm{d}y\, e^{i(x-y)z} f_-(y) \oplus (H-z)^{-1} f + iT_*(\overline{z})^* \int_{-\infty}^{0} \mathrm{d}y\, e^{-iyz} f_-(y) \\ & \oplus i\int_{0}^{x} \mathrm{d}y\, e^{i(x-y)z} f_+(y) + ie^{izx} T(z) f + i\Theta_H(\overline{z})^* \int_{-\infty}^{0} \mathrm{d}y\, e^{i(x-y)z} f_-(y) \end{aligned} \tag{2.33}$$

for $\mathrm{Im}(z) > 0$ and

$$\begin{aligned} (K-z)^{-1}(f_- \oplus f \oplus f_+) = {} & -i\int_{x}^{0} \mathrm{d}y\, e^{i(x-y)z} f_-(y) - ie^{izx} T_*(z) f - i\Theta_H(z) \int_{0}^{\infty} \mathrm{d}y\, e^{i(x-y)z} f_+(y) \\ & \oplus (H^*-z)^{-1} f - iT(\overline{z})^* \int_{0}^{\infty} \mathrm{d}y\, e^{-iyz} f_+(y) \oplus -i\int_{x}^{\infty} \mathrm{d}y\, e^{i(x-y)z} f_+(y) \end{aligned} \tag{2.34}$$

for $\mathrm{Im}(z) < 0$. The generalized eigenfunctions $\vec{\psi}^-(\cdot, \lambda, \tau)$, $\lambda \in \mathbb{R}$, $\tau = a, b$, of K are given by

$$\vec{\psi}^-(x,\lambda,\tau) := \psi_-^-(x,\lambda,\tau) \oplus \psi^-(x,\lambda,\tau) \oplus \psi_+^-(x,\lambda,\tau)$$
$$= \frac{1}{\sqrt{2\pi}} e^{ix\lambda} e_\tau \oplus \frac{1}{\sqrt{2\pi}} (T_*(\lambda) * e_\tau)(x) \oplus \frac{1}{\sqrt{2\pi}} e^{ix\lambda} \Theta_H(\lambda) * e_\tau, \tag{2.35}$$

where

$$e_b := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad e_a := \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.36}$$

The functions are mutually orthogonal, i.e., one has

$$(\vec{\psi}^-(\cdot,\lambda,\tau), \vec{\psi}^-(\cdot,\lambda',\tau'))_{L^2(\hat{\Omega})} = \delta(\lambda-\lambda')\,\delta_{\tau\tau'}, \tag{2.37}$$

in the sense of distribution for $\lambda,\lambda' \in \mathbb{R}$, $\tau,\tau' = a,b$. Moreover, elements of the form

$$\int_{\mathbb{R}} d\lambda \sum_{\tau=a,b} \vec{\psi}^-(\cdot,\lambda,\tau)\hat{g}^\tau(\lambda) \tag{2.38}$$

where $\hat{g}^\tau(\cdot)$, $\tau = a,b$, are smooth functions with compact support, are dense in $\mathfrak{k}$. We note that the generalized eigenfunctions $\vec{\psi}^-(\cdot,\lambda,\tau)$ are usually called the incoming eigenfunctions. Using the incoming eigenfunctions one defines a transformation $\Phi_- : \mathfrak{k} \to \hat{\mathfrak{k}} = L^2(\mathbb{R},\mathbb{C}^2)$,

$$(\Phi_- \vec{g})(\lambda) =: \hat{g}(\lambda) = \begin{pmatrix} \hat{g}^b(\lambda) \\ \hat{g}^a(\lambda) \end{pmatrix}, \tag{2.39}$$

where

$$\hat{g}^\tau(\lambda) := \int_{\hat{\Omega}} dx\ (\vec{g}(x), \vec{\psi}^-(x,\lambda,\tau)), \quad \tau = a,b. \tag{2.40}$$

Φ_- is unitary and called the incoming Fourier transformation. The inverse incoming Fourier transformation Φ_-^{-1} is given by

$$(\Phi_-^{-1}\hat{g})(x) = \int_{\mathbb{R}} d\lambda \sum_{\tau=a,b} \vec{\psi}^-(x,\lambda,\tau)\hat{g}^\tau(\lambda), \quad \hat{g} \in L^2(\mathbb{R},\mathbb{C}^2). \tag{2.41}$$

We note that

$$\Phi_- K \Phi_-^{-1} = M, \tag{2.42}$$

where M is the multiplication operator by the independent variable λ on $\hat{\mathfrak{k}}$, i.e.,

$$\mathrm{dom}(M) := \{\hat{g} \in L^2(\mathbb{R},\mathbb{C}^2) : \lambda\hat{g}(\lambda) \in L^2(\mathbb{R},\mathbb{C}^2)\},$$
$$(M\hat{g})(\lambda) := \lambda\hat{g}(\lambda), \quad \hat{g} \in \mathrm{dom}(M). \tag{2.43}$$

The representation (2.43) induced by Φ_- is called the incoming spectral representation of K.

Finally, we note that each bounded self-adjoint operator G on $\mathfrak{k}$, which commutes with K, corresponds to a measurable family $\{G(\lambda)\}_{\lambda\in\mathbb{R}}$ of two-by-two matrices, which are uniformly bounded, i.e., $G(\cdot) \in L^\infty(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$, such that the multiplication operator $\hat{G}$ on $L^2(\mathbb{R},\mathbb{C}^2)$ defined by

$$\begin{aligned} \mathrm{dom}(\hat{G}) &:= \{\hat{g} \in L^2(\mathbb{R}, \mathbb{C}^2) : G(\lambda)\hat{g}(\lambda) \in L^2(\mathbb{R}, \mathbb{C}^2)\}, \\ (\hat{G}\hat{g})(\lambda) &:= G(\lambda)\hat{g}(\lambda), \quad \hat{g} \in \mathrm{dom}(\hat{G}(\cdot)) \end{aligned} \tag{2.44}$$

is unitarily equivalent to G, i.e.,

$$\Phi_- G \Phi_-^{-1} = \hat{G}. \tag{2.45}$$

Indeed, if G commutes with K, then $\hat{G}$ commutes with M. Applying Theorem VII.2.3 of Ref. 19 one immediately gets that $\hat{G}$ is a multiplication operator of type (2.44). The representation (2.44) is called the incoming spectral representation of G.

III. CARRIER DENSITY

In the following we call an operator $\varrho : \mathfrak{k} \to \mathfrak{k}$ a density matrix if ϱ is a bounded, non-negative operator. The operator ϱ is called a steady state if ϱ commutes with K. Obviously, a steady state does not change in time. If ϱ is a steady state, then there is a measurable matrix-valued function $\varrho(\cdot) \in L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ such that the multiplication operator $\hat{\varrho}$ on $L^2(\mathbb{R}, \mathbb{C}^2)$ generated by $\varrho(\cdot)$ is unitarily equivalent to ϱ, i.e.,

$$\varrho = \Phi_-^{-1} \hat{\varrho} \Phi_-, \tag{3.1}$$

see above. Obviously, the measurable function $\varrho(\cdot)$ takes the form

$$\varrho(\lambda) = \begin{pmatrix} \varrho^{bb}(\lambda) & \varrho^{ba}(\lambda) \\ \varrho^{ab}(\lambda) & \varrho^{aa}(\lambda) \end{pmatrix}, \tag{3.2}$$

where $\varrho^{\tau\nu}(\cdot) \in L^\infty(\mathbb{R})$, $\tau, \nu = a, b$. Since $\varrho \geqslant 0$ one gets that $\varrho(\lambda) \geqslant 0$ a.e. (with respect to the Lebesgue measure).

Definition 3.1: A bounded self-adjoint operator A on $\mathfrak{k}$ is called an observable. We say the observable A

(i) is admissible with respect to ϱ if ϱA is a nuclear operator on $\mathfrak{k}$, i.e., $\varrho A \in \mathcal{L}_1(\mathfrak{k})$,
(ii) is admissible with respect to K if $E_K(\Delta)A \in \mathcal{L}_1(\mathfrak{k})$ for each bounded interval $\Delta \subseteq \mathbb{R}$ where $E_K(\cdot)$ denotes the spectral measure of K.

If the observable A is admissible with respect to ϱ, then its expectation value $\mathbb{E}_\varrho(A)$ with respect to the density matrix ϱ is defined by

$$\mathbb{E}_\varrho(A) := \mathrm{tr}(\varrho A). \tag{3.3}$$

In the following we show that the admissibility of A with respect to K leads to a certain localization in the incoming spectral representation:

Proposition 3.2: Assume $m + 1/m \in L^\infty([a,b])$, $V \in L^2([a,b])$ *and* $\kappa_a, \kappa_b \in \mathbb{C}_+$. *If the observable A is admissible with respect to K, then there exists a measurable matrix-valued function* $A(\cdot) \in L^1_{loc}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$, *such that* $A(\lambda) = A(\lambda)^*$ *for a.e.* $\lambda \in \mathbb{R}$ *and*

$$\mathrm{tr}(\varrho A E_K(\Delta)) = \int_\Delta d\lambda \, \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)A(\lambda)) \tag{3.4}$$

for any bounded Borel set $\Delta \subseteq \mathbb{R}$ *and any steady state* ϱ *of K. The measurable function* $A(\cdot)$ *is uniquely defined up to a Borel set of Lebesgue measure zero.*

If the observable A is in addition admissible with respect to the steady state ϱ, *then* $\mathrm{tr}_{\mathbb{C}^2}(\varrho(\cdot)A(\cdot)) \in L^1(\mathbb{R})$ *and the representation*

$$\mathrm{tr}(\varrho A)=\int_{\mathbb{R}} d\lambda\ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)A(\lambda)) \tag{3.5}$$

holds.

Proof: Notice that the spectral measure $E_K(\cdot)$ of K is absolutely continuous with respect to the Lebesgue measure. Hence, the set function

$$\mu_{\varrho,A}(\Delta):=\mathrm{tr}(\varrho A E_K(\Delta)), \tag{3.6}$$

where Δ is bounded Borel set of $\mathbb{R}$, is in fact a Lebesgue absolutely continuous measure. Let $d\mu_{\rho,A}/d\lambda$ denote its Radon–Nikodym derivative and define

$$T_A(\hat{\varrho}):=\frac{d\mu_{\varrho,A}}{d\lambda}. \tag{3.7}$$

Then $T_A(\cdot)$ maps $L^\infty(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$ continuously into $L^1_{\mathrm{loc}}(\mathbb{R})$ (the latter in its canonic Fréchet topology) and, additionally, one has

$$\mathrm{tr}(\varrho A E_K(\Delta))=\int_\Delta d\lambda\ \frac{d\mu_{\varrho,A}}{d\lambda}(\lambda)=\int_\Delta d\lambda\ T_A(\hat{\varrho})(\lambda) \tag{3.8}$$

for any bounded Borel set $\Delta\subset\mathbb{R}$. It is not hard to see that (3.8) implies the equality

$$T_A(\chi_\Delta\hat{\varrho})=\chi_\Delta T_A(\hat{\varrho}) \tag{3.9}$$

for any bounded Borel set $\Delta\subseteq\mathbb{R}$ where χ_Δ denotes its indicator function. We put

$$e_{bb}:=\begin{pmatrix}1&0\\0&0\end{pmatrix},\quad e_{ba}:=\begin{pmatrix}0&1\\0&0\end{pmatrix},\quad e_{ab}:=\begin{pmatrix}0&0\\1&0\end{pmatrix},\quad e_{aa}:=\begin{pmatrix}0&0\\0&1\end{pmatrix} \tag{3.10}$$

and define for any $h\in L^\infty(\mathbb{R})$,

$$A_{ij}(h):=T_A(h\cdot e_{ji}),\quad i,j=a,b. \tag{3.11}$$

Clearly, each of the mappings $A_{ij}(\cdot)$ then maps $L^\infty(\mathbb{R})$ continuously into $L^1_{\mathrm{loc}}(\mathbb{R})$ and (3.11) implies

$$A_{ij}(\chi_\Delta h)=\chi_\Delta A_{ij}(h) \tag{3.12}$$

for any $h\in L^\infty(\mathbb{R})$ and any Borel set Δ. Taking in particular $h\equiv 1$, this yields

$$A_{ij}(\chi_\Delta)=\chi_\Delta A_{ij}(1). \tag{3.13}$$

Obviously, by the linearity of the mappings $A_{ij}(\cdot)$, this last equation remains true if χ_Δ is there replaced by any (finite) linear combination of indicator functions. Because the set of finite linear combinations of indicator functions is dense in $L^\infty(\mathbb{R})$, one gets for all $h\in L^\infty(\mathbb{R})$

$$A_{ij}(h)=h\cdot A_{ij}(1). \tag{3.14}$$

Since

$$\varrho(\cdot)=\varrho^{bb}(\cdot)e_{bb}+\varrho^{ba}(\cdot)e_{ba}+\varrho^{ab}(\cdot)e_{ab}+\varrho^{aa}(\cdot)e_{aa} \tag{3.15}$$

one gets

$$\mathrm{tr}(\varrho A E_K(\Delta)) = \int_\Delta \mathrm{d}\lambda\, T_A(\hat{\varrho})(\lambda) = \sum_{i,j=a,b} \int_\Delta \mathrm{d}\lambda\, A_{ij}(\varrho^{ij})(\lambda)$$

$$= \sum_{i,j=a,b} \int_\Delta \mathrm{d}\lambda\, \varrho^{ij}(\lambda) A_{ji}(1)(\lambda). \tag{3.16}$$

Setting

$$A(\cdot) := \begin{pmatrix} A_{bb}(1)(\cdot) & A_{ba}(1)(\cdot) \\ A_{ab}(1)(\cdot) & A_{aa}(1)(\cdot) \end{pmatrix} \tag{3.17}$$

we finally obtain (3.4) for any bounded Borel set $\Delta \subset \mathbb{R}$ and any steady state ϱ of K.

Assume that $\tilde{A}(\cdot)$ obeys also the conditions of the proposition. Setting $G(\lambda) := A(\lambda) - \tilde{A}(\lambda)$, $\lambda \in \mathbb{R}$, one gets that

$$\int_\Delta \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda) G(\lambda)) = 0 \tag{3.18}$$

for any bounded Borel set Δ and any steady state ϱ. Hence $\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)G(\lambda)) = 0$ for a.e. λ and any steady state ϱ which immediately yields $G(\lambda) = 0$ or $A(\lambda) = \tilde{A}(\lambda)$ for a.e. $\lambda \in \mathbb{R}$.

If ϱ is admissible with respect to A, then $|\mathrm{tr}(\varrho A E_K(\Delta)| < \|\varrho A\|_{\mathcal{L}_1}$ for any Borel set $\Delta \subseteq \mathbb{R}$. By (3.4) this implies that $\mathrm{tr}(\varrho(\cdot)A(\cdot)) \in L^1(\mathbb{R})$. Since one has $\lim_{\Delta \uparrow \mathbb{R}} \mathrm{tr}(\varrho A E_K(\Delta)) = \mathrm{tr}(\varrho A)$ we obtain from (3.4) the equality (3.5). □

Proposition 3.2 says that the averaging procedure localizes with respect to the incoming spectral representation. Indeed, the quantity $\mathrm{tr}(\varrho(\lambda)A(\lambda))$ can be regarded as the local average of the observable $A(\lambda)$ with respect to the density matrix $\varrho(\lambda)$ at energy $\lambda \in \mathbb{R}$, i.e.,

$$\mathbb{E}_{\varrho(\lambda)}(A(\lambda)) := \mathrm{tr}(\varrho(\lambda)A(\lambda)). \tag{3.19}$$

Formula (3.5) has the meaning that the total average $\mathbb{E}_\varrho(A)$ is the sum of the local averages $\mathbb{E}_{\varrho(\lambda)}(A(\lambda))$, i.e.,

$$\mathbb{E}_\varrho(A) = \int_{\mathbb{R}} \mathrm{d}\lambda\, \mathbb{E}_{\varrho(\lambda)}(A(\lambda)). \tag{3.20}$$

Proposition 3.2 gives rise to the following

Definition 3.3: Let A be an observable which is admissible with respect to K. An element $A(\cdot) \in L^1_{\mathrm{loc}}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ is called a localizer of A with respect to K if $A(\lambda)^* = A(\lambda)$ for a.e. $\lambda \in \mathbb{R}$ and

$$\mathrm{tr}(\varrho A E_K(\Delta)) = \int_\Delta \mathrm{d}\lambda\, \mathrm{tr}(\varrho(\lambda)A(\lambda)) \tag{3.21}$$

holds for any bounded Borel subset $\Delta \subseteq \mathbb{R}$ and any steady state ϱ.

Proposition 3.2 says that an observable which is admissible with respect to K has always a unique localizer.

To calculate the carrier density we consider the observable $U(\omega)$, $\omega \subseteq \Omega$, given by

$$(U(\omega)\vec{f})(x) = 0 \oplus \chi_\omega(x) f(x) \oplus 0, \quad \vec{f} \in L^2(\hat{\Omega}), \tag{3.22}$$

for any Borel subset $\omega \subseteq \Omega$. We note that the observable $U(\omega)$ is a projection on $\mathfrak{k}$ with $\mathrm{ran}(U(\omega)) \subseteq \mathfrak{h}$. Loosely speaking, the projection acts in fact only on the subspace $\mathfrak{h} \subseteq \mathfrak{k}$.

Lemma 3.4: Assume $m+1/m \in L^{\infty}([a,b])$, $V \in L^2([a,b])$ *and* $\kappa_a, \kappa_b \in \mathbb{C}_+$. *Then for any Borel set* $\omega \subseteq \Omega$ *the observable* $U(\omega)$ *is admissible with respect to the minimal self-adjoint dilation* K *of the maximal dissipative operator* H. *If the steady state* ϱ *satisfies the condition*

$$C_{\hat{\varrho}} := \sup_{\lambda \in \mathbb{R}} \sqrt{\lambda^2+1}\,\|\varrho(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} < \infty, \tag{3.23}$$

then for any Borel set $\omega \subseteq \Omega$ *the observable* $U(\omega)$ *is admissible with respect to* ϱ.

Proof: Relation (2.33) implies

$$U(\omega)(K-z)^{-1}\vec{f} = 0 \oplus \chi_\omega (H-z)^{-1} f + i\chi_\omega T_*(\overline{z})^* \int_{-\infty}^{0} dy\, e^{-iyz} f_-(y) \oplus 0 \tag{3.24}$$

for $\vec{f} \in \mathfrak{k}$ and $z \in \mathbb{C}_+$. By Theorem 3.1 of Ref. 5 one gets that $(H-z)^{-1}$ is a trace class operator for each $z \in \mathbb{C}_+$. Hence $U(\omega)(H-z)^{-1}$ is a trace class operator for each $\omega \subseteq \Omega$. Since the operator $T_*(\overline{z})^*$ acts from the two-dimensional Hilbert space $\mathbb{C}^2$ into $\mathfrak{h}$ one easily gets that the second addend of (3.24) is a trace class operator, too. Hence $U(\omega)(K-z)^{-1} \in \mathcal{L}_1(\mathfrak{k})$ for each Borel set $\omega \subseteq \Omega$ and $z \in \mathbb{C}_+$. Using the representation

$$U(\omega)E_K(\Delta) = U(\omega)(K-z)^{-1}(K-z)E_K(\Delta), \quad z \in \mathbb{C}_+, \tag{3.25}$$

we find that $U(\omega)E_K(\Delta)$ is a trace class operator for each Borel sets $\omega \subseteq \Omega$ and each bounded interval $\Delta \subseteq \mathbb{R}$. Hence, the observable $U(\omega)$ is admissible with respect to K for each Borel set $\omega \subseteq \Omega$.

Moreover, taking into account (3.23) and the representation

$$U(\omega)\varrho = U(\omega)(K-i)^{-1}(K-i)\varrho \tag{3.26}$$

one immediately gets that $U(\omega)\,\varrho$ is a trace class operator for each $\omega \subseteq \Omega$, because $(K-i)\varrho$ is bounded. Hence, $\varrho\, U(\omega)$ is a trace class operator for each Borel set $\omega \subseteq \Omega$ which yields that $U(\omega)\,\varrho$ is admissible with respect to ϱ. □

Since $U(\omega)$ is admissible with respect to K for any Borel set $\omega \subseteq \Omega$ by Proposition 3.2 there is a unique localizer $U(\omega)(\cdot): \mathbb{R} \to \mathcal{B}(\mathbb{C}^2)$. We are going to calculate this localizer.

Proposition 3.5: Assume $m+1/m \in L^{\infty}([a,b])$, $V \in L^2([a,b])$ *and* $\kappa_a, \kappa_b \in \mathbb{C}_+$. *Then for any Borel set* $\omega \subseteq \Omega$ *the localizer of* $U(\omega)(\cdot)$ *of the observable* $U(\omega)$ *is given by*

$$U(\omega)(\lambda) = \int_\omega dx\, D(x,\lambda), \tag{3.27}$$

where

$$D(x,\lambda) := \begin{pmatrix} |\psi^-(x,\lambda,b)|^2 & \psi^-(x,\lambda,a)\overline{\psi^-(x,\lambda,b)} \\ \psi^-(x,\lambda,b)\overline{\psi^-(x,\lambda,a)} & |\psi^-(x,\lambda,a)|^2 \end{pmatrix} \tag{3.28}$$

$x \in \Omega,\ \lambda \in \mathbb{R}$.

If the steady state ϱ *satisfies the condition (3.23), then*

$$\mathbb{E}_\varrho(U(\omega)) = \int_{\mathbb{R}} d\lambda\, \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)U(\omega)(\lambda)) \tag{3.29}$$

for any Borel subset $\omega \subseteq \Omega$.

Proof: By Lemma 3.4 the observable $U(\omega)$ is admissible for any Borel set $\omega\subseteq\Omega$. By Proposition 3.2 there is a unique localizer $U(\omega)(\cdot)\in L^1_{\mathrm{loc}}(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$ such that (3.21) is satisfied for any bounded Borel set $\Delta\subseteq\mathbb{R}$ and any steady state ϱ. Following the proof of Proposition 3.2 we consider the measure

$$\mu_{\varrho,U(\omega)}(\Delta)=\mathrm{tr}(\varrho U(\omega)E_K(\Delta)) \tag{3.30}$$

for any bounded Borel set $\Delta\subseteq\mathbb{R}$. We set

$$\hat{U}(\omega):=\Phi_- U(\omega)\Phi_-^{-1},\quad \hat{U}_\Delta(\omega):=E_M(\Delta)\hat{U}E_M(\Delta),$$

where $M=\Phi_- K\Phi_-^{-1}$, see (2.42). By Lemma 3.4 the operator $\hat{U}_\Delta(\omega)$ is nuclear. Hence, we find

$$\mu_{\varrho,U(\omega)}(\Delta)=\mathrm{tr}(\hat{\varrho}\hat{U}_\Delta(\omega)). \tag{3.31}$$

Let us calculate the kernel of $\hat{U}_\Delta(\omega)$. To this end we consider the scalar product $(\hat{U}_\Delta(\omega)\hat{g},\hat{f})$, $\hat{g},\hat{f}\in L^2(\Delta,\mathbb{C}^2)$. Using (2.41) one has

$$(\hat{U}_\Delta(\omega)\hat{g},\hat{f})=\int_\omega \mathrm{d}x\int_\Delta \mathrm{d}\lambda\sum_{\tau=a,b}\psi^-(x,\lambda,\tau)\hat{g}^\tau(\lambda)\overline{\int_\Delta \mathrm{d}\mu\sum_{\xi=a,b}\psi^-(x,\mu,\xi)\hat{f}^\xi(\mu)}. \tag{3.32}$$

Setting

$$U_\Delta^{\tau\xi}(\omega)(\mu,\lambda):=\int_\omega \mathrm{d}x\,\psi^-(x,\lambda,\xi)\overline{\psi^-(x,\mu,\tau)},\quad \tau,\xi=a,b, \tag{3.33}$$

we get

$$(\hat{U}_\Delta(\omega)\hat{g},\hat{f})=\int_\Delta \mathrm{d}\mu\left(\int_\Delta \mathrm{d}\lambda\begin{pmatrix}U_\Delta^{bb}(\omega)(\mu,\lambda) & U_\Delta^{ba}(\omega)(\mu,\lambda)\\ U_\Delta^{ab}(\omega)(\mu,\lambda) & U_\Delta^{aa}(\omega)(\mu,\lambda)\end{pmatrix}\begin{pmatrix}\hat{g}^b(\lambda)\\ \hat{g}^a(\lambda)\end{pmatrix},\begin{pmatrix}\hat{f}^b(\mu)\\ \hat{f}^a(\mu)\end{pmatrix}\right), \tag{3.34}$$

which shows that

$$U_\Delta(\omega)(\mu,\lambda):=\begin{pmatrix}U_\Delta^{bb}(\omega)(\mu,\lambda) & U_\Delta^{ba}(\omega)(\mu,\lambda)\\ U_\Delta^{ab}(\omega)(\mu,\lambda) & U_\Delta^{aa}(\omega)(\mu,\lambda)\end{pmatrix} \tag{3.35}$$

is the kernel of the integral operator $\hat{U}_\Delta(\omega)$. Setting

$$D(x,\mu,\lambda):=\begin{pmatrix}\psi^-(x,\lambda,b)\overline{\psi^-(x,\mu,b)} & \psi^-(x,\lambda,a)\overline{\psi^-(x,\mu,b)}\\ \psi^-(x,\lambda,b)\overline{\psi^-(x,\mu,a)} & \psi^-(x,\lambda,a)\overline{\psi^-(x,\mu,a)}\end{pmatrix} \tag{3.36}$$

we obtain the representation

$$U_\Delta(\omega)(\mu,\lambda)=\int_\omega \mathrm{d}x\,D(x,\mu,\lambda),\quad \mu,\lambda\in\Delta. \tag{3.37}$$

Since $U_\Delta(\omega)(\mu,\lambda)=U_{\Delta'}(\omega)(\mu,\lambda)$ for $\mu,\lambda\in\Delta\subseteq\Delta'$ it makes sense to define $U(\omega)(\mu,\lambda):=\lim_{\Delta\uparrow\mathbb{R}}U_\Delta(\omega)(\mu,\lambda)$, $\mu,\lambda\in\mathbb{R}$. Hence $U_\Delta(\omega)(\mu,\lambda)=U(\omega)(\mu,\lambda)$ for $\mu,\lambda\in\Delta$ and

$$U(\omega)(\mu,\lambda)=\int_\omega \mathrm{d}x\,D(x,\mu,\lambda),\quad \mu,\lambda\in\Delta. \tag{3.38}$$

Since the kernel depends continuously on μ and λ one gets that

$$\mathrm{tr}(\hat{\varrho}\hat{U}_\Delta(\omega))=\int_\Delta \mathrm{d}\lambda\ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)U(\omega)(\lambda,\lambda)) \tag{3.39}$$

for any bounded Borel set $\Delta\subseteq\mathbb{R}$ and any steady state ϱ. From (3.38) we find that $U(\omega)(\lambda,\lambda)^* = U(\omega)(\lambda,\lambda)$ for $\lambda\in\mathbb{R}$. Since the eigenfunctions $\psi^-(x,\lambda,b)$ and $\psi^-(x,\lambda,a)$ are bounded on compact sets of x and λ we obtain that $U(\omega)(\lambda,\lambda)\in L^1_{loc}(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$. By (3.39) the matrix-valued function $U(\omega)(\lambda):=U(\omega)(\lambda,\lambda)$, $\lambda\in\mathbb{R}$, is the unique localizer of the observable $U(\omega)$. By condition (3.23) the observable $U(\omega)$ is admissible with respect to ϱ. Applying Proposition 3.2 we verify (3.29).

It remains to verify (3.27) and (3.28). From (3.38) and (3.39) we obtain the representation

$$\mathrm{tr}(\hat{\varrho}\ \ \hat{U}_\Delta(\omega))=\int_\Delta \mathrm{d}\lambda\ \ \int_\omega \mathrm{d}x\ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda,\lambda)). \tag{3.40}$$

Setting $D(x,\lambda):=D(x,\lambda,\lambda)$, $x\in\Omega$, $\lambda\in\mathbb{R}$, we immediately obtain (3.27) and (3.28). □

We set

$$u_{\hat{\varrho}}(x,\lambda):=\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)) \tag{3.41}$$

for $x\in\Omega$ and $\lambda\in\mathbb{R}$. A simple computation shows that the eigenvalues of $D(x,\lambda)$ are equal to $|\psi^-(x,\lambda,b)|^2$ and $|\psi^-(x,\lambda,a)|^2$, which shows that the matrix $D(x,\lambda)$ is non-negative for each $x\in\Omega$ and $\lambda\in\mathbb{R}$. Since for a.e. $\lambda\in\mathbb{R}$ the matrix $\varrho(\lambda)$ is non-negative, too, one gets that $u_{\hat{\varrho}}(x,\lambda)\geqslant 0$ for $x\in\Omega$ and a.e. $\lambda\in\mathbb{R}$. This fact can also be verified taking into account the representation

$$u_{\hat{\varrho}}(x,\lambda)=\left\langle \varrho^t(\lambda)\begin{pmatrix}\psi^-(x,\lambda,b)\\ \psi^-(x,\lambda,a)\end{pmatrix},\begin{pmatrix}\psi^-(x,\lambda,b)\\ \psi^-(x,\lambda,a)\end{pmatrix}\right\rangle, \tag{3.42}$$

where $\varrho^t(\lambda)$ is the transposed matrix to (3.2). Moreover, if condition (3.23) is satisfied, then from Proposition (3.5) we obtain the representation

$$\mathbb{E}_\varrho(U(\omega))=\int_{\mathbb{R}} \mathrm{d}\lambda\ \ \int_\omega \mathrm{d}x\ u_{\hat{\varrho}}(x,\lambda) \tag{3.43}$$

for Borel sets $\omega\subseteq\Omega$. Taking into account Fubini's theorem we find that

$$\mathbb{E}_\varrho(U(\omega))=\int_\omega \mathrm{d}x\ u_{\hat{\varrho}}(x), \tag{3.44}$$

where

$$u_{\hat{\varrho}}(x):=\int_{\mathbb{R}} \mathrm{d}\lambda\ u_{\hat{\varrho}}(x,\lambda)\geqslant 0,\quad x\in\Omega, \tag{3.45}$$

and $u_{\hat{\varrho}}\in L^1(\Omega)$. The representation (3.44) shows that $\mathbb{E}_\varrho(U(\cdot))$ defines a measure on Ω which is absolutely continuous with respect to the Lebesgue measure. Since the expectation value $\mathbb{E}_\varrho(U(\omega))$ has the meaning of the number of carriers in $\omega\subseteq\Omega$ its Radon–Nikodym derivative can be interpreted as the carrier density of the system described by K and mutatis mutandis by H.

Definition 3.6: Assume $m+1/m\in L^\infty([a,b])$, $V\in L^2([a,b])$ and $\kappa_a,\kappa_b\in\mathbb{C}_+$. Then the matrix $D(x,\lambda)$, $x\in\Omega$, and the value $u_{\hat{\varrho}}(x,\lambda)$ are called carrier density observable and carrier density at $x\in\Omega$ and at energy $\lambda\in\mathbb{R}$ of the system described by H, respectively.

This definition is justified by the fact that by (3.41) the carrier density $u_{\hat{\varrho}}(x,\lambda)$ is the expectation value of the carrier density observable $D(x,\lambda)$, i.e., $u_{\hat{\varrho}}(x,\lambda)=\mathbb{E}_{\varrho(\lambda)}(D(x,\lambda))$ at $x\in\Omega$ and at $\lambda\in\mathbb{R}$. Moreover, we note that (3.45) can be written as

$$u_{\hat{\varrho}}(x)=\int_{\mathbb{R}} d\lambda\ \mathbb{E}_{\varrho(\lambda)}(D(x,\lambda)),\quad x\in\Omega, \tag{3.46}$$

i.e, the carrier density at $x\in\Omega$ is the sum of expectation values of the carrier density observable at $x\in\Omega$ over all energies.

On the Hilbert space $\mathfrak{k}=L^2(\hat{\Omega})$ we consider the multiplication operator $M(h)$,

$$(M(h)\vec{f})(x)=0\oplus h(x)f(x)\oplus 0,\quad x\in\Omega, \tag{3.47}$$

for real functions $h\in L^\infty(\Omega)$. We note that $M(\chi_\omega)=U(\omega)$ for any Borel set $\omega\subseteq\Omega$. In particular, one has $M(\chi_\Omega)=U(\Omega)=P^{\mathfrak{k}}_{\mathfrak{h}}$. Obviously, the representation

$$\varrho M(h)=\varrho U(\Omega)M(h),\quad h\in L^\infty(\Omega) \tag{3.48}$$

is valid. Since the observable $U(\Omega)$ is admissible with respect to ϱ the product $\varrho U(\Omega)$ is a nuclear operator on $\mathfrak{k}$ which yields that $\varrho M(h)$ is a nuclear operator on $\mathfrak{k}$, i.e., the observable $M(h)$ is admissible with respect to ϱ.

Proposition 3.7: Assume $m+1/m\in L^\infty([a,b])$, $V\in L^2([a,b])$ and $\kappa_a,\kappa_b\in\mathbb{C}_+$. If the steady state ϱ satisfies the condition (3.23), then the carrier density $u_{\hat{\varrho}}$ defined by (3.45) is a nonnegative L^1-function such that

$$\mathrm{tr}(\varrho M(h))=\int_\Omega dx\, u_{\hat{\varrho}}(x)h(x) \tag{3.49}$$

for real functions $h\in L^\infty(\Omega)$. In particular, one has

$$\|u_{\hat{\varrho}}\|_{L^1(\omega)}=\mathrm{tr}(\varrho\ U(\omega))\leqslant C_{\hat{\varrho}}\|(K-i)^{-1}P^{\mathfrak{k}}_{\mathfrak{h}}\|_{\mathcal{L}_1(\mathfrak{k})} \tag{3.50}$$

for each Borel set $\omega\subseteq\Omega$.

Proof: Setting $\omega=\Omega$ we obtain from (3.44) that $u_{\hat{\varrho}}\in L^1(\Omega)$. We choose $h=\chi_\omega$, $\omega\subseteq\Omega$. By (3.44) we get

$$\mathrm{tr}(\varrho M(\chi_\omega))=\int_\Omega dx\, u_{\hat{\varrho}}(x)\chi_\omega(x). \tag{3.51}$$

By linearity this equation extends to

$$\mathrm{tr}(\varrho M(h))=\int_\Omega dx\, u_{\hat{\varrho}}(x)h(x), \tag{3.52}$$

where h is an arbitrary step function on Ω. Since $u_{\hat{\varrho}}$ is from $L^1(\Omega)$ and $\varrho U(\Omega)$ is a nuclear operator both sides of (3.52) admit a continuation to L^∞-functions which verifies (3.49).

It remains to show the estimate (3.50). From (3.44) we immediately get

$$\int_\Omega dx\, u_g(x)=\mathrm{tr}(\varrho U(\Omega))=\mathrm{tr}(\varrho(K-i)(K-i)^{-1}U(\Omega)). \tag{3.53}$$

Since $U(\Omega)(K-i)^{-1}\in\mathcal{L}_1(\mathfrak{k})$ and $\varrho(K-i)$ is a bounded operator which norm can be estimated by $C_{\hat{\varrho}}$ we obtain

$$\mathrm{tr}(\varrho(K-i)(K-i)^{-1}U(\omega)) \leqslant C_{\hat{\varrho}} \|(K-i)^{-1}P_{\mathfrak{h}}^{\mathfrak{k}}\|_{\mathcal{L}_1(\mathfrak{k})}, \tag{3.54}$$

which verifies (3.50). □

Obviously, the relation (3.49) takes the form

$$\mathrm{tr}(\varrho M(h)) = \langle u_{\hat{\varrho}}, h\rangle_{L^1} \tag{3.55}$$

where by $\langle \cdot, h\rangle_{L^1}$, $h \in L^\infty(\Omega)$, we denote the linear functionals on $L^1(\Omega)$.

We conclude this section with some considerations which we need in the following section. Since $\{\varrho(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of non-negative self-adjoint operators there is a measurable family $\{V(\lambda)\}_{\lambda\in\mathbb{R}}$ of unitary operators on $\mathbb{C}^2$ such that

$$\varrho(\lambda) = V(\lambda)\begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda)\end{pmatrix} V(\lambda)^* \tag{3.56}$$

for a.e. $\lambda \in \mathbb{R}$ where $\mu_b(\lambda)$ and $\mu_a(\lambda)$ are the non-negative eigenvalues of $\varrho(\lambda)$. From (3.56) we get that

$$\varrho^t(\lambda) = V^t(\lambda)^*\begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda)\end{pmatrix} V^t(\lambda) \tag{3.57}$$

for a.e. $\lambda \in \mathbb{R}$ where $V^t(\lambda)$ is the transposed matrix to $V(\lambda)$. Inserting (3.57) into (3.42) we obtain

$$u_{\hat{\varrho}}(x,\lambda) = \left\langle \begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda)\end{pmatrix} V^t(\lambda)\begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a)\end{pmatrix}, V^t(\lambda)\begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a)\end{pmatrix}\right\rangle. \tag{3.58}$$

Let us introduce the unit vectors $e_\tau(\lambda)$,

$$e_\tau(\lambda) = V(\lambda)e_\tau, \quad \tau = b,a \tag{3.59}$$

which perform an orthonormal basis in $\mathbb{C}^2$. We set

$$\begin{aligned}\vec{\psi}(x,\lambda,e_\tau(\lambda)) &:= \psi_-(x,\lambda,e_\tau(\lambda)) \oplus \psi(x,\lambda,e_\tau(\lambda)) \oplus \psi_+(x,\lambda,e_\tau(\lambda)) \\ &= \frac{1}{\sqrt{2\pi}} e^{ix\lambda} e_\tau(\lambda) \oplus \frac{1}{\sqrt{2\pi}} (T_*(\lambda)^* e_\tau(\lambda))(x) \oplus \frac{1}{\sqrt{2\pi}} e^{ix\lambda}\Theta_H(\lambda)^* e_\tau(\lambda).\end{aligned} \tag{3.60}$$

Obviously, the system $\{\vec{\psi}(x,\lambda,e_\tau(\lambda))\}_{\tau=b,a}$ performs an orthonormal basis of generalized eigenfunctions. Moreover, a straightforward computation shows that

$$V^t(\lambda)\begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a)\end{pmatrix} = \begin{pmatrix} \psi(x,\lambda,e_b(\lambda)) \\ \psi(x,\lambda,e_a(\lambda))\end{pmatrix}, \tag{3.61}$$

which leads to

$$u_{\hat{\varrho}}(x,\lambda) = \mu_b(\lambda)|\psi(x,\lambda,e_b(\lambda))|^2 + \mu_a(\lambda)|\psi(x,\lambda,e_a(\lambda))|^2 \tag{3.62}$$

for $x \in \Omega$ and $\lambda \in \mathbb{R}$.

IV. CURRENT DENSITY

In accordance with (1.8) the current density $j_{\hat{\varrho}}(x,\lambda)$ for the energy $\lambda \in \mathbb{R}$ is defined by

$$j_{\hat{\varrho}}(x,\lambda) := \mu_b(\lambda)\mathrm{Im}\left(\frac{1}{m(x)}\psi(x,\lambda,e_b(\lambda))'\overline{\psi(x,\lambda,e_b(\lambda))}\right) + \mu_a(\lambda)\mathrm{Im}\left(\frac{1}{m(x)}\psi(x,\lambda,e_a(\lambda))'\overline{\psi(x,\lambda,e_a(\lambda))}\right), \tag{4.1}$$

$x \in \Omega$, where the eigenfunctions $\psi(x,\lambda,e_\tau(\lambda))$, $\tau = a,b$, are defined by (3.61). We are going to relate the current density to the characteristic function of the maximal dissipative operator H.

Proposition 4.1: Assume $m + 1/m \in L^\infty([a,b])$, $V \in L^2([a,b])$ *and* $\kappa_a, \kappa_b \in \mathbb{C}_+$. *Further, let* ϱ *be a steady state. Then the current density* $j_{\hat{\varrho}}(x,\lambda)$, $x \in \Omega$, $\lambda \in \mathbb{R}$, *is independent of* x *and admits the representation*

$$j_{\hat{\varrho}}(\lambda) = \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)C(\lambda)) \tag{4.2}$$

where

$$C(\lambda) := -\frac{1}{2\pi i}\frac{\alpha_a\alpha_b}{\overline{W(\lambda)}}E\Theta_H(\lambda)^* = \frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)}\Theta_H(\lambda)E, \tag{4.3}$$

$\lambda \in \mathbb{R}$. *Moreover, if* $\mathrm{tr}_{\mathbb{C}^2}(\varrho(\cdot)) \in L^1(\mathbb{R})$, *then the total current* $j_{\hat{\varrho}}$,

$$j_{\hat{\varrho}} := \int_{\mathbb{R}} d\lambda\, j_{\hat{\varrho}}(\lambda), \tag{4.4}$$

is finite and satisfies the estimate

$$|j_{\hat{\varrho}}| \leqslant \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\, \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)). \tag{4.5}$$

Proof: From the definition (4.2) one gets that

$$j_{\hat{\varrho}}(x,\lambda) = \mathrm{Im}\left(\left\langle \begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda) \end{pmatrix} \begin{pmatrix} \frac{1}{m(x)}\psi(x,\lambda,e_b(\lambda))' \\ \frac{1}{m(x)}\psi(x,\lambda,e_a(\lambda))' \end{pmatrix}, \begin{pmatrix} \psi(x,\lambda,e_b(\lambda)) \\ \psi(x,\lambda,e_a(\lambda)) \end{pmatrix} \right\rangle\right). \tag{4.6}$$

Taking into account (3.57) and (3.61) we get

$$j_{\hat{\varrho}}(x,\lambda) = \mathrm{Im}\left(\left\langle \varrho^t(\lambda) \begin{pmatrix} \frac{1}{m(x)}\psi^-(x,\lambda,b)' \\ \frac{1}{m(x)}\psi^-(x,\lambda,a)' \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix} \right\rangle\right) \tag{4.7}$$

which can be expressed by

$$j_{\hat{\varrho}}(x,\lambda) = \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)C(x,\lambda)), \tag{4.8}$$

where

$$C(x,\lambda):=\mathrm{Im}\left(\begin{pmatrix} \frac{1}{m(x)}\psi^-(x,\lambda,b)'\overline{\psi^-(x,\lambda,b)} & \frac{1}{m(x)}\psi^-(x,\lambda,a)'\overline{\psi^-(x,\lambda,b)} \\ \frac{1}{m(x)}\psi^-(x,\lambda,b)'\overline{\psi^-(x,\lambda,a)} & \frac{1}{m(x)}\psi^-(x,\lambda,a)'\overline{\psi^-(x,\lambda,a)} \end{pmatrix}\right). \tag{4.9}$$

We note that

$$C(x,\lambda)=\frac{1}{i}\begin{pmatrix} W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,b)) & W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,a)) \\ W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,b)) & W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,a)) \end{pmatrix} \tag{4.10}$$

where $W(\cdot,\cdot)$ is the Wronskian defined by (2.5). Since

$$W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,b))=-\frac{i}{2\pi}\frac{\alpha_b^2\alpha_a^2}{|W(\lambda)|^2}, \tag{4.11}$$

$$W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,b))=\frac{1}{2\pi}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\{W(\lambda)-i\alpha_b^2 v_a(b,\lambda)\}, \tag{4.12}$$

$$W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,a))=-\frac{1}{2\pi}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\{W(\lambda)-i\alpha_a^2 v_b(a,\lambda)\}, \tag{4.13}$$

$$W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,a))=\frac{i}{2\pi}\frac{\alpha_a^2\alpha_b^2}{|W(\lambda)|^2}, \tag{4.14}$$

we find

$$C(x,\lambda)=\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\begin{pmatrix} -i\alpha_b\alpha_a & -(W(\lambda)-i\alpha_a^2 v_b(a,\lambda)) \\ W(\lambda)-i\alpha_b^2 v_a(b,\lambda) & i\alpha_a\alpha_b \end{pmatrix}. \tag{4.15}$$

This yields

$$C(x,\lambda)=-\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} W(\lambda)-i\alpha_b^2 v_a(b,\lambda) & i\alpha_b\alpha_a \\ i\alpha_b\alpha_a & W(\lambda)-i\alpha_a^2 v_b(a,\lambda) \end{pmatrix}. \tag{4.16}$$

From (2.21) we obtain

$$\Theta_H(\lambda)^*=\frac{1}{W(\lambda)}\begin{pmatrix} W(\lambda)-i\alpha_b^2 v_a(b,\lambda) & i\alpha_b\alpha_a \\ i\alpha_b\alpha_a & W(\lambda)-i\alpha_a^2 v_b(a,\lambda) \end{pmatrix}. \tag{4.17}$$

Hence, one has

$$C(x,\lambda)=-\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{\overline{W(\lambda)}}E\Theta_H(\lambda)^*, \tag{4.18}$$

where

$$E:=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{4.19}$$

This shows that $C(x,\lambda)$ is actually independent of $x\in\Omega$. By (4.8) this leads to the representation

$$j_{\hat{\varrho}}(x,\lambda) = -\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{\overline{\overline{W(\lambda)}}}\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)E\Theta_H(\lambda)^*), \tag{4.20}$$

which shows that the current density is also independent of $x\in\Omega$. Thus it makes sense to denote $C(x,\lambda)$ and $j_{\hat{\varrho}}(x,\lambda)$ by $C(\lambda)$ and $j_{\hat{\varrho}}(\lambda)$, respectively. Hence, we have proved one part of the assertion (4.2) and (4.3). Taking into account the identity

$$\frac{1}{\overline{\overline{W(\lambda)}}}E\Theta_H(\lambda)^* = -\frac{1}{W(\lambda)}\Theta_H(\lambda)E \tag{4.21}$$

we verify the other part.

It remains to show (4.4) and (4.5). To this end we note that from (4.17) one gets

$$J\Theta_H(\lambda)^* = J + \frac{i}{W(\lambda)}\begin{pmatrix} \alpha_b\alpha_a & -\alpha_a^2 v_b(a,\lambda) \\ -\alpha_b^2 v_a(b,\lambda) & \alpha_b\alpha_a \end{pmatrix}, \tag{4.22}$$

where

$$J := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.23}$$

Hence we find

$$\mathrm{tr}_{\mathbb{C}^2}(J\Theta_H(\lambda)^*) = 2i\frac{\alpha_b\alpha_a}{W(\lambda)}, \tag{4.24}$$

which yields

$$\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)} = -\frac{1}{4\pi}\mathrm{tr}_{\mathbb{C}^2}(J\Theta_H(\lambda)^*). \tag{4.25}$$

Using the definition (4.3) we finally obtain

$$j_{\hat{\varrho}}(\lambda) = -\frac{1}{4\pi}\mathrm{tr}_{\mathbb{C}^2}(J\Theta_H(\lambda)^*)\ \ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)\Theta_H(\lambda)E). \tag{4.26}$$

This leads to the estimate

$$|j_{\hat{\varrho}}(\lambda)| \leqslant \frac{1}{4\pi}\|\Theta_H(\lambda)^*\|_{\mathcal{L}_1(\mathbb{C}^2)}\|\varrho(\lambda)\|_{\mathcal{L}_1(\mathbb{C}^2)}. \tag{4.27}$$

Since $\|\Theta_H(\lambda)^*\|_{\mathcal{L}_1(\mathbb{C}^2)} \leqslant 2$ and $\|\varrho(\lambda)\|_{\mathcal{L}_1(\mathbb{C}^2)} = \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda))$ we find

$$|j_{\hat{\varrho}}(\lambda)| \leqslant \frac{1}{2\pi}\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)), \tag{4.28}$$

which immediately proves (4.5). □

In correspondence to the carrier density it seems to be useful to introduce the following definition.

Definition 4.2: Assume $m+1/m\in L^\infty([a,b])$, $V\in L^2([a,b])$ and $\kappa_a,\kappa_b\in\mathbb{C}_+$. Then the matrix $C(\lambda)$ and the value $j_\varrho(\lambda)$ are called the current density observable and the current density at energy $\lambda\in\mathbb{R}$ of the system described by H, respectively.

The definition is again justified by the fact that the current density at energy $\lambda \in \mathbb{R}$ is the expectation value of the current density observable at energy $\lambda \in \mathbb{R}$, i.e., $j_{\hat{\varrho}}(\lambda) = \mathbb{E}_{\varrho(\lambda)}(C(\lambda))$ for $\lambda \in \mathbb{R}$. Using this notation formula (4.4) takes the form

$$j_{\hat{\varrho}} = \int_{\mathbb{R}} d\lambda \, \mathbb{E}_{\varrho(\lambda)}(C(\lambda)). \tag{4.29}$$

In the following corollary we consider the case that the steady state ϱ is a function of K, i.e.,

$$\varrho = f(K), \tag{4.30}$$

where, of course, $f(\cdot) \in L^{\infty}(\mathbb{R})$ and $f(\lambda) \geqslant 0$ for a.e. $\lambda \in \mathbb{R}$ and. In this case the density matrix ϱ belongs to the bicommutant of K.

Corollary 4.3: Assume $m + 1/m \in L^{\infty}([a,b])$, $V \in L^2([a,b])$ *and* $\kappa_a, \kappa_b \in \mathbb{C}_+$. *If the steady state* ϱ *is given by (4.30) with a non-negative function* $f(\cdot) \in L^{\infty}(\mathbb{R})$, *then* $j_{\hat{\varrho}}(\lambda) = 0$ *for a.e.* $\lambda \in \mathbb{R}$.

Proof: In this case one has

$$\varrho(\lambda) = f(\lambda) I_{\mathbb{C}^2}, \quad \lambda \in \mathbb{R}. \tag{4.31}$$

which gives

$$j_{\hat{\varrho}}(\lambda) = f(\lambda)\mathrm{tr}(C(\lambda)) = -\frac{1}{2\pi i} f(\lambda) \frac{\alpha_b \alpha_a}{\overline{W(\lambda)}} \mathrm{tr}_{\mathbb{C}^2}(E\Theta_H(\lambda)^*). \tag{4.32}$$

By (4.17) we immediately get that $\mathrm{tr}_{\mathbb{C}^2}(E\Theta_H(\lambda)^*) = 0$ for $\lambda \in \mathbb{R}$. □

If the steady state ϱ has the form

$$\varrho(\lambda) = \begin{pmatrix} \varrho^{bb}(\lambda) & 0 \\ 0 & \varrho^{aa}(\lambda) \end{pmatrix}, \tag{4.33}$$

then the current density is given by

$$j_{\hat{\varrho}}(\lambda) = -\frac{1}{2\pi} \frac{\alpha_a^2 \alpha_b^2}{|W(\lambda)|^2} (\varrho^{bb}(\lambda) - \varrho^{aa}(\lambda)). \tag{4.34}$$

This current density is different from zero if $\varrho^{bb}(\lambda) \neq \varrho^{aa}(\lambda)$ at least for a set of positive Lebesgue measure. So a current density different from zero arises only if we have an occupation disparity between the two eigenstates $\psi^-(x,\lambda,b)$ and $\psi^-(x,\lambda,a)$. This is the case if the steady state ϱ belongs to the commutant of K but not to the bicommutant. In other words, the density matrix (1.5) used for self-adjoint boundary conditions and generalized by (4.30) to the dissipative case leads to a zero current density.

V. CONCLUDING REMARKS

A. Density and current

The carrier density $u_{\hat{\varrho}}(\cdot)$ defined by (3.41) and (3.44) is a straightforward generalization of the corresponding definition (1.3) of the carrier density in the self-adjoint case. Indeed, this correspondence relies on the replacements

$$
\begin{gathered}
l \leftrightarrow \{a,b,\lambda\}, \\
\{\psi_l\}_{l=1}^{\infty} \leftrightarrow \{\vec{\psi}(\cdot,\lambda,\tau)\}_{\lambda\in\mathbb{R},\tau=a,b}, \\
\sum_{l=1}^{\infty} \leftrightarrow \int_{\lambda\in\mathbb{R}} d\lambda \sum_{\tau=a,b} \\
\varrho_l \leftrightarrow \varrho(\lambda).
\end{gathered}
\tag{5.1}
$$

The same holds true for the current density defined by (4.1) which is a straightforward generalization of (1.8). However, in contrast to the self-adjoint case the current density now is not necessarily zero.

B. Lax–Phillips scattering theory

There is consensus in the conviction that scattering states are responsible for the current. This usually leads to a a relation between current density and scattering matrix. Actually, the same takes place here. Formulas (4.2) and (4.3) relate the current density $j_{\hat{\varrho}}(\lambda)$ with the characteristic function $\Theta_{H*}(\lambda)$ of H^*. It turns out that the characteristic function $\Theta_{H*}(\lambda)$ of H^* can be regarded as the scattering matrix of an associated scattering system. Indeed, with the self-adjoint dilation K one can associate a Lax–Phillips scattering theory.[20,21] To this end one introduces the Hilbert space $\mathfrak{k}_0$,

$$
\mathfrak{k}_0 := L^2(\mathbb{R},\mathbb{C}^2) = \mathcal{D}_- \oplus \mathcal{D}_+ \subseteq \mathfrak{k}. \tag{5.2}
$$

and the identification operators $J_\pm : \mathfrak{k}_0 \to \mathfrak{k}$,

$$
\begin{aligned}
\vec{f} = J_- f &:= P_{\mathcal{D}_-}^{\mathfrak{k}_0} f \oplus 0 \oplus 0, \quad f \in \mathfrak{k}_0, \\
\vec{f} = J_+ f &:= 0 \oplus 0 \oplus P_{\mathcal{D}_+}^{\mathfrak{k}_0} f, \quad f \in \mathfrak{k}_0.
\end{aligned}
\tag{5.3}
$$

The subspaces $\mathcal{D}_-$ and $\mathcal{D}_+$ are called incoming and outgoing subspaces, respectively. On the Hilbert space $\mathfrak{k}_0$ one defines the self-adjoint operator K_0,

$$
(K_0 f)(x) = -i \frac{d}{dx} f(x) \tag{5.4}
$$

with the domain $\mathrm{dom}(K_0) := W^{1,2}(\mathbb{R},\mathbb{C}^2)$. The Lax–Phillips wave operators

$$
W_\pm = s - \lim_{t\to\pm\infty} e^{itK} J_\pm e^{-itK_0} \tag{5.5}
$$

exist and are complete, i.e., $\mathrm{ran}(W_\pm) = \mathfrak{k}$. The corresponding Lax–Phillips scattering operator $S = W_+^* W_- : \mathfrak{k}_0 \to \hat{\mathfrak{k}}$, is unitary and commutes with the self-adjoint operator K_0. By $\mathcal{F}: \mathfrak{k}_0 \to \hat{\mathfrak{k}}$ we denote the Fourier transform

$$
(\mathcal{F} f)(\lambda) = \hat{f}(\lambda) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dx\, e^{-i\lambda x} f(x), \quad f \in \mathfrak{k}_0, \quad \lambda \in \mathbb{R}. \tag{5.6}
$$

We note that $\mathcal{F} K_0 \mathcal{F}^{-1} = M$ where M is defined by (2.43). Since S commutes with K_0 the operator $\hat{S} = \mathcal{F} S \mathcal{F}^{-1} : \hat{\mathfrak{k}} \to \hat{\mathfrak{k}}$ commutes with M. Hence $\hat{S}$ is a multiplication operator given by

$$
(\hat{S}\hat{f})(\lambda) = S(\lambda)\hat{f}(\lambda), \quad \hat{f} \in \hat{\mathfrak{k}}, \quad \lambda \in \mathbb{R}, \tag{5.7}
$$

where $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of unitary operators which is called the Lax–Phillips scattering matrix. A rather involved computation shows that

$$S(\lambda)=\Theta_{H^*}(\lambda) \tag{5.8}$$

for a.e. $\lambda\in\mathbb{R}$, see, e.g., Ref. 22. By the way one has

$$\Phi_-=\mathcal{F}W_+^*, \quad \Phi_+=\mathcal{F}W_-^*, \tag{5.9}$$

where is Φ_- is the incoming Fourier transformation, cf. (2.41) and (2.42), and Φ_+ is the so-called outgoing Fourier transform which was introduced in Ref. 9.

C. Continuity equation

As mentioned above the quantity $N_\varrho(\omega)$,

$$N_\varrho(\omega):=\|u_{\hat{\varrho}}\|_{L^1(\omega)}=\int_\omega \mathrm{d}x\, u_{\hat{\varrho}}(x), \tag{5.10}$$

has the meaning of the number of carriers on the Borel set subset $\omega\subseteq\Omega=[a,b]$. By (3.44) one has the representation

$$N_\varrho(\omega)=\mathrm{tr}(\varrho U(\omega)). \tag{5.11}$$

Obviously $N:=N_\varrho(\Omega)$ is the total number of carriers on the interval $[a,b]$. We note that under condition (3.23) by Proposition 3.7 the total number of carriers in Ω is always finite.

In accordance with Ref. 8 the time evolution of the density matrix ϱ is given by

$$\varrho(t)=e^{-itK}\varrho e^{itK}, \quad t\in\mathbb{R}. \tag{5.12}$$

Hence, the number of particles at time $t\in\mathbb{R}$ on ω is given by

$$N_{\varrho(t)}(\omega):=\mathrm{tr}(\varrho(t)U(\omega)), \quad t\in\mathbb{R}. \tag{5.13}$$

Since ϱ commutes with K one has $\varrho(t)=\varrho$ and $N_{\varrho(t)}(\omega)=N_\varrho(\omega)$ or

$$\frac{\mathrm{d}}{\mathrm{d}t}N_{\varrho(t)}(\omega)=0, \quad \omega\subseteq\Omega, \quad t\in\mathbb{R}. \tag{5.14}$$

If the condition

$$C_{\hat{\varrho}}:=\sup_{\lambda\in\mathbb{R}}(1+\lambda^2)\|\varrho(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)}<\infty \tag{5.15}$$

is satisfied, then

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}N_{\varrho(t)}(\omega)&=-i\,\mathrm{tr}(K\varrho(t)U(\omega))+i\,\mathrm{tr}(\varrho(t)KU(\omega))\\&=-i\,\mathrm{tr}(K\varrho U(\omega))+i\,\mathrm{tr}(\varrho KU(\omega))\\&=-i\int_{\mathbb{R}}\mathrm{d}\lambda\int_\omega \mathrm{d}x\,\lambda\,\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda))+i\int_{\mathbb{R}}\mathrm{d}\lambda\int_\omega \mathrm{d}x\,\lambda\,\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)).\end{aligned} \tag{5.16}$$

By formula (3.42) we find

$$\int_\omega dx\,\lambda\left(\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)\right)=\int_\omega dx\,\lambda\left\langle \varrho^t(\lambda)\begin{pmatrix}\psi^-(x,\lambda,b)\\ \psi^-(x,\lambda,a)\end{pmatrix},\begin{pmatrix}\psi^-(x,\lambda,b)\\ \psi^-(x,\lambda,a)\end{pmatrix}\right\rangle. \tag{5.17}$$

Since $l(\psi^-(x,\lambda,\tau))=\lambda\psi^-(x,\lambda,\tau)$ one gets

$$\int_\omega dx\,\lambda\left(\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)\right)=\int_\omega dx\left\langle \varrho^t(\lambda)\begin{pmatrix}l(\psi^-(x,\lambda,b))\\ l(\psi^-(x,\lambda,a))\end{pmatrix},\begin{pmatrix}\psi^-(x,\lambda,b)\\ \psi^-(x,\lambda,a)\end{pmatrix}\right\rangle. \tag{5.18}$$

Hence

$$\begin{aligned}\frac{d}{dt}N_{\varrho(t)}(\omega)=&-i\int_{\mathbb{R}}d\lambda\int_\omega dx\left\langle \varrho^t(\lambda)\begin{pmatrix}l(\psi^-(x,\lambda,b))\\ l(\psi^-(x,\lambda,a))\end{pmatrix},\begin{pmatrix}\psi^-(x,\lambda,b)\\ \psi^-(x,\lambda,a)\end{pmatrix}\right\rangle\\ &+i\int_{\mathbb{R}}d\lambda\int_\omega dx\left\langle \varrho^t(\lambda)\begin{pmatrix}\psi^-(x,\lambda,b)\\ \psi^-(x,\lambda,a)\end{pmatrix},\begin{pmatrix}l(\psi^-(x,\lambda,b))\\ l(\psi^-(x,\lambda,a))\end{pmatrix}\right\rangle.\end{aligned} \tag{5.19}$$

Let $\omega=[c,d]\subseteq[a,b]$. Integrating by parts and taking into account formula (4.7) we get

$$\frac{d}{dt}N_{\varrho(t)}(\omega)=\int_{\mathbb{R}}d\lambda\{j_{\hat\varrho}(c,\lambda)-j_{\hat\varrho}(d,\lambda)\}. \tag{5.20}$$

The total current $j_{\hat\varrho}(x)$ at the point $x\in[a,b]$ is defined by

$$j_{\hat\varrho}(x):=\int_{\mathbb{R}}d\lambda\,j_{\hat\varrho}(x,\lambda). \tag{5.21}$$

This yields

$$\frac{d}{dt}N_{\varrho(t)}(\omega)=j_{\hat\varrho}(c)-j_{\hat\varrho}(d) \tag{5.22}$$

which shows that the change of the number of carriers in the set $[c,d]$ is equal to the difference between the incoming current $j_{\hat\varrho}(c)$ at point c and the outgoing current $j_{\hat\varrho}(d)$ at point d which very well corresponds to the physical intuition. Since by Proposition 4.1 the current density $j_{\hat\varrho}(x,\lambda)$ does not depend on $x\in[a,b]$ one gets $j_{\hat\varrho}(d)=j_{\hat\varrho}(c)$ which again verifies (5.14). Relation (5.22) is the integral form of the continuity equation which has the differential form

$$\frac{\partial}{\partial t}u_{\hat\varrho(t)}(x)+\frac{\partial}{\partial x}j_{\hat\varrho(t)}(x)=0,\quad t\in\mathbb{R},\quad x\in\Omega, \tag{5.23}$$

where $u_{\hat\varrho(t)}(x)$ is the carrier density at time $t\in\mathbb{R}$ and $j_{\hat\varrho(t)}(x)$ is the current density at time t given by (5.21). Since $u_{\hat\varrho(t)}(x)=u_{\hat\varrho}(x)$ is independent of t and $j_{\hat\varrho(t)}(x)$ is independent of x the continuity equation (5.23) obviously holds in the present situation.

D. Schrödinger–Poisson systems

Schrödinger–Poisson systems are of great interest in semiconductor physics, see, e.g., Ref. 1. In the following we are interested in a Schrödinger–Poisson system on the interval $\Omega=[a,b]$ of the real axis $\mathbb{R}$. Systems of this type were considered in Ref. 6. By φ we denote the electrostatic potential on Ω which is determined by Poisson's equation

$$-\frac{d}{dx}\epsilon(x)\frac{d}{dx}\varphi=q(C(x)+u^+-u^-),\quad x\in\Omega, \tag{5.24}$$

where u^+ and u^- are the densities of holes and electrons, respectively, q is the magnitude of the elementary charge, $C(\cdot)$ is a given concentration of ionized dopants, and $\epsilon=\epsilon(x)>0$ denotes the dielectric permittivity which satisfies the condition

$$\epsilon(\cdot)+\frac{1}{\epsilon(\cdot)}\in L^\infty([a,b]). \tag{5.25}$$

The Poisson equation (5.24) is completed by the boundary conditions

$$\varphi(a)=\varphi_a, \quad \text{and} \quad \varphi(b)=\varphi_b. \tag{5.26}$$

Next we have to specify Schrödinger-operators of the type (2.1) for different species of particles—holes and electrons indexed by $\pm$, respectively. We assume that for these species the effective masses $m_\pm$, external potentials $V_0^\pm$, and coefficients $\kappa_a^\pm, \kappa_b^\pm \in \mathbb{C}_+$ are given. For each species this leads to different dissipative Schrödinger operators $H^\pm(V_\pm)$ defined in accordance with (1.9), (2.1), and (2.2). The potential V entering into the definition of the Schrödinger operators has the form

$$V_\pm := V_0^\pm \pm \varphi(u), \tag{5.27}$$

where the electrostatic potential φ is a solution of the Poisson equation (5.24) with boundary condition (5.26). The carrier densities $u^\pm$ entering into Poisson's equation are obtained from the dissipative Schrödinger operators $H^\pm(V_\pm)$ in accordance with Sec. III. To this end we assume that the families of matrices $\{\varrho_\pm(\lambda)\}_{\lambda\in\mathbb{R}}$, which obey

$$C_{\hat{\varrho}_\pm} := \sup_{\lambda\in\mathbb{R}} \sqrt{\lambda^2+1}\,\|\varrho_\pm(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} < \infty, \tag{5.28}$$

are given. If $D^\pm(V_\pm)(x)$ are the carrier density observables at $x\in\Omega$ and at energy $\lambda\in\mathbb{R}$, then the carrier densities are computed by

$$u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x)=\int_{\mathbb{R}} d\lambda\, u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x,\lambda), \quad x\in\Omega, \tag{5.29}$$

where

$$u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x,\lambda)=\mathrm{tr}_{\mathbb{C}^2}(\varrho_\pm(\lambda)D^\pm(V_\pm)(x,\lambda)), \quad x\in\Omega, \quad \lambda\in\mathbb{R}. \tag{5.30}$$

Moreover, if $\mathrm{tr}_{\mathbb{C}^2}(\varrho_\pm(\cdot))\in L^1(\mathbb{R})$ is valid, then the current densities $j^\pm_{\hat{\varrho}_\pm}$,

$$j^\pm_{\hat{\varrho}_\pm}=\int_{\mathbb{R}} d\lambda\, j^\pm_{\hat{\varrho}_\pm}(V_\pm)(\lambda) \tag{5.31}$$

are also well-defined and finite, cf. Sec. IV. The so described system is called a dissipative Schrödinger–Poisson system. We note that the total number of carriers $N^\pm(V_\pm)$ is given by

$$N^\pm(V_\pm)=\int_\Omega dx\, u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x) \tag{5.32}$$

and is not fixed.

In a forthcoming paper[23] we show that under suitable conditions on $\epsilon(\cdot)$, $C(\cdot)$, $m_\pm(\cdot)$, $V_0^\pm(\cdot)$, $\kappa_b^\pm$, $\kappa_a^\pm$ and $\varrho_\pm$ this dissipative Schrödinger–Poisson system always admits a self-consistent solution.

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SU(*N*) coherent states

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We generalize Schwinger boson representation of SU(2) algebra to SU(N) and define coherent states of SU(N) using $2(2^{N-1}-1)$ bosonic harmonic oscillator creation and annihilation operators. We give an explicit construction of all (N-1) Casimirs of SU(N) in terms of these creation and annihilation operators. The SU(N) coherent states belonging to any irreducible representations of SU(N) are labeled by the eigenvalues of the Casimir operators and are characterized by (N-1) complex orthonormal vectors describing the SU(N) manifold. The coherent states provide a resolution of identity, satisfy the continuity property, and possess a variety of group theoretic properties. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The idea of a coherent state for a quantum system was realized by Schrödinger[1] way back in 1926 in the context of quantum state of classical motion for a harmonic oscillators. This simplest coherent state construction is associated with the Heisenberg–Weyl group whose Lie algebra is given in terms of a harmonic oscillator creation and annihilation operators. These states have been widely used in physics.[2–4] Later, coherent states associated with an arbitrary Lie group in a given representation were constructed[5] by applying group operators to a weight vector in that particular representation. In the special case of the SU(2) group, another equivalent way of constructing the coherent states was by exploiting the Schwinger representation of the SU(2) algebra.[6] This representation involves a doublet of harmonic oscillator creation annihilation operators in terms of which one generalizes the simplest Heisenberg–Weyl coherent state construction to the SU(2) group. In Ref. 7, using the Schwinger representation of SU(3) algebra, we had constructed coherent states belonging to an arbitrary representation of SU(3). The motivation of the present work is: (a) to further generalize this Schwinger representation of SU(3) to SU(N) Lie algebra for arbitrary N, (b) exploit it to construct coherent states belonging to arbitrary irreducible representations of SU(N). We also give an explicit characterization of the SU(N) coherent states in terms of (N-1) complex N-plets describing the SU(N) manifold. In Ref. 8, SU(N) coherent states were constructed by applying the standard procedure of applying SU(N) group operator on the highest weight state of a SU(N) representation.

The organization of the paper is as follows. In Sec. II we will briefly describe the Heisenberg–Weyl and SU(2) coherent states in terms of harmonic oscillators. Sec. II is not only for the sake of completeness but also for setting up notation and language in a simpler setting before dealing with the larger SU(N) groups. This section also emphasizes the common spirit between them and our SU(N) coherent state formalism. However, with these groups being too simple, many features of larger SU(N) groups become redundant and hence this section fails to bring out a technique which can be generalized to SU(N). Therefore, in Sec. III, we briefly mention the SU(3) coherent state construction in a framework which is equivalent to the one in Ref. 7 but can be easily generalized to SU(N). In Sec. IV, we generalize this SU(3) procedure and explicitly construct SU(N) coherent states for arbitrary N.

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II. HEISENBERG–WEYL AND SU(2) COHERENT STATES

Given a group G and its manifold $\mathcal{M}$, the coherent states in a given representation R are functions of q parameters denoted by $\{z^1,z^2,\ldots,z^q\}$ describing $\mathcal{M}$, and are defined as

$$|\vec{z}\rangle_R \equiv T_R(g(\vec{z}))\ \ |0\rangle_R . \tag{1}$$

Here $T_R(g(\vec{z}))$ is a group element in the representation R, and $|0\rangle_R$ is a fixed vector belonging to R. In the simplest example of the Heisenberg–Weyl group, the Lie algebra contains three generators. It is defined in terms of creation–annihilation operators $(a,a^\dagger)$ satisfying

$$[a,a^\dagger]=\mathcal{I},\quad [a,\mathcal{I}]=0,\quad [a^\dagger,\mathcal{I}]=0. \tag{2}$$

This algebra has only one infinite dimensional irreducible representation which can be characterized by occupation number states

$$|n\rangle \equiv \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$$

with $n=0,1,2,\ldots$. A generic group element in Eq. (1) can be characterized by $T(g)=\exp(i\alpha\mathcal{I}+za^\dagger-\overline{z}a)$ with an angle α and a complex parameter z. Therefore,

$$\begin{aligned} |\alpha,z\rangle_\infty &= \exp(i\alpha)\ \ |z\rangle_\infty , \\ |z\rangle_\infty &= \exp(za^\dagger-\overline{z}a)\ \ |0\rangle = \sum_{n=0}^{\infty} F_n(z)\ \ |n\rangle, \end{aligned} \tag{3}$$

where the sum runs over all the basis vectors of the infinite dimensional representation, and

$$F_n(z)=\frac{z^n}{\sqrt{n!}} \tag{4}$$

are the coherent state expansion coefficients. This feature, i.e., an expansion of the coherent states in terms of basis vectors of a given representation with analytic functions of complex variables $(F_n(z))$ as coefficients, will also be present in the case of SU(N) groups. It is easy to see that Eq. (3) provides a resolution of identity with the measure $d\mu(z)=dz\,d\overline{z}\exp(-|z|^2/2)$.

We now briefly review the next simplest example, i.e., the Schwinger representation of SU(2) Lie algebra and the associated coherent states. The Lie algebra is

$$[J^a,J^b]=i\epsilon^{abc}J^c. \tag{5}$$

The algebra (5) can be realized in terms of a doublet of harmonic oscillator creation and annihilation operators $a\equiv(a^1,a^2)$ and $\vec{a}^\dagger\equiv(a_1^\dagger,a_2^\dagger)$, respectively.[6] They satisfy the simpler bosonic commutation relation $[a^i,a_j^\dagger]=\delta^i_j$ with $i,j=1,2$. The vacuum state is $|0,0\rangle$. In terms of these operators,

$$Q^a \equiv \tfrac{1}{2}a_i^\dagger(\sigma^a)^i_j a^j, \tag{6}$$

where σ^a denote the Pauli matrices. (We will generally use the convention that repeated indices are summed over.) It is easy to check that the operators in (6) satisfy the SU(2) Lie algebra

$$[Q^a,Q^b]=i\epsilon^{abc}Q^c. \tag{7}$$

We also note that

$$[Q^a, a_i^\dagger] = a_j^\dagger \tfrac{1}{2}(\sigma^a)_i^j. \tag{8}$$

Equation (8) implies that $(a_1^\dagger, a_2^\dagger)$ transform like a SU(2) doublet. This fundamental representation of SU(2) will be denoted by the Young diagram $\Sigma_{[1]}$, which is a single box. Therefore, we can realize all SU(2) irreducible representations on the Hilbert space of harmonic oscillators created by creation operators acting on the vacuum which is a direct product of the vacuum states for a_1 and a_2. The SU(2) Casimir operator is given by

$$\mathcal{C} = \sum_{i=1}^{2} a_i^\dagger \cdot a^i \equiv a^\dagger \cdot a. \tag{9}$$

The eigenvalues of the Casimir $\mathcal{C}$ will be denoted by C. The various irreducible representations of SU(2) are characterized by the eigenvalues of the Casimir (or occupation number operator) in (9). We also know that any irreducible representation of SU(2) can also be defined by its Young diagram, which is obtained by arranging a certain number of boxes in a row. It is easy to see that $\mathcal{C}$ just counts this number. The basis vectors of the SU(2) irreducible representation with $\mathcal{C} = C$ are given by

$$\|i_1 i_2 \cdots i_C\rangle \equiv a_{i_1}^\dagger a_{i_2}^\dagger \cdots a_{i_C}^\dagger |0\rangle. \tag{10}$$

The dimension of the above-given irreducible representation is $(C+1)$. With the harmonic oscillator creation and annihilation operators, SU(2) coherent states can be obtained by directly generalizing (3). We define a doublet of complex numbers (z^1, z^2) with the constraint:

$$|z|^2 \equiv |z^1|^2 + |z^2|^2 = 1. \tag{11}$$

The above-given constraint gives three independent real compact parameters which define the sphere $\mathcal{M} = S^3$. The SU(2) coherent state in the representation C is now defined as

$$|z\rangle_C \equiv |z^1, z^2\rangle_C = \exp(\vec{z}\cdot\vec{a}^\dagger)|0,0\rangle|_{\vec{a}^\dagger\cdot\vec{a}=C} \cdot = F^{i_1 i_2 \cdots i_C} a_{i_1}^\dagger a_{i_2}^\dagger \cdots a_{i_C}^\dagger |0\rangle = F^{i_1 i_2 \cdots i_C} \|i_1 i_2 \cdots i_C\rangle, \tag{12}$$

where

$$F^{i_1 i_2 \cdots i_C} = \frac{1}{C!} z^{i_1} z^{i_2} \cdots z^{i_C}. \tag{13}$$

Note that F in (13) are analytic functions of z^1 and z^2. Under SU(2) transformations:

$$z^i \to z'^i = \exp i\left(\theta^a \frac{\sigma^a}{2}\right)_j^i z^j. \tag{14}$$

Thus the constraint (11) remains invariant under the SU(2) transformations (14). Therefore, the coherent states $|z\rangle \equiv |z_1, z_2\rangle$ transform amongst themselves on S^3. It is easy to check the resolution of identity:

$$\int d^2 z^1 d^2 z^2 \delta(|z^1|^2 + |z^2|^2 - 1)|z\rangle_{CC}\langle z| = \frac{1}{1+C} \sum_{i_1,\ldots,i_C=1}^{2} \|i_1 i_2 \ldots i_C\rangle\langle i_1 i_2 \cdots i_C\|. \tag{15}$$

III. THE SCHWINGER SU(3) REPRESENTATION

The basic technique behind the construction of SU(N) coherent states is to generalize the Schwinger representation of SU(3) Lie algebra[7] to SU(N) Lie algebra. We will, therefore, briefly

describe the construction of SU(3) Lie algebra in terms of harmonic oscillators here in a new framework which is equivalent to that in Ref. 7 but is directly generalizable to SU(N).

The rank of the SU(3) group is 2 and therefore it has two fundamental representations: Any SU(3) irreducible representation can be built up from the two fundamental representations, a triplet 3 and an anti-triplet $\bar{3}$. The latter is an antisymmetric combination of the two triplets. The two fundamental representations will be associated with the two (fundamental) Young diagrams $\Sigma_{[1,0]}$, for the triplet representation and $\Sigma_{[0,1]}$, for its conjugate (anti-triplet) representation. The Young diagram $\Sigma_{[1,0]}$ is one box and $\Sigma_{[0,1]}$ is two boxes arranged vertically. We will also label the fundamental representations by the Greek indices $[\alpha]$,$[\beta]$ taking values 1 and 2. The components of any irreducible tensor T transforming according to $\Sigma_{[1,0]}(\Sigma_{[0,1]})$ will be denoted by $T[\alpha=1]_{i_1}(T[\alpha=2]_{i_1 i_2} \equiv -T_{i_1 i_2}, (i_1, i_2 = 1,2,3))$. (The components of the complex conjugate of these tensors will be denoted by $T^*[1]^{j_1} T^*[2]^{j_1 j_2}$.) Further, the eight representation matrices corresponding to these two fundamental representations will be denoted by $\lambda^a[\alpha]$. (Note that $\lambda^a[2]^{i_1 i_2}_{j_1 j_2} \equiv \frac{1}{2}\epsilon^{i_1 i_2 k}\epsilon_{j_1 j_2 l}(-\lambda^{*a}[1])^l_k$.) If Q^a are the generators of SU(3) then under the SU(3) they transform as

$$
\begin{aligned}
[Q^a, T[1]_{i_1}] &= T[1]_{j_1}\lambda^a[1]^{j_1}_{i_1}, \\
[Q^a, T[2]_{i_1 i_2}] &= T[2]_{j_1 j_2}\lambda^a[2]^{j_1 j_2}_{i_1 i_2}.
\end{aligned}
\tag{16}
$$

The matrices on the right-hand side of (16) are the matrices belonging to the fundamental representations of SU(3) and satisfy the SU(3) Lie algebra:

$$
\begin{aligned}
[\lambda^a[1], \lambda^b[1]] &= i f^{abc}\lambda^c[1], \\
[\lambda^a[2], \lambda^b[2]] &= i f^{abc}\lambda^c[2].
\end{aligned}
\tag{17}
$$

The direct product of these two tensors (representations) span the whole SU(3) representation space. In fact, any irreducible tensor can be obtained by taking direct products of C_1 of T[1] and C_2 of T[2] tensors. The corresponding Young diagram is represented by arranging C_2 of $\Sigma[2]$ Young diagrams and C_1 of $\Sigma[1]$ diagrams from left to right side by side. Following Schwinger's representation of SU(2) Lie algebra, we introduce two sets of creation–annihilation operators $a[\alpha], a^\dagger[\alpha], \alpha = 1,2$. The set $a[\alpha=1]$ represents three annihilation operators denoted by $a^{i_1}[1] \equiv (a[1]^1, a[1]^2, a[1]^3)$ and $a[\alpha=2]$ represents another set of three annihilation operators, $a[2]^{i_1 i_2} = -a[2]^{i_2 i_1}$ having three independent components $(a[2]^{12}, a[2]^{23}, a[2]^{31})$. (In Ref. 7, we had chosen $b_1 = a[2]^{23}, b_2 = a[2]^{31}, b_3 = a[2]^{12}$.) We impose the following commutation relations on them:

$$
\begin{aligned}
&[a[1]^{i_1}, a^\dagger[1]_{j_1}] = \delta^{i_1}_{j_1}, \quad [a^{i_1}[1], a^{i_2}[1]] = 0, \\
&[a[2]^{i_1 i_2}, a^\dagger[2]_{j_1 j_2}] = \delta^{i_1}_{j_1}\delta^{i_2}_{j_2} - \delta^{i_1}_{j_2}\delta^{i_2}_{j_1}, \quad [a[2]^{i_1 i_2}, a[2]^{j_1 j_2}] = 0, \\
&[a[1]^{i_1}, a[2]^{i_2 i_3}] = 0, \quad [a^\dagger[1]_{i_1}, a[2]^{i_2 i_3}] = 0.
\end{aligned}
\tag{18}
$$

We now define the SU(3) generators in the Hilbert space of Harmonic oscillators as:

$$
Q^a = a^\dagger[1]_{i_1}\lambda^a[1]^{i_1}_{i_2}a[1]^{i_2} + \frac{1}{2!}a^\dagger[2]_{i_1 i_2}\lambda^a[2]^{i_1 i_2}_{j_1 j_2}a[2]^{j_1 j_2}. \tag{19}
$$

Using (18), it is easy to check that

$$
[Q^a, Q^b] = i f^{abc} Q^c. \tag{20}
$$

Further,

$$[Q^a,a^\dagger[1]_{i_1}]=a^\dagger[1]_{j_1}\lambda^a[1]^{j_1}_{i_1},$$
$$[Q^a,a^\dagger[2]_{i_1i_2}]=a^\dagger[2]_{j_1j_2}\lambda^a[2]^{j_1j_2}_{i_1i_2}. \tag{21}$$

Equation (21) implies that $a^\dagger[1]$ and $a^\dagger[2]$ transform like $\Sigma_{[1,0]}$ and $\Sigma_{[0,1]}$ fundamental representations, respectively. Therefore, all the irreducible representations of (20) can be realized on the Hilbert space created by creation operators $a^\dagger[1]_{i_1}$ and $a^\dagger[2]^{i_1i_2}$ acting on the vacuum state $|0\rangle$, which is direct product of vacuum states associated with each of the six harmonic oscillators. Further, the two Casimir operators of SU(3) in this generalization of Schwinger representation are given by

$$\mathcal{C}[1]=\sum_{i_1=1}^{3} a^\dagger_{i_1}[1]a^{i_1}[1],$$
$$\mathcal{C}[2]=\sum_{i_1,i_2=1}^{3} a^\dagger_{i_1i_2}[2]a^{i_1i_2}[2]. \tag{22}$$

The eigenvalues of the two Casimirs in (22) will be denoted by C_1 and C_2, respectively.

A. Irreducible representations of SU(3)

The eigenvalues of Casimirs (C_1,C_2) characterize all the irreducible representations of SU(3). On the other hand, we can also define irreducible representations by its Young diagram, which is built up by arranging certain numbers of $\Sigma_{[1,0]}$ followed by $\Sigma_{[0,1]}$ horizonally from right to left. It is easy to see that $\mathcal{C}_1$ and $\mathcal{C}_2$ just count these numbers. Therefore, we will denote a general SU(3) Young diagram by $\Sigma_{[C_1,C_2]}$ which contains C_1 of $\Sigma_{[1,0]}$ and C_2 of $\Sigma_{[2]}$ put together from from right to left. Therefore, a general basis vector in $\Sigma_{[C_1,C_2]}$ can be written as

$$\|i^1_1i^2_1\cdots i^{C_2+C_1}_1;i^1_2i^2_2\cdots i^{C_2}_2\rangle_{\Sigma_{[C_1,C_2]}}$$
$$\equiv(e_{\Sigma_{[C_1,C_2]}})a^\dagger[2]_{i^1_1i^1_2}a^\dagger[2]_{i^2_1i^2_2}\cdots a^\dagger[2]_{i^{C_2}_1i^{C_2}_2}[2]a^\dagger[1]_{i^{C_2+1}_1}a[1]^\dagger_{i^{C_2+2}_1}\cdots a^\dagger[1]_{i^{C_2+C_1}_1}|0\rangle. \tag{23}$$

In (23), we have characterized the basis vectors of $\Sigma_{[C_1,C_2]}$ representation by the various box indices appearing in the Young Tableau $\Sigma_{[C_1,C_2]}$. More explicitly, the index i^c_r represents the index corresponding to the box appearing in the rth row and cth column. $e_{\Sigma_{[C_1,C_2]}}$ is the idempotent associated with the Young tableau $\Sigma_{[C_1,C_2]}$. In general, it is an element of group algebra corresponding to the permutation group $S(C_1+2C_2)$. It is defined as the product of the two symmetrizers $\mathcal{S}_1$ (symmetrizing the indices in the first row $(i^1_1,i^2_1,\ldots,i^{C_1+C_2}_1)$, $\mathcal{S}_2$ (symmetrizing the indices in the second row $(i^1_2,i^2_2,\ldots,i^{C_1+C_2}_2)$, and C_2 antisymmetrizers (acting on the C_2 columns indices $((i^1_1,i^1_2),(i^2_1,i^2_2),\ldots,(i^{C_2}_1,i^{C_2}_2))$. In fact, the idempotent for a particular Young tableau can be constructed in two different ways, first symmetrizing the indices in each row and then antisymmetrizing the indices in each column or first antisymmetrizing the indices in each column followed by symmetrizing the indices of each row. Both procedures lead to equivalent results. Here, since the column indices are already antisymmetric, we choose the latter alternative and need to consider only the two symmetry operations along the two rows of $\Sigma_{[C_1,C_2]}$

respectively:

$$\mathcal{S}[1]=\sum_{p\in S_{C_2+C_1}} p, \tag{24}$$

$$\mathcal{S}[2]=\sum_{p\in S_{C_2}} p. \tag{25}$$

(In (24) and (25), $p\in S_n$ is an element of the permutation group S_n and it denotes the permutation $\binom{1\ 2\ \ldots N}{p_1\ p_2\ \ldots p_N}$ element of the permutation group S_N. Henceforth, we follow this notation throughout the paper.) The idempotent is just the product of (24) and (25) and is given by

$$e_{\Sigma_{[C_1,C_2]}}=\mathcal{S}[1]_{[i]}\mathcal{S}[2]_{[j]}. \tag{26}$$

One can easily see that:

$$\begin{aligned}\mathcal{C}[1]|i_1^1 i_1^2\cdots i_1^{C_2+C_1};i_2^1 i_2^2\ldots i_2^{C_2}\rangle&=C_1|i_1^1 i_1^2\cdots i_1^{C_2+C_1};i_2^1 i_2^2\cdots i_2^{C_2}\rangle,\\ \mathcal{C}[2]|i_1^1 i_1^2\cdots i_1^{C_2+C_1};i_2^1 i_2^2\cdots i_2^{C_2}\rangle&=C_2|i_1^1 i_1^2\cdots i_1^{C_2+C_1};i_2^1 i_2^2\cdots i_2^{C_2}\rangle.\end{aligned} \tag{27}$$

Thus all the irreducible representations are eigenvectors of the two casimirs $\mathcal{C}[1]$ and $\mathcal{C}[2]$. As an example we consider $C_1=C_2=1$ corresponding to the octet representation of SU(3). For this representation, $\mathcal{S}[1]=(e+(i_1^1,i_1^2))$ and $\mathcal{S}[2]=e$. Therefore, (1,1) representation is given by: $\|i_1^1,i_1^2;i_2^1\rangle_{\Sigma_{[1,1]}}=[a^\dagger[2]_{i_1^1 i_2^1}a^\dagger[1]_{i_1^2}+a^\dagger[2]_{i_1^2 i_2^1}a^\dagger[1]_{i_1^1}]|0\rangle$.

In Ref. 9 similar results as in this section have been obtained by using Bargmann's techniques for SU(3). More recently, SU(3) multiplicity problem has been analyzed by exploiting the above-given Schwinger construction and a mutually commuting Sp(2,R) group.[10]

B. The SU(3) coherent states

We consider two triplets of complex numbers $z[\alpha](=z^1[\alpha],z^2[\alpha],z^3[\alpha]),\alpha=1,2$ describing the Euclidean manifold $R^6\otimes R^6$. We impose the orthonormality conditions:

$$\overline{z}[\alpha]\cdot z[\beta]\equiv\sum_{i=1}^{3} z_i^*[\alpha]z^i[\beta]=\delta_{\alpha,\beta}. \tag{28}$$

We now define another vector $z[1,2]$ transforming as $\Sigma_{[0,1]}$ with components:

$$z^{i_1 i_2}[12]\equiv\sqrt{\frac{1}{2}}(z[1]^{i_1}z[2]^{i_2}-z[2]^{i_1}z[1]^{i_1})=\sqrt{\frac{1}{2}}\,\epsilon^{\alpha_1\alpha_2}z[\alpha_1]^{i_1}z[\alpha_2]^{i_2}. \tag{29}$$

Using (28), we find:

$$\begin{aligned}z[1,2]\cdot z[1,2]^*&\equiv z^{i_1 i_2}[[12]z^*_{i_1 i_2}[12]=1,\\ \tilde{z}[12]\cdot z[1]\equiv\epsilon_{i_1 i_2 i_3}z^{i_1 i_2}[12]z^{i_3}[1]=0,&\quad \tilde{z}[12]\cdot z[2]\equiv\epsilon_{i_1 i_2 i_3}z^{i_1 i_2}[12]z^{i_3}[2]=0.\end{aligned} \tag{30}$$

We can now construct any 3×3 SU(3) matrix $\mathcal{U}_3$ in terms of $z[1]$ and $z[2]$:

$$\mathcal{U}_3=\begin{pmatrix} z[1]_1 & z[1]_2 & z[1]_3\\ z[2]_1 & z[2]_2 & z[2]_3\\ \tilde{z}[12]_1 & \tilde{z}[12]_2 & \tilde{z}[12]_3\end{pmatrix}. \tag{31}$$

Thus we immediately see that $z[1]$ and $z[2]$ with (28) and (30) completely describe the SU(3) manifold. At this stage we define the SU(3) coherent states generating function as

$$|z[1],z[2]\rangle_{C_1,C_2}\equiv\exp(z[1]^{i_1}a^\dagger[1]_{i_1}+z[1,2]^{i_1i_2}a^\dagger[2]_{i_1i_2})|0\rangle|^{a^\dagger[1]\cdot a[1]=C_1}_{a^\dagger[2]\cdot a[2]=C_2}. \tag{32}$$

One can see that in the expansion of (32), due to the constraints (28) and (30), each irreducible representation occurs *once and only once*. We will now show that (32) indeed generates all the coherent states of SU(3). The constraints on the right-hand side of (32), ($a^\dagger[1]\cdot a[1]=C_1$ and $a^\dagger[2]\cdot a[2]=C_2$), select different possible irreducible representations of SU(3). Note that the states in (32) are characterized by the continuous parameters ($z[1],z[2]$) on the SU(3) manifold. It is easy to check the SU(3) transformation properties of $z[1]$ and $z[1,2]$,

$$\begin{aligned} z[1]^{i_1}&\to z'[1]^{i_1}=(\exp i\theta^a\lambda^a[1])^{i_1}_{i_2}z[1]^{i_2},\\ z[1,2]^{i_1i_2}&\to z'[12]^{i_1i_2}=(\exp i\theta^a\lambda^a[12])^{i_1i_2}_{j_1j_2}z[1,2]^{j_1j_2}. \end{aligned} \tag{33}$$

In (33) θ^a are the eight transformations associated with the SU(3) group transformation. Therefore, under SU(3) transformations both $z[1]$ and $z[2]$ transform like a triplet and the orthonormality conditions (28) and (30) remain invariant under the SU(3) transformations and the state in (32) defined at a point ($z[1],z[2]$) transforms to the coherent state at ($z'[1],z'[2]$) on the SU(3) manifold.

From the generating function (32) we find:

$$|z[1],z[2]\rangle_{C_1,C_2}=F^{i_1^1\cdots i_1^{C_1+C_2};i_2^1\cdots i_2^{C_2}}a[2]^\dagger_{i_1^1i_2^1}\cdots a^\dagger[2]_{i_1^{C_2}i_2^{C_2}}a^\dagger[1]_{i_1^{C_2+1}}\cdots a^\dagger[1]_{i_1^{C_2+C_1}}|0\rangle, \tag{34}$$

where

$$\begin{aligned} &C_1!C_2!F(z[1],z[2])^{i_1^1\cdots i_1^{C_1+C_2};i_2^1\cdots i_2^{C_2}}\\ &\quad=z[1,2]^{i_1^1i_1^1}z[1,2]^{i_1^2i_2^2}\cdots z[1,2]^{i_1^{C_2}i_2^{C_2}}z[1]^{i_1^{C_2+1}}z[1]^{i_1^{C_2+2}}\cdots z[1]^{i_1^{C_2+C_1}}\\ &\quad=P_2z[1]^{i_1^1i_2^1}z[1]^{i_1^2}\cdots z[1]^{i_1^{C_2}}z[1]^{i_1^{C_2+1}}\cdots z[1]^{i_1^{C_2+C_1}}z[2]^{i_2^1i_2^2}z[2]^{i_2^2}\cdots z[2]^{i_2^{C_2}}. \end{aligned} \tag{35}$$

In the second step in (35), we have used the antisymmetry properties of $a^\dagger[2]'s$ under the interchange of its two indices leading to $P_2=(2!)^{C_2/2}$. Equation (35) clearly illustrates the following two important properties of the tensor $F(z[1],z[2])$.

(1) It is an analytic function of ($z[1]$, $z[2]$) which describes the SU(3) manifold.

(2) It has exactly the same symmetry as that of $e_{\Sigma_{[C_1,C_2]}}$, i.e.,

$$F(z[1],z[2])^{i_1^1\cdots i_1^{C_1+C_2};i_2^1\cdots i_2^{C_2}}=F(z[1],z[2])^{i_1^1\cdots i_1^{C_1+C_2};i_2^1\cdots i_2^{C_2}}e_{\Sigma_{[C_1,C_2]}}. \tag{36}$$

Therefore, we can write (34) as

$$\begin{aligned} |z[1],z[2]\rangle_{C_1,C_2}&=F^{i_1\cdots i_{C_1+C_2}j_1\cdots j_{C_2}}e_{\Sigma_{[C_1,C_2]}}a[2]^\dagger_{i_1j_1}\cdots a^\dagger[2]_{i_{C_2}j_{C_2}}a[1]^\dagger_{i_{C_2+1}}\cdots a[1]^\dagger_{i_{C_2+C_1}}|0\rangle\\ &=F^{i_1\cdots i_{C_1+C_2}j_1\cdots j_{C_2}}\|i_1j_1,i_2j_2\cdots i_{C_2}j_{C_2}i_{C_2+1},i_{C_2+2}\cdots i_{C_2+C_1}\rangle_{[C_1,C_2]}. \end{aligned} \tag{37}$$

All these features are similar to Heisenberg–Weyl and SU(2) Schwinger coherent states of the previous section and are discussed in detail in Ref. 7.

We now check the resolution of identity. The Haar measure on SU(3) manifold is given by

$$\int \mathrm{d}\mu(z) \equiv \left(\int \prod_{\alpha=1}^{2} \mathrm{d}z[\alpha] \right) \left(\prod_{\alpha,\beta} \delta(z[\alpha]\cdot z^*[\beta] - \delta_{\alpha,\beta}) \right). \tag{38}$$

We construct an operator $\mathcal{O}_{[3]}$:

$$\mathcal{O}_3 \equiv \int \mathrm{d}\mu(z) |z[1],z[2]\rangle_{C_1,C_2\ C_1,C_2} \langle z[1],z[2]| \,. \tag{39}$$

Under SU(3) transformations (33), $\mathcal{O}_{[3]}$ remains invariant. Therefore,

$$[Q^a, \mathcal{O}_{[3]}] = 0, \quad \forall a = 1,2,\ldots,8. \tag{40}$$

Schur's Lemma implies:

$$\mathcal{O}_{[3]} = K I_{[C_1,C_2]} \,. \tag{41}$$

In (41), K is a constant and $I_{[C_1,C_2]}$ is the identity operator in the $\Sigma_{[C_1,C_2]}$ irreducible representation subspace. Thus we finally get:

$$\begin{aligned}
&\int \mathrm{d}\mu(z[1],z[2]) |z[1],z[2]\rangle_{C_1,C_2 C_1,C_2} \langle z[1],z[2]| \\
&= \int \mathrm{d}^6 z[1] \mathrm{d}^6 z[2] \prod_{\alpha,\beta=1}^{2} \delta(z^*[\alpha]\cdot z[\beta] \\
&\quad - \delta_{\alpha,\beta}) F^{i_1\cdots i_{C_1+C_2} j_1\cdots j_{C_2}} F^*{}_{k_1\cdots k_{C_1+C_2} l_1\cdots l_{C_2}} \big|_{i_1 j_1\cdots i_{C_2} j_{C_2}; i_{C_2+1}\cdots i_{C_2+C_1}} \big\rangle_{[C_1,C_2]\ [C_1,C_2]} \\
&\quad \times \big\langle {}^{k_1 l_1\cdots k_{C_2} l_{C_2}; k_{C_2+1}\cdots k_{C_2+C_1}} \big| \\
&= K \big|_{i_1 j_1, i_2 j_2\cdots i_{C_2} j_{C_2}; i_{C_2+1}\cdots i_{C_2+C_1}} \big\rangle_{[C_1,C_2]\ [C_1,C_2]} \big\langle {}^{i_1 j_1, i_2 j_2\cdots i_{C_2} j_{C_2}; i_{C_2+1}\cdots i_{C_2+C_1}} \big| \equiv K I_{[C_1,C_2]} \,.
\end{aligned} \tag{42}$$

IV. THE SCHWINGER SU(N) REPRESENTATION

We now generalize the ideas developed in Sec. III in the case of SU(3) to the group SU(N) for arbitrary N. The rank of the SU(N) group is (N-1). Therefore, there are (N-1) fundamental representations denoted by the Young diagrams with 1,2,…., (N-1) vertical boxes, respectively. Any irreducible representation of SU(N) can be built by taking direct products of the above-mentioned (N-1) fundamental representations. Following SU(2) and SU(3), we introduce (N-1) sets of creation–annihilations operators $(a[1]^{i_1}, a^\dagger[1]_{i_1}); (a[2]^{i_1 i_2}, a^\dagger[2]_{i_1 i_2}); \ldots; (a[N-1]^{i_1 i_2\cdots i_{N-1}}, a^\dagger[N-1]_{i_1 i_2\cdots i_{N-1}})$, which can be written in a compact form as $(a[\alpha]^{i_1 i_2\cdots i_\alpha}, a^\dagger[\alpha]_{i_1 i_2\cdots i_\alpha}), \alpha = 1,2\cdots(N-1)$. The commutation relations are straightforward generalizations of (18) and are given by

$$\begin{aligned}
[a[\alpha]^{i_1 i_2\cdots i_\alpha}, a^\dagger[\beta]_{j_1 j_2\cdots j_\beta}] &= \delta_{\alpha,\beta} \sum_{p\in S_\alpha} (-)^{|p|} \delta^{i_1}_{j_{p_1}} \delta^{i_2}_{j_{p_2}} \cdots \delta^{i_\alpha}_{j_{p_\alpha}} \,, \\
[a[\alpha]^{i_1 i_2\cdots i_\alpha}, a[\beta]^{j_1 j_2\cdots j_\beta}] &= 0, \quad [a^\dagger[\alpha]_{i_1 i_2\cdots i_\alpha}, a^\dagger[\beta]_{j_1 j_2\cdots j_\beta}] = 0.
\end{aligned} \tag{43}$$

In (43), $|p| = 0$ if p is an even permutation and $|p| = 1$ if it is an odd permutation. We denote the (N-1) generators belonging to (N-1) fundamental representation of SU(N) by $\lambda^a[\alpha]$, $a = 1,2,\ldots,(N^2-1)$. They satisfy the SU(N) algebra:

$$[\lambda^a[\alpha], \lambda^b[\alpha]] = i f^{abc} \lambda^c[\alpha], \quad \alpha = 1,2,\ldots,(N-1). \tag{44}$$

In (44) f^{abc} are the SU(N) structure constants. The SU(3) generators in terms of harmonic oscillators are given by

$$\begin{aligned} Q^a &= a^\dagger[1]_{i_1}[1]\lambda^a[1]^{i_1}_{i_2}a[1]^{i_2} + \frac{1}{2!}a^\dagger[2]_{i_1 i_2}\lambda^a[2]^{i_1 i_2}_{j_1 j_2}a[2]^{j_1 j_2} + \cdots \\ &\quad + \frac{1}{(N-1)!}a^\dagger[N-1]_{i_1 i_2 \cdots i_{N-1}}\lambda^a[N-1]^{i_1 \cdots i_{N-1}}_{j_1 \cdots j_{N-1}}a[N-1]^{j_1 j_2 \cdots j_{N-1}} \\ &= \sum_{\alpha=1}^{N-1}\frac{1}{\alpha!}a^\dagger[\alpha]_{i_1, i_2 \cdots i_\alpha}\lambda^a[\alpha]^{i_1 i_2 \cdots i_\alpha}_{j_1 j_2 \cdots j_\alpha}a[\alpha]^{j_1 j_2 \cdots j_\alpha}. \end{aligned} \tag{45}$$

The commutation relations (43) imply

$$[Q^a, Q^b] = i f^{abc} Q^c. \tag{46}$$

It is easy to verify that under SU(3) transformations the various creation operators belonging to the αth representation transform amongst themselves as

$$[Q^a, a^\dagger_{i_1 i_2 \cdots i_\alpha}[\alpha]] = a^\dagger_{j_1 j_2 \cdots j_\alpha}[\alpha](\lambda^a)^{j_1 j_2 \cdots j_\alpha}_{i_1 i_2 \cdots i_\alpha}[\alpha]. \tag{47}$$

This implies that all the irreducible representations of SU(N) can be realized on the Hilbert space created by the above-given creation operators acting on the vacuum. Further, the (N-1) Casimir operators are just the (N-1) number operators corresponding to (N-1) types of creation–annihilation operators and are given by

$$\begin{aligned} \mathcal{C}[1] &= \sum_{i_1=1}^{N} a^\dagger[1]_{i_1}a[1]^{i_1}, \\ \mathcal{C}[2] &= \frac{1}{2!}\sum_{i_1, i_2=1}^{N} a^\dagger[2]_{i_1 i_2}a[2]^{i_1 i_2}, \\ &\cdots \\ \mathcal{C}[N-1] &= \frac{1}{(N-1)!}\sum_{i_1, i_2, \ldots, i_{N-1}=1}^{N} a^\dagger[N-1]_{i_1 i_2 \cdots i_{N-1}}a[N-1]^{i_1 i_2 \cdots i_{N-1}}. \end{aligned} \tag{48}$$

It is easy to check that the (N-1) Casimir operators in (48) commute with all the (N^2-1) SU(N) generators in (45).

A. The irreducible representations of SU(N)

All irreducible representations of SU(N) can be constructed by taking direct products of the (N-1) fundamental representations and then applying appropriate projection operators. Like the SU(3) case in the previous section, we now consider the most general SU(N) irreducible representation $\Sigma_{[C_1, C_2 \cdots C_{N-1}]}$ containing C_α copies of the αth fundamental representations. We formally write:

$$|C_1, C_2, \ldots, C_{N-1}\rangle \equiv e_{\Sigma_{[C_1 \cdots C_{N-1}]}}(a^\dagger[1])^{C_1}(a^\dagger[2])^{C_2}(a^\dagger[3])^{C_3}\cdots(a^\dagger[N-1])^{C_{N-1}}|0\rangle. \tag{49}$$

(The explicit form of these basis vectors are given at the end of Sec. IV B—(64) and (65).) Just as in the case of SU(3) in the previous sections, all the creation operators being completely antisymmetric in their indices, the idempotent $e_{\Sigma_{[C_1\cdots C_{N-1}]}}$ in (49) is constructed by multiplying all (N-1) symmetrizers:

$$e_{\Sigma_{[C_1\cdots C_{N-1}]}}=\mathcal{S}_1\mathcal{S}_2\cdots\mathcal{S}_{N-1}, \tag{50}$$

where $\mathcal{S}_1,\mathcal{S}_2\cdots\mathcal{S}_{N-1}$ are the elements of permutation group algebras associated with the permutation groups $S_{C_1+\cdots+C_{N-1}},S_{C_2+\cdots+C_{N-1}},\ldots,S_{C_{N-1}}$, respectively,

$$\begin{aligned}
\mathcal{S}_1&\equiv\frac{1}{(C_1+\cdots+C_{N-1})!}\sum_{p\in S_{C_1+\cdots+C_{N-1}}}p,\\
\mathcal{S}_2&\equiv\frac{1}{(C_2+\cdots+C_{N-1})!}\sum_{p\in S_{C_2+\cdots+C_{N-1}}}p,\\
&\cdots\\
\mathcal{S}_{N-1}&\equiv\frac{1}{(C_{N-1})!}\sum_{p\in S_{C_{N-1}}}p.
\end{aligned} \tag{51}$$

Again, as in the case of SU(3), it is easy to verify:

$$\mathcal{C}_\alpha|C_1,C_2,..,C_{N-1}\rangle=C_\alpha|C_1,C_2,..,C_{N-1}\rangle. \tag{52}$$

Therefore, the Casimir operator $\mathcal{C}_\alpha$ acting on an irreducible representation generated by the basis vectors $\mathcal{C}_\alpha|C_1,C_2,\ldots,C_{N-1}\rangle$ just counts the number of times the αth fundamental representation appears in it. This is again similar to the SU(3) case in the previous section. We now exploit this feature to construct the SU(N) coherent states.

B. The SU(N) coherent states

We consider (N-1) N-plets of complex numbers $z[\alpha](=z^1[\alpha],z^2[\alpha],\ldots,z^N[\alpha]),\alpha=1,2,...,N-1$ describing the Eucledian manifold which is a direct product of (N-1) R^{2N}. We impose the orthonormality conditions:

$$z^*[\alpha]\cdot z[\beta]=\delta_{\alpha,\beta}. \tag{53}$$

We now define another vector $z[1,N-1]$ with components:

$$\begin{aligned}
z^{i_1i_2\cdots i_{N-1}}[1,N-1]&\equiv\sqrt{\frac{1}{(N-1)!}}\sum_{p\in S_{N-1}}(-)^{|p|}(z[1]^{i_{p_1}}z[2]^{i_{p_2}}\cdots z[N-1]^{i_{p_{N-1}}})\\
&=\sqrt{\frac{1}{(N-1)!}}\,\epsilon^{\alpha_1\alpha_2\cdots\alpha_{N-1}}z[\alpha_1]^{i_1}z[\alpha_2]^{i_2}\cdots z[\alpha_{N-1}].
\end{aligned} \tag{54}$$

Using (53), we find:

$$\begin{aligned}
z[1,N-1]\cdot z[1,N-1]^*&\equiv z^{i_1i_2\cdots i_{N-1}}[1,N-1]z^*{}_{i_1i_2\cdots i_{N-1}}[1,N-1]=1,\\
\tilde{z}[1,N-1]\cdot z[\alpha]&\equiv\epsilon_{i_1i_2\cdots i_N}z^{i_1i_2\cdots i_{N-1}}[1,N-1]z^{i_N}[\alpha]=0.
\end{aligned} \tag{55}$$

We can now construct any $N\times N$ SU(N) matrix $\mathcal{U}_N$ in terms of $z[1]$, $z[2],\ldots,z[N-1]$:

$$\mathcal{U}_N=\begin{pmatrix} z[1]^1 & z[1]^2 & \dots\ z[1]^N \\ z[2]^1 & z[2]^2 & \dots\ z[2]^N \\ \vdots & & \\ \vdots & & \\ z[N-1]^1 & z[N-1]^2 & \dots z[N-1]^N \\ \bar{z}[1\cdots N-1]^1 & \bar{z}[1\cdots N-1]^2 & \bar{z}[1\cdots N-1]^N \end{pmatrix}. \tag{56}$$

Thus we immediately see that $z[1]$, $z[2],\dots,z[N-1]$ with (55) describe SU(N) manifold. We will now exploit this simple characterization of SU(N) manifold to construct coherent states belonging to all the irreducible representations of SU(N) group. For this purpose, we construct a new set of (N-1) parameters:

$$z[1,1]^{i_1}\equiv z[1]^{i_1},$$

$$z[1,2]^{i_1 i_2}\equiv \sqrt{\frac{1}{2!}}\sum_{p\in S_2}(-)^{|p|}z[1]^{i_{p_1}}z[2]^{i_{p_2}},$$

$$z[1,3]^{i_1 i_2 i_3}\equiv \sqrt{\frac{1}{3!}}\sum_{p\in S_3}(-)^{|p|}z[1]^{i_{p_1}}z[2]^{i_{p_2}}z[3]^{i_{p_3}}, \tag{57}$$

$$\dots$$

$$z[1,N-1]^{i_1 i_2\cdots i_{N-1}}\equiv \sqrt{\frac{1}{(N-1)!}}\sum_{p\in S_{N-1}}(-)^{|p|}z[1]^{i_{p_1}}z[2]^{i_{p_2}}\cdots z[N-1]^{i_{p_{N-1}}}.$$

We now define the SU(N) coherent states generating function as:

$$\begin{aligned} &|z[1],z[2],\dots,z[N-1]\rangle_{C_1,C_2\cdots C_{N-1}} \\ &\quad\equiv\exp\left(\sum_{\beta=1}^{N-1} z[1,\beta]\cdot a^\dagger[\beta]\right)|0\rangle|_{a^\dagger[\alpha]\cdot a[\alpha]=C_\alpha} \\ &\quad\equiv\exp(z[1]^{i_1^1}a^\dagger[1]_{i_1^1}+z[1,2]^{i_1^2 i_2^2}a^\dagger[2]_{i_1^2 i_2^2} \\ &\qquad+\cdots+z[1,N-1]^{i_1^{N-1}i_2^{N-1}\cdots i_{N-1}^{N-1}}a^\dagger[N-1]_{i_1^{N-1}i_2^{N-1}\cdots i_{N-1}^{N-1}})|0\rangle|_{a^\dagger[\alpha]\cdot a[\alpha]=C_\alpha}. \end{aligned} \tag{58}$$

The constraints on the right-hand side of the generating function (58) ensure that we only generate the states which are eigenstates of all the (N-1) Casimir operators and thus selecting all possible irreducible representations of SU(N), i.e.,

$$\mathcal{C}[\alpha]|z[1],z[2],\dots,z[N-1]\rangle_{C_1,C_2\cdots C_{N-1}}=C[\alpha]|z[1],z[2],\dots,z[N-1]\rangle_{C_1,C_2\cdots C_{N-1}} \tag{59}$$

for $\alpha=1,2,\dots,(N-1)$. We will now show that the states thus obtained are the coherent states. All states in (58) are defined continuously over the SU(N) manifold parametrized by $(z[1],z[2],\dots,z[N-1])$. It is easy to check the SU(N) transformation properties of $z[1,\alpha],\alpha=1,2,...(N-1)$,

$$z[1,\alpha]^{i_1\cdots i_\alpha}\to z'[1,\alpha]^{i_1\cdots i_\alpha}=\left(\exp i\sum_{a=1}^{N^2-1}\theta^a\lambda^a[\alpha]\right)^{j_{1_1\cdots i_\alpha}}_{i_1\cdots j_\alpha} z[1,\alpha]^{j_1\cdots j_\alpha}. \tag{60}$$

In (60) θ^a are (N^2-1) parameters describing a point on the SU(N) manifold. Equation (60) implies that all $z[\alpha]$ ($\alpha=1,2,...,N-1$) transform as N-plets of SU(N), i.e.,

$$z[\alpha]\to z'[\alpha]=\left(\exp i\sum_{a=1}^{N^2-1}\theta^a\lambda^a[1]\right)^{i_1}_{j_1}z[\alpha]^{j_1}. \tag{61}$$

We see that the orthonormality conditions (53) remain invariant under the SU(N) transformations. The coherent states defined at a point $(z[1],z[2],\ldots,z[1,N-1])$ transform to the coherent states at $(z'[1],z'[2],\cdot z'[1,N-1])$ of the SU(N) manifold.

Expanding the exponential we find:

$$\begin{aligned}&|z[1],\ldots,z[N-1]\rangle_{C_1,\ldots,C_{N-1}}\\&\quad=P\left[\prod_{h=1}^{h_{\max}}\prod_{v=1}^{(C_h+C_{h+1}\cdots+C_{N-1})}z^{i^v_h}[h]\right]\left[\prod_{v(1)=1}^{C_{N-1}}a^\dagger[N-1]_{i_1^{v(1)}i_2^{v(1)}\ldots i_{N-1}^{v(1)}}\right]\\&\qquad\times\left[\prod_{v(2)=C_{N-1}+1}^{C_{N-1}+C_{N-2}}a^\dagger[N-2]_{i_1^{v(2)}i_2^{v(2)}\ldots i_{N-2}^{v(2)}}\right]\cdots\left[\prod_{v(N-1)=C_{N-1}+\cdots+C_2+1}^{C_{N-1}+\cdots+C_1}a^\dagger[1]_{i_1^{v(N-1)}}\right]|0\rangle.\end{aligned} \tag{62}$$

In (62), we have chosen those terms in the expansion which are eigenvectors of the Casimir operators $\mathcal{C}_\beta$ with eigenvalues C_β and $h_{\max}$ is the maximum value of β such that $C_\beta\neq 0$. $P=[\Pi_{\alpha=1}^{N-1}P_\alpha]$ with $P_\alpha=(\alpha!)^{C_\alpha/2}$. (In (62) $h=1,2\cdots h_{\max}$ counts the horizontal rows and v is used to count the vertical columns of $\Sigma_{[C_1,\ldots,C_{N-1}]}$. Note that it is the maximum number of horizontal rows in the Young diagram.) We note the following important symmetry and anti-symmetry properties of (62):

(1) The $(z[1],z[2],\ldots,z[N-1])$ dependent part of (62) has inbuilt invariance under interchange of any two indices along a row of the Young tableau $\Sigma_{[C_1,C_2,\ldots,C_{N-1}]}$, i.e., it is invariant under all the symmetry operations given in (51),

$$\left(\prod_{h=1}^{h_{\max}}\prod_{v=1}^{(C_h+C_{h+1}\cdots+C_{N-1})}z^{i^v_h}[h]\right)\mathcal{S}_\alpha=\left(\prod_{h=1}^{h_{\max}}\prod_{v=1}^{(C_h+C_{h+1}\cdots+C_{N-1})}z^{i^v_h}[h]\right). \tag{63}$$

(2) The harmonic oscillator dependent part of (62) has inbuilt antisymmetric properties along any column indices of the Young tableau $\Sigma_{[C_1,C_2,\ldots,C_{N-1}]}$.

Therefore, we can write (62) as:

$$\begin{aligned}|z[1],\ldots,z[N-1]\rangle_{C_1,\ldots,C_{N-1}}=&\prod_{h=1}^{h_{\max}}\prod_{v=1}^{(C_h+C_{h+1}\cdots+C_{N-1})}z^{i^v_h}[h]\quad e_{\Sigma_{[C_1,C_2,\ \ldots\ ,C_{N-1}]}}\\&\times\prod_{v(1)=1}^{C_{N-1}}a^\dagger[N-1]_{i_1^{v(1)}i_2^{v(1)}\ldots i_{N-1}^{v(1)}}\prod_{v(2)=C_{N-1}+1}^{C_{N-1}+C_{N-2}}a^\dagger[N\\&-2]_{i_1^{v(2)}i_2^{v(2)}\ldots i_{N-2}^{v(2)}}\cdots\prod_{v(N-1)=C_{N-1}+\cdots C_2+1}^{C_{N-1}+\cdots+C_1}a^\dagger[1]_{i_1^{v(N-1)}}|0\rangle.\end{aligned} \tag{64}$$

In (64), $e_{\Sigma_{[C_1,C_2,\ldots,C_{N-1}]}}$ is defined by Eq. (50). In fact, these are exactly basis vectors of the irreducible representation $\Sigma_{[C_1,C_2,\ldots,C_{N-1}]}$. We denote them by

$$\|(i_1^1 i_1^2 \cdots i_1^{C_1+\cdots+C_{N-1}});(i_2^1 i_2^2 \cdots i_2^{C_2+\cdots+C_{N-1}});\ldots;(i_{N-1}^1 i_{N-1}^2 \cdots i_{N-1}^{C_2+\cdots+C_{N-1}})\rangle_{\Sigma_{[C_1,C_2,\ \ldots\ ,C_{N-1}]}}$$

$$\equiv e_{\Sigma_{[C_1,C_2,\ldots,C_{N-1}]}} \prod_{v(1)=1}^{C_{N-1}} a^\dagger[N-1]_{i_1^{v(1)} i_2^{v(1)} \ldots i_{N-1}^{v(1)}} \prod_{v(2)=C_{N-1}+1}^{C_{N-1}+C_{N-2}} a^\dagger[N-2]_{i_1^{v(2)} i_2^{v(2)} \ldots i_{N-2}^{v(2)}}$$

$$\cdots \prod_{v(N-1)=C_{N-1}+\cdots C_2+1}^{C_{N-1}+\cdots+C_1} a^\dagger[1]_{i_1^{v(N-1)}}|0\rangle. \tag{65}$$

Thus the states belonging to $\Sigma_{[C_1,\ldots,C_{N-1}]}$ in (58) irreducible representations are given by

$$|z[1],z[2],\ldots,z[N-1]\rangle_{C_1,C_2\cdot C_{N-1}}$$

$$= \left(\prod_{h=1}^{h_{\max}} \prod_{v=1}^{(C_h+C_{h+1}\cdots+C_{N-1})} z_h^{i^v}[h] \right) \|(i_1^1 i_1^2 \cdots i_1^{C_1+\cdots+C_{N-1}});(i_2^1 i_2^2 \cdots i_2^{C_2+\cdots+C_{N-1}});\ldots;$$

$$\times (i_{N-1}^1 i_{N-1}^2 \cdots i_{N-1}^{C_2+\cdots+C_{N-1}})\rangle_{\Sigma_{[C_1,C_2,\ \ldots\ ,C_{N-1}]}}. \tag{66}$$

We now check the resolution of identity. This is similar to the SU(3) case in the previous sections. The SU(N) Haar measure is

$$\int \mathrm{d}\mu(z) \equiv \left(\int \prod_{\alpha=1}^{N-1} \mathrm{d}z[\alpha] \right) \left(\prod_{\alpha,\beta} \delta(z[\alpha]\cdot z^*[\beta] - \delta_{\alpha,\beta}) \right). \tag{67}$$

We construct an operator $\mathcal{O}_{[N]}$:

$$\mathcal{O}_N \equiv \left(\int \mathrm{d}\mu(z) \left| z[1],z[2],\ldots,z[N-1] \right\rangle \right)_{C_1,C_2\cdots C_{N-1}} \quad {}_{C_1,C_2\cdots C_{N-1}} \langle z[1],z[2],\ldots,z[N-1]|. \tag{68}$$

Under SU(N) transformations (60), $\mathcal{O}_{[3]}$ remains invariant. Therefore,

$$[Q^a,\mathcal{O}_{[N]}]=0, \quad \forall a=1,2,\ldots,N^2-1 \tag{69}$$

The Schur's Lemma implies

$$\mathcal{O}_{[N]} = K I_{[C_1,C_2,\ldots,C_{N-1}]}. \tag{70}$$

In (70), K is a constant and $I_{[C_1,\ldots,C_{N-1}]}$ is the identity operator in the $\Sigma_{[C_1,\ldots,C_{N-1}]}$ irreducible representation subspace. Therefore, the states in (66) are indeed the coherent states. We have thus constructed all the SU(N) coherent states belonging to different irreducible representations of SU(N).

V. SUMMARY AND DISCUSSION

We have generalized Schwinger representation of SU(2) algebra in terms of harmonic oscillators to the group SU(N). We have exploited this construction to construct SU(N) coherent states and characterized SU(N) manifold in terms of complex vectors. In this sense our SU(N) coherent states definition is analogous to that of Heisenberg–Weyl coherent states. This method is quite general and can be generalized to other Lie groups and their manifolds. We feel our approach is more useful for practical calculations compared to the standard group theoretical approach and can be applied to various problems. In condensed matter physics, coherent states for the Lie group SU(2) have been very useful for studying Heisenberg spin systems using the path integral formalism.[11–15] These studies have been generalized to systems with SU(N) symmetry, although

such studies have usually been restricted to the completely symmetric representations.[12,16] Therefore, our formulation can be used to write down the field theory for the SU(N) Heisenberg model and study its spectrum and topological aspects as in the SU(2) case.[17] Using the techniques discussed in the paper, one can also construct SU(N) coherent states with fixed values of Cartan diagonal generators. The special cases of SU(2) coherent states with fixed charge and SU(3) nonlinear coherent states with fixed charge and hypercharge were constructed in Refs. 18 and 19, respectively.

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On bound states for systems of weakly coupled Schrödinger equations in one space dimension

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We establish the Birman–Schwinger relation for a class of Schrödinger operators $-d^2/dx^2\otimes 1_{\mathcal{H}}+V$ on $L^2(\mathbb{R},\mathcal{H})$, where $\mathcal{H}$ is an auxiliary Hilbert space and V is an operator-valued potential. As an application we give an asymptotic formula for the bound states which may arise for a weakly coupled Schrödinger operator with a matrix potential (having one or more thresholds). In addition, for a two-channel system with eigenvalues embedded in the continuous spectrum we show that, under a small perturbation, such eigenvalues turn into resonances. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1510175]

I. INTRODUCTION

In a recent paper[22] (see also Ref. 21) we studied spectral and scattering theory for the two-channel Schrödinger operator

$$\mathbf{H}=\tilde{\mathbf{H}}_0+\mathbf{V}=\begin{pmatrix} -\dfrac{d^2}{dx^2} & 0 \\ 0 & -\dfrac{d^2}{dx^2}+1 \end{pmatrix}+\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \tag{1.1}$$

on the Hilbert space $L^2(\mathbb{R})\oplus L^2(\mathbb{R})$. In the low-energy limit, where the spectral parameter tends to the boundary point of the continuous spectrum of $\mathbf{H}$, viz. the point zero, we deduced asymptotic expansions for the resolvent of $\mathbf{H}$ and, as an application, we obtained asymptotic expansions for the scattering matrix associated with the pair $(\mathbf{H},\tilde{\mathbf{H}}_0)$ as the energy parameter tends to zero. Besides being interesting from the mathematical point of view, the study of spectral and scattering theory for $\mathbf{H}$, having thresholds at 0 and 1, also works as a useful exercise towards analogous investigations for various multichannel quantum system with more than one threshold (see, e.g., Ref. 23) because it describes many actual physical phenomena to a good approximation.

If we replace $\tilde{\mathbf{H}}_0$ in (1.1) by $\mathbf{H}_0=-d^2/dx^2\otimes 1_{\mathbb{C}^N}$ and $\mathbf{V}$ by an $N\times N$ matrix potential, we obtain the (usual) matrix Schrödinger operator on $L^2(\mathbb{R},\mathbb{C}^N)$ having a single threshold at 0. The latter, of course, has attracted a lot of attention during the years. Among recent results we mention low-energy asymptotics for the corresponding scattering matrix,[2,3] Levinson's theorem,[14] Lieb–Thirring inequalities[4,20] and quantum design.[7]

A natural question, which seems not to have been addressed in the literature, concerns how negative energy levels may arise in a system of weakly coupled Schrödinger equations. In the scalar-valued setting, weakly coupled bound states for Schrödinger operators have been investigated in various dimensions (see Ref. 19, Chapter VI, and Refs. 31, 15, and 16).

In this work we generalize the scalar-valued result obtained by Simon in dimension one[31] to the analogous matrix-valued setting.

We begin in the more abstract framework of Schrödinger operators with operator-valued potentials given formally by $H=-d^2/dx^2\otimes 1_{\mathcal{H}}+V$ on $L^2(\mathbb{R},\mathcal{H})$, where $\mathcal{H}$ is an auxiliary Hilbert

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space and the potential V is a $\mathcal{B}(\mathcal{H})$-valued, measurable function on $\mathbb{R}$ such that $V(x)$ is symmetric for almost all x. In Sec. III we define the Hamiltonian H by means of quadratic forms (Proposition 3.1) and in Sec. IV we establish the celebrated Birman–Schwinger relation (Proposition 4.2), which transforms the eigenvalue problem for H into an eigenvalue problem for a compact operator; the so-called Birman–Schwinger operator.

Equipped with the Birman–Schwinger relation we study weakly coupled bound states in Sec. V. We restrict our attention to Schrödinger operators with matrix-valued potentials. In Sec. V A we consider two-channel Hamiltonians with one and two thresholds, respectively. First we consider $\mathbf{H}(g)=-d^2/dx^2\otimes 1_{\mathbb{C}^2}+g\mathbf{V}(x)$, where $\mathbf{V}$ is a 2×2 matrix potential. Theorem 5.2 reveals how nonpositive eigenvalues of an auxiliary matrix $\mathbf{S}$, defined in (5.2), give rise to negative eigenvalues E_{ij} of $\mathbf{H}(g)$ provided g is small enough. The eigenvalues E_{ij} satisfy an asymptotic perturbation formula in which we derive the first few coefficients explicitly [see (5.3)]. Second, we consider the above-mentioned Hamiltonian (1.1), henceforth denoted $\tilde{\mathbf{H}}(g)$, having thresholds at 0 and 1. In Theorem 5.6 we show how a negative eigenvalue of an auxiliary matrix $\tilde{\mathbf{S}}$, defined in (5.9), generates a negative eigenvalue of $\tilde{\mathbf{H}}(g)$. However, if one compares the proofs of Theorems 5.2 and 5.6 (in particular, the expressions for the matrices $\mathbf{T}_0$ and $\tilde{\mathbf{T}}_0$), it seems that the argument used in the proof of Theorem 5.2 (ii) cannot be modified in order to treat the situation where zero is an eigenvalue of $\tilde{\mathbf{S}}$. Thus, it remains an attractive open problem to show that the zero eigenvalue of $\tilde{\mathbf{S}}$ (may) gives rise to a negative eigenvalue of $\tilde{\mathbf{H}}(g)$. In Sec. V B we state the generalization of Theorem 5.2 to the N-channel Hamiltonian $-d^2/dx^2\otimes 1_{\mathbb{C}^N}+\mathbf{V}(x)$, where $\mathbf{V}$ is an $N\times N$ matrix potential.

Having studied how negative eigenvalues arise for multichannel Hamiltonians under weak coupling, it is natural to address the problem of perturbation of embedded eigenvalues for a multichannel Schrödinger operator with a matrix-valued potential. In Sec. VI we consider a two-channel Hamiltonian having eigenvalues embedded in its continuous spectrum. When perturbed by a ''short range'' potential, we show that such eigenvalues move into the complex plane and become resonances. In particular, we verify Fermi's golden rule (see, e.g., Refs. 27 and 32).

There is a vast literature on 2×2 operator-valued matrices, e.g., in system theory (see, e.g., Ref. 8) and in semigroup theory (see, e.g., Ref. 11). Most notably in this context is the substantial number of questions of a general nature which have been answered on spectral theory recently, see, e.g., the survey in Ref. 33. However, the methods therein are not related to ours although some of the questions addressed clearly are, e.g., the appearance of resonances discussed by Mennicken and Motovilov.[24]

II. PRELIMINARIES

A. Vector-valued functions

Let $\mathcal{H}$ be a separable Hilbert space with scalar product and norm denoted by $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ and $\|\cdot\|_{\mathcal{H}}$. Then a function $\psi(x)$ from $\mathbb{R}$ to $\mathcal{H}$ is measurable if the scalar-valued functions $\langle\psi(x),\phi\rangle_{\mathcal{H}}$ are measurable, where ϕ denotes an arbitrary vector of $\mathcal{H}$. If $\psi(x)$ is such a measurable function, then $\|\psi(x)\|_{\mathcal{H}}$ is also measurable (as a function with non-negative values). Thus $L^p(\mathbb{R},\mathcal{H})$ is defined as the set of equivalence classes of measurable functions $\psi(x)$ from $\mathbb{R}$ to $\mathcal{H}$, which satisfy that $\int_{\mathbb{R}}\|\psi(x)\|_{\mathcal{H}}^p dx$ is finite if $p<\infty$ and $\|\psi\|_\infty=\operatorname{ess\,sup}\|\psi(x)\|_{\mathcal{H}}<\infty$ if $p=\infty$. The measure dx is the Lebesgue measure. For any p the $L^p(\mathbb{R},\mathcal{H})$ space is a Banach space with norm $\|\cdot\|_p=(\int_{\mathbb{R}}\|\cdot\|_{\mathcal{H}}^p dx)^{1/p}$. In the case $p=2$, $L^2(\mathbb{R},\mathcal{H})$ is a complex and separable Hilbert space with scalar product $\langle\phi,\psi\rangle_2=\int_{\mathbb{R}}\langle\phi,\psi\rangle_{\mathcal{H}}dx$ and corresponding norm $\|\psi\|_2=\langle\psi,\psi\rangle_2^{1/2}$. For $n\in\mathbb{N}$, $1\leqslant p<\infty$, the Sobolev space $W^{n,p}(\mathbb{R},\mathcal{H})$ is defined as the space of those $\psi\in L^p(\mathbb{R},\mathcal{H})$, for which all derivatives (weak sense) up to order n are in $L^p(\mathbb{R},\mathcal{H})$. If $p=2$, $W^{n,2}(\mathbb{R},\mathcal{H})$ is a separable Hilbert space denoted by $H^n(\mathbb{R},\mathcal{H})$ with scalar product $\langle\phi,\psi\rangle_{H^n(\mathbb{R},\mathcal{H})}=\int_{\mathbb{R}}\Sigma_{\alpha=0}^n\langle(d/dx)^\alpha\phi,(d/dx)^\alpha\psi\rangle_{\mathcal{H}}$ and norm denoted by $\|\psi\|_{H^n(\mathbb{R},\mathcal{H})}$.

B. Operators

Below $\mathcal{H}$, $\mathcal{H}_1$, $\mathcal{H}_2$ are separable Hilbert spaces. For a linear operator T, the notations $\mathcal{D}(T)$, $\mathrm{Ran}(T)$, $\mathrm{Ker}(T)$, T^*, $\overline{T}$, $\sigma(T)$, $\rho(T)$ are standard (see, for example, Ref. 25). By I we denote the identity operator. The resolvent of a self-adjoint operator T is denoted by $R(T,z)=(T-zI)^{-1}$. By $\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)$ and $\mathbf{S}_\infty(\mathcal{H}_1,\mathcal{H}_2)$ we denote respectively the sets of bounded and compact operators acting from $\mathcal{H}_1$ into $\mathcal{H}_2$. With the usual operator norm $\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)$ is a Banach space. We set $\mathcal{B}(\mathcal{H}):=\mathcal{B}(\mathcal{H},\mathcal{H})$ and $\mathbf{S}_\infty(\mathcal{H}):=\mathbf{S}_\infty(\mathcal{H},\mathcal{H})$.

C. Trace classes of compact operators

If $T\in\mathbf{S}_\infty(\mathcal{H})$, then the nonzero eigenvalues of $|T|=\sqrt{T^*T}$ are called the singular numbers or s-numbers of T. Let $\{s_j(T)\}$ denote the (possibly finite) nonincreasing sequence of the singular numbers of T; every number counted according to its multiplicity as an eigenvalue of $|T|$. For $0<p<\infty$ the von Neumann–Schatten class $\mathbf{S}_p(\mathcal{H}_1,\mathcal{H}_2)$ is the set of $T\in\mathbf{S}_\infty(\mathcal{H}_1,\mathcal{H}_2)$ for which the functional

$$\|T\|^p_{\mathbf{S}_p(\mathcal{H}_1,\mathcal{H}_2)}:=\sum_j\,[s_j(T)]^p$$

is finite. The functional $\|\cdot\|_{\mathbf{S}_p(\mathcal{H}_1,\mathcal{H}_2)}$ is a norm for $p\geqslant 1$ and the normed space $\mathbf{S}_p(\mathcal{H}_1,\mathcal{H}_2)$ is a Banach space. For $p<1$ the functional is a quasinorm. For additional properties of the spaces $\mathbf{S}_p$ of compact operators we refer to Ref. 5, Chap. 11. The sets $\mathbf{S}_1(\mathcal{H}_1,\mathcal{H}_2)$ and $\mathbf{S}_2(\mathcal{H}_1,\mathcal{H}_2)$ are called the trace class and Hilbert–Schmidt class, respectively.

D. Operator-valued functions

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two separable Hilbert spaces. From above, a function $\mathbb{R}\ni x\to\psi(x)\in\mathcal{H}$ is measurable if and only if all the functions $\mathbb{R}\ni x\to\langle\psi(x),\phi\rangle_{\mathcal{H}}\in\mathbb{C}$ are measurable. As a result of the Pettis measurability theorem (see, e.g., Ref. 10 Theorem II.1.2) the following properties are equivalent for a $\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)$-valued function $\mathbb{R}\ni x\mapsto T(x)$:

(i) $\forall\,\phi\in\mathcal{H}_2$, $\forall\,\psi\in\mathcal{H}_1$, $\mathbb{R}\ni x\to\langle\phi,T(x)\psi\rangle_{\mathcal{H}_2}\in\mathbb{C}$ is measurable, and
(ii) $\forall\,\psi\in\mathcal{H}_1$, $\mathbb{R}\ni x\to T(x)\psi\in\mathcal{H}_2$ is measurable.

We say that a function $\mathbb{R}\ni x\mapsto T(x)\in\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)$ is measurable if it satisfies any one of the above properties (i)–(ii). In the affirmative case, $\|T(x)\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)}$ is also measurable because

$$\|T(x)\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)}=\sup_{\psi\in\mathcal{D}_1}(\|T(x)\psi\|_{\mathcal{H}_2}/\|\psi\|_{\mathcal{H}_1}),$$

where $\mathcal{D}_1$ is a countable dense subset of $\mathcal{H}_1$. Moreover, we can define $L^p(\mathbb{R},\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2))$ as the linear space of (equivalence classes of) measurable functions $T:\mathbb{R}\to\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)$ such that $\|T(\cdot)\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)}\in L^p(\mathbb{R})$.

For the functional calculus for self-adjoint operators we recall the following result which can be found in, e.g., Ref. 6, Proposition V.1.2.

Proposition 2.1: If for each $x\in\mathbb{R}$, $T(x)$ is a self-adjoint operator on $\mathcal{H}$ and $\{E_{T(x)}(A);A\,\text{Borel set of}\,\mathbb{R}\}$ denotes its resolution of the identity, the following three properties are equivalent:

(i) $\mathbb{R}\ni x\to E_{T(x)}(A)\in\mathcal{B}(\mathcal{H})$ *is measurable for all Borel sets A,*
(ii) $\mathbb{R}\ni x\to e^{-itT(x)}\in\mathcal{B}(\mathcal{H})$ *is measurable for all $t\in\mathbb{R}$, and*
(iii) $\mathbb{R}\ni x\to(T(x)-\zeta)^{-1}\in\mathcal{B}(\mathcal{H})$ *is measurable for all $\zeta\in\mathbb{C}\setminus\mathbb{R}$.*

E. Fourier transform

Suppose $\psi \in L^1(\mathbb{R}^d,\mathcal{H})$. Then we define its Fourier transform $(\mathcal{F}\psi)(\xi)=\hat{\psi}(\xi) := (2\pi)^{-1/2}\int_{\mathbb{R}} e^{ix\xi}\psi(x)\,dx$ which is an element of $L^\infty(\mathbb{R},\mathcal{H})$. If $\psi \in L^1(\mathbb{R},\mathcal{H})\cap L^2(\mathbb{R},\mathcal{H})$, then $\hat{\psi} \in L^2(\mathbb{R},\mathcal{H})$ with $\|\hat{\psi}\|_{L^2}=\|\psi\|_{L^2}$. The Fourier transform can then be extended by continuity to a unitary mapping of the Hilbert space $L^2(\mathbb{R},\mathcal{H})$ into itself.

We have the following criterion.

Lemma 2.2: Let T be an operator on $L^2(\mathbb{R},\mathcal{H})$ defined by

$$(T\phi)(x)=\int_{\mathbb{R}} t(x,\xi)\phi(\xi)\,d\xi, \tag{2.1}$$

where $t(x,\xi)\in\mathcal{B}(\mathcal{H})$ for each (x,ξ). Then T is a Hilbert–Schmidt operator on $L^2(\mathbb{R},\mathcal{H})$ if and only if

$$\int_{\mathbb{R}_x}\int_{\mathbb{R}_\xi} \mathrm{tr}_{\mathcal{H}}[t(x,\xi)^* t(x,\xi)]\,d\xi dx<\infty.$$

In this case,

$$\|T\|^2_{\mathbf{S}_2(L^2(\mathbb{R},\mathcal{H}))}=\int_{\mathbb{R}_x}\int_{\mathbb{R}_\xi} \mathrm{tr}_{\mathcal{H}}[t(x,\xi)^* t(x,\xi)]\,d\xi dx.$$

Proof: The Hilbert space $\mathcal{H}$ is isomorphic to some $L^2(Y)$ space and therefore it suffices to establish the statement for an operator T on $L^2(\mathbb{R},L^2(Y))$ defined by (2.1) for some $t(x,\xi)\in\mathcal{B}(L^2(Y))$. Since $L^2(\mathbb{R},L^2(Y))$ is isomorphic to $L^2(\mathbb{R}\times Y)$, the rephrased assertion follows immediately from Ref. 25, Theorem VI.23. □

III. THE HAMILTONIAN $H=H_0+V$

As in the scalar-valued case the quadratic form

$$h_0[\psi,\psi] := \int_{\mathbb{R}} \|(d/dx)\psi(x)\|^2_{\mathcal{H}}\,dx \tag{3.1}$$

is closed in $L^2(\mathbb{R},\mathcal{H})$ on the domain $H^1(\mathbb{R},\mathcal{H})$. Thus, this form generates a self-adjoint operator H_0 on $L^2(\mathbb{R},\mathcal{H})$. The free Hamiltonian H_0 corresponds to the "Laplacian" $-d^2/dx^2\otimes 1_{\mathcal{H}}$ on $L^2(\mathbb{R},\mathcal{H})$.

A potential V is a $\mathcal{B}(\mathcal{H})$-valued, measurable function on $\mathbb{R}$. Assume that $V(x)$ is symmetric for almost all x, i.e., $V(x)^*=V(x)$ for almost all x. The operator $V(x)\in\mathcal{B}(\mathcal{H})$ has a unique representation in the form $V(x)=U(x)|V(x)|$, where $|V(x)|$ is the modulus of $V(x)$ defined by $|V(x)|=(V(x)^*V(x))^{1/2}=(V(x)V(x))^{1/2}$. (The representation is not unique if the potential vanishes on a set of positive measure.) We have that $|V(x)|$ is a non-negative, self-adjoint operator belonging to $\mathcal{B}(\mathcal{H})$ and, moreover, $\||V(x)|\|_{\mathcal{B}(\mathcal{H})}=\|V(x)\|_{\mathcal{B}(\mathcal{H})}$. The operator $U(x)$ is a partial isometry with initial domain $\overline{\mathrm{Ran}|V(x)|}$, final domain $\overline{\mathrm{Ran}V(x)}$ and $\mathrm{Ker}\,U(x)=\mathrm{Ker}\,V(x)$. Observe that $U(x)^*U(x)=P_{\overline{\mathrm{Ran}\,|V(x)|}}$ and $U(x)U(x)^*=P_{\overline{\mathrm{Ran}\,V(x)}}$, where P_M denotes the orthogonal projection onto a closed subspace M. The modulus $|V(x)|$ possesses exactly one non-negative, self-adjoint square-root $|V(x)|^{1/2}\in\mathcal{B}(\mathcal{H})$. The square-root $|V(x)|^{1/2}$ commutes with every bounded operator which commutes with $|V(x)|$. We may define $V(x)^{1/2}=U(x)|V(x)|^{1/2}$ such that $V(x)=V(x)^{1/2}|V(x)|^{1/2}$. Moreover, $V(x)^{1/2}\in\mathcal{B}(\mathcal{H})$ with $\|V(x)^{1/2}\|_{\mathcal{B}(\mathcal{H})}=[\|V(x)\|_{\mathcal{B}(\mathcal{H})}]^{1/2}$ and adjoint $(V(x)^{1/2})^*=|V(x)|^{1/2}U(x)^*$. From Proposition 2.1 it follows that $|V|$, $|V|^{1/2}$ and $V^{1/2}$ are $\mathcal{B}(\mathcal{H})$-valued measurable functions on $\mathbb{R}$.

We want to establish the following result.

Proposition 3.1:

(i) If $V\in L^1(\mathbb{R},\mathcal{B}(\mathcal{H}))$, then the real-valued quadratic form

$$v[\psi,\psi]:=\int_{\mathbb{R}}\langle V(x)^{1/2}\psi(x),|V(x)|^{1/2}\psi(x)\rangle_{\mathcal{H}}\,dx$$

is H_0 form-bounded with relative bound zero.

(ii) If $V\in L^1(\mathbb{R},\mathbf{S}_2(\mathcal{H}))$, then v is H_0 form-compact.

It follows from Proposition 3.1 (i) and the KLMN theorem (Ref. 26, Theorem X.17) that the form sum

$$h[\psi,\psi]:=h_0[\psi,\psi]+v[\psi,\psi]$$

is closed and semi-bounded from below on $H^1(\mathbb{R}^d,\mathcal{H})$ and thus generates a self-adjoint operator $H=H_0+V$ on $L^2(\mathbb{R},\mathcal{H})$. From Proposition 3.1 (ii) and Weyl's essential spectrum theorem it follows that $\sigma_{\mathrm{ess}}(H)=\sigma_{\mathrm{ess}}(H_0)=[0,\infty)$.

Proof of Proposition 3.1: The "kernel" of the resolvent of H_0 is given by (see, e.g., Ref. 28, Theorem 9.5.2)

$$Q(x-y;\ \sqrt{|E|})=\frac{e^{-\sqrt{|E|}|x-y|}}{2\sqrt{|E|}},\quad E<0. \tag{3.2}$$

(i) To show that the form v is infinitesimally H_0 form-bounded, it suffices to show that the form

$$w[\phi]=\langle|V|^{1/2}(H_0-E)^{-1/2}\phi,V^{1/2}(H_0-E)^{-1/2}\phi\rangle_{L^2(\mathbb{R},\mathcal{H})}$$

is bounded on $L^2(\mathbb{R},\mathcal{H})$ and that its norm

$$\|w\|:=\inf_{\phi\in L^2(\mathbb{R},\mathcal{H})}\frac{|\langle|V|^{1/2}(H_0-E)^{-1/2}\phi,V^{1/2}(H_0-E)^{-1/2}\phi\rangle|}{\|\phi\|^2}$$

tends to zero as $E\to-\infty$. By the definition of $\|w\|$, and since U in $V^{1/2}=U|V|^{1/2}$ is a partial isometry, we have that

$$\|w\|\leqslant\||V|^{1/2}(H_0-E)^{-1/2}\|^2_{\mathcal{B}(L^2(\mathbb{R},\mathcal{H}))}. \tag{3.3}$$

Therefore, it is enough to show that the right-hand side of the latter tends to zero as $E\to-\infty$.

We consider first $V\in L^\infty(\mathbb{R},\mathcal{B}(\mathcal{H}))$. For such V we have that

$$\||V|^{1/2}(H_0-E)^{-1/2}\|^2_{\mathcal{B}(L^2)}=\||V|^{1/2}(H_0-E)^{-1}|V|^{1/2}\|_{\mathcal{B}(L^2)}. \tag{3.4}$$

Let $\alpha=\sqrt{|E|}$ and $\phi\in L^2(\mathbb{R},\mathcal{H})$. Then Hölder's inequality yields that

$$\|[|V|^{1/2}(H_0+\alpha^2)^{-1}|V|^{1/2}\phi](x)\|_{\mathcal{H}}\leqslant\frac{1}{2\alpha}\|V(x)\|^{1/2}_{\mathcal{B}(\mathcal{H})}\|V\|_{L^1(\mathbb{R},\mathcal{B}(\mathcal{H}))}\|\phi\|_{L^2(\mathbb{R},\mathcal{H})}.$$

The latter implies that

$$\begin{aligned}\||V|^{1/2}(H_0+\alpha^2)^{-1}|V|^{1/2}\phi\|^2_{L^2(\mathbb{R},\mathcal{H})}&\leqslant\int_{\mathbb{R}}\frac{1}{4\alpha^2}\|V(x)\|_{\mathcal{B}(\mathcal{H})}\|V\|^2_{L^1(\mathbb{R},\mathcal{B}(\mathcal{H}))}\|\phi\|^2_{L^2(\mathbb{R},\mathcal{H})}\,dx\\&\leqslant\frac{1}{4\alpha^2}\|V\|^3_{L^1(\mathbb{R},\mathcal{B}(\mathcal{H}))}\|\phi\|^2_{L^2(\mathbb{R},\mathcal{H})}.\end{aligned}$$

In conjunction with (3.4), the latter shows that the right-hand side of (3.3) tends to zero as $E \to -\infty$, which establishes assertion (i) for $V \in L^{\infty}(\mathbb{R},\mathcal{H})$. A standard approximation argument yields the assertion for general V.
(ii) It suffices to show that the form

$$w[\phi]=\langle |V|^{1/2}(H_0-E)^{-1/2}\phi, V^{1/2}(H_0-E)^{-1/2}\phi\rangle$$

defines a compact operator in $L^2(\mathbb{R},\mathcal{H})$. Under the assumption in (i) we already know that w generates a bounded, self-adjoint operator W in $L^2(\mathbb{R},\mathcal{H})$. Let us show that W is a Hilbert–Schmidt operator. From

$$\mathrm{tr}_{L^2}(W^*W)=\mathrm{tr}(V^{1/2}(H_0-E)^{-1}(V^{1/2})^*|V|^{1/2}(H_0-E)^{-1}(|V|^{1/2})^*),$$

we see that it is enough to show that $W_1=|V|^{1/2}(H_0-E)^{-1}(|V|^{1/2})^*$ and $W_2=V^{1/2}(H_0-E)^{-1}(V^{1/2})^*$ are Hilbert-–Schmidt operators on $L^2(\mathbb{R},\mathcal{H})$. It is enough to show it for W_2; the proof for W_1 is similar. The operator W_2 has integral "kernel"

$$K_{W_2}(x-y;\alpha)=V(x)^{1/2}(2\alpha)^{-1}e^{-\alpha|x-y|}(V(y)^{1/2})^*, \quad \alpha=\sqrt{-E}>0.$$

Using the criterion in Lemma 2.2 and the assumption in (ii), we estimate as follows:

$$\begin{aligned}
&\int_{\mathbb{R}}\int_{\mathbb{R}} \mathrm{tr}_{\mathcal{H}}[K_{W_2}(x-y;\alpha)^*K_{W_2}(x-y;\alpha)]\,dxdy\\
&\quad=\int_{\mathbb{R}}\int_{\mathbb{R}}\left(\frac{e^{-\alpha|x-y|}}{2\alpha}\right)^2 \mathrm{tr}_{\mathcal{H}}[(V(y)^{1/2})^{**}(V(x)^{1/2})^*V(x)^{1/2}(V(y)^{1/2})^*]\,dxdy\\
&\quad=\int_{\mathbb{R}}\int_{\mathbb{R}}\left(\frac{e^{-\alpha|x-y|}}{2\alpha}\right)^2 \mathrm{tr}_{\mathcal{H}}[V(y)^{1/2}|V(x)|^{1/2}U(x)^*U(x)|V(x)|^{1/2}(V(y)^{1/2})^*]\,dxdy\\
&\quad=\int_{\mathbb{R}}\int_{\mathbb{R}}\left(\frac{e^{-\alpha|x-y|}}{2\alpha}\right)^2 \mathrm{tr}_{\mathcal{H}}[|V(x)||V(y)|]\,dxdy\\
&\quad\leqslant\frac{1}{4\alpha^2}\int_{\mathbb{R}}\|V(x)\|_{\mathbf{s}_2(\mathcal{H})}\,dx\int_{\mathbb{R}}\|V(y)\|_{\mathbf{s}_2(\mathcal{H})}\,dy.
\end{aligned}$$

This shows that W_2 is a Hilbert–Schmidt operator in $L^2(\mathbb{R},\mathcal{H})$. □

We note that $V \in L^1(\mathbb{R},\mathcal{B}(\mathcal{H}))$ implies that $|V| \in L^1(\mathbb{R},\mathcal{B}(\mathcal{H}))$ and, in view of Proposition 3.1 (i), $|V|$ is infinitesimally H_0 form-bounded. Consequently, the following mappings are bounded:

$$V,|V|: \quad H^1(\mathbb{R},\mathcal{H})\to H^{-1}(\mathbb{R},\mathcal{H}), \tag{3.5}$$

$$|V|^{1/2},V^{1/2}: \quad H^1(\mathbb{R},\mathcal{H})\to L^2(\mathbb{R},\mathcal{H}), \tag{3.6}$$

$$|V|^{1/2},V^{1/2}: \quad L^2(\mathbb{R},\mathcal{H})\to H^{-1}(\mathbb{R},\mathcal{H}). \tag{3.7}$$

The qualitative behavior of any possible negative eigenvalues of H_0+gV as $g\to 0$ is described by the following simple result.

Proposition 3.2: If $V \in L^1(\mathbb{R},\mathcal{B}(\mathcal{H}))$, then any negative eigenvalues of H_0+gV approach zero as g tends to zero.

Proof: Following Ref. 31 it suffices to show that there are positive constants g_0 and C such that $H_0+gV \geqslant -Cg$ for all $g_0>g>0$.

Let $\mathcal{F}$ denote the Fourier transform of vector-valued functions in $L^2(\mathbb{R},\mathcal{H})$ (see Sec. II E). We observe that, as for scalar-valued functions, a function ϕ whose Fourier transform is integrable is bounded and continuous with the usual estimate

$$\|\phi(x)\|_{\mathcal{H}} \leqslant \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \|\mathcal{F}\phi(\xi)\|_{\mathcal{H}}\, d\xi. \tag{3.8}$$

For an arbitrary $\gamma>0$, Hölder's inequality yields that

$$\begin{aligned}\left(\int_{\mathbb{R}} \|\mathcal{F}\phi(\xi)\|_{\mathcal{H}}\, d\xi \right)^2 &\leqslant \left(\int_{\mathbb{R}} (\xi^2+\gamma^2)^{-1}\, d\xi \right) \left(\int_{\mathbb{R}} (\xi^2+\gamma^2) \|\mathcal{F}\phi(\xi)\|_{\mathcal{H}}^2\, d\xi \right) \\ &= \frac{\pi}{\gamma} \|(-i\xi+\gamma)\mathcal{F}\phi\|_{L^2(\mathbb{R},\mathcal{H})}^2 \\ &= \frac{\pi}{\gamma} \|(H_0^{1/2}+\gamma)\phi\|_{L^2(\mathbb{R},\mathcal{H})}^2 \\ &\leqslant \frac{2\pi}{\gamma} \{\|H_0^{1/2}\phi\|_{L^2(\mathbb{R},\mathcal{H})}^2 + \|\gamma\phi\|_{L^2(\mathbb{R},\mathcal{H})}^2\}. \end{aligned} \tag{3.9}$$

Let $d=\max\{1/\gamma,1\}$. Then (3.8) and (3.9) imply that

$$\|\phi(x)\|_{\mathcal{H}} \leqslant d\{\|H_0^{1/2}\phi\|_{L^2(\mathbb{R},\mathcal{H})}^2 + \|\phi\|_{L^2(\mathbb{R},\mathcal{H})}^2\} \tag{3.10}$$

for any $\phi \in \mathcal{D}(H_0^{1/2}) = H^1(\mathbb{R},\mathcal{H})$. The Sobolev type inequality (3.10) implies that

$$h_g[\phi] \geqslant \|H_0^{1/2}\|_{L^2(\mathbb{R},\mathcal{H})}^2 - g\int_{\mathbb{R}} \|V(x)\|_{\mathcal{B}(\mathcal{H})} \|\phi(x)\|_{\mathcal{H}}^2\, dx \geqslant (1-gd_1)\|H_0^{1/2}\|_{L^2(\mathbb{R},\mathcal{H})}^2 - gd_1\|\phi\|_{L^2(\mathbb{R},\mathcal{H})}^2,$$

where $d_1 = d\|V\|_{L^1(\mathbb{R},\mathcal{B}(\mathcal{H}))}^2$. When we take $C=d_1$, $g_0=d_1^{-1}$ and $0<g<g_0$, we arrive at $h_g[\phi] \geqslant -Cg$ as desired. □

IV. THE BIRMAN–SCHWINGER RELATION

The Birman–Schwinger relation has been established rigorously for various classes of operators in the scalar-valued setting (see, e.g., Ref. 30, 31, and 17). It asserts that E is a negative eigenvalue of $H=-d^2/dx^2+V$ if and only if -1 is an eigenvalue of the operator $V^{1/2}(-d^2/dx^2-E)^{-1}|V|^{1/2}$. Formally this is obvious since $\phi=V^{1/2}\psi$ is a solution to $V^{1/2}(-d^2/dx^2-E)^{-1}|V|^{1/2}\phi=-\phi$.

Here we provide a simple proof of the Birman–Schwinger relation in our concrete operator-valued setting. For this purpose we introduce the Birman–Schwinger operator $K_E(V)=V^{1/2}(H_0-E)^{-1}|V|^{1/2}$, $E<0$, where H_0 is the non-negative, self-adjoint operator associated with the quadratic form h_0 in (3.1). Setting $\alpha^2=-E$, its integral "kernel" is given by

$$K_\alpha(x,y) = V(x)^{1/2}(2\alpha)^{-1}e^{-\alpha|x-y|}|V(y)|^{1/2}, \quad \alpha>0.$$

We have the following result.

Lemma 4.1: If $V\in L^1(\mathbb{R},\mathbf{S}_2(\mathcal{H}))$, then the Birman–Schwinger operator $K_E(V)$, $E<0$, is a Hilbert–Schmidt operator on $L^2(\mathbb{R},\mathcal{H})$; in particular $K_E(V)$ is a compact operator. Moreover, $\|K_E(V)\|_{\mathcal{B}(L^2(\mathbb{R},\mathcal{H}))}\to 0$ as $E\to-\infty$.

Proof: We argue as for the operator W_2 in the proof of Proposition 3.1 (ii). We omit the details. □

Having introduced the compact Birman–Schwinger operator we may formulate the Birman–Schwinger relation.

Proposition 4.2: Let $V\in L^1(\mathbb{R},\mathbf{S}_2(\mathcal{H}))$. *Then $E<0$ is an eigenvalue of $H=H_0+V$ (defined by a quadratic form) having multiplicity $\varkappa$ if and only if -1 is an eigenvalue of $K_E(V)$ having geometric multiplicity $\varkappa$.*

To establish Proposition 4.2 we need the following two results.

Lemma 4.3: If $V\in L^1(\mathbb{R},\mathcal{B}(\mathcal{H}))$, *then for* $E<0$ *the operators* $|V|^{1/2}\times(H_0-E)^{-1/2}$ *and* $V^{1/2}(H_0-E)^{-1/2}$ *are bounded on* $L^2(\mathbb{R},\mathcal{H})$.

Proof: Since V is H_0 form-bounded, it follows immediately from (3.6) and (3.7) in conjunction with the fact that the operator $(H_0-E)^{-1/2}$ is a bounded map from the domain $L^2(\mathbb{R},\mathcal{H})$ to the range $H^1(\mathbb{R},\mathcal{H})$. □

Lemma 4.4: Let S *and* T *be bounded operators on the Hilbert space* $\mathcal{K}$. *Then* $\sigma(ST)\setminus\{0\}=\sigma(TS)\setminus\{0\}$. *Moreover,* $\lambda\neq 0$ *is an eigenvalue of* ST *having geometric multiplicity* m *if and only if* λ *is an eigenvalue of* TS *having geometric multiplicity* m.

Proof: This is a simplified version of Theorem 2 (i) in Ref. 9. □

Proof Proposition 4.2: Let h_0 be the form of H_0, let v be the form of V and let $h=h_0+v$ be their form sum. According to Lemma 4.3 the operators $|V|^{1/2}(H_0-E)^{-1/2}$ and $V^{1/2}(H_0-E)^{-1/2}$ are bounded on $L^2(\mathbb{R},\mathcal{H})$ and, consequently, the operator $I+[|V|^{1/2}(H_0-E)^{-1/2}]^*V^{1/2}$ $(H_0-E)^{-1/2}$ is bounded on $L^2(\mathbb{R},\mathcal{H})$. Moreover, the operator $A^{-1}=(H_0-E)^{1/2}$ has domain $H^1(\mathbb{R},\mathcal{H})$ and range $L^2(\mathbb{R},\mathcal{H})$. Thus, we may introduce an auxiliary sesquilinear form a defined on the form domain $H^1(\mathbb{R},\mathcal{H})\times H^1(\mathbb{R},\mathcal{H})$ by

$$a[\phi,\psi]=\langle[I+(|V|^{1/2}A)^*V^{1/2}A]A^{-1}\phi,A^{-1}\psi\rangle. \tag{4.1}$$

We rewrite a and find that

$$a[\phi,\psi]=\underbrace{\langle A^{-1}\phi,A^{-1}\psi\rangle}_{a_1[\phi,\psi]}+\underbrace{\langle(|V|^{1/2}A)^*V^{1/2}AA^{-1}\phi,A^{-1}\psi\rangle}_{a_2[\phi,\psi]}.$$

Clearly,

$$a_1[\phi,\psi]=h_0[\phi,\psi]-E\langle\phi,\psi\rangle \tag{4.3}$$

and, since $|V|^{1/2}A$ is bounded on $L^2(\mathbb{R},\mathcal{H})$,

$$a_2[\phi,\psi]=\langle V^{1/2}AA^{-1}\phi,[|V|^{1/2}A]^{**}A^{-1}\psi\rangle=\langle V^{1/2}\phi,|V|^{1/2}AA^{-1}\psi\rangle=v[\phi,\psi]. \tag{4.4}$$

Hence, (4.2)–(4.4) shows that the forms a and $h-E$ are identical.

Suppose that $E<0$ is an eigenvalue of $H=H_0+V$, i.e., there exists an eigenfunction $\psi\in\mathcal{D}(H)$, $\psi\neq 0$, such that $(H-E)\psi=0$. This is equivalent to $(h-E)[\psi,\phi]=0$ for all $\phi\in H^1(\mathbb{R},\mathcal{H})$. Since the forms h and a are identical, we may introduce $u=A^{-1}\phi$ and deduce that

$$\begin{aligned}0=a[\psi,\phi]&=\langle[I+(|V|^{1/2}A)^*V^{1/2}A]A^{-1}\psi,A^{-1}\phi\rangle,\quad \forall\,\phi\in H^1(\mathbb{R},\mathcal{H}),\\&=\langle[I+(|V|^{1/2}A)^*V^{1/2}A]A^{-1}\psi,u\rangle,\ \ \forall\,\phi\in L^2(\mathbb{R},\mathcal{H}),\end{aligned}$$

because u runs through $L^2(\mathbb{R},\mathcal{H})$ as ϕ runs through $H^1(\mathbb{R},\mathcal{H})$. Consequently, $(I+[|V|^{1/2}A]^*V^{1/2}A)v=0$, where $v=A^{-1}\psi=(H_0-E)^{1/2}\psi$, so $-1\in\sigma_p([|V|^{1/2}A]^*V^{1/2}A)$. By reversing the arguments leading to the latter conclusion, we infer that

$$E\in\sigma_p(H_0+V)\ \text{ if and only if }\ -1\in\sigma_p([|V|^{1/2}A]^*V^{1/2}A). \tag{4.5}$$

Since $(H_0-E)^{1/2}$ is injective from the domain $L^2(\mathbb{R},\mathcal{H})$ to the range $H^1(\mathbb{R},\mathcal{H})$, the arguments above also show that the multiplicities of the eigenvalues E and -1 must be equal. In view of Lemma 4.4 and the definition of A, (4.5) implies that

$$E\in\sigma_p(H_0+V)\ \text{ if and only if }\ -1\in\sigma_p(V^{1/2}(H_0-E)^{-1/2}[|V|^{1/2}(H_0-E)^{-1/2}]^*) \tag{4.6}$$

and the multiplicities of E and -1 are equal. But $[|V|^{1/2}(H_0-E)^{-1/2}]^*=(H_0-E)^{-1/2}|V|^{1/2}$ and, therefore, in view of the definition of $K_E(V)$, (4.6) yields that $E\in\sigma_p(H_0+V)$ if and only if $-1\in\sigma_p(K_E(V))$. □

If g is fixed and $\lambda(\alpha)$ is an eigenvalue of $K_\alpha(V)$, then the Birman–Schwinger relation asserts that any solution $\alpha_g>0$ of

$$g\lambda(\alpha_g)=-1 \tag{4.7}$$

is associated to the eigenvalue $E(g)=-\alpha_g^2$ of $H(g)$. The latter equation plays a crucial role in Sec. V.

Define the operators L_α and M_α by their ''kernels:''

$$L_\alpha(x,y)=\frac{1}{2\alpha}V(x)^{1/2}|V(y)|^{1/2}, \tag{4.8}$$

$$M_\alpha(x,y)=\frac{1}{2\alpha}V(x)^{1/2}[[e^{-\alpha|x-y|}-1]|V(y)|^{1/2}. \tag{4.9}$$

Moreover, we introduce the operator M_0 with ''kernel''

$$M_0(x,y)=-\tfrac{1}{2}V(x)^{1/2}|x-y||V(y)|^{1/2}. \tag{4.10}$$

Imitating Ref. 31 we obtain the following result.

Lemma 4.5: If $\int_{\mathbb{R}}(1+|x|^2)\|V(x)\|_{\mathbf{s}_2(\mathcal{H})}\,dx<\infty$, *then the following assertions are valid:*

(i) The operator M_0 *is Hilbert–Schmidt on* $L^2(\mathbb{R},\mathcal{H})$.
(ii) As $\alpha\downarrow 0$, *the operator* M_α *converges to* M_0 *in the Hilbert–Schmidt norm on* $L^2(\mathbb{R},\mathcal{H})$.
(iii) The Birman–Schwinger operator $gK_\alpha(V)$ *has eigenvalue* -1 *if and only if the same is true for* $g(1+gM_\alpha)^{-1}L_\alpha$.

Proof:

(i) It follows from the estimate

$$\int_{\mathbb{R}}\int_{\mathbb{R}}\mathrm{tr}_{\mathcal{H}}[M_0(x,y)^*M_0(x,y)]\,dxdy\leqslant\frac{1}{2}\int\int(|x|^2+|y|^2)\|\,|V(x)|\,\|_{\mathbf{s}_2(\mathcal{H})}\|\,|V(y)|\,\|_{\mathbf{s}_2(\mathcal{H})}\,dxdy<\infty.$$

(ii) We want to show that

$$\int\int\mathrm{tr}_{\mathcal{H}}[(M_\alpha-M_0)(x,y)^*(M_\alpha-M_0)(x,y)]\,dxdy\to 0 \tag{4.11}$$

as $\alpha\downarrow 0$. Now,

$$\mathrm{tr}_{\mathcal{H}}[(M_\alpha-M_0)(x,y)^*(M_\alpha-M_0)(x,y)]=\left|\frac{1}{2\alpha}(e^{-\alpha|x-y|}-1)+\frac{1}{2}|x-y|\right|^2\mathrm{tr}_{\mathcal{H}}[|V(x)||V(y)|],$$

and since $|(1/2\alpha)(e^{-\alpha|x-y|}-1)+(1/2)|x-y||\to 0$ as $\alpha\downarrow 0$, we have the pointwise convergence

$$\mathrm{tr}_{\mathcal{H}}[(M_\alpha-M_0)(x,y)^*(M_\alpha-M_0)(x,y)]\to 0\ \text{ as }\ \alpha\downarrow 0. \tag{4.12}$$

Moreover,

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}[M_\alpha(x,y)^* M_\alpha(x,y)] &= \left|\frac{1}{2\alpha}(e^{-\alpha|x-y|}-1)\right|^2 \mathrm{tr}_{\mathcal{H}}[|V(x)||V(y)|] \\ &\leqslant |\tfrac{1}{2}|x-y||^2 \mathrm{tr}_{\mathcal{H}}[|V(x)||V(y)|] \\ &= \mathrm{tr}_{\mathcal{H}}[M_0(x,y)^* M_0(x,y)]. \end{aligned} \tag{4.13}$$

It follows from (i) and (4.12) and (4.13) in conjunction with Lebesgue's dominated convergence theorem that (4.11) holds.

(iii) It follows from (4.13) that $\|M_\alpha\|_{\mathcal{B}(L^2(\mathbb{R},\mathcal{H}))} \leqslant \|M_\alpha\|_{HS} \leqslant \|M_0\|_{HS}$. Hence, $\|M_\alpha\|_{\mathcal{B}(L^2(\mathbb{R},\mathcal{H}))}$ is bounded *independently* of $\alpha \in (0,\alpha_0]$ for some $\alpha_0 > 0$. Therefore, for g small enough, $\|gM_\alpha\|_{\mathcal{B}(L^2(\mathbb{R},\mathcal{H}))} < 1$ and, consequently, $(1+gM_\alpha)^{-1}$ exists and is bounded for these g and α. In particular, we may write $1+gK_\alpha(V) = (1+gM_\alpha)[1+g(1+gM_\alpha)^{-1}L_\alpha]$ from which the assertion follows. □

V. WEAKLY COUPLED BOUND STATES

Throughout this section operators (resp. vectors) are denoted by boldface capital (resp. small) letters to emphasize their matrix (resp. vector) structure.

A. Two-channel Hamiltonians with matrix-valued potentials

We consider the case where the potential is a 2×2 matrix-valued potential $\mathbf{V}(x)$ with measurable functions V_{ij} on $\mathbb{R}$ as entries. The Euclidean inner product and norm in $\mathbb{C}^2$ are denoted by $\langle \cdot,\cdot \rangle_{\mathbb{C}^2}$ and $\|\cdot\|_{\mathbb{C}^2}$, respectively.

Assumption 5.1:

(a) $\mathbf{V}(x)$ is symmetric, i.e., $\overline{V_{ji}} = V_{ij}$.

(b) $\int_{\mathbb{R}} (1+|x|^2)\|\mathbf{V}(x)\|_{\mathcal{B}(\mathbb{C}^2)}\, dx < \infty$.

(c) The functions V_{ij} are real-valued.

1. Two-channel Hamiltonian with a single threshold

First we consider the Hamiltonian $\mathbf{H}(g) = \mathbf{H}_0 + g\mathbf{V}(x)$ in $L^2(\mathbb{R},\mathbb{C}^2)$, defined in Proposition 3.1 by means of forms. Formally, we may write the Hamiltonian as

$$\mathbf{H}(g) = \mathbf{H}_0 + g\mathbf{V} = \begin{pmatrix} -\dfrac{d^2}{dx^2} & 0 \\ 0 & -\dfrac{d^2}{dx^2} \end{pmatrix} + g\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \tag{5.1}$$

in $L^2(\mathbb{R},\mathbb{C}^2) = L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$. Under Assumption 5.1 we know that its essential spectrum equals the half-axis starting at the (threshold) point zero.

Define the matrices $\mathbf{S}$ and $\mathbf{T}$ by

$$\mathbf{S} = \int_{\mathbb{R}} \mathbf{V}(x)\, dx, \quad \mathbf{T}_0 = -\frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} \mathbf{V}(x)|x-y|\mathbf{V}(y)\, dy dx. \tag{5.2}$$

We establish the following result.

Theorem 5.2: *Let* $\mathbf{V}$ *obey Assumption 5.1 (a) and (b) and let* $\mathbf{H}(g) = \mathbf{H}_0 + g\mathbf{V}(x)$ *be the self-adjoint Hamiltonian on* $L^2(\mathbb{R},\mathbb{C}^2)$ *defined in Proposition 3.1 by means of forms.*

(i) Assume that the matrix $\mathbf{S}$*, defined in (5.2), has* $n(\leqslant 2)$ *negative eigenvalues, denoted by* s_i*, with multiplicities* $\varkappa_i$*. Then, for a small enough* g*, the two-channel Hamiltonian* $\mathbf{H}(g)$ *has precisely* $\Sigma_{i=1}^n \varkappa_i$ *negative eigenvalues (taking into account multiplicity)* E_{ij} *satisfying the formulas*

$$(-E_{ij}(g))^{1/2}=-\frac{g}{2}s_i+\frac{g^2}{2}\langle \mathbf{v}_{ij},\mathbf{T}_0\mathbf{v}_{ij}\rangle_{\mathbb{C}^2}+O(g^3),$$
$$i=1,\ldots,n,\quad j=1,\ldots,\varkappa_i, \tag{5.3}$$

where $\mathbf{T}_0$ *is defined in (5.2) and* $\mathbf{v}_{ij}$ *are the eigenvectors corresponding to the eigenvalue* s_i *of* $\mathbf{S}$.

(ii) Suppose that $\mathbf{V}$ *obey Assumption 5.1(c) and that the matrix* $\mathbf{S}$ *has n nonpositive eigenvalues, denoted by* s_i, *with multiplicities* $\varkappa_i$. *If the eigenvectors* $\mathbf{v}_{0j}$, $j=1,\ldots,\varkappa_i$, *associated with the eigenvalue zero of* $\mathbf{S}$ *satisfy* $\langle \mathbf{v}_{0j},\mathbf{T}_0\mathbf{v}_{0j}\rangle_{\mathbb{C}^2}\neq 0$, *then the conclusion of part (i) remains valid.*

Proof: According to the Birman–Schwinger relation formulated in Proposition 4.2, $E(g)<0$ is an eigenvalue of $\mathbf{H}(g)$ if and only if -1 is an eigenvalue of $g\mathbf{K}_\alpha(\mathbf{V})$ with $\alpha^2=-E(g)$. Furthermore, in view of Lemma 4.5(iii), the operator $g\mathbf{K}_\alpha(\mathbf{V})$ has eigenvalue -1 if and only if the same is true for $g(1+g\mathbf{M}_\alpha)^{-1}\mathbf{L}_\alpha$. Now let us denote the (unknown) eigenvalues and eigenfunctions of $(1+g\mathbf{M}_\alpha)^{-1}\mathbf{L}_\alpha$ by $\mu_k(g,\alpha)$ and $\mathbf{\Psi}_k(x;g,\alpha)$, respectively, viz.

$$(1+g\mathbf{M}_\alpha)^{-1}\mathbf{L}_\alpha\mathbf{\Psi}_k(x;g,\alpha)=\mu_k(g,\alpha)\mathbf{\Psi}_k(x;g,\alpha). \tag{5.4}$$

Let $\mathbf{u}_k\in\mathbb{C}^2$ be a constant vector. We insert

$$\mathbf{\Psi}_k(x;g,\alpha)=\frac{1}{2\alpha}(1+g\mathbf{M}_\alpha)^{-1}|\mathbf{V}(x)|^{1/2}\mathbf{u}_k$$

into (5.4) and obtain

$$\mathbf{R}_g\mathbf{u}_k=\mu_k(g,\alpha)\mathbf{u}_k, \tag{5.5}$$

where $\mathbf{R}_g$ is the matrix

$$\mathbf{R}_g=\frac{1}{2\alpha}\int_{\mathbb{R}}\mathbf{V}^{1/2}(x)[(1+g\mathbf{M}_\alpha)^{-1}|\mathbf{V}|^{1/2}](x)\,dx.$$

Define $\mathbf{S}$ as in (5.2) and, moreover, define

$$\mathbf{T}(\alpha)=\int_{\mathbb{R}}\mathbf{V}^{1/2}(x)[\mathbf{M}_\alpha|\mathbf{V}|^{1/2}](x)\,dx.$$

Then we have that

$$\mathbf{R}_g=\frac{1}{2\alpha}\mathbf{S}-\frac{g}{2\alpha}\mathbf{T}(\alpha)+\mathrm{O}(g^2)$$

for small g.

(i) By assumption the matrix $\mathbf{S}$ has n negative eigenvalues, denoted by s_k. For simplicity we assume that the eigenvalues s_k are simple. The corresponding eigenvectors are denoted by $\mathbf{v}_k$. We apply the regular perturbation theory to the eigenvalue problem (5.5) and we find that

$$\mu_k(g,\alpha)=\frac{1}{2\alpha}s_k-\frac{g}{2\alpha}\langle \mathbf{v}_k,\mathbf{T}(\alpha)\mathbf{v}_k\rangle_{\mathbb{C}^2}+\mathrm{O}(g^2).$$

Define the matrix $\mathbf{T}_0$ as in (5.2) and

$$\mathbf{T}_1=\frac{1}{4}\int_{\mathbb{R}}\int_{\mathbb{R}}\mathbf{V}(x)|x-y|^2\mathbf{V}(y)\,dxdy.$$

Then we have that $\mathbf{T}(\alpha)=\mathbf{T}_0+\alpha\mathbf{T}_1+\mathrm{O}(\alpha^2)$. In this way we find that the eigenvalues associated with the eigenvalue problem (5.5) are

$$\mu_k(g,\alpha)=\frac{1}{2\alpha}s_k-\frac{g}{2\alpha}\langle\mathbf{v}_k,\mathbf{T}_0\mathbf{v}_k\rangle_{\mathbb{C}^2}+\mathrm{O}(g^2).$$

Together with the comments following the proof of Proposition 4.2, the latter implies that the solution to (4.7) is

$$\alpha_g=-\frac{g}{2}s_k+\frac{g^2}{2}\langle\mathbf{v}_k,\mathbf{T}_0\mathbf{v}_k\rangle_{\mathbb{C}^2}+\mathrm{O}(g^2). \tag{5.6}$$

Clearly, (5.6) implies that each negative eigenvalue s_k of $\mathbf{S}$ gives rise to precisely one negative eigenvalue $E_k(g)$ of $\mathbf{H}(g)$ obeying the asymptotic formula

$$(-E_k(g))^{1/2}=-\frac{g}{2}s_k+\frac{g^2}{2}\langle\mathbf{v}_k,\mathbf{T}_0\mathbf{v}_k\rangle_{\mathbb{C}^2}+\mathrm{O}(g^3).$$

(ii) We investigate the situation where zero is an eigenvalue of $\mathbf{S}$ (as above we restrict ourselves to the case where zero is simple). Let $\mathbf{S}\mathbf{v}_0=0$ for some $\mathbf{v}_0\neq 0$. Taylor's formula yields

$$\begin{aligned}\left\langle \mathbf{v}_0,\int_{\mathbb{R}}\int_{\mathbb{R}}\mathbf{V}(x)\frac{e^{-\alpha|x-y|}}{2\alpha}\mathbf{V}(y)\,dx\,dy\mathbf{v}_0\right\rangle_{\mathbb{C}^2}&\\ =\frac{1}{2\alpha}\langle\mathbf{v}_0,\mathbf{S}^2\mathbf{v}_0\rangle_{\mathbb{C}^2}-\frac{1}{2}\left\langle \mathbf{v}_0,\int_{\mathbb{R}}\int_{\mathbb{R}}\mathbf{V}(x)|x-y|\mathbf{V}(y)\,dx\,dy\mathbf{v}_0\right\rangle_{\mathbb{C}^2}&\\ +\alpha\left\langle \mathbf{v}_0,\int_{\mathbb{R}}\int_{\mathbb{R}}\mathbf{V}(x)O(|x-y|^2)\mathbf{V}(y)\,dx\,dy\mathbf{v}_0\right\rangle_{\mathbb{C}^2}.&\end{aligned}$$

Since $\mathbf{S}\mathbf{v}_0=0$ by assumption, the first term equals zero. As $\alpha\downarrow 0$, we obtain that

$$\begin{aligned}\langle\mathbf{v}_0,\mathbf{T}_0\mathbf{v}_0\rangle_{\mathbb{C}^2}&=\lim_{\alpha\downarrow 0}\left\langle \mathbf{v}_0,\int\int\mathbf{V}(x)\frac{e^{-\alpha|x-y|}}{2\alpha}\mathbf{V}(y)\,dxdy\,\mathbf{v}_0\right\rangle_{\mathbb{C}^2}\\ &=\lim_{\alpha\downarrow 0}\sum_{i,j,k}\int\int\frac{e^{-\alpha|x-y|}}{2\alpha}V_{ik}(x)V_{kj}(y)(\mathbf{v}_0)_i\overline{(\mathbf{v}_0)_j}\,dxdy.\end{aligned} \tag{5.7}$$

Let $\mathcal{F}$ denote the one-dimensional Fourier transform and let $(\mathcal{F}\mathbf{V})(\xi)$ denote the matrix with elements $(\mathcal{F}\mathbf{V})_{ij}(\xi)=(\mathcal{F}V_{ij})(\xi)$ satisfying $\mathcal{F}V_{ij}=\mathcal{F}V_{ji}$ because V is symmetric and V_{ij} are real-valued. Using the latter in conjunction with the Fourier transform of $(1/2\alpha)e^{-\alpha|x|}$, which equals $1/(\xi^2+\alpha^2)$, we find that

$$\begin{aligned}\text{rhs of (5.7)}&=\lim_{\alpha\downarrow 0}\sum_{i,j,k}\int\frac{1}{\xi^2+\alpha^2}(\mathcal{F}V_{ik})(\xi)\overline{(\mathcal{F}V_{kj})(\xi)}(\mathbf{v}_0)_i\overline{(\mathbf{v}_0)_j}\,d\xi\\ &=\int\frac{1}{\xi^2}\langle\mathbf{v}_0,(\mathcal{F}\mathbf{V})^*(\xi)(\mathcal{F}\mathbf{V})(\xi)\mathbf{v}_0\rangle_{\mathbb{C}^2}\,d\xi\\ &=\int\frac{1}{\xi^2}\|(\mathcal{F}\mathbf{V})(\xi)\mathbf{v}_0\|_{\mathbb{C}^2}^2\,d\xi\geqslant 0,\end{aligned} \tag{5.8}$$

By assumption, $\langle \mathbf{v}_0, \mathbf{T}_0 \mathbf{v}_0 \rangle_{\mathbb{C}^2} \neq 0$ and therefore (5.8) implies that there is also a negative eigenvalue of $\mathbf{H}(g)$ associated with the eigenvalue zero of $\mathbf{S}$. □

Remark 5.3: The reasoning in the proof of Theorem 5.2(ii) requires that the entries V_{ij} in the potential $\mathbf{V}$ are real-valued. A substantial improvement would be to establish the result for complex-valued entries.

Example 5.4 (Square-well potentials): Let $\chi_{[0,1]}$ denote the characteristic function associated with the interval $[0,1]$. Choose the following entries of **V:**

$$V_{11}(x) = -5\chi_{[0,1]}(x), \quad V_{22}(x) = -3\chi_{[0,1]}(x),$$

$$V_{12}(x) = V_{21}(x) = -3a\chi_{[0,1]}(x), \quad a > 0.$$

Then the matrix $\mathbf{S}$ equals

$$\mathbf{S} = \begin{pmatrix} -5 & -3a \\ -3a & -3 \end{pmatrix}$$

and it has two real eigenvalues given by $-4 \pm \sqrt{1+9a^2}$. Thus the following cases are possible: (1) If $a > \sqrt{\frac{5}{3}}$, there is exactly one negative eigenvalue of $\mathbf{S}$, namely $-4-\sqrt{1+9a^2}$. (2) If $a < \sqrt{\frac{5}{3}}$ there are two negative eigenvalues of $\mathbf{S}$, namely $-4 \pm \sqrt{1+9a^2}$. (3) If $a = \sqrt{\frac{5}{3}}$, there are two nonpositive eigenvalues of $\mathbf{S}$, namely $-4-\sqrt{1+9a^2}$ and 0.

2. Two-channel Hamiltonian with two thresholds

As an example of a Hamiltonian with more than one threshold, we consider the one in (1.1), having thresholds at 0 and 1. Henceforth, its free Hamiltonian is denoted by $\tilde{\mathbf{H}}_0$. The essential spectrum of $\tilde{\mathbf{H}}_0$ is the union of the half-axes starting at the thresholds, i.e., $\sigma_{\mathrm{ess}}(\tilde{\mathbf{H}}_0) = [0,\infty)$. The resolvent of $\tilde{\mathbf{H}}_0$ is given by

$$(\tilde{\mathbf{H}}_0 + \alpha^2)^{-1} = \begin{pmatrix} (-d^2/dx^2 + \alpha^2)^{-1} & 0 \\ 0 & (-d^2/dx^2 + \alpha^2 + 1)^{-1} \end{pmatrix}, \quad \alpha > 0,$$

where the entries have the integral kernels

$$\frac{1}{2\alpha} e^{-\alpha|x-y|} \quad \text{and} \quad \frac{1}{2\sqrt{\alpha^2+1}} e^{-\sqrt{\alpha^2+1}|x-y|}.$$

It is easy to show that the assertions of Proposition 3.1 are valid if one replaces $\mathbf{H}_0$ by $\tilde{\mathbf{H}}_0$. In this way we obtain a self-adjoint realization of the formal Hamiltonian $\tilde{\mathbf{H}}_0 + g\mathbf{V}$ in $L^2(\mathbb{R}, \mathbb{C}^2)$. Moreover, the Birman–Schwinger relation in Proposition 4.2 holds for $\tilde{\mathbf{H}}(g) = \tilde{\mathbf{H}}_0 + g\mathbf{V}$.

Define the operators $\tilde{\mathbf{L}}_\alpha$ and $\tilde{\mathbf{M}}_\alpha$ by their "kernels"

$$\tilde{\mathbf{L}}_\alpha(x,y) = \frac{1}{2\alpha} \mathbf{V}(x)^{1/2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} |\mathbf{V}(y)|^{1/2},$$

$$\tilde{\mathbf{M}}_\alpha(x,y) = \mathbf{V}(x)^{1/2} \begin{pmatrix} \frac{1}{2\alpha}[e^{-\alpha|x-y|} - 1] & 0 \\ 0 & \frac{e^{-\sqrt{\alpha^2+1}|x-y|}}{2\sqrt{\alpha^2+1}} \end{pmatrix} |\mathbf{V}(y)|^{1/2}.$$

Moreover, we introduce the operator $\tilde{\mathbf{M}}_0$ by its kernel

$$\tilde{\mathbf{M}}_0(x,y)=\mathbf{V}(x)^{1/2}\begin{pmatrix} -\frac{1}{2}|x-y| & 0 \\ 0 & \frac{1}{2}e^{-|x-y|} \end{pmatrix}|\mathbf{V}(y)|^{1/2}.$$

By making a few obvious changes to the proof of Lemma 4.5 we obtain the following result.

Lemma 5.5: Assume that $\int_{\mathbb{R}}(1+|x|^2)\|\mathbf{V}(x)\|_{\mathcal{B}(\mathbb{C}^2)}\,dx<\infty$. *If* K_α, L_α, M_α *and* M_0 *in Lemma 4.5 are replaced by* $\tilde{\mathbf{K}}_\alpha$, $\tilde{\mathbf{L}}_\alpha$, $\tilde{\mathbf{M}}_\alpha$ *and* $\tilde{\mathbf{M}}_0$, *then the assertions (i)–(iii) of Lemma 4.5 are still valid.*

Define the matrices

$$\tilde{\mathbf{S}}=\begin{pmatrix} \int_{\mathbb{R}}V_{11}(x)\,dx & \int_{\mathbb{R}}V_{12}(x)\,dx \\ 0 & 0 \end{pmatrix}, \tag{5.9}$$

$$\tilde{\mathbf{T}}_0=\int_{\mathbb{R}}\int_{\mathbb{R}}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\mathbf{V}(x)\begin{pmatrix} -\frac{1}{2}|x-y| & 0 \\ 0 & \dfrac{e^{-|x-y|}}{2} \end{pmatrix}\mathbf{V}(y)\,dxdy. \tag{5.10}$$

For the Hamiltonian $\tilde{\mathbf{H}}(g)$ we are able to derive an analog of part (i) in Theorem 5.2.

Theorem 5.6: *Let* $\mathbf{V}$ *obey Assumption 5.1(a)–(c) and let* $\tilde{\mathbf{H}}(g)=\tilde{\mathbf{H}}_0+g\mathbf{V}(x)$ *be the self-adjoint Hamiltonian on* $L^2(\mathbb{R},\mathbb{C}^2)$ *defined in Proposition 3.1 by means of forms.*

Assume that the matrix $\tilde{\mathbf{S}}$, *defined in (5.9), has a negative eigenvalue* $\tilde{s}$ *(such an eigenvalue is simple if it exists). Then, for a small enough coupling constant* g, *the eigenvalue* $\tilde{s}$ *of* $\tilde{\mathbf{S}}$ *gives rise to exactly one negative eigenvalue* $\tilde{E}$ *of the two-channel Hamiltonian* $\tilde{\mathbf{H}}(g)$. *The negative eigenvalue* $\tilde{E}$ *satisfies the formula*

$$(-\tilde{E}(g))^{1/2}=-\frac{g}{2}\tilde{s}+\frac{g^2}{2}\langle\tilde{\mathbf{v}},\tilde{\mathbf{T}}_0\tilde{\mathbf{v}}\rangle_{\mathbb{C}^2}+O(g^3), \tag{5.11}$$

where $\tilde{\mathbf{T}}_0$ *is defined in (5.10) and* $\tilde{\mathbf{v}}$ *is the eigenvector corresponding to the eigenvalue* $\tilde{s}$ *of* $\tilde{\mathbf{S}}$.

Proof: Imitating the proof of Theorem 5.2 we arrive at the eigenvalue problem

$$\tilde{\mathbf{R}}_g\mathbf{u}_k=\mu_k(g,\alpha)\mathbf{u}_k, \tag{5.12}$$

where $\tilde{\mathbf{R}}_g$ is the matrix

$$\tilde{\mathbf{R}}_g=\frac{1}{2\alpha}\int_{\mathbb{R}}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\mathbf{V}^{1/2}(x)[(1+g\tilde{\mathbf{M}}_\alpha)^{-1}|\mathbf{V}|^{1/2}](x)\,dx.$$

Define the matrix $\tilde{\mathbf{S}}$ as in (5.9) and, moreover, define

$$\tilde{\mathbf{T}}(\alpha)=\int_{\mathbb{R}}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\mathbf{V}^{1/2}(x)[\tilde{\mathbf{M}}_\alpha|\mathbf{V}|^{1/2}](x)\,dx.$$

Then we may write

$$\tilde{\mathbf{R}}_g=\frac{1}{2\alpha}\tilde{\mathbf{S}}-\frac{g}{2\alpha}\tilde{\mathbf{T}}(\alpha)+\mathrm{O}(g^2)$$

for small g. From here on everything depends on the possible eigenvalues of $\tilde{\mathbf{S}}$. Let

$$a=\int_{\mathbb{R}} V_{11}(x)\,dx.$$

The following cases may occur: (I) If $a\neq 0$, then there are two subcases. (I.1) If $a>0$, then $\tilde{\mathbf{S}}$ has the eigenvalue zero and the positive eigenvalue a, each of multiplicity one. (I.2) If $a<0$, then $\tilde{\mathbf{S}}$ has the eigenvalue zero and the negative eigenvalue a, each having multiplicity one. (II) If $a=0$, then $\tilde{\mathbf{S}}$ has the eigenvalue zero with multiplicity one.

Repeating the reasoning in the first part of the proof of Theorem 5.2 we show that a negative eigenvalue of $\tilde{\mathbf{S}}$ [from (I.2) it has multiplicity one] generates exactly one negative eigenvalue of $\tilde{\mathbf{H}}(g)$ provided g is small enough. □

Remark 5.7: The matrix $\tilde{\mathbf{S}}$ always has the eigenvalue zero. It remains an open problem to settle whether or not the latter gives rise to a negative eigenvalue of $\tilde{\mathbf{H}}(g)$ for a sufficiently small g.

B. *N*-channel Hamiltonian with matrix-valued potentials

In this section we consider the case where the potential is a $N\times N$ matrix-valued potential $\mathbf{V}(x)$ with measurable functions V_{ij} on $\mathbb{R}$ as entries.

Assumption 5.8:

(a) $\mathbf{V}(x)$ is symmetric, i.e., $\overline{V_{ji}}=V_{ij}$.

(b)

$$\int_{\mathbb{R}}(1+|x|^2)\|V(x)\|_{\mathcal{B}(\mathbb{C}^N)}\;dx<\infty.$$

(c) The functions V_{ij} are real-valued.

Define the matrices $\mathbf{S}$ and $\mathbf{T}_0$ by

$$\mathbf{S}=\int_{\mathbb{R}}\mathbf{V}(x)\,dx,\quad \mathbf{T}_0=-\frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}}\mathbf{V}(x)|x-y|\mathbf{V}(y)\,dydx. \tag{5.13}$$

We have the following result.

Theorem 5.9: *Let* $\mathbf{V}$ *obey Assumption 5.8 (a) and (b) and let* $\mathbf{H}(g)=\mathbf{H}_0+g\mathbf{V}(x)$ *be the self-adjoint Hamiltonian on* $L^2(\mathbb{R},\mathbb{C}^2)$ *defined in Proposition 3.1 by means of forms.*

(i) Assume that the matrix $\mathbf{S}$*, defined in (5.13), has n negative eigenvalues, denoted by* s_i*, with multiplicities* $\varkappa_i$*. Then, for a small enough* g*, the N-channel Hamiltonian* $\mathbf{H}(g)$ *has precisely* $\Sigma_{i=1}^{n}\varkappa_i$ *negative eigenvalues (taking into account multiplicity)* E_{ij} *satisfying the formulas*

$$(-E_{ij}(g))^{1/2}=-\frac{g}{2}s_i+\frac{g^2}{2}\langle\mathbf{v}_{ij},\mathbf{T}_0\mathbf{v}_{ij}\rangle_{\mathbb{C}^N}+O(g^3), \tag{5.14}$$

$$i=1,\ldots,n,\quad j=1,\ldots,\varkappa_i,$$

where $\mathbf{T}_0$ *is defined in (5.13) and* $\mathbf{v}_{ij}$ *are the eigenvectors corresponding to the eigenvalue* s_i *of* $\mathbf{S}$.

(ii) Suppose that $\mathbf{V}$ *obey Assumption 5.8(c) and that the matrix* $\mathbf{S}$ *has n nonpositive eigenvalues, denoted by* s_i*, with multiplicities* $\varkappa_i$*. If the eigenvectors* $\mathbf{v}_{0j}$*,* $j=1,\ldots,\varkappa_i$*, associated with the eigenvalue zero of* $\mathbf{S}$ *satisfy* $\langle\mathbf{v}_{0j},\mathbf{T}_0\mathbf{v}_{0j}\rangle_{\mathbb{C}^N}\neq 0$*, then the conclusion of part (i) remains valid.*

Proof: The proof is a straightforward generalization of the proof of Theorem 5.2. □

Remark 5.10: One of the referees pointed out that Theorem 5.9 was proven in Šeba.[29] Therein, however, Theorem 3 is incorrect because the quantity $\int_{\mathbb{R}}(1/p^2)(\mathbf{a}_0,\mathcal{F}(V)^2(p)\mathbf{a}_0)_n\,dp$ (in Šeba's notation) is not necessarily different from zero. Moreover, the Birman–Schwinger relation (in the matrix-valued setting) is stated without proof.

VI. PERTURBATION OF EMBEDDED EIGENVALUES

For the sake of completeness we consider perturbation of two-channel diagonal Hamiltonians with one-dimensional Schrödinger operators as component Hamiltonians, having eigenvalues embedded in its continuous spectrum.

A. Two-channel Hamiltonians

Consider the formal expression

$$\mathbf{H}(g)=\mathbf{H}(0)+g\mathbf{V}=\begin{pmatrix} H_{11} & 0 \\ 0 & H_{22} \end{pmatrix}+g\begin{pmatrix} V_{11}(x) & V_{12}(x) \\ V_{21}(x) & V_{22}(x) \end{pmatrix} \tag{6.1}$$

in $\mathcal{H}=L^2(\mathbb{R})\oplus L^2(\mathbb{R})$, where

$$H_{11}=-\frac{d^2}{dx^2}+W_{11}(x) \quad \text{and} \quad H_{22}=-\frac{d^2}{dx^2}+1+W_{22}(x). \tag{6.2}$$

We impose the following assumptions on the potentials W_{jj}, $j=1,2$.

Assumption 6.1: Suppose that the real-valued, measurable functions W_{jj}, $j=1,2$, satisfy the following.

(a) $W_{jj}\neq 0$.

(b) The bound

$$|W_{jj}(x)|\leqslant C\,(1+|x|^2)^{-1-\delta} \tag{6.3}$$

holds for some $C,\delta>0$ and all x.

(c) $\int_{\mathbb{R}} W_{jj}(x)\,dx\leqslant 0$.

(d) W_{jj} extends to a function analytic in the sector

$$\mathcal{A}_{\alpha_0}=\{\,z\in\mathbb{C}:|\arg z|\leqslant\alpha_0\,\}$$

for some $\alpha_0>0$. Moreover, the bound (6.3) holds in this sector.

Under Assumption 6.1(a)–(c) the operator $H_{11}=-d^2/dx^2+W_{11}(x)$ is self-adjoint in $L^2(\mathbb{R})$ and $\sigma(H_{11})=\sigma_d(H_{11})\cup\sigma_{\text{ess}}(H_{11})=\sigma_d(H_{11})\cup[0,\infty)$ with a nonempty discrete spectrum $\mu_1<\mu_2<\cdots<\mu_N<0$, which is simple and finite.[31] The corresponding normalized eigenfunctions ϕ_n, $n=1,2,\ldots,N$, are exponentially decaying. The analyticity requirement in Assumption 6.1(d) is convenient to adopt for analyzing the resonance behavior. Similarly, the operator $H_{22}=-d^2/dx^2+1+W_{22}(x)$ is self-adjoint in $L^2(\mathbb{R})$ and $\sigma(H_{22})=\sigma_d(H_{22})\cup\sigma_{\text{ess}}(H_{22})=\sigma_d(H_{22})\cup[1,\infty)$ with a nonempty discrete spectrum $\nu_1<\nu_2<\cdots<\nu_M<1$ which is simple and finite. The corresponding normalized eigenfunctions χ_m, $m=1,2,\ldots,M$, are exponentially decaying.

Consider the unperturbed Hamiltonian $\mathbf{H}(0)=\text{diag}\,(H_{11},H_{22})$. Assumption 6.1 ensures that

$$\sigma_c(\mathbf{H}(0))=\sigma_{\text{ess}}(\mathbf{H}(0))=\sigma_{\text{ess}}(H_{11})\cup\sigma_{\text{ess}}(H_{22})=[0,\infty)\cup[1,\infty)=[0,\infty).$$

Thus, the continuous spectrum of $\mathbf{H}(0)$ is the union of the two halflines starting at 0 and 1. This motivates the definition of the threshold set $\mathsf{T}=\{0,1\}$. Furthermore, $\sigma_p(\mathbf{H}(0))=\sigma_p(H_{11})\cup\sigma_p(H_{22})$. Among this (finite) set of eigenvalues, a (finite) subset is isolated or situated at the threshold 0, while the rest satisfying the condition $0<\nu_m<1$ is embedded in the continuous spectrum of $\mathbf{H}(0)$. For the sake of simplicity we make the following assumption.

Assumption 6.2: Suppose that none of the embedded eigenvalues ν_m of $\mathbf{H}(0)$ coincide with the threshold 0.

We impose the following conditions on the components of the perturbation $\mathbf{V}$.

Assumption 6.3: Suppose that the real-valued, measurable functions V_{ij}, $i,j=1,2$, satisfy the following.

(a) The bound

$$|V_{ij}(x)| \leqslant C\,(1+|x|^2)^{-1-\delta} \tag{6.4}$$

holds for some $C,\delta>0$ and all x.

(b) V_{ij} extends to a function analytic in the sector $\mathcal{A}_{\alpha_0}$ [see Assumption 6.1(d)] for some $\alpha_0>0$. Moreover, the bound (6.4) holds in this sector.

B. Complex dilation

We use a complex deformation. For θ real define S_θ on $L^2(\mathbb{R})$ by the unitary operator

$$(S_\theta\psi)=e^{\theta/2}\psi(e^\theta x),\quad \psi\in L^2(\mathbb{R}). \tag{6.5}$$

S_θ is a one-parameter unitary group on $L^2(\mathbb{R})$. It is easy to see that S_θ leave $\mathcal{D}(-d^2/dx^2)=H^2(\mathbb{R})$ invariant and that

$$H_{11,\theta}:=S_\theta H_{11}S_\theta^{-1}=-e^{-2\theta}\frac{d^2}{dx^2}+W_{11,\theta}(x)=-e^{-2\theta}\frac{d^2}{dx^2}+W_{11}(e^\theta x).$$

Let $\mathcal{A}_0=\{\theta:|\mathrm{Im}\,\theta|\leqslant\min\{\alpha_0,\pi/4\}$ [cf. Assumption 6.1(d)]. Under Assumption 6.1, $H_{11,\theta}$ obviously has a continuation to a type (A) family of m-sectorial operators analytic in the sense of Kato[13] for $\theta\in\mathcal{A}_0$. Likewise,

$$H_{22,\theta}:=S_\theta H_{22}S_\theta^{-1}=-e^{-2\theta}\frac{d^2}{dx^2}+1+W_{22,\theta}(x)=-e^{-2\theta}\frac{d^2}{dx^2}+1+W_{22}(e^\theta x)$$

has a continuation to a type (A) analytic family of operators on $\mathcal{A}_0$. From standard Aguilar–Combes theory[1] we determine the spectra of $H_{11,\theta}$ and $H_{22,\theta}$:

$$\sigma(H_{11,\theta})=\{\mu_1,\mu_2,\ldots,\mu_N\}\cup\{e^{-2\theta}\lambda:\lambda\in[0,\infty)\},$$

$$\sigma(H_{22,\theta})=\{\nu_1,\nu_2,\ldots,\nu_M\}\cup\{e^{-2\theta}\lambda+1:\lambda\in[0,\infty)\}.$$

Having extended S_θ in (6.5) analytically to $\mathcal{A}_0$ we may define

$$\mathbf{S}_\theta\Psi=\begin{pmatrix}S_\theta & 0\\ 0 & S_\theta\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix},\quad \Psi\in\mathcal{H}.$$

Due to its diagonal structure, the Hamiltonian

$$\mathbf{H}_\theta(0):=\mathbf{S}_\theta\mathbf{H}(0)\mathbf{S}_\theta^{-1}=\begin{pmatrix}H_{11,\theta} & 0\\ 0 & H_{22,\theta}\end{pmatrix}$$

has a continuation to a type (A) analytic family of operators in the sector $\mathcal{A}_0$. Furthermore,

$$\sigma(\mathbf{H}_\theta(0))=\sigma(H_{11,\theta})\cup\sigma(H_{22,\theta})=\{\mu_1,\mu_2,\ldots,\mu_N\}\cup\{\nu_1,\nu_2,\ldots,\nu_M\}\cup\{e^{-2\theta}\lambda:\lambda\in[0,\infty)\}\cup\{e^{-2\theta}\lambda+1:\lambda\in[0,\infty)\}.$$

In particular, the eigenvalues embedded in $\sigma(\mathbf{H}(0))$ are discrete eigenvalues of $\mathbf{H}_\theta(0)$ for θ nonreal.

Henceforth E_0 denotes any of the embedded eigenvalues ν_m of $\mathbf{H}(0)$. Let $\mathbf{R}_0(\theta;\zeta)$ denote the resolvent of $\mathbf{H}_\theta(0)$. Since E_0 is an isolated eigenvalue of $\mathbf{H}_\theta(0)$, we may choose a contour Γ

around E_0 such that Γ belongs to the resolvent set of $\mathbf{H}_\theta(0)$ and E_0 is the only eigenvalue of $\mathbf{H}_\theta(0)$ contained inside of Γ. Moreover, let $\mathbf{P}_\theta$ denote the eigenprojection associated with the eigenvalue E_0 and put

$$\mathbf{S}_\theta^{(p)} := \frac{1}{2\pi i}\int_\Gamma \frac{\mathbf{R}_0(\theta;\zeta)}{(E_0-\zeta)^p}\,d\zeta, \quad p \geqslant 1. \tag{6.6}$$

Then $\mathbf{P}_\theta = -\mathbf{S}_\theta^{(0)}$ and $\hat{\mathbf{R}}_0(\theta;\zeta) := \mathbf{S}_\theta^{(1)}$ is the reduced resolvent of $\mathbf{H}_\theta(0)$ at the point ζ. Define

$$\mathbf{V}_\theta = \mathbf{S}_\theta \mathbf{V} \mathbf{S}_\theta^{-1} = \begin{pmatrix} V_{11,\theta} & V_{12,\theta} \\ V_{21,\theta} & V_{22,\theta} \end{pmatrix} \quad \text{with} \quad V_{ij,\theta}(x) = V_{ij}(e^\theta x).$$

Then we have the following result.

Lemma 6.4: Let Assumptions 6.1 and 6.3 hold. Let Γ *be the contour described above and let* $\mathbf{S}_\theta^{(p)}$ *be defined in (6.6).*

(i) If $\operatorname{Im}\theta \in (0,\alpha_0)$ *then there exists a constant* $C_\theta > 0$ *such that*

$$\max_{\zeta\in\Gamma} \|g\mathbf{V}_\theta \mathbf{R}(\theta;\zeta)\| \leqslant C_\theta |g|. \tag{6.7}$$

If ζ *is replaced by* $\zeta_0 = \min\{\mu_1,\nu_1\} - 1$, *then the constant in (6.7) is independent of* θ *and the estimate holds for all* $|\operatorname{Im}\theta| < \alpha_0$.

(ii) For $p \geqslant 0$ *there exists a constant* $C_\theta > 0$ *such that*

$$\|g\mathbf{V}_\theta \mathbf{S}_\theta^{(p)}\| \leqslant C_\theta \frac{|\Gamma|}{2\pi} \frac{|g|}{[\operatorname{dist}(E_0,\Gamma)]^p}.$$

Proof: The contour Γ is by assumption contained in the resolvent of $\mathbf{H}_\theta(0)$. Since $\mathbf{R}_0(\theta;\cdot)$ is bounded and continuous and Γ is compact, there exists a constant $\tilde{C}_\theta$ such that $\max_{\zeta\in\Gamma}\|\mathbf{R}_0(\theta;\zeta)\| \leqslant \tilde{C}_\theta$.

Thus, $\max_{\zeta\in\Gamma}\|\mathbf{V}_\theta \mathbf{R}_0(\theta;\zeta)\| \leqslant \tilde{C}_\theta C_{\mathbf{V}}$, where $C_{\mathbf{V}}$ denotes a bound on the norm of $\mathbf{V}_\theta$, which is independent of θ by Assumption 6.3(b). This shows the first claim. Moreover, ζ_0 is to the left of the numerical range $\Theta(\mathbf{H}_\theta(0))$ of $\mathbf{H}_\theta(0)$ at the unit distance. Hence $\|\mathbf{R}_0(\theta;\zeta_0)\| = 1/[\operatorname{dist}(\zeta_0,\Theta(\mathbf{H}_\theta(0)))] = 1$. Therefore the constant $\tilde{C}_\theta$ in the above estimate may be replaced by 1. This verifies (i). The assertion (ii) follows immediately. □

Hence, provided g is small enough, it follows from Lemma 6.4(i) that $g\mathbf{V}_\theta$ is $\mathbf{H}_\theta(0)$-compact. The latter, in conjunction with Ref. 27, Lemma 1, p. 16, implies that the perturbed operators $\mathbf{H}_\theta(g) = \mathbf{H}_\theta(0) + g\mathbf{V}_\theta$ are a type (A) analytic family of operators for $\theta \in \mathcal{A}_0$ and suitable small g. Since E_0 is an isolated, simple eigenvalue of $\mathbf{H}_\theta(0)$, the analyticity of $\mathbf{H}_\theta(g)$ allows us to apply regular perturbation theory. The next section is devoted to this task.

C. Perturbation series and Fermi's golden rule

Following Kato (Ref. 13, Secs. II.2 and VII.1) and using Lemma 6.4 we infer that $\mathbf{H}_\theta(g)$ has an eigenvalue near E_0 given by a convergent power series in g. The convergent series is given by

$$E(g) = E_0 + \sum_{j=1}^{\infty} E_j(g), \tag{6.8}$$

where

$$E_j(g) = \sum_{p_1+\cdots+p_j=j-1} \frac{(-1)^j}{j} \operatorname{tr} \prod_{i=1}^{j} g\mathbf{V}_\theta \mathbf{S}_\theta^{(p_i)}. \tag{6.9}$$

In view of Lemma 6.4(ii), we see that $E_j(g)=O(g^j)$.

Let us compute the lowest-order terms of the series (6.8). Since Rank $\mathbf{P}_\theta=1$, $\mathbf{P}_\theta$ can be represented as

$$\mathbf{P}_\theta=\left\langle \cdot,\begin{pmatrix}0\\ \chi_m^\theta\end{pmatrix}\right\rangle\begin{pmatrix}0\\ \chi_m^\theta\end{pmatrix}$$

with $\chi_m^\theta:=S_\theta\chi_m$, where χ_m is the eigenfunction associated with the eigenvalue E_0 of H_{22}. Indeed, $H_{22,\theta}=\chi_m^\theta=S_\theta H_{22}S_\theta^{-1}S_\theta\chi_m=E_0S_\theta\chi_m=E_0\chi_m^\theta$ and, consequently,

$$\mathbf{H}_\theta(0)\begin{pmatrix}0\\ \chi_m^\theta\end{pmatrix}=\begin{pmatrix}H_{11,\theta}&0\\ 0&H_{22,\theta}\end{pmatrix}\begin{pmatrix}0\\ \chi_m^\theta\end{pmatrix}=E_0\begin{pmatrix}0\\ \chi_m^\theta\end{pmatrix}.$$

We compute $E_1(g)$:

$$E_1(g)=\mathrm{tr}(g\mathbf{V}_\theta\mathbf{P}_\theta)=g\left\langle\begin{pmatrix}0\\ \chi_m^\theta\end{pmatrix},\ \mathbf{V}_\theta\begin{pmatrix}0\\ \chi_m^\theta\end{pmatrix}\right\rangle_{\mathcal{H}}=g\left\langle\begin{pmatrix}0\\ \chi_m\end{pmatrix},\mathbf{V}\begin{pmatrix}0\\ \chi_m\end{pmatrix}\right\rangle_{\mathcal{H}}=g\langle\chi_m,V_{22}\chi_m\rangle_{L^2(\mathbb{R})}. \tag{6.10}$$

We see that the first-order term is real and does not contribute to the resonance width. Next, we consider $E_2(g)$. According to (6.9),

$$E_2(g)=-g^2\mathrm{tr}\,(\mathbf{P}_0\mathbf{V}_\theta\hat{\mathbf{R}}_0(\theta;E_0-i0)\mathbf{V}_\theta\mathbf{P}_0).$$

Due to the standard constancy-in-θ argument (see, e.g., Ref. 27, pp. 55–56), we may take the limit $\mathrm{Im}\,\theta\to0$ and in this way we arrive at

$$\begin{aligned}E_2(g)&=-g^2\mathrm{tr}\,(\mathbf{P}_0\mathbf{V}\hat{\mathbf{R}}_0(0;E_0-i0)\mathbf{V}\mathbf{P}_0)\\&=-g^2\left\langle\begin{pmatrix}0\\ \chi_m\end{pmatrix},\ \mathbf{V}\hat{\mathbf{R}}_0(0;E_0-i0)\mathbf{V}\begin{pmatrix}0\\ \chi_m\end{pmatrix}\right\rangle_{\mathcal{H}}\\&=-g^2\langle\chi_m,V_{21}[(H_{11}-E_0+i0)^{-1}]\hat{}\,V_{12}\chi_m\rangle_{L^2}-g^2\langle\chi_m,V_{22}[(H_{22}-E_0+i0)^{-1}]\hat{}\,V_{22}\chi_m\rangle_{L^2}\\&=-g^2\langle V_{12}\chi_m,[(H_{11}-E_0+i0)^{-1}]\hat{}\,V_{12}\chi_m\rangle_{L^2}-g^2\langle V_{22}\chi_m,[(H_{22}-E_0+i0)^{-1}]\hat{}\,V_{22}\chi_m\rangle_{L^2},\end{aligned} \tag{6.11}$$

where the notation $[(H_{jj}-E_0+i0)^{-1}]\hat{}$ refers to the reduced resolvent of H_{jj}, $j=1,2$.

We restrict our focus to the imaginary part of $E_2(g)$, which determines the resonance width to leading order. For this purpose we introduce

$$R_k=((-d^2/dx^2+W_{kk}(x)-E_0+\mathfrak{t}_k-i0)^{-1})\hat{}\,,\quad k=1,2,$$

where $\mathfrak{t}_1=0$ and $\mathfrak{t}_2=1$ are the thresholds. Clearly,

$$\mathrm{Im}\,E_2(g)=-g^2\sum_{k=1}^{2}\langle V_{k2}\chi_m(\mathrm{Im}\,R_k)V_{k2}\chi_m\rangle_{L^2(\mathbb{R})}. \tag{6.12}$$

Now, for $E>0$, the resolvent equation yields that

$$\mathrm{Im}\,(-d^2/dx^2+W_{kk}(x)-E-i0)^{-1}=t_k(E+i0)^*\mathrm{Im}\,(-d^2/dx^2-E-i0)^{-1}t_k(E+i0), \tag{6.13}$$

where

$$t_k(\zeta)=[I+|W_{kk}|^{1/2}(-\partial_x^2-\zeta)^{-1}|W_{kk}|^{1/2}\mathrm{Sgn}\,(W_{kk})]^{-1}.$$

The quantities $t_k(E+i0)$ are well-defined in view of Assumption 6.1. Furthermore, again for $E>0$,

$$\mathrm{Im}\,(-d^2/dx^2-E-i0)^{-1}=\frac{\pi}{2\sqrt{E}}\sum_{\sigma=\pm}(\gamma_E^\sigma)^*\gamma_E^\sigma, \tag{6.14}$$

where $\gamma_E^\sigma: H^1\to\mathbb{C}$ is the trace operator which acts on the first Sobolev space $H^1(\mathbb{R})$ as follows (see, e.g., Ref. 18, Sec. IV.1),

$$\gamma_E^\sigma\phi:=\hat{\phi}(\sigma\sqrt{E}),\quad \sigma=\pm,\quad E>0.$$

Here, as usual, $\hat{\phi}$ denotes the Fourier transform of ϕ. Using (6.13) and (6.14) we can rewrite the expression (6.12) in the following way:

$$\begin{aligned}
\mathrm{Im}\,E_2(g)&=-g^2\sum_{k=1}^{2}\langle V_{k2}\chi_m,(\mathrm{Im}\,R_k)V_{k2}\chi_m\rangle_{L^2}\\
&=-g^2\sum_{k=1}^{2}\langle V_{k2}\chi_m,t_k(E_0-\mathfrak{t}_k+i0)^*\\
&\quad\times\mathrm{Im}\,(-d^2/dx^2-E_0+\mathfrak{t}_k-i0)^{-1}t_k(E_0-\mathfrak{t}_k+i0)V_{k2}\chi_m\rangle_{L^2}\\
&=-g^2\sum_{k=1}^{2}\langle t_k(E_0-\mathfrak{t}_k+i0)V_{k2}\chi_m,\mathrm{Im}\,(-d^2/dx^2-E_0+\mathfrak{t}_k-i0)^{-1}\\
&\quad\times t_k(E_0-\mathfrak{t}_k+i0)V_{k2}\chi_m\rangle_{L^2}\\
&=-g^2\sum_{k=1}^{2}\sum_{\sigma=\pm}\frac{\pi}{2\sqrt{E_0-\mathfrak{t}_k}}\langle\gamma^\sigma_{E_0-\mathfrak{t}_k}t_k(E_0-\mathfrak{t}_k+i0)V_{k2}\chi_m,\gamma^\sigma_{E_0-\mathfrak{t}_k}\\
&\quad\times t_k(E_0-\mathfrak{t}_k+i0)V_{k2}\chi_m\rangle_{\mathbb{C}}\\
&=-g^2\sum_{k=1}^{2}\sum_{\sigma=\pm}\frac{\pi}{2\sqrt{E_0-\mathfrak{t}_k}}|\gamma^\sigma_{E_0-\mathfrak{t}_k}t_k(E_0-\mathfrak{t}_k+i0)V_{k2}\chi_m|^2.
\end{aligned}\tag{6.15}$$

In this way we have established the following result.

Theorem 6.5: *Let Assumptions 6.1 and 6.3 hold. Let ν_m be a simple eigenvalue of the operator H_{22} defined in (6.2) giving rise to the eigenvalue $E_0=\nu_m$ embedded in the continuous spectrum of $\mathbf{H}(0)$. Let E_0 satisfy Assumption 6.2. For a small enough coupling constant g, the eigenvalue E_0 of $\mathbf{H}(0)$ turns into a resonance, i.e., $E_0\notin\sigma(\mathbf{H}(g))$. The coordinates of its corresponding pole is given by (6.9)–(6.11). In particular, Fermi's golden rule takes the explicit form (6.15).*

Remark 6.6: If Assumption 6.2 is not fulfilled, i.e., we have an eigenvalue of H_{22} at the threshold point 0 of the continuous spectrum of $\mathbf{H}(0)$, complex dilation breaks down. An insight into this problem was established in Ref. 12. For abstract Hamiltonians $\mathbf{H}(g)$ having the structure found in (6.1), it was shown that under small off-diagonal perturbations this eigenvalue never moves into the continuous spectrum.

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Scattering into cones and flux across surfaces in quantum mechanics: A pathwise probabilistic approach

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We show how the scattering-into-cones and flux-across-surfaces theorems in quantum mechanics have very intuitive pathwise probabilistic versions based on some results by Carlen about large time behavior of paths of Nelson's diffusions. The quantum mechanical results can then be recovered by taking expectations in our pathwise statements. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The problem of finding the basic mathematical relationships between theoretical previsions and experimental observable quantities has been, for a long time, an open problem in quantum theory of scattering.

In this direction there exists two relevant theorems. The first one is due to Dollard (1969) and states that the probability of asympotically observing the particle in some cone $C\subset\mathbb{R}^3$ with vertex in the scattering center is equal to the probability of finding its asymptotic momentum exactly in the same cone, i.e.,

$$\lim_{t\uparrow\infty}\int_C \mathrm{d}x|\psi_t(x)|^2=\lim_{t\uparrow\infty}\int_{C\cap B_R^c}\mathrm{d}x|\psi_t(x)|^2=\int_C \mathrm{d}k\,|\hat{\psi}_{\mathrm{out}}(k)|^2, \tag{1.1}$$

where B_R^c is the complement of B_R, the ball of radius R, $\hat{\psi}_{\mathrm{out}}$ denotes the Fourier transform of the outgoing state $\psi_{\mathrm{out}}:=\Omega_+^*\psi_0$, Ω_+ being the wave operator. It is well known that the differential cross section for the time-independent scattering theory can be derived from the right-hand side of (1.1). Nevertheless the importance of (1.1) is primarily conceptual since the probability of observation which it refers to is a time-asymptotic one.

Instead, in the usual experimental situation, the detector being sufficiently far away from the scattering center, one actually measures the probability that the particle crosses the active surface of the detector $C\cap S_R$ (S_R denoting the sphere of radius R) at some random time. The theorem which takes care of this experimental setting is the so-called flux-across-surfaces theorem. It was conjectured in 1975 by Combes, Newton, and Shtokhamer under the form of the following relation:

$$\lim_{R\uparrow\infty}\int_{t_0}^{+\infty}\mathrm{d}t\int_{C\cap S_R} d\sigma(x)\,J^{\psi_t}(x)\cdot n(x)=\int_C \mathrm{d}k|\hat{\psi}_{\mathrm{out}}(k)|^2, \tag{1.2}$$

where $J^{\psi_t}:=\mathrm{Im}\,\psi_t^*\nabla\psi_t$ is the quantum probability current density, n denotes the outward unit normal vector along $C\cap S_R$, and σ is the surface measure.

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No rigorous proof of this conjecture was known until 1996 when Daumer, Dürr, Goldstein, and Zanghì proved the flux-across-surfaces theorem in the free case. Successively the result has been extended to the interacting case by Amrein and Zuleta (1997) and by Teufel, Dürr, and Münch-Berndl (1999) for short-range potentials, and by Amrein and Pearson (1997) for long-range potentials. The case with zero-energy resonances or eigenvalues has been treated by Dell'Antonio and Panati (2001) in and the case with a delta interaction by Panati and Teta (2000).

In view of our approach, the most interesting proof is the one given in Amrein and Pearson (1997). From such a paper one can extract the following clarifying scheme:

Integrating with respect to time the equation of continuity for quantum probability density

$$\frac{\partial}{\partial t}|\psi_t|^2+\nabla J^{\psi_t}=0 \tag{1.3}$$

and inserting the result into relation (1.1) given by Dollard's theorem one obtains

$$\int_C \mathrm{d}k|\hat{\psi}_{\mathrm{out}}(k)|^2=\int_{C\cap B_R^c}\mathrm{d}x|\psi_{t_0}(x)|^2-\lim_{t\uparrow\infty}\int_{t_0}^t \mathrm{d}s\int_{C\cap B_R^c}\mathrm{d}x\,\nabla J^{\psi_s}(x).$$

Then by taking the limit $R\uparrow\infty$ and by Gauss–Green divergence theorem one has

$$\int_C \mathrm{d}k|\hat{\psi}_{\mathrm{out}}(k)|^2=\lim_{R\uparrow\infty}\lim_{t\uparrow\infty}\int_{t_0}^t \mathrm{d}s\int_{(C\cap S_R)\cup(\partial C\cap B_R^c)}\mathrm{d}\sigma(x)\,n(x)\cdot J^{\psi_s}(x),$$

and so the flux-across-surfaces theorem is a consequence of the scattering-into-cones theorem plus the condition

$$\lim_{R\uparrow\infty}\lim_{t\uparrow\infty}\int_{t_0}^t \mathrm{d}s\int_{\partial C\cap B_R^c}\mathrm{d}\sigma(x)\,n(x)\cdot J^{\psi_s}(x)=0, \tag{1.4}$$

i.e., the flux across the lateral boundary of the cone asymptotically vanishes.

In this paper we give a pathwise formulation of scattering-into-cones and flux-across-surfaces theorems following in some way the pathwise analog of the above-given analytic argument. This has the advantage of giving a pictorial view of the scattering behavior. In doing that we exploit the relevant results, obtained by Carlen (1985), about potential scattering in stochastic mechanics.

It is known that stochastic mechanics, introduced by Nelson in 1966 [see also Nelson (1967) and (1985)], allows a pathwise approach to quantum mechanics by providing a suitable class of diffusion processes. Indeed to a solution ψ_t of the Schrödinger equation there is associated a well-defined (see Theorem 1) diffusion process X_t solution of the stochastic differential equation

$$\mathrm{d}X_t=b(t,X_t)\mathrm{d}t+dB_t,$$

where B_t is a Brownian motion and the drift vector field $b_t(x)\equiv b(t,x)$ is given by

$$b_t=|\psi_t|^{-2}(\nabla|\psi_t|^2+J^{\psi_t}).$$

Moreover the probability density of the process X_t is given by $|\psi_t|^2$ and it satisfies the continuity (or Fokker–Planck) equation (1.3). In connection with the problem of potential scattering, Carlen studied the time evolution of the process $(1/t)\,X_t$ proving the following (see Theorem 3).

(1) The scattering diffusions (i.e., the ones associated with the scattering states of the corresponding Schrödinger equation) are such that the limit

$$\lim_{t\uparrow\infty}\frac{1}{t}X_t=p_+$$

exists almost surely.

(2) The random variable p_+ is square integrable and has the same distribution as does the quantum mechanical final momentum.

These facts imply that almost surely the diffusion paths are definitively inside or outside the cone C, a pathwise analog of (1.4). Then the following pathwise version of Dollard's theorem immediately follows:

$$\lim_{t\uparrow\infty}\chi_C(X_t)=\lim_{t\uparrow\infty}\chi_{C\cap B_R^c}(X_t)=\chi_C(p_+),$$

χ_D denoting the characteristic function of the set D; the usual quantum mechanical version is then obtained by taking expectations (see Theorems 4 and 5).

As regards the flux-across-surfaces theorem the situation is almost equally simple. If $N_{C\cap S_R}$ were finite, where

$$N_{C\cap S_R}:=N^+_{C\cap S_R}-N^-_{C\cap S_R},$$

$N^+_{C\cap S_R}(\gamma)$ [respectively, $N^-_{C\cap S_R}(\gamma)$] denoting the number of outward (respectively, inward) crossing by the path $t\mapsto\gamma(t)$ of $C\cap S_R$, then, again by (1) and (2) noted previously, one would obtain the following pathwise version of the flux-across-surfaces theorem:

$$\lim_{R\uparrow\infty}N_{C\cap S_R}=\chi_C(p_+). \tag{1.5}$$

Let us remark here that the relevance of $N_{C\cap S_R}$ for the flux-across-surfaces theorem was already pointed out (in the framework of Bohmian mechanics) in Daumer *et al.* (1997). The problem here is that almost surely the diffusion X_t intersects $C\cap S_R$ on a set of times that has no isolated point and is uncountable. Therefore the above-given definition of $N_{C\cap S_R}$ makes no sense in general. However, by a suitable redefinition of $N_{C\cap S_R}$ as the total mass of an almost surely compactly supported random distribution (see Sec. III for details), (1.5) can be made rigorous (see Theorem 6). After showing (see Theorem 7) how to explicitly compute, by using the continuity equation (1.3), the expectation of $N_{C\cap S_R}$ in terms of the quantum probability current density J^{ψ_t}, the flux-across-surfaces theorem then follows by taking expectation in (1.5) (see Theorem 9).

In our opinion these results show how the probabilistic approach we use is very fruitful and extremely intuitive from the physical point of view.

As regards the analytical hypotheses we impose, our proofs of the pathwise results need, beside the existence of the asymptotic velocity (see Hypotheses 3 and 4 in definition 2), the following condition on the quantum evolution:

$$\int_{t_0}^{+\infty}\frac{\mathrm{d}t}{t}\left\|\left(P-\frac{Q}{t}\right)\psi_t\right\|_{L^2}<+\infty,\quad t_0>0, \tag{1.6}$$

where $P\psi(x):=-i\nabla\psi(x)$ and $Q\psi(x)=x\phi(x)$ denote the usual momentum and position operators of quantum mechanics in Schrödinger representation. Let us remark that the original results by Carlen were obtained by requiring the existence and completeness of wave operators, which is a hypothesis stronger than our Hypotheses 3 and 4. It is not clear to us if our weaker hypotheses together with (1.6) in any case imply the existence and completeness of wave operators. Therefore it could be interesting to find examples (if any) of cases in which the pathwise scattering-into-cones and flux-across-surfaces theorems hold true notwithstanding there are no wave operators.

In order to obtain then the quantum mechanical results by taking expectations, (1.6) is still sufficient to get Dollard's theorem, whereas the flux-across-surfaces theorem requires that the property of paths being definitively always inside or outside cone C holds not only pathwise but in the mean, i.e, as we already know, (1.4) must be true. This condition is a consequence of

$$\int_{t_0}^{+\infty} \mathrm{d}t \, \| \theta(Q) \psi_t \|_{H^1} \left\| \left(P - \frac{Q}{t} \right) \psi_t \right\|_{H^1} < +\infty, \tag{1.7}$$

where $\theta \in C_b^2(\mathbb{R}^3;\mathbb{C})$, $\theta = 1$ on a neighborhood of $\partial C \cap B_R^c$ for some $R>0$, and $H^s(\mathbb{R}^3)$ denotes the Sobolev space of tempered distributions with a Fourier transform which is integrable with respect to the measure with density $(1+|x|^2)^s$.

Conditions (1.6) and (1.7) both follow from propagation estimates on ψ_t. This is a well-known topic in mathematical physics and much literature exists on them. Thus by using known results on time-decay of the solutions of the Schrödinger equation it is possible to deduce (1.6) and (1.7) from explicit conditions imposed on the initial state ψ_0 and on the potential V, which are the natural prescriptions for a physicist. In particular, beside some technical condition on the initial state ψ_0, (1.6) holds true with potential functions decaying at infinity like $\|x\|^{-\epsilon}$, $\epsilon>0$, whereas (1.7) requires potentials decaying faster that $\|x\|^{-2/3}$ (see Sec. V for more details). These conditions on ψ_0 and V also lead to the existence and completeness of (modified) wave operators.

Our probabilistic proof remains unchanged in the case of the presence either of a time-dependent potential or of a magnetic field, the only difference being, if A denotes the magnetic potential, the replacement of P by $P-A$ and of J^{ψ_t} by $J^{\psi_t} - |\psi_t|^2 A$. We plan to work out the details in a future work.

Finally let us remark that all our results hold true every time we can find a stochastic process X_t having $|\psi_t|^2$ as its density and for which Theorem 3 can be proven. By Theorem 1 we realized such a process as a Nelson diffusion, but this is not the only possible choice. Another one is given by Bohmian mechanics (see Durr, Goldstein, and Zanghì (1992) for a thorough introduction to the subject], where one considers the stochastic process $\tilde{X}_t$, solution of the ordinary differential equation $(\mathrm{d}/\mathrm{d}t)\, \tilde{X}_t = |\psi_t(\tilde{X}_t)|^{-2} J^{\psi_t}(\tilde{X}_t)$ with a random initial condition with density $|\psi_0|^2$. Also in this case, under the same hypotheses plus the technical condition $\psi_{t_0} \in C^\infty(\mathbb{R}^3)$ [the Bohmian analog of Theorem 1, see Berndl *et al.* (1995), needs more regularity], Theorem 3 holds true, the proof being essentially the same, and so all our results can be stated in a Bohmian context. We decided to work with Nelson's stochastic mechanics since it does not necessarily need the Schrödinger equation in its formulation. Indeed it can be derived either from a stochastic analog of Newton's law [see Nelson (1966, 1967)] or from a stochastic variational principle [see Guerra and Morato (1983); Nelson (1985)].

II. POTENTIAL SCATTERING IN STOCHASTIC MECHANICS

At first let us recall that, by Nelson's stochastic mechanics [see Nelson (1966, 1967, 1985)], it is possible to associate to a solution ψ_t of the Schrödinger equation a diffusion process which has $|\psi_t|^2$ as its density. More precisely one has the following [in Carlen (1984) V is a Rellich-class potential but the results obtained there can be extended to the more general potentials used here by proceeding as in Dell'Antonio and Posilicano (1991), Theorem 2.1]:

Theorem 1: *Let $V = V_1 + V_2$, with V_1 bounded from below and V_2 $(-\Delta)$-form-bounded with relative bound smaller than one. Let $H = -\frac{1}{2}\Delta + V$ be defined as a sum of quadratic forms, and let ψ_0 be a normalized state in its form domain $\mathcal{Q}(H) = H^1(\mathbb{R}^3) \cap \mathcal{Q}(V_1)$. If $\psi_t := e^{-itH}\psi_0$, then define*

$$b(t,x) := b_t(x), \quad b_t := |\psi_t|^{-2}(\nabla |\psi_t|^2 + J^{\psi_t}).$$

Consider the measurable space $(\Omega,\mathcal{F})$, with $\Omega = C([t_0,+\infty);\mathbb{R}^d)$, $t_0 \geqslant 0$, $\mathcal{F}$ the Borel σ-algebra, and let $(\Omega,\mathcal{F},\mathcal{F}_t,X_t)$ be the evaluation stochastic process $X_t(\gamma) := \gamma(t)$, with $\mathcal{F}_t = \sigma(X_s, t_0 \leqslant s \leqslant t)$ the natural filtration. Then there exists a unique Borel probability measure $\mathbb{P}$ on $(\Omega,\mathcal{F})$ such that:

(a) $(\Omega,\mathcal{F},\mathcal{F}_t,X_t,\mathbb{P})$ is a Markov process;
(b) the image of $\mathbb{P}$ under X_t has density $|\psi_t|^2$;

(c) $B_t := X_t - X_{t_0} - \int_{t_0}^t \mathrm{d}s\, b(s,X_s)$ *is a* $(\mathbb{P},\mathcal{F}_t)$*-Brownian motion, i.e.,* $\mathbb{P}$ *is a weak solution of the stochastic differential equation* $\mathrm{d}X_t = b(t,X_t)\,\mathrm{d}t + \mathrm{d}B_t$ with initial density $|\psi_{t_0}|^2$.

From now on we will assume $t_0 > 0$ and $d = 3$.

Definition 2: With the same notation and hypotheses as in Theorem 1, let us call the couple (ψ_0, V) *weakly admissible* if

Hypothesis 1: ψ_0 is in $\mathcal{H}_c$, the spectral subspace corresponding to the continuous spectrum of H.

Hypothesis 2:

$$\int_{t_0}^{+\infty} \frac{\mathrm{d}t}{t} \left\| \left(P - \frac{Q}{t} \right) \psi_t \right\|_{L^2} < +\infty.$$

Hypothesis 3: The asymptotic velocity exists in the following sense:

$$\forall\, g \in C_c^\infty(\mathbb{R}^3), \quad \text{w-}\lim_{t\uparrow\infty} \Pi_c\, e^{itH}\, g\left(\frac{Q}{t}\right) e^{-itH} \Pi_c = \Pi_c\, g(P_+)\, \Pi_c,$$

where w-lim means the limit in the weak operator norm topology, Π_c denotes the projection onto $\mathcal{H}_c$, and P_+ is a vector of commuting self-adjoint operators;

A weakly admissible couple (ψ_0, V) is then called *admissible* if:

Hypothesis 4: ψ_0 is in the spectral subspace corresponding to the absolutely continuous spectrum of P_+.

Remark: If the (modified) wave operators $\Omega_\pm$ exist and are complete then

$$P_+ \Pi_c = \Omega_+ P \Omega_+^* \Pi_c$$

and, given $\psi_0 \in \mathcal{H}_c$,

$$\langle \psi_0, \chi_A(P_+)\psi_0 \rangle = \langle \psi_0, \Omega_+ \chi_A(P) \Omega_+^* \psi_0 \rangle = \int_A |\hat{\psi}_{\text{out}}(k)|^2\, \mathrm{d}k.$$

Thus in this case Hypothesis 4 holds true for all $\psi_0 \in \mathcal{H}_c$. Therefore Hypothesis 3 and 4 can be interpreted as a weaker substitute for existence and completeness of wave operators.

For explicit conditions on ψ_0 and V ensuring admissibility the reader is referred to Sec. V.

The above-given definitions permit us to extend (with the same proof) Carlen's results [see Carlen (1985), the free case $V = 0$ was already studied in Shucker (1980)] to the case where the hypothesis of existence of the wave operators is replaced by the weaker Hypothesis 3.

Theorem 3: *Let* (ψ_0, V) *be weakly admissible and let* $(\Omega, \mathcal{F}, \mathcal{F}_t, X_t, \mathbb{P})$ *be as in Theorem 1. Then*

$$\lim_{t\uparrow\infty} \frac{1}{t} X_t = p_+, \quad \mathbb{P}\text{-a.s.}, \tag{2.1}$$

for some random variable p_+. *Moreover* p_+ *is* $\mathbb{P}$*-square integrable and it has, under* $\mathbb{P}$*, the same distribution as does the quantum mechanical final momentum* P_+*, i.e., for every Borel set A one has*

$$\mathbb{E}(\chi_A(p_+)) = \langle \psi_0, \chi_A(P_+)\psi_0 \rangle,$$

where $\mathbb{E}$ *denotes expectation with respect to* $\mathbb{P}$.

Proof: The existence of the limit $\lim_{t\uparrow\infty}(1/t)\, X_t$ is proven in Carlen (1985), lemma 1. For the convenience of the reader we reproduce here the main steps of such a proof. Defining the stochastic process $\pi_t := (1/t)\, X_t$, one has the following stochastic differential equation:

$$\mathrm{d}\pi_t=\frac{1}{t}(b(t,X_t)-\pi_t)\,\mathrm{d}t+\frac{1}{t}\mathrm{d}B_t\,.$$

This implies

$$\mathbb{P}\left(\sup_{t>T}\|\pi_t-\pi_T\|>\epsilon\right)\leqslant\mathbb{P}\left(\int_T^{+\infty}\frac{\mathrm{d}t}{t}\|(b(t,X_t)-\pi_t)\|>\epsilon\right)+\mathbb{P}\left(\sup_{t>T}\left\|\int_T^t\frac{1}{t}\mathrm{d}B_t\right\|>\epsilon\right).$$

By Doob's martingale maximal inequality and the Chebychev inequality the second term on the right-hand side can be estimated by $2\epsilon^{-2}T^{-1}$. As regards the first term, by the definition of b one has

$$\begin{aligned}\mathbb{P}\left(\int_T^{+\infty}\frac{1}{t}\|(b(t,X_t)-\pi_t)\|\mathrm{d}t>\epsilon\right)&\leqslant\frac{1}{\epsilon}\int_T^{+\infty}\frac{1}{t}\mathbb{E}(\|(b(t,X_t)-\pi_t)\|)\,\mathrm{d}t\\&\leqslant\frac{1}{\epsilon}\int_T^{+\infty}\frac{1}{t}\mathbb{E}(\|(b(t,X_t)-\pi_t)\|^2)^{1/2}\,\mathrm{d}t\\&\leqslant\frac{\sqrt{2}}{\epsilon}\int_T^{+\infty}\left\|\left(-P-\frac{Q}{t}\right)\psi_t\right\|_{L^2}\frac{\mathrm{d}t}{t}.\end{aligned}$$

The above-given estimates and Hypothesis 2 say that we can find a T_n large enough that

$$\mathbb{P}\left(\bigcup_{s,t>T_n}\left\{\left\|\pi_t-\pi_s\right\|>\frac{1}{n}\right\}\right)<\frac{1}{2^n}.$$

Then, by the Borel–Cantelli lemma, one has

$$\mathbb{P}\left(\bigcap_{m=1}^{\infty}\bigcap_{n>m}\bigcup_{s,t>T_n}\left\{\left\|\pi_t-\pi_s\right\|>\frac{1}{n}\right\}\right)=0,$$

which exactly means that $\lim_{t\uparrow\infty}\pi_t$ exists $\mathbb{P}$-a.s.

By a density argument p_+ has the same distribution as does the quantum mechanical final momentum P_+ if $\mathbb{E}(g(p_+))=\langle\psi_0,g(P_+)\psi_0\rangle$ for all $g\in C_c^\infty(\mathbb{R}^3)$. By Hypothesis 3 there follows

$$\mathbb{E}(g(p_+))=\lim_{t\uparrow\infty}\mathbb{E}(g(\pi_t))=\lim_{t\uparrow\infty}\langle\psi_t,g(Q/t)\psi_t\rangle=\langle\psi_0,g(P_+)\psi_0\rangle,$$

and the proof is done. □

Remark: The proof of the above-given theorem shows that

$$\text{Hypothesis } 2\Rightarrow\frac{1}{t}X_t\to p_+ \quad \text{almost surely,}$$

$$\text{Hypothesis } 3\Leftrightarrow\frac{1}{t}X_t\to p_+ \quad \text{in distribution.}$$

Remark: Under the stronger Hypothesis 2.1

$$\int_{t_0}^{+\infty}\left\|\left(P-\frac{Q}{t}\right)\psi_t\right\|_{L^2}^2\mathrm{d}t<+\infty$$

it is possible to prove [see Carlen (1986)] that the random variable p_+ generates the tail σ-algebra

$$\mathcal{T}:=\bigcap_{t>t_0}\sigma(X_s,\ s\geqslant t).$$

This is the probabilistic analog of the fact that in quantum mechanics the only scattering observables are functions of the final momentum P_+. However we will not need such a nice result here.

Under Hypothesis 2.1, according to Carlen (1986), the proof of Theorem 3 becomes simpler:

Let $\widetilde{\mathbb{P}}$ be the weak solution of the simple stochastic differential equation

$$\mathrm{d}X_t=\frac{1}{t}X_t\,\mathrm{d}t+\mathrm{d}\widetilde{B}_t.$$

Therefore

$$\mathrm{d}\left(\frac{1}{t}X_t\right)=-\frac{1}{t^2}X_t\,\mathrm{d}t+\frac{1}{t}\mathrm{d}X_t=\frac{1}{t}\widetilde{B}_t$$

and so

$$\frac{1}{t}X_t=\frac{1}{t_0}X_{t_0}+\int_{t_0}^{t}\frac{1}{s}\mathrm{d}\widetilde{B}_s.$$

Since

$$\widetilde{\mathbb{E}}\left(\int_{t_0}^{+\infty}\frac{1}{s}\mathrm{d}\widetilde{B}_s\right)^2=\int_{t_0}^{+\infty}\frac{\mathrm{d}s}{s^2}<+\infty,$$

by Doob's martingale convergence theorem one gets $\widetilde{\mathbb{P}}$-a.s. convergence of $(1/t)\ X_t$. Thus the proof of Theorem 3 is then concluded by observing that Hypothesis 2.1 implies

$$\mathbb{E}\left(\int_{t_0}^{+\infty}\mathrm{d}t\|b(t,X_t)-X_t/t\|^2\right)<+\infty$$

and so, by Ershov (1972)—Proposition 2.11, $\mathbb{P}$ is absolutely continuous with respect to $\widetilde{\mathbb{P}}$.

III. THE PATHWISE SCATTERING-INTO-CONES AND FLUX-ACROSS-SURFACES THEOREMS

From now on by an open cone C we will mean a set of the kind

$$\{\lambda x\in\mathbb{R}^3\ :\ x\in\Sigma,\ \lambda>0\},$$

where Σ is an open subset of the unit sphere with $\partial\Sigma$ a finite union of C^1 manifolds.

In the framework of stochastic mechanics, thanks to Theorem 3, the pathwise version of Dollard's scattering-into-cones theorem [see Dollard (1969)] is obvious:

Theorem 4: *Let (ψ_0,V) be admissible and let $(\Omega,\mathcal{F},\mathcal{F}_t,X_t,\mathbb{P})$ be as in Theorem 1. Then for every open cone C and for every ball B_R of radius R one has*

$$\lim_{t\uparrow\infty}\chi_{C\cap B_R^c}(X_t)=\lim_{t\uparrow\infty}\chi_C(X_t)=\chi_C(p_+),\quad \mathbb{P}\text{-a.s.}$$

Proof: By Theorem 3 and Hypothesis 4 $p_+\notin\partial C$, $\mathbb{P}$-a.s.. Thus by (2.1) X_t is $\mathbb{P}$-a.s. definitively either in C or in $\overline{C}^c$ for every open cone C. Moreover, by (2.1) again, being $p_+\neq 0$ $\mathbb{P}$-a.s. by Hypothesis 4, we have

$$\lim_{t\uparrow\infty}\|X_t\|=+\infty,\quad \mathbb{P}\text{-a.s.} \tag{3.1}$$

Therefore

$$\lim_{t\uparrow\infty}\chi_{C\cap B_R^c}(X_t)=\lim_{t\uparrow\infty}\chi_C(X_t)=\lim_{t\uparrow\infty}\chi_C\left(\frac{1}{t}X_t\right)=\chi_C(p_+),\quad \mathbb{P}\text{-a.s.}$$

□

Let us now come to the flux-across-surfaces theorem.
We would like to define the function

$$N_{C\cap S_R}(\gamma):=N^+_{C\cap S_R}(\gamma)-N^-_{C\cap S_R}(\gamma),$$

where $N^+_{C\cap S_R}(\gamma)$ [respectively, $N^-_{C\cap S_R}(\gamma)$] denotes the number of outward (respectively, inward) crossing by $[t_0,+\infty)\ni t\mapsto\gamma(t)$ of $C\cap S_R$, the intersection of the cone C with S_R, the sphere of radius R. The problem is that the above-given definition makes no sense since $\mathbb{P}$-a.s. the set $\{t:X_t\in C\cap S_R\}$ has no isolated point and is uncountable. Therefore we are forced to proceed in an alternative way:

Let us observe that if $\#\{t:\gamma(t)\in C\cap S_R\}<+\infty$ then $N_{C\cap S_R}(\gamma)$ is the total mass of the random distribution

$$\sum_{t\in\{s:\gamma(s)\in C\cap S_R\}}c(t)\,\delta_t,$$

where $c(t)=+1$ if t corresponds to an outward crossing and $c(t)=-1$ if t corresponds to an inward crossing. Since $t\mapsto\gamma(t)$ is definitively either in C or in $\overline{C^c}$ by Hypothesis 4 and (2.1), if R is sufficiently large (then we will consider the limit $R\uparrow\infty$) one has

$$\sum_{t\in\{s:\gamma(s)\in C\cap S_R\}}c(t)\,\delta_t=\sum_{t\in\{s:\gamma(s)\in(C\cap S_R)\cup(\partial C\cap B_R^c)\}}c(t)\,\delta_t=\frac{\mathrm{d}}{\mathrm{d}t}\chi_{C\cap\overline{B_R^c}}(\gamma(t)),$$

where the derivative has to be intended in distributional sense. The advantage of this rewriting is that for every path γ the distribution $(\mathrm{d}/\mathrm{d}t)\chi_{C\cap\overline{B_R^c}}(\gamma(t))$ is well defined.

Definition: Given an open domain D, we define the random distribution

$$\mu_D:\Omega\to\mathcal{D}'(\mathbb{R})$$

by

$$\mu_D(\gamma):=\frac{\mathrm{d}}{\mathrm{d}t}\chi_D(\tilde\gamma(t)),\quad \tilde\gamma(t):=\begin{cases}\gamma(t) & \text{for } t\geqslant t_0\\ \gamma(t_0) & \text{for } t<t_0,\end{cases}$$

i.e., for every test function $\phi\in\mathcal{D}(\mathbb{R})\equiv C_c^\infty(\mathbb{R})$,

$$\langle\mu_D(\gamma),\phi\rangle:=-\chi_D(\gamma(t_0))\,\phi(t_0)-\int_{t_0}^{+\infty}\mathrm{d}t\,\chi_D(\gamma(t))\,\dot\phi(t).$$

Note that $\mathrm{supp}[\mu_D(\gamma)]=\gamma^{-1}(\partial D)$. In the case $\mu_D(\gamma)\in\mathcal{E}'(\mathbb{R})$, i.e., it has compact support, we define as usual its mass by

$$M_D(\gamma):=\langle\mu_D(\gamma),\phi_\gamma\rangle,$$

where ϕ_γ is a test function such that $\phi_\gamma=1$ on a neighborhood of $\mathrm{supp}[\mu_D(\gamma)]$.

By the previous definition and by Theorem 3 we then have the following pathwise version of the flux-across-surfaces theorem:

Theorem 5: *Let* (ψ_0,V) *be admissible and let* $(\Omega,\mathcal{F},\mathcal{F}_t,X_t,\mathbb{P})$ *be as in Theorem 1. Then*

$$\mu_{C\cap\overline{B_R^c}}\in\mathcal{E}'(\mathbb{R}),\quad \mathbb{P}\text{-}a.s.$$

and, defining $N_{C\cap S_R}:=M_{C\cap\overline{B_R^c}}$, *one has*

$$\lim_{R\uparrow\infty} N_{C\cap S_R}=\chi_C(p_+),\quad \mathbb{P}\text{-}a.s.$$

Proof: Let

$$\tau_R(\gamma):=\sup\{t\in\mathbb{R}:X_t(\gamma)\in\partial(C\cap\overline{B_R^c})\}.$$

By (3.1) and since X_t is $\mathbb{P}$-a.s. definitively either in C or in $\overline{C^c}$ by Hypothesis 4 and Theorem 3, one has $\tau_R<+\infty$, $\mathbb{P}$-a.s. Thus $\mu_{C\cap\overline{B_R^c}}\in\mathcal{E}'(\mathbb{R})$, $\mathbb{P}$-$a.s.$, being $\mathrm{supp}[\mu_{C\cap\overline{B_R^c}}]\subseteq[t_0,\tau_R(\gamma)]$.

Let $\phi_\gamma\in\mathcal{D}(\mathbb{R})$ such that $\phi_\gamma=1$ on a neighborhood of $[t_0,\tau_R(\gamma)]$. By the definition of $\mu_{C\cap\overline{B_R^c}}$ one has

$$\begin{aligned}\langle\mu_{C\cap\overline{B_R^c}}(\gamma),\phi_\gamma\rangle&=-\chi_{C\cap\overline{B_R^c}}(\gamma(t_0))-\chi_C(p_+(\gamma))\int_{\tau_R(\gamma)}^{+\infty}\mathrm{d}t\,\dot\phi_\gamma(t)\\&=-\chi_{C\cap\overline{B_R^c}}(\gamma(t_0))+\chi_C(p_+(\gamma)),\end{aligned}$$

and the thesis then immediately follows by taking the limit $R\uparrow\infty$. □

IV. THE SCATTERING-INTO-CONES AND FLUX-ACROSS-SURFACES THEOREMS IN QUANTUM MECHANICS

By taking expectations in Theorem 4 and by dominated convergence theorem one immediately obtains Dollard's theorem:

Theorem 6: *For every open cone* C, *every ball* B_R *of radius* R, *and for every admissible couple* (ψ_0,V), *one has*

$$\lim_{t\uparrow\infty}\int_{C\cap B_R^c}\mathrm{d}x|\psi_t(x)|^2=\lim_{t\uparrow\infty}\int_C\mathrm{d}x|\psi_t(x)|^2=\langle\psi_0,\chi_C(P_+)\psi_0\rangle.$$

In order to prove the flux-across-surfaces theorem we need now to compute the expectation of $\mu_{C\cap\overline{B_R^c}}$. To this end we state the following:

Theorem 7: *Let* ψ_t *and* $\mathbb{P}$ *be as in Theorem 1, with* $\psi_0\in H^2(\mathbb{R}^3)$ *and* V *a* $(-\Delta)$*-operator-bounded potential, with relative bound smaller than one. For every open domain* D, *with* ∂D *a finite union of* C^1 *manifolds, and for every test function* ϕ *one has*

$$\mathbb{E}(\langle\mu_D,\phi\rangle)=-\int_{t_0}^{+\infty}\mathrm{d}t\,\phi(t)\int_{\partial D}\mathrm{d}\sigma(x)\,J^{\psi_t}(x)\cdot n(x),$$

where n *denotes the outward unit normal vector along* ∂D *and* σ *is the surface measure.*

Proof: Since $|\psi_t|^2$ is the density of X_t under $\mathbb{P}$,

$$\mathbb{E}\langle\mu_D,\phi\rangle=-\phi(t_0)\int_D\mathrm{d}x|\psi_{t_0}(x)|^2-\int_{t_0}^{+\infty}\mathrm{d}t\,\dot\phi(t)\int_D\mathrm{d}x|\psi(t,x)|^2.$$

Since ψ_t solves the Schrödinger equation, one has [see, e.g., Carlen (1984)] for all $f \in C_b^1(\mathbb{R}^3)$ and for a.e. t, the continuity equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^3} \mathrm{d}x\, |\psi_t(x)|^2 f(x) = \int_{\mathbb{R}^3} \mathrm{d}x\, J^{\psi_t}(x)\cdot \nabla f(x).$$

Since $\psi_t \in H^2(\mathbb{R}^3)$ by our hypotheses on ψ_0 and V, ∇J^{ψ_t} is an integrable function. Therefore one has, integrating by parts, for all $f \in C_b^1(\mathbb{R}^3)$,

$$\int_{t_0}^{+\infty} \mathrm{d}t\, \dot{\phi}(t) \int_{\mathbb{R}^3} \mathrm{d}x\, |\psi_t(x)|^2 f(x) = -\phi(t_0)\int_{\mathbb{R}^3} \mathrm{d}x\, |\psi_{t_0}(x)|^2 f(x) + \int_{t_0}^{+\infty} \mathrm{d}t\, \phi(t) \int_{\mathbb{R}^3} \mathrm{d}x\, \nabla J^{\psi_t}(x) f(x).$$

Taking now a uniformly bounded sequence $\{f_n\}_1^\infty \subset C_b^1(\mathbb{R}^3)$, pointwise converging to χ_D, by the dominated convergence theorem one obtains

$$\int_{t_0}^{+\infty} \mathrm{d}t\, \dot{\phi}(t) \int_{D} \mathrm{d}x\, |\psi_t(x)|^2 = -\phi(t_0)\int_{D} \mathrm{d}x\, |\psi_{t_0}(x)|^2 + \int_{t_0}^{+\infty} \mathrm{d}t\, \phi(t) \int_{D} \mathrm{d}x\, \nabla J^{\psi_t}(x).$$

Since $\psi_t \in H^2(\mathbb{R}^3)$, one has $\nabla \psi_t \in H^1(\mathbb{R}^3)$, so that both ψ_t and $\nabla \psi_t$ have traces in $L^2(\partial D)$ [see, e.g., Burenkov (1998)]. Thus J^{ψ_t} has a trace in $L^1(\partial D)$ by

$$\|J^{\psi_t}\|_{L^1(\partial D)} \leqslant \|\psi_t\|_{L^2(\partial D)} \|\nabla \psi_t\|_{L^2(\partial D)} \leqslant c\, \|\psi_t\|_{H^1(D)} \|\nabla \psi_t\|_{H^1(D)},$$

and the proof is then concluded by the Gauss–Green theorem. □

Definition 8: The admissible couple (ψ_0, V) is said to be *strongly admissible* if

Hypothesis 5: $\psi_0 \in H^2(\mathbb{R}^3)$, V is a $(-\Delta)$-operator-bounded potential and

$$\int_{t_0}^{\infty} \mathrm{d}t \| \theta(Q)\psi_t\|_{H^1} \left\| \left(P - \frac{Q}{t} \right) \psi_t \right\|_{H^1} < +\infty$$

where $\theta \in C_b^2(\mathbb{R}^3;\mathbb{C})$ such that $\theta = 1$ on a neighborhood of $\partial C \cap B_R^c$ for some $R > 0$.

In the next section we will give explicit conditions on ψ_0 and V ensuring strong admissibility.

By combining Theorems 5 and 7 the flux-across-surfaces theorem now follows:

Theorem 9: *For every open cone C and for every strongly admissible couple (ψ_0, V) one has*

$$\lim_{R\uparrow\infty} \lim_{T\uparrow\infty} \int_{t_0}^{T} \mathrm{d}t \int_{C\cap S_R} \mathrm{d}\sigma(x)\, J^{\psi_t}(x)\cdot n(x) = \langle \psi_0, \chi_C(P_+)\psi_0 \rangle.$$

Proof: By pointwise approximating, on the compact interval $[t_0, \tau_R(\gamma)]$, $t \mapsto \gamma(t)$ with a sequence of polynomials paths, the wildly oscillating function $t \mapsto \chi_{C\cap \overline{B}_R^c}(\gamma(t))$ can be pointwise approximated with a sequence $\{\chi_n\}_1^\infty$ of characteristic functions of finite unions $\cup_{k=0}^{m(n)} [s_k^{(n)}, t_k^{(n)}]$ of disjoint intervals. Therefore one obtains

$$\begin{aligned} |\langle \mu_{C\cap \overline{B}_R^c}(\gamma), \phi \rangle| &\leqslant \chi_{C\cap \overline{B}_R^c}(\gamma(t_0))\, |\phi(t_0)| + \lim_{n\uparrow\infty} \sum_{k=0}^{m(n)} \left| \int_{s_k^{(n)}}^{t_k^{(n)}} \mathrm{d}t\, \dot{\phi}(t) \right| \\ &= \chi_{C\cap \overline{B}_R^c}(\gamma(t_0))\, |\phi(t_0)| + \lim_{n\uparrow\infty} \sum_{k=0}^{m(n)} |\phi(t_k^{(n)}) - \phi(s_k^{(n)})| \\ &\leqslant \chi_{C\cap \overline{B}_R^c}(\gamma(t_0))\, |\phi(t_0)| + \mathrm{var}(\phi). \end{aligned}$$

Now let us note that in Theorem 5 we can alternatively define $N_{C\cap S_R}$ by

$$N_{C\cap S_R}(\gamma) := \lim_{n\uparrow\infty}\lim_{m\uparrow\infty}\langle \mu_{C\cap B_R^c}(\gamma), \phi_{n,m}\rangle,$$

where $\{\phi_{n,m}\}_{n,m\geqslant 1}$ is a double sequence of test functions such that $\phi_{n,m}=1$ on $[t_0,n]$, $\phi_{n,m}\to\chi_{[t_0,n]}$ pointwise. Then if we choose such test functions $\phi_{n,m}$ in such a way that their variation is bounded uniformly in n and m, by the dominated convergence theorem and by Theorem 5 one has

$$\begin{aligned}\langle \psi_0, \chi_C(P_+)\psi_0\rangle &= \mathbb{E}(\chi_C(p_+))\\ &= \lim_{R\uparrow\infty}\lim_{n\uparrow\infty}\lim_{m\uparrow\infty}\mathbb{E}(\langle \mu_{C\cap B_R^c}, \phi_{n,m}\rangle)\\ &= \lim_{R\uparrow\infty}\lim_{n\uparrow\infty}\int_{t_0}^{n}\mathrm{d}t\int_{(C\cap S_R)\cup(\partial C\cap B_R^c)}\mathrm{d}\sigma(x)\, J^{\psi_t}(x)\cdot n(x).\end{aligned}$$

The proof is then conlcuded by proving that

$$\lim_{R\uparrow\infty}\lim_{n\uparrow\infty}\int_{t_0}^{n}\mathrm{d}t\int_{\partial C\cap B_R^c}\mathrm{d}\sigma(x)\, J^{\psi_t}(x)\cdot n(x)=0. \tag{4.1}$$

Since $n\cdot x=0$ on ∂C and $\|J^{\psi_t}\|\leqslant\|\psi_t^*\nabla\psi_t\|=\|\psi_t P\psi_t\|$, one has

$$\begin{aligned}\left|\int_{t_1}^{n}\mathrm{d}t\int_{\partial C\cap B_R^c}\mathrm{d}\sigma(x) J^{\psi_t}(x)\cdot n(x)\right| &\leqslant \int_{t_1}^{n}\mathrm{d}t\int_{\partial C\cap B_R^c}\mathrm{d}\sigma(x)\,\|\psi_t(x)P\psi_t(x)\|\\ &= \int_{t_1}^{n}\mathrm{d}t\int_{\partial C\cap B_R^c}\mathrm{d}\sigma(x)\left\|\psi_t(x)\left(P-\frac{Q}{t}\right)\psi_t(x)\right\|.\end{aligned}$$

Thus, since $\psi_t P\psi_t\in L^1(\partial C)$, by the monotone convergence theorem, (4.1) follows from

$$\int_{t_0}^{\infty}\mathrm{d}t\int_{\partial C\cap B_R^c}\mathrm{d}\sigma(x)\left\|\psi_t(x)\left(P-\frac{Q}{t}\right)\psi_t(x)\right\|<+\infty \tag{4.2}$$

for some $R>0$. By trace estimates on functions in $H^1(\mathbb{R}^3)$ of the kind

$$\|\cdot\|_{L^2(\partial C)}\leqslant c\|\cdot\|_{H^1(\mathbb{R}^3)},$$

(see, e.g., Burenkov 1998, Chap. 5) one has

$$\begin{aligned}&\int_{\partial C\cap B_R^c}\mathrm{d}\sigma(x)\left\|\psi_t(x)\left(P-\frac{Q}{t}\right)\psi_t(x)\right\|\left(\int_{\partial C\cap B_R^c}\mathrm{d}\sigma(x)|\,\theta(x)\psi_t(x)|^2\right)^{1/2}\\ &\quad\times\left(\int_{\partial C\cap B_R^c}\mathrm{d}\sigma(x)\left\|\left(P-\frac{Q}{t}\right)\psi_t(x)\right\|^2\right)^{1/2}\leqslant c\|\,\theta(Q)\psi_t\|_{H^1}\left\|\left(P-\frac{Q}{t}\right)\psi_t\right\|_{H^1},\end{aligned}$$

so that (4.2) is a consequence of Hypothesis 5. □

V. ON THE ADMISSIBILITY CONDITIONS

When $V=0$, $\psi_0\in H^2(\mathbb{R}^3)$, and $|Q|\psi_0\in L^2(\mathbb{R}^3)$, by the explicit espression for $e^{it\Delta}\psi_0$ one has

$$\left\|\left(P-\frac{1}{t}Q\right)\psi_t\right\|_{L^2}=\frac{1}{t}\|Q\psi_0\|_{L^2},$$

and therefore the free case satisfies the admissibility Hypotheses 2–4 (with $P_+ = P$).

Now we come to the interacting case. Hypothesis 3 gives no trouble: it follows from fairly general hypotheses on the potential function V. Indeed by Derezinski [(1997)—Theorem 4.1]

$$V(-\Delta+1)^{-1} \text{ is compact} \tag{5.1}$$

and

$$\int_1^{+\infty} \mathrm{d}R \left\| (-\Delta+1)^{-1} \nabla V \chi_{[1,+\infty)} \left(\frac{\|Q\|}{R} \right) (-\Delta+1)^{-1} \right\|_{L^2,L^2} < +\infty, \tag{5.2}$$

imply (a stronger version of) Hypothesis 3. By Hilsop and Sigal [(1996), Theorem 14.9], if for all $\epsilon > 0$ we can decompose $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$, with $\|V_2\|_\infty < \epsilon$, then (5.1) holds true. If, outside some ball, V is differentiable with its first derivatives decaying at infinity faster than $\|x\|^{-1}$ then condition (5.2) follows.

As regards Hypothesis 2, by the proof of Carlen [(1985), lemma 4] one has

$$\left\| \left(P - \frac{Q}{t} \right) \psi_t \right\|_{L^2} \leqslant \frac{1}{t} \|(P-Q)\psi_1\|_{L^2} + \frac{1}{t} \int_1^t \mathrm{d}s \, s \|\psi_s \nabla V\|_{L^2}.$$

By (5.1) V is infinitesimally $(-\Delta)$-operator-bounded [see, e.g., Hilsop and Sigal (1996), Theorem 14.2] and so [see Carlen (1984), Theorem 2.1(iv)] $\|(-P-Q)\psi_t\|_{L^2} < +\infty$ for all t if

$$\psi_0 \in H^2(\mathbb{R}^3), \quad |Q|\psi_0 \in L^2(\mathbb{R}^3).$$

Therefore Hypothesis 2 follows from

$$\|\psi_t \nabla V\|_{L^2} \leqslant c(1+|t|)^{-\sigma}, \quad \sigma > 1. \tag{5.3}$$

We introduce the notations $\langle x \rangle$ for the function $(1+\|x\|^2)^{1/2}$ and $\langle Q \rangle$ for the corresponding multiplication operator.

In the case $\langle Q \rangle^s \nabla V \in L^\infty(\mathbb{R}^3)$ and $\langle Q \rangle^s \psi_0 \in L^2(\mathbb{R}^3)$ for some s, (5.3) then follows from

$$\|\langle Q \rangle^{-s} e^{-itH} \langle Q \rangle^{-s}\|_{L^2,L^2} \leqslant c(1+|t|)^{-\sigma}. \tag{5.4}$$

Such a kind of estimates were obtained in many papers about propagation estimates for solution of Schrödinger equations [see e.g., Amrein *et al.* (1987); Cycon and Perry (1984); Jensen and Kato (1979); Jensen, Mourre, and Perry (1984); and Journé, Soffer, and Sogge (1991)]. For example, by Cycon and Perry [(1984), Theorem 1], one obtains that Hypothesis 2 holds true under the following hypotheses:

$$\psi_0 \in H^2(\mathbb{R}^3), \quad \langle Q \rangle^s \psi_0 \in L^2(\mathbb{R}^3), \quad \phi(H)\psi_0 = \psi_0, \tag{5.5}$$

$$V = V_S + V_L, \quad V_S \in C^1(\mathbb{R}^3), \quad V_L \in C^{k+3}(\mathbb{R}^3), \tag{5.6}$$

$$\|D^\alpha V_S(x)\| \leqslant c\langle x \rangle^{-2k-|\alpha|-\epsilon}, \quad |\alpha| \leqslant 1, \tag{5.7}$$

$$\|D^\alpha V_L(x)\| \leqslant c\langle x \rangle^{-|\alpha|-\epsilon}, \quad |\alpha| \leqslant k+1, \tag{5.8}$$

where $\phi \in C^\infty(0,+\infty)$ is equal to zero on a (arbitrarily small) neighborhood of zero and

$$\epsilon > 0, \quad k \geqslant 3, \quad 1 < s \leqslant k, \quad s\left(1 - \frac{1}{k}\right) > 1 \tag{5.9}$$

[$s(1-1/k) > 3/2$ gives Hypothesis 2.1].

Note that under these conditions (5.1) and (5.2) hold true. Moreover, by Hilsop and Sigal [(1996), Theorem 1] there are no strictly positive eigenvalues and, by Dereziński and Gerard [(1997), Theorem 4.7.1], one also has the existence and completeness of the (modified) wave operators, so that, for every Borel set A,

$$\langle \psi_0, \chi_A(P_+)\psi_0\rangle = \int_A \mathrm{d}k\, |\hat{\psi}_{\mathrm{out}}(k)|^2.$$

Thus Hypothesis 4 holds true and in conclusion

$$(5.5)-(5.9) \Rightarrow \text{admissibility}.$$

Remark: By Jensen and Kato [(1979), Theorem 10.3] the low energy cutoff hypothesis can be removed when 0 is neither an eigenvalue nor a resonance, $\epsilon>3$ and $s>5/2$. If 0 is not an eigenvalue but is a resonance then ψ_0 has to be orthogonal to the function corresponding to the resonance, otherwise in (5.4) one has $\sigma=1/2$, see Jensen and Kato [(1979), Theorem 10.5].

As regards strong admissibility, i.e., Hypothesis 5, the main point in the paper by Amrein and Pearson (1997) was just to find the conditions on ψ_0 and V leading to such an hypothesis. By using again (5.4) and commutator estimates, by Amrein and Pearson [(1997), Lemmas 5–8] one obtains

$$(5.5)-(5.9) \text{ with } s>5/3 \text{ and } \epsilon>2/3 \Rightarrow \text{strong admissibility}.$$

In Amrein and Pearson [(1997), Sec. 6] it is then shown how to avoid regularity hypotheses on the short-range component of V. However in this situation the hypotheses on the initial state ψ_0 become less transparent. Indeed there one requires $W_+^*\psi_0=\varphi(H_1)W_+^*\psi_0$, $\langle Q\rangle^s W_+^*\psi_0\in L^2(\mathbb{R}^3)$, $s>2$, $\varphi\in C_c(0,+\infty)$, $H_1:=-\Delta+V_1$, V_1 the smooth part of V, W_+ the relative wave operator $W_+:=\lim_{t\uparrow\infty}e^{-itH}e^{itH_1}$.

We conclude the section by listing the conditions on the couple (ψ_0,V) used in other papers (beside those of Amrein and Pearson) already quoted in order to obtain the flux-across-surfaces theorem [$\mathcal{S}(\mathbb{R}^3)$ denoting the space of functions of rapid decrease]:

(1) In Daumer *et al.* (1996) is it assumed that $V=0$ and $\psi_0\in\mathcal{S}(\mathbb{R}^3)$.

(2) In Amrein and Zuleta (1997) it is assumed that $\langle Q\rangle^s\psi_{\mathrm{out}}\in L^2(\mathbb{R}^3)$, $s>5/2$, $\psi_{\mathrm{out}}=\varphi(-\Delta)\psi_{\mathrm{out}}$, $\varphi\in C_c^\infty(0,+\infty)$, V either has local singularities and decays faster than $\|x\|^{-2}$ at infinity or is in $C^4(\mathbb{R}^3)$ and decays faster than $\|x\|^{-1}$ (in this case $\hat{\psi}_{\mathrm{out}}$ has to be in $C_c^4(\mathbb{R}^3\backslash\{0\})$). By Jensen and Nakamura (1992), when V is smooth, the condition on the outgoing state ψ_{out} is implied by a similar one (with $s>7/2$) on ψ_0.

(3) In Teufel, Dürr, and Münch-Berndl (1999) it is assumed that $\psi_{\mathrm{out}}\in\mathcal{S}(\mathbb{R}^3)$, that $V\in L^2(\mathbb{R}^3)$ is locally Hölder continuous except at a finite number of points and is decaying faster than $\|x\|^{-4}$, and that 0 is neither an eigenvalue nor a resonance. No energy cutoff condition on ψ_0 is required.

(4) In Dell'Antonio and Panati (2001) and the results in Teufel, Dürr, and Münch-Berndl (1999) are extended to the case in which 0 is either a zero-energy eigenvalue or resonance. There it is assumed that $\psi_0\in\mathcal{S}(\mathbb{R}^3)$, $V\in L^2(\mathbb{R}^3)$ is locally Hölder continuous except at a finite number of points and is decaying faster than $\|x\|^{-n}$ for all $n\in\mathbb{N}$, $\hat{\psi}_{\mathrm{out}}\in C^5(\mathbb{R}^3\backslash\{0\})$ and $\|D^\alpha\hat{\psi}_{\mathrm{out}}(k)\|\leqslant c\langle k\rangle^{-3-|\alpha|-\epsilon}$, $|\alpha|\leqslant 5$, $\epsilon>0$, $\|k\|\geqslant K_\alpha>0$.

(5) In Panati and Teta (2000) and Dell'Antonio and Panati (2001) the flux-across-surfaces theorem is proven in the case in which $\psi_0\in\mathcal{S}(\mathbb{R}^3)$ and H is the self-adjoint operator describing the Laplacean with a delta point interaction.

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Coherent state triplets and their inner products

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It is shown that if $\mathbb{H}$ is a Hilbert space for a representation of a group G, then there are triplets of spaces $(\mathcal{F}_{\mathbb{H}},\mathbb{H},\mathcal{F}^{\mathbb{H}})$, in which $\mathcal{F}^{\mathbb{H}}$ is a space of coherent state or vector coherent state wave functions and $\mathcal{F}_{\mathbb{H}}$ is its dual relative to a conveniently defined measure. It is shown also that there is a sequence of maps $\mathcal{F}_{\mathbb{H}}\to\mathbb{H}\to\mathcal{F}^{\mathbb{H}}$ which facilitates the construction of the corresponding inner products. After completion if necessary, the spaces $(\mathcal{F}_{\mathbb{H}},\mathbb{H},\mathcal{F}^{\mathbb{H}})$ become isomorphic Hilbert spaces. It is shown that the inner product for $\mathbb{H}$ is often easier to evaluate in $\mathcal{F}_{\mathbb{H}}$ than in $\mathcal{F}^{\mathbb{H}}$. Thus, we obtain integral expressions for the inner products of coherent state and vector coherent state representations. These expressions are equivalent to the algebraic expressions of K-matrix theory, but they are frequently more efficient to apply. The construction is illustrated by many examples. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1509851]

I. INTRODUCTION

Coherent state representations provide a unification of the various constructions for inducing representations of groups and Lie algebras. The method of induced representations, known originally as the ''Frobenius method,'' was introduced into physics by Wigner in two classic papers: in the first[1] he considered the vibrational spectra of molecules and, in the second,[2] he constructed all the irreducible unitary representations of the Poincaré group for positive mass particles. The theory of induced representations became an important tool in mathematics and physics following the developments of Mackey.[3] Other inducing constructions[4] are given by the Borel–Weil theorem and Harish-Chandra's constructions[5] of holomorphic discrete series representations.

Coherent states were first defined by Schrödinger[6] in 1926 as minimal uncertainty wave packets and used to exhibit the classical behavior of harmonic oscillators within the framework of quantum mechanics. Such applications has been particularly effective in quantum optics.[7] They were given general group-theoretic definitions by Klauder,[8] Perelomov,[9] and Gilmore.[10] Coherent state representations were introduced by Bargmann[11] and Segal[12] and defined more generally by Perelomov[13] and Onofri.[14] They were subsequently extended to vector-valued representations.[15,16]

It is now known that the inducing constructions are expressed naturally as coherent state, and vector coherent state, representations.[17] Moreover, the coherent state perspective adds new insights and has the advantage of being physically intuitive and easy to apply. In particular, it reveals the correspondence between the unitary representations of quantum mechanics and the nonunitary representations of classical mechanics and is closely related to the methods of geometric quantization.[18] Thus, coherent state representation theory is of considerable practical and pedagogic value.

A scalar coherent state representation is a representation of a group (or Lie algebra) on a space of complex-valued functions on a coset space. It is a representation induced from a one-dimensional representation of a subgroup. The prototype is the well-known Bargmann–Segal representation[11,12] of the Heisenberg–Weyl group on a Hilbert space of entire analytic functions. A

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vector coherent state (VCS) representation is a representation of a group (or Lie algebra) on a space of vector-valued functions. It is a representation induced from a multi-dimensional representation of a subgroup. Such representations have been used widely in the construction of explicit representations of Lie algebras and Lie groups,[19–22] in the construction of shift tensors,[23] and for the computation of Clebsch–Gordan coefficients for reducing tensor product representations.[24,25]

In constructing a coherent state representation, one needs to identify the space of wave functions and an appropriate inner product. When the group is compact or when it is noncompact but the representation belongs to the discrete series, there are standard methods for determining a suitable volume element relative to which the coherent state wave functions are square integrable and the coherent state representation unitary. The methods are summarized for the holomorphic representations in the book of Perelomov[13] and generalized to VCS representations, by the methods of Rowe, Rosensteel and Gilmore.[16]

Central to the standard construction is the so-called "resolution of the identity." If T denotes a UIR (unitary irreducible representation) on a Hilbert space $\mathbb{H}$ of a Lie group G with invariant measure $\mathrm{d}\mu$, then, if $|0\rangle$ is any state in $\mathbb{H}$, it follows by Schur's lemma that the operator

$$\hat{I}=\int T^{\dagger}(g)|0\rangle\langle 0|T(g)\mathrm{d}\mu(g), \tag{1}$$

when defined, is a multiple of the identity. Thus, with a suitable normalization of the invariant measure, the inner product of two states of $\mathbb{H}$ is expressed

$$\langle\psi|\varphi\rangle=\int_G \Psi^*(g)\Phi(g)\mathrm{d}\mu(g), \tag{2}$$

where Φ, defined by

$$\Phi(g)=\langle 0|T(g)|\varphi\rangle, \tag{3}$$

is a coherent state wave function for the state $|\varphi\rangle$. In particular situations, these expressions simplify. For example, if H is the isotropy subgroup

$$H=\{h\in G|T(h)|0\rangle=|0\rangle\chi(h)\}, \tag{4}$$

where $\chi(h)$ is a phase factor, and if K is a set of coset representives for $H\backslash G$ so that any element $g\in G$ can be factored $h=hk$, with $h\in H$ and $k\in K$, then the coherent state wave functions can be restricted to K and their inner products defined by

$$\langle\psi|\varphi\rangle=\int_K \Psi^*(k)\Phi(k)\mathrm{d}\mu(k), \tag{5}$$

where $\mathrm{d}\mu(k)$ is the measure on K inherited from the invariant measure on G.

A problem encountered in the practical application of such methods is that the integrals are difficult to evaluate and in some cases may not converge. For this reason, an alternative K-matrix theory has been developed[15,20,17] which provides numerically tractable recursive algorithms for constructing orthonormal bases for coherent state and VCS representations. Such bases, which are needed for the explicit construction of the matrices of Lie algebra representations, have been determined by K- matrix methods (reviewed in Ref. 26) for representatives of all the classical series of Lie algebras.[15,19,20] This approach works well for the matrices of Lie algebra representations. However, for other purposes, particularly when working at the group level, it is important to have explicit integral expressions for inner products. Thus, we consider here integral expressions for the results of K-matrix theory and show that they are generally easier to derive and use than the standard methods. In this article, we consider coherent state triplets for scalar coherent state representations. VCS triplets will be considered in a following paper.

The new method makes use of overlap kernels such as

$$\mathcal{S}(g_1,g_2)=\langle 0|T(g_1)T^\dagger(g_2)|0\rangle. \tag{6}$$

Thus, if a state $|\varphi\rangle\in\mathbb{H}$ is represented by a wave function φ defined over G such that

$$|\varphi\rangle=\int T^\dagger(g)|0\rangle\varphi(g)\mathrm{d}v(g), \tag{7}$$

where $\mathrm{d}v$ is any convenient measure on the group, then the inner product of states is given by

$$\langle\psi|\varphi\rangle=\int\int \psi^*(g_1)\mathcal{S}(g_1,g_2)\varphi(g_2)\mathrm{d}v(g_1)\mathrm{d}v(g_2). \tag{8}$$

Likewise, matrix elements of the representation are given by

$$\langle\psi|T(g)|\varphi\rangle=\int\int \psi^*(g_1)\mathcal{S}(g_1g,g_2)\varphi(g_2)\mathrm{d}v(g_1)\mathrm{d}v(g_2). \tag{9}$$

The new and old methods are related as follows. From Eqs. (3) and (7), it is seen that the coherent state wave function Φ for the state $|\varphi\rangle$ is related to φ by

$$\Phi(g)=\int \mathcal{S}(g,g_2)\varphi(g_2)\mathrm{d}v(g_2). \tag{10}$$

Moreover, the inner product of two states $|\psi\rangle$ and $|\varphi\rangle$ is given by

$$\langle\psi|\varphi\rangle=\int \psi^*(g)\Phi(g)\mathrm{d}v(g). \tag{11}$$

Thus, the wave functions φ and Φ are dual to one another relative to the volume $\mathrm{d}v$. The advantage of using the space of functions dual to the coherent state wave functions with inner product given by Eq. (8) is the freedom to choose the volume $\mathrm{d}v$ such that the integrals are easy to define and evaluate. It will be shown in the following, in a number of representative examples, that there are natural choices in given situations.

The new techniques greatly facilitate the use of algebraic and group structures in the solution of physical problems. Indeed, they were developed following the discovery, while computing SU(3) Clebsch–Gordan coefficients,[25] that it is generally very much easier to compute inner products by means of Eq. (8) than by using the coherent state inner product (5) directly.

II. SCALAR COHERENT STATE TRIPLETS

A. Finite-dimensional representations

Let T be a unitary irrep (irreducible represesentation) of a real algebraic Lie group G on a finite dimensional Hilbert space $\mathbb{H}$ with inner product of two vectors $|\psi\rangle$ and $|\varphi\rangle$ denoted by $\langle\psi|\varphi\rangle$. Assume there is an extension to a representation of G^c, the complex extension of G, which is compatible with the natural complex extension of its Lie algebra. Let $|0\rangle$ be a fixed vector in $\mathbb{H}$ and let N be a subset of G^c, such that the states

$$\{T^\dagger(z)|0\rangle; z\in N\} \tag{12}$$

span $\mathbb{H}$. Then, any state $|\psi\rangle\in\mathbb{H}$ is uniquely defined by the overlaps

$$\Psi(z)=\langle 0|T(z)|\psi\rangle, \quad z\in N. \tag{13}$$

The complex function Ψ on N is a coherent-state wave function for the state $|\psi\rangle$ and the space $\mathcal{F}^{\mathbb{H}}$ of such coherent-state wave functions carries a representation Γ of G isomorphic to T and defined by

$$[\Gamma(g)\Psi](z)=\langle 0|T(z)T(g)|\psi\rangle, \quad g\in G. \tag{14}$$

For example, if $P\subset G^c$ is the isotropy subgroup

$$P=\{p\in G^c|\langle 0|T(p)|\psi\rangle=\chi(p)\langle 0|\psi\rangle, \quad \forall|\psi\rangle\in\mathbb{H}\}, \tag{15}$$

where χ is a character of a one-dimensional irrep of P, then N is often chosen to be a set of $P\backslash G^c$ coset representatives or some subgroup of G^c complementary to P such that any element $g\in G$ can be factored as $g=pz$ for some $z\in N$ and some $p\in P$.

To identify the space $\mathcal{F}^{\mathbb{H}}$ of coherent state wave functions, consider first a space $\mathcal{F}=\mathcal{L}^2(N,\mathrm{d}v)$, defined by a convenient volume element $\mathrm{d}v$ such that the map

$$\mathcal{F}\to\mathbb{H}:\varphi\to|\varphi\rangle=\int \mathrm{d}v(z)T^\dagger(z)|0\rangle\varphi(z) \tag{16}$$

is well-defined and surjective onto $\mathbb{H}$. There is then a sequence of maps $\mathcal{F}\to\mathbb{H}\to\mathcal{F}^{\mathbb{H}}$ defined by

$$\psi\to|\psi\rangle\to\Psi=\hat{\mathcal{S}}\psi, \tag{17}$$

with

$$|\psi\rangle=\int T^\dagger(x)|0\rangle\psi(x)\mathrm{d}v(x) \tag{18}$$

and

$$\Psi(z)=\langle 0|T(z)|\psi\rangle=\int \mathcal{S}(z,x)\psi(x)\mathrm{d}v(x)=[\hat{\mathcal{S}}\psi](z), \tag{19}$$

where

$$\mathcal{S}(z,x)=\langle 0|T(z)T^\dagger(x)|0\rangle. \tag{20}$$

Thus, if

$$\mathcal{F}_0=\{\varphi\in\mathcal{F}|\langle\varphi|\varphi\rangle=0\} \tag{21}$$

denotes the kernel of the map $\mathcal{F}\to\mathbb{H}$ and $\mathcal{F}_{\mathbb{H}}$ is the quotient space $\mathcal{F}/\mathcal{F}_0$, it follows that the spaces $\mathcal{F}_{\mathbb{H}}$ and $\mathcal{F}^{\mathbb{H}}$ are dual to one another relative to the volume element $\mathrm{d}v$, i.e.,

$$\langle\varphi|\psi\rangle=\int \varphi^*(z)(\hat{\mathcal{S}}\psi)(z)\mathrm{d}v(z)=\int \varphi^*(z)\Psi(z)\mathrm{d}v(z). \tag{22}$$

It also follows that matrix elements of the representation T are given by

$$\langle\varphi|T(g)|\psi\rangle=\int \varphi^*(z)[\Gamma(g)\hat{\mathcal{S}}\psi](z)\mathrm{d}v(z)]=\int \varphi^*(z)[\Gamma(g)\Psi](z)\mathrm{d}v(z). \tag{23}$$

We refer to the triple of spaces $(\mathcal{F}_{\mathbb{H}},\mathbb{H},\mathcal{F}^{\mathbb{H}})$ as a *coherent state triplet*.

The space $\mathcal{F}^{\mathbb{H}}$ of coherent state wave functions is clearly a Hilbert space with respect to an inner product inherited from $\mathbb{H}$. Thus, if the space $\mathcal{F}_{\mathbb{H}}$ is equipped with the inner product

$$(\varphi,\psi)=\langle\varphi|\psi\rangle=\int\int \mathrm{d}v(z)\varphi^*(z)\mathcal{S}(z,x)\psi(x)\mathrm{d}v(x), \tag{24}$$

the three spaces $(\mathcal{F}_{\mathbb{H}},\mathbb{H},\mathcal{F}^{\mathbb{H}})$ become isomorphic to one another. One can then use whichever gives the simplest expression in any situation. Examples will be given in the following in which it is easiest to evaluate inner products in $\mathcal{F}_{\mathbb{H}}$. One can then construct an orthonormal basis for $\mathcal{F}_{\mathbb{H}}$ and corresponding orthornormal bases for $\mathbb{H}$ and $\mathcal{F}^{\mathbb{H}}$, e.g., if $\{\psi_\nu\}$ is an orthonormal basis for $\mathcal{F}_{\mathbb{H}}$, then $\{\Phi_\nu=\hat{\mathcal{S}}\psi_\nu\}$ is an orthonormal basis for $\mathcal{F}^{\mathbb{H}}$.

The relationship of the above to K-matrix theory[26] is obtained by noting that, since $\hat{\mathcal{S}}$ is a positive definite operator on $\mathcal{F}_{\mathbb{H}}$, it can be factored

$$\hat{\mathcal{S}}=\hat{K}\hat{K}^\dagger, \tag{25}$$

and the inner product for $\mathcal{F}_{\mathbb{H}}$ expressed

$$\langle\varphi|\psi\rangle=\int(\hat{K}^\dagger\varphi)^*(z)(\hat{K}^\dagger\psi)(z)\mathrm{d}v(z). \tag{26}$$

Thus, if $\{\psi_\nu\}$ is an orthonormal basis for $\mathcal{F}_{\mathbb{H}}$, the functions $\{\varphi_\nu=\hat{K}^\dagger\psi_\nu\}$ satisfy the equation

$$\int \varphi_\mu^*(z)\varphi_\nu(z)\mathrm{d}v(z)=\delta_{\mu\nu}, \tag{27}$$

and the corresponding orthonormal coherent state basis is given by $\{\Psi_\nu=\hat{K}\hat{K}^\dagger\psi_\nu=\hat{K}\varphi_\nu\}$. Hence, if $\{\varphi_\nu\}$ is an orthonormal basis for $\mathcal{F}$, the operator $\hat{K}$ maps this basis to an orthonormal basis $\{\Psi_\nu=\hat{K}\varphi_\nu\}$ for $\mathcal{F}^{\mathbb{H}}$ by annihilating the unwanted states of $\mathcal{F}$.

The above construction of coherent state wave functions and their inner products has a powerful and, for practical applications, very significant attribute of facilitating the construction of representations in bases which reduce some desired subgroup $H\subset G$. Basically what has to be done is to choose a measure $\mathrm{d}v$ for $\mathcal{F}$ such that the restriction of the action of Γ to the subgroup $H\subset G$ is unitary on $\mathcal{F}$. Then, $\mathcal{S}$ becomes H-invariant, in the sense that

$$\mathcal{S}(zh,xh)=\langle 0|T(z)T(h)T^\dagger(h)T^\dagger(x)|0\rangle=\mathcal{S}(z,x), \tag{28}$$

and $\hat{\mathcal{S}}$ block diagonal in a basis for $\mathcal{F}$ that reduces the unitary representation of H. Specifically, if $\mathcal{F}=\Sigma_{\alpha\kappa}\mathcal{F}^{\alpha\kappa}$ is a decomposition of $\mathcal{F}$ as a direct sum of irreducible H-invariant subspaces, where κ labels an irrep of H and α distinguishes equivalent irreps, and if $\{\varphi_{\alpha\kappa\nu}\}$ is an orthonormal basis for $\mathcal{F}^{\alpha\kappa}$, then

$$\langle\varphi_{\alpha\kappa\mu}|\varphi_{\beta\kappa'\nu}\rangle=\int\int\varphi_{\alpha\kappa\mu}^*(z)\mathcal{S}(z,x)\varphi_{\beta\kappa'\nu}(x)\mathrm{d}v(z)\mathrm{d}v(x)=\delta_{\kappa\kappa'}\delta_{\mu\nu}\mathcal{S}_{\alpha\kappa\beta}. \tag{29}$$

It then follows that an orthonormal basis $\{\varphi_{\alpha\kappa\nu}\}$ for $\mathcal{F}$ which diagonalizes the matrix $\mathcal{S}_\kappa$, i.e., for which $\mathcal{S}_{\alpha\kappa\beta}=\delta_{\alpha\beta}K_{\alpha\kappa}^2$, defines a corresponding orthonormal basis $\{\Psi_{\alpha\kappa\nu}=K_{\alpha\kappa}\varphi_{\alpha\kappa\nu}\}$ of coherent state wave functions. It is shown explicitly how this is done in the following examples.

The above definitions can be generalized in several ways. For example, the condition that $\mathbb{H}$ should be irreducible can be relaxed. The representation Γ is then isomorphic to a subrepresentation of T. Moreover, if $|0\rangle$ belongs to an irreducible subspace of $\mathbb{H}$, then the space spanned by $\{T^\dagger(z)|0\rangle;z\in N\}$, as well as the corresponding coherent state representation, is irreducible.

B. Infinite-dimensional representations

The above construction extends easily to infinite-dimensional representations. However, although the extension is natural in most situations, there are technical constraints that must be

respected in the choice of state $|0\rangle$ and subset $N\subset G^c$ to ensure that the operators $\{\langle 0|T(z),z \in N\}$ are well defined and have the properties required to define a coherent state representation. For simplicity, it will be assumed here that the representation T is irreducible and unitary. One concern is that an infinite-dimensional irrep T of a real group G on a Hilbert space $\mathbb{H}$ does not automatically extend to a representation of the complex group G^c. For, whereas a real Lie algebra $\mathfrak{g}$ has a natural extension to $\mathfrak{g}^c$ by linearity,

$$T(z\otimes X)=zT(X), \quad \text{for} \quad X\in\mathfrak{g},z\in\mathbb{C}, \tag{30}$$

it can happen, for example, that if $\hat{X}=T(X)$ is the operator representing an element $X\in\mathfrak{g}^c$, then the action of the associated group element $e^{\hat{X}}=T(e^X)$ on a state $|\psi\rangle\in\mathbb{H}$ may not converge to a normalizable state $e^{\hat{X}}|\psi\rangle\in\mathbb{H}$. Nevertheless, as we show by examples in the following, it is frequently possible to choose a functional $\langle 0|$ and a subset $N\subset G^c$ so that the techniques described above can be generalized. In doing this, it is not possible to expect that the representation T can be extended so that N acts on all of $\mathbb{H}$, or that the functional $\langle 0|$ will be normalizable. Both these difficulties can be handled by working with a dense subspace of $\mathbb{H}$. A good example to keep in mind is the delta function, which is not defined on all of $\mathcal{L}^2(\mathbb{R})$, but does make sense on the dense subspace of continuous functions in $\mathcal{L}^2(\mathbb{R})$.

Specifically, what is required is a dense subspace $\mathbb{H}_D\subset\mathbb{H}$ of the Hilbert space; a subset $N\subset G^c$; an extension of the representation T from G to operators $T(z)$, $z\in N$, which are defined on $\mathbb{H}_D$; and a linear functional $\langle 0|$ on the space spanned by $\{T(z)|\psi\rangle:|\psi\rangle\in\mathbb{H}_D,z\in N\}$. The extension of T to N must be compatible at the level of the Lie algebra with Eq. (30) and have the property that

$$\{\langle 0|T(z);z\in N\} \tag{31}$$

are well-defined functionals on $\mathbb{H}_D$ and are a *sufficient set*, in the sense that any $|\psi\rangle\in\mathbb{H}_D$ is uniquely defined by the overlaps

$$\Psi(z)=\langle 0|T(z)|\psi\rangle, \quad z\in N. \tag{32}$$

The complex function Ψ on N is then a coherent-state wave function for the state $|\psi\rangle$. When the subspace $\mathbb{H}_D$ is invariant under the (real) group action, then the space $\mathcal{F}^{\mathbb{H}_D}$ of all such coherent-state wave functions carries a representation Γ of G, isomorphic to T, defined by

$$[\Gamma(g)\Psi](z)=\langle 0|T(z)T(g)|\psi\rangle, \quad g\in G. \tag{33}$$

However, sometimes it will be convenient to choose a dense subspace that is not G-invariant. The group action, defined by Eq. (33), is then extended to the G-invariant completion of the space of coherent state wave functions relative to the inner product inherited from $\mathbb{H}$.

The final step is to generalize the map (16). Since $\langle 0|$ is in general not an element of $\mathbb{H}$ (i.e., not normalizable), it is necessary to choose the measure and the space of functions carefully. Specifically, what is required is a space $\mathcal{F}$ of functions on N and a measure $\mathrm{d}\nu$ on N such that, for every $\varphi\in\mathcal{F}$, the integral

$$\int \mathrm{d}\nu(z)\varphi(z)^*\langle 0|T(z) \tag{34}$$

converges to an element of $\mathbb{H}_D^*$, the dual of the dense subspace $\mathbb{H}_D$ of $\mathbb{H}$ for which coherent state wave functions are defined. This integral then gives a map

$$\mathcal{F}\to\mathbb{H}_D^*:\varphi\to\langle\varphi|=\int \mathrm{d}\nu(z)\varphi(z)^*\langle 0|T(z) \tag{35}$$

which is well-defined for all elements of $\mathcal{F}$. We also require that the image of this map contains $\mathbb{H}_D$ and write $\mathcal{F}_D$ for the space of all elements of $\mathcal{F}$ which the map takes to elements of $\mathbb{H}_D$.

There is now a sequence of maps $\mathcal{F}_D \to \mathbb{H}_D \to \mathcal{F}^{\mathbb{H}_D}$ for which

$$\psi \to |\psi\rangle \to \Psi = \hat{\mathcal{S}}\psi, \tag{36}$$

with

$$|\psi\rangle = \int T^\dagger(x)|0\rangle \psi(x) \mathrm{d}v(x) \tag{37}$$

and

$$\Psi(z) = [\hat{\mathcal{S}}\psi](z) = \int \mathcal{S}(z,x)\psi(x)\mathrm{d}v(x), \tag{38}$$

where

$$\mathcal{S}(z,x)\psi(x) = \langle 0|T(z)T^\dagger(x)|0\rangle. \tag{39}$$

Let

$$\mathcal{F}_0 = \{\varphi \in \mathcal{F} | \langle \varphi|\varphi\rangle = 0\} \tag{40}$$

denote the kernel of the map $\mathcal{F} \to \mathbb{H}_D^*$ given in (35), i.e., $\mathcal{F}_0$ is the set of all functions in $\mathcal{F}$ that map to functionals that are zero on all of $\mathbb{H}_D$, and define $\mathcal{F}_\mathbb{H}$ to be the completion of the space $\mathcal{F}_D/\mathcal{F}_0$, relative to the inner product

$$(\varphi,\psi) = \langle \varphi|\psi\rangle = \int\int \mathrm{d}v(z)\varphi^*(z)\mathcal{S}(z,x)\psi(x)\mathrm{d}v(x), \tag{41}$$

where

$$\mathcal{S}(z,x) = \langle 0|T(z)T^\dagger(x)|0\rangle. \tag{42}$$

Then $\mathcal{F}_\mathbb{H}$ is a Hilbert space isomorphic to $\mathbb{H}$ and, if $\mathcal{F}^\mathbb{H}$ is the completion of the space of coherent state wave functions relative to the inner product inherited from $\mathbb{H}$, it too is isomorphic to $\mathbb{H}$.

Finally observe that, if the map $\mathcal{F} \to \mathbb{H}_D^*$ takes $\varphi \to \langle\varphi|$ and if a state $|\psi\rangle \in \mathbb{H}_D$ has coherent state wave function $\Psi \in \mathcal{F}^{\mathbb{H}_D}$, then

$$\langle \varphi|\psi\rangle = \int \varphi^*(z)(\hat{\mathcal{S}}\psi)(z)\mathrm{d}v(z) = \int \varphi(z)^*\Psi(z)\mathrm{d}v(z). \tag{43}$$

It follows that $\mathcal{F}_\mathbb{H}$ and $\mathcal{F}^\mathbb{H}$ are in duality relative to the volume element $\mathrm{d}v$. It also follows that matrix elements of the representation T are given by

$$\langle \varphi|T(g)|\psi\rangle = \int \varphi^*(z)[\Gamma(g)\hat{\mathcal{S}}\psi](z)\mathrm{d}v(z)] = \int \varphi^*(z)[\Gamma(g)\Psi](z)\mathrm{d}v(z). \tag{44}$$

We again refer to the triple of spaces $(\mathcal{F}_\mathbb{H}, \mathbb{H}, \mathcal{F}^\mathbb{H})$ as a *coherent state triplet*.

III. SIMPLE EXAMPLES

The following well-known examples are developed in some detail as prototypes of four classes of application of the triplets method: holomorphic representations of compact and non-

compact semisimple Lie groups; nonholomorphic representations induced from a noncanonical subgroup; and Mackey type representations[3] of a semidirect product group induced from an Abelian normal subgroup.

A. SU(2)

Let $\{J_0, J_+, J_-\}$ with commutation relations

$$[J_+, J_-] = 2J_0, \quad [J_0, J_\pm] = \pm J_\pm, \tag{45}$$

be a standard basis for the Lie algebra $\mathfrak{su}(2)^c$. Let $T^j: J_k \to \hat{J}_k$ be a UIR (unitary irreducible representation) of SU(2) of angular momentum j on a (finite-dimensional) Hilbert space $\mathbb{H}^j$ with (normalized) highest weight state $|jj\rangle$ satisfying

$$\hat{J}_+|jj\rangle = 0, \quad \hat{J}_0|jj\rangle = j|jj\rangle. \tag{46}$$

With fixed state $|0\rangle$ set equal to the highest weight state $|jj\rangle$, a natural choice of $N \subset \mathrm{SU}(2)^c$ is the nilpotent subgroup

$$N = \{e^{zJ_+}; z \in \mathbb{C}\}, \tag{47}$$

and a convenient measure $\mathrm{d}v$ on N is the Bargmann measure, relative to which the polynomial functions $\{\varphi_\nu\}$, with $\varphi_\nu(z) = z^\nu/\sqrt{\nu!}$, satisfy the orthogonality relationship

$$\int \varphi_\mu^*(z)\varphi_\nu(z)\mathrm{d}v(z) = \delta_{\mu\nu}. \tag{48}$$

The space $\mathcal{F} = \mathcal{L}^2(N, \mathrm{d}v)$ is then the Bargmann space[11] of entire analytic functions of z that are square integrable relative to $\mathrm{d}v$.

The overlap kernel, $\mathcal{S}(z,x) = \langle 0|e^{z\hat{J}_+}e^{x^*\hat{J}_-}|0\rangle$, is evaluated by noting that almost any $\mathrm{SL}(2,\mathbb{C})$ matrix has Gauss factorization

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ x & 1 \end{pmatrix}\begin{pmatrix} a & 0 \\ 0 & a^{-1} \end{pmatrix}\begin{pmatrix} 1 & z \\ 0 & 1 \end{pmatrix} = e^{xJ_-}a^{2J_0}e^{zJ_+} \tag{49}$$

with $z = b/a$ and $x = c/a$. It follows that, as elements of $\mathrm{SL}(2,\mathbb{C})$,

$$e^{zJ_+}e^{x^*J_-} = \begin{pmatrix} 1+zx^* & z \\ x^* & 1 \end{pmatrix} = e^{\alpha x^* J_-}(1+zx^*)^{2J_0}e^{\alpha z J_+}, \tag{50}$$

with $\alpha = (1+zx^*)^{-1}$. Thus, the overlap kernel is given by

$$\mathcal{S}(z,x) = \langle 0|(1+zx^*)^{2\hat{J}_0}|0\rangle = (1+zx^*)^{2j} \tag{51}$$

and has expansion

$$\mathcal{S}(z,x) = \sum_{\nu=0}^{2j} \frac{(2j)!}{(2j-\nu)!\,\nu!}(zx^*)^\nu = \sum_{\nu=0}^{2j} K_\nu^2 \varphi_\nu(z)\varphi_\nu^*(x), \tag{52}$$

with

$$K_\nu^2 = \frac{(2j)!}{(2j-\nu)!}. \tag{53}$$

The space $\mathcal{F}_j$ is now defined as the Hilbert space of holomorphic functions of a complex variable z with inner product

$$\langle\varphi|\psi\rangle=\int\int \psi^*(z)\mathcal{S}(z,x)\varphi(x)\mathrm{d}v(z)\mathrm{d}v(x). \tag{54}$$

With respect to this $\mathcal{F}_j$ inner product, the overlaps of the functions $\{\varphi_\nu\}$ are given by

$$\langle\varphi_\mu|\varphi_\nu\rangle=\delta_{\mu\nu}\times\begin{cases}K_\nu^2 & \text{for } \nu\leqslant 2j,\\ 0 & \text{for } \nu>2j.\end{cases} \tag{55}$$

Thus, with the substitution $\nu=j-m$ (to conform to convention), and choosing the positive square root of K_ν^2, an orthonormal basis for $\mathcal{F}_j$ is given by the set of holomorphic functions

$$\left\{\psi_{jm}(z)=\frac{1}{K_{j-m}}\varphi_{j-m}(z)=\sqrt{\frac{(j+m)!}{(2j)!(j-m)!}}z^{j-m};m=-j,\ldots,j\right\}. \tag{56}$$

The map $\mathcal{F}_j\to\mathbb{H}^j$, in which

$$\psi_{jm}\to|jm\rangle=\int e^{z^*\hat{J}_-}|0\rangle\psi_{jm}(z)\mathrm{d}v(z), \tag{57}$$

and the coherent-state map $\mathbb{H}^j\to\mathcal{F}^j$, given by

$$|jm\rangle\to\Psi_{jm}(z)=\langle 0|e^{z\hat{J}_+}|jm\rangle=\int\langle 0|e^{z\hat{J}_+}e^{x^*\hat{J}_-}|0\rangle\psi_{jm}(x)\mathrm{d}v(x), \tag{58}$$

are isomorphisms. Thus, orthonormal bases for $\mathbb{H}^j$ and $\mathcal{F}^j$, corresponding to the basis (56) for $\mathcal{F}_j$, are given by

$$\left\{|jm\rangle=\frac{1}{K_{j-m}}|\varphi_{j-m}\rangle=\sqrt{\frac{(j+m)!}{(2j)!(j-m)!}}(\hat{J}_-)^{j-m}|0\rangle;\quad m=-j,\ldots,j\right\}, \tag{59}$$

$$\left\{\Psi_{jm}(z)=K_{j-m}\varphi_{j-m}(z)=\sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}z^{j-m};\quad m=-j,\ldots,j\right\}, \tag{60}$$

respectively.

The coherent state representation Γ^j of SU(2) on $\mathcal{F}^j$ is defined by

$$[\Gamma^j(g)\Psi](z)=\langle 0|e^{z\hat{J}_+}T^j(g)|\psi\rangle \tag{61}$$

[cf. Eq. (14)]. From the identity

$$e^{zJ_+}\begin{pmatrix}a & b\\ -b^* & a^*\end{pmatrix}=\begin{pmatrix}a-zb^* & b+za^*\\ -b^* & a^*\end{pmatrix}=e^{-\alpha b^*J_-}(a-b^*z)^{2J_0}e^{\alpha(b+a^*z)J_+} \tag{62}$$

with $\alpha=(a-b^*z)^{-1}$, the action of $\Gamma^j(g)$ is determined to be

$$[\Gamma^j(g)\Psi](z)=(a-b^*z)^{2j}\Psi(z\cdot g), \tag{63}$$

with

$$g=\begin{pmatrix}a & b\\ -b^* & a^*\end{pmatrix},\quad z\cdot g=\frac{b+a^*z}{a-b^*z}. \tag{64}$$

Finally, since the inner product can be written in the form $\langle\psi|\varphi\rangle=\int\psi^*(z)\Phi(z)\mathrm{d}\upsilon(z)$, matrix elements of the representation T are given by

$$\langle\psi|T^j(g)|\varphi\rangle=\int\psi^*(z)[\Gamma^j(g)\Phi](z)\mathrm{d}\upsilon(z), \tag{65}$$

where φ, $|\varphi\rangle$, and Φ are related by the $\mathcal{F}_j\to\mathbb{H}^j\to\mathcal{F}^j$ maps given by Eqs. (57) and (58). For example, setting $c=\cos\beta/2$ and $s=\sin\beta/2$ and

$$g=\begin{pmatrix} c & -s \\ s & c \end{pmatrix}, \tag{66}$$

one obtains, from Eq. (65), an expression for the Wigner function

$$\begin{aligned} d^j_{mn}(\beta)=\langle jm|T^j(g)|jn\rangle&=\int\psi^*_{j-m}(z)[\Gamma^j(g)\Psi_{j-n}](z)\mathrm{d}\upsilon(z)\\ &=\frac{K_{j-n}}{K_{j-m}}\int\varphi^*_{j-m}(z)[\Gamma^j(g)\varphi_{j-n}](z)\mathrm{d}\upsilon(z)\\ &=\frac{K_{j-n}}{K_{j-m}}\int\varphi^*_{j-m}(z)(c+sz)^{j+n}\varphi_{j-n}(-s+cz)\mathrm{d}\upsilon(z), \end{aligned} \tag{67}$$

which integrates to the standard result.

The coherent state representation of the $\mathfrak{su}(2)$ Lie algebra, defined by

$$[\Gamma^j(J_k)\Psi](z)=\langle jj|e^{z\hat{J}_+}\hat{J}_k|\psi\rangle, \tag{68}$$

yields the known expressions

$$\Gamma^j(J_+)=\frac{d}{dz},\quad \Gamma^j(J_0)=j-z\frac{d}{dz},\quad \Gamma^j(J_-)=2jz-z^2\frac{d}{dz}. \tag{69}$$

Acting on the orthonormal coherent state basis wave functions of Eq. (60), they give the expected results

$$\begin{aligned} \Gamma^j(J_0)\Psi_{jm}&=m\Psi_{jm},\\ \Gamma^j(J_\pm)\Psi_{jm}&=\sqrt{(j\mp m)(j\pm m+1)}\Psi_{j,m\pm1}. \end{aligned} \tag{70}$$

The above expressions may be compared to those of the standard holomorphic representations of SU(2). The latter are identical to the coherent state representations but specify the inner product for the Hilbert space $\mathcal{F}^j$ by

$$\langle\psi|\varphi\rangle=\frac{2j+1}{\pi}\int\frac{\Psi^*(z)\Phi(z)}{(1+|z|^2)^{2j+2}}\mathrm{d}^2z, \tag{71}$$

where the integral is over the complex plane with $\mathrm{d}^2z=\mathrm{d}x\mathrm{d}y$ and $z=x+iy$; cf. Ref. 13 and the Appendix. Thus, whereas $\mathcal{F}^j$ is a space of holomorphic functions with norm defined by this inner product, the space $\mathcal{F}_j$, isomorphic to $\mathcal{F}^j$, is the space of holomorphic functions with inner product

$$\langle\psi|\varphi\rangle=\int\int\psi^*(z)(1+zx^*)^{2j}\varphi(x)\mathrm{d}\upsilon(z)\mathrm{d}\upsilon(x). \tag{72}$$

The latter integrals are easier to evaluate and by regarding $\mathcal{F}_j$ and $\mathcal{F}^j$ as mutual duals, we have the still simpler hybrid expression

$$\langle \psi | \varphi \rangle = \int \psi^*(z)\Phi(z)\mathrm{d}v(z). \tag{73}$$

B. SU(1,1)

Let $\{J_0, J_+, J_-\}$ with commutation relations

$$[J_-, J_+] = 2J_0, \quad [J_0, J_\pm] = \pm J_\pm, \tag{74}$$

be a standard basis for the Lie algebra $\mathfrak{su}(1,1)^c$. Let T^λ be a UIR (unitary irreducible representation) of SU(1,1) of lowest weight λ on an infinite-dimensional Hilbert space $\mathbb{H}^\lambda$, where λ is a positive integer, defined such that, if $|0\rangle$ is the lowest weight state, then

$$\hat{J}_-|0\rangle = 0, \quad 2\hat{J}_0|0\rangle = \lambda|0\rangle, \tag{75}$$

where $\hat{J}_k = T^\lambda(J_k)$.

Gauss factorization of almost any $\mathrm{SL}(2,\mathbb{C})$ matrix gives

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix} \begin{pmatrix} d^{-1} & 0 \\ 0 & d \end{pmatrix} \begin{pmatrix} 1 & 0 \\ z & 1 \end{pmatrix} = e^{-xJ_+}(d)^{-2J_0}e^{zJ_-}, \tag{76}$$

with $x = b/d$ and $z = c/d$. This implies that, if g is the SU(1,1) matrix

$$g = \begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix} \quad \text{with} \quad aa^* - bb^* = 1, \tag{77}$$

then $T^\lambda(g)$ can be expanded

$$T^\lambda(g) = e^{-x\hat{J}_+}(a^*)^{-2\hat{J}_0}e^{z\hat{J}_-} \tag{78}$$

and

$$\langle 0|T^\lambda(g)|\psi\rangle = (a^*)^{-\lambda}\langle 0|e^{z\hat{J}_-}|\psi\rangle, \tag{79}$$

with $x = b/a^*$ and $z = b^*/a^*$. Thus, a natural choice of $N \subset \mathrm{SU}(1,1)^c \cong \mathrm{SL}(2,\mathbb{R})^c$ is the Borel subgroup

$$N = \{e^{zJ_-}; z \in \mathbb{C}\}. \tag{80}$$

With this choice of N, the functionals

$$\{\langle 0|e^{z\hat{J}_-}; z \in \mathbb{C}\} \tag{81}$$

are well-defined on the dense subspace $\mathbb{H}_D$ of finite linear combinations of the weight vectors (the so-called K-finite vectors). Thus, a coherent state wave function for a state $|\psi\rangle \in \mathbb{H}_D$ is defined by

$$\Psi(z) = \langle 0|e^{z\hat{J}_-}|\psi\rangle. \tag{82}$$

These coherent state wave functions are polynomials in z.

Let $\mathcal{F}$ denote the Bargmann Hilbert space of holomorphic functions over $\mathbb{C}$ with orthonormal (polynomial) basis $\{\varphi_\nu; \nu = 0,1,2,\ldots\}$, where $\varphi_\nu(z) = z^\nu/\sqrt{\nu!}$. Now observe that the map

$$\varphi \to \langle \varphi | = \int \mathrm{d}v(z)\, \varphi(z)^* \langle 0 | e^{z\hat{J}_-} \tag{83}$$

takes any function $\varphi \in \mathcal{F}$ to a well-defined functional on $\mathbb{H}_D$. The image of this $\mathcal{F} \to \mathbb{H}_D^*$ map contains $\mathbb{H}_D$. Moreover, $\mathcal{F}_D \subset \mathcal{F}$ is identified as the dense subspace of finite polynomials. Thus, if $\mathcal{F}^\lambda = \mathcal{F}^{\mathbb{H}_D}$ is the space of coherent state wave functions for states in $\mathbb{H}_D$, then composition of the maps $\mathcal{F}_D \to \mathbb{H}_D$ and $\mathbb{H}_D \to \mathcal{F}^{\mathbb{H}_D}$ gives the map

$$\hat{\mathcal{S}}: \mathcal{F}_D \to \mathcal{F}^{\mathbb{H}_D}; \psi \mapsto \Psi = \hat{\mathcal{S}}\psi, \tag{84}$$

with

$$\Psi(z) = \int \mathcal{S}(z,x)\, \psi(x)\, \mathrm{d}v(x), \tag{85}$$

and

$$\mathcal{S}(z,x) = \langle 0 | e^{z\hat{J}_-} e^{x^*\hat{J}_+} | 0 \rangle. \tag{86}$$

Claim: The overlap integral $\mathcal{S}(z,x)$ is the distribution on $\mathcal{F}_D$,

$$\mathcal{S}(z,x) = \sum_\nu^\infty K_\nu^2 \varphi_\nu(z)\, \varphi_\nu^*(x), \tag{87}$$

with

$$K_\nu^2 = \frac{(\lambda+\nu-1)!}{(\lambda-1)!}. \tag{88}$$

Proof: First observe that, from its definition (86), $\mathcal{S}(z,x)$ is holomorphic in z and x^*. Thus, it is sufficient to prove the claim for z and x^* lying in some open domain of $\mathbb{C}$. In fact, the $\mathrm{SU}(1,1)^c = \mathrm{SL}(2,\mathbb{C})$ expansion

$$e^{zJ_-} e^{x^*J_+} = \begin{pmatrix} 1 & 0 \\ z & 1 \end{pmatrix} \begin{pmatrix} 1 & -x^* \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & -x^* \\ z & 1-zx^* \end{pmatrix} \tag{89}$$

$$= e^{\alpha x^* J_+} (\alpha)^{2J_0} e^{\alpha z J_-}, \tag{90}$$

with $\alpha = (1-zx^*)^{-1}$, together with the assumption that

$$T^\lambda (e^{\alpha x^* J_+} (1-zx^*)^{-2J_0} e^{\alpha z J_-}) = e^{\alpha x^* \hat{J}_+} (1-zx^*)^{-2\hat{J}_0} e^{\alpha z \hat{J}_-}, \tag{91}$$

gives the correct result for $|zx^*| < 1$:

$$\mathcal{S}(z,x) = \langle 0 | (1-zx^*)^{-2\hat{J}_0} | 0 \rangle = (1-zx^*)^{-\lambda} = \sum_\nu^\infty K_\nu^2 \varphi_\nu(z)\, \varphi_\nu^*(x), \quad \text{for} \quad |zx^*| < 1. \tag{92}$$

However, this result could be questioned because the representation T^λ of $\mathrm{SU}(1,1)$ does not in general extend to all of $\mathrm{SL}(2,\mathbb{C})$, so applying it to elements of the complex group is not, in general, justified; an infinite-dimensional irrep of $\mathrm{SL}(2,\mathbb{C})$ does not remain irreducible on restriction to $\mathrm{SU}(1,1)$. Nevertheless, Eq. (92) is valid for $|z|^2 < 1$ and $|x|^2 < 1$, because there exist matrices

$$Z_+(z^*)=\begin{pmatrix} a^{-1} & az^* \\ 0 & a \end{pmatrix}, \quad Z_-(x)=\begin{pmatrix} b^{-1} & 0 \\ -b^*x & b \end{pmatrix}, \tag{93}$$

with $|a|^2=(1-|z|^2)^{-1}$ and $|b|^2=(1-|x|^2)^{-1}$, such that

$$Z_+(z^*)e^{zJ_-}=\begin{pmatrix} a^{-1} & a^*z^* \\ 0 & a \end{pmatrix}\begin{pmatrix} 1 & 0 \\ z & 1 \end{pmatrix}=\begin{pmatrix} a^* & a^*z^* \\ az & a \end{pmatrix}, \tag{94}$$

$$e^{x^*J_+}Z_-(x)=\begin{pmatrix} 1 & -x^* \\ 0 & 1 \end{pmatrix}\begin{pmatrix} b^{-1} & 0 \\ -b^*x & b \end{pmatrix}=\begin{pmatrix} b^* & -bx^* \\ -b^*x & b \end{pmatrix} \tag{95}$$

are elements of the real Lie group SU(1,1). Factorization of the product of real SU(1,1) group elements

$$Z_+(z^*)e^{zJ_-}e^{x^*J_+}Z_-(x)=Z_+(z^*)e^{\alpha x^*J_+}(\alpha)^{2J_0}e^{\alpha zJ_-}Z_-(x), \tag{96}$$

with $\alpha=(1-zx^*)^{-1}$, then gives the result (92) and confirms the validity of the claim. Q.E.D.

For polynomial functions ψ, φ, the inner product

$$\langle\psi|\varphi\rangle=\int\int \psi^*(z)\mathcal{S}(z,x)\varphi(x)\mathrm{d}\nu(z)\mathrm{d}\nu(x)=\sum_\nu K_\nu^2\int \psi^*(z)\varphi_\nu(z)\mathrm{d}\nu(z)\int \varphi_\nu^*(x)\varphi(x)\mathrm{d}\nu(x) \tag{97}$$

is now well-defined. In particular, the wave functions $\{\varphi_\nu\}$ have inner products $\langle\varphi_\mu|\varphi_\nu\rangle=\delta_{\mu\nu}K_\nu^2$ and norms that are nonvanishing for all integers $\nu\geqslant 0$. Thus, the Hilbert space $\mathcal{F}_\lambda$, isomorphic to $\mathbb{H}^\lambda$, is the completion of the space of holomorphic polynomials with respect to the inner product (97). Relative to this inner product, the normalized functions

$$\left\{\psi_{\lambda\nu}(z)=\frac{1}{K_\nu}\varphi_\nu(z)=\sqrt{\frac{(\lambda-1)!}{(\lambda+\nu-1)!\,\nu!}}z^\nu;\quad \nu=0,1,2,\ldots\right\} \tag{98}$$

form an orthonormal basis for $\mathcal{F}_\lambda$.

The (densely defined) map $\mathcal{F}_\lambda\to\mathbb{H}^\lambda$, with

$$\psi_{\lambda\nu}\to|\lambda\,\nu\rangle=\int e^{z^*\hat{J}_+}|0\rangle\psi_{\lambda\nu}(z)\mathrm{d}\nu(z), \tag{99}$$

and the coherent state map $\mathbb{H}^\lambda\to\mathcal{F}^\lambda;|\lambda\,\nu\rangle\to\Psi_{\lambda\nu}$, with

$$\Psi_{\lambda\nu}(z)=\langle 0|e^{z\hat{J}_-}|\lambda\,\nu\rangle=\int\langle 0|e^{z\hat{J}_-}e^{x^*\hat{J}_+}|0\rangle\psi_{\lambda\nu}(x)\mathrm{d}\nu(x)=\int\mathcal{S}(z,x)\psi_{\lambda\nu}(x)\mathrm{d}\nu(x), \tag{100}$$

define corresponding orthonormal bases

$$\left\{|\lambda\,\nu\rangle=\frac{1}{K_\nu}|\varphi_\nu\rangle=\sqrt{\frac{(\lambda-1)!}{(\lambda+\nu-1)!\,\nu!}}(\hat{J}_+)^\nu|0\rangle;\quad \nu=0,1,2,\ldots\right\}, \tag{101}$$

$$\left\{\Psi_{\lambda\nu}(z)=K_\nu\varphi_\nu(z)=\sqrt{\frac{(\lambda+\nu-1)!}{(\lambda-1)!\,\nu!}}z^\nu;\quad \nu=0,1,2,\ldots\right\}, \tag{102}$$

for $\mathbb{H}^\lambda$ and $\mathcal{F}^\lambda$, respectively.

Proceeding as for SU(2), we find that the coherent state representation Γ^λ of SU(1,1) acts on $\Psi(z)\in\mathcal{F}^\lambda$ by

$$[\Gamma^{\lambda}(g)\Psi](z)=(a^*+bz)^{-\lambda}\Psi(z\cdot g), \tag{103}$$

with

$$g=\begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix}, \quad z\cdot g=\frac{b^*+az}{a^*+bz}. \tag{104}$$

Matrices of the representation Γ^{λ} are easily evaluated in the basis (101). For example, for

$$g=\begin{pmatrix} c & s \\ s & c \end{pmatrix}, \quad c=\cosh\beta/2, \quad s=\sinh\beta/2, \tag{105}$$

an SU(1,1) Wigner function is given by

$$\begin{aligned}\langle\lambda\mu|T^{\lambda}(g)|\lambda\nu\rangle&=\int \psi^*_{\lambda\mu}(z)[\Gamma^{\lambda}(g)\Psi_{\lambda\nu}](z)\mathrm{d}v(z)\\ &=\frac{K_{\nu}}{K_{\mu}}\int \varphi^*_{\mu}(z)[\Gamma^{\lambda}(g)\varphi_{\nu}](z)\mathrm{d}v(z)\\ &=\sqrt{\frac{(\lambda+\nu-1)!}{(\lambda+\mu-1)!\mu!\nu!}}\int (z^*)^{\mu}(s+cz)^{\nu}(c+sz)^{-(\lambda+\nu)}\mathrm{d}v(z)\\ &=\sqrt{\frac{\mu!\nu!}{(\lambda+\mu-1)!(\lambda+\nu-1)!}}\sum_{n=0}^{\mu}(-1)^n\frac{(\lambda+\nu+n-1)!}{(\nu-\mu+n)!(\mu-n)!n!}\\ &\quad\times(\cosh\beta/2)^{\mu-\nu-\lambda-2n}(\sinh\beta/2)^{\nu-\mu+2n},\end{aligned} \tag{106}$$

cf. expressions obtained by Dunne[27] and Ui.[28]

Coherent state representations of the $\mathfrak{su}(1,1)$ Lie algebra have the known expressions

$$\Gamma^{\lambda}(J_+)=\lambda z+z^2\frac{d}{dz}, \quad \Gamma^{\lambda}(J_0)=\frac{1}{2}\lambda+z\frac{d}{dz}, \quad \Gamma^{\lambda}(J_-)=\frac{d}{dz}. \tag{107}$$

Acting on the orthonormal basis wave functions of Eq. (102), they give

$$\begin{aligned}\Gamma^{\lambda}(J_0)\Psi_{\lambda\nu}&=\tfrac{1}{2}(\lambda+2\nu)\Psi_{\lambda\nu},\\ \Gamma^{\lambda}(J_+)\Psi_{\lambda\nu}&=\sqrt{(\lambda+\nu)(\nu+1)}\,\Psi_{\lambda,\nu+1},\\ \Gamma^{\lambda}(J_-)\Psi_{\lambda,\nu}&=\sqrt{(\lambda+\nu-1)\nu}\,\Psi_{\lambda,\nu-1}.\end{aligned} \tag{108}$$

The inner product for $\mathcal{F}^{\lambda}$ is known to be given, for a holomorphic discrete series representation (for which λ is an integer greater than 1), by

$$\langle\psi|\varphi\rangle=\frac{\lambda-1}{\pi}\int_{|z|<1}\Psi^*(z)\Phi(z)(1-|z|^2)^{\lambda-2}\mathrm{d}^2z, \tag{109}$$

where $\Psi=\hat{\mathcal{S}}\psi$, $\Phi=\hat{\mathcal{S}}\varphi$ and the integral is over the interior of the unit disk.[27] When $\lambda>1$, this inner product is identical to that given for $\mathcal{F}_{\lambda}$ by Eq. (97). However, the latter is easier to evaluate. Moreover, unlike the integral of Eq. (109), it is defined for all non-negative values of λ and gives results, not only for SU(1,1), but also for its universal covering group.

C. The semidirect product group $[\mathbb{R}^6]$SO(3)

Let G be the semidirect product $[\mathbb{R}^6]\mathrm{SO}(3)$ of an Abelian normal subgroup $\mathbb{R}^6$, isomorphic to the additive group of real symmetric 3×3 matrices, and the rotation group SO(3). Elements of $[\mathbb{R}^6]\mathrm{SO}(3)$ are pairs of group elements, $\{(Q,\Omega);Q\in\mathbb{R}^6,\Omega\in\mathrm{SO}(3)\}$ with product

$$(Q,\Omega)\circ(Q',\Omega')=(Q+\Omega Q'\tilde{\Omega},\Omega\Omega'), \tag{110}$$

where $\tilde{\Omega}=\Omega^{-1}$ is the transpose of Ω. With Q expressed as a sum $Q=\Sigma_{ij}Q_{ij}\mathfrak{I}_{ij}$, where $\{\mathfrak{I}_{ij}\}$ is a basis of real symmetric matrices, this group is interpreted as the dynamical group of a rotor for which the corresponding Lie algebra is spanned by moments $\{\mathfrak{I}_{ij}\}$ of an inertia tensor $\mathfrak{I}$ and components $\{L_k\}$ of angular momentum [infinitesimal generators of SO(3)].

Let T be a UIR of G on a Hilbert space $\mathbb{H}$. The coherent-state construction of such an irrep mimics Mackey's induction.[3] The construction starts with a one-dimensional unitary irrep of the $\mathbb{R}^6$ subalgebra defined by a so-called *intrinsic inertia tensor* $\bar{\mathfrak{I}}$ which assigns numerical values $\bar{\mathfrak{I}}_{ij}$ to the moments of inertia $\mathfrak{I}_{ij}$; i.e.,

$$\bar{\mathfrak{I}}:\mathfrak{I}_{ij}\to\bar{\mathfrak{I}}_{ij}=\delta_{ij}\bar{\mathfrak{I}}_i. \tag{111}$$

A corresponding one-dimensional unitary irrep of the $\mathbb{R}^6$ group is then defined by

$$Q\to\chi^{-}_{\bar{\mathfrak{I}}}(Q)=e^{i\mathrm{Tr}(Q\bar{\mathfrak{I}})}. \tag{112}$$

Now let

$$D=\{\omega\in\mathrm{SO}(3)\,|\,\omega\bar{\mathfrak{I}}\tilde{\omega}=\bar{\mathfrak{I}}\}, \tag{113}$$

with $(\omega\bar{\mathfrak{I}}\tilde{\omega})_{ij}=\Sigma_{kl}\omega_{ik}\bar{\mathfrak{I}}_{kl}\omega_{jl}$, denote the isotropy subgroup of rotations that leave the intrinsic moments of inertia invariant. To be specific, we take the intrinsic moments of inertia $(\bar{\mathfrak{I}}_1,\bar{\mathfrak{I}}_2,\bar{\mathfrak{I}}_3)$ to be positive and distinct. Then D is the discrete group D_2 comprising the four rotations (parametrized in terms of Euler angles):

$$\omega_1\sim(0,0,0),\quad \omega_2\sim(0,\pi,0),\quad \omega_3\sim(\pi,0,0),\quad \omega_4=\omega_3\omega_2\sim(\pi,\pi,0). \tag{114}$$

This group has four irreps, all of which are one-dimensional. Thus, an irrep $\rho^{-}_{\bar{\mathfrak{I}},\varepsilon}$ of $[\mathbb{R}^6]D_2$ is defined by

$$(Q,\omega_i)\to\rho^{-}_{\bar{\mathfrak{I}},\varepsilon}(Q,\omega_i)=\chi^{-}_{\bar{\mathfrak{I}}}(Q)\varepsilon(\omega_i),\quad i=1,\ldots,4, \tag{115}$$

with $\varepsilon(\omega_1)=1$, $\varepsilon(\omega_2)=\pm 1$, $\varepsilon(\omega_3)=\pm 1$ and $\varepsilon(\omega_4)=\varepsilon(\omega_2)\varepsilon(\omega_3)$.

Let $\langle\bar{\mathfrak{I}},\varepsilon|$ be a functional on a suitably defined dense subspace $\mathbb{H}_D$ of $\mathbb{H}$ which *picks out* a particular irrep of the subgroup $[\mathbb{R}^6]D_2\subset[\mathbb{R}^6]\mathrm{SO}(3)$ in the sense that

$$\langle\bar{\mathfrak{I}},\varepsilon|T(Q,\omega)|\psi\rangle=\chi^{-}_{\bar{\mathfrak{I}}}(Q)\varepsilon(\omega)\langle\bar{\mathfrak{I}},\varepsilon|\psi\rangle,\quad \forall|\psi\rangle\in\mathbb{H}_D,\quad \forall\,\omega\in D_2. \tag{116}$$

A suitable dense subspace $\mathbb{H}_D$ is the SO(3)-invariant space of K-finite vectors in $\mathbb{H}$ comprising all states that are finite linear combinations of vectors from a multiplicity of SO(3) irreps. A coherent state wave function Ψ for a vector $|\psi\rangle\in\mathbb{H}_D$ is then defined by

$$\Psi(\Omega)=\langle\bar{\mathfrak{I}},\varepsilon|\hat{R}(\Omega)|\psi\rangle. \tag{117}$$

The space of such wave functions, $\mathcal{F}^{\mathbb{H}_D}$, carries a representation of $[\mathbb{R}^6]\mathrm{SO}(3)$ defined by

$$[\Gamma(Q,\Omega)\Psi](\Omega')=\langle\bar{\mathfrak{I}},\varepsilon|T(\Omega' Q\tilde{\Omega}',\Omega'\Omega)|\psi\rangle=\chi^{-}_{\bar{\mathfrak{I}}}(\Omega' Q\tilde{\Omega}')\Psi(\Omega'\Omega). \tag{118}$$

The action of Γ defined by Eq. (118) is unitary on $\mathcal{L}^2(\mathrm{SO}(3))$. Thus, we infer from Eq. (116) that the coherent state representation is realized on an irreducible subspace of $\mathcal{L}^2(\mathrm{SO}(3))$ that satisfies the constraint

$$\Psi(\omega\Omega)=\varepsilon(\omega)\Psi(\Omega), \quad \forall\,\omega\in D_2. \tag{119}$$

To construct the triplet, we start with an orthonormal basis for the space $\mathcal{F}=\mathcal{L}^2(\mathrm{SO}(3))$ given by functions

$$\varphi_{KLM}=\sqrt{\frac{2L+1}{8\pi^2}}\mathcal{D}^L_{KM}, \tag{120}$$

where $\mathcal{D}^L_{KM}$ is an SO(3) Wigner function. Consider the map $\mathcal{F}^*\to\mathbb{H}_D^*$ which sends

$$\varphi^*_{KLM}\mapsto\langle KLM|=\sqrt{\frac{2L+1}{8\pi^2}}\int \mathrm{d}\Omega\mathcal{D}^L_{KM}(\Omega)^*\langle\bar{\mathfrak{I}},\varepsilon|R(\Omega). \tag{121}$$

As a functional on $\mathbb{H}_D$, $\langle KLM|$ is nonzero on the finite-dimensional subspace consisting of copies of the SO(3) irrep with angular momentum L, but it is zero on the orthogonal complement of this space. In particular, it can be regarded as a linear functional on a finite-dimensional space, so it must actually be given by a vector in that space. The inner products of such vectors in $\mathbb{H}$ are then expressed

$$\begin{aligned}\langle K'L'M'|KLM\rangle&=\delta_{L'L}\delta_{M'M}\frac{2L+1}{8\pi^2}\int\int \mathcal{D}^L_{K'M}(\Omega')^*\langle\bar{\mathfrak{I}},\varepsilon|\hat{R}(\Omega'\Omega^{-1})|\bar{\mathfrak{I}},\varepsilon\rangle\mathcal{D}^L_{KM}(\Omega)\mathrm{d}\Omega\,\mathrm{d}\Omega'\\&=\delta_{L'L}\delta_{M'M}\int \mathcal{D}^L_{K'K}(\Omega)^*\langle\bar{\mathfrak{I}},\varepsilon|\hat{R}(\Omega)|\bar{\mathfrak{I}},\varepsilon\rangle\mathrm{d}\Omega.\end{aligned} \tag{122}$$

Thus, we obtain a densely defined sequence of maps $\mathcal{F}_D\to\mathbb{H}_D\to\mathcal{F}^{\mathbb{H}_D}$ in which $\varphi_{KLM}\mapsto|KLM\rangle\mapsto\Phi_{KLM}$, where the coherent state wave function Φ_{KLM} for the state $|KLM\rangle$ is given by

$$\Phi_{KLM}(\Omega)=\langle\bar{\mathfrak{I}},\varepsilon|\hat{R}(\Omega)|KLM\rangle=\int \mathcal{S}(\Omega\tilde{\Omega}')\varphi_{KLM}(\Omega')\mathrm{d}\Omega' \tag{123}$$

and $\mathcal{S}$ is the functional on $\mathcal{F}$ given by

$$\mathcal{S}(\Omega)=\langle\bar{\mathfrak{I}},\varepsilon|\hat{R}(\Omega)|\bar{\mathfrak{I}},\varepsilon\rangle. \tag{124}$$

Thus, the inner product for $\mathbb{H}$ is expressed in terms of the $\{|KLM\rangle\}$ basis,

$$\langle K'L'M'|KLM\rangle=\int \varphi^*_{K'L'M'}(\Omega)\Phi_{KLM}(\Omega)\mathrm{d}\Omega. \tag{125}$$

Clearly the functions φ_{KLM} and Φ_{KLM} are dual representations of the state vector $|KLM\rangle$ relative to the measure $\mathrm{d}\Omega$.

The norm of the functional $\langle\bar{\mathfrak{I}},\varepsilon|$, and hence of $\mathcal{S}$, is arbitrary. The essential requirement is that the coherent state functions $\{\Phi_{KLM}\}$ obtained from all basis functions $\{\varphi_{KLM}\}$ of $\mathcal{F}$ should satisfy the constraint condition of Eq. (119). Thus, $\mathcal{S}$ must satisfy the equation

$$\mathcal{S}(\omega\Omega)=\varepsilon(\omega)\mathcal{S}(\Omega), \quad \forall\,\omega\in \mathrm{D}_2. \tag{126}$$

From its definition, Eq. (124), $\mathcal{S}$ also satisfies the equation

$$(\Omega\bar{\mathcal{I}}\tilde{\Omega})\mathcal{S}(\Omega)=\bar{\mathcal{I}}\mathcal{S}(\Omega),\quad \forall\Omega\in \mathrm{SO}(3). \tag{127}$$

Thus, to within an arbitrary norm factor, it has the unique solution

$$\mathcal{S}(\Omega)=\frac{1}{4}\sum_{\omega\in \mathrm{D}_2}\varepsilon(\omega)\delta(\Omega,\omega). \tag{128}$$

With this normalization,

$$\begin{aligned}\Phi_{KLM}(\Omega)&=\sqrt{\frac{2L+1}{8\pi^2}}\int \mathrm{d}\Omega'\mathcal{S}(\Omega\tilde{\Omega}')\mathcal{D}^L_{KM}(\Omega')\\ &=\sqrt{\frac{2L+1}{8\pi^2}}\frac{(1+(-1)^K\varepsilon_3)}{4}(\mathcal{D}^L_{KM}(\Omega)+(-1)^{L+K}\varepsilon_2\mathcal{D}^L_{-K,M}(\Omega)),\end{aligned} \tag{129}$$

where $\varepsilon_2=\varepsilon(\omega_2)$ and $\varepsilon_3=\varepsilon(\omega_3)$.

It is seen that the states $\{|KLM\rangle\}$ are not all linearly independent. In particular, the wave functions Φ_{KLM} with $(-1)^K\varepsilon(\omega_3)=-1$ vanish as do those with $K=0$ and $(-1)^L\varepsilon_2=-1$. Moreover, the wave functions $\Phi_{\pm KLM}$ differ by only a phase factor. Thus, it is appropriate to restrict to labels KLM with $K\geqslant 0$ and nonvanishing wave functions Φ_{KLM}. The subspace of $\mathcal{F}$ spanned by the corresponding restricted basis functions $\{\varphi_{KLM}\}$ is then isomorphic, as a vector space, to the space obtained by factoring out the kernel of the map $\mathcal{F}\to\mathbb{H}$.

With $|KLM\rangle$ restricted in this way, the overlaps are given by

$$\langle K'L'M'|KLM\rangle=\int \varphi^*_{K'L'M'}(\Omega)\Phi_{KLM}(\Omega)d\Omega=\frac{1}{2}(1+\delta_{K,0})\,\delta_{L'L}\delta_{M'M}\delta_{K'K}. \tag{130}$$

The triplet of Hilbert spaces $\mathcal{F}_{\mathrm{H}}\sim\mathbb{H}\sim\mathcal{F}^{\mathrm{H}}$ is then defined with orthornormal bases given, respectively, by

$$\begin{gathered}\left\{\psi_{KLM}=\sqrt{\frac{2L+1}{4\pi^2(1+\delta_{K,0})}}\mathcal{D}^L_{KM};\quad K\geqslant 0\right\},\\ \left\{\sqrt{\frac{2}{(1+\delta_{K,0})}}|KLM\rangle;\quad K\geqslant 0\right\},\\ \left\{\Psi_{KLM}=\sqrt{\frac{2L+1}{16\pi^2(1+\delta_{K,0})}}[\mathcal{D}^L_{KM}+\varepsilon_2(-1)^{L+K}\mathcal{D}^L_{-K,M}];\quad K\geqslant 0\right\},\end{gathered} \tag{131}$$

with K restricted to even or odd integer values according as $\varepsilon_3=\pm 1$ and with L restricted to even or odd integer values when $K=0$ according as $\varepsilon_2=\pm 1$.

These wave functions satisfy the orthogonality relations

$$\int \psi^*_{KLM}(\Omega)\psi_{K'L'M'}\mathrm{d}\Omega=\delta_{LL'}\delta_{KK'}\delta_{MM'}. \tag{132}$$

In addition, with the chosen norm for $\mathcal{S}(\Omega)$, the coherent state wave functions on their own also satisfy

$$\int \Psi^*_{KLM}(\Omega)\psi_{K'L'M'}\mathrm{d}\Omega=\delta_{LL'}\delta_{KK'}\delta_{MM'}. \tag{133}$$

This is a special case that arises because the appropriate volume element for the Hilbert space of coherent-state wave functions for the rotor group happens to be the SO(3)-invariant volume. A

similar result occurs for the Heisenberg–Weyl group with the Bargmann measure. It is nevertheless useful to see this special case in the context of the general construction which can be applied when the end results are less easily anticipated. The following derivation of SU(3) irreps in an SO(3) basis is an example for which the construction is used with considerable advantage.

D. SU(3)⊃SO(3)

Let $|\lambda\mu\rangle$ denote a highest weight state for an SU(3) irrep $T^{(\lambda\mu)}$ of highest weight (λ,μ) with respect to the diagonal Cartan subgroup. It is known that the Hilbert space $\mathbb{H}^{(\lambda\mu)}$ for such an irrep is spanned by the set of states generated by rotating the state $|\lambda\mu\rangle$ with the elements of the subgroup $\mathrm{SO}(3)\subset\mathrm{SU}(3)$.[29] Thus, we may take N to be SO(3) and consider the coherent state representation in which a vector $|\psi\rangle\in\mathbb{H}^{(\lambda\mu)}$ is represented by a wave function over SO(3) with values

$$\Psi(\Omega)=\langle\lambda\mu|\hat{R}(\Omega)|\psi\rangle,\quad \Omega\in\mathrm{SO}(3), \tag{134}$$

where $\hat{R}$ is the restriction of $T^{(\lambda\mu)}$ to the $\mathrm{SO}(3)\subset\mathrm{SU}(3)$ subgroup.

Let $\mathcal{F}=\mathcal{L}^2(\mathrm{SO}(3))$ be the square integrable functions on SO(3) relative to its invariant measure $\mathrm{d}\Omega$. The map $\mathcal{F}\to\mathbb{H}^{(\lambda\mu)}$ is then

$$\varphi\to|\varphi\rangle=\int \hat{R}(\Omega^{-1})|\lambda\mu\rangle\varphi(\Omega)\mathrm{d}\Omega \tag{135}$$

and the space $\mathcal{F}_{(\lambda\mu)}$ isomorphic to $\mathbb{H}^{(\lambda\mu)}$ is defined by the inner product

$$(\psi,\varphi)=\langle\psi|\varphi\rangle=\int\int \psi^*(\Omega')\mathcal{S}(\Omega'\tilde{\Omega})\varphi(\Omega)\mathrm{d}\Omega'\mathrm{d}\Omega, \tag{136}$$

where

$$\mathcal{S}(\Omega)=\langle\lambda\mu|\hat{R}(\Omega)|\lambda\mu\rangle. \tag{137}$$

The overlap kernel $\mathcal{S}$ is easily evaluated by considering a realization of the SU(3) irrep in a Bargmann space[11] in which the highest weight state $|\lambda\mu\rangle$ is represented by the wave function $\phi_{\lambda\mu}$ with values

$$\phi_{\lambda\mu}(\mathbf{r},\mathbf{r}')\propto z^\lambda Y^\mu, \tag{138}$$

where z is a component of a complex vector $\mathbf{r}\equiv(x,y,z)$ and Y is a component of $\mathbf{r}\times\mathbf{r}'\equiv(X,Y,Z)$. Thus, with

$$[\hat{R}(\Omega)\phi_{\lambda\mu}](\mathbf{r},\mathbf{r}')=\phi_{\lambda\mu}(\mathbf{r}\Omega,\mathbf{r}'\Omega), \tag{139}$$

and $\Omega\equiv(\alpha,\beta,\gamma)$ parametrized by Euler angles, $\mathcal{S}$ is given by[30]

$$\mathcal{S}(\Omega)=\langle\lambda\mu|\hat{R}(\Omega)|\lambda\mu\rangle=(\cos\beta)^\lambda(\cos\alpha\cos\gamma-\sin\alpha\cos\beta\sin\gamma)^\mu. \tag{140}$$

From the Bargmann representation, it is also apparent that the state $|\lambda\mu\rangle$ spans a one-dimensional representation of the D_2 subgroup of SO(3) in which, in the notations of Eq. (114),

$$\hat{R}(\omega)|\lambda\mu\rangle=\varepsilon(\omega)|\lambda\mu\rangle,\quad \omega\in D_2, \tag{141}$$

with

$$\varepsilon(\omega_2)=(-1)^\lambda,\quad \varepsilon(\omega_3)=(-1)^\mu. \tag{142}$$

Thus, the SU(3) coherent state wave functions satisfy the symmetry property

$$\Psi(\omega\Omega)=\varepsilon(\omega)\Psi(\Omega), \quad \omega\in D_2. \tag{143}$$

According to the Peter–Weyl theorem,[31] a basis for $\mathcal{F}=\mathcal{L}^2(\mathrm{SO}(3))$ is given by the functions

$$\varphi_{KLM}=\sqrt{\frac{2L+1}{8\pi^2}}\mathcal{D}^L_{KM}, \tag{144}$$

where $\mathcal{D}^L_{KM}$ is an SO(3) Wigner (matrix coefficient) function. These functions satisfy

$$\int \varphi^*_{KLM}(\Omega)\varphi_{K'L'M'}(\Omega)\mathrm{d}\Omega=\delta_{LL'}\delta_{KK'}\delta_{MM'}. \tag{145}$$

The map $\mathcal{F}\to\mathbb{H}^{(\lambda\mu)}$ then gives

$$\varphi_{KLM}\to|KLM\rangle=\sqrt{\frac{2L+1}{8\pi^2}}\int \hat{R}(\Omega^{-1})|\lambda\mu\rangle\mathcal{D}^L_{KM}(\Omega)\mathrm{d}\Omega. \tag{146}$$

A maximal linearly independent subset of the states $\{|KLM\rangle\}$ comprises a so-called *Elliott basis* for $\mathbb{H}^{(\lambda\mu)}$. From Eq. (136), the overlaps of Elliott states are given by

$$\begin{aligned}\langle K'L'M'|KLM\rangle&=\delta_{L'L}\delta_{M'M}\frac{2L+1}{8\pi^2}\int\int \mathcal{D}^L_{K'M}(\Omega')^*\mathcal{S}(\Omega'\tilde{\Omega})\mathcal{D}^L_{KM}(\Omega)\mathrm{d}\Omega'\mathrm{d}\Omega\\&=\delta_{L'L}\delta_{M'M}\int \mathcal{D}^L_{K'K}(\Omega)^*\mathcal{S}(\Omega)\mathrm{d}\Omega.\end{aligned} \tag{147}$$

Let $\mathcal{S}^L$ be the SO(3)-invariant matrix of overlaps with elements

$$\mathcal{S}^L_{K'K}=\langle K'LM|KLM\rangle=\int \mathcal{D}^L_{K'K}(\Omega)^*\mathcal{S}(\Omega)\mathrm{d}\Omega. \tag{148}$$

From the symmetry property (143), it follows that

$$\mathcal{S}^L_{K'K}=(-1)^{\mu+K'}\mathcal{S}^L_{K'K}=(-1)^{\mu+K}\mathcal{S}^L_{K'K}=(-1)^{\lambda+L+K'}\mathcal{S}^L_{-K',K}=(-1)^{\lambda+L+K}\mathcal{S}^L_{K',-K}. \tag{149}$$

Thus, $\mathcal{S}^L_{K'K}$ is zero unless $(-1)^{K'}=(-1)^K=(-1)^\mu$ and, for K or $K'=0$, unless $(-1)^{\lambda+L}=1$. Then, with $\{|KLM\rangle\}$ restricted to a maximal linearly independent set of states with nonzero norms, the matrix $\mathcal{S}^L$ is Hermitian positive definite and can be expressed as a product $\mathcal{S}^L=\mathcal{K}(L)\mathcal{K}^\dagger(L)$; i.e.,

$$\mathcal{S}^L_{K'K}=\sum_\gamma \mathcal{K}_{K'\gamma}(L)\mathcal{K}^*_{K\gamma}(L). \tag{150}$$

Now, if we define $\overline{\mathcal{K}}(L)$ to be the inverse of the matrix $\mathcal{K}^\dagger(L)$, so that

$$\sum_{K\geqslant 0}\mathcal{K}^*_{K\beta}(L)\overline{\mathcal{K}}_{K\alpha}(L)=\delta_{\alpha\beta}, \tag{151}$$

then the transformed basis states,

$$|\alpha LM\rangle=\sum_K |KLM\rangle\overline{\mathcal{K}}_{K\alpha}(L), \tag{152}$$

satisfy

$$\langle \beta L' M' | \alpha L M \rangle = \delta_{LL'} \delta_{MM'} \sum_{K' K \gamma} \overline{\mathcal{K}}^*_{K' \beta}(L) \mathcal{K}_{K' \gamma}(L) \mathcal{K}^*_{K \gamma}(L) \overline{\mathcal{K}}_{K \alpha}(L) = \delta_{LL'} \delta_{MM'} \delta_{\beta \alpha} \quad (153)$$

and form an orthonormal basis.

Coherent state wave functions corresponding to the nonorthonormal $\{|KLM\rangle\}$ states are given by

$$\Phi_{KLM}(\Omega') = [\hat{\mathcal{S}} \varphi_{KLM}](\Omega') = \int \mathcal{S}(\Omega' \tilde{\Omega}) \varphi_{KLM}(\Omega) \mathrm{d}\Omega. \quad (154)$$

Therefore, the coefficients in the expansion

$$\Phi_{KLM}(\Omega) = \sum_{K'} a_{K'}(KL) \mathcal{D}^L_{K' M}(\Omega) \quad (155)$$

are given by

$$a_{K'}(KL) = \frac{2L+1}{8\pi^2} \int \mathcal{D}^L_{K' M}(\Omega)^* \Phi_{KLM}(\Omega) \mathrm{d}\Omega = \sqrt{\frac{2L+1}{8\pi^2}} \int \mathcal{D}^L_{K' K}(\Omega)^* \mathcal{S}(\Omega) \mathrm{d}\Omega. \quad (156)$$

It follows that

$$\begin{aligned} a_{K'}(KL) &= \sqrt{\frac{2L+1}{8\pi^2}} \mathcal{S}^L_{K' K}, \\ a_{-K'}(KL) &= (-1)^{\lambda + L + K'} a_{K'}(KL), \end{aligned} \quad (157)$$

and

$$\Phi_{KLM}(\Omega) = \sum_{K' \geqslant 0} \sqrt{\frac{2L+1}{8\pi^2}} [\mathcal{D}^L_{K' M}(\Omega) + (-1)^{\lambda + L + K'} \mathcal{D}^L_{-K' M}(\Omega)] \frac{1}{1+\delta_{K'0}} \mathcal{S}^L_{K' K}. \quad (158)$$

Because of the symmetries of the $\mathcal{S}$ matrix, given by Eq. (149), these wave functions vanish unless $(-1)^{\mu+K} = 1$ and, for $K = 0$, unless $(-1)^{\lambda+L} = 1$. Furthermore, the wave functions $\Phi_{\pm KLM}$ differ by only a phase factor. Thus, with L and K restricted to a subset of values such that the matrices $\mathcal{S}^L$ are positive definite (so that no linear combinations of the wave functions Φ_{KLM} vanish), an orthornormal basis for $\mathcal{F}_{\lambda \mu}$ is given by wave functions

$$\psi_{KLM}(\Omega) = \sum_{K \geqslant 0} \overline{\mathcal{K}}_{K \alpha}(L) \varphi_{KLM}(\Omega) = \sqrt{\frac{2L+1}{8\pi^2}} \sum_{K \geqslant 0} \overline{\mathcal{K}}_{K \alpha}(L) \mathcal{D}^L_{KM}(\Omega) \quad (159)$$

and a corresponding orthonormal basis of coherent state wave functions is given by

$$\begin{aligned} \Psi_{\alpha LM}(\Omega) &= \sum_{K \geqslant 0} \overline{\mathcal{K}}_{K \alpha}(L) \Phi_{KLM}(\Omega) \\ &= \sum_{K \geqslant 0} \sqrt{\frac{2L+1}{8\pi^2}} \frac{\mathcal{K}_{K \alpha}(L)}{1+\delta_{K0}} [\mathcal{D}^L_{KM}(\Omega) + (-1)^{\lambda+L+K} \mathcal{D}^L_{-KM}(\Omega)]. \end{aligned} \quad (160)$$

These expressions are in agreement with known results.[32,25] An explicit expression for the overlap kernel $\mathcal{S}^L_{K' K}$ is given in Ref. 25.

For a multiplicity-free representation, the $\mathcal{K}$ matrices reduce to simple numbers. For example, for an irrep of highest weight $(\lambda,\mu=0)$,

$$|\mathcal{K}(L)|^2=\langle LM|LM\rangle=4\pi^2\int_0^\pi d^L_{00}(\beta)(\cos\beta)^\lambda\sin\beta\mathrm{d}\beta. \tag{161}$$

The identity

$$\int_0^\pi d^L_{00}(\beta)(\cos\beta)^\lambda\sin\beta\mathrm{d}\beta=\int_0^1 P_L(x)x^\lambda\mathrm{d}x=\frac{\lambda!}{(\lambda-L)!!(\lambda+L+1)!!}, \tag{162}$$

inferrred from Eq. 8.14.15 of Abramowitz and Stegun,[33] then gives

$$|\mathcal{K}(L)|^2=4\pi^2\frac{\lambda!}{(\lambda-L)!!(\lambda+L+1)!!}[1+(-1)^{\lambda+L}]. \tag{163}$$

The corresponding ratios

$$\left|\frac{\mathcal{K}(L)}{\mathcal{K}(L-2)}\right|^2=\frac{\lambda-L+2}{\lambda+L+1} \tag{164}$$

agree with those derived previously[32] by requiring the representation to be unitary.

The coherent state representation of the su(3) Lie algbra is relatively simple and given explicitly in Ref. 32. The action of a group element $g\in\mathrm{SU}(3)$ on a coherent state wave function Ψ, defined by

$$[\Gamma(g)\Psi](\Omega)=\langle\lambda\mu|T^{\lambda\mu}(\Omega g)|\psi\rangle,\quad \Omega\in\mathrm{SO}(3)\subset\mathrm{SU}(3), \tag{165}$$

is more complicated. It can be obtained from the generalized Iwasawa factorization for which

$$g=Z(g)\omega(g), \tag{166}$$

where $Z(g)$ is a lower triangular matrix of the form

$$Z(g)=\begin{pmatrix} z_{11}(g) & 0 & 0\\ z_{21}(g) & z_{22}(g) & 0\\ z_{31}(g) & z_{32}(g) & z_{33}(g)\end{pmatrix} \tag{167}$$

and $\omega(g)\in\mathrm{SO}(3,\mathbb{C})$ is a complex orthogonal matrix. It follows that

$$[\Gamma(g)\Psi](\Omega)=(z_{11}(\Omega g))^{\lambda+\mu}(z_{22}(\Omega g))^{\mu}\Psi(\omega(\Omega g)), \tag{168}$$

where

$$\begin{aligned} z^2_{11}(g)&=\sum_i g^2_{1i},\\ z^2_{11}(g)z^2_{22}(g)&=\sum_i g^2_{1i}\sum_j g^2_{2j}-\sum_i (g_{1i}g_{2i})^2. \end{aligned} \tag{169}$$

The above techniques for constructing orthornormal bases were used effectively in Ref. 25 for computing SU(3) Clebsch-Gordan in an SO(3)-coupled basis.

IV. SCALAR COHERENT-STATE REPRESENTATIONS OF SEMISIMPLE LIE GROUPS

There are four classes of scalar holomorphic discrete series representations of semisimple Lie groups all of which are expressible as coherent state representations over classical domains. They are constructed when a coherent-state representation of a semisimple Lie group G is induced from a one-dimensional irrep ρ of a subgroup $K\subset G$ for which G/K is a Hermitian symmetric space. These spaces have been studied in depth by Helgason.[34] The classical domains which we discuss here were identified by Cartan.[35] The associated coherent state representations have been summarized by Hua[36] and Perelomov.[13]

Hermitian symmetric spaces[34] are easily identified at the Lie algebra level. If G is semisimple and H is a reductive subgroup of G, then G/H is a Hermitian symmetric space if the complex extension $\mathfrak{g}^c$ of the Lie algebra of G has decomposition

$$\mathfrak{g}^c=\mathfrak{h}^c+\mathfrak{n}_+ +\mathfrak{n}_- , \tag{170}$$

such that $\mathfrak{g}^c$ and $\mathfrak{h}^c$ have a Cartan subalgebra in common, $\mathfrak{n}_\pm$ are Abelian, and

$$[C,A]\in\mathfrak{n}_+ , \quad [C,B]\in\mathfrak{n}_- , \quad [A,B]\in\mathfrak{h}^c, \tag{171}$$

for all $A\in\mathfrak{n}_+$, $B\in\mathfrak{n}_-$, and $C\in\mathfrak{h}^c$. There are then holomorphic representations of G with highest weight states which carry one-dimensional irreps of H. These representations have simple expressions as scalar coherent state representations.

A. SU($p+q$) and SU(p,q)

The Lie algebras of SU$(p+q)$ and SU(p,q) have a common complex extension $\mathfrak{su}(n)^c \sim A_{n-1}=\mathfrak{sl}(n,\mathbb{C})$ with $n=p+q$. The latter is spanned by traceless linear combinations of the matrices $\{C_{\alpha\beta}\}$, where $C_{\alpha\beta}$ is an $n\times n$ matrix with entries $(C_{\alpha\beta})_{ij}=\delta_{\alpha i}\delta_{\beta j}$.

Let T^σ denote an irrep of A_{n-1}, with $T^\sigma(C_{\alpha\beta})=\hat{C}_{\alpha\beta}$, on a Hilbert space $\mathbb{H}^\sigma$ having highest weight state $|0\rangle$ and highest weight $(\sigma\ldots\sigma;0\ldots0)$ defined by

$$\begin{aligned}&\hat{C}_{i\nu}|0\rangle=\hat{C}_{ij}|0\rangle=\hat{C}_{\mu\nu}|0\rangle=0,\\ &\hat{C}_{ii}|0\rangle=\sigma|0\rangle, \quad \hat{C}_{\nu\nu}|0\rangle=0, \quad i<j<\mu<\nu,\end{aligned} \tag{172}$$

where i and j run over the range $1,\ldots,p$ and μ and ν run over the range $p+1,\ldots,n=p+q$. If λ is a positive integer, then, when $\sigma=+\lambda$, this irrep integrates to a unitary irrep of SU$(p+q)$; it integrates to a unitary irrep of SU(p,q) when $\sigma=-\lambda$. In both cases, the subgroup of elements that leave the highest weight state $|0\rangle$ invariant (to within a phase factor) is the subgroup of U$(p)\times$U(q) matrices

$$\mathrm{S}[\mathrm{U}(p)\times\mathrm{U}(q)]=\left\{\begin{pmatrix}a&0\\0&b\end{pmatrix}\middle| a\in\mathrm{U}(p),b\in\mathrm{U}(q),\det b=[\det a]^{-1}\right\}. \tag{173}$$

It follows that the highest weight state $|0\rangle$ is a single basis vector for the one-dimensional irrep ρ_σ of S$[\mathrm{U}(p)\times\mathrm{U}(q)]$ for which

$$\rho_\sigma\begin{pmatrix}a&0\\0&b\end{pmatrix}=[\det a]^\sigma. \tag{174}$$

Let $\mathbb{H}_D\subseteq\mathbb{H}^\sigma$ be the space of "K-finite vectors," that is, the vectors obtained by applying polynomials in the lowering operators to the state $|0\rangle$. For $G=\mathrm{SU}(p+q)$, where $\mathbb{H}^\sigma$ is finite-dimensional, this will be all of $\mathbb{H}^\sigma$, but for $G=\mathrm{SU}(p,q)$, it is a dense subspace.

Gauss factorization of almost any SL$(p+q,\mathbb{C})$ matrix gives

$$g=\begin{pmatrix} a & b \\ c & d \end{pmatrix}=\begin{pmatrix} I_p & 0 \\ x & I_q \end{pmatrix}\begin{pmatrix} a & 0 \\ 0 & d-cz \end{pmatrix}\begin{pmatrix} I_p & z \\ 0 & I_q \end{pmatrix} \tag{175}$$

with $z=a^{-1}b$, $x=ca^{-1}$, and with I_p the $p\times p$ identity matrix. It follows that, for an irrep T^σ of $G=\mathrm{SU}(p+q)$ or $G=\mathrm{SU}(p,q)$ with highest weight state $|0\rangle$ and highest weight $(\sigma\ldots\sigma;0\ldots0)$, the coherent state wave functions satisfy

$$\langle 0|T^\sigma(g)|\psi\rangle=[\det a]^\sigma\langle 0|e^{\hat{z}}|\psi\rangle, \quad g=\begin{pmatrix} a & b \\ c & d \end{pmatrix}\in G, \tag{176}$$

where $\hat{z}=\Sigma_{i\nu}z_{i\nu}\hat{C}_{i\nu}$, for any $|\psi\rangle\in\mathbb{H}_D$. Accordingly, a suitable choice of $N\subset\mathrm{SU}(p+q)^c$ is the subgroup of upper triangular matrices

$$N=\left\{\begin{pmatrix} I_p & z \\ 0 & I_q \end{pmatrix};z\in\mathbb{C}^{p\times q}\right\}. \tag{177}$$

A coherent state wave function Ψ for a state $|\psi\rangle\in\mathbb{H}_D$ is then defined by

$$\Psi(z)=\langle 0|e^{\hat{z}}|\psi\rangle \tag{178}$$

and is seen to be a polynomial in the matrix coefficients of z.

The coherent state action $\Gamma(g)$ of a matrix

$$g=\begin{pmatrix} a & b \\ c & d \end{pmatrix}\in G, \tag{179}$$

defined for $\psi\in\mathbb{H}_D$ by

$$[\Gamma(g)\Psi](z)=\langle 0|e^{\hat{z}}T^\sigma(g)|\psi\rangle, \tag{180}$$

is determined by the generalized Gauss factorization of the product

$$\begin{pmatrix} I_p & z \\ 0 & I_q \end{pmatrix}\begin{pmatrix} a & b \\ c & d \end{pmatrix}=\begin{pmatrix} I_p & 0 \\ x & I_q \end{pmatrix}\begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix}\begin{pmatrix} I_p & y \\ 0 & I_q \end{pmatrix}, \tag{181}$$

with

$$\alpha=a+zc, \quad y=(a+zc)^{-1}(b+zd). \tag{182}$$

This gives

$$\langle 0|e^{\hat{z}}T(g)|\psi\rangle=[\det\alpha]^\sigma\langle 0|e^{\hat{y}}|\psi\rangle \tag{183}$$

and

$$[\Gamma(g)\Psi](z)=[\det(a+zc)]^\sigma\Psi((a+zc)^{-1}(b+zd)). \tag{184}$$

The space $\mathcal{F}^{\mathbb{H}}$ of coherent state wave functions is identified in the standard way. Let $\mathcal{F}$ be the Bargmann space of entire analytic functions in the z variables, i.e., $\mathcal{F}$ is the space $\mathcal{L}^2(\mathbb{C}^{p\times q},\mathrm{d}v)$, where $\mathrm{d}v$ is the Bargmann measure on $\mathbb{C}^{p\times q}$. The map of Eq. (35)

$$\mathcal{F}^*\to\mathbb{H}_D^*;\varphi^*\mapsto\langle\varphi|=\int \mathrm{d}v(z)\varphi^*(z)\langle 0|T^\sigma(z) \tag{185}$$

then takes a polynomial $\varphi^* \in \mathcal{F}^*$ to a vector $\langle 0|\varphi(\hat{C})^\dagger$ in $\mathbb{H}^* \cong \mathbb{H}$, where $\varphi(\hat{C})$ is the operator obtained by replacing every $z_{i\nu}$ in $\varphi(z)$ by the corresponding operator $\hat{C}_{i\nu}$. It follows that the dense subspace $\mathcal{F}_D$ of polynomials in $\mathcal{F}$ maps onto the dense subspace $\mathbb{H}_D \subset \mathbb{H}$ as required. Thus, the Hilbert space $\mathcal{F}_{\mathbb{H}}$ is a space of holomorphic functions with inner product

$$\langle \varphi|\psi\rangle = \int \varphi^*(z)\mathcal{S}^\sigma(z,x)\psi(x)\mathrm{d}v(z)\mathrm{d}v(x), \tag{186}$$

where $\mathcal{S}^\sigma(z,x)$ is the overlap kernel

$$\mathcal{S}^\sigma(z,x) = \langle 0|e^{\hat{z}}e^{\hat{x}^\dagger}|0\rangle. \tag{187}$$

Let $\{\psi_n\}$ denote an orthonormal polynomial basis for $\mathcal{F}_{\mathbb{H}}$. An orthonormal basis$\{|n\rangle\}$ for $\mathbb{H}$ is then defined by the map

$$\mathcal{F}_D \to \mathbb{H}_D ; \psi_n \mapsto |n\rangle \tag{188}$$

and a corresponding orthonormal basis $\{\Psi_n\}$ of coherent state wave functions for $\mathcal{F}^{\mathbb{H}}$ is defined by

$$\Psi_n(z) = \int \mathcal{S}^\sigma(z,x)\psi_n(x)\mathrm{d}v(x). \tag{189}$$

These bases for $\mathcal{F}_{\mathbb{H}}$ and $\mathcal{F}^{\mathbb{H}}$ are in duality relative to the inner product defined by $\mathrm{d}v$, i.e.,

$$\langle m|n\rangle = \int \psi_m^*(z)\Psi_n(z)\mathrm{d}v(z), \tag{190}$$

and matrix elements of the representation are given by

$$\langle m|T(g)|n\rangle = \int \psi_m^*(z)[\Gamma(g)\Psi_n](z)\mathrm{d}v(z). \tag{191}$$

For a finite-dimensional irrep, the raising and lowering operators satisfy the Hermitian adjoint relationship

$$\hat{C}_{i\nu}^\dagger = \hat{C}_{\nu i}. \tag{192}$$

Therefore, the overlap kernel for a unitary irrep of SU$(p+q)$, derived as for SU(2), is given by

$$\mathcal{S}^{\sigma=\lambda}(z,x) = \langle 0|e^{\hat{z}}e^{\hat{x}^\dagger}|0\rangle = [\det(I_p + zx^\dagger)]^\lambda. \tag{193}$$

For an infinite-dimensional unitary representation of SU(p,q), for which $\hat{C}_{i\nu}^\dagger = -\hat{C}_{\nu i}$, the overlap kernel is calculated in a manner analogous to that used to find Eq. (92) for SU(1,1); the result is given formally by

$$\mathcal{S}^{\sigma=-\lambda}(z,x) = \langle 0|e^{\hat{z}}e^{\hat{x}^\dagger}|0\rangle = [\det(I_p - zx^\dagger)]^{-\lambda}. \tag{194}$$

This expression does not converge for $|zx^\dagger| \geqslant 1$. However, it is well-defined as a distribution over the polynomial functions of $\mathcal{F}_D$ with the understanding that $\hat{\mathcal{S}}^{-\lambda}\psi$ is defined by the integral

$$[\hat{\mathcal{S}}^{-\lambda}\psi](z) = \int \mathrm{Taylor}(\mathcal{S}^{-\lambda}(z,x))\psi(x)\mathrm{d}v(x), \tag{195}$$

where Taylor $(\mathcal{S}^{-\lambda}(z,x))$ is an expansion of $\mathcal{S}^{-\lambda}(z,x)$ as a Taylor series in $zx^\dagger$ and the integration is performed term by term.

It is useful to note that, for both $G=\mathrm{SU}(p+q)$ and $G=\mathrm{SU}(p,q)$, the above construction leads naturally to irreps in bases that reduce the subgroup $\mathrm{S}[\mathrm{U}(p)\times\mathrm{U}(q)]\subset G$. First observe that the action on $\mathcal{F}$ of an element

$$h=\begin{pmatrix} a & 0 \\ 0 & d \end{pmatrix} \in \mathrm{S}[\mathrm{U}(p)\times\mathrm{U}(q)], \tag{196}$$

given by Eq. (184), i.e.,

$$[\Gamma(h)\varphi](x)=[\det a]^{\sigma}\varphi(a^{\dagger}xd), \tag{197}$$

is unitary. This follows from the observation that the inner product for $\mathcal{F}$, which is expressible in the form

$$\int \psi^*(x)\varphi(x)\mathrm{d}v(x)=[\psi(\partial/\partial x)\varphi(x)]_{x=0}, \tag{198}$$

satisfies the identity

$$\int \psi^*(a^{\dagger}xd)\varphi(a^{\dagger}xd)\mathrm{d}v(x)=\int \psi^*(x)\varphi(x)\mathrm{d}v(x), \tag{199}$$

and is manifestly $\mathrm{S}[\mathrm{U}(p)\times\mathrm{U}(q)]$ invariant. Thus, if $\{\varphi_{\kappa\nu}\}$ is an orthonormal $\mathrm{S}[\mathrm{U}(p)\times\mathrm{U}(q)]$-coupled basis for $\mathcal{F}$, then $\hat{\mathcal{S}}^{\sigma}$ is diagonal and $\mathcal{S}^{\sigma}(z,x)$ is expressible

$$\mathcal{S}^{\sigma}(z,x)=\sum_{\kappa\nu} K_{\kappa}^2\varphi_{\kappa\nu}(z)\varphi_{\kappa\nu}^*(x), \tag{200}$$

where

$$K_{\kappa}^2=\int\int \varphi_{\kappa\nu}^*(z)\mathcal{S}^{\sigma}(z,x)\varphi_{\kappa\nu}(x)\mathrm{d}v(z)\mathrm{d}v(x), \tag{201}$$

is independent of ν.

It is now relatively straightforward to construct an orthonormal $\mathrm{S}[\mathrm{U}(p)\times\mathrm{U}(q)]$ basis for the Bargmann space $\mathcal{F}$ and to map it to orthonormal bases for $\mathcal{F}_{\mathrm{H}}$ and $\mathcal{F}^{\mathrm{H}}$. First observe that, in the coherent state representation, the $\mathrm{U}(p)$ and $\mathrm{U}(q)$ operators are given, respectively, by

$$\Gamma(C_{ij})=\sigma\delta_{ij}-\sum_{\nu} z_{j\nu}\partial_{i\nu}, \tag{202}$$

$$\Gamma(C_{\mu\nu})=\sum_{i} z_{i\mu}\partial_{i\nu}, \tag{203}$$

where

$$\partial_{i\nu}=\frac{\partial}{\partial z_{i\nu}}. \tag{204}$$

To simplify the notation, relabel the z indices such that $z_{p+1-i,p+\nu}$ becomes $z_{i\nu}$. The variables $\{z_{i\nu}\}$ are then ordered by their weights with $z_{i\mu}$ being of higher weight than $z_{j\nu}$ if $i<j$ or if $i=j$ and $\mu<\nu$. The space $\mathcal{F}$ is now seen to be a direct sum of irreducible $\mathrm{S}[\mathrm{U}(p)\times\mathrm{U}(q)]$ subspaces spanned by homogeneous polynomials in the $\{z_{i\nu}\}$ variables. Consider the polynomial

$$\varphi_{\kappa\kappa}(z)=N_{\kappa}Z_1^{\kappa_1-\kappa_2}(z)Z_2^{\kappa_2-\kappa_3}(z)\cdots Z_m^{\kappa_m}(z), \tag{205}$$

indexed by a sequence $\kappa=(\kappa_1,\kappa_2,\ldots,\kappa_m)$ of m positive integers, satisfying the inequalities

$$\kappa_1\geqslant\kappa_2\geqslant\cdots\kappa_m\geqslant 0, \quad m\leqslant\min(p,q), \tag{206}$$

with $(Z_1(z),Z_3(z),Z_3(z),\ldots)$ the sequence of determinants

$$Z_1(z)=z_{11}, \quad Z_2(z)=\begin{vmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{vmatrix}, \quad Z_3(z)=\begin{vmatrix} z_{11} & z_{12} & z_{13} \\ z_{21} & z_{22} & z_{23} \\ z_{31} & z_{32} & z_{33} \end{vmatrix}, \quad \ldots; \tag{207}$$

N_{κ} is a normalization factor. The polynomial $\varphi_{\kappa\kappa}(z)$ is seen from Eqs. (202) and (203) to be of $\mathrm{U}(p)\otimes\mathrm{U}(q)$ weight

$$(\sigma,\ldots,\sigma-\kappa_m,\ldots\sigma-\kappa_1)\otimes(\kappa_1,\ldots,\kappa_m,\ldots,0). \tag{208}$$

Thus, it is the highest weight polynomial of an irreducible $\mathrm{S}[\mathrm{U}(p)\times\mathrm{U}(q)]$ invariant subspace $\mathcal{F}^{\kappa}$ of $\mathcal{F}$. Let $\{\varphi_{\kappa\tau}\}$ denote an orthonormal basis for $\mathcal{F}^{\kappa}$.

The norm factor N_{κ} is determined by the requirement that

$$\int \varphi^*_{\kappa\kappa}(z)\varphi_{\kappa\kappa}(z)\mathrm{d}v(z)=[\varphi^*_{\kappa\kappa}(\nabla)\varphi_{\kappa\kappa}(z)]_{z=0}=1, \tag{209}$$

where

$$\varphi^*_{\kappa\kappa}(\nabla)=N^*_{\kappa}\nabla_1^{\kappa_1-\kappa_2}\nabla_2^{\kappa_2-\kappa_3}\cdots\nabla_m^{\kappa_m} \tag{210}$$

with

$$\nabla_1=\partial_{11}, \quad \nabla_2=\begin{vmatrix} \partial_{11} & \partial_{12} \\ \partial_{21} & \partial_{22} \end{vmatrix}, \quad \nabla_3=\begin{vmatrix} \partial_{11} & \partial_{12} & \partial_{13} \\ \partial_{21} & \partial_{22} & \partial_{23} \\ \partial_{31} & \partial_{32} & \partial_{33} \end{vmatrix}, \ldots. \tag{211}$$

The overlap integral (209) is evaluated by use of the Capelli identity[37]

$$\nabla_n Z_n(z)=\begin{vmatrix} n+z_1\cdot\partial_1 & z_1\cdot\partial_2 & z_1\cdot\partial_3 & \cdots & \cdots & z_1\cdot\partial_n \\ z_2\cdot\partial_1 & n-1+z_2\cdot\partial_2 & z_2\cdot\partial_3 & \cdots & \cdots & z_2\cdot\partial_n \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ z_n\cdot\partial_1 & +z_n\cdot\partial_2 & z_n\cdot\partial_3 & \cdots & \cdots & 1+z_n\cdot\partial_n \end{vmatrix}, \tag{212}$$

where

$$z_i\cdot\partial_j=\sum_{\nu} z_{i\nu}\partial_{j\nu} \tag{213}$$

and it is understood that a determinant of noncommuting operators is ordered by columns, e.g.,

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix}=AD-CB. \tag{214}$$

Thus, when acting on a highest weight polynomial $\varphi_{\kappa\kappa}$ for which $\kappa_n\neq 0$ but $\kappa_{n+1}=0$,

$$\nabla_n Z_n(z)\varphi_{\kappa\kappa}=(n+\kappa_1)(n-1+\kappa_2)\cdots(1+\kappa_n)\varphi_{\kappa\kappa}. \tag{215}$$

By repeated use of this identity we obtain the expression for the norm factors

$$N_\kappa^2=\frac{\Pi_{i<j}(\kappa_i-\kappa_j+j-i)}{\Pi_{i=1}^m(\kappa_i+m-i)!}. \tag{216}$$

It is interesting to note that this norm factor is related to the dimensionality of an irrep of S_N labeled by a partition κ of $N=\Sigma_i\kappa_i$ as follows:

$$\dim\ \kappa=N!N_\kappa^2. \tag{217}$$

The overlap kernel for SU$(p+q)$, given by Eq. (193), is

$$\mathcal{S}^\lambda(z,x)=\begin{vmatrix} 1+z_1\cdot x_1^* & z_1\cdot x_2^* & z_1\cdot x_3^* & \cdots & \cdots & z_1\cdot x_p^* \\ z_2\cdot x_1^* & 1+z_2\cdot x_2^* & z_2\cdot x_3^* & \cdots & \cdots & z_2\cdot x_p^* \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ z_p\cdot x_1^* & z_p\cdot x_2^* & z_p\cdot x_3^* & \cdots & \cdots & 1+z_p\cdot x_p^* \end{vmatrix}^\lambda, \tag{218}$$

where

$$z_i\cdot x_j^*=\sum_\nu z_{i\nu}x_{j\nu}^*. \tag{219}$$

Thus, $\mathcal{S}^\lambda$ is the λ power of a sum of diagonal minors of a determinant, i.e., determinants of submatrices obtained by deleting some number of rows and corresponding columns. Moreover, since $\varphi_{\kappa\kappa}$ is a highest weight polynomial, it follows that

$$\int \mathcal{S}^\lambda(z,x)\varphi_{\kappa\kappa}\mathrm{d}v(x)=\int\left(1+\sum_{n=1}^{\min(p,q)}\Lambda_n(z,x)\right)^\lambda\varphi_{\kappa\kappa}(x)\mathrm{d}v(x), \tag{220}$$

where

$$\Lambda_n(z,x)=\begin{vmatrix} z_1\cdot x_1^* & z_1\cdot x_2^* & \cdots & z_1\cdot x_n^* \\ \cdots & \cdots & \cdots & \cdots \\ z_n\cdot x_1^* & z_n\cdot x_2^* & \cdots & z_n\cdot x_n^* \end{vmatrix}=Z_n(z)Z_n^*(x). \tag{221}$$

We conclude that

$$\int \mathcal{S}^\lambda(z,x)\varphi_{\kappa\kappa}\mathrm{d}v(x)=\binom{\lambda}{(\kappa_1-\kappa_2)(\kappa_2-\kappa_3)\ldots\kappa_p}N_\kappa^{-2}\,\varphi_{\kappa\kappa}(z), \tag{222}$$

where ( ) is a multinomial coefficient, and that

$$\mathcal{S}^\lambda(z,x)=\sum_{\kappa\nu}K_\kappa^2\,\varphi_{\kappa\nu}(z)\varphi_{\kappa\nu}^*(x), \tag{223}$$

with

$$K_\kappa^2=\frac{\lambda!}{(\lambda-\kappa_1)!(\kappa_1-\kappa_2)!(\kappa_2-\kappa_3)!\ldots\kappa_p!}N_\kappa^{-2}. \tag{224}$$

For SU(p,q), instead of Eq. (220), we have

$$\int \mathcal{S}^{-\lambda}(z,x)\varphi_{\kappa\kappa}(x)\mathrm{d}v(x)=\left(1-\sum_{n=1}^{p}\Lambda_n(z,x)\right)^{-\lambda}\varphi_{\kappa\kappa}(z). \tag{225}$$

Thus, for SU(p,q), $\mathcal{S}^{-\lambda}(z,x)$ is again of the form

$$\mathcal{S}^{-\lambda}(z,x)=\sum_{\kappa\nu}K_\kappa^2\,\varphi_{\kappa\nu}(z)\varphi^*_{\kappa\nu}(x), \tag{226}$$

but now with

$$K_\kappa^2=\frac{(\lambda+\kappa_1-1)!}{(\lambda-\kappa_1)!(\kappa_1-\kappa_2)!(\kappa_2-\kappa_3)!\ldots\kappa_p!}N_\kappa^{-2}. \tag{227}$$

B. Sp$(n,\mathbb{R})$ and Sp(n)

The compact symplectic group Sp(n) is isomorphic to the subgroup of unitary matrices in Sp$(n,\mathbb{C})$; it is isomorphic to

$$\mathrm{Sp}(n)\cong\mathrm{Sp}(n,\mathbb{C})\cap\mathrm{U}(2n), \tag{228}$$

which means that an element of Sp(n) is a $2n\times 2n$ matrix of the form

$$g=\begin{pmatrix}\alpha & -\beta\\ \beta^* & \alpha^*\end{pmatrix} \tag{229}$$

with

$$\alpha\alpha^\dagger+\beta\beta^\dagger=I_n,\quad \alpha\tilde{\beta}=\beta\tilde{\alpha}, \tag{230}$$

where I_n is the $n\times n$ identity matrix and $\tilde{\beta}$ is the transpose of β. Similarly Sp$(n,\mathbb{R})$ is given by the isomorphism

$$\mathrm{Sp}(n,\mathbb{R})\cong\mathrm{Sp}(n,\mathbb{C})\cap\mathrm{U}(n,n) \tag{231}$$

and an element of Sp$(n,\mathbb{R})$ is a $2n\times 2n$ matrix of the form

$$g=\begin{pmatrix}\alpha & \beta\\ \beta^* & \alpha^*\end{pmatrix} \tag{232}$$

with

$$\alpha\alpha^\dagger-\beta\beta^\dagger=I_n,\quad \alpha\tilde{\beta}=\beta\tilde{\alpha}. \tag{233}$$

The Lie algebras of the groups Sp$(n,\mathbb{R})$ and Sp(n) have a common complex extension C_n. Let E_{ij} denote the matrix with entries $(E_{ij})_{kl}=\delta_{ik}\delta_{jl}$. Then the complex Lie algebra C_n is spanned by the matrices

$$C_{ij}=\begin{pmatrix}E_{ij} & 0\\ 0 & -E_{ji}\end{pmatrix},\quad i,j=1,\ldots,n, \tag{234}$$

$$A_{ij}=A_{ji}=\begin{pmatrix}0 & -E_{ij}-E_{ji}\\ 0 & 0\end{pmatrix},\quad i,j=1,\ldots,n, \tag{235}$$

$$B_{ij}=B_{ji}=\begin{pmatrix} 0 & 0 \\ E_{ij}+E_{ji} & 0 \end{pmatrix}, \quad i,j=1,\ldots,n, \tag{236}$$

which generate the group elements

$$g(x,y)=\exp\sum_{ij}\,[x_{ij}C_{ij}+y_{ij}A_{ij}+y_{ij}^{*}B_{ij}] \quad \in \mathrm{Sp}(n), \tag{237}$$

$$g(x,y)=\exp\sum_{ij}\,[x_{ij}C_{ij}+y_{ij}A_{ij}-y_{ij}^{*}B_{ij}] \quad \in \mathrm{Sp}(n,\mathbb{R}), \tag{238}$$

with x skew Hermitian (i.e., $x_{ij}=-x_{ji}^{*}$).

Let T denote an irrep of C_n with lowest weight in which the matrices A_{ij}, B_{ij}, and C_{ij} are mapped to linear operators $\hat{A}_{ij}$, $\hat{B}_{ij}$, and $\hat{C}_{ij}$ on a Hilbert space $\mathbb{H}$. We consider an irrep T defined by an integer σ for which the lowest weight state satisfies

$$\hat{B}_{ij}|0\rangle=0, \quad \hat{C}_{ij}|0\rangle=\delta_{ij}\sigma|0\rangle. \tag{239}$$

When $\sigma<0$, T integrates to a unitary irrep of $\mathrm{Sp}(n)$ for which

$$\hat{A}_{ij}^{\dagger}=-\hat{B}_{ij}, \quad \hat{C}_{ij}^{\dagger}=\hat{C}_{ji}. \tag{240}$$

And when $\sigma>0$, it integrates to a unitary irrep of $\mathrm{Sp}(n,\mathbb{R})$ for which

$$\hat{A}_{ij}^{\dagger}=\hat{B}_{ij}, \quad \hat{C}_{ij}^{\dagger}=\hat{C}_{ji}. \tag{241}$$

The special case $\sigma=0$ is the trivial identity representation. Note that one also obtains irreps of C_n when σ is a positive half-odd integer. These restrict to irreps of $\mathrm{sp}(n,\mathbb{R})$ that integrate to unitary irreps of the metaplectic double cover of the group $\mathrm{Sp}(n,\mathbb{R})$. In all nontrivial cases, the subgroup of elements that leave the lowest-weight state invariant is $\mathrm{U}(n)$.

As in the previous example, let $\mathbb{H}_D$ be the space of K-finite vectors. Let D denote the vector space of complex symmetric $n\times n$ matrices and let N be the group

$$N=\left\{\begin{pmatrix} I_n & 0 \\ z & I_n \end{pmatrix}; z\in D\right\}. \tag{242}$$

An element of N is then represented by the operator $\hat{z}=\exp[1/2\ \Sigma_{ij}z_{ij}\hat{B}_{ij}]$ on $\mathbb{H}_D$ and a coherent state wave function Ψ for a state $|\psi\rangle\in\mathbb{H}_D$ is defined by

$$\Psi(z)=\langle 0|e^{\hat{z}}|\psi\rangle. \tag{243}$$

Again, these coherent state wave functions are polynomials in the matrix coefficients of z.

The coherent state action $\Gamma(g)$ of an $\mathrm{Sp}(n,\mathbb{R})$ or $\mathrm{Sp}(n)$ matrix

$$g=\begin{pmatrix} \alpha & b \\ \beta^{*} & \alpha^{*} \end{pmatrix}, \quad b=\pm\beta, \tag{244}$$

defined by

$$[\Gamma(g)\Psi](z)=\langle 0|e^{\hat{z}}T(g)|\psi\rangle, \tag{245}$$

is determined by the generalized Gauss (Harish-Chandra) factorization of the product

$$\begin{pmatrix} I & 0 \\ z & I \end{pmatrix}\begin{pmatrix} \alpha & b \\ \beta^* & \alpha^* \end{pmatrix}=\begin{pmatrix} I & x \\ 0 & I \end{pmatrix}\begin{pmatrix} a & 0 \\ 0 & \tilde{a}^{-1} \end{pmatrix}\begin{pmatrix} I & 0 \\ y & I \end{pmatrix}, \quad z\in D, \tag{246}$$

with

$$a=(\alpha^\dagger+\tilde{b}z)^{-1}, \quad x=b(\alpha^*+zb)^{-1}, \quad y=(\alpha^*+zb)^{-1}(\beta^*+z\alpha). \tag{247}$$

This gives

$$\langle 0|e^{\hat{z}}T(g)|\psi\rangle=[\det a]^\sigma\langle 0|e^{\hat{y}}|\psi\rangle \tag{248}$$

and

$$[\Gamma(g)\Psi](z)=[\det(\alpha^\dagger+\tilde{b}z)]^{-\sigma}\Psi((\alpha^*+zb)^{-1}(\beta^*+z\alpha)). \tag{249}$$

For a unitary irrep of Sp(n), for which $\hat{B}_{ij}^\dagger=-\hat{A}_{ij}$, we derive the overlap kernel

$$\mathcal{S}^{\sigma=-\lambda}(z,x^\dagger)=\langle 0|e^{\hat{z}}e^{\hat{x}^\dagger}|0\rangle=[\det(I_n+zx^\dagger)]^\lambda, \tag{250}$$

where $\hat{x}^\dagger=-1/2\,\Sigma_{ij}x_{ij}^*\hat{A}_{ij}$. The Hilbert space $\mathcal{F}_{\mathbb{H}}$ is then the space of holomorphic functions in the matrix coefficients of z with inner product

$$\langle\varphi|\psi\rangle=\int\int\varphi^*(z)[\det(I_n+zx^\dagger)]^\lambda\psi(x)\mathrm{d}v(z)\mathrm{d}v(x), \tag{251}$$

where the integral is over D, which can be identified with the $n(n+1)/2$-dimensional complex plane and the measure $\mathrm{d}v$ is the corresponding Bargmann measure.

For a unitary representation of Sp($n,\mathbb{R}$), for which $\hat{B}_{ij}^\dagger=\hat{A}_{ij}$,

$$\mathcal{S}^{\sigma=\lambda}(z,x^\dagger)=\langle 0|e^{\hat{z}}e^{\hat{x}^\dagger}|0\rangle=[\det(I_n-zx^\dagger)]^{-\lambda}, \tag{252}$$

when $\det(I_n-zx^\dagger)>0$, and $\mathcal{F}_{\mathbb{H}}$ is the Hilbert space of holomorphic functions obtained by completing the space of polynomials with the inner product

$$\langle\varphi|\psi\rangle=\int\int\varphi^*(z)\psi(x)\ \mathrm{Taylor}\,([\det(I_n-zx^\dagger)]^{-\lambda})\mathrm{d}v(z)\mathrm{d}v(x), \tag{253}$$

where the integral is again over the whole $n(n+1)/2$-dimensional complex plane with the understanding that Taylor $([\det(I_n-zx^\dagger)]^{-\lambda})$ is an expansion of $[\det(I_n-zx^\dagger)]^{-\lambda}$ as a Taylor series in $zx^\dagger$ and the integration is performed term by term.

In both cases, if the map $\mathcal{F}_{\mathbb{H}}\to\mathbb{H}$ sends $\varphi\to|\varphi\rangle$ and the map $\mathbb{H}\to\mathcal{F}^{\mathbb{H}}$ sends $|\psi\rangle\to\Psi$, then the inner product of the two states is the overlap

$$\langle\varphi|\psi\rangle=\int\varphi^*(z)\Psi(z)\mathrm{d}v(z). \tag{254}$$

Thus, as usual, the spaces $\mathcal{F}_{\mathbb{H}}$ and $\mathcal{F}^{\mathbb{H}}$ are in duality with respect to the measure $\mathrm{d}v$ and matrix elements of the representation are given by

$$\langle\varphi|T(g)|\psi\rangle=\int\varphi^*(z)[\Gamma(g)\Psi](z)\mathrm{d}v(z). \tag{255}$$

An orthonormal U(n) basis $\{\varphi_{\kappa\nu}\}$ for the Bargmann space $\mathcal{F}$ can be constructed following the techniques given in Sec. IV A albeit using a generalization of the Capelli identity.[38] Similarly, by

an expansion of the overlap kernels as in Eq. (200), one can determine the renormalization factors $\{K_\kappa\}$ which map this basis for $\mathcal{F}$ to orthonormal bases $\{\psi_{\kappa\nu}=K_\kappa^{-1}\varphi_{\kappa\nu}\}$ and $\{\Psi_{\kappa\nu}=K_\kappa\varphi_{\kappa\nu}\}$ for $\mathcal{F}_{\mathbb{H}}$ and $\mathcal{F}^{\mathbb{H}}$, respectively.

C. SO(2n) and SO*(2n)

The real orthogonal group $\mathrm{SO}(2n)$ is isomorphic to the subgroup of unitary matrices in the complex orthogonal group $\mathrm{SO}(2n,\mathbb{C})$;

$$\mathrm{SO}(2n)\cong\mathrm{SO}(2n,\mathbb{C})\cap\mathrm{U}(2n). \tag{256}$$

Thus, if $\mathrm{SO}(2n,\mathbb{C})$ is realized as the group of matrices

$$\mathrm{SO}(2n,\mathbb{C})=\{M\in\mathrm{SL}(2n,\mathbb{C})\,|\,M\tilde{J}\tilde{M}=J\}, \tag{257}$$

where

$$J=\begin{pmatrix}0 & I_n\\ I_n & 0\end{pmatrix}, \tag{258}$$

then an element $g\in\mathrm{SO}(2n)$ is a $2n\times 2n$ matrix of the form

$$g=\begin{pmatrix}\alpha & \beta\\ \beta^* & \alpha^*\end{pmatrix} \tag{259}$$

with

$$\alpha\alpha^\dagger+\beta\beta^\dagger=I_n,\quad \alpha\tilde{\beta}+\beta\tilde{\alpha}=0. \tag{260}$$

Similarly, $\mathrm{SO}^*(2n)$ is given by the isomorphism

$$\mathrm{SO}^*(2n)\cong\mathrm{SO}(2n,\mathbb{C})\cap\mathrm{U}(n,n) \tag{261}$$

and an element of $\mathrm{SO}^*(2n)$ is a $2n\times 2n$ matrix of the form

$$g=\begin{pmatrix}\alpha & \beta\\ -\beta^* & \alpha^*\end{pmatrix} \tag{262}$$

with

$$\alpha\alpha^\dagger-\beta\beta^\dagger=I_n,\quad \alpha\tilde{\beta}+\beta\tilde{\alpha}=0. \tag{263}$$

The Lie algebras of the groups $\mathrm{SO}(2n)$ and $\mathrm{SO}^*(2n)$ have common complex extension D_n. Let E_{ij} denote the matrix with entries $(E_{ij})_{kl}=\delta_{ik}\delta_{jl}$. Then the complex Lie algebra D_n is spanned by the matrices

$$C_{ij}=\begin{pmatrix}E_{ij} & 0\\ 0 & -E_{ji}\end{pmatrix},\quad i,j=1,\ldots,n, \tag{264}$$

$$A_{ij}=\begin{pmatrix}0 & E_{ij}-E_{ji}\\ 0 & 0\end{pmatrix}=-A_{ji},\quad i,j=1,\ldots,n, \tag{265}$$

$$B_{ij}=\begin{pmatrix}0 & 0\\ E_{ij}-E_{ji} & 0\end{pmatrix}=-B_{ji},\quad i,j=1,\ldots,n, \tag{266}$$

which generate the group elements

$$g(x,y)=\exp\sum_{ij}\,[x_{ij}C_{ij}+y_{ij}A_{ij}+y_{ij}^{*}B_{ij}]\quad\in \mathrm{SO}(2n), \tag{267}$$

$$g(x,y)=\exp\sum_{ij}\,[x_{ij}C_{ij}+y_{ij}A_{ij}-y_{ij}^{*}B_{ij}]\quad\in \mathrm{SO}^{*}(2n), \tag{268}$$

with x skew Hermitian (i.e., $x_{ij}=-x_{ji}^{*}$).

Let T denote an irrep of D_n with lowest weight in which the matrices A_{ij}, B_{ij}, and C_{ij} are mapped to linear operators $\hat{A}_{ij}$, $\hat{B}_{ij}$, and $\hat{C}_{ij}$ on a Hilbert space $\mathbb{H}$. We consider an irrep T defined by an integer σ for which the lowest weight state satisfies

$$\hat{B}_{ij}|0\rangle=0,$$

$$\hat{C}_{ij}|0\rangle=\delta_{ij}\sigma|0\rangle. \tag{269}$$

For $\sigma\leqslant 0$ this D_n irrep integrates to a unitary irrep of $\mathrm{SO}(2n)$ for which

$$\hat{A}_{ij}^{\dagger}=-\hat{B}_{ij},\quad \hat{C}_{ij}^{\dagger}=\hat{C}_{ji}. \tag{270}$$

For $\sigma>0$ it integrates to a unitary irrep of $\mathrm{SO}^{*}(2n)$ and

$$\hat{A}_{ij}^{\dagger}=\hat{B}_{ij},\quad \hat{C}_{ij}^{\dagger}=\hat{C}_{ji}. \tag{271}$$

The special case $\sigma=0$ is the trivial identity representation. One also obtains spinor irreps when σ is a half-odd integer. In all nontrivial cases, the subgroup of elements that leave the lowest-weight state invariant is $\mathrm{U}(n)$.

Let $\mathbb{H}_D$ be the subspace of K-finite vectors in $\mathbb{H}$. Let D denote the vector space of complex symmetric $n\times n$ matrices and let N be the group of lower triangular matrices

$$N=\left\{\begin{pmatrix} I_n & 0\\ z & I_n\end{pmatrix};z\in D\right\}. \tag{272}$$

An element of N is then represented by the operator $e^{\hat{z}}$ with $\hat{z}=1/2\,\Sigma_{ij}z_{ij}\hat{B}_{ij}$ on $\mathbb{H}_D$ and a coherent state wave function Ψ for a state $|\psi\rangle\in\mathbb{H}_D$ is defined by

$$\Psi(z)=\langle 0|e^{\hat{z}}|\psi\rangle. \tag{273}$$

Again, these coherent state wave functions are polynomials in the matrix coefficients of z.

The coherent state action $\Gamma(g)$ of an $\mathrm{SO}(2n)$ or $\mathrm{SO}^{*}(2n)$ matrix

$$g=\begin{pmatrix}\alpha & \beta\\ b^{*} & \alpha^{*}\end{pmatrix},\quad b=\pm\beta, \tag{274}$$

defined by

$$[\Gamma(g)\Psi](z)=\langle 0|e^{\hat{z}}T(g)|\psi\rangle, \tag{275}$$

is determined by the generalized Gauss (Harish-Chandra) factorization of the product

$$\begin{pmatrix} I & 0\\ z & I\end{pmatrix}\begin{pmatrix}\alpha & \beta\\ b^{*} & \alpha^{*}\end{pmatrix}=\begin{pmatrix} I & x\\ 0 & I\end{pmatrix}\begin{pmatrix} a & 0\\ 0 & \tilde{a}^{-1}\end{pmatrix}\begin{pmatrix} I & 0\\ y & I\end{pmatrix},\quad z\in D, \tag{276}$$

with

$$x=\beta(\alpha^*+z\beta)^{-1},\quad a=(\alpha^\dagger-\tilde{\beta}z)^{-1},\quad y=(\alpha^*+z\beta)^{-1}(b^*+z\alpha). \tag{277}$$

This gives

$$\langle 0|e^{\hat{z}}T(g)|\psi\rangle=[\det a]^\sigma\langle 0|e^{\hat{y}}|\psi\rangle \tag{278}$$

and

$$[\Gamma(g)\Psi](z)=[\det(\alpha^\dagger-\tilde{\beta}z)]^{-\sigma}\Psi((\alpha^*+z\beta)^{-1}(b^*+z\alpha)). \tag{279}$$

For a unitary irrep of SO$(2n)$, the overlap kernel is

$$\mathcal{S}^{\sigma=-\lambda}(z,x^\dagger)=\langle 0|e^{(1/2)\,\Sigma z_{ij}\hat{B}_{ij}}e^{-(1/2)\,\Sigma x^*_{ij}\hat{A}_{ij}}|0\rangle=[\det(I+zx^\dagger)]^\lambda \tag{280}$$

and the inner product is defined by

$$\langle\psi|\varphi\rangle=\int\int\psi^*(z)[\det(I+x^\dagger z)]^\lambda\varphi(x)\mathrm{d}v(z)\mathrm{d}v(x), \tag{281}$$

where the integral is over D, which can be identified with the $n(n-1)/2$-dimensional complex plane, and the measure $\mathrm{d}v$ is the corresponding Bargmann measure. For a unitary representation of SO$^*(2n)$,

$$\mathcal{S}^{\sigma=\lambda}(z,x^\dagger)=\langle 0|e^{(1/2)\,\Sigma z_{ij}\hat{B}_{ij}}e^{(1/2)\,\Sigma x^*_{ij}\hat{A}_{ij}}|0\rangle=[\det(I-zx^\dagger)]^{-\lambda}, \tag{282}$$

when $\det(I-zx^\dagger)>0$, and the inner product is

$$\langle\psi|\varphi\rangle=\int\int\psi^*(z)\ \mathrm{Taylor}\,([\det(I-x^\dagger z)]^{-\lambda})\varphi(x)\mathrm{d}v(z)\mathrm{d}v(x), \tag{283}$$

where the integral is again over the $n(n-1)/2$-dimensional complex plane with the understanding that Taylor $([\det(I_n-zx^\dagger)]^{-\lambda})$ is an expansion of $[\det(I_n-zx^\dagger)]^{-\lambda}$ as a Taylor series in $zx^\dagger$ and the integration is performed term by term.

D. SO($p+2$) and SO(p,2)

The groups SO$(p+2)$ and SO$(p,2)$ are defined by

$$\mathrm{SO}(p+2)=\{M\in\mathrm{SL}(p+2,\mathbb{R})\,|\,MJ^+_{p+2}\tilde{M}=J^+_{p+2}\}, \tag{284}$$

$$\mathrm{SO}(p,2)=\{M\in\mathrm{SL}(p+2,\mathbb{R})\,|\,MJ^-_{p+2}\tilde{M}=J^-_{p+2}\}, \tag{285}$$

where

$$J^\pm_{p+2}=\begin{pmatrix}\pm I_2 & 0\\ 0 & I_p\end{pmatrix}; \tag{286}$$

I_p and I_2 are, respectively, the $p\times p$ and 2×2 identity matrices.

Let

$$L_{\alpha\beta}=-i(E_{\alpha\beta}-E_{\beta\alpha}),\quad \alpha,\beta=1,\ldots,p+2, \tag{287}$$

denote the infinitesimal generators (angular momenta) of SO$(p+2)$; they satisfy the commutation relations

$$[L_{\alpha\beta},L_{\gamma\delta}]=-i(\delta_{\beta\gamma}L_{\alpha\delta}-\delta_{\beta\delta}L_{\alpha\gamma}+\delta_{\alpha\delta}L_{\beta\gamma}-\delta_{\alpha\gamma}L_{\beta\delta}). \tag{288}$$

The common complex extension of the Lie algebras SO($p+2$) and SO(p,2) is then spanned by the matrices

$$\begin{gathered} L_{12} \quad \text{infinitesimal generator of SO(2)}, \\ L_{\alpha\beta} \quad \alpha,\beta=3,\ldots,p+2, \\ A_\alpha=L_{1\alpha}+iL_{2\alpha} \quad \alpha=3,\ldots,p+2, \\ B_\alpha=L_{1\alpha}-iL_{2\alpha} \quad \alpha=3,\ldots,p+2. \end{gathered} \tag{289}$$

For example, L_{12} is the matrix of block form

$$L_{12}=\begin{pmatrix} l_{12} & 0 \\ 0 & 0 \end{pmatrix}, \quad l_{12}=\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{290}$$

Group elements are then expressed in terms of this basis by

$$g(\varphi,\theta,x)=\exp i\left[\varphi L_{12}+\sum_{\alpha\beta}\ \theta_{\alpha\beta}L_{\alpha\beta}+\sum_{\alpha}\ (x_\alpha A_\alpha+x_\alpha^* B_\alpha)\right] \quad \in \mathrm{SO}(p+2), \tag{291}$$

$$g(\varphi,\theta,x)=\exp i\left[\varphi L_{12}+\sum_{\alpha\beta}\ \theta_{\alpha\beta}L_{\alpha\beta}+\sum_{\alpha}\ (x_\alpha A_\alpha-x_\alpha^* B_\alpha)\right] \quad \in \mathrm{SO}(p,2), \tag{292}$$

where φ is real, $\theta_{\alpha\beta}$ is real and antisymmetric, and x_α is complex.

By Gauss factorization, an SO($p+2$) or SO(p,2) matrix g is expressed as a product

$$g=e^{z\cdot A}\begin{pmatrix} a & 0 \\ 0 & d \end{pmatrix}e^{x^*\cdot B}, \tag{293}$$

with $a\in \mathrm{SO}(2,\mathbb{C})$ and $d\in \mathrm{SO}(p,\mathbb{C})$, where $z=(z_3,\ldots,z_{p+2})$ and $x^*=(x_3^*,\ldots,x_{p+2}^*)$ are p-component complex vectors, and

$$z\cdot A=\sum_\alpha\ z_\alpha A_\alpha, \quad x^*\cdot B=\sum_\alpha\ x_\alpha^* B_\alpha. \tag{294}$$

Therefore, as matrices,

$$z\cdot A=\begin{pmatrix} 0 & ez \\ -\tilde{z}\tilde{e} & 0 \end{pmatrix}, \quad e^{z\cdot A}=\begin{pmatrix} I_2-\dfrac{1}{2}(z\cdot z)e\tilde{e} & ez \\ -\tilde{z}\tilde{e} & I_p \end{pmatrix}, \tag{295}$$

$$x^*\cdot B=\begin{pmatrix} 0 & -e^*x^* \\ x^\dagger e^\dagger & 0 \end{pmatrix}, \quad e^{x^*\cdot B}=\begin{pmatrix} I_2-\dfrac{1}{2}(x^*\cdot x^*)e^*e^\dagger & -e^*x^* \\ x^\dagger e^\dagger & I_p \end{pmatrix}, \tag{296}$$

where $\tilde{z}$ denotes the transpose (column vector) of z, and e, e^*, $\tilde{e}$, and $e^\dagger$ are the vectors

$$e=\begin{pmatrix} -i \\ 1 \end{pmatrix}, \quad e^*=\begin{pmatrix} i \\ 1 \end{pmatrix}, \quad \tilde{e}=(-i,1), \quad e^\dagger=(i,1). \tag{297}$$

The matrix a is expressible as a function of a complex parameter ϕ in the form

$$a(\phi)=e^{\phi L_{12}}=\begin{pmatrix}\cosh\phi & -i\sinh\phi\\ i\sinh\phi & \cosh\phi\end{pmatrix}. \tag{298}$$

It has the useful property that

$$e^{\dagger}a(\phi)=e^{\phi}e^{\dagger},\quad a(\phi)e=e^{\phi}e. \tag{299}$$

We now consider a representation T with highest weight state $|0\rangle$, which maps $L_{\alpha\beta}\rightarrow\hat{L}_{\alpha\beta}$, etc., and which, for integer values of σ, satisfies the equations

$$\hat{A}_{\alpha}|0\rangle=0,\quad \hat{L}_{12}|0\rangle=\sigma|0\rangle,\quad \hat{L}_{\alpha\beta}|0\rangle=0. \tag{300}$$

For $\sigma\geqslant 0$, this irrep is finite dimensional and integrates to a unitary irrep of $\mathrm{SO}(p+2)$ for which

$$\hat{A}_{\alpha}^{\dagger}=\hat{B}_{\alpha}. \tag{301}$$

For $\sigma<0$, it is infinite dimensional and integrates to a unitary irrep of $\mathrm{SO}(p,2)$ with

$$\hat{A}_{\alpha}^{\dagger}=-\hat{B}_{\alpha}. \tag{302}$$

The special case $\sigma=0$ is the trivial identity representation. The highest weight state $|0\rangle$ is seen to span a one-dimensional irrep of the subgroup $\mathrm{SO}(2,\mathbb{C})\times\mathrm{SO}(p,\mathbb{C})$ with

$$T\begin{pmatrix}a(\phi) & 0\\ 0 & d\end{pmatrix}|0\rangle=e^{\phi\hat{L}_{12}}|0\rangle=e^{\sigma\phi}|0\rangle. \tag{303}$$

A vector $|\psi\rangle$ in the space of K-finite vectors has holomorphic coherent state wave function

$$\Psi(z)=\langle 0|e^{z\cdot\hat{A}}|\psi\rangle. \tag{304}$$

The action of a group element on coherent state wave functions is obtained by considering the actions of each of the factors in the Gauss factorization. One obtains immediately

$$[\Gamma(e^{z\cdot A})\Psi](z')=\langle 0|e^{z'\cdot\hat{A}}e^{z\cdot\hat{A}}|\psi\rangle=\Psi(z'+z). \tag{305}$$

And, from the identity

$$e^{z\cdot\hat{A}}\begin{pmatrix}a(\phi) & 0\\ 0 & d\end{pmatrix}=\begin{pmatrix}a(\phi) & 0\\ 0 & d\end{pmatrix}e^{(e^{-\phi}zd)\cdot\hat{A}}, \tag{306}$$

it follows that

$$\left[\left[\Gamma\begin{pmatrix}a(\phi) & 0\\ 0 & d\end{pmatrix}\Psi\right](z)=e^{\sigma\phi}\Psi(e^{-\phi}zd).\right. \tag{307}$$

The action

$$[\Gamma(e^{x^{*}\cdot B})\Psi](z)=\langle 0|e^{z\cdot\hat{A}}e^{x^{*}\cdot B}|\psi\rangle \tag{308}$$

is determined by Gauss factorization of the product

$$e^{z\cdot A}e^{x^{*}\cdot B}=e^{X^{*}\cdot B}\begin{pmatrix}a(\phi) & 0\\ 0 & d\end{pmatrix}e^{Z\cdot A}. \tag{309}$$

This $(p+2)\times(p+2)$ matrix identity is equivalent to the four matrix equations

$$[I_2-\tfrac{1}{2}(X^*\cdot X^*)e^*e^\dagger]a[I_2-\tfrac{1}{2}(Z\cdot Z)e\tilde{e}]+(X^*d\tilde{Z})e^*\tilde{e}$$
$$=[I_2-\tfrac{1}{2}(z\cdot z)e\tilde{e}][I_2-(x^*\cdot x^*)e^*e^\dagger]+(z\cdot x^*)ee^\dagger, \tag{310}$$

$$e^\phi eZ-e^\phi(X^*\cdot X^*)e^*Z-e^*X^*d=ez-e^*x^*+(z\cdot z)ex^*, \tag{311}$$

$$e^\phi X^\dagger e^\dagger-e^\phi(Z\cdot Z)X^\dagger\tilde{e}-d\tilde{Z}\tilde{e}=x^\dagger e^\dagger-\tilde{z}\tilde{e}+(x^*\cdot x^*)\tilde{z}e^\dagger, \tag{312}$$

$$2e^\phi X^\dagger Z+d=I_p+2\tilde{z}x^\dagger, \tag{313}$$

where we have used Eq. (299). The 2×2 matrix Eq. (310) is equivalent to the four equations

$$e^\phi=1+(x^*\cdot x^*)(z\cdot z)+2(x^*\cdot z), \tag{314}$$

$$e^\phi(Z\cdot Z)=z\cdot z, \tag{315}$$

$$e^\phi(X^*\cdot X^*)=x^*\cdot x^*, \tag{316}$$

$$e^\phi X^*dZ=x^*\cdot z, \tag{317}$$

and the $2\times p$ matrix Eq. (311) is equivalent to the two equations

$$e^\phi Z+e^\phi(X^*\cdot X^*)Z+X^*d=z+x^*+(z\cdot z)x^*, \tag{318}$$

$$e^\phi Z-e^\phi(X^*\cdot X^*)Z-X^*d=z-x^*+(z\cdot z)x^*. \tag{319}$$

Thus, we obtain

$$Z=e^{-\phi}[z+(z\cdot z)x^*]. \tag{320}$$

These results imply that

$$[\Gamma(e^{x^*\cdot B)}\Psi](z)=e^{\sigma\phi}\Psi(e^{-\phi}[z+(z\cdot z)x^*]) \tag{321}$$

with e^ϕ given by Eq. (314).

Equations (305), (308), and (321) are all special cases of the general expression

$$[\Gamma(g)\Psi](z)=e^{\sigma\phi(g)}\Psi(zg), \tag{322}$$

where, for

$$g=\begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{323}$$

$$e^\phi(g)=\tfrac{1}{2}(e^\dagger-z\cdot z\tilde{e})Ae+zCe, \tag{324}$$

$$zg=e^{-\phi}\{\tfrac{1}{2}(e^\dagger-z\cdot z\tilde{e})B+zD\}. \tag{325}$$

For $\sigma=\lambda>0$ [unitary irrep of $O(p+2)$], the overlap integral

$$\mathcal{S}^\lambda(z,x)=\langle 0|e^{z\cdot A}e^{x^*\cdot B}|0\rangle \tag{326}$$

is determined, from Eqs. (308) and (321), to be given by

$$\mathcal{S}^{\lambda}(z,x)=[1+(z\cdot z)(x^*\cdot x^*)+2z\cdot x^*]^{\lambda}. \tag{327}$$

This expression is well-defined for all z and x^* in the p-dimensional complex plane. For $\sigma=-\lambda<0$ [unitary irrep of O(p,2)],

$$\mathcal{S}^{-\lambda}(z,x)=\langle 0|e^{z\cdot A}e^{-x^*\cdot B}|0\rangle=[1+(z\cdot z)(x^*\cdot x^*)-2z\cdot x^*]^{-\lambda} \tag{328}$$

for all z and x^* in the domain

$$D=\{z\in\mathbb{C}^p|1+|z\cdot z|^2-2z^*\cdot z>0\}. \tag{329}$$

Because $\mathcal{S}^{-\lambda}(z,x)$ is holomorphic in the components of z and $x^\dagger$, it is now defined by Eq. (328) for all z and x by the Taylor series expansion

$$\mathcal{S}^{-\lambda}(z,x)=\text{Taylor}[1+(z\cdot z)(x^*\cdot x^*)-2z\cdot x^*]^{-\lambda}, \tag{330}$$

as in (87) for SU(1,1). The integral expression given below for the inner product then makes sense for all polynomials; for any polynomials ψ, φ, only finitely many terms in the series make nonzero contributions.

In both cases, the inner products are given by

$$\langle\psi|\varphi\rangle=\int\int \psi^*(z)\mathcal{S}^{\sigma}(z,x)\varphi(x)\mathrm{d}v(z)\mathrm{d}v(x), \tag{331}$$

where the integrals are with respect to the Bargmann measure over the whole p-dimensional complex plane.

V. CONCLUDING REMARKS

The above examples show that the coherent state method is very versatile and gives all the standard irreps induced from one-dimensional subgroups. Moreover, it does so in a way that considerably simplifies the evaluation of inner products. Such simplification is invaluable in practical applications of the inducing construction, e.g., to problems in physics. For example, the analysis of Sec. IV C has recently been used effectively for the calculation of SU(3) Clebsch–Gordan coefficients in an SO(3) basis,[25] coefficients that are used widely, for example, in nuclear physics.

The above techniques become even more powerful and much more general in their extension to the vector coherent state induction of irreps from multi-dimensional irreps of a subgroup. Applications of the triplets method to VCS representations will be given in a sequel to the present article.

APPENDIX: INNER PRODUCTS FOR STANDARD HOLOMORPHIC REPRESENTATIONS

Let T be an irrep of SU(2) on a Hilbert space $\mathbb{H}$ with highest weight state $|0\rangle$. The standard method of finding the inner product of coherent state wave functions for this representation[13] makes use of the resolution of the identity

$$\hat{I}=\int_{G_0} T^{\dagger}(g)|0\rangle\langle 0|T(g)\mathrm{d}\mu(g), \tag{A1}$$

where $\mathrm{d}\mu$ is a right-invariant measure for the group G. Substituting the Gauss factorization for an SU(2) matrix

$$\begin{pmatrix} a & -b^* \\ b & a^* \end{pmatrix}=\begin{pmatrix} 1 & 0 \\ b/a & 1 \end{pmatrix}\begin{pmatrix} a & 0 \\ 0 & 1/a \end{pmatrix}\begin{pmatrix} 1 & -b^*/a \\ 0 & 1 \end{pmatrix}=e^{b/a\,J_-}a^{2J_0}e^{(-b^*/a)\,J_+}, \tag{A2}$$

and setting $z=-b^*/a$ with the constraint $|a|^2=(1+|z|^2)^{-1}$, we then have

$$\hat{I}=\int T^\dagger(z)|0\rangle\langle 0|T(z)(1+|z|^2)^{-2j}\,\mathrm{d}\sigma(z), \tag{A3}$$

where $\mathrm{d}\sigma(z)$ is the (suitably normalized) right G-invariant measure for $N=\{e^{zJ_+};z\in\mathbb{C}\}$. Taking matrix elements between states of $\mathbb{H}$ gives the inner product

$$\langle\psi|\varphi\rangle=\int \Psi^*(z)\Phi(z)(1+|z|^2)^{-2j}\mathrm{d}\sigma(z), \tag{A4}$$

in terms of coherent state wave functions. The SU(2)-invariant measure $\mathrm{d}\sigma$ for N is determined by considering the right translations of N by SU(2). The appropriate SU(2): $N\to N;z\mapsto z\cdot g$ action is obtained by observing that

$$\begin{pmatrix}1 & z\\ 0 & 1\end{pmatrix}\begin{pmatrix}a & -b^*\\ b & a^*\end{pmatrix}=\begin{pmatrix}1 & 0\\ \dfrac{b}{bz+a} & 1\end{pmatrix}\begin{pmatrix}bz+a & 0\\ 0 & \dfrac{1}{bz+a}\end{pmatrix}\begin{pmatrix}1 & \dfrac{a^*z-b^*}{bz+a}\\ 0 & 1\end{pmatrix}, \tag{A5}$$

which implies that

$$z\cdot g=\frac{a^*z-b^*}{bz+a}. \tag{A6}$$

By computing the Jacobian of the $z\to z\cdot g$ transformation, one determines the invariant volume element

$$\mathrm{d}\sigma(z)\propto(1+|z|^2)^{-2}\mathrm{d}x\mathrm{d}y \tag{A7}$$

with $z=x+iy$; the factor $(1+|z|^2)^{-2}$ which gives an SU(2)-invariant volume in terms of the corresponding Euclidean volume is known as a Bergman kernel.[36] Finally, the normalization constant is fixed by requiring the coherent-state wave function for the highest weight state to be normalized to unity. Thus, one obtains the inner product

$$\langle\psi|\varphi\rangle=\frac{2j+1}{\pi}\int\int\frac{\Psi^*(z)\Phi(z)}{(1+|z|^2)^{2j+2}}\mathrm{d}x\mathrm{d}y. \tag{A8}$$

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Weak pseudo-Hermiticity and antilinear commutant

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We inquire into some properties of diagonalizable pseudo-Hermitian operators, showing that their definition can be relaxed and that the pseudo-Hermiticity property is strictly connected with the existence of an antilinear symmetry. This result is then illustrated by considering the particular case of the complex Morse potential. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1504485]

I. INTRODUCTION

In the last several years the study of some non-Hermitian Hamiltonians with a real spectrum, and the conjecture on the connection between the reality of the spectrum and the PT-invariance of these Hamiltonians due to Bender and Boettcher,[1] have given rise to a growing interest in the literature.[2] Indeed, the above-mentioned Hamiltonians form a subclass of the class of ''pseudo-Hermitian'' operators, i.e., those operators which satisfy

$$A^\dagger = \eta A \eta^{-1} \tag{1}$$

with

$$\eta = \eta^\dagger. \tag{2}$$

Pseudo-Hermitian operators were introduced in the early 1940s by Dirac[3] and Pauli[4] in order to overcome some divergence difficulties in physics by using an indefinite metric associated with η, and were later resumed by Lee and Wick[5] (who first, to the best of our knowledge, used the term ''pseudo-Hermiticity''). More recently, many interesting properties of such operators have been examined and their spectrum has been suitably characterized.[6,7]

In the present paper we aim to point out further properties of pseudo-Hermitian operators that are relevant from a physical viewpoint. To this end, we introduce in Sec. II the possibly broader class of *weakly* pseudo-Hermitian operators, i.e., those operators which satisfy Eq. (1) without any constraint on the (linear, invertible) operator η, and show that, whenever one considers only diagonalizable operators, this class actually coincides with the class of all pseudo-Hermitian operators. Hence the condition in Eq. (2) can be dropped when defining (diagonalizable) pseudo-Hermitian operators, which is useful from several viewpoints [in particular, it simplifies checking Eq. (1)]. Moreover, we show in Sec. III that a diagonalizable operator H is (weakly) pseudo-Hermitian if and only if an antilinear involutory operator exists which commutes with it. This result has a number of relevant consequences; in particular, in every theory which admits a time-reversal invariance, or a CPT-invariance, the Hamiltonian must necessarily be a (weakly) pseudo-Hermitian operator. Furthermore, the above-mentioned result is strictly intertwined with an old theorem[8] of group representation theory, according to which a set of operators admits an involutory antilinear mapping that commutes with it if and only if all the operators in the set can assume conjointly a real form in a suitable basis. Indeed, by using this theorem together with the above-given results, we conclude in Sec. IV that for any diagonalizable (weakly) pseudo-

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Hermitian operator H a basis exists in which H has a real form. If this basis coincides with the eigenbasis of H, then H also has a real spectrum. Finally, we illustrate our results by means of an example, considering the special case of the complex Morse potential[9] in Sec. V.

II. THE SPECTRA OF WEAKLY PSEUDO-HERMITIAN OPERATORS

As we wrote in Sec. I, here we introduce a new class of operators, whose properties will be studied in the following.

Definition 1: A linear operator A is said to be weakly pseudo-Hermitian *if a linear, invertible operator* η *exists such that*

$$\eta A \eta^{-1} = A^{\dagger}. \tag{3}$$

The above-given definition generalizes the definition of pseudo-Hermitian operators since we do not assume $\eta = \eta^{\dagger}$ as is required in the standard definition of pseudo-Hermitian operators.[5,6]

As in Refs. 6 and 7, here we consider only diagonalizable operators; moreover, for the sake of simplicity, we consider only discrete spectra (see, however, Sec. V, where a potential with a continuous spectrum is explicitly studied). Whenever H is a diagonalizable operator with a discrete spectrum, a complete biorthonormal eigenbasis $\{|\psi_n,a\rangle,|\phi_n,a\rangle\}$ exists,[10] i.e., a basis such that

$$H|\psi_n,a\rangle = E_n|\psi_n,a\rangle, \quad H^{\dagger}|\phi_n,a\rangle = E_n^*|\phi_n,a\rangle, \tag{4}$$

$$\langle \phi_m,b|\psi_n,a\rangle = \delta_{mn}\delta_{ab}, \tag{5}$$

$$\sum_n \sum_{a=1}^{d_n} |\phi_n,a\rangle\langle\psi_n,a| = \sum_n \sum_{a=1}^{d_n} |\psi_n,a\rangle\langle\phi_n,a| = 1, \tag{6}$$

where d_n denotes the degeneracy of E_n, and a and b are degeneracy labels.

The operator H can then be written in the form

$$H = \sum_n \sum_{a=1}^{d_n} |\psi_n,a\rangle E_n \langle\phi_n,a|.$$

For the sake of brevity we also write the above-given basis $\{|\psi_m\rangle,|\phi_m\rangle\}$ in the following, with an obvious meaning of symbols. Then H can also be written in the form

$$H = \sum_m |\psi_m\rangle E_m \langle\phi_m|$$

(where it may occur that $E_m = E_{m'}$ even if $m \neq m'$). Furthermore, if $\{u_m\}$ is any complete, orthonormal basis in our space, we put in the following:

$$O = \sum_m |\psi_m\rangle\langle u_m|. \tag{7}$$

By using Eq. (6), we get

$$O^{-1} = \sum_m |u_m\rangle\langle\phi_m|$$

and

$$O^{-1}HO = \sum_m |u_m\rangle\langle\phi_m| \sum_{m'} |\psi_{m'}\rangle E_{m'} \langle\phi_{m'}| \sum_{m''} |\psi_{m''}\rangle\langle u_{m''}| = \sum_m |u_m\rangle E_m \langle u_m|.$$

Moreover,

$$(OO^\dagger)H^\dagger(OO^\dagger)^{-1}=\sum_m |\psi_m\rangle E_m^*\langle\phi_m|. \tag{8}$$

We can now state the following proposition, which embodies some results in Ref. 6 on pseudo-Hermitian operators.

Proposition 1: Let H be a diagonalizable operator with a discrete spectrum. Then, the following conditions are equivalent:

(i) H is weakly pseudo-Hermitian;
(ii) the eigenvalues of H occur in complex conjugate pairs, and for each pair the multiplicities of both the eigenvalues are the same;
(iii) H is pseudo-Hermitian.

Proof: The implication *(iii)⇒(ii)* is proven in Proposition 7 of Ref. 6. By observing that only the invertibility of η is used in this proof, in order to show that η^{-1} maps the eigensubspace of $H^\dagger$ associated with E_n to that of H associated with E_n^*, and both the subspaces have the same dimension, one immediately transforms this proof into a proof of the implication *(i)⇒(ii)*.

The implication *(ii)⇒(iii)* is also proven in Ref. 6. We provide here, however, a somewhat different proof of it, which produces a useful decomposition of η [see Eq. (12)].

Let us therefore assume that condition (ii) holds, and use (whenever it is necessary) the subscript "$_0$" to denote real eigenvalues and the corresponding eigenvectors, and the subscript "$_\pm$" to denote the complex eigenvalues with positive or negative imaginary part, respectively, and the corresponding eigenvectors.

Then, let us consider the involutory operator T, defined as follows:

$$T|\psi_{n_\pm},a\rangle=|\psi_{n_\mp},a\rangle, \quad \text{hence,} \quad T|\psi_{n_0},a\rangle=|\psi_{n_0},a\rangle. \tag{9}$$

The explicit form of T is

$$T=T\left(\sum_{n_0}\sum_{a=1}^{d_{n_0}}|\psi_{n_0},a\rangle\langle\phi_{n_0},a|+\sum_{n_+}\sum_{a=1}^{d_{n_+}}|\psi_{n_+},a\rangle\langle\phi_{n_+},a|+\sum_{n_-}\sum_{a=1}^{d_{n_-}}|\psi_{n_-},a\rangle\langle\phi_{n_-},a|\right)$$

$$=\sum_{n_0,a}|\psi_{n_0},a\rangle\langle\phi_{n_0},a|+\sum_{n_+,n_-,a}(|\psi_{n_-},a\rangle\langle\phi_{n_+},a|+|\psi_{n_+},a\rangle\langle\phi_{n_-},a|).$$

The action of T on the bras $\langle\phi_{n_\pm},a|$ easily follows from the above-given expression:

$$\langle\phi_{n_\pm},a|T=\langle\phi_{n_\mp},a|, \quad \text{hence,} \quad \langle\phi_{n_0},a|T=\langle\phi_{n_0},a|. \tag{10}$$

Then, by simple calculations, one has

$$THT=\sum_m |\psi_m\rangle E_m^*\langle\phi_m|, \tag{11}$$

and finally, comparing Eqs. (8) and (11), it follows

$$THT=(OO^\dagger)H^\dagger(OO^\dagger)^{-1},$$

hence condition *(iii)* follows at once, with

$$\eta=(OO^{\dagger})^{-1}T=\sum_{n_0,a}|\phi_{n_0},a\rangle\langle\phi_{n_0},a|+\sum_{n_+,n_-,a}(|\phi_{n_+},a\rangle\langle\phi_{n_-},a|+|\phi_{n_-},a\rangle\langle\phi_{n_+},a|)=\eta^{\dagger}. \tag{12}$$

Finally, the proof of the Proposition can be completed by observing that the implication $(iii)\Rightarrow(i)$ is obvious. ■

The introduction of the operator T on the above-given proof and the decomposition $\eta=(OO^{\dagger})^{-1}T$ in Eq. (12) allows one to obtain immediately the characterization of the case of real spectrum. Indeed, noting that $T=\mathsf{1}$ if and only if the spectrum of H is real, the following statement holds (see also the Theorem in Ref. 7).

Proposition 2: The spectrum of a diagonalizable weakly pseudo-Hermitian (hence, of a diagonalizable pseudo-Hermitian) operator H is real if and only if an operator η exists such that $\eta=(OO^{\dagger})^{-1}$.

Furthermore, the existence of an Hermitian operator η whenever H is weakly pseudo-Hermitian implies that also in this case one can introduce an Hermitian, indefinite inner product[4–6,11] which is invariant under the time translation generated by H.

III. WEAKLY PSEUDO-HERMITIAN OPERATORS AND ANTILINEAR SYMMETRIES

In order to properly discuss the next argument, we state the following definition.

Definition 2 (Ref. 8): Given the biorthonormal basis $\mathsf{E}=\{|\psi_m\rangle,|\phi_m\rangle\}$ in a Hilbert space, we call conjugation *associated with it the involutory antilinear operator*

$$\Theta_{\mathsf{E}}=\sum_m|\psi_m\rangle K\langle\phi_m|, \tag{13}$$

where the operator K acts transforming each complex number on the right into its complex conjugate.

Let us discuss now the connection between the (weak) pseudo-Hermiticity condition and the *antilinear commutant*[8] of H (i.e., the set of the antilinear, invertible operators which commute with it). This connection was already acknowledged in Ref. 7, where the author shows that, if H commutes with an antilinear operator A, then condition (ii) of Proposition 1 holds, and that a Hamiltonian with an antilinear symmetry A has a real spectrum if and only if the symmetry is *exact*[7] (i.e., its eigenvectors are invariant under the action of A). The latter statement can be rephrased, using Definition 2, by saying that *the spectrum of H is real if and only if* $[H,\Theta_{\mathsf{E}}]=0$.

However, the above-given results enlighten only partially the key role of the antilinear commutant of H. Indeed, the following, more complete proposition holds.

Proposition 3: Let H be a diagonalizable operator with a discrete spectrum. Then, the following conditions are equivalent:

(i) an antilinear, invertible operator Ω exists such that $[H,\Omega]=0$;

(ii) H is (weakly) pseudo-Hermitian;

(iii) an antilinear, involutory operator $\hat{\Omega}$ exists such that $[H,\hat{\Omega}]=0$.

Proof: $(i)\Rightarrow(ii)$. Let Ω exist. Then, the linear operator

$$\eta=(OO^{\dagger})^{-1}\Theta_{\mathsf{E}}\Omega$$

[where E is the biorthonormal basis associated with H, and O and Θ_{E} are defined as in Eqs. (7) and (13), respectively] fulfils the condition stated by Eq. (3), hence H is (weakly) pseudo-Hermitian. Indeed,

$$\Theta_{\mathsf{E}} H \Theta_{\mathsf{E}}^{-1} = \Theta_{\mathsf{E}} H \Theta_{\mathsf{E}} = \sum_m |\psi_m\rangle E_m^* \langle \phi_m|, \tag{14}$$

so that, recalling Eq. (8),

$$\eta H \eta^{-1} = (OO^\dagger)^{-1} \Theta_{\mathsf{E}} \Omega H \Omega^{-1} \Theta_{\mathsf{E}} (OO^\dagger) = (OO^\dagger)^{-1} \Theta_{\mathsf{E}} H \Theta_{\mathsf{E}} (OO^\dagger) = H^\dagger.$$

$(ii) \Rightarrow (iii)$. If H is (weakly) pseudo-Hermitian, the eigenvalues of H occur in complex conjugate pairs, and for each pair the multiplicities of both the eigenvalues are the same (Proposition 1). Then, one easily sees, recalling the definition of the operator T provided in the proof of Proposition 1 and Eq. (11), that

$$\Theta_{\mathsf{E}} H \Theta_{\mathsf{E}} = THT.$$

Hence the antilinear operator

$$\hat{\Omega} = \Theta_{\mathsf{E}} T = \sum_{n_0, a} |\psi_{n_0}, a\rangle K \langle \phi_{n_0}, a| + \sum_{n_+, n_-, a} (|\psi_{n_+}, a\rangle K \langle \phi_{n_-}, a| + |\psi_{n_-}, a\rangle K \langle \phi_{n_+}, a|) \tag{15}$$

commutes with H. Finally, $\hat{\Omega}$ is involutory, (i.e., $\hat{\Omega}^2 = \mathbb{1}$) as one can immediately verify by using the explicit expression of $\hat{\Omega}$ in Eq. (15).

$(iii) \Rightarrow (i)$. Obvious. ■

Proposition 3 has an interesting physical interpretation, as we have emphasized in Sec. I. Indeed, whenever H is the Hamiltonian of some physical system, it establishes a link between the properties of H (and of its spectrum) and the symmetries of the physical system described by it. For, the time-reversal symmetry is associated, in complex quantum mechanics, with an antilinear operator. Hence, whenever a physical system admits such a symmetry (or else, more generally, it is invariant under the combined action of the time-reversal operator times a linear one) the antilinear commutant of its Hamiltonian must be nonvoid, hence H is a (weakly) pseudo-Hermitian operator. Conversely, any (weakly) pseudo-Hermitian Hamiltonian admits an antilinear (involutory) symmetry.

Finally, since in the case of real spectrum the operator T defined in the proof of Proposition 1 is such that $T = \mathbb{1}$, hence $\hat{\Omega} = \Theta_{\mathsf{E}}$, one obtains the following proposition.

Proposition 4: A diagonalizable, weakly pseudo-Hermitian operator H has a real spectrum if and only if it commutes with the conjugation associated with its eigenbasis.

Remark: While we were writing the final version of this paper, some similar results have been obtained by other authors[12] [in particular, having in mind the equivalence *(i)⇔(iii)* in our Proposition 1, Theorem 2 of Ref. 12 essentially states the equivalence *(i)⇔(ii)* of our Proposition 3]. Nevertheless, our presentation is rather different and embodies the new condition *(iii)* in Proposition 3, which has a number of interesting consequences, which we are going to explore in Sec. IV.

IV. REAL FORM OF THE (WEAKLY) PSEUDO-HERMITIAN OPERATORS

According to Proposition 3, for any (weakly) pseudo-Hermitian operator H, at least one involutory antilinear operator exists which commutes with it. Then, it has been proven elsewhere[8] that any involutory antilinear operator $\hat{\Omega}$ is a conjugation in some suitable basis; moreover, in the basis associated with $\hat{\Omega}$, any operator commuting with $\hat{\Omega}$ has a real form.

The proof of the latter statement can be sketched as follows. If we denote by S the linear part of $\hat{\Omega}$, i.e., $\hat{\Omega} = SK$ (where K is the complex conjugation operator, see Sec. III), then $\hat{\Omega}^2 = \mathbb{1}$ implies $SS^* = \mathbb{1}$ and this is possible if and only if an U exists such that $S = UU^{*-1}$. Then $[H, \hat{\Omega}] = 0$ implies $HUU^{*-1} = UU^{*-1}H^*$, hence

$$U^{-1}HU=(U^{*-1}H^{*}U^{*})=(U^{-1}HU)^{*}.$$

Referring to the notation introduced in the present paper, let $\mathsf{F}=\{|v_m\rangle,|w_m\rangle\}$ be the biorthonormal basis associated, in the above-given sense, to the conjugation $\hat{\Omega}$ which commutes with H (of course, F may be an orthonormal basis, which occurs if and only if, for all m, $|v_m\rangle=|w_m\rangle$), and let us consider the matrix elements of H in such basis. It is easy to verify that they are real; indeed, on one hand,

$$\langle w_i|H|v_k\rangle=\langle w_i|\sum_n |\psi_n\rangle E_n\langle \phi_n|v_k\rangle$$

and, on the other hand

$$\begin{aligned}\langle w_i|\hat{\Omega}H\hat{\Omega}|v_k\rangle&=\langle w_i|\sum_m |v_m\rangle K\langle w_m|\sum_n |\psi_n\rangle E_n\langle \phi_n|\sum_{m'} |v_{m'}\rangle K\langle w_{m'}|v_k\rangle\\&=\sum_{m,m',n}\delta_{im}K\langle w_m|\psi_n\rangle E_n\langle \phi_n|v_{m'}\rangle K\delta_{m',k}\\&=\langle v_k|\sum_n |\phi_n\rangle E_n^{*}\langle \psi_n|w_i\rangle\\&=\left(\langle w_i|\sum_n |\psi_n\rangle E_n\langle \phi_n|v_k\rangle\right)^{*}.\end{aligned}$$

Since, trivially, every operator which assumes a real form in some basis B commutes with the conjugation associated with B, we have thus proven the following proposition.

Proposition 5: An operator H is (weakly) pseudo-Hermitian if and only if a basis exists in which it assumes a real form.

The results in Propositions 1, 3, and 5 can be collected together, obtaining a set of six equivalent conditions which can be useful in order to characterize the Hamiltonians that we are considering. In particular, the statement in Proposition 5 can be used to write a (weakly) pseudo-Hermitian operator in a more manageable form (an example of basis transformation which puts a particular Hamiltonian in real form is given in Sec. V).

V. AN EXAMPLE: THE COMPLEX MORSE POTENTIAL

Let us verify the results obtained in the previous sections in the special case of the complex Morse potential.[9] This was extensively studied, for instance, in Ref. 9, and its spectrum was predicted to be real by means of group theoretic techniques.[13]

The Morse potential is given by

$$V(x)=(A+iB)^2e^{-2x}-(A+iB)(2C+1)e^{-x}\quad (A,B,C\in\mathsf{R}). \tag{16}$$

Putting $\rho=\sqrt{A^2+B^2}$, $\theta=\arctan(2B/A)$, $k=2C+1$, we get

$$V(x)=\rho^2e^{-2x+i\theta}-k\rho e^{-x+i\theta/2}. \tag{17}$$

Following Ref. 9, let us introduce the (Hermitian) operator $e^{-\theta p}(\theta\in\mathsf{R}, p=-i(d/dx))$. Hence, we obtain[9]

$$e^{-\theta p}V(x)e^{\theta p}=V(x+i\theta)=V^{*}(x). \tag{18}$$

Equation (18) shows that V is a pseudo-Hermitian (but non-PT-symmetric) operator. Let us put now $\hat{\Omega}=SK=e^{\theta p}K$. By using Eq. (18) one gets

$$\hat{\Omega} V = V \hat{\Omega},$$

which agrees with Proposition 3. Then, a straightforward calculation shows that $S^* = e^{-\theta p} = S^{-1}$, hence $\hat{\Omega}$ is involutory, which also agrees with Proposition 3. Moreover, one gets by inspection that

$$S = e^{\theta p/2}(e^{\theta p/2})^{*-1} = UU^{*-1}.$$

Thus, finally,

$$U^{-1}VU = e^{-\theta p/2} V e^{\theta p/2} = V(x + i\theta/2) = \rho^2 e^{-2x} - k\rho e^{-x} = (U^{-1}VU)^*$$

which agrees with Proposition 5.

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Quantum optical versus quantum Brownian motion master equation in terms of covariance and equilibrium properties

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Structures of quantum Fokker–Planck equations are characterized with respect to the properties of complete positivity, covariance under symmetry transformations and satisfaction of equipartition, referring to recent mathematical work on structures of unbounded generators of covariant quantum dynamical semigroups. In particular the quantum optical master equation and the quantum Brownian motion master equation are shown to be associated to U(1) and R symmetry, respectively. Considering the motion of a Brownian particle, where the expression of the quantum Fokker–Planck equation is not completely fixed by the aforementioned requirements, a recently introduced microphysical kinetic model is briefly recalled, where a quantum generalization of the linear Boltzmann equation in the small energy and momentum transfer limit straightforwardly leads to quantum Brownian motion. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1505126]

I. INTRODUCTION

A theory of quantum dissipation, even restricted to the Markovian case, is a subject of major interest for many different scientific communities, ranging from mathematicians to physicists and chemists, according to various perspectives. Among these in first line experimental applications in phenomena where spontaneous emission, decoherence and dissipation play an important role, but also theoretical studies regarding the connection between quantum and classical description of dynamics, since, thanks to the lack of simple quantization recipes, such as the correspondence principle, dissipative systems become a fruitful working area where typical quantum structures may emerge. This interest has led to a huge number of proposals of Markovian master equations for the description of such dissipative phenomena, based on microphysical, phenomenological or purely mathematical approaches (see references in Refs. 1–3), not always accompanied by clear statements with regard to obeyed physical and mathematical properties, thus often leading to amendments of these models in view of some missing desired feature. This is in particular true with respect to the property of positivity or complete positivity,[4] proper distinction between Hamiltonian and dissipative part,[5] translational invariance,[6,7] and decoherence effects.[8]

As a result some efforts have been made to compare and characterize the different proposals in view of relevant mathematical and physical properties: preservation of the positivity of the statistical operator, existence of a suitable canonical stationary state, and translational invariance.[9–11,2,12] The main starting point for this research work was the result of Lindblad for the most general structure of bounded generator of a completely positive quantum dynamical semigroup,[13] together with his paper on quantum Brownian motion,[14] in which some of these issues were already considered. Complete positivity, actually equivalent to positivity for the considered Markovian quasi-free systems,[15] ensures that the statistical operator preserves positivity during the time evolution, and has emerged as a typical quantum feature, corresponding to the requirement that positivity of the time evolution is preserved under entanglement. It is in fact by

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now an essential property in the realm of quantum communication,[16] even though its origins lie in the theory of quantum measurement.[17] The result of Lindblad rigorously holds for bounded operators, though it is usually exploited as a starting point also for unbounded operators, leaving in this case the task open, to show that the considered structure is a proper generator of a completely positive quantum dynamical semigroup.

In this article we will try to further clarify the situation, showing that if besides complete positivity and equipartition, i.e., existence of a suitable canonical stationary solution, proper covariance properties of the generator of the dynamics, reflecting the relevant symmetries of the reservoir (and therefore not necessarily only translational invariance), are taken into account, a suitable characterization of two different classes of master equations can be given in a very neat way. In particular, with the two one-dimensional Lie groups U(1) and R two distinct type of master equations are associated, describing respectively the damped harmonic oscillator (the so-called quantum optical master equation) and the motion of a Brownian particle (the so-called quantum Brownian motion master equation), which, despite the fact that their physical realm of validity is essentially well-understood,[18] are sometimes mixed up,[7] their characterization in connection to underlying symmetry of the reservoir being usually neglected.[18] Recent work on completely positive quantum dynamical semigroups has shown that, asking for suitable covariance properties, a characterization of generators of such semigroups can be given also in the case of unbounded operators, where very few results are available,[19] so that one can check whether a proposed formal Lindblad structure is indeed a proper generator of a quantum dynamical semigroup. The room left by these mathematical and physical requirements should be covered by microphysical approaches, determining their relevance and predictive power. It turns out that the quantum optical master equation is in essence fixed by these requirements, while in the quantum Brownian motion case there is a nontrivial freedom left, thus explaining the huge, sometimes contradictory, literature devoted to the quantum Brownian motion master equation. In this connection a recently obtained[20–22] microphysical model for the quantum description of the motion of a Brownian particle is presented, derived from a quantum version of the linear Boltzmann equation,[23,24] extending previous phenomenological models[25] where dissipation effects leading to the correct stationary solution could not be accounted for. For further work relying on symmetry properties in the case of a fermionic oscillator, see Ref. 26.

The article is organized as follows: in Sec. II we recall the most general Lindblad structure corresponding to a quantum Fokker–Planck equation, further showing the expressions that come out asking for shift-covariance or translation-covariance; in Sec. III we outline the results of a microphysical model for the description of quantum Brownian motion, obtained from a quantum linear Boltzmann equation expressed in terms of the operator-valued dynamic structure factor of the reservoir; in Sec. IV we briefly comment on our results, indicating possible future extensions.

II. GENERAL EXPRESSION OF THE QUANTUM FOKKER–PLANCK EQUATION WITH A LINDBLAD STRUCTURE

In order to give a quantum description of dissipative phenomena which at the classical level are described by second-order Fokker–Planck equations, we first concentrate on generalizations of the quantum Liouville equation which preserve trace and positivity of the statistical operator, also possibly accounting for friction effects. This can be done considering the most general expression of generator of a completely positive quantum dynamical semigroup (complete positivity being for these Markovian quasi-free systems necessary in order to preserve positivity[15]), given by a Lindblad structure in which position and momentum operator for the microsystem (respectively $\hat{x}$ and $\hat{p}$) appear restricted to bilinear expressions, according to the classical approximations leading to a friction term proportional to velocity. The general expression of a Markovian quantum Fokker–Planck equation preserving the positivity of the statistical operator is thus given, in the one-dimensional case to which we will restrict for simplicity, by[14,27,10]

$$\mathcal{M}_{\hat{x}\hat{p}}[\hat{\rho}]=-\frac{i}{\hbar}\left[H_0(\hat{x},\hat{p})+\frac{\mu}{2}\{\hat{x},\hat{p}\},\hat{\rho}\right]+\sum_{i=1}^{2}\left[\hat{V}_i\hat{\rho}\hat{V}_i^{\dagger}-\frac{1}{2}\{\hat{V}_i^{\dagger}\hat{V}_i,\hat{\rho}\}\right],$$
$$\hat{V}_i=\alpha_i\hat{p}+\beta_i\hat{x},\quad \alpha_i,\beta_i\in\mathrm{C},\quad \mu\in\mathrm{R}, \tag{1}$$

where H_0 is a self-adjoint operator given by a quadratic expression in $\hat{x}$ and $\hat{p}$ describing the free system, and the added Hamiltonian term proportional to μ has been introduced for later convenience. For the sake of comparison with classical Fokker–Planck equations, in order to make the intuitive physical meaning of the different contributions clear, (1) is usually conveniently written in the following form using nested commutators and anticommutators:[10]

$$\mathcal{L}_{\hat{x}\hat{p}}[\hat{\rho}]=-\frac{i}{\hbar}[H_0(\hat{x},\hat{p}),\hat{\rho}]-\frac{i(\mu-\gamma)}{\hbar\quad 2}[\{\hat{x},\hat{p}\},\hat{\rho}]-\frac{i}{\hbar}\gamma[\hat{x},\{\hat{p},\hat{\rho}\}]-\frac{D_{pp}}{\hbar^2}[\hat{x},[\hat{x},\hat{\rho}]]$$
$$-\frac{D_{xx}}{\hbar^2}[\hat{p},[\hat{p},\hat{\rho}]]+\frac{D_{px}}{\hbar^2}[\hat{x},[\hat{p},\hat{\rho}]]+\frac{D_{xp}}{\hbar^2}[\hat{p},[\hat{x},\hat{\rho}]], \tag{2}$$

where due to $[\hat{p},[\hat{x},\cdot]]=[\hat{x},[\hat{p},\cdot]]$ actually $D_{xp}=D_{px}$ and the new coefficients are related to α_i and β_i through the equations

$$D_{xx}=\frac{\hbar}{2}\sum_{i=1}^{2}|\alpha_i|^2,\quad D_{pp}=\frac{\hbar}{2}\sum_{i=1}^{2}|\beta_i|^2,\quad D_{px}=-\frac{\hbar}{2}\Re\sum_{i=1}^{2}\alpha_i^*\beta_i,\quad \gamma=\frac{\hbar}{2}\Im\sum_{i=1}^{2}\alpha_i^*\beta_i,$$

so that the following inequalities hold,

$$D_{xx}\geqslant 0,\quad D_{pp}\geqslant 0,\quad D_{xx}D_{pp}-D_{px}^2\geqslant\frac{\gamma^2\hbar^2}{4}, \tag{3}$$

which are necessary and sufficient conditions for an expression of the form (2) to be cast in Lindblad form, corresponding to the requirement that the matrix of coefficients[27]

$$\mathbf{D}=\begin{pmatrix} D_{xx} & D_{px}+i\frac{\hbar}{2}\gamma \\ D_{px}-i\frac{\hbar}{2}\gamma & D_{pp}\end{pmatrix} \tag{4}$$

has a non-negative determinant.

An alternative but equivalent expression for (2) can be given introducing, with the aid of a length l, whose physical meaning and expression will depend on the system to be described, creation and annihilation operators $\hat{a}$ and $\hat{a}^{\dagger}$:

$$\hat{a}=\frac{1}{l\sqrt{2}}\left(\hat{x}+\frac{i}{\hbar}l^2\hat{p}\right)\quad \hat{a}^{\dagger}=\frac{1}{l\sqrt{2}}\left(\hat{x}-\frac{i}{\hbar}l^2\hat{p}\right), \tag{5}$$

satisfying the commutation relation $[\hat{a},\hat{a}^{\dagger}]=1$. One thus obtains the expression

$$\mathcal{L}_{\hat{a}\hat{a}^{\dagger}}[\hat{\rho}]=-\frac{i}{\hbar}[H_0(\hat{a},\hat{a}^{\dagger}),\hat{\rho}]-\frac{(\mu-\gamma)}{2}[\hat{a}^2-\hat{a}^{\dagger 2},\hat{\rho}]$$
$$-\frac{\gamma}{2}[[\hat{a},\{\hat{a},\hat{\rho}\}]-[\hat{a},\{\hat{a}^{\dagger},\hat{\rho}\}]]+\mathrm{h.c.}$$
$$-\frac{1}{2}\left(\frac{D_{xx}}{l^2}+\frac{D_{pp}l^2}{\hbar^2}\right)[\hat{a}^{\dagger},[\hat{a},\hat{\rho}]]+\frac{1}{2}\left(\frac{D_{xx}}{l^2}-\frac{D_{pp}l^2}{\hbar^2}-2i\frac{D_{px}}{\hbar}\right)[\hat{a},[\hat{a},\hat{\rho}]]+\mathrm{h.c.},$$

or, equivalently, collecting terms as in (1),

$$\mathcal{M}_{\hat{a}\hat{a}^\dagger}[\hat{\rho}] = -\frac{i}{\hbar}[H_0(\hat{a},\hat{a}^\dagger),\hat{\rho}] - \frac{\mu}{2}[\hat{a}^2 - \hat{a}^{\dagger 2},\hat{\rho}]$$
$$+\left(\frac{D_{xx}}{l^2} + \frac{D_{pp}l^2}{\hbar^2} + \gamma\right)\left[\hat{a}\hat{\rho}\hat{a}^\dagger - \frac{1}{2}\{\hat{\rho},\hat{a}^\dagger\hat{a}\}\right]$$
$$+\left(\frac{D_{xx}}{l^2} + \frac{D_{pp}l^2}{\hbar^2} - \gamma\right)\left[\hat{a}^\dagger\hat{\rho}\hat{a} - \frac{1}{2}\{\hat{\rho},\hat{a}\hat{a}^\dagger\}\right]$$
$$-\left(\frac{D_{xx}}{l^2} - \frac{D_{pp}l^2}{\hbar^2} - 2i\frac{D_{px}}{\hbar}\right)\left[\hat{a}\hat{\rho}\hat{a} - \frac{1}{2}\{\hat{\rho},\hat{a}^2\}\right] + \text{h.c.} \tag{6}$$

The recalled expressions essentially give the possible Lindblad structures at most bilinear in the operators $\hat{x}$ and $\hat{p}$ or $\hat{a}$ and $\hat{a}^\dagger$.

A. Shift-covariance

We now analyze the behavior of the considered expressions with respect to suitable symmetry transformations. Consider a locally compact group G and a unitary representation $\hat{U}(g)$, with $g \in G$, on the Hilbert space of the system: following Ref. 28 we say that a mapping $\mathcal{F}$ in the Schrödinger picture is G-covariant if it commutes with the mapping $\mathcal{U}_g[\,\cdot\,] = \hat{U}(g)\cdot\hat{U}^\dagger(g)$ for all $g \in G$:

$$\mathcal{F}[\mathcal{U}_g[\,\cdot\,]] = \mathcal{U}_g[\mathcal{F}[\,\cdot\,]]. \tag{7}$$

Let us now consider the following unitary representation of the group U(1),

$$\hat{U}_\phi = e^{i\phi\hat{N}},$$

where $\hat{N} = \hat{a}^\dagger\hat{a}$ is the number operator and $\phi \in [0,2\pi]$. If we now ask for the general expression (6) invariance under the action of the group U(1), i.e., shift-covariance according to[29]

$$\mathcal{M}_{\hat{a}\hat{a}^\dagger}[e^{i\phi\hat{N}}\cdot e^{-i\phi\hat{N}}] = e^{i\phi\hat{N}}\mathcal{M}_{\hat{a}\hat{a}^\dagger}[\,\cdot\,]e^{-i\phi\hat{N}}, \tag{8}$$

then the Hamiltonian has to be a function of the generator of the transformation $\hat{N}$, and the following stringent requirements appear:

$$D_{xx} = D_{pp}\frac{l^4}{\hbar^2}, \quad D_{px} = 0, \quad \mu = 0.$$

Note that the condition $\mu = 0$ appears here as a necessary condition for shift-covariance or invariance under the relevant symmetry group and not as a natural or most simple choice as sometimes advocated.[2] From a physical point of view the master equation is expected to reflect the relevant symmetry of the reservoir the microscopic system is interacting with. Considering, for example, a single mode (harmonic oscillator) interacting with the electro-magnetic field, one has a U(1) symmetry and condition (8) is actually equivalent to the rotating wave approximation, essentially saying that the master equation is invariant under the transformation

$$\hat{a} \to \hat{a}e^{-i\theta}, \quad \hat{a}^\dagger \to \hat{a}^\dagger e^{+i\theta},$$

or, equivalently, in terms of $\hat{x}$ and $\hat{p}$,

$$\hat{x} \to \hat{x}\cos\theta + \hat{p}\sin\theta, \quad \hat{p} \to -\hat{x}\sin\theta + \hat{p}\cos\theta. \tag{9}$$

The rotating wave approximation is therefore strictly linked to a U(1) symmetry and one cannot expect or try to obtain translational invariance in this case.[7]

If now one further makes the choice $H_0(\hat{\mathsf{N}})=\hbar\omega(\hat{\mathsf{N}}+\frac{1}{2})$ corresponding to a single mode (harmonic oscillator) and asks that an operator with the canonical structure $\hat{\rho}_0=e^{-\beta H_0(\hat{\mathsf{N}})}$ be a stationary solution, i.e., $\mathcal{M}_{\hat{\mathsf{a}}\hat{\mathsf{a}}^\dagger}[\hat{\rho}_0]=0$, a further connection between the coefficients of the master equation appears,[10]

$$2\frac{D_{pp}l^2}{\hbar^2}=\gamma\coth\left(\frac{1}{2}\beta\hbar\omega\right),$$

where β is the inverse temperature characterizing the thermal electromagnetic field the mode is interacting with. The requirements of complete positivity, shift-covariance and existence of the expected canonical stationary solution then fix the quantum Fokker–Planck equation to be of the form

$$\begin{aligned}\mathcal{M}^{\mathrm{QO}}_{\hat{\mathsf{a}}\hat{\mathsf{a}}^\dagger}[\hat{\rho}]=&-\frac{i}{\hbar}[H_0(\hat{\mathsf{N}}),\hat{\rho}]\\&+\gamma\left[\coth\left(\frac{1}{2}\beta\hbar\omega\right)+1\right]\left[\hat{\mathsf{a}}\hat{\rho}\hat{\mathsf{a}}^\dagger-\frac{1}{2}\{\hat{\rho},\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}}\}\right]\\&+\gamma\left[\coth\left(\frac{1}{2}\beta\hbar\omega\right)-1\right]\left[\hat{\mathsf{a}}^\dagger\hat{\rho}\hat{\mathsf{a}}-\frac{1}{2}\{\hat{\rho},\hat{\mathsf{a}}\hat{\mathsf{a}}^\dagger\}\right],\end{aligned}\tag{10}$$

or in terms of the average of the number operator over a thermal distribution,

$$N_\beta(\omega)=\frac{1}{e^{\beta\hbar\omega}-1}=\frac{1}{2}\left[\coth\left(\frac{1}{2}\beta\hbar\omega\right)-1\right],$$

setting $\eta=2\gamma$,

$$\mathcal{M}^{\mathrm{QO}}_{\hat{\mathsf{a}}\hat{\mathsf{a}}^\dagger}[\hat{\rho}]=-\frac{i}{\hbar}[H_0(\hat{\mathsf{N}}),\hat{\rho}]+\eta(N_\beta(\omega)+1)\left[\hat{\mathsf{a}}\hat{\rho}\hat{\mathsf{a}}^\dagger-\frac{1}{2}\{\hat{\rho},\hat{\mathsf{a}}^\dagger\hat{\mathsf{a}}\}\right]+\eta N_\beta(\omega)\left[\hat{\mathsf{a}}^\dagger\hat{\rho}\hat{\mathsf{a}}-\frac{1}{2}\{\hat{\rho},\hat{\mathsf{a}}\hat{\mathsf{a}}^\dagger\}\right],$$

i.e., the well-known quantum optical master equation for the description of a damped harmonic oscillator (for a recent review, see Ref. 30), where the only free parameter is the decay rate η and a further freedom appears in the commutator term, where a function of $\hat{\mathsf{N}}$ corresponding to a frequency shift may be considered. The quantum optical master equation is therefore essentially fixed by formal requirements, well in accordance with its stability with respect to microphysical derivations, which are in fact predictive in so far as they give explicit expressions for η and the energy shift. As a last step, using as natural length of the problem $l=\sqrt{\hbar/M\omega}$, (10) may be written in terms of $\hat{\mathsf{x}}$ and $\hat{\mathsf{p}}$ as

$$\begin{aligned}\mathcal{M}^{\mathrm{QO}}_{\hat{\mathsf{x}}\hat{\mathsf{p}}}[\hat{\rho}]=&-\frac{i}{\hbar}\left[\frac{\hat{\mathsf{p}}^2}{2M}+\frac{1}{2}M\omega^2\hat{\mathsf{x}}^2,\hat{\rho}\right]-\frac{i\gamma}{\hbar 2}([\hat{\mathsf{x}},\{\hat{\mathsf{p}},\hat{\rho}\}]-[\hat{\mathsf{p}},\{\hat{\mathsf{x}},\hat{\rho}\}])\\&-\frac{1\gamma}{\hbar 2}\coth\left(\frac{1}{2}\beta\hbar\omega\right)\left(M\omega[\hat{\mathsf{x}},[\hat{\mathsf{x}},\hat{\rho}]]+\frac{1}{M\omega}[\hat{\mathsf{p}},[\hat{\mathsf{p}},\hat{\rho}]]\right),\end{aligned}$$

where invariance under (9) can be easily checked.

That U(1) symmetry or shift-covariance may lead, under suitable restrictions, to the quantum optical master equation can also be seen considering the recently obtained most general structure of a proper generator of a shift-covariant completely positive quantum dynamical semigroup given in Ref. 29, where also the unboundedness of the operators appearing in the formal Lindblad structure has been taken in due account, using the notion of form-generator. The formal operator expression associated to the form-generator is

$$\mathcal{L}[\hat{\rho}]=-\frac{i}{\hbar}[H(\hat{\mathrm{N}}),\hat{\rho}]+\left[A_0(\hat{\mathrm{N}})\hat{\rho}A_0^{\dagger}(\hat{\mathrm{N}})-\frac{1}{2}\{\hat{\rho},A_0^{\dagger}(\hat{\mathrm{N}})A_0(\hat{\mathrm{N}})\}\right]$$
$$+\sum_{m=1}^{\infty}\left[\hat{\mathrm{W}}^{\dagger m}A_{-m}(\hat{\mathrm{N}})\hat{\rho}A_{-m}^{\dagger}(\hat{\mathrm{N}})\hat{\mathrm{W}}^{m}-\frac{1}{2}\{\hat{\rho},A_{-m}^{\dagger}(\hat{\mathrm{N}})\hat{\mathrm{W}}^{m}\hat{\mathrm{W}}^{\dagger m}A_{-m}(\hat{\mathrm{N}})\}\right]$$
$$+\sum_{m=1}^{\infty}\left[\hat{\mathrm{W}}^{m}A_{m}(\hat{\mathrm{N}})\hat{\rho}A_{m}^{\dagger}(\hat{\mathrm{N}})\hat{\mathrm{W}}^{\dagger m}-\frac{1}{2}\{\hat{\rho},A_{m}^{\dagger}(\hat{\mathrm{N}})A_{m}(\hat{\mathrm{N}})\}\right], \tag{11}$$

where $H(\cdot)=H^{*}(\cdot)$, $A_i(\cdot)$ are functions of the number operator, and $\hat{\mathrm{W}}=\Sigma_{n=0}^{\infty}|n+1\rangle\langle n|$ it the so-called shift-operator.[31] Recalling the polar decompositions $\hat{\mathrm{a}}^{\dagger}=\hat{\mathrm{W}}\sqrt{\hat{\mathrm{N}}+1}$ and $\hat{\mathrm{a}}=\hat{\mathrm{W}}^{\dagger}\sqrt{\hat{\mathrm{N}}}$, for the following simple choice of functions,

$$H(n)=H_0(n)=\hbar\omega\left(n+\frac{1}{2}\right),$$
$$A_m(n)=0,\quad m=0,\quad |m|>1,$$
$$A_1(n)=\sqrt{\gamma(\beta)}\sqrt{n+1},$$
$$A_{-1}(n)=e^{\beta/2}\sqrt{\gamma(\beta)}\sqrt{n},$$

where

$$\gamma(\beta)=\gamma\left[\coth\left(\frac{1}{2}\beta\hbar\omega\right)-1\right],$$

one recovers from (11) the quantum optical master equation.

It is interesting to observe that complete positivity, shift-covariance and the requirement of a canonical stationary solution also allow as a proper generator of a quantum dynamical semigroup the following expression:

$$\mathcal{L}[\hat{\rho}]=-\frac{i}{\hbar}[H_0(\hat{\mathrm{N}}),\hat{\rho}]-\gamma_0[\hat{\mathrm{N}},[\hat{\mathrm{N}},\hat{\rho}]]$$
$$+\sum_{m=1}^{\infty}\gamma_m\left\{\left[\coth\left(\frac{1}{2}\beta\hbar\omega\right)+1\right]^{m}\left[\hat{\mathrm{a}}^{m}\hat{\rho}\hat{\mathrm{a}}^{\dagger m}-\frac{1}{2}\{\hat{\rho},\hat{\mathrm{a}}^{\dagger m}\hat{\mathrm{a}}^{m}\}\right]\right.$$
$$\left.+\left[\coth\left(\frac{1}{2}\beta\hbar\omega\right)-1\right]^{m}\left[\hat{\mathrm{a}}^{\dagger m}\hat{\rho}\hat{\mathrm{a}}^{m}-\frac{1}{2}\{\hat{\rho},\hat{\mathrm{a}}^{m}\hat{\mathrm{a}}^{\dagger m}\}\right]\right\}, \tag{12}$$

corresponding to the functions

$$A_0(n)=\sqrt{\gamma_0}n,$$
$$A_m(n)=\sqrt{\gamma_m(\beta)}\sqrt{\frac{(n+m)!}{n!}},$$
$$A_{-m}(n)=e^{m\beta/2}\sqrt{\gamma_m(\beta)}\sqrt{\frac{n!}{(n-m)!}},$$

where

$$\gamma_m(\beta)=\gamma_m\left[\coth\left(\frac{1}{2}\beta\hbar\omega\right)-1\right]^{m}.$$

Equation (12) provides a generalization of the quantum optical master equation in which both phase-diffusion, related to the coefficient γ_0, and m-photon processes with decay rates $\eta_m = 2^m \gamma_m$, which should quickly approach zero in order to allow for nonexplosion of the associated Markov process, can be considered. Thus far we have dealt with the case of shift-covariance, corresponding to U(1) symmetry of the system with many degrees of freedom acting as reservoir and determining the non-Hamiltonian dynamics of the microsystem.

B. Translation-covariance

We now consider the case in which the relevant symmetry is invariance under translations, corresponding to a homogeneous reservoir. Given the unitary representation of the translation group

$$\hat{U}(b) = e^{-(i/\hbar)\, b\hat{\mathrm{p}}},$$

where $\hat{\mathrm{p}}$ is the momentum operator of the microsystem and $b \in \mathrm{R}$, translation-covariance according to Ref. 32 amounts to the requirement

$$\mathcal{L}_{\hat{\mathrm{x}}\hat{\mathrm{p}}}[e^{-(i/\hbar)\, b\hat{\mathrm{p}}} \cdot e^{+(i/\hbar)\, b\hat{\mathrm{p}}}] = e^{-(i/\hbar)\, b\hat{\mathrm{p}}} \mathcal{L}_{\hat{\mathrm{x}}\hat{\mathrm{p}}}[\,\cdot\,] e^{+(i/\hbar)\, b\hat{\mathrm{p}}}. \tag{13}$$

Invariance under the group R of translations thus implies for the structure of the quantum Fokker–Planck equation that the Hamiltonian has to be a function of the generator of the transformation $\hat{\mathrm{p}}$ and the following simple requirement in the coefficients appearing in (2):

$$\mu = \gamma.$$

Considering, for example, a free particle interacting with a homogeneous reservoir, one has R symmetry corresponding to invariance under translations, which is reflected by the fact that according to (13) the master equation is invariant under the transformation

$$\hat{\mathrm{x}} \to \hat{\mathrm{x}} + b, \quad \hat{\mathrm{p}} \to \hat{\mathrm{p}},$$

or, equivalently, in terms of $\hat{\mathrm{a}}$ and $\hat{\mathrm{a}}^\dagger$,

$$\hat{\mathrm{a}} \to \hat{\mathrm{a}} + \frac{1}{\sqrt{2}} \frac{b}{l}, \quad \hat{\mathrm{a}}^\dagger \to \hat{\mathrm{a}}^\dagger + \frac{1}{\sqrt{2}} \frac{b}{l}.$$

Further, making the obvious choice $H_0(\hat{\mathrm{p}}) = \hat{\mathrm{p}}^2/2M$, corresponding to a free particle of mass M and asking that an operator with the canonical structure $\hat{\rho}_0 = e^{-\beta H_0(\hat{\mathrm{p}})}$ be a stationary solution, i.e., $\mathcal{L}_{\hat{\mathrm{x}}\hat{\mathrm{p}}}[\hat{\rho}_0] = 0$, one has the condition

$$D_{pp} = \gamma \frac{2M}{\beta},$$

with β the inverse temperature of the homogeneous reservoir. The requirement, of complete positivity, translation-covariance and existence of the expected stationary solution thus constrain the quantum Fokker–Planck equation to be of the form

$$\mathcal{L}^{\mathrm{QBM}}_{\hat{\mathrm{x}}\hat{\mathrm{p}}}[\hat{\rho}] = -\frac{i}{\hbar}[H_0(\hat{\mathrm{p}}), \hat{\rho}] - \frac{i}{\hbar}\gamma[\hat{\mathrm{x}}, \{\hat{\mathrm{p}}, \hat{\rho}\}] - \gamma \frac{2M}{\beta\hbar^2}[\hat{\mathrm{x}}, [\hat{\mathrm{x}}, \hat{\rho}]] - \frac{D_{xx}}{\hbar^2}[\hat{\mathrm{p}}, [\hat{\mathrm{p}}, \hat{\rho}]] + 2\frac{D_{px}}{\hbar^2}[\hat{\mathrm{x}}, [\hat{\mathrm{p}}, \hat{\rho}]], \tag{14}$$

i.e., the typical structure one finds in the extensive physical literature aiming at the description of quantum Brownian motion (see Refs. 1 and 3 for a review). With respect to the case of the

quantum optical master equation (10), the remaining freedom in the structure is much bigger: apart from the friction coefficient γ and a real function of $\hat{\mathrm{p}}$ correcting the Hamiltonian, the coefficients D_{xx} and D_{px} are undetermined except for the relation

$$\gamma\frac{2M}{\beta}D_{xx}-D_{px}^2\geqslant\frac{\gamma^2\hbar^2}{4}$$

stemming from (3). This is reflected by the fact that a much wider literature has been devoted to the subject, looking for microphysical derivations of the quantum Brownian motion master equation, in order to obtain expressions for the undetermined parameters.

We now compare the result (14) with the general structure of a proper generator of a translation-covariant quantum dynamical semigroup, given in Ref. 32, where also the case of an unbounded generator has been considered, introducing the notion of form-generator and specifying a suitable domain for the mapping. Restricting to the continuous component of the generator, corresponding to a quantum Fokker–Planck equation describing friction and diffusion, one has for the formal operator expression associated to the form-generator the following result:

$$\begin{gathered}\mathcal{L}[\hat{\rho}]=-\frac{i}{\hbar}[\beta\hat{\mathrm{x}}+H(\hat{\mathrm{p}}),\hat{\rho}]+\alpha\hat{\mathrm{V}}\hat{\rho}\hat{\mathrm{V}}^{\dagger}-\hat{\mathrm{K}}\hat{\rho}-\hat{\rho}\hat{\mathrm{K}}^{\dagger},\quad \beta\in\mathrm{R},\quad \alpha\geqslant 0,\\ \hat{\mathrm{V}}=\hat{\mathrm{x}}+L(\hat{\mathrm{p}}),\quad \hat{\mathrm{K}}=\frac{\alpha}{2}[\hat{\mathrm{x}}^2+2\hat{\mathrm{x}}L(\hat{\mathrm{p}})+L^{\dagger}(\hat{\mathrm{p}})L(\hat{\mathrm{p}})],\end{gathered}\tag{15}$$

$H(\cdot)=H^*(\cdot)$, $L(\cdot)$ being functions of the momentum operator $\hat{\mathrm{p}}$, and $\beta\neq 0$ implying, e.g., a constant gravitational or electric field. According to (15) one has a single operator of the form $\hat{\mathrm{V}}=\hat{\mathrm{x}}+L(\hat{\mathrm{p}})$ (or one for each Cartesian coordinate considering higher dimensions) instead of two as considered in (1). Expressing (15) in terms of nested commutators and anticommutators as in (2), restricting to the case in which $L(\cdot)$ is a linear function, according to the fact that we are considering friction effects at most linear in the velocity, the inequalities in (3), corresponding to the fact that the determinant of the matrix given in (4) be zero or positive, now become more restrictive:

$$D_{xx}\geqslant 0,\quad D_{pp}\geqslant 0,\quad D_{xx}D_{pp}-D_{px}^2=\frac{\gamma^2\hbar^2}{4},$$

corresponding to $\det\mathbf{D}=0$. Coming back to (14), this implies the further restriction

$$D_{xx}=\gamma\frac{\beta\hbar^2}{8M}+\frac{\beta}{2\gamma M}D_{px}^2,$$

so that apart from the overall multiplying coefficient γ only another coefficient D_{px} is left free, and one has

$$\begin{aligned}\mathcal{L}_{\hat{\mathrm{x}}\hat{\mathrm{p}}}^{\mathrm{QBM}}[\hat{\rho}]=&-\frac{i}{\hbar}[H_0(\hat{\mathrm{p}}),\hat{\rho}]-\frac{i}{\hbar}\gamma[\hat{\mathrm{x}},\{\hat{\mathrm{p}},\hat{\rho}\}]-\gamma\frac{2M}{\beta\hbar^2}[\hat{\mathrm{x}},[\hat{\mathrm{x}},\hat{\rho}]]-\gamma\frac{\beta}{8M}[\hat{\mathrm{p}},[\hat{\mathrm{p}},\hat{\rho}]]\\ &-\frac{\beta}{2\gamma M}\frac{D_{px}^2}{\hbar^2}[\hat{\mathrm{p}},[\hat{\mathrm{p}},\hat{\rho}]]+2\frac{D_{px}}{\hbar^2}[\hat{\mathrm{p}},[\hat{\mathrm{x}},\hat{\rho}]].\end{aligned}\tag{16}$$

Therefore, a predictive microphysical model of quantum Brownian motion essentially has to indicate an explicit expression for the coefficients γ and D_{px}.

It is interesting to express (16) in terms of the creation and annihilation operators given in (5). Setting $\beta\hbar^2/4M=\lambda_{\mathrm{th}}^2$, the square of the thermal wavelength of the microsystem undergoing Brownian motion, one has

$$\mathcal{L}^{\mathrm{QBM}}_{\hat{a}\hat{a}^\dagger}[\hat{\rho}] = -\frac{i}{\hbar}[H_0(\hat{a},\hat{a}^\dagger),\hat{\rho}] - \frac{\gamma}{2}[\hat{a}^2-\hat{a}^{\dagger 2},\hat{\rho}]$$
$$+\left[\frac{\gamma}{2}\left(\frac{\lambda_{\mathrm{th}}^2}{l^2}+\frac{l^2}{\lambda_{\mathrm{th}}^2}+2\right)+\frac{1}{\gamma\hbar^2}\frac{2\,\lambda_{\mathrm{th}}^2}{l^2}D_{px}^2\right]\left[\hat{a}\hat{\rho}\hat{a}^\dagger-\frac{1}{2}\{\hat{\rho},\hat{a}^\dagger\hat{a}\}\right]$$
$$+\left[\frac{\gamma}{2}\left(\frac{\lambda_{\mathrm{th}}^2}{l^2}+\frac{l^2}{\lambda_{\mathrm{th}}^2}-2\right)+\frac{1}{\gamma\hbar^2}\frac{2\,\lambda_{\mathrm{th}}^2}{l^2}D_{px}^2\right]\left[\hat{a}^\dagger\hat{\rho}\hat{a}-\frac{1}{2}\{\hat{\rho},\hat{a}\hat{a}^\dagger\}\right]$$
$$-\left[\frac{\gamma}{2}\left(\frac{\lambda_{\mathrm{th}}^2}{l^2}-\frac{l^2}{\lambda_{\mathrm{th}}^2}\right)+2\frac{D_{px}}{\hbar}\left(\frac{1}{\gamma}\frac{\lambda_{\mathrm{th}}^2}{l^2}\frac{D_{px}}{\hbar}-i\right)\right]\left[\hat{a}\hat{\rho}\hat{a}-\frac{1}{2}\{\hat{\rho},\hat{a}^2\}\right]+\mathrm{h.c.} \tag{17}$$

Equation (17) strongly simplifies if one takes for the length l, used in order to introduce the operators $\hat{a}$ and $\hat{a}^\dagger$ in terms of the operator position and momentum of the particle, the value $l=\lambda_{\mathrm{th}}=\sqrt{\beta\hbar^2/4M}$, naturally suggested by the underlying physics. With l the thermal de Broglie wavelength (17) reduces to

$$\mathcal{L}^{\mathrm{QBM}}_{\hat{a}\hat{a}^\dagger}[\hat{\rho}] = -\frac{i}{\hbar}[H_0(\hat{a},\hat{a}^\dagger),\hat{\rho}] - \frac{\gamma}{2}[\hat{a}^2-\hat{a}^{\dagger 2},\hat{\rho}] + 2\gamma\left[\hat{a}\hat{\rho}\hat{a}^\dagger-\frac{1}{2}\{\hat{\rho},\hat{a}^\dagger\hat{a}\}\right]$$
$$+\frac{2D_{px}^2}{\gamma\hbar^2}\left[\hat{a}\hat{\rho}\hat{a}^\dagger-\frac{1}{2}\{\hat{\rho},\hat{a}^\dagger\hat{a}\}+\hat{a}^\dagger\hat{\rho}\hat{a}-\frac{1}{2}\{\hat{\rho},\hat{a}\hat{a}^\dagger\}\right]$$
$$-2\frac{D_{px}}{\hbar}\left(\frac{1}{\gamma}\frac{D_{px}}{\hbar}-i\right)\left[\hat{a}\hat{\rho}\hat{a}-\frac{1}{2}\{\hat{\rho},\hat{a}^2\}\right]+\mathrm{h.c.}, \tag{18}$$

where the last three contributions can only vanish if the real coefficient D_{px} is equal to zero, corresponding to $L(\cdot)=-L^*(\cdot)$ in (15). Equation (16) or equivalently (18) expresses the general structure of a quantum Fokker–Planck equation which is invariant under translation, warrants the existence of the expected canonical expression as a stationary solution, thus recovering equipartition, and is furthermore a proper generator of a completely positive quantum dynamical semigroup.

C. Covariance and uniqueness of the stationary solution

In recent work[2,12] aiming at comparing and clarifying different approaches to quantum dissipation, which relies on[14] but neglects the more recent and thorough results of Refs. 32 and 29, the statement can be found that *no Markovian theory can satisfy all three criteria of positivity, translational invariance, and asymptotic approach to the canonical equilibrium state* $e^{-\beta H_0}$, *except in special cases*. This statement is always correct in view of the last observation, and these simple exceptional cases, which are usually not spelled out, can be read in (11): the microsystem has to be a free particle apart from an effective correction to the Hamiltonian, given by a real function of $\hat{p}$ describing, for example, an effective mass, and a potential term depending linearly on position (such as, e.g., a constant gravitational or electric field). These cases are often neglected, having in mind that translational invariance, mainly seen as an abstract property rather than the expression of homogeneity of the reservoir, should be always asked for. In this spirit translational invariance, i.e., R symmetry, is asked for also for the damped harmonic oscillator.

The three physical requirements one can reasonably ask together for Markovian systems in the weak-coupling limit are complete positivity, existence of the stationary solution predicted by equipartition, and invariance under the relevant symmetry, not necessarily translational invariance. Having translational invariance apart from the potential term is not physically significant since the potential term actually breaks this invariance, and would furthermore lead to high nonuniqueness of the stationary state, as argued below. The dynamics of the microsystem is driven by both the potential term (which could also arise as a mean field effect) and the contributions describing

decoherence and dissipation, so that a physically relevant symmetry should pertain to the system as a whole. Let us in fact consider a mapping $\mathcal{F}$ covariant with respect to a given symmetry group G according to (7), which admits a stationary solution $\hat{\rho}_0$, i.e., $\mathcal{F}[\hat{\rho}_0]=0$. If the operator $\hat{\rho}_0$ is not invariant under the unitary representation $\mathcal{U}_g$ of G, so that

$$\hat{\rho}_g=\mathcal{U}_g[\hat{\rho}_0]$$

is linearly independent from $\hat{\rho}_0$ at least for some g in G, due to the G-covariance of $\mathcal{F}$, $\hat{\rho}_g$ still is a stationary solution

$$\mathcal{F}[\hat{\rho}_g]=\mathcal{F}[\mathcal{U}_g[\hat{\rho}_0]]=\mathcal{U}_g[\mathcal{F}[\hat{\rho}_0]]=0,$$

so that one cannot have the expected uniqueness of the solution. In the case of the one-dimensional Lie groups considered in Sec. II, for example, a stationary solution can be unique only if it commutes with the generator of the group. Note that this simple argument is independent on whether the mapping $\mathcal{F}$ ensures complete positivity of the time evolution or not, so that the clash between the requirement of translation invariance and the existence of the correct stationary state corresponding to equipartition is not due to the requirement of complete positivity of the time evolution mapping.

III. QUANTUM FOKKER–PLANCK EQUATION FOR THE MOTION OF A BROWNIAN PARTICLE

As we have shown in Sec. II A, in the case of an underlying U(1) symmetry formal requirements are enough to essentially fix structure and coefficients of the quantum Fokker–Planck equation, apart from an energy shift and an overall coefficient. The same is not true in the case of R symmetry describing translational invariance. In this paragraph we therefore quickly recall a recently proposed quantum Fokker–Planck equation for the description of the motion of a heavy Brownian particle interacting through collisions with a homogeneous fluid made up of much lighter particles (see Refs. 20, 21, and 23 for details). This result has been obtained within a kinetic approach, where the dynamics is driven by single events described as collisions in which one generally has momentum and energy transfer, alternative to the Zwanzig Caldeira Leggett approach,[33] recently criticized in Ref. 34, where one describes the reservoir as a collection of harmonic oscillators coupled to the microsystem through its position, usually performing calculations in terms of path-integral techniques.

In the aforementioned approach one obtains in the first instance a kinetic equation for the statistical operator analogous to the classical linear Boltzmann equation given by the simple expression

$$\mathcal{L}[\hat{\rho}]=-\frac{i}{\hbar}[H_0(\hat{\mathrm{p}}),\hat{\rho}]+\frac{2\pi}{\hbar}(2\pi\hbar)^3 n\int_{\mathbf{R}^3}d^3\mathbf{q}\,|\tilde{t}(q)|^2\Big[e^{(i/\hbar)\,\mathbf{q}\cdot\hat{\mathrm{x}}}\sqrt{S(\mathbf{q},\hat{\mathrm{p}})}\hat{\rho}\sqrt{S(\mathbf{q},\hat{\mathrm{p}})}e^{-(i/\hbar)\,\mathbf{q}\cdot\hat{\mathrm{x}}}$$
$$-\frac{1}{2}\{S(\mathbf{q},\hat{\mathrm{p}}),\hat{\rho}\}\Big], \tag{19}$$

where $\tilde{t}(q)$ is the Fourier transform of the T-matrix describing the microphysical collisions and the function $S(\mathbf{q},\mathbf{p})$ appearing operator-valued in (19) is a positive two-point correlation function known in the physical community as dynamic structure factor,[35] usually expressed as a function of momentum and energy transfer, $\mathbf{q}$ and E, according to

$$S(\mathbf{q},\mathbf{p})\equiv S(\mathbf{q},E),\quad E(\mathbf{q},\mathbf{p})=\frac{(\mathbf{p}+\mathbf{q})^2}{2M}-\frac{\mathbf{p}^2}{2M},$$

with M the mass of the Brownian particle. The dynamic structure factor $S(\mathbf{q},E)$ is the Fourier transform of the two-point time dependent density autocorrelation function of the fluid

$$S(\mathbf{q},E)=\frac{1}{2\pi\hbar}\int_{\mathbf{R}}dt\int_{\mathbf{R}^3}d^3\mathbf{x}\,e^{(i/\hbar)[E(\mathbf{q},\mathbf{p})t-\mathbf{q}\cdot\mathbf{x}]}\frac{1}{N}\int_{\mathbf{R}^3}d^3\mathbf{y}\,\langle N(\mathbf{y})N(\mathbf{y}+\mathbf{x},t)\rangle, \tag{20}$$

and is always positive since it is proportional to the energy dependent scattering cross-section of a microscopic probe off a macroscopic sample,[36] giving the spectrum of its spontaneous fluctuations. Equation (19) also has the three properties of complete positivity, translational invariance and canonical stationary solution, and it actually gives a physical example of the general structure of generator of a translation-covariant quantum dynamical semigroup,[32] going beyond the diffusive case considered in (11). In order to recover from the general integral kinetic Eq. (19) a quantum Fokker–Planck equation for the description of the Brownian motion of a heavy particle, one has to consider the limit of small momentum transfer and small energy transfer (corresponding to the Brownian limit in which the mass of the test particle is much heavier than the particles of the fluid). Considering a gas of free particles obeying Maxwell–Boltzmann statistics, due to

$$S_{\mathrm{MB}}(\mathbf{q},\mathbf{p})=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}z\exp\left[-\frac{\beta}{8m}\frac{(2mE(\mathbf{q},\mathbf{p})+q^2)^2}{q^2}\right] \tag{21}$$

one has[23]

$$\mathcal{L}[\hat{\rho}]=-\frac{i}{\hbar}[H_0(\hat{\mathrm{p}}),\hat{\rho}]-\frac{i}{\hbar}\gamma\sum_{i=1}^{3}[\hat{\mathrm{x}}_i,\{\hat{\mathrm{p}}_i,\hat{\rho}\}]-\frac{D_{pp}}{\hbar^2}\sum_{i=1}^{3}[\hat{\mathrm{x}}_i,[\hat{\mathrm{x}}_i,\hat{\rho}]]-\frac{D_{xx}}{\hbar^2}\sum_{i=1}^{3}[\hat{\mathrm{p}}_i,[\hat{\mathrm{p}}_i,\hat{\rho}]]. \tag{22}$$

In this kinetic case the free parameters in (16) are now determined as

$$D_{px}=0,\quad \gamma=\frac{1}{3}z\frac{\pi^2m^2}{\beta\hbar}\int_{\mathbf{R}^3}d^3\mathbf{q}\,|\tilde{t}(q)|^2qe^{-(\beta/8m)\,q^2}$$

with $z=e^{\beta\mu}$ the fugacity of the gas,[37] while D_{xx} and D_{pp} are expressed in terms of γ as can be read in (16):

$$D_{xx}=\frac{\beta\hbar^2}{8M}\gamma,\quad D_{pp}=\frac{2M}{\beta}\gamma.$$

Also the expression of (22) in terms of the operators $\hat{\mathrm{a}}_i$ and $\hat{\mathrm{a}}_i^\dagger$ according to (18) takes in this case a particularly simple form

$$\mathcal{L}[\hat{\rho}]=-\frac{i}{\hbar}[H_0(\hat{\mathrm{a}}_i,\hat{\mathrm{a}}_i^\dagger),\hat{\rho}]-\frac{\gamma}{2}\sum_{i=1}^{3}[\hat{\mathrm{a}}_i^2-\hat{\mathrm{a}}_i^{\dagger 2},\hat{\rho}]+2\gamma\sum_{i=1}^{3}\left[\hat{\mathrm{a}}_i\hat{\rho}\hat{\mathrm{a}}_i^\dagger-\frac{1}{2}\{\hat{\rho},\hat{\mathrm{a}}_i^\dagger\hat{\mathrm{a}}_i\}\right], \tag{23}$$

so that one has a single $\hat{\mathrm{a}}_i=\sqrt{2M/\beta\hbar^2}(\hat{\mathrm{x}}_i+i\,(\beta\hbar^2/4M)\hat{\mathrm{p}}_i)$ operator for each Cartesian coordinate.

IV. CONCLUSIONS AND OUTLOOK

The main scope of this article was to show how relevant symmetries can be in the determination of structures of quantum Fokker–Planck equation. While in the literature only translational invariance is considered and asked for also in the case of the damped harmonic oscillator, leading to no go statements regarding the possibility of having quantum Fokker–Planck equations with all the physically relevant features (complete positivity, covariance and equipartition), we here considered both one-dimensional Lie groups U(1) and R, showing that they are connected to two distinct classes of quantum Fokker–Planck equations: the quantum optical master equation associated to shift-covariance and the quantum Brownian motion master equation associated to translation-covariance. That these two classes of models actually correspond to different physics can also be seen in connection with recent studies on their properties with respect to decoherence.[8]

In particular, independently of complete positivity of the time evolution, it has been shown that covariance properties put severe restrictions on the structure of the stationary solution, provided uniqueness is asked for.

In the case of shift-covariance a generalization of the quantum optical master equation has been proposed, in which also m-photon processes can be considered. Moreover, recent mathematical results by Holevo have been considered, concerning the structure of generators of completely positive quantum dynamical semigroups and leading to further restrictions in the quantum Brownian motion case. For the Brownian motion of a test particle in a fluid, where formal requirements are not enough to essentially fix the structure of the quantum Fokker–Planck equation describing the phenomenon, a recent microphysical approach has been briefly recalled, based on scattering theory, where the quantum Fokker–Planck equation is obtained as the small momentum and energy transfer limit of a quantum generalization of the classical linear Boltzmann equation. Covariance properties with respect to some physically relevant group, typically reflecting a symmetry under certain transformations of the given reservoir, can therefore be a most useful requirement in the determination of structures of quantum Fokker–Planck equations or more generally of linear kinetic equations.

An interesting extension of this work would entail the study of generators of the dynamics of systems in which one has an important correlation between internal and translational degrees of freedom, both coupled through different interactions to some reservoir, a problem recently considered in Ref. 38, where the translational degrees of freedom are treated in a classical way, assuming decoherence is strong enough. Such models could be of interest for the implementation of quantum computing, where indeed some experimental scheme actually relies on a coupling between internal and center of mass degrees of freedom.[39]

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Quantum group covariance and the braided structure of deformed oscillators

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The connection between braided Hopf algebra structure and quantum group covariance of the deformed oscillators is constructed explicitly. In this context we provide deformations of the Hopf algebra of functions on SU(1,1). Quantum subgroups and their representations are also discussed. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1509088]

I. INTRODUCTION

The covariance of the oscillator algebras attracted a lot of attention and is discussed in different contexts.[1] The covariance of an algebra under the action of a noncommutative algebra deforms the notion of defining identical copies in the transformed algebra and this leads to the deformation of the usual tensor product namely braided tensor product. The Hopf algebra axioms are replaced by the braided Hopf algebra axioms.[2] Hence braided group theory (self-contained reviews can be found in Ref. 3) unifies the notions of symmetry and statistics. Recently, we found the general braided Hopf algebra solutions of the generalized oscillators.[4] In this work we show that some of these solutions are connected with the quantum group covariance and we find the **R** matrices controlling the braiding structure and the quantum group. We also discuss the representations of quantum subgroups.

II. THE GENERALIZED OSCILLATOR, ITS COVARIANCE AND BRAIDED HOPF STRUCTURE

Suppose that the generalized oscillator algebra

$$\begin{aligned} aa^* - Q_1 a^* a &= q^{2N}, \\ a q^N &= q q^N a, \\ q^N a^* &= q a^* q^N \end{aligned} \tag{1}$$

is covariant under the transformation

$$\begin{aligned} (a)' &= aK_1 + q^N K_2 + a^* K_3, \\ (a^*)' &= a^* K_1^* + q^N K_2^* + a K_3^*, \\ (q^N)' &= a L_1 + q^N L_2 + a^* L_1^*, \end{aligned} \tag{2}$$

where the deformation parameters Q_1 and q are positive and with the $*$-structure $(a^*)^* = a$ and $(q^N)^* = q^N$. The elements K_1, K_1^*, K_2, K_2^*, K_3, K_3^*, L_1, L_1^*, and L_2 ($L_2^* = L_2$) generate some algebra. Our aim is to find that algebra if the transformation is a quantum group transformation. We write the above transformation as a co-vector transformation

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$$\mathbf{x}' = \mathbf{x}\mathbf{t}, \tag{3}$$

where

$$\mathbf{x} = (a \;\; a^* \;\; q^N) \quad \text{and} \quad \mathbf{t} = \begin{pmatrix} K_1 & K_3^* & L_1 \\ K_3 & K_1^* & L_1^* \\ K_2 & K_2^* & L_2 \end{pmatrix}. \tag{4}$$

The matrix $\mathbf{t}$ is a quantum matrix satisfying

$$\mathbf{R}\mathbf{t}_1\mathbf{t}_2 = \mathbf{t}_2\mathbf{t}_1\mathbf{R} \tag{5}$$

and $\mathbf{R}$ satisfies QYBE

$$\mathbf{R}_{12}\mathbf{R}_{13}\mathbf{R}_{23} = \mathbf{R}_{23}\mathbf{R}_{13}\mathbf{R}_{12}. \tag{6}$$

To find the $\mathbf{R}$ matrix and hence the quantum group, we write the oscillator algebra as a co-vector algebra

$$\mathbf{x}_1\mathbf{x}_2 = \mathbf{x}_2\mathbf{x}_1\mathbf{R}, \tag{7}$$

where

$$\mathbf{x}_1\mathbf{x}_2 = (a^2 \;\; aa^* \;\; aq^N \;\; a^*a \;\; (a^*)^2 \;\; a^*q^N \;\; q^Na \;\; q^Na^* \;\; q^{2N}), \tag{8}$$

$$\mathbf{x}_2\mathbf{x}_1 = (a^2 \;\; a^*a \;\; q^Na \;\; aa^* \;\; (a^*)^2 \;\; q^Na^* \;\; aq^N \;\; a^*q^N \;\; q^{2N}), \tag{9}$$

and the general form of the $\mathbf{R}$ matrix

$$\mathbf{R} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_1 & 0 & A_6 & 0 & 0 & 0 & 0 & A_{15} \\ 0 & 0 & A_4 & 0 & 0 & 0 & A_{11} & 0 & 0 \\ 0 & A_2 & 0 & A_7 & 0 & 0 & 0 & 0 & A_{16} \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & A_9 & 0 & A_{13} & 0 \\ 0 & 0 & A_5 & 0 & 0 & 0 & A_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & A_{10} & 0 & A_{14} & 0 \\ 0 & A_3 & 0 & A_8 & 0 & 0 & 0 & 0 & A_{17} \end{pmatrix}. \tag{10}$$

The constants (A_i) appearing in the $\mathbf{R}$ matrix is to be determined from the consistency of (7) with the oscillator relations (1) and from (6). The covariance of a co-vector algebra under the action of a quantum group induces a braided Hopf algebra structure whose axioms are collectively given by

$$m\circ(id\otimes m) = m\circ(m\otimes id),$$

$$m\circ(id\otimes \eta) = m\circ(\eta\otimes id) = id,$$

$$(id\otimes\Delta)\circ\Delta = (\Delta\otimes id)\circ\Delta,$$

$$(\epsilon\otimes id)\circ\Delta = (id\otimes\epsilon)\circ\Delta = id,$$

$$m\circ(id\otimes S)\circ\Delta = m\circ(S\otimes id)\circ\Delta = \eta\circ\epsilon,$$

$$\begin{gathered}
\psi\circ(m\otimes id)=(id\otimes m)\circ(\psi\otimes id)\circ(id\otimes\psi),\\
\psi\circ(id\otimes m)=(m\otimes id)\circ(id\otimes\psi)\circ(\psi\otimes id),\\
(id\otimes\Delta)\circ\psi=(\psi\otimes id)\circ(id\otimes\psi)\circ(\Delta\otimes id),\\
(\Delta\otimes id)\circ\psi=(id\otimes\psi)(\psi\otimes id)\circ(id\otimes\Delta),\\
\Delta\circ m=(m\otimes m)(id\otimes\psi\otimes id)\circ(\Delta\otimes\Delta),\\
S\circ m=m\circ\psi\circ(S\otimes S),\\
\Delta\circ S=(S\otimes S)\circ\psi\circ\Delta,\\
\epsilon\circ m=\epsilon\otimes\epsilon,\\
(\psi\otimes id)\circ(id\otimes\psi)\circ(\psi\otimes id)=(id\otimes\psi)\circ(\psi\otimes id)\circ(id\otimes\psi).
\end{gathered}\tag{11}$$

The $*$-structure for a braided algebra B is different from the nonbraided one such that

$$\begin{gathered}
\Delta\circ *=\pi\circ(*\otimes *)\circ\Delta,\\
S\circ *=*\circ S,\\
(a\otimes b)^*=b^*\otimes a^*,\quad \forall a,b\in B.
\end{gathered}\tag{12}$$

The braided co-vector algebra has a braided Hopf algebra structure

$$\Delta(\mathbf{x})=\mathbf{x}\otimes 1+1\otimes\mathbf{x},\quad \epsilon(\mathbf{x})=0,\quad S(\mathbf{x})=-\mathbf{x}\tag{13}$$

with the braiding relations

$$\psi(\mathbf{x}_1\otimes\mathbf{x}_2)=\mathbf{x}_2\otimes\mathbf{x}_1\mathbf{R}',\quad \text{i.e.,}\quad \psi(x_i\otimes x_j)=x_b\otimes x_a R'^{ab}_{ij}.\tag{14}$$

The matrix $\mathbf{R}'$ which controls the braiding relations should satisfy the following conditions:

$$\begin{gathered}
\mathbf{R}'_{12}\mathbf{R}'_{13}\mathbf{R}'_{23}=\mathbf{R}'_{23}\mathbf{R}'_{13}\mathbf{R}'_{12},\\
\mathbf{R}'_{12}\mathbf{R}'_{13}\mathbf{R}_{23}=\mathbf{R}_{23}\mathbf{R}'_{13}\mathbf{R}'_{12},\\
\mathbf{R}_{12}\mathbf{R}'_{13}\mathbf{R}'_{23}=\mathbf{R}'_{23}\mathbf{R}'_{13}\mathbf{R}_{12},\\
(\mathbf{P}\mathbf{R}'+1)(\mathbf{P}\mathbf{R}-1)=0,\\
\mathbf{R}'_{21}\mathbf{R}=\mathbf{R}_{21}\mathbf{R},
\end{gathered}\tag{15}$$

where **P** is the permutation matrix. Hence the problem of finding the quantum group leaving the generalized oscillator algebra covariant and the braidings induced by the quantum group is reduced to finding the matrices **R** and **R′**.

The general form of the matrix **R′** can be written as

$$\mathbf{R}'=\begin{pmatrix} C_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & C_2 & 0 & C_7 & 0 & 0 & 0 & 0 & C_{12} \\ 0 & 0 & C_5 & 0 & 0 & 0 & C_{11} & 0 & 0 \\ 0 & C_3 & 0 & C_8 & 0 & 0 & 0 & 0 & C_{13} \\ 0 & 0 & 0 & 0 & C_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{10} & 0 & C_6 & 0 \\ 0 & 0 & C_6 & 0 & 0 & 0 & C_{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{11} & 0 & C_5 & 0 \\ 0 & C_4 & 0 & C_9 & 0 & 0 & 0 & 0 & C_{14} \end{pmatrix} \tag{16}$$

which gives the general form of the braiding relations.

For the three deformation parameters Q_1 and q free, it turns out that there is a unique solution for the matrices **R** and **R′**, namely,

$$R=\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{Q_1^2}{q^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{Q_1}{q} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{(q^2-Q_1)}{q^2} & 0 & \frac{1}{Q_1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{q} & 0 & \frac{(q^2-Q_1)}{q^2} & 0 \\ 0 & 0 & \frac{(q^2-Q_1)}{q^2} & 0 & 0 & 0 & \frac{1}{q} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{Q_1}{q} & 0 \\ 0 & \frac{Q_1}{q^2} & 0 & -\frac{1}{Q_1} & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{17}$$

and

$$\mathbf{R}'=\begin{pmatrix}
\frac{q^2}{Q_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & Q_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & q & 0 & 0 & 0 & 0 & 0 & 0\\
0 & \frac{q^2-Q_1}{Q_1} & 0 & \frac{q^2}{Q_1^2} & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & \frac{q^2}{Q_1} & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & \frac{q}{Q_1} & 0 & \frac{q^2-Q_1}{Q_1} & 0\\
0 & 0 & \frac{q^2-Q_1}{Q_1} & 0 & 0 & 0 & \frac{q}{Q_1} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & q & 0\\
0 & 1 & 0 & -\frac{q^2}{Q_1^2} & 0 & 0 & 0 & 0 & \frac{q^2}{Q_1}
\end{pmatrix}. \tag{18}$$

Similar to the R matrix of $\mathrm{SU}_q(2)$ the matrix R' is proportional to R ($R'=q^2Q_1^{-1}R$). The entries of the quantum matrix (4) generate the algebra

$$\begin{gathered}
K_1K_1^*=K_1^*K_1+q^2Q_1^{-2}L_1^*L_1+q^{-2}Q_1(q^2-Q_1)K_3^*K_3,\\
K_1K_2=qQ_1^{-1}K_2K_1,\\
K_1K_2^*=q^{-1}Q_1K_2^*K_1+qQ_1^{-1}L_2L_1+q^{-2}Q_1(q^2-Q_1)K_3^*K_2,\\
K_1K_3=q^2Q_1^{-2}K_3K_1,\\
K_1K_3^*=Q_1K_3^*K_1+L_1^2,\\
K_1L_1=qL_1K_1,\\
K_1L_1^*=qQ_1^{-1}L_1^*K_1+q^{-1}(q^2-Q_1)L_1K_3,\\
K_1L_2=L_2K_1+q^{-1}(q^2-Q_1)L_1K_2,\\
K_2K_2^*=Q_1K_2^*K_2+q^{-2}Q_1^2K_3^*K_3-K_1^*K_1+L_2^2,\\
K_2K_3=qQ_1^{-1}K_3K_2,\\
K_2K_3^*=q^{-1}Q_1^2K_3^*K_2+L_2L_1,\\
K_2L_1=Q_1L_1K_2,\\
K_2L_1^*=L_1^*K_2+q^{-1}(q^2-Q_1)L_2K_3,\\
K_2L_2=qL_2K_2-qQ_1^{-1}L_1^*K_1+q^{-1}Q_1L_1K_3),\\
K_3K_3^*=q^{-2}Q_1^3K_3^*K_3+L_1^*L_1,
\end{gathered} \tag{19}$$

$$K_3L_1=q^{-1}Q_1^2L_1K_3,$$

$$K_3L_1^*=qL_1^*K_3,$$

$$K_3L_2=Q_1L_2K_3,$$

$$L_1L_1^*=q^2Q_1^{-2}L_1^*L_1,$$

$$L_1L_2=qQ_1^{-1}L_2L_1.$$

The Hopf algebra structure is given by the group Hopf algebra

$$\Delta(\mathbf{t})=\mathbf{t}\otimes\mathbf{t},\quad \epsilon(\mathbf{t})=1,\quad S(\mathbf{t})=\mathbf{t}^{-1}, \tag{20}$$

where the inverse matrix is given by

$$\mathbf{t}^{-1}=\begin{pmatrix} L_2K_1^*-qQ_1^{-1}L_1^*K_2^* & -Q_1^{-2}L_2K_3^*+q^{-1}Q_1^{-1}L_1K_2^* & qQ_1^{-2}L_1^*K_3^*-q^{-1}L_1K_1^* \\ -Q_1^2L_2K_3+qQ_1L_1^*K_2 & L_2K_1-q^{-1}Q_1L_1K_2 & q^{-1}Q_1^2L_1K_3-qL_1^*K_1 \\ q^2Q_1^{-1}K_3K_2^*-qK_2K_1^* & q^{-2}Q_1K_3^*K_2-q^{-1}K_2^*K_1 & K_1^*K_1-q^{-2}Q_1^2K_3^*K_3 \end{pmatrix}\delta^{-1}. \tag{21}$$

The element δ which is defined to be

$$\delta\equiv L_2K_1^*K_1-q^{-2}Q_1^2L_2K_3^*K_3+L_1K_3K_2^*+L_1^*K_3^*K_2-qQ_1^{-1}L_1^*K_2^*K_1-q^{-1}Q_1L_1K_2K_1^* \tag{22}$$

has grouplike Hopf algebra structure

$$\Delta(\delta)=\delta\otimes\delta,\quad \epsilon(\delta)=1,\quad S(\delta)=\delta^{-1} \tag{23}$$

and satisfies

$$K_1\delta=\delta K_1,\ K_2\delta=q^{-1}Q_1^2\delta K_2,\ K_3\delta=q^{-2}Q_1^4\delta K_3,\ L_1\delta=qQ_1^{-2}\delta L_1,\ L_2\delta=\delta L_2 \tag{24}$$

and their *-conjugates with $\delta^*=\delta$.

The braided Hopf algebra structure of the generalized oscillator (1) implied by the quantum group covariance is given by the co-products

$$\Delta(q^N)=q^N\otimes 1+1\otimes q^N,\ \Delta(a)=a\otimes 1+1\otimes a,\ \Delta(a^*)=a^*\otimes 1+1\otimes a^*, \tag{25}$$

the co-units

$$\epsilon(q^N)=\epsilon(a)=\epsilon(a^*)=0, \tag{26}$$

the antipodes

$$S(q^N)=-q^N,\ S(a)=-a,\ S(a^*)=-a^* \tag{27}$$

and the braidings implied by (18),

$$\psi(q^N\otimes q^N)=q^2Q_1^{-1}q^N\otimes q^N,$$

$$\psi(q^N\otimes a)=qQ_1^{-1}a\otimes q^N,$$

$$\psi(a^*\otimes q^N)=qQ_1^{-1}q^N\otimes a^*,$$

$$\psi(q^N\otimes a^*)=qa^*\otimes q^N+Q_1^{-1}(q^2-Q_1)q^N\otimes a^*,$$
$$\psi(a\otimes q^N)=qq^N\otimes a+Q_1^{-1}(q^2-Q_1)a\otimes q^N,$$
$$\psi(a\otimes a)=q^2Q_1^{-1}a\otimes a,$$
$$\psi(a^*\otimes a^*)=q^2Q_1^{-1}a^*\otimes a^*,$$
$$\psi(a\otimes a^*)=Q_1^{-1}(q^2-Q_1)a\otimes a^*+Q_1a^*\otimes a+q^N\otimes q^N,$$
$$\psi(a^*\otimes a)=-q^2Q_1^{-2}q^N\otimes q^N+q^2Q_1^{-2}a\otimes a^*. \tag{28}$$

In contrast to the three parameter deformed case where there is a unique solution for the braidings, the two parameter deformed case $Q_1=q^2$ has three more solutions apart from the solution obtained by substituting $Q_1=q^2$ into (28). These solutions are as follows:

sol1,

$$C_1=1,\ C_2=q^2,\ C_3=0,\ C_4=0,\ C_5=q,\ C_6=0,\ C_7=0,$$
$$C_8=q^{-2},\ C_9=0,\ C_{10}=q^{-1},\ C_{11}=0,\ C_{12}=0,\ C_{13}=0,\quad C_{14}=-1; \tag{29}$$

sol2,

$$C_1=1,\ C_2=q^2,\ C_3=0,\ C_4=2,\ C_5=q,\ C_6=0,\ C_7=0,$$
$$C_8=q^{-2},\ C_9=0,\ C_{10}=q^{-1},\ C_{11}=0,\ C_{12}=0,\ C_{13}=0,\quad C_{14}=1; \tag{30}$$

sol3

$$C_1=1,\ C_2=q^2,\ C_3=0,\ C_4=0,\ C_5=q,\ C_6=0,\ C_7=0,$$
$$C_8=q^{-2},\ C_9=-2q^{-2},\ C_{10}=q^{-1},\ C_{11}=0,\ C_{12}=0,\quad C_{13}=0,\ C_{14}=1. \tag{31}$$

The $Q_1=q^2$ case is special not only because there are three more solutions for the braidings, but also the $\mathbf{R}$ matrix is triangular ($\mathbf{R}_{12}^{-1}=\mathbf{R}_{21}$) and $S^2=id$ is satisfied for the quantum group. We also note that in the general braided Hopf algebra solutions given in Ref. 4, only the solutions we give in this section are related with the quantum group covariance.

We should also note that when $L_1=L_1^*=K_2=K_2^*=0$ and $L_2=1$ the transformation matrix is an element of SU(1,1) in the $q=Q_1=1$ limit. Hence the group we define can be interpreted as deformations of SU(1,1).

III. SUBGROUPS AND REPRESENTATIONS

In the general form of the transformation of the generalized oscillator, the invariance quantum group is a nine-parameter quantum group with three deformation parameters. This quantum group has seven and five parameter subgroups which we discuss.

(A) The seven parameter subgroup can be obtained by setting $L_1=L_1^*=0$ in (19). Then the consistency of the relations requires $Q_1=q^2$, i.e., for the oscillator

$$aa^*-q^2a^*a=q^{2N},$$
$$aq^N=qq^Na, \tag{32}$$
$$q^Na^*=qa^*q^N$$

the transformation

$$(a \;\; a^* \;\; q^N)' = (a \;\; a^* \;\; q^N)\begin{pmatrix} K_1 & K_3^* & 0 \\ K_3 & K_1^* & 0 \\ K_2 & K_2^* & L_2 \end{pmatrix} \tag{33}$$

leaves the algebra covariant where the entries of the quantum matrix satisfy

$$\begin{gathered} K_1K_1^* = K_1^*K_1, \\ K_1K_2 = q^{-1}K_2K_1, \\ K_1K_2^* = qK_2^*K_1, \\ K_1K_3 = q^{-2}K_3K_1, \\ K_1K_3^* = q^2K_3^*K_1, \\ K_1L_2 = L_2K_1, \\ K_2K_2^* = q^2K_2^*K_2 + q^2K_3^*K_3 - K_1^*K_1 + L_2^2, \\ K_2K_3 = q^{-1}K_3K_2, \\ K_2K_3^* = q^3K_3^*K_2, \\ K_2L_2 = qL_2K_2, \\ K_3K_3^* = q^4K_3^*K_3, \\ K_3L_2 = q^2L_2K_3. \end{gathered} \tag{34}$$

The Hopf algebra structure is given by the group Hopf algebra, i.e.,

$$\Delta(\mathbf{t}) = \mathbf{t}\otimes\mathbf{t}, \quad \boldsymbol{\epsilon}(\mathbf{t}) = 1, \quad \mathbf{S}(\mathbf{t}) = \mathbf{t}^{-1} \tag{35}$$

and the matrix inverse is

$$\mathbf{t}^{-1} = \begin{pmatrix} L_2K_1^* & -q^{-4}L_2K_3^* & 0 \\ -q^4L_2K_3 & L_2K_1 & 0 \\ K_3K_2^* - qK_2K_1^* & K_3^*K_2 - q^{-1}K_2^*K_1 & K_1^*K_1 - q^2K_3^*K_3 \end{pmatrix}\delta^{-1}, \tag{36}$$

where the element

$$\delta \equiv L_2(K_1^*K_1 - q^2K_3^*K_3) \tag{37}$$

is grouplike

$$\Delta(\delta) = \delta\otimes\delta, \quad \epsilon(\delta) = 1, \quad S(\delta) = \delta^{-1} \tag{38}$$

and satisfies

$$K_1\delta = \delta K_1, \quad K_2\delta = q^3\delta K_2, \quad K_3\delta = q^6\delta K_3, \quad L_2\delta = \delta L_2, \quad \delta^* = \delta. \tag{39}$$

To construct the representation, we take the generators of this algebra as operators acting on some space. We first find the simultaneously diagonalizible operators: the operators L_2, K_1, and

K_1^* commute among themselves and taking into account that $L_2^*=L_2$ we can take these operators as diagonal operators. We take the eigenvalue of the Hermitian operator as

$$L_2|n\rangle=Aq^n|n\rangle, \tag{40}$$

where A is a real constant. The relations of the algebra suggest that

$$K_2|n\rangle\sim|n-1\rangle, \quad K_3|n\rangle\sim|n-2\rangle \tag{41}$$

and hence we take the actions of the generators as

$$\begin{gathered} K_1|n\rangle=k_{1,n}|n\rangle, \quad K_2|n\rangle=k_{2,n}|n-1\rangle, \quad K_3|n\rangle=k_{3,n}|n-2\rangle, \\ K_1^*|n\rangle=k_{1,n}^*|n\rangle, \quad K_2^*|n\rangle=k_{2,n+1}^*|n+1\rangle, \quad K_3^*|n\rangle=k_{3,n+2}^*|n+2\rangle. \end{gathered} \tag{42}$$

Substituting these into (34) we obtain

$$k_{1,n}=Bq^n, \quad k_{2,n}=Cq^n, \quad k_{3,n}=Dq^n, \tag{43}$$

where B, C, and D are complex constants satisfying

$$|B|^2=A^2+q^2|D|^2. \tag{44}$$

We note that the representation is infinite dimensional.

(B) The five parameter subgroup can be obtained by setting $L_1=L_1^*=K_3=K_3^*=0$ in the transformation (2), i.e., for the algebra

$$\begin{gathered} aa^*-Q_1a^*a=q^{2N}, \\ aq^N=qq^Na, \\ q^Na^*=qa^*q^N, \end{gathered} \tag{45}$$

the transformation

$$(a \;\; a^* \;\; q^N)'=(a \;\; a^* \;\; q^N)\begin{pmatrix} K_1 & 0 & 0 \\ 0 & K_1^* & 0 \\ K_2 & K_2^* & L_2 \end{pmatrix} \tag{46}$$

leaves the algebra covariant where the entries of the quantum matrix satisfy

$$\begin{gathered} K_1K_1^*=K_1^*K_1, \\ K_1K_2=qQ_1^{-1}K_2K_1, \\ K_1K_2^*=q^{-1}Q_1K_2^*K_1, \\ K_1L_2=L_2K_1, \\ K_2K_2^*=Q_1K_2^*K_2-K_1^*K_1+L_2^2, \\ K_2L_2=qL_2K_2. \end{gathered} \tag{47}$$

The Hopf algebra structure is given by the group Hopf algebra

$$\Delta(\mathbf{t})=\mathbf{t}\otimes\mathbf{t}, \quad \boldsymbol{\epsilon}(\mathbf{t})=\mathbf{1}, \quad \mathbf{S}(\mathbf{t})=\mathbf{t}^{-1}. \tag{48}$$

The inverse matrix is

$$\mathbf{t}^{-1}=\begin{pmatrix} L_2K_1^* & 0 & 0 \\ 0 & L_2K_1 & 0 \\ -qK_2K_1^* & -q^{-1}K_2^*K_1 & K_1^*K_1 \end{pmatrix}\delta^{-1}, \tag{49}$$

where

$$\delta\equiv L_2K_1^*K_1 \tag{50}$$

is grouplike,

$$\Delta(\delta)=\delta\otimes\delta, \quad \epsilon(\delta)=1, \quad S(\delta)=\delta^{-1}, \tag{51}$$

and satisfies

$$K_1\delta=\delta K_1, \quad K_2\delta=q^{-1}Q_1^2\delta K_2, \quad L_2\delta=\delta L_2. \tag{52}$$

Similar to the construction of the representation of the seven parameter subgroup, the elements L_2 and K_1 can be taken as diagonal operators and K_2 and K_2^* can be taken as lowering and raising operators, respectively. We take the eigenvalue of the Hermitian operator as

$$L_2|n\rangle=Aq^n|n\rangle \tag{53}$$

and for the other operators we take

$$\begin{aligned} &K_1|n\rangle=k_{1,n}|n\rangle, \quad K_2|n\rangle=k_{2,n}|n-1\rangle, \\ &K_1^*|n\rangle=k_{1,n}^*|n\rangle, \quad K_2^*|n\rangle=k_{2,n+1}^*|n+1\rangle. \end{aligned} \tag{54}$$

Substituting these into (47) we obtain

$$k_{1,n}=B\left(\frac{Q_1}{q}\right)^n, \quad |k_{2,n}|^2=A^2\frac{Q_1^n-q^{2n}}{Q_1-q^2}-|B|^2\frac{Q_1^n-\left(\frac{Q_1}{q}\right)^{2n}}{Q_1-\left(\frac{Q_1}{q}\right)^2}, \tag{55}$$

where A is real and B is complex. The quadratic Casimir of the algebra which is found to be

$$C=K_1^*K_1+(q^{-2}-1)K_2^*K_2+q^{-2}L_2^2 \tag{56}$$

has the eigenvalue

$$C|n\rangle=(A^2+q^{-2}|B|^2)|n\rangle. \tag{57}$$

In the algebra (47), when we identify

$$L_2\equiv q^H, \quad K_1=K_1^*\equiv q^{-H}, \quad K_2\equiv(q-q^{-1})^{1/2}X_-, \quad K_2^*\equiv(q-q^{-1})^{1/2}X_+, \quad Q_1=1, \tag{58}$$

the algebra turns out to be

$$q^HX_\pm=q^{\pm1}X_\pm q^H, \quad X_+X_--X_-X_+=\frac{q^{2H}-q^{-2H}}{q-q^{-1}}, \tag{59}$$

which generates $U_q(\mathrm{su}(2))$ with the *-structure

$$(q^H)^* = q^H, \quad (X_\pm)^* = X_\mp . \tag{60}$$

The transformation

$$(a \;\; a^* \;\; q^N)' = (a \;\; a^* \;\; q^N)\begin{pmatrix} q^{-H} & 0 & 0 \\ 0 & q^{-H} & 0 \\ X_- & X_+ & q^H \end{pmatrix} \tag{61}$$

leaves the commutation relations between a, a^*, and q^N invariant. The matrix multiplication gives the co-multiplication of the generators of the algebra

$$\Delta(q^H) = q^H \otimes q^H, \quad \Delta(q^{-H}) = q^{-H} \otimes q^{-H}, \quad \Delta(X_\pm) = X_\pm \otimes q^{-H} + q^H \otimes X_\pm \tag{62}$$

and the co-unit map

$$\epsilon(q^{\pm H}) = 1, \quad \epsilon(X_\pm) = 0 \tag{63}$$

is a map to the identity of the quantum group. The antipodes

$$S(q^{\pm H}) = q^{\mp H}, \quad S(X_\pm) = -q^{\mp 1} X_\pm \tag{64}$$

give the inverse of the transformation matrix.

IV. CONCLUSION

At the level of a single oscillator, the deformation of the oscillator results in a noncommutativity in the algebra whose co-action leaves the oscillator algebra covariant. At the level of two (or more) oscillators, this induces a noncommutativity (called outer noncommutativity) between independent copies. This noncommutativity is described by the braiding relations. The discussion of the n-fold braided tensor product for q-Heisenberg algebra is done in Ref. 5. Hence we give not only a generalization of the oscillator algebra but also the interaction pattern of these oscillators among themselves via the quantum group covariance. This may contribute to understand the possible connections between quantum groups and nonextensive statistical mechanics.[6] In this work we use real deformation parameters, however, the fractional supersymmetric structures require at least one of the deformation parameters to be a root of unity[7] as the generalization of the (-1) factor in the fermionic case. One more thing which deserves a separate study is the decoupling of the oscillators or the unbraiding transformations.[8]

The braided co-vector algebras covariant under quantum groups are also covariant under the braided groups obtained from quantum groups by a transmutation process.[3] The main ingredient of this construction is the **R** matrix. Hence the **R** matrix we found defines a new braided group which we do not consider here.

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The global existence in the Cauchy problem of the Maxwell–Chern–Simons–Higgs system

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In this article we prove the global existence of solution of the classical Maxwell–Chern–Simons–Higgs equations in $(2+1)$-dimensional Minkowski space–time in the Lorentz gauge. We also prove that the topological solution of the Maxwell–Chern–Simons–Higgs system converges to that of Maxwell–Higgs system as the Chern–Simons constant κ goes to zero, reproducing the classical result by Moncrief [J. Math. Phys. **21**, 2291 (1980)] on the global existence of the Maxwell–Klein–Gordon system in $(2+1)$-dimension. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1507609]

I. INTRODUCTION

The Maxwell–Chern–Simons–Higgs model in $(2+1)$-space–time was proposed to construct a self-dual system having both the Maxwell and the Chern–Simons terms.[1] The Lagrangian is

$$\mathcal{L}=-\frac{1}{4}F^{\mu\nu}F_{\mu\nu}+\frac{\kappa}{4}\epsilon^{\mu\nu\rho}F_{\mu\nu}A_\rho+D_\mu\phi\overline{D^\mu\phi}+\frac{1}{2}\partial_\mu N\partial^\mu N-\frac{1}{2}(e|\phi|^2+\kappa N-ev^2)^2-e^2N^2|\phi|^2, \tag{1}$$

where $g_{\mu\nu}=\mathrm{diag}(1,-1,-1)$ is the $(2+1)$-dimensional Minkowskian metric in $\mathbf{R}^3$, ϕ is a complex scalar field, N is a real scalar field, $A=(A_0,A_1,A_2)$ is a gauge field, $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$, $D_\mu=\partial_\mu-ieA_\mu$, e is the charge of the electron, and $\kappa>0$ is the Chern–Simons constant. We are using the summation convention for Greek indices ranging 0,1,2 and for Latin indices ranging 1,2. We raise and lower the tensor indices by $g^{\mu\nu}=(g_{\mu\nu})^{-1}=\mathrm{diag}(1,-1,-1)$ and $g_{\mu\nu}$, respectively. The corresponding Euler–Lagrange equations via variation of the action taken with respect to (A,ϕ,N) are

$$\begin{aligned}&\partial_\lambda F^{\lambda\rho}+\frac{\kappa}{2}\epsilon^{\mu\nu\rho}F_{\mu\nu}+2eIm(\phi\overline{D^\rho\phi})=0,\\ &D_\mu D^\mu\phi+U_{\bar\phi}(|\phi|^2,N)=0,\\ &\partial_\mu\partial^\mu N+U_N=0,\end{aligned} \tag{2}$$

where

$$U(|\phi|^2,N)=\tfrac{1}{2}(e|\phi|^2+\kappa N-ev^2)^2+e^2N^2|\phi|^2,$$

and $U_{\bar\phi}$, U_N are formal derivations of $U(|\phi|^2,N)$ with respect to $\bar\phi$, N:

$$U_{\bar\phi}(|\phi|^2,N)=(e|\phi|^2+\kappa N-ev^2)\phi+e^2N^2|\phi|^2,$$

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$$U_N(|\phi|^2,N)=\kappa(e|\phi|^2+\kappa N-ev^2)+2e^2N|\phi|^2.$$

Setting $\rho=0$ in the first equation of (2), we obtain the Gauss–Law constraint

$$\partial_j F_{j0}-\kappa F_{12}-2e\ \mathrm{Im}(\phi\overline{D_0\phi})=0. \tag{3}$$

The energy functional for the system is

$$E=\int_{\mathbf{R}^2}\left[\frac{1}{2}F_{0i}^2+\frac{1}{2}F_{12}^2+|D_\mu\phi|^2+|\partial_\mu N|^2+U(|\phi|^2,N)\right]dx. \tag{4}$$

We note that, if (A,ϕ,N) is a solution that makes E finite, then either

$$\phi\to 0 \quad \text{and} \quad N\to\frac{ev^2}{\kappa}, \tag{5}$$

or

$$|\phi|^2\to v^2 \quad \text{and} \quad N\to 0 \tag{6}$$

as $|x|\to\infty$. The former is called nontopological boundary condition, and the latter is called topological boundary condition. In the static case, integrating by parts and using (3), we can rewrite the energy functional (4) as

$$E=\int |(D_1\pm iD_2)\phi|^2+|D_0\phi\mp ie\phi N|^2+\frac{1}{2}|F_{12}\pm(e|\phi|^2+\kappa N-e)|^2dx\pm e\int F_{12}dx.$$

This implies the following lower bound for the energy:

$$E\geqslant e\left|\int F_{12}dx\right|. \tag{7}$$

The lower bound is achieved if

$$\begin{aligned}(D_1\pm iD_2)\phi&=0,\\ D_0\mp ie\phi N&=0,\\ F_{12}\pm(e|\phi|^2+\kappa N-e)&=0.\end{aligned} \tag{8}$$

The above system (8) together with (3) is called the self-dual Maxwell–Chern–Simons–Higgs system. The self-dual system was studied extensively under each of the two conditions (5) and (6) by D. Chae *et al.*,[2,3] and on a periodic boundary condition, by Tarantello.[4] They also verified the unifying feature of Maxwell–Chern–Simons–Higgs which was heuristically described in Ref. 1.

On the Cauchy problem to the Maxwell–Chern–Simons–Higgs, to the authors' knowledge there is no previous result in the literature. As a related one, Moncrief has shown the global existence of solutions for the Maxwell–Klein–Gordon equations using the Lorentz gauge in $(2+1)$-space–time.[5] The Lagrangian of the Maxwell–Klein–Gordon system is

$$\mathcal{L}=-\tfrac{1}{4}F^{\mu\nu}F_{\mu\nu}+D_\mu\phi\overline{D^\mu\phi}-m^2|\phi|^2.$$

He proved the global existence of solutions by showing that a suitably defined higher order energy, though not strictly conserved, does not blow up in a finite time. In this article, we prove the global existence of Maxwell–Chern–Simons–Higgs in both nontopological and topological cases in the

Lorentz gauge, and prove that our topological solution converges to that of the Maxwell–Higgs system in the limit, $\kappa \to 0$. We remark that a similar convergence problem was considered for the static cases in Refs. 2 and 4.

In Sec. II we drive sets of equations for Maxwell–Chern–Simons–Higgs from (2) in the Lorentz gauge, and obtain the local existence result by the standard contraction mapping argument. In Sec. III we define the higher order energy and prove that it does not blow up in a finite time. From this result, we show that the $H^2 \times H^1$ norm of a solution can not blow up in any bounded interval of time, which completes the global existence proof. We remark that we could obtain the global boundedness of $H^2 \times H^1$ norm for a solution without introducing the Coulomb transform used in Ref. 5, instead we use the covariant Sobolev inequality which was already used in Ref. 6. Finally, in Sec. IV we verify that the topological solution of Maxwell–Chern–Simons–Higgs converges to that of Maxwell–Higgs which is identified with the Maxwell–Klein–Gordon system by setting $v=0$.

II. THE LOCAL EXISTENCE

The unknowns for the Maxwell–Chern–Simons–Higgs system consist of a vector potential A, a complex scalar field ϕ and a neutral scalar field N. The Lagrangian (1) is invariant through the gauge transformation,

$$A_i' = A_i + \partial_i \lambda,$$

$$\phi' = \exp(i\lambda)\phi.$$

In this article, we fix the gauge by giving the Lorentz gauge condition $\partial^\mu A_\mu = 0$ to the system (2). Using the relation $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, the Euler–Lagrange equations (2) are rewritten in terms of (A, ϕ, N) in the Lorentz gauge by

$$\begin{aligned} \Box A_0 &= -\kappa F_{12} - 2e\ \mathrm{Im}(\phi \overline{D_0 \phi}), \\ \Box A_i &= -\kappa \epsilon^{ij} F_{0j} - 2e\ \mathrm{Im}(\phi \overline{D_i \phi}), \\ \Box \phi &= 2ieA_0 \partial_0 \phi - 2ieA_j \partial_j \phi - e^2 A_j^2 \phi + e^2 A_0^2 \phi - U_{\bar{\phi}}, \\ \Box N &= -U_N, \end{aligned} \tag{9}$$

with given initial data $A_\mu(0,x)$, $\phi(0,x)$, $N(0,x)$, $\partial_0 A_\mu(0,x)$, $\partial_0 \phi(0,x)$, $\partial_0 N(0,x)$ satisfying

$$\begin{aligned} &\partial_\mu A^\mu = 0, \\ &\Delta A_0 - \partial_j \partial_0 A_j - \kappa F_{12} - 2e\ \mathrm{Im}(\phi \overline{D_0 \phi}) = 0. \end{aligned} \tag{10}$$

We write the Maxwell–Chern–Simons–Higgs equations in first order form as follows. Let us introduce the new unknowns $(P_\mu, \psi_\mu, \Omega_\mu)$ defined by

$$P_\mu = \partial_t A_\mu, \quad \psi_\mu = D_\mu \phi, \quad \Omega_\mu = \partial_\mu N.$$

In terms of those unknowns, the Maxwell–Chern–Simons–Higgs system in the Lorentz gauge is written as follows:

$$\partial_0 A_0 = P_0,$$

$$\partial_0 P_0 = \Delta A_0 - \kappa F_{12} - 2e\ \mathrm{Im}(\phi \overline{\psi_0}),$$

$$\partial_0 A_j = P_j,$$

$$\begin{gathered}\partial_0 P_j=\Delta A_j-\kappa\epsilon^{ji}F_{0i}-2e\ \mathrm{Im}(\phi\overline{\psi_j}),\\ \partial_0\phi=\psi_0+ieA_0\phi,\\ \partial_0\psi_0=D_j\psi_j+ieA_0\psi_0-U_{\bar{\psi}},\\ \partial_0\psi_j=D_j\psi_0-ieA_0\psi_j-ieF_{0j}\phi,\\ \partial_0 N=\Omega_0,\\ \partial_0\Omega_0=\partial_j\Omega_j-U_N,\\ \partial_0\Omega_j=\partial_j\Omega_0,\end{gathered}\tag{11}$$

supplemented by constraints (10).

Introduce $\tilde{N}$ satisfying $\tilde{N}+ev^2/\kappa=N$ for the nontopological boundary condition. Then we have

$$(A,\phi,\tilde{N})\to 0 \quad \text{as} \quad |x|\to\infty.$$

In this case the system (11) changes harmlessly (i.e., $U_N\to U_{\tilde{N}}$). For the topological case we may assume $\lim_{|x|\to\infty}\phi=\lambda$ for a complex scalar λ with $|\lambda|=v$. Introducing φ satisfying $\varphi+\lambda=\phi$, we also have

$$(A,\varphi,N)\to 0 \quad \text{as} \quad |x|\to\infty.$$

Let us remark on notations. If no confusion arises, we denote $u=(A,\phi,\tilde{N})$ or (A,φ,N), where $A=(A_0,A_1,A_2)$. Then we denote

$$\|u(t)\|_{H^s}=\|A(t)\|_{H^s}+\|\phi(t)\|_{H^s}+\|\tilde{N}(t)\|_{H^s},$$

in the nontopological case, while

$$\|u(t)\|_{H^s}=\|A(t)\|_{H^s}+\|\varphi(t)\|_{H^s}+\|N(t)\|_{H^s}$$

in the topological case. We also denote

$$\|u(t)\|_{H^s\times H^{s-1}}=\|u(t)\|_{H^s}+\|\partial_0 u(t)\|_{H^{s-1}}.$$

Let $u_0=u(0,\cdot)$. Then $\|u_0\|_{H^2\times H^1}=\|u(0)\|_{H^2}+\|\partial_0 u(0)\|_{H^1}$.

The following is our local existence result for the Maxwell–Chern–Simons–Higgs systems.

Theorem 2.1: *Consider the Maxwell–Chern–Simons–Higgs system (9) with Lorentz gauge constraints (10). Given a data set* $u_0\in H^2\times H^1$ *satisfying* (10) *and either nontopological or topological boundary conditions, there exists a unique local solution u of the Maxwell–Chern–Simons–Higgs system (9) and (10) such that*

$$u\in C([0,T];H^2(\mathbf{R}^2))\cap C^1([0,T];H^1(\mathbf{R}^2)).$$

The existence time interval $[0,T]$ *depends only on* $\|u_0\|_{H^2\times H^1}$.

Proof: We present the local existence proof for the nontopological case only. The topological case is completely similar. We set

$$X_T=C([0,T);H^2(\mathbf{R}^2))\cap C^1([0,T);H^1(\mathbf{R}^2)).$$

Given $T>0$, we introduce the norm $\|\cdot\|_{X_T}$ by $\|f\|_{X_T}=\sup_{0\leqslant t\leqslant T}\|f(t)\|_{H^2\times H^1}$. We seek constants T and Δ_0 so that the equation (9) induces a contraction mapping $\mathcal{F}$ on the closed ball

$$\mathcal{B}=\{(u,\partial_0 u)\in C([0,T];H^2\times H^1):\|u\|_{X_T}\leqslant\Delta_0\},$$

subject to the given initial data $(u_o,\partial_0 u_0)\in H^2\times H^1$. We define the mapping $\mathcal{F}:X_T\to X_T$ as follows: $(A,\phi,\tilde{N})=\mathcal{F}(A',\phi',\tilde{N}')$ solves the following linear wave equations:

$$\begin{aligned}
\Box A_0&=-\kappa(\partial_1 A_2'-\partial_2 A_1')-2e\,\mathrm{Im}(\phi'\overline{D_0'\phi'}),\\
\Box A_i&=-\kappa\epsilon^{ij}(\partial_0 A_j'-\partial_j A_0')-2e\,\mathrm{Im}(\phi'\overline{D_i'\phi'}),\\
\Box\phi&=2ieA_0'\partial_0\phi'-2ieA_j'\partial_j\phi'-e^2A_j'^2\phi'+e^2A_0'^2\phi'-U'_{\overline{\phi'}},\\
\Box\tilde{N}&=-U_{\tilde{N}'}.
\end{aligned}\tag{12}$$

Let $\|u_0\|_{H^2\times H^1}=d$. Applying the standard energy estimates to (12), we have

$$\|A(t)\|_{H^2\times H^1}\leqslant d+C\int_0^t\|\partial A'(s)\|_{H^1}+\|(\mathrm{Im}\,\phi'\overline{D'\phi'})\|_{H^1}ds,$$

$$\|\phi(t)\|_{H^2\times H^1}\leqslant d+C\int_0^t\|(A'\partial\phi')(s)\|_{H^1}+\|(A'^2\phi')(s)\|_{H^1}+\|U'_{\overline{\phi'}}(s)\|_{H^1}ds,$$

$$\|N(t)\|_{H^2\times H^1}\leqslant d+C\int_0^t\|U'_{\tilde{N}'}(s)\|_{H^1},$$

where the symbol ∂ represents a space–time derivative, ∂_0 or ∂_j, and D represents D_0 or D_j, and C depends on κ, e. We use the Nirenberg–Gagliardo inequality, $\|u\|_{L^4}\leqslant\|u\|_{L^2}^{1/2}\Sigma_{j=1}^2\|\partial_j u\|_{L^2}^{1/2}$, and the Sobolev embedding, $\|u\|_{L^\infty}\leqslant C\|u\|_{H^2}$, to estimate the terms in the time integral. The highest order terms are estimated by

$$\begin{aligned}
\|A'\partial\phi'\|_{H^1}&\leqslant\|A'\partial\phi'\|_{L^2}+\sum_{j=1}^2(\|\partial_j A'\partial\phi'\|_{L^2}+\|A'\partial_j\partial\phi'\|_{L^2})\\
&\leqslant C\|A'\|_{H^2}\|\partial\phi'\|_{L^2}+\sum_{i,j,k=1}^2\|\partial_j A'\|_{L^2}^{1/2}\|\partial\phi'\|_{L^2}^{1/2}\|\partial_i\partial_j A'\|_{L^2}^{1/2}\|\partial_k\partial\phi'\|_{L^2}^{1/2}\\
&\quad+C\|A'\|_{H^2}\|\phi'\|_{H^2\times H^1}\leqslant C\|u'\|_{H^2\times H^1},
\end{aligned}$$

and, similarly,

$$\|\phi'\overline{D'\phi'}\|_{H^1}\leqslant C\|u'\|_{H^2\times H^1}.$$

Then we find easily

$$\|u(t)\|_{H^2\times H^1}\leqslant d+C\int_0^t(1+\|u'(s)\|_{H^2\times H^1}^2)\;ds.$$

Using $\|u'\|_{X_T}\leqslant\Delta_0$, we have

$$\|u(t)\|_{H^2\times H^1}\leqslant d+C(1+\Delta_0^2)t$$

for $0\leqslant t\leqslant T$. Therefore, taking $\Delta_0=d+1$ and $T<1/C(1+(d+1)^2)$, we obtain $\|u\|_{X_T}\leqslant\Delta_0$, i.e., we find $\mathcal{F}:\mathcal{B}\to\mathcal{B}$. Using this, we compute easily that

$$\|(\mathcal{F}(u')-\mathcal{F}(v'))(t)\|_{H^2\times H^1}\leqslant C\int_0^t(1+\Delta_0^2)\|(u'-v')(s)\|_{H^2\times H^1}ds$$

for $0\leqslant t\leqslant T$. Choosing T small so that

$$C(1+\Delta_0^2)T\leqslant\tfrac{1}{2}, \tag{13}$$

we deduce that the mapping $\mathcal{F}:\mathcal{B}\to\mathcal{B}$ is a contraction mapping. We can apply the fixed point argument to obtain the unique solution of (9) with $u\in C([0,T];H^2(R^2))\cap C^1([0,T];H^1(R^2))$. To show continuous dependence on the initial data of the solution, we let u,v be each solution to the initial data u_0,v_0. If $\|u_0\|_{H^2},\|v_0\|_{H^2}\leqslant d$, we find that

$$\|u-v\|_{X_T}\leqslant\|u_0-v_0\|_{H^2}+C(1+d^2)T\|u-v\|_{X_T}$$

similarly. Choosing T so small as to T satisfying (13), we obtain

$$\|u-v\|_{X_T}\leqslant 2\|u_0-v_0\|_{X_T}.$$

Next, we show that the constraint equations (10) are propagated by the evolution equations following the argument in Ref. 5. We write

$$\begin{aligned} U&\equiv P_0-\partial_iA_i,\\ V&\equiv\partial_i(\partial_iA_0-\partial_0A_i)-\kappa F_{12}-2e\ \mathrm{Im}\ \phi\overline{D_0\phi}, \end{aligned} \tag{14}$$

and compute, using (11),

$$\frac{d}{dt}\begin{pmatrix}U\\V\end{pmatrix}=\begin{pmatrix}0&I\\\Delta&0\end{pmatrix}\begin{pmatrix}U\\V\end{pmatrix}.$$

We note from the expression (14) that $U\in H^2$ and $V\in H^1$ whenever $u(t)\in H^3\times H^2$. Since the linear wave equation has a unique global solution on $H^2\times H^1$, it follows $U(t)$, $V(t)$ vanish throughout the interval of existence of u. For initial data $u_0\in H^2\times H^1$, we obtain the desired result by the standard density argument. □

III. THE GLOBAL EXISTENCE

In this section we estimate various gauge invariant quantities constructed from $(F_{\mu\nu},\phi,\psi)$. The conserved, gauge invariant energy $E_0(t)$ for Maxwell–Chern–Simons–Higgs is

$$E_0(t)=\int_{\mathbf{R}^2}\left[\frac{1}{2}F_{0i}^2+\frac{1}{2}F_{12}^2+|D_\mu\phi|^2+|\partial_\mu N|^2+U(|\phi|^2,N)\right]dx. \tag{15}$$

Following Ref. 5 we introduce the pseudo-energy $E_1(t)$ defined by

$$E_1(t)=\int_{\mathbf{R}^2}\left[\frac{1}{2}(\partial_lF_{0i})^2+\frac{1}{2}(\partial_lF_{12})^2+|D_l\psi_\mu|^2+(\partial_l\Omega_\mu)^2\right]dx$$

where $\psi_\mu=D_\mu\phi$, $\Omega_\mu=\partial_\mu N$.

The global existence result will be established after several lemmas.

Lemma 3.1: Let $u \in C([0,T];H^2(\mathbf{R}^2)) \cap C^1([0,T];H^1(\mathbf{R}^2))$ *be the solution of systems (9) and (10) with initial data given either nontopological or topological boundary conditions. Then* $\|u(t)\|_{L^2}$ *is estimated in terms of the initial data for all* $t \in [0,T]$.

Proof: We first need to bound $\|A(t)\|_{L^2}$ by the initial data. To derive this, consider the integral

$$\|A(t)\|_{L^2}^2 = \int_{\mathbf{R}^2} A_0^2 + A_i^2 dx.$$

Taking the time derivative of this integral and using the Lorentz gauge condition, we obtain

$$\frac{d}{dt}\|A(t)\|_{L^2}^2 = -\int_{\mathbf{R}^2} 2A_i F_{0i}\ dx \leqslant 2E_0^{1/2}\|A(t)\|_{L^2},$$

where E_0 is the conserved energy of the solution considered. It follows that, for $t \geqslant 0$,

$$\|A(t)\|_{L^2} \leqslant \|A(0)\|_{L^2} + 2E_0^{1/2} t. \tag{16}$$

In a similar way, we obtain the bounds for $(\phi, \tilde{N})$ and (φ, N):

$$\frac{d}{dt}\|\phi(t)\|_{L^2}^2 = 2\ \mathrm{Re}\int_{\mathbf{R}^2} \overline{\phi}\partial_0\phi = 2\ \mathrm{Re}\int_{\mathbf{R}^2} \overline{\phi} D_0\phi dx \leqslant 2E_0^{1/2}\|\phi(t)\|_{L^2},$$

$$\frac{d}{dt}\|\tilde{N}(t)\|_{L^2}^2 = 2\int_{\mathbf{R}^2} \tilde{N}\partial_0 N\ dx \leqslant 2E_0^{1/2}\|\tilde{N}(t)\|_{L^2},$$

$$\frac{d}{dt}\|N(t)\|_{L^2}^2 = 2\int_{\mathbf{R}^2} N\partial_0 N\ dx \leqslant 2E_0^{1/2}\|N(t)\|_{L^2}.$$

To obtain the bound for $\|\varphi(t)\|_{L^2}$, recall $\varphi = \phi - \lambda$. Then we have

$$\|D_0\varphi(t)\|_{L^2} \leqslant \|D_0\phi(t)\|_{L^2} + ev^2\|A(t)\|_{L^2} \leqslant E_0^{1/2} + ev(\|A(0)\|_{L^2} + 2E_0^{1/2} t) \ \text{ by (16)},$$

from which we obtain

$$\frac{d}{dt}\|\varphi(t)\|_{L^2}^2 \leqslant 2\ \mathrm{Re}\int_{\mathbf{R}^2} \overline{\varphi} D_0\varphi dx \leqslant 2\|\varphi(t)\|_{L^2}(E_0^{1/2} + ev(\|A(0)\|_{L^2} + 2E_0^{1/2} t)).$$

The above inequalities imply that

$$\|u(t)\|_{L^2} \leqslant C\|u_0\|_{L^2} + (1+2t)E_0^{1/2} \tag{17}$$

for both $u = (A, \phi, \tilde{N})$ and (A, φ, N). □

Now consider the gauge invariant pseudo-energy $E_1(t)$. We shall show that $E_1(t)$ does not blow up in a finite time.

Lemma 3.2: Let $u \in C([0,T];H^2(\mathbf{R}^2)) \cap C^1([0,T];H^1(\mathbf{R}^2))$ *be the solution of the systems (9) and (10) with an initial data given either nontopological or topological boundary conditions. Then*

(*i*) $E_1(t)$ *is differentiable in time and*

$$\frac{d}{dt}E_1(t) = \int_{\mathbf{R}^2} -2e\partial_j F_{0i}\,\mathrm{Im}(\psi_i\overline{\psi_j}) - 2e\partial_j U_N\partial_j\Omega_0\ dx + 2\ \mathrm{Re}\int_{\mathbf{R}^2} \overline{D_j\psi_0}\cdot(ieF_{ij}\psi_i + ieF_{j0}\psi_0$$

$$-D_j U_{\overline{\phi}})\ dx + 2\ \mathrm{Re}\int_{\mathbf{R}^2} \overline{D_j\psi_i}\cdot(ieF_{ij}\psi_0 - F_{0i}\psi_j + ieF_{j0}\psi_i)\ dx. \tag{18}$$

(*ii*) $E_1(t)$ *is estimated in terms of the initial data for all* $t \in [0,T]$.

We will use the following covariant Sobolev inequality.

Lemma 3.3:[6] *Let* $1\leqslant q,r\leqslant\infty$ *and let* σ *and* p *satisfy* $0\leqslant\sigma\leqslant 1$, $1\leqslant p\leqslant\infty$, *and*

$$\frac{1}{p}=\frac{(1-\sigma)}{r}+\sigma\left(\frac{1}{q}-\frac{1}{n}\right).$$

If $p=\infty$, *then* $r<\infty$ *and* $\sigma<1$. *Let* $D_j=\partial_j-ieA_j$. *Then there exists a constant* C, *depending only on* n, p, q, r, *such that, for any* $u\in L^r$ *for which* $\partial_j u\in L^q$ *and* $A_j u\in L^q$, $j=1,\ldots,n$, *the following inequality holds:*

$$\|u\|_p\leqslant C\|u\|_r^{1-\sigma}\left(\sum_{j=1,2}\|D_j u\|_q\right)^{\sigma}.$$

Proof: See Proposition A.1 in Ref. 6. □

In case $n=2$, $r=2$, we have in particular

$$\|u\|_{L^p}\leqslant C\|u\|_{L^2}^{2/p}\left(\sum_{j=1,2}\|D_j u\|_{L^2}\right)^{1-2/p},\quad 2<p<\infty. \tag{19}$$

Proof of Lemma 3.2: (i) Let us assume an initial data u_0 in $H^3\times H^2$. By the local existence result, we obtain u, the solution of systems (9) and (10) in $C([0,T];H^3(\mathbf{R}^2))\cap C^1([0,T];H^2(\mathbf{R}^2))$. We freely differentiate $E_1(t)$, the pseudo-energy of u, and compute (18) using the equations of motion (11). For an initial data u_0 in $H^2\times H^1$, choose u_0^n in $H^3\times H^2$ so $u_0^n\to u_0$ in the $H^2\times H^1$ sense. Let u^n be the local solution evolving from u_0^n and $E_1^n(t)$ be the corresponding pseudo-energy. Noting that continuous dependence on initial data of the solution assures the uniform existence time interval $[0,T]$ of $\{u_n\}$, we obtain $E_1^n(t)\to E_1(t)$ since $u^n\to u$ in $C([0,T];H^2\times H^1(\mathbf{R}^2))$ by passing to $n\to\infty$. Therefore we obtain the desired result.

(ii) We may express the right hand side of (18), ignoring subscripts, as

$$\int_{\mathbf{R}^2}\partial F\cdot\psi^2+\partial U_N\cdot\partial\Omega+D\psi\cdot\psi\cdot F+D\psi\cdot DU_{\bar{\phi}}dx. \tag{20}$$

We will show that each term of (20) is estimated to be at most linear with respect to $E_1(t)$.

Let us begin with the nontopological case. From (19) we have

$$\|\phi\|_{L^p}\leqslant C\|\phi\|_{L^2}^{2/p}\|\psi\|_{L^2}^{1-2/p}\leqslant C(\|u_0\|_{L^2}+tE_0^{1/2})^{2/p}E_0^{(1/2)}(1-2/p),\quad 2<p<\infty,$$

$$\|\psi\|_{L^4}\leqslant C\|\psi\|_{L^2}^{1/2}\|D\psi\|_{L^2}^{1/2}\leqslant CE_0^{1/4}E_1^{1/4}(t).$$

Note that any power of $\|\phi\|_{L^p}$ $(2<p<\infty)$ is estimated by the initial data since E_0 is conserved. We get

$$\int_{\mathbf{R}^2}\partial F\cdot\psi^2 dx\leqslant\|\partial F\|_{L^2}\|\psi\|_{L^4}^2\leqslant CE_1^{1/2}(t)\|\psi(t)\|_{L^2}\|D\psi(t)\|_{L^2}\leqslant CE_0^{1/2}E_1(t),$$

and

$$\begin{aligned}\int_{\mathbf{R}^2}DF\cdot\psi\cdot F dx&\leqslant\|\psi(t)F(t))\|_{L^2}\|D\psi\|_{L^2}\\&\leqslant C\|F(t)\|_{L^4}\|\psi(t)\|_{L^4}E_1^{1/2}(t)\\&\leqslant C\|\psi(t)\|_{L^2}^{1/2}\|D\psi(t)\|_{L^2}^{1/2}\|F(t)\|_{L^2}^{1/2}\|\partial F(t)\|_{L^2}^{1/2}E_1^{1/2}(t)\leqslant CE_0^{1/2}E_1(t).\end{aligned}$$

Next, we estimate $\partial U_N \cdot \partial\Omega$, $D\psi \cdot DU_{\bar{\phi}}$. Note that ∂U_N, $DU_{\bar{\phi}}$ are expressed by gauge invariant terms using $\partial_l |\phi|^2 = 2\,\mathrm{Re}(\bar{\phi} D_l \phi)$:

$$\partial U_N = 2\kappa(2e\,\mathrm{Re}\,\psi\bar{\phi} + \kappa\Omega) + 2e\kappa^2\left(\Omega|\phi|^2 + 2\left(\tilde{N} + \frac{ev^2}{\kappa}\right)\mathrm{Re}\,\psi\bar{\phi}\right), \tag{21}$$

$$DU_{\bar{\phi}} = \psi|\phi|^2 + 2\phi\,\mathrm{Re}\,\psi\bar{\phi} + \kappa(\phi\Omega + \tilde{N}\psi) + e\kappa^2\left(\tilde{N} + \frac{ev^2}{\kappa}\right)\left(2\Omega\phi + \left(\tilde{N} + \frac{ev^2}{\kappa}\right)\psi\right). \tag{22}$$

Let us pick up $\psi\phi\tilde{N}$ in (21). We may consider $\partial\Omega \cdot \psi\phi\tilde{N}$ term only since other terms of $\partial U_N \cdot \partial\Omega$, $D\psi \cdot DU_{\bar{\phi}}$ are to be estimated in a completely analogous way. First we get

$$\begin{aligned}\int_{\mathbf{R}^2} \psi\phi\tilde{N}\partial\Omega\ dx &\leqslant \|(\psi\tilde{N}\phi)(t)\|_{L^2}\|\partial\Omega\|_{L^2} \\ &\leqslant \|\tilde{N}(t)\|_{L^\infty}\|\psi(t)\|_{L^4}\|\phi(t)\|_{L^4}E_1^{1/2}(t) \\ &\leqslant \|\tilde{N}\|_{L^{2(1-a)/a}}^{1-a}\|\partial^2\tilde{N}\|_{L^2}^{a}\|\psi\|_{L^2}^{1/2}\|D\psi\|_{L^2}^{1/2}\|\phi\|_{L^2}^{1/2}\|\psi\|_{L^2}^{1/2}E_1^{1/2}(t), \quad 0<a<1,\end{aligned}$$

where we use the usual Nirenberg–Gagliardo inequality to $\|\tilde{N}\|_{L^\infty}$ and the covariant Sobolev inequality to $\|\psi\|_{L^4}$, $\|\phi\|_{L^4}$. Applying the Nirenberg–Gagliardo inequality again to $\|\tilde{N}\|_{L^{2(1-a)/a}}$, we get

$$\begin{aligned}\int_{\mathbf{R}^2} \psi\phi\tilde{N}\partial\Omega\,dx &\leqslant \|\tilde{N}(t)\|_{L^2}^{a}\|\partial\tilde{N}(t)\|_{L^2}^{1-2a}\|\partial^2\tilde{N}(t)\|_{L^2}^{a}\|\phi(t)\|_{L^2}^{1/2}E_0^{1/2}E_1^{3/4}(t) \\ &\leqslant C\|u(t)\|_{L^2}^{a+1/2}E_0^{1-a}E_1^{3/4+a/2}(t), \quad 0<a<\tfrac{1}{2}.\end{aligned}$$

Now, choosing $a = 1/4$, we obtain the estimate we want.

Summing up all the estimations of the above, we arrive at

$$\frac{d}{dt}E_1(t) \leqslant C(\|u_0\|_{L^2} + (1+2t^2)E_0^{1/2})E_0^{3/4}(1+E_1(t)) \tag{23}$$

with C depending on κ, e, v and the conserved energy E_0 of the solution considered. Finally, from Gronwall's inequality, it follows that

$$E_1(t) \leqslant C_1(t)E_1(0) + C_2(t),$$

where $C_1(t)$, $C_2(t)$ are smooth functions depending on κ, e, v, E_0 and $\|u(0)\|_{L^2}$. We also prove that for the topological solution $(d/dt)E_1(t)$ is bounded as (23), by applying the covariant Sobolev inequality to φ instead of ϕ in this case. Let $\tilde{\psi}_j = D_j\varphi$. Then

$$\tilde{\psi}_j = \psi_j - ie\lambda A_j.$$

Applying (19) with respect to φ, we find

$$\|\varphi\|_{L^p} \leqslant \|\varphi\|_{L^2}^{2/p}\|\tilde{\psi}\|_{L^2}^{1-2/p} \leqslant C\|\varphi\|_{L^2}^{2/p}(\|\psi\|_{L^2}^{1-2/p} + e\lambda\|A\|_{L^2}^{1-2/p}) \leqslant C(E_0, \|u_0\|_{L^2})(\|\psi\|_{L^2}^{1-2/p} + 1).$$

The last inequality follows from Lemma 3.1. The remaining estimates can be done similarly to the nontopological case. Observe that the Chern–Simons coupling parameter κ appears only on estimating $\partial U_N \cdot \partial\Omega$, $D\psi \cdot DU_{\bar{\phi}}$ with them depending on κ by polynomial order. Thus $E_1(t)$ is continuously increasing with respect to κ. We also see that E_0 for the topological case behaves in the same way. This fact will be used in Sec. IV. □

The following is our main theorem of this section.

Theorem 3.4. (Global existence of smooth solutions): *Consider the Maxwell–Chern–Simons–Higgs system. Then any given initial data* $(u_0,\partial_0 u_0)\in H^2\times H^1$ *satisfying (10) admits a unique, global solution in the Lorentz gauge such that*

$$(A,\phi,\tilde{N})\in C([0,\infty);H^2(\mathbf{R}^2))\cap C^1([0,\infty);H^1(\mathbf{R}^2))$$

in the nontopological case, and

$$(A,\varphi,N)\in C([0,\infty);H^s(\mathbf{R}^2))\cap C^1([0,\infty);H^1(\mathbf{R}^2))$$

in the topological case.

Proof: In order to extend our local solution globally, we show that $\|u(t)\|_{H^2\times H^1}$ is uniformly bounded on any finite interval $[0,T]$. It is sufficient to verify the nontopological case. Consider the Maxwell equations in (9),

$$\begin{aligned}\Box A_0&=-\kappa F_{12}-2e\ \mathrm{Im}(\phi\overline{D_0\phi})\equiv\mathcal{J}_0,\\ \Box A_i&=-\kappa\epsilon^{ij}F_{0j}-2e\ \mathrm{Im}(\phi\overline{D_i\phi})\equiv\mathcal{J}_i.\end{aligned}\tag{24}$$

We compute the spatial derivatives of $\mathcal{J}_0$, $\mathcal{J}_i$ as

$$\partial_j\mathcal{J}_0=-\kappa\partial_jF_{12}-2e\ \mathrm{Im}(\psi_j\overline{\psi_0}+\phi\overline{D_j\psi_0}),$$

$$\partial_j\mathcal{J}_i=-\kappa\epsilon^{ik}\partial_jF_{0k}-2e\ \mathrm{Im}(\psi_j\overline{\psi_i}+\phi\overline{D_j\psi_i}).$$

Then applying energy estimates to (24) with subscripts ignored, we have

$$\begin{aligned}\|A(t)\|_{H^2\times H^1}&\leq\|u_0\|_{H^2\times H^1}+\int_0^t\|\mathcal{J}_\mu\|_{L^2}+\|\partial_j\mathcal{J}_\mu(s)\|_{L^2}ds\\ &\leq\|u_0\|_{H^2\times H^1}+C(\kappa,e)\int_0^t\|F\|_{L^2}+\|\phi\psi\|_{L^2}+\|\partial F\|_{L^2}+\|\psi^2\|_{L^2}+\|\phi D\psi F\|_{L^2}ds\\ &\leq\|u_0\|_{H^2\times H^1}+C(\kappa,e)\int_0^t E_0^{1/2}+\|\phi\|_{L^4}\|\psi\|_{L^4}^2+E_1^{1/2}(s)+\|\psi\|_{L^4}+\|\phi\|_{L^\infty}E_1^{1/2}(s)ds.\end{aligned}$$

Applying the covariant Sobolev inequality (19) repeatedly, we get

$$\|\phi\|_{L^\infty}\leq C\|\phi\|_{L^2}^{\epsilon}\|\psi\|_{L^2}^{1-2\epsilon}\|D\psi\|_{L^2}^{\epsilon},\quad 0<\epsilon<\tfrac{1}{2}.$$

Thus, if $\epsilon=1/4$,

$$\begin{aligned}\|A(t)\|_{H^2\times H^1}&\leq\|u_0\|_{H^2\times H^1}+C(\kappa,e)\int_0^t E_0^{1/2}+\|\phi\|_{L^2}^{1/2}E_0^{1/2}E_a^{1/4}(s)+E_1^{1/2}+E_0^{1/2}E_1^{1/2}(s)\\ &\quad+\|\phi\|_{L^2}^{\epsilon}E_0^{(1-2\epsilon)/2}E_1^{(1+\epsilon)/2}(s)ds\\ &\leq\|u_0\|_{H^2\times H^1}+C(\kappa,e)\int_0^t(1+\|u\|_{L^2})(1+E_0^{1/2})(1+E_1^{1/2}(s))ds.\end{aligned}$$

From Lemmas 3.1 and 3.3, we find that $\|A(t)\|_{H^2\times H^1}$ does not blow up in any finite time. Next we consider $\|\phi\|_{H^2\times H^1}$. We begin by rewriting

$$|\partial_\mu\phi|^2=|D_\mu\phi|^2+ieA_\mu\overline{D_\mu\phi}-ieA_\mu\overline{\phi_\mu D_\mu}\phi+e^2A_\mu^2|\phi|^2\tag{25}$$

$$= |\psi|^2 + ieA_\mu \overline{\psi_\mu} - ieA_\mu \overline{\phi_\mu \psi_\mu} + e^2 A_\mu^2 |\phi|^2, \tag{26}$$

and

$$|\partial_j \partial_\mu \phi|^2 = |D_j \psi_\mu + ieA_j \psi_\mu + ie\partial_j A_\mu \cdot \phi + ieA_\mu \phi_j - e^2 A_\mu A_j \phi|^2. \tag{27}$$

Each term in (26), (27) are shown to be $L^2(R^2)$ and estimated by $\|A(t)\|_{H^2\times H^1}$ and E_0, $E_1(t)$. We present here one of those estimations

$$\begin{aligned}\int_{\mathbf{R}^2} A\psi \cdot \partial A \cdot \phi &\leqslant \|A\|_{L^\infty} \|\partial A\|_{L^2} \|\phi\psi\|_{L^2} \\ &\leqslant C\|A\|^2_{H^2\times H^1} \|\phi\|_{L^4} \|\psi\|_{L^4} \\ &\leqslant \|A\|^2_{H^2\times H^1} \|\phi\|^{1/2}_{L^2} \|\psi\|_{L^2} \|D\psi\|^{1/2}_{L^2} \leqslant C\|A\|^2_{H^2\times H^1} \|\phi\|^{1/2}_{L^2} E_0^{1/2} E_1^{1/4}(t).\end{aligned}$$

Then from the previous result on $\|A(t)\|_{H^2\times H^1}$ and Lemmas 3.1, and 3.3, we find that $\|\phi\|_{H^2\times H^1}$ is uniformly bounded in any finite time. Note that we estimate $\|\tilde{N}(t)\|_{H^2\times H^1}$ by tE_0 and $E_1(0)$ directly from Lemmas 3.1 and 3.3. We are done. □

IV. THE MAXWELL–HIGGS LIMIT

We recall the Lagrangian of Maxwell–Chern–Simons–Higgs system is

$$\mathcal{L} = -\frac{1}{4} F^{\mu\nu} F_{\mu\nu} + \frac{\kappa}{4} \epsilon^{\mu\nu\rho} F_{\mu\nu} A_\rho + D_\mu \phi \overline{D^\mu \phi} + \frac{1}{2} \partial_\mu N \partial^\mu N - \frac{1}{2}(e|\phi|^2 + \kappa N - ev^2)^2 - e^2 N^2 |\phi|^2, \tag{28}$$

and observe that setting $N=0$, $\kappa=0$ into the above formally, (28) becomes the Lagrangian of the well-known Maxwell–Higgs model,

$$\mathcal{L} = -\tfrac{1}{4} F^{\mu\nu} F_{\mu\nu} + D_\mu \phi \overline{D^\mu \phi} - \tfrac{1}{2} e^2 (|\phi|^2 - v^2)^2,$$

as was mentioned in Sec. I. We rigorously verify this connection between the two models by proving the convergence result as follows. In the case $\kappa=0$, the Euler–Lagrange equations of (28) are written by

$$\begin{aligned} \Box A_0 &= -2e \,\mathrm{Im}(\phi \overline{D_0 \phi}), \\ \Box A_i &= -2e \,\mathrm{Im}(\phi \overline{D_i \phi}), \\ \Box \phi &= 2ieA_0 \partial_0 \phi - 2ieA_j \partial_j \phi - e^2 A_j^2 \phi + e^2 A_0^2 \phi - (e|\phi|^2 - ev^2)\phi - eN^2 \phi, \\ \Box N &= -2e^2 N |\phi|^2, \end{aligned} \tag{29}$$

with given initial data $A_\mu(0,x)$, $\phi(0,x)$, $N(0,x)$, $\partial_0 A_\mu(0,x)$, $\partial_0 \phi(0,x)$, $\partial_0 N(0,x)$ satisfying

$$\begin{aligned} \partial_\mu A^\mu &= 0, \\ \Delta A_0 - \partial_j \partial_0 A_j - 2e \,\mathrm{Im}(\phi \overline{D_0 \phi}) &= 0. \end{aligned} \tag{30}$$

In particular, if we set $N(0,x) = \partial_0 N(0,x) = 0$, we have

$$\|N(t)\|_{H^2\times H^1} \leqslant \int_0^t C(s) \|N(s)\|_{H^1} ds,$$

applying the energy estimate to the equation for N of (29), where we use $\|u(t)\|_{H^2\times H^1}\leqslant C(t)$. Then, by Gronwall's inequality we obtain $N(t)=0$ in any finite time.

Theorem 4.1 (Maxwell–Higgs limit): *Consider the topological case of Maxwell–Chern–Simons–Higgs systems. Let u^κ be the global solution of (9) with coupling constant κ of $H^2\times H^1$ initial data u_0^κ and let u be the global solution of (29) of $H^2\times H^1$ initial data u_0. Let us suppose that $u_0^\kappa\to u_0$ in $H^2\times H^1$. Then, $\|u^\kappa(t)-u(t)\|_{H^2\times H^1}\to 0$ as $\kappa\to 0$ uniformly on any finite time interval.*

Proof: From (9) and (29) we write the equations satisfied by $u^\kappa-u$ in the form

$$\begin{aligned}
&\Box(A_0^\kappa-A_0)=-\kappa F_{12}^\kappa-2e\ \mathrm{Im}(\phi^\kappa\overline{D_0\phi^\kappa}-\phi\overline{D_0\phi}),\\
&\Box(A_i^\kappa-A_i)=\kappa\epsilon^{ij}F_{0j}^\kappa-2e\ \mathrm{Im}(\phi^\kappa\overline{D_i\phi^\kappa}-\phi\overline{D_i\phi}),\\
&\Box(\varphi^\kappa-\varphi)=2ie(A_0^\kappa\partial_0\phi^\kappa-A_0\partial_0\phi)-2ie(A_j^\kappa\partial_j\phi^\kappa-A_j\partial_j\phi)-e^2((A_j^\kappa)^2\phi^\kappa-A_j^2\phi)-(U_{\overline{\phi_\kappa}}+U_{\overline{\phi}}),\\
&\Box(N^\kappa-N)=-U_{N^\kappa}+U_N.
\end{aligned}\tag{31}$$

Let $\Delta^\kappa u$ denote $u^\kappa-u$. Then, ignoring subscripts, we get from first two equations of (31),

$$\|\Delta^\kappa A(t)\|_{H^2\times H^1}\leqslant\|\Delta^\kappa u_0\|_{H^2\times H^1}+C\int_0^t\kappa\|F^\kappa\|_{H^1}+\|\phi^\kappa\Delta^\kappa\psi\|_{L^2}+\|\psi\Delta^\kappa\phi\|_{H^1}ds.$$

Noting

$$\begin{aligned}
&\Delta^\kappa\phi=\Delta^\kappa\varphi,\\
&\Delta^\kappa\psi=D\Delta^\kappa\varphi=\partial\Delta^\kappa\varphi+A\Delta^\kappa\varphi,\\
&\partial\Delta^\kappa\psi=\partial^2\Delta^\kappa\varphi+\partial A\cdot\Delta^\kappa\varphi+A\partial\Delta^\kappa\varphi,
\end{aligned}$$

we obtain

$$\begin{aligned}
&\|\Delta^\kappa\phi\|_{L^4}\leqslant\|\Delta^\kappa u\|_{H^1},\\
&\|\Delta^\kappa\psi\|_{L^4}\leqslant\|\Delta^\kappa u\|_{L^4}+\|A\|_{L^\infty}\|u\|_{L^4}\leqslant\|u\|_{H^2}+\|u\|_{H^2}\|\Delta^\kappa u\|_{H^1}.
\end{aligned}\tag{32}$$

We already know that $\sup_{0\leqslant\kappa\leqslant 1}\|u^\kappa(t)\|_{H^2\times H^1}$ is bounded by a smooth function of t in the proof of Theorem 3.4. Replacing all $\|u^\kappa(t)\|_{H^2}$ terms with $C(t)$ and using (32), we get

$$\|\Delta^\kappa A\|_{H^2\times H^1}\leqslant\|\Delta^\kappa u_0\|_{H^2\times H^1}+C(t)\left(\kappa+\int_0^t\|\Delta^\kappa u(s)\|_{H^2}ds\right).$$

Similarly, we estimate $\|\Delta^\kappa\varphi\|_{H^2\times H^1}$, $\|\Delta^\kappa N\|_{H^2\times H^1}$. Thus we have

$$\|\Delta^\kappa u(t)\|_{H^2\times H^1}\leqslant\|\Delta^\kappa u_0\|_{H^2\times H^1}+C(t)\left(\kappa+\int_0^t\|\Delta^\kappa u(s)\|_{H^2}ds\right).\tag{33}$$

Applying Gronwall's inequality to the above, we obtain

$$\|(u^\kappa-u)(t)\|_{H^2\times H^1}\leqslant\kappa C(t)+\|u_0^\kappa-u_0\|_{H^2\times H^1},\tag{34}$$

thus

$$\|(u^\kappa-u)(t)\|_{H^2\times H^1}\to 0\ \text{ uniformly with respect to }\ t\tag{35}$$

as $\kappa \to 0$. If we set $u_0=(A,\varphi,0), \partial_0 u_0=(\partial_0 A, \partial_0 \varphi, 0)$, we deduce from (35) that $(A^\kappa, \varphi^\kappa, N^\kappa)$ converges to $(A,\varphi,0)$ such that $(A,\varphi+\lambda)$ is the finite energy solution of the Maxwell–Higgs system with

$$(A,\varphi) \in C([0,\infty);H^s(\mathbf{R}^2)) \cap C^1([0,\infty);H^1(\mathbf{R}^2)).$$

We complete the proof of Theorem 4.1. □

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Scale invariant Euclidean field theory in any dimension

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We discuss a D-dimensional scalar field interacting with a metric field. The metric depends on d-dimensional coordinates (where $d<D$). We choose formal Gaussian scale invariant correlation functions for the metric field. By a projection to a lower dimensional subspace we obtain a scale invariant non-Gaussian model of Euclidean quantum field theory in $D-d$ or d dimensions. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1510971]

I. INTRODUCTION

We consider a new method of a construction of Euclidean fields. A scalar field in D dimensions is interacting with a metric depending on d-dimensional coordinates. An averaging over the metric and a projection of the scalar field to an s-dimensional subspace leads to a scalar field which is Euclidean invariant in R^s (we consider $s=D-d$ and $s=d$). If the metric field is scale invariant with a scaling dimension 2γ, then the scalar field is also scale invariant with a scaling dimension depending on γ. We discuss two models for the random metric. In the first model we consider a square of a Gaussian random field. We are unable to derive an upper bound for correlation functions in this model. Then, we consider formal scale invariant Gaussian correlation functions for the metric field. Such correlation functions do not arise from any rigorous functional integral. We treat the Gaussian averaging as a tool for constructing models. We obtain scale invariant correlation functions of a scalar field with explicit upper and lower bounds. Our primary interest in this class of models[1,2] comes from quantum gravity. However, the method may be useful for a construction of relativistic quantum fields (although at the moment we are unable to prove the crucial Osterwalder–Schrader positivity[3]). The model can be interesting for statistical physics as a continuum version of spin glass models.[4]

II. *D*-DIMENSIONAL SCALAR FIELDS

We consider a complex scalar matter field Φ in D dimensions interacting with a metric varying only on a d-dimensional submanifold. We split the coordinates as $x=(X,\mathbf{x})$ with $\mathbf{x}\in R^d$. Without a self-interaction the $\Phi\Phi^*$ correlation function averaged over the metric is denoted by

$$\langle \mathcal{A}^{-1}(x,y)\rangle, \tag{1}$$

where

$$-\mathcal{A}=\frac{1}{2}\sum_{\mu=0,\nu=0}^{D-d-1} g^{\mu\nu}(\mathbf{x})\partial_\mu\partial_\nu+\frac{1}{2}\sum_{k=D-d}^{D-1}\partial_k^2. \tag{2}$$

In Eq. (2) $-2\mathcal{A}$ is the Laplace–Beltrami operator on a D-dimensional manifold with a trivial unit metric on the d-dimensional submanifold. In order to calculate the average (1) we repeat some steps of Refs. 1 and 2. We represent the Green's function by means of the proper time method

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$$\mathcal{A}^{-1}(x,y)=\int_0^\infty d\tau(\exp(-\tau\mathcal{A}))(x,y). \tag{3}$$

For a calculation of $(\exp(\tau\mathcal{A}))(x,y)$ we apply the functional integral

$$K_\tau(x,y)=(\exp(-\tau\mathcal{A}))(x,y)$$
$$=\int \mathcal{D}x\exp\left(-\frac{1}{2}\int\frac{d\mathbf{x}}{dt}\frac{d\mathbf{x}}{dt}-\frac{1}{2}\int g^{\mu\nu}(\mathbf{x})\frac{dX_\mu}{dt}\frac{dX_\nu}{dt}\right)\delta(x(0)-x)\,\delta(x(\tau)-y). \tag{4}$$

In the functional integral (4) we make a change of variables $(x\to b)$ determined by Stratonovitch stochastic differential equations[5]

$$dx^\Omega(s)=e_A^\Omega(x(s))db^A(s), \tag{5}$$

where for $\Omega=0,1,\ldots,D-d-1$,

$$e_a^\mu e_a^\nu=g^{\mu\nu}$$

and $e_A^\Omega=\delta_A^\Omega$ if $\Omega>D-d-1$.

After such a change of variables the functional integral in Eq. (4) becomes Gaussian. In fact, this is the standard Wiener integral and $b_A(t)$ for each A are independent Brownian motions

$$E[b_A(t)b_C(s)]=\delta_{AC}\min(s,t).$$

The solution q_τ of Eq. (5) consists of two vectors $(\mathbf{Q},\mathbf{q})$ where

$$\mathbf{q}(\tau,\mathbf{x})=\mathbf{x}+\mathbf{b}(\tau) \tag{6}$$

and $\mathbf{Q}$ has the components (for $\mu=0,\ldots,D-d-1$)

$$Q^\mu(\tau,\mathbf{X})=X^\mu+\int_0^\tau e_a^\mu(\mathbf{q}(s,\mathbf{x}))dB^a(s). \tag{7}$$

The kernel is

$$K_\tau(x,y)=E[\delta(y-q_\tau(x))]=E\left[\delta(\mathbf{y}-\mathbf{x}-\mathbf{b}(\tau))\prod_\mu\delta(Y_\mu-Q_\mu(\tau,X))\right].$$

Using Eq. (7) and the Fourier representation of the δ-function we write the kernel K_τ in the form

$$K_\tau(x,y)=(2\pi)^{-D+d}\int d\mathbf{P}\exp(i\mathbf{P}(\mathbf{Y}-\mathbf{X}))$$
$$\times E\left[\delta(\mathbf{y}-\mathbf{x}-\mathbf{b}(\tau))\exp\left(-i\int P_\mu e_a^\mu(\mathbf{q}(s,\mathbf{x}))dB^a(s)\right)\right]. \tag{8}$$

We may choose a Gaussian field as a model for the tetrad in order to perform the averaging in Eq. (1) (as we did in Ref. 1):

$$\langle e_a^\mu(\mathbf{x})e_b^\nu(\mathbf{y})\rangle=\Gamma_{ab}^{\mu\nu}(\mathbf{x}-\mathbf{y})=\alpha_{ab}^{\mu\nu}|\mathbf{x}-\mathbf{y}|^{-2\gamma}, \tag{9}$$

where α is a scale invariant tensor. Then

$$\langle K_\tau(x,y)\rangle=(2\pi)^{-D+d}\int d\mathbf{P}\exp(i\mathbf{P}(\mathbf{Y}-\mathbf{X}))$$
$$\times E\left[\delta(\mathbf{y}-\mathbf{x}-\sqrt{\tau}\mathbf{b}(1))\exp\left(-\tau^{1-\gamma}P_\mu P_\nu\int_0^1 dB^a(s)\int_0^s dB^c(s')\Gamma^{\mu\nu}_{ac}(\mathbf{b}(s)-\mathbf{b}(s'))\right)\right], \tag{10}$$

where we have changed the time $s\to\tau s$, and used the equivalence $b(\tau s)=\sqrt{\tau}b(s)$ and the scale invariant form of the two-point function (9). Moreover, we renormalized the kernel K_τ removing from it the term (see Refs. 1 and 6)

$$\exp(-\tfrac{1}{2}\tau\Gamma^{\mu\nu}_{aa}(0)P_\mu P_\nu).$$

It can be seen that this procedure is equivalent to the normal ordering of the metric as a square of the tetrad

$$g^{\mu\nu}(x)=e^\mu_a(x)e^\nu_a(x)\to:e^\mu_a(x)e^\nu_a(x):=e^\mu_a(x)e^\nu_a(x)-\langle e^\mu_a(x)e^\nu_a(x)\rangle. \tag{11}$$

We can prove that the double stochastic integral in Eq. (10) is a finite square integrable random variable if $2\gamma<1$. However, it remains unclear whether the momentum integral in Eq. (10) is finite.

We can work without the stochastic integrals (8) if we explicitly integrate over B. The random variables $\mathbf{b}$ and B^a are independent. Hence, using the formula[5]

$$E\left[\exp i\int f_a(\mathbf{q})dB^a\right]=E\left[\exp\left(-\frac{1}{2}\int f_a f_a ds\right)\right],$$

we can rewrite Eq. (8) solely in terms of the metric tensor

$$K_\tau(x,y)=(2\pi)^{-D+d}\int d\mathbf{P}\exp(i\mathbf{P}(\mathbf{Y}-\mathbf{X}))$$
$$\times E\left[\delta(\mathbf{y}-\mathbf{x}-\mathbf{b}(\tau))\exp\left(-\frac{1}{2}\int_0^\tau P_\mu g^{\mu\nu}(\mathbf{q}(s,\mathbf{x}))P_\nu ds\right)\right]. \tag{12}$$

Let $\mathcal{J}$ be the characteristic function of $g^{\mu\nu}$

$$\mathcal{J}(h)=\langle\exp(-\tfrac{1}{2}g(h))\rangle \tag{13}$$

Then, the mean value of the kernel (12) can be expressed in the form

$$\langle K_\tau(x,y)\rangle=(2\pi)^{-D+d}\int d\mathbf{P}\exp(i\mathbf{P}(\mathbf{Y}-\mathbf{X}))$$
$$\times E[\delta(\mathbf{y}-\mathbf{x}-\mathbf{b}(\tau))\mathcal{J}(h)] \tag{14}$$

where $g(h)=\int d\mathbf{z}g^{\mu\nu}(\mathbf{z})h_{\mu\nu}(\mathbf{z})$ and

$$h_{\mu\nu}(\mathbf{z})=P_\mu P_\nu\int_0^\tau\delta(\mathbf{z}-\mathbf{x}-\mathbf{b}(s))ds.$$

If e^μ_a is Gaussian, then $\mathcal{J}$ can be calculated explicitly

$$\langle\exp(-\tfrac{1}{2}g(h))\rangle=\det(1+h\Gamma)^{-1/2}, \tag{15}$$

where on the rhs the renormalization of the determinant [through a multiplication by $\exp(\frac{1}{2}Tr(\Gamma h))$ defining $\det_2$, see Ref. 7 is equivalent to the normal ordering (11) [and subsequently to the renormalization of the kernel (10)].

We consider next another model where the averaging is performed under the assumption that the metric is described by a formal Gaussian field with the two-point correlation function

$$\langle g^{\mu\nu}(\mathbf{x})g^{\sigma\rho}(\mathbf{y})\rangle = -2D^{\mu\nu;\sigma\rho}(\mathbf{x}-\mathbf{y}) = -C^{\mu\nu;\sigma\rho}|\mathbf{y}-\mathbf{x}|^{-4\gamma}, \tag{16}$$

where C (a scale invariant operator) must be positive definite if the momentum integrals in the final formula are to exist. This requirement is not satisfied in a linearized Einstein gravity[8] [e.g., in the transverse-traceless gauge $p_\Omega p_\Gamma g^{\Omega\Gamma}(x)$ would be zero in a covariant D-dimensional gravity; however our gravity is d-dimensional]. Moreover, the averaging cannot be considered as a well-defined functional integral. Concerning the choice of the tensor $C^{\mu\nu;\sigma\rho}$, let us mention that the conformally flat metric $C^{\mu\nu;\sigma\rho}=\delta^{\mu\nu}\delta^{\sigma\rho}$ would be a satisfactory model for our purposes.

The average over g in Eq. (12) can be calculated

$$\langle K_\tau(x,y)\rangle = (2\pi)^{-D+d}\int d\mathbf{P}\exp(i\mathbf{P}(\mathbf{Y}-\mathbf{X})) \times E\left[\delta(\mathbf{y}-\mathbf{x}-\sqrt{\tau}\mathbf{b}(1))\exp\left(-\frac{1}{4}\tau^{2-2\gamma}\int_0^1 P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\mathbf{b}(s)-\mathbf{b}(s'))dsds'\right)\right] \tag{17}$$

[as in Eq. (10) we have changed the time $s\to\tau s$]. By a scaling of momenta we can bring the propagator of Eq. (3) to the form

$$\langle \mathcal{A}^{-1}(x,y)\rangle = \int_0^\infty d\tau\tau^{-d/2-(D-d)(1-\gamma)/2}F_2(\tau^{-1/2}(\mathbf{y}-\mathbf{x}),\tau^{-1/2+\gamma/2}(\mathbf{Y}-\mathbf{X})). \tag{18}$$

III. A PROJECTION TO $D-d$ DIMENSIONS

The two-point function (18) has a different scaling behavior in $\mathbf{x}$ and $\mathbf{X}$ directions. We obtain a fixed scaling behavior setting $\mathbf{x}=\mathbf{y}=0$. Then, we have

$$\langle \mathcal{A}^{-1}(x,y)\rangle = R|\mathbf{X}-\mathbf{Y}|^{-D+2-[\gamma/(1-\gamma)](d-2)}, \tag{19}$$

where R is a positive constant. Hence, if all the correlation functions are scale invariant, then

$$\Phi(0,\mathbf{X}) \simeq \lambda^{(D-2)/2+[\gamma/(1-\gamma)](d-2)/2}\Phi(0,\lambda\mathbf{X}), \tag{20}$$

where the equivalence means that both sides have the same correlation functions.

In order to prove that R is finite and not zero we need upper and lower bounds for the Gaussian model (17). We show first that the bilinear form $(f_j,\langle\mathcal{A}^{-1}\rangle f_l)$ is finite and nonzero on a dense set of functions f. For this purpose we choose

$$f_{\mathbf{k}}(\mathbf{X}) = (2\pi a)^{-d/2}\exp\left(-\frac{a}{2}\mathbf{X}^2+i\mathbf{k}\mathbf{X}\right),$$

Then (we keep $\mathbf{x}\neq\mathbf{y}$ in order to show that the model of Sec. 2 is nontrivial; for a scale invariant model of this section $\mathbf{x}=\mathbf{y}=\mathbf{0}$),

$$(f_{\mathbf{k}},\langle\mathcal{A}^{-1}\rangle f_{\mathbf{k}'}) = (2\pi)^{-D+d}\int_0^\infty d\tau\tau^{-d/2}\int d\mathbf{P} \times E\left[\delta\left(\tau^{-1/2}(\mathbf{y}-\mathbf{x})-\mathbf{b}(1)\right) \times\exp\left(-\frac{1}{2a}(\mathbf{P}-\mathbf{k})^2-\frac{1}{2a}(\mathbf{P}-\mathbf{k}')^2 -\frac{1}{4}\tau^{2-2\gamma}\int_0^1 P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\mathbf{b}(s)-\mathbf{b}(s'))dsds'\right)\right]. \tag{21}$$

In our estimates we apply Jensen inequalities in the form (for real functions A and f)

$$E[\exp A] \geqslant \exp E[A] \tag{22}$$

and

$$E\left[\exp\left(-\int_0^1 ds ds' f(s,s')\right)\right] \leqslant \int_0^1 ds ds' E[\exp(-f(s,s'))]. \tag{23}$$

An upper bound can be obtained by means of the Jensen inequality (23) expressed in the form

$$\begin{aligned}(f_{\mathbf{k}},\langle \mathcal{A}^{-1}\rangle f_{\mathbf{k}'}) \leqslant 2\int_0^\infty d\tau \int_0^1 ds \int_0^s ds' \int d\mathbf{u}_1 d\mathbf{u}_2 d\mathbf{P} \tau^{-d/2} \\ \times \exp\left(-\frac{1}{2a}(\mathbf{P}-\mathbf{k})^2 - \frac{1}{2a}(\mathbf{P}-\mathbf{k}')^2\right) p(s',\mathbf{u}_1) p(s-s',\mathbf{u}_2-\mathbf{u}_1) \\ \times p(1-s,\tau^{-1/2}(\mathbf{y}-\mathbf{x})-\mathbf{u}_2) \exp\left(-\frac{\tau^{2-2\gamma}}{4} P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\mathbf{u}_1-\mathbf{u}_2)\right),\end{aligned} \tag{24}$$

where $p(s,\mathbf{u}) = (2\pi s)^{-d/2} \exp(-\mathbf{u}^2/2s)$. We can convince ourselves by means of explicit calculations (using a proper change of variables) that the integral on the rhs of Eq. (24) is finite. For the lower bound it will be useful to introduce the Brownian bridge[9] starting from **0** and ending in **u** defined on the time interval [0,1]

$$\mathbf{a}(\mathbf{u},s) = \mathbf{u}s + \mathbf{c}(s),$$

where **c** is the Gaussian process starting from **0** and ending in **0** with mean equal zero and the covariance

$$E[c_j(s')c_k(s)] = \delta_{jk} s'(1-s)$$

for $s' \leqslant s$. Then, the δ function in Eq. (21) determines the Brownian bridge and the Jensen inequality (22) takes the form

$$\begin{aligned}(f_{\mathbf{k}},\langle \mathcal{A}^{-1}\rangle f_{\mathbf{k}'}) \geqslant (2\pi)^{-D+d} \int_0^\infty d\tau \tau^{-d/2} \int d\mathbf{P} \\ \times \exp\left(-\frac{1}{2a}(\mathbf{P}-\mathbf{k})^2 - \frac{1}{2a}(\mathbf{P}-\mathbf{k}')^2 \right. \\ - \frac{1}{4}\tau^{2-2\gamma} \int_0^1 P_\mu P_\sigma P_\nu P_\rho E[D^{\mu\nu;\sigma\rho}(\mathbf{a}(\tau^{-1/2}\mathbf{y} - \tau^{-1/2}\mathbf{x}, s) - \mathbf{a}(\tau^{-1/2}\mathbf{y} \\ \left. - \tau^{-1/2}\mathbf{x}, s'))ds ds']\right),\end{aligned} \tag{25}$$

where the expectation value in the exponential on the rhs of Eq. (25) is equal to

$$\begin{aligned}\int d\mathbf{u} \int ds \int_0^s ds' (2\pi\omega(s,s'))^{-d/2} \exp\left(-\frac{1}{2\omega(s,s')}\mathbf{u}^2\right) \\ \times |\mathbf{u} - \tau^{-1/2} s(\mathbf{y}-\mathbf{x}) + \tau^{-1/2} s'(\mathbf{y}-\mathbf{x})|^{-4\gamma},\end{aligned} \tag{26}$$

where $\omega(s,s')=(s-s')(1-s+s')$. It is finite if $\gamma<\frac{1}{2}$ [the form (16) of the graviton two-point function is assumed].

We compute now higher order correlation functions in the Gaussian model,

$$\begin{aligned}
&\langle\Phi(x)\Phi(x')\Phi^*(y)\Phi^*(y')\rangle\\
&\quad=\langle\mathcal{A}^{-1}(x,y)\mathcal{A}^{-1}(x',y')\rangle+(x\to x')\\
&\quad=(2\pi)^{-2D+2d}\int d\tau_1 d\tau_2\int d\mathbf{P}d\mathbf{P}'\exp(i\mathbf{P}(\mathbf{Y}-\mathbf{X})+i\mathbf{P}'(\mathbf{Y}'-\mathbf{X}'))\\
&\qquad\times E\Big[\delta(\mathbf{y}-\mathbf{x}-\mathbf{b}(\tau_1))\,\delta(\mathbf{y}'-\mathbf{x}'-\mathbf{b}'(\tau_2))\\
&\qquad\times\exp\Big(-\frac{1}{4}\int_0^{\tau_1}\int_0^{\tau_1}P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\mathbf{b}(s)-\mathbf{b}(s'))dsds'\\
&\qquad-\frac{1}{4}\int_0^{\tau_2}\int_0^{\tau_2}P'_\mu P'_\sigma P'_\nu P'_\rho D^{\mu\nu;\sigma\rho}(\mathbf{b}'(s)-\mathbf{b}'(s'))dsds'\\
&\qquad-\frac{1}{2}\int_0^{\tau_1}\int_0^{\tau_2}P_\mu P_\nu P'_\rho P'_\sigma D^{\mu\nu;\sigma\rho}(\mathbf{x}-\mathbf{x}'+\mathbf{b}(s)-\mathbf{b}'(s'))dsds'\Big)\Big]+(x\to x'),
\end{aligned}\tag{27}$$

where $(x\to x')$ means the same expression in which x is exchanged with x'. The fourlinear form (27) calculated on the basis f reads

$$\begin{aligned}
&\langle\Phi(f_{\mathbf{k}_1})\Phi(f_{\mathbf{k}_3})\Phi^*(f_{\mathbf{k}_2})\Phi^*(f_{\mathbf{k}_4})\rangle\\
&\quad=(2\pi)^{-2D+2d}\int d\tau_1 d\tau_2\int d\mathbf{P}d\mathbf{P}'E\Big[\delta(\mathbf{y}-\mathbf{x}-\mathbf{b}(\tau_1))\,\delta(\mathbf{y}'-\mathbf{x}'-\mathbf{b}'(\tau_2))\\
&\qquad\times\exp\Big(-\frac{1}{2a}(\mathbf{P}-\mathbf{k}_1)^2-\frac{1}{2a}(\mathbf{P}-\mathbf{k}_2)^2-\frac{1}{2a}(\mathbf{P}'-\mathbf{k}_3)^2-\frac{1}{2a}(\mathbf{P}'-\mathbf{k}_4)^2\Big)\\
&\qquad\times\exp\Big(-\frac{1}{4}\int_0^{\tau_1}\int_0^{\tau_1}P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\mathbf{b}(s)-\mathbf{b}(s'))dsds'\\
&\qquad-\frac{1}{4}\int_0^{\tau_2}\int_0^{\tau_2}P'_\mu P'_\sigma P'_\nu P'_\rho D^{\mu\nu;\sigma\rho}(\mathbf{b}'(s)-\mathbf{b}'(s'))dsds'\\
&\qquad-\frac{1}{2}\int_0^{\tau_1}\int_0^{\tau_2}P_\mu P_\nu P'_\rho P'_\sigma D^{\mu\nu;\sigma\rho}(\mathbf{x}-\mathbf{x}'+\mathbf{b}(s)-\mathbf{b}'(s'))dsds'\Big)\Big]\\
&\qquad+(1,2\to 3,4),
\end{aligned}\tag{28}$$

where the last term means the same expression with exchanged wave numbers. We introduce the spherical coordinates on the (τ_1,τ_2)-plane $\tau_1=r\cos\theta$ and $\tau_2=r\sin\theta$. Let us rescale the momenta $\mathbf{k}=\mathbf{p}\sqrt{r}$, $\mathbf{k}'=\mathbf{p}'\sqrt{r}$, $\mathbf{K}=\mathbf{P}r^{1/2-\gamma/2}$ and $\mathbf{K}'=\mathbf{P}'r^{1/2-\gamma/2}$. Then, we can see that the four-point function (27) takes the form

$$\langle \Phi(x)\Phi(x')\Phi^*(y)\Phi^*(y')\rangle = \int d\theta dr r r^{-d-(1-\gamma)(D-d)} F_4(\theta, r^{-1/2}(\mathbf{x}-\mathbf{y}), r^{-1/2}(\mathbf{x}'-\mathbf{y}'), r^{-1/2}(\mathbf{x}'-\mathbf{x}), r^{-1/2}(\mathbf{x}'-\mathbf{y}), r^{-1/2}(\mathbf{y}'-\mathbf{x}), r^{-1/2+\gamma/2}(\mathbf{X}-\mathbf{Y}), r^{-1/2+\gamma/2}(\mathbf{X}'-\mathbf{Y}'), r^{-1/2+\gamma/2}(\mathbf{X}'-\mathbf{Y}), r^{-1/2+\gamma/2}(\mathbf{X}-\mathbf{Y}')). \tag{29}$$

It follows just by scaling of coordinates [the r-integral scales as twice the τ-integral in Eq. (18)] that at $\mathbf{x}=\mathbf{x}'=\mathbf{y}=\mathbf{y}'=0$ the correlations are scale invariant with the same scaling dimension as in Eq. (20).

It is clear from Eq. (28) that in the same way as we did it in Eqs. (24) and (25) we can obtain finite upper and lower bounds on the correlation functions (28) by means of the Jensen inequalities.

We could continue with higher order correlation functions. Again through an introduction of spherical coordinates in the $(\tau_1,\ldots,\tau_3)$ space we can show that

$$\langle \Phi(x_1)\ldots\Phi(x_3)\Phi^*(y_1)\ldots\Phi^*(y_3)\rangle \tag{30}$$

scales with the same dimension as in Eq. (20). The scaling of higher order correlation functions is now evident. We introduce the spherical coordinates for the τ-integrals. The resulting scaling is a consequence of the fact that the τ-volume and $\mathbf{P}$ integrals have the scaling dimensions proportional to the order of the correlation function.

IV. A PROJECTION TO *d* DIMENSIONS

There is still another option that we let all $X=Y=0$. In such a case

$$\langle K_\tau(\mathbf{x},\mathbf{y})\rangle = (2\pi)^{-D+d}\int d\mathbf{P} E\left[\delta(\mathbf{y}-\mathbf{x}-\sqrt{\tau}\mathbf{b}(1)) \times \exp\left(-\frac{1}{4}\tau^{2-2\gamma}\int_0^1 P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\mathbf{b}(s)-\mathbf{b}(s'))dsds'\right)\right]. \tag{31}$$

By a scaling of momenta we can bring the propagator of Eq. (3) to the form

$$\langle \mathcal{A}^{-1}(x,y)\rangle = \int_0^\infty d\tau \tau^{-d/2-(D-d)(1-\gamma)/2} F_2(\tau^{-1/2}(\mathbf{y}-\mathbf{x})). \tag{32}$$

Hence

$$\langle \mathcal{A}^{-1}(\mathbf{x},\mathbf{y})\rangle = R|\mathbf{x}-\mathbf{y}|^{-d+2-(D-d)(1-\gamma)}, \tag{33}$$

where R is a positive constant. Hence, if all the correlation functions are scale invariant, then

$$\Phi(\mathbf{x},0) \simeq \lambda^{(d-2)/2+(D-d)(1-\gamma)/2}\Phi(\lambda\mathbf{x},0). \tag{34}$$

We can prove all the inequalities of Sec. III in this model. So, the upper bound for the two-point function reads

$$|\langle \mathcal{A}^{-1}(\mathbf{x},\mathbf{y})\rangle| \leqslant 2\int_0^\infty d\tau \int_0^1 ds \int_0^s ds' \int d\mathbf{u}_1 d\mathbf{u}_2 d\mathbf{P} \tau^{-d/2} p(s',\mathbf{u}_1) p(s-s',\mathbf{u}_2-\mathbf{u}_1)$$
$$\times p(1-s,\tau^{-1/2}(\mathbf{y}-\mathbf{x})-\mathbf{u}_2)\exp\left(-\frac{\tau^{2-2\gamma}}{4} P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\mathbf{u}_1-\mathbf{u}_2)\right). \tag{35}$$

The lower bound takes the form

$$|\langle \mathcal{A}^{-1}(\mathbf{x},\mathbf{y})\rangle| \geqslant (2\pi)^{-D+d}\int_0^\infty d\tau \tau^{-d/2}\int d\mathbf{P}$$
$$\times \exp\left(-\frac{1}{4}\tau^{2-2\gamma}\int_0^1 P_\mu P_\sigma P_\nu P_\rho E[D^{\mu\nu;\sigma\rho}(\mathbf{a}(\tau^{-1/2}\mathbf{y}-\tau^{-1/2}\mathbf{x},s)\right.$$
$$\left.-\mathbf{a}(\tau^{-1/2}\mathbf{y}-\tau^{-1/2}\mathbf{x},s'))dsds']\right), \tag{36}$$

where the expectation value in the exponential on the rhs of Eq. (36) is equal to

$$\int d\mathbf{u}\int ds\int_0^s ds'(2\pi\omega(s,s'))^{-d/2}\exp\left(-\frac{1}{2\omega(s,s')}\mathbf{u}^2\right)$$
$$\times|\mathbf{u}-\tau^{-1/2}s(\mathbf{y}-\mathbf{x})+\tau^{-1/2}s'(\mathbf{y}-\mathbf{x})|^{-4\gamma}, \tag{37}$$

where $\omega(s,s')=(s-s')(1-s+s')$. It is finite if $\gamma<\frac{1}{2}$. The bounds (35) and (36) in fact have the form

$$R_1 \leqslant |\mathbf{x}-\mathbf{y}|^{d-2+(D-d)(1-\gamma)}\langle \mathcal{A}^{-1}(\mathbf{x},\mathbf{y})\rangle \leqslant R_2 \tag{38}$$

with certain positive R_1 and R_2.

The inequalities (38) can be proved from the inequlities (35) and (36) just by rescaling of variables. It is more tedious to show that the constants R_1 and R_2 are finite and not zero (but the estimates reduce to finite dimensional integrals and are straightforward).

We can project now to R^d higher order correlation functions:

$$\langle \Phi(\mathbf{x})\Phi(\mathbf{x}')\Phi^*(\mathbf{y})\Phi^*(\mathbf{y}')\rangle = \langle \mathcal{A}^{-1}(\mathbf{x},\mathbf{y})\mathcal{A}^{-1}(\mathbf{x}',\mathbf{y}')\rangle + (\mathbf{x}\to\mathbf{x}')$$
$$= (2\pi)^{-2D+2d}\int d\tau_1 d\tau_2 \int d\mathbf{P}d\mathbf{P}' E\left[\delta(\mathbf{y}-\mathbf{x}-\mathbf{b}(\tau_1))\,\delta(\mathbf{y}'-\mathbf{x}'\right.$$
$$-\mathbf{b}'(\tau_2))\exp\left(-\frac{1}{4}\int_0^{\tau_1}\int_0^{\tau_1} P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\mathbf{b}(s)\right.$$
$$-\mathbf{b}(s'))dsds' - \frac{1}{4}\int_0^{\tau_2}\int_0^{\tau_2} P'_\mu P'_\sigma P'_\nu P'_\rho D^{\mu\nu;\sigma\rho}(\mathbf{b}'(s)$$
$$-\mathbf{b}'(s'))dsds' - \frac{1}{2}\int_0^{\tau_1}\int_0^{\tau_2} P_\mu P_\nu P'_\rho P'_\sigma D^{\mu\nu;\sigma\rho}(\mathbf{x}-\mathbf{x}'+\mathbf{b}(s)$$
$$\left.\left.-\mathbf{b}'(s'))dsds'\right)\right] + (x\to x'), \tag{39}$$

where $(x\to x')$ means the same expression in which x is exchanged with x'. We introduce the spherical coordinates on the (τ_1,τ_2)-plane $\tau_1=r\cos\theta$, $\tau_2=r\sin\theta$ and we rescale the momenta $\mathbf{k}=\mathbf{p}\sqrt{r}$, $\mathbf{k}'=\mathbf{p}'\sqrt{r}$, $\mathbf{K}=\mathbf{P}r^{1/2-\gamma/2}$. Then, we can see that the four-point function (39) takes the form

$$\langle\Phi(\mathbf{x})\Phi(\mathbf{x}')\Phi^*(\mathbf{y})\Phi^*(\mathbf{y}')\rangle = \int d\theta dr r r^{-d-(1-\gamma)(D-d)} F_4(\theta, r^{-1/2}(\mathbf{x}-\mathbf{y}), r^{-\frac{1}{2}}(\mathbf{x}'-\mathbf{y}'), r^{-1/2}(\mathbf{x}'-\mathbf{x}), r^{-1/2}(\mathbf{x}'-\mathbf{y}), r^{-1/2}(\mathbf{y}'-\mathbf{x})). \tag{40}$$

The upper bound now reads

$$\begin{aligned}
&|\langle\Phi(\mathbf{x})\Phi(\mathbf{x}')\Phi^*(\mathbf{y})\Phi^*(\mathbf{y}')\rangle| \\
&\leqslant 2(2\pi)^{-2D+2d}\int d\tau_1 d\tau_2 \int_0^1 ds \int_0^s ds' \int d\mathbf{P} d\mathbf{P}' E\Big[\delta(\mathbf{y}-\mathbf{x}-\sqrt{\tau_1}\mathbf{b}(1)) \\
&\quad\times\delta(\mathbf{y}'-\mathbf{x}'-\sqrt{\tau_2}\mathbf{b}'(1)) \\
&\quad\times\exp\Big(-\frac{\tau_1^2}{4}P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\sqrt{\tau_1}\mathbf{b}(s)-\sqrt{\tau_1}\mathbf{b}(s')) \\
&\quad-\frac{\tau_2^2}{4}P'_\mu P'_\sigma P'_\nu P'_\rho D^{\mu\nu;\sigma\rho}(\sqrt{\tau_2}\mathbf{b}'(s)-\sqrt{\tau_2}\mathbf{b}'(s')) \\
&\quad-\frac{\tau_1\tau_2}{2}P_\mu P_\nu P'_\rho P'_\sigma D^{\mu\nu;\sigma\rho}(\mathbf{x}-\mathbf{x}'+\sqrt{\tau_1}\mathbf{b}(s)-\sqrt{\tau_2}\mathbf{b}'(s'))\Big)\Big] \\
&\quad+(\mathbf{x}\to\mathbf{x}').
\end{aligned} \tag{41}$$

The expectation value (41) can be expressed by the transition functions (as usual for the Wiener process). The bound is scale invariant and the scale invariant function on the rhs could be calculated explicitly. The lower bound takes the form

$$\begin{aligned}
&\langle\Phi(\mathbf{x})\Phi(\mathbf{x}')\Phi^*(\mathbf{y})\Phi^*(\mathbf{y}')\rangle \\
&\geqslant(2\pi)^{-2D+2d}\int d\tau_1 d\tau_2 \int d\mathbf{P} d\mathbf{P}' \\
&\quad\times\exp\Big(-E\Big[\frac{1}{4}\int_0^{\tau_1}\int_0^{\tau_1} P_\mu P_\sigma P_\nu P_\rho D^{\mu\nu;\sigma\rho}(\mathbf{a}(s)-\mathbf{a}(s'))dsds' \\
&\quad+\frac{1}{4}\int_0^{\tau_2}\int_0^{\tau_2} P'_\mu P'_\sigma P'_\nu P'_\rho D^{\mu\nu;\sigma\rho}(\mathbf{a}'(s)-\mathbf{a}'(s'))dsds' \\
&\quad+\frac{1}{2}\int_0^{\tau_1}\int_0^{\tau_2} P_\mu P_\nu P'_\rho P'_\sigma D^{\mu\nu;\sigma\rho}(\mathbf{a}(s)-\mathbf{a}'(s'))dsds'\Big]\Big)+(\mathbf{x}\to\mathbf{x}').
\end{aligned} \tag{42}$$

Here

$$\mathbf{a}(s)=\mathbf{x}+(\mathbf{y}-\mathbf{x})\frac{s}{\tau_1}+\sqrt{\tau_1}\mathbf{c}\Big(\frac{s}{\tau_1}\Big)$$

and

$$\mathbf{a}'(s)=\mathbf{x}'+(\mathbf{y}'-\mathbf{x}')\frac{s}{\tau_2}+\sqrt{\tau_2}\mathbf{c}'\Big(\frac{s}{\tau_2}\Big).$$

In the exponential of the formula (42) we have the expectation over three Gaussian processes. The first is with the mean $(\mathbf{y}-\mathbf{x})(s-s')/\tau_1$ and the covariance $(s-s')(\tau_1-s+s')/\tau_1$, the second has the mean $(\mathbf{y}'-\mathbf{x}')(s-s')/\tau_2$ and the covariance $(s-s')(\tau_2-s+s')/\tau_2$, and the third has the

mean $\mathbf{x}-\mathbf{x}'+(\mathbf{y}-\mathbf{x})s/\tau_1-(\mathbf{y}'-\mathbf{x}')s'/\tau_2$ and the covariance $s(\tau_1-s)/\tau_1+s'(\tau_2-s')/\tau_2$. The lower bound can be explicitly calculated and is given by a scale invariant function. It is clear how to calculate the higher order scale invariant functions and their scale invariant lower and upper bounds.

V. DISCUSSION

The model discussed in Sec. III is invariant under Euclidean rotations in $D-d$ dimensions. Euclidean fields with the Osterwalder–Schrader positivity cannot be more regular than the free field (this follows from the Källen–Lehman representation). In D dimensions the short distance behavior of the correlation functions (18) is more regular than the one of the free fields. However, after setting all $\mathbf{x}=0$, the behavior is more singular than the canonical one in $D-d$ dimensions. For the model (11) where the metric is a square of a Gaussian field we can suggest a lattice model whose formal continuum limit coincides with the scale invariant Euclidean field theory. The simplest possibility is to take the conformally flat metric placed on a sublattice just between the lattice sites of the scalar field (as the gauge fields in Ref. 10). The model (11) could be reflection positive (reflection positivity of lattice spin models is discussed in Ref. 11, reflection positivity of lattice versions of generalized free fields is shown in Ref. 12). However, models of the type (11) require the Wick normal ordering. After this renormalization the finiteness of the τ-integral (3) and the **P** integral (10) is doubtful. However, (if finite) the continuum limit and the subsequent analytic continuation to Minkowski space would give a model of relativistic quantum field theory satisfying all Wightman axioms. The Wick square of a Gaussian field is an example of an infinitely divisible field.[13] An infinitely divisible field can take non-negative values. Its characteristic function has an explicit integral representation. Such a field can be a good candidate for a random metric.

The models of Sec. IV are more promising. The lattice version of the Lagrangian

$$L=g^{\mu\nu}(\mathbf{x})\frac{\partial}{\partial X^{\mu}}\Phi\frac{\partial}{\partial X^{\nu}}\Phi^*+\nabla_{\mathbf{x}}\Phi\nabla_{\mathbf{x}}\Phi^*$$

will have the form $-L=F+\theta F+M\theta M$ where θ is the reflection in the plane perpendicular to one of the coordinates $\mathbf{x}$ (which will be chosen as time). This representation holds true because the random metric does not mix the temporal coordinates in $\nabla_{\mathbf{x}}\Phi\nabla_{\mathbf{x}}\Phi^*$. Then, the reflection positivity results (see Ref. 11). In the lattice approximation we have to replace the (formal) Gaussian measure with a negative definite covariance (16) by a non-Gaussian measure on the metrics which has a formal Gaussian limit (e.g., replacing $\frac{1}{2}x^2$ by $1-\cos x$). There remains to be proven that such a lattice approximation is convergent to the continuum. Without such a proof the Gaussian averaging discussed in this article must be considered solely as a formal tool for a construction of scale invariant Euclidean field theories whose relevance for a quantum field theory in the Minkowski space remains obscure.

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The foliation operator in history quantum field theory

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As a preliminary to discussing the quantization of the foliation in a history form of general relativity, we show how the discussion in an earlier work [J. Math. Phys. **43**, 3053 (2002)] of a history version of free, scalar quantum field theory can be augmented in such a way as to include the quantization of the unit-length, timelike vector that determines a Lorentzian foliation of Minkowski space–time. We employ a Hilbert bundle construction that is motivated by (*i*) discussing the role of the external Lorentz group in the existing history quantum field theory [J. Math. Phys. **43**, 3053 (2002)] and (*ii*) considering a specific representation of the extended history algebra obtained from the multi-symplectic representation of scalar field theory. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1507605]

I. INTRODUCTION

The goal of the present article is to extend the discussion in Ref. 1 of the construction of a history version of quantum scalar field theory in Minkowski space–time. In particular, we shall show how the formalism can be developed to include the quantization of the four-vector n that determines the space–time foliation that plays a central role in the theory. The motivation for such a step, and the relevant background information, is as follows.

The ''consistent-histories'' approach to quantum theory was originally introduced to provide a novel way of reinterpreting standard quantum theory, particularly in regard to the role played by measurement. However, because of the novel way in which time is handled, consistent-history theory also has the potential for providing new and powerful ways of studying quantum theories of gravity. Most recently, in Ref. 2 the formalism was applied to construct a history version of the canonical form of classical general relativity. The possibility also arises to use this formalism in the context of generalized ideas of time and space: for example, in models where space–time is not represented by a differentiable manifold.

A first step in developing the framework with this goal in mind was taken in Ref. 3 where a new mathematical formalism—the ''History Projection Operator'' (HPO) method—was introduced. This places emphasis on the idea of ''quantum temporal logic,'' and potentially allows substantial generalizations of the notion of time. The heart of this formalism is the idea that propositions about the *temporal history* of a system should be represented by projection operators on a ''history'' Hilbert space. (This is to be contrasted with the situation in standard quantum theory in which projection operators represent propositions about the system at a *single* time.) In the case of simple, Newtonian time, and histories labeled by a finite set of discrete time points, the history Hilbert space is a tensor product of a copy of the standard canonical Hilbert space for each such time point.

The idea of representing history propositions by projection operators lead in turn to the notion of a ''*history group*.'' This is the history analog of the Weyl group and its associated canonical commutation relations; in particular, the spectral projectors of the history operators in the Lie algebra of the history group represent propositions about the associated history quantities.

The introduction of a history group is particularly useful in the context of histories with a

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continuous time label, since it is by no means a trivial matter to define the continuous analog of a tensor product. Instead, one finds the history Hilbert space by looking for representations of the appropriate history algebra.

For example, for the case of a point particle moving in one dimension, the history algebra for histories labeled with a continuous time parameter t is[4,5]

$$[\hat{x}_t,\hat{x}_{t'}]=0 \tag{1.1}$$

$$[\hat{p}_t,\hat{p}_{t'}]=0, \tag{1.2}$$

$$[\hat{x}_t,\hat{p}_{t'}]=i\hbar\tau\delta(t-t'), \tag{1.3}$$

and the basic history propositions in the theory refer to the value of time-averaged quantities such as $(1/\tau)\int dtx_t f(t)$ and $(1/\tau)\int dtp_t h(t)$ where f and h are smearing functions. Note that, in Eq. (1.3), τ is a new constant in the theory with the dimension of time. The role of this constant is discussed in more detail (following a private communication from Tulsi Dass) in Ref. 6; from now on we shall choose units so that $\tau=1$.

In Eqs. (1.1)–(1.3), the label t on the operators $\hat{x}_t$ and $\hat{p}_t$ refers to the time at which propositions about the system are asserted—the time of ''temporal logic.'' It was to include in an explicit way such a time of temporal logic that the HPO formalism was originally developed. However, a clear notion of dynamics was not implemented for the naturally time-averaged physical quantities of the theory.

A major advance in the HPO formalism took place when time was introduced in a completely new way.[6,7] It was realized that it is natural to consider time in a twofold manner: the ''time of being''—the time at which events ''happen'' [and from this perspective, the time label t in Eqs. (1.1)–(1.3) and in Eq. (1.4) can be regarded as such], and the ''time of becoming''—the time of dynamical change, represented by a time label s. This *second* time appears in the history analog $\hat{x}_t(s)$ of the Heisenberg picture, which is defined as

$$\hat{x}_t(s):=e^{is\hat{H}/\hbar}\hat{x}_t e^{-is\hat{H}/\hbar} \tag{1.4}$$

where $\hat{H}:=\int dt\hat{H}_t$ is the history quantity that represents the time average of the energy of the system. The notion of time evolution is now recovered for the time-averaged physical quantities, for example,

$$\hat{x}_f(s):=e^{is\hat{H}/\hbar}\hat{x}_f e^{-is\hat{H}/\hbar}, \tag{1.5}$$

where $f(t)$ is a smearing function.

Associated with these two manifestations of the concept of time are two types of time transformation: the ''external'' translation

$$\hat{x}_t(s)\mapsto\hat{x}_{t+t'}(s), \tag{1.6}$$

and the ''internal'' translation

$$\hat{x}_t(s)\mapsto\hat{x}_t(s+s'). \tag{1.7}$$

The external time translation is generated by the ''Liouville'' operator[7]

$$\hat{V}:=\int dt\hat{p}_t\frac{d\hat{x}_t}{dt}, \tag{1.8}$$

whereas the internal time translation is generated by the time-averaged energy operator $\hat{H}$.

More importantly, it was shown in Ref. 7 that the generator of time translation in the HPO theory is the "action" operator $\hat{S}$ defined as

$$\hat{S} := \int dt \hat{p}_t \frac{d\hat{x}_t}{dt} - \hat{H} = \hat{V} - \hat{H}. \tag{1.9}$$

Hence the action operator is the generator of *both* types of time translation

$$\hat{x}_t(s) \mapsto \hat{x}_{t+t'}(s+s'). \tag{1.10}$$

It is a very striking result that in the HPO theory the quantum analog of the classical action functional is an actual operator in the formalism, and is the generator of time translations.[7]

The idea of "two times"—and the associated two types of time translation—has recently been generalized to relativistic field theory[1] where, in particular, it is shown that the analog of the two types of time translation is the existence of two *Poincaré* groups. The goal of the present article is to develop the ideas in Ref. 1 in one particular respect: namely, the way in which space–time foliations enter the theory.

That the idea of a Lorentzian space–time foliation should play an important role in a history quantum field theory is understandable. (By "Lorentzian" we mean that each leaf of the foliation is a hyperplane in the Minkowski space–time.) Indeed, the obvious analog of the history algebra Eqs. (1.1)–(1.3) for a quantum scalar field theory is (choosing units from now on such that $\tau = 1$)

$$[{}^n\hat{\phi}(t,\underline{x}), {}^n\hat{\phi}(t',\underline{x}')] = 0, \tag{1.11}$$

$$[{}^n\hat{\pi}(t,\underline{x}), {}^n\hat{\pi}(t',\underline{x}')]) = 0, \tag{1.12}$$

$$[{}^n\hat{\phi}(t,\underline{x}), {}^n\hat{\pi}(t',\underline{x}')] = i\hbar\,\delta(t-t')\,\delta^3(\underline{x}-\underline{x}'), \tag{1.13}$$

where, for each $t \in \mathbb{R}$, the fields ${}^n\hat{\phi}(t,\underline{x})$ and ${}^n\hat{\pi}(t,\underline{x})$ are defined on the spacelike hypersurface characterized by the unit length timelike vector n, and by the foliation parameter t. In particular, the three-vector $\underline{x}$ in ${}^n\hat{\phi}(t,\underline{x})$ or in ${}^n\hat{\pi}(t,\underline{x})$ denotes a vector in this spacelike hypersurface. Note that the pair $(t,\underline{x})$ can be used to identify a unique point X in space–time, and hence to write ${}^n\hat{\phi}(t,\underline{x})$ as ${}^n\hat{\phi}(X)$. The history algebra Eqs. (1.11)–(1.13) can then be written in the more covariant looking form

$$[\hat{\phi}(X), \hat{\phi}(X')] = 0, \tag{1.14}$$

$$[\hat{\pi}(X), \hat{\pi}(X)] = 0, \tag{1.15}$$

$$[\hat{\phi}(X), \hat{\pi}(X')] = i\hbar\,\delta^4(X-X'), \tag{1.16}$$

where we have dropped the n superscript on the fields since the algebra itself is n-independent. Of course, this does not stop individual *representations* from depending on the foliation vector n; indeed, as we shall see below, this is precisely what happens.

In what follows we shall denote by $H_+ := \{n \in M \,|\, n \cdot n = 1, n^0 > 0\}$ the set of all unit length, forward pointing timelike vectors on Minkowski space–time M. We are using a metric $\eta_{\mu\nu}$ on M with the signature $(+,-,-,-)$; also we use the notation $a \cdot b := a^\mu b^\nu \eta_{\mu\nu}$ for any four-vectors a and b in M.

It was shown in Ref. 1 that for each fixed n in H_+ it is possible to find a representation of the history algebra Eqs. (1.11)–(1.13) on a Hilbert space $\mathcal{H}_n$ with the property that the time-averaged energy exists as a well-defined self-adjoint operator ${}^n\hat{H}$ (this is the history analog of an old theorem of Araki in the context of canonical quantum field theory[8]). This operator generates

translations along the timelike direction n and, as such, is one of the generators of the *internal* Poincaré group that exists for each n: full expressions for all these generators are given in Ref. 1.

One of the key questions for our present purposes is how the external Poincaré group acts for each fixed choice of the foliation vector n. The translation part should obviously act in analog to Eq. (1.6) by taking ${}^n\hat{\phi}(X)$ to ${}^n\hat{\phi}(X+a)$ for any four-vector n. Thus there should be an operator $\hat{U}(a)$ such that

$$\hat{U}(a)\,{}^n\hat{\phi}(X)\hat{U}(a)^{-1} = {}^n\hat{\phi}(X+a), \tag{1.17}$$

with a similar action on ${}^n\hat{\pi}(X)$.

The Lorentz subgroup of the Poincaré group is more interesting since as well as acting on the space–time points, it might also be expected to act on the foliation vector n, and hence to take us out of the Hilbert space $\mathcal{H}_n$. In Ref. 1 this problem is solved by showing that even though the representations of the field algebra (1.11)–(1.13) are unitarily inequivalent for different choices of n, it is nevertheless possible to construct the fields for all n on a *common* Fock space $\mathcal{F}$ (see Sec. II of the present article for details). Hence it is meaningful to look for a unitary operator $\hat{U}(\Lambda)$ such that, for all Lorentz transformations Λ,

$$\hat{U}(\Lambda)\,{}^n\hat{\phi}(X)\hat{U}(\Lambda)^{-1} = {}^{\Lambda n}\hat{\phi}(\Lambda X), \tag{1.18}$$

and similarly for ${}^n\hat{\pi}(X)$, where the operators are all defined on $\mathcal{F}$. Of course, the operators $\hat{U}(\Lambda)$ are expected to form a unitary representation of the Lorentz group in the sense that

$$\hat{U}(\Lambda')\hat{U}(\Lambda) = \hat{U}(\Lambda'\Lambda). \tag{1.19}$$

In the present article we shall extend this formalism by quantizing the foliation vector n itself. The main motivation for this step is our belief—following the conjecture by one of us[2]—that, when constructing the quantum history theory of general relativity,[2] it will be necessary to include the space–time foliation as a genuine ''history variable,'' and which must therefore be represented by operators in the corresponding quantum theory. (In Ref. 9 also, the analog of the foliation is a part of the postulated history group, this time in the context of the Bosonic string.) In the context of our present discussion, the vector n is the Minkowskian analog of a foliation of a general space–time: hence an investigation into what is meant by quantizing n is a valuable precursor to the study of the quantization of foliations of a general space–time.

As an introduction to the quantization of n, it is useful to return to the idea that, for each n, the theory is defined on a Hilbert space $\mathcal{H}_n$, and to ask again how the external Lorentz group might act. In these circumstances, Eq. (1.18) is not meaningful since the operators ${}^n\hat{\phi}(X)$ and ${}^{\Lambda n}\hat{\phi}(\Lambda X)$ are defined on different Hilbert spaces ($\mathcal{H}_n$ and $\mathcal{H}_{\Lambda n}$, respectively). The natural thing instead is to seek a family of unitary intertwining operators $\hat{U}(n;\Lambda):\mathcal{H}_n \to \mathcal{H}_{\Lambda n}$ with the property that

$$\hat{U}(n;\Lambda)\,{}^n\hat{\phi}(X) = {}^{\Lambda n}\hat{\phi}(\Lambda X)\hat{U}(n;\Lambda), \tag{1.20}$$

$$\hat{U}(n;\Lambda)\,{}^n\hat{\pi}(X) = {}^{\Lambda n}\hat{\pi}(\Lambda X)\hat{U}(n;\Lambda), \tag{1.21}$$

which can usefully be represented by the commutative diagram

$$\begin{array}{ccc} \mathcal{H}_n & \xrightarrow{\hat{U}(n;\Lambda)} & \mathcal{H}_{\Lambda n} \\ \downarrow {}^n\hat{\phi}(X) & & \downarrow {}^{\Lambda n}\hat{\phi}(\Lambda X) \\ \mathcal{H}_n & \xrightarrow{\hat{U}(n;\Lambda)} & \mathcal{H}_{\Lambda n} \end{array} \tag{1.22}$$

and similarly for the operator ${}^{n}\hat{\pi}(X)$.

These operators $\hat{U}(n;\Lambda):\mathcal{H}_n\to\mathcal{H}_{\Lambda n}$ are expected to give a type of "representation" of the external Lorentz group in the sense that, for all $n\in H_+$ and for all Lorentz transformations Λ, we have

$$\hat{U}(\Lambda n;\Lambda')\hat{U}(n;\Lambda)=\hat{U}(n;\Lambda'\Lambda), \tag{1.23}$$

which is the appropriate analog of the genuine representation Eq. (1.19). The specific form of Eq. (1.23) follows by considering the commutative diagram

$$\begin{array}{ccccc}
 & & \overset{\hat{U}(n;\Lambda)}{\longrightarrow} & & \overset{\hat{U}(\Lambda n,\Lambda')}{\longrightarrow} \\
\mathcal{H}_n & & \mathcal{H}_{\Lambda n} & & \mathcal{H}_{\Lambda'\Lambda n} \\
\downarrow {}^{n}\hat{\phi}(X) & & \downarrow {}^{\Lambda n}\hat{\phi}(\Lambda X) & & \downarrow {}^{\Lambda'\Lambda n}\hat{\phi}(\Lambda'\Lambda X) \\
\mathcal{H}_n & & \mathcal{H}_{\Lambda n} & & \mathcal{H}_{\Lambda'\Lambda n} \\
 & & \underset{\hat{U}(n;\Lambda)}{\longrightarrow} & & \underset{\hat{U}(\Lambda n,\Lambda')}{\longrightarrow}
\end{array} \tag{1.24}$$

whose outer square should equal the diagram

$$\begin{array}{ccc}
 & \overset{\hat{U}(n;\Lambda'\Lambda)}{\longrightarrow} & \\
\mathcal{H}_n & & \mathcal{H}_{\Lambda'\Lambda n} \\
\downarrow {}^{n}\hat{\phi}(X) & & \downarrow {}^{\Lambda'\Lambda n}\hat{\phi}(\Lambda'\Lambda X). \\
\mathcal{H}_n & & \mathcal{H}_{\Lambda'\Lambda n} \\
 & \underset{\hat{U}(n;\Lambda'\Lambda)}{\longrightarrow} &
\end{array} \tag{1.25}$$

We note that Eq. (1.23) is the type of relation that occurs naturally whenever we have a group G that acts on some G-set X, together with a family of operators $U_x(g)$, $x\in X$, defined on vector spaces V_x, $x\in X$, and satisfying the equation [cf. Eq. (1.23)]

$$\hat{U}(gx,g')\hat{U}(x,g)=\hat{U}(x,g'g) \tag{1.26}$$

for all $x\in X$ and g, $g'\in G$. There is also a version of Eq. (1.26) that uses a multiplier, but we shall not need that here.

Mathematically speaking, the appropriate picture [for the specific case of Eq. (1.23)] is a bundle of Hilbert spaces $\mathcal{H}_n$, $n\in H_+$, with base space H_+, in which the action $n\mapsto\Lambda n$ of the external Lorentz group SO(3, 1) on H_+ is lifted to the bundle by the maps $\hat{U}(n,\Lambda):\mathcal{H}_n\to\mathcal{H}_{\Lambda n}$; note that Eq. (1.23) is precisely the statement that the operators $\hat{U}(n,\Lambda)$ "cover" the action of SO(3, 1) on the base space H_+.

Under these circumstances, it is natural to consider the new Hilbert space formed by the *cross-sections* of this vector bundle. However, this Hilbert space is quite different from the individual spaces $\mathcal{H}_n$, $n\in H_+$: in particular, the foliation vector itself becomes an operator under the natural action on a section Ψ as

$$\{\hat{n}^{\mu}\Psi\}(n):=n^{\mu}\Psi(n) \tag{1.27}$$

for all $n\in H_+$.

All this will be discussed properly in Sec. III, but for the moment it suffices to summarize our remarks above by saying that the mathematical formalism for a history quantum field theory developed in Ref. 1 itself suggests a natural way in which the foliation vector could become a quantum operator.

Such a step is also understandable from a more conceptual perspective, for we should recall that the consistent history theory deals with "beables" (albeit contextualized by the choice of a

particular consistent set of histories) not observables. Thus, in quantizing n, we are not saying that the foliation is something that is determined by nature—in particular, something that must be observed—but rather that the existing history QFT formalism depends on the choice of n in such an intrinsic way that it is natural to formulate propositions about things in the context of specifying n. (This also suggests that a topos approach could be useful: we shall make a few remarks about this later on in the article.) And, as we have seen, one way of doing this in a form that is coherent with respect to the action of the external Lorentz group is to let n become a quantum operator.

The challenge now arises of finding a proper theory of a quantized foliation vector, and thereby justifying the rather heuristic ideas presented above. In particular, in the spirit of our approach to history theories, we must find the correct extension of the history field algebra to include an operator $\hat{n}_\mu$ and its conjugate variables.

We will address this issue in Sec. III A by considering the *multi-symplectic* approach to a scalar field theory. There is a relation between multi-symplectic structures and history theory, and—as we shall see—in the case of a scalar field, attempting to quantize the corresponding multi-symplectic structure leads naturally to a quantized foliation vector in the context of a history group whose Lie algebra generators include n and an appropriate set of conjugate variables.

The plan of the article is as follows. We start in Sec. II by summarizing the results in Ref. 1 for constructing the quantum history theory of a free scalar field. Then in Sec. III we study the main problem of quantizing the foliation vector. We base the first few steps in constructing the appropriate history algebra on the discussion in Sec. III A of the multi-symplectic formalism as applied to the relativistic scalar field. The quantization of this formalism is discussed in Sec. III B, and this is completed in Sec. III C, where we apply group-theoretical quantization techniques to a classical system whose configuration space is the set H_+ of all foliation vectors. Then in Sec. IV we discuss the representations of this algebra, and show how a particularly simple one reproduces the heuristic ideas of a Hilbert bundle sketched above.

II. THE QUANTUM HISTORY THEORY OF A SCALAR FIELD

A. The field operators

The starting point for the construction in Ref. 1 of a quantum history version of a free, scalar field is a Fock space $\mathcal{F}$ defined via annihilation and creation operators, $\hat{b}(X)$ and $\hat{b}^\dagger(X)$, respectively, that satisfy the commutation relations:

$$[\hat{b}(X),\hat{b}(X')]=0, \tag{2.1}$$

$$[\hat{b}^\dagger(X),\hat{b}^\dagger(X')]=0, \tag{2.2}$$

$$[\hat{b}(X),\hat{b}^\dagger(X')]=\hbar\,\delta^4(X-X'). \tag{2.3}$$

This bosonic Fock space has (generalized) basis vectors $|X_1,X_2,\ldots,X_k\rangle$ defined by

$$|X_1,X_2,\ldots,X_k\rangle := \hat{b}^\dagger(X_1)\hat{b}^\dagger(X_2)\cdots\hat{b}^\dagger(X_k)|0\rangle \tag{2.4}$$

where $|0\rangle$ is the cyclic "vacuum" state of the Fock space.

On this Fock space $\mathcal{F}$, field operators for each $n\in H_+$ can be defined as

$${}^n\hat{\phi}(X) := \frac{1}{\sqrt{2}}\,{}^n\Gamma^{-1/4}(\hat{b}(X)+\hat{b}^\dagger(X)) \tag{2.5}$$

$${}^n\hat{\pi}(X) := \frac{1}{i\sqrt{2}}\,{}^n\Gamma^{1/4}(\hat{b}(X)-\hat{b}^\dagger(X)), \tag{2.6}$$

where ${}^n\Gamma$ is the elliptic, partial differential operator on $L^2(\mathbb{R}^4)$ defined as

$$ {}^n\Gamma := (\eta^{\mu\nu} - n^\mu n^\nu)\partial_\mu \partial_\nu + m^2, \tag{2.7} $$

where m is the mass parameter in the theory. It is easy to check that, for each foliation vector $n \in H_+$, the fields ${}^n\hat{\phi}(X)$ and ${}^n\hat{\pi}(X)$ defined in Eqs. (2.5) and (2.6) satisfy the history algebra Eqs. (1.14)–(1.16). We note that, as promised, these fields are all defined on the *same* space $\mathcal{F}$ even though the associated representations of the history algebra are unitarily inequivalent for different choices of $n \in H_+$.

The time-averaged energy for each n is represented by the operator

$$ {}^n\hat{H} = \frac{1}{2} : \int d^4X \{ {}^n\hat{\pi}(X)^2 + {}^n\hat{\phi}(X)\, {}^n\Gamma\, {}^n\hat{\phi}(X) \} : \tag{2.8} $$

$$ = \int d^4X \hat{b}^\dagger(X) \sqrt{{}^n\Gamma}\, \hat{b}(X), \tag{2.9} $$

which is a well-defined self-adjoint operator. It is to guarantee the existence of these operators for all $n \in H_+$ that the basic fields ${}^n\hat{\phi}(X)$ and ${}^n\hat{\pi}(X)$ are defined as they are in Eqs. (2.5) and (2.6); see Refs. 5, 6 and 1 for more information on these matters.

B. The external Poincaré group

There is a natural unitary representation of the "external" Poincaré group on the Fock space $\mathcal{F}$. This is defined in the obvious way on the basic vectors $|X_1, X_2, \ldots, X_k\rangle$ as

$$ \hat{U}(\Lambda)|0\rangle := |0\rangle, \tag{2.10} $$

$$ \hat{U}(\Lambda)|X_1, X_2, \ldots, X_k\rangle := |\Lambda X_1, \Lambda X_2, \ldots, \Lambda X_k\rangle, \tag{2.11} $$

$$ \hat{U}(a)|0\rangle := |0\rangle, \tag{2.12} $$

$$ \hat{U}(a)|X_1, X_2, \ldots, X_k\rangle := |X_1 + a, X_2 + a, \ldots, X_k + a\rangle. \tag{2.13} $$

This induces the action on the annihilation operators of

$$ \hat{U}(\Lambda)\hat{b}(X)\hat{U}(\Lambda)^{-1} = \hat{b}(\Lambda X), \tag{2.14} $$

$$ \hat{U}(a)\hat{b}(X)\hat{U}(a)^{-1} = \hat{b}(X + a). \tag{2.15} $$

and similarly for the creation operators $\hat{b}^\dagger(X)$. It is straightforward to show that, as anticipated, the basic field operators ${}^n\hat{\phi}(X)$ and ${}^n\hat{\pi}(X)$ transform as

$$ \hat{U}(\Lambda)\, {}^n\hat{\phi}(X)\hat{U}(\Lambda)^{-1} = {}^{\Lambda n}\hat{\phi}(\Lambda X), \tag{2.16} $$

$$ \hat{U}(\Lambda)\, {}^n\hat{\pi}(X)\hat{U}(\Lambda)^{-1} = {}^{\Lambda n}\hat{\pi}(\Lambda X), \tag{2.17} $$

$$ \hat{U}(a)\, {}^n\hat{\phi}(X)\hat{U}(a)^{-1} = {}^n\hat{\phi}(X + a), \tag{2.18} $$

$$ \hat{U}(a)\, {}^n\hat{\pi}(X)\hat{U}(a)^{-1} = {}^n\hat{\pi}(X + a). \tag{2.19} $$

We note that it is possible to define another set of fields by

$$ \hat{\Phi}(X) := \frac{1}{\sqrt{2}} (\hat{b}(X) + \hat{b}^\dagger(X)), \tag{2.20} $$

$$\hat{\Pi}(X) := \frac{1}{i\sqrt{2}}(\hat{b}(X) - \hat{b}^{\dagger}(X)), \tag{2.21}$$

which satisfy the basic history field algebra Eqs. (1.14)–(1.16). Under the action of the external Poincaré group, we have

$$\hat{U}(\Lambda)\hat{\Phi}(X)\hat{U}(\Lambda)^{-1} = \hat{\Phi}(\Lambda X), \tag{2.22}$$

$$\hat{U}(a)\hat{\Phi}(X)\hat{U}(a)^{-1} = \hat{\Phi}(X + a), \tag{2.23}$$

and similarly for the conjugate variable $\hat{\Pi}(X)$.

The role of these ''covariant'' fields in the theory is intriguing. The relation of $\hat{\Phi}(X)$ to the fields ${}^{n}\hat{\phi}(X)$ suggests strongly that the former should be thought of as the history analog of the *Newton–Wigner* field (which, in standard quantum field theory, creates and annihilates localized *particle* states). However, we note that—in the history theory—$\hat{\Phi}(X)$ is a genuine scalar field, whereas in standard quantum field theory the Newton–Wigner field transforms in a non-covariant way.

The formal explanation of this difference lies in the way the internal and external times interface with each other in the history theory. In particular, the history field $\hat{\Phi}(X)$ is a ''Schrödinger picture'' object in the sense that it does not carry any dynamical information. On the other hand, the remarks above about the standard Newton–Wigner field apply in the Heisenberg picture: in the history case, this would involve invoking the second, internal time.

III. QUANTIZING THE FOLIATION VECTOR

A. The multi-symplectic formalism for a scalar field

One might be tempted to construct the classical history theory for a scalar field by positing the Poisson bracket algebra [cf. Eqs. (1.14)–(1.16)]:

$$\{\phi(X), \phi(X')\} = 0, \tag{3.1}$$

$$\{\pi(X), \pi(X')\} = 0, \tag{3.2}$$

$$\{\phi(X), \pi(X')\} = \delta^4(X - X'), \tag{3.3}$$

which has the advantage of appearing to be manifestly covariant under the action of the external Poincaré group (on the assumption that ϕ and π are scalar fields). However, this covariance is deceptive in the sense that the conjugate variable $\pi(X)$ has no clear *physical* meaning; not least because the actual field momentum for a physical system is manifestly foliation dependent: i.e., it means the momentum along some specified timelike direction n.

This problem is circumscribed in the approach summarized in Sec. II since the *representations* of the quantum algebra Eqs. (1.14)–(1.16) are manifestly n-dependent, and indeed an explicit n-label becomes attached to both the scalar field and its conjugate momentum via Eqs. (2.5) and (2.6). However, these explicit forms are chosen so that the *quantum* average-energy operator ${}^{n}\hat{H}$ exists, and to some extent therefore this leaves open the question of the structure of the underlying *classical* history theory. We shall now address this issue with the aid of some ideas drawn from an, apparently, quite different scheme: namely, the multi-symplectic formalism.

The multi-symplectic formalism arose from attempts to modify the standard classical *canonical* formalism so that it would be manifestly covariant under the appropriate group of space–time transformations.[10] In the case of a scalar field on Minkowski space–time M, the idea is to intro-

duce a pair of space–time fields $\phi(X)$ and $\pi_\mu(X)$ where, physically, for any vector V, $V^\mu\pi_\mu(X)$ can be interpreted as the field momentum along the space–time direction V^μ. Then, for each choice of foliation vector n, there is defined the Poisson bracket

$$\{F,G\}_n(\phi,\pi) := \int_M d^4X \left(\frac{\delta F}{\delta\phi(X)} \frac{\delta G}{\delta\pi_\mu(X)} - \frac{\delta G}{\delta\phi(X)} \frac{\delta F}{\delta\pi_\mu(X)} \right) n_\mu , \tag{3.4}$$

where F and G are functionals of ϕ and π. By this means, a family of symplectic structures is introduced, and the whole system is manifestly covariant under an action of the Poincaré group in which (*i*) ϕ and π_μ transform as genuine space–time objects in the obvious way; and (*ii*) the symplectic structure labeled by a foliation vector n is transformed into that labeled by Λn for all Lorentz transformations Λ.

The nature of this covariance is particularly clear if we look at the basic Poisson brackets that follow from Eq. (3.4):

$$\{\phi(X),\phi(X')\}_n = 0, \tag{3.5}$$

$$\{\pi_\mu(X),\pi_\nu(X')\}_n = 0, \tag{3.6}$$

$$\{\phi(X),\pi_\mu(X')\}_n = n_\mu \delta^4(X-X'), \tag{3.7}$$

where X and X' are points in Minkowski space–time M.

As remarked above, the multi-symplectic formalism was developed in the context of standard canonical theory. However—in so far as they are space–time objects—we could clearly think of ϕ and π_μ as classical *history* fields, and try to develop a history theory based on Eqs. (3.5)–(3.7) instead of Eqs. (3.1)–(3.3). As a mathematical possibility, this makes good sense. However, we should emphasize that, physically speaking, the history interpretation of the multi-symplectic formalism is quite different from the standard one.

For example, a frequent comment in the literature on the multi-symplectic formalism is that the basic Poisson brackets Eqs. (3.5)–(3.7) are not compatible with the equations of motion. But viewed as a history theory, this is no longer the case since the equations of motion are now to be associated with the introduction of the ''internal'' time label. This is closely related to the fact that, from a history perspective, the fields ϕ and π_μ are the classical analogue of *Schrödinger* picture objects, and are used in a temporal logic sense as the carriers of propositions about the history of the system; they are *not* dynamical fields.

B. First steps to the quantum history algebra

We must now address the question of the quantum analog of the parametrized (by n) family of Poisson brackets given in Eqs. (3.5)–(3.7). It is noteworthy that very little has been said in the literature on the multi-symplectic formalism about quantizing such Poisson bracket relations, and by hindsight we can understand why: it is only in the context of a quantum *history* theory—for example, the consistent history theory—that the quantization makes any physical sense.

If we approach quantization in the traditional way of replacing Poisson brackets with operator commutators, then the first issue is how to handle the n-subscript that appears on the left hand side of the equations (3.5)–(3.7). Attaching a subscript to an operator commutator does not have any *a priori* meaning other than, perhaps, to indicate different representations of an algebra, and one is tempted therefore to postulate the simple algebra (from now on we set $\hbar = 1$)

$$[\hat{\phi}(X),\hat{\phi}(X')] = 0, \tag{3.8}$$

$$[\hat{\pi}_\mu(X),\hat{\pi}_\nu(X')] = 0, \tag{3.9}$$

$$[\hat{\phi}(X),\hat{\pi}_\mu(X')] = i n_\mu \delta^4(X-X'), \tag{3.10}$$

with the understanding that the physically appropriate representation may depend on n.

However, the quantity n_μ now appears as a fixed c-number, and the manifest Poincaré covariance is lost. For example, one would like to postulate an action of the external Lorentz group of the form

$$\hat{U}(\Lambda)\hat{\phi}(X)\hat{U}(\Lambda)^{-1}=\hat{\phi}(\Lambda X), \tag{3.11}$$

$$\hat{U}(\Lambda)\hat{\pi}_\mu(X)\hat{U}(\Lambda)^{-1}=\Lambda_\mu^{\ \nu}\hat{\pi}_\nu(\Lambda X), \tag{3.12}$$

but this is incompatible with the right-hand side of Eq. (3.10) because, since n_μ is a c-number, we have $\hat{U}(\Lambda)n_\mu\hat{U}(\Lambda)^{-1}=n_\mu$. The obvious resolution of this problem is to make n_μ itself into an *operator* with modified form

$$[\hat{\phi}(X),\hat{\phi}(X')]=0, \tag{3.13}$$

$$[\hat{\pi}_\mu(X),\hat{\pi}_\nu(X')]=0, \tag{3.14}$$

$$[\hat{\phi}(X),\hat{\pi}_\mu(X')]=i\hat{n}_\mu\delta^4(X-X') \tag{3.15}$$

of the algebra in Eqs. (3.8)–(3.10), and then to augment the transformations Eqs. (3.11) and (3.12) with

$$\hat{U}(\Lambda)\hat{n}_\mu\hat{U}(\Lambda)^{-1}=\Lambda_\mu^{\ \nu}\hat{n}_\nu \tag{3.16}$$

so that the whole set is now compatible.

We now have four main tasks:

(1) Extend Eqs. (3.13)–(3.15) to a complete history theory; in particular we must discuss the form of the conjugate variables to the quantized foliation vector $\hat{n}_\mu$.
(2) Find a physically appropriate representation of the extended algebra.
(3) Show how dynamics is implemented in this scheme. In particular, how the idea arises of a second, ''internal'' time and associated internal Poincaré group.
(4) Give a physical interpretation of the algebra.

Of course, these different issues are closely related. For example, the average-energy operator for the system could be anticipated to be

$$\hat{H}=\frac{1}{2}:\int d^4X\{(\hat{n}^\mu\hat{\pi}_\mu(X))^2+(\hat{n}^\mu\hat{n}^\nu-\eta^{\mu\nu})\partial_\mu\hat{\phi}(X)\partial_\nu\hat{\phi}(X)+m^2\hat{\phi}(X)^2\}: \tag{3.17}$$

which should be compared with the expression in Eq. (2.8) for a fixed n-vector. Note that there is no longer an n-superscript on $\hat{H}$: there is now just a single operator. It is natural, therefore, to seek to fix the representation of the final history algebra by requiring that the expression in Eq. (3.17) exists as a genuine (essentially) self-adjoint operator.

C. Completing the history algebra

1. The conjugate variables to n

The next step is to consider the conjugate variables for the foliation vector. The key observation in this context is that, before quantization, the vector n is timelike, and is of unit length in the sense that

$$n\cdot n:=n^\mu n^\nu\eta_{\mu\nu}=1. \tag{3.18}$$

It seems appropriate that the quantization of n should preserve these constraints, but this requirement is incompatible with the obvious commutator algebra

$$[\hat{p}^{\mu},\hat{n}_{\nu}]=-i\,\delta^{\mu}_{\nu} \tag{3.19}$$

since the conjugate $\hat{p}^{\mu}$ would then generate translations in $\hat{n}_{\mu}$, and these do not preserve the constraints.

What we are faced with is the quantization of a system whose classical configuration space is not a vector space but rather the hyperboloid $H_{+}:=\{n\in\mathbb{R}^4|n^{\mu}n_{\mu}=1,n^0>0\}$ in $\mathbb{R}^4$, which can be viewed as a noncompact version of the three-sphere S^3. The quantization of systems whose configuration spaces are not vector spaces was discussed at length in Ref. 11 which, in particular, contains a detailed description of the quantization of a system whose classical configuration space is an n-sphere. The conclusion was that the appropriate canonical group is not the standard Weyl group (that is associated with the normal canonical commutation relations) but rather the euclidean group $\mathrm{SO}(n+1)\copyright\mathbb{R}^{n+1}$ where © denotes the semi-direct product.

The same general discussion applies in the present case with the hyperboloid H_{+} as configuration space. The result is that the appropriate history group for the foliation variable is the semi-direct product $\mathrm{SO}(3,1)\copyright\mathbb{R}^4$, with the Lie algebra relations

$$[\hat{n}_{\alpha},\hat{n}_{\beta}]=0, \tag{3.20}$$

$$[\hat{p}^{\alpha\beta},\hat{p}^{\gamma\delta}]=i(\eta^{\alpha\gamma}\hat{p}^{\beta\delta}-\eta^{\beta\gamma}\hat{p}^{\alpha\delta}+\eta^{\beta\delta}\hat{p}^{\alpha\gamma}-\eta^{\alpha\delta}\hat{p}^{\beta\gamma}), \tag{3.21}$$

$$[\hat{n}_{\alpha},\hat{p}^{\beta\gamma}]=i(\delta^{\beta}_{\alpha}\hat{n}^{\gamma}-\delta^{\gamma}_{\alpha}\hat{n}^{\beta}), \tag{3.22}$$

where $\hat{p}^{\alpha\beta}=-\hat{p}^{\beta\alpha}$.

We note the following.

(i) Equation (3.20) shows that the variables $\hat{n}_{\alpha}$ span the Lie algebra of the abelian group $\mathbb{R}^4$.
(ii) Equation (3.21) shows that the conjugate variables $\hat{p}^{\alpha\beta}$ satisfy the Lie algebra of the Lorentz group SO(3,1).
(iii) Equation (3.22) reflects the semi-direct structure given by the action of SO(3,1) on $\mathbb{R}^4$.

This group-theoretic scheme works because $\eta^{\mu\nu}\hat{n}_{\mu}\hat{n}_{\nu}$ is a Casimir operator for the algebra in Eqs. (3.20)–(3.22). Hence it is meaningful to look for a representation in which $\eta^{\mu\nu}\hat{n}_{\mu}\hat{n}_{\nu}$ has the constant value 1, thus maintaining compatibility with the classical constraint in Eq. (3.18).

Of course $\mathrm{SO}(3,1)\copyright\mathbb{R}^4$ is nothing but the familiar Poincaré group. But this should not be confused with either the internal or the external Poincaré groups to which we have referred earlier: the present group has arisen as a direct result of quantizing the foliation vector n_{μ}.

2. Completing the history algebra

We must now try to complete the history algebra by considering the cross commutators between the pair $\hat{\phi}(X)$, $\hat{\pi}_{\mu}(X)$, and the pair $\hat{n}_{\mu}$, $\hat{p}^{\alpha\beta}$. As a first step we take the commutator of both sides of Eq. (3.15) with $\hat{p}^{\alpha\beta}$, then use the Jacobi identity on the left-hand side, and the commutator Eq. (3.22) on the right-hand side, to give

$$[\hat{\phi}(X),[\hat{p}^{\alpha\beta},\hat{\pi}_{\mu}(X')]]+[\hat{\pi}_{\mu}(X'),[\hat{\phi}(X),\hat{p}^{\alpha\beta}]]=(\delta^{\alpha}_{\mu}\hat{n}^{\beta}-\delta^{\beta}_{\mu}\hat{n}^{\alpha})\,\delta^4(X-X'). \tag{3.23}$$

It is natural to think of $\hat{\phi}(X)$ and $\hat{n}_{\mu}$ as disjoint configuration variables, which suggests that

$$[\hat{\phi}(X),\hat{n}_{\mu}]=0=[\hat{\pi}_{\alpha}(X),\hat{n}_{\mu}], \tag{3.24}$$

and for this reason it is arguably also natural to assume that $[\hat{\phi}(X),\hat{p}^{\alpha\beta}]=0$. We note that a more general possibility is

$$[\hat{\phi}(X),\hat{p}^{\alpha\beta}]=ia(\hat{n}^{\alpha}\hat{\pi}^{\beta}(X)-\hat{n}^{\beta}\hat{\pi}^{\alpha}(X)) \tag{3.25}$$

for some real constant a. However, this is rather ugly in the sense that the right-hand side of Eq. (3.25) is a nonlinear function of our basic fields, and from now on we shall assume that $a=0$.

We note that, by virtue of Eq. (3.14) and the assumption in Eq. (3.24), even if the commutator in Eq. (3.25) is nonzero, it does not contribute to the left-hand side of Eq. (3.23). Thus, even if $a\neq 0$, the obvious choice for the commutator $[\hat{p}^{\alpha\beta},\hat{\pi}_{\mu}(X)]$ is

$$[\hat{p}^{\alpha\beta},\hat{\pi}_{\mu}(X)]=-i(\delta^{\alpha}_{\mu}\hat{\pi}^{\beta}(X)-\delta^{\beta}_{\mu}\hat{\pi}^{\alpha}(X)). \tag{3.26}$$

In summary, the entire history algebra is postulated to be as follows:

$$[\hat{\phi}(X),\hat{\phi}(X')]=0, \tag{3.27}$$

$$[\hat{\pi}_{\mu}(X),\hat{\pi}_{\nu}(X')]=0, \tag{3.28}$$

$$[\hat{\phi}(X),\hat{\pi}_{\mu}(X')]=i\hat{n}_{\mu}\delta^{4}(X-X'), \tag{3.29}$$

$$[\hat{n}_{\alpha},\hat{n}_{\beta}]=0, \tag{3.30}$$

$$[\hat{p}^{\alpha\beta},\hat{p}^{\gamma\delta}]=i(\eta^{\alpha\gamma}\hat{p}^{\beta\delta}-\eta^{\beta\gamma}\hat{p}^{\alpha\delta}+\eta^{\beta\delta}\hat{p}^{\alpha\gamma}-\eta^{\alpha\delta}\hat{p}^{\beta\gamma}), \tag{3.31}$$

$$[\hat{n}_{\alpha},\hat{p}^{\beta\gamma}]=i(\delta^{\beta}_{\alpha}\hat{n}^{\gamma}-\delta^{\gamma}_{\alpha}\hat{n}^{\beta}), \tag{3.32}$$

$$[\hat{\phi}(X),\hat{n}_{\alpha}]=0, \tag{3.33}$$

$$[\hat{\pi}_{\mu}(X),\hat{n}_{\alpha}]=0, \tag{3.34}$$

$$[\hat{\phi}(X),\hat{p}^{\alpha\beta}]=0, \tag{3.35}$$

$$[\hat{\pi}_{\mu}(X),\hat{p}^{\alpha\beta}]=i(\delta^{\alpha}_{\mu}\hat{\pi}^{\beta}(X)-\delta^{\beta}_{\mu}\hat{\pi}^{\alpha}(X)). \tag{3.36}$$

It is easy to check that the Jacobi identities are satisfied for this algebra.

3. An ansatz for the operator $\hat{\pi}_{\mu}(X)$

At this point we note that Eqs. (3.29) and (3.33) imply that

$$[\hat{\phi}(X),\hat{\pi}_{\mu}(X')-\hat{n}_{\mu}\hat{n}_{\nu}\hat{\pi}^{\nu}(X')]=0 \tag{3.37}$$

in a representation in which $\hat{n}\cdot\hat{n}=1$. For an arbitrary value of this Casimir operator we have instead

$$[\hat{\phi}(X),\hat{n}\cdot\hat{n}\,\hat{\pi}_{\mu}(X')-\hat{n}_{\mu}\hat{n}_{\nu}\hat{\pi}^{\nu}(X')]=0. \tag{3.38}$$

Because of Eq. (3.27), Eq. (3.37) suggests that $\hat{\pi}_{\mu}(X)-\hat{n}_{\mu}\hat{n}_{\nu}\hat{\pi}^{\nu}(X)$ might be a function of $\hat{\phi}(X)$, although from Eq. (3.33) it could also be a function of $\hat{n}_{\mu}$. In any event, clearly one natural possibility is to set

$$\hat{\pi}_{\mu}(X)-\hat{n}_{\mu}\hat{n}_{\nu}\hat{\pi}^{\nu}(X)=0, \tag{3.39}$$

which suggests that $\hat{\pi}_{\mu}(X)$ can be defined using a single "master" field $\hat{\varpi}(X)$ as

$$\hat{\pi}_{\mu}(X):=\hat{n}_{\mu}\hat{\varpi}(X). \tag{3.40}$$

We shall discuss this option at some length below. Note that it is compatible with the supposed commutator $[\hat{\pi}_\mu(X),\hat{\pi}_\nu(X')]=0$ if we postulate that $[\hat{\varpi}(X),\hat{\varpi}(X')]=0$. It is also compatible with the remaining commutators in Eqs. (3.27)–(3.36) that involve $\hat{\pi}_\mu(X)$.

A natural generalization of the definition Eq. (3.40) of the operator $\hat{\pi}_\mu(X)$ in terms of a single $\hat{\varpi}(X)$ is

$$\hat{\pi}_\mu(X) := \hat{n}_\mu \hat{\varpi}(X) + b(\partial_\mu \hat{\phi}(X) - \hat{n}_\mu \hat{n}\cdot\partial\hat{\phi}(X)) \tag{3.41}$$

for some real constant b. Bearing in mind that (assuming that $\hat{n}\cdot\hat{n}=1$)

$$\hat{n}^\mu(\partial_\mu \hat{\phi}(X) - \hat{n}_\mu \hat{n}\cdot\partial\hat{\phi}(X)) \equiv 0, \tag{3.42}$$

we see that Eq. (3.41) can be viewed as the decomposition of $\hat{\pi}_\mu(X)$ into a "longitudinal" part $\hat{n}_\mu\hat{\varpi}(X)$ and a "transverse part" $\partial_\mu\hat{\phi}(X)-\hat{n}_\mu\hat{n}\cdot\partial\hat{\phi}(X)$, with the implication in particular that the transverse part is essentially the spatial derivatives of the field $\hat{\phi}(X)$. There are several attractive features to assuming Eq. (3.41). However, it does have the implication that

$$[\hat{\pi}_\mu(X),\hat{\pi}_\nu(X')] = 2ib(\hat{n}_{(\nu}\partial_{\mu)} - \hat{n}_\mu\hat{n}_\nu\hat{n}\cdot\partial)\,\delta^4(X-X'), \tag{3.43}$$

where the partial derivatives on the right-hand side are with respect to the X label. This would mean making a change in the postulated commutator in Eq. (3.28).

D. The external and internal Poincaré groups

1. The action of the external Poincaré group

There is a natural automorphism of the complete history algebra Eqs. (3.27)–(3.36) by the external Poincaré group, which we might hope could be unitarily implemented as an extension of Eqs. (3.11), (3.12) and (3.16):

$$\hat{U}(\Lambda)\hat{\phi}(X)\hat{U}(\Lambda)^{-1} = \hat{\phi}(\Lambda X), \tag{3.44}$$

$$\hat{U}(\Lambda)\hat{\pi}_\mu\hat{U}(X)\hat{U}(\Lambda)^{-1} = \Lambda_\mu^{\ \nu}\hat{\pi}_\nu(\Lambda X), \tag{3.45}$$

$$\hat{U}(\Lambda)\hat{n}_\mu\hat{U}(\Lambda)^{-1} = \Lambda_\mu^{\ \nu}\hat{n}_\nu, \tag{3.46}$$

$$\hat{U}(\Lambda)\hat{p}^{\alpha\beta}\hat{U}(\Lambda)^{-1} = \Lambda^\alpha{}_\mu\Lambda^\beta{}_\nu\hat{p}^{\mu\nu}, \tag{3.47}$$

and with the translations acting as

$$\hat{U}(a)\hat{\phi}(X)\hat{U}(a)^{-1} = \hat{\phi}(X+a), \tag{3.48}$$

$$\hat{U}(a)\hat{\pi}_\mu(X)\hat{U}(a)^{-1} = \hat{\pi}_\mu(X+a), \tag{3.49}$$

$$\hat{U}(a)\hat{n}_\mu\hat{U}(a)^{-1} = \hat{n}_\mu, \tag{3.50}$$

$$\hat{U}(a)\hat{p}^{\alpha\beta}\hat{U}(a)^{-1} = \hat{p}^{\alpha\beta}. \tag{3.51}$$

2. The internal Poincaré group

The situation with the internal Poincaré group is interesting. As remarked above, we expect the average-energy operator of the system to be

$$\hat{H} = \frac{1}{2}{:}\int d^4X\{(\hat{n}^\mu\hat{\pi}_\mu(X))^2 + (\hat{n}^\mu\hat{n}^\nu - \eta^{\mu\nu})\partial_\mu\hat{\phi}(X)\partial_\nu\hat{\phi}(X) + m^2\hat{\phi}(X)^2\}{:}. \tag{3.52}$$

However, in this situation, $\hat{H}$ is not defined with respect to any *particular* foliation [unlike, for example, the time-averaged energy in Eq. (2.8)], and hence it cannot be identified as the timelike component of a four-vector $\hat{P}_\mu$ in any obvious way.

The resolution of this issue is as follows. In the original form of history quantum field theory, summarized in Sec. II, there is a four-vector operator ${}^n\hat{P}_\mu$ that is related to the associated time-averaged energy operator ${}^n\hat{H}$ by

$$ {}^n\hat{P}_\mu := n_\mu\, {}^n\hat{H} + \int d^4X (\partial_\mu\, {}^n\hat{\phi}(X) - n_\mu n\cdot\partial\, {}^n\hat{\phi}(X))\, {}^n\hat{\pi}(X), \tag{3.53}$$

and where we note that

$$ n^\mu \int d^4X (\partial_\mu\, {}^n\hat{\phi}(X) - n_\mu n\cdot\partial\, {}^n\hat{\phi}(X)) {}^n\hat{\pi}(X) \equiv 0. \tag{3.54}$$

Thus the "*n*-longitudinal" part of ${}^n\hat{P}_\mu$ is ${}^n\hat{H} \equiv n^\mu\, {}^n\hat{P}_\mu$, whereas the "*n*-transverse" part is $\int d^4X (\partial_\mu\hat{\phi}(X) - n_\mu n\cdot\partial\hat{\phi}(X)) {}^n\hat{\pi}(X)$.

In the present case, where n is quantized, the expression in Eq. (3.53) suggests that we define the translation generators of the internal Poincaré group by

$$ {}^{\text{int}}\hat{P}_\mu := \hat{n}_\mu\hat{H} + \int d^4X (\partial_\mu\hat{\phi}(X) - \hat{n}_\mu\hat{n}\cdot\partial\hat{\phi}(X))\hat{n}^\mu\hat{\pi}_\mu(X), \tag{3.55}$$

where $\hat{H}$ is defined in Eq. (3.52). The remaining generators of the internal Poincaré group can be defined in a similar way using the expressions given in Ref. 1 where the foliation vector n is fixed.

We note that, according to Eqs. (3.44) and (3.45), under the action of the external Lorentz group, the generators of the translations of the internal Poincaré group transform as

$$ \hat{U}(\Lambda)\, {}^{\text{int}}\hat{P}_\mu \hat{U}(\Lambda)^{-1} = \Lambda_\mu^{\ \nu}\, {}^{\text{int}}\hat{P}_\nu, \tag{3.56}$$

whereas, for a fixed n, we have

$$ \hat{U}(\Lambda)\, {}^n\hat{P}_\mu \hat{U}(\Lambda)^{-1} = \Lambda_\mu^{\ \nu}\, {}^{\Lambda n}\hat{P}_\nu. \tag{3.57}$$

3. The internal time

In the context of the discussion above of the internal Poincaré group, it is clear that one way in which a second, internal time variable s could enter the formalism is by the definition of a "Heisenberg picture" field $\hat{\phi}(X;s)$ as

$$ \hat{\phi}(X;s) := e^{is\hat{H}}\hat{\phi}(X)e^{-is\hat{H}}. \tag{3.58}$$

We see that, in this approach, there is now a *single* extra time variable s—for each choice of a foliation vector n—and this is not associated with any particular foliation vector. However, it is still true that the interpretation of the formalism should be such that s automatically has the correct meaning in the correct context. (See Ref. 7 for a detailed discussion of the interpretation of the time variable s.)

However, this is not the only option. For example, it is arguably more natural to have a separate internal time variable $s(n)$ for each value of $n \in H_+$, and such that $s(n) \geqslant 0$ for all n. In the quantum case, an operator $s(\hat{n})$ can be defined using the spectral theorem for the self-adjoint operator $\hat{n}$, and then we can define [cf. Eq. (3.52)]

$$ \hat{H}[s] := \frac{1}{2} : \int d^4X s(\hat{n}) \{ (\hat{n}^\mu\hat{\pi}_\mu(X))^2 + (\hat{n}^\mu\hat{n}^\nu - \eta^{\mu\nu})\partial_\mu\hat{\phi}(X)\partial_\nu\hat{\phi}(X) + m^2\hat{\phi}(X)^2 \} : . \tag{3.59}$$

This suggests defining an associated "generalized Heisenberg picture" object $\hat{\phi}(X;s]$ [cf. Eq. (3.58)] as

$$\hat{\phi}(X;s] := e^{i\hat{H}[s]}\hat{\phi}(X)e^{-i\hat{H}[s]}, \tag{3.60}$$

where the brackets in $\hat{\phi}(X;s]$ serve to remind us that $\hat{\phi}$ is a function of the space–time point X, but a *functional* of the function $s: H_+ \to \{0\} \cup \mathbb{R}_+$.

IV. REPRESENTATIONS OF THE HISTORY ALGEBRA

A. The Hilbert bundle construction

From what has been said above, it is clear that one way of satisfying the history algebra Eqs. (3.27)–(3.36) would be to have a single "master" momentum field $\hat{\varpi}(X)$, and then to define

$$\hat{\pi}_\mu(X) := \hat{n}_\mu \hat{\varpi}(X) \tag{4.1}$$

with the assumption that $\hat{n}_\mu$ commutes with $\hat{\varpi}(X)$ so that there are no operator-ordering problems. This gives us the simpler algebra

$$[\hat{\phi}(X), \hat{\phi}(X')] = 0, \tag{4.2}$$

$$[\hat{\varpi}(X), \hat{\varpi}(X')] = 0, \tag{4.3}$$

$$[\hat{\phi}(X), \hat{\varpi}(X')] = i\delta^4(X - X'), \tag{4.4}$$

$$[\hat{n}_\alpha, \hat{n}_\beta] = 0, \tag{4.5}$$

$$[\hat{p}^{\alpha\beta}, \hat{p}^{\gamma\delta}] = i(\eta^{\alpha\gamma}\hat{p}^{\beta\delta} - \eta^{\beta\gamma}\hat{p}^{\alpha\delta} + \eta^{\beta\delta}\hat{p}^{\alpha\gamma} - \eta^{\alpha\delta}\hat{p}^{\beta\gamma}), \tag{4.6}$$

$$[\hat{n}_\alpha, \hat{p}^{\beta\gamma}] = i(\delta^\beta_\alpha \hat{n}^\gamma - \delta^\gamma_\alpha \hat{n}^\beta), \tag{4.7}$$

with all other commutators vanishing. Of course, this is just the direct sum of the field algebra Eqs. (4.2)–(4.4) with the algebra Eqs. (4.5)–(4.7). Note that the commutator $[\hat{\pi}_\mu(X), \hat{p}^{\alpha\beta}] = i(\delta^\alpha_\mu \hat{\pi}^\beta(X) - \delta^\beta_\mu \hat{\pi}^\alpha(X))$ in Eq. (3.36) need no longer be assumed since it is implied now by the commutation relation $[\hat{n}_\alpha, \hat{p}^{\beta\gamma}] = i(\delta^\beta_\alpha \hat{n}^\gamma - \delta^\gamma_\alpha \hat{n}^\beta)$ in Eq. (4.7).

We anticipate that the key average-energy operator (that will eventually be associated with translations along the internal time direction) is [cf. Eq. (3.52)]

$$\hat{H} := \frac{1}{2} : \int d^4X \{\hat{\varpi}(X)^2 + (\hat{n}^\mu \hat{n}^\nu - \eta^{\mu\nu})\partial_\mu \hat{\phi}(X)\partial_\nu \hat{\phi}(X) + m^2 \hat{\phi}(X)^2\} :, \tag{4.8}$$

in which case the main task is to find a representation of the history algebra Eqs. (4.2)–(4.7) in which Eq. (4.8) exists as a genuine self-adjoint operator.

We proceed as follows. For each $n \in H_+$ we construct the Hilbert space $\mathcal{H}_n$ that carries operators ${}^n\hat{\phi}(X)$, ${}^n\hat{\pi}(X)$ that satisfy the history algebra Eqs. (1.14)–(1.16):

$$[{}^n\hat{\phi}(X), {}^n\hat{\phi}(X')] = 0, \tag{4.9}$$

$$[{}^n\hat{\pi}(X), {}^n\hat{\pi}(X)] = 0, \tag{4.10}$$

$$[{}^n\hat{\phi}(X), {}^n\hat{\pi}(X')] = i\delta^4(X - X'), \tag{4.11}$$

and with the property that the average-energy operator in Eq. (2.8),

$$ {}^n\hat{H} := \frac{1}{2} : \int d^4X \{ {}^n\hat{\pi}(X)^2 + (n^\mu n^\nu - \eta^{\mu\nu}) \partial_\mu {}^n\hat{\phi}(X) \partial_\nu {}^n\hat{\phi}(X) + m^2 {}^n\hat{\phi}(X)^2 \} : , \tag{4.12} $$

exists as a genuine self-adjoint operator. The *n*-superscripts on the fields in Eqs. (4.9)–(4.11) serve to indicate that we have chosen the representation of the abstract history algebra Eqs. (1.14)–(1.16) in which this operator ${}^n\hat{H}$ exists. In fact, as we know from the work in Ref. 1, for all $n \in H_+$ these fields can be constructed on the same abstract Fock space even though the corresponding representations of the history field algebra are unitarily inequivalent for different *n*. However, for our present purposes, it is clearer if we continue to refer to the Hilbert space on which ${}^n\hat{H}$ exists as $\mathcal{H}_n$.

We now link up with the heuristic ideas in the Introduction by constructing a Hilbert bundle whose base space is the hyperboloid H_+, and in which the fiber over each $n \in H_+$ is defined to be the Hilbert space $\mathcal{H}_n$. [We note that the SO(3, 1) subgroup of the history group (i.e., the part associated with the $\hat{n}_\mu$ variables) acts transitively on H_+ with stability group SO(3), so that $H_+ \simeq \mathrm{SO}(3,1)/\mathrm{SO}(3)$. Thus we have the principle bundle

$$ \mathrm{SO}(3) \to \mathrm{SO}(3,1) \to \mathrm{SO}(3,1)/\mathrm{SO}(3) \simeq H_+ := \{ n \in \mathbb{R}^4 \,|\, n \cdot n = 1, n^0 > 0 \}. \tag{4.13} $$

This suggests that we could try using a nontrivial representation of SO(3) to ''twist'' the fibers of the Hilbert bundle. However, we shall not explore that option here.] The Hilbert space of our history theory is then defined to be the direct integral

$$ \mathcal{H} := \int_{H_+}^{\oplus} \mathcal{H}_n d\mu(n). \tag{4.14} $$

Here $d\mu(n)$ is the usual SO(3,1)-invariant measure on the hyperboloid H_+: it is just the standard measure used in normal quantum field theory, but now applied to *n*-space rather than momentum space.

The vectors in this direct-integral Hilbert space $\mathcal{H}$ are defined to be the cross-sections of the Hilbert bundle: i.e., maps $\Psi : H_+ \to \cup_{n \in H_+} \mathcal{H}_n$ with the property that $\Psi(n) \in \mathcal{H}_n$ for all $n \in H_+$. The inner product between a pair of such cross-sections Ψ_1 and Ψ_2 is defined as

$$ \langle \Psi_1, \Psi_2 \rangle := \int_{H_+} d\mu(n) \langle \Psi_1(n), \Psi_2(n) \rangle_{\mathcal{H}_n}, \tag{4.15} $$

where $\langle , \rangle_{\mathcal{H}_n}$ denotes the inner product in the Hilbert space fiber $\mathcal{H}_n$.

Of course, if we make the specific identification of each Hilbert space $\mathcal{H}_n$ with the Fock space $\mathcal{F}$, as summarized in Sec. II, then the new Hilbert space $\mathcal{H}$ can be viewed as the vector space of all measurable functions $\Psi : H_+ \to \mathcal{F}$ with the inner product

$$ \langle \Psi_1, \Psi_2 \rangle := \int_{H_+} d\mu(n) \langle \Psi_1(n), \Psi_2(n) \rangle_{\mathcal{F}}. \tag{4.16} $$

Note that there is a natural cyclic ''ground'' state which is defined to be the cross-section Ω such that, for all $n \in H_+$,

$$ \Omega(n) := |0\rangle_n , \tag{4.17} $$

where $|0\rangle_n$ is the ground state of the average-energy operator ${}^n\hat{H}$ in the Hilbert-space $\mathcal{H}_n$.

B. The field and foliation operators

1. The field operators

The next step is to define the history field operators $\hat{\phi}(X)$ and $\hat{\varpi}(X)$ on $\mathcal{H} := \int_{H_+}^{\oplus} \mathcal{H}_n d\mu(n)$ as follows:

$$\{\hat{\phi}(X)\Psi\}(n) := {}^n\hat{\phi}(X)\Psi(n), \tag{4.18}$$

$$\{\hat{\varpi}(X)\Psi\}(n) := {}^n\hat{\pi}(X)\Psi(n) \tag{4.19}$$

for all $n \in H_+$. These equations are meaningful since the vectors $\Psi(n)$, $n \in H_+$, on the right-hand sides belong to the Hilbert space $\mathcal{H}_n$ on which the field operators ${}^n\hat{\phi}(X)$ and ${}^n\hat{\pi}(X)$ are defined. In other words, the maps $n \mapsto {}^n\hat{\phi}(X)$ and $n \mapsto {}^n\hat{\pi}(X)$ define fields of operators over the base space H_+, and are hence well-defined operators on the direct integral $\int_{H_+}^{\oplus} \mathcal{H}_n d\mu(n)$. (Of course, to do this rigorously one needs to discuss the domains of the various operators concerned, but we shall not dwell on such niceties here.)

It is clear that the operators defined by Eqs. (4.18) and (4.19) satisfy the history algebra Eqs. (4.2)–(4.4). For example,

$$\{\hat{\phi}(X)\hat{\varpi}(X')\Psi\}(n) = {}^n\hat{\phi}(X)\{\hat{\varpi}(X')\Psi\}(n) = {}^n\hat{\phi}(X)\,{}^n\hat{\pi}(X')\Psi(n) \tag{4.20}$$

and similarly

$$\{\hat{\varpi}(X')\hat{\phi}(X)\Psi\}(n) = {}^n\hat{\pi}(X')\{\hat{\phi}(X)\Psi\}(n) = {}^n\hat{\pi}(X')\,{}^n\hat{\phi}(X)\Psi(n), \tag{4.21}$$

so that, for all $n \in H_+$,

$$\{[\hat{\phi}(X), \hat{\varpi}(X')]\Psi\}(n) = [{}^n\hat{\phi}(X), {}^n\hat{\pi}(X')]\Psi(n) = i\delta^4(X - X')\Psi(n), \tag{4.22}$$

which means that (modulo subtleties about domains) we have the basic history field commutator $[\hat{\phi}(X), \hat{\varpi}(X')] = i\delta^4(X - X')$.

Note that, if we exploit the fact that the Hilbert spaces can all be identified with the same Fock space $\mathcal{F}$, then using the definitions in Eqs. (2.5) and (2.6), we can further write

$$\{\hat{\phi}(X)\Psi\}(n) := {}^n\hat{\phi}(X)\Psi(n) = \frac{1}{\sqrt{2}}\,{}^n\Gamma^{-1/4}(\hat{b}(X) + \hat{b}^\dagger(X))\Psi(n), \tag{4.23}$$

$$\{\hat{\varpi}(X)\Psi\}(n) := {}^n\hat{\pi}(X)\Psi(n) = \frac{1}{i\sqrt{2}}\,{}^n\Gamma^{1/4}(\hat{b}(X) - \hat{b}^\dagger(X))\Psi(n). \tag{4.24}$$

Here the operator $\hat{b}(X)$ [and similarly for $\hat{b}^\dagger(X)$] is defined as the constant field of operators over H_+ obtained by identifying each fiber of the Hilbert bundle with the Fock space $\mathcal{F}$.

2. The foliation operators

The operators that represent the foliation vector are easy to define in the Hilbert space $\int_{H_+}^{\oplus} \mathcal{H}_n d\mu(n)$. Specifically,

$$\{\hat{n}_\mu\Psi\}(n) := n_\mu\Psi(n) \tag{4.25}$$

and

$$\{\hat{p}^{\alpha\beta}\Psi\}(n) := i\left\{ n_\alpha \frac{\partial}{\partial n_\beta} - n_\beta \frac{\partial}{\partial n_\alpha} \right\} \Psi(n). \tag{4.26}$$

Note that, strictly speaking, if the history states are considered as sections of the Hilbert bundle, then the right-hand side of Eq. (4.26) involves taking the difference between vectors belonging to different Hilbert-space fibers, and hence it is only meaningful if there is a *connection* in the bundle. However, this is not a problem in our case since the fibers $\mathcal{H}_n$, $n \in H_+$, can all be identified with the basic Fock space $\mathcal{F}$, and this is assumed to have been done when writing Eq. (4.26).

3. The time-averaged energy operator

The natural way of defining a time-averaged energy operator is to exploit the fact that, on each Hilbert space fiber $\mathcal{H}_n$, $n \in H_+$, the operator ${}^n\hat{H}$ defined in Eq. (4.12) exists, and represents the time-averaged value of the energy for that particular foliation. Thus we can define an operator $\hat{H}$ by

$$\{\hat{H}\Psi\}(n) := {}^n\hat{H}\Psi(n) \tag{4.27}$$

for all $n \in H_+$. (As usual, to be fully rigorous we should worry about domains of essential self-adjointness for these operators.) Note that, as anticipated in Eq. (4.8), the operator thus defined can be written in terms of the basic history fields as

$$\hat{H} := \frac{1}{2} : \int d^4X \{ \hat{\varpi}(X)^2 + (\hat{n}^\mu \hat{n}^\nu - \eta^{\mu\nu}) \partial_\mu \hat{\phi}(X) \partial_\nu \hat{\phi}(X) + m^2 \hat{\phi}(X)^2 \} : . \tag{4.28}$$

The remaining generators of the internal Poicaré group can be defined in an analogous way.

4. The internal time function

If an internal time function is introduced as in Eq. (3.59), then the action of the operator $\hat{H}[s]$ on a section Ψ of the Hilbert bundle is

$$\{\hat{H}[s]\Psi\}(n) := s(n)\, {}^n\hat{H}\Psi(n), \tag{4.29}$$

which shows clearly the sense in which $s(n)$ is the internal time associated with the foliation vector n.

This suggests an interesting application of the ideas discussed in Ref. 12 of possible uses of topos theory in quantum gravity and quantum theory. In particular, one might try to view the construction above as being, rather than of a bundle, instead of a sheaf of Hilbert spaces over the base space H_+, which is now construed as the category of ''contexts'' in which assertions about the history system are to be made.

By viewing our construction as an object in the topos of sheaves over H_+, we can exploit the existence in any topos of both external and internal views: ''external'' in the sense of how things look from the perspective of normal mathematics, and ''internal'' in the sense of how things look from the perspective of the mathematical structure based on the topos itself. In particular, when viewed externally, the time function $n \mapsto s(n)$ appears precisely as that: i.e., a function. On the other hand, when viewed internally, it corresponds to a real number in the topos of sheaves over H_+. Thus what we have called the ''internal time *function*'' is just a *real number* when viewed internally in the topos. We intend to devote a future paper to the general question of the ways in which topos ideas can be productively applied to history theory.

C. The external Poincaré group

The key step in constructing a representation of the external Lorentz group in the Hilbert space $\mathcal{H}$ of cross-sections is to have a family of intertwining operators $\hat{U}(n;\Lambda):\mathcal{H}_n\to\mathcal{H}_{\Lambda n}$ that satisfy the conditions given in Eq. (1.23):

$$\hat{U}(\Lambda n;\Lambda')\hat{U}(n;\Lambda)=\hat{U}(n;\Lambda'\Lambda). \tag{4.30}$$

Indeed, the conditions in Eq. (4.30) mean precisely that the intertwining operators $\hat{U}(n;\Lambda)$ "cover" (i.e., act coherently with respect to) the action of SO(3,1) on the base space H_+ of the Hilbert bundle.

In these circumstances, for each $\Lambda\in\mathrm{SO}(3,1)$, we can define an operator $\hat{W}(\Lambda):\mathcal{H}\to\mathcal{H}$ by

$$\{\hat{W}(\Lambda)\Psi\}(n):=\hat{U}(\Lambda^{-1}n;\Lambda)\Psi(\Lambda^{-1}n) \tag{4.31}$$

for all $n\in H_+$. This is clearly unitary since

$$\begin{aligned}\langle\hat{W}(\Lambda)\Psi,\hat{W}(\Lambda)\Psi\rangle_{\mathcal{H}}&=\int_{H_+}d\mu(n)\langle\{\hat{W}(\Lambda)\Psi\}(n),\{\hat{W}(\Lambda)\Psi\}(n)\rangle_{\mathcal{H}_n}\\&=\int_{H_+}d\mu(n)\langle\hat{U}(\Lambda^{-1}n;\Lambda)\Psi(\Lambda^{-1}n),\hat{U}(\Lambda^{-1}n;\Lambda)\Psi(\Lambda^{-1}n)\rangle_{\mathcal{H}_n}\\&=\int_{H_+}d\mu(n)\langle\Psi(\Lambda^{-1}n),\Psi(\Lambda^{-1}n)\rangle_{\mathcal{H}_{\Lambda^{-1}n}}\\&=\int_{H_+}d\mu(n)\langle\Psi(n),\Psi(n)\rangle_{\mathcal{H}_n}=\langle\Psi,\Psi\rangle_{\mathcal{H}},\end{aligned} \tag{4.32}$$

where have used (*i*) the assumed unitarity of the intertwining operators $\hat{U}(n;\Lambda):\mathcal{H}_n\to\mathcal{H}_{\Lambda n}$, and (*ii*) the invariance of the measure $d\mu$ on H_+ under the action of SO(3,1).

To see that $\hat{W}(\Lambda)$ defined in Eq. (4.31) satisfies the group law we compute as follows:

$$\begin{aligned}\{\hat{W}(\Lambda_2)\hat{W}(\Lambda_1)\Psi\}(n)&=\hat{U}(\Lambda_2^{-1}n;\Lambda_2)(\{\hat{W}(\Lambda_1)\Psi\}(\Lambda_2^{-1}n))\\&=\hat{U}(\Lambda_2^{-1}n;\Lambda_2)\hat{U}(\Lambda_1^{-1}\Lambda_2^{-1}n;\Lambda_1)\Psi(\Lambda_1^{-1}\Lambda_2^{-1}n).\end{aligned} \tag{4.33}$$

But, from Eq. (4.30) we have

$$\hat{U}(\Lambda_2^{-1}n;\Lambda_2)\hat{U}(\Lambda_1^{-1}\Lambda_2^{-1}n;\Lambda_1)=\hat{U}(\Lambda_1^{-1}\Lambda_2^{-1}n;\Lambda_2\Lambda_1)=\hat{U}((\Lambda_2\Lambda_1)^{-1}n;\Lambda_2\Lambda_1), \tag{4.34}$$

and, hence, for all $n\in H_+$,

$$\{\hat{W}(\Lambda_2)\hat{W}(\Lambda_1)\Psi\}(n)=\hat{U}((\Lambda_2\Lambda_1)^{-1}n;\Lambda_2\Lambda_1)\Psi((\Lambda_2\Lambda_1)^{-1}n)=\{\hat{W}(\Lambda_2\Lambda_2)\Psi\}(n) \tag{4.35}$$

as is required to give a representation of the Lorentz group.

As was mentioned earlier, in our particular case, the existence of intertwining operators $\hat{U}(n;\Lambda):\mathcal{H}_n\to\mathcal{H}_{\Lambda n}$ satisfying Eq. (4.30) is demonstrated rather easily by exploiting the fact that the Hilbert spaces $\mathcal{H}_n$, $n\in H_+$, can all be identified naturally with the same Fock space generated by creation and annihilation operators $\hat{b}(X)^\dagger$ and $\hat{b}(X)$. Indeed, as discussed earlier, we simply get operators $\hat{U}(\Lambda):\mathcal{F}\to\mathcal{F}$ which in themselves give a representation of the external Lorentz group, and which satisfy Eqs. (2.16) and (2.17).

The translation subgroup of the external Poincaré group is easier to define since the translations do not act on H_+. Thus we have the simple definition

$$\{\hat{W}(a)\Psi\}(n) := {}^n\hat{U}(a)\Psi(n) \quad \forall n \in H_+, \tag{4.36}$$

where ${}^n\hat{U}(a)$ denotes the operators of the translation subgroup of the external Poincaré group in $\mathcal{H}_n$.

V. CONCLUSIONS

We have shown how the discussion in Ref. 1 of a history version of scalar quantum field theory can be augmented in such a way as to include the quantization of the unit-length, timelike vector n that determines the Lorentzian foliation of Minkowski space–time. The Hilbert bundle construction that we employed was motivated by (*i*) a heuristic discussion of the role of the external Lorentz group in the existing history quantum field theory,[1] and (*ii*) a more technical discussion of a specific representation of the extended history algebra obtained from the multi-symplectic representation of classical scalar field theory. In the latter context it should be remarked that there exist representations of this algebra other than the simple one given here—the significance of such representations is a subject for future research.

The construction of a Hilbert bundle over $H_+ := \{n \in M | n \cdot n = 1, n^0 > 0\}$ is a natural idea at a technical level, but it is also interesting from a conceptual perspective. For example, the direct integral representation of the history Hilbert space—together with the postulated nondependence of the average energy operator on the variables conjugate to $\hat{n}^\mu$—suggests that we have a type of history analog of what, in ordinary quantum theory, would be regarded as a system with continuous super-selection sectors labeled by $n \in H_+$. But in a 'neo-realist' theory such as consistent histories, the role of super-selection sectors is somewhat different from that which arises in an instrumentalist theory such as standard quantum mechanics.

The specific form of the quantization of the foliation vector presented in this paper is determined by the reduction of the full history algebra Eqs. (3.27)–(3.36) to the simplified algebra Eqs. (4.2)–(4.7) via the ansatz Eq. (4.1). In this situation, we would not expect the quantization of n to generate any physical results that are different from those of the original paper.[1] Of course, it may be possible to find representations of the full history algebra that are *not* generated by representations of the simplified algebra, and it would then be important to see if these have any physical implications. In particular, this would give some physical meaning to the multi-symplectic formalism from which we derived the full history algebra. These issues are a matter for further research.

However, the main motivation behind the present article is to present certain mathematical techniques that can be proved useful when quantizing the space–time foliations that are expected to arise in a history version of general relativity. This important issue in the history approach to quantum gravity is something to which we shall return in a later paper.

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Microlocal analysis of quantum fields on curved space–times: Analytic wave front sets and Reeh–Schlieder theorems

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We show in this article that the Reeh–Schlieder property holds for states of quantum fields on real analytic curved space–times if they satisfy an analytic microlocal spectrum condition. This result holds in the setting of general quantum field theory, i.e., without assuming the quantum field to obey a specific equation of motion. Moreover, quasifree states of the Klein–Gordon field are further investigated in the present work and the (analytic) microlocal spectrum condition is shown to be equivalent to simpler conditions. We also prove that any quasifree ground or KMS state of the Klein–Gordon field on a stationary real analytic space–time fulfills the analytic microlocal spectrum condition. © *2002 American Institute of Physics.*
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I. INTRODUCTION

One of the remarkable features of quantum field theory is the ubiquity of fluctuations and, connected with that, the generic appearance of long-range correlations. What is even more remarkable is the fact that, using suitable selective operations and applying them, say, in an arbitrary space–time region to the vacuum, one may produce in this way any given state in any other causally separated space–time region up to arbitrary precision. This is known as the Reeh–Schlieder theorem.[40] Let us recall its statement in the setting of the operator-algebraic approach to quantum field theory. Suppose that we are given a space–time manifold (M,g) (i.e., M is a smooth, n-dimensional manifold, and g is a Lorentzian metric on M) and a family ("local net") $\{\mathcal{A}(O)\}_{O\subset M}$ of von Neumann algebras, all acting on a Hilbert-space $\mathcal{H}$; the family is indexed by the open, relatively compact subsets of M, and is subject to the conditions of isotony and locality:

$$O_1\subset O\Rightarrow\mathcal{A}(O_1)\subset\mathcal{A}(O)\quad\text{and}\quad O_1\subset O^{\perp}\Rightarrow\mathcal{A}(O_1)\subset\mathcal{A}(O)'.$$

Here, $O^{\perp}$ denotes the causal complement of O, i.e., the set of all points in M which cannot be connected to O by any causal curve, and $\mathcal{A}(O)'$ denotes the commutant algebra of $\mathcal{A}(O)$ in $B(\mathcal{H})$. These conditions are the minimal assumptions in order that $\{\mathcal{A}(O)\}_{O\subset M}$ may be viewed as a net of local observable algebras of a (relativistic) physical system situated in M, see Ref. 2 for discussion. One now says that a unit vector $\Omega\in\mathcal{H}$ satisfies the **Reeh–Schlieder property** with respect to the region $O\subset M$ if Ω is cyclic for the algebra $\mathcal{A}(O)$ of observables localized in O, that is, the set of vectors $\mathcal{A}(O)\Omega=\{A\Omega:A\in\mathcal{A}(O)\}$ is dense in $\mathcal{H}$. Moreover, one says that Ω has the

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Reeh–Schlieder property if Ω is cyclic for $\mathcal{A}(O)$ for each $O \subset M$ which is open, nonvoid, and relatively compact. By the locality assumption, this then implies that Ω is also separating for all local algebras $\mathcal{A}(O)$ (as long as $O^{\perp}$ contains a nonvoid open set) and this means that $A\Omega = 0 \Rightarrow A = 0$ for all $A \in \mathcal{A}(O)$. (A vector $\Omega \in \mathcal{H}$ which is cyclic and separating for all local algebras $\mathcal{A}(O)$ is sometimes also called a standard vector for the family $\{\mathcal{A}(O)\}_{O \subset M}$.)

The generic occurrence of the Reeh–Schlieder property for large sets of physical states in quantum field theory—as so far known in quantum field theory on manifolds possessing suitable groups of isometries[1,3–9]—is a mathematically precise way of expressing that long-range correlations are a fundamental feature of quantum field theory. Furthermore, the Reeh–Schlieder property plays a very important role in analyzing the mathematical structure of quantum field theory. For instance, it is being used at some stages in the development of charge superselection theory (see Refs. 4 and 10, and references cited there). Another very important aspect of the Reeh–Schlieder property is that one may naturally associate with each von Neumann algebra together with a cyclic and separating vector the so-called Tomita–Takesaki modular objects.[11] In the seminal work of Bisognano and Wichmann[12,13] it has been shown that the Tomita–Takesaki modular objects associated with the vacuum-vector and the von Neumann algebra $\mathcal{A}(W)$ of a ''wedge-region'' (which is actually infinitely extended) in a Wightman-type quantum field theory on Minkowski space–time have a specific geometric significance. This insight has initiated considerable progress in the mathematical development of general quantum field theory on which the recent review by Borchers[14] reports exhaustively; therefore we refer the reader to that reference for further discussion. We limit ourselves to mentioning that quite promising generalized forms of such a ''geometric modular action'' that are applicable to quantum field theories on curved space–times have been suggested and investigated more recently.[15,16] The Reeh–Schlieder property is also responsible for (maximal) violations of Bell's inequalities in quantum field theory,[17] and more recently, Reeh–Schlieder properties have been found to imply various forms of long-range entanglement of states in relativistic quantum field theory;[18–20] see also Refs. 21 and 22 for related discussions. A possible significance of Reeh–Schlieder properties for questions related to cosmology has been proposed in Ref. 23.

As indicated previously, Reeh–Schlieder properties have, either in the model-independent approach or for concrete quantum field models, so far only been established under the assumption that the space–time in which the quantum system is situated possesses a sufficient amount of space–time symmetries. This constitutes a considerable limitation, and the question is if Reeh–Schlieder-like properties can also be established for quantum field theories on space–times not admitting any isometries. This is feasible since the main mathematical argument leading to the Reeh–Schlieder theorem in the case where there are sufficiently many space–time symmetries is an analytical argument of the type of the edge-of-the-wedge-theorem[3] or Schwartz' reflection principle in order to derive a certain global property of a quantum state from local information, and these arguments do not use space–time symmetries (in particular, timelike isometry groups) directly. On the other hand, commonly the analytic properties of correlation functions in quantum field theory are consequences of the relativistic spectrum condition whose formulation requires a form of time-translation symmetry. Time-translation symmetry is also required in order to formulate conditions of thermal equilibrium in relativistic quantum field theory from which Reeh–Schlieder properties may also be deduced.[6]

At any rate, certain analytical properties of correlation functions are prerequisite in order to establish Reeh–Schlieder theorems in quantum field theory and the question arises how to generalize the analyticity properties known to hold, e.g., for ground states or thermal equilibrium states with respect to a time-symmetry group to more general situations. A way to proceed in more general situations may be to follow, and to refine, the approach pioneered by Radzikowski,[24,25] who proved that, for a free scalar quantum field on generic curved space–times, the condition that a quasifree state be a Hadamard state can equivalently be expressed as a condition on the wave front set of the two-point function of that state (see also Refs. 26–28 for related work). Since it can convincingly be argued that Hadamard states are most likely candidates for physical states of quantum fields obeying linear wave-equations,[29] it appears natural to sharpen the condition on the

two-point function of a physical state by demanding that it applies to the analytic wave front set and not only, as in most previous considerations, to the C^∞ wave front set. In order that this makes sense independently of particular coordinates, the underlying space-time manifold ought to be real analytic.

Thus, we will propose a stricter form of the wave front set spectrum condition formulated in Ref. 24, or of the microlocal spectrum condition,[30] for the n-point functions of a generic scalar quantum field on a real analytic space–time in terms of their analytic wave front sets, and we will show that such states possess the Reeh–Schlieder property. In doing so, we will present a transcription of the (analytic) microlocal spectrum condition for a two-point function as a condition on the wave front set of a certain Hilbert-space valued distribution. It turns out that working with wave front sets of Hilbert-space valued distributions has several advantages. One of those is that in terms of Hilbert-space valued distributions the (analytic) microlocal spectrum condition (for two-point functions of free fields) assumes a very simple and elegant form which is, in fact, most reminiscent of the usual spectrum condition in quantum field theory in Minkowski space–time. Part of this analysis appears already in Ref. 31 for the case of the C^∞ wave front set where the calculus of Hilbert space valued distributions is used for the definition of Wick products of free fields. This appeared motivation enough to discuss several aspects of microlocal analysis of Hilbert-space valued distributions more systematically, and that discussion thus forms the first part of the present article in Sec. II.

In Sec. III we summarize some basics on the description of general scalar quantum fields on curved space–times, together with the example of the free scalar Klein–Gordon field.

We recapitulate the definition of the microlocal spectrum condition (''μSC''), referring to the C^∞ wave front sets of n-point functions of quantum fields on manifolds, according to Ref. 30 in Sec. IV. In the same section, we introduce our analytic microlocal spectrum condition (''aμSC'') which will be defined similarly to μSC but now using analytic wave front sets of n-point functions of quantum fields on real analytic manifolds. (We should note that Hollands and Wald[32] have recently also introduced a similar concept of analytic microlocal spectrum condition which refers to a whole class of states, and is used in a different context.)

In Sec. V we will present our main result, which is a Reeh–Schlieder theorem for quantum field states fulfilling the aμSC. Here, we draw on results of Sec. II, and also on a microlocal version of the edge-of-the-wedge theorem, which appears as Theorem 8.5.6′ in Ref. 33.

Finally, in Sec. VI we present the characterization of aμSC and of μSC for two-point functions of a free scalar field on a manifold in terms of a simple conic form of the wave front set of certain Hilbert-space valued distributions. Moreover, we prove that ground and KMS states of the free scalar field on a real analytic stationary space–time obey the aμSC. This shows in particular that the Hartle–Hawking state on the Schwarzschild space–time satisfies the aμSC.

II. MICROLOCAL ANALYSIS FOR HILBERT SPACE VALUED DISTRIBUTIONS

Assume we are given a Hilbert space $\mathcal{H}$ and a smooth manifold M which is second countable and Hausdorff. The space $\mathcal{D}'(M,\mathcal{H})$ of $\mathcal{H}$ valued distributions is defined to be the set of all weakly continuous linear maps

$$C_0^\infty(M)\to\mathcal{H}.$$

Note that due to the nuclearity of $C_0^\infty(M)$ these maps are automatically strongly continuous. If $X\subset\mathbb{R}^n$ is an open subset a linear map $\psi: C_0^\infty(X)\to\mathcal{H}$ is in $\mathcal{D}'(X,\mathcal{H})$ if and only if for each compact subset $K\subset X$ there are constants $C>0$ and $\alpha\in\mathbb{N}_0$ such that

$$\|\psi(f)\|<C\sum_{|k|\leqslant\alpha}\sup_x|(\partial^k f)(x)|, \tag{1}$$

for all $f \in C_0^\infty(K)$. If α can be chosen independently of K, then we say that ψ is of order α and write $\psi \in \mathcal{D}'^{\alpha}(X,\mathcal{H})$. The set of $\psi \in \mathcal{D}'(X,\mathcal{H})$ with compact support in X will be denoted by $\mathcal{E}'(X,\mathcal{H})$. If ψ has compact support then one can easily extend ψ to a linear map $C^\infty(X) \to \mathcal{H}$ and we have for all compact sets K which contain $\mathrm{supp}(\psi)$,

$$\|\psi(f)\| < C \sum_{|k| \leqslant \alpha} \sup_{x \in K} |(\partial^k f)(x)|, \quad \forall f \in C^\infty(X), \tag{2}$$

for some $C > 0, \alpha \in \mathbb{N}_0$. Conversely, if there exists a compact set K such that for a given linear map $\psi: C^\infty(X) \to \mathcal{H}$ the inequality (2) holds for some C and α, then ψ is a distribution with support in K. Therefore, $\mathcal{E}'(X,\mathcal{H})$ can be identified with the set of strongly continuous maps $C^\infty(X) \to \mathcal{H}$. If a subset L of $\mathcal{E}'(X,\mathcal{H})$ is bounded then (2) holds for all $\psi \in L$ and $f \in C^\infty(X)$ with constants C and α independent of ψ. We define $\mathcal{E}'^{\alpha}(X,\mathcal{H}) := \mathcal{E}'(X,\mathcal{H}) \cap \mathcal{D}'^{\alpha}(X,\mathcal{H})$ and obviously $\mathcal{E}'(X,\mathcal{H}) = \cup_\alpha \mathcal{E}'^{\alpha}(X,\mathcal{H})$.

If $\psi \in \mathcal{E}'(\mathbb{R}^n,\mathcal{H})$ one may define the Fourier transform $\hat{\psi}$ in the same way as this is done for ordinary distributions. Namely, the Fourier transform $\hat{\psi}$ is the $\mathcal{H}$ valued function on $\mathbb{R}^n$ given by $\hat{\psi}(k) := \psi(e^{-ik\cdot})$.

Definition 2.1: Let X be open in $\mathbb{R}^n$ and let ψ be in $\mathcal{D}'(X,\mathcal{H})$. Then a point $(x,k) \in X \times (\mathbb{R}^n \backslash \{0\})$ is called regular directed for ψ if the following holds: There exists a function $f \in C_0^\infty(X)$ with $f(x) = 1$ and an open conic neighborhood Γ of k such that for each $N \in \mathbb{N}$ there exists a constant C_N with

$$\sup_{\lambda \in \Gamma} (1 + |\lambda|)^N \|\widehat{f\psi}(\lambda)\| < C_N. \tag{3}$$

The set of regular directed points is open. Its complement in $X \times (\mathbb{R}^n \backslash \{0\})$ is called the wave front set $\mathrm{WF}(\psi)$ *of ψ.*

The following proposition shows that microlocal analysis of Hilbert space valued distributions is analogous to the case of ordinary distributions. See also Ref. 31 for related discussion.

Proposition 2.2: Let X be open in $\mathbb{R}^n$ and let $\psi \in \mathcal{D}'(X,\mathcal{H})$ be a Hilbert space valued distribution.

(1) If (3) *holds for $f \in C_0^\infty(X)$ then it also holds with f replaced by gf for any $g \in C^\infty(X)$.*

(2) If ψ has compact support then $\hat{\psi}$ is polynomially bounded in the norm, i.e., there is a constant C and an integer M, such that

$$\|\hat{\psi}(k)\| < C(1 + |k|)^M. \tag{4}$$

If moreover a subset $L \in \mathcal{E}'(X,\mathcal{H})$ is bounded then (4) *holds for all $\psi \in L$ with C and M independent of ψ.*

(3) If $\mathrm{WF}(\psi)$ *is empty then ψ is smooth in the norm.*

(4) If we define the distribution $w \in \mathcal{D}'(X \times X)$ by $w(f,g) = \langle \psi(\overline{f}), \psi(g) \rangle$, then

$$(x,k) \in \mathrm{WF}(\psi) \Leftrightarrow ((x,-k),(x,k)) \in \mathrm{WF}(w), \tag{5}$$

and moreover, if $(x,k) \notin \mathrm{WF}(\psi)$ with $k \neq 0$, then

$$((x,-k),(x_1,k_1)) \notin \mathrm{WF}(w) \quad \textit{and} \quad ((x_1,k_1),(x,k)) \notin \mathrm{WF}(w), \tag{6}$$

for arbitrary $(x_1,k_1) \in X \times \mathbb{R}^n$.

(5) Under change of coordinates $\mathrm{WF}(\psi)$ *transforms as a subset of the cotangent bundle. Hence,* $\mathrm{WF}(\phi)$ *may be defined for distributions $\phi \in \mathcal{D}'(M,\mathcal{H})$, for a smooth manifold M and* $\mathrm{WF}(\phi) \subset T^*M \backslash 0$. *Here $T^*M \backslash 0$ is the cotangent bundle with zero section removed.*

Proof: The first statement is proved in the same manner as for ordinary distributions (cf. Ref. 33, Lemma 8.1.1). The inequality (2) immediately gives the second statement if $f(x) = e^{-ikx}$. To

see that (3) holds we first note that $\mathrm{WF}(\psi)=\varnothing$ implies that for each point $x\in X$ there is a C_0^∞ function with $f(x)=1$ such that $\|\widehat{f\psi}\|$ is rapidly decreasing. The same arguments as in the complex valued case show that $f\psi$ can be represented by the inverse Fourier transform of $\widehat{f\psi}$, which is a smooth function, i.e., all derivatives in the norm sense exist and are given by $D^\alpha(f\psi)(x)=2\pi((-\mathrm{i}k)^\alpha\widehat{f\psi}(k)(-x)$. (5) is a simple consequence of (4) and it remains to show (4). Assume first that $(x,-k,x,k)$ is regular directed for w. Then there is a function $f_1\in C_0^\infty(X\times X)$ such that $\widehat{f_1 w}$ decays rapidly in a conic neighborhood of $(x,-k,x,k)$. Because of (1) we may choose f_1 to be of the form $f\otimes f$, where $f\in C_0^\infty(X)$ is a positive function. Since

$$\|\widehat{f\psi}(k)\|^2=((\widehat{f\otimes f})w(-k,k), \tag{7}$$

(x,k) is regular directed for ψ. Suppose conversely we knew that (x,k) is regular directed for ψ. By the Cauchy inequality we have

$$|((\widehat{f\otimes g})w(k_1,k_2)|\leqslant\|\psi(\overline{f}(\cdot)e^{\mathrm{i}k_1\cdot})\|\cdot\|\psi(g(\cdot)e^{-\mathrm{i}k_2\cdot})\|. \tag{8}$$

By assumption there is a $g\in C_0^\infty(X)$ with $g(x)=1$ such that in a conic neighborhood of k the second factor is rapidly decreasing. Since the other is polynomially bounded for any $f\in C_0^\infty(X)$, (x_1,k_1,x,k) is a regular directed point for w for any (x_1,k_1). In the same way one shows that $(x,-k,x_1,k_1)$ is regular directed. This concludes the proof. □

The fourth statement in the above-given proposition allows one to take over many results known for ordinary distributions.

Proposition 2.3: If $P:C^\infty(M)\to C^\infty(M)$ is a differential operator and $\psi\in\mathcal{D}'(M,\mathcal{H})$ such that $\psi\circ P^*=0$, where P^* is the formal adjoint of P, then

$$\mathrm{WF}(\psi)\subset\mathrm{char}(P).$$

Here $\mathrm{char}(P)$ *is the characteristic set of P, i.e., the set of points (x,k) in $T^*M\backslash 0$ on which the principal symbol σ_P of P vanishes.*

Proof: We define w as in Proposition 2.2. Note that $((x,-k),(x,k))$ is in the characteristic set of the operator $L:=\overline{P}\otimes P$ if and only if (x,k) is in the characteristic set of P. Moreover, $Lw=0$. The result follows now from the fourth statement in Proposition 2.2. □

One may also define the analytic wave front set of a Hilbert space valued distribution. We follow the definition in Ref. 33 (Definition 8.4.3).

Definition 2.4: Let X be an open subset of $\mathbb{R}^n$ and $\psi\in\mathcal{D}'(X,\mathcal{H})$. We denote by $\mathrm{WF}_A(\psi)$ *the complement in $X\times(\mathbb{R}^n\backslash\{0\})$ of the set of points (x_0,k_0) such that there is a neighborhood $U\subset X$ of x_0, a conic neighborhood Γ of k_0 and a bounded sequence ψ_N of distributions with compact support which is equal to ψ in U, such that there exists a constant C with*

$$\||k|^N\hat{\psi}_N(k)\|\leqslant C(C(N+1))^N, \tag{9}$$

for all $k\in\Gamma$.

The bounded sequence ψ_N can always be chosen to be the product $f_N\psi$, where f_N is a sequence of smooth functions. One has

Lemma 2.5: Let $\psi\in\mathcal{D}'(X,\mathcal{H})$, K a compact subset of X, and let F be a closed cone in $\mathbb{R}^n$ such that $\mathrm{WF}_A(\psi)\cap(K\times F)=\varnothing$. If $f_N\in C_0^\infty(K)$ and for all α

$$|D^{\alpha+\beta}f_N|\leqslant C_\alpha(C_\alpha(N+1))^{|\beta|},\quad |\beta|\leqslant N=1,2,\ldots, \tag{10}$$

then $f_N\psi$ is a bounded sequence and we have

$$\||k|^N\hat{\psi}_N(k)\|\leqslant C(C(N+1))^N, \tag{11}$$

for all $k \in F$. Moreover, if x is a point in the interior of K, there always exists a neighborhood $\mathcal{U}$ of x and a sequence of functions f_N such that (10) is satisfied and $f_N = 1$ on $\mathcal{U}$.

Proof: The proof of this statement is the same as for ordinary distributions (see Ref. 33, Lemma 8.4.4). □

Proposition 2.6: Let X be an open set in $\mathbb{R}^n$ and let $\psi \in \mathcal{D}'(X,\mathcal{H})$ be a Hilbert space valued distribution.

(1) If $\mathrm{WF}_A(\psi)$ is empty then ψ is strongly real analytic.

(2) If we define the distribution $w \in \mathcal{D}'(X \times X)$ by $w(f,g) = \langle \psi(\overline{f}), \psi(g) \rangle$, then

$$(x,k) \in \mathrm{WF}_A(\psi) \Leftrightarrow ((x,-k),(x,k)) \in \mathrm{WF}_A(w), \tag{12}$$

and moreover, if $(x,k) \notin \mathrm{WF}_A(\psi)$ with $k \neq 0$, then

$$((x,-k),(x_1,k_1)) \notin \mathrm{WF}_A(w) \quad \textit{and} \quad ((x_1,k_1),(x,k)) \notin \mathrm{WF}_A(w), \tag{13}$$

for arbitrary $(x_1,k_1) \in X \times \mathbb{R}^n$.

(3) Under analytic change of coordinates $\mathrm{WF}_A(\psi)$ transforms as a subset of the cotangent bundle. Hence, $\mathrm{WF}_A(\phi)$ may be defined for distributions $\phi \in \mathcal{D}'(M,\mathcal{H})$, for a smooth real analytic manifold M and $\mathrm{WF}_A(\phi) \subset T^*M \backslash 0$.

Proof: We start with (2). Assume that $(x,-k,x,k) \notin \mathrm{WF}_A(w)$. We choose a sequence of functions f_N in $C_0^\infty(X)$ which satisfies the inequality (10) and which is equal to 1 in a neighborhood of x. Then the sequence $g_N := \overline{f_N} \otimes f_N \in C_0^\infty(X \times X)$ also satisfies an inequality of the form (10), and hence

$$|(-k_1,k_1)|^N |\widehat{(g_N w)}(-k_1,k_1)| \leq C(C(N+1))^N, \tag{14}$$

for some constant $C > 0$ and all k_1 in a conic neighborhood of k. We have

$$\|\widehat{f_N \psi}(k_1)\|^2 = \widehat{(g_N w)}(-k_1,k_1), \tag{15}$$

and a quick estimate shows that for all k_1 in a conic neighborhood of k we have

$$\| |k_1|^N \widehat{(f_N \psi)}(k_1) \| \leq \widetilde{C}(\widetilde{C}(N+1))^N, \tag{16}$$

for some constant $\widetilde{C}$. Therefore, $(x,k) \notin \mathrm{WF}_A(\psi)$. Suppose conversely that $(x_1,k_1) \notin \mathrm{WF}_A(\psi)$. Hence, there is a sequence ψ_N bounded in $\mathcal{E}'(X,\mathcal{H})$ and equal to ψ in a neighborhood of x_1 such that the inequality (9) holds in a conic neighborhood of k_1. Choose another function g which is equal to 1 in a neighborhood of a point x_2. Then the distribution w_N defined by $w_N(h_1,h_2) := \langle \psi(g \cdot \overline{h_1}), \psi_N(h_2) \rangle$ is bounded in $\mathcal{E}'(X \times X)$. Moreover, an application of the Cauchy inequality shows that

$$|\hat{w}_N(k_2,k)| \leq \|\psi(g e^{\mathrm{i}k_2 \cdot})\| \cdot \|\psi_N(e^{-\mathrm{i}k \cdot})\|. \tag{17}$$

The first factor is bounded by $C_M(1+|k_2|)^M$ for some $M \in \mathbb{N}$ and a simple estimate shows that for all k_2 there is a conic neighborhood Γ of (k_2,k_1) and a $C > 0$ with

$$|(k_2',k)|^N \cdot |\hat{w}_{N+M}(k_2',k)| \leq C(C(N+1))^N, \tag{18}$$

for all $(k_2',k) \in \Gamma$. Since w_N is equal to w in a neighborhood of (x_2,x_1), we get

$$((x_2,k_2),(x_1,k_1)) \notin \mathrm{WF}_A(w).$$

In the same way one shows that

$$((x_1,-k_1),(x_2,k_2)) \notin \mathrm{WF}_A(w).$$

Statement (3) is an immediate consequence of (2) since the analytic wave front set of an ordinary distribution transforms as a subset of the cotangent bundle. The first statement can be shown in the same way as for ordinary distributions (see Ref. 33, Theorem 8.4.5). This concludes the proof.□

Proposition 2.7: If $P:C^\infty(M)\to C^\infty(M)$ *is a differential operator with real analytic coefficients on a real analytic manifold* M *and* $\psi\in\mathcal{D}'(M,\mathcal{H})$ *such that* $\psi\circ P^*=0$, *where* P^* *is the formal adjoint of* P, *then*

$$\mathrm{WF}_A(\psi)\subset\mathrm{char}(P),$$

where $\mathrm{char}(P)$ *is the characteristic set of* P.

Proof: Analogous to the proof of Proposition 2.3. □

Theorem 2.8: *Let* $X\subset\mathbb{R}^n$ *be an open subset and assume* $\psi\in\mathcal{D}'(X,\mathcal{H})$. *Assume that there is a smooth* $\mathcal{H}$*-valued function* $G:I\times X\to\mathcal{H}$, *with* $I=(0,\epsilon)$, *such that*

$\lim_{t\to 0}G(t,\cdot)=\psi$ *in the sense of distributions,*

$(\partial_t G)(t,x_1,\ldots,x_n)=\mathrm{i}(\partial_{x_1}G)(t,x_1,\ldots,x_n)$.

Then $\mathrm{WF}_A(\psi)\subset\{(x_1,\ldots,x_n)\times(y_1,\ldots,y_n)\in X\times\mathbb{R}^n\backslash\{0\};y_1\geqslant 0\}$.

Proof: The proof is a variation of the proof of Theorem 8.4.8 in Ref. 33. Since the statement is local we can assume without loss of generality that $X=X_1\times\cdots\times X_n$ and that ψ. First note that for each given $g\in C_0^\infty(X_2\times\ldots\times X_n)$ the function

$$H(x+\mathrm{i}y):=\int_{X_2\times\cdots\times X_n}G(y,x,y_2,\ldots,y_n)g(y_2,\ldots,y_n)\mathrm{d}y_2\cdots\mathrm{d}y_n \tag{19}$$

is defined on the strip $X_1+\mathrm{i}I$ and is holomorphic. Moreover, it has a distributional boundary value $\psi(\cdot\otimes g)$. We will slightly vary the proof of Theorem 3.1.14 in Ref. 33 to show that the following bound holds:

$$\|H(x+\mathrm{i}y)\|\leqslant C'y^{-m-1} \tag{20}$$

if $(x,y)\in\tilde{X}_1\times I/2$ and $\mathrm{clo}(\tilde{X}_1)\subset X_1$ for some $m>0$. Let $f\in C_0^\infty(X_1\times I)$ be a function with support in $K\times I$, where K is a compact subset of X_1, such that f is equal to 1 in a neighborhood of $\overline{Z}$, where $Z:=\tilde{X}_1\times I/2$. Cauchy's integral formula applied to fH in the set $\Im z>\Im(\zeta/2)$ shows that if $\zeta=\xi+\mathrm{i}\eta\in Z$,

$$\begin{aligned}H(\zeta)=&-\pi^{-1}\int\int_{y>\eta/2}H(x+\mathrm{i}y)\partial f(x,y)/\partial\overline{z}(z-\zeta)^{-1}\mathrm{d}x\,\mathrm{d}y\\&+(2\pi\mathrm{i})^{-1}\int f(x,\eta/2)(x-\xi-\mathrm{i}\eta/2)^{-1}H(x+\mathrm{i}\eta/2)\mathrm{d}x.\end{aligned} \tag{21}$$

An application of the uniform boundedness principle (Banach–Steinhaus theorem) shows that $\|\int_{X_1}H(x+\mathrm{i}y)h(x)\mathrm{d}x\|\leqslant C\Sigma_{\alpha\leqslant m}\sup|\partial^\alpha h|$ for all $h\in C_0^\infty(K)$ with constants C and m independent of y (cf. Ref. 33, Theorem 2.1.8). Therefore, the last integral in (21) can be estimated in the norm by

$$C_1\sum_{\alpha\leqslant m}\sup|\partial_x^\alpha(x,\eta/2)(x-\xi-\mathrm{i}\eta/2)^{-1}|\leqslant C_2|\eta|^{-m-1}. \tag{22}$$

The first integral in (21) is bounded and this proves the inequality (20).

Since the statement of the theorem is local we can always replace X_1 by $\tilde{X}_1$ and I by $I/2$ and we can therefore assume without loss of generality that the bound (20) holds in $X_1\times I$. From Stokes integral formula one gets for y, $Y\in\mathbb{R}_+$ and $N\in\mathbb{N}$ such that $y+Y<\epsilon/2$ the following formula (compare 3.1.19 in Ref. 33) for any $\tilde{\phi}\in C_0^\infty(X)$ with $\tilde{\phi}=\phi\otimes g$:

$$\int_X \tilde{\phi}(\mathbf{x})G(y,\mathbf{x})\mathrm{d}\mathbf{x} = \int_{X_1} \Theta(x,Y)H(x+\mathrm{i}y+\mathrm{i}Y)\mathrm{d}x + (N+1)\int_{X_1}\mathrm{d}x\int_{0<t<1}\mathrm{d}t\, H(x+\mathrm{i}tY+\mathrm{i}y)(\partial^N\phi)(x)\frac{(\mathrm{i}Y)^N}{N!}t^N, \tag{23}$$

where

$$\Theta(x,y) := \sum_{j=0}^{N} \partial^j\phi(x)(\mathrm{i}y)^j/j!. \tag{24}$$

Because of the bound (20) the integrand under the double integral in (23) is uniformly bounded by an integrable function if $N>(m+1)$ and the first term even converges uniformly as $y\to 0$. Therefore, we have for $N>(m+1)$,

$$\psi(\tilde{\phi}) = \int_{X_1}\Theta(x,Y)H(x+\mathrm{i}Y)\mathrm{d}x + (N+1)\int_{X_1}\mathrm{d}x\int_{0<t<1}\mathrm{d}t\, H(x+\mathrm{i}tY)(\partial^N\phi)(x)\frac{(\mathrm{i}Y)^N}{N!}t^N. \tag{25}$$

Now let $\mathbf{x}'=(x_1',\ldots,x_n')$ be a point in X and let ϕ_ν be a sequence of functions on X_1 which are all equal to 1 in a common neighborhood of x_1' such that

$$|\partial^\alpha\phi_\nu| \leqslant (C_1(\nu+1))^\alpha, \quad \alpha\leqslant\nu+1. \tag{26}$$

Assume that g is equal to 1 in a neighborhood of $(x_2',\ldots,x_n')$. With

$$\Theta_\nu(x,y) := \sum_{j=0}^{\nu}\partial^j\phi_\nu(x)(\mathrm{i}y)^j/j! \tag{27}$$

we get from (25) for $\nu>(m+1)$,

$$\widehat{(\phi_\nu\otimes g)}\psi(k) = \int_X G(Y,\mathbf{x})\Theta_\nu(x_1,Y)g(x_2,\ldots,x_n)e^{-\mathrm{i}(\mathbf{x}+\mathrm{i}\mathbf{Y},k)}d\mathbf{x} + (\nu+1)\int_X d\mathbf{x}\int_{0<t<1}dtG(tY,\mathbf{x})e^{-\mathrm{i}(\mathbf{x}+\mathrm{i}t\mathbf{Y},k)}\cdot(\partial^\nu\phi_\nu)(x_1)g(x_2,\ldots,x_n)\frac{(\mathrm{i}Y)^\nu}{\nu!}t^\nu. \tag{28}$$

Here we used the notations $\mathbf{x}=(x_1,\ldots,x_n)$ and $\mathbf{Y}=(Y,0,\ldots,0)$. With $C_2=2e^{C_1Y}$ we have $|\Theta_\nu(x,Y)|\leqslant C_2^{\nu+1}$ and because of the bound (20) we get

$$\|(\phi_\nu\otimes g)\psi(k)\| \leqslant C_3^{\nu+1}(e^{(Y,k)}+(\nu-m-1)!(-\mathbf{Y},k)^{m-\nu}), \quad (\mathbf{Y},k)<0. \tag{29}$$

We define $\psi_\nu := (\phi_{m+\nu}\otimes g)\psi$ and if $(\mathbf{Y},k)<-c|k|$ for a fixed c, we obtain for some C_4,

$$\|\hat{\psi}_\nu(k)\| \leqslant C_4^{\nu+1}\nu!|k|^{-\nu}, \tag{30}$$

since $e^{-c|k|}\leqslant\nu!(c|k|)^{-\nu}$. If we chose ϕ_ν bounded in C_0^∞, then ψ_ν is bounded in $\mathcal{E}'(X,\mathcal{H})$. We have shown that

$$\mathrm{WF}_A(\psi)\subset X\times\{k,(\mathbf{Y},k)\geqslant 0\}.$$

□

An immediate corollary of this theorem is

Corollary 2.9: Let $X\subset\mathbb{R}^n$ be an open subset. Suppose that V is an open cone in $\mathbb{R}^n\backslash\{0\}$ and Z is an open neighborhood of 0 in $\mathbb{R}^n$. Denote by V° the dual cone. (The dual cone V° of an open cone V is defined as the set $V^\circ=\{\xi\in\mathbb{R}^n:\langle v,\xi\rangle\geqslant 0\,\forall\, v\in V\}$, where $\langle\,.\,,.\,\rangle$ denotes the Euclidean scalar product on $\mathbb{R}^n$.) If $\psi\in\mathcal{D}'(X,\mathcal{H})$ is the boundary value in the sense of distributions of a function G which is analytic in $X\times(V\cap Z)$, then $\mathrm{WF}_A(\psi)\subset X\times V^\circ$.

III. QUANTUM FIELD THEORY ON CURVED SPACE–TIMES

By a space–time we mean in the following a connected smooth manifold of dimension $n\geqslant 2$ which is second countable and Hausdorff and which is endowed with a Lorentzian metric g such that M is both oriented and time-oriented. A spacelike hypersurface $\mathcal{C}$ in a space–time M is called Cauchy surface if each inextendible causal curve intersects $\mathcal{C}$ exactly once. In case there exists a Cauchy surface the space–time M is said to be globally hyperbolic (see, e.g., Refs. 34 and 35 for further discussion).

A. Scalar fields on curved space–times

The Borchers–Uhlmann algebra $\mathcal{B}$ of a manifold M is defined to be the topological tensor algebra

$$\mathcal{B}:=\mathbb{C}\oplus\bigoplus_{m=1}^{\infty}\otimes^m C_0^\infty(M) \tag{31}$$

endowed with a star defined by $(f_1\otimes\cdots\otimes f_k)^*=\overline{f_k}\otimes\cdots\otimes\overline{f_1}$. A state ω over $\mathcal{B}$ determines a sequence of distributions $\omega_m\in\mathcal{D}'(M^m)$, the so-called m-point functions, by

$$\omega_m(f_1,\ldots,f_m):=\omega(f_1\otimes\cdots\otimes f_m). \tag{32}$$

If $\mathcal{H}$ is a Hilbert space and D a dense subset we denote by $\mathcal{L}_D^+$ the set of (possibly unbounded) operators A on $\mathcal{H}$ with the properties

$$\mathrm{dom}(A)=D,\quad AD\subset D,\quad \mathrm{dom}(A^*)\supset D,\quad A^*D\subset D. \tag{33}$$

The involution $A^+:=A^*|_D$ and the locally convex topology defined by the seminorms $p_{\phi,\psi}(A):=|\langle\phi,A\psi\rangle|$, $\phi,\psi\in D$ turn $\mathcal{L}_D^+$ into a locally convex topological $*$-algebra.

Each state over the Borchers–Uhlmann algebra $\mathcal{B}$ determines, by the GNS construction, a Hilbert space $\mathcal{H}$ with a dense domain D and an $*$-representation $\pi:\mathcal{B}\to\mathcal{L}_D^+$ with cyclic vector $\Omega\in D$ such that $\pi(\mathcal{B})\Omega=D$. If $M=\mathbb{R}^4$ is the Minkowski space it is well known that Wightman fields can be constructed from states over the Borchers–Uhlmann algebra which satisfy certain requirements like translation invariance or the spectrum condition. The field is, in this case, the operator valued distribution $f\mapsto\Phi(f):=\pi(0\oplus f\oplus 0\oplus\cdots)$. We will think of a quantum field on a curved space–time in the same way, i.e., a quantum field can be defined by a state over the Borchers–Uhlmann algebra of test functions on the underlying space–time. A state is called quasifree if all the odd m-point functions vanish and the even m-point functions can be expressed by

$$\omega_m(f_1,\ldots,f_m)=\sum_P\prod_r\omega_2(f_{(r,1)},f_{(r,2)}), \tag{34}$$

where P denotes a partition of the set $\{1,\ldots,m\}$ into subsets which are pairings of points labeled by r.

For quantum fields on Minkowski space–time one usually requires the properties of Poincaré covariance, spectrum condition, existence of an invariant vacuum vector as well as local commutativity (for observable fields) to hold (see, e.g., Refs. 3 and 2). Due to the lack of an analog of the Poincaré group, only the last requirement can straightforwardly be generalized to curved space–

times. However, as will be seen in Sec. IV, there is a microlocal version of the spectrum condition which can be stated independently of the coordinate system and hence can be applied to quantum fields on curved space–times.

For a field $\Phi(\cdot)$ defined by a state ω over the Borchers–Uhlmann algebra we can associate a net of von Neumann algebras $\{\mathcal{A}(O)\}_{O\subset M}$ in the following way. Let as previously D be the dense domain $\pi(\mathcal{B})\Omega$ arising by the GNS construction from ω. For a subset $S\subset\mathcal{L}_D^+$ the weak commutant S_w' of S is defined to be the set of bounded operators A on $\mathcal{H}$ such that

$$\langle B^*\phi, A\psi\rangle = \langle A^*\phi, B\psi\rangle, \quad \forall \ B\in S, \ \ \phi,\psi\in D. \tag{35}$$

A net of von Neumann algebras $\{\mathcal{A}(O)\}_{O\subset M}$ is then defined by

$$\mathcal{A}(O) := (\{\Phi(f);\ \ \mathrm{supp}(f)\subset O\}_w')'. \tag{36}$$

The requirement of local commutativity may now be formulated by demanding that the von Neumann algebras associated with causally separated regions commute, i.e.,

$$\mathcal{A}(O_1)\subset\mathcal{A}(O)' \quad \text{if} \quad O_1\subset O^\perp.$$

This is a strong form of local commutativity which is to be seen as a selective constraint on the Hilbert-space representation π of the Borchers–Uhlmann algebra $\mathcal{B}$ induced by the state ω, and hence as a constraint on ω itself. It implies in particular spacelike commutativity of field operators, $[\Phi(f),\Phi(h)]=0$ whenever the supports of f and h are causally separated.

B. The Klein–Gordon field on curved space–times

Since the construction of free fields relies heavily on the presence of a Cauchy surface (time-zero formalism) we restrict our considerations of quantum fields on curved space–times to the globally hyperbolic case. The evolution of the free scalar field of mass m and with coupling κ on a globally hyperbolic space–time is described by the Klein–Gordon equation

$$P\phi := (\Box_g + m^2 + \kappa R)\phi = 0, \quad \phi\in C^\infty(M). \tag{37}$$

Here $\Box_g$ is the Laplace operator with respect to the metric and R is the scalar curvature of M. The operator P is a differential operator of second order acting on the smooth functions on M. It has unique advanced and retarded fundamental solutions (see Refs. 36 and 37) $E^\pm: C_0^\infty(M)\to C^\infty(M)$ satisfying

$$PE^\pm = E^\pm P = \mathrm{id} \quad \text{on} \quad C_0^\infty(M),$$

$$\mathrm{supp}(E^\pm f)\subset J^\pm(\mathrm{supp}(f)),$$

where $J^\pm(O)$ denotes the causal future/past of a set O, i.e., the set of points which can be reached by future/past directed causal curves emanating from O. The difference $E := E^+ - E^-$ is the so-called commutator function. It maps $C_0^\infty(M)$ onto the space of smooth solutions to the Klein–Gordon equation which have compactly supported restriction to all Cauchy surfaces. The map $E: C_0^\infty(M)\to C^\infty(M)$ is continuous and hence has a distributional kernel in $\mathcal{D}'(M\times M)$ which we also denote by E, i.e., $E(f,h)=\int_M f(Eh)$ where integration is taken with respect to the Lorentzian metric-volume form. The field algebra $\mathcal{F}$ of the Klein–Gordon field is defined to be the unital $*$-algebra generated by the symbols $\phi(f)$, $f\in C_0^\infty(M)$ and the relations

(1) $f\mapsto\phi(f)$ is complex linear,
(2) $\phi(f)^* = \phi(\overline{f})$,
(3) $\phi(Pf)=0$,
(4) $[\phi(f_1),\phi(f_2)] = \mathrm{i}E(f_1,f_2)$.

Clearly, each state ω over $\mathcal{F}$ with the further property that the $\omega(\phi(\cdot)\cdots\phi(\cdot))$ are distributions defines a state $\tilde{\omega}$ over the Borchers–Uhlmann algebra by

$$\tilde{\omega}(f_1\otimes\cdots\otimes f_m) := \omega(\phi(f_1)\cdots\phi(f_m)). \tag{38}$$

The corresponding quantum field $\Phi: C_0^\infty(M)\to\mathcal{L}_D^+$ satisfies the Klein–Gordon equation

$$\Phi(P\cdot)=0, \tag{39}$$

and the canonical commutation relations

$$[\Phi(f_1),\Phi(f_2)] = \mathrm{i}E(f_1,f_2)\mathbb{I}|_D. \tag{40}$$

Since the commutator function E vanishes for spacelike separation of the arguments the field satisfies the requirement of local commutativity, i.e., $[\Phi(f),\Phi(h)]=0$ if the supports of f and h are spacelike separated. For many states, among them the quasifree states, also the stronger requirement of local commutativity at the level of the net of von Neumann algebras $\{\mathcal{A}(O)\}_{O\subset M}$ in their GNS-representations described previously is fulfilled. In the following we call states over the Borchers–Uhlmann algebra arising in this way states for the Klein–Gordon field.

IV. THE MICROLOCAL SPECTRUM CONDITION

In the investigation of the Klein–Gordon field a crucial role is played by the so-called Hadamard states (see, e.g., Refs. 38–40). They are thought of as the appropriate counterpart of the vacuum in Minkowski space and are characterized by the short distance behavior of their two-point function. The investigation of such states is partially motivated by the result of Wald[29] that the expectation value of the energy momentum tensor $T_{\mu\nu}$ with respect to a Hadamard state can be made sense of in a satisfactory way. This is a very important feature of Hadamard states, since it is this expectation value that appears in the Einstein equations in the semiclassical theory of gravity coupled to the Klein–Gordon field. We will not give the original definition of Hadamard states here, since such states can as well be characterized by the wave front set of their two-point function. This was shown by Radzikowski[24,25] and relies heavily on the work of Duistermaat and Hörmander[41,42] on Fourier integral operators. We first would like to note that the wave front set of the commutator distribution E for the wave operator P on a globally hyperbolic space–time with metric g is given by

$$\begin{aligned}\mathrm{WF}(E)=\{&((x_1,-k_1),(x_2,k_2));(x_1,k_1)\sim(x_2,k_2)\\ &\text{and } g^{\mu\nu}(k_1)_\mu(k_1)_\nu=g^{\mu\nu}(k_2)_\mu(k_2)_\nu=0\},\end{aligned} \tag{41}$$

where $(x_1,k_1)\sim(x_2,k_2)$ means that there is a lightlike geodesic γ connecting x_1 and x_2 such that k_1 is coparallel to the tangent vector of the curve at x_1 and k_2 is the parallel transport of k_1 from x_1 to x_2. Radzikowski's result is that a quasifree state ω for the Klein–Gordon field is a Hadamard state if and only if the wave front set of its two-point function ω_2 is given by

$$\mathrm{WF}(\omega_2)=\{((x_1,-k_1),(x_2,k_2))\in\mathrm{WF}(E);(k_2)_0>0\}, \tag{42}$$

where $(k_2)_0>0$ is shorthand for "k_2 is future-pointing."

The microlocal characterization of Hadamard states has meanwhile led to a rich theory. In fact, it turned out that quasifree Hadamard states allow for a construction of Wick polynomials of field operators[30,32] and a perturbative construction of interacting fields on curved space–times.[31,43] It was shown in Ref. 44 that such states are locally quasiequivalent and therefore (at least locally) distinguish a single folium of states. A passive state for a free quantum field theory on a stationary space–time is always a Hadamard state (see Refs. 45 and 46 for the statement in its full generality). The Hadamard condition can also be formulated almost without change for arbitrary free

quantum fields. Radzikowski's result is known to hold also in these cases.[28] Adiabatic vacuum states satisfy a similar condition with the wave front set replaced by an appropriate Sobolev wave front set as shown in Ref. 47.

Motivated by the observations just mentioned, a microlocal spectrum condition (μSC) that applies to general quantum fields on curved space–times was introduced by Brunetti, Fredenhagen, and Köhler;[30] we shall now summarize its definition. We denote by $\mathcal{G}_k$ the set of all finite graphs with vertices $\{1,\ldots,k\}$ such that for every element $G\in\mathcal{G}_k$ all edges occur in both admissible directions. We write $s(e)$ and $r(e)$ for the source and the target of an edge, respectively. Following Ref. 30 we define an immersion of a graph $G\in\mathcal{G}_k$ into a space–time M an assignment of the vertices ν of G to points $x(\nu)$ in M, and of edges e of G to piecewise smooth curves $\gamma(e)$ in M with source $s(\gamma(e))=x(s(e))$ and range $r(\gamma(e))=x(r(e))$, together with a covariantly constant causal covector field k_e on γ such that

(1) If e^{-1} denotes the edge with opposite direction as e, then the corresponding curve $\gamma(e^{-1})$ is the inverse of $\gamma(e)$.
(2) For every edge e the covector field k_e is directed toward the future whenever $s(e)<r(e)$.
(3) $k_{e^{-1}}=-k_e$.

Definition 4.1 (μSC, Ref. 30)*: A state ω over the Borchers–Uhlmann algebra $\mathcal{B}$ is said to satisfy the microlocal spectrum condition iff its m-point functions $\omega_m\in\mathcal{D}'(M^m)$ satisfy*

$$\mathrm{WF}(\omega_m)\subset\{(x_1,k_1;\ldots;x_m,k_m)\in T^*M^m\setminus 0;\ \ \exists G\in\mathcal{G}_m$$

and an immersion (x,γ,k) of G in, such that

$$x_i=x(i)\quad \forall i=1,\ldots,m \quad and$$

$$k_i=-\sum_{e,\ s(e)=i} k_e(x_i)\}=\Gamma_m .$$

We note here that quasifree Hadamard states of the Klein–Gordon field satisfy the microlocal spectrum condition. For a motivation of this definition and further properties of states satisfying the μSC we refer the reader to Ref. 30. For later purposes we will need the following property of the sets Γ_m which is Lemma 4.2 in Ref. 30.

Proposition 4.2: The sets Γ_m are stable under addition, i.e., $\Gamma_m+\Gamma_m\subset\Gamma_m$. Moreover, if $(x,k)\in\Gamma_m$ then $(x,-k)\notin\Gamma_m$.

V. THE ANALYTIC MICROLOCAL SPECTRUM CONDITION AND THE REEH–SCHLIEDER PROPERTY

In the following we restrict our consideration to the case when M is a real analytic space–time, i.e., M is real analytic as a manifold and the metric g is analytic. Passing from the smooth to the analytic category it seems reasonable to require that the state satisfies a microlocal spectrum condition with the wave front set WF replaced by the analytic wave front set WF_A. (See Ref. 32 for a related concept.)

Definition 5.1 (aμSC)*: A state ω over the Borchers–Uhlmann algebra is said to satisfy the analytic microlocal spectrum condition* (aμSC) *iff its m-point functions satisfy*

$$\mathrm{WF}_A(\omega_m)\subset\Gamma_m ,$$

where the notations of Definition 4.1 are used.

For Wightman fields in Minkowski space–time the spectrum condition is equivalent to the requirement that the m-point functions are boundary values of functions which are analytic in the tube

$$T_m := \{(z_1,\ldots,z_m);\ \Im(z_{j+1}-z_j)\in V_+,\quad j=1,\ldots,m-1\}, \tag{43}$$

where V_+ is the forward lightcone.

Theorem 5.2: *Suppose that M is the n-dimensional Minkowski space–time ($n\geqslant 2$) and let ω be a state over the Borchers–Uhlmann algebra such that its m-point functions are boundary values in the sense of distributions of functions that are analytic in $T_m\cap Z$, where Z is a complex neighborhood of $(\mathbb{R}^n)^m\subset(\mathbb{C}^n)^m$. Then ω satisfies* aμSC.

Proof: Clearly, T_m is of the form $T_m=(\mathbb{R}^n)^m+i\mathcal{C}$, where the cone $\mathcal{C}$ is defined by $\mathcal{C}=\{(k_1,\ldots,k_m);\ k_{j+1}-k_j\in V_+\}$. The dual cone $\mathcal{C}^\circ$ can easily be calculated and the result is

$$\mathcal{C}^\circ=\left\{(k_1,\ldots,k_m);\ k_m,k_{m-1}+k_m,\ldots,\sum_{j=2}^m k_j\in\overline{V}_+,\quad \sum_{j=1}^m k_j=0\right\}. \tag{44}$$

Hence, by Corollary 2.9, the set $\mathrm{WF}_A(\omega_m)$ is contained in $(\mathbb{R}^n)^m\times\mathcal{C}^\circ$. The set

$$\left\{(x_1,k_1;\ldots;x_m,k_m);\ k_m,k_{m-1}+k_m,\ldots,\sum_{j=2}^m k_j\in\overline{V}_+,\quad \sum_{j=1}^m k_j=0\right\}$$

is contained in Γ_m (see, e.g., the proof of Theorem 4.6 in Ref. 30) which concludes the proof.□

This theorem applies to the vacuum state of Wightman fields in Minkowski space–time and, provided that the invariant domain of all field operators includes, e.g., the C^∞-vectors for the energy, it applies also to vector states which are analytic in the energy (in vacuum representation, see, e.g., Chap. 12 in Ref. 4); moreover, it applies also to states which satisfy the relativistic KMS condition proposed by Buchholz and Bros.[48,49] Quasifree states for the Klein–Gordon field on the de Sitter space–time that satisfy the weak spectral condition[50–52] can also be shown to satisfy aμSC.

Let as before $(\pi,\Omega,D,\mathcal{H})$ be the GNS-representation of the state ω and denote by Φ the corresponding quantum field. We will now show that a state that satisfies aμSC has the Reeh–Schlieder property, i.e., the set $\{\Phi(f_1)\cdots\Phi(f_n)\Omega;\ \mathrm{supp}(f_i)\subset O, m\in\mathbb{N}\}$ is total in $\mathcal{H}$ for each nonvoid open set $O\subset M$.

The main technical tool for proving this is a microlocal version of the *edge of the wedge* theorem (Theorem 8.5.6' in Ref. 33).

Proposition 5.3: Let M be a real analytic connected manifold and $u\in\mathcal{D}'(M)$ a distribution with the property that $\mathrm{WF}_A(u)\cap -\mathrm{WF}_A(u)=\varnothing$. Then the following conclusion holds for each nonvoid open subset $O\in M$:

$$u|_O=0\Rightarrow u=0.$$

Proof: For a closed subset $X\subset M$ the exterior normal set $N_e(X)\subset T^*M\setminus 0$ is defined to be the set of all (x,k) such that $x\in X$ and there is a real valued function $f\in C^2(M)$ with $\mathrm{d}f(x)=k\neq 0$ and $f(y)\leqslant f(x)$ for all $y\in X$. The normal set $N(X)$ is the union $N_e(X)\cup -N_e(X)$. Theorem 8.5.6' in Ref. 33 states that $N(\mathrm{supp}(u))\subset\mathrm{WF}_A(u)$ and since $N(\mathrm{supp}(u))=-N(\mathrm{supp}(u))$ the assumption implies that $N(\mathrm{supp}(u))=\varnothing$. Consequently, $N_e(\mathrm{supp}(u))=\varnothing$. Proposition 8.5.8 in Ref. 33 states that the projection of $N_e(X)$ in M is dense in ∂X. Therefore, $\partial(\mathrm{supp}(u))=\varnothing$. Since M is connected this implies that either $\mathrm{supp}(u)=\varnothing$ or $\mathrm{supp}(u)=M$. The latter is excluded by $u|_O=0$. □

Our main result is stated in the following theorem.

Theorem 5.4: *Let ω be a state over the Borchers–Uhlmann algebra on a real analytic space–time and suppose furthermore that ω satisfies* aμSC. *Denote by $(\pi,\Omega,D,\mathcal{H})$ its GNS-representation and by Φ the associated quantum field. Then the set*

$$\{\Omega\}\cup\{\Phi(f_1)\cdots\Phi(f_m)\Omega;\ \mathrm{supp}(f_i)\subset O,\quad m\in\mathbb{N}\}$$

is total in $\mathcal{H}$ for each nonvoid open set $O\subset M$.

Proof: We define a Hilbert space valued distribution $\psi_m \in \mathcal{D}'(M^m, \mathcal{H})$ by

$$\psi_m(f_1,\ldots,f_m) := \Phi(f_1)\cdots\Phi(f_m)\Omega. \tag{45}$$

Note that due to Proposition 2.6 a point $(x,k) \in T^*M^m \setminus 0$ is in $\mathrm{WF}_A(\psi_m)$ if and only if $(x, -k; x, k) \in \mathrm{WF}_A(w_{2m})$, where the distribution $w_{2m} \in \mathcal{D}'(M^{2m})$ is defined by

$$w_{2m}(f_1,\ldots,f_m,g_1,\ldots,g_m) := \omega_{2m}(f_m,\ldots,f_1,g_1,\ldots,g_m). \tag{46}$$

Proposition 4.2 implies that $\mathrm{WF}_A(w_{2m}) \cap -\mathrm{WF}_A(w_{2m}) = \varnothing$ and therefore $\mathrm{WF}_A(\psi_m) \cap -\mathrm{WF}_A(\psi_m) = \varnothing$.

Suppose now that $\phi \in \mathcal{H}$ is orthogonal to the set

$$\{\Omega\} \cup \{\Phi(f_1)\cdots\Phi(f_m)\Omega;\ \mathrm{supp}(f_i) \subset O, \quad m \in \mathbb{N}\}. \tag{47}$$

Then the distributions $v_m(\cdot) = \langle \phi, \psi_m(\cdot)\rangle \in \mathcal{D}'(M^m)$ vanish on O^m and satisfy $\mathrm{WF}_A(v_m) \cap -\mathrm{WF}_A(v_m) = \varnothing$. By Proposition 5.3 we conclude that $v_m = 0$ for all m. Therefore, ϕ is even orthogonal to the set

$$\{\Omega\} \cup \{\Phi(f_1)\cdots\Phi(f_m)\Omega;\ f_i \in C_0^\infty(M), \quad m \in \mathbb{N}\}, \tag{48}$$

which is total in $\mathcal{H}$. We conclude that $\phi = 0$ which proves the theorem. □

An immediate corollary is the Reeh–Schlieder property of the associated net of local algebras.

Corollary 5.5: Let the assumptions of Theorem 5.4 be fulfilled and denote by $\{\mathcal{A}(O)\}_{O \subset M}$ the associated local net of von Neumann algebras. Then $\mathcal{A}(O)\Omega$ is dense in $\mathcal{H}$ for each nonvoid open set O.

Remark 5.6: (a) Clearly, the conclusion of Theorem 5.4 also holds if we impose the weaker condition $\mathrm{WF}_A(\omega_{2m}) \cap -\mathrm{WF}_A(\omega_{2m}) = \varnothing$ on the state instead of the analytic microlocal spectrum condition. Our result is therefore insensitive to the precise form of analytic microlocal spectrum condition as long as an analog of Proposition 4.2 holds.

(b) The same method works for fields with values in an analytic vector bundle. Note that local commutativity is not an assumption of Theorem 5.4 and therefore it applies to fermionic fields as well.

(c) The existence of states fulfilling aμSC *on generic, real analytic, globally hyperbolic space–times remains an open problem, even for free field theories. See our comments at the end of this article on this point.*

VI. QUASIFREE STATES AND THE KLEIN–GORDON FIELD

As indicated in Sec. I the microlocal spectrum condition can be simplified for quasifree states of the Klein–Gordon field using microlocal analysis of Hilbert space valued distributions. This will allow us to give a rather simple proof of the fact that quasifree ground and KMS states for the Klein–Gordon field on (analytic) stationary spacetimes are (analytic) Hadamard states.

Proposition 6.1: Let M be a globally hyperbolic space–time and let ω be a quasifree state for the Klein–Gordon field on M. Let Φ and Ω be as in Sec. V and denote by ψ the Hilbert space valued distribution $\Phi(\cdot)\Omega$. Then the following statements are equivalent.

(1) ω satisfies μSC.

(2) $\mathrm{WF}(\psi) \subset \overline{V}_+$.

(3) $\mathrm{WF}(\psi) = N_+$.

(4) ω is a Hadamard state.

Here $\overline{V}_+$ denotes the set of future directed causal covectors (x,k) and N_+ is the set of future directed non-zero null-covectors.

Proof: We first show that (1)⇒(2). Suppose that $(x,k) \in \mathrm{WF}(\psi)$. Then by Proposition 2.2 we get $(x, -k; x, k) \in \mathrm{WF}(\omega_2)$. By μSC the covector (x,k) must be in $\overline{V}_+$. (2)⇒(3) is a simple consequence of the fact that ψ solves the Klein–Gordon equation and Proposition 2.3. The impli-

cation (4)⇒(1) is Proposition 4.3 in Ref. 30 and it remains to show (3)⇒(4). By Proposition 2.2 we conclude that if $(x_1,k_1;x_2,k_2)\in \mathrm{WF}(\omega_2)$ then $k_2\in \overline{V}_+$ and $k_1\in \overline{V}_-$. Therefore, $\mathrm{WF}(\tilde{\omega}_2)\cap \mathrm{WF}(\omega_2)=\varnothing$ with $\tilde{\omega}_2(f_1,f_2):=\omega_2(f_2,f_1)$. Note that $\tilde{\omega}_2-\omega_2$ is proportional to the commutator function E and consequently $\mathrm{WF}(\omega_2)\cup \mathrm{WF}(\tilde{\omega}_2)=\mathrm{WF}(E)$. This implies Eq. (42) and thus concludes the proof. □

Remark 6.2: It was shown in Ref. 31 that a vector Ω inducing a quasifree Hadamard state is contained in the microlocal domain of smoothness (introduced in the same article), which implies the conclusion (4)⇒(3). *Proposition 6.1 shows that the microlocal domain of smoothness coincides with the set of vectors inducing quasifree Hadamard states.*

A completely analogous statement holds in the analytic category.

Proposition 6.3: Let M be a globally hyperbolic analytic space–time and let ω be a quasifree state for the Klein–Gordon field on M. With the same notation as in Theorem 6.1 the following statements are equivalent.

(1) ω satisfies aμSC.

(2) $\mathrm{WF}_A(\psi)\subset \overline{V}_+$.

(3) $\mathrm{WF}_A(\psi)=N_+$.

(4) ω is an analytic Hadamard state, meaning that (42) is satisfied with WF *replaced by* WF_A.

Proof: Taking into account Propositions 2.6 and 2.7 the proof is identical to that of Proposition 6.1 with WF replaced by WF_A.

A space–time M with metric tensor g is called stationary if there exists a one-parameter group h_t of isometries of M with timelike orbits whose Killing vector fields are (by convention) future pointing. This one-parameter group can be understood as a group of time-translations and it is therefore interesting to investigate passive states with respect to this group action as states which are physically reasonable replacements for the vacuum. For example the Schwarzschild space–time is stationary and the Hartle–Hawking state for the Klein–Gordon field is a KMS state with respect to the group of time translations. Other examples are the Rindler wedge and wedge-like regions in the de Sitter space. We investigate in the following ground and KMS states for the Klein–Gordon field on a stationary space–time. Let us first fix some notation. The push-forward h_{t*} defined by $(h_{t*}f)(x):=f(h_{-t}x)$ acts on the space $C_0^\infty(M)$ and this action lifts uniquely to an action α_t on the Borchers–Uhlmann algebra $\mathcal{B}$ by *-automorphisms. A state ω over $\mathcal{B}$ is called ground state if the function $t\mapsto\omega(A\alpha_t B)$ is bounded for all $A,B\in\mathcal{B}$ and

$$\int_{-\infty}^{+\infty}\hat{f}(t)\,\omega(A\alpha_t(B))\,\mathrm{d}t=0, \tag{49}$$

holds for all $f\in C_0^\infty((-\infty,0))$. A state ω is called KMS state at inverse temperature $\beta>0$ if the function $t\to\omega(A\alpha_t B)$ is bounded for all $A,B\in\mathcal{B}$ and

$$\int_{-\infty}^{+\infty}\hat{f}(t)\,\omega(A\alpha_t(B))\,\mathrm{d}t=\int_{-\infty}^{+\infty}\hat{f}(t+\mathrm{i}\beta)\,\omega(\alpha_t(B)A)\,\mathrm{d}t, \tag{50}$$

for all $f\in C_0^\infty(\mathbb{R})$. Note that ground and KMS states are necessarily invariant, i.e. $\omega(\alpha_t(\cdot))=\omega(\cdot)$.

Theorem 6.4: *Let M be a globally hyperbolic stationary space–time and suppose that ω is a quasifree KMS- or ground-state for the Klein–Gordon field. Then ω satisfies the microlocal spectrum condition. If moreover M is real analytic (as a space–time) and the flow $\mathbb{R}\times M\to M$ induced by h_t is analytic, then ω satisfies the analytic microlocal spectrum condition.*

Proof: Let $(\pi,\Omega,\mathcal{H},D)$ be the GNS representation of ω. Let $\Phi(\cdot)$ be the associated field and define $\psi(\cdot):=\Phi(\cdot)\Omega$. Since ω is invariant there exists a strongly continuous one-parameter group $U(t)=e^{\mathrm{i}t\mathbf{H}}$ on $\mathcal{H}$, such that $U(t)\psi(\cdot)=\psi(h_t\cdot)$ and $U(t)\Omega=\Omega$. If ω is a β-KMS state it follows from the KMS condition that the vectors $\psi(f)$ are in the domain of $e^{-(\beta/2)\mathbf{H}}=U(\mathrm{i}\beta/2)$ for all $f\in C_0^\infty(M)$. If ω is a ground state this is even true for all $\beta>0$. Therefore, we may define the

distribution $G \in \mathcal{D}'((0,\beta/2)\times M,\mathcal{H})$ by $G(t,x)=U(\mathrm{i}t)\psi(x)$. We use a local coordinate system $(x_0,\ldots,x_{n-1})$ such that the vector field ∂_{x_0} generates locally the flow h_t. Then G satisfies the system of equations

$$(\partial_t^2+\partial_{x_0}^2)G=0, \tag{51}$$

$$(\mathrm{id}\otimes P)G=0. \tag{52}$$

This system is elliptic and therefore G is indeed a smooth function satisfying the conditions of Theorem 2.8. It follows that $\mathrm{WF}_A(\psi)$ is a subset of the set $\{(x,k)\in T^*M;k(\partial_{x_0}(x))>0\}$ in this coordinate system. Since ψ solves the Klein–Gordon equation $\mathrm{WF}(\psi)$ is confined to the forward light cone. If M is real analytic and the flow $\mathbb{R}\times M\to M$ induced by h_t is analytic we can choose the local coordinate system to be analytic and therefore $\mathrm{WF}_A(\psi)\subset\overline{V}_+$. □

The part of Theorem 6.4 stating that ground and KMS states on smooth stationary space–times are Hadamard states was shown before in Ref. 46, cf. also Ref. 45. The method we used in our proof is however rather different from the methods employed there. The advantage of our approach is that it applies to the analytic case without any changes.

As a simple consequence of Theorem 6.4 the Hartle–Hawking state on the Schwarzschild space–time is an analytic Hadamard state. On the de Sitter space–time the so-called Euclidian vacuum state (also called Bunch–Davies vacuum) is known to be a KMS state when restricted to certain stationary wedge-like regions (see, e.g., Refs. 53 and 54, and references therein). As a consequence this state satisfies the aμSC. One can also conclude this more directly from the fact that the two-point function of this state is the boundary value of a function holomorphic in a certain complex tuboid.[54]

Whereas the existence of Hadamard states for the Klein–Gordon field on an arbitrary globally hyperbolic space–time is well established a general construction of analytic Hadamard states seems to be a rather difficult task. In the literature there exist two methods of construction of Hadamard states that apply to generic space–time manifolds. The method used by Fulling *et al.*[45] takes advantage of the fact that any globally hyperbolic space–time can be deformed to a space–time that is static in the past of a given Cauchy surface and coincides with the original space–time in its future. Such a C^∞-deformation, however, destroys the analyticity of the metric and thus this method cannot be exploited for the construction of analytic Hadamard states. Another construction of Hadamard states is due to Junker (Ref. 55). His method relies heavily on the calculus of (smooth) pseudodifferential operators and we are so far not aware of a calculus that would allow it to carry over that method to the analytic case.

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Covariant Hamiltonian boundary conditions in General Relativity for spatially bounded space–time regions

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We investigate the covariant Hamiltonian symplectic structure of General Relativity for spatially bounded regions of space–time with a fixed time-flow vector. For existence of a well-defined Hamiltonian variational principle taking into account a spatial boundary, it is necessary to modify the standard Arnowitt–Deser–Misner Hamiltonian by adding a boundary term whose form depends on the spatial boundary conditions for the gravitational field. The most general mathematically allowed boundary conditions and corresponding boundary terms are shown to be determined by solving a certain equation obtained from the symplectic current pulled back to the hypersurface boundary of the space–time region. A main result is that we obtain a covariant derivation of Dirichlet, Neumann, and mixed type boundary conditions on the gravitational field at a fixed boundary hypersurface, together with the associated Hamiltonian boundary terms. As well, we establish uniqueness of these boundary conditions under certain assumptions motivated by the form of the symplectic current. Our analysis uses a Noether charge method which extends and unifies several results developed in recent literature for General Relativity. As an illustration of the method, we apply it to the Maxwell field equations to derive allowed boundary conditions and boundary terms for the existence of a well-defined Hamiltonian variational principle for an electromagnetic field in a fixed spatially bounded region of Minkowski space–time. [DOI: 10.1063/1.1505984]

I. INTRODUCTION

The mathematical structure of General Relativity as a Hamiltonian field theory is well-understood for asymptotically flat space–times. As first shown by Regge and Teitelboim,[1] with asymptotic falloff conditions on the metric, there is a modification of the standard Arnowitt–Deser–Misner (ADM) Hamiltonian[2] whose field equations obtained from the Hamiltonian variational principle yield a $3+1$ split of the Einstein equations. The ADM Hamiltonian itself yields the $3+1$ Einstein equations only if compact support variations of the metric are used in the variational principle. For metric variations satisfying asymptotic falloff conditions, the ADM Hamiltonian does not give a well-defined variational principle since its variation produces asymptotic boundary terms that do not vanish. However, the boundary terms can be canceled by the addition of a surface integral term at spatial infinity to the ADM Hamiltonian. The resulting Regge–Teitelboim Hamiltonian yields a well-defined variational principle for the Einstein equations with asymptotic falloff conditions on the metric. On solutions of the Einstein equations the Hamiltonian reduces to a surface integral expresssion over spatial infinity, which turns out to yield

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the physically important ADM definition of total energy, momentum, and angular momentum for asymptotically flat space–times. Various modern, covariant formulations of this Hamiltonian structure are known.[3–7]

A natural question to investigate is whether this Hamiltonian structure can be extended to spatially bounded regions of space–time. An important motivation is astrophysical applications where asymptotically flat boundary conditions are not appropriate, e.g., collapse to a black hole, mergers of binary stars, or collision of black holes. Another important application is for numerical solution methods of the Einstein equations. In these situations the spatial boundary is not an actual physical boundary in space–time, but rather is viewed as a mathematically defined timelike hypersurface whose boundary conditions effectively replace the dynamics of the gravitational field in the exterior region.

In this paper and a sequel,[8] we work out the covariant Hamiltonian structure of General Relativity for arbitrary spatially compact regions of space–time $\Sigma\times\mathbb{R}$ whose spacelike slices Σ prossess a closed two-surface boundary $\partial\Sigma$, with a fixed time-flow vector tangent to the timelike boundary hypersurface $\partial\Sigma\times\mathbb{R}$. Rather than start with given boundary conditions on the metric, we instead seek to determine both the most general surface integral term necessary to be added to the ADM Hamiltonian in covariant form together with the most general corresponding boundary conditions on the metric at $\partial\Sigma$ such that the modified Hamiltonian has well-defined variational derivatives. This would yield the most general mathematically allowed variational principle for the Einstein equations with spatial boundary conditions on the metric. To carry out the analysis we employ the covariant Hamiltonian formalism (referred to as the Noether charge method) developed in Refs. 4, 9, and 10.

The main results are that we find Dirichlet and Neumann type boundary conditions for the metric at a spatial boundary two-surface and obtain the associated Hamiltonian surface integrals. Under some natural assumptions motivated by the symplectic structure arising from the ADM Hamiltonian, the most general allowed boundary conditions are shown to be certain types of mixtures of the Dirichlet and Neumann ones. We also investigate the geometrical structure of the Dirichlet and Neumann covariant Hamiltonians. These each turn out to involve an underlying ''energy-momentum'' vector at each point in the tangent space of the space–time at the two-surface. In the Dirichlet case, this vector depends only on the extrinsic geometry of the spatial boundary two-surface. Most strikingly, when the vector is decomposed into tangential and normal parts with respect to the two-surface, the normal part yields a direction in which the two-surface has zero expansion in the spacetime.

In Sec. II we first apply the Noether charge formalism to investigate, as an illustrative example, the covariant Hamiltonian structure of the free Maxwell equations on spatially compact regions of Minkowski space–time. We show that this analysis leads to Dirichlet and Neumann type boundary conditions on the electromagnetic field, corresponding to conductor and insulator type boundaries, as well as mixed type boundary conditions which are linear combinations of the Dirichlet and Neumann ones. We also investigate more general boundary conditions which give rise to a well-defined Hamiltonian variational principle for the Maxwell equations, and we obtain a uniqueness result for the mixed and pure type Dirichlet and Neumann boundary conditions under some assumptions. The associated Dirichlet and Neumann Hamiltonians are shown to reduce to expressions for the total energy of the electromagnetic field, including contributions from surface electric charge and current due to the boundary conditions.

In Sec. III we carry out the corresponding analysis of the covariant Hamiltonian structure of General Relativity for arbitrary spatially compact regions of space–time with a closed two-surface boundary, without matter fields. We make some concluding remarks in Sec. IV. In an Appendix we develop the Noether charge method for general Lagrangian field theories with a time symmetry. This approach extends and unifies some aspects of the covariant Hamiltonian formalism introduced in recent literature.[4,9–11] (Throughout we use the notation and conventions of Ref. 12.)

Inclusion of matter fields and analysis of the geometrical properties of the resulting Dirichlet and Neumann Hamiltonians for General Relativity will be investigated in Ref. 8. It is also left to that paper to discuss the relation between these Hamiltonians and the Regge–Teitelboim Hamil-

tonian in the case when the two-surface boundary is taken in a limit to be spatial infinity in an asymptotically flat space–time.

II. ELECTRODYNAMICS

To illustrate our basic approach and the covariant Hamiltonian (Noether charge) formalism, we consider the free Maxwell field theory in four-dimensional Minkowski space–time $(\mathbb{R}^4, \eta_{ab})$.

We use the standard electromagnetic field Lagrangian, where the field variable is the electromagnetic potential one-form A_a, with the field strength two-form defined as $F_{ab}=\partial_{[a}A_{b]}$. The Lagrangian four-form for the field A_a is given by

$$L_{abcd}(A)=\tfrac{1}{2}\epsilon_{abcd}F_{mn}F^{mn}=3F_{[ab}{*F}_{cd]}, \tag{2.1}$$

where ${*F}_{ab}=\epsilon_{ab}{}^{cd}F_{cd}$ is the dual field strength two-form defined using the volume form ϵ_{abcd}. A variation of this Lagrangian gives

$$\delta L_{abcd}(A)=\partial_{[a}\Theta_{bcd]}(A,\delta A)+6\,\delta A_{[a}(\partial_b {*F}_{cd]}), \tag{2.2}$$

where

$$\Theta_{bcd}(A,\delta A)=6\,\delta A_{[b}{*F}_{cd]} \tag{2.3}$$

defines the symplectic potential three-form. From Eq. (2.2), one obtains the field equations

$$\mathcal{E}_{bcd}(A)=6\,\partial_{[b}{*F}_{cd]}=0, \tag{2.4}$$

or equivalently, after contraction with the volume form,

$$\partial^a F_{ab}=\partial^a\partial_{[a}A_{b]}=0 \tag{2.5}$$

which is the source-free Maxwell equations for A_a.

Let $\xi^a=(\partial/\partial t)^a$ be a timelike isometry of the Minkowski metric, with unit normalization $\xi^a\xi^b\eta_{ab}=-1$, and let Σ be a region contained in a spacelike hyperplane $t=0$ orthogonal to ξ^a with the boundary of the region being a closed two-surface $\partial\Sigma$. Denote the unit outward spacelike normal to $\partial\Sigma$ in Σ by s^a, and denote the metric and volume form on $\partial\Sigma$ by $\sigma_{ab}=\eta_{ab}-s_a s_b+\xi_a\xi_b$ and $\epsilon_{ab}=\epsilon_{abcd}s^c\xi^d$. Let Σ_t and $\partial\Sigma_t$ be the images of Σ and $\partial\Sigma$ under the one-parameter diffeomorphism generated by ξ^a on Minkowski space–time. Denote the metric compatible derivative operator on $\partial\Sigma$ by $\mathcal{D}_a$. Let

$$\mathcal{L}_\xi A_a=\xi^e\partial_e A_a+A_e\partial_a\xi^e=2\,\xi^e\partial_{[e}A_{a]}+\partial_a(\xi^e A_e), \tag{2.6}$$

which is the Lie derivative of A_a with respect to ξ^e.

The Noether current three-form associated with ξ^a is given by

$$J_{abc}(\xi,A)=\Theta_{abc}(A,\mathcal{L}_\xi A)+4\,\xi^d L_{abcd}(A)=6{*F}_{[bc}\mathcal{L}_\xi A_{a]}+12\xi^d F_{[ab}{*F}_{cd]}, \tag{2.7}$$

which simplifies to

$$J_{abc}(\xi,A)=6\,\partial_{[a}({*F}_{bc]}\xi^d A_{d)})+2\,\xi^e\epsilon_{abcd}(\delta^d_e F_{mn}F^{mn}-4F_{en}F^{dn})-\xi^e A_e\mathcal{E}_{abc}(A) \tag{2.8}$$

after use of Eqs. (2.4) and (2.6). Hence, one obtains the Noether current on solutions A_a,

$$J_{abc}(\xi,A)=6\,\partial_{[a}({*F}_{bc]}\xi^d A_{d)})+2\,\xi^e\epsilon_{abcd}(\delta^d_e F_{mn}F^{mn}-4F_{en}F^{dn}). \tag{2.9}$$

(Note, one easily sees that this three-form $J_{abc}(\xi,A)$ is closed but is not exact, i.e., there does not exist a Noether current potential $Q_{bc}(\xi,A)$ satisfying $J_{abc}(\xi,A)=3\partial_{[a}Q_{bc]}(\xi,A)$.) Correspondingly, the Noether charge on solutions A_a is given by

$$Q_\Sigma(\xi)=\int_\Sigma J_{abc}(\xi;A)=\int_\Sigma \epsilon_{abcd}\xi^e(-8F_{en}F^{dn}+2\,\delta^d_e F_{mn}F^{mn})+\oint_{\partial\Sigma}2{*}F_{bc}\xi^d A_d\,. \quad (2.10)$$

This expression simplifies in terms of the electromagnetic stress-energy tensor defined by

$$T_e{}^d(F)=2F_{en}F^{dn}-\tfrac{1}{2}\delta_e{}^d F_{mn}F^{mn}. \quad (2.11)$$

Thus,

$$\tfrac{1}{4}\Omega_\Sigma(\xi)=\int_\Sigma \xi^e\xi^d T_{de}(F)\mathrm{d}^3x+\oint_{\partial\Sigma}\xi^a A_a\xi^d s^e F_{de}\mathrm{d}S, \quad (2.12)$$

where d^3x and $\mathrm{d}S$ denote the coordinate volume elements on Σ and $\partial\Sigma$ obtained from the volume forms $\epsilon_{abcd}\xi^d$ and ϵ_{bc}, respectively.

A. Covariant Hamiltonian formulation

The symplectic current, defined by the antisymmetrized variation of $\Theta_{bcd}(A,\delta A)$, is given by the three-form

$$\tfrac{1}{6}\omega_{bcd}(\delta_1A,\delta_2A)=\delta_1A_{[b}\delta_2{*}F_{cd]}-\delta_2A_{[b}\delta_1{*}F_{cd]}\,. \quad (2.13)$$

Then the presymplectic form on Σ is given by

$$\Omega_\Sigma(\delta_1A,\delta_2A)=\int_\Sigma \omega_{bcd}(\delta_1A,\delta_2A). \quad (2.14)$$

A Hamiltonian conjugate to ξ on Σ is a function $H_\Sigma(\xi;A)=\int_\Sigma \mathcal{H}_{abc}(\xi;A)$ for some locally constructed three-form $\mathcal{H}_{abc}(\xi;A)$ such that

$$\delta H_\Sigma(\xi;A)\equiv H'_\Sigma(\xi;A,\delta A)=\Omega_\Sigma(\delta A,\mathcal{L}_\xi A) \quad (2.15)$$

for arbitrary variations δA_a away from solutions A_a.

From the expression (2.7) for the Noether current, the presymplectic form yields

$$\Omega_\Sigma(\delta A,\mathcal{L}_\xi A)=\int_\Sigma \delta J_{abc}(\xi,A)+4\xi^d\delta A_{[d}\mathcal{E}_{abc]}(A)-\oint_{\partial\Sigma}\xi^c\Theta_{abc}(A,\delta A). \quad (2.16)$$

Hence, for compact support variations δA_a away from solutions A_a, the Noether current gives a Hamiltonian (2.15) with $\mathcal{H}_{abc}(\xi;A)=J_{abc}(\xi,A)$, up to an inessential boundary term. The simplified expression (2.8) for $J_{abc}(\xi,A)$ thereby yields the Hamiltonian

$$H(\xi;A)=4\int_\Sigma \xi^e\xi^d(T_{de}(F)+A_e\partial^cF_{cd})\mathrm{d}^3x. \quad (2.17)$$

On solutions A_a, this Hamiltonian is equal to the total electromagnetic field energy on Σ, $H(\xi;A)=4\int_\Sigma \xi^e\xi^d T_{de}(F)\mathrm{d}^3x$.

To define a Hamiltonian (2.15) for variations δA_a without compact support, it follows that the term $\xi^c\Theta_{abc}(A,\delta A)$ in Eq. (2.16) needs to be a total variation at the boundary $\partial\Sigma$, i.e. there must exist a locally constructed three-form $\tilde{B}_{abc}(A)$ such that one has

$$\xi^c\Theta_{abc}(A,\delta A)|_{\partial\Sigma}=(\xi^c\delta\tilde{B}_{abc}(A)+\partial_{[a}\alpha_{b]}(\xi;A,\delta A))|_{\partial\Sigma}\,, \quad (2.18)$$

where $\alpha_b(\xi;A,\delta A)$ is a locally constructed one-form. This equation holds if and only if, by taking an antisymmetrized variation,[10] one has

$$\epsilon^{bc}\xi^a\omega_{abc}(\delta_1A,\delta_2A)|_{\partial\Sigma}=\mathcal{D}_c\tilde{\beta}^c(\xi;\delta_1A,\delta_2A)|_{\partial\Sigma}, \tag{2.19}$$

where

$$\tilde{\beta}^c(\xi;\delta_1A,\delta_2A)=\epsilon^{cb}\delta_1\alpha_b(\xi;A,\delta_2A)-\epsilon^{cb}\delta_2\alpha_b(\xi;A,\delta_1A) \tag{2.20}$$

is a locally constructed vector, in $T(\partial\Sigma)$, which is skew bilinear in δ_1A, δ_2A. The term involving the symplectic current is given by

$$\epsilon^{bc}\xi^a\omega_{abc}(\delta_1A,\delta_2A)=8s^ch^{de}(\delta_1A_e\delta_2F_{cd}-\delta_2A_e\delta_1F_{cd}) \tag{2.21}$$

with $h_{ab}=\eta_{ab}-s_as_b=\sigma_{ab}-\xi_a\xi_b$. Given a solution of Eq. (2.19), one can then determine $\tilde{B}_{abc}(A)$ from Eq. (2.18) by

$$\epsilon^{ab}\xi^c\tilde{B}_{abc}(A)=\epsilon^{ab}(\xi^c\Theta_{abc}(A,\delta A)-\partial_a\alpha_b(\xi;A,\delta A))=8s^ch^{de}F_{cd}\delta A_e-\mathcal{D}_a\tilde{\alpha}^a(\xi;A,\delta A), \tag{2.22}$$

where

$$\tilde{\alpha}^a(\xi;A,\delta A)=\epsilon^{ab}\alpha_b(\xi;A,\delta A). \tag{2.23}$$

This leads to the following main result.

Proposition 2.1: A Hamiltonian conjugate to ξ^a on Σ exists for variations δA_a with support on $\partial\Sigma$ if and only if

$$8h^{bc}s^a(\delta_1A_b\partial_{[a}\delta_2A_{c]}-\delta_2A_b\partial_{[a}\delta_1A_{c]})|_{\partial\Sigma}=\mathcal{D}_c\tilde{\beta}^c(\xi;\delta_1A,\delta_2A) \tag{2.24}$$

for some locally constructed vector $\tilde{\beta}_a(\xi,\delta_1A,\delta_2A)$, in $T(\partial\Sigma)$, which is skew bilinear in δ_1A, δ_2A. The solutions of Eq. (2.24) of the form $\delta\mathcal{F}_a(A)|_{\partial\Sigma}=0$ give the allowed boundary conditions $\mathcal{F}_a(A)|_{\partial\Sigma}$ for a Hamiltonian formulation of the Maxwell equations in the local space–time region Σ_t, $t\geqslant 0$. For each boundary condition, there is a corresponding Hamiltonian given by the Noether charge plus a boundary term

$$H_\Sigma(\xi;A)=\int_\Sigma J_{abc}(\xi,A)-\oint_{\partial\Sigma}\xi^a\tilde{B}_{abc}(A)\equiv H(\xi;A)+H_B(\xi;A), \tag{2.25}$$

with

$$H(\xi;A)=4\int_\Sigma\xi^e\xi^d(T_{de}(F)+A_e\partial^cF_{cd})\mathrm{d}^3x, \tag{2.26}$$

$$H_B(\xi;A)=\oint_{\partial\Sigma}\xi^a(4A_a\xi^ds^eF_{de}-\tfrac{1}{2}\tilde{B}_a(A))\mathrm{d}S, \tag{2.27}$$

where $\tilde{B}_a(A)=\epsilon^{bc}\tilde{B}_{abc}(A)$ is determined from

$$(\xi^a\tilde{B}_a(A)-8s^ch^{de}F_{cd}\delta A_e)|_{\partial\Sigma}=\mathcal{D}_a\tilde{\alpha}^a(\xi;A,\delta A)|_{\partial\Sigma} \tag{2.28}$$

with $\tilde{\alpha}^a(\xi;A,\delta A)$ given by Eqs. (2.20) and (2.23). Note, $\tilde{B}_a(A)$ is unique up to addition of an arbitrary covector function of the fixed boundary data $\mathcal{F}_a(A)$.

The results in Proposition 2.1 take a more familiar form when expressed in terms of the electric and magnetic fields on Σ defined by $E_a=2\xi^bF_{ab}$, $B_a=\xi^b{*}F_{ab}$, which are vectors in $T(\Sigma)$ (i.e., $\xi^aE_a=\xi^aB_a=0$). A convenient notation now is to write vectors in $T(\Sigma)$ using an

overarrow, and for tensors on M, to denote tangential and normal components with respect to Σ by subscripts $\|$ and $\perp$, and denote components orthogonal to Σ_t by a subscript 0. Then we have

$$\vec{E} = \vec{\partial} A_0 - \partial_0 \vec{A}, \quad \vec{B} = \vec{\partial} \times \vec{A}. \tag{2.29}$$

In this notation, the presymplectic form (2.14) and the Hamiltonian (2.25) reduce to the expressions

$$\begin{aligned} \tfrac{1}{4}\Omega_\Sigma(\delta_1 A, \delta_2 A) &= \int_\Sigma (\delta_2 \vec{A} \cdot \delta_1 \vec{E} - \delta_1 \vec{A} \cdot \delta_2 \vec{E}) \mathrm{d}^3 x \\ &= \int_\Sigma (\delta_1 \vec{A} \cdot (\partial_0 \delta_2 \vec{A} - \vec{\partial} \delta_2 A_0) - \delta_2 \vec{A} \cdot (\partial_0 \delta_1 \vec{A} - \vec{\partial} \delta_1 A_0)) \mathrm{d}^3 x \end{aligned} \tag{2.30}$$

and

$$\tfrac{1}{2} H_\Sigma(\xi; A) = \int_\Sigma \tfrac{1}{2}(\vec{E}^2 + \vec{B}^2) + A_0 \vec{\partial} \cdot \vec{E}_\perp \mathrm{d}^3 x - \oint_{\partial\Sigma} A_0 E_\perp + \tfrac{1}{4} \tilde{B}_0(A) \mathrm{d}S. \tag{2.31}$$

Note that the Hamiltonian field equations obtained from $H_\Sigma(\xi; A)$ are given by the variational principle

$$H'_\Sigma(\xi; A, \delta A) = \Omega_\Sigma(\delta A, \mathcal{L}_\xi A) \tag{2.32}$$

for arbitrary variations $\delta A_a|_\Sigma$. These field equations split into dynamical equations and constraint equations, corresponding to a decomposition of A_a into dynamical and nondynamical components, respectively, $\vec{A}$ and A_0, determined by[4] the degeneracy of the presymplectic form (2.30). In particular, this yields the Gauss-law constraint equation

$$\vec{\partial} \cdot \vec{E} = \Delta A_0 - \partial_0 \vec{\partial} \cdot \vec{A} = 0 \tag{2.33}$$

obtained from $H'_\Sigma(\xi; A, \delta A_0) = 0$ through variation of A_0, and the dynamical Maxwell evolution equation

$$\partial_0 \vec{E} - \vec{\partial} \times \vec{B} = (-\partial_0^2 + \Delta)\vec{A} + \vec{\partial}(\partial_0 A_0 - \vec{\partial} \cdot \vec{A}) = 0 \tag{2.34}$$

obtained from $H'_\Sigma(\xi; A, \delta \vec{A}) = \Omega_\Sigma(\delta \vec{A}, \mathcal{L}_\xi A)$ through variation of $\vec{A}$, where $\Delta = \vec{\partial} \cdot \vec{\partial}$ is the Laplacian on Σ. Thus, the Noether charge (covariant Hamiltonian) formalism here is equivalent to the standard canonical formulation[12] of the Maxwell equations.

B. Dirichlet and Neumann boundary conditions

Two immediate solutions of the determining equation (2.24) with $\tilde{\beta}^a = 0$ are boundary conditions associated with fixing components of A_a or $F_{bc} = \partial_{[b} A_{c]}$ at $\partial\Sigma_t$ for $t \geqslant 0$.

Consider

$$\text{(D)} \quad \sigma_b{}^a \delta A_a|_{\partial\Sigma_t} = 0, \quad \xi^a \delta A_a|_{\partial\Sigma_t} = 0, \quad t \geqslant 0, \tag{2.35}$$

or equivalently $\delta \vec{A}_\| = \delta A_0 = 0$, for $t \geqslant 0$, called Dirichlet boundary conditions, i.e.,

$$\mathcal{F}^{\mathrm{D}}_a(A) = h_a{}^b A_b; \tag{2.36}$$

$$\text{(N)} \quad \sigma_b{}^a s^c \delta F_{ac}|_{\partial\Sigma_t} = 0, \ \ s^a \xi^c \delta F_{ac}|_{\partial\Sigma_t} = 0, \quad t \geqslant 0, \tag{2.37}$$

or equivalently $\vec{\partial}_\perp \times \delta\vec{A}_\parallel - \vec{\partial}_\parallel \times \delta\vec{A}_\perp = \vec{\partial}_\perp \delta A_0 - \partial_0 \delta\vec{A}_\perp = 0$, for $t \geqslant 0$, called Neumann boundary conditions, i.e.,

$$\mathcal{F}^{\mathrm{N}}_a(A) = h_a{}^b s^c F_{bc}\,. \tag{2.38}$$

Theorem 2.2: *For the boundary conditions* (D) *or* (N), *a Hamiltonian conjugate to* ξ^a *on* Σ, *evaluated on solutions* A_a, *is given by*

$$\tfrac{1}{2} H^{\mathrm{D}}(\xi;A) = 2\int_\Sigma \epsilon_{dabc}(2\xi^e F_{en}F^{dn} - \tfrac{1}{2}\xi^d F_{mn}F^{mn}) + 2\oint_{\partial\Sigma} \epsilon_{bc}\xi^a A_a \xi^d s^e F_{de} \tag{2.39}$$

$$= \tfrac{1}{2}\int_\Sigma \vec{E}^2 + \vec{B}^2 \mathrm{d}^3x - \oint_{\partial\Sigma} A_0 E_\perp \mathrm{d}S, \tag{2.40}$$

$$\tfrac{1}{2} H^{\mathrm{N}}(\xi;A) = 2\int_\Sigma \epsilon_{dabc}(2\xi^e F_{en}F^{dn} - \tfrac{1}{2}\xi^d F_{mn}F^{mn}) + 2\oint_{\partial\Sigma} \epsilon_{bc}\sigma^{bd} A_b s^e F_{de} \tag{2.41}$$

$$= \tfrac{1}{2}\int_\Sigma \vec{E}^2 + \vec{B}^2 \mathrm{d}^3x - \oint_{\partial\Sigma} (\vec{A}\times\vec{B})_\perp \mathrm{d}S. \tag{2.42}$$

Proof: For (D), one has

$$\epsilon^{bc}\xi^a \Theta_{abc}(A, \mathcal{L}_\xi A) = 6\epsilon^{bc}\xi^a \delta A_{[a} * F_{bc]} = 8(\xi^a \delta A_a \xi^d s^e F_{de} - \sigma^{ad}\delta A_a s^e F_{de}) = 0 \tag{2.43}$$

and hence $\tilde{B}_{abc}(A) = 0$, so thus $\xi^a \tilde{B}_a(A) = 0$. For (N), one has

$$\begin{aligned}\epsilon^{bc}\xi^a \Theta_{abc}(A, \mathcal{L}_\xi A) &= 6\epsilon^{bc}\xi^a(\delta A_{[a} * F_{bc]} = 6\epsilon^{bc}\xi^a(\delta(A_{[a} * F_{bc]}) - A_{[a}\delta * F_{bc]}) \\ &= \delta(6\epsilon^{bc}\xi^a A_{[a} * F_{bc]}) + 8(-\xi^a A_a \xi^d s^e \delta F_{de} + A_a \sigma^{ad} s^e \delta F_{de}) \\ &= \delta(\epsilon^{bc}\xi^a \tilde{B}_{abc})\end{aligned} \tag{2.44}$$

with $\tilde{B}_{abc}(A) = 6A_{[a} * F_{bc]}$. Thus,

$$\xi^a \tilde{B}_a(A) = 6\epsilon^{bc}\xi^a A_{[a} * F_{bc]} = 8 s_d A_e F^{de}. \tag{2.45}$$

□

Note that for both boundary conditions (D) and (N), the surface integral terms in the Hamiltonian take the form

$$H_B(\xi;A) = 4\oint_{\partial\Sigma} \xi^a P_a(A)\mathrm{d}S, \tag{2.46}$$

where

$$P^{\mathrm{D}}_a(A) = A_a \xi^b s^c F_{bc}\,, \tag{2.47}$$

$$P^{\mathrm{N}}_a(A) = -\xi_a s^d \sigma^{bc} A_b F_{cd}\,. \tag{2.48}$$

There is simple physical interpretation of the (D) and (N) boundary conditions: (D) involves fixing A_0 and $\vec{A}_\parallel$ at $\partial\Sigma_t$ for $t \geqslant 0$, which means

$$\vec{E}_\parallel = \vec{\partial}_\parallel A_0 - \partial_0 \vec{A}_\parallel\,, \quad \vec{B}_\perp = \vec{\partial}_\parallel \times \vec{A}_\parallel \tag{2.49}$$

are specified data at the boundary surface (analogous to a conductor) as a function of time. Note, consequently, $\vec{E}_\perp$ and $\vec{B}_\parallel$ are left free by the boundary condition (D) and therefore are induced data for solutions A_0, $\vec{A}$ of the Hamiltonian field equations; (N) reverses the role of the induced and fixed data at the boundary surface, so now $\vec{E}_\perp$ and $\vec{B}_\parallel$ are specified as a function of time (analogous to an insulator), while the induced data for solutions A_0, $\vec{A}$ of the Hamiltonian field equations are $\vec{E}_\parallel$ and $\vec{B}_\perp$. Note the fixed data here are gauge-equivalent to specifying the normal derivative of A_0 and $\vec{A}_\parallel$ at $\partial\Sigma_t$ in Σ_t for $t\geqslant 0$,

$$\vec{E}_\perp = \vec{\partial}_\perp(A_0 - \partial_0\chi), \quad \vec{B}_\parallel = \vec{\partial}_\perp \times (\vec{A}_\parallel - \vec{\partial}_\parallel \chi), \tag{2.50}$$

where χ is given by $\vec{\partial}_\perp \chi = \vec{A}_\perp$.

Moreover, the Hamiltonians (2.40) and (2.42) on solutions A_0, $\vec{A}$ have the interpretation as expressions for the total energy of the electromagnetic fields, with the surface integral parts representing the energy contribution[13] from an effective (fictitious) surface charge density in the case (D), and effective (fictitious) surface current density in the case (N), associated with the specified data at the boundary surface. In particular, effective surface charges and currents arise, respectively, when $\vec{E}_\perp$ or $\vec{A}_\parallel$ are left free[13] on the boundary surface.

We remark that similar boundary terms arise in the asymptotic case when the boundary surface is taken to be a two-sphere at spatial infinity on Σ (see Ref. 14).

C. Determination of allowed boundary conditions

The symplectic current component $\epsilon^{bc}\xi^a\omega_{abc}(\delta_1 A, \delta_2 A)$ involves only the field variations $h_a{}^b\delta A_b$, $h_a{}^b s^c \partial_{[b}\delta A_{c]}$. We refer to the components $\sigma_b{}^c A_c$, $\xi^c A_c$, $\sigma_b{}^c s^a F_{ac}$, $\xi^c s^a F_{ac}$, or equivalently $\vec{A}_\parallel$, A_0, $\vec{B}_\parallel$, $\vec{E}_\perp$, as *symplectic boundary data* at $\partial\Sigma$. Hence, in solving the determining equation (2.24) for the allowed boundary conditions on A_a, it is then natural to restrict attention to boundary conditions involving only this data. (Some remarks on more general boundary conditions are made at the end of this section.) To proceed, we suppose that the possible boundary conditions are linear, homogeneous functions of the symplectic boundary data, with coefficients locally constructed out of the geometrical quantities ξ^a, s^a, σ_{bc}, ϵ_{bc} at the boundary surface. We call this type of boundary condition a *symplectic* boundary condition.

Theorem 2.3: *The most general allowed symplectic boundary conditions*

$$\mathcal{F}_b(h_c{}^d A_d, h_c{}^d s^e F_{de}; \xi^c, s^c, \sigma_{de}, \epsilon_{de}) \tag{2.51}$$

for existence of a Hamiltonian conjugate to ξ^a on Σ are given by

$$\mathcal{F}_b = b_0\sigma_b{}^c A_c + a_0\sigma_b{}^c s^a F_{ac} + b_1\xi_b\xi^c A_c + a_1\xi_b\xi^c s^a F_{ca}, \tag{2.52}$$

or equivalently,

$$\sigma_b{}^c(b_0\delta A_c + a_0 s^a \delta F_{ac})|_{\partial\Sigma_t} = 0, \quad t\geqslant 0, \tag{2.53}$$

$$\xi^c(b_1\delta A_c + a_1 s^a \delta F_{ac})|_{\partial\Sigma_t} = 0, \quad t\geqslant 0 \tag{2.54}$$

for any constants a_0, b_0 (not both zero), a_1, b_1 (not both zero).

Proof: First, we show that $\tilde{\beta}^a = 0$ without loss of generality in the determining equation (2.24) for boundary conditions of the form (2.51). Note that the left-hand side of Eq. (2.24) is algebraic in δA_a, $\delta F_{ab} = \partial_{[a}\delta A_{b]}$. Since the right-hand side necessarily involves at least one derivative on δA_a, we must have

$$\tilde{\beta}^a = \delta_1 A_b \delta_2 A_c \beta^{abc} \tag{2.55}$$

for some tensor

$$\beta^{abc} = \sigma_e{}^a \beta^{e[bc]}. \tag{2.56}$$

We substitute expression (2.55) into Eq. (2.24) and collect all terms that do not involve just the symplectic boundary data, namely $s^c A_c$, $\xi^c \sigma_d{}^a F_{ac}$, $\sigma_b{}^c \sigma_d{}^a F_{ac}$, and $\partial_{(a} A_{b)}$. The coefficients of these terms yield algebraic equations

$$s_c \beta^{(ab)c} = 0, \quad s_c \beta^{[ab]c} = 0, \quad s^{[d} \beta^{ab]c} = 0. \tag{2.57}$$

Then, since β^{abc} has the form (2.56), we find that the solution of the equations in (2.57) is

$$\beta^{abc} = 0 \tag{2.58}$$

and so $\tilde{\beta}^a = 0$.

Hence, the determining equation (2.24) reduces to

$$h^{bc} s^a (\delta_1 A_b \partial_{[a} \delta_2 A_{c]} - \delta_1 A_b \partial_{[a} \partial_1 A_{c]})|_{\partial\Sigma} = 0, \tag{2.59}$$

which we are now free to solve as a purely algebraic equation in terms of the variables δA_b and $\delta F_{ac} = \partial_{[a} \delta A_{c]}$, i.e.,

$$h^{bc} s^a (\delta_1 A_b \delta_2 F_{ac} - \delta_1 A_b \delta_2 F_{ac}) = 0. \tag{2.60}$$

It is straightforward to show from the form of Eq. (2.60) that the only solution which is linear, homogeneous in the previous variables is given by

$$\Pi_{1b}{}^c \delta A_c = \Pi_{2b}{}^c s^a \delta F_{ac}, \tag{2.61}$$

where $\Pi_1{}^{bc}$ and $\Pi_2{}^{bc}$ are some symmetric tensors orthogonal to s^a, such that Eq. (2.61) can be solved for either $\xi^b \delta A_b$ or $\xi^b s^a \delta F_{ab}$, and either $\sigma_c{}^b \delta A_b$ or $\sigma_c{}^b s^a \delta F_{ab}$. Since we require the coefficients in the boundary conditions under consideration to be locally constructed out of ξ^a, s^a, σ_{bc}, ϵ_{bc}, we see that

$$\Pi_1{}^{bc} = b_0 \sigma^{bc} + b_1 \xi^b \xi^c, \quad \Pi_2{}^{bc} = a_0 \sigma^{bc} + a_1 \xi^b \xi^c, \tag{2.62}$$

for some constants a_0, a_1, b_0, b_1 with $a_0 \neq 0$ or $b_0 \neq 0$, and $a_1 \neq 0$ or $b_1 \neq 0$. This yields the general solution (2.53) and (2.54) given in the Theorem. □

The boundary conditions given by Theorem 2.3 comprise the following separate types: (i) for $a_0 = a_1 = 0$ or $b_0 = b_1 = 0$, one obtains, respectively, Dirichlet (2.35) and Neumann (2.37) boundary conditions; (ii) for $b_0 = 0 (a_0 \neq 0)$, $b_1 \neq 0$, the boundary conditions yield a one-parameter $a_1/b_1 \equiv c_1$ family of the form

$$\sigma_b{}^c s^a \delta F_{ac}|_{\partial\Sigma_t} = 0, \quad \xi^c \delta A_c|_{\partial\Sigma_t} = -c_1 s^a \xi^c \delta F_{ac}|_{\partial\Sigma_t}, \quad t \geqslant 0, \tag{2.63}$$

or equivalently, $\delta \vec{B}_\parallel = \vec{s} \delta A_0 + c_1 \frac{1}{2} \delta \vec{E}_\perp = 0$, for $t \geqslant 0$; (iii) similarly, for $b_1 = 0 (a_1 \neq 0)$, $b_0 \neq 0$, the boundary conditions yield another one-parameter $a_0/b_0 \equiv c_0$ family of the form

$$\sigma_b{}^c \delta A_c|_{\partial\Sigma_t} = -c_0 s^a \delta F_{ab}|_{\partial\Sigma_t}, \quad \xi^c s^a \delta F_{ac}|_{\partial\Sigma_t} = 0, \quad t \geqslant 0, \tag{2.64}$$

or equivalently, $\vec{s} \times \delta \vec{A}_\parallel + c_0 \frac{1}{2} \delta \vec{B}_\parallel = \delta \vec{E}_\perp = 0$, for $t \geqslant 0$; (iv) finally, for $b_0 \neq 0$, $b_1 \neq 0 (a_0 \neq 0, a_1 \neq 0)$, we obtain a two-parameter $a_1/b_1 \equiv c_1$ and $a_0/b_0 \equiv c_0$ family of the boundary conditions

$$\sigma_b{}^c \delta A_c|_{\partial\Sigma_t} = -c_0 s^a \delta F_{ab}|_{\partial\Sigma_t}, \quad \xi^c \delta A_c|_{\partial\Sigma_t} = -c_1 s^a \xi^c \delta F_{ac}|_{\partial\Sigma_t}, \quad t \geqslant 0, \tag{2.65}$$

or equivalently, $\vec{s}\times\delta\vec{A}_\parallel + c_0\tfrac{1}{2}\delta\vec{B}_\parallel = \vec{s}\,\delta A_0 + c_1\tfrac{1}{2}\delta\vec{E}_\perp = 0$, for $t\geqslant 0$.

The fixed data for these boundary conditions (2.63)–(2.65) correspond to specifying, respectively, the field components

$$\vec{s}A_0 + c_1\tfrac{1}{2}\vec{E}_\perp, \quad \vec{B}_\parallel, \quad c_1\neq 0, \tag{2.66}$$

$$\vec{E}_\perp, \quad \vec{s}\times\vec{A}_\parallel + c_0\tfrac{1}{2}\vec{B}_\parallel, \quad c_0\neq 0, \tag{2.67}$$

$$\vec{s}A_0 + c_1\tfrac{1}{2}\vec{E}_\perp, \quad \vec{s}\times\vec{A}_\parallel + c_0\tfrac{1}{2}\vec{B}_\parallel, \quad c_0\neq 0, c_1\neq 0, \tag{2.68}$$

at the boundary surface Σ_t for $t\geqslant 0$. From Proposition 2.1, we readily obtain the Hamiltonian boundary terms corresponding to these boundary conditions (by a proof similar to that for Theorem 2.2).

Theorem 2.4: *For boundary conditions (2.63)–(2.65), there is a respective Hamiltonian (2.25) conjugate to ξ^a on Σ, with boundary terms given by*

$$H_B(\xi;A) = 4\oint_{\partial\Sigma} \epsilon_{bc}(\xi^a A_a \xi^d s^e F_{de} + \sigma^{ad} A_a s^e F_{de} - c_1(\xi^d s^e F_{de})^2)$$

$$= -\oint_{\partial\Sigma} 2(\vec{A}\times\vec{B})_\perp + c_1\vec{E}_\perp{}^2\,\mathrm{d}S, \tag{2.69}$$

$$H_B(\xi;A) = 4\oint_{\partial\Sigma} \epsilon_{bc} c_0 \sigma^{de} s^a F_{ad} s^m F_{me} = \oint_{\partial\Sigma} c_0\vec{B}_\parallel{}^2\mathrm{d}S, \tag{2.70}$$

$$H_B(\xi;A) = 4\oint_{\partial\Sigma} \epsilon_{bc}(\xi^a A_a \xi^d s^e F_{de} - c_1(\xi^d s^e F_{de})^2 + c_0\sigma^{de} s^m F_{md} s^n F_{ne})$$

$$= -\oint_{\partial\Sigma} 2A_0\vec{E}_\perp + c_1 E_\perp{}^2 - c_0\vec{B}_\parallel{}^2\mathrm{d}S. \tag{2.71}$$

Interestingly, among the allowed boundary conditions given by Theorem 2.3, we observe that the Hamiltonian boundary terms vanish identically in one (and only one) case, when $c_0=0$ in boundary condition (2.64), i.e.,

$$\sigma_b{}^c\delta A_c|_{\partial\Sigma_t} = 0, \quad \xi^c s^a \delta F_{ac}|_{\partial\Sigma_t} = 0, \quad t\geqslant 0, \tag{2.72}$$

or equivalently, $\delta\vec{A}_\parallel = \delta\vec{E}_\perp = 0$, for $t\geqslant 0$. The resulting Hamiltonian (2.25) reduces, on solutions A_a, simply to the expression for the total energy of the electromagnetic fields, $H(\xi;A) = 4\int_\Sigma \xi^e\xi^d T_{de}(F)\mathrm{d}^3x = \int_\Sigma \vec{E}^2 + \vec{B}^2\mathrm{d}^3x$. The fixed data corresponding to the boundary condition (2.72) are $\vec{A}_\parallel$ and $\vec{E}_\perp$, which means that the normal components of the electric and magnetic fields at $\partial\Sigma$ are specified for $t\geqslant 0$,

$$\vec{B}_\perp = \vec{\partial}_\parallel\times\vec{A}_\parallel, \quad \vec{E}_\perp = \vec{\partial}_\perp A_0 - \partial_0\vec{A}_\perp. \tag{2.73}$$

Since $\vec{A}_\parallel$ and $\vec{E}_\perp$ are fixed, there are no effective charges and currents associated with the boundary surface. Thus, the total electromagnetic energy involves no surface integral contributions in this case.

D. Remarks

We conclude with some short remarks on the uniqueness of the boundary conditions obtained in Theorem 2.3.

Note that the symplectic boundary conditions (2.53) and (2.54) are linear combinations of the tangential and normal parts of the Dirichlet and Neumann boundary conditions, referred to as mixed boundary conditions. In physical terms, they correspond to specifying $b_0\sigma_b{}^c A_c + a_0 s^a \sigma_b{}^c F_{ac}$ and $b_1 \xi^c A_c + a_1 \xi^c s^a F_{ca}$ as boundary data at $\partial\Sigma_t$ for $t \geqslant 0$. Theorem 2.3 gives a uniqueness result for these mixed boundary conditions under the natural assumption (2.51) about the general type of boundary condition considered on the fields at the boundary surface. If this assumption is loosened, then there exist additional boundary conditions allowed by the determining equation (2.24).

In particular, one can trade off some of the mixed boundary conditions on the symplectic boundary data for boundary conditions involving the symmetrized derivatives of A_a at $\partial\Sigma$. For example, an allowed boundary condition satisfying Eq. (2.24) is given by $\mathcal{F}(A) = (\xi^a A_a, \sigma^{ab}\partial_a A_b, \sigma^{ab} s^c \partial_{(b} A_{c)})$, or equivalently

$$\xi^a \delta A_a|_{\partial\Sigma_t} = 0, \quad \sigma^{ab}\partial_a \delta A_b|_{\partial\Sigma_t} = 0, \quad \sigma^{ab} s^c \partial_{(b}\delta A_{c)}|_{\partial\Sigma_t} = 0, \quad t \geqslant 0, \tag{2.74}$$

with $\alpha_a = 8\epsilon_a{}^b A_b s^c \delta A_c$. From Eq. (2.28) one obtains

$$\tfrac{1}{8}\xi^a \tilde{B}_a = s^e \sigma^{cd}(A_c \partial_{(d} A_{e)} - A_e \partial_c A_{d)}) - \tfrac{1}{2} A_d A_e \mathcal{D}^d s^e, \tag{2.75}$$

where $\mathcal{D}_d s_e = \sigma_d{}^m \sigma_e{}^n \partial_m s_n$ is the extrinsic curvature of $\partial\Sigma$ in Σ. Hence the corresponding boundary term in the Hamiltonian is given by Eq. (2.46) with

$$P_a(A) = A_a s^d \xi^e F_{de} - s^e \sigma^{cd}(A_c \partial_{(d} A_{e)} - A_e \partial_c A_{d)}) + \tfrac{1}{2} A_d A_e \mathcal{D}^d s^e. \tag{2.76}$$

III. ANALYSIS OF GENERAL RELATIVITY

We now apply the Noether charge analysis to General Relativity, specifically to the vacuum Einstein equations for the gravitational field in a spatially bounded space–time region with a fixed time-flow vector field. It is straightforward to also include matter fields, as we discuss in Ref. 8.

For General Relativity without matter sources, the starting point is the standard Lagrangian formulation of the Einstein equations with the space–time metric as the field variable. It turns out, however, that the analysis is considerably simplified by introduction of a tetrad (orthonormal frame). Moreover, taking into account local rotations and boosts of the tetrad, the boundary conditions and resulting Hamiltonians that arise in the tetrad formulation are equivalent to those obtained purely using the metric formulation, up to a boundary term in the presymplectic form.

After setting up some preliminary notation and results in Sec. III A, we will first consider a Dirichlet boundary condition as explained in Sec. III B. Then we will carry out details of the Noether charge analysis with the Dirichlet boundary condition using the tetrad formulation of General Relativity in Sec. III C. The resulting covariant Dirichlet Hamiltonian for General Relativity is summarized in Sec. III D where we will discuss the equivalence between the metric and tetrad formulations. In Sec. III E we will investigate a Neumann boundary condition and corresponding Hamiltonian, along with more general boundary conditions and Hamiltonians. The main result will be to establish uniqueness of mixed Dirichlet–Neumann boundary conditions for the existence of a Hamiltonian formulation of General Relativity. Finally, in Sec. III F we will briefly discuss the form of the Dirichlet and Neumann covariant Hamiltonians, and relate these to an analysis of boundary terms for the ADM Hamiltonian using the standard (noncovariant) ADM canonical variables.

A. Preliminaries

On a given smooth orientable four-dimensional space–time manifold M, let g_{ab} be the space–time metric tensor, $\epsilon_{abcd}(g)$ be the volume form normalized with respect to the metric, and ${}^g\nabla_a$ be the covariant (torsion-free) derivative operator determined by the metric.

Now, let ξ^a be a complete, smooth timelike vector field on M, and let Σ be a region contained in a spacelike hypersurface with the boundary of the region being a closed orientable two-surface

$\partial\Sigma$. Let s^a denote the unit outward spacelike normal to $\partial\Sigma$ orthogonal to ξ^a, let t^a denote the unit future timelike normal to $\partial\Sigma$ orthogonal to s^a. Denote the metric tensor and volume form on $\partial\Sigma$ by

$$\sigma_{ab} = g_{ab} - s_a s_b + t_a t_b, \tag{3.1}$$

$$\epsilon_{ab} = \epsilon_{abcd}(g) s^c t^d. \tag{3.2}$$

This yields the decompositions

$$g_{ab} = \sigma_{ab} + s_a s_b - t_a t_b, \tag{3.3}$$

$$\epsilon_{abcd}(g) = 12 t_{[a} s_b \epsilon_{cd]}. \tag{3.4}$$

Note that one has

$$\xi^a = N t^a + N^a, \quad N^a s_a = \xi^a s_a = 0 \tag{3.5}$$

for some scalar function N and vector function N^a on $\partial\Sigma$. It is convenient to extend the previous structures off $\partial\Sigma$ as follows. Let $\mathcal{V}$ be the space–time region foliated by the images of Σ under a one-parameter diffeomorphism on M generated by ξ^a, and let $\mathcal{B}$ be the timelike boundary of $\mathcal{V}$ foliated by the images of $\partial\Sigma$. Fix a time function t which is constant on each of the spacelike slices diffeomorphic to Σ under ξ^a in $\mathcal{V}$ and which is normalized by $\xi^a \partial_a t = 1$, such that $t = 0$ corresponds to Σ. Then $\mathcal{B}$ is a timelike hypersurface in M whose intersection with spacelike hypersurfaces Σ_t given by $t = \text{const}$ in $\mathcal{V}$ consists of spacelike two-surfaces $\partial\Sigma_t$ diffeomorphic to $\partial\Sigma$. Finally, let s^a, t^a, σ_{ab}, ϵ_{ab}, N, N^a be extended to $\partial\Sigma_t$, and let n_a denote the unit future timelike normal to Σ_t parallel to $\partial_a t$.

Note that, by construction, s_a is hypersurface orthogonal to $\mathcal{B}$ and hence

$$s_{[c} \partial_b s_{a]} = 0. \tag{3.6}$$

If t_a is expressed as a linear combination of s_a, $\partial_a t$, then since $\partial_a t$ obviously is hypersurface orthogonal to $\partial\Sigma_t$, it follows that

$$s_{[d} t_c \partial_b t_{a]} = 0. \tag{3.7}$$

In addition, note that $s^a \partial_a t$ measures the extent to which Σ_t fails to be orthogonal to $\mathcal{B}$.

Let $(\mathcal{P}_{\partial\Sigma})_a{}^b$ and $(\mathcal{P}_t)_a{}^b$ be coordinate projection operators onto the respective tangent spaces of the two-surface $\partial\Sigma_t$ and the integral curve of t^a, and let $(\mathcal{P}_{\mathcal{B}})_a{}^b = (\mathcal{P}_{\partial\Sigma})_a{}^b + (\mathcal{P}_t)_a{}^b$, which is the projection operator onto the tangent space of the timelike hypersurface $\mathcal{B}$. Note that these operators are independent of the space–time metric, as they involve only the manifold structure of $\mathcal{B}$ and $\partial\Sigma_t$ in local coordinates in M.

Hereafter we work in terms of an orthonormal frame θ_a^μ (i.e., tetrad) for g_{ab} on M. The frame components of s^a, t^a, n^a, σ_{ab}, ϵ_{ab}, g_{ab}, $\epsilon_{abcd}(g)$ are given by

$$s^\mu = s^a \theta_a^\mu, \quad t^\mu = t^a \theta_a^\mu, \quad n^\mu = n^a \theta_a^\mu, \tag{3.8}$$

$$\sigma^{\mu\nu} = \sigma^{ab} \theta_a^\mu \theta_b^\nu, \quad \epsilon^{\mu\nu} = \epsilon^{ab} \theta_a^\mu \theta_b^\nu, \tag{3.9}$$

$$\eta^{\mu\nu} = g^{ab} \theta_a^\mu \theta_b^\nu, \quad \epsilon^{\alpha\beta\mu\nu} = \epsilon^{abcd}(g) \theta_a^\alpha \theta_b^\beta \theta_c^\mu \theta_c^\nu, \tag{3.10}$$

where $\eta^{\mu\nu} = \sigma^{\mu\nu} + s^\mu s^\nu - t^\mu t^\nu = \text{diag}(-1,1,1,1)$ is the Minkowski frame-metric, with $\sigma^{\mu\nu} = \text{diag}(0,0,1,1)$. This leads to an orthonormal frame for the metric σ_{ab}, given by

$$\sigma_a{}^\mu = \sigma_a{}^b \theta_b^\mu \tag{3.11}$$

satisfying

$$s_\mu \sigma_a{}^\mu = t_\mu \sigma_a{}^\mu = 0. \tag{3.12}$$

Let the inverse orthonormal frame for g_{ab} and for σ_{ab} be denoted by

$$\theta^a_\mu = g^{ab}\theta^\mu_b, \quad \sigma_\mu{}^a = \sigma^{ab}\sigma_b{}^\mu. \tag{3.13}$$

Then, one has the decompositions

$$\theta^\mu_a = \sigma_a{}^\mu + s_a s^\mu - t_a t^\mu, \quad \theta^a_\mu = \sigma_\mu{}^a + s^a s_\mu - t^a t_\mu. \tag{3.14}$$

For later use, we will partially fix the SO(3,1) local gauge freedom in θ^a_μ by choosing the coefficients s_μ, t_μ in the frame decomposition (3.14) to be fixed functions on M, so that under a variation δg_{ab},

$$\delta s_\mu = \delta t_\mu = \delta \sigma_{\mu\nu} = 0 \tag{3.15}$$

and hence, correspondingly,

$$\delta s_a = s_\mu \delta\theta^\mu_a, \quad \delta t_a = t_\mu \delta\theta^\mu_a, \tag{3.16}$$

$$\delta\sigma_{ab} = 2\sigma_{\mu\nu}\theta^\mu_{(a}\delta\theta^\nu_{b)} = 2\sigma_{(a}{}^\mu \delta\sigma_{b)\mu}. \tag{3.17}$$

Similarly, one then also has

$$\delta\epsilon_{abcd}(\theta) = 4\epsilon_{\alpha\beta\mu\nu}\theta^\alpha_{[a}\theta^\beta_b\theta^\mu_c\delta\theta^\nu_{d]} = \epsilon_{abcd}(\theta)\theta^c_\mu\delta\theta^\mu_c, \tag{3.18}$$

$$\delta\epsilon_{ab} = 2\epsilon_{\mu\nu}\theta^\mu_{[a}\delta\theta^\nu_{b]} = \epsilon_{ab}\sigma_\mu{}^c\delta\sigma_c{}^\mu, \tag{3.19}$$

and thus

$$\delta\epsilon_{\mu\nu} = \delta\epsilon_{\alpha\beta\mu\nu} = 0. \tag{3.20}$$

Consequently, some useful identities are given by

$$\delta\theta^\mu_a = \delta\sigma_a{}^\mu + s^\mu\delta s_a - t^\mu\delta t_a, \tag{3.21}$$

$$\delta\theta^a_\mu = -\theta^a_\nu\theta^c_\mu\delta\theta^\nu_c = \delta\sigma_\mu{}^a + s_\mu\delta s^a - t_\mu\delta t^a. \tag{3.22}$$

Now, a variation of the space–time metric δg_{ab} can be decomposed into the parts

$$\delta g_{ab} = \delta\sigma_{ab} + 2s_{(a}\delta s_{b)} - 2t_{(a}\delta t_{b)}. \tag{3.23}$$

By hypersurface orthogonality, one has the identities

$$\delta s_a = s_a s^b \delta s_b, \quad \delta t_a = s_a s^b \delta t_b - t_a t^b \delta t_b \tag{3.24}$$

and

$$\delta\sigma_{ab} = \sigma_a{}^c\sigma_b{}^d\delta\sigma_{cd} + \sigma_a{}^c s_b s^d \delta\sigma_{cd} - \sigma_a{}^c t_b t^d \delta\sigma_{cd}. \tag{3.25}$$

Then, from the relation

$$\delta g^{ab} = \delta\sigma^{ab} + 2s^{(a}\delta s^{b)} - 2t^{(a}\delta t^{b)} = -g^{ac}g^{bd}\delta g_{cd}, \tag{3.26}$$

it straightforwardly follows that

$$\delta\sigma^{ab} = -\sigma^{ac}\sigma^{bd}\delta\sigma_{cd}, \tag{3.27}$$

$$\delta s^a = \sigma_b{}^a \delta s^b + s^a s_b \delta s^b - t^a t_b \delta s^b, \tag{3.28}$$

$$\delta t^a = \sigma_b{}^a \delta t^b - t^a t_b \delta t^b, \tag{3.29}$$

where

$$\sigma_{ab}\delta s^b = -s^b \delta\sigma_{ab}, \quad \sigma_{ab}\delta t^b = -t^b \delta\sigma_{ab}, \tag{3.30}$$

$$s_b \delta s^b = -s^b \delta s_b, \quad t_b \delta s^b = -t^b \delta s_b, \quad t_b \delta t^b = -t^b \delta t_b, \tag{3.31}$$

and again by hypersurface orthogonality,

$$s_a \delta\sigma^{ab} = t_a \delta\sigma^{ab} = 0, \quad s_a \delta t^a = 0. \tag{3.32}$$

Thus, the linearly independent parts of $\delta\theta^\mu_a$, or equivalently of $\delta\theta^a_\mu$, are given by

$$\delta\sigma_\mu{}^a, \sigma_b{}^a \delta s^b, \ \sigma_b{}^a \delta t^b, \ s_b \delta s^b, \ t_b \delta s^b, \ t_b \delta t^b. \tag{3.33}$$

Throughout, the time-flow vector field ξ^a is taken to be fixed, $\delta\xi^a = 0$, under variations of g_{ab}.

B. Dirichlet boundary condition

There is a natural motivation for a Dirichlet boundary condition on the gravitational field in the Einstein equations in analogy with the Maxwell equations where the tangential components of the electromagnetic field potential A_a are specified at the boundary. For General Relativity, similarly, one can introduce a Dirichlet boundary condition given by specifying the tangential components of the space–time metric g_{ab} at the two-surfaces $\partial\Sigma_t$. This boundary condition is expressed equivalently by conditions on the variation of the metric tensor

$$\delta\sigma_{ab}|_{\partial\Sigma_t} = 0, \quad \delta t_a|_{\partial\Sigma_t} = 0, \quad t \geqslant 0. \tag{3.34}$$

Geometrically, this means that the metric given by

$$h_{ab} = \sigma_{ab} - t_a t_b \tag{3.35}$$

on the timelike boundary hypersurface $\mathcal{B}$ is specified data, so it is held fixed under variations of g_{ab},

$$\delta h_{ab} = 0 \ \text{ on } \ \mathcal{B}. \tag{3.36}$$

The geometrical form (3.36) of the Dirichlet boundary condition is often introduced when one considers an action principle for General Relativity on a spacetime manifold with a fixed global timelike boundary hypersurface.[12,15–17] We will see in Sec. III C that this boundary condition in the form (3.34) emerges naturally from the Noether charge analysis for the existence of a Hamiltonian formulation of General Relatively for a spatially bounded local space-time region.

Note that, from the relations (3.27) to (3.31), one can decompose the Dirichlet boundary condition (3.34) into an intrinsic part

$$\delta h^{ab}|_{\partial\Sigma_t} = -h^{ac}h^{bd}\delta h_{cd}|_{\partial\Sigma_t} = 0, \quad t \geqslant 0 \tag{3.37}$$

and an extrinsic part

$$h_{ab}\delta s^b|_{\partial\Sigma_t} = -s^b \delta h_{ab}|_{\partial\Sigma_t} = 0, \quad t \geqslant 0 \tag{3.38}$$

with respect to the timelike hypersurface $\mathcal{B}$. The intrinsic part corresponds to fixing just the metric $\mathcal{P}_{\mathcal{B}}h_{ab}$ restricted to the tangent space of $\mathcal{B}$, where the projection $\mathcal{P}_{\mathcal{B}}$ removes components of the hypersurface metric proportional to s_a. Correspondingly, note that the volume form

$$\epsilon_{abc}(h)=\epsilon_{abcd}(g)s^d=3\epsilon_{[ab}t_{c]} \tag{3.39}$$

on this surface is also fixed, $\delta\epsilon_{abc}(h)=0$ on $\mathcal{B}$, since

$$\delta\epsilon_{abc}(h)=\tfrac{1}{2}\epsilon_{abc}(h)h^{mn}\delta h_{mn}=-\tfrac{1}{2}\epsilon_{abc}(h)h_{mn}\delta h^{mn}. \tag{3.40}$$

The Dirichlet boundary condition has a simple formulation in terms of the orthonormal frame θ_a^μ. It is convenient to introduce a frame for the metric h_{ab} by

$$h_a{}^\mu=h_a{}^b\theta_b^\mu=\sigma_a{}^\mu-t_at^\mu, \tag{3.41}$$

and inverse frame

$$h^{a\mu}=h^{ab}h_b{}^\mu. \tag{3.42}$$

Then the Dirichlet boundary condition (3.34) is equivalent to

$$\delta h_a{}^\mu|_{\partial\Sigma_t}=0,\quad t\geqslant 0, \tag{3.43}$$

with intrinsic part

$$\delta h^{a\mu}|_{\partial\Sigma_t}=0,\quad t\geqslant 0, \tag{3.44}$$

which is equivalent to Eq. (3.37). These equivalences are immediate consequences of the identities $h_{ab}=h_a{}^\mu h_b{}^\nu\eta_{\mu\nu}$ and $h^{ab}=h_\mu{}^a h_\nu{}^b\eta^{\mu\nu}$. From these identities, one also has

$$\delta h_{ab}=2h_{(a}{}^\mu\delta h_{b)\mu}, \tag{3.45}$$

$$\delta\epsilon_{abc}(h)=h_\mu{}^d\delta h_d{}^\mu. \tag{3.46}$$

An additional useful identity is given by

$$\delta h_a{}^c=-(s^c\delta s_a+s_a\delta s^c)=-s_a h_b{}^c\delta s^b \tag{3.47}$$

and therefore $\mathcal{P}_{\mathcal{B}}\delta h_a{}^c=0$.

Finally, note that the intrinsic part of the Dirichlet boundary condition on the frame decomposes into

$$\delta\sigma^{a\mu}|_{\partial\Sigma_t}=0,\quad \delta t^a|_{\partial\Sigma_t}=0,\quad t\geqslant 0. \tag{3.48}$$

The full, extrinsic Dirichlet boundary condition is necessary and sufficient for $\delta h_a{}^c|_{\partial\Sigma_t}=0$, $t\geqslant 0$.

C. Noether charge analysis

We consider the standard tetrad formulation of General Relativity, using an orthonormal frame θ_a^μ for g_{ab} and a frame-connection

$$\Gamma_a{}^{\mu\nu}(\theta)=\theta^{b\mu}\,{}^g\nabla_a\theta_b^\nu=2\theta^{b[\mu}\partial_{[a}\theta_{b]}^{\nu]}-\theta^{b\mu}\theta^{c\nu}\theta_{a\alpha}\partial_{[b}\theta_{c]}^\alpha. \tag{3.49}$$

Here the expression in the second equality is obtained from the relation

$$\theta^\nu_{[b}\Gamma_{a]\nu}{}^\mu(\theta)={}^g\nabla_{[a}\theta^\nu_{b]}=\partial_{[a}\theta^\mu_{b]}. \tag{3.50}$$

The curvature of this connection (3.49) is given by

$$R_{ab}{}^{\mu\nu}(\theta) = 2\partial_{[a}\Gamma_{b]}{}^{\mu\nu}(\theta) + 2\Gamma_{[a}{}^{\mu\sigma}(\theta)\Gamma_{b]\sigma}{}^{\nu}(\theta) = R_{abcd}(g)\,\theta^{c\mu}\theta^{d\nu}, \tag{3.51}$$

related to the Riemann curvature tensor $R_{abcd}(g)$ of g_{ab}.

With θ_a^μ as the field variable, the Lagrangian four-form for General Relativity (without matter sources) is given by

$$L_{abcd}(\theta) = \epsilon_{abcd}(\theta)R(\theta) = 6\,\theta^\mu_{[a}\theta^\nu_b\tilde{R}_{cd]\mu\nu}(\theta), \tag{3.52}$$

where

$$\tilde{R}_{cd}{}^{\mu\nu}(\theta) = R_{cd\alpha\beta}(\theta)\,\epsilon^{\alpha\beta\mu\nu} = 2\partial_{[a}\tilde{\Gamma}_{b]}{}^{\mu\nu} - \Gamma_{[a}{}^{\sigma[\mu}(\theta)\tilde{\Gamma}_{b]\sigma}{}^{\nu]}(\theta) \tag{3.53}$$

in terms of $\tilde{\Gamma}_{a\mu\nu}(\theta) = \Gamma_a{}^{\alpha\beta}(\theta)\epsilon_{\alpha\beta\mu\nu}$. Then the variation of $L_{abcd}(\theta)$ gives, after integration by parts and use of the connection equation (3.50),

$$\tfrac{1}{6}\delta L_{abcd}(\theta) = 2\,\delta\theta^\mu_{[a}(\theta^\nu_b\tilde{R}_{cd]\mu\nu}(\theta)) + \tfrac{1}{6}\partial_{[a}\Theta_{bcd]}(\theta,\delta\theta), \tag{3.54}$$

where

$$\Theta_{bcd}(\theta,\delta\theta) = 12\theta^\mu_{[c}\theta^\nu_d\delta\tilde{\Gamma}_{b]\mu\nu}(\theta) \tag{3.55}$$

defines the symplectic potential three-form. The field equations for θ_a^μ, obtained from the coefficient of $\delta\theta_a^\mu$ in Eq. (3.54), are given by

$$\mathcal{E}^\mu_{bcd}(\theta) = 12\theta^\nu_{[b}\tilde{R}_{cd]\mu\nu}(\theta) = 8\,\epsilon_{bcda}(\theta)(R^{a\mu}(\theta) - \tfrac{1}{2}\theta^{a\mu}R(\theta)) = 0. \tag{3.56}$$

Thus θ_a^μ satisfies $R^{a\mu}(\theta) = 0$, which is equivalent to the vacuum Einstein equations for the space–time metric

$$R_{ab}(g) = 0 \tag{3.57}$$

arising as the stationary points of the action functional $S(g) = \int_M \epsilon_{abcd}(g)R(g)$ under compact support variations of g_{ab}.

The Noether current associated with ξ^a is given by the three-form

$$J_{abc}(\xi,\theta) = \Theta_{abc}(\theta,\mathcal{L}_\xi\theta) + 4\,\xi^d L_{abcd}(\theta) = 12\theta^\mu_{[b}\theta^\nu_c\mathcal{L}_\xi\tilde{\Gamma}_{a]\mu\nu}(\theta) + 24\xi^d\theta^\mu_{[c}\theta^\nu_d\tilde{R}_{ab]\mu\nu}(\theta) \tag{3.58}$$

with the first term obtained from the variation of the frame connection (3.49) after replacement of $\delta\theta_a^\mu$ by the Lie derivative $\mathcal{L}_\xi\theta_a^\mu = \xi^e\partial_e\theta_a^\mu + \theta_e^\mu\partial_a\xi^e$ and use of the fact that Lie derivatives commute with exterior (skew) derivatives. We now simplify the first term in Eq. (3.58) as follows. First we express

$$\mathcal{L}_\xi\Gamma_a{}^{\mu\nu}(\theta) = \partial_a(\xi^e\Gamma_e{}^{\mu\nu}(\theta)) + \xi^e(R_{ea}{}^{\mu\nu}(\theta) - 2\Gamma_{[e}{}^{\mu\sigma}(\theta)\Gamma_{a]\sigma}{}^{\nu}(\theta)). \tag{3.59}$$

Hence we obtain

$$12\theta^\mu_{[b}\theta^\nu_c\mathcal{L}_\xi\tilde{\Gamma}_{a]\mu\nu}(\theta) = \partial_{[a}(12\theta^\mu_b\theta^\nu_{c]}\xi^e\tilde{\Gamma}_{e\mu\nu}(\theta)) - 12\xi^e\theta^\mu_{[b}\theta^\nu_c\tilde{R}_{a]e\mu\nu}(\theta) \tag{3.60}$$

through use of the identity (3.53). Next we combine the second terms in both Eqs. (3.58) and (3.60) to get

$$-12\xi^e\theta^\mu_{[b}\theta^\nu_c\tilde{R}_{a]e\mu\nu}(\theta) + 24\xi^d\theta^\mu_{[c}\theta^\nu_d\tilde{R}_{ab]\mu\nu}(\theta) = \xi^e\epsilon_{abcd}(g)(4\,\delta^d_e R(g) - 8R_e{}^d(g)). \tag{3.61}$$

Thus, one obtains the Noether current

$$J_{abc}(\xi;\theta)=3\partial_{[a}Q_{bc]}(\xi;\theta)-\xi^e\theta_{e\mu}\mathcal{E}^{\mu}_{abc}(\theta), \tag{3.62}$$

where

$$Q_{bc}(\xi;\theta)=4\xi^d\tilde{\Gamma}_{d\mu\nu}(\theta)\theta^{\mu}_b\theta^{\nu}_c \tag{3.63}$$

is the Noether current potential two-form.

On vacuum solutions θ^{μ}_a, the Noether current reduces to an exact three-form

$$J_{abc}(\xi;\theta)=3\partial_{[a}Q_{bc]}(\xi;\theta). \tag{3.64}$$

Therefore, the Noether charge for vacuum solutions is given by the boundary two-surface integral

$$Q_{\Sigma}(\xi)=\int_{\Sigma}J_{abc}(\xi;\theta)=\int_{\partial\Sigma}\epsilon_{bc}4\xi^d\tilde{\Gamma}_{d\mu\nu}(\theta)\epsilon^{\mu\nu}=\int_{\partial\Sigma}8\xi^d\Gamma_{d\mu\nu}(\theta)t^{\mu}s^{\nu}\mathrm{d}S, \tag{3.65}$$

where dS is the volume element on $\partial\Sigma$ corresponding to the volume form ϵ_{bc} in local coordinates.

Now the symplectic current, defined by the antisymmetrized variation of $\Theta_{bcd}(\theta,\delta\theta)$, is given by the three-form

$$\tfrac{1}{24}\omega_{bcd}(\theta,\delta_1\theta,\delta_2\theta)=\theta^{\mu}_{[c}\delta_1\theta^{\nu}_d\delta_2\tilde{\Gamma}_{b]\mu\nu}(\theta)-\theta^{\mu}_{[c}\delta_2\theta^{\nu}_d\delta_1\tilde{\Gamma}_{b]\mu\nu}(\theta). \tag{3.66}$$

Then the presymplectic form on Σ is defined by

$$\Omega_{\Sigma}(\theta,\delta_1\theta,\delta_2\theta)=\int_{\Sigma}\omega_{bcd}(\theta,\delta_1\theta,\delta_2\theta)=24\int_{\Sigma}\theta^{\mu}_{[c}\delta_1\theta^{\nu}_d\delta_2\tilde{\Gamma}_{b]\mu\nu}(\theta)-\theta^{\mu}_{[c}\delta_2\theta^{\nu}_d\delta_1\tilde{\Gamma}_{b]\mu\nu}(\theta). \tag{3.67}$$

A Hamiltonian conjugate to ξ on Σ is a function $H_{\Sigma}(\xi;\theta)=\int_{\Sigma}\mathcal{H}_{abc}(\xi;\theta)$ for some locally constructed three-form $\mathcal{H}_{abc}(\xi;\theta)$ such that

$$\delta H_{\Sigma}(\xi;\theta)\equiv H'_{\Sigma}(\xi;\theta,\delta\theta)=\Omega_{\Sigma}(\delta\theta,\mathcal{L}_{\xi}\theta) \tag{3.68}$$

holds for arbitrary variations $\delta\theta^{\mu}_a$ away from vacuum solutions θ^{μ}_a.

In terms of the Noether current (3.62), the presymplectic form on Σ yields

$$\Omega_{\Sigma}(\theta,\delta\theta,\mathcal{L}_{\xi}\theta)=\int_{\Sigma}J_{abc}(\xi;\theta)-4\xi^d\mathcal{E}^{\mu}_{[abc}(\theta)\delta\theta_{d]\mu}-\int_{\partial\Sigma}\xi^c\Theta_{abc}(\theta,\delta\theta). \tag{3.69}$$

Consequently, for variations $\delta\theta^{\mu}_a$ with compact support on the interior of Σ, the Noether current defines a Hamiltonian conjugate to ξ^a,

$$H(\xi;\theta)=\int_{\Sigma}J_{abc}(\xi;\theta)=8\int_{\Sigma}\xi^e\theta_{e\mu}\mathcal{E}^{\mu}_{abc}(\theta)+\int_{\partial\Sigma}Q_{ab}(\xi;\theta), \tag{3.70}$$

which is equal to the Noether charge (3.65) when θ^{μ}_a is a vacuum solution. Explicitly, from Eqs. (3.56) and (3.63), one has

$$\begin{aligned}H(\xi;\theta)&=8\int_{\Sigma}\epsilon_{dabc}(\xi^e\theta^d_{\mu}R_e{}^{\mu}(\theta)-\tfrac{1}{2}\xi^dR(\theta))+4\int_{\partial\Sigma}\epsilon_{bc}\xi^d\tilde{\Gamma}_{d\mu\nu}(\theta)\epsilon^{\mu\nu}\\&=8\int_{\Sigma}\xi^en_{\mu}(R_e{}^{\mu}(\theta)-\tfrac{1}{2}\theta^{\mu}_eR(\theta))\mathrm{d}\Sigma+8\int_{\partial\Sigma}\xi^d\Gamma_{d\mu\nu}(\theta)t^{\mu}s^{\nu}\,\mathrm{d}S,\end{aligned} \tag{3.71}$$

where $d\Sigma$ is the coordinate volume element on Σ obtained from the volume form $\epsilon_{abcd}n^d$.

To define a Hamiltonian $H_\Sigma(\xi;\theta)$ for variations $\delta\theta^\mu_a$ without compact support, it follows that the term $\xi^c\Theta_{abc}(\theta,\delta\theta)$ in Eq. (3.69) needs to be a total variation at the boundary $\partial\Sigma$, i.e., there must exist a locally constructed three-form $\tilde{B}_{abc}(\theta)$ such that one has

$$\xi^c\Theta_{abc}(\theta,\delta\theta)|_{\partial\Sigma}=(\xi^c\delta\tilde{B}_{abc}(\theta)+\partial_{[a}\alpha_{b]}(\xi;\theta,\delta\theta))|_{\partial\Sigma}, \tag{3.72}$$

where $\alpha_b(\xi;\theta,\delta\theta)$ is a locally constructed one-form. This equation is equivalent to

$$\epsilon^{ab}\xi^c\Theta_{abc}(\theta,\delta\theta)|_{\partial\Sigma}=\epsilon^{ab}\xi^c\delta\tilde{B}_{abc}(\theta,\delta\theta)|_{\partial\Sigma}+\sigma_c{}^d\partial_d\tilde{\alpha}^c(\xi;\theta,\delta\theta)|_{\partial\Sigma}, \tag{3.73}$$

where $\tilde{\alpha}^c(\xi;\theta,\delta\theta)=\epsilon^{cb}\alpha_b(\xi;\theta,\delta\theta)$ and the symplectic potential term is given by

$$\epsilon^{ab}\xi^c\Theta_{abc}(\theta,\delta\theta)=32\xi^c t_{[\alpha}s_{\nu]}\theta^\alpha_c\theta^a_\mu\delta\Gamma_a{}^{\mu\nu}(\theta). \tag{3.74}$$

Hence we now have the following result.

Proposition 3.1: A Hamiltonian conjugate to ξ^a on Σ exists for variations $\delta\theta^\mu_a$ with support on $\partial\Sigma$ if and only if

$$\epsilon^{ab}\xi^c\delta\tilde{B}_{abc}(\theta)|_{\partial\Sigma}=32(\xi^c t_{[\alpha}s_{\nu]}\theta^\alpha_c\theta^a_\mu\delta\Gamma_a{}^{\mu\nu}(\theta))|_{\partial\Sigma}-\sigma_c{}^d\partial_d\tilde{\alpha}^c(\xi;\theta,\delta\theta)|_{\partial\Sigma} \tag{3.75}$$

for some locally constructed three-form $\tilde{B}_{abc}(\theta)$ in $T^*(\Sigma)$ and locally constructed vector $\tilde{\alpha}^c(\xi;\theta,\delta\theta)$ in $T(\partial\Sigma)$. The Hamiltonian is given by the Noether charge plus an additional boundary term

$$\begin{aligned}H_\Sigma(\xi;\theta)&=\int_\Sigma J_{abc}(\xi;\theta)-\int_{\partial\Sigma}\xi^c\tilde{B}_{abc}(\theta)\\&=8\int_\Sigma\xi^e\theta_{e\mu}\mathcal{E}^\mu_{abc}(\theta)+\int_{\partial\Sigma}Q_{ab}(\xi;\theta)-\xi^c\tilde{B}_{abc}(\theta)\\&=8\int_\Sigma\xi^e n_\mu(R_e{}^\mu(\theta)-\tfrac{1}{2}\theta^\mu_e R(\theta))d\Sigma+\int_{\partial\Sigma}\xi^d(8\Gamma_{d\mu\nu}(\theta)t^\mu s^\nu-\tfrac{1}{2}\tilde{B}_d(\theta))dS\end{aligned} \tag{3.76}$$

with $\tilde{B}_d(\theta)=\epsilon^{bc}\tilde{B}_{bcd}(\theta)$.

We now show that equation (3.75) for the existence of a Hamiltonian (3.76) is satisfied for the intrinsic Dirichlet boundary condition on θ^μ_a,

$$\delta h^{a\mu}|_{\partial\Sigma_t}=0,\quad t\geqslant 0, \tag{3.77}$$

and then we derive the corresponding Hamiltonian boundary term. Henceforth we take θ^μ_a to satisfy the gauge conditions (3.15)–(3.17) naturally associated with the boundary hypersurface $\mathcal{B}$.

Consider the left-hand side of Eq. (3.75). The boundary condition (3.77) yields $\delta\sigma^{a\mu}|_{\partial\Sigma}=0$ and hence, from Eq. (3.19), $\delta\epsilon^{ab}=\epsilon^{ab}\sigma_{c\mu}\delta\sigma^{c\mu}|_{\partial\Sigma}=0$. Thus, we have

$$\epsilon^{ab}\xi^c\delta\tilde{B}_{abc}(\theta)|_{\partial\Sigma}=\delta(\epsilon^{ab}\xi^c\tilde{B}_{abc}(\theta))|_{\partial\Sigma}. \tag{3.78}$$

Next consider the right-hand side of Eq. (3.75). We integrate by parts with respect to the variation in the first term to get

$$\xi^c t_{[\alpha}s_{\nu]}\theta^\alpha_c\theta^a_\mu\delta\Gamma_a{}^{\mu\nu}(\theta)=\delta(\xi^c t_{[\alpha}s_{\nu]}\theta^\alpha_c\theta^a_\mu\Gamma_a{}^{\mu\nu}(\theta))-\xi^c t_{[\alpha}s_{\nu]}\Gamma_a{}^{\mu\nu}(\theta)(\theta^a_\mu\delta\theta^\alpha_c+\theta^\alpha_c\delta\theta^a_\mu). \tag{3.79}$$

Then, using orthogonality relations (3.5) and (3.24), we find that the second term in Eq. (3.79) vanishes as follows. First,

$$\xi^c t_{[\alpha} s_{\nu]} \delta\theta^\alpha_c = \tfrac{1}{2}\xi^c (s_\nu \delta t_c - t_\nu \delta s_c) = -s_\nu \xi^c t_c t_b \delta t^b = 0 \tag{3.80}$$

since $\delta t^b|_{\partial\Sigma} = 0$ by the boundary condition (3.77). In addition,

$$\xi^c t_{[\alpha} s_{\nu]} \theta^\alpha_c \delta\theta^a_\mu = \tfrac{1}{2}\xi^c t_c s_\nu (\delta h_\mu{}^a + s_\mu \delta s^a) = -\tfrac{1}{2} N s_\nu s_\mu \delta s^a. \tag{3.81}$$

Hence, the second term in Eq. (3.79) reduces to

$$\tfrac{1}{2} N s_\nu s_\mu \Gamma_a{}^{\mu\nu}(\theta)\, \delta s^a = 0 \tag{3.82}$$

since $\Gamma_a{}^{(\mu\nu)}(\theta) = 0$.

Consequently, returning to Eq. (3.75), we obtain

$$\delta(\xi^c \tilde{B}_c(\theta) - 32 t_{[a} s_{\nu]} \xi^c \theta^\alpha_c \theta^a_\mu \Gamma_a{}^{\mu\nu}(\theta))|_{\partial\Sigma} = -\sigma_c{}^d \partial_d \tilde{\alpha}^c(\xi; \theta, \delta\theta)|_{\partial\Sigma}, \tag{3.83}$$

which obviously is satisfied by

$$\xi^c \tilde{B}_c(\theta) = 32 t_{[\alpha} s_{\nu]} \xi^c \theta^\alpha_c \theta^d_\mu \Gamma_d{}^{\mu\nu}(\theta) \tag{3.84}$$

and $\tilde{\alpha}^c(\xi; \theta, \delta\theta) = 0$. This verifies Proposition 3.1 using the intrinsic Dirichlet boundary condition (3.77).

Finally, from expressions (3.84) for $\xi^c \tilde{B}_c(\theta)$ and (3.63) for $Q_{bc}(\xi, \theta)$, we obtain a Hamiltonian (3.76) with the boundary term given by

$$H_B(\xi, \theta) = \int_{\partial\Sigma} Q_{ab}(\xi, \theta) - \xi^c \tilde{B}_{abc}(\theta, \delta\theta) = 8 \int_{\partial\Sigma} \epsilon_{ab} \xi^c (t_\mu s_\nu \Gamma_c{}^{\mu\nu}(\theta) - 2 t_{[\alpha} s_{\nu]} \theta^\alpha_c \theta^d_\mu \Gamma_d{}^{\mu\nu}(\theta)). \tag{3.85}$$

Hence, the Hamiltonian boundary term takes the form

$$H_B(\xi, \theta) = 8 \int_{\partial\Sigma} \xi^c P_c(\theta) \mathrm{d}S, \tag{3.86}$$

where $P_c(\theta) = t_\mu s_\nu \Gamma_c{}^{\mu\nu}(\theta) - t_c s_\nu \theta^a_\mu \Gamma_a{}^{\mu\nu}(\theta) + s_c t_\nu \theta^a_\mu \Gamma_a{}^{\mu\nu}(\theta)$. This expression is simplified by the identities (3.3) and (3.14), which yield

$$P_c(\theta) = t^a s_\nu \sigma_c{}^{d\ g} \nabla_d \theta^\nu_a - t_c s_\nu \sigma^{bd\ g} \nabla_b \theta^\nu_d + s_c t_\nu \sigma^{bd\ g} \nabla_b \theta^\nu_d. \tag{3.87}$$

Thus, we have the following main result.

Theorem 3.2: *For the intrinsic Dirichlet boundary condition (3.77), a Hamiltonian conjugate to ξ^a on Σ is given by*

$$H_\Sigma(\xi; \theta) = 8 \int_\Sigma \xi^e n_\mu (R_e{}^\mu(\theta) - \tfrac{1}{2} \theta^\mu_e R(\theta)) \mathrm{d}\Sigma + 8 \int_{\partial\Sigma} \xi^c P_c(\theta) \mathrm{d}S. \tag{3.88}$$

On vacuum solutions θ^μ_a, the Hamiltonian reduces to the surface integral (3.86), (3.87).

Note, this Hamiltonian is unique up to adding an arbitrary covector function of the Dirichlet boundary data $h_\mu{}^a$ to $P_c(\theta)$.

D. Dirichlet Hamiltonian

On vacuum solutions of the Einstein equations, the Hamiltonian (3.88) with the Dirichlet boundary condition (3.77) holding on the timelike hypersurface $\mathcal{B}$ bounding a local space–time region $\mathcal{V}$ takes a simple form if the frame θ^μ_a is adapted to the boundary two-surfaces $\partial\Sigma_t$ and ξ^a. Let

$$\vartheta_a^0 = t_a\,, \quad \vartheta_a^1 = s_a\,, \quad \vartheta_{[a}^2 \vartheta_{b]}^3 = \epsilon_{ab}\,, \quad \vartheta_a^2 = \epsilon_a{}^b \vartheta_b^3, \tag{3.89}$$

which defines a preferred orthonormal frame ϑ_a^μ. It follows that

$$t^\nu = t^a \vartheta_a^\nu = -\delta_0^\nu, \quad s^\nu = s^a \vartheta_a^\nu = \delta_1^\nu. \tag{3.90}$$

This choice of frame is unique up to rotations of ϑ_a^2, ϑ_a^3.

Theorem 3.3: *For the Dirichlet boundary condition (3.77), the Hamiltonian (3.88) conjugate to ξ^a on Σ, evaluated in the orthonormal frame (3.89) for vacuum solutions ϑ_a^μ, is given by the surface integral*

$$H^{\mathrm{D}}(\xi;\vartheta) = 8\int_{\partial\Sigma} \xi^c P_c^{\mathrm{D}}(\vartheta)\mathrm{d}S, \tag{3.91}$$

where

$$P_c^{\mathrm{D}}(\vartheta) = t^a \sigma_c{}^{d\,g} \nabla_d s_a - t_c \sigma^{bd\,g} \nabla_b s_d + s_c \sigma^{bd\,g} \nabla_b t_d\,. \tag{3.92}$$

We refer to $H^{\mathrm{D}}(\xi;\vartheta)$ as the *Dirichlet Hamiltonian* for the gravitational field in the local space–time region $\mathcal{V}$, and $P_c^{\mathrm{D}}(\vartheta)$ as the *Dirichlet symplectic vector* associated with the boundary two-surfaces $\partial\Sigma_t$. Note that since ξ^a lies in $\mathcal{B}$, only the first two terms in $P_c^{\mathrm{D}}(\vartheta)$ contribute to $H^{\mathrm{D}}(\xi;\vartheta)$. The significance of the full expression for $P_c^{\mathrm{D}}(\vartheta)$ and its resulting geometrical properties are discussed in Ref. 8.

The general form of the Hamiltonian boundary term (3.86) and (3.87) differs from the special form (3.91) and (3.92) when evaluated in an orthonormal frame not adapted to $\partial\Sigma_t$ and ξ^a. In particular, we obtain the relation

$$P_c(\theta) = P_c^{\mathrm{D}}(\vartheta) - \sigma_c{}^d t^\nu \partial_d s_\nu + t_c \sigma^{b\nu} \partial_b s_\nu - s_c \sigma^{b\nu} \partial_b t_\nu \tag{3.93}$$

and so the general form of the symplectic vector $P_c(\theta)$ differs from $P_c^{\mathrm{D}}(\vartheta)$ by various gradient terms. These terms can be understood by considering a change of orthonormal frame

$$\theta_a^\mu \to U^\mu{}_\nu \theta_a^\nu, \tag{3.94}$$

where $U^\mu{}_\nu$ is a SO(3,1) transformation acting in the frame bundle of the space–time (M,g) at $\partial\Sigma_t$. Such transformations are defined by $U^{-1\mu}{}_\nu = U^\alpha{}_\beta \eta_{\alpha\nu} \eta^{\mu\beta}$ and $\det(U)=1$, where $U^{-1\mu}{}_\nu$ is the inverse of $U^\mu{}_\nu$, given by $U^{-1\mu}{}_\nu U^\nu{}_\alpha = \delta_\alpha^\mu = U^\mu{}_\nu U^{-1\nu}{}_\alpha$.

The transformations (3.94) are a gauge symmetry of the tetrad formulation for General Relativity. Under the change of orthonormal frame, one has

$$\begin{aligned}\Gamma_{a\mu}{}^\nu(\theta) = \theta_\mu^{b\,g} \nabla_a \theta_b^\nu \to \Gamma_{\alpha\mu}{}^\nu(U\theta) &= U^{-1\alpha}{}_\mu \theta_\alpha^b (U^\nu{}_\beta \theta_b^\beta) \\ &= U^{-1\alpha}{}_\mu U^\nu{}_\beta \Gamma_{a\alpha}{}^\beta(\theta) + U^{-1\alpha}{}_\mu \partial_a U^\nu{}_\alpha,\end{aligned} \tag{3.95}$$

and so, through substitution of the transformation (3.95) into the curvature (3.51),

$$R_{ab\mu}{}^\nu(\theta) \to R_{ab\mu}{}^\nu(U\theta) = U^{-1\alpha}{}_\mu U^\nu{}_\beta R_{ab\alpha}{}^\beta(\theta) \tag{3.96}$$

after cancellations of terms. Hence the Lagrangian (3.52) for the field variable θ_a^μ is gauge invariant. As a consequence, it is straightforward to see that the symplectic structure given by the symplectic potential (3.55) and current (3.66) must be gauge invariant. In particular, note that one has $\delta\Gamma_{a\mu}{}^\nu(U\theta) = U^{-1\alpha}{}_\mu U^\nu{}_\beta \delta\Gamma_{a\alpha}{}^\beta(\theta)$ where the gradient term from Eq. (3.95) drops out of the variation since it has no dependence on θ_a^μ. This explicitly establishes the gauge invariance of $\Theta_{abc}(\theta, \delta\theta)$ and hence of $\omega_{abc}(\theta, \delta_1\theta, \delta_2\theta)$.

However, the Noether charge (3.63) fails to be gauge invariant due to its explicit dependence on the frame connection. Consequently, it follows that the gradient terms in the symplectic vector (3.93) originate from a gauge transformation on the frame connection under (3.94) as given by a transformation relating the adapted orthonormal frame to a general orthonormal frame, $\theta^{\mu}_{a} = U^{\mu}{}_{0} t_a + U^{\mu}{}_{1} \sigma_a{}^{1} + U^{\mu}{}_{2} \sigma_a{}^{2} + U^{\mu}{}_{4} s_a$.

The gauge invariance of the symplectic structure arising from the tetrad formulation of the Lagrangian means that the symplectic potential (3.55) and current (3.66) are equivalent to manifestly gauge-invariant expressions derived using the metric formulation of General Relativity with g_{ab} as the field variable. It can be shown that one has

$$\Theta_{abc}(g, \delta g) = \Theta_{abc}(\theta, \delta\theta) + 6\partial_{[c}\psi_{ab]}(g, \delta g), \tag{3.97}$$

where $\psi_{ab}(g, \delta g)$ is a locally constructed two-form, and so the symplectic potentials are equivalent to within an exact three-form. This contributes a boundary term to the presymplectic form obtained from the metric Lagrangian $L_{abcd}(g) = \epsilon_{abcd}(g) R(g)$,

$$\Omega_{\Sigma}(g, \delta g, \mathcal{L}_{\xi} g) = \Omega_{\Sigma}(\theta, \delta\theta, \mathcal{L}_{\xi}\theta) + \int_{\partial\Sigma} \epsilon^{ab} (\delta\psi_{ab}(g, \mathcal{L}_{\xi} g) - \mathcal{L}_{\xi}\psi_{ab}(g, \delta g)) \mathrm{d}S. \tag{3.98}$$

Correspondingly, the Noether charge two-form $Q_{ab}(\xi, g)$ arising in the metric formulation differs from $Q_{ab}(\xi, \theta)$ in the tetrad formulation by the term $2\psi_{ab}(g, \mathcal{L}_{\xi} g)$. Explicitly, using the metric Lagrangian, one finds that[11]

$$\tfrac{1}{4}\epsilon^{ab} Q_{ab}(\xi, g) = -4 t_{[c} s_{d]}{}^{g}\nabla^{c}\xi^{d} = 4\xi^{d} t^{c\,g}\nabla_{c} s_{d} - 2(s^{c}\mathcal{L}_{\xi} t_{c} + t^{c}\mathcal{L}_{\xi} s_{c}). \tag{3.99}$$

Here the first term in Eq. (3.99) is simply the Noether charge (3.63) evaluated in the adapted orthonormal frame (3.89),

$$\epsilon^{ab} Q_{ab}(\xi, \vartheta) = 4\xi^{c}\Gamma_{c}{}^{\mu\nu}(\vartheta)\epsilon^{ab}\epsilon_{abmn}(g)\vartheta^{m}_{\mu}\vartheta^{n}_{\nu} = 16\xi^{c} t_{\mu} s_{\nu}\vartheta^{b\mu\,g}\nabla_{c}\vartheta^{\nu}_{b} = 16\xi^{c} t^{d\,g}\nabla_{c} s_{d} \tag{3.100}$$

since $\mathcal{P}_{\mathcal{B}}({}^{g}\nabla_{[c} s_{d]}) = 0$ by hypersurface orthogonality of s_d. The second term in Eq. (3.99) simplifies through the hypersurface orthogonality relations (3.6) and (3.7), leading to

$$t^{c}\mathcal{L}_{\xi} s_{c} = t^{c}(2\xi^{b\,g}\nabla_{[b} s_{c]} + \partial_{c}(\xi^{b} s_{b})) = 0 \tag{3.101}$$

and

$$s^{c}\mathcal{L}_{\xi} t_{c} = -\xi^{a}\frac{N}{\alpha}\partial_{a}\beta, \tag{3.102}$$

where α, β, N are scalar functions defined by

$$s_{a} = \alpha\partial_{a} s, \quad t_{a} = -N(\partial_{a} t + \beta\partial_{a} s) \tag{3.103}$$

with

$$\mathcal{L}_{\xi} t = \xi^{e}\partial_{e} t = 1, \quad \mathcal{L}_{\xi} s = \xi^{e}\partial_{e} s = 0. \tag{3.104}$$

Hence we obtain the relation

$$\epsilon^{ab} Q_{ab}(\xi, g) = \epsilon^{ab} Q_{ab}(\xi, \vartheta) + 8\xi^{a}\frac{N}{\alpha}\partial_{a}\beta. \tag{3.105}$$

A similar relation can be shown to hold between the respective symplectic vectors arising in the tetrad and metric Hamiltonian formulations of General Relativity. In particular, by direct

calculation with g_{ab} as the field variable, one finds that the full Dirichlet boundary condition (3.34) yields a Hamiltonian conjugate to ξ^a on Σ whose boundary term is given by

$$H^{\mathrm{D}}(\xi;g)=8\int_{\partial\Sigma}\xi^c P_c^{\mathrm{D}}(g)\mathrm{d}S, \tag{3.106}$$

where

$$P_c^{\mathrm{D}}(g)=P_c^{\mathrm{D}}(\vartheta)+\frac{N}{\alpha}\partial_c\beta. \tag{3.107}$$

This differs from the symplectic vector in the tetrad formulation by the same gradient term occurring in the Noether charges (3.105). The extrinsic part (3.38) of the Dirichlet boundary condition is necessary in obtaining this Hamiltonian, because of the boundary term in the presymplectic form (3.98). Interestingly, in the case when ξ^a is orthogonal to Σ_t, then $\beta=0$, and one finds that the weaker, intrinsic Dirichlet boundary condition (3.37) is sufficient for existence of the metric Hamiltonian (3.106) and (3.107). Moreover, in this case the presymplectic form (3.98) and symplectic vector (3.107) are exactly the same as those obtained in the tetrad formulation using the adapted orthonormal frame (3.89).

An expression for the Dirichlet Hamiltonian boundary term (3.106) in terms of the standard ADM canonical variables associated with Σ, and its relation to quasilocal quantities of Brown and York,[16,17] will be derived in Sec. III F.

E. Determination of allowed boundary conditions

A necessary and sufficient condition[10] on variations $\delta\theta_a^\mu$ for the existence of a Hamiltonian (3.76) conjugate to ξ^a on Σ is given by the antisymmetrized variation of the equation (3.72) for the boundary term. This yields

$$\epsilon^{ab}\xi^c\omega_{abc}(\theta,\delta_1\theta,\delta_2\theta)\big|_{\partial\Sigma}=\sigma_a{}^b\partial_b\tilde{\beta}^a(\xi,\gamma;\delta_1\theta,\delta_2\theta)\big|_{\partial\Sigma} \tag{3.108}$$

with

$$\tilde{\beta}^a(\xi,\theta;\delta_1\theta,\delta_2\theta)=\epsilon^{ab}\delta_1\alpha_b(\xi,\theta;\delta_2\theta)-\epsilon^{ab}\delta_2\alpha_b(\xi,\theta;\delta_1\theta). \tag{3.109}$$

To begin, we simplify the expression (3.66) for $\omega_{abc}(\theta,\delta_1\theta,\delta_2\theta)$. First, using Eq. (3.74) for $\Theta_{abc}(\theta,\delta\theta)$ and taking into account the orthogonality $\xi^a s_a=0$, we have

$$\tfrac{1}{16}\epsilon^{ab}\xi^c\Theta_{abc}(\theta,\delta\theta)=\xi^c t_c h_\mu{}^a\delta(s_\nu h^{b\mu g}\nabla_a\theta_b^\nu) \tag{3.110}$$

through the frame decomposition (3.41) and the relation $\Gamma_a{}^{\mu\nu}(\theta)=\theta^{c\mu\,g}\nabla_a\theta_c^\nu=-\theta^{c\nu\,g}\nabla_a\theta_c^\mu$. Now we substitute the identity ${}^g\nabla_a\theta_b^\nu=h_a{}^{c\,g}\nabla_c\theta_b^\nu-s_a s^{c\,g}\nabla_c\theta_b^\nu$ and then use the relations $h^{a\mu}\delta s_a=0$, $h^{a\mu}s_a=0$ to simplify the term

$$h_\mu{}^a\delta(s_\nu s_a h^{b\mu}s^{c\,g}\nabla_c\theta_b^\nu)=0. \tag{3.111}$$

Thus, Eq. (3.110) becomes

$$\tfrac{1}{16}\epsilon^{ab}\xi^c\Theta_{abc}(\theta,\delta\theta)=\xi^c t_c h^{a\mu}\delta(s_\nu h_\mu{}^b h_a{}^{c\ g}\nabla_c\theta_b^\nu). \tag{3.112}$$

Finally, we substitute $\xi^c t_c=\frac{1}{2}\epsilon^{ab}\xi^c\epsilon_{abc}(h)$.

Hence, we obtain

$$\mathcal{P}_{\mathcal{B}}\Theta_{abc}(\theta,\delta\theta)=8\,\epsilon_{abc}(h)h_\mu{}^d\delta K_d{}^\mu, \tag{3.113}$$

where we define

$$K_a{}^\mu = s_\nu h^{b\mu} h_a{}^c{}^g \nabla_c \theta_b^\nu = s_\nu h_a{}^c \Gamma_c{}^{\mu\nu}(\theta). \tag{3.114}$$

Note that $s^a K_a{}^\mu = 0$ and $s_\mu K_a{}^\mu = 0$. From Eq. (3.113), by taking an antisymmetric variation and then using Eq. (3.46) for the variation of $\epsilon_{abc}(h)$, we have

$$\mathcal{P}_{\mathcal{B}} \omega_{abc}(\theta, \delta_1\theta, \delta_2\theta) = 8\epsilon_{abc}(h)((\delta_1 h_\mu{}^d - h_\mu{}^d h_e{}^\nu \delta_1 h_\nu{}^e)\delta_2 K_d{}^\mu - (\delta_2 h_\mu{}^d - h_\mu{}^d h_e{}^\nu \delta_2 h_\nu{}^e)\delta_1 K_d{}^\mu). \tag{3.115}$$

Substitution of this expression into Eq. (3.108) yields the following result.

Theorem 3.4: *A Hamiltonian conjugate to ξ^a on Σ exists for variations $\delta\theta_a^\mu$ with support on $\partial\Sigma$ if and only if*

$$\begin{aligned}&((\delta_1 h_\mu{}^d - h_\mu{}^d h_e{}^\nu \delta_1 h_\nu{}^e)\delta_2 K_d{}^\mu - (\delta_2 h_\mu{}^d - h_\mu{}^d h_e{}^\nu \delta_2 h_\nu{}^e)\delta_1 K_d{}^\mu)\big|_{\partial\Sigma} \\ &\quad = \frac{1}{16N}\sigma_a{}^b \partial_b \tilde{\beta}^a(\xi, \theta; \delta_1\theta, \delta_2\theta)\big|_{\partial\Sigma}\end{aligned} \tag{3.116}$$

for some $\tilde{\beta}^a(\xi, \theta; \delta_1\theta, \delta_2\theta)$ of the form (3.109). The Hamiltonian is given by

$$H_\Sigma(\xi; \theta) = 8\int_\Sigma \xi^e n_\mu (R_e{}^\mu(\theta) - \tfrac{1}{2}\theta_e^\mu R(\theta))\mathrm{d}\Sigma + H_B(\xi; \theta) \tag{3.117}$$

with boundary term

$$H_B(\xi, \theta) = \int_{\partial\Sigma} Q_{ab}(\xi, \theta) - \xi^c \tilde{B}_{abc}(\theta), \tag{3.118}$$

where $\tilde{B}_{abc}(\theta)$ is determined from

$$\xi^c(\mathcal{P}_{\mathcal{B}}\delta\tilde{B}_{abc}(\theta) - 8\epsilon_{abc}(h)h_\mu{}^d \delta K_d{}^\mu) = \mathcal{P}_{\mathcal{B}}\partial_{[a}\alpha_{b]}(\xi, \theta; \delta\theta). \tag{3.119}$$

Thus, equation (3.116) determines the allowed boundary conditions on variations $\delta\theta_a^\mu$ for the existence of a Hamiltonian formulation (3.117) for the vacuum Einstein equations. To proceed, we now parallel the analysis of the similar boundary condition determining equation for the Maxwell equations in Sec. II C.

Two obvious solutions of the determining equation (3.116) with $\tilde{\beta}^a(\xi, \theta; \delta_1\theta, \delta_2\theta) = 0$ are given by $\delta h_\mu{}^a|_{\partial\Sigma_t} = 0$, $t \geqslant 0$, which is the Dirichlet boundary condition (3.77) already considered; and by

$$\delta K_a{}^\mu|_{\partial\Sigma_t} = 0, \quad t \geqslant 0, \tag{3.120}$$

which we call the *Neumann boundary condition*. For the boundary condition (3.120), it follows from Eqs. (3.76) and (3.119) that the corresponding Hamiltonian boundary term is given by

$$H^{\mathrm{N}}(\xi; \theta) = 8\int_{\partial\Sigma} \xi^c P_c^{\mathrm{N}}(\theta)\mathrm{d}S, \tag{3.121}$$

where

$$P_c^{\mathrm{N}}(\theta) = t_\mu s_\nu \Gamma_c{}^{\mu\nu}(\theta) = t^a s_\nu{}^g \nabla_c \theta_a^\nu \tag{3.122}$$

by a derivation similar to Eq. (3.87). In the orthonormal frame (3.89) adapted to the boundary two-surfaces $\partial\Sigma_t$, we have

$$P_c^{\mathrm{N}}(\vartheta) = t^{ag}\nabla_c s_a . \tag{3.123}$$

We refer to this as the *Neumann symplectic vector* associated with the boundary two-surfaces $\partial\Sigma_t$. Moreover, in this frame the Neumann boundary condition (3.120) becomes

$$\delta K_a{}^{\mu}|_{\partial\Sigma_t} = \delta(h^{b\mu}K_{ab})|_{\partial\Sigma_t} = 0, \quad t \geqslant 0 \tag{3.124}$$

in terms of

$$K_{ab} = h_a{}^c h_b{}^d \nabla_c s_d , \tag{3.125}$$

which is the extrinsic curvature of the timelike boundary hypersurface $\mathcal{B}$ in (M,g). Thus, geometrically, the Neumann boundary condition corresponds to fixing the frame components of the boundary hypersurface extrinsic curvature,

$$\delta(h^{b\mu}h_a{}^{c\,g}\nabla_c s_b) = 0 \quad \text{on } \mathcal{B}. \tag{3.126}$$

These components measure the rotation and boost of the hypersurface normal s_a with respect to the frame h_a^{μ} under displacement on $\mathcal{B}$.

We now investigate more general boundary conditions. Note that, on the left-hand side of the determining equation (3.116), $\epsilon^{ab}\xi^c\omega_{abc}(\theta,\delta_1\theta,\delta_2\theta)$ involves only the field variations $\mathcal{P}_{\mathcal{B}}\delta h_{\mu}{}^a$ and $\mathcal{P}_{\mathcal{B}}\delta K_a{}^{\mu} = \mathcal{P}_{\mathcal{B}}\delta(s_\nu h_a{}^c \Gamma_a{}^{\mu\nu}(\theta))$. We call $h_{\mu}{}^a$ and $K_a{}^{\mu}$ the *symplectic boundary data* at $\partial\Sigma_t$ and consider boundary conditions of the form

$$\delta\mathcal{F}_a^{\mu}(h_c{}^{\nu}, K_c{}^{\nu})|_{\partial\Sigma_t} = 0, \quad t \geqslant 0, \tag{3.127}$$

where $\mathcal{F}_a^{\mu}(h_c{}^{\nu}, K_c{}^{\nu})$ is locally constructed as an algebraic expression in terms of the symplectic boundary data and fixed quantities (including the space–time coordinates). We call (3.127) a *mixed Dirichlet–Neumann* boundary condition if $\mathcal{F}_a^{\mu}(h_c{}^{\nu}, K_c{}^{\nu})$ is a constant-coefficient linear combination of the parts $\mathcal{P}_{\partial\Sigma}h_a{}^{\mu}$, $\mathcal{P}_t h_a{}^{\mu}$, $\mathcal{P}_{\partial\Sigma}K_a{}^{\mu}$, $\mathcal{P}_t K_a{}^{\mu}$ of the Dirichlet and Neumann boundary data in (3.77) and (3.120). Here the projections with respect to $\mathcal{P}_{\partial\Sigma}$ and $\mathcal{P}_t$ remove all components proportional to s_a.

An analysis of the boundary condition determining equation (3.116), given later, leads to the following main results.

Theorem 3.5: *The only allowed mixed Dirichlet–Neumann boundary conditions for the existence of a Hamiltonian (3.76) conjugate to ξ^a on Σ are given by*

$$\mathcal{P}_{\mathcal{B}}(a_0\delta K_a{}^{\mu} + b_0\delta h_a{}^{\mu})|_{\partial\Sigma_t} = 0, \quad t \geqslant 0, \tag{3.128}$$

or equivalently

$$\mathcal{F}_a^{\mu}(h_c{}^{\nu}, K_c{}^{\nu}) = a_0 K_a{}^{\mu} + b_0 h_a{}^{\mu} \tag{3.129}$$

for constants a_0, b_0 (and $\beta^a = 0$ in Eq. (3.116)). In the cases $a_0 = 0$ or $b_0 = 0$, respectively Dirichlet or Neumann boundary conditions, the corresponding Hamiltonian boundary terms are given by Eqs. (3.91) and (3.87), and Eqs. (3.121) and (3.122). In the case $a_0 \neq 0$, $b_0 \neq 0$, the corresponding Hamiltonian boundary term is given by

$$H^{\mathrm{DN}}(\xi;\theta) = 8\int_{\partial\Sigma} \xi^c P_c(\theta)\,\mathrm{d}S \tag{3.130}$$

where, now,

$$P_c(\theta) = P_c^{\mathrm{N}}(\theta) + 6\frac{b_0}{a_0}t_c\,. \tag{3.131}$$

(Note, the boundary terms here are unique up to adding an arbitrary covector function of the boundary data (3.129) to $P_c(\theta)$.)

A similar covariant derivation of the pure Dirichlet and Neumann boundary terms is presented in Refs. 18 and 19 from a different perspective. In Theorem 3.5, note that Eq. (3.128) represents a one-parameter a_0/b_0 family of boundary conditions. In particular, in contrast to the two-parameter family of analogous mixed Dirichlet–Neumann boundary conditions (2.52) allowed for the Maxwell equations, here decompositions of the symplectic boundary data with respect to $\mathcal{P}_{\partial\Sigma}$ and $\mathcal{P}_\xi$ do not yield boundary conditions satisfying the determining equation (3.116).

The form of the mixed Dirichlet–Neumann boundary condition (3.128) suggests we also consider boundary conditions specified by a trace part and trace-free part with respect to the boundary hypersurface frame $h_a{}^\mu$:

$$\delta\hat{\mathcal{F}}(h_c{}^\nu, K_c{}^\nu)\big|_{\partial\Sigma_t} = 0, \quad \delta\hat{\mathcal{F}}_a^\mu(h_c{}^\nu, K_c{}^\nu)\big|_{\partial\Sigma_t} = 0, \quad t \geqslant 0 \tag{3.132}$$

with $h_\mu{}^a\hat{\mathcal{F}}_a^\mu(h_c{}^\nu, K_c{}^\nu) = 0$. Taking the trace of the symplectic boundary data variations yields

$$h_\mu{}^a\delta K_a{}^\mu = \delta K + h_\mu{}^b h_\nu{}^a K_a{}^\mu \delta h_b{}^\nu \tag{3.133}$$

and

$$h_\mu{}^a\delta h_a{}^\mu = \delta\ln|h|\,, \tag{3.134}$$

where $K = h_\mu{}^a K_a{}^\mu$ is the trace of $K_a{}^\mu$ and $h = \det(h_a{}^\mu)$ is the determinant of the frame components $h_a{}^\mu$ in local coordinates.

Theorem 3.6: *Allowed boundary conditions (3.132) for the existence of a Hamiltonian (3.76) conjugate to ξ^a on Σ are given by*

$$\mathcal{P}_{\mathcal{B}}\delta(K_a{}^\mu - \tfrac{1}{3}h_a{}^\mu K)\big|_{\partial\Sigma_t} = 0, \quad t \geqslant 0, \tag{3.135}$$

$$(a_0\delta K + b_0\delta\ln|h|)\big|_{\partial\Sigma_t} = 0, \quad t \geqslant 0, \tag{3.136}$$

or equivalently

$$\hat{\mathcal{F}}(h,K) = a_0 K + b_0\ln|h|, \quad \hat{\mathcal{F}}_a^\mu(h_c{}^\nu, K_c{}^\nu) = \mathcal{P}_{\mathcal{B}}(K_a{}^\mu - \tfrac{1}{3}h_a{}^\mu K) \tag{3.137}$$

for constants a_0, b_0 (and $\beta^a = 0$ in Eq. (3.116)). The corresponding Hamiltonian boundary term is given by

$$H_B(\xi,\theta) = 8\int_{\partial\Sigma}\xi^c\left(\frac{1}{3}P_c^{\mathrm{D}}(\theta) + \frac{2}{3}P_c^{\mathrm{N}}(\theta) + 4\frac{b_0}{a_0}t_c\right)\mathrm{d}S \tag{3.138}$$

(which is unique up to adding a term depending on an arbitrary covector function of the boundary data (3.137)).

Finally, we remark that the mixed boundary conditions in Theorems 3.5 and 3.6 admit the following two generalizations.

First,

$$\hat{\mathcal{F}}_a^\mu(h_c{}^\nu, K_c{}^\nu) = a(x,K,\ln|h|)\mathcal{P}_{\mathcal{B}}(K_a{}^\mu - \tfrac{1}{3}h_a{}^\mu K), \tag{3.139}$$

$$\hat{\mathcal{F}}(h,K) = b(x,K,\ln|h|), \quad \partial_K b \neq 0 \tag{3.140}$$

for arbitrary functions $a(x,K,\ln|h|)$, $b(x,K,\ln|h|)$.

Second,

$$\mathcal{F}^{\mu}_{a}(h_c{}^{\nu},K_c{}^{\nu}) = a(x,K,\ln|h|)\mathcal{P}_{\mathcal{B}}(K_a{}^{\mu} + b(x,K,\ln|h|)h_a{}^{\mu}), \quad b \neq -\tfrac{1}{3}K \tag{3.141}$$

for an arbitrary function $b(x,K,\ln|h|)$, with the function $a(x,K,\ln|h|)$ now satisfying the linear partial differential equation

$$(\partial_K\hat{b})\partial_{\ln|h|}a + (\hat{b} + \partial_{\ln|h|}\hat{b})\partial_K a = \tfrac{2}{9}(-1 + 3\partial_K\hat{b})a, \quad \hat{b} = b + \tfrac{1}{3}K \tag{3.142}$$

obtained from the determining equation (3.116). The general form of a is given by solving the characteristic ordinary differential equations

$$\frac{\mathrm{d}\ln|h|}{\partial_K\hat{b}} = \frac{\mathrm{d}K}{\hat{b} + \partial_{\ln|h|}\hat{b}} = \frac{\mathrm{d}a}{\frac{2}{9}(-1 + 3\partial_K\hat{b})a} \tag{3.143}$$

in terms of the variables $\ln|h|$, K, a. For instance, if b is taken to be linear homogeneous in K, then one has $b = \lambda K$, $a = f(x,\lambda K\ln|h|)|h|^{(2/3)\lambda/(3\lambda-1)}$, where $\lambda = \text{const}$ and f is an arbitrary function.

Proofs of Theorems: Since any boundary condition locally constructed from the symplectic boundary data is linear homogeneous in $\mathcal{P}_{\mathcal{B}}\delta h_a{}^{\mu}$ and $\mathcal{P}_{\mathcal{B}}\delta K_a{}^{\mu}$, we begin by finding all such solutions of the determining equation (3.116).

First we show that $\tilde{\beta}^a = 0$. The right-hand side of Eq. (3.116) necessarily involves terms with at least one derivative on $\delta\theta^{\mu}_a$, while only first-order derivatives of $\delta\theta^{\mu}_a$ appear on the left-hand side of Eq. (3.116) through

$$\mathcal{P}_{\mathcal{B}}\delta K_a{}^{\mu} = s_{\nu}h_a{}^{c}\delta\Gamma_c{}^{\mu\nu}(\theta) \tag{3.144}$$

due to Eqs. (3.114) and (3.47). Thus, for a balance in numbers of derivatives, we must have

$$\alpha_a = \alpha_{a\mu}{}^{b}(\theta)\,\delta\theta^{\mu}_b \tag{3.145}$$

for some $\alpha_{a\mu}{}^{b}(\theta)$ locally constructed out of θ^{μ}_a and fixed quantities. This yields, for the antisymmetrized variation of α_a,

$$\beta_a = \alpha_{a\mu\nu}{}^{bc}(\theta)\,\delta_1\theta^{\mu}_b\delta_2\theta^{\nu}_c \tag{3.146}$$

where $\alpha_{a\mu\nu}{}^{bc}(\theta) = -\alpha_{a\nu\mu}{}^{cb}(\theta)$ is the curl of $\alpha_{a\mu}{}^{b}(\theta)$ with respect to θ^{ν}_c. Then, using Eqs. (3.109) and (3.50), we collect all the terms on the left-hand side of Eq. (3.116) linearly independent of $\delta h_a{}^{\mu}$, $\delta K_a{}^{\mu}$. Through Eqs. (3.144) and (3.49), the coefficients of these terms yield

$$s_c\tilde{\alpha}^{(be)c}{}_{\mu\nu}(\theta) = 0, \quad s_b\tilde{\alpha}^{[be]c}{}_{\mu\nu}(\theta) = 0, \quad s_c\tilde{\alpha}^{[be]c}{}_{\mu\nu}(\theta) = 0, \tag{3.147}$$

where

$$\tilde{\alpha}^{ebc}{}_{\mu\nu}(\theta) = \epsilon^{ae}\alpha_{a\mu\nu}{}^{bc}(\theta) = -\tilde{\alpha}^{ecb}{}_{\nu\mu}(\theta). \tag{3.148}$$

These algebraic equations are straightforward to solve, leading to

$$\alpha^{abc}{}_{\mu\nu}(\theta) = t^{[b}\alpha_1{}^{c]a}{}_{\mu\nu}(\theta) + \alpha_2{}^{abc}{}_{\mu\nu}(\theta) + t^b t^c\alpha_3{}^{a}{}_{\mu\nu}(\theta) + t^{(b}\alpha_4{}^{c)a}{}_{\mu\nu}(\theta) \tag{3.149}$$

for some

$$\begin{gathered}\alpha_1{}^{ca}{}_{\mu\nu} = \sigma_b{}^{c}\sigma_d{}^{a}\alpha_1{}^{bd}{}_{(\mu\nu)}, \quad \alpha_2{}^{abc}{}_{\mu\nu} = -\sigma_e{}^{a}\sigma_d{}^{b}\sigma_f{}^{c}\alpha_2{}^{edf}{}_{\nu\mu}, \\ \alpha_3{}^{a}{}_{\mu\nu} = \sigma_e{}^{a}\alpha_3{}^{e}{}_{[\mu\nu]}, \quad \alpha_4{}^{ca}{}_{\mu\nu} = \sigma_b{}^{c}\sigma_d{}^{a}\alpha_4{}^{bd}{}_{[\mu\nu]}.\end{gathered} \tag{3.150}$$

Then, returning to Eq. (3.145), we note that $\alpha_{a\mu}{}^{b}(\theta)=\theta_a^{\alpha}\theta^b_{\beta}\alpha^{\beta}_{\mu\alpha}$ for some $\alpha^{\beta}_{\mu\alpha}$ that is locally constructed only from fixed quantities since it is a scalar expression. Thus we immediately obtain

$$\alpha^{abc}_{\mu\nu}(\theta)=\theta^b_{\beta}\theta^c_{\gamma}\theta^{a\alpha}(\alpha^{\beta}_{\nu\mu}\delta^{\gamma}_{\alpha}-\alpha^{\gamma}_{\mu\nu}\delta^{\beta}_{\alpha}-\alpha^{\gamma}_{\alpha\mu}\delta^{\beta}_{\nu}+\alpha^{\beta}_{\alpha\mu}\delta^{\gamma}_{\nu}). \tag{3.151}$$

By equating expressions (3.149) and (3.151), we find that after some algebraic analysis

$$\alpha^{\gamma}_{\nu\mu}=\delta^{\gamma}_{\nu}\alpha_{0\mu} \tag{3.152}$$

for some $\alpha_{0\mu}$. Now, substitution of expression (3.152) back into Eqs. (3.149) and (3.151) easily leads to the result

$$\alpha_{1\mu\nu}{}^{ca}=\alpha_{2\mu\nu}{}^{abc}=\alpha_{3\mu\nu}{}^{a}=\alpha_{4\mu\nu}{}^{ca}=0. \tag{3.153}$$

Hence, from Eq. (3.149), we have $\alpha_{a\mu\nu}{}^{bc}(\theta)=0$ and so $\beta_a=0$. This establishes that $\tilde{\beta}^a=0$.

Consequently, the determining equation (3.116) reduces to

$$(\delta_1 h_{\mu}{}^{d}-h_{\mu}{}^{d}h_e{}^{\nu}\delta_1 h_{\nu}{}^{e})\delta_2 K_d{}^{\mu}-(\delta_2 h_{\mu}{}^{d}-h_{\mu}{}^{d}h_e{}^{\nu}\delta_2 h_{\nu}{}^{e})\delta_1 K_d{}^{\mu}=0, \tag{3.154}$$

which is equivalent to

$$h_{[\nu}{}^{d}h_{\mu]}{}^{e}(\delta_1 h_e{}^{\nu}\delta_2 K_d{}^{\mu}-\delta_2 h_e{}^{\nu}\delta_1 K_d{}^{\mu})=0. \tag{3.155}$$

Then the algebraic solution of Eq. (3.155) in terms of $\mathcal{P}_{\mathcal{B}}\delta h_e{}^{\nu}$ and $\mathcal{P}_{\mathcal{B}}\delta K_d{}^{\mu}$ has the form

$$\Pi_1{}^{\mu b}_{a\nu}\mathcal{P}_{\mathcal{B}}\delta h_b{}^{\nu}+\Pi_2{}^{\mu b}_{a\nu}\mathcal{P}_{\mathcal{B}}\delta K_b{}^{\nu}=0 \tag{3.156}$$

for some coefficient tensors $\Pi^{\mu b}_{a\nu}$ such that

$$\Pi^{\mu b}_{a\nu}h_{[\alpha}{}^{a}h_{\mu]}{}^{c}=\Pi^{\mu c}_{a\alpha}h_{[\nu}{}^{a}h_{\mu]}{}^{b}. \tag{3.157}$$

It is straightforward to show that Eq. (3.157) holds iff

$$\Pi^{\mu b}_{a\nu}=\hat{\Pi}^{\mu b}_{a\nu}-h_a{}^{\mu}\hat{\Pi}^{b}_{\nu}+h_{\nu}{}^{b}\hat{\Pi}^{\mu}_{a}, \tag{3.158}$$

where $\hat{\Pi}^{\mu b}_{a\nu}h_{\alpha}{}^{a}h_{\mu}{}^{c}=\hat{\Pi}^{\mu c}_{a\alpha}h_{\nu}{}^{a}h_{\mu}{}^{b}$ is the symmetric part of $\Pi^{\mu b}_{a\nu}$ in the index pairs (a,μ) and (b,ν), and where $\hat{\Pi}^{b}_{\nu}=h_{\mu}{}^{a}\hat{\Pi}^{\mu b}_{a\nu}$, $\hat{\Pi}^{\mu}_{a}=h_b{}^{\nu}\hat{\Pi}^{\mu b}_{a\nu}$ is the trace part of $\Pi^{\mu b}_{a\nu}$ in the frame $h_a{}^{\mu}$. Thus, we have established the following result.

Lemma 3.7: All solutions of the determining equation (3.116) for allowed boundary conditions that are linear homogeneous in $\mathcal{P}_{\mathcal{B}}\delta h_a{}^{\mu}$ and $\mathcal{P}_{\mathcal{B}}\delta K_a{}^{\mu}$ have the form (3.156) where the coefficient tensors are given by Eq. (3.158).

Now, for mixed Dirichlet–Neumann boundary conditions, we take

$$\Pi_1{}^{\mu b}_{a\nu}=a_1(\mathcal{P}_{\partial\Sigma})_a{}^{b}\sigma_{\nu}{}^{\mu}+a_0(\mathcal{P}_t)_a{}^{b}t_{\nu}t^{\mu}, \tag{3.159}$$

$$\Pi_2{}^{\mu b}_{a\nu}=b_1(\mathcal{P}_{\partial\Sigma})_a{}^{b}\sigma_{\nu}{}^{\mu}+b_0(\mathcal{P}_t)_a{}^{b}t_{\nu}t^{\mu}, \tag{3.160}$$

where a_0, a_1, b_0, b_1 are constants. Then the requirement (3.158) leads directly to

$$a_0=a_1, \quad b_0=b_1. \tag{3.161}$$

Substitution of Eqs. (3.159)–(3.161) into Eq. (3.156) yields the mixed Dirichlet–Neumann boundary conditions (3.128).

Finally, the other boundary conditions (3.135) and (3.136) arise from

$$\Pi_{1a\nu}^{\mu b}=\frac{1}{2}\frac{b_0}{a_0}h_a{}^{\mu}h_{\nu}{}^{b}-\frac{1}{3}Kh_d{}^{e}h_{\nu}{}^{\mu}, \tag{3.162}$$

$$\Pi_{2a\nu}^{\mu b}=h_a{}^{b}h_{\nu}{}^{\mu}, \tag{3.163}$$

which are easily verified to satisfy the requirement (3.158).

This completes the proofs of Theorems 3.5 and 3.6. □

As a concluding remark, we note that Lemma 3.7 yields the following necessary and sufficient determining equations for finding all boundary conditions (3.127).

Lemma 3.8: All allowed boundary conditions of the form $\mathcal{F}_a^{\mu}(h_c{}^{\nu},K_c{}^{\nu})|_{\partial\Sigma}=0$ *for the existence of a Hamiltonian conjugate to* ξ^a *on* Σ *are given by the solutions of*

$$\frac{\partial\mathcal{F}_a^{\mu}}{\partial h_b{}^{\nu}}h_{[\alpha}{}^{a}h_{\mu]}{}^{c}=\frac{\partial\mathcal{F}_a^{\mu}}{\partial h_c{}^{\alpha}}h_{[\nu}{}^{a}h_{\mu]}{}^{b}, \tag{3.164}$$

$$\frac{\partial\mathcal{F}_a^{\mu}}{\partial K_b{}^{\nu}}h_{[\alpha}{}^{a}h_{\mu]}{}^{c}=\frac{\partial\mathcal{F}_a^{\mu}}{\partial K_c{}^{\alpha}}h_{[\nu}{}^{a}h_{\mu]}{}^{b}. \tag{3.165}$$

We will leave a general analysis of the boundary condition determining equations (3.164) and (3.165) for elsewhere.

F. Relation between covariant and canonical Hamiltonians and boundary terms

To conclude this section, we first give a brief discussion of the Hamiltonian field equations for General Relativity using the covariant symplectic structure and Noether charge Hamiltonian in Sec. III C. Then we discuss the boundary terms in the Dirichlet and Neumann Hamiltonians expressed in standard ADM canonical variables.

For a Hamiltonian (3.76) conjugate to ξ^a on Σ, the associated field equations are obtained through the presymplectic form (3.69) by the variational principle

$$\Omega_{\Sigma}(\theta,\delta\theta,\mathcal{L}_{\xi}\theta)-H'_{\Sigma}(\xi;\theta,\delta\theta)=\int_{\Sigma}8\xi^d n_d(R_{\mu}{}^{e}(\theta)-\tfrac{1}{2}\theta_{\mu}^{e})\delta\theta_e^{\mu}\mathrm{d}\Sigma=0 \tag{3.166}$$

for arbitrary variations $\delta\theta_e^{\mu}|_{\Sigma}$. These field equations split into evolution equations and constraint equations with respect to Σ corresponding to a decomposition of θ_a^{μ} into dynamical and nondynamical components determined by[4] the degeneracy of

$$\Omega_{\Sigma}(\theta,\delta_1\theta,\delta_2\theta)=\int_{\Sigma}\omega_{abc}(\theta,\delta_1\theta,\delta_2\theta)=\int_{\Sigma}\tfrac{1}{6}\epsilon^{abcd}n_d\omega_{abc}(\theta,\delta_1\theta,\delta_2\theta)\mathrm{d}\Sigma. \tag{3.167}$$

For this purpose, it is convenient to partially fix the SO(3,1) local gauge freedom in θ_e^{μ} analogously to conditions (3.15)–(3.17) by choosing the frame components $n^{\mu}=n^a\theta_a^{\mu}$ to be fixed constants on M. Then, through a simplification of the symplectic current here similar to Eq. (3.115), we obtain

$$\tfrac{1}{48}\epsilon^{abcd}n_d\omega_{abc}(\theta,\delta_1\theta,\delta_2\theta)=-(\delta_1q_{\mu}{}^{d}-q_{\mu}{}^{d}q_e{}^{\nu}\delta_1q_{\nu}{}^{e})\delta_2p_d{}^{\mu}+(\delta_2q_{\mu}{}^{d}-q_{\mu}{}^{d}q_e{}^{\nu}\delta_2q_{\nu}{}^{e})\delta_1p_d{}^{\mu}, \tag{3.168}$$

where we define

$$q_a{}^{\mu}=\theta_a^{\mu}+n_an^{\mu},\quad p_a{}^{\mu}=n_{\nu}q^{b\mu}q_a{}^{c}\,{}^{g}\nabla_c\theta_b^{\nu}=n_{\nu}q_a{}^{c}\Gamma_c{}^{\mu\nu}(\theta) \tag{3.169}$$

with $q_{ab}=g_{ab}+n_an_b$, which are counterparts of $h_a{}^{\mu}$, $K_a{}^{\mu}$ associated with the spacelike hypersurface Σ. (Geometrically, $q_a{}^{\mu}$ is a frame for the hypersurface metric $q_{ab}=q_a{}^{\mu}q_b{}^{\nu}\eta_{\mu\nu}$, while $p_a{}^{\mu}$

represents the frame components of the hypersurface extrinsic curvature $\mathcal{K}_{ab}=q_a{}^\mu p_b{}^\nu \eta_{\mu\nu} = q_a{}^c\, {}^g\nabla_c n_b$.) Hence, the degeneracy directions of the presymplectic form (3.167) are given by variations $\delta\theta_a^\mu$ satisfying

$$\delta(q_a{}^\mu/|q|) = \delta p_a{}^\mu = 0, \tag{3.170}$$

where $|q| = \det(q_a{}^\mu)$ and $\delta \ln |q| = q_\nu{}^b \delta q_b{}^\nu$. This immediately leads to the following result, analogous to the discussion in Sec. II A for the Maxwell equations.

Proposition 3.9: For a Hamiltonian $H_\Sigma(\xi;\theta)$ conjugate to ξ^a on Σ, let $\theta_{\ker\omega}$ denote the field components of θ_a^μ and $\Gamma_a{}^{\mu\nu}(\theta)$ invariant under the symplectic degeneracy directions (3.170), and let θ_ω denote the remaining field components modulo $\theta_{\ker\omega}$. Then there is corresponding decomposition of the Hamiltonian field equations given by $H'_\Sigma(\xi;\theta,\delta\theta_{\ker\omega})=0$ and $H'_\Sigma(\xi;\theta,\delta\theta_\omega) = \Omega_\Sigma(\theta,\delta\theta_\omega,\mathcal{L}_\xi\theta)$, which, respectively, yield

$$n^a R_a{}^\mu(\theta) - \tfrac{1}{2} n^\mu R(\theta) = 0, \tag{3.171}$$

$$q_a{}^b R_b{}^\mu(\theta) = 0. \tag{3.172}$$

These field equations arise equivalently by variation of $\mathcal{P}_n\theta_a^\mu = -n_a n^\mu$ and $\mathcal{P}_\Sigma\theta_a^\mu = q_a{}^\mu$ in the Lagrangian (3.52).

Equations (3.171) and (3.172) are the frame components of the standard $3+1$ split of the vacuum Einstein equations[12] into constraint equations and time-evolution equations for the hypersurface metric q_{ab}. Thus, the Hamiltonian field equations given by the variational principle (3.166) constitute a covariant formulation of the standard ADM Hamiltonian equations for General Relativity.

With respect to the spacelike hypersurface Σ, one has a decomposition of ξ^a into normal and tangential parts

$$\xi^a = \mathcal{N} n^a + \mathcal{N}^a, \tag{3.173}$$

where $\mathcal{N}^a = \mathcal{P}_\Sigma(\xi^a)$ and $\mathcal{N} = -\xi^a n_a$ define the lapse and shift of the time flow vector field ξ^a. By use of the Gauss–Codacci equations, we straightforwardly see that the volume part of a Hamiltonian (3.76) conjugate to ξ^a on Σ is given by the "pure constraint form" [11]

$$H(\xi;\theta) = 4\int_\Sigma \mathcal{N}(\mathcal{R} + \mathcal{K}^2 - \mathcal{K}_{ab}\mathcal{K}^{ab}) + 2\mathcal{N}^c(\mathcal{D}^b\mathcal{K}_{bc} - \mathcal{D}_c\mathcal{K})\,\mathrm{d}\Sigma, \tag{3.174}$$

where $\mathcal{R}_{ab}$ and $\mathcal{K}_{ab}$ are the Ricci curvature and extrinsic curvature of the metric $\mathcal{P}_{\Sigma g_{ab}} = q_{ab}$, $\mathcal{R} = \mathcal{R}_a{}^a$ and $\mathcal{K} = \mathcal{K}_a{}^a$ are the corresponding scalar curvatures, and $\mathcal{D}_a$ is the derivative operator associated with q_{ab}. (An analogous result holds more generally for any diffeomorphism covariant Lagrangian field theory.[4]) This demonstrates, explicitly, that our covariant analysis of allowed boundary conditions and corresponding boundary terms for General Relativity in Secs. III B and III E is equivalent to a canonical analysis of the ADM Hamiltonian.

Now, consider Dirichlet or Neumann boundary conditions imposed at the two-surfaces $\partial\Sigma_t$, for $t \geqslant 0$. On solutions of the Hamiltonian field equations, the total Hamiltonian $H_\Sigma(\xi;\theta)$ reduces, respectively, to the Dirichlet and Neumann boundary terms (3.91) and (3.121). Let u^a denote the outward unit normal to $\partial\Sigma_t$ in Σ_t. Let $\mathfrak{d}_a^\mu$ be an orthonormal frame adapted to Σ_t given by

$$\mathfrak{d}_a^0 = n_a, \mathfrak{d}_a^1 = u_a, \mathfrak{d}_{[a}^2 \mathfrak{d}_{b]}^3 = \epsilon_{ab}, \mathfrak{d}_a^2 = \epsilon_a{}^b \mathfrak{d}_b^3, \tag{3.175}$$

which is related to the frame ϑ_a^μ adapted to $\mathcal{B}$ by a boost in the normal space $T^\perp(\partial\Sigma_t)$ to the boundary two-surface $\partial\Sigma_t$,

$$t^a = n^a \cosh\chi + u^a \sinh\chi, \quad s^a = u^a \cosh\chi + n^a \sinh\chi. \tag{3.176}$$

Through the corresponding boost relation (3.95) applied to the symplectic vectors (3.92) and (3.123), the Hamiltonian boundary terms take the respective form

$$\xi^c P_c^{\mathrm{D}}(\tilde{\vartheta}) = \xi^c (n^a \sigma_c{}^{d\,g} \nabla_d u_a - n_c \sigma^{bd\,g} \nabla_b u_d + u_c \sigma^{bd\,g} \nabla_b n_d - \sigma_c{}^{d\,g} \nabla_d \chi), \tag{3.177}$$

$$\xi^c P_c^{\mathrm{N}}(\tilde{\vartheta}) = \xi^c (n^{a\,g} \nabla_c u_a - {}^g\nabla_c \chi). \tag{3.178}$$

These expressions can be simplified in terms of the hypersurface metric q_{ab}, extrinsic curvature $\mathcal{K}_{ab}$, and acceleration $a_b = n^{e\,g} \nabla_e n_b$. We find that

$$\xi^c P_c^{\mathrm{D}}(\tilde{\vartheta}) = \mathcal{N}\kappa - \mathcal{N}^a u^b \mathcal{K}_{ab} - \mathcal{N}_\parallel^a \partial_a \chi, \tag{3.179}$$

$$\xi^c P_c^{\mathrm{N}}(\tilde{\vartheta}) = -\mathcal{N} u^b a_b - \mathcal{N}^a u^b \mathcal{K}_{ab} - \mathcal{N}\partial_t \chi - \mathcal{N}_\perp u^a \partial_a \chi - \mathcal{N}_\parallel^a \partial_a \chi, \tag{3.180}$$

where $\mathcal{N}_\parallel^a = \mathcal{P}_{\partial\Sigma}(\mathcal{N}^a)$, $\mathcal{N}_\perp = u_a \mathcal{N}^a$ are the tangential and normal parts of the shift with respect to $\partial\Sigma_t$, and $\kappa = \sigma^{ab\,g} \nabla_a u_b$ is the mean extrinsic curvature of $\partial\Sigma_t$ in Σ_t.

We note that this form of the Dirichlet and Neumann boundary terms (3.179) and (3.180) agrees with the canonical analysis of boundary terms for the ADM Hamiltonian carried out in Refs. 16 and 17. Moreover, in the case when Σ_t is orthogonal to $\mathcal{B}$, i.e., $\chi = 0$, the surface integral $\int_{\partial\Sigma} \xi^c P_c^{\mathrm{D}}(\tilde{\vartheta}) \mathrm{d}S$ for suitable choice of ξ^c reproduces Brown and York's expressions for quasilocal energy, normal momentum, and tangential momentum quantities (respectively, $\mathcal{N}=1$, $\mathcal{N}^a=0$; $\mathcal{N}=0$, $\mathcal{N}_\parallel^a=0$, $\mathcal{N}_\perp=1$; $\mathcal{N}=\mathcal{N}_\perp=0$, $\mathcal{N}_\parallel^a\neq 0$). Further discussion of quasilocal quantities associated with the Dirichlet and Neumann symplectic vectors (3.92) and (3.123) will be left for elsewhere.

IV. CONCLUDING REMARKS

In this paper we have given a mathematical investigation of boundary conditions on the gravitational field required for the existence of a well-defined covariant Hamiltonian variational principle for General Relativity when spatial boundaries are considered, with a fixed time-flow vector field. In particular, a main result is that we obtain a covariant derivation of Dirichlet, Neumann, and mixed type boundary conditions for the gravitational field in any fixed spatially bounded region of space–time. We show that the resulting Dirichlet and Neumann Hamiltonians lead to covariant Hamiltonian field equations which are equivalent to the standard $3+1$ split of the Einstein equations into constraint equations and time-evolution equations. In addition, we obtain a uniqueness result for the allowed boundary conditions based on the covariant symplectic structure associated with the Einstein equations.

However, we do not address the purely analytical issue of whether the boundary-initial value problem for the Einstein equations is well-posed with these boundary conditions (i.e., do there exist solutions of the Einstein equations satisfying the boundary conditions, initial conditions, and constraints). For work in that direction, see e.g. Ref. 20.

A further interesting generalization of our results would be to treat a space–time region whose spatial boundary is dynamical, e.g., a black-hole horizon or Cauchy boundary. We note that boundary conditions for this situation may be investigated by allowing the time-flow vector field to depend on the space–time metric instead of being a fixed quantity. This analysis will be pursued elsewhere.

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APPENDIX: NOETHER CHARGE METHOD

First of all, consider in n space–time dimensions a general Lagrangian field theory for a set of fields denoted collectively by ϕ. It will be assumed that these fields are defined as sections of a vector bundle E over the space–time manifold M, using local coordinates on M and E. The theory

will be assumed to be described by a Lagrangian n-form $L(\phi)$ that is locally constructed out of the fields ϕ and their partial derivatives $\partial^k\phi$ to some finite order k (and fixed background structure, if any, on M and E).

The Lagrangian $L(\phi)$ provides a variational principle

$$S(\phi)=\int_M L(\phi), \tag{A1}$$

which yields the field equations $\mathcal{E}(\phi)=0$ obtained as the stationary points of $S(\phi)$,

$$\delta S(\phi)=\int_M \delta L(\phi)=\int_M \mathcal{E}(\phi)\,\delta\phi=0, \tag{A2}$$

under variations $\delta\phi$ of ϕ with compact support on M. For arbitrary variations $\delta\phi$, which are not restricted to have compact support, one then has a variational identity

$$L'(\phi,\delta\phi)\equiv\delta L(\phi)=\mathcal{E}(\phi)\,\delta\phi+d\Theta(\phi,\delta\phi), \tag{A3}$$

where $\Theta(\phi,\delta\phi)$ is an $(n-1)$-form, called the *symplectic potential*, derived through formal integration by parts. This yields a well-defined locally constructed formula for $\mathcal{E}(\phi)$ and $\Theta(\phi,\delta\phi)$ in terms of ϕ, $\delta\phi$, and their partial derivatives to a finite order. The symplectic potential is used to define the *presymplectic form* on a fixed hypersurface Σ,

$$\Omega_\Sigma(\phi,\delta_1\phi,\delta_2\phi)\equiv\int_\Sigma \omega(\phi,\delta_1\phi,\delta_2\phi) \tag{A4}$$

in terms of the *symplectic current* $(n-1)$-form ω given by

$$\omega(\phi,\delta_1\phi,\delta_2\phi)\equiv\delta_1\Theta(\phi,\delta_2\phi)-\delta_2\Theta(\phi,\delta_1\phi). \tag{A5}$$

The symplectic current satisfies $\mathrm{d}\omega(\phi,\delta_1\phi,\delta_2\phi)=\mathcal{E}'(\phi,\delta_2\phi)\,\delta_1\phi-\mathcal{E}'(\phi,\delta_1\phi)\,\delta_2\phi$ with $\mathcal{E}'(\phi,\delta\phi)\equiv\delta\mathcal{E}(\phi)$. Hence, $\omega(\phi,\delta_1\phi,\delta_2\phi)$ is closed for variations on solutions,

$$\mathrm{d}\omega(\Phi,\delta_1\Phi,\delta_2\Phi)=0, \tag{A6}$$

where Φ denotes ϕ restricted to satisfy $\mathcal{E}(\phi)=0$, and $\delta\Phi$ denotes $\delta\phi$ restricted to satisfy $\mathcal{E}'(\Phi,\delta\phi)=0$, i.e., $\delta\Phi$ is, formally, a tangent vector field on the space of solutions. Consequently, $\Omega_\Sigma(\phi,\delta_1\phi,\delta_2\phi)$ is unchanged by deformations of the spacelike surface Σ in any compact region of M.

In the previous constructions, a change of coordinates on M or E leaves $\mathcal{E}(\phi)$ unchanged,[21] while $\Theta(\phi,\delta\phi)$ changes in general by an exact locally constructed $(n-1)$-form $\mathrm{d}\nu(\phi,\delta\phi)$. However, one can show that[4] if the Lagrangian $L(\phi)$ is at most second order in partial derivatives $\partial^k\phi$ $(k\leqslant 2)$ of ϕ, then $\Theta(\phi,\delta\phi)$ is independent of the choice of coordinates on M and E and thus the presymplectic form $\Omega_\Sigma(\phi,\delta_1\phi,\delta_2\phi)$ is then coordinate invariant. Moreover, note that $L(\phi)$ can be freely changed by addition of a locally constructed exact form $\mathrm{d}\mu(\phi)$, without affecting the field equations $\mathcal{E}(\phi)$. This changes $\Theta(\phi,\delta\phi)$ by addition of a locally constructed $(n-1)$-form $\mathrm{d}\delta\mu(\phi)$, but leaves $\Omega_\Sigma(\phi,\delta_1\phi,\delta_2\phi)$ unchanged. Therefore, up to its dependence on Σ, the symplectic structure $\Omega_\Sigma(\phi,\delta_1\phi,\delta_2\phi)$ is uniquely determined by $\mathcal{E}(\phi)$ in this situation.

Now consider a complete, nowhere vanishing vector field ξ on M. It will be assumed that there exists a well-defined Lie derivative acting on ϕ associated with the diffeomorphism generated by ξ on M. Let Σ be a connected region contained in a fixed hypersurface in M with a closed boundary $\partial\Sigma$. (Note, if Σ is simply connected, $\partial\Sigma$ is a closed $n-2$-surface in M bounding Σ. If Σ is multiply connected, then $\partial\Sigma$ is a disjoint union of closed $n-2$-surfaces. Also, if Σ extends to "infinity," then $\partial\Sigma$ contains a corresponding "asymptotic boundary" $n-2$-surface.)

Definition A.1: A Hamiltonian conjugate to ξ *on* Σ *is a function* $H_\Sigma(\xi;\phi)=\int_\Sigma \mathcal{H}(\xi;\phi)$ *for some locally constructed* $(n-1)$*-form* $\mathcal{H}(\xi;\phi)$ *such that, on solutions* Φ,

$$H'_\Sigma(\xi;\Phi,\delta\phi)=\Omega_\Sigma(\Phi,\delta\phi,\mathcal{L}_\xi\Phi), \tag{A7}$$

where $\mathcal{L}_\xi$ *denotes the Lie derivative, and* $H'_\Sigma(\xi;\phi,\delta\phi)\equiv\delta H_\Sigma(\xi;\phi)$.

This is a covariant formulation of the standard Hamiltonian symplectic structure, with the ''time'' direction defined by ξ, called the *time flow* vector field. (In particular, Ref. 4 outlines a construction of a standard phase space and Hamiltonian equations of motion determined from this covariant structure.) Note that a Hamiltonian, if it exists, is automatically conserved along ξ for solutions Φ, i.e., $\mathcal{L}_\xi H_\Sigma(\xi;\Phi)=0$. It will now be shown that when ξ is a ''time symmetry'' of the Lagrangian $L(\phi)$, then a Hamiltonian conjugate to ξ exists and is simply given by the Noether charge associated to ξ.

Given any vector field ζ on M, consider the variation $\delta_\zeta\phi\equiv\mathcal{L}_\zeta\phi$. If this is a symmetry of the Lagrangian, so that

$$\delta_\zeta L(\phi)=L'(\phi,\mathcal{L}_\zeta\phi)=\mathrm{d}(i_\zeta L(\phi))=\mathcal{L}_\zeta L(\phi) \tag{A8}$$

by means of the identity $\mathcal{L}_\zeta L(\phi)=\mathrm{d}(i_\zeta L(\phi))$, then one can define a conserved *Noether current* $(n-1)$-form $J(\zeta;\phi)$ by

$$J(\zeta;\phi)=\Theta(\phi,\mathcal{L}_\zeta\phi)-i_\zeta L(\phi), \tag{A9}$$

where i_ζ is the interior product. Conservation of this current simply means that, on solutions Φ, $J(\zeta;\phi)$ is closed

$$\mathrm{d}J(\zeta;\Phi)=\mathrm{d}\Theta(\Phi,\mathcal{L}_\zeta\Phi)-\mathrm{d}(i_\zeta L(\Phi))=L'(\Phi,\delta\Phi)-\mathcal{L}_\zeta L(\Phi)=0 \tag{A10}$$

through the symmetry condition (A8). The integral of $J(\zeta;\Phi)$ over Σ defines the *Noether charge*

$$Q_\Sigma(\zeta)=\int_\Sigma J(\zeta;\Phi). \tag{A11}$$

One finds that the ''time'' derivative of this charge with respect to ξ is given by

$$\mathcal{L}_\xi Q_\Sigma(\zeta)=\int_\Sigma \mathcal{L}_\xi J(\zeta;\Phi)=\int_\Sigma i_\xi \mathrm{d}J(\zeta;\Phi)+\mathrm{d}(i_\xi J(\zeta;\Phi))=\oint_{\partial\Sigma} i_\xi J(\zeta;\Phi), \tag{A12}$$

where $i_\xi J(\zeta;\phi)$ is called the *flux* of the Noether current. Hence, if the flux vanishes on $\partial\Sigma$, then the charge is conserved for solutions Φ.

Examples of field theories which admit a symmetry $\delta_\zeta\phi=\mathcal{L}_\zeta\phi$ are (i) any generally covariant theory on a fixed, background space–time (M,g) with an isometry vector field ζ (i.e., $\mathcal{L}_\zeta g=0$), where $L(\phi)$ is purely a function of g, ϕ and its metric-covariant derivatives $\nabla\phi$; (ii) any diffeomorphism-covariant theory, whose field variables ϕ include the space–time metric g, where $L(\phi)$ is purely a function of ϕ, curvature tensor of g, and their metric-covariant derivatives.

For a diffeomorphism-covariant theory, $\delta_\zeta\phi$ is a symmetry for all vector fields ζ. Consequently, since $J(\zeta;\phi)$ is locally constructed out of ζ, one can show that in this case[4]

$$J(\zeta;\Phi)=\mathrm{d}Q(\zeta;\Phi) \tag{A13}$$

for some locally constructed $(n-2)$-form $Q(\zeta;\phi)$, called the *Noether current potential*. Then the Noether charge reduces to a surface integral

$$Q_\Sigma(\zeta)=\int_\Sigma J(\zeta;\phi)=\oint_{\partial\Sigma} Q(\zeta;\phi). \tag{A14}$$

In contrast, for a generally covariant theory, $J(\zeta;\Phi)$ is related to the conserved stress-energy tensor $T(\phi)$ defined by considering variations of g,

$$*\delta_g L(\phi) = -\tfrac{1}{2} T(\phi)\,\delta g + *\mathrm{d}\Theta(\phi,\delta g). \tag{A15}$$

One can show that,[9] on solutions Φ,

$$J(\zeta;\Phi) = *i_\zeta T(\Phi) + \mathrm{d}\tau(\zeta;\Phi) \tag{A16}$$

for some locally constructed $(n-2)$-form $\tau(\zeta;\phi)$.

Proposition A2: For any symmetry $\delta_\zeta\phi = \mathcal{L}_\zeta\phi$ admitted by a Lagrangian $L(\phi)$, the field equations and symplectic potential satisfy

$$\delta_\zeta \mathcal{E}(\phi) = \mathcal{L}_\zeta \mathcal{E}(\phi), \tag{A17}$$

$$\delta_\zeta\Theta(\phi,\delta\phi) = \mathcal{L}_\zeta\Theta(\phi,\delta\phi) + \mathrm{d}\psi(\zeta;\phi,\delta\phi), \tag{A18}$$

where $\psi(\zeta;\phi,\delta\phi)$ is some locally constructed $(n-2)$-form.

Proof: Consider an arbitrary variation of the Lagrangian symmetry condition (A8),

$$0 = \delta(\delta_\zeta L(\phi) - \mathcal{L}_\zeta L(\phi)) = \delta_\zeta \delta L(\phi) - \mathcal{L}_\zeta \delta L(\phi). \tag{A19}$$

From Eq. (A3), one has

$$\mathcal{L}_\zeta(\delta L(\phi)) = \mathcal{L}_\zeta(\mathcal{E}(\phi)\,\delta\phi) + \mathcal{L}_\zeta d\Theta(\phi,\delta\phi) = (\mathcal{L}_\zeta\mathcal{E}(\phi))\,\delta\phi + \mathcal{E}(\phi)\,\delta\mathcal{L}_\zeta\phi + d\mathcal{L}_\zeta\Theta(\phi,\delta\phi), \tag{A20}$$

and similarly

$$\delta_\zeta(\delta L(\phi)) = (\delta_\zeta\mathcal{E}(\phi))\,\delta\phi + \mathcal{E}(\phi)\,\delta\mathcal{L}_\zeta\phi + d\,\delta_\zeta\Theta(\phi,\delta\phi), \tag{A21}$$

since $\delta_\zeta\phi = \mathcal{L}_\zeta\phi$. Hence, Eq. (A19) yields

$$(\delta_\zeta\mathcal{E}(\phi) - \mathcal{L}_\zeta\mathcal{E}(\phi))\,\delta\phi = \mathrm{d}(\mathcal{L}_\zeta\Theta(\phi,\delta\phi) - \delta_\zeta\Theta(\phi,\delta\phi)) \tag{A22}$$

holding for all $\delta\phi$. By taking $\delta\phi$ to have compact support and integrating Eq. (A22) over M, one obtains $\int_M(\delta_\zeta\mathcal{E}(\phi) - \mathcal{L}_\zeta\mathcal{E}(\phi))\,\delta\phi = 0$, which immediately yields Eq. (A17). Then Eq. (A22) shows that $\mathcal{L}_\zeta\Theta(\phi,\delta\phi) - \delta_\zeta\Theta(\phi,\delta\phi)$ is a closed $(n-1)$-form holding for all ϕ. Since this expression is locally constructed in terms of ϕ, it follows that[21,22] Eq. (A18) holds. □

From these results, one finds that the variation of the Noether current is given by

$$\begin{aligned} J'(\zeta;\phi,\delta\phi) \equiv \delta J(\zeta;\phi) &= \delta\Theta(\phi,\mathcal{L}_\zeta\phi) - i_\zeta\delta L(\phi) \\ &= \omega(\phi,\delta\phi,\mathcal{L}_\zeta\phi) + \delta_\zeta\Theta(\phi,\delta\phi) - i_\zeta(\mathrm{d}\Theta(\phi,\delta\phi) + \mathcal{E}(\phi)\,\delta\phi) \\ &= \omega(\phi,\delta\phi,\mathcal{L}_\zeta\phi) - i_\zeta(\mathcal{E}(\phi)\,\delta\phi) + \mathrm{d}(i_\zeta\Theta(\phi,\delta\phi) + \psi(\zeta;\phi,\delta\phi)) \end{aligned} \tag{A23}$$

using the identity $i_\zeta(\mathrm{d}\Theta(\phi,\delta\phi)) = \mathcal{L}_\zeta\Theta(\phi,\delta\phi) - \mathrm{d}(i_\zeta\Theta(\phi,\delta\phi))$.

Lemma A.3: On solutions Φ,

$$\Omega_\Sigma(\Phi,\mathcal{L}_\zeta\Phi,\delta\phi) = -\int_\Sigma J'(\zeta;\Phi,\delta\phi) + \oint_{\partial\Sigma} i_\zeta\Theta(\Phi,\delta\phi) + \psi(\zeta;\Phi,\delta\phi). \tag{A24}$$

Thus, for variations $\delta\phi$ with compact support in the interior of Σ, i.e., $\delta\phi|_{\partial\Sigma} = 0$,

$$\Omega_\Sigma(\Phi, \mathcal{L}_\zeta \Phi, \delta\phi) = -\int_\Sigma J'(\zeta; \Phi, \delta\phi). \tag{A25}$$

One can then apply this result to the time flow vector field $\zeta = \xi$ to obtain a Hamiltonian.

Theorem A.4: *The Noether current $J(\xi;\phi)$ yields a Hamiltonian conjugate to ξ on Σ given by $H_\Sigma(\xi;\phi) = \int_\Sigma J(\xi;\phi)$ under compact support variations $\delta\phi$. For solutions Φ, $H_\Sigma(\xi;\Phi) = Q_\Sigma(\xi)$ is the conserved Noether charge associated with ξ.*

For variations $\delta\phi$ without compact support, there exists a Hamiltonian if and only if one can find a locally constructed $(n-2)$-form $B(\xi;\phi)$ such that

$$\oint_{\partial\Sigma} B'(\xi;\Phi,\delta\phi) - i_\xi \Theta(\Phi,\delta\phi) - \psi(\xi;\Phi,\delta\phi) = 0, \tag{A26}$$

where $B'(\xi;\phi,\delta\phi) \equiv \delta B(\xi;\phi)$. If one restricts to variations $\delta\phi = \delta\Phi$, then by considering a second variation and antisymmetrizing in this equation, one obtains the necessary condition

$$\oint_{\partial\Sigma} \delta_1(i_\xi \Theta(\Phi,\delta_2\Phi) + \psi(\xi;\Phi,\delta_2\Phi)) - \delta_2(i_\xi \Theta(\Phi,\delta_1\Phi) + \psi(\xi;\Phi,\delta_1\Phi)) = 0 \tag{A27}$$

for existence of $B(\xi;\phi)$. This condition can also be shown to be sufficient.[10]

Definition A.5: An allowed boundary condition on ϕ is a set of field components $\mathcal{F}(\phi)|_{\partial\Sigma}$ locally constructed from ϕ, partial derivatives $\partial^k\phi$, and space–time quantities associated with ξ, Σ, $\partial\Sigma$, such that for all variations $\delta\phi$ satisfying $\mathcal{F}'(\phi,\delta\phi)|_{\partial\Sigma} = 0$, where $\mathcal{F}'(\phi,\delta\phi) \equiv \delta\mathcal{F}(\phi)$, there exists a Hamiltonian $H_\Sigma(\xi;\phi)$ conjugate to ξ on Σ.

One now has the following main result.

Theorem A.6: *A Hamiltonian conjugate to ξ on Σ exists under variations $\delta\phi$ without compact support if and only if*

$$\oint_{\partial\Sigma} i_\xi \omega(\Phi,\delta_1\Phi,\delta_2\Phi) = \oint_{\partial\Sigma} \psi'(\xi;\Phi,\delta_1\Phi,\delta_2\Phi) \tag{A28}$$

on solutions Φ, where $\psi'(\xi;\phi,\delta_1\phi,\delta_2\phi) \equiv \delta_1\psi(\xi;\phi,\delta_2\psi) - \delta_2\psi(\xi;\phi,\delta_1\phi)$. This determines the allowed boundary conditions $\mathcal{F}(\phi)|_{\partial\Sigma}$ for the field equations to admit a covariant Hamiltonian formulation. Then the Hamiltonian is

$$H_\Sigma(\xi;\phi) = \int_\Sigma J(\xi;\phi) - \mathrm{d}B(\xi;\phi) \tag{A29}$$

with $B(\xi;\phi)$ given by Eq. (A26) up to an arbitrary function of the boundary data $\mathcal{F}(\phi)$ and ξ. Furthermore, under the allowed boundary conditions, the Hamiltonian and symplectic structure are independent of choice of Σ.

The surface integral $\oint_{\partial\Sigma} i_\xi \omega(\Phi,\delta_1\Phi,\delta_2\Phi)$ will be referred to as the *symplectic flux* through $\partial\Sigma$.

For a diffeomorphism-covariant theory, or a generally covariant theory on a background space–time, one can show that $\psi(\xi;\phi,\delta\phi) \equiv 0$. Hence the necessary and sufficient condition for existence of a Hamiltonian becomes

$$\oint_{\partial\Sigma} i_\xi \omega(\Phi,\delta_1\Phi,\delta_2\Phi) = 0 \tag{A30}$$

and, furthermore, from relation (A26) between $\Theta(\Phi,\delta\phi)$ and $B(\xi;\phi)$, it follows that one has

$$B(\xi;\phi)|_{\partial\Sigma} = (i_\xi \tilde{B}(\phi))|_{\partial\Sigma}, \tag{A31}$$

where $\tilde{B}(\phi)$ is a locally constructed $(n-1)$-form. Then on solutions Φ the Hamiltonian takes the following form: in the case of a diffeomorphism-covariant theory,

$$H_B(\xi;\Phi) = \oint_{\partial\Sigma} Q(\xi;\Phi) - i_\xi \tilde{B}(\Phi), \tag{A32}$$

which is a surface integral; and in the case of a generally covariant theory,

$$H(\xi;\Phi) + H_B(\xi;\Phi) = \int_\Sigma * i_\zeta T(\Phi) + \oint_{\partial\Sigma} \tau(\xi;\Phi) - i_\xi \tilde{B}(\Phi), \tag{A33}$$

where $H(\xi;\Phi) = \int_\Sigma * i_\zeta T(\Phi)$ is the canonical energy associated with Φ on Σ, and $H_B(\xi;\Phi)$ is the surface integral term.

To conclude, some further features of the Noether charge Hamiltonian will now be developed.

Definition A.7: The coefficient of an arbitrary compact support variation $\delta\phi|_\Sigma$ in the equation

$$\int_\Sigma \Omega_\Sigma(\phi, \delta\phi, \mathcal{L}_\xi\phi) - H'_\Sigma(\xi;\phi,\delta\phi) \equiv \int_\Sigma \mathcal{E}_H(\xi;\phi)\,\delta\phi = 0 \tag{A34}$$

yields the Hamiltonian field equations for ϕ, $\mathcal{E}_H(\xi;\phi) = 0$.

Theorem A.8: *The Hamiltonian field equations $\mathcal{E}_H(\xi;\phi) = 0$ are equivalent to the Lagrangian field equations $\mathcal{E}(\phi) = 0$.*

Proof: The Hamiltonian (A29) satisfies the variational identity

$$\Omega_\Sigma(\phi, \delta\phi, \mathcal{L}_\xi\phi) - H'_\Sigma(\xi;\phi,\delta\phi) = \int_\Sigma i_\xi(\mathcal{E}(\phi)\,\delta\phi) \tag{A35}$$

derived from Eqs. (A23) and (A26). Hence, for arbitrary compact support variations $\delta\phi|_\Sigma$, $\mathcal{E}(\phi) = 0$ holds if and only if ϕ satisfies $\mathcal{E}_H(\xi;\phi) = 0$. □

A field variation, denoted by $\delta\phi_\mathcal{N}$, is a *symplectic degeneracy direction* if $\Omega_\Sigma(\phi, \delta\phi, \delta\phi_\mathcal{N}) = 0$ holds for arbitrary compact support variations $\delta\phi$. Such degeneracies arise whenever the Lagrangian $L(\phi)$ admits a gauge symmetry (i.e., a symmetry $\delta_\chi\phi$ that is locally constructed from ϕ, partial derivatives $\partial^k\phi$, and that depends linearly on a set of parameters χ freely specifiable as functions on M). Note that the set $\{\delta\phi_\mathcal{N}\}$ of all degeneracy directions is a vector space. Then, a nondegeneracy direction, denoted by $\delta\phi_\mathcal{D}$, is represented as an equivalence class in the vector space of all field variations $\{\delta\phi\}$ quotiented by all symplectic degeneracy directions $\{\delta\phi_\mathcal{N}\}$, namely $\delta\phi_\mathcal{D} = \delta\phi/\delta\phi_\mathcal{N}$. This decomposition yields a break up of the Hamiltonian field equations (A34) into nondynamical constraint equations,

$$H'_\Sigma(\xi;\phi,\delta\phi_\mathcal{N}) = 0, \tag{A36}$$

and dynamical evolution equations,

$$H'_\Sigma(\xi;\phi,\delta\phi_\mathcal{D}) = \Omega_\Sigma(\phi, \delta\phi_\mathcal{D}, \mathcal{L}_\xi\phi), \tag{A37}$$

through arbitrary variations $\delta\phi_\mathcal{N}$, $\delta\phi_\mathcal{D}$ with compact support on Σ.

Since it assumed that the set $\{\phi\}$ of all fields has a linear (vector bundle) structure, the symplectic degeneracy directions $\delta\phi_\mathcal{N}$ can be identified with a corresponding set of field components, denoted $\phi_\mathcal{N}$, which will be called nondynamical with respect to Σ. Similarly, the nondegeneracy directions $\delta\phi_\mathcal{D}$ determine a set of equivalence classes of field components, denoted $\phi_\mathcal{D}$, which will be called dynamical with respect to Σ. (Note these components $\phi_\mathcal{D}$ and $\phi_\mathcal{N}$ are locally constructed from ϕ, partial derivatives $\partial^k\phi$, and space–time quantities associated with Σ.) Then,

from the Hamiltonian variational identity (A35), one can view the constraint equations (A36) and evolution equations (A37) as arising equivalently through the action principle (A1) by variations with respect to $\phi_{\mathcal{N}}$ and $\phi_{\mathcal{D}}$.

In summary, the Noether charge formalism presented here gives a covariant Hamiltonian formulation for Lagrangian field theories in the situation where the underlying time flow is given by a symmetry of the Lagrangian.

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The maximum dimension of the inheriting algebra in perfect fluid space–times

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We determine the maximum dimension of the Lie algebra of inheriting conformal Killing vectors in perfect fluid space–times. For the case of conformally flat space–times the maximum dimension is eight and for the case of nonconformally flat space–times the maximum dimension is found to be five. We illustrate each case with examples. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1509087]

I. INTRODUCTION

We are interested in space–times which admit conformal Killing vector fields and, in particular, fluid space–times which admit inheriting conformal Killing vector fields. A conformal Killing vector field is said to be an inheriting conformal Killing vector field if fluid flow lines **u** are mapped conformally by the conformal Killing vector field (see Sec. II and Coley and Tupper[1]). The motivation for studying inheriting conformal Killing vector fields was discussed in Ref. 1 and inheriting conformal Killing vector fields in perfect fluid space–times were studied in Refs. 2 and 3. For general space–times, from a kinematical description of matter it has been shown[4] that in order for there to be zero entropy production there must exist a conformal Killing vector field parallel to the fluid four-velocity (which is consequently inheriting).

In this article we determine the maximum dimension of the Lie algebra of inheriting conformal Killing vectors in perfect fluid space–times. For the case of conformally flat space–times the maximum dimension is eight and for the case of nonconformally flat space–times the maximum dimension is found to be five.

In Sec. II we define conformal Killing vector fields and state a number of theorems concerning the maximum dimension of Lie algebras of conformal Killing vector fields. We also address the reducibility of a Lie algebra of conformal Killing vector fields (to a Lie algebra of Killing vector fields) with respect to a conformal scaling of the metric. We consider some cases where the inheriting condition is automatically satisfied. In Sec. III we consider the maximum dimension of the inheriting Lie algebra for conformally flat space–times and present the space–times which admit this maximum number. In Sec. IV we determine the maximum dimension of the inheriting

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Lie algebra for the nonconformally flat space–times. In Sec. V we discuss the results and outline possible future work.

II. CONFORMAL KILLING VECTORS AND INHERITANCE

Let M be a four-dimensional spacetime manifold with metric tensor $\mathbf{g}$ of Lorentz signature. Any vector field $\mathbf{X}$ which satisfies

$$\mathcal{L}_{\xi}\mathbf{g}=2\psi(x^{\alpha})\mathbf{g} \tag{1}$$

is said to be a *conformal Killing vector* (CKV) of $\mathbf{g}$. If ψ is not constant on M, then ξ is called a *proper conformal Killing vector*; if ψ is constant on M, then ξ is called a *homothetic Killing vector* (HKV); and if ψ is constant and $\psi\neq 0$ on M, then ξ is called *proper homothetic*. If $\psi_{;\alpha\beta}=0$, then ξ is called a *special conformal Killing vector* (SCKV), and if $\psi=0$, then ξ is said to be a Killing vector (KV).

The set of all CKV (respectively, HKV and KV) form a finite dimensional Lie algebra denoted by $\mathcal{C}$ (respectively, $\mathcal{H}$ and $\mathcal{G}$) whose maximum dimension is 15 (respectively, 11 and 10). If $\dim\mathcal{C}=15$, M is conformally flat. If the dimension of $\mathcal{G}$ is 10, then M is of constant curvature. If M is not of constant curvature, then this algebra has dimension at most 7. The algebra of HKV has dimension equal to or at most one greater than that of the KV algebra so that each given space–time admits a basis for $\mathcal{H}$ containing at most one HKV (i.e., all other HKV can be constructed by the addition of a KV). If the algebra $\mathcal{H}$ has its maximum dimension of 11, then M is flat. Any CKV field in a flat space–time is a SCKV and so the maximum dimension of the SCKV algebra is 15. If this occurs, M is flat, while if M is nonflat, its maximum dimension is 8. For details and proofs, see Ref. 5 and references therein (see Ref. 6 for a summary). It will be assumed throughout this article that the space–times considered admit no local (nonglobalizable) conformal Killing vector fields.

We would like to know the maximum dimension of $\mathcal{C}$ in the nonconformally flat case. First, we need to introduce the following terminology. A point $p\in M$ is called a *zero* (or a *fixed point*) of the CKV ξ if $\xi(p)=0$. A zero p of ξ is called *isometric* if $\psi(p)=0$ and *homothetic* if $\psi(p)\neq 0$.

The Petrov type of the Weyl tensor is a statement about the Weyl tensor at a point $p\in M$, and may vary from point to point. If the Petrov type is the same at all points of M, then one can speak of the Petrov type of M.

The following theorem is known,[7–10] but is collected together here for convenience.

Theorem 1: *Let (M,g) be a nonconformally flat space–time and let $\mathcal{C}$ be the conformal algebra of M. Then we have the following.*

(i) *If the Petrov type is N at some $p\in M$, $\dim\mathcal{C}\leqslant 7$.*
(ii) *If the Petrov type is D at some $p\in M$, $\dim\mathcal{C}\leqslant 6$.*
(iii) *If the Petrov type is III at some $p\in M$, $\dim\mathcal{C}\leqslant 5$.*
(iv) *If the Petrov type is I or II at some $p\in M$, $\dim\mathcal{C}\leqslant 4$.*

In fact it can be shown (using theorem 2 below) that part (iii) of theorem 1 may be strengthened by saying that if the Petrov type is III over some non-empty subset of M then $\dim\mathcal{C}(M)\leqslant 4$.

The following theorem is due to Hall and Steele[8] (see also Ref. 11).

Theorem 2: *Let (M,g) be a space–time that admits an r-dimensional conformal algebra $\mathcal{C}$ and suppose that the Petrov type and the dimension and nature of the orbits associated with $\mathcal{C}$ are the same at each $p\in M$ and that M admits no local (nonglobalizable) conformal vector fields. Then for each $p\in M$ there exists an open neighborhood U of p and a function $\sigma: U\mapsto\mathbf{R}$ such that $\mathcal{C}$ (restricted to U) is a Lie algebra of special conformal vector fields on U with respect to the metric $g'=e^{2\sigma}g$ on U. If the Petrov type is not O, the above local scaling function σ can always be chosen such that $\mathcal{C}$ restricts to a Lie algebra of homothetic Killing vector fields with respect to*

g' on U, and, if (M,g) is not locally conformally related to a generalized plane-wave space–time about any $p \in M$, the above local scaling can always be chosen such that $\mathcal{C}$ restricts to a Lie algebra of Killing vector fields with respect to g' on U.

See Ref. 8 for the definition of a *generalized plane wave*. Minkowski space–time admits 15 (special) CKV fields, (admitting a ten-dimensional subalgebra of KV fields) and it follows that the Lie algebra of CKVs of a conformally flat space–time can, in principle, be locally reduced to a corresponding set of special CKVs with a ten-dimensional subalgebra of KVs. For space–times conformal to the (nonconformally flat) pp-wave space–times, the Lie algebra of CKVs can be locally reduced to a Lie algebra of homotheties,[11] that is, if $\dim\mathcal{C}=7$, then $\mathcal{C}$ can be locally reduced to a seven-dimensional homothety Lie algebra (e.g., 6 KV and 1 HKV); if $\dim\mathcal{C}=6$, then $\mathcal{C}$ can be locally reduced to a six-dimensional homothety Lie algebra (e.g., 5 KV and 1 HKV); and if $\dim\mathcal{C}<6$, then $\mathcal{C}$ can be locally reduced to a Lie algebra of KVs.

The energy momentum tensor for a perfect fluid space–time is given by

$$T_{ab}=(\mu+p)u_a u_b+pg_{ab}, \tag{2}$$

where u^a is the normalized fluid four-velocity and μ and p are, respectively, the energy-density and the pressure. A CKV in a perfect fluid space–time is said to be inheriting if fluid flow lines $\mathbf{u}$ are mapped conformally by the CKV ξ, i.e.,

$$\mathcal{L}_\xi \mathbf{u}=-\psi\mathbf{u}. \tag{3}$$

We shall refer to such a CKV as an ICKV. For an HKV or proper CKV which is parallel to the fluid four-velocity vector $\mathbf{u}$, Eq. (3) is automatically true.[1]

We note that the set of ICKVs form a subalgebra $\mathcal{I}$ of the Lie algebra $\mathcal{C}$ and we refer to this as the inheriting algebra. This is proved in Sec. 3.7 of Ref. 12. Thus, the conditions required for a perfect fluid space–time to admit n independent ICKVs are as follows: there must exist n independent vector fields ξ_I, $I=1,\ldots,n$, which satisfy Eqs. (1) and (3). Therefore, in order to determine the maximum dimension of the Lie algebra of ICKV in a space–time, we can either consider the compatibility of these conditions generally or find the answer on a case by case basis.

III. CONFORMALLY FLAT SPACE–TIMES

In the conformally flat (CF) case, in which $\dim\mathcal{C}=15$, it has been shown that the maximum dimension of the inheriting algebra in a perfect fluid space–time is eight (see Sec. 6 in Ref. 13). Since the maximum dimension of the conformal algebra for any non-CF space–time is seven,[7,8] it follows that

$$\mathrm{MAX}(\dim\mathcal{I})=8.$$

In particular, it is known that the Friedmann–Robertson–Walker model with flat spatial geometry admits precisely eight ICKV.[1,2]

Recently, as part of an investigation into the general CKV admitted by CF perfect fluid space–times,[14] all such space–times admitting the maximum eight ICKV and also all admitting seven ICKV have been discovered. Here we present only the results with a brief indication of the calculation that led to the discovery of these space–times.

The CF perfect fluid space–times are all known[15] and fall into two classes, namely the nonexpanding $(\Theta=0)$ generalized Schwarzschild interior solution and the expanding $[\Theta=\Theta(t)\neq 0]$ generalized FRW solution. The space–time metric of each of these classes can be written in the form

$$ds^2=V^{-2}(-F^2dt^2+dx^2+dy^2+dz^2), \tag{4}$$

where $F(t,x,y,z)$ is of the form

$$F(t)=a(t)r^2+b(t)x+c(t)y+d(t)z+e(t), \tag{5}$$

a, b, c, d, e are arbitrary functions of t and $r^2=x^2+y^2+z^2$. For the nonexpanding models, V is given by

$$V=(1+r^2)C/2, \tag{6}$$

where C is a constant and F is of the particular form

$$F=-\tfrac{1}{2}(Cf_4+1)r^2+f_1x+f_2y+f_3z+\tfrac{1}{2}(Cf_4-1), \tag{7}$$

with f_1, f_2, f_3, f_4 arbitrary functions of t. For the expanding models, V is given by

$$V=Hr^2-2Hx_0x-2Hy_0y-2Hz_0z+V_0+Hr_0^2, \tag{8}$$

where H, x_0, y_0, z_0, V_0 are arbitrary functions of t, $r_0^2=x_0^2+y_0^2+z_0^2$ and F is given by

$$F=3\Theta^{-1}\frac{dV}{dt}. \tag{9}$$

In all cases the fluid four-velocity is comoving, i.e., $u^a=VF^{-1}\partial/\partial t$. However, since the condition (3) is conformally invariant, we may consider the ICKV of the underlying space–time

$$d\sigma^2=-F^2dt^2+dx^2+dy^2+dz^2 \tag{10}$$

with four-velocity $u'^a=F^{-1}\partial/\partial t$.

For the space–time (10) the ICKV equations for ξ^a imply that $\xi^0_{,\alpha}=\xi^\alpha_{,0}=0$ ($\alpha=1,2,3$) and lead to

$$\begin{aligned}
\xi^0&=G(t),\\
\xi^1&=\tfrac{1}{2}A(x^2-y^2-z^2)+Bxy+Cxz+Dx-My+Nz+Q,\\
\xi^2&=\tfrac{1}{2}B(-x^2+y^2-z^2)+Ayx+Cyz+Mx+Dy-Pz+R,\\
\xi^3&=\tfrac{1}{2}C(-x^2-y^2+z^2)+Azx+Bzy-Nx+Py+Dz+S,\\
\psi&=Ax+By+Cz+D,
\end{aligned} \tag{11}$$

where A, B, C, D, M, N, P, Q, R, S are constants, together with the set of equations

$$\begin{aligned}
\frac{d}{dt}(Ga)&=\frac{1}{2}(bA+cB+dC-2aD),\\
\frac{d}{dt}(Gb)&=eA+dN-cM-2aQ,\\
\frac{d}{dt}(Gc)&=eB-dP+bM-2aR,\\
\frac{d}{dt}(Gd)&=eC+cP-bN-2aS,\\
\frac{d}{dt}(Ge)&=eD-bQ-cR-dS.
\end{aligned} \tag{12}$$

A. Space–times admitting eight ICKV

To find those space–times admitting the maximum number of ICKV we must find those functions a, b, c, d, e, G which result in the maximum number of nonzero constants A, $B,\ldots,S$. This is found to occur only when $a=b=c=d=0$, $e\neq 0$ or when $b=c=d=e=0$, $a\neq 0$. However, when the appropriate conformal factor V^{-2} is restored, the second case results only in space–times which are coordinate transformed ($r\mapsto 1/r$) versions of those occuring in the first case, which is thus the only one we need to consider. A transformation of the coordinate t enables us to put $e=1$, so the underlying space–time (10) is Minkowski space–time with $u'^a=\partial/\partial t$. Using the notation of Maartens and Maharaj[16] the eight ICKV are then

$$P_a=\frac{\partial}{\partial x^a},\quad H=x^a\frac{\partial}{\partial x^a},\quad M_{\alpha\beta}=x_\alpha\frac{\partial}{\partial x^\beta}-x_\beta\frac{\partial}{\partial x^\alpha}, \tag{13}$$

where $a=0,1,2,3$ and $\alpha,\beta=1,2,3$. From expressions (8) and (9) the corresponding form of V for the expanding case is

$$V=\alpha r^2+\beta x+\gamma y+\delta z+f(t), \tag{14}$$

where α, β, γ, δ are arbitrary constants and $f(t)$ is an arbitrary function of t. Thus the expanding perfect fluid space–times admitting the maximum number of eight ICKV are all of the form

$$ds^2=[\alpha r^2+\beta x+\gamma y+\delta z+f(t)]^{-2}(-dt^2+dx^2+dy^2+dz^2), \tag{15}$$

and the corresponding nonexpanding space–times have V given by (6). There are three cases to consider:

1. Case (i) $\alpha\Theta\neq 0$

A translation of the origin of the form

$$x'=x+\frac{\beta}{2\alpha},\quad y'=y+\frac{\gamma}{2\alpha},\quad z'=z+\frac{\delta}{2\alpha}$$

transforms the metric into

$$ds^2=[f(t)+\alpha r^2]^{-2}(-dt^2+dx^2+dy^2+dz^2), \tag{16}$$

where we have dropped the primes and absorbed the constants into $f(t)$. This is the space–time $S1$ of Ref. 2 with $k=0$ which was shown to admit five proper ICKV, namely P_a and H, together with the three KV of spherical symmetry.

2. Case (ii) $\alpha=0$, $\Theta\neq 0$

A rotation of the spatial axes brings the metric into the form

$$ds^2=[f(t)+kx]^{-2}(-dt^2+dx^2+dy^2+dz^2), \tag{17}$$

where k is an arbitrary constant. This is the plane symmetric model listed under (a) with $k=0$ in Table 1 of in Ref. 3. In addition to the three KV of plane symmetry, this model admits five proper ICKV (a fact not recognized in Ref. 3—see the Appendix), namely P_0, P_1, H, M_{21}, M_{13}. The corresponding conformal scalars ψ are given by

$$(f+kx)\psi=-\frac{df}{dt},\quad -k,\quad f-t\frac{df}{dt},\quad -ky,\quad -kz, \tag{18}$$

respectively. The density of the model is $\mu=3[(df/dt)^2-k^2]$, so we must have $(df/dt)^2>k^2$.

3. Case (iii) $\Theta=0$

For the nonexpanding model, Eq. (6) leads to the metric

$$ds^2=4C^{-2}(1+r^2)^{-2}(-dt^2+dx^2+dy^2+dz^2), \tag{19}$$

i.e., Eq. (7) with $f_1=f_2=f_3=Cf_4+1=0$. This is a special case of the static Schwarzschild interior solution which is known[2] to admit four proper ICKV together with four KV.

The space–times with metrics (16), (17) and (19) are the only perfect fluid space–times admitting the maximum number of eight ICKV.

B. Space–times admitting seven ICKV

Perfect fluid models admitting seven ICKV are found to occur if and only if the functions a, b, c, d, e in Eq. (5) are constant multiples of each other so that, by a redefinition of the time coordinate, we may write the function F in the form

$$F=\alpha r^2+\beta x+\gamma y+\delta z+\epsilon, \tag{20}$$

where α, β, γ, δ, ϵ are constants. For the expanding models, from Eqs. (8) and (9), V is of the form

$$V=K(t)F+\lambda_1 r^2+\lambda_2 x+\lambda_3 y+\lambda_4 z+\lambda_5, \tag{21}$$

where $3dK/dt=\Theta$ and λ_1, λ_2, λ_3, λ_4, λ_5 are constants of integration. For the nonexpanding models V is given by (6). There are three cases to consider:

1. Case (i) $\alpha\Theta\neq 0$

A translation to a new origin, a rotation of the spatial axes and a rescaling of the time coordinate results in the spacetime metric

$$ds^2=[K(t)(1+\alpha r^2)+\omega r^2+\lambda x]^{-2}[-(1+\alpha r^2)^2dt^2+dx^2+dy^2+dz^2], \tag{22}$$

where ω, λ are constants. When $\lambda=0$ these solutions are the spherical symmetric $S1$ models of Ref. 2 with $k\neq 0$. If, in addition, $\omega=0$, these are the $k=\pm 1$ FRW models.

The ICKV of (22) and the corresponding conformal scalars are

$$\xi_{(1)}=\frac{\partial}{\partial t},\quad \psi_{(1)}=-(1+\alpha r^2)V^{-1}\frac{dK}{dt},$$

$$\xi_{(2)}=[\alpha(x^2-y^2-z^2)+1]\frac{\partial}{\partial x}+2\alpha xy\frac{\partial}{\partial y}+2\alpha zx\frac{\partial}{\partial z},\quad \psi_{(2)}=(2\alpha\omega r^2x+\lambda\alpha r^2-\lambda)V^{-1},$$

$$\xi_{(3)}=2\alpha xy\frac{\partial}{\partial x}+[\alpha(-x^2+y^2-z^2)+1]\frac{\partial}{\partial y}+2\alpha zy\frac{\partial}{\partial z},\quad \psi_{(3)}=2\alpha\omega r^2yV^{-1},$$

$$\xi_{(4)}=2\alpha xz\frac{\partial}{\partial x}+2\alpha yz\frac{\partial}{\partial y}+[\alpha(-x^2-y^2+z^2)+1]\frac{\partial}{\partial z},\quad \psi_{(4)}=2\alpha\omega r^2zV^{-1}, \tag{23}$$

$$\xi_{(5)}=-y\frac{\partial}{\partial x}+x\frac{\partial}{\partial y},\quad \psi_{(5)}=\lambda yV^{-1},$$

$$\xi_{(6)}=z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z},\quad \psi_{(6)}=-\lambda zV^{-1},$$

$$\xi_{(7)}=-z\frac{\partial}{\partial y}+y\frac{\partial}{\partial z},\quad \psi_{(7)}=0.$$

No linear combination of $\xi_{(1)}$ to $\xi_{(6)}$ will result in a vanishing or constant conformal scalar, so this model admits six proper ICKV and one KV. Putting $\lambda=0$, we see that the $S1$ models admit four proper ICKV and three KV, as shown in Ref. 3, and putting $\lambda=\omega=0$, we see that the $k=\pm1$ FRW models admit one proper ICKV and six KV, as shown in Ref. 1.

2. Case (ii) $\alpha=0$, $\Theta\neq0$

A translation to a new spatial origin, a rotation of the spatial axes and a rescaling of the time coordinate results in the space–time metric

$$ds^2=[hr^2+L(t)x+m]^{-2}[-x^2dt^2+dx^2+dy^2+dz^2], \tag{24}$$

where h,m are constants and $L(t)$ is an arbitrary function of time. This space–time admits four proper ICKV, namely,

$$\xi_{(1)}=\frac{\partial}{\partial t},\quad \xi_{(2)}=\frac{\partial}{\partial y},\quad \xi_{(3)}=\frac{\partial}{\partial z},\quad \xi_{(4)}=x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}+z\frac{\partial}{\partial z}, \tag{25}$$

and three KV, namely,

$$\begin{aligned}\xi_{(5)}&=-z\frac{\partial}{\partial y}+y\frac{\partial}{\partial z},\\ \xi_{(6)}&=2hxy\frac{\partial}{\partial x}+[m+h(-x^2+y^2-z^2)]\frac{\partial}{\partial y}+2hzy\frac{\partial}{\partial z},\\ \xi_{(7)}&=2hxz\frac{\partial}{\partial x}+2hyz\frac{\partial}{\partial y}+[m+h(-x^2-y^2+z^2)]\frac{\partial}{\partial z}.\end{aligned} \tag{26}$$

When $h=0$, the space–time is plane symmetric and again admits four proper ICKV and three KV.

3. Case (iii) $\Theta=0$

For the nonexpanding model, using Eqs. (6) and (20) together with a rotation of the spatial axes and a rescaling of the time coordinate, we obtain

$$ds^2=4C^{-2}(1+r^2)^{-2}[-(\alpha r^2+\beta x+1)^2dt^2+dx^2+dy^2+dz^2]. \tag{27}$$

This space–time admits three proper ICKV, namely,

$$\begin{aligned}\xi_{(1)}&=[\alpha(x^2-y^2-z^2)+\beta x+1]\frac{\partial}{\partial x}+y(2\alpha x+\beta)\frac{\partial}{\partial y}+z(2\alpha x+\beta)\frac{\partial}{\partial z},\\ \xi_{(2)}&=2\alpha xy\frac{\partial}{\partial x}+[\alpha(-x^2+y^2-z^2)+1]\frac{\partial}{\partial y}+2\alpha yz\frac{\partial}{\partial z},\\ \xi_{(3)}&=2\alpha xz\frac{\partial}{\partial x}+2\alpha yz\frac{\partial}{\partial y}+[\alpha(-x^2-y^2+z^2)+1]\frac{\partial}{\partial z},\end{aligned} \tag{28}$$

and the four KV,

$$\begin{aligned}\xi_{(4)}&=\frac{\partial}{\partial t},\quad \xi_{(5)}=-z\frac{\partial}{\partial y}+y\frac{\partial}{\partial z},\\ \xi_{(6)}&=2y(1-\alpha+\beta x)\frac{\partial}{\partial x}+[\beta(1-x^2+y^2-z^2)+2(\alpha-1)]\frac{\partial}{\partial y}+2\beta yz\frac{\partial}{\partial z},\\ \xi_{(7)}&=2z(1-\alpha+\beta x)\frac{\partial}{\partial x}+2\beta yz\frac{\partial}{\partial y}+[\beta(1-x^2-y^2+z^2)+2(\alpha-1)]\frac{\partial}{\partial z}.\end{aligned} \tag{29}$$

When $\beta=0$, $\xi_{(4)}$ and $\xi_{(5)}$ are KV; the resulting metric is that of the general spherically symmetric Schwarzschild interior solution which is known[2] to admit three proper ICKV and four KV.

The space–times with metrics (22), (24) and (27) are the only CF perfect fluid space–times admitting precisely seven ICKV. Some, but not all, are known admitting precisely six ICKV; none of the known models admit six proper ICKV, thus, so far, the solution (22) is unique in this regard.

IV. NON-CONFORMALLY FLAT SPACE–TIMES

For the case of nonconformally flat space–times, Theorem 1 tells us that $\dim\mathcal{C}\leqslant 7$ and so $\dim\mathcal{I}\leqslant 7$. It is known that the Gödel space–time admits 5 ICKV: This is a perfect fluid homogeneous Petrov type *D* space–time with 5 KVs. Thus, we ask the question: Does there exist a perfect fluid space–time with $\dim\mathcal{I}=7$ or $\dim\mathcal{I}=6$? From Theorem 1, we only need to consider Petrov types *N* and *D*.

First, we give some notation. Let ξ be a CKV. From (1) it follows that $\xi_{a;b}=\psi g_{ab}+F_{ab}$. Now suppose $\xi\not\equiv 0$ but $\xi(p)=0$ for some $p\in M$. Then[9,17] we have the following:

Theorem 3: *(i) If $\psi(p)=0$ (isometric zero), the Petrov type at p is N, D or O. Also, if $F_{ab}(p)=0$, then the Petrov type at p is O. If the Petrov type at p is D, then $F_{ab}(p)\neq 0$ and is a linear combination of the bivectors $l_{[a}n_{b]}$ and $x_{[a}y_{b]}$ where l,n,x,y is a null tetrad ($l_an^a=x_ax^a=y_ay^a=1$, others zero) at p with l and n repeated principle null directions of the Weyl tensor at p. If the Petrov type at p is N, then $F_{ab}(p)\propto l_{[a}x_{b]}$ where l is the repeated principle null direction of the Weyl tensor at p and $l^ax_a=0$.*

(ii) If $\psi(p)\neq 0$ (homothetic zero), the Petrov type at p is III, N or O. If the Petrov type is III or N, $F_{ab}(p)\neq 0$ and timelike.

Corollary: If ξ is a CKV with $\xi\not\equiv 0$ and $\xi(p)=0$ and the Petrov type at p is not O, then $F_{ab}(p)\neq 0$.

Theorem 4: *If ξ is an ICKV and $\xi\not\equiv 0$ and $\xi(p)=0$, then, if u is the fluid flow velocity at p, $F_{ab}u^b=0$ at p (the fluid flow is assumed nowhere zero).*

Proof: Use $\mathcal{L}_\xi u\propto u$ at p and put $\xi(p)=0$.

□

Theorem 5: *If a perfect fluid space–time is not conformally flat, the dimension of the ICKV algebra is at most 5. If such a space–time admits a maximal ICKV algebra (of dimension 5), it must be of Petrov type D with $F_{ab}\propto x_{[a}y_{b]}$.*

Proof: Suppose this dimension is $\geqslant 6$. Then by taking linear combinations of members of the ICKV algebra one can arrange to have ξ, η as two (i.e., 6−4) independent ICKV such that

$$\xi_{a;b}=\psi g_{ab}+F_{ab},\quad \xi(p)=0,\quad \xi\neq 0,\quad \mathcal{L}_\xi u\propto u,\quad F_{ab}u^b=0,$$

$$\eta_{a;b}=\phi g_{ab}+G_{ab},\quad \eta(p)=0,\quad \eta\neq 0,\quad \mathcal{L}_\eta u\propto u,\quad G_{ab}u^b=0$$

hold at any $p\in M$. Also, by taking linear combinations of ξ and η, we can assume that at least one of ψ and ϕ vanishes at p.

Case (a): $\psi(p)=\phi(p)=0$ and $F_{ab}u^b=G_{ab}u^b=0$. Then from Theorem 3 (i) the (necessarily spacelike) blades of F_{ab} and G_{ab} at p must coincide. Hence $F_{ab}=\mu G_{ab}$ at p ($0\neq\mu\in\mathbf{R}$). Now construct $Z=\xi-\mu\eta$ which is not identically zero. Then Z is an ICKV and $Z_{a;b}=(\psi-\mu\phi)g_{ab}+(F_{ab}-\mu G_{ab})$ with $(\psi-\mu\phi)(p)=0$, $(F_{ab}-\mu G_{ab})(p)=0$ which contradicts nonconformal flatness by Theorem 3 (i).

Case (b): $\psi=0$, $\phi\neq 0$. $F_{ab}u^b=0$, $G_{ab}u^b=0$. Theorem 3 (ii) then shows that $G_{ab}(p)$ is nonzero and timelike (contradicting $G_{ab}u^b=0$ at p), i.e., timelike bivectors cannot have a timelike vector annihilating them.

The second assertion of the theorem follows immediately from this proof and Theorem 3, and is due to the fact that the relevant bivectors are necessarily spacelike.

□

Corollary: The maximum dimension of the ICKV algebra for Petrov type N and type III perfect fluid space–times is at most four.

These results also may be obtained by somewhat tedious direct calculations without recourse to the fixed point theorems of Ref. 17.

A. Examples of Petrov type *D* space–times with five ICKV

(a) The Gödel space–time

$$ds^2=a^2[-(dt+e^x dz)^2+dx^2+dy^2+\tfrac{1}{2}e^{2x}dz^2], \tag{30}$$

when considered as a perfect fluid space–time with zero cosmological constant, has energy density μ and pressure p given by $\mu=p=a^{-2}/2$. It admits five ICKV, all of which are KV.

(b) The plane symmetric Kasner type model

$$ds^2=-dt^2+dx^2+t(dy^2+dz^2) \tag{31}$$

admits four KV and one HKV given by

$$\mathbf{H}=t\frac{\partial}{\partial t}+x\frac{\partial}{\partial x}+\frac{y}{2}\frac{\partial}{\partial y}+\frac{z}{2}\frac{\partial}{\partial z}. \tag{32}$$

The four-velocity is comoving, $\mu=p=t^{-2}/4$.

The space–time with metric

$$d\sigma^2=\omega^{-2}ds^2, \tag{33}$$

where ds^2 is the metric (31) and

$$\omega=a(x^2-2t^2)+b, \tag{34}$$

a and b being nonzero constants, is also a perfect fluid space–time. In this case the KV

$$X=\frac{\partial}{\partial x}$$

becomes a proper ICKV with $\psi_X=-2ax/\omega$ and the HKV H given by (32) also becomes a proper ICKV with $\psi_H=-1+2b/\omega$.

(c) The static spherically symmetric model

$$ds^2=-r^{2m}dt^2+(1+2m-m^2)dr^2+r^2(d\theta^2+\sin^2\theta d\phi^2) \tag{35}$$

has $\mu=(1+2m-m^2)^{-1}m(2-m)r^{-2}$ and $p=m(2-m)^{-1}\mu$ and all energy conditions hold for $0<m\leqslant 1$. The space–time admits four KV and one HKV given by

$$\mathbf{H}=(1-m)t\frac{\partial}{\partial t}+r\frac{\partial}{\partial r}. \tag{36}$$

The space–time with metric

$$d\Sigma^2=U^{-2}ds^2, \tag{37}$$

where ds^2 is the metric (35) and $U=a+br^2$, a and b being positive constants, is also a perfect fluid space–time. The four KV of (35) remain as KV but the HKV given by (36) is now a proper ICKV with $\psi=(a-br^2)/(a+br^2)$.

(d) The static spherically symmetric space–time

$$ds^2 = \mathrm{sech}^2\left(\frac{r}{\sqrt{2}}\right)(-dt^2+dr^2+d\theta^2+\sin^2\theta d\phi^2) \tag{38}$$

satisfies the energy conditions. It admits the four KV associated with static spherical symmetry together with the proper ICKV

$$\mathbf{I} = \frac{\partial}{\partial r}.$$

V. DISCUSSION

The results of Secs. III and IV may be summarized in the following theorem:

Theorem 6: *For conformally flat perfect fluid space–times* $\dim\mathcal{I}$ *is at most eight and all such space–times are known. The maximum number of independent proper ICKV is six. For nonconformally flat perfect fluid space–times* $\dim\mathcal{I}$ *is at most five, in which case the space–time is of Petrov type D*.

The example given by (33) and (34) is the only known nonconformally flat perfect fluid solution admitting more than one independent proper ICKV.

It is also of interest to determine the maximum dimension of $\mathcal{I}$ for types *N*, *III*, *II* and *I* separately. From the analysis of Sec. IV we see that for each of those Petrov types $\dim\mathcal{I}\leqslant 4$. The determination of the exact maximum number in each case may require techniques other than the geometrical approach used here.

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APPENDIX A: ERRATA TO COLEY AND CZAPOR[3]

The result in Sec. III that the plane symmetric CF model given by Eq. (17) admits eight ICKV contradicts Theorem 1 of Ref. 3 which states, in effect, that M_{21} and M_{13} cannot be ICKV (it can be easily checked that they are indeed ICKV). The proof of Theorem 1 in Ref. 3 is correct up to and including Eq. (2.24), but Eq. (2.25) is wrong. In fact, using Eqs. (2.23) and (2.24), Eq. (2.9) becomes (using the notation of Ref. 3)

$$w_x(w_t w_{xt}+w_x w_{tt}-w_{ttx})=0,$$

and, since $w_x\neq 0$, it follows that $w_t w_{xt}+w_x w_{tt}-w_{ttx}=0$; i.e.,

$$(w_t w_x - w_{tx})_x = 0.$$

But Eq. (2.23) states that

$$(w_t w_x - w_{tx})_t = 0,$$

so $w_t w_x - w_{tx} = \text{const}$, which does not contradict the later correct result $w_t w_x = w_{tx}$. [Note Eqs. (2.33a) and (2.33b) are wrong since they are derived from the incorrect Eq. (2.25).] Thus there is no contradiction and solutions do exist for which $\Lambda\neq 0$. Equation (2.37) is correct and substituting this into Eq. (2.9) leads to $w_x^2 w_{xx}+w_{xx}^2-w_x w_{xxx}=0$, and putting $e^{-w}=p(t)+s(x)$ we obtain $s_{xx}^2 = s_x s_{xxx}$. If $s_{xx}=0$, we obtain the solution (18), otherwise we obtain $s=\beta e^{\alpha x}$ which is the first solution in Table I of Ref. 3; i.e., the $k\neq 0$ case. Thus this also admits the "exceptional" ICKV

(using the terminology of Ref. 2) but admits only seven ICKV (4 proper ICKV and 3 KV). Thus the plane symmetric case admits models with the ''exceptional'' ICKV corresponding to those in the spherically symmetric case.

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Wavefronts, caustic sheets, and caustic surfing in gravitational lensing

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Very little attention has been paid to the properties of optical wavefronts and caustic surfaces due to gravitational lensing. Yet the wavefront-based point of view is natural and provides insights into the nature of the caustic surfaces on a gravitationally lensed lightcone. We derive analytically the basic equations governing the wavefronts, lightcones, caustics on wavefronts, and caustic surfaces on lightcones in the context of weak-field, thin-screen gravitational lensing. These equations are all related to the potential of the lens. In the process, we also show that the standard single-plane gravitational lensing map extends to a new mapping, which we call a wavefront lensing map. Unlike the standard lensing map, the Jacobian matrix of a wavefront lensing map is not symmetric. Our formulas are then applied to caustic ''surfing.'' By surfing a caustic surface, a space–borne telescope can be fixed on a gravitationally lensed source to obtain an observation of the source at very high magnification over an extended time period, revealing structure about the source that could not otherwise be resolved. Using our analytical expressions for caustic sheets, we present a scheme for surfing a caustic sheet of a lensed source in rectilinear motion. Detailed illustrations are also presented of the possible types of wavefronts and caustic sheets due to nonsingular and singular elliptical potentials, and singular isothermal spheres, including an example of caustic surfing for a singular elliptical potential lens. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Among relativistic concepts of direct application to gravitational lensing, the observer's past lightcone is perhaps the most fundamental. The lightcone concept unifies the temporal and spatial properties of lensing events in a geometrical manner that makes the multiplicity, magnification, and time delay of the images arise naturally. In this view, gravitational lensing by dark and luminous matter causes the observer's past lightcone to curve into a singular three-dimensional hypersurface that self-intersects and folds sharply. It is the singular ''folding'' of the lightcone that is responsible for most features of interest in gravitational lensing, such as image multiplicity, magnification, and time delay. Additionally, in this view, caustics—so relevant to observational lensing—literally acquire a new dimension, turning into caustic sheets (possibly multiple) contained within the lightcone itself, and carrying a sense of time as well as spatial location. The lightcone concept is most naturally built by imagining an optical wavefront emanating from an observer and traveling out and towards the past or future. At the start, the wavefront is convex and almost perfectly spherical. Upon encountering gravitational lenses, the wavefront becomes nonuniformly retarded, acquiring dents. No matter how small and insignificant these dents in the wavefront are soon after leaving the neighborhood of the lens, in time the normal propagation enhances them, inevitably developing crossings and sharp ridges. The surface traced out in space–time by a wavefront is a (past or future) lightcone. The trace of the wavefront's sharp ridges and

''swallowtail'' points is called a ''comoving caustic surface'' if thought of as embedded in three-space, and a ''caustic surface'' if viewed in space–time. In other words, a caustic surface is built out of caustic sheets with cusp ridges and higher-order singularities (e.g., swallowtails, elliptic umbilics, and hyperbolic umbilics). Remarkably, in spite of the naturalness of this concept, very little attention has been paid to the greater significance of the caustics as sheets or surfaces. As a result, to our knowledge, the properties of optical wavefronts and caustic surfaces in gravitational lensing have not progressed much beyond the generic local classification of caustic singularities of the general theory as developed by Thom, Arnold, and others. Our goal is to initiate a program that investigates optical wavefronts and caustics as they relate to the matter distribution of the gravitational lenses in the space–time.

The vast majority of gravitational lenses can be modeled extremely well using a small-angle approximation of weak-field perturbations of a Friedmann–Lemaître universe, and projecting the deflectors into planes (thin-screen approximation)—see the monographs by Schneider, Ehlers, and Falco[1] and Petters, Levine, and Wambsganss[2] for a detailed treatment. An enormous advantage of weak-field, thin-screen gravitational lensing is that we can obtain explicit analytical expressions for the associated lightcones, optical wavefronts, and caustics on both the wavefronts and lightcones. Indeed, one of the reasons there has been limited progress in the study of quantitative properties of the optical caustic surfaces and wavefronts due to gravitating matter is the lack of computable physical models with observational relevance. Thin-screen, weak-field gravitational lensing provides us with such a setting.

Gravitational lensing from a wavefront perspective was used by Refsdal[3] to relate the Hubble constant to the time delay between lensed images (see Ref. 3, Kayser and Refsdal[4,5] for more). Arnold's singularity theory was used by Petters[6] to treat the local qualitative properties of caustic surfaces (big caustics) in gravitational lensing. Friedrich and Stewart,[7] Stewart,[8] Hasse, Kriele, and Perlick,[9] Low,[10] and Ehlers and Newman[11] also used Arnold's theory to treat wavefronts and caustics in general relativity with varied motivations. In the case of a strong gravitational field, Rauch and Blandford[12] numerically computed the caustic sheets due to the Kerr metric. Wavefronts in the context of liquid droplet lenses have been studied extensively by Berry, Hannay, Nye, Upstill, and others—see Berry and Upstill,[13] Nye,[14] and references therein. Readers may also benefit from the popular article by Nityananda[15] on wavefronts in gravitational lensing.

Our paper calculates explicitly the equations governing the wavefronts and caustic surfaces in gravitational lensing with the standard approximations, and analytically relates the wavefronts and caustic surfaces to the gravitational potential of the lens. This allows us to give a first quantitative treatment of *caustic surfing*, a futuristic notion suggested by Blandford[16] in his millennium essay. The motivation for caustic surfing is to lock a satellite on a gravitationally lensed moving source so as to observe the source at a high magnification over an extended time period. We derive the starting equations for the trajectory to be followed in order to surf the caustic surface. The appeal of caustic surfing lies in its potential as a tool to obtain information about a distant moving source that could not otherwise be resolved.

Our paper is organized as follows. Section II derives an explicit expression for the present optical path length in units of time of light signals that reach the observer in the thin-screen approximation. In Sec. III this expression is used to define a new lensing map in which the sources lie on an instantaneous wavefront, rather than on a lens plane. The caustic surfaces and sheets are related to the wavefront lensing map in Sec. IV. Section V develops some fundamentals of the concept of caustic surfing. Applications to the case of nonsingular and singular elliptical potential models, as well as singular isothermal spheres, are given in Sec. VI. The latter section also gives full classifications of the singularities of the wavefronts and caustic surfaces of the noted lenses, and explicitly illustrates the caustic surfing concept. We conclude in Sec. VII with some remarks and an outlook of future applications. The research reported in this paper extends preliminary results on wavefronts in gravitational lensing first reported by Frittelli and Petters[17] at the Ninth Marcel Grossmann Meeting.

II. THE PRESENT PROPER LENGTH FUNCTION AND LENS EQUATION

We shall calculate the present optical length of gravitationally lensed light rays from a source to the observer using Fermat's principle and coordinates in space. This will include a formula (lensing map) relating the position of a lensed source to the impact positions at the gravitational lens of lensed light rays from the source to observer. For the convenience of readers who are new to gravitational lensing, Secs. II A and II B 1 give an introduction overviewing those aspects of lensing relevant to our wavefront and caustic surface considerations. Readers already familiar with the basics of gravitational lensing can skip to Sec. II B 2, where we cast the lens equation in comoving form.

A. Cosmological model for lensing

We use the usual cosmological setting of gravitational lensing, namely, a weak-field perturbation of a Friedmann–Lemaître space–time. These models are quite robust and fit extremely well with observations. A detailed treatment of the assumptions and approximations used to model most gravitational lensing scenarios is given in Chap. 3 of Ref. 2.

The space–time geometry in the vicinity of a weak-field gravitational lens system [i.e., source, lens(es), observer, and light rays between source and observer] is approximated by the following space–time metric:

$$\mathbf{g}^{\mathsf{K}}_{\mathrm{GL}} = -\left(1+2\frac{\phi}{c^2}\right)c^2\,d\tau^2 + a^2(\tau)\left(1-2\frac{\phi}{c^2}\right)dS^2_{\mathsf{K}} = a^2(\mathsf{t})\left[-\left(1+2\frac{\phi}{c^2}\right)d\mathsf{t}^2 + \left(1-2\frac{\phi}{c^2}\right)dS^2_{\mathsf{K}}\right]. \tag{1}$$

The quantity τ is cosmic time, t is conformal time related to τ by

$$d\mathsf{t} = \frac{c}{a(\tau)}\,d\tau, \tag{2}$$

with $a(\tau)$ a positive function called the *expansion factor* and we use the notation $a(\mathsf{t}) = a(\tau(\mathsf{t}))$. Also ϕ represents the time-independent Newtonian potential of the density perturbation due to the lens(es), and dS^2_{K} the metric of space with constant curvature $\mathsf{K} = -1,0,1$. The weak-field limit is assumed (i.e., $|\phi|/c^2 \ll 1$), so we ignore terms of order greater than ϕ/c^2. Note that the potential ϕ obeys the cosmological Poisson equation—see Sec. II B 2. The weak-field assumption near a gravitational lens ensures that the bending angles $\hat{\alpha}$ of light rays deflected by the lens are small, i.e., $\hat{\alpha} \ll 1$. In addition to the latter assumption, we suppose that the lens is ''thin.'' This means that along the line of sight, the diameter of the matter distribution of the lens or source is very small compared to the distances between lens and observer, and between lens and source. We shall treat the gravitational lens and the point sources as lying on planes—called the *lens plane* and *light source plane*—approximately orthogonal to an axis defined by the observer and some central point on the lens—referred to as the optical axis. All these assumptions allow us to consistently restrict lensing to small observation angles as measured from the optical axis.

Now consider the gravitational lensing metric $\mathbf{g}^{\mathsf{K}}_{\mathrm{GL}}$ in (1). There are coordinates (R,θ,φ) in space, called *comoving coordinates*, such that the Riemannian metric dS^2_{K} becomes

$$dS^2_{\mathsf{K}} = \frac{dR^2}{1-\mathsf{K}R^2} + R^2(d\theta^2 + \sin^2\theta\, d\varphi^2). \tag{3}$$

We assume that the comoving coordinates are dimensionless, the expansion factor $a(\tau)$ has physical dimensions of length, and the potential ϕ has physical dimensions of $[\text{length}]^2/[\text{time}]^2$. The cosmic time τ has dimension of time, while the conformal time t is dimensionless. Away from the neighborhood of the lens, the gravitational lensing metric $\mathbf{g}^{\mathsf{K}}_{\mathrm{GL}}$ is approximated by the Friedmann–Lemaître (FL) metric

$$\mathbf{g}_{\mathrm{FL}}^{\mathsf{K}} = -c^2\, d\tau^2 + a^2(\tau) dS_{\mathsf{K}}^2 = a^2(\mathrm{t})[-d\mathrm{t}^2 + dS_{\mathsf{K}}^2].$$

This employs the assumption that the Newtonian potential ϕ decreases to zero sufficiently fast away from the lens with the lens-source and observer-lens angular diameter distances sufficiently large. In a realistic physical sense, the Newtonian potential of an isolated body decays no faster than r^{-1}. Some plausible ways to justify the use of this metric as intended are discussed in Ref. 18 and references therein. Still, it is not at all clear how to improve on this assumption rigorously. Indeed, there are some unresolved technical mathematical issues with the standard approximations in gravitational lensing, but it is not our intention to address them here.

In this work we will restrict our discussion to a flat cosmological setting. *Henceforth, we shall assume that the gravitational lensing metric* $\mathbf{g}_{\mathrm{GL}}^{\mathsf{K}}$ has $\mathsf{K}=0$. The associated FL metric then reduces to the Einstein–de Sitter metric

$$\mathbf{g}_{\mathrm{Ed}} \equiv \mathbf{g}_{\mathrm{FL}}^{0} = a^2(\mathrm{t}) ds_{\mathrm{flat}}^2, \tag{4}$$

where

$$ds_{\mathrm{flat}}^2 = -d\mathrm{t}^2 + dS_0^2, \quad dS_0^2 = dR^2 + R^2(d\theta^2 + \sin^2\theta\, d\varphi^2) \tag{5}$$

with $0 \leqslant R < \infty$, $0 \leqslant \theta < \pi$, $0 \leqslant \varphi < 2\pi$. Note that for $\mathsf{K}=0$ the comoving coordinates (R,θ,φ) define spherical coordinates in space. The conformal relationship (4) yields that the Minkowski metric ds_{flat}^2 is very important for our study, because $\mathbf{g}_{\mathrm{Ed}}$ and ds_{flat}^2 have the same null geodesics up to an affine parameter. The topology of our space–time with a gravitational lens now takes the form $I \times E$, where I is an open interval of $\mathbf{R}$ and E an open subset of $\mathbf{R}^3$. In most applications of gravitational lensing, we have $E = \mathbf{R}^3 - A$, where A is a finite set of points corresponding to singularities (e.g., point masses) in the lens. These singularities would include points where the density perturbation of the lens or the Newtonian potential ϕ diverge. This yields a lens plane L that is $\mathbf{R}^2$ minus a finite set of points. We call E the *comoving space* and $\tau \times E$ the *proper three-space* at cosmic time τ. Away from the lens, the metrics on E and $\tau \times E$ are the standard Euclidean metric dS_0^2 and metric $a^2(\tau) dS_0^2$, respectively. When we study the caustic surfaces along our past lightcone, we project them into E.

B. The present proper length function and the comoving lens equation

1. Physical setting for present proper length of light rays

We must discuss the basic physical setting needed to determine the present optical length of light rays via Fermat's principle (see pp. 65–76 of Ref. 2 for a detailed treatment). Suppose that a light signal emanates from a source at cosmic time τ_S and arrives at the observer at the present cosmic time τ_0. Assume that the observer is at the origin $\mathbf{0}$ of the spherical coordinate system (R,θ,φ) in the comoving space S and the source at comoving position $p_S = (R_S, \theta_S, \varphi_S)$. Assume that the light ray undergoes deflection by a gravitational lens on some intermediate lens plane L. Since the deflection angle at the lens plane is assumed small, we approximate the light ray's trajectory by an FL piecewise-smooth null geodesic consisting of an FL null geodesic from the source to L and one from L to the observer. Fix an optical axis through an arbitrary comoving point p_L on L (e.g., center of mass of the lens); say, $p_L = (R_L, \theta_L, \varphi_L)$ with (R, θ_L, φ_L) defining the optical axis. Take p_L to be the origin of L. We now consider the set $\mathcal{N}$ of all piecewise-smooth null FL geodesics that left the source at cosmic time τ_S and arrive at the observer at roughly the present cosmic time τ_0 after undergoing deflection at L. The travel time differences between these null rays are assumed to be significantly smaller than the Hubble time $(1/H_0)$ and so the scale factor is assumed to change negligibly during these time differences. In particular, the scale factor is taken to be approximately $a(\tau_0)$ when the different rays arrive. Fixing τ_S and τ_0, the set $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$ of null rays can be parametrized by their comoving impact vectors $\mathbf{r}$ on L (relative to the origin of L). The rays in $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$ will be denoted by $\nu_{\mathbf{r}}$.

But not all the rays in $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$ represent actual light rays. By Fermat's principle (e.g., pp. 66–67, Ref. 2), the actual physical light rays (within our approximations) are given by the rays in $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$ whose present proper lengths are stationary with respect to variations of the comoving impact vector $\mathbf{r}$. To characterize the light rays, we first determine a formula for the present proper lengths of the rays in $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$. Our space–time with

$$\mathbf{g}_{\mathrm{GL}} \equiv \mathbf{g}_{\mathrm{GL}}^0 = a^2(\mathrm{t})\left[-\left(1+2\frac{\phi}{c^2}\right) d\mathrm{t}^2 + \left(1-2\frac{\phi}{c^2}\right) dS_0^2 \right] \tag{6}$$

can be viewed as an Einstein–de Sitter universe with a medium having the following time-independent refractive index (e.g., p. 54, Ref. 2):

$$n = 1 - \frac{2}{c^2}\phi. \tag{7}$$

Along a null ray $\nu_{\mathbf{r}}(s) = (\tau(s), \hat{\nu}_{\mathbf{r}}(s))$ in $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$, where s is a parameter along the ray and $\hat{\nu}_{\mathbf{r}}(s)$ is the spatial path of $\nu_{\mathbf{r}}$ in E, Eq. (6) shows that

$$n(\nu_{\mathbf{r}}(s)) = 1 - \frac{2}{c^2}\phi(\hat{\nu}_{\mathbf{r}}(s)) = \left|\frac{d\mathrm{t}}{d\ell}\right|, \tag{8}$$

where the dimensionless incremental length $d\ell$ along $\hat{\nu}_{\mathbf{r}}(s)$ is relative to the Euclidean metric dS_0^2. The rightmost equality in Eq. (8) uses the assumption that $|\phi|/c^2 \ll 1$ and terms of order higher than ϕ/c^2 are ignored.

The present proper length $L_{\tau_0}(\nu_{\mathbf{r}})$ of a ray $\nu_{\mathbf{r}}$ in $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$ is then the ray's optical length relative to the refractive medium in the hypersurface $\tau_0 \times E$. In other words,

$$L_{\tau_0}(\nu_{\mathbf{r}}) = \int_{\hat{\nu}_{\mathbf{r}}} n(\hat{\nu}_{\mathbf{r}})\, d\ell_{\tau_0}.$$

Here the increment of length $d\ell_{\tau_0}$ is with respect to the spatial metric $a_0^2\, dS_0^2$ on $\tau_0 \times E$, where

$$a_0 \equiv a(\mathrm{t}(\tau_0)).$$

Note that $d\ell_{\tau_0} = a_0\, d\ell$. Using (7), the present proper length of $\nu_{\mathbf{r}}$ in units of time is

$$\mathcal{T}(\nu_{\mathbf{r}}) = \frac{L_{\tau_0}(\nu_{\mathbf{r}})}{c} = \frac{a_0}{c}\int_{\hat{\nu}_{\mathbf{r}}} \left(1 - \frac{2}{c^2}\phi(\hat{\nu}_{\mathbf{r}})\right) d\ell. \tag{9}$$

Henceforth, we shall refer to $\mathcal{T}$ simply as a present proper length function and assume that its values are in units of time.

By Fermat's principle, the light rays are characterized by those rays in $\nu_{\mathbf{r}}$ for which $\mathcal{T}(\nu_{\mathbf{r}})$ is a stationary value of $\mathcal{T}$. In the next section, we shall obtain an explicit formula that determines these stationary values.

2. Present proper length function and lens equation via comoving coordinates

We shall now provide a practical expression of the present proper length (in units of time) in terms of rectangular coordinates in the comoving space E of our lensing space–time $(I \times E, \mathbf{g}_{\mathrm{GL}})$. First, let's transform the dimensionless spherical coordinates (R, θ, φ) to dimensionless rectangular coordinates (x, y, z) such that the observer is at (0,0,0) and the optical axis (R, θ_L, φ_L) corresponds to the z axis. The lens plane L is the xy plane located at z_l along the positive z axis.

We shall relabel the rectangular coordinates on L as $(\mathbf{r},z_l)$, where $\mathbf{r}=(r_1,r_2)$ and $z_l>0$ is fixed. The source is assumed to be located at $(\mathbf{s},z)$, where $\mathbf{s}=(s_1,s_2)$. When $z>z_l$, the source is behind the lens (and so is gravitationally lensed).

The cosmological Poisson equation at the present cosmic time $\tau=\tau_0$ is

$$\nabla_{\mathsf{x}}^2\phi(\mathsf{x})=4\pi G a_0^2\rho(\mathsf{x}), \tag{10}$$

where $\mathsf{x}=(x,y,z)$, ∇_{x}^2 is the Laplace operator relative to x, G is the gravitational constant, and ρ is the cosmological volume mass density. Here ρ has units of $[\text{mass}]/[\text{length}]^3$. Set

$$\tilde{\rho}\equiv a_0^3\rho, \quad \tilde{\phi}\equiv a_0\phi.$$

Since (10) is solved by

$$\phi(\mathsf{x})=-a_0^2G\int_{\mathbf{R}^3}\rho(\mathsf{x}')\frac{d\mathsf{x}'}{|\mathsf{x}-\mathsf{x}'|},$$

we have

$$\tilde{\phi}(\mathsf{x})=-G\int_{\mathbf{R}^3}\tilde{\rho}(\mathsf{x}')\frac{d\mathsf{x}'}{|\mathsf{x}-\mathsf{x}'|},$$

which has units of $[\text{length}]^3/[\text{time}]^2$. Integrating (10) along the optical axis from the source to the observer, we obtain the cosmological 2D–Poisson equation:

$$\nabla_{\mathbf{r}}^2\Psi(\mathbf{r})=\frac{8\pi G a_0^2}{c^2}\sigma(\mathbf{r}), \tag{11}$$

where

$$\Psi(\mathbf{r})\equiv\frac{2}{c^2}\int_z^0\phi(\mathbf{r},z')a_0\,dz', \quad \sigma(\mathbf{r})\equiv\int_z^0\rho(\mathbf{r},z')a_0\,dz'.$$

Note that $\Psi(\mathbf{r})$ has units of length, while $\sigma(\mathbf{r})$ has units of $[\text{mass}]/[\text{length}]^2$. Let

$$\tilde{\Psi}(\mathbf{r})=\frac{2}{c^2}\int_z^0\tilde{\phi}(\mathbf{r},z')dz', \quad \tilde{\sigma}(\mathbf{r})=\int_z^0\tilde{\rho}(\mathbf{r},z')dz'.$$

It follows that $\tilde{\Psi}=\Psi$ and $\tilde{\sigma}=a_0^2\sigma$. Equation (11) then yields the comoving 2D–Poisson equation

$$\nabla_{\mathbf{r}}^2\tilde{\Psi}(\mathbf{r})=\frac{8\pi G}{c^2}\tilde{\sigma}(\mathbf{r}), \tag{12}$$

where $\tilde{\Psi}$ and $\tilde{\sigma}$ have units of length and mass, respectively. The function $\tilde{\Psi}$ can be expressed formally as a solution of (12) by

$$\tilde{\Psi}(\mathbf{r})=\frac{4G}{c^2}\int_{\mathbf{R}^2}d\mathbf{r}'\,\tilde{\sigma}(\mathbf{r}')\ln\left|\frac{\mathbf{r}'-\mathbf{r}}{\xi_0}\right|,$$

where ξ_0 is an arbitrary, dimensionless, fixed constant.

Equation (9) yields that the present proper length of a null ray $\nu_{\mathbf{r}}$ in $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$ separates into two terms

$$\mathcal{T}(\nu_{\mathbf{r}}) = \frac{a_0}{c}[L(\hat{\nu}_{\mathbf{r}}) - \hat{\Psi}(\mathbf{r})], \tag{13}$$

where

$$L(\hat{\nu}_{\mathbf{r}}) \equiv \int_{\hat{\nu}_{\mathbf{r}}} d\ell, \quad \hat{\Psi}(\mathbf{r}) \equiv \frac{2}{c^2}\int_{\hat{\nu}_{\mathbf{r}}} \phi(\hat{\nu}_{\mathbf{r}})\, d\ell$$

with $L(\hat{\nu}_{\mathbf{r}})$ the (dimensionless) Euclidean length of $\hat{\nu}_{\mathbf{r}}$. Since bending angles are assumed small, we approximate the line integral of ϕ over $\hat{\nu}_{\mathbf{r}}$ by an integral along the optical axis, i.e.,

$$\hat{\Psi}(\mathbf{r}) = \frac{2}{c^2}\int_z^0 \phi(\mathbf{r}, z')\, dz' = \frac{\tilde{\Psi}(\mathbf{r})}{a_0}.$$

Note that the scaled comoving potential $\hat{\Psi}(\mathbf{r})$ is dimensionless.

The contribution of the term $a_0 L(\hat{\nu}_{\mathbf{r}})/c$ to Eq. (13) is the time due to the present proper length of the light's geometric path relative to the Euclidean metric, while the term $a_0\hat{\Psi}(\mathbf{r})/c$ contributes the relativistic time dilation (Shapiro time delay) due to the gravitational potential ϕ of the lens. We have

$$L(\hat{\nu}_{\mathbf{r}}) = \ell_l + \ell_{ls}, \tag{14}$$

where ℓ_l is the Euclidean length of the segment of $\hat{\nu}_{\mathbf{r}}$ consisting of the straight line from comoving impact vector $\mathbf{r}$ to the observer and ℓ_{ls} the Euclidean length of the straight-line segment from the source to $\mathbf{r}$. Expressing the null ray $\nu_{\mathbf{r}}$ parametrically as $\nu_{\mathbf{r}}(s) = (\tau(s), \hat{\nu}_{\mathbf{r}}(s))$, we obtain

$$0 = \mathbf{g}_{\mathrm{Ed}}\left(\frac{d\hat{\nu}_{\mathbf{r}}}{ds}, \frac{d\hat{\nu}_{\mathbf{r}}}{ds}\right) = -c^2\left(\frac{d\tau}{ds}\right)^2 + a^2(\tau)\left|\frac{d\hat{\nu}_{\mathbf{r}}}{ds}\right|^2,$$

where the squared magnitude of the comoving velocity $d\hat{\nu}_{\mathbf{r}}/ds$ is relative to dS_0^2. This implies

$$\ell_l = \int_{s_L}^{s_0} \left|\frac{d\hat{\nu}_{\mathbf{r}}}{ds}\right| ds = \int_{\tau_L}^{\tau_0} \frac{c}{a(\tau)}\frac{d\tau}{ds}\, ds = \int_{\mathrm{t}_L}^{\mathrm{t}_0} d\mathrm{t} = \mathrm{t}_0 - \mathrm{t}_L,$$

where τ_L is the cosmic time when $\nu_{\mathbf{r}}$ arrives at the lens plane, s_0 and s_L are the respective parameter values corresponding to τ_0 and τ_L, and $\mathrm{t}_0 = \mathrm{t}(\tau_0)$, $\mathrm{t}_L = \mathrm{t}(\tau_L)$. Similarly,

$$\ell_{ls} = \mathrm{t}_L - \mathrm{t}_S,$$

where $\mathrm{t}_S = \mathrm{t}(\tau_S)$ with τ_S the cosmic time when $\nu_{\mathbf{r}}$ left the source. Hence, the present proper length function $\mathcal{T}(\nu_{\mathbf{r}})$ can be expressed in terms of conformal time as

$$\mathcal{T}(\nu_{\mathbf{r}}) = \frac{a_0}{c}[(\mathrm{t}_0 - \mathrm{t}_S) - \hat{\Psi}(\mathbf{r})]. \tag{15}$$

We now express the present proper length function in terms of our comoving rectangular coordinates. In the approximation of small angles, we have

$$\begin{aligned} \ell_l &= \sqrt{z_l^2 + |\mathbf{r}|^2} = z_l + \frac{|\mathbf{r}|^2}{2z_l}, \\ \ell_{ls} &= \sqrt{(z - z_l)^2 + |\mathbf{r} - \mathbf{s}|^2} = z - z_l + \frac{|\mathbf{r} - \mathbf{s}|^2}{2(z - z_l)}. \end{aligned} \tag{16}$$

By (14) and (16), the present proper length of the null ray $\nu_{\mathbf{r}}$ becomes

$$\mathcal{T}(\mathbf{r},\mathbf{s},z)\equiv\mathcal{T}(\nu_{\mathbf{r}})=\frac{a_0}{c^2}\mathsf{T}(\mathbf{r},\mathbf{s},z), \tag{17}$$

where

$$\mathsf{T}(\mathbf{r},\mathbf{s},z)\equiv z+\frac{|\mathbf{r}|^2}{2z_l}+\frac{|\mathbf{r}-\mathbf{s}|^2}{2(z-z_l)}-\hat{\Psi}(\mathbf{r}). \tag{18}$$

Equation (15) implies that the function $\mathsf{t}(\mathbf{r},\mathbf{s},z)$ is the conformal time of the null ray $\nu_{\mathbf{r}}$. Fixing $\mathbf{s}$ and z, Fermat's principle yields that the light rays from source to observer are determined by those null rays in $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$ with comoving impact vectors $\mathbf{r}$ satisfying

$$\mathrm{grad}_{\mathbf{r}}\,\mathcal{T}(\mathbf{r},\mathbf{s},z)=\mathbf{0}. \tag{19}$$

where $\mathrm{grad}_{\mathbf{r}}$ is the gradient operator in rectangular coordinates $\mathbf{r}$. By (17) and (18), Eq. (19) is equivalent to

$$\mathbf{s}=\frac{z}{z_l}\mathbf{r}-(z-z_l)\hat{\boldsymbol{\alpha}}(\mathbf{r})\equiv\mathbf{s}(\mathbf{r},z), \tag{20}$$

where $\hat{\boldsymbol{\alpha}}(\mathbf{r})\equiv_{\mathbf{r}}\hat{\Psi}(\mathbf{r})$ is the change in direction through which the light signal $\nu_{\mathbf{r}}$ bends at the lens plane, and its magnitude is referred to as the (*comoving*) *bending angle*. Equation (20) is called the (*comoving*) *lens equation*. It determines the comoving impact vectors $\mathbf{r}$ of the light rays from $\mathbf{s}$ to the observer.

For fixed z, Eq. (20) defines a map

$$\mathbf{s}_z:L\to S:\mathbf{s}_z(\mathbf{r})=\mathbf{s}(\mathbf{r},z),$$

called a *(comoving) standard lensing map* from the lens plane L to the *light source plane* S (i.e., the xy plane at position z on the optical axis), and carries no sense of time. This is the comoving version of the cosmological lensing map commonly used in gravitational lensing—see (28). Note that the Jacobian matrix of $\mathbf{s}_z$ is symmetric:

$$(\mathrm{Jac}\,\mathbf{s}_z)(\mathbf{r})=\frac{z}{z_l}\mathbf{I}-(z-z_l)[\mathrm{Hess}_{\mathbf{r}}\hat{\Psi}](\mathbf{r}). \tag{21}$$

Here $\mathbf{I}$ is the 2×2 identity matrix and $\mathrm{Hess}_{\mathbf{r}}\hat{\Psi}$ is the Hessian matrix of $\hat{\Psi}$ relative to $\mathbf{r}=(r_1,r_2)$.

The present proper length of each light ray in $\mathcal{N}_{\tau_S}^{\tau_0}(\mathbf{r})$ depends on the comoving position $\mathbf{s}$ of the source on the source plane. Inserting (20) in (18), we obtain an expression for the present proper length

$$\mathcal{T}(\mathbf{r},z)\equiv\frac{a_0}{c}\mathsf{T}(\mathbf{r},z), \tag{22}$$

where

$$\mathsf{T}(\mathbf{r},z)\equiv\mathsf{T}(\mathbf{r},\mathbf{s}(\mathbf{r},z),z)=z+\frac{1}{2}\left[z\frac{|\mathbf{r}|^2}{z_l^2}+(z-z_l)\left(|\hat{\boldsymbol{\alpha}}(\mathbf{r})|^2-2\frac{\mathbf{r}\cdot\hat{\boldsymbol{\alpha}}(\mathbf{r})}{z_l}\right)\right]-\hat{\Psi}(\mathbf{r}) \tag{23}$$

with $\mathbf{s}(\mathbf{r},z)$ given by (20). *The function $\mathcal{T}(\mathbf{r},z)$ has the convenient property that the source coordinate z appears linearly*. We will take advantage of this fact later in this work.

Notice that though Eqs. (18), (20), and (22) are stated for $z>z_l$, they actually hold for all z if we assume that $\hat{\Psi}(\mathbf{r})\equiv 0$ when $-\infty<z\leqslant z_l$. For example, if $z=0$, then $\mathcal{T}(\mathbf{r},0)=0$. If a light ray starts out from a source at position $(\mathbf{s},z)$ in E with $z_l\leqslant z<\infty$, then $\mathbf{r}$ is the light ray's comoving impact vector on the lens plane L at position z_l. For $0<z<z_l$, the vector $\mathbf{r}$ is the comoving position on L of the light ray's spatial path when extended backward from $(\mathbf{s},z)$ to L. If $-\infty<z<0$, then $\mathbf{r}$ is the ray's impact position on L when the light ray is extended forward from $(\mathbf{s},z)$ to the observer to L. Since the case that is of interest to us is when the wavefront has passed through the lens, *we shall assume, unless stated to the contrary, that* $z\geqslant z_l$.

3. Present proper length function via angular diameter distances, redshifts, and proper vectors

In the majority of the gravitational lensing literature, the comoving coordinates of the preceding sections have not been exploited. In order to make a connection with standard gravitational lensing, we now show that the present proper length function $\mathcal{T}(\mathbf{r},\mathbf{s},z)$ in (17), which uses comoving coordinates, can be expressed in terms of the FL angular diameter distances, redshifts, and proper impact vectors commonly used in gravitational lensing.

Equations (13) and (14) yield

$$\mathcal{T}(\mathbf{r},\mathbf{s},z)=\frac{a_0}{c}[(\ell_l+\ell_{ls}-\ell_s)-\hat{\Psi}(\mathbf{r})]+\frac{a_0\ell_s}{c}. \tag{24}$$

Since $a_0\equiv a(\mathsf{t}(\tau_0))=a(\tau_0)=(1+\mathsf{z}_S)a(\tau_S)$ and the FL angular diameter distance from observer to source is $d_S=a(\tau_S)\ell_s$ for $\mathsf{K}=0$, we get

$$\frac{a_0\ell_s}{c}=\frac{1+\mathsf{z}_S}{c}d_S. \tag{25}$$

The first term on the right-hand side of (24) is the time delay of $\nu_{\mathbf{r}}$ relative to the FL light ray from the source to observer in the absence of the lens. Using the formula for the time delay (e.g., p. 74 of Ref. 2 and p. 146, Ref. 1), we obtain

$$\mathcal{T}(\mathbf{r},\mathbf{s},z)=\frac{1+\mathsf{z}_L}{c}\frac{d_L d_S}{d_{L,S}}\left[\frac{1}{2}\left|\frac{\mathsf{r}}{d_L}-\frac{\mathsf{s}}{d_S}\right|^2-\frac{d_{L,S}}{d_L d_S}\Psi(\mathsf{r})\right]+\frac{1+\mathsf{z}_S}{c}d_S\equiv\mathcal{T}(\mathsf{r},\mathsf{s},d_S), \tag{26}$$

where z_L is the redshift of the lens; d_L is the FL angular diameter distance from observer to lens and $d_{L,S}$ the angular diameter distance from lens to source; $\mathsf{r}=a(\tau_L)\mathbf{r}$ is the proper impact vector of the ray at the lens plane at approximately cosmic time τ_L and $\mathsf{s}=a(\tau_S)\mathbf{s}$ is the proper vector of the source relative to the optical axis at cosmic time τ_S; and $\Psi_L(\mathsf{r})\equiv a_L\hat{\Psi}(\mathbf{r})$ with $a_L=a(\mathsf{t}(\tau_L))$. Note that Ψ_L has units of length and is the two-dimensional cosmological potential at cosmic time $\tau=\tau_L$. Fixing s and d_S, Fermat's principle yields that light rays are determined by $\mathrm{grad}_{\mathsf{r}}\mathcal{T}(\mathsf{r},\mathsf{s},d_S)=\mathbf{0}$. Equation (26) now shows that the latter is equivalent to the usual (cosmological) lens equation:

$$\mathsf{s}=\frac{d_S}{d_L}\mathsf{r}-d_{L,S}\,\mathsf{r}\,\Psi(\mathsf{r}). \tag{27}$$

This induces the standard *cosmological lensing map* in the gravitational lensing literature (e.g., Ref. 2, p. 77):

$$\boldsymbol{\eta}:\mathsf{L}\to\mathsf{S}:\boldsymbol{\eta}(\mathsf{r})=\frac{d_S}{d_L}\mathsf{r}-d_{L,S}\,\mathrm{grad}_{\mathsf{r}}\Psi(\mathsf{r}), \tag{28}$$

where $\mathsf{L}=\{a(\tau_L)\mathbf{r}:\mathbf{r}\in L\}$ and $\mathsf{S}=\{a(\tau_S)\mathbf{s}:\mathbf{r}\in S\}$ are the cosmological lens plane and light source planes, respectively.

III. LIGHTCONES, WAVEFRONTS, AND WAVEFRONT LENSING MAPS

Consider a gravitational lensing situation with an observer receiving light from sources beyond the lens plane where deflectors are located. Even though each light source emits perhaps in all directions, generating their own lightcones, the observer receives only those rays that belong to his past lightcone. Consequently, we shall study the observer's past lightcone, rather than a source's future lightcone. We are also interested in constant-time sections of the observer's past lightcone, which we refer to as wavefronts. In this section, we shall determine parametric equations for the past lightcone and for the wavefronts generating the lightcone.

A. Lensed lightcones

The observer's past lightcone $\mathcal{L}^-$ in the space–time $(I\times E,\mathbf{g}_{\mathrm{GL}})$ is the subset of $I\times E$ consisting of all past-pointing light rays originating from the observer at $(\tau_0,0,0,0)$. Equivalently, the lightcone $\mathcal{L}^-$ is the set of all space–time events in $(I\times E,\mathbf{g}_{\mathrm{GL}})$ from which a light ray arrives at the observer at cosmic time τ_0. To obtain a formula for the points in $\mathcal{L}^-$, consider a light ray $\nu_{\mathbf{r}}$ starting out at event $(\tau_S,\mathbf{s}_s,z_s)$, where z_s may be positive or negative, and arriving at the observer at $(\tau_0,0,0,0)$. Here $\mathbf{r}$ is the light ray's comoving impact position on the lens plane L at z_l, resulting possibly from extending the ray backwards or forwards to L—see discussion at end of Sec. II B 2. Then the (comoving) lens equations (20) and present proper length equation (22), show that $\nu_{\mathbf{r}}$ can be expressed as follows with z as parameter:

$$\nu_{\mathbf{r}}(z)=(\tau_0-\mathcal{T}(\mathbf{r},z),\mathbf{s}(\mathbf{r},z),z), \tag{29}$$

where z varies from z_s to 0, $\mathcal{T}(\mathbf{r},0)=0$, and $\mathbf{s}(\mathbf{r},z_s)=\mathbf{s}_s$. Alternatively, Eq. (29) holds for a light ray from the observer to $(\tau_S,\mathbf{s}_s,z_s)$ by varying z from 0 to z_s. Hence, by allowing z and $\mathbf{r}$ to vary, we obtain the following expression for the observer's past lightcone:

$$\mathcal{L}^-=\{(\tau_0-\mathcal{T}(\mathbf{r},z),\ \mathbf{s}(\mathbf{r},z),\ z):z\in\mathbf{R},\mathbf{r}\in L\}. \tag{30}$$

The set $\mathcal{L}^-$ is a three-dimensional hypersurface in the space–time $(I\times S,\mathbf{g}_{\mathrm{GL}})$ and typically has singularities due to distortions caused by the lens. In Sec. IV, we shall give equations that characterize these singularities. Notice that in the conformally equivalent space–time $(I\times S,\mathbf{g}_{\mathsf{GL}})$, where

$$\mathbf{g}_{\mathsf{GL}}\equiv\frac{\mathbf{g}_{\mathrm{GL}}}{a^2(\mathrm{t})}=-\left(1+2\frac{\phi}{c^2}\right)d\mathrm{t}^2+\left(1-2\frac{\phi}{c^2}\right)dS_0^2,$$

the observer's past lightcone becomes

$$\mathsf{L}^-=\{(\mathsf{T}_0-\mathsf{T}(\mathbf{r},z),\mathbf{s}(\mathbf{r},z),\ z):\ z\in\mathbf{R},\mathbf{r}\in L\}, \tag{31}$$

where $\mathsf{T}_0=c\tau_0/a_0$. The observer's future lightcone $\mathcal{L}^+$ and conformal future lightcone L^+ are given, respectively, as follows:

$$\mathcal{L}^+=\{(\tau_0+\mathcal{T}(\mathbf{r},z),\mathbf{s}(\mathbf{r},z),\ z):\ z\in\mathbf{R},\mathbf{r}\in L\},$$

$$\mathsf{L}^+=\{(\mathsf{T}_0+\mathsf{T}(\mathbf{r},z),\ \mathbf{s}(\mathbf{r},z),\ z):\ z\in\mathbf{R},\mathbf{r}\in L\}.$$

B. Lensed wavefronts and wavefront lensing maps

With fixed z, we saw that Eq. (20) defines a lensing map from the lens plane to the light source plane at z. There is an alternative interpretation of the lensing map stemming from the lightcone point of view. We can consider (20) and (22) jointly with the condition of fixed conformal travel time, instead of fixed z.

We define a *comoving (optical) wavefront* in E as a surface of constant conformal present proper length $\mathsf{T}(\mathbf{r},z)$. One should keep in mind that conformal time flows at a rate different from that of cosmological time—see Eq. (2). However, the surfaces of constant conformal time T are the same as those of constant present proper length $\mathcal{T}$; they are only labeled differently—see (22). Since we are not particularly interested in the specific labels of the wavefronts, which are not observable, we prefer to use the conformal time

$$T \equiv \mathsf{T}(\mathbf{r},z)$$

to describe the wavefronts. We shall refer to T as a conformal present proper length function.

Due to the linearity of (23) in the variable z, we obtain a parametric expression in terms of $(\mathbf{r},T)$ for all the z coordinates of the comoving wavefront by solving for z:

$$z(\mathbf{r},T) = \frac{T - \mathbf{r}\cdot\hat{\boldsymbol{\alpha}}(\mathbf{r}) + \dfrac{z_l}{2}|\hat{\boldsymbol{\alpha}}(\mathbf{r})|^2 + \hat{\Psi}(\mathbf{r})}{1 + \dfrac{|\mathbf{r}|^2}{2z_l^2} + \dfrac{|\hat{\boldsymbol{\alpha}}(\mathbf{r})|^2}{2} - \dfrac{\mathbf{r}\cdot\hat{\boldsymbol{\alpha}}(\mathbf{r})}{z_l}}. \tag{32}$$

The values of $z(\mathbf{r},T)$ are assumed to obey $z(\mathbf{r},T) \geqslant z_l$. In other words, we are interested primarily in the lensed portion of the front, i.e., the portion of the front with z values on the optical axis from the lens plane onward. Note that if we allow $z(\mathbf{r},T) < z_l$, then it is assumed that $\hat{\Psi}(\mathbf{r}) \equiv 0$ in (32)—see the end of Sec. II B 2.

Equation (32) can now be used in (20) to obtain an expression for the points of the wavefront that are on the xy plane at position $z(\mathbf{r},T)$:

$$\mathbf{s}(\mathbf{r},T) \equiv \mathbf{s}(\mathbf{r},z(\mathbf{r},T)) = z(\mathbf{r},T)\left(\frac{\mathbf{r}}{z_l} - \hat{\boldsymbol{\alpha}}(\mathbf{r})\right) + z_l\hat{\boldsymbol{\alpha}}(\mathbf{r}). \tag{33}$$

In other words, the pair $(\mathbf{s},z)$ determined by (33) and (32) defines a chart (possibly with singularities) on the portion of the wavefront that went through the lens plane. Of course, the pair can also be used as a chart for the portion of the front behind the lens plane [e.g., by setting $\hat{\Psi}(\mathbf{r}) \equiv 0$]. The *comoving wavefront* at conformal time T is then given by

$$\mathcal{W}(T) \equiv \{(\mathbf{s}(\mathbf{r},T), z(\mathbf{r},T)) : \mathbf{r} \in L\} \subseteq E, \tag{34}$$

which is a two-dimensional surface that generically has singularities due to lensing. Notice that if we allow $-\infty < z < \infty$ and $0 \leqslant T \leqslant T_0$, then $\mathcal{W}(T)$ traces out the conformal light cone L^- in (31).

For the cosmological present proper length

$$t \equiv \mathcal{T}(\mathbf{r},z),$$

the wavefront is given in the space–time $(I\times E, \mathbf{g}_{\mathrm{GL}})$ at cosmic time τ_0 by

$$\mathcal{W}_0(t) \equiv \{(\tau_0 - t, \mathbf{s}(\mathbf{r},t), z(\mathbf{r},t)) : \mathbf{r} \in L\} \subseteq I\times E,$$

where $\mathbf{s}(\mathbf{r},t) \equiv \mathbf{s}(\mathbf{r},T(t))$ and $z(\mathbf{r},t) \equiv z(\mathbf{r},T(t))$ with $T(t) = ct/a_0$. Equation (30) shows that $\mathcal{W}_0(t)$ is a subset of the past lightcone $\mathcal{L}^-$. The wavefront $\mathcal{W}_0(t)$ is the set of positions of all sources whose light rays left at the same cosmic time $\tau_0 - t$ and arrive at the observer at roughly the present cosmic time τ_0. Most observed lensed light sources are at distances ranging from of

order tens of kiloparsecs (e.g., microlensing) to gigaparsecs (e.g., quasar lensing). The observation time is typically of order weeks to a few years. Consequently, we expect the wavefront $\mathcal{W}_0(t)$ to change negligibly during the observing time, unless the front happens to pass through a higher order singularity during the observation.

The wavefront $\mathcal{W}_0(t)$ lies in the proper space $\{\tau_0-t\}\times E$. Projecting the front into the comoving space, we obtain

$$\mathcal{W}_0^E(t)\equiv\{(\mathbf{s}(\mathbf{r},t),z(\mathbf{r},t)):\mathbf{r}\in L\}\subseteq E,$$

which is a constant cosmic time slice of $\mathcal{L}^-$ (namely, $\tau_0-t=$constant). The wavefront $\mathcal{W}_0^E(t)$ differs from $\mathcal{W}(T)$ in E merely by the label $T=ct/a_0$. The two wavefronts are isometric as singular spaces in the comoving space with the Euclidean metric.

Now for fixed T, the lens Eq. (20) determines a mapping

$$\mathbf{w}_T:L\to\mathcal{W}(T)\subseteq\mathbf{R}^3,$$

called a *comoving wavefront lensing map*, defined by

$$\mathbf{w}_T(\mathbf{r})=(\mathbf{s}(\mathbf{r},T),z(\mathbf{r},T)).$$

By allowing for z values with $z(\mathbf{r},T)<z_l$, the map $\mathbf{w}_T$ can be separated into two single-valued maps

$$\mathbf{w}_T(\mathbf{r})=\begin{cases}\mathbf{w}_T^+(\mathbf{r}) & \text{if } z(\mathbf{r},T)\geqslant z_l,\\ \mathbf{w}_T^-(\mathbf{r}) & \text{if } z(\mathbf{r},T)<z_l\end{cases},$$

where $\mathbf{w}_T^+:L\to\mathcal{W}^+(T)$ and $\mathbf{w}_T^-:L\to\mathcal{W}^-(T)$ with $\mathcal{W}^+(T)$ the subset of $\mathcal{W}(T)$ for which $z\geqslant z_l$, while $\mathcal{W}^-(T)$ is the subset with $z<z_l$. In other words, the map $\mathbf{w}_T$ defines two (possibly singular) coordinate patches on $\mathcal{W}(T)$. Since $\mathcal{W}^-(T)$ did not pass through the lens, it has no singularities and so the map $\mathbf{w}_T^-$ is of little interest for our purposes. Instead, we shall focus primarily on $\mathbf{w}_T$. *Unless stated to the contrary, we shall assume that* $\mathbf{w}_T(\mathbf{r})=\mathbf{w}_T^+(\mathbf{r})$.

It is important to emphasize that rather than the usual mapping from a lens plane to the light source plane (such as given by the comoving and cosmological lensing maps $\mathbf{s}_z:L\to S$ and $\boldsymbol{\eta}:$L $\to$S), *we now have a new mapping—one from the lens plane to a wavefront*. This gives us an alternative interpretation of gravitational lensing where the light source plane is dispensed with and substituted with a wavefront: the locus of points that can be reached in a given time by light signals emitted simultaneously from the observer in all possible directions, after passing through the lens plane. It should also be kept in mind that even though the wavefront as a surface is different from a source plane, in typical lensing scenarios the wavefront surface lies very close to a plane in the region of interest, namely around the optical axis.

IV. CAUSTICS ON WAVEFRONTS AND LIGHTCONES

As a surface in the comoving space $E\subseteq\mathbf{R}^3$, the wavefront $\mathcal{W}^+(T)$ typically develops singularities—called *caustics*—due to the distortions caused by the lens. More precisely, a point $\mathbf{r}$ in the lens plane L is a *critical point* of the wavefront lensing map

$$\mathbf{w}_T:L\to\mathcal{W}^+(T)\subseteq\mathbf{R}^3,\quad \mathbf{w}_T(\mathbf{r})=(\mathbf{s}(\mathbf{r},T),z(\mathbf{r},T))$$

if $\operatorname{rank}[(\operatorname{Jac}\mathbf{w}_T)(\mathbf{r})]<2$, where $\operatorname{Jac}\mathbf{w}_T$ is the Jacobian matrix of $\mathbf{w}_T$ and $z(\mathbf{r},T)\geqslant z_l$. The set of critical points of $\mathbf{w}_T$ will be denoted by $\operatorname{Crit}(\mathbf{w}_T)$. The set of *caustic points* of $\mathbf{w}_T$ or on $\mathcal{W}^+(T)$ is the set

$$\operatorname{Caustics}[\mathcal{W}^+(T)]\equiv\mathbf{w}_T[\operatorname{Crit}(\mathbf{w}_T)]$$

of all critical values of $\mathbf{w}_T$.

The Jacobian matrix of $\mathbf{w}_T$ is the following 3×2 matrix:

$$\operatorname{Jac}\mathbf{w}_T=\begin{bmatrix}\dfrac{\partial \mathbf{s}(\mathbf{r},T)}{\partial \mathbf{r}}\\[2ex] \dfrac{\partial z(\mathbf{r},T)}{\partial \mathbf{r}}\end{bmatrix}, \tag{35}$$

where $z=z(\mathbf{r},T)$ is given by (32) and $\mathbf{s}=\mathbf{s}(\mathbf{r},T)$ by (33). Define a function $f:L\to\mathbf{R}$ by

$$f(\mathbf{r})=z_l+\frac{|\mathbf{r}|^2}{2z_l}-\hat{\Psi}(\mathbf{r}). \tag{36}$$

Note that $f(\mathbf{r})=\ell_l-\hat{\Psi}(\mathbf{r})$ within our approximations [see (16)], so $a_0 f(\mathbf{r})/c$ is the present proper length of a light ray from the point $\mathbf{r}$ on the lens plane to the observer. By (20), we see that

$$\mathbf{s}(\mathbf{r},T)=\mathbf{s}(\mathbf{r},z(\mathbf{r},T))=z(\mathbf{r},T)\nabla_{\mathbf{r}}f(\mathbf{r})+z_l\hat{\boldsymbol{\alpha}}(\mathbf{r}).$$

Consequently, the Jacobian matrix of $\mathbf{s}(\mathbf{r},T)$ relative to $\mathbf{r}$ can then be expressed as

$$\frac{\partial \mathbf{s}}{\partial \mathbf{r}}=\begin{bmatrix} f_1\dfrac{\partial z}{\partial r_1}+zf_{11}+z_l\hat{\Psi}_{11} & f_1\dfrac{\partial z}{\partial r_1}+zf_{12}+z_l\hat{\Psi}_{12}\\[2ex] f_2\dfrac{\partial z}{\partial r_1}+zf_{21}+z_l\hat{\Psi}_{21} & f_2\dfrac{\partial z}{\partial r_2}+zf_{22}+z_l\hat{\Psi}_{22}\end{bmatrix}, \tag{37}$$

where f_i, f_{ij}, and $\hat{\Psi}_{ij}$ denote the usual partial derivatives relative to $\mathbf{r}=(r_1,r_2)$. Note that the Jacobian matrix in (37) is *not* symmetric, unlike the usual Jacobian matrices $\partial \mathbf{s}_z/\partial \mathbf{r}$ and $\partial \boldsymbol{\eta}/\partial \mathbf{r}$ of the comoving and cosmological lensing maps. If z is fixed, then (37) reduces to the usual comoving symmetric case—see Eq. (21),

$$\frac{\partial \mathbf{s}(\mathbf{r},T)}{\partial \mathbf{r}}=\frac{\partial \mathbf{s}_z(\mathbf{r})}{\partial \mathbf{r}}=\frac{z}{z_l}\mathbf{I}-(z-z_l)(\operatorname{Hess}_{\mathbf{r}}\hat{\Psi})(\mathbf{r}).$$

We have $\operatorname{rank}[(\operatorname{Jac}\mathbf{w}_T)(\mathbf{r})]<2$ if and only if every 2-square minor of $\operatorname{Jac}\mathbf{w}_T$ vanishes,

$$\det\frac{\partial \mathbf{s}}{\partial \mathbf{r}}=0, \tag{38}$$

$$\det\begin{bmatrix}\dfrac{\partial s_1}{\partial \mathbf{r}}\\[2ex] \dfrac{\partial z}{\partial \mathbf{r}}\end{bmatrix}=\frac{\partial s_1}{\partial r_1}\frac{\partial z}{\partial r_2}-\frac{\partial s_1}{\partial r_2}\frac{\partial z}{\partial r_1}=0, \tag{39}$$

$$\det\begin{bmatrix}\dfrac{\partial s_2}{\partial \mathbf{r}}\\[2ex] \dfrac{\partial z}{\partial \mathbf{r}}\end{bmatrix}=\frac{\partial s_2}{\partial r_1}\frac{\partial z}{\partial r_2}-\frac{\partial s_2}{\partial r_2}\frac{\partial z}{\partial r_1}=0, \tag{40}$$

where $\mathbf{s}=(s_1,s_2)$. Since the conformal time T is fixed when studying $\mathcal{W}^+(T)$, we have

$$\mathsf{T}(\mathbf{r},\mathbf{s}(\mathbf{r},T),z(\mathbf{r},T))=T=\text{constant},$$

which yields

$$\frac{\partial \mathsf{T}}{\partial \mathbf{r}} + \frac{\partial \mathsf{T}}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{r}} + \frac{\partial \mathsf{T}}{\partial z} \frac{\partial z}{\partial \mathbf{r}} = \mathbf{0}. \tag{41}$$

By (19), we get

$$\frac{\partial \mathsf{T}}{\partial \mathbf{r}} = \mathbf{0}, \tag{42}$$

while Eq. (18) yields $\partial \mathsf{T}/\partial \mathbf{s} = (\mathbf{s}-\mathbf{r})/(z-z_l)$. The latter vanishes if and only if $\hat{\boldsymbol{\alpha}}(\mathbf{r}) = \mathbf{r}/z_l$ [apply (42) or (20)], which holds if and only if $\mathbf{r}$ is a critical point of the function f in (36). Note that for $\mathbf{r}$ to be a critical point of ξ it must solve

$$\frac{\mathbf{r}}{z_l} - \hat{\boldsymbol{\alpha}}(\mathbf{r}) = \frac{\partial f}{\partial \mathbf{r}}(\mathbf{r}) = \mathbf{0}.$$

Generically, the critical points of f are nondegenerate and so are isolated points (e.g., p. 240, Petters *et al.*[2]). For this reason, *we shall assume—unless stated to the contrary—that* $\mathbf{r} \neq \mathbf{s}$. Consequently,

$$\frac{\partial \mathsf{T}}{\partial \mathbf{s}} = \frac{\mathbf{s}-\mathbf{r}}{z-z_l} \neq \mathbf{0}, \quad \frac{\partial \mathsf{T}}{\partial z} = -\frac{|\mathbf{r}-\mathbf{s}|^2}{2(z-z_l)^2} \neq 0. \tag{43}$$

Equation (41) yields

$$\frac{\partial z}{\partial \mathbf{r}} = \left[\frac{(\partial \mathsf{T}/\partial \mathbf{s})}{(\partial \mathsf{T}/\partial z)}\right] \frac{\partial \mathbf{s}}{\partial \mathbf{r}}, \tag{44}$$

where by (43) the bracketed term is nonzero. Plugging $\partial z/\partial r_1$ and $\partial z/\partial r_2$ from (44) into (39) and (40) implies that

$$\frac{\partial s_1}{\partial r_1}\frac{\partial z}{\partial r_2} - \frac{\partial s_1}{\partial r_2}\frac{\partial z}{\partial r_1} = \left[\frac{(\partial \mathsf{T}/\partial s_2)}{(\partial \mathsf{T}/\partial z)}\right] \det \frac{\partial \mathbf{s}}{\partial \mathbf{r}}, \tag{45}$$

$$\frac{\partial s_2}{\partial r_1}\frac{\partial z}{\partial r_2} - \frac{\partial s_2}{\partial r_2}\frac{\partial z}{\partial r_1} = -\left[\frac{(\partial \mathsf{T}/\partial s_1)}{(\partial \mathsf{T}/\partial z)}\right] \det \frac{\partial \mathbf{s}}{\partial \mathbf{r}}. \tag{46}$$

Equations (38)–(40), (45), (46), along with our assumption in (43), then show that the Jacobian matrix of $\mathbf{w}_T$ has rank below 2 if and only if the Jacobian determinant of $\mathbf{s}$ vanishes. Thus, at the conformal time T the caustics on the wavefront are given by

$$\text{Caustics}[\mathcal{W}(T)] = \{(\mathbf{s}(\mathbf{r},T), z(\mathbf{r},T))\}, \tag{47}$$

where $\mathbf{r} \in L$, $\mathbf{s}(\mathbf{r},T)$ is given by (33) with T fixed, and $\mathbf{s} = \mathbf{s}(\mathbf{r},T)$ is subjected to the constraint

$$\det \frac{\partial \mathbf{s}}{\partial \mathbf{r}}(\mathbf{r},T) = 0. \tag{48}$$

Equation (47) extends to wavefront lensing maps the usual concept of caustics in gravitational lensing, where lensing maps are from a lens plane to a light source plane. Allowing the conformal time T to vary in (47) yields evolving caustics on the wavefront as the front propagates. The caustics on a wavefront trace out a *caustic surface* on the conformal past lightcone L^- is given by

$$\text{Caustics}[\mathsf{L}^-] = \{(T_0 - T(\mathbf{r}), \mathbf{s}(\mathbf{r}, T(\mathbf{r})), z(\mathbf{r}, T(\mathbf{r})))\}, \tag{49}$$

where $T_0 = c\tau_0/a_0$, $\mathbf{r} \in L$, and $\mathbf{s}(\mathbf{r},T)$ obeys (48). Since T varies in the case of a caustic surface, the vanishing-determinant condition (48) forces T to be a function of $\mathbf{r}$, which we have expressed by $T(\mathbf{r})$. Also, note that the caustics lie on the portion of L^- with $z \geqslant z_l$. Projecting Caustics$[\mathsf{L}^-]$ into the comoving space E, we obtain the *comoving caustic surface*

$$\text{Caustics}_E[\mathsf{L}^-] = \{(\mathbf{s}(\mathbf{r},T(\mathbf{r})), z(\mathbf{r},T(\mathbf{r})))\}, \tag{50}$$

where $\mathbf{r} \in L$ and $\mathbf{s}(\mathbf{r},T(\mathbf{r}))$ satisfies (48). In the space–time $(I \times E, \mathbf{g}_{GL})$, the caustic is given by

$$\text{Caustics}[\mathcal{L}^-] = \{(\tau_0 - \tau(\mathbf{r}), \mathbf{s}(\mathbf{r},T(\mathbf{r})), z(\mathbf{r},T(\mathbf{r})))\}, \tag{51}$$

where τ_0 is the present cosmic time and $\tau(\mathbf{r}) \equiv a_0 T(\mathbf{r})/c$, $\mathbf{r} \in L$, and $\mathbf{s}(\mathbf{r},T(\mathbf{r}))$ obeys (48). Projecting Caustics$[\mathcal{L}^-]$ into E yields a surface that is isometric to Caustics$_E[\mathsf{L}^-]$ as singular spaces relative to the Euclidean metric on E. Analogous to Eqs. (49)–(51), the caustics of the future lightcone and their projection into the comoving space are given as follows:

$$\text{Caustics}[\mathcal{L}^+] = \{(\tau_0 + \tau(\mathbf{r}), \mathbf{s}(\mathbf{r},T(\mathbf{r})), z(\mathbf{r},T(\mathbf{r})))\}, \tag{52}$$

$$\text{Caustics}[\mathsf{L}^+] = \{(T_0 + T(\mathbf{r}), \mathbf{s}(\mathbf{r},T(\mathbf{r})), z(\mathbf{r},T(\mathbf{r})))\}, \tag{53}$$

$$\text{Caustics}_E[\mathsf{L}^+] = \{(\mathbf{s}(\mathbf{r},T(\mathbf{r})), z(\mathbf{r},T(\mathbf{r})))\}, \tag{54}$$

where $\mathbf{r} \in L$ and $\mathbf{s}(\mathbf{r},T)$ satisfies (48).

The previous discussion traces out the caustic surfaces of an observer's past lightcone using constant time slices. The caustic surfaces can also be traced out using constant z slices. Slices of the caustic sheet by constant z planes are curves on the light source plane, and coincide with what are commonly referred to in the lensing literature as ''caustics.'' We shall refer to such caustics as *z-sliced caustic curves*. These caustic curves can also have singularities, such as cusps. It is important to add that our discussion shows that points on a z-sliced caustic curve actually occur at different cosmic (or conformal) times. Often times, points on caustic curves are treated in the lensing literature as if they occur at the same cosmic time.

In order to calculate the points on the comoving caustic sheet, we impose the condition that the Jacobian of the lens map be singular—see (50) and (54):

$$\det \frac{\partial \mathbf{s}}{\partial \mathbf{r}} = 0.$$

This condition can be imposed either at constant z or constant T if the intention is to produce the caustic sheet. For constant T, we have that $\mathbf{s}$ is given by the wavefront lensing map (33), i.e., $\mathbf{s} = \mathbf{s}(\mathbf{r},z(\mathbf{r},T))$, while for constant z the function $\mathbf{s}$ is given by the standard lensing map (20), i.e., $\mathbf{s} = \mathbf{s}_z(\mathbf{r})$. In the latter case, we consider the caustics of the mapping $\mathbf{s} = \mathbf{s}_z$ from the lens plane to the light source plane, with the intention of eventually letting the light source plane at z sweep (along the optical axis) the entire range behind the lens.

By Eq. (21)—equivalently, Eq. (37) with z fixed—we see that the Jacobian matrix of $\mathbf{s}_z$ depends linearly on z,

$$\frac{\partial \mathbf{s}_z}{\partial \mathbf{r}} = \begin{bmatrix} 1 + (z - z_l) f_{11} & -(z - z_l)\hat{\Psi}_{12} \\ -(z - z_l)\hat{\Psi}_{21} & 1 + (z - z_l) f_{22} \end{bmatrix}, \tag{55}$$

where f is given by (36). Consequently, the determinant of (55) is a quadratic in z. Explicitly, the vanishing of the Jacobian determinant of $\mathbf{s}_z$ is

$$0 = 1 + (z - z_l)(2z_l^{-1} - \hat{\Psi}_{11} - \hat{\Psi}_{22}) + (z - z_l)^2[(z_l^{-1} - \hat{\Psi}_{11})(z_l^{-1} - \hat{\Psi}_{22}) - \hat{\Psi}_{12}^2]. \tag{56}$$

There are two solutions for z as a function of $\mathbf{r}$, representing the z coordinate of points on the caustic surface,

$$z_{\pm}(\mathbf{r}) \equiv z_l + \frac{\hat{\Psi}_{11} + \hat{\Psi}_{22} - 2z_l^{-1} \pm \sqrt{(\hat{\Psi}_{11} - \hat{\Psi}_{22})^2 + 4\hat{\Psi}_{12}^2}}{2[(z_l^{-1} - \hat{\Psi}_{11})(z_l^{-1} - \hat{\Psi}_{22}) - \hat{\Psi}_{12}^2]}. \tag{57}$$

Evaluating $\mathbf{s}_z = \mathbf{s}(\mathbf{r},z)$ at $z_{\pm}(\mathbf{r})$, we obtain the transverse coordinates of points on the caustic surface:

$$\mathbf{s}_{\pm}(\mathbf{r}) \equiv \mathbf{s}(\mathbf{r}, z_{\pm}(\mathbf{r})) = \frac{z_{\pm}(\mathbf{r})}{z_l}\mathbf{r} - (z_{\pm}(\mathbf{r}) - z_l)\hat{\boldsymbol{\alpha}}(\mathbf{r}). \tag{58}$$

By varying $\mathbf{r}$ across the lens plane, the pair $(\mathbf{s}_{\pm}(\mathbf{r}), z_{\pm}(\mathbf{r}))$ traces out the comoving caustic surface for either the future or past conformal lightcone:

$$\begin{aligned} \mathrm{Caustics}_E[\mathsf{L}^+] &= \{(\mathbf{s}_{\pm}(\mathbf{r}), z_{\pm}(\mathbf{r})) : \ \mathbf{r} \in L\} \\ &= \mathrm{Caustics}_E[\mathsf{L}^-]. \end{aligned} \tag{59}$$

V. SURFING A CAUSTIC SHEET

In his Millennium Essay, Blandford[16] speculated about some possible novel gravitational lensing ways of probing the cosmos. One of these dealt with caustic sheets: ''Our observations need not be passive. ... For example, suppose that we launch an array of robotic telescopes and use three of them to measure the velocity of a caustic sheet (from by a bright source) as it passes Earth; a fourth telescope could be made to ''surf'' the wave and observe the source with considerable magnification for a long time.''

We now apply the results of the previous section to show how a telescope may surf a sheet of a caustic surface. This will be done in two steps.

First, change the point of view by assuming that the telescope is the observer. We shall then consider the past comoving caustic surface of the telescope and the future comoving caustic surface of the source simultaneously, and determine the analytical form of the equations for these surfaces. Assume that the telescope lies somewhere on the future comoving caustic surface of the source (i.e., the source is seen at an extremely high magnification corresponding to being on a caustic). For the time being, we shall also suppose that the source is at rest relative to the lens. The past comoving caustic surface of the telescope is given by an expression of the form

$$S_0(\mathsf{x}) = 0,$$

where $\mathsf{x} = (\mathbf{s},z)$. In principle, one can find S_0 by solving for $\mathbf{r}$ in terms of $\mathbf{s}_{\pm}$ using (58) and inserting those values of $\mathbf{r}$ into (57) to obtain $z_{\pm}$ in terms of $\mathbf{s}_{\pm}$, say, $z_{\pm} = F_{\pm}(\mathbf{s}_{\pm})$. In this case, the past comoving caustic surface of the telescope is given by

$$S_0(\mathsf{x}) \equiv z_{\pm} - F_{\pm}(\mathbf{s}_{\pm}) = 0. \tag{60}$$

Since we are using the small-angle approximation, we can approximate the future comoving caustic surface of the source by (60) if $\mathbf{s}$ and z are transformed as follows:

$$\mathbf{s} \to -\mathbf{s}\frac{\ell_{\mathrm{tl}}}{\ell_{\mathrm{sl}}}, \quad z \to \ell_{\mathrm{tl}} + \ell_{\mathrm{sl}}$$

where ℓ_{tl} and ℓ_{sl} are the telescope-lens and lens-source Euclidean distances, respectively. Hence, we suppose that there is an expression for the future comoving caustic surface of the source of the form

$$S_0(\mathsf{x})=0. \tag{61}$$

Second, suppose that a source moving relative to the lens with slowly varying 3-velocity V in comoving coordinates is observed extremely magnified by a telescope at a given instant of conformal time, say, $\mathsf{t}=0$. Assuming that the telescope lies somewhere on a caustic sheet of the source away from singularities (e.g., cusp ridges, swallowtails, elliptic umbilics, hyperbolic umbilics), what should the subsequent motion of the telescope be in order to track the image of the source at a peak brightness? Suppose that during a time increment $\delta\mathsf{t}$ the source moves keeping the distance to the lens plane approximately the same, and assuming its motion to be relatively slow, the caustic sheet of the source in motion will not differ from that of the source at rest other than by a general translation in the direction of motion, i.e.,

$$S(\mathsf{x},\delta\mathsf{t})=S_0(\mathsf{x}-\mathsf{V}\ \ \delta\mathsf{t})=0.$$

If the telescope lies on the caustic sheet at point x_0 at time $\mathsf{t}=0$, then

$$S(\mathsf{x}_0,0)=0=S_0(\mathsf{x}_0).$$

For the telescope to see a bright image of the source during a length of time $\delta\mathsf{t}$, the telescope needs to move with velocity v to another point on the caustic sheet, i.e., to a point $\mathsf{x}=\mathsf{x}_0+\mathsf{v}\delta\mathsf{t}$ so that

$$S(\mathsf{x},\delta\mathsf{t})=0=S_0(\mathsf{x}_0+(\mathsf{v}-\mathsf{V})\,\delta\mathsf{t}).$$

Taylor expanding to first order in $\delta\mathsf{t}$, this is equivalent to

$$\nabla S_0\cdot(\mathsf{v}-\mathsf{V})=0, \tag{62}$$

where ∇S_0 is evaluated at the original position of the telescope x_0 and $\cdot$ stands for the Euclidean scalar product of the two vectors. This means that the telescope's velocity must differ from that of the source at most by a vector tangent to the caustic sheet. Clearly $\mathsf{v}=\mathsf{V}$ would be one way to stay on the caustic sheet, but it may require more energy than necessary. We want the smallest speed needed to stay on the caustic sheet. In order words, we shall minimize $|\mathsf{v}|^2$ for a fixed spatial position and time subjected to the constraint in (62). This will be valid for the time increment $\delta\mathsf{t}$, i.e., we are considering only the zeroth iterate of caustic surfing. The vanishing gradient of the Lagrangian $\mathcal{L}=v_1^2+v_2^2+v_3^2+\lambda\ \nabla S_0\cdot(\mathsf{v}-\mathsf{V})$ with respect to $\mathsf{v}=(v_1,v_2,v_3)$ and the multiplier λ yields $\lambda=-\mathsf{V}\cdot\nabla S_0/|\nabla S_0|^2$. Hence, we obtain the minimum velocity

$$\mathsf{v}_{\min}=-\lambda\nabla S_0=\frac{\mathsf{V}\cdot\nabla S_0}{|\nabla S_0|^2}\nabla S_0, \tag{63}$$

where ∇S_0 is evaluated at x_0. In other words, the minimum velocity is the projection of V to the normal vector ∇S_0 to the caustic surface at x_0. This is physically the minimum speed since ∇S_0 points along the shortest direction between the caustic sheet at time $\mathsf{t}=0$ and the sheet at $\mathsf{t}=\delta\mathsf{t}$. The speed $|\mathsf{v}_{\min}|$ might be considerably smaller than the source's speed $|\mathsf{V}|$ depending on the circumstances. The normal unit vector to the caustic $\nabla S_0/|\nabla S_0|$ can be calculated either from the expression (61) if available or from the parametric version of the caustic map given by (57) and (58).

In a physically realistic situation the telescope will spend some time to reach this velocity, and one will need to adjust the velocity continuously even if the source is moving at constant speed, due to the curvature of the caustic sheet.

We shall illustrate the caustic surfing concept with a singular-elliptical-potential example in Sec. VI B.

VI. EXAMPLES AND ILLUSTRATIONS

In this section we illustrate explicitly the construction of the wavefronts in some of the most widely used models for the deflection potential in astrophysics. In all the cases that we deal with the expressions for the deflection potentials stated are assumed to hold only in the vicinity of the optical axis. This assumption is maintained in the construction of all the figures.

A. Nonsingular elliptical potential lens

In this section we illustrate the case of an elliptical potential, which has the following form:

$$\hat{\Psi}_{\mathrm{ep}}(\mathbf{r}) \equiv A_0 \sqrt{r_c^2 + (1-\epsilon) r_1^2 + (1+\epsilon) r_2^2}, \tag{64}$$

where A_0 is a dimensionless constant. This potential is often used to model elliptical galaxies with A_0 proportional to the velocity dispersion of the lens, whereas the dimensionless parameters $r_c > 0$ and $\epsilon \geqslant 0$ determine the core radius and ellipticity of the lens. A nonvanishing core radius r_c guarantees a nonsingular surface mass density, which in turn ensures that no light rays are obstructed in their passage through the lens. The bending angle is given by

$$\hat{\boldsymbol{\alpha}}_{\mathrm{ep}}(\mathbf{r}) = \nabla_{\mathbf{r}} \hat{\Psi}_{\mathrm{ep}}(\mathbf{r}) = \frac{A_0((1+\epsilon) r_1, (1-\epsilon) r_2)}{\sqrt{r_c^2 + (1-\epsilon) r_1^2 + (1+\epsilon) r_2^2}}.$$

For fixed parameter values of A_0, r_c, and ϵ, these two explicit expressions for the potential and bending angle can be used in $z(\mathbf{r},T)$ and $\mathbf{s}(\mathbf{r},T)$ to produce plots of the constant-time wavefronts embedded in three-dimensional space beyond the lens plane. At early times beyond the lens plane, the wavefront is essentially spherical, but as it progresses away from the lens plane the central section of the wavefront begins to lag behind the rest of the wavefront, eventually folding and developing multiple sheets. The progression of the wavefront in time shows different regimes, from smooth to various singular types. In the following, we produce a representative surface of each regime, effectively classifying the singularities of the wavefronts of an elliptical lens. This extends the brief summary of such wavefronts given in Ref. 17. Note that formally our treatment is along the future lightcone of the observer, which can be interpreted as the past lightcone in a time coordinate running towards the past, because the space–time is static.

1. Wavefront singularities

We arbitrarily fix the values of the parameters at $A_0 = 1.01, z_l = 90, \epsilon = 0.0002$, and $r_c = 1.001$. These values are chosen for purely pedagogical reasons. Notwithstanding, in making our choice we took care to ensure that the approximation of small angles was met, in order for the plots to be qualitatively representative of lensing problems.

Let T_l be the time at which the ray that passes through the center of the lens (i.e., the origin) reaches the lens plane. With our choice of parameters, it takes the value $T_l = 90$. We find that for times at least as late as $T = T_l + 8900$, the wavefronts are regular on the other side of the lens plane, but sometime before $T = T_l + 9800$ the first singularity occurs in the form of a single point on the wavefront. The time scales in this particular example are irrelevant; in physically accurate lensing situations the time scale should agree with the distance scale to the lens plane in order of magnitude. The time of the first singular wavefront is about $T = T_l + 9699.27$, and is calculated in Sec. VI A 2. After the first singularity, the wavefront successively goes through four more distinct singularity regimes.

The regular regime is illustrated in Fig. 1, which shows a field view of the wavefront. The observer is located to the far right, at (0,0,0) in the plot coordinates. The wavefront is distorted with respect to a sphere, and develops a dent that points toward the observer along the optical axis. The scale of the optical axis is greatly magnified (about 10^4 times) with respect to the transversal axes in order to better show the retardation effect on the wavefront. The ''spike'' has a total length of about 10^{-3} on a sphere of radius about 9×10^3, so the effect is small in the proper scales and

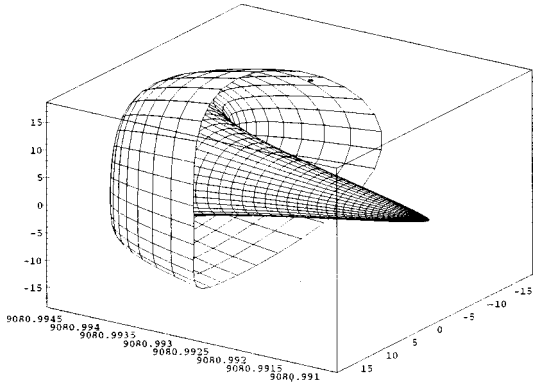

FIG. 1. A portion of the wavefront of an elliptical potential in the regular regime, i.e., early times past the lens plane (in this case, $T=T_l+8900$). The observer is to the right at (0,0,0).

is well within the approximation of small angles. The tip of the ''spike'' is perfectly smooth and presents a convex surface to the observer. There are no singularities anywhere in the wavefront at this time ($T=T_l+8900$).

At a later time, the first singular regime develops, illustrated in Fig. 2. The tip of the spike, which earlier was convex toward the observer, develops a self-intersection and a sharp cuspidal ridge in the form of horizontal ''lips.'' Our use of the term ''lips'' in this context is entirely for descriptive purposes and should not be understood in the technical sense used in Arnold's theory, in which the term ''lips'' refers to the $A_3(+)$ planar caustic metamorphosis (e.g., pp. 375–376, 381 of Ref. 2). The surface of the wavefront that faces the observer is now concave, and limited by the two cuspidal ridges outlining the ''lips.'' The two cuspidal ridges pinch off the back convex

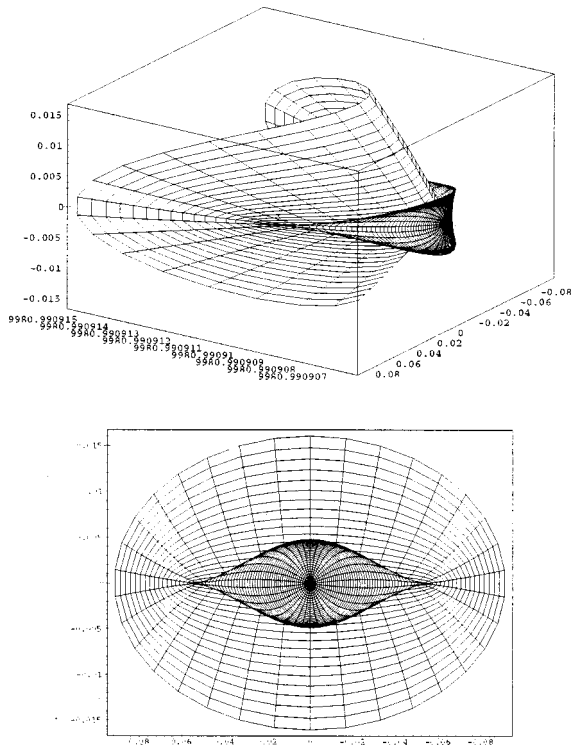

FIG. 2. The single lips regime ($T=T_l+9800$). The bottom panel shows a front view of the lips singularity.

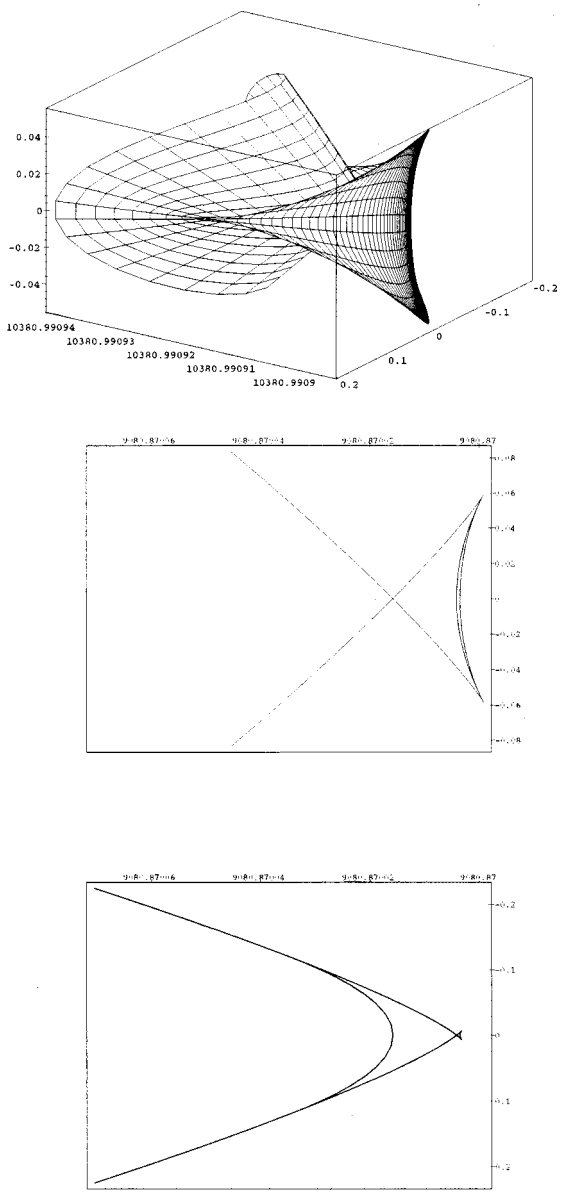

FIG. 3. Typical wavefront in the criss-cross lip regime ($T=T_l+10\,200$), where two nested perpendicular cuspidal ridges are present. The middle panel is a vertical slice of the top panel, while the bottom panel is a horizontal slice. Both slices are through the optical axis.

sheet of the wavefront at two symmetrical swallowtail points. The swallowtails are best appreciated in the top panel, where a side view of the wavefront is shown. The bottom panel shows a front view, where the lip character of the cuspidal ridge can be appreciated. The wavefronts in this regime all have this horizontal lip singularity, but the ''lips'' grow in time continuously after starting out from a single point at the center. The picture shows the wavefront at $T=T_l+9800$, which is still quite early in this regime. One notable fact about this wavefront is that, locally, it is indistinguishable from the early singular wavefronts in the implosion of a triaxial ellipsoid,[18] in which case, the cuspidal lip-ridge lies ''in the outside.'' For the gravitational lensing case that we are illustrating, in a global sense, the cuspidal lip-ridge lies ''inside.''

The next singular regime is illustrated in Fig. 3. The point at the center of the concave sheet of the wavefront facing the observer turns momentarily singular at approximately $T=T_l$

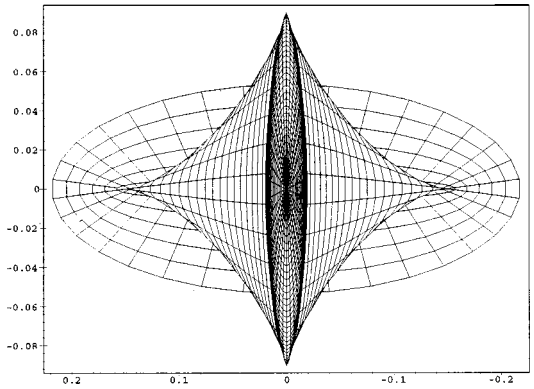

FIG. 4. The critical wavefront ($T=T_l+10\,420$).

$+10\,148.84$, and grows another lips singularity, this time vertically oriented. These vertical ''lips'' ride on top of the now mixed convex–concave section of the wavefront and present a concave surface to the observer, as can be appreciated from the two slices in the middle and bottom panels. The middle panel shows a vertical slice of the wavefront through the optical axis. It may be difficult to appreciate that the foremost sheet pinches off the underlying originally existing sheet well before touching the originally existing cuspidal ridges at the top and bottom. The bottom panel shows an optical-axis horizontal slice, where the cuspidal character of the newly created forefront sheet is evident. The two ends of the vertical ''lips'' are two symmetrical swallowtails. All the wavefronts in this regime have two perpendicular lips, yielding a total of four swallowtails. The perpendicular lips grow continuously in time, but the inner lip starts at the center and grows until it touches the outer lips. This picture shows the wavefront at $T=10\,200$, which is quite late within this regime since the inner lip is about to merge with the outer one.

The next regime consists entirely of a single wavefront at the critical time when the inner lip singularity merges with the outer one. This wavefront is represented in Fig. 4. The singular ridge on the wavefront has the general outline of a football in a vertical position, inscribed in an outer astroid or diamond. The ''football'' outline is the distorted last expression of the inner lip-ridge, whereas the astroid is the distorted last expression of the outer (original) horizontal lips. At this time the two cuspidal ridges merge right before they undergo a permanent change. The wavefront at this critical time has two swallowtails symmetrically located along the horizontal direction, and two singular points symmetrically located along the vertical direction where the two lips merge. In the context of wavefronts, these points have no greater significance than the merger of a cusp ridge and a swallowtail surface. However, their greater significance is that they are indicators of the presence of hyperbolic umbilic points in the caustic sheet, which we describe in the next section. The figure represents the time $T=10\,420$, which is close enough to the critical time at the resolution that we are using.

The last regime comprises all the wavefronts later than the critical time at which the inner ''lips'' merge with the outer ''lips.'' All such late wavefronts have a ''regular'' cuspidal ridge delimiting a concave surface that faces the observer, namely, a cuspidal ridge which is smooth as a curve in three space. Behind the foremost concave cap, the wavefront self-intersects and has another cuspidal ridge with four singular points in the general shape of an astroid or diamond. One such wavefront at time $T=T_l+10\,900$ is shown in Fig. 5. In this front view, the foremost oval cuspidal ridge is clearly distinguishable, as are the two swallowtails in the back. However, there are two other swallowtails completing the diamond, which lie behind the foremost oval cap and are blocked from view in this picture. The qualitative structure of the wavefront in the diamond-ridge neighborhood is shown in the bottom panel of Fig. 6.

A very late wavefront at time $T=T_l+55\,000$ is shown in Fig. 6. It can be seen that as time moves on, the oval and diamond cuspidal ridges remain essentially unchanged except that the oval ridge in the foreground grows at a much faster rate than the diamond-shaped ridge in the back, and

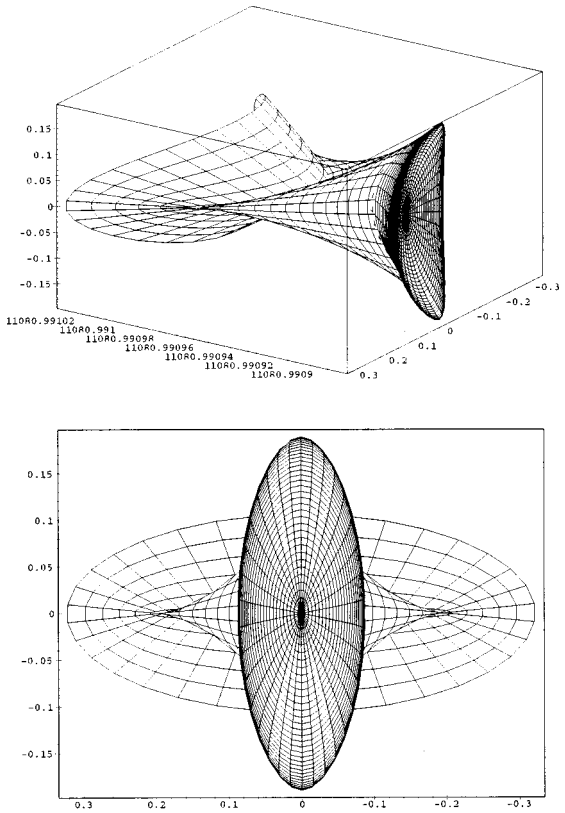

FIG. 5. Typical wavefront early in the late regime ($T=T_I+10\,900$). The bottom panel shows a front view.

the wavefront eventually acquires a shape resembling that of a goblet. The figure shows both a field view of the ''goblet'' and a magnification of the goblet's throat to show the diamond ridge. The diamond ridge structure is almost ubiquitous in wavefront evolutions that are not axisymmetric. For another view of one of these local diamond ridges in wavefronts, we refer the reader to the bottom panel of Fig. 10. The global ''goblet'' wavefront is typical of spherically symmetric regular potentials, with the major difference that the throat of the goblets in the spherically symmetric case degenerates down to a single point, lacking the complicated diamond structure for the case of elliptical symmetry. The diamond ridge represents the nondegenerate version of the throat of the goblet. The goblet's throat has three wavefront sheets, each generically giving rise to an image of the light source.

What we have described in this section are precisely the singularities and metamorphosis of wavefronts in the observer's lightcone in the case of an elliptical potential. In this case, we found that the wavefronts have three types of singularities: cuspidal ridges, swallowtail points, and points of transversal self-intersections. These three singularity types are shared by generic wavefronts in space—see p. 55 of Ref. 19. We also showed that two kinds of metamorphosis occur for the wavefronts due to an elliptical potential. In the first place, we have found two occurrences of the birth of ''lips'' on the wavefront. Second, we have found two hyperbolic umbilic metamorphoses, i.e, the two symmetrical occurrences on the wavefront of the exchange of a swallowtail point from one cuspidal ridge to another. Both metamorphosis are part of Arnold's list of metamorphoses of fronts in space—see, for instance, the first and fourth perestroikas in Fig. 258 on p. 489 of Ref. 20.

2. Caustic sheet

If we think of the family of wavefronts for all times T as spatial slices of the observer's lightcone, then the collection of all the caustic singularities (i.e., cuspidal ridges, swallowtail

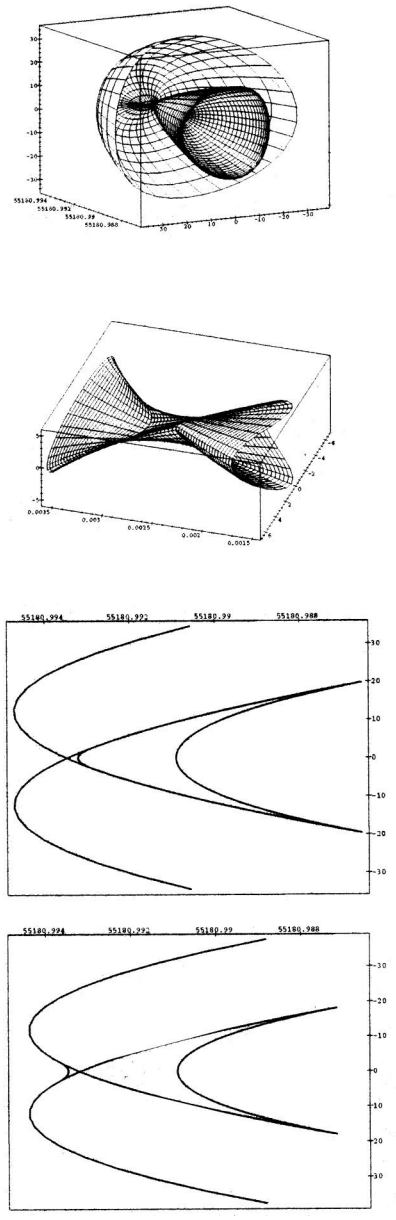

FIG. 6. Typical ''goblet'' wavefront in the very late regime (in this case, $T = T_l + 55\,000$). The middle-top panels shows a magnification of the throat. The middle-bottom and bottom panels show vertical and horizontal slices, respectively.

points) on the instantaneous wavefronts forms a two-surface in space–time. The projection of this two-surface into the comoving space E is referred to as a comoving caustic surface.

As a surface in the three-space E, the caustic surface is traced in time by the caustics of the traveling wavefront as the front moves away from the observer. The metamorphoses of the wavefront's caustics thus build up a picture of the caustic surface's singularities. The generic singularities of a caustic surface in three-space are of five different types: folds, cuspidal ridges, swallowtail points, elliptic umbilic points, and hyperbolic umbilic points.[21]

We showed that the caustic surface on an observer's lightcone is given by Eq. (59). In the particular case of the elliptical potential, the resulting caustic surface is shown in Fig. 7. A significant feature of our caustic surface in three-space is that it consists of two separate intersecting sheets, one for each nontrivial root (57) of the Jacobian determinant in (56). The two bottom

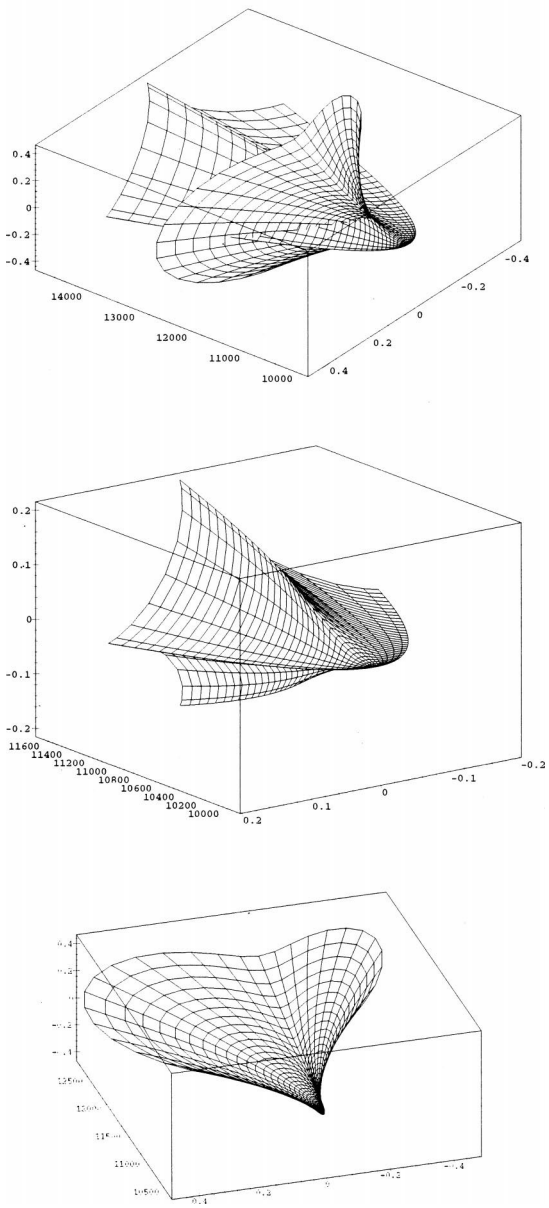

FIG. 7. Caustic sheet of the elliptical potential. The two component sheets are represented separately in the middle and bottom panels.

panels in the figure show the two component sheets. One sheet starts closer to the observer as a horizontal ''beak'' and then develops a diamond cross section. The second sheet starts inside the first one as a vertical ''beak'' and eventually opens up into a smooth surface with an oval cross section. The transitions of both sheets take place at the points where they intersect. The points of intersection where the vertical beak disappears from the second component sheet and the vertical cusp ridge appears on the first component sheet are hyperbolic umbilic points—there are two such points.

We can also at this point give the exact value of the time of the first singular wavefront. This is the smaller of $T(\mathbf{s}_+(\mathbf{0}),z_+(\mathbf{0}))$ and $T(\mathbf{s}_-(\mathbf{0}),z_-(\mathbf{0}))$ since rays passing through the origin have the longest delay (as is evidenced from the spike). For the preceding section, we have

$T(\mathbf{s}_+(\mathbf{0}),z_+(\mathbf{0}))=T_l+9699.27$ and $T(\mathbf{s}_-(\mathbf{0}),z_-(\mathbf{0}))=T_l+10\,148.84$, i.e., the first singular wavefront is the surface at $T=T_l+9699.27$, as anticipated.

By slicing the caustic sheet with constant-z surfaces we obtain a series of planar caustics representing the metamorphosis of the hyperbolic umbilic. These are shown in Fig. 8 and coincide with the well-known caustic curves in the gravitational lensing literature for an elliptical potential—e.g., p. 386 of Ref. 2. Beautiful photographs of caustic metamorphoses are shown in Ref. 14—see p. 68 for the hyperbolic umbilic metamorphosis.

B. Singular elliptical potential lens

We shall illustrate the wavefront singularities and caustic surface due to a singular elliptical potential, namely, the case of vanishing core radius ($r_c=0$). In this case, it is simpler to use polar coordinates (r,ϑ) on the lens plane. We have for the potential,

$$\hat{\Psi}^{\mathrm{sing}}_{\mathrm{ep}}(r,\vartheta)\equiv A_0\sqrt{(1-\epsilon)r_1^2+(1+\epsilon)r_2^2}=A_0 r\sqrt{1+\epsilon\cos(2\vartheta)},$$

and for the associated bending angle,

$$\hat{\boldsymbol{\alpha}}^{\mathrm{sing}}_{\mathrm{ep}}(r,\vartheta)=\frac{A_0}{\sqrt{1+\epsilon\cos(2\vartheta)}}((1+\epsilon)\cos\vartheta,(1-\epsilon)\sin\vartheta),$$

which has no dependence on r. The potential vanishes at the origin $r=0$. This case is singular because the surface mass density associated with the potential blows up at the origin of the lens plane (i.e., $\nabla^2_{\mathbf{r}}\hat{\Psi}^{\mathrm{sing}}_{\mathrm{ep}}(\mathbf{r})\to\infty$ as $\mathbf{r}\to\mathbf{0}$). The center of the lens (i.e., the origin) thus acts as an obstruction to the light rays—see Ref. 22) and p. 544 of Ref. 2 for a detailed treatment of obstruction points. Soon after going through the lens plane, the wavefronts evolve markedly differently from the nonsingular case. For our illustrations, we have used the following values of the lens parameters: $A_0=0.3,\epsilon=0.02,z_l=4000$. As in the regular case, these values are chosen for pedagogical reasons, although taking care to respect the approximations of small angles.

1. Wavefront singularities

Due to the obstruction at the center of the lens (i.e., the origin), all the wavefronts are singular and there are only two regimes. The first regime consists entirely of a single wavefront (the earliest one to make it past the lens plane) with an interior spike pointing towards the observer, as did the wavefronts of the nonsingular elliptical potential. However, in this singular case the spike is conical, and touches the lens plane at the origin. The point at the tip of the spike is removed. This wavefront, $T=T_l=4000$, is shown in Fig. 9. The figure shows both a field view of the wavefront, and a side view of the tip of the spike magnified to make the conical character apparent.

At all times afterwards, the wavefronts resemble a goblet—the second regime. However, these goblets are markedly different from those that resulted at late times in the nonsingular elliptical potential case. There is a single diamond-shaped cuspidal ridge, which lies at the throat of the goblet. The rim of the goblet is removed and acts as a boundary of the wavefront. These goblets lack the interior concave surface facing the observer that characterizes the goblets in the nonsingular case. The throat of the goblet has three sheets, each typically giving rise to an image of the source. One such wavefront in this regime ($T=T_l+1000$) is illustrated in Fig. 10, where a field view evidences the resemblance to a goblet. The bottom panel in the figure shows a magnified view of the throat of the ''goblet'' where the diamond structure is evident.

Two questions relating to this imperfect ''goblet'' wavefront arise. In the first place, do the wavefronts ever detach from the lens plane, or, on the contrary, do they reach out to the obstruction point? As one can appreciate in Fig. 11, where a given portion of the initial wavefront at $T=T_l$ is followed up and plotted again at $T=T_l+1000$, *the wavefront does not remain attached to the lens plane*.

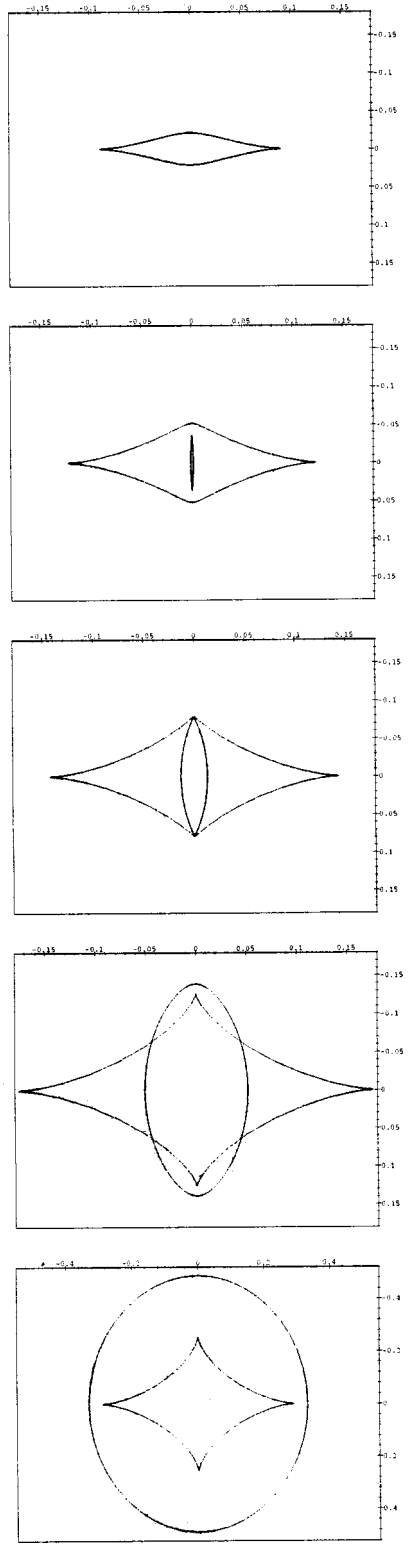

FIG. 8. The metamorphosis of the planar caustics arising from z-plane slices of the caustic surface.

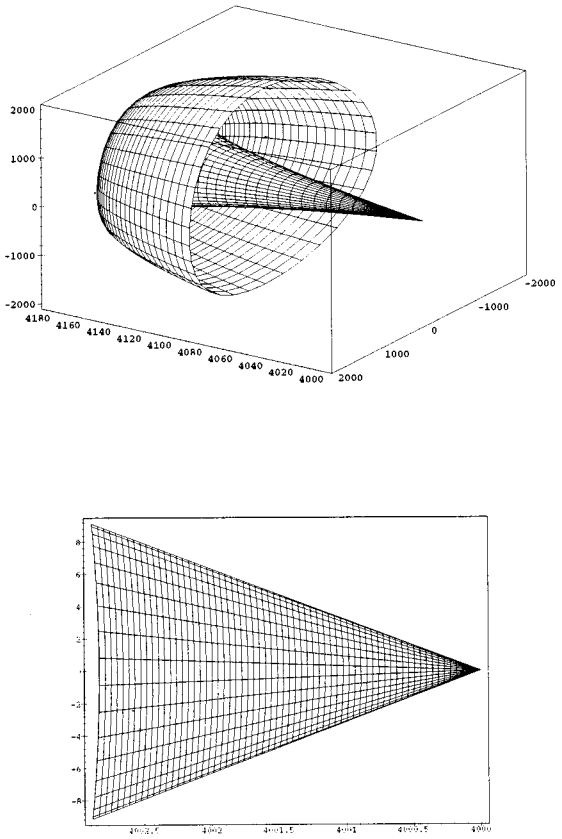

FIG. 9. The unique wavefront in the early regime ($T=T_l$) in the singular case. The bottom panel shows a side view of the tip of the spike.

The second question is whether the rim of the goblet is planar, namely, whether it lies on a constant-z plane. *The answer is no.* The rim of the goblet is a space curve, which is plotted in Fig. 12. It must be kept in mind that the rim is the boundary of the wavefront. This rim is removed because it is the image of the point $r=0$ on the lens plane under the wavefront lensing map, i.e., $\mathbf{w}^{\rm sing}_{T,\rm ep}(0,\vartheta)=(\mathbf{s}(0,\vartheta,T),z(0,\vartheta,T))$, which is a space curve for fixed T. Explicitly, Eqs. (32) and (33) yield that

$$\mathbf{s}(0,\vartheta,T)=\frac{-(T+z_l|\hat{\boldsymbol{\alpha}}^{\rm sing}_{\rm ep}(\vartheta)|^2/2)\,\hat{\boldsymbol{\alpha}}^{\rm sing}_{\rm ep}(\vartheta)}{1+|\hat{\boldsymbol{\alpha}}^{\rm sing}_{\rm ep}(\vartheta)|^2/2}+z_l\hat{\boldsymbol{\alpha}}^{\rm sing}_{\rm ep}(\vartheta),$$
$$z(0,\vartheta,T)=\frac{T+z_l|\hat{\boldsymbol{\alpha}}^{\rm sing}_{\rm ep}(\vartheta)|^2/2}{1+|\hat{\boldsymbol{\alpha}}^{\rm sing}_{\rm ep}(\vartheta)|^2/2}. \tag{65}$$

As is seen from these equations, the ultimate reason why the wavefronts have a whole elliptical curve's worth of boundary points instead of only one point is that the bending angle vector field $\hat{\boldsymbol{\alpha}}^{\rm sing}_{\rm ep}$ does not depend on r.

In rectangular coordinates, the map $\hat{\boldsymbol{\alpha}}^{\rm sing}_{\rm ep}$ is ill-defined at the origin $\mathbf{r}=\mathbf{0}$. It has a singularity of the type 0/0 since

$$\hat{\boldsymbol{\alpha}}^{\rm sing}_{\rm ep}(\mathbf{r})=\frac{A_0^2((1-\epsilon)r_1,(1+\epsilon)r_2)}{\hat{\Psi}^{\rm sing}_{\rm ep}(\mathbf{r})}.$$

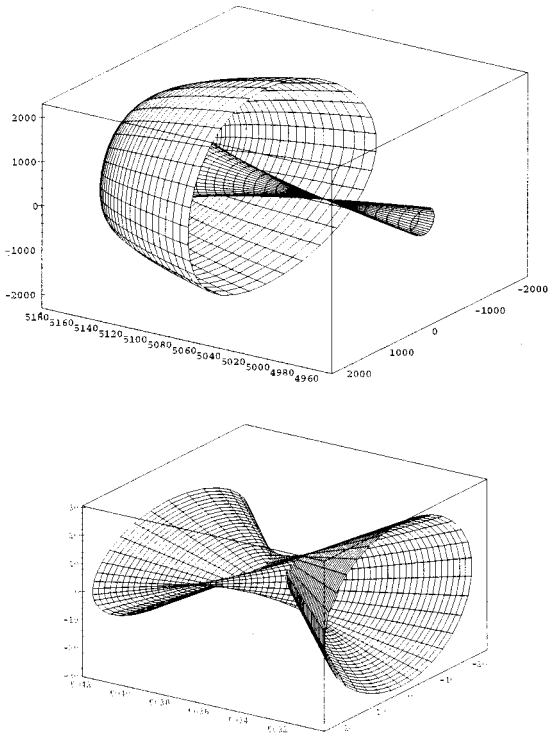

FIG. 10. Typical wavefront in the late regime ($T=T_l+1000$) in the singular case. The bottom panel shows a magnified view of the ''throat'' of the goblet.

One can approach the singular point from different directions in the lens plane and hope that the limit would be the same in all directions. However, the limiting value of the $\hat{\boldsymbol{\alpha}}_{\rm ep}^{\rm sing}(\mathbf{r})$ as $\mathbf{r}\to\mathbf{0}$ is direction dependent, as signaled by the direction-dependent bending angle ϑ in (65). In this atypically singular case, obstructing one light ray (the one that passes through the center of the lens) removes an elliptical curve's worth of points on the wavefront. If a source is outside the rim, then one lensed image is seen of the source, while two images are seen if the source is inside the rim. This phenomenon seems to have been first noted on p. 188 of Ref. 2 for the case of a singular isothermal sphere (i.e., $r_c=\epsilon=0$), where the rim is a circle, as discussed in Sec. VI C.

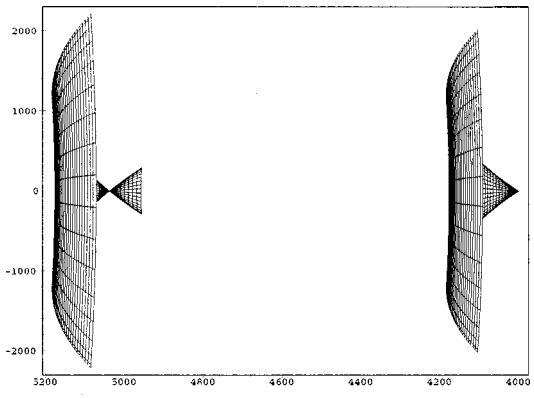

FIG. 11. Progression of a portion of the wavefront in the singular case. The observer is on the right.

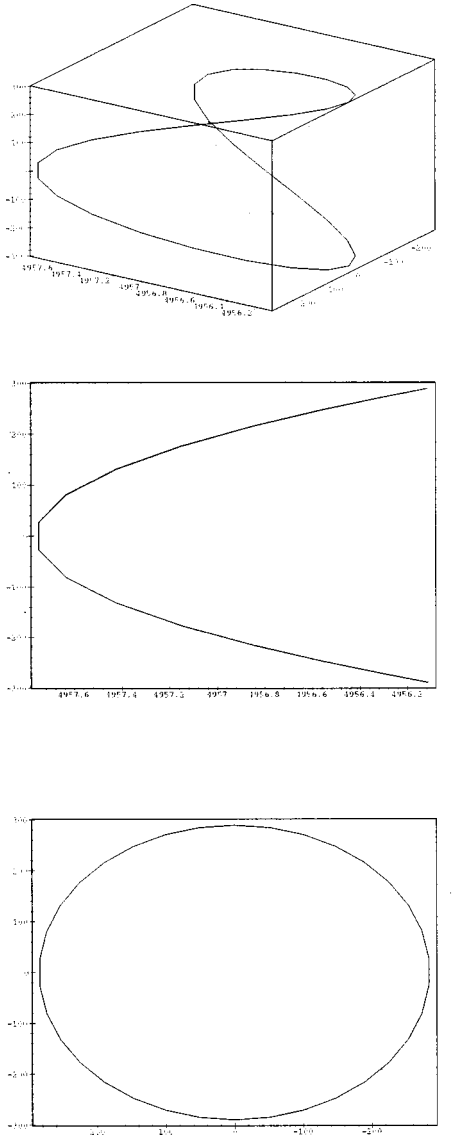

FIG. 12. The boundary of the wavefront in the critical case. Middle and bottom panels show side and front views.

2. Caustic sheet

The caustic sheet in this case is obtained by the same method as in the case of a nonsingular elliptical potential. The use of polar coordinates (r,ϑ) simplifies the calculation. We have

$$\det\frac{\partial \mathbf{s}_z}{\partial \mathbf{r}}=\cos(2\vartheta)\det\frac{\partial \mathbf{s}_z(\mathbf{r})}{\partial(r,\vartheta)}=\cos(2\phi)\left(\frac{\partial x}{\partial r}\frac{\partial y}{\partial \vartheta}-\frac{\partial x}{\partial \vartheta}\frac{\partial y}{\partial r}\right),$$

where x and y are the Cartesian components of the lensing map $\mathbf{s}_z$. In this case, the components reduce to

$$x=\left(\frac{z}{z_l}r-\frac{(z-z_l)A_0(1+\epsilon)}{\sqrt{1+\epsilon\cos(2\vartheta)}}\right)\cos\vartheta,$$

(66)

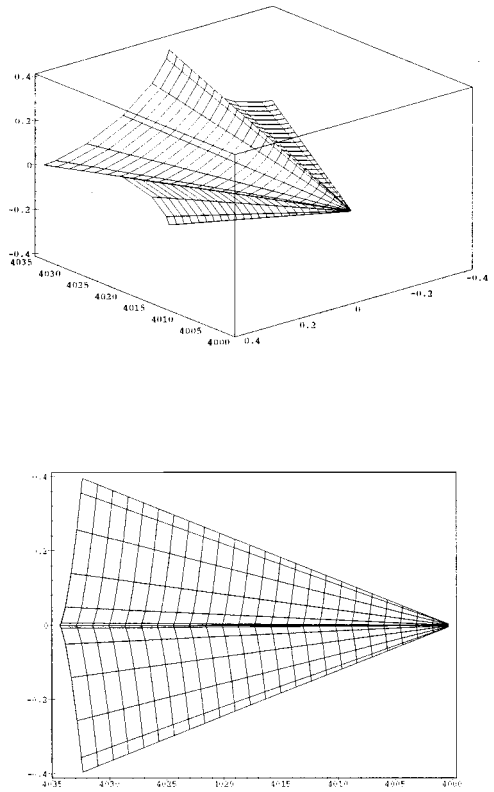

FIG. 13. The caustic sheet in the singular case.

$$y=\left(\frac{z}{z_l}r-\frac{(z-z_l)A_0(1-\epsilon)}{\sqrt{1+\epsilon\cos(2\vartheta)}}\right)\sin\vartheta,$$

and the vanishing of the Jacobian determinant—see Eq. (56)—becomes

$$0=\det\frac{\partial\mathbf{s}_z}{\partial\mathbf{r}}=\frac{z\cos(2\vartheta)}{z_l(1+\epsilon\cos(2\vartheta))^{3/2}}\left[z\left((1+\epsilon\cos(2\vartheta))^{3/2}\frac{r}{z_l}-A_0(1-\epsilon^2)\right)+z_lA_0(1-\epsilon^2)\right].$$

The unphysical root $z=0$, which defines the plane of the observer, is responsible for the absence of a second component caustic sheet, the most notable aspect of the caustic sheet in the singular case. The (one component) caustic sheet is obtained from the nontrivial root, i.e.,

$$z=z_c(r,\vartheta)\equiv-\frac{z_lA_0(1-\epsilon^2)}{(1+\epsilon\cos(2\vartheta))^{3/2}\ r/z_l-A_0(1-\epsilon^2)}. \tag{67}$$

A plot of the caustic sheet is shown in Fig. 13. The surface has four cuspidal ridges with a conical profile, which can clearly be appreciated in the bottom panel of the figure. The tip of the caustic surface lies at the center of the lens (origin) and is removed. Slicing the caustic sheet with constant-z planes we obtain the z-planar caustic curves. The planar caustics are astroid-shaped curves with four cusps, as can be seen in Fig. 14. A source inside the caustic curve has four lensed images, while a source outside has two.

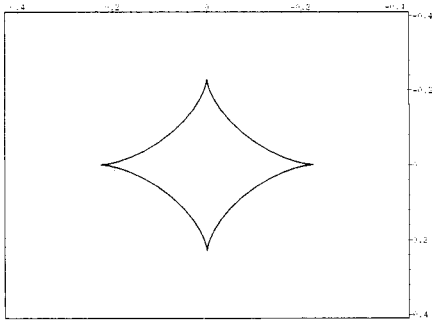

FIG. 14. Typical planar caustic in the singular case.

3. Caustic surfing

The singular elliptical potential provides an excellent opportunity to illustrate the caustic surfing scheme. We start by pointing out that the caustic sheet, which is parametrically given by (66) and (67), can equivalently be given by the following expression:

$$S_0(\mathsf{x}) \equiv ((1+\epsilon)x^2)^{1/3} + ((1-\epsilon)y^2)^{1/3} - (2\epsilon A_0(z-z_l))^{2/3} = 0.$$

This expression assumes that the apex of the lightcone where the caustic lies is at the origin of coordinates, and the lens plane is at a distance z_l from it.

Suppose now that a source is moving on the light source plane with an approximately constant velocity $\mathsf{V}=(V_1,V_2,0)$, carrying its own lightcone with it. Then the caustic on the source's lightcone moves as well, and at any given instant of conformal time t, assuming the motion is sufficiently slow, the caustic surface can be given as $S(\mathsf{x},\mathsf{t}) = S_0(\mathsf{x}-\mathsf{V}\mathsf{t})$. Assume that a space-borne telescope observes at time $\mathsf{t}=0$ an image of the source at peak magnification. From the location of the image, by the (comoving) lens map we can determine the location $\mathbf{s}$ of the source on the source plane. But for our purposes we need to switch the point of view and think of the lightcone of the source instead: The source lies at the origin and the telescope at a location $(x_0,y_0,z_0) = (-\mathbf{s}\ell_{\mathrm{tl}}/\ell_{\mathrm{sl}}, \ell\mathrm{tl}+\ell_{\mathrm{sl}})$, where ℓ_{tl} and ℓ_{sl} are the distance between the telescope and the lens plane, and between the lens plane and the source plane, resp. Because (x_0,y_0,z_0) lies on the comoving future caustic sheet of the source at $\mathsf{t}=0$, we have

$$S_0(\mathsf{x}_0) = 0 = ((1+\epsilon)x_0^2)^{1/3} + ((1-\epsilon)y_0^2)^{1/3} - (2\epsilon A_0 \ell_{\mathrm{tl}})^{2/3}, \tag{68}$$

where we have made the substitution $z_l = \ell_{\mathrm{tl}}$. Now, we calculate the speed $\mathsf{v}_{\min}$ that the telescope needs to stay on the caustic sheet during the time increment $\delta\mathsf{t}$. From our discussion in Sec. V, specifically Eq. (63), we have

$$\mathsf{v}_{\min} = \frac{V_1[(1+\epsilon)/x_0]^{1/3} + V_2[(1-\epsilon)/y_0]^{1/3}}{[(1+\epsilon)/x_0]^{2/3} + [(1-\epsilon)/y_0]^{2/3} + [4\epsilon^2 A_0^2/\ell_{\mathrm{tl}}]^{2/3}} \times \left(\left(\frac{1+\epsilon}{x_0}\right)^{1/3}, \left(\frac{1-\epsilon}{y_0}\right)^{1/3}, -\left(\frac{4\epsilon^2 A_0^2}{\ell_{\mathrm{tl}}}\right)^{1/3} \right).$$

In this expression, all the symbols are known in principle. The values of x_0 and y_0 can be found via the lens mapping at the observation event, as explained above. Clearly, this may be a technically complex procedure, considering that it is only a first step in a iterative scheme to place the telescope on the caustic sheet. Our main purpose is to show that the calculation is feasible in principle.

C. Singular isothermal sphere lens

For a singular isothermal sphere lens, we have $r_c = \epsilon = 0$. The potential and bending angle vector are given respectively as follows:

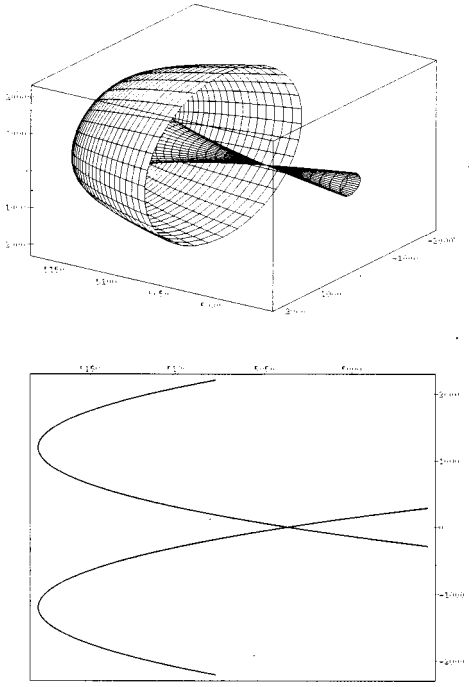

FIG. 15. Wavefront due to a singular isothermal sphere. The top panel shows a field view, and the bottom panel shows a slice or profile of the wavefront. Notice that the wavefront is a surface of revolution around the optical axis.

$$\hat{\Psi}_{ep}^{\mathrm{sis}}(r,\vartheta)=A_0 r, \quad \hat{\boldsymbol{\alpha}}_{\mathrm{ep}}^{\mathrm{sis}}(r,\vartheta)=A_0(\cos\vartheta,\sin\vartheta).$$

The wavefronts are similar to those of the singular elliptical potential, except that the throat of the goblet is a point and the singular rim of the goblet is a circle—see Fig. 15. The caustic surface collapses to a line coinciding with the portion of the optical axis beyond the lens plane (i.e., $z > z_l$). Note the origin on the lens plane, which is a singularity of the lens, is not a part of the caustic line. We have that each z-planar caustic is a point.

VII. CONCLUDING REMARKS AND OUTLOOK

We have shown how to construct a lensing map that takes points on the lens plane into points on a wavefront surface, as opposed to a source plane. This represents a sort of ''instantaneous'' lens map, carrying a sense of constant time. By contrast, the standard lens map carries no sense of time at all. Additionally, the wavefront lensing map has an asymmetric Jacobian matrix. Notice that, barring multiple sheets, the wavefront surface lies very close to a plane in the weak-field case, as illustrated in most of our figures. In the figures the optical axis is magnified several times in order to appreciate the distance between the different sheets in the folded wavefront. Our intial motivation for explicitly constructing a wavefront-lens mapping was inspired by several works (e.g., Refs. 6, 13, 15, 18, and 23). In this respect, it appears that an extension of our constructions in Secs. III and IV beyond the weak field domain is feasible.[24,25]

We took advantage of the conformally flat nature of the flat FL universe in order to make use of a comoving lens equation, which in addition to being comoving is also a conformal lens equation. A conformally related flat space–time exists, of course, in all three types of FL universes, so in principle, our wavefront map could be adapted for interpretation in the open or closed universes. However, in such universes the conformal factor relating the FL universes to the corresponding flat space–time depends on the space point, as well as the time, and the translation of our conformal present proper length function to a cosmological present proper length is not at all as direct as we found it in this work. Some of the subtleties that would be involved in the

translation in the open and closed cases are treated in detail by Frittelli, Kling, and Newman,[26] where the conformally flat lens map and time delay are transformed into the cosmological lensing map and time delay. Nonetheless, we do not need to rely on the conformally related flat space to calculate our present proper length function.

The individual wavefronts for the potentials illustrated proved useful in visualizing the relationship between the location of the source in reference to the caustic, and the number of images observed. Additionally, the wavefronts of the singular potentials helped explain the anomalous counting of images observed by Petters, Levine, and Wambsganss,[2] p. 188. The latter showed that in the case of the singular potentials there is a simple closed curve, that is not a caustic, but that separates regions in the source plane where the number of images differs by one, rather than two. We have here shown that such a curve is the boundary of the wavefront, it is not a caustic, and the number of images differs by one less than in the regular case because one whole sheet of the wavefront is missing due to an obstruction in the lens plane.

Lastly, we have taken a step towards a preliminary scheme for caustic surfing in a meaningful and consistent manner. The form of the subsequent iterations remains an open problem, as does the implementation of the procedure, particularly the measurement of the transverse velocity of the the moving source that one intends to follow. Clearly the caustic surfing proposal depends only on the caustic surface, and not on the method used to obtain it. But the point is that optimal caustic surfing (with the least effort) is achieved only by allowing the telescope to surf the caustic sheet, rather than the planar caustics at fixed distance from the source. One could also imagine scenarios where a telescope may not ride a caustic sheet, but move so as to stay inside certain chambers of the caustic surface (compare with Gaudi and Gould[27]), possibly near higher order singularities. Future studies of the aforementioned issues are clearly warranted.

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Continuum spin foam model for 3d gravity

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An example illustrating a continuum spin foam framework is presented. This covariant framework induces the kinematics of canonical loop quantization, and its dynamics is generated by a *renormalized* sum over colored polyhedra. Physically the example corresponds to 3d gravity with cosmological constant. Starting from a kinematical structure that accommodates local degrees of freedom and does not involve the choice of any background structure (e.g., triangulation), the dynamics reduces the field theory to have only global degrees of freedom. The result is *projectively* equivalent to the Turaev–Viro model. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1509850]

I. INTRODUCTION

Several TQFTs can be written as a sum over assignments of spins to polyhedra: that is, as spin foam models. A trend in today's research is to try to find a model of a similar type that is related to 4d gravity.[1] Regarding these models as fundamental amounts to postulating that gravity is only effectively a field theory, but fundamentally it has only finitely many degrees of freedom and a privileged polyhedron (or triangulation), comes along with space–time. It has been proposed to get rid of this extra structure with a sum over triangulations.[2] In this article we will explore another route. We will regard the continuum as fundamental and take the diffeomorphism invariance of general relativity as the guiding symmetry. We share this principle with canonical loop quantization.[3]

In this article we present an example. It is defined in the continuum, but it turns out to be equivalent to the Turaev–Viro model.[4] The interest of our example relies on the fact that it is a continuum spin foam model. More precisely, the construction induces the kinematics of q-deformed loop quantization in the spatial slices, and the projector to the space of physical states is constructed as a renormalized sum over colored (by spins) polyhedra.

The construction does not involve the choice of any background structure, and the diffeomorphism group acts faithfully at the kinematical level.

The strategy used to generate this family of examples (one for every value of a deformation parameter) can be adapted to other spin foam models. A ''renormalizability condition'' determines whether the continuum theory exists. The proof that other topological models satisfy the condition proceeds almost in complete parallel to the proof given here. Interestingly, there are reasons to believe that there are other examples corresponding to genuine field theories. In the case of compact QED, the first steps in this direction have already been taken.[5]

In Sec. II we construct the example and prove the equivalence with the Turaev–Viro model. Section III gives an interpretation of the projector as a renormalized sum over quantum geometries.

II. A CONTINUUM SPIN FOAM MODEL

This is the central section of the article. In the beginning we present the construction of the example and show its main properties. With minor modification of the proofs, the construction

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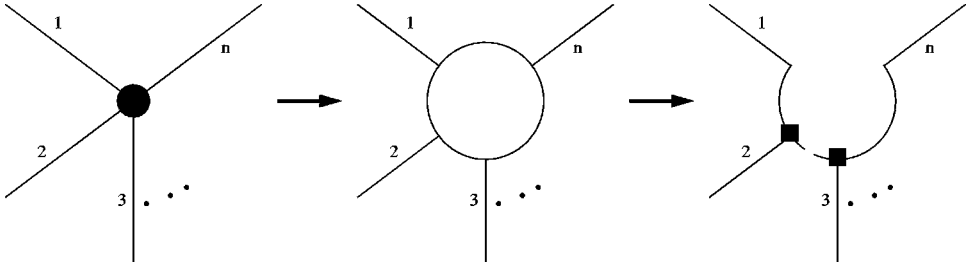

FIG. 1. The construction uses an arbitrary numbering of the edges coming to a vertex. Internal vertices are shown as square dots and internal edges are dashed lines.

applies to other topological spin foam models and the same strategy could apply to other less trivial spin foam models as well. In the last subsection, we prove the projective equivalence with the Turaev–Viro model.

A. Embedded graphs and embedded polyhedra

In this work all the spaces and maps are piecewise linear.

Consider a compact surface without boundary Σ. By an embedded graph Γ we mean a finite one-dimensional CW-complex all of whose vertices have valence two or bigger, together with an embedding into Σ. The set of all graphs embedded into a given surface will be denoted by $G(\Sigma)$. This set has a natural partial order given by inclusion and it is directed.

Similarly, consider a three-manifold with boundary M. By an embedded polyhedron X we mean a finite two-dimensional CW-complex all of whose internal edges have valence two or bigger, together with an embedding into M such that $X\cap\partial M$ denoted by ∂X belongs to $G(\partial M)$. The set of all polyhedra embedded into a given three-manifold will be denoted by $P(M)$. Again, this set is partially ordered and directed.

B. Data from lattice gauge theory

Our construction starts with data generated by ''lattice gauge theory'' on all lattices embedded into given space–times.

For every $\Gamma\in G(\Sigma)$ we are given a complex vector space $C(\Gamma)$ and for every $X\in P(M)$ we are given a linear functional $\Omega_X^n: C(\partial X)\to\mathbb{C}$. Thus, for each surface Σ we get a collection of vector spaces labeled by embedded graphs and for each three-manifold M we get a collection of linear functionals labeled by embedded polyhedra. Our work is based on the compatibility of these collections of structures with the partial order of the labeling sets.

Now we define these objects in the example presented here. We follow the notation of Turaev and Viro[4] as closely as possible as well as their conventions and normalizations.

Fix an integer $r\geqslant 3$ and denote by I the set of spins $\{0,1/2,\ldots,(r-2)/2\}$. A triple of spins is admissible, $(i,j,k)\in adm$, if $i+j+k$ is an integer and

$$i\leqslant j+k,\quad j\leqslant k+i,\quad k\leqslant i+j,\quad i+j+k\leqslant r-2.$$

Given an embedded graph $\Gamma\in G(\Sigma)$ we assign to it an abstract simple graph Γ_s. The vertices of a simple graph are always trivalent; a graph dual to a triangulation is an example of a simple graph.

Γ_s is constructed by blowing up the vertices of Γ as we explain below. To each edge of Γ corresponds one edge in Γ_s and to each vertex of Γ we assign several ''internal vertices'' and ''internal edges'' in Γ_s in the manner indicated by Fig. 1.

A coloring α of Γ is an assignment of spins to its edges and intertwiners to its vertices. An intertwiner is a coloring (with spins) of the internal edges assigned to the vertex. Clearly, a

coloring α of Γ induces a coloring of Γ_s, an assignment of spins to its edges. The coloring is admissible, $\alpha \in adm(\Gamma)$, if at each vertex v of Γ_s the triple $(\alpha(e_1(v)),\alpha(e_2(v)),\alpha(e_3(v))) \in adm$.

Then $C(\Gamma)$ is defined by

$$C(\Gamma)=\mathbb{C}[adm(\Gamma)],$$

where $\mathbb{C}[adm(\Gamma)]$ is the complex vector space freely generated by the elements of $adm(\Gamma)$; in addition, the inner product makes $adm(\Gamma)$ an orthonormal set. A different choice of internal structure in the construction of Γ_s results in an *a priori* different vector space; however, ''recoupling moves'' on the internal edges define an isomorphism between any two spaces generated by different choices. This is reviewed in the Appendix. We identify all these isomorphic vector spaces and call them $C(\Gamma)$.

In the non-q-deformed case, when the set of spins is infinite, the space just constructed is the space of square integrable functions of (generalized) SU(2)-connections,[6] and it is the heart of the kinematics of canonical loop quantum gravity.[3]

X_s, a simple abstract polyhedron, is constructed by blowing up the edges and vertices of $X \in P(M)$ as we explain below. We proceed in complete parallel to the case of graphs. First, we surround every edge by a cylindrical neighborhood and every vertex by a spherical neighborhood; in this way we created an internal (empty) bubble for each edge and vertex of X in analogy with the middle picture of Fig. 1. Then, we will erase one internal face in each internal bubble, as we did in the last picture of Fig. 1, to create X_s. There are only two rules to select the face to be erased from each internal bubble. In the case of edge-bubbles, we erase one of the lateral faces (not a face shared with a vertex-bubble). And in the case of the vertex-bubbles, we erase one of the faces shared with an edge-bubble. Notice that the valence of any edge in X_s is three and that at every vertex of X_s six faces meet.

A coloring φ of X is an assignment of spins to its faces and intertwiners to its edges. An intertwiner is a coloring (with spins) of the internal faces assigned to the edge. The coloring is admissible, $\varphi \in adm(X)$, if at each edge e of X_s the triple $(\varphi(f_1(e)),\varphi(f_2(e)),\varphi(f_3(e))) \in adm$.

Each colored polyhedra is assigned a weight. This assignment is a simple extension of the Turaev and Viro weight to embedded (not necessarily simple) polyhedra. The Turaev–Viro weight is constructed as the product of weights assigned to its vertices and faces (with a correction due to the boundary edges):[4]

$$|X|_\varphi = |X_s|^{TV}_\varphi = w^{-2\chi(X_s)+\chi(\partial X_s)} \prod_{f\in F(X_s)} w^{2\chi(f)}_{\varphi(f)} \prod_{e\in E(X_s)} w^{\chi(e)}_{\partial\varphi(e)} \prod_{v\in V(X_s)} |\hat{T}_v|_\varphi .$$

Here χ denotes Euler characteristic. $w_{\varphi(f)}$ and $w_{\partial\varphi(e)}$ denote the quantum group analog of the dimension of the spin j representation for $j=\varphi(f)$ and $j=\partial\varphi(e)$, respectively. $|\hat{T}_v|_\varphi$ is the quantum $6j$ symbol corresponding to the six-tuple of spins of the faces meeting at vertex v.

Then $\Omega_X : C(\partial(X)) \to \mathbb{C}$ is defined by $\Omega_X(\alpha)=\Sigma_\varphi |X|_\varphi$, where the sum runs over the colorings $\varphi \in adm(X)$ that induce α in the boundary. We will work with the linear functional normalized dividing by the ''vacuum to vacuum amplitude'' $\Omega_X(j=0)$,

$$\Omega^n_X(\alpha)=\frac{\Omega_X(\alpha)}{\Omega_X(j=0)}.$$

Note that $\Omega^n_X(\alpha)$ can also be defined from $\Omega'_X(\alpha)=\Sigma_\varphi |X|'_\varphi$ which is defined from a less refined Turaev–Viro weight $|X|'_\varphi$ in which the normalizing factor $w^{-2\chi(X_s)+\chi(\partial X)}$ is omitted.

The construction of X_s involves a choice of ''internal structure'' on the edges of X. However, the invariance results of Turaev and Viro imply that Ω_X and Ω'_X are independent of this choice. This is reviewed in the Appendix.

The weight assigned to a colored polyhedron is what defines the dynamics of this example. We extended the Turaev–Viro weight in a simple manner, but it is possible to derive a weight assignment for general polyhedra that reduces to the Turaev–Viro weight in the case of simple polyhedra.[7]

C. From lattices to the continuum

Now we will leave single ''lattices'' and go to the continuum.

Consider two embedded graphs $\Gamma_1 \leqslant \Gamma_2$ in $G(\Sigma)$. It is easy to see that $\alpha \in adm(\Gamma_1)$ defines an admissible coloring in Γ_2 by simply extending the coloring with color $j=0$ in the additional edges and extending the intertwiners also coloring with $j=0$ in the additional internal edges. Thus, we can take this natural inclusion for granted and write $C(\Gamma_1) \subset C(\Gamma_2)$. Due to this property we can define $C(\Sigma)$ as the inductive limit or co-limit[8] of the nested spaces labeled by graphs,

$$C(\Sigma) = \text{co-}\lim_{\Gamma \to \Sigma} C(\Gamma).$$

Similarly, for $\alpha \in C(\partial M)$ induced by $\alpha \in adm(\Gamma)$ we define

$$\Omega^n_M(\alpha) = \lim_{X \to M} \Omega^n_X(\alpha), \quad \partial X \geqslant \Gamma. \tag{1}$$

When the limit exists it defines $\Omega^n_M : C(\partial M) \to \mathbb{C}$. In our example we prove its existence in the next subsection. However, the analogous limit in theories constructed from other lattice gauge theories may not exist. The existence of the limit should be interpreted as a renormalizability condition.

Note that the extendibility of colorings from subgraphs implies that $adm(\Sigma)$ and similarly $adm(M)$ can be defined. A coloring in $\alpha \in adm(\Sigma)$ should be thought of as a coloring of all graphs, bigger than a certain minimal graph $\Gamma(\alpha)$, that is compatible with inclusion of graphs. We then have the equivalent definition $C(\Sigma) = \mathbb{C}[adm(\Sigma)]$.

D. Renormalizability and cellular decompositions

A polyhedron $X \in M$ induces a cellular decomposition for (M,Γ), where $\Gamma \in G(\partial M)$, if $\partial X = \Gamma$ and $M - \partial M - X$ is a disjoint union of open balls.

Theorem 1: *Given any polyhedron $X \in P(M)$ there is a finer polyhedron $X' \in P(M)$, $X \leqslant X'$, such that X' induces a cellular decomposition for (M,Γ) for some $\Gamma \geqslant \partial X$.*

Proof: First note that for every manifold with boundary one can find embedded polyhedra inducing cellular decompositions. Take for example the cellular complex dual to any triangulation of the manifold. Once we have one cellular decomposition, we can generate many by subdivision of the induced cells adding faces to the original polyhedron.

Let $X'' \in P(M)$ induce a cellular decomposition that is sufficiently fine in the sense that for each open ball in $\cup_{r=1}^n B_r = M - \partial M - X''$ we have that $B_r - X$ is a finite union of open balls, $B_r - X = \cup_{s=1}^{m_r} B'_{r,s}$.

Since we are working with piecewise-linear spaces, such a X'' can be constructed from an initial cellular decomposition after finitely many refinements.

Let $X' = X'' \cup X$. Then $M - \partial M - X' = \cup_{r=1}^n \cup_{s=1}^{m_r} B'_{r,s}$. □

Theorem 2: *Fix $X \in P(M)$ a polyhedron inducing a cellular decomposition of (M,Γ). For any finer polyhedron $X' \in P(M)$, $X \leqslant X'$, we have*

$$\Omega^n_X = \Omega^n_{X'}|_{C(\partial X)}.$$

The proof of this theorem requires some previous definitions and lemmas presented after the following corollary.

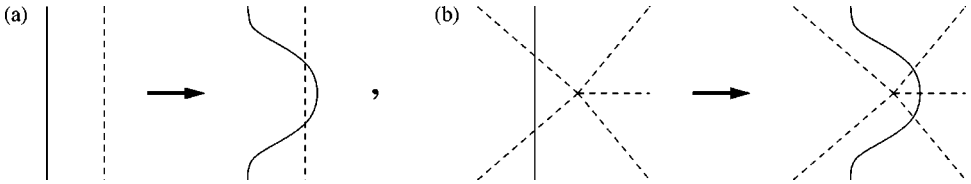

FIG. 2. In each picture the paper corresponds to a set of faces of a portion of the polyhedron. The solid lines indicate edges where one (or more) faces meet the paper from above. The dashed lines correspond to faces that are below the paper. (a) Illustrates a top face(s) sliding through a wedge with bottom face(s). (b) Illustrates a top face(s) sliding through a corner with bottom faces.

Corollary 1 (renormalizability): In the definition

$$\Omega_M^n = \lim_{X \to M} \Omega_X^n$$

the limit exists. In this sense, the theory defined by the collection of linear functionals Ω_X' *is renormalizable*.

We should mention that for the linear functionals Ω_X' and Ω_X the limit does not exist. Only the renormalized functional exists in the continuum.

Wedge and corner moves generalize the lune $\mathcal{L}$ and Matveev $\mathcal{M}$ moves (and their inverses) on simple polyhedra. Wedge moves describe a face of an embedded polyhedron $X \in P(M)$ sliding through a wedge, while in corner moves a face slides through a corner. See Fig. 2.

Lemma 1 (Invariance under wedge and corner moves): Let $X \in P(M)$ *and* $\alpha \in adm(\partial X)$. *Then* $\Omega_X'(\alpha)$ *is invariant under wedge and corner moves*.

Proof: It is clear that a wedge move in X induces a sequence of $\mathcal{L}$ or $\mathcal{L}^{-1}$ moves in X_s. Similarly, a corner move in X induces a sequence of $\mathcal{M}$ and/or $\mathcal{M}^{-1}$ and/or $\mathcal{L}$ and/or $\mathcal{L}^{-1}$ in X_s. Thus, this lemma is a direct consequence of the similar invariance lemmas of Turaev and Viro.[4]□

The following lemma is a well-known consequence of the definition a properties of $|X|_\varphi'$; see Refs. 4 and 9.

Lemma 2 (The color $j=0$ *is invisible): Let* $X \in P(M)$ *and* $\varphi \in adm(X)$. *Construct the polyhedron* $X(\varphi)$ *erasing from* X *the "invisible" two-strata, the ones colored with* $j=0$. *Then*

$$|X(\varphi)|_\varphi' = |X|_\varphi'.$$

Also, for $\alpha \in adm(\partial X)$ *construct* $X(\alpha)$ *erasing from* X *the two-strata meeting* ∂X *in edges colored with* $j=0$. *Then*

$$\Omega_{X(\alpha)}'(\alpha) = \Omega_X'(\alpha).$$

Proof of Theorem 2: Consider a collection of nested polyhedra $\{X_r\}$ such that $X = X_1 \leqslant X_2 \leqslant \cdots \leqslant X_n = X'$ where $X_{r+1} - X_r \subset B_{s(r)}$ for some cell B_s in $\cup_{s=1}^n B_s = M - \partial M - X$ with $B_{s(r)} \neq B_{s(t)}$ if $r \neq t$.

We will show that $\Omega_{X_{r+1}}^n|_{C(\partial X_r)} = \Omega_{X_r}^n$.

Let $\partial B_{s(r)} - \partial M = \cup_{u=1}^m F_u$ with F_u faces of X.

The closures of the faces in $X_{r+1} - X_r$ may intersect several of the faces of $\partial B_{s(r)}$, but we can use wedge and corner moves on X_{r+1} (inside $B_{s(r)}$) until only F_1 (and ∂M if $B_{s(r)}$ is a boundary cell) is intersected. Call the resulting polyhedron Y_{r+1}'. Remove from Y_{r+1}' the two-strata meeting $\partial Y_{r+1}' - \partial X_r$; we call this polyhedron Y_{r+1}.

Let $B \subset M$ be an open ball such that $Y_{r+1} - X_r \subset B$, and $B \cap X_r$ lies in the interior of F_1.

Then

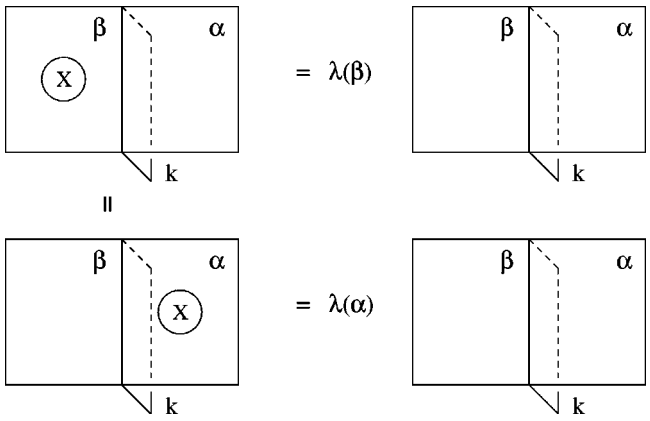

FIG. 3. The pictures should be thought of as Ω' evaluations with the indicated boundary coloring.

$$\Omega'_{X_{r+1}}|_{C(\partial X_r)}(\alpha)=\Omega'_{Y_{r+1}}(\alpha)=\sum_{\beta\in adm(Y_{r+1}\cap\partial B)}\Omega'_{Y_{r+1}\cap B^c}(\alpha\cup\beta)\Omega'_{Y_{r+1}\cap\overline{B}}(\beta)$$

$$=\sum_{\beta\in adm(X_r\cap\partial B)}\Omega'_{X_r\cap B^c}(\alpha\cup\beta)\Omega'_{Y_{r+1}\cap\overline{B}}(\beta)$$

$$=\lambda\sum_{\beta\in adm(X_r\cap\partial B)}\Omega'_{X_r\cap B^c}(\alpha\cup\beta)\Omega'_{X_r\cap\overline{B}}(\beta)=\lambda\Omega'_{X_r}(\alpha),$$

where B^c and $\overline{B}$ denote the complement and the closure of B, respectively. In the first equality Lemmas 1 and 2 were used. In the second and fifth equalities the associativity of Ω' was used. The fourth equality is due to the following lemma.

Lemma 3: The quotient $\Omega'_{Y_{r+1}\cap\overline{B}}(\beta)/\Omega'_{X_r\cap\overline{B}}(\beta)=\lambda$ *is independent of the coloring.*

Proof of the Lemma: Let $(\beta,\alpha,k)\in adm$. The proof follows picture in Fig. 3.

In the upper left picture the face with a circle and an X inside represents $Y_{r+1}\cap\overline{B}$; the rest of the faces play only an auxiliary role. Using wedge moves the X slides through the edge. The result is the picture in the bottom left. There we can again identify the face with a circle and an X with $Y_{r+1}\cap\overline{B}$. From the pictures in the left to the ones in the right we have only used $\Omega'_{Y_{r+1}\cap\overline{B}}(\gamma)=\lambda(\gamma)\Omega'_{X_r\cap\overline{B}}(\gamma)$.

The lemma follows from the fact that the set of spins is adm-connected; given any two spins there is a chain of admissible triples linking them. □

This completes the proof of Theorem 2. □

E. Spaces of physical states and propagators

We will now define adequate spaces of physical states and propagators. To do this cleanly we need to use the language of cobordism theory. A cobordism W is defined by the triple

Corollary 1 (renormalizability): In the definition $W=(M;i_{\Sigma_0}:\Sigma_0\to\partial M,i_{\Sigma_1}:\Sigma_1\to\partial M)$ where M is a three-manifold with boundary, Σ_0 and Σ_1 are compact surfaces without boundary, $\partial M=i_{\Sigma_0}(\Sigma_0)\cup i_{\Sigma_1}(\Sigma_1)$ and $i_{\Sigma_0}(\Sigma_0)\cap i_{\Sigma_1}(\Sigma_1)=\emptyset$. Cobordisms can be composed in an obvious way. Also, there is a special cobordism for each Σ compact surface without boundary, $id_\Sigma=(\Sigma\times I;i_0(p)=(p,0),i_1(p)=(p,1))$.

To every Σ we assign a space of physical states $H(\Sigma)\subset C(\Sigma)^*$ defined by $H(\Sigma)=\Omega^n_{\Sigma\times I}(C(\Sigma))$. In the jargon of the field $\Omega^n_{\Sigma\times I}$ is referred to as the "generalized projector," even though $H(\Sigma)\subset C(\Sigma)^*$. It is useful to note that $H(\Sigma)$ is spanned by vectors $\overline{\alpha}$ defined by

$$\overline{\alpha}[\delta]=\Omega^n_{\Sigma\times I}(i_0^{-1}{}^*\alpha\cup i_1^{-1}{}^*\delta),$$

where $\alpha,\delta\in C(\Sigma)$ and we have used the pull back maps $i_0^{-1}{}^*:adm(\Sigma)\to adm(\partial(\Sigma\times I)_{t=0})$, $i_1^{-1}{}^*:adm(\Sigma)\to adm(\partial(\Sigma\times I)_{t=1})$. The inner product in $H(\Sigma)$ is defined by

$$(\overline{\alpha},\overline{\beta})=\overline{\alpha}(\beta).$$

Now for a general cobordism define the map $\Phi^n_W:H(\Sigma_0)\to C(\Sigma_1)^*$ by

$$\Phi^n_W(\overline{\alpha})[\delta]=\Omega^n_M(i_0^{-1}{}^*\alpha\cup i_1^{-1}{}^*\delta).$$

Theorem 3: $\Phi^n_W(H(\Sigma_0))\subset H(\Sigma_1)$

Proof: Consider a regular neighborhood M'' of $i_{\Sigma_1}\Sigma_1$ in M; it has the $\Sigma_1\times I$ topology. Denote its boundary by $\partial M''=\Sigma_1'\cup\Sigma_1$. Also call $M'=M-M''$; clearly $M'\approx M$ and $\partial M''=\Sigma_0\cup\Sigma_1'$.

We are going to compute $\Phi^n_W(\overline{\alpha})[\delta]$ using the following auxiliary structures: First, two boundary graphs Γ_0,Γ_1 such that $\Gamma_0\geqslant\Gamma(\alpha)$ and $\Gamma_1\geqslant\Gamma(\delta)$; second, $X\in P(M)$ inducing a cellular decomposition of $(M;i_{\Sigma_0}\Gamma_0\cup i_{\Sigma_1}\Gamma_1)$ such that $X|_{M''}\in P(M'')$ induces a cellular decomposition of $(M'';i_{\Sigma_0}\Gamma_0\cup i_{\Sigma_1'}\Gamma_1')$, and $X|_{M'}\in P(M')$ induces a cellular decomposition of $(M';i_{\Sigma_1'}\Gamma_1'\cup i_{\Sigma_1}\Gamma_1)$:

$$\begin{aligned}\Phi^n_W(\overline{\alpha})[\delta]&=\frac{\Omega'_X(\alpha\cup\delta)}{\Omega'_X(j=0)}\\&=\sum_\beta\frac{\Omega'_{X|_{M'}}(\alpha\cup\beta)\Omega'_{X|_{M''}}(\beta\cup\delta)}{\Omega'_X(j=0)}\\&=\left(\frac{\Omega'_{X|_{M'}}(j=0)\Omega'_{X|_{M''}}(j=0)}{\Omega'_X(j=0)}\right)\sum_\beta\ \Omega^n_{M'}(i_{\Sigma_0}^{-1}{}^*\alpha\cup i_{\Sigma_1'}^{-1}{}^*\beta)\Omega^n_{M''}(i_{\Sigma_1'}^{-1}{}^*\beta\cup i_{\Sigma_1}^{-1}{}^*\delta)\\&=\lambda(\Gamma_1')\sum_\beta\ \Omega^n_M(i_{\Sigma_0}^{-1}{}^*\alpha\cup i_{\Sigma_1}^{-1}{}^*\beta)\Omega^n_{\Sigma\times I}(i_0^{-1}{}^*\beta\cup i_1^{-1}{}^*\delta).\end{aligned}\tag{2}$$

The sums are over $\beta\in adm(\Gamma_1')$. In the last equality we used the invariance under homeomorphisms; this property follows from the definitions and will be described in the next subsection. We could have used another cellular decomposition to perform the calculation or another auxiliary surface Σ_1'. The result would have been another expression for the same element of $H(\Sigma)$.

The desired result follows from the above equation. □

Note that the maps assigned to identity cobordisms are identity maps, $\Phi^n_{id_\Sigma}|_{H(\Sigma)}=id_{H(\Sigma)}$. Now we show that Φ^n_W satisfies the projectivized propagator condition.

Theorem 4: *For any two composable cobordisms,* $W_1=(M_1;i_{\Sigma_0},i_{\Sigma_1})$ *and* $W_2=(M_2;i'_{\Sigma_1},i_{\Sigma_2})$, *we have* $\Phi^n_{W_2}\circ\Phi^n_{W_1}=\lambda\Phi^n_{W_2\circ W_1}$.

Proof: The definition of Φ^n_W requires that its argument is written in a canonical form. We use (2). We follow the strategy of the previous theorem's proof: with X an auxiliary polyhedron giving a cellular decomposition for W_1 and Y for W_2, we will write the expression in terms of Ω' to use associativity. Then we will rewrite in terms of the renormalized objects of $X\cup Y$, which is an auxiliary polyhedron giving a cellular decomposition for $W_2\circ W_1$.

$$\Phi^n_{W_2}\circ\Phi^n_{W_1}(\overline{\alpha})(\delta)=\lambda(\Gamma_1')\sum_\beta\ \Omega^n_{M_1}(i_{\Sigma_0}^{-1}{}^*\alpha\cup i_{\Sigma_1}^{-1}{}^*\beta)\Omega^n_{M_2}(i'^{-1}_{\Sigma_1}{}^*\beta\cup i_{\Sigma_2}^{-1}{}^*\delta)$$

$$=\lambda(\Gamma_1')\left(\frac{\Omega'_{X\cup Y}(j=0)}{\Omega'_X(j=0)\Omega'_Y(j=0)}\right)\Omega^n_{X\cup Y}(\alpha\cup\delta)$$

$$=\lambda(\Gamma_1')\Lambda(\Gamma_1)\Phi^n_{W_2\circ W_1}(\overline{\alpha})(\delta).$$

□

Here we proved the last two theorems for the example that we are presenting, but the proofs extend with very little change to the general case in which the renormalizability condition (1) holds.

F. Action of the homeomorphism group

A homeomorphism between two manifolds with boundary $f:M\to N$ induces a map among the spaces of embedded polyhedra. Colorings are pulled back by this map. Similarly, the restriction of the map to the boundaries induces a pull back map among the spaces of colorings which leads to $U_f:C(\partial M)\to C(\partial N)$ defined by the action $U_f(\alpha)=f^{-1}{}^*(\alpha)$. The following identities describe the action of homeomorphisms

$$|X|'_\varphi=|f(X)|'_{f^{-1}{}^*\varphi},\quad \Omega'_X(\alpha)=\Omega'_{f(X)}(f^{-1}{}^*\alpha),\quad \Omega^n_M=\Omega^n_{f(M)}\circ U_f.$$

Note that the action of f is not trivial due to its action in the boundaries. The language of the last subsection already assumes this level of invariance; W is only sensible to M up to a homeomorphism preserving the boundary. By dual action of U_f we have a representation of the modular group (mapping class group) of Σ on $H(\Sigma)$. Indeed, if f and g are two isotopic homeomorphisms, U_f and U_g induce the same map in $H(\Sigma)$. In particular, if f is connected to the identity,

$$U_f|_{H(\Sigma)}=id_{H(\Sigma)}.$$

Thus, for homeomorphisms connected with the identity we have $\Omega^n_{f(M)}=\Omega^n_M$.

In relation with canonical loop quantum gravity we have the following question: *Is it possible to find first the space of homeomorphism invariant states and construct $H(\Sigma)$ from it?* The next section gives a satisfactory affirmative answer to this question. Here we present a preliminary answer.

Define the space of states invariant under homeomorphisms connected with the identity $\mathcal{H}_{hom}(\Sigma)\subset C(\Sigma)^*$ as in Ref. 3. This space is spanned by elements of the type

$$\tilde{\alpha}[\beta]=s(\Gamma(\alpha))\,\delta_{[\Gamma(\alpha)][\Gamma(\beta)]}(\alpha,f_0^{-1}{}^*\beta),$$

where the factor $s(\Gamma(\alpha))$ depends on the symmetry of the graph, and f_0 is a homeomorphism (connected with the identity) on Σ taking $\Gamma(\beta)$ to $\Gamma(\alpha)$.

Clearly, $\tilde{\alpha}=\tilde{\beta}$ only if there is homeomorphism (connected with the identity) f_0 such that $U_{f_0}(\tilde{\beta})=\tilde{\alpha}$. Thanks to the invariance properties stated above, we can define

$$P(\tilde{\alpha})=\overline{\alpha}. \tag{3}$$

In this way the Reisenberger–Rovelli projector, $P(\mathcal{H}_{hom}(\Sigma))=H(\Sigma)$,[10] reconstructs the space of physical states from the space of homeomorphism invariant states.

G. Projective equivalence with the Turaev–Viro model

A particularization of the construction of Turaev and Viro[4] can be described as follows. *To each triangulated surface T assign the vector space $C(T^*)$, where T^* is the graph dual to the triangulation. Similarly, to each cobordism between triangulated surfaces W assign the map $\Phi_W: C(T_0^*) \to C(T_1^*)$ by the formula*

$$\Phi_W(\alpha) = \sum_{\beta} \Omega_{\Delta^*}(i_{T_0}^{-1*}\alpha \cup i_{T_1}^{-1*}\beta)\beta,$$

where α and β are admissible colorings of the graphs dual to the triangulations T_0 and T_1, respectively, and Δ is a triangulation of the interpolating manifold of W.

The structures are then refined to construct a TQFT. The spaces of physical states are $Q(T^*) = C(T^*)/\ker\Phi_{id_T}$ with inner product $([\alpha],[\beta]) = \Omega_{T\times I}(\alpha,\beta)$. The propagators are induced by Φ_W, $\Psi_W: Q(T_0^*) \to Q(T_1^*)$, $\Psi_W[\alpha] = \Sigma_\beta \Omega_{\Delta^*}(\alpha,\beta)[\beta]$.

The invariance result says that two spaces $Q(T)$ constructed from different triangulations of the same surface are isomorphic, and that the map $\Psi_W: Q(T_0^*) \to Q(T_1^*)$ is independent of the triangulation up to conjugacy by the mentioned isomorphisms.

Now we compare the Turaev–Viro model with our construction.

Theorem 5: *For any triangulation T of a surface Σ, the map $\overline{i_{T^*}}: Q(T^*) \to H(\Sigma)$ defined by $\overline{i_{T^*}}([\alpha]) = \overline{\alpha}$ is an isomorphism, and for any cobordism W*

$$\overline{i_{T_1^*}}^{-1} \circ \Phi_W^n \circ \overline{i_{T_0^*}} = \Lambda \Psi_W.$$

Proof: Since the dual of any triangulation of a three-manifold gives a cellular decomposition, it is easy to verify that $\overline{i_{T^*}}$ is a dilatation (a multiple of an isometry) by $\lambda = (\Omega_{\Delta^*_{id_\Sigma}}(j=0))^{-1/2}$ (where Δ_{id_Σ} is a triangulation of $\Sigma \times I$ compatible with T in both boundaries), and that the map taking $\overline{\alpha}$ to $\lambda^2 \Sigma_\beta \overline{\alpha}(\beta)[\beta]$ is its inverse.

$\overline{i_{T_1^*}}^{-1} \circ \Phi_W^n \circ \overline{i_{T_0^*}} = \Lambda \Psi_W$ follows from a simple application of definitions. We obtain $\Lambda = (\Omega_{\Delta^*_{id_{\Sigma_1}}}(j=0)\Omega_{\Delta_W^*}(j=0))^{-1}$, where Δ_W is a triangulation of the interpolating manifold of W compatible with T_0 and T_1. □

III. INTERPRETATION AS A RENORMALIZED SUM OVER QUANTUM GEOMETRIES

A. Preliminaries

Recall that we gave an alternative definition of $C(\Sigma)$ as $\mathbb{C}[adm(\Sigma)]$. Similarly, after having enunciated the "color $j=0$ is invisible" lemma, we can give an equivalent definition of the linear functional Ω'_X:

$$\Omega'_X(\alpha) = \sum_{\varphi} |X(\varphi)|'_\varphi,$$

where the sum runs over colorings $\varphi \in adm(M)$ such that $\partial\varphi = \alpha$ and $X(\varphi) \leqslant X$. That is, X serves only to restrict the set of colorings allowed in Ω'_X.

In this way, we can see Ω_M^n of formula (1) as a renormalized sum over colorings in which the "restricting box" X grows infinitely large.

In particular, *the "generalized projector" $\Omega^n_{\Sigma\times I}$ is a renormalized sum over quantum geometries.*

The term *quantum geometry* means a history in the form of a colored polyhedron because any slice of it defines a quantum geometry in canonical loop quantum gravity. In formal path integral quantization of general relativity the central object is an integral over diffeomorphism classes of metrics. Our quantum geometries are not analogous to diffeomorphism classes of metrics because

they are defined for a fixed embedding. *Is there an interpretation of the "generalized projector" as a sum over knot classes of colored polyhedra?* Below we give an affirmative answer.

B. Summing over knot classes of colorings

Consider $X \in P(M)$, $Y \in [X]$ if and only if there is a homeomorphism $f: M \to M$ such that $f|_{\partial M} = id$ and $f(Y) = X$. The set of such classes will be denoted by $KP(M)$.

There is a natural partial ordering in $KP(M)$ defined by $[X] \leqslant [Y]$ if and only if there are representatives $X \in [X]$, $Y \in [Y]$ satisfying $X \leqslant Y$. It is easy to verify that this defines a partial ordering; in addition, $KP(M)$ is directed with respect to this partial ordering.

Our goal now will be to use $[X]$ as a restricting box for a sum over classes of colorings. Then we will remove the restriction for the renormalized sum.

Recall that a homeomorphism $f: M \to M$ acts on admissible colorings $\varphi \in adm(M)$ by $f^{-1} * \varphi \in adm(M)$. We will denote by $[\varphi]$ the class of colorings with respect to the group of homeomorphisms that restrict to the identity on ∂M. Note that $[X(\varphi)]$ is independent of the representative $\varphi \in [\varphi]$.

Since $|X(f^{-1} * \varphi)|'_{f^{-1} * \varphi} = |X(\varphi)|'_{\varphi}$ we can define $|[\varphi]| = |X(\varphi)|'_{\varphi}$ and for $\alpha \in adm(\partial M)$

$$\Omega'_{[X]}(\alpha) = \sum_{[\varphi]} |[\varphi]|' s([X(\varphi)],[X]),$$

where the sum runs over all classes of colorings such that $\partial[\varphi] = \alpha$ and $[X(\varphi)] \leqslant [X]$. The symmetry factor $s([X(\varphi)],[X])$ counts in how many distinct ways can $[X(\varphi)]$ fit in $[X]$. Then, we have the following interpretative result concerning the central object of this work.

Theorem 6: Ω^n_M, *as defined in Eq. (1), is a renormalized sum over knot classes of colorings. That is,*

$$\Omega^n_M(\alpha) = \lim_{[X] \to M} \Omega^n_{[X]}(\alpha).$$

The same techniques can be applied using the notion of class resulting from the group of homeomorphisms that preserves each connected component of ∂M. The analysis proceeds in complete parallel to the one described above, but the resulting linear functional acts naturally on $\mathcal{H}_{hom}$. In addition, the space of physical states and the projective propagator are naturally isomorphic to the ones constructed here. This construction is of interest to loop quantization because it gives a construction of the Reisenberger–Rovelli projector (3) as a renormalized sum over quantum geometries.

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APPENDIX: INDEPENDENCE OF INTERNAL STRUCTURE

A choice of internal structure is needed to construct the simple graph Γ_s from $\Gamma \in G(\Sigma)$. In the next paragraphs we will see that different choices lead to naturally isomorphic vector spaces $C(\Gamma_s)$ which in the main body of the article are denoted collectively by $C(\Gamma)$.

Consider a portion of a graph adjacent to a vertex with valence higher than three; call it $\Gamma(v)$. Use the prescription of Sec. II B (Fig. 1) to generate a simple graph $\Gamma(v)_s$. Fix a coloring α of $\Gamma(v)$'s edges, and define $C(\Gamma(v)_s, \alpha) = \mathbb{C}[adm(\Gamma(v)_s, \alpha)]$ as the complex vector space generated by the admissible colorings of $\Gamma(v)_s$ that are compatible with α.

Construct $\Gamma(v)^3_s$ from $\Gamma(v)_s$ simply by sliding "edge 1" counter clockwise past "edge 3" (see Fig. 1). Continue sliding "edge 1" in the same direction to generate a sequence of graphs $(\Gamma(v)_s, \Gamma(v)^3_s, \Gamma(v)^4_s, \ldots, \Gamma(v)^{n-1}_s)$. Note that $\Gamma(v)^{n-1}_s$ corresponds to the graph $\Gamma(v)_s$ obtained using a different numbering of the edges. With this set of moves we can generate all the graphs $\Gamma(v)_s$ obtained with any counter-clockwise (or clockwise) oriented numbering of edges.

Now we are going to show that the spaces $C(\Gamma(v)_s^i,\alpha)$, $C(\Gamma(v)_s^{i+1},\alpha)$ are naturally isomorphic. After we do so, we will know that any two counter-clockwise (or clockwise) oriented numberings of edges produce different simple graphs $\Gamma(v)_s^a \neq \Gamma(v)_s^b$, but naturally isomorphic vector spaces $C(\Gamma(v)_s^a,\alpha) \approx C(\Gamma(v)_s^b,\alpha)$. Clearly, this implies that different choices of Γ_s for a given Γ lead to naturally isomorphic vector spaces.

Consider the graph $\Gamma(v)_s^i$ described above. Its internal edges can be labeled as $(e_{3,4},e_{4,5},\ldots,e_{i,1},e_{1,i+1},\ldots,e_{n-2,n-1})$. Similarly, the internal edges of the graph $\Gamma(v)_s^{i+1}$ can be labeled as $(e_{3,4},e_{4,5},\ldots,e_{i,i+1},e_{i+1,1},\ldots,e_{n-2,n-1})$. Using an abbreviated notation for the internal edges, we can write the generators of $C(\Gamma(v)i_s,\alpha)$ as $(\ldots,j_{i,1},j_{1,i+1},j_{i+1,i+2}\ldots)_i$. There is one generator for each choice of ''internal spins'' that is compatible with the coloring of the external edges $\alpha=(j_1,j_2,\ldots,j_n)$. In a similar fashion, the generators of $C(\Gamma(v)_s^{i+1},\alpha)$ are denoted by $(\ldots,j_{i,i+1},j_{i+1,1},j_{1,i+2},\ldots)_{i+1}$. The isomorphism is given by the recoupling move,[9] which sends the generator $(\ldots,j_{i,1},j_{1,i+1},j_{i+1,i+2},\ldots)_i$ to

$$\sum_{j_{3,1}} w_{j_{1,i+1}} w_{j_{i+1,1}} \begin{vmatrix} j_{i,1} & j_1 & j_{1,i+1} \\ j_{1,i+2} & j_{i+1} & j_{i+1,1} \end{vmatrix} (\ldots,j_{i,i+1},j_{i+1,1},j_{1,i+2},\ldots)_{i+1}.$$

If we slide back ''edge 1'' to its position in $\Gamma(v)_s^i$ the recoupling move gives us another $6j$ symbol. The resulting sum of products of two $6j$ symbols is just the orthogonality relation, meaning that sliding back ''edge 1'' induces just the inverse transformation. This completes the proof; any two choices of internal structure for $\Gamma \in G(\Sigma)$ lead to naturally isomorphic vector spaces.

Let us now show that Ω'_X is independent of the choice of X_s used to define it. To do it, we will construct a sequence of lune and Matveev moves that interpolates between any two choices of X_s leaving Ω'_X unchanged. We will describe a sequence of moves that changes the internal structure of an edge and a sequence that changes the internal structure of a vertex. Composing these sequences of moves we can generate any of the possible choices of internal structure starting from a particular choice.

We will start describing how to change the internal structure of edges. First take the case of an edge with at least one end in the boundary. In this case the internal structure of the edge is fixed by the structure of the vertex in the boundary; there is no choice of internal structure. (If the edge has two vertices in the boundary, they are assumed to have compatible structures.)

Take now the case of an edge that starts and ends at two distinct vertices that lie in the interior of M. We will change the internal structure of the edge sliding ''face 1'' in the same spirit used to change the internal structure of a vertex in the case of boundary graphs. That is, we will slide ''face 1'' around the lateral faces of the edge-bubble until it is connected to ''face n.'' Iterating this process, we can change the location of the hole in the edge-bubble to be any of the lateral faces. In the next paragraph we describe a sequence of Matveev and lune moves that slides ''face 1'' as we need.

''Face 1'' meets two vertex bubbles, the bubbles corresponding to the vertices at the extremes of the edge. Then we can use Matveev moves to slide ''face 1'' past ''face 3'' on the surface of both vertex-bubbles. Then we simply pull ''face 1'' through the surface of the edge-bubble past ''face 3'' using an inverse lune move. We can iterate this process to slide ''face 1'' until it is connected to ''face n.'' At this point we have moved the position of the hole in the edge-bubble, but we may have not finished our job yet. One of the vertex-bubbles may have had its hole connecting it to the edge-bubble. In this case, the sequence of Matveev moves has made ''face 1'' surround all the internal vertices of the vertex bubble. To finish we have to slide ''face 1'' on the surface of the vertex-bubble past all these vertices using Matveev and inverse Matveev moves.

Finally, consider the case of an edge that closes in itself. ''Face 1'' can be slid using the technique explained above for the case in which the edge ended in two internal vertices. We have described how to change the internal structure of an edge with any location in M. In the next paragraph we explain how to change the internal structure at vertices.

Each vertex-bubble has a hole connecting it to an edge-bubble. We may want to change the location of the hole in a way that connects the vertex-bubble to another edge-bubble. To do it we can simply move the face that occupies the place where we want the hole to be to the old location of the hole. This moving of the face can be achieved by a sequence of Matveev and inverse Matveev moves done inside the vertex-bubble. This finishes the construction; any two choices of internal structure for $X \in P(M)$ are connected by a sequence of lune and Matveev moves (and their inverses). Thus, Ω'_X is independent of any choice.

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Generalization of Berry's geometric phase, equivalence of the Hamiltonian nature, quantizability and strong stability of linear oscillatory systems, and conservation of adiabatic invariants

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A linear set of ordinary differential equations with a matrix depending on a set of adiabatically varying parameters is considered. Its asymptotic solutions are constructed to an arbitrary accuracy in the adiabaticity parameter ε. By extending the phase space of the system not only with the space of parameters, like in the theory of Berry's phase, but also with the space of their derivatives, it proves possible to represent the phase of the solution as a sum of the dynamic phase and a generalized geometric phase (determined by a contour integral in the space of parameters and derivatives). Hence, it is possible to obtain the asymptotic results to any degree of accuracy in ε, while earlier they were obtainable only in the first-order adiabatic approximation. Namely, for linear oscillatory adiabatic systems, the quantizability, parametric stability, and the Hamiltonian nature of the system are equivalent properties. As a consequence, one can obtain the well-known result regarding conservation with accuracy to any power of ε of adiabatic invariants in a Hamiltonian system on a torus. An important point is that the generalized geometric phase can appear, in contrast to Berry's phase, with only one real varying parameter. [DOI: 10.1063/1.1506954]

I. INTRODUCTION

This paper develops the ideas of Refs. 1 and 2 that proposed to analyze nonautonomous dynamic systems with the help of a functional approach. In this case the phase space of a dynamic system is extended not only by adding the dimension of time but also a space of parameters varying with time. As a result, solutions to the equations, changes of variables, etc., are considered as functionals (generally speaking, nonlocal) of the parameters and not just as functions of time. As it occurs, the approach allows one to obtain essential results of considerable interest. For example, the theory of Berry's phases[3] provides a prominent example of the functional approach to nonautonomous dynamic systems.

Note that an essential feature of the functional approach is the possibility to separate coordinate substitutions into local and nonlocal ones. The local substitutions involve only current values of system parameters and their derivatives, and hence cannot result in qualitative distortions of the system's phase portrait. Whereas nonlocal substitutions are, for the most part, integral functionals of parameters containing the system's prior history. Such substitutions always distort the global qualitative phase portrait.[1,2]

Reference 1 was an attempt to develop a consistent theory of linear adiabatic systems from the viewpoint of the functional approach. Special attention was paid to oscillatory systems, i.e., the systems with purely imaginary current eigenvalues. For such systems, adiabatic equivalence was proven (i.e., equivalence to the first order in the adiabatic parameter ε) of the quantizability, strong stability, and Hamiltonian property of the system. It was exactly the functional approach that made

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the proof possible, and the notion of complex geometric phases was used essentially.

In the present paper we will show that a consistent application of the technique permits extending the formalism up to any order of ε. As a result, the notion of the *generalized geometric phase* is introduced, and the above-mentioned statements of Ref. 1 are proved in a similar way, however to a new accuracy. It is important that the generalized geometric phase, while being described analogously to Berry's phase and representing similar physical effects, can appear under adiabatic changes of only one real parameter. In this paper, some modifications of the strong stability property are introduced for parameter-dependent systems in a more rigorous way than in Ref. 1, namely the parametric stability and strong stability in a class. It is noteworthy that from the formalism introduced and the theorems proved in the paper some well-known results follow immediately. Namely, adiabatic invariants of the Hamiltonian system whose phase trajectories lie, under constant parameters, on an n-dimensional torus, remain unchanged with accuracy to any power of ε.[4–6]

The central idea of this work, allowing an efficient extension of the known results to any degree of accuracy, consists in analyzing the system in a generalized space of parameters that involves not only the dimensions of the parameters but of their derivatives as well.

II. GENERAL FORMALISM

Consider the linear system described by an n-dimensional vector equation in $\mathbf{C}^n$,

$$\mathbf{x}' = \mathbf{A}(\bar{\mu})\mathbf{x}. \tag{1}$$

[Let us note that all conclusions of this paper can be obtained in a similar way for the initial system in $\mathbf{R}^{2n}$. Besides, the results can be derived in an almost identical way for the initial system with the matrix of form $\mathbf{A}=\mathbf{A}(\bar{\mu},\bar{\mu}',\ldots,\bar{\mu}^{(m)})$.] Here $\mathbf{x}=(x_1,\ldots,x_n)$ is the vector-function to be found (its components will be called coordinates), the prime stands for differentiation with respect to the independent real variable t (further referred to as time), $\mathbf{A}(\bar{\mu})$ is a linear operator defined by a square nondegenerate matrix, which is an infinitely differentiable function of the set of s adiabatically varying parameters $\bar{\mu}=(\mu_1,\ldots,\mu_s)$, and $\bar{\mu}$ is a vector from a compact simply connected domain $\wp\subset\mathbf{R}^s$.

The eigenvalues of the matrix $\mathbf{A}(\bar{\mu})$ are assumed to satisfy the following conditions for all values of the parameters:

$$0<|\lambda_j(\bar{\mu})|<\infty, \quad j=1,...,n; \quad \lambda_j(\bar{\mu})\neq\lambda_l(\bar{\mu}) \quad \text{for} \quad j\neq l \tag{1a}$$

The latter requirement is necessary to permit the use of independent adiabatic solutions of (1). [Applicability criteria of the adiabatic approximation for the case when eigenvalues are closing in can be found in Ref. 7.]

The system parameters are subject to an arbitrary adiabatical variation with time:

$$\bar{\mu}=\bar{\mu}(\varepsilon t), \quad \varepsilon\ll 1. \tag{2}$$

Here, ε is the adiabaticity parameter, and the vector-function $\bar{\mu}(\varepsilon t)$ is assumed to be infinitely differentiable. From here on, referring to system (1), we also imply all the above-listed requirements.

Notice that there is no need to require the nonresonance character of the $\bar{\mu}(\varepsilon t)$ dependence as was done in Ref. 1. The point is that even in the presence of parametric resonance in the adiabatic oscillatory system the growth rate is exponentially small,[8,9] being a value of the form $\alpha\exp(-\beta\varepsilon^{-1})$. [In the case of parametric resonance with nonadiabatic sections of the function $\bar{\mu}(t)$, the growth rate generally is of order ε^1, where ε is the reciprocal of the period.[9]] For this reason, parametric resonances are beyond the scope of this paper treating power-series approximations in ε. Furthermore, the statements and theorems discussed here utilize the function $\bar{\mu}(\varepsilon t)$ only as an auxiliary tool. In fact they deal with the system as a whole, i.e., structure of the $\mathbf{A}(\bar{\mu})$ dependence.

To construct asymptotic solutions to system (1) we will use the following idea proposed by Neishtadt.[10] (Compare also with the method of successive diagonalizations in Ref. 4.) Let us bring the parameter-dependent matrix $\mathbf{A}(\overline{\mu})$ to a diagonal form by applying a linear substitution of coordinates. In terms of new coordinates, the matrix of the transformed system will be only slightly nondiagonal (the off-diagonal terms are proportional to the first-order time derivatives of parameters and have the order of ε). Let us further diagonalize the matrix obtained to a first order in ε through the next linear substitution of coordinates. In these coordinates the off-diagonal matrix elements will be small terms of order ε^2 being proportional to second-order time derivatives. This procedure can be similarly reiterated. Thus, the initial system can be reduced, for any finite order in ε, to a diagonal form, for which exact solutions can be easily written. The sequence of recurrence relations to describe the procedure is given in Appendix A.

Equation (1), upon k successive diagonalizations, takes the form

$$\mathbf{x}'_{[k]}=[\mathbf{\Lambda}_{[k]}+\mathbf{\Delta}_{[k]}]\mathbf{x}_{[k]}, \tag{3}$$

where the variables $\mathbf{x}_{[k]}$ are related to the initial ones through a certain reversible local substitution without singularities of the form $\mathbf{x}=\mathbf{B}(\overline{\mu},\overline{\mu}',\ldots,\overline{\mu}^{(k)})\mathbf{x}_{[k]}$; the subscript in the square brackets stands for the diagonalization number; $\mathbf{\Lambda}_{[k]}$ is the diagonal matrix containing terms of order ε^k and under, while the components of the matrix $\mathbf{\Delta}_{[k]}$ are of order ε^{k+1}. The matrix $\mathbf{\Lambda}_{[k]}$ can be written in the form [see (A5)]

$$\mathbf{\Lambda}_{[k]}=\mathbf{\Lambda}+\sum_{j=0}^{k-1}\mathrm{dg}\,\mathbf{\Delta}_{[j]}. \tag{4}$$

Here $|\mathbf{\Delta}_{[j]}|\sim\varepsilon^{j+1}$, the operator dg rejects off-diagonal components of the matrix, and $\mathbf{\Lambda}\equiv\mathbf{\Lambda}_{[0]}=\mathrm{diag}(\lambda_1,\ldots,\lambda_n)$, with the values $\lambda_j=\lambda_j(\overline{\mu})\sim\varepsilon^0$ being current eigenvalues of the matrix $\mathbf{A}(\overline{\mu})$ of the initial equation (1).

Let us determine the form of the matrices $\mathbf{\Delta}_{[j]}$. In view of their proportionality to the corresponding power of ε and with account of Eq. (2), it can be seen that $\mathbf{\Delta}_{[1]}$ is proportional to the first-order time derivative of $\overline{\mu}(\varepsilon t)$ and has the general form like

$$\mathbf{\Delta}_{[0]}=\overline{\mathbf{F}}_{[0]}(\overline{\mu}(\varepsilon t))\overline{\mu}'(\varepsilon t),$$

where $\overline{\mathbf{F}}_{[0]}(\overline{\mu}(\varepsilon t))$ is the matrix field over the $\overline{\mu}$-space of parameters. The nonpotential component of this field gives rise to Berry's geometric phase, or Hannay's angle (see Refs. 1 and 3). Similarly, $\mathbf{\Delta}_{[2]}$ can be written in general form as

$$\mathbf{\Delta}_{[1]}=\overline{\mathbf{F}}_{[1]}(\overline{\mu}(\varepsilon t))\overline{\mu}''(\varepsilon t)+\mathbf{F}_{[1]}(\overline{\mu}(\varepsilon t))(\overline{\mu}'(\varepsilon t))^2,$$

where $\overline{\mathbf{F}}_{[1]}(\overline{\mu}(\varepsilon t))$ also is a matrix field and $\mathbf{F}_{[1]}(\overline{\mu}(\varepsilon t))$ is a scalar (with respect to the $\overline{\mu}$-space) matrix-function.

Continuing the procedure, we see that the diagonal matrix $dg\,\mathbf{\Delta}_{[j]}$ can be represented as a sum of elements that are proportional to different orders of derivatives of $\overline{\mu}(\varepsilon t)$. Besides, in each term, the sum of products of the derivative order by the power it is raised to is equal to $j+1$.

Now we turn to solving Eq. (3). Its solutions can be written as follows:

$$\mathbf{x}_{[k]}(t)\approx\mathbf{x}_{[k]}(0)\exp\left\{\int_0^t\left[\mathbf{\Lambda}+\sum_{j=0}^{k-1}\mathrm{dg}\,\mathbf{\Delta}_{[j]}+O(\varepsilon^{k+1})\right]\mathrm{d}\tau\right\}. \tag{5}$$

From what has been said previously on the form of the matrices in the integrand, it appears that the solution (5) can be written like

$$\mathbf{x}_{[k]}(t)\approx\mathbf{x}_{[k]}(0)\exp\left\{\int_0^t\mathbf{\Lambda}(\overline{\mu}(\varepsilon\tau))\mathrm{d}\tau+\int_0^t\vec{\mathbf{F}}(\vec{M}(\varepsilon\tau))\vec{M}'(\varepsilon\tau)\mathrm{d}\tau\right\}+O(\varepsilon^{k+1}t). \tag{6}$$

Here we have introduced the space $\vec{M}$, which we suggest calling the *generalized parameter space*. Its dimensions are constituted by dimensions of the set of the values $(\overline{\mu}(\varepsilon t),\overline{\mu}'(\varepsilon t),\ldots,\overline{\mu}^{(k-1)}(\varepsilon t))$ (with regard to the properties of this space see Appendix B). The value $\vec{\mathbf{F}}(\vec{M})$ represents a field of diagonal matrices over this space. Finally, similarly to the geometric phase theory, the second term in the integrand of Eq. (6) can be easily transformed into a contour integral in the $\vec{M}$-space:

$$\mathbf{x}_{[k]}(t)\approx\mathbf{x}_{[k]}(0)\exp\left\{\int_0^t\mathbf{\Lambda}(\overline{\mu}(\varepsilon\tau))\mathrm{d}\tau+\int_L\vec{\mathbf{F}}(\vec{M})\mathrm{d}\vec{M}\right\}+O(\varepsilon^{k+1}t), \tag{7}$$

where L is the contour along which the representative point of the system moves in the generalized parameter space.

The solution (7) is fully identical in its form to the known adiabatic solution [Eq. (8) of Ref. 1] that was specified to within ε^1, however its accuracy is ε^k. The first term in Eq. (7) is the standard ''fast'' dynamic phase. The second term is the ''slow'' phase, whose nonlocal part represents the *generalized geometric phase*. It has the form of the standard Berry phase, however written in the generalized parameter space.

Equation (7) can be easily separated by the degrees of freedom of the system in $\mathbf{C}^n$, because it contains diagonal matrices alone. From here on, we will separately consider the projections of the solutions,

$$x_{[k]j}(t)\approx x_{[k]j}(0)\exp\left\{\int_0^t\lambda_j(\overline{\mu}(\varepsilon\tau))\mathrm{d}\tau+\int_L\vec{f}_j(\vec{M})d\vec{M}\right\}+O(\varepsilon^{k+1}t), \tag{8}$$

where $j=1,\ldots,n$ and $\vec{f}_j(\vec{M})\equiv\vec{\mathbf{F}}_{jj}(\vec{M})$.

Let us isolate the potential component of $\vec{f}_j(\vec{M})$, representing the field as

$$\vec{f}_j(\vec{M})=\mathrm{grad}[\varphi_j(\vec{M})]+\vec{f}_j^{(c)}(\vec{M}), \tag{9}$$

where $\varphi_j(\vec{M})$ is a scalar function, while $\vec{f}_j^{(c)}(\vec{M})$ is the nonpotential component of $\vec{f}_j(\vec{M})$. By substituting Eq. (9) into Eq. (8), we obtain

$$x_{[k]j}(t)\approx x_{[k]j}(0)\exp\left\{\int_0^t\lambda_j(\overline{\mu}(\varepsilon\tau))\mathrm{d}\tau+\varphi_j(\vec{M}(\varepsilon t))-\varphi_j(\vec{M}(0))+\int_L\vec{f}_j^{(c)}(\vec{M})\mathrm{d}\vec{M}\right\}+O(\varepsilon^{k+1}t). \tag{10}$$

The contribution of the potential field component $\vec{f}_j(\vec{M})$ to the solutions (8), (10) is *local*. It is determined only by boundary values of the parameters and their derivatives, and is independent of the integration contour in the $\vec{M}$-space. Therefore, it is the component that determines the connection between the slow amplitude of the solution and *current* values of parameters and their derivatives, and is responsible for the construction of adiabatic invariants.

The contribution of the nonpotential component, $\vec{f}_j^{(c)}(\vec{M})$, is, on the contrary, *nonlocal*. It depends essentially on the geometry of the contour L (i.e., on all *prior* values of the parameters), being nonzero even for cyclic variations of the parameters that correspond to closed contours in the $\vec{M}$-space. The last term in the exponent of Eq. (10) is the complex generalized geometric phase.

For the convenience of further consideration we will separate the real and the imaginary part of the generalized geometric phase. Its imaginary part will be called the generalized geometric phase proper,

$$\psi_j(L)=\mathrm{Im}\int_L \vec{f}_j^{(c)}(\vec{M})\mathrm{d}\vec{M}, \tag{11}$$

while its real part will be spoken of as the generalized geometric amplitude,

$$\gamma_j(L)=\mathrm{Re}\int_L \vec{f}_j^{(c)}(\vec{M})\mathrm{d}\vec{M}, \tag{12}$$

since it is exactly its changes that bring forth the variations of the solution amplitude. Note that the $\vec{M}$-space is multidimensional even in the case of only one varying real parameter in the system ($s=1$). For this reason generalized geometric phases and amplitudes may appear even when Berry's phase certainly does not exist (the $\overline{\mu}$-space is one-dimensional).

The potential component of $\vec{f}_j(\vec{M})$ can be easily reduced to zero via the local substitution $x_{[k]j}(t)=\exp[\varphi_j(\vec{M}(\varepsilon t))-\varphi_j(\vec{M}(0))]z_j(t)$. As a result, from (10) we obtain:

$$z_j(t)\approx z_j(0)\exp\left\{\int_0^t \lambda_j(\overline{\mu}(\varepsilon\tau))\mathrm{d}\tau+\int_L \vec{f}_j^{(c)}(\vec{M})\mathrm{d}\vec{M}\right\}+O(\varepsilon^{k+1}t). \tag{13}$$

We will also write the equation corresponding to projections of Eq. (3) in terms of these variables:

$$z_j'=(\lambda_j+\vec{f}_j^{(c)}\vec{M}')z_j+O(\varepsilon^{k+1}t). \tag{14}$$

These expressions coincide in form with those obtained in Ref. 1 [Eqs. (7)–(14) of this work correspond to Eqs. (8), (11), (13)–(16), (20), and (19) of paper Ref. 1]. In what follows we will derive analogous results, therefore in the following discussion we will only write out the fundamental propositions, referring the reader to Ref. 1 for details of the proofs. All one needs to do is to replace the parameter space and geometric terms with their generalized analogs.

III. MAIN RESULTS

A. Global qualitative portrait of the system

Statement I: The generalized geometric terms, together with the current eigenvalues λ_j, *determine the qualitative portrait of a linear adiabatic system.*

Indeed, to describe the system we can introduce, similar to Ref. 1, the efficient eigenvalues corresponding to the solutions (13) over a given time interval,

$$\lambda_j^{\mathrm{eff}}(t)=\frac{\ln z_j(t)-\ln z_j(0)}{t}. \tag{15}$$

By substituting the solutions (13) into Eq. (15), we obtain:

$$\lambda_j^{\mathrm{eff}}(t)=\langle\lambda_j\rangle_t+\frac{\gamma_j+i\psi_j}{t}+O(t^{-1},\varepsilon^{k+1}), \tag{16}$$

where $\langle\lambda_j\rangle_t\equiv(1/t)\int_0^t\lambda_j(\overline{\mu}(\varepsilon\tau))\mathrm{d}\tau$ are average values of the current eigenvalues. The second term in Eq. (16) contains terms of different orders ranging from ε to ε^k and, generally speaking, do not tend to zero together with t^{-1}, since during continuous circulation of the system's representative point in the $\vec{M}$-space the geometric terms increase infinitely. If there is a limit $\tilde{\lambda}_j^{\mathrm{eff}}=\lim_{t\to\infty}\lambda_j^{\mathrm{eff}}(t)$, then the behavior of the solutions for large times (strictly speaking, for times large enough so that $\lambda_j^{\mathrm{eff}}(t)$ does not leave the small vicinity of its limiting value) can be "roughly" (i.e., without account of local deviations) described by the formula $z_j(t)\approx z_j(0)\exp(\tilde{\lambda}_j^{\mathrm{eff}}t)$. For example, under periodic (of period $T\sim\varepsilon^{-1}$) variations of the parameters the value $\lambda_j^{\mathrm{eff}}(t)$ tends asymptotically to the limit

$$\tilde{\lambda}_j^{\text{eff}} = \langle \lambda_j \rangle_T + \frac{\gamma_j(L_T) + i\psi_j(L_T)}{T} + O(\varepsilon^{k+1}),$$

where L_T is the closed contour corresponding to one period. The above-derived solutions as well as the analysis presented are applicable over times $t \ll \varepsilon^{-(k+1)}$. It is significant that the system's portrait analyzed in z-coordinates is qualitatively equivalent to the portrait of the initial system (1). Indeed, we used only local coordinate substitutions that leave the system's fundamental characteristics (current eigenvalues and generalized geometric phases, i.e., efficient eigenvalues) invariant (see Ref. 2 and Appendix B in Ref. 1).

B. Adiabatic and integral invariants

Statement II: A degree of freedom of the system possesses an adiabatic invariant of action, conserved to the order of ε^k, if and only if

$$\begin{aligned} \operatorname{Re} \lambda_j &= 0, \\ \gamma_j &= 0. \end{aligned} \tag{17}$$

Indeed, if the conditions (17) are met, then Eq. (13) yields

$$I_j(t) \equiv |z_j(t)|^2 \approx \text{const}. \tag{18}$$

The values I_j are known as the adiabatic invariants of action. Each I_j corresponds to conservation of the phase flux of the jth degree of freedom in the **z**-space. In terms of the initial coordinates, the adiabatic invariants determine, under given initial conditions, an unambiguous relation between the amplitude of the approximate solution and current values of the parameters. Note that the conditions (17) are equivalent to the requirement that the real part of the effective eigenvalue λ_j^{eff} specified previously, be equal to zero. In other words, this is the requirement of conservation of oscillatory nature of the system movement over large times with adiabatically varying parameters.

Following Ref. 1, it can be easily shown that the existence of Poincaré's first integral invariant is equivalent to the presence in the system of a complete set of n adiabatic invariants (once again, this is true up to the order of ε^k). [It should be noted at this point that we do not consider the case of Hamiltonian systems with $\operatorname{Re} \lambda_j \neq 0$. Such systems also possess Poincaré's integral invariants, however adiabatic invariants are absent. The complex structure suggested here and integral invariants in these systems have different form as compared with Hamiltonian systems on a torus ($\operatorname{Re} \lambda_j = 0$), which mostly are considered in this paper.] In addition, the condition for conservation of the system's phase volume to the accuracy ε^k (Poincaré's nth integral invariant, or Liouville's theorem) are:

$$\begin{aligned} \sum_{j=1}^{n} \operatorname{Re} \lambda_j &= 0, \\ \sum_{j=1}^{n} \gamma_j &= 0. \end{aligned} \tag{19}$$

C. Hamiltonian formalism

We will further consider oscillatory systems, i.e., such systems that

$$\operatorname{Re} \lambda_j = 0, \quad j = 1,...,n. \tag{20}$$

Theorem I: *The system (1) with purely imaginary current eigenvalues [Eq. (20)] coincides, to accuracy* ε^k*, with a Hamiltonian system if and only if all of its generalized geometric amplitudes are equal to zero:*

$$\gamma_j = 0, \quad j = 1,...,n. \tag{21}$$

The Hamiltonian of such a system is represented by the Hamiltonian of a sum of independent oscillators:

$$H(p,q) = \sum_{j=1}^{n} H_j(p_j, q_j) = \frac{1}{2} \sum_{j=1}^{n} \omega_j (p_j^2 + q_j^2), \tag{22}$$

where $i\omega_j = \lambda_j + \vec{f}_j^{(c)} \vec{M}$.

Carrying out the realification of **z**-space, $p_j = \mathrm{Re}\, z_j$ and $q_j = \mathrm{Im}\, z_j$, we obtain from Eq. (14) with account of Eqs. (20) and (21),

$$\begin{aligned} p_j' &= -\,\mathrm{Im}(\lambda_j + \vec{f}_j^{(c)} \vec{M}') q_j + O(\varepsilon^{k+1} t), \\ q_j' &= \mathrm{Im}(\lambda_j + \vec{f}_j^{(c)} \vec{M}') p_j + O(\varepsilon^{k+1} t). \end{aligned} \tag{23}$$

To within the order ε^k, this is a Hamiltonian system with the Hamiltonian (22). Thus, the sufficiency of the condition (21) for the system to be a Hamiltonian one has been proven. The necessity of condition (21) can be proved following Ref. 1 by replacing the parameter space and the geometric values involved with their generalized analogs (also see Appendix B).

Note that points of the unperturbed system trajectory (in the proofs of Theorems I and III) should not belong to the boundary of the considered compact region $\wp$ in the $\overline{\mu}$-space.

D. System quantization

Theorem II: *System (1) with purely imaginary current eigenvalues [Eq. (20)] coincides, to accuracy* ε^k*, with a quantizable system if and only if all of its generalized geometric amplitudes are equal to zero [Eq. (21)].*

The proof can be performed following Ref. 1 by replacing the parameter space and the geometric values involved with their generalized analogs.

E. Strong stability properties

Now we turn to stability properties of the systems considered. In Ref. 1 equivalence of the Hamiltonian nature and quantizability of the system to a special version of strong stability was proven. Here we will introduce the property of a *parametric stability*, which we think is more adequate when discussing parametric systems. Next, we will formulate a strong stability property, which could be more properly referred to as *strong stability in a class*. It will be shown that the parametric stability is a primary property for systems with parameters. The strong stability property can be introduced only for the class of parametrically stable systems.

Definition I: System (1) with a specific (rather than arbitrary) $\overline{\mu}(\varepsilon t)$ *dependence is said to be a realization of system (1).*

In essence, the notion of realization emphasizes that in the functional approach we operate in fact with a set of systems characterized by a variety of $\overline{\mu}(\varepsilon t)$ dependencies, whereas in the temporal approach we consider a single system.

Definition II: Let a realization $\overline{\mu} = \overline{\mu}_0(\varepsilon t)$ *of system (1) with the matrix* $\mathbf{A}(\overline{\mu})$ *be stable, i.e., all of its solutions are bounded, if there exists a* $\delta > 0$*, such that any perturbed realization* $\overline{\mu} = \overline{\mu}_1(\varepsilon t)$ *of the same system satisfying the inequality*

$$|\overline{\mu}_1(\varepsilon t) - \overline{\mu}_0(\varepsilon t)| < \delta, \quad \forall t, \tag{24}$$

is also stable, then the initial realization of the system is called parametrically stable.

The system is parametrically stable if all of its realizations are parametrically stable.

As noted at the beginning of Sec. II, parametric resonances in adiabatic systems go beyond the accuracy of the approximation considered here. Talking of stability here and in the following, we will not consider parametric resonances again, since we operate in the framework of the approximation adopted.

Definition III: Let system (1) with the matrix $\mathbf{A}=\mathbf{A}_0(\overline{\mu})$ *from a certain class* $\aleph$ *be parametrically stable. If there exists a* $\delta>0$, *such that any perturbed system (1) with the matrix* $\mathbf{A}=\mathbf{A}_1(\overline{\mu})$ *from the same class* $\aleph$, *satisfying the inequality*

$$\|\mathbf{A}_1(\overline{\mu})-\mathbf{A}_0(\overline{\mu})\|<\delta, \quad \forall \overline{\mu}\subset\wp, \tag{25}$$

is also parametrically stable, then the initial system is called strongly stable in the class $\aleph$.

In essence, the property of parametric stability reflects the stability of a system against small variations of its parameters. The property of strong stability in a class describes stability under small variations in the system matrix, however, demanding that the matrix does not leave the given class, which is to be determined in every particular problem. Like in Ref. 1, we speak here of strong stability in the class of Hamiltonian oscillatory systems with different eigenvalues. (This kind of stability was proven previously for systems with periodic coefficients.[11–13]) Apparently, small variations in the system matrix that take the system out of that class will readily produce loss of the system's stability. This is the reflection of the fact that Hamiltonian oscillatory systems are *structurally unstable*.[13] More specifically, when the system loses its oscillatory nature, it may become simply *unstable* (parametrically unstable even more so) even for fixed values of its parameters (if $\mathrm{Re}\,\lambda_j>0$). At the same time, if a system leaves the class of Hamiltonian ones, while retaining its oscillatory nature, then the system becomes parametrically unstable (a property opposite to the one of parametric stability).

Remark: If we choose a class in which all the systems are parametrically stable, then they will be also strongly stable in the class.

As a consequence of the Remark, it is the parametric stability property that can be naturally assumed to be primary: it determines the class of systems in which they possess the property of strong stability.

Theorem III: *System (1) with purely imaginary current eigenvalues [Eq. (20)] is parametrically stable to the order of* ε^k *if and only if its generalized geometric amplitudes are all equal to zero [Eq. (21)].*

Once again, the proof is carried out following the pattern of Theorem III in Ref. 1, however replacing the parameter space and the geometric values involved with their generalized analogs (also see Appendix B).

F. Corollaries

By virtue of Eq. (21) representing the necessary and sufficient condition for all of the above-given theorems, the following conclusions can be drawn.

Corollary I: The Hamiltonian nature, parametric stability, and quantizability are equivalent properties with accuracy to any power of ε, *for system (1) with purely imaginary current eigenvalues.*

Also, the property of parametric stability (Theorem III) determines the strong stability class of the oscillatory systems (1):

Corollary II: Systems (1) are strongly stable, with accuracy to any power of ε, *in the class of oscillatory Hamiltonian systems. Moreover, the class of Hamiltonian systems is the complete strong stability class among the oscillatory systems (1), i.e., none of the oscillatory systems not belonging to this set is strongly stable.*

It is clear that the complete class of strongly stable systems (1) represents a union of the set of Hamiltonian systems with $\mathrm{Re}\,\lambda_j=0$, $j=1,...,n$, and the set of systems with a negative real part of current eigenvalues ($\mathrm{Re}\,\lambda_j<0$, $j=1,...,n$). The strong stability in the latter set is clear enough and is not discussed here.

Corollary III: Let the phase curves of a linear Hamiltonian system for fixed values of parameters represent the winding of an n-dimensional torus with various rotation periods. Then n adiabatic invariants exist in the system that are retained during slow variations of the system parameters with accuracy to any power of ε.

Indeed, if the system is a Hamiltonian one and the conditions (20) are met, then its generalized geometric amplitudes are equal to zero (Theorem I) for any k. And hence (Statement II), the system possesses a set of n adiabatic invariants that are conserved to within the accuracy ε^k with arbitrary k.

IV. CONCLUSIONS

The paper considered a linear dynamic system of the general kind, described by the complex vector equation (1) with a nondegenerate matrix possessing different nonzero eigenvalues. The system matrix is assumed to depend on a set of parameters varying adiabatically in time. The principal results reported in the paper are as follows:

(1) A procedure has been suggested for constructing asymptotic solutions (5) that satisfy the system (1) to terms of any given order in ε.

(2) The notion of the generalized parameter space $\vec{M}=(\overline{\mu}(\varepsilon t),\overline{\mu}'(\varepsilon t),\ldots,\overline{\mu}^{(k-1)}(\varepsilon t))$ has been introduced that allows representing asymptotic solutions as an exponential function of the sum of the dynamic phase and the generalized geometric phase. The latter can be represented as a contour integral of some field on the $\vec{M}$-space. Thus the problem has been formally reduced to the case (already considered in Ref. 1) of adiabatic solutions determined with an accuracy of ε. The $\vec{M}$-space is multidimensional even in the case of a single real varying parameter in the system ($s=1$). Hence, generalized geometric phases can appear when Berry's phase is certainly absent. The appearance of such phases may produce interesting effects in physical systems that are similar to the appearance of Berry's phase for higher orders of ε. [In the papers now being prepared for publication the author shows that the generalized geometric phase can appear even in very simple systems, such as an oscillator with a varying eigenfrequency or the rotating polarization plane of light in a one-dimensionally inhomogeneous medium.]

(3) Making use of the analogy with the adiabatic problem already analyzed to within ε, we have shown the generalized geometric terms, along with current eigenvalues, to be fundamental characteristics of the system. They determine its global qualitative portrait over times up to ε^{-k}. The real part of the complex generalized geometric phase, i.e., the generalized geometric amplitude, plays a special role in the system analysis. The geometric amplitudes determine the system's Lyapunov indices.

(4) The necessary and sufficient conditions (17) for constructing the adiabatic invariant for one degree of freedom have been formulated (under the assumption that the invariant is conserved to within ε^k). These are the absence of the generalized geometric amplitude and zero value for the real part of the current eigenvalue for the given degree of freedom. Within the same approximation, Poincaré's first integral invariant is equivalent to the complete set of n adiabatic invariants. In other words, the conditions for its existence are an oscillatory nature of the system and zero values for all geometric amplitudes. The conditions of the Liouville theorem (the nth Poincaré integral invariant) demand that real parts of the current eigenvalues be zeros, as well as the sum of generalized geometric amplitudes.

(5) The central results of the paper are the following equivalence relationships. For the oscillatory systems (1) equivalence has been proved of the Hamiltonian nature of the system, its quantizability, and parametric stability with accuracy to any power of ε. These properties are implemented if and only if the generalized geometric amplitudes of the oscillatory system are all equal to zero.

(6) Particularly discussed have been the properties of parametric stability and strong stability in a class that are modifications of the strong stability property as applied to parametric systems. As has been shown, it is natural to assume the parametric stability as the primary property. It determines the class of strong stability of parametric systems. In the case under consideration, the complete class of strongly stable oscillatory systems (1) is formed by Hamiltonian oscillatory systems.

(7) It is of interest that a direct consequence of the theorems proven here is the known result concerning adiabatic invariants. Namely, a Hamiltonian system with constant-parameter phase trajectories lying on an n-dimensional torus supports a complete set of n adiabatic invariants that are conserved with accuracy to any power of ε.[4–6]

It appears to us that the equivalence relationships proven here and in Ref. 1 do not just have an abstract, mathematical meaning but also possess a physical if not philosophical significance. They show the role of the Hamiltonian nature of our world. It is well known that the principal, elemental oscillatory systems are described by Hamiltonian equations equally in quantum and classical mechanics and in the wave theory. One could think that the form of these equations is somewhat accidental and they might well have different form. However, the results presented in this work offer a clear view of the following fact: if the equations for linear physical oscillators had not been of Hamiltonian nature, then our world would not have been so stable against small perturbations. Besides, it would not have been of quantum nature either, or at least there would have not existed such a correlation between the micro- and macroworld theories.

In conclusion, we stress once again that the derivation of all of these results has become possible exclusively due to the functional approach to nonautonomous systems (see Sec. I and Refs. 1 and 2).

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APPENDIX A: CONSTRUCTION OF ASYMPTOTIC SOLUTIONS

Consider in more detail Neishtadt's method of successive diagonalizations proposed in Sec. II (Compare also with method in Ref. 4.). Let upon the kth diagonalization the initial equation (1) take the form

$$\mathbf{x}'_{[k]}=[\mathbf{\Lambda}_{[k]}+\mathbf{\Delta}_{[k]}]\mathbf{x}_{[k]}, \tag{A1}$$

where $|\mathbf{\Delta}_{[k]}|\sim\varepsilon^{k+1}$ and $\mathbf{\Lambda}_{[k]}$ is a diagonal matrix containing the terms up to the order ε^k inclusive. Next let us perform the $(k+1)$th diagonalization. Let us make the substitution

$$\mathbf{x}_{[k]}=\mathbf{D}_{[k]}\mathbf{x}_{[k+1]}, \tag{A2}$$

where

$$\mathbf{D}_{[k]jl}=\frac{\mathbf{\Delta}_{[k]jl}}{(\mathbf{\Lambda}_{[k]jj}-\mathbf{\Lambda}_{[k]ll})}, \quad j\neq l; \quad \mathbf{D}_{[k]jj}=1. \tag{A3}$$

The substitution (A2) always exists and allows inversion, because it is close to the unit matrix (the diagonal elements of $\mathbf{\Lambda}_{[k]}$ are different according to the initial assumptions).

After the substitution (A2), Eq. (A1) will take the form

$$\mathbf{x}'_{[k+1]}=\mathbf{D}^{-1}_{[k]}\{[\mathbf{\Lambda}_{[k]}+\mathbf{\Delta}_{[k]}]\mathbf{D}_{[k]}-\mathbf{D}'_{[k]}\}\mathbf{x}_{[k+1]}. \tag{A4}$$

Then we set in (A4)

$$\mathbf{\Lambda}_{[k+1]}=\mathbf{\Lambda}_{[k]}+\mathrm{dg}\,\mathbf{\Delta}_{[k]}, \tag{A5}$$

(recall that the operator dg denotes rejection of the off-diagonal matrix terms)

$$\mathbf{\Delta}_{[k+1]}=\mathbf{D}_{[k]}^{-1}[\mathbf{\Lambda}_{[k]}+\mathbf{\Delta}_{[k]}]\mathbf{D}_{[k]}-\mathbf{\Lambda}_{[k]}-\mathrm{dg}\,\mathbf{\Delta}_{[k]}-\mathbf{D}_{[k]}^{-1}\mathbf{D}'_{[k]}. \tag{A6}$$

By substituting Eq. (A3) into Eq. (A6) we can easily verify that the components of $\mathbf{\Delta}_{[k+1]}$ are proportional to the derivatives of the $\mathbf{\Delta}_{[k]}$ components, i.e., they are terms of order ε^{k+2}. Finally, by substituting Eqs. (A5) and (A6) into Eq. (A4) we obtain:

$$\mathbf{x}'_{[k+1]}=[\mathbf{\Lambda}_{[k+1]}+\mathbf{\Delta}_{[k+1]}]\mathbf{x}_{[k+1]}. \tag{A7}$$

Thus, we have completely described the recurrent step from Eq. (A1) to Eq. (A7). It only remains to derive the initial equation of the form (A1) to apply the induction.

Since the matrix $\mathbf{A}$ of the initial equation (1) possesses different nonzero eigenvalues, there exists a matrix $\mathbf{D}$ such that $\mathbf{D}^{-1}\mathbf{A}\mathbf{D}=\mathbf{\Lambda}$ (The matrix $\mathbf{\Lambda}$ was introduced in Sec. II.) By carrying out the substitution $\mathbf{x}=\mathbf{D}\mathbf{x}_{[0]}$, we obtain from Eq. (1)

$$\mathbf{x}'_{[0]}=[\mathbf{\Lambda}-\mathbf{D}^{-1}\mathbf{D}']\mathbf{x}_{[0]}.$$

By setting $\mathbf{\Lambda}_{[0]}\equiv\mathbf{\Lambda}$ and $\mathbf{\Delta}_{[0]}\equiv-\mathbf{D}^{-1}\mathbf{D}'$, we obtain Eq. (A1) for $k=0$. Equations (A2)–(A7) allow one to repeat the diagonalization procedure as many times as necessary, reducing the initial equation to a diagonal form with accuracy to any power of ε.

APPENDIX B: ON PROPERTIES OF THE $\vec{M}$-SPACE AND SYSTEM TRAJECTORIES IN IT

It should be noted that the dimensions of the generalized parameter space ($\vec{M}$-space), strictly speaking, are not independent. Indeed, consider, for instance, a closed oriented contour of the system's representative point in the plane (μ_j,μ'_j) (Fig. 1). It is easy to see that the contour shown by a dashed line cannot be realized. Along the sections of decreasing μ_j, the value μ'_j should be negative, and hence this section of the contour should lie in the lower half-plane. The contour depicted in Fig. 1 by a solid line meets the requirement, and thus it can be realized.

By generalizing the example, we can suggest the following requirement, which does not, however, exhaust the relations between the coordinates in the $\vec{M}$-space (certain constraints are also imposed on the trajectories in the planes of $(\mu_j^{(l)},\mu_j^{(l-2)})$ type and others). At the same time, only the relations considered in the following are essential for proving the theorems of this paper.

Statement: Let $\vec{M}=\vec{M}(\tau)$ be some parametrization of a trajectory of the system's representative point in the $\vec{M}$-space. Also, let the τ parameter be a smooth, monotonically increasing function of the real time t $(\mathrm{d}\tau/\mathrm{d}t>0)$. Then the following equality should hold at any point of the trajectory:

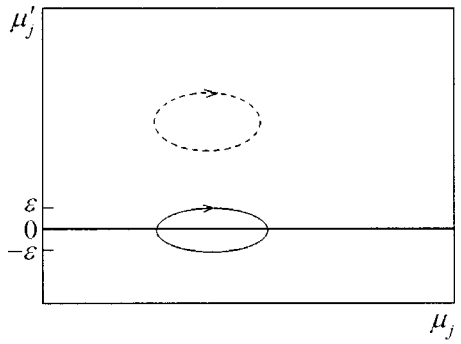

FIG. 1. Realizable (solid line) and nonrealizable (dashed line) contours of the system's representative point in a (μ_j,μ'_j) plane of the $\vec{M}$-space.

$$\operatorname{sign}\frac{d\mu_j^{(l-1)}}{d\tau}=\operatorname{sign}\mu_j^{(l)} \tag{B1}$$

for all components $j=1,...,n$ *and all the derivatives* $l=1,...,k-1$ *used.*

Let us analyze how the constraints (B1) imposed on the coordinates of the $\vec{M}$-space affect the proofs of Theorems I–III. To this end, first note that due to the adiabaticity condition (2) the system trajectories are located in the $\vec{M}$-space near the hyperplane of the $\bar{\mu}$-space. For example, the values μ_j' should be of the order ε. Hence, the trajectory of the system's representative point in the plane shown in Fig. 1 in fact is attached to the band $\mu_j'\in(-\varepsilon,\varepsilon)$ and cannot move far away from it. Similarly, the dimensions of the higher-order derivatives $\mu_j^{(l)}$ are attached to even narrower bands of width ε^l.

Let us turn now to the proof of Theorem I (see Ref. 1). It is clear that the nonperturbed realization of the system used there (an arbitrary point in the considered region of $\vec{M}$-space) is located in the hyperplane of the $\bar{\mu}$-space. The perturbed realization of the system is represented by an arbitrary closed contour around the point considered whose projections are tied to bands $\mu_j^{(l)}\in(-\varepsilon^l,\varepsilon^l)$ in the planes $(\mu_j^{(l)},\mu_j^{(l-1)})$. The admissible closed contour satisfying the conditions (B1) must intersect with the hyperplane $\mu_j^{(l)}=0$ (see Fig. 1), and hence the height of its projection on the plane $(\mu_j^{(l)},\mu_j^{(l-1)})$ is of order ε^l. In terms of μ_j dimensions, no restrictions on the contour geometry are posed, so it can always be chosen arbitrarily small. Meanwhile, in terms of μ_j' dimensions its value is generally bounded both from *above* and from *below* by the order ε. This could prevent us from selecting a sufficiently small arbitrary contour for the perturbed system realization. However, *all* the admissible contours can be made arbitrarily small in the dimensions $\mu_j^{(l)}$, $l\geqslant 1$ by choosing a sufficiently small value of ε. Thus, it only remains to choose the necessarily small shape of the contour in the $\bar{\mu}$-space; its projections onto other dimensions will always be sufficiently small in order to use the theorem on the strong stability of Hamiltonian systems with periodic coefficients. Evidently, the Hamiltonian nature as well as the presence of generalized geometric amplitudes in a system does not depend on the magnitude of ε. So the proof remains valid for any small ε.

The proof of Theorem II does not face any additional difficulties as compared with the one given in Ref. 1. As for the proof of Theorem III, it involves, as in the case of Theorem I, the trajectory of the unperturbed realization of the system, as well as the closely lying trajectory of a perturbed realization, spiraling around the former one. The problem of existence of a sufficiently close perturbed trajectory can be resolved if we follow the logic pattern of the previous paragraph. Any admissible trajectory can be made arbitrarily close (in terms of dimensions $\mu_j^{(l)}$, $l\geqslant 1$) to the initial unperturbed one by choosing a sufficiently small value of ε, then utilizing the fact that the properties in question do not depend on the magnitude of the small ε.

In conclusion, let us note one more interesting point. The theory of Berry's phase is remarkable in that the phase growth in the solution is determined only by the shape of the trajectory of the system's representative point in the $\bar{\mu}$-space, rather than by the explicit time dependence of the parameters. A single trajectory may correspond to an infinitely large number of various realizations of the system. When considering the system trajectories in the generalized $\vec{M}$-space, the freedom in recovering the system's realization (i.e., the $\bar{\mu}(\varepsilon t)$ dependence) is substantially restricted. Indeed, not only the sequence of variations in $\bar{\mu}$ values is specified, but also their derivatives up to the $(k-1)$th order. Still, a single contour corresponds as yet to an infinitely large number of realizations. For example, a closed contour in the $\vec{M}$-space does not necessarily correspond to periodic variations of the parameters: it is quite possible that the contour would be open in further dimensions ($\bar{\mu}^{(k)}$th). However, in the infinite-dimensional space $\vec{M}^{(\infty)}=(\bar{\mu}(\varepsilon t),\bar{\mu}'(\varepsilon t),...,\bar{\mu}^{(k)}(\varepsilon t),...)$, in which all the parameter derivatives are taken into account, the system realization can be recovered unambiguously (if, say, the function $\bar{\mu}(\varepsilon t)$ is analytical) from knowledge of a contour in that space. Closed trajectories in that space correspond to periodic variations in $\bar{\mu}(\varepsilon t)$ values. Moreover, an analytical function $\bar{\mu}(\varepsilon t)$, as well as the corresponding trajectories, can be unambiguously reconstructed from one point on this trajectory. It is readily

seen that the coordinates of this point determine all the coefficients of the Taylor series. The $\vec{M}^{(\infty)}$-space can be regarded as a certain representation of the space of analytic functions. Here every function corresponds to a certain trajectory, and conversely: each point in the $\vec{M}^{(\infty)}$-space corresponds to a unique trajectory containing this point and a function.

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Elliptic Ruijsenaars operators and functional equations

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We study mutually commutative difference operators introduced by Ruijsenaars, which are regarded as elliptic analogs of Macdonald operators and consist of the Jacobi theta functions and shift operators. These operators are constructed in terms of R-operators due to Shibukawa and Ueno or root algebras introduced by Cherednik, which give rise to a set of functional equations. We investigate solutions of these functional equations for generalizations of elliptic Ruijsenaars operators.
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I. INTRODUCTION

Ruijsenaars introduced a family of mutually commutative operators, whose coefficients consist of theta functions, as a relativistic quantum many-body system in Ref. 10. These operators are regarded as an elliptic analog of Macdonald operators. Since the Macdonald operators are associated with affine root systems, their elliptic analogs are also expected to have generalizations to arbitrary root systems. From this viewpoint, first an analog for the BC-type root system was introduced by van Diejen,[13] and later for arbitrary root systems in Ref. 6. In the latter, the operators are constructed in terms of an algebra called root algebra due to Cherednik,[4] which is a generalization of the Yang–Baxter equation. In this framework, Shibukawa–Ueno's R-operator[12] is regarded as a representation of the root algebras for simply-laced root systems. For the other root systems, we need to construct corresponding elliptic R-operators, which give rise to a set of functional equations and is not yet investigated thoroughly. In this article, we study solutions of these functional equations to find out generalizations of elliptic Ruijsenaars operators.

This article is organized as follows: In Sec. II, we give the notation and definitions, and outline the construction of elliptic Ruijsenaars operators following Ref. 6 as a motivation. In Sec. III, we put four types of equations associated with the root systems of type $A_1\times A_1$, A_2, B_2 and G_2 and set our basic assumption in this article. Since in our setting, the $A_1\times A_1$-type equation gives no functional equation, we first investigate the functional equations of type A_2, in Sec. IV. One of these functional equations coincides with the one of the classical Yang–Baxter equation.[2] Due to their result, we can exhaust all the solutions. It should be noted that a detailed study on R-operators of type A_2 was given in Ref. 11 in a little different setting. In Sec. V, we study the B_2-type equations. Since in affine root systems other than $C_2^{(1)}$, $D_3^{(2)}$ and $A_4^{(2)}$, they are combined with A_2-type equations, the solutions are obtained due to the results in Sec. IV and in Ref. 7. Although general solutions purely subject to the B_2-type equations are not obtained, we present an exceptional solution corresponding to the solution studied in Refs. 8 and 9. The last section is devoted to the G_2-type equations. In this system, the equations are much more complicated than the others, and are not fully investigated. We give partial results and find 22 solutions under an assumption called extensibility.

In this article, we obtain R-operators by solving functional equations. However, it is strongly hoped that they are obtained in a natural way or from smaller algebra as the representation of double affine Hecke algebras in Macdonald theory.[3]

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II. AFFINE ROOT SYSTEMS AND ELLIPTIC RUIJSENAARS OPERATORS

We give some well-known facts about affine root systems and affine Weyl groups,[1,4,5] and outline the construction of elliptic Ruijsenaars operators following Ref. 6. In this article we only treat nontwisted root systems for simplicity.

Let $\mathring{V}$ be a real vector space equipped with inner product $(\cdot,\cdot)$. For $\alpha\in V$, define $\alpha^\vee := 2\alpha/(\alpha,\alpha)$. Let $\mathring{\Delta}$ be an irreducible reduced root system, $\mathring{I}=\{1,\ldots,l\}$, $\mathring{\Pi}=\{\alpha_i|i\in\mathring{I}\}$, the set of simple roots and $\mathring{\Pi}^\vee=\{\alpha_i^\vee|i\in\mathring{I}\}$, the set of simple coroots. Let $\mathring{\Lambda}:=\{\lambda_i|i\in\mathring{I}\}$ be a dual basis of $\mathring{\Pi}$. Let $\mathring{Q}^\vee$ and $\mathring{P}^\vee$ be the coroot lattice and the coweight lattice generated by $\mathring{\Pi}$ and $\mathring{\Lambda}$, respectively. Let $V:=\mathring{V}\oplus\mathbb{R}\delta$ with $(\delta,V)=0$. Let $\Delta:=\mathring{\Delta}\times\mathbb{Z}\delta$ be the corresponding nontwisted affine root system. Let $I=\{0,\ldots,l\}$, $\Pi=\{\alpha_i|i\in I\}$ and $\Pi^\vee=\{\alpha_i^\vee|i\in I\}$. Let Δ_+ and Δ_- be the set of positive roots and negative roots, respectively. Then one has the disjoint union $\Delta=\Delta_+\cup\Delta_-$. For $\alpha\in\Delta$, let s_α be a reflection defined by

$$s_\alpha(v):=v-(v,\alpha^\vee)\alpha,\quad v\in V. \tag{2.1}$$

The Weyl group $\mathring{W}$ is generated by the fundamental reflections $\{s_i:=s_{\alpha_i}|i\in\mathring{I}\}$ and the affine Weyl group W is generated by $\{s_i|i\in I\}$. The defining relations are given by $s_i^2=id$ and the Coxeter relations:

$$(s_i\ s_j)^{m_{ij}}=id,\quad \text{for } i\neq j\in I, \tag{2.2}$$

where $m_{ij}=2$ if α_i and α_j are disconnected in the Dynkin diagram and $m_{ij}=3,4,6$ if 1,2,3 lines respectively connect α_i and α_j. For $\mu\in\mathring{V}$, we define endomorphisms τ_μ of the vector space V by

$$\tau_\mu(\lambda):=\lambda-(\lambda,\mu)\delta. \tag{2.3}$$

The actions of s_α, τ_μ are naturally induced on $x\in V^*$ by transposition as follows:

$$s_\alpha(x)=x-\langle x,\alpha\rangle\alpha^\vee, \tag{2.4}$$

$$\tau_\mu(x)=x+\langle x,\delta\rangle\mu, \tag{2.5}$$

where $\langle\cdot,\cdot\rangle$ denotes the pairing of V^* and V, and $\alpha^\vee$, μ are identified with $(\alpha^\vee,\cdot)$, $(\mu,\cdot)$, respectively. For an arbitrary lattice L, we denote by $T(L)$ the corresponding group of translations of L.

Proposition 2.1: The affine Weyl group W is the semidirect product $W=\mathring{W}\ltimes T(\mathring{Q}^\vee)$.

Definition 2.2: The extended affine Weyl group $\hat{W}$ is the semidirect product $\hat{W}:=\mathring{W}\ltimes T(\mathring{P}^\vee)$.

Let Ω be the subgroup of $\hat{W}$ which stabilizes the affine Weyl chamber.

Proposition 2.3: The extended affine Weyl group $\hat{W}$ is isomorphic to the semidirect product $W\rtimes\Omega$.

Definition 2.4: (1) The length $\ell(w)$ of $w\in W$ is the length ℓ of the reduced decomposition:

$$w=s_{i_1}\ldots s_{i_\ell},\quad \text{for}\quad i_k\in I, \tag{2.6}$$

$$\ell(id)=0. \tag{2.7}$$

(2) The length $\ell(\hat{w})$ of $\hat{w}\in\hat{W}$ is the number of the negative roots made positive by $\hat{w}$:

$$\ell(\hat{w}):=|\Delta_{\hat{w}}|,\quad \Delta_{\hat{w}}:=\Delta_+\cap\hat{w}\Delta_-, \tag{2.8}$$

which is equivalent to the definition $\ell(w)$ for $w\in W$. The reduced decomposition of $\hat{w}\in\hat{W}$ is $\hat{w}=w\omega=s_{i_1}\cdots s_{i_\ell}\omega$, where $\omega\in\Omega$ and $\ell=\ell(\hat{w})=\ell(w)$.

The set $\Delta_{\hat{w}}$ is explicitly described as $\Delta_{\hat{w}}=\{\alpha^{(1)}=\alpha_{i_1},\alpha^{(2)}=s_{i_1}(\alpha_{i_2}),\ldots,\alpha^{(\ell)}=ws_{i_\ell}(\alpha_{i_\ell})\}$. By definition, $\Delta_{\hat{w}}$ is independent of reduced expressions.

Definition 2.5: A coweight $\lambda\in\mathring{P}^\vee$ is said to be minuscule if $\Delta_{\tau_{-\lambda}}\subset\mathring{\Delta}_+$.

We shall define the root algebras after Cherednik.[4] Let $\mathcal{T}$ be the tensor algebra over $\mathbb{C}$ generated by independent variables $\{R_\alpha|\alpha\in\Delta\}$. Then the action of $\hat{w}\in\hat{W}$ on Δ induces an action on $\mathcal{T}$ by ${}^{\hat{w}}:R_\alpha\mapsto R_{\hat{w}(\alpha)}$.

Definition 2.6: Let $\mathcal{I}$ be the two-sided ideal in $\mathcal{T}$ which is generated by all the elements of the form for $i\neq j\in I$, and $\hat{w}\in\hat{W}$:

$$\underbrace{{}^{\hat{w}}(R_{\alpha_i}\otimes R_{s_i\alpha_j}\otimes R_{s_is_j\alpha_i}\otimes\cdots)}_{m_{ij}\ \text{factors}}-\underbrace{{}^{\hat{w}}(R_{\alpha_j}\otimes R_{s_j\alpha_i}\otimes R_{s_js_i\alpha_j}\otimes\cdots)}_{m_{ij}\ \text{factors}}. \tag{2.9}$$

The root algebra $\tilde{\mathcal{R}}$ is $\mathcal{T}/\mathcal{I}$. $\{R_\alpha|\alpha\in\Delta\}$ are called the R-matrices.

Because of the $\hat{W}$-invariance of $\mathcal{I}$, the action of $\hat{W}$ is induced on $\tilde{\mathcal{R}}$. For simplicity, we write products in $\tilde{\mathcal{R}}$ in the usual way for associative algebras.

Theorem 2.7 (Cherednik): *(1) There exists a unique set $\{R_{\hat{w}}|\hat{w}\in\hat{W}\}\subset\tilde{\mathcal{R}}$ satisfying the relations*

$$R_{vw}=R_v{}^vR_w,\quad R_{s_i}=R_{\alpha_i}\quad(i\in I),\quad R_\omega=1, \tag{2.10}$$

where $\omega\in\Omega$, $v,w\in\hat{W}$ and $\ell(v\ w)=\ell(v)+\ell(w)$.

(2) We have the R-matrix for $\hat{w}\in\hat{W}$ and its arbitrary reduced decomposition $\hat{w}=w\omega=s_{i_1}\cdots s_{i_\ell}\omega$ as

$$\begin{gathered}R_{\hat{w}}=R_{\alpha^{(1)}}\cdots R_{\alpha^{(\ell)}},\\ \alpha^{(1)}=\alpha_{i_1},\quad \alpha^{(2)}=s_{i_1}(\alpha_{i_2}),\quad\ldots,\quad \alpha^{(\ell)}=ws_{i_\ell}(\alpha_{i_\ell})\in\Delta_{\hat{w}}.\end{gathered} \tag{2.11}$$

Instead of the original root algebra, we use the following extension, where $\tilde{\mathcal{R}}$ is combined with the translation group $T(\mathring{P}^\vee)$:

Definition 2.8: $\mathcal{R}:=\tilde{\mathcal{R}}\rtimes T(\mathring{P}^\vee)$,

$$(R\tau_\lambda)(R'\tau_\mu)=R({}^{\tau_\lambda}R')\tau_{\lambda+\mu}, \tag{2.12}$$

where $R,R'\in\tilde{\mathcal{R}}$ and $\lambda,\mu\in\mathring{P}^\vee$.

Theorem 2.9: *The subalgebra $\mathcal{S}\subset\mathcal{R}$ generated by $\{Y^\lambda:=R_{\tau_\lambda}\ \tau_\lambda|\lambda\in\mathring{P}^\vee_-\}$ forms a commutative algebra and is generated by $\{Y^{-\lambda_i}|i\in\mathring{I}\}$.*

We consider such a representation that R_α acts on the space of the meromorphic functions $\mathcal{M}$ on $\mathbb{C}\otimes V^*$ and takes the form

$$(R_\alpha\ f)(x):=H_\alpha(\langle\alpha,x\rangle,\mu_\alpha)f(x)-H_\alpha(\langle\alpha,x\rangle,(\alpha^\vee,\xi))f(s_\alpha(x)), \tag{2.13}$$

where $\xi\in\mathring{V}$ is a parameter called spectral parameter, $\mu_\alpha\in\mathbb{C}$ is a $\hat{W}$-invariant constant, $f\in\mathcal{M}$ and $H_\alpha(z,\mu)$ is a meromorphic function of z on $\mathbb{C}$. Furthermore, we assume that (2.13) satisfies unitarity:

$$R_{-\alpha}R_\alpha=c_\alpha((\alpha^\vee,\xi)), \tag{2.14}$$

where $c_\alpha(z)$ is a meromorphic function on $\mathbb{C}$ and $c_\alpha(-\mu_\alpha)=0$.

For some $\lambda \in \mathring{P}^\vee_-$, the explicit forms of Y^λ on the space $\mathcal{V}=\mathcal{M}^{\mathring{W}}$ are calculated as follows:

Theorem 2.10: *Let $\xi=-\mathring{\rho}_\mu:=\Sigma_{\alpha\in\mathring{\Delta}}\mu_\alpha\alpha$ and let λ be minuscule. Then we have*

$$Y^{-\lambda}|_{\mathcal{V}}=\frac{1}{|\mathring{W}_\lambda|}\sum_{w\in\mathring{W}} w\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\lambda,\alpha)=1}} H_\alpha(\mu_\alpha)\tau_{-\lambda}\right)\Bigg|_{\mathcal{V}}, \tag{2.15}$$

$$Y^{-\theta^\vee}|_{\mathcal{V}}=\frac{1}{|\mathring{W}_{\theta^\vee}|}\sum_{w\in\mathring{W}} w\left(\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\alpha,\theta^\vee)>0}} H_\alpha(\mu_\alpha)\right)(H_{\theta+\delta}(\mu_{\alpha_0})\tau_{-\theta^\vee}-H_{\theta+\delta}(-(\theta^\vee,\mathring{\rho}_\mu)))\right)\Bigg|_{\mathcal{V}}, \tag{2.16}$$

where $H_\alpha(\mu)$ denotes the multiplication operator of $H_\alpha(\cdot,\mu)$ and $\mathring{W}_\nu$ is the stabilizer of ν in $\mathring{W}$.

For an appropriate function H_α, they give actually generalizations of elliptic Ruijsenaars operators. In the following sections, we investigate R-operators in more general settings.

III. FUNCTIONAL EQUATIONS ASSOCIATED WITH ROOT ALGEBRAS

Motivated by the previous section, we will investigate the representation of the root algebras. Following Definition 2.6 in root systems of rank 2, we have the following equations:

$$R_\alpha\ R_\beta = R_\beta\ R_\alpha, \tag{3.1}$$

$$R_\alpha\ R_{\alpha+\beta}\ R_\beta = R_\beta\ R_{\alpha+\beta}\ R_\alpha, \tag{3.2}$$

$$R_\alpha\ R_{\alpha+\beta}\ R_{\alpha+2\beta}\ R_\beta = R_\beta\ R_{\alpha+2\beta}\ R_{\alpha+\beta}\ R_\alpha, \tag{3.3}$$

$$R_\alpha\ R_{\alpha+\beta}\ R_{2\alpha+3\beta}\ R_{\alpha+2\beta}\ R_{\alpha+3\beta}\ R_\beta = R_\beta\ R_{\alpha+3\beta}\ R_{\alpha+2\beta}\ R_{2\alpha+3\beta}\ R_{\alpha+\beta}\ R_\alpha, \tag{3.4}$$

where $|\alpha|\geqslant|\beta|$. In root systems of higher rank, we see that for any two roots α and β, R_α and R_β satisfy one of the equations (3.1)–(3.4). So it is sufficient to consider the above systems.

Let $\mathcal{M}_0$ be the set of meromorphic functions defined in a neighborhood of the origin of $\mathbb{C}$ with a possible pole at the origin. Let $\mathcal{H}_0$ be the set of holomorphic functions defined in a similar manner.

Although we considered the representation of the form (2.13), we relax the condition in the following. Namely, R_α acts on $\mathcal{M}_0$ and takes the form

$$(R_\alpha\ f)(x):=G_\alpha(\langle\alpha,x\rangle)f(x)+H_\alpha(\langle\alpha,x\rangle)f(s_\alpha(x)), \tag{3.5}$$

where $G_\alpha, H_\alpha \in \mathcal{M}_0$.

We study solutions G_α and H_α of (3.1), (3.2), (3.3) or (3.4) such that either G_α or H_α is not identically zero. Since the $A_1\times A_1$-type relation (3.1) does not require any constraint in G_α, H_α, we first investigate general solutions of the A_2-type (3.2).

Define for $\Im\tau>0$

$$\sigma_{a,b}(x,\lambda;\tau):=e^{-2\pi i b\lambda}\frac{\theta_1'(0;\tau)\theta_1(x+a+b\tau-\lambda;\tau)}{\theta_1(x+a+b\tau;\tau)\theta_1(-\lambda;\tau)}, \tag{3.6}$$

where $\theta_1(x;\tau)$ is the Jacobi theta function.

IV. A_2 CASE

A. Functional equations

Proposition 4.1: In the root system of type A_2, *the operators* R_γ *satisfy* (3.2) *if and only if* G_γ *and* H_γ *satisfy, up to an overall factor, the following equations:*

$$G_\alpha(u)=G_{\alpha+\beta}(u)=G_\beta(u), \tag{4.1a}$$

$$H_\alpha(u)H_{\alpha+\beta}(v)+H_{\alpha+\beta}(u+v)H_\beta(-u)-H_\alpha(u+v)H_\beta(v)=0, \tag{4.1b}$$

$$\begin{aligned}G_\alpha(u)G_\alpha(-u)-G_\alpha(v)G_\alpha(-v)&=H_\alpha(u)H_\alpha(-u)-H_\alpha(v)H_\alpha(-v)\\&=H_\beta(u)H_\beta(-u)-H_\beta(v)H_\beta(-v).\end{aligned} \tag{4.1c}$$

Proof: Substituting (3.5) into (3.2), we obtain functional equations as follows:

$$(G_{\alpha+\beta}(v)G_\beta(u+v)-G_{\alpha+\beta}(u+v)G_\beta(v))H_\alpha(u)=0, \tag{4.2a}$$

$$(G_\alpha(u+v)G_{\alpha+\beta}(u)-G_\alpha(u)G_{\alpha+\beta}(u+v))H_\beta(v)=0, \tag{4.2b}$$

$$\begin{aligned}&(G_\alpha(u)G_\beta(-u)-G_\alpha(-v)G_\beta(v))H_{\alpha+\beta}(u+v)+H_\alpha(u)H_{\alpha+\beta}(v)H_\beta(u)\\&-H_\alpha(v)H_{\alpha+\beta}(u)H_\beta(v)=0,\end{aligned} \tag{4.2c}$$

$$\begin{aligned}&G_\beta(u)H_\alpha(u)H_{\alpha+\beta}(v)+G_\alpha(u)H_{\alpha+\beta}(u+v)H_\beta(-u)\\&-G_{\alpha+\beta}(u)H_\alpha(u+v)H_\beta(v)=0,\end{aligned} \tag{4.2d}$$

$$\begin{aligned}&-G_\beta(v)H_\alpha(-v)H_{\alpha+\beta}(u+v)+G_{\alpha+\beta}(v)H_\alpha(u)H_\beta(u+v)\\&-G_\alpha(v)H_{\alpha+\beta}(u)H_\beta(v)=0,\end{aligned} \tag{4.2e}$$

where we have set $u:=\langle x,\alpha\rangle$ and $v:=\langle x,\beta\rangle$. From (4.2a) and (4.2b), since either H_α or H_β is not identically zero, we deduce $G_\alpha(u)=G_{\alpha+\beta}(u)=G_\beta(u)$ without loss of generality and obtain (4.1a). Then (4.2d) and (4.2e) are identical and implies (4.1b). The equation (4.1c) is obtained from (4.2c) by applying (4.1b). □

The equation (4.1b) appears in the classical, i.e., differential, case and was solved in Ref. 2.

Theorem 4.2([2]): *Consider the functional equation*

$$f(u)g(-v)+g(-u-v)h(-u)+h(v)f(u+v)=0. \tag{4.3}$$

(1) The only nontrivial solutions of (4.3) holomorphic around the origin are

$$f(u)=\frac{1}{\lambda}e^{pu},\quad g(u)=-\left(\frac{1}{\lambda+\mu}\right)e^{-(p+q)u},\quad h(u)=\frac{1}{\mu}e^{qu}, \tag{4.4}$$

where $\lambda,\mu,p,q\in\mathbb{C}$ *are arbitrary such that* $\lambda,\mu,\lambda+\mu\neq 0$.

(2) The only nontrivial solutions of (4.3) which have a pole at the origin are

$$\begin{aligned}f(u)&=a\sigma_{0,0}(bu,\lambda;\tau)e^{pu},\\g(u)&=a\sigma_{0,0}(bu,-\lambda-\mu;\tau)e^{-(p+q)u},\\h(u)&=a\sigma_{0,0}(bu,\mu;\tau)e^{qu},\end{aligned} \tag{4.5}$$

where $a,b,\lambda,\mu,p,q\in\mathbb{C}$ *are arbitrary such that* $a,b\neq 0$, $\lambda,\mu,\lambda+\mu\notin\mathbb{Z}+\mathbb{Z}\tau$. *In the above,* ∞ *as a period or a certain limit is also permitted.*[11]

Theorem 4.2 can be applied to $f(u)=H_\alpha(u)$, $g(u)=-H_{\alpha+\beta}(-u)$ and $h(u)=H_\beta(u)$.

B. Holomorphic solutions

Theorem 4.3: *The following functions exhaust all the nontrivial solutions of the equation (4.1) holomorphic around the origin*:

$$H_\alpha(u)=\frac{1}{\lambda}e^{pu},\quad H_{\alpha+\beta}(u)=\left(\frac{1}{\lambda+\mu}\right)e^{(p+q)u},\quad H_\beta(u)=\frac{1}{\mu}e^{qu},\tag{4.6a}$$

$$G_\alpha(u)=G_{\alpha+\beta}(u)=G_\beta(u)=\frac{1}{\nu}\phi(u),\tag{4.6b}$$

where $\lambda,\mu,\nu,p,q\in\mathbb{C}$ *are arbitrary such that* $\lambda,\mu,\nu,\lambda+\mu\neq 0$ *and* $\phi\in\mathcal{M}_0$ *satisfies* $\phi(u)\phi(-u)=1$.

C. Meromorphic solutions

Theorem 4.4: *The following functions exhaust all the nontrivial solutions of the equation (4.1) which has a pole at the origin:*

$$\begin{aligned}H_\alpha(u)&=a\sigma_{0,0}(bu,\lambda;\tau)e^{pu},\\ H_{\alpha+\beta}(u)&=a\sigma_{0,0}(bu,\lambda+\mu;\tau)e^{(p+q)u},\\ H_\beta(u)&=a\sigma_{0,0}(bu,\mu;\tau)e^{qu},\end{aligned}\tag{4.7a}$$

$$G_\alpha(u)=G_{\alpha+\beta}(u)=G_\beta(u)=a\sigma_{0,0}(bu,\nu;\tau)\phi(u),\tag{4.7b}$$

where $a,b,\lambda,\mu,\nu,p,q\in\mathbb{C}$ *such that* $a,b\neq 0$, $\lambda,\mu,\nu,\lambda+\mu\notin\mathbb{Z}+\mathbb{Z}\tau$ *and* $\phi\in\mathcal{M}_0$ *satisfies* $\phi(u)\phi(-u)=1$. *In the above,* ∞ *as a period or a certain limit is also permitted.*

Remark 4.5: The solution in Theorem 4.4 has the following principal part at the origin:

$$H_\alpha(u)=\frac{a}{bu}+\cdots.\tag{4.8}$$

V. B_2 CASE

A. Functional equations

Proposition 5.1: *In the root system of type* B_2, *the operators* R_γ *satisfy (3.3) if and only if* G_γ *and* H_γ *satisfy, up to an overall factor, the following equations:*

$$G_\alpha(u)=G_{\alpha+2\beta}(u),\quad G_{\alpha+\beta}(u)=G_\beta(u),\tag{5.1a}$$

$$H_{\alpha+\beta}(u+v)H_\alpha(-u-2v)+H_\beta(v)H_{\alpha+2\beta}(u)+H_{\alpha+\beta}(-v)H_{\alpha+2\beta}(u+2v)=H_\beta(u+v)H_\alpha(u),\tag{5.1b}$$

$$\begin{aligned}G_\alpha(u)G_\alpha(-u)-G_\alpha(v)G_\alpha(-v)&=H_\alpha(u)H_\alpha(-u)-H_\alpha(v)H_\alpha(-v)\\ &=H_{\alpha+2\beta}(u)H_{\alpha+2\beta}(-u)-H_{\alpha+2\beta}(v)H_{\alpha+2\beta}(-v),\end{aligned}\tag{5.1c}$$

$$G_\beta(u)G_\beta(-u)-G_\beta(v)G_\beta(-v)=H_\beta(u)H_\beta(-u)-H_\beta(v)H_\beta(-v)$$
$$=H_{\alpha+\beta}(u)H_{\alpha+\beta}(-u)-H_{\alpha+\beta}(v)H_{\alpha+\beta}(-v). \tag{5.1d}$$

Proof: Substituting (3.5) into (3.3), we obtain functional equations as follows:

$$(G_{\alpha+\beta}(v)G_\beta(u+v)-G_{\alpha+\beta}(u+v)G_\beta(v))G_{\alpha+2\beta}(u+2v)H_\alpha(u)=0, \tag{5.2a}$$

$$(G_\alpha(u+2v)G_{\alpha+2\beta}(u)-G_\alpha(u)G_{\alpha+2\beta}(u+2v))H_\beta(v)G_{\alpha+\beta}(u+v)=0, \tag{5.2b}$$

$$(G_\alpha(u)G_{\alpha+2\beta}(-u)-G_\alpha(-u)G_{\alpha+2\beta}(u))H_{\alpha+\beta}(u+v)H_\beta(v)$$
$$=(G_{\alpha+\beta}(v)G_\beta(-v)-G_{\alpha+\beta}(-v)G_\beta(v))H_\alpha(u)H_{\alpha+2\beta}(u+2v), \tag{5.2c}$$

$$G_\beta(u+v)G_{\alpha+2\beta}(u)H_{\alpha+\beta}(v)H_\alpha(u)+G_{\alpha+\beta}(u+v)G_\alpha(u)H_\beta(-u-v)H_{\alpha+2\beta}(u+2v)$$
$$+G_\beta(u+v)G_\alpha(u)H_{\alpha+\beta}(u+v)H_{\alpha+2\beta}(-u)$$
$$=G_{\alpha+\beta}(u+v)G_{\alpha+2\beta}(u)H_\beta(v)H_\alpha(u+2v), \tag{5.2d}$$

$$G_\beta(v)G_{\alpha+2\beta}(u+2v)H_{\alpha+\beta}(u+v)H_\alpha(-u-2v)+G_{\alpha+\beta}(v)G_\alpha(u+2v)H_\beta(v)H_{\alpha+2\beta}(u)$$
$$+G_\beta(v)G_\alpha(u+2v)H_{\alpha+\beta}(-v)H_{\alpha+2\beta}(u+2v)$$
$$=G_{\alpha+\beta}(v)G_{\alpha+2\beta}(u+2v)H_\beta(u+v)H_\alpha(u), \tag{5.2e}$$

$$G_\beta(v)G_\alpha(u)G_{\alpha+2\beta}(-u)H_{\alpha+\beta}(u+v)+G_\beta(v)H_{\alpha+\beta}(v)H_\alpha(u)H_{\alpha+2\beta}(u)$$
$$+G_{\alpha+\beta}(v)H_\beta(-v)H_\alpha(u)H_{\alpha+2\beta}(u+2v)$$
$$=G_\beta(v)H_{\alpha+\beta}(-v)H_\alpha(u+2v)H_{\alpha+2\beta}(u+2v)+G_{\alpha+\beta}(v)H_\beta(v)H_\alpha(u+2v)H_{\alpha+2\beta}(u)$$
$$+G_\beta(v)G_\alpha(-u-2v)G_{\alpha+2\beta}(u+2v)H_{\alpha+\beta}(u+v), \tag{5.2f}$$

$$G_{\alpha+2\beta}(u)H_{\alpha+\beta}(v)H_\beta(u+v)H_\alpha(u)+G_\alpha(u)H_{\alpha+\beta}(u+v)H_\beta(u+v)H_{\alpha+2\beta}(-u)$$
$$+G_{\alpha+\beta}(u+v)G_\beta(-u-v)G_\alpha(u)H_{\alpha+2\beta}(u+2v)$$
$$=G_{\alpha+2\beta}(u)H_{\alpha+\beta}(u+v)H_\beta(v)H_\alpha(-u)+G_\alpha(u)H_{\alpha+\beta}(v)H_\beta(v)H_{\alpha+2\beta}(u)$$
$$+G_{\alpha+\beta}(-v)G_\beta(v)G_\alpha(u)H_{\alpha+2\beta}(u+2v), \tag{5.2g}$$

where we have set $u:=\langle x,\alpha\rangle$ and $v:=\langle x,\beta\rangle$. First we see that from (5.2a) and (5.2b), $G_\alpha(u)=G_{\alpha+2\beta}(u)$ and $G_{\alpha+\beta}(u)=G_\beta(u)$, which implies (5.1a). Then (5.2c) vanishes and (5.2d) and (5.2e) result in the same equation as (5.1b). By applying (5.1b) to (5.2f) and (5.2g), we obtain (5.1c) and (5.1d). □

A solution of these equations possesses the duality:

Lemma 5.2: If $\tilde{G}_\gamma$ and $\tilde{H}_\gamma$ are a solution of (5.1), then

$$\begin{aligned} G_\alpha(u)&=\tilde{G}_\beta(u), \quad H_\alpha(u)=\tilde{H}_\beta(u),\\ G_\beta(u)&=\tilde{G}_\alpha(2u), \quad H_\beta(u)=\tilde{H}_\alpha(2u),\\ G_{\alpha+\beta}(u)&=\tilde{G}_{\alpha+2\beta}(2u), \quad H_{\alpha+\beta}(u)=\tilde{H}_{\alpha+2\beta}(2u),\\ G_{\alpha+2\beta}(u)&=\tilde{G}_{\alpha+\beta}(u), \quad H_{\alpha+2\beta}(u)=\tilde{H}_{\alpha+\beta}(u) \end{aligned} \tag{5.3}$$

are also a solution of (5.1).

Proof: This can be checked by a direct calculation. □

In the root systems of type $C_2^{(1)}$, $D_3^{(2)}$ or $A_4^{(2)}$, we have only the equation (3.3) and we actually need the general solution for the equations (5.1). However, it is a very difficult problem to obtain the general solution and we assume that H_α and $H_{\alpha+2\beta}$ are given by Theorem 4.3 or Theorem 4.4, which is not an assumption and is imposed in the other root systems.

B. Solutions associated with holomorphic solutions

We assume that H_α and $H_{\alpha+2\beta}$ are given by Theorem 4.3.

Lemma 5.3: Let

$$H_\alpha(u)=\frac{1}{\lambda}e^{pu},\quad H_{\alpha+2\beta}(u)=\frac{1}{\mu}e^{qu}, \tag{5.4}$$

where $\lambda,\mu\neq 0$. *Then the solution of (5.1b) is*

$$H_\beta(u)=e^{(-p+q)u}(b+\varphi(u)),\quad H_{\alpha+\beta}(u)=e^{(p+q)u}(a+\varphi(u)), \tag{5.5}$$

where $\varphi\in\mathcal{M}_0$ *is an arbitrary odd function and* $a,b\in\mathbb{C}$ *are arbitrary such that* $a(\lambda+\mu)+b(\lambda-\mu)=0$.

Proof: We assume that $\lambda\neq\mu$. By substituting (5.4) and $H_\beta(u)=f(u)e^{(-p+q)u}$ and $H_{\alpha+\beta}(u)=g(u)e^{(p+q)u}$ into the equation (5.1b), we obtain

$$\lambda f(v)-\mu f(u+v)+\lambda g(-v)+\mu g(u+v)=0, \tag{5.6}$$

and thus by setting $u=0$,

$$f(v)=\frac{\lambda g(-v)+\mu g(v)}{-\lambda+\mu}. \tag{5.7}$$

Substituting this into (5.6) and setting $u=0$ after the differentiation by u, we arrive at

$$(g(v)+g(-v))'=0. \tag{5.8}$$

This differential equation yields

$$g(v)=a+\varphi(v), \tag{5.9}$$

where $a\in\mathbb{C}$ is an arbitrary constant and $\varphi\in\mathcal{M}_0$ is an arbitrary odd function. Again substituting this function into (5.6), we can check that they are really a solution of (5.1b). If $\lambda=\mu$, then by exchanging the roles of f and g, the statement follows. □

Theorem 5.4: *Let*

$$H_\alpha(u)=\frac{1}{\lambda}e^{pu},\quad H_{\alpha+2\beta}(u)=\frac{1}{\mu}e^{qu}, \tag{5.10a}$$

$$G_\alpha(u)=G_{\alpha+2\beta}(u)=\frac{1}{\nu}\phi(u), \tag{5.10b}$$

where $\lambda,\mu\neq 0$ *and* $\phi\in\mathcal{M}_0$ *satisfies* $\phi(u)\phi(-u)=1$. *Then the following functions exhaust all the nontrivial solutions of the equation (5.1):*

$$H_\beta(u)=e^{(-p+q)u}(b+\varphi(u)),\quad H_{\alpha+\beta}(u)=e^{(p+q)u}(a+\varphi(u)), \tag{5.11a}$$

$$G_\beta(u)=G_{\alpha+2\beta}(u)=\psi(u)(c+\varphi(u)), \tag{5.11b}$$

where $\varphi \in \mathcal{M}_0$ *is odd and* $a,b,c \in \mathbb{C}$ *are such that* $a(\lambda+\mu)+b(\lambda-\mu)=0$ *and* $\psi \in \mathcal{M}_0$ *satisfies* $\psi(u)\psi(-u)=1$.

C. Solutions associated with meromorphic solutions

We assume that H_α and $H_{\alpha+2\beta}$ are given by Theorem 4.4 and consider the following equation:

$$H_{\alpha+\beta}(v)H_\alpha(u-v)+H_\beta(-u)H_{\alpha+2\beta}(u+v)+H_{\alpha+\beta}(u)H_{\alpha+2\beta}(-u+v) = H_\beta(v)H_\alpha(u+v), \tag{5.1b$'$}$$

which is obtained by replacing u by $u+v$ and v by $-u$ in (5.1b).

Set

$$H_\beta(u)=\sum_{i\geqslant -p} H_\beta^{(i)}u^i, \quad H_{\alpha+\beta}(u)=\sum_{i\geqslant -q} H_{\alpha+\beta}^{(i)}u^i. \tag{5.12}$$

Lemma 5.5: If either H_β *or* $H_{\alpha+\beta}$ *has a pole at the origin, then both* H_β *and* $H_{\alpha+\beta}$ *have a simple pole at the origin and* $H_\beta^{(-1)}=H_{\alpha+\beta}^{(-1)}$.

Proof: We assume H_β has a pole at the origin of order $p>0$. By substituting (5.12) and the Taylor expansions of $H_\alpha(u+v)$, $H_\alpha(u-v)$, $H_{\alpha+2\beta}(u+v)$ and $H_{\alpha+2\beta}(-u+v)$ with respect to u into the equation (5.1b$'$), we see that $H_{\alpha+\beta}$ has the same order as H_β at the origin. Comparing the coefficient of u^{-p}, we have

$$H_{\alpha+\beta}^{(-p)}=(-1)^{-p+1}H_\beta^{(-p)}. \tag{5.13}$$

If $p>1$, we have the following equation by comparing the coefficient of u^{-p+1}:

$$(H_{\alpha+\beta}^{(-p+1)}+(-1)^{-p+1}H_\beta^{(-p+1)})H_{\alpha+2\beta}(v)-2H_{\alpha+\beta}^{(-p)}H'_{\alpha+2\beta}(v)=0, \tag{5.14}$$

where we have used (5.13). Since $H_\beta(v)$ is not of the form ae^{bv}, we have $H_{\alpha+\beta}^{(-p)}=0$, which contradicts to the assumption and implies $p=1$. The case that $H_{\alpha+\beta}$ has a pole at the origin is shown similarly. □

By substituting the form $H_\gamma(u)=\Sigma_{i=-1}^{\infty}H_\gamma^{(i)}u^i$ and $H_\alpha^{(-1)}=H_{\alpha+2\beta}^{(-1)}$ and $H_\beta^{(-1)}=H_{\alpha+\beta}^{(-1)}$, we obtain for all $l,m\geqslant 0$,

$$\begin{aligned}
&-H_\alpha^{(-1)}((-1)^mH_{\alpha+\beta}^{(l+m+1)}+H_\beta^{(l+m+1)})+H_\beta^{(-1)}\Bigg(((-1)^{l+m+1}+(-1)^{m+1})\binom{l+m+1}{m}H_\alpha^{(l+m+1)}\\
&\quad+((-1)^{m+1}-1)\binom{l+m+1}{m+1}H_{\alpha+2\beta}^{(l+m+1)}\Bigg)+\sum_{k=0}^{l}\binom{m+k}{k}((-1)^{m+k}H_{\alpha+\beta}^{(l-k)}H_\alpha^{(m+k)}\\
&\quad-(-1)^mH_\beta^{(l-k)}H_\alpha^{(m+k)})+\sum_{k=0}^{m}\binom{l+k}{k}((-1)^kH_\beta^{(m-k)}H_{\alpha+2\beta}^{(l+k)}+(-1)^{m-k}H_{\alpha+\beta}^{(m-k)}H_{\alpha+2\beta}^{(l+k)})\\
&\quad=0.
\end{aligned} \tag{5.15}$$

Lemma 5.6: H_β *and* $H_{\alpha+\beta}$ *are determined by* $H_\beta^{(-1)}$, $H_\beta^{(0)}$, $H_\beta^{(1)}$ *and* $H_{\alpha+\beta}^{(0)}$.

Proof: In (5.15), by setting $l=n-m-1$ we obtain two equations for $m=0,1$, which are written in the form

$$-H_\alpha^{(-1)}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}H_\beta^{(n)}\\ H_{\alpha+\beta}^{(n)}\end{pmatrix}=\Phi_n, \tag{5.16}$$

where Φ_n consists of $H_\beta^{(i)}$ and $H_{\alpha+\beta}^{(i)}$ for $-1\leqslant i<n$ and $H_\alpha^{(i)}$ and $H_{\alpha+2\beta}^{(i)}$ for $-1\leqslant i\leqslant n$. Since $H_\alpha^{(-1)}\neq 0$, we see by induction that $H_\beta^{(n)}$ and $H_{\alpha+\beta}^{(n)}$ for $n\geqslant 2$ are determined by $H_\beta^{(-1)}$, $H_\beta^{(0)}$, $H_\beta^{(1)}$, $H_{\alpha+\beta}^{(0)}$, $H_{\alpha+\beta}^{(1)}$, and $H_\alpha^{(i)}$ and $H_{\alpha+2\beta}^{(i)}$ for $i\geqslant -1$. The $l=m=0$ case of (5.15) yields

$$H_\alpha^{(0)}(H_\beta^{(0)}-H_{\alpha+\beta}^{(0)})+H_\alpha^{(-1)}(H_\beta^{(1)}+H_{\alpha+\beta}^{(1)})+2H_\beta^{(-1)}(H_\alpha^{(1)}+H_{\alpha+2\beta}^{(1)})=H_{\alpha+2\beta}^{(0)}(H_\beta^{(0)}+H_{\alpha+\beta}^{(0)}) \tag{5.17}$$

and shows that $H_{\alpha+\beta}^{(1)}$ and thus H_β and $H_{\alpha+\beta}$ are determined by $H_\beta^{(-1)}$, $H_\beta^{(0)}$, $H_\beta^{(1)}$ and $H_{\alpha+\beta}^{(0)}$.□

By Lemma 5.6, we see that $H_\beta^{(-1)}$, $H_\beta^{(0)}$, $H_{\alpha+\beta}^{(0)}$ and $H_\beta^{(1)}$ may be taken arbitrarily as long as the series converges.

Now we return to the whole system (5.1).

Theorem 5.7: *Let*

$$H_\alpha(u)=a\sigma_{0,0}(b\,u,\lambda;\tau)e^{pu},\quad H_{\alpha+2\beta}(u)=a\sigma_{0,0}(b\,u,\mu;\tau)e^{qu}, \tag{5.18a}$$

$$G_\alpha(u)=G_{\alpha+2\beta}(u)=a\sigma_{0,0}(b\,u,\nu;\tau)\phi(u), \tag{5.18b}$$

where $a,b,\lambda,\mu,\nu,p,q\in\mathbb{C}$ *such that* $a,b\neq 0$, $\lambda,\mu,\nu,-\lambda+\mu,\lambda+\mu\notin\mathbb{Z}+\mathbb{Z}\tau$ *and* $\phi\in\mathcal{M}_0$ *satisfies* $\phi(u)\phi(-u)=1$. *Then the following functions exhaust all the nontrivial solutions of the equations (5.1):*

$$H_\beta(u)=\sum_{m,n=0}^{1}a_{m,n}\sigma_{m/2,n/2}(b\,u,-\lambda+\mu;\tau)e^{(-p+q)u},$$

$$H_{\alpha+\beta}(u)=\sum_{m,n=0}^{1}a_{m,n}\sigma_{m/2,n/2}(b\,u,\lambda+\mu;\tau)e^{(p+q)u}, \tag{5.19a}$$

$$G_\beta(u)=G_{\alpha+\beta}(u)=\sum_{m,n=0}^{1}a_{m,n}\sigma_{m/2,n/2}(b\,u,\eta;\tau)\psi(u), \tag{5.19b}$$

where $\eta,a_{m,n}\in\mathbb{C}$ *for* $0\leqslant m,\ n\leqslant 1$ *are arbitrary such that* $\eta\notin\mathbb{Z}+\mathbb{Z}\tau$ *and* $\psi\in\mathcal{M}_0$ *satisfies* $\psi(u)\psi(-u)=1$.

Proof: We know that the equation (5.1b) has at most four free parameters. It is known that for arbitrary $a_{m,n}\in\mathbb{C}$, (5.19a) satisfies the equation (5.1b).[7]

By a direct calculation we have

$$A\begin{pmatrix}a_{0,0}\\ a_{1/2,0}\\ a_{1/2,1/2}\\ a_{0,1/2}\end{pmatrix}=\begin{pmatrix}H_\beta^{(-1)}\\ H_\beta^{(0)}\\ H_{\alpha+\beta}^{(0)}\\ H_\beta^{(1)}\end{pmatrix}, \tag{5.20}$$

where A is a matrix whose determinant is $f(\lambda+\mu,-\lambda+\mu)$ and

$$\begin{aligned}f(x,y)=&-\frac{\theta_1'^{\,3}(0)}{\theta_0(0)\theta_2(0)\theta_3(0)\theta_1(x)\theta_1(y)^2}(-\theta_3(x)\theta_2(y)\theta_0'(y)+\theta_2(x)\theta_3(y)\theta_0'(y)\\&+\theta_3(x)\theta_0(y)\theta_2'(y)-\theta_0(x)\theta_3(y)\theta_2'(y)-\theta_2(x)\theta_0(y)\theta_3'(y)+\theta_0(x)\theta_2(y)\theta_3'(y))\end{aligned} \tag{5.21}$$

$$=\frac{\theta_1((x-y)/2)^2\theta_1((x+y)/2)^2}{\theta_1(x)}g(y), \tag{5.22}$$

with $g(y)$ a meromorphic function which has simple poles at $\mathbb{Z}+\mathbb{Z}\tau$ and no zeros. By the assumption $\lambda,\mu\notin\mathbb{Z}+\mathbb{Z}\tau$, we see that the determinant is always nonzero and A is invertible. □

Remark 5.8: In Theorem 5.7, the $\lambda+\mu\in\mathbb{Z}+\mathbb{Z}\tau$ or $-\lambda+\mu\in\mathbb{Z}+\mathbb{Z}\tau$ case is not investigated.

D. Exceptional solutions

As mentioned before, the general solution of (5.1) is not known. But we found another solution experimentally.

Theorem 5.9: *The following is a solution of the equations (5.1):*

$$\begin{aligned}
H_\alpha(u)&=a\sigma_{0,0}(cu,\lambda;\tau)e^{pu}+b\sigma_{0,0}(cu,2\lambda;2\tau)e^{pu},\\
H_{\alpha+2\beta}(u)&=a\sigma_{0,0}(cu,\mu;\tau)e^{qu}+b\sigma_{0,0}(cu,2\mu;2\tau)e^{qu},\\
H_\beta(u)&=a'\sigma_{0,0}(cu,-\lambda+\mu;\tau)e^{(-p+q)u}+b'\sigma_{0,0}(2cu,-\lambda+\mu;2\tau)e^{(-p+q)u},\\
H_{\alpha+\beta}(u)&=a'\sigma_{0,0}(cu,\lambda+\mu;\tau)e^{(p+q)u}+b'\sigma_{0,0}(2cu,\lambda+\mu;2\tau)e^{(p+q)u},
\end{aligned}\tag{5.23a}$$

$$\begin{aligned}
G_\alpha(u)&=G_{\alpha+2\beta}(u)=a\sigma_{0,0}(cu,\nu;\tau)\phi(u)+b\sigma_{0,0}(cu,2\nu;2\tau)\phi(u),\\
G_\beta(u)&=G_{\alpha+\beta}(u)=a'\sigma_{0,0}(cu,\eta;\tau)\varphi(u)+b'\sigma_{0,0}(2cu,\eta;2\tau)\varphi(u),
\end{aligned}\tag{5.23b}$$

where $a,b,c,a',b',\lambda,\mu,\nu,\eta,p,q$ *are arbitrary complex numbers, and* $\phi,\varphi\in\mathcal{M}_0$ *satisfy* $\phi(u)\phi(-u)=\varphi(u)\varphi(-u)=1$.

Proof: This follows from the linearity of the equation (5.1b), Lemma 5.2 and the following identity. □

Lemma 5.10:

$$\begin{pmatrix}\sigma_{0,0}(2u,\mu;\tau)\\ \sigma_{0,0}(u,\mu;\tau/2)\\ \sigma_{0,0}(2u,2\mu;2\tau)\\ \sigma_{0,0}(u,2\mu;\tau)\end{pmatrix}=\begin{pmatrix}\frac12&\frac12&\frac12&\frac12\\ 0&1&0&1\\ 0&0&\frac12&\frac12\\ 0&0&0&1\end{pmatrix}\begin{pmatrix}\sigma_{1/2,1/2}(u,2\mu;\tau)\\ \sigma_{0,1/2}(u,2\mu;\tau)\\ \sigma_{1/2,0}(u,2\mu;\tau)\\ \sigma_{0,0}(u,2\mu;\tau)\end{pmatrix}.\tag{5.24}$$

Remark 5.11: We can choose a,b,a',b' so that $H_\gamma\in\mathcal{H}_0$. Such a solution indicates that in the B_2 case, holomorphy does not simplify solutions as in the A_2 case. See Theorem 4.3. The solution in Theorem 5.9 corresponds to the system studied in Refs. 8 and 9.

VI. G_2 CASE

In this section, we study the solution related to the G_2 system. The functional equations are much more complicated than the A_2 or the B_2 case and we have not completed the investigation of general solutions.

A. Functional equations

In the following, we make an assumption called extensibility:[4]

$$R_\alpha\ R_{2\alpha+3\beta}\ R_{\alpha+3\beta}=R_{\alpha+3\beta}\ R_{2\alpha+3\beta}\ R_\alpha.\tag{6.1}$$

Then we have the following equivalent condition to (3.4):

Theorem 6.1: *The operators* R_γ *satisfy (3.4) if and only if* G_γ *and* H_γ *satisfy, up to an overall factor, the following equations:*

$$G_{\alpha+\beta}(u)=G_{\alpha+2\beta}(u)=G_\beta(u),\tag{6.2a}$$

$$H_\alpha(u)H_\beta(u+v)-H_\alpha(-2u-3v)H_{\alpha+\beta}(u+v)-H_\beta(v)H_{\alpha+3\beta}(u)-H_{\alpha+2\beta}(-v)H_{\alpha+3\beta}(u+3v)$$
$$-H_{\alpha+2\beta}(u+2v)H_{2\alpha+3\beta}(-u-3v)-H_{\alpha+\beta}(-u-2v)H_{2\alpha+3\beta}(2u+3v)=0, \tag{6.2b}$$

$$G_\beta(u)G_\beta(-u)-G_\beta(v)G_\beta(-v)=H_\beta(u)H_\beta(-u)-H_\beta(v)H_\beta(-v), \tag{6.2c}$$

$$G_\alpha(-u)G_\alpha(u)H_{\alpha+\beta}(u+v)H_{\alpha+2\beta}(v)+G_\alpha(-2u-3v)G_\alpha(2u+3v)H_\beta(-u-v)H_{\alpha+2\beta}(u+2v)$$
$$-G_\alpha(-2u-3v)G_\alpha(2u+3v)H_\beta(v)H_{\alpha+\beta}(u+2v)+G_\beta(-u-v)G_\beta(u+v)$$
$$\times H_{\alpha+3\beta}(-u)H_{2\alpha+3\beta}(2u+3v)+G_\beta(-v)G_\beta(v)H_\alpha(u)H_{2\alpha+3\beta}(u+3v)$$
$$-G_\beta(-v)G_\beta(v)H_\alpha(2u+3v)H_{\alpha+3\beta}(u+3v)+H_\alpha(u)H_{\alpha+\beta}(v)H_{\alpha+2\beta}(u+v)H_{\alpha+3\beta}(-u)$$
$$+H_\alpha(u)H_{\alpha+\beta}(v)H_{\alpha+2\beta}(v)H_{2\alpha+3\beta}(u)+H_\alpha(u)H_{\alpha+\beta}(v)H_\beta(-u-v)H_{\alpha+3\beta}(2u+3v)$$
$$-H_\alpha(2u+3v)H_\beta(v)H_{\alpha+\beta}(-u-v)H_{2\alpha+3\beta}(2u+3v)-H_\alpha(2u+3v)H_\beta(v)H_{\alpha+2\beta}(u+v)$$
$$\times H_{2\alpha+3\beta}(-u)-H_\alpha(2u+3v)H_\beta(v)H_{\alpha+2\beta}(v)H_{\alpha+3\beta}(u)+H_{\alpha+\beta}(u+v)H_{\alpha+2\beta}(u+v)$$
$$\times H_{\alpha+3\beta}(-u)H_{2\alpha+3\beta}(-u)+H_\beta(-u-v)H_{\alpha+\beta}(u+v)H_{\alpha+3\beta}(2u+3v)H_{2\alpha+3\beta}(-u)$$
$$+H_\beta(-u-v)H_{\alpha+2\beta}(-u-v)H_{\alpha+3\beta}(2u+3v)H_{2\alpha+3\beta}(2u+3v)=0, \tag{6.2d}$$

$$G_\alpha(-u)G_\alpha(u)H_\beta(u+v)H_{\alpha+\beta}(u+v)H_{\alpha+2\beta}(v)-G_\alpha(-u)G_\alpha(u)H_\beta(v)H_{\alpha+\beta}(v)H_{\alpha+2\beta}(u+v)$$
$$-G_\alpha(-u-3v)G_\alpha(u+3v)G_\beta(-v)G_\beta(v)H_{\alpha+2\beta}(u+2v)+G_\alpha(-2u-3v)G_\alpha(2u+3v)$$
$$\times G_\beta(-u-v)G_\beta(u+v)H_{\alpha+2\beta}(u+2v)+G_\beta(-u-v)G_\beta(u+v)$$
$$\times H_\alpha(u)H_{\alpha+\beta}(v)H_{\alpha+3\beta}(2u+3v)-G_\beta(-u-v)G_\beta(u+v)H_\alpha(-u)H_\beta(v)$$
$$\times H_{2\alpha+3\beta}(2u+3v)+G_\beta(-u-v)G_\beta(u+v)H_{\alpha+\beta}(u+v)H_{\alpha+3\beta}(2u+3v)H_{2\alpha+3\beta}(-u)$$
$$+G_\beta(-u-v)G_\beta(u+v)H_{\alpha+2\beta}(-u-v)H_{\alpha+3\beta}(2u+3v)H_{2\alpha+3\beta}(2u+3v)+G_\beta(-u-v)$$
$$\times G_\beta(u+v)H_\beta(u+v)H_{\alpha+3\beta}(-u)H_{2\alpha+3\beta}(2u+3v)+G_\beta(-v)G_\beta(v)H_\alpha(u)H_\beta(u+v)$$
$$\times H_{2\alpha+3\beta}(u+3v)-G_\beta(-v)G_\beta(v)H_\alpha(-u)H_{\alpha+\beta}(u+v)H_{\alpha+3\beta}(u+3v)-G_\beta(-v)$$
$$\times G_\beta(v)H_{\alpha+\beta}(v)H_{\alpha+3\beta}(u+3v)H_{2\alpha+3\beta}(u)-G_\beta(-v)G_\beta(v)H_{\alpha+2\beta}(-v)$$
$$\times H_{\alpha+3\beta}(u+3v)H_{2\alpha+3\beta}(u+3v)-G_\beta(-v)G_\beta(v)H_\beta(v)H_{\alpha+3\beta}(u)H_{2\alpha+3\beta}(u+3v)$$
$$+H_\alpha(u)H_\beta(u+v)H_{\alpha+\beta}(v)H_{\alpha+2\beta}(u+v)H_{\alpha+3\beta}(-u)+H_\alpha(u)H_\beta(u+v)$$
$$\times H_{\alpha+\beta}(v)H_{\alpha+2\beta}(v)H_{2\alpha+3\beta}(u)-H_\alpha(-u)H_\beta(v)H_{\alpha+\beta}(u+v)H_{\alpha+2\beta}(u+v)H_{2\alpha+3\beta}(-u)$$
$$-H_\alpha(-u)H_\beta(v)H_{\alpha+\beta}(u+v)H_{\alpha+2\beta}(v)H_{\alpha+3\beta}(u)+H_\beta(u+v)H_{\alpha+\beta}(u+v)H_{\alpha+2\beta}(u+v)$$
$$\times H_{\alpha+3\beta}(-u)H_{2\alpha+3\beta}(-u)-H_\beta(v)H_{\alpha+\beta}(v)H_{\alpha+2\beta}(v)H_{\alpha+3\beta}(u)H_{2\alpha+3\beta}(u)=0, \tag{6.2e}$$

$$G_\alpha(-u)G_\alpha(u)G_\beta(-u-v)G_\beta(u+v)H_{2\alpha+3\beta}(2u+3v)+G_\alpha(-u)$$
$$\times G_\alpha(u)H_\alpha(u)H_{\alpha+\beta}(v)H_{\alpha+2\beta}(u+v)-G_\alpha(-u)G_\alpha(u)H_\alpha(u+3v)H_\beta(v)$$
$$\times H_{\alpha+2\beta}(u+v)+G_\alpha(-u)G_\alpha(u)H_{\alpha+\beta}(u+v)H_{\alpha+2\beta}(u+v)H_{2\alpha+3\beta}(-u)$$
$$+G_\alpha(-u)G_\alpha(u)H_{\alpha+\beta}(u+v)H_{\alpha+2\beta}(v)H_{\alpha+3\beta}(u)+G_\alpha(-u)G_\alpha(u)H_\beta(-v)H_{\alpha+\beta}(u+v)$$
$$\times H_{\alpha+3\beta}(u+3v)-G_\alpha(-u-3v)G_\alpha(u+3v)G_\beta(-u-2v)G_\beta(u+2v)H_{2\alpha+3\beta}(2u+3v)$$
$$+G_\alpha(-u-3v)G_\alpha(u+3v)H_\alpha(u)H_\beta(-v)H_{\alpha+2\beta}(u+2v)-G_\alpha(-u-3v)G_\alpha(u+3v)$$
$$\times H_\alpha(u+3v)H_{\alpha+\beta}(-v)H_{\alpha+2\beta}(u+2v)-G_\alpha(-u-3v)G_\alpha(u+3v)H_{\alpha+\beta}(u+2v)$$

$$
\begin{aligned}
&\times H_{\alpha+2\beta}(u+2v)H_{2\alpha+3\beta}(-u-3v)-G_{\alpha}(-u-3v)G_{\alpha}(u+3v)H_{\alpha+\beta}(u+2v)\\
&\times H_{\alpha+2\beta}(-v)H_{\alpha+3\beta}(u+3v)-G_{\alpha}(-u-3v)G_{\alpha}(u+3v)H_{\beta}(v)H_{\alpha+\beta}(u+2v)H_{\alpha+3\beta}(u)\\
&+G_{\beta}(-v)G_{\beta}(v)H_{\alpha}(u)H_{\alpha+3\beta}(u)H_{2\alpha+3\beta}(u+3v)-G_{\beta}(-v)G_{\beta}(v)H_{\alpha}(u+3v)\\
&\times H_{\alpha+3\beta}(u+3v)H_{2\alpha+3\beta}(u)+H_{\alpha}(u)H_{\alpha+\beta}(v)H_{\alpha+2\beta}(v)H_{\alpha+3\beta}(u)H_{2\alpha+3\beta}(u)\\
&-H_{\alpha}(u+3v)H_{\alpha+\beta}(-v)H_{\alpha+2\beta}(-v)H_{\alpha+3\beta}(u+3v)H_{2\alpha+3\beta}(u+3v)\\
&+H_{\alpha}(u)H_{\beta}(-v)H_{\alpha+\beta}(v)H_{\alpha+3\beta}(u+3v)H_{2\alpha+3\beta}(u)+H_{\alpha}(u)H_{\beta}(-v)H_{\alpha+2\beta}(-v)\\
&\times H_{\alpha+3\beta}(u+3v)H_{2\alpha+3\beta}(u+3v)-H_{\alpha}(u+3v)H_{\beta}(v)H_{\alpha+2\beta}(v)H_{\alpha+3\beta}(u)H_{2\alpha+3\beta}(u)\\
&-H_{\alpha}(u+3v)H_{\beta}(v)H_{\alpha+\beta}(-v)H_{\alpha+3\beta}(u)H_{2\alpha+3\beta}(u+3v)=0. \qquad (6.2f)
\end{aligned}
$$

We omit the proof, since it is straightforward but lengthy. We remark that the equations (6.2a)–(6.2c) are comparable to the equation (4.1) or (5.1), while the others do not seem to be simplified.

B. Solutions associated with holomorphic solutions

We assume that H_{α}, $H_{2\alpha+3\beta}$ and $H_{\alpha+3\beta}$ are given by Theorem 4.3.

Lemma 6.2: Let

$$
H_{\alpha}(u)=\frac{1}{\lambda}e^{pu},\quad H_{2\alpha+3\beta}(u)=\left(\frac{1}{\lambda+\mu}\right)e^{(p+q)u},\quad H_{\alpha+3\beta}(u)=\frac{1}{\mu}e^{qu}, \qquad (6.3)
$$

where $\lambda,\mu,\lambda+\mu\neq 0$. *Then the solution of (6.2b) is*

$$
\begin{aligned}
H_{\beta}(u)&=e^{(-p+q)u}(a+\varphi(u)),\\
H_{\alpha+2\beta}(u)&=e^{(p+2q)u}(b-\varphi(-u)),\\
H_{\alpha+\beta}(u)&=e^{(2p+q)u}(c+\varphi(u)),
\end{aligned} \qquad (6.4)
$$

where $\varphi\in\mathcal{M}_0$ *and* $a,b,c\in\mathbb{C}$ *are such that*

$$
a(\lambda+\mu)(\lambda-\mu)+b\lambda(\lambda+2\mu)+c\mu(2\lambda+\mu)=0. \qquad (6.5)
$$

Proof: We assume that $\lambda\neq\mu$. By substituting (6.3) and $H_{\beta}(u)=f(u)e^{(-p+q)u}$, $H_{\alpha+\beta}(u)=g(u)e^{(2p+q)u}$ and $H_{\alpha+2\beta}(u)=h(u)e^{(p+2q)u}$ into the equation (6.2b), we obtain

$$
\begin{aligned}
&\lambda(\lambda+\mu)f(v)-\mu(\lambda+\mu)f(u+v)+\mu(\lambda+\mu)g(u+v)\\
&\quad+\lambda(\lambda+\mu)h(-v)+\lambda\mu(g(-u-2v)+h(u+2v))=0,
\end{aligned} \qquad (6.6)
$$

and thus by setting $u=0$,

$$
f(v)=\frac{\lambda\mu g(-2v)+\mu(\lambda+\mu)g(v)+\lambda(\lambda+\mu)h(-v)+\lambda\mu h(2v)}{-\lambda^2+\mu^2}. \qquad (6.7)
$$

Substituting this and $g(v)=c+\varphi(v)$ and $h(v)=a(v)-\varphi(-v)$ into (6.6), we have the following equations for $a(v)$ by setting $u=0$ after the differentiation by u, and $u=-3v$:

$$
(a(-v)+a(2v))'=0, \qquad (6.8)
$$

$$
a(-4v)-2a(-v)+a(2v)=0. \qquad (6.9)
$$

The first equation is solved as

$$a(-v)+a(2v)=2b, \tag{6.10}$$

where $b\in\mathbb{C}$ is an arbitrary constant, and consequently the second as $a(v)=b$. Hence by (6.7), we see that f, g and h should be of the form

$$f(u)=-\frac{c\mu(2\lambda+\mu)+b\lambda(\lambda+2\mu)}{\lambda^2-\mu^2}+\varphi(v), \tag{6.11}$$

$$g(u)=c+\varphi(u), \tag{6.12}$$

$$h(u)=b-\varphi(-u) \tag{6.13}$$

for some $\varphi\in\mathcal{M}_0$. Substituting these functions into (6.6), we can check that they are really a solution of (6.2b) for any $\varphi\in\mathcal{M}_0$. If $\lambda=\mu$, then by exchanging the roles of f and g, the statement follows. □

Theorem 6.3: *Let*

$$H_\alpha(u)=\frac{1}{\lambda}e^{pu},\quad H_{2\alpha+3\beta}(u)=\left(\frac{1}{\lambda+\mu}\right)e^{(p+q)u},\quad H_{\alpha+3\beta}(u)=\frac{1}{\mu}e^{qu}, \tag{6.14a}$$

$$G_\alpha(u)=G_{2\alpha+3\beta}(u)=G_{\alpha+3\beta}(u)=\frac{1}{\nu}\phi(u), \tag{6.14b}$$

where $\lambda,\mu,\nu,\lambda+\mu,2\lambda+\mu,\mu+2\lambda\neq 0$ *and* $\phi\in\mathcal{M}_0$ *satisfies* $\phi(u)\phi(-u)=1$. *Then the following functions exhaust all the nontrivial solutions of the equations (6.2) if* $a\neq -b$:

$$\begin{aligned} H_\beta(u)&=e^{(-p+q)u}(a+\varphi(u)),\\ H_{\alpha+2\beta}(u)&=e^{(p+2q)u}(b-\varphi(-u)), \end{aligned} \tag{6.15a}$$

$$\begin{aligned} H_{\alpha+\beta}(u)&=e^{(2p+q)u}(c+\varphi(u)),\\ G_\beta(u)=G_{\alpha+2\beta}(u)&=G_{\alpha+\beta}(u)=\psi(u)(\kappa+\varphi(u)), \end{aligned} \tag{6.15b}$$

where $a,b,c,\kappa\in\mathbb{C}$ *and*

$$\varphi(u)=\eta/u,\quad \eta\in\mathbb{C}, \tag{6.16a}$$

$$\begin{aligned} &-a(\lambda-\mu)=b(\lambda+2\mu)=c(2\lambda+\mu)\quad \textit{or}\\ &-a(2\nu^2-\lambda\mu-\mu^2)=b(2\nu^2+\lambda\mu),\quad a(2\nu^2-\lambda^2-\lambda\mu)=c(2\nu^2+\lambda\mu), \end{aligned} \tag{6.16b}$$

or

$$\varphi(u)=d\coth(du/\eta),\quad \eta\in\mathbb{C}\backslash\{0\}, \tag{6.17a}$$

$$a(\lambda+\mu)(\lambda-\mu)+b\lambda(\lambda+2\mu)+c\mu(2\lambda+\mu)=0, \tag{6.17b}$$

$$d^2=\frac{ab(\lambda^2+\lambda\mu-2\nu^2)}{\lambda(\lambda+\mu)}-\frac{ac\lambda(\lambda\mu+\mu^2-2\nu^2)}{\mu(\lambda+\mu)}+\frac{bc(\lambda+\mu)(\lambda\mu+2\nu^2)}{\lambda\mu}, \tag{6.17c}$$

and $\psi\in\mathcal{M}_0$ *satisfies* $\psi(u)\psi(-u)=1$.

Proof: Substituting (6.4) with (6.5) into the equation (6.2f), we have

$$(a+b)(\varphi(-u)+\varphi(u)-\varphi(-u-v)-\varphi(u+v))=0, \tag{6.18}$$

where we have used $\lambda,\lambda+2\mu,2\lambda+\mu\neq 0$ and the equation (6.2c). By the proof of Lemma 6.2, we assume without loss of generality that $\varphi(u)$ has no constant term in the Laurent expansion at the origin.

Since we assume $a\neq -b$, then $\varphi(u)$ is an odd function. By the equation (6.2d), we have

$$\varphi(u)\varphi(v)-\varphi(v)\varphi(u+v)-\varphi(u)\varphi(u+v)=d^2, \tag{6.19}$$

where

$$d^2=\frac{ab(\lambda^2+\lambda\mu-2\nu^2)}{\lambda(\lambda+\mu)}-\frac{ac\lambda(\lambda\mu+\mu^2-2\nu^2)}{\mu(\lambda+\mu)}+\frac{bc(\lambda+\mu)(\lambda\mu+2\nu^2)}{\lambda\mu}. \tag{6.20}$$

If $\varphi\in\mathcal{H}_0$, then $\varphi(0)=0$ and thus $\varphi(v)=d=0$ by (6.19). In this case, we have (6.16b) by using (6.5). If $\varphi\in\mathcal{M}_0$ with a pole at the origin, then it should be simple. Replacing $\varphi(u)$ by $1/f(u)$, we have

$$f(u+v)-f(u)-f(v)=d^2f(u)f(v)f(u+v). \tag{6.21}$$

Dividing both sides by u and letting $u\to 0$, we obtain

$$f'(v)-f'(0)=d^2f'(0)f(v)^2. \tag{6.22}$$

This Riccati-type ordinary differential equation has a unique solution:

$$\begin{gathered} f(u)=\tanh(du/\eta)/d, \quad \text{if } d\neq 0, \\ f(u)=u/\eta, \quad \text{if } d=0, \end{gathered} \tag{6.23}$$

for an arbitrary constant $\eta\neq 0$, and it is checked that $\varphi(u)=d\coth(du/\eta)$ or $\varphi(u)=\eta/u$ is actually a solution of (6.19). □

Remark 6.4: If $a=-b$, then by (6.5) we have $b=c$ and the following functional equation is necessary and sufficient for $\gamma(u)=\varphi(u)-b$:

$$\gamma(u-v)\gamma(-v)+\gamma(u)\gamma(v)+\gamma(-u)\gamma(-u+v)=0, \tag{6.24}$$

which is not completely solved yet. However, (6.16a) or (6.17a) is a solution of (6.24).

C. Solutions associated with meromorphic solutions

Similarly to the B_2-type system, the equation (6.2b) has linearity of the solutions for fixed H_α, $H_{2\alpha+3\beta}$ and $H_{\alpha+3\beta}$. Moreover, we can show the following lemma. Set $H_\gamma(u)=\Sigma_{i\geqslant p}H_\gamma^{(i)}u^i$.

Lemma 6.5: *In the equation (6.2b), if one of H_β, $H_{\alpha+2\beta}$ or $H_{\alpha+\beta}$ has a pole at the origin, then all have a simple pole at the origin and $H_\beta^{(-1)}=H_{\alpha+2\beta}^{(-1)}=H_{\alpha+\beta}^{(-1)}$. H_β, $H_{\alpha+\beta}$ and $H_{\alpha+2\beta}$ are determined by $H_\beta^{(-1)}$, $H_\beta^{(0)}$, $H_{\alpha+2\beta}^{(0)}$, $H_{\alpha+\beta}^{(0)}$, $H_\beta^{(1)}$, $H_{\alpha+2\beta}^{(1)}$, $H_\beta^{(2)}$, $H_\beta^{(3)}$ and $H_{\alpha+2\beta}^{(3)}$.*

Theorem 6.6: *Let*

$$\begin{gathered} H_\alpha(u)=a\sigma_{0,0}(bu,\lambda;\tau)e^{pu}, \\ H_{2\alpha+3\beta}(u)=a\sigma_{0,0}(bu,\lambda+\mu;\tau)e^{(p+q)u}, \\ H_{\alpha+3\beta}(u)=a\sigma_{0,0}(bu,\mu;\tau)e^{qu}, \end{gathered} \tag{6.25}$$

where $a,b,\lambda,\mu,p,q\in\mathbb{C}$ *are arbitrary such that* $a,b\neq 0$, $\lambda,\mu,\lambda+\mu,\lambda-\mu,\lambda+2\mu,2\lambda+\mu\notin\mathbb{Z}+\mathbb{Z}\tau$. *Then the following functions are solutions of the equation (6.2b):*

$$\begin{aligned}
H_\beta(u)&=\sum_{m,n=0}^{2} a_{m,n}\sigma_{m/3,n/3}(b\,u,-\lambda+\mu;\tau)e^{(-p+q)u},\\
H_{\alpha+2\beta}(u)&=-\sum_{m,n=0}^{2} a_{m,n}\sigma_{m/3,n/3}(-b\,u,-\lambda-2\mu;\tau)e^{(p+2q)u},\\
H_{\alpha+\beta}(u)&=\sum_{m,n=0}^{2} a_{m,n}\sigma_{m/3,n/3}(b\,u,2\lambda+\mu;\tau)e^{(2p+q)u},
\end{aligned}\tag{6.26}$$

where $a_{m,n}\in\mathbb{C}$ *are arbitrary*.

Remark 6.7: Although the solution in Theorem 6.6 has nine parameters, it is not known whether or not they exhaust all the nontrivial solutions since the same process as in Theorem 5.7 is too complicated to execute.

Theorem 6.8: *Under the same condition as in Theorem 6.6, the following functions are solutions of the equations (6.2):*

$$\begin{aligned}
H_\beta(u)&=\sum_{m,n=0}^{2} a_{m,n}\sigma_{m/3,n/3}(b\,u,-\lambda+\mu;\tau)e^{(-p+q)u},\\
H_{\alpha+2\beta}(u)&=-\sum_{m,n=0}^{2} a_{m,n}\sigma_{m/3,n/3}(-b\,u,-\lambda-2\mu;\tau)e^{(p+2q)u},\\
H_{\alpha+\beta}(u)&=\sum_{m,n=0}^{2} a_{m,n}\sigma_{m/3,n/3}(b\,u,2\lambda+\mu;\tau)e^{(2p+q)u},
\end{aligned}\tag{6.27a}$$

$$G_\beta(u)=G_{\alpha+2\beta}(u)=G_{\alpha+\beta}(u)=\sum_{m,n=0}^{2} a_{m,n}\sigma_{m/3,n/3}(b\,u,\eta;\tau)\psi(u),\tag{6.27b}$$

where $\eta\in\mathbb{C}$ *is arbitrary,* $\psi\in\mathcal{M}_0$ *satisfies* $\psi(u)\psi(-u)=1$, *and* $\{a_{m,n}\in\mathbb{C}\}$ *is one of the following:*

	$a_{0,0}$	$a_{0,1}$	$a_{0,2}$	$a_{1,0}$	$a_{1,1}$	$a_{1,2}$	$a_{2,0}$	$a_{2,1}$	$a_{2,2}$
I	1	0	0	0	0	0	0	0	0
II	1	1	1	c	c	c	c^2	c^2	c^2
	1	c	c^2	1	c	c^2	1	c	c^2
	1	c	c^2	c^2	1	c	c	c^2	1
	1	c	c^2	c	c^2	1	c^2	1	c
III	1	c	c^2	0	0	0	0	0	0
IV	1	0	0	c	0	0	c^2	0	0
V	1	0	0	0	c	0	0	0	c^2
VI	1	0	0	0	0	c	0	c^2	0

(6.28)

where c *is one of cubic roots of unity*.

This is checked by comparing the poles and periodicity for the equations (6.2c)–(6.2f).

Remark 6.9: There are 22 solutions and the function $\Sigma_{m,n=0}^{2} a_{m,n}\sigma_{m/3,n/3}(u,3\mu;\tau)$ is simplified up to constant factor as follows except V and VI:

				(6.29)
I		$\sigma_{0,0}(3\mu,u;\tau)$		
II	$\sigma_{0,0}(\mu,3u;\tau)$	$\sigma_{1/3,0}(\mu,3u;\tau)$	$\sigma_{2/3,0}(\mu,3u;\tau)$	
	$\sigma_{0,1/3}(\mu,3u;\tau)$	$\sigma_{1/3,1/3}(\mu,3u;\tau)$	$\sigma_{2/3,1/3}(\mu,3u;\tau)$	
	$\sigma_{0,2/3}(\mu,3u;\tau)$	$\sigma_{1/3,2/3}(\mu,3u;\tau)$	$\sigma_{2/3,2/3}(\mu,3u;\tau)$	
III	$\sigma_{0,0}(\mu,u;\tau/3)$	$\sigma_{1/3,0}(\mu,u;\tau/3)$	$\sigma_{2/3,0}(\mu,u;\tau/3)$	
IV	$\sigma_{0,0}(3\mu,3u;3\tau)$	$\sigma_{0,1/3}(3\mu,3u;3\tau)$	$\sigma_{0,2/3}(3\mu,3u;3\tau)$	

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Lie algebroid structures on a class of affine bundles

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We introduce the notion of a Lie algebroid structure on an affine bundle whose base manifold is fibered over $\mathbb{R}$. It is argued that this is the framework which one needs for coming to a time-dependent generalization of the theory of Lagrangian systems on Lie algebroids. An extensive discussion is given of a way one can think of forms acting on sections of the affine bundle. It is further shown that the affine Lie algebroid structure gives rise to a coboundary operator on such forms. The concept of admissible curves and dynamical systems whose integral curves are admissible brings an associated affine bundle into the picture, on which one can define in a natural way a prolongation of the original affine Lie algebroid structure. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1510958]

I. INTRODUCTION

There has been a lot of interest recently in the study of dynamical systems which have a Lie algebroid as carrying space (see, e.g., Refs. 1–6). A Lie algebroid is a vector bundle $\pi: V \to M$, which comes equipped with two operators. To begin with, there is a bracket operation on $Sec(\pi)$, the set of sections of π, which provides it with a real Lie algebra structure. Second, there is a linear bundle map $\rho: V \to TM$, called the anchor map, which establishes a Lie algebra homomorphism between $Sec(\pi)$ and the real Lie algebra of vector fields on M and does this in such a way that there is a certain compatibility also with the module structure over $C^\infty(M)$. To be precise, we have

$$[\rho(\sigma),\rho(\eta)]=\rho([\sigma,\eta]) \quad \text{and} \quad n[\sigma,f\eta]=f[\sigma,\eta]+\rho(\sigma)(f)\eta,$$

for all $\sigma,\eta \in Sec(\pi)$ and $f \in C^\infty(M)$.

Weinstein's paper on Lagrangian mechanics and groupoids[6] roused new interest into the field of algebroids and groupoids. Weinstein introduces "Lagrangian systems" on a Lie algebroid by means of a Legendre-type map from V to V^*, associated to a given function L on V. The local coordinate expression of such equations reads

$$\begin{aligned} \dot{x}^i &= \rho^i_\alpha(x)y^\alpha, \\ \frac{d}{dt}\left(\frac{\partial L}{\partial y^\alpha}\right) &= \rho^i_\alpha \frac{\partial L}{\partial x^i} - C^\gamma_{\alpha\beta} y^\beta \frac{\partial L}{\partial y^\gamma}, \end{aligned} \tag{1}$$

where the x^i are coordinates on M, y^α are fiber coordinates on V and the $C^\gamma_{\alpha\beta}$ are structure functions coming from the Lie algebroid structure. Applications for such model equations can be found, e.g., in the theory of systems with symmetries on principal fiber bundles and in rigid body dynamics. Note that, more generally, equations of the form

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$$\dot{x}^i=\rho^i_\alpha(x)y^\alpha,$$
$$\dot{y}^\alpha=f^\alpha(x,y), \tag{2}$$

were called ''second-order equations on a Lie algebroid'' by Weinstein. They are indeed, to some extent, the analogs of second-order dynamics on a tangent bundle. It is clear, however, that these equations truly are second-order differential equations only when the base manifold and the fibers have the same dimension and ρ is injective. We will therefore rather call them ''pseudo-second-order ordinary differential equations,'' pseudo-SODEs for short. Weinstein also raised the question whether there would be a geometrical way of defining equations of the form (1), much in the line of the geometrical construction of classical Lagrange equations, which makes use of the intrinsic structures living on a tangent bundle.

One of us has recently resolved this issue[5] by introducing a kind of lifted Lie algebroid, where suitable analogs can be introduced of the dilation vector field and the vertical endomorphism on a tangent bundle.

In the present article, we wish to set the stage for an appropriate generalization of this theory to nonautonomous systems of differential equations. We believe that, for example, at the level of pseudo-second-order equations, the right generalization is not just a matter of allowing the functions ρ^i_α and f^α to depend on time, but rather should produce equations of the form

$$\dot{x}^i=\rho^i_\alpha(t,x)y^\alpha+\lambda^i(t,x),$$
$$\dot{y}^\alpha=f^\alpha(t,x,y). \tag{3}$$

The reason for this simply is that we wish the structure of the equations to be invariant under time-dependent coordinate transformations. As for Lagrange-type equations, our only concern at the moment is to have an idea of what a time-dependent generalization of (1) should look like. Now, there is a way of developing a kind of formal calculus of variations approach which leads to equations of the form (1), and in which the first set of equations are treated as constraints. We have shown in Ref. 7 that if such an approach is adopted when the Lagrangian is allowed to depend on time and the constraints are as in (3), one obtains equations of the form

$$\dot{x}^i=\rho^i_\alpha(t,x)y^\alpha+\lambda^i(t,x),$$
$$\frac{d}{dt}\left(\frac{\partial L}{\partial y^\alpha}\right)=\rho^i_\alpha\frac{\partial L}{\partial x^i}-(C^\gamma_{\alpha\beta}y^\beta-C^\gamma_\alpha)\frac{\partial L}{\partial y^\gamma}, \tag{4}$$

where the functions ρ^i_α, λ^i, $C^\gamma_{\alpha\beta}$, C^γ_α satisfy the relations

$$\rho^i_\alpha\frac{\partial\rho^j_\beta}{\partial x^i}-\rho^i_\beta\frac{\partial\rho^j_\alpha}{\partial x^i}=\rho^j_\gamma C^\gamma_{\alpha\beta}, \tag{5}$$

$$\frac{\partial\rho^j_\beta}{\partial t}+\lambda^i\frac{\partial\rho^j_\beta}{\partial x^i}-\rho^i_\beta\frac{\partial\lambda^j}{\partial x^i}=\rho^j_\alpha C^\alpha_\beta. \tag{6}$$

Thus, we want to address the question of explaining the nature of the conditions (5) and (6), which presumably should again have something to do with a Lie algebroid structure.

Inspired by these analytical considerations, we will introduce the notion of a Lie algebroid structure on an affine bundle $\pi:E\to M$, where the base manifold M in addition is assumed to be fibered over $\mathbb{R}$. The assumption about the additional fibration of M is a very natural one to start the development of this new theory, because the canonical example of an affine Lie algebroid (when the anchor map reduces to the identity) should be the model of time-dependent mechanics, which traditionally is described on the first-jet bundle of a manifold fibered over $\mathbb{R}$ (see, e.g., Ref. 8). For

the present paper, we will limit ourselves to a number of basic features of such a theory. In particular, we shall show in Sec. III that our defining relations for an affine Lie algebroid are fully consistent with the expectation of being able to develop an exterior differential calculus of sections of the extended dual of this bundle (and its exterior products). We shall further show in Sec. IV that vector fields on E, whose integral curves are "admissible curves" and which in fact model differential equations of the pseudo-SODE type, can be identified in a natural way with special sections of a kind of prolongation of the original affine bundle. This then brings us to a final test, for this article, of the internal coherence of the newly defined structures: we will verify in Sec. V whether the prolongation of a Lie algebroid, as constructed in Ref. 5 for the vector bundle situation, carries over to the present more general situation.

The final section lists a number of other topics of interest, which will be the subject of forthcoming publications. One of our objectives is to arrive at an intrinsic geometrical construction of the time-dependent Lagrangian equations of type (4). For the time being, however, the conditions (5) and (6) merely serve as benchmarks, to be met by our model of an affine Lie algebroid.

The basic ingredients for our theory are an affine bundle $\pi:E\to M$, where the base manifold M is further fibered over $\mathbb{R}$. In Sec. II, we define the concept of a Lie algebroid on π. In Sec. III, we show that the axioms for such a Lie algebroid structure give rise to a consistent development of an exterior calculus on sections of the extended dual of E. In Sec. IV, we discuss a special class of curves on E, which are said to be admissible by the anchor map, and we look into the concept of dynamical systems whose integral curves all belong to this special class. In Sec. V, we define the prolongation $\pi_1:J^1_\lambda E\to E$ of $\pi:E\to M$ and show that it inherits the Lie algebroid structure from π.

II. AFFINE LIE ALGEBROIDS

Let M be an $(n+1)$-dimensional smooth manifold, which is fibered over $\mathbb{R}$, $\tau:M\to\mathbb{R}$. We denote the first jet bundle of τ by $\tau_1^0:J^1M\to M$. It is an affine bundle modeled on the bundle of tangent vectors to M which are vertical with respect to τ; this vector bundle will be denoted by $\overline{\tau}_1^0:VM\to M$. To fix notations further, if $\pi:E\to M$ is an affine bundle and $\overline{\pi}:V\to M$ its associated vector bundle, sections of π will be denoted by ordinary Greek characters, whereas boldface Greek type will be used for sections of $\overline{\pi}$.

Definition 1: An affine Lie algebroid over M is an affine bundle $\pi:E\to M$, with the following properties:

(1) $Sec(\overline{\pi})$, the set of sections of the vector bundle $\overline{\pi}:V\to M$ on which E is modeled, is equipped with a skew-symmetric and bilinear (over $\mathbb{R}$) bracket $[\cdot,\cdot]$.

(2) The affine space $Sec(\pi)$ acts by derivations on the real algebra $Sec(\overline{\pi})$, that is to say, if the same bracket notation $[\zeta,\boldsymbol{\sigma}]$ is used to denote the way $\zeta\in Sec(\pi)$ acts on $\boldsymbol{\sigma}\in Sec(\overline{\pi})$, we have $[\zeta,\boldsymbol{\sigma}]\in Sec(\overline{\pi})$ and

$$[\zeta,\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2]=[\zeta,\boldsymbol{\sigma}_1]+[\zeta,\boldsymbol{\sigma}_2],\quad [\zeta+\boldsymbol{\sigma},\boldsymbol{\eta}]=[\zeta,\boldsymbol{\eta}]+[\boldsymbol{\sigma},\boldsymbol{\eta}], \tag{7}$$

$$[\zeta,[\boldsymbol{\sigma},\boldsymbol{\eta}]]=[[\zeta,\boldsymbol{\sigma}],\boldsymbol{\eta}]+[\boldsymbol{\sigma},[\zeta,\boldsymbol{\eta}]]. \tag{8}$$

(3) There exists an affine bundle map $\lambda:E\to J^1M$ (over the identity on M), with corresponding vector bundle homomorphism $\rho:V\to VM$, such that the following compatibility condition holds for all $f\in C^\infty(M)$,

$$[\zeta,f\boldsymbol{\sigma}]=f[\zeta,\boldsymbol{\sigma}]+\lambda(\zeta)(f)\boldsymbol{\sigma}. \tag{9}$$

Both the affine map $\lambda:E\to J^1M$ and its linear part $\rho:V\to VM$ will be called anchor maps.

Note that we make no notational distinction between, on the one hand, the affine and linear anchor maps, regarded as maps between total spaces of bundles, and their action on sections of bundles on the other hand. Needless to say, for the interpretation of the bracket in the left-hand side of (12), both $\lambda(\zeta)$ and $\rho(\boldsymbol{\sigma})$ are regarded as vector fields on M.

Let us derive some further properties which follow from this definition. First of all, if we replace ζ in (8) by $\zeta+\boldsymbol{\xi}$, for an arbitrary $\boldsymbol{\xi}\in Sec(\overline{\pi})$, it follows that $\forall\,\boldsymbol{\xi},\boldsymbol{\sigma},\boldsymbol{\eta}\in Sec(\overline{\pi})$:

$$[\boldsymbol{\xi},[\boldsymbol{\sigma},\boldsymbol{\eta}]]=[[\boldsymbol{\xi},\boldsymbol{\sigma}],\boldsymbol{\eta}]+[\boldsymbol{\sigma},[\boldsymbol{\xi},\boldsymbol{\eta}]]. \tag{10}$$

This means, in view of the first hypothesis, that the bracket on $Sec(\overline{\pi})$ actually provides $Sec(\overline{\pi})$ with a real Lie algebra structure. Second, making the same substitution for ζ in (9), recalling that $\lambda(\zeta+\boldsymbol{\xi})=\lambda(\zeta)+\rho(\boldsymbol{\xi})$, it follows that

$$[\boldsymbol{\xi},f\boldsymbol{\sigma}]=f[\boldsymbol{\xi},\boldsymbol{\sigma}]+\rho(\boldsymbol{\xi})(f)\boldsymbol{\sigma}. \tag{11}$$

This means that the linear anchor map $\rho:V\to VM$ defines a Lie algebra homomorphism from $Sec(\overline{\pi})$ into the real Lie algebra of vertical vector fields on M, and that we have a classical Lie algebroid structure on the vector bundle $\overline{\pi}:V\to M$ (although its image cannot reach the whole of TM). Third, replacing $\boldsymbol{\eta}$ by $f\boldsymbol{\eta}$ in (8) and making use of (9) and (11), one obtains the additional compatibility property

$$[\lambda(\zeta),\rho(\boldsymbol{\sigma})]=\rho([\zeta,\boldsymbol{\sigma}]), \tag{12}$$

from which it further follows that

$$[\rho(\boldsymbol{\xi}),\rho(\boldsymbol{\sigma})]=\rho([\boldsymbol{\xi},\boldsymbol{\sigma}]). \tag{13}$$

Remark: For an alternative and equivalent definition of an affine Lie algebroid, we could impose first the Lie algebra structure (10) of the bracket on $Sec(\overline{\pi})$, together with the compatibility condition (11) for the anchor map ρ, and subsequently require that the properties (7)–(9) hold true for at least one $\zeta\in Sec(\pi)$ and for an affine map $\lambda:E\to J^1M$ whose linear part is ρ. It then follows that such properties hold for all ζ.

We can now further extend the bracket operation to $Sec(\pi)$, as follows.

Definition 2: (i) *For* $\boldsymbol{\sigma}\in Sec(\overline{\pi})$ *and* $\zeta\in Sec(\pi)$, *we put* $[\boldsymbol{\sigma},\zeta]=-[\zeta,\boldsymbol{\sigma}]$. (ii) *For every two sections* $\zeta_1,\zeta_2\in Sec(\pi)$ *with* $\boldsymbol{\zeta}_{12}=\zeta_2-\zeta_1$, $[\zeta_1,\zeta_2]=[\zeta_1,\boldsymbol{\zeta}_{12}]$.

Observe that the extended bracket in (ii) is a map from $Sec(\pi)\times Sec(\pi)$ to $Sec(\overline{\pi})$. As we will show below, it has Lie algebra-type properties, which could justify talking about an ''affine Lie algebra structure,'' were it not that this term is in use already in the literature, with an entirely different meaning. The extended bracket also has Lie algebroid type properties with respect to the anchor maps λ and ρ.

Proposition 1: The bracket $[\,\cdot\,,\cdot\,]:Sec(\pi)\times Sec(\pi)\to Sec(\overline{\pi})$, *has the following properties:*

$$[\zeta_1,\zeta_2+\boldsymbol{\sigma}]=[\zeta_1,\zeta_2]+[\zeta_1,\boldsymbol{\sigma}], \tag{14}$$

$$[\zeta_1,\zeta_2]=-[\zeta_2,\zeta_1], \tag{15}$$

$$[[\zeta_1,\zeta_2],\zeta_3]+[[\zeta_2,\zeta_3],\zeta_1]+[[\zeta_3,\zeta_1],\zeta_2]=\mathbf{0}, \tag{16}$$

$$\rho([\zeta_1,\zeta_2])=[\lambda(\zeta_1),\lambda(\zeta_2)]. \tag{17}$$

Proof: The first property follows immediately from the definition and (7). Next, we have $[\zeta_2,\zeta_1]=[\zeta_2,\boldsymbol{\zeta}_{21}]=-[\zeta_1+\boldsymbol{\zeta}_{12},\boldsymbol{\zeta}_{12}]=-[\zeta_1,\zeta_2]$. For the Jacobi identity, using a simple summation sign to indicate the cyclic sum over the three sections in each summand, we have

$$\sum\,[[\zeta_1,\zeta_2],\zeta_3]=\sum\,[[\zeta_1,\zeta_2],\zeta_2+\boldsymbol{\zeta}_{23}]=\sum\,[[\zeta_1,\zeta_2],\boldsymbol{\zeta}_{23}],$$

in view of the linearity properties and the skew-symmetry of the bracket. Substituting subsequently $\zeta_1+\boldsymbol{\zeta}_{12}$ for ζ_2, we obtain

$$\sum [[\zeta_1,\zeta_2],\zeta_3]=\sum [[\zeta_1,\boldsymbol{\zeta}_{12}],\boldsymbol{\zeta}_{23}],$$

which is zero in view of (8). Finally, the compatibility property (17) easily follows in the same way from the definition of the extended bracket and (12). □

To understand what an affine Lie algebroid structure means in coordinates, let us coordinatize E in the usual way, as follows: t denotes the coordinate on $\mathbb{R}$; $(x^i)_{1\leqslant i\leqslant n}$ are fiber coordinates on M; we further choose a local section e_0 of π to play the role of zero section and a local basis $(\mathbf{e}_\alpha)_{1\leqslant\alpha\leqslant k}$ for $Sec(\overline{\pi})$. Then, if e is a point in the fiber E_m over $m\in M$, it can be written in the form: $e=e_0(m)+y^\alpha\mathbf{e}_\alpha(m)$; (t,x^i,y^α) are coordinates of e $[(t,x^i)$ being the coordinates of $m]$.

We have

$$[\mathbf{e}_\alpha,\mathbf{e}_\beta]=C^\gamma_{\alpha\beta}(t,x)\mathbf{e}_\gamma,\quad [e_0,\mathbf{e}_\alpha]=C^\beta_\alpha(t,x)\mathbf{e}_\beta, \tag{18}$$

for some *structure functions* $C^\gamma_{\alpha\beta}=-C^\gamma_{\beta\alpha}$ and C^β_α on M. The affine map λ and its linear part ρ are fully determined by

$$\lambda(e_0)=\frac{\partial}{\partial t}+\lambda^i(t,x)\frac{\partial}{\partial x^i},\quad \rho(\mathbf{e}_\alpha)=\rho^i_\alpha(t,x)\frac{\partial}{\partial x^i}. \tag{19}$$

The further characterization of the Lie algebroid structure now has the following coordinate translation. The derivation property (8) and the resulting Jacobi identity (10) mean that we have

$$\frac{\partial C^\mu_{\alpha\beta}}{\partial t}+\lambda^i\frac{\partial C^\mu_{\alpha\beta}}{\partial x^i}+C^\gamma_{\alpha\beta}C^\mu_\gamma=C^\mu_{\alpha\gamma}C^\gamma_\beta-C^\mu_{\beta\gamma}C^\gamma_\alpha+\rho^i_\alpha\frac{\partial C^\mu_\beta}{\partial x^i}-\rho^i_\beta\frac{\partial C^\mu_\alpha}{\partial x^i}, \tag{20}$$

$$\sum_{\alpha,\beta,\gamma}\left(\rho^i_\alpha\frac{\partial C^\mu_{\beta\gamma}}{\partial x^i}+C^\mu_{\alpha\nu}C^\nu_{\beta\gamma}\right)=0, \tag{21}$$

where the summation this time refers to a cyclic sum over α, β, γ and also the compatibility conditions (9) and (11) have been invoked. Finally, the properties (12) and (13), for which it is sufficient to express that $[\lambda(e_0),\rho(\mathbf{e}_\alpha)]=\rho([e_0,\mathbf{e}_\alpha])$ and $[\rho(\mathbf{e}_\alpha),\rho(\mathbf{e}_\beta)]=\rho([\mathbf{e}_\alpha,\mathbf{e}_\beta])$, require that

$$\frac{\partial\rho^j_\beta}{\partial t}+\lambda^i\frac{\partial\rho^j_\beta}{\partial x^i}-\rho^i_\beta\frac{\partial\lambda^j}{\partial x^i}=C^\alpha_\beta\rho^j_\alpha, \tag{22}$$

$$\rho^i_\alpha\frac{\partial\rho^j_\beta}{\partial x^i}-\rho^i_\beta\frac{\partial\rho^j_\alpha}{\partial x^i}=C^\gamma_{\alpha\beta}\rho^j_\gamma. \tag{23}$$

These are precisely the relations (5) and (6) we encountered in the Introduction, in the context of Lagrangian equations of type (4).

It is of some interest to look at the way the various structure and anchor map functions transform under coordinate transformations. There are two distinct levels in making a change of coordinates on E, which we will describe separately. First, we could choose a different (local) zero section $\overline{e_0}$ and a different local basis $\overline{\mathbf{e}}_\beta$ for $Sec(\overline{\pi})$: say that $\mathbf{e}_\alpha=A^\beta_\alpha\overline{\mathbf{e}}_\beta$ and $e_0=\overline{e_0}+B^\alpha\overline{\mathbf{e}}_\alpha$. This amounts to making an affine change of coordinates in the fibers of the form $\overline{y^\alpha}=A^\alpha_\beta(t,x)y^\beta+B^\alpha(t,x)$. Putting $[\overline{\mathbf{e}}_\alpha,\overline{\mathbf{e}}_\beta]=\overline{C}^\gamma_{\alpha\beta}\overline{\mathbf{e}}_\gamma$, $[\overline{e_0},\overline{\mathbf{e}}_\alpha]=\overline{C}^\beta_\alpha\overline{\mathbf{e}}_\beta$, and also $\lambda(\overline{e_0})=\partial/\partial t+\overline{\lambda^i}\,\partial/\partial x^i$, $\rho(\overline{\mathbf{e}}_\alpha)=\overline{\rho}^j_\alpha\partial/\partial x^j$, one can verify that the following transformation rules apply:

$$\rho^i_\alpha=A^\beta_\alpha\overline{\rho}^i_\beta,\quad \overline{\lambda^i}=\lambda^i-B^\alpha\overline{\rho}^i_\alpha,$$

and further

$$C^{\gamma}_{\alpha\beta}A^{\mu}_{\gamma}=\overline{C}^{\mu}_{\gamma\nu}A^{\gamma}_{\alpha}A^{\nu}_{\beta}+\rho^{i}_{\alpha}\frac{\partial A^{\mu}_{\beta}}{\partial x^{i}}-\rho^{i}_{\beta}\frac{\partial A^{\mu}_{\alpha}}{\partial x^{i}},$$

$$C^{\gamma}_{\beta}A^{\alpha}_{\gamma}=\overline{C}^{\alpha}_{\mu}A^{\mu}_{\beta}+\overline{C}^{\alpha}_{\gamma\mu}B^{\gamma}A^{\mu}_{\beta}+\frac{\partial A^{\alpha}_{\beta}}{\partial t}+\lambda^{i}\frac{\partial A^{\alpha}_{\beta}}{\partial x^{i}}-\rho^{i}_{\beta}\frac{\partial B^{\alpha}}{\partial x^{i}}.$$

At a different level, one can make a change of coordinates on M, of the form: $t'=t$, $x'^{i}=x'^{i}(t,x)$. This has an effect on the anchor map functions of the form

$$\rho'^{j}_{\alpha}=\rho^{i}_{\alpha}\frac{\partial x'^{j}}{\partial x^{i}},\quad \lambda'^{j}=\frac{\partial x'^{j}}{\partial t}+\lambda^{i}\frac{\partial x'^{j}}{\partial x^{i}}.$$

A general change of adapted coordinates is of course a composition of the two steps described above.

III. EXTERIOR CALCULUS ON AN AFFINE LIE ALGEBROID

We first recall some features of the by now standard theory of Lie algebroids on a vector bundle (see Ref. 9). Considering sections of exterior powers of the dual bundle, one gets a notion of forms on sections of the vector bundle, on which an exterior derivative can be defined which involves the Lie algebroid bracket and the anchor map. It then turns out that the Jacobi identity of the Lie algebroid bracket and the compatibility with the bracket of vector fields via the anchor map are exactly the conditions for this exterior derivative to have the co-boundary property $d^2=0$ (see also Refs. 10, 11, and 5). In our opinion, such a feature in itself gives a strong indication that the generalization from Lie algebra to Lie algebroid is indeed a meaningful step. We shall therefore investigate in this section whether a similar support can be detected for our extension to Lie algebroids on affine bundles.

The extended dual of the affine space E_m is the space of real valued affine functions on E_m and will be denoted by $E^{\dagger}_m$. The union of these spaces over all points $m\in M$ gives us a bundle $\pi^{\dagger}:E^{\dagger}\to M$ say. Although this is in fact a vector bundle, we are interested in the action of its sections (and sections of its exterior powers) on sections of the affine bundle π. This brings some subtleties into the picture which need to be investigated in sufficient detail. We will write $\overline{\pi}^{*}:V^{*}\to M$ for the dual bundle of $\overline{\pi}$ and also use boldface type for its sections (and the sections of its exterior powers). Now, to begin with, if θ is a section of $\pi^{\dagger}$ and $\zeta\in Sec(\pi)$, $\theta(\zeta)$ is a function on M defined by $\theta(\zeta)(m)=\theta_m(\zeta_m)$. θ_m being an affine function on E_m, there exists an associated element $\boldsymbol{\theta}_m\in V^{*}_m$ such that $\forall e_m\in E_m$, $\boldsymbol{\sigma}_m\in V_m$, we have $\theta_m(e_m+\boldsymbol{\sigma}_m)=\theta_m(e_m)+\boldsymbol{\theta}_m(\boldsymbol{\sigma}_m)$. Expressed in slightly different terms and now at the level of sections again, a $\theta\in Sec(\pi^{\dagger})$ is such that there exist a $\theta_0\in Sec(\pi^{\dagger})$ and a $\boldsymbol{\theta}\in Sec(\overline{\pi}^{*})$, such that for all $\zeta\in Sec(\pi)$,

$$\theta(\zeta)=\theta_0(\zeta_0)+\boldsymbol{\theta}(\boldsymbol{\zeta}), \tag{24}$$

where ζ_0 is any section and then $\zeta=\zeta_0+\boldsymbol{\zeta}$. The two composing elements θ_0 (which, in fact, is simply θ itself here) and $\boldsymbol{\theta}$ do not depend on the choice of ζ_0. With sections of $\pi^{\dagger}$ as our notion of one-forms on $Sec(\pi)$, there is of course no linearity with respect to multiplication by functions on M. We can now come in a similar way to the following concept of k-forms on $Sec(\pi)$ [thereby taking for granted that the meaning of a k-form on a vector bundle such as $Sec(\overline{\pi})$ is known].

Definition 3: A k-form on the affine bundle $Sec(\pi)$ $(k\geqslant 1)$ is a map $\omega:Sec(\pi)\times\cdots\times Sec(\pi)\to C^{\infty}(M)$, for which there exists a k-form $\boldsymbol{\omega}$ on the associated vector bundle $Sec(\overline{\pi})$ and a map $\omega_0:Sec(\pi)\times Sec(\overline{\pi})\times\cdots\times Sec(\overline{\pi})\to C^{\infty}(M)$ with the following properties:

(1) ω_0 is skew-symmetric and $C^{\infty}(M)$-linear in its $k-1$ vector arguments;

(2) $\forall\zeta\in Sec(\pi)$ and $\forall\boldsymbol{\sigma},\boldsymbol{\zeta}_j\in Sec(\overline{\pi})$, we have

$$\omega_0(\zeta+\boldsymbol{\sigma},\boldsymbol{\zeta}_1,\ldots,\boldsymbol{\zeta}_{k-1})=\omega_0(\zeta,\boldsymbol{\zeta}_1,\ldots,\boldsymbol{\zeta}_{k-1})+\boldsymbol{\omega}(\boldsymbol{\sigma},\boldsymbol{\zeta}_1,\ldots,\boldsymbol{\zeta}_{k-1}); \tag{25}$$

(3) $\forall \zeta_i \in Sec(\pi)$, *if we choose an arbitrary* $\zeta_0 \in Sec(\pi)$ *and put* $\zeta_i = \zeta_0 + \boldsymbol{\zeta}_i$, *we have*

$$\omega(\zeta_1,\ldots,\zeta_k) = \sum_{i=1}^{k} (-1)^{i-1}\omega_0(\zeta_0,\boldsymbol{\zeta}_1,\ldots,\hat{\boldsymbol{\zeta}}_i,\ldots,\boldsymbol{\zeta}_k) + \boldsymbol{\omega}(\boldsymbol{\zeta}_1,\ldots,\boldsymbol{\zeta}_k). \tag{26}$$

There are a number of properties to be checked to make sure that this definition makes sense. First of all, one can verify that with two different choices of a reference section, ζ_0 and ζ_0', for example, related through $\zeta_0 = \zeta_0' + \boldsymbol{\sigma}$, it follows from the second requirement that

$$\sum_{i=1}^{k} (-1)^{i-1}\omega_0(\zeta_0,\boldsymbol{\zeta}_1,\ldots,\hat{\boldsymbol{\zeta}}_i,\ldots,\boldsymbol{\zeta}_k) + \boldsymbol{\omega}(\boldsymbol{\zeta}_1,\ldots,\boldsymbol{\zeta}_k)$$

$$= \sum_{i=1}^{k} (-1)^{i-1}\omega_0(\zeta_0',\boldsymbol{\zeta}_1',\ldots,\hat{\boldsymbol{\zeta}}_i',\ldots,\boldsymbol{\zeta}_k') + \boldsymbol{\omega}(\boldsymbol{\zeta}_1',\ldots,\boldsymbol{\zeta}_k').$$

Second, the two elements ω_0 and $\boldsymbol{\omega}$ which make up ω are unique. Indeed, assuming there would be a second couple ω_0' and $\boldsymbol{\omega}'$ making up the same ω, it follows by choosing $\zeta_0 = \zeta_1$ (such that $\boldsymbol{\zeta}_1 = 0$) that $\omega_0 = \omega_0'$, after which it is clear that also $\boldsymbol{\omega} = \boldsymbol{\omega}'$. Note finally that the definition implies that ω itself is skew-symmetric in all its arguments.

The set of forms on $Sec(\pi)$, which we will denote by $\Lambda(\pi^\dagger)$, is a module over the ring $C^\infty(M)$, which also constitutes the set of zero-forms. The wedge product of two forms is defined in the usual way. By way of example, if α and β are one-forms, we have

$$(\alpha\wedge\beta)(\zeta_1,\zeta_2) = \alpha(\zeta_1)\beta(\zeta_2) - \alpha(\zeta_2)\beta(\zeta_1),$$

which for every choice of a reference section ζ_0 gives rise to

$$(\alpha\wedge\beta)(\zeta_1,\zeta_2) = \alpha(\zeta_0)\boldsymbol{\beta}(\boldsymbol{\zeta}_2 - \boldsymbol{\zeta}_1) - \beta(\zeta_0)\boldsymbol{\alpha}(\boldsymbol{\zeta}_2 - \boldsymbol{\zeta}_1) + (\boldsymbol{\alpha}\wedge\boldsymbol{\beta})(\boldsymbol{\zeta}_1,\boldsymbol{\zeta}_2). \tag{27}$$

It follows that $\boldsymbol{\alpha}\wedge\boldsymbol{\beta}$ is the two-form on $Sec(\overline{\pi})$ corresponding to $\alpha\wedge\beta$, and

$$(\alpha\wedge\beta)_0(\zeta,\boldsymbol{\sigma}) = \alpha(\zeta)\boldsymbol{\beta}(\boldsymbol{\sigma}) - \beta(\zeta)\boldsymbol{\alpha}(\boldsymbol{\sigma}). \tag{28}$$

Similarly, for the wedge product of three one-forms, we have

$$(\alpha\wedge\beta\wedge\gamma)_0(\zeta,\boldsymbol{\zeta}_1,\boldsymbol{\zeta}_2) = (\alpha(\zeta)(\boldsymbol{\beta}\wedge\boldsymbol{\gamma}) + \beta(\zeta)(\boldsymbol{\gamma}\wedge\boldsymbol{\alpha}) + \gamma(\zeta)(\boldsymbol{\alpha}\wedge\boldsymbol{\beta}))(\boldsymbol{\zeta}_1,\boldsymbol{\zeta}_2). \tag{29}$$

These examples suggest to formalize the representation of k-forms a bit further. As a preliminary remark, it may sometimes be of interest to extend the interpretation of the operator ω_0 in such a way that its single affine section argument need not necessarily be the first. This can simply be achieved by declaring ω_0 to be skew-symmetric in all its arguments [but still $C^\infty(M)$-linear in its vector arguments only]. More importantly, we shall take the sum of ω_0-terms in (26) to define another operator, denoted by ω^0, as follows:

$$\omega^0(\zeta_1,\ldots,\zeta_k) = \sum_{i=1}^{k} (-1)^{i-1}\omega_0(\zeta_0,\boldsymbol{\zeta}_1,\ldots,\hat{\boldsymbol{\zeta}}_i,\ldots,\boldsymbol{\zeta}_k) = \sum_{i=1}^{k} \omega_0(\boldsymbol{\zeta}_1,\ldots,\check{\underset{i}{\zeta}}_0,\ldots,\boldsymbol{\zeta}_k), \tag{30}$$

where the second expression takes the above remark into account and the symbol $\check{\zeta}_{0_i}$then indicates that ζ_0 has been inserted in the ith argument. The other important new convention we will adopt is to regard $\boldsymbol{\omega}$ also as acting on affine sections:

$$\boldsymbol{\omega}(\zeta_1,\ldots,\zeta_k) = \boldsymbol{\omega}(\boldsymbol{\zeta}_1,\ldots,\boldsymbol{\zeta}_k). \tag{31}$$

This way, we can formally write

$$\omega = \omega^0 + \boldsymbol{\omega}, \tag{32}$$

whereby it is to be understood that the two composing terms ω^0 and $\boldsymbol{\omega}$ are not k-forms on $Sec(\pi)$ by themselves. In fact, to compute their value when acting on k sections ζ_i, a reference section ζ_0 has to be chosen, but as argued above, the value of the sum $\omega^0 + \boldsymbol{\omega}$ in the end does not depend on that choice.

The rather formal looking decomposition (32) now greatly facilitates the representation of wedge products and will make the general coordinate representation of a form more transparent. For example, the result (29) means that

$$(\alpha \wedge \beta \wedge \gamma)_0 = \alpha^0 \otimes (\boldsymbol{\beta} \wedge \boldsymbol{\gamma}) + \beta^0 \otimes (\boldsymbol{\gamma} \wedge \boldsymbol{\alpha}) + \gamma^0 \otimes (\boldsymbol{\alpha} \wedge \boldsymbol{\beta}), \tag{33}$$

which then implies from (30) that

$$(\alpha \wedge \beta \wedge \gamma)^0 = \alpha^0 \wedge \boldsymbol{\beta} \wedge \boldsymbol{\gamma} + \boldsymbol{\alpha} \wedge \beta^0 \wedge \boldsymbol{\gamma} + \boldsymbol{\alpha} \wedge \boldsymbol{\beta} \wedge \gamma^0, \tag{34}$$

as expected. More generally, it follows directly from the defining formula for wedge products that for $\omega = \omega^0 + \boldsymbol{\omega}$ and $\rho = \rho^0 + \boldsymbol{\rho}$,

$$\omega \wedge \rho = \omega^0 \wedge \rho^0 + \omega^0 \wedge \boldsymbol{\rho} + \boldsymbol{\omega} \wedge \rho^0 + \boldsymbol{\omega} \wedge \boldsymbol{\rho}, \tag{35}$$

where the sum of the first three terms is $(\omega \wedge \rho)^0$.

Suppose that, for a coordinatization of E, we have chosen a zero section e_0 and a local basis of vector sections $\mathbf{e}_\alpha$. Denote by $\{\mathbf{e}^\beta\}$ the dual basis for $Sec(\overline{\pi}^*)$. There exists a global section of $\pi^\dagger$ which for each m selects in $E_m^\dagger$ the constant function 1. We will call it e^0. The local zero section e_0 of $Sec(\pi)$ can now play the role of the reference section ζ_0 in our general considerations. Writing $\zeta = e_0 + \zeta^\alpha \mathbf{e}_\alpha$ for an arbitrary section ζ, we have for each one-form θ: $\theta(\zeta) = \theta(e_0) + \zeta^\alpha \boldsymbol{\theta}(\mathbf{e}_\alpha)$. Putting $\boldsymbol{\theta}(\mathbf{e}_\alpha) = \theta_\alpha$ and $\theta(e_0) = \theta_0$, we see that θ has the local representation

$$\theta = \theta_0 e^0 + \theta_\alpha \mathbf{e}^\alpha, \tag{36}$$

where, in agreement with the general decomposition (32), $\mathbf{e}^\alpha$ has to be regarded now as acting on $Sec(\pi)$ and $\theta^0 = \theta_0 e^0$. To be precise, putting

$$e_\alpha = e_0 + \mathbf{e}_\alpha, \tag{37}$$

the action of $\mathbf{e}^\beta$ on affine sections, which can be given a meaning only after introducing a reference section, is determined by

$$\mathbf{e}^\beta(e_0) = 0, \quad \mathbf{e}^\beta(e_\alpha) = \delta_\alpha^\beta. \tag{38}$$

There is another slight abuse of notation in (36) since θ_0 could have a double meaning: in (36) it represents a local function on M, whereas it also could refer to the operator introduced in (24) and more generally in Definition 3. We will, however, seldom use the notation θ_0 in the latter sense when dealing with coordinate calculations, so that the meaning will always be clear from the context.

Let us now see how all these notations fit together when we start wedging one-forms. For two one-forms $\alpha = \alpha^0 + \boldsymbol{\alpha}$ and $\beta = \beta^0 + \boldsymbol{\beta}$ we find, for example from (28) and (30), that

$$(\alpha \wedge \beta)^0 = \alpha^0 \wedge \boldsymbol{\beta} - \beta^0 \wedge \boldsymbol{\alpha}. \tag{39}$$

This is in agreement with the general formula (35) since obviously $\alpha^0 \wedge \beta^0 = 0$. Expressing α and β with respect to the basis $(e^0, \mathbf{e}^\alpha)$, we find

$$\alpha \wedge \beta = (\alpha_0 \beta_\gamma - \beta_0 \alpha_\gamma) e^0 \wedge \mathbf{e}^\gamma + \tfrac{1}{2}(\alpha_\gamma \beta_\delta - \alpha_\delta \beta_\gamma) \mathbf{e}^\gamma \wedge \mathbf{e}^\delta. \tag{40}$$

Similarly, for the wedge product of three one-forms with local representations of the form (36), we obtain

$$\alpha\wedge\beta\wedge\gamma=\tfrac{1}{2}(\alpha_0(\beta_\mu\gamma_\nu-\beta_\nu\gamma_\mu)+\beta_0(\gamma_\mu\alpha_\nu-\gamma_\nu\alpha_\mu)+\gamma_0(\alpha_\mu\beta_\nu-\alpha_\nu\beta_\mu))e^0\wedge\mathbf{e}^\mu\wedge\mathbf{e}^\nu+\boldsymbol{\alpha}\wedge\boldsymbol{\beta}\wedge\boldsymbol{\gamma}. \tag{41}$$

It should now be clear without going into any further detail that a general k-form on $Sec(\pi)$ locally has the following representation,

$$\omega=\frac{1}{(k-1)!}\,\omega_{0\mu_1\cdots\mu_{k-1}}\,e^0\wedge\mathbf{e}^{\mu_1}\wedge\cdots\wedge\mathbf{e}^{\mu_{k-1}}+\frac{1}{k!}\,\omega_{\mu_1\cdots\mu_k}\mathbf{e}^{\mu_1}\wedge\cdots\wedge\mathbf{e}^{\mu_k}, \tag{42}$$

where the coefficients are functions on M, which are skew-symmetric in all their indices (including the zero for the first term); we have

$$\omega_{0\mu_1\cdots\mu_{k-1}}=\omega(e_0,e_{\mu_1},\ldots,e_{\mu_{k-1}}), \tag{43}$$

$$\omega_{\mu_1\cdots\mu_k}=\omega(e_{\mu_1},\ldots,e_{\mu_k})-\sum_{i=1}^{k}\omega_{\mu_1\cdots\overset{\check{}}{0}\cdots\mu_k}, \tag{44}$$

where $\overset{\check{}}{0}$ again means that the index μ_i has been replaced by 0.

Before arriving at our main goal, the development of an exterior calculus on forms, we will recall a few generalities about derivations. Derivations on $\Lambda(\pi^\dagger)$ are defined in the usual way. Following the standard work of Frölicher and Nijenhuis,[12] one easily shows that derivations are local operators and that they are completely determined by their action on functions and one-forms. The commutator of two derivations D_i, of degree r_i say, is again a derivation, of degree r_1+r_2, defined by

$$[D_1,D_2]=D_1\circ D_2-(-1)^{r_1r_2}D_2\circ D_1. \tag{45}$$

Perhaps the simplest type of derivation is contraction with a section.

Definition 4: For $\omega\in\Lambda^k(\pi^\dagger)$ and $\zeta\in Sec(\pi)$, $i_\zeta\omega\in\Lambda^{k-1}(\pi^\dagger)$ is defined by

$$i_\zeta\omega(\zeta_1,\ldots,\zeta_{k-1})=\omega(\zeta,\zeta_1,\ldots,\zeta_{k-1}). \tag{46}$$

The proof that this is a derivation of degree -1 is standard and does not depend on the peculiarities of our present theory. But perhaps we have to convince ourselves in the first place that $i_\zeta\omega$ is indeed a form in the sense of Definition 3.

Proposition 2: $i_\zeta\omega$ is a $(k-1)$-form which, in the sense of the general defining relation (26), is determined by an operator $(i_\zeta\omega)_0$ and a k-form $\mathbf{i}_{\boldsymbol{\zeta}}\boldsymbol{\omega}$ on $Sec(\overline{\pi})$, defined as follows: for all $\boldsymbol{\zeta}_i\in Sec(\overline{\pi})$, $\zeta_0\in Sec(\pi)$,

$$(i_\zeta\omega)_0(\zeta_0,\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_{k-1})=-\omega_0(\zeta_0,\boldsymbol{\zeta},\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_{k-1}),\quad \textit{where}\quad \boldsymbol{\zeta}=\zeta-\zeta_0, \tag{47}$$

$$\mathbf{i}_{\boldsymbol{\zeta}}\boldsymbol{\omega}(\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_k)=\omega_0(\zeta,\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_k). \tag{48}$$

We further have the property (with $\boldsymbol{\zeta}_1=\boldsymbol{\zeta}$)

$$i_\zeta\omega(\zeta_2,\ldots,\zeta_k)=\sum_{i=1}^{k}(-1)^{i-1}(i_\zeta\omega_0)(\boldsymbol{\zeta}_1,\ldots,\hat{\boldsymbol{\zeta}}_i,\ldots,\boldsymbol{\zeta}_k). \tag{49}$$

Proof: A direct computation, using (46) and (26), gives

$$
\begin{aligned}
i_{\zeta}\omega(\zeta_2,\ldots,\zeta_k) &= \omega(\zeta,\zeta_2,\ldots,\zeta_k)\\
&= \omega_0(\zeta_0,\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_k)+\sum_{j=1}^{k-1}(-1)^j\omega_0(\zeta_0,\boldsymbol{\zeta},\boldsymbol{\zeta}_2,\ldots,\hat{\boldsymbol{\zeta}}_j,\ldots,\boldsymbol{\zeta}_k)+\boldsymbol{\omega}(\boldsymbol{\zeta},\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_k)\\
&= \sum_{j=1}^{k-1}(-1)^j\omega_0(\zeta_0,\boldsymbol{\zeta},\boldsymbol{\zeta}_2,\ldots,\hat{\boldsymbol{\zeta}}_j,\ldots,\boldsymbol{\zeta}_k)+\omega_0(\zeta,\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_k),
\end{aligned}
$$

from which we are led to introduce $(i_{\zeta}\omega)_0$ and $\mathbf{i}_{\boldsymbol{\zeta}}\boldsymbol{\omega}$ as in (47) and (48). It is then straightforward to verify that these two operators are linked by a property of type (25), so the first statement follows. Observe that, with an obvious meaning for contraction of the operator ω_0 with ζ, we can write $\mathbf{i}_{\boldsymbol{\zeta}}\boldsymbol{\omega}=i_{\zeta}\omega_0$. The somewhat peculiar feature of the additional property is that $i_{\zeta}\omega$ can be completely computed from $i_{\zeta}\omega_0$. To prove this we again start from (26) to write (with $\zeta_1=\zeta$)

$$
i_{\zeta}\omega(\zeta_2,\ldots,\zeta_k)=\sum_{i=1}^{k}(-1)^{i-1}\omega_0(\zeta_0,\boldsymbol{\zeta}_1,\ldots,\hat{\boldsymbol{\zeta}}_i,\ldots,\boldsymbol{\zeta}_k)+\boldsymbol{\omega}(\boldsymbol{\zeta}_1,\ldots,\boldsymbol{\zeta}_k).
$$

This time, we substitute $\zeta_1-\boldsymbol{\zeta}_1$ for ζ_0 and observe that the second part of the sum involving ω_0, in view of (25), then precisely cancels the last term. □

Maintaining the same line of approach requires that also for the exterior derivative $d\omega$, we identify the associated $(d\omega)_0$ and the form $\mathbf{d}\boldsymbol{\omega}$ on $Sec(\overline{\pi})$ in the sense of Definition 3. Before we can introduce $d\omega$, we need to give a meaning also to the value of a k-form ω, when say its first argument is taken to be a vector section.

Definition 5: If ω is a k-form on $Sec(\pi)$, then for $\boldsymbol{\sigma}\in Sec(\overline{\pi})$ and $\zeta_i\in Sec(\pi)$, we put

$$
\omega(\boldsymbol{\sigma},\zeta_2,\ldots,\zeta_k)=\omega(\zeta_1+\boldsymbol{\sigma},\zeta_2,\ldots,\zeta_k)-\omega(\zeta_1,\zeta_2,\ldots,\zeta_k), \tag{50}
$$

where ζ_1 is chosen arbitrarily.

For this to make sense, of course, we need to be sure that the result does not depend on the choice of ζ_1. Now, if we evaluate the right-hand side of the defining relation by using (26), we obtain

$$
\omega(\boldsymbol{\sigma},\zeta_2,\ldots,\zeta_k)=\boldsymbol{\omega}(\boldsymbol{\sigma},\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_k)+\sum_{i=2}^{k}(-1)^{i-1}\omega_0(\zeta_0,\boldsymbol{\sigma},\boldsymbol{\zeta}_2,\ldots,\hat{\boldsymbol{\zeta}}_i,\ldots,\boldsymbol{\zeta}_k). \tag{51}
$$

The right-hand side of this explicit expression makes no mentioning of ζ_1 anymore. It might seem at first sight that we have shifted the problem, because it does depend on the reference section ζ_0. However, we have argued before that (26) does not depend on the choice of such a reference section, whence our newly defined concept makes sense.

The explicit formula (51) further shows that $i_{\boldsymbol{\sigma}}\omega$ is well defined as a $(k-1)$-form, in the sense of Definition 3. The first term on the right identifies its associated form on $Sec(\overline{\pi})$, whereas the second term, upon swapping the first two arguments, reveals that $(i_{\boldsymbol{\sigma}}\omega)_0=i_{\boldsymbol{\sigma}}\omega_0$. As for local computations, it follows from the definition (50) that $e^0(\boldsymbol{\sigma})=0$, whereas the $\mathbf{e}^{\alpha}$ act on $\boldsymbol{\sigma}$ simply as duals of $Sec(\overline{\pi})$.

Definition 6: The exterior derivative of ω, denoted by $d\omega$ is defined by

$$
\begin{aligned}
d\omega(\zeta_1,\ldots,\zeta_{k+1}) &= \sum_{i=1}^{k+1}(-1)^{i-1}\lambda(\zeta_i)(\omega(\zeta_1,\ldots,\hat{\zeta}_i,\ldots,\zeta_{k+1}))\\
&\quad+\sum_{1\leqslant i<j\leqslant k+1}(-1)^{i+j}\omega([\zeta_i,\zeta_j],\zeta_1,\ldots,\hat{\zeta}_i,\ldots,\widehat{\zeta_j},\ldots,\zeta_{k+1}).
\end{aligned} \tag{52}
$$

Note first that we are making use of Definition 5 in the second term on the right, because the bracket of two affine sections is a vector section. It is fairly obvious that $d\omega$ is skew-symmetric in all its arguments. To further justify this definition in the sense of the defining property (26) of forms, note first that we of course have an exterior derivative at our disposal for the k-form $\boldsymbol{\omega}$ on $Sec(\overline{\pi})$ which we denote by d also. We know that $d\boldsymbol{\omega}$ has a property of type (52) (or can be defined that way), with vector sections replacing affine sections and ρ as anchor map instead of λ. It remains to give a meaning to $d\omega_0$.

Definition 7: For $\omega_0 : Sec(\pi)\times Sec(\overline{\pi})\times\cdots\times Sec(\overline{\pi})\to C^\infty(M)$, *we define* $d\omega_0$, *an operator of the same type, but depending on one more vector section, by*

$$\begin{aligned} d\omega_0(\zeta,\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_{k+1}) &= \lambda(\zeta)(\boldsymbol{\omega}(\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_{k+1})) + \sum_{i=2}^{k+1}(-1)^{i-1}\rho(\boldsymbol{\zeta}_i)(\omega_0(\zeta,\boldsymbol{\zeta}_2,\ldots,\hat{\boldsymbol{\zeta}}_i,\ldots,\boldsymbol{\zeta}_{k+1})) \\ &\quad + \sum_{j=2}^{k+1}(-1)^{j+1}\boldsymbol{\omega}([\zeta,\boldsymbol{\zeta}_j],\boldsymbol{\zeta}_2,\ldots,\hat{\boldsymbol{\zeta}}_j,\ldots,\boldsymbol{\zeta}_{k+1}) \\ &\quad - \sum_{2\leqslant i<j\leqslant k+1}(-1)^{i+j}\omega_0(\zeta,[\boldsymbol{\zeta}_i,\boldsymbol{\zeta}_j],\boldsymbol{\zeta}_2,\ldots,\hat{\boldsymbol{\zeta}}_i,\ldots,\hat{\boldsymbol{\zeta}}_j,\ldots,\boldsymbol{\zeta}_{k+1}). \end{aligned} \tag{53}$$

This expression may look rather exotic at first, but it is obtained by formally copying the definition (52) and writing in that process either λ or ρ, and either ω_0 or $\boldsymbol{\omega}$, in such a way that every term in the right-hand side has a proper meaning. There are two important observations to be made here. First of all, the required linearity of $d\omega_0$ in its vector arguments relies on the properties (9) and (11) of our Lie algebroid bracket. Second, replacing the affine section ζ in the definition by $\zeta+\boldsymbol{\sigma}$, we find

$$d\omega_0(\zeta+\boldsymbol{\sigma},\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_{k+1}) = d\omega_0(\zeta,\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_{k+1}) + d\boldsymbol{\omega}(\boldsymbol{\sigma},\boldsymbol{\zeta}_2,\ldots,\boldsymbol{\zeta}_{k+1}). \tag{54}$$

We now know what to expect for the decomposition (26) of $d\omega$ and this is confirmed by the following result.

Proposition 3: We have $(d\omega)_0 = d\omega_0$ *and* $\mathbf{d}\boldsymbol{\omega} = d\boldsymbol{\omega}$.

The proof involves a rather technical but straightforward calculation and therefore is omitted. It is of some interest, however, to work out some simple cases in detail. For a function $f\in C^\infty(M)$, df is defined by

$$df(\zeta) = \lambda(\zeta)(f) = \lambda(\zeta_0)(f) + \rho(\boldsymbol{\zeta})(f), \tag{55}$$

from which we learn that $(df)_0 = df$ (as expected) and $\mathbf{df}(\boldsymbol{\sigma}) = \rho(\boldsymbol{\sigma})(f)$. If θ is a one-form, the defining relation (52) for its exterior derivative reads

$$d\theta(\zeta_1,\zeta_2) = \lambda(\zeta_1)(\theta(\zeta_2)) - \lambda(\zeta_2)(\theta(\zeta_1)) - \boldsymbol{\theta}([\zeta_1,\zeta_2]). \tag{56}$$

Introducing an arbitrary reference section ζ_0, it is easy to verify that this can be rewritten as

$$d\theta(\zeta_1,\zeta_2) = (d\theta)_0(\zeta_0,\boldsymbol{\zeta}_2) - (d\theta)_0(\zeta_0,\boldsymbol{\zeta}_1) + \mathbf{d}\boldsymbol{\theta}(\boldsymbol{\zeta}_1,\boldsymbol{\zeta}_2), \tag{57}$$

where $\mathbf{d}\boldsymbol{\theta} = d\boldsymbol{\theta}$ and

$$(d\theta)_0(\zeta,\boldsymbol{\sigma}) = \lambda(\zeta)(\boldsymbol{\theta}(\boldsymbol{\sigma})) - \rho(\boldsymbol{\sigma})(\theta(\zeta)) - \boldsymbol{\theta}([\zeta,\boldsymbol{\sigma}]). \tag{58}$$

This is in perfect agreement with the results of Proposition 3 and Definition 7.

Concerning derivation properties, it is trivial to verify that for the product of functions: $d(fg) = fdg + gdf$. Also, from (56) applied to $f\theta$ we get

$$d(f\theta)(\zeta_1,\zeta_2)=\lambda(\zeta_1)(f\theta(\zeta_2))-\lambda(\zeta_2)(f\theta(\zeta_1))-f\theta([\zeta_1,\zeta_2])$$
$$=df(\zeta_1)\theta(\zeta_2)-df(\zeta_2)\theta(\zeta_1)+f(\lambda(\zeta_1)(\theta(\zeta_2))-\lambda(\zeta_2)(\theta(\zeta_1))-\theta([\zeta_1,\zeta_2])),$$

from which we conclude that

$$d(f\theta)=fd\theta+df\wedge\theta, \tag{59}$$

i.e., d has the right derivation property for the action on functions and one-forms. Recalling now the general statements about derivations we made before, we can conclude that there is a unique derivation of degree 1 on $\Lambda(\pi^\dagger)$, which coincides with our d on functions and one-forms. Not surprisingly, this is the d we have introduced by (52), but we again omit the rather technical proof of this claim.

We now reach the main question which is about the relationship between d^2 and the compatibility requirements in the definition of an affine Lie algebroid. To appreciate the meaning of the following lemma, we take a step back and assume now that the bracket $[\zeta_i,\zeta_j]$ figuring in the definition (52) of d satisfies the ''Leibniz-type property'' (9) with respect to the module structure of $Sec(\pi)$ [and the resulting property (11)], but no further compatibility or Lie algebra conditions *a priori*. Remember that the property (9) of the bracket was necessary to make sure that $d\omega$ is a form in the first place.

Lemma 1: For all $\omega\in\Lambda^k(\pi^\dagger)$ *and* $\zeta_i\in Sec(\pi)$, *we have*

$$d^2\omega(\zeta_1,...,\zeta_{k+2})=\sum_{1\leqslant i<j\leqslant k+2}(-1)^{i+j}(\rho([\zeta_i,\zeta_j])-[\lambda(\zeta_i),\lambda(\zeta_j)])(\omega(\zeta_1,...,\hat{\zeta}_i,...,\hat{\zeta}_j,...,\zeta_{k+2}))$$
$$+\sum_{1\leqslant i<j<l\leqslant k+2}(-1)^{i+j+l}\omega\Big(\sum_{i,j,l}[\zeta_i,[\zeta_j,\zeta_l]],\zeta_1,.,\hat{\zeta}_i,.,\hat{\zeta}_j,.,\hat{\zeta}_l,.,\zeta_{k+2}\Big) \tag{60}$$

(where the smaller summation sign of course refers again to a cyclic sum over the three indices involved).

In fact this lemma, with suitable adaptations, also has a rather universal validity, though we were unable to find similar statements in the literature. For this reason, we give a sketch of the proof here.

If ω is a k-form, then $d^2\omega$ is a $(k+2)$-form with

$$d^2\omega(\zeta_1,\ldots,\zeta_{k+2})=\sum_{i=1}^{k+2}(-1)^{i-1}\lambda(\zeta_i)(d\omega(\zeta_1,\ldots,\hat{\zeta}_i,\ldots,\zeta_{k+2}))$$
$$+\sum_{1\leqslant i<j\leqslant k+2}(-1)^{i+j}d\omega([\zeta_i,\zeta_j],\zeta_1,\ldots,\hat{\zeta}_i,\ldots,\hat{\zeta}_j,\ldots,\zeta_{k+2}). \tag{61}$$

If we plug in the definition of $d\omega$, the first term on the right will further decompose into two parts, one involving double and the other involving triple sums. After some elementary multiple sum manipulations, it can be written in the form

$$\sum_{1\leqslant i<j\leqslant k+2}(-1)^{i+j}(\lambda(\zeta_j)\lambda(\zeta_i)-\lambda(\zeta_i)\lambda(\zeta_j))(\omega(\zeta_1,\ldots,\hat{\zeta}_i,\ldots,\hat{\zeta}_j,\ldots,\zeta_{k+2}))$$
$$+\sum_{1\leqslant i<j<l\leqslant k+2}(-1)^{i+j+l-1}\sum_{i,j,l}\{\lambda(\zeta_i)(\omega([\zeta_j,\zeta_l]\},\zeta_1,.,\hat{\zeta}_i,.,\hat{\zeta}_j,.,\hat{\zeta}_l,.,\zeta_{k+2})), \tag{62}$$

where the smaller summation sign stands for a cyclic sum, the range of which is delimited by the curly brackets. For the second term on the right in (61), we have to remember that the first argument is a vector section. Using the defining relation (50), applied to $d\omega$, we obtain

$$d\omega(\boldsymbol{\sigma},\zeta_1,\ldots,\zeta_k)=\rho(\boldsymbol{\sigma})(\omega(\zeta_1,\ldots,\zeta_k))+\sum_{i=1}^{k}(-1)^i\lambda(\zeta_i)(\omega(\boldsymbol{\sigma},\zeta_1,\ldots,\hat{\zeta}_i,\ldots,\zeta_k))$$
$$+\sum_{j=1}^{k}(-1)^j\omega([\boldsymbol{\sigma},\zeta_j],\zeta_1,\ldots,\hat{\zeta}_j,\ldots,\zeta_k)$$
$$+\sum_{1\leqslant i<j\leqslant k}(-1)^{i+j}\omega([\zeta_i,\zeta_j],\boldsymbol{\sigma},\zeta_1,\ldots,\hat{\zeta}_i,\ldots,\hat{\zeta}_j,\ldots,\zeta_k). \tag{63}$$

The last line here has two vector arguments, but this is consistent with the application of Definition 5 to a form of type $i_\zeta\omega$. We look at the effect of each of these four terms, when inserted in the second sum of (61). The first one simply gives

$$\sum_{1\leqslant<i<j\leqslant k+2}(-1)^{i+j}\rho([\zeta_i,\zeta_j])(\omega(\zeta_1,\ldots,\hat{\zeta}_i,\ldots,\hat{\zeta}_j,\ldots,\zeta_{k+2})). \tag{64}$$

The second one is easily seen to give rise to terms which cancel exactly the second sum in (62). The third term of (63) gives rise to expressions involving double brackets, which combine to

$$\sum_{1\leqslant i<j<l\leqslant k+2}(-1)^{i+j+l}\omega\left(\sum_{i,j,l}[[\zeta_i,\zeta_j],\zeta_l],\zeta_1,\ldots,\hat{\zeta}_i,\ldots,\hat{\zeta}_j,\ldots,\hat{\zeta}_l,\ldots,\zeta_{k+2}\right). \tag{65}$$

The fourth term of (63) finally creates terms which involve two double sums, and in each of the summands the first two arguments of ω are brackets. One can show by a suitable reshuffling of summations that all terms in this part cancel out. What we are left with in the end is the first term of (62), (64) and (65): they precisely combine to the statement in the lemma.

Proposition 4: The exterior derivative has the property $d^2=0$ if and only if the bracket further satisfies the Jacobi identity (16) [or equivalently (8)].

Proof: If (9) and (16) hold true, we also have (8) and know from previous considerations that (12) then holds as well. The above lemma this way trivially implies $d^2=0$. For the converse, we observe that $d^2f=0$, for $f\in C^\infty(M)$, implies (17), from which it subsequently follows that $d^2\theta=0$, with $\theta\in\Lambda^1(\pi^\dagger)$, implies (16). □

It remains now to list coordinate expressions for the basic exterior derivatives. Let (t,x^i) as before be coordinates on M. For their exterior derivatives we obtain the following: for all $\zeta\in Sec(\pi)$,

$$dt(\zeta)=\lambda(\zeta)(t)=1,\quad dx^i(\zeta)=\lambda(\zeta)(x^i),$$

from which it follows that $\mathbf{dt}=\mathbf{0}$ and $\mathbf{dx}^i(\boldsymbol{\sigma})=\rho(\boldsymbol{\sigma})(x^i)$ [and of course $(dt)_0=dt$, $(dx^i)_0=dx^i$]. In terms of the general representation (36) of a one-form, we thus have

$$dt=e^0, \tag{66}$$

$$dx^i=\lambda^i e^0+\rho^i_\alpha\mathbf{e}^\alpha. \tag{67}$$

Obviously, we have $de^0=0$. We further calculate, making use, for example, of (43) and (44), the general formula (56) and the coordinate expressions (18), that

$$d\mathbf{e}^\alpha=-C^\alpha_\beta e^0\wedge\mathbf{e}^\beta-\frac{1}{2}C^\alpha_{\beta\gamma}\mathbf{e}^\beta\wedge\mathbf{e}^\gamma. \tag{68}$$

It is instructive to verify that expressing the properties $d^2\mathbf{e}^\alpha=0$ and $d^2x^i=0$ is indeed equivalent to the requirements (20) and (21) and (22) and (23), respectively.

To complete the picture of basic derivations on $\Lambda(\pi^\dagger)$, we have a closer look at the analog of the classical Lie derivative.

Definition 8: For every $\zeta\in Sec(\pi)$, the derivation d_ζ of degree zero is defined as

$$d_\zeta=[i_\zeta,d]=i_\zeta\circ d+d\circ i_\zeta. \tag{69}$$

So, since d_ζ is defined as a commutator of derivations, we know that it will itself be a derivation of degree zero:

$$d_\zeta(\omega\wedge\mu)=d_\zeta\omega\wedge\mu+\omega\wedge d_\zeta\mu. \tag{70}$$

Likewise, we can rely on proofs similar to those in the standard theory to conclude that the following commutator properties will hold true:

$$[d_\zeta,i_\eta]=i_{[\zeta,\eta]},\quad [d_\zeta,d]=0,\quad [d_\zeta,d_\eta]=d_{[\zeta,\eta]}. \tag{71}$$

Note, however, that a Lie-type derivation with respect to a vector section turns up in the last property, and this is indeed well defined also as $d_{\boldsymbol{\sigma}}=[i_{\boldsymbol{\sigma}},d]$. It is further natural to extend the action of d_ζ to $Sec(\pi)$ by duality. It then follows, as expected, that for $\eta,\zeta\in Sec(\pi)$,

$$d_\zeta\eta=[\zeta,\eta]. \tag{72}$$

As a result of such an extension, d_ζ has Leibniz-type properties also with respect to the evaluation of forms on the appropriate number of affine (or vector) sections; the following property, which could be verified by a direct computation from the definition of d_ζ, thus becomes self-evident:

$$d_\eta\omega(\zeta_1,\ldots,\zeta_k)=\lambda(\eta)(\omega(\zeta_1,\ldots,\zeta_k))+\sum_{j=1}^{k}(-1)^j\omega([\eta,\zeta_j],\zeta_1,\ldots,\hat{\zeta}_j,\ldots,\zeta_k). \tag{73}$$

In the interest of doing computations, we list the Lie-type derivatives of functions $f\in C^\infty(M)$ and the local basis of one-forms. For $\zeta=e_0+\zeta^\alpha\mathbf{e}_\alpha$,

$$d_\zeta f=\lambda(\zeta)(f),\quad d_\zeta e^0=0,\quad d_\zeta\mathbf{e}^\alpha=C^\alpha_\beta\zeta^\beta e^0-C^\alpha_\beta\mathbf{e}^\beta+C^\alpha_{\beta\gamma}\zeta^\gamma\mathbf{e}^\beta+d\zeta^\alpha.$$

IV. λ-ADMISSIBLE CURVES AND DYNAMICS

As we expressed in the Introduction, the model of affine Lie algebroids we are developing should in the first place offer an environment in which one can accommodate the time-dependent Lagrange-type equations (4). At present, we wish to look in more detail at the geometric nature of the more general dynamical systems, which we call pseudo-second-order equations, and are those described by differential equations of the form (3). For this purpose, in fact, we do not need the full machinery of algebroids: it suffices to assume that E is an affine bundle over M and $\lambda:E\to J^1M$ an affine bundle map over the identity.

Definition 9: A curve ψ in E, which is a section of $\tau\circ\pi$, is said to be λ-admissible, if $\lambda\circ\psi=j^1(\pi\circ\psi)$.

One could say that ψ is the λ-prolongation of a curve in M. In coordinates, we have

$$\psi:t\mapsto(t,x^i(t),y^\alpha(t)),\quad \text{with}\quad \dot{x}^i(t)=\lambda^i(t,x(t))+\rho^i_\alpha(t,x(t))y^\alpha(t).$$

Note in passing that, not unexpectedly, one can characterize λ-admissibility via a concept of contact forms: putting $\Theta^i=\lambda^*\theta^i$, where the θ^i are the contact forms on J^1M, we have that ψ is a λ-admissible curve in E if and only if $\psi^*\Theta^i=0$.

Pseudo-second-order equation fields on E are vector fields whose integral curves all are λ-admissible curves. As in the standard theory of SODEs on a tangent bundle or first jet bundle, however, there is a simple direct characterization of such vector fields.

Definition 10: $\Gamma \in \mathcal{X}(E)$ *is a pseudo-second-order equation field if*

$$T\pi \circ \Gamma = i \circ \lambda,$$

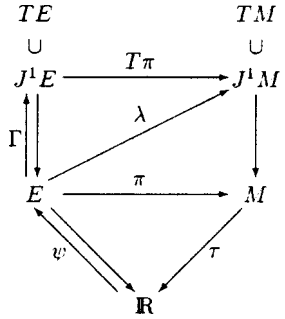
where i *is the injection of* J^1M *into* TM.

Clearly, in coordinates, a pseudo-SODE is of the form

$$\Gamma = \frac{\partial}{\partial t} + (\lambda^i(t,x) + \rho^i_\alpha(t,x)y^\alpha)\frac{\partial}{\partial x^i} + f^\alpha(t,x,y)\frac{\partial}{\partial y^\alpha}, \tag{74}$$

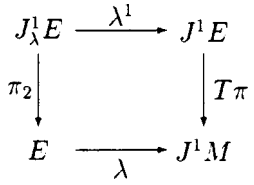
for some functions f^α, and it is obvious that all its integral curves will be λ-admissible.

The following diagram visualizes the notions of λ-admissible curves and pseudo-SODEs.



An important point now, however, is that there is a natural way of interpreting the vector field Γ as section of a different bundle.

From the above definition, it is clear that a pseudo-SODE is actually a section of $(\tau \circ \pi)^0_1 : J^1E \to E$, with the additional property that for all $p \in E$, $T\pi|_{J^1E}(\Gamma(p)) = \lambda(p)$. An equivalent way of saying the same thing, by definition of the concept of a pullback bundle, is that $(p,\Gamma(p))$ is a point of $\lambda^* J^1E$, with J^1E regarded as fibered over J^1M via $T\pi|_{J^1E}$. From now on, we will write $J^1_\lambda E$ for $\lambda^* J^1E$, and denote its two projections as indicated in the following diagram:



If we finally put $\pi_1 = (\tau \circ \pi)^0_1 \circ \lambda^1$, there is yet another way of expressing the characterization of a pseudo-SODE. Indeed, from the trivial observation that $(\tau \circ \pi)^0_1(\Gamma(p)) = p = \pi_2((p,\Gamma(p)))$, it follows that a pseudo-SODE Γ can be regarded also as a section of the bundle $\pi_1 : J^1_\lambda E \to E$, with the property that $\pi_2 \circ \Gamma = \pi_1 \circ \Gamma$.

The various spaces and projections, described in this discussion, are depicted in the diagram of the next section. This diagram immediately suggests the following question: if we put more structure into the scheme by assuming now again that $\pi : E \to M$ carries an affine Lie algebroid structure, is it possible to prolong this structure to the bundle $\pi_1 : J^1_\lambda E \to E$, in such a way of course that λ^1 becomes the anchor map of the induced affine Lie algebroid?

V. PROLONGATION OF AFFINE LIE ALGEBROIDS

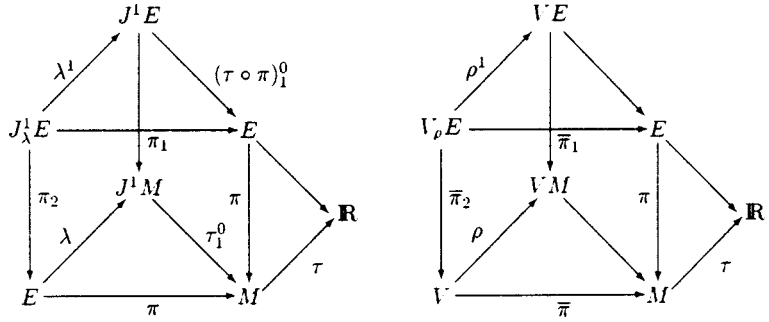
We shall now look in more detail at the bundle $\pi_1 : J^1_\lambda E \to E$. Its total space is the manifold

$$J^1_\lambda E = \lambda^* J^1 E = \{(q,Z) \in E \times J^1 E \,|\, \lambda(q) = T\pi|_{J^1 E}(Z)\},$$

but the fibration we want to focus on is not one of the projections which define $J^1_\lambda E$, but rather the map $\pi_1 = (\tau \circ \pi)^0_1 \circ \lambda^1$. As such, we are looking at an affine bundle, modeled on the vector bundle $\overline{\pi}_1 : V_\rho E \to E$, with total space

$$V_\rho E = \{(\mathbf{v},\mathbf{V}) \in V \times VE \,|\, \rho(\mathbf{v}) = T\pi|_{VE}(\mathbf{V})\}.$$

The affine bundles involved, and their underlying vector bundles, are illustrated below.



A section Z of π_1 is completely determined once we know the maps $\pi_2 \circ Z : E \to E$ and $\lambda^1 \circ Z : E \to J^1 E$. Likewise, vector sections $\mathbf{Z}$ of $\overline{\pi}_1$ are determined by $\overline{\pi}_2 \circ \mathbf{Z}$ and $\rho^1 \circ \mathbf{Z}$. For example, let $e \in E$ be a point with coordinates (t,x^i,y^α), so that (t,x^i) are the coordinates of $\pi(e) \in M$ and e has the representation $e = e_0 + y^\alpha \mathbf{e}_\alpha$. If then Z is a section of π_1, we will have

$$\pi_2 \circ Z: \quad (t,x,y) \mapsto (t,x,z^\alpha(t,x,y)),$$

$$\lambda^1 \circ Z: \quad (t,x,y) \mapsto \left(\frac{\partial}{\partial t} + (\lambda^i + \rho^i_\alpha z^\alpha) \frac{\partial}{\partial x^i} + Z^\alpha \frac{\partial}{\partial y^\alpha} \right)\Bigg|_e,$$

and determining Z in coordinates of course amounts to assigning the functions (z^α, Z^α) on E.

It is worthwhile looking at the representation of such a Z with respect to suitably selected local sections of π_1 and $\overline{\pi}_1$, which will exhibit the affine structure of π_1 and are adapted to the basis which was selected to coordinatize E. To this end, we introduce two sets of local sections $\boldsymbol{\mathcal{X}}_\alpha$ and $\boldsymbol{\mathcal{V}}_\alpha$ of $\overline{\pi}_1$ which will span $Sec(\overline{\pi}_1)$, and select a zero section $\mathcal{E}_0$ as follows. The $\boldsymbol{\mathcal{V}}_\alpha$ span 'vertical sections' and are determined by: $\overline{\pi}_2 \circ \boldsymbol{\mathcal{V}}_\alpha = \mathbf{0}$, while for $e \in E_m$ we let $\rho^1 \circ \boldsymbol{\mathcal{V}}_\alpha(e)$ be the tangent vector to the curve $s \mapsto e + s\mathbf{e}_\alpha(m)$ in E_m. Verticality is an intrinsic property whereas, as usual, there is no intrinsic notion of horizontality. The determination of the $\boldsymbol{\mathcal{X}}_\alpha$ and $\mathcal{E}_0$ will therefore rely on pure coordinate arguments. For the projection onto V we put $\overline{\pi}_2 \circ \boldsymbol{\mathcal{X}}_\alpha = \mathbf{e}_\alpha \circ \pi$ and then, fixing $\rho^1 \circ \boldsymbol{\mathcal{X}}_\alpha$ (as a vector field on E) further requires making a prescription for the vertical components, which we simply take to be zero. Similarly, for the choice of a zero section, we could take any vector field on E which projects under $T\pi$ onto $\lambda(e_0) \in \mathcal{X}(M)$ (and as such defines also a section of π_1), but we will fix it also by taking the vertical components to be zero. Thus we have

$$\boldsymbol{\mathcal{X}}_\alpha(e) = \left(\mathbf{e}_\alpha(\pi(e)), \rho^i_\alpha(t,x) \frac{\partial}{\partial x^i}\Big|_e \right), \quad \boldsymbol{\mathcal{V}}_\alpha(e) = \left(\mathbf{0}(\pi(e)), \frac{\partial}{\partial y^\alpha}\Big|_e \right), \tag{75}$$

and

$$\mathcal{E}_0(e)=\left(e_0(\pi(e)),\left(\frac{\partial}{\partial t}+\lambda^i(t,x)\frac{\partial}{\partial x^i}\right)\Big|_e\right). \tag{76}$$

The general section Z of π_1 then has the local representation

$$Z=\mathcal{E}_0+z^\alpha(t,x,y)\boldsymbol{\mathcal{X}}_\alpha+Z^\alpha(t,x,y)\boldsymbol{\mathcal{V}}_\alpha. \tag{77}$$

Note that pseudo-SODEs, as discussed in the previous section, are precisely those sections Γ of π_1, for which $z^\alpha(t,x,y)=y^\alpha$.

Let now E be equipped with an affine Lie algebroid structure. To be in line with the notations we used in Definition 1, we will from now on also write $\lambda^1(Z)$ instead of $\lambda^1\circ Z$, and likewise for the π_2-projection and the corresponding projections of vector sections.

We wish to establish that there is an induced Lie algebroid structure on the affine bundle π_1. To this end, following the scheme of Definition 1, we have to identify a bracket on $\overline{\pi}_1$ and an action of affine sections on vector sections, such that all the necessary requirements are met. The idea is to define such brackets by requiring roughly that its two projections are determined by the known brackets of the projected sections. But there are some technical complications which we will address now.

For $\mathbf{Z}_1,\mathbf{Z}_2\in Sec(\overline{\pi}_1)$, a preliminary observation is that the Lie bracket of their image under ρ^1 (which gives rise to vector fields on E), belongs to the image of ρ^1. A coordinate calculation can confirm this. Putting

$$\rho^1(\mathbf{Z}_i)=z_i^\alpha\rho_\alpha^j\frac{\partial}{\partial x^j}+Z_i^\alpha\frac{\partial}{\partial y^\alpha},$$

we have

$$[\rho^1(\mathbf{Z}_1),\rho^1(\mathbf{Z}_2)]=(\rho^1(\mathbf{Z}_1)(z_2^\alpha)-\rho^1(\mathbf{Z}_2)(z_1^\alpha))\rho_\alpha^j\frac{\partial}{\partial x^j}+(z_2^\alpha\rho^1(\mathbf{Z}_1)(\rho_\alpha^j)$$

$$-z_1^\alpha\rho^1(\mathbf{Z}_2)(\rho_\alpha^j))\frac{\partial}{\partial x^j}+\cdots\frac{\partial}{\partial y^\alpha}.$$

The first term on the right manifestly belongs to the image of ρ^1, whereas the last term is irrelevant for that purpose. The middle term can be rewritten as

$$z_2^\alpha z_1^\beta\left(\rho_\beta^j\frac{\partial\rho_\alpha^i}{\partial x^j}-\rho_\alpha^j\frac{\partial\rho_\beta^i}{\partial x^j}\right)\frac{\partial}{\partial x^i},$$

which is seen to belong to the image of ρ^1 in view of the property (23). It is therefore natural to impose right away that the bracket $[\cdot,\cdot]^1$ under construction, which of course is required to be skew-symmetric and $\mathbb{R}$-bilinear, should satisfy

$$\rho^1([\mathbf{Z}_1,\mathbf{Z}_2]^1)=[\rho^1(\mathbf{Z}_1),\rho^1(\mathbf{Z}_2)]. \tag{78}$$

This will have for consequence that for $F_i\in C^\infty(E)$,

$$\rho^1([F_1\mathbf{Z}_1,F_2\mathbf{Z}_2]^1)=F_1F_2[\rho^1(\mathbf{Z}_1),\rho^1(\mathbf{Z}_2)]+F_1\rho^1(\mathbf{Z}_1)(F_2)\rho^1(\mathbf{Z}_2)-F_2\rho^1(\mathbf{Z}_2)(F_1)\rho^1(\mathbf{Z}_1).$$

It remains then to make sure that the projection under $\overline{\pi}_2$ can be specified in a compatible way. The above coordinate calculation to some extent illustrates how one should proceed. If we apply $T\pi$ to the preceding equality, we get (pointwise)

$$T\pi(\rho^1([F_1\mathbf{Z}_1,F_2\mathbf{Z}_2]^1))=(F_1F_2)T\pi([\rho^1(\mathbf{Z}_1),\rho^1(\mathbf{Z}_2)])+F_1\rho^1(\mathbf{Z}_1)(F_2)\rho(\overline{\pi}_2(\mathbf{Z}_2))$$
$$-F_2\rho^1(\mathbf{Z}_2)(F_1)\rho(\overline{\pi}_2(\mathbf{Z}_1)).$$

In general, the $\rho(\overline{\pi}_2(\mathbf{Z}_i))$ are vector fields along π for which there is no standard Lie bracket available. If the $\mathbf{Z}_i$ are projectable, however, meaning that there exist $\boldsymbol{\zeta}_i\in Sec(\overline{\pi})$ such that $\overline{\pi}_2\circ\mathbf{Z}_i=\boldsymbol{\zeta}_i\circ\pi$, the vector fields $\rho^1(\mathbf{Z}_i)$ on E are π-related to the vector fields $\rho(\boldsymbol{\zeta}_i)$ on M. Hence, the corresponding brackets are also π-related, meaning that for projectable $\mathbf{Z}_i$, we can put

$$\overline{\pi}_2([\mathbf{Z}_1,\mathbf{Z}_2]^1)=[\overline{\pi}_2(\mathbf{Z}_1),\overline{\pi}_2(\mathbf{Z}_2)], \tag{79}$$

and then the property (13) [which in coordinates gives (23)] ensures that

$$T\pi(\rho^1([\mathbf{Z}_1,\mathbf{Z}_2]^1))=\rho\circ\overline{\pi}_2([\mathbf{Z}_1,\mathbf{Z}_2]^1)$$

as it should. The expression for $T\pi(\rho^1([F_1\mathbf{Z}_1,F_2\mathbf{Z}_2]^1))$ further shows that the $\overline{\pi}_2$ and ρ^1 projections of the bracket under construction will still match up if for projectable $\mathbf{Z}_i$ and for any $F_i\in C^\infty(E)$, we define

$$\overline{\pi}_2([F_1\mathbf{Z}_1,F_2\mathbf{Z}_2]^1)=F_1F_2[\overline{\pi}_2(\mathbf{Z}_1),\overline{\pi}_2(\mathbf{Z}_2)]+F_1\rho^1(\mathbf{Z}_1)(F_2)\overline{\pi}_2(\mathbf{Z}_2)-F_2\rho^1(\mathbf{Z}_2)(F_1)\overline{\pi}_2(\mathbf{Z}_1). \tag{80}$$

It then follows that

$$[F_1\mathbf{Z}_1,F_2\mathbf{Z}_2]^1=F_1F_2[\mathbf{Z}_1,\mathbf{Z}_2]^1+F_1\rho^1(\mathbf{Z}_1)(F_2)\mathbf{Z}_2-F_2\rho^1(\mathbf{Z}_2)(F_1)\mathbf{Z}_1, \tag{81}$$

since both sides have the same $\overline{\pi}_2$ and ρ^1 projections.

The final point to observe now is that sections of $\overline{\pi}_1$ (locally) are finitely generated, over the ring $C^\infty(E)$, by projectable sections. Hence, the defining relations (78) and (80) are sufficient to define the bracket $[\cdot,\cdot]^1$ on vector sections. The property (81) will hold by extension for all vector sections and the bracket will satisfy the Jacobi identity as a result of the Jacobi identity of the Lie algebroid bracket we start from and the same identity for vector fields on E.

To define the action of $Z\in Sec(\pi_1)$ on $\mathbf{V}\in Sec(\overline{\pi}_1)$, we proceed in exactly the same manner. First, one easily verifies that the Lie bracket of $\lambda^1(Z)$ and $\rho^1(\mathbf{V})$ belongs to the image of ρ^1, this time in view of the properties (22) and (23). Hence, it makes sense to put

$$\rho^1([Z,\mathbf{V}]^1)=[\lambda^1(Z),\rho^1(\mathbf{V})], \tag{82}$$

and we of course require the bracket $[\cdot,\cdot]^1$ to have linearity properties of the kind of (7). For projectable sections, we can put

$$\overline{\pi}_2([Z,\mathbf{V}]^1)=[\pi_2(Z),\overline{\pi}_2(\mathbf{V})], \tag{83}$$

and be assured of consistency with the projection (82). Next, still for projectable Z and $\mathbf{V}$ and for any $F\in C^\infty(E)$, we define

$$\overline{\pi}_2([Z,F\mathbf{V}]^1)=F[\pi_2(Z),\overline{\pi}_2(\mathbf{V})]+\lambda^1(Z)(F)\overline{\pi}_2(\mathbf{V}). \tag{84}$$

Sections of π_1 can be written as a projectable zero section, plus a linear combination of projectable vector sections with coefficients in $C^\infty(E)$. In combination with the earlier arguments for vector sections, we are again led to the conclusion that the requirements (82) and (84) are sufficient to define $[Z,\mathbf{V}]^1$ for arbitrary $Z\in Sec(\pi_1)$ and $\mathbf{V}\in Sec(\overline{\pi}_1)$ and that we will have the property

$$[Z,F\mathbf{V}]^1=F[Z,\mathbf{V}]^1+\lambda^1(Z)(F)\mathbf{V}. \tag{85}$$

The final requirement of type (8) then also easily follows, which concludes the construction of the prolonged affine Lie algebroid.

For computational purposes, it remains to list the brackets of the local sections which are used in the general representation of a section of π_1 as in (77). We have

$$[\mathcal{E}_0, \boldsymbol{\mathcal{X}}_\alpha]^1 = C_\alpha^\beta \boldsymbol{\mathcal{X}}_\beta, \quad [\mathcal{E}_0, \boldsymbol{\mathcal{V}}_\alpha]^1 = \mathbf{0},$$

$$[\boldsymbol{\mathcal{X}}_\alpha, \boldsymbol{\mathcal{X}}_\beta]^1 = C_{\alpha\beta}^\gamma \boldsymbol{\mathcal{X}}_\gamma, \quad [\boldsymbol{\mathcal{X}}_\alpha, \boldsymbol{\mathcal{V}}_\beta]^1 = \mathbf{0}, \quad [\boldsymbol{\mathcal{V}}_\alpha, \boldsymbol{\mathcal{V}}_\beta]^1 = \mathbf{0}.$$

It is perhaps worthwhile to repeat hereby that the two projections have to be looked at to verify these statements, although of course they are bound to match up if our new bracket has been defined consistently. Thus we have, for example:

$$\overline{\pi}_2([\mathcal{E}_0, \boldsymbol{\mathcal{X}}_\alpha]^1) = [\pi_2(\mathcal{E}_0), \overline{\pi}_2(\boldsymbol{\mathcal{X}}_\alpha)] = [e_0, \mathbf{e}_\alpha] = C_\alpha^\beta \mathbf{e}_\beta,$$

$$\rho^1([\mathcal{E}_0, \boldsymbol{\mathcal{X}}_\alpha]^1) = [\lambda^1(\mathcal{E}_0), \rho^1(\boldsymbol{\mathcal{X}}_\alpha)] = \left[\frac{\partial}{\partial t} + \lambda^i \frac{\partial}{\partial x^i}, \rho_\alpha^j \frac{\partial}{\partial x^j}\right] = C_\alpha^\beta \rho^1(\boldsymbol{\mathcal{X}}_\beta),$$

where (22) has been used again in the last line.

VI. DISCUSSION AND OUTLOOK FOR FUTURE WORK

The form of equations (4), which we claim to be the appropriate generalization of Lagrangian systems on Lie algebroids to a situation where explicit time dependence is involved, has brought us to the introduction of the new concept of Lie algebroids on affine bundles which are fibered over $\mathbb{R}$. More precisely, the first guidance for developing this concept was provided by the conditions (5) and (6) which the various functions appearing in (4) have to satisfy. Ultimately, of course, we want to arrive at an intrinsic geometrical construction of such Lagrangian systems. There are many aspects to be explored yet, but we have sufficiently paved the way already to be able to predict what the outcome of subsequent studies will bring.

One of us has shown[5] that the prolongation of a Lie algebroid (in the standard situation of vector bundles) provides a platform where there exist analog of the intrinsic structures living on a tangent bundle and these in turn give rise to an intrinsic definition of Lagrangian systems via Poincaré–Cartan-type forms. This is the reason why we were keen to verify immediately that the same notion of prolongation exists in our affine set-up. There is little doubt now that we will find intrinsic objects on such a prolonged affine Lie algebroid, which are analogs of what is known to give rise to an intrinsic definition of time-dependent Lagrangian systems on the first jet bundle of a manifold fibered over $\mathbb{R}$. But there is more to it. Even when there is no Lagrangian for the dynamics under consideration and we are, in other words, talking about pseudo-SODEs on a Lie algebroid, we expect to be able to develop a machinery of associated nonlinear and linear connections, which again is analogous to the standard theory of connections associated to SODEs on a tangent bundle or first jet bundle. A paper on these issues is in preparation.

One of the features we examined in this article as a kind of test for the relevance and internal consistency of the generalized notion of Lie algebroids was the existence of an associated coboundary operator d. But, of course, there are still other interesting properties which standard Lie algebroids are known to exhibit. Let us briefly highlight another one here and show that it also survives our generalization, namely the existence of an associated Poisson structure. Specifically, we want to establish that there exists a canonically defined Poisson structure on the extended dual $E^\dagger$.

Sections of π (respectively $\overline{\pi}$) can be identified with linear functions on $E^\dagger$ (respectively V^*). Explicitly, if $\zeta \in Sec(\pi)$, we consider the function $\hat{\zeta} \in C^\infty(E^\dagger)$ defined by: for each $p \in E^\dagger$, $p \in E_m^\dagger$ say, $\hat{\zeta}(p) = p(\zeta_m)$. Likewise, if $\boldsymbol{\sigma} \in Sec(\overline{\pi})$, we denote by $\hat{\boldsymbol{\sigma}} \in C^\infty(V^*)$ the function defined

by $\hat{\boldsymbol{\sigma}}(\mathbf{p})=\mathbf{p}(\boldsymbol{\sigma}_m)$, where $\mathbf{p}\in V_m^*$. In coordinates, if $\zeta=e_0+\zeta^\alpha \mathbf{e}_\alpha$ and $p\in E^\dagger$ has coordinates (t,x^i,p_0,p_α), then $\hat{\zeta}(p)=p_0+p_\alpha\zeta^\alpha(t,x)$ and similarly for $\hat{\boldsymbol{\sigma}}$. Now, for any two sections $\zeta,\eta \in Sec(\pi)$, we define the function $\{\hat{\zeta},\hat{\eta}\}$ on $E^\dagger$ by

$$\{\hat{\zeta},\hat{\eta}\}(p)=[\widehat{\zeta,\eta}](\mathbf{p}), \tag{86}$$

whereby we recall that $[\zeta,\eta]$ is a section of $\overline{\pi}$ and, for $p\in E_m^\dagger$, $\mathbf{p}$ is the associated element of V_m^*. If further f,g are functions on M and we make no notational distinction for their pullback to $E^\dagger$, internal consistency of (86) for the action of $Sec(\overline{\pi})$ on $Sec(\pi)$ requires that we further put

$$\{\hat{\zeta},f\}=-\{f,\hat{\zeta}\}=\lambda(\zeta)(f),\quad \{f,g\}=0. \tag{87}$$

The construction then uniquely extends to a skew-symmetric, $\mathbb{R}$-bilinear bracket operation on $E^\dagger$ with the required derivation property. This bracket satisfies the Jacobi identity as a result of the Lie algebroid Jacobi identity (16).

The brackets for the coordinate functions on $E^\dagger$ are found to be

$$\{t,t\}=0,\quad \{t,x^i\}=0,\quad \{x^i,x^j\}=0,$$

$$\{p_0,t\}=1,\quad \{p_0,x^i\}=\lambda^i,\quad \{p_0,p_\beta\}=C^\gamma_\beta p_\gamma,$$

$$\{p_\alpha,t\}=0,\quad \{p_\alpha,x^i\}=\rho^i_\alpha,\quad \{p_\alpha,p_\beta\}=C^\gamma_{\alpha\beta}p_\gamma.$$

There is an interesting observation to be made here. Recall that $E^\dagger$ is actually a vector bundle and note now that the bracket we have constructed preserves the subset of functions on $E^\dagger$ which are linear in the fiber coordinates. As a result, we know that there is an induced Lie algebroid structure on the bundle $(E^\dagger)^*\to M$. There are many new insights to be gained from approaching the subject of a Lie algebroid structure on the affine bundle $E\to M$ from this angle; that is to say, by regarding $E\to M$ as an affine subbundle of $(E^\dagger)^*\to M$ and taking an appropriate Lie algebroid structure on $(E^\dagger)^*\to M$ as the starting point. Also this is the subject of a forthcoming paper[13] and is the point of view also in the preprint[14] which came out during the revision process of the present work. One of the main advantages which such an approach offers is that it enables us to get beyond the assumption about the extra fibration of M and thus gives rise to a more general concept of affine Lie algebroids. It further leads to considerable simplifications in proving results about the calculus of forms, as discussed here in Sec. III. We believe, nevertheless, that the present approach preserves its merits mainly for two reasons: one is the repeatedly mentioned motivation coming from time-dependent mechanics; the second one is that the theory of differential forms on sections of an affine bundle $E\to M$, as investigated in Sec. III from a kind of ''internal point of view,'' i.e., without recourse to the larger vector bundle in which E can be imbedded, is something which is being developed here (to the best of our knowledge) for the first time.

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On generalizations of the Calogero–Moser–Sutherland quantum problem and WDVV equations

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It is proved that if the Schrödinger equation $L\psi=\lambda\psi$ of Calogero–Moser–Sutherland type with $L=-\Delta+\Sigma_{\alpha\in\mathcal{A}_+}[m_\alpha(m_\alpha+1)(\alpha,\alpha)/\sin^2(\alpha,x)]$ has a solution of the product form $\psi_0=\Pi_{\alpha\in\mathcal{A}_+}\sin^{-m_\alpha}(\alpha,x)$, then the function $F(x)=\Sigma_{\alpha\in\mathcal{A}_+}m_\alpha(\alpha,x)^2\log(\alpha,x)^2$ satisfies the generalized WDVV equations. This explains the relation between these equations and the deformed CMS quantum problems observed in an earlier work [Phys. Lett. A **261**, 297 (1999)]. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1505651]

I. INTRODUCTION

Let $\mathcal{A}$ be a finite set of vectors α in the Euclidean space $\mathbf{R}^n$ which generates the space and is invariant under the symmetry $x\to -x$. We assume that $-\alpha$ is the only vector from $\mathcal{A}$ which is proportional to α. Let $\mathcal{A}_+$ be its half positive with respect to some linear form. Let us prescribe to each vector $\alpha\in\mathcal{A}$ a real number (''multiplicity'') m_α such that $m_{-\alpha}=m_\alpha$.

Consider the following Schrödinger operator:

$$L=-\Delta+\sum_{\alpha\in\mathcal{A}_+}\frac{m_\alpha(m_\alpha+1)(\alpha,\alpha)}{\sin^2(\alpha,x)}. \tag{1}$$

When $\mathcal{A}$ is a root system with the multiplicities invariant under the corresponding Weyl group W this is an integrable generalization of the Calogero–Moser–Sutherland (CMS) operator[1,2] suggested by Olshanetsky and Perelomov.[3] As it has been shown in Refs. 4 and 5 there are also nonsymmetric integrable generalizations of this problem. This discovery led to the notion of the locus configurations which play a crucial role in the theory of the Huygens' principle.[6]

It turned out[7,8] that the locus configurations discovered in Refs. 4–6 can be used also to construct new solutions of the generalized Witten–Dijgraaf–Verlinde–Verlinde (WDVV) equations:

$$F_iF_k^{-1}F_j=F_jF_k^{-1}F_i,\quad i,j,k=1,\ldots,n. \tag{2}$$

Here F_m is the $n\times n$ matrix constructed from the third partial derivatives of the unknown function $F=F(x^1,\ldots,x^n)$:

$$(F_m)_{pq}=\frac{\partial^3F}{\partial x^m\partial x^p\partial x^q}. \tag{3}$$

In this form these equations have been written by Marshakov, Mironov and Morozov, who showed that the Seiberg–Witten prepotential in $N=2$ four-dimensional supersymmetric gauge theories

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satisfies this system.[9] Originally these equations have been introduced first in topological field theory as some associativity conditions[10,11] and have been later investigated in this context by Dubrovin.[12]

However, in Ref. 13 we have shown that the relation discovered in Ref. 7 between the locus configurations and WDVV equations does not always work, which raised the question what exactly is the property behind this relation.

The aim of this article is to present the answer to this question. The main result is the following:

Theorem: *If the Schrödinger equation $L\psi=\lambda\psi$ of Calogero–Moser–Sutherland type (1) has a solution of the product form*

$$\psi_0=\prod_{\alpha\in\mathcal{A}_+}\sin^{-m_\alpha}(\alpha,x),$$

then the function

$$F(x)=\sum_{\alpha\in\mathcal{A}_+}m_\alpha(\alpha,x)^2\log(\alpha,x)^2$$

satisfies the generalized WDVV equations.

We should mention that the eigenfunctions of the product form play a special role in the theory of the original CMS problem giving the ground states of the system.[1,2] For the deformed CMS problem this becomes more complicated because these solutions become singular on some hyperplanes, so we can consider these solutions as the eigenfunctions only in the formal sense.

II. SPECIAL CLASS OF SOLUTIONS TO GENERALIZED WDVV EQUATIONS

In this section we essentially follow the analysis of the special solutions to WDVV equations from Refs. 7 and 8.

It is known[9,14] that WDVV equations (2) and (3) are equivalent to the equations

$$F_iG^{-1}F_j=F_jG^{-1}F_i,\quad i,j=1,\ldots,n, \tag{4}$$

where $G=\Sigma_{k=1}^n\eta^kF_k$ is any particular invertible linear combination of F_i with the coefficients, which may depend on x. Introducing the matrices $\check{F}_i=G^{-1}F_i$, one can rewrite (4) as the commutativity relations

$$[\check{F}_i,\check{F}_j]=0,\quad i,j=1,\ldots,n. \tag{5}$$

We will consider the following particular class of the solutions to these equations.

Let V be a real vector space of dimension n, V^* be its dual space consisting of the linear functions on V (covectors), and $\mathfrak{A}$ be a finite set of noncollinear covectors $\alpha\in V^*$ generating V^*.

Consider the following function on V:

$$F^{\mathfrak{A}}=\sum_{\alpha\in\mathfrak{A}}(\alpha,x)^2\log(\alpha,x)^2, \tag{6}$$

where $(\alpha,x)=\alpha(x)$ is the value of covector $\alpha\in V^*$ on a vector $x\in V$. For any basis $e_1,\ldots,e_n$ we have the corresponding coordinates $x^1,\ldots,x^n$ in V and the matrices F_i defined according to (3). In a more invariant form for any vector $a\in V$ one can define the matrix

$$F_a=\sum_{i=1}^n a^iF_i.$$

One can easily check that F_a is the matrix of the following bilinear form on V,

$$F_a^{\mathfrak{A}}=\sum_{\alpha\in\mathfrak{A}}\frac{(\alpha,a)}{(\alpha,x)}\alpha\otimes\alpha,$$

where $\alpha\otimes\beta(u,v)=\alpha(u)\beta(v)$ for any $u,v\in V$ and $\alpha,\beta\in V^*$. Define G as F_x, i.e.,

$$G=\sum_{i=1}^{n}x^iF_i,$$

which is actually the matrix of the bilinear form

$$G^{\mathfrak{A}}=\sum_{\alpha\in\mathfrak{A}}\alpha\otimes\alpha, \tag{7}$$

which does not depend on x. Since the covectors $\alpha\in\mathfrak{A}$ generate V^*, the form $G^{\mathfrak{A}}$ is nondegenerate. This means that the natural linear mapping $\varphi_{\mathfrak{A}}:V\to V^*$ defined by the formula

$$(\varphi_{\mathfrak{A}}(u),v)=G^{\mathfrak{A}}(u,v),\quad u,v\in V,$$

is invertible. We will denote $\varphi_{\mathfrak{A}}^{-1}(\alpha),\alpha\in V^*$, as $\alpha^\vee$. By definition

$$\sum_{\alpha\in\mathfrak{A}}\alpha^\vee\otimes\alpha=Id$$

as an operator in V^* or, equivalently,

$$(\alpha,v)=\sum_{\beta\in\mathfrak{A}}(\alpha,\beta^\vee)(\beta,v), \tag{8}$$

for any $\alpha\in V^*,v\in V$. Now according to (5) the WDVV equations (2) and (3) for the function (6) can be rewritten as

$$[\check{F}_a^{\mathfrak{A}},\check{F}_b^{\mathfrak{A}}]=0 \tag{9}$$

for any $a,b\in V$, where the operators $\check{F}_a^{\mathfrak{A}}$ are defined as

$$\check{F}_a^{\mathfrak{A}}=\sum_{\alpha\in\mathfrak{A}}\frac{(\alpha,a)}{(\alpha,x)}\alpha^\vee\otimes\alpha. \tag{10}$$

Let $G_{\mathfrak{A}}$ be the form on V^* induced by $G^{\mathfrak{A}}$:

$$G_{\mathfrak{A}}(\alpha,\beta)=G^{\mathfrak{A}}(\alpha^\vee,\beta^\vee).$$

Its matrix in the corresponding basis is G^{-1}. A simple calculation shows that (9) can be rewritten as

$$\sum_{\alpha\neq\beta,\alpha,\beta\in\mathfrak{A}}\frac{G_{\mathfrak{A}}(\alpha,\beta)B_{\alpha,\beta}(a,b)}{(\alpha,x)(\beta,x)}\alpha\wedge\beta\equiv 0, \tag{11}$$

where

$$\alpha\wedge\beta=\alpha\otimes\beta-\beta\otimes\alpha$$

and

$$B_{\alpha,\beta}(a,b)=\alpha\wedge\beta(a,b)=\alpha(a)\beta(b)-\alpha(b)\beta(a).$$

One can check that the relations (11) are equivalent to

$$\sum_{\beta\neq\alpha,\beta\in\Pi\cap\mathfrak{A}}\frac{G_{\mathfrak{A}}(\alpha,\beta)B_{\alpha,\beta}(a,b)}{(\beta,x)}\alpha\wedge\beta|_{(\alpha,x)=0}\equiv 0$$

for any $\alpha\in\mathfrak{A}$ and any two-dimensional plane Π containing α, and therefore to

$$\sum_{\beta\neq\alpha,\beta\in\Pi\cap\mathfrak{A}}G_{\mathfrak{A}}(\alpha,\beta)B_{\alpha,\beta}(a,b)=0 \tag{12}$$

for any such α and Π.

Summarizing we have the following result (cf. Refs. 7 and 8).

Proposition 1: The function (6) satisfies the generalized WDVV equations (2) and (3) iff the relations (12) are satisfied for any $\alpha\in\mathfrak{A}$ and any two-dimensional plane Π such that $\alpha\in\Pi$.

Remark: In Refs. 7 and 8 the conditions (12) have been reformulated in geometric terms ($\vee$-conditions). For the purpose of the present article it is more convenient to use these conditions in the original form.

Any Coxeter root system satisfies these conditions, but there are many more examples (see Refs. 7, 8, and 13).

III. MAIN IDENTITY AND PROOF OF THE THEOREM

Let now $\mathcal{A}$ be a finite set of the vectors α in the Euclidean space $\mathbf{R}^n$ with multiplicities m_α. We will assume that this set is invariant under the symmetry $x\to -x$ and that $-\alpha$ is the only vector from $\mathcal{A}$ which is proportional to α. By $\mathcal{A}_+$ we mean the positive half of $\mathcal{A}$:

$$\mathcal{A}_+=\{\alpha\in\mathcal{A}:(\alpha,v)>0\}$$

for some $v\in\mathbf{R}^n$ which is generic in the sense that $(\alpha,v)\neq 0$ for all $\alpha\in\mathcal{A}$.

Consider the Schrödinger equation

$$L\psi=\lambda\psi, \tag{13}$$

where

$$L=-\Delta+\sum_{\alpha\in\mathcal{A}_+}\frac{m_\alpha(m_\alpha+1)(\alpha,\alpha)}{\sin^2(\alpha,x)}.$$

Let us look for the solutions of this equation of the form

$$\psi_0=\prod_{\alpha\in\mathcal{A}_+}\sin^{-m_\alpha}(\alpha,x). \tag{14}$$

By straightforward calculation one can check the following result (cf. Ref. 15).

Lemma 1: The function (14) satisfies the equation (13) for some λ iff the following main identity holds:

$$\sum_{\alpha\neq\beta,\alpha,\beta\in\mathcal{A}_+}m_\alpha m_\beta(\alpha,\beta)(\cot(\alpha,x)\cot(\beta,x)+1)\equiv 0. \tag{15}$$

The eigenvalue λ in that case has a form $\lambda=|\rho(m)|^2$ where $\rho(m)=\Sigma_{\alpha\in\mathcal{A}_+}m_\alpha\alpha$.

Actually, first we have the condition that the sum

$$S=\sum_{\alpha\neq\beta,\alpha,\beta\in\mathcal{A}_+} m_\alpha m_\beta(\alpha,\beta)\cot(\alpha,x)\cot(\beta,x)$$

must be a constant in x. Considering then $x=itv$ with a large positive t and v from the definition of $\mathcal{A}_+$, we see that this constant must be equal to

$$S=-\sum_{\alpha\neq\beta,\alpha,\beta\in\mathcal{A}_+} m_\alpha m_\beta(\alpha,\beta).$$

This leads also to the formula for the eigenvalue λ. It is worthy to note that this formula implies that the vector $\rho(m)$ which depends on the choice of the positive part $\mathcal{A}_+$ (i.e., on the choice of v) has the norm $|\rho(m)|$ independent on this choice.

Remark: The gauged operator $\tilde{L}=\hat{\psi}_0^{-1}L\hat{\psi}_0$, where $\hat{\psi}_0$ is the operator of multiplication by ψ_0, in this case has the form $\tilde{L}=-L^{\mathrm{rad}}+|\rho(m)|^2$,

$$L^{\mathrm{rad}}=\Delta-2\sum_{\alpha\in\mathcal{A}_+} m_\alpha\cot(\alpha,x)\partial_\alpha.$$

When $\mathcal{A}$ is a root system with special multiplicities L^{rad} is the radial part of Laplace–Beltrami operator on some symmetric space.[16] Thus, the property of L we discuss is equivalent to the existence of the "radial gauge." We should mention that the relation between the radial parts of the Laplace operators and quantum many-body problems was first observed [in the case of the symmetric spaces $\mathrm{SU}(n)/\mathrm{SO}(n)$] by Berezin, Pokhil, and Finkelberg[17] and was investigated in details by Olshanetsky and Perelomov in Ref. 15.

The main identity is equivalent to the following identities:

$$\sum_{\beta\in\mathcal{A}_+,\beta\neq\alpha} m_\alpha m_\beta(\alpha,\beta)\cot(\beta,x)|_{(\alpha,x)=k\pi}\equiv 0, \tag{16}$$

for each $\alpha\in\mathcal{A}_+$ and $k\in\mathbf{Z}$. In particular,

$$\sum_{\beta\in\mathcal{A}_+,\beta\neq\alpha} m_\alpha m_\beta(\alpha,\beta)\cot(\beta,x)|_{(\alpha,x)=0}\equiv 0 \tag{17}$$

must be satisfied on all the hyperplanes $(\alpha,x)=0$. It is easy to see that the last identities are equivalent to the set of identities:

$$\sum_{\beta\in\mathcal{A}_+\cap\Pi,\beta\neq\alpha} m_\alpha m_\beta(\alpha,\beta)\cot(\beta,x)|_{(\alpha,x)=0}\equiv 0 \tag{18}$$

hold for any plane Π containing vector $\alpha\in\mathcal{A}_+$.

Let us look now at these two-dimensional identities. Let Π be the plane generated by $\alpha,\beta\in\mathcal{A}_+,\alpha\neq\beta$. We can assume that $(\alpha,\beta)\neq 0$ since otherwise the identity is trivially satisfied. All the vectors $\gamma\in\mathcal{A}_+\cap\Pi$ can be split into equivalence classes $\Gamma_1,\ldots,\Gamma_p$ according to the equivalence relation: $\gamma\sim\gamma'$ if

$$\gamma'=\pm\gamma+\mu\alpha \tag{19}$$

for some μ. I would like to mention that similar equivalence has been considered by M. V. Feigin in the theory of trigonometric locus configurations.[18]

The restrictions of $\cot(\gamma,x)$ and $\cot(\gamma',x)$ on the intersection line of Π with the hyperplane $(\alpha,x)=0$ are the same up to a sign. To take care of this sign let us introduce a skew-symmetric bilinear form $B=B_{a,b}(\alpha,\beta)$ related to a pair of vectors $a,b\in\mathbf{R}^n$ by the formula

$$B_{a,b}(\alpha,\beta)=(\alpha,a)(\beta,b)-(\alpha,b)(\beta,a).$$

It is easy to check that the identity (18) for the plane Π is equivalent to the set of relations

$$\sum_{\gamma\in\Gamma_s,\,\gamma\neq\alpha} m_\alpha m_\gamma(\alpha,\gamma)B(\alpha,\gamma)=0 \tag{20}$$

for all the equivalence classes $\Gamma_1,\ldots,\Gamma_p$. As a corollary we have the same relation on each plane Π:

$$\sum_{\beta\neq\alpha,\beta\in\mathcal{A}_+\cap\Pi} m_\alpha m_\beta(\alpha,\beta)B(\alpha,\beta)=0, \tag{21}$$

and thus in the whole space

$$\sum_{\beta\neq\alpha,\beta\in\mathcal{A}_+} m_\alpha m_\beta(\alpha,\beta)B(\alpha,\beta)=0 \tag{22}$$

for any $\alpha\in\mathcal{A}_+$.

Let us introduce now the operators M_α in $\mathbf{R}^n$ by the relation

$$M_\alpha=m_\alpha\alpha\otimes\alpha,$$

where by definition $\alpha\otimes\beta(x)=(\beta,x)\alpha$. Let M be the sum

$$M=\sum_{\alpha\in\mathcal{A}_+} m_\alpha\alpha\otimes\alpha.$$

Now we need the following natural definition. We will call a configuration $\mathcal{A}$ *irreducible* if it cannot be split into two nontrivial orthogonal parts.

Lemma 2: The main identity (15) implies that all the operators $M_\alpha,\alpha\in\mathcal{A}_+$ commute with M. For irreducible configurations this means that M is a scalar operator: $M=\mu I$ for some μ.

Indeed, the commutator $C_\alpha=[M,M_\alpha]$ is $C_\alpha=[\Sigma_{\beta\in\mathcal{A}_+}m_\beta\beta\otimes\beta,m_\alpha\alpha\otimes\alpha]$ $=-\Sigma_{\beta\neq\alpha,\beta\in\mathcal{A}_+}m_\alpha m_\beta(\alpha,\beta)(\alpha\otimes\beta-\beta\otimes\alpha)$. It is easy to see that the relations (22) are equivalent to $(C_\alpha(a),b)=0$ for arbitrary $a,b\in\mathbf{R}^n$ which imply that $C_\alpha=0$. The commutativity of the operator M with M_α means that any $\alpha\in\mathcal{A}$ is an eigenvector of the (self-adjoint) operator M. If M has two different eigenvalues, then $\mathcal{A}$ can be split into two orthogonal parts which is impossible in the irreducible case. This proves the lemma.

Now everything is ready for the proof of our main result. For a given configuration $\mathcal{A}$ let us define the set $\mathfrak{A}$ in the Euclidean space $V=\mathbf{R}^n\simeq V^*$ by taking all the vectors of the form $\sqrt{m_\alpha}\alpha,\alpha\in\mathcal{A}_+$.

Lemma 3: If $\mathcal{A}$ is irreducible and satisfies the main identity, then $\mathfrak{A}$ satisfies the relations (12) from the previous section.

Indeed, due to Lemma 2 in this case $G^{\mathfrak{A}}=\Sigma_{\alpha\in\mathcal{A}_+}m_\alpha\alpha\otimes\alpha$ is proportional to the scalar product in $\mathbf{R}^n$. The same is obviously true for $G_{\mathfrak{A}}$ so the relations (12) are reduced to (21).

Remark: Strictly speaking we should consider only positive multiplicities in order to stay on reals but one can easily check that the resulting function

$$F(x)=\sum_{\alpha\in\mathcal{A}_+} m_\alpha(\alpha,x)^2\log(\alpha,x)^2$$

is real even in the case of negative multiplicities and all the arguments work in the complex case as well.

Combining these three lemmas with Proposition 1 we have the proof of the theorem in the irreducible case. The reducible case then easily follows.

Now using the results of Refs. 7 and 8 we have the following:

Corollary: For any configuration $\mathcal{A}$ satisfying the main identity the corresponding set $\mathfrak{A}$ is a $\vee$-system in the sense of Ref. 7. In particular the following differential operators of the Knizhnik–Zamolodchikov type,

$$\nabla_a = \partial_a - \sum_{\alpha \in \mathcal{A}_+} m_\alpha \frac{(\alpha,a)}{(\alpha,x)} \alpha \otimes \alpha, \tag{23}$$

commute and therefore define a flat connection in $\mathbf{R}^n$.

As the examples one can consider the following "locus configurations" $A_n(m)$ and $C_{n+1}(m,l)$ which have been introduced in Refs. 4–6. They consist of the following vectors in $\mathbf{R}^{n+1}$:

$$A_n(m) = \begin{cases} e_i - e_j, & 1 \leqslant i < j \leqslant n, \quad \text{with multiplicity } m, \\ e_i - \sqrt{m} e_{n+1}, & i = 1,\ldots,n, \quad \text{with multiplicity } 1, \end{cases}$$

and

$$C_{n+1}(m,l) = \begin{cases} e_i \pm e_j, & 1 \leqslant i < j \leqslant n, \quad \text{with multiplicity } k, \\ 2e_i, & i = 1,\ldots,n, \quad \text{with multiplicity } m, \\ e_i \pm \sqrt{k} e_{n+1}, & i = 1,\ldots,n, \quad \text{with multiplicity } 1, \\ 2\sqrt{k} e_{n+1}, & \text{with multiplicity } l, \end{cases}$$

where $k = (2m+1)/(2l+1)$. The fact that they satisfy the main identity (for all values of the parameters) can be checked by direct calculation. Our theorem thus explains the observation[7] that the corresponding functions F satisfy the generalized WDVV equation.

IV. CONCLUDING REMARKS

We have seen that the main identity is behind the relation between the locus configurations and WDVV equation. Since there are locus configurations without this property this explains also why this relation does not always work.[13] An interesting problem is to classify all locus configurations which satisfy the main identity. The fact that this is true for the series $A_n(m)$ and $C_{n+1}(m,l)$ seems to be very important. In particular, as it follows from our analysis in the previous section these configurations (with integer parameters) are the "vector systems" in the Borcherds' sense.[19] Their role in Borcherds' theory deserves a special investigation.

We have already mentioned the relations with the theory of symmetric spaces and the radial parts of the Laplace operators for the usual root systems. It is interesting that the operators related to $A_n(m)$ and $C_{n+1}(m,l)$ also can be interpreted in a similar way using the Lie superalgebras and symmetric superspaces as it was recently discovered by A. N. Sergeev.[20] This relation gives some new interesting examples of the integrable deformations of Calogero–Sutherland operators satisfying the main identity[21] (and therefore new solutions for the WDVV equation).

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Scattering relations for point sources: Acoustic and electromagnetic waves

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The problem of scattering of spherical waves by a bounded obstacle is considered. General scattering theorems are proved. These relate the far-field patterns due to scattering of waves from a point source put in any two different locations. The scatterer can have any of the usual properties, penetrable or impenetrable. The optical theorem is recovered as a corollary. Mixed scattering relations are also established, relating the scattered fields due to a point source and a plane wave. [DOI: 10.1063/1.1509089]

I. INTRODUCTION

In classical scattering theory, there are some general results that connect the solutions of two related problems. The most familiar of these is *reciprocity*: the scattered field at A due to a source at B is simply related to the scattered field at B due to a source at A.

There are also internal relations within a single problem. A well-known example is the *optical theorem* for scattering of plane waves: it relates the far-field pattern in the forward direction to a certain integral of the far-field pattern over all directions.

In this article, we derive some general relations for scattering of waves emanating from point sources. Thus, we relate one problem with a point source at A to a similar problem with a point source at B. By setting $A=B$ and then letting A recede to infinity, we recover the optical theorem. If we keep A fixed and let B recede to infinity, we obtain so-called *mixed scattering theorems*, relating plane-wave incidence to point-source incidence. An example of these is the *mixed reciprocity theorem*, which has found much use recently in methods for solving inverse scattering problems.[1]

As Logan[2] points out, Clebsch considered the scattering of elastic waves from a point source by a rigid sphere 140 years ago, a decade before Lord Rayleigh published his solution for the scattering of a plane sound wave by a sphere. Collected results for scattering of point-source fields by simple shapes are given in Ref. 3. More recently, Dassios and his co-workers have studied incident waves generated by a point source in the vicinity of a scatterer; see, for example, Refs. 4–6. There is also some recent work on near-field inverse problems: in addition to the previous papers, we note the work by Coyle[7] and Potthast,[1] as well as recent work by three of the present authors.[8,9] The revival of interest in problems related to point-generated wave fields has several reasons. One is due to the variety of applications coming from the theory of composite materials and of acoustic emission, from the theoretical analysis of biological studies at the cell level, from nondestructive testing and evaluation, from geophysics, from modeling in medicine and health

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sciences, and from scattering problems connected to environmental data analysis. Another reason is due to the fact that a point-source field is more easily realizable in a laboratory.

We give results for both acoustic and electromagnetic waves, and we permit all the usual kinds of scattering obstacles, penetrable and impenetrable. Extensions to elastic-wave problems are expected.

II. FORMULATION: ACOUSTICS

Let Ω^- be a bounded three-dimensional obstacle with a smooth closed boundary S (the scatterer). The exterior $\mathbb{R}^3\backslash\Omega^- = \Omega$ of the scatterer is an infinite homogeneous isotropic lossless acoustic medium, that is the compressional viscosity δ is zero, and with mass density ρ, phase velocity c, mean compressibility γ and real wave number $k=\omega\sqrt{\gamma\rho}$, ω being the angular frequency. The interior of the scatterer Ω^- is filled with a lossy medium, in general, with corresponding physical parameters δ^-, ρ^-, c^- and γ^-. We consider an incident spherical acoustic wave due to a source located at a point with position vector $\mathbf{a}$. Suppressing the harmonic time dependence $\exp\{-\mathrm{i}\omega t\}$, and following the normalization introduced by Dassios and Kamvyssas,[4] we assume the following form for the incident field:

$$u_a^{\mathrm{i}}(\mathbf{r}) = a\,\mathrm{e}^{-\mathrm{i}ka}\frac{\mathrm{e}^{\mathrm{i}k|\mathbf{r}-\mathbf{a}|}}{|\mathbf{r}-\mathbf{a}|}, \quad \mathbf{r}\neq\mathbf{a}, \tag{1}$$

where $a=|\mathbf{a}|$. We note that when $a\to\infty$, the spherical wave reduces to a plane wave with direction of propagation $-\hat{\mathbf{a}}$, where $\mathbf{a}=a\hat{\mathbf{a}}$.[4] The total field u_a^{t} in the exterior of the scatterer is given by

$$u_a^{\mathrm{t}}(\mathbf{r}) = u_a^{\mathrm{i}}(\mathbf{r}) + u_a^{\mathrm{s}}(\mathbf{r}), \quad \mathbf{r}\in\Omega\backslash\{\mathbf{a}\}, \tag{2}$$

where u_a^{s} is the scattered acoustic field, and solves the Helmholtz equation

$$\nabla^2 u_a^{\mathrm{t}}(\mathbf{r}) + k^2 u_a^{\mathrm{t}}(\mathbf{r}) = 0, \quad \mathbf{r}\in\Omega. \tag{3}$$

The scattered as well as the incident fields are solutions of Helmholtz's equation that satisfy the Sommerfeld radiation condition

$$\hat{\mathbf{r}}\cdot\nabla u(\mathbf{r}) - \mathrm{i}ku(\mathbf{r}) = o(r^{-1}), \quad r\to\infty, \tag{4}$$

uniformly in all directions $\hat{\mathbf{r}}\in S^2$, where S^2 is the unit sphere. We note that u_a^{t} also satisfies the Sommerfeld radiation condition.

In our analysis, we can permit impenetrable or penetrable scatterers. In the former case, we could have Dirichlet ($u_a^{\mathrm{t}}=0$), Neumann ($\partial u_a^{\mathrm{t}}/\partial n=0$) or Robin conditions on S; the Robin (or impedance) condition is

$$\left(\frac{\partial}{\partial n} + \mathrm{i}k\lambda\right) u_a^{\mathrm{t}}(\mathbf{r}) = 0, \quad \mathbf{r}\in S, \tag{5}$$

where λ is a dimensionless real parameter. In the penetrable case, the incident wave is transmitted into the scatterer; let u_a^- be the total acoustic field in Ω^-. Then the following *transmission conditions* must hold on the scatterer's surface

$$u_a^{\mathrm{t}}(\mathbf{r}) = u_a^-(\mathbf{r}) \quad \text{and} \quad \frac{\partial u_a^{\mathrm{t}}(\mathbf{r})}{\partial n} = \beta\frac{\partial u_a^-(\mathbf{r})}{\partial n}, \quad \mathbf{r}\in S, \tag{6}$$

where the constant $\beta=(\rho/\rho^-)(1-\mathrm{i}kc\,\delta^-\gamma^-)$ is complex for a lossy scatterer and real for a lossless scatterer. More details on the physical parameters of the above problems can be found in Ref. 6. The field u_a^- solves the Helmholtz equation in Ω^-,

$$\nabla^2 u_a^-(\mathbf{r}) + \eta^2 k^2 u_a^-(\mathbf{r}), \quad \mathbf{r} \in \Omega^-, \tag{7}$$

where $\eta = (c/c^-)(1 - ikc\gamma^- \delta^-)^{-1/2}$ is the (complex) index of refraction between the two media in Ω and Ω^-. The choice of the branch of the square root is such that $\mathrm{Im}(\eta) \geqslant 0$ and hence $\mathrm{Im}(\eta k) \geqslant 0$.

In addition, in order to cover various cases that arise in applications, we can easily extend our analysis to include an impenetrable core in the interior of the scatterer.

As it is well known, all the above problems are well posed.

The behavior of the scattered wave in the far field is given by

$$u_a^s(\mathbf{r}) = g_a(\hat{\mathbf{r}}) h_0(kr) + O(r^{-2}), \quad r \to \infty, \tag{8}$$

where $h_0(x) = e^{ix}/(ix)$ is the spherical Hankel function of the first kind and order zero. Moreover,

$$g_a(\hat{\mathbf{r}}) = -\frac{ik}{4\pi} \int_S \left[\frac{\partial u_a^s(\mathbf{r}')}{\partial n} + ik(\hat{\mathbf{r}} \cdot \hat{\mathbf{n}}) u_a^s(\mathbf{r}') \right] e^{-ik\hat{\mathbf{r}} \cdot \mathbf{r}'} ds(\mathbf{r}') \tag{9}$$

is the far-field pattern.[5]

III. GENERAL SCATTERING THEOREM

In what follows, we consider two locations for the point source, **a** and **b**, from which the time-harmonic incident spherical waves emanate. Each source generates a corresponding scattered field, u_a^s and u_b^s, respectively. We are interested in relations between these fields.

Let S_r denote a large sphere of radius r, surrounding the points **a** and **b**, and let

$$S_{a,\varepsilon} = \{\mathbf{r} \in \mathbb{R}^3 : |\mathbf{a} - \mathbf{r}| = \varepsilon\}, \tag{10}$$

a small sphere of radius ε, surrounding the point **a**. Then, we introduce the following notation,

$$[u, v]_S = \int_S \left(\overline{u} \frac{\partial v}{\partial n} - v \frac{\partial \overline{u}}{\partial n} \right) ds,$$

where the overbar denotes complex conjugation; in particular, we write $[u, v] \equiv [u, v]_S$.

Lemma 1: Let u_a^i be a point source at **a**. *Let u_b^i be a point source at* **b**, *with corresponding scattered field u_b^s and far-field pattern g_b. Then*

$$\lim_{r \to \infty} [u_a^i, u_b^s]_{S_r} = 2a e^{ika} \int_{S^2} g_b(\hat{\mathbf{r}}) e^{ik\hat{\mathbf{r}} \cdot \mathbf{a}} ds(\hat{\mathbf{r}}) \tag{11}$$

and

$$\lim_{\varepsilon \to 0} [u_a^i, u_b^s]_{S_{a,\varepsilon}} = 4\pi a e^{ika} u_b^s(\mathbf{a}), \tag{12}$$

where S_r is a large sphere of radius r surrounding **a** *and* **b**, *and $S_{a,\varepsilon}$ is the small sphere defined by Eq. (10).*

Proof: For Eq. (11), we use the asymptotic relations

$$|\mathbf{r} - \mathbf{a}| = r - \hat{\mathbf{r}} \cdot \mathbf{a} + O(r^{-1}) \quad \text{and} \quad |\mathbf{r} - \mathbf{a}|^{-1} = r^{-1} + O(r^{-2}), \tag{13}$$

as $r \to \infty$, and obtain

$$u_a^i(\mathbf{r}) = h_0(kr) g_a^i(\hat{\mathbf{r}}) + O(r^{-2}), \quad r \to \infty, \tag{14}$$

where $g_a^{\mathrm{i}}(\hat{\mathbf{r}})=\mathrm{i}ka\exp\{-\mathrm{i}ka(1+\hat{\mathbf{a}}\cdot\hat{\mathbf{r}})\}$ is the far-field pattern of the point-source incident wave. Using Eqs. (8) and (14) gives Eq. (11).

For Eq. (12), we evaluate $\overline{u_a^{\mathrm{i}}}$ and its normal derivative on $S_{a,\varepsilon}$. There, we have $\overline{u_a^{\mathrm{i}}}=(a/\varepsilon)\mathrm{e}^{\mathrm{i}k(a-\varepsilon)}$ and $(\partial/\partial n)\overline{u_a^{\mathrm{i}}}=-(\mathrm{i}k+\varepsilon^{-1})\overline{u_a^{\mathrm{i}}}(\mathbf{r})$, where $\partial/\partial n$ denotes normal differentiation in the outward direction. Using the mean value theorem and letting $\varepsilon\to 0$, Eq. (12) is proved. □

Now, for two point sources, with position vectors **a** and **b**, we define a *spherical far-field pattern generator* for spherical acoustic waves by

$$G_b(\mathbf{a})=\mathrm{i}ka\mathrm{e}^{\mathrm{i}ka}\left[u_b^{\mathrm{s}}(\mathbf{a})-\frac{1}{2\pi}\int_{S^2}g_b(\hat{\mathbf{r}})\mathrm{e}^{\mathrm{i}k\mathbf{a}\cdot\hat{\mathbf{r}}}ds(\hat{\mathbf{r}})\right]. \tag{15}$$

This terminology and definition are appropriate for the following reason [see Eq. (50) later in this work]. When both the point source and the observation point recede to infinity, $G_b(\mathbf{a})$ reduces to the far-field pattern for an incident plane wave propagating in the direction $-\hat{\mathbf{b}}$. Using this notation, the general scattering theorem for spherical waves is formulated as follows.

Theorem 2: *For any two point-source locations in* Ω, **a** *and* **b**, *we have*

$$G_b(\mathbf{a})+\overline{G_a(\mathbf{b})}+\frac{1}{2\pi}\int_{S^2}g_b(\hat{\mathbf{r}})\overline{g_a(\hat{\mathbf{r}})}ds(\hat{\mathbf{r}})=\mathcal{E}_{a,b}, \tag{16}$$

where

$$\mathcal{E}_{a,b}=-\frac{\mathrm{i}k}{4\pi}[u_a^{\mathrm{t}},u_b^{\mathrm{t}}]. \tag{17}$$

The value of $\mathcal{E}_{a,b}$ *depends on the scatterer:*

$$\mathcal{E}_{a,b}=0 \quad \textit{for Dirichlet or Neumann conditions on } S; \tag{18}$$

$$\mathcal{E}_{a,b}=-\frac{k^2\lambda}{2\pi}\int_S u_b^{\mathrm{t}}(\mathbf{r})\overline{u_a^{\mathrm{t}}(\mathbf{r})}ds \quad \textit{for the Robin condition (5) on } S; \tag{19}$$

or

$$\mathcal{E}_{a,b}=-\frac{k}{2\pi}\mathrm{Im}(\beta)\int_{\Omega^-}\nabla\overline{u_a^-(\mathbf{r})}\cdot\nabla u_b^-(\mathbf{r})dv(\mathbf{r}) \quad \textit{for a penetrable scatterer,} \tag{20}$$

where β *is the constant in the transmission conditions (6).*

Proof: Let us first evaluate $\mathcal{E}_{a,b}$ directly. For Dirichlet ($u^{\mathrm{t}}=0$) or Neumann ($\partial u^{\mathrm{t}}/\partial n=0$) conditions, we immediately obtain Eq. (18). Similarly, the Robin condition (5) gives Eq. (19). For a penetrable scatterer, we use the transmission conditions (6), apply Green's first theorem and take into account that $\mathrm{Im}(\beta\eta^2)=0$ (see p. 9 of Ref. 6); this gives Eq. (20).

Next, we give an alternative evaluation of $\mathcal{E}_{a,b}$. Thus, by the relations $u_\alpha^{\mathrm{t}}=u_\alpha^{\mathrm{i}}+u_\alpha^{\mathrm{s}}$ for $\alpha=a,b$ we have

$$[u_a^{\mathrm{t}},u_b^{\mathrm{t}}]=[u_a^{\mathrm{i}},u_b^{\mathrm{i}}]+[u_a^{\mathrm{s}},u_b^{\mathrm{i}}]+[u_a^{\mathrm{i}},u_b^{\mathrm{s}}]+[u_a^{\mathrm{s}},u_b^{\mathrm{s}}]. \tag{21}$$

Since $\overline{u_a^{\mathrm{i}}}$ and u_b^{i} are regular solutions of the Helmholtz equation in Ω^-, Green's second theorem gives

$$[u_a^{\mathrm{i}},u_b^{\mathrm{i}}]=0. \tag{22}$$

For the other terms in Eq. (21), we consider two small spheres, S_{a,ε_1} and S_{b,ε_2}, centered at **a** and **b** with radii ε_1 and ε_2, respectively, with $S_{a,\varepsilon_1}\cap S_{b,\varepsilon_2}=\varnothing$, as well as a large sphere S_R centered

at the origin surrounding the whole system of the scatterer and the two small spheres. Since $\overline{u_a^{\mathrm{i}}}(\mathbf{r})$ and $u_b^{\mathrm{s}}(\mathbf{r})$ are solutions of the Helmholtz equation, for $\mathbf{r}\neq\mathbf{a},\mathbf{b}$, Green's second theorem gives

$$[u_a^{\mathrm{i}},u_b^{\mathrm{s}}]=[u_a^{\mathrm{i}},u_b^{\mathrm{s}}]_{S_R}-[u_a^{\mathrm{i}},u_b^{\mathrm{s}}]_{S_{a,\varepsilon_1}}-[u_a^{\mathrm{i}},u_b^{\mathrm{s}}]_{S_{b,\varepsilon_2}}.$$

The third term is zero because $\overline{u_a^{\mathrm{i}}}$ and u_b^{s} are regular solutions of the Helmholtz equation in the interior of S_{b,ε_2}. Then, letting $R\to\infty$ and $\varepsilon_1\to 0$, using Lemma 1, we obtain

$$[u_a^{\mathrm{i}},u_b^{\mathrm{s}}]=-4\pi a\mathrm{e}^{\mathrm{i}ka}u_b^{\mathrm{s}}(\mathbf{a})+2a\mathrm{e}^{\mathrm{i}ka}\int_{S^2}g_b(\hat{\mathbf{r}})\mathrm{e}^{\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{a}}ds(\hat{\mathbf{r}}). \tag{23}$$

As $[u_a^{\mathrm{s}},u_b^{\mathrm{i}}]=-\overline{[u_b^{\mathrm{i}},u_a^{\mathrm{s}}]}$, we easily deduce that

$$[u_a^{\mathrm{s}},u_b^{\mathrm{i}}]=4\pi b\mathrm{e}^{-\mathrm{i}kb}\overline{u_a^{\mathrm{s}}(\mathbf{b})}-2b\mathrm{e}^{-\mathrm{i}kb}\int_{S^2}\overline{g_a(\hat{\mathbf{r}})}\mathrm{e}^{-\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{b}}ds(\hat{\mathbf{r}}). \tag{24}$$

Finally, in view of the regularity of $\overline{u_a^{\mathrm{s}}}$ and u_b^{s} in the region exterior to S, we have

$$[u_a^{\mathrm{s}},u_b^{\mathrm{s}}]=[u_a^{\mathrm{s}},u_b^{\mathrm{s}}]_{S_R}.$$

Then, letting $R\to\infty$, we pass to the radiation zone and thus we can use the asymptotic form (8), giving

$$[u_a^{\mathrm{s}},u_b^{\mathrm{s}}]=\frac{2\mathrm{i}}{k}\int_{S^2}\overline{g_a(\hat{\mathbf{r}})}g_b(\hat{\mathbf{r}})ds(\hat{\mathbf{r}}). \tag{25}$$

Substituting Eqs. (22)–(25) in Eq. (21), making use of Eq. (17) and its evaluation, gives Eq. (16), and the theorem is proved. □

Let us make two remarks. First, if the scatterer is a lossless penetrable obstacle, that is, the physical parameter β is real, then we obtain $\mathcal{E}_{a,b}=0$ in Eq. (16), just as for soft or hard scatterers.

Second, suppose that we have a penetrable scatterer with a core S^- on which $u^-=0$ or $\partial u^-/\partial n=0$. Then, the relation (20) still holds, where, now, Ω^- denotes the part of the scatterer between the surfaces S and S^-.

IV. RECIPROCITY RELATIONS

The proof of Theorem 2 uses two evaluations of $[u_a^{\mathrm{t}},u_b^{\mathrm{t}}]$. If, instead, we start from $[\overline{u_a^{\mathrm{t}}},u_b^{\mathrm{t}}]$, we obtain a reciprocity theorem. This is not surprising, because u_a^{t} can be regarded as the exact Green's function for the scattering problem. The reciprocity theorem can be found on p. 48 of Ref. 6, for example. We quote it here, using our normalizations.

Theorem 3: *For any two point-source locations in* Ω, **a** *and* **b**, *and for any scatterer, we have*

$$h_0(ka)u_a^{\mathrm{s}}(\mathbf{b})=h_0(kb)u_b^{\mathrm{s}}(\mathbf{a}), \tag{26}$$

where $h_0(x)=\mathrm{e}^{\mathrm{i}x}/(\mathrm{i}x)$.

From Eq. (1), we see that the same reciprocity relation holds for the incident fields, as well: $h_0(ka)u_a^{\mathrm{i}}(\mathbf{b})=h_0(kb)u_b^{\mathrm{i}}(\mathbf{a})$. Hence, by Eq. (2) we conclude that the total exterior fields satisfy $h_0(ka)u_a^{\mathrm{t}}(\mathbf{b})=h_0(kb)u_b^{\mathrm{t}}(\mathbf{a})$.

We note that the presence of the multiplicative constant in the above reciprocity relation is due to the form of the modified spherical wave, Eq. (1). If we consider the point sources lying on the same sphere, that is, $a=b$, then we obtain the following results:

$$u_a^{\mathrm{s}}(\mathbf{b})=u_b^{\mathrm{s}}(\mathbf{a}),\quad u_a^{\mathrm{i}}(\mathbf{b})=u_b^{\mathrm{i}}(\mathbf{a}),\quad u_a^{\mathrm{t}}(\mathbf{b})=u_b^{\mathrm{t}}(\mathbf{a}). \tag{27}$$

These relations express the fact that interchanging the excitation with the observation point, the scattered, incident and total fields remain unchanged. From Eq. (26) we cannot have a reciprocity relation for the corresponding spherical far-field patterns, because when the point sources go to infinity the spherical waves reduce to plane waves.

V. THE OPTICAL THEOREM

In Ref. 8, an optical theorem for spherical waves incident upon a soft scatterer has been proved. Now, this theorem as well as optical theorems for scatterers of other types can be derived as corollaries of the general scattering theorem. First we define the scattering cross-section due to a point source at **a** (Ref. 6) as

$$\sigma_a^{\mathrm{s}}=\frac{1}{k^2}\int_{S^2}|g_a(\hat{\mathbf{r}})|^2 ds(\hat{\mathbf{r}}), \tag{28}$$

the absorption cross-section as

$$\sigma_a^{\mathrm{a}}=\frac{1}{k}\,\mathrm{Im}\int_S u_a^{\mathrm{t}}\frac{\partial\overline{u_a^{\mathrm{t}}}}{\partial n}ds, \tag{29}$$

and the extinction cross-section as

$$\sigma_a^{\mathrm{e}}=\sigma_a^{\mathrm{s}}+\sigma_a^{\mathrm{a}}. \tag{30}$$

If we put $\mathbf{a}=\mathbf{b}$ in Theorem 2, we obtain

$$2\,\mathrm{Re}\{G_a(\mathbf{a})\}+\frac{1}{2\pi}\int_{S^2}|g_a(\hat{\mathbf{r}})|^2 ds(\hat{\mathbf{r}})=\mathcal{E}_{a,a}.$$

We can rewrite this equation using Eq. (28) to give

$$\sigma_a^{\mathrm{s}}=-4\pi k^{-2}\,\mathrm{Re}\{G_a(\mathbf{a})\}+2\pi k^{-2}\mathcal{E}_{a,a}. \tag{31}$$

From the definitions (17) and (29), we have

$$\sigma_a^{\mathrm{a}}=\tfrac{1}{2}\mathrm{i}k^{-1}[u_a^{\mathrm{t}},u_a^{\mathrm{t}}]=-2\pi k^{-2}\mathcal{E}_{a,a}. \tag{32}$$

Hence, adding Eqs. (31) and (32), Eq. (30) gives

$$\sigma_a^{\mathrm{e}}=-4\pi k^{-2}\,\mathrm{Re}\{G_a(\mathbf{a})\}. \tag{33}$$

The value of $\mathcal{E}_{a,a}$ is given in Theorem 2. In particular, for a penetrable scatterer, we obtain

$$\sigma_a^{\mathrm{a}}=-\frac{1}{k}\,\mathrm{Im}(\beta)\int_{\Omega^-}|\nabla u_a^-(\mathbf{r})|^2 dv(\mathbf{r}), \tag{34}$$

whereas for an impedance surface, we have

$$\sigma_a^{\mathrm{a}}=\lambda k\int_S|u_a^{\mathrm{t}}|^2 ds.$$

We remark that the absorption cross-section σ_a^{a} provides a measure of the total energy taken from the incident spherical wave and absorbed by the surface of the scatterer in the impedance boundary case, or by the lossy medium occupying Ω^- in the penetrable case. It is clear that $\sigma_a^{\mathrm{a}}=0$ for the soft and hard scatterers and $\sigma_a^{\mathrm{a}}\geqslant 0$ for the other cases.

VI. MIXED SCATTERING RELATIONS

For inverse problems, one effective reconstruction method is the point-source method.[1] One of the main steps of this method is the derivation of mixed reciprocity relations. These relations were introduced in Ref. 10 for sound-soft scatterers, and in Ref. 1 for sound-hard scatterers.

In this section, we allow one of the two point sources considered previously to recede to infinity, so that we have one spherical incident wave and one plane incident wave. We let both sources recede to infinity at the end of this section, and recover known results for plane-wave incidence.

An incident plane wave propagating in the direction of the unit vector $\hat{\mathbf{d}}$ is given by

$$u^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{d}}) = \exp\{\mathrm{i}k\hat{\mathbf{d}}\cdot\mathbf{r}\}. \tag{35}$$

We have already noted that $u_a^{\mathrm{i}}(\mathbf{r}) \to u^{\mathrm{i}}(\mathbf{r};-\hat{\mathbf{a}})$ as $a\to\infty$.

For an incident plane wave, Eq. (35), we denote the total field in Ω, the scattered field and the far-field pattern by $u^{\mathrm{t}}(\mathbf{r};\hat{\mathbf{d}})$, $u^{\mathrm{s}}(\mathbf{r};\hat{\mathbf{d}})$ and $g(\hat{\mathbf{r}};\hat{\mathbf{d}})$, respectively, indicating the dependence on the incident direction $\hat{\mathbf{d}}$. We have[4]

$$u_a^{\mathrm{s}}(\mathbf{r}) \to u^{\mathrm{s}}(\mathbf{r};-\hat{\mathbf{a}}), \quad \text{as} \quad a\to\infty \tag{36a}$$

and

$$g_a(\hat{\mathbf{r}}) \to g(\hat{\mathbf{r}};-\hat{\mathbf{a}}), \quad \text{as} \quad a\to\infty. \tag{36b}$$

Now, consider our previous results, involving $\mathbf{a}$ and $\mathbf{b}$, and let $b\to\infty$. Lemma 1 gives the following results.

Lemma 4: Let $u_a^{\mathrm{i}}(\mathbf{r})$ be an incident spherical wave and let $u^{\mathrm{i}}(\mathbf{r};-\hat{\mathbf{b}})$ be an incident plane wave. Then

$$\lim_{r\to\infty}[u_a^{\mathrm{i}}, u^{\mathrm{s}}(\cdot,-\hat{\mathbf{b}})]_{S_r} = 2a\mathrm{e}^{\mathrm{i}ka}\int_{S^2} g(\hat{\mathbf{r}};-\hat{\mathbf{b}})\mathrm{e}^{\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{a}}ds(\hat{\mathbf{r}}) \tag{37}$$

and

$$\lim_{\varepsilon\to 0}[u_a^{\mathrm{i}}, u^{\mathrm{s}}(\cdot,-\hat{\mathbf{b}})]_{S_{a,\varepsilon}} = 4\pi a\mathrm{e}^{\mathrm{i}ka}u^{\mathrm{s}}(\mathbf{a};-\hat{\mathbf{b}}). \tag{38}$$

Next, we define a *plane far-field pattern generator* by

$$G(\mathbf{a};-\hat{\mathbf{b}}) = \lim_{b\to\infty} G_b(\mathbf{a}) \tag{39}$$

$$= \mathrm{i}ka\mathrm{e}^{\mathrm{i}ka}\left[u^{\mathrm{s}}(\mathbf{a};-\hat{\mathbf{b}}) - \frac{1}{2\pi}\int_{S^2} g(\hat{\mathbf{r}};-\hat{\mathbf{b}})\mathrm{e}^{\mathrm{i}k\mathbf{a}\cdot\hat{\mathbf{r}}}ds(\hat{\mathbf{r}})\right], \tag{40}$$

where the spherical far-field pattern generator $G_b(\mathbf{a})$ is defined by Eq. (15). We will also require $\lim_{a\to\infty} G_b(\mathbf{a})$; this limit is contained in the following theorem.

Theorem 5: *For two incident spherical waves, u_a^{i} and u_b^{i}, we have*

$$\lim_{a\to\infty} G_b(\mathbf{a}) = g_b(-\hat{\mathbf{a}}) \tag{41}$$

and

$$\lim_{a\to\infty} G(\mathbf{a};-\hat{\mathbf{b}}) = g(-\hat{\mathbf{a}};-\hat{\mathbf{b}}). \tag{42}$$

Proof: We prove Eq. (41); a very similar argument gives Eq. (42).

We choose coordinates so that the point source at $\mathbf{a}$ is on the z-axis. Then, take spherical polar coordinates (θ, φ) on S^2, so that $\hat{\mathbf{a}}\cdot\hat{\mathbf{r}} = \cos\theta$. Hence for $\theta = 0$ we have $\hat{\mathbf{r}} = \hat{\mathbf{a}}$, while for $\theta = \pi$ we have $\hat{\mathbf{r}} = -\hat{\mathbf{a}}$. If we define

$$F_b(\theta) = \int_0^{2\pi} g_b(\hat{\mathbf{r}})\, d\varphi, \tag{43}$$

then we have $F_b(0) = 2\pi g_b(\hat{\mathbf{a}})$ and $F_b(\pi) = 2\pi g_b(-\hat{\mathbf{a}})$. Hence

$$\begin{aligned}\int_{S^2} g_b(\hat{\mathbf{r}})\mathrm{e}^{\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{a}} ds(\hat{\mathbf{r}}) &= \int_0^{\pi} F_b(\theta)\mathrm{e}^{\mathrm{i}ka\cos\theta}\sin\theta\, d\theta \\ &= \frac{\mathrm{i}}{ka}\int_0^{\pi} F_b(\theta)\frac{d}{d\theta}(\mathrm{e}^{\mathrm{i}ka\cos\theta})\, d\theta \\ &= \frac{2\pi\mathrm{i}}{ka}[g_b(-\hat{\mathbf{a}})\mathrm{e}^{-\mathrm{i}ka} - g_b(\hat{\mathbf{a}})\mathrm{e}^{\mathrm{i}ka}] - \frac{\mathrm{i}}{ka}\int_0^{\pi}\mathrm{e}^{\mathrm{i}ka\cos\theta}\frac{dF_b(\theta)}{d\theta}\, d\theta.\end{aligned}$$

From this equation and Eq. (15), we find that

$$G_b(\mathbf{a}) = \mathrm{i}ka\mathrm{e}^{\mathrm{i}ka}u_b^s(\mathbf{a}) + \mathrm{e}^{\mathrm{i}ka}[g_b(-\hat{\mathbf{a}})\mathrm{e}^{-\mathrm{i}ka} - g_b(\hat{\mathbf{a}})\mathrm{e}^{\mathrm{i}ka}] + \frac{\mathrm{e}^{\mathrm{i}ka}}{2\pi}\int_0^{\pi}\mathrm{e}^{\mathrm{i}ka\cos\theta}\frac{dF_b(gv)}{d\theta}\, d\theta. \tag{44}$$

In view of Eq. (8) and taking into account that the integral in Eq. (44) tends to zero as $a\to\infty$, by the Riemann-Lebesgue lemma, we get Eq. (41).

We can now let $b\to\infty$ in the general scattering theorem, Theorem 2; this gives the following results.

Theorem 6: *Let $u_a^{\mathrm{i}}(\mathbf{r})$ be an incident spherical wave and let $u^{\mathrm{i}}(\mathbf{r};-\hat{\mathbf{b}})$ be an incident plane wave. Then*

$$G(\mathbf{a};\hat{\mathbf{b}}) + \overline{g_a(-\hat{\mathbf{b}})} + \frac{1}{2\pi}\int_{S^2} g(\hat{\mathbf{r}};-\hat{\mathbf{b}})\overline{g_a(\hat{\mathbf{r}})}\, ds(\hat{\mathbf{r}}) = \mathcal{M}_a(-\hat{\mathbf{b}}), \tag{45}$$

where $\mathcal{M}_a(-\hat{\mathbf{b}}) = \lim_{b\to\infty}\mathcal{E}_{a,b}$:

$$\mathcal{M}_a(-\hat{\mathbf{b}}) = 0 \quad \textit{for Dirichlet or Neumann conditions on } S; \tag{46}$$

$$\mathcal{M}_a(-\hat{\mathbf{b}}) = -\frac{k^2\lambda}{2\pi}\int_S u^t(\mathbf{r};-\hat{\mathbf{b}})\overline{u_a^t(\mathbf{r})}\, ds(\hat{\mathbf{r}}) \quad \textit{for the Robin condition (5) on } S; \tag{47}$$

or

$$\mathcal{M}_a(-\hat{\mathbf{b}}) = -\frac{k}{2\pi}\mathrm{Im}(\beta)\int_{\Omega^-}\nabla\overline{u_a^-(\mathbf{r})}\cdot\nabla u^-(\mathbf{r};-\hat{\mathbf{b}})\, dv(\mathbf{r}) \quad \textit{for a penetrable scatterer.} \tag{48}$$

The mixed reciprocity principle is contained in the next theorem.

Theorem 7: *Let $u_a^{\mathrm{i}}(\mathbf{r})$ be an incident spherical wave and let $u^{\mathrm{i}}(\mathbf{r};-\hat{\mathbf{b}})$ be an incident plane wave. Then, we have the following reciprocity relation:*

$$g_a(\hat{\mathbf{b}}) = \mathrm{i}ka\,\mathrm{e}^{-\mathrm{i}ka} u^s(\mathbf{a}; -\hat{\mathbf{b}}). \tag{49}$$

Proof: Let $b \to \infty$ in Theorem 3, using Eqs. (8) and (36a). □

This result means that the spherical far-field pattern of the point source at $\mathbf{a}$ in the direction $\hat{\mathbf{b}}$ is proportional to the scattered field at $\mathbf{a}$ due to the incident plane wave with direction of propagation $-\hat{\mathbf{b}}$.

Finally, if we combine Eqs. (36b), (39), (41) and (42), we obtain

$$\lim_{a\to\infty}\lim_{b\to\infty} G_b(\mathbf{a}) = \lim_{b\to\infty}\lim_{a\to\infty} G_b(\mathbf{a}) = g(-\hat{\mathbf{a}}; -\hat{\mathbf{b}}). \tag{50}$$

We can then check that letting both point sources recede to infinity, $a \to \infty$ and $b \to \infty$, yields the known scattering and optical theorems for plane-wave scattering; see Refs. 11–13, 6, and 8.

VII. FORMULATION: ELECTROMAGNETICS

In the remainder of the article, we consider electromagnetic problems. The exterior Ω is an infinite homogeneous medium with electric permittivity ε, magnetic permeability μ, phase velocity c and conductivity $\sigma = 0$. The scatterer Ω^- is filled with a homogeneous medium with corresponding physical parameters ε^-, μ^-, c^- and $\sigma^- \neq 0$.

We consider an incident spherical electromagnetic wave due to a source located at a point with position vector $\mathbf{a}$, with respect to the origin $\mathcal{O}$. This incident wave $(\mathbf{E}_a^{\mathrm{i}}, \mathbf{H}_a^{\mathrm{i}})$ has the form[9]

$$\mathbf{E}_a^{\mathrm{i}}(\mathbf{r}; \hat{\mathbf{p}}) = \frac{a\,\mathrm{e}^{-\mathrm{i}ka}}{\mathrm{i}k} \nabla \times \left(\frac{\mathrm{e}^{\mathrm{i}k|r-a|}}{|\mathbf{r}-\mathbf{a}|} \hat{\mathbf{a}} \times \hat{\mathbf{p}} \right), \tag{51}$$

$$\mathbf{H}_a^{\mathrm{i}}(\mathbf{r}; \hat{\mathbf{p}}) = (\mathrm{i}k)^{-1} (\varepsilon/\mu)^{1/2} \nabla \times \mathbf{E}_a^{\mathrm{i}}(\mathbf{r}; \hat{\mathbf{p}}), \tag{52}$$

where $\hat{\mathbf{p}}$ is a constant unit vector with $\hat{\mathbf{p}} \cdot \hat{\mathbf{a}} = 0$, $k = \omega\sqrt{\varepsilon\mu} > 0$ is the free-space wave number, and $a = |\mathbf{a}|$. Physically, $(\mathbf{E}_a^{\mathrm{i}}, \mathbf{H}_a^{\mathrm{i}})$ represents the field generated by a magnetic dipole with dipole moment $\hat{\mathbf{a}} \times \hat{\mathbf{p}}$; see p. 163 of Ref. 14 or p. 23 of Ref. 6. The coefficient $a\mathrm{e}^{-\mathrm{i}ka}/(\mathrm{i}k)$ in Eq. (51) assures that when the point source tends to infinity the spherical wave reduces to a plane electric wave with direction of propagation $-\hat{\mathbf{a}}$ and polarization $\hat{\mathbf{p}}$. The total electric exterior field $\mathbf{E}_a^{\mathrm{t}}$ is given by

$$\mathbf{E}_a^{\mathrm{t}}(\mathbf{r}; \hat{\mathbf{p}}) = \mathbf{E}_a^{\mathrm{i}}(\mathbf{r}; \hat{\mathbf{p}}) + \mathbf{E}_a^{\mathrm{s}}(\mathbf{r}; \hat{\mathbf{p}}), \quad \mathbf{r} \in \Omega \backslash \{\mathbf{a}\}, \tag{53}$$

where $\mathbf{E}_a^{\mathrm{s}}(\mathbf{r}; \hat{\mathbf{p}})$ is the scattered electric field, which satisfies the Silver-Müller radiation condition

$$\lim_{r\to\infty} (\mathbf{r} \times \nabla \times \mathbf{E}_a^{\mathrm{s}} + \mathrm{i}kr\mathbf{E}_a^{\mathrm{s}}) = \mathbf{0} \tag{54}$$

uniformly in all directions $\hat{\mathbf{r}} \in S^2$, where S^2 is the unit sphere. $\mathbf{E}_a^{\mathrm{t}}$ solves the equation

$$\nabla \times \nabla \times \mathbf{E}_a^{\mathrm{t}} = k^2 \mathbf{E}_a^{\mathrm{t}} \text{ in } \Omega. \tag{55}$$

We note that the incident electric field satisfies the radiation condition (54), and hence the total electric field also satisfies Eq. (54).

The surface of the scatterer may be perfectly conducting, in which case

$$\hat{\mathbf{n}} \times \mathbf{E}_a^{\mathrm{t}} = \mathbf{0} \text{ on } S, \tag{56}$$

or it may be an impedance surface, in which case

$$\hat{\mathbf{n}} \times \nabla \times \mathbf{E}_a^{\mathrm{t}} = -(\mathrm{i}k/Z_s) \hat{\mathbf{n}} \times (\hat{\mathbf{n}} \times \mathbf{E}_a^{\mathrm{t}}) \text{ on } S, \tag{57}$$

where the dimensionless parameter Z_s denotes the surface impedance relative to the characteristic impedance of the medium and may vary on S.

If the scatterer is a dielectric, the incident electromagnetic waves are transmitted into the scatterer. Let $\mathbf{E}_a^-$ be the total electric field in the interior. Then $\mathbf{E}_a^-$ satisfies

$$\nabla\times\nabla\times\mathbf{E}_a^- = \eta^2 k^2 \mathbf{E}_a^- \quad \text{in} \quad \Omega^-, \tag{58}$$

where the complex constant η is the relative index of refraction; on the surface of the scatterer we have the following transmission conditions:

$$\hat{\mathbf{n}}\times\mathbf{E}_a^t = \hat{\mathbf{n}}\times\mathbf{E}_a^- \quad \text{and} \quad \hat{\mathbf{n}}\times\nabla\times\mathbf{E}_a^t = (\mu/\mu^-)\hat{\mathbf{n}}\times\nabla\times\mathbf{E}_a^- \quad \text{on} \quad S.$$

The behavior of the scattered electric field in the radiation zone is given by

$$\mathbf{E}_a^s(\mathbf{r}) = h_0(kr)\mathbf{g}_a(\hat{\mathbf{r}}) + O(r^{-2}), \quad r\to\infty, \tag{59}$$

where $\mathbf{g}_a(\hat{\mathbf{r}})$ is the far-field pattern.

More details on the physical parameters of the above problems can be found in Ref. 6. Each problem has a unique and stable classical solution.[14,15]

VIII. GENERAL SCATTERING THEOREM: ELECTROMAGNETICS

In the sequel, for an incident time-harmonic spherical wave $\mathbf{E}_a^i(\mathbf{r};\hat{\mathbf{p}})$ due to a point source located at $\mathbf{a}$, we will denote the total field in Ω, the scattered field and the far-field pattern by writing $\mathbf{E}_a^t(\mathbf{r};\hat{\mathbf{p}})$, $\mathbf{E}_a^s(\mathbf{r};\hat{\mathbf{p}})$ and $\mathbf{g}_a(\hat{\mathbf{r}};\hat{\mathbf{p}})$, respectively, indicating the dependence on the position $\mathbf{a}$ of the point source and the polarization $\hat{\mathbf{p}}$. Also, the total electric field in Ω^- will be denoted by $\mathbf{E}_a^-(\mathbf{r};\hat{\mathbf{p}})$. We consider a point source at $\mathbf{a}$ with polarization $\hat{\mathbf{p}}_1$ and another point source at $\mathbf{b}$ with polarization $\hat{\mathbf{p}}_2$.

For a shorthand notation, we use

$$\{\mathbf{E},\mathbf{E}'\}_S = \int_S [(\hat{\mathbf{n}}\times\overline{\mathbf{E}})\cdot(\nabla\times\mathbf{E}') - (\hat{\mathbf{n}}\times\mathbf{E}')\cdot(\nabla\times\overline{\mathbf{E}})]ds;$$

in particular, we write $\{\mathbf{E},\mathbf{E}'\}\equiv\{\mathbf{E},\mathbf{E}'\}_S$.

Lemma 8: Let $\mathbf{E}_a^i(\mathbf{r};\hat{\mathbf{p}}_1)$ *be a point source at* $\mathbf{a}$. *Let* $\mathbf{E}_b^i(\mathbf{r};\hat{\mathbf{p}}_2)$ *be a point source at* $\mathbf{b}$, *with corresponding scattered field* $\mathbf{E}_b^s(\mathbf{r};\hat{\mathbf{p}}_2)$ *and far-field pattern* $\mathbf{g}_b(\hat{\mathbf{r}};\hat{\mathbf{p}}_2)$. *Then*

$$\lim_{r\to\infty}\{\mathbf{E}_a^i(\cdot;\hat{\mathbf{p}}_1),\mathbf{E}_b^s(\cdot;\hat{\mathbf{p}}_2)\}_{S_r} = 2a\mathrm{e}^{\mathrm{i}ka}\int_{S^2}\mathbf{g}_b(\hat{\mathbf{r}};\hat{\mathbf{p}}_2)\cdot(\hat{\mathbf{r}}\times(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1))\mathrm{e}^{\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{a}}ds(\hat{\mathbf{r}}) \tag{60}$$

and

$$\lim_{\varepsilon\to 0}\{\mathbf{E}_a^i(\cdot;\hat{\mathbf{p}}_1),\mathbf{E}_b^s(\cdot,\hat{\mathbf{p}}_2)\}_{S_{a,\varepsilon}} = 4\pi\mathrm{i}(a/k)\mathrm{e}^{\mathrm{i}ka}(\nabla\times\mathbf{E}_b^s(\mathbf{a};\hat{\mathbf{p}}_2))\cdot(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1), \tag{61}$$

where S_r *is a large sphere of radius r enclosing* $\mathbf{a}$ *and* $\mathbf{b}$, *and* $S_{a,\varepsilon}$ *is a small sphere surrounding* $\mathbf{a}$, *defined by Eq. (10).*

Proof: For Eq. (60), we use the asymptotic forms (13). These show that the incident electric wave takes the form

$$\mathbf{E}_a^i(\mathbf{r};\hat{\mathbf{p}}_1) = h_0(kr)\mathbf{g}_a^i(\hat{\mathbf{r}};\hat{\mathbf{p}}_1) + O(r^{-2}), \quad r\to\infty, \tag{62}$$

where $\mathbf{g}_a^i(\hat{\mathbf{r}};\hat{\mathbf{p}}_1) = \mathrm{i}ka\exp\{-\mathrm{i}ka(1+\hat{\mathbf{r}}\cdot\hat{\mathbf{a}})\}\ (\hat{\mathbf{r}}\times(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1))$ is the far-field pattern of the point source incident wave. Using Eqs. (59) and (62) we establish Eq. (60). Note that $\hat{\mathbf{r}}\cdot\mathbf{g}_a^i(\hat{\mathbf{r}};\hat{\mathbf{p}}_1) = 0$.

For Eq. (61), some calculations show that

$$\{\mathbf{E}_a^{\mathrm{i}}(\cdot,\hat{\mathbf{p}}_1),\mathbf{E}_b^{\mathrm{s}}(\cdot,\hat{\mathbf{p}}_2)\}_{S_{a,\varepsilon}}=a\mathrm{e}^{\mathrm{i}ka}\Bigg\{\int_{S_{a,\varepsilon}}\hat{\mathbf{n}}\cdot\nabla\times[((\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1)\cdot\overline{\nabla h_0(k|\mathbf{r}-\mathbf{a}|)})\mathbf{E}_b^{\mathrm{s}}]ds$$
$$+\int_{S_{a,\varepsilon}}(\mathrm{i}k+|\mathbf{r}-\mathbf{a}|^{-1})\overline{h_0(k|\mathbf{r}-\mathbf{a}|)}(\nabla\times\mathbf{E}_b^{\mathrm{s}})\cdot(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1)ds$$
$$-k^2\int_{S_{a,\varepsilon}}\hat{\mathbf{n}}\cdot[\mathbf{E}_b^{\mathrm{s}}\times(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1)]\overline{h_0(k|\mathbf{r}-\mathbf{a}|)}ds\Bigg\}.$$

The first integral on the right-hand side vanishes by Stokes's theorem. Applying the mean value theorem on the remaining integrals and letting $\varepsilon\to 0$, we obtain Eq. (61). □

For two incident spherical electric waves, $\mathbf{E}_a^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{p}}_1)$ and $\mathbf{E}_b^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{p}}_2)$, we define a *spherical far-field pattern generator*, as follows:

$$\mathbf{G}_b(\mathbf{a};\hat{\mathbf{p}}_2)=\mathrm{e}^{\mathrm{i}ka}\mathbf{a}\times\left[\nabla\times\mathbf{E}_b^{\mathrm{s}}(\mathbf{a};\hat{\mathbf{p}}_2)-\frac{\mathrm{i}k}{2\pi}\int_{S^2}\hat{\mathbf{r}}\times\mathbf{g}_b(\hat{\mathbf{r}};\hat{\mathbf{p}}_2)\mathrm{e}^{\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{a}}ds(\hat{\mathbf{r}})\right]. \tag{63}$$

As we shall see later, when the point sources recede to infinity, $\mathbf{G}_b(\mathbf{a};\hat{\mathbf{p}}_2)$ is reduced to the far-field pattern for an incident plane electric wave propagating in the direction $-\hat{\mathbf{a}}$ and of polarization $\hat{\mathbf{p}}_2$. Using this notation, the general scattering theorem for spherical electric waves is formulated as follows.

Theorem 9: *For any two point-source locations in* Ω, **a** *and* **b**, *and for any polarizations,* $\hat{\mathbf{p}}_1$ *and* $\hat{\mathbf{p}}_2$, *we have*

$$\hat{\mathbf{p}}_1\cdot\mathbf{G}_1(\mathbf{a};\hat{\mathbf{p}}_2)+\hat{\mathbf{p}}_2\cdot\overline{\mathbf{G}_a(\mathbf{b};\hat{\mathbf{p}}_1)}+\frac{1}{2\pi}\int_{S^2}\mathbf{g}_b(\hat{\mathbf{r}};\hat{\mathbf{p}}_2)\cdot\overline{\mathbf{g}_a(\hat{\mathbf{r}};\hat{\mathbf{p}}_1)}ds(\hat{\mathbf{r}})=\mathcal{E}_{a,b}(\hat{\mathbf{p}}_1;\hat{\mathbf{p}}_2), \tag{64}$$

where

$$\mathcal{E}_{a,b}(\hat{\mathbf{p}}_1;\hat{\mathbf{p}}_2)=-\frac{\mathrm{i}k}{4\pi}\{\mathbf{E}_a^{\mathrm{t}}(\cdot,\hat{\mathbf{p}}_1),\mathbf{E}_b^{\mathrm{t}}(\cdot,\hat{\mathbf{p}}_2)\}. \tag{65}$$

The value of $\mathcal{E}_{a,b}$ *depends on the scatterer:*

$$\mathcal{E}_{a,b}=0 \quad \textit{for a perfectly conducting surface;} \tag{66}$$

$$\mathcal{E}_{a,b}(\hat{\mathbf{p}}_1;\hat{\mathbf{p}}_2)=-\frac{k^2}{2\pi}\int_S\frac{\mathrm{Re}(Z_S)}{|Z_S|^2}(\hat{\mathbf{n}}\times\overline{\mathbf{E}_a^{\mathrm{t}}(\hat{\mathbf{r}};\hat{\mathbf{p}}_1)})\cdot(\hat{\mathbf{n}}\times\mathbf{E}_b^{\mathrm{t}}(\hat{\mathbf{r}};\hat{\mathbf{p}}_2))ds(\mathbf{r}) \tag{67}$$

for the impedance boundary condition (57); or

$$\mathcal{E}_{a,b}(\hat{\mathbf{p}}_1;\hat{\mathbf{p}}_2)=-\frac{k^3\mu}{2\pi\mu^-}\mathrm{Im}(\eta^2)\int_{\Omega^-}\overline{\mathbf{E}_a^-(\hat{\mathbf{r}};\hat{\mathbf{p}}_1)}\cdot\mathbf{E}_b^-(\hat{\mathbf{r}};\hat{\mathbf{p}}_2)dv \tag{68}$$

for a dielectric scatterer.

Proof: We proceed exactly as in the proof of Theorem 2. First, we evaluate $\mathcal{E}_{a,b}$ directly, using the boundary or transmission conditions on S; for the dielectric scatterer, we have to apply the divergence theorem in Ω^-. This gives the stated expressions for $\mathcal{E}_{a,b}$.

Next, we give an alternative evaluation of $\mathcal{E}_{a,b}$, using the relations $\mathbf{E}_\alpha^{\mathrm{t}}=\mathbf{E}_\alpha^{\mathrm{i}}+\mathbf{E}_\alpha^{\mathrm{s}}$, for $\alpha=a,\ b$. Formally, the calculations proceed as before, with $\{\cdot,\cdot\}$ in place of $[\cdot,\cdot]$. We also use the vector version of Green's second theorem, which gives

$$\{\mathbf{E}_a^{\mathrm{i}},\mathbf{E}_b^{\mathrm{i}}\}=0, \tag{69}$$

$$\{\mathbf{E}_a^{\mathrm{i}},\mathbf{E}_b^{\mathrm{s}}\}=-4\pi\mathrm{i}(a/k)\mathrm{e}^{\mathrm{i}ka}(\nabla\times\mathbf{E}_b^{\mathrm{s}}(\mathbf{a};\hat{\mathbf{p}}_2))\cdot(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1)+2a\mathrm{e}^{\mathrm{i}ka}\int_{S^2}\mathbf{g}_b(\hat{\mathbf{r}};\hat{\mathbf{p}}_2)\cdot(\hat{\mathbf{r}}\times(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1))\mathrm{e}^{\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{a}}ds(\hat{\mathbf{r}}) \tag{70}$$

and

$$\{\mathbf{E}_a^{\mathrm{s}},\mathbf{E}_b^{\mathrm{s}}\}=\frac{2\mathrm{i}}{k}\int_{S^2}\overline{\mathbf{g}_a(\hat{\mathbf{r}};\hat{\mathbf{p}}_1)}\cdot\mathbf{g}_b(\hat{\mathbf{r}};\hat{\mathbf{p}}_2)ds(\hat{\mathbf{r}}). \tag{71}$$

The remaining details are omitted. □

There is also a reciprocity theorem, as $\mathbf{E}_a^{\mathrm{t}}$ is an exact Green's function. It can be found on p. 63 of Ref. 6, for example. With our normalizations, it takes the following form.

Theorem 10: *For any two point-source locations in* Ω, **a** *and* **b**, *for any polarizations,* $\hat{\mathbf{p}}_1$ *and* $\hat{\mathbf{p}}_2$, *and for any scatterer, we have*

$$h_0(ka)(\hat{\mathbf{b}}\times\hat{\mathbf{p}}_2)\cdot(\nabla\times\mathbf{E}_a^{\mathrm{s}}(\hat{\mathbf{b}};\hat{\mathbf{p}}_1))=h_0(kb)(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1)\cdot(\nabla\times\mathbf{E}_b^{\mathrm{s}}(\hat{\mathbf{a}};\hat{\mathbf{p}}_2)). \tag{72}$$

IX. OPTICAL THEOREM: ELECTROMAGNETICS

In Ref. 9, an optical theorem for spherical waves incident upon a perfect conductor has been proved. Here, we generalize this result to other scatterers, using the general scattering theorem.

First we define the scattering cross-section due to a point source at **a** (Ref. 6) as

$$\sigma_a^{\mathrm{s}}=\frac{1}{k^2}\int_{S^2}|\mathbf{g}_a(\hat{\mathbf{r}};\hat{\mathbf{p}})|^2ds(\hat{\mathbf{r}}), \tag{73}$$

the absorption cross-section as

$$\sigma_a^{\mathrm{a}}=\frac{1}{k}\mathrm{Im}\int_S\hat{n}\cdot(\mathbf{E}_a^{\mathrm{t}}\times\nabla\times\overline{\mathbf{E}_a^{\mathrm{t}}})ds \tag{74}$$

and the extinction cross-section, σ_a^{e}, by Eq. (30).

If we put $\mathbf{a}=\mathbf{b}$ and $\hat{\mathbf{p}}_1=\hat{\mathbf{p}}_2=\hat{\mathbf{p}}$ in Theorem 9, we obtain

$$2\,\mathrm{Re}[\hat{\mathbf{p}}\cdot\mathbf{G}_a(a;\hat{\mathbf{p}})]+\frac{1}{2\pi}\int_{S^2}|\mathbf{g}_a(\hat{\mathbf{r}};\hat{\mathbf{p}})|^2ds(\hat{\mathbf{r}})=\mathcal{E}_{a,a}(\hat{\mathbf{p}};\hat{\mathbf{p}}),$$

which we can rewrite as

$$\sigma_a^{\mathrm{s}}=-4\pi k^{-2}\,\mathrm{Re}[\hat{\mathbf{p}}\cdot\mathbf{G}_a(\mathbf{a};\hat{\mathbf{p}})]+2\pi k^{-2}\mathcal{E}_{a,a}(\hat{\mathbf{p}};\hat{\mathbf{p}}). \tag{75}$$

From the definitions (65) and (74), we have

$$\sigma_a^{\mathrm{a}}=\tfrac{1}{2}\mathrm{i}k^{-1}\{\mathbf{E}_a^{\mathrm{t}}(\cdot,\hat{\mathbf{p}}),\mathbf{E}_a^{\mathrm{t}}(\cdot,\hat{\mathbf{p}})\}=-2\pi k^{-2}\mathcal{E}_{a,a}(\hat{\mathbf{p}};\hat{\mathbf{p}}). \tag{76}$$

Hence, adding Eqs. (75) and (76), the definition (30) gives

$$\sigma_a^{\mathrm{e}}=-4\pi k^{-2}\,\mathrm{Re}[\hat{\mathbf{p}}\cdot\mathbf{G}_a(\mathbf{a};\hat{\mathbf{p}})]. \tag{77}$$

The value of $\mathcal{E}_{a,a}(\hat{\mathbf{p}};\hat{\mathbf{p}})$ is given in Theorem 9; it depends on the scatterer's properties.

X. MIXED SCATTERING RELATIONS

Let

$$\mathbf{E}^{\mathrm{i}}(r;\hat{\mathbf{d}},\hat{\mathbf{p}})=\hat{\mathbf{p}}\exp\{\mathrm{i}k\hat{\mathbf{d}}\cdot\mathbf{r}\}. \tag{78}$$

be an incident time-harmonic plane electric wave, where the unit vector $\hat{\mathbf{d}}$ describes the direction of propagation and the unit vector $\hat{\mathbf{p}}$ gives the polarization. We will indicate the dependence of the total field in Ω, the total field in Ω^-, the scattered field and the electric far-field pattern on the incident direction $\hat{\mathbf{d}}$ and the polarization $\hat{\mathbf{p}}$ by writing $\mathbf{E}^{\mathrm{t}}(\mathbf{r};\hat{\mathbf{d}},\hat{\mathbf{p}})$, $\mathbf{E}^{-}(\mathbf{r};\hat{\mathbf{d}},\hat{\mathbf{p}})$, $\mathbf{E}^{\mathrm{s}}(\mathbf{r};\hat{\mathbf{d}},\hat{\mathbf{p}})$ and $\mathbf{g}(\hat{\mathbf{r}};\hat{\mathbf{d}},\hat{\mathbf{p}})$, respectively.

Here, we consider mixed situations, and relate fields due to one spherical electric wave $\mathbf{E}_a^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{p}}_1)$ and one plane electric wave $\mathbf{E}^{\mathrm{i}}(\mathbf{r};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)$; we do this by letting $b\to\infty$ in our previous results.

Using the asymptotic forms (13), we can easily show that for the spherical electric wave (51) we have

$$\lim_{b\to\infty}\mathbf{E}_b^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{p}})=\mathbf{E}^{\mathrm{i}}(\mathbf{r};-\hat{\mathbf{b}},\hat{\mathbf{p}}), \tag{79}$$

that is the spherical electric wave, when the point source goes to infinity, reduces to a plane electric wave with direction of propagation $-\hat{\mathbf{b}}$ and polarization $\hat{\mathbf{p}}$. Similarly, we have $\mathbf{E}_b^{\mathrm{t}}(\mathbf{r};\hat{\mathbf{p}})\to\mathbf{E}^{\mathrm{t}}(\mathbf{r};-\hat{\mathbf{b}},\hat{\mathbf{p}})$, $\mathbf{E}_b^{\mathrm{s}}(\mathbf{r};\hat{\mathbf{p}})\to\mathbf{E}^{\mathrm{s}}(\mathbf{r};-\hat{\mathbf{b}},\hat{\mathbf{p}})$ and $\mathbf{g}_b(\hat{\mathbf{r}};\hat{\mathbf{p}})\to\mathbf{g}(\hat{\mathbf{r}};-\hat{\mathbf{b}},\hat{\mathbf{p}})$ as $b\to\infty$.

Next, let $b\to\infty$ in Lemma 8 to give the following result.

Lemma 11: Let $\mathbf{E}_a^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{p}}_1)$ *be an incident spherical electric wave and let* $\mathbf{E}^{\mathrm{i}}(\mathbf{r};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)$ *be an incident plane electric wave. Then*

$$\lim_{r\to\infty}\{\mathbf{E}_a^{\mathrm{i}}(\cdot;\hat{\mathbf{p}}_1),\mathbf{E}^{\mathrm{s}}(\cdot;-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)\}_{S_r}=2a\mathrm{e}^{\mathrm{i}ka}\int_{S^2}\mathbf{g}(\hat{\mathbf{r}};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)\cdot(\hat{\mathbf{r}}\times(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1))\mathrm{e}^{\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{a}}ds(\hat{\mathbf{r}})$$

and

$$\lim_{\varepsilon\to 0}\{\mathbf{E}_a^{\mathrm{i}}(\cdot;\hat{\mathbf{p}}_1),\mathbf{E}^{\mathrm{s}}(\cdot;-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)\}_{S_{a,\varepsilon}}=4\pi\mathrm{i}(a/k)\mathrm{e}^{\mathrm{i}ka}(\nabla\times\mathbf{E}^{\mathrm{s}}(\mathbf{a};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2))\cdot(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1).$$

We define a *plane far-field pattern generator* by the formula

$$\mathbf{G}(\mathbf{a};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)=\lim_{b\to\infty}\mathbf{G}_b(\mathbf{a};\hat{\mathbf{p}}_2)=\mathrm{e}^{\mathrm{i}ka}\mathbf{a}\times\left[\nabla\times\mathbf{E}^{\mathrm{s}}(\mathbf{a};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)-\frac{\mathrm{i}k}{2\pi}\int_{S^2}\hat{\mathbf{r}}\times\mathbf{g}(\hat{\mathbf{r}};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)\mathrm{e}^{\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{a}}ds(\hat{\mathbf{r}})\right],$$

where $\mathbf{G}_b(\mathbf{a};\hat{\mathbf{p}}_2)$ is defined by Eq. (63). Other limiting values are given in the next theorem.

Theorem 12: *For two incident point source electric waves,* $\mathbf{E}_a^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{p}}_1)$ *and* $\mathbf{E}_b^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{p}}_2)$*, we have*

$$\lim_{a\to\infty}\mathbf{G}_b(\mathbf{a};\hat{\mathbf{p}})=\mathbf{g}_b(-\hat{\mathbf{a}};\hat{\mathbf{p}}_2) \tag{80}$$

and

$$\lim_{a\to\infty}\mathbf{G}(\mathbf{a};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)=\mathbf{g}(-\hat{\mathbf{a}};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2). \tag{81}$$

Proof: For Eq. (80), we use spherical polar coordinates (θ, φ) as in the proof of Theorem 5, and define

$$\mathbf{F}_b(\theta)=\int_0^{2\pi}\hat{\mathbf{r}}\times\mathbf{g}_b(\hat{\mathbf{r}};\hat{\mathbf{p}}_2)d\varphi.$$

In particular, we have $\mathbf{F}_b(0)=2\pi\hat{\mathbf{a}}\times\mathbf{g}_b(\hat{\mathbf{a}};\hat{\mathbf{p}}_2)$ and $\mathbf{F}_b(\pi)=-2\pi\hat{\mathbf{a}}\times\mathbf{g}_b(-\hat{\mathbf{a}};\hat{\mathbf{p}}_2)$. Hence

$$\int_{S^2}\hat{\mathbf{r}}\times\hat{\mathbf{g}}_b(\hat{\mathbf{r}};\hat{\mathbf{p}}_2)\mathrm{e}^{\mathrm{i}k\hat{\mathbf{r}}\cdot\mathbf{a}}ds(\hat{\mathbf{r}})=\int_0^{\pi}\mathbf{F}_b(\theta)\mathrm{e}^{\mathrm{i}ka\cos\theta}\sin\theta d\theta$$

$$=\frac{\mathrm{i}}{ka}[\mathbf{F}_b(\pi)\mathrm{e}^{-\mathrm{i}ka}-\mathbf{F}_b(0)\mathrm{e}^{\mathrm{i}ka}]-\frac{\mathrm{i}}{ka}\int_0^{\pi}\mathrm{e}^{\mathrm{i}ka\cos\theta}\frac{d\mathbf{F}_b(\theta)}{d\theta}d\theta$$

$$\sim-\frac{2\pi\mathrm{i}}{ka}\hat{\mathbf{a}}\times[\mathbf{g}_b(-\hat{\mathbf{a}};\hat{\mathbf{p}}_2)\mathrm{e}^{-\mathrm{i}ka}+\mathbf{g}_b(\hat{\mathbf{a}};\hat{\mathbf{p}}_2)\mathrm{e}^{\mathrm{i}ka}]$$

for large a. From this equation and Eq. (63), we arrive at Eq. (80). The proof of Eq. (81) is similar. □

We can now let $b\to\infty$ in the general scattering theorem, Theorem 9.

Theorem 13: *Let* $\mathbf{E}_a^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{p}}_1)$ *be an incident spherical electric wave and let* $\mathbf{E}^{\mathrm{i}}(\mathbf{r};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)$ *be an incident plane electric wave. Then*

$$\hat{\mathbf{p}}_1\cdot\mathbf{G}(\mathbf{a};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)+\hat{\mathbf{p}}_2\cdot\overline{\mathbf{g}_a(\hat{\mathbf{b}};\hat{\mathbf{p}}_1)}+\frac{1}{2\pi}\int_{S^2}\mathbf{g}(\hat{\mathbf{r}};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)\cdot\overline{\mathbf{g}_a(\hat{\mathbf{r}};\hat{\mathbf{p}}_1)}ds(\hat{\mathbf{r}})=\mathcal{M}_a(-\hat{\mathbf{b}};\hat{\mathbf{p}}_1,\hat{\mathbf{p}}_2),$$

where $\mathcal{M}_a(-\hat{\mathbf{b}};\hat{\mathbf{p}}_1,\hat{\mathbf{p}}_2)=\lim_{b\to\infty}\mathcal{E}_{a,b}(\hat{\mathbf{p}}_1;\hat{\mathbf{p}}_2)$:

$$\mathcal{M}_a(-\hat{\mathbf{b}};\hat{\mathbf{p}}_1,\hat{\mathbf{p}}_2)=0 \tag{82}$$

for a perfectly conducting surface;

$$\mathcal{M}_a(-\hat{\mathbf{b}};\hat{\mathbf{p}}_1,\hat{\mathbf{p}}_2)=-\frac{k^2}{2\pi}\int_S\frac{\mathrm{Re}(Z_S)}{|Z_S|^2}(\hat{\mathbf{n}}\times\mathbf{E}^{\mathrm{t}}(\hat{\mathbf{r}};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2))\cdot(\hat{\mathbf{n}}\times\overline{\mathbf{E}_a^{\mathrm{t}}(\hat{\mathbf{r}};\hat{\mathbf{p}}_1)})ds(\hat{\mathbf{r}}) \tag{83}$$

for the impedance boundary condition; or

$$\mathcal{M}_a(-\hat{\mathbf{b}};\hat{\mathbf{p}}_1,\hat{\mathbf{p}}_2)=-\frac{k^3\mu}{2\pi\mu^-}\mathrm{Im}(\eta^2)\int_{\Omega^-}\overline{\mathbf{E}_a^-(\hat{\mathbf{r}};\hat{\mathbf{p}}_1)}\cdot\mathbf{E}^-(\hat{\mathbf{r}};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)dv \tag{84}$$

for a dielectric scatterer.

Proof: The proof is similar to that of Theorem 9. The only substantial difference appears in the formula for $\{\mathbf{E}_a^{\mathrm{s}},\mathbf{E}^{\mathrm{i}}\}$; cf. Eq. (70). Now, using the plane electric wave (78), we find that (see p. 59 of Ref. 6)

$$\{\mathbf{E}_a^{\mathrm{s}}(\cdot;\hat{\mathbf{p}}_1),\mathbf{E}^i(\cdot;-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)\}=\hat{\mathbf{p}}_2\cdot\int_S[\hat{\mathbf{n}}\times\nabla\times\overline{\mathbf{E}_a^{\mathrm{s}}(\mathbf{r};\hat{\mathbf{p}}_1)}+\mathrm{i}k\hat{\mathbf{b}}\times(\hat{\mathbf{n}}\times\overline{\mathbf{E}_a^{\mathrm{s}}(\mathbf{r};\hat{\mathbf{p}}_1)})]\mathrm{e}^{-\mathrm{i}k\hat{\mathbf{b}}\cdot\mathbf{r}}ds(\mathbf{r})$$

$$=4\pi\mathrm{i}k^{-1}\hat{\mathbf{p}}_2\cdot\overline{\mathbf{g}_a(-\hat{b},\hat{\mathbf{p}}_1)}.$$

□

The mixed reciprocity relation for perfect conductors is Theorem 2.3.4 in Ref. 1. It is valid more generally, as follows.

Theorem 14: *Let* $\mathbf{E}_a^{\mathrm{i}}(\mathbf{r};\hat{\mathbf{p}}_1)$ *be an incident spherical electric wave and let* $\mathbf{E}^{\mathrm{i}}(\mathbf{r};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)$ *be an incident plane electric wave. Then*

$$\hat{\mathbf{p}}_2\cdot\mathbf{g}_a(\hat{\mathbf{b}},\hat{\mathbf{p}}_1)=\mathrm{e}^{-\mathrm{i}ka}\hat{\mathbf{p}}_1\cdot[(\nabla\times\mathbf{E}^{\mathrm{s}}(\mathbf{a};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2))\times\hat{\mathbf{a}}]. \tag{85}$$

Proof: Working as in the proof of Theorem 10 and taking into account that

$$\{\overline{\mathbf{E}_a^{\mathrm{i}}(\cdot;\hat{\mathbf{p}}_1)},\mathbf{E}^{\mathrm{s}}(\cdot;-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)\}=4\pi\mathrm{i}(a/k)\mathrm{e}^{-\mathrm{i}ka}(\nabla\times\mathbf{E}^{\mathrm{s}}(\mathbf{a};-\hat{\mathbf{b}},\hat{\mathbf{p}}_1))\cdot(\hat{\mathbf{a}}\times\hat{\mathbf{p}}_1)$$

and

$$\{\overline{\mathbf{E}_a^s(\cdot;\hat{\mathbf{p}}_1)},\mathbf{E}^i(\cdot;-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)\}=-4\pi ik^{-1}\hat{\mathbf{p}}_2\cdot\mathbf{g}_a(\hat{\mathbf{b}},\hat{\mathbf{p}}_1),$$

Theorem 14 is proved. □

To conclude, we note that we also have

$$\lim_{a\to\infty}\lim_{b\to\infty}\mathbf{G}_b(\mathbf{a};\hat{\mathbf{p}}_2)=\lim_{b\to\infty}\lim_{a\to\infty}\mathbf{G}_b(\mathbf{a};\hat{\mathbf{p}}_2)=\mathbf{g}(-\hat{\mathbf{a}};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2).$$

This can be used to verify that the known scattering relations for plane-wave incidence[14,6] are recovered when $a\to\infty$ and $b\to\infty$. Furthermore, Eq. (81) and the reciprocity principle for plane waves[6] gives the following limiting property:

$$\lim_{a\to\infty}\hat{\mathbf{p}}_1\cdot\mathbf{G}(\mathbf{a};-\hat{\mathbf{b}},\hat{\mathbf{p}}_2)=\lim_{b\to\infty}\hat{\mathbf{p}}_2\cdot\mathbf{G}(-\mathbf{b};\hat{\mathbf{a}},\hat{\mathbf{p}}_1).$$

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Born–Infeld type equations for electrostatic fields

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In this paper we consider the field equations deduced by the second order approximation of the Born–Infeld Lagrangian density for the electromagnetic field. In particular we prove the existence of finite energy electrostatic fields, both in the case of a point charge and in the case of L^1 charge density. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1508433]

I. INTRODUCTION

A. Classical Maxwell's equations

The classical Maxwell's equations for an electrostatic field $\mathbf{E}$, in the vacuum, with a suitable choice of physical constants, are

$$\nabla \times \mathbf{E} = 0, \tag{1}$$

$$\frac{1}{4\pi} \nabla \cdot \mathbf{E} = \rho, \tag{2}$$

where ρ is the charge density. Standard procedures immediately give the expression of the energy

$$\mathcal{H} = \frac{1}{8\pi} \int |\mathbf{E}|^2 dx.$$

From (1) we deduce

$$\mathbf{E} = -\nabla \phi,$$

then Eq. (2) becomes

$$-\Delta \phi = 4\pi\rho. \tag{3}$$

This classical theory does not cover some physically interesting cases, namely $\rho = \delta$ and $\rho \in L^1(\mathbf{R}^3)$.

(i) If $\rho = \delta$ (point charge), then the solution of (3) is

$$\phi = \frac{1}{|x|},$$

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but the energy

$$\mathcal{H}=\frac{1}{8\pi}\int |\nabla\phi|^2 dx,$$

is infinite;

(ii) if, as it is natural, we assume $\rho\in L^1(\mathbf{R}^3)$ it is not clear if (3) admits solutions such that

$$\mathcal{H}=\frac{1}{8\pi}\int |\nabla\phi|^2 dx<+\infty.$$

Remark 1: By the Sobolev inequality

$$\left(\int |\phi|^6 dx\right)^{1/6}\leqslant c\left(\int |\nabla\phi|^2 dx\right)^{1/2},$$

it is easy to deduce that for any $\rho\in L^{6/5}(\mathbf{R}^3)\simeq(L^6(\mathbf{R}^3))'$ *there exists a unique solution of (3) with finite energy [simply take* ϕ *as test function in (3) and use Hölder inequality].*

If $\rho\in L^1(\mathbf{R}^3)$ *we can give a partial counterexample about the nonexistence of finite energy solutions. Infact consider the charge density*

$$\rho(x)=\frac{1}{|x|^{5/2}+|x|^{7/2}}.$$

Then it is easy to see that $\rho\in L^1(\mathbf{R}^3)\setminus L^{6/5}(\mathbf{R}^3)$ *and Eq. (3) has no radial solutions such that* $\mathcal{H}<+\infty$.

Remark 2: When we consider a bounded domain Ω*, it is well known that (3), with Dirichlet boundary conditions, admits a unique solution* ϕ *such that*

$$\int_\Omega |\nabla\phi|^q dx<+\infty \quad \forall q<\tfrac{3}{2},$$

for any datum $\rho\in L^1(\Omega)$ *[see Ref. 1].*

A way to overcome these difficulties was proposed by Born and Infeld in 1933–34.

The starting point for their theory is the set of Maxwell's equations

$$\nabla\times\mathbf{E}+\frac{\partial\mathbf{B}}{\partial t}=0, \tag{4}$$

$$\nabla\cdot\mathbf{B}=0, \tag{5}$$

$$\nabla\cdot\mathbf{D}=\rho, \tag{6}$$

$$\nabla\times\mathbf{H}-\frac{\partial\mathbf{D}}{\partial t}=\mathbf{J}, \tag{7}$$

where **E** and **H** are, respectively, the electric and the magnetic field, **D** and **B** are, respectively, the electric and the magnetic induction field, ρ and **J** are, respectively, the charge and the current density.

In the vacuum we have the relations

$$\mathbf{D}=\frac{1}{4\pi}\mathbf{E}, \tag{8}$$

$$\mathbf{H}=\frac{1}{4\pi}\mathbf{B}, \tag{9}$$

so we can write the second pair of Maxwell's equations as follows:

$$\frac{1}{4\pi}\nabla\cdot\mathbf{E}=\rho, \tag{10}$$

$$\frac{1}{4\pi}\nabla\times\mathbf{B}-\frac{1}{4\pi}\frac{\partial\mathbf{E}}{\partial t}=\mathbf{J}. \tag{11}$$

If we describe $(\mathbf{E},\mathbf{B})$ by means of the gauge potential $(\phi,\mathbf{A})$

$$\mathbf{E}=-(\mathbf{A}_t+\nabla\phi),$$

$$\mathbf{B}=\nabla\times\mathbf{A},$$

then the first couple of Maxwell's equations (4) and (5) is immediately satisfied.

The other two equations [Eqs. (10) and (11)] are the Euler–Lagrange equations with respect to the Lagrangian density

$$\mathcal{L}_{\mathrm{M}}=\frac{1}{4\pi}\mathcal{I}+\mathbf{J}\cdot\mathbf{A}-\rho\phi, \tag{12}$$

where

$$\mathcal{I}=\tfrac{1}{2}(|\mathbf{E}|^2-|\mathbf{B}|^2).$$

B. The Born–Infeld theory

As we pointed out the electrostatic field of a point charge has infinite energy. In order to overcome this difficulty Born and Infeld[2] (and references therein) proposed to modify equations (10) and (11).

Born and Infeld introduced a parameter $b\gg 1$ and considered the Lagrangian density

$$\mathcal{L}_{\mathrm{BI}}=\frac{b^2}{4\pi}\left(1-\sqrt{1-\frac{2}{b^2}\mathcal{I}}\right)+\mathbf{J}\cdot\mathbf{A}-\rho\phi. \tag{13}$$

If we set

$$\mathbf{D}_{\mathrm{BI}}=\frac{1}{4\pi}\frac{\mathbf{E}}{\sqrt{1-\frac{2}{b^2}\mathcal{I}}}, \tag{14}$$

$$\mathbf{H}_{\mathrm{BI}}=\frac{1}{4\pi}\frac{\mathbf{B}}{\sqrt{1-\frac{2}{b^2}\mathcal{I}}}, \tag{15}$$

then the Euler–Lagrange equations relative to (13) can be written as follows:

$$\nabla\cdot\mathbf{D}_{\mathrm{BI}}=\rho, \tag{16}$$

$$\nabla \times \mathbf{H}_{\mathrm{BI}} - \frac{\partial \mathbf{D}_{\mathrm{BI}}}{\partial t} = \mathbf{J}. \tag{17}$$

These equations, which substitute (10) and (11), are formally identical with the second pair of Maxwell's equations (6) and (7).

In the Born–Infeld theory the electrostatic field of a point charge has finite energy.

In fact consider the electrostatic case, i.e.,

$$\mathbf{B} = 0, \tag{18}$$

$$\frac{\partial \mathbf{E}}{\partial t} = 0, \tag{19}$$

$$\mathbf{J} = 0, \tag{20}$$

and assume

$$\rho = q\,\delta.$$

Equation (17) is immediately satisfied; an explicit solution of (16) is indeed

$$\mathbf{E} = \frac{q}{r_0^2 \sqrt{1 + (|x|/r_0)^4}} \frac{x}{|x|}, \tag{21}$$

where the constant $r_0 = q/b$ can be interpreted as the radius of the electron.

The energy for the Lagrangian density $\mathcal{L}_{\mathrm{BI}}$ is [see Ref. 3]

$$\mathcal{H}_{\mathrm{BI}} = \int T_{00}^{\mathrm{BI}}\, dx,$$

where

$$T_{00}^{\mathrm{BI}} = \frac{\partial \mathcal{L}_{\mathrm{BI}}}{\partial u_t} \cdot u_t - \mathcal{L}_{\mathrm{BI}},$$

and $u_t = (\phi_t, \mathbf{A}_t)$. A direct calculation shows that

$$T_{00}^{\mathrm{BI}} = \frac{1}{4\pi} \left[\frac{|\mathbf{E}|^2}{\sqrt{1 - \frac{2}{b^2}\mathcal{I}}} - b^2 \left(1 - \sqrt{1 - \frac{2}{b^2}\mathcal{I}} \right) \right] - \mathbf{J} \cdot \mathbf{A}. \tag{22}$$

Substituting (21) into (22), and taking into account (18)–(20) we can verify that $\mathcal{H}_{\mathrm{BI}}$ is finite.

Remark 3: As far as we know, it is not clear if the Born–Infeld theory could avoid also the divergence of the energy arising in presence of L^1 charge density (see discussion in Sec. I A).

C. Statement of the results

In the following we propose a slight variation of Born–Infeld theory which also permits us to get a finite energy electrostatic field with L^1 charge density.

Set

$$\beta = \frac{1}{2b^2} \ll 1,$$

then (13) becomes

$$\mathcal{L}_{\mathrm{BI}}=\frac{1}{8\pi\beta}(1-\sqrt{1-4\beta\mathcal{I}})+\mathbf{J}\cdot\mathbf{A}-\rho\phi. \tag{23}$$

We point out that the first order expansion of $\mathcal{L}_{\mathrm{BI}}$, for β small, is $\mathcal{L}_{\mathrm{M}}$ (see 12). In this paper we consider the second order expansion, that is

$$\mathcal{L}^*=\frac{1}{4\pi}(\mathcal{I}+\beta\mathcal{I}^2)+\mathbf{J}\cdot\mathbf{A}-\rho\phi.$$

The Euler–Lagrange equations relative to $\mathcal{L}^*$, which substitute (10) and (11), are

$$\nabla\cdot(1+2\beta\mathcal{I})\mathbf{E}=4\pi\rho, \tag{24}$$

$$\nabla\times(1+2\beta\mathcal{I})\mathbf{B}-\frac{\partial}{\partial t}(1+2\beta\mathcal{I})\mathbf{E}=4\pi\mathbf{J}. \tag{25}$$

Now, if we set

$$\mathbf{D}^*=\frac{1}{4\pi}(1+2\beta\mathcal{I})\mathbf{E}, \tag{26}$$

$$\mathbf{H}^*=\frac{1}{4\pi}(1+2\beta\mathcal{I})\mathbf{B}, \tag{27}$$

then (24) and (25) can be written again as in (6) and (7), namely

$$\nabla\cdot\mathbf{D}^*=\rho,$$

$$\nabla\times\mathbf{H}^*-\frac{\partial\mathbf{D}^*}{\partial t}=\mathbf{J}.$$

A straightforward calculation shows that now the energy is

$$\mathcal{H}^*=\int\left(\frac{\partial\mathcal{L}^*}{\partial u_t}\cdot u_t-\mathcal{L}^*\right)dx=\int\left\{\frac{1}{8\pi}[(|\mathbf{E}|^2+|\mathbf{B}|^2)+\beta\mathcal{I}(3|\mathbf{E}|^2+|\mathbf{B}|^2)]-\mathbf{J}\cdot\mathbf{A}\right\}dx.$$

Now consider the electrostatic situation described by (18)–(20).

Since (5) is obviously satisfied, the first couple of equations (4) and (5) reduces to

$$\nabla\times\mathbf{E}=0. \tag{28}$$

Moreover, since (25) is satisfied the second couple reduces to

$$\nabla\cdot[(1+\beta|\mathbf{E}|^2)\mathbf{E}]=4\pi\rho, \tag{29}$$

with $\beta>0$.

In this case the energy of the solutions is

$$\mathcal{H}^*=\frac{1}{8\pi}\int\left(|\mathbf{E}|^2+\frac{3}{2}\beta|\mathbf{E}|^4\right)dx.$$

The following theorems hold.

Theorem 4: *If we consider a point charge $\rho = q\,\delta$, there exists a solution of (28) and (29) having finite energy.*

We point out that, as well as in case of Born–Infeld equations, we shall give an explicit solution.

Theorem 5: *For every charge density $\rho \in L^1(\mathbf{R}^3)$, there exists a unique solution of (28) and (29) having finite energy.*

In particular, for $\rho = 0$, we have only the trivial solution. Hence the quasi-linear structure does not give rise to an effective source term, as well as in the Born–Infeld theory [see Ref. 4].

II. PROOF OF THEOREM 4

A. Estimate of the energy

Using (28) it easy to see that

$$\nabla \times [(1+\beta|\mathbf{E}|^2)\mathbf{E}] = 0,$$

then

$$(1+\beta|\mathbf{E}|^2)\mathbf{E} = -\nabla v, \tag{30}$$

and (29) becomes

$$-\Delta v = 4\pi q\,\delta,$$

which gives

$$v = \frac{q}{|x|}. \tag{31}$$

(30) and (31) imply

$$|\mathbf{E}| + \beta|\mathbf{E}|^3 = \frac{q}{|x|^2},$$

which gives

$$|\mathbf{E}| \leqslant \frac{q}{|x|^2}, \tag{32}$$

$$|\mathbf{E}| \leqslant \sqrt[3]{\frac{q}{\beta}}\frac{1}{|x|^{2/3}}. \tag{33}$$

From (32) we deduce that $|\mathbf{E}|^2$ and $|\mathbf{E}|^4$ are summable at infinity; from (33) we deduce that $|\mathbf{E}|^4$ and $|\mathbf{E}|^2$ are summable at 0. Hence

$$\mathcal{H}^* = \frac{1}{8\pi}\int_{\mathbf{R}^3}\left(|\mathbf{E}|^2 + \frac{3}{2}\beta|\mathbf{E}|^4\right)dx < +\infty.$$

B. Existence of a solution

For the sake of simplicity assume

$$q = 1.$$

By (28)

$$\mathbf{E} = -\nabla\phi,$$

so we have to solve

$$-\Delta\phi - \beta\Delta_4\phi = 4\pi\delta, \tag{34}$$

where

$$\Delta_p\phi = \mathrm{div}[(|\nabla\phi|^{p-2})\nabla\phi].$$

Since

$$-\mathrm{div}\left(\nabla\frac{1}{|x|}\right) = 4\pi\delta,$$

it is sufficient to solve

$$(1+\beta|\nabla\phi|^2)\nabla\phi = \nabla\frac{1}{|x|} = -\frac{x}{|x|^3}. \tag{35}$$

Let $\varphi:\mathbf{R}\to\mathbf{R}$ denote the inverse function of

$$\psi(t) = t + \beta t^3.$$

Using the asymptotic estimates on φ

$$\varphi(t) \simeq t \quad \text{for } t\to 0,$$

$$\varphi(t) \simeq \sqrt[3]{t/\beta} \quad \text{for } t\to+\infty,$$

we deduce that the integral

$$\int_0^{+\infty} \varphi(1/r^2)\,dr,$$

is convergent; indeed

$$\varphi(1/r^2) \simeq 1/\sqrt[3]{\beta r^2} \quad \text{for } r\to 0,$$

$$\varphi(1/r^2) \simeq 1/r^2 \quad \text{for } r\to+\infty.$$

So we can define

$$\phi(x) = \int_{|x|}^{+\infty} \varphi(1/r^2)\,dr. \tag{36}$$

We claim that ϕ satisfies (35). In fact we have

$$\nabla\phi(x) = -\varphi(1/|x|^2)\frac{x}{|x|},$$

hence

$$|\nabla\phi(x)| = \varphi(1/|x|^2).$$

Therefore

$$(1+\beta|\nabla\phi|^2)\nabla\phi = -(1+\beta\varphi^2(1/|x|^2))\,\varphi(1/|x|^2)\,\frac{x}{|x|}$$

$$= -\psi(\varphi(1/|x|^2))\,\frac{x}{|x|}$$

$$= -\frac{x}{|x|^3}.$$

Remark 6: For $|x|$ large, $\phi(x)$ is asymptotically equivalent to the Coulomb potential $1/|x|$.

Remark 7: We recall that if Ω is a bounded set in $\mathbf{R}^3$, then the solution of $-\Delta_4\phi=\delta$, with Dirichlet boundary data belongs to the Sobolev space $W_0^{1,4}(\Omega)$; so that, in particular

$$\int_\Omega |\nabla\phi|^4 dx < +\infty.$$

Indeed the space of measures on Ω is embedded in the dual space of $W_0^{1,4}(\Omega)$ and so the existence of a solution follows from well-known results on monotone operators in duality [see Ref. 5]. This is not the case for the solution of $-\Delta\phi=\delta$, which is of infinite energy. So the modification of Eq. (3) is used only to control *the energy of the solution near the origin. Note that the operator $-\Delta_4$ can be substituted (always having finite energy solutions) with $-\Delta_p$, for any $p>3$. In this way, however, the equation is no longer obtained as the Euler–Lagrange equation of the second order expansion of $\mathcal{L}_{\mathrm{BI}}$ [defined in (23)] for β near 0.*

III. PROOF OF THEOREM 5

As in the previous section, by (28)

$$\mathbf{E} = -\nabla\phi.$$

So (29) is reduced to

$$-\Delta\phi - \beta\Delta_4\phi = 4\pi\rho.$$

The energy of the solutions is

$$\mathcal{H}^* = \frac{1}{8\pi}\int \left(|\nabla\phi|^2 + \frac{3}{2}\beta|\nabla\phi|^4 \right) dx.$$

Then the natural functional space for finite energy solutions is the closure D of $C_0^\infty(\mathbf{R}^3)$ with respect to this norm

$$\|\phi\|_D = \|\nabla\phi\|_{L^2} + \|\nabla\phi\|_{L^4}.$$

Proposition 8: The Banach space D is continuously embedded in $L^\infty(\mathbf{R}^3)$, that is there exists $M>0$ such that, for every $\phi\in D$

$$\|\phi\|_{L^\infty} \leq M\|\phi\|_D.$$

Proof: It is well known that $D^{1,2}(\mathbf{R}^3)$ is continuously embedded in $L^6(\mathbf{R}^3)$. Consider a family of cubes $Q_k\subset\mathbf{R}^3$ such that

$$|Q_k| = 1$$

$$\bigcup_k Q_k = \mathbf{R}^3.$$

Fixed $\phi \in C_0^\infty(\mathbf{R}^3)$, for every $x \in \mathbf{R}^3$

$$\begin{aligned}|\phi(x)| &\leq \left| \int_{Q_k} \phi dx \right| + M\|\nabla\phi\|_{L^4(Q_k)} \\ &\leq M_1\|\phi\|_{L^6(Q_k)} + M\|\nabla\phi\|_{L^4(Q_k)} \\ &\leq M_1\|\phi\|_{L^6(\mathbf{R}^3)} + M\|\nabla\phi\|_{L^4(\mathbf{R}^3)} \\ &\leq M_2\|\nabla\phi\|_{L^2(\mathbf{R}^3)} + M\|\nabla\phi\|_{L^4(\mathbf{R}^3)}.\end{aligned}$$

Then we easily deduce the thesis. ■

Theorem 5 is a consequence of the following result.

Proposition 9: For every $\rho \in L^1(\mathbf{R}^3)$ there exists a unique $\phi \in D$ such that

$$-\Delta\phi - \beta\Delta_4\phi = \rho. \tag{37}$$

If we call $T(\rho)$ such a solution, the map $T: L^1(\mathbf{R}^3) \to D$ is continuous and bounded, in the sense that it maps bounded sets in bounded sets.

Proof: The solutions of (37) can be characterized as critical points of the functional

$$J(\phi) = \frac{1}{2}\|\nabla\phi\|_{L^2}^2 + \frac{\beta}{4}\|\nabla\phi\|_{L^4}^4 - \int_{\mathbf{R}^3} \phi\rho dx.$$

By Proposition 8 and Hölder inequality, this functional is bounded from below and coercive; furthermore it is weakly lower semicontinuous on D. Then it has a minimizer, which is a solution of (37).

The solution is unique. Indeed observe first that the operator

$$\mathcal{A} = -\Delta - \beta\Delta_4,$$

is monotone; that is, for every $\phi_1, \phi_2 \in D$

$$c(\|\nabla\phi_1 - \nabla\phi_2\|_{L^2}^2 + \|\nabla\phi_1 - \nabla\phi_2\|_{L^4}^4) \leq \langle \mathcal{A}\phi_1 - \mathcal{A}\phi_2, \phi_1 - \phi_2 \rangle, \tag{38}$$

being c a suitable positive constant [see, e.g., Lemma 9 in Ref. 6].

Now if ϕ_1 and ϕ_2 are solutions of (37) in D, then

$$\mathcal{A}\phi_1 - \mathcal{A}\phi_2 = 0.$$

Hence, by (38), $\phi_1 = \phi_2$.

The continuity of the inverse map $T = \mathcal{A}^{-1}$ can be obtained using again (38) and arguments similar to those of Theorem 30 in Benci *et al.*[6]

In order to show that T maps bounded sets in bounded sets we multiply (37) by the solution ϕ. After integration by parts, we obtain, by Proposition 8,

$$\|\nabla\phi\|_{L^2}^2 + \beta\|\nabla\phi\|_{L^4}^4 \leq \|\rho\|_{L^1}\|\phi\|_{L^\infty} \leq M\|\rho\|_{L^1}(\|\nabla\phi\|_{L^2} + \|\nabla\phi\|_{L^4}).$$

Then we easily deduce that, if $\|\rho\|_{L^1}$ is bounded, also $\|\phi\|_D = \|\nabla\phi\|_{L^2} + \|\nabla\phi\|_{L^4}$ is bounded. ■

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Optimal regularity in a variational problem for current sheets in ideal magnetohydrodynamics

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We characterize local behavior, and establish optimal local regularity, for minimizers of the functional $E(\psi)=\int_\Omega|\nabla\psi|^2$ over collections $\mathcal{C}$ that are weakly closed in $H^1(\Omega)$, closed under local smooth domain perturbations, and for which $E(\psi)$ controls $\int_\Omega\psi^2$. Minimizers ψ satisfy a weak magnetohydrodynamic (MHD) equation and correspond to fields in low density ideal plasmas under cylindrical symmetry where the field component in the direction of the axis of symmetry is zero. We prove that $(\partial\psi/\partial x+i\partial\psi/\partial y)^2$ is complex analytic, and locally $\psi=f(\phi)$ for some ϕ, f, with $\Delta\phi=0$ and f Lipschitz continuous with $|f'|=1$ almost everywhere, near points where $\nabla\psi\neq 0$. An analogous but more elaborate characterization is established at points where $\nabla\psi=0$. This characterization forms the basis for a general theory of the existence of current sheets due to imposed topological and boundary constraints. Results carry over to functions that are stationary points of $E(\psi)$ with respect to local smooth domain variations. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1508437]

I. INTRODUCTION

The analysis of current sheets in low density ideal plasmas has important applications in the study of the sun's corona, for instance in understanding the extreme heating that occurs in the corona. We study the problem in cylindrical symmetry, so our results apply to models of solar coronal arcades. Our characterization of local behavior forms the basis for results on existence of current sheets in general boundary value problems with topological constraints that will appear in the companion paper.[8]

Consider a z independent magnetic field B. This can be expressed as

$$B=\left(\frac{\partial\psi}{\partial y},-\frac{\partial\psi}{\partial x},Q\right), \tag{1}$$

where ψ,Q are scalar functions of x,y. We will assume that

$$Q=0. \tag{2}$$

In the context of basic coronal arcade models the condition $Q=0$ corresponds to the case where there is no footpoint motion in the z direction (footpoints being the points where field lines are anchored in the x,z plane, which models the photospheric boundary of the sun's corona). In this setting we avoid the highly nonlinear constraints usually satisfied by Q but retain the conservation of field line topology thought to generate current sheets.

The variational problem, of minimizing the energy

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$$E(\psi)=\int_{\Omega}|\nabla\psi|^2, \tag{3}$$

over the collection C of functions $\psi=\psi_0(d)$ with ψ_0 a fixed element of $H^1(\Omega)$, and $d:\Omega\to\Omega$ any smooth domain diffeomorphism, models the relaxation of a field to minimum energy constrained by fixed field line topology imposed by ideal MHD. To produce a function ψ that is energy minimizing it is necessary to extract weak limits. Thus it is natural to minimize (3) over the weak closure of C.

To put this problem in historical context note that many examples of current sheets are present in the astrophysics literature. For the most part however these are particular examples generated by explicit mathematical formulas. Although there is a great deal of analysis of one sort or another on the subject, what is lacking is a complete, rigorous theory where current sheets arise in general global energy minimization problems due to prescribed field line topology and boundary data. Such a theory, carried out in settings relevant to solar physics, would substantiate on a rigorous mathematical level an important scientific theory.

Prior to our current results, work of Aly and Amari,[1–3] comes the closest to accomplishing this goal. In Ref. 1 Aly and Amari analyze QPSEs, that is, quasi-potential singular equilibrium states, which are fields B that are solutions of the equations of MHD under the assumption that ψ is harmonic away from a finite union of differentiable (possibly intersecting) curve segments on which ψ is constant and across which $\nabla\psi$ is discontinuous in accord with standard jump conditions. This analysis forms the basis for a careful characterization of what is expected in energy minimizing states that are conjectured to have current sheets. In Refs. 2 and 3 various basic field topologies of interest to solar physics are considered. Integral formulas are given as solutions of general boundary value problems, usually under the assumption of y symmetry in ψ (ψ as above). Except in one basic example, which can be reduced to a consideration of a boundary value problem for harmonic functions, Aly and Amari do not establish that such solutions are energy minimizers, although the solutions are undoubtedly stationary points in a sense we discuss later. In addition the methods are limited to fairly simple geometries due to reliance on integral formulas.

In Refs. 6 and 7 we presented a general existence theory for minimizers of variational problems such as the one described at (3) (also including the $Q\neq 0$ case). In the present paper we characterize local behavior of such minimizers and give an optimal local regularity result. In the companion paper[8] we will apply our general techniques to a model problem first introduced by Low and Wolfson[10] to give the first rigorous proof of the existence of current sheets in energy minimizers of a general boundary value problem with topological constraints, at least for topologies where the problem is not easily reducible to consideration of global harmonic functions. The approach is general in that it easily extends to arbitrarily complex field line topologies.

We now describe more completely the results of the present paper. It is easily seen that a minimizer exists for the variational problem of minimizing (3) over a collection of functions that is weakly closed in H^1, closed under local smooth domain perturbations, and for which (3) controls the H^1 norm, see (9), the latter occurring for example if boundary values are specified. For such a minimizer ψ our first result is that $B^2=(\partial\psi/\partial x+i\partial\psi/\partial y)^2$ is complex analytic, which follows from the Euler equations for the functional (3). Note in Ref. 4 Arnold and Khesin consider the analog of this in the general setting of Riemannian manifolds, however they assume *a priori* that the minimizer is smooth. The analyticity of B^2 also appears for instance in the work of Aly and Amari[1] under the assumption that ψ is harmonic away from a finite union of differentiable curve segments on which ψ is constant and across which $\nabla\psi$ is discontinuous in accord with standard jump conditions. We establish the analyticity here in a much weaker setting where energy minimizers and associated free boundaries can be quite irregular. At first the possibility of highly irregular minimizers is surprising since one is minimizing the simple functional $\int|\nabla\psi|^2$. However note that $|\nabla f(\psi)|=|f'(\psi)\nabla\psi|=|\nabla\psi|$ for Lipschitz continuous functions f satisfying $|f'|=1$ so $\int|\nabla\psi|^2=\int|\nabla f(\psi)|^2$. Thus if ψ is a minimizer of the variational problem described above it can be seen that $f(\psi)$ is a minimizer for a related collection $\mathcal{C}$. Current sheets, i.e., discontinuities in the gradient of a minimizer, can thus occur in general on a dense subset of the domain. Another

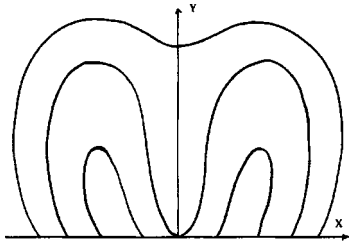

FIG. 1.

perspective is that when one, roughly speaking, takes a square root of $B^2=(\partial\psi/\partial x+i\partial\psi/\partial y)^2$ one gets that $\nabla\psi(p)=s(p)\nabla\phi(p), s(p)=\pm 1$ for some ϕ that is harmonic except possibly on a cut. Intuitively this implies that ψ is locally constant on level curves $\{\phi=c\}$, however, when one moves orthogonally to such a curve the function $s(p)$ possibly introduces wild flips in the direction of $\nabla\psi$.

A corollary of our analyticity result is that $\nabla\psi$ has discontinuities in a subdomain O of Ω if and only if ψ is not harmonic in all of O. This verifies in this weak setting the traditional view that a field must develop currents sheets if it cannot relax to a potential state, due to preservation of field line topology.

A second corollary is that $\nabla\psi$ is locally bounded, so ψ is locally Lipschitz continuous. This is in fact an optimal **local** regularity result due to the observation above relating ψ and $f(\psi)$.

To get a more precise sense of both where ψ is regular, but also where current sheets exist, one must analyze the field line topology, or equivalently the topological structure of levels sets $\{\psi=c\}$. In the setting of $Q=0$ such topology can only be sustained by prescribed boundary conditions. However, boundary conditions are not enough to prescribe such topology. In Ref. 8 we use the results of the present paper, in combination with methods for handling weak topology of level sets introduced in Refs. 6 and 7, to carefully examine a model of a solar coronal arcade first introduce by Low and Wolfson[10] and studied by a number of authors including Aly and Amari.[3] This example involves a topological level set structure that is one of the simplest of relevance to astrophysics in which one expects current sheets to exist (or not exist, depending on imposed boundary values), but that is also complex enough so one cannot trivially reduce the analysis to consideration of a globally harmonic function. In this context we establish a rigorous proof of the existence of currents sheets. In Fig. 1 one sees sample level curves corresponding to an initial field before it relaxes to minimum energy. The level curves correspond to field lines. These are anchored on the x axis, which models the surface of the photosphere. In Fig. 2 we see a typical level curve configuration for the field after it relaxes to minimum energy. In Ref. 10 Low and Wolfson give a specific example of such a field where there is a current sheet in the curve segment shown emanating from the origin up to the point where the level curve moves away from the y axis, the flux function ψ being harmonic away from the current sheet. In Ref. 3 Aly and Amari give an integral formula for such fields for general boundary conditions under the assumption of y symmetry, as well a condition on the boundary values that characterizes whether a current sheet in fact

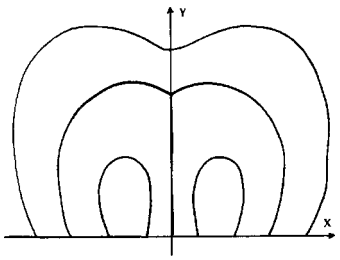

FIG. 2.

occurs or not. They do not prove that such fields are energy minimizing but they do verify that the fields satisfy the correct jump condition, which in this case is that the gradient of ψ has continuous magnitude but reverses direction across the current sheet, which as in the Low, Wolfson example emanates from the origin and lies on the y axis. As before, the flux function ψ associated with the field is harmonic away from the current sheet. In Ref. 8 we use results of the present paper as well as those from Refs. 6 and 7 to prove the existence of energy minimizers in this particular topological class and for general boundary conditions. We show that such minimizers are harmonic away from a current sheet which is an analytic curve emanating from the origin, and across which the gradient has continuous magnitude but changes sign. No symmetry assumption is made on the boundary data. The method handles much more general topological classes, which are discussed more in Sec. III A. The results of Ref. 8 are set in a bounded domain while those of Aly and Amari, and Low and Wolfson are in a half space. In Ref. 9 we will extend our results to unbounded domains.

To properly appreciate these results one must separate them from current sheet examples that arise trivially from field reversal examples created from harmonic functions. Note that if $\phi \in H^1(\mathbb{R}^2)$ is harmonic in a bounded domain Ω and f is Lipschitz continuous with $|f'|=1$ then as mentioned earlier $\int_\Omega |\nabla \phi|^2 = \int_\Omega |\nabla f(\phi)|^2$ so one can show that $\psi = f(\phi)$ is a minimizer over the weak closure of the set of all functions $\psi(d)$ where $d:\Omega \to \Omega$ is any smooth domain diffeomorphism. ψ is thus an energy minimizer of the sort we are discussing which has current sheets at all values of t in the range of ψ where f' has a discontinuity. Such examples are not of great interest because the topological classes associated with these are not of a type that is usually studied in astrophysics. Note, however, that the Low–Wolfson geometry is such that reflections of the type introduced by f cannot reduce ψ to a harmonic function. It is the contrast between these two examples that helps put the results of the present paper in context. In the local theory tackled in the present paper one must cope with the possibility of arbitrarily bad field reversals. It is only in the context of a global problem where boundary values and topology of fields lines are prescribed that one can control where current sheets occur. However, the basic local regularity and structure results of this paper form a foundation for exploiting the global constraints considered in Ref. 8.

We now elaborate on our local characterization results for minimizers of (3). Near points where $\nabla \psi \neq 0$ we prove that $\psi = f(\phi)$ for some ϕ, f with $\Delta \phi = 0$ and f Lipschitz continuous with $|f'|=1$ almost everywhere. Near points p where $\nabla \psi = 0$ (which are isolated) we show for some integer $m \geqslant 3$ that there are analytic curves γ_i, $i=1,2,\ldots,m$ which are asymptotic (as the curves approach p) to m line segments emanating from p at equally spaced angles (relative to p), and a function ϕ that is harmonic, except on γ_1 if m is odd, and zero on $\cup_i \gamma_i$, such that for each $i = 1,2,\ldots,m$ we have $\psi = f_i(\phi)$ near p in the region between γ_i, γ_{i+1}, for Lipschitz continuous functions f_i with $|f_i'|=1$ almost everywhere.

II. INITIAL TECHNICAL DEFINITIONS

Let $B(x,r)=\{y \in \mathbb{R}^2 : |x-y|<r\}$. For any open set $\Omega \subset \mathbb{R}^2$ let $L^1(\Omega)$ be the set of Lebesgue integrable functions defined on Ω, $C(\Omega)$ the set of continuous real valued functions defined on Ω, $C^1(\Omega)$ the subset of $C(\Omega)$ whose elements have continuous first derivatives, $C^\infty(\Omega)$ the set of infinitely differentiable real valued functions defined on Ω, and $C_0^\infty(\Omega)$ the subset of $C^\infty(\Omega)$ whose elements have compact support in Ω. Given the norm $\|u\|_\Omega = [\int_\Omega (|u|^2 + |\nabla u|^2)]^{1/2}$ let $H^1(\Omega)$ be the closure of $\{u \in C^\infty(\Omega) | \|u\|_\Omega < \infty\}$ in $\|\cdot\|_\Omega$, and $H_0^1(\Omega)$ the closure of $C_0^\infty(\Omega)$ in $\|\cdot\|_\Omega$.

For simplicity we follow the convention of treating any two elements of $H^1(\Omega)$ as being equal if they are equal pointwise almost everywhere (that is everywhere except on a set of zero Lebesgue measure). The Lebesgue measure of a set E will be represented by $|E|$. The closure of a set E is denoted by $\overline{E}$.

Given an open set Ω and functions u_n, $u \in H^1(\Omega)$ we say that u_n converges weakly to u in $H^1(\Omega)$ if

$$\int_\Omega u_n v + \nabla u_n \cdot \nabla v \to \int_\Omega uv + \nabla u \cdot \nabla v, \tag{4}$$

for all $v \in H^1(\Omega)$.

A functional $F: H^1(\Omega) \to \mathbb{R}$ is said to be weakly lower semi-continuous if for any sequence $(u_n) \subset H^1(\Omega)$ converging weakly to u in $H^1(\Omega)$ we have

$$\liminf_{n\to\infty} F(u_n) \geqslant F(u). \tag{5}$$

Note that $\int_\Omega |\nabla u|^2$ is weakly lower semicontinuous.

III. GENERAL VARIATIONAL PROBLEM

Definition 1: Given an open bounded set $\Omega \subset \mathbb{R}^2$ let

$$\tilde{\Omega} = \{x + iy \in \mathbb{C} | (x,y) \in \Omega\} \tag{6}$$

and

$$\mathcal{D}(\Omega) = \{d: \Omega \to \Omega | d \text{ is a } C^\infty \text{ diffeomorphism,}$$

$$d = I \text{ in a neighborhood of } \partial\Omega, \det Dd > 0\}, \tag{7}$$

where I is the identity map $I(p) = p$. A collection of functions $\mathcal{C}$ with domain Ω will be said to be closed under smooth domain variations if for all $f \in \mathcal{C}$ and $d \in \mathcal{D}(\Omega)$ we have $f(d) \in \mathcal{C}$.

Recall

$$E(u) = \int_\Omega |\nabla u|^2. \tag{8}$$

Lemma 1: Given an open bounded set $\Omega \subset \mathbb{R}^2$ and a nonempty collection of functions $\mathcal{C} \subset H^1(\Omega)$ that is weakly closed in $H^1(\Omega)$, closed under smooth domain variations, and satisfies the property that for any sequence $(u_n) \subset \mathcal{C}$

$$\{E(u_n) | n = 1,2,\ldots\} \text{ bounded } \Rightarrow \{\|u_n\|_\Omega | n = 1,2,\ldots\} \text{ bounded,} \tag{9}$$

then there exists a function $\psi_1 \in \mathcal{C}$ such that

$$E(\psi_1) \leqslant \inf_{\psi \in \mathcal{C}} (E\psi). \tag{10}$$

For any such ψ_1 the function $(\partial\psi_1/\partial x - i\partial\psi_1/\partial y)^2$ is a complex analytic function on $\tilde{\Omega}$ (after possible redefinition of $\nabla\psi$ on a set of Lebesgue measure zero).

Remark 1: Property (9) holds for instance if functions in $\mathcal{C}$ satisfy a prescribed weak boundary condition, for example if they are restrictions to Ω of functions in $\mathcal{C}' \subset H^1(\mathbb{R}^2)$ with $u = f$ on $\mathbb{R}^2 \backslash \Omega$ for all $u \in \mathcal{C}'$, and some fixed $f \in H^1(\mathbb{R}^2)$. See the next section for more details.

Lemma 2: If $\psi \in H^1(\Omega)$ with $(\partial\psi/\partial x - i\partial\psi/\partial y)^2$ a complex analytic function on $\tilde{\Omega}$ then

$$|\nabla\psi|^4 \text{ is real analytic so } \psi \text{ is locally Lipschitz continuous in } \Omega \tag{11}$$

and

$$\Delta\psi = 0 \text{ in any subdomain of } \Omega \text{ on which } \nabla\psi \text{ is continuous.} \tag{12}$$

Corollary 1: Let ψ be as in Lemma 2 and $O\subseteq\Omega$ be open. If ψ is not harmonic throughout O then $\psi\notin C^1(O)$.

Lemmas 1,2 tell us the nature of a minimizer ψ in regions where ψ is C^1. The following result indicates behavior near points where $\nabla\psi$ may not be continuous.

Theorem 1: *Given a nonconstant ψ as in Lemma 2, if $|\nabla\psi(p)|\neq 0$ then there exist $R>0$, a Lipschitz continuous function $f:\mathbb{R}\to\mathbb{R}$ satisfying*

$$|f'|=1 \ \text{almost everywhere}, \tag{13}$$

and a harmonic function $\phi:B(p,R)\to\mathbb{R}$ such that

$$\psi=f(\phi) \ \text{in} \ B(p,R). \tag{14}$$

Points p where $|\nabla\psi(p)|=0$ are isolated. If $|\nabla\psi(p)|=0$ then for some $R>0$ and some integer $m\geqslant 3$ there are analytic curves $\gamma_i:[0,R]\to\Omega, \gamma_i(0)=p, i=1,2,\ldots,m$ which are asymptotic (as the curves approach p) to m line segments emanating from p at equally spaced angles (relative to p), the set $B(p,R)\setminus(\cup_i\gamma_i([0,R]))$ being the union of m open, pairwise disjoint, simply connected regions $D_i, i=1,2,\ldots,m$ (each bounded by three connected arcs, two being subarcs of γ_i, γ_j for $j=i+1$ unless $i=m$ when $j=1$, and the third a subarc of $\partial B(p,R)$), and a Lipschitz continuous function ϕ which is harmonic in $B(p,R)\setminus\gamma_1$ with $\{\phi=0\}\cap B(0,R)=\cup_i\gamma_i([0,R])$, such that for each $i=1,2,\ldots,m$ there exists a Lipschitz continuous function $f_i:\mathbb{R}\to\mathbb{R}$ satisfying $f_i(p)=\psi(p)$, $|f_i'|=1$ almost everywhere such that

$$\psi=f_i(\phi) \ \text{in the closure of} \ D_i. \tag{15}$$

If m is even then ϕ may be taken to be harmonic in all of $B(p,r)$, while if m is odd one can take $|\nabla\phi|$ to be continuous with $\nabla\phi$ reversing direction across γ_1. Moreover ϕ can be chosen so that the discontinuity in $\nabla\phi$ occurs on any one of the γ_i.

Remark 2: It is fairly easy to see that Theorem 1 is optimal in describing local regularity. Given ψ, p, R, ϕ as in the statement of the theorem, one has $\int_{B(p,R)}|\nabla\psi|^2=\int_{B(p,R)}|\nabla\phi|^2$ in both the $\nabla\psi(p)\neq 0$ and $\nabla\psi(p)=0$ cases (if $f:\mathbb{R}\to\mathbb{R}$ is a Lipschitz continuous function with $|f'|=1$ almost everywhere then $|\nabla(f(\psi))|=|\nabla\psi|$ for $\psi\in H^1(B(p,R))$—see discussion at Lemma 1, in Ref. 6 for technical details beyond the use of the weak chain rule; also $\phi\chi_{D_i}\in H^1(B(p,R)), i=1,\ldots,m$ for ϕ, D_i as above, and $\chi_E(p)=1$ for $p\in E$, $\chi_E(p)=0$ for $p\notin E$). Thus for fixed ϕ one can redefine f or $f_i, i=1,\ldots,m$ arbitrarily (of course maintaining the $|f'|=1, |f_i'|=1$ condition, and taking $f_i(p)$ independent of i), and thus redefine ψ [as in (14), (15)], and ψ is still a minimizer of $\int_{B(p,R)}|\nabla\psi|^2$ over the weak closure of $\{\psi(d)|d\in\mathcal{D}(B(p,R))\}$.

Proof of Lemma 1: The lemma can be deduced from Noether's Theorem (see, for example, Proposition 2, p.168 of Ref. 5; note in Ref. 5 minimizers are assumed to be C^1, but this is used only to justify use of the chain rule which is true much more generally). However, due to the simplicity of the functional we present a self contained elementary proof.

We first verify that there exists a minimizer ψ of the variational problem (10). Recall that $\mathcal{C}\neq\emptyset, \mathcal{C}\subset H^1(\Omega)$ so $\inf_{\psi\in\mathcal{C}}E(\psi)<\infty$, and there exists a sequence $(\psi_n)\subset\mathcal{C}$ such that $E(\psi_n)\to\inf_{\psi\in\mathcal{C}}E(\psi)$ as $n\to\infty$. Such a sequence is bounded in $H^1(\Omega)$ by (9), so one can extract a subsequence that converges weakly in $H^1(\Omega)$ to some $\psi\in H^1(\Omega)$. The weak closedness of $\mathcal{C}$ implies $\psi\in\mathcal{C}$, and the weak lower semi-continuity of E implies that $E(\psi)\leqslant\inf_{\psi\in\mathcal{C}}E(\psi)<\infty$, so ψ is a minimizer.

Given $w\in C_0^\infty(\Omega)\times C_0^\infty(\Omega)$ let $d_t(p)=p+tw(p)$ so there exists $t_0>0$ such that $d_t\in\mathcal{D}(\Omega)$ for $|t|<t_0$. For $|t|<t_0$ let $\psi_t(q)=\psi(d_t^{-1}(q))$ so

$$\nabla\psi_t(q)=\nabla\psi(d_t^{-1}(q))Dd_t^{-1}(q)=\nabla\psi(p)[Dd_t(p)]^{-1}, \tag{16}$$

for $p=d_t^{-1}(q)$.

Note for any 2×2 matrix A that

$$|(x,y)A^{-1}| = \left|A\begin{pmatrix} y \\ -x \end{pmatrix}\right| \Big/ |\det A|, \tag{17}$$

so

$$\int_\Omega |\nabla \psi_t(q)|^2 dq = \int_\Omega |\nabla \psi(p)[Dd_t(p)]^{-1}|^2 \det Dd_t(p) dp, \tag{18}$$

$$= \int_\Omega |Dd_t(p)\begin{pmatrix} \psi_y(p) \\ -\psi_x(p) \end{pmatrix}|^2 \det{}^{-1} Dd_t(p) dp. \tag{19}$$

Also note that

$$Dd_t = I + tDw, \quad \det Dd_t = 1 + t\nabla\cdot w + t^2 \det Dw, \tag{20}$$

so

$$\frac{\partial Dd_t}{\partial t} = Dw, \quad \left.\frac{\partial \det Dd_t}{\partial t}\right|_{t=0} = \nabla\cdot w. \tag{21}$$

Consequently we can differentiate (19) with respect to t and evaluate at $t=0$ to get

$$\int_\Omega 2(\psi_y, -\psi_x) Dw \begin{pmatrix} \psi_y \\ -\psi_x \end{pmatrix} - |\nabla\psi|^2 \nabla\cdot w = 0. \tag{22}$$

Take $w=(-\eta,0)$ to get

$$\int_\Omega (\psi_x^2 - \psi_y^2)\eta_x + 2\psi_y\psi_x\eta_y = 0. \tag{23}$$

Similarly using $w=(0,\eta)$ we get

$$\int_\Omega (\psi_x^2 - \psi_y^2)\eta_y - 2\psi_y\psi_x\eta_x = 0. \tag{24}$$

Note that these are the weak form of the Cauchy–Riemann equations for $(\psi_x^2-\psi_y^2)-2\psi_y\psi_x i$ so we claim, possibly after redefinition of $\nabla\psi$ on a set of measure zero, that

$$(\psi_x^2 - \psi_y^2) - 2\psi_y\psi_x i \ \text{ is complex analytic,} \tag{25}$$

thought of as a function of $z=x+iy$.

To verify the claim let $u=\psi_x^2-\psi_y^2$ and $v=-2\psi_y\psi_x$ so from (23) and (24) we get

$$\int_\Omega u\eta_x - v\eta_y = 0, \int_\Omega u\eta_y + v\eta_x = 0. \tag{26}$$

Take $\eta=\alpha_x$ in the first equation and $\eta=\alpha_y$ in the second to get

$$\int_\Omega u\alpha_{xx} - v\alpha_{xy} = 0, \int_\Omega u\alpha_{yy} + v\alpha_{xy} = 0. \tag{27}$$

Adding the two equation we see that

$$\int_\Omega u\Delta\alpha = 0, \tag{28}$$

so u is a distributional solution of $\Delta u = 0$. Standard results then imply that u is classically harmonic.

A similar calculation implies that v is harmonic, and thus smooth, so using integration by parts in (26) confirms that the classical Cauchy–Riemann equations hold for $u+iv$. Note that the redefinition of u,v on a set of measure zero can be accomplished by redefining $\nabla\psi$ because the equations $u=a^2-b^2$, $v=-ab$ always have a solution.

Proof of Lemma 2: Let $\psi\in H^1(\Omega)$ be such that $a(z)=(\partial\psi/\partial x - i\partial\psi/\partial y)^2$ is a complex analytic function on $\tilde{\Omega}$. Thus $|a(z)|^2=|\partial\psi/\partial x - i\partial\psi/\partial y|^4=|\nabla\psi|^4$ is real analytic, and so is locally bounded in Ω. Consequently ψ is locally Lipschitz in Ω.

Now assume $\psi\in C^1(O)$, O a connected open subset of Ω. Given a point p such that $\nabla\psi(p)\neq 0$ let $B\subset O$ be an open ball centered at p such that $\nabla\psi$ is close to $\nabla\psi(0)$ in B, so for instance $\nabla\psi\neq 0$, but mainly so we can use the complex analytic square root function with cut chosen so that the square root is analytic on the image of B under the map $(\psi_x-\psi_y i)^2$. Thus we can conclude that $\psi_x-\psi_y i$ is analytic. Consequently ψ is harmonic in B due to the Cauchy–Riemann equations.

Next note that complex analytic functions are either constant or have isolated zeros. In the later case the above argument implies that ψ is harmonic in O minus an at most countable set of isolated points. A point is a removable discontinuity for $\Delta\psi=0$ due to $\psi\in H^1$ so in fact ψ is harmonic in all of O.

Proof of Theorem 1: Let ψ be a nonconstant function in $H^1(\Omega)$ such that $a=(\partial\psi/\partial x - i\partial\psi/\partial y)^2$ is a complex analytic function in $\tilde{\Omega}$. Note that a cannot be identically zero otherwise ψ would be constant contrary to assumption.

The following paragraph is strictly for purposes of motivation. The functions q,ϕ will be defined differently in the actual proof. First consider a point $p_0=(x_0,y_0)\in\Omega$ such that $a(z)\neq 0$ in a neighborhood of $z_0=x_0+y_0 i$, and assume $\nabla\psi$ is continuous in a neighborhood of p_0. For $p=(x,y)$, $z=x+yi$ choose a cut for the square root function that avoids $a(z_0)$ and define

$$q(z)=\int_{p_0}^{z}\sqrt{a(w)}\,dw, \quad \phi(x,y)=\mathrm{Re}(q(z)), \tag{29}$$

so $\phi_x-\phi_y i = dq/dz = \pm(\psi_x-\psi_y i)$, $\nabla\phi=\pm\nabla\psi$, and

$$\psi=\psi(p_0)\pm\phi \ \text{ with } \ \Delta\phi=0 \ \text{ near } \ p_0, \tag{30}$$

and so ψ is represented locally in a simple manner in terms of the harmonic function ϕ. We now drop the assumptions that $a(z)\neq 0$ and $\nabla\psi$ is continuous. This makes the analysis more intricate, though we will basically emulate the above construction. Also the sign in (30) will possibly vary with z forcing the introduction of Lipschitz continuous functions f, f_i.

For simplicity we take $z_0=0$. Note that $(\psi_x-\psi_y i)^2=\tilde{c}z^n j(z)$ in a neighborhood of 0 for some complex number $\tilde{c}\neq 0$, integer $n\geq 0$, and analytic function $j(z)$ satisfying $j(0)=1$.

For some $r_0,\beta,0\leq\beta<2\pi$, $\tilde{c}=r_0 e^{i\beta}$. We will define $\tilde{c}^{1/2}=r_0^{1/2}\,e^{i\beta/2}$, but all other fractional exponents will be calculated with respect to the following cut. Let k_0 be the largest integer k such that $\theta_k=((2k+1)\pi-\beta)/(n+2)<0$. Let $\overline{\gamma_k}$ be the half line $r\geq 0$, $\theta=\theta_k$, (r,θ) being the polar coordinates associated with (x,y) with $z=x+iy$. We will use the cut $\overline{\gamma_{k_0}}$ to define z^α for fractional α, except for $\tilde{c}^{1/2}$. More precisely, representing $z=re^{i\theta}$ for $r\geq 0$, $\theta_{k_0}\leq\theta<2\pi+\theta_{k_0}$, define $z^\alpha=r^\alpha e^{i\alpha\theta}$. This particular cut insures that $\mathrm{Re}(\tilde{c}^{1/2}\,z^{(n+2)/2})$ is continuous, which will be important in defining ϕ as a continuous function. In fact note that $\mathrm{Re}(\tilde{c}^{1/2}\,z^{(n+2)/2})=0$ precisely on the sets $\overline{\gamma_k}$, k an integer, of which there are only $m=n+2$ distinct sets. In addition $z=1$ is represented by $\theta=0$, so small neighborhoods of $z=1$ will get mapped to small neighborhoods of 1 by the fractional powers used below.

Let $k(z)=j^{1/2}(z)$, so k is analytic in a small neighborhood of 0 with $k(0)=1$. Thus $k(z)=1+\Sigma_{j=1}^{\infty}c_j z^j$. Note that $\ell(z)=1+\Sigma_{j=1}^{\infty}[(n+2)c_j z^j/(n+2j+2)]$ has the same radius of convergence, so $h(z)=\ell^{2/(n+2)}(z)$ is a well defined analytic function in a small neighborhood of 0, with values close to 1. Define

$$q(z)=\frac{2\tilde{c}^{1/2}}{n+2}(zh(z))^{n+2/2}. \tag{31}$$

Note for $b(z)=zh(z)$ that $db/dz=1$ at $z=0$, thus if $b(z)=u(x,y)+iv(x,y)$, $z=x+iy$, and we define $S(x,y)=(u(x,y),\ v(x,y))$, then the map $S:B(0,R)\to T(B(0,R))$ is an analytic diffeomorphism for small $R>0$, and S approaches the identity map as $R\to 0$. Also let $\gamma_k=b^{-1}(\overline{\gamma_k})$ (with $b^{-1}(z)$ being the inverse function of $b(z)$), so $q(z)$ is analytic in $\tilde{B}(0,R)$ (recall Definition 1) if n is even, and in $\tilde{B}(0,R)\backslash\gamma_{k_0}$ if n is odd.

For small enough R there is a ball $B\subset B(0,R)$, so $B,b(B)$ both lie in the positive quadrant, therefore, in $\tilde{B}$

$$q(z)=\frac{2\tilde{c}^{1/2}}{n+2}z^{n+2/2}\ell(z),\quad \frac{dq}{dz}=\tilde{c}^{1/2}z^{n/2}k(z), \tag{32}$$

due to the explicit power series for $\ell(z)$, thus

$$\left(\frac{dq}{dz}\right)^2=(\phi_x-i\phi_y)^2=(\psi_x-i\psi_y)^2, \tag{33}$$

for

$$\phi(x,y)=\mathrm{Re}(q(z)),z=x+iy. \tag{34}$$

However $(dq/dz)^2$ and $(\psi_x-i\psi_y)^2$ are both analytic in $\tilde{B}(0,R)\backslash\gamma_{k_0}$ (and in $\tilde{B}(0,R)$ if n is even), so (33) holds there as well.

We now characterize the behavior of ψ near 0. First assume $n=0$ so that ϕ is harmonic in $B(0,R)$ and $\nabla\phi(0)\neq 0$. From (33) we see that $\phi_x-i\phi_y=s(x,y)(\psi_x-i\psi_y)$, with $s(x,y)=\pm 1$ for each (x,y), so

$$\nabla\phi=s(x,y)\nabla\psi, \tag{35}$$

which intuitively indicates that ψ is locally constant on level sets of ϕ. To make this rigorous we introduce a change of variables that makes ϕ linear near 0. We can then take advantage of the fact that $H^1(\Omega)$ functions are absolutely continuous along almost all lines, which is enough regularity to compare ψ and ϕ. Choose axes so that $\nabla\phi(0)/|\nabla\phi(0)|=(0,1)$ and note by the implicit function theorem that in a neighborhood of 0 (recall $\phi(0)=0$) there exists a function $l(x,t)$ with $l(0,0)=0$ such that $\phi(x,l(x,t))=t$. Also note that we can assume $T(x,t)=(x,l(x,t))$ is smooth and 1-1 close to 0 so if we define $\overline{\phi}=\phi(T),\overline{\psi}=\psi(T)$ then $\overline{\phi}(x,t)=\phi(x,l(x,t))=t$ so

$$(0,1)=\nabla\overline{\phi}=\nabla\phi(T)DT=s(T)\nabla\psi(T)DT=s(T)\nabla\overline{\psi}, \tag{36}$$

and $\nabla\overline{\psi}=(0,s(T))$. Thus $\partial\overline{\psi}/\partial x=0$, which in conjunction with the fact that $\overline{\psi}$ is absolutely continuous on almost every line (due to $\overline{\psi}\in H^1$), implies that $\overline{\psi}=f(t)$ on almost every line $\mathbb{R}\times\{t\}$ for some function f. However, ψ is continuous so this extends to all t with f continuous. An immediate consequence is that $\psi=f(\phi)$ in a neighborhood of 0. Choosing a line $\{x\}\times\mathbb{R}$ on which $\overline{\psi}$ is absolutely continuous we see that f is absolutely continuous and $\partial\overline{\psi}/\partial t(x,t)=f'(t)$ so $|f'|=1$ almost everywhere due to $\nabla\overline{\psi}=(0,s(T))$.

If $n>0$ then $\nabla\phi(0)=0$. However, isolation of zeros of analytic functions implies that this is the only zero of $\nabla\phi$ in some neighborhood of 0. Thus $\nabla\phi\neq 0$ in each of the open regions $D_i = D_i(R)\subset B(0,R)$, bounded by $\gamma_i, \gamma_{i+1}, \partial B(0,R)$.

Fix i, and recall that the basic idea of the $n=0$ case is that near a point where $\nabla\psi\neq 0$ the identity (35) implies that ψ is constant on level sets of ϕ. This is a local result but it is easily extended to apply to connected components of level sets of ϕ as discussed below. However, that is the best one can do in general. To see this note that in the $n>0$ case $\phi=c$ has several components for many c, each component in a different D_i, as can be seen from the basic example where $k\equiv 1$ [k as defined above (31)]. In such a case it is easy to construct functions ψ satisfying $\nabla\psi=\pm\nabla\phi$ ($\pm$ consistent within each D_i but changing from one D_i to another) such that ψ has opposite signs on two different components of $\{\phi=c\}$. Thus the identity $\psi=f(\phi)$ is not possible because f cannot be defined consistently on all components of $\{\phi=c\}$. Because of this we are forced to analyze the level set structure of ϕ.

Given $c\in\mathbb{R}$ let

$$\overline{\gamma_i}(c)=\left\{ z\in\mathbb{C}\middle|\,\mathrm{Re}\left(\frac{2\tilde{c}^{1/2}}{n+2}z^{(n+2)/2}\right)=c\right\}\cap D_i, \tag{37}$$

which in polar coordinates is described by

$$r=\left(\frac{(n+2)c}{2r_0^{1/2}\cos\left(\dfrac{(n+2)\theta+\beta}{2}\right)}\right)^{2/(n+2)}, \quad \theta_i<\theta<\theta_{i+1}, \tag{38}$$

when c and $\cos([(n+2)\theta+\beta]/2)$ have the same sign, and is empty otherwise.

Thus if $\{\phi=c\}\cap D_i\neq\emptyset$ then for small R it equals $\gamma_i(c)=b^{-1}(\overline{\gamma_i}(c))$, which is a smooth connected curve with no self-intersections, and with endpoints in $\partial B(0,R)$. Let $\gamma:[0,1]\to\mathbb{R}^2$ parameterize $\{\phi=c\}\cap\overline{D_i}$ (where $\overline{D_i}$ is the closure of D_i) with $\gamma(0),\gamma(1)\in\partial B(0,R)$. Let $E=\{t\in[0,1]\,|\,\psi(\gamma(t))=\psi(\gamma(0))\}$. Note that E is closed due to continuity of ψ, γ so we can define $t_0=\max E$. Also the $n=0$ case above tells us that ψ is constant on $\{\phi=c\}$ near $\gamma(t_0)$ which contradicts the definition of t_0 unless $t_0=1$. Thus ψ is constant on $\{\phi=c\}\cap D_i$ so the function $f=f_i$ from the $n=0$ case is consistently defined in $D_i(R)$.

Note that one can take any of the curves $\overline{\gamma_k}$ to use as the cut in defining fractional powers simply by choosing the x,y axes differently. Thus if ϕ_k is the ϕ arising from using the cut $\overline{\gamma_k}$ (after a change of coordinates so we are using one consistent choice of axes for all k), then the above analysis, with ψ replaced by ϕ_j, shows on each D_i that $\phi_j=f_{i,j,k}(\phi_k)$ with $f_{i,j,k}(0)=0, |f'_{i,j,k}|=1$ almost everywhere. However, ϕ_j, ϕ_k are harmonic with nonzero gradient in D_i so $f'_{i,j,k}$ cannot have discontinuities, thus $f'_{i,j,k}$ is identically 1 or identically -1. Therefore, in each D_i either $\phi_j=\phi_k$ or $\phi_j=-\phi_k$. The claims about the discontinuity of $\nabla\phi$ follow directly from comparing $\phi=\phi_{k_0}$ with a ϕ_j corresponding to a different cut, since then ϕ_j is harmonic across γ_{k_0}.

A. Examples of weak classes

Given a function $\psi_0\in H^1(\mathbb{R}^2)$, if $\psi_0\in\mathcal{C}$, with $\mathcal{C}$ a collection as in Lemma 1, then

$$W(\psi_0)=\{\psi_0(d)\,|\,d\in\mathcal{D}(\Omega)\}\subset\mathcal{C}, \tag{39}$$

since $\mathcal{D}$ is closed under smooth domain variations (see Definition 1), and

$$\overline{W}(\psi_0)=\text{Weak Closure of } \{\psi_0(d)\,|\,d\in\mathcal{D}(\Omega)\} \text{ in } H^1(\Omega)\subset\mathcal{C}, \tag{40}$$

since $\mathcal{C}$ is weakly closed (for simplicity, as in the above definition, we will use $\psi_0(d)$ to denote both a function in $H^1(\Omega)$ and a function in $H^1(\Omega')$ for open sets Ω' containing Ω). Therefore it follows from Lemma 3 that $\overline{W}(\psi_0)$ is the smallest collection of the type described in Lemma 1 that contains ψ_0.

Thus our results apply to $\overline{W}(\psi_0)$, however, it is difficult to say much more about the global nature of the discontinuities in the gradients of functions in $\overline{W}(\psi_0)$ due to the fact that the ''topological structure'' of such functions is not explicit. To rectify this deficiency we consider the function classes described after Lemma 3 which very explicitly encode topological structure.

Lemma 3: If $\psi_0 \in H^1(\mathbb{R}^2)$ then $W(\psi_0) \subset H^1(\Omega)$, and $\overline{W}(\psi_0)$ is weakly closed in $H^1(\Omega)$, satisfies (9), and is closed under smooth domain variations, as defined in Definition 1.

Remark 3: Note that one need only assume that $\psi_0 \in H^1(\Omega')$ for some open set Ω' containing the closure of Ω.

Proof: Let $B_r = B(0,r)$, where r is chosen such that $\Omega \subset B_{r/3}$. By multiplying by a smooth cutoff function which equals 1 in $B_{r/2}$, and 0 in $\mathbb{R}^2 \backslash B_r$, one can assume $\psi_0 \in H_0^1(B_r)$.

To confirm the first claim of the lemma take $\psi \in W(\psi_0)$, i.e., $\psi = \psi_0(d)$ for some $d \in \mathcal{D}$. Note that (18), (19) hold with d replacing d_t, thus there is a constant $c(d)$ dependent on d, such that

$$\int_\Omega |\nabla \psi|^2 \leqslant c(d) \int_\Omega |\nabla \psi_0|^2, \tag{41}$$

since Dd is smooth and equals the identity map in a neighborhood of $\partial\Omega$, and thus in addition $\det Dd$ is bounded, and uniformly bounded from zero (with bound dependent on d). However, using the convention above with $\Omega' = B_r$, $\psi = \psi_0$ in $B_r \backslash \Omega$, so

$$\int_{B_r} |\nabla \psi|^2 \leqslant (c(d)+1) \int_{B_r} |\nabla \psi_0|^2, \tag{42}$$

so the first claim follows from the inequality:

$$\int_{B_r} u^2 \leqslant c \int_{B_r} |\nabla u|^2 \tag{43}$$

which holds for all $u \in H_0^1(B_r)$ for some $c = c(r)$.

The second claim of the lemma is clearly true since a weak closure is weakly closed. To confirm (9) holds for $\overline{W}(\psi_0)$ first consider $\psi \in \overline{W}(\psi_0)$. By definition there exists a sequence $(\psi_n) \subset W(\psi_0)$ with $\psi_n \to \psi$ weakly in $H^1(\Omega)$. Thus (ψ_n) is bounded in $H^1(\Omega)$, however $\psi_n = \psi_0$ in $B_r \backslash \Omega$ so ψ_n is bounded in $H_0^1(B_r)$. One can then extract a subsequence which converges weakly in $H_0^1(B_r)$. Weak convergence in $H^1(\Omega)$, or in $H_0^1(B_r)$, implies pointwise convergence almost everywhere on a subsequence, so the later limit must equal ψ in Ω and ψ_0 in $B_r \backslash \Omega$. In summary, any element of $\psi \in \overline{W}(\psi_0)$ can be extended to equal ψ_0 in B_r so that $\psi \in H_0^1(B_r)$.

Now assume $\psi_n \in \overline{W}(\psi_0)$ with $E(\psi_n) \leqslant M$. Extending ψ_n as above we have

$$\int_{B_r} (\psi_n)^2 \leqslant c \int_{B_r} |\nabla \psi_n|^2 \leqslant c \left(\int_{B_r \backslash \Omega} |\nabla \psi_0|^2 + M \right), \tag{44}$$

and (9) is verified.

Finally given $\psi \in \overline{W}(\psi_0), d \in \mathcal{D}$ we need to show that $\psi(d) \in \overline{W}(\psi_0)$. By definition there exist $\psi_n \in W(\psi_0)$ with $\psi_n \to \psi$ weakly in $H^1(\Omega)$. As above we can take ψ, ψ_n equal to ψ_0 in $B_r \backslash \Omega$ with $\psi_n \to \psi$ weakly in $H_0^1(B_r)$ on a subsequence. But $\psi_n = \psi_0(d_n)$ for some $d_n \in \mathcal{D}$ so $\psi_n(d) = \psi_0(d_n(d)) \in W(\psi_0)$ since $d_n(d) \in \mathcal{D}$. Also $E(\psi_n(d)) \leqslant c(d) E(\psi_n)$ as in (41) so

$$\int_{B_r} (\psi_n(d))^2 \leqslant c \int_{B_r} |\nabla(\psi_n(d))|^2 \leqslant c(c(d)+1) \int_{B_r} |\nabla \psi_n|^2, \tag{45}$$

since $\psi_n(d)=\psi_n=\psi_0$ on $B_r\backslash\Omega$. However as before weak convergence of ψ_n in $H^1(\Omega)$ implies (ψ_n) is bounded in $H_0^1(B_r)$ so (45) implies that $(\psi_n(d))$ is bounded in $H_0^1(B_r)$, and so on a subsequence converges weakly in $H_0^1(B_r)$, the limit equaling $\psi(d)$ by pointwise almost everywhere convergence on a subsequence. Thus $\psi(d) \in \overline{W}(\psi_0)$ since $\psi_n(d) \in W(\psi_0)$ and the proof of the lemma is complete.

Next we consider function classes with explicit topological structure. For simplicity assume Ω is a simply connected open set with closure in $B(0,R)$ for some $R>0$. We have strong evidence to indicate that any $\psi \in H_0^1(B(0,R))$ can be decomposed as

$$\psi = \sum_{i \in I} f_i(\psi_i), \tag{46}$$

where I is a finite or countable index set, functions $f_i:\mathbb{R}\to\mathbb{R}$ are Lipschitz continuous with $|f'|=1$ almost everywhere and $f(0)=0$, and functions $\psi_i \in H_0^1(B(0,R)) \cap C(\mathbb{R}^2)$ are "topologically simple" in the sense that $\psi_i \geqslant 0$, and sets $\{\psi_i > t\}$ are simply connected for all t, and in addition ψ_i satisfy 'support conditions' defined in terms of a collection of constants $\{t_{i,j}: i,j \in I, i<j\}$, namely $\psi_i = t_{i,j}$ on $\psi_j > 0$ for all $i<j$.

From methods in Ref. 7, augmented as in Ref. 8, one can prove that the collection of all such functions, with fixed $I, f_i, t_{i,j}$, and with functions ψ_i fixed in $B(0,R)\backslash\Omega$ such that $\max \psi_i = \max_{\partial\Omega} \psi_i$, is weakly closed in $H_0^1(B(0,R))$ (and thus, as in Lemma 3, the collection restricted to Ω is weakly closed in $H^1(\Omega)$). Condition (9) is satisfied due to the inequality $\int_{B(0,R)} \psi^2 \leqslant c \int_{B(0,R)} |\nabla \psi|^2$ which holds due to $\psi \in H_0^1(B(0,R))$. Also it is easy to see that such a collection is closed under smooth domain variations of Ω as in Definition 1. Thus our present results apply so there is a minimizer ψ satisfying various regularity properties. Note the appearance of Lipschitz functions f_i both in Theorem 1 and in the decomposition above. More importantly the decomposition in some sense encodes topological information in that the level sets of ψ can be reconstructed from the level sets of the functions ψ_i, after taking into account the constants $t_{i,j}$ and the "folding" effect of the functions f_i. It remains, however, to analyze the set on which $\nabla\psi$ is discontinuous. This is left to Ref. 8 where a fairly simple example is used to illustrate a general approach to studying discontinuities.

IV. STATIONARY POINTS

Lemma 1 deals with energy minimizers. However, the proof carries over to stationary points of the energy defined in the following manner. Thus all our results carry over to this more general situation.

Definition 2: A function $\psi_0 \in H^1(\Omega)$ is a stationary point of

$$E(\psi) = \int_\Omega |\nabla \psi|^2, \tag{47}$$

with respect to local smooth domain variations if for any $p_0 \in \Omega$ there exists $r, 0<r<\operatorname{dist}(p_0, \partial\Omega)$ such that

$$\frac{d}{dt} E(\psi_t)\bigg|_{t=0} = 0, \tag{48}$$

for all $\psi_t, \psi_t(p,t) = \psi_0(X(p,t))$, X being any smooth map $X:\Omega\times(-\epsilon,\epsilon)\to\Omega$ defined for some $\epsilon>0$ such that $X(\cdot,0)=I$ (I the identity map) and $X(\cdot,t)$ is a diffeomorphism of Ω onto Ω for each t, such that $X(p,t)=p$ for all $p \in \Omega\backslash B(p_0,r)$ and $t \in (-\epsilon,\epsilon)$.

Theorem 2: *If ψ is a stationary point of E then $(\partial\psi/\partial x - i\partial\psi/\partial y)^2$ is a complex analytic function (after possible redefinition of $\nabla\psi$ on a set of Lebesgue measure zero), and consequently Lemma 2, Theorem 1, and Corollary 1 hold for ψ.*

Proof: Given $p_0 \in \Omega$ let r be as in the statement of the theorem. Given $w \in C_0^\infty(B(p_0,r)) \times C_0^\infty(B(p_0,r))$ let $d_t(p) = p + tw(p)$. Thus there exists $\epsilon > 0$ such that for all $|t| < \epsilon$ the map d_t is a smooth diffeomorphism from Ω onto Ω with $\det Dd_t \geqslant c > 1/2$. Consequently $X(\cdot,t) = d_t^{-1}$ satisfies the conditions in Definition 2 so

$$\frac{d}{dt} E(\psi_t)\bigg|_{t=0} = 0, \tag{49}$$

for ψ_t defined by $\psi_t(p,t) = \psi_0(X(p,t))$ for $(p,t) \in \Omega \times (-\epsilon, \epsilon)$. The argument is completed as in the proof of Lemma 1.

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Image system for Stokes-flow singularity between two parallel planar walls

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Using a recently developed image representation for Stokes flow in a half-space bounded by a planar wall [Cichocki and Jones, Physica A **258**, 273 (1998)], the image system is constructed for the flow field produced by a force multipole in the space bounded by two parallel walls. The image singularities are expressed in terms of products of double-reflection matrices, and the expansion is simplified using symmetries of the double-reflection operation. Our analysis yields recurrence relations for the strengths of the image multipoles. The relations are solved explicitly, and a complete image system is obtained for an arbitrary source-force multipole. Applications of our image representation for evaluating the hydrodynamic friction and mobility matrices of particles interacting with two parallel planar walls are indicated. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1508812]

I. INTRODUCTION

Dynamics of particles suspended in a viscous fluid that occupies the space bounded by a planar interface[1–8] or two planar walls[9–15] has recently attracted much attention. Hydrodynamic interactions of particles in such geometries are affected by the flow field reflected from the walls. An important tool for investigating particle motion in wall-bounded systems is the image representation of the reflected flow.[16]

The Stokes flow reflected from a single no-slip wall was originally discussed by Lorentz,[17] and the image of a Stokeslet was derived by Blake.[18] Recently, a complete image representation for a force multipole of an arbitrary order was obtained by Cichocki and Jones.[4] This image representation was used to determine single-particle[4] and many-particle[8] friction and mobility coefficients for the motion of spherical particles near a rigid wall.

In the present article we derive the image representation for a flow field generated by a force multipole between two parallel rigid walls. In an earlier study,[19] the image solution was considered only for a special case of Stokeslet, but a complete multiple-reflection singularity representation was not found. The difficulty of the analysis stems from the form of the one-wall solution: unlike the reflection of an electrostatic charge multipole from a conducting plane, the image of a force multipole of an order l involves a combination of multipoles of orders $l' \neq l$. For this reason, the multiple-reflection series for Stokes flow in a space bounded by two parallel walls involves complicated combinations of image multipoles of different orders and strengths, placed at the positions corresponding to multiple mirror reflections of the source in the bounding planes.

A key ingredient of our analysis is the double-reflection identity that results from a symmetry between the source and the image flows in a system with a single reflection plane. Both of these flows satisfy Stokes equations, and their sum vanishes on the plane; thus, the reflection operation applied twice, first to the source and then to the image flow, yields the original source flow. The double-reflection identities are used to simplify the multiple-reflection sequences in a two-wall system and to derive simple recurrence relations for the strength of the image force multipoles. The recurrence relations are solved explicitly.

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This article is organized as follows. In Sec. II, basic notation is introduced, and image singularities are represented in terms of a complete set of Stokes-flow fields. The image representation for a force multipole in a system with a single wall is discussed in Sec. III, where the double-reflection identities are derived. The identities are used in Sec. IV to obtain the image solution for a force multipole between two walls. The results are discussed in Sec. V.

II. FORMULATION

We consider Stokes flow produced by a multipolar force distribution $\mathbf{F}$ located at $\mathbf{r}=0$ in a region bounded by two infinite parallel planar walls (a) and (b) located at

$$z=-h^{(a)}, \quad z=h^{(b)}. \tag{2.1}$$

At the walls, the flow field $\mathbf{u}$ satisfies no-slip boundary conditions.

The incident flow $\mathbf{v}$, produced by the force distribution $\mathbf{F}$ in infinite space, can be expanded in a complete set of basis solutions of Stokes equations. We choose here the representation introduced by Cichocki *et al.*,[20]

$$\mathbf{v}(\mathbf{r})=\sum_{lm\sigma} f_{lm\sigma}\mathbf{v}^{-}_{lm\sigma}(\mathbf{r}), \tag{2.2}$$

where $f_{lm\sigma}$ are the multipole moments of the distribution $\mathbf{F}$, and the basis velocity fields are of the form

$$\mathbf{v}^{-}_{lm\sigma}(\mathbf{r})=\mathbf{V}_{lm\sigma}(\theta,\phi)r^{-(l+\sigma)}. \tag{2.3}$$

Here (r,θ,ϕ) represent vector $\mathbf{r}$ in spherical coordinates, and the indices assume values $l=1,2,\ldots$; $m=-l,\ldots,l$; and $\sigma=0,1,2$. The functions $\mathbf{V}_{lm\sigma}(\theta,\phi)$ are combinations of vector spherical harmonics with angular and azimuthal quantum numbers l and m. This property and the r-dependence in Eq. (2.3) define the functions $\mathbf{v}^{-}_{lm\sigma}(\mathbf{r})$ up to a normalization constant; we use here the same normalization as in Ref. 20. Explicit expressions for the functions $\mathbf{V}_{lm\sigma}(\theta,\phi)$ are listed in Appendix A.

In the presence of the walls, the reflected flow field

$$\mathbf{v}_{\mathrm{s}}=\mathbf{u}-\mathbf{v} \tag{2.4}$$

can be represented in terms of image singularities. In a system with the source singularity at $\mathbf{r}_{\mathrm{s}}=z_{\mathrm{s}}\mathbf{e}_z$ and a single wall at $z=z_{\mathrm{w}}$, the image singularity is at $\mathbf{r}_{\mathrm{i}}=(2z_{\mathrm{w}}-z_{\mathrm{s}})\mathbf{e}_z$, and

$$\mathbf{v}_{\mathrm{s}}(\mathbf{r})=\sum_{lm\sigma} f^{*}_{lm\sigma}\mathbf{v}^{-}_{lm\sigma}(\mathbf{r}-\mathbf{r}_{\mathrm{i}}), \tag{2.5}$$

where $f^{*}_{lm\sigma}$ are the multipole moments of the image, and $\mathbf{e}_z$ is the unit vector in the z direction.

For two walls, the image representation can be obtained from (2.5) in a form of a multiple-reflection sequence. Accordingly,

$$\mathbf{v}_{\mathrm{s}}(\mathbf{r})=\sum_{\alpha=a,b}\sum_{i=1}^{\infty}\mathbf{v}_{\mathrm{s}}^{(i\alpha)}(\mathbf{r}), \tag{2.6}$$

where

$$\mathbf{v}_{\mathrm{s}}^{(i\alpha)}(\mathbf{r})=\sum_{lm\sigma} f^{(i\alpha)}_{lm\sigma}\mathbf{v}^{-}_{lm\sigma}(\mathbf{r}-\mathbf{r}^{(i\alpha)}). \tag{2.7}$$

For the geometry (2.1), the positions of the image singularities are $\mathbf{r}^{(i\alpha)}=H^{(i\alpha)}\mathbf{e}_z$, with

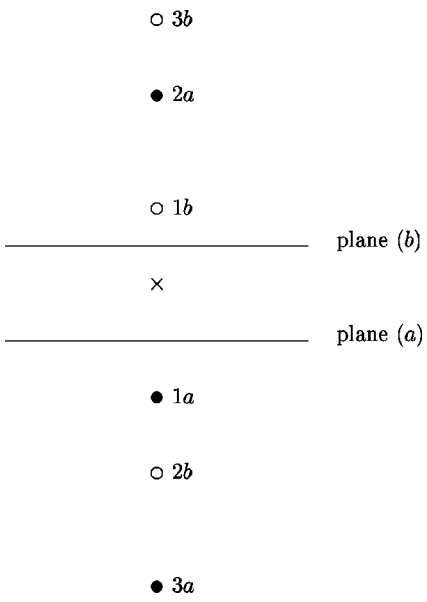

FIG. 1. Positions $\mathbf{r}^{(ia)}$ and $\mathbf{r}^{(ib)}$ $(i=1,2,\ldots)$ of image singularities in two families (a) and (b).

$$\begin{aligned} H^{(2r\,a)}&=2rh, \quad H^{(2r+1\,a)}=-2(h^{(a)}+rh),\\ H^{(2r\,b)}&=-2rh, \quad H^{(2r+1\,b)}=2(h^{(b)}+rh), \end{aligned} \tag{2.8}$$

where $h=h^{(a)}+h^{(b)}$ is the distance between walls, $H^{(0a)}=H^{(0b)}=0$ describes the position of the source singularity, and the index $r=0,1,2...$ characterizes the double-reflection order. The family of images at $\mathbf{r}^{(i\alpha)}$, $i=1,2,\ldots$, corresponds to the multiple-reflection sequence with the initial reflection on the plane (α), as illustrated in Fig. 1. The explicit expressions for the multipole moments $f^{(i\alpha)}_{lm\sigma}$ are derived in the following sections.

III. SINGLE-REFLECTION MATRIX

A. Multipoles of image force

By linearity of Stokes equations, the multipole moments of the source and image force distributions are linearly related,

$$f^{*}_{lm\sigma}=\sum_{l'm'\sigma'} R(H,lm\sigma|l'm'\sigma')f_{l'm'\sigma'}, \tag{3.1}$$

where R is the reflection matrix, and $H=z_{\mathrm{s}}-z_{\mathrm{w}}$ describes the relative position of the source singularity and the wall. The explicit form of the reflection matrix has recently been derived by Cichocki and Jones,[4] and we follow here their notation.

The successive images in the families $\alpha=a,b$ are obtained by a sequence of reflections

$$f^{(i\alpha)}_{lm\sigma}=\sum_{l'm'\sigma'} R(H^{(i-1\alpha)}_{\mathrm{w}},lm\sigma|l'm'\sigma')f^{(i-1\alpha)}_{l'm'\sigma'}, \quad i=1,2,\ldots, \tag{3.2}$$

where

$$H^{(i\alpha)}_{\mathrm{w}}=\tfrac{1}{2}(H^{(i\alpha)}-H^{(i+1\alpha)}). \tag{3.3}$$

The reflection is on the plane α for $i=2r+1$ and at the plane $\beta\neq\alpha$ for $i=2r$.

B. Structure of reflection matrix

Due to the rotational symmetry with respect to the axis z, the matrix R is diagonal in the angular quantum number m,

$$R(H,lm\sigma|l'm'\sigma')=R(H,lm\sigma|l'm\sigma')\,\delta_{mm'}. \tag{3.4}$$

The dependence of $R(H,lm\sigma|l'm'\sigma')$ on the relative coordinate H and the azimuthal quantum numbers l, l' can be derived from the Lorentz's reflection formula[16,17] for the reflected field,

$$\mathbf{v}_s=\hat{\mathrm{P}}(\hat{\mathbf{R}}_0+H\hat{\mathbf{R}}_1+H^2\hat{\mathbf{R}}_2)\cdot\mathbf{v}, \tag{3.5}$$

where

$$\hat{\mathbf{R}}_0=-\mathbf{I}_z-2\bar{z}\boldsymbol{\nabla}\mathbf{e}_z+\bar{z}^2\nabla^2\mathbf{I}, \tag{3.6}$$

$$\hat{\mathbf{R}}_1=-2\boldsymbol{\nabla}\mathbf{e}_z+2\bar{z}\nabla^2\mathbf{I}, \tag{3.7}$$

$$\hat{\mathbf{R}}_2=\nabla^2\mathbf{I}. \tag{3.8}$$

In the above relations, $\bar{z}=z-z_s$ is the coordinate relative to the source position, $\mathbf{I}$ is the identity tensor, $\mathbf{I}_z=\mathbf{I}-2\mathbf{e}_z\mathbf{e}_z$, and $\hat{\mathrm{P}}$ is the reflection operator with respect to the plane $z=z_w$,

$$[\hat{\mathrm{P}}\mathbf{w}](x,y,z)=\mathbf{I}_z\cdot\mathbf{w}(x,y,2z_w-z). \tag{3.9}$$

Since the operators (3.6)–(3.8) can be decomposed into a linear combination of tensor operators with azimuthal quantum numbers $l''\leqslant 2$, the matrix elements (3.4) vanish for $|l-l'|>2$, because of the triangle property of Clebsch–Gordan coefficients.[21] Moreover, operators $\hat{\mathbf{R}}_i$ are homogeneous of the order $-i$ in $\mathbf{r}$, according to Eqs. (3.6)–(3.8). It thus follows from relations (2.3) and (3.5) that

$$\begin{aligned}R(H,n-\sigma\ m\ \sigma|n'-\sigma'\ m\ \sigma')=&R_{n\,n}(\sigma\sigma',m)\,\delta_{n'n}+HR_{n\,n-1}(\sigma\sigma',m)\,\delta_{n'n-1}\\&+H^2R_{n\,n-2}(\sigma\sigma',m)\,\delta_{n'n-2}.\end{aligned} \tag{3.10}$$

The explicit expressions for the matrix elements $R_{n\,n'}(\sigma\sigma',m)$ are listed in Appendix B.

C. Reduced matrix notation

Relations (3.4) and (3.10) allow us to introduce a compact matrix notation. Accordingly, we define a vector space $\mathcal{S}$ of infinite column vectors f with components f_n $(n=1,2,\ldots)$, where each component itself consists of three components $\mathsf{f}_n(\sigma)$ $(\sigma=0,1,2)$. We also define matrices A acting in $\mathcal{S}$: each element $\mathsf{A}_{n\,n'}$ of such a matrix is itself a three-dimensional matrix with the elements $\mathsf{A}_{n\,n'}(\sigma\sigma')$. In the space $\mathcal{S}$, the products Af and AB are defined in a natural way,

$$(\mathsf{Af})_n=\sum_{n'=1}^{\infty}\mathsf{A}_{n\,n'}\mathsf{f}_{n'},\quad (\mathsf{AB})_{n\,n''}=\sum_{n'=1}^{\infty}\mathsf{A}_{n\,n'}\mathsf{B}_{n'n''}, \tag{3.11}$$

where $\mathsf{A}_{n\,n'}\mathsf{f}_{n'}$ and $\mathsf{A}_{n\,n'}\mathsf{B}_{n'n''}$ are the inner products in the corresponding three-dimensional space.

In this notation, the single-reflection matrix (3.10) is represented by the matrix $\mathsf{R}(H)$ with a three-diagonal structure

$$\mathsf{R}_{n\,n-i}(H)=\begin{cases}H^i\bar{\mathsf{R}}_{n\,n-i}, & i=0,1,2,\\ 0, & \text{otherwise},\end{cases} \tag{3.12}$$

where

$$\bar{\mathsf{R}}_{n\,n'}(\sigma\sigma') = R_{n\,n'}(\sigma\sigma', m). \tag{3.13}$$

The arrays of source and image multipoles are represented by the arrays f and f^* with elements

$$\mathsf{f}_n(\sigma) = f_{n-\sigma\,m\,\sigma}, \quad \mathsf{f}^*_n(\sigma) = f^*_{n-\sigma\,m\,\sigma}. \tag{3.14}$$

Taking into account diagonal form (3.4) of the matrix R, relation (3.1) can be rewritten as

$$\mathsf{f}^* = \mathsf{R}(H)\mathsf{f}, \tag{3.15}$$

where, for simplicity, the dependence on the index m is not indicated.

D. Double-reflection identities

The reflection of the image f^* with respect to the plane of the original reflection returns the source force distribution f. This symmetry and Eq. (3.15) imply the double-reflection identity

$$\mathsf{R}(-H)\mathsf{R}(H) = \mathsf{I}^{\mathcal{S}}, \tag{3.16}$$

where $\mathsf{I}^{\mathcal{S}}$ is the unit matrix in the space $\mathcal{S}$. For the individual matrix components (3.12), Eq. (3.16) yields

$$\bar{\mathsf{R}}_{n\,n}\bar{\mathsf{R}}_{n\,n} = \mathsf{I}, \tag{3.17}$$

$$\bar{\mathsf{R}}_{n\,n-1}\bar{\mathsf{R}}_{n-1\,n-1} - \bar{\mathsf{R}}_{n\,n}\bar{\mathsf{R}}_{n\,n-1} = 0, \tag{3.18}$$

$$\bar{\mathsf{R}}_{n\,n-2}\bar{\mathsf{R}}_{n-2\,n-2} - \bar{\mathsf{R}}_{n\,n-1}\bar{\mathsf{R}}_{n-1\,n-2} + \bar{\mathsf{R}}_{n\,n}\bar{\mathsf{R}}_{n\,n-2} = 0, \tag{3.19}$$

$$\bar{\mathsf{R}}_{n\,n-2}\bar{\mathsf{R}}_{n-2\,n-3} - \bar{\mathsf{R}}_{n\,n-1}\bar{\mathsf{R}}_{n-1\,n-3} = 0, \tag{3.20}$$

$$\bar{\mathsf{R}}_{n\,n-2}\bar{\mathsf{R}}_{n-2\,n-4} = 0, \tag{3.21}$$

where I is the identity matrix in three dimensions corresponding to indices σ, σ' in the relation (3.13).

IV. TWO WALL SOLUTION

A. Double-reflection expansion

The double-reflection identities (3.17)–(3.21) can be used to derive explicit expressions for the multipolar moments of the image singularities $f^{(i\alpha)}_{lm\sigma}$ in the two-wall system. The problem is formulated in terms of multiple-reflection matrices $\mathsf{R}^{(i\alpha)}$, which are defined by the linear relation

$$\mathsf{f}^{(i\alpha)} = \mathsf{R}^{(i\alpha)}(h^{(\alpha)}, h)\mathsf{f}, \tag{4.1}$$

where the dependence of R on the wall position (2.1) and the separation of the walls are indicated. The array $\mathsf{f}^{(i\alpha)}$ is related to the elements $f^{(i\alpha)}_{lm\sigma}$ as implied by Eq. (3.14). By invariance with respect to the transformation $z \to -z$, the reflection matrices representing two families of images (a) and (b) are related,

$$\mathsf{R}^{(ib)}(H, h) = \mathsf{R}^{(ia)}(-H, -h). \tag{4.2}$$

In what follows, we thus consider only the family $\alpha = a$, and we set $H = h^{(a)}$.

The structure of matrices $\mathsf{R}^{(ia)}$ is analyzed by factorizing them into a double-reflection sequence. To this end, we introduce abbreviated notation

$$\mathsf{R}^{(2r\,a)}(H,h)=\mathsf{P}^{(r)} \tag{4.3}$$

and

$$\mathsf{R}^{(2r+1\,a)}(H,h)=\tilde{\mathsf{P}}^{(r)}. \tag{4.4}$$

Equations (3.2) and (4.1) imply that the odd-reflection matrices can be obtained from the relation

$$\tilde{\mathsf{P}}^{(r)}=\mathsf{R}(H_r)\mathsf{P}^{(r)}, \tag{4.5}$$

and the even-reflection matrices can be factorized

$$\mathsf{P}^{(r)}=\prod_{i=1}^{r}\mathsf{Q}(H_{i-1}). \tag{4.6}$$

Here

$$H_r=H+2rh \tag{4.7}$$

is the distance between the plane (a) and the image at the position $\mathbf{r}^{(2r\,a)}$, consistent with Eq. (3.3). The double-reflection matrix is defined

$$\mathsf{Q}(H)=\mathsf{R}(-H-h)\mathsf{R}(H), \tag{4.8}$$

and the order of the matrix product is $\Pi_{i=1}^{k}\mathsf{M}_i=\mathsf{M}_k\ldots\mathsf{M}_1$.

B. Simplified form of even-reflection matrices

Definitions (4.6) and (4.8) imply that the even-reflection matrix has the following structure,

$$\mathsf{P}^{(r)}_{n\,n'}=\sum_{\{n_j\}}\left[\alpha(\{n_j\})\prod_{k=1}^{2r}\bar{\mathsf{R}}_{n_k\,n_{k-1}}\right], \tag{4.9}$$

where the summation is over all sets $\{n_j\}$ of integer elements n_j $(j=0,1,\ldots,2r)$ that satisfy relations

$$n_0=n',\quad n_{2r}=n,\quad n_j-n_{j-1}=0,1,2. \tag{4.10}$$

The matrix $\mathsf{P}^{(r)}_{nn'}$ depends on H and h only through the coefficients

$$\alpha(\{n_j\})=\prod_{i=1}^{r}\left[(-h-H_{i-1})^{n_{2i}-n_{2i-1}}H_{i-1}^{n_{2i-1}-n_{2i-2}}\right], \tag{4.11}$$

which can be shown using Eq. (3.12).

Equation (4.9) can be considerably simplified by using the double-reflection identities (3.17)–(3.21). Accordingly, the commutation relations (3.18) and (3.20) are used to shift matrices $\bar{\mathsf{R}}_{k\,k-1}$ to the left; in the resulting formula products $\bar{\mathsf{R}}_{k\,k-1}\bar{\mathsf{R}}_{k-1\,k-2}$ are eliminated using (3.19), and products $\bar{\mathsf{R}}_{k\,k}\bar{\mathsf{R}}_{k\,k}$ and $\bar{\mathsf{R}}_{k\,k-2}\bar{\mathsf{R}}_{k-2\,k-4}$ are reduced using (3.17) and (3.21). Following this procedure, the even-reflection matrices $\mathsf{P}^{(r)}_{n\,n'}$ can be represented as linear combinations

$$\mathsf{P}^{(r)}_{n\,n-2s}=a(r,s)\mathsf{A}_{n\,n-2s}+b(r,s)\mathsf{B}_{n\,n-2s}, \tag{4.12}$$

$$\mathsf{P}^{(r)}_{n\,n-2s-1}=c(r,s)\mathsf{C}_{n\,n-2s-1}+d(r,s)\mathsf{D}_{n\,n-2s-1}, \tag{4.13}$$

where

$$\mathsf{A}_{n\,n}=\mathsf{B}_{n\,n}=\mathsf{I}, \tag{4.14}$$

$$\mathsf{A}_{n\,n-2s}=\prod_{i=n-2s}^{n-2}{}' \ (\bar{\mathsf{R}}_{i+2\,i}\bar{\mathsf{R}}_{i\,i}), \quad s=1,2,\ldots, \tag{4.15}$$

$$\mathsf{B}_{n\,n-2s}=\prod_{i=n-2s}^{n-2}{}' \ (\bar{\mathsf{R}}_{i+2\,i+2}\bar{\mathsf{R}}_{i+2\,i}), \quad s=1,2,\ldots, \tag{4.16}$$

$$\mathsf{C}_{n\,n-2s-1}=\bar{\mathsf{R}}_{n\,n}\bar{\mathsf{R}}_{n\,n-1}\mathsf{A}_{n-1\,n-1-2s}, \quad s=0,1,\ldots, \tag{4.17}$$

$$\mathsf{D}_{n\,n-2s-1}=\bar{\mathsf{R}}_{n\,n-1}\bar{\mathsf{R}}_{n-1\,n-3}\mathsf{B}_{n-3\,n-3-2(s-1)}, \quad s=1,2,\ldots, \tag{4.18}$$

and the remaining elements of $\mathsf{A}_{n\,n'}$, $\mathsf{B}_{n\,n'}$, $\mathsf{C}_{n\,n'}$, $\mathsf{D}_{n\,n'}$ are set equal to zero.

Explicit expressions for the matrices A, B are given in Appendix C; the matrices C and D can be obtained from these results using Eqs. (4.17) and (4.18) and the expressions listed in Appendix B. The scalar coefficients a, b, c, and d are evaluated in the following section.

C. Recurrence relations

To proceed with our analysis, we rewrite Eq. (4.6) in the form

$$\mathsf{P}^{(r+1)}=\mathsf{Q}(H_r)\mathsf{P}^{(r)}, \tag{4.19}$$

which in the component notation yields

$$\mathsf{P}^{(r+1)}_{n\,n-q}=\sum_{p=0}^{4}\mathsf{Q}_{n\,n-p}(H_r)\mathsf{P}^{(r)}_{n-p\,n-q}, \tag{4.20}$$

according to Eqs. (4.8) and (3.12). The elements of the matrix Q are simplified by using the double-reflection identities (3.17)–(3.21). It follows that

$$\mathsf{Q}_{n\,n}(H)=I, \tag{4.21}$$

$$\mathsf{Q}_{n\,n-1}(H)=-h\bar{\mathsf{R}}_{n\,n}\bar{\mathsf{R}}_{n\,n-1}, \tag{4.22}$$

$$\mathsf{Q}_{n\,n-2}(H)=h[(H+h)\bar{\mathsf{R}}_{n\,n-2}\bar{\mathsf{R}}_{n-2\,n-2}-H\bar{\mathsf{R}}_{n\,n}\bar{\mathsf{R}}_{n\,n-2}], \tag{4.23}$$

$$\mathsf{Q}_{n\,n-3}(H)=hH(H+h)\bar{\mathsf{R}}_{n\,n-1}\bar{\mathsf{R}}_{n-1\,n-3}, \tag{4.24}$$

$$\mathsf{Q}_{n\,n-4}(H)=0, \tag{4.25}$$

and all other elements $\mathsf{Q}_{n\,n'}$ vanish. Two pairs of coupled recurrence relations for the coefficients a, b, c, d in Eqs. (4.12) and (4.13) are derived from relation (4.20) by using the above expressions for Q and definitions (4.14)–(4.18),

$$\begin{aligned}a(r+1,s)=a(r,s)-h\,c(r,s-1)+h(h+H_r)[\delta_{s1}+(1-\delta_{s1})a(r,s-1)]\\ +h(h+H_r)\,H_r c(r,s-2),\end{aligned} \tag{4.26}$$

$$c(r+1,s)=c(r,s)-h[\delta_{s0}+(1-\delta_{s0})a(r,s)]-h\,H_r c(r,s-1), \tag{4.27}$$

and

$$b(r+1,s)=b(r,s)-h[d(r,s-1)-rh\delta_{s1}]-h\,H_r[\delta_{s1}+(1-\delta_{s1})b(r,s-1)], \tag{4.28}$$

$$\begin{aligned} d(r+1,s)=&d(r,s)-h(1-\delta_{s0})b(r,s)+h\,(h+H_r)[d(r,s-1)-rh\delta_{s1}]\\ &+h(h+H_r)\,H_r[\delta_{s1}+(1-\delta_{s1})b(r,s-1)]. \end{aligned} \tag{4.29}$$

The initial conditions for the above relations are obtained from the identity

$$\mathsf{P}^{(1)}_{nn'}=\mathsf{Q}_{n\,n'}(H) \tag{4.30}$$

and Eqs. (4.21)–(4.25), which imply

$$\begin{gathered} a(1,0)=1,\quad a(1,1)=h(h+H),\\ b(1,0)=0,\quad b(1,1)=-hH,\\ c(1,0)=-h,\quad c(1,1)=0,\\ d(1,0)=0,\quad d(1,1)=h(h+H)H, \end{gathered} \tag{4.31}$$

and

$$a(1,s)=b(1,s)=c(1,s)=d(1,s)=0,\qquad \text{for}\quad s>1\quad\text{or}\quad s<0. \tag{4.32}$$

We assumed here $a(1,0)=1$; however, because of Eq. (4.14), only $a(1,0)+b(0,1)=1$ is required.

The recurrence relations (4.26)–(4.29) with initial conditions (4.31) and (4.32) can be explicitly solved. It can be verified by induction that the solution is

$$a(r,s)=\frac{(-1)^{s+1}(r+s-1)!}{(2s)!(r-s)!}h^{2s-1}[2sH+(4sr-r-s)h], \tag{4.33}$$

$$b(r,s)=\frac{(-1)^{s}(r+s-1)!}{(2s)!(r-s)!}h^{2s-1}[2sH+(r-s)h](1-\delta_{s0}), \tag{4.34}$$

$$c(r,s)=\frac{(-1)^{s+1}(r+s)!}{(2s+1)!(r-s-1)!}h^{2s+1}, \tag{4.35}$$

$$\begin{aligned} d(r,s)=&\frac{(-1)^{s+1}(r+s-1)!}{(2s+1)!(r-s)!}h^{2s-1}\{2s(2s+1)[H^2+(2r-1)Hh]\\ &+(r-s)(r-s+4rs)h^2\}(1-\delta_{s0}). \end{aligned} \tag{4.36}$$

Using in the above equations the relation $k!=\infty$ for $k=-1,-2,\ldots$, we find

$$a(r,s)=b(r,s)=c(r,s)=d(r,s)=0,\qquad \text{for}\quad s<0,\quad\text{or}\quad s>r, \tag{4.37}$$

which is equivalent to

$$\mathsf{P}^{(r)}_{n\,n-q}=0\qquad \text{for}\quad q<0\quad\text{or}\quad q>2r+1. \tag{4.38}$$

The limit $r\to 0$ yields relations $a(0,0)+b(0,0)=1$ and $c(0,0)=d(0,0)=0$ corresponding to $\mathsf{P}^{(0)}=\mathsf{I}^{\mathcal{S}}$.

D. Odd-reflection matrices

Odd-reflection matrices $\tilde{\mathsf{P}}^{(r)}$ can be evaluated from our solution for the even-reflection problem. By inserting relations (4.12) and (4.13) into (4.5) and using identities (3.17)–(3.21), we find

$$\tilde{\mathsf{P}}^{(r)}_{n\,n-2s}=\tilde{a}(r,s)\bar{\mathsf{R}}_{n\,n}\mathsf{A}_{n\,n-2s}+\tilde{b}(r,s)\bar{\mathsf{R}}_{n\,n-2}\mathsf{B}_{n-2\,n-2s}, \tag{4.39}$$

$$\tilde{\mathsf{P}}^{(r)}_{n\,n-2s-1}=\tilde{c}(r,s)\bar{\mathsf{R}}_{n\,n-1}\mathsf{A}_{n-1\,n-2s-1}+\tilde{d}(r,s)\bar{\mathsf{R}}_{n\,n-1}\mathsf{B}_{n-1\,n-2s-1}, \tag{4.40}$$

where

$$\tilde{a}(r,s)=a(r,s)+H_r c(r,s-1), \tag{4.41}$$

$$\tilde{b}(r,s)=b(r,s)+H_r[d(r,s-1)+c(r,0)\,\delta_{s1}]+H_r^2[b(r,s-1)+\delta_{s1}], \tag{4.42}$$

$$\tilde{c}(r,s)=c(r,s)+H_r a(r,s)+H_r^2 c(r,s-1), \tag{4.43}$$

$$\tilde{d}(r,s)=d(r,s)+H_r b(r,s). \tag{4.44}$$

The above expressions, along with the results (4.12)–(4.18) and (4.33)–(4.36) for $\mathsf{P}^{(r)}$, provide a complete image representation of the flow reflected from the walls.

V. CONCLUSIONS

We have explored the structure of the multiple-reflection series for a Stokes-flow singularity in the space bounded by two parallel planar walls. Explicit expressions for the multipole moments of the images were derived using the symmetry properties of the reflection matrices to simplify the problem.

Accordingly, symmetries of the Lorentz's reflection operator were applied to show that the single-reflection matrix R has a lower-triangular/tri-diagonal structure in a properly chosen basis. The symmetry between the source and image singularities was shown to yield commutation identities for the elements of R. These identities were used to simplify the matrices $\mathsf{P}^{(r)}$ that represent even-order reflections of the flow field from the walls. In this form, $\mathsf{P}^{(r)}$ depends on the position of the source singularity and the reflection order r only through scalar prefactors, which are independent of the multipolar order l of the source. The prefactors were evaluated using recurrence formulas associated with subsequent even-order reflections.

Our image representation can be applied in investigations that involve the motion of particles suspended in a fluid confined between two parallel walls. Such problems include particle dynamics in highly asymmetric colloidal mixtures[22] and suspension flows in slit pores.[9–15] Single- and multi-particle mobility matrices for particles between two walls can be evaluated using the induced-force representation of the particles[23] and our image solution for the flow reflected from the walls. By this approach, the force multipoles induced on the particles are determined using appropriate multipole-expansion algorithms.[8,24] Our image representation can also be used to develop boundary-integral algorithms[25] for the motion of deformable drops between two walls.

Extensions of our work may include derivation of an image solution for a force multipole in a space bounded by two planar surfactant-free[1] or surfactant-covered[5] fluid-fluid interfaces. Such solutions would be useful in investigations of the dynamics of colloidal-particle- or micelle-stabilized thin liquid films.[26,27]

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APPENDIX A: FUNDAMENTAL SET OF VELOCITY FIELDS

Following definitions given in Ref. 20, we list expressions for the functions $\mathbf{V}_{lm\sigma}(\theta,\phi)$ that characterize angular dependence of the velocity fields (2.3):

$$\mathbf{V}_{lm0}=\frac{1}{(2l+1)^2}\left[\frac{l+1}{l(2l-1)}\hat{\mathbf{A}}_{lm}-\frac{1}{2}\hat{\mathbf{B}}_{lm}\right], \tag{A1}$$

$$\mathbf{V}_{lm1}=\frac{\mathrm{i}}{l(l+1)(2l+1)}\hat{\mathbf{C}}_{lm}, \tag{A2}$$

$$\mathbf{V}_{lm2}=\frac{l}{(l+1)(2l+1)^2(2l+3)}\hat{\mathbf{B}}_{lm}. \tag{A3}$$

Here

$$\hat{\mathbf{A}}_{lm}=r^{-l+1}\boldsymbol{\nabla}(r^l\hat{Y}_{lm}),\quad \hat{\mathbf{B}}_{lm}=r^{l+2}\boldsymbol{\nabla}(r^{-l-1}\hat{Y}_{lm}),\quad \hat{\mathbf{C}}_{lm}=\hat{\mathbf{A}}_{lm}\times\mathbf{e}_r \tag{A4}$$

(with $r=|\mathbf{r}|$ and $\mathbf{e}_r=\mathbf{r}/r$) are the unnormalized vector spherical harmonics, where

$$\hat{Y}_{lm}=(-1)^m P_l^m(\cos\theta)e^{im\phi} \tag{A5}$$

are the unnormalized scalar spherical harmonics.

APPENDIX B: ELEMENTS OF REFLECTION MATRIX

Here we list expressions for nonzero elements of the reflection matrix $\bar{\mathsf{R}}_{n\,n'}(\sigma\sigma')$, defined by Eqs. (3.10) and (3.13),

$$\bar{\mathsf{R}}_{n\,n}(00)=(-1)^{(n+m+1)}\left[1+\frac{2(n-2)(n+m)(n-m)}{n(2n-1)}\right], \tag{B1}$$

$$\bar{\mathsf{R}}_{n\,n}(01)=(-1)^{(n+m)}\frac{4m(n+m)}{n(n-1)}, \tag{B2}$$

$$\bar{\mathsf{R}}_{n\,n}(02)=(-1)^{(n+m+1)}\frac{4(n-2)(n+m)(n+m-1)}{(n-1)(2n-1)(2n-3)}, \tag{B3}$$

$$\bar{\mathsf{R}}_{n\,n}(10)=(-1)^{(n+m+1)}\frac{2(n-2)m(n-m)}{n(2n-1)}, \tag{B4}$$

$$\bar{\mathsf{R}}_{n\,n}(11)=(-1)^{(n+m+1)}\left[1-\frac{4m^2}{(n-1)n}\right], \tag{B5}$$

$$\bar{\mathsf{R}}_{n\,n}(12)=(-1)^{(n+m+1)}\frac{4(n-2)m(n-1+m)}{(n-1)(2n-3)(2n-1)}, \tag{B6}$$

$$\bar{\mathsf{R}}_{n\,n}(20)=(-1)^{(n+m)}\frac{(n+1)(2n-3)(n-m-1)(n-m)}{n(2n-1)}, \tag{B7}$$

$$\bar{\mathsf{R}}_{n\,n}(21)=(-1)^{(n+m+1)}\frac{2m(n+1)(2n-3)(n-m-1)}{(n-2)(n-1)n}, \tag{B8}$$

$$\bar{\mathsf{R}}_{n\,n}(22)=(-1)^{(n+m+1)}\left[1-\frac{2(n+1)(n-m-1)(n+m-1)}{(n-1)(2n-1)}\right], \tag{B9}$$

$$\bar{\mathsf{R}}_{n\,n-1}(00)=(-1)^{(n+m+1)}2(n+m), \tag{B10}$$

$$\bar{\mathsf{R}}_{n\,n-1}(10)=(-1)^{(n+m+1)}2m, \tag{B11}$$

$$\bar{\mathsf{R}}_{n\,n-1}(20)=(-1)^{(n+m)}4n(n-m-1), \tag{B12}$$

$$\bar{\mathsf{R}}_{n\,n-1}(21)=(-1)^{(n+m+1)}\frac{2m(2n-3)(2n-1)}{(n-2)^2}, \tag{B13}$$

$$\bar{\mathsf{R}}_{n\,n-1}(22)=(-1)^{(n+m)}\frac{2(n-3)(n-1)(2n-1)(n+m-2)}{(2n-5)(n-2)^2}, \tag{B14}$$

$$\bar{\mathsf{R}}_{n\,n-2}(20)=(-1)^{(n+m)}\frac{(n-1)(2n-3)(2n-1)}{n-2}. \tag{B15}$$

In the above expressions we set

$$\bar{\mathsf{R}}_{n\,n'}(\sigma\sigma')=0 \quad \text{for} \quad n'-\sigma'<1. \tag{B16}$$

Equations (B1)–(B15) are equivalent to Eqs. (A20) in Ref. 4.

APPENDIX C: PRODUCTS OF MATRICES $\bar{\mathsf{R}}$

Here we list expressions for nonzero elements of matrices A and B, defined by Eqs. (4.15) and (4.16),

$$\mathsf{A}_{n\,n-2s}=f(n,s)\mathsf{A}'_{n\,n-2s}, \tag{C1}$$

$$\mathsf{B}_{n\,n-2s}=f(n,s)\mathsf{B}'_{n\,n-2s}, \tag{C2}$$

where $s\geqslant 1$, and

$$f(n,s)=(-4)^s\frac{(n-1)(2n-1)(2n-3)}{n-2}\,\frac{(n+m-2)!}{(n+m-2s)!}, \tag{C3}$$

$$\mathsf{A}'_{n\,n-2s}(20)=\frac{1}{4}\left[1+\frac{2(n-2s-2)(n-2s-m)(n-2s+m)}{(2n-4s-1)(n-2s)}\right], \tag{C4}$$

$$\mathsf{A}'_{n\,n-2s}(21)=-\frac{m(m+n-2s)}{(n-2s-1)(n-2s)}, \tag{C5}$$

$$\mathsf{A}'_{n\,n-2s}(22)=\frac{(m+n-2s-1)(m+n-2s)(n-2s-2)}{(2n-4s-3)(2n-4s-1)(n-2s-1)}, \tag{C6}$$

$$\mathsf{B}'_{n\,n-2s}(00)=\frac{(n-2)(m+n)(m+n-1)}{(n-1)(2n-1)(2n-3)}, \tag{C7}$$

$$\mathsf{B}'_{n\,n-2s}(10)=\frac{(n-2)m(m+n-1)}{(n-1)(2n-1)(2n-3)}, \tag{C8}$$

$$\mathsf{B}'_{n\,n-2s}(20)=\frac{1}{4}\left[1-\frac{2(n+1)(n-m-1)(n+m-1)}{(n-1)(2n-1)}\right]. \tag{C9}$$

In the above expressions we set

$$\mathsf{A}_{n\,n'}(\sigma\sigma')=\mathsf{B}_{n\,n'}(\sigma\sigma')=0 \quad \text{for} \quad n'-\sigma'<1. \tag{C10}$$

Relations (C1)–(C10) can be verified by induction using definitions (4.15) and (4.16) and the expressions in Appendix B.

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Bethe ansatz for the Gaudin model and its relation with Knizhnik–Zamolodchikov equations

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We recall the construction of the common eigenvectors of Gaudin Hamiltonians based on the Bethe ansatz. In the case of an arbitrary Lie algebra, this construction can be done either recursively or explicitly and we prove the equivalence of the two methods. We also prove that Bethe vectors are singular only if the Bethe equations are satisfied. In each eigenspace of the spin operator we construct additional common eigenvectors, having the same eigenvalue as the vacuum vector and which can not be obtained by the Bethe ansatz. These eigenvectors are not singular. We also recall the connection between Bethe vectors and integral solutions of the KZ equation. In an analogous way, the additional vectors lead to solutions of KZ equation which are not singular vectors and do not have an integral representation. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1501168]

I. INTRODUCTION

The Gaudin model is an example of a statistical integrable model associated to a quantum interacting system. The prototype of such a model is the system of N spin particles with magnetic interaction. It was formulated as a spin model related to the Lie algebra SL(2). The set of N independent and commuting Hamiltonians which allows us to integrate this model with N degrees of freedom was proposed by Gaudin.[1] For this model two fundamental problems have been discussed. The first one is the integration of the Hamiltonian system by means of the classical methods: construction of action-angle variables, integration of equations of motion.[2] The second one is the diagonalization of the family of Hamiltonians. The present article is concerned with this second problem.

In the simplest case of the Lie algebra SL(2), the problem of the diagonalization of the Hamiltonians was first discussed by Gaudin.[3] Using the method introduced by Bethe,[4] known as the Bethe ansatz, Gaudin constructed common eigenstates for all Hamiltonians (Bethe sums) and obtained the corresponding eigenvalues.

Integrable systems can be associated to any semi-simple complex Lie algebra. For such a system, generalizations of the set of Gaudin Hamiltonians have been constructed.[5] The methods proposed for diagonalization of these Hamiltonians are based on a remarkable connection between integrable models and two dimensional conformal field theories.

In Ref. 5, the structure of the Bethe vectors for the Gaudin model is related to the representation theory of affine Lie algebras. The diagonalization of Gaudin Hamiltonians is based on a concept of invariant functionals (correlation functions) on the tensor product of representations of an affine Lie algebra at the critical level.

Another approach for the problem of diagonalization[6,7] is related to the connection between eigenvectors of the Gaudin Hamiltonians and the solutions[8] of the Knizhnik–Zamolodchikov (KZ) equations.[9] In this approach, the common eigenvectors are constructed inductively, and it is shown that each eigenvector leads to an integral solution of the KZ equations. Conversely, it was proved[10] that, in the quasi-classical limit, the first term of the asymptotic solutions of the KZ equation leads

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to a common eigenvector of Hamiltonians. In this case the Bethe equations for the Gaudin model appear as conditions of critical points.

Another method to construct eigenvectors in statistical models associated to a simple Lie algebra G is to find a sequence of embeddings of Lie algebras into G and to solve inductively the problem of diagonalization of Hamiltonians for each subalgebra.[11]

In the second section we review some aspects concerning the Gaudin model, originally formulated for the Lie algebra SL(2). We recall the expression of the N commuting Hamiltonians, introduced by Gaudin and their common eigenvectors, constructed with the Bethe method. The space Ω of physical states is defined as a tensor product of N finite dimensional highest weight representations of the Lie algebra SL(2). It is decomposed as a direct sum of eigenspaces of the spin operator, i.e., $\Omega=\oplus\mathcal{V}_m$ and we search for common eigenvectors for Hamiltonians in each eigenspace $\mathcal{V}_m$.

With the Bethe ansatz, the number of common eigenvectors obtained in each subspace $\mathcal{V}_m$ is equal to the number of distinct solutions of the Bethe equations. A brief analysis of these equations shows that this constructive method does not provide all the common eigenvectors of Hamiltonians. There is at least one more vector in each subspace $\mathcal{V}_m$, common to all Hamiltonians, which can not be constructed with this method. The expression of such a vector is given as well as its eigenvalue. This result shows that the fundamental state is degenerate.

The third section is devoted to a discussion of the generalized model associated to an arbitrary simple Lie algebra. We recall the generalization of the Gaudin Hamiltonians and we explain how the Bethe ansatz works to construct common eigenvectors for these Hamiltonians. This construction can be done either recursively or explicitly. The main result of this section is the theorem which proves the equivalence of these two methods. The constructive method does not ensure the completeness of the system of eigenvectors. In each eigenspace of the spin operator we construct additional common eigenvectors, corresponding to the same eigenvalue as the vacuum vector and which can not be obtained by the Bethe ansatz.

The Bethe vectors are eigenvectors of the family of Hamiltonians only if the Bethe equations are satisfied and, in this case, we prove that they are also singular vectors in the tensor product representation. This is the main result of Sec. IV. The additional eigenvectors proposed here are not singular.

Section V recalls the connection between Bethe vectors and integral solutions of the KZ equation. In an analogous way, the additional vectors lead to solutions of the KZ equation which do not have an integral representation. Moreover, these solutions are not singular vectors.

Conclusions are presented in Sec. VI.

II. GAUDIN MODEL FOR SL(2) LIE ALGEBRA

In this section we recall the Gaudin model and Bethe ansatz procedure. Consider the Lie algebra SL(2) with generators E, F and H and commutation relations:

$$[E,F]=H;\quad [H,E]=2E;\quad [H,F]=-2F.$$

For this algebra, consider also N finite-dimensional highest weight modules: $V_{\lambda_1},\ldots,V_{\lambda_N}$ with highest weights $\lambda_1,\ldots,\lambda_N$ and highest weight vectors $v_{\lambda_1},\ldots,v_{\lambda_N}$.

The tensor product of these N modules is the space of physical states for a system of N spin particles:

$$\Omega=V_{\lambda_1}\otimes\cdots\otimes V_{\lambda_N}.$$

For each Lie algebra element A consider the following operator on the space Ω:

$$A^{(i)}=1\otimes\cdots\otimes A\otimes\cdots\otimes 1:\Omega\to\Omega,\quad A^{(i)}v_1\otimes\cdots\otimes v_N=v_1\otimes\cdots\otimes Av_i\otimes\cdots\otimes v_N, \qquad (1)$$

which acts as A on the ith module and as the identity operator on all other factors.

The system could be integrated if N independent and commuting Hamiltonians are found. Gaudin proposed a set of N Hamiltonians, which are operators on Ω depending on N distinct, complex parameters $z_1,\ldots,z_N$:

$$\mathcal{H}_i(z_1,\ldots,z_N)=\sum_{j=1,j\neq i}^{N}\frac{1}{z_i-z_j}\left[\frac{1}{2}H^{(i)}H^{(j)}+E^{(i)}F^{(j)}+F^{(i)}E^{(j)}\right],\quad \forall\ i=1,\ldots,N.$$

All these operators commute:

$$[\mathcal{H}_i,\mathcal{H}_j]=0,\quad \forall\ i,j=1,\ldots,N,$$

but they are not independent because $\Sigma_{i=1}^{N}\mathcal{H}_i=0$. We can prove that, up to a constant, this is the only vanishing linear combination of operators $\mathcal{H}_i$ with nonzero coefficients. As a consequence, this family of Hamiltonians is not enough to integrate a system of N spin particles. There is another family of commuting operators $\{H^{(i)}\}_{i=1,\ldots,N}$ introduced by the Cartan generator. Gaudin Hamiltonians do not commute with each $H^{(i)}$, but only with their sum, called the total spin operator:

$$\mathcal{S}=\sum_{i=1}^{N}H^{(i)}\quad\text{and}\quad[\mathcal{H}_i,\mathcal{S}]=0.$$

Then, there is a system of N commuting operators on Ω, which are independent. The problem discussed in this article is to find common eigenvectors for these operators. This can be done using the following ''general constructive procedure.''

Let A and B be two commuting operators on a finite dimensional space Ω. Suppose that for the operator A all the eigenvalues and the complete system of eigenvectors, which form a basis in Ω, are known. Denote by $\{a_n\}_n$ the spectrum of A, by g_n the multiplicity of a_n and by ϕ_{nr}, $r=1,\ldots,g_n$, the eigenvectors, $A\phi_{nr}=a_n\phi_{nr}$, which form a basis of the eigenspace $\mathcal{V}_n$ of A, associated to the eigenvalue a_n. If A and B commute, then $B\phi_{nr}$ is also an eigenvector for A, corresponding to the same eigenvalue a_n:

$$A(B\phi_{nr})=a_nB\phi_{nr}.$$

Therefore, $\mathcal{V}_n$ is an invariant subspace of B and the vector $B\phi_{nr}$, as an element of the eigenspace $\mathcal{V}_n$, has the following expansion:

$$B\phi_{nr}=\sum_{s=1}^{g_n}c_{sr}\phi_{ns}.$$

In the eigenspace $\mathcal{V}_n$ consider now the vector

$$\Phi_n=\sum_{r=1}^{g_n}d_r\phi_{nr}.$$

Then Φ_n is an eigenvector for the operator B, corresponding to an eigenvalue b_n if the coefficients $\{d_r\}_{r=1,g_n}$ satisfy the following system of g_n homogeneous equations:

$$\sum_{r=1}^{g_n}d_rc_{sr}=b_nd_s,\quad s=1,g_n. \tag{2}$$

This system has a nontrivial solution if its determinant is zero:

$$\Delta=\mathrm{Det}|c_{sr}-b_n\delta_{sr}|=0. \tag{3}$$

This is an equation of order g_n for the eigenvalue b_n of B, which has g_n complex roots (not necessarily distinct). For each distinct root b_n^k there is at least one solution $\{d_r^k\}_{r=1,g_n}$ of the system (2) and

$$\Phi_n^k = \sum_{r=1}^{g_n} d_r^k \phi_{nr}$$

is an eigenvector for the operator B with eigenvalue b_n^k and also for the operator A with eigenvalue a_n.

This procedure can be extended to an arbitrary number of commuting operators.

We use this scheme in Sec. II C to prove that the Bethe ansatz does not give all the common eigenvectors and to find an additional eigenvector. The expression of this eigenvector suggests to us how to look for other additional common eigenvectors.

A. Eigenvectors of the spin operator $\mathcal{S}$

The presence of the spin operator $\mathcal{S}$ in the system of commuting operators is important because, for this operator, all the eigenvalues and the complete system of eigenvectors, which form a basis in Ω, are known (see Lemma 1). Then, we look for common eigenvectors of Gaudin Hamiltonians as linear combinations of eigenvectors of $\mathcal{S}$, with some unknown coefficients.

The eigenvectors of $\mathcal{S}$ have a particular form which is explained by the theory of highest weight representations of the Lie algebra SL(2).

The space Ω is a tensor product of N highest weight representations V_λ of SL(2), with highest weight λ. Such a representation is completely determined by a highest weight vector v_λ, on which the action of the algebra is given by

$$Hv_\lambda = \lambda v_\lambda, \quad Ev_\lambda = 0, \quad Fv_\lambda \in \Omega.$$

The representation space V_λ is generated by vectors

$$\{v_n = F^n \; v_\lambda\}_{n \in \mathbb{N}},$$

and the action of the Lie algebra on these vectors is

$$Hv_n = (\lambda - 2n)v_n,$$

$$Ev_n = n(\lambda - n + 1)v_{n-1},$$

$$Fv_n = v_{n+1}.$$

If the highest weight λ is not a positive integer, the representation V_λ is infinite dimensional and irreducible. If $\lambda \in \mathbb{N}$, then in $\{v_n = F^n \; v_\lambda\}_{n \in \mathbb{N}}$ there is an invariant subspace, generated by $\{v_{\lambda+1}, v_{\lambda+2}, \ldots\}$ and the quotient representation is an irreducible, finite dimensional representation, of dimension $\lambda + 1$, generated by vectors $\{v_n = F^n \; v_\lambda\}_{n=0,\ldots,\lambda}$.

We consider Ω as a tensor product of finite dimensional representations, which is completely determined by the vector $v_0 = v_{\lambda_1} \otimes \cdots \otimes v_{\lambda_N}$, called vacuum vector and is generated by vectors $\{v_{n_1 \ldots n_N} = F^{n_1} \otimes F^{n_2} \cdots \otimes F^{n_N} v_0\}_{n_i = 0, \lambda_i;\; i=1,N}$. Remark that a vector $v_{n_1 \ldots n_N}$, with n_i operators F applied on the ith component, can be written as a product of $m = n_1 + n_2 + \cdots + n_N$ operators of type (1), denoted

$$v_m^{(k_1, \ldots, k_m)} = F^{(k_1)} F^{(k_2)} \cdots \; F^{(k_m)} v_0,$$

with $k_1,k_2,\ldots,k_m=1,\ldots,N$. Such a simplified notation is useful for explicit calculations since this model is applied to systems with a very large number N of particles, greater than m, which is related to the Lie algebra representation. Note that for finite dimensional representations, m can vary between 0 and a maximal value $m_{\max}=\Sigma_i^N\lambda_i$.

Knowing the structure of the space Ω, we can determine the eigenvectors and eigenvalues of the spin operator $\mathcal{S}$ on Ω. Obviously, the vacuum state is an eigenstate for the total spin operator and also for all Gaudin Hamiltonians:

$$\mathcal{S}v_0=\left(\sum_{k=1}^{N}\lambda_k\right)v_0,$$

$$\mathcal{H}_iv_0=\left(\frac{1}{2}\sum_{j=1,j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}\right)v_0. \tag{4}$$

Moreover, applying a finite number m of generators F on the vacuum state we get an eigenvector of $\mathcal{S}$:

Lemma 1: For a finite m, the vectors $v_m^{(k_1,\ldots,k_m)}=F^{(k_1)}F^{(k_2)}\cdots F^{(k_m)}v_0$ of the basis of Ω, with $k_1,\ldots,k_m=1,\ldots,N$, are eigenvectors of the total spin operator $\mathcal{S}$:

$$\mathcal{S}F^{(k_1)}F^{(k_2)}\cdots F^{(k_m)}v_0=\left(\sum_{i=1}^{N}\lambda_i-2m\right)F^{(k_1)}F^{(k_2)}\cdots F^{(k_m)}v_0.$$

The eigenvalue $\Sigma_{i=1}^N\lambda_i-2m$ is determined by the number m of operators F. Its eigenspace $\mathcal{V}_m$ is generated by vectors $\{v_m^{(k_1,\ldots,k_m)}=F^{(k_1)}F^{(k_2)}\cdots F^{(k_m)}v_0\}_{k_i=1,\ldots,N}$, called states of spin deviation m.

Since the spin deviation m can take a finite number of positive integer values, $\mathcal{S}$ has a finite number of eigenvalues and the representation space Ω can be written as the direct sum of eigenspaces of spin deviation m: $\Omega=\oplus_{m=0}^{m_{\max}}\mathcal{V}_m$.

The construction of common eigenvectors for Gaudin Hamiltonians is based on the fact that the eigenspaces of the operator $\mathcal{S}$ are invariant subspaces for $\mathcal{H}_i$. Therefore, in each eigenspace $\mathcal{V}_m$ we can look for common eigenvectors for Hamiltonians as expansions on the basis of $\mathcal{V}_m$:

$$\psi_m=\sum_{k_1=1}^{N}\cdots\sum_{k_m=1}^{N}c_{k_1\ldots k_m}F^{(k_1)}\cdots F^{(k_m)}v_0.$$

To determine the coefficients $c_{k_1\ldots k_m}$ one could use the "general constructive procedure," presented at the begining of this section, and solve the system (2) with the condition (3). Another approach is to consider a particular form for these coefficients, as rational complex functions:

$$c_{k_1\ldots k_m}=\frac{1}{w_1-z_{k_1}}\cdots\frac{1}{w_m-z_{k_m}}$$

with some unknown distinct, complex parameters: $w_1,\ldots,w_m$. This approach is essentially known as the Bethe ansatz method.

We present hereafter both approaches.

B. Bethe vectors of spin deviation $m=1$

The eigenspace $\mathcal{V}_1$ is generated by vectors $\{F^{(k)}v_0\}_{k=1,\ldots,N}$. A Bethe vector of spin deviation $m=1$ is defined as an expansion on this basis, with rational coefficients depending on one complex parameter w:

$$\psi_1(w)=\sum_{k=1}^{N}\frac{1}{w-z_k}F^{(k)}v_0.$$

Denote $\mathcal{F}(w)$ the operator on Ω:

$$\mathcal{F}(w)=\sum_{k=1}^{N}\frac{1}{w-z_k}F^{(k)}. \tag{5}$$

Straightforward calculations give the commutator:

$$[\mathcal{H}_i,\mathcal{F}(w)]=\sum_{j=1,j\neq i}^{N}\frac{1}{(w-z_i)(w-z_j)}(H^{(i)}F^{(j)}-F^{(i)}H^{(j)}). \tag{6}$$

Applying this operator on v_0 we obtain

$$[\mathcal{H}_i,\mathcal{F}(w)]v_0=\frac{\lambda_i}{w-z_i}\mathcal{F}(w)v_0-\left(\sum_{k=1}^{N}\frac{\lambda_k}{w-z_k}\right)\frac{F^{(i)}}{w-z_i}v_0. \tag{7}$$

Then the action of a Gaudin Hamiltonian $\mathcal{H}_i$ on $\psi_1(w)$ is

$$\mathcal{H}_i\ \ \psi_1(w)=\left(\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\frac{\lambda_i}{w-z_i}\right)\psi_1(w)-\left(\sum_{k=1}^{N}\frac{\lambda_k}{w-z_k}\right)\frac{F^{(i)}}{w-z_i}v_0$$

and we have the following lemma.

Lemma 2: Given N distinct complex numbers $\{z_i\}_{i=1,\ldots,N}$ *and fixed positive, integer highest weights* $\{\lambda_i\}_{i=1,\ldots,N}$, *the Bethe vector* $\psi_1(w)$ *of spin deviation* $m=1$ *is an eigenvector for all Gaudin Hamiltonians:*

$$\mathcal{H}_i\ \ \psi_1(w)=s_i^1\psi_1(w),\quad \forall\ \ i=1,\ldots,N,$$

if the complex parameter w satisfies the following condition:

$$\sum_{k=1}^{N}\frac{\lambda_k}{w-z_k}=0, \tag{8}$$

called Bethe equation associated to $\mathcal{V}_1$. *The eigenvalue* s_i^1 *of* $\mathcal{H}_i$ *depends on the solution w of this equation:*

$$s_i^1(w)=\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\frac{\lambda_i}{w-z_i}.$$

C. Additional eigenvector in $\mathcal{V}_1$

In the eigenspace $\mathcal{V}_1$ of $\mathcal{S}$, which has dimension N, the Bethe construction gives a number of common eigenvectors equal to the number of distinct solutions of the equation (8). It is a polynomial equation of degree $N-1$ and therefore it has $N-1$ complex solutions (not necessarily distinct). The following lemma gives one more eigenvector in $\mathcal{V}_1$, common to all Hamiltonians, which can not be constructed with the Bethe ansatz (and also from linear combinations of vectors obtained from the Bethe ansatz).

Lemma 3: The vector ψ_1^0 *in* $\mathcal{V}_1$,

$$\psi_1^0=\sum_{k=1}^{N} F^{(k)}v_0,$$

is an eigenvector for each Hamiltonian $\mathcal{H}_i$*:*

$$\mathcal{H}_i\ \ \psi_1^0=\left(\frac{1}{2}\sum_{j=1,j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}\right)\psi_1^0. \tag{9}$$

This vector has equal coefficients, as expansion on the basis of $\mathcal{V}_1$. This possibility is not allowed by the Bethe construction, where these coefficients, chosen in the form $1/(w-z_i)$ with distinct z_i, are necessarily distinct. Remark also that the eigenvalue of this vector is the same as the eigenvalue of the vacuum vector (4).

Finally, remark that the Bethe equation (8) is nothing else that the condition (3) of the ''general constructive procedure,'' presented at the begining of this section, which gives the eigenvalues of the Hamiltonians. To see this let us write the action of a Hamiltonian $\mathcal{H}_i$ on each generator $F^{(k)}v_0$ of $\mathcal{V}_1$:

$$\begin{aligned}
\mathcal{H}_iF^{(i)}v_0&=\left(\sum_{j=1,j\neq i}^{N}\frac{\frac{1}{2}\lambda_i\lambda_j-\lambda_j}{z_i-z_j}\right)F^{(i)}v_0+\sum_{j=1,j\neq i}^{N}\frac{\lambda_i}{z_i-z_j}F^{(j)}v_0,\\
\mathcal{H}_iF^{(k)}v_0&=\left(\frac{1}{2}\sum_{j=1,j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}-\frac{\lambda_i}{z_i-z_k}\right)F^{(k)}v_0+\frac{\lambda_k}{z_i-z_k}F^{(i)}v_0,\quad \forall k\neq i.
\end{aligned} \tag{10}$$

A vector Φ of $\mathcal{V}_1$, $\Phi=\Sigma_{r=1}^{N}d_rF^{(r)}v_0$, is a common eigenvector for all Hamiltonians $\mathcal{H}_i$, corresponding to eigenvalues b_i, $\mathcal{H}_i\Phi=b_i\Phi$, if the set of coefficients $\{d_r\}_{r=1,N}$ is a common solution of the systems of type (2):

$$\sum_{r=1}^{N} d_rc_{sr}^{i}=b_id_s,\quad s=1,\ldots,N \tag{11}$$

(one system for each Hamiltonian $\mathcal{H}_i$), where the coefficients $\{c_{sr}^{i}\}_{s,r=1,\ldots,N}$ are given by (10). The determinant of the ith system, $\Delta_i=\mathrm{Det}(c_{sr}^{i}-b_i\delta_{sr})$, is

$$\Delta_i=\begin{vmatrix}
\tilde{b}-\frac{\lambda_i}{z_i-z_1} & 0 & \ldots & \frac{\lambda_i}{z_i-z_1} & 0 & \ldots & 0\\
0 & \tilde{b}-\frac{\lambda_i}{z_i-z_2} & \ldots & \frac{\lambda_i}{z_i-z_2} & 0 & \ldots & 0\\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \\
\frac{\lambda_1}{z_i-z_1} & \frac{\lambda_2}{z_i-z_2} & \ldots & \tilde{b}-\sum_{j\neq i}^{N}\frac{\lambda_j}{z_i-z_j} & \frac{\lambda_{i+1}}{z_i-z_{i+1}} & \ldots & \frac{\lambda_N}{z_i-z_N}\\
0 & 0 & \ldots & \frac{\lambda_i}{z_i-z_{i+1}} & \tilde{b}-\frac{\lambda_i}{z_i-z_{i+1}} & \ldots & 0\\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots\\
0 & 0 & \ldots & \frac{\lambda_i}{z_i-z_N} & 0 & \ldots & \tilde{b}-\frac{\lambda_i}{z_i-z_N}
\end{vmatrix},$$

where $\tilde{b}=\frac{1}{2}\Sigma_{j=1,j\neq i}^{N}\lambda_i\lambda_j/(z_i-z_j)-b_i$. The determinant can be calculated,

$$\Delta_i=\tilde{b}\left\{\prod_{j=1;j\neq i}^{N}\left(\tilde{b}-\frac{\lambda_i}{z_i-z_j}\right)-\sum_{k=1;k\neq i}^{N}\frac{\lambda_k}{z_i-z_k}\prod_{j=1;j\neq i,k}^{N}\left(\tilde{b}-\frac{\lambda_i}{z_i-z_j}\right)\right\},$$

and gives a polynomial equation of degree N in $\tilde{b}$ with N complex roots.

One of them is $\tilde{b}=0$, which gives the eigenvalue $b_i=\frac{1}{2}\Sigma_{j=1,j\neq i}^{N}\lambda_i\lambda_j/(z_i-z_j)$. In this case the nontrivial common solution of the systems (11) is $d_1=d_2=\cdots=d_N$, which gives, up to a constant, the particular eigenvector ψ_1^0 of Lemma 3, common to all Hamiltonians.

It is more difficult to find the other roots of Δ_i. We can verify that $\lambda_i/(z_i-z_k)$ is not a root of Δ_i for any $k=1,\ldots,N$, $k\neq i$. Then we can choose $\tilde{b}$ as the rational function,

$$\tilde{b}(w)=-\frac{\lambda_i}{w-z_i}$$

depending on the unknown complex variable w, with $w\neq z_k$, for all $k=1,\ldots,N$ and we have

$$\Delta_i=-\left\{\sum_{j=1}^{N}\frac{\lambda_j}{w-z_j}\right\}\left(\frac{\lambda_i}{w-z_i}\right)^{N-1}\prod_{k=1;k\neq i}^{N}\left(\frac{w-z_k}{z_k-z_i}\right).$$

The conditions (3), for each Δ_i, give the same equation:

$$\sum_{j=1}^{N}\frac{\lambda_j}{w-z_j}=0,$$

which is the Bethe equation (8) for the eigenspace $\mathcal{V}_1$. In this case the nontrivial common solution of the systems (11) is $d_k=1/(w-z_k)$, $\forall\ k=1,\ldots,N$, which gives the Bethe eigenvector $\psi_1(w)$, with eigenvalues $b_i=\frac{1}{2}\Sigma_{j=1,j\neq i}^{N}\lambda_i\lambda_j/(z_i-z_j)+\lambda_i(w-z_i)$.

D. States of spin deviation *m*

In the general case of spin deviation m, the eigenspace $\mathcal{V}_m$ is generated by vectors $\{F^{(k_1)}\cdots F^{(k_m)}v_0\}_{1\leqslant k_1\leqslant\ldots\leqslant k_m\leqslant N}$. A Bethe vector of spin deviation m is defined as an expansion on the basis, with coefficients depending on m complex parameters $w_1,\ldots,w_m$:

$$\psi_m(w_1,\ldots,w_m)v_0=\sum_{i_1=1}^{N}\frac{F^{(i_1)}}{w_1-z_{i_1}}\cdots\sum_{i_m=1}^{N}\frac{F^{(i_m)}}{w_m-z_{i_m}}v_0=\mathcal{F}(w_1)\cdots\mathcal{F}(w_m)v_0. \tag{12}$$

The order of the operators $\mathcal{F}$ is not significant because they commute.

The action of a Gaudin Hamiltonian $\mathcal{H}_i$ on this state is calculated by induction on m:

$$\begin{aligned}\mathcal{H}_i\psi_m(w_1,\ldots,w_m)v_0&=\mathcal{H}_i\mathcal{F}(w_m)\psi_{m-1}(w_1,\ldots,\ w_{m-1})v_0\\&=\mathcal{F}(w_m)\mathcal{H}_i\psi_{m-1}(w_1,\ldots,\ w_{m-1})v_0+\psi_{m-1}(w_1,\ldots,\ w_{m-1})\\&\quad\times[\mathcal{H}_i,\mathcal{F}(w_m)]v_0+[[\mathcal{H}_i,\mathcal{F}(w_m)],\psi_{m-1}(w_1,\ldots,\ w_{m-1})]v_0.\end{aligned}$$

The first term is computed from the induction hypothesis, the second from (7), and for the last term we use the commutator formula:

$$[[\mathcal{H}_i,\mathcal{F}(w_1)],\mathcal{F}(w_2)]=\frac{2}{w_1-w_2}\left(\frac{F^{(i)}}{w_1-z_i}\mathcal{F}(w_2)-\frac{F^{(i)}}{w_2-z_i}\mathcal{F}(w_1)\right), \tag{13}$$

which can be obtained from (6). Putting all together it follows:

$$\mathcal{H}_i\psi_m(w_1,\ldots,\ w_m)v_0=\left(\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\sum_{k=1}^{m}\frac{\lambda_i}{w_k-z_i}\right)\psi_m(w_1,\ldots,\ w_m)v_0$$
$$-\sum_{k=1}^{m}\left(\sum_{j=1}^{N}\frac{\lambda_j}{w_k-z_j}+\sum_{l=1;l\neq k}^{m}\frac{2}{w_l-w_k}\right)\frac{F^{(i)}}{w_k-z_i}\psi_{m-1}(\ldots,\widehat{w_k},\ldots)v_0, \tag{14}$$

where $\psi_{m-1}(\ldots,\widehat{w_k},\ldots)$ denotes $\psi_{m-1}(w_1,\ldots,\ w_{k-1},w_{k+1},\ldots,w_m)$. Hence, we obtain the following theorem:

Theorem 4: *The Bethe vector $\psi_m(w_1,\ldots,\ w_m)v_0$ of spin deviation m is a common eigenvector for all Gaudin Hamiltonians:*

$$\mathcal{H}_i\psi_m(w_1,\ldots,\ w_m)v_0=s_i^m\psi_m(w_1,\ldots,\ w_m)v_0,\quad \forall\ \ i=1,\ldots,N,$$

if the complex parameters $w_1,\ldots,w_m$ satisfy the Bethe equations associated to $\mathcal{V}_m$:

$$\sum_{j=1}^{N}\frac{\lambda_j}{w_k-z_j}+\sum_{l=1;l\neq k}^{m}\frac{2}{w_l-w_k}=0,\quad \forall k=1,\ldots,m. \tag{15}$$

The eigenvalues s_i^m depend on the solution of these equations:

$$s_i^m(w_1,\ldots,\ w_m)=\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\sum_{k=1}^{m}\frac{\lambda_i}{w_k-z_i}.$$

E. Additional eigenvector in $\mathcal{V}_m$

As remarked in Ref. 12, the number of distinct solutions of the Bethe equations (15) is at most C_{N+m-2}^m (the standard binomial coefficient), which is less than the dimension of the space $\mathcal{V}_m$:

$$\dim\mathcal{V}_m=\sum_{1\leqslant k_1\leqslant\ldots\leqslant k_m\leqslant N}1=\sum_{1\leqslant j_1\ \ldots\ <j_m\leqslant N+m-1}1=C_{N+m-1}^m.$$

Therefore, the system of Bethe eigenvectors ψ_m is not complete. We can construct one more common vector in $\mathcal{V}_m$, which has equal coefficients and with the same eigenvalues as the vacuum vector (4).

Theorem 5: *The vector $\psi_m^0\in\mathcal{V}_m$,*

$$\psi_m^0=\sum_{k_1=1}^{N}\ \cdots\ \sum_{k_m=1}^{N}F^{(k_1)}\cdots\ F^{(k_m)}v_0 \tag{16}$$

is an eigenvector for each Hamiltonian $\mathcal{H}_i$:

$$\mathcal{H}_i\ \ \psi_m^0=\left(\frac{1}{2}\sum_{j=1,j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}\right)\psi_m^0.$$

The proof follows from (4) and using the fact that $[\mathcal{H}_i,\Sigma_{k=1}^{N}F^{(k)}]=0$.

F. Conclusions

In this section, eigenvalues for Gaudin Hamiltonians are determined and by the Bethe method common eigenvectors for these operators are constructed in each eigenspace of the spin operator. This constructive method does not ensure the completeness of the system of common eigenvec-

tors, but it can be used for large values of spin deviation. On the other hand, the "general constructive procedure," presented at the begining of the section, could give additional common eigenvectors, but it is difficult to apply it, even for $m=2$.

For each value of spin deviation we have constructed one additional common eigenvector which can not be obtained by the Bethe ansatz. From Lemma 3 and Theorem 5 it follows that the eigenvalue $s_0^i=\frac{1}{2}\Sigma_{j=1,j\neq i}^N \lambda_i\lambda_j/(z_i-z_j)$ of the Hamiltonian $\mathcal{H}_i$ is degenerate and its eigenspace contains not only the vacuum state v_0, but all the states ψ_m^0.

Unlike the case $m=1$, where the additional vector ψ_1^0 could complete the system of eigenvectors, if the Bethe equation (8) has distinct solutions, in the case $m>1$ the number of "missing vectors" is greater than one. The additional vector ψ_m^0 is only one of them. An alternative construction, which gives a larger system of eigenvectors, was proposed in Ref. 13.

III. GENERALIZATION OF THE GAUDIN MODEL FOR AN ARBITRARY SIMPLE LIE ALGEBRA *G*

Consider a simple Lie algebra G, of dimension d and rank r. We denote Δ the root system of G, Δ_+ the system of positive roots and Δ_0 the system of simple roots. The Cartan basis of G is formed by the Cartan generators $\{H_i\}_{i=1,r}$, the generators of positive roots $\{E_\alpha\}_{\alpha\in\Delta_+}$ and the generators of negative roots $\{F_\alpha=E_{-\alpha}\}_{\alpha\in\Delta_+}$. The commutation relations are

$$[E_\alpha,F_\alpha]=\frac{2}{\langle\alpha,\alpha\rangle}H_\alpha;\quad [H,E_\alpha]=\alpha(H)E_\alpha;\quad [H,F_\alpha]=-\alpha(H)F_\alpha;$$

$$[E_\alpha,E_\beta]=N_{\alpha,\beta}E_{\alpha+\beta},\quad \forall\,\alpha,\beta\in\Delta \text{ such that } \alpha+\beta\in\Delta.$$

Recall that the Killing form of G defines a symmetrical, G-invariant, bilinear form $\langle,\rangle$ on G. This scalar product allows us to identify the Cartan subalgebra $\mathcal{K}$ of G with its dual $\mathcal{K}^*$ by the isomorphism which associates to each element $\alpha\in\mathcal{K}^*$ one element $H_\alpha\in\mathcal{K}$, defined by $\alpha(H)=\langle H_\alpha,H\rangle$, for all $H\in\mathcal{K}$. The scalar product on $\mathcal{K}$ induces a scalar product on its dual $\mathcal{K}^*$, which is nondegenerate,

$$\langle\alpha,\beta\rangle=\langle H_\alpha,H_\beta\rangle,$$

normalized such that $\langle\alpha_l,\alpha_l\rangle=2$ for a long root α_l.

All generators of G are orthogonal with respect to this scalar product except the pairs (E_α,F_α) and (H_i,H_i), for which we have[14]

$$\langle H_i,H_i\rangle=\frac{1}{2}\chi,\forall i=1,\ldots,r,\quad \langle E_\alpha,F_\alpha\rangle=\frac{2}{\langle\alpha,\alpha\rangle},\forall\alpha\in\Delta_+,$$

where $\chi=\Sigma_{i=1}^r\alpha_l^2(H_i)$ is the square of the length of a long root. Then, for the Cartan basis we can define the dual basis with respect to this scalar product:

$$\tilde{H}_i=\frac{2}{\chi}H_i,\quad \tilde{E}_\alpha=\frac{\langle\alpha,\alpha\rangle}{2}F_\alpha,\quad \tilde{F}_\alpha=\frac{\langle\alpha,\alpha\rangle}{2}E_\alpha,$$

such that $\langle H_i,\tilde{H}_j\rangle=\delta_{ij}$ and $\langle E_\alpha,\tilde{E}_\beta\rangle=\langle F_\alpha,\tilde{F}_\beta\rangle=\delta_{\alpha\beta}$.

For this algebra, consider N finite-dimensional highest weight G-modules: $V_{\lambda_1},\ \ldots,\ V_{\lambda_N}$, with dominant integral highest weights $\lambda_1,\ \ldots,\ \lambda_N$ and highest weight vectors $v_{\lambda_1},\ \ldots,\ v_{\lambda_N}$. The tensor product of these N G-modules is the space of physical states for the system of N spin particles:

$$\Omega=V_{\lambda_1}\otimes\cdots\otimes V_{\lambda_N}.$$

To introduce the Hamiltonian operators on Ω, we consider $\{I_a\}_{a=1,\ldots,d}$ a basis of G and $\{\tilde{I}_a\}_{a=1,\ldots,d}$ its dual with respect to the scalar product. The generalized Gaudin Hamiltonians are defined as

$$\mathcal{H}_i(z_1,\ldots,z_N)=\sum_{j=1,j\neq i}^{N}\frac{1}{z_i-z_j}\sum_{a=1}^{d}I_a^{(i)}\tilde{I}_a^{(j)},\quad \forall i=1,\ldots,N,$$

where $z_1,\ldots,z_N$ are N distinct, complex numbers. A remarkable property of the sum $\Sigma_{a=1}^{d}I_a^{(i)}\tilde{I}_a^{(j)}$ is that it is independent of the choice of the basis.[14] In particular, we can consider the Cartan basis, so that the Hamiltonians are given by

$$\mathcal{H}_i=\sum_{j=1,j\neq i}^{N}\frac{1}{z_i-z_j}\left\{\frac{2}{\chi}\sum_{l=1}^{r}H_l^{(i)}H_l^{(j)}+\sum_{\alpha\in\Delta_+}\frac{\langle\alpha,\alpha\rangle}{2}(E_\alpha^{(i)}F_\alpha^{(j)}+F_\alpha^{(i)}E_\alpha^{(j)})\right\}.$$

All these operators commute:

$$[\mathcal{H}_i,\mathcal{H}_j]=0,\quad \forall i,j=1,\ldots,N,$$

but they are not independent, since $\Sigma_{i=1}^{N}\mathcal{H}_i=0$. There is another family of commuting operators on Ω, introduced by the r Cartan generators:

$$\{H_\alpha^{(i)}\}_{i=1,\ldots,N;\ \alpha\in\Delta_0}.$$

We can define r spin operators $\mathcal{S}_\alpha=\Sigma_{i=1}^{N}H_\alpha^{(i)}$ and Gaudin Hamiltonians commute with each one of them:

$$[\mathcal{H}_i,\mathcal{S}_\alpha]=0,\quad \forall\ \ i=1,\ldots,N;\ \ \forall\ \ \alpha\in\Delta_0.$$

Then, there is a system of $N+r-1$ commuting operators on Ω, which are independent.

Our goal is to find common eigenvectors for these operators.

A. Eigenvectors and eigenvalues for generalized Gaudin Hamiltonians

In this section, we discuss the possibility to generalize the Bethe ansatz to the case of an arbitrary simple Lie algebra G.

The space Ω of physical states is a tensor product of N highest weight representations V_λ of G. Such a representation is completely determined by a highest weight vector v_λ, on which the action of the algebra is given by

$$H_\alpha v_\lambda=\langle\alpha,\lambda\rangle v_\lambda,\quad E_\alpha v_\lambda=0,\quad F_\alpha v_\lambda\in\Omega.$$

As in the SL(2) case, the representation space V_λ is linearly generated by monomials in generators of negative roots:

$$\{v_{\alpha_1\ldots\alpha_l}^{n_1\ldots n_l}=F_{\alpha_1}^{n_1}\cdots F_{\alpha_l}^{n_l}v_\lambda\}_{\alpha_i\in\Delta_+,\ n_i\in\mathbb{N}},$$

but in this case, the monomials are ordered with respect to the roots. The necessity to consider an ordered system of positive roots comes from the Poincaré-Birkhoff-Witt theorem,[15] which gives the basis of the enveloping algebra $\mathcal{U}(G)$ of G.

These vectors are eigenvectors for the Cartan generators:

$$H_\alpha v_{\alpha_1\ldots\alpha_l}^{n_1\ldots n_l}=\left(\langle\alpha,\lambda\rangle-\sum_{\beta\in\Delta_+}n_\beta\langle\alpha,\beta\rangle\right)v_{\alpha_1\ldots\alpha_l}^{n_1\ldots n_l}.$$

We can also compute the action of a positive root generator on monomials $v_\alpha^{n_\alpha}$:

$$E_\alpha v_\alpha^{n_\alpha} = n_\alpha \left(2\frac{\langle \lambda, \alpha \rangle}{\langle \alpha, \alpha \rangle} - n_\alpha + 1 \right) v_\alpha^{n_\alpha - 1}.$$

The dimension of a highest weight representation V_λ of G, with highest weight λ, is related to the notion of dominant integral weight. The set of dominant integral weights is

$$\left\{ \lambda \in \mathcal{K}^* \middle| 2\frac{\langle \lambda, \alpha \rangle}{\langle \alpha, \alpha \rangle} \in \mathbb{N}, \ \ \forall \ \ \alpha \in \Delta_0 \right\}.$$

If the highest weight λ is not a dominant integral weight, then the representation V_λ is infinite dimensional and irreducible. If λ is a dominant integral weight, then, denoting $r_\alpha = 2\langle \lambda, \alpha \rangle / \langle \alpha, \alpha \rangle \in \mathbb{N}$, for all $\alpha \in \Delta_0$, there exists an invariant subspace and the quotient representation is an irreducible, finite dimensional representation of G, generated by ordered monomials:

$$\{ v_{\alpha_1 \dots \alpha_l}^{n_1 \dots n_l} = F_{\alpha_1}^{n_1} \dots F_{\alpha_l}^{n_l} \ v_\lambda \}_{\alpha_j \in \Delta_+, \ n_j = 0, \dots, r_{\alpha_j}}.$$

As in the SL(2) case, we are interested in finite dimensional representations. The space Ω of physical states is then a tensor product of finite dimensional representations, completely determined by the vacuum vector $v_0 = v_{\lambda_1} \otimes \cdots \otimes v_{\lambda_N}$ and generated by vectors $v_{\alpha_1^1 \dots \alpha_l^1}^{n_1^1 \dots n_l^1} \otimes v_{\alpha_1^2 \dots \alpha_l^2}^{n_1^2 \dots n_l^2} \dots \otimes v_{\alpha_1^N \dots \alpha_l^N}^{n_1^N \dots n_l^N}$. To simplify this hard notation, remark that such a vector, which has on the ith component n_1^i operators F_{α_1}, ..., n_l^i operators F_{α_l}, can be written as a product of $m = \Sigma_{i=1}^N \Sigma_{k=1}^l n_k^i$ operators of negative roots of type (1). We denote

$$v_{\alpha_1 \dots \alpha_m}^{(k_1 \dots k_m)} = F_{\alpha_1}^{(k_1)} F_{\alpha_2}^{(k_2)} \dots F_{\alpha_m}^{(k_m)} v_0,$$

with $k_1, k_2, \dots, k_m = 1, \dots, N$. Note that for finite dimensional representations, m can vary between 0 and a maximal value $m_{\max} = \Sigma_{i=1}^N \Sigma_{\alpha \in \Delta_+} r_\alpha^i$.

B. Eigenvectors of the spin operator $\mathcal{S}_\beta$

As in the case of the Lie algebra SL(2), the problem of eigenvectors and eigenvalues for the spin operators $\mathcal{S}_\beta$ on Ω can be completely solved. The vacuum state is an eigenvector for all spin operators and also for all Gaudin Hamiltonians:

$$\mathcal{S}_\beta v_0 = \left(\sum_{k=1}^N \langle \lambda_k, \beta \rangle \right) v_0, \beta \in \Delta_0,$$

$$\mathcal{H}_i v_0 = \left(\sum_{j=1, j \neq i}^N \frac{\langle \lambda_i, \lambda_j \rangle}{z_i - z_j} \right) v_0, \quad i = 1, \dots, N. \tag{17}$$

Moreover, applying a finite number m of generators of negative roots on the vacuum state we get an eigenvector of $\mathcal{S}_\beta$:

Lemma 6: The vectors $v_{\alpha_1 \dots \alpha_m}^{(k_1 \dots k_m)} = F_{\alpha_1}^{(k_1)} F_{\alpha_2}^{(k_2)} \cdots F_{\alpha_m}^{(k_m)} v_0$ *in* Ω, *for all positive roots* $\alpha_1, \dots, \alpha_m \in \Delta_+$ *and* $k_1, \dots, k_m = 1, \dots, N$, *are eigenvectors of the spin operators* $\mathcal{S}_\beta$:

$$\mathcal{S}_\beta \ F_{\alpha_1}^{(k_1)} \cdots \ F_{\alpha_m}^{(k_m)} v_0 = \left(\sum_{i=1}^N \langle \lambda_i, \beta \rangle - \sum_{j=1}^m \langle \alpha_j, \beta \rangle \right) F_{\alpha_1}^{(k_1)} \cdots \ F_{\alpha_m}^{(k_m)} v_0.$$

As in the case of the Lie algebra SL(2), the eigenvalue $\Sigma_{i=1}^{N}\lambda_i(\beta)-\Sigma_{j=1}^{m}\alpha_j(\beta)$ is degenerate but its eigenspace is no more completely determined by the number of operators of negative roots, applied on the vacuum vector. Each eigenspace is determined by the value of the sum of positive roots $\Sigma_{j=1}^{m}\alpha_j$, which can be written as a sum of simple roots, with positive integer coefficients, in a unique way. Then the eigenspaces of $\mathcal{S}_\beta$ will be labeled by a family of simple roots: $\mathcal{V}_{\delta_1\ldots\delta_s}$, with $\delta_1,\ldots,\delta_s\in\Delta_0$ not necessarily distinct and satisfying $\Sigma_{k=1}^{s}\delta_k=\Sigma_{j=1}^{m}\alpha_j$. We call $\mathcal{V}_{\delta_1\ldots\delta_s}$ the subspace of spin deviation $\delta_1,\ldots,\delta_s$.

In view of the discussion concerning the finite dimension of Ω, m can take a finite number of positive integer values and then $\mathcal{S}_\beta$ has a finite number of eigenvalues. Therefore, the tensor product representation space Ω can be written as the direct sum of eigenspaces of $\mathcal{S}_\beta$:

$$\Omega=\bigoplus_{\delta_1,\ldots,\delta_s}\mathcal{V}_{\delta_1\ldots\delta_s},\quad \delta_1,\ldots,\quad \delta_s\in\Delta_0.$$

As in the previous section, for the model related to the Lie algebra SL(2), we search common eigenvectors for all generalized Gaudin Hamiltonians in each eigenspace of the spin operator, as expansions on the basis of eigenvectors of $\mathcal{S}_\beta$. The coefficients of these expansions have a particular form similar to that of the Bethe ansatz.

C. States of spin deviation α

Consider a simple root α. For a spin deviation α, the equation of eigenvectors for a spin operator $\mathcal{S}_\beta$ is

$$\mathcal{S}_\beta F_\alpha^{(k)}v_0=\left(\sum_{i=1}^{N}\lambda_i(\beta)-\alpha(\beta)\right)F_\alpha^{(k)}v_0. \tag{18}$$

The eigenspace $\mathcal{V}_\alpha$ of spin deviation α corresponding to the eigenvalue $\Sigma_{i=1}^{N}\lambda_i(\beta)-\alpha(\beta)$ is generated by vectors $\{F_\alpha^{(k)}v_0\}_{k=1,\ldots,N}$. A Bethe vector of spin deviation α is defined as an expansion on the basis, with rational coefficients depending on one complex parameter w:

$$\psi_1(w,\alpha)=\sum_{i=1}^{N}\frac{F_\alpha^{(i)}}{w-z_i}v_0=\mathcal{F}(w,\alpha)v_0. \tag{19}$$

To give the action of a Hamiltonian $\mathcal{H}_i$ on this vector is useful to calculate the commutator:

$$[\mathcal{H}_i,\mathcal{F}(w,\alpha)]=\mathcal{F}(w,\alpha)\frac{H_\alpha^{(i)}}{w-z_i}-\frac{F_\alpha^{(i)}}{w-z_i}\left(\sum_{j=1}^{N}\frac{H_\alpha^{(j)}}{w-z_j}\right)+\sum_{\beta\in\Delta_+,\beta>\alpha}\frac{\langle\beta,\beta\rangle}{2}N_{\beta,-\alpha}$$
$$\times\left\{\mathcal{F}(w,\beta)\frac{E_{\beta-\alpha}^{(i)}}{w-z_i}-\frac{F_\beta^{(i)}}{w-z_i}\sum_{j=1}^{N}\frac{E_{\beta-\alpha}^{(j)}}{w-z_j}\right\}. \tag{20}$$

Applied on the vacuum vector all the terms of the last sum vanish and then.

$$[\mathcal{H}_i,\mathcal{F}(w,\alpha)]v_0=\frac{\langle\alpha,\lambda_i\rangle}{w-z_i}\mathcal{F}(w,\alpha)v_0-\left(\sum_{j=1}^{N}\frac{\langle\alpha,\lambda_j\rangle}{w-z_j}\right)\frac{F_\alpha^{(i)}}{w-z_i}v_0. \tag{21}$$

Hence, the action of a Gaudin Hamiltonian $\mathcal{H}_i$ on the vector (19) is

$$\mathcal{H}_i\psi_1(w,\alpha)=\left(\sum_{j=1;j\neq i}^{N}\frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j}+\frac{\langle\alpha,\lambda_i\rangle}{w-z_i}\right)\psi_1(w,\alpha)-\left(\sum_{k=1}^{N}\frac{\langle\alpha,\lambda_k\rangle}{w-z_k}\right)\frac{F_\alpha^{(i)}}{w-z_i}v_0 \tag{22}$$

and we have the following lemma.

Lemma 7: Given N complex numbers $\{z_i\}_{i=1,N}$ and dominant integral highest weights $\{\lambda_i\}_{i=1,N}$, the Bethe vector $\psi_1(w,\alpha)$ of spin deviation α is an eigenvector for all Gaudin Hamiltonians:

$$\mathcal{H}_i\psi_1(w,\alpha)=s_i^1(w,\alpha)\psi_1(w,\alpha), \quad \forall \ i=1,\ldots,N,$$

if the complex parameter w satisfies the Bethe equation

$$\sum_{k=1}^{N}\frac{\langle\alpha,\lambda_k\rangle}{w-z_k}=0. \tag{23}$$

The eigenvalue $s_i^1(w,\alpha)$ of the Hamiltonian $\mathcal{H}_i$ depends on the solution of this equation:

$$s_i^1(w,\alpha)=\sum_{j=1;j\neq i}^{N}\frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j}+\frac{\langle\alpha,\lambda_i\rangle}{w-z_i}, \quad i=1,\ldots,N.$$

1. Additional eigenvector in $\mathcal{V}_\alpha$

As in the case of the model related to the Lie algebra SL(2), this constructive method does not provide all the common eigenvectors in $\mathcal{V}_\alpha$. In the eigenspace $\mathcal{V}_\alpha$, which has dimension N, the number of common eigenvectors obtained is equal to the number of distinct solutions of the equation (23), which is at most $N-1$. One more common eigenvector, which is not of the form (19), is given by the following lemma.

Lemma 8: The vector $\psi_\alpha^0\in\mathcal{V}_\alpha$,

$$\psi_\alpha^0=\sum_{k=1}^{N}F_\alpha^{(k)}v_0,$$

is an eigenvector for each Hamiltonian $\mathcal{H}_i$:

$$\mathcal{H}_i \ \ \psi_\alpha^0=\left(\sum_{j=1,j\neq i}^{N}\frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j}\right)\psi_\alpha^0. \tag{24}$$

This vector has equal coefficients as an expansion on the basis of $\mathcal{V}_\alpha$ and it has the same eigenvalue as the vacuum vector (17).

2. The case of a nonsimple root α

Lemma 7 is no longer true for a positive root α which is not simple. In this case the action (22) of $\mathcal{H}_i$ on the state $\psi_1(w,\alpha)$ presents a number of additional terms of type

$$\frac{1}{w-z_i}F_\gamma^{(i)}\mathcal{F}(w,F_{\alpha-\gamma})v_0$$

with some numerical coefficients, where $\gamma\in\Delta_+$ are positive roots $\gamma\neq\alpha$ such that $\alpha-\gamma\in\Delta_+$. Such terms exist only if α is not a simple root and they do not vanish for any parameter w. Therefore, $\psi_1(w,\alpha)$ can not be an eigenvector for the Hamiltonians $\mathcal{H}_i$. This fact has the following explanation: If α is not simple, the expression (19) for $\psi_1(w,\alpha)$ has to be modified, because the eigenspace "$\mathcal{V}_\alpha$" is in fact $\mathcal{V}_{\alpha_1\alpha_2\ldots}$ and is generated not only by vectors $F_\alpha^{(i)}v_0$, but also by "higher order" vectors $F_{\alpha_1}^{(i)}F_{\alpha_2}^{(i)}\cdots$ with $\alpha_1+\alpha_2+\cdots=\alpha$ and therefore the expansion (19) is not complete.

In particular, if the nonsimple root α is the sum of two simple roots α_1 and α_2, the action of a Hamiltonian $\mathcal{H}_i$ on the state $\psi_1(w,\alpha)$ presents two additional terms and we have the following formula, which will be useful in the next section, for the case of two spin deviation α_1, α_2:

$$\mathcal{H}_i\psi_1(w,[F_{\alpha_1},F_{\alpha_2}])=\left(\sum_{j=1;j\neq i}^{N}\frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j}+\frac{\alpha(\lambda_i)}{w-z_i}\right)\psi_1(w,[F_{\alpha_1},F_{\alpha_2}])$$
$$-\left(\sum_{k=1}^{N}\frac{\alpha(\lambda_k)}{w-z_k}\right)\frac{[F_{\alpha_1},F_{\alpha_2}]^{(i)}}{w-z_i}v_0-\langle\alpha_1,\alpha_2\rangle$$
$$\times\left\{\mathcal{F}(w,\alpha_1)\frac{F_{\alpha_2}}{w-z_i}-\frac{F_{\alpha_1}}{w-z_i}\mathcal{F}(w,\alpha_2)\right\}v_0. \tag{25}$$

D. States of spin deviation α_1, α_2

Consider two simple roots α_1 and α_2, which are not necessarily distinct. For spin deviation α_1, α_2, the equation of eigenvectors for the spin operator $\mathcal{S}_\beta$ is

$$\mathcal{S}_\beta F_{\alpha_1}^{(k_1)}F_{\alpha_2}^{(k_2)}v_0=\left(\sum_{i=1}^{N}\lambda_i(\beta)-\alpha_1(\beta)-\alpha_2(\beta)\right)F_{\alpha_1}^{(k_1)}F_{\alpha_2}^{(k_2)}v_0. \tag{26}$$

The eigenspace $\mathcal{V}_{\alpha_1,\alpha_2}$ of spin deviation α_1, α_2, corresponding to the eigenvalue $\Sigma_{i=1}^{N}\lambda_i(\beta)-\alpha_1(\beta)-\alpha_2(\beta)$ is generated by vectors $\{F_{\alpha_1}^{(k_1)}F_{\alpha_2}^{(k_2)}v_0\}_{k_1,k_2=1,\ldots,N;k_1\neq k_2}$ with two generators of negative roots applied on two distinct components of v_0, but also by vectors $\{(F_{\alpha_1}F_{\alpha_2})^{(k)}v_0\}_{k=1,\ldots,N}$ and $\{(F_{\alpha_2}F_{\alpha_1})^{(k)}v_0\}_{k=1,\ldots,N}$ with two generators of negative roots applied on the same component of v_0. A Bethe vector of spin deviation α_1, α_2 is defined as an expansion on all these vectors, with some particular coefficients depending on two complex parameters w_1,w_2:

$$\psi_2(w_1,\alpha_1;w_2,\alpha_2)=\sum_{k_1=1}^{N}\sum_{k_2\neq k_1}^{N}\frac{F_{\alpha_1}^{(k_1)}F_{\alpha_2}^{(k_2)}}{(w_1-z_{k_1})(w_2-z_{k_2})}v_0+\frac{1}{w_1-w_2}\sum_{k=1}^{N}\frac{F_{\alpha_1}^{(k)}F_{\alpha_2}^{(k)}}{w_2-z_k}v_0$$
$$+\frac{1}{w_2-w_1}\sum_{k=1}^{N}\frac{F_{\alpha_2}^{(k)}F_{\alpha_1}^{(k)}}{w_1-z_k}v_0. \tag{27}$$

As an element of the representation space V_{λ_k}, one of the two last terms is not a good ordered monomial and we must write, for instance, $F_{\alpha_2}^{(k)}F_{\alpha_1}^{(k)}=F_{\alpha_1}^{(k)}F_{\alpha_2}^{(k)}+[F_{\alpha_2}^{(k)},F_{\alpha_1}^{(k)}]$. Then this vector can also be written in the following form, using the operators $\mathcal{F}$:

$$\psi_2(w_1,\alpha_1;w_2,\alpha_2)=\mathcal{F}(w_1,\alpha_1)\mathcal{F}(w_2,\alpha_2)v_0+\frac{1}{w_1-w_2}\mathcal{F}(w_1,[F_{\alpha_1},F_{\alpha_2}])v_0.$$

With this construction, the vector ψ_2 is symmetrical in the pairs (w,α):

$$\psi_2(w_1,\alpha_1;w_2,\alpha_2)=\psi_2(w_2,\alpha_2;w_1,\alpha_1).$$

To calculate the action of a Hamiltonian $\mathcal{H}_i$ on the vector ψ_2,

$$\mathcal{H}_i\psi_2(w_1,\alpha_1;w_2,\alpha_2)=[\mathcal{H}_i,\mathcal{F}(w_1,\alpha_1)]\mathcal{F}(w_2,\alpha_2)v_0+\mathcal{F}(w_1,\alpha_1)\mathcal{H}_i\mathcal{F}(w_2,\alpha_2)v_0$$
$$+\frac{1}{w_1-w_2}\mathcal{H}_i\mathcal{F}(w_1,[F_{\alpha_1},F_{\alpha_2}])v_0, \tag{28}$$

we use the result (20) for the first term and (22) for the second term, but not for the third term, because it corresponds to a positive root $\alpha_1+\alpha_2$ which is no longer simple. For this one we apply the formula (25). Then, the action of a Hamiltonian $\mathcal{H}_i$ on the vector ψ_2 is

$$\mathcal{H}_i\psi_2(w_1,\alpha_1;w_2,\alpha_2)=s_i^2(w_1,w_2)\psi_2(w_1,\alpha_1;w_2,\alpha_2)$$
$$-f_1\left(\frac{F^{(i)}_{\alpha_1}}{w_1-z_i}\mathcal{F}(w_2,\alpha_2)+\frac{1}{w_1-w_2}\frac{[F^{(i)}_{\alpha_1},F^{(i)}_{\alpha_2}]}{w_1-z_i}\right)v_0$$
$$-f_2\left(\mathcal{F}(w_1,\alpha_1)\frac{F^{(i)}_{\alpha_2}}{w_2-z_i}+\frac{1}{w_1-w_2}\frac{[F^{(i)}_{\alpha_1},F^{(i)}_{\alpha_2}]}{w_1-z_i}\right)v_0,$$

where

$$s_i^2=\sum_{j=1;j\neq i}^{N}\frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j}+\frac{\langle\alpha_1,\lambda_i\rangle}{w_1-z_i}+\frac{\langle\alpha_2,\lambda_i\rangle}{w_2-z_i},$$

$$f_1=\sum_{k=1}^{N}\frac{\langle\alpha_1,\lambda_k\rangle}{w_1-z_k}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_2-w_1},$$

$$f_2=\sum_{k=1}^{N}\frac{\langle\alpha_2,\lambda_k\rangle}{w_2-z_k}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_1-w_2}.$$

Lemma 9 follows from these considerations.

Lemma 9: The Bethe vector $\psi_2(w_1,\alpha_1;w_2,\alpha_2)$ of spin deviation α_1,α_2 is an eigenvector for all Gaudin Hamiltonians

$$\mathcal{H}_i\psi_2(w_1,w_2)=s_i^2\psi_2(w_1,\alpha_1;w_2,\alpha_2)$$

if the parameters w_1,w_2 satisfy the Bethe equations:

$$f_1=\sum_{k=1}^{N}\frac{\langle\alpha_1,\lambda_k\rangle}{w_1-z_k}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_2-w_1}=0,$$
$$f_2=\sum_{k=1}^{N}\frac{\langle\alpha_2,\lambda_k\rangle}{w_2-z_k}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_1-w_2}=0. \tag{29}$$

Remarks:

(1) As discussed in the previous section, if the roots α_1 and α_2 are not simple the result of the previous lemma is not true and the expression (27) of ψ_2 has to be completed.

(2) The number of distinct solutions of Bethe equations is less than the dimension of the eigenspace $\mathcal{V}_{\alpha_1,\alpha_2}$. Therefore, other common eigenvectors could exist. It can be proved that

$$\psi^0_{\alpha_1,\alpha_2}=\left(\sum_{k_1=1}^{N}F^{(k_1)}_{\alpha_1}\right)\left(\sum_{k_2=1}^{N}F^{(k_2)}_{\alpha_2}\right)v_0 \quad\text{and}\quad \psi^0_{\alpha_1+\alpha_2}=\sum_{k=1}^{N}[F_{\alpha_1},F_{\alpha_2}]^{(k)}v_0$$

are also common eigenvectors of Hamiltonians, with the same eigenvalue as the vacuum vector.

E. States of spin deviation $\alpha_1,\ldots,\alpha_m$

For m simple roots $\alpha_1,\ldots,\alpha_m$, which are not necessarily distinct, the eigenspace $\mathcal{V}_{\alpha_1,\ldots,\alpha_m}$ of spin deviation $\alpha_1,\ldots,\alpha_m$, corresponding to the eigenvalue $\Sigma_{i=1}^{N}\lambda_i(\beta)-\Sigma_{l=1}^{m}\alpha_l(\beta)$, is generated by ordered monomials $F^{(k_1)}_{\gamma_1}\cdots F^{(k_n)}_{\gamma_n}v_0$ for all $k_1,\ldots,k_n=1,\ldots,N$ and $\gamma_1,\ldots,\gamma_n$ positive roots with $\Sigma_{i=1}^{n}\gamma_i=\Sigma_{l=1}^{m}\alpha_l$. Common eigenvectors of Hamiltonians are defined as expansions on all the monomials, but, in this general case, a particular form of coefficients (depending on m complex parameters $w_1,\ldots w_m$) can hardly be justified.

It was claimed in Ref. 6 that such a vector can be determined in each subspace $\mathcal{V}_{\alpha_1,\ldots,\alpha_m}$ through a recursive procedure in the number m of simple roots:

$$\begin{aligned}&\psi_m(w_1,\alpha_1;\ldots;w_m,\alpha_m)v_0\\&\quad=\psi_{m-1}(w_1,\alpha_1;\ldots;w_{m-1},\alpha_{m-1})\mathcal{F}(w_m,\alpha_m)v_0\\&\qquad+\sum_{j=1}^{m-1}\frac{1}{w_j-w_m}\psi_{m-1}(w_1,\alpha_1;\ldots;w_j,[F_{\alpha_j},F_{\alpha_m}];\ldots;w_{m-1},\alpha_{m-1})v_0,\end{aligned}\tag{30}$$

with $\psi_1(w,\alpha)=\mathcal{F}(w,\alpha)v_0$, and that the action of a Hamiltonian $\mathcal{H}_i$ on the vector $\psi_m v_0$ is

$$\mathcal{H}_i\psi_m(w_1,\alpha_1;\ldots;w_m,\alpha_m)v_0=s_i^m\psi_m(w_1,\alpha_1;\ldots;w_m,\alpha_m)v_0-\sum_{k=1}^{m}f_k^m\overline{\psi}_m^k v_0,\tag{31}$$

where

$$\begin{aligned}s_i^m&=\sum_{j=1;j\neq i}^{N}\frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j}+\sum_{k=1}^{m}\frac{\langle\alpha_k,\lambda_i\rangle}{w_k-z_i},\\f_k^m&=\sum_{j=1}^{N}\frac{\langle\alpha_k,\lambda_j\rangle}{w_k-z_j}+\sum_{l=1}^{m}\frac{\langle\alpha_k,\alpha_l\rangle}{w_l-w_k},\quad\forall k=1,\ldots,m,\end{aligned}\tag{32}$$

and $\overline{\psi}_m^k v_0$ are some vectors in $\mathcal{V}_{\alpha_1,\ldots,\alpha_m}$.

Such a recursive construction of the common eigenvectors seems to be appropriate for inductive calculations. For example, we can verify by induction that the vector ψ_m is symmetrical in the pairs (w,α):

$$\psi_m(\ldots;w_k,\alpha_k;\ldots;w_l,\alpha_l;\ldots)=\psi_m(\ldots w_l,\alpha_l;\ldots;w_k,\alpha_k;\ldots).$$

However, an inductive calculation for the action (31) of Hamiltonians on these vectors is very difficult. As remarked for the case of spin deviation α_1, α_2, the serious problem comes from the presence in (30) of roots which are not simple and therefore the induction step can not be applied.

For the eigenvector ψ_m an explicit form is given by the following theorem (for simplicity F_i denotes F_{α_i})

Theorem 10: *The recursion relation (30) has the following result:*

$$\begin{aligned}&\psi_m(w_1,\alpha_1;\ldots;w_m,\alpha_m)v_0\\&\quad=\sum_{\mathcal{P}_m}\prod_{j=1}^{N}\sum_{\sigma\in\mathcal{S}(I^j)}\frac{(F_{\sigma(i_1^j)}\ldots F_{\sigma(i_{l_j}^j)})^{(j)}}{(w_{\sigma(i_1^j)}-w_{\sigma(i_2^j)})(w_{\sigma(i_2^j)}-w_{\sigma(i_3^j)})\ldots(w_{\sigma(i_{l_j}^j)}-z_j)}v_0.\end{aligned}\tag{33}$$

In this relation the first sum is taken over all N-fold partitions $(I^1,\ldots,I^N)$, $I^1\cup\ldots\cup I^N=\{1,\ldots,m\}$ *of the set of indices* $\{1,\ldots,m\}$ *of the m simple roots* $\alpha_1,\ldots,\alpha_m$. *The partitions are considered with N disjoint subsets, which can be empty, as well:* $I^j=\{i_1^j,\ldots,i_{l_j}^j\}$, *with* $0\leqslant l_j\leqslant m$. *The product is taken over all components* V_{λ_j} *of the tensor product representation* Ω. *The second sum is taken over the set* $\mathcal{S}(I^j)$ *of all permutations in the subset* I^j.

For example, in the case of two simple roots, there are two types of partitions of the set $\{1,2\}$:

$$\text{type } I:\begin{cases}I^k=\{1,2\}\\I^l=\phi\end{cases}\quad\text{together with its permutation}\quad\begin{cases}I^k=\{2,1\}\\I^l=\phi\end{cases}\qquad k,l=1,\ldots,N,l\neq k,$$

$$\text{type } II: \begin{cases} I^k=\{1\} \\ I^l=\{2\} \end{cases} \qquad k,l=1,\ldots,N, l\neq k, \text{ and the others are empty.}$$

Then the sum (33) over these partitions reduces to (27).

Theorem 10 was announced in Ref. 6, where it was also remarked that (33) is exactly the same vector function (45), appearing in the integral solutions of the KZ equation. In Sec. V we will briefly analyze the connection between the problem of common eigenvectors for Gaudin Hamiltonians and the solutions of the KZ equation.

In the rest of the present section we give a proof of Theorem 10 which is based on two lemmas.

Lemma 11: Let $A=\{i_1,i_2,\ldots,i_n\}$ be a set of indices, E an expression depending on these indices and $\mathcal{S}(A)$ the set of permutations of A. Then, for any fixed $i_a\in A$ we have

$$\sum_{\sigma\in\mathcal{S}(A)} E(\sigma(i_1),\ldots,\sigma(i_n)) = \sum_{\sigma'\in\mathcal{S}(A\setminus\{i_a\})}\sum_{q=1}^{n} E(\sigma'(i'_1),\ldots,\sigma'(i'_{q-1}),i_a,\sigma'(i'_q),\ldots,\sigma'(i'_{n-1})),$$

where $\{i'_1,i'_2,\ldots,i'_{n-1}\}=A\setminus\{i_a\}$.

It means that a sum over the permutations of n elements can be rearranged as follows: fix one of these elements, make the sum over the permutations of the resting $n-1$ elements and for each such permutation make the sum of the expressions E in which the fixed element is placed successively on all positions from 1 to n.

The second lemma is a result of straightforward calculations:

Lemma 12: For some distinct complex numbers $w_1,\ldots,w_n,w_\beta,z$, let

$$Q_s(w_1,\ldots,w_n,w_\beta)=\sum_{q=1}^{s}\frac{1}{(w_1-w_2)\cdots(w_{q-1}-w_\beta)(w_\beta-w_q)\cdots(w_{n-1}-w_n)(w_n-z)}, \quad \forall s=1,\ldots,n+1,$$

where the first term (for $q=1$) is $1/[(w_\beta-w_1)(w_1-w_2)\cdots(w_{n-1}-w_n)(w_n-z)]$ and the term for $q=n+1$ is $1/[(w_1-w_2)\cdots(w_{n-1}-w_n)(w_n-w_\beta)(w_\beta-z)]$. Then

$$Q_s(w_1,\ldots,w_n,w_\beta)=\frac{1}{(w_1-w_2)\ldots(w_{n-1}-w_n)(w_n-z)}\frac{1}{(w_\beta-w_s)}, \quad \forall s=1,\ldots,n, \tag{34}$$

$$Q_{n+1}(w_1,\ldots,w_n,w_\beta)=\frac{1}{(w_1-w_2)\ldots(w_{n-1}-w_n)(w_n-z)}\frac{1}{(w_\beta-z)}. \tag{35}$$

Proof of the theorem: In the expression (33) of ψ_m, the sum over the partitions $(J^1,\ldots,J^N)\in\mathcal{P}_m$ of the indices $\{1,2,\ldots,m\}$ is rewritten as the sum over the partitions $(I^1,\ldots,I^N)\in\mathcal{P}_{m-1}$ of the indices $\{1,2,\ldots,m-1\}$, and for each partition in $\mathcal{P}_{m-1}$, the index m is successively placed in each subset $I^k=\{i^k_1,\ldots,i^k_{l_k}\}: J^l=I^l$, $\forall l\neq k$ and $J^k=I^k\cup\{m\}$. It follows

$$\psi_m=\sum_{\mathcal{P}_{m-1}}\sum_{k=1}^{N}\left(\prod_{j=1,j\neq k}^{N}\sum_{\sigma\in\mathcal{S}(I^j)}\frac{(F_{\sigma(i^j_1)}\cdots F_{\sigma(i^j_{l_j})})^{(j)}}{(w_{\sigma(i^j_1)}-w_{\sigma(i^j_2)})\cdots(w_{\sigma(i^j_{l_j})}-z_j)}\right) \times\left(\sum_{\sigma\in\mathcal{S}(J^k)}\frac{(F_{\sigma(i^k_1)}\cdots F_{\sigma(i^k_{l_k})}F_{\sigma(m)})^{(k)}}{(w_{\sigma(i^k_1)}-w_{\sigma(i^k_2)})\cdots(w_{\sigma(i^k_{l_k})}-w_{\sigma(m)})(w_{\sigma(m)}-z_k)}\right). \tag{36}$$

Then we compute the last sum and, to simplify the writing, we leave out the index k. Using Lemma 11 we obtain

$$\sum_{\sigma\in\mathcal{S}(J\setminus\{m\})}\sum_{q=1}^{l+1}\frac{F_{\sigma(i_1)}\cdots F_{\sigma(i_{q-1})}F_mF_{\sigma(i_q)}\cdots F_{\sigma(i_l)}}{(w_{\sigma(i_1)}-w_{\sigma(i_2)})\cdots(w_{\sigma(i_{q-1})}-w_m)(w_m-w_{\sigma(i_q)})\cdots(w_{\sigma(i_l)}-z_k)}. \tag{37}$$

At the numerator, we commute successively F_m, up to the last position:

$$\begin{aligned}&F_{\sigma(i_1)}\cdots F_{\sigma(i_{q-1})}F_mF_{\sigma(i_q)}\cdots F_{\sigma(i_l)}\\&\quad=F_{\sigma(i_1)}\cdots F_{\sigma(i_l)}F_m+\sum_{s=q}^{l}F_{\sigma(i_1)}\cdots F_{\sigma(i_{s-1})}[F_m,F_{\sigma(i_s)}]\cdots F_{\sigma(i_l)},\quad\forall q=1,\ldots,l.\end{aligned}$$

In this relation, the first term does not depend on q and can be factorized out of the sum over q in (37). It multiplies a sum of fractions which forms the sum $Q_l(w_{\sigma(i_1)},\ldots,w_{\sigma(i_l)},w_m)$, given by the relation (35) of Lemma 12.

For the second term we change in (37) the order of the two sums, over s and over q. Then the operator product $F_{\sigma(i_1)}\cdots F_{\sigma(i_{s-1})}[F_m,F_{\sigma(i_s)}]\cdots F_{\sigma(i_l)}$ can also be factorized out of the sum over q and it multiplies the sum $Q_s(w_{\sigma(i_1)},\ldots,w_{\sigma(i_l)},w_m)$, which is given by the relation (34) of Lemma 12, for all $s=1,\ldots,l$. Hence, for (37) we obtain

$$\begin{aligned}\sum_{\sigma\in\mathcal{S}(I)}\Bigg(&\frac{F_{\sigma(i_1)}\ldots F_{\sigma(i_l)}}{(w_{\sigma(i_1)}-w_{\sigma(i_2)})\ldots(w_{\sigma(i_l)}-z_k)}\frac{F_m}{w_m-z_k}\\&+\sum_{s=1}^{l}\frac{1}{w_m-w_{\sigma(i_s)}}\frac{F_{\sigma(i_1)}\ldots F_{\sigma(i_{s-1})}[F_m,F_{\sigma(i_s)}]\ldots F_{\sigma(i_l)}}{(w_{\sigma(i_1)}-w_{\sigma(i_2)})\ldots(w_{\sigma(i_l)}-z_k)}\Bigg).\end{aligned} \tag{38}$$

Replacing the first part of (38) in the expression (36) of ψ_m, we obtain

$$\sum_{\mathcal{P}_{m-1}}\left(\prod_{j=1}^{N}\sum_{\sigma\in\mathcal{S}(I^j)}\frac{(F_{\sigma(i_1^j)}\cdots F_{\sigma(i_{l_j}^j)})^{(j)}}{(w_{\sigma(i_1^j)}-w_{\sigma(i_2^j)})\cdots(w_{\sigma(i_{l_j}^j)}-z_j)}\right)\sum_{k=1}^{N}\frac{F_m^{(k)}}{w_m-z_k}, \tag{39}$$

which is exactly the term $\psi_{m-1}(w_1,\alpha_1;\ldots;w_{m-1},\alpha_{m-1})\mathcal{F}(w_m,\alpha_m)$ of the recursion relation (30).

Using lemma 11, the second part of the relation (38) can be rewritten as

$$\sum_{s=1}^{l}\frac{1}{w_m-w_{i_s}}\sum_{\sigma\in\mathcal{S}(I\setminus\{i_s\})}\sum_{q=1}^{l}\frac{F_{\sigma(j_1)}\ldots F_{\sigma(j_{q-1})}[F_m,F_{i_s}]\ldots F_{\sigma(j_{l-1})}}{(w_{\sigma(j_1)}-w_{\sigma(j_2)})\cdots(w_{\sigma(j_{q-1})}-w_{\sigma(i_s)})(w_{\sigma(i_s)}-w_{\sigma(j_q)})\cdots(w_{\sigma(j_{l-1})}-z_k)},$$

where $\{j_1,\ldots,j_{l-1}\}$ is the subset $I\setminus\{i_s\}$ of I. Applying again Lemma 11, it becomes

$$\sum_{s=1}^{l}\frac{1}{w_m-w_{i_s}}\left\{\sum_{\sigma\in\mathcal{S}(I)}\frac{F_{\sigma(i_1)}\cdots F_{\sigma(i_l)}}{(w_{\sigma(i_1)}-w_{\sigma(i_2)})\cdots(w_{\sigma(i_l)}-z_k)}\right\}_{F_{i_s}\hookrightarrow[F_m,F_{i_s}]},$$

where $\{\text{expr}\}_{F_{i_s}\hookrightarrow[F_m,F_{i_s}]}$ is the expression expr in which the operator F_{i_s} is replaced by the commutator $[F_m,F_{i_s}]$. Replacing this term in the expression (36) of ψ_m, we obtain

$$\sum_{\mathcal{P}_{m-1}} \sum_{k=1}^{N} \sum_{s=1}^{l_k} \frac{1}{w_m - w_{i_s^k}} \left(\prod_{\substack{j=1 \\ j\neq k}}^{N} \sum_{\sigma\in\mathcal{S}(I^j)} \frac{(F_{\sigma(i_1^j)}\cdots F_{\sigma(i_{l_j}^j)})^{(j)}}{(w_{\sigma(i_1^j)} - w_{\sigma(i_2^j)})\cdots} \right)$$
$$\times \left\{ \sum_{\sigma\in\mathcal{S}(I^k)} \frac{(F_{\sigma(i_1^k)}\cdots F_{\sigma(i_{l_k}^k)})^{(k)}}{(w_{\sigma(i_1^k)} - w_{\sigma(i_2^k)})\cdots(w_{\sigma(i_{l_k}^k)} - z_k)} \right\}_{F_{i_s^k}\hookrightarrow[F_m, F_{i_s^k}]}.$$

In this expression, for each partition $(I^1,\ldots,I^N)$ and for each index $r=1,\ldots,m-1$, the factor $1/(w_m - w_r)$ occurs once only. Therefore, this expression can be rearranged in the following form:

$$\sum_{r=1}^{m-1} \frac{1}{w_m - w_r} \sum_{\mathcal{P}_{m-1}} \left(\prod_{\substack{j=1 \\ j\neq k, r\in I^k}}^{N} \sum_{\sigma\in\mathcal{S}(I^j)} \frac{(F_{\sigma(i_1^j)}\cdots F_{\sigma(i_{l_j}^j)})^{(j)}}{(w_{\sigma(i_1^j)} - w_{\sigma(i_2^j)})\cdots} \right)$$
$$\times \left\{ \sum_{\sigma\in\mathcal{S}(I^k)} \frac{(F_{\sigma(i_1^k)}\cdots F_{\sigma(i_{l_k}^k)})^{(k)}}{(w_{\sigma(i_1^k)} - w_{\sigma(i_2^k)})\cdots(w_{\sigma(i_{l_k}^k)} - z_k)} \right\}_{F_r\hookrightarrow[F_m, F_r]},$$

which is exactly the term $\Sigma_{j=1}^{m-1} 1/(w_j - w_m)\, \psi_{m-1}(w_1,\alpha_1;\ldots;w_j,[F_{\alpha_j},F_{\alpha_m}];\ldots;w_{m-1},\alpha_{m-1})$ of the recursion (30).

1. Additional eigenvectors

The recursion relation (30) gives only a part of common eigenvectors. As in the cases of spin deviation α and α_1, α_2, additional eigenvectors can be found:

Lemma 13: For any ordered set of simple roots $\alpha_1,\alpha_2,\ldots,\alpha_m$, the vector

$$\psi^0_{\alpha_1,\ldots,\alpha_m} = \left(\sum_{k_1=1}^{N} F^{(k_1)}_{\alpha_1} \right) \cdots \left(\sum_{k_m=1}^{N} F^{(k_m)}_{\alpha_m} \right) v_0 \tag{40}$$

is an eigenvector of Hamiltonians $\mathcal{H}_i$ corresponding to the same eigenvalue as the vacuum vector:

$$\mathcal{H}_i \psi^0_{\alpha_1,\ldots,\alpha_m} = \left(\sum_{j=1, j\neq i}^{N} \frac{\langle \lambda_i, \lambda_j \rangle}{z_i - z_j} \right) \psi^0_{\alpha_1,\ldots,\alpha_m}.$$

Remark that these vectors of Ω lie in $\mathcal{V}_{\alpha_1,\ldots,\alpha_m}$ only if the roots α_i are all simple. The lemma is a consequence of the following property of the operators $\mathcal{H}_i$:

$$\left[\mathcal{H}_i, \sum_{k=1}^{N} F^{(k)}_{\alpha} \right] = 0, \quad \forall \alpha \in \Delta_0.$$

IV. SINGULAR AND NONSINGULAR EIGENVECTORS

In the previous sections we have constructed two types of eigenvectors for the Gaudin Hamiltonians: the Bethe vectors $\psi_m(w_1,\ldots,w_m)v_0$ in (12) and $\psi_m(w_1,\alpha_1,\ldots,w_m,\alpha_m)v_0$ in (33) and the additional eigenvectors ψ^0_m in (16) and $\psi^0_{\alpha_1,\ldots,\alpha_m}$ in (40). In this section we prove that Bethe vectors are singular only if the Bethe equations are satisfied and that the additional eigenvectors are not singular.

A vector v of the tensor product representation Ω is called singular if

$$E_\alpha v=\sum_{i=1}^{N} E_\alpha^{(i)} v=0, \quad \forall \alpha\in\Delta_0 .$$

In the case of the Lie algebra SL(2) the Bethe vectors $\psi_m(w_1,\ldots,w_m)v_0$ given by (12) are singular only for those values of $w_1,\ldots,w_m$ which are solutions of the Bethe equations (15), since

$$E\psi_m(w_1,\ldots,w_m)v_0=\sum_{k=1}^{m}\left(\sum_{j=1}^{N}\frac{\lambda_j}{w_k-z_j}+\sum_{l=1;l\neq k}^{m}\frac{2}{w_l-w_k}\right)\psi_{m-1}(\ldots,\widehat{w_k},\ldots)v_0 .$$

Therefore the Bethe equations (15) appear also as conditions that Bethe vectors be singular vectors of Ω.

Unlike Bethe vectors, the additional eigenvectors ψ_m^0 are not singular, since

$$E\psi_m^0=m\left(\sum_{j=1}^{N}\lambda_j-m+1\right)\psi_{m-1}^0\neq 0, \quad \forall m=1,\ldots,m_{\max}, \quad m_{\max}=\sum_{j=1}^{N}\lambda_j .$$

A similar result holds in the case of an arbitrary Lie algebra G:

Theorem 14: *For any simple root β, the action of the operator E_β on the Bethe vector (33) is given by*

$$E_\beta\psi_m(w_1,\alpha_1,\ldots,w_m,\alpha_m)v_0=\sum_{i=1}^{m}\frac{2\delta_{\beta\alpha_i}}{\langle\alpha_i,\alpha_i\rangle}\left[\sum_{j=1}^{N}\frac{\langle\alpha_i,\lambda_j\rangle}{w_i-z_j}-\sum_{j=1,j\neq i}^{m}\frac{\langle\beta,\alpha_j\rangle}{w_i-w_j}\right]\psi_{m-1}(\ldots,\widehat{w_i,\alpha_i},\ldots)v_0 . \tag{41}$$

Therefore, the Bethe vectors $\psi_m(w_1,\alpha_1,\ldots,w_m\alpha_m)v_0$ are singular only for those values of $w_1,\ldots,w_m$ which are solutions of the Bethe equations $f_j^m=0, \forall j=1,\ldots,m$ in (32).

Proof: Using similar considerations as for Theorem 10, we compute the commutator $[E_\beta,\psi_m]=[\Sigma_{k=1}^{N}E_\beta^{(k)},\psi_m]$, which is

$$\sum_{k=1}^{N}\sum_{\mathcal{P}_m}\left(\prod_{j=1,j\neq k}^{N}\sum_{\sigma\in\mathcal{S}(I^j)}\frac{(F_{\sigma(i_1^j)}\cdots F_{\sigma(i_{l_j}^j)})^{(j)}}{(w_{\sigma(i_1^j)}-w_{\sigma(i_2^j)})\cdots(w_{\sigma(i_{l_j}^j)}-z_j)}\right)\times\left(\sum_{\sigma\in\mathcal{S}(I^k)}\frac{[E_\beta,F_{\sigma(i_1^k)}\cdots F_{\sigma(i_{l_k}^k)}]^{(k)}}{(w_{\sigma(i_1^k)}-w_{\sigma(i_2^k)})\cdots(w_{\sigma(i_{l_k}^k)}-z_k)}\right). \tag{42}$$

Using the relation

$$[E_\beta,F_{\alpha_1}\cdots F_{\alpha_l}]=\sum_{n=1}^{l}\delta_{\beta,\alpha_n}\frac{2}{\langle\alpha_n,\alpha_n\rangle}F_{\alpha_1}\cdots\widehat{F_{\alpha_n}}\cdots F_{\alpha_l}\left(H_{\alpha_n}-\sum_{s=n+1}^{l}\langle\alpha_n,\alpha_s\rangle\right),$$

and applying Lemma 11, the last factor of (42) becomes (for simplicity, we leave out the index k)

$$\sum_{n=1}^{l}\sum_{\sigma\in\mathcal{S}_n}\sum_{q=1}^{l}\frac{2\delta_{\beta,\alpha_{i_n}}}{\langle\alpha_{i_n},\alpha_{i_n}\rangle}\frac{F_{\sigma(i_1)}\cdots F_{\sigma(i_{q-1})}\widehat{F_{i_n}}F_{\sigma(i_q)}\cdots F_{\sigma(i_{l-1})}(H_\beta-\Sigma_{s=q}^{l-1}\langle\beta,\alpha_{\sigma(i_s)}\rangle)}{(w_{\sigma(i_1)}-w_{\sigma(i_2)})\cdots(w_{\sigma(i_{q-1})}-w_{i_n})(w_{i_n}-w_{\sigma(i_q)})\cdots(w_{\sigma(i_{l-1})}-z_k)},$$

where, for each n, $\mathcal{S}_n$ are the permutations of the subset $\{i_1,\ldots,i_{l-1}\}=I\setminus\{i_n\}$ of I. To compute the sum over q we use Lemma 12 and we obtain

$$\sum_{n=1}^{l}\sum_{\sigma\in\mathcal{S}_n}\frac{2\delta_{\beta,\alpha_{i_n}}}{\langle\alpha_{i_n},\alpha_{i_n}\rangle}\frac{F_{\sigma(i_1)}\cdots F_{\sigma(i_{l-1})}}{(w_{\sigma(i_1)}-w_{\sigma(i_2)})\cdots(w_{\sigma(i_{l-1})}-z_k)}\left(\frac{H_\beta}{w_{i_n}-z_k}-\sum_{s=1}^{l-1}\frac{\langle\beta,\alpha_{\sigma(i_s)}\rangle}{w_{i_n}-w_{\sigma(i_s)}}\right).$$

In this expression, since σ is a bijection, it holds

$$\sum_{s=1}^{l-1}\frac{\langle\beta,\alpha_{\sigma(i_s)}\rangle}{w_{i_n}-w_{\sigma(i_s)}}=\sum_{s=1}^{l-1}\frac{\langle\beta,\alpha_{i_s}\rangle}{w_{i_n}-w_{i_s}},$$

and therefore the last parenthesis can be factorized out of the sum over permutations. Replacing this result in (42) we obtain

$$\sum_{\mathcal{P}_m}\sum_{k=1}^{N}\sum_{n=1}^{l_k}\frac{2\delta_{\beta,\alpha_{i_n}}}{\langle\alpha_{i_n},\alpha_{i_n}\rangle}\left(\prod_{\substack{j=1\\ j\neq k}}^{N}\sum_{\sigma\in\mathcal{S}(I^j)}\cdots\right)\sum_{\sigma\in\mathcal{S}_n}\frac{(F_{\sigma(i_1^k)}\cdots F_{\sigma(i_{l-1}^k)})^{(k)}}{(w_{\sigma(i_1^k)}-w_{\sigma(i_2^k)})\cdots(w_{\sigma(i_{l_k-1}^k)}-z_k)}$$
$$\times\left(\frac{H_\beta^{(k)}}{w_{i_n^k}-z_k}-\sum_{s\in I^k\setminus\{i_n^k\}}\frac{\langle\beta,\alpha_s\rangle}{w_{i_n^k}-w_s}\right).$$

For each partition $I^1,\ldots,I^N$ of $\mathcal{P}_m$ and for each index $r=1,\ldots,m$, there is only one index k such that $r\in I^k$. Therefore, in the last expression, there is only one term, containing $2\delta_{\beta,\alpha_r}/\langle\alpha_r,\alpha_r\rangle$. Hence the last expression is

$$\sum_{r=1}^{m}\frac{2\delta_{\beta,\alpha_r}}{\langle\alpha_r,\alpha_r\rangle}\sum_{\mathcal{P}_m}\left(\prod_{j=1,j\neq k}^{N}\sum_{\sigma\in\mathcal{S}(I^j)}\cdots\right)\left(\sum_{\sigma\in\mathcal{S}(I^k\setminus\{r\})}\cdots\right)\left(\frac{H_\beta^{(k)}}{w_r-z_k}-\sum_{s\in I^k\setminus\{r\}}\frac{\langle\beta,\alpha_s\rangle}{w_r-w_s}\right).$$

For each $r=1,\ldots,m$, the sum over the partitions $\mathcal{P}_m$ of the indices is rewritten as the sum over the partitions $(J^1,\ldots,J^N)\in\mathcal{P}_{m-1}$ of the indices $\{1,2,\ldots,m\}\setminus\{r\}$ and the index r is successively placed in each subset J^q. Hence we obtain

$$\sum_{r=1}^{m}\frac{2\delta_{\beta,\alpha_r}}{\langle\alpha_r,\alpha_r\rangle}\sum_{\mathcal{P}_{m-1}}\sum_{q=1}^{N}\left(\prod_{j=1,j\neq q}^{N}\sum_{\sigma\in\mathcal{S}(J^j)}\cdots\right)\left(\sum_{\sigma\in\mathcal{S}(J^q)}\cdots\right)\left(\frac{H_\beta^{(q)}}{w_r-z_q}-\sum_{s\in J^q}\frac{\langle\beta,\alpha_s\rangle}{w_r-w_s}\right).$$

We identify in this expression the vectors $\psi_{m-1}(\ldots,\widehat{w_r,\alpha_r},\ldots)$, given by (33), and we obtain (41).

V. BETHE ANSATZ AND KNIZHNIK–ZAMOLODCHIKOV EQUATION

Knizhnik–Zamolodchikov equations

$$\frac{\partial\Phi}{\partial z_i}(z_1,\ldots,z_N)=\frac{1}{\kappa}\mathcal{H}_i(z_1,\ldots,z_N)\Phi(z_1,\ldots,z_N),\quad i=1,\ldots,N,\tag{43}$$

were first introduced[9] as a system of partial differential equations for correlation functions of primary fields in a WZW model of conformal field theory. The number κ is the sum of the dual Coxeter number of the Lie algebra G and the central charge of the model.

Such a system is defined by N operators:

$$\mathcal{H}_i(z_1,\ldots,z_N)=\sum_{j=1,j\neq i}^{N}\frac{1}{z_i-z_j}\sum_{a=1}^{d}I_a^{(i)}\tilde{I}_a^{(j)},\quad\forall i=1,\ldots,N,$$

on a tensor product representation Ω, which are rational functions of complex variables $z_1,\ldots,z_N$. The ''coefficients'' $\mathcal{H}_i(z_1,\ldots,z_N)$ of this system commute and verify

$$\frac{\partial \mathcal{H}_i}{\partial z_j}=\frac{\partial \mathcal{H}_j}{\partial z_i},$$

which means that the differential form $\Sigma_{i=1}^{N}\mathcal{H}_i\,dz_i$ is closed. Hence the conditions of integrability of the system are fulfilled.

This system is rather difficult to solve, but there is a simple exception in the case of four variables, when the partial differential equation can be reduced to an ordinary differential equation of hypergeometric type. In this case, the four-point correlation functions for a model related to the SL(2) Lie algebra was determined.[16] This has led to the idea that such correlation functions admit representations as generalized hypergeometric integrals (also known as Feigin–Fuchs integrals). For KZ equations associated to arbitrary Lie algebra, Varchenko and Schechtman[17,8] gave a set of solutions in terms of generalized hypergeometric integrals. We present here these solutions.

Consider the KZ equations in the tensor product representation Ω, which is also a graduate space with its weight decomposition $\Omega=\oplus\mathcal{V}_\mu$. In each weight subspace $\mathcal{V}_\mu$, of weight $\mu=\Sigma_{i=1}^{N}\lambda_i-\Sigma_{j=1}^{m}\alpha_j$, a solution of the KZ equations with values in the subspace of singular vectors $\mathrm{Sing}\mathcal{V}_\mu$ is given by

$$\Phi(z_1,\ldots,z_N)=\int_\gamma \chi(z_1,\ldots,z_N;w_1,\ldots,w_m)\,\psi(w_1,\alpha_1;\ldots;w_m,\alpha_m)\,dw_1\cdots dw_m. \tag{44}$$

Here χ is the multivalued complex function:

$$\chi_m(\mathbf{z},\mathbf{w})=\prod_{1\leqslant j<k\leqslant N}(z_j-z_k)^{\langle\lambda_j,\lambda_k\rangle/\kappa}\prod_{j=1}^{N}\prod_{l=1}^{m}(w_l-z_j)^{-\langle\alpha_l,\lambda_j\rangle/\kappa}\prod_{1\leqslant l<n\leqslant m}(w_l-w_n)^{\langle\alpha_l,\alpha_n\rangle/\kappa}$$

with $\mathbf{z}=(z_1,\ldots,z_N)$, $\mathbf{w}=(w_1,\ldots,w_m)$ and γ is a m-cycle in the complement in $\mathbb{C}^{N+m}$ of all hyperplanes

$$z_j-z_k=0;\quad w_l-w_n=0;\quad w_l-z_j=0;\quad \forall j,k=1,\ldots,N;\quad l,n=1,\ldots,m,$$

on which $\chi(\mathbf{z},\mathbf{w})$ is a single-valued function of $\mathbf{w}$. The vector valued function $\psi\in V_\mu$ is a sum of ordered monomials with rational complex coefficients:

$$\psi_m(w_1,\alpha_1;\ldots;w_m,\alpha_m)=\sum_{\mathcal{P}}\prod_{j=1}^{N}\frac{(F_{i_1^j}\cdots F_{i_{l_j}^j})^{(j)}}{(w_{i_1^j}-w_{i_2^j})(w_{i_2^j}-w_{i_3^j})\cdots(w_{i_{l_j}^j}-z_j)}v_0, \tag{45}$$

where the product is taken over all components V_{λ_j} of the tensor product representation Ω and the sum is taken over all ordered partitions $I^1\cup\cdots\cup I^N$ of the set of indices $\{1,\ldots,m\}$ of the m simple roots $\alpha_1,\ldots,\alpha_m$. The ordered partitions are considered with N disjoint subsets, which can be empty, as well: $I^j=\{i_1^j,\ldots,i_{l_j}^j\}$, with $0\leqslant l_j\leqslant m$.

In this form, the solution (44) of KZ equations seems to be rather complicated, but a simple direct calculation can be performed to obtain

$$\kappa\frac{\partial\chi_m}{\partial z_i}(\mathbf{z},\mathbf{w})=\left(\sum_{j=1;j\neq i}^{N}\frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j}+\sum_{k=1}^{m}\frac{\langle\alpha_k,\lambda_i\rangle}{w_k-z_i}\right)\chi_m=s_i^m(\mathbf{z},\mathbf{w})\chi_m(\mathbf{z},\mathbf{w}),$$

$$\kappa\frac{\partial\chi_m}{\partial w_k}(\mathbf{z},\mathbf{w})=\left(\sum_{l=1;l\neq k}^{m}\frac{\langle\alpha_k,\alpha_l\rangle}{w_k-w_l}-\sum_{j=1}^{N}\frac{\langle\alpha_k,\lambda_j\rangle}{w_k-z_j}\right)\chi_m=-f_k^m(\mathbf{z},\mathbf{w})\chi_m(\mathbf{z},\mathbf{w})$$

for all $i=1,\ldots,N$ and $k=1,\ldots,m$. The particular form of the denominator of (45) allows us to change the derivative of ψ_m with respect to z_i into a sum of derivatives with respect to w_k:

$$\frac{\partial \psi_m}{\partial z_i}(\mathbf{z},\mathbf{w}) = -\sum_{k=1}^{m} \frac{\partial}{\partial w_k} \overline{\psi}_m^{ik}(\mathbf{z},\mathbf{w}), \quad \forall i = 1,\ldots,N,$$

where $\overline{\psi}_m^{ik}$ is also a vector of $\mathcal{V}_\mu$.

Using the last three relations we can formally compute

$$\left(\frac{\partial}{\partial z_i} - \frac{1}{\kappa}\mathcal{H}_i\right)\Phi = \int_\gamma \chi_m(\mathbf{z},\mathbf{w})\left\{\mathcal{H}_i(\mathbf{z})\psi_m(\mathbf{z},\mathbf{w}) - s_i^m(\mathbf{z},\mathbf{w})\psi_m(\mathbf{z},\mathbf{w}) + \sum_{k=1}^{m} f_k^m(\mathbf{z},\mathbf{w})\overline{\psi}_m^{ik}(\mathbf{z},\mathbf{w})\right\} \mathrm{d}\mathbf{w}. \tag{46}$$

To obtain this formula we have supposed that the derivatives $\partial/\partial z_i$ commute with the integral and that it is possible to choose a basis of contours γ such that integrals along them of total derivatives vanish.

It is clear from (46) that the generalized Bethe ansatz and the KZ equations are closely related. If we suppose that we know how to calculate the action of a Hamiltonian $\mathcal{H}_i$ on the vector valued function $\psi_m(\mathbf{z},\mathbf{w})$ given by (45) and if

$$\mathcal{H}_i(\mathbf{z})\psi_m(\mathbf{z},\mathbf{w}) = s_i^m(\mathbf{z},\mathbf{w})\psi_m(\mathbf{z},\mathbf{w}) - \sum_{k=1}^{m} f_k^m(\mathbf{z},\mathbf{w})\overline{\psi}_m^{ik}(\mathbf{z},\mathbf{w}),$$

then the function (44) is a solution of the KZ equation. In particular, this relation holds if all the coefficients $f_k^m(\mathbf{z},\mathbf{w})$ vanish for some $\overline{\mathbf{w}}(\mathbf{z})$ and if $\psi_m(\mathbf{z},\overline{\mathbf{w}}(\mathbf{z}))$ is an eigenvector of $\mathcal{H}_i$ with eigenvalue $s_i^m(\mathbf{z},\overline{\mathbf{w}}(\mathbf{z}))$. In the case of the Lie algebra SL(2), all these suppositions are fulfilled since the vector valued function (45) reduces to the Bethe vector (12) and the action of a Hamiltonian $\mathcal{H}_i$ on it is given by (14).

Conversely, it was proved[17] that (44) is a solution of the KZ equation. It follows from (46) that the integrand is a total derivative with respect to $\mathbf{w}$, but we can not conclude that it vanishes.

A. Additional solutions of KZ equation

All the integral solutions (44) proposed by Varchenko and Schechtman are singular vectors in the tensor product representation Ω. Moreover, in the case of the Lie algebra SL(2), it was proved [17] that, under certain conditions, the family of integral solutions is complete in $\mathrm{Sing}\mathcal{V}_\lambda$. However, other solutions which are not singular vectors may exist.

In this article we have introduced additional eigenvectors ψ_m^0 and $\psi_{\alpha_1,\ldots\alpha_m}^0$. These vectors are not singular. They lead to solutions of the KZ equations which do not have an integral form and which are not singular vectors.

In the case of the Lie algebra SL(2), each vector ψ_m^0 introduces one vector valued function:

$$\Phi_m^0(z_1,\ldots,z_N) = \chi^0(z_1,\ldots,z_N)\psi_m^0,$$

where

$$\chi^0(z_1,\ldots,z_N) = \prod_{1\leqslant j} \prod_{<k\leqslant N} (z_j - z_k)^{\langle \lambda_j,\lambda_k\rangle/\kappa},$$

for which we can verify directly that it is a solution of KZ equations, observing that

$$\kappa\frac{\partial}{\partial z_i}\chi^0 = \left(\sum_{j=1,j\neq i}^{N} \frac{\langle \lambda_i,\lambda_j\rangle}{z_i - z_j}\right)\chi^0 = s_i^0\chi^0.$$

In the case of an arbitrary Lie algebra G, with the same function $\chi^0(z_1,\ldots,z_N)$, for any vector $\psi_{\alpha_1,\ldots\alpha_m}^0$ we can construct in an analogous way solutions of KZ equations:

$$\Phi^0_{\alpha_1,\ldots\alpha_m}(z_1,\ldots,z_N)=\chi^0(z_1,\ldots,z_N)\psi^0_{\alpha_1,\ldots\alpha_m}.$$

VI. CONCLUSIONS

In this article, we recall the construction of the common eigenvectors of generalized Gaudin Hamiltonians based on generalized Bethe ansatz. This constructive method does not ensure the completeness of the system of eigenvectors. In each eigenspace of the spin operator we have constructed common eigenvectors, corresponding to the same eigenvalue as the vacuum vector and which can not be obtained by the Bethe ansatz.

The Bethe vectors are eigenvectors of the family of Hamiltonians only if the Bethe equations are satisfied and in this case they are also singular vectors in the tensor product representation. The additional eigenvectors proposed here are not singular.

We recall also the connection between Bethe vectors and integral solutions of the KZ equations. In an analogous way, the additional vectors lead to solutions of KZ equations which do not have integral representations. Moreover, these solutions are not singular vectors.

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$\mathcal{W}_\infty$-algebras in n complex dimensions and Kodaira–Spencer deformations: A symplectic approach

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It is shown that the notion of $\mathcal{W}_\infty$-algebra originally carried out over a (compact) Riemann surface can be extended to n complex dimensional (compact) manifolds within a symplectic geometrical setup. The relationships with the Kodaira–Spencer deformation theory of complex structures are discussed. Subsequently, some field theoretical aspects at the classical level are briefly underlined. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1513653]

I. INTRODUCTION

It is fair to say that the concept of dimensionality plays an important role in Physics. In particular, the developments in quantum field theory as well as in statistical mechanics have greatly enlarged its importance. In renormalization theory, string field models, the concept of dimension is found to be not only a characterization of the background space where the physical phenomena are supposed to take place, but also a physical regularizing parameter. Indeed, a world with a given dimension very often shows merits and faults not found in some others of different dimensions. This led to the search for hyperspaces which could gather together the praises and avoid the imperfections of the theoretical models.

For instance, two-dimensional models show the great relevance of complex structures[1] in quantum field theory. Moreover, this approach produces a dimensional halving, but, in spite of the low dimensionality, the conformal models are described by means of an infinite dimensional algebra.[2]

So, the wide class of these ''new'' symmetries has been supporting the conjecture that life in two dimensions could be easier and more convenient.[3] The so-called $\mathcal{W}$-algebras[4] were a byproduct of this feasibility in two-dimensional spaces. For an extensive review on the various possibilities offered by these kinds of symmetries we refer to Ref. 5. Thus the question of extending this type of symmetries to higher dimensional spaces comes naturally. The extension required the use of the Kodaira–Spencer deformation theory.[6] In particular, chiral symmetries have already been extended from 2D conformal models built on a Riemann surface to models to an n complex dimensional complex manifold.[7–9] Note that Kodaira–Spencer-type deformation theories have already been used to describe $\mathcal{W}_\infty$ in two (or more) dimensions[10–12] in order to study holomorphic properties (chiral splitting) or mirror manifolds of arbitrary complex dimension.[7,8,13–16]. Their cohomologies have been investigated both in Lagrangian field theory models[9] and in more general mathematical aspects in Refs. 17 and 18.

Therefore we shall address in the present paper the extension to n complex dimensions of our

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BRS treatment for $\mathcal{W}_\infty$-algebra grounded on a symplectic approach.[19–21] In the latter, the algebra emerges from a ghost realization geometrically constructed from the symplectic approach and as a byproduct the infinite number of chiral ghost fields $\mathcal{C}^{(n)}$, $n=1,2,\ldots$, turn out to be $(-n,0)$-conformal fields and their infinitesimal variations have a well-defined geometrical setting. To be more specific, let us remind how the chiral $\mathcal{W}_\infty$-algebra is recovered in the bidimensional case over a Riemann surface. For any positive integer n, the local variations of the chiral ghosts are

$$\mathcal{S}\mathcal{C}^{(n)}(z,\overline{z})=\sum_{m=1}^{n} m\mathcal{C}^{(m)}(z,\overline{z})\partial_z\mathcal{C}^{(n-m+1)}(z,\overline{z}). \tag{1.1}$$

Introducing by duality to each ghost a local operator $T_{(n)}(z,\overline{z})$ in order to construct the anticommuting functional BRS operator,[22]

$$\delta=\sum_{n\geqslant 1}\int_\Sigma \mathrm{d}\overline{z}\wedge\mathrm{d}z\left(\mathcal{C}^{(n)}(z,\overline{z})T_{(n)}(z,\overline{z})+\mathcal{S}\mathcal{C}^{(n)}(z,\overline{z})\frac{\delta}{\delta\mathcal{C}^{(n)}(z,\overline{z})}\right), \tag{1.2}$$

namely, $\{\delta,\delta\}=0$, leads to the following local commutation relations:

$$\begin{aligned}[T_{(n)}(z,\overline{z}),T_{(m)}(z',\overline{z}')]=&\,n\partial_{z'}\delta^{(2)}(z'-z)T_{(n+m-1)}(z,\overline{z})\\&-m\partial_z\delta^{(2)}(z-z')T_{(n+m-1)}(z',\overline{z}'),\end{aligned} \tag{1.3}$$

which turn out to be a realization of the so-called W_∞-algebra if one goes to the Fourier modes.

We stress that the well-defined ghost realization allows one to write down the extension of the $\mathcal{W}_\infty$-algebra to higher dimensions. Moreover we want to take advantage of the symplectic description for incompressible flows in order to extend to n dimensions the notion of $\mathcal{W}_\infty$-algebra, which in two dimensions is related to area preserving diffeomorphisms, see for instance Ref. 23, and references therein.

The algebra will be described in our approach by means of the Kodaira–Spencer deformation theory of complex structures but reformulated in a symplectic framework. The physical motivation of investigating the subject is connected to the so-called W-gravity and also on the fact that quantizing a conformal gravitational theory would incorporate all the possible configurations of the gravitational fields. By the way, ''well-defined'' gravitational conformal models are fully described by means of the complex structure of the surrounding space. Therefore a complete description just at the classical level of all its possible deformations might be relevant for a successful quantum improvement.

The paper is organized as follows. We shall first briefly introduce, in a nontechnical way, the Kodaira–Spencer deformations, referring the reader to the book by Kodaira[6] for a more complete survey, especially Chaps. 2, 4, and 5. Then Sec. III will give a geometrical setting of symplectomorphisms in a generic n complex dimensional space in order to introduce the BRS formulation of the (infinitesimal) diffeomorphisms of a symplectic space. Furthermore in Sec. IV the specific Kodaira–Spencer deformation of complex structures related to $\mathcal{W}_\infty$-algebra will be presented through a symplectic approach by using a ghost representation. It is recalled that the symplectic treatment of the two-dimensional case for $\mathcal{W}$-algebras[19] provides a well-defined geometrical definition of the ghost fields and their BRS variations as well. In the present paper we avail ourselves of that symplectic approach, in order to address the problem of extending to arbitrary complex dimensions the notion of $\mathcal{W}_\infty$-algebra and its consequences, in particular, for the study of Lagrangians subject to that type of symmetry to which a very brief section will be devoted.

II. A BRIEF ACCOUNT ON THE KODAIRA–SPENCER DEFORMATION

Let M be an n dimensional (compact) complex manifold described in terms of background local complex coordinates:

$$(z^k) := (z^1, z^2, \ldots, z^n), \quad k = 1, \ldots, n \tag{2.1}$$

and the subordinated differentiable structure $(z^k, \overline{z^k})$ turns M into a $2n$ real dimensional manifold.

Its complex structure is determined by the $\overline{\partial} \equiv \Sigma_{i=1}^{n} d\overline{z^i} \overline{\partial_i}$ operator. In order to control the deformation, usually a complex deformation parameter $t = (t_1, \ldots, t_n)$ is introduced. Basically the physical implications of this mathematical field of interest, rises from the primitive idea that a complex manifold is composed of a set of coordinate neighborhoods patched together. Obviously the patching procedure sewing should be irrelevant to the manifold description. In this philosophy a deformation of M is considered to be the sewing of the same patches, through a fit of the parameters t via various identifications. For our purpose the dimension of the parameter space will be exactly equal to that of M. According to Chap. 5 of Ref. 6 one considers a complex family of compact complex manifolds such as a complex manifold $\mathcal{M}$ and a holomorphic map $\varpi: \mathcal{M} \to \mathcal{B}$ where $\mathcal{B}$ is a domain in $\mathbb{C}^n$ such that $\varpi^{-1}(t) = M_t$ is a compact complex manifold. For $\Delta \subset \mathcal{B}$ sufficiently small, $\mathcal{M}_\Delta := \varpi^{-1}(\Delta)$ can be identified as a complex manifold with the complex structure defined on the smooth manifold $M \times \Delta$ since the subordinated smooth structure is always the same and does not depend on t (Ref. 6 Theorem 2.3). Accordingly, local complex coordinates on $\mathcal{M}_\Delta$ will be given by the system of local complex coordinates $(\mathcal{Z}^\alpha((z,\overline{z}),t), t^\alpha)$, $\alpha = 1, \ldots, n$ and for fixed t, M_t is the complex structure of the differentiable manifold M defined by the system of local complex coordinates $(\mathcal{Z}^\alpha((z,\overline{z}),t))$, $\alpha = 1, \ldots, n$ considered as a smooth change of local complex coordinates on M, i.e., the Jacobian does not vanish.

On the other hand, the deformation of complex structure is thus described by the change of the $\overline{\partial}$-operator,[6]

$$\overline{\partial} \to \overline{\partial} - \sum_{\ell=1}^{n} \mu^\ell((z,\overline{z}),t)\partial_\ell, \tag{2.2}$$

the $\mu^\ell((z,\overline{z}),t)$ are unique smooth (0,1)-forms on $M \times \Delta$. In this way, one can describe both infinitesimal and finite deformations. Indeed, by looking for, at fixed t, the local solutions $\mathcal{Z}^\alpha((z,\overline{z}),t)$ of this family of deformed $\overline{\partial}$-operators

$$\left(\overline{\partial} - \sum_{\ell=1}^{n} \mu^\ell((z,\overline{z}),t)\partial_\ell\right)\mathcal{Z}^\alpha((z,\overline{z}),t) = 0, \tag{2.3}$$

then they will patch together holomorphically with respect to the complex structure M_t and thus they will define a new complex structure parametrized by the μ on M.

To be consistent with the deformation philosophy discussed before, the previous equation (2.3) must be coupled (Newlander–Nirenberg integrability theorem)[6] with the Kodaira–Spencer (integrability) equation,

$$\overline{\partial}\mu((z,\overline{z}),t) - \tfrac{1}{2}[\mu((z,\overline{z}),t), \mu((z,\overline{z}),t)] = 0, \tag{2.4}$$

where $\mu((z,\overline{z}),t) = \mu^\ell((z,\overline{z}),t)\partial_\ell$, is a smooth (1,0)-vector field valued (0,1)-form on M and the graded brackets $[,]$ means the commutator of two vector fields and wedging.

To sum up, two solutions of Eq. (2.4) correspond to the same complex structure if they differ by an holomorphic diffeomorphism. Since for $t = 0$ both (z^k) and $(\mathcal{Z}^\alpha(z,0))$ are local complex coordinates on the complex manifold M, then $\mathcal{Z}^\alpha(z,0)$ are holomorphic functions of (z^k), showing that $\mu(z,0) = 0$. The construction of the new local complex coordinates $\mathcal{Z}^\alpha((z,\overline{z}),t)$ for each fixed t will correspond to a smooth change of local complex coordinates $(z^k) \mapsto (\mathcal{Z}^\alpha((z,\overline{z}),t))$. The construction holds in each holomorphic sector in t. Embedding in a symplectic framework generates an infinite sequence of changes of local complex coordinates. It is the signature of their behavior under symplectomorphisms which gives rise to an algebra. The latter extends to higher dimensions the usual $\mathcal{W}_\infty$-algebra (1.3).

For this reason, if we now wish to settle the Kodaira–Spencer deformation in a symplectic framework, we may consider the deformation parameters as the conjugate variables (by symplectic doubling, as it will be better specified later on) to those of the configuration space by identifying locally, as differentiable manifolds, the cotangent space T^*M with $\mathcal{M}_\Delta$ endowed with local smooth coordinates $(z^k,\overline{z^k},t,\overline{t})$. Then all the requirements to perform a Kodaira–Spencer deformation will be satisfied, so that this mathematical artillery will be at our disposal to investigate the possible extension of our symplectic approach to an n complex dimensional manifold and the consequences for physical models, in particular higher spin fields and their sources.

III. SYMPLECTOMORPHISMS IN 2*n* COMPLEX DIMENSIONAL COMPLEX SYMPLECTIC SPACE

Symplectomorphisms describe diffeomorphisms preserving a given symplectic structure on the cotangent bundle T^*M. They can be, respectively, described in terms of local coordinates, namely,

$$\begin{aligned}\mathcal{U}(z,y)&=(z^1\cdots z^n,\overline{z^1}\cdots\overline{z^n};y_1\cdots y_n,\overline{y_1}\cdots\overline{y_n}),\\ \mathcal{U}(Z,\mathcal{Y})&=(Z^1\cdots Z^n,\overline{Z^1}\cdots\overline{Z^n};\mathcal{Y}_1\cdots\mathcal{Y}_n,\overline{\mathcal{Y}_1}\cdots\overline{\mathcal{Y}_n})\end{aligned}\tag{3.1}$$

and, respectively, endowed with the symplectic fundamental two-form which, in full generality, locally writes according to the system of local coordinates—not necessarily Darboux's ones,

$$\Omega_{\mathcal{U}(z,y)}=\sum_{i,j=1}^{n}\omega^i_j\mathrm{d}z^j\wedge\mathrm{d}y_i+\mathrm{c.c.}=\mathrm{d}\theta_{\mathcal{U}(z,y)},\tag{3.2}$$

$$\Omega_{\mathcal{U}(Z,\mathcal{Y})}=\sum_{\alpha,\beta=1}^{n}\omega^\alpha_\beta\,\mathrm{d}Z^\beta\wedge d\mathcal{Y}_\alpha+\mathrm{c.c.}=\mathrm{d}\theta_{\mathcal{U}(Z,\mathcal{Y})}\tag{3.3}$$

with the following local requirements:

$$\det|\omega_{(i,j)}|\neq 0,\quad \det|\omega_{(\beta,\alpha)}|\neq 0,\quad d_z\omega^i_j=d_y\omega^i_j=d_Z\omega^\alpha_\beta=d_{\mathcal{Y}}\omega^\alpha_\beta=0.\tag{3.4}$$

and the invariance of the fundamental two-form is locally expressed by

$$\Omega_{\mathcal{U}(z,y)}=\Omega_{\mathcal{U}(Z,\mathcal{Y})}.\tag{3.5}$$

Locally, this implies on $\mathcal{U}(z,y)\cap\mathcal{U}(Z,\mathcal{Y})\neq\varnothing$ that

$$\theta_{\mathcal{U}(z,y)}-\theta_{\mathcal{U}(Z,\mathcal{Y})}=\mathrm{d}F.\tag{3.6}$$

From now on, we shall work locally in terms of the ''mixed'' local independent coordinates $(z,\mathcal{Y})$,

$$\mathcal{U}(z,\mathcal{Y})=(z^1\cdots z^n,\overline{z^1}\cdots\overline{z^n};\mathcal{Y}_1\cdots\mathcal{Y}_n,\overline{\mathcal{Y}_1}\cdots\overline{\mathcal{Y}_n}),\tag{3.7}$$

where we define the differential operators (from now on the Einstein's convention for summation will be used throughout the paper):

$$d=d_z+\mathrm{d}_{\mathcal{Y}},\quad d_z=\mathrm{d}z^i\frac{\partial}{\partial z^i}+\mathrm{d}\overline{z^i}\frac{\partial}{\partial\overline{z^i}}=\mathrm{d}z^i\partial_i+\mathrm{d}\overline{z^i}\bar{\partial}_i,\quad d_{\mathcal{Y}}=\mathrm{d}\mathcal{Y}_\alpha\frac{\partial}{\partial\mathcal{Y}_\alpha}+\mathrm{d}\overline{\mathcal{Y}_\alpha}\frac{\partial}{\partial\overline{\mathcal{Y}_\alpha}}.\tag{3.8}$$

The corresponding generating function $\Phi(z,\mathcal{Y})$ is obtained through the Legendre transformation

$$d\Phi(z\mathcal{Y}) = d(F + \omega^{\alpha}_{\beta} Z^{\beta}\mathcal{Y}_{\alpha} + \text{c.c.}) = \omega^{i}_{j} y_{i} dz^{j} + \omega^{\alpha}_{\beta} Z^{\beta} d\mathcal{Y}_{\alpha} + \text{c.c.}. \tag{3.9}$$

In the cotangent space T^*M endowed with this system of local coordinates, the mappings:

$$\mathbf{y}_i(z,\mathcal{Y}) \equiv \omega^{j}_{i} y_j = \frac{\partial \Phi(z,\mathcal{Y})}{\partial z^{i}} \equiv \partial_i \Phi(z,\mathcal{Y}), \tag{3.10}$$

$$\mathcal{Z}^{\alpha}(z,\mathcal{Y}) \equiv \omega^{\alpha}_{\beta} Z^{\beta} = \frac{\partial \Phi(z,\mathcal{Y})}{\partial \mathcal{Y}_{\alpha}} \tag{3.11}$$

are canonical and define new canonical variables via the ω matrices.

Several ways can settle this canonical procedure: Poisson brackets (or something similar), flow analysis of hierarchical structures. We shall be concerned with the study of this aspect in a field theoretical language by using the BRS formulation. Moreover we can rewrite:

$$\begin{aligned}\Omega_{\mathcal{U}(z,\mathcal{Y})} &= \partial_i \mathcal{Z}^{\alpha}(z,\mathcal{Y}) dz^{i} \wedge d\mathcal{Y}_{\alpha} + \overline{\partial_i} \mathcal{Z}^{\alpha}(z,\mathcal{Y}) d\overline{z^{i}} \wedge d\mathcal{Y}_{\alpha} + \partial_i \overline{\mathcal{Z}^{\alpha}}(z,\mathcal{Y}) dz^{i} \wedge d\overline{\mathcal{Y}_{\alpha}} + \overline{\partial_i}\,\overline{\mathcal{Z}^{\alpha}}(z,\mathcal{Y}) d\overline{Z^{\alpha}} \wedge d\overline{\mathcal{Y}_{\alpha}} \\ &= \frac{\partial}{\partial \mathcal{Y}_{\alpha}} \mathbf{y}_i(z,\mathcal{Y}) dz^{i} \wedge d\mathcal{Y}_{\alpha} + \frac{\partial}{\partial \mathcal{Y}_{\alpha}} \overline{\mathbf{y}_i}(z,\mathcal{Y}) d\overline{z^{i}} \wedge d\mathcal{Y}_{\alpha} + \frac{\partial}{\partial \overline{\mathcal{Y}_{\alpha}}} \mathbf{y}_i(z,\mathcal{Y}) dz^{i} \wedge d\overline{\mathcal{Y}_{\alpha}} \\ &\quad + \frac{\partial}{\partial \overline{\mathcal{Y}_{\alpha}}} \overline{\mathbf{y}_i}(z,\mathcal{Y}) d\overline{z^{i}} \wedge d\overline{\mathcal{Y}_{\alpha}} = d_z d_{\mathcal{Y}} \Phi(z,\mathcal{Y})\end{aligned} \tag{3.12}$$

from which we get the relations of duality (with their complex conjugate expressions as well):

$$\partial_i \mathcal{Z}^{\alpha}(z,\mathcal{Y}) = \frac{\partial}{\partial \mathcal{Y}_{\alpha}} \mathbf{y}_i(z,\mathcal{Y}), \quad \overline{\partial_i} \mathcal{Z}^{\alpha}(z,\mathcal{Y}) = \frac{\partial}{\partial \mathcal{Y}_{\alpha}} \overline{\mathbf{y}_i}(z,\mathcal{Y}). \tag{3.13}$$

In order to parametrize our space we define[19–21] the Hessian matrix elements by

$$\partial_i \frac{\partial}{\partial \mathcal{Y}_{\alpha}} \Phi(z,\mathcal{Y}) \equiv \lambda^{\alpha}_{i}(z,\mathcal{Y}), \tag{3.14}$$

$$\overline{\partial_j} \frac{\partial}{\partial \mathcal{Y}_{\alpha}} \Phi(z,\mathcal{Y}) \equiv \lambda^{\alpha}_{i}(z,\mathcal{Y}) \mu^{i}_{j}(z,\mathcal{Y}) \equiv \overline{\lambda^{\beta}_{j}}(z,\mathcal{Y}) \overline{\mu^{\alpha}_{\beta}}(z,\mathcal{Y}) \tag{3.15}$$

with $\det|\lambda| \neq 0$ for nonsingularity requirement and also for the complex conjugate expressions. From Eqs. (3.14) and (3.15) we get the following identities:

$$\partial_j \lambda^{\alpha}_{i}(z,\mathcal{Y}) = \partial_i \lambda^{\alpha}_{j}(z,\mathcal{Y}), \quad \frac{\partial}{\partial \mathcal{Y}_{\beta}} \lambda^{\alpha}_{i}(z,\mathcal{Y}) = \frac{\partial}{\partial \mathcal{Y}_{\alpha}} \lambda^{\beta}_{i}(z,\mathcal{Y}), \tag{3.16}$$

$$\overline{\partial_j} \lambda^{\alpha}_{i}(z,\mathcal{Y}) = \partial_i(\lambda^{\alpha}_{r}(z,\mathcal{Y}) \mu^{r}_{j}(z,\mathcal{Y})), \quad \frac{\partial}{\partial \overline{\mathcal{Y}_{\beta}}} \lambda^{\alpha}_{i}(z,\mathcal{Y}) = \frac{\partial}{\partial \mathcal{Y}_{\alpha}}(\overline{\lambda^{\beta}_{r}}(z,\mathcal{Y}) \overline{\mu^{r}_{i}}(z,\mathcal{Y})), \tag{3.17}$$

$$\overline{\partial_j} \lambda^{\alpha}_{i}(z,\mathcal{Y}) = \partial_i(\overline{\lambda^{\alpha}_{j}}(z,\mathcal{Y}) \overline{\mu^{\alpha}_{\alpha}}(z,\mathcal{Y})), \quad \frac{\partial}{\partial \overline{\mathcal{Y}_{\beta}}} \lambda^{\alpha}_{i}(z,\mathcal{Y}) = \frac{\partial}{\partial \mathcal{Y}_{\alpha}}(\lambda^{\sigma}_{i}(z,\mathcal{Y}) \mu^{\beta}_{\sigma}(z,\mathcal{Y})). \tag{3.18}$$

So from Eqs. (3.13) to (3.15) we have the following two main identities which must be viewed within the Kodaira–Spencer spirit of Eq. (2.3):

$$(\overline{\partial_j} - \mu_j^r(z,\mathcal{Y})\partial_r)\mathcal{Z}^\alpha(z,\mathcal{Y}) \equiv \mathcal{L}_j(z,\mathcal{Y})\mathcal{Z}^\alpha(z,\mathcal{Y}) = 0, \tag{3.19}$$

$$\left(\frac{\partial}{\partial\overline{\mathcal{Y}_\alpha}} - \mu_\beta^{\overline{\alpha}}(z,\mathcal{Y})\frac{\partial}{\partial\mathcal{Y}_\beta}\right)\mathbf{y}_r(z,\mathcal{Y}) \equiv \mathcal{L}^{\overline{\alpha}}(z,\mathcal{Y})\mathbf{y}_r(z,\mathcal{Y}) = 0, \tag{3.20}$$

where the role of the parameter t of deformation is presently played by the covariant coordinates $(\mathcal{Y},\overline{\mathcal{Y}})$ in the former or by the background complex coordinates $(z,\overline{z})$ in the latter. The first of the two equations tells us that a local deformation of the complex structure on the base complex manifold M can be implemented by using the symplectic structure on the cotangent bundle T^*M, while the second one governs the vertical deformation. This coincidence justifies our point of view of taking the conjugate variables as the deformation parameter. Hence, the complex family of complex manifolds $M_{\mathcal{Y}}$ is locally recasted as the symplectic cotangent bundle TM when the differentiable structure is considered.

Let us write down the following Pfaff system:

$$\begin{aligned} d_z\mathcal{Z}^\alpha(z,\mathcal{Y}) &= \lambda_i^\alpha(z,\mathcal{Y})(dz^i + \mu_j^i(z,\mathcal{Y})d\overline{z^j}) =: (dz + d\overline{z}\cdot\mu(z,\mathcal{Y}))\cdot\lambda(z,\mathcal{Y}), \\ d_{\mathcal{Y}}\mathbf{y}_i(z,\mathcal{Y}) &= \lambda_i^\alpha(z,\mathcal{Y})(d\mathcal{Y}_\alpha + \mu_\alpha^{\overline{\alpha}}(z,\mathcal{Y})d\overline{\mathcal{Y}_\alpha}). \end{aligned} \tag{3.21}$$

The system serves to define two types of Kodaira–Spencer differentials, namely, $\mu_j^i(z,\mathcal{Y})$ and $\mu_\beta^\alpha(z,\mathcal{Y})$ which parametrize the complex structures on the base space M with background local complex coordinates $(z,\overline{z})$ and the fibers with local coordinates $(\mathcal{Y},\overline{\mathcal{Y}})$, respectively. These complex structures are interlinked by the duality relations Eqs. (3.13)–(3.15)

$$\mu_j^i(z,\mathcal{Y}) = \overline{\partial_j}\mathcal{Z}^\beta(z,\mathcal{Y})[\lambda(z,\mathcal{Y})^{-1}]_\beta^i, \tag{3.22}$$

$$\mu_\beta^{\overline{\alpha}}(z,\mathcal{Y}) = [\overline{\lambda}(z,\mathcal{Y})^{-1}]_\beta^r\partial_r\overline{\mathcal{Z}^\alpha}(z,\mathcal{Y}). \tag{3.23}$$

Inverting the previous formulas (3.21) by matrix inversion

$$\partial_i = \lambda_i^\alpha(z,\mathcal{Y})\partial_\alpha + \overline{\mu_i^j}(z,\mathcal{Y})\overline{\lambda_j^\alpha}(z,\mathcal{Y})\partial_{\overline{\alpha}} = \lambda_i^\alpha(z,\mathcal{Y})(\partial_\alpha + \mu_\alpha^{\overline{\alpha}}(z,\mathcal{Y})\partial_{\overline{\alpha}}), \tag{3.24}$$

where

$$\partial_\alpha = \frac{\partial}{\partial\mathcal{Z}^\alpha(z,\mathcal{Y})},$$

one gets

$$\frac{\partial}{\partial\mathcal{Y}_\alpha} = \lambda_i^\alpha(z,\mathcal{Y})\left(\frac{\partial}{\partial\mathbf{y}_i} + \mu_j^i(z,\mathcal{Y})\frac{\partial}{\partial\overline{\mathbf{y}_j}}\right) \equiv \lambda_i^\alpha(z,\mathcal{Y})\mathcal{D}^i(z,\mathcal{Y}). \tag{3.25}$$

It is now easy to derive from Eqs. (3.15) to (3.25) another description of the Kodaira–Spencer differentials

$$\mu_j^i(z,\mathcal{Y}) = \mathcal{D}^i\partial_{\overline{j}}\Phi(z,\mathcal{Y}), \tag{3.26}$$

where $\mathcal{Y}=\mathcal{Y}(z,y)$ has to be taken into account. The most relevant properties of the $\mathcal{D}^i(z,\mathcal{Y})$ and $\partial/\partial\mathbf{y}_i$ operators can be summarized as

$$[\mathcal{D}^i(z,\mathcal{Y}),\mathcal{D}^j(z,\mathcal{Y})]=0, \quad \left[\frac{\partial}{\partial \mathbf{y}_i},\frac{\partial}{\partial \mathbf{y}_j}\right]=0, \quad \left[\frac{\partial}{\partial \mathbf{y}_i},\frac{\partial}{\partial \overline{\mathbf{y}}_i}\right]=0. \tag{3.27}$$

The third-order derivatives of Φ yield the integrability conditions (2.4) for the deformation of complex structures in the $(z,\overline{z})$ and $(\mathcal{Y},\overline{\mathcal{Y}})$ spaces, written respectively, as

$$\mathcal{L}_{\overline{i}}(z,\mathcal{Y})\mu^s_{\overline{j}}(z,\mathcal{Y})=\mathcal{L}_{\overline{j}}(z,\mathcal{Y})\mu^s_{\overline{i}}(z,\mathcal{Y}), \tag{3.28}$$

$$\lambda^\beta_i(z,\mathcal{Y})\partial_j\mu^{\overline{\alpha}}_{\overline{\beta}}(z,\mathcal{Y})=\lambda^\beta_j(z,\mathcal{Y})\partial_i\mu^{\overline{\alpha}}_{\overline{\beta}}(z,\mathcal{Y}). \tag{3.29}$$

Moreover in the $(\mathcal{Y},\overline{\mathcal{Y}})$ space, the partner of the Kodaira–Spencer equations can be immediately recovered computing $\partial_j(\partial/\partial\overline{\mathcal{Y}}_{\overline{\alpha}})(\partial/\partial\overline{\mathcal{Y}}_{\overline{\beta}})\Phi(z,\mathcal{Y})$,

$$\mathcal{L}^{\overline{\alpha}}(z,\mathcal{Y})\mu^{\overline{\beta}}_{\overline{\lambda}}(z,\mathcal{Y})=\mathcal{L}^{\overline{\beta}}(z,\mathcal{Y})\mu^{\overline{\alpha}}_{\overline{\lambda}}(z,\mathcal{Y}) \tag{3.30}$$

with the consistency conditions:

$$[\mathcal{L}_{\overline{i}}(z,\mathcal{Y}),\mathcal{L}_{\overline{j}}(z,\mathcal{Y})]=0, \quad [\mathcal{L}^{\overline{\alpha}}(z,\mathcal{Y}),\mathcal{L}^{\overline{\beta}}(z,\mathcal{Y})]=0. \tag{3.31}$$

BRS setting of symplectomorphisms in $2n$ *complex dimensions*. As said before the Kodaira–Spencer deformations reparametrize in a consistent way the space of complex structures. Furthermore, we shall study the action of reparametrizations on symplectic space (symplectomorphisms).

The BRS setting for symplectomorphisms can be performed along the lines developed in Ref. 19. Let us define by $\mathcal{S}$ the nilpotent BRS operation associated with the infinitesimal symplectomorphisms. Locally, $\mathcal{S}$ will be represented in $(z,\mathcal{Y})$ coordinates by

$$\mathcal{S}\Phi(z,\mathcal{Y})=\Lambda(z,\mathcal{Y}), \quad \mathcal{S}\Lambda(z,\mathcal{Y})=0. \tag{3.32}$$

The infinitesimal BRS transformation of the deformed coordinate $\mathcal{Z}^\alpha(z,\overline{z})$ can be calculated from its canonical definition Eqs. (3.10) and (3.11),

$$\mathcal{S}\mathcal{Z}^\alpha(z,\mathcal{Y})=\frac{\partial}{\partial\mathcal{Y}_\alpha}\Lambda(z,\mathcal{Y})=\lambda^\alpha_i(z,\mathcal{Y})\mathcal{D}^i(z,\mathcal{Y})\Lambda(z,\mathcal{Y})=\mathcal{C}^i(z,\mathcal{Y})\partial_i\mathcal{Z}^\alpha(z,\mathcal{Y}), \tag{3.33}$$

where the chiral ghost fields $\mathcal{C}^i(z,\mathcal{Y})$ naturally emerge and are related to the ordinary diffeomorphism ghosts $c^i(z,\mathcal{Y})$, $\overline{c^j}(z,\mathcal{Y})$ on T^*M within this symplectic framework by

$$\mathcal{C}^i(z,\mathcal{Y})\equiv\mathcal{D}^i\Lambda(z,\mathcal{Y})=\left(\frac{\partial\Lambda(z,\mathcal{Y})}{\partial\mathbf{y}_i}+\mu^{\overline{i}}_{\overline{j}}(z,\mathcal{Y})\frac{\partial\Lambda(z,\mathcal{Y})}{\partial\overline{\mathbf{y}}_j}\right)=c^i(z,\mathcal{Y})+\mu^{\overline{i}}_{\overline{j}}(z,\mathcal{Y})\overline{c^j}(z,\mathcal{Y}), \tag{3.34}$$

which explicitly corresponds to a change of generators for symplectomorphisms. Their BRS variations read

$$\mathcal{S}\mathcal{C}^i(z,\mathcal{Y})=\mathcal{C}^j(z,\mathcal{Y})\partial_j\mathcal{C}^i(z,\mathcal{Y}), \tag{3.35}$$

$$\mathcal{S}c^i(z,\mathcal{Y})=[c^j(z,\mathcal{Y})\partial_j+\overline{c^j}(z,\mathcal{Y})\overline{\partial_j}]c^i(z,\mathcal{Y}). \tag{3.36}$$

These BRS transformations correspond to an infinitesimal reparametrization of $\mathcal{Z}^\alpha(z,\mathcal{Y})$ due to an infinitesimal shift of the $(z,\overline{z})$ background, keeping $(\mathcal{Y},\overline{\mathcal{Y}})$ fixed.

We can easily derive:

$$\mathcal{S}\lambda^\alpha_i(z,\mathcal{Y})=\partial_i(\lambda^\alpha_j(z,\mathcal{Y})\mathcal{C}^j(z,\mathcal{Y})), \tag{3.37}$$

$$\mathcal{S}(\lambda_r^{\alpha}(z,\mathcal{Y})\mu_j^{r}(z,\mathcal{Y}))=\overline{\partial_j}(\lambda_r^{\alpha}(z,\mathcal{Y})\mathcal{C}^{r}(z,\mathcal{Y})), \tag{3.38}$$

so that

$$\mathcal{S}\mu_j^{i}(z,\mathcal{Y})=\mathcal{C}^{l}(z,\mathcal{Y})\partial_l\mu_j^{i}(z,\mathcal{Y})-\partial_l\mathcal{C}^{i}(z,\mathcal{Y})\mu_j^{l}(z,\mathcal{Y})+\overline{\partial_j}\mathcal{C}^{i}(z,\mathcal{Y}). \tag{3.39}$$

The nonchiral representation of this algebra can be easily given following the lines of Ref. 9, where we have stressed the relevance of the $(z,\overline{z})$ counterpart of the Kodaira–Spencer equation (3.30).

Moreover the ordinary ghosts $c^{i}(z,\mathcal{Y})$ transform as

$$\mathcal{S}c^{i}(z,\mathcal{Y})=(c^{l}(z,\mathcal{Y})\partial_l+\overline{c^{t}}(z,\mathcal{Y})\overline{\partial_l})c^{i}(z,\mathcal{Y}). \tag{3.40}$$

Finally, note the important commutators coming from the combination of the commutators

$$\left[\mathcal{S},\frac{\partial}{\partial\mathcal{Y}_{\alpha}}\right]=0=\left[\partial_i,\frac{\partial}{\partial\mathcal{Y}_{\alpha}}\right]$$

with (3.16) and (3.25):

$$\begin{aligned}[\mathcal{S},\mathcal{D}^{i}(z,\mathcal{Y})]&=-[\lambda(z,\mathcal{Y})^{-1}]_{\alpha}^{i}\partial_i(\lambda_j^{\alpha}(z,\mathcal{Y})\mathcal{C}^{j}(z,\mathcal{Y}))\mathcal{D}^{j}(z,\mathcal{Y})\\&=-\partial_r\mathcal{C}^{i}(z,\mathcal{Y})\mathcal{D}^{r}(z,\mathcal{Y})+\mathcal{C}^{r}(z,\mathcal{Y})[\partial_r,\mathcal{D}^{i}(z,\mathcal{Y})].\end{aligned} \tag{3.41}$$

Conversely, from Eqs. (3.10) and (3.11) we can derive the infinitesimal transformation of $\mathbf{y}_i(z,\mathcal{Y})$ due to an infinitesimal reparametrization on $(\mathcal{Y},\overline{\mathcal{Y}})$ space, keeping the $(z,\overline{z})$ background fixed,

$$\begin{aligned}\mathcal{S}\mathbf{y}_i(z,\mathcal{Y})=\partial_i\Lambda(z,\mathcal{Y})&=\lambda_i^{\alpha}(z,\mathcal{Y})(\partial_{\alpha}+\mu_{\alpha}^{\overline{\alpha}}(z,\mathcal{Y})\partial_{\overline{\alpha}})\Lambda(z,\mathcal{Y})\\&=(\omega_{\alpha}(z,\mathcal{Y})+\mu_{\alpha}^{\overline{\alpha}}(z,\mathcal{Y})\omega_{\overline{\alpha}}(z,\mathcal{Y}))\frac{\partial}{\partial\mathcal{Y}_{\alpha}}\mathbf{y}_i(z,\mathcal{Y})\\&=\mathcal{O}_{\alpha}(z,\mathcal{Y})\frac{\partial}{\partial\mathcal{Y}_{\alpha}}\mathbf{y}_i(z,\mathcal{Y}),\end{aligned} \tag{3.42}$$

where it has been set

$$\omega_{\alpha}(z,\mathcal{Y})=\partial_{\alpha}\Lambda(z,\mathcal{Y}) \tag{3.43}$$

and:

$$\mathcal{S}\mathcal{O}_{\alpha}(z,\mathcal{Y})=\mathcal{O}_{\beta}(z,\mathcal{Y})\frac{\partial}{\partial\mathcal{Y}_{\beta}}\mathcal{O}_{\alpha}(z,\mathcal{Y}). \tag{3.44}$$

Now the generating function $\Phi(z,\mathcal{Y})$ for such canonical transformations will be so chosen in order to view the holomorphic deformation process in the $\mathcal{Y}$ direction as being a canonical transformation.

For this purpose it will be convenient to use a multi-index notation. Let A,B denote multi-indices on the fibers related to Greek indices, while I,J denote multi-indices on M related to Latin indices. For $A=(a_1,\ldots,a_n)$ with positive integers $a_{\alpha}\geqslant 0$, $|A|=\Sigma_{\alpha=1}^{n}a_k$ will be the order of A and one sets $A+1_{\beta}=(a_1,\ldots,a_{\beta-1},a_{\beta}+1,a_{\beta+1},\ldots,a_n)$, $A!=\Pi_{\alpha=1}^{n}a_{\alpha}!$. For the sake of notational completeness, on the base M one will similarly use $I+1_k=(i_1,\ldots,i_{k-1},i_k+1,i_{k+1},\ldots,i_n)$. Now, one *chooses* a $\mathcal{Y}$-holomorphically split generating function

$$\Phi(z,\mathcal{Y})=\sum_{|A|\geqslant 1}\mathcal{Z}^{(A)}(z,\overline{z})\mathcal{Y}_A+\text{c.c.}, \tag{3.45}$$

where for $|A|\geqslant 1$ and $\mathcal{Y}_A:=\Pi_{\alpha=1}^{n}(\mathcal{Y}_\alpha)^{a_\alpha}$, we have set

$$\mathcal{Z}^{(A)}(z,\overline{z}):=\frac{1}{|A|!}\frac{\partial^{|A|}\Phi(z,\mathcal{Y})}{\partial\mathcal{Y}_A}\bigg|_{\mathcal{Y}=0}:=\frac{1}{|A|!}\frac{\partial^{|A|}\Phi(z,\mathcal{Y})}{(\partial\mathcal{Y}_1)^{a_1}\cdots(\partial\mathcal{Y}_n)^{a_n}}\bigg|_{\mathcal{Y}=0} \tag{3.46}$$

for the

$$\frac{(|A|+n-1)!}{|A|!(n-1)!}$$

independent derivatives of order $|A|$. With such a generating function the symplectic two-form (3.12) is locally written as

$$\Omega=\sum_{|A|\geqslant 1}d_z\mathcal{Z}^{(A)}(z,\overline{z})\wedge d_{\mathcal{Y}}\mathcal{Y}_A+\text{c.c.}, \tag{3.47}$$

while the new coordinates defined in (3.10) and (3.11) are, respectively, given by

$$\mathbf{y}_i(z,\mathcal{Y})=\sum_{|A|\geqslant 0}\partial_i\mathcal{Z}^{(A)}(z,\overline{z})\mathcal{Y}_A+\sum_{|B|\geqslant 0}\partial_i\overline{\mathcal{Z}^{(B)}}(z,\overline{z})\overline{\mathcal{Y}_B}, \tag{3.48}$$

$$\begin{aligned}\mathcal{Z}^{\alpha}(z,\mathcal{Y})&=\sum_{|A|\geqslant 0}\sum_{\alpha=1}^{n}(a_\alpha+1)\mathcal{Z}^{(A+1_\alpha)}(z,\overline{z})\mathcal{Y}_A\\&=\mathcal{Z}^{\alpha}(z,\overline{z})+\sum_{|A|\geqslant 1}\sum_{\alpha=1}^{n}(a_\alpha+1)\mathcal{Z}^{(A+1_\alpha)}(z,\overline{z})\mathcal{Y}_A.\end{aligned} \tag{3.49}$$

Note that $\mathcal{Z}^{\alpha}(z,\mathcal{Y})|_{\mathcal{Y}=0}=\mathcal{Z}^{\alpha}(z,\overline{z})$ showing that the complex structure given by the local complex coordinates $\mathcal{Z}^{\alpha}$ is the one which is actually deformed. Recall that the latter are local complex coordinates solutions of (3.19) at $\mathcal{Y}_\alpha=\overline{\mathcal{Y}_{\overline{\alpha}}}=0$ and have already been treated in the context n complex dimensional manifolds in Ref. 9.

As explicitly shown above, the local coefficients $\mathcal{Z}^{(A)}(z,\overline{z})$, $|A|\geqslant 1$ thus describe the response to the deformation of the $\mathcal{Z}^{\alpha}(z,\overline{z})$ complex coordinates. Combining the decomposition (3.47) with the covariance requirement (3.5) leads to an infinite sequence of changes of local complex coordinates $(z^k)\rightarrow(\mathcal{Z}^{(A)}(z,\overline{z}))$ whose algebra of infinitesimal transformations can be derived by means of BRS techniques.

Furthermore, the role of the complex structures involved in the present approach can be deepened. Indeed, the Kodaira–Spencer differentials $\mu^{i}_{\overline{j}}(z,\mathcal{Y})$ reflect the general behavior [see Eq. (3.26)] of the generating function of the canonical transformations. Their infinitesimal behavior in the $(z,\overline{z})$ and $(\mathcal{Y},\overline{\mathcal{Y}})$ spaces are constrained by both Eqs. (3.29) and (3.30). Now the explicit complex deformation will be chosen as a particular case of Ref. 6, according to

$$\mu^{i}_{\overline{j}}(z,\mathcal{Y})=\sum_{|A|\geqslant 0}\mu^{i(A)}_{\overline{j}}(z,\overline{z})\mathcal{Y}_A, \tag{3.50}$$

with

$$\mu^{i(A)}_{\overline{j}}(z,\overline{z})=\frac{1}{|A|!}\frac{\partial^{|A|+1}}{\partial\mathcal{Y}_{A+1_\beta}}(\overline{\partial_j}\Phi(z,\mathcal{Y})[\lambda(z,\mathcal{Y})^{-1}]^{i}_{\beta})\bigg|_{\mathcal{Y}=0}.$$

This series converges in a Holder norm[6] and represents a deformation of the integrable complex structure defined by $\mu_j^{i(0)}$ with the role of deformation parameters played by $\mathcal{Y}$ as already said before. Since the use of this space doubling is to introduce a symplectic structure in order that the smooth local changes of complex coordinates $(z^k)\to(\mathcal{Z}^{(A)}(z,\bar{z}))$ are interpreted as coming from a symplectomorphism symmetry. Recall that the generating function (3.45) for the canonical transformations has been chosen to be compatible with the deformation (3.50). The holomorphic character of the deformations will define, in a BRS framework, a series of infinitesimal symmetry transformations which will reproduce the n complex dimensional extension of the $\mathcal{W}_\infty$-algebra as will be shown in Sec. IV.

The link of the parametrization in Eq. (3.49) with the one of (3.50) is given through (3.15) for $|A|\geqslant 0$ and for each $\alpha=1,\ldots,n$-no summation over α-

$$(a_\alpha+1)\bar{\partial}_j\mathcal{Z}^{(A+1_\alpha)}(z,\bar{z})=\sum_{\substack{|B|,|C|\geqslant 0\\ B+C=A}}(b_\alpha+1)\partial_i\mathcal{Z}^{(B+1_\alpha)}(z,\bar{z})\mu_j^{i(C)}(z,\bar{z}) \tag{3.51}$$

which, in the particular case of $|A|=0$, reduces to the usual Beltrami equations

$$\bar{\partial}_j\mathcal{Z}^\alpha(z,\bar{z})=\partial_r\mathcal{Z}^\alpha(z,\bar{z})\mu_j^{r(0)}(z,\bar{z}), \tag{3.52}$$

which were fully treated in Ref. 9 in the two-dimensional case. In this context the integrability condition (3.28) is transferred on the jet coordinates $\mu_j^{i(A)}(z,\bar{z})$ with $|A|\geqslant 0$, as follows:

$$\bar{\partial}_i\mu_j^{r(A)}(z,\bar{z})-\bar{\partial}_j\mu_i^{r(A)}(z,\bar{z})=\sum_{\substack{|B|,|C|\geqslant 0\\ B+C=A}}(\mu_i^{s(B)}(z,\bar{z})\partial_s\mu_j^{r(C)}(z,\bar{z})-\mu_j^{s(B)}(z,\bar{z})\partial_s\mu_i^{r(C)}(z,\bar{z})). \tag{3.53}$$

For $|A|\geqslant 1$,

$$\bar{\partial}_j\mathcal{Z}^{(A)}(z,\bar{z})=\frac{1}{A!}\frac{\partial^{|A|}}{\partial\mathcal{Y}_A}\bar{\partial}_j\Phi(z,\mathcal{Y})\bigg|_{\mathcal{Y}=0}=\sum_{1\leqslant|I|\leqslant|A|}\mathcal{G}_{(I)}^{(A)}(z,\bar{z})\mu_j^{(I)}(z,\bar{z}), \tag{3.54}$$

where we have set for $|I|\geqslant 1$,

$$\mu_j^{(I)}(z,\bar{z}):=\frac{1}{I!}\mathcal{D}^{(I)}(z,\mathcal{Y})\bar{\partial}_j\Phi(z,\mathcal{Y})\bigg|_{\mathcal{Y}=0}:=\prod_{k=1}^n\left(\frac{1}{i_k!}(\mathcal{D}^k(z,\mathcal{Y}))^{i_k}\right)\bar{\partial}_j\Phi(z,\mathcal{Y})\bigg|_{\mathcal{Y}=0} \tag{3.55}$$

as representing the n-dimensional version for the $\mathcal{W}$-extension of the Beltrami multipliers introduced by Bilal, Fock, and Kogan.[24] It is worthwhile to say that the coefficients $\mathcal{G}_{(I)}^{(A)}(z,\bar{z})$ are very intricate nonlocal expressions depending on the derivatives up to order $|A|$ of $\mathcal{Z}^{(B)}$, with $1\leqslant|B|\leqslant|A|$. Writing (3.54) in more precise terms one has for $|A|\geqslant 1$,

$$\begin{aligned}\bar{\partial}_j\mathcal{Z}^{(A)}(z,\bar{z})&=\mu_j^r(z,\bar{z})\partial_r\mathcal{Z}^{(A)}(z,\bar{z})+\cdots\\ &\quad+\sum_{\alpha=1}^n\sum_{|I^\alpha|=a_\alpha}\frac{(I^1+\cdots+I^n)!}{I^1!\cdots I^n!}\left(\prod_{\beta=1}^n\lambda_{I^\beta}^\beta(z,\bar{z})\right)\mu_j^{(I^1+\cdots+I^n)}(z,\bar{z}),\end{aligned} \tag{3.56}$$

where on the multi-indices $I^\alpha=(i_1^\alpha,\ldots,i_n^\alpha)$ the summand $I=\Sigma_{\alpha=1}^n I^\alpha$ is the linear addition on the monoid of positive integers $\mathbb{N}^n$ while $\lambda_{I^\beta}^\beta(z,\bar{z})=\Pi_{r=1}^n(\partial_r\mathcal{Z}^\beta(z,\bar{z}))^{i_r^\beta}$. Moreover, in the above-given expansion μ_j^r must be identified with $\mu_j^{r(0)}$—see (3.51) and (3.52).

Furthermore, the symplectic structure of the space ought to provide by virtue of (3.50) a recursive construction for the coefficients $\mu_j^{i\,(A)}$ defined in (3.50) for the complex structure in terms of those of Bilal–Fock–Kogan defined in (3.55). This certainly allows one to write

$$\mu_j^i(z,\mathcal{Y})=\sum_{|I|\geqslant 1}\mathcal{F}^i_{(I)}(z,\mathcal{Y})\,\mu_j^{(I)}(z,\overline{z}), \tag{3.57}$$

where the very complicated coefficients $\mathcal{F}^i_{(I)}(z,\mathcal{Y})$ depending on $\mathcal{G}$ carry a well-defined geometrical meaning.

IV. CLASSICAL $\mathcal{W}_\infty$-ALGEBRA IN n-COMPLEX DIMENSIONS

Due to the holomorphically split expansion (3.45), the action of the BRS operator $\mathcal{S}$ on the theory can be parametrized by means of new ghost fields directly obtained from this expansion. These will be intimately related to the $\mathcal{W}_\infty$-algebra. Indeed, since $\mathcal{S}\mathcal{Y}_\alpha=0$, by using (3.46), for $|A|\geqslant 1$, one gets the same combinatorial expansion as (3.54),

$$\mathcal{S}\mathcal{Z}^{(A)}(z,\overline{z})=\frac{1}{A!}\frac{\partial^{|A|}}{\partial\mathcal{Y}_A}\Lambda(z,\mathcal{Y})\bigg|_{\mathcal{Y}=0}=\sum_{1\leqslant|I|\leqslant|A|}\mathcal{G}^{(A)}_{(I)}(z,\overline{z})\mathcal{C}^{(I)}(z,\overline{z}), \tag{4.1}$$

where we have introduced the independent ghost fields

$$\mathcal{C}^{(I)}(z,\overline{z})\coloneqq\frac{1}{I!}\mathcal{D}^{(I)}(z,\mathcal{Y})\Lambda(z,\mathcal{Y})\bigg|_{\mathcal{Y}=0}\coloneqq\prod_{k=1}^{n}\left(\frac{1}{i_k!}(\mathcal{D}^k(z,\mathcal{Y}))^{i_k}\right)\Lambda(z,\mathcal{Y})\bigg|_{\mathcal{Y}=0}. \tag{4.2}$$

Note that from the very definitions, the dependence on the generalized Bilal, Fock, and Kogan pararameters can be isolated and turns out to be coupled to the ghost $\overline{c}^{\overline{I}}\coloneqq\overline{c}^{(0,i)}$,

$$\mathcal{C}^{(I)}(z,\overline{z})=\mu_i^{(I)}(z,\overline{z})\overline{c}^{(0,i)}(z,\overline{z})+\cdots,\quad \overline{c}^{(0,i)}(z,\overline{z})\coloneqq\frac{\partial\Lambda(z,\mathcal{Y})}{\partial\overline{\mathbf{y}}_\mathbf{i}}\bigg|_{\mathcal{Y}=0}, \tag{4.3}$$

the full detailed expression will be given in the following–see (4.10).

Notably, after a tedious combinatorial calculation based upon the commutators (3.41), the BRS variations of the ghosts defined by (4.2) turn out to be local (in the sense that they do not depend on the λ fields), namely, for $|I|\geqslant 1$,

$$\mathcal{S}\mathcal{C}^{(I)}(z,\overline{z})=\sum_{k=1}^{n}(1-\delta_{0i_k})\sum_{J^{(k)}\leqslant I^{(k)}-1_k}\frac{(I-J^{(k)}-1_k+1_r)!}{(I-J^{(k)}-1_k)!}\times\mathcal{C}^{(I-J^{(k)}-1_k+1_r)}(z,\overline{z})\partial_r\mathcal{C}^{(J^{(k)}+1_k)}(z,\overline{z}), \tag{4.4}$$

where the notation $J^{(k)}$ means $J^{(k)}=(j_1,\ldots,j_k,0,\ldots,0)$ (and similarly for $I^{(k)}$), $J\leqslant I$ is a shorthand for $j_k\leqslant i_k$, $k=1,\ldots,n$ and

$$\frac{(I-J^{(k)}-1_k+1_r)!}{(I-J^{(k)}-1_k)!}=\begin{cases} i_r-j_r+1 & \text{if } 1\leqslant r\leqslant k-1\\ i_k-j_k & \text{if } r=k\\ i_r+1 & \text{if } k+1\leqslant r\leqslant n\end{cases}. \tag{4.5}$$

This formula represents the extended version to n complex dimensions of the *chiral* $\mathcal{W}_\infty$-algebra. Indeed, let us consider $n=1$ a complex curve which represents a bidimensional theory built on a Riemann surface. In that case, the multi-index I reduces to a simple index and for $|I|=i_1=m, J^{(1)}=(j_1)=j$, $r=k=1$, the formula (4.4) reduces (with $\ell=m-j$) to that found in Refs. 19 and 20,

$$\mathcal{S}\mathcal{C}^{(m)}(z,\overline{z})=\sum_{\ell=1}^{m}\ \ell\,\mathcal{C}^{(\ell)}(z,\overline{z})\partial\mathcal{C}^{(m-\ell+1)}(z,\overline{z}), \tag{4.6}$$

and recalled in Sec. I—see (1.1). Going back to the general case, at first order $|I|=1$, we refind the usual BRS transformations for the chiral ghosts $\mathcal{C}^i$ under diffeomorphisms of M,[9]

$$\mathcal{S}\mathcal{C}^i(z,\overline{z})=\mathcal{C}^\ell(z,\overline{z})\partial_\ell\mathcal{C}^i(z,\overline{z}), \tag{4.7}$$

showing that diffeomorphisms are actually captured by the $\mathcal{W}_\infty$-symmetry. In order to exemplify once more (4.4), at the second order $|I|=2$, for $1\leqslant i\leqslant j\leqslant n$, the multi-index $I=(0,\ldots,0,1,0,\ldots,0,1,0,\ldots,0)$, where 1 at both the ith and jth places will be shorthandly written as $I=(ij)$ in order to recover a tensorial notation. With this notation, one gets

$$\begin{aligned}\mathcal{S}\mathcal{C}^{(ij)}(z,\overline{z})=&\mathcal{C}^r(z,\overline{z})\partial_r\mathcal{C}^{(ij)}(z,\overline{z})+2\mathcal{C}^{(ii)}(z,\overline{z})\partial_i\mathcal{C}^j(z,\overline{z})+2\mathcal{C}^{(jj)}(z,\overline{z})\partial_j\mathcal{C}^i(z,\overline{z})\\&+\sum_{\substack{r=1\\r\neq i}}^{n}\mathcal{C}^{(ir)}(z,\overline{z})\partial_r\mathcal{C}^j(z,\overline{z})+\sum_{\substack{r=1\\r\neq j}}^{n}\mathcal{C}^{(jr)}(z,\overline{z})\partial_r\mathcal{C}^i(z,\overline{z}),\end{aligned}$$

(no summation on i and j and recall that the independent ghosts are $\mathcal{C}^{(ij)}$). In particular, the case $i=j$ is obtained by dividing both sides of the above equation by the symmetry factor 2,

$$\mathcal{S}\mathcal{C}^{(ii)}(z,\bar{z})=\underbrace{\mathcal{C}^r(z,\bar{z})\partial_r\mathcal{C}^{(ii)}(z,\bar{z})+2\mathcal{C}^{(ii)}(z,\bar{z})\partial_i\mathcal{C}^i(z,\bar{z})}_{\text{as in (4.6) with } m=2}+\sum_{r\neq i}\mathcal{C}^{(ri)}(z,\bar{z})\partial_r\mathcal{C}^i(z,\bar{z})$$

where $I=(ii)$ means 2 at the ith place, a shorthand notation saying that the multi-index entries are $i_k=2\,\delta_{ki}$. Of course, there is the complex conjugate expression to (4.4) as well.

Following the BRS method recalled in Sec. I, the algebra of the $\mathcal{W}_\infty$-generators in the n complex dimensional case will be obtained by duality through the corresponding BRS functional operator (1.2) from the BRS transformations (4.4) of the chiral ghost fields themselves. By performing this construction for the chiral ghosts, one should directly get a generalization to n dimensions of the chiral $\mathcal{W}_\infty$-algebra (1.3).

Accordingly, the BRS variations of the generalized Bilal–Fock–Kogan parameters (3.55) can be directly computed from (4.4) by using a trick related to diffeomorphisms,[25] namely, $\{\mathcal{S},\partial/\partial\overline{c^i}\}=\overline{\partial_i}$,, together with (4.3),

$$\begin{aligned}\mathcal{S}\mu_j^{(I)}(z,\overline{z})=&\overline{\partial_j}\mathcal{C}^{(I)}(z,\overline{z})+\sum_{k=1}^{n}(1-\delta_{0i_k})\sum_{J^{(k)}\leqslant I^{(k)}-1_k}\frac{(I-J^{(k)}-1_k+1_r)!}{(I-J^{(k)}-1_k)!}\\&\times(\mathcal{C}^{(I-J^{(k)}-1_k+1_r)}(z,\overline{z})\partial_r\mu_j^{(J^{(k)}+1_k)}(z,\overline{z})-\mu_j^{(I-J^{(k)}-1_k+1_r)}(z,\overline{z})\partial_r\mathcal{C}^{(J^{(k)}+1_k)}(z,\overline{z})).\end{aligned} \tag{4.8}$$

By using once more the previous trick on (4.8) one ends up with the counterpart of the integrability condition (3.30) in terms of the external fields (3.55) for $|I|\geqslant 1$, and with the aforementioned notation

$$\overline{\partial_i}\mu_j^{(I)}(z,\overline{z})-\overline{\partial_j}\mu_i^{(I)}(z,\overline{z})=\sum_{k=1}^{n}(1-\delta_{0i_k})\sum_{J^{(k)}\leqslant I^{(k)}-1_k}\frac{(I-J^{(k)}-1_k+1_r)!}{(I-J^{(k)}-1_k)!}$$
$$\times(\mu_{\overline{i}}^{(I-J^{(k)}-1_k+1_r)}(z,\overline{z})\partial_r\mu_{\overline{j}}^{(J^{(k)}+1_k)}(z,\overline{z})$$
$$-\mu_{\overline{j}}^{(I-J^{(k)}-1_k+1_r)}(z,\overline{z})\partial_r\mu_{\overline{i}}^{(J^{(k)}+1_k)}(z,\overline{z})). \tag{4.9}$$

The chiral ghost fields $\mathcal{C}^{(I)}$ admit a local decomposition in terms of the fields (3.55) which generalizes the well-known conformal one[26] in two dimensions. The latter has already been extended in Ref. 19 for Riemann surfaces. By definition the promised detailed expression for (4.3) is written as

$$\mathcal{C}^{(I)}(z,\overline{z})=\sum_{|P|,|Q|=0}^{|I|}\overline{Q}!\sum_{\substack{P+a_1J_1+\cdots+a_{|I|}J_{\underline{|I|}}=I\\ a_1+\cdots+a_{|I|}=|Q|}}$$
$$\times\left(\sum_{\substack{\overline{S}_1+\cdots+\overline{S}_{|I|}=\overline{Q}\\ |\overline{S}_k|=a_k,\ k=1,\ldots,|I|}}\prod_{k=1}^{|I|}\left(\frac{1}{\overline{S}_k!}(\mu^{(J_k)}(z,\overline{z}))_{\overline{S}_k}\right)\right)c^{(P,\overline{Q})}(z,\overline{z}), \tag{4.10}$$

where in the second summand a_k enumerates the number of multi-indices identical to J_k, $J_k\neq J_\ell$ for $k\neq\ell$ and $k,\ell=1,\ldots,|I|$, $(0\leqslant a_k\leqslant|I|)$, the sum goes with no repetition, and, for a given multi-index $\overline{S}_k=(\overline{s}_1^{(k)},\ldots,\overline{s}_n^{(k)})$,

$$(\mu^{(J_k)}(z,\overline{z}))_{\overline{S}_k}:=(\mu_{\overline{1}}^{(J_k)}(z,\overline{z}))^{\overline{s}_1^{(k)}}\cdots(\mu_{\overline{n}}^{(J_k)}(z,\overline{z}))^{\overline{s}_n^{(k)}} \tag{4.11}$$

and where new independent ghost fields have been introduced by

$$c^{(P,\overline{Q})}(z,\overline{z}):=\frac{1}{P!\overline{Q}!}\frac{\partial^{|P|}}{\partial\mathbf{y}_P}\frac{\partial^{|\overline{Q}|}}{\partial\overline{\mathbf{y}}_{\overline{Q}}}\Lambda(z,\mathcal{Y})\bigg|_{Y=0}. \tag{4.12}$$

Note that expression (4.10) which expresses a change of generators for the $\mathcal{W}$-symmetry is local. For instance, the case $|I|=1$ gives

$$\mathcal{C}^i(z,\overline{z})=c^{(i,0)}(z,\overline{z})+\mu_{\overline{s}}^i(z,\overline{z})c^{(0,\overline{s})}(z,\overline{z}),$$

which is the expression of the chiral ghost fields in terms of the true ghost fields $c^{(i,0)}$ and $c^{(0,\overline{s})}$ for (infinitesimal) diffeomorphisms of M,[9] while $|I|=2$ yields, respectively, for $I=(ii)$ and $I=(ij)$, $i<j$,

$$\mathcal{C}^{(ii)}(z,\overline{z})=c^{(ii,0)}(z,\overline{z})+\mu_{\overline{s}}^i(z,\overline{z})c^{(i,\overline{s})}(z,\overline{z})+(\mu_{\overline{s}}^i(z,\overline{z}))^2c^{(0,\overline{ss})}(z,\overline{z})+\mu_{\overline{s}}^{(ii)}(z,\overline{z})c^{(0,\overline{s})}(z,\overline{z})$$
$$+\sum_{\underline{r<s}}\mu_{\overline{r}}^i(z,\overline{z})\mu_{\overline{s}}^i(z,\overline{z})c^{(0,\overline{rs})}(z,\overline{z}),$$

$$\mathcal{C}^{(ij)}(z,\overline{z})=c^{(ij,0)}(z,\overline{z})+\mu_{\overline{s}}^i(z,\overline{z})c^{(j,\overline{s})}(z,\overline{z})+\mu_{\overline{s}}^j(z,\overline{z})c^{(i,\overline{s})}(z,\overline{z})+\mu_{\overline{s}}^{(ij)}(z,\overline{z})c^{(0,\overline{s})}(z,\overline{z})$$
$$+2\mu_{\overline{s}}^i(z,\overline{z})\mu_{\overline{s}}^j(z,\overline{z})c^{(0,\overline{ss})}(z,\overline{z})+\sum_{\underline{r<s}}(\mu_{\overline{r}}^i(z,\overline{z})\mu_{\overline{s}}^j(z,\overline{z})+\mu_{\overline{r}}^j(z,\overline{z})\mu_{\overline{s}}^i(z,\overline{z}))c^{(0,\overline{rs})}(z,\overline{z}).$$

The ghosts $c^{(R,\overline{S})}(z,\overline{z})$ satisfy rather elaborate BRS transformations, which generalize formula (4.4) to the nonchiral sectors. They can be obtained either from the very definition Eq. (4.12) or from the combined action of the decomposition Eq. (4.10) and the BRS variations (4.4) and (4.8). For $|P|+|\overline{Q}|\geqslant 1$ the variations look like

$$\begin{aligned}
\mathcal{S}c^{(P,\overline{Q})}(z,\overline{z}) = & \sum_{\overline{S}\leqslant\overline{Q}} \sum_{k=1}^{n} (1-\delta_{0p_k}) \sum_{R^{(k)}\leqslant P^{(k)}-1_k} \frac{(P-R^{(k)}-1_k+1_r)!}{(P-R^{(k)}-1_k)!} \\
& \times c^{(P-R^{(k)}-1_k+1_r,\overline{Q}-\overline{S})}(z,\overline{z})\partial_r c^{(R^{(k)}+1_k,\overline{S})}(z,\overline{z}) \\
& + (1-\delta_{0\overline{Q}}) \frac{(P+1_r)!}{P!} \sum_{\overline{S}\leqslant\overline{Q},|S|\geqslant 1} c^{(P+1_r,\overline{Q}-\overline{S})}(z,\overline{z})\partial_r c^{(0,\overline{S})}(z,\overline{z}) \\
& + \sum_{R\leqslant P} \sum_{k=1}^{n} (1-\delta_{0\overline{q_k}}) \sum_{\overline{S}^{(k)}\leqslant\overline{Q}^{(k)}-\overline{1_k}} \frac{(\overline{Q}-\overline{S}^{(k)}-\overline{1_k}+\overline{1_s})!}{(\overline{Q}-\overline{S}^{(k)}-\overline{1_k})!} \\
& \times c^{(P-R,\overline{Q}-\overline{S^k}-\overline{1_k}+\overline{1_s})}(z,\overline{z})\overline{\partial_s} c^{(R,\overline{S^k}+\overline{1_k})}(z,\overline{z}) \\
& + (1-\delta_{0P}) \frac{(\overline{Q}+\overline{1_s})!}{\overline{Q}!} \sum_{R\leqslant P,|R|\geqslant 1} c^{(P-R,\overline{Q}+\overline{1_s})}(z,\overline{z})\overline{\partial_s} c^{(R,0)}(z,\overline{z}), \qquad (4.13)
\end{aligned}$$

and, according to the BRS technique briefly recalled in Sec. I, give rise to the $\mathcal{W}_\infty$-structure at a nonchiral level. These results provide (in the $(z,\overline{z})$ submanifold characterized by $\mathcal{Y}_\alpha=\overline{\mathcal{Y}_{\overline{\alpha}}}=0$ in the symplectic space) an infinite $\mathcal{W}_\infty$-algebra of which the first step describes the reparametrization invariance $(z,\overline{z})\to(\mathcal{Z}^\alpha(z,\overline{z}),\overline{\mathcal{Z}^\alpha}(z,\overline{z}))$ studied in Ref. 9.

Here, what is left over is the relic of the deformation process for $\mathcal{Y}_\alpha,\overline{\mathcal{Y}_{\overline{\alpha}}}\neq 0$ given by an infinite hierarchy of smooth changes of local complex coordinates $(z,\overline{z})\to(\mathcal{Z}^{(A)}(z,\overline{z}),\overline{\mathcal{Z}^{(A)}}(z,\overline{z}))$ on the base (the $(z,\overline{z})$-space) of the symplectic space. The new $\mathcal{W}_\infty$-algebra really encodes the behavior under symplectomorphisms of this hierarchy.

V. TOWARD A LAGRANGIAN FORMULATION

If we now wish to construct a Lagrangian field theory whose classical limit is invariant under this n-dimensional extension of a $\mathcal{W}_\infty$-algebra, it would retain the imprinting of the infinite expansion from which the algebra is extracted, by reproducing a theory which is badly packed in the $(z,\overline{z})$ space and makes an attempt to get away in the full symplectic space. The ''classical'' fields whose dynamics serve to probe the $\mathcal{Y}_\alpha,\overline{\mathcal{Y}_{\overline{\alpha}}}\neq 0$ sector are the generalized Bilal–Fock–Kogan parameters $\mu_j^{(I)}(z,\overline{z})$ defined in (3.55). Indeed they are the only ''true'' local fields from which the pure gravitational theory would depend on. They are sources related to higher spin fields as in the unidimensional complex case, see, e.g., Ref. 24.

So from the BRS approach an infinite set of Ward operators $\mathcal{W}_{(I)}(z,\overline{z})$ can be obtained and from which a classical action Γ^{Cl} may be defined in the vacuum sector as follows. For $|I|\geqslant 1$,

$$\begin{aligned}
\mathcal{W}_{(I)}(z,\overline{z})\Gamma^{\mathrm{Cl}} = & -\overline{\partial_j}\frac{\delta\Gamma^{\mathrm{Cl}}}{\mu_j^{(I)}(z,\overline{z})} + \sum_{|L|\geqslant 1} ((i_r+\ell_r)(\partial_r\mu_j^{(L)}(z,\overline{z})) + \ell_r\,\mu_j^{(L)}(z,\overline{z})\partial_r)\frac{\delta\Gamma^{\mathrm{Cl}}}{\mu_j^{(I+L-1_r)}(z,\overline{z})} \\
= & 0. \qquad (5.1)
\end{aligned}$$

These encapsulate the first-order case $|I|=|L|=1$ already treated in Ref. 9. Remark also that in order to know the $\overline{\partial}$ divergence of the higher spin current, dual to $\mu_j^{(I)}$, the infinite collection of higher spin fields must be known first.

Using the usual techniques, which in the two-dimensional limit lead from Ward identities to O.P.E. expansion,[24] we can derive a generalization of the ''O.P.E.'' algebra which would promote the present symplectic approach, since an n complex dimensional short-distance product could generally be a difficult task to manage.

For both $|I|$ and $|J|$ greater than 0, one obtains

$$\pi\sum_{j=1}^{n}\int_{\mathbb{C}^{n-1}}\left(\prod_{\substack{\ell=1\\ \ell\neq j}}^{n}\frac{d\overline{w}^{\ell}\wedge dw^{\ell}}{2i(w^{\ell}-z'^{\ell})}\right)\frac{\delta^2\Gamma^{\mathrm{Cl}}}{\delta\mu_j^{(I)}(w^1,\ldots,z'^j,\ldots,w^n,\overline{w}^1,\ldots,\overline{z}'^j,\ldots,\overline{w}^n)\,\delta\mu_k^{(J)}(z,\overline{z})}\Bigg|_{\mu=0}$$
$$+\sum_{r=1}^{n}\left(\frac{i_r+j_r}{(z^r-z'^r)^2}-\frac{i_r}{z^r-z'^r}\right)\left(\prod_{\substack{\ell=1\\ \ell\neq r}}^{n}\frac{1}{z^{\ell}-z'^{\ell}}\right)\frac{\delta\Gamma^{\mathrm{Cl}}}{\delta\mu_j^{(I+J-1_r)}(z,\overline{z})}\Bigg|_{\mu=0}=0. \tag{5.2}$$

leading to a convolution algebra, where the directional properties of the (short) distance limit is taken into account, for the Green functions generated by the generalized Bilal–Fock–Kogan fields. Its two-dimensional limit gives the usual classical O.P.E. expansion.

Anyhow, due to the anomalous character of the diffeomorphism symmetry at the quantum level, we must foresee whether this defect would be transmitted to the residual part of the algebra. Hence quantum corrections would be required to give a meaning to the theoretical model and are still under investigation.

VI. CONCLUSIONS

It has been shown how a symplectic approach gives a strong geometrical way of extending the notion of $\mathcal{W}_\infty$-algebra as a symmetry arising in the one complex dimensional case to a generic n complex dimensional (compact) manifold.

This symmetry appears from consistent deformations of integrable complex structures in the spirit of Kodaira–Spencer deformation. The decomposition in terms of local quantities such as the Bilal–Fock–Kogan coefficients considered as generalized sources for higher spin fields naturally emerges from the construction. However, in this symplectic framework, a truncation process analogous to the one for Riemann surfaces[21] from $\mathcal{W}_\infty$-algebra to a finite $\mathcal{W}$-algebra is still lacking. In particular, the latter could be of some interest in both string and brane theories (see, e.g., Ref. 12) where higher spin fields appear in four real dimensions. In these theories, the fields seem to be related to some finite $\mathcal{W}$-algebra. However theoretical models with explicit higher spin fields still remain to be constructed.

More generally, even if the topic ought to seem, according to the physical context, rather technical and strongly grounded on mathematics, we would emphasize that the important problem of a metric or a complex structure for a physical theory embedded in a gravitational model is far from being understood. So any little step in that direction could be profitable in discovering the role of Nature and the intricacies of geometrical implications within the formulation of physical theories.

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Analog of secondary invariants for holomorphic vector bundles

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Given a pair of holomorphic structures on a complex vector bundle over a complex manifold, Dolbeault cohomological invariants are constructed. The construction is based on the construction of Chern–Simons secondary classes. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1510972]

I. INTRODUCTION

Let E be a C^∞ complex vector bundle over a complex manifold M. Holomorphic structures on E are defined by giving a Dolbeault operator. We recall that a Dolbeault operator is a first order differential operator

$$\overline{\partial}_E : E \to \Omega^{0,1}_M(E)$$

satisfying the Leibniz identity and the integrability condition $\overline{\partial}_E \bigcirc \overline{\partial}_E = 0$. The Leibniz identity says that $\overline{\partial}_E(fs) = f\overline{\partial}_E(s) + s \otimes \overline{\partial} f$, where f is a locally defined smooth function on M and s is a locally defined smooth section of E. The (locally defined) solutions of the operator are the holomorphic sections of the corresponding holomorphic vector bundle.

Let $\overline{\partial}_0$ and $\overline{\partial}_1$ be two Dolbeault operators on E. We construct a differential form $D_k(\overline{\partial}_0, \overline{\partial}_1)$ of degree $2k+1$ on M. This form $D_k(\overline{\partial}_0, \overline{\partial}_1)$ is of Hodge type $(0,2k+1)$ and it is $\overline{\partial}$ closed. Therefore, $D_k(\overline{\partial}_0, \overline{\partial}_1)$ gives a Dolbeault cohomology class in $H^{2k+1}(M, \mathcal{O}_M)$, where $\mathcal{O}_M$ is the coherent analytic sheaf of holomorphic functions.

The construction of $D_k(\overline{\partial}_0, \overline{\partial}_1)$ relies on the construction of secondary classes, and it has some of the properties enjoyed by secondary classes.

If $\overline{\partial}_2$ is a holomorphic structure on E such that $\overline{\partial}_1$ and $\overline{\partial}_2$ lies in the same path connected component in the space of all holomorphic structures on E, then for any $k \geqslant 1$, the Dolbeault cohomology class represented by $D_k(\overline{\partial}_0, \overline{\partial}_1)$ coincides with the one represented by $D_k(\overline{\partial}_0, \overline{\partial}_2)$ (Proposition 3.3).

If $\overline{\partial}_0$ and $\overline{\partial}_1$ are two holomorphic structures on E related by a C^∞ automorphism of E, then the cohomology class represented by $D_k(\overline{\partial}_0, \overline{\partial}_2)$ is contained in the image of the homomorphism

$$H^{2k+1}(M, (2\pi\sqrt{-1})^{k+1}\mathbb{Z}) \to H^{2k+1}(M, \mathcal{O}_M)$$

defined by the obvious inclusion of the constant sheaf $(2\pi\sqrt{-1})^{k+1}\mathbb{Z}$ in the sheaf $\mathcal{O}_M$ of holomorphic functions (Theorem 4.2).

II. SECONDARY INVARIANTS

Let M be a smooth manifold. Let E be a C^∞ complex vector bundle over M. The space of sections of $\mathrm{End}(E) \otimes \wedge T^*M$ has an obvious algebra structure which is defined using the (associative) multiplication of the fibers of $\mathrm{End}(E)$ and the exterior algebra structure of $\wedge T^*M$. The multiplication operation of $\mathrm{End}(E)$-valued forms will also be denoted $\wedge$. There is a natural ho-

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momorphism $\mathrm{End}(E)\otimes\wedge T^*M\to\wedge T^*M$ of vector bundles that sends any $s\otimes\omega$, where $s\in\mathrm{End}(E_x)$ and $\omega\in\wedge T^*_xM$ are in the fiber over any point $x\in M$, to $\mathrm{trace}(s)\omega$. This homomorphism will be denoted by trace.

Lemma 2.1: Take $\theta_i\in C^\infty(M,\mathrm{End}(E)\otimes\wedge^{n_i}T^*M)$, *where* $i\in[1,d]$. *The identity*

$$\mathrm{trace}(\theta_1\wedge\theta_2\wedge\cdots\wedge\theta_d)=(-1)^{n_1(n_2+n_3+\cdots+n_d)}\mathrm{trace}(\theta_2\wedge\theta_3\wedge\cdots\wedge\theta_d\wedge\theta_1)$$

is valid.

Proof: This is an immediate consequence of the fact that $\mathrm{trace}(AB)=\mathrm{trace}(BA)$, where $A,B\in M(n,\mathbb{C})$.

Let ∇ be a connection on E. The differential operator

$$C^\infty(E\otimes\wedge^iT^*M)\to C^\infty(E\otimes\wedge^{i+1}T^*M),$$

where $i\geqslant 1$, induced by ∇ will also be denoted by ∇. The curvature $\nabla\circ\nabla$ of ∇ will be denoted by K_∇. So $K_\nabla\in C^\infty(\mathrm{End}(E)\otimes\wedge^2T^*M)$. We will often use the notation ∇^2 to denote the curvature of ∇.

Lemma 2.2: If there is a $\mathrm{End}(E)$*-valued one form* θ *on* M *such that*

$$K_\nabla=\theta\wedge\theta,$$

then the $2k$*-form* $\mathrm{trace}((K_\nabla)^k)$ *vanishes identically*.

Proof: Since $(K_\nabla)^k=(\theta\wedge\theta)^k=\theta\wedge\theta^{2k-1}$, by setting $d=2$, $\theta_1=\theta$, and $\theta_2=\theta^{2k-1}$ in Lemma 2.1 we obtain that $\mathrm{trace}((K_\nabla)^k)=-\mathrm{trace}((K_\nabla)^k)$, and hence the lemma follows. □

The Hermitian–Yang–Mills connection on a polystable Higgs bundle is an example of a connection satisfying the condition in Lemma 2.2.[1] Let X be a compact connected Kähler manifold and V a holomorphic vector bundle over X. Let

$$\phi\in H^0(X,\mathrm{End}(V)\otimes\Omega^1_X)$$

be a holomorphic section with $\phi\wedge\phi=0$. Here Ω^1_X is the holomorphic cotangent bundle of X. For notational convenience, the vector bundle $\mathrm{End}(V)\otimes\Omega^1_X$ will be denoted by $\Omega^1_X(\mathrm{End}(V))$. If the pair (V,ϕ), which is called a *Higgs bundle*, is stable and $c_1(E)=0=c_2(E)$, then V admits a unique Hermitian connection satisfying the Yang–Mills equation.[1] If H is a Hermitian metric on V and ∇^H the corresponding Chern connection, then the Yang–Mills equation is the flatness condition

$$(\nabla^H+\phi+\phi^*)^2=0 \tag{2.1}$$

of the connection $\nabla^H+\phi+\phi^*$, where $\phi^*\in C^\infty(M,\Omega^{0,1}_X(\mathrm{End}(V)))$ is the adjoint of ϕ defined using H. It is easy to see that (2.1) is equivalent to the equation $(\nabla^H)^2=-(\phi+\phi^*)^2$. Therefore, a Hermitian–Yang–Mills connection ∇^H satisfies the condition in Lemma 2.2 with $\theta=\sqrt{-1}(\phi+\phi^*)$.

Take two connections ∇_0 and ∇_1 on E. Set $\omega:=\nabla_1-\nabla_0$, which is a $\mathrm{End}(E)$-valued one-form, and for any $t\in[0,1]$, let

$$\nabla_t:=\nabla_0+t\omega$$

be the connection on E. For any $k\geqslant 0$, consider the smooth differential form

$$C_k(\nabla_0,\nabla_1):=\int_0^1\mathrm{trace}(\omega\wedge(\nabla_t^2)^k)\in C^\infty(M,\wedge^{2k+1}T^*M) \tag{2.2}$$

of degree $2k+1$ on M. Note that the integration is defined using the vector space structure of the space of forms. The following lemma is essentially a consequence of Lemma 2.2.

Lemma 2.3: If both ∇_0 and ∇_1 satisfy the condition in Lemma 2.2, then the differential form $C_k(\nabla_0,\nabla_1)$ defined in (2.2) is closed.

Proof: Let $p:M\times[0,1]\to M$ be the projection map. The family of connections ∇_t gives a connection, which we will denote by $\overline{\nabla}$, on p^*E. For each $t\in[0,1]$, the connection induced on $(p^*E)|_{M\times\{t\}}$ by $\overline{\nabla}$ is ∇_t, and for any $x\in M$, the induced connection on $(p^*E)|_{\{x\}\times[0,1]}$ coincides with the natural trivialization of a pullback bundle on a fiber of the projection. These two properties evidently determine $\overline{\nabla}$. The Bianchi identity, says that for a connection ∇' on a vector bundle E', the $\mathrm{End}(E')$-valued three-form $\nabla'\circ\nabla'\circ\nabla'$ vanishes identically. Using the Bianchi identity for $\overline{\nabla}$ it follows that

$$dC_k(\nabla_0,\nabla_1)=\frac{1}{k+1}\int_0^1\frac{d}{dt}\mathrm{trace}((\nabla_t^2)^{k+1})=\frac{\mathrm{trace}((\nabla_1^2)^{k+1})}{k+1}-\frac{\mathrm{trace}((\nabla_0^2)^{k+1})}{k+1}$$

(see Ref. 2, Appendix for details). Now Lemma 2.2 completes the proof. □

For two connections ∇_0 and ∇_1 as in Lemma 2.3 (satisfying the condition in Lemma 2.2), the de Rham cohomology class in $H^{2k+1}(M,\mathbb{C})$ represented by the closed form $C_k(\nabla_0,\nabla_1)$ is an analog of the Chern–Simons secondary invariant for flat connections.[3] See Ref. 4 for construction of secondary invariants of Hermitian–Yang–Mills connections.

Although in the construction of $C_k(\nabla_0,\nabla_1)$ we use the straight-line segment defined by $t\mapsto\nabla_t$ in the affine space of connections on E, the cohomology class represented by the closed form $C_k(\nabla_0,\nabla_1)$ is independent of the choice of path connecting ∇_1 to ∇_0. To prove this, let γ be a smooth map from $[0,1]$ to $\mathrm{Conn}(E)$, the space of connections on E, such that $\gamma(0)=\nabla_0$ and $\gamma(1)=\nabla_1$. Let

$$\Omega_t\in C^\infty(M,\mathrm{End}(E)\otimes\wedge^2T^*M) \tag{2.3}$$

be the curvature of $\gamma(t)$. Now define

$$C_k^\gamma(\nabla_0,\nabla_1):=\int_0^1\mathrm{trace}\left(\frac{d\gamma(t)}{dt}\wedge(\Omega_t)^k\right)dt. \tag{2.4}$$

Note that $d\gamma(t)/dt\in C^\infty(M,\mathrm{End}(E)\otimes T^*M)$.

Proposition 2.4. The form $C_k^\gamma(\nabla_0,\nabla_1)$ is closed. The cohomology class in $H^{2k+1}(M,\mathbb{C})$ represented by it coincides with the one represented by $C_k(\nabla_0,\nabla_1)$ defined in (2.2).

Proof: If $k=0$, then $C_k^\gamma(\nabla_0,\nabla_1)$ and $C_k(\nabla_0,\nabla_1)$ coincide with $\nabla_1-\nabla_0$. So assume $k\geqslant 1$. Let

$$q:M\times[0,1]\times[0,1]\to M$$

be the natural projection map. Consider the map

$$\overline{\gamma}:[0,1]\times[0,1]\to\mathrm{Conn}(E)$$

that sends any (s,t) to $(1-s)\nabla_t+s\gamma(t)$. The map $\overline{\gamma}$ defines a connection on q^*E over $M\times[0,1]\times[0,1]$. The connection on q^*E, which we will denote by $\overline{\nabla}$, is determined by the following two conditions. For any $(s,t)\in[0,1]\times[0,1]$, the restriction of $\overline{\nabla}$ to $(q^*E)|_{M\times\{s\}\times\{t\}}$ coincides with the connection $\overline{\gamma}(s,t)$, and for any $x\in M$, the restriction of $\overline{\nabla}$ to $(q^*E)|_{\{x\}\times[0,1]\times[0,1]}$ coincides with the connection defined by the natural trivialization of $(q^*E)|_{\{x\}\times[0,1]\times[0,1]}$.

The curvature of the connection $\overline{\gamma}(s,t)$ will be denoted by $\Theta(s,t)$. Let ψ denote the one-form on $[0,1]\times[0,1]$ with values in $C^\infty(M,\wedge^{2k+1}T^*M)$ defined by

$$\psi(s,t)(v)=\mathrm{trace}\left(\frac{\partial\overline{\gamma}}{\partial v}(s,t)\wedge\Theta(s,t)^k\right),$$

where $(s,t)\in[0,1]\times[0,1]$, v is a tangent vector to $[0,1]\times[0,1]$ at (s,t) and $\partial/\partial v$ is the directional derivative. So, we have

$$\int_{\partial([0,1]\times[0,1])}\psi = C_k^{\gamma}(\nabla_0,\nabla_1)-C_k(\nabla_0,\nabla_1),$$

where $\partial([0,1]\times[0,1])$ denotes the boundary of $[0,1]\times[0,1]$ with the anticlockwise orientation. Therefore, Stokes' theorem gives

$$C_k^{\gamma}(\nabla_0,\nabla_1)-C_k(\nabla_0,\nabla_1)=\int_{[0,1]\times[0,1]} d\psi.$$

It suffices to show that the form on M defined by the right-hand side is exact.

Let $\overline{\nabla}^2$ be the curvature of the connection $\overline{\nabla}$ on q^*E. Consider the differential form of degree $2k+2$ on $M\times[0,1]\times[0,1]$ defined by $\mathrm{trace}((\overline{\nabla}^2)^{k+1})$. It is straightforward to check that the Künneth component of this form in $\wedge^{2k+1}T^*M\otimes\wedge^1([0,1]\times[0,1])$ coincides with form defined by ψ.

Now it follows that $d\psi$ coincides with the two-form that sends any ordered pair of tangent vectors v_1, $v_2\in T_{(s,t)}[0,1]\times[0,1]$ at any point (s,t) to

$$k\,d\,\mathrm{trace}\left(\frac{\partial\overline{\gamma}}{\partial v_1}(s,t)\wedge\frac{\partial\overline{\gamma}}{\partial v_2}(s,t)(\Theta(s,t))^{k-1}\right).$$

Therefore, $d\psi$ is a two-form on $[0,1]\times[0,1]$ with values in exact $(2k+1)$-forms on M. Consequently, $\int_{[0,1]\times[0,1]}d\psi$ is an exact $(2k+1)$-form on M. This completes the proof of the proposition. □

The Proposition 2.4 has the following consequence. Let ∇_0 and ∇_1 be two connections as in Proposition 2.4 both satisfying the condition in Lemma 2.2. Suppose that ∇_0 and ∇_1 are such that there is a smooth path γ in $\mathrm{Conn}(E)$ connecting ∇_0 with ∇_1 and satisfying the condition that each $\gamma(t)$ is a flat connection, that is each Ω_t in (2.3) vanishes identically. Then the closed form $C_k(\nabla_0,\nabla_1)$ is exact for each $k\geqslant 1$, where $C_k(\nabla_0,\nabla_1)$ is defined in (2.2). Indeed, $C_k(\nabla_0,\nabla_1)$ and $C_k^{\gamma}(\nabla_0,\nabla_1)$ [defined in (2.4)] represent the same cohomology class (Proposition 2.4), and the form $C_k^{\gamma}(\nabla_0,\nabla_1)$ is identically zero for such a path γ provided $k\geqslant 1$.

III. INVARIANTS FOR HOLOMORPHIC BUNDLES

Let M be a complex manifold, and $\overline{\partial}_i$, $i=0,1$, be two holomorphic structures on E. So $\overline{\partial}_i: E\to\Omega_M^{0,1}(E)$ is a first order differential operator satisfying the Leibniz identity

$$\overline{\partial}_i(fs)=f\overline{\partial}_i s+s\otimes\overline{\partial}f,$$

where f is a C^{∞} (local) function and s is a locally defined smooth section of E. In order to be a holomorphic structure, the operator $\overline{\partial}_i$ must satisfy the integrability condition $\overline{\partial}_i\circ\overline{\partial}_i=0$. In other words, such an operator $\overline{\partial}_i$ can be thought of as a flat connection of type (0,1). We denote $\overline{\partial}_1-\overline{\partial}_0$ by ω, which is a section of $\Omega_M^{0,1}(\mathrm{End}(E))$. So ω is a $\mathrm{End}(E)$ valued form of Hodge type (0,1).

For any $t\in[0,1]$, define

$$\overline{\partial}_t=(1-t)\overline{\partial}_0+t\overline{\partial}_1=\overline{\partial}_0+t\omega.$$

The Leibniz identity is clearly satisfied by $\overline{\partial}_t$, but the integrability condition is not necessarily satisfied. Let Θ_t denote $\overline{\partial}_t \circ \overline{\partial}_t$, which is a section of $\Omega_M^{0,2}(\mathrm{End}(E))$. It may be noted that the Bianchi identity $\overline{\partial}_t(\Theta_t)=0$ is satisfied by $\overline{\partial}_t$.

As in (2.2), define

$$D_k(\overline{\partial}_0,\overline{\partial}_1) := \int_0^1 \mathrm{trace}(\omega \wedge (\Theta_t)^k)\,dt \tag{3.1}$$

which is a differential form of Hodge type $(0,2k+1)$ on M.

We have the following analog of Lemma 2.3.

Lemma 3.1: The form $D_k(\overline{\partial}_0,\overline{\partial}_1)$ is $\overline{\partial}$-closed.

We recall that the exterior derivative $d=\partial+\overline{\partial}$. In other words, a smooth differential form ψ of Hodge type $(0,k_0)$ is $\overline{\partial}$ closed if and only if $d\psi$ is of Hodge type $(1,k_0)$. The proof of Lemma 3.1 is identical to that of Lemma 2.3.

So, $D_k(\overline{\partial}_0,\overline{\partial}_1)$ gives an element in the Dolbeault cohomology $H_{\overline{\partial}}^{2k+1}(M)$ of M. Recall that $H_{\overline{\partial}}^{j}(M)$ coincides with $H^j(M,\mathcal{O}_M)$, where $\mathcal{O}_M$ is the structure sheaf of M (the sheaf of holomorphic functions).

For notational convenience, let $\mathrm{Dol}(E)$ denote the space of first order operators

$$\overline{\partial}_E : E \to \Omega_M^{0,1}(E)$$

on E satisfying the Leibniz identity and $\mathrm{Hol}(E)\subset \mathrm{Dol}(E)$ the subset consisting of all those operators that satisfy the integrability condition $\overline{\partial}_E \circ \overline{\partial}_E = 0$. So, $\mathrm{Dol}(E)$ is an affine space for the vector space $C^\infty(M,\Omega_M^{0,1}(\mathrm{End}(E)))$ [the space of $\mathrm{End}(E)$ valued forms of type $(0,1)$].

As in Proposition 2.4, if instead of the line segment in $\mathrm{Dol}(E)$ defined by $t\mapsto\overline{\partial}_t$ we choose a different path smooth γ in $\mathrm{Dol}(E)$ connecting $\overline{\partial}_1$ with $\overline{\partial}_0$, then the corresponding form is also $\overline{\partial}$ closed, and furthermore, the cohomology class in $H_{\overline{\partial}}^{2k+1}(M)$ represented by it coincides with the one represented by $D_k(\overline{\partial}_0,\overline{\partial}_1)$. The proof is exactly identical to Proposition 2.4.

As in Sec. II, we have the following corollary.

Corollary 3.2: If there is a path γ connecting $\overline{\partial}_1$ with $\overline{\partial}_0$ such that each $\gamma(t)$ is an integrable holomorphic structure on E, then the cohomology class in $H_{\overline{\partial}}^{2k+1}(M)$ represented by $D_k(\overline{\partial}_0,\overline{\partial}_1)$ vanishes if $k\geqslant 1$.

Let $\overline{\partial}_2 \in \mathrm{Hol}(E)$ be a third integrable Dolbeault operator. The above corollary has the following generalization.

Proposition 3.3: If there is a path γ connecting $\overline{\partial}_1$ with $\overline{\partial}_2$ such that each $\gamma(t)$ is an integrable holomorphic structure on E, then for any $k\geqslant 1$, the cohomology class in $H_{\overline{\partial}}^{2k+1}(M)$ represented by $D_k(\overline{\partial}_0,\overline{\partial}_2)$ coincides with the one represented by $D_k(\overline{\partial}_0,\overline{\partial}_1)$.

Proof: Since the cohomology class $D_k(\overline{\partial}_0,\overline{\partial}_2)$ does not depend on the choice of the path connecting $\overline{\partial}_0$ to $\overline{\partial}_2$ (see the paragraph before Corollary 3.2) we will compute $D_k(\overline{\partial}_0,\overline{\partial}_2)$ by constructing a path.

Fix a path δ in $\mathrm{Dol}(E)$ connecting $\overline{\partial}_0$ to $\overline{\partial}_2$ that passes through $\overline{\partial}_1$. The path is assumed to pass through $\overline{\partial}_1$ exactly once. Since $\mathrm{Dol}(E)$ is an affine space, such a path exists. Let δ_1 denote the part of δ from $\overline{\partial}_0$ to $\overline{\partial}_1$ and δ_2 the rest, namely the part from $\overline{\partial}_1$ to $\overline{\partial}_2$. Since the integral [as in (3.1)] over δ is the sum of integrals over δ_1 and δ_2, and by Corollary 3.2 the cohomology class represented by the integral over δ_2 is zero, the proof is complete. □

Instead of holomorphic structures on E, we can consider a differential operator

$$\partial_E : E \to \Omega_M^{1,0}(E)$$

satisfying the Leibniz identity $\partial_E(fs)=f\partial_E s+s\partial f$ and the integrability condition $\partial_E\circ\partial_E=0$. If ∂_0 and ∂_1 are two such differential operators, then imitating (3.1) define

$$D'_k(\partial_0,\partial_1):=\int_0^1 \mathrm{trace}((\partial_1-\partial_0)\wedge(\partial_t\circ\partial_t)^k), \tag{3.2}$$

where $\partial_t:=(1-t)\partial_0+t\partial_1$. The $(2k+1,0)$-form $D'_k(\partial_0,\partial_1)$ is ∂ closed, and hence gives a cohomology class in $H^{2k+1}_{\partial}(M)$.

Fix a Hermitian structure on the C^∞ vector bundle E. Given any $\overline{\partial_E}\in\mathrm{Hol}(E)$, there is a unique connection on E, known as the *Chern connection*, determined by the following two conditions: the connection preserves the Hermitian structure and the (0,1) part of the connection coincides with $\overline{\partial_E}$.

The (1,0) part of the Chern connection is a differential operator of the above type. Take $\overline{\partial_i}\in\mathrm{Hol}(E)$, $i=0,1$, and let ∂_i be the (1,0) part of the corresponding Chern connection. It is easy to check that

$$D_k(\overline{\partial_0},\overline{\partial_1})=-\overline{D'_k(\partial_0,\partial_1)},$$

where D_k and D'_k are defined in (3.1) and (3.2), respectively. Indeed, this follows immediately from the fact that if $\partial_2+\overline{\partial_2}$ is a connection on E preserving the Hermitian structure, then the connection $(\partial_2-\beta^*)+(\overline{\partial_2}+\beta)$ on E also preserves the Hermitian structure, where β is any $\mathrm{End}(E)$-valued (0,1)-form.

The construction of the cohomology class $D_k(\overline{\partial_0},\overline{\partial_1})$ can be generalized as follows.

Let T be a compact oriented smooth manifold of dimension $d+1$. The manifold T is assumed to have a boundary. Let $S=\partial T$ be the boundary.

Take a smooth map

$$f:S\to\mathrm{Dol}(E). \tag{3.3}$$

Since $\mathrm{Dol}(E)$ is an affine space, f extends to a smooth map

$$F:T\to\mathrm{Dol}(E).$$

Indeed, any smooth function on S extends to T as a smooth function. Since $\mathrm{Dol}(E)$ is isomorphic to a vector space, this extension property remains valid for functions with values in $\mathrm{Dol}(E)$.

For the Dolbeault operator $F(t)$, the obstruction to integrability, namely $F(t)\circ F(t)$ will be denoted by $F(t)^2$. So, $F(t)^2\in C^\infty(M,\Omega^{0,2}_M(\mathrm{End}(E)))$. Using F, we have a $(d+1)$-form on T, with values in $C^\infty(M,\Omega^{0,2k-l+2}_M)$ which is defined as follows. Take any $t\in T$ and let

$$dF(t):T_tT\to C^\infty(M,\Omega^{0,1}_M(\mathrm{End}(E)))$$

be the differential of the map F. [Recall that $\mathrm{Dol}(E)$ is an affine space for the vector space $C^\infty(M,\Omega^{0,1}_M(\mathrm{End}(E)))$.] Take two integers $k,l\geqslant 0$. Associating to tangent vectors $v_i\in T_tT$, $i\in[1,l]$, the form

$$\mathrm{trace}((dF(t)(v_1)\wedge dF(t)(v_2)\wedge\cdots\wedge dF(t)(v_l))\wedge(F(t)^2)^{k-l+1})\in C^\infty(M,\Omega^{0,2k-l+2}_M)$$

we get a l-form on T with values in $C^\infty(M,\Omega^{0,2k-l+2}_M)$. This form on T will be denoted by Θ_l.

Lemma 3.4: The integral

$$\int_T\Theta_{d+1}\in C^\infty(M,\Omega^{0,2k+1-d}_M)$$

is $\overline{\partial}$ closed. Furthermore, its Dolbeault cohomology class is independent of the extension F. In other words, it depends only on f in (3.3).

Proof: It is a straightforward computation to check that the identity

$$(d\Theta_l)(v_1,v_2,\ldots,v_{l+1})=(k+1-l)\overline{\partial}(\Theta_{l+1}(v_1,v_2,\ldots,v_{l+1})) \tag{3.4}$$

is valid, where $v_i \in T_tT$.

For the inclusion map of S, the pullback of Θ_d to S vanishes identically. Now using (3.4), Stokes' theorem for the form Θ_d on T says that $\int_T \Theta_{d+1}$ is a $\overline{\partial}$-closed form.

Suppose F and F_1 are two extensions of f to T. Set $\overline{T}=T\times[0,1]$ and define

$$\overline{F}:\overline{T}\to \mathrm{Dol}(E)$$

by $\overline{F}(z,s)=(1-s)F(z)+sF_1(z)$, where $z\in T$ and $s\in[0,1]$. Now in (3.4), set $T=\overline{T}$ and $F=\overline{F}$. From Stokes' theorem in (3.4) with $l=d+1$, it follows immediately that $\int_T \Theta_{d+1}$ represents the same cohomology class for both F and F_1. This completes the proof of the lemma.

The identity (3.4) shows that the cohomology class represented by $\int_T \Theta_{d+1}$ does not depend on T. Indeed, let T' be another oriented manifold with boundary such that $\partial T'=S$. Denote $T\cup_S T'$, the gluing of T with T' along S, by T_2. So T_2 is an oriented manifold without boundary. The identity (3.4) says that the form Θ_{d+1} is exact. Consequently,

$$\int_{T_2}\Theta_{d+1}=0.$$

In other words, $\int_T \Theta_{d+1}=\int_{T'}\Theta_{d+1}$. Therefore, we have the following theorem.

Theorem 3.5: *Given any map*

$$f:S\to \mathrm{Dol}(E),$$

where S is a boundary of some smooth oriented manifold, the integral

$$\int_T \Theta_{d+1}\in C^\infty(M,\Omega_M^{0,2k+1-d}),$$

where T is a manifold with boundary given by S, gives a cohomology class in $H_{\overline{\partial}}^{2k+1-d}(M)$ which depends only on f and, in particular, it is independent of the choices of T and the extension of the map f to T.

In the next section, some rigidity properties of the cohomology classes defined in Lemma 2.3 and Lemma 3.1 are described.

IV. RIGIDITY PROPERTIES

Let ∇ be a connections on E whose curvature coincides with θ^2, where θ is a $\mathrm{End}(E)$ valued one-form. Let A be a C^∞ automorphism of E. Set $\nabla_1=A^*\nabla$. Therefore, the curvature of the connection ∇_1 coincides with $(A^*\theta)^2$.

Proposition 4.1: The cohomology class $C_k(\nabla,\nabla_1)\in H^{2k+1}(M,\mathbb{C})$ defined in Lemma 2.3 is contained in the image of $H^{2k+1}(M,(2\pi\sqrt{-1})^{k+1}\mathbb{Z})$.

Proof: Consider the pullback of E to $M\times[0,1]$ using the natural projection to M. Construct the vector bundle $\overline{E}$ over $M\times S^1$ identifying this pullback bundle along $M\times\{0\}$ and $M\times\{1\}$ using the automorphism A of E. Let $\overline{\nabla}$ be the connection on $\overline{E}$ which is $t\nabla+(1-t)\nabla_1$ on $M\times\{t\}$ and coincides with the trivialization in the direction of $[0,1]$. Consider the Künneth decomposition of the Chern character form $(k+1)!\mathrm{Ch}^{k+1}(\overline{E})$ over $M\times S^1$ of the connection $\overline{\nabla}$ over $\overline{E}$. The Künneth component of type $(2k+1,1)$ coincides with the form $C_k(\nabla,\nabla_1)\otimes dt$, where

$C_k(\nabla,\nabla_1)$ is defined in (2.2) and dt is the natural one-form on $S^1=\mathbb{R}/\mathbb{Z}$. Since the cohomology class represented by $(k+1)!\mathrm{Ch}^{k+1}(\overline{E})$ is in the image of $H^{2k+2}(M\times S^1,(2\pi\sqrt{-1})^{k+1}\mathbb{Z})$, each of its Künneth components are also in the image of the cohomology group with values in $(2\pi\sqrt{-1})^{k+1}\mathbb{Z}$. Therefore, the cohomology class represented by $C_k(\nabla,\nabla_1)$ is in the image of $H^{2k+1}(M,(2\pi\sqrt{-1})^{k+1}\mathbb{Z})$ and the proposition is proved. □

We will show that if $\overline{\partial}_0$ and $\overline{\partial}_1$ are two holomorphic structures on a C^∞ vector bundle E related by an automorphism of E, then the cohomology class represented by the form $D_k(\overline{\partial}_0,\overline{\partial}_1)$ is integral.

Let M be a complex manifold. For any $n\geqslant 0$, consider the natural projection

$$\tau(n):C^\infty(M,\wedge^n T^*_{\mathbb{C}}M)\to C^\infty(M,\Omega^{0,n}_M)$$

that sends a complex n form to its component of type $(0,n)$. Here $T^*_{\mathbb{C}}M:=T^*M\otimes_{\mathbb{R}}\mathbb{C}$ is the complexified cotangent bundle. The following diagram of homomorphisms

$$\begin{array}{ccc} C^\infty(M,\wedge^n T^*_{\mathbb{C}}M) & \stackrel{d}{\to} & C^\infty(M,\wedge^{n+1} T^*_{\mathbb{C}}M) \\ \downarrow\tau(n) & & \downarrow\tau(n+1) \\ C^\infty(M,\Omega^{0,n}_M) & \stackrel{\bar\partial}{\to} & C^\infty(M,\Omega^{0,n+1}_M) \end{array}$$

is commutative. Therefore, $\tau(n)$ induces a homomorphism

$$\hat\tau(n):H^n(M,\mathbb{C})\to H^n_{\mathrm{Dol}}(M) \tag{4.1}$$

from the complex de Rham cohomology to the Dolbeault cohomology.

Consider the inclusion map of the constant sheaf $\mathbb{C}$ on M in the structure sheaf $\mathcal{O}_M$. This map induces a homomorphism

$$H^n(M,\mathbb{C})\to H^n(M,\mathcal{O}_M)=H^n_{\mathrm{Dol}}(M)$$

which obviously coincides with $\hat\tau(n)$ constructed in (4.1).

Let E be a holomorphic vector bundle over M defined by a Dolbeault operator $\overline{\partial}_0$. Take a C^∞ automorphism A of E. Set

$$\overline{\partial}_1:=A^{-1}\circ\overline{\partial}_0\circ A$$

to be the new holomorphic structure on E defined by A.

Theorem 4.2: *The Dolbeault cohomology class $D_k(\overline{\partial}_0,\overline{\partial}_1)$ defined in* (3.1) *is in the image of $H^{2k+1}(M,(2\pi\sqrt{-1})^{k+1}\mathbb{Z})$ for the map $\hat\tau(2k+1)$ defined in* (4.1).

Proof: Take a connection ∇ on E such that the (0,1) component of ∇ coincides with $\overline{\partial}_0$. For example, ∇ can be the Chern connection for a Hermitian structure on the holomorphic vector bundle E.

Set $\nabla_1:=A^*\nabla$. Consider the vector bundle $\overline{E}$ over $M\times S^1$ constructed in the proof of Proposition 4.1, and construct the connection $\overline{\nabla}$ on $\overline{E}$ exactly as in the proof of Proposition 4.1.

Let

$$\beta\in H^{2k+1}(M,\mathbb{C})\otimes H^1(S^1,\mathbb{C})$$

be the Künneth component of the Chern character form $(k+1)!\mathrm{Ch}^{k+1}(\overline{E})$ for the connection $\overline{\nabla}$. Using the natural isomorphism $H^1(S^1,\mathbb{C})\cong\mathbb{C}$, the cohomology class β gives an element $\hat\beta\in H^{2k+1}(M,\mathbb{C})$. It was noted in the proof of Proposition 4.1 that $\hat\beta$ is in the image of $H^n(M,(2\pi\sqrt{-1})^{k+1}\mathbb{Z})$.

From the definition of the form $D_k(\overline{\partial}_0, \overline{\partial}_1)$ given in (3.1) it follows immediately that the differential form $\tau(2k+1)(\hat{\beta})$ on M of Hodge type $(0,2k+1)$ coincides with $D_k(\overline{\partial}_0, \overline{\partial}_1)$. This completes the proof of the theorem. □

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How to generate spinor representations in any dimension in terms of projection and nilpotent operators

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We present a technique to construct a spinor space basis as products of certain nilpotents and projections formed from γ^a for which we only need to know that they obey the Clifford algebra. The technique works for all dimensions and signatures. We use this technique to deliver a concrete choice of γ-matrices and Lorentz group generators for (fundamental representations of) spinors in a rather systematic and transparent way. We further develop the formalism by proposing the corresponding graphic presentation of basic states, which offers an easy way to see all the quantum numbers of states with respect to the generators of the Lorentz group, as well as transformation properties of the states under any element of the Clifford algebra. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1505125]

I. INTRODUCTION

If one wants to work with the Dirac (or the Weyl) spinor states, one *a priori* has the problem that one must choose a certain representation of the γ^a-matrices before writing down in a safe way any state of the spinor. It is therefore often attractive to avoid as long as possible writing down explicit spinor states. In this article, we propose the construction of a basis for spinors made out of products of the formal Clifford algebra objects, presented later in this article. Looking for how the left multiplication with γ^a transforms these formal Clifford algebra objects, we construct representations for the γ^a and accordingly for all the products of γ^a. These technique enables us accordingly to find solutions of the Weyl or the Dirac equation without making a choice of a special representation for γ^a operators.

The technique is built on the property of spinors that eigenstates of a particular member of the Cartan subalgebra of the Lorentz group can be expressed as nilpotents and projectors, expressions which are constructed out of γ^a's as odd and even objects in γ^a's, respectively, and accordingly a spinor basis can be expressed as products of nilpotents and projectors, operating on an (unimportant) ''vacuum state.''

We indeed start by taking γ^a's as abstract objects, fulfilling the Clifford algebra (Sec. II). We then construct a series of the Clifford algebra elements, which can be used as a basis for the representation of the Clifford algebra in the following sense: When multiplying from the left these special Clifford algebra elements, which we call our ''basis,'' with any of the Clifford algebra elements, we get a linear combination of these ''basic'' elements back. In other words, our ''basis'' spans a left ideal. (The reader should see also Chap. 3 of Chevalley's book.[1,2]) We can consider the action of left multiplication by an element of the Clifford algebra on the space spanned by the ''basis'' as a representation of the Clifford algebra. Accordingly we show by this procedure the (well known[3]) fact that the Clifford algebra has an operator representation, which is known as the

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spinor space. So we can consider elements of our special ''basis'' as a proposal for a basis for spinors.

The proposed technique was initiated and developed by one of the authors of this article, when proposing an approach[4–6] in which all the internal degrees of freedom of either spinors or vectors can be described in the space of d-anticommuting (Grassmann) coordinates, if the dimension of ordinary space is also d. In this approach (two kinds of) γ^a operators were defined. One of the two kinds of γ^a's was used to generate nilpotents and projectors—eigenstates of the Cartan subalgebra of the Lorentz group—products of which define, when operating on a vacuum state, basic vectors. These 2^d basic vectors are polynomials of anticommuting coordinates and are orthonormal with respect to the inner product defined as an integral over anticommuting coordinates, with an appropriately chosen weight function. They form an orthonormal basis for spinors.

Both authors of this work then used the results of this approach in the space of differential forms to generalize[7] the approach of Kähler,[8] who defined in the space of differential forms spins of spinors.

We recognized that mapping of ideals to spinor representations can lead either to only one irreducible representation or to ''families'' of representations (Sec. V) (which we have noticed before[5,6]). We investigate the consequence of seeking to keep all the basis spinors corresponding to our basis in the Clifford algebra linearly independent. That of course means that a reducible representation of the Clifford algebra is needed and it is to have for d even $2^{d/2}$ replicas and for d odd $2^{(d+1)/2}$ replicas of the usual irreducible spinor representation. Usually, of course, we deal with only one ''family,'' that is with only one Dirac spinor.

Using this technique, it is then straightforward, for example, to find solutions of the Dirac equation, for either massless or massive spinors, for any dimension d and for any signature (Sec. IX), or to apply any operator to a spin state (Secs. III C and VII), or to find irreducible representations of subgroups of the Lorentz group $\mathrm{SO}(q,d-q)$, where q means the number of timelike coordinates.

We further propose a very simple graphic representation (Sec. VI), which makes the technique transparent by enabling us to easily see all the quantum numbers of states with respect to the generators of the Lorentz group, as well as how states transform when operated on by the operators.

We demonstrate (Sec. VIII) the proposed technique as well as the graphic representation of this technique for $d=3$ and $d=4$ and the Minkowski metric.

In this article, we assume an arbitrary signature of space–time so that our metric tensor η^{ab}, with $a,b \in \{0,1,2,3,5,\ldots\}$, is diagonal with values $\eta^{aa}=\pm 1$, depending on the chosen signature ($+1$ for timelike coordinates and -1 for spacelike coordinates).

II. CLIFFORD AND LORENTZ ALGEBRA

It is well known that there exist for any dimension d and any signature the operators γ^a which fulfill the Clifford algebra. Following the Dirac procedure (a similar procedure with quadratic forms can be found in Ref. 1), one finds the algebra which γ^a's have to fulfill by assuming the equation of motion for a particle, which is called a spinor, to be linear in the momentum p^a. A momentum p^a is a vector in a d-dimensional space, in which the metric tensor η_{ab} (assumed for simplicity diagonal) has q diagonal elements being 1 and $p=d-q$ being -1. For this purpose the operators γ^a, with a vector index a, have to be introduced, which commute with p^a, and operate on some abstract space which is called the spinor space. So, when considering γ^a, we understand that we are making a basis in the vector space marked with the index a.

In order that an equation of motion linear in the momentum p^a and therefore of the form $\gamma_a p^a \psi=0$ for a wave function ψ should lead to the Klein–Gordon equation $p^a \eta_{ab} p^b \psi=0$ (when multiplied from the left by $\gamma_a p^a$, say), it should be required that the operators on the spinor space γ^a should obey the algebra, called the Clifford algebra,

$$\{\gamma^a,\gamma^b\}_+ = I2\,\eta^{ab}, \quad \text{for} \quad a,b \in \{0,1,2,3,5,\ldots,d\}, \tag{1}$$

for any d, even or odd, and with I, which is the unit element in the Cliffird algebra. Here $\{\gamma^a,\gamma^b\}_\pm=\gamma^a\gamma^b\pm\gamma^b\gamma^a$.

In this article, we start by assuming abstract objects γ^a for which we only need to know that they fulfill the Clifford algebra [Eq. (1)]. We do not assume that they are the operators. We deduce that they can be represented by operators operating on a space spanned by a certain basis which we construct out of the Clifford algebra objects γ^a themselves.

We are therefore considering a Clifford algebra $\mathcal{C}$ over a d-dimensional vector space and denote a set of elements corresponding to an orthonormal basis in the vector space for which this Clifford algebra [Eq. (1)] is defined as γ^a $(a\in\{0,1,2,3,5,6,\ldots d-1,d\})$. The quadratic form, for which this Clifford algebra is defined, is taken to be given by the metric $Q(x)=p^a\eta_{ab}p^b$, with p^a being vectors in the d-dimensional vector space.

We can impose an antilinear anti-automorphism for elements A,B,C of the Clifford algebra, which we denote by $(^\dagger)$,

$$\begin{aligned}(AB\cdots C)^\dagger&=C^\dagger\cdots B^\dagger A^\dagger,\\(\alpha A+\beta C)^\dagger&=\alpha^* A^\dagger+\beta^* B^\dagger,\end{aligned}\tag{2}$$

with $(^*)$ meaning complex conjugation. We easily see a possible choice for such an operation $(^\dagger)$ for elements made out of γ^a's by defining the "Hermiticity" property for γ^a's,

$$\gamma^{a\dagger}=\eta^{aa}\gamma^a,\tag{3}$$

in order that γ^a are compatible with (1) and formally unitary, i.e., $\gamma^{a\dagger}\gamma^a=I$, and I is the unity operator.

We also define the Clifford algebra objects

$$S^{ab}=\frac{i}{4}[\gamma^a,\gamma^b]:=\frac{i}{4}(\gamma^a\gamma^b-\gamma^b\gamma^a),\tag{4}$$

which close the Lie algebra of the Lorentz group

$$\{S^{ab},S^{cd}\}_-=i(\eta^{ad}S^{bc}+\eta^{bc}S^{ad}-\eta^{ac}S^{bd}-\eta^{bd}S^{ac})\tag{5}$$

and have the following "Hermiticity" property

$$S^{ab\dagger}=\eta^{aa}\eta^{bb}S^{ab}.\tag{6}$$

We also see that these objects of the Lorentz algebra being imbedded in the Clifford algebra fulfill the relation

$$\{S^{ab},S^{ac}\}_+=\tfrac{1}{2}\eta^{aa}\eta^{bc},\tag{7}$$

which is true only for the Dirac (or the Weyl) spinors (known also as the fundamental representation of the Lorentz group).

We recognize the similarity transformation properties of γ^a's with respect to the Lorentz group

$$e^{i\omega_{cd}S^{cd}}\gamma^a e^{-i\omega_{cd}S^{cd}}=\Lambda^a{}_b(\omega)\gamma^b.\tag{8}$$

Recognizing from Eq. (5) that two Clifford algebra objects S^{ab},S^{cd} with all indices different commute, we readily select the Cartan subalgebra of the algebra of the Lorentz group, which has a basis of

$$m=d/2, \text{ for } d \text{ even},$$

$$m=(d-1)/2, \text{ for } d \text{ odd}, \tag{9}$$

commuting objects.

It is useful also to define one of the Casimirs of the Lorentz group (which will later be used to determine the handedness of an irreducible representation of the Lorentz group). (To see the definition of the operator Γ for any spin in even-dimensional spaces, see Refs. 5, 9–12, and 7.) When once the representation will be built

$$\Gamma: \ =(i)^{d/2}\prod_a \ (\sqrt{\eta^{aa}}\gamma^a), \text{ if } d=2n,$$

$$\Gamma: \ =(i)^{(d-1)/2}\prod_a \ (\sqrt{\eta^{aa}}\gamma^a), \text{ if } d=2n+1, \tag{10}$$

for any integer n. We understand the product of γ^a's in the ascending order with respect to the index a: $\gamma^0\gamma^1\cdots\gamma^d$. Since $(\sqrt{\eta^{aa}}\gamma^a)^\dagger=\sqrt{\eta^{aa}}\gamma^a$ and $(\sqrt{\eta^{aa}}\gamma^a)^2=I$, which is the unit element in the Clifford algebra, then it follows for any choice of the signature η^{aa} that Γ is "Hermitian" in the sense of the antilinear antiautomorphism of Eqs. (2), and (3) and its square is equal to the unity element

$$\Gamma^\dagger=\Gamma,$$

$$\Gamma^2=I. \tag{11}$$

One also finds that in even-dimensional spaces Γ "anticommutes" while in odd-dimensional spaces Γ "commutes." Two formal Clifford objects A and B "commute" or "anticommute," if they fulfill the relation $\{A,B\}_\mp=0$, with $(-)$ and $(+)$, respectively, under the left multiplication, with γ^a's

$$\{\Gamma,\gamma^a\}_+=0, \text{ for } d \text{ even},$$

$$\{\Gamma,\gamma^a\}_-=0, \text{ for } d \text{ odd}. \tag{12}$$

Accordingly, Γ always "commutes" with the generators of the Lorentz algebra S^{ab}.

III. BASIS IN SPINOR SPACE *S*

In this section we are constructing successively a set of 2^d Clifford algebra elements, which if any one of them is multiplied from the left by any of the $d/2$ members S^{ab} of the chosen basis for the Cartan subalgebra of the Lorentz group, Eq. (4) is mapped up to a factor to the same element of the set. We shall start by constructing for each member S^{ab} a set of four of the Clifford algebra elements $(\frac{1}{2})(\gamma^a+ik\gamma^b)$, $(\frac{1}{2})(1+ik\gamma^a\gamma^b)$, with $k^2=\eta^{aa}\eta^{bb}$ and $k=\pm1$ or $\pm i$, depending on the signature η^{aa} and η^{bb}. We shall call two of them "nilpotents" and two of them "projectors," since, when squared, nilpotents map into zero while projectors map into themselves.

We shall then construct the basis for spinors out of $d/2$ factors of these nilpotents and projectors, each member of the Cartan subalgebra being represented by one out of four possibilities. The spinor representation for the Lorentz group will be selected by the application of (all) the elements of the Lorentz algebra on a starting object of $d/2$ factors. A representation will be called the Weyl representation. All the elements of the Clifford algebra will select what we call a Dirac spinor representation. This will lead to the basis for the Clifford algebra elements, which we shall recognize as spinor representation for the Lorentz group. We shall accordingly show that the Clifford algebra objects can be represented as operators acting on these basic states. The procedure

will enable us to construct an explicit matrix representation with concretely constructible matrices representing the γ^a-matrices. These means that we construct the basis in the spinor space from a basis in the vector space M. We shall tell what specifications we need for the construction. The basis in the vector space M used will be taken to be an orthonormal basis so that the different basis vectors are normalized to $Q(e^a)=\pm 1$ according to whether the basic vector in question is space- or timelike.

We shall make our construction formulated for general dimension and signature (i.e., for general index also).

A. Decisions for choosing a basis in spinor space

It is obvious that by specifying whatever properties of a set of spinors, say basis, belong to $\mathcal{S}$ concerning the linear operation of the representatives of the Clifford algebra, say of the γ^a's, we can never specify the overall phase for this set, i.e., if we have a basis ψ_i, $i=1,\ldots,n$, with $n=2^{d/2}$ for d even and $n=2^{(d-1)/2}$ for d odd (the well-known spinor space dimensions will come out also of our formalism below) fulfilling a set of specifications, then so do $e^{i\phi}\psi_i$.

So we only can (and have to) specify the *relative* phase of the various basis spinors, which will also specify phases in the explicit matrix representation of the Clifford algebra. We attempt to make an as simple as possible choice of the basis and its relative phases (putting all phases equal to one) so that the reader can easily remember and reproduce the procedure.

The basis elements for spinors will be chosen as eigenstates under the left multiplication of the chosen basis for the Cartan subalgebra for the Lorentz/orthogonal group $\mathcal{G}$.

B. Eigenstates of Cartan subalgebra elements

We consider the left multiplication with the elements of the Cartan subalgebra. We call ψ an eigenstate of the Cartan subalgebra basis $\{S^{ab},S^{cd},\ldots\}$, if the left multiplication of ψ with the Cartan subalgebra basis maps ψ back to itself up to a complex number. We look for a basis of 2^d eigenstates of the Cartan subalgebra.

According to the algebra of the Lorentz group [Eq. (5)], one can make infinitely many choices of a set [of $d/2$ for d even and $(d-1)/2$ for d odd], commuting elements of the Cartan subalgebra out of $d(d-1)/2$ elements of the Lorentz algebra. In order to be able at the end to present elements of the Clifford algebra as operators—operating on the spinors, which we are constructing successively in this article—in terms of numbers, we make an explicit choice of elements of the Cartan subalgebra.

We shall select elements belonging to the Cartan subalgebra in a given coordinate system as follows,

$$\begin{aligned} &S^{0d},S^{12},S^{35},\ldots,S^{d-2d-1}, \ \text{if} \ d=2n, \\ &S^{12},S^{35},\ldots,S^{d-1d}, \ \text{if} \ d=2n+1, \end{aligned} \tag{13}$$

with raising indices from the left to the right and within each of a chosen element of the Lorentz algebra.

One can easily see that for spinors [Eq. (7)] the element of the Clifford algebra Γ, which will be chosen to determine what we call handedness of eigenstates of the Cartan subalgebra, can for even-dimensional spaces be written in terms of the elements of the Cartan subalgebra as follows:

$$\Gamma=2^{d/2}\prod_a \sqrt{\eta^{aa}}\ S^{0d}S^{12}S^{35}\cdots S^{d-2d-1}, \ \text{if} \ d=2n. \tag{14}$$

For odd-dimension we can write

$$\Gamma=2^{(d-1)/2}\prod_a \sqrt{\eta^{aa}}\ \gamma^0 S^{12}S^{35}\cdots S^{d-1d}, \ \text{if} \ d=2n+1. \tag{15}$$

We can now present a trivial theorem which helps, however, to find eigenstates of the above chosen Cartan subalgebra of the Lorentz group.

Theorem 1a: Let S^{ab} be the element of the Cartan subalgebra of Eq. (9), for which $\eta^{aa}\eta^{bb}=1$. Then elements of the Clifford algebra

$$\overset{ab}{(\pm)} := \frac{1}{2}\left(\gamma^a \pm \frac{\eta^{bb}}{i}\gamma^b\right), \quad \overset{ab}{[\pm]} := \frac{1}{2}(1 \pm i\gamma^a\gamma^b), \tag{16}$$

are eigenstates for the left multiplication with S^{ab} with the eigenvalues $\pm(\frac{1}{2})$ in both cases.

Proof: To prove this theorem we only have to make the left multiplication of $\overset{ab}{(\pm)}$ and $\overset{ab}{[\pm]}$ by $S^{ab}=(i/2)\gamma^a\gamma^b$, $a\neq b$. We easily find the above result.

Theorem 1b: Let S^{ab} be the generator of the Cartan subalgebra of Eq. (9) for which $\eta^{aa}\eta^{bb}=-1$. Then elements of the Clifford algebra

$$\overset{ab}{(\pm i)} := \tfrac{1}{2}(\gamma^a \pm \eta^{bb}\gamma^b), \quad \overset{ab}{[\pm i]} := \tfrac{1}{2}(1 \pm \gamma^a\gamma^b), \tag{17}$$

are eigenstates for the left multiplication with S^{ab} with the eigenvalues $\pm(i/2)$ in both cases.

Proof: The proof follows the proof of Theorem 1a.

According to these two theorems, we can construct states which are eigenstates of all the Cartan subalgebra elements by making products of expressions from Theorems 1a and 1b.

We find that while elements of the Clifford algebra either $\overset{ab}{[\pm]}$ or $\overset{ab}{[\pm i]}$ are idempotent,

$$\overset{ab}{[\pm]}^2 = \overset{ab}{[\pm]}, \quad \overset{ab}{[\pm i]}^2 = \overset{ab}{[\pm i]}, \tag{18}$$

the elements $\overset{ab}{(\pm)}$ and $\overset{ab}{(\pm i)}$ are nilpotent

$$\overset{ab}{(\pm)}^2 = 0, \quad \overset{ab}{(\pm i)}^2 = 0. \tag{19}$$

According to the above theorem, it is straightforward to prove the following theorem.

Theorem 2: For an even dimension $(d=2n)$ the states

$$(\gamma^0 \pm \sqrt{-\eta^{00}\eta^{dd}}\gamma^d)(\gamma^1 \pm \sqrt{-\eta^{11}\eta^{22}}\gamma^2)\cdots(\gamma^{d-2} \pm \sqrt{-\eta^{d-2d-2}\eta^{d-1d-1}}\gamma^{d-1}), \tag{20}$$

or any state which follows from one of the states of Eq. (20) by replacing any of the expressions $(\gamma^a \pm \sqrt{-\eta^{aa}\eta^{bb}}\gamma^b)$ by the corresponding $(1 \pm \sqrt{-\eta^{aa}\eta^{bb}}\gamma^a\gamma^b)$, are the eigenstates of all the elements of the Cartan subalgebra of Eq. (13) for an even dimension, with the eigenvalue of the chosen S^{ab} determined by Theorems 1a and 1b, while the eigenvalue of the element of the Clifford algebra defining handedness [Eq. (10)] can easily be calculated by taking into account Eqs. (14) and (15) and the fact that $\gamma^a\gamma^b=-2iS^{ab}$.

For an odd dimension $(d=2n+1)$ the states

$$(1\pm\Gamma)\gamma^0(\gamma^1 \pm \sqrt{-\eta^{11}\eta^{22}}\gamma^2)(\gamma^3 \pm \sqrt{-\eta^{33}\eta^{55}}\gamma^5)\cdots(\gamma^{d-1} \pm \sqrt{-\eta^{d-1d-1}\eta^{dd}}\gamma^d), \tag{21}$$

or any state which follows from one of the states of Eq. (21) by replacing any of the expressions $(\gamma^a \pm \sqrt{-\eta^{aa}\eta^{bb}}\gamma^b)$ by the corresponding $(1 \pm \sqrt{-\eta^{aa}\eta^{bb}}\gamma^a\gamma^b)$, are the eigenstates of all the elements of the Cartan subalgebra of Eq. (13) of odd dimension, with the eigenvalues of the chosen S^{ab} determined in Theorems 1a and 1b and with the eigenvalue of Γ which follow if taking into account Eq. (10).

The proof for d even or d odd follows from Theorems 1a and 1b and the fact that Γ commutes with all S^{ab}.

It is simple to count the number of basic states, which is 2^d.

C. Irreducible representations of Lorentz group for spinors

In Sec. III B we constructed eigenstates of the basis of the Cartan subalgebra. From Eqs. (14) and (15) one easily sees that they are at the same time also the eigenstates of Γ, which defines handedness of states. We make a choice of one of these states, calling it a ''starting state.'' It is not difficult to prove that one gets an irreducible representation of the Lorentz group by the left multiplication of this state with all the elements of the Lorentz algebra S^{ab}, which do not belong to the Cartan subalgebra [Eq. (13)] [or by the left multiplication of the ''starting state'' by a group element $O(\omega)=\exp(-(i/2)\omega_{ab}S^{ab})$]. (To prove that a set of states, which follows from the ''starting state'' by the application of all the members of the Lorentz algebra, forms an irreducible representation, one only has to count the number of states in this particular set of states [which is for d even $2^{d/2-1}$ and since in the Dirac representation left and right handed states are required one has to multiply this number by 2 and for d odd the number of states is $2^{(d-1)/2}$ (Sec. V)] and then also the number of ''families'' [which is for d even equal to $2^{d/2}$ and for d odd $2^{(d+1)/2}$ (Sec. V)] to see that the number of all the states is equal to 2^d, as it should be.)

We present theorems, which help to find all the irreducible representations of the Lorentz group.

Theorem 3: Let S^{ab} and S^{cd} be the two elements of the Cartan subalgebra. Then the two vectors

$$\begin{aligned}&(\gamma^a+\sqrt{-\eta^{aa}\eta^{bb}}\gamma^b)(\gamma^c+\sqrt{-\eta^{cc}\eta^{dd}}\gamma^d),\\&\left(1+\frac{1}{\eta^{aa}}\sqrt{-\eta^{aa}\eta^{bb}}\gamma^a\gamma^b\right)\left(1+\frac{1}{\eta^{cc}}\sqrt{-\eta^{cc}\eta^{dd}}\gamma^c\gamma^d\right)\end{aligned}\tag{22}$$

belong to the same representation of the left action of the Lorentz algebra.

Proof: To prove the theorem we multiply from the left by $S^{ac}=(i/2)\gamma^a\gamma^c$ (or by S^{ad} or S^{bc} or S^{bd}) the first state

$$\begin{aligned}&\frac{i}{2}\gamma^a\gamma^c(\gamma^a+\sqrt{-\eta^{aa}\eta^{bb}}\gamma^b)(\gamma^c+\sqrt{-\eta^{cc}\eta^{dd}}\gamma^d)\\&\quad=-\frac{i}{2}\eta^{aa}\eta^{cc}\left(1+\frac{1}{\eta^{aa}}\sqrt{-\eta^{aa}\eta^{bb}}\gamma^a\gamma^b\right)\left(1+\frac{1}{\eta^{cc}}\sqrt{-\eta^{cc}\eta^{dd}}\gamma^c\gamma^d\right).\end{aligned}\tag{23}$$

The theorem which follows, generalizes Theorem 3.

Theorem 3a: The generators of the Lorentz transformations which do not belong to the Cartan subalgebra transform a pair of nilpotents (or a pair of a nilpotent and a projector, or a projector and a nilpotent, or two projectors) with the positive eigenvalues of the Cartan subalgebra to a pair of two projectors (or a pair of a projector and a nilpotent, or a nilpotent and a projector, or two nilpotents) with the negative values of the Cartan subalgebra. In resume, the left multiplication of the generators S^{ab} of the Lorentz transformations which do not belong to the Cartan subalgebra leaves all but the two elements, which include indices ab, of a state unchanged, while the two concerned elements change the type (that is each one changes from nilpotency to idempotency or opposite) and the eigenvalues of the corresponding Cartan subalgebra.

Theorem 4: In an odd-dimensional space the two states

$$\begin{aligned}&(1\pm\Gamma)\gamma^0(\gamma^1+\sqrt{-\eta^{11}\eta^{22}}\gamma^2)(\gamma^3+\sqrt{-\eta^{33}\eta^{55}}\gamma^5)\cdots,\\&(1\pm\Gamma)(\gamma^1+\sqrt{-\eta^{11}\eta^{22}}\gamma^2)(\gamma^3+\sqrt{-\eta^{33}\eta^{55}}\gamma^5)\cdots\end{aligned}\tag{24}$$

are proportional to each other.

Proof: We first notice that $\Gamma =: \Gamma^{(d)} = \sqrt{\eta^{00}}\gamma^0\Gamma^{(d-1)}$. The indices (d) and $(d-1)$ were added to point out that $\Gamma^{(d-1)}$ includes all the γ^a's, except the first one with factors which guarantee that either $\Gamma^{(d)}$ or $\Gamma^{(d-1)}$ fulfills the conditions of Eq. (11). Then we see that when $\Gamma^{(d)}$ is applied to the state $\gamma^0(\gamma^1+\sqrt{-\eta^{11}\eta^{22}}\gamma^2)(\gamma^3+\sqrt{-\eta^{33}\eta^{55}}\gamma^5)\cdots$, it gives $\sqrt{\eta^{00}}\eta^{00}\ \varepsilon(\gamma^1+\sqrt{-\eta^{11}\eta^{22}}\gamma^2)\times(\gamma^3+\sqrt{-\eta^{33}\eta^{55}}\gamma^5)\cdots$, where $\varepsilon(=\pm 1)$ is the eigenvalue of $\Gamma^{(d-1)}$ on the chosen state. Then it follows $(1\pm\Gamma)\gamma^0(\gamma^1+\sqrt{-\eta^{11}\eta^{22}}\gamma^2)(\gamma^3+\sqrt{-\eta^{33}\eta^{55}}\gamma^5)\cdots = \pm\varepsilon\,\eta^{00}\sqrt{\eta^{00}}(1\pm\Gamma)(\gamma^1+\sqrt{-\eta^{11}\eta^{22}}\gamma^2)(\gamma^3+\sqrt{-\eta^{33}\eta^{55}}\gamma^5)\cdots$. This completes the proof.

As a consequence of Theorem 4 the following statement follows:

Statement 1: In odd-dimensional spaces γ^a's do not transform one irreducible representation of the Lorentz group into another as they do in even-dimensional spaces.

The proof is self-evident if we take account of Theorem 4 and the fact that $\gamma^0\gamma^a = -2iS^{0a}$. (From Theorems 3 and 4 it follows that by applying to a chosen state the elements $S^{01},S^{03},\ldots,S^{0d-2},S^{13},\ldots,S^{1d-2},\ldots$ for an even d and $S^{01},S^{05},\ldots,S^{0d-1},S^{15},\ldots,S^{1d-1},\ldots$ for an odd d, we obtain all the members of a particular irreducible representation.)

Statement 2a: We find accordingly for d even $2^{d/2-1}$ and for d odd $2^{(d-1)/2}$ basis vectors of an irreducible representation, which is either left (with Γ eigenvalue equal to -1) or right (with Γ eigenvalues equal to $+1$) handed.

We can easily count the number of states in one representation following Theorem 3a just by counting the number of different products, generated by the elements of the Lorentz algebra:

Even case: Since the action of the Lorentz generators (from left multiplication) exchanges both nilpotency-versus-idempotency-character and eigenvalue sign there are in one representation only two combinations for each Cartan algebra generator and thus there can at least be made use of no more than $2^{d/2}$ in the even case, but now it is the even case, so that the S^{cb} generators change two cases at a time and thus say the number of nilpotent factors can only change by an even number as we go along inside the representation. This means that we really only get half as many products needed in the representation. That makes it have $2^{d/2-1}$ dimensions in the even case.

Odd case: In the odd case there is one of the γ^a's for which there is no place in the Cartan subalgebra generators (we made a choice of γ^0). As seen by Theorem 4 the action of this particular γ^0 from the left makes no change—except for a sign—on our products (states) and thus the generators involving this special γ^0 such as $S^{0b}=i/2\gamma^0\gamma^b$ act as a γ^b effectively and change just one of the factors, i.e., an odd number of them. This makes there being no rule guaranteeing an odd number of said nilpotents. Thus the number of products in the representation we can make to close it is $2^{(d-1)/2}$, which is thus the dimension of the found representation in the odd case.

We call these representations the Weyl spinor representations. In Sec. VI we present a graphic way of looking for representations.

Statement 2b: By applying any of the γ^a's to any of the states belonging to the above-obtained irreducible representation of the chosen handedness for an even d, the corresponding Weyl irreducible representation of the opposite handedness follows.

In even-dimensional spaces, left multiplication by γ^a's change the handedness of states, since Γ commutes with S^{ab} and anticommutes with γ^a. The representation we can close under the γ^a's has double dimension relative to the one we found for the Lorentz generators. Two Weyl spinors of the opposite handedness together have $2^{d/2}$ states for even d. We call such a representation the Dirac representation.

In an odd case, multiplication from the left brings according to Theorem 4 no extension compared to the Lorentz algebra representation.

IV. INNER PRODUCT AND SPINOR SPACE $\mathcal{S}_\rho$

Until now we considered the Clifford algebra elements as just abstract objects or elements. We found representations of these elements or the special ones among them being Lorentz generators (or products of Lorentz generators) which form the even part $\mathcal{C}_+$ of the Clifford algebra $\mathcal{C}$. Let us now formally define the (spinor) representation (map) ρ corresponding to the left multiplication

already described. That is to say, we define for any element $v \in \mathcal{C}$, i.e., for v being any linear combination of products of γ^a's, an endomorphism $\rho(v)$, i.e., a linear map $\rho(v)$ of the space $\mathcal{S}$ spanned by those basis vectors in the basis for the Clifford algebra which we have constructed and which correspond to one single representation as we found for γ^a's. For example, we easily saw that if we start from a product with factors only being our nilpotent expressions with eigenvalues of the Cartan subalgebra generators under left multiplication being $+\frac{1}{2}$ or $+i/2$ (for rotation and Lorentz boosts respectively), then we shall get in this representation under left multiplication by γ^a's only the following types of expressions (Theorem 1a and 1b):

$$\begin{aligned}
\overset{ab}{(+)} &= \frac{1}{2}\left(\gamma^a + \frac{\eta^{bb}}{i}\gamma^b\right),\\
\overset{ab}{(+i)} &= \frac{1}{2}(\gamma^a + \eta^{bb}\gamma^b),\\
\overset{ab}{[-]} &= \frac{1}{2}(1 - i\gamma^a\gamma^b),\\
\overset{ab}{[-i]} &= \frac{1}{2}(1 - \gamma^a\gamma^b).
\end{aligned} \tag{25}$$

We denote by $\mathcal{S}$ just the space spanned by these products containing just these mentioned factors. Then we simply define for $\hat{\psi} \in \mathcal{S}$

$$\rho(v)\hat{\psi} = v\hat{\psi}, \tag{26}$$

where the multiplication on the right hand side of the equation (26) $v\hat{\psi}$ is just the product of two Clifford elements. The idea, of course, is to suggest that the space $\mathcal{S}$ is the space of spinors.

We can consider our construction as a realization with an explicit basis of the same spinor space identification with an ideal in the Clifford algebra as used in the book by Chevalley[1] in Sec. III, wherein the spinor space is identified with a minimal left ideal $\mathcal{C}f = \mathcal{C}^N f$ where f is a product of basis vectors in a certain maximally totally singular subspace of the space of d-vectors identified into the Clifford algebra. The subalgebra $\mathcal{C}^N$ is one generated in the Clifford algebra from some other maximally singular subspace of the space M of d-vectors. So really it is the subalgebra $\mathcal{C}^N$ which gets identified with the space of spinors.

Strictly speaking this is not the case since the Lorentz transformation properties usually assigned to spinors only agree with the ones of the elements of $\mathcal{S}$ provided one uses only the left but not also the right multiplication by the Lorentz generators. For states to be identified with spinor states, being the part of the Hilbert space, one would like to define also the inner product. We shall construct an inner product in the next subsection.

A. Inner product and Hilbert space for spinors $\mathcal{S}_\rho$

After we have found that we can use our "basis" of the Clifford algebra elements as a basis on which to represent this algebra, i.e., as the spinor space $\mathcal{S}$, we would like to construct an inner product or Hilbert product on this space, the ideal, spanned by this basis.

It shall turn out that having chosen that the "Hermitian conjugation" operation (†) on the Clifford algebra elements γ^a defined in Sec. II is given by the equation $\gamma^{a\dagger} = \eta^{aa}\gamma^a$ (3) we have essentially specified the inner product in the sense that it only could change by a normalization overall factor.

It is actually easily seen for any pair of "spinors" v, u, (both being linear combinations of our basis vectors for the representation space $\mathcal{S}$) that using the Clifford algebra equipped with (†) have

$$v^\dagger u = c\prod [-]\prod [-i], \tag{27}$$

where c is a complex number. For the space $\mathcal{S}$ it was assumed that we only used those products as basis vectors which could be constructed alone from the expressions $(+),[-],(i),[-i]$ (which is a possible but not at all a unique choice). One can easily prove that any expression resulting when combining various terms in $v^\dagger$ and u gives either zero or a c-number times the product of the expressions $[-]$ and $[-i]$. In fact, one can see that $\overset{ab}{(+)}^\dagger = \eta^{aa}\overset{ab}{(-)}$, $\overset{ab}{(-)}\overset{ab}{(+)}\eta^{aa}\overset{ab}{[-]}$ with the same, and that also $\overset{ab}{[-]}\overset{ab}{[-]}=\overset{ab}{[-]}$ and $\overset{ab}{[-]}^\dagger=\overset{ab}{[-]}$, $\overset{ab}{[-]}\overset{ab}{(+)}=0$ as can be found in Sec. VI in more detailed form, including same relations with $\pm i$ instead of $\pm$.

This formula (27) means that we can propose the c-number c to be identified with the inner product by defining

$$\langle v|u\rangle = c, \quad \text{where} \quad v^\dagger u = c\prod [-]\cdot\prod [-i], \tag{28}$$

or

$$v^\dagger u = \langle v|u\rangle\prod [-]\prod [-i]. \tag{29}$$

Actually we can see that this definition is extremely suggestive if we assumed that we already had a representation, now on a spinor space $\mathcal{S}_\rho$, of the Clifford algebra with $(^\dagger)$ and ρ, i.e., we had

$$\begin{aligned} &\rho(AB)=\rho(A)\rho(B),\\ &\rho(aA+bB)=a\rho(A)+b\rho(B),\\ &\rho(A^\dagger)=\rho(A)^\dagger. \end{aligned} \tag{30}$$

So, for example, $\rho(\gamma^a)$ is the usual γ^a when conceived of as a matrix or operator acting on spinor states. It means accordingly that all the Clifford algebra is mapped into operators and so are our $\overset{ab}{(k)}$ and $\overset{ab}{[k]}$. It further means that we have assumed spinor states $\in\mathcal{S}_\rho$ on which these products of expressions (operators) work. So indeed we can select now one state ψ_0, which we call a ''vacuum state'' and for which we assume, in order to be able to use Eq. (29), that $\rho(\Pi[-]\Pi[-i])\psi_0$ is different from zero. Even having in mind that $\rho([-])$ or $\rho([-i])$ are projectors, we realize that this is indeed a very mild requirement.

After selecting the ''vacuum state'' one can produce the correspondence between the ''spinor states'' $\mathcal{S}$ equal to the left ideal (as Chevalley did in Chap. III in his book) and spinors in $\mathcal{S}_\rho$. The relation is of course

$$u\to\rho(u)\psi_0. \tag{31}$$

If there is an inner product defined on the space of spinors $\mathcal{S}_\rho$ $(\langle\psi_1|\psi_2\rangle_\rho)$, then the corresponding inner product on $\mathcal{S}$ is suggested to be $\langle v|u\rangle=\langle\rho(v)\psi_0|\rho(u)\psi_0\rangle$. Now we have

$$\begin{aligned} \langle\rho(v)\psi_0|\rho(u)\psi_0\rangle_\rho &= \langle\psi_0|\rho(v)^\dagger\rho(u)\psi_0\rangle_\rho = \langle\psi_0|\rho(v^\dagger u)\psi_0\rangle_\rho\\ &= \langle v|u\rangle\cdot\left\langle\psi_0\middle|\rho\left(\prod [-]\prod [-i]\right)\psi_0\right\rangle_\rho, \end{aligned} \tag{32}$$

where $\langle v|u\rangle$ is the expression from Eq. (29). We would now like to justify this inner product on $\mathcal{S}$ as a well chosen definition. To do that we have to evaluate the factor $\langle\psi_0|\rho(\Pi[-]\Pi[-i])\psi_0\rangle_\rho$ from Eq. (32), justifying that it is not important. We assumed already above that $\rho(\Pi[-]\Pi[-i])\psi_0$ is nonzero, which means that the ''vacuum state'' ψ_0 contains spinor states which have the corresponding quantum numbers so that the projector on such a state is nonzero. But since the factor $\langle\psi_0|\rho(\Pi[-]\Pi[-i])\psi_0\rangle_\rho$ does not depend on either u or v it can only be a constant, which goes into normalization. That confirms that the ''vacuum state'' only manifests itself in an overall factor. We conclude that $\langle v|u\rangle$ was a good choice [Eqs. (29) and (27)].

We have the correspondence between the Clifford algebra objects in the left ideal $\mathcal{S}$ spanned by our basis [we made a choice of $(+)(+i)$ as a starting state] and the Hilbert space of spinors $\mathcal{S}_\rho$. Having a set of products in Theorem 3, used for a basis for $\mathcal{S}$, we can now find the corresponding basis in the spinor space $\mathcal{S}_\rho$, just as an example for $d=4$:

$$\begin{aligned}&(\gamma^a+\sqrt{-\eta^{aa}\eta^{bb}}\gamma^b)(\gamma^c+\sqrt{-\eta^{cc}\eta^{dd}}\gamma^d)\psi_0,\\&\left(1+\frac{1}{\eta^{aa}}\sqrt{-\eta^{aa}\eta^{bb}}\gamma^a\gamma^b\right)\left(1+\frac{1}{\eta^{cc}}\sqrt{-\eta^{cc}\eta^{dd}}\gamma^c\gamma^d\right)\psi_0.\end{aligned}\tag{33}$$

These two states belong to one Weyl representation. To get the full basis for the representation $\mathcal{S}_\rho$ for the whole Clifford algebra (two Weyl spinors) one has to add the following two spinor basis states:

$$\begin{aligned}&(\gamma^a+\sqrt{-\eta^{aa}\eta^{bb}}\gamma^b)\left(1+\frac{1}{\eta^{cc}}\sqrt{-\eta^{cc}\eta^{dd}}\gamma^c\gamma^d\right)\psi_0,\\&\left(1+\frac{1}{\eta^{aa}}\sqrt{-\eta^{aa}\eta^{bb}}\gamma^a\gamma^b\right)(\gamma^c+\sqrt{-\eta^{cc}\eta^{dd}}\gamma^d)\psi_0.\end{aligned}\tag{34}$$

One can easily see that these states are orthonormalized provided that the vacuum state ψ_0 is properly normalized, which means in our example

$$\left\langle\psi_0\left|\frac{1}{2}\left(1+\frac{1}{\eta^{aa}}\sqrt{-\eta^{aa}\eta^{bb}}\gamma^a\gamma^b\right)\frac{1}{2}\left(1+\frac{1}{\eta^{cc}}\sqrt{-\eta^{cc}\eta^{dd}}\gamma^c\gamma^d\right)\psi_0\right.\right\rangle=1.\tag{35}$$

In the general case the normalization condition is

$$\left\langle\psi_0\left|\prod\,[-]\prod\,[-i]\psi_0\right.\right\rangle=1.\tag{36}$$

We may realize that only one component along the common eigenstates of the Cartan subalgebra generators $\rho(S^{ab}),\rho(S^{cd})$ matters in our normalization condition Eq. (36).

We conclude the subsection with the statement that each state ${}^h\psi_i$ belonging to a representation of handedness h, is, due to appropriately chosen ''vacuum state,'' orthonormal to any other state $|{}^{h'}\psi_j\rangle$, where ψ_i are basis states of spinors, generated in the way we presented above:

$$\langle{}^h\psi_i|{}^{h'}\psi_j\rangle=\delta^{hh'}\delta^{ij}.\tag{37}$$

V. "FAMILIES"

In the construction of our basis for a left ideal, which at the end got identified with the spinor space $\mathcal{S}$ and mapped into $\mathcal{S}_\rho$, we made at a point a selection of a ''starting object.'' We had chosen for the ''starting object'' the product of $d/2$ for even d [respectively $(d-1)/2$ for odd d] nilpotent

constructions with $+\frac{1}{2}$ or $+i/2$ as the eigenvalues of the left multiplication Cartan algebra generators: $\overset{ab}{(+)}=1/2(\gamma^a+\eta^{aa}/i\gamma^b)$, $\overset{ab}{(+i)}=1/2(\gamma^a+\eta^{bb}\gamma^b)$. By acting on the starting basis with γ^a's we reached other basis elements belonging to our Clifford basis. We ended with a closing involving $2^{d/2}$ for even d (and $2^{(d-1)/2}$ for odd d) basis constructions.

We noticed already that none of the Clifford algebra object can transform $\overset{ab}{(+)}$ into $\overset{ab}{[+]}$ or opposite (Sec. III C), and also not $\overset{ab}{(-)}$ into $\overset{ab}{[-]}$. We see that whenever $\overset{ab}{(+)}$ is replaced by $\overset{ab}{[+]}$ a new ''starting state'' is generated leading to a new representation. We can count the number of different representations, finding $2^{d/2}$ for d even and $2^{(d+1)/2}$ for d odd, respectively. [In the odd d case left and right handed objects transform under the Clifford algebra left multiplication into themselves (Theorem 4), that is, without changing handedness.]

Each of these $2^{d/2}$ (or $2^{(d+1)/2}$ for d odd) different representations leads to a different left ideal and, thus, if we identify the ideals with $\mathcal{S}$, we would get, strictly speaking, different $\mathcal{S}$ in each case. If we let there be, as above, a representation ρ of the Clifford algebra on a spinor space $\mathcal{S}_\rho$, each of these choices of representations, or rather of ideals, would in general lead to a different basis in the space $\mathcal{S}_\rho$. If ρ is an *irreducible* representation, it is well-known that in the even case the dimension of $\mathcal{S}_\rho$ is equal to $2^{d/2}$, which falls into two irreducible representations of the Lorentz group.

Let us remind that we previously showed that when we construct the states (33) and (34) they only extract from the ''vacuum state'' ψ_0 the component along the common eigenspace of the representations $\rho(S^{03})$, $\rho(S^{12})$, etc. of the Cartan algebra generators, namely the one with $-\frac{1}{2}$ or $-i/2$ eigenvalues. If we choose another ideal, belonging to another starting state, the component extracted from ψ_0 will be another one. We find the following rule: (i) If for the Cartan subalgebra generators S^{ab}, in the starting state and accordingly the basis use the pair $\overset{ab}{(+)}$ and $\overset{ab}{[-]}$ is contained, say for $\eta^{aa}=1=\eta^{bb}$, then the extracted component is from a common eigenspace for the Cartan subalgebra generators with the eigenvalue for S^{ab} being $-\frac{1}{2}$. If, however, the pair $\overset{ab}{(-)}$ and $\overset{ab}{[+]}$ is used in the starting state, the extracted component of the common eigenspace will be S^{ab} having the eigenvalue $\frac{1}{2}$. All these different basis states coming from different ideals are independent of the ''vacuum states'' except for normalization. Of course, the basis states in $\mathcal{S}_\rho$, induced by the choice of one ideal, can not be orthogonal to the basis induced by another ideal, when we talk about basis vectors in only one irreducible representation space $\mathcal{S}_\rho$. Actually, the basis vectors in $\mathcal{S}_\rho$, reached by using different representations $\mathcal{S}$, induced by different ideals, are essentially the same. In fact, to get into essentially the same basis vector in $\mathcal{S}_\rho$ from one ideal to another one can use the replacement of $\overset{ab}{(+)}$ into $\overset{ab}{[+]}$ and $\overset{ab}{(-)}$ into $\overset{ab}{[-]}$, because eigenvectors in $\mathcal{S}$ are characterized by their eigenvalues of the Cartan subalgebra generators.

But we could have required that all $2^{d/2}$ different $\mathcal{S}$, belonging to different ideals, should be mapped into $2^{d/2}$ for d even (and similarly for d odd) orthogonal basis vectors in an enlarged $\mathcal{S}_\rho$, which then would be a reducible representation of the Clifford algebra, which would lead to, for instance, block-diagonal representations of blocks of the dimension $2^{d/2}$ in even d case,[4,5]

$$\mathcal{S}_\rho=\sum_i^{N_{gen}} \mathcal{S}_{ir,i}, \tag{38}$$

where N_{gen} is equal $2^{d/2}$ and $\mathcal{S}_{ir,i}$ denotes the ith irreducible representation.

In a generic case, we could have the number of what we call ''families'' greater than one and smaller than $2^{d/2}$ for even d and $2^{(d+1)/2}$ for d odd.

Taking into account the orthogonality of all the 2^d polynomials of the γ^a operators and assuming that these polynomials act on a ''vacuum state'' which assures the orthogonality of all

the obtained states, we find $2^{d/2}$ copies of the two-Weyl spinors (that is, of the Dirac spinor). We count the number of all states, which is for d-dimensional space 2^d, and compare for d even this number with twice the number of states in one Weyl spinor irreducible representation (since we count states of both handedness), which is $2\times 2^{d/2-1}$. For d odd we find accordingly $2^{(d+1)/2}$ copies of the Weyl spinor. We call these $2^{d/2}$ copies for d even and $2^{(d+1)/2}$ copies for d odd ''families'' of spinors. Each ''family'' differs from all the others in the choice of the starting state, on which the irreducible representation is built, and accordingly on all the states.

To achieve the required orthogonality, we make a choice of phases for states belonging to different ''families'' in such a way that, when choosing the ''vacuum state'' $|\psi_0\rangle$ to be the sum of not only all the states in one ''family'' but of all the states of all the ''families,'' each state appearing with the same coefficient, not only the expectation values of the operators S^{ab}, belonging to the Cartan subalgebra, but also the expectation values of γ^a are for such $|\psi_0\rangle$ equal to zero, that is $\langle\psi_0|\gamma^a|\psi_0\rangle=0$, for d even and odd. Given such a choice of the ''vacuum state,'' all states belonging to any ''family'' are orthonormal:

$$\langle {}^a\psi_i|{}^b\psi_j\rangle=\delta^{ab}\delta^{ij}. \tag{39}$$

We use index a or b to numerate a ''family'' and index i or j to numerate states within a ''family.''

VI. GRAPHIC PRESENTATION

We shall present in this section a simple and transparent graphic technique for finding irreducible representations of the Lorentz group for spinors for any dimension—even or odd. We start by introducing the notation (already seen in Theorem 1)

$$\begin{aligned}
\overset{ab}{(k)} &:= \frac{1}{2}\left(\gamma^a+\frac{\eta^{bb}}{i}k\gamma^b\right)=\frac{1}{2}\left(\gamma^a+\frac{\eta^{aa}}{ik}\gamma^b\right),\\
\overset{ab}{[k]} &:= \frac{1}{2}(1+ik\eta^{aa}\eta^{bb}\gamma^a\gamma^b)=\frac{1}{2}\left(1+\frac{i}{k}\gamma^a\gamma^b\right),\\
\overset{+}{\bigcirc} &:= \tfrac{1}{2}(1+\Gamma),\\
\overset{-}{\bullet} &:= \tfrac{1}{2}(1-\Gamma),
\end{aligned} \tag{40}$$

under the assumption that the eigenvalue k of $2S^{ab}$ (supposedly one of the Cartan-algebra generators) being of course restricted by $k^2=\eta^{aa}\eta^{bb}$, since it is real for a and b corresponding both to time or both to space index, while it is purely imaginary for opposite signatures. We see that Theorem 1 above tells us

$$\begin{aligned}
S^{ab}\overset{ab}{(k)} &= \tfrac{1}{2}k\overset{ab}{(k)},\\
S^{ab}\overset{ab}{[k]} &= \tfrac{1}{2}k\overset{ab}{[k]}.
\end{aligned} \tag{41}$$

We have of course for d different from a and b

$$\begin{aligned}
\gamma^d\overset{ab}{(k)} &= -\overset{ab}{(k)}\gamma^d,\\
\gamma^d\overset{ab}{[k]} &= \overset{ab}{[k]}\gamma^d.
\end{aligned} \tag{42}$$

We can easily find

$$\begin{gathered}\overset{ab}{\gamma^a}(k)=\eta^{aa}\overset{ab}{[}-k],\\ \overset{ab}{\gamma^b}(k)=-ik\overset{ab}{[}-k],\\ \overset{ab}{\gamma^a}[k]=\overset{ab}{(}-k),\\ \overset{ab}{\gamma^b}[k]=-ik\,\eta^{aa}\overset{ab}{(}-k).\end{gathered}\tag{43}$$

From Eqs. (42) and (43) it follows that

$$\begin{gathered}\overset{ab\ cd}{S^{ac}}(k)(k)=-\frac{i}{2}\eta^{aa}\eta^{cc}\overset{ab}{[}-k]\overset{cd}{[}-k],\\ \overset{ab\ cd}{S^{ac}}[k][k]=\frac{i}{2}\overset{ab}{(}-k)\overset{cd}{(}-k),\\ \overset{ab\ cd}{S^{ac}}(k)[k]=-\frac{i}{2}\eta^{aa}\overset{ab}{[}-k]\overset{cd}{(}-k),\\ \overset{ab\ cd}{S^{ac}}[k](k)=\frac{i}{2}\eta^{cc}\overset{ab}{(}-k)\overset{cd}{[}-k].\end{gathered}\tag{44}$$

We also find

$$\overset{ab}{(k)}^{\dagger}=\eta^{aa}\overset{ab}{(}-k),\tag{45}$$

$$\overset{ab}{[k]}^{\dagger}=\overset{ab}{[}k],\tag{46}$$

and

$$\begin{gathered}\overset{ab\ ab}{(k)(k)}=0,\quad \overset{ab\ ab}{(k)(}-k)=\eta^{aa}\overset{ab}{[}k],\quad \overset{ab\ ab}{(}-k)(k)=\eta^{aa}\overset{ab}{[}-k],\quad \overset{ab\ ab}{(}-k)(-k)=0,\\ \overset{ab\ ab}{[k][}k]=\overset{ab}{[}k],\quad \overset{ab\ ab}{[k][}-k]=0,\quad \overset{ab\ ab}{[}-k][k]=0,\quad \overset{ab\ ab}{[}-k][-k]=\overset{ab}{[}-k],\\ \overset{ab\ ab}{(k)[}k]=0,\quad \overset{ab\ ab}{[k](}k)=\overset{ab}{(}k),\quad \overset{ab\ ab}{(}-k)[k]=\overset{ab}{(}-k),\quad \overset{ab\ ab}{(}-k)[-k]=0,\\ \overset{ab\ ab}{(k)[}-k]=\overset{ab}{(}k),\quad \overset{ab\ ab}{[k](}-k)=0,\quad \overset{ab\ ab}{[}-k](k)=0,\quad \overset{ab\ ab}{[}-k](-k)=\overset{ab}{(}-k).\end{gathered}\tag{47}$$

According to Eqs. (46) and (47) and discussions in Sec. IV we find

$$\overset{ab\ ab}{(k)^{\dagger}(k)}=\overset{ab}{[}-k],\quad \langle\overset{ab\ ab}{(k)^{\dagger}(k)}\rangle=1,\tag{48}$$

$$\overset{ab}{[k]}{}^{\dagger}\overset{ab}{[k]}=\overset{ab}{[k]}, \quad \langle \overset{ab}{[k]}{}^{\dagger}\overset{ab}{[k]}\rangle = 1. \tag{49}$$

Let us conclude this section by presenting graphically a Weyl spinor irreducible representation for d-dimensional space, with d even and with the handedness [Eq. (14)] Γ equal to $\Pi_a \sqrt{\eta^{aa}}\, \Pi_{\text{Cartan ab}}\, k_{ab}$. The first product runs over all the indices a, while the second product runs over the eigenvectors k_{ab} [Eq. (41)] of the Cartan subalgebra elements [Eq. (9)]. This irreducible representation of the chosen handedness is one out of $2^{d/2}$ possible ones. All the pairs $S^{ab}, S^{cd}, \ldots$ are members of the Cartan subalgebra of the Lorentz group:

$$\begin{aligned}
&\overset{ab}{(k_{ab})}\overset{cd}{(k_{cd})}\overset{ef}{(k_{ef})}\cdots\overset{gh}{(k_{gh})}\cdots\psi_0\\
&\overset{ab}{[-k_{ab}]}\overset{cd}{[-k_{cd}]}\overset{ef}{(k_{ef})}\cdots\overset{gh}{(k_{gh})}\cdots\psi_0\\
&\overset{ab}{[-k_{ab}]}\overset{cd}{(k_{cd})}\overset{ef}{[-k_{ef}]}\cdots\overset{gh}{(k_{gh})}\cdots\psi_0\\
&\qquad\vdots\\
&\overset{ab}{[-k_{ab}]}\overset{cd}{(k_{cd})}\overset{ef}{(k_{ef})}\cdots\overset{gh}{[-k_{gh}]}\cdots\psi_0\\
&\overset{ab}{(k_{ab})}\overset{cd}{[-k_{cd}]}\overset{ef}{[-k_{ef}]}\cdots\overset{gh}{(k_{gh})}\cdots\psi_0\\
&\qquad\vdots
\end{aligned} \tag{50}$$

States, belonging to one multiplet with respect to the group $\mathrm{SO}(q,d-q)$, that is to one irreducible representation, can have any phase. We made a choice of the simplest one, taking all phases equal to one.

What we learn from the above graphic representation is that one obtains all the states of an irreducible Weyl representation by transforming all possible pairs of $\overset{ab}{(k_{ab})}\overset{mn}{(k_{mn})}$ to $\overset{ab}{[-k_{ab}]}\overset{mn}{[-k_{mn}]}$. The procedure gives $2^{(d/2-1)}$ states. We shall use the presented graphical search to find the Weyl spinors for $d=3$ and $d=4$ in the next section.

VII. MATRIX REPRESENTATION OF γ^a AND S^{ab}

In this section we present matrix elements for the Clifford algebra elements γ^a's and for the generators of the Lorentz group S^{ab}.

As we learned in Sec. VI (and can be very easily checked), transforms γ^a the nilpotent $\overset{ab}{(k)} = \frac{1}{2}(\gamma^a + (\eta^{aa}/ik)\,\gamma^b)$ [Eq. (43)] into the projector $\eta^{aa}\overset{ab}{[-k]} = \eta^{aa}\frac{1}{2}(1 - i/k\,\gamma^a\gamma^b)$. A basic state has for a chosen dimension d, $d/2$ factors, which are either nilpotents or projectors, but only one among those nilpotents or projectors has the index ab. We shall therefore first look at the matrix elements between the two states $\overset{ab}{(k)}$ and $\overset{ab}{[-k]}$, for example. The only difference in matrix elements between this case and the case with a general $d/2$ factors in a basic state is in a phase factor, which we shall comment on later.

Following the definition of the inner product in Sec. IV and taking into account Eq. (43) in Sec. VI, one easily finds matrix elements of the Clifford algebra operators γ^a between any two states for any d of what we called the Dirac representation, if we first recognize the relations

$$\langle\psi_0|\overset{ab}{[-k]}^\dagger\gamma^a\overset{ab}{(k)}\psi_0\rangle=\eta^{aa}\langle\psi_0|\overset{ab}{[-k]}^\dagger\overset{ab}{[-k]}\psi_0\rangle=\eta^{aa},$$

$$\langle\psi_0|\overset{ab}{[-k]}^\dagger\gamma^b\overset{ab}{(k)}\psi_0\rangle=-ik_{ab}\langle\psi_0|\overset{ab}{[-k]}^\dagger\overset{ab}{[-k]}\psi_0\rangle=-ik_{ab}, \tag{51}$$

$$\langle\psi_0|\overset{ab}{(k)}^\dagger\gamma^a\overset{ab}{[-k]}\psi_0\rangle=\langle\psi_0|\overset{ab}{(k)}^\dagger\overset{ab}{(k)}\psi_0\rangle=1,$$

$$\langle\psi_0|\overset{ab}{(k)}^\dagger\gamma^b\overset{ab}{[-k]}\psi_0\rangle=ik_{ab}\eta^{aa}\langle\psi_0|\overset{ab}{(k)}^\dagger\overset{ab}{(k)}\psi_0\rangle=ik_{ab}\eta^{aa},$$

where the ''vacuum state'' has to be understood as explained in Sec. IV and k_{ab} means k, which belongs to the nilpotent $\overset{ab}{(k)}$ or to the projector $\overset{ab}{[k]}$, with $k_{ab}^2=\eta^{aa}\eta^{bb}$.

In the space of the two vectors $\overset{ab}{(k)}\psi_0$ and $\overset{ab}{[-k]}\psi_0$ the matrix representations of γ^a and γ^b are

$$\gamma^a=\begin{pmatrix}0 & 1\\ \eta^{aa} & 0\end{pmatrix},\quad \gamma^b=\begin{pmatrix}0 & ik_{ab}\eta^{aa}\\ -ik_{ab} & 0\end{pmatrix}, \tag{52}$$

with k_{ab} belonging to the nilpotent $\overset{ab}{(k)}$ and $-k_{ab}$ belonging to the projector $\overset{ab}{[-k]}$. If γ^{a_k} operates on a state $\overset{a_1a_2}{\{k\}}\cdots\overset{a_ia_j}{\{k\}}\ \overset{a_ka_l}{(k)}\cdots\psi_0$, where $\{k\}$ stands for either nilpotents (k) or for projectors $[k]$, one obtains

$$\gamma^{a_k}\overset{a_1a_2}{\{k\}}\cdots\overset{a_ia_j}{\{k\}}\overset{a_ka_l}{(k)}\cdots\psi_0=(-)^{n_0}\eta^{a_ka_k}\overset{a_1a_2}{\{k\}}\cdots\overset{a_ia_j}{\{k\}}\overset{a_ka_l}{[-k]}\cdots\psi_0, \tag{53}$$

where n_0 means the number of nilpotents among all the $\{k\}$, which γ^{a_k} has to jump over. Accordingly the phase $(-)^{n_0}$ of the new state is either $+$ or $-$ factor, for an even or odd number of nilpotents, respectively. If, in Eq. (53), the state $\overset{a_ka_l}{(k)}$ is replaced by the state $\overset{a_ka_l}{[-k]}$, it follows

$$\gamma^{a_k}\overset{a_1a_2}{\{k\}}\cdots\overset{a_ia_j}{\{k\}}\overset{a_ka_l}{[-k]}\cdots\psi_0=(-)^{n_0}\overset{a_1a_2}{\{k\}}\cdots\overset{a_ia_j}{\{k\}}\overset{a_ka_l}{(k)}\cdots\psi_0, \tag{54}$$

where again n_0 means the number of nilpotents among all the $\{k\}$, which γ^{a_k} has to jump over. By taking into account Eqs. (52)–(54) and accordingly by counting the number of nilpotents, which γ^a's have to jump over, one easily finds the matrix representation for γ^a's for any dimension and any signature.

When looking for matrix representations of $S^{ab}(=(i/4)[\gamma^a,\gamma^b])$, which are not elements of the Cartan subalgebra, the space of at least two factors of nilpotents or projectors has to be considered, since each of γ^a and γ^b transforms one factor as we know from above. In the space of the two vectors $\overset{ab}{(k)}\ \overset{cd}{(k)}\ \psi_0$ and $\overset{ab}{[-k]}\ \overset{cd}{[-k]}\ \psi_0$, for example, one finds the following matrix representations for the generators of the Lorentz group S^{ac}, S^{bd}, S^{ad} and S^{bc},

$$S^{ac}=\frac{1}{2}\begin{pmatrix}0 & i\\ -i\eta^{aa}\eta^{cc} & 0\end{pmatrix},\quad S^{bd}=\frac{1}{2}k_{ab}k_{cd}\begin{pmatrix}0 & -i\eta^{aa}\eta^{cc}\\ i & 0\end{pmatrix},$$

$$S^{ad}=\frac{1}{2}k_{cd}\begin{pmatrix}0 & -\eta^{cc}\\ -\eta^{aa} & 0\end{pmatrix},\quad S^{bc}=\frac{1}{2}k_{ab}\begin{pmatrix}0 & -\eta^{aa}\\ -\eta^{cc} & 0\end{pmatrix}. \tag{55}$$

If $S^{a_k a_p}$ operates on a state $\stackrel{a_1 a_2}{\{k\}}\cdots\stackrel{a_i a_j}{\{k\}}\stackrel{a_k a_l}{(k)}\stackrel{a_m a_n}{\{k\}}\cdots\stackrel{a_p a_r}{(k)}\cdots\psi_0$, where $\{k\}$ stands again for either nilpotents (k) or for projectors $[k]$, one obtains

$$S^{a_k a_p}\stackrel{a_1 a_2}{\{k\}}\cdots\stackrel{a_i a_j a_k a_l a_m a_n}{\{k\}(k)\{k\}}\cdots\stackrel{a_p a_r}{(k)}\cdots\psi_0$$

$$=-(-)^{(n_{0_k}+n_{0_p})}\frac{i}{2}\eta^{a_k a_k}\eta^{a_p a_p}\stackrel{a_1 a_2}{\{k\}}\cdots\stackrel{a_i a_j}{\{k\}}\stackrel{a_k a_l}{[-k]}\stackrel{a_m a_n}{\{k\}}\cdots\stackrel{a_p a_r}{[-k]}\cdots\psi_0, \tag{56}$$

where $\underset{a_k a_l}{n_{0_k}}$ and $\underset{a_p a_r}{n_{0_p}}$ counts the number of nilpotents among all the $\{k\}$ between $S^{a_k a_p}$ and either $\stackrel{a_k a_l}{(k)}$ or $\stackrel{a_p a_r}{(k)}$, respectively.

By taking into account Eqs. (55) and (56) one easily finds matrix elements of all the nondiagonal elements of the Lorentz algebra, while the matrix elements of the Cartan subalgebra very easily follow from Eq. (41).

Up to now we only have paid attention to even dimensions. For odd dimensions, the application of γ^a on a state, if $a\neq 0$, is due to Theorem 4 equivalent to the application of $\gamma^a\gamma^0=2iS^{0a}$ on the state, since Theorem 4 says that $\gamma^a\gamma^0(1\pm\Gamma)\stackrel{a_1 a_2}{\{k\}}\cdots\stackrel{a_i a_j}{\{k\}}\stackrel{a_k a_l}{(k)}\cdots\psi_0=\pm\sqrt{\underset{a_1 a_2}{\eta^{00}}}\eta^{00}\varepsilon(1\pm\Gamma)\gamma^a\stackrel{a_1 a_2}{\{k\}}\cdots\stackrel{a_i a_j}{\{k\}}\stackrel{a_k a_l}{(k)}\cdots\psi_0$, where ε is the handedness of the $(d-1)$-dimensional part $\stackrel{a_1 a_2}{\{k\}}\cdots\stackrel{a_i a_j}{\{k\}}\stackrel{a_k a_l}{(k)}\cdots\psi_0$ of the state, that is, of the even part, which does not include γ^0. We took into account that in odd-dimensional spaces γ^a and Γ commute. The evaluation of γ^a on the rest of the state follows from the above derivations.

We are concluding this section with the statement that the simplest choice of the relative phases (by just taking all the phases equal to one) in Eq. (50) leads for $d=4$ and for the Minkowski metric to the representation known as the chiral representation for spinors. We present matrix representations of γ^a and S^{ab} for $d=3$ and $d=4$ in the next section.

VIII. DEMONSTRATION OF IRREDUCIBLE REPRESENTATIONS OF WEYL SPINORS

In this section we demonstrate what we have learned, on two cases: We look for the irreducible representations of spinors with respect to the Lorentz group for a three-dimensional and a four-dimensional case. In both cases we shall assume the Minkowski metric: $\eta^{00}=-\eta^{ii}$, with $i=1,2$ for $d=3$ and $i=1,2,3$ for $d=4$. The ''vacuum state'' ψ_0 is chosen in such a way that all the 2^d linearly independent polynomials of γ^a are orthonormalized [as explained in Sec. IV].

A. Weyl spinors for $d=3$

There is only one $[(d-1)/2=1]$ operator of the Cartan subalgebra of the Lorentz algebra. According to Eq. (13) we choose S^{12} as the member of the Cartan subalgebra of the Lorentz algebra which the operators S^{01}, S^{02}, S^{12} close. Following Eq. (10) we find $\Gamma=i\gamma^0\gamma^1\gamma^2$. There are 2^3, that is eight, basic states, which we arange to be eigenstates of S^{12}, Γ and γ^0:

$$(\tfrac{1}{2})^2(1\pm\Gamma)(\gamma^1\pm i\gamma^2),\quad (\tfrac{1}{2})^2\gamma^0(1\pm\Gamma)(1\pm i\gamma^1\gamma^2). \tag{57}$$

We find the eigenvalues of the only member of the Cartan subalgebra S^{12} according to Theorem 1 [or by using Eq. (41), since S^{12} commutes with Γ] for the eight states of Eq. (57) to be $\pm\frac{1}{2}$. Using Theorem 4 one easily finds that the eigenvalues of γ^0 are $+1$ for those states, in which both factors appear with the same sign, otherwise they are -1. We arrange these eight orthonormal states into four ''families'' as presented in Table I.

Any of the four ''families'' can be used as the Weyl basis (or the Dirac; for odd dimensions the Weyl and the Dirac basis coincide) when solving the massless or massive Dirac equation, as it will be demonstrated in next section [Sec. IX].

TABLE I. Four "families" of the Lorentz group SO(1,2). All vectors are eigenvectors of S^{12}, γ^0 and Γ. They are orthonormalized according to Sec. IV. The graphical presentation follows the procedure described in Sec. VI. We add also a simplified version of the graphical presentation of states.

a	i	${}^a\psi_i$	S^{12}	γ^0	Γ	Graphic presentation
1	1	$(\frac{1}{2})^2(1+\Gamma)(\gamma^1+i\gamma^2)\psi_0$	$\frac{1}{2}$	1	1	$\overset{+}{\bigcirc}\overset{12}{(+)}$ or $\bigcirc(+)$
1	2	$(\frac{1}{2})^2(1+\Gamma)(1-i\gamma^1\gamma^2)\psi_0$	$-\frac{1}{2}$	-1	1	$\overset{+}{\bigcirc}\overset{12}{[-]}$ or $\bigcirc[-]$
2	1	$(\frac{1}{2})^2(1-\Gamma)(\gamma^1+i\gamma^2)\psi_0$	$\frac{1}{2}$	-1	-1	$\overset{-}{\bullet}\overset{12}{(+)}$ or $\bullet(+)$
2	2	$(\frac{1}{2})^2(1-\Gamma)(1-i\gamma^1\gamma^2)\psi_0$	$-\frac{1}{2}$	1	-1	$\overset{-}{\bullet}\overset{12}{[-]}$ or $\bullet[-]$
3	1	$(\frac{1}{2})^2(1+\Gamma)(1+i\gamma^1\gamma^2)\psi_0$	$\frac{1}{2}$	1	1	$\overset{+}{\bigcirc}\overset{12}{[+]}$ or $\bigcirc[+]$
3	2	$(\frac{1}{2})^2(1+\Gamma)(\gamma^1-i\gamma^2)\psi_0$	$-\frac{1}{2}$	-1	1	$\overset{+}{\bigcirc}\overset{12}{(-)}$ or $\bigcirc(-)$
4	1	$(\frac{1}{2})^2(1-\Gamma)(1+i\gamma^1\gamma^2)\psi_0$	$\frac{1}{2}$	-1	-1	$\overset{-}{\bullet}\overset{12}{[+]}$ or $\bullet[+]$
4	2	$(\frac{1}{2})^2(1-\Gamma)(\gamma^1-i\gamma^2)\psi_0$	$-\frac{1}{2}$	1	-1	$\overset{-}{\bullet}\overset{12}{(-)}$ or $\bullet(-)$

According to Sec. VII we find for the generators of the Lorentz group $S^{0i}(=(i/2)\,\gamma^0\gamma^i)$ for the first (and the third "family"), for $\eta^{00}=1=-\eta^{11}=-\eta^{22}$, just by multiplying γ^0 [which is diagonal with diagonal elements 1 and -1 (by Theorem 4)] and γ^i [from Eq. (52)] the following matrix presentation,

$$S^{01}=\frac{i}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad S^{02}=\frac{i}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad S^{12}=\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \tag{58}$$

which are, up to a factor, just the Pauli matrices $S^{01}=(i/2)\,\sigma_1$, $S^{02}=(i/2)\,\sigma_2$, $S^{12}=\frac{1}{2}\sigma_3$. The matrix γ^0 is equal to $2S^{12}=\sigma_3$. The matrices γ^1 and γ^2 are equal to $-2i\gamma^0S^{01}=i\sigma^2$ and $-2i\gamma^0S^{02}=-i\sigma^1$, respectively. We could, of course, calculate these matrices directly, using Table I. For example, the second element of the first row in S^{01} is equal to

$$\begin{aligned}&\langle\psi_0|((\tfrac{1}{2})^2(1+\Gamma)(1-i\gamma^1\gamma^2))^\dagger S^{01}(\tfrac{1}{2})^2(1+\Gamma)(\gamma^1+i\gamma^2)\psi_0\rangle\\ &\quad=\frac{i}{2}\langle\psi_0|((\tfrac{1}{2})^2(1+\Gamma)(1-i\gamma^1\gamma^2))^\dagger\gamma^0\gamma^1(\tfrac{1}{2})^2(1+\Gamma)(\gamma^1+i\gamma^2)\psi_0\rangle\\ &\quad=-\frac{i}{2}\langle\psi_0|((\tfrac{1}{2})^2(1+\Gamma)(1-i\gamma^1\gamma^2))^\dagger(\tfrac{1}{2})^2\gamma^0(1+\Gamma)(1-i\gamma^1\gamma^2)\psi_0\rangle=\frac{i}{2},\end{aligned} \tag{59}$$

since, due to the Clifford algebra properties, $\{\gamma^a,\gamma^b\}_+=2\,\eta^{ab}$. [The second and the third "families" have $S^{01}=-(i/2)\,\sigma_1$, $S^{02}=-(i/2)\,\sigma_2$, $S^{12}=\frac{1}{2}\sigma_3$ and $\gamma^0=-\sigma_3$.]

B. Weyl spinors for $d=4$

There are two $(d/2=2)$ operators of the Cartan subalgebra of the Lorentz algebra, which is closed by the operators S^{01}, S^{02}, S^{03}, S^{12}, S^{13}, S^{23}. According to Eq. (13) we choose S^{03} and S^{12} as members of the Cartan subalgebra. Following Eq. (10) we find $\Gamma=i\gamma^0\gamma^1\gamma^2\gamma^3$. There are 2^4, that is 16, basic states, all of them being eigenstates of S^{12} and S^{03}:

TABLE II. Four ''families'' of the two Weyl spinors of the Lorentz group SO(1,3). Basic vectors are eigenvectors of the two operators of the Cartan subalgebra S^{12} and S^{03}. The eigenvalues of the operator of handedness $\Gamma=2^2 i S^{03}S^{12}$ are also presented. All the basic states are orthonormalized as discussed in Sec. IV. Two types of graphic presentation are added, a simplified version in addition to the ordinary one. We made the simplest choice of relative phases—assuming all phases to be equal to $+1$, as discussed in Sec. IV.

a	i	${}^a\psi_i$	S^{12}	S^{03}	Γ	Graphic presentation
1	1	$(\frac{1}{2})^2(\gamma^0-\gamma^3)(\gamma^1+i\gamma^2)\psi_0$	$\frac{1}{2}$	$\frac{i}{2}$	-1	$\overset{03}{(+i)}\overset{12}{(+)}$ or $(+i)(+)$
1	2	$(\frac{1}{2})^2(1-\gamma^0\gamma^3)(1-i\gamma^1\gamma^2)\psi_0$	$-\frac{1}{2}$	$-\frac{i}{2}$	-1	$\overset{03}{[-i]}\overset{12}{[-]}$ or $[-i][-]$
2	1	$(\frac{1}{2})^2(1-\gamma^0\gamma^3)(\gamma^1+i\gamma^2)\psi_0$	$\frac{1}{2}$	$-\frac{i}{2}$	1	$\overset{03}{[-i]}\overset{12}{(+)}$ or $[-i](+)$
2	2	$(\frac{1}{2})^2(\gamma^0-\gamma^3)(1-i\gamma^1\gamma^2)\psi_0$	$-\frac{1}{2}$	$\frac{i}{2}$	1	$\overset{03}{(+i)}\overset{12}{[-]}$ or $(+i)[-]$
3	1	$(\frac{1}{2})^2(1+\gamma^0\gamma^3)(1+i\gamma^1\gamma^2)\psi_0$	$\frac{1}{2}$	$\frac{i}{2}$	-1	$\overset{03}{[+i]}\overset{12}{[+]}$ or $[+i][+]$
3	2	$(\frac{1}{2})^2(\gamma^0+\gamma^3)(\gamma^1-i\gamma^2)\psi_0$	$-\frac{1}{2}$	$-\frac{i}{2}$	-1	$\overset{03}{(-i)}\overset{12}{(-)}$ or $(-i)(-)$
4	1	$(\frac{1}{2})^2(\gamma^0+\gamma^3)(1+i\gamma^1\gamma^2)\psi_0$	$\frac{1}{2}$	$-\frac{i}{2}$	1	$\overset{03}{(-i)}\overset{12}{[+]}$ or $(-i)[+]$
4	2	$(\frac{1}{2})^2(1+\gamma^0\gamma^3)(\gamma^1-i\gamma^2)\psi_0$	$-\frac{1}{2}$	$\frac{i}{2}$	1	$\overset{03}{[+i]}\overset{12}{(-)}$ or $[+i](-)$
5	1	$(\frac{1}{2})^2(1+\gamma^0\gamma^3)(\gamma^1+i\gamma^2)\psi_0$	$\frac{1}{2}$	$\frac{i}{2}$	-1	$\overset{03}{[+i]}\overset{12}{(+)}$ or $[+i](+)$
5	2	$(\frac{1}{2})^2(\gamma^0+\gamma^3)(1-i\gamma^1\gamma^2)\psi_0$	$-\frac{1}{2}$	$-\frac{i}{2}$	-1	$\overset{03}{(-i)}\overset{12}{[-]}$ or $(-i)[-]$
6	1	$(\frac{1}{2})^2(\gamma^0+\gamma^3)(\gamma^1+i\gamma^2)\psi_0$	$\frac{1}{2}$	$-\frac{i}{2}$	1	$\overset{03}{(-i)}\overset{12}{(+)}$ or $(-i)(+)$
6	2	$(\frac{1}{2})^2(1+\gamma^0\gamma^3)(1-i\gamma^1\gamma^2)\psi_0$	$-\frac{1}{2}$	$\frac{i}{2}$	1	$\overset{03}{[+i]}\overset{12}{[-]}$ or $[+i][-]$
7	1	$(\frac{1}{2})^2(\gamma^0-\gamma^3)(1+i\gamma^1\gamma^2)\psi_0$	$\frac{1}{2}$	$\frac{i}{2}$	-1	$\overset{03}{(+i)}\overset{12}{[+]}$ or $(+i)[+]$
7	2	$(\frac{1}{2})^2(1-\gamma^0\gamma^3)(\gamma^1-i\gamma^2)\psi_0$	$-\frac{1}{2}$	$-\frac{i}{2}$	-1	$\overset{03}{[-i]}\overset{12}{(-)}$ or $[-i](-)$
8	1	$(\frac{1}{2})^2(1-\gamma^0\gamma^3)(1+i\gamma^1\gamma^2)\psi_0$	$\frac{1}{2}$	$-\frac{i}{2}$	1	$\overset{03}{[-i]}\overset{12}{[+]}$ or $[-i][+]$
8	2	$(\frac{1}{2})^2(\gamma^0-\gamma^3)(\gamma^1-i\gamma^2)\psi_0$	$-\frac{1}{2}$	$\frac{i}{2}$	1	$\overset{03}{(+i)}\overset{12}{(-)}$ or $(+i)(-)$

$$
\begin{aligned}
&(\tfrac{1}{2})^2(\gamma^0\pm\gamma^3)(\gamma^1\pm i\gamma^2), \quad (\tfrac{1}{2})^2(\gamma^0\pm\gamma^3)(1\pm i\gamma^1\gamma^2),\\
&(\tfrac{1}{2})^2(1\pm\gamma^0\gamma^3)(\gamma^1\pm i\gamma^2), \quad (\tfrac{1}{2})^2(1\pm\gamma^0\gamma^3)(1\pm i\gamma^1\gamma^2).
\end{aligned}
\tag{60}
$$

According to Theorem 1, the eigenvalues of the Cartan operator S^{12} for four times four basic states of Eq. (60) are $\pm\frac{1}{2}$ for the $\pm$ sign in the second factor of the states and the eigenvalues of the Cartan operator S^{03} for the four times four basic states are $\mp i/2$ for the $\pm$ sign in the first factor of the states. All 16 basic states are orthonormal.

We arrange these 16 states into four ''families'' as presented in Sec. IV. Each ''family'' includes two Weyl spinors, one left and one right handed. We come from one Weyl spinor, say left, to another, say right, by applying γ^a's to the left one. These four ''families'' are presented in Table II.

Using expressions for basis states from Table II and the orthogonality properties of states we can easily evaluate matrix elements of, say, S^{01}. The second matrix element of the first row for $S^{01}(=(i/2)\,\gamma^0\gamma^1)$, for example, is

$$\left\langle \psi_0 \left| \left(\left(\frac{1}{2}\right)^2 (1-\gamma^0\gamma^3)(1-i\gamma^1\gamma^2) \right)^\dagger S^{01} \left(\frac{1}{2}\right)^2 (\gamma^0-\gamma^3)(\gamma^1+i\gamma^2)\psi_0 \right\rangle \right. \tag{61}$$

$$= -\frac{i}{2} \left\langle \psi_0 \left| \left(\left(\frac{1}{2}\right)^2 (1-\gamma^0\gamma^3)(1-i\gamma^1\gamma^2) \right)^\dagger \left(\frac{1}{2}\right)^2 \gamma^0(\gamma^0-\gamma^3)\gamma^1(\gamma^1+i\gamma^2)\psi_0 \right\rangle \right. = \frac{i}{2}. \tag{62}$$

We present below the matrix representations for the generators of the Lorentz algebra and of the γ^a's for the first family (and the second family):

$$S^{0i}=\frac{i}{2}\begin{pmatrix} \sigma_i & 0 \\ 0 & -\sigma_i \end{pmatrix}, \quad S^{ij}=\sum_k \varepsilon_{ijk}\frac{1}{2}\begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}, \quad i\in\{1,2,3\},$$
$$\gamma^o=\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \quad \gamma^i=\begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad i\in\{1,2,3\}. \tag{63}$$

The above representation is known as the chiral representation for the Lorentz group.

[The matrix representations for the third and the fourth ''families'' differ with respect to Eq. (63) in an overall sign for γ^i, $i=1,2,3$, and accordingly also for S^{0i} but not for S^{ij}.]

Any of the four ''families'' can be used to present the solution of the Dirac equation for a massive spinor, while the massless spinors are either left- or right-handed, so that only half of the space of the massive case is needed to find the solution. We shall present solutions of the Dirac equation for a massless or a massive case in the next section.

IX. SOLUTIONS OF WEYL AND DIRAC EQUATIONS FOR THE THREE- AND FOUR-DIMENSIONAL CASES

We shall demonstrate the usefulness of the presented technique by finding solutions of the Dirac equation for massless and massive cases in three- and four-dimensional spaces with one time ($\eta^{00}=1$) and $(d-1)$ space (η^{ii}, $i=1,..,d-1$) dimensions. We shall work, as one usually does, with only one family, making a choice of the first one in each of the two tables. Looking for solutions of the Dirac equation one proceeds as usual when solving the eigenvalue problem: one makes a superposition of basic states of one ''family'' with unknown coefficients solving the eigenvalue problem for the Dirac equation of the motion operator with the eigenvalue zero, either by taking into account equations from Sec. VI, or by just operating from the left on this superposition by the operator of the Dirac equation and taking into account the Clifford algebra properties of γ^a's.

A. Solution of the Dirac equation for spinors in $d=3$

To find the solution of the Dirac equation (using units in which $c=1=\overline{h}$)

$$(\gamma^a p_a - m=0)\,\psi, \tag{64}$$

we shall use the basic states presented in Table I as the first ''family'' of two basic vectors and find what γ^a does when operating on a linear superposition of basic states. Looking for the solution as a plane wave with a wave vector $p^a=(p^0,p^1,p^2)$ we find that the state

$$\psi=e^{-ip^a x_a}\mathcal{N}\left(\frac{1}{2}\right)^2(1+\Gamma)\left\{(\gamma^1+i\gamma^2)+\frac{p^1+ip^2}{p^0+m}(1-i\gamma^1\gamma^2)\right\}\psi_0, \tag{65}$$

or graphically

$$\psi = e^{-ip^a x_a} \mathcal{N} \left\{ \overset{+}{\circlearrowright}\overset{12}{(+)} + \frac{p^1 + ip^2}{p^0 + m} \overset{+}{\circlearrowright}\overset{12}{[-]} \right\} \psi_0 , \tag{66}$$

solves the Dirac equation for a massive case with $\mathcal{N} = \sqrt{(p^0+m)/(2p^0)}$ and $(p^0)^2 = (p^1)^2 + (p^2)^2 + m^2$. For the massless case we need only to set m equal to zero. Then the normalization factor $\mathcal{N}$ simplifies to $1/\sqrt{2}$. The first state appears with the weight 1 and the second with the weight $(p^1 + ip^2)/p^0$. It is evident that both solutions—for the massless and the massive case—are linear combinations of exactly the same number of basic states.

B. Solution of the Dirac equation for spinors in $d=4$

We shall first look for one of the two solutions of the massless Weyl equation

$$(\gamma^a p_a = 0)|\psi\rangle . \tag{67}$$

Using the first irreducible representation of only left handedness from Table II, we find

$$\psi = e^{-ip^a x_a} \mathcal{N} \left\{ \left(\frac{1}{2}\right)^2 (\gamma^0 - \gamma^3)(\gamma^1 + i\gamma^2) + \frac{p^1 + ip^2}{p^0 + p^3} \left(\frac{1}{2}\right)^2 (1 - \gamma^0\gamma^3)(1 - i\gamma^1\gamma^2) \right\} \psi_0 , \tag{68}$$

or graphically

$$\psi = e^{-ip^a x_a} \mathcal{N} \left\{ \overset{03}{(+i)}\overset{12}{(+)} + \frac{p^1 + ip^2}{p^0 + p^3} \overset{03}{[-i]}\overset{12}{[-]} \right\} \psi_0 , \tag{69}$$

with $\mathcal{N} = \sqrt{(p^0+p^3)/(2p^0)}$ and $(p^0)^2 = (p^1)^2 + (p^2)^2 + (p^3)^2$.

A massive case

$$(\gamma^a p_a - m = 0)|\psi\rangle \tag{70}$$

can only be solved within left and right handed irreducible representations. We find

$$\begin{aligned} \psi = e^{-ip^a x_a} \mathcal{N} \{ & (p^0 + p^3)(\tfrac{1}{2})^2 (\gamma^0 - \gamma^3)(\gamma^1 + i\gamma^2) + (p^1 + ip^2)(\tfrac{1}{2})^2 (1 - \gamma^0\gamma^3)(1 - i\gamma^1\gamma^2) \\ & + m(\tfrac{1}{2})^2 (1 - \gamma^0\gamma^3)(\gamma^1 + i\gamma^2) \} \psi_0 , \end{aligned} \tag{71}$$

or graphically

$$\psi = e^{-ip^a x_a} \mathcal{N} \{ (p^0 + p^3) \overset{03}{(+i)}\overset{12}{(+)} + (p^1 + ip^2) \overset{03}{[-i]}\overset{12}{[-]} + m \overset{03}{[-i]}\overset{12}{(+)} \} \psi_0 , \tag{72}$$

with $\mathcal{N} = 1/\sqrt{(p^0+p^3)(2p^0)}$ and $(p^0)^2 = (p^1)^2 + (p^2)^2 + (p^3)^2 + m^2$.

X. CONCLUSION

In this article we demonstrated a simple technique for finding the representations of the Lorentz group (Weyl spinors) and for Clifford algebra (Dirac spinors) for spinors for any-dimensional space, even or odd, of any signature, solely started from the abstract objects γ^a for which we only needed to know that they fulfill the Clifford algebra: $\gamma^a\gamma^b + \gamma^b\gamma^a = 2\eta^{ab}$. We first constructed the basis for the whole Clifford algebra made out, of course, of formal Clifford objects—Clifford algebra elements, each basis vector being a products of two types of objects: nilpotent ones and idempotent ones.

Introducing the ''Hermitian conjugation'' in the space of the Clifford algebra as a formal antiautomorphism specified by the signature $\gamma^{a\dagger} = \eta^{aa}\gamma^a$, we were able to define an inner product.

Introducing the vacuum state, which turned out to be (almost) generic, we were able to map the basis for abstract Clifford objects into the spinor basis forming the Hilbert space and accordingly the abstract Clifford objects into operators.

We further derived a simple and transparent graphic technique, which enables us to easily find matrix elements of all the Clifford operators in our basis—γ^a matrices and generators of the Lorentz transformations S^{ab} in particular.

By formally playing the game, that all 2^d linear independent polynomials of γ^a's, if applied to appropriately chosen "vacuum state," generate 2^d orthogonal states, we get $2^{d/2}$ "families" of twice $2^{d/2-1}$ Weyl spinors for d even and $2^{(d+1)/2}$ families of $2^{(d-1)/2}$ Weyl spinors for d odd. If a "vacuum state" contains the space of only one Dirac spinors, all the polynomials, applied to such a state, generate of course only one Dirac spinor, that is only one "family."

Taking advantage of the fact that the generators of the Lorentz group are binomials of the γ^a operators enables us to find eigenstates of any operator (say the Weyl or the Dirac operator), as well as the application of any operator to a given state, without making a choice of the representation of the operators γ^a.

Except for the orthonormalization procedure, this technique follows Refs. 4–7, 11, 12.

We also present a transparent graphic representation of basic states, as well as the application of operators to these states.

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The embedding of the space–time in five dimensions: An extension of the Campbell–Magaard theorem

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We extend the Campbell–Magaard embedding theorem by proving that any n-dimensional semi-Riemannian manifold can be locally embedded in an $(n+1)$-dimensional Einstein space. We work out some examples of application of the theorem and discuss its relevance in the context of modern higher-dimensional spacetime theories. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The old idea that our universe is fundamentally higher-dimensional with $n=4+d$ space–time dimensions seems to be gaining grounds very rapidly in recent years. Mathematical schemes by which our ordinary space–time is viewed as a hypersurface embedded in a higher dimensional space have been considered in several different contexts, such as strings,[1] D-branes,[2] Randall-Sundrum[3] models and noncompactified versions of Kaluza–Klein theories.[4]

On the other hand, local isometric embeddings of Riemannian manifolds have long been studied in differential geometry. Of particular interest is a well known theorem which states that if the embedding space is flat, then the minimum number of extra dimensions needed to analytically embed a n-dimensional Riemannian manifold is d, with $0 \leqslant d \leqslant n(n-1)/2$.[5]

It turns out, however, that if the embedding space is allowed to be Ricci-flat, then the minimum number of extra dimensions that are necessary for the embedding falls dramatically to $d=1$. This is the content of a little known but powerful theorem due to Campbell,[6] the proof of which was given by Magaard.[7] Campbell–Magaard's result has acquired fundamental relevance for granting the mathematical consistency of five-dimensional embedding theories and also has been applied to investigate how lower-dimensional theories could be related to $(3+1)$-dimensional vacuum Einstein gravity.[8]

The increasing attention given to the Randall–Sundrum model[3] in which the embedding space, i.e., the bulk, corresponds to an Einstein space, rather than a Ricci-flat one, has led us to wonder whether Campbell–Magaard theorem could be generalized and what sort of generalization could be done. Research in this direction, where a scheme for extending Campbell–Magaard theorem for embedding spaces with a non-null Ricci tensor has been put forward quite recently by Anderson and Lidsey.[9]

The purpose of the present article is to prove that Campbell–Magaard theorem can, indeed, be extended to include Einstein spaces. Our proof is entirely inspired by Magaard's reasoning, although some adaptations to the more general semi-Riemannian character of the spaces had to be made.

The article is organized as follows. Section II is devoted to stating and proving an extension of Campbell–Magaard theorem, in which the embedding manifold is an Einstein space. The proof is rather involved and resorts to auxiliary theorems and lemmas. In Sec. III we apply the general result to some examples and, finally, Sec. 4 contains our conclusion.

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II. ISOMETRIC EMBEDDING IN AN EINSTEIN SPACE

The Campbell–Magaard theorem for local isometric embedding in Ricci-flat space refers to Riemannian manifolds, i.e., those endowed with positive-definite metrics. It turns out that for our purposes of generalization this restrictive condition is not essential, so in what follows we shall consider a semi-Riemannian manifold with metrics of indefinite signature instead. First let us introduce some definitions, set the notation and present preliminary theorems and lemmas.

An n-dimensional manifold M^n is termed semi-Riemannian if it is endowed with a metric, i.e., a symmetric and nondegenerated second-rank tensor field of arbitrary signature. (In this article we are considering only manifolds and metrics which are analytic.)

Definition 1: Consider a differential map Φ: $U\subset M^n\rightarrow N^{n+k}$, *where* U *is an open subset of* M^n, *and* N^{n+k} $(k\geqslant 0)$ *is a manifold of dimension* $n+k$. *Then* Φ *is called a local isometric embedding if the following conditions hold:*

(i) $d\Phi_p: T_pM^n\rightarrow T_{\Phi(p)}N^{n+k}$ *is injective for all* $p\in U$.
(ii) $g_p(v,w)=\tilde{g}_{\Phi(p)}(d\Phi(v),d\Phi(w))$ *for all* v, $w\in T_pM^n$, *where* $\tilde{g}$ *denotes the metric of* N^{n+k}.
(iii) Φ *is a homeomorphism onto its image in the induced topology.*

If Φ is of class C^k (*analytic*), then the embedding is said to be of class C^k (*analytic*). Naturally, a local isometric embedding may be characterized in terms of coordinates. For instance, let $\mathbf{x}=\{x^1,\ldots,x^n\}$ and $\mathbf{y}=\{y^1,\ldots,y^{n+k}\}$ denote coordinate patches for $U\subset M^n$ and $V\subset N^{n+k}$, respectively, with $\Phi(p)\in V$. The embedding Φ determines a relation between the coordinates denoted by

$$y^\alpha=\sigma^\alpha(x^1,\ldots,x^n), \tag{1}$$

where $\sigma=\mathbf{y}\circ\Phi\circ\mathbf{x}^{-1}:\mathbf{x}(U)\subset\mathbb{R}^n\rightarrow\mathbb{R}^{n+k}$. (Throughout Latin and Greek indices will run from 1 to n and 1 to $n+k$, respectively.)

In this way the isometric condition leads to

$$g_{ij}=\frac{\partial\sigma^\alpha}{\partial x^i}\frac{\partial\sigma^\beta}{\partial x^j}\tilde{g}_{\alpha\beta}, \tag{2}$$

where the functions g_{ij} and $\tilde{g}_{\alpha\beta}$ are the components of metric with respect to the coordinate bases $\{\partial_{x^i}\}$ and $\{\partial_{y^\alpha}\}$, respectively. We, therefore, say that M^n can be local and isometrically embedded in N^{n+k} if there exist $n+k$ differentiable functions $y^\alpha=\sigma^\alpha(x^1,\ldots,x^n)$, (embedding functions) such that the Jacobian matrix $\partial\sigma^\alpha/\partial x^i$ has rank n and (2) holds.

Given two arbitrary semi-Riemannian manifolds M^n and N^{n+k} it may happen that there exists no isometric embedding between them. Thus, it is of interest to find out conditions assuring or not the existence of embedding, in particular, if the embedding space N^{n+k} is not specified except that its belongs to a collection of manifolds, $\mathcal{M}_\pi$, whose members, say, share a certain geometrical property. For example, π may express a restriction of the following kinds: to be flat, to have constant curvature, to be Ricci-flat, to be an Einstein space, and so forth. This way of formulating the problem motivates the definition below.

Definition 2: We say that a semi-Riemannian manifold M^n *has an embedding in the set* $\mathcal{M}_\pi$, *if there is at least a member of* $\mathcal{M}_\pi$, *say* N^{n+k}, *in which* M^n *is embeddable.*

The following is a theorem which establishes necessary and sufficient conditions for the existence of local isometric embedding of an n-dimensional semi-Riemannian space (M^n,g) in the set $\mathcal{M}_\pi^{n+1}$ of $(n+1)$-dimensional semi-Riemannian spaces $(N^{n+1},\tilde{g})$ that satisfy the (nonspecified) property π. The original version of this theorem is due to Magaard[7] and is restricted to the Riemannian case, though the extension to semi-Riemannian manifold is straightforward.

Theorem 1: *Let* (M^n,g) *constitute a semi-Riemannian manifold,* $\mathcal{M}_\pi^{n+1}=\{(N^{n+1},\tilde{g})$, *which satisfy the property* $\pi\}$ *and* $\mathbf{x}=\{x^1,\ldots,x^n\}$ *a coordinate system covering a neighborhood* U *of* $p\in M^n$. *A necessary and sufficient condition for a local analytical embedding of* M^n *at* p, *with line element*

$$ds^2 = g_{ik}dx^i dx^k, \tag{3}$$

in $\mathcal{M}_\pi^{n+1}$ *is the following.*

(i) There exist analytic functions,

$$\overline{g}_{ik} = \overline{g}_{ik}(x^1,\ldots,x^n,x^{n+1}), \tag{4}$$

$$\overline{\phi} = \overline{\phi}(x^1,\ldots,x^n,x^{n+1}), \tag{5}$$

defined in some open set $D \subset \mathbf{x}(U)\times\mathbb{R}$ *containing the point* $(x_p^1,\ldots,x_p^n,0)$ *and satisfying the conditions*

$$\overline{g}_{ik}(x^1,\ldots,x^n,0) = g_{ik}(x^1,\ldots,x^n) \tag{6}$$

in an open set $A \subset \mathbf{x}(U)$;

$$\overline{g}_{ik} = \overline{g}_{ki}, \tag{7}$$

$$|\overline{g}_{ik}| \neq 0, \tag{8}$$

$$\overline{\phi} \neq 0 \tag{9}$$

in D. ($|\overline{g}_{ik}|$ *denotes the determinant of* $\overline{g}_{ik}$).

(ii) Also,

$$ds^2 = \overline{g}_{ik}dx^i dx^k + \varepsilon\,\overline{\phi}^2 dx^{n+1}dx^{n+1}, \tag{10}$$

where $\varepsilon^2 = +1$, *be a line element in a certain coordinate neighborhood V of some manifold* $N^{n+1} \in \mathcal{M}_\pi^{n+1}$.

The essential idea of this theorem is that there exists a coordinate system ''adapted'' to the embedding in such a manner that the image of the embedding coincide with the hypersurface $x^{n+1}=0$ of the embedding space and the condition of isometry reduces to (6).

While the sufficient condition is easily demonstrated, the proof of the necessary condition of this theorem is very long and will be omitted.[7,10]

We now consider an $(n+1)$-dimensional semi-Riemannian manifold $(N^{n+1},\tilde{g})$ and $\{y^1,\ldots,y^{n+1}\}$ a coordinate system defined in an open set of $V \subset N^{n+1}$. Let $\tilde{g}_{\alpha\beta}$ and $\tilde{R}_{\alpha\beta}$ denote the components of the metric and Ricci tensor, respectively. The manifold $(N^{n+1},\tilde{g})$ is called an Einstein space if

$$\tilde{R}_{\alpha\beta} = \frac{2\Lambda}{1-n}\tilde{g}_{\alpha\beta}, \tag{11}$$

where $n \geqslant 2$ and Λ is a constant. Of course (11) is equivalent to $\tilde{G}_{\alpha\beta} = \Lambda\tilde{g}_{\alpha\beta}$, $\tilde{G}_{\alpha\beta}$ being the components of the Einstein tensor, and for this reason Λ will be occasionally referred to as the cosmological constant.

As is well known, at each point of an arbitrary semi-Riemannian space N^{n+1} there exists a coordinate neighborhood in which the metric has the form

$$ds^2 = \overline{g}_{ik}dy^i dy^k + \varepsilon\,\overline{\phi}^2 (dy^{n+1})^2. \tag{12}$$

Let us now consider the inclusion map $\iota(y^1,\ldots,y^n) = (y^1,\ldots,y^n,0)$. This map determines an embedding of the hypersurface Σ_0, defined by $y^{n+1}=0$, in N^{n+1}. This hypersurface endowed with the induced metric by the inclusion map, which is given by

$$g_{ik}(y^1,\ldots,y^n)=\frac{\partial \iota^\alpha}{\partial y^i}\frac{\partial \iota^\beta}{\partial y^k}\tilde{g}_{\alpha\beta}=\overline{g}_{ik}(y^1,\ldots,y^n,0), \tag{13}$$

constitutes a semi-Riemannian space. The intrinsic curvature of Σ_0 and the curvature of N^{n+1} calculated at Σ_0 are related by the Gauss–Codazzi equations. In the coordinates (12), the Gauss–Codazzi relations can be written in the form[5]

$$R_{mkij}=\tilde{R}_{mkij}+\varepsilon(\Omega_{ik}\Omega_{jm}-\Omega_{jk}\Omega_{im}), \tag{14}$$

$$\nabla_j\Omega_{ik}-\nabla_i\Omega_{jk}=\frac{1}{\phi}\tilde{R}_{(n+1)kij}, \tag{15}$$

where R_{mkij} and $\tilde{R}_{mkij}$ ($R^l_{kij}=\Gamma^l_{ik,j}-\Gamma^l_{jk,i}+\Gamma^l_{jm}\Gamma^m_{ik}-\Gamma^l_{im}\Gamma^m_{jk}$) are the components of the curvature tensor of Σ_0 and of N^{n+1}, respectively, ∇_i denoting the covariant derivative with respect to the metric g_{ik}, and Ω_{ik} (the covariant components of the extrinsic curvature tensor of Σ_0) are given by

$$\Omega_{ik}=-\frac{1}{2\overline{\phi}}\frac{\partial \overline{g}_{ik}}{\partial y^{n+1}}, \tag{16}$$

in the coordinates (12). We are now interested in obtaining the components of the Ricci tensor $R_{\alpha\beta}=g^{\delta\gamma}R_{\delta\alpha\gamma\beta}$ in the coordinates (12). With the help of the Gauss–Codazzi equations and from the expression

$$\tilde{R}^{(n+1)}_{i(n+1)k}=\left(-\frac{\varepsilon}{\phi}\frac{\partial\Omega_{ik}}{\partial y^{n+1}}+\frac{1}{\phi}\nabla_i\nabla_k\phi-\varepsilon g^{jm}\Omega_{jk}\Omega_{im}\right),$$

which can be obtained by a straightforward calculation, we are left with

$$\tilde{R}_{ik}=R_{ik}+\varepsilon g^{jm}(\Omega_{ik}\Omega_{jm}-2\Omega_{jk}\Omega_{im})-\frac{\varepsilon}{\phi}\frac{\partial\Omega_{ik}}{\partial y^{n+1}}+\frac{1}{\phi}\nabla_i\nabla_k\phi, \tag{17}$$

$$\tilde{R}_{i(n+1)}=\phi g^{jk}(\nabla_j\Omega_{ik}-\nabla_i\Omega_{jk}), \tag{18}$$

$$\tilde{R}_{(n+1)(n+1)}=\varepsilon\phi^2 g^{ik}\left(-\frac{\varepsilon}{\phi}\frac{\partial\Omega_{ik}}{\partial y^{n+1}}+\frac{1}{\phi}\nabla_i\nabla_k\phi-\varepsilon g^{jm}\Omega_{jk}\Omega_{im}\right). \tag{19}$$

At this stage, it should be clear that the results just obtained may be carried over to any hypersurface Σ_c defined by $y^{n+1}=c=\text{const}$. Owing to this we shall henceforth introduce a slightly different notation: the metric induced on any Σ_c, i.e., $\overline{g}_{ik}(y^1,\ldots,y^n,c)$, will be denoted simply by $\overline{g}_{ik}$; likewise all quantities associated with $\overline{g}_{ik}$ will be marked with a bar sign. However, for convenience, only the metric induced on Σ_0 may also be denoted by g_{ik} (without the bar).

Now let us turn our attention to the case when the embedding manifold N^{n+1} is an Einstein space. Since we can assume that any point $q\in N^{n+1}$ lies in some hypersurface Σ_c, we can use the equations above for decomposing the Ricci tensor of the embedding manifold in terms of its intrinsic and extrinsic parts with respect to any hypersurface Σ_c, with $c=y^{n+1}_q$. If N^{n+1} is an Einstein space, then it follows from (10) that

$$\tilde{R}_{ik}=\overline{R}_{ik}+\varepsilon\overline{g}^{jm}(\overline{\Omega}_{ik}\overline{\Omega}_{jm}-2\overline{\Omega}_{jk}\overline{\Omega}_{im})-\frac{\varepsilon}{\overline{\phi}}\frac{\partial\overline{\Omega}_{ik}}{\partial y^{n+1}}+\frac{1}{\overline{\phi}}\overline{\nabla}_i\overline{\nabla}_k\overline{\phi}=\frac{2\Lambda}{1-n}\overline{g}_{ik}, \tag{20}$$

$$\tilde{R}_{i(n+1)}=\overline{\phi}\overline{g}^{jk}(\overline{\nabla}_j\overline{\Omega}_{ik}-\overline{\nabla}_i\overline{\Omega}_{jk})=0, \tag{21}$$

$$\tilde{G}^{(n+1)}_{(n+1)} = -\tfrac{1}{2}\overline{g}^{ik}\overline{g}^{jm}(\overline{R}_{ijkm} + \varepsilon(\overline{\Omega}_{ik}\overline{\Omega}_{jm} - \overline{\Omega}_{jk}\overline{\Omega}_{im})) = \Lambda, \tag{22}$$

where in the last equation, from the definition of the Einstein tensor, $\tilde{G}^{(n+1)}_{(n+1)} = \tilde{R}^{(n+1)}_{(n+1)} - 1/2\tilde{R}$, $\tilde{R}$ being the curvature scalar $\tilde{R} = \tilde{g}^{\alpha\beta}\tilde{R}_{\alpha\beta}$.

After writing the equations above let us concentrate on the problem of embedding a semi-Riemannian manifold in an Einstein space. The equations (20)–(22) may be looked upon as a set of partial differential equations for $\overline{g}_{ik}$ and $\overline{\phi}$. At this point, our strategy is to show that if the components $g_{ik}(x^1,\ldots,x^n)$ of a metric of M^n with respect to some coordinate system are given, then there exists an open set of $\mathbb{R}^{n+1}$ where the above-mentioned equations admit a solution $\overline{g}_{ik}(y^1,\ldots,y^n,y^{n+1})$ and $\overline{\phi}(y^1,\ldots,y^n,y^{n+1})$, which satisfies the initial condition $\overline{g}_{ik} = g_{ik}$ at Σ_0. Moreover, it will be shown that the functions $\overline{g}_{ik}$ and $\overline{\phi}$ possess all properties which are necessary to constitute a line element of an $(n+1)$-dimensional semi-Riemannian manifold. Then, as $\overline{g}_{ik}$ and $\overline{\phi}$ satisfy Eqs. (20)–(22), the metric originated by them represents that of an Einstein space. Then, by virtue of Theorem 1, the existence of the embedding will be guaranteed. However, before proceeding to the final demonstration we shall make use of two lemmas. Let us consider the first one.

Lemma 1: Let the functions $\overline{g}_{ik}$ and $\overline{\phi}$ be analytic at $(0,\ldots,0) \in \Sigma_0 \subset \mathbb{R}^{n+1}$ and satisfy the conditions (7)–(9), and the equation (20) in an open set of $\mathbb{R}^{n+1}$ which contains $(0,\ldots,0,0) \in \mathbb{R}^{n+1}$. If, in addition, $\overline{g}_{ik}$ and $\overline{\phi}$ satisfy (21) and (22) at Σ_0, then $\overline{g}_{ik}e\overline{\phi}$ also satisfy (21) and (22) in some open set of $\mathbb{R}^{n+1}$ containing $(0,\ldots, 0, 0)$.

Proof: By assumption $\overline{g}_{ik}$ and $\overline{\phi}$ satisfy (7)–(9), hence the functions $\tilde{g}_{\alpha\beta}$ defined by $\tilde{g}_{ik} = \overline{g}_{ik}$, $\tilde{g}_{n+1n+1} = \overline{\phi}^2$ and $\tilde{g}_{in+1} = 0$ for $i, k = 1,\ldots,n$, may be considered as the components of an $(n+1)$-dimensional metric tensor $\tilde{g}$. The coefficients of the connection and the components of the curvature tensor associated to the metric $\tilde{g}_{\alpha\beta}$ can be calculated as usual. Let us now define the tensor $\tilde{F}_{\alpha\beta} = \tilde{G}_{\alpha\beta} - \Lambda\tilde{g}_{\alpha\beta}$, where $\tilde{G}_{\alpha\beta}$ is the Einstein tensor. Then, as a consequence of Bianchi identities for the curvature tensor, it follows that $\tilde{F}_{\alpha\beta}$ is divergenceless, i.e.,

$$\tilde{\nabla}_\alpha \tilde{F}^\alpha_\beta = 0. \tag{23}$$

This equation can be rewritten as

$$\frac{\partial \tilde{F}^{n+1}_\beta}{\partial y^{n+1}} = -\frac{\partial \tilde{F}^i_\beta}{\partial y^i} - \tilde{\Gamma}^\mu_{\mu\lambda}\tilde{F}^\lambda_\beta + \tilde{\Gamma}^\mu_{\lambda\beta}\tilde{F}^\lambda_\mu. \tag{24}$$

We have assumed that $\overline{g}_{ik}$ and $\overline{\phi}$ satisfy the equations (20)–(22) at Σ_0, hence $\tilde{F}^\alpha_\beta = 0$ at Σ_0. Moreover, $\partial\tilde{F}^i_\beta/\partial y^i\big|_{y^{n+1}=0} = (\partial/\partial y^i)(\tilde{F}^i_\beta\big|_{y^{n+1}=0}) = 0$. Therefore, we conclude from (24) that

$$\left.\frac{\partial \tilde{F}^{n+1}_\beta}{\partial y^{n+1}}\right|_{y^{n+1}=0} = 0. \tag{25}$$

Let us look into Eq. (24) separately for $\beta = n+1$ and $\beta = i$. Taking first $\beta = n+1$ gives

$$\frac{\partial \tilde{F}^{n+1}_{n+1}}{\partial y^{n+1}} = -\frac{\partial \tilde{F}^i_{n+1}}{\partial y^i} - \tilde{\Gamma}^\mu_{\mu\lambda}\tilde{F}^\lambda_{n+1} + \tilde{\Gamma}^{n+1}_{\lambda n+1}\tilde{F}^\lambda_{n+1} + \tilde{\Gamma}^i_{n+1n+1}\tilde{F}^{n+1}_i + \tilde{\Gamma}^i_{kn+1}\tilde{F}^k_i. \tag{26}$$

From the definition of the Einstein tensor we can write $\tilde{G}^i_j = \tilde{R}^i_j - \delta^i_j(\tilde{R}^k_k + \tilde{G}^{n+1}_{n+1})$. By assumption, $\tilde{R}_{ij} = [2\Lambda/(1-n)]\overline{g}_{ij}$ not only at the hypersurface $y^{n+1} = 0$, but also for some open set $V \subset \mathbb{R}^{n+1}$, with $0 \in U$. Thus, the equality $\tilde{F}^k_i = -\delta^k_i\tilde{F}^{n+1}_{n+1}$ holds in V. This implies that

$$\frac{\partial \tilde{F}^{n+1}_{n+1}}{\partial y^{n+1}} = -\frac{\partial \tilde{F}^{i}_{n+1}}{\partial y^{i}} - \tilde{\Gamma}^{\mu}_{\mu\lambda}\tilde{F}^{\lambda}_{n+1} + \tilde{\Gamma}^{n+1}_{\lambda n+1}\tilde{F}^{\lambda}_{n+1} + \tilde{\Gamma}^{i}_{n+1n+1}\tilde{F}^{n+1}_{i} - \tilde{\Gamma}^{i}_{in+1}\tilde{F}^{n+1}_{n+1}. \tag{27}$$

In terms of the components of $\tilde{F}^{n+1}_{n+1}$ and $\tilde{F}^{n+1}_{i}$ the equation above may be written as

$$\frac{\partial \tilde{F}^{n+1}_{n+1}}{\partial y^{n+1}} = -\varepsilon\,\overline{\phi}^{2}\overline{g}^{ij}\frac{\partial \tilde{F}^{n+1}_{i}}{\partial y^{j}} - 2\tilde{\Gamma}^{i}_{in+1}\tilde{F}^{n+1}_{n+1} + \left(-\varepsilon\,\frac{\partial(\overline{\phi}^{2}\overline{g}^{ij})}{\partial y^{j}} - \varepsilon\,\overline{\phi}^{2}\overline{g}^{ij}\tilde{\Gamma}^{k}_{kj} + \tilde{\Gamma}^{i}_{n+1n+1}\right)\tilde{F}^{n+1}_{i}. \tag{28}$$

Analogously for $\beta = i$ we obtain

$$\frac{\partial \tilde{F}^{n+1}_{i}}{\partial y^{n+1}} = \frac{\partial \tilde{F}^{n+1}_{n+1}}{\partial y^{i}} + 2\tilde{\Gamma}^{n+1}_{n+1i}\tilde{F}^{n+1}_{n+1} + (\tilde{\Gamma}^{k}_{n+1i} + \varepsilon\,\overline{\phi}^{2}\overline{g}^{kj}\tilde{\Gamma}^{n+1}_{ij} - \tilde{\Gamma}^{\mu}_{n+1\mu}\delta^{k}_{i})\tilde{F}^{n+1}_{k}. \tag{29}$$

By taking into account (28) and (29) it can be easily shown by mathematical induction that

$$\left.\frac{\partial^{r}\tilde{F}^{n+1}_{\beta}}{\partial (y^{n+1})^{r}}\right|_{y^{n+1}=0} = 0 \tag{30}$$

for any integer $r \geqslant 0$. As a consequence we conclude that $\tilde{F}^{n+1}_{\beta} = 0$ in a neighborhood of the origin. Indeed, as $\overline{g}_{ik}$ and $\overline{\phi}$ are analytic at $0 \in \mathbb{R}^{n+1}$, then there exists such a neighborhood in which $\tilde{F}^{n+1}_{\beta}$ can be expressed as a Taylor series about $0 \in \mathbb{R}^{n+1}$, with each term of this series being null. Since the equation $\tilde{F}^{n+1}_{\beta} = 0$ is equivalent to the equations (21) and (22), then the lemma is proved.

A. The Cauchy–Kowalewski theorem and the existence of the embedding

Although essential to the main result to be presented later, Lemma 1 says nothing about the existence of the solutions $\overline{g}_{ik}$ and $\overline{\phi}$. Thus we have to resort to the following theorem.

Theorem (Cauchy-Kowalewski): *Let us consider the set of partial differential equations:*

$$\frac{\partial^{2}u^{A}}{\partial (y^{n+1})^{2}} = F^{A}\left(y^{\alpha}, u^{B}, \frac{\partial u^{B}}{\partial y^{\alpha}}, \frac{\partial^{2}u^{B}}{\partial y^{\alpha}\partial y^{i}}, \right), \quad A = 1,...,m, \tag{31}$$

where $u^{1},\ldots,u^{m}$ *are* m *unknown functions of the* $n+1$ *variables* $y^{1},\ldots,y^{n},y^{n+1}$, $\alpha = 1,...,n+1$, $i = 1,...,n$, $B = 1,...,m$. *Also, let* $\xi^{1},\ldots,\xi^{m}$, $\eta^{1},\ldots,\eta^{m}$, *functions of the variables* $y^{1},\ldots,y^{n}$, *be analytic at* $0 \in \mathbb{R}^{n}$. *If the functions* F^{A} *are analytic with respect to each of their arguments around the values evaluated at the point* $y^{1} = \cdots = y^{n} = 0$, *then there exists a unique solution of Eqs.* (31) *which is analytic at* $0 \in \mathbb{R}^{n+1}$ *and that satisfies the initial condition*

$$u^{A}(y^{1},\ldots,y^{n},0) = \xi^{A}(y^{1},\ldots,y^{n}), \tag{32}$$

$$\frac{\partial u^{A}}{\partial y^{n+1}}(y^{1},\ldots,y^{n},0) = \eta^{A}(y^{1},\ldots,y^{n}), \quad A = 1,...,m. \tag{33}$$

By using (16), we can rewrite (20) as

$$\frac{\partial^{2}\overline{g}_{ik}}{\partial (y^{n+1})^{2}} = \varepsilon\,\frac{4\Lambda}{1-n}\,\overline{\phi}^{2}\overline{g}_{ik} + \frac{1}{\overline{\phi}}\frac{\partial \overline{\phi}}{\partial y^{n+1}}\frac{\partial \overline{g}_{ik}}{\partial y^{n+1}} - \frac{1}{2}\overline{g}^{jm}\left(\frac{\partial \overline{g}_{ik}}{\partial y^{n+1}}\frac{\partial \overline{g}_{jm}}{\partial y^{n+1}} - 2\,\frac{\partial \overline{g}_{im}}{\partial y^{n+1}}\frac{\partial \overline{g}_{jk}}{\partial y^{n+1}}\right)$$

$$-2\varepsilon\,\overline{\phi}\left(\frac{\partial^{2}\overline{\phi}}{\partial y^{i}\partial y^{k}} - \frac{\partial \overline{\phi}}{\partial y^{j}}\overline{\Gamma}^{j}_{ik}\right) - 2\varepsilon\,\overline{\phi}^{2}\overline{R}_{ik}. \tag{34}$$

Owing to the symmetry condition $\overline{g}_{ik}=\overline{g}_{ki}$, we can express Eq. (34) in terms of the functions $\overline{g}_{ik}$ with $i\leqslant k$. If $\overline{\phi}$ is regarded as a known function, then (34) becomes a set of partial differential equations for the $m=n(n+1)/2$ unknown function $\overline{g}_{ik}(i\leqslant k)$. This set of equations has the same form as (31). We also note that the right-hand side of (34) consists of rational functions of the coordinates y, the functions $\overline{g}_{ik}(i\leqslant k)$ and their derivatives (up to first order with respect to y^{n+1} and up to second order relative to the other coordinates). Therefore, if we take $\overline{\phi}\neq 0$ analytic at $0\in\mathbb{R}^{n+1}$ and if the initial conditions

$$\underset{i\leqslant k}{\overline{g}_{ik}}(y^1,\ldots,y^n,0)=\underset{i\leqslant k}{g_{ik}}(y^1,\ldots,y^n), \tag{35}$$

$$\underset{i\leqslant k}{\frac{\partial\overline{g}_{ik}}{\partial y^{n+1}}}(y^1,\ldots,y^n,0)=-2\,\overline{\phi}(y^1,\ldots,y^n,0)\underset{i\leqslant k}{\Omega_{ik}}(y^1,\ldots,y^n) \tag{36}$$

hold in some neighborhood of the point $0\in\mathbb{R}^n$, where g_{ik} and Ω_{ik} are arbitrary analytic functions with $|g_{ik}|\neq 0$ at the origin, then the right-hand side of (34) will also be analytic at

$$y^1=0\ldots y^{n+1}=0;\quad \underset{i\leqslant k}{\overline{g}_{ik}}\Big|_0\ ;\quad \underset{i\leqslant k}{\frac{\partial\overline{g}_{ik}}{\partial y^1}}\Big|_0\ \cdots\ \underset{i\leqslant k}{\frac{\partial\overline{g}_{ik}}{\partial y^{n+1}}}\Big|_0\ ;\quad \underset{i\leqslant k}{\frac{\partial^2\overline{g}_{ik}}{\partial y^j\partial y^m}}\Big|_0\ . \tag{37}$$

We conclude, then, from the Cauchy–Kowalewski theorem, that Eq. (34) admits a unique solution $\overline{g}_{ik}(y^1,\ldots,y^{n+1})$ which is analytic at $0\in\mathbb{R}^{n+1}$ and also satisfies the given initial conditions. It should be noted that the determinant $|\overline{g}_{ik}|$ (which due to the initial conditions is non-null at the origin) remains non-null in some open set of $\mathbb{R}^{n+1}$ as a consequence of the continuity of the solution. These results may be summed up in the following lemma.

Lemma 2: Let $g_{ik}(y^1,\ldots,y^n)$ and $\Omega_{ik}(y^1,\ldots,y^n)$, for $i,k=1,\ldots,n$, and $\overline{\phi}(y^1,\ldots,y^n,y^{n+1})$, be arbitrary functions which are analytic at $0\in\mathbb{R}^n$ and $0\in\mathbb{R}^{n+1}$, respectively, with $g_{ik}=g_{ki}$, $|g_{ik}|\neq 0$, $\Omega_{ik}=\Omega_{ki}$ in some open set of $\mathbb{R}^n$ containing $0\in\mathbb{R}^n$, and $\overline{\phi}\neq 0$ in some open set of $\mathbb{R}^{n+1}$ containing $0\in\mathbb{R}^{n+1}$. Then there exists a unique set of functions $\overline{g}_{ik}(y^1,\ldots,y^n,y^{n+1})$, which are analytic at $0\in\mathbb{R}^{n+1}$, that satisfy (i) the conditions (7) and (8) and the equation (20) in a neighborhood of $0\in\mathbb{R}^{n+1}$; and (ii) the initial conditions (6) and (36).

Now if we identify the functions g_{ik} of the initial conditions with the components of a semi-Riemannian manifold M^n, then from Lemmas 1 and 2 and Theorem 1 we can prove the following theorem:

Theorem 2: *Let M^n be an n-dimensional semi-Riemannian manifold with metric given by*

$$ds^2=g_{ik}dx^i dx^j,$$

in coordinate system $\{x^i\}$ of M^n. Let $p\in M^n$ have coordinates $x^1_p=\cdots=x^n_p=0$. Then, M^n has a local isometric and analytic embedding (at the point p) in an $(n+1)$-dimensional Einstein space with cosmological constant Λ if and only if there exist functions $\Omega_{ik}(x^1,\ldots,x^n)$ $(i,k=1,\ldots,n)$ that are analytic at $0\in\mathbb{R}^n$ and such that

$$\Omega_{ik}=\Omega_{ki}, \tag{38}$$

$$g^{jk}(\nabla_j\Omega_{ik}-\nabla_i\Omega_{jk})=0, \tag{39}$$

$$g^{ik}g^{jm}(R_{ijkm}+\varepsilon(\Omega_{ik}\Omega_{jm}-\Omega_{jk}\Omega_{im}))=-2\Lambda. \tag{40}$$

Proof: Let $\mathcal{M}_{\Lambda}^{n+1}$ be the collection of all $(n+1)$-dimensional Einstein spaces with cosmological constant Λ. If M^n has a local and analytic embedding in $\mathcal{M}_{\Lambda}^{n+1}$, at the point p, then in accordance with Theorem 1, there exist functions $\overline{g}_{ik}(x^1,\ldots,x^{n+1})$, satisfying (6), and $\overline{\phi}(x^1,\ldots,x^{n+1})$ that are analytic at $0\in\mathbb{R}^{n+1}$ such that

$$ds^2=\overline{g}_{ik}dx^i dx^k+\varepsilon\overline{\phi}^2 dx^{n+1}dx^{n+1} \tag{41}$$

is the line element of some member of $\mathcal{M}_{\Lambda}^{n+1}$ expressed in a conveniently chosen coordinate system. Therefore, this metric satisfies the equations (20)–(22) in a neighborhood of $0\in\mathbb{R}^{n+1}$. In particular, this is true for points lying on the hypersurface $x^{n+1}=0$, where $\overline{g}_{ik}=g_{ik}$, from (6). Thus, if we define $\Omega_{ik}(x^1,\ldots,x^n)=\overline{\Omega}_{ik}(x^1,\ldots,x^n,0)$, then the functions Ω_{ik} necessarily satisfy (38)–(40).

Let us consider the sufficient condition. First, we choose $\overline{\phi}(x^1,\ldots,x^{n+1})\neq 0$ and analytic at $0\in\mathbb{R}^{n+1}$. According to Lemma 2, there exists a unique set of functions $\overline{g}_{ik}(x^1,\ldots,x^{n+1})$ satisfying (6)–(8), (16), and (20) and the condition $\overline{\Omega}_{ik}(x^1,\ldots,x^n,0)=\Omega_{ik}(x^1,\ldots,x^n)$. If Ω_{ik} and g_{ik} satisfy (39) and (40), then, from Lemma 1, the functions $\overline{g}_{ik}(x^1,\ldots,x^{n+1})$ satisfy (20)–(22) in a neighborhood of $0\in\mathbb{R}^{n+1}$, which in turn implies that the line element formed with $\overline{g}_{ik}$ and $\overline{\phi}$ is that of an Einstein space with cosmological constant Λ. Then, Theorem 1 tell us that M^n has a local isometric and analytical embedding in $\mathcal{M}_{\Lambda}^{n+1}$. □

We now want to show that once the functions g_{ik} are given, the equations (38)–(40) always admit a solution for Ω_{ik}. These equations constitute a set of n partial differential equations [Eq. (39)] plus a constraint equation [Eq. (40)] for $n(n+1)/2$ independent functions Ω_{ik}. Except for $n=1$, the number of unknown functions is greater than [or equal to $(n=2)$] the number of equations. Out of the set of functions Ω_{ik} we pick n functions to be regarded as the unknowns. We proceed to put (39) in the form required for application of the Cauchy–Kowalewski (first-order derivative version) theorem to assure the existence of the solution. The detailed proof is a bit laborious, so we shall omit some of its parts.

For the sake of the argument and with no loss of generality we assume that we are using a coordinate system in which $g_{11}\neq 0$ and $g_{1k}=0$, $k=2,\ldots,n$. Thus, $g^{11}=1/g_{11}$ and $g^{1k}=0$. Equation (39) can be written as

$$g^{rs}(\Omega_{sk,r}-\Omega_{rs,k}+\Omega_{rt}\Gamma^t_{sk}-\Omega_{kt}\Gamma^t_{sr})=0. \tag{42}$$

Recalling that $\Omega_{ik}=\Omega_{ki}$, it is not difficult to see that (42) may be put in the form

$$g^{rs}\left(\underset{s\leqslant k}{\Omega_{sk,r}}+\underset{k<s}{\Omega_{ks,r}}-2\underset{r<s}{\Omega_{rs,k}}\right)-g^{rr}\Omega_{rr,k}+g^{rs}\left(\underset{t\leqslant r}{\Omega_{tr}\Gamma^t_{sk}}+\underset{r<t}{\Omega_{rt}\Gamma^t_{sk}}-\underset{t\leqslant k}{\Omega_{tk}\Gamma^t_{sr}}-\underset{k<t}{\Omega_{kt}\Gamma^t_{sr}}\right)=0. \tag{43}$$

Likewise and taking advantage of the special form of the metric we can write Eq. (40) as

$$\begin{aligned}2g^{11}\Omega_{11}\underset{r,s>1}{g^{rs}}\left(\underset{r\leqslant s}{\Omega_{rs}}+\underset{s<r}{\Omega_{sr}}\right)-2g^{11}\underset{r,s>1}{g^{rs}}\,\Omega_{1r}\Omega_{1s}+\underset{r,s,t,u>1}{g^{rs}g^{tu}}\Bigg[&\left(\underset{r\leqslant s}{\Omega_{rs}}+\underset{s<r}{\Omega_{rs}}\right)\left(\underset{t\leqslant u}{\Omega_{tu}}+\underset{u<t}{\Omega_{ut}}\right)\\&-\left(\underset{r\leqslant u}{\Omega_{ru}}+\underset{u<r}{\Omega_{ur}}\right)\left(\underset{s\leqslant t}{\Omega_{st}}+\underset{t<s}{\Omega_{ts}}\right)\Bigg]+\varepsilon R=-2\varepsilon\Lambda.\end{aligned} \tag{44}$$

Our next step is to identify in Eq. (43) the terms containing derivatives of Ω_{ik} with respect to the coordinate x^1. Let us consider first the case $k=1$. Thus, we have

$$g^{rs}\left(\underset{r,s>1}{\Omega_{1s,r}}-2\underset{1<r<s}{\Omega_{rs,1}}\right)-g^{rr}\underset{r>1}{\Omega_{rr,1}}+\underset{r,s>1}{g^{rs}}\left(\underset{t\leqslant r}{\Omega_{tr}\Gamma^t_{s1}}+\underset{r<t}{\Omega_{rt}\Gamma^t_{s1}}-\Omega_{11}\Gamma^1_{sr}-\underset{t<1}{\Omega_{1t}\Gamma^t_{sr}}\right)=0. \tag{45}$$

In order to write (45) in the form specified by Cauchy–Kowalewski (in its first-derivative version) we should decide what among the functions $\Omega_{ik}(i\leqslant k)$ are to be chosen as unknowns. We also

note that since $|g_{ik}|\neq 0$ there exists at least an index $r'>1$ such that $g^{r'n}\neq 0$. We choose $\Omega_{r'n}$ as one of the unknown functions and solve (45) for $\partial\Omega_{r'n}/\partial x^1$. Thus, it is possible to put (45) in the form

$$\frac{\partial\Omega_{r'n}}{\partial x^1}=\frac{1}{g^{r'n}(\delta_{r'n}-2)}\Bigg[-\sum_{r,s>1} g^{rs}\,\Omega_{1s,r}+2\sum_{\substack{1<r<s\\ r,s\neq r',n}} g^{rs}\Omega_{rs,1}+\sum_{\substack{r>1\\ r\neq r'}} g^{rr}\Omega_{rr,1}+g^{r'r'}\Omega_{r'r',1}(1-\delta_{r'n})$$
$$-\sum_{r,s>1} g^{rs}\Bigg(\sum_{t\leqslant r}\Omega_{tr}\Gamma^t_{s1}+\sum_{r<t}\Omega_{rt}\Gamma^t_{s1}-\Omega_{11}\Gamma^1_{sr}-\sum_{t<1}\Omega_{1t}\Gamma^t_{sr}\Bigg)\Bigg], \tag{46}$$

where no sum over r' is implied.

For $k\geqslant 2$ we have

$$\frac{\partial\Omega_{1k}}{\partial x^1}=g_{11}\Bigg[-\sum_{r,s>1} g^{rs}\Bigg(\sum_{s\leqslant k}\Omega_{sk,r}+\sum_{k<s}\Omega_{ks,r}-2\sum_{r<s}\Omega_{rs,k}\Bigg)-g^{11}\Omega_{11,k}-\sum_{r>1} g^{rr}\Omega_{rr,k}$$
$$-g^{rs}\Bigg(\sum_{t\leqslant r}\Omega_{tr}\Gamma^t_{sk}+\sum_{r<t}\Omega_{rt}\Gamma^t_{sk}-\sum_{t\leqslant k}\Omega_{tk}\Gamma^t_{sr}-\sum_{k<t}\Omega_{kt}\Gamma^t_{sr}\Bigg)\Bigg],\quad k\geqslant 2. \tag{47}$$

From (44) we can express Ω_{11} in terms of the other Ω_{ik}. Thus

$$\Omega_{11}=\frac{1}{2g^{11}\sum_{r,s>1} g^{rs}\Big(\sum_{r\leqslant s}\Omega_{rs}+\sum_{s<r}\Omega_{sr}\Big)}\Bigg[2g^{11}\sum_{r,s>1} g^{rs}\,\Omega_{1r}\Omega_{1s}-\sum_{r,s,tu>1} g^{rs}g^{tu}\Bigg[\Big(\sum_{r\leqslant s}\Omega_{rs}+\sum_{s<r}\Omega_{sr}\Big)\Big(\sum_{t\leqslant u}\Omega_{tu}+\sum_{u<t}\Omega_{ut}\Big)$$
$$-\Big(\sum_{r\leqslant u}\Omega_{ru}+\sum_{u<r}\Omega_{ur}\Big)\Big(\sum_{s\leqslant t}\Omega_{st}+\sum_{t<s}\Omega_{ts}\Big)\Bigg]-\varepsilon(R+\Lambda)\Bigg]. \tag{48}$$

Finally, substituting Ω_{11} from (48) into (46) and (47) we obtain a set of partial differential equations for the functions Ω_{ik}, $(i,k)\neq(1,1)$. If we regard the functions $\Omega_{ik}(i\leqslant k)$ with $i>1$ and $(i,k)\neq(r',n)$ as analytic functions already known, then we apply the Cauchy–Kowalewski theorem (first derivative version) to this set of differential equations considering $\Omega_{1k}(k>1)$ and $\Omega_{r'n}$ as the unknown functions. We, then, choose $\Omega_{ik}\,(x^1,\ldots,x^n)$ $[i\leqslant k, i>1, (i,k)\neq(r',n)]$ and the initial conditions $\Omega_{1k}\,(0,x^2,\ldots,x^n)=f_k(x^2,\ldots,x^n)$ $(k>1)$ and $\Omega_{r'n}(0,x^2,\ldots,x^n)=f_1(x^2,\ldots,x^n)$. Of course the chosen functions must be analytic at $0\in\mathbb{R}^n$ and satisfy the condition

$$\sum_{r,s>1} g^{rs}\Big(\sum_{r\leqslant s}\Omega_{rs}+\sum_{s<r}\Omega_{sr}\Big)\Big|_0\neq 0. \tag{49}$$

It should be noted that it is always possible to have functions Ω_{ik} that satisfy the condition above. For instance, if we take $\Omega_{ik}=0$ $[i\leqslant k, i>1, (i,k)\neq(r',n)]$, this condition reduces to $g^{r'n}\Omega_{r'n}|_0\neq 0$. Hence we just choose $\Omega_{r'n}\neq 0$.

Once we have specified the functions $\Omega_{ik}(x^1,\ldots,x^n)$ $[i\leqslant k, i>1, (i,k)\neq(r',n)]$, the right-hand sides of (46) and (47) become a function of the arguments

$$x^1,\ldots,x^n;\quad \sum_{k>1}\Omega_{1k},\Omega_{r'n};\quad \sum_{k,j>1}\Omega_{1k,j},\sum_{j>1}\Omega_{r'n,j}, \tag{50}$$

which is analytic at

$$x^1=0,\ldots,x^n=0;\quad \sum_{k>1}\Omega_{1k}\Big|_0,\Omega_{r'n}|_0;\quad \sum_{k,j>1}\Omega_{1k,j}\Big|_0,\sum_{j>1}\Omega_{r'n,j}\Big|_0. \tag{51}$$

Therefore, the Cauchy–Kowalewski theorem asserts that there exists a unique set of functions $\Omega_{1k}(x^1,x^2,\ldots,x^n)$ $(k>1)$ and $\Omega_{r'n}(x^1,x^2,\ldots,x^n)$, analytic at $0\in\mathbb{R}^{n+1}$ which satisfy the equations (46) and (47). We determine Ω_{11} from (48) by taking the chosen functions $\Omega_{ik}(x^1,\ldots,x^n)$ $[i\leqslant k,i>1,(i,k)\neq(r',n)]$ and the solutions of the system of equations. From (49) and due to the analyticity of g_{ik} and of the solution we conclude that Ω_{11} is analytic at the origin. Therefore, the existence of analytic functions Ω_{ik} satisfying (38)–(40) is demonstrated. The above may be summarized in the following lemma:

Lemma 3: Let $g_{ik}(x^1,\ldots,x^n)$ *and* $\Omega_{ik}(x^1,\ldots,x^n)$ $[i\leqslant k,i>1,(i,k)\neq(r',n)]$ *be analytic functions at the origin* $0\in\mathbb{R}^n$, *with* Ω_{ik} *satisfying the initial conditions* $\Omega_{1k}(0,x^2,\ldots,x^n)=f_k(x^2,\ldots,x^n)$ $(k>1)$ and $\Omega_{r'n}(0,x^2,\ldots,x^n)=f_1(x^2,\ldots,x^n)$, *where* f_k *are analytic at* $0\in\mathbb{R}^n$. *If, in addition, the condition* (49) *is fulfilled, then there exists a unique set of functions* $\Omega_{ik}(x^1,\ldots,x^n)$ $(i,k=1,...,n)$, *analytic at* $0\in\mathbb{R}^{n-1}$, *which satisfy the equations (38)–(40).*

Therefore, according to the lemma above, if we are given a set of analytic functions g_{ik}, then the existence of analytic functions Ω_{ik} which satisfy the equations (38)–(40) is assured. In this way Lemma 3 tell us that the sufficient conditions of Theorem 2 are satisfied, so we can state the final theorem.

Theorem 3: *Let* M^n $(n>1)$ *be a semi-Riemannian space with line element*

$$ds^2=g_{ik}dx^i dx^k,$$

expressed in a coordinate system which covers a neighborhood of a point $p\in M^n$ *whose coordinates are* $x_p^1=\cdots=x_p^n=0$. *If* g_{ik} *are analytic functions at* $0\in\mathbb{R}^n$, *then* M^n *can be embedded at p in some* $(n+1)$*-dimensional Einstein space* $N^{n+1}\in\mathcal{M}_\Lambda$.

Two comments are in order. First, if the $n(n-1)/2-1$ specified arbitrary functions $\Omega_{ik}(x^1,\ldots,x^n)$ $[i\leqslant k,i>1,(i,k)\neq(r',n)]$ obey the conditions

(i) the functions Ω_{ik} $[i\leqslant k,i>1,(i,k)\neq(r',n)]$ are analytic at $0\in\mathbb{R}^n$;
(ii) the n functions $\Omega_{1k}(0,x^2,\ldots,x^n)=f_k(x^2,\ldots,x^n)$ $(k>1)$ and $\Omega_{r'n}(0,x^2,\ldots,x^n)=f_1(x^2,\ldots,x^n)$ are analytic at $0\in\mathbb{R}^{n-1}$, with $g^{rs}_{r,s>1}\,(\Omega_{\substack{rs\\ r\leqslant s}}+\Omega_{\substack{sr\\ s<r}})\big|_0\neq 0$;
(iii) a function $\overline{\phi}(x^1,\ldots,x^{n+1})\neq 0$, analytic at $0\in\mathbb{R}^{n+1}$, is chosen;

then the line element of the embedding space as referred to in Theorem 1 is unique.

Second, if we consider the case $\Lambda=0$, then clearly this theorem reduces to the Campbell–Magaard theorem, which establishes the existence of local analytic embedding of any Riemannian manifold in the set of Ricci-flat spaces. In this sense, Theorem 3 is a generalization of the Campbell–Magaard theorem.

III. APPLICATION OF THE EXTENDED CAMPBELL–MAGAARD THEOREM

Let us consider some cases where (M^n,g) is a Lorentzian manifold of dimension $n=4$. We know from Theorem 3 that there exists at least one Einstein space of dimension $n=5$ in which (M^4,g) can be embedded. In this section, we shall discuss and exhibit explicitly the embedding of four-dimensional Einstein spaces into five-dimensional embedding Einstein spaces.

Let us suppose (M^4,g) is an Einstein space, that is,

$$R_{ik}=-\lambda g_{ik}. \tag{52}$$

Our aim is to find a five-dimensional $(M^5,\tilde{g})$ with a given arbitrary cosmological constant Λ in which (M^4,g) can be embedded.

Let us assume the following *ansatz*,

$$\overline{g}_{ik}=f(u)g_{ik} \tag{53}$$

with $f(0)=1$. Since we now have $R=-4\lambda$, the equation (40) can be satisfied only if $f'(0)=\sqrt{-2\varepsilon\Lambda/3+4\varepsilon\lambda/3}$.

Owing to the fact that $\overline{g}_{ik}$ and g_{ik} are related by a conformal transformation which depends on the extra coordinate u only, it follows that $\overline{R}_{ik}=R_{ik}=-\lambda g_{ik}$. Thus, Eq. (34) is equivalent to

$$f''+\frac{f'^2}{f}+\frac{4\varepsilon\Lambda}{3}f-2\varepsilon\lambda=0. \tag{54}$$

It is not difficult to show that the solution which satisfies the initial conditions imposed on f is given by[9]

$$f(u)=\left[\cosh\left(\sqrt{-\frac{\varepsilon\Lambda}{6}}u\right)+\left(1-2\frac{\lambda}{\Lambda}\right)\sinh\left(\sqrt{-\frac{\varepsilon\Lambda}{6}}u\right)\right]^2. \tag{55}$$

In this way we conclude that the Einstein space (M^4,g) can be embedded in the Einstein space

$$ds^2=f(u)g_{ik}dx^i dx^j+\varepsilon du^2, \tag{56}$$

with $f(u)$ being given by (55).

Let us briefly note that embeddings of Minkowski and Schwarzschild space–times may be easily obtained as a particular case of the example above if we take $\lambda=0$.

IV. CONCLUSION

The recent appearance of physical models which regard the ordinary space–time as a hypersurface embedded in a five-dimensional manifold has naturally raised the question of what kind of mathematical conditions both the embedded and the spaces are subject to. An answer to this question necessarily involves a careful account of the mathematical theory of embedding. Particularly useful and clarifying are the Campbell–Magaard theorem and its extension to the case in which the embedding manifold is an Einstein space. Belonging to the latter kind is the embedding considered in the Randall–Sundrum braneworld. On the other hand, embeddings in Ricci-flat five-dimensional manifolds are crucial for the noncompactified approach to Kaluza–Klein gravity.[4] Of course, if according to some new physical model the five-dimensional surrounding manifolds should obey some field equations, e.g., Einstein field equations, it would be of importance to investigate whether further extensions of Campbell–Magaard theorem could be achieved in order to accommodate these models. We are currently doing some research in this direction.

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Quaternionic eigenvalue problem

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We discuss the (right) eigenvalue equation for $\mathbb{H}$, $\mathbb{C}$ and $\mathbb{R}$ linear quaternionic operators. The possibility to introduce an isomorphism between these operators and real/complex matrices allows us to translate the quaternionic problem into an *equivalent* real or complex counterpart. Interesting applications are found in solving differential equations within quaternionic formulations of quantum mechanics. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1511789]

I. INTRODUCTION

The full understanding of the subtleties of the quaternionic eigenvalue problem still represents an intriguing challenge for mathematicians and physicists. The recent study of the eigenvalue problem for complex linear quaternionic operators[1] played a fundamental role in solving quaternionic differential equations.[2] In the last few years, interesting applications of quaternionic analysis and linear algebra were investigated in quantum mechanics.[3] In particular, the solution of the Schrödinger equation in the presence of quaternionic perturbations was explicitly given for constant potentials and deviations from standard (complex) quantum mechanics discussed.[4] In this article, we aim to complete the study begun in Ref. 1, where preliminary steps in solving the eigenvalue problem for complex linear quaternionic operators were traced. In order to extend to the $\mathbb{R}$-linear case the results obtained for the $\mathbb{H}$- and $\mathbb{C}$-linear quaternionic matrices, we have to introduce a system of *coupled* equations which represents the *new* eigenvalue problem for $\mathbb{R}$ linear quaternionic operators. It is important to observe that no attempt to develop a complete theory of the quaternionic eigenvalue problem has been made here; this exceeds the scope of our article. A satisfactory discussion of the eigenvalue problem for quaternionic operators is at present far from being given. We could have directly investigated the eigenvalue equation in the quaternionic space, but we have preferred a more practical approach and chosen to handle the problem by finding a more familiar real or complex space isomorphic to the quaternionic one. We shall show that the isomorphism between $\mathbb{H}$-, $\mathbb{C}$-, and $\mathbb{R}$-linear quaternionic operators and real/complex matrices immediately allows us to translate the quaternionic (right) eigenvalue problem in a corresponding real or complex counterpart. The study of the new translated problem gives important information about the quaternionic solution. The results obtained are very useful in solving polynomial and differential equations. This could represent a fundamental step in understanding the potentiality of using quaternions in formulating quantum mechanics (by investigating *quaternionic* deviations from the standard theory[3,4]) and gauge theory (by suggesting *new* unification groups[5]).

Throughout the article we shall denote by $\mathbb{R}$, $\mathbb{C}$, and $\mathbb{H}$ the sets of real, complex, and quaternionic numbers, $\mathbb{R}\subset\mathbb{C}\subset\mathbb{H}$, and by $V[n,\mathbb{X}]$ and $M[n,\mathbb{X}]$, respectively, the n-tuples and the $n\times n$ matrices over $\mathbb{X}$. Linear quaternionic operators will be distinguished by their linearity from the

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right. In what follows, the notation $\mathcal{O}_{\mathbb{X}}$ stands for quaternionic operators linear (from the right) over the field $\mathbb{X}$.

II. QUATERNIONIC ALGEBRA AND LINEAR OPERATORS

We now introduce the quaternionic algebra and some useful properties of $\mathbb{H}$-, $\mathbb{C}$-, and $\mathbb{R}$-linear operators. The (real) quaternionic skew-field $\mathbb{H}$ is an associative (division) algebra of rank 4 over $\mathbb{R}$,

$$q=q_0+iq_1+jq_2+kq_3, \quad q_{0,1,2,3}\in\mathbb{R}, \tag{1}$$

where

$$i^2=j^2=k^2=ijk=-1, \tag{2}$$

endowed with an involutory anti-automorphism (*conjugation*)

$$q\to\overline{q}=q_0-iq_1-jq_2-kq_3.$$

Due to the noncommutative nature of quaternions, we must distinguish between the left and right action of the quaternionic imaginary units i, j, and k. To do it, we introduce the operators

$$L_\mu=(1,L_i,L_j,L_k) \quad \text{and} \quad R_\mu=(1,R_i,R_j,R_k), \quad \mu=0,1,2,3,$$

which act on quaternionic vectors $\psi\in V[n,\mathbb{H}]$ in the following way:

$$L_\mu\psi=h_\mu\psi \quad \text{and} \quad R_\mu\psi=\psi h_\mu, \quad h_\mu=(1,i,j,k).$$

These operators satisfy

$$L_i^2=L_j^2=L_k^2=L_iL_jL_k=R_i^2=R_j^2=R_k^2=R_kR_jR_i=-1, \tag{3}$$

and

$$[L_\mu,R_\nu]=0, \quad \mu,\nu=0,1,2,3. \tag{4}$$

Note that $\mathbb{H}$-linear quaternionic operators acting on a finite n-dimensional quaternionic vector space,

$$\mathcal{O}_{\mathbb{H}}(\psi_1q_1+\psi_2q_2)=(O_{\mathbb{H}}\psi_1)q_1+(O_{\mathbb{H}}\psi_2)q_2, \quad q_{1,2}\in\mathbb{H}, \quad \psi_{1,2}\in V[n,\mathbb{H}],$$

are in one-to-one correspondence with $n\times n$ quaternionic matrices:

$$\mathcal{O}_{\mathbb{H}}\leftrightarrow M_{\mathbb{H}}\in M[n,\mathbb{H}]. \tag{5}$$

Consequently, $\mathbb{R}$- and $\mathbb{C}$-linear quaternionic operators,[6]

$$\mathcal{O}_{\mathbb{R}}(\psi_1r_1+\psi_2r_2)=(\mathcal{O}_{\mathbb{R}}\psi_1)r_1+(\mathcal{O}_{\mathbb{R}}\psi_2)r_2, \quad r_{1,2}\in\mathbb{R}, \quad \psi_{1,2}\in V[n,\mathbb{H}],$$

$$\mathcal{O}_{\mathbb{C}}(\psi_1c_1+\psi_2c_2)=(\mathcal{O}_{\mathbb{C}}\psi_1)c_1+(\mathcal{O}_{\mathbb{C}}\psi_2)c_2, \quad c_{1,2}\in\mathbb{C}, \quad \psi_{1,2}\in V[n,\mathbb{H}],$$

can be represented by $n\times n$ quaternionic matrices $M_{\mathbb{H}}$ and right acting operators R_μ as follows:

$$\mathcal{O}_{\mathbb{R}}\leftrightarrow M_{\mathbb{R}}=\sum_{\mu=0}^{3}M_{\mu,\mathbb{H}}R_\mu \quad \text{and} \quad \mathcal{O}_{\mathbb{C}}\leftrightarrow M_{\mathbb{C}}=\sum_{s=0}^{1}M_{s,\mathbb{H}}R_s. \tag{6}$$

Thus, $\mathbb{R}$-linear quaternionic operators consist of right multiplication by quaternionic numbers ($\mu=0,1,2,3$) whereas $\mathbb{C}$-linear quaternionic operators are restricted to right multiplication by complex numbers ($s=0,1$).

III. THE EIGENVALUE PROBLEM

In this section, we briefly discuss the left and right eigenvalue equation for $\mathbb{H}$-, $\mathbb{C}$-, and $\mathbb{R}$-linear quaternionic operators. As explicitly shown below, the conceptual difficulties which characterize the left eigenvalue problem readily disappear by resorting to right eigenvalues. The need to apply similarity transformations on $\mathbb{H}$-, $\mathbb{C}$-, and $\mathbb{R}$-linear quaternionic matrices introduces *complex* or *real* constraints on the right eigenvalues. The choice of complex or real (right) eigenvalues will be extremely useful in finding a practical method of resolution and manipulating quaternionic matrices.

A. Left eigenvalues

The left eigenvalue problem for $\mathbb{H}$-linear quaternionic operators reads

$$\mathcal{O}_{\mathbb{H}}\psi=q\psi, \quad \psi\in V[n,\mathbb{H}], \quad q\in\mathbb{H}. \tag{7}$$

This problem has been recently studied in the mathematical literature.[7,8] Nevertheless, no systematic way to approach the problem has been given. We point out some difficulties which appear in solving the left eigenvalue equation.

1. Similarity transformations

In finding the solution of Eq. (7), a first difficulty is represented by the impossibility to apply similarity transformations, $S_{\mathbb{H}}\in M[n,\mathbb{H}]$, without losing the formal structure of the left eigenvalue equation. In fact, by observing that $S_{\mathbb{H}}q\neq qS_{\mathbb{H}}$, the quaternionic matrices

$$M_{\mathbb{H}} \quad \text{and} \quad S_{\mathbb{H}}M_{\mathbb{H}}S_{\mathbb{H}}^{-1} \tag{8}$$

do *not* necessarily satisfy the same eigenvalue equation. Consequently, we can have quaternionic matrices with the same left eigenvalue spectrum, but *no* similarity transformation relating them. Explicit examples are found in Ref. 1.

2. Hermitian operators

Let $\mathcal{O}_{\mathbb{H}}$ be a Hermitian quaternionic operator and ψ be the eigenvector corresponding to the eigenvalue q. By using Eq. (7) and denoting by $\langle\varphi|\psi\rangle$ the inner product in $V[n,\mathbb{H}]$, we obtain

$$0=\langle\mathcal{O}_{\mathbb{H}}\psi|\psi\rangle-\langle\psi|\mathcal{O}_{\mathbb{H}}\psi\rangle\Rightarrow 0=\langle q\psi|\psi\rangle-\langle\psi|q\psi\rangle\neq(\overline{q}-q)\langle\psi|\psi\rangle.$$

Consequently, the left eigenvalue problem for Hermitian operators could admit *quaternionic* solutions.[9]

3. Square operators and eigenvalues

As a last difficulty in the use of left eigenvalues, we observe that if ψ is an $\mathcal{O}_{\mathbb{H}}$ eigenvector with eigenvalue q, it will not necessarily be an $\mathcal{O}_{\mathbb{H}}^2$ eigenvector with eigenvalue q^2. In fact,

$$\mathcal{O}_{\mathbb{H}}^2\psi=\mathcal{O}_{\mathbb{H}}q\psi\neq q\mathcal{O}_{\mathbb{H}}\psi=q^2\psi.$$

B. Right eigenvalues

The right eigenvalue equation for $\mathbb{H}$-linear transformations reads

$$\mathcal{O}_{\mathbb{H}}\psi=\psi q, \quad \psi\in V[n,\mathbb{H}], \quad q\in\mathbb{H}. \tag{9}$$

Such an equation can be reduced to a right complex eigenvalue equation rephasing the quaternionic eigenvalues by unitary quaternions u,

$$\mathcal{O}_{\mathrm{H}}\psi u=\psi u\bar{u}qu=\psi uz, \quad z\in\mathbb{C}. \tag{10}$$

This trick obviously fails for complex and real linear transformations. In fact, due to the presence of the operators R_i in $\mathcal{O}_{\mathrm{C}}$ and $\mathbf{R}\equiv(R_i,R_j,R_k)$ in $\mathcal{O}_{\mathbb{R}}$, we cannot apply unitary transformations from the right. Observe that

$$(\mathcal{O}_{\mathbb{R},\mathrm{C}}\psi)u\neq\mathcal{O}_{\mathbb{R},\mathrm{C}}(\psi u), \quad u\in\mathbb{H}. \tag{11}$$

The failure of the *associativity* in Eq. (11) suggests that we should consider *complex* eigenvalue equations for $\mathbb{C}$-linear quaternionic operators,

$$\mathcal{O}_{\mathrm{C}}\psi=\psi z, \quad z\in\mathbb{C}, \tag{12}$$

and *real* eigenvalues for $\mathbb{R}$-linear quaternionic operators,

$$\mathcal{O}_{\mathbb{R}}\psi=\psi r, \quad r\in\mathbb{R}. \tag{13}$$

These equations are formally invariant under $\mathbb{C}$- and $\mathbb{R}$-linear similarity transformations. Moreover, it can easily be proved that

$$\mathcal{O}^n_{\mathrm{H}}\psi=\psi q^n, \quad \mathcal{O}^n_{\mathrm{C}}\psi=\psi z^n, \quad \mathcal{O}^n_{\mathbb{R}}\psi=\psi r^n.$$

It is important to note here that $\mathbb{R}$-linear quaternionic operators admit real eigenvalues only in particular cases. Thus, Eq. (13) has to be generalized. As shown later, a satisfactory discussion of the eigenvalue problem for $\mathbb{R}$-linear quaternionic operators will require the use of a system of *coupled* equations.

IV. CANONICAL FORMS

In this section, following the procedure introduced in the paper of Ref. 1, we discuss the canonical forms for $\mathbb{H}$-, $\mathbb{C}$-, and $\mathbb{R}$-linear quaternionic matrices. The results we will establish find an immediate application in the theory of quaternionic differential operators. In fact, by using the canonical form $J_{\mathbb{X}}$ of a given matrix $M_{\mathbb{X}}$ we can readily obtain the exponential

$$\exp[M_{\mathbb{X}}x]=S_{\mathbb{X}}\exp[J_{\mathbb{X}}x]S^{-1}_{\mathbb{X}}$$

and, consequently, avoiding tedious calculations, solve quaternionic differential equations with constant coefficients.[2]

A. $\mathbb{H}$-linear matrices

While matrices over commutative rings have gained much attention, the literature on matrices with quaternionic entries is often fragmentary. The main difficulty is that, due to the noncommutative nature of quaternions, the standard method of resolution breaks down. Consequently, finding eigenvalues and canonical forms represents a more delicate problem. The recent renewed interest in quaternionic matrix theory[1,10] and its applications[2] shed new light on this intriguing research field. To facilitate access to the individual topics, we recall the main properties of $\mathbb{H}$-linear quaternionic matrices[11–14] and repeat the relevant theorems from Refs. 1, 10, 15, and 16 without proofs, thus making our exposition self-contained.

In approaching the problem of diagonalization we have to consider a right quaternionic eigenvalue equation. In fact, from

$$M_{\mathrm{H}}\psi_k=\psi_k q_k, \quad k=1,\ldots,n, \quad \psi_k\in V[n,\mathbb{H}], \tag{14}$$

in the case $M_{\mathbb{H}}$ is diagonalizable, we immediately get the following matrix equation

$$M_{\mathbb{H}}S_{\mathbb{H}}[\psi_1,\psi_2,\ldots,\psi_n]=S_{\mathbb{H}}[\psi_1,\psi_2,\ldots,\psi_n]D_{\mathbb{H}},$$

where

$$D_{\mathbb{H}}=\mathrm{diag}[q_1,q_2,\ldots,q_n]$$

and $S_{\mathbb{H}}=S_{\mathbb{H}}[\psi_1,\psi_2,\ldots,\psi_n]$ is defined by $Col_k(S_{\mathbb{H}})=\psi_k$.

Consequently, the diagonalization of the matrix $M_{\mathbb{H}}$,

$$M_{\mathbb{H}}=S_{\mathbb{H}}D_{\mathbb{H}}S_{\mathbb{H}}^{-1},$$

is obtained by solving the corresponding right eigenvalue problem. It is important to note here that we have *infinite* ways to diagonalize a quaternionic matrix $M_{\mathbb{H}}$,

$$\mathrm{diag}[u_1,u_2,\ldots,u_n]\mathrm{diag}[q_1,q_2,\ldots,q_n]\mathrm{diag}[\overline{u_1},\overline{u_2},\ldots,\overline{u_n}].$$

Geometrically speaking this means that $\mathrm{Im}[q]$ can arbitrarily be fixed on the sphere of ray $|\mathrm{Im}[q]|$. By a particular choice of the unitary matrix

$$U_{\mathbb{H}}=\mathrm{diag}[u_1,u_2,\ldots,u_n]$$

we can set a preferred space direction, for example the positive i axis, and consequently a *complex* (positive) eigenvalue spectrum.

Let us now briefly recall some properties of the eigenvalue spectrum of $\mathbb{H}$-linear quaternionic matrices. By using the symplectic decomposition of the matrix $M_{\mathbb{H}}$,

$$M_{\mathbb{H}}=M_1+jM_2,\quad M_{1,2}\in M[n,\mathbb{C}],$$

and the symplectic decomposition of the vector ψ,

$$\psi=\psi_1+j\psi_2,\quad \psi_{1,2}\in V[n,\mathbb{C}],$$

we can rewrite Eq. (10) in the following (complex) form:

$$\tilde{M}_{\mathbb{H}}\tilde{\psi}=z\,\tilde{\psi}, \tag{15}$$

where

$$\tilde{M}_{\mathbb{H}}=\begin{pmatrix} M_1 & -M_2^* \\ M_2 & M_1^* \end{pmatrix}\in M[2n,\mathbb{C}]\quad\text{and}\quad \tilde{\psi}=\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}\in V[2n,\mathbb{C}]. \tag{16}$$

The mapping

$$f:M_{\mathbb{H}}\mapsto\tilde{M}_{\mathbb{H}} \tag{17}$$

is an isomorphism of the ring of quaternionic matrices $M_{\mathbb{H}}$ into the ring of the corresponding complex counterparts $\tilde{M}_{\mathbb{H}}$. It is important to observe that this isomorphism do not preserve the inner product of eigenvectors.[9] Nevertheless, the choice of a *complex projection* of quaternionic inner products[17] opens the door to interesting applications in relativistic quantum mechanics.[18] The *complex* orthogonality of quaternionic eigenvectors (instead of a quaternionic orthogonality) implies a doubling of solution in the two-dimensional quaternionic Dirac equation.[17] The *four* (complex) orthogonal quaternionic solutions describe particle/antiparticle with spin up/down. The use of *complex* inner products is also a fundamental ingredient in the formulation of gauge theories by geometric algebras.[5]

The next theorem states the main property of the eigenvalue spectrum of $\mathbb{H}$-linear quaternionic matrices. For a detailed discussion, see Refs. 14–16.

Theorem 1: *Let $\tilde{M}_{\mathrm{H}}$ be the matrix given in Eq. (16). Then, its eigenvalues appear in complex conjugate pairs.*

By using the result of Theorem 1 and the Gram–Schmidt method, we can readily obtain the triangular form for $\mathbb{H}$-linear quaternionic matrices.

Theorem 2: *Every M_{H} is unitarily similar to an upper triangular matrix.*

Moreover, a Jordan form can be given for every $\mathbb{H}$-linear quaternionic matrix.

Theorem 3: *Every $n\times n$ matrix with real quaternion elements is similar under a matrix transformation with real quaternion elements to a matrix in (complex) Jordan normal form with diagonal elements in the complex field.*

To prove Theorem 3, we can use the isomorphism defined in (17). To any $\tilde{M}_{\mathrm{H}}$ corresponds a $2n\times 2n$ matrix B in the (complex) Jordan form $B=B_{\mathrm{H}}\oplus B_{\mathrm{H}}^{*}$, such that $\tilde{M}_{\mathrm{H}}P=PB$, where the (nonsingular) matrix P has the form

$$P=\begin{pmatrix} P_1 & -P_2^{*} \\ P_2 & P_1^{*} \end{pmatrix}.$$

This implies that

$$(P_1+jP_2)^{-1}M_{\mathrm{H}}(P_1+jP_2)=B_{\mathrm{H}}=D_{\mathrm{H}}+N_{\mathrm{H}}, \tag{18}$$

where D_{H} and N_{H} respectively denote the diagonal and the nilpotent parts of B_{H}.

B. $\mathbb{C}$-linear matrices

Let us now consider $\mathbb{C}$-linear transformations. We can associate to any $n\times n$ $\mathbb{C}$-linear quaternionic matrix a $2n$-dimensional complex matrix by the following mapping.

$$M_{\mathrm{C}}=M_{\mathrm{H}}+M'_{\mathrm{H}}R_i\leftrightarrow\tilde{M}_{\mathrm{C}}=f(M_{\mathrm{H}})+if(M'_{\mathrm{H}})=\begin{pmatrix} M_1 & -M_2^{*} \\ M_2 & M_1^{*} \end{pmatrix}+i\begin{pmatrix} M'_1 & -M'^{*}_2 \\ M'_2 & M'^{*}_1 \end{pmatrix}, \tag{19}$$

where f denotes the isomorphism defined in (17). Then the following proposition holds:

Proposition 1: Let M_{C} be a $\mathbb{C}$-linear quaternionic matrix and $\tilde{M}_{\mathrm{C}}$ its complex counterpart [see Eq. (19)]. The mapping

$$g:M_{\mathrm{C}}\mapsto\tilde{M}_{\mathrm{C}} \tag{20}$$

is an isomorphism of the ring of the n-dimensional $\mathbb{C}$-linear matrices into the ring of 2n-dimensional complex matrices.

Indeed, if

$$A_{\mathrm{C}}=A_{0,\mathrm{H}}+A_{1,\mathrm{H}}R_i \quad\text{and}\quad B_{\mathrm{C}}=B_{0,\mathrm{H}}+B_{1,\mathrm{H}}R_i$$

are two $\mathbb{C}$-linear matrices, their corresponding complex counterparts are given by

$$g(A_{\mathrm{C}})=f(A_{0,\mathrm{H}})+if(A_{1,\mathrm{H}}),\quad g(B_{\mathrm{C}})=f(B_{0,\mathrm{H}})+if(B_{1,\mathrm{H}}).$$

Then,

$$\begin{aligned} A_{\mathrm{C}}B_{\mathrm{C}}=C_{\mathrm{C}}&=A_{0,\mathrm{H}}B_{0,\mathrm{H}}+A_{1,\mathrm{H}}R_iB_{0,\mathrm{H}}+A_{0,\mathrm{H}}B_{1,\mathrm{H}}R_i+A_{1,\mathrm{H}}R_iB_{1,\mathrm{H}}R_i \\ &=A_{0,\mathrm{H}}B_{0,\mathrm{H}}-A_{1,\mathrm{H}}B_{1,\mathrm{H}}+(A_{0,\mathrm{H}}B_{1,\mathrm{H}}+A_{1,\mathrm{H}}B_{0,\mathrm{H}})R_i \end{aligned}$$

and

$$g(A_{\mathbb{C}})g(B_{\mathbb{C}})=f(A_{0,\mathbb{H}})f(B_{0,\mathbb{H}})-f(A_{1,\mathbb{H}})f(B_{1,\mathbb{H}})+if(A_{1,\mathbb{H}})f(B_{0,\mathbb{H}})+if(A_{0,\mathbb{H}})f(B_{1,\mathbb{H}})$$
$$=f(A_{0,\mathbb{H}}B_{0,\mathbb{H}}-A_{1,\mathbb{H}}B_{1,\mathbb{H}})+if(A_{0,\mathbb{H}}B_{1,\mathbb{H}}+A_{1,\mathbb{H}}B_{0,\mathbb{H}})=g(C_{\mathbb{C}}).$$

□

By using this isomorphism, the right eigenvalue spectrum of $\mathbb{C}$-linear quaternionic matrices can easily be determined.[1] The following result,

"*A* $\mathbb{C}$*-linear matrix is diagonalizable if the corresponding complex counterpart is diagonalizable,*"

was proven in Ref. 1 (where a preliminary discussion of the eigenvalue problem for $\mathbb{C}$-linear quaternionic matrix operators was given). It is worth pointing out that the converse of the previous statement is, in general, not true. For instance, let us consider the complex matrix

$$\tilde{G}_{\mathbb{C}}=\begin{pmatrix} z_1 & 0 & 1 & 0 \\ 0 & z_2 & 0 & 1 \\ 0 & 0 & z_1 & 0 \\ 0 & 0 & 0 & z_2 \end{pmatrix}. \tag{21}$$

This matrix admits a corresponding *diagonalizable* $\mathbb{C}$-linear quaternionic matrix given by

$$G_{\mathbb{C}}=D_{\mathbb{C}}+N_{\mathbb{C}}=\begin{pmatrix} \mathrm{Re}(z_1)+\mathrm{Im}(z_1)R_i & 0 \\ 0 & \mathrm{Re}(z_2)+\mathrm{Im}(z_2)R_i \end{pmatrix}+\frac{1}{2}\begin{pmatrix} -j+kR_i & 0 \\ 0 & -j+kR_i \end{pmatrix}, \tag{22}$$

where $N_{\mathbb{C}}$ is nilpotent, diagonal, and commutes with $D_{\mathbb{C}}$.

The normal form of a $\mathbb{C}$-linear quaternionic matrix can easily be calculated. Indeed, given any $\mathbb{C}$-linear transformation $M_{\mathbb{C}}$ and its corresponding complex counterpart $\tilde{M}_{\mathbb{C}}$ [see Eq. (19)], from the known properties of the Jordan form of complex matrices, we can immediately obtain

$$\tilde{S}_{\mathbb{C}}^{-1}\tilde{M}_{\mathbb{C}}\tilde{S}_{\mathbb{C}}=\tilde{J}_{\mathbb{C}}=\tilde{D}_{\mathbb{C}}+\tilde{N}_{\mathbb{C}},$$

where $\tilde{D}_{\mathbb{C}}$ is diagonal, $\tilde{N}_{\mathbb{C}}$ is nilpotent, and $[\tilde{D}_{\mathbb{C}},\tilde{N}_{\mathbb{C}}]=0$. Then, the quaternionic $\mathbb{C}$-linear matrices $M_{\mathbb{C}},S_{\mathbb{C}},D_{\mathbb{C}}$, and $N_{\mathbb{C}}$ are uniquely determined by the isomorphism stated in Proposition 1.

C. $\mathbb{R}$-linear matrices

In the n-dimensional quaternionic vector space $V[n,\mathbb{H}]$, the $\mathbb{R}$-linear transformations are represented by

$$M_{\mathbb{R}}=\sum_{\mu=0}^{3} M_{\mu,\mathbb{H}}R_{\mu}, \tag{23}$$

where $M_{\mu,\mathbb{H}}$ represent $\mathbb{H}$-linear quaternionic matrices and R_{μ} are the right acting operators defined

in the second section. Any $M_{\mathbb{R}}$ is then characterized by $16n^2$ real parameters. We can translate $\mathbb{R}$-linear $n\times n$ matrices into equivalent $4n\times 4n$ real matrices, and vice versa, by the following translation rules:

$$R_i \leftrightarrow \mathbf{I} = \begin{pmatrix} 0 & -\mathbf{1}_n & 0 & 0 \\ \mathbf{1}_n & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1}_n \\ 0 & 0 & -\mathbf{1}_n & 0 \end{pmatrix},$$

$$R_j \leftrightarrow \mathbf{J} = \begin{pmatrix} 0 & 0 & -\mathbf{1}_n & 0 \\ 0 & 0 & 0 & -\mathbf{1}_n \\ \mathbf{1}_n & 0 & 0 & 0 \\ 0 & \mathbf{1}_n & 0 & 0 \end{pmatrix}, \tag{24}$$

$$R_k \leftrightarrow \mathbf{K} = \begin{pmatrix} 0 & 0 & 0 & -\mathbf{1}_n \\ 0 & 0 & \mathbf{1}_n & 0 \\ 0 & -\mathbf{1}_n & 0 & 0 \\ \mathbf{1}_n & 0 & 0 & 0 \end{pmatrix},$$

and

$$M_{\mu,\mathbb{H}} = M_0 + iM_1 + jM_2 + kM_3 \leftrightarrow \hat{M}_{\mu,\mathbb{H}} = \begin{pmatrix} M_0 & -M_1 & -M_2 & -M_3 \\ M_1 & M_0 & -M_3 & M_2 \\ M_2 & M_3 & M_0 & -M_1 \\ M_3 & -M_2 & M_1 & M_0 \end{pmatrix}, \tag{25}$$

where $M_{\mu,\mathbb{H}} \in M[n,\mathbb{H}]$, $M_{0,\ldots,3} \in M[n,\mathbb{R}]$, and $\hat{M}_{\mu,\mathbb{H}} \in M[4n,\mathbb{R}]$. It is easy to verify that $\mathbf{I},\mathbf{J},\mathbf{K}$ commute with $\hat{M}_{\mu,\mathbb{H}}$:

$$[\mathbf{I},\hat{M}_{\mu,\mathbb{H}}] = [\mathbf{J},\hat{M}_{\mu,\mathbb{H}}] = [\mathbf{K},\hat{M}_{\mu,\mathbb{H}}] = 0$$

and

$$\mathbf{I}^2 = \mathbf{J}^2 = \mathbf{K}^2 = \mathbf{KJI} = -\mathbf{1}.$$

The following proposition holds.

Proposition 2: Let $M_{\mathbb{R}}$ be a $\mathbb{R}$-linear matrix and $\hat{M}_{\mathbb{R}}$ its real counterpart. Then the mapping

$$h: M_{\mathbb{R}} = M_{0,\mathbb{H}} + M_{1,\mathbb{H}}R_i + M_{2,\mathbb{H}}R_j + M_{3,\mathbb{H}}R_k \mapsto \hat{M}_{\mathbb{R}} = \hat{M}_{0,\mathbb{H}} + \hat{M}_{1,\mathbb{H}}\mathbf{I} + \hat{M}_{2,\mathbb{H}}\mathbf{J} + \hat{M}_{3,\mathbb{H}}\mathbf{K}$$

is an isomorphism of the ring of the n-dimensional $\mathbb{R}$-linear matrices into the ring of $4n$-dimensional real matrices $\hat{M}_{\mathbb{R}}$.

Observe that $\widehat{M_{\mathbb{H}}M'_{\mathbb{H}}} = \hat{M}_{\mathbb{H}}\hat{M}'_{\mathbb{H}}$. Let

$$A_{\mathbb{R}} = A_{0,\mathbb{H}} + A_{1,\mathbb{H}}R_i + A_{2,\mathbb{H}}R_j + A_{3,\mathbb{H}}R_k \quad \text{and} \quad B_{\mathbb{R}} = B_{0,\mathbb{H}} + B_{1,\mathbb{H}}R_i + B_{2,\mathbb{H}}R_j + B_{3,\mathbb{H}}R_k$$

be two $\mathbb{R}$-linear quaternionic matrices. Their corresponding real counterparts are given by

$$h(A_{\mathbb{R}}) = \hat{A}_{0,\mathbb{H}} + \mathbf{I}\hat{A}_{1,\mathbb{H}} + \mathbf{J}\hat{A}_{2,\mathbb{H}} + \mathbf{K}\hat{A}_{3,\mathbb{H}} \quad \text{and} \quad h(B_{\mathbb{R}}) = \hat{B}_{0,\mathbb{H}} + \mathbf{I}\hat{B}_{1,\mathbb{H}} + \mathbf{J}\hat{B}_{2,\mathbb{H}} + \mathbf{K}\hat{B}_{3,\mathbb{H}}.$$

Then,

$$A_{\mathbb{R}}B_{\mathbb{R}}=C_{\mathbb{R}}=(A_{0,\mathbb{H}}B_{0,\mathbb{H}}-A_{1,\mathbb{H}}B_{1,\mathbb{H}}-A_{2,\mathbb{H}}B_{2,\mathbb{H}}-A_{3,\mathbb{H}}B_{3,\mathbb{H}})+(A_{0,\mathbb{H}}B_{1,\mathbb{H}}+A_{1,\mathbb{H}}B_{0,\mathbb{H}}+A_{2,\mathbb{H}}B_{3,\mathbb{H}}-A_{3,\mathbb{H}}B_{2,\mathbb{H}})R_i+(A_{0,\mathbb{H}}B_{2,\mathbb{H}}+A_{2,\mathbb{H}}B_{0,\mathbb{H}}+A_{3,\mathbb{H}}B_{1,\mathbb{H}}-A_{1,\mathbb{H}}B_{3,\mathbb{H}})R_j+(A_{0,\mathbb{H}}B_{3,\mathbb{H}}+A_{3,\mathbb{H}}B_{0,\mathbb{H}}+A_{1,\mathbb{H}}B_{2,\mathbb{H}}-A_{2,\mathbb{H}}B_{1,\mathbb{H}})R_k$$

and

$$h(A_{\mathbb{R}})h(B_{\mathbb{R}})=(\hat{A}_{0,\mathbb{H}}\hat{B}_{0,\mathbb{H}}-\hat{A}_{1,\mathbb{H}}\hat{B}_{1,\mathbb{H}}-\hat{A}_{2,\mathbb{H}}\hat{B}_{2,\mathbb{H}}-\hat{A}_{3,\mathbb{H}}\hat{B}_{3,\mathbb{H}})+(\hat{A}_{0,\mathbb{H}}\hat{B}_{1,\mathbb{H}}+\hat{A}_{1,\mathbb{H}}\hat{B}_{0,\mathbb{H}}+\hat{A}_{2,\mathbb{H}}\hat{B}_{3,\mathbb{H}}-\hat{A}_{3,\mathbb{H}}\hat{B}_{2,\mathbb{H}})\mathbf{I}+(\hat{A}_{0,\mathbb{H}}\hat{B}_{2,\mathbb{H}}+\hat{A}_{2,\mathbb{H}}\hat{B}_{0,\mathbb{H}}+\hat{A}_{3,\mathbb{H}}\hat{B}_{1,\mathbb{H}}-\hat{A}_{1,\mathbb{H}}\hat{B}_{3,\mathbb{H}})\mathbf{J}+(\hat{A}_{0,\mathbb{H}}\hat{B}_{3,\mathbb{H}}+\hat{A}_{3,\mathbb{H}}\hat{B}_{0,\mathbb{H}}+\hat{A}_{1,\mathbb{H}}\hat{B}_{2,\mathbb{H}}-\hat{A}_{2,\mathbb{H}}\hat{B}_{1,\mathbb{H}})\mathbf{K}=h(C_{\mathbb{R}})$$ □

We now discuss the canonical forms of $\mathbb{R}$-linear matrices. Let $A_{\mathbb{R}}$ be an $\mathbb{R}$-linear transformation, $\hat{A}_{\mathbb{R}}$ its real counterpart, $\{\lambda_1+i\mu_1,\lambda_2+i\mu_2,\ldots,\lambda_s+i\mu_s\}$ the complex eigenvalues of $\hat{A}_{\mathbb{R}}$, and $\{\lambda_{2s+1},\ldots,\lambda_{4n}\}$ the real eigenvalues of $\hat{A}_{\mathbb{R}}$. As is well known,[19,20] there exists a real orthogonal matrix O such that

$$\hat{J}_{\mathbb{R}}=O\hat{A}_{\mathbb{R}}O^T,$$

where

$$\hat{J}_{\mathbb{R}}=\begin{pmatrix} X_1 & & & & & & \\ & X_2 & & & & P & \\ & & \ddots & & & & \\ & & & X_s & & & \\ & 0 & & & \lambda_{2s+1} & & \\ & & & & & \ddots & \\ & & & & & & \lambda_{4n} \end{pmatrix}$$

$$=\begin{pmatrix} X_1 & & & & & & \\ & X_2 & & & & 0 & \\ & & \ddots & & & & \\ & & & X_s & & & \\ & 0 & & & \lambda_{2s+1} & & \\ & & & & & \ddots & \\ & & & & & & \lambda_{4n} \end{pmatrix}+\begin{pmatrix} 0 & & & & & & \\ & 0 & & & & P & \\ & & \ddots & & & & \\ & & & 0 & & & \\ & 0 & & & 0 & & \\ & & & & & \ddots & \\ & & & & & & 0 \end{pmatrix}$$

$$=\hat{D}_{\mathbb{R}}+\hat{N}_{\mathbb{R}}. \tag{26}$$

In the previous equation, X_r represents a 2×2 real matrix with eigenvalues $\lambda_r\pm i\mu_r$. An appropriate choice of O guarantees that

$$X_r=\begin{pmatrix} \lambda_r & -\mu_r \\ \mu_r & \lambda_r \end{pmatrix}. \tag{27}$$

Let us come back to the $\mathbb{R}$-linear transformation $A_{\mathbb{R}}$. By using the translation rules given in Eqs. (24) and (25), we can immediately give its canonical form

$$J_{\mathbb{R}}=D_{\mathbb{R}}+N_{\mathbb{R}}.$$

In particular, the diagonal elements of $D_{\mathbb{R}}$ corresponding to the quaternionic translation of the real blocks

$$\hat{D}_{1,\mathbb{R}}=\begin{pmatrix} \lambda_m & -\mu_m & 0 & 0 \\ \mu_m & \lambda_m & 0 & 0 \\ 0 & 0 & \lambda_{m+1} & -\mu_{m+1} \\ 0 & 0 & \mu_{m+1} & \lambda_{m+1} \end{pmatrix},$$

$$\hat{D}_{2,\mathbb{R}}=\begin{pmatrix} \lambda_m & -\mu_m & 0 & 0 \\ \mu_m & \lambda_m & 0 & 0 \\ 0 & 0 & \lambda_{m+1} & 0 \\ 0 & 0 & 0 & \lambda_{m+2} \end{pmatrix}, \tag{28}$$

$$\hat{D}_{3,\mathbb{R}}=\begin{pmatrix} \lambda_m & 0 & 0 & 0 \\ 0 & \lambda_{m+1} & 0 & 0 \\ 0 & 0 & \lambda_{m+2} & 0 \\ 0 & 0 & 0 & \lambda_{m+3} \end{pmatrix}$$

are respectively given by

$$\begin{aligned} D_{1,\mathbb{R}}&=\tfrac{1}{2}[\lambda_m(1-L_iR_i)+\mu_m(L_i+R_i)+\lambda_{m+1}(1+L_iR_i)+\mu_{m+1}(L_i-R_i)], \\ D_{2,\mathbb{R}}&=\tfrac{1}{2}[\lambda_m(1-L_iR_i)+\mu_m(L_i+R_i)+\tfrac{1}{2}\lambda_{m+1}(1+L_iR_i-L_jR_j+L_kR_k) \\ &\quad+\tfrac{1}{2}\lambda_{m+2}(1+L_iR_i+L_jR_j-L_kR_k)], \\ D_{3,\mathbb{R}}&=\tfrac{1}{4}[\lambda_m(1-L_iR_i-L_jR_j-L_kR_k)+\lambda_{m+1}(1-L_iR_i+L_jR_j+L_kR_k) \\ &\quad+\lambda_{m+2}(1+L_iR_i-L_jR_j+L_kR_k)+\lambda_{m+3}(1+L_iR_i+L_jR_j-L_kR_k)]. \end{aligned} \tag{29}$$

As happens for $\mathbb{C}$-linear quaternionic matrices, an $\mathbb{R}$-linear quaternionic matrix is diagonalizable if the corresponding real counterpart is diagonalizable. The converse is not necessarily true.

V. THE EIGENVALUE PROBLEM FOR $\mathbb{R}$-LINEAR MATRICES

Let us now consider the eigenvalue problem for $\mathbb{R}$-linear quaternionic matrices. Equation (13) is obviously too restrictive. In fact, such an equation sets the real eigenvalue spectrum of $\mathbb{R}$-linear quaternionic operators. No information is given about the remaining eigenvalues. In particular, if the real counterpart $\hat{M}_{\mathbb{R}}$ of the $\mathbb{R}$-linear quaternionic matrix $M_{\mathbb{R}}$ does not have real eigenvalues, Eq. (13) does not admit solution. This is very embarrassing if we consider, for example, $\mathbb{R}$-linear anti-Hermitian quaternionic operators. Thus, we need to modify Eq. (13). The discussion regarding the ''pseudo-triangular'' form of the matrices $\hat{A}_{\mathbb{R}}$ [see Eq. (26)] suggests as a $\mathbb{R}$-linear eigenvalue problem the following system of *coupled* equations:

$$\begin{aligned} M_{\mathbb{R}}\psi&=a\psi+b\varphi, \\ M_{\mathbb{R}}\varphi&=c\varphi+d\psi, \end{aligned} \tag{30}$$

where

$$a,b,c,d\in\mathbb{R}, \quad \psi=\psi_0+i\psi_1+j\psi_2+k\psi_3, \quad \varphi=\varphi_0+i\varphi_1+j\varphi_2+k\varphi_3,$$
$$\psi_{0,\ldots,3},\varphi_{0,\ldots,3}\in V[n,\mathbb{R}].$$

It can be shown that the real coefficients a,b,c,d are related to the real and imaginary parts of the $\hat{M}_{\mathbb{R}}$ eigenvalues. In fact, by translating the system (30) into its real matrix counterpart, we find

$$\begin{pmatrix} \hat{M}_{\mathbb{R}} & 0 \\ 0 & \hat{M}_{\mathbb{R}} \end{pmatrix} \begin{pmatrix} \hat{\psi} \\ \hat{\varphi} \end{pmatrix} = \begin{pmatrix} a\mathbf{1}_{4n} & b\mathbf{1}_{4n} \\ c\mathbf{1}_{4n} & d\mathbf{1}_{4n} \end{pmatrix} \begin{pmatrix} \hat{\psi} \\ \hat{\varphi} \end{pmatrix}, \tag{31}$$

where

$$\hat{\psi} = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}, \quad \hat{\varphi} = \begin{pmatrix} \varphi_0 \\ \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix} \quad \in V[4n,\mathbb{R}].$$

The matrix equation (31) admits nontrivial solutions if and only if

$$\det\left[\begin{pmatrix} \hat{M}_{\mathbb{R}} - a\mathbf{1}_{4n} & -b\mathbf{1}_{4n} \\ -c\mathbf{1}_{4n} & \hat{M}_{\mathbb{R}} - d\mathbf{1}_{4n} \end{pmatrix} \right] = 0. \tag{32}$$

By rewriting the matrix $\hat{M}_{\mathbb{R}}$ in terms of the similarity matrix $\hat{S}_{\mathbb{R}}$ and of its Jordan form $\hat{J}_{\mathbb{R}}$, i.e.,

$$\hat{M}_{\mathbb{R}} = \hat{S}_{\mathbb{R}} \hat{J}_{\mathbb{R}} \hat{S}_{\mathbb{R}}^{-1},$$

and by using the cyclic property of the determinant, we reduce Eq. (32) to

$$\det\left[\begin{pmatrix} \hat{J}_{\mathbb{R}} - a\mathbf{1}_{4n} & -b\mathbf{1}_{4n} \\ -c\mathbf{1}_{4n} & \hat{J}_{\mathbb{R}} - d\mathbf{1}_{4n} \end{pmatrix} \right] = 0. \tag{33}$$

By simple algebraic manipulations,[20] we obtain

$$\begin{aligned} \det\left[\begin{pmatrix} \hat{J}_{\mathbb{R}} - a\mathbf{1}_{4n} & -b\mathbf{1}_{4n} \\ -c\mathbf{1}_{4n} & \hat{J}_{\mathbb{R}} - d\mathbf{1}_{4n} \end{pmatrix} \right] &= \det[(\hat{J}_{\mathbb{R}} - a\mathbf{1}_{4n})(\hat{J}_{\mathbb{R}} - d\mathbf{1}_{4n}) - bc\mathbf{1}_{4n}] \\ &= \det[\hat{J}_{\mathbb{R}}^2 - (a+d)\hat{J}_{\mathbb{R}} + (ad-bc)\mathbf{1}_{4n}] \\ &= \prod_i [z_i^2 - (a+d)z_i + (ad-bc)] = 0, \end{aligned}$$

where z_i represent the eigenvalues of the real matrix $\hat{M}_{\mathbb{R}}$. The previous equation explicitly shows the relation between the real coefficients a,b,c,d (which appear in the $\mathbb{R}$-linear eigenvalue problem) and the eigenvalues z of the real counterpart of the quaternionic matrix $M_{\mathbb{R}}$. In the case of complex eigenvalues z, we find

$$\Delta = (a+d) - 4(ad-bc) = (a-d)^2 + bc < 0. \tag{34}$$

This condition guarantees that the eigenvalues of the real matrix

$$Z = \begin{pmatrix} a\mathbf{1}_{4n} & b\mathbf{1}_{4n} \\ c\mathbf{1}_{4n} & d\mathbf{1}_{4n} \end{pmatrix}$$

appear in conjugate pairs. Consequently, we can find a real similarity transformation T such that

$$TZT^{-1}=\begin{pmatrix} \lambda \mathbf{1}_{4n} & -\mu \mathbf{1}_{4n} \\ \mu \mathbf{1}_{4n} & \lambda \mathbf{1}_{4n} \end{pmatrix}.$$

Finally, without loss of generality, we can consider the following eigenvalue problem for $\mathbb{R}$-linear transformations

$$\begin{aligned} M_{\mathbb{R}}\psi &= \lambda\psi - \mu\varphi, \\ M_{\mathbb{R}}\varphi &= \lambda\varphi + \mu\psi. \end{aligned} \tag{35}$$

VI. FINAL REMARKS

These final remarks aim to give a concluding discussion on the ''coupled'' eigenvalue problem and a brief summary of mathematical and physical applications motivating our interest in this research. In particular, we are interested to bring together two areas: quaternionic differential operators and quantum mechanics.

A. Coupled eigenvalue equations

In the previous section, we have introduced, for $\mathbb{R}$-linear transformations, the eigenvalue problem (35) which represents the *natural* generalization of (13). In particular, as we observed above, the study of system (35) instead of Eq. (13) allows us to take into account the existence of complex eigenvalues and, consequently, complete the eigenvalue spectrum of $\mathbb{R}$-linear quaternionic operators. Actually, the eigenvalue problem (35) also applies to $\mathbb{H}$- and $\mathbb{C}$-linear transformations. It can be considered as an equivalent formulation of Eqs. (9) and (12). To show that, let us consider the equation

$$M_{\mathbb{C}}\psi = \psi z = \psi\lambda + \psi i\mu. \tag{36}$$

We limit ourselves to discussing $\mathbb{C}$-linear transformations. Obviously, if a preferred complex direction is chosen for the eigenvalues of $\mathbb{H}$-linear quaternionic operators, all the arguments in what follows also hold for $\mathbb{H}$-linear transformations. By using the $\mathbb{C}$-linearity, we find

$$(M_{\mathbb{C}}\psi)i = M_{\mathbb{C}}(\psi i) = \psi i\lambda - \psi\mu.$$

The pair of eigenvector $(\psi, \varphi = \psi i)$, where ψ is solution of Eq. (36), satisfies the coupled equations

$$\begin{aligned} M_{\mathbb{C}}\psi &= \lambda\psi - \mu\varphi, \\ M_{\mathbb{C}}\varphi &= \mu\psi + \lambda\varphi. \end{aligned} \tag{37}$$

Vice versa, let $M_{\mathbb{C}}$ and (37) be respectively a $\mathbb{C}$-linear transformation and the corresponding eigenvalue problem. We denote by (ψ, φ) a solution of the system (37). If ψ satisfies Eq. (36), too, then, comparing Eq. (36) and the first equation in (37), one immediately obtains $\varphi = \psi i$. If, on the contrary, ψ is not a solution of Eq. (36), by using the $\mathbb{C}$-linearity, we obtain

$$M_{\mathbb{C}}(\varphi i) = (M_{\mathbb{C}}\varphi)i = \mu\psi i + \varphi i.$$

Thus,

$$M_{\mathbb{C}}(\psi + \varphi i) = (\psi + \varphi i)z. \tag{38}$$

Hence, it is possible to associate to any solution (ψ, φ) of the system (37) a corresponding eigenvector of $M_{\mathbb{C}}$.

It is worth pointing out that the coupled system (35) can be obtained by solving the eigenvalue problem (13) for *complexified* quaternionic eigenvectors and *complexified* real eigenvalues. In fact, by imposing that

$$\psi \to \Psi = \psi + I\varphi \quad \in \mathbb{H}(1,i,j,k) \otimes \mathbb{C}(1,I),$$

and

$$r \to Z = \lambda + I\mu \quad \in \mathbb{C}(1,I),$$

from the *complexified* eigenvalue problem (13),

$$M_{\mathbb{R}}\Psi = \Psi Z,$$

we immediately get the coupled system (35).

B. Applications

Many physical problems dealing with differential operators are greatly simplified by using the matrix formalism and solving the corresponding eigenvalue problem.

Let us first consider a very simple case, that is, the $\mathbb{H}$-linear second order homogeneous ordinary differential equation

$$\ddot{\psi}(x) - \alpha\dot{\psi}(x) - \beta\psi(x) = 0, \quad \alpha,\beta \in \mathbb{H}, \quad x \in \mathbb{R}. \tag{39}$$

In looking for quaternionic exponential solution $\psi(x) = \exp[qx]$ and observing that the derivative of $\exp[qx]$ with respect to the real variable x is $q\exp[qx]$, we reduce the previous problem to find the solutions of the following quadratic equation

$$q^2 = \alpha q + \beta. \tag{40}$$

This equation can be rewritten in matrix form as follows:

$$M_{\mathbb{H}}\begin{pmatrix} q \\ 1 \end{pmatrix} = \begin{pmatrix} q^2 \\ q \end{pmatrix}, \quad M_{\mathbb{H}} = \begin{pmatrix} \alpha & \beta \\ 1 & 0 \end{pmatrix}. \tag{41}$$

As seen in this article, the $\mathbb{H}$-linear quaternionic matrix $M_{\mathbb{H}}$ satisfies a right (complex) eigenvalue equation

$$M_{\mathbb{H}}\begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} v \\ w \end{pmatrix} z, \quad z \in \mathbb{C}, \quad v,w \in \mathbb{H}, \quad w\overline{w} = 1. \tag{42}$$

Due to the particular form of $M_{\mathbb{H}}$, the components of the $M_{\mathbb{H}}$-eigenvectors satisfy the following condition

$$v = wz. \tag{43}$$

Multiplying (from the right) Eq. (42) by $\overline{w}$ and using the constraint (43), we obtain

$$M_{\mathbb{H}}\begin{pmatrix} wz\overline{w} \\ 1 \end{pmatrix} = \begin{pmatrix} wz^2\overline{w} \\ wz\overline{w} \end{pmatrix}. \tag{44}$$

Comparing Eq. (41) with Eq. (44), we immediately get

$$q = wz\overline{w}. \tag{45}$$

The problem of finding exponential solutions for a $\mathbb{H}$-linear differential with constant coefficients and, consequently, zeros of $\mathbb{H}$-linear polynomial equations,[21] is thus equivalent to solving the right (complex) eigenvalue problem for the associated matrix. Obviously, the previous considerations also hold for the n-dimensional case.

The solutions of $\mathbb{X}$-linear quaternionic differential equations with constant coefficients

$$\psi^{(n)}(x)-A_{n-1,\mathbb{X}}\psi^{(n-1)}(x)-A_{n-2,\mathbb{X}}\psi^{(n-2)}(x)-\cdots -A_{0,\mathbb{X}}\psi(x)=0, \quad \mathbb{X}=\mathbb{R},\mathbb{C},\mathbb{H}, \tag{46}$$

can be given in terms of the eigenvalues and eigenvectors of the matrix

$$\begin{pmatrix} A_{n-1,\mathbb{X}} & A_{n-2,\mathbb{X}} & \cdots & A_{0,\mathbb{X}} \\ 1 & 0 & \cdots & 0 \\ . & . & \cdots & . \\ . & . & \cdots & . \\ . & . & \cdots & . \\ 0 & 0 & ..1 & 0 \end{pmatrix}.$$

Interesting $\mathbb{C}$-linear differential equations appear in quaternionic quantum mechanics.[3] For example, by studying quaternionic tunneling effects as a candidate to possible phenomenological deviations from the standard (complex) theory, we have to solve the following $\mathbb{H}$-linear Schrödinger equation,

$$\partial_t\Psi(x,t)=\left[\frac{i}{\hbar}\left(\frac{\hbar^2}{2m}\partial_{xx}-iV\right)+\frac{j}{\hbar}W\right]\Psi(x,t), \tag{47}$$

where $(j/\hbar)W$ represents the *new* quaternionic perturbation. The quaternionic stationary state wave function

$$\Psi(x,t)=\psi(x)\exp\left[-\frac{i}{\hbar}Et\right] \tag{48}$$

is a solution of Eq. (47) on the condition that $\psi(x)$ be a solution of the following time-independent $\mathbb{C}$-linear (ordinary) differential equation:

$$i\frac{\hbar^2}{2m}\ddot{\psi}(x)-iV\psi(x)+jW\psi(x)+\psi(x)iE=0. \tag{49}$$

Observe that the choice of the imaginary unit i in the Laplacian operator ∂_{xx}, Eq. (47), and in the time exponential, Eq. (48), is fundamental to recover the standard results in the complex limit. In this formalism, quaternionic potentials are treated as perturbation effects on standard quantum mechanics. We also point out that the right position of the time exponential is fundamental to perform the separation of variables.

The solution of Eq. (49) can be given in terms of the eigenvalues and eigenvectors of the $\mathbb{C}$-linear matrix

$$\begin{pmatrix} 0 & A_{0,\mathbb{C}} \\ 1 & 0 \end{pmatrix},$$

where

$$A_{0,\mathbb{C}}=\frac{2m}{\hbar^2}(V+L_kW+L_iR_iE).$$

A detailed phenomenological discussion of the quaternionic tunneling effect is found in the paper of Ref. 4.

C. Outlooks

As seen in this article, the choice of right (complex) eigenvalues for $\mathbb{H}$- and $\mathbb{C}$-linear operators plays a fundamental role in discussing canonical forms and in finding solutions of polynomial and differential equations. It was shown that the right (complex) eigenvalue problem is equivalent to a ''coupled'' system and this was extremely important to study the eigenvalue problem for $\mathbb{R}$-linear quaternionic matrices, where a pair of real eigenvalues must be introduced. This work was intended as an attempt at motivating the study of $\mathbb{R}$- and $\mathbb{C}$-linear quaternionic operators in view of possible applications in quantum mechanics and gauge theory. It would be desirable to give a complete theory of $\mathbb{X}$-linear quaternionic matrices and differential operators. More realistically, this article touches only a few aspects of the theory and shows how the choice of the right eigenvalue equation seems to be the best to investigate quaternionic formulations of physical theory. It was not our purpose to study here differential operators. The results in this field are far from being conclusive and some questions represent at present intriguing challenges: variations of parameters; order reduction; not invertible higher derivative $\mathbb{R}$- and $\mathbb{C}$-linear constant coefficients; variable coefficients; and integral transforms. Finally, it would be desirable to extend the discussion on the eigenvalue problem by matrix translation to the nonassociative case.[22–24]

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Matrix models for beta ensembles

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This paper constructs tridiagonal random matrix models for general ($\beta>0$) β-Hermite (Gaussian) and β-Laguerre (Wishart) ensembles. These generalize the well-known Gaussian and Wishart models for $\beta=1,2,4$. Furthermore, in the cases of the β-Laguerre ensembles, we eliminate the exponent quantization present in the previously known models. We further discuss applications for the new matrix models, and present some open problems. © *2002 American Institute of Physics.*
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I. INTRODUCTION

A. Overview

Classical random matrix theory focuses on the random matrix models in the following 3×3 table:

	Real, $\beta=1$	**Complex**, $\beta=2$	**Quaternion**, $\beta=4$
Hermite	GOE	GUE	GSE
Laguerre	Real Wishart	Complex Wishart	(Quaternion Wishart)
Jacobi	Real MANOVA	Complex MANOVA	(Quaternion MANOVA)

The two entries in parentheses (in the third column) correspond to less-studied random matrix models; the others are mainstream and have been extensively researched and publicized. The three columns correspond to Dyson's ''threefold way'' $\beta=1,2$, and 4; the three rows correspond to the weight function associated to the random matrix model. Other weight functions have also been considered (for example, the uniform weight on the unit circle corresponds to the circular ensembles).

Zirnbauer[33] and Ivanov[12] produced a more general taxonomy of random matrix models. Their characterizations (''tenfold,'' and ''twelvefold,'' respectively) are based on symmetric spaces, and include Hermite, Laguerre, and Jacobi cases, and also the circular ensembles (each of their models can be associated with $\beta=1,2$ or 4).

We propose a random matrix program of study that would generalize β beyond the above-mentioned threefold way, thus generalizing the 3×3 Cartesian product to $3\times\infty$, making the leap from discrete characterizations to continuous ones. A step in this direction has been initiated by Forrester,[2,10] who studied the β-ensembles in connection with multivariate orthogonal polynomials and Calogero–Sutherland-type quantum systems. Furthermore, in the case of the classical Laguerre and Jacobi models, our program goes beyond the quantized exponents forced by the classical models, and proposes continuous ones.

For the benefit of the reader we have expanded the 3×3 table with detailed information in Fig. 1.

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Random Matrix Ensembles

Joint Eigenvalue Distributions: $c\,|\Delta|^{\beta}\prod_{i=1}^{n} V(\lambda_i)$

Technical name	Traditional name	β	Field	Property	Invariance	Connected Matrix Problem
Hermite ensembles	**Gaussian ensembles**					(EIG)
$V(\lambda)=e^{-\lambda^2/2}$	GOE	1	$\mathbb{R}$	Symmetric	$A \leftarrow Q^T A Q$	Symmetric Eigenvalue Problem
	GUE	2	$\mathbb{C}$	Hermitian	$A \leftarrow U^H A U$	
	GSE	4	$\mathbb{H}$	Self–Dual	$A \leftarrow S^D A S$	
Laguerre ensembles	**Wishart ensembles**					(SVD)
$V(\lambda)=\lambda^a e^{-\lambda/2}$	Wishart real	1	$\mathbb{R}$	Positive Semi–Definite	$A \leftarrow Q^T A Q$	Singular Value Decomposition
$a=\frac{\beta}{2}(n-m+1)-1$	Wishart complex	2	$\mathbb{C}$		$A \leftarrow U^H A U$	
	Wishart quaternion	4	$\mathbb{H}$		$A \leftarrow S^D A S$	
Jacobi ensembles	**MANOVA ensembles**					(QZ)
$V(\lambda)=\lambda^a(1-\lambda)^b$	MANOVA real	1	$\mathbb{R}$	Positive Semi–Definite	$X \leftarrow Q^T X Q_1$, $Y \leftarrow Q^T Y Q_1$	Generalized Symmetric Eigenvalue Problem
$a=\frac{\beta}{2}(n_1-m+1)-1$	MANOVA complex	2	$\mathbb{C}$		$X \leftarrow U^H X U_1$, $Y \leftarrow U^H Y U_1$	
$b=\frac{\beta}{2}(n_2-m+1)-1$	MANOVA quaternion	4	$\mathbb{H}$		$X \leftarrow S^D X S_1$, $Y \leftarrow S^D Y S_1$	

Type of ensemble	β	**MATLAB** code
Hermite	1	A = randn(n); A = (A+A') / 2;
	2	A = randn(n) + i * randn(n); A = (A+A') / 2;
	4	X = randn(n) + i * randn(n); Y = randn(n) + i * randn(n); A = [X Y; −conj(Y) conj(X)]; A = (A+A') / 2;
Laguerre	1	A = randn(m, n); A = A * A';
	2	A = randn(m, n) + i * randn(m, n); A = A * A';
	4	X = randn(m, n) + i * randn(m, n); Y = randn(m, n) + i * randn(m, n); A = [X Y; −conj(Y) conj(X)]; A = A * A';
Jacobi	1	X = randn(m, n_1); Y = randn(m, n_2); A = (X * X') / (X * X' + Y * Y');
	2	X = randn(m, n_1) + i * randn(m, n_1); Y = randn(m, n_2) + i * randn(m, n_2); A = (X * X') / (X * X' + Y * Y');
	4	X_1 = randn(m, n_1) + i * randn(m, n_1); X_2 = randn(m, n_1) + i * randn(m, n_1); Y_1 = randn(m, n_2) + i * randn(m, n_2); Y_2 = randn(m, n_2) + i * randn(m, n_2); X = [X_1 X_2; −conj(X_2) conj(X_1)]; Y = [Y_1 Y_2; −conj(Y_2) conj(Y_1)]; A = (X * X') / (X * X' + Y * Y');

FIG. 1. Random matrix ensembles. As a guide to MATLAB notation, randn(m,n) produces an $m\times n$ matrix with i.i.d. standard normal entries, conj(X) produces the complex conjugate of the matrix X, and the apostrophe $(')$ operator produces the conjugate transpose of a matrix. Also $[X\ Y;\ Z\ W]$ produces a 2×2 block matrix.

B. Background

The Gaussian (or Hermite) ensembles arise in physics, and are identified by Dyson[7] by the group over which they are invariant: Gaussian Orthogonal or for short GOE (with real entries), Gaussian Unitary or GUE (with complex entries), and Gaussian Symplectic or GSE (with quaternion entries). The Wishart ensembles arise in statistics, and the three corresponding models could be named Wishart real, Wishart complex, and Wishart quaternion.

The three Gaussian ensembles have joint eigenvalue probability density function

$$\text{HERMITE: } f_\beta(\lambda)=c_H^\beta \prod_{i<j} |\lambda_i-\lambda_j|^\beta \exp\left(-\sum_{i=1}^{n} \lambda_i^2/2\right), \tag{1}$$

with $\beta=1$ corresponding to the reals, $\beta=2$ to the complexes, $\beta=4$ to the quaternions, and with

$$c_H^\beta=(2\pi)^{-n/2}\prod_{j=1}^{n}\frac{\Gamma\left(1+\frac{\beta}{2}\right)}{\Gamma\left(1+\frac{\beta}{2}j\right)}. \tag{2}$$

The best references are Mehta[18] and the original paper by Dyson.[7]

Similarly, the Wishart (or Laguerre) models have joint eigenvalue p.d.f.

$$\text{LAGUERRE: } f_\beta(\lambda)=c_L^{\beta,a}\prod_{i<j}|\lambda_i-\lambda_j|^\beta\prod_i \lambda_i^{a-p}\exp\left(\sum_{i=1}^n \lambda_i/2\right), \tag{3}$$

with $a=(\beta/2)\,n$ and $p=1+(\beta/2)\,(m-1)$. Again, $\beta=1$ for the reals, $\beta=2$ for the complexes, and $\beta=4$ for the quaternions. The constant

$$c_L^{\beta,a}=2^{-ma}\prod_{j=1}^m \frac{\Gamma\left(1+\frac{\beta}{2}\right)}{\Gamma\left(1+\frac{\beta}{2}j\right)\Gamma\left(a-\frac{\beta}{2}(m-j)\right)}. \tag{4}$$

Good references are Refs. 21, 8, and 13, and for $\beta=4$, Ref. 17.

To complete the triad of classical orthogonal polynomials, we will mention the β-MANOVA ensembles, which are associated with the multivariate analysis of variance (MANOVA) model. They are better known in the literature as the Jacobi ensembles, with joint eigenvalue p.d.f.

$$\text{JACOBI: } f_\beta(\lambda)=c_J^{\beta,a_1,a_2}\prod_{i<j}|\lambda_i-\lambda_j|^\beta\prod_{j=1}^n \lambda_i^{a_1-p}(1-\lambda_i)^{a_2-p}, \tag{5}$$

with $a_1=(\beta/2)\,n_1$, $a_2=(\beta/2)\,n_2$, and $p=1+(\beta/2)\,(m-1)$. As usual, $\beta=1$ for real and $\beta=2$ for complex; also

$$c_J^{\beta,a_1,a_2}=\prod_{j=1}^m \frac{\Gamma\left(1+\frac{\beta}{2}\right)\Gamma\left(a_1+a_2-\frac{\beta}{2}(m-j)\right)}{\Gamma\left(1+\frac{\beta}{2}j\right)\Gamma\left(a_1-\frac{\beta}{2}(m-j)\right)\Gamma\left(a_2-\frac{\beta}{2}(m-j)\right)}. \tag{6}$$

The MANOVA real and complex cases ($\beta=1$ and 2) have been studied by statisticians (see Ref. 21).

Though ''Gaussian,'' ''Wishart,'' and ''MANOVA'' are the traditional names for the three types of β-ensembles, we prefer the sometimes used and technically more informative names ''Hermite,'' ''Laguerre,'' and ''Jacobi'' ensembles. These technical names reflect the fact that the p.d.f.s for the ensembles correspond to the p.d.f.s $\text{etr}(-A^2/2)$, $\det(A)^{a-p}\text{etr}(-A/2)$, and $\det(A)^{a_1-p}\det(I-A)^{a_2-p}$ over their respective spaces of matrices. In turn, these functions correspond to three sets of orthogonal polynomials (Hermite, Laguerre, Jacobi). Throughout this paper, we will use the term ''general β-Hermite, -Laguerre, -Jacobi ensembles'' for general β in the p.d.f.s (1), (3), (5).

Though it was believed that no other choice of β would correspond to a matrix model constructed with entries from a classical distribution, there have been studies of general β-Hermite ensembles as theoretical eigenvalue distributions. They turn out to have important applications in lattice gas theory (see Refs. 10 and 2).

The general β ensembles appear to be connected to a broad spectrum of mathematics and physics, among which we list lattice gas theory, quantum mechanics, and Selberg-type integrals. Also, the β ensembles are connected to the theory of Jack polynomials (with the correspondence $\alpha=2/\beta$ where α is the Jack parameter), which are currently objects of intensive research (see Refs. 27, 17, and 23).

TABLE I. Random matrix constructions.

Hermite matrix $n \in \mathbb{N}$	$H_\beta \sim \frac{1}{\sqrt{2}} \begin{pmatrix} N(0,2) & \chi_{(n-1)\beta} & & & & \\ \chi_{(n-1)\beta} & N(0,2) & \chi_{(n-2)\beta} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \chi_{2\beta} & N(0,2) & \chi_\beta & \\ & & & \chi_\beta & N(0,2) \end{pmatrix}$
Laguerre matrix $m \in \mathbb{N}$ $a \in \mathbb{R}$ $a > \frac{\beta}{2}(m-1)$	$L_\beta = B_\beta B_\beta^T$, where $B_\beta \sim \begin{pmatrix} \chi_{2a} & & & \\ \chi_{\beta(m-1)} & \chi_{2a-\beta} & & \\ & \ddots & \ddots & \\ & & \chi_\beta & \chi_{2a-\beta(m-1)} \end{pmatrix}$

C. Our results

Dyson's original threefold way is a byproduct of the invariance assumptions as in the ''Invariance'' column of Fig. 1. By necessity, any invariant distribution is generically dense. Further, the invariance approach forces the consideration of the complex and quaternion division algebras.

In this paper, we drop the invariance requirement. What we gain are ''sparse'' models (with only $O(n)$ nonzero parameters) over the reals numbers *only*. As an additional bonus, we go beyond the quantizations of the classical cases $\beta = 1,2,4$ and obtain continuous exponents (see Sec. IV for further discussion of this point).

We provide real tridiagonal random matrix models for all β-Gaussian (or Hermite) and β-Wishart (or Laguerre) ensembles, and we discuss the possibility of constructing a real matrix model for the β-MANOVA (or Jacobi) ensembles.

We obtain our results by extrapolating the classical cases, thereby providing concrete models for what have previously been considered purely theoretical distributions.

In Sec. II we establish results for symmetric tridiagonal matrices, and we use them to construct tridiagonal models for the β-Hermite ensembles. Along the way, we obtain a short proof based on random matrix theory for the Jacobian of the transformation $T \to (q, \lambda)$, where T is a symmetric tridiagonal matrix, λ is its set of eigenvalues, and q is the first row of its eigenvector matrix. In Sec. III we construct tridiagonal models for the β-Laguerre ensembles, by building on the same set of ideas that we use in Sec. II. In Sec. IV we present some immediate applications of the new classes of ensembles and we discuss the β-Jacobi ensembles and other interesting open problems.

We display our random matrix constructions in Table I.

II. THE β-HERMITE (GAUSSIAN) ENSEMBLES

A. Motivation: Tridiagonalizing the GOE, GUE, and GSE

The joint distribution $f_\beta(\lambda)$ of the eigenvalues for the GOE, GUE, and GSE is

$$f_\beta(\Lambda) = c_H^\beta |\Delta(\lambda)|^\beta \exp\left(-\frac{1}{2} \sum_i \lambda_i^2 \right), \tag{7}$$

where $\beta = 1,2,4$.[18] Here the Vandermonde determinant notation $\Delta(\lambda)$ stands for $\Pi_{i \neq j}(\lambda_i - \lambda_j)$, and c_H^β is given by (2).

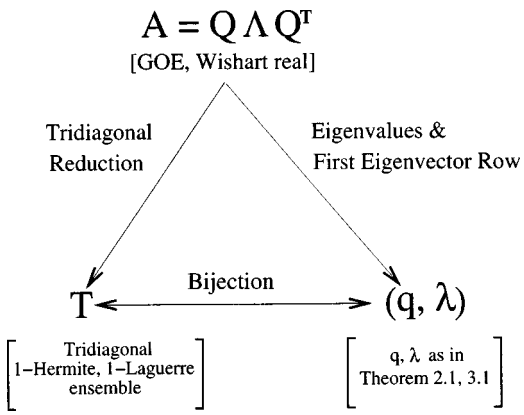

FIG. 2. A dense symmetric matrix A can be tridiagonalized (left-hand side) or diagonalized (right-hand side). In brackets, we provide the distributions starting with that of A (GOE or Wishart real).

We will prove in Sec. II B that the tridiagonal β-Hermite random matrix displayed in Table I has the joint eigenvalue p.d.f. given by general β in (7). For motivation, we will begin with a quick ''back-door'' proof for $\beta=1$ by tridiagonalizing the GOE; then we will extend the result to the GUE and GSE.

To illustrate the proof and help the reader follow it more easily, we have included the diagram of Fig. 2.

Theorem 2.1: *If A is an $n\times n$ matrix from the GOE, then reduction of A to tridiagonal form shows that the matrix T from the 1-Hermite ensemble has joint eigenvalue p.d.f. given by (7) with $\beta=1$.*

Proof: We write $A=\left(\begin{smallmatrix} a_n & x^T \\ x & B \end{smallmatrix}\right)$. Here a_n is a standard Gaussian, x is a vector of $(n-1)$ i.i.d. Gaussians of mean 0 and variance 1/2, and B is an $(n-1)\times(n-1)$ matrix from the GOE; a_n, x and B are all independent from each other.

Let H be any $(n-1)\times(n-1)$ orthogonal matrix (depending only on x) such that

$$Hx=[\|x\|_2\ 0...0]^T\equiv\|x\|_2 e_1,$$

where $e_1=[1,0,\ldots,0]^T$. Then clearly

$$\begin{pmatrix} 1 & 0 \\ 0 & H \end{pmatrix}\begin{pmatrix} a_n & x^T \\ x & B \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & H^T \end{pmatrix}=\begin{pmatrix} a_n & \|x\|_2 e_1^T \\ \|x\|_2 e_1 & HBH^T \end{pmatrix}.$$

Since A is from the GOE and H depends only on x, we can readily identify the distributions of a_n, $\|x\|_2$, and HBH^T (these three quantities are clearly independent). The entry a_n is unchanged and thus a standard normal with variance 1. Being the length of a multivariate Gaussian of mean 0 and entry variance 1/2, $\|x\|_2$ has the distribution $(1/\sqrt{2})\,\chi_{n-1}$. It is worth mentioning that the p.d.f. of $\|x\|_2$ is given by

$$\frac{2}{\Gamma\left(\frac{n-1}{2}\right)}y^{n-2}e^{-y^2}.$$

Finally, by the orthogonal invariance of the GOE, HBH^T is an $(n-1)\times(n-1)$ matrix from the GOE.

Proceeding by induction completes the tridiagonal construction.

Because the only operations we perform on A are orthogonal similarity transformations, which do not affect the eigenvalues, the conclusion of the theorem follows. □

We recall that matrices from the GOE have the following properties:

Property 1: The joint eigenvalue density is $c_H^1|\Delta(\lambda)|\exp(-\frac{1}{2}\Sigma_i\lambda_i^2)$.[18]

Property 2: The first row of the eigenvector matrix is distributed uniformly on the sphere, and it is independent of the eigenvalues.

The second property is an immediate consequence of the fact that the eigenvector matrix of a GOE matrix is independent from the eigenvalues [Ref. 18, (3.1.3) and (3.1.16), pp. 55–58], and has the Haar (uniform) distribution because of the orthogonal invariance.

The following corollary is easily established.

Corollary 2.2: If T is a matrix from the 1-Hermite ensemble, with eigendecomposition $T=Q\Lambda Q^T$, then the first row q of the eigenvector matrix Q is independent of Λ, and is distributed uniformly on the sphere.

Proof: If $A=Q_1\Lambda Q_1^T$ and $T=HAH^T$, then $Q=HQ_1$. Since each one of the reflectors which form H has first row e_1, multiplication by H does not affect the first row of Q_1. The conclusion follows. □

Reduction to tridiagonal form is a familiar algorithm which solves the symmetric eigenvalue problem. The special ''reflector'' matrix H used in practice for a vector $x=[x_1,\ldots,x_{n-1}]^T$ is

$$H=I-2\frac{uu^T}{u^Tu},$$

where $u=x\pm x_1\ e_1$. This special matrix H is known as the ''Householder reflector'' (see Ref. 11, p. 209).

The tridiagonal reduction algorithm can be applied to any real symmetric, complex hermitian, or quaternion self-dual matrix; the resulting matrix is always a real, symmetric tridiagonal. Using the algorithm similarly on a GUE or GSE matrix one gets the following.

Corollary 2.3: When $\beta=2,4$, reduction to tridiagonal form of matrices from the GUE, respectively, GSE, shows that the tridiagonal 2-Hermite, respectively, 4-Hermite, random matrix has the distribution given by (7). Note that β "counts" the number of independent Gaussians in each entry of the matrix.

Remark 2.4: The observation that numerical linear algebra algorithms may be performed statistically is not new; it may be found in the literature (see Trotter—Ref. 31, Silverstein—Ref. 26, and Edelman—Ref. 8).

B. Tridiagonal matrix lemmas

In this section we prove lemmas that will be used in our constructions in Secs. II C and III B.

Given a tridiagonal matrix T defined by the diagonal $a=(a_n,\ldots,a_1)$ and subdiagonal $b=(b_{n-1},\ldots,b_1)$, with all b_i positive, let $T=Q\Lambda Q^T$ be the eigendecomposition of T as in Theorem 2.12. Let q be the first row of Q and $\lambda=\mathrm{diag}(\Lambda)$.

Lemma 2.5: Under the above-given assumptions, starting from q and λ, one can uniquely reconstruct Q and T.

Proof: This is a special case of the more general Theorem 7.2.1 in Parlett.[24] □

Remark 2.6: It follows that, except for sets of measure 0, the map $T\to(q,\lambda)$ is a bijection from the set of tridiagonal matrices of size n with positive subdiagonal, to the set of pairs (q,λ), with q a unit norm n-dimensional vector of positive real entries, and λ a strictly increasingly ordered sequence of n real numbers. Let the bijection's Jacobian be denoted by J

$$J=\left\{\frac{\partial(a,b)}{\partial(q,\lambda)}\right\}.$$

Our next lemma establishes a formula for the Vandermonde determinant of the eigenvalues of a tridiagonal matrix.

Lemma 2.7: The Vandermonde determinant for the ordered eigenvalues of a symmetric tridiagonal matrix with positive subdiagonal $b=(b_{n-1},\ldots,b_1)$ is given by

$$\Delta(\lambda)=\prod_{i<j}(\lambda_i-\lambda_j)=\frac{\Pi_{i=1}^{n-1}b_i^i}{\Pi_{i=1}^{n}q_i},$$

where $(q_1,\ldots,q_n)$ *is the first row of the eigenvector matrix.*

Proof: Let $\lambda_i^{(k)}$, $i=1...k$, be the eigenvalues of the $k\times k$ lower right-corner submatrix of T. Then $P_k(x)=\Pi_{i=1}^{k}(x-\lambda_i^{(k)})$ is the associated characteristic polynomial of that submatrix.

For $k=1,\ldots,n$ we have the three-term recurrence

$$P_k(x)=(x-a_k)P_{k-1}(x)-b_{k-1}^2P_{k-2}(x), \tag{8}$$

and the two-term relation

$$\prod_{\substack{1\leqslant i\leqslant k\\ 1\leqslant j\leqslant k-1}}|\lambda_i^{(k)}-\lambda_j^{(k-1)}|=\prod_{i=1}^{k}|P_{k-1}(\lambda_i^{(k)})|=\prod_{j=1}^{k-1}|P_k(\lambda_j^{(k-1)})|. \tag{9}$$

From (8) we get

$$\left|\prod_{i=1}^{k-1}P_k(\lambda_i^{(k-1)})\right|=b_{k-1}^{2(k-1)}\left|\prod_{i=1}^{k-1}P_{k-2}(\lambda_i^{(k-1)})\right|. \tag{10}$$

By repeatedly applying (8) and (2.9) we obtain

$$\prod_{i=1}^{n-1}|P_n(\lambda_i^{(n-1)})|=b_{n-1}^{2(n-1)}\qquad\prod_{i=1}^{n-2}|P_{n-1}(\lambda_i^{(n-2)})| \tag{11}$$

$$=b_{n-1}^{2(n-1)}\quad b_{n-2}^{2(n-2)}\quad\left|\prod_{i=1}^{n-2}P_{n-3}(\lambda_i^{(n-2)})\right| \tag{12}$$

$$=\ldots \tag{13}$$

$$=\prod_{i=1}^{n-1}b_i^{2i}. \tag{14}$$

Finally, we use the following formula due to Paige, found in Ref. 24, as the more general Theorem 7.9.2:

$$q_i^2=\left|\frac{P_{n-1}(\lambda_i)}{P_n'(\lambda_i)}\right|=\left|\frac{P_{n-1}(\lambda_i^{(n)})}{P_n'(\lambda_i^{(n)})}\right|. \tag{15}$$

It follows that

$$\prod_{i=1}^{n}q_i^2=\frac{\Pi_{i=1}^{n}|P_{n-1}(\lambda_i^{(n)})|}{\Delta(\lambda)^2}=\frac{\Pi_{i=1}^{n-1}b_i^{2i}}{\Delta(\lambda)^2}, \tag{16}$$

which proves the result.

Remark 2.8: The Vandermonde determinant formula of Lemma 2.7 can also be obtained from the Heine formula, as presented in Deift (Ref. 5, p. 44).

The next lemma computes the Jacobian J by relating the tridiagonal and diagonal forms of a GOE matrix, as in Fig. 2.

Lemma 2.9: The Jacobian J can be written as

$$J=\frac{\Pi_{i=1}^{n-1}b_i}{\Pi_{i=1}^{n}q_i}.$$

Proof: To obtain the Jacobian, we will study the transformation from GOE to 1-Hermite ensemble (see Fig. 2). Note that J does *not* depend on β; hence computing the Jacobian for this case is sufficient.

Let T be a 1-Hermite matrix. We know from Sec. II A that the eigenvalues of T are distributed as the eigenvalues of a symmetric GOE matrix A, from which T can be obtained via tridiagonal reduction ($T=HAH^T$ for some orthogonal H, which is the product of the consecutive reflections described in Sec. II A).

The joint element distribution for the matrix T is

$$\mu(a,b)=c_{a,b}\exp\left(-\frac{1}{2}\sum_{i=1}^{n}a_i^2\right)\prod_{i=1}^{n}b_i^{i-1}\exp\left(-\sum_{i=1}^{n}b_i^2\right),$$

where

$$c_{a,b}=\frac{2^{n-1}}{(2\pi)^{n/2}\Pi_{i=1}^{n-1}\Gamma\left(\frac{i}{2}\right)}.$$

Let

$$\mathrm{d}a=\wedge_{i=1}^{n}\mathrm{d}a_i,\quad \mathrm{d}b=\wedge_{i=1}^{n-1}\mathrm{d}b_i,\quad \mathrm{d}\lambda=\wedge_{i=1}^{n}\lambda_i,$$

and $\mathrm{d}q$ be the surface element of the n-dimensional sphere. Let $\mu(a(q,\lambda),b(q,\lambda))$ be the expression for $\mu(a,b)$ in the new variables q,λ. We have that

$$\mu(a,b)\mathrm{d}a\,\mathrm{d}b=J\ \ \mu(a(q,\lambda),b(q,\lambda))\mathrm{d}q\,\mathrm{d}\lambda\equiv\nu(q,\lambda)\ \ \mathrm{d}q\,\mathrm{d}\lambda. \tag{17}$$

We combine Properties 1 and 2 of Sec. II A to get the joint p.d.f. $\nu(q,\lambda)$ of the eigenvalues and first eigenvector row of a GOE matrix, and rewrite it as

$$\nu(q,\lambda)\mathrm{d}q\,\mathrm{d}\lambda=n!c_H^1\frac{2^{n-1}\Gamma\left(\frac{n}{2}\right)}{\pi^{n/2}}\Delta(\lambda)\exp\left(-\frac{1}{2}\sum_i\lambda_i^2\right)\mathrm{d}q\,\mathrm{d}\lambda.$$

We have introduced the $n!$ and removed the absolute value from the Vandermonde, because the eigenvalues are ordered. We have also included the distribution of q (as mentioned in Property 2, it is uniform, but only on the all-positive 2^{-n}th of the sphere because of the condition $q_i\geqslant 0$.)

Since orthogonal transformations do not change the Frobenius norm $\|A\|_F=\Sigma_{i,j=1}^{n}a_{ij}^2$ of a matrix A, from (17), it follows that

$$J=\frac{\nu(q,\lambda)}{\mu(a,b)}=\frac{n!c_H^1\dfrac{2^{n-1}\Gamma\left(\frac{n}{2}\right)}{\pi^{n/2}}}{c_{a,b}}\frac{\Delta(\lambda)}{\Pi_{i=1}^{n}b_i^{i-1}}.$$

All constants cancel, and by Lemma 2.7 we obtain

$$J=\frac{\Pi_{i=1}^{n-1}b_i}{\Pi_{i=1}^{n}q_i}.$$

Note that we have not expressed $\mu(a,b)$ in terms of q and λ in the above, and have thus obtained the expression for the Jacobian neither in the variables q and λ, nor a and b, solely; but rather in a mixture of the two sets of variables. The reason for this is that of simplicity. □

Remark 2.10: Our derivation of the Jacobian is a true random matrix derivation. Alternate derivations of the Jacobian can be obtained either via symplectic maps or through direct calculation.

The last lemma of this section computes one more Jacobian, which will be needed in Sec. III B.

Let B be a bidiagonal matrix with positive diagonal $x=(x_m,\ldots,x_1)$ and positive subdiagonal $y=(y_{m-1},\ldots,y_1)$. Let $T=BB^T$; denote by $a=(a_m,\ldots,a_1)$ and $b=(b_{m-1},\ldots,b_1)$, respectively, the diagonal and the subdiagonal part of T. Since T is a positive definite matrix, the transformation $B\to T$ is a bijection from the set of bidiagonal matrices with positive entries to the set of positive definite tridiagonal matrices.

Lemma 2.11: The Jacobian $J_{(B\to T)}$ is

$$J_{(B\to T)}=\left(2^m x_1\prod_{i=2}^{m} x_i^2\right)^{-1}.$$

Proof: We compute $J_{(B\to T)}$ from the formula

$$\mathrm{d}x\,\mathrm{d}y=J_{(B\to T)}\mathrm{d}a\,\mathrm{d}b,$$

where $\mathrm{d}z=\wedge_i \mathrm{d}z_i$ for all $z\in\{a,b,x,y\}$.

We have that

$$a_m=x_m^2, \tag{18}$$

$$a_i=y_i^2+x_i^2, \tag{19}$$

$$b_i=y_i x_{i+1}, \tag{20}$$

for all $i=m-1,m-2,\ldots,1$.

Hence by computing differentials we get

$$\mathrm{d}a_m=2x_m\,\mathrm{d}x_m$$

$$\mathrm{d}a_i=2(x_i\,\mathrm{d}x_i+y_i\,\mathrm{d}y_i),\quad \forall i=m-1,m-2,\ldots,1$$

$$\mathrm{d}b_i=x_{i+1}\mathrm{d}y_i+y_i\,\mathrm{d}x_{i+1},\quad \forall i=m-1,m-2,\ldots,1,$$

from which the formula follows. □

C. The eigendistribution of the β-Hermite ensemble

Let H_β be a random real symmetric, tridiagonal matrix whose distribution we schematically depict as

$$H_\beta\sim\frac{1}{\sqrt{2}}\begin{pmatrix} N(0,2) & \chi_{(n-1)\beta} & & & & \\ \chi_{(n-1)\beta} & N(0,2) & \chi_{(n-2)\beta} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \chi_{2\beta} & N(0,2) & \chi_\beta & \\ & & & \chi_\beta & N(0,2) & \end{pmatrix}.$$

By this we mean that the n diagonal elements and the $n-1$ subdiagonals are mutually independent, with standard normals on the diagonal, and $1/\sqrt{2}\,\chi_{k\beta}$ on the subdiagonal.

Theorem 2.12: *Let $H_\beta = Q\Lambda Q^T$ be the eigendecomposition of H_β; fix the signs of the first row of Q to be non-negative and order the eigenvalues in increasing order on the diagonal of $\lambda = \mathrm{diag}(\Lambda)$. Then λ and q, the first row of Q, are independent. Furthermore, the joint density of the eigenvalues is*

$$f_\beta(\lambda) = c_H^\beta \prod_{i<j} |\lambda_i - \lambda_j|^\beta \exp\left(-\frac{1}{2}\sum_{i=1}^n \lambda_i^2\right) = c_H^\beta |\Delta(\lambda)|^\beta \exp\left(-\frac{1}{2}\sum_{i=1}^n \lambda_i^2\right),$$

and $q = (q_1,\ldots,q_n)$ is distributed as $(\chi_\beta,\ldots,\chi_\beta)$, normalized to unit length.

Proof of Theorem 2.12: Just as before, we denote by $a = (a_n,\ldots,a_1)$ the diagonal of H_β, and by $b = (b_{n-1},\ldots,b_1)$ the subdiagonal. The differentials $\mathrm{d}a, \mathrm{d}b, \mathrm{d}q, \mathrm{d}\lambda$ are the same as in Lemma 2.9.

For general β, we have that

$$(\mathrm{d}H_\beta) \equiv \mu(a,b)\,\mathrm{d}a\,\mathrm{d}b = c_{a,b} \prod_{k=1}^{n-1} b_k^{k\beta-1} \exp\left(-\frac{1}{2}\|T_1\|_F\right)\mathrm{d}a\,\mathrm{d}b$$

$$= c_{a,b} J \prod_{k=1}^{n-1} b_k^{k\beta-1} \exp\left(-\frac{1}{2}\|T_1\|_F\right)\mathrm{d}q\,\mathrm{d}\lambda,$$

where

$$c_{a,b} = \frac{2^{n-1}}{(2\pi)^{n/2}\prod_{k=1}^{n-1}\Gamma\left(\frac{\beta}{2}k\right)}.$$

With the help of Lemmas 2.7 and 2.9 this identity becomes

$$(\mathrm{d}H_\beta) = c_{a,b}\frac{\prod_{k=1}^{n-1} b_k}{\prod_{k=1}^n q_k} \prod_{k=1}^{n-1} b_k^{k\beta-1} \exp\left(-\frac{1}{2}\|T_1\|_F\right)\mathrm{d}q\,\mathrm{d}\lambda \tag{21}$$

$$= c_{a,b}\frac{\prod_{k=1}^{n-1} b_k^{k\beta}}{\prod_{i=1}^n q_i^\beta} \prod_{i=1}^{n} q_i^{\beta-1} \exp\left(-\frac{1}{2}\sum_i \lambda_i^2\right)\mathrm{d}q\,\mathrm{d}\lambda. \tag{22}$$

Thus

$$(\mathrm{d}H_\beta) = \left(c_q^\beta \prod_{i=1}^n q_i^{\beta-1}\,\mathrm{d}q\right)\left(n!\,c_H^\beta \Delta(\lambda)^\beta \exp\left(-\frac{1}{2}\sum_i \lambda_i^2\right)\mathrm{d}\lambda\right).$$

Since the joint density function of q and λ separates, q and λ are independent. Moreover, once we drop the ordering imposed on the eigenvalues, it follows that the joint eigenvalue density of H_β is $c_H^\beta |\Delta(\lambda)|^\beta \exp(-\frac{1}{2}\Sigma_i \lambda_i^2)$, and q is distributed as $(\chi_\beta,\ldots,\chi_\beta)$, normalized to unit length. From (22), it also follows that

$$c_q^\beta = \frac{2^{n-1}\Gamma\left(\frac{\beta}{2}n\right)}{\left[\Gamma\left(\frac{\beta}{2}\right)\right]^n}. \tag{23}$$

III. THE β-LAGUERRE (WISHART) ENSEMBLES

A. Motivation: Tridiagonalizing the Wishart ensembles

The preceding section gives tridiagonal random matrix models for all β-Hermite ensembles. In the following we define the β-Laguerre ensembles, and give tridiagonal random matrix models for them.

The Wishart ensembles have joint eigenvalue density

$$f_\beta(\lambda)=c_L^{\beta,a}|\Delta(\lambda)|^\beta\prod_{i=1}^m \lambda_i^{a-p}\exp\left(-\sum_{i=1}^m \lambda_i/2\right), \tag{24}$$

again with $a=(\beta/2)\,n$, $p=1+(\beta/2)\,(m-1)$, and with, respectively, $\beta=1$ for real, and $\beta=2$ for complex. Here $c_L^{\beta,a}$ as the same as in (4).

From now on p will always denote the quantity $1+(\beta/2)\,(m-1)$, following the notation of Muirhead for $\beta=1$ (Ref. 21, Chap. 7) and Forrester[10] (Forrester uses $1+(1/\alpha)\,(m-1)$, where $\alpha=2/\beta$ is the Jack parameter). Its presence is implicit in the p.d.f. of all β-Laguerre ensembles; hence we will identify the ensembles by β and by a (we call the latter the ''Laguerre'' parameter, generalizing from the univariate case $\beta=1$, $m=1$).

As in Sec. II A, we will provide the most basic case for our construction: the case $\beta=1$ and Wishart real exponent $(n-m-1)/2$ (also referred to as the case $\beta=1$ and Laguerre parameter $a=n/2$).

Theorem 3.1: *Let G be an $m\times n$ matrix of i.i.d. standard Gaussians; then $W=GG^T$ is a Wishart real matrix. By reducing G to bidiagonal form B one obtains that the matrix $T=BB^T$ from the 1-Laguerre ensemble of Laguerre parameter $a=n/2$ (defined as in Table I) has the joint eigenvalue p.d.f. given by (24).*

Proof: We write

$$G=\begin{pmatrix} x^T \\ G_1 \end{pmatrix},$$

with x^T a row multivariate standard Gaussian of length n and G_1 a $(m-1)\times n$ matrix of i.i.d. standard Gaussians. Let R be a right reflector corresponding to the vector x^T ($R^Tx=\|x\|_2\,e_1^T$) which is independent of G_1. Hence G_1R is a matrix of i.i.d. standard Gaussians.

Write $G_1R=[y,G_2]$, where y is a column multivariate standard Gaussian of length $m-1$ and G_2 is a $(m-1)\times(n-1)$ matrix of i.i.d. standard Gaussians. Let L be a left reflector corresponding to y ($Ly=\|y\|_2\,e_1$) which is independent of G_2. Then we have that

$$\begin{pmatrix} 1 & 0 \\ 0 & L \end{pmatrix} GR=\begin{pmatrix} \|x\|_2 & 0 \\ \|y\|_2\,e_1 & LG_2 \end{pmatrix}.$$

As we have seen before, $\|x\|_2$ is distributed like χ_{n-1}, $\|y\|_2$ is distributed like χ_{m-1}, and LG_2 is a matrix of i.i.d. standard Gaussians (since L and G_2 are independent).

We proceed inductively to finish the bidiagonal construction of B.

Because the operations we have performed on G are orthogonal left and right multiplications, which do not affect the singular values, it follows that the singular values of G and B are the same. Since the squares of the singular values of G and B, respectively, are the eigenvalues of W and T, respectively, the conclusion of the theorem follows. □

Remark 3.2: The bidiagonalization process presented above is part of a familiar numerical linear algebra algorithm for computing the singular values of a matrix.

Corollary 3.3: The same process of bidiagonalization performed on $\tilde{G}$, a matrix of i.i.d. standard complex (standard quaternion) Gaussians, shows that the matrix $\tilde{W}=\tilde{G}\tilde{G}^T$ and the matrix T from the 2-Laguerre (4-Laguerre) ensemble of parameter $a=n$ ($a=2n$) has the joint

eigenvalue p.d.f. given by (24). In all three cases (real, complex, quaternion) we say that T represents the tridiagonalization of the Wishart (real, complex, quaternion) ensemble.

In Sec. III B we prove the general form of the theorem.

B. The Eigendistribution of β-Laguerre ensemble

Let

$$B_\beta \sim \begin{pmatrix} \chi_{2a} & & & \\ \chi_{\beta(m-1)} & \chi_{2a-\beta} & & \\ & \ddots & \ddots & \\ & & \chi_\beta & \chi_{2a-\beta(m-1)} \end{pmatrix},$$

by this we mean that all of the $2m-1$ diagonal and subdiagonal elements are mutually independent with the corresponding χ distribution.

Let $L_\beta = B_\beta B_\beta^T$ be the corresponding tridiagonal matrix.

Theorem 3.4: *Let $L_\beta = Q\Lambda Q^T$ be the eigendecomposition of L_β; fix the signs of the first row of Q to be non-negative and order the eigenvalues increasingly on the diagonal of Λ. Then Λ and the first row q of Q are independent. Furthermore, the joint density of the eigenvalues is*

$$f_\beta(\lambda) = c_L^{\beta,a} |\Delta(\lambda)|^\beta \prod_{i=1}^n \lambda_i^{a-p} \exp\left(-\sum_{i=1}^n \lambda_i/2 \right),$$

where $p = 1 + (\beta/2)(m-1)$, and q is distributed as $(\chi_\beta, \ldots, \chi_\beta)$ normalized to unit length.

Proof of Theorem 3.4: We will use throughout the results of Lemma 2.7, Lemma 2.9, Lemma 2.11, and Remark 2.6, which are true in the context of tridiagonal symmetric matrices with positive subdiagonal entries. By definition, L_β is such a matrix.

We will again use the notations of Lemma 2.9 and 2.11 for the differentials da, db, dq, $d\lambda$, dx, and dy.

We define (dB_β) to be the joint element distribution on B_β

$$(dB_\beta) \equiv \mu(x,y)\,dx\,dy = c_{x,y} \prod_{i=0}^{m-1} x_{m-i}^{a-\beta_i-1} \exp(-x_i^2/2) \prod_{i=1}^{m-1} y_i^{\beta_i-1} \exp(-y_i^2/2)\,dx\,dy.$$

By using Lemma 24 we obtain the joint element distribution on L_β as

$$(dL_\beta) \equiv J_{B\to T}^{-1} \mu(x,y)\,dx\,dy \tag{25}$$

$$= 2^{-m} c_{x,y} x_1^{2a-\beta(m-1)-2} \exp(-x_1^2/2) \prod_{i=0}^{m-2} x_{m-i}^{a-\beta_i-3}$$

$$\times \exp(-x_i^2/2) \prod_{i=1}^{m-1} y_i^{\beta_i-1} \exp(-y_i^2/2)\,dx\,dy, \tag{26}$$

where

$$c_{x,y} = \frac{\Pi_{i=1}^{m-1} \Gamma\left(i\frac{\beta}{2} \right) \Pi_{i=1}^{m} \Gamma\left(a - \frac{\beta}{2}(i-1) \right)}{2^{2m-1}}.$$

We rewrite (26) in terms of x, y, λ, and q:

$$
\begin{aligned}
(dL_\beta) &= 2^{-m} c_{x,y} \exp\left(-\sum_{i=1}^{m} x_i^2/2 \right) \exp\left(-\sum_{i=1}^{m-1} y_i^2/2 \right) \frac{\Pi_{i=1}^{m-1}(x_{i+1}y_i)}{\Pi_{i=1}^{m} q_i} x_1^{2a-\beta(m-1)-2} \\
&\quad \times \prod_{i=0}^{m-2} x_{m-i}^{2a-\beta(m-i)-3} \prod_{i=1}^{m-1} y_i^{\beta_i - 1} \mathrm{d}q \, \mathrm{d}\lambda \\
&= 2^{-m} c_{x,y} \exp\left(-\sum_{i=1}^{m} x_i^2/2 \right) \\
&\quad \times \exp\left(-\sum_{i=1}^{m-1} y_i^2/2 \right) \frac{\Pi_{i=0}^{m-1} x_{m-i}^{2a-\beta(m-i)-2} \Pi_{i=1}^{m-1} y_i^{\beta_i}}{\Pi_{i=1}^{m} q_i} \, \mathrm{d}q \, d\lambda .
\end{aligned}
$$

Since the Vandermonde with respect to b and q and the ordered eigenvalues λ can be written as

$$
\Delta(\lambda) = \frac{\Pi_{i=1}^{m-1} b_i^i}{\Pi_{i=1}^{m} q_i},
$$

it follows that

$$
\Delta(\lambda) = \frac{\Pi_{i=1}^{m-1} (x_{i+1}y_i)^i}{\Pi_{i=1}^{m} q_i}.
$$

This means that we can rewrite

$$
\begin{aligned}
(dL_\beta) &= 2^{-m} c_{x,y} \exp\left(-\sum_{i=0}^{m-1} x_{m-i}^2/2 \right) \exp\left(-\sum_{i=1}^{m-1} y_i^2/2 \right) \frac{\Pi_{i=1}^{m-1}(x_{i+1}y_i)^{\beta_i}}{\Pi_{i=1}^{m} q_i^{\beta}} \\
&\quad \times \prod_{i=1}^{m-1} q_i^{\beta-1} \prod_{i=0}^{m-1} x_{m-i}^{2a-\beta(m-1)-2} \mathrm{d}q \, \mathrm{d}\lambda \\
&= 2^{-m} c_{x,y} \exp\left(-\sum_{i=0}^{m-1} x_{m-i}^2/2 \right) \exp\left(-\sum_{i=1}^{m-1} y_i^2/2 \right) \Delta(\lambda)^{\beta} \\
&\quad \times \prod_{i=1}^{m-1} q_i^{\beta-1} \left(\prod_{i=0}^{m-1} x_{m-i} \right)^{2a-\beta(m-1)-2} \mathrm{d}q \, \mathrm{d}\lambda .
\end{aligned}
$$

The trace and the determinant are invariant under orthogonal similarity transformations, so $\mathrm{tr}(L_\beta) = \mathrm{tr}(\Lambda)$, and $\det(L_\beta) = \det(\Lambda)$. This is equivalent to

$$
\sum_{i=0}^{m-1} x_{m-i}^2 + \sum_{i=1}^{m-1} y_i^2 = \sum_{i=1}^{m} \lambda_i ,
$$

$$
\prod_{i=0}^{m-1} x_{m-i}^2 = \prod_{i=1}^{m} \lambda_i .
$$

Using this, and substituting p for $1 + \beta/2\,(m-1)$, we obtain that

$$
(dL_\beta) = \left(c_q^\beta \prod_{i=1}^{m-1} q_i^{\beta-1} \, \mathrm{d}q \right) \left(m! c_L^{\beta,a} e^{-\sum_{i=1}^{m} \lambda_i/2} \Delta(\lambda)^\beta \prod_{i=1}^{m} \lambda_i^{a-p} \, \mathrm{d}\lambda \right),
$$

where c_q^β is the same as in (23).

From the above we see that q and λ are independent, and once we drop the ordering the joint eigenvalue density is given by the β-Laguerre ensemble of parameter a, while q is distributed like a normalized vector of χ_β's.

This concludes the proof of Theorem 3.4. □

IV. APPLICATIONS AND OPEN PROBLEMS

As we mentioned in Sec. I, we believe that there should be many applications for the new tridiagonal ensembles. Here we illustrate some (in Sec. IV A), in the hope that researchers will find many more. Some of the applications we believe are new results (Applications 1, 3, 5, and 6), and some are simplifications of known results (Applications 2 and 4).

We discuss the open problem of constructing a matrix model for the β-Jacobi ensembles in the beginning of Sec. IV B. To facilitate the finding of new results, we conclude with a few open "general β-ensemble" problems.

A. Applications

1. Interpolating Laguerre exponents

Our β-Laguerre ensembles have "continuous" Laguerre parameters a which, even in the cases $\beta=1,2,4$, interpolate the Wishart parameters. Though β-Laguerre ensembles with general ("continuous") parameter a have been studied by many researchers (Refs. 2, 14, and 21), no nonquantized matrix realizations (i.e., explicit random matrix models) of β-Laguerre ensembles are found in the literature. By "quantized" we mean that the exponent a is either an even integer, an integer, or a half-integer (depending on the value of β). In particular, all models corresponding to a Laguerre (or Jacobi) weight found in Refs. 33 and 12 are quantized.

Thus, our β-Laguerre random matrix constructions extend the pre-existing ones in two ways: through β and through the Laguerre parameter a.

2. The expected characteristic polynomial

The result in the following might be seen as an extension of the classical Heine theorem (see Szegö[25] and Deift[5]) which has $\beta=2$. Note that for $\beta\neq 2$, $\Delta(\lambda)^\beta$ can no longer be written as the determinant of a Vandermonde matrix times its transpose, and the proof cannot be duplicated.

The same result is found in a slightly more general form in Ref. 8, and its Jacobi case was first derived by Aomoto.[1]

Theorem 4.1: *The expected characteristic polynomial $P_n(y)=\det(yI_n-S)$ over S in the β-Hermite and β-Laguerre ensembles, respectively, are proportional to*

$$H_n\left(\frac{y}{\sqrt{2\beta}}\right), \quad L_n^{(2a/\beta)-n}\left(\frac{y}{2\beta}\right).$$

Here H_n and $L_n^{(2a/\beta)-n}$ are, respectively, the Hermite and Laguerre polynomials, and the constant of proportionality accounts for the fact that $P_n(y)$ is monic.

Proof: Both formulas follow immediately from the 3-term recurrence for the characteristic polynomial of a tridiagonal matrix (see formula (8)) and from the independence of the variables involved in the recurrence. □

3. Expected values of symmetric polynomials

Using the three-term recurrence for the characteristic polynomial of a tridiagonal matrix, we obtain Theorem 4.2.

Theorem 4.2: *Let p be any fixed (independent of β) multivariate symmetric polynomial on n variables. Then the expected value of p over the β-Hermite or β-Laguerre ensembles is a polynomial in β.*

We remark that it is difficult to see this from the eigenvalue density.

Proof: The elementary symmetric functions

$$e_i(x_1,x_2,\ldots,x_n)=\sum_{1\leq j_1<\cdots<j_i\leq n} x_{j_1}x_{j_2}\ldots x_{j_i}, \quad i=0,1,\ldots,n,$$

can be used to generate any symmetric polynomial of degree n (in particular p).

The e_i evaluated at the eigenvalues of a matrix are the coefficients of its characteristic polynomial, and hence they can be written in terms of the matrix entries. Thus p can be written as a polynomial of the $n\times n$ tridiagonal matrix entries (which corresponds, respectively, to the Hermite and Laguerre cases).

To obtain the expected value of p over the β-Hermite or β-Laguerre ensemble, one can write p in terms of the corresponding matrix entries, use the symmetry to condense the expression, then replace the powers of the matrix entries by their expected values.

The diagonal matrix entries are either normal random variables in the Hermite case or sums of χ^2 random variables in the Laguerre case. The subdiagonal entries appear only raised at even powers in the e_i and hence in p (this is an immediate consequence of the three-term recurrence for the characteristic polynomial, (8)). Since all even moments of the involved χ distributions are polynomials in $\beta/2$, it follows that the expectation of p will be a polynomial in β. □

As an easy consequence we have the following corollary.

Corollary 4.3: *All moments of the determinant of a β-Hermite matrix are integer-coefficient polynomials in $\beta/2$.*

Proof: Note that even moments of the $\chi_{\beta i}$ distribution are integer-coefficient polynomials in $\beta/2$, and that the determinant is e_n. □

4. A new proof for Hermite and Laguerre forms of the Selberg integral

Here is a quick proof for the Hermite and Laguerre forms of the Selberg integral (Ref. 18), using respectively, the β-Hermite, and β-Laguerre ensembles.

The Hermite Selberg integral is

$$I_H(\beta,n)\equiv\int_{\mathbb{R}^n}|\Delta(\lambda)|^\beta\exp\left(-\sum_{i=1}^n\lambda_i^2/2\right)d\lambda.$$

We have that

$$I_H(\beta,n)=n!\left(\int_{0\leqslant\lambda_1\leqslant\cdots\leqslant\lambda_n<\infty}\Delta(\lambda)^\beta\exp\left(-\sum_{i=1}^n\lambda_i^2/2\right)d\lambda\right)\left(c_q^\beta\int_{S_+^{n-1}}\prod_{i=1}^n q_i^{\beta-1}\,dq\right),$$

where c_q^β is as in (23). We introduce the $n!$ because in the first integral we have ordered the eigenvalues; S_+^{n-1} signifies that all q_i are positive.

Note that c_q^β can easily be computed independently of the β-Hermite ensembles.

Using the formula for the Vandermonde given by Lemma 2.7, the formula for the Jacobian J given in Lemma 2.9, and the fact that the Frobenius norm of a matrix in the tridiagonal 1-Hermite ensemble is the same as the Frobenius norm of its eigenvalue matrix, one obtains

$$I_H(\beta,n)=n!c_q^\beta\int_{\mathbb{R}^n\times(0,\infty)^{n-1}}\frac{\Pi_{i=1}^n q_i}{\Pi_{i=1}^{n-1}b_i}\frac{\Pi_{i=1}^{n-1}b_i^{\beta i}}{\Pi_{i=1}^n q_i^\beta}\prod_{i=1}^n q_i^{\beta-1}\exp\left(-\sum_{i=1}^{n-1}b_i^2-\sum_{i=1}^n a_i^2/2\right)da\,db$$

$$=n!c_q^\beta(2\pi)^{n/2}\prod_{i=1}^{n-1}\int_{(0,\infty)}b_i^{\beta i-1}e^{-b_i^2}db_i=n!\frac{2^{n-1}\Gamma\left(\frac{\beta}{2}n\right)}{\left(\Gamma\left(\frac{\beta}{2}\right)\right)^n}(2\pi)^{n/2}\prod_{i=1}^{n-1}\frac{\Gamma\left(\frac{\beta}{2}i\right)}{2}=\frac{1}{c_H^\beta}.$$

The same reasoning yields the Laguerre Selberg integral formula

$$I_L^{\beta,a,n}=\frac{1}{c_L^{\beta,a}}.$$

5. Moments of the discriminant

The discriminant of a polynomial equation of order m is the square of the Vandermonde determinant of the m zeroes of the equation. Thus, the discriminant of the characteristic polynomial of a β-Hermite or β-Laguerre ensemble matrix is simply $D(\lambda)=\Delta(\lambda)^2$.

A simple calculation shows that the kth moment of $D(\lambda)$ is, respectively,

$$\frac{c_H^{\beta}}{c_H^{\beta+2k}}=\prod_{j=1}^{n}\frac{\left(1+\frac{\beta}{2}j\right)_{kj}}{\left(1+\frac{\beta}{2}\right)_k},$$

$$\frac{c_L^{\beta,a}}{c_L^{\beta+2k,a+k(m-1)}}=2^{km(m-1)}\prod_{j=1}^{m}\frac{\left(1+\frac{\beta}{2}j\right)_{kj}\left(a-\frac{\beta}{2}(m-j)\right)_{k(j-1)}}{\left(1+\frac{\beta}{2}\right)_k},$$

where n and m are, respectively, the matrix sizes for the Hermite and Laguerre cases, and the rising factorial $(x)_k\equiv\Gamma(x+k)/\Gamma(x)$.

Using the Selberg integral, one obtains that the moments of the discriminant for the β-Jacobi case are

$$\frac{c_J^{\beta,a_1,a_2}}{c_J^{\beta+2k,a_1+k(m-1),a2+k(m-1)}}=\prod_{j=1}^{m}\frac{\left(1+\frac{\beta}{2}j\right)_{kj}\left(a_1-\frac{\beta}{2}(m-j)\right)_{k(j-1)}\left(a_2-\frac{\beta}{2}(m-j)\right)_{k(j-1)}}{\left(1+\frac{\beta}{2}\right)_k\left(a_1+a_2-\frac{\beta}{2}(m-j)\right)_{k(m+j-2)}}.$$

6. Software for application 3: Computing eigenvalue statistics for the β-ensembles

Application 3 suggests that integrals of the form

$$E_{\beta}[p]\equiv c_H^{\beta}\int_{\mathbb{R}^n}p(\lambda)|\Delta(\lambda)|^{\beta}\exp\left(-\sum_{i=1}^{n}\lambda_i^2/2\right)d\lambda$$

may be evaluated with software.

One example of this would be computing moments of the determinant over the β-Hermite ensemble. There are explicit formulas for the cases $\beta=1,2$ and 4, due to Mehta[19] and to Delannay and Le Caër,[6] which can be used to evaluate these moments.

In the absence of a closed-form, explicit formula, like the one for $\beta=1$ provided in Ref. 6, the computation of these moments cannot be made polynomial; thus it is inherently slow.

For the general β case, one can compute the moments in terms of a multivariate Hermite polynomial evaluated at 0 (see Refs. 4 and 2). Using this technique, the complexity of the computation might exceed that of symbolically taking the determinant of a tridiagonal matrix, expanding the power, and replacing all powers of the entries by their expected values (which are all known). Writing a Mathematica code to implement this algorithm is an easy exercise, and such a code would allow the author to compute these moments in a reasonable amount of time, provided that the product between the power and the size of the matrix is not very large. A template for a special case when $\beta=1$ can be found in Ref. 9, Appendix A.

B. Open problems

1. β-Jacobi (MANOVA) ensembles

Sections II and III of the paper provide tridiagonal matrix models for the β-Hermite and β-Laguerre ensembles. The natural question is whether such models exist for the last member of the classical triplet, Jacobi. The β-Jacobi ensembles have been intensively studied as theoretical distributions, especially in connection with Selberg-type integrals and Jack (or Jack–Selberg) polynomials (see Refs. 1, 15, 16, and 3). Finding a random matrix model that corresponds to them would be of much interest.

If the two matrix factorization problems that are associated with the Hermite and Laguerre ensembles are the EIG and the SVD, the one associated with the Jacobi should be the QZ (the generalized symmetric eigenvalue problem). This idea is supported by the fact that the MANOVA real and complex distributions, which correspond to the Jacobi $\beta=1,2$ ensembles, are indeed connected to the QZ algorithm. A good reference for QZ is Ref. 11.

Though we have not studied this problem sufficiently, we believe that a concrete (perhaps sparse, perhaps tridiagonal) matrix model may be constructed for the β-Jacobi ensembles.

2. Level densities

The level density of an ensemble is the distribution of a random eigenvalue of that ensemble (and by the Wigner semicircular law we know that the limiting distribution as $n\to\infty$ of such an eigenvalue is semicircular). The three functions found to be the level densities of the Gaussian models depend on the univariate Hermite polynomials.

Recently, Forrester[10] has found a formula for the level densities of the β-Hermite ensembles which works for β an even integer. This formula depends on a multivariate Hermite polynomial.

Finding a unified formula for the general β case would be of interest.

3. Level spacings

The level spacings are the distances between the eigenvalues of an ensemble, usually normalized so that the average consecutive spacing is 1. These spacings have been well-studied in the case of the Gaussian ensembles ($\beta=1,2,4$). The limiting probability density of a random spacing in these cases is known in terms of spheroidal functions (see Ref. 18).

A surprising connection exists between the limiting probability density of a GUE random spacing and the probability density of the zeroes of the Riemann zeta function. Inspired by the theoretical work of Montgomery,[20] Odlyzko[22] has shown experimentally that the two probability densities are very close; the subsequent conjecture that the two probability densities coincide has been named the Montgomery–Odlyzko law.

To the best of our knowledge, the level spacing of the general β-Hermite ensembles has not been investigated.

4. Bulk and edge scaling limits

Finally, a very important application would be the generalization of the bulk and edge scaling limits for the GOE, GUE, and GSE obtained by Tracy and Widom (the latter are known as the Tracy–Widom distributions F_1, F_2, and F_4).

The edge scaling limit refers to the distribution of the largest eigenvalue of a matrix in the ensemble; the bulk scaling limit refers to the distribution of an eigenvalue in the ''bulk'' of the spectrum. See Refs. 29, 30 or 28. The Tracy–Widom distributions are defined in terms of Painlevé functions, which are solutions to certain differential equations, with asymptotics given by Airy functions. For a good treatment of Painlevé equations in relationship with Gaussian (Hermite), Laguerre, and Jacobi random matrix models, see Pierre van Moerbeke's notes (Ref. 32, Sec. 4). Recently, Johnstone[14] has found that the limiting distributions F_1 and F_2 apply to real (respectively, complex) Wishart matrices.

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Monopoles and dyons in SO(3) gauged Skyrme models: Corrigendum

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The axially symmetric solutions of a gauged Skyrme model previously studied in an earlier work [J. Math. Phys. **42**, 3270 (2001)] are reconsidered. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1509090]

I. INTRODUCTION

A few years ago topologically stable solutions with nonvanishing magnetic flux were constructed[1] in a particular SU(2) gauged $SU(2)\otimes SU(2)$ sigma model. This model differs essentially from the (gauged) Skyrme model[2] because in place of the usual pion-mass potential of the latter, it is characterized by a potential which results in the breaking of the SU(2) symmetry down to U(1), resulting in a monopole charge. The gauging prescription is given by Eq. (6) of Ref. 1 and we employ the constrained field ϕ^a, $a=1,2,3,4$ $[\Sigma_{a=1}^4(\phi^a)^2=1]$, instead of $U=\phi^a\sigma_a$ $U^\dagger=\phi^a\tilde{\sigma}_a$.

Recently, we discovered that the boundary conditions used to solve the axially symmetric equations of the above model are not strong enough to provide continuously differentiable profiles for the ϕ^a fields. In Ref. 1, our inability to specify the boundary conditions satisfactorily stems from our use of an axially symmetric ansatz in which the Skyrme field was represented by two functions in a ''polar parametrization.'' In this corrigendum, to overcome this obstacle, we employ instead a ''vector parametrization'' ansatz. The new results change some of the qualitative conclusions of our results in the case of a vanishing Skyrme term, but also confirm those obtained for the ''full'' system.

The numerical analysis carried out with the new ansatz, however, is unfortunately more limited than that attempted in Ref. 1. We encounter severe difficulties when the coupling constant κ_2 of the quartic (Skyrme) term in Eq. (8) of Ref. 1 is nonvanishing. Thus our main analysis is carried out in the special case of vanishing κ_2. We have, however, presented a heuristic analysis of the $\kappa_2\neq 0$ case, at least for small κ_2, using a simple perturbative prescription.

II. AXIALLY SYMMETRIC ANSATZ

In order to construct axially symmetric solution of the above mentioned model, the following ''polar parametrization'' ansatz was considered in Ref. 1 for the Skyrme field:

$$\phi_4=\cos f, \quad \vec{\phi}=\sin f(\sin g\sin\theta+\cos g\cos\theta)\vec{e}_r^{\,n}+\sin f(\sin g\cos\theta-\cos g\sin\theta)\vec{e}_\theta^{\,n}, \qquad (1)$$

with (e_r^n, e_θ^n) defined in Eq. (34) of Ref. 1 and where f,g are functions of r and θ only. Severe

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TABLE I. The energy per winding number E/n, the maximal value of the energy $\mathcal{E}_M$, and the radius x_M of the annulus of the maximal value of the energy density are presented for the gauged skyrmion for winding number $n=1,2,3,4$.

n	1	2	3	4
E/n	2.95	3.05	3.09	3.10
$\mathcal{E}_M$	0.47	0.066	0.031	0.02
x_M	0.0	0.68	0.81	0.86

numerical difficulties using this ansatz had forced us to attempt to construct solutions numerically subject to the boundary conditions for the functions parametrizing the Skyrme field at the origin $(r=0)$:

$$f(r=0,\theta)=\pi, \quad \partial_r g|_{r=0,\theta}=0. \tag{2}$$

Unfortunately, it turned out that these boundary conditions are too weak to ensure the continuity of the partial derivatives of the fields at the origin. We therefore reconsider here the equations by using a ''vector parametrization'' ansatz:

$$\phi_4=\sqrt{1-g_5^2-g_6^2}, \quad \vec{\phi}=g_5\ \vec{e}_r^{\,n}+g_6\ \vec{e}_\theta^{\,n}, \tag{3}$$

where g_5, g_6 are functions of r and θ.

Now, the boundary conditions necessary to ensure regular and finite energy solutions read

$$g_5(r=0,\theta)=0, \quad g_5(r=\infty,\theta)=1, \tag{4}$$

$$g_6(r=0,\theta)=0, \quad g_6(r=\infty,\theta)=0, \tag{5}$$

$$\frac{\partial g_k}{\partial\theta}(r,\theta=0)=0, \quad \frac{\partial g_k}{\partial\theta}\left(r,\theta=\frac{\pi}{2}\right)=0, \ \ k=5,6. \tag{6}$$

III. NUMERICAL RESULTS

With this set of boundary conditions [completed by those for the gauge fields, see Eqs. (35), (37), (39), and (40) in Ref. 1] we succeeded in solving the classical equations numerically for $n=1,2,3,4$. The energy per winding number E/n, the maximal value of the energy density $\mathcal{E}_M$ and the value of the coordinate x_M [represented by means of the compactified coordinate $x \equiv r/(1+r)$] at which the energy density attains its maximum are presented in Table I.

Some features are worth noticing. First we observe that the energy per winding number increases with n, that is to say, at least classically, the solutions for $n>1$ are unstable against decaying into n separate solitons. This contrasts with the case of BPS magnetic monopole where the self-duality equation ensures that the ratio $E(n)/n$ is independent on n. The excess of energy

TABLE II. The energy per winding number E/n, the maximal value of the energy density $\mathcal{E}_M$, and the radius x_M of the annulus of the maximal value of the energy density are presented for the BPS monopoles for winding number $n=1,2,3,4$.

n	1	2	3	4
E/n	1.0	1.0	1.0	1.0
$\mathcal{E}_M$	0.21	0.037	0.019	0.012
x_M	0.0	0.68	0.79	0.84

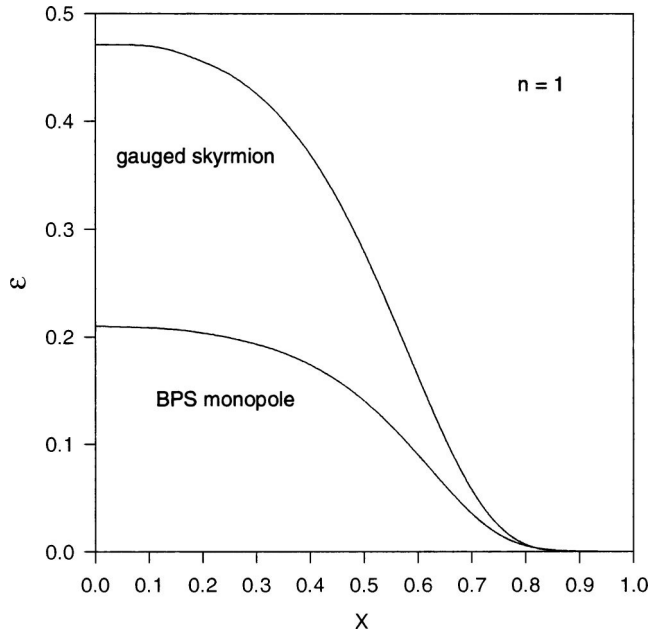

FIG. 1. The profiles of the energy density ε of the gauged skyrmion (solid) and of the BPS monopole (dotted) are shown for $n=1$.

of the $n=2$ gauged skyrmion solution is about 3% of the classical energy of the spherically symmetric soliton. This conclusion is the opposite of what was claimed in Ref. 1.

As a second feature of the axially symmetric solutions we point out that the radius of the annulus (in the plane orthogonal to the symmetry axis, the x,y-plane in our case) increases with n, that is to say, the lump occupies a larger volume in space. We observe that the values of these radii are very close to their corresponding values in the BPS monopole case; this statement can be

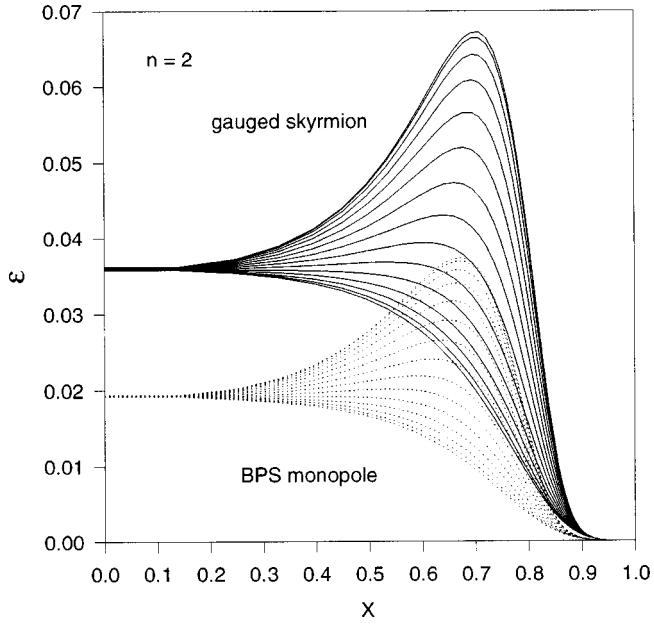

FIG. 2. The profiles of the energy density ε of the gauged skyrmion (solid) and of the BPS monopole (dotted) are shown for $n=2$ and several values of θ between $\theta=0$ and $\theta=\pi/2$. Note that the curve's height increases with θ.

checked easily in Table II which is the counterpart of Table I, for BPS monopoles. The energy densities corresponding to the gauged skyrmion and to the monopole, respectively, are presented in Fig. 1 for the spherically symmetric solutions and in Fig. 2 for the axially symmetric solutions with winding number $n=2$.

A natural question to raise now is whether the addition of a Skyrme term to the model can lead to qualitatively different properties for axially symmetric solutions. We expect that the reinstalment of the Skyrme term should lead to bound states of higher magnetic charges, as is known to be the case for the analogous gauged Higgs models.[3,4] Unfortunately this question leads to severe technical problems in the numerical integrations which we do not have under control at the present. However, we have some heuristic results indicating that, when a nonvanishing Skyrme term [i.e., the term in $\kappa_2^4 \equiv \kappa$ Eqs. (7) and (8) of Ref. 1] is considered, the solutions with $n>2$ become stable for large enough values of κ. The argument is based on the observation that the ''Skyrme term energy,''

$$E_{sk}=\int d^3x \frac{1}{2}|D_{[i}\phi^a D_{j]}\phi^b|^2 \tag{7}$$

evaluated with the solutions constructed for $\kappa=0$, gives

$$E_{sk}\approx 0.368 \quad \text{for} \quad n=1, \quad E_{sk}/2\approx 0.092 \quad \text{for} \quad n=2. \tag{8}$$

This allows us to approximate the total energy with the first order correction:

$$E_a(\kappa)=E+\kappa E_{sk}\,. \tag{9}$$

In the spherically symmetric case we checked that this approximation is correct within 1% up to values of $\kappa\approx 0.2$. Using the values of the energy given in Table I, together with the first order correction to the energy (9), we find the ''binding energy''

$$\Delta(\kappa)\equiv \tfrac{1}{2}E_a(\kappa)|_{n=2}-E_a(\kappa)|_{n=1}\approx 0.1-\kappa 0.278. \tag{10}$$

Equation (10) strongly indicates that Δ decreases for $\kappa>0$ and thus that, at least the $n=2$, solution becomes stable for a large enough value of κ. This kind of approximation, whose validity definitely needs to be confirmed by a direct integration of the full equations, can be justified heuristically as follows. In a two-dimensional system where the charge (vorticity) n solution can be constructed by integrating one-dimensional differential equations, the inclusion of a quartic kinetic term (a Skyrme term) does not result in the numerical difficulties encountered here with two dimensional integrations. Thus a perturbative evaluation of the energy like that used above can be rigorously tested. The heuristic step we have taken here is that we proceed with this perturbative construction in our three-dimensional model, on the justification that it works for two-dimensional models. This approximation gave very good results when applied in the context of the (higher order) Born–Infeld correction to various topological solitons.[5]

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Wigner functions for curved spaces. I. On hyperboloids

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We propose a Wigner quasiprobability distribution function for Hamiltonian systems in spaces of constant curvature, in this article on hyperboloids, which returns the correct marginals and has the covariance of the Shapiro functions under SO(D,1) transformations. To the free systems obeying the Laplace–Beltrami equation on the hyperboloid, we add a conic-oscillator potential in the hyperbolic coordinate. As an example, we analyze the one-dimensional case on a hyperbola branch, where this conic-oscillator is the Pöschl–Teller potential. We present the analytical solutions and plot the computed results. The standard theory of quantum oscillators is regained in the contraction limit to the space of zero curvature. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1518139]

I. INTRODUCTION

In Hamiltonian systems which a have flat $\mathfrak{R}^D$ configuration space, among the phase space quasiprobability distribution functions the Wigner function[1] is the only one covariant under Euclidean translations of phase space.[2,3] The present article, and others that will follow it, aim to the construction of Wigner functions on configuration spaces that are conic surfaces, hyperboloids and spheres, which transform under the Lorentz and rotation groups respectively, and which reproduce the traditional Wigner function when the conic contracts to the plane. Quantum motion on spaces of constant curvature is of current interest in various fields of theoretical physics, such as quantum gravity and string theory,[4] noncommutative geometry,[5] and quantum chaos.[6] Hamiltonian systems on conic manifolds have a natural kinetic energy given by the Laplace–Beltrami operator, and, moreover, on these conics also a natural oscillator ''potential'' can be proposed. In one dimension, this oscillator turns out to be one of the Pöschl–Teller potentials.[7]

In this article, subtitled I, we propose a Wigner function on the D-dimensional hyperboloid $\mathcal{H}^D_+$, which generalizes the ordinary Wigner function on flat phase space. It displays the correct marginals, and returns the traditional form of the Wigner function under Inönü–Wigner contraction to the zero-curvature limit. The elements and background for this assertion are contained in Sec. II, including the Shapiro solutions $\Phi^{(D)}_{\mathbf{p}}(\mathbf{x})$ to the Laplace–Beltrami equation.[8] In Sec. III we present our proposed definition of Wigner function on the hyperboloid, and verify the properties of marginality and the contraction limit to flat phase space. Covariance remains an issue because the Wigner function that we propose here follows from the covariance of the basis of wavefunctions, between the argument $\mathbf{x}$ and the index $\mathbf{p}$, as if they were canonically conjugate variables. In this context, we reexamine the interpretation of momentum coordinates.

In Sec. IV we exemplify the D-dimensional theory with a one-dimensional *sui generis* oscillator on one branch of a hyperbola. This example may appear to be trivial, because the hyperbola is in most respects equivalent to a straight line. Nevertheless, the resulting Pöschl–Teller potential is of particular interest because the wavefunctions are also the Clebsch–Gordan (Wigner coupling) coefficients for the three-dimensional Lorentz algebra, $\mathrm{so}(2,1)=\mathrm{sp}(2,\mathfrak{R})=\mathrm{su}(1,1)$.[9] We display

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the Wigner functions of some Pöschl–Teller wavefunctions; these have not been examined before. Finally, in Sec. V we recapitulate the aim and offer the present outlook of our program.

II. ELEMENTS OF PHASE SPACE AND HYPERBOLOIDS

In his fundamental article,[1] Wigner proposed a distribution function to represent on phase space the wavefunctions of pure and of mixed states in quantum systems. In this section we recall the definition and properties that we shall generalize from flat to conic spaces, using the Laplace–Beltrami operator and the Shapiro functions.

A. Wigner function on flat phase space

In D-dimensional flat configuration space $\mathbf{x}\in\mathfrak{R}^D$, the generalized Dirac basis of plane waves solves the free-space Schrödinger equation, which is identical to the Helmholtz equation

$$-\Delta\,\phi(\mathbf{x})=p^2\,\phi(\mathbf{x}),\quad \phi_{\mathbf{p}}(\mathbf{x})=\exp(i\mathbf{p}\cdot\mathbf{x}),\quad \mathbf{p}\in\mathfrak{R}^D. \tag{1}$$

When we write $p=+(\mathbf{p}\cdot\mathbf{p})^{1/2}$, $\mathbf{n}=\mathbf{p}/p$, and call $\mathbf{p}=p\mathbf{n}$ the momentum or wavenumber vector, the functions $\phi_{\mathbf{p}}(\mathbf{x})$ represent plane waves in the direction of the unit vector $\mathbf{n}\in\mathcal{S}^{D-1}$ in the $(D-1)$-dimensional sphere manifold. In the quantum model with natural units $\hbar=1$, p has units of inverse length; in the wave optical model, p is the wavenumber of light.

The basis of plane wave functions (1) plays many roles: it provides the Fourier transform kernel which bridges the configuration and momentum realizations, it constitutes a basis for representations of the Euclidean group, and it serves for the construction of the $\mathfrak{R}^{2D}$-Wigner function of wavefields $f(\mathbf{x})$, $g(\mathbf{x})$ through the equivalent expressions

$$W_{\mathfrak{R}^D}(f,g|\mathbf{x},\mathbf{p})=\frac{1}{(2\pi)^D}\int_{\mathfrak{R}^D}d^D\mathbf{z}\,f\left(\mathbf{x}-\frac{1}{2}\mathbf{z}\right)^*e^{-i\mathbf{p}\cdot\mathbf{z}}g\left(\mathbf{x}+\frac{1}{2}\mathbf{z}\right) \tag{2}$$

$$=\frac{1}{(2\pi)^D}\int_{\mathfrak{R}^D}d^D\mathbf{z}\,f\left(\mathbf{x}-\frac{1}{2}\mathbf{z}\right)^*\times e^{+i\mathbf{p}\cdot(\mathbf{x}-(1/2)\mathbf{z})}e^{-i\mathbf{p}\cdot(\mathbf{x}+(1/2)\mathbf{z})}g\left(\mathbf{x}+\frac{1}{2}\mathbf{z}\right)$$

$$=\frac{1}{(2\pi)^D}\int_{\mathfrak{R}^D}d^D\mathbf{x}'\int_{\mathfrak{R}^D}d^D\mathbf{x}''\,f(\mathbf{x}')^*\,g(\mathbf{x}'')\times\phi_{\mathbf{p}}(\mathbf{x}')\,\delta^D\left(\mathbf{x}-\frac{1}{2}(\mathbf{x}'+\mathbf{x}'')\right)\phi_{\mathbf{p}}(\mathbf{x}'')^*. \tag{3}$$

This has the well-known properties of being sesquilinear in the functions, real for $f=g$, with the marginal projections $\int_{\mathfrak{R}^D}d\mathbf{p}W=f(\mathbf{x})^*g(\mathbf{x})$, $\int_{\mathfrak{R}^D}d\mathbf{x}W=\tilde{f}(\mathbf{p})^*\,\tilde{g}(\mathbf{p})$ (the tilde indicates ordinary Fourier transformation, $F:f=\tilde{f}$), and covariant under translations in coordinate and momentum spaces

$$T_{\mathbf{a}}:f(\mathbf{x})=f(\mathbf{x}-\mathbf{a})\Rightarrow W_{\mathfrak{R}^D}(T_{\mathbf{a}}:f,T_{\mathbf{a}}:g|\mathbf{x},\mathbf{p})=W_{\mathfrak{R}^D}(f,g|\mathbf{x}-\mathbf{a},\mathbf{p}), \tag{4}$$

$$\tilde{T}_{\mathbf{b}}:f(\mathbf{x})=e^{i\mathbf{b}\cdot\mathbf{x}}f(\mathbf{x})\Rightarrow W_{\mathfrak{R}^D}(\tilde{T}_{\mathbf{b}}:f,\tilde{T}_{\mathbf{b}}:g|\mathbf{x},\mathbf{p})=W_{\mathfrak{R}^D}(f,g|\mathbf{x},\mathbf{p}-\mathbf{b}), \tag{5}$$

$$F:f(\mathbf{x})=\tilde{f}(\mathbf{x})\Rightarrow W_{\mathfrak{R}^D}(F:f,F:g\,|\mathbf{x},\mathbf{p})=W_{\mathfrak{R}^D}(f,g\,|\mathbf{p},-\mathbf{x}). \tag{6}$$

The last intertwining by the Fourier transform was known when García–Calderón and Moshinsky noticed that the Wigner function is covariant also under the larger group of $\mathrm{Sp}(2D,\mathfrak{R})$ linear canonical transformations of phase space.[10] This is exceptional in the sense that the Heisenberg–Weyl algebra [whose generators are the phase space translations (4) and (5)—and the unit that

generates a commuting phase factor] has the outer automorphism group $\mathrm{Sp}(2D,\Re)$. This accident does not occur for Lorentz algebras, so we should not expect similar covariances of the Wigner function under groups larger than $\mathrm{SO}(D,1)$.

B. Laplace–Beltrami operator on the hyperboloid

The purpose of this article is to generalize the expression of the Wigner function (2) and (3) with functions on a D-dimensional space $\mathbf{x}\in\Re^D$ of constant curvature. This manifold can be seen in an "ambient" space of $D+1$ dimensions as a hyperboloid, with vectors $x=(x_0,\mathbf{x})\in\Re^{D+1}$.

Consider the upper sheet of the two-sheeted hyperboloid $\mathcal{H}_+^D\subset\Re^{D+1}$ of hyperbolic radius $R>0$,

$$|x|^2=x_0^2-\mathbf{x}^2=R^2,\quad \mathbf{x}^2=x_1^2+x_2^2+\cdots+x_D^2. \tag{7}$$

In this ambient Minkowski space, the isometry group is the Poincaré group $\mathrm{ISO}(D,1)_+^{\uparrow}$, in place of the Euclidean group $\mathrm{ISO}(D)_+$ of flat space. The Lie algebra $\mathrm{so}(D,1)$ has then the standard realization

$$M_{j,k}=x_j\partial_{x_k}-x_k\partial_{x_j},\quad M_{0,k}=x_0\partial_{x_k}+x_k\partial_{x_0},\quad j,k=1,2,\ldots,D. \tag{8}$$

The second-order Casimir operator, $\mathcal{C}$, which is an invariant under the group $\mathrm{SO}(D,1)_+^{\uparrow}$, is ($-R^2$ times) the Laplace–Beltrami operator on $\mathcal{H}_+^D$, namely

$$\frac{1}{R^2}\mathcal{C}=-\Delta_{\mathrm{LB}}=\frac{1}{R^2}\left(\sum_{1\leqslant j<k\leqslant D}M_{j,k}^2-\sum_{1\leqslant k\leqslant D}M_{0,k}^2\right). \tag{9}$$

This operator replaces the Laplacian in the Schödinger equation for hyperbolic curved space. Thus, the Schrödinger equation on this space with a potential $V(\mathbf{x})$ is

$$\left(\frac{-1}{2\mu}\Delta_{\mathrm{LB}}+R^2V(\mathbf{x})\right)f(\mathbf{x})=R^2Ef(\mathbf{x}). \tag{10}$$

In quantum mechanics $\mu=m/\hbar^2$, where m is the particle mass. For application in paraxial wave optics, we recall the interpretation where the extra term characterizes the refractive index anomaly of the medium,

$$n(\mathbf{x})=n_\circ-\nu(\mathbf{x}),\quad n_\circ=n(0),\qquad \begin{matrix} n_\circ\leftrightarrow\mu,\\ \nu(\mathbf{x})\leftrightarrow V(\mathbf{x}).\end{matrix} \tag{11}$$

First we consider the case when the potential is identically zero, $V(\mathbf{x})=0$; a nonzero oscillator potential will be introduced in Sec. II E.

For the free case, in the unitary irreducible representation spaces of the D-dimensional Lorentz group belonging to the most degenerate continuous series indicated by p,[11] the operator (9) has a real lower-bound spectrum, as does (1). The wavefunctions of the free system on the hyperboloid are the solutions to the equation

$$\Delta_{\mathrm{LB}}f(\mathbf{x})=-\left[\left(\frac{D-1}{2R}\right)^2+p^2\right]f(\mathbf{x})=-\frac{\lambda(\lambda+D-1)}{R^2}f(\mathbf{x}),$$
$$p\in\Re_0^+=[0,\infty),\quad \lambda=-\frac{1}{2}(D-1)-ipR. \tag{12}$$

Any wavefield of a given wavenumber p is a solution of this equation.

C. Shapiro functions

A privileged basis for the solutions of the Laplace–Beltrami equation (12) was given by Gel'fand, Graev and Shapiro[8] in the form of D-dimensional plane waves of momentum $\mathbf{p}=p\mathbf{n}$, with positive wavenumber p and in the direction of a unit vector on the sphere $\mathbf{n}\in\mathcal{S}^{D-1}$,

$$\Phi_{\mathbf{p}}^{(D)}(x)=\left(\frac{x_0-\mathbf{n}\cdot\mathbf{x}}{R}\right)^{-(1/2)(D-1)-ipR}=(\cosh\chi-\mathbf{n}\cdot\boldsymbol{\xi}\sinh\chi)^{-(1/2)(D-1)-ipR}, \tag{13}$$

where functions $f(x)$ on the hyperboloid $x\in\mathcal{H}_+^D$ $(x^2=R^2)$ will be denoted, according to convenience, by

$$\begin{aligned} &x_0=+\sqrt{R^2+\mathbf{x}^2}=R\cosh\chi\geqslant R,\\ f(x)=f(x_0,\mathbf{x})=f(\mathbf{x}),\qquad &\\ &\mathbf{x}=R\boldsymbol{\xi}\sinh\chi\in\mathfrak{R}^D,\ \ \chi\in\mathfrak{R}_0^+,\ \ \boldsymbol{\xi}\in\mathcal{S}^{D-1}. \end{aligned} \tag{14}$$

The *Shapiro* functions (13) are a Dirac basis for functions on the hyperboloid, which are orthogonal and complete over **x**- and **p**-spaces:

$$\frac{R}{(2\pi)^D}\int_{\mathbf{x}\in\mathfrak{R}^D}\frac{d^D\mathbf{x}}{x_0}\Phi_{\mathbf{p}}^{(D)}(x)^*\,\Phi_{\mathbf{p}'}^{(D)}(x)=N^{(D)}(p)\,\delta^D(\mathbf{p}-\mathbf{p}'), \tag{15}$$

$$\frac{1}{(2\pi)^D}\int_{\mathbf{p}\in\mathfrak{R}^D}\frac{d^D\mathbf{p}}{N^{(D)}(p)}\Phi_{\mathbf{p}}^{(D)}(x)^*\,\Phi_{\mathbf{p}}^{(D)}(x')=\delta^D(x,x'), \tag{16}$$

with the measure and Dirac δ under $\int_{\mathcal{H}_+^D}d^Dx=R\int_{\mathfrak{R}^D}d^D\mathbf{x}/x_0$,

$$N^{(D)}(p)=\left|\frac{\Gamma(ipR)}{\Gamma\left(\frac{1}{2}(D-1)+ipR\right)}\right|^2(pR)^{D-1}, \tag{17}$$

$$\delta^D(x,x')=\frac{x_0}{R}\,\delta^D(\mathbf{x}-\mathbf{x}')=\sqrt{1+\frac{\mathbf{x}^2}{R^2}}\,\delta^D(\mathbf{x}-\mathbf{x}'). \tag{18}$$

In particular, $N^{(1)}(p)=1$, $N^{(2)}(p)=\coth(pR)$, and $N^{(3)}(p)=1$.

The Inönu–Wigner contraction limit of the Lorentz to the Euclidean group $\mathrm{SO}(D,1)_+^\uparrow\to\mathrm{ISO}(D)_+$ is the limit $R\to\infty$ in our expressions for vectors with $x_0\approx R$, $\mathbf{x}^2\ll R^2$, and $\mathbf{p}=p\mathbf{n}$ as before, i.e.,

$$\lim_{R\to\infty}\Phi_{\mathbf{p}}^{(D)}(x)=\lim_{R\to\infty}\left(\frac{x_0-\mathbf{x}\cdot\mathbf{n}}{R}\right)^{-(1/2)(D-1)-ipR}\approx\lim_{R\to\infty}\left(1-\frac{\mathbf{x}\cdot\mathbf{n}}{R}\right)^{-ipR}=\exp(i\mathbf{x}\cdot\mathbf{p}). \tag{19}$$

Correspondingly, $\lim_{R\to\infty}N^{(D)}(p)=1$ and $\delta^D(x,x')\to\delta^D(\mathbf{x}-\mathbf{x}')$.

D. Momentum space for the hyperboloid

The Shapiro functions $\{\Phi_{\mathbf{p}}^{(D)}(\mathbf{x})\}_{\mathbf{p}\in\mathfrak{R}^D}$ in (13) serve as the integral transform kernel between functions of **x** on the hyperboloid, $f(\mathbf{x})$, and conjugate functions of **p**, that has the interpretation of momentum or wavenumber space, and is indicated $\tilde{f}(\mathbf{p})$. Using (14) for $\mathbf{x},\mathbf{p}\in\mathfrak{R}^D$, one writes

$$\tilde{f}(\mathbf{p})=\frac{R}{(2\pi)^{D/2}}\int_{\mathbf{x}\in\mathfrak{R}^D}\frac{d^D\mathbf{x}}{x_0}\Phi_{\mathbf{p}}^{(D)}(\mathbf{x})^*\,f(\mathbf{x}), \tag{20}$$

$$f(\mathbf{x})=\frac{1}{(2\pi)^{D/2}}\int_{\mathbf{p}\in\Re^D}\frac{d^D\mathbf{p}}{N^{(D)}(p)}\Phi_{\mathbf{p}}^{(D)}(\mathbf{x})\,\tilde{f}(\mathbf{p}). \tag{21}$$

This *Shapiro transform* has been used as a relativistic analog of the Fourier transform (the physical context here, though, is **not** that of space–time relativity, as we shall clarify below), and is a vector form of one of the two branches of the bilateral Mellin transform.[12] Here the Shapiro transform replaces the traditional Fourier transform in the definition of a momentum space $\mathbf{p}\in\Re^D$, canonically conjugate with respect to this basis, to a configuration space of constant curvature. The corresponding Parseval relation is

$$R\int_{\mathbf{x}\in\Re^D}\frac{d^D\mathbf{x}}{x_0}f(\mathbf{x})^*\,g(\mathbf{x})=(f,\,g)_{\mathcal{H}_+^D}=\int_{\mathbf{p}\in\Re^D}\frac{d^D\mathbf{p}}{N^{(D)}(p)}\tilde{f}(\mathbf{p})^*\,\tilde{g}(\mathbf{p}). \tag{22}$$

The manifold of momentum $\mathbf{p}=p\mathbf{n}\in\Re^D$ ($p\in\Re^+$ and $\mathbf{n}\in\mathcal{S}^{D-1}$) can be placed also in a $(D+1)$-dimensional "ambient" space, where it occupies the cone $\varpi=(p,\mathbf{p})\in\vee^+$. The momentum thus defined by the Shapiro functions has certain features, however, which do not correspond to those of a standard relativistic momentum vector. If $f(\mathbf{x})$ is a monochromatic wavefield with a definite value of p, this wavenumber will not change under SO(D,1) translations of the hyperboloid ("boosts"), because it is the invariant value of the Casimir operator (9)–(12). Only the direction of momentum, $\mathbf{n}$, can shift over the sphere; it will do so following the well-known Bargmann deformation of the circle,[13] where the colatitude angle "boosts" as $\tan\frac{1}{2}\phi\mapsto e^{-\zeta}\tan\frac{1}{2}\phi$ for rapidity $\zeta\in\Re$. Quotation marks are used for "boost" because here we mean a translation in the hyperboloid, and not the well-known relativistic acceleration.

E. Oscillators on conics

The Laplace–Beltrami equation (9)–(12) provides the free fields (whose energy is purely kinetic) on the hyperboloid. In Eq. (10) we allowed a potential energy term as in the Schrödinger equation of quantum mechanics, by adding a function of position $V(\mathbf{x})$.[7,14,15] A straightforward and useful generalization of the SO(D)-isotropic harmonic oscillator potential from flat to conic D-dimensional configuration space is[14]

$$V(\mathbf{x})=\frac{1}{2}\mu\omega^2R^2\frac{|\mathbf{x}|^2}{x_0^2}=\frac{1}{2}\mu\omega^2R^2\tanh^2\chi=\frac{1}{2}\mu\omega^2R^2\,(1-\operatorname{sech}^2\chi), \tag{23}$$

where $\chi\in\Re_0^+$ is the hyperbolic angle coordinate defined in Eqs. (14). This is the Pöschl–Teller "secant-hyperbolic-squared" trough.

III. WIGNER FUNCTION ON THE HYPERBOLOID

With the Shapiro basis of wavefunctions of the free system, we construct now our proposed Wigner function following the double-integral form in Eq. (3) for two wavefunctions, $f(x)$ and $g(x)$, by means of integrals on two hyperboloids, $|x'|=R$ and $|x''|=R$.

A. Definition

With the measures in Eqs. (15) and the Shapiro functions in (13), we define the Wigner function on the hyperboloid by

$$W_{\mathcal{H}}(f,g|\mathbf{x},\mathbf{p})=\frac{R^2}{(2\pi)^D}\int_{\mathbf{x}'\in\Re^D}\frac{d^D\mathbf{x}'}{x_0'}\int_{\mathbf{x}''\in\Re^D}\frac{d^D\mathbf{x}''}{x_0''}f(x')^*\,g(x'')$$
$$\times\Phi_{\mathbf{p}}^{(D)}(x')\,\Delta^D(x;x',x'')\,\Phi_{\mathbf{p}}^{(D)}(x'')^*, \tag{24}$$

where $\Delta^D(x;x',x'')$ takes the place of the Dirac delta $\delta^D(\mathbf{x}-\frac{1}{2}(\mathbf{x}'+\mathbf{x}''))$ on flat space, Eq. (3), and which will be detailed below.

The crucial property that we must require of this "binding-Δ" in (24) is that it should guarantee that x be the midpoint of the *geodesic* between x' and x'', so that all three points lie on the hyperboloid $\mathcal{H}_+^D$. We achieve this in the following way:[16] given $x \in \mathfrak{R}^{D+1}$ in the upper sheet of a two-sheeted hyperboloid, we build any $y \in \mathfrak{R}^{D+1}$ on a one-sheeted hyperboloid $\tilde{\mathcal{H}}^D$ of the same radius R, such that it be Minkowski-orthogonal to x,

$$y=(y_0,\mathbf{y}), \quad |y|^2=y_0^2-\mathbf{y}^2=-R^2, \quad x_0y_0-\mathbf{x}\cdot\mathbf{y}=0. \tag{25}$$

Then, we can express x' and x'' as vectors obtained from x and y as follows:

$$x'=x\cosh\tfrac{1}{2}\tau-y\sinh\tfrac{1}{2}\tau, \quad x''=x\cosh\tfrac{1}{2}\tau+y\sinh\tfrac{1}{2}\tau, \tag{26}$$

where $x',x'' \in \mathcal{H}_+^D$ for all $\tau \in \mathfrak{R}$. Also, it is easy to show that

$$x_0'x_0''-\mathbf{x}'\cdot\mathbf{x}''=R^2\cosh\tau, \quad x_0x_0'-\mathbf{x}\cdot\mathbf{x}'=x_0x_0''-\mathbf{x}\cdot\mathbf{x}''=R^2\cosh\tfrac{1}{2}\tau, \tag{27}$$

i.e., the geodesic distance between x' and x'' is $R\tau$, while x is at $\frac{1}{2}R\tau$ from both x' and x''. The arguments x' and x'' in the expression (24) thus emulate the arguments $\mathbf{x}\pm\frac{1}{2}\mathbf{z}$ in (2) with the parameter $\frac{1}{2}\tau$.

Using (18) and the parameter τ in (27), we propose the binding-Δ in (24) to be

$$\Delta^D(x;x',x'')=\frac{x_0}{R}\,\delta^D\left(\mathbf{x}-\frac{\mathbf{x}'+\mathbf{x}''}{2\cosh\frac{1}{2}\tau}\right). \tag{28}$$

This will yield the correct marginals (to be seen below) due to its properties

$$\Delta^D(x;x',x')=\frac{x_0}{R}\,\delta^D(\mathbf{x}-\mathbf{x}'), \quad R\int_{\mathbf{x}\in\mathfrak{R}^D}\frac{d^D\mathbf{x}}{x_0}\,\Delta^D(x;x',x'')=1. \tag{29}$$

B. Integral forms

The $2D$-fold integral form of the Wigner function in (24) contains Dirac δ's; it can therefore be brought to a $(D+1)$-fold integral noting that the definition of $y \in \tilde{\mathcal{H}}^D$ leaves the freedom of rotating $\mathbf{y}$ around $\mathbf{x}$ on a sphere $\mathcal{S}^{D-1}$. When we change variables from x' and x'' to x and y according to (26), we reduce the integration to $\mathbf{y}$ and τ while keeping Minkowski-orthogonality. The proposed Wigner function (24) then becomes

$$\begin{aligned} W_{\mathcal{H}}(f,g|\mathbf{x},\mathbf{p})=\frac{R^2}{(2\pi)^D}\int_0^\infty(\sinh\tau)^{D-1}\,d\tau\int_{y\in\tilde{\mathcal{H}}^D}d^D\mathbf{y}\;\delta(x_0y_0-\mathbf{x}\cdot\mathbf{y}) \\ \times f\left(x\cosh\frac{1}{2}\tau-y\sinh\frac{1}{2}\tau\right)^*\,g\left(x\cosh\frac{1}{2}\tau+y\sinh\frac{1}{2}\tau\right) \\ \times\Phi_{\mathbf{p}}^{(D)}\left(x\cosh\frac{1}{2}\tau-y\sinh\frac{1}{2}\tau\right)\Phi_{\mathbf{p}}^{(D)}\left(x\cosh\frac{1}{2}\tau+y\sinh\frac{1}{2}\tau\right)^*. \end{aligned} \tag{30}$$

The Dirac δ remaining in (30) can be used to find a third alternative form of the Wigner function. This is obtained with the parametrization of the ambient-space vectors given by

$$x=(x_0,\mathbf{x})=R(\cosh\chi,\boldsymbol{\xi}\sinh\chi), \quad y=(y_0,\mathbf{y})=R(\sinh\omega,\boldsymbol{\eta}\cosh\omega), \tag{31}$$

where $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ are unit vectors on the sphere $\mathcal{S}^{D-1}$ and $\chi,\omega \in \mathfrak{R}_0^+$. The Dirac δ in Eq. (30) is then

$$\delta(x_0 y_0 - \mathbf{x}\cdot\mathbf{y}) = \frac{1}{R^2}\frac{\cosh\Omega}{\cosh\chi}\,\delta(\omega-\Omega), \quad \text{with} \quad \tanh\Omega = \boldsymbol{\xi}\cdot\boldsymbol{\eta}\tanh\chi. \tag{32}$$

The differential $d^D\mathbf{y}$ of the integral in $y\in\tilde{\mathcal{H}}_+^D$ becomes $R^D(\cosh\omega)^{D-1}d\omega\, d^{D-1}\boldsymbol{\eta}$, so the Wigner function (24) becomes a D-fold integral with the structure of (2), viz.,

$$\begin{aligned} W_{\mathcal{H}}(f,g|\mathbf{x},\mathbf{p}) = \frac{1}{(2\pi)^D}\int_0^\infty (\sinh\tau)^{D-1}\,d\tau \int_{\mathcal{S}^{D-1}} \frac{|\mathbf{y}|^D}{\cosh\chi}\,d^{D-1}\boldsymbol{\eta} \\ \times f\left(x\cosh\frac{1}{2}\tau - y\sinh\frac{1}{2}\tau\right)^* g\left(x\cosh\frac{1}{2}\tau + y\sinh\frac{1}{2}\tau\right) \\ \times \Phi_{\mathbf{p}}^{(D)}\left(x\cosh\frac{1}{2}\tau - y\sinh\frac{1}{2}\tau\right)\Phi_{\mathbf{p}}^{(D)}\left(x\cosh\frac{1}{2}\tau + y\sinh\frac{1}{2}\tau\right)^*, \end{aligned} \tag{33}$$

with

$$y = R(\sinh\Omega,\ \ \boldsymbol{\eta}\cosh\Omega) = R\,\frac{(\boldsymbol{\xi}\cdot\boldsymbol{\eta}\tanh\chi,\ \ \boldsymbol{\eta})}{\sqrt{1-(\boldsymbol{\xi}\cdot\boldsymbol{\eta}\tanh\chi)^2}}. \tag{34}$$

C. Marginal projections

The marginal projections obtained by integrating the proposed Wigner function (24) over momentum and configuration space should yield, respectively, $f(\mathbf{x})^* g(\mathbf{x})$ and $\tilde{f}(\mathbf{p})^*\tilde{g}(\mathbf{p})$ as defined in (20) and (21). The two marginals follow from the orthogonality and completeness relations of the Shapiro functions, Eqs. (15) and (16).

The integration of the Wigner function over $\mathfrak{R}^D$ momentum space with the measure $1/N^{(D)}(p)$ in (17) is

$$\begin{aligned} M_{\mathcal{H}}(f,g|\mathbf{x}) &= \int_{\mathbf{p}\in\mathfrak{R}^D}\frac{d^D\mathbf{p}}{N^{(D)}(p)}\,W_{\mathcal{H}}(f,g|\mathbf{x},\mathbf{p}) \\ &= R^2\int_{\mathbf{x}'\in\mathfrak{R}^D}\frac{d^D\mathbf{x}'}{x_0'}\int_{\mathbf{x}''\in\mathfrak{R}^D}\frac{d^D\mathbf{x}''}{x_0''}\,f(x')^*\,g(x'')\,\Delta^D(x;x',x'')\,\delta^D(x',x'') \\ &= R\int_{\mathbf{x}'\in\mathfrak{R}^D}\frac{d^D\mathbf{x}'}{x_0'}\,f(x')^*\,g(x')\,\Delta^D(x;x',x') = f(\mathbf{x})^*\,g(\mathbf{x}), \end{aligned} \tag{35}$$

where we used (16), (18), and the first property of the binding-Δ in (29).

Similarly, the integration over $\mathfrak{R}^D$ configuration space with the measure R/x_0 in (18) is

$$\begin{aligned} M_{\mathcal{H}}(f,g|\mathbf{p}) &= R\int_{\mathbf{x}\in\mathfrak{R}^D}\frac{d^D\mathbf{x}}{\sqrt{R^2+\mathbf{x}^2}}\,W_{\mathcal{H}}(f,g|\mathbf{x},\mathbf{p}) \\ &= \frac{R^2}{(2\pi)^D}\int_{\mathbf{x}'\in\mathfrak{R}^D}\frac{d^D\mathbf{x}'}{x_0'}\,f(x')^*\,\Phi_{\mathbf{p}}^{(D)}(x')\int_{\mathbf{x}''\in\mathfrak{R}^D}\frac{d^D\mathbf{x}''}{x_0''}\,g(x'')\,\Phi_{\mathbf{p}}^{(D)}(x'')^* = \tilde{f}(\mathbf{p})^*\,\tilde{g}(\mathbf{p}), \end{aligned} \tag{36}$$

where we used the second property of the binding-Δ in (29) and the Shapiro transform (20).

Finally, integrating over the whole of phase space with the appropriate measures in the Parseval relation (22), we have the total probability

$$R\int_{\mathbf{x}\in\mathfrak{R}^D}\frac{d^D\mathbf{x}}{x_0}M_{\mathcal{H}}(f,g|\mathbf{x})=(f,g)_{\mathcal{H}_+^D}=\int_{\mathbf{p}\in\mathfrak{R}^D}\frac{d^D\mathbf{p}}{N^{(D)}(p)}M_{\mathcal{H}}(f,g|\mathbf{p}). \tag{37}$$

D. Covariance under rotations and conic translations

Under rotations $\mathbf{R}\in \mathrm{SO}(D)$, wavefunctions $f(x_0,\mathbf{x})$ transform through

$$T(\mathbf{R}):f(x)=f(x_0,\mathbf{R}^{-1}\mathbf{x}). \tag{38}$$

In particular, the basis of Shapiro functions (13) transforms as

$$T(\mathbf{R}):\Phi_{p\,\mathbf{n}}^{(D)}(x_0,\mathbf{x})=\Phi_{p\,\mathbf{n}}^{(D)}(x_0,\mathbf{R}^{-1}\,\mathbf{x})=\Phi_{p\,\mathbf{Rn}}^{(D)}(x_0,\mathbf{x}). \tag{39}$$

Applying rotations $T(\mathbf{R})$ to the wavefields f and g in the Wigner function (24), we next change variables to $\mathbf{x}'=\mathbf{R}\overline{\mathbf{x}'}$ and $\mathbf{x}''=\mathbf{R}\overline{\mathbf{x}''}$ (the ambient x_0-components behave as scalars), then use (39) for $\mathbf{R}^{-1}$, noting that the binding-Δ in (28) is invariant, $\Delta^D(\overline{x};\overline{x}',\overline{x}'')=\Delta^D(x;x',x'')$ for $\overline{\mathbf{x}}=\mathbf{R}^{-1}\mathbf{x}$, and so are the measures $d^D\mathbf{x}'=d^D\overline{\mathbf{x}'}$. It thus follows that the Wigner function (24) is covariant under rotations, fulfilling

$$W_{\mathcal{H}}(T(\mathbf{R}):f,T(\mathbf{R}):g|\mathbf{x},\mathbf{p})=W_{\mathcal{H}}(f,g|\mathbf{R}^{-1}\mathbf{x},\mathbf{R}^{-1}\mathbf{p}). \tag{40}$$

Now consider translations by ζ (''boosts'' of rapidity ζ) $\mathbf{B}_{\mathbf{m}}(\zeta)\in \mathrm{SO}(D,1)_+^{\uparrow}$ in the direction of unit $\mathbf{m}\in\mathcal{S}^{D-1}$, which transform the ambient space vectors preserving the constant-curvature subspaces $x\in\mathcal{H}_+^D$ for each radius $R>0$. We denote by $\mathbf{x}_{\parallel\mathbf{m}}$ and $\mathbf{x}_{\perp\mathbf{m}}$ the projections of $\mathbf{x}$ parallel and perpendicular to the direction of $\mathbf{m}$, so that $\mathbf{x}=\mathbf{x}_{\parallel\mathbf{m}}+\mathbf{x}_{\perp\mathbf{m}}$. Then, wavefunctions on the hyperboloid transform as

$$T(\mathbf{B}_{\mathbf{m}}(\zeta)):f\begin{pmatrix}x_0\\ \mathbf{x}_{\parallel\mathbf{m}}\\ \mathbf{x}_{\perp\mathbf{m}}\end{pmatrix}=f\begin{pmatrix}x_0\cosh\zeta-\mathbf{m}\cdot\mathbf{x}\sinh\zeta\\ \mathbf{x}_{\parallel\mathbf{m}}\cosh\zeta-x_0\,\mathbf{m}\sinh\zeta\\ \mathbf{x}_{\perp\mathbf{m}}\end{pmatrix}. \tag{41}$$

When this transformation is applied to the plane-wave basis of Shapiro functions, their directions $\mathbf{n}$ on the sphere change, and they acquire a multiplier factor:

$$T(\mathbf{B}_{\mathbf{m}}(\zeta)):\Phi_{p\,\mathbf{n}}^{(D)}(x_0,\mathbf{x})=(\cosh\zeta+\mathbf{m}\cdot\mathbf{n}\sinh\zeta)^{-(1/2)(D-1)-ipR}\,\Phi_{p\,\mathbf{n}'}^{(D)}(x_0,\mathbf{x}), \tag{42}$$

where the components of $\mathbf{n}'\in\mathcal{S}^{D-1}$ that are orthogonal and parallel to $\mathbf{m}$ are

$$\mathbf{n}'_{\perp\mathbf{m}}=\frac{\mathbf{n}_{\perp\mathbf{m}}}{\cosh\zeta+\mathbf{n}\cdot\mathbf{m}\sinh\zeta},\quad \mathbf{n}'_{\parallel\mathbf{m}}=\frac{\mathbf{n}\cdot\mathbf{m}\cosh\zeta+\sinh\zeta}{\cosh\zeta+\mathbf{n}\cdot\mathbf{m}\sinh\zeta}\,\mathbf{m}, \tag{43}$$

within the same $\mathrm{SO}(D,1)_+^{\uparrow}$ irreducible representation characterized by the invariant wavenumber, p. If the angle from $\mathbf{m}$ to $\mathbf{n}$ is ϕ, it will transform through the well-known Bargmann SO(2,1) map of the circle.

The expression in the multiplier factor of Eq. (42),

$$\mu(\mathbf{m},\zeta;\mathbf{n})=\cosh\zeta+\mathbf{m}\cdot\mathbf{n}\sinh\zeta, \tag{44}$$

is, not coincidentally, p'/p—if the $(D+1)$-vector $\varpi=(p,\mathbf{p})\in\vee^+$ were allowed to transform as a ''lightlike'' vector in relativity, i.e., without being constrained to its p-sphere. Under the inner product (16), the $\mathrm{SO}(D,1)$ boost with the multiplier (42) is unitary nonetheless, because the measure in $\mathbf{p}$-space is $d^D\mathbf{p}=p^D dp d^{N-1}\mathbf{n}$, and while p is invariant, from (43) it follows that $d^{D-1}\mathbf{n}=\mu(\mathbf{m},\zeta;\mathbf{n})^{D-1}d^{D-1}\mathbf{n}'$. This cancels the absolute square of the multiplier (44) in the

Shapiro functions (41). This type of covariance modulo a multiplier function is determined by the Shapiro function basis; we may call Eqs. (41) and (42) the *Shapiro covariance* between the conjugate transformations in **x** and **p**.

When the wavefields in the Wigner function (24) are translated within the hyperboloid by (41), the ambient vectors x are multiplied by a $(D+1)\times(D+1)$ ('boost') matrix $\mathbf{B_m}(\zeta)$, to $x'\mapsto\overline{x'}=\mathbf{B_m}(\zeta)^{-1}x'$ and $x''\mapsto\overline{x''}=\mathbf{B_m}(\zeta)^{-1}x''$. Under this transformation, the measures are again invariant, $d^D\mathbf{x}'/x_0'=d^D\overline{\mathbf{x}'}/\overline{x_0'}$, etc., and so is $\Delta^D(x;x',x'')=\Delta^D(\overline{x};\overline{x'},\overline{x''})$; hence, $\overline{x}=\mathbf{B_m}(\zeta)^{-1}x$ will appear in the first argument of the transformed Wigner function. But the corresponding transformation of **p** in each of the two Shapiro functions, Eqs. (42) and (44), yields a multiplier factor. The imaginary exponents of $\mu(\mathbf{m},\zeta;\mathbf{n})$ cancel, and there remains a positive net multiplier factor:

$$W_{\mathcal{H}}(T[\mathbf{B_m}(\zeta)]:f,\,T[\mathbf{B_m}(\zeta)]:g|\mathbf{x},p\,\mathbf{n})=(\mu(\mathbf{m},\zeta;\mathbf{n}))^{-D+1}\,W_{\mathcal{H}}(f,g|\mathbf{B}(\zeta)^{-1}:\mathbf{x},\;\; p\,\mathbf{B_m}(\zeta)^{-1}:\mathbf{n}), \tag{45}$$

where $\mathbf{n}'=\mathbf{B_m}(\zeta)^{-1}:\mathbf{n}$ is given by (43). Note that in the $D=1$-dimensional case, the multiplier factor is 1.

Covariance of the Wigner function is usually understood in the simple form it has under rotations, as given by (40). Under these transformations, the hyperboloid in the ambient x-space rotates on its axis, and in the momentum plane the circles **n** of all radii p rotate in synchrony. Translations within the hyperboloid (45), on the other hand, deform the ambient and projected space vectors, x and **x**, through (41); momentum space is concurrently squeezed in the direction of the translation so that its points move on constant-p circles and with a common Bargmann deformation of the angle. Since areas are not conserved in momentum space, a multiplier function of **p** is necessary for the Wigner function to ensure the total conservation of probability (37).

E. Contraction limit

We now show that, when $f(x)$ and $g(x)$ are significantly different from zero only within a small, essentially flat patch of the hyperboloid, the definition of the Wigner function in Eq. (33) reduces to the standard Wigner function for flat space in Eq. (3). In (33), the integrand for $\boldsymbol{\eta}$ [recall Eqs. (31) and (34)] will be significant only when $\mathfrak{R}^D$ norms of the vectors fulfill

$$\left|\mathbf{x}\cosh\frac{1}{2}\tau\pm\mathbf{y}\sinh\frac{1}{2}\tau\right|\ll R\Rightarrow\begin{cases}|\mathbf{x}|\cosh\frac{1}{2}\tau\ll R & \Rightarrow\quad \sinh\chi\ll 1\\ |\mathbf{y}|\sinh\frac{1}{2}\tau\ll R & \Rightarrow\quad \sinh\tau\ll 1\end{cases} \tag{46}$$

$$\Rightarrow x\approx R(1,\chi\,\boldsymbol{\xi}),\quad y\approx R(\chi\,\boldsymbol{\xi}\cdot\boldsymbol{\eta},\boldsymbol{\eta}). \tag{47}$$

Also, using the limit in (19), and approximating $\sinh\tau\approx\tau$ and $\cosh\frac{1}{2}\tau\approx\cosh\chi\approx\cosh\omega\approx 1$, the Wigner function in Eq. (33) reduces to

$$W_{\mathcal{H}}(f,g|\mathbf{x},\mathbf{p})=\frac{R^D}{(2\pi)^D}\int_0^\infty\tau^{D-1}\,d\tau\int_{\mathcal{S}^{D-1}}d^{D-1}\boldsymbol{\eta}$$
$$\times f\left(x_0,\mathbf{x}-\frac{1}{2}R\tau\boldsymbol{\eta}\right)^*\exp(-iR\tau\,\boldsymbol{\eta}\cdot\mathbf{p})\,g\left(x_0,\mathbf{x}+\frac{1}{2}R\tau\boldsymbol{\eta}\right). \tag{48}$$

Finally, changing variables to $\mathbf{z}=R\tau\,\boldsymbol{\eta}$ and noticing that

$$\int_{\mathfrak{R}^D}d^D\mathbf{z}\cdots=R^D\int_0^\infty\tau^{D-1}\,d\tau\int_{\mathcal{S}^{D-1}}d^{D-1}\boldsymbol{\eta}\cdots, \tag{49}$$

we see that (48) reduces to (2).

F. Special case of one dimension

In the case $D=1$, the Wigner function (33) actually coincides in form with the corresponding one-dimensional standard flat space form (2), as we now proceed to show.

First, notice that the unit vectors $\mathbf{n}$ and $\boldsymbol{\xi}$ in Eq. (13) are now the unit scalars $n,\xi=\pm 1$, and that the Shapiro functions become simple exponentials:

$$\Phi_p^{(1)}(R\xi\cosh\chi,R\xi\sinh\chi)=[\exp(-n\xi\chi)]^{-ipR}=\exp(in\xi pR\chi). \tag{50}$$

We can now let $np\mapsto p$ and $\xi\chi\mapsto\chi$ with $p,\chi\in(-\infty,\infty)$, and recognize that (50) is a 1:1 function of only one variable, $x_1\in\mathfrak{R}$,

$$\Phi_p^{(1)}(x_1)=\exp(i\chi pR),\quad x_1=R\sinh\chi. \tag{51}$$

The arguments $x=(x_0,x_1)$ of the functions f and g in (33) then simplify, in components, to

$$x=\begin{pmatrix}x_0\\x_1\end{pmatrix}\mapsto x\cosh\frac{1}{2}\tau\pm y\sinh\frac{1}{2}\tau=R\begin{pmatrix}\cosh(\chi\pm\frac{1}{2}\eta\tau)\\ \sinh(\chi\pm\frac{1}{2}\eta\tau)\end{pmatrix}. \tag{52}$$

For short, we indicate $f(R\cosh\chi,R\sinh\chi)=f(\chi)$. The unit vector $\boldsymbol{\eta}$ in (33) and (34) also becomes a unit scalar, $\eta=\pm 1$, and the integral extends over $y=\eta R(\sinh\chi,\cosh\chi)$, and $\Omega=\eta\chi$ [see Eq. (32)]. Finally, the integral over $\boldsymbol{\eta}$ reduces to a sum over $\eta=\pm 1$, and for $\tau\mapsto\eta\tau\in(-\infty,\infty)$, the Wigner function (33) becomes

$$W_{\mathcal{H}}(f,g|x,p)=\frac{R}{2\pi}\int_{-\infty}^{\infty}d\tau f\left(\chi-\frac{1}{2}\tau\right)^{*}e^{-ipR\tau}g\left(\chi+\frac{1}{2}\tau\right) \tag{53}$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\upsilon\tilde{f}\left(p-\frac{1}{2}\upsilon\right)^{*}e^{+iR\upsilon x}\tilde{g}\left(p+\frac{1}{2}\upsilon\right). \tag{54}$$

The last expression is the usual flat-space Wigner function in terms of the conjugate wavefunctions on momentum space. Finally, note that for $D=1$, the net multiplier which appears under "boost" transformations in (45) is unity, so standard and Shapiro covariances coincide.

IV. EXAMPLE: OSCILLATOR ON THE HYPERBOLA

We consider the open one-dimensional space which is the upper branch of a hyperbola of fixed radius $R>0$,

$$\mathcal{H}_{+}^{1}=\{(x_0,x_1)\in\mathfrak{R}^2|x_0^2-x_1^2=R^2\}, \tag{55}$$

parametrized as usual by the hyperbolic angle $\chi\in\mathfrak{R}$.

A. Laplace–Beltrami operator and the oscillator

When the potential $V(\mathbf{x})$ is a constant (corresponding to a homogeneous optical medium), the $D=1$ Schrödinger equation (10) is the free wave equation, and its Shapiro solutions are simply the oscillating exponentials (51), with energy $E=p^2/2\mu\geqslant 0$.

Since the Laplace–Beltrami operator on the hyperbola (55) is $\Delta_{\mathrm{LB}}=R^{-2}d^2/d\chi^2$, the Schrödinger equation for the conic oscillator (23) is

$$\left(\frac{-1}{2\mu}\frac{d^2}{d\chi^2}-R^2E_0\,\mathrm{sech}^2\,\chi\right)f(\chi)=R^2\,(E-E_0)\,f(\chi),\quad E_0=\frac{1}{2}\mu\omega^2R^2, \tag{56}$$

$$V(\chi)=\frac{1}{2}\mu\omega^2R^2\frac{x_1^2}{x_0^2}=\sqrt{s(s+1)}\,(1-\mathrm{sech}^2\chi), \tag{57}$$

$$s=-\tfrac{1}{2}+\sqrt{(\mu\omega R^2)^2+\tfrac{1}{4}}. \tag{58}$$

The bound solutions are[17]

$$\begin{aligned}\psi_n^s(\chi)&=\frac{2^{-(s-n)}}{\Gamma(s-n+1)}\sqrt{\frac{(s-n)\,\Gamma(2s-n+1)}{n!}}\,\mathrm{sech}^{s-n}\chi\,{}_2F_1\left(\begin{matrix}-n,\,2s-n+1\\ s-n+1\end{matrix}\middle|\,\frac{1-\tanh\chi}{2}\right)\\&=\sqrt{\frac{(s-n)\,n!}{\pi\,\Gamma(2s-n+1)}}\,\Gamma\left(s-n+\frac{1}{2}\right)(2\,\mathrm{sech}\,\chi)^{s-n}\,C_n^{s-n+1/2}(\tanh\chi),\end{aligned} \tag{59}$$

where n is a non-negative integer bounded by $s+1$, and $C_n^{\alpha}(\xi)$ are the Gegenbauer (or ultraspherical) polynomials[18] for $\alpha>-\frac{1}{2}$. The corresponding quantized values of the energy are quadratic in n, and counted from the lowest level up by

$$E_n^s=\frac{\mu\omega^2R^2}{2}-\frac{1}{2\mu R^2}(n-s)^2,\quad n=0,1,2,\ldots<s+1. \tag{60}$$

As a check on our concepts, we verify that the contraction limit $R\to\infty$ of this system, when the radius of the hyperbola grows without bound, is the harmonic oscillator on flat space. Since the coefficient s correspondingly grows as $s\approx\mu\omega R^2$, the linear-quadratic spectrum of energies in Eq. (60) becomes the linear spectrum of the quantum harmonic oscillator $E_n=\omega(n+\frac{1}{2})$. To implement this limit on the wavefunctions (59), it is convenient to use the following forms for the Gegenbauer polynomials in $\xi=\tanh\chi$:

$$C_n^{\alpha}(\xi)=\begin{cases}(-1)^{(1/2)\,n}\dfrac{\Gamma(\alpha+\frac{1}{2}\,n)}{(\frac{1}{2}n)!\,\Gamma(\alpha)}\,{}_2F_1\left(\begin{matrix}-\frac{1}{2}n,\,\frac{1}{2}n+\alpha\\ \frac{1}{2}\end{matrix}\middle|\,\xi^2\right), & n\text{ even},\\[2ex](-1)^{(1/2)(n-1)}\dfrac{\Gamma(\alpha+\frac{1}{2}(n+1))}{(\frac{1}{2}(n-1))!\,\Gamma(\alpha)}\,2\xi\,{}_2F_1\left(\begin{matrix}-\frac{1}{2}(n-1),\,\frac{1}{2}(n+1)+\alpha\\ \frac{3}{2}\end{matrix}\middle|\,\xi^2\right), & n\text{ odd}.\end{cases} \tag{61}$$

Then, for $\alpha=s-n+\frac{1}{2}\to\infty$, the hypergeometric polynomials simplify: for n even, ${}_2F_1(-\frac{1}{2}n,\,\alpha;\frac{1}{2};\xi^2)\approx{}_1F_1(-\frac{1}{2}n;\frac{1}{2};\alpha\xi^2)=H_n(\sqrt{\alpha}\xi)$, and similarly for n odd. Replacing this into Eq. (59), with $\xi=\tanh\chi\approx\sinh\chi=x_1/R$ and $\cosh^{-s+n}\chi\approx\exp(-s\tanh^2\frac{1}{2}\chi)$, we obtain the harmonic oscillator wavefunctions on flat space,

$$\frac{1}{\sqrt{R}}\psi_n^s(\chi)\approx\frac{1}{\sqrt{2^n n!\,\sqrt{\pi/\mu\omega}}}\,e^{-\mu\omega x_1^2/2}\,H_n(\sqrt{\mu\omega}\,x_1). \tag{62}$$

The factor $\sqrt{R}$ restores the proper normalization on the x_1 axis.

In addition to the bound states, the sech-trough Pöschl–Teller potential also has free states with energy above the asymptotic value of the potential $\lim_{\chi\to\pm\infty}V(\chi)=\frac{1}{2}\mu\omega^2R^2$. These scattering solutions contain associated Legendre polynomials of imaginary upper index:

$$p = R\sqrt{2\mu E - \mu^2\omega^2 R^2} > 0,$$

$$\psi_p(\chi) = \frac{|\Gamma(1-ip)|}{2\pi} P_\sigma^{ip}(\tanh\chi), \tag{63}$$

$$\sigma = \tfrac{1}{2} \pm \sqrt{\omega^2\mu^2 R^4 + \tfrac{1}{4}}.$$

These wavefunctions are Dirac-orthonormal.

B. Momentum representation of the wavefunctions

The bound wavefunctions of the Pöschl–Teller sech-trough potential in the momentum representation, $\tilde{\psi}_n^s(p)$, are found through the ordinary Fourier transform [Eqs. (20) and (21) for $D=1$ and (51)] of the wavefunctions $\psi_n^s(\chi)$ found in Eq. (59). The result is

$$\tilde{\psi}_n^s(p) = \sqrt{\frac{R}{2\pi}} \int_{-\infty}^{\infty} d\chi \exp(-ipR\chi)\, \psi_n^s(\chi)$$

$$= \frac{R}{2}\sqrt{\frac{\Gamma(2s-n+1)}{\pi(s-n)n!}} \frac{|\Gamma(\frac{1}{2}(s-n-ipR))|^2}{\Gamma(s-n)^2}\, {}_3F_2\left(\begin{matrix} -n,\, 2s-n+1, \frac{1}{2}(s-n-ipR) \\ s-n+1, s-n \end{matrix} \middle| 1 \right) \tag{64}$$

$$= \frac{(-i)^n R}{2\sqrt{\pi}} \frac{\sqrt{(s-n)\,n!\,\Gamma(2s-n+1)}}{\Gamma(s)\,\Gamma(s+1)} \left| \Gamma\left(\frac{1}{2}(s-n-ipR) \right) \right|^2$$

$$\times R_n\left(-\frac{1}{2}ipR; \frac{1}{2}(s-n), \frac{1}{2}(s-n), \frac{1}{2}(s-n), \frac{1}{2}(s-n)+1 \right), \tag{65}$$

where $R_n(z;\alpha,\beta,\gamma,\delta)$ are the continuous Hahn polynomials.[19] On the other hand, the unbound solutions (63) are not square-integrable, so their Fourier transform must be performed allowing for the phase difference between asymptotic incoming and outgoing waves, as determined by the scattering properties of this Pöschl–Teller potential. We shall not further detail the free states here; they can be found in Ref. 9 among the coupling coefficients between the $D^+ \times D^- \to \Sigma D^+ + \int C$ irreducible representations series of SO(2,1).

C. Wigner function for the oscillator eigenstates on the hyperbola

On the one-dimensional hyperbola $\mathcal{H}_+^1$, the Wigner function (24) collapses to (53) and (54), its usual form in Eqs. (2) and (3) for $D=1$.

We are interested in the single-function form $W(f|\mathbf{x},\mathbf{p}) \equiv W(f,f|\mathbf{x},\mathbf{p}) = W(\tilde{f},\tilde{f}|\mathbf{p},-\mathbf{x})$ for the Pöschl–Teller wavefunctions, whose explicit form is in Eq. (59) for $\psi_n^s(x)$, and in Eq. (64) for $\tilde{\psi}_n^s(p)$; we find the latter more amenable to analytic solution. We change the integration to a contour along the imaginary axis, and find

$$W(\psi_n^s|\chi,p) = \frac{R^2}{8\pi^2} \frac{s-n}{n!\,\Gamma(2s-n+1)} \sum_{m,l=0}^{n} \frac{(-n)_m (-n)_l}{\Gamma(s-n+m)\,\Gamma(s-n+l)}$$

$$\times \frac{\Gamma(2s-n+m+1)\,\Gamma(2s-n+l+1)}{\Gamma(s-n+m+1)\,\Gamma(s-n+l+1)} \frac{1}{l!m!} I_n^s(\chi,p), \tag{66}$$

where

$$I_n^s(\chi,p)=-\frac{4i}{R}\int_{-i\infty}^{i\infty}dz\,\Gamma\left(\frac{1}{2}(s-n)-\frac{1}{2}ipR-z\right)\Gamma\left(\frac{1}{2}(s-n)+\frac{1}{2}ipR+z+m\right)$$
$$\times e^{-4\chi z}\,\Gamma\left(\frac{1}{2}(s-n)+\frac{1}{2}ipR-z\right)\Gamma\left(\frac{1}{2}(s-n)-\frac{1}{2}ipR+z+l\right). \tag{67}$$

The last integral can be computed in the complex plane straightforwardly, and leads to a pair of complex conjugate ${}_2F_1$-functions of $e^{-4\chi}$. We thus finally have

$$W(\psi_n^s|\chi,p)=\frac{2R\,(s-n)\,n!\,e^{-2\chi(s-n)}}{\pi\Gamma(2s-n+1)}\sum_{m,l=0}^{n}\frac{\Gamma(2s-n+m+1)\,\Gamma(2s-n+l+1)}{\Gamma(s-n+l+1)\,\Gamma(s-n+m+1)\,\Gamma(s-n+l)}$$
$$\times\frac{(-1)^{l+m}}{l!m!(n-m)!(n-l)!}\,\mathrm{Re}\left\{\Gamma(ipR)\,\Gamma(s-n+l-ipR)\,e^{2ipR\chi}\right.$$
$$\left.\times{}_2F_1\left(\begin{matrix}s-n+m,s-n+l-ipR,\\1-ipR\end{matrix}\middle|\,e^{-4\chi}\right)\right\}. \tag{68}$$

We note that this expression is suitable for numerical computation only for $\chi>0$ because it converges fast, but it holds everywhere analytically, with the reflection symmetries $W(\psi_n^s|\chi,p)=W(\psi_n^s|-\chi,p)=W(\psi_n^s|\chi,-p)$.

The Wigner functions, together with their marginal projections $|\psi_n^s(x)|^2$ and $|\tilde{\psi}_n^s(p)|^2$, are shown in Fig. 1, for $n=0,1,2,3$, and for the potential depth parameter $s=4$ and 30. It can be appreciated that the Wigner function of the most tightly bound states resemble the familiar Gaussian-bell form of the harmonic oscillator ground state. According to (60), for $s=4$ there are only five bound states ($n=0,\ldots,4$), and as the energy of the state approaches the binding energy, the wavefunction stretches in space with ever-smaller momentum in a neighborhood of the classical turning point. The contraction limit can be appreciated in the $s=30$ column, corresponding to a large binding energy; the Wigner functions for the eigenstates in Eq. (59) approach the familiar Laguerre–Gaussian form that corresponds to the Wigner function of the harmonic oscillator wavefunctions on flat space.

V. CONCLUDING REMARKS

We have generalized the Wigner quasiprobability distribution function by replacing the oscillating exponential functions of the standard version, which are Dirac solutions of the free Schrödinger equation on flat space, by the Shapiro functions, because they are solutions to the Laplace–Beltrami equation on a simply connected hyperbolic space, while respecting the midpoint condition through an appropriate Dirac-like $\Delta^D(x;x',x'')$. The role of the Fourier transform in the standard version is transfered by the Shapiro functions to a Mellin-like transform between the position and momentum coordinates of phase space. Indeed, the relation between what were called position and momentum variables is actually defined by the argument and index of the basis of Shapiro functions. Thus built, the proposed Wigner function is covariant under the group SO(D,1) of motions of the hyperbola, with the hyperbolic translations extracting a multiplier factor. The correct marginals are found and the contraction limit to flat space returns the standard Wigner function.

The transformations of the momentum direction under translations of the hyperbola are the (unique) action of SO(D,1) on the sphere $\mathcal{S}^D$.[13] There are several models of Hamiltonian systems where momentum is restricted to a sphere, such as geometric and Helmholtz (monochromatic) optics.[20,21] In the first model, a ''Descartes sphere'' of momentum vectors $\mathbf{p}$, which is of radius $|\mathbf{p}|=n(\mathbf{x})$ (the refractive index), is associated to each point $\mathbf{x}$ in space. This sphere of momentum vectors has been subject to Bargmann's ''boost'' transformation in Ref. 22 (which is unique for Lorentz groups acting on spheres) and here given by (43), with a canonically conjugate transformation of the ray positions at a plane screen. The resulting phenomenon has been called relativ-

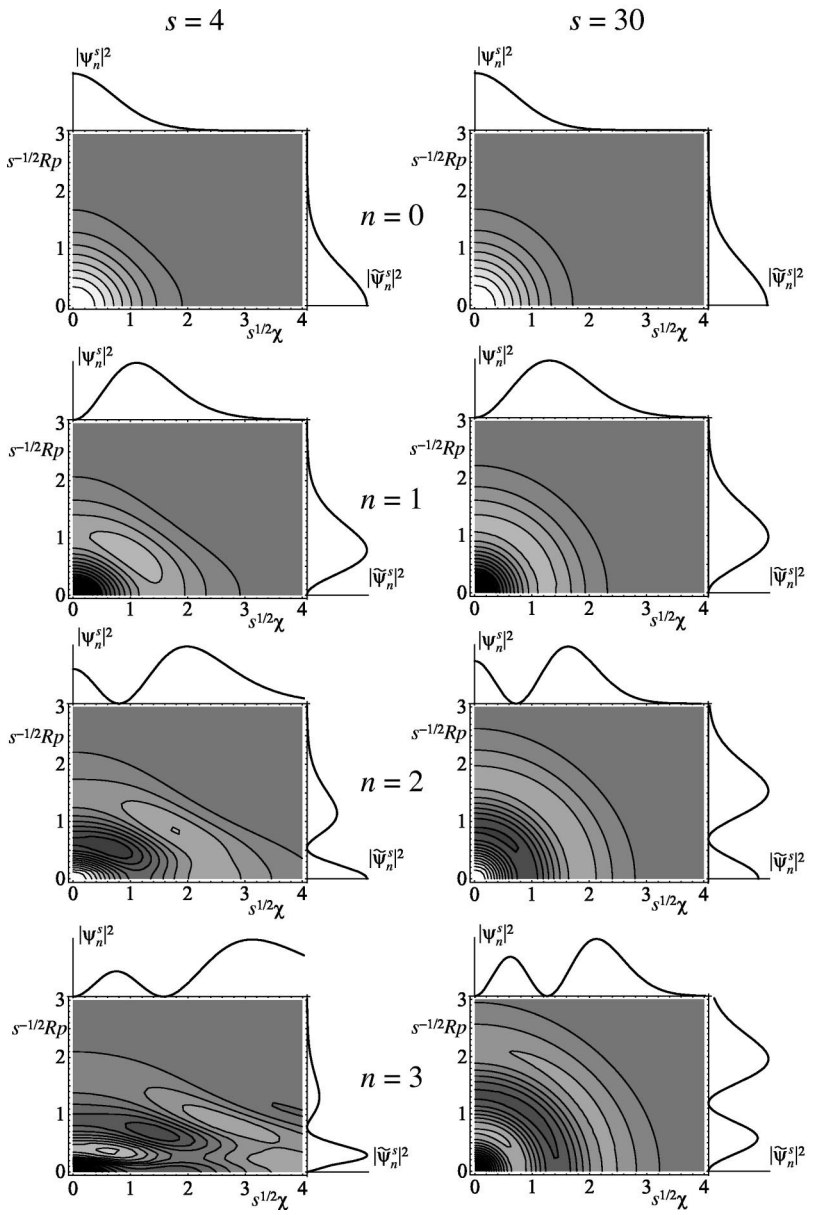

FIG. 1. Wigner functions of the Pöschl–Teller eigenfunctions $\psi_n^s(\chi)$ on a quadrant of phase space (axes are position $\chi\sqrt{s}$ and momentum $pR/\sqrt{s}$; the quadrants have reflection symmetry across the axes). Rows are numbered by the mode $n=0,1,2,3$. Left: $s=4$ (so only five states, $n=0,\ldots,4$, are bound); right: $s=30$ (so states are bound up to $n=30$). White is the maximum, black is the minimum; the shade at the upper right corner corresponds to zero. From each Wigner function we project up the marginal distribution of position $|\psi_n^s(\chi)|^2$, and right the marginal of momentum $|\tilde{\psi}_n^s(p)|^2$.

istic coma, because the aberration in the images projected on moving screens in vacuum is comatic. The Doppler effect is of course absent, so this transformation cannot be called physically relativistic in the Helmholtz case, which involves a configuration space with a nonlocal metric. Indeed, the difference between the various models consists in their space of positions; here, it is the hyperboloid. A Wigner function on spheres will be examined in part II of this title; it is expected to clarify further the use of function bases to define conjugate variables as a simile or substitute for phase space.

The context of this work has a wider significance as a model for phase space with noncom-

mutative geometry, although here the noncommutativity is restricted to momentum space only. In one dimension this argument does not apply, but the example of the one-dimensional Wigner function of Pöschl–Teller wavefunctions is of interest on its own for the traditional quantum mechanical model, and also for the paraxial propagation of light along shallow nonharmonic waveguides whose index of refraction has a sech^2 profile, as given by Eq. (11). One of the manifestations of higher symmetry is the appearance of ''closed-form'' wavefunctions expressed in terms of well-known (and some not-so-well-known) special functions. Generally, the Fourier transforms and Wigner functions of such wavefunctions are again known special functions because symmetry, when it occurs, is displayed in phase space.

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Fixed points of quantum operations

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Quantum operations frequently occur in quantum measurement theory, quantum probability, quantum computation, and quantum information theory. If an operator A is invariant under a quantum operation ϕ, we call A a ϕ-fixed point. Physically, the ϕ-fixed points are the operators that are not disturbed by the action of ϕ. Our main purpose is to answer the following question. If A is a ϕ-fixed point, is A compatible with the operation elements of ϕ? We shall show in general that the answer is no and we shall give some sufficient conditions under which the answer is yes. Our results will follow from some general theorems concerning completely positive maps and injectivity of operator systems and von Neumann algebras. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1519669]

I. INTRODUCTION

Let $\mathcal{H}$ be a Hilbert space and let $\mathcal{B}(\mathcal{H})$ be the set of bounded linear operators on $\mathcal{H}$. We use the notation

$$\mathcal{B}(\mathcal{H})^+ = \{A \in \mathcal{B}(\mathcal{H}) : A \geqslant 0\}, \quad \mathcal{E}(\mathcal{H}) = \{A \in \mathcal{B}(\mathcal{H}) : 0 \leqslant A \leqslant I\},$$

that is, $\mathcal{B}(\mathcal{H})^+$ is the positive cone for $\mathcal{B}(\mathcal{H})$ and $\mathcal{E}(\mathcal{H})$ is the set of **quantum effects**.[1–4] Quantum effects correspond to yes–no quantum measurements that may be unsharp. Denoting the set of trace class operators on $\mathcal{H}$ by $\mathcal{T}(\mathcal{H})$, the set of **states** (or **density operators**) of a quantum system is described by

$$\mathcal{D}(\mathcal{H}) = \{\rho \in \mathcal{T}(\mathcal{H})^+ : \mathrm{tr}(\rho) = 1\}.$$

The probability that an effect A occurs (has a yes answer) in the state ρ is given by $P_\rho(A) = \mathrm{tr}(\rho A)$.

Quantum measurements that have more than two values (not just yes–no) are frequently described by effect-valued measures. In this paper we shall only consider discrete effect-valued measures. These are described by a sequence $E_i \in \mathcal{E}(\mathcal{H})$, $i = 1,2,\ldots$, satisfying $\Sigma E_i = I$, where the sum converges in the strong operator topology. In this case the probability that outcome i occurs in the state ρ is $P_\rho(E_i)$ and the postmeasurement state given that i occurs is $E_i^{1/2}\rho E_i^{1/2}/\mathrm{tr}(\rho E_i)$. Moreover, the resulting state after the measurement is executed but no observation is performed is given by

$$\phi(\rho) = \sum E_i^{1/2}\rho E_i^{1/2}.$$

More general quantum measurements will be discussed later when we consider quantum operations. Notice that ϕ is an affine map from $\mathcal{D}(\mathcal{H})$ into $\mathcal{D}(\mathcal{H})$. Also, ϕ extends to a unital, trace-

preserving, completely positive map on $\mathcal{B}(\mathcal{H})$. (Detailed definitions will be given subsequently.) An important physical question is whether the measurement disturbs the state ρ. The fact that the measurement does not disturb ρ is given mathematically by the equation $\phi(\rho)=\rho$. It is shown in Ref. 5 that $\phi(\rho)=\rho$ if and only if ρ commutes with every E_i, $i=1,2,\ldots$. We then say that ρ is **compatible** with E_i, $i=1,2,\ldots$, and this result is called the generalized Lüders theorem.

In the dual picture, the probability that an effect A occurs in the state ρ given that the measurement was performed is

$$P_{\phi(\rho)}(A)=\mathrm{tr}\left[A\sum\ E_i^{1/2}\rho E_i^{1/2}\right]=\mathrm{tr}\left(\sum\ E_i^{1/2}AE_i^{1/2}\rho\right).$$

If A is not disturbed by the measurement in any state we have

$$\sum\ E_i^{1/2}AE_i^{1/2}=A. \tag{1.1}$$

Again, defining $\phi(A)=\Sigma E_i^{1/2}AE_i^{1/2}$, Eq. (1.1) reduces to $\phi(A)=A$. But, now A may not be in $\mathcal{T}(\mathcal{H})^+$ and the previous proof of the generalized Lüders theorem does not go through. In fact, we shall show that $\phi(A)=A$ does not necessarily imply that A is compatible with E_i, $i=1,2,\ldots$. (This solves an open problem posed in Refs. 5 and 3.) Another way that (1.1) comes about is from the law of total probability, which is given by

$$\mathrm{tr}(\rho A)=P_\rho(A)=\sum\ P_\rho(E_i)P_\rho(A|E_i)=\sum\ \mathrm{tr}(\rho E_i)\frac{\mathrm{tr}(E_i^{1/2}\rho E_i^{1/2}A)}{\mathrm{tr}(\rho E_i)}=\mathrm{tr}\left(\rho\sum\ E_i^{1/2}AE_i^{1/2}\right).$$

If this law holds for every $\rho\in\mathcal{D}(\mathcal{H})$, we again obtain $\phi(A)=A$.

An application of our result can be found in axiomatic quantum field theory. Suppose a measurement $\{E_i:i=1,2,\ldots\}$ is performed in a bounded spacetime region X and $A\in\mathcal{E}(\mathcal{H})$ is a measurement performed in another space–time region Y that is spacelike separated from X. According to Einstein causality, the measurement in X should not disturb A so that $\phi(A)=A$. But, applying our result, A may not be compatible with E_i, $i=1,2,\ldots$. Thus, the axiom of local commutativity does not follow from Einstein causality. We conclude that this axiom may be too strong and it should be replaced by a weaker axiom.

More general measurements are frequently considered in quantum dynamics, quantum computation, and quantum information theory.[1,2,6] Let $A_i\in\mathcal{B}(\mathcal{H})$, $i=1,2,\ldots$, and let $\mathcal{A}=\{A_i,A_i^*:i=1,2,\ldots\}$. Assume for now that $\Sigma A_i^*A_i=I$ (trace preserving) and that $\Sigma A_iA_i^*=I$ (unitality). (The unitality condition is sometimes omitted and the trace-preserving condition is sometimes relaxed to $\Sigma A_i^*A_i\leqslant I$.) For $B\in\mathcal{B}(\mathcal{H})$, define $\phi_\mathcal{A}(B)=\Sigma A_iBA_i^*$. It can be shown that $\phi_\mathcal{A}:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ is a normal, completely positive map. Moreover, $\phi_\mathcal{A}(I)=I$ (unital) and $\mathrm{tr}[\phi_\mathcal{A}(B)]=\mathrm{tr}(B)$ for all $\mathcal{B}\in\mathcal{T}(\mathcal{H})$ (trace preserving). In fact, if $\mathcal{H}$ is separable, then any map satisfying these conditions has the form $\phi_\mathcal{A}$ for some $\mathcal{A}$.[2] There are various interpretations for $\phi_\mathcal{A}$. For example, $\phi_\mathcal{A}$ can describe a quantum measurement, an interaction of a quantum system with an environment followed by a unitary evolution, a noisy quantum channel, or a quantum error correction map. We call $\phi_\mathcal{A}$ a **quantum operation** and we call $\mathcal{A}$ the set of **operation elements** for $\phi_\mathcal{A}$. Note that our previous examples are a special type of quantum operations. This can be seen by letting $A_i=E_i^{1/2}$.

We say that $B\in\mathcal{B}(\mathcal{H})$ is a $\phi_\mathcal{A}$ **fixed point** if $\phi_\mathcal{A}(B)=B$, and denote the set of $\phi_\mathcal{A}$ fixed points by $\mathcal{B}(\mathcal{H})^{\phi_\mathcal{A}}$. It is clear that the commutant $\mathcal{A}'\subseteq\mathcal{B}(\mathcal{H})^{\phi_\mathcal{A}}$. The main purpose of this paper is to study $\mathcal{B}(\mathcal{H})^{\phi_\mathcal{A}}$ and the question of whether $\mathcal{B}(\mathcal{H})^{\phi_\mathcal{A}}=\mathcal{A}'$. We shall show that in general $\mathcal{B}(\mathcal{H})^{\phi_\mathcal{A}}\neq\mathcal{A}'$ and shall give sufficient conditions under which equality holds. For example, in quantum computation it is assumed that $\dim\mathcal{H}<\infty$. For this case we shall show that $\mathcal{B}(\mathcal{H})^{\phi_\mathcal{A}}=\mathcal{A}'$. Thus, a noisy quantum channel does not disturb a state ρ if and only if ρ is compatible with the operation elements A_i, $i=1,2,\ldots$. Related results and methods may be found in Ref. 7.

II. COMPLETELY POSITIVE MAPS

This section studies completely positive maps on von Neumann algebras. Such maps give a unifying generalization of quantum operations and many of our results will follow from these general considerations.

An **operator system** is a linear subspace of $\mathcal{B}(\mathcal{H})$ that is closed under the involution * and contains the identity operator. Let $\mathcal{M}_k$ be the C^* algebra of $k\times k$ complex matrices which we identify with $\mathcal{B}(\mathbb{C}^k)$. For an operator system $\mathcal{S}\subseteq\mathcal{B}(\mathcal{H})$ we consider $\mathcal{S}\otimes\mathcal{M}_k$ embedded in the C^* algebra $\mathcal{B}(\mathcal{H})\otimes\mathcal{M}_k$. Then, $\mathcal{S}\otimes\mathcal{M}_k$ carries the natural operator norm and the natural operator order. Given operator systems $\mathcal{V}$ and $\mathcal{W}$ and a linear map $\phi:\mathcal{V}\to\mathcal{W}$, for any integer $k\geqslant 1$, there is defined a linear map $\phi_k:\mathcal{V}\otimes\mathcal{M}_k\to\mathcal{W}\otimes\mathcal{M}_k$ given by

$$\phi_k(v)=[\phi(v_{ij})],\quad \text{where}\quad v=[v_{ij}]\in\mathcal{V}\otimes\mathcal{M}_k,\quad i,j=1,\ldots,k.$$

We then have a nondecreasing sequence of operator norms

$$\|\phi\|=\|\phi_1\|\leqslant\|\phi_2\|\leqslant\|\phi_3\|\leqslant\cdots.$$

The map ϕ is called **completely bounded** if

$$\|\phi\|_{\mathrm{cb}}=\sup_{k\geqslant 1}\|\phi_k\|<\infty.$$

It follows that $\|\cdot\|_{\mathrm{cb}}$ is a norm on the linear space $\mathcal{CB}(\mathcal{V},\mathcal{W})$ of completely bounded maps from $\mathcal{V}$ into $\mathcal{W}$. If $\|\phi\|_{\mathrm{cb}}\leqslant 1$, then ϕ is called **completely contractive**. If ϕ_k is positive for all k, then ϕ is called **completely positive**. Any completely positive map ϕ is completely bounded and

$$\|\phi(I)\|=\|\phi\|=\|\phi\|_{\mathrm{cb}}.$$

In particular, if $\phi(I)=I$ then ϕ is completely contractive.[8]

Now, let $\mathcal{V}\subseteq\mathcal{B}(\mathcal{H})$ be an operator system. A map $\psi:\mathcal{V}\to\mathcal{V}$ is **idempotent** if $\psi\circ\psi=\psi$. A completely contractive idempotent map ψ from $\mathcal{B}(\mathcal{H})$ onto $\mathcal{V}$ is called a **projection** onto $\mathcal{V}$. If there exists a projection from $\mathcal{B}(\mathcal{H})$ onto $\mathcal{V}$, then $\mathcal{V}$ is **injective**. A linear map ψ from a C^* subalgebra $\mathcal{M}$ into itself is a **conditional expectation** if ψ is a positive idempotent, its range is a C^* subalgebra $\mathcal{N}$ of $\mathcal{M}$ and $\psi(CB)=\psi(C)B$ and $\psi(BC)=B\psi(C)$ for every $B\in\mathcal{N}$ and $C\in\mathcal{M}$. A C^* algebra $\mathcal{M}\subseteq\mathcal{B}(\mathcal{H})$ is injective if and only if there exists a conditional expectation on $\mathcal{B}(\mathcal{H})$ with range $\mathcal{M}$.[9] A von Neumann algebra $\mathcal{M}$ is injective if and only if $\mathcal{M}'$ is injective.[10,11] A **state** on a C^* algebra $\mathcal{M}$ is a positive linear functional $\omega:\mathcal{M}\to\mathbb{C}$ with norm $\|\omega\|=1$. [If $\mathcal{M}$ has a unit I, the condition $\|\omega\|=1$ is equivalent to $\omega(I)=1$.] We say that ω is **faithful** if $\omega(A^*A)=0$ implies $A=0$.

In the sequel we shall need the following theorem of Choi.[12]

Theorem 2.1: *Suppose that ϕ is a completely contractive and completely positive map from a unital C^* algebra $\mathcal{C}$ into $\mathcal{B}(\mathcal{H})$. Then, $\phi(C)^*\phi(C)\leqslant\phi(C^*C)$ for every $C\in\mathcal{C}$. Moreover, if $\phi(C)^*\phi(C)=\phi(C^*C)$ for some $C\in\mathcal{C}$, then for all $B\in\mathcal{C}$ we have $\phi(BC)=\phi(B)\phi(C)$, $\phi(CB)=\phi(C)\phi(B)$.*

If $\phi:\mathcal{M}\to\mathcal{M}$ is a unital completely positive map and ω is a state on $\mathcal{M}$, then $\omega\circ\phi$ is again a state on $\mathcal{M}$. We say that ω is **ϕ-invariant** of $\omega\circ\phi=\omega$. We say that $A\in\mathcal{M}$ is a **fixed point** of ϕ if $\phi(A)=A$ and denote the set of fixed points of ϕ by $\mathcal{M}^\phi$.[7] Notice that $\mathcal{M}^\phi$ is an operator system. In general, $\mathcal{M}^\phi$ is not an algebra.[7] It is easy to check that

$$\mathcal{I}(\phi)=\{A\in\mathcal{M}:\phi(AB)=A\phi(B),\phi(BA)=\phi(B)A\ \text{ for every }\ B\in\mathcal{M}\}$$

is a C^* algebra in $\mathcal{M}$ and $\mathcal{I}(\phi)\subseteq\mathcal{M}^\phi$. Moreover, if ϕ is weakly continuous, then $\mathcal{I}(\phi)$ is a von Neumann subalgebra of $\mathcal{M}$ and $\mathcal{M}^\phi$ is a weakly closed operator system.

Lemma 2.2: The following statements are equivalent. (a) $\mathcal{M}^\phi=\mathcal{I}(\phi)$. (b) $\mathcal{M}^\phi$ *is a C^* algebra.* (c) If $A\in\mathcal{M}^\phi$, *then* $A^*A\in\mathcal{M}^\phi$.

Proof: (a)⇒(b)⇒(c) is clear. To prove that (c) implies (a) suppose (c) holds and $A \in \mathcal{M}^{\phi}$. Then, $A^*A \in \mathcal{M}^{\phi}$ so that

$$\phi(A)^*\phi(A) = A^*A = \phi(A^*A).$$

It follows from Theorem 2.1 that for every $B \in \mathcal{M}$ we have

$$\phi(AB) = \phi(A)\phi(B) = A\phi(B),$$

and

$$\phi(BA) = \phi(B)\phi(A) = \phi(B)A.$$

Hence, $A \in \mathcal{I}(\phi)$. □

Theorem 2.3: *If ϕ admits a faithful invariant state ω,* then $\mathcal{M}^{\phi} = \mathcal{I}(\phi)$.

Proof: Suppose that $A \in \mathcal{M}^{\phi}$. By Theorem 2.1 we have

$$A^*A = \phi(A)^*\phi(A) \leqslant \phi(A^*A),$$

so that $\phi(A^*A) - A^*A \in \mathcal{M}^{+}$. Since

$$\omega[\phi(A^*A) - A^*A] = \omega \circ \phi(A^*A) - \omega(A^*A) = 0,$$

we conclude that $\phi(A^*A) = A^*A$. Hence, $A^*A \in \mathcal{M}^{\phi}$. Applying Lemma 2.2 we have that $\mathcal{M}^{\phi} = \mathcal{I}(\phi)$. □

For $\phi: \mathcal{M} \to \mathcal{M}$ we denote the map obtained by composing ϕ with itself n times by ϕ^n. If $\psi: \mathcal{M} \to \mathcal{M}$ we denote the composition $\psi \circ \phi$ by $\psi\phi$.

Theorem 2.4: *Let $\phi: \mathcal{M} \to \mathcal{M}$ be a weakly continuous, unital, completely positive map.* (a) *There exists an idempotent, unital, completely positive map $\psi: \mathcal{M} \to \mathcal{M}$ with range* $\mathrm{ran}(\psi) = \mathcal{M}^{\phi}$. (b) $\mathcal{M}^{\phi} = \mathcal{I}(\phi)$ *if and only if ψ is a conditional expectation.* (c) *If $\mathcal{M} = \mathcal{B}(\mathcal{H})$ and $\mathcal{M}^{\phi} = \mathcal{I}(\phi)$, then $\mathcal{I}(\phi)$ is an injective von Neumann algebra.*

Proof: (a) Let $\psi_n: \mathcal{M} \to \mathcal{M}$ be the sequence of Cesàro means

$$\psi_n = \frac{1}{n} \sum_{i=1}^{n} \phi^i.$$

Then, ψ_n, $n = 1,2,\ldots$, are unital completely positive (and hence completely contractive) maps. Since $\mathcal{M}$ has a predual, it follows from the Alaoglu theorem that the closed unit ball of $\mathcal{M}$ is compact in the weak * topology. Hence, the closed unit ball of $\mathcal{CB}(\mathcal{M})$ is compact in the point-weak topology. It follows that there exists a subsequence ψ_{n_k} and a unital completely positive map $\psi: \mathcal{M} \to \mathcal{M}$ such that

$$w\text{-}\lim_{k \to \infty} \psi_{n_k}(A) = \psi(A) \tag{2.1}$$

for every $A \in \mathcal{M}$. For any integer $n \geqslant 1$ we have

$$\|\psi_n - \phi\psi_n\| = \frac{1}{n}\|\phi - \phi^{n+1}\| \leqslant \frac{2}{n}, \tag{2.2}$$

and hence $\psi_n - \phi\psi_n$ converges uniformly to 0. For any $k \geqslant 1$ we have

$$\phi\psi - \psi = (\phi\psi - \phi\psi_{n_k}) + (\phi\psi_{n_k} - \psi_{n_k}) + (\psi_{n_k} - \psi).$$

Note that the point-weak limit of the expression of the right side is 0 as $n_k \to \infty$. Indeed, $\psi_{n_k} - \psi \to 0$ by the definition of ψ, $\psi_{n_k} - \phi\psi_{n_k} \to 0$ by (2.2) and

$$\phi\psi - \phi\psi_{n_k} = \phi(\psi - \psi_{n_k}) \to 0,$$

because ϕ is weakly continuous. In a similar way we have $\psi\phi = \psi$ and thus

$$\phi\psi = \psi\phi = \psi. \tag{2.3}$$

By induction we see that $\phi^k\psi = \psi\phi^k = \psi$ for all $k \geqslant 1$, and hence

$$\psi_{n_k}(\psi(A)) = \psi(A), \tag{2.4}$$

for all $A \in \mathcal{M}$. Taking the weak limit in (2.4) as $k \to \infty$, we conclude that ψ is idempotent. In particular, $\mathrm{ran}(\psi) = \mathcal{M}^{\psi}$. Applying (2.3), we have $\mathrm{ran}(\psi) \subseteq \mathcal{M}^{\phi}$. To prove the converse inclusion, let $A \in \mathcal{M}^{\phi}$. Then $\psi_{n_k}(A) = A$ for all $k \geqslant 1$ and by (2.1) we have $\psi(A) = A$. Hence, $\mathrm{ran}(\psi) = \mathcal{M}^{\phi}$.

(b) If $\mathcal{M}^{\phi} = \mathcal{I}(\phi)$, then $\mathrm{ran}(\psi) = \mathcal{M}^{\phi}$ is a von Neumann subalgebra of $\mathcal{M}$. For $A \in \mathrm{ran}(\psi)$, we have

$$\psi(A)^*\psi(A) = A^*A = \psi(A^*A).$$

Hence, by Theorem 2.1 we obtain

$$\psi(AB) = \psi(A)\psi(B) = A\psi(B),$$

and

$$\psi(BA) = \psi(B)\psi(A) = \psi(B)A$$

for all $B \in \mathcal{M}$. Thus, ψ is a conditional expectation. Conversely, if ψ is a conditional expectation, then $\mathcal{M}^{\phi} = \mathrm{ran}(\psi)$ is a C^* subalgebra of $\mathcal{M}$, so applying Lemma 2.2, we conclude that $\mathcal{M}^{\phi} = \mathcal{I}(\phi)$.

(c) If $\mathcal{M}^{\phi} = \mathcal{I}(\phi)$, then by (b), ψ is a conditional expectation with $\mathrm{ran}(\psi) = \mathcal{I}(\phi)$ so $\mathcal{I}(\phi)$ is an injective von Neumann algebra. □

Corollary 2.5: Let $\phi: \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be a weakly continuous, unital, completely positive map. If $\mathcal{I}(\phi)$ is not injective, then $\mathcal{B}(\mathcal{H})^{\phi} \neq \mathcal{I}(\phi)$.

III. QUANTUM OPERATIONS

Let $\mathcal{A}$ be a set of operators $\mathcal{A} = \{A_i, A_i^* : i = 1,2,\ldots\}$, where $A_i \in \mathcal{B}(\mathcal{H})$ satisfy $\Sigma A_i A_i^* \leqslant I$. A map $\phi: \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ of the form $\phi_{\mathcal{A}}(B) = \Sigma A_i B A_i^*$ is called a **quantum operation**. If $B \geqslant 0$ then this series gives an increasing sequence of positive operators that is bounded above by $\|B\|I$ so it converges in the strong operator topology. It follows that the series converges in the strong operator topology for any $B \in \mathcal{B}(\mathcal{H})$. It is easy to see that a quantum operation is completely positive. If $\phi_{\mathcal{A}}(I) = I$ or equivalently if $\Sigma A_i A_i^* = I$, then $\phi_{\mathcal{A}}$ is **unital**. If $\Sigma A_i^* A_i = I$ then $\phi_{\mathcal{A}}$ is **trace preserving**. If the A_i are self-adjoint then $\phi_{\mathcal{A}}$ is **self-adjoint**. An important example of a self-adjoint quantum operation is **Lüders operation**

$$L_{\mathcal{A}}(B) = \sum A_i^{1/2} B A_i^{1/2},$$

where $A_i \geqslant 0$ and $\Sigma A_i = I$. A quantum operation $\phi_{\mathcal{A}}$ is **faithful** if $\phi_{\mathcal{A}}(B^*B) = 0$ implies that $B = 0$.

Theorem 3.1: *Let $\phi_{\mathcal{A}}$ be a quantum operation.* (a) *$\phi_{\mathcal{A}}$ is a weakly continuous completely positive map.* (b) *If $\phi_{\mathcal{A}}$ is trace preserving then $\phi_{\mathcal{A}}$ is faithful and* $\mathrm{tr}(\phi_{\mathcal{A}}(B)) = \mathrm{tr}(B)$ *for every $B \in \mathcal{T}(\mathcal{H})$.*

Proof: (a) Let ℓ_2 denote the Hilbert space of square summable complex sequences and let $\ell_2(\mathcal{H})=\ell_2\otimes\mathcal{H}$ be the Hilbert space of square summable sequences with elements in $\mathcal{H}$. Let $V:\mathcal{H}\to\ell_2(\mathcal{H})$ be the linear operator defined by

$$Vh=(A_1^*h,A_2^*h,\ldots).$$

Now, $V\in\mathcal{B}(\mathcal{H},\ell_2(\mathcal{H}))$ because

$$\|Vh\|^2=\sum\ \langle A_i^*h,A_i^*h\rangle=\sum\ \langle A_iA_i^*h,h\rangle=\left\langle\sum\ A_iA_i^*h,h\right\rangle\leqslant\|h\|^2.$$

The adjoint $V^*\in\mathcal{B}(\ell_2(\mathcal{H}),\mathcal{H})$ is given by

$$V^*(h_1,h_2,\ldots)=\sum\ A_ih_i.$$

It follows that $\phi_{\mathcal{A}}(B)=V^*(I\otimes B)V$ for all $B\in\mathcal{B}(\mathcal{H})$. Since the map $B\mapsto I\otimes B$ from $\mathcal{B}(\mathcal{H})$ to $\mathcal{B}(\ell_2(\mathcal{H}))$ is weakly continuous[13] and completely positive, it follows that $\phi_{\mathcal{A}}$ is weakly continuous and completely positive.

(b) Suppose that $\phi_{\mathcal{A}}$ is trace preserving. To show $\phi_{\mathcal{A}}$ is faithful, suppose $\phi_{\mathcal{A}}(B^*B)=0$. Then, for every $h\in\mathcal{H}$ we have

$$0=\langle\phi_{\mathcal{A}}(B^*B)h,h\rangle=\left\langle\sum\ A_iB^*BA_i^*h,h\right\rangle=\sum\ \langle BA_i^*h,BA_i^*h\rangle.$$

Hence, $BA_i^*h=0$ for every $h\in\mathcal{H}$ so that $BA_i^*=0$. But, then

$$B=B\sum\ A_i^*A_i=0.$$

Finally, let $B\in\mathcal{T}(\mathcal{H})^+$. Then, the operators $A_iBA_i^*$ and $A_i^*A_iB$ are trace class and

$$\mathrm{tr}\left(\sum_{i=1}^n A_iBA_i^*\right)=\mathrm{tr}\left(\sum_{i=1}^n A_i^*A_iB\right)\leqslant\left\|\sum_{i=1}^n A_i^*A_i\right\|\mathrm{tr}(B)\leqslant\mathrm{tr}(B).$$

Since $\Sigma_{i=1}^n A_iBA_i^*$ is a nondecreasing sequence of positive operators converging strongly to $\phi_{\mathcal{A}}(B)$, and since the trace is continuous with respect to such sequences, we have

$$\mathrm{tr}(\phi_{\mathcal{A}}(B))=\lim_{n\to\infty}\mathrm{tr}\left(\sum_{i=1}^n A_iBA_i^*\right)\leqslant\mathrm{tr}(B).$$

Hence, $\phi_{\mathcal{A}}(B)\in\mathcal{T}(\mathcal{H})^+$. Again by the continuity of trace on bounded nondecreasing sequences we have

$$\mathrm{tr}(\phi_{\mathcal{A}}(B))=\lim_{n\to\infty}\mathrm{tr}\left(\sum_{i=1}^n A_i^*A_iB\right)=\mathrm{tr}\left(\sum_{i=1}^\infty A_i^*A_iB\right)=\mathrm{tr}(B).$$

The result for arbitrary $B\in\mathcal{T}(\mathcal{H})$ now follows. □

Let $\phi_{\mathcal{A}}$ be a unital quantum operation and define the fixed point set $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ as before. We then have the von Neumann algebras $\mathcal{I}(\phi_{\mathcal{A}})$ and $\mathcal{A}'$ as well as the weakly closed operator system $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$, and it is clear that

$$\mathcal{A}'\subseteq\mathcal{I}(\phi_{\mathcal{A}})\subseteq\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}.$$

We are now interested in when these sets coincide; that is, when $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} \subseteq \mathcal{A}'$. The next theorem generalizes a result in Ref. 5 and has essentially the same proof.

Theorem 3.2: *Let $\phi_{\mathcal{A}}$ be a self-adjoint quantum operation. If $B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ is positive and has pure point spectrum which can be totally ordered in decreasing order, then $B \in \mathcal{A}'$.*

Proof: Let h be a unit eigenvector of B corresponding to the largest eigenvalue $\lambda_1 = \|B\|$. Then, $\phi_{\mathcal{A}}(B) = B$ implies that

$$\lambda_1 = \sum \langle BA_i h, A_i h\rangle \leqslant \|B\| \sum \|A_i h\|^2 = \lambda_1 \sum \langle A_i^2 h, h\rangle \leqslant \lambda_1 .$$

Since $\langle BA_i h, A_i h\rangle \leqslant \lambda_1 \langle A_i^2 h, h\rangle$, it follows that

$$\langle (\lambda_1 I - B) A_i h, A_i h\rangle = 0.$$

Hence, $(\lambda_1 I - B) A_i h = 0$ for every eigenvector h corresponding to λ_1. Thus, A_i leaves the λ_1-eigenspace invariant. Letting P_1 be the corresponding spectral projection of B, we have $P_1 A_i P_1 = A_i P_1$, which implies that $A_i P_1 = P_1 A_i$, $i = 1,2,\ldots$. Now, $B = \lambda_1 P_1 + B_1$ where B_1 is a positive operator with a largest eigenvalue. Since

$$\lambda_1 P_1 + B_1 = B = \phi_{\mathcal{A}}(B) = \lambda_1 \phi_{\mathcal{A}}(P_1) + \phi_{\mathcal{A}}(B_1) = \lambda_1 P_1 + \phi_{\mathcal{A}}(B_1),$$

we have $\phi_{\mathcal{A}}(B_1) = B_1$. Proceeding by induction, $B \in \mathcal{A}'$. □

We shall show later that Theorem 3.2 cannot be extended to an arbitrary positive $B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$. Moreover, it cannot be extended to a non-self-adjoint $\phi_{\mathcal{A}}$ even in the case where B is positive with finite spectrum and $\mathcal{A}$ contains only two operation elements. The next result follows from Lemmas 3.1 and 3.3 of Ref. 7. However, we present a simpler and more algebraic proof.

Lemma 3.3: If $\phi_{\mathcal{A}}$ is a unital quantum operation, then the following statements are equivalent. (a) $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} = \mathcal{A}'$. (b) $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ *is a von Neumann algebra.* (c) $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} = \mathcal{I}(\phi_{\mathcal{A}})$. (d) If $B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$, *then* $B^*B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$.

Proof: (a)⇒(b) is clear, (b)⇒(c) follows from Lemma 2.2, and (c)⇒(d) is clear. To show that (d) implies (a) assume that (d) holds and $B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$. Then, $B^*B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$. Notice that

$$\begin{aligned} 0 \leqslant [B,A_i][B,A_i]^* &= (BA_i - A_iB)(A_i^*B^* - B^*A_i^*) \\ &= BA_iA_i^*B^* + A_iBB^*A_i^* - A_iBA_i^*B^* - BA_iB^*A_i^* . \end{aligned}$$

Summing over i yields

$$0 \leqslant \sum [B,A_i][B,A_i]^* = BB^* + \phi_{\mathcal{A}}(BB^*) - \phi_{\mathcal{A}}(B)B^* - B\phi_{\mathcal{A}}(B^*) = \phi_{\mathcal{A}}(BB^*) - BB^* = 0.$$

Hence, $[B,A_i] = 0$ for all $i = 1,2,\ldots$. In a similar way, we have $[B,A_i^*] = 0$. Hence, $B \in \mathcal{A}'$ so that $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} = \mathcal{A}'$. □

Corollary 3.4: Let $\phi_{\mathcal{A}}$ be a unital quantum operation. If $B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$, then $B \in \mathcal{A}'$ if and only if $B^*B, BB^* \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$.

An operator $W \in \mathcal{T}(\mathcal{H})$ is **faithful** if for any $A \in \mathcal{B}(\mathcal{H})$, $\mathrm{tr}(W^*A^*AW) = 0$ implies $A = 0$.

Theorem 3.5: *Let $\phi_{\mathcal{A}}$ be a trace preserving, unital, quantum operation.*
(a) If $\dim(\mathcal{H}) < \infty$, *then* $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} = \mathcal{A}'$. (b) *If there exists a faithful operator* $W \in \mathcal{T}(\mathcal{H}) \cap \mathcal{A}'$, *then* $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} = \mathcal{A}'$. (c) *If* $B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ *and* $B = C + D$ *for* $C \in \mathcal{A}'$, $D \in \mathcal{T}(\mathcal{H})$, *then* $B \in \mathcal{A}'$. (d) $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} \cap \mathcal{T}(\mathcal{H}) = \mathcal{A}' \cap \mathcal{T}(\mathcal{H})$.

Proof: (a) If $\dim(\mathcal{H}) = n < \infty$, then $\omega(B) = \mathrm{tr}(B)/n$ is a faithful ϕ-invariant state. The result follows from Theorem 2.3 and Lemma 3.3. (b) By the proof of Lemma 3.3, if $B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ then

$$\phi_{\mathcal{A}}(B^*B) - B^*B \geqslant 0.$$

Since $W \in \mathcal{T}(\mathcal{H}) \cap \mathcal{A}'$, by Theorem 3.1 (b) we have

$$\text{tr}\,[W^*(\phi_{\mathcal{A}}(B^*B) - B^*B)W] = \text{tr}\,[\phi_{\mathcal{A}}(W^*B^*BW)] - \text{tr}(W^*B^*BW) = 0.$$

Hence, $\phi_{\mathcal{A}}(B^*B) = B^*B$ so that $B^*B \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$. Applying Lemma 3.3 gives $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} = \mathcal{A}'$. (c) Since

$$C + D = \phi_{\mathcal{A}}(C + D) = \phi_{\mathcal{A}}(C) + \phi_{\mathcal{A}}(D) = C + \phi_{\mathcal{A}}(D),$$

we have $D \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$. Now, $D^*D \in \mathcal{T}(\mathcal{H})$ and by the proof of Lemma 3.3

$$\phi_{\mathcal{A}}(D^*D) - D^*D \geqslant 0.$$

Since $\phi_{\mathcal{A}}$ is trace preserving, we have

$$\text{tr}\,[\phi_{\mathcal{A}}(D^*D) - D^*D] = 0.$$

Hence, $\phi_{\mathcal{A}}(D^*D) = D^*D$ so that $D^*D \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$. Similarly, $DD^* \in \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ so by Corollary 3.4, $D \in \mathcal{A}'$. Hence, $B \in \mathcal{A}'$. (d) follows from (c). □

The next result follows from Theorem 2.4 and Lemma 3.3.

Theorem 3.6: *Let $\phi_{\mathcal{A}}$ be a unital quantum operation.* (a) *There exists an idempotent, unital, completely positive map $\psi: \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ with* $\text{ran}(\psi) = \mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$. (b) $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} = \mathcal{A}'$ *if and only if ψ is a conditional expectation.* (c) *If $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} = \mathcal{A}'$ then $\mathcal{A}'$ is an injective von Neumann algebra.*

IV. EXAMPLE

It follows from Theorem 3.6(c) that if $\mathcal{A}'$ is not injective then $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} \neq \mathcal{A}'$. We can apply this observation to obtain examples for various conjectures. For instance, the following counter-example shows: (a) If $\phi_{\mathcal{A}}(B) = \Sigma A_i^{1/2} B A_i^{1/2}$, $A_i \geqslant 0$, $\Sigma A_i = I$, is a Lüders operation, then $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} \neq \mathcal{A}'$ in general. (This answers a question posed in Refs. 5 and 3.) (b) If $\phi_{\mathcal{A}}(B) = A_1 B A_1^* + A_2 B A_2^*$ is a trace-preserving, unital, quantum operation, then $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} \neq \mathcal{A}'$ in general. (It has been shown that if A_1 and A_2 are positive, then $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}} = \mathcal{A}'$.[5,3])

Example: Let $\mathbb{F}_2$ be the free group on two generators g_1, g_2 with identity e. It is clear that $\mathbb{F}_2$ is countable. Let $\mathcal{H} = \ell_2(\mathbb{F}_2)$ be the separable complex Hilbert space

$$\mathcal{H} = \ell_2(\mathbb{F}_2) = \left\{ f: \mathbb{F}_2 \to \mathbb{C}: \sum |f(x)|^2 < \infty \right\}.$$

For $x \in \mathbb{F}_2$ define $\delta_x: \mathbb{F}_2 \to \mathbb{C}$ by

$$\delta_x(y) = \begin{cases} 1 & \text{if } y = x \\ 0 & \text{if } y \neq x \end{cases}.$$

Then $\{\delta_x : x \in \mathbb{F}_2\}$ is an orthonormal basis for $\mathcal{H}$. Define the unitary operators U_1, U_2 on $\mathcal{H}$ by $U_1 \delta_x = \delta_{g_1 x}$, $U_2 \delta_x = \delta_{g_2 x}$. The von Neumann algebra generated by U_1 and U_2 is denoted by $\mathcal{N} = L(\mathbb{F}_2)$. It is known that $\mathcal{N}$ and hence $\mathcal{N}'$ are not injective.[14,15]

Lemma 4.1: Suppose $B \in \mathcal{B}(\mathcal{H})$ has the form $B\delta_x = \lambda_x \delta_x$, $0 \leqslant \lambda_x \leqslant 1$. Then, $B \in \mathcal{E}(\mathcal{H})$ and if $B \in \mathcal{N}'$, then $B = \lambda_e I$.

Proof: It is clear that $B \in \mathcal{E}(\mathcal{H})$. Now, suppose that $B \in \mathcal{N}'$. Then

$$\lambda_{g_1} \delta_{g_1} = B \delta_{g_1} = B U_1 \delta_e = U_1 B \delta_e = \lambda_e U_1 \delta_e = \lambda_e \delta_{g_1}.$$

Hence, $\lambda_{g_1} = \lambda_e$ and in a similar way

$$\lambda_{g_1^{-1}} = \lambda_{g_2} = \lambda_{g_2^{-1}} = \lambda_e.$$

Now, suppose $x\in\mathbb{F}_2$ has the form $x=g_1y$ for some $y\in\mathbb{F}_2$. Then

$$\lambda_x\delta_x=B\delta_x=B\delta_{g_1y}=BU_1\delta_y=U_1B\delta_y=\lambda_yU_1\delta_y=\lambda_y\delta_{g_1y}=\lambda_y\delta_x.$$

Hence, $\lambda_{g_1y}=\lambda_y$ for every $y\in\mathbb{F}_2$. Similarly

$$\lambda_{g_1^{-1}y}=\lambda_{g_2y}=\lambda_{g_2^{-1}y}=\lambda_y$$

for every $y\in\mathbb{F}_2$. Continuing by induction, we conclude that $\lambda_x=\lambda_e$ for every $x\in\mathbb{F}_2$. Hence, $B=\lambda_eI$. □

Let $A_1=2^{-1/2}U_1$ and $A_2=2^{-1/2}U_2$ and let $\mathcal{A}=\{A_1,A_2\}$. Then, $\mathcal{A}'=\mathcal{N}'$ and

$$A_1A_1^*+A_2A_2^*=A_1^*A_1+A_2^*A_2=I.$$

Thus, $\phi_{\mathcal{A}}$ is a trace-preserving, unital quantum operation. Now, a B of the form in Lemma 4.1 satisfies $B\in\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ if and only if

$$\tfrac{1}{2}\lambda_{g_1^{-1}x}+\tfrac{1}{2}\lambda_{g_2^{-1}x}=\lambda_x \tag{4.1}$$

for all $x\in\mathbb{F}_2$. Define $B\in\mathcal{B}(\mathcal{H})$ by $B\delta_x=\lambda_x\delta_x$ where $\lambda_x=0$ if x ends in g_2^{-1}, $\lambda_x=1$ if x ends in g_1^{-1}, and $\lambda_x=1/2$ otherwise. Then, it is easy to check that (4.1) is satisfied. Hence, $B\in\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ and by Lemma 4.1 $B\notin\mathcal{A}'$. Thus, $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}\neq\mathcal{A}'$.

Theorem 4.2: *There exists a Lüders operation $\phi_{\mathcal{A}}$ on $\mathcal{H}=\ell_2(\mathbb{F}_2)$ such that $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}\neq\mathcal{A}'$. More precisely, there exists a $B\in\mathcal{E}(\mathcal{H})$ such that $B\in\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ but $B\notin\mathcal{A}'$.*

Proof: By taking the real and imaginary parts of $U_1=V_1+iV_2$, $U_2=V_3+iV_4$, we see that $\mathcal{N}$ is generated by four self-adjoint operators V_1,V_2,V_3,V_4. Moreover, $\mathcal{N}$ is generated by the four positive operators $C_i=\|V_i\|I-V_i$, $i=1,2,3,4$. Let $A_i=C_i/4\|C_i\|$, $i=1,2,3,4$, and let $A_5=I-\Sigma_{i=1}^4A_i$. Then, $A_i\in\mathcal{E}(\mathcal{H})$, $i=1,\ldots,5$, $\Sigma A_i=I$ and $\mathcal{A}=\{A_i:i=1,\ldots,5\}$ generates $\mathcal{N}$. Now, $\phi_{\mathcal{A}}$ is a Lüders operation and since $\mathcal{N}'=\mathcal{A}'$ is not injective we have $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}\neq\mathcal{A}'$. Hence, there exists a $B\in\mathcal{B}(\mathcal{H})$ such that $B\in\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}\backslash\mathcal{A}'$. Now, the real part or the imaginary part B_1 of B also satisfies $B_1\in\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}\backslash\mathcal{A}'$. Letting $B_2=\|B_1\|I-B_1$ we see that $B_2\geqslant0$ and that $B_3=B_2/\|B_2\|\in\mathcal{E}(\mathcal{H})$. Moreover, $B_3\in\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}\backslash\mathcal{A}'$. □

Although the B in Theorem 4.2 exists, it appears to be quite difficult to construct a concrete example of such a B.

V. CONCLUDING REMARKS

We have seen that the injectivity of the commutant of the set of operation elements $\mathcal{A}'$ of a Lüders operation $\phi_{\mathcal{A}}$ plays a role in deciding whether the set of fixed points $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ coincides with $\mathcal{A}'$ or not. However, the following question remains: if $\mathcal{A}'$ is injective, does this imply that $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}=\mathcal{A}'$? On the other hand, it has been proved that for a Lüders operation with only two operation elements, we have $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}=\mathcal{A}'$.[5,3] In this case, $\mathcal{A}$ is commutative and it follows that $\mathcal{A}$ and $\mathcal{A}'$ are injective. It is then natural to ask whether the result is true for any commutative set of operation elements $\mathcal{A}$. Finally, we ask the following general question. Is it true that $\mathcal{B}(\mathcal{H})^{\phi_{\mathcal{A}}}$ is an injective envelope of either $\mathcal{A}'$ or $\mathcal{I}(\phi_{\mathcal{A}})$?[8]

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Classicality criteria

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We present two possible criteria quantifying the degree of classicality of an arbitrary (finite dimensional) dynamical system. The inputs for these criteria are the classical dynamical structure of the system together with the quantum and the classical data providing the two alternative descriptions of its initial time configuration. It is proved that a general quantum system satisfying the criteria up to some extend displays a time evolution consistent with the classical predictions up to some degree and thus it is argued that the criteria provide a suitable measure of classicality. The features of the formalism are illustrated through two simple examples. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1516626]

I. INTRODUCTION

It is generally accepted that quantum mechanics yields the most fundamental description of all physical systems. Such status requires the theory to provide a suitable description of every day classical like phenomena. However, quantum mechanics faces a considerable number of problems to explain the emergence of a classical domain. In a broad sense, this is called the problem of the semiclassical limit of quantum mechanics.[1–6]

This is a difficult topic not least because there are a variety of different ways of relating classical and quantum mechanics. The standard approach is to take the limit $\hbar \to 0$, or equivalently, the limit of a large number of particles $N \to \infty$. Under some general conditions one can derive the classical evolution from the quantum dynamics.[7] Alternatively, one may start with a set of quantum initial data with minimal spread and show that its quantum time evolution remains very peaked around the classical orbits. Coherent states[8] (and squeezed states[9,10]) have been extensively studied in this context.[11–17] It has been proved, using several different approaches and for a large class of dynamical systems, that coherent states evolve, up to a prescribed error and during a prescribed lapse of time, peaked around the classical paths.[14,16–18] Coherent states methods have also been used to prove that in the limit $\hbar \to 0$ and for times shorter than Eherenfest's time, the quantum and the classical predictions coincide exactly.[10,18–20] Related results have been obtained using the tools of pseudodifferential calculus[21–23] and microlocal analysis.[24–26] These have played an important part in several attempts to understand the semiclassical behavior of classically chaotic systems.[24,27]

Two other significant approaches are the Wigner (or more generally the quasidistributions)[28] and the dechoerent histories[3,4,29] approaches. The aim is to (either by identifying proper quantum phase space distributions, or by coupling the quantum system to a suitable environment) recover the classical statistical predictions from the quantum formulation of the system. All these views are of course not antagonic, but complementary, meaning that the classical behavior can emerge in a variety of different regimes.

Despite the importance of these results there are still several open problems in the field of the semiclassical limit of quantum mechanics. The common view is that classical mechanics is an approximate description of quantum mechanics. This approximation is not always valid. In fact, one expects it to be only valid for some particular set of quantum initial data and even in this case not for all dynamical systems (consider for instance a particle hitting a potential barrier). An

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important question is then what is the degree of validity of the classical approximation? Clearly this question does not have a single answer. It depends on the dynamical structure of the system and on the quantum and also the classical data providing the two alternative descriptions of the initial time configuration. Let us assume that we are given this information. Can we compare the classical and the quantum descriptions of the dynamical system and produce a statement about the degree of validity of the classical description? Or, in other words, can we produce a statement about the degree of classicality of the quantum description? The answer to these questions should be affirmative since we are given all the necessary ingredients. However, and despite the fact that the pertinence of these questions have been recognized by several authors,[3–5] the problem of establishing a measure of classicality is still lacking an unique solution.

Closely related to this topic is the problem of establishing a clear relation between the quantum initial state and the classical like behavior. Very few studies elaborate on this subject. Instead, one typically assumes a particular quantum initial state and works from there to prove the ''classicality'' of the quantum dynamics. A weak point in the procedure is that we are still lacking a precise definition of ''classicality.'' For instance in Refs. 10, 14, and 16 the aim is to provide minimal bounds for the spreading of the time evolution of a specific quantum initial data (typically a coherent or squeezed state). But the questions that remain are: are these results extendable to a wider class of quantum initial states, or more generally, what is the relation between the spreading of the wave function through time and the quantum initial state? And further, how is the spreading of the wave function related to classicality?

In this paper we attempt to provide a partial answer to these questions. In general terms we study the inverse problem of Refs. 10, 14, and 16: we start by imposing the bounds (which will be related to the error margins of the classical time evolution) and attempt to identify those initial quantum states which display a time evolution that satisfies these bounds for all times. In doing so we identify a (possible) set of general conditions an arbitrary, finite dimensional quantum system should satisfy so that it evolves in agreement with the classical predictions. These conditions will be of the form of a sequence of restrictions on the initial quantum state (the higher the classicality the more stringent the conditions) and provide the basic mathematical structure to construct a measure of classicality.

More precisely our approach will be as follows: We work in the context of the standard *Copenhagen* formulation of quantum mechanics[30–33] and consider a general dynamical system with N degrees of freedom. Its initial time configuration might be described by a set of quantum initial data or, alternatively, by a set of classical initial data. The classical description is given by a set of values a_i^0 for a complete set of classical observables a_i $(i=1\cdots 2N)$, together with their associated error margins δ_i. The quantum description is given by the initial time wave function $|\psi\rangle$. Classical mechanics states that the output of a measurement of an observable a_i will belong to the interval $[a_i^0-\delta_i, a_i^0+\delta_i]$. Quantum mechanics, in turn, states that there is some probability $p_i \leqslant 1$ that a measurement of the observable $\hat{a}_i$ yields a value inside the former interval. Clearly the two statements are not equivalent. However, there are a number of fairly intuitive ways by which one can measure the consistency (i.e., the agreement) of the two former descriptions of the initial time configuration. We will propose two such *consistency criteria* in Sec. II.

Unfortunately, the fact that the two descriptions of the initial time configuration are consistent up to some degree does not imply that the classical and the quantum descriptions of a future configuration will also be consistent up to the same degree. Our aim is then to identify the conditions that should be satisfied by the initial time configuration so that the degree of consistency is preserved through time evolution. These conditions are obtained (they are given by a set of relations between the classical initial data (a_i^0, δ_i) and the spreads of the initial wave function $|\psi\rangle$) and used to construct two alternative classicality criteria. Given the classical initial data these conditions constitute a sequence of growing restrictions on the functional form of the initial data wave function. When $|\psi\rangle$ satisfies the n first former conditions we say that $|\psi\rangle$ is *n-order classical*. When $|\psi\rangle$ satisfies the full set of conditions we say that $|\psi\rangle$ is a *classical limit initial data wave function*.

The main property of the classicality criteria is that if the classical and the quantum initial data satisfy the classicality criteria up to some degree then the time evolution of the classical initial data (obtained using classical mechanics) and the time evolution of the quantum initial data (obtained using quantum mechanics) will display a minimum degree of consistency for all times. Hence, the classicality criteria supply a suitable (although clearly not unique) measure of classicality that might be computed, for an arbitrary dynamical system, at the kinematical level.

These results are not limited to some specific type of systems displaying a particular dynamical behavior or having some particular quantum initial data. On the contrary, for an arbitrary dynamical system the classicality criteria can be used to determine the set of quantum initial data that displays a n-order classical time evolution (a quantum time evolution n-order consistent with the classical predictions). This will be done explicitly for the two physical examples presented in Secs. VI and VII.

Further applications of the criteria are given in Refs. 34, 35, and 36.

II. CONSISTENCY CRITERIA

Let us consider a general dynamical system with N degrees of freedom. The phase space T^*M has the structure of the cotangent bundle of the configuration space M, and henceforth will be also assumed to have the structure of a *flat* sympletic manifold. Therefore a global Darboux chart can be defined in T^*M. Let us choose a set of canonical variables $a_i, i=1\cdots 2N$ (where $a_i=q_i, i=1\cdots N$ and $a_i=p_{i-N}, i=N+1\cdots 2N$). They yield the sympletic structure as the 2-form $w=dq_i\wedge dp_i$.

The classical description of a specific time configuration of the system is given by a set of values a_i^0 for the complete set of observables a_i together with the associated error margins δ_i. The classical statement is that a measurement of a_i will yield a value a_i^1 belonging to the classical error interval $I_i=[a_i^0-\delta_i, a_i^0+\delta_i]$.

Alternatively, quantum mechanics describes the same configuration of the system with a wave function $|\psi\rangle$ belonging to the physical Hilbert space $\mathcal{H}$ and the quantum statement is that there is some probability $p(a_i)=\Sigma_k|\langle a_i,k|\psi\rangle|^2$ that a measurement of the observable $\hat{a}_i$ yields the value a_i (where the states $|a_i,k\rangle$ form a complete set of eigenvectors of $\hat{a}_i$ that spans the Hilbert space $\mathcal{H}$, a_i are the associated eigenvalues and k is the degeneracy index). For notational convenience we will assume that $\hat{A}$ displays a discrete spectrum, but all results can be easily rewritten for the continuous case.

A straightforward way of measuring the consistency between the two descriptions is given by the following criterion.

Definition: First consistency criterion. Let us calculate the probabilities p_i—generated by the wave function $|\psi\rangle$ in the representation of each of the observables $\hat{a}_i$, $i=1\cdots 2N$—that a measurement of $\hat{a}_i$ yields a value belonging to the classical error interval $I_i=[a_i^0-\delta_i, a_i^0+\delta_i]$, i.e.,

$$p_i=\sum_{a_i\in I_i,k}|\langle a_i,k|\psi\rangle|^2. \tag{1}$$

The minimum value of the set $\{p_i: i=1\cdots 2N\}$ provides a suitable measure of the consistency between the classical and the quantum descriptions of the configuration of the dynamical system. If this minimum value above is for instance p_0 we say that the classical and the quantum descriptions are p_0-*consistent*. Furthermore, if $p_0=1$ then the two descriptions are fully consistent and $|\psi\rangle$ is named a *classical limit wave function.* □

Another, probably less intuitive, consistency criterion is given by the following definition:

Definition: Second consistency criterion. Let $0\leqslant p<1$ be an arbitrary probability and let $M\in\mathcal{N}$. To each classical observable a_i we associate the set of intervals of the form:

$$I_i(p,M)=\left[a_i^0-\frac{\delta_i}{(1-p)^{1/(2M)}},a_i^0+\frac{\delta_i}{(1-p)^{1/(2M)}}\right]. \tag{2}$$

In each of the former intervals we can calculate the probability p_i generated by the wave function $|\psi\rangle$, in the representation of the corresponding quantum observable $\hat{a}_i$:

$$p_i(p,M)=\sum_{a_i\in I_i(p,M),k}|\langle a_i,k|\psi\rangle|^2. \tag{3}$$

For given values of the classical and quantum data a_i^0, δ_i, and $|\psi\rangle$ this probability is an exclusive function of p and M. The second consistency criterion is defined as follows: The classical and the quantum data, describing a given configuration of the dynamical system, are *M-order consistent* if and only if for all $0\leqslant p<1$ and for all $i=1\cdots 2N$ the condition $p_i(p,M)\geqslant p$ is satisfied, i.e.,

$$\sum_{a_i\in I_i(p,M),k}|\langle a_i,k|\psi\rangle|^2\geqslant p,\quad \forall_{p\in[0,1[},\forall_{i=1\cdots 2N}, \tag{4}$$

where $I_i(p,M)$ is given by (2). If $M=\infty$ the classical and the quantum descriptions are fully consistent, in which case $|\psi\rangle$ is a *classical limit* wave function. □

The former criterion provides a measure of how peaked is the wave function—in the representation of each of the quantum observables—around the classical error margin of the corresponding classical observable. This will became clear in the sequel (16).

As a first remark let us point out that the two alternative definitions of a classical limit wave function (using the first and the second consistency criterion) are, in fact, equivalent, i.e. $p=1\Leftrightarrow M=+\infty$, which in turn, is equivalent to the statement that

$$|\psi\rangle=\sum_{a_i\in I_i,k}\langle a_i,k|\psi\rangle|a_i,k\rangle,\quad \forall_{i=1\cdots 2N}, \tag{5}$$

where, as before $I_i=[a_i^0-\delta_i,a_i^0+\delta_i]$, (a_i^0,δ_i) is the classical data and $|a_i,k\rangle$ is the general eigenstate of the operator $\hat{a}_i$.

As a second remark let us notice that in some cases it is not possible to construct a wave function satisfying Eq. (5) exactly. One should keep in mind that Eq. (5) stands for the limit $M\rightarrow\infty$ or $p\rightarrow 1$ which may, or may not admit an explicit realization in terms of some wave function $|\psi\rangle$.

Some emphasis will be put in the study of the time evolution of a general classical limit initial data wave function. Although, for some systems, we might be unable to write $|\psi\rangle$ [satisfying (5)] explicitly, its time evolution can be obtained, in the Heisenberg picture, using the standard rules of quantum mechanics. This study will prove to be useful allowing us to develop a set of techniques that will later be used to obtain the classicality criteria and, in the sequel, to study physical systems with general initial data.

III. ERROR KET FRAMEWORK

Let us introduce dynamics by specifying a general Hamiltonian H. The quantum time evolution of an arbitrary fundamental observable $\hat{A}$ (with $\hat{A}=\hat{a}_i$ for some $i=1\cdots 2N$) is given by

$$\hat{A}(t)=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{t}{i\hbar}\right)^n[\cdots[[\hat{A},\hat{H}],\hat{H}]\cdots]. \tag{6}$$

Alternatively, the standard classical treatment of the same system provides the predictions

$$A(t)=\sum_{n=0}^{\infty}\frac{t^n}{n!}\{\cdots\ \{\{A,H\},H\}\cdots\ \},$$

$$\delta_A(t)=\sum_{n=1}^{+\infty}\frac{1}{n!}\sum_{k_1,\ldots,k_n=1}^{2N}\left|\frac{\partial^n A(t)}{\partial a_{k_1}\ldots\partial a_{k_n}}\right|\delta_{k_1}\cdots\ \delta_{k_n}, \tag{7}$$

where the error margins δ_{k_i} are taken at the initial time. Notice that, in general, it is possible to obtain more accurate predictions than those of (7), i.e., with smaller error margins. Such estimates have the disadvantage of requiring a case by case evaluation, while Eq. (7) is valid in general.

To avoid some possible misunderstandings we will, from now on, focus on the case of the second consistency criterion. In Sec. V our results will then be rewritten using the language of the first consistency criterion. Let us then assume that the classical and the quantum initial data are M-consistent. The question we would like to answer is then: which are the conditions that should be satisfied so that the quantum description of the system at a time t—given by the initial data wave function $|\psi\rangle$ in the representation of the observables $\hat{a}_i(t)$ (6)—is also M-consistent with the classical description given by (7)?

This is not an easy task. We start by presenting a framework that will later be used to give a precise answer to this question.

A. Definition and properties of $|E\rangle$ and Δ

Let us start by introducing the relevant definitions. Let $\hat{A}$ be an operator acting on the quantum Hilbert space $\mathcal{H}$. Let $|a,k\rangle$ be a complete set of eigenvectors of $\hat{A}$, with associated eigenvalues a and k being the degeneracy index. This set forms a complete orthogonal basis of $\mathcal{H}$. Finally, let $|\psi\rangle$ be the wave function describing the system.

Definition: Error Ket. We define the nth-order error ket $|E^n(\hat{A},\psi,a^0)\rangle$, as the quantity

$$|E^n(\hat{A},\psi,a^0)\rangle=(\hat{A}-a^0)^n|\psi\rangle, \tag{8}$$

where $n\in\mathcal{N}$, $a^0\in\mathcal{C}$ and $\hat{A}$ does not need to be self-adjoint. The error bra $\langle E^n(\hat{A},\psi,a^0)|$ is defined accordingly to the definition of the error ket.

Let now $\hat{A}_z$, $z=1,...,n$ be a set of operators acting on $\mathcal{H}$. For each value of z let $|a_z,k_z\rangle$ be a complete set of eigenvectors of $\hat{A}_z$, with eigenvalues a_z, and k_z being the degeneracy index. Moreover let $a_z^0\in\mathcal{C}$. The nth-order mixed error ket $|E(\hat{A}_1,\hat{A}_2,\ldots,\hat{A}_n,\psi,a_1^0,a_2^0,\ldots,a_n^0)\rangle$, is defined as the quantity

$$|E(\hat{A}_1,\hat{A}_2,\ldots,\hat{A}_n,\psi,a_1^0,a_2^0,\ldots,a_n^0)\rangle=(\hat{A}_n-a_n^0)\cdots\ (\hat{A}_2-a_2^0)(\hat{A}_1-a_1^0)|\psi\rangle. \tag{9}$$

When there is no risk of confusion we will use the short notations $|E^n\rangle$ or $|E_A^n\rangle$ for the nth-order error ket and $|E_{A_1,A_2,\ldots,A_n}\rangle$ for the mixed error ket. □

We shall now study some of the properties of this quantity.

(a) *Explicit form of the error ket.* Let us start with the 1st-order error ket. We have: $|E(\hat{A},\psi,a^0)\rangle=\Sigma_{a,k}(a-a^0)\langle a,k|\psi\rangle|a,k\rangle$. This result is easily extended to the case of the nth-order mixed error ket $|E_{A_1,A_2,\ldots,A_n}\rangle$:

$$|E_{A_1,A_2,\ldots,A_n}\rangle=\sum_{a_1,k_1}\sum_{a_2,k_2}\ldots\sum_{a_n,k_n}(a_1-a_1^0)(a_2-a_2^0)\cdots\ (a_n-a_n^0)\langle a_1,k_1|\psi\rangle\langle a_2,k_2|a_1,k_1\rangle$$
$$\times\langle a_3,k_3|a_2,k_2\rangle\ldots\langle a_n,k_n|a_{n-1},k_{n-1}\rangle|a_n,k_n\rangle, \tag{10}$$

and if $\hat{A}_1=\hat{A}_2=\cdots\ =\hat{A}_n=\hat{A}$ we have $|E_{A_1,A_2,\ldots,A_n}\rangle=|E_A^n\rangle$ which give us the explicit expression for the nth-order error:

$$|E_A^n\rangle=(\hat{A}-a^0)^n|\psi\rangle=\sum_{a,k}(a-a^0)^n\langle a,k|\psi\rangle|a,k\rangle. \tag{11}$$

(b) *Relation between the n*th*-order error ket and the mean second-order deviation*. Let us calculate the value of $\langle E_A^n|E_A^n\rangle$:

$$\langle E_A^n|_A^n\rangle=\sum_{a,k}((a-a^0)^*(a-a^0))^n|\langle a,k|\psi\rangle|^2, \tag{12}$$

and if $\hat{A}$ is self-adjoint and $a^0=\langle\psi|\hat{A}|\psi\rangle$ then $\langle E_A^n|E_A^n\rangle$ is just the mean $2n$th-order deviation of $\hat{A}$: $(\Delta\hat{A})^{2n}$ (if $n=1$ then $\langle E_A^1|E_A^1\rangle$ is just the mean square deviation).

(c) *N*th*-order error ket of a classical limit initial data wave function*. Let us consider the case in which the initial time configuration of the dynamical system is described by a classical limit initial data wave function $|\psi\rangle$. Let A be a fundamental observable of the system and let the classical initial data associated to A be given by a^0 with error margin δ_A. From Eqs. (5) and (12) it is straightforward to obtain the relation:

$$\langle E_A^n|E_A^n\rangle=\sum_{a,k}|a-a^0|^{2n}|\langle a,k|\psi\rangle|^2\leqslant\delta_A^{2n}\sum_{a,k}|\langle a,k|\psi\rangle|^2=\delta_A^{2n}, \tag{13}$$

which is valid for all $n\in\mathcal{N}$ and for all fundamental observables $A=a_i(i=1\cdots 2N)$.

(d) *Probabilistic distribution function from the n*th*-order error ket*. Let $\hat{A}$ be self-adjoint, let $|\psi\rangle$ be the state of the system and let a^0 be a real number. Given $\langle E^n(\hat{A},\psi,a^0)|E^n(\hat{A},\psi,a^0)\rangle$, to each "quantity of probability" $0\leqslant p<1$ we can associate an interval I_n around a^0, $I_n=[a^0-\Delta_n,a^0+\Delta_n]$, such that the probability of obtaining a value $a\in I_n$ from a measurement of $\hat{A}$ is at least p. The range of the interval I_n is dependent of $\hat{A},\psi$ and a^0 only through the value of $\langle E_A^n|E_A^n\rangle$. The quantity $\Delta_n(\langle E_A^n|E_A^n\rangle,p)$ is named the *n*th*-order spread* of the wave function. Let us show that if $\Delta_n=\Delta_n(\hat{A},\psi,a^0,p)$ is given by

$$\Delta_n(\hat{A},\psi,a^0,p)=\left(\frac{\langle E_A^n|E_A^n\rangle}{1-p}\right)^{1/2n} \tag{14}$$

then the probability of obtaining a value $a\in I_n$ from a measurement of $\hat{A}$ is at least p. From (12), (14) we have

$$(\Delta_n)^{2n}(1-p)=\sum_{k,a}|a-a^0|^{2n}|\langle a,k|\psi\rangle|^2,$$

$$\geqslant\sum_{k,a\notin I_n}|a-a^0|^{2n}|\langle a,k|\psi\rangle|^2\geqslant(\Delta_n)^{2n}\sum_{k,a\notin I_n}|\langle a,k|\psi\rangle|^2, \tag{15}$$

and this implies: $\Sigma_{k,a\notin I_n}|\langle a,k|\psi\rangle|^2\leqslant 1-p$, which is the result we were looking for. If $\hat{A}$ is not self-adjoint the former result can also be obtained, but in this case I_n is a ball of radius Δ_n in the complex plane.

(e) *Corollary of (d)*. A straightforward consequence of the previous result is the following: If for some positive integer M the condition:

$$\langle E^M(\hat{a}_i,\psi,a_i^0)|E^M(\hat{a}_i,\psi,a_i^0)\rangle\leqslant\delta_i^{2M} \tag{16}$$

holds for all $i=1\cdots 2N$ then the classical and the quantum descriptions [given by $(a_i^0,\delta_i,i=1\cdots 2N)$ and $|\psi\rangle$, respectively] are, accordingly to the second consistency criterion, M-order consistent.

B. Time evolution of $|E\rangle$ and Δ

The aim is now to determine the nth-order error ket and the nth-order spread associated to the operator $\hat{A}(t)$ given in (6), as a function of the error kets and spreads associated with the initial time operators. The calculations might seem, in a first reading, complicated and cumbersome. Nevertheless, the final result will be simple and physically appealing.

1. Evolving the error ket

We will start by calculating the 1st-order error ket associated with the sum and with the product of two arbitrary operators $\hat{A}$ and $\hat{B}$ and with the product of an operator by a scalar. Let the state of the system be $|\psi\rangle$, let $|E(\hat{A},\psi,a)\rangle$ and $|E(\hat{B},\psi,b\rangle$ be the first-order error kets associated to $\hat{A}$ and $\hat{B}$ and let $a,b,c\in\mathcal{C}$.

Theorem: The first-order error kets associated to the operators $\hat{A}+\hat{B}$, $c\hat{A}$, and $\hat{A}\hat{B}$ are, respectively,

$$|E(\hat{A}+\hat{B},\psi,a+b)\rangle=|E(\hat{A},\psi,a)\rangle+|E(\hat{B},\psi,b)\rangle, \tag{17}$$

$$|E(c\hat{A},\psi,ca)\rangle=c|E(\hat{A},\psi,a)\rangle, \tag{18}$$

$$|E(\hat{A}\hat{B},\psi,ab)\rangle=a|E(\hat{B},\psi,b)\rangle+b|E(\hat{A},\psi,a)\rangle+|E(\hat{B},\hat{A},\psi,b,a)\rangle. \tag{19}$$

Proof: For the sum of operators we have

$$|E_{A+B}\rangle=(\hat{A}+\hat{B}-(a+b))|\psi\rangle=(\hat{A}-a)|\psi\rangle+(\hat{B}-b)|\psi\rangle=|E_A\rangle+|E_B\rangle. \tag{20}$$

The proof of the product by a scalar and of the product of two operators follows the same lines, this time using the relations $(c\hat{A}-ca)=c(\hat{A}-a)$ and

$$(\hat{A}\hat{B}-ab)=a(\hat{B}-b)+b(\hat{A}-a)+(\hat{A}-a)(\hat{B}-b), \tag{21}$$

that when applied to the state $|\psi\rangle$ provide the desired results. □

Let us now extend these results to the case of several products and sums of fundamental operators. Let $\hat{A}$ be a general hermitian operator displayed as a sum of multiple products of fundamental operators and let A^0 be the classical function that is functionally identical to $\hat{A}$:

$$\hat{A}=\sum_{i=1}^{n} c_i\hat{B}_i=\sum_{i=1}^{n} c_i\prod_{j=1}^{m}\hat{x}_{ij}, \quad A^0=\sum_{i=1}^{n} c_iB_i^0=\sum_{i=1}^{n} c_i\prod_{j=1}^{m} x_{ij}, \tag{22}$$

where $\hat{x}_{ij}$ is one of the fundamental operators ($\hat{x}_{ij}\in\{\hat{I},\hat{q}_1,\ldots,\hat{q}_N,\hat{p}_1,\ldots,\hat{p}_N\}$ where N is the dimension of the classical system), n and m are arbitrary positive integers, c_i are complex numbers and $\hat{B}_i$, B_i are multiple products of the fundamental observables and multiple products of the corresponding classical observables, respectively. The map from $\hat{A}$ to A^0 will be named *unquantization*. Clearly, the procedure (22) is beset by order problems (i.e., if $\hat{A}$ is displayed in different orders we get different A^0). The consequences of this will be discussed later on.

The aim now is to expand $(\hat{A}-A^0)$ in terms of $(\hat{x}_{ij}-x_{ij})$. The first step is to set $(\hat{A}-A^0)=\Sigma_{i=1}^{n}c_i(\hat{B}_i-B_i^0)$. Using Eq. (21) we get

$$\begin{aligned}\hat{B}_i-B_i^0&=\hat{x}_{i1}\prod_{j=2}^{m}\hat{x}_{ij}-x_{i1}\prod_{j=2}^{m}x_{ij}\\&=x_{i1}\left(\prod_{j=2}^{m}\hat{x}_{ij}-\prod_{j=2}^{m}x_{ij}\right)+\prod_{j=2}^{m}x_{ij}(\hat{x}_{i1}-x_{i1})+(\hat{x}_{i1}-x_{i1})\left(\prod_{j=2}^{m}\hat{x}_{ij}-\prod_{j=2}^{m}x_{ij}\right),\end{aligned} \tag{23}$$

and using (21) once again to expand $(\Pi_{j=2}^{m}\hat{x}_{ij}-\Pi_{j=2}^{m}x_{ij})$ in terms of $(\hat{x}_{i2}-x_{i2})$ and $(\Pi_{j=3}^{m}\hat{x}_{ij}-\Pi_{j=3}^{m}x_{ij})$ and so on, after using the relation (21) m times we will obtain

$$\hat{B}_i-B_i^0=\sum_{L=1}^{+\infty}\sum_{j_1<j_2\cdots<j_L=1}^{m}\frac{\partial^L B_i^0}{\partial x_{ij_1}\ldots\partial x_{ij_L}}(\hat{x}_{ij_1}-x_{ij_1})\ldots(\hat{x}_{ij_L}-x_{ij_L}) \tag{24}$$

where the sum in L can be truncated at the mth term. The next step is to multiply each term in i by c_i and after sum in i. We get

$$\hat{A}-A^0=\sum_{L=1}^{+\infty}\sum_{i=1}^{n}\sum_{j_1<j_2\cdots<j_L=1}^{m}\frac{\partial^L A^0}{\partial x_{ij_1}\ldots\partial x_{ij_L}}(\hat{x}_{ij_1}-x_{ij_1})\ldots(\hat{x}_{ij_L}-x_{ij_L}). \tag{25}$$

Notice that this is just a ''Taylor expansion'' of an operator around the classical observable with the same functional form. The sums in the expansions (24) and (25) are taken over $j_1<j_2\cdots<j_L$ to preserve the order in which the operators $\hat{x}_{ij}$ appear in $\hat{B}_i$ since in general $(\hat{x}_{ik}-x_{ik})(\hat{x}_{ij}-x_{ij})\neq(\hat{x}_{ij}-x_{ij})(\hat{x}_{ik}-x_{ik})$. Because of this the analysis of the expansion (25) is tricky. The order in which the classical variables appear in A^0 is relevant. For instance if $\hat{A}=\hat{p}\hat{q}-\hat{q}\hat{p}$ then $A^0=pq-qp$ and this form, and not $A^0=0$, should be the one used to calculate the partial derivatives in (25).

Let us now consider the operator $(\hat{A})_+=\Sigma_{i=1}^{n}c_i(\Pi_{j=1}^{m}\hat{x}_{ij})_+$ obtained from a general hermitian operator $\hat{A}$ (22) by a term by term symmetrization: $(\hat{A})_+=\Sigma_{i=1}^{n}c_i(\hat{B}_i)_+$, where $(\hat{B}_i)_+$ is the completly symmetric operator obtained from $\hat{B}_i$. In general $(\hat{A})_+\neq\hat{A}$ but the classical observables obtained from $\hat{A}$ and $(\hat{A})_+$, given by (22), are identical, i.e., $A^0=(A)_+^0$. For this operator the expansion (25) might be written

$$(\hat{A})_+-A^0=\sum_{L=1}^{+\infty}\frac{1}{L!}\sum_{i=1}^{n}\sum_{j_1,j_2,..,j_L=1}^{m}\frac{\partial^L A^0}{\partial x_{ij_1}\ldots\partial x_{ij_L}}(\hat{x}_{ij_1}-x_{ij_1})\ldots(\hat{x}_{ij_L}-x_{ij_L}) \tag{26}$$

Our next step is to understand under which conditions, if any, is the expansion (26) a valid approximation to the expansion (25). To do this the first step is to define the unquantization map more precisely.

Definition: Unquantization V_0. Let $\mathcal{A}(\mathcal{H})$ be the algebra of linear operators acting on the physical Hilbert space $\mathcal{H}$ and let $\mathcal{A}(T^*M)$ be the algebra of complex functions over the classical phase space T^*M. V_0 is the map:

$$V_0:\mathcal{A}(\mathcal{H})\to\mathcal{A}(T^*M);\quad A^0=V_0(\hat{A}), \tag{27}$$

that satisfies the following *requirements*.

(a) The action of V_0 on a fundamental operator provides the corresponding classical fundamental observable: $V_0(\hat{q}_i)=q_i$ and $V_0(\hat{p}_i)=p_i$, $i=1\cdots N$. Moreover $V_0(\hat{I})=1$.

(b) The action of V_0 on a general operator $\hat{A}$, displayed in an arbitrary order, is given by $V_0(\hat{A})=V_0(\hat{A}_R)$ where $\hat{A}_R=\hat{A}$ but displayed in an order in which (i) $\hat{A}$ is the sum of an hermitian term with an anti-Hermitian term and (ii) all the commutators present in $\hat{A}$ have been resolved ($\hat{A}_R$ does not contain antisymmetric terms).

If $\hat{A}$ is displayed in the required order, $\hat{A}_R$ then

(c) V_0 is linear, i.e., if $\hat{A}_R=b\hat{B}+c\hat{C}$ then $V_0(\hat{A}_R)=bV_0(\hat{B})+cV_0(\hat{C})$; $b,c\in\mathcal{C}$.

(d) The product rule is valid: if $\hat{A}_R=\cdots+\hat{B}\hat{C}+\cdots$ then $V_0(\hat{A}_R)=V_0(\cdots)+V_0(\hat{B})V_0(\hat{C})+V_0(\cdots)$. □

One should notice that the map V_0 is not equivalent to the procedure (22). However, for a general operator $\hat{A}$, all the classical observables $V_0(\hat{A})$ can also be obtained using the procedure

(22) (by displaying $\hat{A}$ in appropriate order). Therefore all the results that were valid for A^0 obtained in (22), are also valid for $A^0=V_0(\hat{A})$. Further properties of the map V_0 will be discussed in Sec. IV.

Let us proceed with the analysis of expansions (25) and (26). We realize that if $\hat{A}$ is displayed in the required order $\hat{A}_R$ then the difference between $\hat{A}$ and $(\hat{A})_+$ is, at the most, proportional to a factor of $\hbar^2$. Since $A^0=V_0(\hat{A})$ is identical to $V_0((\hat{A})_+)$ we conclude that if $A^0=V_0(\hat{A})$ then the difference between the right hand sides of equations (25) and (26) is at the most proportional to a factor of $\hbar^2$ which, in the context of the results of this paper is of negligible magnitude. In conclusion, if $A^0=V_0(\hat{A})$ then the right-hand side of (26) is a valid approximation to $\hat{A}-A^0$.

Let us proceed: since $\hat{x}_{ij}$—in the expansion (26)—is one of the $2N$ fundamental operators the former expansion can be cast in the form

$$\hat{A}-A^0=\sum_{L=1}^{+\infty}\frac{1}{L!}\sum_{j_1,\ldots,j_L=1}^{2N}\frac{\partial^L A^0}{\partial a_{j_1},\ldots,\partial a_{j_L}}(\hat{a}_{j_1}-a_{j_1})\ldots(\hat{a}_{j_L}-a_{j_L}). \tag{28}$$

Finally, if we apply this expansion to the quantum state $|\psi\rangle$, we get

$$|E(\hat{A},\psi,A^0)\rangle=\sum_{L=1}^{+\infty}\frac{1}{L!}\sum_{j_1,\ldots,j_L=1}^{2N}\frac{\partial^L A^0}{\partial a_{j_1}\ldots\partial a_{j_L}}|E_{a_{j1},\ldots,a_{jL}}\rangle. \tag{29}$$

The generalization of the former set of results to the case of the mth-order error ket, $|E_A^m\rangle=(\hat{A}-A^0)^m|\psi\rangle$ can be obtained by exponentiating the expansion (28) to the mth power. Up to the lowest order we get

$$|E_A^m\rangle=(\hat{A}-A^0)^m|\psi\rangle=\sum_{k_1,\ldots,k_m=1}^{2N}\left(\prod_{i=1}^{m}\frac{\partial A^0}{\partial a_{k_i}}\right)|E_{a_{k1},\ldots,a_{km}}\rangle, \tag{30}$$

which is our final result concerning the error ket of an operator $\hat{A}$ functional of the fundamental operators. Notice that the former results are valid in general, irrespectively of the specific functional form of the wave function $|\psi\rangle$.

2. Evolving Δ_m

We shall now concentrate on the case of a system with a classical limit initial data. The aim is to calculate, in the representation of $\hat{A}$ (22), the value of the mth-order spread of a wave function $|\psi\rangle$ satisfying (5). To do this the main point is to calculate the norm of a general error ket: $\langle E_{x_1,\ldots,x_n}|E_{x_1,\ldots,x_n}\rangle$, where $x_1,\ldots,x_n$ is an arbitrary sequence of fundamental observables: $x_i\in\{q_1,\cdots,q_N,p_1,\cdots p_N\}, i=1\cdots n, n\in\mathcal{N}$. The following theorem will do this.

Theorem: If $|\psi\rangle$ is a classical limit initial data wave function then the norm of the error ket $|E(\hat{x}_1,..,\hat{x}_n,\psi,x_1^0,..,x_n^0)\rangle$ satisfies the following relation:

$$\langle E_{x_1,\ldots,x_n}|E_{x_1,\ldots,x_n}\rangle\leqslant\delta_1^2\ldots\delta_n^2, \tag{31}$$

where $(x_i^0,\delta_i), i=1\cdots n$ is the classical initial data associated to the observable x_i.

Proof: This result will be proved by induction:

(i) For $n=1$ and x_1 an arbitrary fundamental observable Eq. (5) immediately implies (result (3.1c): $\langle E_{x_1}|E_{x_1}\rangle\leqslant\delta_1^2$.

(ii) For an arbitrary n we use (10) and write

$$\langle E_{x_1,\ldots,x_n}|E_{x_1,\ldots,x_n}\rangle=\sum_{s,x_n}\langle E_{x_1,\ldots,x_{n-1}}|x_n,s\rangle\langle x_n,s|E_{x_1,\ldots,x_{n-1}}\rangle|(x_n-x_n^0)|^2, \tag{32}$$

where x_n are the eigenvalues of the operator $\hat{x}_n$, with degeneracy index s. We want to show that for all eigenvalues $x_n \notin I_n$, where $I_n=[x_n^0-\delta_n, x_n^0+\delta_n]$, we have

$$\langle x_n,s|E_{x_1,\ldots,x_{n-1}}\rangle=\langle x_n,s|\prod_{i=1}^{n-1}(\hat{x}_i-x_i^0)|\psi\rangle=0, \quad \forall_{x_n\notin I_n}. \tag{33}$$

To prove this let us expand the wave function $|\psi\rangle$ using a second set of eigenstates of $\hat{x}_n$,

$$\langle x_n,s|\prod_{i=1}^{n-1}(\hat{x}_i-x_i^0)|\psi\rangle=\sum_{x_n'\in I_n,s'}\langle x_n,s|\prod_{i=1}^{n-1}(\hat{x}_i-x_i^0)|x_n',s'\rangle\langle x_n',s'|\psi\rangle, \tag{34}$$

where x_n' are eigenvalues of $\hat{x}_n$ with degeneracy index s'. Notice that in the representation of $\hat{x}_n$ the wave function is completely confined to the interval I_n. To prove the result (33) is then sufficient to show that

$$\langle x_n,s|\prod_{i=1}^{j}\hat{x}_i|x_n',s'\rangle=0, \quad \forall_{x_n\notin I_n, x_n'\in I_n}, \forall_{j<n}. \tag{35}$$

Let us then prove the former identity

$$\langle x_n,s|\prod_{i=1}^{j}\hat{x}_i|x_n',s'\rangle=\frac{1}{x_n'}\langle x_n,s|\prod_{i=1}^{j}\hat{x}_i\hat{x}_n|x_n',s'\rangle=\frac{1}{x_n'}\langle x_n,s|\hat{x}_n\prod_{i=1}^{j}\hat{x}_i+\left[\prod_{i=1}^{j}\hat{x}_i,\hat{x}_n\right]|x_n',s'\rangle \tag{36}$$

and if $\langle x_n,s|[\Pi_{i=1}^{j}\hat{x}_i,\hat{x}_n]|x_n',s'\rangle=0$ then

$$\langle x_n,s|\prod_{i=1}^{j}\hat{x}_i|x_n',s'\rangle=\frac{1}{x_n'}\langle x_n,s|\hat{x}_n\prod_{i=1}^{j}\hat{x}_i|x_n',s'\rangle=\frac{x_n}{x_n'}\langle x_n,s|\prod_{i=1}^{j}\hat{x}_i|x_n',s'\rangle. \tag{37}$$

Since $x_n\neq x_n'$ Eq. (37) immediately implies (35) and thus the result (33) is valid. The problem is now reduced to prove that $\langle x_n,s|[\Pi_{i=1}^{j}\hat{x}_i,\hat{x}_n]|x_n',s'\rangle=0$, which in turn, and using the same procedure, will be reduced to prove that $\langle x_n,s|[[\Pi_{i=1}^{j}\hat{x}_i,\hat{x}_n],\hat{x}_n]|x_n',s'\rangle=0$, and so on until we obtain at the most a j-commutator which will always have the value zero (notice that $\hat{x}_i$ are fundamental operators). Inserting the result (33) into (32) we get

$$\begin{aligned}\langle E_{x_1,\ldots,x_n}|E_{x_1,\ldots,x_n}\rangle&=\sum_{s,x_n\in I_n}\langle E_{x_1,\ldots,x_{n-1}}|x_n,s\rangle\langle x_n,s|E_{x_1,\ldots,x_{n-1}}\rangle|(x_n-x_n^0)|^2\\&\leqslant\langle E_{x_1,\ldots,x_{n-1}}|E_{x_1,\ldots,x_{n-1}}\rangle\delta_n^2,\end{aligned} \tag{38}$$

which proves the theorem. □

A straightforward corollary of the former result is the one obtained by using the Schwartz inequality:

$$|\langle E_{x_1,\ldots,x_n}|E_{y_1,\ldots,y_m}\rangle|\leqslant\delta_{x_1}\cdots\delta_{x_n}\delta_{y_1}\cdots\delta_{y_m}, \tag{39}$$

where $x_1,\ldots,x_n$ and $y_1,\ldots,y_m$ are two arbitrary sequences of fundamental observables.

Let us return to the calculation of the m-order spread of the wave function $|\psi\rangle$, satisfying (5), in the representation of $\hat{A}$. The relevant calculation is that of $\langle E_A^m|E_A^m\rangle$. From Eqs. (28) and (39), we get

$$\langle E_A^m|E_A^m\rangle=\langle\psi|(\hat{A}-A^0)^{2m}|\psi\rangle\leqslant\left(\sum_{L=1}^{+\infty}\frac{1}{L!}\sum_{j_1,\ldots,j_L=1}^{2N}\left|\frac{\partial^L A^0}{\partial a_{j_1}\ldots\partial a_{j_L}}\right|\delta_{j_1}\ldots\delta_{j_L}\right)^{2m}=\delta_{A^0}^{2m}, \tag{40}$$

a result that is valid for all $m\in\mathcal{N}$. The m-order spread then reads

$$\Delta_m(\hat{A},\psi,A^0,p)=\left(\frac{\langle E_A^m|E_A^m\rangle}{1-p}\right)^{1/2m}\leqslant\frac{\delta_{A^0}}{(1-p)^{1/2m}}, \tag{41}$$

which, for all $p<1$ converges to the classical error margin δ_{A^0} as $m\to\infty$.

From the results (3.1d) and (41) we can draw the conclusion that the classical limit initial data wave function $|\psi\rangle$, in the representation of an arbitrary observable $\hat{A}$, is completely confined to an interval around A^0 with the range of the classical error margin of A^0, the relation between $\hat{A}$ and A^0 being the one given by (27).

IV. UNQUANTIZATION

In the last section we proved that the wave function $|\psi\rangle$—satisfying (5)—in the representation of a given quantum operator $\hat{A}$, which in the end is to be identified with $\hat{A}(t)$ given in (6), is completely confined to an interval centered at the value of the classical observable A^0 and with the range of the classical error interval of A^0. This implies that the output of a measurement of $\hat{A}$, performed with an experimental apparatus of any resolution, will certainly belong to the previous error interval, which is exactly the classical prediction for the output of a measurement of the classical observable A^0.

However these are not our final results, yet. The reason is straightforward: Let $\hat{A}=\hat{A}(t)$, what remains to be proven is simply that $A^0=V_0(\hat{A}(t))=A(t)$, i.e., that the classical observable A^0, obtained from the quantum observable $\hat{A}(t)$ using the map V_0, coincides with the classical observable $A(t)$ obtained by evolving $A(0)=V_0(\hat{A}(0))$ using the classical theory.

Hence the relevant questions are: Is the map V_0 well defined? And will it map a quantum observable $\hat{A}(t)$ to the classical observable $A(t)$ given by (7)?

Starting with the first question it is easy to see that the map V_0 is not well defined. In general $\hat{A}$ can be displayed in several different functional forms (all of them satisfying the order requirement), each of which will be mapped by V_0 to a *different* (however very similar) classical observable. A simple example will elucidate this point: let $\hat{A}=1/2(\hat{x}\hat{y}\hat{z}+\hat{z}\hat{y}\hat{x})$ with $\hat{x}=\hat{q}_1\hat{p}_2$, $\hat{y}=\hat{p}_1$ and $\hat{z}=\hat{q}_1\hat{q}_2$ where q_1, p_1, q_2, p_2 are the canonical variables of a two dimensional system. Alternatively, $\hat{A}$ might be written as $\hat{A}=1/4(\hat{x}\hat{y}\hat{z}+\hat{z}\hat{y}\hat{x}+\hat{x}\hat{z}\hat{y}+\hat{y}\hat{z}\hat{x})+1/4[\hat{x},[\hat{y},\hat{z}]]$. The first form of $\hat{A}$ is mapped by V_0 to the classical observable $A^0=xyz$ while the second form is mapped to the observable $A^0=xyz-1/4\hbar^2 q_1$. Moreover for each different classical observable obtained we will, in general, also get a different associated error ket and error margin. This does not mean that the former results (30), (41) concerning the error ket and the spread of the wave function are incorrect. These results have been proved to be valid (up to a correction term proportional to $\hbar^2$) for all different orders we may choose for the operator $\hat{A}$, and consequently for all different A^0 obtained from $\hat{A}$, providing the order requirement is satisfied.

Notice however that this ambiguity would be problematic if the difference between two different classical observables, obtained from a single quantum one, had meaningful values. However, one can easily realize that if A_1^0 and A_2^0 are two such observables [i.e., $A_1^0=V_0(\hat{A})$ and also $A_2^0=V_0(\hat{A})$] then $A_1^0-A_2^0$ is proportional to a factor of, at the most $\hbar^2$. An imprecision of this magnitude is not meaningful when compared to the errors associated to the classical observables. That is the predictions A_1^0 and A_2^0 are well within the error interval of each other $|A_1^0-A_2^0|$

$\ll \delta_{A_1^0 \text{or} A_2^0}$. Hence, the two predictions are consistent with each other and we conclude that A_1^0 and A_2^0 are equally valid candidates for a classical description of the quantum observable $\hat{A}$.

This takes us to the second question, which now can be restated as: will the classical observable $A(t)$, given by (7), be one of the images of $V_0(\hat{A}(t))$?

To answer this question let us start by presenting a second proposal for the unquantization map:

Definition: Unquantization V. Using the notation of the previous definition we define the new unquantization V to be the map:

$$V: \mathcal{A}(\mathcal{H}) \to \mathcal{A}(T^*M), \quad A = V(\hat{A}), \tag{42}$$

that satisfies the following requirement: $V \circ \wedge = 1$ where $\wedge$ is the Dirac quantization map.[32,37] That is V is the inverse of the Dirac quantization map $\wedge$. The properties of V follow immediately from the properties of $\wedge$:

(a) $V(\hat{q}_i) = q_i$, $V(\hat{p}_i) = p_i$, $i = 1 \cdots N$, and $V(\hat{I}) = 1$.

(b) $V(1/i\hbar[\hat{A}, \hat{B}]) = \{V_0(\hat{A}), V_0(\hat{B})\}$ for all $\hat{A}$ and $\hat{B}$.

For a general operator $\hat{A}$ displayed in the required order (see definition of V_0):

(c) V is linear: if $\hat{A} = b\hat{B} + \hat{C}$ then $V(\hat{A}) = bV(\hat{B}) + V(\hat{C})$, $b \in \mathcal{C}$.

(d) The product rule is valid: if $\hat{A} = \cdots + \hat{B}\hat{C} + \cdots$ then $V(\hat{A}) = V(\cdots) + V(\hat{B})V(\hat{C}) + V(\cdots)$. □

We should point out that, since the Dirac quantization map $\wedge$ is not injective, the unquantization map V is also nonunivocous. The simple example above—$\hat{A} = 1/2(\hat{x}\hat{y}\hat{z} + \hat{z}\hat{y}\hat{x})$—can also be used here to make this point clear. Being beset by the same type of order problems still V displays an important advantage over V_0: it is straightforward to recognize that when V is applied to the operator $\hat{A}(t)$—given by (6)—yields the classical observable $A(t)$:

$$V(\hat{A}(t)) = V\left[\sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{t}{i\hbar}\right)^n [\cdots[\hat{A}, \hat{H}], \hat{H}]\cdots\right] = \sum_{n=0}^{\infty} \frac{t^n}{n!}\{\cdots\{A, H\}, H\}\cdots\}. \tag{43}$$

Let us now consider a general operator $\hat{X}$. We want to prove that $V(\hat{X})$ provides a set of classical observables that is included in the set $V_0(\hat{X})$. Clearly the action of the two maps on an operator that does not contain antisymmetric components is identical. Moreover the two commutation relations $1/i\hbar[,]$ and $\{,\}$ have "compatible" algebraic structures, that is we can resolve $1/i\hbar[\hat{A}, \hat{B}]$ and express the result in such an order that when we perform the substitution of the quantum observables by the corresponding classical ones (i.e., when we unquantize $1/i\hbar[\hat{A}, \hat{B}]$ using the map V_0) we get exactly the same final result as if we just compute $\{A, B\}$ (i.e., as if we use the map V to unquantize $1/i\hbar[\hat{A}, \hat{B}]$). Thus, if $\hat{X}$ contains antisymmetric components the classical observable $V(\hat{X})$ might be obtained by displaying $\hat{X}$ in an adequate order and calculating $V_0(\hat{X})$. Hence, it is always possible to obtain the classical observables $V(\hat{X})$ using the map V_0. This is the result we were looking for. It means that expansion (28) and thus all subsequent results are valid for $A^0 = V(\hat{A})$.

Finally, we are able to state that the quantum mechanical predictions for an arbitrary dynamical system with a classical limit initial data wave function are that a measurement of an arbitrary fundamental observable $\hat{A}(t)$ at the time t will yield the value given by (43) with an error margin given by (41) (with $m \to \infty$). These are exactly the predictions of the classical mechanical treatment of the same system.

V. CRITERIA OF CLASSICALITY

In the last section we proved that a dynamical system with a quantum initial data satisfying (5) will evolve *exactly* accordingly to the predictions of classical mechanics, that is the system is ∞-consistent for all times. The main interest of this result is formal since, in most cases we are unable to provide a wave function satisfying the classical limit criterion (5).

To proceed we will now study dynamical systems with general physical initial data. The aim is to use the formalism developed in the previous sections to derive two criteria providing a measure of the degree of classicality of an arbitrary quantum system with arbitrary initial data.

Let then $|\phi\rangle$ be the initial data wave function of a N dimensional dynamical system with canonical variables a_k, $(k=1\cdots 2N)$. Let $\hat{S}_{k_i}=(\hat{a}_{k_1},\hat{a}_{k_2},\ldots,\hat{a}_{k_n})$, $k_i\in\{1\cdots 2N\}$ be a sequence of fundamental operators associated to the n-terms sequence k_i $(i=1\cdots n; n\in\mathcal{N})$. The relevant quantities that we have to calculate will be the n-order mixed error kets associated to the sequences $\hat{S}_{k_i}$:

$$|E_{S_{ki}}\rangle=(\hat{a}_{k_1}-a^0_{k_1})(\hat{a}_{k_2}-a^0_{k_2})\cdots(\hat{a}_{k_n}-a^0_{k_n})|\phi\rangle, \tag{44}$$

where $a^0_{k_i}$ is the classical initial value of the canonical variable a_{k_i}, i.e., $a^0_{k_i}=a_{k_i}(t=0)$.

A. First criterion

The first step is to obtain the time evolution of the canonical variables using the standard classical formulation of the system

$$a_j(t)=\sum_{m=0}^{\infty}\frac{t^m}{m!}\{\ldots\{a_j,H\}\ldots,H\}=F_j(a_k,t). \tag{45}$$

We then consider the sequences S_{k_i} such that

$$\frac{\partial F_j}{\partial S_{k_i}}=\frac{\partial^n F_j}{\partial a_{k_1}\partial a_{k_2}\cdots\partial a_{k_n}}\neq 0, \tag{46}$$

for at least one $j=1\cdots 2N$. For each of these sequences we construct the associated error ket (44). This way we obtain a set of error kets. The first order classicality criterion is given by the following conditions:

$$\langle E_{S_{ki}}|E_{S_{ki}}\rangle\leqslant(\delta_{S_{ki}})^2=(\delta_{k_1}\delta_{k_2}\cdots\delta_{k_n})^2, \tag{47}$$

where the inequalities should hold for all the sequences determined in (46). In (47) δ_{k_i} is the initial data classical error margin associated to the classical observable a_{k_i}, $i=1\cdots n$. If the initial data wave function satisfies the former conditions we say that the dynamical system is *first order classical*.

To proceed we construct the sequences $S^M_{k_i}$ formed by $M\in\mathcal{N}$ original sequences S_{k_i}, that is $S^M_{k_i}=S_{k_i},S_{k_i'},\ldots,S_{k_i''}$, where each of the M former sequences S_{k_i} might be any of the ones determined in (46). Once again, we calculate the values of $\langle E_{S^M_{ki}}|E_{S^M_{ki}}\rangle$ and compare them with $(\delta_{S^M_{ki}})^2$. If the initial data satisfies:

$$\langle E_{S^M_{ki}}|E_{S^M_{ki}}\rangle\leqslant(\delta_{S^M_{ki}})^2, \tag{48}$$

for all possible sequences $S^M_{k_i}$ we say that the dynamical system is M-order classical.

Let us make two remarks: the first one to say that the classification of a given initial data as M-order classical is *dependent* on the scales (error margins δ_k) that characterize the classical description. In particular for $\delta_k=\infty$ all dynamical systems will be ∞-order classical (and will have a classical limit initial data) while for scales smaller than the Planck scale none will even be

first-order classical. The second remark is to point out that if a system is M-order classical then [result (3.1d)] its initial data wave function, in the representation of any of the observables $\hat{a}_k(0)$, will have a minimum probability p in the interval $I_k=[a_k(0)-\delta_k/(1-p)^{1/(2M)},a_k(0)+\delta_k/(1-p)^{1/(2M)}]$, where $a_k(0)$ is the value of the classical observable a_k at the initial time, $t=0$. That is the initial data is M-order consistent. This is because in (46) we always determine the $2N$ single value sequences $S_{k_1}=a_k$, $(k=1\cdots 2N)$.

Furthermore, if the classical and the quantum initial data satisfy the inequalities (48) then we can substitute $\langle E_{S_{ki}^M}|E_{S_{ki}^M}\rangle$ by $(\delta_{S_{ki}^M})^2$ when computing (40) for $A^0=a_j(t)$. The result (41) can then be easily obtained being valid up to the order $m=M$. Hence, using the result (3.1d) we can state that an arbitrary M-order classical system, as defined above, will evolve in such a way that in the representation of $\hat{a}_j(t)$ (for all $j=1\cdots 2N$ and for all t) the initial data wave function has at least a probability p confined to the interval $I_j(t)=[a_j(t)-\delta_j(t)/(1-p)^{1/(2M)},a_j(t)+\delta_j(t)/(1-p)^{1/(2M)}]$ with $a_j(t)$ and $\delta_j(t)$ being the classical time evolution of the canonical variable a_j and associated error margin. According to the second consistency criterion this means that the classical and the quantum data describing the system at the time t are M-order consistent.

We conclude that if M is the order of classicality of a given dynamical system then: first the classical and the quantum data describing the initial time configuration of the system are M-order consistent and, second the degree of consistency is preserved through the time evolution.

Finally, notice that the higher the order of classicality M of the dynamical system the more similar will be the range of $I_j(t)$ and the classical error margin. When M goes to infinity we obtain the classical limit description of the system.

B. Second criterion

A second classicality criterion can be easily devised. Once again the first step is to calculate the time evolution of the canonical variables a_j using the classical formulation of the theory (45). Again we use this result to obtain the sequences of fundamental operators $\hat{S}_{k_i}$ (46) and the associated error kets (44). Using these error kets we can write the second classicality criterion:

$$\langle E_{S_{ki}}|E_{S_{ki}}\rangle \leqslant (\delta_{S_{ki}})^2(1-p_0)=(\delta_{k_1}\delta_{k_2}\ldots\ldots\delta_{k_n})^2(1-p_0), \quad \forall S_{k_i} \quad \text{in (46)}. \tag{49}$$

If the classical and the quantum initial data satisfy the former inequalities for a given p_0 $(0\leqslant p_0<1)$ and for all sequences determined in (46), then we say that the dynamical system is p_0-order classical. A straightforward use of the result (3.1d) will prove that a p_0-order classical system is described by an initial data wave function that, in the representation of any of its fundamental observables $\hat{a}_k(t=0)$, $k=1\cdots 2N$, has at least a probability p_0 confined to the classical error interval $[a_k(0)-\delta_k,a_k(0)+\delta_k]$. That is the initial time configuration is p_0-order consistent (according to the first consistency criterion).

Now, let us concentrate on the dynamical evolution of the former initial data. If the inequalities (49) are satisfied we can perform the substitution of $\langle E_{S_{ki}}|E_{S_{ki}}\rangle$ by $(\delta_{S_{ki}})^2(1-p_0)$ when computing (40) for $m=1$. Notice that there will be an extra factor of $(1-p_0)$ in the final expression in (40). We can then proceed and obtain the result (41) for $\Delta_1(\hat{a}_j(t),\phi,a_j(t),p)$ [which still contains the extra factor $(1-p_0)^{1/2}$]. More precisely we make $p=p_0$ in (41) and get for all $j=1\cdots 2N$:

$$\Delta_1(\hat{a}_j(t),\phi,a_j(t),p_0)=\left(\frac{\langle E_{a_j(t)}|E_{a_j(t)}\rangle}{1-p_0}\right)^{1/2}$$
$$\leqslant \frac{1}{(1-p)^{1/2}}\sum_{L=1}^{+\infty}\frac{1}{L!}\sum_{k_1,\ldots,k_L=1}^{2N}\left|\frac{\partial^L a_j(t)}{\partial a_{k_1}\ldots\partial a_{k_L}}\right|\delta_{k_1}\cdots\delta_{k_L}(1-p_0)^{1/2}=\delta_j(t). \tag{50}$$

The previous result together with (3.1d) implies that in the representation of $\hat{a}_j(t)$ (for all $j=1\cdots 2N$) the initial data wave function has at least a probability p_0 confined to the classical error interval $[a_j(t)-\delta_j(t), a_j(t)+\delta_j(t)]$, i.e., the classical and the quantum descriptions of the configuration of the system at the time t are p_0-order consistent. This result is valid for all times. We conclude that if a dynamical system is p_0-order classical then the classical and the quantum descriptions of the configuration of the system are p_0-order consistent for all times. Once again, when $p_0 \to 1$ we obtain the classical limit description of the system.

VI. EXAMPLE—HARMONIC OSCILLATOR

To illustrate the use of the first classicality criterion (Sec. V A), let us obtain the classicality conditions for the simple example of the harmonic oscillator. The classical Hamiltonian is given by $H=\frac{1}{2}(q^2+p^2)$, where q and p are a pair of canonical variables and, to make it simple we made $w=m=1$. Solving the equations of motion we obtain the classical time evolution of the canonical variables and the corresponding error margins

$$\begin{aligned} &q(t)=q(0)\cos t+p(0)\sin t, \quad \delta_q(t)=|\cos t|\,\delta_q(0)+|\sin t|\,\delta_p(0),\\ &p(t)=q(0)\sin t+p(0)\cos t, \quad \delta_p(t)=|\sin t|\,\delta_q(0)+|\cos t|\,\delta_p(0). \end{aligned} \tag{51}$$

Let $|\phi\rangle$ be the initial data wave function for the quantum harmonic oscillator. Let us then determine the conditions that $|\phi\rangle$ should satisfy so that the quantum system allows for a consistent M-order classical description. Following the general prescription of Sec. V A the first step is to determine the fundamental sequences (46). They are the single value sequences

$$S_1=q \quad \text{and} \quad S_2=p. \tag{52}$$

For a M-order classical system the relevant sequences are arrays of M fundamental sequences:

$$S^M=(z_1,\ldots,z_M), \quad z_i=q\vee p, \quad i=1\cdots M, \tag{53}$$

and the condition of M-order classicality (48) reads

$$\begin{aligned} &\langle E_{S^M}|E_{S^M}\rangle \leqslant \delta^2_{S^M}, \quad \forall S^M \quad \text{in (53)}\\ \Leftrightarrow &\langle\phi|(\hat{z}_1-z_1(0))\ldots(\hat{z}_M-z_M(0))(\hat{z}_M-z_M(0))\ldots(\hat{z}_1-z_1(0))|\phi\rangle \leqslant \delta^2_{z_1}(0)\ldots\delta^2_{z_M}(0). \end{aligned} \tag{54}$$

Given the classical initial data $\{q(0),p(0),\delta_q(0),\delta_p(0)\}$, Eq. (54) constitute a system of inequalities to be satisfied by initial data wave function $|\phi\rangle$. For a first-order classical system the classicality conditions take their simpler form

$$\begin{aligned} &\langle\phi|(\hat{q}-q(0))^2|\phi\rangle \leqslant \delta^2_q(0)\\ &\langle\phi|(\hat{p}-p(0))^2|\phi\rangle \leqslant \delta^2_p(0) \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} &\int (q-q(0))^2|\phi(q)|^2dq \leqslant \delta^2_q(0)\\ &\int (p-p(0))^2|\phi(p)|^2dp \leqslant \delta^2_p(0). \end{aligned} \tag{55}$$

To obtain explicit solutions we may want to consider Gaussian wave packets [notice however that, in general, there are many solutions of (55) which are not Gaussians]:

$$\phi_c(q_0,p_0,\Delta q,q)=\frac{1}{(2\pi(\Delta q)^2)^{1/4}}\exp\left\{-\frac{(q-q_0)^2}{4(\Delta q)^2}+ip_0q/\hbar\right\}, \tag{56}$$

where q_0, p_0 and Δq are parameters and the wave function was displayed in the $\hat{q}$ representation. If we make $q_0=q(0)$ and $p_0=p(0)$ and substitute $\phi_c(q(0),p(0),\Delta q,q)$ in (55) we get the equivalent set of inequalities:

$$\Delta q \leqslant \delta_q(0) \quad \wedge \quad \frac{\hbar}{2^{1/2}\Delta q} \leqslant \delta_p(0). \tag{57}$$

As expected, if $\delta_p(0)\delta_q(0) < \hbar/(2^{1/2})$ there is no coherent state (and actually no wave function) that might satisfy the former inequalities, while for larger values of the classical error margins there are many solutions of (55), including the coherent states with a parameter Δq satisfying (57). We see that the classicality criteria provide a comparative notion of classicality but not an absolute one. In fact the degree of classicality is always relative to the classical description supplied.

The main result of the formalism is that a wave function satisfying (55), and in particular a coherent state satisfying (57) displays a time evolution first order consistent with the classical predictions (51), which means that for all t:

$$\int_{q(t)-\delta_q(t)/(1-P)^{1/2}}^{q(t)+\delta_q(t)/(1-P)^{1/2}} |\phi(q,t)|^2 dq \geqslant P, \quad \wedge \quad \int_{p(t)-\delta_p(t)/(1-P)^{1/2}}^{p(t)+\delta_p(t)/(1-P)^{1/2}} |\phi(p,t)|^2 dp \geqslant P, \quad \forall_{0\leqslant P<1}, \tag{58}$$

where $q(t)$, $p(t)$, $\delta_q(t)$, $\delta_p(t)$ are given by (51), $|\phi(t)\rangle$ is the solution of the Schrödinger equation:

$$i\hbar\,\partial/\partial t|\phi(t)\rangle = 1/2(\hat{q}^2+\hat{p}^2)|\phi(t)\rangle, \quad |\phi(t=0)\rangle = |\phi\rangle,$$

and P is an arbitrary probability. Take for instance $P=0.99$, Eq. (58) states that 99% of the probability of the wave function $|\phi(t)\rangle$, in both the representations of $\hat{q}$ and $\hat{p}$, is confined to the classical intervals $[q(t)-10\delta_q(t), q(t)+10\delta_q(t)]$ and $[p(t)-10\delta_p(t), p(t)+10\delta_p(t)]$, respectively. This statement is valid for all times and, for the case of coherent states can be easily verified by numerical computation of the integrals (58).

To see what happens when the degree of classicality is increased let us consider a 10th-order classical system. In this case the initial data wave function should satisfy the conditions (54) for all $M=10$ sequences (53). If we consider Gaussian type solutions (56) and substitute (56) in (54) we get the following set of inequalities for the parameter Δq:

$$\frac{(2M-1)!}{2^{M-1}((M-1)!)}(\Delta q)^{2M} \leqslant \delta_q^{2M}(0) \quad \wedge \quad \frac{(2M-1)!}{2^{M-1}((M-1)!)}\left(\frac{\hbar}{2^{1/2}\Delta q}\right)^{2M} \leqslant \delta_p^{2M}(0), \tag{59}$$

where $M=10$. Clearly, for the same classical initial data the set of solutions of (59) is just a subset of the set of solutions of (57).

The solutions of (54) with $M=10$ and in particular the coherent states satisfying (59), display a time evolution 10th-order consistent with the classical predictions (Sec. V A). In particular for $P=0.99$ we have $(1-P)^{1/20}=0.79$ and thus

$$\int_{q(t)-1.25\delta_q(t)}^{q(t)+1.25\delta_q(t)} |\phi(q,t)|^2 dq \geqslant 0.99 \quad \wedge \quad \int_{p(t)-1.25\delta_p(t)}^{p(t)+1.25\delta_p(t)} |\phi(p,t)|^2 dp \geqslant 0.99, \tag{60}$$

where $|\phi(t)\rangle$ is the quantum time evolution of a general initial data wave function satisfying (54) for $M=10$. The result is valid for all times and can be checked explicitly for an arbitrary coherent state satisfying (59).

One of the most interesting properties of coherent states is that its quantum time evolution is (in some sense) ''consistent'' with the classical predictions. Because of this coherent states might be seen as ''classical states.'' We see that the classicality criteria provide a systematic procedure to obtain ''classical states'' for an arbitrary dynamical system: by solving the classicality conditions (54) we obtain a large set of classical states (much larger than the coherent states set) for which the quantum time evolution is consistent with the classical predictions. Moreover, and most important, the imprecise notions of ''consistency'' and of ''classical states'' are made fully precise in this formalism.

VII. FURTHER EXAMPLE

To further illustrate the use of the criteria let us consider the two-dimensional system described by the Hamiltonian:

$$H=\frac{P^2}{2M}+\frac{p^2}{2m}+kQp^2, \tag{61}$$

where (Q,P) are the canonical variables of a particle of mass M, (q,p) the ones of the particle of mass m and k is a coupling constant. The classical time evolution is obtained by solving the Hamiltonian equations of motion which yield

$$\begin{aligned} Q(t)&=Q(0)+\frac{P(0)}{M}t-\frac{k}{2M}p(0)^2t^2,\\ P(t)&=P(0)-kp(0)^2t,\\ q(t)&=q(0)+\left\{\frac{p(0)}{m}+2kQ(0)p(0)\right\}t+\frac{k}{M}P(0)p(0)t^2-\frac{k^2}{3M}p(0)^3t^3,\\ p(t)&=p(0) \end{aligned} \tag{62}$$

with error margins (taking into account all orders in the initial time error margins):

$$\begin{aligned} \delta_Q(t)&=\delta_Q(0)+\left|\frac{t}{M}\right|\delta_P(0)+\left|\frac{kp(0)t^2}{M}\right|\delta_p(0)+\left|\frac{kt^2}{2M}\right|\delta_p^2(0),\\ \delta_P(t)&=\delta_P(0)+|2kp(0)t|\,\delta_p(0)+|kt|\,\delta_p^2(0),\\ \delta_q(t)&=\delta_q(0)+\left|\left(\frac{1}{m}+2kQ(0)\right)t+\frac{kP(0)t^2}{M}-\frac{k^2p(0)^2t^3}{M}\right|\delta_p(0)+|2kp(0)t|\,\delta_Q(0)\\ &\quad+\left|\frac{kp(0)t^2}{M}\right|\delta_P(0)+|kt|\,\delta_Q(0)\,\delta_p(0)+\left|\frac{kt^2}{2M}\right|\delta_P(0)\,\delta_p(0)+\left|\frac{k^2p(0)t^3}{M}\right|\delta_p^2(0)+\left|\frac{k^2t^3}{M}\right|\delta_p^3(0),\\ \delta_p(t)&=\delta_p(0). \end{aligned} \tag{63}$$

For this dynamical system the fundamental sequences (46) are (the indexes 1, 2, 3, and 4 refer to the canonical variables q, p, Q, and P, respectively)

$$\begin{aligned} &S_1=q,\quad S_2=p,\quad S_3=Q,\quad S_4=P,\\ &S_{22}=(p,p),\quad S_{23}=(p,Q),\quad S_{24}=(p,P),\quad S_{222}=(p,p,p) \end{aligned} \tag{64}$$

and the first order classicality condition reads

$$\langle E_{S_{ki}}|E_{S_{ki}}\rangle\leqslant\delta_{S_{ki}}^2,\quad \forall S_{k_i}\quad \text{in (64)}. \tag{65}$$

To make the discussion simpler let us consider solutions of the form $|\xi\rangle=|\psi\rangle|\phi\rangle$, where $|\psi\rangle$ is the quantum state of the particle of mass m, and $|\phi\rangle$ is that of the particle of mass M. In the $(\hat{q},\hat{Q})$ representation we have $\xi(q,Q)=\psi(q)\phi(Q)$. To proceed we notice that if the condition (65) is satisfied for the sequences S_1, S_2, S_3 and S_4 then is also satisfied for S_{23} and S_{24}. Furthermore, if it is satisfied for S_{222} is also for S_{22} and S_2. Hence, the system of eight inequalities (65) is reduced to the system of four inequalities: $\langle E_{S_{ki}}|E_{S_{ki}}\rangle\leqslant\delta_{S_{ki}}^2$, $S_{ki}\in\{S_1,S_3,S_4,S_{222}\}$. Moreover, the former system splits into two independent systems:

$$\begin{array}{ll} \langle\psi|(\hat{q}-q(0))^2|\psi\rangle \leqslant \delta_q^2(0) & \langle\phi|(\hat{Q}-Q(0))^2|\phi\rangle \leqslant \delta_Q^2(0) \\ & \text{and} \\ \langle\psi|(\hat{p}-p(0))^6|\psi\rangle \leqslant \delta_p^6(0) & \langle\phi|(\hat{P}-P(0))^2|\phi\rangle \leqslant \delta_P^2(0). \end{array} \tag{66}$$

For Gaussian type solutions $\xi_c(Q_0,P_0,q_0,p_0,\Delta Q,\Delta q,q,Q)=\phi_c(Q_0,P_0,\Delta Q,Q)\psi_c(q_0,p_0,\Delta q,q)$ it reduces to the form

$$\begin{array}{ll} \Delta q \leqslant \delta_q(0) & \Delta Q \leqslant \delta_Q(0) \\ & \text{and} \\ (15)^{1/6}\dfrac{\hbar}{2^{1/2}\Delta q} \leqslant \delta_p(0) & \dfrac{\hbar}{2^{1/2}\Delta Q} \leqslant \delta_P(0), \end{array} \tag{67}$$

where we used Eq. (59) to obtain the second inequality of the first system. Any Gaussian wave function satisfying the former conditions displays a time evolution (solution of the Schrödinger equation: $i\hbar\,\partial/\partial t|\xi(t)\rangle=\hat{H}|\xi(t)\rangle$, $|\xi(0)\rangle=|\xi\rangle$) first order consistent with the classical predictions (62) and (63). This means that for any of the canonical variables $Z=q,p,Q\vee P$ and for all times:

$$\int_w \int_{Z(t)-\delta_Z(t)/(1-P)^{1/2}}^{Z(t)+\delta_Z(t)/(1-P)^{1/2}} |\langle\xi(t)|z,w\rangle|^2 dz dw \geqslant P, \quad \forall_{0\leqslant P<1}, \tag{68}$$

where $|z,w\rangle$ is the general eigenstate of the observable $\hat{Z}$ with associated eigenvalue z and degeneracy index w, P is a probability and $(Z(t),\delta_Z(t))$ are the classical time evolution of the canonical variable Z and its error margin which are given by Eqs. (62) and (63), respectively.

Just like in the example of the harmonic oscillator we can increase the order of classicality of the system by requiring the initial data wave function to satisfy higher order classicality conditions. Likewise, this will increase the degree of consistency between the classical and the quantum predictions.

VIII. CONCLUSIONS

A general procedure leading to the construction of a measure of classicality was presented. The procedure can be summarized in two main steps.

(1) Definition of a consistency criterion. This is a kinematical criterion. It should provide a suitable measure of the degree of agreement between the classical and the quantum descriptions of a single, specific time configuration of the system. Two intuitive definitions of consistency criteria were presented and certainly other, possible more interesting criteria might be defined.

(2) Using the consistency criterion the problem of studying the overall consistency between the classical and the quantum descriptions of a general dynamical system is reduced to a simpler and more precisely formulated problem: that of identifying the conditions that should be satisfied so that the degree of consistency between the classical and the quantum initial data is preserved through time evolution. These conditions were explicitly obtained and used to construct a classicality criterion for each of the consistency criteria proposed at the beginning. We expect that the same general procedure might be used to derive the classicality criterion associated to other proposals of consistency criteria.

Ultimately, the two measures of classicality obtained are arbitrary in nature since they are a direct consequence of the definition of a consistency criterion. Therefore, they should be tested in physical examples to see if they yield sensible results. The criteria of this paper were applied to two simple dynamical systems and yield expected results. Namely, Gaussian wave functions were obtained as ''classical-like states'' (solutions of the classicality conditions).

Further applications of the criteria have been developed in Refs. 34, 35, and 36. Other possible future applications which might be of considerable interest are in the field of nonlinear dynamical systems, where the connection between classical and quantum mechanics becomes more involved.

To finish let us make a few remarks.

(i) The degree of classicality of a given quantum system is always relative to the classical description supplied (more precisely, to the classical initial data supplied). Therefore, the criteria do not provide an absolute classification of classicality but only a comparative one.

(ii) The fully classical behavior (i.e., the complete consistency with the classical predictions) is obtained in the limit case in which the quantum system fully satisfies one of the classicality criteria to all orders or equivalently, if the quantum and the classical initial data are fully consistent. Notice that consistency and classicality, in this case and in general only in this case, are equivalent notions: the results of Sec. III B 2 imply this statement directly.

(iii) The classicality conditions vary from one dynamical system to another. More precisely, once the classical initial data is given the M-order classicality conditions on the quantum initial data are more restrictive for some systems (for instance, the second example) than for others (for instance, the first example). This is not surprising, as neither is the fact that for some dynamical systems, the classicality conditions are so restrictive that there is no wave function that, for typical values of the classical data, might satisfy even the first order classicality conditions (consider for instance the system of a particle in a potential step).

(iv) The classicality criteria provide only a partial answer to the problem of measuring the degree of classicality of a general dynamical system. We were able to prove that a general dynamical system will evolve in agreement with the classical predictions up to some degree if its initial time configuration satisfies the classicality conditions up to some extent. However, these are sufficient but not necessary conditions: the system may very well not satisfy even the first order classicality criterion and still present a fairly classical-like evolution.

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Superintegrability with third-order integrals in quantum and classical mechanics

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We consider here the coexistence of first- and third-order integrals of motion in two-dimensional classical and quantum mechanics. We find explicitly all potentials that admit such integrals, and all their integrals. Quantum superintegrable systems are found that have no classical analog, i.e., the potentials are proportional to $\hbar^2$, so their classical limit is free motion. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In classical mechanics, an n-dimensional Hamiltonian system is called Liouville integrable if it allows n functionally independent integrals of motion in involution (including the Hamiltonian), that is,

$$\{H,X_i\}=0,$$
$$\{X_i,X_j\}=0,\forall i,j. \tag{1.1}$$

The Hamiltonian $H=H(x_1,\ldots,x_n,p_1,\ldots,p_n)$ and the integrals of motion $X_i=X_i(x_1,\ldots,x_n,p_1,\ldots,p_n)$ must be well defined functions on phase space.[2,13] The system is superintegrable if it allows more than n functionally independent integrals, n of them in involution. The best known superintegrable systems in n dimensions are the harmonic oscillator $V=\omega r^2$ and the Coulomb potential $V=\alpha/r$, both of them allowing $2n-1$ independent integrals of motion, the maximal number possible for an interacting system. Bertrand's theorem[2,3] tells us that these are the only rotationally invariant systems for which all finite trajectories are closed, a fact intimately related to their maximal superintegrability.

In quantum mechanics, a Hamiltonian system is said to be integrable if there exists a set $\{X_i\}$ of n well defined, algebraically independent operators (including the Hamiltonian) that commute pairwise. It is superintegrable if it possesses further independent operators, $\{Y_j\}$ that commute with the Hamiltonian. The Y_j do not necessarily commute with each other, nor with the X_i.

The definition of the independence of quantum operators is not unique, and this may give rise to different types of quantum superintegrability.

A good working definition, which may be appropriate for applications in quantum mechanics, soliton theory and for instance in the study of the Huygens principle, is that operators are considered independent unless one of them can be expressed as a polynomial in the others.[4,5,15,18] The fact that commuting operators can be useful even if they are functionally dependent in the classical limit was clearly demonstrated by Hietarinta.[15–18] This definition is in itself not quite satisfactory

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since it ignores more general polynomial or functional relations between integrals. This may lead to important differences between classical and quantum integrability. Moreover, it is not appropriate for nonpolynomial integrals. Finding an appropriate and rigorous definition of the independence of quantum operators is not an easy problem, but it is worth investigating as wrong or ambiguous definitions may give rise to incorrect results. For a discussion of related problems, see, e.g., Refs. 17 and 30.

Previous systematic searches for superintegrable systems concentrated on integrals of motion of at most second order in momenta.[7–9,12,23,31] This ''quadratic superintegrability'' has been shown to be related to multiseparability of the Schrödinger or Hamilton–Jacobi equations. More recently, it was related to generalized symmetries[27] and exact solvability.[28]

Quadratic superintegrability has been considered in spaces of nonzero constant curvature[22,25] and of nonconstant curvature.[20] For superintegrable systems in n dimensions see Ref. 26.

Our purpose in this article is to start a systematic search for superintegrable systems with higher-order integrals of motion. We consider a two-dimensional real Euclidian space with a one-particle Hamiltonian;

$$H=\frac{1}{2}(p_x^2+p_y^2)+V(x,y).$$

We request the existence of two additional integrals of motion: one of first order in the momenta and the other of third order.

The classical and quantum mechanical cases will be treated separately. When second-order integrals of motion are considered, classical and quantum integrable and superintegrable potentials coincide. For third-order integrals this is no longer the case (as was pointed out by Hietarinta in Ref. 15). For integrable systems with third- or higher-order integrals in classical mechanics, see also Refs. 6, 10, 11, 14, 19, 21, and 24.

II. CONDITIONS FOR THE EXISTENCE OF A THIRD-ORDER INVARIANT IN CLASSICAL MECHANICS

We are looking for a classical integral of motion that is a polynomial in the momenta with coefficients depending on the spatial coordinates, i.e.,

$$X=\sum_{j,k} f_{jk}(x,y)p_1^j p_2^k,$$

that Poisson-commutes with the Hamiltonian;

$$\begin{aligned} 0&=\{H,X\},\\ H&=\frac{p_1^2+p_2^2}{2}+V(x,y). \end{aligned} \tag{2.1}$$

We can simplify our search by using the fact that Eq. (2.1) implies that X is a constant over any trajectory:

$$\frac{dX}{dt}=\frac{\partial X}{\partial q_i}\dot{q}_i+\frac{\partial X}{\partial p_i}\dot{p}_i=0, \tag{2.2}$$

with

$$\begin{aligned} \dot{p}_i&=-V_{q_i}(q_1,q_2),\\ \dot{q}_i&=p_i. \end{aligned} \tag{2.3}$$

If we write explicitly X in (2.2), we find

$$\sum_{j+k=1}^{n}\left(\frac{\partial f_{jk}}{\partial x}p_1^{j+1}p_2^k+\frac{\partial f_{jk}}{\partial y}p_1^j p_2^{k+1}-f_{jk}V_x j p_1^{j-1}p_2^k-f_{jk}V_y k p_1^j p_2^{k-1}\right)=0. \tag{2.4}$$

Since the monomials $p_1^a p_2^b$'s form a basis, the coefficients for each (a,b) must vanish separately, thus (2.4) gives relations between the f_{ij} with odd and even $i+j$ separately. If we are looking for an integral of odd (even) degree in the momenta, the even (odd) terms will play no role and we can without loss of generality consider only integrals that have terms only of odd (even) parity. Moreover, we may notice, in (2.4), that the terms of leading order in the p_i's imply a relation independent of V between the $f_{i,j}$ with $i+j=n$. This allows us to find immediately the form of the leading-order terms, so the integral of motion in the third-order case takes the form

$$\begin{gathered}X=\sum_{i+j+k=3}A_{ijk}L^i p_1^j p_2^k+g_1(x,y)p_1+g_2(x,y)p_2,\\ L=xp_2-yp_1,\end{gathered} \tag{2.5}$$

where the A_{ijk} are arbitrary real constants.

The requirement $dX/dt=0$ and the Hamilton equations (2.3) yield four equations:

$$0=g_1V_x+g_2V_y, \tag{2.6}$$

$$(g_1)_x=3f_1(y)V_x+f_2(x,y)V_y, \tag{2.7}$$

$$(g_2)_y=f_3(x,y)V_x+3f_4(x)V_y, \tag{2.8}$$

$$(g_1)_y+(g_2)_x=2(f_2(x,y)V_x+f_3(x,y)V_y), \tag{2.9}$$

where

$$\begin{gathered}f_1(y)=-A_{300}y^3+A_{210}y^2-A_{120}y+A_{030},\\ f_2(x,y)=3A_{300}xy^2-2A_{210}xy+A_{201}y^2+A_{120}x-A_{111}y+A_{021},\\ f_3(x,y)=-3A_{300}x^2y+A_{210}x^2-2A_{201}xy+A_{111}x-A_{102}y+A_{012},\\ f_4(x)=A_{300}x^3+A_{201}x^2+A_{102}x+A_{003}.\end{gathered}$$

Requiring that Eqs. (2.7), (2.8), and (2.9) be compatible, we obtain a linear compatibility condition for the potential, namely

$$\begin{aligned}0=&-f_3V_{xxx}+(2f_2-3f_4)V_{xxy}+(-3f_1+2f_3)V_{xyy}-f_2V_{yyy}+2(f_{2y}-f_{3x})V_{xx}\\&+2(-3f_{1y}+f_{2x}+f_{3y}-3f_{4x})V_{xy}+2(-f_{2y}+f_{3x})V_{yy}+(-3f_{1yy}+2f_{2xy}-f_{3xx})V_x\\&+(-f_{2yy}+2f_{3xy}-3f_{4xx})V_y.\end{aligned} \tag{2.10}$$

Requiring that all four equations (2.6), (2.7), (2.8), (2.9) be compatible, we obtain further third-order equations for the potential, this time nonlinear ones. They are the limit case (for $\hbar\to 0$) of the corresponding quantum compatibility conditions (3.7)–(3.9) given below.

These conditions, together with (2.10), form an overdetermined system for the potential $V(x,y)$. The solution space will hence be rather restricted. Indeed, in 1935, Drach[6] posed the problem of finding classical Hamiltonian systems with one third-order integral. In a complex Euclidian space $E_2(\mathbf{C})$, he found ten such potentials, each one depending on arbitrary constants, not, however, on arbitrary functions. We recall that in the case of second-order integrals, one

obtains four families of potentials, each of them depending on two arbitrary functions of one variable.[12,31] They are the four most general potentials that allow the separation of variables in Cartesian, polar, parabolic and elliptic coordinates, respectively.

III. CONDITIONS FOR THE EXISTENCE OF A THIRD-ORDER INVARIANT IN QUANTUM MECHANICS

Here we are interested in the existence of third-order operators, i.e.,

$$X=\sum_{i+j=0}^{3} P_{ij}(x,y)p_1^i p_2^j,$$

$$p_1=-i\hbar\partial_x,\quad p_2=-i\hbar\partial_y,$$

that commute with the Hamiltonian. An equivalent way of writing this operator is

$$X=\sum_{i+j=0}^{3} \{P_{ij}(x,y),p_1^i p_2^j\}.$$

Here the bracket means the anticommutator:

$$\{f,p_1^j p_2^k\}=fp_1^j p_2^k+p_1^j p_2^k f.$$

Each of these anticommutators can be expressed as

$$\{f,p_1^j p_2^k\}^+ + i\{f,p_1^j p_2^k\}^- = \{\Re e[f],p_1^j p_2^k\}+i\{\Im m[f],p_1^j p_2^k\}.$$

Hence we can write the operator X in the form

$$X=X^+ + iX^-,$$

where X^+ and X^- are self-adjoint operators. As the Hamiltonian itself is self-adjoint, $X^\dagger = X^+ - iX^-$ must also commute, as well as X^+ and X^-. These two last operators commute under the same conditions, so we may restrict our search without loss of generality to self-adjoint operators. This turns out to be quite useful in view of the following result.

Proposition 3.1: For each self-adjoint integral of motion of order n, there exists one integral of order n with definite parity, i.e.,

$$X_n=\sum_{j=0}^{[n/2]}\sum_{k=0}^{n-2j} \{P_{n-2j,k}(x,y),p_1^k p_2^{n-2j-k}\}, \tag{3.1}$$

where P is a real function.

Proof: This is simply due to the fact that we have a real Hamiltonian and a purely imaginary momentum operator, so terms of even order, which are real, must commute independently of the terms of odd order, which are purely imaginary. □

In the case $n=3$ we restrict ourselves to third-order integrals of the form

$$X_3=\sum_{i+j=3} \{f_{ij}(x,y),p_1^j p_2^k\}+\{g_1(x,y),p_1\}+\{g_2(x,y),p_2\}.$$

Requesting

$$0=[H,X],$$

$$H=\frac{1}{2m}(p_1^2+p_2^2)+V(x,y),$$

we find a set of 15 differential equations, of which the first nine can be explicitly solved to give

$$X=\sum_{\substack{i,j,k\\ i+j+k=3}} A_{ijk}\{L_3^i,p_1^j p_2^k\}+\{g_1(x,y),p_1\}+\{g_2(x,y),p_2\}, \tag{3.2}$$

where the A_{ijk} are arbitrary real constants. So far this is similar to the classical case.

Remark 1: The argument used in demonstrating Proposition 3.1 can be generalized to any expression involving the anticommutators of self-adjoint operators homogeneous in the p_i's, for example, to terms of the form $\{L_3^i,p_1^j p_2^k\}$, as long as the coefficients of the p_i's are real.

We could get rid of the $\hbar$ and m factors by a dilation of the undetermined functions,

$$V(x,y)=\frac{\hbar^2}{2m}\tilde{V}(x,y),$$

$$g_1(x,y)=\hbar^2 g_1'(x,y),$$

$$g_2(x,y)=\hbar^2 g_2'(x,y).$$

This is equivalent to setting $\hbar$ and m equal to one, which we could do, but we prefer to keep track of the dependence on $\hbar$ (while setting $m=1$), in order to see the classical limit.

We are left with a set of 6 equations, two of which are consequences of the other four, so that, as in the classical case, we have to solve four equations:

$$0=g_1V_x+g_2V_y-\frac{\hbar^2}{4}(f_1V_{xxx}+f_2V_{xxy}+f_3V_{xyy}+f_4V_{yyy}+8A_{300}(xV_y-yV_x)$$
$$+2(A_{210}V_x+A_{201}V_y)), \tag{3.3}$$

$$(g_1)_x=3f_1(y)V_x+f_2(x,y)V_y\equiv h_1, \tag{3.4}$$

$$(g_2)_y=f_3(x,y)V_x+3f_4(x)V_y\equiv h_2, \tag{3.5}$$

$$(g_1)_y+(g_2)_x=2(f_2(x,y)V_x+f_3(x,y)V_y)\equiv h_3. \tag{3.6}$$

Equations (3.4) to (3.6) are the same as in the classical case, however, Eq. (3.3) differs from Eq. (2.6) by the terms proportional to $\hbar^2$. Both in the classical and quantum cases we can eliminate g_1 and g_2 and obtain compatibility conditions for the potentials.

We shall write these in a unified manner for both cases. One such compatibility condition is the third-order linear equation (2.10). To write three more conditions we introduce the notation

$$\phi_1=\frac{V_y}{V_x},$$

$$\phi_2=-\hbar^2\frac{(f_1V_{xxx}+f_2V_{xxy}+f_3V_{xyy}+f_4V_{yyy}+8A_{300}(xV_y-yV_x)+2(A_{210}V_x+A_{201}V_y))}{4V_x},$$

and use h_1, h_2 and h_3 introduced in (3.4), (3.5) and (3.6). In the classical case we have $\phi_2=0$. The three (independent) nonlinear compatibility conditions are

$$-\phi_{2x}+\left(\frac{\phi_1(h_3\phi_1+h_2\phi_1^2+\phi_1\phi_{2y}+\phi_{2x}+h_1)}{\phi_{1x}+\phi_1\phi_{1y}}\right)_x=h_1, \tag{3.7}$$

$$\left(\frac{\phi_1^2h_2+\phi_1\phi_{2y}+\phi_1h_3+\phi_{2x}+h_1}{\phi_{1x}+\phi_1\phi_{1y}}\right)_y=-h_2, \tag{3.8}$$

$$\begin{aligned}&h_1(\phi_{1xy}+\phi_{1y}^2)+h_2(\phi_1^2\phi_{1xy}-\phi_{1x}^2-2\phi_1\phi_{1x}\phi_{1y})+h_3(\phi_1\phi_{1xy}-\phi_{1x}\phi_{1y})\\&\quad-(h_{1y}+\phi_1h_{2x})(\phi_{1x}+\phi_1\phi_{1y})\\&\quad=-\phi_{2x}(\phi_{1xy}+\phi_{1y}^2)+\phi_{2y}(\phi_{1x}\phi_{1y}-\phi_{1xy}\phi_1)+\phi_{2xy}(\phi_{1x}+\phi_1\phi_{1y}).\end{aligned} \tag{3.9}$$

In the quantum case these are fifth-order equations for the potential. They can be used to express ϕ_{2xy}, ϕ_{2xx} and ϕ_{2yy} in terms of ϕ_{2x}, ϕ_{2y} and ϕ_2. In the classical case we set $\phi_2=0$, but the equations remain algebraically independent. They can be used to determine ϕ_{1xy}, ϕ_{1xx} and ϕ_{1yy} in terms of ϕ_{1x}, ϕ_{1y} and ϕ_1. The nonlinear equations for $V(x,y)$ are third-order ones in the classical case.

In deriving these equations we have assumed

$$\begin{aligned}\phi_{1x}+\phi_1\phi_{1y}&\neq 0,\\ \phi_{1xy}\phi_1-\phi_{1x}\phi_{1y}&\neq 0.\end{aligned} \tag{3.10}$$

The cases when the above conditions do not hold must be considered separately. This will actually be the case for potentials considered in Sec. IV.

We also mention the interesting fact, already noticed by Hietarinta,[16] that a classical integrable potential is also quantum integrable, if and only if it respects the compatibility condition

$$f_1V_{xxx}+f_2V_{xxy}+f_3V_{xyy}+f_4V_{yyy}+8A_{300}(xV_y-yV_x)+2(A_{210}V_x+A_{201}V_y)=0. \tag{3.11}$$

In that case the equations are invariant under a simultaneous dilation of the potential and the g_i's. Thus any potential that is a solution to both (2.6) to (2.9) and (3.11) can be multiplied by an arbitrary factor, which can be used to "absorb" the $\hbar^2$ factor so the solution does not vanish in the classical limit.

Even if a classical superintegrable potential does not satisfy this relation, there could exist corresponding quantum superintegrable systems. In that case, though, the equations are not invariant under a dilation of the potential as in the previous case, so terms that do not satisfy both (3.11) and (2.6) to (2.9) must be proportional to $\hbar^2$ and vanish in the classical limit.

We will show that condition (3.11) cannot be the consequence of Eqs. (3.4), (3.5) and (3.6) for in that case the classical and quantum integrable potentials would be the same.

IV. SUPERINTEGRABLE SYSTEMS WITH ONE THIRD-ORDER AND ONE FIRST-ORDER INTEGRAL

A. Integral of first order

A potential $V(x,y)$ allows an integral that is of first order in the momenta if and only if it is invariant under either rotations or translations. Thus the potential must satisfy

$$aL_3V+bp_1V+cp_2V=0.$$

Without loss of generality, we can take the potential and first-order integral to be one of the following:

- $a\neq 0$: $\quad V=V(r), \quad X=L_3,$

- $a=0,\ b^2+c^2\neq 0:\ \ V=V(x),\ \ X=p_2.$

B. Quantum and classical superintegrable potentials invariant under rotations

Compatibility conditions obtained from Eqs. (2.6) to (2.9) or (3.3) to (3.6) leave us with only two possibilities, namely,

$$V=\frac{\alpha}{r},$$

$$V=\omega^2 r^2,$$

the Coulomb potential and the harmonic oscillator, which are the best-known superintegrable potentials in any dimension. In addition to angular momentum L_3, the Coulomb potential in E_2 allows two second-order integrals, namely the components of the Laplace–Runge–Lenz vector:

$$X_1^C=\{L_3,p_1\}-\frac{2\alpha y}{r};$$

$$X_2^C=\{L_3,p_2\}+\frac{2\alpha x}{r}.$$

The harmonic oscillator, in addition to angular momentum, allows two second-order integrals which are the components of a quadrupole tensor;

$$X_1^h=-\tfrac{1}{2}p_1^2+\tfrac{1}{2}p_2^2+\omega^2x^2-\omega^2y^2;$$

$$X_2^h=-p_1p_2+2\omega^2xy.$$

Commuting (or Poisson commuting) second-order integrals, we in general find third-order integrals.

The third-order integrals obtained for these potentials are indeed direct consequences of integrals at order one and two.

C. Classical superintegrable potentials invariant under translation

In the classical case, the remaining equations are readily solved. If we set $V_y=0$, Eqs. (2.6) to (2.9) simplify to

$$0=g_1,$$

$$0=A_{300}=A_{210}=A_{120}=A_{030},$$

$$(g_2)_y=f_3(x,y)V_x,$$

$$(g_2)_x=2\,f_2(x,y)V_x.$$

We can at once set A_{021} and A_{003} to 0, for they correspond to trivial constants of motion, p_2^3 and Hp_2, that can be subtracted from the constant (2.5).

The compatibility condition between the two last equations forces one of the three following conditions to be satisfied (up to a translation in x):

$$V=ax, \tag{4.1}$$

$$V=\frac{a}{x^2}, \tag{4.2}$$

$$A_{201}=A_{111}=A_{102}=A_{012}=0. \tag{4.3}$$

The first two potentials correspond to superintegrable systems that have one first- and at least one second-order integral. Their third-order integrals can be obtained by commutation of these lower-order ones.

The last conditions forbid the existence of a nontrivial third-order commuting operator for any other potentials than (4.1) and (4.2).

D. Quantum superintegrable potentials invariant under translation

Here the situation is more interesting. Equations (3.3) to (3.6) reduce to

$$0=g_1V_x-\frac{\hbar^2}{4}(f_1V_{xxx}-8yA_{300}V_x+2A_{210}V_x), \tag{4.4}$$

$$(g_1)_x=3f_1(y)V_x, \tag{4.5}$$

$$(g_2)_y=f_3(x,y)V_x, \tag{4.6}$$

$$(g_1)_y+(g_2)_x=2(f_2(x,y)V_x). \tag{4.7}$$

The linear compatibility condition leads to two equations (since coefficients of y^0 and of y^1 must vanish separately), namely,

$$\begin{aligned}0&=(A_{210}x^2+A_{111}x+A_{012})V_{xxx}+4(2A_{210}x+A_{111})V_{xx}+12A_{210}V_x;\\ 0&=(3A_{300}x^2+2A_{201}x+A_{102})V_{xxx}+4(6A_{300}x+2A_{201})V_{xx}+36A_{300}V_x.\end{aligned} \tag{4.8}$$

The two equations are similar and easy to solve, but it turns out their only solutions that also satisfy (4.4) to (4.7) are again the potentials $V=ax$ and $V=a/x^2$. Their third-order integrals in general are direct consequences of lower-order commuting operators, that is, they can be obtained by commuting their second-order integrals. In the $V=a/x^2$ case, we find three third-order integrals:

$$X_1=\{L_3^2,p_2\}+a\left\{2\frac{y^2}{x^2},p_2\right\},$$

$$X_2=\{L_3,p_1p_2\}-a\left\{2\frac{y}{x^2},p_2\right\},$$

$$X_3=2p_1^2p_2+a\left\{\frac{2}{x^2},p_2\right\}.$$

The integrals X_2 and X_3 can be obtained by commuting X_1 with the first-order integral p_2.

In the particular case $V=\hbar^2/x^2$, we find four more integrals, again related to each other by commutation with p_2:

$$X_4=2L_3^3+\hbar^2\left\{\frac{3y^2}{x}+x,p_2\right\}+\hbar^2\left\{\frac{-3y^3}{x^2}-2y,p_1\right\},$$

$$X_5=\{L_3^2,p_1\}-\hbar^2\left\{\frac{2y}{x},p_2\right\}+\frac{\hbar^2}{2}\left\{\frac{6y^2}{x^2}+1,p_1\right\},$$

$$X_6=\{L_3,p_1^2\}+\hbar^2\left\{\frac{1}{x},p_2\right\}+\hbar^2\left\{\frac{-3y}{x^2},p_1\right\},$$

$$X_7=2p_1^3+\hbar^2\left\{\frac{3}{x^2},p_1\right\}.$$

In this case we find nine third-order integrals, two of which are trivial (Hp_2 and p_2^3), and four are purely quantum integrals. In the classical limit they correspond to integrals of the free motion. Only the first three can be associated with the corresponding classical integrals of $V=a/x^2$.

The most interesting potentials are obtained by setting all the A_{ijk} involved in (4.8) equal to 0. The expressions for f_1, f_2, f_3, f_4 greatly simplify and Eqs. (4.4) to (4.7) can be solved directly. The nonlinear compatibility condition for these four equations reduces to

$$\hbar^2V'(x)^2=4V(x)^3+\alpha V(x)^2+\beta V(x)+\gamma, \tag{4.9}$$

where the α, β, γ are arbitrary real integration constants. Equation (4.9) is the well-known equation for elliptic functions which can be rewritten as

$$\hbar^2V'(x)^2=4(V(x)-A_1)(V(x)-A_2)(V(x)-A_3). \tag{4.10}$$

The constants A_i are either all real, or one of them is real and the other two are complex conjugated. If all three constants are real, we obtain either finite or singular potentials of the form

$$V_1=(\hbar\omega)^2k^2sn^2(\omega x,k),$$
$$V_2=\frac{(\hbar\omega)^2}{sn^2(\omega x,k)}, \tag{4.11}$$

respectively.

If we have, e.g., $A_3=A_2^*$ and $\mathrm{Im}\,A_2\neq 0$, we obtain the singular potential

$$V_3=\frac{(\hbar\omega)^2}{2(cn(\omega x,k)+1)}$$

(throughout we have $0\leqslant k\leqslant 1$, $\omega\in\mathbf{R}$).

The special cases with $k=0$ or $k=1$, which arise when two roots coincide, can be expressed in terms of elementary functions. The most interesting example is the ''soliton'' potential,

$$V_{1a}=\frac{(\hbar\omega)^2}{\cosh^2(\omega x)},$$

obtained by setting $k=1$ in V_1. If we set $k=0$, or $k=1$ in V_2, we get a singular periodic, or nonperiodic potential, respectively, namely

$$V_{2a}=\frac{(\hbar\omega)^2}{\sin^2(\omega x)},$$

$$V_{2b}=\frac{(\hbar\omega)^2}{\sinh^2(\omega x)}.$$

For all these potentials ω is an arbitrary constant, hence there exist potentials of arbitrary amplitude for all nonzero values of $\hbar$.

Finally, if all roots coincide, we reobtain the known superintegrable potential,

$$V_4=\frac{\hbar^2}{x^2},$$

which explains the extra integrals found previously for that potential.

The other potentials V_1, V_2, V_3 also satisfy

$$\frac{\hbar^2}{4}\frac{V_{xxx}}{V_x}-3V=-\sigma, \quad \sigma=A_1+A_2+A_3,$$

a consequence of (4.9).

The two nontrivial integrals of motion for all these potentials can be written as

$$X_1=\{L_3,p_1^2\}+\{(\sigma-3V(x))y,p_1\}+\left\{-\sigma x+2xV(x)+\int V(x)dx,p_2\right\},$$
$$X_2=p_1^3+\frac{1}{2}\{3V(x)-\sigma,p_1\}. \tag{4.12}$$

The second integral can be trivially obtained by the commutation of the first one with p_2.

V. CONCLUSION

We have found all potentials in two-dimensional Euclidian space E_2 that allow one first- and at least one third-order integral of motion. In the classical case the result provides no new superintegrable potentials; all the potentials found allow second-order integrals and the third-order integrals are consequences of the second-order ones. In the case of quantum mechanics the result is quite different. Any potential satisfying the elliptic function equation (4.9) will be superintegrable in the above sense, i.e., it will allow the first-order integral p_2 and two nontrivial third-order integrals. All those ''behave well'' in the classical limit, that is, they are proportional to $\hbar^2$ and therefore their classical limit is the (superintegrable) free motion.

No new superintegrable systems are found for rotationally invariant potentials $V(r)$, neither in the classical nor in the quantum case. Thus all potentials found above are of the form $V=V(x)$, i.e., are actually one-dimensional. The problem, however, remains two-dimensional as the kinetic energy and the integrals of motion also involve the y direction.

There is also an interesting link with soliton theory.[1] All new superintegrable potentials obtained above are also translationally invariant solutions of the Korteweg-de Vries equation. The same potentials occur in the rational, trigonometric and elliptic Calogero–Moser–Sutherland models.[29]

The difference between classical and quantum integrable and superintegrable systems with higher-order symmetries makes the systematic search for such systems very interesting. First of all, Drach's study of classical integrable systems should be completed. His systems are really complex ones and most of them do not exist in real Euclidian space. Moreover it is not clear how complete his list is. On the other hand, Rañada[24] has shown that 7 out of 10 Drach potentials are ''reducible'' in the sense that they are superintegrable and allow two second-order integrals. The third-order integral found by Drach is the Poisson commutator of the second-order ones.

The problem of classifying quantum systems with third-order integrals remains open and the conditions of Sec. III provide the means for finding all such systems.

Work is in progress on superintegrable systems in two-dimensional Euclidian space with one second- and one third-order invariant, as well as with two third-order ones.

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Convexity and potential sums for Salpeter-type Hamiltonians

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The semirelativistic Hamiltonian $H=\beta\sqrt{m^2+p^2}+V(r)$, where $V(r)$ is a central potential in $\Re^3$, is concave in p^2 and convex in $p\equiv\sqrt{p^2}$. This fact enables us to obtain complementary energy bounds for the discrete spectrum of H. By extending the notion of ''kinetic potential'' we are able to find general energy bounds on the ground-state energy E corresponding to potentials with the form $V=\Sigma_i a_i f^{(i)}(r)$. In the case of sums of powers and the log potential, where $V(r)=\Sigma_{q\neq 0}a(q)\mathrm{sgn}(q)r^q+a(0)\ln(r)$, the bounds can all be expressed in the semiclassical form $E\approx\min_r\{\beta\sqrt{m^2+(1/r^2)}+\Sigma_{q\neq 0}a(q)\mathrm{sgn}(q)(rP(q))^q+a(0)\ln(rP(0))\}$. ''Upper'' and ''lower'' P numbers are provided for $q=-1,1,2$, and for the log potential $q=0$. Some specific examples are discussed, to show the quality of the bounds. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1515381]

I. INTRODUCTION

The Hamiltonian $H=K+V$ for the problems we study has the feature that either the kinetic energy K or the potential energy V is nonlocal. The most important example is the semirelativistic ''spinless-Salpeter'' Hamiltonian[1–4] given by

$$H=K(p)+V(r)=\sqrt{m^2+p^2}+V(r), \tag{1.1}$$

where $r\equiv\|\mathbf{r}\|$, $\mathbf{r}\in\Re^3$, and $p\equiv\|\mathbf{p}\|\equiv\sqrt{\mathbf{p}^2}$. In this form at least $K(p)$ is nonlocal in configuration space and is defined as a multiplicative operator in momentum space. That is to say, $K\psi$ is defined to be what we get when ψ is transformed to momentum space, the multiplicative operator K is applied, and the result is transformed back to coordinate space. Nonlocality is the main source of difficulty for this class of problems. We study the discrete spectra of these Hamiltonians by the use of approaches that make use of convexity and of spectral information already obtained concerning related problems. In an earlier paper[4] we studied the relationship between $H_0=K+h$ and $H=K+g\circ h$, where $g(h(r))$ is a smooth transformation of a 'base' potential $h(r)$. For cases in which g had definite convexity, one could then employ the so-called kinetic-potential[5] formalism and envelope theory[6] to construct upper or lower bounds to the discrete eigenvalues of H by using the known spectrum of H_0.

The present paper has two distinct aspects: we turn our attention firstly to the convexity of K, as a function of p or p^2; and then we look at potentials that are a *sum* of terms $V=\Sigma_i V^{(i)}$. In Sec.

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II we extend the kinetic-potential formalism to include more general kinetic-energy operators than the Schrödinger form $K=p^2$ studied earlier.[5] We have already found[7] some implications of the fact that K is *concave* in p^2. The spectral implications of the *convexity* of K in p demand a new analysis. By using Jensen's inequality[8] we are able to construct a framework in Sec. III which accommodates both cases. Although it may not be immediately apparent, the treatment of potential *sums* also leads to an interesting convexity analysis of a completely different type.[9,10] This in turn yields an optimized general lower bound for the bottom of the spectrum expressed in terms of the kinetic potentials generated by 'component' problems $K+V^{(i)}$. We discuss this in general terms in Sec. IV. In the special case in which the component problems are pure-power potentials or the log potential, that is to say

$$V(r)=\sum_{q\neq 0} a(q)\mathrm{sgn}(q)r^q+a(0)\ln(r), \tag{1.2}$$

the lower bound (Sec. V) and also upper bounds obtained by variational methods (Sec. VI) can all be expressed in terms of a semiclassical expression of the form

$$E\approx\min_r\left\{\sqrt{m^2+\frac{1}{r^2}}+\sum_{q\neq 0} a(q)\mathrm{sgn}(q)(rP(q))^q+a(0)\ln(rP(0))\right\}. \tag{1.3}$$

It is the goal of this paper to develop a general theory which leads to such a result and, in particular, to determine P numbers which guarantee that the approximation (1.3) is an upper or lower bound. We shall find the appropriate upper and lower $P(q)$ for the cases $q=-1,1,2$, and for the log potential $q=0$. In Sec. VII we apply our general results to some specific examples.

Although we obtain very concrete results in the end, our study begins with a somewhat abstract viewpoint. We now make a few general remarks that will help motivate these starting considerations. An idea that runs through the work is one well known to those who study nonlinear problems: we try to use transformations to make the most of any soluble problem that is at hand, or, at least, one for which we have a good approximation. The setting for our ideas is geometrical. We suppose that we have an exact solution (or good bounds) for a base problem with Hamiltonian $\alpha p^2+\beta h(r)$, and we are interested in a Hamiltonian of the form $H=k(p^2)+g(h(r))$, where k and g are monotone increasing smooth transformations. It follows that the tangent spaces to H are Schrödinger operators with the general form $H^{(\mathbf{t})}=a+bp^2+ch(r)$, where the parameters $\{a,b,c\}$ depend on the contact vector $\mathbf{t}$. What we look for is a theory that would allow us to deduce spectral information about H from the known spectrum of its tangents $H^{(\mathbf{t})}$. For example, if the transformation functions k and g are both concave, we would expect to obtain upper bounds via the spectral inequality $H<H^{(\mathbf{t})}$. *Mutatis mutandis*, a complimentary theory is possible with operator tangent spaces of the form $H^{(\mathbf{t})}=a+bp+ch(r)$, where $K(p)$ is *convex* in p and $g(h)$ is convex in h: this leads to energy *lower* bounds. Since we have already explored[4] the potential transformation g, the main thrust of the present paper concerns kinetic-energy transformations with base problems, respectively, p^2+h and $p+h$ and to applications of the results when the potential in H is a sum of terms. The more general case in which neither transformation $k(p)$ nor $g(h)$ is the identity follows immediately by combining the present and earlier results; hence we do not need to discuss this natural generalization in detail here. Coulomb components present a special difficulty for a lower bound with kinetic energy p because the operator $p-v/r$ has no discrete eigenvalues. However, for our main concern, the Salpeter Hamiltonian, we are able to make use of the very good Coulomb lower bound of Martin and Roy[11] and so incorporate the Coulomb contribution smoothly into our general formulation.

II. VARIETY OF KINETIC POTENTIALS

The discrete eigenvalues of the self-adjoint operators we study may be characterized variationally. Thus the bottom of the spectrum E of $H=K+V$ is given by $E=\inf(\psi,H\psi)$, where the

infimum is taken over all normalized functions in the domain $\mathcal{D}(H)\subset L^2(\Re^3)$. The idea behind kinetic potentials is to perform the minimization in two stages: we first find the constrained minimum $\overline{V}(K;s)$ of $(\psi,V\psi)$, keeping the mean kinetic energy $(\psi,K\psi)=s$ constant; then, we recover E by minimizing over the kinetic energy $s>0$. Thus we have

$$\overline{V}(K;s)=\inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}}(\psi,V\psi)\ \Rightarrow\ E=\min_{s>0}\{s+\overline{V}(K;s)\}. \tag{2.1}$$

We call the function $\overline{V}(K;s)$ the kinetic potential of V associated with the kinetic-energy operator K; we shall write simply $\overline{V}(s)$, if the kinetic-energy operator K is fixed or is clear from the context. It follows immediately from the definition that the kinetic potentials absorb a positive coupling parameter in the sense that $\overline{cV}(s)=c\overline{V}(s)$. We note also that the elementary

Comparison theorem:

$$\overline{V}^{(1)}(s)<\overline{V}^{(2)}(s)\ \Rightarrow\ E^{(1)}<E^{(2)}$$

follows immediately from (2.1). The arguments we use are not restricted to dimension $N=3$: this choice allows us to illustrate the general results with some explicit well-known examples, without the distraction of the operator dependencies on N.

The reason for using this description of the spectral problem is that it lends itself to some interesting approximations. First, we have shown in the Schrödinger[5] and Salpeter[4] cases that, if $V(r)=g(h(r))$ and g is monotone increasing and has definite convexity, then the approximation $\overline{V}(s)\approx g(\overline{h}(s))$ leads to lower bounds if g is convex and upper bounds if g is concave. In Sec. IV of the present paper we shall extend to general K the result obtained earlier[10] for the Schrödinger case that kinetic potentials are subadditive, that is to say

$$V(r)=h^{(1)}(r)+h^{(2)}(r)\ \Rightarrow\ \overline{V}(s)\geqslant\overline{h}^{(1)}(s)+\overline{h}^{(2)}(s). \tag{2.2}$$

The lower energy bound then immediately follows from the above-mentioned comparison theorem for kinetic potentials. There is more to this result than meets the eye: it generates the optimum of a family of lower bounds; the details will be given in Sec. IV. Extensions to sums with more than two terms (or, further, to mixtures generated by an integral) are immediate. The principal limitation is that each potential term alone, when added to the kinetic energy, must, for large enough coupling, support a discrete eigenvalue. Thus $V(r)=-1/r+r$ is allowed but $V(r)=1/r+r$ is not.

The component kinetic potential $\overline{h}(s)=\overline{h}(K;s)$ can be constructed by use of a Legendre transformation from the eigenvalue function $E=F(v)$, in which $F(v)$ is the bottom of the spectrum of $H=K+vh(r)$, as a function of the coupling v. In the Schrödinger case $H=p^2+vh(r)$ we have shown that $F(v)$ is concave[5] and moreover the kinetic potential for $K=p^2$ is given in terms of $F(v)$ by the transformation

$$s=F(v)-vF'(v),\quad \overline{h}(K;s)=F'(v). \tag{2.3}$$

The concavity of the eigenvalue function $F(v)$ has been proved for the Schrödinger case[5] and the Salpeter case[4] by the application of a simple variational argument. By exactly similar reasoning we can show that the eigenvalue function for the operator $p+vh(r)$ is also concave in v. Moreover, the Legendre transformation (2.3) is generic: it is valid for all kinetic-energy operators K. This is an immediate consequence of the concavity of $F(v)$, as the following equations clearly demonstrate:

$$F(v)=\min_{u>0}\{F(u)-uF'(u)+vF'(u)\}=\min_{s>0}\{s+v\overline{h}(K;s)\}.$$

Our principal assumption concerning K is that it is at once a convex function of p and a concave function of p^2. This convexity is clearly true for our most important example, the relativistic kinetic energy $K=\sqrt{m^2+p^2}$; however, we shall use this specific form only when we need to.

We now turn from the general to some very specific results. We shall need to have at our disposal some component kinetic potentials for the operators $K+v\ \mathrm{sgn}(q)r^q$, where $K=p$, or the Schrödinger case $K=p^2$. By elementary scaling arguments we can show that the dependence of the energy functions on the coupling v are given by

$$p+v\ \mathrm{sgn}(q)r^q \Rightarrow E=F^{(1)}(q;v)=F^{(1)}(q;1)v^{1/(1+q)} \tag{2.4a}$$

and

$$p^2+v\ \mathrm{sgn}(q)r^q \Rightarrow E=F^{(2)}(q;v)=F^{(2)}(q;1)v^{2/(2+q)}. \tag{2.4b}$$

The Legendre transformation $F\leftrightarrow\overline{h}$ given above in (2.3) now allows us to deduce the precise forms of the corresponding kinetic potentials. For convenience we choose to write the kinetic potentials so obtained in a special way. We change variables for the mean kinetic energy s in the two cases, respectively, to $s=1/r$ and $s=1/r^2$. It then follows from (2.3) by straightforward algebraic computations that the kinetic potentials for $h(r)=\mathrm{sgn}(q)r^q$ have similar convenient forms, namely

$$\overline{h}(p;1/r)=\mathrm{sgn}(q)(P^{(1)}(q)r)^q \tag{2.5a}$$

and

$$\overline{h}(p^2;1/r^2)=\mathrm{sgn}(q)(P^{(2)}(q)r)^q, \tag{2.5b}$$

where the P numbers are *defined* in terms of the $v=1$ eigenvalues $E^{(i)}(q)=F^{(i)}(q;1)$, $i=1,2$, respectively, by the explicit formulas

$$K=p \Rightarrow P^{(1)}(q):=\left|\frac{E^{(1)}(q)}{1+q}\right|^{1+1/q}|q|, \quad q>-1, \quad q\neq 0 \tag{2.6a}$$

and

$$K=p^2 \Rightarrow P^{(2)}(q):=\left|\frac{E^{(2)}(q)}{1+q/2}\right|^{1/2+1/q}\left|\frac{q}{2}\right|^{1/2}, \quad q>-2, \quad q\neq 0. \tag{2.6b}$$

The energies are related to the kinetic potentials by specific realizations of the general formula (2.1): for example, we have in this spectral representation

$$p+v\ \mathrm{sgn}(q)r^q \Rightarrow E=\min_{r>0}\left\{\frac{1}{r}+v\ \mathrm{sgn}(q)(P^{(1)}(q)r)^q\right\}, \quad q>-1, \quad q\neq 0. \tag{2.7}$$

One of our side goals is purely esthetic, namely we wish to end up with attractive formulas: after the changes of variable from s to r, the kinetic potentials look like the original power potentials themselves, but with the P factors inserted. We turn now to the base potential $h(r)=\ln(r)$ and find by scaling arguments that

$$p+v\ \ln(r) \Rightarrow F^{(1)}(v)=vF^{(1)}(1)-v\ \ln(v) \tag{2.8a}$$

and

$$p^2+v\ \ln(r) \Rightarrow F^{(2)}(v)=vF^{(2)}(1)-\tfrac{1}{2}v\ \ln(v). \tag{2.8b}$$

TABLE I. Eigenvalues for $v=1$ and corresponding P numbers [given by (2.6) and (2.10)] for the Coulomb, log, linear, and harmonic-oscillator potentials. The eigenvalues have been computed numerically and are rounded so that the $E^{(1)}(q)$ are lower bounds and the $E^{(2)}(q)$ are upper bounds (and similarly for the derived P numbers). The Coulomb lower bound is treated differently because $H=p-1/r$ has no discrete spectrum.

q	$E^{(1)}(q)$	$P^{(1)}(q)$	$E^{(2)}(q)$	$P^{(2)}(q)$
-1			$-\frac{1}{4}$	1
0	1.063 65	1.0657	1.044 3325	1.218 669
1	2.232 25	1.2457	2.338 1075	1.376 084
2	2.338 107	1.366 687	3	$\frac{3}{2}$

Consequently we obtain from the transformation (2.3),

$$\overline{h}(p;1/r)=\ln(P^{(1)}(0)r), \quad \overline{h}(p^2;1/r^2)=\ln(P^{(2)}(0)r), \tag{2.9}$$

where

$$P^{(1)}(0)=\exp(E^{(1)}(0)-1), \quad P^{(2)}(0)=\frac{1}{\sqrt{2}}\exp\left(E^{(2)}(0)-\frac{1}{2}\right). \tag{2.10}$$

For the discussion of examples we shall need to have some specific P values. For the cases $q=-1,0,1,2$ we supply some of these numerical values in Table I. This table has an eigenvalue symmetry because of the operator equivalence $p+r^2\sim p^2+r$; it also has two omissions corresponding to $q=-1$, because $p-1/r$ has no discrete eigenvalues. We offer now a solution to this Coulomb difficulty. As we shall make clear in Sec. IV, viable Coulomb P numbers are needed for *lower* bounds. For our most important application $K=\sqrt{p^2+m^2}$, a lower bound to the bottom of the spectrum of $H=K-v/r$ is provided by the Martin–Roy bound[11]

$$E\geqslant e_L(v)=m\left(\frac{1+\sqrt{1-4v^2}}{2}\right)^{1/2}, \quad v<\frac{1}{2}. \tag{2.11}$$

The condition $v<\frac{1}{2}$ is a little more restrictive than the fundamental operator restriction $v<2/\pi$: it was proved by Herbst[12] that a Friedrichs extension exists for H only if the Coulomb coupling is sufficiently small. The Coulomb lower bound has the same scaling law with respect to m as does the exact energy: although m originates in the Hamiltonian inside the square root of the kinetic-energy term, it appears in the eigenvalue and in its lower approximation simply as an overall factor.[4] Now we construct a v-dependent P representation for this lower bound. We write [as a definition of $P_L(v)$]

$$e_L(v)=\min_r\left\{\sqrt{m^2+\frac{1}{r^2}}-\frac{v}{P_L(v)r}\right\}. \tag{2.12}$$

An elementary calculation then shows that (2.11) and (2.12) imply $P_L(v)=e_L(v)/m$. This serendipitous discovery fills the gaps in Table I, and will allow us to include the Coulomb component in our lower-bound energy formula for sums of potential terms: we must make the substitution

$$-\frac{v}{P^{(1)}(-1)r}=-\frac{v}{P_L(v)r}=-\frac{mv}{e_L(v)r}, \quad v<\frac{1}{2}. \tag{2.13}$$

III. COMPLEMENTARY CONVEXITY: $p+V$ AND p^2+V

The principal result of this section is best expressed in terms of kinetic potentials by the following.

Theorem 1: *If E is the bottom of the spectrum of the Hamiltonian $H=K+V$, and the kinetic-energy operator K is at once convex in p and concave in p^2, then it follows that*

$$\min_{s>0}\{K(s)+\overline{V}(p;s)\}\leqslant E\leqslant\min_{s>0}\{K(s)+\overline{V}(p^2;s^2)\}. \tag{3.1}$$

It makes sense here to speak of $K(p)$ as though p were a real variable since, by definition, the action of the operator K is effected via the Fourier transform. We shall now prove this result by an application of Jensen's inequality[8] and kinetic potentials defined in (2.1). We consider first the left-hand inequality of the theorem. If ψ is a normalized function in the domain $\mathcal{D}(H)$ of $H=K+V$, then, since $K=K(p)$ is convex in p, by Jensen's inequality, we have

$$E=\inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1}}\{(\psi,K(p)\psi)+(\psi,V\psi)\}\geqslant\inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1}}\{K((\psi,p\psi))+(\psi,V\psi)\}.$$

That is to say,

$$E\geqslant\min_{s>0}\inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,p\psi)=s}}\{K((\psi,p\psi))+(\psi,V\psi)\}=\min_{s>0}\{K(s)+\overline{V}(p;s)\}.$$

The proof of the upper-bound inequality is very similar: we write $K(p)=k(p^2)$, where k is concave; then, setting $t=s^2$, we arrive at the inequality

$$E\leqslant\min_{t>0}\{k(t)+\overline{V}(p^2;t)\}=\min_{s>0}\{K(s)+\overline{V}(p^2;s^2)\},$$

which establishes the theorem. □

This result is an essential ingredient in the proof of the sum approximation in the next section. We now look at an example, namely the Salpeter problem with a linear potential. We have

$$H=\sqrt{m^2+p^2}+V(r),\quad V(r)=vh(r)=vr, \tag{3.2}$$

where v is a positive coupling parameter. In terms of the convenient variable $r>0$ the two kinetic potentials from (2.5) are

$$\overline{h}(p;1/r)=P^{(1)}(1)r,\quad \overline{h}(p^2;1/r^2)=P^{(2)}(1)r, \tag{3.3}$$

where the P numbers are provided in Table I. Theorem 1 then immediately yields the bounds

$$\min_{r>0}\{\sqrt{m^2+r^{-2}}+vP^{(1)}(1)r\}\leqslant E\leqslant\min_{r>0}\{\sqrt{m^2+r^{-2}}+vP^{(2)}(1)r\}. \tag{3.4}$$

In Fig. 1 we plot these bounds as a function of m for the case $v=1$. If we combine Theorem 1 here with Theorem 2 of Ref. 4 (to the effect that $\overline{g\circ h}>g\circ\overline{h}$ when g is convex) we obtain the following class of examples. We suppose that $V(r)$ is monotone increasing and convex in $h(r)=r$ then the two theorems together yield the lower bound

$$E\geqslant\min_{r>0}\left\{\sqrt{m^2+\frac{1}{r^2}}+vV(P^{(1)}(1)r)\right\}. \tag{3.5}$$

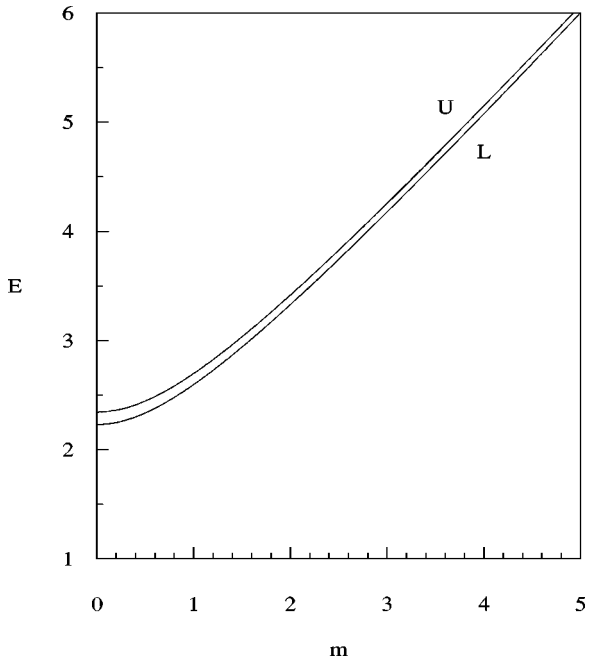

FIG. 1. Complementary upper (U) and lower (L) bounds (3.4) on the lowest eigenvalue $E(m)$ of $H=\sqrt{m^2+p^2}+r$ plotted against m.

Of course, if $V(r)$ is *concave*, then we get an *upper* bound by the same expression provided we use $P^{(2)}(1)$. It is perhaps important to note that with $P=P^{(2)}(r)$ an upper bound would be obtained for every choice of r in the expression on the right-hand side; the expression in (3.5) is however only a lower bound *a priori* at the minimum point.

IV. THE SUM APPROXIMATION: LOWER BOUNDS

Since further generalization easily follows, we first look at the problem of the sum of two potential terms. We assume that each potential $vh^{(i)}(r)$ alone, when added to the kinetic-energy operator K, has a discrete eigenvalue at the bottom of the spectrum for sufficiently large coupling v. We express our result in terms of kinetic potentials and prove the following.

Theorem 2: *If E is the bottom of the spectrum of the Hamiltonian $H=K+V$, and the potential V is the sum $V(r)=h^{(1)}(r)+h^{(2)}(r)$, then it follows that the sum of the component kinetic potentials yields a lower bound to $\overline{V}$, that is to say*

$$\overline{V}(K;s)\geqslant\overline{h^{(1)}}(K;s)+\overline{h^{(2)}}(K;s). \tag{4.1}$$

We shall now prove this theorem, which is in effect an optimized Weyl lower bound;[13–15] this remark will be clarified below, after the proof of the theorem. From the definition (2.1) of kinetic potentials we have

$$\overline{V}(K;s)=\inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}}(\psi,V\psi)=\inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}}(\psi,(h^{(1)}+h^{(2)})\psi).$$

But the latter minimum mean-value is clearly bounded below by the sum of the *separate* minima. Thus we have

$$\overline{V}(K;s) \geqslant \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}} (\psi,h^{(1)}\psi) + \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}} (\psi,h^{(2)}\psi) = \overline{h}^{(1)}(K;s) + \overline{h}^{(2)}(K;s),$$

which inequality establishes the theorem. □

Another approach, which would eventually yield an alternative proof of the theorem, exhibits the relationship between Theorem 2 and the classical Weyl lower bound[13–15] for the eigenvalues of the sum of two operators. Let us suppose that Ψ is the exact normalized lowest eigenfunction of $H=K+V$, so that $H\Psi=E\Psi$. If the positive real parameter w is bounded by 1, $0<w<1$, then $E=(\Psi,(K+V)\Psi)$ may be written as follows:

$$E = w\left(\Psi,\left(K+\frac{1}{w}h^{(1)}(r)\right)\Psi\right) + (1-w)\left(\Psi,\left(K+\frac{1}{1-w}h^{(2)}(r)\right)\Psi\right)$$

$$\geqslant w \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1}}\left(\psi,\left(K+\frac{1}{w}h^{(1)}(r)\right)\psi\right) + (1-w)\inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1}}\left(\psi,\left(K+\frac{1}{1-w}h^{(2)}(r)\right)\psi\right).$$

That is to say, in terms of component kinetic potentials, we arrive at Weyl's inequality for the lowest eigenvalue of the sum $H=wK+h^{(1)}+(1-w)K+h^{(2)}$:

$$E \geqslant w\min_{s>0}\left\{s+\frac{1}{w}\overline{h}^{(1)}(K;s)\right\} + (1-w)\min_{s>0}\left\{s+\frac{1}{1-w}\overline{h}^{(2)}(K;s)\right\}.$$

Since w is an essentially free parameter in the last expression, we may optimize the Weyl lower bound with respect to the choice of w and this forces the individual values of s at the minima, $\{s_1(w),s_2(w)\}$, to be related. More specifically we find from the individual minimizations over s,

$$E \geqslant \mathcal{E}(w) = ws_1(w) + (1-w)s_2(w) + \overline{h}^{(1)}(K;s_1(w)) + \overline{h}^{(2)}(K;s_2(w)),$$

where

$$w = -\frac{\partial\overline{h}^{(1)}}{\partial s}(K;s_1(w)) \quad \text{and} \quad 1-w = -\frac{\partial\overline{h}^{(2)}}{\partial s}(K;s_2(w)).$$

The critical condition $\mathcal{E}'(w)=0$ for the subsequent maximization of the lower bound over w then yields $s_1(w)=s_2(w)$. Thus the best lower energy bound is given by

$$E \geqslant \min_{s>0}\{s+\overline{h}^{(1)}(K;s)+\overline{h}^{(2)}(K;s)\}.$$

The kinetic-potential inequality of Theorem 2 leads, of course, to the same energy lower bound: the optimization just performed above is therefore seen to be automatically built in by the formalism.

It follows immediately from the above kinetic-potential comparison theorem and coupling-parameter absorption that a lower bound to the lowest energy E of the Hamiltonian $H=K+\Sigma_i c_i h^{(i)}(r)$, $\{c_i>0\}$, is provided by the formula

$$E \geqslant \min_{s>0}\left\{s+\sum_i c_i\overline{h}^{(i)}(K;s)\right\}. \tag{4.2}$$

Similarly we can extend this result to continuous sums such as $V(r)=\int_{t_1}^{t_2}c(t)h^{(t)}(r)dt$.

This general theory becomes practically useful when we have good information concerning the components. More particularly, we must have some exact component kinetic potentials, or

lower bounds to them. Outside the well-explored Schrödinger case $K=p^2$, such analytical results are rather sparse. We look at the interesting class of power-law potentials in the next section.

V. SUMS OF POWERS AND THE LOG POTENTIAL

For power-law potentials and the relativistic kinetic energy $K=\sqrt{m^2+p^2}$ we have discussed some lower bounds in Sec. III and we shall now turn these to our advantage. The link between Theorem 1 and Theorem 2 derives from the observation that the equation $K(s)=\sqrt{m^2+s^2}$ allows us to change the minimization variable $s\to r=1/s$. In the first stage of minimization, we have used Jensen's inequality for the lower bound (see proof of Theorem 1); this allows us to keep $(\psi,p\psi)=s=1/r$ constant at first, and then later minimize over s, or, equivalently, over r. We can also easily accommodate a further positive kinetic-energy parameter β. Thus we immediately arrive at the following.

Theorem 3: *A lower bound to the lowest eigenvalue of the semirelativistic spinless-Salpeter operator*

$$H=\beta\sqrt{m^2+p^2}+\sum_{q\neq 0}a(q)\mathrm{sgn}(q)r^q+a(0)\ln(r),$$

where $\beta>0$ *and the potential coefficients* $a(q)\geqslant 0$ *are not all zero, is given by*

$$E\geqslant\min_{r>0}\left\{\beta\sqrt{m^2+\frac{1}{r^2}}+\sum_{q\neq 0}a(q)\mathrm{sgn}(q)(P^{(1)}(q)r)^q+a(0)\ln(P^{(1)}(0)r)\right\},\tag{5.1}$$

where, for the Coulomb component $q=-1$, *we make the substitution*

$$-\frac{a(-1)}{P^{(1)}(-1)r}=-\frac{\beta^2 mv}{e_L(v)r}=-\frac{\beta v}{r}\left(\frac{2}{1+\sqrt{1-4v^2}}\right)^{1/2},\quad v=\frac{a(-1)}{\beta}<\frac{1}{2}.\tag{5.2}$$

The problem presented for the lower bound by the fact that $p-v/r$ has no discrete spectrum was discussed in Sec. II. We have no simple P-number $P(-1)$ but we could derive a running P (2.13) from the Martin–Roy energy bound (2.11); the positive factor β has been inserted in (5.2) by elementary scaling. We shall look at applications of Theorem 3 in Sec. VII when we also have at our disposal the upper-bound P numbers derived in Sec. VI.

VI. VARIATIONAL UPPER BOUNDS

The lower bound for sums discussed in the preceding two sections has the attractive feature that if the component kinetic potentials are exact and only one term is present, then the result is exact. We are unable to construct a general upper bound with this feature. Instead we use a trial wave function $\phi=c\exp(-\frac{1}{2}\alpha r^\nu)$ with a scale parameter $\alpha>0$ and two other parameters $\{c,\nu\}$, and we apply this wave function to the entire problem. One degree of freedom c is used to guarantee normalization, and the scale parameter $\alpha>0$ is expressed in terms of a new variable $t>0$ chosen in such a way that the scale minimization is of an expression with the same form as the lower bound. Initially we use here t rather than r since, during the discussion, we shall need to refer to the potential function $V(r)$. The choice of the remaining parameter $\nu>0$ is left for later optimization.

If we suppose that c has already been chosen so that $\|\phi\|=1$ and, for computational convenience, we use Jensen's inequality, we then obtain the following upper energy bound:

$$E<\mathcal{E}=\beta\sqrt{m^2+(\phi,p^2\phi)}+\left(\phi,\left\{\sum_{q\neq 0}a(q)\mathrm{sgn}(q)r^q+a(0)\ln(r)\right\}\phi\right).\tag{6.1}$$

Now, for each fixed $\nu>0$, we define a new scale variable $t>0$ by the following:

$$(\phi,p^2\phi)=(\phi,-\Delta\phi)=\alpha^{2/\nu}\left(\frac{\nu}{2}\right)^2\frac{\Gamma\left(2+\frac{1}{\nu}\right)}{\Gamma\left(\frac{3}{\nu}\right)}\equiv\frac{1}{t^2}. \tag{6.2}$$

Using this definition of t, we can go on to define the upper P numbers $\mathcal{P}(\nu,q)$ by the relations

$$(\phi,r^q\phi)=\frac{1}{\alpha^{q/\nu}}\frac{\Gamma\left(\frac{q+3}{\nu}\right)}{\Gamma\left(\frac{3}{\nu}\right)}\equiv(\mathcal{P}(\nu,q)t)^q,\quad q\neq 0, \tag{6.3a}$$

and

$$(\phi,\ln(r)\phi)=\ln(\mathcal{P}(\nu,0)t). \tag{6.3b}$$

If we now rename the scale variable $t=r$, and minimize the upper bound $\mathcal{E}$ with respect to scale, we arrive at

Theorem 4: *For each $\nu>0$, an upper bound to the lowest eigenvalue E of the Salpeter operator*

$$H=\beta\sqrt{m^2+p^2}+\sum_{q\neq 0}a(q)\mathrm{sgn}(q)r^q+a(0)\ln(r),$$

where $\beta>0$ and the potential coefficients $a(q)\geqslant 0$ are not all zero, is given by

$$E\leqslant\min_{r>0}\left\{\beta\sqrt{m^2+\frac{1}{r^2}}+\sum_{q\neq 0}a(q)\mathrm{sgn}(q)(\mathcal{P}(\nu,q)r)^q+a(0)\ln(\mathcal{P}(\nu,0)r)\right\}, \tag{6.4}$$

where the upper P numbers are provided by the formulas

$$\mathcal{P}(\nu,q)=\frac{\nu}{2}\left(\frac{\Gamma\left(2+\frac{1}{\nu}\right)}{\Gamma\left(\frac{3}{\nu}\right)}\right)^{1/2}\left(\frac{\Gamma\left(\frac{q+3}{\nu}\right)}{\Gamma\left(\frac{3}{\nu}\right)}\right)^{1/q},\quad q\neq 0, \tag{6.5a}$$

$$\mathcal{P}(\nu,0)=\frac{\nu}{2}\left(\frac{\Gamma\left(2+\frac{1}{\nu}\right)}{\Gamma\left(\frac{3}{\nu}\right)}\right)^{1/2}\exp\left(\frac{1}{\nu}\psi\left(\frac{3}{\nu}\right)\right), \tag{6.5b}$$

and ψ is the digamma function $\psi(t)=\Gamma'(t)/\Gamma(t)$.

Apart from the special Coulomb considerations pertaining to the lower bound (5.1), that formula is essentially identical to the upper bound (6.4): we simply have to use the correct P numbers in each case.

VII. EXAMPLES

We have now assembled the P numbers for our energy-bound formulas (5.1) and (6.4). We shall use the lower P numbers in Table I, lower running P formula for the Coulomb component

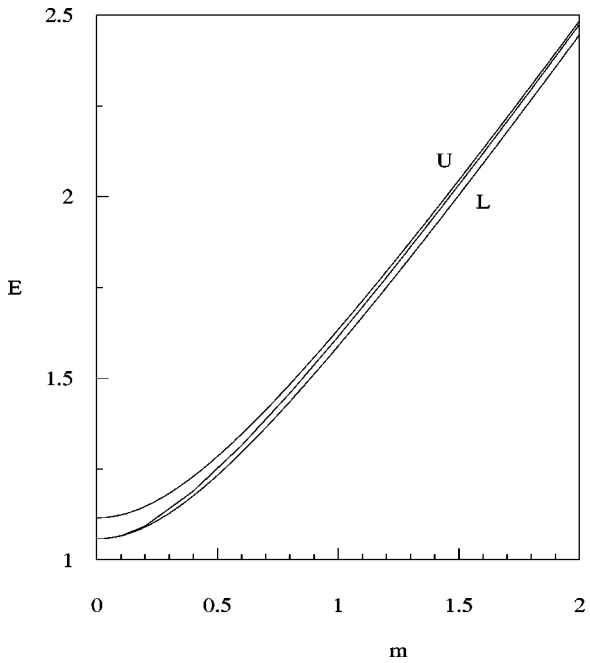

FIG. 2. Lower bounds (L) by (5.1) and upper bounds (U) by (6.4) for the lowest eigenvalue $E(m)$ of $H=\sqrt{m^2+p^2}-0.1/r+0.25r$ plotted against m. The upper bound (U) used the wave-function parameter $\nu=1.6$. The central curve is a very accurate upper bound found by a variational exploration in a 25-dimensional trial space.

(2.13), and the formulas (6.5) for the $\mathcal{P}(\nu,q)$ corresponding to the variational upper bound (6.4). The class of problems we are thus immediately able to consider have the following explicit Hamiltonian form:

$$H=\beta\sqrt{m^2+p^2}-a/r+b\ln(r)+cr+dr^2, \quad a,b,c,d\geqslant 0, \tag{7.1}$$

where $\beta>0$, and the potential parameters $\{a,b,c,d\}$ are not all zero. We look at two examples. In the first, illustrated in Fig. 2, we look at the linear-plus-Coulomb potential $V(r)=-0.1/r+0.25r$ and compare the energy bounds $\{L,U\}$ we find, as functions of the mass m, with some very accurate numerical values (center curve) obtained by minimizing the expectation value of the Hamiltonian in a 25-dimensional trial space. In the next graph, Fig. 3, we plot the energy bounds alone, for the same potential and a wider range of values of the mass m. As a second example we consider the broad linear combination $V(r)=-0.1/r+0.25\ln(r)+0.25r+0.25r^2$ and plot in Fig. 4 the energy bounds as functions of the mass. These illustrations give a clear indication of the quality of the bounds that the theory yields.

VIII. CONCLUSION

The principal theoretical results of this paper are the complementary bounds of Theorem 1, and the sum-approximation lower bound, Theorem 2. In order to arrive at these results we needed first to extend the notion of kinetic potential to allow for more general kinetic-energy operators than the Schrödinger form $K=p^2$. The complementary bounds are based on the assumption that K is a convex function of p and also a concave function of p^2, assumptions clearly satisfied by our prime example and principal motivation, the relativistic kinetic energy $K=\beta\sqrt{m^2+p^2}$. The inequality of Jensen then allows us to learn approximately how special mean values of the problem, the eigenvalues of H, depend on the operator parameters.

By combining Theorem 1 of this paper with Theorem 2 of our earlier paper[4] we obtain a general theory applicable to operator manifolds of the form $H=K(p)+g(h)$ with, on the one

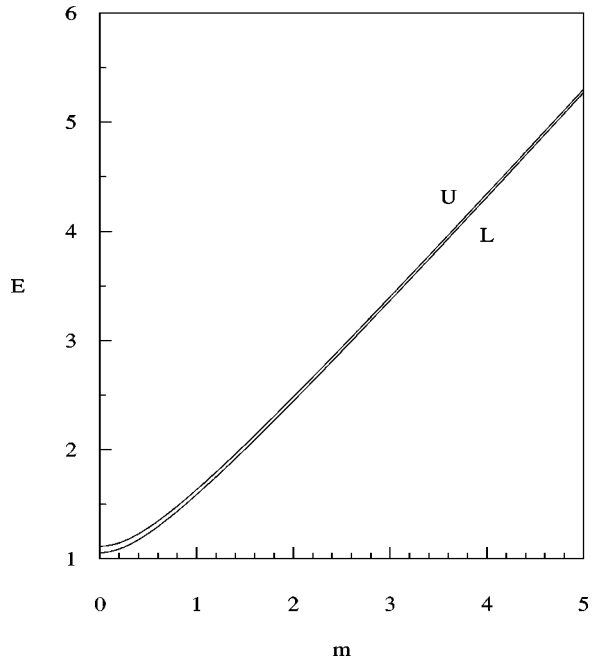

FIG. 3. Lower bounds (L) by (5.1) and upper bounds (U) by (6.4) for the lowest eigenvalue $E(m)$ of $H=\sqrt{m^2+p^2}-0.1/r+0.25r$ plotted against m: this is a continuation of the graph in Fig. 2 to larger m.

hand, tangent spaces spanned by the Schrödinger operators $ap^2+bh(r)+c$, and, on the other, by complementary operators of the form $ap+bh(r)+c$. Given the correct convexities of K and g, energy bounds immediately follow. We looked at one example of this type of problem near the end of Sec. III; and the results were exhibited in Fig. 1.

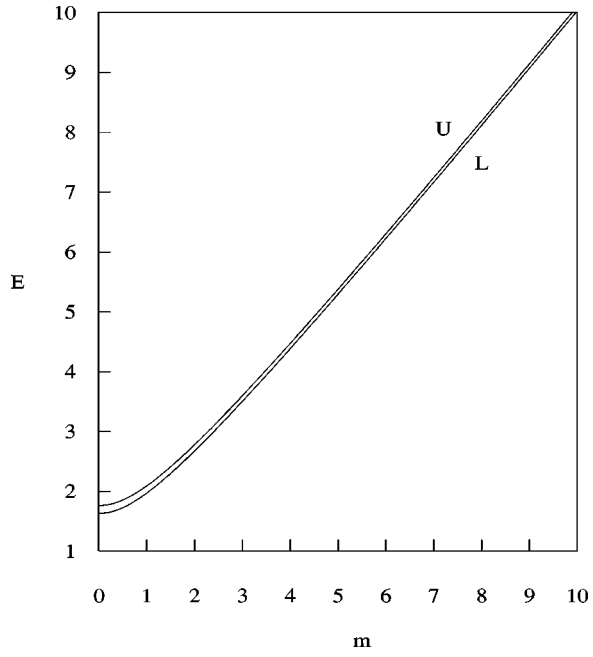

FIG. 4. Lower bounds (L) by (5.1) and upper bounds (U) by (6.4) for the lowest eigenvalue $E(m)$ of $H=\sqrt{m^2+p^2}-0.1/r+0.25\ln(r)+0.25r+0.25r^2$ plotted against m. The upper bound (U) used the wave-function parameter $\nu=1.4$.

A completely different lower bound is provided by Theorem 2, which may be thought of as a spectral expression of the sum structure of the potential, namely the subadditivity of the corresponding kinetic potential, as a sum of components.

In order to make practical use of these theoretical results we need some definite spectral information about component problems. This is provided by the family of pure-power potentials $V(r)=\mathrm{sgn}(q)r^q$. For this family we are able to take advantage of known eigenvalues, or bounds to them, and of simple upper bounds obtained with the aid of Jensen's inequality and a two-parameter family of trial functions. All of our component results can then be expressed in terms of certain P numbers (or, for the lower Coulomb case, $q=-1$, by a P function), which are required by the general lower- and upper-bound formulas of Theorems 3 and 4. These formulas illustrate the effectiveness of the theoretical results and provide recipes for approximate solutions to an interesting class of semirelativistic spectral problems.

ACKNOWLEDGMENTS

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Magnetic translation groups in an *n*-dimensional torus and their representations

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A charged particle in a uniform magnetic field in a two-dimensional torus has a discrete noncommutative translation symmetry instead of a continuous commutative translation symmetry. We study topology and symmetry of a particle in a magnetic field in a torus of arbitrary dimensions. The magnetic translation group (MTG) is defined as a group of translations that leave the gauge field invariant. We show that the MTG in an n-dimensional torus is isomorphic to a central extension of a cyclic group $\mathbf{Z}_{\nu_1}\times\cdots\times\mathbf{Z}_{\nu_{2l}}\times T^m$ by $U(1)$ with $2l+m=n$. We construct and classify irreducible unitary representations of the MTG in a three-torus and apply the representation theory to three examples. We briefly describe a representation theory for a general n-torus. The MTG in an n-torus can be regarded as a generalization of the so-called noncommutative torus. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1513208]

I. INTRODUCTION

Many people have been studying dynamics of an electrically charged particle in a magnetic field for various interests. Landau found that the energy spectrum of an electron becomes discrete when a magnetic field is applied, and explained the diamagnetic property of a metal. The quantum Hall effect looked a peculiar phenomenon when it was first discovered but today it is understood as a universal phenomenon observable in a two-dimensional electron system in a magnetic field. Dynamics of charged particles in a magnetic field is still an active research area.

Here we examine a group-theoretical aspect of the quantum system in a magnetic field. In particular we compare symmetry in a torus with symmetry in a Euclidean space. We would like to understand how the symmetry structure of the dynamical system is affected by the topological structure of the underlying space. It is known that the translation symmetry group becomes noncommutative when a uniform magnetic field is introduced into the Euclidean space. Moreover, the translation symmetry group becomes discrete when the underlying space is replaced by a torus. In this article we consider a vector potential

$$A=\sum_{j,k=1}^{n} x_j\omega_{jk}dx_k+\sum_{j=1}^{n}\alpha_j dx_j \tag{1.1}$$

over an n-dimensional torus $T^n=\mathbf{R}^n/\mathbf{Z}^n$. Here ω_{jk} are arbitrary integers and α_j are real numbers. Then the corresponding magnetic field is given by the two-form

$$B=dA=\sum_{j,k=1}^{n}\frac{1}{2}(\omega_{jk}-\omega_{kj})dx_j\wedge dx_k\,. \tag{1.2}$$

We conclude that the magnetic translation group (MTG) in T^n is

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$$S_A=(\mathbf{R}\times_\omega\Omega^n)/(\mathbf{Z}\times_\omega\mathbf{Z}^n), \tag{1.3}$$

where Ω^n is a subgroup of $\mathbf{R}^n$ defined by $\Omega^n=\{v\in\mathbf{R}^n|(\omega-{}^t\omega)v\in\mathbf{Z}^n\}$ and the group operation in $\mathbf{R}\times_\omega\mathbf{R}^n$ is defined by

$$(x_0,x_1,\ldots,x_n)\cdot(y_0,y_1,\ldots,y_n)=\left(x_0+y_0+\sum_{j,k=1}^{n}x_j\omega_{jk}y_k,x_1+y_1,\ldots,x_n+y_n\right). \tag{1.4}$$

This characterization of the magnetic translation symmetry is one of the main results of this article. The MTG is actually a central extension of a cyclic group

$$\mathbf{Z}_{\mu_1}\times\cdots\times\mathbf{Z}_{\mu_l}\times\mathbf{Z}_{\nu_1}\times\cdots\times\mathbf{Z}_{\nu_l}\times T^m\quad(2l+m=n) \tag{1.5}$$

by $S^1=U(1)$. We build a complete set of irreducible representations of the MTG in T^3. We also describe a method to build irreducible representations of the MTG in T^n.

We would like to briefly review studies by other people on a quantum system in a magnetic field. Brown[1] found that the translation symmetry of an electron in a lattice in a uniform magnetic field is noncommutative and that the quantum system obeys a projective representation of the translation group. At the almost same time[2] and later[3] Zak built a representation theory of the lattice translation group in a magnetic field. Ashby and Miller[4] considered a space–time lattice of a finite size in uniform electric and magnetic fields and proposed an electromagnetic translation group. Avron, Herbst, and Simon have been studying spectral problems of the Schrödinger operators in a magnetic field in a series of papers.[5–8] Particularly, in Ref. 6 they examined a system of particles in a uniform magnetic field and characterized a constant of motion analogous to the total momentum. Dubrovin and Novikov[9,10] studied the spectrum of the Pauli operator in a two-dimensional lattice with a periodic magnetic field and intensively analyzed the gap structure above the ground state. Asch, Over, and Seiler[11] clarified how the inequivalent Hamiltonians on a torus in a magnetic field are induced from a Hamiltonian on the universal covering space of the torus. In a series of studies[12–17] Lulek, Florek, Lipinski, and Walcerz established a systematic method to construct central extensions of a finitely generated Abelian group. Their results are equivalent to the MTGs in a lattice. Kuwabara[18,19] is studying relations between the trajectories of a classical particle and the spectra of its quantized system and has obtained many results. Gruber[20] also examined quantization of a particle on a Riemannian manifold in a magnetic field from a view point of geometric quantization.

As reviewed above, a lot of studies on dynamics and symmetry in a magnetic field have been done. Although MTGs in a finite lattice and in an infinite lattice have been much investigated, the MTG in a torus of arbitrary dimensions is not yet fully investigated. Motivated by a recent study[21,22] on extra dimensions of the space–time, Sakamoto *et al.*[23–25] are developing field theoretical models in which the translation symmetry of an extra circle is spontaneously broken by a nontrivial boundary condition in the extra S^1. Moreover, we are developing models[26,27] in which the rotation symmetry of an extra two-sphere is spontaneously broken by a magnetic monopole in the extra S^2. So we would like to understand how a background gauge field in a compact space influences symmetry structure of a quantum system. Hence we decide to investigate symmetry in a magnetic field in a torus.

This article is organized as follows. In Sec. II we shall examine how symmetry of a quantum system in a magnetic field is changed when the underlying two-dimensional Euclidean space is replaced by a two-dimensional torus. In Sec. III we extend our discussion to an n-dimensional torus. We introduce a noncommutative group structure into $\mathbf{R}^{n+1}$ and use it to construct a magnetic fiber bundle, which is a bundle over T^n with a fiber S^1. In Sec. IV we classify topological structures of the bundles. In Sec. V we define connections, which are generalizations of a vector potential, and classify them. In Sec. VI we define a magnetic translation group as a group of lifted translations that leave the connection invariant. In Sec. VII we build a representation theory of the MTG for T^3 and illustrate the theory by a few examples. In Sec. VIII we describe an outline of the

representation theory of the MTG for a general T^n. Section IX is devoted to conclusions and discussions. To reach the main result quickly the reader may read only Secs. III, V, and VI.

II. SYMMETRIES IN A MAGNETIC FIELD

This section is devoted to exercises to get ideas about the problem. The reader may skip this section and restart from Sec. III without missing the main course of the article.

A. Euclidean space

Let us begin our discussion by examining symmetry of quantum mechanics of a particle in the uniform magnetic field in $\mathbf{R}^2$. It is a well-known system and becomes a starting point to explore further nontrivial systems.

A uniform magnetic field $Bdx\wedge dy=dA$ is derived from a vector potential $A=Bx\ dy$. The Schrödinger equation is

$$H\psi=\left[-\frac{1}{2}\left(\frac{\partial}{\partial x}\right)^2-\frac{1}{2}\left(\frac{\partial}{\partial y}-iBx\right)^2\right]\psi(x,y)=E\psi. \tag{2.1}$$

Then the operators

$$\tilde{P}_x:=-i\frac{\partial}{\partial x}-By, \quad P_y:=-i\frac{\partial}{\partial y} \tag{2.2}$$

commute with H. These generate unitary transformations

$$(U_x(a)\psi)(x,y)=e^{-i\tilde{P}_x a}\psi(x,y)=e^{iBay}\psi(x-a,y), \tag{2.3}$$

$$(U_y(b)\psi)(x,y)=e^{-iP_y b}\psi(x,y)=\psi(x,y-b). \tag{2.4}$$

It is to be noted that $U_x(a)$ is a combination of a translation in the x-direction by the length a and a gauge transformation. It is also to be noted that the translation in the x-direction and the one in the y-direction do not commute but satisfy

$$U_x(a)U_y(b)(U_x(a))^{-1}(U_y(b))^{-1}=e^{iBab}. \tag{2.5}$$

The momentum generates a continuous symmetry and enables us to separate the variables. For example, if we put the eigenvalue of P_y as k, the wave function is factorized as

$$\psi(x,y)=e^{iky}\phi(x). \tag{2.6}$$

Then the Schrödinger equation (2.1) is rewritten as

$$H\psi=e^{iky}\left[-\frac{1}{2}\left(\frac{\partial}{\partial x}\right)^2+\frac{1}{2}(k-Bx)^2\right]\phi(x)=e^{iky}E\phi(x) \tag{2.7}$$

and is reduced to the equation of a harmonic oscillator. Hence the energy eigenvalues are given by

$$E=|B|(n+\tfrac{1}{2}) \quad (n=0,1,2,\ldots) \tag{2.8}$$

and are called the Landau levels. Each eigenvalue is infinitely degenerated with respect to $-\infty<k<\infty$.

B. Torus

Next we turn to a two-dimensional torus. The two-torus T^2 is defined as the quotient space $\mathbf{R}^2/\mathbf{Z}^2$. Namely, the points in $\mathbf{R}^2$,

$$(x,y)\sim(x+1,y)\sim(x,y+1), \tag{2.9}$$

are identified as a single point in T^2. If we impose a pseudoperiodic condition

$$\psi(x+1,y)=e^{iBy}\psi(x,y), \quad \psi(x,y+1)=\psi(x,y), \tag{2.10}$$

on the wave function, the Schrödinger equation (2.1) is well defined over T^2. In other words, on the space of functions satisfying the pseudoperiodic condition, the operator H becomes self-adjoint. To make the two conditions in (2.10) compatible each other we need to have

$$\psi(x+1,y+1)=e^{iB(y+1)}\psi(x,y+1)=e^{iB}e^{iBy}\psi(x,y)=\psi(x+1,y)=e^{iBy}\psi(x,y). \tag{2.11}$$

Hence we should have $e^{iB}=1$. Namely, in the magnetic field strength

$$B=2\pi\nu, \tag{2.12}$$

ν must be an integer. We call ν the magnetic flux number of the torus.

The operators $\tilde{P}_x$ and P_y in (2.2) commute with H defined in (2.1). However, when they act on a wave function satisfying the pseudoperiodic condition (2.10), they do not give back a function satisfying the pseudoperiodic condition but instead give

$$P_y\psi(x+1,y)=e^{iBy}(P_y+B)\psi(x,y), \tag{2.13}$$

$$\tilde{P}_x\psi(x,y+1)=(\tilde{P}_x-B)\psi(x,y). \tag{2.14}$$

Hence, the actions of these operators are not closed in the space of pseudoperiodic functions. Thus we get a lesson that *the generator of infinitesimal translation does not exist in the torus*. However, it is still possible to construct operators for finite translations. We let the finite translation operators (2.3) and (2.4) act on a pseudoperiodic function (2.10), and examine whether the resultant functions satisfy the pseudoperiodic condition. Using the flux quantization (2.12) we get

$$\begin{aligned}(U_x(a)\psi)(x,y+1)&=e^{iBa(y+1)}\psi(x-a,y+1)\\&=e^{iBa}e^{iBay}\psi(x-a,y)\\&=e^{2\pi i\nu a}(U_x(a)\psi)(x,y),\end{aligned} \tag{2.15}$$

$$\begin{aligned}(U_y(b)\psi)(x+1,y)&=\psi(x+1,y-b)\\&=e^{iB(y-b)}\psi(x,y-b)\\&=e^{-iBb}e^{iBy}\psi(x,y-b)\\&=e^{-2\pi i\nu b}e^{iBy}(U_y(b)\psi)(x,y).\end{aligned} \tag{2.16}$$

Therefore, the transformed wave functions, $U_x(a)\psi$ and $U_y(b)\psi$, satisfy the pseudoperiodic condition (2.10) if and only if

$$\nu a,\nu b\in\mathbf{Z}. \tag{2.17}$$

Consequently, the lengths of shifts, a and b, are restricted to integral multiples of $1/\nu$. Moreover, on a pseudoperiodic function the shifts by the unit length act as

$$(U_x(1)\psi)(x,y)=e^{iBy}\psi(x-1,y)=\psi(x,y), \tag{2.18}$$

$$(U_y(1)\psi)(x,y)=\psi(x,y-1)=\psi(x,y). \tag{2.19}$$

Hence $U_x(1)$ and $U_y(1)$ are identity operators. Thus the operators $U_x(1/\nu)$ and $U_y(1/\nu)$ generate a cyclic group $\mathbf{Z}_\nu=\mathbf{Z}/\nu\mathbf{Z}$ of the order ν. However, as seen in (2.5) their commutator produces a nontrivial phase factor. Thus we conclude that the symmetry of the quantum system in the torus magnetic field is described by a projective representation of $\mathbf{Z}_\nu\times\mathbf{Z}_\nu$.

The group of translations of the quantum system in the magnetic field is called a magnetic translation group (abbreviated as MTG). A more precise definition of the MTG will be given in Sec. VI. In the torus the MTG becomes discrete and finite. Its representation is constructed as follows. Let $\{|0\rangle,|1\rangle,\ldots,|\nu-1\rangle\}$ be a basis of the representation space. Then we define the action of the translation operators by

$$U_x(n_x/\nu)|q\rangle=e^{2\pi i n_x q/\nu}|q\rangle, \tag{2.20}$$

$$U_y(n_y/\nu)|q\rangle=|q+n_y(\mathrm{mod}\ \ \nu)\rangle, \tag{2.21}$$

for $n_x,n_y\in\mathbf{Z}$. We can easily verify that they satisfy

$$U_x(n_x/\nu)U_y(n_y/\nu)(U_x(n_x/\nu))^{-1}(U_y(n_y/\nu))^{-1}|q\rangle=e^{i(2\pi\nu)(n_x/\nu)(n_y/\nu)}|q\rangle, \tag{2.22}$$

which is homomorphic to the commutator (2.5). This representation is irreducible and its dimension is ν. Hence each energy eigenvalue (2.8) is degenerated by ν folds.

C. Three-torus

Let us examine the case of a three-dimensional torus briefly to motivate further discussion. With real constants (b_1,b_2,b_3) a vector potential

$$A=b_1x_2dx_3+b_2x_3dx_1+b_3x_1dx_2 \tag{2.23}$$

gives rise to a magnetic field

$$B=dA=b_1dx_2\wedge dx_3+b_2dx_3\wedge dx_1+b_3dx_1\wedge dx_2. \tag{2.24}$$

The Hamiltonian is then given by

$$H\psi=-\frac{1}{2}\left[\left(\frac{\partial}{\partial x_1}-ib_2x_3\right)^2+\left(\frac{\partial}{\partial x_2}-ib_3x_1\right)^2+\left(\frac{\partial}{\partial x_3}-ib_1x_2\right)^2\right]\psi(x_1,x_2,x_3). \tag{2.25}$$

On the three-torus the wave function must satisfy a set of conditions

$$\begin{aligned}\psi(x_1+1,x_2,x_3)&=e^{ib_3x_2}\psi(x_1,x_2,x_3),\\ \psi(x_1,x_2+1,x_3)&=e^{ib_1x_3}\psi(x_1,x_2,x_3),\\ \psi(x_1,x_2,x_3+1)&=e^{ib_2x_1}\psi(x_1,x_2,x_3),\end{aligned} \tag{2.26}$$

which is a generalization of the the pseudoperiodic condition (2.10) of the two-torus.

We would like to find a complete set of translation operators that commute with H and are compatible with the pseudoperiodic condition (2.26). Of course, if the magnetic field is parallel to one of the axes, the system is reduced to the two-torus as has been discussed by Zak.[3] For example, if $(b_1,b_2,b_3)=(0,0,B)$, the Hamiltonian (2.25) and the condition (2.26) are reduced to (2.1) and (2.10), respectively. However, it is a highly nontrivial and not yet fully solved problem to find a complete symmetry group for an inclined magnetic field (b_1,b_2,b_3). Thus we decide to develop a more systematic method to construct the translation symmetry group for a generic magnetic field in the n-torus.

III. MAGNETIC FIBER BUNDLE

We shall extend the previous consideration on the two-dimensional torus to arbitrary dimensions. What we will do in the rest of this article is to construct $U(1)$ principal fiber bundles over an n-dimensional torus T^n, to classify the bundles, to introduce $U(1)$ connections with constant curvatures over T^n, to define the MTG as the stability group of each connection, and to construct the representations of the MTGs. Throughout this article we are identifying S^1 with $U(1)$.

Let us begin with construction of S^1 principal fiber bundles over T^n. For this purpose we introduce a noncommutative group structure into $\mathbf{R}^{n+1}$ as follows. Take an $n\times n$ matrix ω which consists of integers, $\omega_{jk}\in\mathbf{Z}$ $(j,k=1,\ldots,n)$. The matrix ω is not necessarily antisymmetric. Define a product of $(x_0,x_1,\ldots,x_n),(y_0,y_1,\ldots,y_n)\in\mathbf{R}^{n+1}$ by

$$(x_0,x_1,\ldots,x_n)\cdot(y_0,y_1,\ldots,y_n):=\left(x_0+y_0+\sum_{j,k=1}^{n}x_j\omega_{jk}y_k,x_1+y_1,\ldots,x_n+y_n\right). \tag{3.1}$$

In the following we abbreviate the notation of the vectors as $x=(x_1,\ldots,x_n)\in\mathbf{R}^n$. We write the inner product of vectors as $xy=\Sigma_{j=1}^{n}x_j\,y_j$ and the bilinear form as $x\omega y=\Sigma_{j,k=1}^{n}x_j\omega_{jk}y_k$. It is easily verified that the set $\mathbf{R}^{n+1}$ becomes a group with this product operation; the associativity is satisfied as

$$\begin{aligned}((x_0,x)\cdot(y_0,y))\cdot(z_0,z)&=(x_0+y_0+x\omega y,x+y)\cdot(z_0,z)\\&=(x_0+y_0+z_0+x\omega y+(x+y)\omega z,(x+y)+z)\\&=(x_0+y_0+z_0+x\omega y+x\omega z+y\omega z,x+y+z)\\&=(x_0+y_0+z_0+x\omega(y+z)+y\omega z,x+(y+z))\\&=(x_0,x)\cdot((y_0,y)\cdot(z_0,z)),\end{aligned} \tag{3.2}$$

the unit element is given by $(0,0)\in\mathbf{R}\times\mathbf{R}^n$, and the inverse element of $(x_0,x)\in\mathbf{R}\times\mathbf{R}^n$ is given by

$$(x_0,x)^{-1}=(-x_0+x\omega x,-x). \tag{3.3}$$

The set $\mathbf{R}^{n+1}$ equipped with this group structure is denoted by $\mathbf{R}\times_\omega\mathbf{R}^n$. A commutator is calculated as

$$\begin{aligned}(x_0,x)\cdot(y_0,y)\cdot(x_0,x)^{-1}\cdot(y_0,y)^{-1}&=(x_0+y_0+x\omega y,x+y)\cdot(-x_0+x\omega x,-x)\cdot(-y_0+y\omega y,-y)\\&=(y_0+x\omega y+x\omega x-(x+y)\omega x,y)\cdot(-y_0+y\omega y,-y)\\&=(x\omega y+x\omega x-(x+y)\omega x+y\omega y-y\omega y,0)=(x\omega y-y\omega x,0),\end{aligned} \tag{3.4}$$

and therefore $\mathbf{R}\times_\omega\mathbf{R}^n$ is Abelian if and only if ω is a symmetric matrix. The natural projection map $\mathbf{R}\times_\omega\mathbf{R}^n\to\mathbf{R}^n$ becomes a group homomorphism. As its kernel $\mathbf{R}\times_\omega\{0\}$ is contained in the center of $\mathbf{R}\times_\omega\mathbf{R}^n$, the group $\mathbf{R}\times_\omega\mathbf{R}^n$ is a central extension of $\mathbf{R}^n$ by $\mathbf{R}$.

The subset $\mathbf{Z}\times_\omega\mathbf{Z}^n=\{(m_0,m_1,\ldots,m_n)|m_0,m_j\in\mathbf{Z}\}$ is also a subgroup of $\mathbf{R}\times_\omega\mathbf{R}^n$ but it is not isomorphic to the standard Abelian group $\mathbf{Z}^{n+1}$. The subgroup $\mathbf{Z}\times_\omega\mathbf{Z}^n$ acts freely on $\mathbf{R}\times_\omega\mathbf{R}^n$ from the left via the group operation. Hence the space of orbits

$$P_\omega^{n+1}:=(\mathbf{Z}\times_\omega\mathbf{Z}^n)\backslash(\mathbf{R}\times_\omega\mathbf{R}^n) \tag{3.5}$$

becomes a smooth manifold.

The group operation also induces action of the group $\mathbf{R}\times_\omega\mathbf{R}^n$ on the space P_ω^{n+1} from the right. The subgroups $\mathbf{Z}\times_\omega\{0\}\subset\mathbf{R}\times_\omega\{0\}$ are contained in the center of $\mathbf{R}\times_\omega\mathbf{R}^n$ and hence their actions from the right are equivalent to those from the left. The subgroups $\mathbf{R}\times_\omega\{0\}$ and $\mathbf{Z}$

$\times_\omega\{0\}$ are isomorphic to $\mathbf{R}$ and $\mathbf{Z}$, respectively. Thus $\mathbf{R}$ acts on P_ω^{n+1} but its subgroup $\mathbf{Z}$ acts trivially on P_ω^{n+1} since $\mathbf{Z}$ is contained in the dividing group $\mathbf{Z}\times_\omega\mathbf{Z}^n$ of the quotient space (3.5). Therefore the action of $\mathbf{R}$ is reduced to the effective action of $S^1=\mathbf{R}/\mathbf{Z}$ on P_ω^{n+1}. The space of orbit P_ω^{n+1}/S^1 is diffeomorphic to a torus T^n. Consequently we obtain a principal fiber bundle with the canonical projection map $\pi_\omega: P_\omega^{n+1}\to T^n$ with a structure group S^1. We call this fiber bundle a *magnetic fiber bundle twisted by the matrix* ω. The procedure to construct the magnetic fiber bundle is summarized by the following commutative diagram:

$$\begin{array}{ccccc} \mathbf{Z}\times_\omega\{0\} & \to & \mathbf{Z}\times_\omega\mathbf{Z}^n & \to & \mathbf{Z}^n \\ \downarrow & & \downarrow & & \downarrow \\ \mathbf{R}\times_\omega\{0\} & \to & \mathbf{R}\times_\omega\mathbf{R}^n & \to & \mathbf{R}^n \\ \downarrow & & \downarrow & & \downarrow \\ S^1 & \to & P_\omega^{n+1} & \underset{\pi_\omega}{\to} & T^n \end{array}. \tag{3.6}$$

A function $f: P_\omega^{n+1}\to\mathbf{C}$ is identified with a function $f:\mathbf{R}\times_\omega\mathbf{R}^n\to\mathbf{C}$ that is invariant under action of $\mathbf{Z}\times_\omega\mathbf{Z}^n$ from the left as

$$f(m_0+x_0+m\omega x, m+x)=f(x_0,x), \quad (m_0,m)\in\mathbf{Z}\times_\omega\mathbf{Z}^n. \tag{3.7}$$

Moreover, when the function $f: P_\omega^{n+1}\to\mathbf{C}$ satisfies

$$f(x_0+t,x)=e^{-2\pi it}f(x_0,x), \quad t\in\mathbf{R}, \tag{3.8}$$

it is called an equivariant function on P_ω^{n+1}. Hence the equivariant function f has the property

$$f(x_0,x+m)=e^{2\pi im\omega x}f(x_0,x), \quad m\in\mathbf{Z}^n. \tag{3.9}$$

This is a generalization of the pseudoperiodic condition (2.10),

$$\psi(x+1,y)=e^{2\pi i\nu y}\psi(x,y), \quad \psi(x,y+1)=\psi(x,y). \tag{3.10}$$

In fact, if we take the matrix

$$\omega=\begin{pmatrix} 0 & \nu \\ 0 & 0 \end{pmatrix}, \tag{3.11}$$

the general condition (3.9) of T^n is reduced to the specific one (3.10) of T^2.

IV. EQUIVALENT MAGNETIC BUNDLES

In the above construction each magnetic fiber bundle is specified by an integral matrix ω. However, it can happen that different matrices ω and ω' give rise to equivalent fiber bundles. In this section we prove that ω and ω' induce equivalent fiber bundles if and only if the difference $\omega'-\omega$ is a symmetric integral matrix. Therefore, we may choose a representative matrix ω such that $\omega_{jk}=0$ for $j\geqslant k$. Namely, the upper triangle matrix

$$\omega=\begin{pmatrix} 0 & \omega_{12} & \omega_{13} & \cdots & \omega_{1,n-1} & \omega_{1n} \\ 0 & 0 & \omega_{23} & \cdots & \omega_{2,n-1} & \omega_{2n} \\ 0 & 0 & 0 & \cdots & \omega_{3,n-1} & \omega_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \omega_{n-1,n} \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \tag{4.1}$$

with integers ω_{jk} can be taken as a standard form of the matrix ω. The reader will not miss the main result of the article even if he skips this section and restarts from Sec. V.

Here we introduce three kinds of isomorphisms that convert a bundle specified by a matrix ω to a bundle specified by another matrix ω'.

Let us introduce the first kind of bundle isomorphism. When a symmetric matrix σ of integral elements, $\sigma_{jk}=\sigma_{kj}\in\mathbf{Z}$, satisfies

$$\sum_{j,k=1}^{n} m_j\sigma_{jk}m_k\in 2\mathbf{Z} \tag{4.2}$$

for any $m=(m_1,\ldots,m_n)\in\mathbf{Z}^n$, we call σ an even symmetric matrix. This requirement for σ is equivalent to demanding that the off-diagonal elements σ_{jk} are integers and that the diagonal elements σ_{jj} are even integers. Here we will show that two magnetic bundles P_{ω}^{n+1} and $P_{\omega+\sigma}^{n+1}$ are isomorphic each other for any even symmetric matrix σ. For this purpose let us define a map $\phi_\sigma:\mathbf{R}\times_\omega\mathbf{R}^n\to\mathbf{R}\times_{\omega+\sigma}\mathbf{R}^n$ by

$$\phi_\sigma(x_0,x):=(x_0+\tfrac{1}{2}x\sigma x,x). \tag{4.3}$$

Existence of the inverse map is obvious; it is given by $\phi_\sigma^{-1}(x_0,x)=(x_0-\frac{1}{2}x\sigma x,x)$. It is easily verified that the map ϕ_σ is a group isomorphism as

$$\begin{aligned}\phi_\sigma((x_0,x)\cdot_\omega(y_0,y)) &= \phi_\sigma(x_0+y_0+x\omega y,x+y)\\ &=(x_0+y_0+x\omega y+\tfrac{1}{2}(x+y)\sigma(x+y),x+y)\\ &=(x_0+y_0+\tfrac{1}{2}x\sigma x+\tfrac{1}{2}y\sigma y+x(\omega+\sigma)y,x+y)\\ &=(x_0+\tfrac{1}{2}x\sigma x,x)\cdot_{\omega+\sigma}(y_0+\tfrac{1}{2}y\sigma y,y)\\ &=\phi_\sigma(x_0,x)\cdot_{\omega+\sigma}\phi_\sigma(y_0,y),\end{aligned} \tag{4.4}$$

where we have distinguished the product operation of $\mathbf{R}\times_{\omega+\sigma}\mathbf{R}^n$ from that of $\mathbf{R}\times_\omega\mathbf{R}^n$. The map ϕ_σ sends the integer subgroup $\mathbf{Z}\times_\omega\mathbf{Z}^n$ to $\mathbf{Z}\times_{\omega+\sigma}\mathbf{Z}^n$, since σ is even as required in (4.2). Therefore, ϕ_σ induces a diffeomorphism

$$(\phi_\sigma)_*:(\mathbf{Z}\times_\omega\mathbf{Z}^n)\backslash(\mathbf{R}\times_\omega\mathbf{R}^n)\to(\mathbf{Z}\times_{\omega+\sigma}\mathbf{Z}^n)\backslash(\mathbf{R}\times_{\omega+\sigma}\mathbf{R}^n). \tag{4.5}$$

Moreover, since ϕ_σ is the identity map when it is restricted on $\mathbf{R}\times_\omega\{0\}$,

$$\phi_\sigma((t,0)\cdot_\omega(x_0,x))=\phi_\sigma(t,0)\cdot_{\omega+\sigma}\phi_\sigma(x_0,x)=(t,0)\cdot_{\omega+\sigma}\phi_\sigma(x_0,x), \tag{4.6}$$

thus $(\phi_\sigma)_*$ is equivariant with respect to the action of S^1. It is also clear that $\pi_\omega=\pi_{\omega+\sigma}\circ(\phi_\sigma)_*$. Thus we conclude that the map $(\phi_\sigma)_*$ is an isomorphism between the principal fiber bundles P_{ω}^{n+1} and $P_{\omega+\sigma}^{n+1}$.

Next we shall introduce the second kind of bundle isomorphism. We identify a diagonal matrix $\Delta=\mathrm{diag}(\Delta_1,\Delta_2,...,\Delta_n)$ with a vector $\Delta=(\Delta_1,\Delta_2,\ldots,\Delta_n)\in\mathbf{Z}^n$. Then we define a map $\phi_\Delta:\mathbf{R}\times_\omega\mathbf{R}^n\to\mathbf{R}\times_{\omega+\Delta}\mathbf{R}^n$ by

$$\phi_\Delta(x_0,x):=\left(x_0+\frac{1}{2}x\Delta x+\frac{1}{2}\Delta x,x\right)=\left(x_0+\frac{1}{2}\sum_{j=1}^{n}(x_j\Delta_jx_j+\Delta_jx_j),x\right). \tag{4.7}$$

It is also easily verified that ϕ_Δ is a group isomorphism as

$$\begin{aligned}\phi_\Delta((x_0,x)\cdot_\omega(y_0,y)) &= \phi_\Delta(x_0+y_0+x\omega y,x+y)\\ &= (x_0+y_0+x\omega y+\tfrac{1}{2}(x+y)\Delta(x+y)+\tfrac{1}{2}\Delta(x+y),x+y)\\ &= (x_0+y_0+\tfrac{1}{2}x\Delta x+\tfrac{1}{2}\Delta x+\tfrac{1}{2}y\Delta y+\tfrac{1}{2}\Delta y+x(\omega+\Delta)y,x+y)\\ &= (x_0+\tfrac{1}{2}x\Delta x+\tfrac{1}{2}\Delta x,x)\cdot_{\omega+\Delta}(y_0+\tfrac{1}{2}y\Delta y+\tfrac{1}{2}\Delta y,y)\\ &= \phi_\Delta(x_0,x)\cdot_{\omega+\Delta}\phi_\Delta(y_0,y). \end{aligned} \tag{4.8}$$

Note that when x_j is an integer, $x_j^2+x_j=x_j(x_j+1)$ is always an even integer and hence $\frac{1}{2}\Delta_j(x_j^2+x_j)$ is an integer. Therefore the map ϕ_Δ sends the integer subgroup $\mathbf{Z}\times_\omega\mathbf{Z}^n$ to $\mathbf{Z}\times_{\omega+\Delta}\mathbf{Z}^n$. Moreover, ϕ_Δ sends $\mathbf{R}\times_\omega\{0\}$ to $\mathbf{R}\times_{\omega+\Delta}\{0\}$ identically. Thus the induced map $(\phi_\Delta)_*$ becomes an isomorphism between the principal fiber bundles P_ω^{n+1} and $P_{\omega+\Delta}^{n+1}$.

There is the third kind of bundle isomorphism, which will be used when we classify connections later. For each $\varepsilon=(\varepsilon_1,\varepsilon_2,\ldots,\varepsilon_n)\in\mathbf{Z}^n$ we define a map $\phi_\varepsilon:\mathbf{R}\times_\omega\mathbf{R}^n\to\mathbf{R}\times_\omega\mathbf{R}^n$ by

$$\phi_\varepsilon(x_0,x):=(x_0+\varepsilon x,x)=\left(x_0+\sum_{j=1}^n\varepsilon_j x_j,x\right). \tag{4.9}$$

It is also easily verified that ϕ_ε is a group isomorphism as

$$\begin{aligned}\phi_\varepsilon((x_0,x)\cdot_\omega(y_0,y)) &= \phi_\varepsilon(x_0+y_0+x\omega y,x+y)\\ &= (x_0+y_0+x\omega y+\varepsilon(x+y),x+y)\\ &= (x_0+\varepsilon x+y_0+\varepsilon y+x\omega y,x+y)\\ &= (x_0+\varepsilon x,x)\cdot_\omega(y_0+\varepsilon y,y)=\phi_\varepsilon(x_0,x)\cdot_\omega\phi_\varepsilon(y_0,y). \end{aligned} \tag{4.10}$$

The map ϕ_ε sends the integer subgroup $\mathbf{Z}\times_\omega\mathbf{Z}^n$ to $\mathbf{Z}\times_\omega\mathbf{Z}^n$. Moreover, ϕ_ε sends $\mathbf{R}\times_\omega\{0\}$ to $\mathbf{R}\times_\omega\{0\}$ identically. Thus the group isomorphism ϕ_ε induces an automorphism $(\phi_\varepsilon)_*$ of the principal fiber bundle P_ω^{n+1}.

As a summary, we write down a combined isomorphism of the three kinds of maps

$$(\phi_\varepsilon\circ\phi_\Delta\circ\phi_\sigma)(x_0,x):=(x_0+\tfrac{1}{2}x(\sigma+\Delta)x+\tfrac{1}{2}\Delta x+\varepsilon x,x). \tag{4.11}$$

By adding an integral diagonal matrix Δ to an even symmetric matrix σ, we can make any integral symmetric matrix $\sigma'=\sigma+\Delta$. Therefore, by combining the first and second kinds of isomorphisms, ϕ_σ and ϕ_Δ, we can establish an isomorphism between P_ω^{n+1} and $P_{\omega+\sigma'}^{n+1}$ for any integral symmetric matrix σ'. In other words, the set of magnetic fiber bundles has a one-to-one correspondence with $\mathrm{Mat}(n,\mathbf{Z})/\mathrm{Sym}(n,\mathbf{Z})$, where the quotient is taken in the sense of additive groups.

V. CONNECTION

In this section we define the vector potentials that yield uniform magnetic fields in an n-dimensional torus. We use the words, a vector potential, a gauge field, and a connection, to describe the same notion. Magnetic field strength and curvature are an identical notion.

Let us define a differential one-form A on $\mathbf{R}\times_\omega\mathbf{R}^n$ by

$$A:=-dx_0+\sum_{j,k=1}^n x_j\omega_{jk}dx_k+\sum_{j=1}^n\alpha_j dx_j=-dx_0+x\omega dx+\alpha dx \tag{5.1}$$

with a real vector $\alpha\in\mathbf{R}^n$. These parameters $\alpha=(\alpha_1,\ldots,\alpha_n)$ characterize the Aharonov–Bohm effect. The action of $(m_0,m)\in\mathbf{Z}\times_\omega\mathbf{Z}^n$ from the left of $\mathbf{R}\times_\omega\mathbf{R}^n$ defines a map $\varphi:(x_0,x)\mapsto(m_0+x_0+m\omega x,m+x)$. Note that the one-form A is invariant under the transformation by φ as

$$\varphi^*A=-(dx_0+m\omega dx)+(m+x)\omega dx+\alpha dx=A. \tag{5.2}$$

Thus A can be regarded as a one-form on $P_\omega^{n+1}=(\mathbf{Z}\times_\omega\mathbf{Z}^n)\backslash(\mathbf{R}\times_\omega\mathbf{R}^n)$. It is also obvious that A is invariant under a transformation $(x_0,x)\mapsto(x_0+t,x)$ for any $t\in\mathbf{R}$. Moreover, A satisfies

$$\left\langle\frac{\partial}{\partial x_0},A\right\rangle=-1 \tag{5.3}$$

by the definition. In the above equation, $\langle\cdot,\cdot\rangle$ denotes the pairing of a vector and a one-form. Thus A satisfies the axiom of a connection form of the principal bundle $\pi_\omega:P_\omega^{n+1}\to T^n$.

We can classify the connections using isomorphism maps introduced in the last section. The connection $A_{\omega,\alpha}$ defined by (5.1) is parametrized by an integral matrix $\omega\in\mathrm{Mat}(n,\mathbf{Z})$ and a real vector $\alpha\in\mathbf{R}^n$. For any even symmetric matrix $\sigma\in\mathrm{EvenSym}(n,\mathbf{Z})$ and integral vectors $\Delta,\varepsilon\in\mathbf{Z}^n$, the combined isomorphism (4.11) induces a transformation

$$\begin{aligned}
&(\phi_\varepsilon\circ\phi_\Delta\circ\phi_\sigma)^*A_{\omega+\sigma+\Delta,\alpha+1/2\,\Delta+\varepsilon}\\
&\quad=-d(x_0+\tfrac{1}{2}x(\sigma+\Delta)x+\tfrac{1}{2}\Delta x+\varepsilon x)+x(\omega+\sigma+\Delta)dx+(\alpha+\tfrac{1}{2}\Delta+\varepsilon)dx\\
&\quad=-dx_0-x(\sigma+\Delta)dx-\tfrac{1}{2}\Delta dx-\varepsilon dx+x(\omega+\sigma+\Delta)dx+(\alpha+\tfrac{1}{2}\Delta+\varepsilon)dx\\
&\quad=-dx_0+x\omega dx+\alpha dx\\
&\quad=A_{\omega,\alpha}
\end{aligned} \tag{5.4}$$

via pullback. Thus the connections are classified by the equivalence relation

$$(\omega,\alpha)\sim(\omega+\sigma+\Delta,\alpha+\tfrac{1}{2}\Delta+\varepsilon),\quad \sigma\in\mathrm{EvenSym}(n,\mathbf{Z});\Delta,\varepsilon\in\mathbf{Z}^n \tag{5.5}$$

among $(\omega,\alpha)\in\mathrm{Mat}(n,\mathbf{Z})\times\mathbf{R}^n$.

Next we define a covariant derivative of the equivariant function f by

$$Df:=df-2\pi iAf. \tag{5.6}$$

Of course, on the right-hand side, $i=\sqrt{-1}$. The curvature form F is defined by

$$F:=dA=\sum_{j,k=1}^{n}\omega_{jk}dx_j\wedge dx_k=\sum_{j,k=1}^{n}\frac{1}{2}(\omega_{jk}-\omega_{kj})dx_j\wedge dx_k, \tag{5.7}$$

which gives a constant magnetic field. Hence the first Chern class is uniquely specified by the integral antisymmetrized matrix $(\omega-{}^t\omega)$. It is known[28] that an S^1-fiber bundle has a one-to-one correspondence with the first Chern class. Therefore, by choosing $\omega\in\mathrm{Mat}(n,\mathbf{Z})$ appropriately, we can construct any principal fiber bundles over T^n with the fiber S^1.

VI. MAGNETIC TRANSLATION GROUP

Now we shall examine translation symmetry of the vector potential A of the uniform magnetic field. In this section we shall give a precise definition of the MTG in T^n and express the MTG in a more concrete form. We will prove that the MTG is

$$S_A=(\mathbf{R}\times_\omega\Omega^n)/(\mathbf{Z}\times_\omega\mathbf{Z}^n), \tag{6.1}$$

where Ω^n is a subgroup of $\mathbf{R}^n$ defined by $\Omega^n=\{v\in\mathbf{R}^n|(\omega-{}^t\omega)v\in\mathbf{Z}^n\}$ and the group operation is taken in the sense of (3.1). This is one of the main results of this article.

We begin by defining the MTG. A vector $v\in\mathbf{R}^n$ generates a translation of T^n by

$$\tau_v : T^n \to T^n, \quad x \mapsto x+v. \tag{6.2}$$

When a map $\tilde{\tau}_v : P_\omega^{n+1} \to P_\omega^{n+1}$ satisfies the commutative diagram

$$\begin{array}{ccc} & S^1 & \\ \swarrow & & \searrow \\ P_\omega^{n+1} & \overset{\tilde{\tau}}{\to} & P_\omega^{n+1} \\ \pi_\omega \downarrow & & \downarrow \pi_\omega \\ T^n & \overset{\tau}{\to} & T^n \end{array} \tag{6.3}$$

the map $\tilde{\tau}_v$ is called a lift of the translation τ_v. The lifted translations that leave the connection A invariant form a group

$$S_A := \{\tilde{\tau}_v : P_\omega^{n+1} \to P_\omega^{n+1} | v \in \mathbf{R}^n, \pi_\omega \circ \tilde{\tau}_v = \tau_v \circ \pi_\omega ; \ \tilde{\tau}_v^* A = A\}. \tag{6.4}$$

We call it the stability group of A, or the magnetic translation group (MTG).

Let us write down the lifted translation in a more explicit form. We use $(x_0, x) \in \mathbf{R}^{n+1}$ as a coordinate of P_ω^{n+1}. Since $\pi_\omega \circ \tilde{\tau}_v = \tau_v \circ \pi_\omega$, the lift $\tilde{\tau}_v$ of (6.2) must have the form

$$\tilde{\tau}_v : (x_0, x) \mapsto (x_0 + \theta(x_0, x, v), x+v). \tag{6.5}$$

To make $\tilde{\tau}_v$ commutative with the action of $e^{2\pi i w_0} \in S^1$ the function θ must satisfy

$$x_0 + w_0 + \theta(x_0 + w_0, x, v) = x_0 + \theta(x_0, x, v) + w_0, \tag{6.6}$$

namely, θ must satisfy

$$\theta(x_0 + w_0, x, v) = \theta(x_0, x, v) \tag{6.7}$$

for any $w_0 \in \mathbf{R}$. Therefore, the function θ is independent of x_0. To become a map of P_ω^{n+1}, the map $\tilde{\tau}_v$ must send an orbit of the left-action of $\mathbf{Z} \times_\omega \mathbf{Z}^n$ to an orbit of the same group. In other words, for any $(m_0, m) \in \mathbf{Z} \times_\omega \mathbf{Z}^n$ there must exist an element $(m_0', m') \in \mathbf{Z} \times_\omega \mathbf{Z}^n$ that satisfies

$$\tilde{\tau}_v((m_0, m) \cdot (x_0, x)) = (m_0', m') \cdot \tilde{\tau}_v(x_0, x). \tag{6.8}$$

The above equation is rewritten as

$$(m_0 + x_0 + m\omega x + \theta(m+x, v), m+x+v) = (m_0' + x_0 + \theta(x, v) + m'\omega(x+v), m'+x+v),$$

which is equivalent to a set of equations

$$m = m', \tag{6.9}$$

$$m_0 + m\omega x + \theta(m+x, v) = m_0' + \theta(x, v) + m'\omega(x+v). \tag{6.10}$$

The last equation implies that

$$\theta(m+x, v) - \theta(x, v) - m\omega v = m_0' - m_0 \in \mathbf{Z} \tag{6.11}$$

for any $m \in \mathbf{Z}^n$. In reverse order, any function $\theta(x, v)$ satisfying the condition (6.11) defines a lifted translation $\tilde{\tau}_v$ by (6.5). The lifted translation $\tilde{\tau}_v$ is actually a combination of a spatial shift by v with a gauge transformation by θ. Hence, we finish characterizing the lifted translations.

Let the lifted translation $\tilde{\tau}_v$ act on the connection form A of (5.1) via pull-back. Then it gives

$$\tilde{\tau}_v^* A = -(dx_0 + d\theta) + (x+v)\omega d(x+v) + \alpha d(x+v) = A - d\theta + v\omega dx. \tag{6.12}$$

Hence, to leave the connection invariant as $\tilde{\tau}_v^* A = A$, the function θ must satisfy a differential equation $d\theta = v\omega dx$. Thus we have

$$\theta(x,v) = v\omega x + v_0 \tag{6.13}$$

with a constant $v_0 \in \mathbf{R}$. To make $\tilde{\tau}_v$ a map of P_ω^{n+1}, the function θ must satisfy the condition (6.11), which requires that

$$\theta(m+x,v) - \theta(x,v) - m\omega v = v\omega m - m\omega v = -m(\omega - {}^t\omega)v \in \mathbf{Z} \tag{6.14}$$

for any $m \in \mathbf{Z}^n$. Therefore, the vector $v \in \mathbf{R}^n$ is required to satisfy

$$(\omega - {}^t\omega)v \in \mathbf{Z}^n. \tag{6.15}$$

We call the vector v satisfying (6.15) a magnetic shift. A set of the magnetic shifts is denoted by

$$\Omega^n := \{v \in \mathbf{R}^n \mid (\omega - {}^t\omega)v \in \mathbf{Z}^n\}. \tag{6.16}$$

The set Ω^n becomes an additive subgroup of $\mathbf{R}^n$. When the antisymmetrized matrix $(\omega - {}^t\omega)$ is nondegenerated, Ω^n is discrete. The lifted translation $\tilde{\tau}_v$ defined by (6.5) with (6.13) becomes

$$\tilde{\tau}_v : (x_0,x) \mapsto (x_0 + \theta(x_0,x,v), x+v) = (x_0 + v\omega x + v_0, x+v) = (v_0,v)\cdot(x_0,x), \tag{6.17}$$

and therefore the action of $\tilde{\tau}_v$ is identified with the action of $(v_0,v) \in \mathbf{R} \times_\omega \Omega^n$ on P_ω^{n+1} from the left. However, the subgroup $\mathbf{Z} \times_\omega \mathbf{Z}^n \subset \mathbf{R} \times_\omega \Omega^n$ acts on P_ω^{n+1} trivially. Thus the stability group S_A of the connection A is identified as

$$S_A = (\mathbf{R} \times_\omega \Omega^n)/(\mathbf{Z} \times_\omega \mathbf{Z}^n). \tag{6.18}$$

This is one of the main results of this article. Note that S_A is a central extension of a compact Abelian group $\Omega^n/\mathbf{Z}^n$ by $S^1 = \mathbf{R}/\mathbf{Z}$.

Actually, there is another way to characterize the group S_A. The group $\mathbf{R} \times_\omega \Omega^n$ is a normalizer of $N = \mathbf{Z} \times_\omega \mathbf{Z}^n$ in $G = \mathbf{R} \times_\omega \mathbf{R}^n$. In other words, the subgroup H defined by

$$H := \{h \in G \mid \forall n \in N, hnh^{-1} \in N\} \tag{6.19}$$

coincides with $\mathbf{R} \times_\omega \Omega^n$. The above statement is easily proved as follows. A straightforward calculation yields

$$(x_0,x)\cdot(m_0,m)\cdot(x_0,x)^{-1} = (m_0 + x(\omega - {}^t\omega)m, m). \tag{6.20}$$

Therefore the necessary and sufficient condition for $(x_0,x) \in \mathbf{R} \times_\omega \mathbf{R}^n$ to bring the above element into $N = \mathbf{Z} \times_\omega \mathbf{Z}^n$ is that $(\omega - {}^t\omega)x \in \mathbf{Z}^n$, or that $x \in \Omega^n$. Thus $N = \mathbf{Z} \times_\omega \mathbf{Z}^n$ is a normal subgroup of $H = \mathbf{R} \times_\omega \Omega^n$, and hence the quotient group $S_A = H/N$ is well defined.

VII. REPRESENTATIONS OF THE MTG IN A THREE-TORUS

A unitary representation theory of the MTG is significant for spectral analyses of the Laplace operator and the Dirac operator in a background gauge field. In this section we examine a three-dimensional torus and construct a complete set of representations. This is another main result of this article. In the next section we will discuss an outline of the representation theory of the MTG for arbitrary dimensions.

A. Method

The MTG was identified as $S_A=(\mathbf{R}\times_\omega\Omega^n)/(\mathbf{Z}\times_\omega\mathbf{Z}^n)$ at (6.18). We would like to express the MTG in terms of generators and relations. Here we concentrate on the three-dimensional torus. Let us take the matrix

$$\omega=\begin{pmatrix}0 & b_3 & -b_2\\ 0 & 0 & b_1\\ 0 & 0 & 0\end{pmatrix} \tag{7.1}$$

with positive integers b_1, b_2, and b_3. Then antisymmetrization of ω yields

$$\omega-{}^t\omega=\begin{pmatrix}0 & b_3 & -b_2\\ -b_3 & 0 & b_1\\ b_2 & -b_1 & 0\end{pmatrix}. \tag{7.2}$$

The characteristic equation of $(\omega-{}^t\omega)$ is

$$\det(\lambda-(\omega-{}^t\omega))=\lambda(\lambda^2+b_1^2+b_2^2+b_3^2). \tag{7.3}$$

Hence, its eigenvalues are

$$\lambda=0,\pm iB \tag{7.4}$$

with $B:=\sqrt{b_1^2+b_2^2+b_3^2}$. We assume that $B\neq 0$. The eigenspace for $\lambda=0$ is spanned by

$$b=\begin{pmatrix}b_1\\ b_2\\ b_3\end{pmatrix}. \tag{7.5}$$

The action of $(\omega-{}^t\omega)$ on a vector $v\in\mathbf{R}^3$ is equivalent to the vector product $(\omega-{}^t\omega)v=v\times b$. The magnetic shift group (6.16) now becomes

$$\Omega^3=\{v\in\mathbf{R}^3|(\omega-{}^t\omega)v\in\mathbf{Z}^3\}. \tag{7.6}$$

The linear subspace $\mathbf{R}b$ spanned by b of (7.5) is a subgroup of Ω^3. Let us define a generator e_0 by

$$D_0:=\mathrm{GCD}\{b_1,b_2,b_3\}, \tag{7.7}$$

$$e_0:=\frac{1}{D_0}\begin{pmatrix}b_1\\ b_2\\ b_3\end{pmatrix}. \tag{7.8}$$

Here the GCD is an abbreviation of the greatest common divisor while the LCM is an abbreviation of the least common multiple. It is obvious that e_0 is in $\mathbf{Z}^3$ and that $(\omega-{}^t\omega)e_0=0$. The vector e_0 is a minimal integral vector in the sense that there is no real number s such that $0<s<1$ and $se_0\in\mathbf{Z}^3$. There exist other vectors e_1, e_2, $\in\mathbf{Q}^3$ that generate Ω^3 as

$$\Omega^3=\mathbf{R}e_0\oplus\mathbf{Z}e_1\oplus\mathbf{Z}e_2. \tag{7.9}$$

Here $\mathbf{Q}$ is the whole set of rational numbers. From (7.6) these generators e_1 and e_2 must satisfy

$$(\omega-{}^t\omega)e_1,(\omega-{}^t\omega)e_2\in\mathbf{Z}^3. \tag{7.10}$$

These vectors $\{e_1,e_2\}$ are minimal magnetic shifts in the sense that there is no real number s such that

$$0<s<1, \quad s(\omega-{}^t\omega)e_i\in\mathbf{Z}^3, \tag{7.11}$$

for each $i=1,2$. Moreover, there are positive integers ν_1 and ν_2 such that

$$\nu_1 e_1, \nu_2 e_2\in\mathbf{Z}^3. \tag{7.12}$$

We demand that the integers $\{\nu_1,\nu_2\}$ are the smallest cycles in the sense that there is no integer m such that

$$0<m<\nu_i, \quad me_i\in\mathbf{Z}^3, \tag{7.13}$$

for each $i=1,2$. Consequently, the decomposition (7.9) yields

and

$$\Omega^3/\mathbf{Z}^3=(\mathbf{R}/\mathbf{Z})\oplus(\mathbf{Z}/\nu_1\mathbf{Z})\oplus(\mathbf{Z}/\nu_2\mathbf{Z}). \tag{7.14}$$

Thus an arbitrary element g of $S_A=(\mathbf{R}\times_\omega\Omega^3)/(\mathbf{Z}\times_\omega\mathbf{Z}^3)$ is parametrized as

$$g=(s,te_0+n_1e_1+n_2e_2), \quad s,t\in\mathbf{R}/\mathbf{Z};n_1\in\mathbf{Z}/\nu_1\mathbf{Z};n_2\in\mathbf{Z}/\nu_2\mathbf{Z}. \tag{7.15}$$

Let us examine the commutator (3.4). It is clear that the element $(s,0)$ commutes with any element. Since $(\omega-{}^t\omega)e_0=0$, the element $(0,te_0)$ also commutes with any element. On the other hand, $(0,e_1)$ and $(0,e_2)$ produce a nonvanishing commutator

$$(0,e_1)\cdot(0,e_2)\cdot(0,e_1)^{-1}\cdot(0,e_2)^{-1}=(\gamma,0) \tag{7.16}$$

with

$$\gamma:=e_1(\omega-{}^t\omega)e_2=e_1\cdot(e_2\times b). \tag{7.17}$$

From (7.10) and (7.12) we can see that

$$\nu_1\gamma,\nu_2\gamma\in\mathbf{Z}. \tag{7.18}$$

Hence γ is a rational number. Let d be the greatest common divisor of ν_1 and ν_2. If we put $\nu_1=dp_1$ and $\nu_2=dp_2$, then p_1 and p_2 are mutually prime. The above equation (7.18) implies that $d\gamma$ is an integer. So we have

$$d:=\mathrm{GCD}\{\nu_1,\nu_2\}, \quad \ell:=d\gamma\in\mathbf{Z}. \tag{7.19}$$

Before constructing the representation of the MTG, we need to know how the generators generate an arbitrary element of the MTG. From the multiplication rule of the group $\mathbf{R}\times_\omega\mathbf{R}^n$ we deduce that for $x,y\in\mathbf{R}^n$

$$\begin{aligned}(\tfrac{1}{2}x\omega x,x)\cdot(\tfrac{1}{2}y\omega y,y)&=(\tfrac{1}{2}x\omega x+\tfrac{1}{2}y\omega y+x\omega y,x+y)\\&=(\tfrac{1}{2}x\omega y-\tfrac{1}{2}y\omega x+\tfrac{1}{2}(x+y)\omega(x+y),x+y)\\&=(\tfrac{1}{2}x(\omega-{}^t\omega)y,0)\cdot(\tfrac{1}{2}(x+y)\omega(x+y),x+y)\end{aligned} \tag{7.20}$$

and

$$(\tfrac{1}{2}x\omega x,x)^{-1}=(\tfrac{1}{2}x\omega x,-x). \tag{7.21}$$

Iteration of (7.20) yields

$$(\tfrac{1}{2}x\omega x,x)^n=(\tfrac{1}{2}n^2x\omega x,nx),\quad n\in\mathbf{Z}. \tag{7.22}$$

Furthermore, (7.20) implies

$$(\tfrac{1}{2}s^2x\omega x,sx)\cdot(\tfrac{1}{2}t^2x\omega x,tx)=(\tfrac{1}{2}(s+t)^2x\omega x,(s+t)x),\quad s,t\in\mathbf{R}. \tag{7.23}$$

By a tedious calculation we can show

$$(s,x+y+z)=(s-X,0)\cdot(\tfrac{1}{2}x\omega x,x)\cdot(\tfrac{1}{2}y\omega y,y)\cdot(\tfrac{1}{2}z\omega z,z) \tag{7.24}$$

with

$$X=\tfrac{1}{2}(x+y+z)\omega(x+y+z)+\tfrac{1}{2}x(\omega-{}^t\omega)y+\tfrac{1}{2}x(\omega-{}^t\omega)z+\tfrac{1}{2}y(\omega-{}^t\omega)z. \tag{7.25}$$

Thus an arbitrary element of the MTG is expressed as

$$\begin{aligned}g&=(s,te_0+n_1e_1+n_2e_2)\\&=(s-\tfrac{1}{2}(te_0+n_1e_1+n_2e_2)\omega(te_0+n_1e_1+n_2e_2)-\tfrac{1}{2}\gamma n_1n_2,0)\\&\quad\cdot(\tfrac{1}{2}t^2e_0\omega e_0,te_0)\cdot(\tfrac{1}{2}e_1\omega e_1,e_1)^{n_1}\cdot(\tfrac{1}{2}e_2\omega e_2,e_2)^{n_2}\\&=\phi(s-X)\cdot g_0(t)\cdot(g_1)^{n_1}\cdot(g_2)^{n_2},\end{aligned} \tag{7.26}$$

which is a product of the generators

$$\phi(s):=(s,0), \tag{7.27}$$

$$g_0(t):=(\tfrac{1}{2}t^2e_0\omega e_0,te_0), \tag{7.28}$$

$$g_1:=(\tfrac{1}{2}e_1\omega e_1,e_1), \tag{7.29}$$

$$g_2:=(\tfrac{1}{2}e_2\omega e_2,e_2). \tag{7.30}$$

These generators satisfy the relations

$$\phi(s)\cdot\phi(t)=\phi(s+t), \tag{7.31}$$

$$\phi(1)=1, \tag{7.32}$$

$$g_0(s)\cdot g_0(t)=g_0(s+t), \tag{7.33}$$

$$g_0(1)=\phi(\tfrac{1}{2}z_0), \tag{7.34}$$

$$(g_1)^{\nu_1}=\phi(\tfrac{1}{2}z_1), \tag{7.35}$$

$$(g_2)^{\nu_2}=\phi(\tfrac{1}{2}z_2), \tag{7.36}$$

$$g_1\cdot g_2\cdot g_1^{-1}\cdot g_2^{-1}=\phi(\gamma) \tag{7.37}$$

and other trivial commutators. Here we have defined $\{z_0,z_1,z_2\}$ by

$$z_0 := e_0 \omega e_0 = \left(\frac{1}{D_0}\right)^2 b_1 b_2 b_3, \tag{7.38}$$

$$z_1 := \nu_1^2 e_1 \omega e_1, z_2 := \nu_2^2 e_2 \omega e_2. \tag{7.39}$$

Because e_0 is an integral vector and ω is an integral matrix, z_0 is an integer. Furthermore, (7.12) implies that z_1 and z_2 are also integers.

In reverse order, the generators $\{\phi(s), g_0(t), g_1, g_2\}$ and their relations (7.31)–(7.37) determine the MTG uniquely. These generators with the relations form the MTG in a constructive manner. Consequently, the MTG in T^3 is completely characterized by the set of parameters $(z_0, z_1, z_2, \nu_1, \nu_2, \gamma)$, where $\{z_0, z_1, z_2, \nu_1, \nu_2\}$ are integers and γ is a rational number constrained by the condition (7.18).

Now we discuss the representation theory of the MTG exhaustively. The space of functions $\{f: \mathbf{R}^{n+1} \to \mathbf{C}\}$ provides the regular representation of the group $\mathbf{R} \times_\omega \mathbf{R}^n$ via

$$\begin{aligned} U(v_0, v) f(x_0, x) &:= f((v_0, v)^{-1} \cdot (x_0, x)) \\ &= f((-v_0 + v\,\omega v, -v) \cdot (x_0, x)) \\ &= f(x_0 - v_0 + v\,\omega v - v\,\omega x, x - v). \end{aligned} \tag{7.40}$$

We restrict the representation U on the space of equivariant functions, which are constrained by (3.7) and (3.8). Then we have

$$U(v_0, v) f(x_0, x) = e^{2\pi i (v_0 - v\,\omega v + v\,\omega x)} f(x_0, x - v), \tag{7.41}$$

which reproduces the unitary transformations (2.3) and (2.4) when the twisting matrix (3.11) is taken. Particularly $(v_0, 0)$ is represented by

$$U(v_0, 0) f(x_0, x) = e^{2\pi i v_0} f(x_0, x). \tag{7.42}$$

Hence the representation U induces an isomorphism of (7.31) and (7.32) by

$$U(\phi(s)) = e^{2\pi i s}. \tag{7.43}$$

Moreover, if we put

$$U_0(t) := U(g_0(t)), \quad U_1 := U(g_1), \quad U_2 := U(g_2), \tag{7.44}$$

they satisfy

$$U_0(s) U_0(t) = U_0(s + t), \tag{7.45}$$

$$U_0(1) = e^{\pi i z_0}, \tag{7.46}$$

$$(U_1)^{\nu_1} = e^{\pi i z_1}, \tag{7.47}$$

$$(U_2)^{\nu_2} = e^{\pi i z_2}, \tag{7.48}$$

$$U_1 U_2 U_1^{-1} U_2^{-1} = e^{2\pi i \gamma}, \tag{7.49}$$

since U is a homomorphism of the relations (7.33)–(7.37).

An irreducible representation of $U_0(t)$ is labeled by an integer q_0 and defined by

$$U_0(t) |q_0\rangle = e^{2\pi i (q_0 + (1/2) z_0) t} |q_0\rangle. \tag{7.50}$$

On the other hand, to construct a representation of the algebra generated by U_1 and U_2, we introduce a set of orthogonal vectors $\{|q_1,q_2\rangle | q_1 \in \mathbf{Z}/\nu_1\mathbf{Z}, q_2 \in \mathbf{Z}/\nu_2\mathbf{Z}\}$. We assume identification $|q_1,q_2\rangle = |q_1+k_1\nu_1, q_2+k_2\nu_2\rangle$ for any $k_1,k_2 \in \mathbf{Z}$. Let the operators U_1 and U_2 act on them by

$$U_1|q_1,q_2\rangle = e^{2\pi i(q_1+(1/2)z_1)/\nu_1}|q_1,q_2\rangle, \tag{7.51}$$

$$U_2|q_1,q_2\rangle = e^{2\pi i(q_2+(1/2)z_2)/\nu_2}|q_1+\nu_1\gamma,q_2\rangle. \tag{7.52}$$

The step of q_1 generated by U_2 is

$$\Delta q_1 := \nu_1\gamma = dp_1\frac{\ell}{d} = p_1\ell. \tag{7.53}$$

Then the fundamental relations, (7.47)–(7.49), are satisfied as

$$(U_1)^{\nu_1}|q_1,q_2\rangle = e^{2\pi i(q_1+(1/2)z_1)}|q_1,q_2\rangle = e^{2\pi i(1/2)z_1}|q_1,q_2\rangle, \tag{7.54}$$

$$\begin{aligned}(U_2)^{\nu_2}|q_1,q_2\rangle &= e^{2\pi i(q_2+(1/2)z_2)}|q_1+\nu_1\nu_2\gamma,q_2\rangle \\ &= e^{2\pi i(1/2)z_2}|q_1,q_2\rangle \quad \text{(because } \nu_2\gamma \text{ is an integer)},\end{aligned} \tag{7.55}$$

$$\begin{aligned}U_1U_2U_1^{-1}U_2^{-1}|q_1,q_2\rangle &= U_1U_2U_1^{-1}e^{-2\pi i(q_2+(1/2)z_2)/\nu_2}|q_1-\nu_1\gamma,q_2\rangle \\ &= U_1U_2e^{-2\pi i(q_1-\nu_1\gamma+(1/2)z_1)/\nu_1}e^{-2\pi i(q_2+(1/2)z_2)/\nu_2}|q_1-\nu_1\gamma,q_2\rangle \\ &= U_1\,e^{-2\pi i(q_1-\nu_1\gamma+(1/2)z_1)/\nu_1}|q_1,q_2\rangle = e^{2\pi i\gamma}|q_1,q_2\rangle.\end{aligned} \tag{7.56}$$

Thus the basis $\{|q_1,q_2\rangle\}$ spans a representation space of the algebra generated by U_1 and U_2. This representation space is reducible generally. We can see that the action of U_2 is cyclic. Namely, if we put

$$c := \frac{\mathrm{LCM}\{\Delta q_1,\nu_1\}}{\Delta q_1} = \frac{\mathrm{LCM}\{p_1\ell,p_1d\}}{p_1\ell} = \frac{\mathrm{LCM}\{\ell,d\}}{\ell} = \frac{d}{\mathrm{GCD}\{\ell,d\}}, \tag{7.57}$$

then

$$c\Delta q_1 = \mathrm{LCM}\{\Delta q_1,\nu_1\} \tag{7.58}$$

is an integral multiple of ν_1 and therefore the U_2 action (7.52) iterated by c times gives

$$(U_2)^c|q_1,q_2\rangle = e^{2\pi i(q_2+(1/2)z_2)c/\nu_2}|q_1+c\Delta q_1,q_2\rangle = e^{2\pi i(q_2+(1/2)z_2)c/\nu_2}|q_1,q_2\rangle. \tag{7.59}$$

Moreover,

$$\frac{\nu_1}{c} = \frac{\nu_1\mathrm{GCD}\{\ell,d\}}{d} = \frac{dp_1\mathrm{GCD}\{\ell,d\}}{d} = p_1\mathrm{GCD}\{\ell,d\}, \tag{7.60}$$

$$\frac{\nu_2}{c} = \frac{\nu_2\mathrm{GCD}\{\ell,d\}}{d} = \frac{dp_2\mathrm{GCD}\{\ell,d\}}{d} = p_2\mathrm{GCD}\{\ell,d\} \tag{7.61}$$

are integers. Therefore, each choice of $q_1 \in \mathbf{Z}$ modulo $(\nu_1/c)\mathbf{Z}$ and $q_2 \in \mathbf{Z}$ modulo $(\nu_2/c)\mathbf{Z}$ specifies one of inequivalent irreducible representations. Consequently, the dimension of the irreducible representation is

$$\text{dimension} = c = \frac{d}{\mathrm{GCD}\{d,\ell\}}. \tag{7.62}$$

On the other hand, the number of inequivalent representations for a fixed q_0 is

$$\#\text{inequivalent irreducible representations} = \frac{\nu_1}{c}\cdot\frac{\nu_2}{c} = p_1 p_2 (\mathrm{GCD}\{d,\ell\})^2. \tag{7.63}$$

These numbers give a number

$$(\text{dimension})^2 \times (\#\text{inequivalent irreducible representations}) = c^2 \times \frac{\nu_1\nu_2}{c^2} = \nu_1\nu_2, \tag{7.64}$$

which coincides with the dimension of the algebra generated by U_1 and U_2, as required by the Peter–Weyl theory on group representation.[29] Thus we have obtained the complete set of irreducible representations of the algebra.

In summary, an irreducible representation of the MTG in the three-dimensional torus is specified by

$$\chi = (q_0,[q_1],[q_2]) \in \mathbf{Z}\times\mathbf{Z}_{(\nu_1/c)}\times\mathbf{Z}_{(\nu_2/c)}. \tag{7.65}$$

Using the decomposition (7.26) we have

$$\begin{aligned} &U(s,te_0+n_1e_1+n_2e_2)|q_0,q_1,q_2\rangle \\ &\quad = e^{2\pi i(s-X)}U_0(t)(U_1)^{n_1}(U_2)^{n_2}|q_0,q_1,q_2\rangle \\ &\quad = e^{2\pi i\{(s-X)+(q_0+(1/2)z_0)t+(q_1+\gamma\nu_1 n_2+(1/2)z_1)n_1/\nu_1+(q_2+(1/2)z_2)n_2/\nu_2\}}|q_0,q_1+\gamma\nu_1 n_2,q_2\rangle \end{aligned} \tag{7.66}$$

with X evaluated as

$$X = \tfrac{1}{2}(te_0+n_1e_1+n_2e_2)\omega(te_0+n_1e_1+n_2e_2)+\tfrac{1}{2}\gamma n_1 n_2. \tag{7.67}$$

B. Examples in the three-dimensional torus

Here we apply the previous method of representation of the MTG to three examples of magnetic fields in T^3.

The first example is a magnetic field parallel to the x_3-axis,

$$b = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \nu \end{pmatrix} \tag{7.68}$$

with a positive integer ν. The generators (7.9) of the MTG are chosen as

$$e_0 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad e_1 = \frac{1}{\nu}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad e_2 = \frac{1}{\nu}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \tag{7.69}$$

The vectors $\{e_1,e_2\}$ reproduce the discrete magnetic shifts (2.17) in the plane perpendicular to the magnetic field. The cycles (7.12) of e_1 and e_2 are found to be

$$\nu_1 = \nu, \quad \nu_2 = \nu, \tag{7.70}$$

respectively. Using them we evaluate the parameters of the MTG as

$$d=\mathrm{GCD}\{\nu_1,\nu_2\}=\mathrm{GCD}\{\nu,\nu\}=\nu, \tag{7.71}$$

$$\gamma=e_1(\omega-{}^t\omega)e_2=e_1\cdot(e_2\times b)=\frac{1}{\nu}, \tag{7.72}$$

$$\ell=d\gamma=\nu\frac{1}{\nu}=1, \tag{7.73}$$

$$z_0=z_1=z_2=0. \tag{7.74}$$

The size and the number of irreducible representations are

$$\text{dimension}=c=\frac{d}{\mathrm{GCD}\{\ell,d\}}=\frac{\nu}{\mathrm{GCD}\{1,\nu\}}=\frac{\nu}{1}=\nu, \tag{7.75}$$

$$\#\text{inequivalent irreducible representations}=\frac{\nu_1\nu_2}{c^2}=\frac{\nu^2}{\nu^2}=1. \tag{7.76}$$

In this case (7.51) and (7.52) reproduce the representations (2.20) and (2.21) in T^2.

The second example is a magnetic field perpendicular to the x_1-axis and lying in the middle of the x_2- and x_3-axes,

$$b=\begin{pmatrix}b_1\\b_2\\b_3\end{pmatrix}=\begin{pmatrix}0\\\nu\\\nu\end{pmatrix}, \tag{7.77}$$

with a positive integer ν. The generators of the MTG are chosen as

$$e_0=\begin{pmatrix}0\\1\\1\end{pmatrix},\quad e_1=\frac{1}{\nu}\begin{pmatrix}0\\0\\1\end{pmatrix},\quad e_2=\frac{1}{\nu}\begin{pmatrix}1\\0\\0\end{pmatrix}. \tag{7.78}$$

The cycles of e_1 and e_2 are

$$\nu_1=\nu,\quad \nu_2=\nu, \tag{7.79}$$

and other parameters of the MTG are also evaluated as

$$d=\nu,\ \gamma=\frac{1}{\nu},\ \ell=1,\ z_0=z_1=z_2=0, \tag{7.80}$$

$$\text{dimension}=c=\nu, \tag{7.81}$$

$$\#\text{inequivalent irreducible representations}=\frac{\nu_1\nu_2}{c^2}=1. \tag{7.82}$$

The third example is a magnetic field in the direction of (1,1,1),

$$b=\begin{pmatrix}b_1\\b_2\\b_3\end{pmatrix}=\begin{pmatrix}\nu\\\nu\\\nu\end{pmatrix} \tag{7.83}$$

with a positive integer ν. A calculation similar to the previous ones gives a series of parameters. Here we show only the results

$$e_0=\begin{pmatrix}1\\1\\1\end{pmatrix},\quad e_1=\frac{1}{\nu}\begin{pmatrix}1\\0\\0\end{pmatrix},\quad e_2=\frac{1}{\nu}\begin{pmatrix}0\\1\\0\end{pmatrix}, \tag{7.84}$$

$$\nu_1=\nu,\ \nu_2=\nu,\ d=\nu,\ \gamma=\frac{1}{\nu},\ \ell=1, z_0=\nu, z_1=z_2=0, \tag{7.85}$$

$$\text{dimension}=c=\nu, \tag{7.86}$$

$$\#\text{inequivalent irreducible representations}=\frac{\nu_1\nu_2}{c^2}=1. \tag{7.87}$$

VIII. REPRESENTATION THEORY OF THE MTG IN AN *n*-TORUS

Here we describe how to characterize the MTGs in an n-dimensional torus. We can choose generators $\{e_1,e_2,\ldots,e_l,f_1,f_2,\ldots,f_l,g_1,g_2,\ldots,g_m\}$ $(2l+m=n)$ of the magnetic shift group Ω^n such that

$$e_i,f_i\in\mathbf{Q}^n,\quad(\omega-{}^t\omega)e_i,(\omega-{}^t\omega)f_i\in\mathbf{Z}^n,\quad e_i(\omega-{}^t\omega)f_j=\gamma_i\delta_{ij}\quad(i,j=1,\ldots,l), \tag{8.1}$$

$$g_k\in\mathbf{Z}^n,\quad(\omega-{}^t\omega)g_k=0\quad(k=1,\ldots,m), \tag{8.2}$$

with nonzero rational numbers $\gamma_i\in\mathbf{Q}$. The vectors $\{g_1,\ldots,g_m\}$ are demanded to be minimal integral vectors in the sense that there is no real number s satisfying

$$0<s<1,\quad sg_k\in\mathbf{Z}^n, \tag{8.3}$$

for each $k=1,\ldots,m$. Let $\{\mu_i,\nu_i\}(i=1,\ldots,l)$ be smallest positive integers such that

$$\mu_ie_i,\nu_if_i\in\mathbf{Z}^n \tag{8.4}$$

and that there are no integers $\{m_i,n_i\}$ satisfying

$$0<m_i<\mu_i,\quad m_ie_i\in\mathbf{Z}^n, \tag{8.5}$$

$$0<n_i<\nu_i,\quad n_if_i\in\mathbf{Z}^n. \tag{8.6}$$

Equations (8.1) and (8.4) imply that $\gamma_i\mu_i$ and $\gamma_i\nu_i$ are integers. Thus, by putting

$$d_i:=\mathrm{GCD}\{\mu_i,\nu_i\}, \tag{8.7}$$

we can see that γ_id_i is an integer. Consequently, the group of translations (6.16) is decomposed as

$$\Omega^n=\mathbf{Z}e_1\oplus\cdots\oplus\mathbf{Z}e_l\oplus\mathbf{Z}f_1\oplus\cdots\oplus\mathbf{Z}f_l\oplus\mathbf{R}g_1\oplus\cdots\oplus\mathbf{R}g_m \tag{8.8}$$

and the MTG (6.18) is expressed as

$$S_A\cong S^1\times_\omega(\mathbf{Z}_{\mu_1}\times\cdots\times\mathbf{Z}_{\mu_l}\times\mathbf{Z}_{\nu_1}\times\cdots\times\mathbf{Z}_{\nu_l}\times T^m). \tag{8.9}$$

Finally, we describe an outline of the representation theory of the MTG's in an n-dimensional torus. Let us define integers x_i,y_i,z_j by

$$x_i:=\mu_i^2e_i\omega e_i, \tag{8.10}$$

$$y_i:=\nu_i^2f_i\omega f_i\quad(i=1,\ldots,l), \tag{8.11}$$

$$z_k := g_k \omega g_k \quad (k=1,\ldots,m). \tag{8.12}$$

Generators of the MTG (8.9) are represented by a set of unitary operators

$$T(s) := U(s,0), \quad s \in \mathbf{R}, \tag{8.13}$$

$$U_i := U(\tfrac{1}{2} e_i \omega e_i, e_i), \tag{8.14}$$

$$V_i := U(\tfrac{1}{2} f_i \omega f_i, f_i), \tag{8.15}$$

$$W_k(t) := U(\tfrac{1}{2} t^2 g_k \omega g_k, t g_k), \quad t \in \mathbf{R}. \tag{8.16}$$

They satisfy the equations

$$T(s)T(t) = T(s+t), \tag{8.17}$$

$$T(1) = 1, \tag{8.18}$$

$$(U_i)^{\mu_i} = T(x_i/2), \tag{8.19}$$

$$(V_i)^{\nu_i} = T(y_i/2), \tag{8.20}$$

$$U_i V_i U_i^{-1} V_i^{-1} = T(\gamma_i), \tag{8.21}$$

$$W_k(s) W_k(t) = W_k(s+t), \tag{8.22}$$

$$W_k(1) = T(z_k/2), \tag{8.23}$$

and other trivial commutators. These equations for the n-torus are generalization of the equations (7.31)–(7.37) for the three-torus. A representation space is spanned by the basis vectors

$$|\lambda, p, q, r\rangle = |\lambda, p_1, p_2, \ldots, p_l, q_1, q_2, \ldots, q_l, r_1, r_2, \ldots, r_m\rangle \tag{8.24}$$

labeled by $\lambda \in \mathbf{Z}$, $p_i \in \mathbf{Z}_{\mu_i}$, $q_i \in \mathbf{Z}_{\nu_i}$, and $r_k \in \mathbf{Z}$. The generators act on the basis vectors according to

$$T(s)|\lambda, p, q, r\rangle = e^{2\pi i \lambda s} |\lambda, p, q, r\rangle, \tag{8.25}$$

$$U_i |\lambda, p, q, r\rangle = e^{\pi i \lambda (2p_i + x_i)/\mu_i} |\lambda, p, q, r\rangle, \tag{8.26}$$

$$V_i |\lambda, p, q, r\rangle = e^{\pi i \lambda (2q_i + y_i)/\nu_i} |\lambda, p_1, \ldots, p_i + \gamma_i \mu_i, \ldots, p_l, q, r\rangle, \tag{8.27}$$

$$W_k(t) |\lambda, p, q, r\rangle = e^{\pi i \lambda (2r_k + z_k) t} |\lambda, p, q, r\rangle. \tag{8.28}$$

These are generalization of (7.43) and (7.50)–(7.52). The cycle of V_i is given by

$$c_i := \frac{\mathrm{LCM}\{\gamma_i \mu_i, \mu_i\}}{\gamma_i \mu_i} = \frac{\mathrm{LCM}\{\gamma_i d_i, d_i\}}{\gamma_i d_i} = \frac{d_i}{\mathrm{GCD}\{\gamma_i d_i, d_i\}}. \tag{8.29}$$

Hence an irreducible representation is labeled by

$$\chi = (\lambda, [p_1], \ldots, [p_l], [q_1], \ldots, [q_l], r_1, \ldots, r_m) \in \mathbf{Z} \times \mathbf{Z}_{(\mu_1/c_1)} \times \cdots \times \mathbf{Z}_{(\mu_l/c_l)} \times \mathbf{Z}_{(\nu_1/c_1)} \times \cdots \times \mathbf{Z}_{(\nu_l/c_l)} \times \mathbf{Z}^m. \tag{8.30}$$

The dimension of the irreducible representation is

$$\text{dimension}=\prod_{i=1}^{l} c_i, \tag{8.31}$$

and the number of inequivalent representations is

$$\#\text{inequivalent irreducible representations}=\prod_{i=1}^{l} \frac{\mu_i \nu_i}{c_i^2} \tag{8.32}$$

for fixed $(\lambda, r_1, \ldots, r_m) \in \mathbf{Z}^{m+1}$.

IX. CONCLUSION

Let us summarize our discussions. We began this article with a discussion on symmetry of a charged particle in a uniform magnetic field. We saw that the quantum system in T^2 has a discrete noncommutative translation symmetry. The symmetry is characterized by a central extension of a cyclic group.

In the following part of this article we introduced a noncommutative product into $\mathbf{R}^{n+1}$. Using the group structure, we defined the magnetic fiber bundles P_ω^{n+1}, which is a fiber bundle over T^n with a fiber S^1. Then we showed that the set of magnetic fiber bundles is classified by the quotient space of integral matrices $\mathrm{Mat}(n,\mathbf{Z})/\mathrm{Sym}(n,\mathbf{Z})$. We introduced connections into the fiber bundles and classified them by $\mathrm{Mat}(n,\mathbf{Z})\times\mathbf{R}^n/\mathrm{Sym}(n,\mathbf{Z})\times\mathbf{Z}^n$ as shown in (5.5). The lifted translations leaving the connection invariant form the magnetic translation group of (6.4). We characterized the MTG by (6.18) with (6.16). This characterization of the MTG is one of main results of this article. We found that the magnetic shift group Ω^n is discrete when the characteristic matrix $(\omega - {}^t\omega)$ is nondegenerated.

In the rest of the article we discussed the representation theory of the MTG for T^3 in detail and applied it to a few examples. The dimensions of an irreducible unitary representation is given by c in (7.62) and each irreducible representation is labeled by χ in (7.65). These results may be useful for application to the electron system in a lattice in an inclined magnetic field. We briefly described the representation theory of the MTG for T^n and summarized the result in (8.30) and (8.31).

Here we would like to mention remaining problems. It is desirable to apply the representation theory of the MTG to spectral analyses of the Laplace and Dirac operators. Originally the spectral problem of the quantum mechanics in a torus motivated this study. For this application the Peter–Weyl theory on group representation will play an essential role. In the next study we would like to pursue the analysis of the Laplace operator in the torus with a magnetic field. Moreover, an equilateral torus admits discrete transformations that exchange vertices of the torus and that leave the metric and the magnetic field invariant. It is also desirable to include such discrete transformations into the MTG for the complete spectral analysis.

By developing the theory of the MTG we will find its applications to physics. Inclusion of the supersymmetry into the MTG is an interesting direction for the future development. Sakamoto, Tachibana, and Takenaga[30,31] have pointed out that breaking of the translation symmetry causes breaking of the supersymmetry because the supersymmetry includes the translation symmetry. Hence the magnetic field may trigger supersymmetry breaking. On the other hand, the MTG in an n-torus is regarded as a generalization of the noncommutative torus, which attracted much attention recently in the string theory.[32] The B-field in a compactified space naturally induces a noncommutative structure, which is described by the MTG. Jackiw[33] also showed that how the noncommutative structure emerges in physical situations. If we turn our attention to solid state physics, we find another interesting application of the MTG also in this area. Tranquada[34] observed spontaneous formation of a charge density wave at a nonzero wave number in a copper-

oxide superconductor. This ordered state is called the stripe phase, in which the translation symmetry is broken. A similar stripe phase occurs commonly in a quantum Hall system.[35] Application of the MTG may help understanding of the stripe phases.

Note added in proof. After acceptance for publication of this article we obtained more strong results on the magnetic translation group in n dimensions. As concerns γ_i in (8.1) and μ_i, ν_i in (8.4), we proved that $\mu_i=\nu_i=1/\gamma_i$. Consequently, the definition (8.7) means simply that $d_i=\nu_i$. Eq. (8.29) is also simplified as $c_i=\nu_i$. In (8.31) the dimension of the irreducible representation becomes $\Pi_{i=1}^{l}\nu_i$. Finally, the number of inequivalent reprenentations (8.32) is reduced to one. As a corollary, we can show that $\nu_1=\nu_2=d=c=1/\gamma$ and hence $\ell=d\gamma=1$ in Sec. VII. More strongly, we can prove that $\nu_1=\mathrm{GCD}\{b_1,b_2,b_3\}$ for the three-deimensional magnetic field. Proofs of these statements are to be published elsewhere.

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Theory and application of Fermi pseudo-potential in one dimension

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The theory of interaction at one point is developed for the one-dimensional Schrödinger equation. In analog with the three-dimensional case, the resulting interaction is referred to as the Fermi pseudo-potential. The dominant feature of this one-dimensional problem comes from the fact that the real line becomes disconnected when one point is removed. The general interaction at one point is found to be the sum of three terms, the well-known delta-function potential and two Fermi pseudo-potentials, one odd under space reflection and the other even. The odd one gives the proper interpretation for the $\delta'(x)$ potential, while the even one is unexpected and more interesting. Among the many applications of these Fermi pseudo-potentials, the simplest one is described. It consists of a superposition of the delta-function potential and the even pseudo-potential applied to two-channel scattering. This simplest application leads to a model of the quantum memory, an essential component of any quantum computer. © *2002 American Institute of Physics.*
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I. INTRODUCTION

There are several interrelated motivations for the present investigation. These are discussed in the following.

It was realized several years ago that there are significant differences between scattering in one channel and scattering in two or more coupled channels.[1] For this reason, it may be useful to gain some experience in dealing with coupled channels in general.

The first question is: What is the simplest scattering problem in the case of coupled channels? Once this simplest problem is understood, it is reasonable to expect that many of its features hold also for more general situations. Clearly, for this simplest problem, the number of channels should be chosen to be the smallest, namely two, and the number of spatial dimensions should also be chosen this way, namely one. Thus the scattering problem under consideration, in the time-independent case, deals with the coupled Schrödinger equations

$$\begin{aligned} -\frac{d^2\psi_1(x)}{dx^2}+V_{11}(x)\psi_1(x)+V_{12}(x)\psi_2(x)&=k^2\psi_1(x),\\ -\frac{d^2\psi_2(x)}{dx^2}+V_{21}(x)\psi_1(x)+V_{22}(x)\psi_2(x)&=k^2\psi_2(x), \end{aligned} \tag{1.1}$$

where the 2×2 matrix potential

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$$V(x)=\begin{bmatrix} V_{11}(x) & V_{12}(x) \\ V_{21}(x) & V_{22}(x) \end{bmatrix} \tag{1.2}$$

is such that it cannot be diagonalized simultaneously for all x.

What is the simplest possible choice for this $V(x)$? In the case of one channel, the simplest potential is the one that is proportional to the Dirac delta-function $\delta(x-x_0)$. This potential is localized at the one point x_0, and the corresponding Schrödinger equation is easy to solve. For two coupled channels, it is equally desirable to have the potential localized at one point, say at $x=0$. However, it is not allowed to take $V(x)$ to be the product of $\delta(x)$ and a constant 2×2 matrix because the diagonalization of this constant matrix decouples the channels.

What is needed, therefore, is another one-dimensional potential that is localized at one point. With a linear combination of $\delta(x)$ and this new potential, the 2×2 matrix $V(x)$ can be easily chosen such that it cannot be diagonalized and, hence, the two channels do not decouple.

There are many practical applications of the two-channel scattering problem in one dimension. In this article, let us restrict ourselves to one such application that is of current interest. The coupled channels can be used as a model for quantum memory; a natural approach to resetting, reading, and writing on a quantum memory is to use scattering from such a quantum memory.

In trying to find this second potential that is localized at one point, it is not necessary to study the coupled Schrödinger equations (1.1); it is sufficient to return to the simpler case of the one-channel Schrödinger equation

$$\left[-\frac{d^2}{dx^2}+V(x)\right]\psi(x)=k^2\psi(x). \tag{1.3}$$

A natural first guess for this second potential is the derivative of the Dirac delta-function, i.e., $\delta'(x)$. However, the presence of this $\delta'(x)$ term in Eq. (1.3) implies that the wave function must be discontinuous at this point $x=0$. But the product of $\delta'(x)$ and a function discontinuous at $x=0$ is not well defined. Furthermore, even if this $\delta'(x)$ potential is well defined, it is not suitable for the first application to quantum memory. The reason for this will be discussed later in this article.

A more powerful method is needed to find this desired potential. It is useful here to recall the concept of the Fermi pseudo-potential in three dimensions, which can be written in the form

$$\delta^3(r)\frac{\partial}{\partial r}r, \tag{1.4}$$

as given by Blatt and Weisskopf.[2] The most far-reaching application of this Fermi pseudo-potential is to the study of many-body systems, as initiated by Huang and Yang.[3] For the ground-state energy per particle of a Bose system of hard spheres, the low-density expansion is known to be

$$4\pi a\rho\left[1+\frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2}+8\left(\frac{4\pi}{3}-\sqrt{3}\right)\rho a^3\ln(\rho a^3)+O(\rho a^3)\right]. \tag{1.5}$$

In this expansion, the second term was first obtained by Lee and Yang[4] using the method of binary collision, but the derivation by Lee, Huang and Yang[5] using the Fermi pseudo-potential is somewhat simpler; the third term, which involves the logarithm, was first obtained by using the Fermi pseudo-potential.[6] In the derivation of the third term, it was found inconvenient to use the form (1.4), and thus a limiting process was reintroduced. This point will be of importance in this article. Thus a great deal is known about the Fermi pseudo-potential in three dimensions.

A further motivation for this article is to develop the Fermi pseudo-potential for one-dimensional scattering. In many cases, once a theory has been developed for three dimensions, it

is straightforward to repeat the development for one dimension. In the present case of the Fermi pseudo-potential, this is not the case. Furthermore, the result for one dimension seems qualitatively different from that for three dimensions.

For clarity of presentation, this article is organized into two parts: part A for the theory of the Fermi pseudo-potential in one dimension, and part B for its application to quantum computing. Needless to say, these two parts are closely related to each other. The sections are numbered consecutively throughout the paper.

PART A: THEORY OF ONE-DIMENSIONAL FERMI PSEUDO-POTENTIAL

II. INTERACTION AT ONE POINT

In the absence of V, the Hamiltonian of Eq. (1.3) is

$$H_0 = -\frac{d^2}{dx^2} \tag{2.1}$$

for real x, where the right-hand side is suitably interpreted so that it is self-adjoint. Let k be purely imaginary; define a real, positive κ by

$$\kappa = -ik. \tag{2.2}$$

For such a k, the Green's function, or resolvent, for this H_0 satisfies the differential equation

$$\left(-\frac{d^2}{dx^2} + \kappa^2\right) R_\kappa^{(0)}(x,x') = \delta(x-x'), \tag{2.3}$$

and is given explicitly by

$$R_\kappa^{(0)}(x,x') = (2\kappa)^{-1} e^{-\kappa|x-x'|}. \tag{2.4}$$

Let a potential V be added to this H_0 to give

$$H = H_0 + V, \tag{2.5}$$

which is also self-adjoint. Again for κ positive, the Green's function, or resolvent, for this H satisfies, similar to Eq. (2.3),

$$(H+\kappa^2) R_\kappa(x,x') = \delta(x-x'). \tag{2.6}$$

The interaction V is said to be at the one point x_0 if Eq. (2.6) implies that Eq. (2.3), with $R_\kappa^{(0)}(x,x')$ replaced by $R_\kappa(x,x')$, is satisfied for all x except $x = x_0$.

Because of translational symmetry, this x_0 is chosen to be 0 throughout this article. It is a consequence of Eq. (2.4) and the symmetry of the Green's function that this definition of an interaction at one point implies

$$R_\kappa(x,x') = \frac{1}{2\kappa}[e^{-\kappa|x-x'|} - f(\kappa;\mathrm{sg}x,\mathrm{sg}x') e^{-\kappa(|x|+|x'|)}], \tag{2.7}$$

where sg$x$ and sgx' mean the sign of x and the sign of x', respectively.

Since Eq. (2.7) is the starting point for the present paper, this is the appropriate place to add the following comments.

(1) In the present case of one dimension, the real line with the point $x=0$ removed is not connected. This is a qualitative difference between one dimension and higher dimensions.

(2) It is because of this property that the f in Eq. (2.7) can depend on the signs of x and x'.

(3) In the three-dimensional case, the Fermi pseudo-potential can be obtained in the following way: Take the self-adjoint Hamiltonian $-\nabla^2$, where ∇^2 is the three-dimensional Laplacian, and restrict it to functions that are zero at $\mathbf{r}=0$; the self-adjoint extensions[7] of this restricted operator give the Fermi pseudo-potential, i.e., these self-adjoint extensions can be written as the sum of $-\nabla^2$ and (1.4) multiplied by a constant. Such a procedure applied to the case of one dimension does not give Eq. (2.7).

It is useful to write out explicitly the f of Eq. (2.7) as

$$f(\kappa;\mathrm{sg}x,\mathrm{sg}x')=\begin{cases} f_1(\kappa), & \text{for } x>0,\ x'>0,\\ f_2(\kappa), & \text{for } x<0,\ x'>0,\\ f_3(\kappa), & \text{for } x<0,\ x'<0,\\ f_4(\kappa), & \text{for } x>0,\ x'<0, \end{cases} \tag{2.8}$$

following the four quadrants in the $x-x'$ plane. Note that all of these f's are dimensionless.

III. RESOLVENT EQUATION

In view of Eq. (2.7), it is most convenient to study the resolvent equation in coordinate representation:

$$R_{\kappa_1}(x,x')-R_{\kappa_2}(x,x')+(\kappa_1^2-\kappa_2^2)\int_{-\infty}^{\infty}dx''R_{\kappa_1}(x,x'')R_{\kappa_2}(x'',x')=0, \tag{3.1}$$

where κ_1 and κ_2 are two values of κ.

The substitution of Eq. (2.7) into this resolvent equation (3.1) gives, after a lengthy calculation,

$$\frac{1}{\kappa_1-\kappa_2}f(\kappa_1;\mathrm{sg}x,\mathrm{sg}x')+\frac{1}{\kappa_1+\kappa_2}f(\kappa_1;\mathrm{sg}x,-\mathrm{sg}x')-\frac{1}{\kappa_1-\kappa_2}f(\kappa_2;\mathrm{sg}x,\mathrm{sg}x')+\frac{1}{\kappa_1+\kappa_2}f(\kappa_2;$$
$$-\mathrm{sg}x,\mathrm{sg}x')-\frac{1}{\kappa_1+\kappa_2}[f(\kappa_1;\mathrm{sg}x,-)f(\kappa_2;-,\mathrm{sg}x')+f(\kappa_1;\mathrm{sg}x,+)f(\kappa_2;+,\mathrm{sg}x')]=0 \tag{3.2}$$

for $\kappa_1\neq\kappa_2$. This is the resolvent equation for the interaction at the point $x=0$ as defined in Sec. II.

Equation (3.2) has the following symmetry properties besides space reflection.

(1) Since $f(\kappa;\mathrm{sg}x,\mathrm{sg}x')$ is dimensionless, there is no scale for κ. Thus, Eq. (3.2) is invariant under the scale change

$$\kappa_1\to\lambda\kappa_1 \quad \text{and} \quad \kappa_2\to\lambda\kappa_2. \tag{3.3}$$

Note that λ is positive since the κ's are positive.

(2) There is an additional symmetry

$$f(\kappa;\mathrm{sg}x,\mathrm{sg}x')\to-\mathrm{sg}x\,\mathrm{sg}x'f\left(\frac{1}{\kappa};\mathrm{sg}x,\mathrm{sg}x'\right). \tag{3.4}$$

This discrete symmetry is going to play an important role in this article. In terms of the $f_j(\kappa)$ defined in Eq. (2.8), this symmetry is

$$\kappa\to\frac{1}{\kappa},$$

$$f_1 \to -f_1, \quad f_3 \to -f_3, \tag{3.5}$$

$$f_2 \to f_2, \quad f_4 \to f_4.$$

The next task is to solve the resolvent equation (3.2) for $f(\kappa;\mathrm{sg}x,\mathrm{sg}x')$. Since differential equations are easier to deal with than difference equations, it is convenient to take the limit $\kappa_1 \to \kappa_2$. In this limit, Eq. (3.2) reduces to

$$\frac{d}{d\kappa} f(\kappa;\mathrm{sg}x,\mathrm{sg}x') + \frac{1}{2\kappa}[f(\kappa;\mathrm{sg}x,-\mathrm{sg}x') + f(\kappa;-\mathrm{sg}x,\mathrm{sg}x')]$$

$$- \frac{1}{2\kappa}[f(\kappa;\mathrm{sg}x,-)f(\kappa;-,\mathrm{sg}x') + f(\kappa;\mathrm{sg}x,+)f(\kappa;+,\mathrm{sg}x')] = 0. \tag{3.6}$$

In terms of the $f_j(\kappa)$ of Eq. (2.8), this differential equation (3.6) consists of the following four equations by taking various signs for x and x':

$$f_1'(\kappa) + \frac{1}{2\kappa}[f_2(\kappa)+f_4(\kappa)] - \frac{1}{2\kappa}[f_2(\kappa)f_4(\kappa)+f_1(\kappa)^2] = 0, \tag{3.7a}$$

$$f_2'(\kappa) + \frac{1}{2\kappa}[f_1(\kappa)+f_3(\kappa)] - \frac{1}{2\kappa}[f_2(\kappa)f_3(\kappa)+f_1(\kappa)f_2(\kappa)] = 0, \tag{3.7b}$$

$$f_3'(\kappa) + \frac{1}{2\kappa}[f_2(\kappa)+f_4(\kappa)] - \frac{1}{2\kappa}[f_3(\kappa)^2+f_2(\kappa)f_4(\kappa)] = 0, \tag{3.7c}$$

$$f_4'(\kappa) + \frac{1}{2\kappa}[f_1(\kappa)+f_3(\kappa)] - \frac{1}{2\kappa}[f_3(\kappa)f_4(\kappa)+f_1(\kappa)f_4(\kappa)] = 0. \tag{3.7d}$$

An examination of these four differential equations shows the important role played by the combination $f_1(\kappa)+f_3(\kappa)$, which appears twice in Eq. (3.7b) and twice in Eq. (3.7d). Define $F(\kappa)$ up to an additive constant by

$$F'(\kappa) = \frac{1}{2\kappa}[f_1(\kappa)+f_3(\kappa)]. \tag{3.8}$$

In terms of this $F(\kappa)$, Eqs. (3.7b) and (3.7d) take the form

$$f_2'(\kappa) + F'(\kappa) - f_2(\kappa)F'(\kappa) = 0; \quad f_4'(\kappa) + F'(\kappa) - f_4(\kappa)F'(\kappa) = 0. \tag{3.9}$$

Integration of Eqs. (3.9) gives $f_2(\kappa)$ and $f_4(\kappa)$ in terms of $F(\kappa)$:

$$f_2(\kappa) = 1 + c_2 e^{F(\kappa)}, \quad f_4(\kappa) = 1 + c_4 e^{F(\kappa)}, \tag{3.10}$$

where c_2 and c_4 are two arbitrary constants of integration. Similarly, subtracting Eq. (3.7c) from Eq. (3.7a) gives

$$\frac{d}{d\kappa}[f_1(\kappa)-f_3(\kappa)] = \frac{1}{2\kappa}[f_1(\kappa)^2 - f_3(\kappa)^2] = F'(\kappa)[f_1(\kappa)-f_3(\kappa)], \tag{3.11}$$

or

$$f_1(\kappa) - f_3(\kappa) = 2c_3 e^{F(\kappa)}, \tag{3.12}$$

where c_3 is another arbitrary constant of integration.

It remains to determine $F(\kappa)$, which satisfies the second-order ordinary differential equation obtained from adding Eqs. (3.7a) and (3.7c):

$$2\kappa\frac{d}{d\kappa}\kappa\frac{d}{d\kappa}F(\kappa)=\left[\kappa\frac{d}{d\kappa}F(\kappa)\right]^2-1+(c_3^2+c_2c_4)e^{2F(\kappa)}. \tag{3.13}$$

The solution of this equation is straightforward but somewhat lengthy and is thus relegated to Appendix A.

The results are as follows:

$$f_1(\kappa)=\frac{-\sqrt{c_3^2+c_2c_4-c_1^2}\,[c_0\kappa+(c_0\kappa)^{-1}]-2c_3}{\sqrt{c_3^2+c_2c_4-c_1^2}\,[c_0\kappa-(c_0\kappa)^{-1}]+2c_1}, \tag{3.14a}$$

$$f_2(\kappa)=1-\frac{2c_2}{\sqrt{c_3^2+c_2c_4-c_1^2}\,[c_0\kappa-(c_0\kappa)^{-1}]+2c_1}, \tag{3.14b}$$

$$f_3(\kappa)=\frac{-\sqrt{c_3^2+c_2c_4-c_1^2}\,[c_0\kappa+(c_0\kappa)^{-1}]+2c_3}{\sqrt{c_3^2+c_2c_4-c_1^2}\,[c_0\kappa-(c_0\kappa)^{-1}]+2c_1}, \tag{3.14c}$$

$$f_4(\kappa)=1-\frac{2c_4}{\sqrt{c_3^2+c_2c_4-c_1^2}\,[c_0\kappa-(c_0\kappa)^{-1}]+2c_1}, \tag{3.14d}$$

when

$$c_3^2+c_2c_4-c_1^2>0. \tag{3.15}$$

Similarly,

$$f_1(\kappa)=\frac{-\sqrt{c_1^2-c_3^2-c_2c_4}\,[c_0\kappa-(c_0\kappa)^{-1}]-2c_3}{\sqrt{c_1^2-c_3^2-c_2c_4}\,[c_0\kappa+(c_0\kappa)^{-1}]+2c_1}, \tag{3.16a}$$

$$f_2(\kappa)=1-\frac{2c_2}{\sqrt{c_1^2-c_3^2-c_2c_4}\,[c_0\kappa+(c_0\kappa)^{-1}]+2c_1}, \tag{3.16b}$$

$$f_3(\kappa)=\frac{-\sqrt{c_1^2-c_3^2-c_2c_4}\,[c_0\kappa-(c_0\kappa)^{-1}]+2c_3}{\sqrt{c_1^2-c_3^2-c_2c_4}\,[c_0\kappa+(c_0\kappa)^{-1}]+2c_1}, \tag{3.16c}$$

$$f_4(\kappa)=1-\frac{2c_4}{\sqrt{c_1^2-c_3^2-c_2c_4}\,[c_0\kappa+(c_0\kappa)^{-1}]+2c_1}, \tag{3.16d}$$

when

$$c_3^2+c_2c_4-c_1^2<0. \tag{3.17}$$

In Eqs. (3.14) and (3.16), $c_0>0$ and all square roots are also positive. Although there are five constants c_0, c_1, c_2, c_3 and c_4, effectively there are four because all the quantities do not change under

$$c_j\to\lambda c_j \tag{3.18}$$

for $j=1, 2, 3, 4$, and $\lambda>0$.

It remains to discuss briefly the case

$$c_3^2+c_2c_4-c_1^2=0. \tag{3.19}$$

This case, which was in fact the first case worked out and also the most important one as discussed in Sec. IV, can be recovered by taking the limit $c_3^2+c_2c_4-c_1^2\to 0$ together with either $c_0\to 0$ or $c_0\to\infty$. These two limiting cases are to be considered separately. For definiteness, they are applied to Eqs. (3.16).

(1) $c_3^2+c_2c_4-c_1^2\to 0$ and $c_0\to 0$, such that

$$\gamma=c_0^{-1}\sqrt{c_1^2-c_3^2-c_2c_4} \tag{3.20}$$

is fixed; $\gamma>0$. In this limit,

$$f_1(\kappa)=\frac{\gamma-2c_3\kappa}{\gamma+2c_1\kappa}, \tag{3.21a}$$

$$f_2(\kappa)=1-\frac{2c_2\kappa}{\gamma+2c_1\kappa}, \tag{3.21b}$$

$$f_3(\kappa)=\frac{\gamma+2c_3\kappa}{\gamma+2c_1\kappa}, \tag{3.21c}$$

$$f_4(\kappa)=1-\frac{2c_4\kappa}{\gamma+2c_1\kappa}. \tag{3.21d}$$

(2) $c_3^2+c_2c_4-c_1^2\to 0$ and $c_0\to\infty$, such that

$$\gamma=c_0\sqrt{c_1^2-c_3^2-c_2c_4} \tag{3.22}$$

is fixed; $\gamma>0$. In this limit,

$$f_1(\kappa)=\frac{-\gamma\kappa-2c_3}{\gamma\kappa+2c_1}, \tag{3.23a}$$

$$f_2(\kappa)=1-\frac{2c_2}{\gamma\kappa+2c_1}, \tag{3.23b}$$

$$f_3(\kappa)=\frac{-\gamma\kappa+2c_3}{\gamma\kappa+2c_1}, \tag{3.23c}$$

$$f_4(\kappa)=1-\frac{2c_4}{\gamma\kappa+2c_1}. \tag{3.23d}$$

Note that Eqs. (3.21) and (3.23) are related by the discrete symmetry (3.5) provided that the sign of c_3 is reversed. The same results also follow from Eqs. (3.14).

IV. INTERACTION POTENTIALS

Naively, one would expect it to be straightforward to determine the potential when the Green's function (resolvent) is known. It does not turn out to be so straightforward, and this section is devoted to solving this problem.

The substitution of Eqs. (2.1) and (2.5) into Eq. (2.6) gives

$$V(x)R_\kappa(x,x')=\delta(x-x')-\left(-\frac{d^2}{dx^2}+\kappa^2\right)R_\kappa(x,x'), \tag{4.1}$$

or

$$V(x)R_\kappa(x,x')=-\left(-\frac{d^2}{dx^2}+\kappa^2\right)[R_\kappa(x,x')-R_\kappa^{(0)}(x,x')], \tag{4.2}$$

with the last term defined by Eq. (2.3) or (2.4). This should determine $V(x)$; that this $V(x)$ does not depend on κ is a consequence of $R_\kappa(x,x')$ satisfying the resolvent equation.

More generally, the left-hand side of Eq. (4.2) may be an integral, and this equation takes the form

$$\int_{-\infty}^{\infty}dx''V(x,x'')R_\kappa(x'',x')=-\left(-\frac{d^2}{dx^2}+\kappa^2\right)[R_\kappa(x,x')-R_\kappa^{(0)}(x,x')]. \tag{4.3}$$

If $V(x)$ exists, then

$$V(x,x')=V(x)\,\delta(x-x'). \tag{4.4}$$

Since Eq. (4.2) is simpler than Eq. (4.3), it is useful to study Eq. (4.2) first even though it is less general. The substitution of Eq. (2.7) into Eq. (4.2) gives

$$V(x)R_\kappa(x,x')=\frac{1}{2\kappa}\left(-\frac{d^2}{dx^2}+\kappa^2\right)f(\kappa;\mathrm{sg}x,\mathrm{sg}x')e^{-\kappa(|x|+|x'|)}. \tag{4.5}$$

The difficulty is to give a proper interpretation to this equation. The right-hand side contains a term

$$f(\kappa;\mathrm{sg}x,\mathrm{sg}x')\,\delta(x)e^{-\kappa|x'|}, \tag{4.6}$$

obtained by applying the differential operator to the exponential. As seen from Eqs. (3.14) for example, this expression (4.6) is in general the product of $\delta(x)$ and a function discontinuous at $x=0$. The only reasonable interpretation of such a product is

$$\alpha(x)\,\delta(x)=\frac{1}{2}\left[\left(\lim_{x\to 0+}+\lim_{x\to 0-}\right)\alpha(x)\right]\delta(x). \tag{4.7}$$

As mentioned above, there are effectively four parameters in the solutions as given by either Eqs. (3.14) or Eqs. (3.16). Since the symmetry of the Green's function implies that $c_2=c_4$, the number of parameters is reduced by 1. Therefore, the potential $V(x,x')$ depends on *three* parameters. That there are three parameters instead of two is a major surprise, and this fact is to play a central role in part B of this article, where this interaction potential is applied to study certain aspects of quantum computing.

The three pieces of $V(x,x')$ are of different levels of complication. They are studied in the following three subsections.

A. $\delta(x)$ potential

The simplest piece is the well-known $\delta(x)$ potential, where

$$V_1(x)=g_1\,\delta(x), \tag{4.8}$$

and

$$V_1(x,x')=g_1\,\delta(x)\,\delta(x-x'), \tag{4.9}$$

or equivalently

$$V_1(x,x')=g_1\delta(x)\delta(x'). \tag{4.10}$$

For this potential, the differential equation (2.6) is well defined. Its solution is

$$R_\kappa(x,x')=\frac{1}{2\kappa}\left[e^{-\kappa|x-x'|}-\frac{g_1}{2\kappa+g_1}e^{-\kappa(|x|+|x'|)}\right]. \tag{4.11}$$

Comparison with Eq. (2.7) gives

$$f(\kappa;\mathrm{sg}x,\mathrm{sg}x')=\frac{g_1}{2\kappa+g_1}, \tag{4.12}$$

independent of the signs of x and x'. By Eq. (2.8), this is

$$f_1(\kappa)=f_2(\kappa)=f_3(\kappa)=f_4(\kappa)=\frac{g_1}{2\kappa+g_1}. \tag{4.13}$$

This is a special case of Eqs. (3.21) with

$$c_1=c_2=c_4=\frac{\gamma}{g_1} \quad \text{and} \quad c_3=0. \tag{4.14}$$

It is instructive to recover Eq. (4.8) from Eq. (4.12) by using Eq. (4.5). Since $f(\kappa;\mathrm{sg}x,\mathrm{sg}x')$ does not depend on the signs of x and x', Eq. (4.5) gives

$$V(x)=\left[\frac{g_1}{2\kappa+g_1}\delta(x)e^{-\kappa|x'|}\right]\Bigg/\left\{\frac{1}{2\kappa}\left[e^{-\kappa|x-x'|}-\frac{g_1}{2\kappa+g_1}e^{-\kappa(|x|+|x'|)}\right]\right\}=g_1\delta(x). \tag{4.15}$$

This $V(x)$ is even in x.

B. $\delta'(x)$ potential

As already discussed in Sec. I, the potential $\delta'(x)$ is not acceptable because, in the Schrödinger equation, there is a product of $\delta'(x)$ and a function discontinuous at $x=0$. While $\delta(x)$ is a potential, $\delta'(x)$ has to be understood as a Fermi pseudo-potential in much the same way as the expression (1.4) in three dimensions.

Since $\delta'(x)$ is odd in x, the resolvent must satisfy

$$f_1(\kappa)=-f_3(\kappa) \quad \text{and} \quad f_2(\kappa)=f_4(\kappa). \tag{4.16}$$

Next, consider the *formal* Eq. (2.6) with this $\delta'(x)$ potential

$$\left[-\frac{d^2}{dx^2}+g_2\delta'(x)+\kappa^2\right]R_\kappa(x,x')=\delta(x-x'). \tag{4.17}$$

Since every term on the left-hand side is of dimension x^{-2} times that of $R_\kappa(x,x')$, the resolvent $R_\kappa(x,x')$ must be of the form

$$\kappa^{-1} \text{ function of } \kappa x \text{ and } \kappa x'.$$

A comparison with Eq. (2.7) then shows that $f(\kappa;\mathrm{sg}x,\mathrm{sg}x')$ is independent of κ. This is satisfied with

$$f_1(\kappa)=\alpha, \quad f_3(\kappa)=-\alpha, \quad \text{and} \quad f_2(\kappa)=f_4(\kappa)=-\beta, \tag{4.18}$$

with

$$2\beta+\alpha^2+\beta^2=0. \tag{4.19}$$

With the resolvent known, it is now possible to define the Fermi pseudo-potential

$$V_2(x)=g_2\delta_p'(x). \tag{4.20}$$

Omitting the argument κ in f, Eq. (4.5) takes the form

$$g_2\delta_p'(x)R_\kappa(x,x')=\frac{1}{2\kappa}\left(-\frac{d^2}{dx^2}+\kappa^2\right)f(\mathrm{sg}x,\mathrm{sg}x')e^{-\kappa(|x|+|x'|)}. \tag{4.21}$$

Let x' be positive. Then

$$\left(-\frac{d^2}{dx^2}+\kappa^2\right)f(\mathrm{sg}x,\mathrm{sg}x')e^{-\kappa|x|}=-(f_1-f_2)\delta'(x)+\kappa(f_1+f_2)\delta(x). \tag{4.22}$$

This expression has not only a $\delta'(x)$ term, but also a $\delta(x)$ term. For the left-hand side of Eq. (4.21), it is necessary to evaluate, using Eq. (4.7),

$$\begin{aligned}R_\kappa(x,x')|_{x=0}&=[e^{-\kappa(x'-x)}-f(\mathrm{sg}x,+)e^{-\kappa(|x|+x')}]_{x=0}\\&=e^{-\kappa x'}[1-\tfrac{1}{2}(\lim_{x\to 0+}+\lim_{x\to 0-})f(\mathrm{sg}x,+)e^{-\kappa|x|}]=e^{-\kappa x'}[1-\tfrac{1}{2}(f_1+f_2)]\end{aligned} \tag{4.23}$$

and

$$\begin{aligned}\frac{d}{dx}[e^{-\kappa(x'-x)}-f(\mathrm{sg}x,+)e^{-\kappa(|x|+x')}]_{x=0}&=\kappa[e^{-\kappa(x'-x)}+(\mathrm{sg}x)f(\mathrm{sg}x,+)e^{-\kappa(|x|+x')}]_{x=0}\\&=\kappa e^{-\kappa x'}[1+\tfrac{1}{2}(\lim_{x\to 0+}+\lim_{x\to 0-})(\mathrm{sg}x)f(\mathrm{sg}x,+)e^{-\kappa|x|}]\\&=\kappa e^{-\kappa x'}[1+\tfrac{1}{2}(f_1-f_2)].\end{aligned} \tag{4.24}$$

Suppose the $\delta_p'(x)$ on the left-hand side of Eq. (4.21) is replaced by $\delta'(x)$. Then a comparison of Eq. (4.22) with Eqs. (4.23) and (4.24) gives

$$g_2[1-\tfrac{1}{2}(f_1+f_2)]=f_1-f_2; \quad g_2[1+\tfrac{1}{2}(f_1-f_2)]=f_1+f_2, \tag{4.25}$$

where the identity $x\delta'(x)=-\delta(x)$ has been used. These are the conditions for $x'>0$; similar conditions for $x'<0$ are

$$g_2[1-\tfrac{1}{2}(f_4+f_3)]=f_4-f_3; \quad g_2[-1+\tfrac{1}{2}(f_4-f_3)]=f_4+f_3. \tag{4.26}$$

Solving Eqs. (4.25) and (4.26) gives

$$f_1=\frac{g_2}{1+g_2^2/4}; \quad f_3=\frac{-g_2}{1+g_2^2/4}; \quad f_2=f_4=\frac{g_2^2/2}{1+g_2^2/4}. \tag{4.27}$$

This is consistent with the previous Eqs. (4.18) and (4.19).

Where is the difficulty explained in Sec. I? Another way of asking the same question is: How does $\delta_p'(x)$ differ from $\delta'(x)$?

The answer is to be found in the first step of Eq. (4.24). In differentiating the quantity on the left-hand side of Eq. (4.24), the factor $f(\mathrm{sg}x,+)$ is not differentiated. In other words, the term with $(d/dx)f(\mathrm{sg}x,+)$ has been omitted; if this term were not omitted, there would be a $\delta(x)$, precisely the difficulty explained in Sec. I.

The situation is therefore entirely similar to the Fermi pseudo-potential in three dimensions, where the operator (1.4) performs the function of removing a term proportional to $1/r$. Here, what $\delta_p'(x)$ does is

$$\delta_p'(x)g(x)=\delta'(x)\tilde{g}(x), \tag{4.28}$$

where

$$\tilde{g}(x)=\begin{cases} g(x)-\lim\limits_{x\to 0+} g(x), & \text{for } x>0, \\ g(x)-\lim\limits_{x\to 0-} g(x), & \text{for } x<0. \end{cases} \tag{4.29}$$

This removes the discontinuity of $g(x)$ at $x=0$, which is precisely what is needed.

C. Third potential

At the beginning of this investigation it was thought that, in one dimension, there was one potential (Sec. IV A) and one pseudo-potential (Sec. IV B). But the detailed analysis of the resolvent equation in Sec. III shows that there are three independent parameters in the resolvent, and hence there is an independent third potential, or a second pseudo-potential in one dimension.

This third potential is most easily understood through the discrete symmetry (3.4). Let $c=2/g_1$. Then, from Eq. (4.13), the resolvent for the $\delta(x)$ potential is given by

$$f_1(\kappa)=f_2(\kappa)=f_3(\kappa)=f_4(\kappa)=\frac{1}{1+c\kappa}. \tag{4.30}$$

Application of the discrete symmetry (3.4) to Eq. (4.30) gives the result that the resolvent for the third potential is expressed by

$$f_1(\kappa)=f_3(\kappa)=\frac{-\kappa}{\kappa+c}; \quad f_2(\kappa)=f_4(\kappa)=\frac{\kappa}{\kappa+c}. \tag{4.31}$$

In particular, similar to the resolvent of the first pseudo-potential as given by Eq. (4.27), this resolvent is also not continuous. The relation between the resolvents as expressed by Eqs. (4.30) and (4.31) is a special case of that between Eqs. (3.21) and (3.23).

It remains to determine the potential, or more precisely the pseudo-potential, from Eq. (4.31), which can be written more succinctly as

$$f(\kappa;\mathrm{sg}x,\mathrm{sg}x')=-\frac{\kappa}{\kappa+c}\mathrm{sg}x\,\mathrm{sg}x'. \tag{4.32}$$

Therefore, for the present case of the third potential $V_3(x,x')$, Eq. (4.3) takes the form

$$\int_{-\infty}^{\infty} dx'' V_3(x,x'')\left[e^{-\kappa|x''-x'|}+\frac{\kappa}{\kappa+c}\,\mathrm{sg}x''\mathrm{sg}x' e^{-\kappa(|x''|+|x'|)}\right]$$
$$=\frac{\kappa}{\kappa+c}\left(-\frac{d^2}{dx^2}+\kappa^2\right)[\mathrm{sg}x\mathrm{sg}x' e^{-\kappa(|x|+|x'|)}]. \tag{4.33}$$

Differentiation of the right-hand side gives

$$\frac{d}{dx}[\mathrm{sg}x e^{-\kappa|x|}]=2\delta(x)-\kappa e^{-\kappa|x|},$$

and hence

$$\left(-\frac{d^2}{dx^2}+\kappa^2\right)[\mathrm{sg}x e^{-\kappa|x|}]=-2\delta'(x). \tag{4.34}$$

Thus Eq. (4.33) for $V_3(x,x')$ is explicitly

$$\int_{-\infty}^{\infty} dx'' V_3(x,x'')\left[e^{-\kappa|x''-x'|}+\frac{\kappa}{\kappa+c}\,\mathrm{sg}x''\mathrm{sg}x' e^{-\kappa(|x''|+|x'|)}\right]=-\frac{2\kappa}{\kappa+c}\,\delta'(x)\mathrm{sg}x' e^{-\kappa|x'|}. \tag{4.35}$$

The task is to make sense of this equation and to determine $V_3(x,x')$.

That the resolvent equation is satisfied means that Eq. (4.35), properly understood, does lead to a $V_3(x,x')$. By Eqs. (4.28) and (4.29), the $\delta'(x)$ on the right-hand side of Eq. (4.35) can be replaced by $\delta_p'(x)$, because it is not multiplied by a discontinuous function of x. Therefore, $V_3(x,x')$ is expected to be proportional to $\delta_p'(x)$; that $\delta_p'(x)$ is used instead of $\delta'(x)$ is due to the development in Sec. IV B. With these considerations, an examination of Eq. (4.35) indicates that

$$V_3(x,x')=g_3\delta_p'(x)\delta_p'(x'). \tag{4.36}$$

See also Eq. (4.20).

It remains to substitute Eq. (4.36) into Eq. (4.35) to find the relation between the two constants g_3 and c:

$$g_3\int_{-\infty}^{\infty} dx''\delta_p'(x'')\left[e^{-\kappa|x''-x'|}+\frac{\kappa}{\kappa+c}\,\mathrm{sg}x''\mathrm{sg}x' e^{-\kappa(|x''|+|x'|)}\right]=-\frac{2\kappa}{\kappa+c}\,\mathrm{sg}x' e^{-\kappa|x'|}. \tag{4.37}$$

The evaluation of the first integral is straightforward because $e^{-\kappa|x''-x'|}$ is continuous:

$$\int_{-\infty}^{\infty} dx''\delta_p'(x'')e^{-\kappa|x''-x'|}=\int_{-\infty}^{\infty} dx''\delta'(x'')e^{-\kappa|x''-x'|}=-\kappa\mathrm{sg}x' e^{-\kappa|x'|}. \tag{4.38}$$

After the removal of the common factor

$$\kappa\mathrm{sg}x' e^{-\kappa|x'|},$$

Eq. (4.37) reduces to

$$g_3\left[-1+\frac{1}{\kappa+c}\int_{-\infty}^{\infty} dx''\delta_p'(x'')\mathrm{sg}x'' e^{-\kappa|x''|}\right]=-\frac{2}{\kappa+c}. \tag{4.39}$$

This integral can be evaluated using Eqs. (4.28) and (4.29):

$$\int_{-\infty}^{\infty} dx'' \delta_p'(x'') \mathrm{sg}x'' e^{-\kappa|x''|} = -\int_{-\infty}^{\infty} dx'' \delta(x'') \mathrm{sg}x'' \frac{d}{dx''} e^{-\kappa|x''|} = \kappa. \tag{4.40}$$

Therefore, Eq. (4.39) is simply

$$g_3\left[-1+\frac{\kappa}{\kappa+c}\right] = -\frac{2}{\kappa+c} \quad \text{or} \quad g_3 = \frac{2}{c}. \tag{4.41}$$

This is the desired relation.

It is merely a matter of terminology whether this pseudo-potential $V_3(x,x')$ as given by Eq. (4.36) is called a local potential or not. It is a local potential if the definition is used that the support is the same before and after operating with $V_3(x,x')$.

In summary, the three potentials V_1, V_2, and V_3 are given by Eqs. (4.8), (4.20), and (4.36). Thus the most general Fermi pseudo-potential for the interaction at one point in one dimension is

$$\begin{aligned} V(x,x') &= V_1(x,x') + V_2(x,x') + V_3(x,x') \\ &= g_1 \delta(x)\delta(x-x') + g_2 \delta_p'(x)\delta(x-x') + g_3 \delta_p'(x)\delta_p'(x'). \end{aligned} \tag{4.42}$$

From the above experience of working with $\delta_p'(x)$ and the fact that the product of $\delta'(x)$ and a function discontinuous at $x=0$ is not meaningful, from here on the convention will be adopted that $\delta'(x)$ always means $\delta_p'(x)$. With this convention, Eq. (4.42) is written as

$$V(x,x') = g_1 \delta(x)\delta(x-x') + g_2 \delta'(x)\delta(x-x') + g_3 \delta'(x)\delta'(x'). \tag{4.43}$$

Equation (4.43) can be rewritten in a prettier form as follows. Since

$$\delta(x)\delta(x-x') = \delta(x)\delta(x')$$

and

$$\delta'(x)\delta(x-x') = \delta'(x)\delta(x'-x) = \delta'(x)[\delta(x') - x\delta'(x')] = \delta'(x)\delta(x') + \delta(x)\delta'(x'), \tag{4.44}$$

where use has been made of the identity $\delta'(x)x = -\delta(x)$, a general Fermi pseudo-potential (4.43) can be written as

$$V(x,x') = g_1 \delta(x)\delta(x') + g_2[\delta'(x)\delta(x') + \delta(x)\delta'(x')] + g_3 \delta'(x)\delta'(x'). \tag{4.45}$$

As already mentioned, the first and last terms are even while the middle term is odd. That is, under space inversion

$$x \to -x \quad \text{and} \quad x' \to -x', \tag{4.46}$$

the coupling constants transform as

$$g_1 \to g_1; \quad g_2 \to -g_2; \quad g_3 \to g_3. \tag{4.47}$$

V. SOLVING THE SCHRÖDINGER EQUATION

In applying the Fermi pseudo-potential to various problems, such as the one to be treated in part B of this article, the resolvent equation is difficult to use and it is much more convenient to employ the prescription of Sec. IV to the Schrödinger equation.

This section is devoted to studying the equation

$$\left(-\frac{d^2}{dx^2}+\kappa^2\right)R_\kappa(x,x')+\int_{-\infty}^{\infty}dx''V(x',x'')R_\kappa(x'',x')=\delta(x-x'), \tag{5.1}$$

where $V(x,x')$ is the Fermi pseudo-potential as given by Eq. (4.42). On the one hand, this is an equation for this $V(x,x')$. On the other hand, the procedure of this section is directly applicable to the Schrödinger equation, which differs from Eq. (5.1) only in the absence of the $\delta(x-x')$ term on the right-hand side.

This section serves two distinct purposes. First, the parameters in the known resolvent of Sec. III, especially Eqs. (3.14) and (3.16), are to be related to the coupling constants g_1, g_2, and g_3 in Eq. (4.42). This will give an explicit verification of consistency of the prescriptions given in Sec. IV. Second, the procedure to be followed here serves as a useful introduction to the slightly more complicated problem of the next section, where a two-channel scattering by a Fermi pseudo-potential is taken to be a model for a quantum memory.

The solution $R_\kappa(x,x')$ is given, as in the general case, by Eq. (2.7). The substitution of Eq. (2.7) into Eq. (5.1) gives

$$\left(-\frac{d^2}{dx^2}+\kappa^2\right)\left[-\frac{1}{2\kappa}f(\kappa;\mathrm{sg}x,\mathrm{sg}x')e^{-\kappa(|x|+|x'|)}\right]+\int_{-\infty}^{\infty}dx''V(x,x'')R_\kappa(x'',x')=0. \tag{5.2}$$

Since the first term has been evaluated by Eq. (4.22), Eq. (5.2) can be written alternatively as

$$2\kappa\int_{-\infty}^{\infty}dx''V(x,x'')R_\kappa(x'',x')$$

$$=e^{-\kappa|x'|}\begin{cases}\{-[f_1(\kappa)-f_2(\kappa)]\delta'(x)+\kappa[f_1(\kappa)+f_2(\kappa)]\delta(x)\}, & \text{for } x'>0\\ \{-[f_4(\kappa)-f_3(\kappa)]\delta'(x)+\kappa[f_4(\kappa)+f_3(\kappa)]\delta(x)\}, & \text{for } x'<0.\end{cases} \tag{5.3}$$

Using the knowledge gained from Sec. IV, a fairly lengthy calculation gives more explicitly

$$\begin{aligned}&[g_1\delta(x)+g_2\delta'(x)]e^{-\kappa|x'|}\begin{cases}\{1-\frac{1}{2}[f_1(\kappa)+f_2(\kappa)]\}, & \text{for } x'>0\\ \{1-\frac{1}{2}[f_4(\kappa)+f_3(\kappa)]\}, & \text{for } x'<0\end{cases}\\ &+[g_2\delta(x)+g_3\delta'(x)]\kappa e^{-\kappa|x'|}\begin{cases}\{-1+\frac{1}{2}[-f_1(\kappa)+f_2(\kappa)]\}, & \text{for } x'>0\\ \{1+\frac{1}{2}[-f_4(\kappa)+f_3(\kappa)]\}, & \text{for } x'<0\end{cases}\\ &=e^{-\kappa|x'|}\begin{cases}\{-[f_1(\kappa)-f_2(\kappa)]\delta'(x)+\kappa[f_1(\kappa)+f_2(\kappa)]\delta(x)\}, & \text{for } x'>0\\ \{-[f_4(\kappa)-f_3(\kappa)]\delta'(x)+\kappa[f_4(\kappa)+f_3(\kappa)]\delta(x)\}, & \text{for } x'<0,\end{cases}\end{aligned} \tag{5.4}$$

where Eq. (4.45) has been used. In Eq. (5.4), all dependences on x' cancel out. It therefore only remains to identify the coefficients of $\delta(x)$ and $\delta'(x)$. The results are

$$g_1\{1-\tfrac{1}{2}[f_1(\kappa)+f_2(\kappa)]\}+\kappa g_2\{-1+\tfrac{1}{2}[-f_1(\kappa)+f_2(\kappa)]\}=\kappa[f_1(\kappa)+f_2(\kappa)], \tag{5.5a}$$

$$g_2\{1-\tfrac{1}{2}[f_1(\kappa)+f_2(\kappa)]\}+\kappa g_3\{-1+\tfrac{1}{2}[-f_1(\kappa)+f_2(\kappa)]\}=-[f_1(\kappa)-f_2(\kappa)], \tag{5.5b}$$

$$g_1\{1-\tfrac{1}{2}[f_4(\kappa)+f_3(\kappa)]\}+\kappa g_2\{1+\tfrac{1}{2}[-f_4(\kappa)+f_3(\kappa)]\}=\kappa[f_4(\kappa)+f_3(\kappa)], \tag{5.5c}$$

$$g_2\{1-\tfrac{1}{2}[f_4(\kappa)+f_3(\kappa)]\}+\kappa g_3\{1+\tfrac{1}{2}[-f_4(\kappa)+f_3(\kappa)]\}=-[f_4(\kappa)-f_3(\kappa)]. \tag{5.5d}$$

Solving Eqs. (5.5) gives

$$f_1(\kappa)=D^{-1}[-g_3\kappa+2g_2-g_1\kappa^{-1}], \tag{5.6a}$$

$$f_3(\kappa)=D^{-1}[-g_3\kappa-2g_2-g_1\kappa^{-1}], \tag{5.6b}$$

$$f_2(\kappa)=f_4(\kappa)=1+D^{-1}\tfrac{1}{2}(4+g_1g_3-g_2^2), \tag{5.6c}$$

where

$$D=g_3\kappa-\tfrac{1}{2}(4-g_1g_3+g_2^2)-g_1\kappa^{-1}. \tag{5.7}$$

Equations (5.6) are to be compared with Eqs. (3.14) and (3.16). First, this gives a deeper understanding why there are the two distinct cases (3.14) and (3.16). Equations (3.14) correspond to the situation where g_1 and g_3 have the same sign, while Eqs. (3.16) correspond to g_1 and g_3 having opposite signs. Second, in both cases, it is seen immediately from Eqs. (5.6) that $c_2=c_4$, a fact that has been used before. The results of expressing the five c's in terms of the three g's are the following:

$$c_0=\sqrt{|g_3/g_1|}, \tag{5.8}$$

$$c_1=\tfrac{1}{4}(4-g_1g_3+g_2^2), \tag{5.9a}$$

$$c_2=c_4=\tfrac{1}{4}(4+g_1g_3-g_2^2), \tag{5.9b}$$

$$c_3=g_2. \tag{5.9c}$$

Here use has been made of the scale invariance (3.18). [Strictly speaking, the right-hand sides of the three Eqs. (5.9a)–(5.9c) should all be multiplied by the factor $\mathrm{sg}g_3$. This factor has been omitted because it has no consequences.]

For completeness and also for later use, let the scattering matrix be written down. This involves returning to the more familiar variable k through Eq. (2.2) and then letting $x'\to\pm\infty$. After analytic continuation to positive values of k, the S-matrix is a 2×2 matrix,

$$S=\begin{bmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{bmatrix}, \tag{5.10}$$

where $+$ denotes propagation in the $+x$ direction, and $-$ in the $-x$ direction. For any interaction at the point $x=0$, it follows from Eqs. (2.7) and (2.8) that

$$S=\begin{bmatrix} 1-f(-ik;+,-) & -f(-ik;-,-) \\ -f(-ik;+,+) & 1-f(-ik;-,+) \end{bmatrix}=\begin{bmatrix} 1-f_4(-ik) & -f_3(-ik) \\ -f_1(-ik) & 1-f_2(-ik) \end{bmatrix}. \tag{5.11}$$

Equations (5.6) and (5.7) then give explicitly

$$S=[ig_3k+\tfrac{1}{2}(4-g_1g_3+g_2^2)+ig_1k^{-1}]^{-1}\begin{bmatrix} \tfrac{1}{2}(4+g_1g_3-g_2^2) & ig_3k-2g_2-ig_1k^{-1} \\ ig_3k+2g_2-ig_1k^{-1} & \tfrac{1}{2}(4+g_1g_3-g_2^2) \end{bmatrix}, \tag{5.12}$$

which is unitary.

An interesting special case is that with $g_2=0$; in this case, the pseudo-potential is even and there is left–right symmetry. Explicitly, in this case $g_2=0$, the S-matrix is

$$S=[ig_3k+\tfrac{1}{2}(4-g_1g_3)+ig_1k^{-1}]^{-1}\begin{bmatrix} \tfrac{1}{2}(4+g_1g_3) & ig_3k-ig_1k^{-1} \\ ig_3k-ig_1k^{-1} & \tfrac{1}{2}(4+g_1g_3) \end{bmatrix}. \tag{5.13}$$

This special case $g_2=0$, generalized to the case of coupled channels, is going to play a central role in part B of this article.

This completes the present discussion of the theory of Fermi pseudo-potential in one dimension. Attention is now turned to the first application of this theory.

PART B: APPLICATION OF ONE-DIMENSIONAL FERMI PSEUDO-POTENTIAL

VI. MODEL FOR QUANTUM MEMORY

There are many possible applications of the Fermi pseudo-potential in one dimension. As an example, it is intriguing to ask under what conditions Bethe's hypothesis[8,9] still holds when the delta-function potential is replaced by the $V(x,x')$ of Eq. (4.42). As a first application, however, it is more desirable to begin with a case where the Fermi pseudo-potential is used in a relatively simple situation of current interest.

For decades, computer components have become smaller and smaller, and this trend is expected to continue.[10] When some of the components become sufficiently small, as to be expected in the not-too-distant future, they need to be described in general by quantum mechanics. No matter how quantum computing is to develop in the future, one important component is necessarily the quantum memory, sometimes called the quantum register. The main function of any quantum memory is to store a quantum state.

In order for a quantum memory to be useful, it must be possible to alter the quantum state in the memory in a controlled way. This can only be accomplished by sending a signal from outside of the memory. In other words, the quantum state in the memory is to be controlled by a scattering process.[11]

It is the purpose of Sec. VI to propose a simple model for quantum memory. First, in order to have scattering processes, at least one space dimension is necessary. Otherwise there is no possibility of interference between the incident wave and the scattered wave. As perhaps to be expected, this interference is of central importance. Since the state in the memory must include at least two independent quantum states, it is simplest to describe the quantum memory using the coupled Schrödinger equations for two channels. This is essentially Eq. (1.1) in the Introduction.

It remains to make the simplest choice for the 2×2 matrix potential $V(x)$ of Eq. (1.2). This simplest choice, the Fermi pseudo-potential in one dimension, has been investigated systematically in part A of this article, the general result being given by Eq. (4.42).

The symmetry properties of this $V(x,x')$ under space inversion have been discussed at the end of Sec. IV. In particular, it is symmetrical if $g_2=0$. In order for the model to be suitable for quantum memory, it is essential to concentrate on this special case. The reason is that, only in this case, do the even wave $\cos kx$ and the odd wave $\sin kx$ not mix. This is also the basis for the comment in the Introduction, after Eq. (1.3), why the $\delta'(x)$ potential is not suitable for quantum memory. That this absence of mixing is important is discussed further in Sec. VII for a more general setting.

With this understanding and choice, the present model for the quantum memory is described by the one-dimensional coupled Schrödinger equations

$$\begin{aligned} -\frac{d^2\psi_1(x)}{dx^2}+\int_{-\infty}^{\infty}dx'[V_{11}(x,x')\psi_1(x')+V_{12}(x,x')\psi_2(x')]=k^2\psi_1(x),\\ -\frac{d^2\psi_2(x)}{dx^2}+\int_{-\infty}^{\infty}dx'[V_{21}(x,x')\psi_1(x')+V_{22}(x,x')\psi_2(x')]=k^2\psi_2(x), \end{aligned} \tag{6.1}$$

with the 2×2 matrix potential

$$V(x,x')=\begin{bmatrix} V_{11}(x,x') & V_{12}(x,x') \\ V_{21}(x,x') & V_{22}(x,x') \end{bmatrix}=\begin{bmatrix} g_3\delta'(x)\delta'(x') & g_1\delta(x)\delta(x') \\ g_1\delta(x)\delta(x') & -g_3\delta'(x)\delta'(x') \end{bmatrix}. \tag{6.2}$$

A more elegant way to write this potential is

$$V(x,x')=g_1\delta(x)\delta(x')\sigma_1+g_3\delta'(x)\delta'(x')\sigma_3, \tag{6.3}$$

where the σ's are the Pauli matrices.

When $g_2=0$, the potential $g_1\delta(x)\delta(x')$ does not act on the odd wave, and similarly the potential $g_3\delta'(x)\delta'(x')$ does not act on the even wave. The first part of this claim is easy to obtain, and the second part follows from the definition (4.28) of $\delta'_p(x)$. Alternatively, they can be seen from Eq. (5.13), where $S_{++}=S_{--}$ and $S_{+-}=S_{-+}$. For the even wave, the scattering phase shift is given by

$$S_{++}+S_{+-}=\frac{2k-ig_1}{2k+ig_1} \tag{6.4}$$

independent of g_3, while, for the odd wave, it is

$$S_{++}-S_{+-}=\frac{2-ig_3k}{2+ig_3k} \tag{6.5}$$

independent of g_1. Therefore, for the present case of two coupled channels as described by Eqs. (6.1) and (6.2), the S-matrix for the even and odd cases can be expressed in terms of these quantities as follows. Consider first the case for the odd wave; since the g_1 term does not contribute and can be neglected, the $V(x,x')$ of Eq. (6.2) effectively reduces to

$$V(x,x')=\begin{bmatrix} g_3\delta'(x)\delta'(x') & 0 \\ 0 & -g_3\delta'(x)\delta'(x') \end{bmatrix}, \tag{6.6}$$

which is diagonal, meaning that $\psi_1(x)$ and $\psi_2(x)$ do not couple. Since the behaviors of the two channels differ only in the sign of g_3, the S-matrix for this odd case is given by Eq. (6.5), or more explicitly

$$S_-(k)=\begin{bmatrix} \dfrac{2-ig_3k}{2+ig_3k} & 0 \\ 0 & \dfrac{2+ig_3k}{2-ig_3k} \end{bmatrix}. \tag{6.7}$$

It is instructive to rewrite this expression in terms of σ_3:

$$S_-(k)=\frac{(4-g_3^2k^2)-4ig_3k\sigma_3}{4+g_3^2k^2}=\exp\left[-i\sigma_3\left(2\tan^{-1}\frac{g_3k}{2}\right)\right]. \tag{6.8}$$

For the even wave, it is merely necessary to replace the right-hand side of Eq. (6.5) by that of Eq. (6.4), and also σ_3 by σ_1. Therefore Eq. (6.8) leads to

$$S_+(k)=\frac{(4k^2-g_1^2)-4ig_1k\sigma_1}{4k^2+g_1^2}=\exp\left[-i\sigma_1\left(2\tan^{-1}\frac{g_1}{2k}\right)\right] \tag{6.9}$$

or

$$S_+(k)=\begin{bmatrix} \dfrac{4k^2-g_1^2}{4k^2+g_1^2} & \dfrac{-4ig_1k}{4k^2+g_1^2} \\ \dfrac{-4ig_1k}{4k^2+g_1^2} & \dfrac{4k^2-g_1^2}{4k^2+g_1^2} \end{bmatrix}. \tag{6.10}$$

When neither g_1 nor g_3 is zero, any given element S of SU(2) can be expressed as a finite product of $S_+(k)$ and $S_-(k)$, i.e.,

$$S=S(k_1)S(k_2)\cdots S(k_m), \tag{6.11}$$

where each $S(k_i)$ is suitably chosen as $S_+(k_i)$ or $S_-(k_i)$.

In the language of scattering theory, the meaning of $S_+(k)$ is as follows. [The meaning of $S_-(k)$ is similar.] The in field is

$$\Psi^{\text{in}}=\begin{bmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{bmatrix} e^{-ik|x|}, \tag{6.12}$$

while the out field is

$$\Psi^{\text{out}}=\begin{bmatrix} a_1^{\text{out}} \\ a_2^{\text{out}} \end{bmatrix} e^{ik|x|}. \tag{6.13}$$

Then

$$\begin{bmatrix} a_1^{\text{out}} \\ a_2^{\text{out}} \end{bmatrix} = S_+(k) \begin{bmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{bmatrix}. \tag{6.14}$$

In other words, the quantum state in the memory is $\left[\begin{smallmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{smallmatrix}\right]$ before scattering, and $\left[\begin{smallmatrix} a_1^{\text{out}} \\ a_2^{\text{out}} \end{smallmatrix}\right]$ after scattering. These states before and after scattering are related by Eq. (6.14).

For any memory, classical or quantum, the basic operations are *write*, *read*, and *reset*. Of these three operations, writing is the simplest: Given the initial state $\left[\begin{smallmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{smallmatrix}\right]$ and the desired final state $\left[\begin{smallmatrix} a_1^{\text{out}} \\ a_2^{\text{out}} \end{smallmatrix}\right]$, there is a desired S-matrix S. Express this particular S by Eq. (6.11) as a finite product; then the writing is accomplished by a sequence of these m scatterings.

The question may be asked: While the final state $\left[\begin{smallmatrix} a_1^{\text{out}} \\ a_2^{\text{out}} \end{smallmatrix}\right]$ is the desired state to be stored in the quantum memory, how can one know what the initial state $\left[\begin{smallmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{smallmatrix}\right]$ is? This is where the idea of a standard state s is needed. ''Resetting'' means changing the content of the quantum memory, whatever it is, to the standard state s. For writing, the initial state is the standard state, i.e.,

$$\begin{bmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{bmatrix} = s. \tag{6.15}$$

In other words, before writing on a quantum memory, it is first reset so that Eq. (6.15) is satisfied. The standard state can be chosen to be any quantum state; however, once chosen, the choice is rarely altered.

Since scattering from a quantum memory leads to a unitary transformation of the quantum state in the memory, resetting cannot be accomplished without first finding out the content of the quantum memory. In other words, the first step of ''resetting'' is ''reading.'' After the content of

the quantum memory is known, say $\left[\begin{smallmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{smallmatrix}\right]$, "resetting" involves finding a sequence of scattering $S(k_j)$, $j=1,2,\ldots,m$, via Eq. (6.11) such that the resulting S has the property

$$S\begin{bmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{bmatrix} = s. \tag{6.16}$$

In summary, if "reading" can be accomplished, then so can "resetting;" if "resetting" can be accomplished, so can "writing."

The main task here is therefore to discuss, within the present model, the operation of reading a quantum memory. More precisely, what is involved is the following. When the quantum state in a memory, $\left[\begin{smallmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{smallmatrix}\right]$, is not known, find a suitably chosen sequence of incident waves $\cos k_i x$ or $\sin k_i x$ such that the knowledge about the field can be used to determine the values of a_1^{in} and a_2^{in}. After this determination, the quantum memory is returned to the initial state $\left[\begin{smallmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{smallmatrix}\right]$. (The last step is similar to the classical case in which a core memory is read from an initial state and then returned to it.)

Let the quantum state in the memory be $\left[\begin{smallmatrix} a_1 \\ a_2 \end{smallmatrix}\right]$; the problem is to determine the values of a_1 and a_2 by scattering from this state. Suppose an odd wave is used for the first scattering; then the two-component wave function for $x>0$ is given explicitly by

$$\psi(x) = \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} e^{-ikx} + \begin{bmatrix} a_1 e^{i\phi_-} \\ a_2 e^{-i\phi_-} \end{bmatrix} e^{ikx}, \tag{6.17}$$

where, by Eq. (6.8),

$$\phi_- = -2\tan^{-1}\tfrac{1}{2}g_3 k. \tag{6.18}$$

In particular,

$$\psi(x)^\dagger \psi(x) = 2[1+\cos 2kx\cos\phi_- - (|a_1|^2-|a_2|^2)\sin 2kx\sin\phi_-], \tag{6.19}$$

because $|a_1|^2+|a_2|^2=1$. Therefore, this scattering process gives, through the interference term, the quantity

$$A_1 = |a_1|^2 - |a_2|^2. \tag{6.20}$$

Similarly, if the quantum state in the memory is first returned to the original state by a suitable scattering, then a second scattering with an even wave gives, again through the interference term, the second quantity

$$A_2 = \tfrac{1}{2}[|a_1+a_2|^2+|a_1-a_2|^2] = 2\,\text{Re}\,a_1^* a_2. \tag{6.21}$$

These two quantities, A_1 and A_2, are sufficient to determine the values of the complex numbers a_1 and a_2, except for a common phase. In order to determine this common phase, it is simplest to use the known standard state s. For example, a further interference with this standard state using, say, the odd wave gives a third quantity

$$A_3 = |a_1+s_1|^2 - |a_2+s_2|^2. \tag{6.22}$$

Since s_1 and s_2 are known, these three quantities A_1, A_2 and A_3 determine a_1 and a_2. Returning once more to the original quantum state presents no problem.

This completes the description of the present model of the quantum memory, including the operations of writing, reading, and resetting.

The advantages of this model, based on the Fermi pseudo-potential in one dimension, are its simplicity and its being completely explicit. On the one hand, such an explicit model plays an essential role in the initial understanding of some aspects of a new problem. On the other hand, the usefulness of such a model really lies in the possibility of opening a line of inquiry into these aspects. This is to be discussed in some detail in the next section. That is, in Sec. VII an attempt is to be made to present a general picture concerning the quantum memory, emphasizing the operations of writing, reading, and resetting, all accomplished by repeated scattering.

Some simplifying assumptions introduced in the model of this section are clearly not needed in the general setting of the next section. An example is the choice of using the Fermi pseudo-potential $V(x,x')$ of Eq. (6.2); another one is the use of the Schrödinger equation (6.1) in one dimension. Thus the generalization to the Schrödinger equation in three dimensions with a more general potential is immediate but the results are less explicit. The further generalization to renormalized quantum field theory also does not present any obstacle.

What is less clear, and most important, is the role played by the condition $g_2=0$, used throughout this section. This condition is closely related to, and makes it possible to use, the even waves and the odd waves. In order to appreciate this point, take instead the incoming wave as, say, from the direction of the $-x$ axis, i.e.,

$$\Psi^{\text{in}}=\begin{bmatrix} a_1^{\text{in}} \\ a_2^{\text{in}} \end{bmatrix} e^{-ikx}. \tag{6.23}$$

This is a superposition of an even wave and an odd wave. Since the Schrödinger equation is linear, the even part is operated on by the $S_+(k)$ of Eq. (6.10), and the odd part by the $S_-(k)$ of Eq. (6.7). Since g_1 and g_3 are not zero and thus these $S_+(k)$ and $S_-(k)$ are not equal, the quantum state in the memory for an outgoing wave in the $+x$ direction is different from that for an outgoing wave in the $-x$ direction. In other words, in order to determine the quantum state in the memory after scattering with the Ψ^{in} of Eq. (6.23), it is necessary to detect the direction of the outgoing wave.

In order for a quantum memory to behave as a memory, i.e., as the storage for a quantum state, it is essential that what is in the memory does not depend on the behavior of the scattered wave. Indeed, from the point of view of scattering theory, this characterizes quantum memories. Therefore, for the present model with the Fermi pseudo-potential, some incident waves, such as the even wave and the odd wave, are acceptable or ''admissible,'' while many others, such as e^{-ikx} of Eq. (6.23), are not ''admissible.''

This concept of admissible incident waves is central, not only for the present model but also in general. This is the first topic to be discussed in the next section.

VII. GENERALIZATION

It is the purpose of this section to give a general description of quantum memories. This is to be accomplished by extracting the dominant features from the model of Sec. VI on the basis of the Fermi pseudo-potential in one dimension.

In order to extract the dominant features, consider first the following two generalizations, the first one obvious and the second one less so.

First, that the potential is the Fermi pseudo-potential is not necessary. In other words, the matrix potential $V(x,x')$ of Eq. (6.2) can take a fairly general form. That g_2 is zero translates into the condition that this $V(x,x')$ is symmetrical, i.e.,

$$V(-x,-x')=V(x,x')$$

in general.

Second, that the model is one-dimensional is not essential. For example, the model can be a two-channel scattering in three-dimensional space. In this case, the $V(x,x')$ is replaced by another 2×2 matrix potential $V(\mathbf{r},\mathbf{r}')$, while the symmetry of the $V(x,x')$ becomes the condition that this $V(\mathbf{r},\mathbf{r}')$ is rotationally symmetrical.

While this rotational symmetry is probably not necessary, this symmetry does play an important role. In the one-dimensional case studied in detail in Sec. VI, the symmetry of the $V(x,x')$, coming from $g_2=0$, makes it possible to use the even wave and the odd wave. Similarly, in three dimensions, the rotational symmetry of $V(\mathbf{r},\mathbf{r}')$ makes it possible to use partial waves: the various partial waves do not couple so that each partial in wave leads to only the corresponding partial out wave.

Consider now the more general setting. Let the quantum memory be in a pure state $\Sigma_j a_j|j\rangle$, where $|j\rangle$ is a complete set of linearly independent states for the memory. The standard state s is a particular linear combination of these $|j\rangle$. Let ψ denote the wave function sent in from the outside to interact with the quantum memory; then the in field for the scattering process on the memory is

$$\Psi^{\text{in}}=\left(\sum_j a_j^{\text{in}}|j\rangle\right)\psi^{\text{in}}. \tag{7.1}$$

An example of Ψ^{in} is given by Eq. (6.23). It should be emphasized that ψ^{in} is at our disposal to accomplish whatever the purpose of this scattering is.

It is the fundamental characteristic of the scattering from a quantum memory that not only is the in field Ψ^{in} of the form of Eq. (7.1), but also the out field is of a similar form,

$$\Psi^{\text{out}}=\left(\sum_j a_j^{\text{out}}|j\rangle\right)\psi^{\text{out}}. \tag{7.2}$$

For the special model of Sec. VI, this important point has been discussed near the end of that section. For the present generalization, it is worked out in detail in Appendix B. As already seen in Sec. VI, Eq. (7.2) puts strong conditions on ψ^{in}. More precisely, a ψ^{in} is defined to be *admissible* if, for all $\Sigma_j a_j^{\text{in}}|j\rangle$, the corresponding Ψ^{out} is given by Eq. (7.2).

It should be added parenthetically that this definition of being admissible can be easily generalized by restricting the $\Sigma_j a_j^{\text{in}}|j\rangle$ to certain subsets. This generalization is expected to be useful in future investigations, but is not needed for this article.

In order to perform the operations of writing, reading, and resetting a quantum memory, it is necessary to have a sufficiently large collection of admissible ψ^{in}. This has been verified to be the case for the model of Sec. VI, and will be assumed to be so in this section. Let

$$\psi^{\text{in}}\left(\sum_j a_j^{\text{in}}|j\rangle\rightarrow\sum_j a_j^{\text{out}}|j\rangle\right) \tag{7.3}$$

denote a ψ^{in} with the property that, if Eq. (7.1) holds for this ψ^{in}, then Eq. (7.2) holds. It is assumed that, given any a_j^{in} and a_j^{out}, there is at least one such ψ^{in}. It is possible that there is more than one such ψ^{in}. It has been seen from the model of Sec. VI that this ψ^{in} may actually involve a sequence of ψ^{in}'s; see especially Eq. (6.11). However, for simplicity of notation, the expression (7.3) will be retained.

The operations of writing, reading, and resetting are now to be described in this order. For the purpose of writing after the quantum memory has been reset to the standard state s, it is sufficient to use any one of the $\psi^{\text{in}}(s\rightarrow\Sigma_j a_j|j\rangle)$, where $\Sigma_j a_j|j\rangle$ is the desired quantum state to be put in the memory.

Reading from a quantum memory is more complicated. Let a quantum memory be in a state $\Sigma_j a_j^{\text{in}}|j\rangle$; it is desired to determine the values of these a_j^{in} by interrogating this memory, i.e., by sending a suitably chosen sequence of admissible ψ^{in}'s,

$$\psi^{\text{in}(1)},\ \psi^{\text{in}(2)},\ \psi^{\text{in}(3)},\ldots,\psi^{\text{in}(N)}, \tag{7.4}$$

and scattering them successively by this quantum memory. More precisely, consider the successive scattering processes

$$
\begin{aligned}
&\sum_j a_j^{\mathrm{in}}|j\rangle\psi^{\mathrm{in}(1)}\to\sum_j a_j^{\mathrm{out}(1)}|j\rangle\psi^{\mathrm{out}(1)}\to a_j^{\mathrm{out}(1)}=a_j^{\mathrm{in}(2)}\\
&\to\sum_j a_j^{\mathrm{in}(2)}|j\rangle\psi^{\mathrm{in}(2)}\to\sum_j a_j^{\mathrm{out}(2)}|j\rangle\psi^{\mathrm{out}(2)}\to a_j^{\mathrm{out}(2)}=a_j^{\mathrm{in}(3)}\\
&\to\sum_j a_j^{\mathrm{in}(3)}|j\rangle\psi^{\mathrm{in}(3)}\to\sum_j a_j^{\mathrm{out}(3)}|j\rangle\psi^{\mathrm{out}(3)}\to a_j^{\mathrm{out}(3)}=a_j^{\mathrm{in}(4)}\\
&\to\cdots\\
&\to\sum_j a_j^{\mathrm{in}(N)}|j\rangle\psi^{\mathrm{in}(N)}\to\sum_j a_j^{\mathrm{out}(N)}|j\rangle\psi^{\mathrm{out}(N)}.
\end{aligned}
\tag{7.5}
$$

Corresponding to the list (7.4), there is a list of ψ^{out}'s,

$$
\psi^{\mathrm{out}(1)},\ \psi^{\mathrm{out}(2)},\ \psi^{\mathrm{out}(3)},\ \ldots,\ \psi^{\mathrm{out}(N)}. \tag{7.6}
$$

From the quantities given in (7.4) and (7.6) together with their interference, the values of a_j^{in} are obtained. This has been demonstrated explicitly in Sec. VI for the model there, and it is also shown there that a further interference with the standard state s may be needed to determine the overall phase. The importance of interference cannot be overemphasized.

Once the a_j^{in} are known, the values of $a_j^{\mathrm{out}(N)}$ of the process (7.5) can be obtained. An additional scattering using any one of the admissible $\psi^{\mathrm{in}}(\Sigma_j a_j^{\mathrm{out}(N)}|j\rangle\to\Sigma_j a_j^{\mathrm{in}}|j\rangle)$ returns the quantum memory to its initial state.

With the above process of reading a quantum memory, resetting is now straightforward. Resetting a quantum memory in the initial state $\Sigma_j a_j^{\mathrm{in}}|j\rangle$ to the standard state s consists of the following two steps.

(i) Read the memory to determine a_j^{in}. Note that, after the process of reading is performed, the memory is in the original initial state $\Sigma_j a_j^{\mathrm{in}}|j\rangle$.
(ii) Apply an additional scattering using any one of the admissible $\psi^{\mathrm{in}}(\Sigma_j a_j^{\mathrm{in}}|j\rangle\to s)$.

This completes the description of the quantum memory together with writing, reading, and resetting, all performed through scattering from the memory.

It may be worthwhile to emphasize that the concept of the quantum memory introduced and described here is quite general. In particular, the scattering process

$$
\Psi^{\mathrm{in}}=\left(\sum_j a_j^{\mathrm{in}}|j\rangle\right)\psi^{\mathrm{in}}\to\Psi^{\mathrm{out}}=\left(\sum_j a_j^{\mathrm{out}}|j\rangle\right)\psi^{\mathrm{out}} \tag{7.7}
$$

does not have many restrictions, and may or may not be linear. Also, the linearly independent states $|j\rangle$ are allowed to depend on time, and may or may not be the eigenstates of an operator.

VIII. COMPARISON WITH AN EARLIER MODEL

The idea of quantum computing was first discussed by Benioff in 1980.[12] In this pioneering paper, spatial dependence was retained, although not in the form of the Schrödinger equation. Since then, quantum computing and quantum information have become popular subjects with a vast literature.[13] However, in the majority of the theoretical papers on quantum computing, spatial dependence is omitted entirely. Therefore the usual model for quantum memory consists of a spin system or its generalization, and the operations on the quantum memory consist of applying unitary matrices. This prevailing model for the quantum memory has led to a number of important results.

In the present article, as a first application of the Fermi pseudo-potential in one dimension, an alternative model for the quantum memory is proposed. This model differs from the previous one mainly in the reintroduction of the spatial variables, much in the spirit of the original work of Benioff.[12] From the point of view of physics, the spatial variables are clearly present, whether one wants them or not. Instead of saying that a unitary matrix is applied mathematically to the content of the quantum memory, here the content of the quantum memory is altered in a controlled way by applying suitably chosen scatterings to the memory.

This is much more than a change of language. While the previous model has the advantage of simplicity, which is important because quantum computing is a difficult subject, the present model with the spatial variable or variables may be considered to be desirable from the following two points of view. First, it offers a closer description of the experimental situation. Since a quantum memory is necessarily small in size, for practical reasons scattering is the simplest means of modifying the content of a quantum memory. Second, the presence of the spatial dimensions allows more possibilities of analyzing the quantum memory. It is also worth mentioning that the theory of scattering has been developed over many decades and is well understood, in the context of both quantum mechanics and quantum field theory. It is often advantageous to be able to make use of existing knowledge to study a new subject.

In both the previous model and the present model, the content of a quantum memory is given as a pure state. This content is altered by applying a unitary transformation, directly in the previous model and indirectly through scattering in the present model. The incident, scattered, and total wave functions have no analog in the previous model. In general, the phase shift[2] of scattering is determined from the total wave function, and the analysis of the explicit model in Sec. VI is actually an especially simple application of the usual phase-shift analysis, including the prominent role played by interference. The point is that, while in the definition of an admissible ψ^{in} in Sec. VII both Ψ^{in} [Eq. (7.1)] and Ψ^{out} [Eq. (7.2)] are unentangled so far as the memory and the interrogating wave are concerned, this is not true of the total wave function, which is for example

$$\psi(x)=\begin{bmatrix}\psi_1(x)\\ \psi_2(x)\end{bmatrix}$$

for the model of Sec. VI.

There are many interesting open questions for the present model. The analysis of these questions is beyond the scope of the present article. Nevertheless, here are two examples of such open questions.

(a) In Sec. VII, it is explicitly assumed that there is a sufficiently large class of admissible ψ^{in} of the form (7.3). In the model of Sec. VI, such a large class indeed exists in the form of even waves and odd waves. On the other hand, when $g_2\neq 0$, no such large class exists. What is needed is a more general discussion as to the conditions under which such a sufficiently large class of admissible ψ^{in} is actually available.

Even though examples where such a large class is available are known both in one dimension and in three dimensions, the three-dimensional case seems rather difficult to achieve experimentally. If this observation is true in general, then there may well be significant advantages to connecting the various components of a quantum computer, including quantum memories, by single-mode optical fibers. In particular, sending signals through space rather than fibers may lead to unexpected problems.

(b) Another especially challenging and interesting question for the present model of quantum memory concerns the issue of the so-called no-cloning theorem. This has been derived in the context of the previous model, but such derivations do not seem to be applicable directly to the present model. This is again related to the fact that here there is not only an S-matrix but also the incident, scattered, and total wave functions.

Preliminary analysis indicates that whether the no-cloning theorem holds for the present

model of quantum memory may depend on subtle aspects of the Schrödinger equation. If this is indeed the case, then the no-cloning theorem may need to be stated properly and precisely before it can be derived within the present model of quantum memory.

IX. DISCUSSIONS

The present investigation began as an attempt to understand the $\delta'(x)$ potential in the context of the one-dimensional Schrödinger equation. When simple attempts failed, the powerful method of the resolvent equation was used. The surprise is that, not only can the resolvent equation be solved in general in terms of rational functions, but also the solution yields, in addition to the well-known δ-function potential, not one but *two* linearly independent Fermi pseudo-potentials in one dimension. One of the pseudo-potentials is odd under space reflection and is the proper interpretation of the $\delta'(x)$ potential. The other one is originally unexpected and is even under space reflection.

It is likely that there are many applications of these pseudo-potentials to one-dimensional problems. A possible use in statistical mechanics connected with the Bethe ansatz[8,9] has already been mentioned in Sec. VI. In this article, only the simplest application is discussed. This has nothing to do with the proper interpretation of the $\delta'(x)$ potential, but depends critically on the unexpected, even pseudo-potential. By combining this even pseudo-potential with the δ-function potential, an elegant special case is found for the scattering in two coupled channels. Even though the two channels cannot be decoupled, it is easy to write down the complete solution from the known one-channel case.

In spite of the mathematical simplicity of this application of the Fermi pseudo-potential in one dimension, this example gives a model for the quantum memory (sometimes called the quantum register). While this model is completely explicit, its more important function is to point out a way to gain a general picture concerning the quantum memory.

More generally, the time-independent Schrödinger equation for n coupled channels with interaction at only the one point $x=0$ is

$$-\frac{d^2\psi(x)}{dx^2}+\int_{-\infty}^{\infty}dx'\,V(x,x')\,\psi(x')=k^2\psi(x) \tag{9.1}$$

with

$$\psi(x)=\begin{bmatrix}\psi_1(x)\\ \psi_2(x)\\ \vdots\\ \psi_n(x)\end{bmatrix} \tag{9.2}$$

and

$$V(x,x')=C_1\delta(x)\,\delta(x')+C_2[\,\delta_p'(x)\,\delta(x')+\delta(x)\,\delta_p'(x')\,]+C_3\delta_p'(x)\,\delta_p'(x'). \tag{9.3}$$

Here C_1, C_2 and C_3 are three numerical Hermitian $n\times n$ matrices, while $\delta_p'(x)$ is similar to $\delta'(x)$ and is defined in Sec. IV. For a given k and a given incident wave $\psi_0(x)$ with n components, the solution of Eq. (9.1) takes the form, for $j=1,2,\ldots,n$,

$$\psi_j(x)=\psi_{0j}(x)+\begin{cases}F_{j+}e^{ikx}, & \text{for } x>0,\\ F_{j-}e^{-ikx}, & \text{for } x<0,\end{cases} \tag{9.4}$$

analogous to Eq. (2.7), where the F's are $2n$ coefficients that depend on ψ_{0j} and k. The substitution of Eq. (9.4) into Eq. (9.1) shows that these $2n$ F's satisfy $2n$ linear equations. Indeed, it is the power of the Fermi pseudo-potential that Schrödinger equations reduce to linear algebraic equations. It will be interesting to study the structure of these algebraic equations. Even more

generally, the pseudo-potential (9.3) at $x=0$ may be replaced by a linear superposition of a finite number of such pseudo-potentials at $x=x_1,x_2,\ldots$. The number of coefficients in the solution increases but remains finite, leading to more simultaneous algebraic equations that are still linear. The Green's functions can be treated in a very similar manner.

Needless to say, the range of integration in Eq. (9.1) for x' can be replaced by a semi-infinite or finite interval, and the $V(x,x')$ may contain additional terms such as those from step potentials. A more interesting problem is to apply the Fermi pseudo-potentials to first-order differential equations.

In summary, the theory of the Fermi pseudo-potential in one dimension has been worked out here together with the simplest nontrivial application to a problem of current interest.

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APPENDIX A: SOLUTION FOR EQUATION (3.13)

A possible way to solve Eq. (3.13) for $F(\kappa)$ is as follows. Because of the exponential function in the last term, let

$$x=e^{F(\kappa)} \tag{A1}$$

and

$$y=\ln\kappa. \tag{A2}$$

[This x of Eq. (A1) of course has nothing to do with the space variable in the Schrödinger equation (1.1), for example.] In view of Eq. (3.3), Eq. (3.13) is translationally invariant in y. It is therefore desirable to use x as the independent variable and y as the dependent variable, leading to a first-order ordinary differential equation for

$$z=\frac{dy}{dx}. \tag{A3}$$

This first-order equation is

$$-\frac{2}{x^2z^3}\left[x\frac{dz}{dx}+z\right]=\frac{1}{x^2z^2}-1+(c_3^2+c_2c_4)x^2. \tag{A4}$$

Let

$$u=\frac{1}{x^3z^2}. \tag{A5}$$

Then, after some algebra,

$$\frac{du}{dx}=-\frac{1}{x^2}+(c_3^2+c_2c_4). \tag{A6}$$

Integration yields

$$u=\frac{1}{x}+2c_1+(c_3^2+c_2c_4)x, \tag{A7}$$

where c_1 is the fourth arbitrary constant of integration. The expression for z follows from Eqs. (A5) and (A7):

$$z=\pm x^{-1}[1+2c_1x+(c_3^2+c_2c_4)x^2]^{-1/2}, \tag{A8}$$

where the $\pm$ sign comes from taking the square root of z^2. It is, of course, related to the fact that every term in Eq. (A4) is even in z. In the following, there are many $\pm$ and $\mp$ signs; it is to be understood that these signs are used as a shorthand for two equations, one with the upper sign everywhere and a second one with the lower sign everywhere.

From Eqs. (A3) and (A8), y is given by

$$y=\mp\int\frac{dx'}{\sqrt{(c_3^2+c_2c_4)+2c_1x'+x'^2}}, \tag{A9}$$

where $x'=1/x$. It is fortunate that this integral is elementary. For definiteness, consider the case

$$c_3^2+c_2c_4-c_1^2>0. \tag{A10}$$

In this case, the explicit integration of the right-hand side of Eq. (A9) gives

$$y=\mp\left[\sinh^{-1}\frac{1+c_1x}{\sqrt{c_3^2+c_2c_4-c_1^2}x}+\text{const}\right]. \tag{A11}$$

The rest of the calculation is straightforward although lengthy, and the results are

$$f_1(\kappa)=\frac{-\sqrt{c_3^2+c_2c_4-c_1^2}[c_0\kappa+(c_0\kappa)^{-1}]\mp 2c_3}{\sqrt{c_3^2+c_2c_4-c_1^2}[c_0\kappa-(c_0\kappa)^{-1}]\pm 2c_1}, \tag{A12}$$

$$f_2(\kappa)=1\mp\frac{2c_2}{\sqrt{c_3^2+c_2c_4-c_1^2}[c_0\kappa-(c_0\kappa)^{-1}]\pm 2c_1}, \tag{A13}$$

$$f_3(\kappa)=\frac{-\sqrt{c_3^2+c_2c_4-c_1^2}[c_0\kappa+(c_0\kappa)^{-1}]\pm 2c_3}{\sqrt{c_3^2+c_2c_4-c_1^2}[c_0\kappa-(c_0\kappa)^{-1}]\pm 2c_1}, \tag{A14}$$

$$f_4(\kappa)=1\mp\frac{2c_4}{\sqrt{c_3^2+c_2c_4-c_1^2}[c_0\kappa-(c_0\kappa)^{-1}]\pm 2c_1}. \tag{A15}$$

Since c_1, c_2, c_3 and c_4 are arbitrary constants of integration, their signs can be changed simultaneously. This change then removes all the $\pm$ and $\mp$ signs, and Eqs. (A12)–(A15) reduce to Eqs. (3.14).

The other case, where $c_3^2+c_2c_4-c_1^2<0$, can be treated in an entirely similar manner, leading to Eq. (3.16).

APPENDIX B: DERIVATION OF EQUATION (7.2)

In this Appendix B, the reasoning is given that leads to Eq. (7.2).

Just as the Ψ^{in} of Eq. (7.1) contains information about the initial state of the quantum memory and the behavior of the incoming wave ψ^{in} before scattering, the Ψ^{out} contains information about the final state of the quantum memory and the behavior of the outgoing wave after scattering.

Later the outgoing wave moves away from the memory and the information about this outgoing wave is no longer available. This means that the final state of the memory is given by Ψ^{out} *averaged* over this outgoing wave. This average can be written schematically as

$$M = \int \Psi^{\text{out}} \Psi^{\text{out}\dagger}. \tag{B1}$$

This M is the density matrix for the quantum memory. Here the $\int$ indicates integration and summation over all degrees of freedom associated with the outgoing wave or particle, but not those of the quantum memory. The corresponding differential symbol is omitted: It is $d^3\mathbf{r}$ if the wave is described by the three-dimensional Schrödinger equation; it is $d^3\mathbf{r}$ together with a summation over the spin in the case of the Dirac equation; and it is a functional differential such as $\mathcal{D}A_\mu$ in the context of quantum field theory.

In order for the quantum memory to function, the final state must be a pure state $\Sigma_j a_j^{\text{out}}|j\rangle$, just like the initial state. Therefore, the above M must also be given by

$$M = \sum_j a_j^{\text{out}}|j\rangle \sum_i a_i^{\text{out}*}\langle i|. \tag{B2}$$

Equating the two formulas for M gives

$$\sum_j a_j^{\text{out}}|j\rangle \sum_i a_i^{\text{out}*}\langle i| = \int \Psi^{\text{out}} \Psi^{\text{out}\dagger}. \tag{B3}$$

It remains to derive Eq. (7.2) from Eq. (B3).

Since the $|j\rangle$ form a complete set, Ψ^{out} can always be written in the form

$$\Psi^{\text{out}} = \sum_j |j\rangle \psi_j^{\text{out}}. \tag{B4}$$

The substitution of Eq. (B4) into Eq. (B3) gives

$$a_j^{\text{out}} a_i^{\text{out}*} = \int \psi_j^{\text{out}} \psi_i^{\text{out}\dagger} \tag{B5}$$

for all i and j. For $i \neq j$, define the integral

$$I_{ji} = \int (a_i^{\text{out}} \psi_j^{\text{out}} - a_j^{\text{out}} \psi_i^{\text{out}})(a_i^{\text{out}*} \psi_j^{\text{out}\dagger} - a_j^{\text{out}*} \psi_i^{\text{out}\dagger}). \tag{B6}$$

This I_{ji} is non-negative, and is zero only if

$$a_i^{\text{out}} \psi_j^{\text{out}} - a_j^{\text{out}} \psi_i^{\text{out}} = 0. \tag{B7}$$

But the substitution of Eq. (B5) into Eq. (B6) gives immediately that

$$I_{ji} = 0. \tag{B8}$$

Thus, Eq. (B7) holds for all i and j.

The desired Eq. (7.2) is just Eq. (B4) with Eq. (B7).

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Extension of Bethe ansatz to multiple occupancies for one-dimensional SU(4) fermions with δ-function interaction

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We consider the problem of consistence between the Bethe ansatz (BA) wave function and the multiparticle (more than two) scattering in one-dimensional δ-function interacting SU(4) fermions, which the approach of BA does not explicitly take into account. We find the scattering conditions of three and four particles located at the same position and show that the conditions can be fulfilled by the two-particle connection conditions of the BA wave function. So the definition of the BA wave function can be exactly extended to those cases with multiple occupancies. The inconsistence between the BA and multiparticle interacting on a same site in the degenerate Hubbard model, which makes the BA fail for the model, is shown to vanish in the limit of small site spacing. A correspondence relation of the BA equation and SU(4) symmetry of the system is also indicated for the fermions. The degeneracy of state with BA eigenenergy is given. Singlet lies in the case when there are equal numbers of particles in each inner component. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1515380]

I. INTRODUCTION

Since the Bethe ansatz (BA) approach was proposed to solve exactly the Heisenberg model,[1] it has been applied to many integrable systems such as one-dimensional δ-function interacting bosons[2,3] and spin-1/2 fermions,[4] Hubbard model,[5] Kondo model,[6] spin ladder,[7] etc., and recently there has been much interest in extending the BA to the study of degenerate electrons systems.[8–14] As is well known, the coordinate BA wave functions for N-particle systems are defined on separated regions denoted by $x_{Q_1} < \cdots < x_{Q_N}$ where Q is a permutation of the particles and x_{Q_i} is the coordinate of the Q_ith particle, the connection boundaries between two adjacent regions are those cases in which two (and no more than two) particles interact at the same position, and the two-particle scattering matrices solve the boundary conditions. The matrices transferring amplitudes in the BA wave function from one region to another factorize into products of two-particle S matrices. The diagonalization of the N-particle transfer matrices with periodic conditions leads to the BA equations that determine the whole solutions. So the original BA, as a matter of fact, does not involve the boundaries with more than two particles scattering at the same position or take into account the corresponding scattering conditions. If the scattering conditions of multiple occupations, which are required by models of the degenerate or multicomponent particle systems, cannot be consistently met by the BA wave function, the BA wave function will not be the solutions of the systems. Such a problem of consistence has been encountered in the degenerate Hubbard model, the BA fails to solve the model at configurations with more than two particles on one site,[10] and the theoretical work in the framework of the BA for degenerate Hubbard model has

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been based on the exclusion of such multiply occupied configurations.[11–14] Therefore, whether the BA wave functions are exactly valid for the degenerate systems is still unconfirmed if the consistency between the BA wave function and multiparticle scattering conditions has not been definitely verified.

In the present paper we shall investigate explicitly the problem of consistence between the BA and the multiparticle scattering conditions for one-dimensional δ-function interacting SU(4) fermions which is a spatially continuous system instead of a lattice model. We work out explicitly the scattering boundary conditions of three and four particles located at the same spatial point. We prove that the multiparticle scattering conditions can be fulfilled by the two-particle connection conditions of the BA wave function. Therefore we can extend exactly the definition of the BA wave function to the configurations with multiple occupancies and, unlike in lattice models, the BA is valid for the spatially continuous model without the exclusion of more than two particles interacting at the same position. The inconsistency in the BA for the degenerate Hubbard model is shown to vanish in the limit of small site spacing. An interesting correspondence between the SU(4) symmetry and the BA equation is also pointed out for the δ-function interacting fermions. The states relating to a BA eigenenergy are degenerate, and the degeneracy can be calculated in terms of the highest weight vector of the corresponding SU(4) multiplet.

II. TWO-PARTICLE SCATTERING AND THE BETHE ANSATZ WAVE FUNCTION

The Schrödinger equation of the N-fermion system we shall consider reads

$$\left(-\frac{1}{2}\sum_{i}^{N}\frac{\partial^2}{\partial x_i^2} + c\sum_{i<j}\delta(x_i - x_j)\right)\psi = E\psi. \tag{1}$$

We define the BA wave function in the form of

$$\psi^{(Q)}_{a_1\cdots\ a_N}(x_1,\cdots,x_N) = \sum_{P\in S_N} A^{(Q)}_{a_1\cdots\ a_N}(k_{P_1}\cdots\ k_{P_N})e^{i\Sigma_j k_{P_j}x_j}, \tag{2}$$

where a_j labels the four components of the jth fermions. The inner degree of freedom can be spin–orbital double. Other forms of BA wave function are equivalent, our further proof holds as long as the solution is BA wave function. The BA wave function is defined in the region sector

$$R_Q : x_{Q_1} < \cdots < x_{Q_N}.$$

The wave function (2) surely solves the eigenequation

$$-\frac{1}{2}\sum_{i}^{N}\frac{\partial^2}{\partial x_i^2}\psi^{(Q)} = E_{\mathrm{BA}}\psi^{(Q)} \tag{3}$$

in R_Q with the eigenenergy

$$E_{\mathrm{BA}} = \frac{1}{2}\sum_{i}^{N} k_i^2 . \tag{4}$$

Let $(Q_1\cdots ij\cdots Q_N)$ denote a sector with $Q_r = i$ and $Q_{r+1} = j$ for some r. The two-particle connection condition across the barrier $x_i = x_j$ is given by

$$\left(\frac{\partial}{\partial x_i} - \frac{\partial}{\partial x_j}\right)\psi^{(Q_1\cdots ji\cdots Q_N)}_{a_1\cdots\ a_N}\Big|_{x_j = x_i -} - \left(\frac{\partial}{\partial x_i} - \frac{\partial}{\partial x_j}\right)\psi^{(Q_1\cdots ij\cdots Q_N)}_{a_1\cdots\ a_N}\Big|_{x_j = x_i +} = 2c\,\psi^{(Q_1\cdots ij\cdots Q_N)}_{a_1\cdots\ a_N}\Big|_{x_i = x_j}, \tag{5}$$

which can be obtained by integrating of the eigenequation over a Gauss box at the hyperplane $x_i=x_j$. And on the right-hand side of Eq. (5) the $\psi^{(Q_1\cdots ij\cdots Q_N)}|_{x_j=x_i}$ can be replaced by $\psi^{(Q_1\cdots ji\cdots Q_N)}|_{x_j=x_i}$ because of the continuity of the wave function. Combining the above condition with the uniqueness of the wave function on the two-particle connection boundary, one can find the two-particle S-matrix,[4]

$$S^{ij}=\frac{(k_{P_i}-k_{P_j})I^{ij}+icP^{ij}}{(k_{P_i}-k_{P_j})+ic}, \quad S^{ij}A^{(Q_1\cdots\ ij\cdots\ Q_N)}_{(k_{P_1}\cdots\ k_{P_i}\cdots\ k_{P_j}\cdots\ k_{P_N})}=A^{(Q_1\cdots\ ji\cdots\ Q_N)}_{(k_{P_1}\cdots\ k_{P_i}\cdots\ k_{P_j}\cdots\ k_{P_N})}, \tag{6}$$

where P^{ij} exchanges inner components a_i,a_j and

$$\begin{aligned}
&P^{ij}A^{(Q_1\cdots\ ij\cdots\ Q_N)}_{a_1\cdots\ a_i\cdots\ a_j\cdots\ a_N}(k_{P_1}\cdots\ k_{P_i}\cdots\ k_{P_j}\cdots\ k_{P_N})\\
&\quad=A^{(Q_1\cdots\ ij\cdots\ Q_N)}_{a_1\cdots\ a_j\cdots\ a_i\cdots\ a_N}(k_{P_1}\cdots\ k_{P_i}\cdots\ k_{P_j}\cdots\ k_{P_N})\\
&\quad=-A^{(Q_1\cdots\ ji\cdots\ Q_N)}_{a_1\cdots\ a_i\cdots\ a_j\cdots\ a_N}(k_{P_1}\cdots\ k_{P_j}\cdots\ k_{P_i}\cdots\ k_{P_N}),
\end{aligned}$$

where the minus sign in the second equation comes from the antisymmetry of fermions.

It should be noted that $\psi^{(Q_1\cdots ij\cdots Q_N)}|_{x_j=x_i-}$ and $\psi^{(Q_1\cdots ji\cdots Q_N)}|_{x_j=x_i+}$ in (5) are, respectively, in two regions $(Q_1\cdots ij\cdots Q_N)$ and $(Q_1\cdots ji\cdots Q_N)$ which are neighbor sectors. The transfer matrices for regions not adjacent are products of the two-particle S-matrices. The S-matrices satisfy the Yang–Baxter relations.[4] The diagonalization of the N-particle transfer matrices combined with periodic conditions

$$\psi(\cdots\ x_j\ \cdots\ )=\psi(\cdots\ x_j+L\cdots\ )$$

results in the BA equations by means of the methods in Refs. 15 and 16

$$\begin{aligned}
e^{ik_jL}&=\prod_{\alpha=1}^{M}\frac{k_j-\lambda_\alpha+ic/2}{k_j-\lambda_\alpha-ic/2},\\
1&=-\prod_{j=1}^{N}\frac{\lambda_\alpha-k_j-ic/2}{\lambda_\alpha-k_j+ic/2}\prod_{\alpha'=1}^{M}\frac{\lambda_\alpha-\lambda_{\alpha'}+ic}{\lambda_\alpha-\lambda_{\alpha'}-ic}\prod_{\beta=1}^{M'}\frac{\lambda_\alpha-\mu_\beta-ic/2}{\lambda_\alpha-\mu_\beta+ic/2},\\
1&=-\prod_{\alpha=1}^{M}\frac{\mu_\beta-\lambda_\alpha-ic/2}{\mu_\beta-\lambda_\alpha+ic/2}\prod_{\beta'=1}^{M'}\frac{\mu_\beta-\mu_{\beta'}+ic}{\mu_\beta-\mu_{\beta'}-ic}\prod_{\gamma=1}^{M''}\frac{\mu_\beta-\nu_\gamma-ic/2}{\mu_\beta-\nu_\gamma+ic/2},\\
1&=-\prod_{\beta=1}^{M'}\frac{\nu_\gamma-\mu_\beta-ic/2}{\nu_\gamma-\mu_\beta+ic/2}\prod_{\gamma'=1}^{M''}\frac{\nu_\gamma-\nu_{\gamma'}+ic}{\nu_\gamma-\nu_{\gamma'}-ic},
\end{aligned} \tag{7}$$

which determine the whole solution in the BA approach. The total particle numbers N_1,N_2,N_3,N_4 with inner components 1,2,3,4 are, respectively,

$$\begin{aligned}
&N_1=N-M, \quad N_2=M-M',\\
&N_3=M'-M'', \quad N_4=M''.
\end{aligned} \tag{8}$$

Here we do not intend to discuss the corresponding ground states, excitations or thermodynamics. In the following we shall consider the relation of the BA wave function and the system symmetry as well as the state's degeneracy.

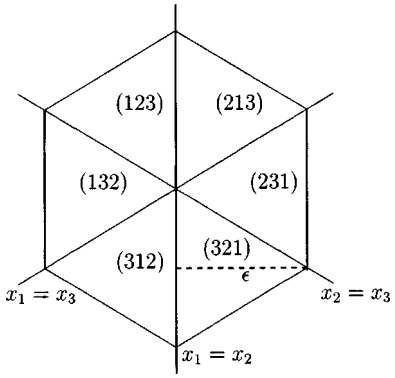


FIG. 1. A cross section of the hexagonal prism in the three-dimensional subspace of x_1, x_2, and x_3. The center axis of the prism is along the intersecting line $x_1=x_2=x_3$, and labels of the three interacting particles ijk have been set to be 123.

As one can see from the above procedure, the BA treatment is built up on the basis of solving the separate noninteracting regions R_Q and the two-particle boundaries which are connections of *two* neighbor regions. The BA indeed does not take into account the multiple-occupancy (more than two) boundaries which are joint boundary of *three* or *four* regions, and the corresponding multiparticle scattering conditions become additional ones; what these conditions are is not explicit and whether they are solved by BA remains to be answered. In fact, it is just by examining this kind of multiparticle scattering that Choy and Haldane found the failure of the BA in the degenerate Hubbard model.[10] In the following we shall explicitly investigate the consistence between the BA and those multiparticle scattering out of the consideration of the BA for the four-component fermions (1).

III. THREE-PARTICLE SCATTERING

With the help of the continuity of the wave function at two-particle scattering boundary, which has been used in the Bethe ansatz, it is easy to prove the single valueness of the wave function for three and four particles at the same point. Without guarantee of the wave function single valueness, further discussion on the problem of consistence would be unnecessary since it had been inconsistent here.

To investigate the consistence between the BA and the three-particle scattering we have to obtain the corresponding scattering boundary condition which is not obvious or explicit to write out. Let us consider three particles i, j, and k at the boundary $x_i=x_j=x_k$. We integrate the eigenequation (1) over an arbitrarily shaped volume through which the intersecting line $x_i=x_j=x_k$ is located in the three-dimensional subspace of x_i, x_j, and x_k. The arbitrarily shaped volume can be cut into an ϵ-sized hexagonal prism of which a cross section is shown in Fig. 1. The integration of the eigenequation over the cutoff part cancels automatically, which is a natural result of (3) and (5), respectively, in the sectors and on the two-particle connecting hyperplanes. Therefore, it's sufficient to consider only the prism left.

Set ϵ to be infinitesimal, carry out the expansion of the Gaussian integral in orders of ϵ and keep the lowest order, we find the three-particle condition to be

$$\left(\frac{\partial}{\partial x_1}-\frac{\partial}{\partial x_2}\right)\left(\psi^{(Q_1\cdots 231\cdots Q_N)}-\psi^{(Q_1\cdots 132\cdots Q_N)}\right)\Big|_{x_1=x_2=x_3}+\left(\frac{\partial}{\partial x_2}-\frac{\partial}{\partial x_3}\right)\left(\psi^{(Q_1\cdots 312\cdots Q_N)}\right.$$
$$\left.-\psi^{(Q_1\cdots 213\cdots Q_N)}\right)\Big|_{x_1=x_2=x_3}+\left(\frac{\partial}{\partial x_3}-\frac{\partial}{\partial x_1}\right)\left(\psi^{(Q_1\cdots 123\cdots Q_N)}-\psi^{(Q_1\cdots 321\cdots Q_N)}\right)\Big|_{x_1=x_2=x_3}$$
$$=12c\,\psi^{(Q_1\cdots 123\cdots Q_N)}\big|_{x_1=x_2=x_3}, \tag{9}$$

where we have set the three particles to be 123 for the sake of clarity, and the infinitesimal notations as in $\psi^{(Q_1\cdots 231\cdots Q_N)}|_{x_1=x_3^+,x_2=x_3^-}$ have been dropped since it has been indicated in the corresponding label Q of region sector. Also on the right-hand side of the above relations, $\psi^{(Q_1\cdots 123\cdots Q_N)}|_{x_1=x_2=x_3}$ can be replaced by wave function with other permutation of the particles 123, while the positions of other particles remain unchanged. On the left-hand side of (9), it should be noted that the pairs of wave functions in a bracket are not in neighbor sectors as those of Eq. (5).

We find the condition (9) can be satisfied in terms of the two-particle connection condition (5). As one knows in the BA, the two-particle S-matrices provide to cancel the amplitudes of a same exponential $\exp(i\Sigma_j k_{P_j} x_j)$, the amplitudes $A^{(Q)}_{k_{P_1}\cdots\ k_{P_N}}$ are independent of the particles coordinates, so it does not affect the cancellation of the amplitudes in (5) when we set the position of a third adjacent particle to be the same as the two particles on the connection boundary and keep all the permutation notation Q's in the amplitudes unchanged. Hence, Eq. (5) still holds at $x_{Q_1}<\cdots<x_i=x_j=x_k<\cdots<x_{Q_N}$,

$$\left(\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_j}\right)(\psi^{(Q_1\cdots jik\cdots Q_N)}-\psi^{(Q_1\cdots ijk\cdots Q_N)})|_{x_i=x_j=x_k}=2c\,\psi^{(Q_1\cdots ijk\cdots Q_N)}|_{x_i=x_j=x_k},$$
$$\left(\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_j}\right)(\psi^{(Q_1\cdots kji\cdots Q_N)}-\psi^{(Q_1\cdots kij\cdots Q_N)})_{x_i=x_j=x_k}=2c\,\psi^{(Q_1\cdots kij\cdots Q_N)}|_{x_i=x_j=x_k}. \tag{10}$$

Also note that the wave functions on the left-hand sides are defined on neighbor regions as in (5). We split the differential operation $\partial/\partial x_1-\partial/\partial x_2$ to be $(\partial/\partial x_1-\partial/\partial x_3)+(\partial/\partial x_3-\partial/\partial x_2)$ and similarly for others, thus the left-hand side of (9) becomes

$$\begin{aligned}&\left(\left(\frac{\partial}{\partial x_1}-\frac{\partial}{\partial x_3}\right)+\left(\frac{\partial}{\partial x_3}-\frac{\partial}{\partial x_2}\right)\right)(\psi^{(Q_1\cdots 231\cdots Q_N)}-\psi^{(Q_1\cdots 132\cdots Q_N)})|_{x_1=x_2=x_3}\\&\quad+\left(\left(\frac{\partial}{\partial x_2}-\frac{\partial}{\partial x_1}\right)+\left(\frac{\partial}{\partial x_1}-\frac{\partial}{\partial x_3}\right)\right)(\psi^{(Q_1\cdots 312\cdots Q_N)}-\psi^{(Q_1\cdots 213\cdots Q_N)})|_{x_1=x_2=x_3}\\&\quad+\left(\left(\frac{\partial}{\partial x_3}-\frac{\partial}{\partial x_2}\right)+\left(\frac{\partial}{\partial x_2}-\frac{\partial}{\partial x_1}\right)\right)(\psi^{(Q_1\cdots 123\cdots Q_N)}-\psi^{(Q_1\cdots 321\cdots Q_N)})|_{x_1=x_2=x_3}\end{aligned}$$

which, as a result of (10), equals to $12c\,\psi^{(Q)}|_{x_1=x_2=x_3}$, exactly the right-hand side of (9). Therefore we have proved that the scattering condition of three particles at a same position can be fulfilled by the two-particle connection conditions in the BA solution.

IV. FOUR-PARTICLE SCATTERING

Now let us consider the case of four particles interacting at the same point. For simplicity we omit the notations of other particles. Similar to the three-particle scattering, it is also sufficient to calculate the integral of the eigenequation over an ϵ-sized Gaussian box at the axis $x_1=x_2=x_3=x_4$. A vector in the sector of (1234) can be built on another set of orthonormal basis

$$\mathbf{r}_{1234}\equiv x_1\mathbf{e}_1+x_2\mathbf{e}_2+x_3\mathbf{e}_3+x_4\mathbf{e}_4=\omega\alpha_{1234}+h\gamma+y\beta_{1234}+y'\beta'_{1234}, \tag{11}$$

where the basis vectors are

$$\alpha_{1234}=-\frac{3\mathbf{e}_1+\mathbf{e}_2-\mathbf{e}_3-3\mathbf{e}_4}{\sqrt{20}},\quad \gamma=\frac{\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3+\mathbf{e}_4}{2},$$
$$\beta_{1234}=\frac{\mathbf{e}_1-\mathbf{e}_2-\mathbf{e}_3+\mathbf{e}_4}{2},\quad \beta'_{1234}=\frac{\mathbf{e}_1-3\mathbf{e}_2+3\mathbf{e}_3-\mathbf{e}_4}{\sqrt{20}}. \tag{12}$$

γ is the direction vector along the center axis $x_1=x_2=x_3=x_4$. The connecting boundary $x_i=x_j$ can be expressed in terms of α_{1234}, γ, β_{1234}, and β'_{1234} according to the above relations. In the (1234) sector the inwards normals of the intersecting hyperplanes $x_1=x_2$, $x_2=x_3$ and $x_3=x_4$ are, respectively, $\mathbf{n}_{21}=\mathbf{e}_2-\mathbf{e}_1$, $\mathbf{n}_{32}=\mathbf{e}_3-\mathbf{e}_2$, and $\mathbf{n}_{43}=\mathbf{e}_4-\mathbf{e}_3$. It is easy to see $\alpha_{1234}\cdot\mathbf{n}_{21}=\alpha_{1234}\cdot\mathbf{n}_{32}=\alpha_{1234}\cdot\mathbf{n}_{43}$. Setting $\omega=\epsilon$, we have a hyperplane which can be the side surface of the Gaussian box in the (1234) region, α_{1234} is the outwards normal direction vector. Other sectors are similar with the subscripts permuted correspondingly. We also set the size parameter ϵ to be infinitesimal, carry out the expansion in the orders of ϵ and keep the lowest order in the integration of the eigenequation. After a careful calculation we find the scattering condition of four particles at one point to be

$$-\frac{1}{2}\sum_{Q\in S_4}\left(3\frac{\partial}{\partial x_{Q_1}}+\frac{\partial}{\partial x_{Q_2}}-\frac{\partial}{\partial x_{Q_3}}-3\frac{\partial}{\partial x_{Q_4}}\right)\psi^{(Q)}(x,x,x,x)=120c\,\psi(x,x,x,x). \tag{13}$$

As we show below, the above four-particle scattering condition is also fulfilled by the two-particle conditions.

Relations in (10) are similarly extended to

$$\left(\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_j}\right)(\psi^{(Q_1\cdots jikl\cdots Q_N)}-\psi^{(Q_1\cdots ijkl\cdots Q_N)})|_{x_i=x_j=x_k=x_l}=2c\,\psi^{(Q_1\cdots ijkl\cdots Q_N)}|_{x_i=x_j=x_k=x_l},$$
$$\left(\frac{\partial}{\partial x_j}-\frac{\partial}{\partial x_k}\right)(\psi^{(Q_1\cdots ikjl\cdots Q_N)}-\psi^{(Q_1\cdots ijkl\cdots Q_N)})|_{x_i=x_j=x_k=x_l}=2c\,\psi^{(Q_1\cdots ijkl\cdots Q_N)}|_{x_i=x_j=x_k=x_l}, \tag{14}$$
$$\left(\frac{\partial}{\partial x_k}-\frac{\partial}{\partial x_l}\right)(\psi^{(Q_1\cdots ijlk\cdots Q_N)}-\psi^{(Q_1\cdots ijkl\cdots Q_N)})|_{x_i=x_j=x_k=x_l}=2c\,\psi^{(Q_1\cdots ijkl\cdots Q_N)}|_{x_i=x_j=x_k=x_l}.$$

And by means of the following trick:

$$\left(3\frac{\partial}{\partial x_{Q_1}}+\frac{\partial}{\partial x_{Q_2}}-\frac{\partial}{\partial x_{Q_3}}-3\frac{\partial}{\partial x_{Q_4}}\right)=\left(3\left(\frac{\partial}{\partial x_{Q_1}}-\frac{\partial}{\partial x_{Q_2}}\right)+4\left(\frac{\partial}{\partial x_{Q_2}}-\frac{\partial}{\partial x_{Q_3}}\right)+3\left(\frac{\partial}{\partial x_{Q_3}}-\frac{\partial}{\partial x_{Q_4}}\right)\right), \tag{15}$$

the differential operations are changed to be of neighbor particles pairs on the left-hand side of (13). To use (14) we note the relation

$$\sum_{Q\in S_4}\left(\frac{\partial}{\partial x_{Q_1}}-\frac{\partial}{\partial x_{Q_2}}\right)\psi^{(Q)}(x,x,x,x)=\frac{1}{2}\sum_{Q\in S_4}\left(\frac{\partial}{\partial x_{Q_1}}-\frac{\partial}{\partial x_{Q_2}}\right)(\psi^{(Q)}(x,x,x,x)-\psi^{(Q')}(x,x,x,x)), \tag{16}$$

where $Q'=(Q_2Q_1Q_3Q_4)$, and the similar relations for the cases of $(\partial/\partial x_{Q_2}-\partial/\partial x_{Q_3})$ and $(\partial/\partial x_{Q_3}-\partial/\partial x_{Q_4})$ with Q' replaced, respectively, by $(Q_1Q_3Q_2Q_4)$ and $(Q_1Q_2Q_4Q_3)$. Applying (14)–(16), we find the four-particle condition (13) is also satisfied. The general case for any four scattering particles among the total N particles can be directly generalized from the results we have obtained.

The configurations with more than four particles at one point are excluded by the Pauli principle (extended to four components), the antisymmetric wave function vanishes in such cases. Thus we have covered all kinds of occupancies and explicitly proven the consistence between the BA and the multiparticle scattering boundary conditions.

V. NARROW-SITES LIMITING IN THE DEGENERATE HUBBARD MODEL

In the above sections we have proven explicitly the consistence between the multiparticle scattering and the BA solution in spatially continuous case. Now let us turn to the lattice case and investigate the limiting process of small site spacing in the Hubbard model. As one knows the Hubbard model, in the limit of small site distance d, approaches to the model of electrons with δ-function interaction which is spatially continuous. The single-band Hubbard model was solved by the SU(2) BA.[5] But the direct generalization of SU(2) BA solution of the single-band Hubbard model to the degenerate SU(N) case for the degenerate Hubbard model fails due to the multiparticle same-site interacting case. In Ref. 10 it is found that there appears to be an unhermition extra interacting term for three bosons occupying the same site in the BA wave function which was proposed with an attempt to solve the boson Hubbard model. This unhermition term extra to the Hubbard on-site interaction $3U$, with the form of

$$\frac{U^2/t}{\cos(k_1+k_2)\cos(k_2+k_3)\cos(k_3+k_1)}, \tag{17}$$

where U is the Hubbard on-site interaction and t is the hopping constant and k_1, k_2, and k_3 are momenta of the interacting bosons, breaks the validity of the BA for boson Hubbard model. The similar thing will happen for degenerate electrons or fermions and the inconsistent extra term has the same form as (17) except a sign difference. According to our explicit proof of consistence between the BA and the multiparticle interacting for δ-function interacting fermions, the inconsistent term should come to vanish in the limit process of site distance going to zero, since the Hubbard model approaches to the model of electrons with δ-function interaction. Let us pick up the site distance d which is usually taken to be unit, and the S-matrix for the Hubbard model is

$$S^{ij}=\frac{(\sin k_s d-\sin k_t d)I^{ij}+iU/2tP^{ij}}{(\sin k_s d-\sin k_t d)+iU/2t} \tag{18}$$

where the notations of P_s, P_t, and P^{ij} are the same as in (6) and $\sin k_s d$ is originated from the discreteness in space coordinate for lattice sites. The above S-matrix becomes

$$\frac{(k_s d-k_t d)I^{ij}+iU/2tP^{ij}}{(k_s d-k_t d)+iU/2t}=\frac{(k_s-k_t)I^{ij}+iU/2tdP^{ij}}{(k_s-k_t)+iU/2td} \tag{19}$$

for small d.

One may mention the large momentum case in which $k_j d$ may not be small. This is true indeed if we have definite total site number. But the problem is naturally solved when we take into account the increasing site number in the limiting process. In fact, the one-dimensional space of the fermions should have a finite length L. So the total site number $N_s=L/d$ should increase with the decreasing d in the limiting process. The momenta are inversely proportional to the site number and site spacing

$$k_j \propto \frac{2\pi}{N_s d}$$

and

$$k_j d \propto \frac{2\pi}{N_s} = \frac{2\pi d}{L} \to 0, \tag{20}$$

where the space length L is definite constant. Thus we still have the limiting result (19).

Besides L, another important parameter

$$c = U/2td$$

should remain to be constant as $d \to 0$ and the S-matrix (19) becomes the same as the S-matrix (6) of δ-function interacting fermions. So we have

$$\frac{U}{t} = 2cd, \tag{21}$$

which means that U/t is proportional to the decreasing site distance d. Therefore the extra term (17) will vanish with the d and inconsistency arising in the lattice case diminishes and disappears in the limiting process to spatially continuous case.

VI. SU(4) SYMMETRY OF THE SYSTEM

Since we have proven that the BA is exactly valid for all occupancies in the four-component fermions with δ-function interactions, we would like to mention an interesting correspondence between the BA equations and system symmetry and then consider the degeneracy of the eigenstates. The system of the four-component fermions, with the second-quantized Hamiltonian

$$H = -\frac{1}{2}\int dx \sum_a \psi_a^*(x)\frac{\partial^2}{\partial x^2}\psi_a(x) + \frac{c}{2}\int dx \sum_{a\neq a'} n_a(x) n_{a'}(x),$$

where $\psi_a^*(x)$ creates a fermion with internal component a at position x and $n_a(x) = \psi_a^*(x)\psi_a(x)$ is the particle number operator, possesses the SU(4) symmetry

$$\mathrm{SU}(4): \{D_m, \quad E_{aa'} | m = 1,2,3; \;\; a, a' = 1,2,3,4, \;\; a \neq a'\}, \tag{22}$$

where the generators are

$$E_{aa'} = \int dx\, \psi_a^*(x)\psi_{a'}(x),$$

$$D_m = N_m - N_{m+1}, \quad N_m = \int dx \psi_m^*(x)\psi_{m'}(x),$$

and a, m label the inner components. The commutation relations are

$$\begin{aligned} [E_{ss'}, E_{tt'}] &= \delta_{s',t}E_{st'} - \delta_{s,t'}E_{ts'}, \\ [D_m, E_{ss'}] &= (\delta_{m,s} - \delta_{m,s'} - \delta_{m+1,s} + \delta_{m+1,s'})E_{ss'} \end{aligned} \tag{23}$$

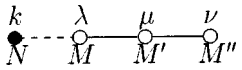
and $\{D_m\}$ forms the commuting Cardan subalgebra of rank 3. As the system is spatially continuous instead of lattice, the symmetry involving pairing creation and annihilation operators as in the simple Hubbard model[17] and spin–orbital case[18,19] does not exist.

The BA equations (7) rewritten as

$$e^{ik_j L} = \prod_{\alpha=1}^{M} \Xi_{1/2}(k_j - \lambda_\alpha),$$

$$
\begin{aligned}
1 &= -\prod_{j=1}^{N} \Xi_{-1/2}(\lambda_\alpha - k_j) \prod_{\alpha'=1}^{M} \Xi_1(\lambda_\alpha - \lambda_{\alpha'}) \prod_{\beta=1}^{M'} \Xi_{-1/2}(\lambda_\alpha - \mu_\beta), \\
1 &= -\prod_{\alpha=1}^{M} \Xi_{-1/2}(\mu_\beta - \lambda_\alpha) \prod_{\beta'=1}^{M'} \Xi_1(\mu_\beta - \mu_{\beta'}) \prod_{\gamma=1}^{M''} \Xi_{-1/2}(\mu_\beta - \nu_\gamma), \\
1 &= -\prod_{\beta=1}^{M'} \Xi_{-1/2}(\nu_\gamma - \mu_\beta) \prod_{\gamma'=1}^{M''} \Xi_{-1/2}(\nu_\gamma - \nu_{\gamma'}),
\end{aligned}
\tag{24}
$$

where $\Xi_n(x) = (x + inc)/(x - inc)$ is easy to remember by means of the Dynkin diagram of A_3 Lie algebra



where the dark dot is added to represent the charge rapidity k_j which takes an angle of 120° relative to the first simple root r_1. The subscripts of $\Xi_n(x)$ in the above form of BA equations correspond, respectively, to the covariant components of the simple roots which are chosen as nonorthogonal basis, $r_1 = (-1/2, 1, -1/2, 0)$, $r_2 = (0, -1/2, 1, -1/2)$, $r_3 = (0, 0, -1/2, 1)$. This connection exists because the system has the above SU(4) symmetry, the generators of which constitute an A_3 Lie algebra. Such a connection was noticed for correlated electrons with twofold orbital degeneracy in SU(4) lattice case[14] and the electrons with spin–exchange interactions in $\mathrm{SU}(2) \times \mathrm{SU}(2)$ case.[20]

The BA eigenstates are the SU(4) highest weight state. Let us assume the highest weight is $w^h = (w_1^h, w_3^h, w_3^h)$ which labels an irreducible representation of the SU(4) group. We obtain the expression

$$
\begin{aligned}
w_1^h &= N_1 - N_2 = N - 2M + M', \\
w_2^h &= N_2 - N_3 = M - 2M' + M'', \\
w_3^h &= N_3 - N_4 = M' - 2M'',
\end{aligned}
\tag{25}
$$

from the Cartan operators and the relations (8) of N_m and M, M', M''. The lower weight states in the SU(4) representation can be obtained by the lowering operators $E_{-\alpha}$ acting on the highest weight state $|w^h\rangle = |\psi_{\mathrm{BA}}\rangle$,

$$
|w^h - \alpha\rangle = E_{-\alpha}|w^h\rangle, \tag{26}
$$

where the lowering operator $E_{-\alpha}$ is a product of the SU(4) generators $E_{ss'}$ which commute with the Hamiltonian. The obtained lower-weight states are also the eigenstates of the system

$$
H|w^h - \alpha\rangle = E_{-\alpha} H|w^h\rangle = E_{-\alpha} E_{\mathrm{BA}}|w^h\rangle = E_{\mathrm{BA}}|w^h - \alpha\rangle \tag{27}
$$

with the same eigenenergy E_{BA} as the BA solution. Therefore the state with energy E_{BA} is degenerate with degeneracy

$$
n_{w^h} = \tfrac{1}{12}(w_1^h + 1)(w_2^h + 1)(w_3^h + 1)(w_1^h + w_2^h + 2)(w_2^h + w_3^h + 2)(w_1^h + w_2^h + w_3^h + 3) \tag{28}
$$

which corresponds to the total weight number and dimension of the SU(4) representation. The only possible nondegenerate case is

$$
w_1^h = w_2^h = w_3^h = 0 \tag{29}
$$

which requires

$$M=\frac{3N}{4},\quad M'=\frac{N}{2},\quad M''=\frac{N}{4},$$

$$N_1=N_2=N_3=N_4=\frac{N}{4}, \tag{30}$$

and the total particle number N should be the integer times 4, i.e., there are an equal number of particles in each state $a=1,2,3,4$. If the condition (30) is not satisfied, all the states will be degenerate including the BA ground state.

VII. BRIEF SUMMERY

In this paper, we have worked out the boundary conditions of three and four particles interacting at the same spatial point for the δ-function interacting SU(4) fermions and shown that they can be solved by the two-particle connection boundary conditions in the BA. Therefore we have explicitly proven the consistence of the BA with the multiparticle scattering boundary conditions and that the BA is valid for all multiple occupancies. Unlike the lattice degenerate Hubbard model, the definition of the BA wave function for the spatially continuous system can be extended to those cases with more than two particles occupying the same positions. We also show that the inconsistence of BA in the degenerate Hubbard model vanishes in the limit of small-site spacing. An interesting correspondence between the BA equations and the system SU(4) symmetry is indicated. The degeneracy is generally given for the state with BA eigenenergy. Singlet exists in the case that there are equal number of particles in each inner component. Our proof for consistence of the BA and the multiparticle scattering is also valid for the δ-function interacting bosons.[2,3] In that case one needs to show the consistency for all the multiple occupancies.

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Results on the Wess–Zumino consistency condition for arbitrary Lie algebras

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The so-called covariant Poincaré lemma on the induced cohomology of the space–time exterior derivative in the cohomology of the gauge part of the BRST differential is extended to cover the case of arbitrary, nonreductive Lie algebras. As a consequence, the general solution of the Wess–Zumino consistency condition with a nontrivial descent can, for arbitrary (super) Lie algebras, be computed in the small algebra of the one-form potentials, the ghosts and their exterior derivatives. For particular Lie algebras that are the semidirect sum of a semisimple Lie subalgebra with an ideal, a theorem by Hochschild and Serre is used to characterize more precisely the cohomology of the gauge part of the BRST differential in the small algebra. In the case of an Abelian ideal, this leads to a complete solution of the Wess–Zumino consistency condition in this space. As an application, the consistent deformations of $2+1$ dimensional Chern–Simons theory based on $iso(2,1)$ are rediscussed. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The algebraic problem that is central for the renormalization of Yang–Mills theory is the computation of $H^{0,n}(s|d)$ and $H^{1,n}(s|d)$, the cohomology of the BRST differential modulo the exterior space–time differential d in ghost number 0 and 1 in the space of fields, external sources (called antifields below) and their derivatives[1] (see also, e.g., Refs. 2–4 for reviews).

So far, local BRST cohomology groups for Yang–Mills and Chern–Simons theories have been investigated exclusively in the context of reductive Lie algebras, i.e., Lie algebras that are the direct sum of a semisimple and Abelian factors. In this case, the invariant metric used in the construction of the actions is necessarily the Killing metric for the semisimple factor (up to an overall constant), complemented by an arbitrary metric for the Abelian factors. Recently, there has been a lot of interest in nonreductive Lie algebras that nevertheless possess an invariant metric,[5] as it is then still possible to construct Wess–Zumino–Witten models and Chern–Simons and Yang–Mills theories (see Ref. 6 and references therein). In particular, the associated Yang–Mills theories have remarkable renormalization properties. This motivates the study of the local BRST cohomology groups for such theories.

An important intermediate step in this study is the computation of the local BRST cohomology $H(\gamma|d)$ of the gauge part γ of the BRST differential in the algebra $\mathcal{A}$ generated by the space–time forms, the gauge potentials, ghosts and a finite number of their derivatives. This computation in turn relies crucially on the so-called covariant Poincaré lemma.[7–9] In the reductive case, the covariant Poincaré lemma states that the cohomology $H(d,H(\gamma,\mathcal{A}))$ is generated by the invariant polynomials in the curvature two-forms F^a and invariant polynomials in the ghosts C^a. The proof of this lemma uses the fact that for reductive Lie algebras, the (Chevalley–Eilenberg) Lie algebra cohomology[10] with coefficients in a finite dimensional module V is isomorphic to the

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tensor product of the invariant subspace of the module (Whitehead's theorem) and the Lie algebra cohomology with coefficients in $\mathbb{R}$, which is itself generated by the primitive elements (see, e.g., Ref. 11 and 12 and also Ref. 13). The consequence for the computation of $H(\gamma|d)$ is that all the solutions of the Wess–Zumino consistency condition[14] with a nontrivial descent can be computed in the small algebra $\mathcal{B}$ generated by the one-form potentials, the ghosts and their exterior derivatives, thus providing an a posteriori justification of the assumptions of Refs. 15–18 (see also Refs. 19–22 for related considerations).

The central result of the present article is the generalization of the covariant Poincaré lemma to arbitrary Lie algebras for which the Lie algebra cohomology is not necessarily explicitly known. In order to do so, we will use a standard decomposition according to the homogeneity in the fields. From the proof, it will also be obvious that the result extends to the case of super/graded Lie algebras.

For particular Lie algebras $\mathcal{G}$ that admit an ideal $\mathcal{J}$ such that the quotient $\mathcal{G}/\mathcal{J}$ is semisimple, we use a theorem by Hochschild and Serre[23] that states that the Lie algebra cohomology of $\mathcal{G}$ with coefficients in V reduces to the tensor product of the Lie algebra cohomology of the semisimple factor $\mathcal{G}/\mathcal{J}$ with coefficients $\mathbb{R}$ and the invariant cohomology of the ideal $\mathcal{J}$ with coefficients in V. As this result is not as widely known as the standard results on reductive Lie algebra cohomology, we will rederive it using ''ghost'' language, i.e., by writing the cochains with coefficients in V as polynomials in the Grassmann odd generators C^a with coefficients in V and by writing the Chevalley–Eilenberg differential as a first order differential operator acting in this space. As a direct application, we explicitly compute $H(\gamma,\mathcal{B})$ for the three dimensional Euclidian and Poincaré algebras $iso(3)$ and $iso(2,1)$.

In the case where the ideal $\mathcal{J}$ is abelian, this leads to a complete characterization of $H(\gamma|d,\mathcal{B})$, allowing us in particular to give exhaustive results for $iso(3)$ and $iso(2,1)$. The covariant Poincaré lemma allows us to extend these results to $H(\gamma|d,\mathcal{A})$.

Finally, we explicitly rediscuss the local BRST cohomology, and more particularly the consistent deformations, of $iso(2,1)$ Chern–Simons theory, whose physical relevance is due to its relation with $2+1$ dimensional gravity.[24,25]

II. GENERALITIES AND CONVENTIONS

We take space–time to be n-dimensional Minkowski space with $n \geqslant 3$ and $\mathcal{A}$ to be either the algebra of form valued polynomials or the algebra of form valued formal power series in the potentials A^a_μ, the ghosts C^a (collectively denoted by ϕ^i) and their derivatives. The algebra $\mathcal{A}$ can be decomposed into subspaces of definite ghost number g, by assigning ghost number 1 to the ghosts and their derivatives and ghost number zero to x^μ, dx^μ, the gauge potentials and their derivatives. Let $\mathcal{B}$ be either the algebra of polynomials or of formal power series generated by A^a, C^a, dA^a, dC^a, with $d = dx^\mu \partial_\mu$ and ∂_μ denoting the total derivative. Let f^c_{ab} be the structure constants of a Lie algebra $\mathcal{G}$. The action of the gauge part γ of the BRST differential is defined by

$$\gamma A^a_\mu = \partial_\mu C^a + f^a_{bc} A^b_\mu C^c, \gamma C^a = -\tfrac{1}{2} f^a_{bc} C^b C^c, \tag{2.1}$$

$$\gamma x^\mu = \gamma dx^\mu = 0, [\gamma, \partial_\mu] = \{\gamma, d\} = 0. \tag{2.2}$$

Let $F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + f^a_{bc} A^b_\mu A^c_\nu$ so that $\gamma F^a_{\mu\nu} = f^a_{bc} F^b_{\mu\nu} C^c$. In $\mathcal{B}$, the action of γ reads

$$\gamma A^a = -DC^a, \tag{2.3}$$

$$\gamma C^a = -\tfrac{1}{2}[C,C]^a. \tag{2.4}$$

The field strength two-form $F^a = dA^a + \frac{1}{2}[A,A]^a$ satisfies

$$\gamma F^a=[F,C]^a,\quad DF^a=0, \tag{2.5}$$

with $D=d+[A,\cdot]$.

In the following, the algebra $\mathcal{E}$ stands for either $\mathcal{A}$ or $\mathcal{B}$. Under the above assumptions, the cohomology of d is known to be trivial in $\mathcal{E}$.[7,26–35] More precisely, in form degree 0, the cohomology of d is exhausted by the constants, and in particular it is trivial in strictly positive ghost numbers. It is also trivial in form degrees $0<p<n$.

A standard technique for computing $H(\gamma|d,\mathcal{E})$ is to use so-called descent equations. As a consequence of the acyclicity of the exterior differential d, the cocyle condition $\gamma\omega^p+d\omega^{p-1}=0$ implies that $\gamma\omega^{p-1}+d\omega^{p-2}=0$. Iterating the descent, there necessarily exists an equation which reads $\gamma\omega^{p-l}=0$ because the form degree cannot be lower than zero. One then tries to compute $H(\gamma|d,\mathcal{E})$ by starting from the last equation. The systematics of this strategy can be captured by the exact couple

$$\mathcal{C}=\langle H(\gamma|d,\mathcal{E}),H(\gamma,\mathcal{E}),\mathcal{D},l^{\#},i^{\#}\rangle, \tag{2.6}$$

$$\begin{array}{ccc} H(\gamma|d,\mathcal{E}) & \overset{\mathcal{D}}{\longrightarrow} & H(\gamma|d,\mathcal{E}) \\ & {\scriptstyle i^{\#}}\nwarrow \quad \swarrow{\scriptstyle l^{\#}} & \\ & H(\gamma,\mathcal{E}) & \end{array} \tag{2.7}$$

and the associated spectral sequence[16] (see also Refs. 36 and 37 for reviews). The various maps are defined as follows: $i^{\#}$ is the map which consists in regarding an element of $H(\gamma,\mathcal{E})$ as an element of $H(\gamma|d,\mathcal{E})$, $i^{\#}:H(\gamma,\mathcal{E})\to H(\gamma|d,\mathcal{E})$, with $i^{\#}[\omega]=[\omega]$. It is well defined because every γ cocycle is a γ cocycle modulo d and every γ coboundary is a γ coboundary modulo d. The descent homomorphism $\mathcal{D}:H^{k,l}(\gamma|d,\mathcal{E})\to H^{k+1,l-1}(\gamma|d,\mathcal{E})$ with $\mathcal{D}[\omega]=[\omega']$, if $\gamma\omega+d\omega'=0$ is well defined because of the triviality of the cohomology of d in form degree $p\leqslant n-1$ (and ghost number $\geqslant 1$). Finally, the map $l^{\#}:H^{k+1,l-1}(\gamma|d,\mathcal{E})\to H^{k+1,l}(\gamma,\mathcal{E})$ is defined by $l^{\#}[\omega]=[d\omega]$. It is well defined because the relation $\{\gamma,d\}=0$ implies that it maps cocycles to cocycles and coboundaries to coboundaries. The differential associated to the exact triangle is $d^{\#}=l^{\#}\circ i^{\#}$.

The exactness of the couple (2.7) implies that

$$H(\gamma,\mathcal{E})\simeq H(d^{\#},H(\gamma,\mathcal{E}))\oplus d^{\#}\mathcal{N}_{\mathcal{E}}\oplus\mathcal{N}_{\mathcal{E}}, \tag{2.8}$$

$$H(\gamma|d,\mathcal{E}))=i^{\#}H(\gamma,\mathcal{E})\oplus\mathcal{D}^{-1}\mathcal{D}H(\gamma|d,\mathcal{E}), \tag{2.9}$$

where $\mathcal{N}_{\mathcal{E}}$ is the subspace of $H(\gamma,\mathcal{E}))$ which cannot be lifted, i.e., $[c]\in\mathcal{N}_{\mathcal{E}}$ if $\gamma c=0$ with $dc+\gamma\omega=0\Rightarrow c=\gamma\omega'$.

In the following, $\omega,a,A\in\mathcal{A}$ and $\varpi,b,B\in\mathcal{B}$.

III. THE FIRST LIFT IN THE SMALL ALGEBRA

In $\mathcal{B}$, the change of generators from A^a,dA^a,C^a,dC^a to $A^a,F^a,C^a,-DC^a$ allows us to isolate the contractible pairs $A^a,-DC^a$ and the cohomology of γ can be computed in the polynomial algebra generated by F^a,C^a. In other words, $\gamma b=0\Leftrightarrow b=P(F,C)+\gamma b'$ with $\gamma P(F,C)=0$, while $P(F,C)=\gamma b'\Rightarrow P(F,C)=\gamma P'(F,C)$. Let us first prove the following lemma:

Lemma 1: Every element of $H(\gamma,\mathcal{B})$ can be lifted at least once and, furthermore, no element of $H(\gamma,\mathcal{B})$ is an obstruction to a lift of an element of $H(\gamma,\mathcal{B})$:

$$H^p(d^{\#},H(\gamma,\mathcal{B}))\simeq H^p(\gamma,\mathcal{B}),\quad \text{for } 0\leqslant p\leqslant n, \tag{3.1}$$

i.e.,

$$\gamma b^p = 0 \Rightarrow d b^p + \gamma \varpi = 0, \tag{3.2}$$

together with

$$\left.\begin{array}{c} b^p = d\bar{b} + \gamma b', \\ \gamma \bar{b} = 0 \end{array}\right\} \Rightarrow b^p = \gamma \varpi'. \tag{3.3}$$

Proof: In terms of the new generators, we have

$$\gamma = -DC^a \frac{\partial}{\partial A^a} + [F,C]^a \frac{\partial}{\partial F^a} - \frac{1}{2}[C,C]^a \frac{\partial}{\partial C^a}, \tag{3.4}$$

$$d = \left(F - \frac{1}{2}[A,A]\right)^a \frac{\partial}{\partial A^a} - [A,F]^a \frac{\partial}{\partial F^a} + (DC - [A,C])^a \frac{\partial}{\partial C^a} + ([F,C] - [A,DC])^a \frac{\partial}{\partial DC^a}. \tag{3.5}$$

Let us introduce the operator[7,38]

$$\lambda = A^a \frac{\partial}{\partial C^a} - \left(F^a - \frac{1}{2}[A,A]^a\right) \frac{\partial}{\partial DC^a}. \tag{3.6}$$

We get

$$d = [\lambda, \gamma]. \tag{3.7}$$

It follows that

$$db + \gamma \lambda b = 0, \tag{3.8}$$

if $\gamma b = 0$. Furthermore, if $b = d\bar{b} + \gamma \varpi$ with $\gamma \bar{b} = 0$, we get $b = \gamma(\varpi - \lambda \bar{b})$.

If $\gamma b = 0$, we also get

$$d\lambda b + \gamma \tfrac{1}{2} \lambda^2 b = \tau b, \tag{3.9}$$

with

$$\tau = \frac{1}{2}[d,\lambda] = F^a \frac{\partial}{\partial C^a}, \tag{3.10}$$

$$\tau^2 = 0, \ \{\tau, \gamma\} = 0. \tag{3.11}$$

It follows that the potential obstructions to lifts of elements of $H(\gamma,\mathcal{B})$ are controlled by the differential τ.

IV. COVARIANT POINCARÉ LEMMA FOR GENERIC (SUPER)-LIE ALGEBRAS

A. Formulation

Theorem 1 (Covariant Poincaré lemma): *The following isomorphism holds:*

$$H^p(d^{\#}, H(\gamma,\mathcal{A})) \simeq H^p(\gamma,\mathcal{B}), \ \ 0 \leqslant p < n. \tag{4.1}$$

Explicitly, this means that

$$\left.\begin{array}{c} \gamma a^p = 0, \\ d a^p + \gamma \omega = 0, \ \ 0 \leqslant p < n \end{array}\right\} \Leftrightarrow \left\{\begin{array}{c} a^p = b^p + d a'^p + \gamma \omega', \\ \gamma b^p = 0 = \gamma a'^p, \end{array}\right. \tag{4.2}$$

together with

$$\left.\begin{array}{c} b^p + da'^p + \gamma\omega' = 0, \\ \gamma b^p = 0 = \gamma a'^p, \quad 0 \leqslant p < n \end{array}\right\} \Rightarrow b^p = \gamma\varpi. \tag{4.3}$$

In fact, we will prove that (4.3) also holds in form degree $p=n$.

B. Associated structure of $\mathcal{D}H(\gamma|d,\mathcal{A})$

As a direct consequence of the covariant Poincaré lemma, the descent homomorphism in $\mathcal{A}$ reduces to that in $\mathcal{B}$.

Corollary 1: The isomorphism (4.1) *implies*

$$(\mathcal{D}H)^p(\gamma|d,\mathcal{A}) \simeq (\mathcal{D}H)^p(\gamma|d,\mathcal{B}), \quad 0 \leqslant p < n. \tag{4.4}$$

More precisely, (4.1) *for* $0 \leqslant p \leqslant m (< n)$ *implies* (4.4) *for* $0 \leqslant p \leqslant m (< n)$.

This last isomorphism is equivalent to

$$\left.\begin{array}{c} \gamma A^p + dA'^{p-1} = 0, \\ dA^p + \gamma\omega = 0, \quad 0 \leqslant p < n, \end{array}\right\} \Leftrightarrow \left\{\begin{array}{c} A^p = B^p + \gamma\omega' + d\omega'', \\ \gamma B^p + dB'^{p-1} = 0, \\ dB^p + \gamma B'' = 0, \end{array}\right. \tag{4.5}$$

together with

$$\left.\begin{array}{c} B^p + \gamma\omega' + d\omega'' = 0, \\ dB^p + \gamma B'' = 0, \quad 0 \leqslant p < n, \end{array}\right\} \Rightarrow B^p = \gamma\varpi + d\varpi'. \tag{4.6}$$

Proof: That the condition (4.5) is necessary ($\Leftarrow$) follows directly from the properties of γ cocycles in the small algebra proved in Sec. III and the fact that d and γ anticommute.

The proof that the condition (4.5) is also sufficient, and the proof of (4.6) proceeds by induction on the form degree. In form degree 0, (4.5) and (4.6) hold, because (4.5) coincides with (4.2), while (4.6) coincides with (4.3). Suppose (4.5) and (4.6) hold in form degree $0 \leqslant p \leqslant m-1$.

For (4.5), it follows by induction that $A'^{m-1} = B'^{m-1} + \gamma\omega'' + d(\ )$. This implies $\gamma(A^m - d\omega'') + dB'^{m-1} = 0$. This gives $dB'^{m-1} + \gamma\overline{B}^m = 0$ and then $A^m = B^m + \overline{a}^m + d\omega''$ with $\gamma\overline{a}^m = 0$. The assumption on A^m implies that $d\overline{B}^m + d\overline{a}^m + \gamma\omega = 0$. From (4.3), we then deduce that $d\overline{B}^m + \gamma\overline{B}'' = 0$, and also that $d\overline{a}^m + \gamma(\omega - \overline{B}'') = 0$. Using (4.2), we get $\overline{a}^m = b^m + da' + \gamma(\ )$. Hence, because of (3.2), the right hand side (4.5) holds with $B^m = \overline{B}^m + b^m$.

For (4.6), we note that the assumptions imply that $\gamma B^m + dB'^{m-1} = 0$. Furthermore, $d(B'^{m-1} + \gamma\omega'') = 0$, so that $B'^{m-1} + \gamma\omega'' + d(\ ) = 0$. By induction, this means that $B'^{m-1} = \gamma\varpi' + d\varpi''$. This implies that $\gamma(B^m - d\varpi') = 0$ so that $B^m = d\varpi' + b^m$. The assumption that B^m can be lifted in the small algebra then gives $db^m = -\gamma B''$. Using (3.3), this implies that $b^m = \gamma\varpi$ so that the r.h.s. of (4.6) holds in form degree m.

C. Associated structure of $H(\gamma,\mathcal{A})$ and $H(\gamma|d,\mathcal{A})$

Taking (4.1) into account, the decomposition (2.8) for $\mathcal{E}=\mathcal{A}$ becomes

$$H^p(\gamma,\mathcal{A}) \simeq H^p(\gamma,\mathcal{B}) \oplus d^{\#}\mathcal{N}_{\mathcal{A}}^{p-1} \oplus \mathcal{N}_{\mathcal{A}}^{p}, \quad 0 \leqslant p < n, \tag{4.7}$$

$$H^n(\gamma,\mathcal{A}) \simeq \mathcal{F}^n \oplus d^{\#}\mathcal{N}_{\mathcal{A}}^{n-1}, \tag{4.8}$$

with $\mathcal{F}^n \simeq H^n(\gamma,\mathcal{A})/d^{\#}\mathcal{N}_{\mathcal{A}}^{n-1}$. This is equivalent to

$$\gamma a^p = 0,\ \ 0 \leqslant p < n \Leftrightarrow \begin{cases} a^p = b^p + d\tilde{a}^{p-1} + \tilde{a}'^p + \gamma\omega, \\ \gamma b^p = 0 = \gamma\tilde{a}^{p-1} = \gamma\tilde{a}'^p, \end{cases} \tag{4.9}$$

together with

$$\left.\begin{matrix} b^p + d\tilde{a}^{p-1} + \tilde{a}'^p + \gamma\omega = 0,\ \ 0 \leqslant p < n, \\ \gamma b^p = 0 = \gamma\tilde{a}^{p-1} = \gamma\tilde{a}'^p \end{matrix}\right\} \Rightarrow \begin{cases} b^p = \gamma\varpi, \\ \tilde{a}^{p-1} = \gamma\omega', \\ \tilde{a}'^p = \gamma\omega'', \end{cases} \tag{4.10}$$

in form degrees $0 \leqslant p < n$ and to

$$\gamma a^n = 0 \Leftrightarrow \begin{cases} a^n = \hat{a}^n + d\tilde{a}^{n-1} + \gamma\omega, \\ \gamma\hat{a}^n = 0 = \gamma\tilde{a}^{n-1}, \end{cases} \tag{4.11}$$

together with

$$\left.\begin{matrix} \hat{a}^n + d\tilde{a}^{n-1} + \gamma\omega = 0, \\ \gamma\hat{a}^n = 0 = \gamma\tilde{a}^{n-1} \end{matrix}\right\} \Rightarrow \begin{cases} \hat{a}^n = \gamma\omega, \\ \tilde{a}^{n-1} = \gamma\omega', \end{cases} \tag{4.12}$$

in form degree n.

Finally, using (4.7) and (4.4), the decomposition (2.9) for $\mathcal{E} = \mathcal{A}$ becomes

$$H^p(\gamma|d,\mathcal{A}) \simeq i^{\#}H^p(\gamma,\mathcal{B}) \oplus \mathcal{N}^p_{\mathcal{A}} \oplus \mathcal{D}^{-1}(\mathcal{D}H)^{p-1}(\gamma|d,\mathcal{B}), 0 \leqslant p < n. \tag{4.13}$$

$$H^n(\gamma|d,\mathcal{A}) \simeq \mathcal{F}^n \oplus \mathcal{D}^{-1}(\mathcal{D}H)^{n-1}(\gamma|d,\mathcal{B}), \tag{4.14}$$

which is equivalent to

$$\gamma A^p + dA'^p = 0,\ \ 0 \leqslant p < n \Leftrightarrow \begin{cases} A^p = \tilde{a}^p + b^p + B^p + \gamma\omega + d\omega', \\ \gamma\tilde{a}^p = 0 = \gamma b^p = \gamma B^p + dB'^{p-1}, \\ d\tilde{a}^p + \gamma\omega'' = 0 \Rightarrow \tilde{a}^p = \gamma\omega''', \\ B'^{p-1} = \gamma\varpi + d\varpi' \Rightarrow B^p = \gamma\varpi'' + d\varpi, \end{cases} \tag{4.15}$$

together with

$$\left.\begin{matrix} \tilde{a}^p + b^p + B^p + \gamma\omega + d\omega' = 0,\ \ 0 \leqslant p < n \\ \gamma\tilde{a}^p = 0 = \gamma b^p = \gamma B^p + dB'^{p-1}, \\ d\tilde{a}^p + \gamma\omega'' = 0 \Rightarrow \tilde{a}^p = \gamma\omega''', \\ B'^{p-1} = \gamma\varpi + d\varpi' \Rightarrow B^p = \gamma\varpi'' + d\varpi \end{matrix}\right\} \Rightarrow \begin{cases} \tilde{a}^p = \gamma\omega^4, \\ b^p = dB''^{p-1} + \gamma\varpi''', \\ B^p = \gamma\varpi''' + d\varpi^4, \end{cases} \tag{4.16}$$

in form degrees $0 \leqslant p < n$, and

$$\gamma A^n + dA'^{n-1} = 0 \Leftrightarrow \begin{cases} A^n = \hat{a}^n + B^n + \gamma\omega + d\omega', \\ \gamma\hat{a}^n = 0 = \gamma B^n + dB'^{n-1}, \\ \left.\begin{matrix} \hat{a}^n + d\tilde{a}^{n-1} + \gamma\omega'' = 0, \\ \gamma\tilde{a}^{n-1} = 0, \end{matrix}\right\} \Rightarrow \begin{cases} \hat{a}^n = \gamma\omega''', \\ \tilde{a}^{n-1} = \gamma\omega^4, \end{cases} \\ B'^{n-1} = \gamma\varpi + d\varpi' \Rightarrow B^n = \gamma\varpi'' + d\varpi, \end{cases} \tag{4.17}$$

together with

$$\left.\begin{matrix} \hat{a}^n + B^n + \gamma\omega + d\omega' = 0, \\ \gamma\hat{a}^n = 0 = \gamma B^n + dB'^{n-1}, \\ B'^{n-1} = \gamma\varpi + d\varpi' \Rightarrow B^n = \gamma\varpi'' + d\varpi \end{matrix}\right\} \Rightarrow \begin{cases} \hat{a}^n = dB''^{n-1} + \gamma\omega''', \\ \gamma B''^{n-1} + dB'''^{p-2} = 0, \\ B^n = \gamma\varpi''' + d\varpi^4, \end{cases} \tag{4.18}$$

in form degree n.

D. Proof of theorem 1

That the condition (4.2) is necessary ($\Leftarrow$) is again direct.

1. Decomposition according to homogeneity and change of variables

If one decomposes the space of polynomials or formal power series into monomials of definite homogeneity, the differential γ splits accordingly into a piece that does not change the homogeneity and a piece that increases the homogeneity by one, $\gamma=\gamma_0+\gamma_1$. Consider the change of variables from A_μ, C^a and their derivatives to

$$y^\alpha \equiv \partial_{(\mu_k}\cdots\partial_{\mu_2}A^a_{\mu_1)}, \tag{4.19}$$

$$z^\alpha \equiv \partial_{\mu_k}\cdots\partial_{\mu_1}C^a, \tag{4.20}$$

$$C^a, F^{0a}_\Delta \equiv \partial_{(\mu_{k-1}}\cdots\partial_{\mu_3}F^{0a}_{\mu_2)\mu_1}, \tag{4.21}$$

with $F^{0a}_{\mu\nu}=\partial_\mu A^a_\nu-\partial_\nu A^a_\mu$. In the new variables,

$$\gamma_0 = z^\alpha\frac{\partial}{\partial y^\alpha}. \tag{4.22}$$

This implies that

$$a(y^\alpha,z^\alpha,F^{0a}_\Delta,C^a)=a(0,0,F^{0a}_\Delta,C^a)+\{\gamma_0,\rho\}a, \tag{4.23}$$

$$\rho\cdot=\int_0^1\frac{dt}{t}\left[y^\alpha\frac{\partial}{\partial z^\alpha}\cdot\right](ty^\alpha,tz^\alpha,F^{0a}_\Delta,C^a). \tag{4.24}$$

Suppose that $\gamma_0 a=0$. It follows that

$$\gamma_0 a=0\Leftrightarrow a=I+\gamma_0\omega, \tag{4.25}$$

for some form valued polynomials $I(x^\mu,dx^\mu,F^{0a}_\Delta,C^a)$. Furthermore,

$$I+\gamma_0\omega=0\Rightarrow I=0. \tag{4.26}$$

2. Properties of γ_1 and γ_0

Let $\mathcal{I}^0$ be the algebra of form valued polynomials or formal power series that do not depend on y^α,z^α, but only on C^a,F^{0a}_Δ, with elements denoted below by I,J and $\mathcal{P}^0$ be the algebra of polynomials or formal power series that depend only on F^{0a},C^a, with elements denoted by P,Q. Polynomials which depend only on the ghosts are denoted by R.

Let us introduce the operator

$$\sigma=\gamma_1-C^a\delta_a, \tag{4.27}$$

where δ_a denotes the representation under which the object transforms. We have

$$\sigma A^a_\mu=0,\ \ \sigma C^a=\tfrac{1}{2}[C,C]^a,\ \ \sigma^2=0,\ \ [\sigma,\partial_\mu]=[\partial_\mu C,\cdot],\ \ \{\sigma,\gamma_0\}=0. \tag{4.28}$$

The point about σ is that when it acts on any expression that depends only on A^a_μ and its derivatives, the result does not involve undifferentiated ghosts. More precisely, $(\sigma f[A^a_\mu])|_{z=0}=0$. We have $\gamma_0\sigma\partial_{\nu_k}\cdots\partial_{\nu_2}F^{0a}_{\nu_1\mu}=0$. It follows that

$$\sigma\partial_{\nu_k}\cdots\partial_{\nu_2}F^{0a}_{\nu_1\mu}=\gamma_0\rho\sigma\partial_{\nu_k}\cdots\partial_{\nu_2}F^{0a}_{\nu_1\mu}. \tag{4.29}$$

Symmetrizing over the ν indices, one gets

$$\sigma F^{0a}_{\Delta} = \gamma_0(\rho\sigma) F^{0a}_{\Delta}. \tag{4.30}$$

3. The differential γ^R

For later use, let us also establish that if

$$\gamma^R J = -[C, F^0_{\Delta}]^a \frac{\partial J}{\partial F^{0a}_{\Delta}} - \frac{1}{2}[C,C]^a \frac{\partial J}{\partial C^a}, \tag{4.31}$$

and

$$v = (\rho\sigma F^{0a}_{\Delta}) \frac{\partial}{\partial F^{0a}_{\Delta}}, \tag{4.32}$$

then

$$\gamma_1 J = \gamma_0(vJ) + \gamma^R J. \tag{4.33}$$

Lemma 2:

$$H(\gamma_1, H(\gamma_0)) \simeq H(\gamma^R, \mathcal{I}^0). \tag{4.34}$$

Proof: The lemma means that

$$\left.\begin{array}{c} \gamma_0 a = 0, \\ \gamma_1 a + \gamma_0 b = 0, \end{array}\right\} \Leftrightarrow \left\{\begin{array}{c} a = J + \gamma_0(\ ), \\ \gamma^R J = 0, \end{array}\right. \tag{4.35}$$

and

$$\left.\begin{array}{c} J = \gamma_1 a' + \gamma_0(\ ), \\ \gamma_0 a' = 0, \end{array}\right\} \Rightarrow J = \gamma^R J'. \tag{4.36}$$

Indeed, the result follows directly from (4.33).

Suppose now that the decomposition of the space of polynomials or of formal power series into monomials of homogeneity M has been made (see the Appendix for notations and more details). Then one has the following:

Lemma 3:

$$H(\gamma, \mathcal{A}) \simeq \oplus_{M \geqslant 0} H_M(\gamma^R, \mathcal{I}^0), \tag{4.37}$$

$$H(\gamma, \mathcal{B}) \simeq \oplus_{M \geqslant 0} H_M(\gamma^R, \mathcal{P}^0). \tag{4.38}$$

Proof: Let us first show that every element $[I_M] \in H(\gamma^R, \mathcal{I}^0)$ can be completed to a γ cocycle. Indeed, let us denote by I^M the expression obtained by replacing in I_M the variables F^{0a}_{Δ} by their non-Abelian counterparts,

$$F^a_{\Delta} \equiv D_{(\mu_{k-1}} \cdots D_{\mu_3} F^a_{\mu_2)\mu_1}, \tag{4.39}$$

where $F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + f^a_{bc} A^b_\mu A^c_\nu$, and $D_\mu = \partial_\mu + A^b_\mu \delta_b$ and the covariant derivatives of $F^a_{\mu\nu}$ transform in the coadjoint representation. Hence, $I^M = I_M|$ where the vertical bar denotes the operation of substitution. Because $\gamma F^a_{\Delta} = -[C, F_{\Delta}]^a$, it follows that

$$\gamma I^M = (\gamma^R I_M)| = 0. \tag{4.40}$$

Similarily,

$$(\gamma^R J_M)| = \gamma J^M. \tag{4.41}$$

Note that if $I_M, J_M \in \mathcal{P}^0$, then $I^M \equiv b^M \in \mathcal{B}$ and $J^M \equiv \varpi^M \in \mathcal{B}$.

Suppose $\gamma a^M = 0$. The equations in homogeneity M and $M+1$ imply that a_M is a cocycle of $H(\gamma_1, H(\gamma_0))$. According to the previous lemma, $a_M = I_M + \gamma_0 \eta_M$ where I_M is a cocycle of $H(\gamma^R, \mathcal{I}^0)$.

Suppose that $a^M = \gamma \omega^{M-B}$. In particular, to orders $\leqslant M$, we have

$$\begin{aligned} a_M = \gamma_0 \omega_M \quad &+ \quad \gamma_1 \omega_{M-1}, \\ \gamma_0 \omega_{M-1} \quad &+ \quad \gamma_1 \omega_{M-2} = 0, \\ &\vdots \\ \gamma_0 \omega_{M-B+1} \quad &+ \quad \gamma_1 \omega_{M-B} = 0, \\ \gamma_0 \omega_{M-B} = 0. & \end{aligned} \tag{4.42}$$

If $B > 1$, the equations for ω_{M-B} imply that $\omega_{M-B} = J_{M-B} + \gamma_0 \eta_{M-B}$ with $\gamma^R J_{M-B} = 0$. The redefinition $\omega^{M-B} \to \omega^{M-B} - \gamma \eta_{M-B}$, which does not affect a^M allows to absorb η_{M-B}. One can then replace ω^{M-B} by $\omega^{M-B+1} = \omega^{M-B} - J^{M-B}$, without affecting a^M. This can be done until $B = 1$, where one finds $I_M = \gamma^R J_{M-1}$. This proves that the map $[a^M] \in H(\gamma) \mapsto [I_M] \in H(\gamma^R, \mathcal{I}^0)$ is well defined. The map is surjective because as shown above, every γ^R cocycle I_M can be extended to a γ cocycle I^M. It is also injective, because as also shown above, if $I_M = \gamma^R J_{M-1}$, then $I^M = \gamma J^{M-1}$, so that $a^M - \gamma(J^{M-1} - \eta_M) = a^{M+1}$ starts at homogeneity $M+1$.

4. $H(\gamma)$ and split of variables adapted to the non-Abelian differential γ

If one is not interested in proving the covariant Poincaré lemma, one can avoid the detour of using the split of variables adapted to the Abelian differential γ_0 given in (4.19)–(4.21) for the characterization of $H(\gamma)$. One can use instead directly the variables

$$Y^\alpha \equiv \partial_{(\mu_k} \cdots \partial_{\mu_2} A^a_{\mu_1)}, \tag{4.43}$$

$$Z^\alpha \equiv \partial_{(\mu_k} \cdots \partial_{\mu_2} D_{\mu_1)} C^a, \tag{4.44}$$

$$C^a, F^a_\Delta \equiv D_{(\mu_{k-1}} \cdots D_{\mu_3} F^a_{\mu_2)\mu_1}, \tag{4.45}$$

with $F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + f^a_{bc} A^b_\mu A^c_\nu$ adapted to the non-Abelian differential γ, which reads

$$\gamma = Z^\alpha \frac{\partial}{\partial Y^\alpha} + \gamma^S, \tag{4.46}$$

$$\gamma^S = C^a \delta_a - \frac{1}{2}[C,C]^a \frac{\partial}{\partial C^a}, \tag{4.47}$$

$$\delta_a = -f^c_{ab} F^b_\Delta \frac{\partial}{\partial F^c_\Delta}. \tag{4.48}$$

The usual argument then shows that $H(\gamma, \mathcal{A})$ and $H(\gamma, \mathcal{B})$ are isomorphic to $H(\gamma^S, \mathcal{I})$, respectively $H(\gamma^S, \mathcal{P})$, where $\mathcal{I}$ is the algebra of form valued polynomials or formal power series that do not depend on Y^α, Z^α, but only on C^a, F^a_Δ, and $\mathcal{P}$ is the algebra of polynomials or formal power series that depend only on F^a, C^a.

5. Exterior derivative and contracting homotopy for the gauge potentials

Let us introduce the total derivative that does not act on the ghosts,

$$\overline{\partial}_\mu = \partial_\mu - \partial_{(\nu)\mu} C^a \frac{\partial}{\partial \partial_{(\nu)} C^a}, \tag{4.49}$$

and also the associated exterior derivative and contracting homotopy,[39]

$$\overline{d} = dx^\mu \overline{\partial}_\mu, \tag{4.50}$$

$$\overline{\rho}\omega^p = \int_0^1 dt \frac{|\lambda|+1}{n-p+|\lambda|+1} \overline{\partial}_{(\lambda)} \left(A^a_\mu \left[\frac{\overline{\delta}}{\delta \partial_{(\lambda)\nu} A^a_\mu} \frac{\partial \omega^p}{\partial dx^\nu} \right] [x, dx, C, tA] \right), \tag{4.51}$$

$$\omega^p[x,dx,C,A] = \omega^p[x,dx,C,0] + \{\overline{\rho}, \overline{d}\}\omega^p, 0 \leqslant p < n, \tag{4.52}$$

where $\overline{\delta}/\delta \partial_{(\lambda)\nu} A^a_\mu$ are the higher order Euler operators with respect to the dependence on A^a_μ only (see Ref. 40, Appendix A for conventions). In the old variables A^a_μ, C^a and their derivatives, consider the split

$$\gamma_1 = \gamma^R + \gamma^{\partial C}, \gamma^R = [\partial_{(\nu)} A_\mu, C]^a \frac{\partial}{\partial \partial_{(\nu)} A^a_\mu} - \frac{1}{2}[C,C]^a \frac{\partial}{\partial C^a}. \tag{4.53}$$

This is consistent with (4.31) when acting on functions that depend only on F^{0a}_Δ, C^a. We have

$$\{\gamma^R, \overline{d}\} = 0 = \{\gamma^R, \overline{\rho}\} = 0. \tag{4.54}$$

The first relation is obvious, while the second follows from the fact that γ^R just rotates all the A^a_μ and their derivatives in the internal space without changing the derivatives, while $\overline{\rho}$ only involves the various derivatives and does not act in the internal space. It can be proved directly using the explicit expression (4.51) for $\overline{\rho}$.

6. Core of the proof

Lemma 4:

$$\left.\begin{array}{c} \gamma a^M = 0, \\ d a^M + \gamma \omega^{M-B} = 0, \end{array}\right\} \Rightarrow \left\{\begin{array}{c} \gamma^R I_M = 0, \\ \overline{d} I_M + \gamma^R J_{M-1} = 0. \end{array}\right. \tag{4.55}$$

Proof: In (4.55), one can assume without loss of generality that $B=1$. This can be shown in the same way as in the corresponding part of the proof of Lemma 3. We then have $a_M = I_M + \gamma_0 \eta_M$ with $\gamma^R I_M = 0$, and $\omega_{M-1} = J_{M-1}$, with $\gamma^R J_{M-1} = 0$. To order M, the l.h.s. of (4.55) then gives the r.h.s. of (4.55).

Lemma 5: In form degree $<n$,

$$\left.\begin{array}{c} \gamma^R I_M = 0, \\ \overline{d} I_M + \gamma^R J_{M-1} = 0, \end{array}\right\} \Leftrightarrow \left\{\begin{array}{c} I_M = P_M + \overline{d} I'_M + \gamma^R J'_{M-1}, \\ \gamma^R P_M = 0 = \gamma^R I'_M. \end{array}\right. \tag{4.56}$$

Proof: That the condition is necessary ($\Leftarrow$) is direct. In order to show that it is sufficient, we are first going to show that

$$\overline{d} I_{N a_1 \ldots a_k} + \gamma^R_k J_{N-1 a_1 \ldots a_k} = 0 \Rightarrow I_{N a_1 \ldots a_k} = P_{N a_1 \ldots a_k} + \overline{d} I'_{N a_1 \ldots a_k} + \gamma^R_k J'_{N-1 a_1 \ldots a_k}, \tag{4.57}$$

where $\gamma^R_k J_{a_1 \ldots a_k} = -\Sigma_{l=1}^k C^b f^c_{b a_l} J_{a_1 \ldots a_{l-1} c a_{l+1} \ldots a_k} + \gamma^R J_{a_1 \ldots a_k}$.

Indeed, in form degree 0, the algebraic Poincaré lemma for $\overline{d}$ implies that $I_{Na_1 \ldots a_k} = R_{Na_1 \ldots a_k} + \overline{\rho}\overline{d} I_{Na_1 \ldots a_k}$. Using the l.h.s. of (4.57) and the fact γ^R_k anticommutes with $\overline{\rho}$, one gets the desired result by putting the y^α to zero.

Suppose now that the result is true in form degrees $<p$ and that $I_{Na_1 \ldots a_k}$ has form degree p. The algebraic Poincaré lemma for $\overline{d}$ implies that $I_{Na_1 \ldots a_k} = \overline{\rho}\overline{d} I_{Na_1 \ldots a_k} + \overline{d}\overline{\rho} I_{Na_1 \ldots a_k}$. Using the l.h.s. of (4.57), we get $I_{Na_1 \ldots a_k} = \gamma^R_k \overline{\rho} J_{N-1 a_1 \ldots a_k} + \overline{d}\overline{\rho} I_{Na_1 \ldots a_k}$. We have $\overline{\rho} I_{Na_1 \ldots a_k} = y^\alpha I_{N-1 \alpha a_1 \ldots a_k} + I'_{Na_1 \ldots a_k}$ and $\overline{\rho} J_{N-1 a_1 \ldots a_k} = y^\beta J_{N-2 \beta a_1 \ldots a_k} + J'_{N-1 a_1 \ldots a_k}$ so that

$$I_{Na_1 \ldots a_k} - \overline{d} I'_{Na_1 \ldots a_k} - \gamma^R_k J'_{N-1 a_1 \ldots a_k} = \overline{d}(y^\alpha I_{N-1 \alpha a_1 \ldots a_k}) + \gamma^R_k (y^\beta J_{N-2 \beta a_1 \ldots a_k}). \tag{4.58}$$

The action of γ^R only rotates the y^β in the internal space; its action on an expression that is linear and homogeneous in the y^β reproduces an expression that is linear and homogeneous in y^β. Supposing that the term in $y^\alpha I_{N-1 \alpha a_1 \ldots a_k}$ with the highest number of derivatives on y^α is

$$A^a_{(\mu, \nu_1 \ldots \nu_m)} I^{(\mu \nu_1 \ldots \nu_m)}_{N-1 a a_1 \ldots a_k},$$

we get, for the term linear in y^α with the highest number of derivatives on y^α, that $dx^\sigma A^a_{(\mu, \nu_1 \ldots \nu_m \sigma)} I^{(\mu \nu_1 \ldots \nu_m)}_{N-1 a a_1 \ldots a_k} + \gamma^R_k (A^a_{(\mu, \nu_1 \ldots \nu_m \sigma)} J^{(\mu \nu_1 \ldots \nu_m \sigma)}_{N-2 a a_1 \ldots a_k}) = 0$. This implies that $J^{(\mu \nu_1 \ldots \nu_m \sigma)}_{N-2 a a_1 \ldots a_k} = dx^{(\sigma} J^{\mu \nu_1 \ldots \nu_m)}_{N-2 a a_1 \ldots a_k}$ and that

$$I^{(\mu \nu_1 \ldots \nu_m)}_{N-1 a a_1 \ldots a_k} = dx^{(\nu_m} I^{(\mu \nu_1 \ldots \nu_{m-1}))}_{N-1 a a_1 \ldots a_k} - \gamma^R_{k+1} J^{(\mu \nu_1 \ldots \nu_m)}_{N-2 a a_1 \ldots a_k}.$$

The redefinition,

$$\begin{aligned} y^\alpha I_{N-1 \alpha a_1 \ldots a_k} \to y^\alpha I_{N-1 \alpha a_1 \ldots a_k} &- \overline{d}(A^a_{(\mu, \nu_1 \ldots \nu_{m-1})} I^{(\mu \nu_1 \ldots \nu_{m-1})}_{N-1 a a_1 \ldots a_k}) \\ &+ \gamma^R_k (A^a_{(\mu, \nu_1 \ldots \nu_m)} J^{(\mu \nu_1 \ldots \nu_m)}_{N-2 a a_1 \ldots a_k}), \end{aligned} \tag{4.59}$$

$$y^\beta J_{N-2 \beta a_1 \ldots a_k} \to y^\beta J_{N-2 \beta a_1 \ldots a_k} + \overline{d}(A^a_{(\mu, \nu_1 \ldots \nu_m)} J^{(\mu \nu_1 \ldots \nu_m)}_{N-2 a a_1 \ldots a_k}), \tag{4.60}$$

does not change the equation (4.58) and allows it to absorb the term linear in y^α with the highest number of derivatives on y^α. These redefinitions can be done until there are no derivatives on the y^α left, so that $y^\alpha I_{N-1 \alpha a_1 \ldots a_k} = A^a I_{N-1 a a_1 \ldots a_k}$, $y^\beta J_{N-2 \beta a_1 \ldots a_k} = A^a J_{N-2 a a_1 \ldots a_k}$. The vanishing of the term proportional to A^a in (4.58) then implies that $\overline{d} I_{N-1 a a_1 \ldots a_k} + \gamma^R_{k+1} J_{N-2 a a_1 \ldots a_k} = 0$. Because this is the l.h.s. of (4.57) in form degree $<p$, we have by induction that $I_{N-1 a a_1 \ldots a_k} = P_{N-1 a a_1 \ldots a_k} + \overline{d} I'_{N-1 a a_1 \ldots a_k} + \gamma^R_{k+1} J'_{N-2 a a_1 \ldots a_k}$. Injecting into (4.58) gives the desired result:

$$\begin{aligned} &I_{Na_1 \ldots a_k} - \overline{d} I'_{Na_1 \ldots a_k} - \gamma^R_k J'_{N-1 a_1 \ldots a_k} \\ &\quad = F^a P_{N-1 a a_1 \ldots a_k} + \overline{d}(F^a I'_{N-1 a a_1 \ldots a_k}) + \gamma^R_k (F^a J'_{N-2 a a_1 \ldots a_k}). \end{aligned} \tag{4.61}$$

The first line on the right hand side of (4.56) then follows as a particular case of (4.57). Applying now γ^R, one gets $\gamma^R P_M - \overline{d} \gamma^R I'_M = 0$. Restriction to the small algebra $\mathcal{B}$ then implies that $\gamma^R P_M = 0 = \overline{d} \gamma^R I'_M$ because $\overline{d}(\gamma^R I'_M)|_{\mathcal{B}} = 0$. We have $I'_M = R'_M + \overline{d}\overline{\rho} I'_M + \overline{\rho}\overline{d} I'_M$. One can then set the variables y^α to zero on the r.h.s. without changing the l.h.s., $I'_M = R'_M + (\overline{d}\overline{\rho} I'_M)|_{y=0}$

$+(\overline{\rho d} I'_M)_{y=0}$. Appling the same reasoning as above then gives $(\overline{d\rho} I'_M)|_{y^\alpha=0} = P'''_M + \overline{d} J''_M$, so that $I'_M = P''_M + \overline{d} J''_M + (\overline{\rho d} I'_M)|_{y=0}$. Because the first two terms do not contribute to $\overline{d} I'_M$, we can assume without loss of generality that $I'_M = (\overline{\rho d} I'_M)|_{y=0}$. For such an I'_M, the relation $\overline{d}\gamma^R I'_M = 0$ implies $\gamma^R I'_M = 0$ by using (4.54).

Completing the proof of (4.2): According to (4.40), we can complete $P^M = P_M|$, $I'^M = (I'_M)|$ such that $\gamma P^M = 0 = \gamma I'^M$, and according to (4.41) $\gamma^R J'_{M-1} = \gamma J'^{M-1} + O(M+1)$. Hence,

$$a^M - P^M - dI'^M - \gamma\left(\eta_M + A^a \frac{\partial I'_M}{\partial C^a} + J'^{M-1}\right) = a^{M+1}. \tag{4.62}$$

Because all the individual terms on the left hand side satisfy the l.h.s. of (4.2), so does a^{M+1}.

Lemma 6:

$$\left.\begin{array}{c} b^M + da'^{M-B} + \gamma\omega'^{M-C} = 0, \\ \gamma b^M = 0 = \gamma a'^{M-B}, \end{array}\right\} \Rightarrow \left\{\begin{array}{c} P_M + \overline{d} I'_M + \gamma^R J'_{M-1} = 0, \\ \gamma^R P_M = 0 = \gamma^R I'_M. \end{array}\right. \tag{4.63}$$

Proof: Proceeding again as in the proof of Lemma 3, one can assume without loss of generality that $C = B+1 \geqslant 1$ by suitably modifying ω'^{M-C}. If $B \geqslant 1$, we have by assumption at the lowest orders

$$\begin{gathered} da'_{M-B} + \gamma_1 \omega'_{M-B-1} + \gamma_0 \omega'_{M-B} = 0, \\ \gamma_0 \omega'_{M-B-1} = 0 = \gamma_0 a'_{M-B} = \gamma_1 a'_{M-B} + \gamma_0 a'_{M-B+1}. \end{gathered} \tag{4.64}$$

We thus have $\omega'_{M-B-1} = J'_{M-B-1} + \gamma_0(\ )$. The γ_0 exact term can be assumed to be absent by a further modification of ω'^{M-B-1} by a γ exact term that does not affect the equations. Because $a'_{M-B} = I'_{M-B} + \gamma_0 \eta_{M-B}$, we get

$$\left\{\begin{array}{c} \overline{d} I'_{M-B} + \gamma^R J'_{M-B-1} = 0, \\ \gamma^R I'_{M-B} = 0. \end{array}\right. \tag{4.65}$$

According to (4.56), this implies

$$\begin{gathered} I'_{M-B} = P'_{M-B} + \overline{d} I''_{M-B} + \gamma^R J''_{M-B-1}, \\ \gamma^R P'_{M-B} = 0 = \gamma^R I''_{M-B}. \end{gathered} \tag{4.66}$$

As in the reasoning leading to (4.62), we get

$$a'^{M-B} - P'^{M-B} - dI''^{M-B} - \gamma\left(\eta_{M-B} + A^a \frac{\partial I'_{M-B}}{\partial C^a} + J''^{M-B-1}\right) = a'^{M-B+1}, \tag{4.67}$$

with $\gamma P'^{M-B} = 0 = \gamma I''^{M-B}$. Because $dP'^{M-B} + \gamma(\ ) = 0$, we can replace on the l.h.s. of (4.63) a'^{M-B} by a'^{M-B+1} by suitably modifying ω'^{M-C}. This can be done until $B = 0$ by the same reasoning as in the beginning of this proof. For $B = 0$, we get the r.h.s. of (4.63), with $b_M = P_M + \gamma_0 \varpi_M$.

Lemma 7: In form degree $\leqslant n$,

$$\left.\begin{array}{c} P_M + \overline{d} I'_M + \gamma^R J'_{M-1} = 0, \\ \gamma^R P_M = 0 = \gamma^R I'_M, \end{array}\right\} \Rightarrow P_M = \gamma^R Q_{M-1}. \tag{4.68}$$

Proof: By restricting to the small algebra $\mathcal{B}$, we get $P_M + \overline{d}(I'_M|_{\mathcal{B}}) + \gamma^R(J'_{M-1}|_{\mathcal{B}}) = 0$. This gives directly the result because $\overline{d}(I'_M|_{\mathcal{B}}) = 0$.

Note that because of the first relation of (4.54), the map

$$\begin{aligned} &\overline{d}^{\#}: H(\gamma^R, \mathcal{I}^0) \to H(\gamma^R, \mathcal{I}^0), \\ &[I] \mapsto [\overline{d} I], \end{aligned} \tag{4.69}$$

is well defined. Lemmas 5 and 7 (for $p<n$) can then be summarized by the following corollary.

Corollary 2:

$$H^p(\overline{d}^{\#}, H(\gamma^R, \mathcal{I}^0)) \simeq H^p(\gamma^R, \mathcal{P}^0), \quad p<n. \tag{4.70}$$

Completing the proof of (4.3): According to (4.41), the expression $Q^{M-1}=Q_{M-1}|$ satisfies $\gamma^R Q_{M-1} = \gamma Q^{M-1} + O(M+1)$ so that $b^M - \gamma(\varpi_M + Q^{M-1}) = b^{M+1}$. This implies that b^{M+1} obeys again the l.h.s. of (4.3).

7. Convergence in the space of polynomials

As they stand, the proofs are valid in the space of formal power series. In order that they apply to the case of polynomials, one needs to be sure that if the l.h.s. of (4.2) and (4.3) are polynomials, i.e., if the degrees of homogeneity of all the elements are bounded from above, then the same holds for the elements that have been constructed on the r.h.s. of these equations. This can be done by controlling the number of derivatives on the A^a_μ and the C^a's. Let

$$K = (|\nu| - 1)\partial_{(\nu)} C^a \frac{\partial}{\partial \partial_{(\nu)} C^a} + |\nu| \partial_{(\nu)} A^a_\mu \frac{\partial}{\partial \partial_{(\nu)} A^a_\mu}. \tag{4.71}$$

Suppose that a^M is a polynomial $a^M = a_M + \ldots + a_{M+L}$. It follows that the K degree of a^M is bounded from above by some k. We will say that a^M is of order k. Note that γ_0 does not modify the order, while γ_1 decreases the order by 1. It follows that the γ_0 exact term and J in (4.35) can be assumed to be of order k as well, while J' in (4.36) can be assumed to be of order $k+1$. The important point is that $I^M - I_M$ and $\gamma J^M - \gamma^R J_M$ are of order $k-1$ if I_M, respectively $\gamma^R J_M$, are of order k.

Since $\overline{d}$ increases the order by 1, I_M and J_{M-1} in (4.55) can be assumed to be of order k, respectively $k+2$, while I'_M can be assumed to be of order $k-1$. It follows that J'_{M-1} in (4.56) can be assumed to be of order $k+1$. This implies that in the recursive construction (4.62) of a^M, after $M+L+1$ steps, i.e., after all of the original $a_M + \ldots + a_{M+L}$ have been absorbed, the order strictly decreases at each step. Since the order is bounded from below, the construction necessarily finishes after a finite number of steps, so that one stays inside the space of polynomials.

Similarily, if b^M on the l.h.s. (4.63) is of order k, P_M, I'_M and J'_{M-1} on the right hand side of (4.63) can be assumed to be of order k, $k-1$ and $k+1$, respectively. It follows that on the r.h.s. of (4.68), Q_{M-1} can be assumed to be of order $k+1$. In the recursive construction of b^M, once the original b^M has been completely absorbed, the order strictly decreases at each step, so that the construction again finishes after a finite number of steps.

8. The case of super or graded Lie algebras

In the case of super or graded Lie algebras, some of the gauge potentials become fermionic, while some of the ghosts become bosonic. By taking due care of sign factors and using graded commutators everywhere, the same proof as above of the covariant Poincaré lemma goes through.

V. $H(\gamma)$ FOR $\mathcal{G}/\mathcal{J}$ SEMISIMPLE

A. Formulation of a theorem by Hochschild and Serre

As shown in the digression in Sec. IV D 4, $H(\gamma, \mathcal{A}) \simeq H(\gamma^S, \mathcal{I})$, respectively $H(\gamma, \mathcal{B}) \simeq H(\gamma^S, \mathcal{P})$. By identifying the ghosts C^a as generators of $\wedge(\mathcal{G}^*)$, the spaces $\mathcal{I}$ and $\mathcal{P}$ can be

identified with $C(\mathcal{G},V^{\mathcal{I}})$, respectively $C(\mathcal{G},V^{\mathcal{P}})$, the spaces of cochains with values in the module $V^{\mathcal{I}}$, respectively $V^{\mathcal{P}}$. Here, $V^{\mathcal{I}}$ is the module of form valued polynomials or formal power series in the F^a_Δ, while $V^{\mathcal{P}}$ is the module of polynomials or formal power series in the F^a. The differential γ^S defined in (4.48) can then be identified with the Chevalley–Eilenberg Lie algebra differential with coeffcients in the module $V^{\mathcal{I}}$, respectively $V^{\mathcal{P}}$. The module $V^{\mathcal{P}}$ decomposes into the direct sum of finite dimensional modules $V^{\mathcal{P}}_M$ of monomials of homogeneity M in the F^a. The module $V_{\mathcal{I}}$ decomposes into the direct sum of modules $\Omega(M)\otimes V^{\mathcal{I}}_M$ of form valued monomials of homogeneity M in the F^a_Δ. The space–time forms can be factorized because the representation does not act on them, and the module $V^{\mathcal{I}}_M$ is finite dimensional.

As mentioned in the Introduction, it is at this stage that, for reductive Lie algebras, one can use standard results on Lie algebra cohomology with coefficients in a finite dimensional module (see, e.g., Ref. 12). But even for non reductive Lie algebras, there exist some general results. We will now review one of these results due to Hochschild and Serre.[23] In order to be self-contained, a simple proof of their theorem in ''ghost'' language is given.

Theorem 2: *Let $\mathcal{G}$ be a real Lie algebra and $\mathcal{J}$ an ideal of $\mathcal{G}$ such that $\mathcal{G}/\mathcal{J}$ is semi-simple. Let V be a finite dimensional $\mathcal{G}$-module. Then the following isomorphism holds,*

$$H(\mathcal{G},V)\simeq H(\mathcal{G}/\mathcal{J},\mathbb{R})\otimes H^{\mathcal{G}}(\mathcal{J},V), \tag{5.1}$$

where $H^{\mathcal{G}}$ means the $\mathcal{G}$-invariant cohomology space.

B. Proof

The above hypothesis implies that there is a semi-simple subalgebra $\mathcal{K}$ of $\mathcal{G}$ isomorphic to $\mathcal{G}/\mathcal{J}$ such that

$$\mathcal{G}=\mathcal{K}\ltimes\mathcal{J}. \tag{5.2}$$

Let $\{e_A,h_\alpha\},(A=1,\ldots,p),(\alpha=1,\ldots,q)$ denote a basis of $\mathcal{G}$, among which the e_A's form a basis of $\mathcal{K}$ and the h_α's a basis of $\mathcal{J}$: the fundamental brackets are given by

$$[e_A,e_B]=f_{AB}^{C}e_C,\quad [h_\alpha,h_\beta]=f_{\alpha\beta}^{\gamma}h_\gamma,\quad [e_A,h_\beta]=f_{A\beta}^{\gamma}h_\gamma. \tag{5.3}$$

If $C^a\equiv(\eta^A,C^\alpha)$, the coboundary operator γ^T can be cast into the form

$$\gamma^T=\eta^A\rho(e_A)+\eta^A\rho_C(e_A)-\frac{1}{2}\eta^A\eta^B f_{AB}^{C}\frac{\partial}{\partial\eta^C}+C^\alpha\rho(h_\alpha)-\frac{1}{2}C^\alpha C^\beta f_{\alpha\beta}^{\gamma}\frac{\partial}{\partial C^\gamma}. \tag{5.4}$$

Here, $\rho_C(e_A)$ is the extension to $\wedge(C)$ of the coadjoint representation of the semi-simple $\mathcal{K}$,

$$\rho_C(e_A)=-f_{A\beta}^{\gamma}C^\beta\frac{\partial}{\partial C^\gamma}, \tag{5.5}$$

while ρ denotes the representation of $\mathcal{G}$ in V. Let

$$N_\eta=\eta^A\frac{\partial}{\partial\eta^A},\quad N_C=C^\alpha\frac{\partial}{\partial C^\alpha}, \tag{5.6}$$

be the counting operators for the η's and C's and the associated gradings gh_η and gh_C on $V\otimes\wedge(C,\eta)$. According to the gh_C–grading, γ^T is the sum

$$\gamma^T=\gamma_0^T+\gamma_1^T,\quad (\gamma^T)^2=(\gamma_0^T)^2=(\gamma_1^T)^2=0,\quad \{\gamma_0^T,\gamma_1^T\}=0, \tag{5.7}$$

with γ_1^T explicitly given by

$$\gamma_1^T = C^\alpha \rho(h_\alpha) - \frac{1}{2} C^\alpha C^\beta f_{\alpha\beta}{}^\gamma \frac{\partial}{\partial C^\gamma} \tag{5.8}$$

and which obey

$$[N_C, \gamma_0^T] = 0, \quad [N_C, \gamma_1^T] = \gamma_1^T, \tag{5.9}$$

which means that γ_0^T conserves the number of C's while γ_1^T increases this number by one. At this stage, γ_0^T can already be identified with the coboundary operator of the Lie algebra cohomology of the semi-simple subalgebra $\mathcal{K}$ with coefficients in the $\mathcal{K}$-module $V \otimes \wedge(C)$, the corresponding representation being defined as $\rho^T(e_A) = \rho(e_A) \otimes \mathbb{I}_C + \mathbb{I}_V \otimes \rho_C(e_A)$. An element $a \in V \otimes \wedge(C, \eta)$ of total ghost number g can be decomposed according to its gh_C components,

$$a = a_0 + a_1 + \cdots + a_g, \quad gh_C a_k = k. \tag{5.10}$$

The cocycle condition $\gamma^T a = 0$ generates the following tower of equations,

$$\gamma_0^T a_0 = 0, \tag{5.11}$$

$$\gamma_1^T a_0 + \gamma_0^T a_1 = 0, \tag{5.12}$$

$$\gamma_1^T a_1 + \gamma_0^T a_2 = 0, \tag{5.13}$$

$$\vdots$$

$$\gamma_1^T a_g = 0, \tag{5.14}$$

and the coboundary condition reads

$$a_0 = \gamma_0^T \omega_0, \tag{5.15}$$

$$a_1 = \gamma_1^T \omega_0 + \gamma_0^T \omega_1, \tag{5.16}$$

$$\vdots$$

$$a_g = \gamma_1^T \omega_{g-1}. \tag{5.17}$$

The above mentioned results on reductive Lie algebra cohomology imply that the general solution of Eq. (5.11) can be written as

$$a_0 = v_0^j \Theta_j + \gamma_0^T \omega_0, \tag{5.18}$$

$$\rho^T(e_A) v_0^j = 0, \tag{5.19}$$

where the $\Theta_j(\eta)$'s form a basis of the cohomology $H(\mathcal{K}, \mathbb{R})$, which is generated by the primitive elements. Furthermore, all $\mathcal{K}$-invariant polynomials v^j, obeying $v^j \Theta_j + \gamma_0^T \omega = 0$ for some ω, have to vanish, $v^j = 0$.

The term $\gamma_0^T \omega_0$ can be absorbed by subtracting $\gamma^T \omega_0$ from a and modifying a_1 appropriately. Injecting then (5.18) in (5.12), one gets, since γ_1^T does not act on the η's,

$$(\gamma_1^T v_0^j) \Theta_j + \gamma_0^T a_1 = 0. \tag{5.20}$$

Now, from $[\rho^T(e_A), \gamma_1^T] = 0$, one sees that $\gamma_1^T v_0^j \in V \otimes \wedge(C)$ is still invariant under $\rho^T(e_A)$. Accordingly, one must have

$$\gamma_1^T v_0^j = 0 \quad \text{and} \quad \gamma_0^T a_1 = 0. \tag{5.21}$$

Again, the general solution of the last equation (5.21) is

$$a_1 = v_1^j \Theta_j + \gamma_0^T \omega_1 \tag{5.22}$$

with $\rho^T(e_A)v_1^j = 0$; subtraction of $\gamma^T\omega_1$ and injection in Eq. (5.13) gives

$$(\gamma_1^T a_1^j)\Theta_j + \gamma_0^T a_2 = 0, \tag{5.23}$$

implying

$$\gamma_1^T v_1^j = 0 \quad \text{and} \quad \gamma_0^T a_2 = 0. \tag{5.24}$$

The same procedure can be repeated until (5.14).

Every γ^T-cocycle is thus of the form

$$a = \sum_{k=0}^{g} v_k^j \Theta_j + \gamma^T \omega, \tag{5.25}$$

with

$$\rho^T(e_A)v_k^j = 0 \Rightarrow v_k^j \in [V \otimes \wedge(C)]^{\mathcal{K}}, \tag{5.26}$$

$$\gamma_1^T v_k^j = 0. \tag{5.27}$$

Let us now analyze the coboundary condition. To order 0, we find

$$v_0^j = 0 \quad \text{and} \quad \gamma_0^T \omega_0 = 0. \tag{5.28}$$

The last equation implies $\omega_0 = w_0^j \Theta_j + \gamma_0^T(\ )$. The γ_0^T exact term can be absorbed by subtracting the corresponding γ^T exact term from ω. To order 1, we then find

$$v_1^j = \gamma_1^T w_0^j \quad \text{and} \quad \gamma_0^T \omega_1 = 0. \tag{5.29}$$

Going on in the same way gives

$$v_k^j = \gamma_1^T w_{k-1}^j, \quad k = 1, \ldots, g. \tag{5.30}$$

In other words,

$$H(\mathcal{G}, V) \simeq H(\mathcal{G}/\mathcal{J}, \mathbb{R}) \otimes H(\gamma_1^T, (V \otimes \wedge(C))^{\mathcal{K}}). \tag{5.31}$$

From $\{\gamma_1^T, \partial/\partial C^\alpha\} = \rho^T(h_\alpha)$, it follows that the elements $[v_k^j]$ of the second space are invariant under the action of $\mathcal{J}$,

$$\rho^T(h_\alpha)v_k^j = \gamma_1^T \frac{\partial}{\partial C^\alpha} v_k^j \Rightarrow (\rho^T(h_\alpha))^{\#}[v_k^j] = 0, \tag{5.32}$$

where $\rho^T(h_\alpha) = \rho(h_\alpha) \otimes \mathbb{I}_C + \mathbb{I}_V \otimes \rho_C(h_\alpha)$. Hence,

$$H(\gamma_1^T, (V \otimes \wedge(C))^{\mathcal{K}}) = H^{\mathcal{G}}(\mathcal{J}, V), \tag{5.33}$$

as required.

C. Explicit computation of $H(\gamma,\mathcal{B})$ for $\mathcal{G}=iso(3)$ or $iso(2,1)$

1. Applicability of the theorem

As a concrete application, we consider the case where $\mathcal{G}=iso(3)$, the three dimensional Euclidian algebra, or $\mathcal{G}=iso(2,1)$, the three dimensional Poincaré algebra. Both of these Lie algebras fulfill the hypothesis of the Hochschild–Serre theorem with $\mathcal{J}$ being the Abelian translation algebra.

Denoting by $\{h_a=P_a, e_a=J_a\}$ a basis of $\mathcal{G}$ where P_a represent the translation generators and J_a represent the rotation (resp. Lorentz) generators, their brackets can be written as

$$[P_a,P_b]=0,\ [J_a,J_b]=\epsilon_{abc}J^c,\ [J_a,P_b]=\epsilon_{abc}P^c. \tag{5.34}$$

The indices are lowered or raised with the Killing metric g_{ab} of the semi-simple subalgebra $\mathcal{K}=so(3)$ or $so(2,1)$.

In the so-called universal algebra, (see Refs. 16 and 37 for more details) the space of polynomials in the F^a, the Abelian curvature two-form associated to the translations, and the G^a, the non-Abelian curvature two-form associated to the rotations/boosts, can be identified with the module $V=S(\mathcal{G}^*)$ transforming under the extension of the coadjoint representation, so that

$$H(\gamma,\mathcal{B}))\simeq H(\gamma^R,\mathcal{P})\equiv H(\mathcal{G},S(\mathcal{G}^*)). \tag{5.35}$$

The coboundary operator γ^R acts on $V\otimes\wedge(C,\eta)$ through

$$\gamma^R=\eta^a\epsilon_{abc}\left[F^c\frac{\partial}{\partial F_b}+G^c\frac{\partial}{\partial G_b}-\frac{1}{2}\eta^b\frac{\partial}{\partial\eta_c}-C^b\frac{\partial}{\partial C_c}\right]+C^a\epsilon_{abc}G^c\frac{\partial}{\partial F_b}. \tag{5.36}$$

As mentioned above, the Lie algebra cohomology $H(\mathcal{K},\mathbb{R})$ is generated by particular ghost polynomials $\Theta_i(\eta)$ representing the primitive elements which are in one-to-one correspondence with the independent Casimir operators. In the particular cases considered here, there is but one primitive element given by

$$\theta_1=\frac{1}{3!}\epsilon_{abc}\eta^a\eta^b\eta^c=(-)^\sigma\hat{\eta}^3, \tag{5.37}$$

where $\sigma=0,1$ for the Euclidean respectively Minkowskian case. The elements of the set $\{1,\theta_1\}$ provide a basis of this cohomology.

2. Invariants, cocycles, coboundaries

a. Order zero. In $gh_C=0$, the invariant space $V^{\mathcal{K}}$ is generated by the following quadratic invariants:

$$f_1=g_{ab}G^aG^b,\ f_2=g_{ab}F^aF^b,\ f_3=g_{ab}F^aG^b. \tag{5.38}$$

An element $a_0\in V^{\mathcal{K}}$ is a polynomial in the three variables

$$a_0=Q(f_1,f_2,f_3). \tag{5.39}$$

To fulfill the cocycle condition $\gamma_1^Ra_0=0$, Q has to obey

$$\epsilon_{abc}G^c\frac{\partial}{\partial F_b}Q=0=\epsilon_{abc}G^c\left[2F^b\frac{\partial}{\partial f_2}+G^b\frac{\partial}{\partial f_3}\right]Q, \tag{5.40}$$

which implies

$$\frac{\partial}{\partial f_2}Q=0. \tag{5.41}$$

The γ_1^R-cocycles of $gh_C=0$ are thus of the form

$$a_0=Q(f_1,f_3). \tag{5.42}$$

Using the following decomposition,

$$Q(f_1,f_2,f_3)=Q(f_1,0,f_3)+f_2\tilde{Q}(f_1,f_2,f_3), \tag{5.43}$$

the coboundaries of $gh_C=1$ are given by

$$t_1=\gamma_1^R[f_2\tilde{Q}(f_1,f_2,f_3)]=2C^a\epsilon_{abc}G^cF^b\frac{\partial}{\partial f_2}[f_2\tilde{Q}(f_1,f_2,f_3)]. \tag{5.44}$$

b. Order one. In $gh_C=1$, the elements of $[V\otimes\wedge(C)]^{\mathcal{K}}$ can be written as

$$\omega_1=C^b\omega_b, \tag{5.45}$$

where the $\omega_b\in S(\mathcal{G}^*)$ transform under $\mathcal{K}$ as the components of a vector. They are of the form

$$C^b\omega_b=C^b[G_bQ(f_k)+F_bR(f_k)+\epsilon_{bcd}G^cF^dS(f_k)]. \tag{5.46}$$

According to (5.44), the last term is γ_1^R-exact. For the other terms, the cocycle condition $\gamma_1^Ra_1=0$ implies

$$C^aC^b\epsilon_{amn}G^n\left[2G_bF^m\frac{\partial Q}{\partial f_2}+\delta_b^mR+2F_bF^m\frac{\partial R}{\partial f_2}\right]=0, \tag{5.47}$$

and imposes

$$R=0 \quad \text{and} \quad \frac{\partial Q}{\partial f_2}=0. \tag{5.48}$$

Hence, the nontrivial $gh_C=1$ cocycles are given by

$$a_1=C^bG_bQ(f_1,f_3). \tag{5.49}$$

The $gh_C=2$ coboundaries are given by

$$t_2=\gamma_1^RC^b[G_bf_2\tilde{Q}(f_k)+F_bR(f_k)], \tag{5.50}$$

or equivalently by

$$t_2=[(GC^2)f_3-(FC^2)f_1]\frac{\partial f_2\tilde{Q}}{\partial f_2}+(GC^2)R+[(GC^2)f_2-(FC^2)f_3]\frac{\partial R}{\partial f_2} \tag{5.51}$$

due to the identities

$$2(C^aG_a)(C^b\epsilon_{bcd}G^cF^d)=(GC^2)f_3-(FC^2)f_1, \tag{5.52}$$

$$2(C^aF_a)(C^b\epsilon_{bcd}G^cF^d)=(GC^2)f_2-(FC^2)f_3, \tag{5.53}$$

in which $(FC^2)=C^aC^b\epsilon_{abc}F^c$ and $(GC^2)=C^aC^b\epsilon_{abc}G^c$.

One deduces from (5.51) that, for all integers L,M,N, the following equalities between γ_1^R equivalences classes hold:

$$[(GC^2)f_1^L f_2^M f_3^{N+1}]=[(FC^2)f_1^{L+1}f_2^M f_3^N], \tag{5.54}$$

$$[(GC^2)f_1^L f_2^M f_3^N]=\left[\frac{M}{M+1}(FC^2)f_1^L f_2^{M-1}f_3^{N+1}\right], \tag{5.55}$$

from which one infers that the elements of the form $(GC^2)U(f_k)$ are equivalent to elements of the form $(FC^2)V(f_k)$ and, furthermore, that all monomials of the form $(FC^2)f_1^L f_2^M f_3^N$ with $L>M$ are coboundaries, while those which have $L\leqslant M$ can be replaced by monomials not containing f_1 according to

$$[(FC^2)f_1^L f_2^M f_3^N]=\left[(FC^2)\frac{(M-L+1)}{M+1}f_2^{M-L}f_3^{N+2L}\right]. \tag{5.56}$$

c. Order two. The $gh_C=2$ elements of $[V\otimes\wedge(C)]^{\mathcal{K}}$ can be written as

$$\omega_2=C^aC^b\omega_{ab}. \tag{5.57}$$

The most general element is of the type

$$\omega_2=C^aC^b\epsilon_{abc}[G^cU(f_k)+F^cV(f_k)+\epsilon^{cmn}G_mF_nW(f_k)], \tag{5.58}$$

but, according to our preceding results, through the addition of an appropriate coboundary, we can remove the U-part and suppose V not depending on f_1. The cocycle condition $\gamma_1^R a_2=0$ then reads

$$C^dC^aC^b\epsilon_{def}G^f\epsilon_{abc}\frac{\partial}{\partial F_e}[F^cV(f_2,f_3)+\epsilon^{cmn}G_mF_nW(f_k)]=0. \tag{5.59}$$

It does not further restrict V but requires $W=0$. The nontrivial $gh_C=2$ cocycles are thus given by

$$a_2=(FC^2)V(f_2,f_3). \tag{5.60}$$

In order to characterize the $gh_C=3$ coboundaries, we use the following identity,

$$\gamma_1^R(F\times G)C^2f_1^Lf_2^Mf_3^N=C^1C^2C^3(4(M+1)f_1^{L+1}f_2^Mf_3^N-4Mf_1^Lf_2^{M-1}f_3^{N+2}), \tag{5.61}$$

from which we infer that all monomials of the form $C^1C^2C^3f_1^Lf_2^Mf_3^N$ for $L>M$ are coboundaries, while those with $L\leqslant M$ are equivalent to monomials involving powers of f_2 and f_3 only.

d. Order three. The $gh_C=3$ invariants are of the form

$$\omega_3=C^1C^2C^3Q(f_1,f_2,f_3). \tag{5.62}$$

All of them are cocycles since $\mathcal{J}$ is of dimension 3, but only those of the form

$$a_3=C^1C^2C^3Q(f_2,f_3) \tag{5.63}$$

are nontrivial.

e. Summary. The nontrivial cocycles of $H(\gamma_1^R,[V\otimes\wedge(C)]^{\mathcal{K}})$ are summarized in Table I, where $\hat{C}^3=C^1C^2C^3$, $CG=C^aG_a$. They provide a basis of $H(\gamma_1^R,[V\otimes\wedge(C)]^{\mathcal{K}})$ as a vector space.

The associated basis of $H(\gamma,\mathcal{B})\simeq H(\gamma_1^R,\mathcal{P})$ is given by

$$\{Q_0(f_1,f_3),CGR_0(f_1,f_3),FC^2S_0(f_2,f_3),\hat{C}^3T_0(f_2,f_3),$$

$$\hat{\eta}^3Q_1(f_1,f_3),\hat{\eta}^3CGR_1(f_1,f_3),\ \hat{\eta}^3FC^2S_1(f_2,f_3),\ \hat{\eta}^3\hat{C}^3T_1(f_2,f_3)\}. \tag{5.64}$$

TABLE I. Cohomology of γ_1^R in the total invariant representation space.

gh_C	$H(\gamma_1^R,[V\otimes\wedge(C)]^{\mathcal{K}})$
0	$Q(f_1,f_3)$
1	$CGR(f_1,f_3)$
2	$FC^2S(f_2,f_3)$
3	$\hat{C}^3S(f_2,f_3)$

VI. $H(\gamma|d)$ FOR $\mathcal{G}/\mathcal{J}$ SEMISIMPLE AND $\mathcal{J}$ ABELIAN

Let $\mathcal{K}$ be a semi-simple Lie algebra and $\mathcal{G}=\mathcal{K}\ltimes\mathcal{J}$ with $\mathcal{J}$ an Abelian ideal. This means that, with respect to Sec. V, the additional assumption $[h_\alpha,h_\beta]=0$ holds. In other words, the only possibly nonvanishing structure constants are given by f_{AB}^C and $f_{A\beta}^\gamma$.

A. $H(\gamma|d,\mathcal{B})$

1. General results

Let B^A and η^A the gauge field one-forms and ghosts associated to $\mathcal{K}$ and A^α and C^α the gauge fields one-forms and ghosts associated to $\mathcal{J}$. The curvature two-form decomposes as $G^A=dB^A+\frac{1}{2}[B,B]^A$ and $F^\alpha=dA^\alpha+[B,A]^\alpha$. Let us consider the algebra $\mathcal{B}$ using the variables C^α, $DC^\alpha=dC^\alpha+[B,C]^\alpha$, A^α, F^α, B^A, G^A, η^A, $D\eta^A=d\eta^A+[B,\eta]^A$. Applying the results of Sec. III, we have

$$d=[\lambda,\gamma]. \tag{6.1}$$

As in Sec. III, if $\gamma b=0$, one has

$$db+\gamma\lambda b=0, \tag{6.2}$$

and

$$d\lambda b+\gamma\tfrac{1}{2}\lambda^2 b=\tau b, \tag{6.3}$$

with

$$\tau=\frac{1}{2}[d,\lambda]=F^\alpha\frac{\partial}{\partial C^\alpha}+G^A\frac{\partial}{\partial\eta^A}, \tag{6.4}$$

$$\tau^2=0,\ \{\tau,\gamma\}=0. \tag{6.5}$$

Furthermore, if

$$\sigma=C^\alpha\frac{\partial}{\partial F^\alpha}, \tag{6.6}$$

$$\sigma^2=0,\ \{\tau,\sigma\}=N_{C,F}, \tag{6.7}$$

$$\{\sigma,\gamma\}=0. \tag{6.8}$$

It is in order for this last relation to hold that one needs the assumption that $\mathcal{J}$ is Abelian. Indeed, in this case, because

$$\gamma = -DC^\alpha \frac{\partial}{\partial A^\alpha} - D\eta^A \frac{\partial}{\partial B^A} + ([F,\eta]+[G,C])^\alpha \frac{\partial}{\partial F^\alpha}$$
$$+[G,\eta]^A \frac{\partial}{\partial G^A} - [\eta,C]^\alpha \frac{\partial}{\partial C^\alpha} - \frac{1}{2}[\eta,\eta]^A \frac{\partial}{\partial \eta^A}, \tag{6.9}$$

the absence of the term $[F,C]^\alpha \partial/\partial F^\alpha$ guarantess that (6.8) holds.

According to (5.25), we can assume $b = v^j \Theta_j$, where $v^j = v^j(F,G,C)$ with

$$\rho^T(e_A) v^j = 0 = \gamma v^j, \tag{6.10}$$

$$\rho^T(e_A) = -f^\gamma_{A\beta} F^\beta \frac{\partial}{\partial F^\gamma} - f^C_{AB} G^B \frac{\partial}{\partial G^C} - f^\gamma_{A\beta} C^\beta \frac{\partial}{\partial C^\gamma}, \tag{6.11}$$

$$\gamma v^j = -[C,G]^\alpha \frac{\partial}{\partial F^\alpha} v^j. \tag{6.12}$$

Applying (6.2) and (6.3), we get

$$dv^j + \gamma \lambda v^j = 0, \tag{6.13}$$

$$d\lambda v^j + \gamma \tfrac{1}{2}\lambda^2 v^j = \tau v^j. \tag{6.14}$$

Furthermore, because $\mathcal{K}$ is semi-simple, there exist $\hat{\Theta}_j$ and $\hat{\hat{\Theta}}_j$ such that

$$d\Theta_j + \gamma \hat{\Theta}_j = 0, \tag{6.15}$$

$$d\hat{\Theta}_j + \gamma \hat{\hat{\Theta}}_j = 0. \tag{6.16}$$

It follows that

$$\gamma(v^j \Theta_j) = 0, \tag{6.17}$$

$$d(v^j \Theta_j) + \gamma((\lambda v^j)\Theta_j + v^j \hat{\Theta}_j) = 0, \tag{6.18}$$

$$d((\lambda v^j)\Theta_j + v^j \hat{\Theta}_j) + \gamma((\tfrac{1}{2}\lambda^2 v^j)\Theta_j + (\lambda v^j)\hat{\Theta}_j + v^j \hat{\hat{\Theta}}_j) = (\tau v^j)\Theta_j. \tag{6.19}$$

The necessary and sufficient condition that $v^j \Theta_j$ "can be lifted twice," i.e., that $[v^j \Theta_j] \in \mathrm{Ker}\, d_1$, with

$$d_1 : H(d, H(\gamma, \mathcal{B})) \to H(d, H(\gamma, \mathcal{B})),$$

$$[v^j \Theta_j] \mapsto d_1[v^j \Theta_j] = [d((\lambda v^j)\Theta_j + v^j \hat{\Theta}_j)],$$

is

$$d((\lambda v^j)\Theta_j + v^j \hat{\Theta}_j) = db' + \gamma(\ ), \tag{6.20}$$

with $\gamma b' = 0$. Because $db' + \gamma(\ ) = 0$, it follows by using (6.19) that this necessary and sufficient condition is

$$(\tau v^j)\Theta_j + \gamma(\ ) = 0. \tag{6.21}$$

Because τ commutes with $\rho^T(e_a)$ and anticommutes with γ, it follows from (5.30) that the condition reduces to

$$(\tau v^j)+\gamma w^j=0,\ \rho^T(e_A)w^j=0, \tag{6.22}$$

for some w^j. Let us decompose v^j as a sum of terms of definite $N_{F,C}$ degree k, $v^j=v_0^j+\Sigma_{k=1}v_k^j$. Using (6.7), this can be rewritten as

$$v^j=v_0^j+\sum_{k=1}\ (\sigma t_k^j+\tau s_k^j), \tag{6.23}$$

where $t_k^j=1/k\ \tau v_k^j$ and $s_k^j=1/k\ \sigma v_k^j$. This decomposition is direct and induces a well defined decomposition in cohomology because γ and τ, respectively σ, anticommute. Furthermore,

$$\tau v_0^j=0,\ \tau(\tau s_k^j)=0, \tag{6.24}$$

$$\tau\sigma t_k^j+\gamma w_k^j=0\Rightarrow\tau v_k^j+\gamma w_k^j=0\Rightarrow\sigma t_k^j=\gamma\frac{1}{k}\sigma w_k^j=0. \tag{6.25}$$

This implies for the decomposition $H(\gamma,\mathcal{B})=E_2\oplus d_1F_1\oplus F_1$, with Ker $d_1=E_2\oplus d_1F_1$, that

$$\text{Ker } d_1=\left\{v_0^j\Theta_j+\sum_{k=1}\ [\tau s_k^j]\,\Theta_j\right\}, \tag{6.26}$$

$$d_1F_1=\left\{\sum_{k=1}\ [\tau s_k^j]\,\Theta_j\right\}, \tag{6.27}$$

$$F_1=\left\{\sum_{k=1}\ [\sigma t_k^j]\,\Theta_j\right\}, \tag{6.28}$$

$$E_2=\{v_0^j\,\Theta_j\}. \tag{6.29}$$

Here, $[\tau s_k^j]$ and $[\sigma t_k^j]$ denote equivalence classes of $\rho^T(e_A)$ invariant cocycles that are τ, respectively σ, exact, up to coboundaries of $\rho^T(e_a)$ invariant elements that are also τ, respectively σ, exact.

Let

$$\lambda^{\#}:F_1\to H(\gamma|d,B),$$

$$[\sigma t_k^j]\Theta_j\mapsto[(\lambda\sigma t_k^j)\Theta_j+\sigma t_k^j\hat{\Theta}_j]. \tag{6.30}$$

That the map is well defined follows from (6.18) and $\lambda\gamma(\sigma w_k^j)\Theta_j+\gamma(\sigma w_k^j)\hat{\Theta}_j=d(\sigma w_k^j\Theta_j+\gamma(\lambda\sigma w_k^j\Theta_j+\sigma w_k^j\hat{\Theta}_j)$ due to (6.1).

Let $\mathcal{B}_\mathcal{K}$ be the restriction of $\mathcal{B}$ to the generators associated to $\mathcal{K}$. Because $E_2\simeq H(\gamma,\mathcal{B}_\mathcal{K})$, we have

$$H(\gamma,\mathcal{B}_\mathcal{G})\simeq H(\gamma,\mathcal{B}_\mathcal{K})\oplus d_1F_1\oplus F_1. \tag{6.31}$$

Furthermore, the general analysis of the exact triangle associated to the descent equations[16] (see also, e.g., Ref. 36) implies that

$$H(\gamma|d,\mathcal{B}_\mathcal{G})\simeq H(\gamma|d,\mathcal{B}_\mathcal{K})\oplus\lambda^{\#}F_1\oplus F_1. \tag{6.32}$$

TABLE II. Nontrivial solutions of the consistency condition in the small algebra.

gh	$H(\gamma\|d,\mathcal{B})$			
0	1	$GAR_0(f_1,f_3)$	0	$\hat{\eta}^0 Q_1(f_1)$
1	$GCR_0(f_1,f_3)$	0	$\hat{\eta}^1 Q_1(f_1)$	0
2	0	$\hat{\eta}^2 Q_1(f_1)+\frac{1}{2}AC^2T_1(f_2,f_3)$	0	0
3	$\hat{\eta}^3 Q_1(f_1)+\hat{C}^3T_0(f_2,f_3)$	$(\hat{\eta}^2 GC+\hat{\eta}^3 GA)R_1(f_1,f_3)$	0	0
4	$\hat{\eta}^3 GCR_1(f_1,f_3)$	0	0	0
5	0	$(\hat{\eta}^2\hat{C}^3+\frac{1}{2}\hat{\eta}^3AC^2)T_1(f_2,f_3)$	0	0
6	$\hat{\eta}^3\hat{C}^3T_1(f_2,f_3)$	0	0	0

This solves the problem because the classification of $H(\gamma|d,\mathcal{B}_\mathcal{K})$ and the associated decomposition of $H(\gamma,\mathcal{B}_\mathcal{K})$ for semi-simple $\mathcal{K}$ has been completely solved[16] (see, e.g., Ref. 37 for a review).

2. Application to $\mathcal{G}=iso(3)$ or $iso(2,1)$

By applying the analysis of the previous subsubsection to the particular case of $iso(3)$, respectively $iso(2,1)$, with $H(\gamma,\mathcal{B})$ given by (5.64), it follows that

$$F_1=\{GC\,R_0(f_1,f_3),\ \hat{C}^3\,T_0(f_2,f_3),\ \hat{\eta}^3\,GC\,R_1(f_1,f_3),\ \hat{C}^3\hat{\eta}^3\,T_1(f_2,f_3)\}, \tag{6.33}$$

$$d_1F_1=\{f_3\,\tilde{Q}_0(f_1,f_3),\ FC^2\,S_0(f_2,f_3),\ \hat{\eta}^3\,f_3\,\tilde{Q}_1(f_2,f_3),\ \hat{\eta}^3\,S_1(f_2,f_3)\}, \tag{6.34}$$

$$E_2=\{Q_0(f_1),\hat{\eta}^3\,Q_1(f_1)\}. \tag{6.35}$$

Furthermore, the general analysis of the semi-simple case applied to $so(3)$, respectively $so(2,1)$, gives

$$E_2=1\oplus d_3F_3\oplus F_3, \tag{6.36}$$

with

$$F_3=\{\hat{\eta}^3\,Q_1(f_1)\}, \tag{6.37}$$

$$d_3F_3=\{f_1\,\tilde{Q}_0(f_1)\}. \tag{6.38}$$

The associated elements of $H(\gamma|d,\mathcal{B})$ are listed in Table II, which involves the following new shorthand notations

$$\hat{\eta}^2=-\tfrac{1}{2}\epsilon_{abc}\,\eta^a\eta^bB^c, \tag{6.39}$$

$$\hat{\eta}^1=\eta^a\,(G_a-\tfrac{1}{2}\,\epsilon_{abc}B^bB^c), \tag{6.40}$$

$$\hat{\eta}^0=B^bG_b-\frac{1}{3!}\,\epsilon_{abc}B^aB^bB^c=g_{ab}B^adB^b+\frac{1}{3}\,\epsilon_{abc}B^aB^bB^c. \tag{6.41}$$

B. $H(\gamma|d,\mathcal{A})$

Using (4.13), respectively (4.14), we have, for $0\leqslant p<n$,

$$H^p(\gamma|d,\mathcal{A})\simeq i_0 H^p(\gamma,\mathcal{B}_\mathcal{K})\oplus F_1\oplus\mathcal{N}^p_\mathcal{A}\oplus\mathcal{D}^{-1}(\mathcal{D}H)^{p-1}(\gamma|d,\mathcal{B}_\mathcal{K})\oplus\lambda^\# F^n_1. \tag{6.42}$$

and in form degree n,

$$H^n(\gamma|d,\mathcal{A})\simeq\mathcal{F}^n\oplus\mathcal{D}^{-1}(\mathcal{D}H)^{n-1}(\gamma|d,\mathcal{B}_\mathcal{K})\oplus\lambda^\# F^n_1, \tag{6.43}$$

with $\mathcal{F}^n\simeq H^n(\gamma,\mathcal{A})/d_0\mathcal{N}^{n-1}_\mathcal{A}$.

VII. APPLICATION TO THE CONSISTENT DEFORMATIONS OF 2+1 DIMENSIONAL GRAVITY

A. Generalities

$2+1$ dimensional gravity with vanishing cosmological constant λ is equivalent to a Chern–Simons theory based on the gauge group $ISO(2,1)$.[24,25]

The Lie algebra $iso(2,1)$ is not reductive and its Killing metric $G_{AB}=f^D_{AC}f^C_{BD}$ is degenerate,

$$G_{AB}=\begin{pmatrix} g_{ab} & 0\\ 0 & 0\end{pmatrix}, \tag{7.1}$$

where g_{ab} is the Killing metric of the semi-simple $so(2,1)$ subalgebra. However, in this case, another invariant, symmetric and nondegenerate metric $\Omega^{(0)}_{AB}$ exists which allows for the construction of the CS Lagrangian. The invariant quadratic form of interest is

$$\Omega^{(0)}_{AB}=\begin{pmatrix}\langle J_a,J_b\rangle & \langle J_a,P_b\rangle\\ \langle P_a,J_b\rangle & \langle P_a,P_b\rangle\end{pmatrix}=\begin{pmatrix}0 & g_{ab}\\ g_{ab} & 0\end{pmatrix}. \tag{7.2}$$

Locally, the relation between $2+1$ dimensional gravity and the Chern–Simons theory is based on the $iso(2,1)$ Lie algebra valued one-form

$$\mathcal{A}_\mu=A^A_\mu T_A=e^a_\mu P_a+\omega^a_\mu J_a \tag{7.3}$$

built from the dreibein fields e^a_μ and the spin connection $\omega^a_\mu=\frac{1}{2}\epsilon^a_{bc}\omega^{bc}_\mu$ of three dimensional Minkowski space–time $\mathcal{M}$ with metric that we choose of signature $(-,+,+)$. In terms of these variables, the Chern–Simons action takes the form of the $2+1$ dimensional Einstein–Hilbert action in vielbein formulation:

$$\begin{aligned} S^{(0)}_{CS}&=\int_\mathcal{M}\Omega^{(0)}_{AB}\left[\frac{1}{2}A^A\,dA^B+\frac{1}{6}A^A\,f^B{}_{CD}\,A^C\,A^D\right]\\ &=\int_\mathcal{M}\frac{1}{2}(e^a\,d\omega_a+\omega^a\,de_a+\epsilon_{abc}\,e^a\,\omega^b\,\omega^c), \qquad (7.4)\\ &=\int_\mathcal{M}e^a\,G_a+\frac{1}{2}d(e^a\,\omega_a). \qquad (7.5)\end{aligned}$$

The gauge transformations are parametrized by two zero-forms ϵ^a and τ^a,

$$\varepsilon=\varepsilon^A T_A=\epsilon^a P_a+\tau^a J_a. \tag{7.6}$$

Explicitly,

$$\delta_\epsilon e^a = -d\epsilon^a - \epsilon^a{}_{bc}(\omega^b \epsilon^c + e^b \tau^c), \tag{7.7}$$

$$\delta_\epsilon \omega^a = -d\tau^a - \epsilon^a{}_{bc}\omega^b \tau^c, \tag{7.8}$$

and are equivalent, on shell, to local diffeomorphisms and local Lorentz rotations. The classical equations of motion express the vanishing of the field strenghts two-forms

$$F_a = \tfrac{1}{2}F_{\mu\nu a}dx^\mu dx^\nu = de_a + \epsilon_{abc}\omega^b e^c, \tag{7.9}$$

$$G_a = \tfrac{1}{2}G_{\mu\nu a}dx^\mu dx^\nu = d\omega_a + \tfrac{1}{2}\epsilon_{abc}\omega^b \omega^c, \tag{7.10}$$

where

$$\mathcal{F}_{\mu\nu} = \mathcal{F}^A_{\mu\nu} T_A = F^a_{\mu\nu} P_a + G^a_{\mu\nu} J_a . \tag{7.11}$$

For invertible dreibeins, the equation $F^a = 0$ can be algebraically solved for ω^a as a function of the e^a's; when substituted into the remaining equation it tells that the space–time Riemann curvature vanishes, which in three dimensions implies that space–time is locally flat.

Our aim is to study systematically all consistent deformations of $2+1$ dimensional gravity. By consistent, we mean deformations of the action by local functionals and simultaneous deformations of the gauge transformations such that the deformed action is invariant under the deformed gauge transformations.

The problem of such consistent deformations can be reformulated[41] (for a review, see Ref. 42) as the problem of deformations of the solution of the master equation and is controlled to first order by the cohomology $H^{0,3}(s|d)$.

B. Results on local BRST cohomology

The analysis of $H(s|d)$ for the Chern–Simons case (see, e.g., Ref. 37, Sec. 14) implies that the cohomology $H(s|d)$ is essentially given by the bottoms $[\frac{1}{2}\hat{\eta}^3]$, $[\hat{C}^3]$, $[\frac{1}{2}\hat{\eta}^3\hat{C}^3]$ of $H(\gamma,\mathcal{B})$ and by their lifts, which are all nontrivial and unobstructed. (The only additional classes correspond to the above bottoms multiplied by nonexact space–time forms.)

It follows that $H^{0,3}(s|d)$ is obtained from the lift (associated to s) of the elements $[\frac{1}{2}\hat{\eta}^3]$ and $[\hat{C}^3]$ of $H^{3,0}(s)$. The former element can be lifted to $\frac{1}{2}\hat{\eta}^0$ with $\hat{\eta}^0$ given in (6.41). It corresponds to the Chern–Simons action built on $so(2,1)$. The results on $H(\gamma|d,\mathcal{B})$ (see Table II) imply that the lift of $\hat{C}^3$ in $H(s|d)$ cannot been done without a nontrivial dependence on the antifields, and hence without a nontrivial deformation of the gauge transformations. Following again, Ref. 37, this lift is given by

$$\epsilon_{abc}[\tfrac{1}{6}e^a e^b e^c + e^a \star\omega^{*b} C^c + \tfrac{1}{2}\star\eta^{*a} C^b C^c], \tag{7.12}$$

where $\star\omega^{*a} = \frac{1}{2}dx^\mu dx^\nu \epsilon_{\mu\nu\rho}\omega^{*a\rho}$ and $\star\eta^*_a = d^3x\,\eta^*_a$. The antifield independent part gives the deformation of the original action.

Note also that $H^{1,3}(s|d)$ is trivial, which implies that there can be no anomalies in a perturbative quantization of $2+1$ dimensional gravity. Furthermore, the starting point Lagrangian three-form eG is trivial, $[eG]=[0]\in H^{0,3}(s|d)$, which is the reason why we do not introduce a separate coupling constant for this term.

C. Maximally deformed 2+1 dimensional gravity

Introducing coupling constants μ and λ (the cosmological constant) for the two first order deformations, they can be easily shown to extend to all orders by introducing a $\lambda\mu$ dependent term in the action. The associated completely deformed theory can be written as a Chern–Simons theory in terms of the deformed invariant metric

$$\Omega^{\lambda,\mu}_{AB}=\Omega^{(0)}_{AB}+G^{\mu,\lambda}_{AB}, \tag{7.13}$$

$$G^{\mu,\lambda}_{AB}=\mu\begin{pmatrix} g_{ab} & 0 \\ 0 & \lambda\, g_{ab}\end{pmatrix}, \tag{7.14}$$

and the deformed structure constants $f^{A(\lambda)}_{BC}$ given by

$$[J_a,J_b]=\epsilon_{abc}\,J^c,[J_a,P_b]=\epsilon_{abc}\,P^c,[P_a,P_b]=\lambda\,\epsilon_{abc}\,J^c. \tag{7.15}$$

For $\lambda>0$, these structure constants are those of the semi-simple Lie algebra $so(2,1)\oplus so(2,1)$. The deformed Chern–Simons action reads explicitly

$$S^{\lambda,\mu}=\int_{\mathcal{M}}\Omega^{\lambda,\mu}_{AB}\left[\frac{1}{2}A^A\,dA^B+\frac{1}{6}A^A\,f^{B(\lambda)}_{CD}\,A^C A^D\right] \tag{7.16}$$

$$=\int_{\mathcal{M}}\left[e^a G_a+\mu\left[\frac{1}{2}\,\omega^a\,d\omega_a+\frac{1}{6}\,\epsilon_{abc}\,\omega^a\,\omega^b\,\omega^c\right]\right.$$

$$\left.+\lambda\,\frac{1}{3!}\,\epsilon_{abc}\,e^a\,e^b\,e^c+\lambda\mu\left[\frac{1}{2}\,e^a\,de_a+\frac{1}{2}\,\epsilon_{abc}\,e^a\,e^b\,\omega^c\right]\right], \tag{7.17}$$

while the deformed gauge transformations read

$$\delta_\epsilon\,e^a=-d\,\epsilon^a-\epsilon^a{}_{bc}(\omega^b\,\epsilon^c+e^b\,\tau^c), \tag{7.18}$$

$$\delta_\epsilon\,\omega^a=-d\,\tau^a-\epsilon^a{}_{bc}(\omega^b\,\tau^c+\lambda\,e^b\,\epsilon^c). \tag{7.19}$$

Thus, our analysis shows that there are no other consistent deformations of $2+1$ dimensional gravity than those already discussed in Ref. 25.

Note added in proof: Two remarks concerning the proof of lemma 5 are in order. (1) The homotopy formula (4.52) has been used in the form $\{\overline{p},d\}=1$. This supposes that the forms on which it applies vanish when the variables A^a_μ and their derivatives are put to zero. In order to complete the reasoning, one should separate each form in such a part and a part that does not depend on those variables, but only on C^a, x^μ and dx^μ. This last part can be treated easily by using the homotopy of the standard Poincaré lemma. The final result, Eq. (4.61) is unchanged. (2) The proof on the top of page 12 that $\gamma^R I'_M=0$ is incorrect. The correct proof proceeds again by induction. More precisely, one shows that if $I_{Na_1\ldots a_k}$ in the l.h.s. of (4.57) is γ^R_k closed, then the $I'_{Na_1\ldots a_k}$ that has been constructed in the r.h.s of (4.57) can be chosen to be γ^R_k closed as well.

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APPENDIX: DESCENTS AND DECOMPOSITION ACCORDING TO HOMOGENEITY

The space $\mathcal{E}$ can be decomposed into monomials of definite homogeneity M in the fields and their derivatives, $\mathcal{E}=\oplus_{M=0}\mathcal{E}_M$, and one can define the spaces of polynomials of homogeneity greater or equal to M, $\mathcal{E}^M=\oplus_{N\geq M}\mathcal{E}_N$.

If

$$\mathcal{C}^M=\langle H(\gamma|d,\mathcal{E}^M),H(\gamma,\mathcal{E}^M),\mathcal{D}^M,l^{\#^M},i^{\#^M}\rangle, \tag{A1}$$

$$\mathcal{C}_M=\langle H(\gamma_0|d,\mathcal{E}_M),H(\gamma_0,\mathcal{E}_M),\mathcal{D}_M,l_M^{\#},i_M^{\#}\rangle, \tag{A2}$$

are the exact couples that describe the descents of γ in $\mathcal{E}^M$, respectively of γ_0 in $\mathcal{E}_M$, one can define mappings between exact couples (see, e.g., Ref. 43) through

$$I_{M+1}=(j_{M+1},k_{M+1}):\mathcal{C}^{M+1}\to\mathcal{C}^M, \tag{A3}$$

$$P_M=(\pi_M,\psi_M):\mathcal{C}^M\to\mathcal{C}_M, \tag{A4}$$

$$G_M=(m_M,n_M):\mathcal{C}_M\to\mathcal{C}^{M+1}. \tag{A5}$$

The map j_{M+1} consists in the natural injection of elements of $H(\gamma|d,\mathcal{E}^{M+1})$ in $H(\gamma|d,\mathcal{E}^M)$ and similarily k_{M+1} consists in the injection of elements of $H(\gamma,\mathcal{E}^{M+1})$ as elements of $H(\gamma,\mathcal{E}^M)$, with

$$\mathcal{D}^M\circ j_{M+1}=j_{M+1}\circ\mathcal{D}^{M+1}, \tag{A6}$$

$$l^{\#^M}\circ j_{M+1}=k_{M+1}\circ l^{\#^{M+1}}, \tag{A7}$$

$$i^{\#^M}\circ k_{M+1}=j_{M+1}\circ i^{\#^{M+1}}. \tag{A8}$$

The map $\pi_M:H(\gamma|d,\mathcal{E}^M)\to H(\gamma_0|d,\mathcal{E}_M)$ is defined by $\pi_M[A^M]=[A_M]$, while $\psi_M:H(\gamma,\mathcal{E}^M)\to H(\gamma_0,\mathcal{E}_M)$ is defined by $\psi_M[a^M]=[a_M]$. Again, the various maps commute,

$$\mathcal{D}_M\circ\pi_M=\pi_M\circ\mathcal{D}^M, \tag{A9}$$

$$l_M^{\#}\circ\pi_M=\psi_M\circ l^{\#^M}, \tag{A10}$$

$$i_M^{\#}\circ\psi_M=\pi_M\circ i^{\#^M}. \tag{A11}$$

Both the maps $m_M:H(\gamma_0|d,\mathcal{E}_M)\to H(\gamma|d,\mathcal{E}^{M+1})$ and $n_M:H(\gamma_0,\mathcal{E}_M)\to H(\gamma,\mathcal{E}^{M+1})$ are defined by the induced action of $\gamma_1:m_M[a_M]=[\gamma_1 a_M]$ and $n_M[a_M]=[\gamma_1 a_M]$, with

$$\mathcal{D}^{M+1}\circ m_M=m_M\circ\mathcal{D}_M, \tag{A12}$$

$$l^{\#^{M+1}}\circ m_M=n_M\circ l_M^{\#}, \tag{A13}$$

$$i^{\#^{M+1}}\circ n_M=m_M\circ i_M^{\#}. \tag{A14}$$

Finally, the triangles

$$\begin{array}{ccc} H(\gamma|d,\mathcal{E}^{M+1}) & \overset{j_{M+1}}{\to} & H(\gamma|d,\mathcal{E}^M) \\ & {\scriptstyle m_M}\nwarrow \quad \swarrow{\scriptstyle \pi_M} & \\ & H(\gamma_0|d,\mathcal{E}_M), & \end{array} \tag{A15}$$

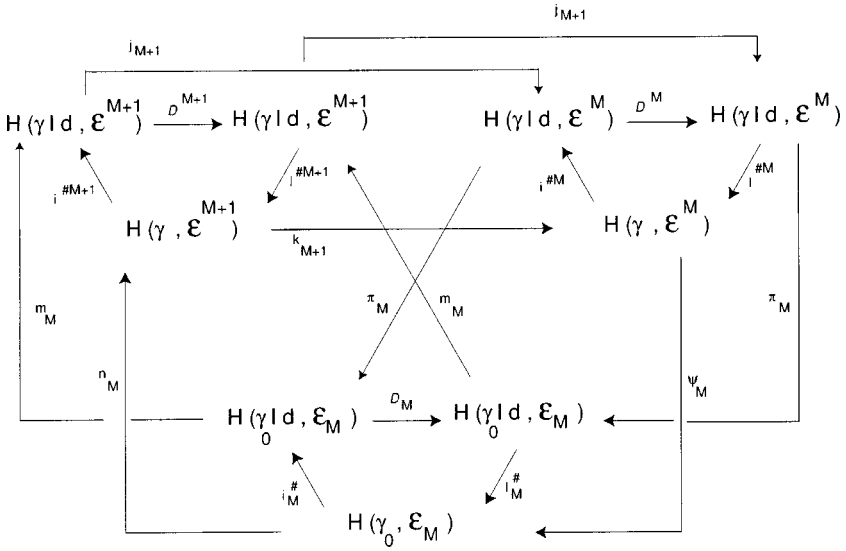

FIG. 1. Exact triangle of exact triangles.

$$
\begin{array}{ccc}
 & & H(\gamma,\mathcal{E}^{M+1}) \\
 & \overset{k_{M+1}}{\nearrow} & \downarrow \\
H(\gamma,\mathcal{E}^{M+1}) & & H(\gamma,\mathcal{E}^{M}) \\
 & {\scriptstyle n_M}\nwarrow \quad \swarrow{\scriptstyle \psi_M} & \\
 & H(\gamma_0,\mathcal{E}_M), &
\end{array}
\tag{A16}
$$

are exact at all corners, implying, if $j_0=1=k_0$, that

$$H(\gamma|d,\mathcal{E})=\oplus_{M=0}^{\infty} j_0 \ldots j_M \pi_M^{-1}\mathrm{Ker}\ \ m_M, \tag{A17}$$

$$H(\gamma,\mathcal{E})=\oplus_{M=0}^{\infty} k_0 \ldots k_M \psi_M^{-1}\mathrm{Ker}\ \ n_M. \tag{A18}$$

All this can be summarized by the commutative diagram of Fig. 1. The corners of the big triangle are itself given by exact triangles and the large triangles obtained by taking a group at the same position of each small triangle are also exact.

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Black-brane solution for C_2 algebra

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Black p-brane solutions for a wide class of intersection rules and Ricci-flat ''internal'' spaces are considered. They are defined up to moduli functions H_s obeying nonlinear differential equations with certain boundary conditions imposed. A new solution with intersections corresponding to the Lie algebra C_2 is obtained. The functions H_1 and H_2 for this solution are polynomials of degree 3 and 4. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1513654]

I. INTRODUCTION

The discovery of various extended objects (D-branes, p-branes, etc.)[1] in superstring theories leads to a new stage in the development of superstring paradigm, e.g., to a notion of M-theory.[2] These extended objects (branes) play a very important role in the description of superstrings in the strong coupling limit and the explanation of dual relations between different superstring theories.

The brane objects may be described as classical solutions in supergravitational models (see, for example, Ref. 3 and references therein). They have BPS properties (i.e., they preserve partial supersymmetry) and are protected from quantum corrections. These solutions lead to extremal black hole solutions after a suitable compactifications of extra dimensions.

Other important objects are non-extremal black brane solutions.[4–6] In the extremal limit they (usually) lead to BPS brane configurations. Nonextremal black branes give also a remarkable microscopical explanation of black hole entropy,[7,8] being a nice polygon for application of different quantum methods (for toy quantum analogues of black branes see Ref. 9).

This paper is devoted to intersecting black-brane solutions with (next to) arbitrary intersections (see Sec. II).[10–13] These black-brane solutions are governed by moduli functions $H_s = H_s(R)$ obeying a set of second order nonlinear differential equations with some boundary relations imposed.

Some general features of the black-brane solutions were investigated earlier (see Ref. 14). More general spherically symmetric (and cosmological solutions) were obtained in Ref. 15 using the sigma-model approach and the Lagrange representation from Refs. 16–18.

In Ref. 10 the following conjecture was suggested (see Sec. III): the moduli functions H_s are polynomials when intersection rules correspond to semisimple Lie algebras. This conjecture was confirmed by special black-brane ''block-orthogonal'' solutions considered earlier in Refs. 14, 19–22 (Sec. III A). It was verified also for A_m and C_m series of Lie algebras in Refs. 11 and 12. An analogue of this conjecture for extremal black holes was considered earlier in Ref. 23.

An example of black brane solution corresponding to Lie algebra $A_2 = \mathrm{sl}(3)$ was considered earlier in Refs. 10 and 11, where some dyonic configurations (e.g., in 11-dimensional supergrav-

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ity) were considered. The A_2 solution is governed by two polynomials H_1 and H_2 of degree 2. The coefficients of polynomials and charges are functions of some parameters P_1 and P_2 and have a rather simple form (Sec. III A). It seems that A_2 solution is the only one that may be obtained "by hands:" the search of solutions for other Lie algebras needs computer calculations.

Here we present a first nontrivial result of such calculations, i.e., a new solution corresponding to the Lie algebra C_2 governed by polynomials of degree 3 and 4 (Sec. III C). The coefficients of polynomials exhibit a nontrivial dependence upon parameters P_1 and P_2, namely: a nontrivial term Δ, that is a square root of a polynomial of degree 4, appears.

II. *p*-BRANE BLACK HOLE SOLUTIONS

Consider a model governed by the action

$$S=\int d^D x\sqrt{|g|}\left\{R[g]-h_{\alpha\beta}g^{MN}\partial_M\varphi^\alpha\partial_N\varphi^\beta-\sum_{a\in\triangle}\frac{\theta_a}{n_a!}\exp[2\lambda_a(\varphi)](F^a)^2\right\}, \tag{1}$$

where $g=g_{MN}(x)dx^M\otimes dx^N$ is a metric, $\varphi=(\varphi^\alpha)\in\mathbb{R}^l$ is a vector of scalar fields, $(h_{\alpha\beta})$ is a constant symmetric nondegenerate $l\times l$ matrix ($l\in\mathbb{N}$), $\theta_a=\pm 1$,

$$F^a=dA^a=\frac{1}{n_a!}F^a_{M_1\cdots M_{n_a}}dz^{M_1}\wedge\cdots\wedge dz^{M_{n_a}} \tag{2}$$

is a n_a-form ($n_a\geqslant 1$), λ_a is a 1-form on $\mathbb{R}^l$: $\lambda_a(\varphi)=\lambda_{\alpha a}\varphi^\alpha$, $a\in\triangle$, $\alpha=1,\ldots,l$. In (1) we denote $|g|=|\det(g_{MN})|$, $(F^a)^2_g=F^a_{M_1\cdots M_{n_a}}F^a_{N_1\cdots N_{n_a}}g^{M_1N_1}\cdots g^{M_{n_a}N_{n_a}}$, $a\in\triangle$. Here $\triangle$ is some finite set. In the models with one time all $\theta_a=1$ when the signature of the metric is $(-1,+1,\ldots,+1)$.

Let us consider (black-brane) solutions to field equations corresponding to the action (1) from Refs. 10–12. These solutions are defined on the manifold

$$M=(R_0,+\infty)\times(M_1=S^{d_1})\times(M_2=\mathbb{R})\times\cdots\times M_n, \tag{3}$$

and have the following form:

$$g=\left(\prod_{s\in S}H_s^{2h_s d(I_s)/(D-2)}\right)\left\{f^{-1}\,dR\otimes dR+R^2\,d\Omega^2_{d_1}-\left(\prod_{s\in S}H_s^{-2h_s}\right)f\,dt\otimes dt\right.$$
$$\left.+\sum_{i=3}^{n}\left(\prod_{s\in S}H_s^{-2h_s\delta_{iI_s}}\right)g^i\right\}, \tag{4}$$

$$\exp(\varphi^\alpha)=\prod_{s\in S}H_s^{h_s\chi_s\lambda^\alpha_{a_s}}, \tag{5}$$

$$F^a=\sum_{s\in S}\delta^a_{a_s}\mathcal{F}^s, \tag{6}$$

where $f=1-2\mu/R^{\overline{d}}$,

$$\mathcal{F}^s=-\frac{Q_s}{R^{d_1}}\left(\prod_{s'\in S}H_{s'}^{-A_{ss'}}\right)dR\wedge\tau(I_s),\quad s\in S_e, \tag{7}$$

$$\mathcal{F}^s=Q_s\tau(\overline{I_s}),\quad s\in S_m. \tag{8}$$

Here $Q_s \neq 0$ $(s \in S)$ are charges, $R_0 > 0$, $R_0^{\overline{d}} = 2\mu > 0$, $\overline{d} = d_1 - 1$. In (4) $g^i = g^i_{m_i n_i}(y_i) dy_i^{m_i} \otimes dy_i^{n_i}$ is a Ricci-flat metric on M_i, $i = 3,\ldots,n$ and $\delta_{iI} = \Sigma_{j \in I} \delta_{ij}$ is the indicator of i belonging to I: $\delta_{iI} = 1$ for $i \in I$ and $\delta_{iI} = 0$ otherwise. Here $g^2 = -dt \otimes dt$, and $g^1 = d\Omega_{d_1}$ be a canonical metric on unit sphere $M_1 = S^{d_1}$,

The p-brane set S is by definition

$$S = S_e \cup S_m, \quad S_v = \cup_{a \in \triangle} \{a\} \times \{v\} \times \Omega_{a,v}, \tag{9}$$

$v = e,m$ and $\Omega_{a,e}, \Omega_{a,m} \subset \Omega$, where $\Omega = \Omega(n)$ is the set of all nonempty subsets of $\{2,\ldots,n\}$, i.e., all p-branes do not "live" in M_1.

Any p-brane index $s \in S$ has the form $s = (a_s, v_s, I_s)$, where $a_s \in \triangle$, $v_s = e,m$ and $I_s \in \Omega_{a_s,v_s}$. The sets S_e and S_m define electric and magnetic p-branes, correspondingly. In (5) $\chi_s = +1,-1$ for $s \in S_e, S_m$, respectively. All p-branes contain the time manifold $M_2 = \mathbb{R}$, i.e.,

$$2 \in I_s, \quad \forall s \in S. \tag{10}$$

All manifolds M_i, $i > 2$, are oriented and connected and

$$\tau_i \equiv \sqrt{|g^i(y_i)|} dy_i^1 \wedge \cdots \wedge dy_i^{d_i}, \tag{11}$$

are volume d_i forms, where $d_i = \dim M_i$, $i = 1,\ldots,n$, with $d_1 > 1$ and $d_2 = 1$. For any $I = \{i_1,\ldots,i_k\} \in \Omega$, $i_1 < \cdots < i_k$, we denote

$$\tau(I) \equiv \tau_{i_1} \wedge \cdots \wedge \tau_{i_k}, \quad d(I) = \sum_{i \in I} d_i. \tag{12}$$

The forms $\mathcal{F}^s$ correspond to electric and magnetic p-branes for $s \in S_e, S_m$, respectively. In (8) we use the notation $\overline{I} = \{1,\ldots,n\} \setminus I$.

The parameters h_s appearing in the solution satisfy the relations: $h_s = (B_{ss})^{-1}$, where

$$B_{ss'} = d(I_s \cap I_{s'}) + \frac{d(I_s) d(I_{s'})}{2 - D} + \chi_s \chi_{s'} \lambda_{\alpha a_s} \lambda_{\beta a_{s'}} h^{\alpha\beta}, \tag{13}$$

$s, s' \in S$, with $(h^{\alpha\beta}) = (h_{\alpha\beta})^{-1}$ and $D = 1 + \Sigma_{i=1}^n d_i$. Here we assume that (i) $B_{ss} \neq 0$, $s \in S$ and (ii) $\det(B_{ss'}) \neq 0$, i.e., the matrix $(B_{ss'})$ is a nondegenerate one.

Let us consider the matrix

$$(A_{ss'}) = (2B_{ss'}/B_{s's'}). \tag{14}$$

Here some ordering in S is assumed.

The functions $H_s = H_s(z) > 0$, $z = 2\mu/R^{\overline{d}} \in (0,1)$, obey the equations

$$\frac{d}{dz}\left(\frac{(1-z)}{H_s} \frac{dH_s}{dz} \right) = B_s \prod_{s' \in S} H_{s'}^{-A_{ss'}}, \tag{15}$$

equipped with the boundary conditions

$$H_s(1-0) = H_{s0} \in (0,+\infty), \tag{16}$$

$$H_s(+0) = 1, \tag{17}$$

$s \in S$. Here $B_s = B_{ss} \epsilon_s Q_s^2 / (2\overline{d}\mu)^2$ and

$$\epsilon_s = (-\epsilon[g])^{(1-\chi_s)/2} \epsilon(I_s) \theta_{a_s}, \tag{18}$$

$s \in S$, $\epsilon[g] \equiv \operatorname{sign}\det(g_{MN})$. More explicitly Eq. (18) reads $\epsilon_s = \epsilon(I_s)\theta_{a_s}$ for $v_s = e$ and $\epsilon_s = -\epsilon[g]\epsilon(I_s)\theta_{a_s}$, for $v_s = m$.

Equations (16) are equivalent to Toda-type equations. The first boundary condition guarantees the existence of a regular horizon at $R^d = 2\mu$. The second condition (17) ensures an asymptotical flatness (for $R \to +\infty$) of the $(2+d_1)$-dimensional section of the metric.

Due to Eqs. (7) and (8), the dimension of p-brane world volume $d(I_s)$ is defined by relations $d(I_s) = n_{a_s} - 1$, $d(I_s) = D - n_{a_s} - 1$, for $s \in S_e, S_m$, respectively. For a p-brane we use a standard notation $p = p_s = d(I_s) - 1$.

The solutions are valid if the following restriction on the sets $\Omega_{a,v}$ is imposed. This restriction guarantees the block-diagonal structure of the stress-energy tensor. We denote $w_1 \equiv \{i | i \in \{2, \ldots, n\},\ d_i = 1\}$ and $n_1 = |w_1|$ (i.e., n_1 is the number of one-dimensional spaces among M_i, $i = 2, \ldots, n$). It is clear, that $2 \in w_1$.

Restriction. Let $(1a)$ $n_1 \leqslant 1$ *or* $(1b)$ $n_1 \geqslant 2$ *and for any* $a \in \Delta$, $v \in \{e, m\}$, $i, j \in w_1$, $i \neq j$, *there are no* $I, J \in \Omega_{a,v}$ *such that* $i \in I$, $j \in J$ *and* $I \backslash \{i\} = J \backslash \{j\}$.

This restriction is satisfied in the noncomposite case: $|\Omega_{a,e}| + |\Omega_{a,m}| = 1$ (i.e., when there are no two p-branes with the same color index a, $a \in \Delta$). The restriction forbids certain intersections of two p-branes with the same color index for $n_1 \geqslant 2$.

The solution under consideration describes a set of charged (by forms) overlapping black p-branes "living" on submanifolds of $M_2 \times \cdots \times M_n$.

III. EXAMPLES OF SOLUTIONS

A. "Block-orthogonal" solutions

The simplest polynomial solutions occur in orthogonal case,[18,24–27] when

$$B_{ss'} = 0, \tag{19}$$

for $s \neq s'$, $s, s' \in S$. In this case $(A_{ss'}) = \operatorname{diag}(2, \ldots, 2)$ is a Cartan matrix for semisimple Lie algebra $A_1 \oplus \cdots \oplus A_1$ and

$$H_s(z) = 1 + P_s z, \tag{20}$$

with $P_s \neq 0$, satisfying

$$P_s(P_s + 1) = -B_s, \tag{21}$$

$s \in S$. For positive parameters $P_s > 0$ we get negative $B_s < 0$.

In Refs. 19, 20, and 22 this solution was generalized to the "block-orthogonal" case,

$$S = S_1 \cup \cdots \cup S_k, \quad S_i \cap S_j = \varnothing, \quad i \neq j, \tag{22}$$

$S_i \neq \varnothing$, i.e., the set S is a union of k nonintersecting (nonempty) subsets $S_1, \ldots, S_k$, and relation (19) is satisfied for all $s \in S_i$, $s' \in S_j$, $i \neq j$; $i, j = 1, \ldots, k$. In this case Eq. (20) is modified as follows:

$$H_s(z) = (1 + P_s z)^{b^s}, \tag{23}$$

where

$$b^s = 2 \sum_{s' \in S} A^{ss'}, \tag{24}$$

$(A^{ss'})=(A_{ss'})^{-1}$ and parameters P_s are coinciding inside blocks, i.e., $P_s=P_{s'}$ for $s,s'\in S_i$, $i=1,\ldots,k$. Parameters $P_s\neq 0$ satisfy the relations (21) and parameters B_s are also coinciding inside blocks, i.e., $B_s=B_{s'}$ for $s,s'\in S_i$, $i=1,\ldots,k$.

Let $(A_{ss'})$ be a Cartan matrix for a finite-dimensional semisimple Lie algebra $\mathcal{G}$. In this case all powers in (24) are natural numbers coinciding with the components of twice the dual Weyl vector in the basis of simple roots,[28] and hence, all functions H_s are polynomials, $s\in S$.

Conjecture (Ref. 10). Let $(A_{ss'})$ be a Cartan matrix for a semisimple finite-dimensional Lie algebra $\mathcal{G}$. Then the solution to Eqs. (15)–(17) (if exists) is a polynomial

$$H_s(z)=1+\sum_{k=1}^{n_s} P_s^{(k)} z^k, \tag{25}$$

where $P_s^{(k)}$ are constants, $k=1,\ldots,n_s$, the integers $n_s=b^s$ are defined in (24) and $P_s^{(n_s)}\neq 0$, $s\in S$.

This conjecture was verified for A_n and C_n series of Lie algebras.[11,12] In the extremal case $\mu=+0$ an a analogue of this conjecture was suggested previously in Ref. 23.

B. Solution for A_2 algebra

Here we present the polynomial solution from Refs. 10 and 11 corresponding to the Lie algebra $A_2=sl(3)$ with the Cartan matrix

$$(A_{ss'})=\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}. \tag{26}$$

The moduli polynomials read in this case as follows:

$$H_s=1+P_s z+P_s^{(2)} z^2, \tag{27}$$

where $P_s=P_s^{(1)}$ and $P_s^{(2)}\neq 0$ are constants and

$$P_s^{(2)}=\frac{P_s P_{s+1}(P_s+1)}{2(P_1+P_2+2)}, \tag{28}$$

$$B_s=-\frac{P_s(P_s+1)(P_s+2)}{P_1+P_2+2}, \tag{29}$$

$s=1,2$. Here $P_1+P_2+2\neq 0$.

In the A_2-case the solution is described by relations (4)–(8) with $S=\{s_1,s_2\}$ and intersection rules following from (13), (14), and (26):

$$d(I_{s_1}\cap I_{s_2})=\frac{d(I_{s_1})d(I_{s_2})}{D-2}-\chi_{s_1}\chi_{s_2}\lambda_{a_{s_1}}\cdot\lambda_{a_{s_2}}-\frac{1}{2}K, \tag{30}$$

$$d(I_{s_i})-\frac{(d(I_{s_i}))^2}{D-2}+\lambda_{a_{s_i}}\cdot\lambda_{a_{s_i}}=K, \tag{31}$$

where $K\neq 0$ and functions $H_{s_i}=H_i$ are defined by relations (27)–(29) with $z=2\mu R^{-\bar{d}}$, $i=1,2$. Here and in what follows $\lambda\cdot\lambda'=\lambda_\alpha\lambda'_\beta h^{\alpha\beta}$.

C. Solutions for C_2 algebra

Now we present the solution related to the Lie algebra $C_2=\mathrm{so}(5)$ with the Cartan matrix

$$(A_{ss'})=\begin{pmatrix} 2 & -1 \\ -2 & 2 \end{pmatrix}. \tag{32}$$

According to "Conjecture" we seek the solution to Eqs. (15)–(17) in the following form:

$$H_1(z)=1+P_1z+P_1^{(2)}z^2+P_1^{(3)}z^3, \tag{33}$$

$$H_2(z)=1+P_2z+P_2^{(2)}z^2+P_2^{(3)}z^3+P_2^{(4)}z^4, \tag{34}$$

where $P_s=P_s^{(1)}$ and $P_s^{(k)}$ are constants, $s=1,2$.

Here we outline the result. For B_s parameters we get the following relations:

$$2B_1=-\Delta+(2P_1+3)(2+P_2), \tag{35}$$

$$B_2=\Delta-2-2P_1(P_1+3)-(2+P_2)^2, \tag{36}$$

and for parameters $P_s^{(k)}$ we obtain

$$4P_1^{(2)}=6+3P_2-\Delta+2P_1(3+P_1+P_2), \tag{37}$$

$$\begin{aligned}12P_1^{(3)}=&-\Delta(2+P_1+P_2)+12+18P_1+2P_1^3+3P_2(4+P_2)\\&+2P_1^2(5+P_2)+P_1P_2(11+2P_2),\end{aligned} \tag{38}$$

$$2P_2^{(2)}=-6-2P_1(3+P_1)-3P_2+\Delta, \tag{39}$$

$$\begin{aligned}6P_2^{(3)}=&\Delta(2+2P_1+P_2)-12-24P_1-4P_1^3-3P_2(4+P_2)\\&-2P_1P_2(7+P_2)-2P_1^2(8+P_2),\end{aligned} \tag{40}$$

$$\begin{aligned}24P_2^{(4)}=&\Delta[2P_1^2+(3+P_2)(2+2P_1+P_2)]-4P_1^4-3(2+P_2)^2(3+P_2)\\&-2P_1(3+P_2)^2(4+P_2)-4P_1^3(6+P_2)-P_1^2(60+30P_2+4P_2^2),\end{aligned} \tag{41}$$

where

$$\Delta=\sqrt{4(3+P_1(3+P_1))^2+(3+2P_1)^2P_2(4+P_2)}. \tag{42}$$

It may be verified that $B_1<0$ and $B_2<0$ for $P_1>0$, $P_2>0$.

The C_2 black-brane solution is described by relations (4)–(8), with $S=\{s_1,s_2\}$, and intersection rules following from (13), (14), and (32):

$$d(I_{s_1}\cap I_{s_2})=\frac{d(I_{s_1})d(I_{s_2})}{D-2}-\chi_{s_1}\chi_{s_2}\lambda_{a_{s_1}}\cdot\lambda_{a_{s_2}}-K, \tag{43}$$

$$d(I_{s_1})-\frac{(d(I_{s_1}))^2}{D-2}+\lambda_{a_{s_1}}\cdot\lambda_{a_{s_1}}=K, \tag{44}$$

$$d(I_{s_2})-\frac{(d(I_{s_2}))^2}{D-2}+\lambda_{a_{s_2}}\cdot\lambda_{a_{s_2}}=2K, \tag{45}$$

where $K \neq 0$ and functions $H_{s_i} = H_i$ are defined by relations (33) and (34) with $z = 2\mu R^{-\bar{d}}$, $i = 1,2$.

A simple test for verification of the relations for H_s-functions is to set $P_1 = 3P$ and $P_2 = 4P$ with $P > 0$. In this case we a get a special "block-orthogonal" solution

$$H_1(z) = (1+Pz)^3, \quad H_2(z) = (1+Pz)^4, \tag{46}$$

in agreement with the relations (23) and (24).

IV. CONCLUSIONS

In this paper we presented a new black-brane solution with two branes and intersection rule corresponding to the Lie algebra C_2. The solutions is governed by polynomials of degree 3 and 4 and the coefficients of polynomials exhibit a nontrivial dependence upon the parameters P_1 and P_2, due to appearance of the nontrivial term Δ [see (42)]. The C_2 solution differs drastically from the A_2 one, that has a rather simple analytical structure. This means that the polynomial solutions for other A_n algebras ($n > 2$) should be also nontrivial. Indeed, the C_2 solution may be extended to a special A_3 one, if we impose a restriction on the moduli polynomials H_1, H_2, H_3 of the following form: $H_1 = H_3$. (Thus, here we obtained by product a special A_3 black-brane solution.) It should be noted that A,D,E (or simply laced) Lie algebras are of much interest, since they appear for p-brane intersection rules in supergravitational models.[18] Other topics of interest are related to black-brane thermodynamics (e.g., relations for the entropy, the Hawking temperature, etc.) and analysis of post-Newtonian effects. On this way one may expect to clarify the appearance of the function Δ in the solution. But the main (mathematical) problem here is to find the polynomial solutions for all Lie algebras. This problem seems to be a very difficult one and may be of interest for mathematicians dealing with polynomials (e.g., appearing in nonlinear ordinary and partial differential equations), Lie algebras, number theory, etc.

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Cluster properties in relativistic quantum mechanics of *N*-particle systems

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A general technique is presented for constructing a quantum theory of a finite number of interacting particles satisfying Poincaré invariance, cluster separability, and the spectral condition. Irreducible representations and Clebsch–Gordan coefficients of the Poincaré group are the central elements of the construction. A different realization of the dynamics is obtained for each basis of an irreducible representation of the Poincaré group. Unitary operators that relate the different realizations of the dynamis are constructed. This technique is distinguished from other solutions [S. N. Sokolov, Dokl. Akad. Nauk USSR **233**, 575 (1977); F. Coester and W. N. Polyzou, Phys. Rev. D **26**, 1348 (1982)] of this problem because it does not depend on the kinematic subgroups of Dirac's forms [P. A. M. Dirac, Rev. Mod. Phys. **21**, 392 (1949)] of dynamics. Special basis choices lead to kinematic subgroups. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1516627]

I. INTRODUCTION

This article illustrates a general method for constructing a relativistic quantum theory of N-interacting particles. The theory has a dynamical unitary representation of the Poincaré group, satisfies cluster separability, and has a four-momentum operator with spectrum in the future-pointing cone. These are the minimal elements of any physically motivated axioms of relativistic quantum theory.

Relativistic quantum theory of particles falls between nonrelativistic quantum theory and local relativistic quantum field theory. It is interesting because it provides a mathematically well-defined framework for realizing the symmetry of special relativity in quantum theories. This makes it useful for applications to systems of a few strongly interacting particles.

The relativistic quantum theory constructed in this article has many properties of local relativistic quantum field theory.[1] Both are quantum theories satisfying Poincaré invariance, cluster separability, and the spectral condition. The most significant distinction between the two theories is that local relativistic quantum field theory satisfies a microscopic locality constraint, which requires an infinite number of degrees of freedom.

The absence of theories that are simultaneously consistent with the axioms of local quantum field theory and applicable to realistic systems suggests that mathematically well-behaved alternatives might be well-suited to applications involving strongly interacting particles.

The essential features of quantum theory of particles are as follows:

(1) The model Hilbert space is the finite tensor product of single-particle Hilbert spaces. This defines the degrees of freedom of the model.

(2) There is a unitary representation of the Poincaré group $\hat{U}(\Lambda, Y)$ on the model Hilbert space. This ensures that the quantum probabilities are independent of inertial frame. This representation necessarily contains the dynamics.

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(3) The four-momentum operators, which are the infinitesimal generators of the space–time translation subgroup of $\hat{U}(\Lambda,Y)$, have a spectrum in the future-pointing light cone. This ensures the stability of the theory.
(4) The operator $\hat{U}(\Lambda,y)$ can be approximated by a tensor product of $\hat{U}_i(\Lambda,y)$'s on vectors describing subsets of particles in asymptotically separated regions. This justifies experiments on isolated subsystems and provides the relation between few- and many-body systems.
(5) The scattering operator is unitary and Poincaré invariant.

While relativistic quantum theory of particles is useful, independent of a relation to local quantum field theory, any local field theory should be well approximated by a quantum theory of particles when it is applied to reactions involving a finite number of particles. Because the defining requirements of relativistic quantum theory of particles are a subset of the axioms of local relativistic quantum field theory, the consequences of these requirements on the structure of the models of interacting particles are the same in both theories.

The Poincaré symmetry makes the problem of constructing a dynamical theory difficult. Poincaré covariance of the dynamics involves nonlinear constraints. The requirement that these constraints are preserved when the system is separated into isolated subsystems introduces additional nonlinear constraints. These difficulties were recognized by Dirac[2] and have been pointed out in a recent text by Weinberg.[3]

The essential role of unitary representations of the Poincaré group in relativistic quantum theory was first emphasized by Wigner[4] in 1939. Most applications to finite systems of interacting particles cite Dirac's[2] 1949 paper, which identified the essential difficulty and introduced kinematic subgroups associated with different ''forms of dynamics.'' These subgroups, which reduce the number of constraints on the interactions, have played a role in all subsequent theoretical development.

The problem of constructing interacting unitary representations of the Poincaré group was first solved for the two-particle system by Bakamjian and Thomas[5] in 1953. A three-particle solution satisfying S-matrix clustering was given by Coester in 1965.[6] The first complete solution of the problem for N particles was given by Sokolov in 1977.[7] A general solution in all of Dirac's forms of dynamics appears in Refs. 8 and 9.

Relativistic quantum theory of particles is a practical framework for applications to few-hadron[10–17] and few-quark systems.[18–22] All of these application are formulated in one of Dirac's forms of dynamics; they are limited to systems where cluster properties can be trivially realized.

The construction in this article is directly motivated by Wigner's 1939 paper and makes essential use of irreducible representations of the Poincaré group. It generalizes the two-body construction of Ref. 23 and leads to a relativistic N-body dynamics satisfying cluster properties and the spectral condition. Groups of unitary transformations that preserve the S-matrix and cluster properties are constructed. In the general construction all of the Poincaré generators may be interaction dependent. The kinematic subgroup symmetries can be implemented by imposing additional constraints on the general construction.

The resulting dynamics has interactions in between three and ten of the Poincaré generators. Unitary operators that preserve the S-matrix and cluster properties redistribute the interactions in ways that may be advantageous for different applications. These unitary operators are elements of a C^* algebra of asymptotic constants, which is relevant for identifying physically equivalent theories.

This article is organized as follows. Section II contains a brief account of Wigner's formulation of relativistic quantum mechanics, which is central to the construction in this paper. Sections III–VI summarize the group theory that is needed to construct the required representations. These sections discuss inhomogeneous $SL(2,C)(ISL(2,C))$, which is the covering group of the Poincaré group, irreducible representations of $ISL(2,C)$, and Clebsch–Gordan coefficients of $ISL(2,C)$. Section VII provides an introduction to relativistic scattering theory, which is used in the general construction. This formulation of scattering theory does not assume the existence of a kinematic

subgroup. Section VIII introduces the cluster separability condition. Section IX introduces the C^* algebra of asymptotic constants and its unitary elements, which are called scattering equivalences. This algebra provides a functional calculus of noncommuting operators that is used to establish cluster properties. Section X introduces the Möbius and Zeta function of the lattice of partitions. These combinatoric tools, which generalize standard Ursell cumulant expansions, are used extensively in the construction of the N-body dynamics. Section XI contains the general solution of the two-body problem, which is the starting point of the recursive construction, and Sec. XII contains the recursive N-body construction. Section XIII constructs scattering and cluster equivalences that relate dynamical models that utilize different bases. Section XIV has conclusions. Technical aspects of the construction are included in the four appendices.

II. RELATIVITY IN QUANTUM MECHANICS

In 1939 Wigner[4] showed that the relativistic invariance of all quantum probabilities

$$P_{\psi\phi} := |\langle \psi | \phi \rangle|^2 \tag{1}$$

is equivalent to the existence of a unitary representation of the Poincaré group. This was refined by Bargmann in 1954,[24] who observed that the dynamics could be realized by a single valued unitary representation of the covering group, $ISL(2,C)$, of the Poincaré group. The central problem of relativistic quantum mechanics is to construct a unitary representation $\hat{U}[\Lambda,Y]$ of $ISL(2,C)$ which implements the dynamics.

III. INHOMOGENEOUS $SL(2,C)$

In this section $ISL(2,C)$ is defined and related to the Poincaré group. Elements of $ISL(2,C)$ consist of ordered pairs of complex 2×2 matrices (Λ,Y), where Λ has determinant 1 and Y is Hermitian. The group product is

$$(\Lambda_2,Y_2)(\Lambda_1,Y_1)=(\Lambda_2\Lambda_1,\Lambda_2 Y_1 \Lambda_2^\dagger + Y_2). \tag{2}$$

The relation to four-dimensional Poincaré transformations follows by representing four vectors x^μ by 2×2 Hermitian matrices X:

$$X := x^\mu \sigma_\mu, \quad x^\mu = \tfrac{1}{2}\mathrm{Tr}(X\sigma_\mu) \tag{3}$$

where σ_0 is the identity and σ_i are the Pauli matrices. In this matrix representation $ISL(2,C)$ transformations are affine transformations of the form

$$X' = \Lambda X \Lambda^\dagger + Y. \tag{4}$$

Any Poincaré transformation continuously connected to the identity can be represented in the form (4).

Elements of $ISL(2,C)$ can be parametrized by three components of a rotation vector $\vec{\theta}$, three components of a rapidity vector $\vec{\rho}$, and a space–time translation four vector y^μ:

$$\Lambda(\vec{\theta},\vec{\rho}) = e^{-(i/2)(\vec{\theta}+i\vec{\rho})\cdot\vec{\sigma}}, \quad Y(y) := y^\mu \sigma_\mu. \tag{5}$$

Thus, the relativistic quantum dynamics, $\hat{U}[\Lambda,Y]$, satisfies

$$\hat{U}^\dagger[\Lambda,Y] = \hat{U}^{-1}[\Lambda,Y] = \hat{U}[\Lambda^{-1}, -\Lambda^{-1}Y(\Lambda^{-1})^\dagger] \tag{6}$$

and

$$\hat{U}[\Lambda_2,Y_2]\hat{U}[\Lambda_1,Y_1] = \hat{U}[\Lambda_2\Lambda_1, \Lambda_2 Y_1 \Lambda_2^\dagger + Y_2]. \tag{7}$$

IV. $ISL(2,C)$ GENERATORS

The infinitesimal generators of $\hat{U}[\Lambda,Y]$ are defined. These operators are used to identify a maximal set of commuting self-adjoint operators. For structureless particles the eigenvalues of these commuting operators label the state of the particle. The spectrum of these operators is determined by the eigenvalues of the invariant mass and spin operators, which define an irreducible subspace, and group theoretic considerations. The single-particle Hilbert space is the space of square integrable functions of these eigenvalues.

The ten parameters $y^\mu, \vec{\theta}, \vec{\rho}$ have the property that if any nine of them are set to zero, the group becomes a one-parameter unitary group with respect to the remaining parameter. These unitary one-parameter groups necessarily have the form $\hat{U}(\lambda)=e^{-i\lambda\hat{G}}$ for a self-adjoint operator $\hat{G}$.[25] Thus a unitary representation $\hat{U}[\Lambda,Y]$ of $ISL(2,C)$ can be parametrized as

$$\hat{U}[\Lambda(\vec{\theta},\vec{\rho}),I]=e^{-i(\vec{\theta}\cdot\hat{\vec{J}}+\vec{\rho}\cdot\hat{\vec{K}})}, \tag{8}$$

$$\hat{U}[I,Y(y)]=e^{i(\vec{y}\cdot\hat{\vec{P}}-y^0\hat{H})}, \tag{9}$$

with self-adjoint generators $\hat{H},\hat{\vec{P}},\hat{\vec{J}}$ and $\hat{\vec{K}}$.

The commutation relations of the generators follow from the group representation property (7) and the definition (8) and (9) of the generators.[26] The commutation relations are consistent with $\hat{P}^\mu:=(\hat{H},\hat{\vec{P}})$ transforming as a four-vector operator

$$\hat{U}[\Lambda,0]\hat{P}^\mu\hat{U}^\dagger[\Lambda,0]=\hat{P}^\nu\Lambda^\mu_\nu, \tag{10}$$

and

$$\hat{J}^{\mu\nu}:=\begin{pmatrix} 0 & \hat{K}^1 & \hat{K}^2 & \hat{K}^3 \\ -\hat{K}^1 & 0 & \hat{J}^3 & -\hat{J}^2 \\ -\hat{K}^2 & -\hat{J}^3 & 0 & \hat{J}^1 \\ -\hat{K}^3 & \hat{J}^2 & -\hat{J}^1 & 0 \end{pmatrix} \tag{11}$$

transforming as a rank-two antisymmetric tensor operator:

$$\hat{U}[\Lambda,0]\hat{J}^{\mu\nu}\hat{U}^\dagger[\Lambda,0]=\hat{J}^{\alpha\beta}\Lambda^\mu_\alpha\Lambda^\nu_\beta. \tag{12}$$

The Pauli–Lubanski vector $\hat{W}^\mu$ is a four-vector valued function of $\hat{P}^\mu$ and $\hat{J}^{\mu\nu}$:

$$\hat{W}^\mu:=\tfrac{1}{2}\epsilon^{\mu\alpha\beta\gamma}\hat{P}_\alpha\hat{J}_{\beta\gamma} \tag{13}$$

satisfying

$$[\hat{J}^j,\hat{W}^k]_-=i\epsilon^{jkl}\hat{W}^l, \quad [\hat{J}^j,\hat{W}^0]_-=0, \tag{14}$$

$$[\hat{K}^j,\hat{W}^k]_-=-i\delta^{jk}\hat{W}^0, \quad [\hat{K}^j,\hat{W}^0]_-=-i\hat{W}^j, \tag{15}$$

$$[\hat{P}^\mu,\hat{W}^\nu]_-=0, \tag{16}$$

$$[\hat{W}^\mu,\hat{W}^\nu]_-=i\epsilon^{\mu\nu\rho\eta}\hat{W}_\rho\hat{P}_\eta, \quad \hat{W}^\mu\hat{P}_\mu=0. \tag{17}$$

The scalar operators

$$\hat{M}^2 = -\hat{P}^\mu \hat{P}_\mu \tag{18}$$

and

$$\hat{W}^2 = \hat{W}^\mu \hat{W}_\mu \tag{19}$$

are the two independent invariant polynomial functions of the generators[27] of $ISL(2,C)$.

When the spectrum of the mass operator is positive, the spin-squared operator is defined by

$$\hat{j}^2 := \frac{\hat{W}^2}{\hat{M}^2}. \tag{20}$$

V. IRREDUCIBLE REPRESENTATIONS OF $ISL(2,C)$

The Hilbert space for an N-particle system is the tensor product of single particle Hilbert spaces. Single particle Hilbert spaces are irreducible representation spaces of $ISL(2,C)$. The irreducible representations are labeled by the mass and spin of a particle. Eigenvalues of additional commuting self-adjoint functions of the $ISL(2,C)$ generators are needed to specify the state of the particle. Simultaneous eigenstates of the commuting self-adjoint operators define a basis in the irreducible representation space. The single particle Hilbert space is the space of square integrable functions of the eigenvalues.

The irreducible representations of the $ISL(2,C)$ were classified by Wigner.[6,28,29,5] The displacement $x_a^\mu - x_b^\mu$ between events a and b can be classified into six invariant classes depending on whether this displacement is zero, lightlike positive time, lightlike negative time, spacelike, timelike positive time, or timelike negative time.

The irreducible representations corresponding to massive particles are the timelike positive-time representations. These irreducible representations of $ISL(2,C)$ are labeled by the invariant eigenvalues of the mass (18) and spin operators (20). For a particle the mass eigenvalue m is discrete and the spin operator has the eigenvalue $j(j+1)$ where j is the spin of the particle.

The state of a structureless particle of mass m and spin j is determined by specifying the eigenvalues of a maximal set of commuting self-adjoint operators. These operators are the invariant mass $\hat{M}$, the spin $\hat{j}^2$ and four independent functions, $\hat{F}^i = F^i(\hat{P}^\mu, \hat{J}^{\mu\nu})$, of the $ISL(2,C)$ generators. The operators $\hat{F}^j$ cannot be invariant. They are arbitrary independent functions of the $ISL(2,C)$ generators subject to the constraints:

$$\hat{F}^i = (\hat{F}^i)^\dagger, \quad [\hat{F}^i, \hat{F}^j] = 0, \tag{21}$$

$$[\hat{F}^i, \hat{M}] = [\hat{F}^i, \hat{j}^2] = 0. \tag{22}$$

For particles with structure, additional invariant degeneracy operators are needed to get a maximal set of commuting operators.

The traditional choice for the operators $\hat{F}^i$ are the three components of the linear momentum $\hat{\vec{P}}$ and the z-component of the canonical[26] spin $\hat{z} \cdot \hat{\vec{j}}_c$. In some applications it is advantageous to use the four velocity, the light-front components of the four momentum, or their conjugate variables. The helicity or light-front spin is sometimes used instead of the canonical spin. Any of the spin observables could be replaced by a component of the Pauli–Lubanski operator. These special cases are treated in Appendix A. Each choice of $\hat{F}^i$ corresponds to a single particle basis. In this article the operators $\hat{F}^i$ are assumed to have a spectrum independent of the mass eigenvalue. This condition is not very restrictive and holds for all conventional choices.

The Hilbert space for a particle of mass m and spin j can be represented as the space of square integrable functions of the eigenvalues of the operators $\hat{F}^i$:

$$\mathcal{H}_{mj}=\left\{\langle f|\psi\rangle\left|\int d\mu(f)|\langle f|\psi\rangle|^2\right.\right\}<\infty, \tag{23}$$

where $f=\{f^1\cdots f^4\}$ and $\int d\mu(f)$ indicates a sum over the discrete eigenvalues and an integral over the continuous eigenvalues of $\hat{F}^i$.

Basis vectors have the form

$$|f\rangle:=|f;m,j\rangle:=|f^1,f^2,f^3,f^4;m,j\rangle. \tag{24}$$

The normalization convention is

$$\langle f|f'\rangle=\delta[f,f'], \tag{25}$$

where $\delta[f,f']$ is the product of Dirac or Kronecker delta functions in the variables f^i.

Irreducibility requires the transformation property:

$$\hat{U}[\Lambda,Y]|f;m,j\rangle=\int|f';m,j\rangle d\mu(f')\mathcal{D}^{m,j}_{f',f}[\Lambda,Y], \tag{26}$$

where

$$\mathcal{D}^{m,j}_{f',f}[\Lambda,Y]\delta_{m'm}\delta_{j'j}:=\langle f';m',j'|\hat{U}[\Lambda,Y]|f;m,j\rangle \tag{27}$$

is the mass m, spin j irreducible representation of $ISL(2,C)$ in the basis $\hat{F}^j$. The $\mathcal{D}$-function includes δ-functions that eliminate the integrals over the continuous spectrum in (26). Unitarity of the group representation property requires

$$\mathcal{D}^{m,j}_{f',f}[\Lambda,Y]=(\mathcal{D}^{m,j}_{f,f'}[\Lambda^{-1},-\Lambda Y\Lambda^{\dagger}])^* \tag{28}$$

and

$$\int\mathcal{D}^{m,j}_{f',f''}[\Lambda_2,Y_2]d\mu(f'')\mathcal{D}^{m,j}_{f'',f}[\Lambda_1,Y_1]=\mathcal{D}^{m,j}_{f',f}[\Lambda_2\Lambda_1,\Lambda_2Y_1\Lambda_2^{\dagger}+Y_2]. \tag{29}$$

The restriction on the spectrum of $\hat{F}^i$ implies that range of values of f in $\mathcal{D}^{m,j}_{f',f}[\Lambda,Y]$ is independent of m.

Explicit representations for the $ISL(2,C)$ Wigner $\mathcal{D}$-functions corresponding to different $\hat{F}^i$ are given in Appendix A. The form of the $\mathcal{D}$-functions is basis dependent.

Irreducible representations in a basis of simultaneous eigenstates of a different set of commuting self-adjoint functions, $\hat{G}^i$, of the generators are related to the representations in the basis $\hat{F}^i$ by

$$\mathcal{D}^{m,j}_{g,g'}[\Lambda,Y]=\int\langle g|f\rangle d\mu(f)\mathcal{D}^{m,j}_{f,f'}[\Lambda,Y]d\mu(f')\langle f'|g'\rangle, \tag{30}$$

where

$$\langle f|g\rangle\delta_{mm'}\delta_{jj'}:=\langle f;m,j|g;m',j'\rangle. \tag{31}$$

The coefficient functions $\langle f|g\rangle$ can depend parametrically on the mass or spin. This parametric dependence on the mass is responsible for the dynamical differences that arise with different basis choices.

VI. CLEBSCH–GORDAN COEFFICIENTS

In this section Clebsch–Gordan coefficients[8,26,28,29] and Racah coefficients of $ISL(2,C)$ are defined. These are used to expand tensor products of irreducible representation as linear superpositions of irreducible representations and to transform between irreducible bases with different degeneracy quantum numbers.

The tensor product of irreducible representations of $ISL(2,C)$ is reducible. The $ISL(2,C)$ generators for a tensor product of two irreducible representations are

$$\hat{P}^\mu = \hat{P}_1^\mu \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{P}_2^\mu, \tag{32}$$

$$\hat{J}^{\mu\nu} = \hat{J}_1^{\mu\nu} \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{J}_2^{\mu\nu}. \tag{33}$$

These operators act on the space

$$\mathcal{H} = \mathcal{H}_{m_1 j_1} \otimes \mathcal{H}_{m_2 j_2}. \tag{34}$$

The operators $\hat{F}^i = F^i(\hat{P}^\mu, \hat{J}^{\mu\nu})$, $\hat{M} = M(\hat{P}^\mu, \hat{J}^{\mu\nu})$, and $\hat{j}^2 = j^2(\hat{P}^\mu, \hat{J}^{\mu\nu})$ are commuting self-adjoint operators on $\mathcal{H}$. Because the tensor product is reducible, these operators do not define a maximal set of commuting self-adjoint operators. There are additional $ISL(2,C)$ invariant degeneracy operators $\hat{D}^j$ that distinguish multiple copies of the same irreducible representation. The degeneracy operators $\hat{D}^i$ normally include the invariant operators $\hat{M}_1$, $\hat{j}_1$, $\hat{M}_2$, $\hat{j}_2$ of the factors of the tensor product and additional operators, $\hat{R}_{12}$, that distinguish multiple copies of the m,j representation in the tensor product of the m_1,j_1 and m_2,j_2 representations.

The operators $\hat{D}^j$ are invariant, self-adjoint functions of the single particle generators. The operators $\hat{M}$, $\hat{j}^2$, $\hat{F}^1,\ldots,\hat{F}^4$, $\hat{D}^1,\ldots,\hat{D}^6$ form a maximal set of commuting self-adjoint operators on $\mathcal{H}$. Examples are given in the Appendix B.

The (f,d) basis is the $ISL(2,C)$-irreducible basis for the tensor product space defined in terms of simultaneous eigenstates, $|f,d;m,j\rangle$ of

$$\{\hat{F}^i, \hat{D}^k; \hat{M}, \hat{j}^2\}. \tag{35}$$

It follows that

$$\hat{U}_1[\Lambda,Y] \otimes \hat{U}_2[\Lambda,Y] |f,d;m,j\rangle = \int |f',d;m,j\rangle d\mu(f') \mathcal{D}^{m,j}_{f',f}[\Lambda,Y], \tag{36}$$

where $\mathcal{D}^{m,j}_{f',f}[\Lambda,Y]$ is the irreducible representation matrix for a single particle of mass m and spin j. The $\mathcal{D}$-function is independent of the invariant degeneracy parameters, d.

The coefficients

$$\langle f_1;m_1,j_1:f_2;m_2,j_2|f,d;m,j\rangle \tag{37}$$

are Clebsch–Gordan coefficients of the Poincaré group in the (f,d) basis. They are the kernel of the unitary transformation that relates tensor products of $ISL(2,C)$ irreducible representations to direct integrals of irreducible representations. The $ISL(2,C)$ Clebsch–Gordan coefficients have similar properties to $SU(2)$ Clebsch–Gordan coefficients:

$$\int \mathcal{D}^{m_1,j_1}_{f_1,f_1'}[\Lambda,Y] \mathcal{D}^{m_2,j_2}_{f_2,f_2'}[\Lambda,Y] d\mu(f_1') d\mu(f_2') \langle f_1';m_1,j_1:f_2';m_2,j_2|f,d;m,j\rangle$$
$$= \int \langle f_1;m_1,j_1:f_2;m_2,j_2|f',d;m,j\rangle d\mu(f') \mathcal{D}^{m,j}_{f',f}[\Lambda,Y]. \tag{38}$$

The new feature is that the irreducible representations are labeled by two Casimir operators and the mass operator has a continuous spectrum.

It is sometimes useful to replace the mass operator $\hat{M}$ of the tensor product of two irreducible representations by the invariant relative momentum $\hat{q}^2$, which has absolutely continuous spectrum, $[0,\infty)$:

$$\hat{q}^2 = q^2(\hat{M}^2,\hat{M}_1^2,\hat{M}_2^2) := \frac{\hat{M}^4+\hat{M}_1^4+\hat{M}_2^4-2\hat{M}_1^2\hat{M}_2^2-2\hat{M}^2\hat{M}_1^2-2\hat{M}^2\hat{M}_2^2}{4\hat{M}^2}. \tag{39}$$

The Clebsch–Gordan coefficients have different forms in different bases. If $(f,d)\rightarrow(g,k)$, then the Clebsch–Gordan coefficients in the (f,d) basis are related to the Clebsch–Gordan coefficients in the (g,k) basis by

$$\begin{aligned}&\langle g_1;m_1,j_1:g_2;m_2,j_2|g,k;m,j\rangle\\ &\quad=\int \langle g_1|f_1'\rangle\langle g_2|f_2'\rangle d\mu(f_1')d\mu(f_2')\langle f_1';m_1,j_1:f_2';m_2,j_2|f',d';m,j\rangle d\mu(f',d')\\ &\qquad\times\langle f',d'|g,k\rangle,\end{aligned} \tag{40}$$

where

$$\langle g_i|f_i'\rangle\delta_{j_ij_i'}\delta_{m_im_i'} := \langle g_i;m_i,j_i|f_i';m_i',j_i'\rangle \tag{41}$$

and

$$\delta_{jj'}\delta(m-m')\langle f,d|g',k'\rangle := \langle f,d;m,j|g',k';m',j'\rangle. \tag{42}$$

The Hilbert space for a system of N-particles is the N-fold tensor product of single particle Hilbert spaces:

$$\mathcal{H}=\mathcal{H}_{m_1j_1}\otimes\cdots\otimes\mathcal{H}_{m_Nj_N}. \tag{43}$$

The noninteracting representation of $ISL(2,C)$ on $\mathcal{H}$ is defined by

$$\hat{U}_0[\Lambda,Y] := \hat{U}_1[\Lambda,Y]\otimes\cdots\otimes\hat{U}_N[\Lambda,Y], \tag{44}$$

where the 0 subscript is used to denote the noninteracting system. It follows that

$$\hat{U}_0[\Lambda,Y]|f_1;m_1,j_1\cdots f_N;m_N,j_N\rangle=\int |f_1';m_1,j_1:\cdots f_N';m_N,j_N\rangle d\mu(f_1'\cdots f_N')\prod_{i=1}^{N}\mathcal{D}_{f_i',f_i}^{m_i,j_i}[\Lambda,Y]. \tag{45}$$

As in the case of $SU(2)$, the tensor product of N irreducible representation spaces can be decomposed into a direct integral of irreducible representation spaces using successive pairwise coupling. The invariant degeneracy operators depend on the order of the coupling. It is also possible to use a simultaneous coupling scheme based on Mackey's[30] theory of induced representations[9] which leads to a symmetric coupling.

Successive pairwise coupling is illustrated for the three-particle system:

$$|f,d_{((12)3)};m,j\rangle = \int |f_1;m_1,j_1:f_2;m_2,j_2:f_3;m_3,j_3\rangle d\mu(f_1)d\mu(f_2)$$
$$\times\langle f_1;m_1,j_1:f_2;m_2,j_2|f_{12},d_{12};m_{12},j_{12}\rangle d\mu(f_{12})d\mu(f_3)d\mu(m_{12},j_{12})$$
$$\times\langle f_{12};m_{12},j_{12}:f_3;m_3,j_3|f,d_{12,3};m,j\rangle, \tag{46}$$

where the invariant degeneracy parameters are

$$d_{12,3}=\{d_{12},m_{12},j_{12},m_3,j_3,r_{12,3}\} \tag{47}$$

with

$$d_{12}=\{m_1,j_1,m_2,j_2,r_{12}\}. \tag{48}$$

Changing the ordering of the coupling from ((12)3) to ((23)1) changes the degeneracy parameters from $\{r_{12},j_{12},m_{12},r_{12,3}\}$ to $\{r_{23},j_{23},m_{23},r_{23,1}\}$, leaving the operators $\hat{M},\hat{j}^2$ and $\hat{F}^i$ unchanged. The overlap coefficients have the general form

$$\langle f,d_{ab,c}(m,j)|f',d'_{ef,g}(m',j')\rangle = \delta[f,f']\delta_{jj'}\delta(m-m')R^{m,j}_{d_{a,bc},d'_{e,fg}}. \tag{49}$$

The invariant quantities $R^{m,j}_{d_{a,bc},d'_{e,fg}}$ are Racah coefficients for $ISL(2,C)$. They are the kernel of the unitary transformation that changes the choice of degeneracy labels in subspaces corresponding the same mass, spin, and vector labels f. They are independent of f.

The Racah coefficients are important for performing computations because, as in the case of rotations, some operators have a simple form when the couplings are done in a specific order. Since many of the operators are defined in specific representations, the Racah coefficients are needed for the evaluation of the abstract operator expressions.

The term Racah coefficient is used to indicate any change of irreducible basis with matrix elements of the form (49). Examples of Racah coefficients in representative bases are given in Appendix B.

VII. RELATIVISTIC SCATTERING THEORY

Relativistic scattering theory is formulated in this section. A kinematic subgroup is not assumed. The two-Hilbert space formulation[6,8,31] is used to treat multichannel scattering theory. The notation of this section follows Ref. 8. Conditions on the interactions that are sufficient for a sensible relativistic scattering theory are discussed. Relativistic two-Hilbert-space wave operators are essential elements of the general construction.

In this section the dynamical representation $\hat{U}[\Lambda,Y]$ of $ISL(2,C)$ is assumed to be given. The construction of $\hat{U}[\Lambda,Y]$ is the main topic of the remainder of this article.

The first step in formulating relativistic scattering theory is to determine the bound states of $\hat{U}[\Lambda,Y]$; subsystem bound states are needed to formulate the asymptotic conditions in multichannel scattering.

Bound states are associated with point eigenvalues of the mass and spin. For each bound-state channel α_b there is an irreducible subspace of $\mathcal{H}$. Vectors in the bound state subspace can be expressed as linear superpositions of simultaneous eigenstates of $\hat{M},\hat{j}^2,\hat{F}^i$:

$$|\phi_{\alpha_b}\rangle = \int |f;m_\alpha,j_\alpha\rangle d\mu(f)\langle f|\chi\rangle, \tag{50}$$

where in this expression $\hat{F}^i=F^i(\hat{P}^\mu,\hat{J}^{\mu\nu})$ are functions of the generators of $\hat{U}[\Lambda,Y]$.

The channel eigenstate $|f;m_{\alpha_b},j_{\alpha_b}\rangle$ can be considered as a mapping, $\hat{\Phi}_{\alpha_b}$, from the channel Hilbert space $\mathcal{H}_{\alpha_b}$,

$$\mathcal{H}_{\alpha_b}=\left\{\langle f|\chi_\alpha\rangle\middle|\int\langle f|\chi_\alpha\rangle|^2 d\mu(f)<\infty\right\}, \tag{51}$$

to the invariant bound-state subspace of the Hilbert space $\mathcal{H}$,

$$\hat{\Phi}_{\alpha_b}|\chi_\alpha\rangle:=|\phi_{\alpha_b}\rangle=\int|f;m_\alpha,j_\alpha\rangle d\mu(f)\langle f|\chi_\alpha\rangle. \tag{52}$$

For each bound channel α_b there is a channel injection operator $\hat{\Phi}_{\alpha_b}$ and a channel Hilbert space $\mathcal{H}_{\alpha_b}$. Since the bound channel spaces are irreducible representation spaces with respect to $\hat{U}[\Lambda,Y]$, the channel eigenstates transform irreducibly

$$\hat{U}[\Lambda,Y]|f;m_{\alpha_b},j_{\alpha_b}\rangle=\int|f';m_{\alpha_b},j_{\alpha_b}\rangle d\mu(f')\mathcal{D}^{m_{\alpha_b},j_{\alpha_b}}_{f',f}[\Lambda,Y]. \tag{53}$$

Equation (53) can be expressed in terms of the channel injection operator as

$$\hat{U}[\Lambda,Y]\hat{\Phi}_{\alpha_b}=\hat{\Phi}_{\alpha_b}\hat{U}_{\alpha_b}[\Lambda,Y]. \tag{54}$$

Scattering states are solutions of the time-dependent Schrödinger equation that look like mutually noninteracting bound or elementary subsystems in the asymptotic past or future. To formulate the asymptotic condition let a denote a partition of N particles into n_a disjoint nonempty clusters. Denote the ith cluster by a_i and the number of particles in the i-th cluster by n_{a_i}.

For any partition a, the N-particle Hilbert space can be factored into a tensor product of subsystem Hilbert spaces $\mathcal{H}_{a_i}$:

$$\mathcal{H}=\otimes_{i=1}^{n_a}\mathcal{H}_{a_i}, \tag{55}$$

$$\mathcal{H}_{a_i}=\otimes_{l\in a_i}\mathcal{H}_{m_l j_l}. \tag{56}$$

A partition a has a scattering channel α if the subsystem dynamics

$$\hat{U}_{a_i}[\Lambda,Y]:\mathcal{H}_{a_i}\to\mathcal{H}_{a_i} \tag{57}$$

associated with each cluster of a is either a one particle cluster or has a bound state.

For each bound subsystem channel, α_i, there is an injection operator, an asymptotic Hilbert space,

$$\hat{\Phi}_{\alpha_i}:\mathcal{H}_{\alpha_i}\to\mathcal{H}_{a_i}, \tag{58}$$

and an irreducible asymptotic representation $\hat{U}_{\alpha_i}[\Lambda,Y]$ of $ISL(2,C)$ on $\mathcal{H}_{\alpha_i}$ satisfying

$$\hat{U}_{a_i}[\Lambda,Y]\hat{\Phi}_{\alpha_i}=\hat{\Phi}_{\alpha_i}\hat{U}_{\alpha_i}[\Lambda,Y]. \tag{59}$$

These relations hold trivially for the one particle clusters. The asymptotic Hilbert space for the scattering channel α is defined as the tensor product of the bound channel subspaces for the subsystems:

$$\mathcal{H}_\alpha=\otimes_{i=1}^{n_a}\mathcal{H}_{\alpha_i}. \tag{60}$$

The channel injection operator

$$\hat{\Phi}_\alpha : \mathcal{H}_\alpha \to \mathcal{H} \tag{61}$$

is defined by

$$\hat{\Phi}_\alpha := \otimes_{i=1}^{n_a} \hat{\Phi}_{\alpha_i}. \tag{62}$$

It follows from (59) that $\hat{\Phi}_\alpha$ satisfies the intertwining relation

$$\hat{U}_a[\Lambda, Y]\hat{\Phi}_\alpha = \hat{\Phi}_\alpha \hat{U}_\alpha[\Lambda, Y], \tag{63}$$

where

$$\hat{U}_a[\Lambda, Y] := \otimes_{i=1}^{n_a} \hat{U}_{a_i}[\Lambda, Y] \tag{64}$$

and

$$\hat{U}_\alpha[\Lambda, Y] := \otimes_{i=1}^{n_a} \hat{U}_{\alpha_i}[\Lambda, Y]. \tag{65}$$

In this notation a scattering state is a solution

$$|\psi_\alpha^\pm(t)\rangle = \hat{U}[I,T]|\psi_\alpha^\pm\rangle, \quad T := t\sigma_0 \tag{66}$$

of the time-dependent Schrödinger equation satisfying the asymptotic condition

$$\lim_{t\to\pm\infty} \| |\psi_\alpha^\pm(t)\rangle - \hat{U}_a[I,T]\hat{\Phi}_\alpha|\chi_\alpha\rangle \| \tag{67}$$

for $|\chi_\alpha\rangle \in \mathcal{H}_\alpha$.

Equation (63) can be used to express the asymptotic condition as

$$\lim_{t\to\pm\infty} \| |\psi_\alpha^\pm\rangle - \hat{U}[I,-T]\hat{\Phi}_\alpha \hat{U}_\alpha[I,T]|\chi_\alpha\rangle \| = 0, \tag{68}$$

which is identically satisfied by the bound-state channels.

Equation (68) can be expressed as

$$|\psi_\alpha^\pm\rangle := \hat{\Omega}_{\alpha\pm}|\chi_\alpha\rangle, \tag{69}$$

where the channel wave operators

$$\hat{\Omega}_{\alpha\pm} : \mathcal{H}_\alpha \to \mathcal{H} \tag{70}$$

are defined by the strong limits

$$\hat{\Omega}_{\alpha\pm} := \lim_{t\to\pm\infty} \hat{U}(I,-T)\hat{\Phi}_\alpha \hat{U}_\alpha(I,T). \tag{71}$$

A sufficient condition for the existence of the channel wave operators is the Cook condition:[32]

$$\int_{t_c}^{\infty} \| \hat{V}_\alpha \hat{U}_\alpha(I, \pm T)|\chi\rangle \| dt < \infty, \tag{72}$$

where t_c is any constant and

$$\hat{V}_\alpha := \hat{H}\hat{\Phi}_\alpha - \hat{\Phi}_\alpha \hat{H}_\alpha . \tag{73}$$

The scattering operator for scattering from channel α to channel β is the mapping from $\mathcal{H}_\alpha \to \mathcal{H}_\beta$ defined by

$$\hat{S}_{\beta\alpha} := \hat{\Omega}^\dagger_{\beta+} \hat{\Omega}_{\alpha-} . \tag{74}$$

This can be expressed compactly in a two-Hilbert-space notation, where the asymptotic Hilbert space, $\mathcal{H}_\mathcal{A}$, is the orthogonal direct sum of all of the channel spaces, including the bound state channel spaces:

$$\mathcal{H}_\mathcal{A} = \oplus_\alpha \mathcal{H}_\alpha . \tag{75}$$

A two-Hilbert-space injection operator $\hat{\Phi}_\mathcal{A}$,

$$\hat{\Phi}_\mathcal{A} : \mathcal{H}_\mathcal{A} \to \mathcal{H}, \tag{76}$$

is defined as the sum of the channel injection operators

$$\hat{\Phi}_\mathcal{A} = \sum_\alpha \hat{\Phi}_\alpha , \tag{77}$$

where it is understood that each $\hat{\Phi}_\alpha$ acts on the channel subspace $\mathcal{H}_\alpha$ of $\mathcal{H}_\mathcal{A}$.

There is a natural unitary representation of $ISL(2,C)$ on $\mathcal{H}_\mathcal{A}$ which transforms the particles or bound states as tensor products of irreducible representations:

$$\hat{U}_\mathcal{A}[\Lambda, Y] = \sum_\alpha \hat{U}_\alpha[\Lambda, Y], \tag{78}$$

where $\hat{U}_\alpha[\Lambda, Y] : \mathcal{H}_\alpha \to \mathcal{H}_\alpha$.

The bound state solutions and the scattering asymptotic conditions can be replaced by one two-Hilbert-space equation:

$$\Omega_\pm(\hat{H}, \hat{\Phi}_\mathcal{A}, \hat{H}_\mathcal{A}) = \lim_{t \to \pm\infty} \hat{U}[I, -T] \hat{\Phi}_\mathcal{A} \hat{U}_\mathcal{A}[I, T], \tag{79}$$

where the limit is a strong limit. The wave operators $\Omega_\pm(\hat{H}, \hat{\Phi}_\mathcal{A}, \hat{H}_\mathcal{A})$ are mappings from $\mathcal{H}_\mathcal{A} \to \mathcal{H}$.

The scattering operator $\hat{S}$ is a mapping from $\mathcal{H}_\mathcal{A} \to \mathcal{H}_\mathcal{A}$ defined by

$$\hat{S} := \Omega^\dagger_+(\hat{H}, \hat{\Phi}_\mathcal{A}, \hat{H}_\mathcal{A}) \Omega_-(\hat{H}, \hat{\Phi}_\mathcal{A}, \hat{H}_\mathcal{A}). \tag{80}$$

The dynamics is asymptotically complete if the two-Hilbert space wave operators $\Omega_\pm(\hat{H}, \hat{\Phi}_\mathcal{A}, \hat{H}_\mathcal{A})$, which include all bound state channels, are unitary mappings from $\mathcal{H}_\mathcal{A}$ to $\mathcal{H}$. In all that follows the two-Hilbert-space wave operators are assumed exist and to be unitary. These properties can be proved using the same methods used in nonrelativistic scattering theory.

Fong and Sucher[8,33–35] showed that relativistic invariance of the scattering operator does not follow from the existence of $\hat{U}[\Lambda, Y]$. This is because the $ISL(2,C)$ transformations must commute with the limiting operations that are used to construct the scattering operator.

Invariance of $\hat{S}$ is equivalent to the condition

$$[\hat{U}_\mathcal{A}[\Lambda, Y], \hat{S}]_- = 0. \tag{81}$$

The following theorem provides a sufficient condition on $\hat{U}[\Lambda,Y]$ for the $ISL(2,C)$ invariance of the S-matrix:

Theorem 1: Let $\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})$ be asymptotically complete two-Hilbert-space wave operators. A sufficient condition for $\hat{S}$ to be $ISL(2,C)$ invariant is that for all Λ and Y

$$\lim_{t\to\pm\infty}(\hat{\Phi}_{\mathcal{A}}-\hat{U}^{\dagger}[\Lambda,Y]\hat{\Phi}_{\mathcal{A}}\hat{U}_{\mathcal{A}}[\Lambda,Y])\hat{U}_{\mathcal{A}}[I,T]=0, \tag{82}$$

and for any Y of the form $Y=\vec{y}\cdot\vec{\sigma}$

$$\lim_{t\to\pm\infty}(\hat{\Phi}_{\mathcal{A}}-\hat{U}^{\dagger}[I,Yt]\hat{\Phi}_{\mathcal{A}}\hat{U}_{\mathcal{A}}[I,Yt])\hat{U}_{\mathcal{A}}[I,T]=0. \tag{83}$$

The limits above are strong limits. They must hold for both time directions.

Theorem 1 provides sufficient conditions on the interactions in the generators for a sensible relativistic scattering theory. The proof of this theorem is given in Appendix C.

The proof of Theorem 1 has a number of useful corollaries:

Corollary 1: If the conditions of Theorem 1 are satisfied, then

$$\hat{U}[\Lambda,Y]\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[\Lambda,Y]. \tag{84}$$

This intertwining property ensures the $ISL(2,C)$ invariance of S.

Corollary 2: If the conditions of Theorem 1 are satisfied, then

$$\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\Omega_{\pm}(\hat{P}\cdot y,\hat{\Phi}_{\mathcal{A}},\hat{P}_{\mathcal{A}}\cdot y), \tag{85}$$

where y is any future-pointing timelike four-vector.

This means that all future pointing timelike directions are equivalent for the purpose of formulating the asymptotic condition.

Corollary 3: If the conditions of Theorem 1 are satisfied, then

$$\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\Omega_{\pm}(\hat{M},\hat{\Phi}_{\mathcal{A}},\hat{M}_{\mathcal{A}}). \tag{86}$$

This shows that in applications the Hamiltonian can be replaced by the mass operator in the wave operators. Both representations of the two-Hilbert-space wave operators are used in the remainder of this article.

Theorem 1 and its corollaries define conditions on the interactions that ensure that the dynamics is consistent with naive expectations for a relativistic scattering theory. In all that follows it is assumed that the two-Hilbert-space wave operators exist, are complete, and the dynamical operators satisfy (82) and (83).

VIII. CLUSTER PROPERTIES

Cluster properties provide the essential connection between the few- and many-body problem. The cluster property requires that few-body interactions in the few-body problem are identical to the few-body interactions in the many-body problem. This establishes the justification for performing experiments on few-body systems.

The difficulty in satisfying cluster properties is that the interactions that appear in the $ISL(2,C)$ generators are uniquely determined by cluster properties up to an N-body interaction. Unfortunately, the $ISL(2,C)$ commutation relations put nonlinear constraints on the N-body interactions which cannot be satisfied by setting these interactions to zero.

To formulate cluster properties let a be a partition of the N-particle systems into n_a disjoint clusters. Let $\hat{U}_{a_i}[\Lambda,Y]$ be the subsystem representation of $ISL(2,C)$ for the particles in the ith cluster of a. Define the cluster translation operator $\hat{T}_a(Y_1,\ldots,Y_{n_a})$ on $\mathcal{H}$ by

$$\hat{T}_a[Y_1,\ldots,Y_{n_a}] := \otimes \hat{U}_{a_i}[I,Y_i]. \tag{87}$$

The dynamical representation of the Poincaré group satisfies strong cluster properties if for all partitions a and all $|\chi\rangle \in \mathcal{H}$

$$\lim_{\min(y_i-y_j)^2\to+\infty} \|(\hat{U}[\Lambda,Y]-\otimes_{i=1}^{n_a}\hat{U}_{a_i}[\Lambda,Y])\hat{T}_a[Y_1,\ldots,Y_{n_a}]|\chi\rangle\| = 0. \tag{88}$$

Cluster properties will hold if (a)

$$\hat{U}[\Lambda,Y]\to U_a[\Lambda,Y] = \otimes_{i=1}^{n_a}\hat{U}_{a_i}[\Lambda,Y], \tag{89}$$

when the interactions involving particles in different clusters of a are set to zero and (b) all of the interactions in each generator $\hat{G}$ satisfy

$$\lim_{\min(y_i-y_j)^2\to+\infty} \|(\hat{G}-\hat{G}_a)\hat{T}_a[Y_1,\ldots,Y_{n_a}]|\chi\rangle\| = 0, \tag{90}$$

where $\hat{G}$ and $\hat{G}_a$ are the $ISL(2,C)$ generators associated with $\hat{U}[\Lambda,Y]$ and $U_a[\Lambda,Y]$, respectively.

Condition (a) is called the algebraic cluster property.[8] It puts the nonlinear constraints on the interactions of a relativistic quantum theory. It ensures that once the interactions between particles in different clusters are turned off, the remainder is a tensor product. This condition is nontrivial because it must hold for every possible clustering.

The condition (b) is related to the range of the interaction. If the operators satisfy algebraic cluster properties, the proof of the short range condition is similar to the nonrelativistic proof[36] of cluster properties. In all that follows the interaction terms are assumed to satisfy condition (b).

When $\hat{U}[\Lambda,Y]$ does not satisfy algebraic cluster properties the limit (88) may not exist. A typical consequence is that the cluster limit eliminates interactions between particles in the *same* cluster.[26]

The cluster condition (88) is a strong form of the cluster condition. It is also possible to formulate a weaker form of the cluster condition that applies only to the scattering matrix.[8] The stronger form is needed for the recursive construction in Secs. XII and XIII.

IX. SCATTERING EQUIVALENCES

There is a large class of dynamical models with the same S-matrix. These models are called scattering equivalent models.[37] The freedom to transform between scattering equivalent models with different properties is an important tool for realizing cluster properties. What separates scattering equivalent models from unitary equivalent models is that scattering equivalent models do not change the description of free particles. They provide a parametrization of the freedom that is created by restricting the class of physical observables to asymptotic quantities ($t\to\pm\infty$).

While scattering equivalences necessarily preserve cluster properties of the S-matrix, they do not preserve cluster properties of the representation $\hat{U}[\Lambda,Y]$. Because of this property, scattering equivalences can be used to restore cluster properties of the dynamics.

The key to understanding scattering equivalences is to understand the algebra of operators that are asymptotically zero. A bounded operator $\hat{Z}$ on the N-particle Hilbert space is asymptotically zero if the following strong limits vanish:

$$\lim_{t\to\pm\infty} \hat{Z}\hat{U}_0[I,T]|\psi\rangle = 0, \tag{91}$$

$$\lim_{t\to\pm\infty}\hat{Z}^\dagger\hat{U}_0[I,T]|\psi\rangle=0, \tag{92}$$

for *both* time limits, where

$$T=t\sigma_0. \tag{93}$$

The subset of bounded operators that are asymptotically zero are denoted by $\mathcal{Z}$. It is straightforward to show that for $\hat{Z}_n\in\mathcal{Z}$ and α complex that

$$\alpha\hat{Z}_1+\hat{Z}_2\in\mathcal{Z}, \tag{94}$$

$$\hat{Z}_1\hat{Z}_2\in\mathcal{Z}, \tag{95}$$

$$\hat{Z}_1^\dagger\in\mathcal{Z}, \tag{96}$$

$$\|\hat{Z}_n-\hat{Z}\|\to 0\Rightarrow\hat{Z}\in\mathcal{Z}. \tag{97}$$

Including the identity makes a C^* algebra, which we call the algebra of asymptotic constants, $\mathcal{C}$.

A scattering equivalence $\hat{A}$ is a unitary member of $\mathcal{C}$ that is asymptotically equal to the identity $\hat{I}$:

$$\lim_{t\to\pm\infty}(\hat{A}-\hat{I})\hat{U}_0[I,T]|\psi\rangle=0; \tag{98}$$

$$\lim_{t\to\pm\infty}(\hat{A}^\dagger-\hat{I})\hat{U}_0[I,T]|\psi\rangle=0. \tag{99}$$

The relation of these operators to scattering is through the following theorems:

Theorem 2: Let $\hat{A}$ be a scattering equivalence. Let $\Omega_\pm(\hat{H},\hat{\Phi}_\mathcal{A},\hat{H}_\mathcal{A})$ be asymptotically complete two-Hilbert-space wave operators. Let $\hat{H}'=\hat{A}\hat{H}\hat{A}^\dagger$ and $\hat{\Phi}'_\mathcal{A}=\hat{A}\hat{\Phi}_\mathcal{A}$. Then $\Omega_\pm(\hat{H}',\hat{\Phi}'_\mathcal{A},\hat{H}_\mathcal{A})$ exist, are asymptotically complete, and give the same S matrix as $\Omega_\pm(\hat{H},\hat{\Phi}_\mathcal{A},\hat{H}_\mathcal{A})$.

The proof follows from the identity

$$\hat{A}\Omega_\pm(\hat{H},\hat{\Phi}_\mathcal{A},\hat{H}_\mathcal{A})=\Omega_\pm(\hat{H}',\hat{\Phi}'_\mathcal{A},\hat{H}_\mathcal{A}). \tag{100}$$

While the structure of the injection operator $\hat{\Phi}_\mathcal{A}$ depends on the representation of the subsystem bound states, it must become the identity in the scattering channel, $(\alpha=\alpha_0)$, corresponding to N free particles. Note that $\hat{\Phi}'_{\alpha_0}=\hat{A}\hat{I}=\hat{I}+\hat{Z}\neq\hat{I}$ where $\hat{Z}$ is asymptotically zero. This ensures that $\hat{\Phi}'_\mathcal{A}$ can be replaced by another injection operator, $\hat{\Phi}''_\mathcal{A}$, with $\hat{\Phi}''_{\alpha_0}=\hat{I}$:

$$\hat{\Phi}''_\mathcal{A}=\hat{\Phi}'_\mathcal{A}-\delta_{\alpha\alpha_0}\hat{Z}. \tag{101}$$

It follows that

$$\Omega_\pm(\hat{H}',\hat{\Phi}'_\mathcal{A},\hat{H}_{\alpha_0})=\Omega_\pm(\hat{H}',\hat{\Phi}''_\mathcal{A},\hat{H}_{\alpha_0}), \tag{102}$$

where $\hat{\Phi}''_{\alpha_0}=\hat{I}$.

Scattering equivalences are naturally constructed from pairs of wave operators that give the same S-matrix.

Theorem 3: Let $\hat{\Omega}_{\pm} := \Omega_{\pm}(\hat{H}, \hat{\Phi}_{\mathcal{A}}, \hat{H}_{\mathcal{A}})$ and $\hat{\Omega}'_{\pm} := \Omega_{\pm}(\hat{H}', \hat{\Phi}'_{\mathcal{A}}, \hat{H}_{\mathcal{A}})$ be asymptotically complete wave operators that give the same scattering matrix. Then there is a scattering equivalence $\hat{A}$ satisfying $\hat{H}' = \hat{A}\hat{H}\hat{A}^{\dagger}$.

To prove Theorem 3 note that the assumptions imply

$$S = \hat{\Omega}_{+}^{\dagger}\hat{\Omega}_{-} = \hat{\Omega}_{+}'^{\dagger}\hat{\Omega}'_{-}. \tag{103}$$

Asymptotic completeness implies

$$\hat{A} := \hat{\Omega}'_{+}\hat{\Omega}_{+}^{\dagger} = \hat{\Omega}'_{-}\hat{\Omega}_{-}^{\dagger}. \tag{104}$$

This definition and the intertwining relations[36] for the Hamiltonian give

$$\hat{A}\hat{H}\hat{A}^{\dagger} = \hat{\Omega}'_{+}\hat{H}_{\mathcal{A}}\hat{\Omega}_{+}^{\dagger}\hat{A}^{\dagger} = \hat{H}'\hat{\Omega}'_{+}\hat{\Omega}_{+}^{\dagger}\hat{A}^{\dagger} = \hat{H}'. \tag{105}$$

Equations (104) and (105) imply

$$\Omega_{\pm}(\hat{H}', \hat{\Phi}'_{\mathcal{A}}, \hat{H}_{\mathcal{A}}) = \hat{A}\Omega_{\pm}(\hat{H}, \hat{\Phi}_{\mathcal{A}}, \hat{H}_{\mathcal{A}}) = \Omega_{\pm}(\hat{H}', \hat{A}\hat{\Phi}_{\mathcal{A}}, \hat{H}_{\mathcal{A}}). \tag{106}$$

The equality of the first and last terms gives the strong limit

$$\lim_{t \to \pm\infty} (\hat{\Phi}'_{\mathcal{A}} - \hat{A}\hat{\Phi}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[I,T] = 0. \tag{107}$$

Unitarity of $\hat{A}$ gives

$$\lim_{t \to \pm\infty} (\hat{A}^{\dagger}\hat{\Phi}'_{\mathcal{A}} - \hat{\Phi}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[I,T] = 0; \tag{108}$$

restricting to the α_0 channel, using $\hat{\Phi}_{\alpha_0} = \hat{\Phi}'_{\alpha_0} = \hat{I}$ and $\hat{U}_{\alpha_0}[I,T] = \hat{U}_0[I,T]$ gives

$$\lim_{t \to \pm\infty} (\hat{A} - \hat{I})\hat{U}_0[I,T] = 0 \tag{109}$$

and

$$\lim_{t \to \pm\infty} (\hat{A}^{\dagger} - \hat{I})\hat{U}_0[I,T] = 0, \tag{110}$$

which establishes that $\hat{A}$ is a scattering equivalence.

This shows that if two asymptotically complete wave operators give the same scattering matrix, then the Hamiltonians are related by a scattering equivalence. Since $\hat{A}$ is unitary it follows that

$$\hat{U}'[\Lambda, Y] := \hat{A}\hat{U}[\Lambda, Y]\hat{A}^{\dagger} \tag{111}$$

is a scattering equivalent representation of $ISL(2,C)$.

The important property of the scattering equivalences is that they are the unitary elements of the C^* algebra of asymptotic constants. The C^* algebra can be used to construct functions of the noncommuting scattering equivalences. When these functions are unitary and can be expressed as uniform limits of elements of this algebra, they are scattering equivalences. This provides the mechanism for constructing scattering equivalences with specialized properties.

X. BIRKHOFF LATTICES:

The construction of operators satisfying cluster properties requires a significant amount of algebra involving cluster expansions of operators. The theory of Birkhoff lattices[8,38–41] facilitates the required algebra. It provides closed-form expressions relating different standard cluster expansions of operators.

Let $\mathcal{P}$ denote the set of all possible partitions of N-particles into disjoint nonempty clusters. There is a natural partial ordering on $\mathcal{P}$ given by

$$a \supseteq b \tag{112}$$

if and only if every pair of particles in the same cluster of b is in the same cluster of a. This means that b can be obtained from a by breaking up clusters.

The Zeta and Möbius functions[38,41] for this partial ordering are integer valued functions on $\mathcal{P}\times\mathcal{P}$ defined by

$$\zeta(a \supseteq b) = \begin{cases} 1, & a \supseteq b, \\ 0, & \text{otherwise}, \end{cases} \tag{113}$$

and

$$\mu(a \supseteq b) = \zeta^{-1}(a \supseteq b) = \begin{cases} (-)^{n_a} \prod_{i=1}^{n_a} (-)^{n_{b_i}} (n_{b_i}-1)!, & a \supseteq b, \\ 0, & \text{otherwise}, \end{cases} \tag{114}$$

where n_{b_i} are the number of clusters of b in the ith cluster of a. Note that both $\zeta(a \supseteq b)$ and $\mu(a \supseteq b)$ vanish unless $a \supseteq b$.

Intersections and unions, $a \cap b$ and $a \cup b$, of two partitions a and b are defined as the greatest lower bound and least upper bound with respect to this partial ordering.

It follows from the definitions that

$$\zeta((a \cap b) \supseteq c) = \zeta(a \supseteq c)\zeta(b \supseteq c), \tag{115}$$

$$\zeta(a \supseteq (b \cup c)) = \zeta(a \supseteq b)\zeta(a \supseteq c). \tag{116}$$

The set of partitions with the operations $\cup$ and $\cap$ form a semimodular lattice,[38] called a partition or Birkhoff lattice. It provides a convenient means for keeping track of interactions. Let $\mathcal{O}$ be an operator that is a function of the physical $ISL(2,C)$ infinitesimal generators. Imagine putting a parameter λ_i in front of each interaction that appears in the physical $ISL(2,C)$ generators. The operator $\mathcal{O}_a$ is defined to be the result of turning off the interactions between particles in different clusters of a. In general the operator $\mathcal{O}_a$ will include the contributions of operators in $\mathcal{O}_b$ for all $a \supset b$. These can be recursively subtracted to construct truncated contributions $[\mathcal{O}]_b$ to $\mathcal{O}_a$. The truncated operators $[\mathcal{O}]_a$ vanish whenever interactions involving particles in *any* cluster of a are turned off. Then the Möbius function can be used to generate closed form expressions for the truncated operators in terms of the untruncated $\mathcal{O}_a$'s:

$$[\mathcal{O}]_a := \sum_b \mu(a \supseteq b)\mathcal{O}_b. \tag{117}$$

This can be inverted using the Zeta function to get

$$\mathcal{O}_a := \sum_b \zeta(a \supseteq b)[\mathcal{O}]_b. \tag{118}$$

If this is applied to the case where a is the one-cluster partition, this becomes

$$\mathcal{O}=\sum_b [\mathcal{O}]_b . \tag{119}$$

While this generates the standard relations between ordinary multipoint functions and truncated multipoint functions based on cluster expansion methods, use of the lattice structure, and specifically the underlying partial ordering, has advantages that are useful in the recursive construction described in Secs. XII and XIII.

XI. TWO-BODY PROBLEM

The construction of two-body models follows.[23] The two-body Hilbert space is the tensor product of single particle spaces

$$\mathcal{H}=\mathcal{H}_{m_1 j_1}\otimes\mathcal{H}_{m_2 j_2}. \tag{120}$$

Choose a basis (f,d) and use the Clebsch–Gordan coefficient,

$$\langle f_1;m_1,j_1:f_2;m_2,j_2|f,d;m,j\rangle, \tag{121}$$

to construct an irreducible free-particle basis. The states

$$|f,d;m,j\rangle \tag{122}$$

transform as mass m, spin j irreducible representations of $ISL(2,C)$ with respect to the noninteracting representation

$$\hat{U}_0[\Lambda,Y]:=\hat{U}_1[\Lambda,Y]\otimes\hat{U}_2[\Lambda,Y]. \tag{123}$$

Using the $ISL(2,C)$ transformation properties it is possible to construct operators $\Delta\hat{F}_0^i$ that change the value of f^i, holding the values of f^j $(j\neq i)$ constant. If $\hat{F}_0^i$ has a continuous spectrum, these operators are proportional to partial derivatives

$$\Delta\hat{F}_0^j=i\frac{\partial}{\partial f^j} \tag{124}$$

holding $f^k;k\neq j$ constant. If F_0^j has discrete eigenvalues, a suitable $\Delta\hat{F}_0^j$ can typically be expressed in terms of a raising or lowering operators.

The operators $\hat{M}_0$, $\hat{j}_0^2$, $\hat{F}_0^i$, $\Delta\hat{F}_0^i$ are functions of the free particle generators. Expression for the generators in terms of these operator can be constructed using the $ISL(2,C)$ $\mathcal{D}$-functions:

$$\langle f,d;m,j|\vec{K}_0|f',d';m,s\rangle:=i\frac{\partial}{\partial\vec{\rho}}\mathcal{D}^{m,j}_{f,f'}[\Lambda(\theta=0,\rho),0]\delta[d,d']\delta(m-m')\delta_{jj'}, \tag{125}$$

$$\langle f,d;m,j|\vec{J}_0|f',d';m,j\rangle:=i\frac{\partial}{\partial\vec{\theta}}\mathcal{D}^{m,j}_{f,f'}[\Lambda(\theta,\rho=0),0]\delta[d,d']\delta(m-m')\delta_{jj'}, \tag{126}$$

$$\langle f,d;m,j|P_0^\mu|f',d';m,j\rangle:=-i\frac{\partial}{\partial y_\mu}\mathcal{D}^{m,j}_{f,f'}[I,Y(y)]\delta[d,d']\delta(m-m')\delta_{jj'}, \tag{127}$$

where all derivatives are computed at 0.

The chain rule gives explicit expressions for the $ISL(2,C)$ generators in terms of the operators $\hat{M}_0,\hat{j}_0^2,\hat{F}_0^i,\Delta\hat{F}_{i0}$:

$$\hat{P}_0^\mu = \hat{P}^\mu(\hat{M}_0, \hat{j}_0, \hat{F}_0^i, \Delta\hat{F}_0^i), \tag{128}$$

$$\hat{J}_0^{\mu\nu} = \hat{J}^{\mu\nu}(\hat{M}_0, \hat{j}_0, \hat{F}_0^i, \Delta\hat{F}_0^i). \tag{129}$$

These expressions can be inverted to express $\hat{M}_0, \hat{j}_0^2, \hat{F}_0^i, \Delta\hat{F}_{i0}$ in terms of the $ISL(2,C)$ generators:

$$\hat{M}_0 = M(\hat{P}_0^\mu, \hat{J}_0^{\mu\nu}), \tag{130}$$

$$\hat{j}_0^2 = j_0(\hat{P}_0^\mu, \hat{J}_0^{\mu\nu}), \tag{131}$$

$$\hat{F}_0^i = F^j(\hat{P}_0^\mu, \hat{J}_0^{\mu\nu}), \tag{132}$$

$$\Delta\hat{F}_{i0} = \Delta F^j(\hat{P}_0^\mu, \hat{J}_0^{\mu\nu}). \tag{133}$$

Examples of these operators for specific basis choices are computed in Appendix A to illustrate the general procedure.

Since $\hat{M}_0^2$ is a Casimir operator for $ISL(2,C)$, it necessarily commutes with $\hat{j}_0^2$, $\hat{F}_0^i$, and $\Delta\hat{F}_0^i$. The $ISL(2,C)$ commutation relations follow as consequences of the commutation relations of $\hat{M}_0$, $\hat{j}_0^2$, $\hat{F}_0^i$, and $\Delta\hat{F}_0^i$.

It follows that in order to construct a dynamical representation of $ISL(2,C)$ it is enough to replace $\hat{M}_0$ by an operator $\hat{M} = \hat{M}_0 + \hat{V}$ which also commutes with $\hat{j}_0^2$, $\hat{F}_{i0}$, and $\Delta\hat{F}_{i0}$. With this choice of interaction it follows that the operators

$$\hat{P}_0^\mu \to \hat{P}^\mu = \hat{P}^\mu(\hat{M}, \hat{j}_0^2, \hat{F}_0^i, \Delta\hat{F}_0^i), \tag{134}$$

$$\hat{J}_0^{\mu\nu} \to \hat{J}^{\mu\nu} = \hat{J}^{\mu\nu}(\hat{M}, \hat{j}_0^2, \hat{F}_0^i, \Delta\hat{F}_0^i) \tag{135}$$

automatically satisfy the $ISL(2,C)$ Lie algebra.

Cluster properties are satisfied for sufficiently short-range interactions. For the interaction to be nontrivial it should also satisfy

$$[\hat{M}, \hat{M}_0] \neq 0 \tag{136}$$

and the spectral condition, $\hat{M}_0 > \hat{V}$. In general the interaction can be treated as a perturbation of different functions of $\hat{M}_0$, such as $\hat{M}_0^2$. In all cases the interactions can be put in the form $\hat{M} = \hat{M}_0 + \hat{V}$ by defining $\hat{V} := \hat{M} - \hat{M}_0$, independent of how $\hat{M}$ is constructed. The spectral condition constrains the interaction.

In the free particle irreducible basis an interaction $\hat{V}$ commuting with $\hat{j}_0^2$, $\hat{F}_0^i$, and $\Delta\hat{F}_0^i$ has a kernel with the structure

$$\langle f,d;m,j|\hat{V}|f',d';m',j'\rangle = \delta[f,f']\delta_{jj'}\langle d,m\|\hat{V}_j\|d',m'\rangle. \tag{137}$$

The dynamical generators are given by (134) and (135) with $\hat{M} = \hat{M}_0 + \hat{V}$. If the expression for a generator in (134) or (135) has an explicit mass dependence, the corresponding operator will be interaction dependent. Depending on the choice of basis (f,d) between three and ten generators will have an explicit interaction dependence. Dirac's forms of dynamics result from specific basis choices. A generic choice will not have a kinematic subgroup.

While it is straightforward to derive explicit expressions for the generators in terms of the $\hat{F}^i$'s, (see Appendix A) it is easier to directly solve for the dynamics in the free particle basis $|f,d;m,j\rangle$.

In this basis $\hat{M}$, $\hat{F}_0^i$, $\hat{j}_0$ can be simultaneously diagonalized:

$$\langle f',d';m',j'|f;m,j\rangle = \delta[f,f']\delta_{jj'}\phi_m^j(d',m'), \tag{138}$$

where $\phi_m^j(d',m')$ is the solution of the mass eigenvalue equation

$$(m-m')\phi_m^j(d',m') = \sum \int dm''dd''\langle d',m'\|\hat{V}_j\|d''m''\rangle\phi_m^j(d'',m''). \tag{139}$$

For suitable interactions $\hat{M}$ will be self-adjoint and the eigenstates $|f,d;m,j\rangle$ will define a complete set of simultaneous eigenstates of $\hat{M}$, $\hat{F}_0^i$, $\hat{j}_0^2$. Solving equation (139) is of comparable difficulty to solving the time-independent nonrelativistic Schrödinger equation. It is assumed that the eigenstates include two-body bound states and scattering states satisfying incoming and outgoing wave asymptotic conditions.

Since the expressions (125)–(127) for the $ISL(2,C)$ generators were derived by evaluating the infinitesimal transformations in an irreducible basis, and $\{\hat{M}_0,\hat{F}_0^i,\Delta\hat{F}_0^i,\hat{j}_0\}$ and $\{\hat{M},\hat{F}_0^i,\Delta\hat{F}_0^i,\hat{j}_0\}$ have the same commutation relations, the action of the dynamical representation of $ISL(2,C)$ on the eigenstates $|f;m,j\rangle$ has the same form as the free dynamics on $|f,d;m_0,j\rangle$, with the eigenvalue of $\hat{M}_0$ replaced by the eigenvalue of $\hat{M}$. It follows that

$$\hat{U}[\Lambda,Y]|f;m,j\rangle = |f';m,j\rangle d\mu(f')\mathcal{D}^{m,j}_{f',f}[\Lambda,Y]. \tag{140}$$

Since the states $|f;j,m\rangle$ are complete, this defines $\hat{U}[\Lambda,Y]$ on $\mathcal{H}$. Since m is the eigenvalue of a dynamical operator, all of the mass dependent parts of $\mathcal{D}^{mj}_{f'f}[\Lambda,Y]$ are interaction dependent.

This construction gives (1) an explicit expressions for the interaction dependent $ISL(2,C)$ Lie algebra, (2) a solution of the two-body dynamics expressed as a direct integral of irreducible representations of $ISL(2,C)$, and (3) and an explicit unitary representation of $ISL(2,C)$ on $\mathcal{H}$.

This construction can be done in any irreducible basis. Consider the same construction in two bases (f,d) and (g,d) where, for simplicity, the degeneracy operators in both bases are assumed to have the same spectrum. In one model the interaction commutes with $\hat{F}^i$, while in the other the interaction commutes with $\hat{G}^i$. Because $\hat{M}$ does not commute with $\hat{M}_0$, if the relation between the (f,d) and (g,d) bases involves the mass, these two interactions cannot be the same.

Nevertheless, the form of the dynamical equation (139) is identical in both cases. Both will give the same bound state masses and scattering matrix elements. It follows, using Theorem 3, that the dynamical models constructed using the free particle bases

$$(\hat{F},\hat{d},\hat{M}_1) \quad \text{and} \quad (\hat{G},\hat{d},\hat{M}_2) \tag{141}$$

are scattering equivalent and are related by

$$\hat{A} = \Omega_{\pm}(\hat{M}_1,\hat{\Phi}_1,\hat{M}_{\mathcal{A}})\Omega_{\pm}^{\dagger}(\hat{M}_2,\hat{\Phi}_2,\hat{M}_{\mathcal{A}}). \tag{142}$$

The transformation $\hat{A}$ is not simply a change of basis; it is interaction dependent and changes the nature of the interactions. This illustrates the relation of the basis choice to the structure of the dynamics.

To understand the nature of the interaction dependence of $\hat{A}$ note that both wave operators in (142) need to be computed in the same basis. This leads to an expression of the form

$$\langle f|\hat{A}|f'\rangle = \int \langle f|\Omega_{\pm}(\hat{M}_f,\hat{\Phi}_f,\hat{M}_{\mathcal{A}})|f''\rangle d\mu(f'')\langle f''|g''\rangle_{\mathcal{A}} d\mu(g'')$$
$$\times\langle g''|\Omega_{\pm}^{\dagger}(\hat{M}_g,\hat{\Phi}_g,\hat{M}_{\mathcal{A}})|g'\rangle d\mu(g')\langle g'|f'\rangle. \tag{143}$$

If the change of basis $f \leftrightarrow g$ involves the mass parametrically, then $\langle f|g\rangle_{\mathcal{A}}$ will involve the physical mass eigenvalues while $\langle g|f\rangle$ involves the noninteracting masses. The interaction dependence is due to having the interacting mass in one of these expressions and the free mass in the inverse expression. In the limit that the interactions are turned off, this becomes the identity.

This completes the construction of the two-body dynamics. The construction provides a relativistic two-body model for any choice of basis and $ISL(2,C)$ Clebsch–Gordan coefficient.

To illustrate the structure of the dynamical equation in a familiar basis consider the case (see Appendix B) that $\hat{F}=\{\hat{\vec{P}},\hat{j}_{cz}\}$, corresponding to the linear momentum and z-component of the canonical spin, and $\hat{D}^i=\{j_1,m_1,j_2,m_2,\hat{l},\hat{s}\}$ where $\hat{l},\hat{s}$ are two-body orbital and spin angular momenta. The matrix elements of $\hat{V}=\hat{M}-\hat{M}_0$ have the form

$$\langle p,\mu,l,s;m,j|\hat{V}|p',\mu',l',s';m',j'\rangle=\delta(\vec{p}-\vec{p}')\,\delta_{\mu\mu'}\,\delta_{jj'}\langle l,s,m\|\hat{V}^j\|l',s',m\rangle. \tag{144}$$

If m is replaced by the kinematic momentum q defined by

$$m=\sqrt{q^2+m_1^2}+\sqrt{q^2+m_2^2}, \tag{145}$$

the matrix element (144) has the same structure as the corresponding nonrelativistic interaction. The eigenvalue equation (139) becomes:

$$\begin{aligned}(m-\sqrt{q^2+m_1^2}+\sqrt{q^2+m_2^2})\,\phi^j_m(l,s,q)&\\ =\sum_{l'=0}^{\infty}\sum_{s'=|j-l|}^{|j+l|}\int_0^\infty q'^2 dq'\langle l,s,q\|\hat{V}^j\|l',s',q'\rangle\,\phi^j_m(l',s',q').&\end{aligned} \tag{146}$$

XII. THE *N*-BODY PROBLEM

The formulation of the N-body problem is by induction. The construction follows.[7–9] What is different is that the notion of ''form of the dynamics'' is replaced by a choice (f,d) of basis for $ISL(2,C)$ irreducible representation spaces and associated Clebsch–Gordan coefficients.

The construction of the N-body dynamics exploits the scattering equivalence of two representations of $ISL(2,C)$. One representation satisfies algebraic cluster properties and the other has a kinematic spin, which is useful for the $ISL(2,C)$ invariant addition of interactions.

The construction begins with the decomposition of the system into interacting subsystems, which are obtained by turning off the interactions between particles in different clusters of a partition a. The tensor product of the subsystem representations define unitary representation of $ISL(2,C)$ on the N-body Hilbert space. These representations are reducible and have interactions in both the N-body mass and spin operators. As a runs over all partitions these representations contain all interactions except the N-body interactions. Because the mass and spin operators for different decompositions into subsystems do not all commute, these tensor product representations are not suited to $ISL(2,C)$ invariant addition of interactions.

In order to facilitate the invariant addition of interactions, scattering equivalences are introduced that transform each of the tensor product representations into scattering equivalent representations of $ISL(2,C)$ where $\hat{j}^2$, $\hat{F}^j$, and $\Delta\hat{F}^j$ are free of interaction. In these representations all of the interactions are in the mass operators. Linear combinations of the mass operators for different decompositions into subsystems can be used to construct an overall N-body mass operator $\overline{M}$ that still commutes with the noninteracting operators j_0^2, $\hat{F}_0^j$, and $\Delta\hat{F}_0^j$.

The existence of the required scattering equivalences follows by induction from properties of the two-body solution. This is different than the solution presented in Ref. 8 where the kinematic subgroup and the $\vec{p}=0$ condition played a central role in establishing the required scattering equivalences.

The properties of $\overline{M}$ guarantee that $ISL(2,C)$ generators expressed as functions of $\overline{M}$, j_0^2, $\hat{F}_0^j$, and $\Delta\hat{F}_0^j$ satisfy the $ISL(2,C)$ commutation relations. The associated unitary representation of

$ISL(2,C)$, which is constructed using the same method used in the two-body construction, does not satisfy algebraic cluster properties for $N>2$. Cluster properties are restored by constructing a suitable scattering equivalence, which introduces additional many-body interactions and introduces a non-trivial interaction dependence in the spin.

The induction begins with the two-body dynamics formulated in the previous section. The dynamical two-body representation, $\hat{U}[\Lambda,Y]$, of $ISL(2,C)$ satisfies the following:

(i) It becomes the tensor product of two one-body representations when the interaction is set to zero:

$$\hat{U}_{(12)}[\Lambda,Y]\rightarrow\hat{U}_1[\Lambda,Y]\otimes\hat{U}_2[\Lambda,Y]. \tag{147}$$

(ii) The two-body mass operator commutes with the noninteracting $\hat{F}^j$, $\Delta\hat{F}^j$, and $\hat{j}^2$:

$$[\hat{M}_{(12)},\hat{F}^j_0]=[\hat{M}_{(12)},\Delta\hat{F}^j_0]=[\hat{M}_{(12)},\hat{j}^2_0]=0. \tag{148}$$

These conditions cannot be simultaneously satisfied for systems of more than two particles. They are replaced by the following induction assumption, which reduces to the above condition when $N=2$:

(i) For each proper subsystem s of the N-body system, there is a dynamical representation $\hat{U}_s[\Lambda,Y]:\mathcal{H}_s\rightarrow\mathcal{H}_s$ with short-range interactions satisfying algebraic cluster properties. This means that if the interactions between particles in different clusters of the subsystem s are set to zero, then

$$\hat{U}_s[\Lambda,Y]\rightarrow\otimes_i\hat{U}_{a_i}[\Lambda,Y]. \tag{149}$$

(ii) For each proper subsystem there is a scattering equivalence $\hat{C}_s$ satisfying

$$\hat{C}_s\hat{U}_s[\Lambda,Y]\hat{C}_s^\dagger=\overline{U}_s[\Lambda,Y] \tag{150}$$

with the property that the mass operator $\overline{M}_s$ of the $\overline{U}_s[\Lambda,Y]$ representation commutes with $\hat{F}^i_s$, $\hat{j}^2_s$, $\Delta\hat{F}^i_s$ of the noninteracting subsystem, s.

These conditions are trivially satisfied by the two-body construction of the previous section for $\hat{C}_s=\hat{I}$ on each single particle Hilbert space.

First we show that if these conditions hold for all proper subsystems, then they hold for any nontrivial partitioning of the N-body system.

The theorem below ensures the scattering equivalence of tensor products of subsystem representations that satisfy (150) to representations with a non-interacting $\hat{j}^2$, $\hat{F}^i$, and $\Delta\hat{F}^i$.

Theorem 4: Let a be a partition of the N-particle system into n_a disjoint mutually noninteracting subsystems, a_i. Assume that each subsystem has a dynamical representation $\hat{U}_{a_i}[\Lambda,Y]$ of $ISL(2,C)$ with an asymptotically complete scattering theory. Assume that each of the representations $\hat{U}_{a_i}[\Lambda,Y]$ is scattering equivalent to a representation that has $\hat{F}^j_{a_i}=\hat{F}^j_{0a_i}$, $\Delta\hat{F}^j_{a_i}=\Delta\hat{F}^j_{0a_i}$, $\hat{j}^2_{a_i}=\hat{j}^2_{0a_i}$. Let

$$\hat{U}_a[\Lambda,Y]:=\otimes_{i=1}^{n_a}\hat{U}_{a_i}[\Lambda,Y] \tag{151}$$

be the tensor product of subsystem representations of $ISL(2,C)$. Then $\hat{U}_a[\Lambda,Y]$ is scattering equivalent to a representation $\overline{U}_a[\Lambda,Y]$ that has $\hat{F}^j_a=\hat{F}^j_0$, $\Delta\hat{F}^j_a=\Delta\hat{F}^j_0$, $\hat{j}_a=\hat{j}_0$.

This states that if the subsystem mass operators are scattering equivalent to the subsystem mass operator with kinematic $\hat{F}^j_{a_i}$, $\Delta\hat{F}^j_{a_i}$, $\hat{j}_{a_i}$ then the tensor product of the subsystems has a mass operator that is scattering equivalent to a mass operator with kinematic $\hat{F}^j$, $\Delta\hat{F}^j$, and $\hat{j}$.

The induction assumptions (150) and (149) and the application of Theorem 4 imply that for every partition a with at least two nonempty clusters there are representations $\hat{U}_a[\Lambda,Y]$, and $\overline{U}_a[\Lambda,Y]$, related by a scattering equivalence $\hat{B}_a$. The proof of Theorem 4 as well as the construction of $\hat{B}_a$ is given in Appendix D.

To establish algebraic cluster properties let $\hat{X}$ be an operator valued function of the interactions. Assume that a coupling constant λ_b is put in front of all interactions involving particles in different clusters of a partition b. Let $(\hat{X})_b$ denote the operator obtained from $\hat{X}$ by setting λ_b to 0.

Theorem 4 implies the following relation:

$$\overline{U}_a[\Lambda,Y]=\hat{B}_a\hat{U}_a[\Lambda,Y]\hat{B}_a^\dagger. \tag{152}$$

Turning off interactions between particles in different clusters of b in (152) gives, using (149) and (151),

$$(\overline{U}_a[\Lambda,Y])_b=(\hat{B}_a)_b\hat{U}_{a\cap b}[\Lambda,Y](\hat{B}_a^\dagger)_b, \tag{153}$$

when $b\cap a$ is a refinement of a.

Applying Theorem 4 directly to the partition $c=b\cap a$ gives

$$\overline{U}_{a\cap b}[\Lambda,A]=\hat{B}_{a\cap b}\hat{U}_{a\cap b}[\Lambda,Y]\hat{B}_{a\cap b}^\dagger. \tag{154}$$

This gives distinct scattering equivalences $\hat{B}_{a\cap b}$ and $(\hat{B}_a)_b$ relating $\hat{U}_{a\cap b}[\Lambda,Y]$ to different representations that commute with $\hat{F}_0^j$, $\Delta\hat{F}_0^j$, and $\hat{j}_0^2$. An illustration of this ambiguity in the four-body system occurs for $a=(123)(4)$, $b=(12)(34)$ and $c=(12)(3)(4)$.

It is desirable that the scattering equivalence obtained by turning off interactions agrees with the scattering equivalence constructed directly by applying Theorem 4 to the tensor products. This can be achieved by recursively replacing the operators $\hat{B}_a$ of Theorem 4 with operators $\hat{A}_a$ that satisfy $(\hat{A}_a)_b=\hat{A}_{a\cap b}$. This replacement involves a redefinition of the $\overline{M}_a$'s.

For $N-1$ cluster partitions define

$$\hat{A}_a:=\hat{B}_a. \tag{155}$$

Because $N-1$ cluster interactions only have two-body interactions, both $\hat{A}_a$ and $\hat{B}_a$ become the identity when the interaction is turned off:

$$(\hat{A}_a)_b=\hat{A}_{a\cap b}=\hat{I}. \tag{156}$$

In this case any nontrivial refinement of a gives N free particles.

Next consider a partition a with k clusters. By induction assume that scattering equivalences $\hat{A}_c$ have have been defined for all partitions c with more than k clusters and that these operators satisfy $(\hat{A}_c)_d=\hat{A}_{c\cap d}$ for $n_c>k$.

Let b be a partition such that $a\cap b$ has more than k clusters. Note that

$$\hat{A}_{a\cap b}(\hat{B}_a^\dagger)_b \tag{157}$$

is defined and commutes with $\hat{F}_0^j$, $\Delta\hat{F}_0^j$, and $\hat{j}_0$.

Define

$$\hat{A}_a:=\left(\frac{\hat{I}-i\hat{\alpha}_a}{\hat{I}+i\hat{\alpha}_a}\right)\hat{B}_a, \tag{158}$$

where

$$\hat{\alpha}_a := -\sum_{b\neq a} \mu(a\supset b)\hat{\alpha}_{a,b} \tag{159}$$

and

$$\hat{\alpha}_{a,b} := i\frac{\hat{I}-\hat{A}_b(\hat{B}_a^\dagger)_b}{\hat{I}+\hat{A}_b(\hat{B}_a^\dagger)_b}. \tag{160}$$

Note that $a\cap b=b$ was used in (160). These expressions utilize Cayley transforms to construct unitary functions of scattering equivalences. The resulting unitary operators will be scattering equivalences provided their Cayley transforms are in the algebra of asymptotic constants. This is not entirely trivial, because the algebra $\mathcal{C}$ is uniformly closed, but not strongly closed. $\hat{A}_a$ will be a scattering equivalence if the Cayley transforms $\hat{\alpha}_{a,b}$ are bounded. This will be assumed in all that follows.

The restriction $b\neq a$ means that the b's appearing in the sum are proper refinements of a and necessarily have more than k clusters. By induction the $\hat{A}_b$'s satisfy $(\hat{A}_b)_c=\hat{A}_{b\cap c}$. It follows for $c\cap a\neq a$ that

$$(\hat{\alpha}_{a,b})_c := i\frac{\hat{I}-\hat{A}_{b\cap c}(\hat{B}_a^\dagger)_{b\cap c}}{\hat{I}+\hat{A}_{b\cap c}(\hat{B}_a^\dagger)_{b\cap c}} = \hat{\alpha}_{a,b\cap c}, \tag{161}$$

which gives

$$(\hat{\alpha}_a)_c = -\sum_{b\neq a} \mu(a\supset b)\hat{\alpha}_{a,b\cap c} = -\sum_{b\neq a} \mu(a\supset b)\zeta((b\cap c)\supset d)\mu(d\supset e)\hat{\alpha}_{a,e}. \tag{162}$$

Using (115) gives

$$-\sum_{b\neq a} \mu(a\supset b)\zeta(b\supset d)\zeta(c\supset d)\mu(d\supset e)\hat{\alpha}_{a,e}. \tag{163}$$

The b sum gives $\mu(a\supset a)\zeta(a\supset d)-\delta_{ad}=\zeta(a\supset d)-\delta_{ad}$. Using this in the above sum and observing that $\zeta(c\supset a)=0$ gives

$$\sum_{d,e} \zeta(a\supset d)\zeta(c\supset d)\mu(d\supset e)\hat{\alpha}_{a,e} = \sum_{d,e} \zeta(a\cap c\supset d)\mu(d\supset e)\hat{\alpha}_{a,e} = \hat{\alpha}_{a,a\cap c}. \tag{164}$$

It follows that

$$(\hat{A}_a)_c = \left(\frac{\hat{I}-i\hat{\alpha}_{a,c}}{\hat{I}+i\hat{\alpha}_{a,c}}\right)(\hat{B}_a)_c = \hat{A}_{a\cap c}(\hat{B}_a^\dagger)_c(\hat{B}_a)_c = \hat{A}_{a\cap c}. \tag{165}$$

This shows that if the result holds for more than k clusters, it holds for k clusters.

This process can be continued recursively until $n_a=2$. The result is a set of scattering equivalences, $\hat{A}_a$, and representations

$$\hat{U}_a[\Lambda,Y], \overline{\hat{U}}_a[\Lambda,Y] \tag{166}$$

with the properties

$$\overline{U}_a[\Lambda,Y]=\hat{A}_a\hat{U}_a[\Lambda,Y]\hat{A}_a^\dagger, \tag{167}$$

$$\hat{U}_a[\Lambda,Y]=\otimes_{i=1}^{n_a}\hat{U}_{a_i}[\Lambda,Y], \tag{168}$$

$$\hat{A}_a\to\hat{A}_{a\cap b}, \tag{169}$$

and

$$\overline{F}_a^i=\hat{F}_0^i, \quad \Delta\overline{F}_a^i=\Delta\hat{F}_0^i, \quad \overline{j}_a^2=\hat{j}_0^2. \tag{170}$$

The final step is to complete the construction of the dynamics. For each partition a of the N-particle system with at least two clusters let $\hat{M}_a$ be the mass operator for the tensor product representation $\hat{U}_a[\Lambda,Y]$. Note that

$$\overline{M}_a=\hat{A}_a\hat{M}_a\hat{A}_a^\dagger \tag{171}$$

is scattering equivalent to $\hat{M}_a$ and commutes with $\hat{F}_0^j$, $\Delta\hat{F}_0^j$, and $\hat{j}_0^2$.

Define

$$\overline{M}:=-\sum_{a\neq 1}\mu(1\supseteq a)\overline{M}_a+[\overline{M}]_N=-\sum_{a\neq 1}\mu(1\supseteq a)\hat{A}_a\hat{M}_a\hat{A}_a^\dagger+[\overline{M}]_N, \tag{172}$$

where $[\overline{M}]_N$ is a possible additional N-body interaction that commutes $\hat{F}_0^j$, $\Delta\hat{F}_0^j$, and $\hat{j}_0^2$. By construction $\overline{M}$ commutes with $\hat{F}_0^j$, $\Delta\hat{F}_0^j$, and $\hat{j}_0^2$. This expansion is equivalent to the cluster expansion of $\overline{M}$. By the induction assumption, turning off the interactions between particles in different clusters of partition b gives

$$\begin{aligned}(\overline{M})_b&:=-\sum_{a\neq 1}\mu(1\supseteq a)(\overline{M}_a)_b=-\sum_{a\neq 1}\mu(1\supseteq a)\hat{A}_{a\cap b}\hat{M}_{a\cap b}\hat{A}_{a\cap b}^\dagger\\&=-\sum_{a\neq 1}\mu(1\supseteq a)\zeta((a\cap b)\supseteq d)\mu(d\supseteq e)\hat{A}_e\hat{M}_e\hat{A}_e^\dagger\\&=-\sum_{a\neq 1}\mu(1\supseteq a)\zeta(a\supseteq d)\zeta(b\supseteq d)\mu(d\supseteq e)\hat{A}_e\hat{M}_e\hat{A}_e^\dagger.\end{aligned} \tag{173}$$

The a sum gives $(1-\delta_{1d})\hat{I}$. Inserting this into (173) gives

$$(\overline{M})_b=\hat{A}_b\hat{M}_b\hat{A}_b^\dagger \tag{174}$$

or

$$(\overline{M})_b=\overline{M}_b. \tag{175}$$

This is not the mass operator $\hat{M}_b$ corresponding to the tensor product of the subsystems associated with the clusters of b. To correct this define the scattering equivalence

$$\hat{A}:=\frac{I+i\hat{\alpha}}{I-i\hat{\alpha}} \tag{176}$$

with

$$\hat{\alpha}=-\sum_{a\neq 1}\mu(1\supseteq a)\hat{\alpha}_a, \tag{177}$$

$$\hat{\alpha}_a:=i\frac{\hat{I}-\hat{A}_a}{\hat{I}+\hat{A}_a}. \tag{178}$$

Using the same algebra used to show that $(\overline{M})_b=\overline{M}_b$, it follows that

$$(\hat{A})_b=\hat{A}_b. \tag{179}$$

Since $\hat{A}$ is a scattering equivalence define

$$\hat{M}:=\hat{A}^\dagger\overline{M}\hat{A}. \tag{180}$$

Since $\overline{M}$ commutes with the kinematic operators $\hat{F}_0^j$, $\Delta\hat{F}_0^j$, and $\hat{j}_0^2$, simultaneous eigenstates of $\overline{M}$, $\hat{F}_0^j$, and $\hat{j}_0^2$ define a complete set of states that transform irreducibly. This can be used to construct a representation $\overline{U}[\Lambda,Y]$ of the $ISL(2,C)$. The scattering equivalence $\hat{A}$ defines a scattering equivalent representation

$$\hat{U}[\Lambda,Y]:=\hat{A}^\dagger\overline{U}[\Lambda,Y]\hat{A} \tag{181}$$

with the property that

$$(\hat{U}[\Lambda,Y])_b:=\hat{A}_b^\dagger\overline{U}_b[\Lambda,Y]\hat{A}_b=\hat{U}_b[\Lambda,Y]=\otimes_{i=1}^{n_b}\hat{U}_{b_i}[\Lambda,Y]. \tag{182}$$

The generators have the form

$$\hat{P}^\mu=\hat{A}^\dagger P^\mu(\overline{M},\hat{j}_0^2,\hat{F}_0^i,\Delta\hat{F}_0^i)\hat{A} \tag{183}$$

and

$$\hat{J}^{\mu\nu}=\hat{A}^\dagger J^{\mu\nu}(\overline{M},\hat{j}_0^2,\hat{F}_0^i,\Delta\hat{F}_0^i)\hat{A}. \tag{184}$$

This completes the proof of the induction.

The operator $\hat{U}[\Lambda,Y]$ defined in (181) is the desired N-body representation of $ISL(2,C)$ that is consistent with the dynamics and satisfies algebraic cluster separability. The effect of the transformation $\hat{A}$ is to cancel the $\hat{A}_a$'s from the subsystems. It generates new many-body interactions that are necessary for the algebraic cluster properties of $\hat{U}[\Lambda,Y]$.

To summarize this construction, tensor products of subsystem dynamics are transformed to scattering equivalent representations where the operators $\hat{F}^j$, $\Delta\hat{F}^j$, and $\hat{j}$ are free of interactions. The transformed mass operators are combined to construct a mass operator for a unitary representation of $ISL(2,C)$ with kinematic $\hat{F}^j,\Delta\hat{F}^j$, and $\hat{j}$. This representation is transformed to a scattering equivalent representation satisfying cluster properties.

The construction, while complex, leads to a simple structure. All of the $ISL(2,C)$ generators can be expressed as sums of one, two, three, ..., N-body interactions. For any $ISL(2,C)$ generator, the k-body interaction in the k-body problem is identical to the k-body interaction in the many-body problem. At each stage of the construction the subsystem interactions remain unchanged. What is new is that cluster properties generate new many-body interactions. These do not change when they are imbedded in systems with more than N particles. The spin, which is a nonlinear function of these generators, is an interaction dependent quantity given by

$$\hat{j}^2 = \hat{A}^\dagger \hat{j}_0^2 \hat{A}. \tag{185}$$

The scattering equivalence $\hat{A}$ is an interaction dependent operator that becomes the identity when the interactions are switched off. While there is freedom to include many-body interactions, there is a class of many-body interactions that cannot be removed without violating cluster properties.

XIII. CLUSTER EQUIVALENCE

The dynamical unitary representation of $ISL(2,C)$ constructed in the previous section satisfies algebraic cluster properties. With suitable short-ranged interactions it will satisfy cluster properties (88) and the spectral condition. The choice of basis (f,d) was an important element of this construction. In this section, this representation is shown to be scattering equivalent to a representation based on a different choice of basis, (g,h). This representation also satisfies algebraic cluster properties.

This illustrates the existence of a subgroup of the group of scattering equivalences that relates the constructions based on different irreducible representation basis choices and preserves algebraic cluster properties. This subgroup will be called the group of cluster equivalences.

It follows that the choice of irreducible basis used in the construction has no fundamental physical significance. This generalizes the equivalence of choices of kinematic subgroups in two ways. First, it extends the result to the general setting of this article where the form of dynamics is replaced by the basis choice (f,d). Second, it shows that this equivalence respects cluster properties.

To illustrate the nature of the required scattering equivalence, first let $\hat{U}^f[\Lambda,Y]$ denote the representation constructed in the previous section using the (f,d) basis. Turning off interactions between particles in different clusters of the partition a gives

$$\hat{U}^f[\Lambda,Y] \to \hat{U}_a^f[\Lambda,Y] = \hat{A}_a^{f\dagger} \overline{U}_a^f[\Lambda,Y] \hat{A}_a^f, \tag{186}$$

where $\hat{A}_a^f$ are the scattering equivalences constructed in the previous section. The superscript f indicates that the (f,d) basis was used in the construction.

Algebraic cluster properties give the relations

$$\begin{aligned}\hat{U}^f[\Lambda,Y] \to \hat{U}_a^f[\Lambda,Y] &= \otimes_{i=1}^{n_a} \hat{U}_{a_i}^f[\Lambda,Y] = \otimes_{i=1}^{n_a} (\hat{A}_{a_i}^{f\dagger} \overline{U}_{a_i}^f[\Lambda,Y] \hat{A}_{a_i}^f) \\ &= (\otimes_{i=1}^{n_a} \hat{A}_{a_i}^{f\dagger})(\otimes_{j=1}^{n_a} \overline{U}_{a_j}^f[\Lambda,Y])(\otimes_{k=1}^{n_a} \hat{A}_{a_k}^f), \end{aligned} \tag{187}$$

where the $\hat{A}_{a_i}^f$ are the $\hat{A}^f$ operators for the subsystem consisting of the particles in the ith cluster of a.

It is useful to introduce the operators

$$\tilde{U}_a^f[\Lambda,Y] := \otimes_{i=1}^{n_a} \overline{U}_{a_i}^f[\Lambda,Y], \tag{188}$$

which are related to $\hat{U}_a^f[\Lambda,Y]$ by the scattering equivalence

$$\hat{B}_a^f := \otimes_{i=1}^{n_a} \hat{A}_{a_i}^f. \tag{189}$$

The construction of the previous section defined $\hat{U}_a^f[\Lambda,Y] := \tilde{U}_a^f[\Lambda,Y]$ for $n_a = N-1$. All of the $\hat{U}_a^f[\Lambda,Y]$'s were recursively constructed from the $n_a = N-1$ cluster representations.

Any of the representations $\overline{U}_a^f[\Lambda,Y]$ are scattering equivalent to a $\overline{U}_a^g[\Lambda,Y]$ representation. This scattering equivalence is realized by making the following replacements in the kernel of the barred mass operators:

$$\langle f,d(m_0,j_0)|\overline{M}^f|f',d'(m_0',j_0')\rangle=\delta[f;f']\delta_{j_0,j_0'}\langle m_0,d||\overline{M}^{j_0}||m_0',d'\rangle \tag{190}$$

by

$$\langle g,h(m_0,j_0)|\overline{M}^g|g',h'(m_0',j_0')\rangle=\delta[g;g']\delta_{j_0,j_0'}\langle m_0,h||\overline{M}^{j_0}||m_0',h'\rangle, \tag{191}$$

where the reduced kernel $\langle m_0,h||\overline{M}^{j_0}||m_0',h'\rangle$ is defined in terms of the reduced kernel $\langle m_0,d||\overline{M}^{j_0}||m_0',d'\rangle$ by a variable change $d\to h$ implemented by kinematic $ISL(2,C)$–Racah coefficients. This means abstract reduced mass operators are identical. The operators $\overline{M}^g$ and $\overline{M}^f$ differ because of the delta functions in f or g, but both operators manifestly give the same S matrix elements and bound-state observables. The operators $\overline{M}^f$ and $\overline{M}^g$ define scattering equivalent representations of $ISL(2,C)$ with the noninteracting $\hat{F}^i,\Delta\hat{F}^i$ or $\hat{G}^i,\Delta\hat{G}^i$, respectively. The scattering equivalence is denoted by $\hat{C}^{gf}$:

$$\hat{C}^{gf}\overline{U}^f[\Lambda,Y]\overline{C}^{gf\dagger}=\overline{U}^g[\Lambda,Y]. \tag{192}$$

Since this equivalence is valid for systems or subsystems, for each partition a the following representations are scattering equivalent:

$$\hat{U}_a^f[\Lambda,Y],\quad \overline{U}_a^f[\Lambda,Y],\quad \tilde{U}_a^f[\Lambda,Y],\quad \overline{U}_a^g[\Lambda,Y],\quad \tilde{U}_a^g[\Lambda,Y]. \tag{193}$$

These representations have the property that $\hat{U}_a^f[\Lambda,Y]=\tilde{U}_a^f[\Lambda,Y]$ for $N-1$ cluster partitions and $\hat{U}_a^f[\Lambda,Y]$ is scattering equivalent to $\overline{U}_a^f[\Lambda,Y]$ for the one-cluster partition.

The goal is to find a $\hat{U}^g[\Lambda,a]$ that is scattering equivalent to $\overline{U}^g[\Lambda,Y]$ and $\overline{U}^f[\Lambda,Y]$ and also satisfies algebraic cluster properties, with $\hat{U}_a^g[\Lambda,Y]=\tilde{U}_a^g[\Lambda,Y]$ for $n_a=N-1$.

The first step is to define

$$\hat{U}_a^g[\Lambda,Y]=\tilde{U}_a^g[\Lambda,Y] \tag{194}$$

for $n_a=N-1$. Following the construction of the previous section, this gives scattering equivalences $\hat{A}_a^g$ relating $\hat{U}_a^g[\Lambda,Y]$ to $\overline{U}_a^g[\Lambda,Y]$ for $n_a=N-1$.

Next, assume by induction that $\hat{U}_a^g[\Lambda,Y]$ has been defined for partitions with more than K clusters satisfying algebraic cluster properties and is scattering equivalent to $\overline{U}_a^g[\Lambda,Y]$. The $\overline{U}_a^g[\Lambda,Y]$ for K-cluster partitions is defined by (192). Its mass operator, $\overline{M}_a^g$, is related to $\overline{M}_a^f$ by replacing delta functions in f by delta functions in g. Since $(\overline{M}_a^f)_b=\overline{M}_{a\cap b}^f$ it follows that $(\overline{M}_a^g)_b=\overline{M}_{a\cap b}^g$ because the kernel of the two operators only differ by delta functions in the overall kinematic operators f or g.

This means that $\overline{M}_a^g$ differs from the cluster expansion

$$\overline{M}_a^{g0}=-\sum_{b\neq a}\mu(a\supseteq b)\overline{M}_b^g \tag{195}$$

by at most an a-connected interaction term, $[\overline{M}]_a^g$. In order to construct the desired representation it is enough to define

$$\hat{U}_a^g[\Lambda,Y]:=\hat{A}_a^{g\dagger}\overline{U}_a^g[\Lambda,Y]\hat{A}_a^g, \tag{196}$$

where

$$\hat{A}^g_a = \frac{I + i\hat{\alpha}^g_a}{I - i\hat{\alpha}^g_a}, \tag{197}$$

$$\hat{\alpha}^g_a := -\sum_{b \neq a} \mu(a,b)\hat{\alpha}^g_b, \tag{198}$$

$$\hat{\alpha}^g_b = i\frac{I + \hat{A}^g_b}{I - \hat{A}^g_b}. \tag{199}$$

Following the algebra used in (173) $\hat{\alpha}^g_a$ has the property that

$$(\hat{\alpha}^g_a)_b = \hat{\alpha}^g_b, \quad b \subset a, \tag{200}$$

and

$$(\hat{U}^g_a)_b[\Lambda, Y] := \hat{A}^{g\dagger}_{a\cap b}\overline{U}^g_{a\cap p}[\Lambda, Y]\hat{A}^g_{a\cap b} = \hat{U}^g_{a\cap b}[\Lambda, Y]. \tag{201}$$

This differs from the result of a direct construction in the (g,h) basis because of the difference $[\overline{M}]^g_a$ between $\overline{M}^g_a$ and $\overline{M}^{g0}_a$. This introduces additional many-body interactions that are needed to maintain the scattering equivalence at each stage of the recursion. Note that in this construction the factor $\mu(a \supseteq b)$ ensures that only the b satisfying $b \subset a$ appear in the sum. These partitions have more than K-clusters. This construction can be continued until $K = 1$, where

$$\hat{U}^g[\Lambda, Y] = \hat{U}^g_1[\Lambda, Y] = \hat{A}^g\overline{U}^g_1\hat{A}^{g\dagger} \tag{202}$$

is the desired representation based on the (g,h) representation. The relevant scattering equivalence is

$$\hat{U}^g[\Lambda, Y] = \hat{A}^{g\dagger}\hat{C}^{gf}\hat{A}^f\hat{U}^f[\Lambda, Y]\hat{A}^{f\dagger}\hat{C}^{gf\dagger}\hat{A}^g. \tag{203}$$

It follows that $\hat{A}^{g\dagger}\hat{C}^{gf}\hat{A}^f$ is the desired scattering equivalence connecting the construction of $\hat{U}[\Lambda, Y]$ using the (f,d) representation to a dynamics satisfying cluster properties based on the (g,h) representation.

It is important to emphasize that the $\hat{A}^g$ constructed in this manner are not identical to the corresponding operators that would have been constructed if one began with the (g,h) basis. This is due to the presence of additional many-body interactions that are determined by the difference between the operators $\overline{M}^{g0}_a$ and $\overline{M}^g_a$ for each a. These differences account for the dynamical differences that occur when the many-body dynamics is formulated with different basis choices, or using different forms of dynamics.

The cluster equivalences transform $ISL(2,C)$ generators in one representation to physically equivalent generators in another representation. In each representation the interactions are distributed differently among the generators. Specific representation have computational advantages.

XIV. SUMMARY AND CONCLUSION

This article provides a general construction of a unitary representation $\hat{U}[\Lambda, Y]$ of $ISL(2,C)$ for a system of N-interacting particles based on the representation theory of $ISL(2,C)$. For suitable interactions the representation satisfies cluster properties and the spectral condition. The representation defines a nontrivial relativistic quantum theory of interacting particles. Unitary operators that preserve the S-matrix and cluster properties, called cluster equivalences, relate the different constructions.

Relativistic quantum theory of N-particles can be applied to model systems of strongly interacting particles. This framework has many features of nonrelativistic quantum mechanics and local relativistic quantum field theory. Like nonrelativistic quantum mechanics, it is a mathematically well behaved theory where exact numerical calculations are possible. Like quantum field theory, it is a quantum theory with an exact $ISL(2,C)$ symmetry that satisfies cluster properties and the spectral condition.

The generality of the construction suggests that any quantum theory dominated by a finite number of particle degrees of freedom which is consistent with Poincaré invariance, cluster properties, and the spectral condition will be related to a theory of the type discussed in this article by a cluster equivalence.

The cluster equivalences introduced in Sec. XIII relate physically equivalent representations of the same model. Cluster equivalent models have the same bound state observables and S-matrix elements. In each representation free particles are represented as tensor products of irreducible representations. The unitary representation of $ISL(2,C)$ that defines the dynamics clusters into tensor products of subsystems representations with the same properties. Cluster equivalence is a stronger condition than unitary equivalence or scattering equivalence. Scattering equivalences were shown to be unitary elements of the C^* algebra of asymptotic constants. Cluster equivalences were shown to be a subgroup of the scattering equivalences.

The practical need to understand the relationship between different formulations of relativistic quantum theory suggests that it would be useful to have an abstract definition of a relativistic quantum theory of particles. The situation is different than the quantum field theory case, where there are several sets of axioms[1] that are designed to define a suitable local field theory, with an absence of examples of realistic theories consistent with these axioms. In relativistic quantum theory there are many applications that claim to be relativistic quantum theories, with no universally accepted criteria of what it means to be a relativistic quantum theory of particles. The absence of an acceptable definition of what constitutes a relativistic quantum theory of particles makes comparison difficult. The construction of this article, which focuses on mathematical formulation of observable physical properties, and how they can be realized in models, suggest minimal elements that need to be included in a set of axioms:

(A1) The Hilbert space $\mathcal{H}$ is the tensor product of irreducible representation spaces of $ISL(2,C)$ associated with the mass and spins of the constituent particles.

(A2) There is a unitary representation $\hat{U}[\Lambda,Y]$ of $ISL(2,C)$ on $\mathcal{H}$ with a positive mass and energy spectrum.

(A3) The Hilbert space can be factored into a tensor product of subsystem spaces, with each one supporting a subsystem unitary representation $\hat{U}_i[\Lambda,Y]$ of $ISL(2,C)$. For each partition a into subsystems a_i the operator $\hat{U}[\Lambda,Y]$ satisfies cluster property (88).

(A4) The dynamics $\hat{U}[\Lambda,Y]$ has an asymptotically complete, $ISL(2,C)$ invariant S-matrix.

These requirements can be used to formulate a precise relationship between different formulations of relativistic quantum theory when they are applied to systems with finite energy and number of degrees of freedom.

The construction in Sec. XII points to some of the general features of relativistic quantum theory of particles. In the physical representations of $ISL(2,C)$ the scattering equivalence $\hat{A}$, which is an interaction dependent operator, normally generates interaction dependent terms in all of the operators using the relations

$$\hat{F}^i=\hat{A}^\dagger\hat{F}_0^i\hat{A}, \tag{204}$$

$$\Delta\hat{F}^i=\hat{A}^\dagger\Delta\hat{F}_0^i\hat{A}, \tag{205}$$

$$j^2=\hat{A}^\dagger j_0^2\hat{A}, \tag{206}$$

$$P^\mu = P^\mu(M, j^2, \hat{F}^i, \Delta\hat{F}^i) = \hat{A}^\dagger P^\mu(\overline{M}, j_0^2, \hat{F}_0^i, \Delta\hat{F}_0^i)\hat{A}, \tag{207}$$

$$J^{\mu\nu} = J^{\mu\nu}(M, j^2, \hat{F}^i, \Delta\hat{F}^i) = \hat{A}^\dagger J^{\mu\nu}(\overline{M}, j_0^2, \hat{F}_0^i, \Delta\hat{F}_0^i)\hat{A}. \tag{208}$$

While the construction begins with representations having kinematic j^2, $\hat{F}^i$, and $\Delta\hat{F}^i$, all of these operators acquire an interaction dependence in the physical representation.

Tensor and spinor operator densities also play an important role in relativistic quantum mechanics. For example, the hadronic electroweak current operators provide the coupling of the hadronic dynamics to electroweak probes. In one-boson exchange approximations these current operators must transform as four-vector densities with respect to $ISL(2,C)$:

$$\hat{U}[\Lambda, Y] I^\mu[X] \hat{U}^\dagger[\Lambda, Y] = I^\nu[\Lambda X \Lambda^\dagger + Y]\Lambda^\mu_\nu. \tag{209}$$

Because $\hat{U}[\Lambda, Y]$ is an interaction dependent operator, the covariance condition (209) requires the existence of many-body contributions to the current.

This is understood by considering covariance condition

$$\langle f; m, j | I^\mu[X] | f'; m', j' \rangle = \int d\mu(f'') d\mu(f''') \langle f''; m, j | I^\nu[\Lambda X \Lambda^\dagger + Y] | f'''; m', j' \rangle \times \mathcal{D}^{*m,j}_{f'',f}[\Lambda, Y] \mathcal{D}^{m',j'}_{f''',f'}[\Lambda, Y]\Lambda^\mu_\nu. \tag{210}$$

In this expression the m and m' in the $\mathcal{D}$-functions are physical mass eigenvalues. This expression fixes a general matrix elements in terms of a set of independent current matrix elements and interaction (m) dependent coefficients. This is essentially the Wigner–Eckart theorem for $ISL(2,C)$. In this interpretation the interaction dependence arises because the Clebsch–Gordan coefficients depend on the physical mass eigenvalues. This means that the operators $\hat{I}^\mu(X)$ necessarily have interaction dependent terms that depend on the specific representation.

The result is that the representation of tensor and spinor densities is related to the representation of the dynamics. Changing the representation of the dynamics by a cluster equivalence changes the representation of the interaction dependent parts of the tensor and spinor densities. This has important implications for modeling electromagnetic probes of hadronic systems.

Dirac's forms of dynamics are obtained for special basis choices. Specifically, if the $ISL(2,C)$ Wigner $\mathcal{D}$ functions, $\mathcal{D}^{m,j}_{f,f'}[\Lambda, Y]$, do not depend explicitly on m for a subgroup $\mathcal{G}$ of $ISL(2,C)$, there are no interactions in the generators of the subgroup. This depends on the choice of commuting operators $\hat{F}^i$ that are used to label vectors in $ISL(2,C)$ irreducible subspaces. Cluster equivalences can be used to relate a general model to an equivalent models in any of Dirac's forms of dynamics.

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APPENDIX A: $ISL(2,C)$ IRREDUCIBLE REPRESENTATIONS: EXAMPLES

Examples of positive mass positive energy irreducible representations of $ISL(2,C)$ are constructed. The construction presented below is not as general as the abstract construction given in Sec. V, but it is general enough to include all of the representations that are commonly used in the literature.

Let $f^i(\vec{p}, m)$, $i = 1,2,3$, be three independent real valued functions of the three momentum and the mass. Since the $\hat{M}$ and $\hat{\vec{P}}$ commute, these three functions become commuting self-adjoint

operators when m and $\vec{p}$ are replaced by operators. Independence means that these functions can be uniquely inverted to express $\vec{p}=\vec{P}(f,m)$ where f denotes the three functions f^i. By the implicit function theorem this will be true provided the Jacobian matrix

$$\frac{\partial f^i}{\partial p^j} \tag{A1}$$

is invertible for any $\vec{p}$ and any m in the spectrum of $\hat{M}$.

Define the operators

$$\hat{F}^i=f^i(\hat{\vec{P}},\hat{M}) \tag{A2}$$

for $i=1$ to 3. Let $L(p)$ be an arbitrary but fixed $SL(2,C)$ valued function of $p=(\sqrt{m^2+\vec{p}^2},\vec{p})$ with properties

$$L(p)L^\dagger(p)=\frac{1}{m}\sigma_\mu p^\mu, \tag{A3}$$

$$L(p_0)L^\dagger(p_0)=\sigma_0, \quad p_0:=(m,0,0,0). \tag{A4}$$

These equations mean that $L(p)$ is an $SL(2,C)$ representation of a Lorentz boost. In general it can differ from the canonical (rotationless boost) by a p-dependent rotation, $R(p)\in SU(2)$:

$$L(p)=L_c(p)R(p), \quad R(p_0)=I. \tag{A5}$$

Given the function $L(p)$ it is possible to define the $SL(2,C)$ valued matrix of operators $L(\hat{P})$ which is obtained by replacing p by the commuting operators $(\hat{\vec{P}},\hat{M})$.

For a given $L(p)$ define the l-spin by

$$\hat{\vec{j}}_l:=\frac{1}{2\hat{M}}\mathrm{Tr}[\vec{\sigma}L(\hat{P})\hat{W}^\mu\sigma_\mu L^\dagger(\hat{P})], \tag{A6}$$

where $\hat{W}^\mu$ is the Pauli Lubanski vector. Since $\hat{W}^\mu$ commutes with $\hat{P}^\nu$, all components of $\hat{\vec{j}}_l$ commute with $\hat{F}^1,\hat{F}^2,\hat{F}^3$. In addition, for any choice of $L(p)$ the components of $\hat{\vec{j}}_l$ satisfy $SU(2)$ commutation relations with $\hat{j}_l^2=\hat{j}^2=\hat{W}^2/\hat{M}^2$. Let $\hat{F}^4=\hat{z}\cdot\hat{\vec{j}}_l$. The operators $\hat{F}^1,\ldots,\hat{F}^4,\hat{M},\hat{j}^2$ define a complete set of commuting self-adjoint operators.

Let $f_0^1=f^1(p_0)$, $f_0^2=f^2(p_0)$, and $f_0^3=f^3(p_0)$. By construction f_0^1,f_0^2,f_0^3 is invariant under rotations, although f does not transform like an $SO(3)$ vector. Let $\vec{f}$ denote the eigenvalues of $\hat{F}^1$, $\hat{F}^2$, and $\hat{F}^3$ and μ denote the eigenvalue of $\hat{F}^4$. Define $f_\Lambda:=f(\vec{p}_\Lambda,m)$, where $p_\Lambda^\mu=\Lambda^\mu_\nu p^\nu$. For fixed Λ, f_Λ is a function of f and m.

Let $|f_0,\mu;j,m\rangle$ denote a rest eigenstate of $\hat{F}^i,\hat{M},\hat{j}^2$ and let R be an $SU(2)$ rotation. Define rotations and translations on the rest states by

$$\hat{U}[R,0]|f_0,\mu;j,m\rangle:=\sum_{\nu=-j}^{j}|f_0,\nu;j,m\rangle D^j_{\nu\mu}(R), \tag{A7}$$

$$\hat{U}[I,Y]|f_0,\mu;j,m\rangle:=e^{-imy^0}|f_0,\mu;j,m\rangle. \tag{A8}$$

Define states of arbitrary $\hat{F}$ by

$$|f,\mu;j,m\rangle := \hat{U}[L(f),0]|f_0,\mu;j,m\rangle \sqrt{\left|\frac{\partial f_0}{\partial f}\right|}. \tag{A9}$$

The expressions for $\hat{U}[R,0]$ and $\hat{U}[I,Y]$ are manifestly unitary. The factor $\sqrt{|\partial f_0/\partial f|}$ assures $\hat{U}[L(f),0]$ unitarity for states with a delta-function normalization. These elementary relations determine a unitary representation $\hat{U}[\Lambda,Y]$ on any state by using the decomposition

$$\hat{U}[\Lambda,Y] = \hat{U}[I,Y]\hat{U}[L(f_\Lambda),0]\hat{U}[R_{wl}(\Lambda,f),0]\hat{U}[L^{-1}(f),0], \tag{A10}$$

where

$$R_{wl}(\Lambda,f) := L^{-1}(f_\Lambda)\Lambda L(f) \tag{A11}$$

is the l-spin Wigner rotation and $L(f)$ is obtained from $L(p)$ by replacing p by $p(f,m)$.

The irreducible representation in this basis follows as a consequence of the above relations:

$$\hat{U}[\Lambda,Y]|f,\mu;j,m\rangle = \sum_{\nu=-j}^{j} |f_\Lambda,\nu;j,m\rangle e^{ip(\vec{f}_\Lambda,m)\cdot y}\left|\frac{\partial f_\Lambda}{\partial f}\right|^{1/2} D^j_{\nu\mu}[R_{wl}(\Lambda,f)]. \tag{A12}$$

Taking matrix elements give the $ISL(2,C)$ $\mathcal{D}$-function

$$\mathcal{D}^{mj}_{f'f}[\Lambda,Y] = e^{ip(\vec{f}',m)\cdot y} D^j_{\mu'\mu}[R_{wl}(\Lambda,f)]\left|\frac{\partial f_\Lambda}{\partial f}\right|^{1/2} \delta^3(f'-f_\Lambda). \tag{A13}$$

The infinitesimal generators of $ISL(2,C)$ in this representation can be computed using (125)–(127). The results are

$$\hat{P}^\mu = p^\mu(\vec{f},m), \tag{A14}$$

$$\hat{j}^j = i\epsilon^{jkl}\frac{\partial f^m}{\partial p^k}\frac{\partial}{\partial f^m}\hat{p}^l + (\hat{c}_1^{jk}(p) + i\epsilon_{jlm}\hat{c}_2^{lk}(p)\hat{p}^m)\hat{j}^k, \tag{A15}$$

$$\hat{K}^j = -\frac{1}{2}\frac{\partial f^m}{\partial \hat{p}^k}[\Delta f^m,\hat{H}]_+ + i(\hat{c}_1^{jk}(p) - H\hat{c}_2^{jk}(p))\hat{j}^k, \tag{A16}$$

where

$$\hat{c}_1^{jk}(p) = \tfrac{1}{2}\mathrm{Tr}(L^{-1}(\hat{p})\sigma_j L(\hat{p})\sigma_k), \tag{A17}$$

$$\hat{c}_2^{jk}(p) = \mathrm{Tr}\left(L^{-1}(\hat{p})\frac{\partial}{\partial p^j}L(\hat{p})\sigma_k\right). \tag{A18}$$

These equations can be inverted to obtain explicit expressions (133) for $\Delta\hat{f}^k$ in terms of the generators

$$\Delta\hat{f}^k = -\frac{i}{2\hat{H}}\frac{\partial\hat{H}}{\partial f^k} - \frac{1}{\hat{H}}\left[\frac{\partial p^j}{\partial f^k}(\hat{K}^j - i(\hat{c}_1^{jm}(p) - \hat{H}\hat{c}_2^{jm}(p))\hat{j}^m)\right] \tag{A19}$$

for $k=1$, 2, or 3. This expression reduces[23] to the Newton–Wigner position operator when $f^i = p^i$ and the l-spin is the canonical spin. The l-spin is given as a function of the infinitesimal generators by (A6). The partial derivatives in this expression are computed with functions which are replaced by the appropriate operators after the differentiation is performed.

The Δf^4 for the spins are the raising and lowering operators

$$\hat{j}_{l\pm} := \hat{j}_{lx} \pm i\hat{j}_{ly}. \tag{A20}$$

This shows explicitly the equivalence between

$$\{\hat{H},\vec{\hat{P}},\vec{\hat{J}},\vec{\hat{K}}\} \quad \text{and} \quad \{\hat{M},\hat{j}^2,\vec{\hat{F}},\Delta\vec{\hat{F}}\}. \tag{A21}$$

The basis choices illustrated above, while restrictive, include all of the basis choices that lead to Dirac's forms of dynamics. The general construction yields a Dirac instant form of dynamics if f^i are taken as the three components of the linear momentum and $L_l(p)$ is a canonical (rotationless) boost. Dirac's point-form dynamics is obtained if f^i is taken as the three components of the four velocity and $L_l(p)$ is the canonical boost. A front form dynamics is obtained if f^i is taken as the three generators of translations tangent to a light front and L_l is taken as corresponding the light front boost. Infinitely many other choices of f^i and $L_l(p)$ are possible.

APPENDIX B: *ISL*(2,*C*) CLEBSCH-GORDAN AND RACAH COEFFICIENTS

The Clebsch–Gordan coefficients for the representations in Appendix A can be computed from the tensor product representation using the same methods that were used to construct the single irreducible representations. The first step is to decompose the tensor product representation of the ''rest state'' into irreducible representation of $SU(2)$. This requires generalized Melosh rotations to ensure that all of the spins undergo the same rotations. The irreducible representation are then boosted with the appropriate l-boost. This generally leads to Wigner rotations. The general result is derived in Ref. 26. The resulting Clebsch–Gordan coefficients for this basis are

$$\begin{aligned}\langle \vec{f}_1,\mu_1,\vec{f}_2,\mu_2|\vec{f},\mu;m,j,l,s\rangle = {} & \delta(\vec{f}-\vec{f}(\vec{f}_1,\vec{f}_2))\,\delta(m-m(\vec{f}_1,\vec{f}_2,m_1,m_2))\left|\frac{\partial(f,k)}{\partial(f_1,f_2)}\right|^{1/2}\frac{1}{k}\frac{\partial k}{\partial m}\\ & \times D^{j_1}_{\mu_1\mu_1'}[R_{wl}(p,k_1)R_{ml}(k_1)]D^{j_2}_{\mu_2\mu_2'}[R_{wl}(p,k_2)R_{ml}(k_2)]\\ & \times Y^l(\hat{k}_1(f_1,f_2))\langle j_1,\mu_1,j_2,\mu_2|s,\mu_s\rangle\langle s,\mu_s,l,\mu_l|j,\mu\rangle,\end{aligned}$$

where $L_c(p)$ is the canonical boost and $L_l(p)$ is a l-boost,

$$k_i = \tfrac{1}{2}\mathrm{Tr}(L_l^{-1}(p)p_i^\mu\cdot\sigma_\mu(L_l^{-1}(p))^\dagger) \tag{B1}$$

and

$$R_{wl}(p,k_i) := L_l^{-1}(p_i)L_l(p)L_l(k_i), \tag{B2}$$

$$R_{mlc}(k_i) := L_l^{-1}(k_i)L_c(k_i). \tag{B3}$$

These are the Wigner and Melosh rotations associated with the l-boost.

The Racah coefficient for this choice of basis can be computed in terms of four Clebsch–Gordan coefficients. It is simplest to compute the invariant part of this coefficient by choosing $p=(m,0,0,0)$ and integrating the result over $SU(2)$. The Racah coefficients for the couplings $((12)(3))\to((23)(1))$ become

$$
\begin{aligned}
&\langle \vec{f}',\mu';m',j',(12,3)|\vec{f},\mu;m,j,(23,1)\rangle \\
&\quad=\delta_{j'j}\delta_{\mu'\mu}\delta(\vec{f}'-\vec{f})\,\delta(m-m')\,\frac{1}{2j+1} \\
&\qquad\times\sum_{\mu_f}\left[\frac{8\pi^2 m_{12}m_{23}\omega_2(q_3'+q_1)}{k_1'k_2q_3'q_1\omega_1(k_1')\omega_2(k_1')\omega_2(k_2)\omega_3(k_2)\omega_{12}(q_3)\omega_{23}(q_1)}\right] \\
&\qquad\times\left[\left|\frac{\partial(f_{12}',f_3')}{\partial(f',q_3')}\right|\left|\frac{\partial(f_{12}',k_1')}{\partial(f_1',f_2')}\right|\left|\frac{\partial(f_{23},k_2)}{\partial(f_2,f_3)}\right|\left|\frac{\partial(f_{23},f_1)}{\partial(f,q_1)}\right|\right]^{1/2} \\
&\qquad\times\langle j,\mu_f|L',\mu_L',S',\mu_S'\rangle\langle S',\mu_S'|j_{12}',\mu_{12}',j_3',\mu_3'\rangle \\
&\qquad\times D^{j_{12}}_{\mu_{12}'\mu_{12}}[R_{mcl}(-q_3')]Y^{L'*}_{\mu_L'}(\hat{q}_3')\langle j_{12}',\mu_{12}|l',\mu_l',s',\mu_s'\rangle\langle s',\mu_s'|j_1',\mu_1',j_2',\mu_2'\rangle Y^{l'*}_{\mu_l'}(\hat{k}_1') \\
&\qquad\times D^{j_3}_{\mu_3'\mu_3}[R_{mcl}(q_3')R_{wl}(-q_1,k_3)R_{mlc}(k_3)]D^{j_1}_{\mu_1\mu_1'}[R_{mcl}(k_1')R_{wl}^{-1}(-q_3',q_1')R_{ml}(q_1)] \\
&\qquad\times D^{j_2}_{\mu_2\mu_2'}[R_{mcl}(k_2')R_{wl}^{-1}(-q_3',q_2')R_{wl}(-q_1,k_2)R_{mlc}(k_2)]Y^{l*}_{\mu_l'}(\hat{k}_2)\langle j_2\mu_2 j_3\mu_3|s\mu_s\rangle \\
&\qquad\times\langle l,\mu_l,s,\mu_s|j_{23}\mu_{23}\rangle Y^{L}_{\mu_L}(\hat{q}_1) \\
&\qquad\times D^{j_{23}}_{\mu_{23}\mu_{23}'}[R_{ml}(-q_1)]\langle j_{23}\mu_{23}j_1\mu_1|S\mu_S\rangle\langle L,\mu_L,S,\mu_S|j\mu_f\rangle,
\end{aligned}
$$

where m is the three-body invariant mass, m_{ij} are the invariant masses of the ij and jk subsystems, $w(k)$ are energies, and q_i are the operators

$$\hat{q}_i := L_l^{-1}(\hat{p})\hat{p}_i\,. \tag{B4}$$

APPENDIX C: PROOF OF THEOREM 1

To prove Theorem 1 first note that condition (82) implies

$$\lim_{t\to\pm\infty}\|\hat{U}[I,-T](\hat{\Phi}_{\mathcal{A}}-\hat{U}^{\dagger}[\Lambda,Y]\hat{\Phi}_{\mathcal{A}}\hat{U}_{\mathcal{A}}[\Lambda,Y])\hat{U}_{\mathcal{A}}[I,T]|\psi\rangle\|=0, \tag{C1}$$

which is equivalent to

$$\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\Omega_{\pm}(\hat{H},\hat{U}^{\dagger}[\Lambda,Y]\hat{\Phi}_{\mathcal{A}}\hat{U}_{\mathcal{A}}[\Lambda,Y],\hat{H}_{\mathcal{A}}). \tag{C2}$$

Since the Hamiltonian commutes with the linear and angular momentum operators, it follows that if (Λ,A) is a rotation or translation, this becomes

$$\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\hat{U}^{\dagger}[R,0]\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[R,0] \tag{C3}$$

and

$$\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\hat{U}^{\dagger}[I,Y]\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[I,Y]. \tag{C4}$$

For the case of a rotationless Lorentz transformation condition (C2) implies

$$\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\Omega_{\pm}(\hat{H},\hat{U}^{\dagger}[\Lambda,0]\hat{\Phi}_{\mathcal{A}}\hat{U}_{\mathcal{A}}[\Lambda,0],\hat{H}_{\mathcal{A}}). \tag{C5}$$

The commutation relations imply

$$\hat{U}^{\dagger}[\Lambda,0]\hat{H}\hat{U}[\Lambda,0]=\Lambda^0_\mu\hat{P}^\mu, \tag{C6}$$

$$\hat{U}^{\dagger}_{\mathcal{A}}[\Lambda,0]\hat{H}_{\mathcal{A}}\hat{U}_{\mathcal{A}}[\Lambda,0]=\Lambda^0_\mu\hat{P}^\mu_{\mathcal{A}}. \tag{C7}$$

It follows that

$$\begin{aligned}\hat{U}^{\dagger}[\Lambda,0]\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[\Lambda,0]&=\hat{U}^{\dagger}[\Lambda,0]\Omega_{\pm}(\hat{H},\hat{U}[\Lambda,0]\hat{\Phi}_{\mathcal{A}}\hat{U}^{\dagger}_{\mathcal{A}}[\Lambda,0],\hat{H}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[\Lambda,0]\\&=\Omega_{\pm}(\Lambda^0_\mu\hat{P}^\mu,\hat{\Phi},\Lambda^0_\mu\hat{P}^\mu_{\mathcal{A}}),\end{aligned} \tag{C8}$$

which can be expressed as

$$\Omega_{\pm}(\Lambda^0_\mu\hat{P}^\mu,\hat{\Phi}_{\mathcal{A}},\Lambda^0_\mu\hat{P}^\mu_{\mathcal{A}})=\lim_{t\to\pm\infty}e^{i\hat{H}\Lambda^0_0t+i\Lambda^0_i\hat{P}_it}\hat{\Phi}_{\mathcal{A}}e^{-i\hat{H}_{\mathcal{A}}\Lambda^0_0t+i\Lambda^0_i\hat{P}_{\mathcal{A}i}t}. \tag{C9}$$

Since $\Lambda^0_0>0$ it is possible to redefine $t\to t'=\Lambda^0_0t$ so the limit $t\to\pm\infty$ is equivalent to the limit the $t'\to\pm\infty$. This gives

$$\lim_{t'\to\pm\infty}e^{i\hat{H}t'}\hat{U}[I,At']\hat{\Phi}_{\mathcal{A}}\hat{U}_{\mathcal{A}}[I,At']e^{-i\hat{H}_{\mathcal{A}}t'}, \tag{C10}$$

where

$$A=\frac{\Lambda^0_i}{\Lambda^0_0}\sigma_i. \tag{C11}$$

Condition (83) then gives

$$\lim_{t'\to\pm\infty}e^{i\hat{H}t'}\hat{U}[I,At]\hat{\Phi}_{\mathcal{A}}\hat{U}_{\mathcal{A}}[I,At']e^{-i\hat{H}_{\mathcal{A}}t'}=\Omega_{\pm}(\hat{H},\hat{\Phi},\hat{H}_{\mathcal{A}}). \tag{C12}$$

Combining (C8) and (C12) gives

$$\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\hat{U}^{\dagger}[\Lambda,0]\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[\Lambda,0]. \tag{C13}$$

To complete the proof of Theorem 1 note that (C3) and (C13) imply

$$\hat{U}[\Lambda,Y]\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\Omega_{\pm}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[\Lambda,Y], \tag{C14}$$

which is the intertwining relation of Corollary 1. Corollary 2 follows by identifying (C9) and (C12).

It follows that

$$\begin{aligned}\hat{U}^{\dagger}_{\mathcal{A}}[\Lambda,Y]\hat{S}\hat{U}_{\mathcal{A}}[\Lambda,Y]&=\hat{U}^{\dagger}_{\mathcal{A}}[\Lambda,Y]\Omega^{\dagger}_{+}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})\Omega_{-}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})\hat{U}_{\mathcal{A}}[\Lambda,Y]\\&=\Omega^{\dagger}_{+}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})\hat{U}^{\dagger}[\Lambda,Y]\hat{U}[\Lambda,Y]\Omega_{-}(\hat{H},\hat{\Phi}_{\mathcal{A}},\hat{H}_{\mathcal{A}})=\hat{S}.\end{aligned} \tag{C15}$$

This completes the proof of Theorem 1.

To prove Corollary 3 note that Eq. (86) is equivalent to

$$s-\lim_{s\to\pm\infty}[e^{-i\hat{M}s}\Omega_{\pm}(\hat{H},\hat{\Phi},\hat{H}_{\mathcal{A}})-\hat{\Phi}e^{-i\hat{M}_{\mathcal{A}}s}]=0. \tag{C16}$$

The intertwining properties that follow from Theorem 1 give the strong limit:

$$s-\lim_{s\to\pm\infty}[(\Omega_{\pm}(\hat{H},\hat{\Phi},\hat{H}_{\mathcal{A}})-\hat{\Phi})]e^{-i\hat{M}_{\mathcal{A}}s}=0. \tag{C17}$$

The proof that this holds on the dense set of asymptotic states with bounded momentum follows the proof of theorem IX.23 of Ref. 36 (see also Refs. 42 and 43). The extension to the strong limit follows the argument in Ref. 8.

APPENDIX D: PROOF OF THEOREM 4

To prove Theorem 4 let $\hat{C}_{a_i}$ be the scattering equivalence that maps $\hat{U}_{a_i}[\Lambda,Y]$ to the representation $\tilde{U}_{a_i}[\Lambda,Y]$ with kinematic $\hat{F}^i_{a_j}$, $\Delta\hat{F}^i_{a_j}$, $\hat{j}_{a_j}$. Define

$$\hat{C}_a:=\otimes_{i=1}^{n_a}\hat{C}_{a_i} \tag{D1}$$

and

$$\tilde{U}_a[\Lambda,Y]:=\hat{C}_a\hat{U}_a[\Lambda,Y]\hat{C}_a^{\dagger}=\otimes_{i=1}^{n_a}(\hat{C}_{a_i}\hat{U}_{a_i}[\Lambda,Y]\hat{C}_{a_i}^{\dagger}). \tag{D2}$$

By assumption, the representations $\hat{U}_a[\Lambda,A]$ and $\tilde{U}_a[\Lambda,A]$ have the same scattering matrix elements, which are products of the single cluster scattering matrix elements. In addition, because

$$(\hat{I}-\hat{C}_a)\hat{U}_0[I,T]=\otimes_{i=1}^{n_a}(I_{a_i}-\hat{C}_{a_i})\hat{U}_{0a_i}[I,T], \tag{D3}$$

it follows that

$$\lim_{t\to\pm\infty}(\hat{I}-\hat{C}_a)\hat{U}_0[I,T]=0, \tag{D4}$$

which shows that $\hat{C}_a$ is a scattering equivalence on the N-body Hilbert space.

The representation $\tilde{U}_a[\Lambda,Y]$ does not have kinematic $\hat{F}_i$, $\Delta\hat{F}_i$, or $\hat{j}$, even though each factor of the tensor product has this property. The advantage of the representation $\tilde{U}_a[\Lambda,Y]$ is that it is scattering equivalent to a representation $\overline{U}_a[\Lambda,Y]$ that has a kinematic $\hat{F}^i$, $\Delta\hat{F}^i$ and $\hat{j}$.

To show this consider the structure of the single cluster $\tilde{H}_{a_i}$ and $\tilde{M}_{a_i}$. The Hamiltonian $\tilde{H}_a$ of the representation $\tilde{U}_a[\Lambda,Y]$ is

$$\tilde{H}_a:=\sum_{i=1}^{n_a}\tilde{H}_{a_i}\otimes\hat{I}_i, \tag{D5}$$

where $\hat{I}_i$ is the identity on the remaining factors in the tensor product. The mass operator $\tilde{M}_a$ is a function of the commuting operators $\tilde{M}_{a_i}\otimes\hat{I}_i$ and $\tilde{\vec{P}}_{a_i}\otimes\hat{I}_i$. Corollary 3 of Theorem 1 give mild conditions on the interactions for $\tilde{H}_a$ and $\tilde{M}_a$ to lead to the same S-matrix.

The matrix elements of $\tilde{M}_{a_i}\otimes\hat{I}_i$ in the tensor product of n_a free particle irreducible representations have the form

$$\begin{aligned}&\langle\otimes_j(f_j,d_j;m_j,j_j)|\tilde{M}_{a_i}\otimes\hat{I}_i|\otimes_k(f'_k,d'_k;m'_k,j'_k)\rangle\\&=\delta[f_i,f'_i]\delta_{j_ij'_i}\langle d_i,m_i\|\tilde{M}^{j_i}_{a_i}\|d'_i,m'_i\rangle\prod_{k\neq i}\delta[f_k,f'_k]\delta[d_k,d'_k]\delta_{j_kj'_k}\delta(m_k-m'_k).\end{aligned} \tag{D6}$$

An irreducible free particle basis for the N-body system can be constructed by successive use of the $ISL(2,C)$ Clebsch–Gordan coefficients to decompose the basis $|\otimes_j(f_j,d_j;m_j,j_j)\rangle$ into a

direct integral of irreducible representations. What is relevant for the proof of this theorem is that the variables m_i, d_i, and j_i that appear in the kernel $\langle d_i, m_i \| \tilde{M}_{a_i}^{j_i} \| d_i', m_i' \rangle$ of $\tilde{M}_{a_j}$ are degeneracy parameters in this representation.

In order to be precise assume that the irreducible free particle basis is obtained by successively coupling clusters in the order $(\cdots(((12)3)4)\cdots n_a)$. In addition, at each stage in the coupling define $\hat{q}_i$ as the solution to

$$\hat{M}_{0(\cdots(12))3)\cdots i+1)} = \sqrt{\hat{q}_i^2 + \hat{M}_{0(i+1)}^2} + \sqrt{\hat{q}_i^2 + \hat{M}_{0(\cdots(12))3)\cdots i)}^2}. \tag{D7}$$

The operators $\hat{q}_i$ are alternate labels for the kinematic invariant masses $\hat{M}_{0(\cdots(12))3)\cdots i)}$.

Define the single cluster mass operators $\overline{M}_{a_i}$ in this irreducible representation,

$$\langle f,d;m,j|\overline{M}_{a_i}|f',d';m',j'\rangle = \delta[f,f']\delta[j,j']\delta_{j_i j_i'}\langle d_i, m_i \| \tilde{M}_{a_i}^{j_i} \| d_i', m_i' \rangle \times JJ' \prod_{k\neq i} \delta_{j_k j_k'} \delta(m_k - m_k') \prod_{l=1}^{n_a} (q_l - q_l') \delta_{r_l r_l'}, \tag{D8}$$

where the q_l's are considered functions of the kinematic invariant masses, the r_l are degeneracy parameters that result when particle l is coupled to the irreducible $(1\cdots l-1)$ system, and J and J' are Jacobians

$$J = \left| \frac{\partial(q_1 \cdots q_{n_a-1})}{\partial(m_{(12)} \cdots m_{0(\cdots((12)\cdots(n_a)))})} \right|^{1/2}. \tag{D9}$$

The three important observations about this definition are the following.

(i) The nontrivial part of this kernel is identical to the nontrivial part of the kernel of $\tilde{M}_{a_i}$ in the tensor product representation (D6).

(ii) Each $\overline{M}_{a_j}$ commutes with $\hat{F}_0^i$, $\Delta\hat{F}_0^i$, $\hat{j}_0$.

(iii) $[\overline{M}_{a_i}, \overline{M}_{a_j}] = 0$.

The relations (D7) can be inverted to express the free mass as a function of the free single cluster mass operators and the q_i's:

$$\hat{M}_0 = M(\hat{M}_{01}, \ldots, \hat{M}_{0n_a}, \hat{q}_1, \ldots, \hat{q}_{n_a-1}). \tag{D10}$$

The commutation relations allow the definition

$$\overline{M}_a := M(\tilde{M}_{a_1}, \ldots, \tilde{M}_{a_{n_a}}, \hat{q}_1, \ldots, \hat{q}_{n_a-1}), \tag{D11}$$

where the $\hat{q}_i$'s in (D11) are identical to the non-interacting $\hat{q}_i$'s in (D10). By construction $\overline{M}_a$ commutes with $\hat{F}_0^i$, $\Delta\hat{F}_0^i$, $\hat{j}_0$. Simultaneous eigenstates of $\overline{M}_a$, $\hat{F}_0^i$, and j_0 transform as mass $\overline{M}_a$ spin j_0 irreducible representations of $ISL(2,)$. This defines the representation $\overline{U}_a[\Lambda, Y]$.

In order to construct a scattering theory we need to define a suitable injection operator to the asymptotic Hilbert space for $\hat{M}_a$. The channel injection operator for the representation $\tilde{U}_a[\Lambda, Y]$ is the tensor product of irreducible eigenstates

$$\tilde{\Phi}_\alpha = |f_1, \alpha_1, \ldots, f_{n_a}, \alpha_1\rangle. \tag{D12}$$

The corresponding channel injection operator for the representation $\overline{U}_a[\Lambda,A]$ is defined as the simultaneous eigenstates of $\overline{M}_a$, $\hat{j}_0^2$, $\hat{F}_0^j$, $\hat{q}_{i0}$, $\hat{r}_i$, and $\tilde{M}_{a_i}$ corresponding the same bound states of the $\tilde{M}_{a_i}$:

$$\overline{\Phi}_\alpha = |f, j_0, q_1, \ldots, q_{n_a-1}, r_1, \ldots, r_{n_a-1}, \alpha_1 \ldots \alpha_{n_a}\rangle. \tag{D13}$$

These differ by the delta functions that multiply the cluster eigenfunctions.

With this definition it follows that

$$\overline{\Omega}_{a\pm} := \Omega_\pm(\overline{M}_a, \overline{\Phi}_{\mathcal{A}a}, H_{\mathcal{A}a}) \tag{D14}$$

exist and are complete. The scattering operator

$$\overline{S}_a = \overline{\Omega}_{a+}^\dagger \overline{\Omega}_{a-} = \delta_{j_0 j_0'} \delta[f, f'] \prod_{i=1}^{n_a-1} \delta(q_i - q_i') \delta[r_i, r_i'] \prod_i \delta_{j_i j_i'} \hat{S}_{a_i} \tag{D15}$$

is identical to $\tilde{S}_a$ if the Clebsch–Gordan coefficients are used to replace the irreducible spectator variables by the single cluster f_i, j_i's. The equivalence follows because the S-matrix elements are determined by the single cluster mass operators, which have identical reduced kernels in representations (D6) and (D8).

This establishes that the representations $\tilde{U}_a[\Lambda,Y]$ and $\overline{U}_a[\Lambda,Y]$ give the same scattering matrix elements. By Theorem 3 they are scattering equivalent. Let $\hat{D}_a$ be the scattering equivalence that relates these two representations:

$$\overline{U}_a[\Lambda,Y] = \hat{D}_a \tilde{U}_a[\Lambda,Y] \hat{D}_a^\dagger. \tag{D16}$$

It follows from (D2) and (D16) that

$$\overline{U}_a[\Lambda,Y] = \hat{B}_a \hat{U}_a[\Lambda,Y] \hat{B}_a^\dagger, \tag{D17}$$

where

$$\hat{B}_a := \hat{D}_a \hat{C}_a. \tag{D18}$$

The operator $\hat{B}_a$ is a scattering equivalence since it is a product of scattering equivalences. This completes the proof of Theorem 4.

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Exactly solvable models of relativistic δ-sphere interactions in quantum mechanics

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We discuss the quantum Hamiltonian $H_{\underline{\underline{G}}}$ describing a δ-sphere interaction introduced in [J. Math. Phys **30**, 2275 (1989)] and formally given by $H_{\underline{\underline{G}}}=H_D+\underline{\underline{G}}\,\delta(|x|-R)$, where H_D is the Dirac Hamiltonian and $\underline{\underline{G}}$ is a real 4×4 matrix defined by $\underline{\underline{G}}=\left(\begin{smallmatrix}A & 0\\ 0 & B\end{smallmatrix}\right)$. We obtain a series of new results for this model, in particular the resolvent equation, the spectral properties, the nonrelativistic limit and the various quantities related to the scattering theory. These results are generalized to the case of an asymmetric δ-sphere interaction and a δ-sphere plus Coulomb interaction, respectively. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In the last two decades, a lot of research has been carried out on point and sphere interactions in quantum mechanics, both from the mathematical point of view and for their applications in physics.[1–15]

For a long time, this research focused on nonrelativistic interactions. The first paper providing a rigorous mathematical analysis of relativistic δ-sphere interactions was published in 1989 by Dittrich *et al.*[7] Using the theory of self-adjoint extensions of symmetric closed operators in Hilbert spaces, Ref. 7 defines the quantum Hamiltonian corresponding to the formal expression:

$$H_{\underline{\underline{G}}}=H_D+\underline{\underline{G}}\,\delta(|x|-R),\quad x\in\mathbb{R}^3,\quad R\in\mathbb{R}, \tag{1}$$

where $\underline{\underline{G}}$ is a real 4×4 matrix of the form $\underline{\underline{G}}=\left(\begin{smallmatrix}A & 0\\ 0 & B\end{smallmatrix}\right)$, H_D is the Dirac Hamiltonian and R is the radius of a sphere in $\mathbb{R}^3$ centered at the origin. Ref. 7 also provides a detailed discussion of the spectral properties of $H_{\underline{\underline{G}}}$.

In Ref. 12, the above results were extended to the case of a δ sphere plus a Coulomb interaction. In Ref. 12, the authors also provide a numerical analysis of the point spectrum and compare the definition of $H_{\underline{\underline{G}}}$ used in Refs. 7 and 12 with an alternative definition proposed by Dominguez-Adame.[8]

More recently, Hounkonnou and Avossevou published a series of papers in which they claim to provide rigorous mathematical definitions and to perform a systematic study of the δ, δ' and finitely many δ-sphere interactions in the particular cases when $A\neq0$, $B=0$ and $A=0$, $B\neq0$.[16–19] Unfortunately, a comparison with Refs. 7 and 12 shows that the boundary conditions used in Refs. 17 and 19 do not correspond to any of the above-mentioned δ-sphere interactions. Actually these boundary conditions do not define any self-adjoint operator. Therefore, the conditions required for

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the application of the Krein formula and the Weyl theorem for the computation of the resolvent equation and the analysis of spectral properties of $H_{\underline{\underline{G}}}$ are not fulfilled which means that all the results presented in Refs. 17–19 are not correct.

The aim of this paper is to provide new results on the relativistic δ-sphere interaction in the general case $A\neq 0$ and $B\neq 0$.

The paper covers several areas which were not considered in Refs. 7 and 12 and therefore provides new insights in the understanding of relativistic δ-sphere interactions. As an example, the nonrelativistic limit leads to a new two-parameters family of nonrelativistic δ-sphere interactions. As in the case of point and nonrelativistic δ-sphere interactions, these results were obtained by applying rigorous concepts and techniques of functional analysis and differential operators.

The applications of point and sphere interactions in physics are greatly facilitated by the fact these interactions are exactly solvable. Point and nonrelativistic δ-sphere interactions are extensively used since the 1930s in order to develop mathematical models in nuclear, solid state, and molecular physics [(see Refs. 2 and 3) and references therein]. More recently, nonrelativistic δ-sphere interactions were used to define a mathematical model of heavy quarkonia mesonic decays.[13] Since relativistic δ-sphere interactions are also exactly solvable, it is anticipated that a better understanding of these interactions will stimulate research on their applications in various areas of physics.

In Sec. II, we define the quantum Hamiltonian describing the interaction, compute the resolvent equation, derive the spectral properties and obtain the nonrelativistic limit of the Hamiltonian. We also discuss the stationary scattering theory for the pair $(h_{jl,G_{jl}};h_D)$ where $h_{jl,G_{jl}}$ and h_D are defined by Eqs. (38) and (42), respectively. In Sec. III, we discuss the generalization of $H_{\underline{\underline{G}}}$ to the so-called asymmetric δ-sphere interactions while in Sec. IV we provide a generalization of the results obtained in Sec. II to the case of a δ-sphere plus a Coulomb interaction.

The special cases $A\neq 0$, $B=0$ and $A=0$, $B\neq 0$ yield the relativistic δ-sphere interactions of the first and second type, respectively. Indeed, as indicated in Sec. II D, the nonrelativistic limits of the Hamiltonians corresponding to these interactions converge in the norm resolvent topology to the Hamiltonians describing the nonrelativistic δ-sphere interactions of the first and second type, respectively.[2,4,5]

In a series of forthcoming papers,[20] we extend the results presented in this publication to the case of a δ' and finitely many sphere interactions and discuss the approximation of $H_{\underline{\underline{G}}}$ by local scaled short range and momentum cutoff Hamiltonians.

II. THE δ-SPHERE INTERACTION

A. Definition of the Hamiltonian

In this section, using the theory of self-adjoint extensions of symmetric closed operators in Hilbert spaces, we provide the mathematical definition of a quantum Hamiltonian describing a relativistic δ-sphere interaction formally given by

$$H_{\underline{\underline{G}}}=H_D+\underline{\underline{G}}\,\delta(|x|-R);\quad x\in\mathbb{R}^3,\quad R\in\mathbb{R}, \tag{2}$$

where $\underline{\underline{G}}$ is a real 4×4 matrix of the form

$$\underline{\underline{G}}=\begin{pmatrix} A & 0\\ 0 & B\end{pmatrix}. \tag{3}$$

1. The radial operators

Consider in the state Hilbert space $\mathcal{H}=L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ the Dirac Hamiltonian H_D defined by

$$\begin{aligned} H_D&=-\mathrm{i}\underline{\underline{\alpha}}\nabla+\underline{\underline{\beta}}\frac{c^2}{2},\\ \mathcal{D}(H_D)&=H^{1,2}(\mathbb{R}^3)\otimes\mathbb{C}^4, \end{aligned} \tag{4}$$

where we have used the following definitions and notations:

(i) c is the velocity of the light,
(ii) $H^{m,n}(\Omega)$ is the Sobolev space of indices (m,n),
(iii) $\underline{\underline{\alpha}}$ and $\underline{\underline{\beta}}$ are 4×4 Dirac matrices given by

$$\underline{\underline{\alpha}}=\begin{pmatrix}0 & \sigma\\ \sigma & 0\end{pmatrix},\quad \underline{\underline{\beta}}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{5}$$

Here σ are Pauli's spin matrices defined by

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{6}$$

Consider in $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ the symmetric closed operator $\overline{H}_D$ defined by

$$\overline{H}_D=H_D,$$

$$D(\overline{H}_D)=\{\psi\in H^{1,2}(\mathbb{R}^3)\otimes\mathbb{C}^4/\psi(S_R)=0\}, \tag{7}$$

where $S_R=\{x\in\mathbb{R}^3:|x|=R\}$ is the sphere of radius R in $\mathbb{R}^3$ centered at the origin.

As indicated in Ref. 7, the operator $\overline{H}_D$ admits a large number of self-adjoint extensions. In this paper, we consider those extensions of $\overline{H}_D$ which correspond to $H_{\underline{\underline{G}}}$.

For this purpose, we restrict ourselves to those extensions of $\overline{H}_D$ which are rotationally and space-reflection symmetric. With these assumptions, one may decompose the space $\mathcal{H}$ in the following way:

$$\mathcal{H}=\bigoplus_{j=1/2}^{\infty}\ \bigoplus_{l=j-1/2}^{j+1/2}\ \bigoplus_{\mu=-j}^{j}\mathcal{H}_{jl\mu}, \tag{8}$$

where we have used the following definitions and notations:

(i)
$$\mathcal{H}_{jl\mu}=\left\{\psi\in\mathcal{H}\,\middle|\,\psi(r,n)=\begin{pmatrix}f(r)\Omega_{jl\mu}(n)\\ g(r)\Omega_{jl'\mu}(n)\end{pmatrix};f,g\in L^2((0,\infty),r^2dr)\right\}, \tag{9}$$

(ii) $\Omega_{jl\mu}$ are spherical spinors defined by[21]

$$\Omega_{jl\mu}(\theta,\varphi)=\begin{pmatrix}\sqrt{\dfrac{j+\mu}{2l+1}}Y_{l,\mu-1/2}(\theta,\varphi)\\ \sqrt{\dfrac{j-\mu}{2l+1}}Y_{l,\mu+1/2}(\theta,\varphi)\end{pmatrix}\quad \text{for } l=j-\frac{1}{2}, \tag{10}$$

$$\Omega_{jl\mu}(\theta,\varphi)=\begin{pmatrix}-\sqrt{\dfrac{j-\mu+1}{2l+1}}Y_{l,\mu-1/2}(\theta,\varphi)\\ \sqrt{\dfrac{j+\mu+1}{2l+1}}Y_{l,\mu+1/2}(\theta,\varphi)\end{pmatrix}\quad \text{for } l=j+\frac{1}{2}, \tag{11}$$

(iii) $l'=j\mp\frac{1}{2}$ for $l=j\pm\frac{1}{2}$.

Next we introduce the isomorphisms U_{jl} defined by

$$U_{jl}:L^2((0,\infty);r^2dr)\otimes\mathbb{C}^2\to\tilde{\mathcal{H}}\equiv L^2((0,\infty);dr)\otimes\mathbb{C}^2, \tag{12}$$

$$(U_{jl}\psi)(r)=\begin{pmatrix} rf(r) \\ (-1)^{j-l-1/2}rg(r)\end{pmatrix} \tag{13}$$

which enable us to represent $\mathcal{H}$ in the form

$$\mathcal{H}=\bigoplus_{j=1/2}^{\infty}\bigoplus_{l=j-1/2}^{j+1/2}\bigoplus_{\mu=-j}^{j}[U_{jl}^{-1}\tilde{\mathcal{H}}]\otimes[\Omega_{jl\mu}(\theta,\varphi)], \tag{14}$$

where $[\Omega_{jl\mu}(n)]$ stands for the vector space generated by the spherical spinors.

With respect to the decomposition (14), $\overline{H}_D$ reads

$$\overline{H}_D=\bigoplus_{j=1/2}^{\infty}\bigoplus_{l=j-1/2}^{j+1/2}[U_{jl}^{-1}h_{jl}U_{jl}]\otimes\mathbb{1}. \tag{15}$$

The operators h_{jl} in $L^2((0,\infty))\otimes\mathbb{C}^2$ are given by

$$h_{jl}=\begin{pmatrix} \dfrac{c^2}{2} & -c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} \\ c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} & -\dfrac{c^2}{2}\end{pmatrix}\equiv\tau, \tag{16}$$

$$\kappa_{jl}=(-1)^{j-l+1/2}(j+\tfrac{1}{2}), \tag{17}$$

$$\begin{aligned} D(h_{jl})=\{&\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\,|\,\psi\in \mathrm{AC}_{\mathrm{loc}}((0,\infty));\quad \psi(R\pm)=0;\\ &\tau\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\},\end{aligned} \tag{18}$$

where $\mathrm{AC}_{\mathrm{loc}}(\Omega)$ denotes the set of locally absolutely continuous functions on Ω and

$$\psi(x\pm)=\lim_{\epsilon\to 0+}\psi(x\pm\epsilon).$$

The adjoint h_{jl}^* of h_{jl} reads

$$h_{jl}^*=\tau,$$

$$\begin{aligned} D(h_{jl}^*)=\{&\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\,|\,\psi\in \mathrm{AC}_{\mathrm{loc}}((0,\infty)\setminus\{R\}),\\ &\tau\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\}.\end{aligned} \tag{19}$$

2. The self-adjoint extensions of h_{jl}

Consider the equation

$$(h_{jl}^*-z)\psi=0,\quad \psi\in\mathcal{D}(h_{jl}^*),\quad z\in\mathbb{C}-\left\{\left(-\infty,-\frac{c^2}{2}\right]\cup\left[\frac{c^2}{2},\infty\right)\right\} \tag{20}$$

which may be written in the form

$$\psi_1''+\left[k(z)^2-\frac{\kappa_{jl}(\kappa_{jl}+1)}{r^2}\right]\psi_1=0,$$
$$\psi_2''+\left[k(z)^2-\frac{\kappa_{jl}(\kappa_{jl}-1)}{r^2}\right]\psi_2=0, \tag{21}$$

where

$$k(z)=\frac{1}{c}\sqrt{z^2-\frac{c^4}{4}}\equiv k. \tag{22}$$

A straightforward computation shows that Eq. (20) has two linearly independent solutions

$$\psi^{(1)}_{jl,z}(r)=\begin{cases}\begin{pmatrix}F_{jl}(z,r)\\ \tilde{F}_{jl}(z,r)\end{pmatrix}, & r<R,\\ \begin{pmatrix}0\\0\end{pmatrix}, & r>R,\end{cases} \tag{23}$$

$$\psi^{(2)}_{jl,z}(r)=\begin{cases}\begin{pmatrix}0\\0\end{pmatrix}, & r<R,\\ \begin{pmatrix}G_{jl}(z,r)\\ \tilde{G}_{jl}(z,r)\end{pmatrix}, & r<R,\end{cases} \tag{24}$$

where

$$F_{jl}(z,r)=\left(\frac{k(z)}{2}\right)^{-\kappa_{jl}-1/2}\Gamma\left(\kappa_{jl}+\frac{3}{2}\right)r^{1/2}J_{\kappa_{jl}+1/2}(k(z)r), \tag{25}$$

$$\tilde{F}_{jl}(z,r)=\frac{1}{c}\left(\frac{1}{2}\right)^{-\kappa_{jl}-1/2}k(z)^{-\kappa_{jl}+1/2}\Gamma\left(\kappa_{jl}+\frac{3}{2}\right)r^{1/2}J_{\kappa_{jl}-1/2}(k(z)r), \tag{26}$$

$$G_{jl}(z,r)=\mathrm{i}\frac{\pi}{2}\left(\frac{k(z)}{2}\right)^{\kappa_{jl}+1/2}\Gamma\left(\kappa_{jl}+\frac{3}{2}\right)^{-1}r^{1/2}H^{(1)}_{\kappa_{jl}+1/2}(k(z)r), \tag{27}$$

$$\tilde{G}_{jl}(z,r)=\mathrm{i}\frac{\pi}{2c}\left(\frac{1}{2}\right)^{\kappa_{jl}+1/2}k(z)^{\kappa_{jl}+3/2}\Gamma\left(\kappa_{jl}+\frac{3}{2}\right)^{-1}r^{1/2}H^{(1)}_{\kappa_{jl}-1/2}(k(z)r),\quad \mathrm{Im}\,k(z)>0. \tag{28}$$

$J_\nu(.)$ is the Bessel function and $H^{(1)}_\nu(.)$ the Hankel function of the first type of order ν.

The solutions (23) and (24) have been normalized in such a way that

$$\det\begin{bmatrix}G_{jl}(z,r) & F_{jl}(z,r)\\ \tilde{G}_{jl}(z,r) & \tilde{F}_{jl}(z,r)\end{bmatrix}=\frac{1}{c}. \tag{29}$$

Therefore, h_{jl} has deficiency indices (2,2) and consequently, all self-adjoint(sa) extensions of h_{jl} are given by a four-parameter family of self-adjoint operators.[22] Since the matrix G in Eq. (34) depends on two parameters, it follows that the sa extension $h_{jl,G}$ of h_{jl} corresponding to the interaction $V(r)=G\,\delta(r-R)$ is a special two-parameters family of sa extensions of h_{jl}.

The relation $h_{jl,G}\subset h^*_{jl}$ implies that the domain $\mathcal{D}(h_{jl,G})$ contains those functions $\psi\in\mathcal{D}(h^*_{jl})$ which satisfy suitable boundary conditions at $r=R$.

Theorem 2.1 (Ref. 7): Any self-adjoint extension $\hat{h}_{jl}$ of h_{jl} reads

$$\hat{h}_{jl}=\begin{pmatrix} \frac{c^2}{2} & -c\frac{d}{dr}+c\frac{\kappa_{jl}}{r} \\ c\frac{d}{dr}+c\frac{\kappa_{jl}}{r} & -\frac{c^2}{2} \end{pmatrix},$$

$$\mathcal{D}(\hat{h}_{jl})=\{\psi\in\mathcal{D}(h_{jl}^{*})/\psi \text{ satisfies } \mathrm{cond}_1 \text{ or } \mathrm{cond}_2\}, \tag{30}$$

$$\mathrm{cond}_1:\psi(R-)=e^{i\theta}\hat{A}\psi(R_+),\quad \theta\in[0,\pi), \tag{31}$$

and $\hat{A}$ is a 2×2 matrix with $\det\hat{A}=1$;

$$\mathrm{cond}_2:\begin{pmatrix} c_1 & c_2 \\ 0 & 0 \end{pmatrix}\psi(R-)+\begin{pmatrix} 0 & 0 \\ d_1 & d_2 \end{pmatrix}\psi(R+)=0, \tag{32}$$

where c_1, c_2, d_1, and d_2 are real and both matrices are nonzero. Conversely, any operator of this form is self-adjoint extension of h_{jl}.

Theorem 2.2 (Ref. 7): The general form of boundary conditions (31) and (32) reads

$$C\psi(R-)+D\psi(R+)=0, \tag{33}$$

where C and D are 2×2 matrices such that the 2×4 matrix (C,D) has rank 2.

Let us now construct the self-adjoint extension corresponding to the radial Dirac operator with the potential

$$V(r)=G_{jl}\delta(r-R),$$

$$G_{jl}=\begin{pmatrix} A_{jl} & 0 \\ 0 & B_{jl} \end{pmatrix},\quad A_{jl},B_{jl}\in\mathbb{R}.$$

Suppose that ψ satisfies the equation

$$[\tau+G_{jl}\delta(r-R)]\psi=z\psi, \tag{34}$$

$$\tau=\begin{pmatrix} \frac{c^2}{2} & -c\frac{d}{dr}+c\frac{\kappa_{jl}}{r} \\ c\frac{d}{dr}+c\frac{\kappa_{jl}}{r} & -\frac{c^2}{2} \end{pmatrix},$$

$$G_{jl}=\begin{pmatrix} A_{jl} & 0 \\ 0 & B_{jl} \end{pmatrix},\quad A_{jl},\ B_{jl}\in\mathbb{R}, \tag{35}$$

and the limits $f(R\pm)$ exist. Integrating Eq. (34) over $(R-\epsilon,R+\epsilon)$, and taking the limit $\epsilon\to0$ we get[7]

$$\left(1-\tau_0\frac{G_{jl}}{2c}\right)\psi(R+)-\left(1+\tau_0\frac{G_{jl}}{2c}\right)\psi(R-)=0, \tag{36}$$

where

$$\tau_0=\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{37}$$

We will accept only those matrices G for which Eq. (36) is compatible with Eqs. (31) and (32). As indicated in Ref. 7 the boundary condition (36) defines a self-adjoint extension of h_{jl} iff $G=G^{+}$.

Consider in $L^2((0,\infty))\otimes\mathbb{C}^2$ the operator $h_{jl,G_{jl}}$ defined by

$$h_{jl,G_{jl}}=\begin{pmatrix} \dfrac{c^2}{2} & -c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} \\ c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} & -\dfrac{c^2}{2} \end{pmatrix}\equiv\tau,$$

$$D(h_{jl,G_{jl}})=\left\{\psi\in\mathcal{D}(h_{jl}^{*})\middle|\left(1-\tau_0\frac{G_{jl}}{2c}\right)\psi(R+)-\left(1+\tau_0\frac{G_{jl}}{2c}\right)\psi(R-)=0\right\}, \tag{38}$$

$$l\in[j-\tfrac{1}{2},j+\tfrac{1}{2}],\quad j\in[\tfrac{1}{2},\infty).$$

The boundary condition (38) may be written in the form

$$C\psi(R-)+D\psi(R+)=0 \tag{39}$$

with

$$C=-\begin{pmatrix} 1 & -\dfrac{B_{jl}}{2c} \\ \dfrac{A_{jl}}{2c} & 1 \end{pmatrix},\quad D=\begin{pmatrix} 1 & \dfrac{B_{jl}}{2c} \\ -\dfrac{A_{jl}}{2c} & 1 \end{pmatrix}. \tag{40}$$

Therefore, according to theorem 2.2, the operator $h_{jl,G_{jl}}$ is a self-adjoint extension of h_{jl}.

By construction, the operator $h_{jl,G_{jl}}$ provides the mathematical definition of the formal expression

$$h_{G_{jl}}=h_D+G_{jl}\delta(r-R), \tag{41}$$

where h_D is the radial Dirac Hamiltonian defined by

$$h_D=\begin{pmatrix} \dfrac{c^2}{2} & -c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} \\ c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} & -\dfrac{c^2}{2} \end{pmatrix},$$

$$\mathcal{D}(h_D)=\{\psi\in\mathcal{D}(h_{jl}^{*})\,|\,\psi(R+)=\psi(R-)\}\quad l\in[j-\tfrac{1}{2},j+\tfrac{1}{2}],j\in[\tfrac{1}{2},\infty). \tag{42}$$

The case $G_{jl}=0$ in Eq. (38) yields the radial Dirac Hamiltonian $h_{jl,0}\equiv h_D$. The case $A_{jl}\neq 0$, $B_{jl}=0$ in Eq. (38) gives the δ-sphere interaction of the first type defined by[23]

$$h_{jl,A_{jl}}=\tau,$$

$$\mathcal{D}(h_{jl,A_{jl}})=\left\{\psi=\begin{pmatrix} f \\ g \end{pmatrix}\in\mathcal{D}(h_{jl}^{*})\middle|\, f(R-)=f(R+)\equiv f(R),\ \ g(R+)-g(R-)=\frac{A_{jl}}{c}f(R)\right\}. \tag{43}$$

The case $A_{jl}=0$, $B_{jl}\neq 0$ leads to a δ-sphere interaction of the second type defined by[23]

$$h_{jl,B_{jl}}=\tau,$$
$$\mathcal{D}(h_{jl,B_{jl}})=\left\{\psi=\begin{pmatrix} f \\ g\end{pmatrix}\in\mathcal{D}(h_{jl}^{*})\,\middle|\, g(R-)=g(R+)\equiv g(R),\ \ f(R+)-f(R-)=-\frac{B_{jl}}{c}g(R)\right\}. \tag{44}$$

Let $\underline{\underline{G}}=\{G_{jl}\};\ j-\frac{1}{2}\leqslant j+\frac{1}{2};\ \frac{1}{2}\leqslant j<\infty$. The decomposition (15), implies that the operator $H_{\underline{\underline{G}}}$ in $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ defined by

$$H_{\underline{\underline{G}}}=\bigoplus_{j=1/2}^{\infty}\ \bigoplus_{l=j-1/2}^{j+1/2} U_{jl}^{-1}h_{jl,G_{jl}}U_{jl}\otimes\mathbb{I} \tag{45}$$

provides the mathematical formulation of the formal expression (2). Actually, $H_{\underline{\underline{G}}}$ in Eq. (45) provides a slight generalization of Eq. (2) since $\underline{\underline{G}}$ may depend on j and l.

The case $\underline{\underline{G}}=0$, i.e., $G_{jl}=0$ for all j and l yields the Dirac Hamiltonian H_D defined by Eq. (4).

B. The resolvent equation

Theorem 2.3: The resolvent of $h_{jl,G_{jl}}$ is given by

$$(h_{jl,G_{jl}}-z)^{-1}=(h_D-z)^{-1}+\vartheta_{jl}(z,A_{jl},B_{jl})\left\{(\overline{\hat{M}_{jl,z}^{(2)}(.)},.)\left[A_{jl}\hat{M}_{jl,z}^{(2)}(.)+\frac{A_{jl}B_{jl}}{2c}\tilde{M}_{jl,z}^{(1)}(.)\right]\right.$$
$$\left.+(\overline{\tilde{M}_{jl,z}^{(2)}(.)},.)\left[B_{jl}\tilde{M}_{jl,z}^{(2)}(.)-\frac{A_{jl}B_{jl}}{2c}\hat{M}_{jl,z}^{(1)}(.)\right]\right\},$$
$$z\in\rho(h_{jl,G_{jl}}),\quad \operatorname{Im}k(z)>0,\quad l\in\left[j-\frac{1}{2},j+\frac{1}{2}\right],\quad j\in\left[\frac{1}{2},\infty\right) \tag{46}$$

[$\rho(.)$ is the resolvent set],
where $(h_D-z)^{-1}$, $\operatorname{Im}k(z)>0$ is the radial Dirac resolvent with kernel

$$G^{(jl)}(z,r,r')=\begin{pmatrix} G_{11}^{(jl)}(z,r,r') & G_{12}^{(jl)}(z,r,r') \\ G_{21}^{(jl)}(z,r,r') & G_{22}^{(jl)}(z,r,r')\end{pmatrix}, \tag{47}$$

where

$$G_{11}^{(jl)}(z,r,r')=\begin{cases} G_{jl}(z,r')F_{jl}(z,r), & r<r', \\ F_{jl}(z,r')G_{jl}(z,r), & r>r', \end{cases} \tag{48}$$

$$G_{12}^{(jl)}(z,r,r')=\begin{cases} \tilde{G}_{jl}(z,r')F_{jl}(z,r), & r<r' \\ \tilde{F}_{jl}(z,r')G_{jl}(z,r), & r>r', \end{cases} \tag{49}$$

$$G_{21}^{(jl)}(z,r,r')=\begin{cases} G_{jl}(z,r')\tilde{F}_{jl}(z,r), & r<r' \\ F_{jl}(z,r')\tilde{G}_{jl}(z,r), & r>r', \end{cases} \tag{50}$$

$$G_{22}^{(jl)}(z,r,r')=\begin{cases} \tilde{G}_{jl}(z,r')\tilde{F}_{jl}(z,r), & r<r' \\ \tilde{F}_{jl}(z,r')\tilde{G}_{jl}(z,r), & r>r', \end{cases} \tag{51}$$

and

$$\vartheta_{jl}(z,A_{jl},B_{jl})=-\left[1-\frac{A_{jl}B_{jl}}{4c^2}+B_{jl}\tilde{F}_{jl}(z,R)\tilde{G}_{jl}(z,R)+A_{jl}F_{jl}(z,R)G_{jl}(z,R)\right]^{-1}, \tag{52}$$

$$\hat{M}^{(m)}_{jl,z}(r)=\begin{cases} G^{(jl)}(z,r,R)\begin{pmatrix}1\\0\end{pmatrix}, & r<R,\\ (-1)^m G^{(jl)}(z,r,R)\begin{pmatrix}1\\0\end{pmatrix}, & r>R, m=1,2,\end{cases} \tag{53}$$

$$\tilde{M}^{(m)}_{jl,z}(r)=\begin{cases} G^{(jl)}(z,r,R)\begin{pmatrix}0\\1\end{pmatrix}, & r<R,\\ (-1)^m G^{(jl)}(z,r,R)\begin{pmatrix}0\\1\end{pmatrix}, & r>R, m=1,2\end{cases} \tag{54}$$

with $F_{jl}(z,r)$, $\tilde{F}_{jl}(z,r)$, $G_{jl}(z,r)$, $\tilde{G}_{jl}(z,r)$, and $k(z)$ defined by (25)–(28) and (22), respectively.

Proof: According to Krein's resolvent formula,[22] we have

$$(h_{jl,G_{jl}}-z)^{-1}=(h_D-z)^{-1}+\sum_{n,m=1}^{2}\lambda_{mn}(z)(\overline{\psi^{(n)}_{jl,z}(.)},.)\psi^{(m)}_{jl,z}(.),\quad z\in\rho(h_{jl,G_{jl}}),\quad \mathrm{Im}\,k(z)>0, \tag{55}$$

where $\psi^{(m)}_{jl,z}(r)$, $m=1,2$ are given by (23) and (24), respectively.

Let $\phi=\binom{\phi_1}{\phi_2}\in L^2((0,\infty))\otimes\mathbb{C}^2$ and define the function $\chi_{jl}(z,r)$ by

$$\chi_{jl}(z,r)=((h_{jl,G_{jl}}-z)^{-1}\phi)(r). \tag{56}$$

Since $\chi_{jl}=\binom{\chi_{jl,1}}{\chi_{jl,2}}\in\mathcal{D}(h_{jl,G_{jl}})$, it follows that χ_{jl} satisfies the boundary conditions in (38).

The implementation of these boundary conditions provides the constants $\lambda_{mn}(z)$. Inserting the λ_{mn} [z into (55) we obtain Eq. (46)].

Remarks:

(i) The resolvent of H_G may be obtained from Eq. (46) and the decomposition (45).

(ii) In the cases $A_{jl}\neq 0$, $B_{jl}=0$ and $A_{jl}=0$, $B_{jl}\neq 0$, the resolvent Eq. (46) simplifies, respectively, to

$$(h_{jl,A_{jl}}-z)^{-1}=(h_D-z)^{-1}+A_{jl}\vartheta_{jl}(z,A_{jl},0)(\overline{\hat{M}^{(2)}_{jl,z}(.)},.)\hat{M}^{(2)}_{jl,z}(.),$$

$$z\in\rho(h_{jl,A_{jl}}),\quad \mathrm{Im}\,k(z)>0,\ \ l\in[;j-\tfrac{1}{2},j+\tfrac{1}{2}],\quad j\in[\tfrac{1}{2},\infty] \tag{57}$$

and

$$(h_{jl,B_{jl}}-z)^{-1}=(h_D-z)^{-1}+B_{jl}\vartheta_{jl}(z,0,B_{jl})(\overline{\tilde{M}^{(2)}_{jl,z}(.)},.)\tilde{M}^{(2)}_{jl,z}(.),$$

$$z\in\rho(h_{jl,B_{jl}}),\quad \mathrm{Im}\,k(z)>0,\ \ l\in[j-\tfrac{1}{2},j+\tfrac{1}{2}],\quad j\in[\tfrac{1}{2},\infty]. \tag{58}$$

C. Spectral properties

Theorem 2.4: For $A_{jl},B_{jl}\in(-\infty,\infty)$, $l\in[j-\frac{1}{2},j+\frac{1}{2}]$, $j\in[\frac{1}{2},\infty)$, the essential spectrum of $h_{jl,G_{jl}}$ is purely absolutely continuous and coincides with $(-\infty,-c^2/2]\cup[c^2/2,\infty)$. Its singularly continuous and residual spectra are empty. Furthermore, $h_{jl,G_{jl}}$ has at most two eigenvalues (with account of multiplicity in $[-c^2/2,c^2/2]$.

Proof:

See, e.g., Ref. 7, Proposition 6.1 and theorem 6.2.

The resonances of $h_{jl,G_{jl}}$ are defined as poles of the resolvent equation (46) in the unphysical sheet $\mathrm{Im}\,k(z)<0$.

D. The nonrelativistic limit

Following the strategy of Gesztesy *et al.*[1,24] in the case of point interactions, one can discuss the nonrelativistic limit of $h_{jl,G_{jl}}$ as $c\to\infty$.

Theorem 2.5: For spin-$\frac{1}{2}$ particules, the operator $h_{jl,G_{jl}}-(c^2/2)$ converges in norm resolvent sense to the Schrödinger operator $h_{l,\hat{\alpha}_l}$ times the projector onto $\tilde{\mathcal{H}}_+=L^2((0,\infty))$:

$$n.\lim_{c\to\infty}\left(h_{jl,G_{jl}}-\frac{c^2}{2}-z\right)^{-1}=(h_{l,\hat{\alpha}_l}-z)^{-1}\otimes\begin{pmatrix}1&0\\0&0\end{pmatrix},\quad z\in\mathbb{C}\backslash\mathbb{R},\tag{59}$$

where $h_{l,\hat{\alpha}_l}$ is defined by

$$h_{l,\hat{\alpha}_l}=-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2},$$

$$\mathcal{D}(h_{l,\hat{\alpha}_l})=\{f\in L^2((0,\infty))\,|\,f,f'\in \mathrm{AC}_{loc}((0,\infty)\backslash\{R\}),\quad f(0+)=0\quad \text{if } l=0,$$

$$f(R+)-f(R-)=\frac{\beta_l}{2}[f'(R+)+f'(R-)],$$

$$f'(R+)-f'(R-)=\frac{\alpha_l}{2}[f(R+)+f(R-)],\quad -f''+l(l+1)r^{-2}f\in L^2((0,\infty))\},$$

$$\hat{\alpha}=\{\beta_l,\alpha_l\};-\infty<\beta_l,\alpha_l\leqslant\infty;\ \ l\in\mathbb{N}_0.\tag{60}$$

One can prove that if $\alpha_l\beta_l-4=0,\alpha_l,\beta_l\in\mathbb{R}$, then the boundary conditions in (60) define a self-adjoint extension of the radial Schrödinger operator $\dot{h}_l$ defined by

$$\dot{h}_l=-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2},$$

$$\mathcal{D}(\dot{h}_l)=\{f\in L^2((0,\infty))\,|\,f,f'\in \mathrm{AC}_{loc}((0,\infty));f(0+)=0\ \text{ if }\ l=0;\ \ f(R\pm)=f'(R\pm)=0-f''+l(l+1)r^{-2}f\in L^2((0,\infty))\}\quad l\in\mathbb{N}_0.\tag{61}$$

Proof:

One may follow step by step[1,24] where a similar result was obtained in the case of the point interactions.

To the best of our knowledge, the Hamiltonian $h_{l,\hat{\alpha}_l}$ defines a new exactly solvable model of nonrelativistic δ-sphere interactions. The cases $\alpha_l\neq 0$, $\beta_l=0$ and $\alpha_l=0$, $\beta_l\neq 0$ in Eq. (60) lead to nonrelativistic δ-sphere interactions of the first and second type, respectively. These interactions have been extensively discussed in Refs. 2, 4, 5, and 15.

E. Scattering theory for the pair $(h_{jl,G_{jl}};h_D)$

Let us define for $k(z)>0$, the function

$$\begin{pmatrix} F_{G_{jl},1}(z,r) \\ F_{G_{jl},2}(z,r) \end{pmatrix} = \begin{pmatrix} F_{jl}(z,r) \\ \tilde{F}_{jl}(z,r) \end{pmatrix} + \vartheta_{jl}(z,A_{jl},B_{jl}) \Bigg\{ G^{(jl)}(z,r,R) \Bigg[A_{jl} \begin{pmatrix} F_{jl}(z,R) \\ 0 \end{pmatrix} + B_{jl} \begin{pmatrix} 0 \\ \tilde{F}_{jl}(z,R) \end{pmatrix} \Bigg] + \frac{A_{jl}B_{jl}}{2c} \hat{G}^{(jl)}(z,r,R) \Bigg[\begin{pmatrix} 0 \\ F_{jl}(z,R) \end{pmatrix} - \begin{pmatrix} \tilde{F}_{jl}(z,R) \\ 0 \end{pmatrix} \Bigg] \Bigg\}, \tag{62}$$

where

$$\hat{G}^{(jl)}(z,r,R) = \begin{cases} G^{(jl)}(z,r,R) & r<R, \\ -G^{(jl)}(z,r,R), & r>R, \end{cases} \tag{63}$$

$G^{(jl)}(z,r,R)$ is the Green matrix of the radial Dirac Hamiltonian defined by the Eq. (47) and the functions $F_{jl}(z,r)$, $\tilde{F}_{jl}(z,r)$, and $\vartheta_{jl}(z,A_{jl},B_{jl})$ are defined by (25), (26), and (52), respectively. A straightforward calculation shows that $\binom{F_{G_{jl},1}(z,r)}{F_{G_{jl},2}(z,r)}$ are the scattering wave functions of $h_{jl,G_{jl}}$. In the particular cases $A_{jl}\neq 0$ and $B_{jl}=0$ and $A_{jl}=0$, $B_{jl}\neq 0$ Eq. (62) simplies, respectively, to

$$\begin{pmatrix} F_{A_{jl},1}(z,r) \\ F_{A_{jl},2}(z,r) \end{pmatrix} = \begin{pmatrix} F_{jl}(z,r) \\ \tilde{F}_{jl}(z,r) \end{pmatrix} + A_{jl}\vartheta_{jl}(z,A_{jl},0) G^{(jl)}(z,r,R) \begin{pmatrix} F_{jl}(z,R) \\ 0 \end{pmatrix} \tag{64}$$

and

$$\begin{pmatrix} F_{B_{jl},1}(z,r) \\ F_{B_{jl},2}(z,r) \end{pmatrix} = \begin{pmatrix} F_{jl}(z,r) \\ \tilde{F}_{jl}(z,r) \end{pmatrix} + B_{jl}\vartheta_{jl}(z,0,B_{jl}) G^{(jl)}(z,r,R) \begin{pmatrix} 0 \\ \tilde{F}_{jl}(z,R) \end{pmatrix}. \tag{65}$$

Equations (64) and (65) define the scattering wave functions corresponding to the Hamiltonians $h_{jl,A_{jl}}$ and $h_{jl,B_{jl}}$ describing relativistic δ-sphere interactions of the first and second type, respectively.

The asymptotic behavior of $\binom{F_{G_{jl},1}(z,r)}{F_{G_{jl},2}(z,r)}$ as $r\to\infty$ yields[25,26]

$$\begin{aligned} \begin{pmatrix} F_{G_{jl},1}(z,r) \\ F_{G_{jl},2}(z,r) \end{pmatrix} &\xrightarrow[r\to\infty]{k(z)>0} \begin{pmatrix} \hat{A}_{jl}(z)\sin\left[kr-\kappa_{jl}\frac{\pi}{2}\right] \\ \hat{B}_{jl}(z)\sin\left[kr-(\kappa_{jl}-1)\frac{\pi}{2}\right] \end{pmatrix} + \vartheta_{jl}(z,A_{jl},B_{jl})\{A_{jl}F_{jl}^2(z,R) \\ &\quad + B_{jl}\tilde{F}_{jl}^2(z,R)\} \begin{pmatrix} \hat{C}_{jl}(z)\exp -i\left[kr-\kappa_{jl}\frac{\pi}{2}\right] \\ \hat{O}_{jl}(z)\exp -i\left[kr-(\kappa_{jl}-1)\frac{\pi}{2}\right] \end{pmatrix} \\ &= \begin{pmatrix} [A_1^2(z)+A_2^2(z)]^{1/2}\sin\left[kr-\kappa_{jl}\frac{\pi}{2}+\delta_{G_{jl}}(z)\right]+0(1) \\ [A_3^2(z)+A_4^2(z)]^{1/2}\sin\left[kr-(\kappa_{jl}-1)\frac{\pi}{2}+\delta_{G_{jl}}(z)\right]+0(1) \end{pmatrix}, \end{aligned} \tag{66}$$

where $\hat{A}_{jl}(z)$, $\hat{C}_{jl}(z)$, $\hat{B}_{jl}(z)$, $\hat{O}_{jl}(z)$ are given by

$$\hat{A}_{jl}(z) = 2^{-\kappa_{jl}}k(z)^{-\kappa_{jl}-1}\Gamma(2\kappa_{jl}+2)\Gamma(\kappa_{jl}+1)^{-1}, \tag{67}$$

$$\hat{C}_{jl}(z) = 2^{\kappa_{jl}}k(z)^{\kappa_{jl}}\Gamma(2\kappa_{jl}+2)^{-1}\Gamma(\kappa_{jl}+1), \tag{68}$$

$$\hat{B}_{jl}(z)=\frac{1}{c}2^{-\kappa_{jl}}k(z)^{-\kappa_{jl}}\Gamma(2\kappa_{jl}+2)\Gamma(\kappa_{jl}+1)^{-1}, \tag{69}$$

$$\hat{O}_{jl}(z)=\frac{1}{c}2^{\kappa_{jl}}k(z)^{\kappa_{jl}+1}\Gamma(2\kappa_{jl}+2)^{-1}\Gamma(\kappa_{jl}+1). \tag{70}$$

The phase shifts corresponding to $h_{jl,G_{jl}}$ are defined as

$$\delta_{G_{jl}}(z)=-\arctan\frac{A_2(z)}{A_1(z)}=-\arctan\frac{A_4(z)}{A_3(z)}=-\arctan\frac{\hat{C}_{jl}(z)\vartheta'_{jl}(z)}{\hat{A}_{jl}(z)-\mathrm{i}\hat{C}_{jl}(z)\vartheta'_{jl}(z,A_{jl},B_{jl})}, \tag{71}$$

where

$$\vartheta'_{jl}(z)=\vartheta_{jl}(z,A_{jl},B_{jl})[A_{jl}F_{jl}(z,R)F_{jl}(z,R)+B_{jl}\tilde{F}_{jl}(z,R)\tilde{F}_{jl}(z,R)]. \tag{72}$$

The elements of the on-shell scattering matrix are given by

$$S_{G_{jl}}(z)=\exp[2\mathrm{i}\delta_{G_{jl}}(z)]. \tag{73}$$

The partial wave scattering amplitude is given by

$$f_{G_{jl}}(z)=\frac{\exp[2\mathrm{i}\delta_{G_{jl}}(z)]-1}{2\mathrm{i}k}. \tag{74}$$

III. THE ASYMMETRIC δ-SPHERE INTERACTION

Consider in dimension $n=3$, the quantum Hamiltonian describing the so-called asymmetric δ-sphere interaction formally given by:[7]

$$H_{\underline{\underline{G}}^{(a)}}=H_D+\underline{\underline{G}}\,\delta_a(|x|-R), \quad a\in\mathbb{C}, \tag{75}$$

where $\underline{\underline{G}}$ is a 4×4 matrix given by $\underline{\underline{G}}=\left(\begin{smallmatrix}A & 0\\ 0 & B\end{smallmatrix}\right)$ and δ_a is defined by

$$\int_{R-\epsilon}^{R+\epsilon}\delta_a(r-R)\psi(r)dr=a\,\psi(R+)+(1-a)\psi(R-). \tag{76}$$

Following the strategy used for the construction of $h_{jl,G_{jl}}$ in Eq. (38), one can show that the self-adjoint extension corresponding to the radial Dirac operator with the potential

$$V_a(r)=G_{jl}\delta_a(r-R);a\in\mathbb{C}, \quad G_{jl}=\begin{pmatrix}A_{jl} & 0\\ 0 & B_{jl}\end{pmatrix}, \quad A_{jl},B_{jl}\in\mathbb{R} \tag{77}$$

is given by

$$h_{jl,G_{jl}^{(a)}}=\begin{pmatrix}\dfrac{c^2}{2} & -c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r}\\ c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} & -\dfrac{c^2}{2}\end{pmatrix}\equiv\tau,$$

$$\mathcal{D}(h_{jl,G_{jl}^{(a)}})=\{g\in\mathcal{D}(h_{jl}^{*})|(1-a\tilde{B})g(R+)-(1+b\tilde{B})g(R-)=0\},$$

$$l\in[j-\tfrac{1}{2},j+\tfrac{1}{2}], \quad j\in[\tfrac{1}{2},\infty), \tag{78}$$

where we have used the following definitions and notations:

$$\tilde{B}=\tau_0 c^{-1}G_{jl}, \quad b=1-a, \quad a\in\mathbb{C} \tag{79}$$

and $G_{jl}-G_{jl}^{+}=(1-2\,\mathrm{Re}\,a)c^{-1}G_{jl}^{+}\tau_0 G_{jl}$.

The case $a=\frac{1}{2}$ gives $h_{jl,G_{jl}}$ defined by Eq. (38). Obviously, all the results obtained in Sec. II may be extended to the case of asymmetric δ-sphere interactions.

IV. THE δ-SPHERE PLUS COULOMB INTERACTION

A. Definition of the Hamiltonian

Now the Hamiltonian of the system is formally given by[12]

$$H_{\gamma,\underline{\underline{G}}}=H_D+\frac{\gamma}{|x|}+\underline{\underline{G}}\,\delta(|x|-R), \quad x\in\mathbb{R}^3, \quad R>0, \tag{80}$$

where $\underline{\underline{G}}$ is a real 4×4 matrix of the form

$$\underline{\underline{G}}=\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}. \tag{81}$$

Consider the decomposition (15) and introduce in $L^2((0,\infty))\otimes\mathbb{C}^2$ the operator

$$\overline{H}_{\gamma,\underline{\underline{G}}}=\bigoplus_{j=1/2}^{\infty}\bigoplus_{l=j-1/2}^{j+1/2}[U_{jl}^{-1}h_{jl,\gamma}U_{jl}]\otimes\mathbb{1}, \tag{82}$$

where $h_{jl,\gamma}$ is given by

$$h_{jl,\gamma}=\begin{pmatrix} \dfrac{c^2}{2}+\dfrac{\gamma}{r} & -c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} \\ c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} & -\dfrac{c^2}{2}+\dfrac{\gamma}{r} \end{pmatrix}\equiv\tau_\gamma, \tag{83}$$

$$D(h_{jl,\gamma})=\{\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\,|\,\psi\in\mathrm{AC}_{loc}((0,\infty)), \quad \psi(R\pm)=0;$$
$$\tau_\gamma\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\}. \tag{84}$$

κ_{jl} is defined by Eq. (17).

The adjoint $\overline{H}^{*}_{\gamma,\underline{\underline{G}}}$ of $\overline{H}_{\gamma,\underline{\underline{G}}}$ is defined by

$$\overline{H}^{*}_{\gamma,\underline{\underline{G}}}=\bigoplus_{j=1/2}^{\infty}\bigoplus_{l=j-1/2}^{j+1/2}[U_{jl}^{-1}h^{*}_{jl,\gamma}U_{jl}]\otimes\mathbb{1}, \tag{85}$$

$$h^{*}_{jl,\gamma}=\begin{pmatrix} \dfrac{c^2}{2}+\dfrac{\gamma}{r} & -c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} \\ c\dfrac{d}{dr}+c\dfrac{\kappa_{jl}}{r} & -\dfrac{c^2}{2}+\dfrac{\gamma}{r} \end{pmatrix}\equiv\tau_\gamma, \tag{86}$$

$$D(h^{*}_{jl,\gamma})=\{\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\,|\,\psi\in\mathrm{AC}_{loc}((0,\infty)\backslash\{R\});$$
$$\tau_\gamma\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\}. \tag{87}$$

The self-adjoint extension of $h_{jl,\gamma}$: Consider the equation

$$(h^*_{jl,\gamma}-z)\psi=0,\psi=\begin{pmatrix} f \\ g \end{pmatrix}\in D(h^*_{jl,\gamma}),z\in\mathbb{C}-\left\{\left(-\infty,-\frac{c^2}{2}\right]\left[\frac{c^2}{2},\infty\right)\right\} \tag{88}$$

and introduce the following notations

$$k(z)=\frac{1}{c}\sqrt{z^2-\frac{c^4}{4}}\equiv k, \tag{89}$$

$$\xi=(\kappa_{jl}^2c^2-\gamma^2)^{1/2}, \tag{90}$$

$$\tilde{\xi}=\frac{1}{c}\xi, \tag{91}$$

$$\tilde{\gamma}=\frac{2z\gamma}{c^2}. \tag{92}$$

A straightforward computation shows that the equation (88) has two linearly independent solutions[25]

$$\psi^{(1)}_{\gamma,z}(r)=\begin{cases} \begin{pmatrix} f_{\gamma,1}(z,r) \\ f_{\gamma,2}(z,r) \end{pmatrix}, & r<R, \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, & r>R, \end{cases} \tag{93}$$

$$\psi^{(2)}_{\gamma,z}(r)=\begin{cases} \begin{pmatrix} 0 \\ 0 \end{pmatrix}, & r<R, \\ \begin{pmatrix} g_{\gamma,1}(z,r) \\ g_{\gamma,2}(z,r) \end{pmatrix}, & r>R, \end{cases} \tag{94}$$

where

$$f_{\gamma,1}(z,r)=\left(1-\frac{\gamma^2}{(\kappa_{jl}c+\xi)^2}\right)^{-1/2}\left[\cos\left(\arctan\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]^{-1/2}\left[F_{jl,\gamma}(z,r)-\frac{\gamma}{\kappa_{jl}c+\xi}\tilde{F}_{jl,\gamma}(z,r)\right], \tag{95}$$

$$f_{\gamma,2}(z,r)=\left(1-\frac{\gamma^2}{(\kappa_{jl}c+\xi)^2}\right)^{-1/2}\left[\cos\left(\arctan\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]^{-1/2}\left[\tilde{F}_{jl,\gamma}(z,r)-\frac{\gamma}{\kappa_{jl}c+\xi}F_{jl,\gamma}(z,r)\right], \tag{96}$$

$$g_{\gamma,1}(z,r)=\left(1-\frac{\gamma^2}{(\kappa_{jl}c+\xi)^2}\right)^{-1/2}\left[\cos\left(\arctan\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]^{-1/2}\left[G_{jl,\gamma}(z,r)-\frac{\gamma}{\kappa_{jl}c+\xi}\tilde{G}_{jl,\gamma}(z,r)\right], \tag{97}$$

$$g_{\gamma,2}(z,r)=\left(1-\frac{\gamma^2}{(\kappa_{jl}c+\xi)^2}\right)^{-1/2}\left[\cos\left(\arctan\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]^{-1/2}\left[\tilde{G}_{jl,\gamma}(z,r)-\frac{\gamma}{\kappa_{jl}c+\xi}G_{jl,\gamma}(z,r)\right], \tag{98}$$

with

$$F_{jl,\gamma}(z,r)=r^{\tilde{\xi}+1}e^{-\mathrm{i}k(z)r}{}_1F_1\left(\tilde{\xi}+1-\mathrm{i}\frac{\tilde{\gamma}}{2k(z)},2\tilde{\xi}+2,2\mathrm{i}k(z)r\right), \tag{99}$$

$$G_{jl,\gamma}(z,r)=\Gamma(2\tilde{\xi}+2)^{-1}\Gamma\left(\tilde{\xi}+1-\frac{\mathrm{i}\tilde{\gamma}}{2k(z)}\right)(2\mathrm{i}k(z))^{2\tilde{\xi}+1}r^{\tilde{\xi}+1}e^{-\mathrm{i}k(z)r}$$
$$\times U\left(\tilde{\xi}+1-\mathrm{i}\frac{\tilde{\gamma}}{2k(z)},2\tilde{\xi}+2,2\mathrm{i}k(z)r\right), \tag{100}$$

$$\tilde{F}_{jl,\gamma}(z,r)=\frac{\tilde{\xi}}{c}(2\tilde{\xi}+1)\left|\Gamma\left(\tilde{\xi}+\frac{\mathrm{i}\tilde{\gamma}}{2k(z)}\right)\right|\left|\Gamma\left(\tilde{\xi}+1+\frac{\mathrm{i}\tilde{\gamma}}{2k(z)}\right)\right|^{-1}r^{\tilde{\xi}}e^{-\mathrm{i}k(z)r}$$
$$\times{}_1F_1\left(\tilde{\xi}-\mathrm{i}\frac{\tilde{\gamma}}{2k(z)},2\tilde{\xi},2\mathrm{i}k(z)r\right), \tag{101}$$

$$\tilde{G}_{jl,\gamma}(z,r)=\frac{\tilde{\xi}^{-1}}{c}(2\tilde{\xi}+1)^{-1}\Gamma(2\tilde{\xi})^{-1}\Gamma\left(\tilde{\xi}+\frac{\mathrm{i}\tilde{\gamma}}{2k(z)}\right)\left|\Gamma\left(\tilde{\xi}+\frac{\mathrm{i}\tilde{\gamma}}{2k(z)}\right)\right|^{-1}$$
$$\times\left|\Gamma\left(\tilde{\xi}+1+\frac{\mathrm{i}\tilde{\gamma}}{2k(z)}\right)\right|k(z)^2(2\mathrm{i}k(z))^{2\tilde{\xi}-1}r^{\tilde{\xi}}e^{-\mathrm{i}k(z)r}U\left(\tilde{\xi}-\mathrm{i}\frac{\tilde{\gamma}}{2k(z)},2\tilde{\xi},2\mathrm{i}k(z)r\right), \tag{102}$$

${}_1F_1(a,b,r)$ ($U(a,b,r)$) denotes the regular (respectively, irregular) confluent hypergeometric functions.[27] The functions $f_{\gamma,n}(z,r),g_{\gamma,n}(z,r),n=1,2$ are normalized in such a way that

$$\det\begin{bmatrix} g_{\gamma,1}(z,r) & f_{\gamma,1}(z,r) \\ g_{\gamma,2}(z,r) & f_{\gamma,2}(z,r)\end{bmatrix}=\frac{1}{c}. \tag{103}$$

We note that the limit $\gamma\to 0+$, yields[26]

$$\begin{pmatrix} f_{\gamma,1}(z,r) \\ f_{\gamma,2}(z,r)\end{pmatrix}\xrightarrow[\gamma\to 0+]{}\begin{pmatrix} F_{jl}(z,r) \\ \tilde{F}_{jl}(z,r)\end{pmatrix}, \tag{104}$$

$$\begin{pmatrix} g_{\gamma,1}(z,r) \\ g_{\gamma,2}(z,r)\end{pmatrix}\xrightarrow[\gamma\to 0+]{}\begin{pmatrix} G_{jl}(z,r) \\ \tilde{G}_{jl}(z,r)\end{pmatrix}, \tag{105}$$

where $F_{jl}(z,r)$, $\tilde{F}_{jl}(z,r)$, $G_{jl}(z,r)$, and $\tilde{G}_{jl}(z,r)$ are defined by (25)–(27) and (28).

The operator $h_{jl,\gamma}$ has deficiency indices (2,2) and consequently all its self-adjoint extensions may be parametrised by a four-parameter family of self-adjoint operators. As in Sec. II A, we consider the following two-parameters family of self-adjoint extensions of $h_{jl,\gamma}$

$$h_{jl,\gamma,G_{jl}}=\begin{pmatrix} \frac{c^2}{2}+\frac{\gamma}{r} & -c\frac{d}{dr}+c\frac{\kappa_{jl}}{r} \\ c\frac{d}{dr}+c\frac{\kappa_{jl}}{r} & -\frac{c^2}{2}+\frac{\gamma}{r}\end{pmatrix}\equiv\tau_\gamma,$$

$$D(h_{jl,\gamma,G_{jl}})=\left\{\psi=\begin{pmatrix} f \\ g\end{pmatrix}\in\mathcal{D}(h^*_{jl,\gamma})\middle|\left(1-\tau_0\frac{G_{jl}}{2c}\right)\psi(R+)-\left(1+\tau_0\frac{G_{jl}}{2c}\right)\psi(R-)=0\right\},$$
$$A_{jl},B_{jl}\in\mathbb{R};\quad l\in[j-\tfrac{1}{2},j+\tfrac{1}{2}];\quad j\in[\tfrac{1}{2},\infty). \tag{106}$$

Following Sec. II A, one can show that the operator $h_{jl,\gamma,G_{jl}}$ gives the mathematical definition of the formal expression

$$h_{\gamma,G_{jl}}=h_D+\frac{\gamma}{r}+G_{jl}\delta(r-R). \tag{107}$$

The case $G_{jl}=0$ in Eq. (106) gives the radial Dirac–Coulomb Hamiltonian $h_{jl,\gamma,0}\equiv h_{\gamma,D}$,

$$h_{\gamma,D}=h_D+\frac{\gamma}{r}\equiv\tau_\gamma,$$

$$\mathcal{D}(h_{\gamma,D})=\{\psi\in\mathcal{D}(h^*_{jl,\gamma})\,|\,\psi(R+)=\psi(R-)\};\quad l\in[j-\tfrac{1}{2},j+\tfrac{1}{2}],\quad j\in[\tfrac{1}{2},\infty). \tag{108}$$

The cases $A_{jl}\neq 0$, $B_{jl}=0$ and $A_{jl}=0$, $B_{jl}\neq 0$ in Eq. (106) yields the δ-sphere plus Coulomb interaction of the first and second types, respectively.

The model (80) is defined in $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ by

$$H_{\gamma,\underline{\underline{G}}}=\bigoplus_{j=1/2}^{\infty}\bigoplus_{l=j-1/2}^{j+1/2}U_{jl}^{-1}h_{jl,\gamma,G_{jl}}U_{jl}\otimes\mathbb{1}. \tag{109}$$

The case $\underline{\underline{G}}=0$ for all j and l leads to the Dirac–Coulomb Hamiltonian $H_{\gamma,D}$,

$$H_{\gamma,D}=H_D+\frac{\gamma}{|x|},\quad \mathcal{D}(H_{\gamma,D})=H^{1,2}(\mathbb{R}^3)\otimes\mathbb{C}^4. \tag{110}$$

B. The resolvent equation

Theorem 4.1: The resolvent of $h_{jl,\gamma,G_{jl}}$ is given by

$$\begin{aligned}(h_{jl,\gamma,G_{jl}}-z)^{-1}=(h_{\gamma,D}-z)^{-1}+\vartheta_{jl,\gamma}(z,A_{jl},B_{jl})\Bigg\{&(\overline{\hat{M}^{(2)}_{jl,z,\gamma}(.)},.)\left[A_{jl}\hat{M}^{(2)}_{jl,z,\gamma}(.)+\frac{A_{jl}B_{jl}}{2c}\tilde{M}^{(1)}_{jl,z,\gamma}(.)\right]\\&+(\overline{\tilde{M}^{(2)}_{jl,z,\gamma}(.)},.)\left[B_{jl}\tilde{M}^{(2)}_{jl,z,\gamma}(.)-\frac{A_{jl}B_{jl}}{2c}\hat{M}^{(1)}_{jl,z,\gamma}(.)\right]\Bigg\},\\ z\in\rho(h_{jl,\gamma,G_{jl}}),\ \ \mathrm{Im}\,k(z)>0,\ \ l\in[j-\tfrac{1}{2},j+\tfrac{1}{2}],\ \ j\in[\tfrac{1}{2},\infty)\end{aligned} \tag{111}$$

[$\rho(.)$ is the resolvent set] where $(h_{\gamma,D}-z)^{-1}$, $\mathrm{Im}\,k(z)>0$ is the radial Dirac–Coulomb resolvent with kernel

$$G^{(jl,\gamma)}(z,r,r')=\begin{pmatrix}G^{(jl,\gamma)}_{11}(z,r,r') & G^{(jl,\gamma)}_{12}(z,r,r')\\ G^{(jl,\gamma)}_{21}(z,r,r') & G^{(jl,\gamma)}_{22}(z,r,r')\end{pmatrix}, \tag{112}$$

where

$$G^{(jl,\gamma)}_{11}(z,r,r')=\begin{cases}g_{\gamma,1}(z,r')f_{\gamma,1}(z,r), & r<r',\\ f_{\gamma,1}(z,r')g_{\gamma,1}(z,r), & r>r',\end{cases} \tag{113}$$

$$G^{(jl,\gamma)}_{12}(z,r,r')=\begin{cases}g_{\gamma,2}(z,r')f_{\gamma,1}(z,r), & r<r',\\ f_{\gamma,2}(z,r')g_{\gamma,1}(z,r), & r>r',\end{cases} \tag{114}$$

$$G^{(jl,\gamma)}_{21}(z,r,r')=\begin{cases}g_{\gamma,1}(z,r')f_{\gamma,2}(z,r), & r<r',\\ f_{\gamma,1}(z,r')g_{\gamma,2}(z,r), & r>r',\end{cases} \tag{115}$$

$$G_{22}^{(jl,\gamma)}(z,r,r')=\begin{cases} g_{\gamma,2}(z,r')f_{\gamma,2}(z,r), & r<r', \\ f_{\gamma,2}(z,r')g_{\gamma,2}(z,r), & r>r', \end{cases} \tag{116}$$

and

$$\vartheta_{jl,\gamma}(z,A_{jl},B_{jl})=-\left[1-\frac{B_{jl}A_{jl}}{4c^2}+A_{jl}f_{\gamma,1}(z,R)g_{\gamma,1}(z,R)+B_{jl}f_{\gamma,2}(z,R)g_{\gamma,2}(z,R)\right]^{-1}, \tag{117}$$

$$\hat{M}_{jl,z,\gamma}^{(m)}(r)=\begin{cases} G^{(jl,\gamma)}(z,r,R)\begin{pmatrix}1\\0\end{pmatrix}, & r<R, \\ (-1)^m G^{(jl,\gamma)}(z,r,R)\begin{pmatrix}1\\0\end{pmatrix}, & r>R, m=1,2, \end{cases} \tag{118}$$

$$\tilde{M}_{jl,z,\gamma}^{(m)}(r)=\begin{cases} G^{(jl,\gamma)}(z,r,R)\begin{pmatrix}0\\1\end{pmatrix}, & r<R, \\ (-1)^m G^{(jl,\gamma)}(z,r,R)\begin{pmatrix}0\\1\end{pmatrix}, & r>R, m=1,2, \end{cases} \tag{119}$$

where Green matrix for the radial Dirac-Coulomb operator defined by the equation (111).

Proof:

One may follow step by step the proof of theorem 2.3.

Remark 1: As in the case of Sec. II B, the resolvent of $H_{\gamma,\underline{G}}$ may be obtained from Eq. (111) and the decomposition (82).

C. Spectral properties

Theorem 4.2: For $A_{jl},B_{jl}\in(-\infty,\infty)$, $l\in[j-\frac{1}{2},j+\frac{1}{2}]$, $j\in[\frac{1}{2},\infty)$ and $\gamma\in\mathbb{R}$, the essential spectrum of $h_{jl,\gamma,G_{jl}}$ is purely absolutely continuous and coincide with $(\infty,-c^2/2]\cup[c^2/2,\infty)$. Its singular continuous and residual spectra are empty.[12] The bound states of $h_{jl,\gamma,G_{jl}}$ in the gap $(-c^2/2,c^2/2)$ coincide with the poles of the resolvent equation (111) in $\mathrm{Im}\,k>0$.

D. The nonrelativistic limit

Theorem 4.3: For spin-$\frac{1}{2}$ particles, i.e., $l=j+\frac{1}{2}$, one obtain

$$n.\lim_{c\to\infty}\left(h_{jl,\gamma,G_{jl}}-\frac{c^2}{2}-z\right)^{-1}=(h_{l,\gamma,\hat{\beta}_l}-z)^{-1}\otimes\begin{pmatrix}1&0\\0&0\end{pmatrix}, \quad z\in\mathbb{C}\backslash\mathbb{R}, \tag{120}$$

where $h_{l,\gamma,\hat{\beta}_l}$ is defined by

$$h_{l,\gamma,\hat{\beta}_l}=-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+\frac{\gamma}{r},$$

$$\mathcal{D}(h_{l,\gamma,\hat{\beta}_l})=\Bigg\{f\in L^2((0,\infty))\Bigg|\, f,f'\in \mathrm{AC}_{loc}((0,\infty)\backslash\{R\});f(0+)=0 \text{ if } l=0;$$

$$f'(R+)-f'(R-)=\frac{\alpha_l}{2}[f(R+)+f(R-)];$$

$$f(R+)-f(R-)=\frac{\beta_l}{2}[f'(R+)+f'(R-)]-f''+l(l+1)r^{-2}f+\gamma r^{-1}f\in L^2((0,\infty))\Bigg\},$$

$$-\infty<\alpha_l,\beta_l\leqslant\infty;\ \ l\in\mathbb{N}_0,\ \ \gamma\in\mathbb{R}. \tag{121}$$

If $\alpha_l\beta_l-4=0,\alpha_l,\beta_l\in\mathbb{R}$, then one can show that the boundary conditions in (121) define a self-adjoint extension of $\dot{h}_{l,\gamma}$ defined by

$$\dot{h}_{l,\gamma}=-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+\frac{\gamma}{r}$$

$$\mathcal{D}(\dot{h}_{l,\gamma})=\{f\in L^2((0,\infty))|f,f'\in \mathrm{AC}((0,\infty));f(0+)=0 \text{ if } l=0;f(R\pm)=f'(R\pm)=0;$$
$$-f''+l(l+1)r^{-2}f+\gamma r^{-1}f\in L^2((0,\infty))\},\quad \gamma\in\mathbb{R},l=0. \tag{122}$$

The Hamiltonian $h_{l,\gamma,\hat{\beta}_l}$ provides a generalization of the nonrelativistic δ-sphere interaction of the first and second kind plus a Coulomb interaction discussed in Ref. 2.

E. Scattering theory for the pair $(h_{jl,\gamma,G_{jl}};h_{\gamma,D})$

For $k(z)>0$, we define the function

$$\begin{pmatrix}F_{\gamma,G_{jl},1}(z,r)\\F_{\gamma,G_{jl},2}(z,r)\end{pmatrix}=\begin{pmatrix}f_{\gamma,1}(z,r)\\f_{\gamma,2}(z,r)\end{pmatrix}+\vartheta_{jl,\gamma}(z,A_{jl},B_{jl})\Bigg\{G^{(jl,\gamma)}(z,r,R)\Bigg[A_{jl}\begin{pmatrix}f_{\gamma,1}(z,R)\\0\end{pmatrix}$$
$$+B_{jl}\begin{pmatrix}0\\f_{\gamma,2}(z,R)\end{pmatrix}\Bigg]+\frac{A_{jl}B_{jl}}{2c}\hat{G}^{(jl,\gamma)}(z,r,R)\Bigg[\begin{pmatrix}0\\f_{\gamma,1}(z,R)\end{pmatrix}-\begin{pmatrix}f_{\gamma,2}(z,R)\\0\end{pmatrix}\Bigg]\Bigg\}, \tag{123}$$

where

$$\hat{G}^{(jl,\gamma)}(z,r,R)=\begin{cases}G^{(jl,\gamma)}(z,r,R), & r<R,\\ -G^{(jl,\gamma)}(z,r,R), & r>R,\end{cases} \tag{124}$$

$G^{(jl,\gamma)}(z,r,R)$ is the Green matrix of the radial Dirac–Coulomb operator defined by the equation (112) and the functions $f_{\gamma,1}(z,r)$, $f_{\gamma,2}(z,r)$, and $\vartheta_{jl,\gamma}(z,A_{jl},B_{jl})$ are defined by (95), (96), and (117), respectively.

A straightforward computation shows that $\binom{F_{\gamma,G_{jl},1}(z,r)}{F_{\gamma,G_{jl},2}(z,r)}$ is the wave scattering function of $h_{jl,\gamma,G_{jl}}$.

The particular cases $A_{jl}\neq 0,B_{jl}=0$ and $A_{jl}=0;\ B_{jl}\neq 0$ in Eq. (123) yield

$$\begin{pmatrix}F_{\gamma,A_{jl},1}(z,r)\\F_{\gamma,A_{jl},2}(z,r)\end{pmatrix}=\begin{pmatrix}f_{\gamma,1}(z,r)\\f_{\gamma,2}(z,r)\end{pmatrix}+A_{jl}\vartheta_{jl,\gamma}(z,A_{jl},0)G^{(jl,\gamma)}(z,r,R)\begin{pmatrix}f_{\gamma,1}(z,R)\\0\end{pmatrix} \tag{125}$$

and

$$\begin{pmatrix}F_{\gamma,B_{jl},1}(z,r)\\F_{\gamma,B_{jl},2}(z,r)\end{pmatrix}=\begin{pmatrix}f_{\gamma,1}(z,r)\\f_{\gamma,2}(z,r)\end{pmatrix}+B_{jl}\vartheta_{jl,\gamma}(z,0,B_{jl})G^{(jl,\gamma)}(z,r,R)\begin{pmatrix}0\\f_{\gamma,2}(z,R)\end{pmatrix}. \tag{126}$$

Equations (125) and (126) define the wave functions corresponding to the δ-sphere plus Coulomb interactions of the first and second type, respectively.

The asymptotic behavior of $\binom{F_{G_{jl},1}(z,r)}{F_{G_{jl},2}(z,r)}$ as $r\to\infty$ is given by[26]

$$\begin{pmatrix}F_{G_{jl},1}(z,r)\\F_{G_{jl},2}(z,r)\end{pmatrix}\xrightarrow[r\to\infty]{k(z)>0}\begin{pmatrix}V_1(z)\sin[x_1+\delta^0_{\xi}(z)]+V_2(z)\cos[x_1+\delta^0_{\xi}(z)]\\V_3(z)\sin[x_2+\delta^0_{\xi-1}(z)]+V_4(z)\cos[x_2+\delta^0_{\xi-1}(z)]\end{pmatrix}$$

$$= \begin{pmatrix} [V_1^2(z)+V_2^2(z)]^{1/2} \sin[x_1+\delta^0_{\tilde{\xi}}(z)+\delta^C_{\gamma,G_{jl},1}(z)] \\ [V_3^2(z)+V_4^2(z)]^{1/2} \sin[x_2+\delta^0_{\tilde{\xi}-1}(z)+\delta^C_{\gamma,G_{jl},2}(z)] \end{pmatrix}, \tag{127}$$

where

$$x_1 = k - \frac{\tilde{\gamma}}{2k}\ln(2kr) - \tilde{\xi}\frac{\pi}{2}, \tag{128}$$

$$x_2 = k - \frac{\tilde{\gamma}}{2k}\ln(2kr) - (\tilde{\xi}-1)\frac{\pi}{2}, \tag{129}$$

and

$$\delta^0_{\tilde{\xi}}(z) = \delta^0_{\tilde{\xi}-1}(z) + \arctan\left(\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right), \tag{130}$$

$$\delta^0_{\tilde{\xi}}(z) = \arg\Gamma\left(\tilde{\xi}+1+\mathrm{i}\frac{\tilde{\gamma}}{2k}\right). \tag{131}$$

The Coulomb modified phase shift $\delta^C_{\gamma,G_{jl}}(z)$ corresponding to $h_{jl,\gamma,G_{jl}}$ is given by

$$\delta^C_{\gamma,G_{jl}}(z) = \begin{pmatrix} \delta^C_{\gamma,G_{jl},1}(z) \\ \delta^C_{\gamma,G_{jl},2}(z) \end{pmatrix}, \tag{132}$$

where

$$\delta^C_{\gamma,G_{jl},1}(z) = -\arctan\frac{V_2(z)}{V_1(z)}, \tag{133}$$

$$\delta^C_{\gamma,G_{jl},2}(z) = -\arctan\frac{V_4(z)}{V_3(z)}. \tag{134}$$

The constants $V_i (i=1,\ldots,4)$ are defined by

$$V_1(z) = d_1(z) + [d_2(z) - \mathrm{i}\vartheta'_{jl,\gamma}(z)d_4(z)]\sin\left[\arctan\left(\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right] - \mathrm{i}\vartheta'_{jl,\gamma}(z)d_3(z)$$
$$- \vartheta'_{jl,\gamma}(z)d_4(z)\cos\left[\arctan\left(\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right], \tag{135}$$

$$V_2(z) = [d_2(z) - \mathrm{i}\vartheta'_{jl,\gamma}(z)d_4(z)]\cos\left[\arctan\left(\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right] + \vartheta'_{jl,\gamma}(z)d_3(z)$$
$$+ \vartheta'_{jl,\gamma}(z)d_4(z)\sin\left[\arctan\left(\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right], \tag{136}$$

$$V_3(z)=\left[-\frac{\gamma}{\kappa_{jl}c+\xi}d_1(z)+\mathrm{i}\vartheta'_{jl,\gamma}(z)\frac{\gamma}{\kappa_{jl}c+\xi}d_3(z)\right]\sin\left[\arctan\left(\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]-\left(\frac{\gamma}{\kappa_{jl}c+\xi}\right)^{-1}d_2(z)$$
$$-\vartheta'_{jl,\gamma}(z)\frac{\gamma}{\kappa_{jl}c+\xi}d_3(z)\cos\left[\arctan\left(\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]+\mathrm{i}\vartheta'_{jl,\gamma}(z)\left(\frac{\gamma}{\kappa_{jl}c+\xi}\right)^{-1}d_4(z), \tag{137}$$

$$V_4(z)=\left[-\frac{\gamma}{\kappa_{jl}c+\xi}d_1(z)+\mathrm{i}\vartheta'_{jl,\gamma}(z)\frac{\gamma}{\kappa_{jl}c+\xi}d_3(z)\right]\cos\left[\arctan\left(\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]$$
$$-\vartheta'_{jl,\gamma}(z)\frac{\gamma}{\kappa_{jl}c+\xi}d_3(z)\sin\left[\arctan\left(\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]-\vartheta'_{jl,\gamma}(z)\left(\frac{\gamma}{\kappa_{jl}c+\xi}\right)^{-1}d_4(z) \tag{138}$$

with $\vartheta'_{jl}(z,A_{jl},B_{jl})$ defined by

$$\vartheta'_{jl}(z)=\vartheta_{jl}(z,A_{jl},B_{jl})[A_{jl}f_{\gamma,1}(z,R)f_{\gamma,1}(z,R)+B_{jl}f_{\gamma,2}(z,R)f_{\gamma,2}(z,R)]. \tag{139}$$

The constants $d_i(z)(i=1,\ldots,4)$ are given by

$$d_1(z)=\left(1-\frac{\gamma^2}{(\kappa_{jl}c+\xi)^2}\right)^{-1/2}\left[\cos\left(\arctan\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]^{-1/2}2^{-\tilde{\xi}}(k)^{-\tilde{\xi}-1}\Gamma(2\tilde{\xi}+2)$$
$$\times\left|\Gamma\left(\tilde{\xi}+1+\mathrm{i}\frac{\tilde{\gamma}}{2k}\right)\right|^{-1}e^{\pi(\tilde{\gamma}/4k)}, \tag{140}$$

$$d_2(z)=-\frac{\gamma}{c(\kappa_{jl}c+\xi)}\left(1-\frac{\gamma^2}{(\kappa_{jl}c+\xi)^2}\right)^{-1/2}\left[\cos\left(\arctan\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]^{-1/2}2^{-\tilde{\xi}}(k)^{-\tilde{\xi}}$$
$$\times\Gamma(2\tilde{\xi}+2)\left|\Gamma\left(\tilde{\xi}+1+\mathrm{i}\frac{\tilde{\gamma}}{2k}\right)\right|^{-1}e^{\pi(\tilde{\gamma}/4k)}, \tag{141}$$

$$d_3(z)=\left(1-\frac{\gamma^2}{(\kappa_{jl}c+\xi)^2}\right)^{-1/2}\left[\cos\left(\arctan\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]^{-1/2}2^{\tilde{\xi}}(k)^{\tilde{\xi}}$$
$$\times\Gamma(2\tilde{\xi}+2)^{-1}\left|\Gamma\left(\tilde{\xi}+1+\mathrm{i}\frac{\tilde{\gamma}}{2k}\right)\right|e^{-\pi(\tilde{\gamma}/4k)}, \tag{142}$$

$$d_4(z)=-\frac{\gamma}{c(\kappa_{jl}c+\xi)}\left(1-\frac{\gamma^2}{(\kappa_{jl}c+\xi)^2}\right)^{-1/2}\left[\cos\left(\arctan\frac{\tilde{\gamma}}{2k\tilde{\xi}}\right)\right]^{-1/2}2^{\tilde{\xi}}(k)^{\tilde{\xi}+1}$$
$$\times\Gamma(2\tilde{\xi}+2)^{-1}\left|\Gamma\left(\tilde{\xi}+1+\mathrm{i}\frac{\tilde{\gamma}}{2k}\right)\right|e^{-\pi(\tilde{\gamma}/4k)}. \tag{143}$$

The limit $\gamma\to 0+$, in (133) and (134) yields

$$\lim_{\gamma\to 0+}\delta^C_{\gamma,G_{jl},1}(z)=\lim_{\gamma\to 0+}\delta^C_{\gamma,G_{jl},2}(z)=\delta_{G_{jl}}(z), \tag{144}$$

where $\delta_{G_{jl}}(z)$ is defined by (71).

The Coulomb modified on-shell scattering matrix is given by

$$S^{C}_{\gamma,G_{jl},n}(z)=e^{2i\delta^{C}_{\gamma,G_{jl},n}(z)},\quad n=1,2. \tag{145}$$

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Boundary states, extended symmetry algebra, and module structure for certain rational torus models

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The massless bosonic field compactified on the circle of rational R^2 is reexamined in the presense of boundaries. A particular class of models corresponding to $R^2 = 1/2k$ is distinguished by demanding the existence of a consistent set of Neumann boundary states. The boundary states are constructed explicitly for these models and the fusion rules are derived from them. These are the ones prescribed by the Verlinde formula from the S-matrix of the theory. In addition, the extended symmetry algebra of these theories is constructed, which is responsible for the rationality of these theories. Finally, the chiral space of these models is shown to split into a direct sum of irreducible modules of the extended symmetry algebra. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1517168]

I. INTRODUCTION

The massless bosonic field compactified on the circle has been particularly useful for studying the moduli space of $c=1$ theories.[1,2] In this case, there are two continuous families of theories corresponding to the torus and the Z_2 orbifold models. Theories in each family are connected by marginal operator deformations. In both cases there is a duality that identifies the model with radius R with the model with radius $1/2R$. Also the theory corresponding to $R=\sqrt{2}$ for the torus models is identified with the $R=1/\sqrt{2}$ theory for the orbifold models. For the self-dual radius $R=1/\sqrt{2}$ the theory possesses an extended $SU(2)\times SU(2)$ symmetry. By dividing this symmetry by the three special discrete subgroups of $SU(2)$, the tetrahedral, octahedral, and icosahedral,[1] we constructed three more theories that are not connected to the others by marginal operator deformations. This list of $c=1$ theories has been shown to be complete in the case where the partition function is a linear combination of toroidal partition functions by Ref. 2. However the partition functions of these theories contain an infinite sum of products of holomorphic times antiholomorphic Virasoro characters, as predicted by a theorem of Ref. 3. In the particular case where R^2 is rational, these products group into a finite sum of holomorphic times antiholomorphic blocks. Furthermore this is the complete list of $c=1$ theories possessing this property as proven in Ref. 4.

Next we consider conformal field theory on surfaces with boundaries.[5] On the finite cylinder it is possible to construct a partition function in two ways: either through a closed string propagating between two boundary states or through an open string satisfying corresponding boundary conditions propagating around a loop. Compatibility between these two points of view gives two conditions on the boundary states. One is the Ishibashi condition[6] arising from the restriction of the conformal field theory to the upper half plane (necessary in the open string picture) and the other is the Cardy condition,[7,8] which arises from the representational compatibility of the two constructions. Cardy, in particular, showed that given the Verlinde formula and a complete set of Ishibashi states it is possible to construct a consistent set of boundary states for diagonal theories. In the particular case where the representation space of the theory splits into a direct sum of irreducible representations of an extended $\widehat{su}(2)$ chiral algebra, the Ishibashi states have been constructed in Ref. 6. The case of the Z_2 orbifold model at radius 1 has been considered in Ref. 9.

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In this case boundary states have been derived that do not correspond to bulk operators.

In this work we study the rational torus models from the boundary CFT point of view. We distinguish a particular class of models ($R=1/\sqrt{2k}$) which posesses a consistent set of Neumann boundary states (or dually Dirichlet boundary states) in the sense of Ref. 7. These boundary states have been constructed explicitly. Next the extended symmetry algebra of these theories has been written down. Finally the infinite direct sum of Fock modules, which constitutes the chiral representation space of this particular set of torus models, is shown to decompose into a finite sum of irreducible extended algebra modules.

II. TORUS MODELS REVISITED

These models correspond to a free massless real bosonic field compactified on a circle of radius R. The action in this case is

$$S=\frac{1}{2\pi}\int \partial X\bar{\partial}X. \tag{1}$$

The partition function for these models turns out to be

$$Z(\beta)=\sum_{m,n}\frac{q^{(1/2)(m/2R+nR)^2}}{\eta(q)}\frac{\bar{q}^{(1/2)(m/2R-nR)^2}}{\eta(\bar{q})}. \tag{2}$$

Here $q=e^{2\pi i\tau}=e^{-2\pi\beta}$, $\beta=-i\tau$, and $\eta(q)$ is the Jacobi eta function. The representation space for these models can be read of from the partition function to be

$$H=\bigoplus_{n,m\epsilon Z} F_{\alpha_{m,n}}\otimes F_{\bar{\alpha}_{m,n}}, \tag{3}$$

where the possible charges are $\alpha_{m,n}=m/2R-nR$ and $\bar{\alpha}_{m,n}=m/2R-nR$.

In the particular case $R^2=p/p'$ the partition function becomes a finite sum of holomorphic times antiholomorphic parts:

$$Z(q)=\sum_{r=0}^{2p-1}\sum_{s=0}^{2p'-1} f_{r,s}(q)f_{r,-s}(\bar{q}), \tag{4}$$

where

$$f_{r,s}(q)=\sum_{n\epsilon Z}\frac{q^{2pp'(n+(r/4p)+(s/2p'))^2}}{\eta(q)}. \tag{5}$$

Now consider the free field more closely. We can view our field as describing an open string propagating along a strip periodic in the horizontal direction but with boundary conditions along the end point lines of the string. What we really have in this way is an open string propagating along the sides of a cylinder, while it obeys boundary conditions on the end point circles. The length of the circumference will be taken to be β, while the height of the cylinder will be 1/2. This one loop open string diagram is equivalent to a closed string propagating along the cylinder from one boundary to the other. The boundaries of the closed string are to be interpreted as states. Following the closed string picture we will take time to be the vertical direction. The free field admits now the following expansion into oscillator modes:

$$\phi(\sigma,t)=\hat{x}+\frac{2\pi}{\beta}R\hat{w}\sigma+\frac{\pi}{\beta}\hat{p}t+\frac{1}{2}i\sum_{n\neq 0}\left(\frac{a_n}{n}\exp\left(-\frac{2\pi i}{\beta}n(t+\sigma)\right)+\frac{\tilde{a}_n}{n}\exp\left(-\frac{2\pi i}{\beta}n(t-\sigma)\right)\right). \tag{6}$$

This splits into left and right modes according to

$$\phi(\sigma,t)=\phi_L(x^+)+\phi_R(x^-), \tag{7}$$

where $x^+=t+\sigma$ and $x^-=t-\sigma$. Here

$$\begin{aligned}\phi_L(x^+)&=\frac{\hat{x}}{2}+\frac{\pi}{\beta}a_0x^+ +\frac{1}{2}i\sum_{n\neq 0}\frac{a_n}{n}\exp\left(-\frac{2\pi i}{\beta}nx^+\right),\\ \phi_R(x^-)&=\frac{\hat{x}}{2}+\frac{\pi}{\beta}\tilde{a}_0x^- +\frac{1}{2}i\sum_{n\neq 0}\frac{\tilde{a}_n}{n}\exp\left(-\frac{2\pi i}{\beta}nx^-\right),\end{aligned} \tag{8}$$

where $a_0=\hat{p}/2+R\hat{w}$ and $\tilde{a}_0=\hat{p}/2-R\hat{w}$. The Hamiltonian in the closed string picture turns out to be

$$H_\beta=\frac{2\pi}{\beta}\left[(R\hat{w})^2+(\hat{p}/2)^2+\sum_{n=1}^{\infty}a_{-n}a_n+\sum_{n=1}^{\infty}\tilde{a}_{-n}\tilde{a}_n-1/12\right]. \tag{9}$$

Using the oscillator mode representation of the Virasoro generators

$$\begin{aligned}L_m&=\frac{1}{2}\sum_{-\infty}^{\infty}:a_{m-n}a_n:,\\ \overline{L}_m&=\frac{1}{2}\sum_{-\infty}^{\infty}:\tilde{a}_{m-n}\tilde{a}_n:,\end{aligned} \tag{10}$$

we have that

$$H_\beta=\frac{2\pi}{\beta}(L_0+\overline{L}_0-1/12). \tag{11}$$

The boundary states of the closed string have to satisfy the Ishibashi condition[6]:

$$(L_n-\overline{L}_{-n})|B\rangle=0. \tag{12}$$

This is certainly satisfied if

$$(a_m\pm\tilde{a}_{-m})|B\rangle=0. \tag{13}$$

The plus sign corresponds to Neumann boundary conditions in the open string picture while the minus sign corresponds to Dirichlet boundary conditions.[9] Solving the conditions (13) we get the following Ishibashi states:

$$\begin{aligned}|\iota^N_{nR}\rangle&=\exp\left(-\sum_{n=1}^{\infty}\frac{a_{-n}\tilde{a}_{-n}}{n}\right)|p=0,\quad w=nR\rangle,\\ |\iota^D_{m/2R}\rangle&=\exp\left(\sum_{n=1}^{\infty}\frac{a_{-n}\tilde{a}_{-n}}{n}\right)\left|\frac{p}{2}=\frac{m}{2R},\quad w=0\right\rangle.\end{aligned} \tag{14}$$

Note that in the Neumann case the zero mode condition demands that there is no momentum while in the Dirichlet case it demands that there is no winding. Now we have the following lemma:

Lemma 1: The Ishibashi states (14) give rise to the following inner products:

$$\langle \iota^N_{nR}|e^{-H_{\beta/2}}|\iota^N_{mR}\rangle = \frac{\tilde{q}^{R^2n^2/2}}{\eta(\tilde{q})}\delta_{n,m},$$

$$\langle \iota^D_{n/2R}|e^{-H_{\beta/2}}|\iota^D_{m/2R}\rangle = \frac{\tilde{q}^{n^2/8R^2}}{\eta(\tilde{q})}\delta_{n,m}, \tag{15}$$

$$\langle \iota^N_{nR}|e^{-H_{\beta/2}}|\iota^D_{m/2R}\rangle = \tilde{q}^{-1/24}\prod_{n=1}^{\infty}\frac{1}{1+\tilde{q}^n}\delta_{n,0}\delta_{m,0} = \frac{\Sigma_{n\epsilon Z}(-1)^n\tilde{q}^{n^2}}{\eta(\tilde{q})}\delta_{n,0}\delta_{m,0},$$

where $\tilde{q}=e^{-2\pi/\beta}$.

The proof of this lemma is a simple free field calculation. Note that it is possible to interchange the Neumann and Dirichlet Ishibashi states by interchanging the directions of t and σ.

There is however another condition that must be satisfied by the boundary states.[7] This states that if $|X_A\rangle$ are the boundary states, then

$$Z_{AB}(\beta)=\langle X_A|e^{-H_{\beta/2}}|X_B\rangle=\sum_i n^i_{AB}\chi_i(q) \tag{16}$$

for some integers n^i_{AB} where $q=e^{-2\pi i\beta}$. In particular there is a special vacuus state $|X_0\rangle$ for which $n^i_{0j}=\delta_{i,j}$. This condition arises from the possibility to see $Z_{AB}(\beta)$ as an one loop amplitude of an open string satisfying the boundary conditions A,B on the boundary circles.

Now let us restrict ourselves to the Neumann sector. Consider the case R^2 is rational, and let us demand that there is a Neumann vacuum boundary state

$$|X^N_0\rangle=\sum_{n\epsilon Z} C_n|\iota^N_{nR}\rangle. \tag{17}$$

Of course demanding a Dirichlet vacuum boundary state is completely equivalent because of the t, σ interchange duality. Consider the partition function on the cylinder with two vacuum boundary states at the boundary circles:

$$Z_{00}(\beta)=\langle X^N_0|e^{-H_{\beta/2}}|X^N_0\rangle=\sum_{n\epsilon Z}|C_n|^2\frac{\tilde{q}^{R^2n^2/2}}{\eta(\tilde{q})}. \tag{18}$$

According to the Cardy condition,[7] $Z_{00}(\beta)$ must be equal to the vacuum character. To change the variable from $\tilde{q}$ to q, we need to use the Poisson resummation formula, which in this case takes the form:

$$\sum_{n\epsilon Z}\frac{\tilde{q}^{A(n+b)^2}}{\eta(\tilde{q})}=\frac{1}{\sqrt{2A}}\sum_{n\epsilon Z}\frac{q^{(n^2/4A)}e^{2\pi inb}}{\eta(q)}. \tag{19}$$

In the case of the rational theories and in order to be able to get the identity character after use of formula (19) there must exist a minimum integer m such that the constants C_n in the classes $n=r \bmod m$ are equal. This gives rise to the following partition function:

$$Z_{00}(\beta)=\sum_{r=0}^{m-1}|C_r|^2\sum_{n\epsilon Z}\frac{\tilde{q}^{(m^2R^2/2)(n+(r/m))^2}}{\eta(\tilde{q})}=\sum_{r=0}^{m-1}\frac{|C_r|^2}{mR}\sum_{n\epsilon Z}\frac{q^{(n^2/2m^2R^2)\rangle}e^{2\pi in(r/m)}}{\eta(q)}. \tag{20}$$

Now letting $n=mn'+s$ we get

$$Z_{00}(\beta)=\sum_{r,s=0}^{m-1}\frac{|C_r|^2}{mR}e^{2\pi irs/m}\sum_{n'\epsilon Z}\frac{q^{[(n'+s/m)^2/2R^2]}}{\eta(q)}. \tag{21}$$

Since $s/m<1$, the power $q^{1/2R^2}$ appears only when $s=0$, and taking into account that in the vacuum character only integer powers of q appear and that

$$\sum_{r=0}^{m-1}\frac{|C_r|^2}{mR}\neq 0$$

we have that

$$R^2=\frac{1}{2k}. \tag{22}$$

These are the values of the radius that we are going to analyze further. For these values the closed string partition function regroups to

$$Z(\beta)=\sum_{s=0}^{2k-1}\chi_s(q)\chi_{-s}(\overline{q}), \tag{23}$$

where

$$\chi_s(q)=\sum_{n\epsilon Z}\frac{q^{k(n+s/2k)^2}}{\eta(q)}. \tag{24}$$

The vacuum character must be a partial sum of $\chi_0(q)$. Comparing this with $Z_{00}(\beta)$ we get that $s=0$, which in turn means that $\chi_0(q)$ itself is the vacuum character. Furthermore it is necessary that all $|C_r|$ are equal, so that the value $s=0$ is the only one that survives the sum over r. So, without loss of generality we can assume that $m=1$. In this case we have

$$Z_{00}(\beta)=\frac{|C|^2}{R}\sum_{n\epsilon Z}\frac{q^{kn^2}}{\eta(q)}. \tag{25}$$

Equality with $\chi_0(q)$ demands that $|C|=\sqrt{R}=1/\sqrt[4]{2k}$. So the corresponding vacuum state is

$$|X_0^N\rangle=\frac{1}{\sqrt[4]{2k}}\sum_{n\epsilon Z}|\iota^N_{n/\sqrt{2k}}\rangle=\frac{1}{\sqrt[4]{2k}}\sum_{l=0}^{2k-1}\sum_{n\epsilon Z}|\iota^N_{\sqrt{2k}(n+l/2k)}\rangle. \tag{26}$$

Now it is necessary (because of the Cardy condition) that

$$Z_{0m}(\beta)=\chi_m(q)=\frac{1}{\sqrt{2k}}\sum_{l=0}^{2k-1}\exp\left(\frac{2\pi ilm}{2k}\right)\chi_l(\tilde{q}). \tag{27}$$

This demands that the other boundary states are

$$|X_m^N\rangle=\frac{1}{\sqrt[4]{2k}}\sum_{l=0}^{2k-1}\exp\left(\frac{2\pi ilm}{2k}\right)\sum_{n\epsilon Z}|\iota^N_{\sqrt{2k}(n+l/2k)}\rangle. \tag{28}$$

It is not too difficult to check that

$$Z_{m_1 m_2}=\frac{1}{2k}\sum_{l,m=0}^{2k-1}\exp\left(2\pi i l\frac{(m_2-m_1+m)}{2k}\right)\chi_m(q)=\chi_{m_1-m_2}(q). \tag{29}$$

This is certainly an integer sum of characters so the Cardy condition is satisfied. It is worth mentioning that since the construction of the boundary states is based on the modular properties of the characters the Verlinde formula gives integer fusion rules as was necessary. In particular we can read from (27) that

$$S_l^j=\frac{1}{\sqrt{2k}}\exp\left(\frac{2\pi i j l}{2k}\right)$$

and from the Verlinde formula

$$\sum_{i=0}^{2k-1} S_i^j N_{k'l}^i=S_k'^j S_l^j/S_0^j \tag{30}$$

we can read the fusion rules

$$N_{k'l}^i=\delta_{(i,k'+l)\bmod 2k}. \tag{31}$$

III. EXTENDED SYMMETRY ALGEBRA

We will now try to find which extended symmetry gives rise to the characters $\chi_m(q)$ for each k. Consider first the identity character

$$\chi_0(q)=\frac{\Sigma_{n\epsilon Z}q^{kn^2}}{\eta(q)}=q^{-1/24}\frac{1+2q^k+2q^{4k}+\cdots+2q^{n^2k}+\cdots}{(1-q)(1-q^2)\cdots(1-q^k)(1-q^{k+1})\cdots}. \tag{32}$$

Expanding in q we get

$$\begin{aligned}\chi_0(q)=q^{-1/24}([1+P(1)q+P(2)q^2+\cdots+P(k-1)q^{k-1}]+q^k[[P(k)+2]+[P(k+1)\\ +2P(1)]q+\cdots+[P(4k-1)+2P(3k-1)]q^{3k-1}]+\cdots+q^{n^2k}[[P(n^2k)+\cdots+2]\\ +\cdots+[P((n+1)^2k-1)+\cdots+2P((2n+1)k-1)]q^{(2n+1)r-1}]+\cdots).\end{aligned} \tag{33}$$

Here $P(n)$ is the number of partitions of n. Now the Fock module built on the zero charge vacuum, F_0, has $P(n)$ linearly independent states at level n. From the above-given expansion we see that at level k we have two extra linearly independent states that are orthogonal to F_0, and since they are the first such states they have to be killed by all a_n for n positive. So they can be taken to be the highest weight Fock states of charge $\alpha_{nm}=\pm\sqrt{2k}$ because the L_0 eigenvalue $h_{nm}=k$. They are generated by the spin k currents

$$J^{\pm}(z)=e^{\pm i\sqrt{2k}\phi(z)}. \tag{34}$$

Here we have taken $\phi(z)=2\phi_L(x^+)$ and $z=e^{2\pi i x^+/\beta}$. Clearly, $J^{\pm}$ adds charge $\pm\sqrt{2k}$ on the states it acts on. There is of course another current, of spin 1, the $U(1)$ current, which we take to be

$$J^0(z)=\frac{1}{\sqrt{2k}}i\partial\phi(z). \tag{35}$$

Now we have the following lemma:

Lemma 2: The modes of the above currents generate the space $\oplus_{n\epsilon Z}F_{n\sqrt{2k}}$.

Proof: To prove this consider the mode expansion of the $J^+(z)$ current acting on the zero charge vacuum:

$$\sum_{n\epsilon Z} J_n^+ z^{-n-k}|0\rangle = \exp\left(\sqrt{2k}\sum_{n>0}\frac{a_{-n}}{n}z^n\right)|\sqrt{2k}\rangle, \tag{36}$$

where by $|\sqrt{2k}\rangle$ we denote the vacuum state of charge $\sqrt{2k}$. From this relation we see that

$$J_0^+|0\rangle = 0, \quad J_{-1}^+|0\rangle = 0,\cdots, \quad J_{-k+1}^+|0\rangle = 0, \quad J_{-k}^+|0\rangle = |\sqrt{2k}\rangle. \tag{37}$$

Similarly we get that $J_{-k}^-|0\rangle = |-\sqrt{2k}\rangle$. These are the extra states at level k. Of course since the modes of $J^0(z)$ can act on those states all the Fock descendents of the states $|\pm\sqrt{2k}\rangle$ are generated by the current modes. If we move to level $k+r$ then the number of them is $2P(r)$. Together with the descendents of $|0\rangle$ we have overall $P(k+r)+2P(r)$ states. This takes account of the second bracket in (33). But at level $4k$ there are again two more states. To take account of them consider the product

$$J^+(z)J_{-k}^+|0\rangle = J^+(z)|\sqrt{2k}\rangle = z^{2k}\exp\left(\sqrt{2k}\sum_{n>0}\frac{a_{-n}}{n}z^n\right)|2\sqrt{2k}\rangle. \tag{38}$$

This means that we have

$$J_0^+J_{-k}^+|0\rangle = 0, \quad J_{-1}^+J_{-k}^+|0\rangle = 0,\cdots, \quad J_{-3k+1}^+J_{-k}^+|0\rangle = 0, \quad J_{-3k}^+J_{-k}^+|0\rangle = |2\sqrt{2k}\rangle. \tag{39}$$

Considering also $J_{-3k}^-J_{-k}^-|0\rangle$ we get the extra two states at level $4k$. Again at level $4k+r$ we have all the Fock descendents of $|0\rangle$, $J_{-k}^\pm|0\rangle = |\pm\sqrt{2k}\rangle$, and $J_{-3k}^\pm J_{-k}^\pm|0\rangle = |\pm 2\sqrt{2k}\rangle$. The number of these states is $P(4k+r)+2P(3k+r)+2P(r)$. Continuing in this fashion we get two extra states appearing at every level of the form n^2k, as indicated by (32). They are of the form

$$J_{-(2n-1)k}^\pm\cdots J_{-3k}^\pm J_{-k}^\pm|0\rangle = |\pm n\sqrt{2k}\rangle. \tag{40}$$

Of course all the Fock descendents of these states are created by the J^0 modes so we have that the current modes generate completely the direct sum $\oplus_{n\epsilon Z}F_{n\sqrt{2k}}$. This ends the proof of the lemma.

The next question is what are the OPEs satisfied by these high spin currents. This is not too difficult to obtain. These are the following:

$$\begin{aligned} J^0(z)J^\pm(w) &= \pm\frac{1}{z-w}J^\pm(w)+\text{reg}, \\ J^+(z)J^-(w) &= \frac{1}{(z-w)^{2k}}\exp n_{O(2k-1)}e^{i\sqrt{2k}(\phi(z)-\phi(w))}+\text{reg}. \end{aligned} \tag{41}$$

The second operator product has to be expressed in terms of the currents. This is possible by expanding $\phi(z)$ near w:

$$\begin{aligned} J^+(z)J^-(w) = \frac{1}{(z-w)^{2k}}\exp n_{O(2k-1)}\exp\Bigg(2k\Bigg[&(z-w)J^0(w)+\cdots \\ &+\frac{(z-w)^{2k-1}}{(2k-1)!}\partial^{2k-2}J^0(w)\Bigg]\Bigg)+\text{reg}. \end{aligned} \tag{42}$$

Here by $\exp n_{O(2k-1)}$ we mean expansion up to and including terms of order $(z-w)^{2k-1}$. At this point it is worth mentioning that our product $J^+(z)J^-(w)$ is a bilocal field in the sense of Ref. 10. There it was remarked that for $k=1/2$ (unaccepted value for us) this product is the generating

function for the $W_{1+\infty}$ algebra. Here however we will restrict our attention to integer values of k. Now, the product (42) can be expanded in terms of Schur polynomials. In general the Schur polynomials are defined by

$$\exp\left(\sum_{k=1}^{\infty} t_k z^k\right)=\sum_{N=0}^{\infty} z^N S_N(t_1,t_2,\ldots,t_k,\ldots) \tag{43}$$

and they turn out to be

$$S_N(t_1,t_2,\ldots,t_k,\ldots)=\sum_{n_1,\ldots,n_k,\ldots}^{\Sigma_{k=1}^{\infty} k n_k=N} \frac{t_1^{n_1}\cdots t_k^{n_k}\cdots}{n_1!\cdots n_k!\cdots}. \tag{44}$$

Let us now define, following Ref. 10, the associated polynomials:

$$f^l(\partial^i J^0(z))=(l)!:S_l\left(J^0(z),\frac{\partial J^0(z)}{2!},\cdots,\frac{\partial^{l-1}J^0(z)}{l!}\right):. \tag{45}$$

They satisfy the following recurrence relation:

$$f^{l+1}(\partial^i J^0(z))=(J^0(z)+\partial)f^l(\partial^i J^0(z))=\cdots=(J^0(z)+\partial)^l J^0(z). \tag{46}$$

Now using these new definitions we have

$$\begin{aligned} J^+(z)J^-(w)&=\frac{1}{(z-w)^{2k}}\left(\sum_{N=0}^{2k-1} S_N(2kJ^0(w),\ldots,2k\partial^{2k-2}J^0(w)/(2k-1)!)(z-w)^N\right)+\text{reg}\\ &=\sum_{N=0}^{2k-1}\frac{f^N(2k\partial^i J^0(w))}{N!}(z-w)^{N-2k}+\text{reg}. \end{aligned} \tag{47}$$

The next question is what is the algebra satisfied by the modes of the currents $J^+(z)$, $J^-(z)$. This can be read from the OPEs:

$$[J_n^+,J_m^-]=\oint_0\frac{dw}{2\pi i}\oint_w\frac{dz}{2\pi i}z^{n+k-1}w^{m+k-1}J^+(z)J^-(w), \tag{48}$$

where the left integral is around the origin and the right is around w. Expanding the product of currents as above we get

$$[J_n^+,J_m^-]=\sum_{N=0}^{2k-1}\frac{\Gamma(n+k)}{\Gamma(2k-N)\Gamma(N+n-k+1)}\oint_0\frac{dw}{2\pi i}w^{n+m+N-1}\frac{f^N(2k\partial^i J^0(w))}{N!}. \tag{49}$$

This suggests the following definition:

$$V^k_{m+n,N}=\oint_0\frac{dw}{2\pi i}w^{n+m+N-1}f^N(2k\partial^i J^0(w))=\oint_0\frac{dw}{2\pi i}w^{n+m+N-1}(2kJ^0(w)+\partial)^{N-1}2kJ^0(w), \tag{50}$$

where we have made use of the recurrence relation (46). In this notation (49) becomes

$$[J_n^+,J_m^-]=\sum_{N=0}^{2k-1}\frac{\Gamma(n+k)}{\Gamma(2k-N)\Gamma(N+n-k+1)\Gamma(N+1)}V^k_{n+m,N}. \tag{51}$$

Following the same procedure for the remaining commutators we get

$$[J_n^0, J_m^0] = \frac{n}{2k}\delta_{n+m}, \quad [J_n^0, J_m^\pm] = \pm J_{m+n}^\pm, \tag{52}$$

while the other commutators are 0.

Note that in particular if $k=1$ then $V_{m+n,0}^1 = \delta_{m+n}$ and $V_{m+n,1}^1 = 2J_{m+n}^0$, so in this case the commutator (51) becomes

$$[J_n^+, J_m^-] = n\delta_{m+n} + 2J_{m+n}^0 \tag{53}$$

giving rise to the $\widehat{su}(2)$ current algebra. Nevertheless it is only for $k=1$ that this algebra closes so nicely. In general the operators V_{m+n}^k belong to the universal enveloping algebra of the U(1) current.

IV. PRIMARY FIELDS

Now that we have the extended symmetry algebra, the next question is what are the primary fields with respect to this algebra. To answer this we need to consider the characters $\chi_m(q)$. Under $q \to e^{2\pi i} q$ we pick a phase $\exp(2\pi i((m^2/4k) - (1/24)))$. So the conformal dimension of the corresponding field is $h_m = m^2/4k$, $0 \leqslant m \leqslant 2k-1$. There are two Virasoro primary fields with this conformal dimension, the fields

$$V_m^\pm(z) = \exp\left(\pm i \frac{m}{\sqrt{2k}} \phi(z) \right). \tag{54}$$

Observe that for $m = 2k$ we get the two currents.

These primary fields satisfy the following operator product expansions:

$$J^0(z) V_m^\pm(w) = \pm \frac{m}{2k} \frac{V_m^\pm(w)}{z-w} + \text{reg},$$

$$\begin{aligned} J^+(z) V_m^-(w) = \frac{1}{(z-w)^m} :V_{2k-m}^+(w) \exp\Bigg(& 2k(z-w)J^0(w) + 2k\frac{(z-w)^2}{2!}\partial J^0(w) + \cdots \\ & + 2k\frac{(z-w)^{m-1}}{(m-1)!}\partial^{m-2} J^0(w) \Bigg) : + \text{reg}, \end{aligned} \tag{55}$$

$$\begin{aligned} J^-(z) V_m^+(w) = \frac{1}{(z-w)^m} :V_{2k-m}^-(w) \exp\Bigg(& -2k(z-w)J^0(w) - 2k\frac{(z-w)^2}{2!}\partial J^0(w) - \cdots \\ & - 2k\frac{(z-w)^{m-1}}{(m-1)!}\partial^{m-2} J^0(w) \Bigg) : + \text{reg}, \end{aligned}$$

where the remaining OPEs are trivial. Note that we can take the fields $V_m^+(z) = e^{i(m/\sqrt{2k})\,\phi(z)}$, $0 \leqslant m \leqslant 2k-1$ as a complete set of primary fields, since they are related to the $V_m^-(z)$ through the last of the relations (55).

V. MODULE STRUCTURE

The primary fields $V_m^+(z)$ add charge $m/\sqrt{2k}$ to the vacuum so we have

$$V_m^+(0)|0\rangle = \left| \frac{m}{\sqrt{2k}} \right\rangle. \tag{56}$$

Recall now that the chiral Fock space associated with the partition function was $H=\oplus_{n,m\epsilon Z}F_{\alpha_{nm}}$, where $\alpha_{nm}=n\sqrt{2k}+m/\sqrt{2k}$. The currents now can only add charges that are multiples of $\sqrt{2k}$. So it is natural to decompose the space H into the sum

$$H=\bigoplus_{m=0}^{2k-1}\mathcal{H}_m, \tag{57}$$

where

$$\mathcal{H}_m=\bigoplus_{n\epsilon Z}F_{m/\sqrt{2k}+n\sqrt{2k}} \tag{58}$$

is the space that is generated by the currents from $V_m^+(0)|0\rangle=|m/\sqrt{2k}\rangle$.

Let us examine now more closely what is the action of the currents on $\mathcal{H}_m$. Again by expanding the character $\chi_m(q)$ as a power series in q we see that there is one extra state appearing at the levels $n^2k-nm+m^2/4k$ and $n^2k+nm+m^2/4k$ for all positive integers n. Considering the product $J^+(z)|m/\sqrt{2k}\rangle$ we get

$$\sum_{n\epsilon Z}J_{-n}^+z^{n-k}|m/\sqrt{2k}\rangle=z^m\exp\left(\sqrt{2k}\sum_{n>0}\frac{a_{-n}}{n}z^n\right)|\sqrt{2k}+m/\sqrt{2k}\rangle. \tag{59}$$

This implies that

$$J_{-(k+m)}^+|m/\sqrt{2k}\rangle=|\sqrt{2k}+m/\sqrt{2k}\rangle \tag{60}$$

and $J_{-r}^+|m/\sqrt{2k}\rangle=0$ for all $r<k+m$. Applying $J^+(z)$ on this new state a number of times we eventually get that

$$J_{-((2n-1)k+m)}^+\cdots J_{-(3k+m)}^+J_{-(k+m)}^+|m/\sqrt{2k}\rangle=|n\sqrt{2k}+m/\sqrt{2k}\rangle. \tag{61}$$

These states account for the extra states at the levels $n^2k+nm+m^2/4k$. Applying $J^-(z)$ similarly a number of times on the state $m/\sqrt{2k}$ we get

$$J_{-((2n-1)k-m)}^-\cdots J_{-(3k-m)}^-J_{-(k-m)}^-|m/\sqrt{2k}\rangle=|-n\sqrt{2k}+m/\sqrt{2k}\rangle \tag{62}$$

and these states account for the extra states at levels $n^2k-nm+m^2/4k$.

Suppose now that the space $\mathcal{H}_m$ is reducible, as a module of our current algebra. Then there must be a state $|v_m\rangle$ other than $|m/\sqrt{2k}\rangle$ such that

$$J_n^\pm|v_m\rangle=0,\quad n>0 \tag{63}$$

and

$$J_n^0|v_m\rangle=0,\quad n>0. \tag{64}$$

Equation (64) forces us to consider the highest weight Fock states. Such states in the module $\mathcal{H}_m$ are the states $|m/\sqrt{2k}+n\sqrt{2k}\rangle$ for n integer. Suppose now that $n>0$. Applying $J^-(z)$ we get

$$\sum_{l\epsilon Z}J_l^-z^{-l-k}|m/\sqrt{2k}+n\sqrt{2k}\rangle=z^{-(m+2nk)}\exp\left(-\sqrt{2k}\sum_{l>0}\frac{a_{-l}}{l}z^l\right)|m/\sqrt{2k}+(n-1)\sqrt{2k}\rangle \tag{65}$$

and this in turn implies that

$$J_{m+(2n-1)k}^-|m/\sqrt{2k}+n\sqrt{2k}\rangle\neq 0. \tag{66}$$

Since $m+(2n-1)k$ is positive for positive n, $J_r^-|m/\sqrt{2k}+n\sqrt{2k}\rangle$ cannot be 0 for all positive r. If now $n=-n'<0$ then we need to apply $J^+(z)$. In this case we get

$$J^+_{-m+(2n'-1)k}|m/\sqrt{2k}-n'\sqrt{2k}\rangle=|m/\sqrt{2k}-(n'-1)\sqrt{2k}\rangle\neq 0. \tag{67}$$

Since $-m+(2n'-1)k$ is positive for positive n' (negative n), $J_r^+|m/\sqrt{2k}+n\sqrt{2k}\rangle$ cannot be 0 for all positive r. So $\mathcal{H}_m$ cannot be reducible. Hence we have the following theorem:

Theorem 1: *The space* $H=\oplus_{n,m\epsilon Z}F_{\alpha_{nm}}$ *where* $\alpha_{nm}=n\sqrt{2k}+m/\sqrt{2k}$ *admits the decomposition* $H=\oplus_{m=0}^{2k-1}\mathcal{H}_m$ *into irreducible modules of the algebra generated by the modes of the spin k currents* $J^{\pm}(z)$ *and the spin 1 current* $J^0(z)$. *In terms of Fock modules we have* $\mathcal{H}_m=\oplus_{n\epsilon Z}F_{m/\sqrt{2k}+n\sqrt{2k}}$.

VI. CONCLUSIONS

What we have achieved in this work is to single out a family of rational torus models by demanding the existence of a consistent set of Newmann (dually Dirichlet) boundary states. For these models we have written down the extended symmetry algebra which restricts the number of blocks to a finite number. Furthermore it is shown that the space of these torus models, which is an infinite sum of Fock modules, splits into a direct sum of a finite number of irreducible extended algebra modules.

The extended symmetry algebra that has appeared is a W-type algebra since it contains high spin currents. It should be thought of as a generalization of the SU(2) current algebra at level one, a theory which corresponds to $k=1$ in our list of theories. It is of interest to identify the algebras corresponding to the general level, in this way getting theories that may not possess free field representations. Some work in this direction has been done in the context of W-algebras in Ref. 11. A study of the representation theory of such algebras may give new examples of rational conformal field theories.

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Scalar-tensor gravity and conformal continuations

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Global properties of vacuum static, spherically symmetric configurations are studied in a general class of scalar-tensor theories (STTs) of gravity in various dimensions. The conformal mapping between the Jordan and Einstein frames is used as a tool. Necessary and sufficient conditions are found for the existence of solutions admitting a conformal continuation (CC). The latter means that a singularity in the Einstein-frame manifold maps to a regular surface $\mathbb{S}_{\text{trans}}$ in the Jordan frame, and the solution is then continued beyond this surface. $\mathbb{S}_{\text{trans}}$ can be an ordinary regular sphere or a horizon. In the second case, $\mathbb{S}_{\text{trans}}$ connect two epochs of a Kantowski-Sachs type cosmology. It is shown that the list of possible types of global causal structure of vacuum space–times in any STT, with any potential function $U(\phi)$, is the same as in general relativity with a cosmological constant. This is even true for conformally continued solutions. A traversable wormhole is shown to be one of the generic structures created as a result of CC. Two explicit examples are presented: the known solution for a conformal field in general relativity, illustrating the emergence of singularities and wormholes due to CC, and a nonsingular three-dimensional model with an infinite sequence of CCs. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1519667]

I. INTRODUCTION

Scalar fields with various potentials are of great significance in various branches of theoretical physics and cosmology: it is sufficient to mention, e.g., the Higgs field in particle theory and numerous quintessence models in modern cosmology. It is thus highly desirable to know which kinds of gravitationally self-bound configurations can be formed by such fields.

This article continues the study of global properties of static, spherically symmetric scalar-vacuum configurations of arbitrary dimension in various theories of gravity begun in Refs. 1–3. We will here consider scalar-tensor theories (STTs) belonging to the Bergmann–Wagoner–Nordtvedt family, where the Lagrangian depends on two essential arbitrary functions of the scalar field. It can be mentioned that STTs are among the viable alternatives to general relativity (GR), and their different versions emerge in the field limits of the candidate ''theories of everything.''

The field equations of an arbitrary STT are reduced by a conformal mapping to the equations of GR with a scalar field possessing a certain potential (the so-called Einstein frame). This article will pay special attention to the properties of such mappings. The point is that, when a manifold $\mathbb{M}[g]$ is conformally mapped to another manifold $\overline{\mathbb{M}}[\overline{g}]$ (relating the metrics by $g_{\mu\nu} = F(x)\overline{g}_{\mu\nu}$), the global properties of both manifolds are the same as long as the conformal factor F is everywhere smooth and finite. It can happen, however, that a singular surface in $\overline{\mathbb{M}}$ maps to a regular surface $\mathbb{S}_{\text{trans}}$ in $\mathbb{M}$ due to a singularity in the conformal factor F. Then $\mathbb{M}$ can be continued in a regular manner through this surface, and the global properties of $\mathbb{M}$ can be considerably richer than those of $\overline{\mathbb{M}}$: in the new region one can possibly find, e.g., new horizons or another spatial infinity. A known example of this phenomenon, to be called *conformal continua-*

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tion, is provided by the properties of the static, spherically symmetric solution for a conformally coupled scalar field in GR[4,5] as compared with the corresponding solution for a minimally coupled scalar field—see Sec. VI.

The Einstein-frame action for vacuum configurations in STT reads

$$S_{\mathrm{E}}=\int d^{D}x\sqrt{g}[\mathcal{R}_{\mathrm{E}}+(\partial\psi)^{2}-2V(\psi)], \tag{1}$$

i.e., coincides with the action of GR with a minimally coupled real scalar field ψ possessing a potential $V(\psi)$.

The field equations due to (1) with nontrivial potentials can be integrated explicitly in very few cases, even for highly symmetric configurations such as cosmological or static, spherically symmetric ones. Nevertheless, rather much can be said about the nature of the solutions. Examples of such general statements for non-negative potentials V are the no-hair theorems[6] discarding nontrivial scalar field for asymptotically flat black holes and the generalized Rosen theorem[7] claiming that an asymptotically flat solution with a positive mass cannot have a regular center.

It is also of interest what can happen if the asymptotic flatness and/or $V\geqslant 0$ assumptions are abandoned. Both assumptions are frequently violated in modern studies. Negative potential energy densities, in particular, the cosmological constant $V=\Lambda<0$ giving rise to the anti-de Sitter (AdS) solution or AdS asymptotic, do not lead to catastrophes (if bound below), are often treated in various aspects and quite readily appear from quantum effects like vacuum polarization.

Our previous papers[1,2] have provided some essential restrictions on the possible behavior of solutions of the theory (1) with arbitrary $V(\psi)$ in D dimensions. It has been shown, in particular, that, whatever is the potential and irrespective of the asymptotic conditions, the variable scalar field adds nothing to the list of causal structures known for $\psi=\mathrm{const}$. In the latter case V becomes a cosmological constant, and the corresponding exact solutions are well known (Schwarzschild, Schwarzschild–de Sitter, Schwarzschild–anti-de Sitter and their multidimensional analogs) along with their causal structures.

The possibility of regular configurations without a center (wormholes and horns) was also ruled out.

As was shown in Refs. 1 and 2, the above results can be extended to (i) generalized scalar field Lagrangians in GR, with an arbitrary dependence on the ψ field and its gradient squared, and (ii) to multiscalar field theories of sigma-model type in GR. To scalar-tensor theories, as is clear from the aforesaid, the same results can be extended only partly and only in the absence of conformal continuation (CC). This phenomenon is of particular interest since it widens the set of possible configurations. A study of possible CCs in the Jordan frames of STT was begun in Ref. 3 and is continued here more systematically and in more detail. Moreover, we will discuss the global properties of conformally continued space–times.

We will here avoid a detailed discussion of which conformal frame (Jordan or Einstein) in STT should be regarded as the physical one, refering to Ref. 8 and references therein. Only one comment is in order: when an STT emerges in a weak-field or low-energy limit of some more fundamental theory, its Lagrangian generally contains the scalar curvature with a ϕ-dependent factor, thus leading to one of numerous possible Jordan frames (e.g., the string metric in models of string origin). So, by origin, it is this formulation of the theory that should be used for studying such fundamental issues as topology, singularities, causal properties, etc., although a comparison with observations may require a different formulation.

The paper is organized as follows. Section II presents the field equations. In Sec. III we review the known results on scalar vacuum structures in GR and configurations described by generic STT solutions. We begin with a brief description of purely vacuum structures in D-dimensional GR with a cosmological constant and then reproduce the no-go theorems of Refs. 1 and 2 on the properties of scalar vacuum in GR and mention some other known theorems and examples. Two theorems, providing the necessary and sufficient conditions under which a given STT contains a CC, are formulated and proved in Sec. IV. In Sec. V we discuss the global properties of Jordan-

frame space–times in the presence of CCs. It turns out, in particular, that even the presence of CCs does not enlarge the number of possible horizons and hence the above list of global causal structures. It is shown that one of the generic structures created by CCs is a traversable wormhole. The whole space–time is then globally regular and static. Some particular kinds of singularities can also be created beyond a CC surface. Section VI contains two explicit examples of STT solutions with CCs. One of them represents the well-known solution for a conformally coupled scalar field in GR, which, in addition to singular cases, contains a family of traversable wormhole solutions.[5,9] The other is a nonsingular model containing an infinite sequence of CCs in three-dimensional gravity with a conformally coupled scalar field having a certain non-negative potential.

To sum up, with all theorems and examples at hand, we now have, even without solving the field equations, rather a clear picture of what can and what cannot be expected from static scalar-vacuum configurations in a general class of STT of gravity with various scalar field potentials.

Throughout the article all relevant functions are assumed to be sufficiently smooth, unless otherwise indicated. The symbol $\sim$, as usual, connects quantities of the same order of magnitude. The ends of theorem proofs are marked with $\square$.

II. FIELD EQUATIONS

The general STT action in a D-dimensional pseudo-Riemannian manifold $\mathbb{M}_J[g]$ is

$$S_{\rm STT}=\int d^D x\sqrt{g}[f(\phi)\mathcal{R}+h(\phi)(\partial\phi)^2-2U(\phi)+L_m], \tag{2}$$

where $g_{\mu\nu}$ is the metric, $\mathcal{R}=\mathcal{R}[g]$ is the scalar curvature, $g=|\det g_{\mu\nu}|$, f, h and U are functions of the real scalar field ϕ, $(\partial\phi)^2=g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi$, and L_m is the matter Lagrangian. The manifold $\mathbb{M}_J[g]$ with the metric $g_{\mu\nu}$ comprises the so-called Jordan conformal frame. The vacuum ($L_m=0$) field equations due to (2) read

$$\nabla_\alpha(h\nabla^\alpha)\phi-\tfrac{1}{2}\mathcal{R}f_\phi=-dU/d\phi, \tag{3}$$

$$f(\phi)(\mathcal{R}_\mu^{\ \nu}-\tfrac{1}{2}\delta_\mu^\nu\mathcal{R})=h(\phi)(-\phi_{,\mu}\phi^{,\nu}+\tfrac{1}{2}\delta_\mu^\nu\phi^{,\alpha}\phi_{,\alpha})-\delta_\mu^\nu U(\phi)-(\nabla_\mu\nabla^\nu-\delta_\mu^\nu\square)f-T^\nu_{\mu({\rm m})}, \tag{4}$$

where $\square=\nabla^\alpha\nabla_\alpha$ is the d'Alembert operator, $\mathcal{R}_\mu^{\ \nu}$ is the Ricci tensor, and the last term in (4) is the energy-momentum tensor of matter. (The usual constant factor $8\pi G$, where G is the gravitational constant, can be restored by proper redefinition of the variables.)

The standard transition to the Einstein frame, which generalizes Wagoner's[10] four-dimensional transformation,

$$g_{\mu\nu}=F(\psi)\overline{g}_{\mu\nu},\quad F=|f|^{-2/(D-2)}, \tag{5}$$

$$\frac{d\psi}{d\phi}=\pm\frac{\sqrt{|l(\phi)|}}{f(\phi)},\quad l(\phi)\overset{\rm def}{=}fh+\frac{D-1}{D-2}\left(\frac{df}{d\phi}\right)^2, \tag{6}$$

removes the nonminimal scalar-tensor coupling expressed in the ϕ-dependent coefficient before $\mathcal{R}$. Putting $L_m=0$ (vacuum), one can write the action (2) in the new manifold $\mathbb{M}_E[\overline{g}]$ with the new metric $\overline{g}_{\mu\nu}$ and the new scalar field ψ as follows (up to a boundary term):

$$S_{\rm E}=\int d^D x\sqrt{\overline{g}}\{{\rm sign}f[\overline{\mathcal{R}}+({\rm sign}l)(\partial\psi)^2]-2V(\psi)\}, \tag{7}$$

where the determinant $\overline{g}$, the scalar curvature $\overline{\mathcal{R}}$ and $(\partial\psi)^2$ are calculated using $\overline{g}_{\mu\nu}$ and

$$V(\psi)=|f|^{-D/(D-2)}(\psi)\,U(\phi). \tag{8}$$

Note that $\mathrm{sign}\,l=-1$ corresponds to the so-called anomalous STT, with a wrong sign of scalar field kinetic energy, while $\mathrm{sign}\,f=-1$ means that the effective gravitational constant in the Jordan frame (which can be defined as $1/f$ up to a constant factor) is negative. So the normal choice of signs is $\mathrm{sign}\,l=\mathrm{sign}\,f=1$, when the scalar-vacuum action takes the form (1). We will adhere to theories with $l>0$ in the whole paper, but we shall see that the continuations to be discussed in Secs. IV–VI lead to $f<0$ in some regions of $\mathbb{M}_{\mathrm{J}}$.

Among the three functions of ϕ entering into (2) only two are independent since there is a freedom of transformations $\phi=\phi(\phi_{\mathrm{new}})$. We assume $h\geqslant 0$ and use this freedom, choosing in what follows $h(\phi)\equiv 1$. {Another standard parametrization is to put $f(\phi)=\phi$ and $h(\phi)=\omega(\phi)/\phi$ [the Brans–Dicke parametrization of the general theory (2)].}

From the viewpoint of the field equations, the transformation (5) and (6) is merely a simplifying substitution. Instead of Eqs. (3) and (4) (assuming $f>0$), we deal in $\mathbb{M}_{\mathrm{E}}$ with simpler equations due to (1):

$$\overline{\Box}\psi+dV/d\psi=0, \tag{9}$$

$$\overline{\mathcal{R}}{}^{\nu}_{\mu}-\tfrac{1}{2}\delta^{\nu}_{\mu}\overline{\mathcal{R}}=-\psi_{,\mu}\psi^{,\nu}+\tfrac{1}{2}\delta^{\nu}_{\mu}(\partial\psi)^2-\delta^{\nu}_{\mu}V(\psi), \tag{10}$$

with the Ricci tensor $\overline{\mathcal{R}}{}^{\nu}_{\mu}$ and the d'Alembert operator $\overline{\Box}$ corresponding to $\overline{g}_{\mu\nu}$.

Consider static, spherically symmetric configurations, so that the metric in $\mathbb{M}_{\mathrm{E}}$ is written as

$$ds^2_{\mathrm{E}}=A(\rho)dt^2-\frac{d\rho^2}{A(\rho)}-r^2(\rho)d\Omega^2_{\overline{d}}, \tag{11}$$

where $d\Omega^2_{\overline{d}}$ is the linear element on the sphere $\mathbb{S}^{\overline{d}}$ of unit radius, and the scalar field is $\psi=\psi(\rho)$.

Then Eq. (9) and some combinations of the Einstein equations (10) have the form

$$(Ar^{\overline{d}}\psi')'=r^{\overline{d}}V_{\psi}; \tag{12}$$

$$(A'r^{\overline{d}})'=-(4/\overline{d})r^{\overline{d}}V; \tag{13}$$

$$\overline{d}r''/r=-\psi'^2; \tag{14}$$

$$A(r^2)''-r^2A''+(\overline{d}-2)r'(2Ar'-A'r)=2(\overline{d}-1); \tag{15}$$

$$\overline{d}(\overline{d}-1)(1-Ar'^2)-\overline{d}A'rr'=-Ar^2\psi'^2+2r^2V, \tag{16}$$

where the prime denotes $d/d\rho$. Only three of these five equations are independent: the scalar equation (12) follows from the Einstein equations, while Eq. (16) is a first integral of the others. Given a potential $V(\psi)$, this is a determined set of equations for the unknowns r, A, ψ.

This choice of the radial coordinate according to the condition $\overline{g}_{tt}\overline{g}_{\rho\rho}=-1$ is preferable for considering Killing horizons, which correspond to zeros of the function $A(\rho)$, since such zeros are regular points of Eqs. (12)–(16), and therefore one can jointly consider regions at both sides of a horizon; moreover, in a close neighborhood of a horizon, the coordinate ρ defined in this way varies (up to a positive constant factor) like manifestly well-behaved Kruskal-like coordinates used for an analytic continuation of the metric.[11] Therefore this coordinate frame can be called *quasiglobal*.

The corresponding metric in $\mathbb{M}_{\mathrm{J}}$ reads

$$ds_J^2 = F(\psi)\left[A(\rho)dt^2 - \frac{d\rho^2}{A(\rho)} - r^2 d\Omega_{\bar{d}}^2\right] = \mathcal{A}(q)dt^2 - \frac{dq^2}{\mathcal{A}(q)} - R^2 d\Omega_{\bar{d}}^2, \tag{17}$$

where we have introduced the quasiglobal coordinate q in $\mathbb{M}_J$, similar to ρ in (11), such that $g_{tt}g_{\rho\rho} = -1$. The quantities in (17) and (11) are related by

$$\pm dq = F d\rho, \quad \mathcal{A}(q) = FA(\rho), \quad R(q) = \sqrt{F} r(\rho). \tag{18}$$

With our convention $h(\phi) \equiv 1$, three independent field equations in $\mathbb{M}_J$ can be written as follows:

$$f\left(\mathcal{A}_{qq} + \bar{d}\mathcal{A}_q \frac{R_q}{R}\right) + \frac{D}{\bar{d}}\mathcal{A}_q f_q + 2\mathcal{A}\frac{R_q}{R} f_q + \frac{2}{\bar{d}}\mathcal{A} f_{qq} + \frac{4}{\bar{d}}U = 0, \tag{19}$$

$$\bar{d} f \frac{R_{qq}}{R} + \phi_q^2 + f_{qq} = 0, \tag{20}$$

$$\frac{f}{R^2}\left[-(\bar{d}-1) + \mathcal{A}RR_{qq} + \mathcal{A}R_q^2 - \frac{1}{2}R^2\mathcal{A}_{qq} + \frac{1}{2}(\bar{d}-2)R_q(2\mathcal{A}R_q - R\mathcal{A}_q)\right] + \left(\frac{\mathcal{A}R_q}{R} - \frac{\mathcal{A}_q}{2}\right) f_q = 0, \tag{21}$$

where the subscript q denotes d/dq.

III. PROPERTIES OF GENERIC STT SOLUTIONS

A. Some known results for the Einstein frame

Let us enumerate some consequences of Eqs. (12)–(16) valid in $\mathbb{M}_E$.

The first important restriction is the nonexistence of regular configurations having no center ($r = 0$), namely, wormholes, horns and flux tubes.[1,2]

For the metric (11), a (traversable, Lorentzian) *wormhole* is, by definition, a configuration with two asymptotics at which $r(\rho) \to \infty$, hence with $r(\rho)$ having at least one regular minimum. A *horn* is a region where, as r tends to some finite value, $g_{tt} = A$ remains finite whereas the length integral $l = \int d\rho/\sqrt{A}$ diverges. In other words, a horn is a configuration ending with a regular, infinitely long $(\bar{d}+1)$-dimensional "tube" of finite radius. Such "horned particles" were discussed as possible remnants of black hole evaporation.[12] Lastly, a *flux tube* is a configuration with $r = \text{const}$, a "cylindrical" space.

Theorem 1: *The field equations due to (1) for $D \geqslant 4$ do not admit (i) solutions where the function $r(\rho)$ has a regular minimum, (ii) solutions describing a horn, and (iii) flux-tube solutions with $\psi \neq \text{const}$.*

The formulation of the theorem and its proof,[1,2] which essentially rests on Eq. (14), do not refer to any kind of asymptotic, therefore wormhole throats or horns are absent in solutions having any large r behavior—flat, de Sitter or any other, or having no large r asymptotic at all.

For $D = 3$ items (*i*) and (*iii*) of Theorem 1 hold, but solutions with a horn can exist; though, a horn can only appear at a maximum of $r(\rho)$, so that horned configurations have no spatial asymptotic.

The global causal structure of space–time is unambiguously determined (up to identification of isometric surfaces, if any) by the disposition of static ($A > 0$) and nonstatic, homogeneous ($A < 0$) regions, separated by horizons.[13–16] The following two theorems severely restrict such possible dispositions.

Theorem 2: *Consider solutions of the theory (1), $D \geqslant 4$, with the metric (11) and $\psi = \psi(\rho)$. Let there be a static region $a < \rho < b \leqslant \infty$. Then:*

(i) all horizons are simple;
(ii) no horizons exist at $\rho<a$ and at $\rho>b$.

Theorem 2a: *A static, circularly symmetric configuration in the theory (1), $D=3$, has either no horizon or one simple horizon.*

The proof of these theorems[1,2] employs the properties of Eq. (15), which can be rewritten in the form

$$r^4B''+(\bar{d}+2)r^3r'B'=-2(\bar{d}-1), \tag{22}$$

where $B(\rho)=A/r^2$. This equation shows that B cannot have a regular minimum, therefore, having once become negative while moving to the left or to the right along the ρ axis, $B(\rho)$ [and hence $A(\rho)$] cannot return to zero or positive values.

Theorems 2 and 2a show that the possible disposition of zeros of the function $A(\rho)$ is the same as in the case of vacuum with a cosmological constant. Therefore the list of possible global causal structures is also the same.

Let us, for reference purposes, enumerate these structures. The metric satisfying Eqs. (13)–(16) with $\psi'=0$, $V=\Lambda=\text{const}$ is

$$ds^2=A(r)dt^2-\frac{dr^2}{A(r)}-r^2d\Omega_{\bar{d}}^2 \tag{23}$$

[it is (11) with $\rho\equiv r$] where

$$A(r)=1-\frac{2m}{r^{\bar{d}-1}}-\frac{2\Lambda r^2}{\bar{d}(\bar{d}+1)}. \tag{24}$$

This is the multidimensional Schwarzschild–de Sitter solution. Its special cases correspond to the Schwarzschild ($\bar{d}=2$, $\Lambda=0$) and Tangherlini (any $\bar{d}$, $\Lambda=0$) solutions and the de Sitter solution in arbitrary dimension when $m=0$, called anti-de Sitter (AdS) in the case $\Lambda<0$.

Different qualitative behaviors of $A(r)$ for different values of Λ and m correspond to the following structures:[17]

(1) $\Lambda=0$, $m\leqslant 0$: curves 1a and 1b in Fig. 1, diagram 1 in Fig. 2 (Minkowski and $m<0$ Schwarzschild, respectively).
(2) $\Lambda<0$, $m\leqslant 0$: curves 2a and 2b in Fig. 1, diagram 2 in Fig. 2 (AdS and $m<0$ Schwarzschild–AdS).
(3) $\Lambda<0$, $m>0$: curve 3 in Fig. 1, diagram 3 in Fig. 2 (Schwarzschild–AdS).
(4) $\Lambda=0$, $m>0$: curve 4 in Fig. 1, diagram 4 in Fig. 2 (Schwarzschild).
(5) $\Lambda>0$, $m\leqslant 0$: curves 5a and 5b in Fig. 1, diagram 5 in Fig. 2 (de Sitter and $m<0$ Schwarzschild–de Sitter).
(6) $\Lambda>0$, $m>0$: curves 6a, 6b and 6c in Fig. 1, and the corresponding diagrams in Fig. 2 (Schwarzschild–de Sitter in case 6a and Kantowski–Sachs homogeneous cosmologies in cases 6b and 6c).

The center $r=0$ is regular for $m=0$ and singular for $m\neq 0$.

In case 6, given a particular value of $\Lambda>0$, the solution behavior depends on the mass parameter m. When m is smaller than the critical value

$$m_{\text{cr}}=\frac{1}{\bar{d}+1}\left[\frac{\bar{d}(\bar{d}-1)}{2\Lambda}\right]^{(\bar{d}-1)/2}, \tag{25}$$

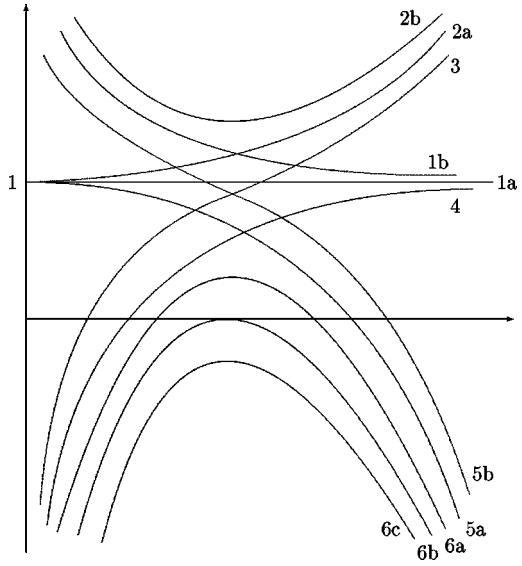

FIG. 1. The behavior of $A(r)$, Eq. (24), for different values of m and Λ.

there are two horizons, the smaller one being interpreted as a black hole horizon and the greater one as a cosmological horizon. If $m=m_{\rm cr}$, the two horizons merge, and one has two homogeneous T regions separated by a double horizon. Lastly, the solution with $m>m_{\rm cr}$ is purely cosmological and has no Killing horizon.

In $(2+1)$-dimensional gravity ($\bar{d}=1$), according to Theorem 2a, the list is even shorter: the structures corresponding to the curves 6a and 6b are absent.

Let us also mention, for completeness, some results known for $D=4$ and most probably admitting a generalization to other dimensions.

No-hair theorems state that (1) if $V\geqslant 0$, an asymptotically flat black hole cannot have a nontrivial scalar field;[6,18,19] and (2) if $V\geqslant 0$ and $d^2V/d\psi^2\geqslant 0$ (a convex potential), an asymptotically anti-de Sitter black hole cannot have a nontrivial scalar field.[20]

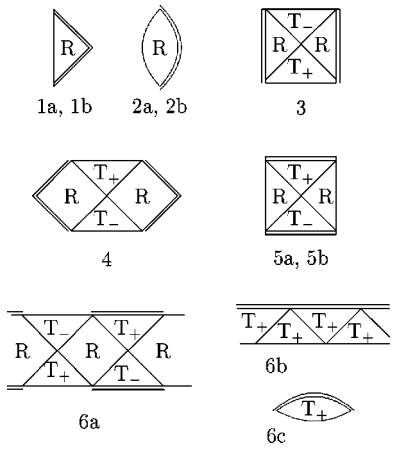

FIG. 2. Carter–Penrose diagrams for different cases of the metric (23) and (24), labeled according to Fig. 1. The R and T letters correspond to R and T space–time regions; T_+ and T_- denote expanding and contracting T region (i.e., with r increasing and decreasing with time, respectively). Single lines on the border of the diagrams denote $r=0$, double lines—$r=\infty$. Diagrams 6b and 6c are drawn for the case of expanding Kantowski–Sachs cosmologies; to obtain diagrams for contracting models, one should merely interchange $r=0$ and $r=\infty$ and replace T_+ with T_-. Diagrams 6a and 6b admit identification of isometric timelike sections.

The generalized Rosen theorem states that, provided $V \geqslant 0$, a particlelike solution with a regular center, a flat asymptotic and positive mass does not exist.[7]

These theorems cannot be directly extended to STT in the Jordan frame and will not be discussed any more, though an attempt to formulate additional conditions able to provide such extensions may be of interest.

Explicit examples have been obtained, confirming the existence of some kinds of solutions admitted by the above theorems. Thus, there exist (1) black holes possessing nontrivial scalar fields (scalar hair), with $V \geqslant 0$, but with nonflat and non-de Sitter asymptotics;[21] (2) black holes with scalar hair and flat asymptotics, but partly negative potentials;[2] and (3) configurations with a regular center, a flat asymptotic and positive mass, but also with partly negative potentials.[2]

Thus black holes with scalar hair are not excluded in general, but such objects as regular black holes,[22] possessing a regular center and a global structure coinciding with that of Reissner–Nordstrom or Reissner–Nordstrom–de Sitter space–time, are ruled out.

B. Generic solutions in the Jordan frame

It should be, above all, noted that when a space–time manifold $\mathbb{M}_{\mathrm{E}}[\overline{g}]$ (the Einstein frame) with the metric (11) is conformally mapped into another manifold $\mathbb{M}_{\mathrm{J}}[g]$ (the Jordan frame), equipped with the same coordinates, according to the law

$$g_{\mu\nu} = F(\rho)\overline{g}_{\mu\nu}, \tag{26}$$

it is easily verified that a horizon $\rho = h$ in $\mathbb{M}_{\mathrm{J}}$ passes into a horizon of the same order in $\mathbb{M}_{\mathrm{E}}$, a center ($r = 0$) and an asymptotic ($r \to \infty$) in $\mathbb{M}_{\mathrm{J}}$ pass into a center and an asymptotic, respectively, in $\mathbb{M}_{\mathrm{E}}$ if the conformal factor $F(\rho)$ is regular (i.e., finite, at least C^2-smooth and positive) at the corresponding values of ρ. A regular center passes to a regular center and a flat asymptotic to a flat asymptotic under evident additional requirements.

The validity of Theorems 1, 2 and 2a in the Jordan frame depends on the nature of the conformal mapping (5) that connects $\mathbb{M}_{\mathrm{J}}[g]$ with $\mathbb{M}_{\mathrm{E}}[\overline{g}]$). There are four variants:

I. $\mathbb{M}_{\mathrm{J}} \leftrightarrow \mathbb{M}_{\mathrm{E}}$,

II. $\mathbb{M}_{\mathrm{J}} \leftrightarrow (\mathbb{M}'_{\mathrm{E}} \subset \mathbb{M}_{\mathrm{E}})$,

III. $(\mathbb{M}'_{\mathrm{J}} \subset \mathbb{M}_{\mathrm{J}}) \leftrightarrow \mathbb{M}_{\mathrm{E}}$,

IV. $(\mathbb{M}'_{\mathrm{J}} \subset \mathbb{M}_{\mathrm{J}}) \leftrightarrow (\mathbb{M}'_{\mathrm{E}} \subset \mathbb{M}_{\mathrm{E}})$,

where $\leftrightarrow$ is a diffeomorphism preserving the metric signature. The last three variants are possible if the conformal factor F vanishes or blows up at some values of ρ, which then mark the boundary of $\mathbb{M}'_{\mathrm{J}}$ or $\mathbb{M}'_{\mathrm{E}}$.

A situation of the kind III or IV can be called a *conformal continuation* (CC) from $\mathbb{M}_{\mathrm{E}}$ into $\mathbb{M}_{\mathrm{J}}$.

One can notice that such continuations can only occur for special solutions: to admit a CC, the singularity in $\mathbb{M}_{\mathrm{E}}$ should be removable by a conformal factor, i.e., be, in a sense, isotropic. Moreover, the factor F should have precisely the behavior needed to remove it.

Thus generic situations are I and II, the latter meaning that the factor F "spoils" the geometry and creates a singularity. In these cases Theorem 2 (or 2a for $D = 3$) on horizon dispositions is obviously valid in $\mathbb{M}_{\mathrm{J}}$.

The manifolds $\mathbb{M}_{\mathrm{J}}$ then cannot have other causal structures than those depicted in Fig. 2. This is manifestly true for STT with $f(\phi) > 0$.

Theorem 1 cannot be directly transferred to $\mathbb{M}_{\mathrm{J}}$ in any case except the trivial one, $F = \mathrm{const}$. In particular, minima of $g_{\theta\theta}$ (wormhole throats) can appear. It is only possible to assert without specifying $F(\psi)$ that wormholes as global entities are impossible in $\mathbb{M}_{\mathrm{J}}$ in case I if the conformal factor F is finite in the whole range of ρ, including the boundary values. Indeed, if we suppose that

there is such a wormhole, it will immediately follow that there are two large r asymptotics and a minimum of $r(\rho)$ between them even in $\mathbb{M}_E$, in contrast to Theorem 1 which is valid there. Wormholes are also absent in case II since we then have a singularity instead of at least one of the asymptotics.

The above-mentioned examples of black holes with scalar hair when the potential is not positive-definite or the asymptotic is nonflat are also directly transferred to $\mathbb{M}_J$ provided $F(\psi)$ is regular at least outside the horizon. Given a particlelike solution in $\mathbb{M}_E$, with a regular center and positive mass, the condition that a solution with similar properties occurs in $\mathbb{M}_J$ can also be easily formulated, but we will not concentrate on this question here.

Conformal continuations, if any, can in principle lead to other, maybe more complex structures. In what follows we will try to answer two questions: (1) under which conditions the mapping (26) creates a conformal continuation in STT and (2) what can be the nature of conformally continued solutions in the Jordan frame.

IV. CONFORMAL CONTINUATION CONDITIONS

A. Preliminaries

A CC from $\mathbb{M}_E$ into $\mathbb{M}_J$ can occur at such values of the scalar field ϕ that the conformal factor F in the mapping (5) is singular while the functions f, h and U in the action (2) are regular. This means that at $\phi=\phi_0$, corresponding to a possible transition surface $\mathbb{S}_{\text{trans}}$, the function $f(\phi)$ has a zero of a certain order n. We then have in the transformation (6) near $\phi=\phi_0$ in the leading order of magnitude

$$f(\phi)\sim\Delta\phi^n, \quad n=1,2,\ldots, \quad \Delta\phi\equiv\phi-\phi_0. \tag{27}$$

One can notice, however, that $n>1$ leads to $l(\phi_0)=0$ [recall that by our convention $h(\phi)\equiv 1$]. This generically leads to a curvature singularity in $\mathbb{M}_J$, as can be seen from the trace of Eqs. (4):

$$l(\phi)\mathcal{R}=-\left(1+2\frac{D-1}{D-2}f_{\phi\phi}\right)\phi^\alpha\phi_\alpha+\frac{2}{D-2}[DU+(D-1)f_\phi U_\phi] \tag{28}$$

(the subscript ϕ denotes $d/d\phi$). If the right-hand side of (28) is nonzero at $\phi=\phi_0$ at which $l=0$, the scalar curvature $\mathcal{R}$ is infinite. There can be special choices of f and U such that this singularity is avoided, but we will ignore this possibility and simply assume $l>0$ at $\mathbb{S}_{\text{trans}}$.

Thus, according to (6), we have near $\mathbb{S}_{\text{trans}}(\phi=\phi_0)$,

$$f(\phi)\sim\Delta\phi\sim e^{-\psi\sqrt{d/(d+1)}}, \tag{29}$$

where without loss of generality we choose the sign of ψ so that $\psi\to\infty$ as $\Delta\phi\to 0$.

In the CC case, the metric $\overline{g}_{\mu\nu}$ specified by (11) is singular on $\mathbb{S}_{\text{trans}}$ while $g_{\mu\nu}=F(\psi)\overline{g}_{\mu\nu}$ is regular. There are two opportunities. The first one, to be called CC-I for short, is that $\mathbb{S}_{\text{trans}}$ is an *ordinary regular surface* in $\mathbb{M}_J$, where both $g_{tt}=\mathcal{A}=FA$ and $-g_{\theta\theta}=R^2=\underline{F}r^2$ (squared radius of $\mathbb{S}_{\text{trans}}$) are finite. (Here θ is one of the angles that parametrize the sphere $\mathbb{S}^d$.) The second variant, to be called CC-II, is that $\mathbb{S}_{\text{trans}}$ is a *horizon* in $\mathbb{M}_J$. In the latter case only $g_{\theta\theta}$ is finite, while $g_{tt}=0$. We will consider these two kinds of CC separately.

In both cases some necessary conditions for CC are easily obtained using the field equations in $\mathbb{M}_E$, but these equations describe the system only on one side of $\mathbb{S}_{\text{trans}}$. Another Einstein frame may be built for the region beyond $\mathbb{S}_{\text{trans}}$, but in this case there arises the problem of matching the solutions obtained in two nonintersecting regions. Therefore to prove sufficient conditions for the existence of solutions in $\mathbb{M}_J$, which are regular on and near $\mathbb{S}_{\text{trans}}$, we have to deal with the field equations in $\mathbb{M}_J$.

B. Continuation through an ordinary sphere (CC-I)

Given a metric $\overline{g}_{\mu\nu}$ of the form (11) in $\mathbb{M}_{\rm E}$, a CC-I can occur if

$$F(\psi)=|f|^{-2/\overline{d}}\sim 1/r^2\sim 1/A \tag{30}$$

as $\psi\to\infty$, while the behavior of f is specified by (29). The surface $\mathbb{S}_{\rm trans}$, being regular in the Jordan frame, is singular in $\mathbb{M}_{\rm E}$ ($r^2\sim A\to 0$): it is either a singular center if the continuation occurs in an R-region, or a cosmological singularity in the case of a T-region.

The following theorem is valid:

Theorem 3: *Consider scalar-vacuum configurations with the metric (17) and $\phi=\phi(q)$ in the theory (2) with $h(\phi)\equiv 1$ and $l(\phi)>0$. Suppose that $f(\phi)$ has a simple zero at some $\phi=\phi_0$, and $|U(\phi_0)|<\infty$. Then*

(i) there exists a solution in $\mathbb{M}_{\rm J}$, smooth in a neighborhood of the surface $\mathbb{S}_{\rm trans}$ ($\phi=\phi_0$), which is an ordinary regular surface in $\mathbb{M}_{\rm J}$; and

(ii) in this solution the ranges of ϕ are different on different sides of $\mathbb{S}_{\rm trans}$.

Proof: Let us begin with item (ii): given a CC-I, we will show that $d\phi/dq\neq 0$ at $\phi=\phi_0$, so that ϕ_0 is not a maximum or minimum of $\phi(q)$.

Indeed, it can be deduced from the conditions (29) and (30) and Eq. (14) that near $\mathbb{S}_{\rm trans}$

$$r(\rho)\sim(\rho-\rho_0)^{1/D}, \tag{31}$$

where $\rho=\rho_0$ is the location of $\mathbb{S}_{\rm trans}$. It then follows that $q_0=q(\rho_0)$ is finite on $\mathbb{S}_{\rm trans}$ and both $\Delta\phi$ and $q-q_0$ behave as $r^{\overline{d}}$ in its neighborhood, hence $d\phi/dq$ is finite.

With this necessary condition, we can prove item (i), seeking a solution to Eqs. (19)–(21) in an appropriate form. Here, the unknowns are $\mathcal{A}(q)$, $R(q)$, $\phi(q)$, while $f(\phi)$ and $U(\phi)$ are prescribed by the choice of the theory. However, since $f(\phi_0)=0$ and $df/d\phi\neq 0$ at $\phi=\phi_0$, we can treat $\phi(f)$ as a known function in a certain neighborhood of $f=0$ and consider $f(q)$ as an unknown instead of $\phi(q)$.

Let $\mathbb{S}_{\rm trans}$ be located (without loss of generality) at $q=0$. It is sufficient to find a solution in the form of a power series in q near $q=0$. Since R and A should be finite at $\mathbb{S}_{\rm trans}$, while $f=0$ and $df/dq\neq 0$, we seek a solution in the form

$$\mathcal{A}(q)=\sum_{n=0}^{\infty}A_n q^n/n!=A_0+A_1 q+\frac{1}{2}A_2 q^2+\ldots,$$

$$R(q)=\sum_{n=0}^{\infty}R_n q^n/n!=R_0+R_1 q+\frac{1}{2}R_2 q^2+\ldots, \tag{32}$$

$$f(q)=\sum_{n=1}^{\infty}f_n q^n/n!=f_1 q+\frac{1}{2}f_2 q^2+\ldots,$$

with nonzero A_0, R_0, f_1.

Substituting (32) into the equations, we see that in the senior order of magnitude, $O(1)$, the coefficients A_1, R_1, f_2 are expressed in terms of A_0, R_0, f_1 and $U(\phi_0)$. Next powers of q express the further expansion factors in terms of the previous ones. Namely, in every order of magnitude $O(q^n)$, $n>0$, Eq. (20) gives

$$(n-1)\overline{d}R_n/R_0+f_{n+1}/f_1=\cdots, \tag{33}$$

where the dots on the right mean various combinations of coefficients of the previous orders as well as power expansion factors of the known functions $U(\phi)$ and $\phi(f)$. Then, excluding f_{n+1} from the other two equations in the order $O(q^n)$, we obtain a set of two linear algebraic equations for A_n/A_0 and R_n/R_0:

$$A_n/A_0 - 2R_n/R_0 = \cdots,$$
$$(n\overline{d}+2)A_n/A_0 - 2\overline{d}(n-2)R_n/R_0 = \cdots, \tag{34}$$

whose determinant is equal to $4(\overline{d}+1)$ for any n. We conclude that all the expansion factors in (32) are uniquely expressed in terms of A_0, R_0, f_1 and the expansion factors of the known functions. This proves the existence of the solution in $\mathbb{M}_J$ near $\mathbb{S}_{trans}$. □

The order of smoothness of the solution obtained depends on the smoothness of the original functions f, h, U. If they are C^∞, as is natural for a field theory, then the metric functions and ϕ are also C^∞.

The existence of such a solution automatically implies the existence of the corresponding solutions on different sides of $\mathbb{S}_{trans}$ in two different Einstein frames. These solutions are special, being restricted by Eq. (30). As follows from the proof, the solution in $\mathbb{M}_J$, and hence its counterparts in both $\mathbb{M}_E$, contain two essential integration constants (R_0 and f_1, whereas A_0 determines the time scale on $\mathbb{S}_{trans}$ and can be chosen arbitrarily).

It is of interest that, under the CC-I conditions, the potential $V(\psi)$ in $\mathbb{M}_E$ (although it may even blow up) is inessential: the solution is close to Fisher's scalar-vacuum solution[23] for $D=4$ or its modification in other dimensions.

In case $D=3$, as follows from Eq. (15), a necessary condition for CC is $A/r^2 = \text{const}$.

One can also notice that no restriction other than regularity is imposed on the potential U, in particular, U may vanish in some region or in the whole space. [The conclusion that $U(\phi)=0$ on $\mathbb{S}_{trans}$, obtained in Ref. 3, appeared there due to an additional assumption on the form of the expansion of $A(\rho)$ in powers of ρ. An inspection shows that this assumption is unnecessary.] The latter case will be used as an explicit example of CC in Sec. VI A.

C. Continuation through a horizon in $\mathbb{M}_J$ (CC-II)

Let us suppose that in the metric (17) a certain value of q (without loss of generality, $q=0$) corresponds to a horizon of order $k \geqslant 1$. This means that $q=0$ is a zero of order k of the function $\mathcal{A}(q)$.

Suppose now that this horizon is $\mathbb{S}_{trans}$, a transition sphere in a CC. In other words, in the vicinity of $q=0$, $f(\phi) \sim \Delta\phi$. One can directly verify that the corresponding value ρ_0 of the coordinate ρ in the Einstein-frame metric (11) is finite, and we can choose for convenience $\rho_0 = 0$. We thus have near $q=0$

$$\mathcal{A}(q) = AF \sim q^k, \quad R^2(q) = Fr^2 = O(1). \tag{35}$$

Now, the question is: under which requirements to the original theory a horizon in $\mathbb{M}_J$, described by (35), can be a transition sphere $\mathbb{S}_{trans}$. An answer is given by the following theorem.

Theorem 4: *Consider scalar-vacuum configurations with the metric (17) and $\phi=\phi(q)$ in the theory (2) with $h(\phi)\equiv 1$ and $l(\phi)>0$. Suppose that $f(\phi)$ has a simple zero at some $\phi=\phi_0$. There exists a solution in $\mathbb{M}_J$, smooth in a neighborhood of the surface $\mathbb{S}_{trans}$ ($\phi=\phi_0$), which is a Killing horizon in $\mathbb{M}_J$,* **if and only if**

(**a**) $D \geqslant 4$,

(**b**) *ϕ_0 is a simple zero of $U(\phi)$, and*

(**c**) *$dU/df > 0$ at $\phi=\phi_0$.*

Then, in addition,

(**d**) *$\mathbb{S}_{trans}$ is a second-order horizon, connecting two T-regions in $\mathbb{M}_J$; and*

(**e**) *the ranges of ϕ are different on the two sides of $\mathbb{S}_{trans}$.*

Proof: Necessity: Given a CC-II, we will prove items (a)–(e).

Let us use Eqs. (13)–(15) in $\mathbb{M}_{\mathrm{E}}$. In particular, Eq. (15), which contains only $A(\rho)$ and $r(\rho)$, can be rewritten in the form

$$[r^D(A/r^2)']' + 2(\overline{d}-1)r^{\overline{d}-2} = 0. \tag{36}$$

Suppose CC-II at $\rho = 0$ $(q=0)$, which is a horizon of order k in $\mathbb{M}_{\mathrm{J}}$. Let us put $\overline{d} > 1$ and assume for certainty, without generality loss, that $q > 0$ as $\rho \to +0$. We have $dq/d\rho \sim F \sim 1/r^2$ and $A/r^2 \sim q^k$. Therefore the first term in (36) at small ρ behaves as

$$(\text{sign } A)\ [r^{\overline{d}} q^{k-1}]'.$$

Since both $r(\rho)$ and q are growing functions of ρ, this derivative is non-negative, whereas the second term in (36) is manifestly positive. The only way to satisfy (36) is to put $A < 0$. In other words, the horizon is approached from a T-region, where we deal with a Kantowski-Sachs type cosmological model.

Such a reasoning applies to approaching the surface $q=0$ from either side, therefore the horizon $\mathbb{S}_{\mathrm{trans}}$ connects two T-regions and is thus of even order.

We must also ascertain that the orders of magnitude of the two terms in (36) are the same. This is only true if $k=2$, as can be easily verified using (31), which now reads $r \sim \rho^{1/D}$. So item (d) is proved.

Equations (29) and (31) can be used to show that the derivative $d\phi/dq$ is finite at $q=0$, leading to item (e).

The behavior of $U(\phi)$ can be determined using Eq. (13), taking into account the relation (8) between U and V and the conditions (35) with $k=2$. We find in this way that $U(\phi) \sim \Delta\phi$ (i.e., the potential has a first-order zero) and that $dU/df > 0$ at $\phi = \phi_0$, so items (b) and (c) hold.

It remains to rule out $\overline{d}=1$ (three-dimensional gravity). In this case (36) leads to $(A/r^2) = c_1/r^3$, $c_1 = \text{const}$. The value $c_1 = 0$ is excluded since we must have $A/r^2 \sim q^k$. For $c_1 \neq 0$ we obtain $(q^k)' = kq^{k-1}dq/d\rho$, where due to (35) $q^{k-1} \sim 1/r \to \infty$, whereas $q \to 0$ and $k \geqslant 1$. This contradiction proves item (a).

Sufficiency: As in Theorem 3, the existence of a solution in $\mathbb{M}_{\mathrm{E}}$, smoothly continued across $\mathbb{S}_{\mathrm{trans}}$, is proved using Eqs. (19)–(21) and a power expansion for a sought-for solution. It is again convenient to treat $\phi(f)$ as a known function and $f(q)$ as an unknown, so again the unknowns are $\mathcal{A}(q)$, $R(q)$ and $f(q)$.

Seeking solutions to Eqs. (19)–(21) as series in q, we use again the expansions (32), but, under the present necessary conditions, we put there $A_0 = A_1 = 0$ and suppose nonzero A_2, R_0, f_1. With these expansions substituted, the equations again lead to a chain of recurrent relations for the coefficients, slightly more involved than in Theorem 3.

In the orders $O(1)$ and $O(q)$, Eq. (19) leads to

$$U(\phi_0) = 0, \quad (\overline{d}+D)A_2 + 4U_{f0} = 0$$

(where $U_{f0} = dU/df|_{f=0}$), hence $U_{f0} > 0$, in agreement with the necessary conditions. Equation (20) $[O(1)]$ expresses f_2 in terms of f_1 and $d\phi/df(f=0)$. Equation (21) $[O(1)]$ gives $A_2 = -(\overline{d}-1)/R_0^2$. Furthermore, Eqs. (19) $[O(q^2)]$ and (21) $[O(q)]$ yield two equations determining R_1 and A_3:

$$\begin{gathered}(3\overline{d}+2)A_3/A_2 + 2\overline{d}(\overline{d}+1)R_1/R_0 = \cdots, \\ 3A_3/A_2 + 2(\overline{d}-1)R_1/R_0 = \cdots,\end{gathered} \tag{37}$$

where the dots on the right replace combinations of previously known constants. The determinant of this set of linear equations with respect to A_3/A_2 and R_1/R_0 is $-4(2\overline{d}+1)<0$ for $\overline{d}>0$. We thus know the coefficients up to R_1, f_2, A_3. Further coefficients are determined recursively from further orders of magnitude in all three equations:

$$(n+D/\overline{d})a_n+n(n-1)(\overline{d}+1)b_n+(n-1)(n+D)c_n/D=\cdots,$$

$$(n+2)\overline{d}b_n+c_n=\cdots, \tag{38}$$

$$(n+1)a_n+n(-n^2+\overline{d}n-\overline{d}+9)b_n+(n-1)c_n=\cdots,$$

where $n\geqslant 3$ and

$$a_n=A_{n+1}/A_2, \quad b_n=R_{n-1}/R_0, \quad c_n=f_n/f_1.$$

The determinant of Eqs. (38) with respect to a_n, b_n, c_n is a multiple (with a nonzero coefficient) of

$$n[\overline{d}(n^2-2n-7)+n^2-9]. \tag{39}$$

This quantity is nonzero for all values of $\overline{d}$ and n of interest: it is negative for $n=3$ and positive for $n>3$. Therefore Eqs. (38) can be consecutively solved for all n, leading to a C^∞ solution to the field equations (19)–(21). The proof is completed. □

Thus the only kind of STT configurations admitting CC-II is a $D\geqslant 4$ Kantowski–Sachs cosmology consisting of two T-regions (in fact, epochs, since ρ is a temporal coordinate), separated by a second-order horizon. The qualitative behavior of the metric function $\mathcal{A}(q)$ is shown by the curve 6b in Fig. 1, and the Carter–Penrose diagram is 6b in Fig. 2. We shall see in the next section that this conclusion does not change even if the same solution undergoes one more CC.

Unlike CC-I, the present case requires specific properties of the potential U. It cannot vanish everywhere, but must behave as const$\cdot(\phi-\phi_0)$ near ϕ_0.

Moreover, when these requirements are satisfied, the solution that realizes a CC-II is even more special than in CC-I. Indeed, in the above series expansion, only the constant f_1 is arbitrary, whereas A_2 and R_0 are expressed via U_{f0}, a constant depending on the potential in the theory chosen.

V. GLOBAL PROPERTIES OF CONFORMALLY CONTINUED SOLUTIONS

A. Horizon dispositions

A solution to the STT equations may *a priori* undergo a number of CCs, so that each region of $\mathbb{M}_\mathrm{J}$ between adjacent surfaces $\mathbb{S}_\mathrm{trans}$ is conformally equivalent to some $\mathbb{M}_\mathrm{E}$. However, the global properties of $\mathbb{M}_\mathrm{J}$ with CCs turn out to be not so diverse as one might expect. The main restriction is that Theorems 2 and 2a on horizon dispositions, which have been proved for $\mathbb{M}_\mathrm{E}$, actually hold in $\mathbb{M}_\mathrm{J}$.

A key point for proving this is the observation that the quantity $B=A/r^2=\mathcal{A}/R^2$ is insensitive to conformal mappings and is thus common to $\mathbb{M}_\mathrm{J}$ and $\mathbb{M}_\mathrm{E}$ equivalent to a given part of $\mathbb{M}_\mathrm{J}$. We have here presented B in terms of the metrics (11) and (17), respectively, so that it may be treated as a function of the quasiglobal coordinates ρ in $\mathbb{M}_\mathrm{E}$ or q in $\mathbb{M}_\mathrm{J}$.

A horizon of order k in $\mathbb{M}_\mathrm{J}$ is evidently a zero of the same order of the function $B(q)$, and between zeros (if more than one) there must be maxima and minima. Theorem 2 rests on the fact that $B(\rho)$ cannot have a regular minimum in $\mathbb{M}_\mathrm{E}$ due to Eq. (22). Hence it follows that $B(q)$ cannot have a regular minimum in any region of $\mathbb{M}_\mathrm{J}$ equivalent to a particular $\mathbb{M}_\mathrm{E}$. A minimum can thus take place only on a transition surface $\mathbb{S}_\mathrm{trans}$ between two such regions. Consider Eq. (21) rewritten in terms of $B(q)$ [an analogue of (22) in $\mathbb{M}_\mathrm{J}$]:

$$f[R^4 B_{qq} + (\overline{d}+2)R^3 R_q B_q + 2(\overline{d}-1)] + R^4 f_q B_q = 0. \tag{40}$$

Assuming that $q=0$ is $\mathbb{S}_{\text{trans}}$ and simultaneously an extremum of $B(q)$ and taking into account Theorems 3 and 4, we can suppose that the Taylor expansions of B, f, R near $q=0$ begin with the terms

$$\begin{aligned} B &= B_0 + \tfrac{1}{2} B_2 q^2 + \cdots, \\ f &= f_1 q + \cdots, \\ R &= R_0 + R_1 q + \cdots, \end{aligned} \tag{41}$$

with nonzero f_1 and R_0. Substituting (41) into (40), we find in the senior order of magnitude $O(q)$:

$$B_2 = -(\overline{d}-1)/R_0^4. \tag{42}$$

Thus $q=0$ is a maximum of $B(q)$—in particular, if $B_0=0$, we are dealing with CC-II, and $\mathbb{S}_{\text{trans}}$ separates two T-regions.

The lack of minima of $B(q)$ means that there can be at most two simple zeros, with $B>0$ between them, or one double zero outside which $B<0$.

We thus obtain the following theorem, extending Theorem 2 to Jordan frames of arbitrary STT:

Theorem 5: *In the theory (2), $D \geqslant 4$, under the conditions $l(\phi)>0$ and $h(\phi)>0$, configurations with the metric (17) and the field $\phi=\phi(q)$ can have at most two simple horizons (and there is then an* R*-region between them), or one double horizon separating two* T*-regions.*

There certainly can be a single simple horizon, as in the Schwarzschild or de Sitter space–times, or no horizons at all. Theorem 5 means that, precisely as in GR, the list of possible causal structures of scalar-vacuum configurations in STT is exhausted by the list presented in Sec. III for systems with a cosmological constant in D-dimensional GR.

The situation is still simpler for $D=3$: in this case a CC (more precisely, CC-I) is only possible under the condition $B=\text{const}\neq 0$, which excludes horizons. A single horizon can exist, but there is then no CC.

B. Multiple CCs, singularities and wormholes

A full classification of STT solution behaviors is beyond the scope of this article; we will instead outline some new features appearing in STT formulated in $\mathbb{M}_{\text{J}}$ as compared with GR or with the Einstein-frame formulation of STT, in particular, in connection with conformal continuations. For simplicity, we will use the STT parametrization such that $h\equiv 1$.

A singularity in $\mathbb{M}_{\text{J}}$ can emerge due to the behavior of the conformal factor $F=|f|^{-2/\overline{d}}$ at points where $\mathbb{M}_{\text{E}}$ is regular. The most evident case is that $f\to\infty$ at some value of ϕ, then $F\to 0$, and we obtain both $\mathcal{A}=g_{tt}\to 0$ and $R^2=g_{\theta\theta}\to 0$.

Two kinds of singularities can appear in an ''anti-gravitational'' region where $f<0$, that is, beyond a CC surface. The first one occurs if ϕ blows up while ψ is finite. Using the relation (6) between ϕ and ψ, one easily finds that this is only possible when, at large $|\phi|$,

$$f(\phi) \approx -\frac{D-2}{4(D-1)}\phi^2, \tag{43}$$

i.e., when the ϕ field is asymptotically conformally coupled to the curvature. The singularity is then again connected with $F\to 0$ that leads to zero $A(q)$ and $R(q)$.

Another kind of singularity is more generic and occurs where

$$l(\phi)=f+\frac{D-1}{D-2}\left(\frac{df}{d\phi}\right)^2\to 0. \tag{44}$$

Recall that we adhere to the assumption $l>0$ in the whole article. In the case (44), the conformal factor F is finite provided $f\neq 0$ but its derivatives generically blow up:

$$\frac{dF}{du}=-\frac{2}{\overline{d}\sqrt{l(\phi)}}\frac{df}{d\phi}\frac{d\psi}{du}$$

(u is any admissible coordinate in $\mathbb{M}_{\rm E}$), which can only be finite if $d\psi/du\to 0$ at the same u. So, a value of ϕ where $l\to 0$ is generically a singular sphere of finite radius. Recall also Eq. (28) showing that, again generically, the scalar curvature $\mathcal{R}$ is infinite where $l=0$. Special solutions where such a sphere is regular are not completely excluded but are not considered here.

Under the assumption $l>0$, *there cannot be more than two values of* ϕ *where CCs are possible*, i.e., those where $f=0$ and $df/d\phi\neq 0$; if they do exist, one has $f>0$ between them. Indeed, if the function $f(\phi)<0$ between two zeros, it has to pass a minimum where $df/d\phi=0$, hence $l<0$, contrary to our assumption.

This does not mean, however, that a STT solution cannot contain more than two CCs. The point is that ϕ as a function of the radial coordinate is not necessarily monotonic, so there can be two or more CCs corresponding to the same value of ϕ; see the second example in Sec. VI. But there can be no more than one CC-II due to Theorem 5: other CCs in the same solution, if any, belong to type CC-I and occur in a T-region.

Though, multiple CCs can appear in rather special (if not artificial) situations since the very existence of a CC imposes restrictions on the solution parameters, such as (30) for CC-I. A transition surface $\mathbb{S}_{\rm trans}\in\mathbb{M}_{\rm J}$ corresponds to a singularity $r=0$ in $\mathbb{M}_{\rm E}$, therefore an Einstein-frame manifold $\mathbb{M}_{\rm E}$, describing a region between two transitions, should contain ''two centers,'' more precisely, two values of the radial coordinate (say, ρ) at which $r(\rho)=0$. This property, resembling that of a closed cosmological model, is quite generic due to $r''\leqslant 0$ in Eq. (14), but a special feature is that the conditions (30) should hold at both centers.

Another generic (and more usual) behavior of $\mathbb{M}_{\rm E}$ is that r varies from zero to infinity. Let there be a family of such static solutions and an STT with $f(\phi)$ having a simple zero. Then, by Theorem 3, there is a subfamily of solutions admitting CC-I. A particular solution from this subfamily can come beyond $\mathbb{S}_{\rm trans}$ either to one of the above-mentioned types of singularities, or, if ''everything is quiet,'' to another spatial asymptotic and will then describe a static, traversable wormhole. Each of the asymptotics can be either flat [if $U(\phi)\to 0$], or anti-de Sitter [if $U(\phi)\to$const<0]. Thus wormholes are among generic structures that emerge due to conformal continuations.

VI. EXAMPLES

We will present two explicit examples of configurations with CC-I. The first example is well known and is given here to illustrate the generic character of wormholes appearing due to CC. The second one is a three-dimensional periodic structure with an infinite sequence of CCs.

A. Conformal scalar field in GR

Conformal scalar field in GR can be viewed as a special case of STT, such that, in Eq. (2), $D=4$ and

$$f(\phi)=1-\phi^2/6,\quad h(\phi)=1,\quad U(\phi)=0. \tag{45}$$

After the transformation (5) $g_{\mu\nu}=F(\psi)\overline{g}_{\mu\nu}$ with

$$\phi=\sqrt{6}\tanh(\psi+\psi_0)/\sqrt{6}),\quad \psi_0=\text{const},$$
$$F(\psi)=\cosh^2[(\psi+\psi_0)/\sqrt{6}], \tag{46}$$

we obtain the action (1) with $D=4$ and $V\equiv 0$, describing a minimally coupled massless scalar field in GR. The corresponding static, spherically symmetric solution is well known: it is the Fisher solution.[23] In terms of the harmonic radial coordinate $u\in\mathbb{R}_+$, specified by the condition $g_{uu}=-g_{tt}(g_{\theta\theta})^2$, the solution is[5]

$$ds_{\mathrm{E}}^2=\mathrm{e}^{-2mu}dt^2-\frac{k^2\mathrm{e}^{2mu}}{\sinh^2(ku)}\left[\frac{k^2du^2}{\sinh^2(ku)}+d\Omega^2\right],$$
$$\psi=Cu, \tag{47}$$

where $d\Omega^2=d\theta^2+\sin^2\theta d\varphi^2$, m (the mass), C (the scalar charge), $k>0$ and u_0 are integration constants, and k is expressed in terms of m and C:

$$k^2=m^2+C^2/2. \tag{48}$$

In the case $C=0$, $k=m$ we recover the Schwarzschild solution, as is easily verified using the coordinate $\rho=2k/(1-\mathrm{e}^{-2ku})$. The metric (47) takes the form (11) with $A(\rho)=(1-2k/\rho)^{m/k}$ and $r^2(\rho)=\rho^2(1-2k/\rho)^{1-m/k}$.

Another convenient form of the solution is obtained in isotropic coordinates: with $y=\tanh(ku/2)$, Eqs. (47) are converted to

$$ds_{\mathrm{E}}^2=A(y)dt^2-\frac{k^2(1-y^2)^2}{y^4A(y)}(dy^2+y^2d\Omega^2),$$
$$A(y)=\left|\frac{1-y}{1+y}\right|^{2m/k},\quad \psi=\frac{C}{k}\ln\left|\frac{1+y}{1-y}\right|. \tag{49}$$

The solution is asymptotically flat at $u\to 0$ ($y\to 0$), has no horizon when $C\neq 0$ (as should be the case according to the no-hair theorem) and is singular at the center ($u\to\infty$, $y\to 1-0$, $\psi\to\infty$).

A feature of importance is the invariance of (49) under the inversion $y\mapsto 1/y$, noticed probably for the first time by Mitskevich.[24] Due to this invariance, the solution (49) considered in the range $y>1$ describes quite a similar configuration, but now $y\to\infty$ is a flat asymptotic and $y\to 1+0$ is a singular center. An attempt to unify the two ranges of y is meaningless due to the singularity at $y=1$. We shall see that such a unification, leading to a wormhole, is achieved when the singularity is smoothed out in $\mathbb{M}_{\mathrm{J}}$ in case $C=\sqrt{6}m$ due to the conformal factor.

The Jordan-frame solution for (45) is described by the metric $ds^2=F(\psi)ds_{\mathrm{E}}^2$ and the ϕ field according to (46). It is the conformal scalar field solution,[4,25] its properties are more diverse and can be described as follows (putting, for definiteness, $m>0$ and $C>0$):

(**1**) $C<\sqrt{6}m$. The metric behaves qualitatively as in the Fisher solution: it is flat at $y\to 0$ ($u\to 0$), and both g_{tt} and $r^2=|g_{\theta\theta}|$ vanish at $y\to 1$ ($u\to\infty$)—a singular attracting center. A difference is that here the scalar field is finite: $\phi\to\sqrt{6}$.

(**2**) $C>\sqrt{6}m$. Instead of a singular center, at $y\to 1$ ($u\to\infty$) one has a repulsive singularity of infinite radius: $g_{tt}\to\infty$ and $r^2\to\infty$. Again $\phi\to\sqrt{6}$.

(**3**) $C=\sqrt{6}m$, $k=2m$. Now the metric and ϕ are regular at $y=1$; this is $\mathbb{S}_{\mathrm{trans}}$, and the coordinate y provides a continuation. The solution acquires the form

$$ds^2=\frac{(1+yy_0)^2}{1-y_0^2}\left[\frac{dt^2}{(1+y)^2}-\frac{m^2(1+y)^2}{y^4}(dy^2+y^2d\Omega^2)\right],$$
$$\phi=\sqrt{6}\,\frac{y+y_0}{1+yy_0}, \tag{50}$$

where $y_0=\tanh(\psi_0/\sqrt{6})$. The range $u\in\mathbb{R}_+$, describing the whole manifold $\mathbb{M}_E$ in the Fisher solution, corresponds to the range $0<y<1$, describing only a region $\mathbb{M}_J'$ of the manifold $\mathbb{M}_J$ of the solution (50). The properties of the latter depend on the sign of y_0.[5] In all cases, $y=0$ corresponds to a flat asymptotic, where $\phi\to\sqrt{6}y_0$, $|y_0|<1$.

(**3a**) $y_0<0$. The solution is defined in the range $0<y<1/|y_0|$. At $y=1/|y_0|$, there is a naked attracting central singularity: $g_{tt}\to 0$, $r^2\to 0$, $\phi\to\infty$. Such singularities have been mentioned in Sec. V B as a characteristic feature of solutions for conformally and asymptotically conformally coupled scalar fields, see Eq. (43).

(**3b**) $y_0>0$. The solution is defined in the range $y\in\mathbb{R}_+$. At $y\to\infty$, we find another flat spatial infinity, where $\phi\to\sqrt{6}/y_0$, $r^2\to\infty$ and g_{tt} tends to a finite limit. This is a *wormhole solution*, found for the first time in Ref. 5 and recently discussed by Barcelo and Visser.[9]

(**3c**) $y_0=0$, $\phi=\sqrt{6}y$, $y\in\mathbb{R}_+$. In this case it is helpful to pass to the conventional coordinate r, substituting $y=m/(r-m)$. The solution

$$ds^2=(1-m/r)^2dt^2-\frac{dr^2}{(1-m/r)^2}-r^2d\Omega^2,$$
$$\phi=\sqrt{6}m/(r-m) \tag{51}$$

is the well-known BH with a conformal scalar field.[4,25] The infinite value of ϕ at the horizon $r=m$ does not make the metric singular since, as is easily verified, the energy-momentum tensor remains finite there. This solution turns out to be unstable under radial perturbations.[26]

Case 3 belongs to variant III in the classification of Sec. III B, and the whole manifold $\mathbb{M}_J$ can be represented as the union

$$\mathbb{M}_J=\mathbb{M}_J'\cup\mathbb{S}_{\rm trans}\cup\mathbb{M}_J'', \tag{52}$$

where $\mathbb{M}_J'$ is the region $y<1$, which is, according to (46), in one-to-one correspondence with the manifold $\mathbb{M}_E$ of the Fisher solution (47). The "antigravitational" [$f(\phi)<0$] region $\mathbb{M}_J''$ ($y>1$) is in similar correspondence with another "copy" of the Fisher solution, where, instead of (46),

$$\phi=\sqrt{6}\coth(\psi/\sqrt{6}),\quad F(\psi)=\sinh^2(\psi/\sqrt{6}). \tag{53}$$

Static wormhole solutions have also been found[9] for more general nonminimally coupled massless scalar fields in GR, represented as STT where

$$f(\phi)=1-\xi\phi^2,\quad h(\phi)=1,\quad U(\phi)=0 \tag{54}$$

with $\xi=\text{const}>0$. In full agreement with the observations of Sec. V B, there appear wormholes similar to (50), but, in the case $\xi<\frac{1}{6}$, some of the conformally continued solutions possess singularities connected with $l(\phi)=1-\xi(1-6\xi)\phi^3\to 0$. In the case $\xi>\frac{1}{6}$ all continued solutions describe wormholes.

All the wormhole solutions mentioned in this section prove to be unstable under radial perturbations,[27] which seems to be a common feature of transitions to regions with $f<0$, where the effective gravitational constant becomes negative. This problem deserves further study. A similar instability was pointed out by Starobinsky[28] for cosmological models with conformally coupled scalar fields.

B. A solution with multiple CCs

Trying to obtain a simple analytical solution, we choose $D=3$ and the functions $f(\phi)$ and $h(\phi)$ in the action (2) corresponding to conformal coupling:

$$f(\phi)=1-\phi^2/8, \quad h(\phi)\equiv 1. \tag{55}$$

The $\phi-\psi$ connection according to (6) (with a proper choice of the integration constant) and the conformal factor $F(\psi)$ in (5) may be written as

$$\begin{gathered}\phi=\sqrt{8}\tanh(\psi/\sqrt{8}),\\ F(\psi)=\cosh^2(\psi/\sqrt{8}) \quad \text{for} \quad \phi^2<8,\end{gathered} \tag{56}$$

$$\begin{gathered}\phi=\sqrt{8}\coth(\psi/\sqrt{8}),\\ F(\psi)=\sinh^2(\psi/\sqrt{8}) \quad \text{for} \quad \phi^2>8.\end{gathered} \tag{57}$$

A solution in $\mathbb{M}_{\mathrm{J}}$, including regions with $|\phi|$ larger and smaller than $\sqrt{8}$, is built from solutions in different $\mathbb{M}_{\mathrm{E}}$ with CC through the surfaces $\mathbb{S}_{\mathrm{trans}}$ on which $\phi^2=8$.

Let us first construct a solution in the Einstein frame, to be put into correspondence to any of the regions (56) and (57) in $\mathbb{M}_{\mathrm{J}}$, in such a way as to avoid $\psi=0$, since otherwise we shall encounter a singularity due to $F(\psi)=0$ in the region (57). We will use the metric in the form (11) and Eqs. (13)–(15) with $\overline{d}=1$.

As follows from the aforesaid, to provide a CC we must choose a solution to (15) in the form

$$A(\rho)=c_A r^2(\rho), \quad c_A=\text{const}, \tag{58}$$

where $c_A>0$ and $c_A<0$ correspond to static and cosmological solutions, respectively.

By (31), near $\mathbb{S}_{\mathrm{trans}}$ ($\rho=\rho_c$) the function $r(\rho)$ behaves as $(\rho-\rho_c)^{1/D}$. Accordingly, let us choose this function as follows:

$$\begin{gathered}r(\rho)=r_0(1-x^4)^{1/3}, \quad x=\rho/\rho_0,\\ \rho_0=\text{const}>0.\end{gathered} \tag{59}$$

Thus a CC-I can occur at $x=\pm 1$.

Now, Eq. (14) makes it possible to find $\psi(\rho)$, or equivalently $\psi(x)$:

$$\pm 3\frac{d\psi}{dx}=\frac{2x\sqrt{9-x^4}}{1-x^4}. \tag{60}$$

Choosing the plus sign and integrating, we find

$$\psi(x)=-\frac{\sqrt{2}}{3}\ln(1-x^2)+\psi_1(x)+\psi_0, \tag{61}$$

where ψ_0 is an integration constant while the function ψ_1 is analytic and finite for all $|x|\leqslant 1$:

$$\psi_1(x)=\arcsin(x^2/3)+\sqrt{2}\ln\frac{(1+x^2)[9-x^2+\sqrt{8(9-x^4)}]}{9+x^2+\sqrt{8(9-x^4)}}. \tag{62}$$

The potential $V(\psi)$ as a function of x is found from (13):

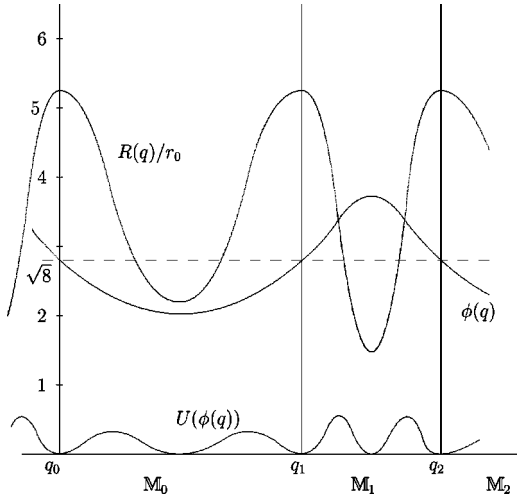

FIG. 3. The behavior of $\phi(q)$, $R(q)$, $U(\phi(q))$ in the model of Sec. VI B with multiple CCs, in the case $\psi_0=\sqrt{8}$, on a segment of the infinite sequence of regions $\mathbb{M}_i$. The latter are separated by vertical lines $q=q_i$ corresponding to the surfaces $\mathbb{S}_{\text{trans}}$. The potential $U(\phi)$ is shown in an arbitrary scale.

$$V(\psi)=2\,\frac{c_A r_0^2}{\rho_0^2}\,\frac{x^2}{(1-x^4)^{1/3}}. \tag{63}$$

This completes the solution in $\mathbb{M}_{\text{E}}$, specified in the range $-1<x<1$. All the constituent functions are even. The potential $V(\psi)$ is well-defined due to monotonicity of $\psi(x)$ in each half-range $0<|x|<1$. At possible CCs, $x=\pm 1$, $\psi\to\infty$, and the minimum value of ψ is $\psi(0)=\psi_0$; assuming $\psi_0>0$, we make sure that $\psi>0$ everywhere.

The corresponding solutions in the Jordan frame are different for $\phi<\sqrt{8}$ and $\phi>\sqrt{8}$, according to (56) and (57) where we put for certainty $\phi>0$.

The solution in $\mathbb{M}_{\text{J}}$ for $\phi<\sqrt{8}$, obtained from $\mathbb{M}_{\text{E}}$ using (56), occupies in $\mathbb{M}_{\text{J}}$ a certain region $\mathbb{M}_0$ parametrized by $x\in(-1.+1)$. The solution can be continued through the surface, say, $x=1$ to $\phi>\sqrt{8}$; to do that one can, i.e., consider the metric coefficients as functions of ϕ and analytically continue them beyond the value $\phi=\sqrt{8}$. However, one cannot do that explicitly since the transcendental equation (61) cannot be resolved with respect to x.

In the new region $\mathbb{M}_1$, which can again be parametrized by $x\in(-1,+1)$, another ''copy'' of the Einstein-frame solution (58)–(63) is valid. To make sure that this is the same solution as the one used in $\mathbb{M}_0$, let us consider the transition between them and recall the proof of Theorem 3 (sufficiency). Namely, there is a unique solution in $\mathbb{M}_{\text{J}}$ near $\mathbb{S}_{\text{trans}}$ (in the form of a power series in q) if the functions $f(\phi)$ and $U(\phi)$ and the constants A_0, R_0 and f_1 are specified. In our case $f(\phi)$ is given, and $U(\phi)$ is not known explicitly but its existence follows from the existence of the analytic continuation in terms of ϕ. So it is sufficient to show that the constants A_0, R_0 and f_1, calculated as the limiting values of $\mathcal{A}=AF$, $R=r\sqrt{F}$ and df/dq, respectively, from the two solutions, are finite and coincide with each other. A direct inspection shows that this is indeed the case if all the parameters of the solutions are the same, including ψ_0.

In $\mathbb{M}_1$ the field ϕ reaches its maximum at $x=0$,

$$\phi_{\max}=\sqrt{8}\,\coth(\psi_0/\sqrt{8}), \tag{64}$$

and returns to the value $\sqrt{8}$ on the other end of the region. One more CC leads to one more region M_2 with $\phi<\sqrt{8}$ and so on. The same happens starting from $x=-1$ of the initial region $\mathbb{M}_0$. We obtain *an infinite sequence of regions* M_i, $i\in\mathbb{Z}$, where adjacent regions are connected by CCs. In

regions with even and odd numbers i, one has $\phi<\sqrt{8}$ and $\phi>\sqrt{8}$, respectively. Each region $\mathbb{M}_i \in \mathbb{M}_J$ corresponds to its own Einstein-frame manifold $\mathbb{M}_{Ei}$, described by the solution (58)–(63) with singularities at $x \to \pm 1$.

The whole manifold $\mathbb{M}_J$ can be parametrized by a unique "radial" coordinate: it can be, e.g., the quasiglobal coordinate q used in Theorem 3, or the proper length $\ell = \int dq/\sqrt{\mathcal{A}}$; both quantities take finite values on the transition surfaces from $\mathbb{M}_i$ to $\mathbb{M}_{i+1}$ and change monotonically inside $\mathbb{M}_i$.

The manifold $\mathbb{M}_J$ is thus nonsingular and has the topology $\mathbb{R}\times\mathbb{R}\times\mathbb{S}^1$: an infinitely long static tube with a periodically changing diameter. This is true if $c_A>0$, when we deal with a static model. One can identify any two $\mathbb{M}_i$ with the numbers i of equal parity, and this leads to the topology $\mathbb{R}\times\mathbb{S}^1\times\mathbb{S}^1$, in other words, two-torus times the time axis. If $c_A<0$, then q is a temporal coordinate, ℓ becomes proper time, and the solution describes a $(2+1)$-dimensional cosmology with a periodically and isotropically (since $A \propto R^2$) changing scale factor. The spatial section is $\mathbb{R}\times\mathbb{S}^1$, but any two points on the t axis (t is now spacelike) may be identified, and we obtain a periodically "breathing" two-torus.

The properties of the model are illustrated in Fig. 3.

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On the nonlocal equations and nonlocal charges associated with the Harry Dym hierarchy

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A large class of nonlocal equations and nonlocal charges for the Harry Dym hierarchy is exhibited. They are obtained from nonlocal Casimirs associated with its bi-Hamiltonian structure. The Lax representation for some of these equations is also given. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1512974]

I. INTRODUCTION

The following nonlinear partial differential equation,

$$w_t=(w^{-1/2})_{xxx}, \tag{1}$$

is known as the Harry Dym equation (see Ref. 1 for a review). It can also be written in the following equivalent forms:

$$v_t=\tfrac{1}{4}v^3v_{xxx},$$

$$u_t=(u_{xx}^{-1/2})_x,$$

for $v=-2^{1/3}w^{-1/2}$ and $u_{xx}=w$, respectively. This equation was obtained by Harry Dym and Martin Kruskal as an evolution equation solvable by a spectral problem based on the string equation instead of the Schrödinger equation. This result was reported in Ref. 2 and rediscovered independently in Refs. 3 and 4. The Harry Dym equation shares many of the properties typical of the soliton equations. It is a completely integrable equation which can be solved by the inverse scattering transform.[5–7] It has a bi-Hamiltonian structure and an infinite number of conservation laws and infinitely many symmetries.[8,9]

The nonlinear hyperbolic equation, which we call the Hunter–Zheng equation,

$$(u_t+uu_x)_{xx}=\tfrac{1}{2}(u_x^2)_x,$$

or the nonlocal version

$$w_t=-(\partial^{-2}w)w_x-2(\partial^{-1}w)w \tag{2}$$

for $u_{xx}=w$, has the same bi-Hamiltonian structure as the Harry Dym equation. The complete integrability of (2) was established in Ref. 10 as well its connection with the Camassa–Holm equation;[11] the former is the high-frequency limit of the latter. Due to the presence of the antiderivative ∂^{-1} the Hunter–Zheng equation (2) is nonlocal.

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As we will describe the Harry Dym equation (1) and the Hunter–Zheng equation (2) belong to the same hierarchy of flows, which we will call the Harry Dym hierarchy. The Hunter–Zheng equation is a member of the positive order equations in this hierarchy while the Harry Dym belongs to the negative order equations. Hierarchies of negative order equations were considered previously through the use of the negative powers of the recursion operator.[12–14] Usually, while the positive order equations are local the negative order ones are nonlocal. For the Harry Dym hierarchy we have the opposite situation, all the positive order equations are nonlocal.

We will show the existence of two new hierarchies of integrable nonlocal equations associated with the Harry Dym hierarchy besides the Hunter–Zheng one. In fact the existence of two nonlocal Casimirs operators implies some sort of degeneracy for the positive order equations.

The paper is organized as follows. In Sec. II we review the bi-Hamiltonian formulation of integrable evolution equations emphasizing the role played by the Casimirs or distinguished functionals of the Hamiltonian operators. We find one more nonlocal Casimir for the modified Kortweg–de Vries equation. In Sec. III we obtain new nonlocal equations as well nonlocal charges for the Harry Dym hierarchy. In Sec. IV we discuss the Lax representation of these equations. The conclusions are given in Sec. V.

II. Bi-HAMILTONIAN SYSTEMS AND CASIMIRS

Central to our discussion is the concept of the bi-Hamiltonian formulation of an integrable evolution equation[8,9]

$$u_t = K_1[u] = \mathcal{D}_1 \frac{\delta H_2}{\delta u} = \mathcal{D}_2 \frac{\delta H_1}{\delta u}.$$

Whenever $\mathcal{D}_1$ and $\mathcal{D}_2$ are compatible this implies the existence of an infinite hierarchy of higher order commuting bi-Hamiltonian systems,

$$u_t^{(n)} = K_n[u] = \mathcal{D}_1 \frac{\delta H_{n+1}}{\delta u} = \mathcal{D}_2 \frac{\delta H_n}{\delta u} \quad \text{with} \quad n \in \mathbb{Z}, \tag{3}$$

where the higher order conservation laws $H_n[u]$ are shared by all members of the hierarchy. This hierarchy of equations can be generated by the recursion operator

$$R = \mathcal{D}_2 \mathcal{D}_1^{-1},$$

since

$$K_{n+1} = R K_n.$$

Also, using

$$\frac{\delta H_{n+1}}{\delta u} = R^{\dagger} \frac{\delta H_n}{\delta u}, \tag{4}$$

where $R^{\dagger} = \mathcal{D}_1^{-1} \mathcal{D}_2$ is the adjoint of R, as a recursion scheme we can obtain the higher Hamiltonians H_n.

We call any functional $H_C[u]$ a Casimir (or distinguished functional) of the Hamiltonian operator $\mathcal{D}$ if

$$\mathcal{D} \frac{\delta H_C}{\delta u} = 0.$$

As a consequence any Hamiltonian system having $\mathcal{D}$ as a Hamiltonian operator,

$$u_t = \mathcal{D}\frac{\delta H}{\delta u},$$

has H_C as a conserved charge. In fact

$$\dot{H}_C = \{H_C, H\} = \int \mathrm{d}x \int \mathrm{d}y \, \frac{\delta H_C}{\delta u(x,t)} \{u(x,t), u(y,t)\} \frac{\delta H}{\delta u(y,t)} = -\int \mathrm{d}x \left(\mathcal{D}\frac{\delta H_C}{\delta u} \right) \frac{\delta H}{\delta u} = 0.$$

When one of the conservation laws in (3) is a Casimir, let us say of $\mathcal{D}_1$, the hierarchy of equations stops except if the Hamiltonian operator $\mathcal{D}_2$ has at least one Casimir.

The Kortweg–de Vries (KdV) equation

$$u_t = u_{xxx} + 3uu_x$$

has the following series of conservation laws:

$$H_0 = \int \mathrm{d}x \, u,$$

$$H_1 = \int \mathrm{d}x \, \frac{1}{2}u^2,$$

$$H_2 = \int \mathrm{d}x \, \frac{1}{2}(u^3 - u_x^2),$$

$$\vdots,$$

and the two compatible Hamiltonian operators

$$\begin{aligned} \mathcal{D}_1 &= \partial, \\ \mathcal{D}_2 &= \partial^3 + u\partial + \partial u. \end{aligned} \tag{5}$$

From (3) we get

$$u_t^{(0)} = \mathcal{D}_1\frac{\delta H_1}{\delta u} = \mathcal{D}_2\frac{\delta H_0}{\delta u} = u_x,$$

$$u_t^{(1)} = \mathcal{D}_1\frac{\delta H_2}{\delta u} = \mathcal{D}_2\frac{\delta H_1}{\delta u} = u_{xxx} + 3uu_x,$$

$$u_t^{(2)} = \mathcal{D}_1\frac{\delta H_3}{\delta u} = \mathcal{D}_2\frac{\delta H_2}{\delta u} = u_{xxxxx} + 5uu_{xxx} + 10u_xu_{xx} + \frac{15}{2}u^2u_x,$$

$$\vdots$$

and apparently we cannot extend this recursion procedure for negatives values of n in (3) since H_0 is a Casimir of $\mathcal{D}_1$ and $\mathcal{D}_2$ appears to have only trivial local distinguished functionals [see Eq. (9)]. Now, the modified KdV equation (mKdV)

$$u_t = u_{xxx} + \tfrac{3}{2}u^2u_x$$

has the following bi-Hamiltonian form:

$$u_t = \mathcal{D}_1 \frac{\delta H_2}{\delta u} = \mathcal{D}_2 \frac{\delta H_1}{\delta u},$$

where

$$\begin{aligned} \mathcal{D}_1 &= \partial, \\ \mathcal{D}_2 &= \partial^3 + \partial u \partial^{-1} u \partial, \end{aligned} \tag{6}$$

and

$$H_1 = \int \mathrm{d}x \frac{1}{2} u^2,$$

$$H_2 = \int \mathrm{d}x \left(\frac{1}{8} u^4 - \frac{1}{2} u_x^2 \right).$$

Of course, $H_0 = \int \mathrm{d}x\, u$ is the Casimir of $\mathcal{D}_1$, however $\mathcal{D}_2$ in (6) admits a nontrivial nonlocal Casimir,[15]

$$H_C = \int \mathrm{d}x \cos(\partial_x^{-1} u).$$

Here we will define the skew-adjoint antiderivative ∂^{-1} acting on functions u, which satisfy $u \to 0$ as $|x| \to \infty$, by

$$(\partial_x^{-1} u) \equiv (\partial^{-1} u)(x) = \int_{-\infty}^{+\infty} \mathrm{d}y\, \epsilon(x-y) u(y), \tag{7}$$

where

$$\epsilon(x-y) = \begin{cases} 1/2 & \text{for } x > y, \\ -1/2 & \text{for } x < y. \end{cases}$$

From now on we will omit the x subscript in (7). It is easy to verify that for functions A and B of u we have the property

$$\int \mathrm{d}x\, A(\partial^{-1} B) = -\int \mathrm{d}x (\partial^{-1} A) B.$$

Now

$$\frac{\delta H_C}{\delta u} = \partial^{-1}(\sin(\partial^{-1} u))$$

and it is easy to show that $\mathcal{D}_2(\delta H_C / \delta u) = 0$. From (3) we get, for $n = -1, -2, \ldots$, a hierarchy of negative order equations

$$
\begin{aligned}
u_t^{(0)} &= \mathcal{D}_1 \frac{\delta H_1}{\delta u} = \mathcal{D}_2 \frac{\delta H_0}{\delta u} = u_x, \\
u_t^{(-1)} &= \mathcal{D}_1 \frac{\delta H_0}{\delta u} = \mathcal{D}_2 \frac{\delta H_{-1}}{\delta u} = 0, \\
u_t^{(-2)} &= \mathcal{D}_1 \frac{\delta H_{-1}}{\delta u} = \mathcal{D}_2 \frac{\delta H_{-2}}{\delta u} = \sin(\partial^{-1} u), \\
&\vdots
\end{aligned}
\tag{8}
$$

where $H_{-1} \equiv H_C$. Introducing the potential function $\psi_x = u$ the last equation in (8) is the sine-Gordon equation

$$\psi_{xt} = \sin \psi.$$

Besides H_0 and H_C we have found that the Hamiltonian operator $\mathcal{D}_2$ also has the following nonlocal Casimir:

$$H_C' = \int \mathrm{d}x \sin(\partial^{-1} u)(\partial^{-1} \cos(\partial^{-1} u)),$$

which will generate another negative order hierarchy of equations.

Returning to the KdV equation, if we set

$$u = -2 \psi^{-1} \psi_{xx},$$

the second Hamiltonian structure in (5) can be written as

$$\mathcal{D}_2 = \psi^{-2} \partial \psi^2 \partial \psi^2 \partial \psi^{-2},$$

and it follows that

$$\psi^2, \quad \psi^2(\partial^{-1} \psi^{-2}), \quad \psi^2 \partial^{-1}(\psi^{-2}(\partial^{-1} \psi^{-2})) \tag{9}$$

are non trivial kernels of $\mathcal{D}_2$. We will not discuss this system here but the Casimirs associated with (9) will give rise to nonlocal KdV hierarchies of equations (see Refs. 12–14, and references therein) and nonlocal charges. Instead, we will perform this analysis in a systematic way for the Harry Dym hierarchy in Sec. III.

III. THE HARRY DYM HIERARCHY

The Harry Dym equation (1) is a completely integrable bi-Hamiltonian system[8,9]

$$w_t = \mathcal{D}_1 \frac{\delta H_{-1}}{\delta w} = \mathcal{D}_2 \frac{\delta H_{-2}}{\delta w},$$

where

$$
\begin{aligned}
\mathcal{D}_1 &= \partial^3, \\
\mathcal{D}_2 &= w \partial + \partial w,
\end{aligned}
\tag{10}
$$

and

$$H_{-1}=\int \mathrm{d}x(2w^{1/2}),$$

$$H_{-2}=\int \mathrm{d}x\left(\frac{1}{8}w^{-5/2}w_x^2\right).$$

It is well known that H_{-1} is a Casimir of $\mathcal{D}_2$ and that

$$H_0=-\int \mathrm{d}x\, w \tag{11}$$

is a Casimir of $\mathcal{D}_1$. So, we can consider equations going ''up'' and ''down'' in Eq. (3). However, we also have the following nonlocal Casimirs for $\mathcal{D}_1$:

$$\begin{aligned} H_0^{(1)}&=\int \mathrm{d}x(\partial^{-1}w),\\ H_0^{(2)}&=\int \mathrm{d}x(\partial^{-2}w). \end{aligned} \tag{12}$$

In this way (3) gets degenerated for $n>0$,

$$\vdots$$

$$\begin{aligned} w_t^{(2,\alpha)}&=\mathcal{D}_1\frac{\delta H_2^{(\alpha)}}{\delta w}=\mathcal{D}_2\frac{\delta H_1^{(\alpha)}}{\delta w},\\ w_t^{(1,\alpha)}&=\mathcal{D}_1\frac{\delta H_1^{(\alpha)}}{\delta w}=\mathcal{D}_2\frac{\delta H_0^{(\alpha)}}{\delta w},\\ w_t^{(0)}&=\mathcal{D}_1\frac{\delta H_0^{(\alpha)}}{\delta w}=\mathcal{D}_2\frac{\delta H_{-1}}{\delta w}=0,\\ w_t^{(-1)}&=\mathcal{D}_1\frac{\delta H_{-1}}{\delta w}=\mathcal{D}_2\frac{\delta H_{-2}}{\delta w}=(w^{-1/2})_{xxx},\\ &\vdots, \end{aligned} \tag{13}$$

where $\alpha=0$, 1, 2 and $H_0^{(0)}=H_0$.

Using (4) and (13) as a recursion scheme we can obtain, after a straightforward but tedious calculation, the first few Hamiltonian functionals and flows for the Harry Dym hierarchy equations. For $n\leqslant 0$ the first conserved charges, some of them already calculated in Ref. 10, are

$$H_0=H_0^{(0)}=\int \mathrm{d}x(-w),$$

$$H_{-1}=\int \mathrm{d}x\, 2w^{1/2},$$

$$H_{-2}=\int \mathrm{d}x\,\frac{1}{8}w^{-5/2}w_x^2,$$

$$H_{-3}=\int \mathrm{d}x\,\frac{1}{16}\left(\frac{35}{16}w^{-11/2}w_x^4-w^{-7/2}w_{xx}^2\right), \tag{14}$$

$$H_{-4}=\int \mathrm{d}x\,\frac{1}{32}\left(\frac{5005}{128}w^{-17/2}w_x^6-\frac{231}{8}w^{-13/2}w_x^2w_{xx}^2+5w^{-11/2}w_{xx}^3+w^{-9/2}w_{xxx}^2\right),$$

$$\vdots$$

and the first flows are

$$w_t^{(0)}=0,$$

$$w_t^{(-1)}=(w^{-1/2})_{xxx},$$

$$w_t^{(-2)}=\tfrac{1}{4}(\tfrac{5}{4}w^{-7/2}w_x^2-w^{-5/2}w_{xx})_{xxx}, \tag{15}$$

$$w_t^{(-3)}=\tfrac{1}{16}(\tfrac{1155}{32}w^{-13/2}w_x^4-\tfrac{231}{4}w^{-11/2}w_x^2w_{xx}+\tfrac{21}{2}w^{-9/2}w_{xx}^2+14w^{-9/2}w_{xxx}w_x-2w^{-7/2}w_{xxxx})_{xxx},$$

$$\vdots.$$

For $n>0$ we have to consider the three cases $\alpha=0$, 1, 2 separately. So, for $\alpha=0$ we get the nonlocal conserved charges

$$H_1^{(0)}=\int \mathrm{d}x\,\frac{1}{2}(\partial^{-1}w)^2,$$

$$H_2^{(0)}=\int \mathrm{d}x\,\frac{1}{2}(\partial^{-2}w)(\partial^{-1}w)^2,$$

$$H_3^{(0)}=\int \mathrm{d}x\left[\frac{1}{4}(\partial^{-2}w)^2(\partial^{-1}w)^2+\frac{1}{8}(\partial^{-1}(\partial^{-1}w)^2)^2\right], \tag{16}$$

$$H_4^{(0)}=\int \mathrm{d}x\left[\frac{1}{12}(\partial^{-2}w)^3(\partial^{-1}w)^2-\frac{1}{4}(\partial^{-1}w)^2\partial^{-2}((\partial^{-2}w)(\partial^{-1}w)^2)\right.$$
$$\left.-\frac{1}{8}(\partial^{-2}w)(\partial^{-1}(\partial^{-1}w)^2)^2\right],$$

$$H_5^{(0)}=\int \mathrm{d}x\Big[\frac{1}{48}(\partial^{-2}w)^4(\partial^{-1}w)^2-\frac{1}{8}(\partial^{-2}w)^2(\partial^{-1}w)^2(\partial^{-2}(\partial^{-1}w)^2)$$
$$-\frac{1}{16}(\partial^{-2}w)^2(\partial^{-1}(\partial^{-1}w)^2)^2+\frac{1}{16}(\partial^{-2}(\partial^{-1}w)^2)^2(\partial^{-1}w)^2$$
$$+\frac{1}{16}(\partial^{-1}w)^2(\partial^{-2}(\partial^{-1}(\partial^{-1}w)^2)^2)+\frac{1}{8}(\partial^{-1}((\partial^{-1}w)\partial^{-1}(\partial^{-1}w)^2))^2\Big],$$
$$\vdots,$$

and the first flows are

$$\begin{gathered} w_t^{(1,0)}=-w_x, \\ w_t^{(2,0)}=-(\partial^{-2}w)w_x-2(\partial^{-1}w)w, \\ w_t^{(3,0)}=-\tfrac{1}{2}(\partial^{-2}w)^2w_x-2(\partial^{-2}w)(\partial^{-1}w)w+\tfrac{1}{2}(\partial^{-2}(\partial^{-1}w)^2)w_x+w(\partial^{-1}(\partial^{-1}w)^2), \\ \vdots. \end{gathered} \tag{17}$$

Note that the flow $w_t^{(2,0)}$ is the Hunter–Zheng equation (2).

From (10) we can construct the recursion operator

$$R=\mathcal{D}_2\mathcal{D}_1^{-1}=2w\partial^{-2}+w_x\partial^{-3}, \tag{18}$$

and since

$$(\partial w+w\partial)^{-1}=\tfrac{1}{2}w^{-1/2}\partial^{-1}w^{-1/2}$$

we have

$$R^{-1}=\tfrac{1}{2}\partial^3w^{-1/2}\partial^{-1}w^{-1/2}.$$

The flows (15) and (17) can now be expressed as the action of powers of R acting on the seed equation $w_t^{(1,0)}=\mathcal{D}_2\,(\delta H_0^{(0)}/\delta w)=-w_x$,

$$w_t^{(n)}=R^{n-1}(-w_x), \quad n=0,-1,-2,..., \tag{19}$$

$$w_t^{(n,0)}=R^{n-1}(-w_x), \quad n=1,2,3,.... \tag{20}$$

To be able to perform the steps in the iteration given in (19) and (20) we must point out that for any function $f(x,t)$ we can use instead of (7) the representation[16,12,13,14]

$$(\partial^{-1}f)(x,t)=\int_{-\infty}^{+\infty}\mathrm{d}y\;\epsilon(x-y)f(y,t)+c(t),$$

where $c(t)$ is a function of t. Here we set $c=0$ for any f, except $f=0$ where we use $c=2$. In this way,

$$w_t^{(0)}=R^{-1}(-w_x)=0$$

and

$$w_t^{(-1)}=R^{-2}(-w_x)=\tfrac{1}{2}\partial^3w^{-1/2}\partial^{-1}0=(w^{-1/2})_{xxx},$$

resulting in the Harry Dym equation.

For $n>0$ and $\alpha=1, 2$ we have the seed equations

$$w_t^{(1,1)}=\mathcal{D}_2\frac{\delta H_0^{(1)}}{\delta w}=-2w-xw_x,$$
$$w_t^{(1,2)}=\mathcal{D}_2\frac{\delta H_0^{(2)}}{\delta w}=2xw+\frac{x^2}{2}w_x, \tag{21}$$

where we have used $(\partial^{-n}1)=x^n/n$, for $n>0$. The respective flows follow from the analog of (20) and they read for $\alpha=1$,

$$w_t^{(1,1)}=-2w-xw_x,$$
$$w_t^{(2,1)}=-2wx(\partial^{-1}w)-w_x(\partial^{-1}(x(\partial^{-1}w))),$$
$$w_t^{(3,1)}=(2w+w_x\partial^{-1})\left(\frac{x}{2}\partial^{-1}(\partial^{-1}w)^2-(\partial^{-1}w)\partial^{-1}(x(\partial^{-1}w))\right), \tag{22}$$
$$\vdots$$

and for $\alpha=2$,

$$w_t^{(1,2)}=2xw+\frac{x^2}{2}w_x,$$
$$w_t^{(2,2)}=2w(\tfrac{1}{2}x^2(\partial^{-1}w)-(\partial^{-3}w))+w_x\partial^{-1}(\tfrac{1}{2}x^2(\partial^{-1}w)-(\partial^{-3}\omega)),$$
$$w_t^{(3,2)}=(2w+w_x\partial^{-1})\left(\frac{1}{2}\partial^{-1}(\partial^{-2}w)^2+\frac{1}{2}\partial^{-3}(\partial^{-2}w)^2-(\partial^{-4}w)(\partial^{-1}w)-\frac{x^2}{4}\partial^{-1}(\partial^{-1}w)^2\right.$$
$$\left.+\frac{1}{2}(\partial^{-1}w)\partial^{-1}(x^2(\partial^{-1}w))\right), \tag{23}$$
$$\vdots.$$

Again using (4) and (13) recursively we obtain the nonlocal conserved charges

$$H_1^{(1)}=-\frac{1}{2}\int \mathrm{d}x\,\partial^{-1}(\partial^{-1}w)^2,$$
$$H_2^{(1)}=\frac{1}{2}\int \mathrm{d}x\,\partial^{-1}((\partial^{-1}w)\partial^{-1}(\partial^{-1}w)^2),$$
$$H_3^{(1)}=-\frac{1}{2}\int \mathrm{d}x\,\partial^{-1}\left[\frac{1}{4}(\partial^{-1}(\partial^{-1}w)^2)^2+(\partial^{-1}w)\partial^{-1}((\partial^{-1}w)\partial^{-1}(\partial^{-1}w)^2)\right], \tag{24}$$
$$\vdots$$

and

$$H_1^{(2)}=-\frac{1}{2}\int \mathrm{d}x[(\partial^{-2}w)^2+(\partial^{-2}(\partial^{-1}w)^2)],$$

$$H_2^{(2)}=\frac{1}{2}\int \mathrm{d}x\left[\frac{1}{3}(\partial^{-2}w)^3+\partial^{-2}((\partial^{-1}w)(\partial^{-1}(\partial^{-1}w)^2))+(\partial^{-4}w)(\partial^{-1}w)^2\right],$$

$$H_3^{(2)}=-\frac{1}{2}\int \mathrm{d}x\left[\frac{1}{12}(\partial^{-1}w)^4+\frac{1}{4}(\partial^{-2}(\partial^{-1}w)^2)^2+\frac{1}{4}\partial^{-2}(\partial^{-1}(\partial^{-1}w)^2)^2\right.$$
$$+\frac{1}{2}(\partial^{-1}w)^2\partial^{-2}(\partial^{-2}w)^2-(\partial^{-1}w)^2\partial^{-1}((\partial^{-4}w)(\partial^{-1}w))$$
$$\left.+\partial^{-2}((\partial^{-1}w)\partial^{-1}((\partial^{-1}w)(\partial^{-1}(\partial^{-1}w)^2)))\right], \tag{25}$$

$$\vdots.$$

These hierarchies of integrable equations become extremely nonlocal as we proceed further in the recursion. $w_t^{(2,1)}$ and $w_t^{(2,2)}$ are equations of the Hunter–Zheng type. It is interesting to note that Eqs. (17), (22), and (23) are in the positive direction (positive flows) of recursion while the Harry Dym equations (15) are in the negative direction (negative flows). Of course this is due to the fact that the recursion operator (18) is completely nonlocal. That is to be compared with the usual situation we have for the KdV recursion operator $R=\partial^2+2u+u_x\partial^{-1}$.

After obtaining Eqs. (22) and (23) we became aware of Refs. 17 and 18 where these equations are given implicitly in a recursion form. However, we have shown here their origin from the Casimirs (11) and (12).

IV. LAX PAIRS

The equations in the Harry Dym hierarchy are integrable since they are bi-Hamiltonian. Therefore we hope to find a Lax representation for all of them. In fact, the Lax pair for the Harry Dym equation (1) is given by[1,19,20]

$$L=\frac{1}{w}\partial^2, \tag{26}$$

$$B=-2w^{-3/2}\partial^3+\tfrac{3}{2}w^{-5/2}w_x\partial^2,$$

$$\frac{\partial L}{\partial t}=[B,L]. \tag{27}$$

Calculating the square-root of L (aided by a computer algebra program) we obtain

$$L^{1/2}=\beta\partial+a_0+a_1\partial^{-1}+a_2\partial^{-2}+a_3\partial^{-3}+a_4\partial^{-4}+a_5\partial^{-5}+O(\partial^{-6}),$$

where

$$\beta=w^{-1/2},$$

$$a_0=-\tfrac{1}{2}\beta_x,$$

$$a_1=\frac{1}{2^2}\beta_{xx}-\frac{1}{2^3}\beta_x^2\beta^{-1},$$

$$a_2=-\frac{1}{2^3}\beta_{xxx}-\frac{3}{2^4}\beta_x^3\beta^{-2}+\frac{3}{2^3}\beta_x\beta_{xx}\beta^{-1},$$

$$a_3=\frac{1}{2^4}\beta_{xxxx}-\frac{3}{2^3}\beta_x\beta_{xx}\beta^{-1}+\frac{37}{2^5}\beta_x^2\beta_{xx}\beta^{-2}-\frac{61}{2^7}\beta_x^4\beta^{-3}-\frac{13}{2^5}\beta_{xx}^2\beta^{-1},$$

$$a_4=-\frac{1}{2^5}\beta_{(5)}+\frac{5\cdot 7}{2^5}\beta_{xx}\beta_{xxx}\beta^{-1}+\frac{5}{2^4}\beta_x\beta_{xxxx}\beta^{-1}-\frac{3\cdot 5\cdot 7}{2^6}\beta_x^2\beta_{xxx}\beta^{-2}-\frac{3\cdot 5\cdot 13}{2^6}\beta_x\beta_{xx}^2\beta^{-2}$$
$$+\frac{3^2\cdot 5\cdot 7}{2^6}\beta_x^3\beta_{xx}\beta_{-3}-\frac{3\cdot 5\cdot 29}{2^8}\beta_x^5\beta^{-4},$$

$$a_5=\frac{1}{2^6}\beta_{(6)}-\frac{7\cdot 17}{2^7}\beta_{xxx}^2\beta^{-1}-\frac{19}{2^4}\beta_{xx}\beta_{xxxx}\beta^{-1}+\frac{43}{2^2}\beta_{xx}\beta_{xxx}\beta_x\beta^{-2}-\frac{3\cdot 5}{2^6}\beta_x\beta_{(5)}\beta^{-1}$$
$$+\frac{241}{2^7}\beta_x^2\beta_{xxxx}\beta^{-2}-\frac{569}{2^6}\beta_x^3\beta_{xxx}\beta^{-3}+\frac{413}{2^7}\beta_{xx}^3\beta^{-2}-\frac{3\cdot 1973}{2^8}\beta_x^2\beta_{xx}^2\beta^{-3}$$
$$+\frac{3\cdot 4493}{2^9}\beta_x^4\beta_{xx}\beta^{-4}-\frac{7\cdot 17\cdot 67}{2^{10}}\beta_x^6\beta^{-5},$$

where $\beta_{(n)}=\mathrm{d}^n\beta/\mathrm{d}x^n$. Now it can be easily recognized that

$$B=-2(L^{3/2})_{\geqslant 2},$$

and $(\ )_{\geqslant 2}$ stands for the differential part of the pseudodifferential operator with terms ∂^n, $n\geqslant 2$. In this way (27) assumes the nonstandard Lax representation

$$\frac{\partial L}{\partial t}=-2[(L^{3/2})_{\geqslant 2},L]. \tag{28}$$

Similarly the whole negative hierarchy of Eq. (15) can be obtained from

$$\frac{\partial L}{\partial t}=-2^n[(L^{(2n+1)/2})_{\geqslant 2},L],\quad n=0,1,2,\ldots. \tag{29}$$

The charges (14) (except by multiplicative constant factors) follow from

$$H_{-(n+1)}=\mathrm{Tr}L^{(2n-1)/2},\quad n=1,2,3,..., \tag{30}$$

where ''Tr'' is the usual Adler trace.[21] We have used (29) and (30) to perform a check of Eq. (15) and charges (14), respectively.

Through ''gauge transformations'' [22] the Lax representation for the Harry Dym hierarchy (27) and (28) can be brought in other forms. For instance, the Harry Dym equation also follows from

$$L'=\partial L\partial^{-1},$$

with the nonstandard Lax representation

$$\frac{\partial L'}{\partial t}=-2[(L'^{3/2})_{\geqslant 1},L'], \tag{31}$$

or even from a standard Lax representation

$$\frac{\partial L''}{\partial t} = -2[(L''^{3/2})_{\geqslant 0}, L''],$$

with

$$L'' = w^{1/2} L w^{-1/2}.$$

So, for the negative flows of the Harry Dym hierarchy we have a complete Lax representation. However, for the positive flows the Lax representation picture is not so complete. It is easy to check that the Lax operator (26) with

$$\frac{\partial L}{\partial t} = -2[B^{(i,\alpha)}, L], \quad i = 1,2,3,\ldots, \quad \alpha = 0,1,2, \tag{32}$$

yields the first equations $w^{(1,\alpha)}$, for the positive flows (17), (22), and (23), if we choose

$$B^{(1,0)} = \tfrac{1}{2}\partial,$$

$$B^{(1,1)} = -\tfrac{1}{4} + \tfrac{1}{2} x \partial,$$

$$B^{(1,2)} = \tfrac{1}{4} x - \tfrac{1}{4} x^2 \partial,$$

respectively. For the equations $w^{(2,\alpha)}$ in (17), (22), and (23) we have obtained, for $i=2$ in (32), the operators

$$B^{(2,0)} = \tfrac{1}{4}(\partial^{-2} w)\partial + \tfrac{1}{4}\partial^{-1}(\partial^{-2} w)\partial^2,$$

$$B^{(2,1)} = \tfrac{1}{4}(\partial^{-1}(x\partial^{-1} w))\partial + \tfrac{1}{4}\partial^{-1}(\partial^{-1}(x\partial^{-1} w))\partial^2 - \tfrac{1}{4}\partial^{-1}(\partial^{-1} w),$$

$$B^{(2,2)} = \tfrac{1}{4}(\partial^{-1}(\tfrac{1}{2}x^2\partial^{-1} w - \partial^{-3} w))\partial + \tfrac{1}{4}\partial^{-1}(\partial^{-1}(\tfrac{1}{2}x^2\partial^{-1} w - \partial^{-3} w))\partial^2 - \tfrac{1}{4}\partial^{-1} x(\partial^{-1} w) + \tfrac{1}{4}\partial^{-1}(\partial^{-2} w) + \tfrac{1}{8}\partial^{-2} x w.$$

In fact $B^{(2,0)}$ was first obtained in Ref. 10 but in the nonstandard Lax representation (31). An interesting question is how, if possible at all, $B^{(i,\alpha)}$ in (32) and the nonlocal charges $H_n^{(\alpha)}$ in (16), (24), and (25) can be obtained from the same Lax operator (26), i.e., what are the analogs of Eqs. (29) and (30) for the positive Harry Dym flows? In the literature we can find Lax representations for equations obtained by the inverse recursion operator,[23,24] such as of the Harry Dym type. However, these Lax representations are not given only in terms of L and use some sort of ansatz. Also, the authors do not try to obtain the relation between the nonlocal charges and the Lax operator. These intriguing points are under investigation and will appear elsewhere.

V. CONCLUSION

We have given a unified picture of the Harry Dym hierarchy of equations which includes local as well a series of three nonlocal hierarchies of equations. We have shown, using the bi-Hamiltonian formulation of integrable models, how the nonlocal Casimirs lead to these nonlocal equations and also to three series of nonlocal charges. Some of the nonlocal equations and nonlocal charges obtained in this way are new. This procedure can also be applied for the KdV and mKdV equations since both equations, in accordance with the discussion in Sec. II, also have three Casimirs associated with the third-order Hamiltonian operator $\mathcal{D}_2$. We believe that the treatment given here for the Harry Dym hierarchy unifies, within the bi-Hamiltonian formulation of the integrable models, some of the results scattered in the literature. We have also tried to understand these nonlocal equations and charges from a Lax representation. Even though we have found explicitly Lax pairs for some of the positive flows a unique Lax representation is still missing.

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Infinite symmetries and conservation laws

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We will consider partial differential equations of a variational problem whose symmetry group generators contain arbitrary function(s) of one or more independent variables. Unlike the Second Noether Theorem we will be interested in the case of arbitrary functions of not all base variables. We will study the relations between infinite symmetries and local conservation laws. We will demonstrate that infinite symmetries may lead to a finite number of conservation laws through appropriate boundary conditions, or to a set of additional constraints for the function and its derivatives. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1517394]

I. INTRODUCTION

The problem of the relationship between symmetries and conservation laws has a long history starting from the famous work by Emmy Noether.[1] A thorough study of the Noether theory with many references can be found in Ref. 2; see also Refs. 3, 4 and references therein, and the paper by Lanczos.[5] Numerous applications of the Noether Theorem are presented in Ref. 6.

In this paper we will discuss a problem somewhat intermediate between the First and the Second Noether Theorems:[1] the correspondence between infinite-dimensional symmetries and conservation laws. We consider differential equations in R^n that admit infinite symmetry algebras with operators depending on an arbitrary function of independent variables, as well as its derivatives. We will be interested in systems corresponding to a well defined variational (action) functional, where symmetries of the functional (variational or Noether symmetries) are at the same time symmetries of our differential system (see, e.g., Ref. 2). Our goal is to generate conservation laws associated with infinite symmetries through the Noether mechanism. By a conservation law, we will mean such a continuity equation, which leads to nonvanishing conserved (in time) quantity. We will consider a general situation of an arbitrary function of $k<n$ independent variables, or their combinations, for a differential equation with a Lagrangian of any order, and will follow the ideology of Ref. 7 where the case of an arbitrary function of one variable: x or t was studied for first order Lagrangians. We will demonstrate that considered infinite symmetries do not lead to an infinite number of conservation laws. We will also show that boundary conditions determine the existence of a finite number of conservation laws.

The paper is organized as follows.

In Sec. II we review the First and Second Noether Theorems. We point out the essential difference between the case of arbitrary functions of all independent variables of the base space and arbitrary functions of some of the base variables.

In Sec. III we consider the case of an arbitrary function of one independent variable, and introduce a ''strict'' boundary condition as a necessary condition for the existence of conservation laws.

In Sec. IV we analyze the correspondence between infinite symmetries and conservation laws for Lagrangian differential equations of the second order associated with one-dimensional infinite symmetries.

In Sec. V a special situation of an arbitrary function of time is considered and the role of boundary conditions for the generation of conservation laws is discussed.

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In Sec. VI we deal withthe correspondence between infinite symmetries and conservation laws for higher order differential equations.

In Sec. VII the generalizations for arbitrary functions of several variables are discussed.

II. FIRST AND SECOND NOETHER THEOREMS

Let

$$S=\int L(x^i,u,u_i,\ldots)d^nx, \tag{1}$$

be the action functional, where L is the Lagrangian density, $x^i=(x,y,\ldots,t)$, $i=1,...,n$ are independent variables and u is a dependent variable, $u_i\equiv\partial u/\partial x^i$, $u_{ij}\equiv\partial^2 u/\partial x^i\,\partial x^j$. Then

$$E(L)\equiv\omega(x,u,u_i,u_{ij},\ldots)=0 \tag{2}$$

is the equation of motion, where E is the Euler–Lagrange operator,

$$E=\frac{\partial}{\partial u}-D_i\frac{\partial}{\partial u_i}+\sum_{i\leqslant j}D_iD_j\frac{\partial}{\partial u_{ij}}+\cdots. \tag{3}$$

Consider an infinitesimal transformation of the form (see, e.g., Ref. 2)

$$\begin{aligned} x'^i&=x^i+\varepsilon\xi^i(x,u,u_j,\ldots)+O(\varepsilon^2),\\ u'&=u+\varepsilon\eta(x,u,u_j,\ldots)+O(\varepsilon^2), \end{aligned} \tag{4}$$

where ε is a small parameter. The operator corresponding to this transformation is

$$X=\xi^i\frac{\partial}{\partial x^i}+\eta\frac{\partial}{\partial u}+\zeta^i\frac{\partial}{\partial u_i}+\cdots. \tag{5}$$

Instead of X, we consider a canonical operator X_α with $\alpha=\eta-\xi^iu_i$:

$$\begin{aligned} X_\alpha&=\alpha\frac{\partial}{\partial u}+\sum_i(D_i\alpha)\frac{\partial}{\partial u_i}+\sum_{i\leqslant j}(D_iD_j\alpha)\frac{\partial}{\partial u_{ij}}+\cdots,\\ &i,j=1,...,m+1. \end{aligned} \tag{6}$$

In the future we will make use of the Noether identity (see Ref. 8 or Ref. 4, or Ref. 9 for a version used here):

$$X_\alpha=\alpha E+\sum_{i=1}D_iR_{\alpha i}, \tag{7}$$

where

$$\begin{aligned} R_{\alpha i}=&\alpha\frac{\partial}{\partial u_i}+\left\{\sum_{k\geqslant i}(D_k\alpha)-\alpha\sum_{k\leqslant i}D_k\right\}\frac{\partial}{\partial u_{ik}}\\ &+\left\{\sum_{k\geqslant j\geqslant i}(D_jD_k\alpha)-\sum_{k\leqslant i\leqslant j}(D_j\alpha)D_k+\alpha\sum_{j\leqslant k\leqslant i}D_JD_k\right\}\frac{\partial}{\partial u_{ijk}}+\cdots. \end{aligned} \tag{8}$$

Variation of the functional S under a transformation (4) with the symmetry vector α and operator X_α is

$$\delta S = \int [X_\alpha L + D_i(\xi^i L)] d^n x. \tag{9}$$

Let the canonical transformation X_α be a variational (Noether) symmetry,

$$X_\alpha L = D_i M_i . \tag{10}$$

The application of Noether identity (7) to L gives

$$X_\alpha L = \alpha\omega + D_i(R_{\alpha i} L). \tag{11}$$

Combining (11) with (10) we will obtain

$$D_i(M_i - R_{\alpha i} L) = \alpha\omega, \tag{12}$$

meaning that on the solution manifold ($\omega = 0$, $D_i\omega = 0, \ldots$) we get a continuity equation

$$D_i(M_i - R_{\alpha i} L) \doteq 0. \tag{13}$$

Thus, any variational symmetry α (in case of a finite Lie group) leads to a corresponding conservation law (continuity equation) (13); which is a statement of the First Noether Theorem.[1]

Consider now a case of an infinite group where the symmetry vector α is of the form

$$\alpha = a p(x) + b_i D_i p(x) + c_{ij} D_i D_j p(x) + \cdots, \tag{14}$$

with an *arbitrary function* $p(x)$. Applying the Noether identity (7) to L,

$$X_\alpha L = \alpha^b E^b(L) + D_i(R_{\alpha i} L), \tag{15}$$

and transforming the rhs of (15) we obtain

$$\begin{aligned} \alpha^b E^b(L) &= (a^b p + b_i^b D_i p + c_{ij}^b D_i D_j p + \cdots)\omega^b \\ &= p a^b \omega^b + D_i(b_i^b \omega^b p) - p D_i(b_i^b \omega^b) + \cdots \\ &= p(x)\{a^b \omega^b - D_i(b_i^b \omega^b) + D_i D_j(c_{ij}^b \omega^b) + \cdots\} + D_i(b_i^b \omega^b p + \cdots). \end{aligned} \tag{16}$$

Thus,

$$\alpha^b E^b(L) = p(x)\tilde{a}(\omega, D_i\omega, \ldots) + D_i K_i , \tag{17}$$

where $K_i \sim p(x), D_k p(x), \ldots,$ and

$$\tilde{a} = a^b \omega^b - D_i(b_i^b \omega^b) + D_i D_j(c_{ij}^b \omega^b) + \cdots . \tag{18}$$

Since α is a variational symmetry using (10), (15) and (17) we obtain

$$D_i M_i = p(x)\tilde{a} + D_i K_i + D_i(R_{\alpha i} L), \tag{19}$$

or

$$D_i T_i = p(x)\tilde{a}, \tag{20}$$

where $T_i = M_i - K_i - R_{\alpha i} L \sim p(x), D_k p(x), \ldots$. Equation (20) has the form of a continuity equation, but in general for arbitrary $p(x)$ it does not imply a conservation law. Let us integrate (20) over the whole space in R^n and apply the Gauss theorem:

$$\int_D D_i T_i \, dV = \int_{\partial D} T_i n_i \, d\sigma = \int_D p(x) \tilde{a} dV. \tag{21}$$

Consider the following cases.

(I) $p = p(x^1, x^2, \ldots, x^n)$, *where* $p(x)$ *is an arbitrary function of all variables in* R^n.

In this case it is possible to choose the function $p(x)$ such that it vanishes on the boundary together with its derivatives,

$$p(x)|_{\partial D} = D_k p(x)|_{\partial D} = \cdots = 0. \tag{22}$$

Then $T_i|_{\partial D} = 0$. From Eq. (21) using arbitrariness of V we can write

$$D_i T_i = 0, \tag{23}$$

and from (20) we conclude that

$$\tilde{a}(\omega, D_i \omega, \ldots) = 0. \tag{24}$$

Therefore,

$$a^b \omega^b - D_i(b_i^b \omega^b) + D_i D_j (c_{ij}^b \omega^b) + \cdots = 0, \tag{25}$$

where $a^b, b_i^b, c_{ij}^b, \ldots,$ are components of the symmetry α (14). Equation (25) expresses the Second Noether Theorem, which states that in case of an infinite variational symmetry group not all equations of the original differential system are independent.[1]

As an interesting example of the Second Noether Theorem in action, let us consider a consequence of local gauge invariance for the Yang–Mills functional,

$$S = \frac{1}{4} \int G_{\mu\nu}^a G^{a\mu\nu} d^4 x, \tag{26}$$

where

$$G_{\mu\nu}^a = A_{\nu,\mu}^a - A_{\mu,\nu}^a + g g^{abc} A_\mu^b A_\nu^c, \quad A_\mu^a = A_\mu^a(x_\nu), \quad \mu, \nu = 1, \ldots, 4, \quad a, b, c = 1, \ldots, N;$$

g is a coupling constant, g_{abc} are structure constants of the (simple) gauge group H of dimension N [for $H = \mathrm{SU}(2)$: $g_{abc} = \varepsilon_{abc}$; we are using the adjoint representation of H]. The Yang–Mills equations $\omega^{a\mu} \equiv E^{a\mu}(L) = 0$ take the form

$$d_\rho G^{a\mu\rho} + g g^{abc} A_\rho^b G^{c\mu\rho} = 0, \tag{27}$$

or

$$D_\rho G^{a\mu\rho} = 0, \tag{28}$$

where

$$D_\rho = d_\rho + g[A_\rho, \ ] = d_\rho + g g^{abc} A_\rho^b \tag{29}$$

is the covariant derivative operator, and $d_\rho \equiv d/dx^\rho$. The Yang–Mills equations (27) are invariant under a local gauge transformation,

$$A_\mu^a \to A_\mu^a - \frac{1}{g} \partial_\mu \varphi^a(x) + g^{abc} \varphi^b A_\mu^c \tag{30}$$

(in infinitesimal form) with arbitrary functions $\varphi^a=\varphi^a(x)$. As was shown in Ref. 10 the gauge transformations (30) can be extended to potentials A^a_μ and their derivatives to give rise to generalized symmetries (Lie–Bäcklund tangent transformation group) with the following operator:

$$X_\varphi=\alpha^a_\mu\frac{\partial}{\partial A^a_\mu}+(d_\rho\alpha^a_\mu)\frac{\partial}{\partial A^a_{\mu,\rho}}+\cdots, \tag{31}$$

where

$$\alpha^a_\mu=-\frac{1}{g}d_\mu\varphi^a+g^{abc}\varphi^bA^c_\mu \tag{32}$$

and $\varphi^a=\varphi^a(x,A^a_\mu,A^a_{\mu,\alpha},A^a_{\mu,\alpha\beta},\ldots)$ are arbitrary functions of all variables. For the coefficients of the symmetry vector α (14) we can write

$$\alpha^a_\mu=a^a_{\mu b}\varphi^b+b^{a\nu}_{\mu b}d_\nu(\varphi^b),\quad a^a_{\mu b}=g^a_{bc}A^c_\mu,\quad b^{a\nu}_{\mu b}=-\frac{1}{g}\delta^a_b\delta^\nu_\mu. \tag{33}$$

Thus, the Second Noether theorem (25) takes the form

$$a^a_{\mu b}\omega^{a\mu}-d_\nu(b^{a\nu}_{\mu b}\omega^{a\mu})=0, \tag{34}$$

which together with Eq. (33) gives rise to the equation

$$D_\mu D_\rho G^{b\mu\rho}=0. \tag{35}$$

The expression (35) is a known identity, which was noted to be related to the Second Noether Theorem.[11] Here we aimed to show how the direct application of the Second Noether Theorem to a gauge invariant functional leads to the condition showing that the set of Yang–Mills equations is under-determined; quite important for the quantization of the gauge fields fact.[11]

(II) $p=p(\theta_1,\theta_2,\ldots,\theta_k)$, where $\theta_i=\theta_i(x)$, $i=1,\ldots,k$, $x\in R^n$, $k<n$ are some independent combinations of $x^1,x^2,\ldots,x^n$, and $p(\theta)$ is arbitrary.

In this case we generally cannot choose $p(x)$ such that it would vanish on the boundary together with its derivatives. Therefore, $T_i\sim p(x)\not\to 0$ as $x_i\to\partial D$ and we can no longer conclude that $\tilde{a}=0$. We will start consideration of this situation with a case $k=1$ (Ref. 7) when generators of a variational symmetry group contain an arbitrary function of one of independent variables or their combination.

III. INFINITE SYMMETRY ALGEBRA WITH ARBITRARY FUNCTION(S) OF ONE VARIABLE. NOETHER AND "STRICT" BOUNDARY CONDITIONS

Let us consider functions $u=u(x)$ defined on a region D of $(m+1)$-dimensional space–time $D\subset R^{m+1}$, $x=(x^1,x^2,\ldots,x^m,t)$. Consider a Noether symmetry α of the form

$$\begin{gathered}\alpha=a\gamma(\theta)+b\gamma'(\theta)+c\gamma''(\theta)+\cdots+h\gamma^{(l)}(\theta),\\ \theta=\theta(x).\end{gathered} \tag{36}$$

We have

$$\delta S=\int\limits_D\int\delta L\,d^{m+1}x=\int\limits_D\int(X_\alpha L)d^{m+1}x=\int\limits_D\int\sum_{i=1}^{m+1}(D_iM_i)d^{m+1}x=0. \tag{37}$$

Therefore,

$$\int\int \sum_{i=1}^{m+1} M_i\Big|_{x_i\to\partial D} d^m x=0, \tag{38}$$

and it follows from (37) that the following conditions for M_i should be satisfied:

$$M_i(x,u,\ldots)|_{x_i\to\partial D}=0, \quad \forall i=1,\ldots,m+1. \tag{39}$$

We will call Eqs. (39) the *Noether boundary conditions*. Equations (39) are usually satisfied for a "regular" asymptotic behavior, $u,u_i\to 0$ as $x\to\pm\infty$, or for periodic solutions.

Let us consider now another type of boundary condition related to the existence of local conserved quantities. Integrating Eq. (12) over the space $(x^1,x^2,\ldots,x^m)$, and restricting ourselves to the solution manifold, we get

$$\int\int dx^1\,dx^2\ldots dx^m \sum_{j=1}^{m+1} D_j(M_j-R_{\alpha j}L)\doteq 0, \tag{40}$$

or

$$\int\int dx^1\,dx^2\ldots dx^m\, D_t(M_t-R_{\alpha t}L)\doteq \int\int dx^1\,dx^2\cdots dx^{i-1}\,dx^{i+1}\cdots dx^m \sum_{i=1}^{m} D_i(R_{\alpha i}L-M_i). \tag{41}$$

Since α is a Noether symmetry, we can apply the Noether boundary condition (39). Requiring also that the lhs of (41) vanishes on the solution manifold[7] we obtain

$$R_{\alpha 1}L|_{x^1\to\partial D}=R_{\alpha 2}L|_{x^2\to\partial D}=\cdots R_{\alpha m}L|_{x^m\to\partial D}=0. \tag{42}$$

We will call Eqs. (42) "*strict*" *boundary conditions*.[6] Thus, in order for the system to possess (Noether) local conserved quantities, conditions (39) and (42) have to be satisfied. Note that in case $L=L(x,u,u_j)$ (second order PDE's) strict boundary conditions (32) take a simple form,

$$\alpha\frac{\partial L}{\partial u_i}\Big|_{x^i\to\partial D}=0, \quad \forall i=1,\ldots,m. \tag{43}$$

If both Noether (39) and strict boundary conditions (42) are satisfied the Noether conservation laws will take a form

$$\int\int dx^1\,dx^2\cdots dx^m\, D_t(M_t-R_{\alpha t}L)\doteq 0. \tag{44}$$

Let us look at the structure of possible Noether conservation laws (44) corresponding to an infinite Lie group on the example of the case $L=L(x^i,u,u_i)$.

IV. CONSERVATION LAWS FOR EQUATIONS WITH FIRST ORDER LAGRANGIANS. NONSINGULAR SPATIAL TRANSFORMATION

Writing M_t as

$$\begin{gathered} M_t=A\gamma(\theta)+B\gamma'(\theta)+C\gamma''(\theta)+\cdots+H\gamma^{(l)}(\theta), \\ \theta=\theta(x^1,\ldots,x^m,t), \end{gathered} \tag{45}$$

and using Eqs. (44) and (36) we obtain

$$D_t\int\int dx^1\,dx^2\cdots dx^m\left[\gamma\left(A-a\frac{\partial L}{\partial u_t}\right)+\gamma'\left(B-b\frac{\partial L}{\partial u_t}\right)+\cdots+\gamma^{(l)}\left(H-h\frac{\partial L}{\partial u_t}\right)\right]\doteq 0. \quad (46)$$

Let us rewrite Eq. (46) in the form

$$D_t\int\int dx^1\,dx^2\cdots dx^m[a_0\gamma(\theta)+a_1\gamma'(\theta)+a_2\gamma''(\theta)+\cdots+a_l\gamma^{(l)}(\theta)]\doteq 0, \quad (47)$$

where

$$a_0=A-a\frac{\partial L}{\partial u_t},\quad a_1=B-b\frac{\partial L}{\partial u_t},\cdots,a_l=H-h\frac{\partial L}{\partial u_t}. \quad (48)$$

Let us go over to new integration variables $(x^1,x^2,\ldots,x^m)\overset{\psi}{\to}(x^1,x^2,\ldots,x^{p-1},\theta,x^{p+1},\ldots,x^m)$, corresponding to the transformation $\tilde{\psi}$ of the whole space R^{m+1}, $(x^1,x^2,\ldots,x^m,t)\overset{\tilde{\psi}}{\to}(x^1,x^2,\ldots,x^{p-1},\theta,x^{p+1},\ldots,x^m,t)$. In case of a nonsingular one-to-one transformation ψ, we can invert the functional relation $\theta=\theta(x^1,x^2,\ldots,x^p,\ldots,x^m,t)$: $x^p=\varphi^p(x^1,x^2,\ldots,x^{p-1},\theta,x^{p+1},\ldots,x^m,t)$ and obtain the Jacobian of the transformation ψ, $J=\partial\varphi^p/\partial\theta$. From (47) we get

$$D_t\int\int d\theta\,dx^1\,dx^2\cdots dx^{p-1}\,dx^{p+1}\cdots dx^m[\overline{a_0}\gamma(\theta)+\overline{a_1}\gamma'(\theta)+\overline{a_2}\gamma''(\theta)+\cdots+\overline{a_l}\gamma^{(l)}(\theta)]\doteq 0, \quad (49)$$

where

$$\overline{a_i}=a_i\frac{\partial\varphi^p}{\partial\theta},\quad \text{for } i=0,\ldots,l,\ p=1,\ldots,m. \quad (50)$$

For the integral (49) we use integration by parts and either choose an arbitrary function $\gamma(\theta)$ to vanish on the boundary along with all its derivatives up to the order $l-1$,

$$\gamma(\theta)|_{\theta\to\partial D}=\gamma'(\theta)|_{\theta\to\partial D}=\gamma''(\theta)|_{\theta\to\partial D}=\cdots=\gamma^{(l-1)}(\theta)|_{\theta\to\partial D}=0, \quad (51a)$$

or impose an *additional boundary condition*,

$$\partial_\theta^i\overline{a_k}|_{\theta\to\partial D}=0,\quad \forall i=0,\ldots,k-1,\quad k=1,\ldots,l, \quad (51b)$$

where $\partial_\theta\equiv\partial/\partial\theta$. Then we get

$$D_t\int\int d\theta\,dx^1\,dx^2\cdots dx^{p-1}\,dx^{p+1}\cdots dx^m\,\gamma(\theta)[\overline{a_0}-\partial_\theta\overline{a_1}+\partial_\theta^2\overline{a_2}+\cdots+(-1)^l\partial_\theta^l\overline{a_l}]\doteq 0. \quad (52)$$

Since $\gamma(\theta)$ is arbitrary we can use a known theorem of analysis (see, e.g., Ref. 12): if $\alpha(x),p(x)$ are continuous functions on $[a,b]$ and $\int_a^b\alpha(x)p(x)dx=0$ for arbitrary $p(x)$ such that $p(a)=p(b)=0$ then $\alpha(x)=0$ for all x in $[a,b]$.

Therefore,

$$D_t\int\int dx^1\,dx^2\cdots dx^{p-1}\,dx^{p+1}\cdots dx^m[\overline{a_0}-\partial_\theta\overline{a_1}+\partial_\theta^2\overline{a_2}+\ldots+(-1)^l\partial_\theta^l\overline{a_l}]\doteq 0. \quad (53)$$

Equation (53) gives an expression of a conserved quantity corresponding to an infinite symmetry α of the form (36) where $\overline{a_i}$, $i=0,\ldots,l$ are determined by coefficients of the symmetry vector α

and Eqs. (48), (50), and all Noether (39), strict (43) and additional boundary conditions (51a) or (51b) are satisfied. In case additional boundary conditions (51b) are not satisfied, symmetries with arbitrary functions $\gamma(\theta)$ whose derivatives do not vanish on the boundary may lead according to (49) only to the following "conservation statements" (which in fact may impose additional constraints on the system instead of producing any conserved quantities):

$$D_t \int \int dx^1\, dx^2 \cdots dx^{p-1}\, dx^{p+1} \cdots dx^m\, \overline{a_i} \doteq 0, \quad i=0,\ldots,l. \tag{54}$$

Thus, an infinite symmetry group with an arbitrary function of independent variables (36) in case of a nonsingular transformation $(x^1,x^2,\ldots,x^m) \overset{\psi}{\rightarrow} (x^1,x^2,\ldots,x^{p-1},\theta,x^{p+1},\ldots,x^m)$, leads to just one conservation law (53) provided that additional boundary conditions (51a) or (51b) are satisfied.

Let us consider a special case when $\theta = x^p$ and α is a Noether symmetry of the form[6]

$$\alpha = aq(x^p) + bq'(x^p) + cq''(x^p) + \cdots + hq^{(l)}(x^p), \tag{55}$$

and

$$M_t = Aq(x^p) + Bq'(x^p) + Cq''(x^p) + \cdots + Hq^{(l)}(x^p). \tag{56}$$

In accordance with Eqs. (53) if either conditions (51a) or (51b) are satisfied we will obtain the following conservation law:

$$D_t \int \int dx^1 \cdots dx^{p-1}\, dx^{p+1} \cdots dx^m \left\{ \left(A - a\frac{\partial L}{\partial u_t} \right) - D_{x^p}\left(B - b\frac{\partial L}{\partial u_t} \right) + \cdots + (-1)^l D_{x^p}^l \left(H - h\frac{\partial L}{\partial u_t} \right) \right\} \doteq 0. \tag{57}$$

In the case for which additional conditions (51b) are satisfied,

$$\left(B - b\frac{\partial L}{\partial u_t} \right)\Big|_{x^p \to \pm\infty} = \left(C - c\frac{\partial L}{\partial u_t} \right)\Big|_{x^p \to \pm\infty} = D_{x^p}\left(C - c\frac{\partial L}{\partial u_t} \right)\Big|_{x^p \to \pm\infty} = \cdots = \left(H - h\frac{\partial L}{\partial u_t} \right)\Big|_{x^p \to \pm\infty}$$
$$= D_{x^p}\left(H - h\frac{\partial L}{\partial u_t} \right)\Big|_{x^p \to \pm\infty} = \cdots = D_{x^p}^{l-1}\left(H - h\frac{\partial L}{\partial u_t} \right)\Big|_{x^p \to \pm\infty} = 0, \tag{58}$$

the conservation law (53) takes a simple form,

$$D_t \int \int dx^1 \cdots dx^{p-1}\, dx^{p+1} \cdots dx^m \left(A - a\frac{\partial L}{\partial u_t} \right) \doteq 0. \tag{59}$$

According to (54) if conditions (51b) [or (58)] are not satisfied then the symmetry (55) with $q(x^p)$ such that its derivatives do not vanish on the boundary $(x^p \to \pm\infty)$ may lead only to the relations

$$D_t \int dy \left(A - a\frac{\partial L}{\partial u_t} \right) \doteq D_t \int dy \left(B - b\frac{\partial L}{\partial u_t} \right) \doteq \cdots \doteq D_t \int dy \left(H - h\frac{\partial L}{\partial u_t} \right) \doteq 0 \tag{60}$$

$(dy \equiv dx^1 \cdots dx^{p-1} dx^{p+1} \cdots dx^m)$. Obviously some relations in (60) imply additional constraints on the function and its derivatives rather than conservation laws.

As an example let us consider the following differential equation:

$$\omega = 2u_{xt} + u_t u_{tt} - u_{yy} = 0, \tag{61}$$

with the Lagrangian

$$L=-u_x u_t-\frac{1}{6}u_t^3+\frac{1}{2}u_y^2. \tag{62}$$

A symmetry transformation for the equation (61) is

$$X=\beta(x)\frac{\partial}{\partial t}+[2\beta'(x)t+2\beta''(x)y^2]\frac{\partial}{\partial u}. \tag{63}$$

We will consider a canonical form of this transformation,

$$\begin{gathered}X_\alpha=\alpha\frac{\partial}{\partial u}+(D_i\alpha)\frac{\partial}{\partial u_i}+\sum_{i\leqslant j}(D_iD_j\alpha)\frac{\partial}{\partial u_{ij}}+\cdots,\\ \alpha=2\beta'(x)t+2\beta''(x)y^2-\beta(x)u_t,\end{gathered} \tag{64}$$

where $\beta(x)$ is an arbitrary function. Calculating $X_\alpha L$ we can see that transformation (64) is a divergence symmetry,

$$X_\alpha L=D_iM_i, \tag{65}$$

$$M_x=-2\beta'(x)u,\quad M_y=4\beta''(x)yu,\quad M_t=-\beta(x)L-2\beta'''(x)y^2u-2t\beta''(x)u.$$

Transformation (64) is a Noether symmetry ($\delta S=0$) if the following (Noether) boundary conditions are satisfied [see (39)]:

$$\beta'(x)u(x,y,t)\Big|_{x\to-\infty}^{x\to\infty}=0,\quad yu(x,y,t)\Big|_{y\to-\infty}^{y\to\infty}=0,\quad u_i\Big|_{t\to-\infty}^{t\to\infty}=tu\Big|_{t\to-\infty}^{t\to\infty}=0, \tag{66}$$

or

$$u(x,y,t)\Big|_{x\to-\infty}^{x\to\infty}=yu(x,y,t)\Big|_{y\to-\infty}^{y\to\infty}=u_i(x,y,t)\Big|_{t\to-\infty}^{t\to\infty}=tu(x,y,t)\Big|_{t\to-\infty}^{t\to\infty}=0. \tag{67}$$

"Strict" boundary conditions (43) take the form

$$[2\beta'(x)t+2\beta''(x)y^2-\beta(x)u_t]u_t\Big|_{x\to-\infty}^{x\to\infty}=[2\beta'(x)t+2\beta''(x)y^2-\beta(x)u_t]u_y\Big|_{y\to-\infty}^{y\to\infty}=0, \tag{68}$$

and for a function $\beta(x)$ vanishing on the boundary along with its first and second derivatives, we get

$$u_t\Big|_{x\to-\infty}^{x\to\infty}=y^2u_y\Big|_{y\to-\infty}^{y\to\infty}=0. \tag{69}$$

Thus, for the equation (61) with symmetry transformation (64) we have [see (65), (55), (56)]

$$a=-u_t,\quad b=2t,\quad c=2y^2,\quad d=0, \tag{70}$$

$$A=u_xu_t+u_t^3/6-u_y^2/2,\quad B=0,\quad C=-2tu,\quad D=-2y^2u.$$

The conservation law (53) corresponding to the symmetry (64) will have the form

$$D_t\int dy\left\{-\left(\frac{u_t^3}{3}+\frac{u_y^2}{2}\right)-(2tu_x+tu_t^2)_x+(-2tu+2y^2u_x+y^2u_t^2)_{xx}-2y^2u_{xxx}\right\}\doteq 0. \tag{71}$$

In case the additional boundary conditions (58) are satisfied,

$$t(2u_x+u_t^2)|_{x\to\pm\infty}=(-2tu+2y^2u_x+y^2u_t^2)|_{x\to\pm\infty}=(-2tu+2y^2u_x+y^2u_t^2)_x|_{x\to\pm\infty}$$
$$=(-2y^2u)|_{x\to\pm\infty}=(-2y^2u_x)|_{x\to\pm\infty}=(-2y^2u_{xx})|_{x\to\pm\infty}=0,$$

or

$$u,u_x,u_t,u_{xx},u_{xt}\Big|_{x\to\pm\infty}=0, \tag{72}$$

the conservation law (71) will take the form

$$D_t\int\int dx\,dy\left(\frac{u_t^3}{3}+\frac{u_y^2}{2}\right)\doteq 0. \tag{73}$$

Note that (73) is the energy conservation law for Eq. (61). This observation is the reflection of a more general rule for Noether symmetries X of the form (55) with an arbitrary function of x^p. When additional boundary conditions (58) are satisfied the conservation law (59) associated with this symmetry will be the energy conservation law, if it belongs in the equivalence class with time translation: $X\sim\partial/\partial t$; or momentum conservation law, if $X\sim\partial/\partial x$. Obviously, these two special cases do not cover the whole variety of different situations. In case the additional boundary conditions (71) are not satisfied, and derivatives of the function $\beta(x)$ do not vanish on the boundary the symmetry (55) may lead only to the relations (60)

$$D_t\int dy\left[\frac{u_t^3}{3}+\frac{u_y^2}{2}\right]\doteq D_t\int dy[2tu_x+tu_t^2]\doteq D_t\int dy[-2tu+2y^2u_x+y^2u_t^2]\doteq D_t\int dy[-y^2u]\doteq 0. \tag{74}$$

It is easy to see that Eqs. (74) imply additional constraints on the function u and its derivatives instead of determining a system of conservation laws, and in this case infinite symmetries do not lead to any local conserved quantities.

Consider a situation when transformation ψ is singular. If $\partial\theta/\partial x^p=0$, but $\exists k\in(1,\ldots,m)$: $\partial\theta/\partial x^k\neq 0$, we can change $x^p\leftrightarrow x^k$, and generate a corresponding conservation law (57) or (59). If $\partial\theta/\partial x^p=0\ \forall p\in(1,\ldots,m)$ then $\theta=t$; this is a case of an arbitrary function of time in the generators of the symmetry group. This case is considered in the next section.

V. INFINITE SYMMETRY ALGEBRA WITH ARBITRARY FUNCTION OF TIME. LAGRANGIAN OF THE FIRST ORDER

Let $x^i=(x^1,x^2,\ldots,x^m,t)$. Consider a Noether symmetry α of the form

$$\alpha=a\,\gamma(t)+b\,\gamma'(t)+c\,\gamma''(t)+\cdots+h\,\gamma^{(l)}(t) \tag{79}$$

for a differential equation with the Lagrangian function $L=L(x^i,u,u_i)$. As earlier, [see (37)] we have

$$\delta S=\int\int\delta L\,d^{m+1}x=\int\int X_\alpha L\,d^{m+1}x=\int\int D_iM_i\,d^{m+1}x=0. \tag{80}$$

Assuming that the Noether and strict boundary conditions (39) and (43) are satisfied we will obtain the corresponding Noether conservation law in the form

$$\int\int dx^1\,dx^2\cdots dx^m\,D_t(M_t-R_{\alpha t}L)\doteq 0. \tag{81}$$

Let us demonstrate that for the symmetry (79) the equation (81) does not lead to an infinite number of conservation laws.[7] In fact, we will show that symmetry with an *arbitrary* function of time does not correspond to any conservation law. As earlier, writing M_t as

$$M_t = A\gamma(t) + B\gamma'(t) + C\gamma''(t) + \cdots + H\gamma^{(l)}(t), \tag{82}$$

and using Eq. (79), we obtain from Eq. (81)

$$D_t \int\int dx^1\, dx^2 \cdots dx^m \left[\gamma(t)\left(A - a\frac{\partial L}{\partial u_t}\right) + \gamma'(t)\left(B - b\frac{\partial L}{\partial u_t}\right) + \cdots + \gamma^{(l)}(t)\left(H - h\frac{\partial L}{\partial u_t}\right)\right] \doteq 0. \tag{83}$$

Since $\gamma(t)$ is an arbitrary function we get

$$\begin{aligned}
&\gamma(t): \quad \int\int dx^1\, dx^2 \cdots dx^m D_t\left(A - a\frac{\partial L}{\partial u_t}\right) \doteq 0,\\
&\gamma'(t): \quad \int\int dx^1\, dx^2 \cdots dx^m \left\{ A - a\frac{\partial L}{\partial u_t} + D_t\left(B - b\frac{\partial L}{\partial u_t}\right)\right\} \doteq 0,\\
&\gamma''(t): \quad \int\int dx^1\, dx^2 \cdots dx^m \left\{ B - b\frac{\partial L}{\partial u_t} + D_t\left(C - c\frac{\partial L}{\partial u_t}\right)\right\} \doteq 0,\\
&\qquad\qquad \cdots\cdots\\
&\gamma^{(l+1)}(t): \quad \int\int dx^1\, dx^2 \cdots dx^m \left\{ H - h\frac{\partial L}{\partial u_t}\right\} \doteq 0.
\end{aligned} \tag{84}$$

The system (84) can be written in the form

$$\begin{aligned}
\int\int dx^1\, dx^2 \cdots dx^m \left\{ A - a\frac{\partial L}{\partial u_t}\right\} &\doteq \int\int dx^1\, dx^2 \cdots dx^m \left\{ B - b\frac{\partial L}{\partial u_t}\right\}\\
&\doteq \ldots \doteq \int\int dx^1\, dx^2 \cdots dx^m \left\{ H - h\frac{\partial L}{\partial u_t}\right\} \doteq 0.
\end{aligned} \tag{85}$$

Obviously, Eqs. (85) in general determine not a system of conservation laws but additional constraints. Thus, Noether symmetries (empowered by strict boundary conditions) with arbitrary functions of time instead of conservation laws lead to a set of additional constraints imposed on the function u and its derivatives. Therefore the satisfaction of the strict boundary conditions (43) [or more general conditions (42)] becomes critical in the sense of avoiding additional constraints (85). Correspondingly, we have three possible situations.

(1) Strict boundary conditions (43) (or (42) can be satisfied for an arbitrary function $\gamma(t)$. Then the system (85) as a consequence of an infinite symmetry (79) provides additional constraints that the function u and its derivatives must satisfy. No conservation laws are associated with the symmetry. This situation can obviously be materialized for the cases when the system (85) is not overly restrictive.
(2) Strict boundary conditions (43) can be satisfied for some particular functions $\gamma(t)$. In this case the (finite) symmetry (79) will lead to the Noether conservation law (83) in agreement with the First Noether Theorem. Additional constraints (85) will not appear in this picture.

(3) Strict boundary conditions cannot be satisfied for any functions $\gamma(t)$. In this case a consequence of an infinite symmetry will be the fact that the solutions of the original differential equation with the strict boundary conditions (43) do not exist.

As an example of the system with one-dimensional infinite symmetry algebra, let us consider the equation of nonstationary transonic gas flows,[13]

$$2u_{xt}+u_xu_{xx}-u_{yy}=0, \tag{86}$$

with Lagrangian

$$L=-u_xu_t-\frac{u_x^3}{6}+\frac{u_y^2}{2}. \tag{87}$$

The Lie point symmetry group for the equation (86) was studied in Ref. 14. An infinite set of conservation laws for this equation is presented in Ref. 6. The symmetry group of the equation (86) includes a number of infinite subgroups:

$$(1) \qquad X=n(t)\frac{\partial}{\partial u}, \tag{88}$$

where $n(t)$ is arbitrary. We have

$$\begin{gathered}\alpha=n(t), \quad X_\alpha L=n'(t)\frac{\partial L}{\partial u_t}=D_x(-n'(t)u), \quad M_x=-n'(t)u, \quad M_y=M_z=0,\\ a=1, \ b=c=0, \ A=B=C=0.\end{gathered} \tag{89}$$

The Noether boundary condition (39) here reads as

$$u(x,y,t)\Big|_{x\to-\infty}^{x\to\infty}=0. \tag{90}$$

The strict boundary conditions (43) have the form

$$n(t)(u_t+u_x^2/2)\Big|_{x\to-\infty}^{x\to\infty}=0, \quad n(t)u_y\Big|_{y\to-\infty}^{y\to\infty}=0. \tag{91}$$

Conditions (91) are easy to satisfy for all $n(t)$. Therefore we are dealing with case (1) and no conservations laws are associated with this symmetry. Equation (85) takes the form

$$\int\int dx\,dy\,u_x\doteq 0. \tag{92}$$

Obviously, Eq. (92) does not imply any ''additional'' constraint on the function u and is automatically satisfied for all Noether symmetries (88) [see the Noether boundary condition (90)]:

$$(2) \qquad X=m(t)y\frac{\partial}{\partial u}, \tag{93}$$

where $m(t)$ is arbitrary. We have

$$\begin{gathered}\alpha=ym(t), \quad X_\alpha L=ym'(t)\frac{\partial L}{\partial u_t}+m(t)\frac{\partial L}{\partial u_y}=D_x(-m'(t)yu)+D_y(m(t)u),\\ M_x=-m'(t)u, \quad M_y=m(t)u, \quad M_z=0,\\ a=y, \ b=c=0, \quad A=B=C=0.\end{gathered} \tag{94}$$

The Noether boundary conditions are

$$u(x,y,t)\Big|_{x\to-\infty}^{x\to\infty}=u(x,y,t)\Big|_{y\to-\infty}^{y\to\infty}=0. \tag{95}$$

The strict boundary conditions are

$$ym(t)(u_t+u_x^2/2)\Big|_{x\to-\infty}^{x\to\infty}=0,\quad ym(t)u_y\Big|_{y\to-\infty}^{y\to\infty}=0. \tag{96}$$

Conditions (96) can be satisfied for any $m(t)$. No conservation laws are associated with given symmetry transformation. The additional constraint,

$$\int\int dx\,dy y u_x \doteq 0, \tag{97}$$

is fulfilled for any Noether symmetry [see (95)]:

$$(3)\qquad X=\gamma(t)\frac{\partial}{\partial x}+(2\gamma'(t)x+2\gamma''(t)y^2)\frac{\partial}{\partial u}, \tag{98}$$

$\gamma(t)$ is arbitrary. We have

$$\begin{gathered}\alpha=2\gamma' x+2\gamma'' y^2-\gamma u_x,\ \ M_x=-\gamma L-2xu\gamma''-2y^2u\gamma''',\ \ M_y=4yu\gamma'',\\ M_t=-2u\gamma',\ \ a=-u_x,\ \ b=2x,\ \ c=2y^2,\quad A=C=0,\ \ B=-2u.\end{gathered} \tag{99}$$

In this case the form of Noether and strict boundary conditions depends on the function $\gamma(t)$.

(a) $\gamma(t)$ *is arbitrary:*

Noether conditions are

$$u_i \xrightarrow[x\to\pm\infty]{} 0,\ \ xu \xrightarrow[x\to\pm\infty]{} 0,\quad yu \xrightarrow[y\to\pm\infty]{} 0,\ \ u \xrightarrow[t\to\pm\infty]{} 0. \tag{100}$$

Strict conditions are

$$xu_t, xu_x^2 \xrightarrow[x\to\pm\infty]{} 0,\ \ y^2u_y \xrightarrow[y\to\pm\infty]{} 0. \tag{101}$$

No local conservation laws are associated with the Noether transformation (98). The additional constraints (85) take the form

$$\int\int u_x^2\,dx\,dy=\int\int(2xu_x-2u)dx\,dy=\int\int 2y^2u_x dx\,dy\doteq 0. \tag{102}$$

Conditions (102) lead only to a trivial solution ($u=ay$). Situation (1) does not materialize.

Let us consider now some specific forms of $\gamma(t)$ [situation (2)] for which we can weaken our "strict" boundary conditions (96) in order to avoid restrictions (102).

(b) $\gamma'(t)=0,\ \gamma(t)=c=\text{const.}$:

Noether conditions are

$$u_i \xrightarrow[x_i\to\pm\infty]{} 0. \tag{103}$$

For "strict" boundary conditions in addition to (103) we have

$$u_x u_y \xrightarrow[y\to\pm\infty]{} 0. \tag{104}$$

According to (83) we will get the following conservation law (conservation of momentum):

$$D_t \int\int u_x^2 dx\, dy \doteq 0, \tag{105}$$

or

$$\int\int u_x^2 dx\, dy \doteq \text{const.} \tag{106}$$

As could be expected, the conservation of momentum corresponds to standard boundary conditions (103)–(104).

(c) $\gamma''(t)=0,\ \gamma(t)=at,\ a=\text{const.}$:

Noether conditions are

$$u_i \xrightarrow[x_i\to\pm\infty]{} 0, \quad u \xrightarrow[t\to\pm\infty]{} 0. \tag{107}$$

For "strict" boundary conditions in addition to (107) we have

$$xu_t, xu_x^2 \xrightarrow[x\to\pm\infty]{} 0, \quad u_y \xrightarrow[y\to\pm\infty]{} 0. \tag{108}$$

The conservation law (83) corresponding to the boundary conditions (107)–(108) has the form

$$D_t \int\int [2(xu_x - u) - tu_x^2] dx\, dy \doteq 0. \tag{109}$$

As we can see strict boundary conditions (108) determined a nontrivial conservation law.

(d) $\gamma''(t)\neq 0$: In this case we will get the same boundary conditions (100)–(101) as in (a) and the same additional constraints (102) which do not leave any nontrivial solutions.

Let us note that the transonic gas equation (86) can be obtained from the equation (61) with the interchange $x\leftrightarrow t$. The analysis above illustrates the difference in conservation laws between these two systems. The strict boundary conditions (42), critical for the derivation of conservation laws, clearly distinguish between x and t. However, in the situation when boundary conditions take a "standard" form: (72) or (103)–(104), the conservation laws for both systems may correspond to similar continuity equations. For example, it can be shown that the conserved densities (73) and (106) are dual in the sense that their corresponding continuity equations transform into each other by the interchange $x\leftrightarrow t$. A full analysis of other infinite subgroups of the symmetry group of the nonstationary transonic gas equation (86), along with corresponding conservation laws, will be given elsewhere. Another interesting application of the above approach for finding conservation laws and asymptotic behavior for systems that admit invariance transformations with arbitrary functions of time, would be the equation of "short waves."[4]

VI. CONSERVATION LAWS FOR EQUATIONS WITH HIGHER ORDER LAGRANGIANS

Let us now consider the more general case of equation of the order $(N+1)$,

$$L = L(x^i, u, u_j, u_{j_1 j_2}, \ldots, u_{j_1 j_2 \ldots j_N}), \tag{110}$$

in R^{m+1}: $u=u(x^1,x^2,\ldots,x^m,x^{m+1}\equiv t)$ with the Noether symmetry vector,

$$\alpha = b_0\gamma(\theta) + b_1\gamma'(\theta) + b_2\gamma''(\theta) + \cdots + b_l\gamma^{(l)}(\theta),$$

$$\theta=\theta(x^j),\quad j=1,\ldots,m+1. \tag{111}$$

As earlier,

$$X_\alpha L=D_i M_i, \tag{112}$$

and since $L=L(\ldots,u_{j_1 j_2 \ldots j_N})$, then according to formula (6),

$$M_t=A_0\gamma(\theta)+A_1\gamma'(\theta)+A_2\gamma''(\theta)+\cdots+A_{N+l}\gamma^{(N+l)}(\theta). \tag{113}$$

As in Sec. III, if both Noether (39) and strict boundary conditions (42) are satisfied, corresponding Noether conservation laws (if any) will take the form (44)

$$\int\int dx^1\,dx^2\ldots dx^m\,D_t(M_t-R_{\alpha t}L)\doteq 0. \tag{114}$$

Let us derive the expression for $R_{\alpha t}L$. We start with the definition (6),

$$X_\alpha L=\alpha\frac{\partial L}{\partial u}+\sum_{i=1}^{m+1}(D_i\alpha)\frac{\partial L}{\partial u_i}+\sum_{i_1\leqslant i_2}(D_{i_1}D_{i_2}\alpha)\frac{\partial L}{\partial u_{i_1 i_2}}+\sum_{i_1\leqslant i_2\leqslant i_3}(D_{i_1}D_{i_2}D_{i_3}\alpha)$$
$$\times\frac{\partial L}{\partial u_{i_1 i_2 i_3}}+\cdots+\sum_{i_1\leqslant i_2\leqslant\ldots\leqslant i_N}(D_{i_1}D_{i_2}\cdots D_{i_N}\alpha)\frac{\partial L}{\partial u_{i_1 i_2\ldots i_N}}, \tag{115}$$

and use integration by parts,

$$\sum_{i=1}^{m+1}(D_i\alpha)\frac{\partial L}{\partial u_i}=\sum_{i=1}^{m+1}D_i\left(\alpha\frac{\partial L}{\partial u_i}\right)-\sum_{i=1}^{m+1}\alpha\left(D_i\frac{\partial L}{\partial u_i}\right),$$

$$\begin{aligned}\sum_{i_1\leqslant i_2}(D_{i_1}D_{i_2}\alpha)\frac{\partial L}{\partial u_{i_1 i_2}}&=\sum_{i_1\leqslant i_2}D_{i_1}\left((D_{i_2}\alpha)\frac{\partial L}{\partial u_{i_1 i_2}}\right)-\sum_{i_1\leqslant i_2}(D_{i_2}\alpha)\left(D_{i_1}\frac{\partial L}{\partial u_{i_1 i_2}}\right)\\&=\sum_{i_1\leqslant i_2}D_{i_1}\left((D_{i_2}\alpha)\frac{\partial L}{\partial u_{i_1 i_2}}\right)-\sum_{i_1\leqslant i_2}D_{i_2}\left(\alpha D_{i_1}\frac{\partial L}{\partial u_{i_1 i_2}}\right)\\&\quad+\sum_{i_1\leqslant i_2}\alpha\left(D_{i_2}D_{i_1}\frac{\partial L}{\partial u_{i_1 i_2}}\right)\\&=\sum_{i_1\leqslant i_2}D_{i_1}\left((D_{i_2}\alpha)\frac{\partial L}{\partial u_{i_1 i_2}}\right)-\sum_{i_1\geqslant i_2}D_{i_1}\left(\alpha D_{i_2}\frac{\partial L}{\partial u_{i_{21} i_1}}\right)\\&\quad+\sum_{i_1\leqslant i_2}\alpha\left(D_{i_2}D_{i_1}\frac{\partial L}{\partial u_{i_1 i_2}}\right),\end{aligned} \tag{116}$$

$$\sum_{i_1\leqslant i_2\leqslant i_3}(D_{i_1}D_{i_2}D_{i_3}\alpha)\frac{\partial L}{\partial u_{i_1 i_2 i_3}}$$
$$=\sum_{i_1\leqslant i_2\leqslant i_3}D_{i_1}\left((D_{i_2}D_{i_3}\alpha)\frac{\partial L}{\partial u_{i_1 i_2 i_3}}\right)+\sum_{i_1\leqslant i_2\leqslant i_3}D_{i_3}\left(\alpha D_{i_2}D_{i_1}\frac{\partial L}{\partial u_{i_1 i_2 i_3}}\right)$$
$$-\sum_{i_2\leqslant i_1\leqslant i_3}D_{i_1}\left((D_{i_3}\alpha)D_{i_2}\frac{\partial L}{\partial u_{i_2 i_1 i_3}}\right)-\sum_{i_1\leqslant i_2\leqslant i_3}\alpha(D_{i_3}D_{i_2}D_{i_1})\frac{\partial L}{\partial u_{i_1 i_2 i_3}}.$$

.....

The sum of the last terms in each expression gives rise to $\alpha E(L)$, in agreement with (7),

$$X_\alpha L = \alpha E(L) + D_i(R_{\alpha i} L). \tag{117}$$

Terms with D_t have the form ($t \equiv x^{m+1}$):

$$\begin{aligned}
&D_t\left(\alpha \frac{\partial L}{\partial u_t}\right) + D_t\left((D_t\alpha)\frac{\partial L}{\partial u_{tt}} - \sum_{j\leqslant t}\alpha\left(D_j \frac{\partial L}{\partial u_{jt}}\right)\right)\\
&\quad + D_t\left((D_t^2\alpha)\frac{\partial L}{\partial u_{ttt}} - (D_t\alpha)\sum_{j\leqslant t} D_j \frac{\partial L}{\partial u_{jtt}} - \sum_{i\leqslant j}\alpha\left(D_j D_i \frac{\partial L}{\partial u_{ijt}}\right)\right) + \cdots\\
&\quad = D_t\Bigg\{\alpha\Bigg[\frac{\partial L}{\partial u_t} - \sum_{j=1}^{m+1} D_j \frac{\partial L}{\partial u_{jt}} + \sum_{j_1\leqslant j_2} D_{j_2}D_{j_1}\frac{\partial L}{\partial u_{j_1 j_2 t}}\\
&\qquad - \sum_{j_1\leqslant j_2\leqslant j_3} D_{j_3}D_{j_2}D_{j_1}\frac{\partial L}{\partial u_{j_1 j_2 t}} - \cdots\Bigg] + (D_t\alpha)\Bigg[\frac{\partial L}{\partial u_{tt}} - \sum_{j=1}^{m+1} D_j \frac{\partial L}{\partial u_{jtt}}\\
&\qquad + \sum_{j_1\leqslant j_2} D_{j_2}D_{j_1}\frac{\partial L}{\partial u_{j_1 j_2 tt}} - \sum_{j_1\leqslant j_2\leqslant j_3} D_{j_3}D_{j_2}D_{j_1}\frac{\partial L}{\partial u_{j_1 j_2 tt}} - \cdots\Bigg]\\
&\qquad + (D_t^2\alpha)\Bigg[\frac{\partial L}{\partial u_{ttt}} - \sum_{j=1}^{m+1} D_j \frac{\partial L}{\partial u_{jttt}} + \sum_{j_1\leqslant j_2} D_{j_2}D_{j_1}\frac{\partial L}{\partial u_{j_1 j_2 ttt}}\\
&\qquad - \sum_{j_1\leqslant j_2\leqslant j_3} D_{j_3}D_{j_2}D_{j_1}\frac{\partial L}{\partial u_{j_1 j_2 ttt}} - \cdots\Bigg] + \cdots\Bigg\}.
\end{aligned} \tag{118}$$

Thus, using (115) and (117) we get

$$\begin{aligned}
R_{\alpha t} L = \sum_{k=0}^{N-1} (D_t^k\alpha)\Bigg\{&\frac{\partial L}{\partial \underbrace{u_{tt\ldots t}}_{k+1}} - \sum_{j=1}^{m+1} D_j \frac{\partial L}{\partial \underbrace{u_{jtt\ldots t}}_{k+1}} + \sum_{j_1\leqslant j_2} D_{j_2}D_{j_1}\frac{\partial L}{\partial u_{j_1 j_2}\underbrace{{}_{tt\ldots t}}_{k+1}} - \cdots\\
&+ (-1)^n \sum_{j_1\leqslant j_2\leqslant\ldots\leqslant j_n} D_{j_n}D_{j_{n-1}}\ldots D_{j_1}\frac{\partial L}{\partial u_{j_1\ldots j_n}\underbrace{{}_{tt\ldots t}}_{k+1}} + \cdots\Bigg\},
\end{aligned} \tag{119}$$

where

$$j_1, j_2, \ldots, j_n = 1, \ldots, m+1,$$

and, obviously,

$$n_{\max} = N - k - 1.$$

Let us analyze the structure of the ''conservation law'' (114). Following the logic of Sec. IV, we can rewrite the equation (114) in the form

$$D_t \int\int dx^1\, dx^2 \ldots dx^m [a_0\gamma(\theta) + a_1\gamma'(\theta) + a_2\gamma''(\theta) + \cdots + a_{N+l}\gamma^{(N+l)}(\theta)] \doteq 0, \tag{120}$$

with corresponding coefficients a_j, determined by coefficients b_j, A_j from (111), (113) and L. As in Sec. IV, we can introduce new integration variables θ and make use of the transformation ψ: $(x^1, x^2, \ldots, x^m) \overset{\psi}{\to} (x^1, x^2, \ldots, x^{p-1}, \theta, x^{p+1}, \ldots, x^m)$. Conservation law (120) can be given the form

$$D_t\int\int d\theta\, dx^1\, dx^2\cdots dx^{p-1}\, dx^{p+1}\cdots dx^m[\overline{a}_0\gamma(\theta)+\overline{a}_1\gamma'(\theta)+\cdots+\overline{a}_{N+l}\gamma^{(N+l)}(\theta)]\doteq 0, \tag{121}$$

where

$$\overline{a}_i=a_i\frac{\partial\varphi^p}{\partial\theta},\text{for}\quad i=0,...,N+l. \tag{122}$$

Like in the case of Eq. (49) for the integral (121), we use integration by parts and either choose an arbitrary function $\gamma(\theta)$ to vanish on the boundary along with all its derivatives up to the order of $N+l-1$ or impose additional boundary conditions (51). We will get

$$D_t\int\int d\theta\, dx^1\, dx^2\cdots dx^{p-1}\, dx^{p+1}\cdots dx^m\,\gamma(\theta)[\overline{a}_0-\partial_\theta\overline{a}_1+\partial_\theta^2\overline{a}_2+\ldots+(-1)^{N+l}\partial_\theta^{N+l}\overline{a}_{N+l}]\doteq 0. \tag{123}$$

Using arbitrariness of the function $\gamma(\theta)$ as in the derivation of (53) we obtain

$$D_t\int\int dx^1\, dx^2\cdots dx^{p-1}\, dx^{p+1}\cdots dx^m[\overline{a}_0-\partial_\theta\overline{a}_1+\partial_\theta^2\overline{a}_2+\cdots+(-1)^{N+l}\partial_\theta^{N+l}\overline{a}_{N+l}]\doteq 0. \tag{124}$$

Equation (124) is an expression for a conserved quantity corresponding to an infinite symmetry α of the form (111), and $\overline{a}_i$, $i=0,\ldots,N+l$ are determined by coefficients of symmetry vector α and M_t. Thus, an infinite symmetry group with an arbitrary function of independent variables in case of a nonsingular one-to-one transformation ψ [if additional boundary conditions (51) are satisfied] leads to just one conservation law (124).

In case additional boundary conditions are not satisfied, symmetries with arbitrary functions $\gamma(\theta)$ whose derivatives do not vanish on the boundary may lead according to (121) only to the following ''conservation statements'' (which in fact may impose additional constraints on the system instead of producing any conserved quantities; in this case infinite symmetries do not lead to any local conserved quantities):

$$D_t\int\int dx^1\, dx^2\cdots dx^{p-1}\, dx^{p+1}\cdots dx^m\,\overline{a}\doteq 0,\quad i=0,\ldots,N+l. \tag{125}$$

Let us analyze the structure of the conservation law (114) for the case of infinite symmetry (111) with $\theta=t$,

$$\int\int dx^1\, dx^2\cdots dx^m\, D_t(M_t-R_{\alpha t}L)\doteq 0. \tag{126}$$

Using (119) we can write

$$R_{\alpha t}L=\sum_{k=0}^{N-1}(D_t^k\alpha)\{S_k\}, \tag{127}$$

where S_k is determined by L; see (119). From (111) we have

$$D_t^k\alpha=D_t^k\sum_{\mu=0}^{l}b_\mu\gamma^{(\mu)}(t)=\sum_{\mu=0}^{l}\sum_{q=0}^{k}C_k^q(D_t^{k-q}b_\mu)\gamma^{(\mu+q)}(t), \tag{128}$$

where C_p^q is the number of combinations of q from p. Using (127), (128) and (113) the ''conservation law'' (114) can be given for

$$D_t\int\int dx^1\,dx^2\ldots dx^m\left[\sum_{\mu=0}^{l}\sum_{k=0}^{N-1}\sum_{q=0}^{k}C_k^q(D_t^{k-q}b_\mu)\{S_k\}\gamma^{(\mu+q)}(t)-\sum_{\mu=0}^{N+l}A_{\bar{\mu}}\gamma^{(\bar{\mu})}(t)\right]\doteq 0. \tag{129}$$

Let us rewrite the equation (129) in the form

$$D_t\int\int dx^1\,dx^2\ldots dx^m\left[\sum_{k=0}^{N-1}\sum_{q=0}^{k}\sum_{r=q}^{q+l}C_k^q(D_t^{k-q}b_{r-q})\{S_k\}\gamma^{(r)}(t)-\sum_{\nu=0}^{N+l}A_\nu\gamma^{(\nu)}(t)\right]\doteq 0, \tag{130}$$

or

$$D_t\int\int dx^1\,dx^2\ldots dx^m\sum_{\nu=0}^{N+l}B_\nu\gamma^{(\nu)}(t)\doteq 0, \tag{131}$$

where coefficients B_ν are determined from the equation (130). Since the function $\gamma(t)$ is arbitrary, similar to (84) we obtain the following system:

$$\begin{aligned}
&\gamma(t): && \int\int dx^1\,dx^2\cdots dx^m D_tB_0\doteq 0,\\
&\gamma'(t): && \int\int dx^1\,dx^2\cdots dx^m\{B_0+D_tB_1\}\doteq 0,\\
&\gamma''(t): && \int\int dx^1\,dx^2\ldots dx^m\{B_1+D_tB_2\}\doteq 0,\\
&&&\cdots\\
&\gamma^{(N+l)}(t): && \int\int dx^1\,dx^2\ldots dx^m\{B_{N+l-1}+D_tB_{N+l}\}\doteq 0,\\
&\gamma^{(N+l+1)}(t): && \int\int dx^1\,dx^2\ldots dx^m B_{N+l}\doteq 0,
\end{aligned} \tag{132}$$

which is equivalent to the system

$$\int\int dx^1\,dx^2\ldots dx^m B_j\doteq 0,\ \ \forall j=1,\ldots,N+l. \tag{133}$$

Equations (133) determine, in general, additional constraints imposed on the function u and its derivatives rather than conservation laws. Similar to the situation with the first order Lagrangian functions, the fact of whether or not the strict boundary conditions (42) can be satisfied is critical in order to avoid additional constraints (133). Again, we have three possible situations.

(1) Strict boundary conditions (42) can be satisfied for the arbitrary function $\gamma(t)$. The system (133) provides the additional constraints the function u and its derivatives must satisfy. No conservation laws are associated with the symmetry. This situation can be materialized for the cases when the system (133) is not overly restrictive.

(2) Strict boundary conditions can be satisfied for some particular functions $\gamma(t)$. In this case the ''finite'' symmetry (111) will lead to the Noether conservation law (130) in agreement with the First Noether Theorem. Additional constraints (133) will not appear.

(3) Strict boundary conditions cannot be satisfied for any functions $\gamma(t)$. Solutions of the original differential equation with the strict boundary conditions (42) do not exist.

An interesting example of the equation with infinite symmetry algebra and a higher (third) order Lagrangian is the potential Kadomtsev–Petviashvili equation; see, e.g., Ref. 15.

VII. ARBITRARY FUNCTION OF TWO OR MORE VARIABLES

Let us consider now a case when the Noether symmetry vector of the equation with a Lagrangian (110) has an arbitrary function of two or more variables:

$$\alpha = b^0 \gamma(\theta_1,\theta_2,\ldots,\theta_k) + \sum_{q=1}^{k} b^1_q \partial_q \gamma(\theta_1,\theta_2,\ldots,\theta_k) + \sum_{q_1,q_2=1}^{k} b^2_{q_1q_2} \partial_{q_1q_2}\gamma(\theta_1,\theta_2,\ldots,\theta_k)$$
$$+\cdots+\sum_{q_i=1}^{k} b^l_{q_1q_2\ldots q_l}\partial_{q_1q_2\ldots q_l}\gamma(\theta_1,\theta_2,\ldots,\theta_k), \tag{134}$$

where

$$\theta=\theta(x^j),\quad j=1,\ldots,m+1,\quad l=1,\ldots,k,\quad k<m+1,$$

and

$$\partial_q=\frac{\partial}{\partial\theta_q},\quad \partial_{q_1q_2}=\frac{\partial^2}{\partial\theta_{q_1}\partial\theta_{q_2}},\ldots,\quad \partial_{q_1q_2\ldots q_l}=\frac{\partial^l}{\partial\theta_{q_1}\partial\theta_{q_2}\ldots\partial\theta_{q_l}}. \tag{135}$$

As earlier,

$$X_\alpha L = D_i M_i, \tag{136}$$

and since $L=L(\ldots,u_{j_1j_2\ldots j_N})$, then similarly to the formula (113) we get

$$M_t = A^0\gamma(\theta_1,\theta_2,\ldots,\theta_k) + \sum_{q=1}^{k} A^1_q\partial_q\gamma(\theta_1,\theta_2,\ldots,\theta_k) + \sum_{q_1,q_2=1}^{k} A^2_{q_1q_2}\partial_{q_1q_2}\gamma(\theta_1,\theta_2,\ldots,\theta_k)$$
$$+\cdots+\sum_{q_i=1}^{k} A^{N+l}_{q_1q_2\ldots q_{N+l}}\partial_{q_1q_2\ldots q_{N+l}}\gamma(\theta_1,\theta_2,\ldots,\theta_k). \tag{137}$$

If the Noether and strict boundary conditions, (39) and (42), are satisfied the corresponding Noether conservation laws (if any) take the form of (114),

$$\int\int dx^1\,dx^2\ldots dx^m\, D_t(M_t - R_{\alpha t}L)\doteq 0. \tag{138}$$

We can rewrite the equation (138) in the form

$$D_t\int\int dx^1\,dx^2\cdots dx^m\Bigg[a^0\gamma(\theta_1,\theta_2,\ldots,\theta_k)+\sum_{q=1}^{k} a^1_q\partial_q\gamma+\sum_{q_i,q_2=1}^{k} a^2_{q_1q_2}\partial_{q_1q_2}\gamma(\theta_1,\theta_2,\ldots,\theta_k)$$
$$+\cdots+\sum_{q_i=1}^{k} a^{N+l}_{q_1q_2\cdots q_{N+l}}\partial_{q_1q_2\cdots q_{N+l}}\gamma(\theta_1,\theta_2,\ldots,\theta_k)\Bigg]\doteq 0, \tag{139}$$

with corresponding coefficients a^j, determined by coefficients b^i, A^j from (134), (137) and L.

Introduce new integration variables θ_i, $i=1,\ldots,k$ and consider a transformation ψ, $(x^1,x^2,\ldots,x^m)\overset{\psi}{\to}(x^1,x^2,\ldots,x^{p_i-1},\theta_i,x^{p_i+1},\ldots,x^m)$ with k inserts $x^{p_i}\to\theta_i\ \forall i=1,\ldots,k$, correspond-

ing to the transformation $\tilde{\psi}$ of the whole space R^{m+1}, $(x^1,x^2,\ldots,x^m,t) \overset{\tilde{\psi}}{\to} (x^1,x^2,\ldots,x^{p_i-1},\theta_i,x^{p_i+1},\ldots,x^m,t)$. In case of a nonsingular one-to-one transformation ψ we get

$$D_t \int\int d\theta_1\, d\theta_2 \cdots d\theta_k\, dx^1\, dx^2 \cdots dx^{p_1-1}\, dx^{p_1+1} \cdots dx^{p_k-1}\, dx^{p_k+1} \cdots dx^m \times \left[\overline{a}^0 \gamma(\theta_1,\theta_2,\ldots,\theta_k) + \sum_{q=1}^{k} \overline{a}^1_q\, \partial_q \gamma + \sum_{q_i,q_2=1}^{k} \overline{a}^2_{q_1q_2}\, \partial_{q_1q_2} \gamma(\theta_1,\theta_2,\ldots,\theta_k) + \cdots + \sum_{q_i=1}^{k} \overline{a}^{N+l}_{q_1q_2\cdots q_{N+l}}\, \partial_{q_1q_2\cdots q_{N+l}} \gamma(\theta_1,\theta_2,\ldots,\theta_k) \right] \doteq 0, \tag{140}$$

where coefficients $\overline{a^j}$ are determined by a^j and the Jacobian of the transformation $\overline{\psi}$. As earlier for the integral (140) we will use integration by parts and either choose an arbitrary function $\gamma(\theta_1,\theta_2,\ldots,\theta_k)$ to vanish on the boundary along with all its derivatives up to the order of $N+l-1$ or impose *additional boundary conditions*:

$$\overline{a}^j_q|_{\theta_q \to \partial D} = 0, \quad j = 1,\ldots,N+l. \tag{141}$$

We get

$$D_t \int\int d\theta_1\, d\theta_2 \cdots d\theta_k\, dx^1\, dx^2 \cdots dx^{p_1-1}\, dx^{p_1+1} \cdots dx^{p_k-1}\, dx^{p_k+1} \cdots dx^m \gamma(\theta_1,\theta_2,\ldots,\theta_k) \times \left[\overline{a}_0 - \sum_{q=1}^{k} \partial_q \overline{a}^1_q + \sum_{q_i,q_2=1}^{k} \partial_{q_1q_2} (\overline{a}^2_{q_1q_2}) + \cdots + (-1)^{N+l} \sum_{q_i=1}^{k} \partial_{q_1q_2\cdots q_{N+l}} (\overline{a}^{N+l}_{q_1q_2\cdots q_{N+l}}) \right] \doteq 0. \tag{142}$$

Using arbitrariness of the function $\gamma(\theta_1,\theta_2,\ldots,\theta_k)$ as in derivation of (53) we obtain

$$D_t \int\int dx^1\, dx^2 \cdots dx^{p_1-1}\, dx^{p_1+1} \cdots dx^{p_k-1}\, dx^{p_k+1} \cdots dx^m \left[\overline{a}^0 - \sum_{q=1}^{k} \partial_q \overline{a}^1_q + \sum_{q_i,q_2=1}^{k} \partial_{q_1q_2} (\overline{a}^2_{q_1q_2}) + \cdots + (-1)^{N+l} \sum_{q_i=1}^{k} \partial_{q_1q_2\cdots q_{N+l}} (\overline{a}^{N+l}_{q_1q_2\cdots q_{N+l}}) \right] \doteq 0. \tag{143}$$

Equation (143) gives an expression of a conserved quantity corresponding to an infinite symmetry α of the form (111) where $\overline{a^j}$, $j=0,\ldots,N+l$ are determined by coefficients of symmetry vector α and M_t, with the aid of Eqs. (134), (137), knowing the specific form of transformation Ψ. Noether strict and additional boundary conditions are assumed satisfied.

Thus, again an infinite symmetry group with an arbitrary function of several independent variables in the case of a nonsingular one-to-one transformation ψ (if additional boundary conditions are satisfied) leads to just one conservation law (143). In case additional boundary conditions (141) are not satisfied, symmetries with arbitrary functions $\gamma(\theta_1,\theta_2,\ldots,\theta_k)$ whose derivatives do not vanish on the boundary may lead according to (140) only to the following "conservation statements" (which in fact may impose additional constraints on the system instead of producing any conserved quantities; in this case infinite symmetries do not lead to any local conserved quantities):

$$D_t \int\int d\theta_1\, d\theta_2 \cdots d\theta_k\, dx^1\, dx^2 \cdots dx^{p-1}\, dx^{p+1} \cdots dx^m\, \overline{a^j} \doteq 0, \quad j = 0,\ldots,N+l. \tag{144}$$

Let us discuss now the situation when transformation ψ is singular. Since we naturally assume all θ_i to be independent, the interesting case to consider is $\theta_r=t$, $1\leqslant r\leqslant k$. Let $\theta_k=t$. Then $\gamma=\gamma(\theta_1,\theta_2,\ldots,\theta_{k-1},t)$ and analogously to (140), we get

$$D_t\int\int d\theta_1\,d\theta_2\ldots d\theta_{k-1}\,dx^1\,dx^2\cdots dx^{p_1-1}\,dx^{p_1+1}\cdots dx^{p_k-1}$$
$$\times dx^{p_k+1}\ldots dx^m\Bigg[\overline{a}^0\gamma(\theta_1,\theta_2,\ldots,\theta_{k-1},t)$$
$$+\sum_{q=1}^{k}\overline{a}^1_q\,\partial_q\gamma+\sum_{q_i,q_2=1}^{k}\overline{a}^2_{q_1q_2}\,\partial_{q_1q_2}\gamma(\theta_1,\theta_2,\ldots,\theta_{k-1},t)+\cdots$$
$$+\sum_{q_i=1}^{k}\overline{a}^{N+l}_{q_1q_2\cdots q_{N+l}}\,\partial_{q_1q_2\cdots q_{N+l}}\gamma(\theta_1,\theta_2,\ldots,\theta_{k-1},t)\Bigg]\doteq 0. \tag{145}$$

As with the integral (140) we can use integration by parts and either choose an arbitrary function $\gamma(\theta_1,\theta_2,\ldots,\theta_{k-1},t)$ to vanish on the boundary along with all its spatial derivatives up to the order of $N+l-1$ or impose additional boundary conditions (141) with $q=1,\ldots,k-1$ to get

$$D_t\int\int dx^1\,dx^2\cdots dx^{p_1-1}\,d\theta_1\,dx^{p_1+1}\cdots dx^{p_2-1}\,d\theta_2\,dx^{p_2+1}\cdots dx^{p_{k-1}-1}$$
$$\times d\theta_{k-1}\,dx^{p_{k-1}+1}\cdots dx^m\sum_{\nu=0}^{N+l}B_\nu(x^j)\,\partial_t^\nu\gamma(\theta_1,\theta_2,\ldots,\theta_{k-1},t)\doteq 0, \tag{146}$$

with some coefficients B_ν determined from (140). As in the case with the equation (121) arbitrariness of the function γ (and its time derivatives) leads us to the system

$$D_t\int\int dx^1\,dx^2\cdots dx^{p_1-1}\,d\theta_1\,dx^{p_1+1}\cdots dx^{p_{k-1}-1}\,d\theta_{k-1}\,dx^{p_{k-1}+1}\cdots dx^m B_\nu(x^j)\doteq 0. \tag{147}$$

As earlier, the system (147) is a system of additional constraints rather than conservation laws. If the strict boundary conditions (42) are satisfied for arbitrary γ, no conservation law is associated with the given symmetry. However, the case when conditions (42) can be satisfied only for some functions γ may lead to local conserved quantities. Every such situation when a function γ satisfying (42) still preserves arbitrariness with respect to other variables $\theta_1,\theta_2,\ldots,\theta_{k-1}$ (but not t), according to the analysis above, may lead to one conservation law.

Note 1. Conclusions made in Secs. III–VI cover two- and higher-dimensional equations. One-dimensional theories, like mechanics or quantum mechanics fall under the Second Noether Theorem (see, e.g., Sec. II).

Note 2. Arbitrary functions of dependent variables and their derivatives were not considered in the paper.

VIII. CONCLUSIONS

We have shown that infinite symmetries with arbitrary functions of not all independent variables lead to a finite number of conservation laws. The set of Noether, ''strict'' and additional boundary conditions determines the existence of associated nontrivial conservation laws. An arbitrary function of spatial variables, or any combination of independent variables with a nonzero spatial part, may lead to one (nontrivial) conservation law. Arbitrary functions of time in general do not correspond to conservation laws; instead they generate a system of additional constraints imposed on the function and its derivatives. However, the system of boundary conditions may determine specific form(s) of arbitrary functions that may lead to a finite number of local conser-

vation laws. The difference in roles of arbitrary functions of spatial variables and time is, obviously related to our understanding of (local) conservation laws as those continuity equations that result in conserved in time quantities $D_t \int \int dx^1\, dx^2 \ldots dx^m\, P_t \doteq 0$. The observation that a differential system possesses infinite symmetries corresponding to (at most) a finite number of conservation laws could be an indication of the fact that our description of such a system is ''richer'' than the very system.

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Soliton-like solutions of higher order wave equations of the Korteweg–de Vries type

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In this work we study second and third order approximations of water wave equations of the Korteweg–de Vries (KdV) type. First we derive analytical expressions for solitary wave solutions for some special sets of parameters of the equations. Remarkably enough, in all these approximations, the form of the solitary wave and its amplitude-velocity dependence are identical to the sech^2 formula of the one-soliton solution of the KdV. Next we carry out a detailed numerical study of these solutions using a Fourier pseudospectral method combined with a finite-difference scheme, in parameter regions where soliton-like behavior is observed. In these regions, we find solitary waves which are stable and behave like solitons in the sense that they remain virtually unchanged under time evolution and mutual interaction. In general, these solutions sustain small oscillations in the form of radiation waves (trailing the solitary wave) and may still be regarded as stable, provided these radiation waves do not exceed a numerical stability threshold. Instability occurs at high enough wave speeds, when these oscillations exceed the stability threshold already at the outset, and manifests itself as a sudden increase of these oscillations followed by a blowup of the wave after relatively short time intervals.
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I. INTRODUCTION

As is well known, the Korteweg–de Vries (KdV) equation represents a first order approximation in the study of long wavelength, small amplitude waves of inviscid and incompressible fluids. Furthermore, if one allows the appearance of higher order terms, more complicated wave equations can be obtained. Such an equation, including second and third order corrections, was proposed in Ref. 1 and was examined, in its second order form, analytically and numerically in Refs. 2, 3, and 4. It was found that, although it is nonintegrable in general, it still possesses solitary wave solutions, which, for small values of parameters, behave like pure solitons.

One problem mentioned in Ref. 4 was that the solitary waves of this second order equation generally possess a nonzero background and thus might be unphysical.

In this work, we study in more detail this second order equation, as well as its third order counterpart proposed in Ref. 1, as approximations for water wave propagation. We first apply the Pickering algorithm[5,6] and introduce an additional arbitrary constant, which allows us to construct zero background solitary waves for both of these equations. Thus we demonstrate the remarkable fact that all these solutions have the same sech^2 form and the same amplitude dependence on the velocity as the one-soliton solution of the KdV.

We then proceed to conduct a numerical study and show that a range of parameters exists for which these solitary waves possess soliton-like behavior, in the sense that they interact nearly elastically with each other and are stable under small perturbations. We also demonstrate that all these results continue to hold in the case of the third order approximation of water wave propagation, for an even larger set of parameters.

Let us consider the famous KdV equation

$$\frac{\partial u}{\partial t}+\frac{\partial u}{\partial x}+\alpha u\frac{\partial u}{\partial x}+\beta\frac{\partial^3 u}{\partial x^3}=0 \tag{1}$$

which constitutes a first approximation of unidirectional wave motion on the surface of a thin layer of an inviscid and incompressible fluid. The function $u(x,t)$ represents the amplitude of the fluid surface with respect to its level at rest, while α and β characterize, respectively, the long wavelength and short amplitude of the waves, compared with the depth of the layer.

In order to obtain a more physically realistic form of (1) one may include second order terms in α and β as suggested in Ref. 1

$$\frac{\partial u}{\partial t}+\frac{\partial u}{\partial x}+\alpha u\frac{\partial u}{\partial x}+\beta\frac{\partial^3 u}{\partial x^3}+\alpha^2\rho_1 u^2\frac{\partial u}{\partial x}+\alpha\beta\left(\rho_2 u\frac{\partial^3 u}{\partial x^3}+\rho_3\frac{\partial u}{\partial x}\frac{\partial^2 u}{\partial x^2}\right)=0, \tag{2}$$

where ρ_1,ρ_2,ρ_3 are considered, for the time being, as free parameters. This equation holds for $\alpha,\beta\ll 1$, obeying $O(\beta)<O(\alpha)$, as, e.g., $\beta\approx\alpha^2$.[1] In Ref. 1 it was also observed that (2) can be transformed—up to terms of second order in α, β—to a completely integrable partial differential equation (pde), through a nonlinear local change of the dependent variable.

As mentioned in Refs. 2 and 3, Eq. (2) is, in general, nonintegrable in the sense that some of its ordinary differential equation (ode) reductions do not possess the Painlevé property and a Lax pair does not seem to exist. However, it was still found to possess the traveling wave solution:[3,4]

$$u(x,t)=K+\frac{3\beta k(A^2-2k)(2\rho_2+\rho_3)\operatorname{sech}^2[\sqrt{k}(x-Ct-x_0)/\sqrt{2}]}{\alpha\rho_1(A-\sqrt{2k}\tanh[\sqrt{k}(x-Ct-x_0)/\sqrt{2}])^2}, \tag{3}$$

where

$$K=\frac{2\rho_1-2\rho_2-\rho_3}{2\alpha\rho_1(\rho_2+\rho_3)}-\frac{\beta(2\rho_2+\rho_3)k}{\alpha\rho_1}, \tag{4}$$

$$C=\frac{4\rho_1-1}{4\rho_1}+\frac{(\rho_2-2\rho_1)^2}{4\rho_1(\rho_2+\rho_3)^2}+\frac{\beta^2\rho_3(2\rho_2+\rho_3)k^2}{\rho_1}, \tag{5}$$

and A,k,x_0 are arbitrary constants.

These waves were studied numerically in Ref. 4 and were found to possess, for small values of β and k, properties of true solitons: i.e., they are stable under small perturbations and interact elastically with each other. However, they also possess a generally nonzero ''background,'' given by (4), which means that they may be thought of as unphysical, since they have infinite energy (when integrated over the full real line).

As we show in this paper, however, this need not be true, since there are particular choices of the ρ_i parameters which make $K=0$ and thus restore to the solitary wave (3) its proper physical meaning. To establish this we use a method due to Pickering[5,6] and introduce an extra free parameter which helps us choose the ρ_i so that (3) finally becomes identical to the sech^2-profile of the KdV one-soliton solution.

Entirely analogous results are obtained if we allow third order terms in (2) and study solitary wave solutions of the pde

$$\frac{\partial u}{\partial t}+\frac{\partial u}{\partial x}+\alpha u\frac{\partial u}{\partial x}+\beta\frac{\partial^3 u}{\partial x^3}+\alpha^2\rho_1 u^2\frac{\partial u}{\partial x}+\alpha\beta\left(\rho_2 u\frac{\partial^3 u}{\partial x^3}+\rho_3\frac{\partial u}{\partial x}\frac{\partial^2 u}{\partial x^2}\right)$$
$$+\alpha^3\rho_4 u^3\frac{\partial u}{\partial x}+\alpha^2\beta\left(\rho_5 u^2\frac{\partial^3 u}{\partial x^3}+\rho_6 u\frac{\partial u}{\partial x}\frac{\partial^2 u}{\partial x^2}+\rho_7\left(\frac{\partial u}{\partial x}\right)^3\right)=0, \tag{6}$$

where $\rho_1,\ldots,\rho_7$ are again considered free parameters. This equation is also found to be valid for $O(\beta)<O(\alpha)$,[1] as e.g., $\beta\approx\alpha^2$, with $0<\alpha\leqslant 1$.

In fact, as we show in Sec. II, (6) possesses a solitary wave that has exactly the sech^2-form of the KdV soliton, for certain choices of the values of the parameters $\rho_1,\ldots,\rho_7$. These solitary wave solutions are obtained at ρ_i values which are different than the ones needed to derive (6) from the pair of pdes of bidirectional wave propagation given by first principles.[1] However, this does not mean that solitary waves cannot be found by other analytical or numerical methods and for other parameter values than those identified in this paper.

We then proceed, in Sec. III, to carry out a detailed numerical investigation of the stability of our solutions, using a combination of a Fourier pseudospectral method in space and a finite difference scheme in time with various step sizes Δt. Establishing first as maximum tolerance for numerical stability, $E=(\Delta t)^2$, we regard a solitary wave as stable if the small radiation waves, occurring due to numerical errors, do not exceed in amplitude this threshold.

Thus, we find regions of parameters for which such stable solutions exist, exhibiting small oscillations that remain bounded for all times. However, when the amplitude of these oscillations exceeds E they are seen to exhibit a sharp increase after relatively short times, leading eventually to blowup of the wave. In Sec. III we also study the interaction of three such stable solitary waves and show that they remain unchanged before and after collision, demonstrating thus their soliton-like character. Finally in Sec. IV we summarize our conclusions and list some open questions for future investigation.

II. ANALYTICAL EXPRESSIONS OF SOLITARY WAVE SOLUTIONS

In order to obtain explicit expressions for solitary wave solutions we shall employ Pickering's algorithm,[5,6] which was also used in Ref. 3 for the derivation of the solution (3)–(5). As can be seen in (4), however, for specific values of $\rho_i\alpha$ and β, K becomes zero only for one value of k. This means that such solutions would exist only for one particular velocity, which is inconsistent with what one finds for the soliton solutions of the KdV. It is possible, however, to obtain a zero background for a wider set of k values by introducing an additional arbitrary constant in (4), as follows:

If we consider a truncated expansion of the solution of (2) of the form

$$u(x,t)=\frac{u_0}{z^2}+\frac{u_1}{z}+u_2+u_3z+u_4z^2, \tag{7}$$

where the u_i's are constants and $z=z(x,t)$ satisfies the equations

$$z_x=1-Az-Bz^2,$$

$$z_t=-C+ACz+BCz^2 \tag{8}$$

with A, B, and C also free constants, we can allow one of the u_i to be arbitrary. This happens, for example, if

$$\rho_1=0 \quad \text{and} \quad \rho_3=-2\rho_2, \tag{9}$$

in which case u_0 is arbitrary and

$$u_1=-Au_0, \quad u_2=\frac{1}{12}(A^2-8B)u_0-\frac{au_0+12b}{12ab\rho_2}, \quad u_3=u_4=0.$$

Substituting relation (7) in (2) and using (8) we finally obtain

$$u(x,t)=K-\frac{B_1(A^2-4B_1)u_0\,\mathrm{sech}^2[\sqrt{B_1}(x-Ct-x_0)]}{(A-2\sqrt{B_1}\tanh[\sqrt{B_1}(x-Ct-x_0)])^2}$$

(where we have set $B_1=B+\frac{1}{4}A^2$) with

$$K=-\frac{1}{\alpha\rho_2}+\frac{1}{12}\left(4B_1-\frac{1}{\beta\rho_2}\right)u_0,$$

$$C=\frac{\rho_2-1}{\rho_2}-\frac{\alpha u_0}{12\beta\rho_2}+\frac{4}{3}\alpha\beta B_1^2\rho_2 u_0,$$

x_0 being the arbitrary location of the ''center'' of the wave. We can now force the background to be zero ($K=0$) by choosing

$$u_0=\frac{12\beta}{\alpha(4\beta\rho_2B_1-1)} \tag{10}$$

(hence u_0 is no longer arbitrary) and conclude with the solution

$$R3U_0:\ u(x,t)=-\frac{B_1(A^2-4B_1)u_0\,\mathrm{sech}^2[\sqrt{B_1}(x-Ct-x_0)]}{(A-2\sqrt{B_1}\tanh[\sqrt{B_1}(x-Ct-x_0)])^2}, \tag{11}$$

where

$$C=1+4\beta B_1$$

is the velocity of the traveling wave.

Observe that (11) can in fact be written in the form of the well-known sech^2-soliton solution of the KdV (1) by a simple transformation: Writing

$$\cosh\theta=\frac{A}{\sqrt{A^2-4B_1}}\quad\text{and}\quad\sinh\theta=\frac{2\sqrt{B_1}}{\sqrt{A^2-4B_1}}\quad\text{for}\ A^2>4B_1$$

and shifting x_0 appropriately, (11) is easily seen to take the form

$$u(x,t)=-\frac{3(C-1)}{\alpha(-1+(C-1)\rho_2)}\,\mathrm{sech}^2\left[\frac{1}{2}\sqrt{\frac{C-1}{\beta}}(x-Ct-x_0)\right]$$

which is exactly the one-soliton solution of the KdV if $\rho_2=0$ in which case (2) reduces exactly to (1).

In the expansion (7) of the Pickering algorithm we may alternatively consider u_2 as an arbitrary constant, by setting

$$\rho_2=2\rho_1\quad\text{and}\quad\rho_3=-2\rho_1 \tag{12}$$

and thus obtain explicit solutions of (3) even in the case $\rho_1\neq0$. Conditions (12) then lead to the solution

$$u(x,t)=K+\frac{12\beta B_1(A^2-4B_1)\mathrm{sech}^2[\sqrt{B_1}(x-Ct-x_0)]}{\alpha(A-2\sqrt{B_1}\tanh[\sqrt{B_1}(x-Ct-x_0)])^2},$$

where

$$K=\frac{3\beta(A^2-4B_1)}{\alpha}+u_2,$$

$$C=1+3A^2\beta-8\beta B_1+\alpha u_2+\rho_1(3A^2\beta-12\beta B_1+\alpha u_2)(3A^2\beta-4\beta B_1+\alpha u_2),$$

and A,B_1,x_0 are again arbitrary constants. Zero background is obtained by setting

$$u_2=-\frac{3\beta(A^2-4B_1)}{\alpha}, \tag{13}$$

whence we arrive at the expression

$$R3U2:\ u(x,t)=\frac{12\beta B_1(A^2-4B_1)\operatorname{sech}^2[\sqrt{B_1}(x-Ct-x_0)]}{\alpha(A-2\sqrt{B_1}\tanh[\sqrt{B_1}(x-Ct-x_0)])^2}, \tag{14}$$

where the velocity of the wave is again $C=1+4\beta B_1$.

It is worth remarking here that if, instead of applying Pickering's approach, we were to consider the traveling wave reductions of (2), $u(x,t)=f(x-Ct)$, for the choice of parameters (12), we can integrate the resulting ode and discover, by a simple phase plane analysis, that it possesses a separatrix along which the solution is

$$u(x,t)=\frac{3(C-1)}{\alpha}\operatorname{sech}^2\left[\frac{1}{2}\sqrt{\frac{C-1}{\beta}}(x-Ct-x_0)\right]. \tag{15}$$

This is exactly the same as the sech^2-soliton solution of KdV (1) for all ρ_1 and also coincides with (14), for $C=1+4\beta B_1$ if we shift x_0 appropriately, as explained below (11).

Finally, let us turn to the third order equation (6). Here it is important to point out that a traveling wave reduction and a derivation of the solitary wave form as done above appears to be quite difficult, as the associated odes are too cumbersome to integrate exactly. Thus we need to turn to the application of Pickering's algorithm and show, as before, that u_0, A, and B remain arbitrary iff ρ_i satisfy the following relations:

$$\rho_3=2(\rho_1-\rho_2),\quad \rho_4=0,\quad \rho_5=2\rho_1(\rho_2-2\rho_1),$$

$$\rho_6=6\rho_1(2\rho_1-\rho_2),\quad \rho_7=3\rho_1(\rho_2-2\rho_1), \tag{16}$$

whence the corresponding solution takes the form

$$u(x,t)=K-\frac{B_1(A^2-4B_1)u_0\operatorname{sech}^2[\sqrt{B_1}(x-Ct-x_0)]}{(A-2\sqrt{B_1}\tanh[\sqrt{B_1}(x-Ct-x_0)])^2},$$

where K and C depend on the parameters of the equation and the arbitrary constants u_0, A, and B_1. The zero background solution $(K=0)$ arises if we set

$$u_0=\frac{12\beta}{\alpha(4\beta B_1\rho_2-8\beta B_1\rho_1-1)}, \tag{17}$$

whence we finally obtain

$$R7U0:\ u(x,t)=-\frac{B_1(A^2-4B_1)u_0\operatorname{sech}^2[\sqrt{B_1}(x-Ct-x_0)]}{(A-2\sqrt{B_1}\tanh[\sqrt{B_1}(x-Ct-x_0)])^2} \tag{18}$$

with $C=1+4\beta B_1$ again the velocity of the wave. Note that, with $\rho_1=0$, solution (18) with (17) coincides exactly with (11) and (10).

In the same way, as with the second order equations, we may also consider u_2 arbitrary and derive the following ρ_i relations:

$$\rho_2=2\rho_1, \quad \rho_3=-2\rho_1, \quad \rho_5=3\rho_4, \quad \rho_6=-6\rho_4, \quad \rho_7=3\rho_4, \tag{19}$$

whence the corresponding solution is

$$u(x,t)=K+\frac{12\beta B_1(A^2-4B_1)\operatorname{sech}^2[\sqrt{B_1}(x-Ct-x_0)]}{\alpha(A-2\sqrt{B_1}\tanh[\sqrt{B_1}(x-Ct-x_0)])^2},$$

where K and C depend again on the parameters of the equation and the arbitrary constants u_2, A and B_1. The zero background solution $(K=0)$ now requires

$$u_2=-\frac{3\beta(A^2-4B_1)}{\alpha} \tag{20}$$

and we finally obtain

$$R7U2: \quad u(x,t)=\frac{12\beta B_1(A^2-4B_1)\operatorname{sech}^2[\sqrt{B_1}(x-Ct-x_0)]}{\alpha(A-2\sqrt{B_1}\tanh[\sqrt{B_1}(x-Ct-x_0)])^2}, \tag{21}$$

where the velocity is $C=1+4\beta B_1$, as in all the cases above. Again here (21) also becomes identical to the KdV soliton (15), with the appropriate shift of the constant x_0, even though it is the solution of a much more complicated pde.

It is important, however, to remark that the ρ_i parameter values, (16) or (19), determined by our approach, are quite different from the ones found in Ref. 1, by the reduction to unidirectional flow from a pair of pdes describing bidirectional wave propagation. The reasons for this difference remains an open question, which clearly requires further investigation.

III. NUMERICAL STABILITY ANALYSIS

The numerical scheme used in the current study is the same as the one employed in Ref. 4 and is based on a combination of finite differences and a Fourier pseudospectral method. In order to demonstrate the application of our algorithm we first describe it on the KdV equation

$$u_t+u_x+\alpha u u_x+\beta u_{xxx}=0 \tag{22}$$

with the initial condition $u(x,0)=f(x)$. The time derivative in (22) is discretized using a finite difference approximation, in terms of central differences

$$u^{n+1}=u^{n-1}-2\Delta t(u_x^n+\alpha u^n u_x^n+\beta u_{xxx}^n)=0. \tag{23}$$

According to the pseudospectral method, we introduce the approximate solution

$$u(x,t)=\sum_{k=0}^{N}\alpha_k(t)\Phi_k(x), \tag{24}$$

where $\Phi_k(x)=e^{ikx}$ are the Fourier exponentials, and $\alpha_k(t)$ are coefficients to be determined, for $k=0,1,...,N$.

The steps used to advance the solution from time step n to $n+1$ are[7]

(i) Given $u_j^n=u(x_j,t_n)$ evaluate $\alpha_k^n=\alpha_k(t_n)$ from (24).
(ii) Given α_k^n evaluate the derivatives, e.g., $[\partial^2 u/\partial x^2]_j^n$ from (24).

(iii) Evaluate the nonlinear terms, e.g., $u_j^n[\partial u/\partial x]_j^n$.
(iv) Evaluate u_j^{n+1} from (23), at $x=x_j$, $t=t_{n+1}$.

Step (i) is the transformation from physical space to spectral space. This transformation is achieved by the use of a fast Fourier transform (FFT) described in Refs. 7 and 8 with a number of operations $(5/2)N\log_2 N$ (N being the number of polynomials), in contrast to the $2N^2$ operations required for a matrix-vector multiplication.[9] Step (ii) occurs in spectral space and the evaluation of the nonlinear term in step (iii) is in physical space, thus avoiding the expensive multiplication of all coefficients in the expansions of the form (24). Step (iv) occurs again in physical space.

The accuracy of our numerical scheme for the time variable t is $O((\Delta t)^2)$, due to central differences and for the space variable x, where we use the pseudospectral method, $O(e^{-qN})$, where q is a constant.[8] Numerical calculations were carried out for various numbers of polynomials $N=128$, 256, 512, and 1024 and time steps $\Delta t=0.0001$ to 0.002, while the spatial step was chosen to be $\Delta x=1$.

We should mention here that, for the time propagation of such types of problems, where the spatial discretization is extremely accurate, the most commonly used method is the fourth order Runke–Kutta integration scheme. Even though this method provides satisfactory results, it may fail because of sensitivity to the initial conditions and inherent instabilities. Thus, since the stability of the waves propagating in time is of more interest than the accuracy, a more stable, central differencing is used for the discretization in time.

In Ref. 4 we carried out several calculations to verify the efficiency of our numerical code. For the KdV equation (1) at $t=0$ with $\alpha=1$, $\beta=0.1$, $x_0=20$ and $c=1.1$, we took as initial condition the well-known exact solitary wave solution

$$u(x,t)=\frac{3(c-1)}{\alpha}\,\mathrm{sech}^2\left[\frac{1}{2}\sqrt{\frac{c-1}{\beta}}(x-ct-x_0)\right], \tag{25}$$

where c is the propagation speed and x_0 is an arbitrary constant.[10,11] We observed that our wave moves along the spatial direction retaining its initial profile for a very long time period of at least $t=2.5\times10^6$ time units with time step $\Delta t=0.01$. A three-soliton interaction was also studied and the results were as expected from the soliton solutions of the KdV, i.e., the waves interact elastically and remain unchanged before and after their interaction. These results were obtained for various time steps and numbers of polynomials N mentioned above, which demonstrates that our code reproduces accurately the fundamental properties of the KdV.

The plethora of free parameters entering into Eqs. (2) and (6) makes the study of the wave solutions, obtained in Sec. II, not a very easy task. However, if we impose the zero background for our solutions, much of the redundancy is removed and our ρ_i's begin to have a more specific meaning. Thus, we investigate the wave solution (11) for Eq. (2), with u_0 given by (10) and for ρ_i, $i=1,2,3$ satisfying (9). This solution is referred to as $R3U0$. For the same equation we also study the solution (14) for u_2 given by (13) and ρ_i, $i=1,2,3$ satisfying (12), which is referred to as $R3U2$. Similarly we name $R7U0$ the solution (18) of Eq. (6) with u_0 given by (17) and for ρ_i, $i=1,...,7$ satisfying (16) and $R7U2$ the solution (21) of the same equation with u_2 given by (20) and for ρ_i, $i=1,...,7$ satisfying (19).

The free parameters now present in the solutions $R3U0$ and $R3U2$ are only α, β, B_1, and ρ_2 for $R3U0$ or ρ_1 for $R3U2$. Therefore, we will first study how they affect the stability of the above-mentioned wave solutions, and then proceed to study the $R7U0$ and $R7U2$ waves, using similar α and β, plus ρ_1 for $R7U0$ and ρ_4 for $R7U2$.

A. A stability criterion

Our ultimate goal, of course, is to examine the values of the parameters in our higher order KdV equations (2) and (6), for which the solitary wave solutions mentioned above preserve their shape and are stable under evolution. By the term ''stable'' we mean that a wave solution, when

substituted in an equation, retains its initial profile for long times, albeit with some smaller oscillations present as radiation waves, due to unavoidable numerical errors produced under time evolution.

Thus, in order to check stability, one way is to track the residual of the solution in time. For the case of KdV, for example, if $\overline{u}$ is an exact solution of (1) it will satisfy

$$\overline{u}_t+\overline{u}_x+\alpha\overline{u}\overline{u}_x+\beta\overline{u}_{xxx}=0. \tag{26}$$

If the approximate solution (24), computed numerically, is substituted into (26) it will not, of course, give zero. Thus we write for it

$$u_t+u_x+\alpha u u_x+\beta u_{xxx}=R,$$

where R is called the residual of the equation. It is expected that R is a continuous function of x and t and if N is sufficiently large then, in principle, the coefficients $\alpha_k(t)$ can be chosen so that R is as small as we wish over the computational domain. In our case we evaluate $R=R_i$ at each x_i, $i=1,...,N$ grid point at specific time moments t_n.

Due to the fact that the wave solutions are computed for sufficiently large values of N (128 to 1024), the spatial error of the pseudospectral method is in agreement with the $O(e^{-qN})$ estimate mentioned above, and is practically zero. The maximum absolute residual, which we refer to as the error, $E=\max_i|R_i|$, will increase due to the central differencing in time, but cannot be greater than $O((\Delta t)^2)$. Several tests have been made for the wave solution (25) of the KdV verifying that for various values of N (128 to 1024) and time step $\Delta t=0.0001$ to 0.02, $E<(\Delta t)^2$ at least for a time period of 10^6 time units.

Therefore, a practical way to verify that a wave solution is stable is to check if the error remains, for long times, less than $O((\Delta t)^2)$. If E increases above this value already from the outset, oscillations will soon grow and become unbounded after relatively short times, not only because of the numerical scheme, but also due to the nonlinear nature of the equations, suggesting that the initial wave solution has become unstable. *This is also supported by the fact that blowup occurs nearly at the same times, irrespective of the values of the Δx and Δt step sizes used in the numerical scheme.*

B. Solutions *R3U0* and *R3U2*

Let us now proceed to the study of $R3$ solutions. In all that follows B_1 satisfies the relations $B_1>0$ and $A>\sqrt{2B_1}$ which are vital in order to have a bounded wave solution. The parameter A does not affect the stability of the wave and in all cases is taken $A=3$.

One way to examine the stability of solutions under investigation is to set α, β fixed and start to increase B_1, the velocity of the wave, by a quantity ΔB_1. Each time we increase B_1, we track the error E for a period of time: If it remains below $(\Delta t)^2$, we consider that the wave is stable for this period, and proceed to increase B_1 by another ΔB_1 until E becomes greater than $(\Delta t)^2$. Once this happens, we set $\Delta B_1=\Delta B_1/2$, decrease B_1 by ΔB_1 and track the error again. In that way, we determine, up to an accuracy ϵ ($\Delta B_1<\varepsilon$), the maximum value of B_1 (speed), $B_1^{\max}$, for which the solitary wave is stable.

The period of time used in the current study is 500 time units, with time step $\Delta t=0.001$ and accuracy $\varepsilon=0.001$. Several tests have been made, e.g., with the KdV, using cases where the exact solution is known to be stable, and as expected, the value of $B_1^{\max}$, estimated in the above way, depends neither on the time step Δt, nor on the number of points N we use.

Figure 1 shows the variation of $B_1^{\max}$ with α for various values of β. The parameter ρ_2 is fixed equal to 1. It is observed that as α increases $B_1^{\max}$ is increasing for small values of β. The variation of $B_1^{\max}$ with α is smaller as β increases and finally no significant changes are observed when $\beta>0.2$. Thus, it can be concluded that α has a stabilizing effect on the solutions, especially for low

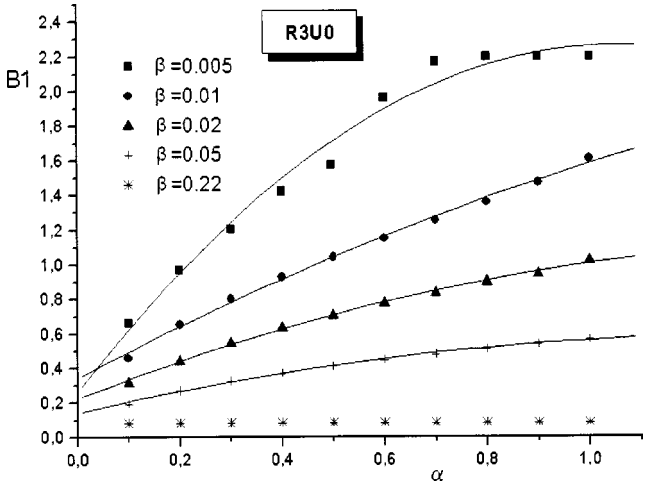

FIG. 1. Variation of $B_1^{\max}$ of solution $R3U0$ with α.

values of β, since its increase makes the range of velocities larger for stable soliton-like waves (in the range of $0<\beta\leqslant 0.1$). The region below each curve (plotted by interpolation) is the region of stability of the wave solution for the corresponding values of parameters.

The variation of the $B_1^{\max}$ with β for various values of α is shown in Fig. 2. Unlike what was observed for α in Fig. 1, we find that $B_1^{\max}$ decays exponentially with the increase of β, and the region where the wave solution is stable is larger for greater values of α. Thus we conclude that increasing β has a destabilizing effect on the solitary waves. The parameter ρ_2 is again kept equal to 1. The variation of $B_1^{\max}$ for the solution $R3U2$ with α or β is qualitatively the same as that for $R3U0$, and any quantitative differences with Figs. 1 and 2 are insignificant.

Similar results were also observed for the $R7U0$ and $R7U2$ solutions. However, because of the additional ρ_i parameters present in these cases, a direct comparison with the $R3$ solutions is not easy to demonstrate pictorially.

It is important to note that these findings are in good agreement with the conditions of the validity of (2) and (6), i.e., that $O(\beta)<O(\alpha)$.[1] In fact, using $\beta\approx\alpha^2$ is seen to yield optimal results in terms of the size of stability regions of our solitary wave solutions.

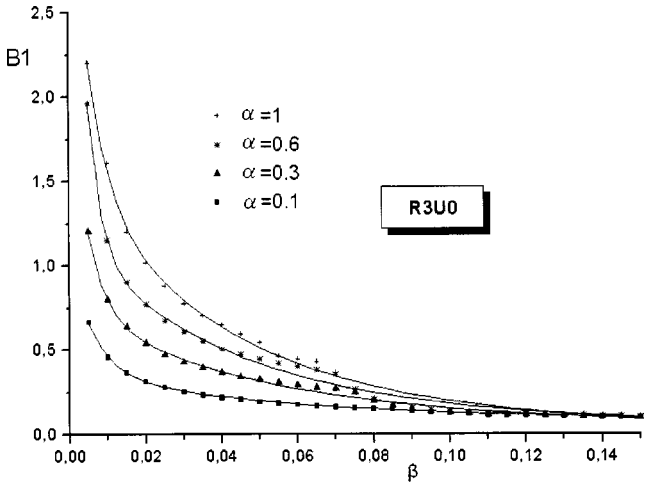

FIG. 2. Variation of $B_1^{\max}$ of solution $R3U0$ with β.

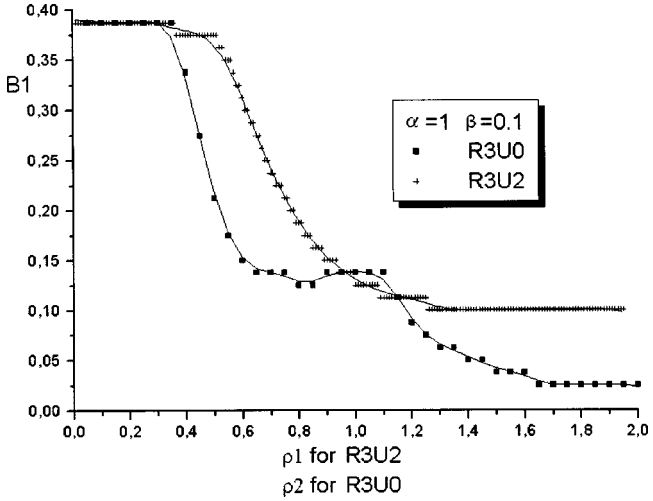

FIG. 3. Variation of $B_1^{\max}$ with ρ_2 for $R3U0$ and ρ_1 for $R3U2$.

In order to examine the effect of ρ_2 on $R3U0$ or ρ_1 on $R3U2$ we can set $\alpha=1$, $\beta=0.1$ and find $B_1^{\max}$ while varying the corresponding ρ_i. Figure 3 shows this variation of $B_1^{\max}$ with ρ_2 for $R3U0$ and ρ_1 for $R3U2$ solitary wave solutions. It is found that for an increase of the corresponding ρ_i up to 0.4 there are no significant changes. When the ρ_i increase beyond 0.4 a rapid decrease of $B_1^{\max}$ takes place. This decrease stops at $\rho_1 \approx 1.2$ for the $R3U2$ solution, while, in the case of $R3U0$ it continues until ρ_2 reaches the value of approximately 1.7.

It is worth mentioning that the results plotted in Figs. 1–3 using $\Delta t=0.001$ and $N=128$, are also obtained for time steps 0.0001, 0.002, and number of points 256 and 512.

C. Error behavior during wave propagation

Before proceeding to the $R7$ solutions, let us discuss some results concerning the error criterion of Sec. III A, in order to understand how wave solutions propagate in time and which of them are considered as stable. The results described below were obtained for the $R7U0$ solution, but are similar to what is observed for $R7U2$.

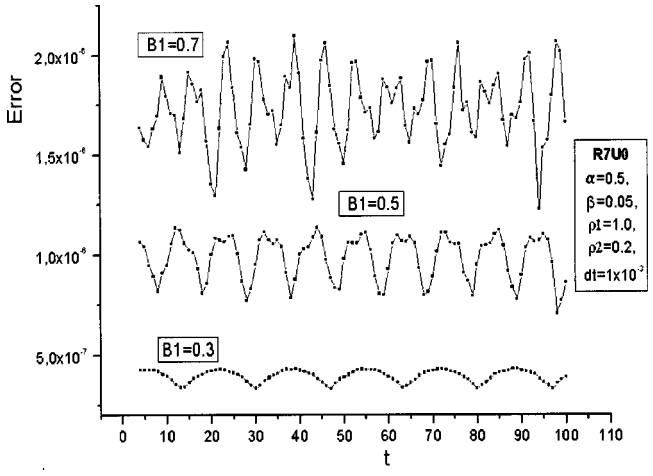

FIG. 4. Error variation with time for three different values of B_1. The case $B_1=0.5$ lies just above the boundary of the stability region $E \leqslant (\Delta t)^2$.

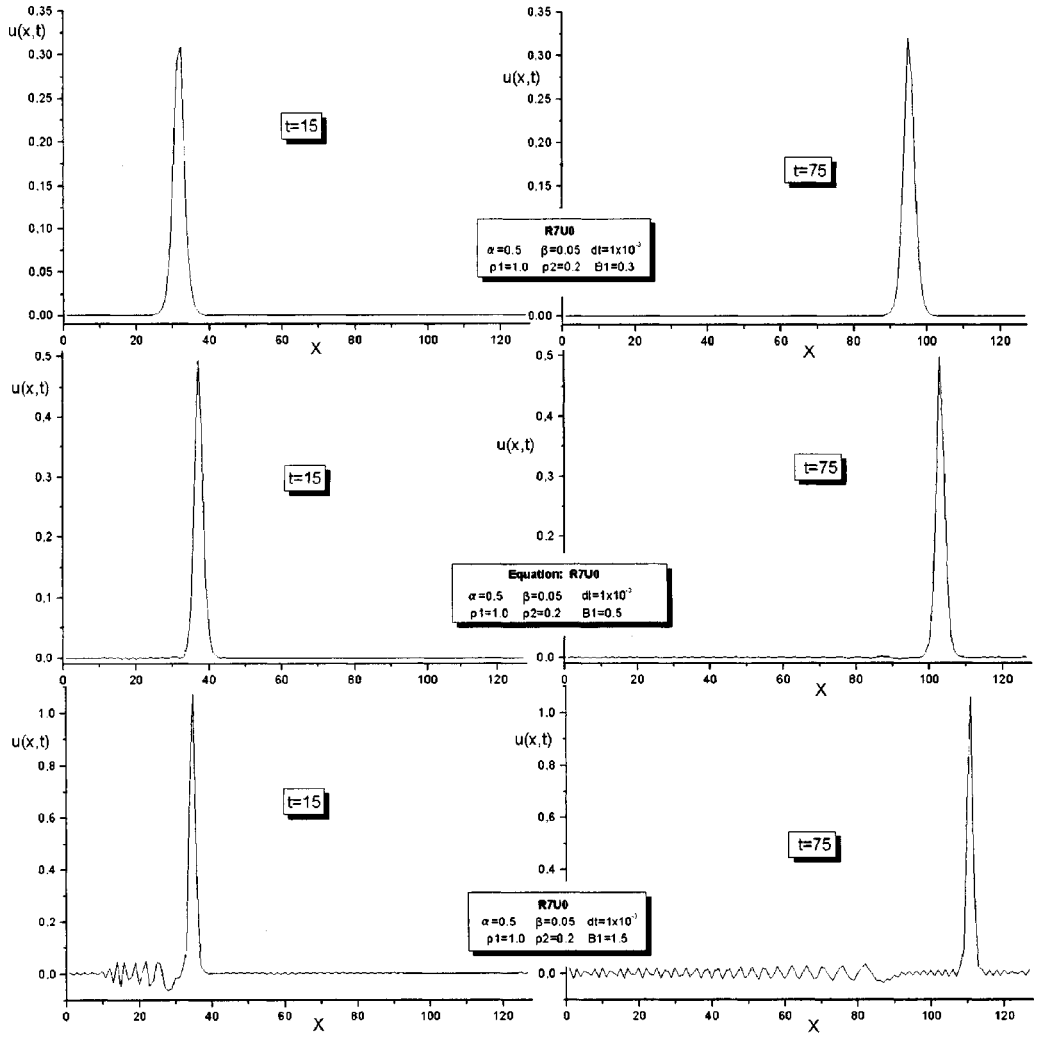

FIG. 5. Evolution of $R7U0$ in time for $B_1=0.3$, 0.5, and 1.5, respectively.

We set $\alpha=0.5$, $\beta=0.05$, $\rho_1=1$, $\rho_2=0.2$ and track the error of $R7U0$ for a period of time of 100 time units, with time step $\Delta t=0.001$, and three different values of B_1, namely 0.3, 0.5, and 0.7. The variation of the errors for these cases are shown in Fig. 4. Note that the error for $B_1=0.3$ is less than $(\Delta t)^2=1\times10^{-6}$.

Figure 5 shows the $R7U0$ solution propagating in time for B_1 equal to 0.3, 0.5 and 1.5, respectively, for the same values of the other parameters as above. It is observed that for $B_1=0.3$ the wave remains virtually unchanged in time and is therefore considered stable, with its radiation waves remaining smaller than $(\Delta t)^2$ for very long times. On the other hand, in the case $B_1=0.5$, bounded oscillations appear where the error slightly exceeds $(\Delta t)^2$. We call this solution unstable, because its radiation waves grow as time increases and become unbounded after a relatively short time. Similarly, for $B_1=1.5$, where these oscillations are even larger at the beginning, blowup occurs after a much shorter time interval. We remark once more that analogous results are obtained for different time steps, and also for the same time step and greater values of N.

It is important to mention that for small $\beta(\beta<0.1)$ and large $\alpha(\alpha\approx1)$ oscillations appear, even when the error E does not exceed $(\Delta t)^2$. These oscillations remain almost the same for a time period comparable to the one used to test the stability of the solutions of KdV. Moreover,

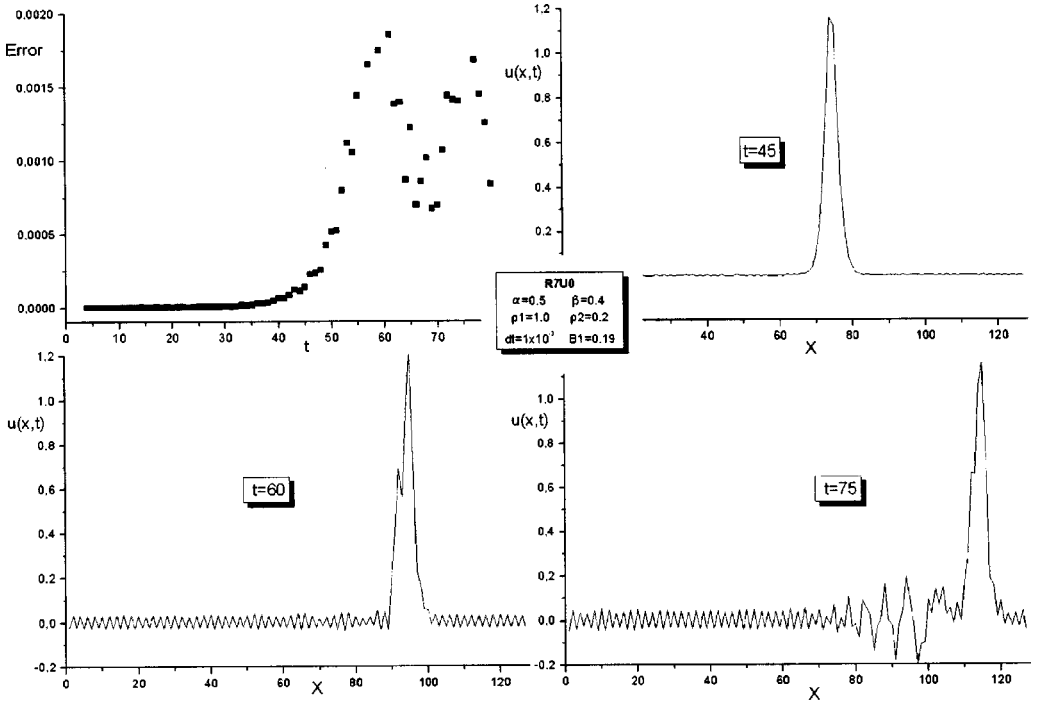

FIG. 6. Evolution of $R7U0$ in time for $B_1=0.19$.

even when $E\approx(\Delta t)^2$ (and β small enough) oscillations can persist over long time intervals as seen in Fig. 5, with $\beta=0.05$, where the oscillations occurring for $B_1=1.5$ remain unchanged and bounded well beyond value of $t=75$ shown in the figure.

However, if the error grows sharply at some point in time, this implies that the oscillation will become unbounded soon thereafter leading to a blowup of the solution. Figure 6 shows the propagation of $R7U0$ for $\alpha=0.5$, $\beta=0.4$, $\rho_1=1$ and $\rho_2=0.2$. In this case, $B_1^{\max}\approx 0.156$, as estimated by the method described above. Consequently, if we set $B_1=0.19$ error oscillations suddenly explode at $t\approx 50$ causing the wave amplitude to increase while at $t\approx 80$ the solution blows up. The same behavior is observed for Δt varying from 0.0001 to 0.002 and N from 128 to 512 indicating that this is not a numerical blowup.

As in the case of $R7U0$ shown in Fig. 6, we have also observed from numerous tests, that if the wave is to blow up, the error will suddenly increase by 2–3 orders of magnitude within the first 200 time units. In some examples, blowup occurs after thousands of time units, but is predicted by our error analysis already within the first 200 time units. Thus, for the calculation of stability results, we adopt the time period of 500 time units of numerical integration.

In order to investigate the stability of the $R7$ solutions we keep the values of α and β fixed at $\alpha=1$, $\beta=0.1$. Moreover, we consider $\rho_1=0.2$ and $\rho_2=0.2$ for $R7U2$ and $R7U0$, respectively. Consequently, the independent parameters are ρ_1 for $R7U0$ and ρ_4 for $R7U2$. The variation of $B_1^{\max}$ with ρ_1 for $R7U0$ and ρ_4 with $R7U2$ is shown in Fig. 7. It is found that the growth of ρ_1 in $R7U0$ results in an increase of $B_1^{\max}$, whereas increasing ρ_4 in $R7U2$ solution results in a decrease of $B_1^{\max}$. For relatively large values of the corresponding ρ_i the stability regions differ considerably and for values greater than unity the corresponding $B_1^{\max}$ can be 4 times greater for $R7U0$ than that of $R7U2$.

D. Elastic three wave interactions

In Ref. 4 a three-wave interaction was performed with Eq. (2), using its solution (3) as initial condition for the three solitary waves. It was reported that due to the different backgrounds of the

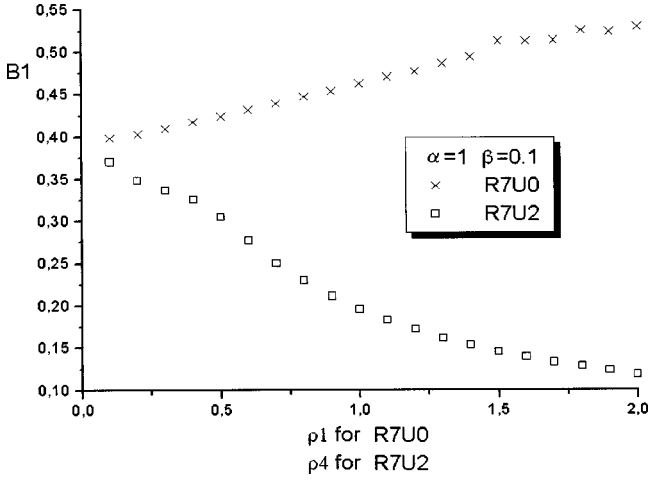

FIG. 7. Variation of the $B_1^{\max}$ with ρ_1, for $R7U0$ and ρ_4 for $R7U2$.

waves a slight displacement of each solution by a constant had to be applied. This can now be avoided using the zero background wave solutions we have obtained here. Thus, we study here the interactions of solitary waves of the form (15), using the third order KdV equation (6).

A preliminary investigation of the $R7$ solutions suggests using the $R7U0$ solitary wave, since its stability region increases with increasing ρ_1, provided we keep the difference between ρ_1 and ρ_2 small. The reason is that the additional nonlinear terms in $R7U0$ are multiplied by $\rho_4,\ldots,\rho_7$ values which are smaller than those of $R7U2$, and thus lead to a larger area of stability.

The next step is to specify values for the α and β parameters. As was shown in Sec. II, the wave speed of propagation is $C=1+4\beta B_1$. Thus, the relative speed between two waves is $4\beta(B_1-B_1')$, where $C'=1+4\beta B_1'$ is the velocity of the second wave. Consequently, we have to use relatively large values of β to see an interaction within a reasonable time. Furthermore, we have to avoid using large α so as to reduce the bounded oscillations described in the preceding section. Therefore, taking into account all these considerations we choose $\alpha=0.4$, $\beta=0.1$, $\rho_1=0.25$, and $\rho_2=0.1$.

For the values of the remaining parameters we set $x_1=10$, $x_2=28$, $x_3=55$ and $B_{11}=0.30$, $B_{12}=0.20$, $B_{13}=0.06$, where x_i and B_{1i} correspond, for $i=1,2,3$, to the first (fastest), second (middle), and third (slowest) wave. The interaction of these solitary waves, as shown in Fig. 8, is seen to occur in exactly the same way as for the KdV equation. No radiation is observed and no differences are found in the shape of the solitary waves (before and after collision) as far as we could determine numerically (with $\Delta t=0.01$ and $N=1024$). These results strongly indicate the existence of wave solutions which ''behave'' as true solitons in water wave equations which represent higher order approximations to the KdV equation.

IV. CONCLUDING REMARKS

In this paper, we have studied the existence and stability of solitary wave solutions of pdes representing second and third order approximations of unidirectional water wave propagation, in the short amplitude, $0<\alpha=a/h\ll 1$, and long wavelength limit, $0<\beta=(h/l)^2\ll 1$ (h is the depth of the fluid layer). To first order in α and β, these pdes reduce to the famous KdV equation, which is completely integrable and possesses solitary waves that interact perfectly elastically with each other and are called solitons.

Our original motivation was the fact that these higher order KdV equations have been shown to be equivalent to completely integrable pdes, by a local nonlinear transformation, at the same order of approximation in α and β.[1] The question therefore naturally arises if these higher order KdV approximations also possess solitary waves exhibiting soliton-like dynamics.

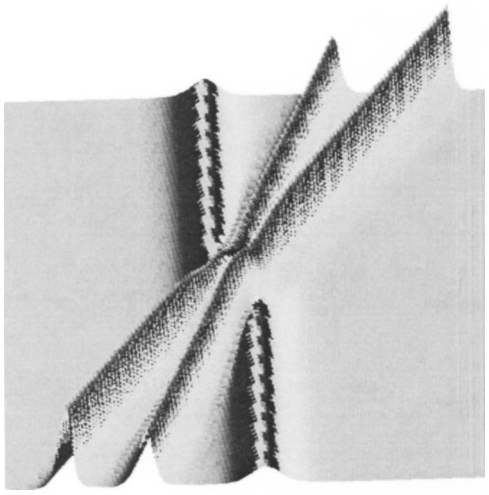

FIG. 8. Elastic interaction of three $R7U0$ solitary waves of Eq. (6).

Adopting the assumption $O(\alpha)<O(\beta)$ (e.g., $\beta\approx\alpha^2$), which eliminates some dispersive terms with higher order derivatives,[1,12] we derive exact, closed form expressions for the solitary waves valid to second and third order in α and β using Pickering's algorithm.[5,6] Choosing then specific values for the free parameters, we force these solutions to have zero background and demonstrate the remarkable fact that they all have the same sech^2 form and velocity dependence as the simple, one-soliton solution of the KdV.

Proceeding to a numerical study of their stability, we use a Fourier pseudospectral method combined with finite difference in time (with step size Δt) and establish a threshold of numerical error tolerance $E=(\Delta t)^2$. Thus we call a solitary wave stable if the small oscillations trailing the wave have amplitude smaller than E and remain bounded for very long times ($\leqslant$500 units).

However, as the speed of the wave increases, these ''radiation'' oscillations also increase and when their amplitude exceeds E, already at the beginning of their evolution, turn out to exhibit a dramatic growth over relatively short times ($\leqslant$200 units) leading eventually to blowup of the wave and characterizing the solution as unstable. Our results are entirely consistent with what is observed for the KdV equation and also agree with the assumption that $O(\beta)<O(\alpha)$ in these pdes.

A number of open questions remain for future investigation: What is the ''physical'' meaning of the values of the free parameters, which we have chosen so that the solitary waves of these pdes have zero background? Why are these values different from those obtained by the reduction of the original water wave equations to unidirectional motion?[1] In fact, we have recently observed that the ode that gives traveling wave solutions for the second order approximation (2) can be easily integrated once and then numerically studied by phase plane analysis to give homoclinic orbits, which correspond to solitary waves for many other ρ_i parameters than the ones identified here.

Can such integrations be carried out also for the third order equation (6) to yield solitary waves, exhibiting similar behavior and reducing to the KdV soliton, as α and β go to zero? Finally, among all these choices, which ρ_i fit best the physical realization of a solitary water wave?

Another question concerns the mathematical form of the solitary waves we have obtained in this paper: Could their simple sech^2 expressions (identical for the second and third order case) imply that they also hold in higher order approximations? Finally, is their presence related to the fact that the corresponding approximation can be transformed to a pde which is completely integrable to the same order in α, β?

In conclusion, we believe that water wave motion still remains an open and fascinating topic of great mathematical and physical interest and hope to be able to answer some of the above questions in a future publication.

ACKNOWLEDGMENTS

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Driven Newton equations and separable time-dependent potentials

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We present a class of time-dependent potentials in R^n that can be integrated by separation of variables: by embedding them into so-called cofactor pair systems of higher dimension, we are led to a time-dependent change of coordinates that allows the time variable to be separated off, leaving the remaining part in separable Stäckel form. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1514833]

I. INTRODUCTION

Newton's law of force in mechanics leads to second order ordinary differential equations $\ddot{q}=M(q,\dot{q},t)$, where $q=(q^1,\ldots,q^n)$ are coordinates on some manifold Q, the configuration space of the system. Often the force M is derived from a potential $V(q,t)$ and the equations can be written in Lagrangian form

$$\frac{\partial L}{\partial q^i}-\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}=0, \quad L(q,\dot{q},t)=\frac{1}{2}g_{ij}\dot{q}^i\dot{q}^j-V(q,t),$$

or, via the Legendre transformation, in Hamiltonian form

$$\dot{q}^i=\frac{\partial H}{\partial p_i}, \quad \dot{p}_i=-\frac{\partial H}{\partial q^i}, \quad H(q,p,t)=\frac{1}{2}g^{ij}p_ip_j+V(q,t).$$

Here g_{ij} is the metric tensor on Q, with inverse g^{ij}, and (q^i,p_j) are (adapted) coordinates on the cotangent bundle T^*Q.

Powerful techniques have been developed for solving such equations; in particular the well-known Hamilton–Jacobi method, where one tries to find new coordinates $u=u(q)$ on Q, in terms of which the Hamilton–Jacobi equation corresponding to H can be solved by separation of variables. If this succeeds, the mechanical system can be integrated by quadratures.

We will restrict ourselves to Euclidean n-space, i.e., $Q=R^n$ and $g_{ij}=\delta_{ij}$. The coordinates will be written with lower indices in this case, and regarded as a column vector $q=(q_1,\ldots,q_n)^T$, the T denoting matrix transposition.

Consider a Newton system which does not contain time t or velocity $\dot{q}$ explicitly,

$$\ddot{q}=M(q).$$

If there is a potential, the system takes the form

$$\ddot{q}=-\nabla V(q), \quad \nabla=\frac{\partial}{\partial q}=\left(\frac{\partial}{\partial q_1},\ldots,\frac{\partial}{\partial q_n}\right)^T,$$

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and then the energy $E=\frac{1}{2}\dot{q}^T\dot{q}+V(q)$ is conserved ($\dot{E}=0$). The separability theory for such time-independent potentials in Euclidean space is highly developed. It is known that separation of the corresponding Hamilton–Jacobi equation can only take place in so-called generalized elliptic coordinates or some degeneration thereof.[4] There even exists an effective algorithm for determining whether or not a given potential $V(q)$, expressed in Cartesian coordinates, is separable, and if so, in which coordinate system.[10]

Less is known in the time-dependent case. One of the aims of this paper is to show how certain Newton systems in R^n with time-dependent potential can be integrated by viewing them as driven systems in R^N, with $N>n$, as the following example illustrates.

Example 1: Consider the time-dependent potential

$$V(x_1,x_2,t)=\frac{1}{x_1x_2-t} \tag{1}$$

and the corresponding Newton system in R^2:

$$\begin{aligned}\ddot{x}_1&=-\frac{\partial V}{\partial x_1}=\frac{x_2}{(x_1x_2-t)^2},\\ \ddot{x}_2&=-\frac{\partial V}{\partial x_2}=\frac{x_1}{(x_1x_2-t)^2}.\end{aligned} \tag{2}$$

In order to integrate this system, we introduce the following auxiliary Newton system in R^3, where the first equation drives the other two:

$$\begin{aligned}\ddot{q}_1&=0,\\ \ddot{q}_2&=\frac{q_3}{(q_2q_3-q_1)^2},\\ \ddot{q}_3&=\frac{q_2}{(q_2q_3-q_1)^2}.\end{aligned} \tag{3}$$

We think of the q coordinates as partitioned into *driving* coordinates y and *driven* coordinates x:

$$\begin{pmatrix} q_1\\ \hline q_2\\ q_3\end{pmatrix}\equiv\begin{pmatrix} y\\ \hline x_1\\ x_2\end{pmatrix}.$$

The particular solution $y(t)\equiv q_1(t)=t$ clearly gives rise to the system (2) under the identification $x_1=q_2$, $x_2=q_3$. The Newton system (3) in R^3 is what we call a *cofactor system* (see Sec. II), which means that it has the form

$$\ddot{q}=-A(q)^{-1}\nabla W(q)=-\frac{1}{\det G(q)}G(q)\nabla W(q),$$

where $A=\operatorname{cof}G=(\det G)G^{-1}$ is the cofactor matrix of a symmetric matrix $G(q)$ of the form

$$G_{ij}(q)=\alpha q_iq_j+\beta_iq_j+\beta_jq_i+\gamma_{ij}.$$

Equivalently, $\frac{1}{2}\dot{q}^TA(q)\dot{q}+W(q)$ is an integral of motion (of *cofactor type*) for the system.

In this specific case, as is easily verified, the system (3) can be written as $\ddot{q}=-G\nabla W/(\det G)$ with

$$G(q)=\begin{pmatrix} 2q_1 & q_2 & q_3 \\ q_2 & 0 & 1 \\ q_3 & 1 & 0 \end{pmatrix}, \quad W(q)=-\frac{q_2^2+q_3^2}{q_2q_3-q_1}.$$

According to the general theory to be developed in this paper, such a driven cofactor system can be integrated using a time-dependent change of coordinates

$$u_1=\lambda_1(t,x_1,x_2),$$

$$u_2=\lambda_2(t,x_1,x_2),$$

where $\lambda_1(q)$ and $\lambda_2(q)$ are the roots of the equation $\det(G(q)-\lambda\tilde{G})=0$, with $\tilde{G}=\mathrm{diag}(0,1,1)$.

It turns out that by defining corresponding momenta s_1 and s_2 appropriately, the equations of motion for (u_1,u_2) can be put in Hamiltonian form with a time-dependent *separable* Hamiltonian. Consequently, $u_1(t)$ and $u_2(t)$ can be found using a variant of the Hamilton–Jacobi method. Changing back to old coordinates, we find $x_1(t)$ and $x_2(t)$, and the problem is solved.

We will fill in the details of this example in Sec. V, after explaining the method in general.

II. QUASIPOTENTIAL NEWTON SYSTEMS OF COFACTOR TYPE

The general framework in which we are working was developed in Refs. 9, 6, and 7. It has been extended[2] to cover also the case of Riemannian manifolds, but here we will restrict ourselves to Euclidean space. We will now quote the definitions and results needed here, some of which have already been hinted at above.

We use the shorthand $\partial_i=\partial/\partial q_i$. The notation $\mathrm{cof}\,X$ means the cofactor matrix of a square matrix X. If X is nonsingular, then $\mathrm{cof}\,X=(\det X)X^{-1}$.

Proposition 2: The "energy-like" function

$$E(q,\dot{q})=\frac{1}{2}\sum_{i,j=1}^{n}A_{ij}(q)\dot{q}_i\dot{q}_j+W(q)=\frac{1}{2}\dot{q}^TA(q)\dot{q}+W(q), \tag{4}$$

with $A(q)$ a symmetric $n\times n$ matrix, is an integral of motion of the Newton system $\ddot{q}=M(q)$ in R^n if and only if

(1) The matrix entries $A_{ij}(q)$ satisfy the cyclic conditions

$$\partial_iA_{jk}+\partial_jA_{ki}+\partial_kA_{ij}=0, \quad i,j,k=1,\ldots,n. \tag{5}$$

[*The general solution of these equations is a subspace, of dimension $\frac{1}{12}n(n+1)^2(n+2)$, of the vector space of symmetric matrices whose entries are polynomials of degree at most two in $q_1,\ldots,q_n$.*]

(2) The force $M(q)$ satisfies $A(q)M(q)+\nabla W(q)=0$.

Definition 3 (quasipotential system): A Newton system of the form

$$\ddot{q}=-A(q)^{-1}\nabla W(q),$$

where the matrix A satisfies the cyclic conditions (5), is called a *quasipotential* system. By the proposition above, $E=\frac{1}{2}\dot{q}^TA\dot{q}+W$ is an integral of motion for the system, and it is said to generate the system, since the system is completely determined by $A(q)$ and $W(q)$, and hence by E. (Special case: if $A=I$ is the identity matrix, then W is a potential for the system and E is the usual energy.)

Definition 4 (elliptic coordinates matrix G): A symmetric matrix of the form

$$G_{ij}(q)=\alpha q_i q_j+\beta_i q_j+\beta_j q_i+\gamma_{ij}, \quad i,j=1,\ldots,n, \tag{6}$$

is called an *elliptic coordinates matrix.* Using matrix multiplication, $G(q)$ can be written

$$G(q)=\alpha qq^T+\beta q^T+q\beta^T+\gamma, \tag{7}$$

with α a scalar, q and β column vectors, and γ a symmetric matrix.

Set briefly, the eigenvalues $u_1(q),\ldots,u_n(q)$ of $G(q)$ give the change of coordinates from Cartesian coordinates q to elliptic coordinates $u=u(q)$. See Ref. 6 for a more detailed explanation.

Definition 5 (associated vector N): To a given elliptic coordinate matrix G we associate the column vector $N=\alpha q+\beta=\frac{1}{2}\nabla \operatorname{tr} G$.

Proposition 6: If G is an elliptic coordinates matrix, N the associated vector, and $A=\operatorname{cof} G$, then

$$\nabla \det G=2AN. \tag{8}$$

The preceding proposition is frequently useful. It implies, for example, that $A=\operatorname{cof} G$ satisfies

$$(\det G)\partial_k A_{ij}=2[AN]_k A_{ij}-[AN]_i A_{kj}-[AN]_j A_{ik}, \tag{9}$$

from which the following remarkable property of elliptic coordinates matrices follows.

Proposition 7: If $G(q)$ is an elliptic coordinates matrix, then $A(q)=\operatorname{cof} G(q)$ satisfies the cyclic conditions (5).

Corollary 8: If $G(q)$ and $\tilde{G}(q)$ are elliptic coordinates matrices, then the matrices $A^{(0)}(q),\ldots,A^{(n-1)}(q)$ defined by the generating function

$$\operatorname{cof}(G+\mu\tilde{G})=\sum_{k=0}^{n-1} A^{(k)}\mu^i \tag{10}$$

all satisfy the cyclic conditions (5).

Remark 9: Note that $A^{(0)}=\operatorname{cof} G$ and $A^{(n-1)}=\operatorname{cof}\tilde{G}$.

We will also need a proposition that does not occur in Ref. 6.

Proposition 10: With G, N, and $A=\operatorname{cof} G$ as above,

$$\nabla(N^TAN)=2\alpha AN. \tag{11}$$

Proof: Equation (9) implies that $\Sigma_{i,j}(\partial_k A_{ij})N_iN_j=0$, from which the statement follows easily. □

Definition 11 (cofactor system): A *cofactor system* is a quasipotential Newton system of the special form

$$\ddot{q}=-A(q)^{-1}\nabla W(q)=-\frac{1}{\det G(q)}G(q)^{-1}\nabla W(q),$$

where $A=\operatorname{cof} G$, and G is a nonsingular elliptic coordinates matrix. The integral of motion $E=\frac{1}{2}\dot{q}^TA\dot{q}+W=\frac{1}{2}\dot{q}^T(\operatorname{cof} G)\dot{q}+W$ is said to be of cofactor type.

Definition 12 (cofactor pair system): A *cofactor pair system* is a Newton system which has two independent integrals of motion of cofactor type,

$$E=\tfrac{1}{2}\dot{q}^T(\operatorname{cof} G)\dot{q}+W \quad \text{and} \quad \tilde{E}=\tfrac{1}{2}\dot{q}^T(\operatorname{cof}\tilde{G})\dot{q}+\tilde{W}.$$

Equivalently, it is a system which can be written as

$$\ddot{q}=-A^{-1}\nabla W=-\tilde{A}^{-1}\nabla\tilde{W}, \tag{12}$$

where $A=\operatorname{cof} G$ and $\tilde{A}=\operatorname{cof}\tilde{G}$.

Theorem 13 (two implies *n*): *A cofactor pair system $\ddot{q}=M(q)$ in R^n has n integrals of motion*

$$E^{(k)}=\tfrac{1}{2}\dot{q}^T A^{(k)}\dot{q}+W^{(k)}, \quad k=0,\ldots,n-1, \tag{13}$$

where the matrices $A^{(k)}$ are given by (10) and the quasipotentials $W^{(k)}$ are determined (up to irrelevant additive constants) by $\nabla W^{(k)}=-A^{(k)}M$.

Remark 14: Note that the original integrals of motion $E=E^{(0)}$ and $\tilde{E}=E^{(n-1)}$ of cofactor type sit at either end of this ''cofactor chain'' of integrals.

Remark 15: It is sometimes convenient to handle the integrals of motion using a generating function

$$E_\mu=\sum_{k=0}^{n-1} E^{(k)}\mu^k=\frac{1}{2}\dot{q}^T\operatorname{cof}(G+\mu\tilde{G})\dot{q}+W_\mu, \tag{14}$$

where $W_\mu=\Sigma_{k=0}^{n-1}W^{(k)}\mu^k$.

Remark 16: For W to be well defined by $\nabla W=-AM$, the compatibility conditions $\partial_i[AM]_j=\partial_j[AM]_i$ have to be satisfied for all i and j. This, of course, is the reason that not every Newton system $\ddot{q}=M(q)$ has a potential V, and also that not every Newton system has a quasipotential W, even though by allowing $A(q)\neq I$ we enlarge the class of systems under consideration.

Now, for $\ddot{q}=M(q)$ to be a cofactor pair system, two sets of compatibility conditions need to be satisfied simultaneously; $\partial_i[AM]_j=\partial_j[AM]_i$ and $\partial_i[\tilde{A}M]_j=\partial_j[\tilde{A}M]_i$. For given G and $\tilde{G}$, this is a rather strong restriction on M. In fact, according to the theorem, it is so strong that if $\partial_i[A^{(k)}M]_j=\partial_j[A^{(k)}M]_i$ holds for $A^{(0)}=A=\operatorname{cof} G$ and $A^{(n-1)}=\tilde{A}=\operatorname{cof}\tilde{G}$, then it must hold for *all* the matrices $A^{(k)}$.

Definition 17 (fundamental equations): The *fundamental equations* associated to a pair $(G,\tilde{G})$ of elliptic coordinates matrices is the following set of $\binom{n}{2}$ second order linear PDEs:

$$\begin{aligned}0=&\sum_{r,s=1}^{n}(G_{ir}\tilde{G}_{js}-G_{jr}\tilde{G}_{is})\partial_{rs}K+3\sum_{r=1}^{n}(G_{ir}\tilde{N}_j+\tilde{G}_{jr}N_i-G_{jr}\tilde{N}_i-\tilde{G}_{ir}N_j)\partial_r K\\&+6(N_i\tilde{N}_j-N_j\tilde{N}_i)K, \quad i,j=1,\ldots,n.\end{aligned} \tag{15}$$

Here $N=\alpha q+\beta$ is the vector associated to G, with the same parameters α and β as in $G=\alpha qq^T+\beta q^T+q\beta^T+\gamma$, and similarly for $\tilde{N}$.

Theorem 18: *Let*

$$\ddot{q}=-(\operatorname{cof} G)^{-1}\nabla W=-(\operatorname{cof}\tilde{G})^{-1}\nabla\tilde{W} \tag{16}$$

be a cofactor pair system. Then the functions $K_1=W/\det G$ and $K_2=\tilde{W}/\det\tilde{G}$, while in general different, both satisfy the fundamental equations (15) associated to the pair $(G,\tilde{G})$.

Conversely, if K satisfies (15) and we set $W=K\det G$, then there is a function $\tilde{W}$ such that (16) holds. And if we set $\tilde{W}=K\det\tilde{G}$, then there is a function W such that (16) holds (but these W and $\tilde{W}$ are in general not the same as those in the previous sentence).

Remark 19: Once again, this is all about compatibility conditions. If G, $\tilde{G}$, and W are given, then $\tilde{W}$ is well defined by (16) if and only if

$$\partial_i[(\operatorname{cof}\tilde{G})(\operatorname{cof} G)^{-1}\nabla W]_j=\partial_j[(\operatorname{cof}\tilde{G})(\operatorname{cof} G)^{-1}\nabla W]_i$$

for all i and j. This is a system of $\binom{n}{2}$ second order linear PDEs for W, with coefficients depending in a complicated way on G and $\widetilde{G}$. Substituting $K=W/\det G$ and forming suitable linear combinations of the equations simplifies this system to precisely the fundamental equations (15). These being completely antisymmetric with respect to coefficients with and without the tilde, the result is the same if we go the other way around, interchanging the roles of W and $\widetilde{W}$.

Remark 20: This theorem leads to a recursive procedure for explicitly constructing infinite families of cofactor pair systems. See Ref. 6 for details.

In Ref. 6 it was shown, using the theory of bi-Hamiltonian systems, that cofactor pair systems generically are completely integrable, but it was not clear if they admit some kind of separation of variables. The special case $\widetilde{G}=I$ corresponds to conservative systems with an extra integral of motion of cofactor type. Such systems are precisely those with potentials separable in the elliptic (or parabolic) coordinates given by the eigenvalues of $G(q)$, so in that case we have a concrete method of integration. Reference 8, which appeared recently, deals with separation of variables for generic cofactor pair systems, with both G and $\widetilde{G}$ nonsingular (and nonconstant, in general). Here, we study the very degenerate case of cofactor pair systems with $\widetilde{G}=\mathrm{diag}(0,\ldots,0,1,\ldots,1)$. As we will see in the next section, these systems admit a somewhat nonstandard integration by separation of variables, and there is a surprising connection with time-dependent potentials.

III. DRIVEN SYSTEMS

From now on we fix positive integers m and n, and let $N=m+n$. Hopefully there is no risk of confusing this integer N with the vector $N(q)$ associated to an elliptic coordinates matrix $G(q)$. Let us begin by defining some notation.

Definition 21 (block notation): If X is an $N\times N$ matrix, with $N=m+n$, then we use arrow subscripts to denote blocks in X, as follows:

$$X=\begin{pmatrix} X_{\nwarrow} & X_{\nearrow} \\ X_{\swarrow} & X_{\searrow} \end{pmatrix} \quad \text{with sizes} \quad \begin{bmatrix} m\times m & m\times n \\ n\times m & n\times n \end{bmatrix}. \tag{17}$$

Similarly, if Y is a column vector in R^N, then

$$Y=\begin{pmatrix} Y_{\uparrow} \\ Y_{\downarrow} \end{pmatrix} \quad \text{with sizes} \quad \begin{bmatrix} m \\ n \end{bmatrix}. \tag{18}$$

So, for instance, $[X_{\nearrow}]_{ij}=X_{i,m+j}$.

We will consider *driven* Newton systems in R^N, where $N=m+n$. By this we mean that the first m equations depend only on the first m variables, so that they form a Newton system in R^m on their own:

$$\begin{gathered} \ddot{q}_1=M_1(q_1,\ldots,q_m), \\ \vdots \\ \ddot{q}_m=M_m(q_1,\ldots,q_m), \\ \ddot{q}_{m+1}=M_{m+1}(q_1,\ldots,q_m;q_{m+1},\ldots,q_{m+n}), \\ \vdots \\ \ddot{q}_{m+n}=M_{m+n}(q_1,\ldots,q_m;q_{m+1},\ldots,q_{m+n}). \end{gathered} \tag{19}$$

This notion is not new; for example Kossowski and Thompson[5] use tangent bundle geometry to study *submersive* systems, which are second order ODEs on manifolds, containing a subsystem depending on fewer variables (possibly after a change of coordinates).

Here, however, our purpose is to investigate what happens when a system is at the same time a driven system and a cofactor system. In this initial stage of investigation we have restricted ourselves to Euclidean space and assume that the systems splits as above in Cartesian coordinates. We hope that further research will clarify the relation between our present results and the geometric picture of Refs. 5 and 2.

Definition 22 (vectors x and y): Since we will consider the time evolution of $q_\uparrow$ and $q_\downarrow$ separately, we write $y=q_\uparrow$ and $x=q_\downarrow$ to simplify the notation.

With this definition, the system (19) can be written as

$$\begin{aligned} \ddot{y} &= M_\uparrow(y), \\ \ddot{x} &= M_\downarrow(y,x). \end{aligned} \tag{20}$$

As in example 1, $(y_1,\ldots,y_m)$ are called *driving* variables and $(x_1,\ldots,x_n)$ are called *driven* variables. The system $\ddot{y}=M_\uparrow(y)$ is called the *driving* system, since its solution $y=y(t)$, when fed into $\ddot{x}=M_\downarrow(y(t),x)$, drives the evolution of the x variables.

An important observation is that if

$$G=\alpha qq^T+\beta q^T+q\beta^T+\gamma$$

is an $N\times N$ elliptic coordinates matrix, then

$$G_{\nwarrow}=\alpha yy^T+\beta_\uparrow y^T+y(\beta_\uparrow)^T+\gamma_{\nwarrow},$$

so that $G_{\nwarrow}(y)$ is an $m\times m$ elliptic coordinates matrix in the y variables. [Similarly for $G_{\searrow}(x)$, but we will not use that here.]

The major part of this paper is devoted to proving the following theorem.

Theorem 23 (driven cofactor systems): *Suppose that a driven Newton system in R^{m+n} is of cofactor type*

$$\ddot{q}=\begin{pmatrix} M_\uparrow(y) \\ M_\downarrow(y,x) \end{pmatrix}=-(\operatorname{cof} G(q))^{-1}\frac{\partial W}{\partial q}(q). \tag{21a}$$

Suppose also that G is not constant (i.e., that α and β are not both zero), that $\det G_{\nwarrow}\neq 0$, *and that there is a potential $V(y,x)$, with y occuring parametrically, such that*

$$M_\downarrow(y,x)=-\frac{\partial V}{\partial x}(y,x). \tag{21b}$$

Then the driving system is a cofactor system in R^m. Namely, there is a function $w(y)$ such that

$$\ddot{y}=-(\operatorname{cof} G_{\nwarrow}(y))^{-1}\frac{\partial w}{\partial y}(y). \tag{22}$$

Moreover, for any given solution $y=y(t)$ of the driving system $\ddot{y}=M_\uparrow(y)$, the system

$$\ddot{x}=M_\downarrow(y(t),x)=-\frac{\partial V}{\partial x}(y(t),x), \tag{23}$$

given by the time-dependent potential $V(y(t),x)$, has n (time-dependent) integrals of motion. Under some technical assumptions, stated in definition 28, its solution $x(t)$ can be found by quadratures.

The proof is quite lengthy, so we have divided it into subsections labeled A through F. First we show that a driven cofactor system can be viewed as a degenerate form of cofactor pair system, with $\tilde{G}=\mathrm{diag}(0,\ldots,0,1,\ldots,1)$. The integrals of motion are given by a cofactor chain that terminates prematurely. We introduce a new system of coordinates, which is given by the m driving Cartesian coordinates together with the n roots of the equation $\det(G(q)-u\tilde{G})=0$. This is similar to defining elliptic coordinates implicitly as the eigenvalues of G. When the integrals of motion are transformed into these new coordinates, which is the most technical part of this paper, it turns out that they take a form similar to that known from classical separability theory (Stäckel systems). This suggests that the system should be solvable by separation of variables. We show that this is indeed the case, since the equations of motion are Hamiltonian and the variables can be separated in the time-dependent Hamilton–Jacobi equation. Perhaps surprisingly, the Hamiltonian does not involve the potential $V(y,x)$ in any direct way, but is instead given by one of the integrals of motion in the cofactor chain, divided by the determinant $\det G$, all expressed in new coordinates.

A. Driven cofactor systems as cofactor pair systems

Definition 24 (matrix J): Let J denote the $N\times N$ diagonal matrix

$$J=\mathrm{diag}(0,\ldots,0,1,\ldots,1), \tag{24}$$

with m zeros and n ones along the diagonal ($N=m+n$).

Proposition 25: A system of the form (21) is a cofactor pair system with

$$\tilde{G}(q)=\lambda G(q)+J=:\tilde{G}_\lambda(q), \tag{25}$$

for any λ such that $\det\tilde{G}_\lambda\neq 0$. Conversely, any such cofactor pair system has the form (21).

We note that since G is assumed nonsingular by the definition of cofactor system, $\det(\lambda G(q)+J)$ cannot vanish identically, so there are λ such that $\det\tilde{G}_\lambda\neq 0$. The reason for taking $\tilde{G}=\tilde{G}_\lambda$ instead of just $\tilde{G}=J$ is that the theorems we use about cofactor pair systems require both G and $\tilde{G}$ to be nonsingular. However, many of the results will be the same as if applying the theorems formally with $\tilde{G}=J$ directly, so we will regard such systems as cofactor pair systems associated with the pair (G,J).

The proof of proposition 25 uses the following lemma, which follows from the algebraic properties of an elliptic coordinates matrix G.

Lemma 26: If $M=-(\det G)^{-1}G\nabla W$, then

$$-\partial_j M_i=\sum_{r=1}^{N} G_{ir}\partial_{rj}K+3N_i\partial_j K \quad (i\neq j),$$

where $K(q)=W(q)/\det G(q)$.

Proof: Proposition 6 implies that $-M=G\nabla(K\det G)/\det G=2KN+G\nabla K$. Differentiating $-M_i=2KN_i+\sum_{r=1}^{N}G_{ir}\partial_r K$ we obtain the result immediately, since for $j\neq i$ we have $\partial_j G_{ir}=\delta_{jr}N_i$ and $\partial_j N_i=0$. □

Proof of proposition 25: By construction, the given cofactor system

$$\ddot{q}=M(q)=-(\mathrm{cof}\,G)^{-1}\nabla W=-(\det G)^{-1}G\nabla W,$$

has an integral of motion of cofactor type $E=\frac{1}{2}\dot{q}^T(\mathrm{cof}\,G)\dot{q}+W$. Now fix some constant λ such that $\det\tilde{G}_\lambda\neq 0$. Theorem 18 says that the system is a cofactor *pair* system with $\tilde{G}=\tilde{G}_\lambda$, i.e., admits an additional integral of motion of cofactor type

$$\tilde{E}_\lambda=\tfrac{1}{2}\dot{q}^T(\mathrm{cof}\,\tilde{G}_\lambda)\dot{q}+\tilde{W}_\lambda,$$

if and only if $K=W/\det G$ satisfies the fundamental equations (15) associated to the pair $(G,\tilde{G}_\lambda)$.

The antisymmetry of the fundamental equations shows that any pair $(G,\lambda G+J)$ gives rise to the same fundamental equations as the pair (G,J), so we simply plug $\tilde{G}=J$ into the fundamental equations (15) (with n replaced by $m+n$). To begin with, since J is diagonal and constant (so that $\tilde{N}=0$), we obtain

$$0=\sum_{r=1}^{m+n} G_{ir}J_{jj}\partial_{rj}K-\sum_{r=1}^{m+n} G_{jr}J_{ii}\partial_{ri}K+3(J_{jj}N_i\partial_j K-J_{ii}N_j\partial_i K),\quad i,j=1,\ldots,m+n. \tag{26}$$

Now $J_{ii}=0$ or 1 as $i\leqslant m$ and $i>m$, respectively. From this it is immediate that (26) is identically satisfied if $i,j\leqslant m$. Using lemma 26 to express the remaining equations (26) for K in terms of $M=-(\det G)^{-1}G\nabla(K\det G)$ gives $0=\partial_j M_i$ for $i\leqslant m<j$, and $0=\partial_i M_j-\partial_j M_i$ for $m<i,j$. Clearly, these equations are equivalent to M having the block structure

$$M(q)=\begin{pmatrix} M_\uparrow(y) \\ M_\downarrow(y,x)\end{pmatrix}$$

and (at least locally) a "partial potential" V such that $M_\downarrow=-\partial V/\partial x$. □

B. Integrals of motion

Proposition 27: The system (21) has $n+1$ integrals of motion $E^{(0)},\ldots,E^{(n)}$ given by the generating function

$$E_\mu=\sum_{k=0}^{n} E^{(k)}\mu^k=\sum_{k=0}^{n}\left(\frac{1}{2}\dot{q}^T A^{(k)}\dot{q}+W^{(k)}\right)\mu^k=\frac{1}{2}\dot{q}^T\operatorname{cof}(G+\mu J)\dot{q}+W_\mu \tag{27}$$

for some functions $W^{(k)}$. The integral $E^{(n)}$ has the form

$$E^{(n)}(y,\dot{y})=\tfrac{1}{2}\dot{y}^T\operatorname{cof}G_{\diagdown}(y)\dot{y}+w(y), \tag{28}$$

and is an integral of motion of the driving system $\ddot{y}=M_\uparrow(y)$, of cofactor type in the y variables.

Proof: According to theorem 13, our cofactor pair system should have a chain of $N=m+n$ integrals of motion. Here, however, that number is reduced since some of them will be linearly dependent. More specifically, for arbitrary λ such that $\det\tilde{G}_\lambda\neq 0$, theorem 13 gives us integrals $E_\lambda^{(0)},\ldots,E_\lambda^{(N-1)}$ which we write using a generating function

$$E_{\lambda,\mu}=\sum_{k=0}^{m+n-1} E_\lambda^{(k)}\mu^k=\frac{1}{2}\dot{q}^T\operatorname{cof}(G+\mu\tilde{G}_\lambda)\dot{q}+W_{\lambda,\mu} \tag{29}$$

as in (14). By construction, $\dot{E}_{\lambda,\mu}=0$ for all values of μ and all λ such that $\det\tilde{G}_\lambda\neq 0$. But $E_{\lambda,\mu}$ depends polynomially on λ and μ, since $\operatorname{cof}(G+\mu\tilde{G}_\lambda)=\operatorname{cof}(G+\mu(\lambda G+J))=\operatorname{cof}((1+\mu\lambda)G+\mu J))$ does. Hence, $\dot{E}_{\lambda,\mu}=0$ identically. In particular, if we set $\lambda=0$ we extract the constant term with respect to λ, which is just the E_μ of (27), a polynomial in μ whose coefficients are integrals of motion.

The reason why E_μ is only of degree n (instead of $m+n-1$) is that the matrix J has so few nonzero elements that the expansion of $\operatorname{cof}(G+\mu J)$ in powers of μ terminates "prematurely" (the details in this expansion are explained below, after the proof):

$$\operatorname{cof}(G+\mu J)=\operatorname{cof} G + \cdots + \begin{pmatrix} A^{(n-1)}_{\nwarrow} & -(\operatorname{cof} G_{\nwarrow})G_{\nearrow} \\ -((\operatorname{cof} G_{\nwarrow})G_{\nearrow})^T & (\det G_{\nwarrow})I_{n\times n}\end{pmatrix}\mu^{n-1}+\begin{pmatrix}\operatorname{cof} G_{\nwarrow} & 0_{m\times n}\\ 0_{n\times m} & 0_{n\times n}\end{pmatrix}\mu^n$$
$$=:\sum_{k=0}^{n} A^{(k)}\mu^k. \tag{30}$$

All the coefficients in the generating function $E_{\lambda,\mu}$ in (29) are linear combinations of these $n+1$ basic integrals $E^{(0)},\ldots,E^{(n)}$, so even though one can obtain a seemingly longer chain (with $N=m+n$ integrals) by taking $\lambda\neq 0$, it would not contain any essentially new integrals of motion. (Note also that the polynomial E_μ is what we would have obtained by applying theorem 13 formally with the singular matrix $\tilde{G}=J$ instead of $\tilde{G}_\lambda$.)

The integral $E^{(n)}$ has the form

$$E^{(n)}=\frac{1}{2}(\dot{y}^T \quad \dot{x}^T)\begin{pmatrix}\operatorname{cof} G_{\nwarrow}(y) & 0_{m\times n}\\ 0_{n\times m} & 0_{n\times n}\end{pmatrix}\begin{pmatrix}\dot{y}\\ \dot{x}\end{pmatrix}+W^{(n)}(y,x)=\frac{1}{2}\dot{y}^T\operatorname{cof} G_{\nwarrow}(y)\dot{y}+w(y), \tag{31}$$

where clearly $W^{(n)}=w(y)$ cannot depend on x if $E^{(n)}$ is to be an integral of motion. Consequently, $E^{(n)}(y,\dot{y})$ must be an integral of motion of the driving system $\ddot{y}=M_\uparrow(y)$, and it is of cofactor type in the y variables. □

In (30) we have written out some blocks in the matrices $A^{(n-1)}$ and $A^{(n)}$ for future reference (in the proof of proposition 36). These can be found either by analyzing the cofactor expansion directly or by writing the identity

$$(G+\mu J)\operatorname{cof}(G+\mu J)=\det(G+\mu J)I_{N\times N}$$

as

$$JA^{(n)}\mu^{n+1}+(JA^{(n-1)}+GA^{(n)})\mu^n+\cdots=(0\,\mu^{n+1}+(\det G_{\nwarrow})\mu^n+\ldots)I_{N\times N}$$

and identifying coefficients block-wise at μ^{n+1} and μ^n, using that the matrices $A^{(i)}$ are symmetric. The block $A^{(n-1)}_{\nwarrow}$ does not enter into this identity until at the power μ^{n-1}, and depends on G in a more complicated way. Fortunately, the only information about $A^{(n-1)}_{\nwarrow}$ that we will need is that $A^{(n-1)}$ satisfies the cyclic conditions (5) which connect derivatives of $A^{(n-1)}_{\nwarrow}$ to derivatives of the other blocks, which are known explicitly.

We have now completed the proof of the first statement of theorem 23, namely, that the driving system is a cofactor system in the y variables.

Moreover, for any given solution $y=y(t)$ of the driving system, we can consider $E^{(0)},\ldots,E^{(n-1)}$ as functions of $(x,\dot{x},t)$, and these constitute n time-dependent integrals of motion of the driven system (23) given by the time-dependent potential $V(y(t),x)$. These are the integrals referred to at the end of theorem 23.

C. Separation coordinates

Our remaining task (which is much more complicated) is to show how to integrate the driven system $\ddot{x}=-(\partial V/\partial x)(y(t),x)$, given a solution $y(t)$ of the driving system $\ddot{y}=M_\uparrow(y)$. This will be accomplished using a change of variables $(y,x)\mapsto(v,u)$ on R^{m+n} defined as follows:

Definition 28 (variables u and v, roots λ): Let $v_i=y_i$ *for* $i=1,\ldots,m$. *Let* $u_j=\lambda_j(y,x)$ *for* $j=1,\ldots,n$, *where* $\lambda_1,\ldots,\lambda_n$ *are the roots of the n*th *degree polynomial equation*

$$\det(G(y,x)-\lambda J)=0. \tag{32}$$

(We assume that this really defines a coordinate system. This requires, to begin with, that all the roots λ_j are nonconstant as functions of q. Moreover, the gradients of the v_i and u_j must be linearly independent. Because of lemma 31 below, this holds at least in a neighborhood of any point where all $\lambda_j(q)$ are distinct.)

Definition 29 [polynomial $U(\mu)$]. Let

$$U(\mu)=(u_1-\mu)(u_2-\mu)\cdots(u_n-\mu). \tag{33}$$

It follows from the definition of the u_k as roots of the polynomial $\det(G-\mu J)$, which has the leading term $(-\mu)^n \det G_{\nwarrow}$, that

$$\det(G-\mu J)=U(\mu)\det G_{\nwarrow}. \tag{34}$$

Our aim is to express the integrals of motion $E^{(0)},\ldots,E^{(n)}$ in terms of the new coordinates v and u, and likewise for the equations of motion for the system [although for that purpose we view $x\mapsto u=\lambda(y(t),x)$, where $y(t)$ is a given solution of the driving system, as a time-dependent change of variables in R^n; more about that later]. The remainder of this subsection contains technical preparations for these tasks.

Definition 30 (matrix Ψ): Let Ψ denote the $N\times N$ matrix of partial derivatives of v and u with respect to y and x, arranged so that the columns of Ψ are the gradients of v and u with respect to $q=\binom{y}{x}$:

$$\Psi=(\nabla v_1\cdots\nabla v_m \;\; \nabla u_1\cdots\nabla u_n)=(e_1\cdots e_m \;\; \nabla\lambda_1\cdots\nabla\lambda_n), \tag{35}$$

where e_i is the column vector with 1 in position i and 0 elsewhere. [In the block notation of (17), $\Psi_{\nwarrow}=I_{m\times m}$ and $\Psi_{\swarrow}=0_{n\times m}$.]

With this definition we have

$$\begin{pmatrix}\dot v\\ \dot u\end{pmatrix}=\Psi^T\dot q, \quad \dot q=\frac{1}{\det\Psi}(\operatorname{cof}\Psi^T)\begin{pmatrix}\dot v\\ \dot u\end{pmatrix}, \tag{36}$$

and also

$$\nabla=\begin{pmatrix}\partial/\partial y\\ \partial/\partial x\end{pmatrix}=\Psi\begin{pmatrix}\partial/\partial v\\ \partial/\partial u\end{pmatrix}. \tag{37}$$

(Note that $\partial/\partial y\neq\partial/\partial v$ even though $y=v$, hence the need for the different names.)

The following lemma will give us information about the last n columns in the matrix Ψ (or, equivalently, about the blocks $\Psi_{\nearrow}$ and $\Psi_{\searrow}$).

Lemma 31 (eigenvalues and eigenvectors): Let $G(q)$ and $\tilde G(q)$ be elliptic coordinates matrices. If $\lambda=\lambda(q)$ is a simple root of $\det(G-\lambda\tilde G)=0$, then $\nabla\lambda(q)$ is the corresponding "eigenvector:"

$$(G(q)-\lambda(q)\tilde G(q))\nabla\lambda(q)=0. \tag{38}$$

If λ_1 and λ_2 are two different such roots, then

$$(\nabla\lambda_1)^T\tilde G\nabla\lambda_2=0. \tag{39}$$

Proof: Let $G_r=G-r\tilde G$ and $p(r)=\det G_r$. For each r, G_r is an elliptic coordinates matrix, with associated vector $N_r=N-r\tilde N$, where $N=\alpha q+\beta$ and $\tilde N=\tilde\alpha q+\tilde\beta$. If we apply proposition 6 to G_r we get $\nabla p(r)=2(\operatorname{cof}G_r)N_r$. Now compute the gradient of $p(\lambda(q))\equiv 0$:

$$0=(\nabla p)(\lambda(q))+p'(\lambda(q))\nabla\lambda(q)=2\operatorname{cof}(G-\lambda(q)\tilde G)(N-\lambda(q)\tilde N)+p'(\lambda(q))\nabla\lambda(q). \tag{40}$$

Multiplying this by $G-\lambda(q)\tilde{G}$ yields, since $\det(G-\lambda(q)\tilde{G})=0$ by definition of λ,

$$0=p'(\lambda(q))\,(G-\lambda(q)\tilde{G})\nabla\lambda(q).$$

But $p'(\lambda(q))\neq 0$ since $\lambda(q)$ is assumed to be a simple root of p. The first statement follows.

The second statement comes from the simple observation that if $GX_1=\lambda_1\tilde{G}X_1$ and $GX_2=\lambda_2\tilde{G}X_2$, then, since G and $\tilde{G}$ are symmetric,

$$0=(GX_1)^TX_2-X_1^T(GX_2)=(\lambda_1-\lambda_2)X_1^T\tilde{G}X_2.$$

□

Lemma 31, with $\tilde{G}=J$, says that

$$G\nabla u_k=u_kJ\nabla u_k, \tag{41}$$

and that $\nabla u_1,\ldots,\nabla u_n$ (which are the last n columns of Ψ) are "J-orthogonal,"

$$(\nabla u_j)^TJ\,(\nabla u_k)=0, \quad \text{if } j\neq k. \tag{42}$$

Thus, the columns $(\nabla u_j)_\downarrow$ of the lower right $n\times n$ block $\Psi_\searrow$ in Ψ are orthogonal in R^n in the ordinary Euclidean sense, with squared lengths $\Delta_1,\ldots,\Delta_n$, where

$$\Delta_k=((\nabla u_k)_\downarrow)^T(\nabla u_k)_\downarrow=\sum_{i=1}^{n}(\Psi_{n+i,n+k})^2. \tag{43}$$

Consequently, since the first m columns in Ψ are just $e_1,\ldots,e_m$, the interpretation of an $n\times n$ determinant as a volume in R^n shows that

$$(\det\Psi)^2=\Delta_1\Delta_2\cdots\Delta_n. \tag{44}$$

It also follows that, with $\Delta=\mathrm{diag}(\Delta_1,\ldots,\Delta_n)$ and $\mathcal{U}=\mathrm{diag}(u_1,\ldots,u_n)$,

$$\Psi^TJ\,\Psi=\begin{pmatrix}0_{m\times m} & 0_{m\times n}\\ 0_{n\times m} & \Delta\end{pmatrix} \tag{45}$$

and

$$\Psi^TG\,\Psi=\begin{pmatrix}G_\nwarrow & 0_{m\times n}\\ 0_{n\times m} & \mathcal{U}\Delta\end{pmatrix}. \tag{46}$$

D. Integrals of motion in separation coordinates

Now we will transform the integrals of motion $E^{(0)},\ldots,E^{(n)}$ given by (27) to the new coordinates (v,u).

Kinetic part: We begin with the "kinetic" part $\dot{q}^T\,\mathrm{cof}(G+\mu J)\dot{q}$. Write $G_\mu=G+\mu J$ for simplicity. Equation (36) gives

$$\dot{q}^T(\mathrm{cof}\,G_\mu)\dot{q}=\frac{1}{(\det\Psi)^2}(\dot{v}^T\ \ \dot{u}^T)\mathrm{cof}(\Psi^TG_\mu\Psi)\begin{pmatrix}\dot{v}\\ \dot{u}\end{pmatrix}.$$

Equations (45) and (46) show that

$$\Psi^TG_\mu\Psi=\begin{pmatrix}G_\nwarrow & 0_{m\times n}\\ 0_{n\times m} & \mathcal{U}_\mu\Delta\end{pmatrix},$$

where

$$\mathcal{U}_\mu = \mathcal{U} + \mu I_{n\times n} = \mathrm{diag}(u_1+\mu,\ldots,u_n+\mu). \tag{47}$$

This, together with (44), gives

$$\frac{1}{(\det\Psi)^2}\,\mathrm{cof}(\Psi^T G_\mu \Psi) = \begin{pmatrix} \det\mathcal{U}_\mu\,\mathrm{cof}G_{\nwarrow} & 0_{m\times n} \\ 0_{n\times m} & (\det G_{\nwarrow})\Delta^{-1}\,\mathrm{cof}\,\mathcal{U}_\mu \end{pmatrix}.$$

Sandwiching this between $(\dot v^T\ \dot u^T)$ and $\binom{\dot v}{\dot u}$, we finally obtain

$$\dot q^T(\mathrm{cof}\,G_\mu)\dot q = (\det\mathcal{U}_\mu)\dot v^T(\mathrm{cof}\,G_{\nwarrow})\dot v + (\det G_{\nwarrow})\dot u^T(\Delta^{-1}\mathrm{cof}\,\mathcal{U}_\mu)\,\dot u. \tag{48}$$

Note that $\det\mathcal{U}_\mu = \Pi_1^n(u_i+\mu)$ is the generating function for the elementary symmetric polynomials in the n variables $\{u_1,\ldots,u_n\}$, while the kth entry in the diagonal matrix $\mathrm{cof}\,\mathcal{U}_\mu$ generates the elementary symmetric polynomials in the $n-1$ variables $\{u_1,\ldots,u_n\}\setminus\{u_k\}$.

Structure of Δ_k: Next we prove a statement about how Δ_k, defined by (43), depends on u and v. This result is important for showing separability later.

Proposition 32: The quantities $\Delta_1,\ldots,\Delta_n$ satisfy

$$\Delta_k(u,v)\,U'(u_k)\det G_{\nwarrow}(v) = f_k(u_k), \quad k=1,\ldots,n, \tag{49}$$

where each of the functions $f_1,\ldots,f_n$ depends on one variable only, as indicated. [But $U'(u_k)$, which is just the derivative of $U(\mu)=\Pi(u_i-\mu)$ evaluated at $\mu=u_k$, depends on all the variables u_i.]

Proof: Recall that $\Delta=\mathrm{diag}(\Delta_1,\ldots,\Delta_n)=(\Psi_{\searrow})^T\Psi_{\searrow}$, by (45). Since the columns ∇u_k make up the blocks $\Psi_{\nearrow}$ and $\Psi_{\searrow}$, the "upper part" of (41) shows that

$$G_{\nwarrow}\Psi_{\nearrow} + G_{\nearrow}\Psi_{\searrow} = 0_{m\times n}. \tag{50}$$

Recall from (34) that

$$\det(G-\mu J) = U(\mu)\det G_{\nwarrow} = \det G_{\nwarrow}\left((-\mu)^n + (-\mu)^{n-1}\left(\sum u_i\right) + \cdots\right).$$

By proposition 6,

$$\nabla\det(G-\mu J) = 2\,\mathrm{cof}(G-\mu J)\,N = 2((-\mu)^n A^{(n)} + (-\mu)^{n-1}A^{(n-1)} + \cdots)\,N.$$

(Note that N is the vector associated to $G-\mu J$ as well as to G, since J is constant.) Hence, in particular,

$$2\,A^{(n-1)}N = \nabla\left((\det G_{\nwarrow})\sum u_i\right).$$

Now, $(\nabla\det G_{\nwarrow})_{\downarrow}=0$ since $G_{\nwarrow}$ depends only on the y variables, and consequently

$$2\,(A^{(n-1)}N)_{\downarrow} = (\det G_{\nwarrow})\sum (\nabla u_i)_{\downarrow} = (\det G_{\nwarrow})\Psi_{\searrow}1_n,$$

where $1_n\in R^n$ is the column vector with all ones. If we use what we know from (30) about the block structure of $A^{(n-1)}$ and divide by $\det G_{\nwarrow}$, this takes the form

$$2\begin{pmatrix} -G_{\nwarrow}^{-1}G_{\nearrow} \\ I_{n\times n}\end{pmatrix}^T N = \Psi_{\searrow}1_n. \tag{51}$$

Combining (50) and (the transpose of) (51), we find

$$2\,N^T\begin{pmatrix}\Psi_{\nearrow}\\ \Psi_{\searrow}\end{pmatrix}=2\,N^T\begin{pmatrix}-G^{-1}_{\nwarrow}G_{\nearrow}\Psi_{\searrow}\\ \Psi_{\searrow}\end{pmatrix}=(\Psi_{\searrow}1_n)^T\Psi_{\searrow}=1_n^T\Delta=(\Delta_1\quad\Delta_2\ldots\Delta_n).$$

In other words,

$$\Delta_k=2\,N^T\nabla u_k,\quad k=1,\ldots,n. \tag{52}$$

As a special case of (40), with $\tilde{G}=J$, $\tilde{N}=0$, $p(\mu)=\det(G-\mu J)=U(\mu)\det G_{\nwarrow}$, and $\lambda=u_k$, we have

$$U'(u_k)\,(\det G_{\nwarrow})\nabla u_k=-2\,\mathrm{cof}(G-u_kJ)\,N, \tag{53}$$

which, because of (52), when multiplied from the left by $2\,N^T$ yields

$$U'(u_k)\,(\det G_{\nwarrow})\,\Delta_k=-4\,N^T\,\mathrm{cof}(G-u_kJ)\,N, \tag{54}$$

The left-hand side here is what we claim depends on u_k only, and we will prove this by showing that the gradient of the right hand side is proportional to ∇u_k. [Clearly, a function $f(v,u)$ depends on u_k alone iff $(\partial f/\partial u_k)\nabla u_k$ is the only contribution when computing ∇f with the chain rule.]

Proposition 10, applied to $G-\mu J$ (which has the same α and N as G), shows that

$$\nabla(N^T\mathrm{cof}(G-\mu J)\,N)=2\,\alpha\mathrm{cof}(G-\mu J)\,N.$$

Hence, by the chain rule,

$$\nabla(N^T\,\mathrm{cof}(G-u_kJ)\,N)=2\,\alpha\,\mathrm{cof}(G-u_kJ)\,N+\frac{d}{d\mu}[N^T\mathrm{cof}(G-\mu J)\,N]_{\mu=u_k}\nabla u_k\,.$$

It is manifest that the second term is proportional to ∇u_k, and so is in fact also the first term, because of (53). This finishes the proof of proposition 32. □

Remark 33: In all the examples we have computed, it turns out that $f_i(q_i)=f(q_i)$ for a single function f, but we have no proof that this is always true. In any case, it is not needed for proving separability here.

Solution of the fundamental equations: We previously (in the proof of proposition 25) investigated the fundamental equations associated to the pair (G,J):

$$0=\frac{\partial M_i}{\partial q_j}\quad\text{for } i\leqslant m<j, \tag{55}$$

$$0=\frac{\partial M_i}{\partial q_j}-\frac{\partial M_j}{\partial q_i}\quad\text{for } m<i,j, \tag{56}$$

where

$$M=-\frac{G\,\nabla(K\det G)}{\det G}$$

is the right-hand side in the cofactor pair system $\ddot{q}=M(q)$ generated by $E^{(0)}=\frac{1}{2}\dot{q}^T(\mathrm{cof}\,G)\dot{q}+K\det G$.

Proposition 34: In terms of the separations coordinates (v,u), the general solution of the fundamental equations(55) and (56) is

$$K(v,u)=\frac{1}{\det G_{\nwarrow}(v)}\left(w(v)+\sum_{k=1}^{n}\frac{g_k(u_k)/u_k}{U'(u_k)}\right), \tag{57}$$

where $g_1(u_1),\ldots,g_n(u_n)$ are arbitrary functions of one variable, and $U'(u_k)$ is as in proposition 32.

Proof: Recall from (37) that

$$\nabla\equiv\begin{pmatrix}\partial_y\\ \partial_x\end{pmatrix}=\Psi\begin{pmatrix}\partial_v\\ \partial_u\end{pmatrix},$$

while (34) shows that $\det G=u_1\ldots u_n\det G_{\nwarrow}(v)$. Hence,

$$-M=G\Psi\begin{pmatrix}\partial_v(K\det G)\\ \partial_u(K\det G)\end{pmatrix}/\det G=\frac{\begin{pmatrix}G_{\nwarrow} & 0\\ G_{\swarrow} & \Psi_{\searrow}\mathcal{U}\end{pmatrix}\begin{pmatrix}u_1\cdots u_n\,\partial_v(K\det G_{\nwarrow})\\ (\det G_{\nwarrow})\partial_u(u_1\cdots u_nK)\end{pmatrix}}{u_1\ldots u_n\det G_{\nwarrow}}$$

$$=\begin{pmatrix}\dfrac{G_{\nwarrow}\partial_v(K\det G_{\nwarrow})}{\det G_{\nwarrow}}\\ \dfrac{G_{\swarrow}\partial_v(K\det G_{\nwarrow})}{\det G_{\nwarrow}}+\Psi_{\searrow}\begin{pmatrix}\partial_{u_1}(u_1K)\\ \vdots\\ \partial_{u_n}(u_nK)\end{pmatrix}\end{pmatrix},$$

where $G\Psi$ was computed using (41). Equation (55) says that the upper part

$$M_{\uparrow}=-\frac{G_{\nwarrow}\partial_v(K\det G_{\nwarrow})}{\det G_{\nwarrow}}$$

depends only on the y (or v) variables, which happens if and only if

$$K\det G_{\nwarrow}=w(v)+F(u).$$

The function $w(y)$ here is the same as in theorem 23, since the driving system $\ddot{y}=M_{\uparrow}$ is generated by $E^{(n)}=\frac{1}{2}\dot{y}^T(\operatorname{cof}G_{\nwarrow})\dot{y}+w(y)$.

The function $F(u)$ is then determined by (56), which obviously is only interesting if $i\neq j$. In this case, if we set $i=m+k$ and $j=m+l$, the first term in

$$M_i=M_{m+k}=-\frac{[G_{\swarrow}]_{\text{row }k}\,\partial_v(K\det G_{\nwarrow})}{\det G_{\nwarrow}}-[\Psi_{\searrow}]_{\text{row }k}\begin{pmatrix}\partial_{u_1}(u_1K)\\ \vdots\\ \partial_{u_n}(u_nK)\end{pmatrix}$$

does not depend on $q_j=x_l$, since row k of $G_{\swarrow}$ depends on x_k and y only. Then, since by the definition of Ψ

$$[\Psi_{\searrow}]_{\text{row }k}=\begin{pmatrix}\dfrac{\partial u_1}{\partial x_k} & \dfrac{\partial u_2}{\partial x_k}\cdots\dfrac{\partial u_n}{\partial x_k}\end{pmatrix},$$

we find

$$\frac{\partial M_i}{\partial q_j}=-\frac{\partial}{\partial x_l}\sum_{s=1}^{n}\frac{\partial u_s}{\partial x_k}\partial_{u_s}(u_sK)=-\sum_{s=1}^{n}\frac{\partial^2u_s}{\partial x_l\partial x_k}\partial_{u_s}(u_sK)-[\Psi_{\searrow}]_{\text{row }k}\frac{\partial}{\partial x_l}\begin{pmatrix}\partial_{u_1}(u_1K)\\ \vdots\\ \partial_{u_n}(u_nK)\end{pmatrix}.$$

In the second term we substitute $K=(w(v)+F(u))/\det G_{\nwarrow}(v)$ and plug what we have into (56). The first term cancels out in the subtraction, leaving

$$0=\frac{\partial M_i}{\partial q_j}-\frac{\partial M_j}{\partial q_i}=-\frac{1}{\det G_{\nwarrow}}\left([\Psi_{\searrow}]_{\text{row }k}\frac{\partial}{\partial x_l}\begin{pmatrix}\partial_{u_1}(u_1F)\\ \vdots\\ \partial_{u_n}(u_nF)\end{pmatrix}-[\Psi_{\searrow}]_{\text{row }l}\frac{\partial}{\partial x_k}\begin{pmatrix}\partial_{u_1}(u_1F)\\ \vdots\\ \partial_{u_n}(u_nF)\end{pmatrix}\right).$$

Now, since $\partial_x=\Psi_{\searrow}\partial_u$, this shows that

$$0=[\Psi_{\searrow}]_{\text{row }l}\,\Omega\,[\Psi^T_{\searrow}]_{\text{column }k}-[\Psi_{\searrow}]_{\text{row }k}\,\Omega\,[\Psi^T_{\searrow}]_{\text{column }l},$$

where Ω (temporarily) denotes the $n\times n$ matrix with entries $\Omega_{ab}=\partial_{u_a}\partial_{u_b}(u_bF)$. In other words, $0=\Psi_{\searrow}(\Omega-\Omega^T)\Psi^T_{\searrow}$, or, finally,

$$\frac{\partial^2}{\partial u_a\partial u_b}((u_a-u_b)F(u))=0,\quad a,b=1,\ldots,n. \tag{58}$$

This equation occurs in classical separability theory in connection with separation in elliptic and parabolic coordinates. It is known to have the general solution

$$F(u)=\sum_{k=1}^{n}\frac{F_k(u_k)}{\prod\limits_{\substack{j=1\\ j\neq k}}^{n}(u_k-u_j)},$$

with arbitrary functions $F_1(u_1),\ldots,F_n(u_n)$ depending on one variable each (see Lemma 1 and Lemma 2 in Ref. 3). Hence, we have the general solution

$$K(v,u)=\frac{1}{\det G_{\nwarrow}(v)}\left(w(v)+\sum_k\frac{F_k(u_k)}{\Pi_{j\neq k}(u_k-u_j)}\right). \tag{59}$$

For our purposes, it turns out to be most convenient to write this in the form (57). □

Potential part: It remains to investigate the form of the "potential" parts $W^{(0)},\ldots,W^{(n)}$ in the (v,u) coordinates.

Proposition 35: The functions $W^{(0)},\ldots,W^{(n-1)}$ take the following form when expressed in the (v,u) coordinates:

$$W^{(a)}(v,u)=\sigma_{n-a}(u)\,w(v)+\sum_{k=1}^{n}\frac{\sigma_{n-a-1}(\check{u}_k)\,g_k(u_k)}{U'(u_k)}, \tag{60}$$

where $\sigma_b(u)$ denotes the elementary symmetric polynomial of degree b in the n variables $\{u_1,\ldots,u_n\}$, and $\sigma_b(\check{u}_k)$ denotes the elementary symmetric polynomial of degree b in the $n-1$ variables $\{u_1,\ldots,u_n\}\backslash\{u_k\}$. As above, $g_1(u_1),\ldots,g_n(u_n)$ are functions of one variable, and $U'(u_k)$ is as in proposition 32.

In particular, the function $W^{(n)}$ depends on the v coordinates only:

$$W^{(n)}=w(v). \tag{61}$$

Proof: We have seen that $W^{(n)}=w(y)$ depends only on y in the original coordinates, hence also $W^{(n)}=w(v)$. We also know that $K=W^{(0)}/\det G$ is a solution of the fundamental equations, so according to (57)

$$W^{(0)}(v,u)=\frac{\det G(v,u)}{\det G_{\nwarrow}(v)}\left(w(v)+\sum_{k=1}^{n}\frac{g_k(u_k)/u_k}{U'(u_k)}\right)=u_1\cdots u_n\,w(v)+\sum_{k=1}^{n}\frac{\sigma_{n-1}(\check{u}_k)\,g_k(u_k)}{U'(u_k)}. \tag{62}$$

With M determined by $W^{(0)}$, the remaining $W^{(a)}$ are determined (up to irrelevant additive constants) by the relation $\nabla W^{(a)}=-A^{(a)}M$, or

$$\nabla W_\mu=\sum_{a=0}^{n}\nabla W^{(a)}\mu^a=-\left(\sum_{a=0}^{n}A^{(a)}\mu^a\right)M=\operatorname{cof}(G+\mu J)\frac{G}{\det G}\nabla W^{(0)}.$$

We multiply by $(\det G)\Psi^T(G+\mu J)$ from the left and use (37), (45), and (46) to obtain the equivalent condition

$$(\det G)\begin{pmatrix}G_{\nwarrow} & 0\\ 0 & (\mathcal{U}+\mu I)\Delta\end{pmatrix}\begin{pmatrix}\partial_v W_\mu\\ \partial_u W_\mu\end{pmatrix}=\det(G+\mu J)\begin{pmatrix}G_{\nwarrow} & 0\\ 0 & \mathcal{U}\Delta\end{pmatrix}\begin{pmatrix}\partial_v W^{(0)}\\ \partial_u W^{(0)}\end{pmatrix}.$$

It is a tedious but fairly straightforward calculation, which we omit, to verify that this is satisfied by

$$W_\mu=\left(\prod_{i=1}^{n}(u_i+\mu)\right)w(v)+\sum_{k=1}^{n}\left(\prod_{\substack{j=1\\ j\neq k}}^{n}(u_j+\mu)\right)\frac{g_k(u_k)}{U'(u_k)},$$

from which $W^{(a)}$ can be read off as the coefficient of μ^a. □

Summary: We have now determined the form of the integrals of motion in separation coordinates (v,u). We have seen that

$$E^{(n)}=\tfrac{1}{2}\dot{v}^T(\operatorname{cof}G_{\nwarrow}(v))\dot{v}+w(v) \tag{63}$$

depends only on v, while the form of $E^{(0)},\ldots,E^{(n-1)}$ is obtained from (48) and (60):

$$E^{(a)}=\sigma_{n-a}(u)\,E^{(n)}+\sum_{k=1}^{n}\sigma_{n-a-1}(\check{u}_k)\left(\frac{1}{2}(\det G_{\nwarrow})\frac{\dot{u}_k^2}{\Delta_k}+\frac{g_k(u_k)}{U'(u_k)}\right). \tag{64}$$

If we let $s_k=\dot{u}_k/\Delta_k$ and use proposition 32, we can write this as

$$E^{(a)}=\sigma_{n-a}(u)\,E^{(n)}+\sum_{k=1}^{n}\frac{\sigma_{n-a-1}(\check{u}_k)}{U'(u_k)}\left(\frac{1}{2}f_k(u_k)\,s_k^2+g_k(u_k)\right). \tag{65}$$

Note in particular that

$$E^{(n-1)}=\left(\sum_{k=1}^{n}u_k\right)E^{(n)}+\sum_{k=1}^{n}\left(\frac{f_k(u_k)\,s_k^2+g_k(u_k)}{U'(u_k)}\right). \tag{66}$$

E. The equations of motion are Hamiltonian

Given some solution $y=y(t)$ [or $v=v(t)$] of the driving system, we now consider $u=u(y(t),x)$ as a time-dependent change of variables in R^n. We want to express the driven system $\ddot{x}=-(\partial V/\partial x)(y(t),x)$ in terms of the u variables. Note that since $E^{(n)}$ is an integral of motion for the driving system, it can from now on be treated as simply a constant, the value of which is determined by which solution $y(t)$ is taken.

Proposition 36: The equations of motion for the u variables can be put into canonical Hamiltonian form

$$\dot{u} = \frac{\partial h}{\partial s}(u,s,t),$$

$$\dot{s} = -\frac{\partial h}{\partial u}(u,s,t),$$

with momenta $s_1,\ldots,s_n$ *defined by*

$$s_k = \frac{\dot{u}_k}{\Delta_k} \tag{67}$$

(Δ_i *as in proposition 32*), *and with the time-dependent Hamiltonian*

$$h(u,s,t) = \frac{1}{\det G_{\diagdown}(y(t))}\left(\left(\sum_{k=1}^{n} u_k\right)E^{(n)} + \sum_{k=1}^{n}\left(\frac{f_k(u_k)\,s_k^2 + g_k(u_k)}{U'(u_k)}\right)\right). \tag{68}$$

Proof: First we see from (66) that h is simply $E^{(n-1)}/\det G_{\diagdown}$, expressed in terms of u, s, and t. Now, with $p=\dot{x}$ the system $\ddot{x} = -(\partial V/\partial x)(y(t),x)$ has a canonical Hamiltonian formulation

$$\dot{x} = \frac{\partial H}{\partial p}(x,p,t),$$

$$\dot{p} = -\frac{\partial H}{\partial x}(x,p,t),$$

where $H(x,p,t) = \frac{1}{2}p^T p + V(y(t),x)$. Consider the extended phase space R^{2n+1} with coordinates (x,p,t). With $T=t$, the variables (u,s,T) constitute a different coordinate system on this space. The vector field in extended phase space that corresponds to the canonical phase flow is encoded in the 1-form $p^T\,dx - H\,dt$ (by spanning the kernel of its exterior derivative). It follows that the equations of motion are canonical in the new coordinates, with Hamiltonian h, if the two 1-forms,

$$p^T\,dx - H\,dt \quad \text{and} \quad s^T\,du - h\,dT,$$

have the same exterior derivative (see Sec. 45 in Ref. 1). Here we view dx and du as column vectors of 1-forms dx_i and du_i, in order to be consistent with our previous matrix notation. Since here we have $dT = dt$, the proof amounts to showing that

$$d(p^T\,dx - s^T\,du + (h-H)\,dt) = 0. \tag{69}$$

The computations will be performed in the (x,p,t) coordinates, and whenever we write y we mean the given function $y(t)$. Note also that since $G_{\diagdown}$ depends only on the y variables, it too will be a function of t only. In particular, $\det G_{\diagdown}$ is a function of t only.

We need to express $s^T\,du$ and h in terms of the (x,p,t) coordinates. Recall that by the definition 30 of the matrix Ψ we have

$$(\nabla u_1,\ldots,\nabla u_n) = \begin{pmatrix} \Psi_{\nearrow} \\ \Psi_{\searrow} \end{pmatrix}.$$

Since

$$du_i = \sum_{k=1}^{m}\frac{\partial u}{\partial y_k}\dot{y}_k\,dt + \sum_{k=1}^{n}\frac{\partial u}{\partial x_k}dx_k$$

we obtain

$$du=(\Psi_{\nearrow})^T\dot{y}\,dt+(\Psi_{\searrow})^T\,dx,$$

that is,

$$\dot{u}=(\Psi_{\nearrow})^T\dot{y}+(\Psi_{\searrow})^T\dot{x}.$$

If we transpose and multiply from the right by $\Delta^{-1}=\mathrm{diag}(\Delta_k^{-1})$, we get

$$s^T=\dot{y}^T\Psi_{\nearrow}\Delta^{-1}+p^T\Psi_{\searrow}\Delta^{-1}.$$

Now we define an $m\times n$ matrix Ξ by

$$\Xi=\Psi_{\nearrow}(\Psi_{\searrow})^{-1}. \tag{70}$$

Since $\Delta=(\Psi_{\searrow})^T\Psi_{\searrow}$, it follows that

$$\Psi_{\searrow}\Delta^{-1}(\Psi_{\nearrow})^T=\Xi^T,$$

$$\Psi_{\nearrow}\Delta^{-1}(\Psi_{\nearrow})^T=\Xi\,\Xi^T.$$

Consequently,

$$s^T\,du=p^T\,dx+(\dot{y}^T\Xi\,\Xi^T\dot{y}+\dot{y}^T\Xi p)dt+\dot{y}^T\Xi\,dx. \tag{71}$$

Furthermore, (50) shows that $G_{\nearrow}=-G_{\nwarrow}\Xi$, so that the expression for the block $A^{(n-1)}_{\nearrow}$ from (30) can be written as

$$A^{(n-1)}_{\nearrow}=-(\mathrm{cof}\,G_{\nwarrow})G_{\nearrow}=(\det G_{\nwarrow})\Xi. \tag{72}$$

Hence, since from (30) we also have $A^{(n-1)}_{\searrow}=(\det G_{\nwarrow})I$, we find the following expression for h:

$$h=\frac{E^{(n-1)}}{\det G_{\nwarrow}}=\frac{1}{\det G_{\nwarrow}}\left(\frac{1}{2}(\dot{y}^T\ \ p^T)A^{(n-1)}\begin{pmatrix}\dot{y}\\ p\end{pmatrix}+W^{(n-1)}\right)=\frac{1}{2}p^Tp+\dot{y}^T\Xi p+\frac{\frac{1}{2}\dot{y}^TA^{(n-1)}_{\nwarrow}\dot{y}+W^{(n-1)}}{\det G_{\nwarrow}}. \tag{73}$$

So far we have

$$p^T\,dx-s^T\,du+(h-H)\,dt=\left(\frac{\frac{1}{2}\dot{y}^TA^{(n-1)}_{\nwarrow}\dot{y}+W^{(n-1)}}{\det G_{\nwarrow}}-V-\dot{y}^T\Xi\,\Xi^T\dot{y}\right)dt-\dot{y}^T\Xi\,dx,$$

and the exterior derivative of this is zero iff

$$\frac{\partial}{\partial x}\left(\frac{\frac{1}{2}\dot{y}^TA^{(n-1)}_{\nwarrow}\dot{y}+W^{(n-1)}}{\det G_{\nwarrow}}-V-\dot{y}^T\Xi\,\Xi^T\dot{y}\right)+\frac{\partial}{\partial t}(\Xi^T\dot{y})=0.$$

Now $(\partial/\partial t)\,(\Xi^T\dot{y})=(\partial\Xi^T/\partial t)\dot{y}+\Xi^T\ddot{y}$, and from $\ddot{q}=-[A^{(n-1)}]^{-1}\nabla W^{(n-1)}$ it follows that

$$\frac{\partial W^{(n-1)}}{\partial x}=-[A^{(n-1)}\ddot{q}]_{\downarrow}=-(A^{(n-1)}_{\nearrow})^T\ddot{y}+A^{(n-1)}_{\searrow}\frac{\partial V}{\partial x}=(\det G_{\nwarrow})\left(-\Xi^T\ddot{y}+\frac{\partial V}{\partial x}\right),$$

so it remains to show that

$$\frac{\partial}{\partial x}\left(\frac{\frac{1}{2}\dot{y}^TA^{(n-1)}_{\nwarrow}\dot{y}}{\det G_{\nwarrow}}-\dot{y}^T\Xi\,\Xi^T\dot{y}\right)+\frac{\partial\Xi^T}{\partial t}\dot{y}=0.$$

To simplify the notation for this final computation, write

$$\det G_{\nwarrow} = D, \quad A^{(n-1)}_{\nwarrow} = (a_{ij}), \quad \text{and } A^{(n-1)}_{\nearrow} = (b_{ij}).$$

Then $(b_{ij}) = -(\operatorname{cof} G_{\nwarrow}) G_{\nearrow} = D\Xi$, by (72). In this notation, what we must show is

$$\frac{1}{2D}\sum_{i,j=1}^{m} \frac{\partial a_{ij}}{\partial x_k}\dot{y}_i\dot{y}_j - \frac{1}{D^2}\sum_{i,j=1}^{m}\sum_{l=1}^{n} \frac{\partial(b_{il}b_{jl})}{\partial x_k}\dot{y}_i\dot{y}_j + \sum_{i=1}^{m}\frac{\partial}{\partial t}\left(\frac{b_{ik}}{D}\right)\dot{y}_i = 0. \tag{74}$$

To begin with, since $G_{\nwarrow}$ is independent of x and $G_{\nearrow}$ is linear in x, we see that b_{ij} is linear in x. More precisely, since

$$\frac{\partial [G_{\nearrow}]_{rj}}{\partial x_k} = \frac{\partial G_{r,m+j}}{\partial q_{m+k}} = \delta_{jk} N_r,$$

applying proposition 6 with y instead of q gives

$$\frac{\partial b_{ij}}{\partial x_k} = -\sum_{r=1}^{m} [\operatorname{cof} G_{\nwarrow}]_{ir}(\delta_{jk}N_r) = -\delta_{jk}[(\operatorname{cof} G_{\nwarrow})N_{\uparrow}]_i = -\frac{\delta_{jk}}{2}\frac{\partial D}{\partial y_i}.$$

Furthermore,

$$\sum_{i=1}^{m}\frac{\partial}{\partial t}\left(\frac{b_{ik}}{D}\right)\dot{y}_i = \sum_{i,j=1}^{m}\frac{\partial}{\partial y_j}\left(\frac{b_{ik}}{D}\right)\dot{y}_i\dot{y}_j.$$

Finally, since $A^{(n-1)}$ satisfies the cyclic conditions,

$$\frac{\partial a_{ij}}{\partial x_k} = \frac{\partial A^{(n-1)}_{ij}}{\partial q_{m+k}} = -\frac{\partial A^{(n-1)}_{j,m+k}}{\partial q_i} - \frac{\partial A^{(n-1)}_{m+k,i}}{\partial q_j} = -\frac{\partial b_{jk}}{\partial y_i} - \frac{\partial b_{ik}}{\partial y_j}.$$

Plugging all this into (74), it is easy to verify that everything cancels out, which completes the proof. □

F. Separation of the time-dependent Hamilton–Jacobi equation

The time-dependent Hamilton–Jacobi equation corresponding to the Hamiltonian $h(u,s,t)$ of proposition 36 is

$$h\left(u, \frac{\partial F}{\partial u}, t\right) + \frac{\partial F}{\partial t} = 0. \tag{75}$$

A complete solution $F(u,\alpha,t)$ can be obtained by separation of variables, as we will now show. We number the parameters $\alpha_0,\ldots,\alpha_{n-1}$ since they will in fact be just the values of the integrals of motion $E^{(0)},\ldots,E^{(n-1)}$, as will be clear by comparing (78) below with (65).

To begin with, since the time variable t appears in K only in the overall multiplicative factor $1/(\det G_{\nwarrow})$, it can be separated off by assuming a solution for F of the form

$$F(u,\alpha,t) = S(u,\alpha) - \alpha_{n-1}\int \frac{1}{\det G_{\nwarrow}(y(t))}\,dt. \tag{76}$$

With the explicit expression for h from proposition 36 we get the following equation for $S(u,\alpha)$:

$$\left(\sum_{k=1}^{n} u_k\right)E^{(n)} + \sum_{k=1}^{n}\left(\frac{\frac{1}{2}f_k(u_k)(\partial S/\partial u_k)^2 + g_k(u_k)}{U'(u_k)}\right) = \alpha_{n-1}. \tag{77}$$

In order to find a complete solution, depending on all the parameters α_i, we will use Stäckel's method. Consider the n equations

$$\sum_{k=1}^{n} \frac{\sigma_{n-a-1}(\breve{u}_k)}{U'(u_k)} \left(\frac{1}{2} f_k(u_k) \left(\frac{\partial S}{\partial u_k} \right)^2 + g_k(u_k) \right) = \alpha_a - \sigma_{n-a}(u) E^{(n)}, \tag{78}$$

where $a=0,\ldots,n-1$. If we can find a solution of this system, it will be a complete solution of (77), since it will depend on all α_i. [Of course it will solve (77) which is just the last equation of the system, corresponding to $a=n-1$.]

Now (78) is a linear system of equations for the expression in parentheses, and the matrix of coefficients is the inverse of a Stäckel matrix (similar to the one occuring when separating in elliptic or parabolic coordinates). In fact, the matrix can be inverted using known properties of symmetric polynomials, resulting in

$$\frac{1}{2} f_k(u_k) \left(\frac{\partial S}{\partial u_k} \right)^2 + g_k(u_k) = -P(-u_k), \quad k=1,\ldots,n, \tag{79}$$

where the polynomial P is given by

$$P(z) = \alpha_0 + \alpha_1 z + \cdots + \alpha_{n-1} z^{n-1} + E^{(n)} z^n. \tag{80}$$

It is now clear that the additive Ansatz

$$S(u,\alpha) = S_1(u_1,\alpha) + \ldots + S_n(u_n,\alpha)$$

yields a separated solution, provided that each function S_k satisfies the separation ODE

$$\frac{1}{2} \left(\frac{dS_k}{du_k} \right)^2 = \frac{-g_k(u_k) - P(-u_k)}{f_k(u_k)}. \tag{81}$$

Consequently,

$$F(u,\alpha,t) = \sum_{k=1}^{n} \int \sqrt{-2 \frac{g_k(u_k) + P(-u_k)}{f_k(u_k)}}\, du_k - \alpha_{n-1} \int \frac{1}{\det G_{\nwarrow}(y(t))}\, dt \tag{82}$$

is a complete solution, and in the usual way it generates a canonical transformation to variables (β,α), where $\beta_i = \partial F / \partial \alpha_i$. These new variables will be constant during the motion, with values determined by the initial condition. One can then (at least in principle) solve for $u=u(\beta,\alpha,t)$, and hence $x=x(\beta,\alpha,t)$. This finishes the proof of theorem 23.

IV. THE CASE OF ONE DRIVEN EQUATION

The case when only the last equation is driven by the other ones is easier to handle, since it does not require the Hamilton–Jacobi method, as we shall soon see. Specializing our previous results to this case by setting $n=1$, we find the following. If a system of the form

$$\begin{aligned} \ddot{y}_1 &= M_1(y_1,\ldots,y_m), \\ &\vdots \\ \ddot{y}_m &= M_m(y_1,\ldots,y_m), \\ \ddot{x} &= -\frac{\partial V}{\partial x}(y_1,\ldots,y_m;x) \end{aligned} \tag{83}$$

has an integral of motion $E^{(0)}$ of cofactor type, then it must have an extra integral of motion $E^{(1)}=\frac{1}{2}\dot{y}^T \operatorname{cof} G_{\nwarrow}(y)\dot{y}+w(y)$ depending only on the variables y. We change to new coordinates $(v_1,\ldots,v_m,u)$, where $v=y$ and u is the zero of the first degree polynomial $\det(G-\lambda J)$. Here $J=\operatorname{diag}(0,\ldots,0,1)$, so $\det(G-\lambda J)=\det G-\lambda \det G_{\nwarrow}$, hence

$$u=\frac{\det G(y,x)}{\det G_{\nwarrow}(y)}.$$

In the new variables, $E^{(1)}$ remains unchanged (with v instead of y), while $E^{(0)}$ takes the form given by (64),

$$E^{(0)}=uE^{(1)}+\frac{1}{2}\frac{\det G_{\nwarrow}(v)}{\Delta}\dot{u}^2+g(u),$$

where, according to (43) and proposition 32,

$$\Delta=\left(\frac{\partial u}{\partial x}\right)^2=\frac{f(u)}{\det G_{\nwarrow}(v)}$$

for some function $f(u)$. Hence,

$$E^{(0)}=uE^{(1)}+\frac{1}{2}\frac{(\det G_{\nwarrow}(v))^2}{f(u)}\dot{u}^2+g(u). \tag{84}$$

Now, for a given solution $v(t)=y(t)$ of the driving system, we write this as

$$\left(\det G_{\nwarrow}(v(t))\frac{du}{dt}\right)^2=2\,f(u)(E^{(0)}-uE^{(1)}-g(u)),$$

or

$$\frac{du}{\sqrt{2\,f(u)(E^{(0)}-uE^{(1)}-g(u))}}=\frac{dt}{\det G_{\nwarrow}(v(t))},$$

which can be integrated by quadrature, since u and t are separated.

This procedure can be applied recursively to ''triangular'' systems, as in the following proposition. Note that for an arbitrary triangular system all we can do in general is to solve the first equation for $q_1(t)$. It is quite surprising that the existence of an integral of motion of cofactor type is enough to allow us to solve the system completely.

Proposition 37 (triangular cofactor systems): Suppose that the "triangular" Newton system

$$\begin{aligned}
\ddot{q}_1&=M_1(q_1),\\
\ddot{q}_2&=M_2(q_1,q_2),\\
\ddot{q}_3&=M_3(q_1,q_2,q_3),\\
&\vdots\\
\ddot{q}_N&=M_N(q_1,q_2,q_3,\ldots,q_N),
\end{aligned} \tag{85}$$

is of cofactor type. Suppose also that no upper left $k\times k$ block in G is constant or singular ($k=1,\ldots,N-1$). Then the system can be integrated by quadratures.

Proof: The whole system is of the type considered above (driven, with $n=1$), so it can be integrated provided that the driving system, consisting of the $N-1$ first equations, can be integrated. By what we said above, the driving system must have an integral of motion of cofactor type, so it is itself a triangular cofactor system, of one dimension less. Since the first equation can be integrated (being one dimensional), the statement follows by induction. □

In each step of the integration procedure one new variable $u=u_k$ is introduced. Denoting the determinant of the upper left $k\times k$ block in G by $D_k(q_1,\ldots,q_k)$, we can write the separation variables $(u_1,\ldots,u_N)$ as

$$u_1=q_1 \quad \text{and} \quad u_i=\frac{D_i}{D_{i-1}}, \quad i=2,\ldots,N.$$

V. EXAMPLES

Example 38 (example 1 continued): We can now fill in the missing details in our first example. We had

$$M(q)=\frac{1}{(q_2q_3-q_1)^2}\begin{pmatrix}0\\ q_3\\ q_2\end{pmatrix}.$$

With

$$G(q)=\begin{pmatrix}2q_1 & q_2 & q_3\\ q_2 & 0 & 1\\ q_3 & 1 & 0\end{pmatrix}, \quad J=\begin{pmatrix}0 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix},$$

we find from $A_\mu=\operatorname{cof}(G+\mu J)$ that

$$A^{(0)}=\operatorname{cof} G=\begin{pmatrix}-1 & q_3 & q_2\\ q_3 & -q_3^2 & q_2q_3-2q_1\\ q_2 & q_2q_3-2q_1 & -q_2^2\end{pmatrix},$$

$$A^{(1)}=\begin{pmatrix}0 & -q_2 & -q_3\\ -q_2 & 2q_1 & 0\\ -q_3 & 0 & 2q_1\end{pmatrix}, \quad A^{(2)}=\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}.$$

The relation $\nabla W^{(k)}=-A^{(k)}M$ then yields

$$W^{(0)}=-\frac{q_2^2+q_3^2}{q_2q_3-q_1}, \quad W^{(1)}=\frac{2q_1}{q_2q_3-q_1}, \quad W^{(2)}=0.$$

We introduce new variables (v,u_1,u_2), where $v=q_1$ and $u_{1,2}$ are the roots of

$$0=\det(G-uJ)=2(q_2q_3-q_1)+(q_2^2+q_3^2)u+(2q_1)u^2.$$

With (y,x_1,x_2) instead of (q_1,q_2,q_3), we see that $u_1+u_2=-(x_1^2+x_2^2)/2y$ and $u_1u_2=2(x_1x_2-y)/2y$, so that

$$\left(\frac{x_1+x_2}{\sqrt{2}}\right)^2 = v(1-u_1)(1-u_2),$$
$$\left(\frac{x_1-x_2}{\sqrt{2}}\right)^2 = -v(1+u_1)(1+u_2). \tag{86}$$

Except for the factor v, the new variables (u_1,u_2) are elliptic coordinates aligned along axes that are rotated $\pi/4$ relative to the Cartesian coordinates (x_1,x_2). With $u_1<-1<u_2<1$, the coordinate curves are ellipses (for u_1) and hyperbolas (for u_2). The example (2) is obtained by taking the particular solution $y(t)=v(t)=q_1(t)=t$ of the driving equation $\ddot{q}_1=0$, and in this case we get a factor t with the effect of expanding the entire coordinate web as time increases, so these coordinates might be called "expanding elliptic coordinates."

We can express (u_1,u_2) in terms of (y,x_1,x_2) as

$$u_{1,2}=\frac{-1}{4y}(x_1^2+x_2^2\pm\sqrt{(x_1^2+x_2^2)^2-16y(x_1x_2-y)}),$$

and then a straightforward computation gives the quantities

$$\Delta_{1,2}=\left(\frac{\partial u_{1,2}}{\partial x_1}\right)^2+\left(\frac{\partial u_{1,2}}{\partial x_2}\right)^2=\frac{1}{2y^2}\left(x_1^2+x_2^2\pm\frac{(x_1^2+x_2^2)^2-8yx_1x_2}{\sqrt{(x_1^2+x_2^2)^2-16y(x_1x_2-y)}}\right).$$

With $U(\mu)=(u_1-\mu)(u_2-\mu)$ we find that $(\det G_{\nwarrow})U'(u_1)\Delta_1=2y(u_1-u_2)\Delta_1=4(1-u_1^2)$ and $(\det G_{\nwarrow})U'(u_2)\Delta_2=2y(u_2-u_1)\Delta_1=4(1-u_2^2)$ depend only on one variable, as predicted by Proposition 32. So in this case we have $f_1=f_2=f$, where $f(u)=4(1-u^2)$.

The functions $W^{(k)}$, expressed in the new variables, take the form

$$W^{(0)}=2\frac{u_1+u_2}{u_1u_2}=u_2\frac{-2/u_1}{U'(u_1)}+u_1\frac{-2/u_2}{U'(u_2)},$$
$$W^{(1)}=\frac{2}{u_1u_2}=\frac{-2/u_1}{U'(u_1)}+\frac{-2/u_2}{U'(u_2)},$$
$$W^{(2)}=0,$$

in accordance with proposition 35.

We can now write down the integrals of motion $E^{(k)}=\frac{1}{2}\dot{q}^TA^{(k)}\dot{q}+W^{(k)}$ in terms of the variables (v,u_1,u_2). With $s_i=\dot{u}_i/\Delta_i$, we find

$$E^{(2)}=\frac{\dot{v}^2}{2},$$
$$E^{(1)}=(u_1+u_2)E^{(2)}+\frac{4(1-u_1^2)\frac{s_1^2}{2}-\frac{2}{u_1}}{U'(u_1)}+\frac{4(1-u_2^2)\frac{s_2^2}{2}-\frac{2}{u_2}}{U'(u_2)},$$
$$E^{(0)}=u_1u_2E^{(2)}+u_2\frac{4(1-u_1^2)\frac{s_1^2}{2}-\frac{2}{u_1}}{U'(u_1)}+u_1\frac{4(1-u_2^2)\frac{s_2^2}{2}-\frac{2}{u_2}}{U'(u_2)}.$$

The new Hamiltonian is $h=E^{(1)}/\det G_{\nwarrow}(v(t))$, or, with $v(t)=t$,

$$h(u,s,t)=\frac{1}{2t}\left(\frac{u_1+u_2}{2}+\frac{4(1-u_1^2)\dfrac{s_1^2}{2}-\dfrac{2}{u_1}}{U'(u_1)}+\frac{4(1-u_2^2)\dfrac{s_2^2}{2}-\dfrac{2}{u_2}}{U'(u_2)}\right).$$

The time-dependent Hamilton–Jacobi equation $h(u,\partial F/\partial u,t)+\partial F/\partial t=0$ admits a separated complete solution of the form

$$F(u_1,u_2,\alpha_1,\alpha_2,t)=S_1(u_1,\alpha_0,\alpha_1)+S_2(u_2,\alpha_0,\alpha_1)-\frac{\alpha_1}{2}\ln|t|,$$

where S_1 and S_2 satisfy the separation equations

$$\frac{1}{2}\left(\frac{dS_1}{du_1}\right)^2=\frac{\dfrac{2}{u_1}-\alpha_0+\alpha_1u_1-\dfrac{u_1^2}{2}}{4(1-u_1^2)},$$

$$\frac{1}{2}\left(\frac{dS_2}{du_2}\right)^2=\frac{\dfrac{2}{u_2}-\alpha_0+\alpha_1u_2-\dfrac{u_2^2}{2}}{4(1-u_2^2)}.$$

From $\beta_k=\partial F/\partial\alpha_k$ we finally obtain

$$\beta_1(u_1,u_2,t,\alpha_0,\alpha_1)=\int^{u_1}\frac{x}{2R}dx+\int^{u_2}\frac{x}{2R}dx-\frac{1}{2}\ln|t|,$$

$$\beta_0(u_1,u_2,t,\alpha_0,\alpha_1)=\int^{u_1}\frac{-1}{2R}dx+\int^{u_2}\frac{-1}{2R}dx,$$

where

$$R(x,\alpha_1,\alpha_2)=\sqrt{2(1-x^2)\left(\frac{2}{x}-\alpha_0+\alpha_1x-\frac{x^2}{2}\right)}.$$

This gives the solution $u(\beta,\alpha,t)$ in implicit form.

Example 39 (a triangular system): An interesting example of a triangular cofactor system appears when applying the recursive method for constructing cofactor pair systems given in Ref. 6 to the matrices

$$G=\begin{pmatrix}0&-1&q_1\\-1&0&q_2\\q_1&q_2&2q_3\end{pmatrix},\quad \tilde{G}=\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix}.$$

Starting with $W^{(0)}=W^{(1)}=0$ and $W^{(2)}=-1$, one obtains after four steps the system

$$\begin{aligned}\ddot{q}_1&=-4q_1,\\ \ddot{q}_2&=6q_1^2-4q_2,\\ \ddot{q}_3&=-10q_1^3+12q_1q_2-4q_3,\end{aligned}\tag{87}$$

which is a cofactor pair system with respect to the given matrices G and $\tilde{G}$. Since the third equation is driven by the first two, the system is also a cofactor pair system with respect to G and $J=\mathrm{diag}(0,0,1)$. In fact, the most general matrix G for which the system has an integral of motion of the form $\frac{1}{2}\dot{q}^T(\mathrm{cof}\,G)\dot{q}+W(q)$ is

$$c_1\begin{pmatrix} 0 & -1 & q_1 \\ -1 & 0 & q_2 \\ q_1 & q_2 & 2q_3 \end{pmatrix}+c_2\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}+c_3\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}+c_4\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

so it might be called a ''cofactor quadruple system.'' [The third matrix comes from the fact that there is a function $U(q)$ such that $M_2=\partial_3 U$ and $M_3=\partial_2 U$.] Anyway, we know from Sec. IV that the driving system is a cofactor system with respect to

$$G_{\nwarrow}=\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}.$$

Since this matrix is constant, we cannot use it for integrating the driving system, but it so happens that the driving system is a cofactor system with respect to any matrix of the form

$$c_1\begin{pmatrix} -1 & q_1 \\ q_1 & 2q_2 \end{pmatrix}+c_2\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}+c_3\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

So, forgetting about (87) for the moment, we consider the two-dimensional driving system

$$\ddot{q}=\begin{pmatrix} -4q_1 \\ 6q_1^2-4q_2 \end{pmatrix}=-\frac{g\nabla w}{\det g}, \tag{88}$$

where now

$$g=\begin{pmatrix} -1 & q_1 \\ q_1 & 2q_2 \end{pmatrix}, \quad w=\tfrac{3}{2}q_1^4+2q_1^2q_2-2q_2^2.$$

[In this example, we use lowercase letters for quantities referring to the two-dimensional system (88).] In the new variables $v=q_1$ and $u=\det g/\det g_{\nwarrow}=q_1^2+2q_2$, we have the integrals of motion

$$e^{(1)}=\tfrac{1}{2}\dot{q}_1^2+2q_1^2=\tfrac{1}{2}\dot{v}^2+2v^2$$

from the first equation, and (after a short calculation)

$$e^{(0)}=\frac{1}{2}\dot{q}^T(\mathrm{cof}\,g)\dot{q}+w(q)=ue^{(1)}-\frac{\dot{u}^2}{8}-\frac{u^2}{2}.$$

The function $v(t)=q_1(t)$ is just a harmonic oscillation, whose amplitude determines the numerical value of $e^{(1)}$ (or the other way around):

$$q_1(t)=\sqrt{\frac{e^{(1)}}{2}}\sin 2(t-t_1). \tag{89}$$

The value of $e^{(0)}$ is determined by the initial conditions for q_1 and q_2. Then $u(t)$, and hence $q_2(t)=(u(t)-v(t)^2)/2$, can be found from the separable ODE

$$\frac{du}{dt}=\sqrt{8\left(ue^{(1)}-\frac{u^2}{2}-e^{(0)}\right)}.$$

This gives

$$u(t)=\sqrt{(e^{(1)})^2-2e^{(0)}}\sin 2(t-t_2)+e^{(1)},$$

so that

$$q_2(t)=\tfrac{1}{2}\left(\sqrt{(e^{(1)})^2-2e^{(0)}}\sin 2(t-t_2)+e^{(1)}\left(1-\tfrac{1}{2}\sin^2 2(t-t_1)\right)\right). \tag{90}$$

Having found $q_1(t)$ and $q_2(t)$, we return to the three-dimensional system (87):

$$\ddot{q}=\begin{pmatrix} -4q_1 \\ 6q_1^2-4q_2 \\ -10q_1^3+12q_1q_2-4q_3 \end{pmatrix}=-\frac{G\nabla W}{\det G},$$

where

$$G=\begin{pmatrix} 0 & -1 & q_1 \\ -1 & 0 & q_2 \\ q_1 & q_2 & 2q_3 \end{pmatrix}, \quad W=6q_1^2q_2^2-4q_1^4q_2+4q_1q_2q_3-2q_3^2-4q_1^3q_3.$$

Here we take new variables $v_1=q_1$, $v_2=q_2$, and $u=\det G/\det G_{\nwarrow}=2(q_1q_2+q_3)$. The integrals of motion turn out to be

$$E^{(1)}=\frac{1}{2}\dot{v}^T\operatorname{cof}\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}\dot{v}+4v_1v_2-2v_1^3$$

and

$$E^{(0)}=\frac{1}{2}\dot{q}^T(\operatorname{cof}G)\dot{q}+W(q)=uE^{(1)}-\frac{\dot{u}^2}{8}-\frac{u^2}{2},$$

so the equation for $u(t)$ can again be separated (in exactly the same way as above). After finding $u(t)$, we finally obtain $q_3(t)=u(t)/2-q_1(t)q_2(t)$, that is

$$q_3(t)=\tfrac{1}{2}\left(\sqrt{E^{(1)}-2E^{(0)}}\sin 2(t-t_3)+E^{(1)}\right)-q_1(t)q_2(t). \tag{91}$$

By inserting the expressions for $q_1(t)$ and $q_2(t)$ into the expression for $E^{(1)}$ we find that it depends on the previous integration constants $e^{(0)}$, $e^{(1)}$, t_1, t_2 through the equation

$$E^{(1)}=\sqrt{2e^{(1)}}\sqrt{e^{(1)}-2e^{(0)}}\cos 2(t_2-t_1).$$

On the other hand, $E^{(0)}$ and t_3 are independent of the previous integration constants.

Example 40 (construction of driven systems): Given a cofactor system

$$\ddot{y}=M_{\uparrow}(y)=-(\operatorname{cof}g(y))^{-1}\frac{\partial w}{\partial y}(y),$$

how can it be extended to a driven system

$$\ddot{q}=\begin{pmatrix} M_{\uparrow}(y) \\ M_{\downarrow}(y,x) \end{pmatrix}=-(\operatorname{cof}G(q))^{-1}\frac{\partial W}{\partial q}(q)$$

of the type considered in this paper? First of all, the restriction that the elliptic coordinates matrix $G(q)$ must have $g(y)=G_{\nwarrow}(y)$ as its upper left block fixes α, $\beta_{\uparrow}$ and $\gamma_{\nwarrow}$. The remaining entries of β and γ can be chosen at will (as long as G is nonsingular). Then we want to find some

extension $M_{\downarrow}$ of the right-hand side which is compatible with the chosen matrix G [i.e., so that $W(q)$ exists]. In separation coordinates, this amounts to specifying the functions $g_k(u_k)$ in the corresponding solution of the fundamental equations (proposition 34), the function $w(v)=w(y)$ already being determined by the driving system. One can find a family of possible $M_{\downarrow}$ in Cartesian coordinates directly by using the recursion formula from Ref. 6. As it stands, this formula requires $\widetilde{G}$ to be nonsingular, but taking $\widetilde{G}=J$ can be justified like in the proof of proposition 27 (however, it only makes sense in the ''downwards'' recursion formula). We then find that if a driven system has integrals of motion given by the generating function $E_\mu=\frac{1}{2}\dot{q}^T A_\mu \dot{q}+W_\mu$ as in (27), then we obtain another driven system with integrals of motion $\frac{1}{2}\dot{q}^T A_\mu \dot{q}+U_\mu$ by setting

$$U_\mu=\frac{1}{\mu}\left(\frac{\det(G+\mu J)}{\det G}W^{(0)}-W_\mu\right). \tag{92}$$

It is clear that U_μ is a polynomial in μ of degree $n-1$, not n, which means that the new system (and any system obtained by iterating this process) is driven in the trivial way ($\ddot{y}=0$). They correspond to solutions (57) of the fundamental equations with $w(y)=0$. Adding

$$\frac{\det(G+\mu J)}{\det G_{\nwarrow}}w(y)$$

to U_μ gives a system with any $w(y)$ desired.

As an example, consider the two-dimensional Garnier potential $V=(q_1^2+q_2^2)^2-(\lambda_1 q_1^2+\lambda_2 q_2^2)$. We will demonstrate how to find G and M_3 such that the system

$$\begin{aligned}\ddot{q}_1&=-\partial_1 V(q_1,q_2),\\ \ddot{q}_2&=-\partial_2 V(q_1,q_2),\\ \ddot{q}_3&=M_3(q_1,q_2,q_3)\end{aligned} \tag{93}$$

is of cofactor type $\ddot{q}=-(G/\det G)\nabla W$. With $G_{\nwarrow}=\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$, corresponding to $w=V$, we have $\alpha=\beta_1=\beta_2=0$, so we choose, for example, $\beta_3=1$ and extend γ with zeros to get

$$G=\begin{pmatrix}1&0&q_1\\0&1&q_2\\q_1&q_2&2q_3\end{pmatrix}.$$

Applying (92) with $W_\mu=1+0\mu$ and $J=\mathrm{diag}(0,0,1)$ gives $U_\mu=(\det G)^{-1}$, corresponding to the trivially driven system

$$\ddot{q}=-\frac{G}{\det G}\nabla\left(\frac{1}{\det G}\right)=\frac{2}{(2q_3-q_1^2-q_2^2)^2}\begin{pmatrix}0\\0\\1\end{pmatrix}.$$

To keep things simple we stop the recursion after this first step, and let

$$E_\mu=\frac{1}{2}\dot{q}^T\,\mathrm{cof}(G+\mu J)\dot{q}+(\det G)^{-1}+\frac{\det(G+\mu J)}{\det G_{\nwarrow}}V(q_1,q_2),$$

which then generates an extended system of the desired form

$$\ddot{q}=-\frac{G}{\det G}\nabla((\det G)^{-1}+(\det G)V)=\begin{pmatrix}-\partial_1 V\\-\partial_2 V\\2(2q_3-q_1^2-q_2^2)^{-2}-2V\end{pmatrix}. \tag{94}$$

Since the Garnier potential is separable in elliptic coordinates it admits an extra integral of motion of cofactor type. This gives us the possibility to instead take

$$G_{\nwarrow} = \begin{pmatrix} \lambda_1 - q_1^2 & -q_1 q_2 \\ -q_1 q_2 & \lambda_2 - q_2^2 \end{pmatrix},$$

corresponding to

$$w = \lambda_2 q_1^4 + \lambda_1 q_2^4 + (\lambda_1 + \lambda_2) q_1^2 q_2^2 - \lambda_1 \lambda_2 (q_1^2 + q_2^2).$$

Here $\alpha = -1$ and $\beta_{\uparrow} = 0$, and we can for example extend $G_{\nwarrow}$ to

$$G = \begin{pmatrix} \lambda_1 - q_1^2 & -q_1 q_2 & -q_1 q_3 \\ -q_1 q_2 & \lambda_2 - q_2^2 & -q_2 q_3 \\ -q_1 q_3 & -q_2 q_3 & \lambda_3 - q_3^2 \end{pmatrix}.$$

In a similar way as above we get in this case (after some computation) the extended system

$$\begin{aligned} \ddot{q} &= -\frac{G}{\det G} \nabla \left(\frac{\det G_{\nwarrow}}{\det G} + \frac{\det G}{\det G_{\nwarrow}} w \right) \\ &= \begin{pmatrix} -\partial_1 V \\ -\partial_2 V \\ \lambda_1 \lambda_2 q_3 \left(\dfrac{2w(q_1, q_2)}{(\det G_{\nwarrow})^2} - \dfrac{2}{(\det G)^2} + \dfrac{q_1 (\partial_1 V)/\lambda_1 + q_2 (\partial_2 V)/\lambda_2}{\det G_{\nwarrow}} \right) \end{pmatrix}, \end{aligned} \tag{95}$$

where $\det G = \lambda_1 \lambda_2 \lambda_3 (1 - q_1^2/\lambda_1 - q_2^2/\lambda_2 - q_3^2/\lambda_3)$ and $\det G_{\nwarrow} = \lambda_1 \lambda_2 (1 - q_1^2/\lambda_1 - q_2^2/\lambda_2)$.

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Uniqueness in MHD in divergence form: Right nullvectors and well-posedness

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Magnetohydrodynamics in divergence form describes a hyperbolic system of covariant and constraint-free equations. It comprises a linear combination of an algebraic constraint and Faraday's equations. Here, we study the problem of well-posedness, and identify a preferred linear combination in this divergence formulation. The limit of weak magnetic fields shows the slow magnetosonic and Alfvén waves to bifurcate from the contact discontinuity (entropy waves), while the fast magnetosonic wave is a regular perturbation of the hydrodynamical sound speed. These results are further reported as a starting point for characteristic based shock capturing schemes for simulations with ultra-relativistic shocks in magnetized relativistic fluids. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Highly relativistic astrophysical fluids have been observed as highly energetic outflows, e.g., jets in active galactic nuclei, including a few optical radio-jets such as 3C273 (Pearson *et al.*, 1981; Thomson *et al.*, 1993; Bahcall *et al.*, 1995), 3C346 (Dey and van Breugel, 1994), M87 (Biretta *et al.*, 1995) and PKS 1229-21 (Le Brun *et al.*, 1997), microquasars in our galaxy (Hjellming and Rupen, 1995; Mirabel and Rodriguez, 1995; Levinson and Blandford, 1996), pulsar winds (Kennel and Coroniti, 1984), and fireballs in recent models of γ-ray bursts (Rees and Meszaros, 1994). These flows are generally time-dependent, or have been produced in a strongly time-variable episode, and hence are relativistically shocked fluid flows. In most cases, shocks are responsible for brightest emission features at the highest energies.

The evolution of strongly magnetized flows can be markedly different from unmagnetized flows. This is already apparent from small amplitude wave-motion in ideal magnetohydrodynamics compared with hydrodynamics, and their distinct shock structures. The nonlinear development of large scale morphology of strongly magnetized jets can result in features such as the formation of a nose cone (Clarke *et al.*, 1986), which is absent in hydrodynamical evolution. Of particular interest is the role of magnetic fields in the large scale, three-dimensional stability of jets and their knotted structures.

Time-dependent simulations may provide the link between the observed emission features and the internal structure such as magnetized field distribution, and boundary conditions at the source. It is hoped that simulations ultimately provide constraints on the flow parameters, perhaps also derived from stability criteria. Higher dimensional simulations of jets are performed by a number of groups in the approximation of relativistic hydrodynamics (van Putten, 1993b; Duncan and Hughes 1994; Martí *et al.*, 1995; Martí *et al.*, 1997) and relativistic magnetohydrodynamics (van Putten 1994a, b, 1996; Nishikawa *et al.*, 1997; Koide *et al.*, 1996, 1998).

The earliest approach for time-dependent simulations on shocked relativistic magnetohydrodynamic flows with dynamically significant magnetic fields uses the equations of magnetohydrodynamics (MHD) in divergence form (van Putten 1991, 1993a). The divergence technique obtains hyperbolic systems from partial differential-algebraic systems of equations, and applies more

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generally to the case of Yang-Mills magnetohydrodynamics in SU(N) (van Putten 1994c, d; Choquet-Bruhat 1994a, b), and general relativity (van Putten and Eardley, 1996). A linear smoothing method has been used as a shock capturing scheme for this formulation (van Putten 1993a, 1994a b, 1995). Both one- and two-dimensional simulations on astrophysical jets are performed (van Putten, 1993b, 1996; Levinson and van Putten, 1997). This method is accurate and stable, and generally performs well for relativistic shocked fluid flow with up to moderately strong shock strengths (van Putten, 1993a), and preserves divergence free magnetic fields to within machine round-off error (van Putten, 1995). A smoothing method, therefore, is appropriate for simulations on the large scale morphology of astrophysical jets.

Advanced shock capturing schemes are commonly based on characteristics, however, such as Roe's method (1981) and its extensions. These methods are generally more stable than smoothing methods for flows with ultra-relativistic shocks, such as in calculations of fire-balls for γ-ray bursts (Rees and Meszaros 1994; Wen *et al.*, 1997). It is therefore of interest to explore applications of these shock capturing schemes to relativistic MHD. Here, we describe a first step in this direction given by studying the computational stability of normalized right nullvectors (i.e., the right eigenvectors) of the characteristic matrix.

The divergence technique incorporates a constraint $c=0$ into a divergence equation of a two-form, $\nabla^a \omega_{ab}=0$, as in Faraday's equation, through the linear combination

$$\nabla^a(\omega_{ab}+\lambda g_{ab}c)=0, \quad \lambda \neq 0. \tag{1}$$

In the context of a Cauchy problem, (1) conserves $c=0$ in the future domain of dependence of the initial hypersurface with physical Cauchy data (van Putten 1991).

In this article, we identify a preferred linear combination in (1), i.e., a choice of λ and overall sign of (1) in its application to the equations of ideal MHD. This follows from two separate analyses: a derivation of the right nullvectors of the characteristic matrix and well-posedness. Somewhat remarkably, both analyses agree in their preferred linear combinations. This suggests to consider this preferred linear combination in future applications in characteristic based methods to MHD in divergence form.

The problem of linearized perturbations in relativistic MHD has been considered previously by Anile (1989) and that of Alfvén waves by Komissarov (1997). The well-posedness proof uses an extension to the Friedrichs–Lax symmetrization procedure from earlier work on Yang–Mills magnetohydrodynamics (van Putten, 1994c, d).

In Sec. II we describe nonuniqueness in the original version of the divergence technique. In Sec. III, a new derivation of the right nullvectors is given. Section IV briefly summarizes well-posedness obtained by embedding of physical solutions in a symmetric hyperbolic system of equations.

II. MHD IN DIVERGENCE FORM

Ideal MHD describes an inviscid, perfectly conductive plasma in a single fluid description with velocity four-vector, u^b $(u^c u_c=-1)$. It is given by energy-momentum conservation, $\nabla_a T^{ab}=0$, where T^{ab} is the stress-energy tensor of both the fluid and the electromagnetic field, Faraday's equations, $\nabla_a(u^{[a}h^{b]})=0$ subject to the algebraic constraint $u^c h_c=0$, and conservation, $\nabla_a(ru^a)=0$, of baryon number, r. For a polytropic equation of state with polytropic index γ, we have $T^{ab}=(r+[\gamma/(\gamma-1)](P/r)+h^2)u^a u^b+(P+h^2/2)g^{ab}-h^a h^b$, P is the hydrostatic pressure and g^{ab} is the metric tensor. The theory of relativistic magnetohydrodynamics is contained in the conservation laws of energy-momentum, $\nabla_a T^{ab}=0$, and baryon number, $\nabla_a(ru^a)=0$, together with Faraday's equations and a constraint,

$$\nabla_a(h^{[a}u^{b]})=0, \quad u^c h_c=0. \tag{2}$$

The divergence technique considers a constraint-free formulation by taking a linear combination

$$\nabla_a(h^{[a}u^{b]}+\lambda u^c h_c)=0. \tag{3}$$

Provided $\lambda \neq 0$, (3) preserves $u^c h_c = 0$ during dynamical evolution in response to physical initial data (van Putten, 1991), and no constraint violating wave-motion occurs.

Algebraically, the linear combination (3) establishes a rank-one update to its Jacobian, and hence of that of the full equations of MHD. Clearly, symmetry conditions of the Jacobian may enter a particular choice of λ. Below, we consider the choice

$$\lambda = 1, \tag{4}$$

so that

$$\begin{gathered} \nabla_a T^{ab} = 0, \\ -\nabla_a (h^{[a} u^{b]} + g^{ab} u^c h_c) = 0, \\ \nabla_a (r u^a) = 0, \\ \nabla_a (\xi^a (u^2 + 1)) = 0, \end{gathered} \tag{5}$$

where ξ is any timelike vector field and $U = (u^b, h^b, r, P)$. The minus sign in front of the present linear combination is chosen also in regards to the structure of the Jacobian of (5). This will be made explicit below.

Upon expansion, (5) obtains the system

$$A^a \partial_a U + \cdots = 0, \tag{6}$$

where the matrices $A^{aA}_B = A^{aA}_B(U) = \partial F^{aA} / \partial U^B$ are 10 by 10, and the dots refer coupling terms to the Christoffel symbols. The infinitesimal wave-structure is given by characteristic wave-fronts at given U (since the A^a are coordinate independent). The simple wave ansatz $U = U(\phi)$ obtains

$$A^a \partial_a \phi U' + \cdots = 0. \tag{7}$$

The wave-fronts are characteristic surfaces, whenever the matrix $A^a \partial_a \phi$ is singular. The directions $\nu_a = \partial_a \phi$ then are the normals to these surfaces. The small amplitude perturbations in these simple waves are given by the right nullvectors of $A^a \nu_a$. Stated differently, the small amplitude perturbations are right eigenvectors, R, of $(A^t)^{-1} A^x \nu_x$, when the wave moves along the x direction, following

$$((A^t)^{-1} A^x - v) R = 0, \tag{8}$$

where v is the velocity of propagation.

The divergence technique provides an embedding of the theory of ideal MHD in a system of ten equations. Physical initial data are properly propagated by it, without exiting nonphysical wave-modes. The physical waves (entropy waves, Alfvén and magnetohydrodynamic waves) are all contained within the light cone. Here, adding $g^{ab} u^c h_c$ (or a multiple thereof) to Faraday's equations provides a rank-one update to the characteristic matrix $A^c \nu_c$. On the light cone, however, $\nu^2 = 0$, and this linear combination no longer regularizes the characteristic determinant. (This results from insisting on covariance in the divergence formulation.) Kommissarov (1997) attempts to discuss MHD in divergence form outside the context of the initial value problem with physical initial data, and hence erroneously concludes the presence of nonphysical wave-modes.

III. THE CHARACTERISTIC MATRIX

We have

$$A^{aA}(U) = \frac{\partial F^{aA}}{\partial U^B} \nu_a = \frac{\partial F^{aA} \nu_a}{\partial U^B}; \tag{9}$$

with $\rho = r + [\gamma/(\gamma-1)]P + h^2 = rf + h^2$, we have

$$F^{cA}\nu_c = \begin{cases} \rho(u^c\nu_c)u^a + (P + h^2/2)\nu^a - (h^c\nu_c)h^a, \\ -\{(h^c\nu_c)u^a - (u^c\nu_c)h^a + \nu^a u^c h_c\}, \\ r(u^c\nu_c), \\ (\xi^c\nu_c)(u^2+1). \end{cases} \tag{10}$$

The system of 10×10 equations for $U^B = (u^b, h^b, r, P)$ can be reduced to 8×8 in the variables $V^B = (v^s, h^b, r)$ by expressing u^b in terms of the spatial three-velocity $u^b = \Gamma(1, v^s)$, $\Gamma = 1/\sqrt{1-v^2}(1, v^s)$, $s = 1,2,3$, noting that linearized wave-motion conserves entropy, so that $\mathrm{d}P = \gamma(P/r)\mathrm{d}r$. In V^B, the equation of energy conservation, $\nabla_a T^{at} = 0$ and the last equation of (5) are automatically satisfied, whence they can be ignored. In what follows, A^a shall denote the resulting 8×8 matrix, obtained from the original 10×10 matrix by deletion of the first and last row, addition of the last column (multiplied by $\gamma P/r$) to the one-but last column (associated with r), followed by deletion of the first and last columns.

The linearized wave-structure is given by the characteristic problem

$$A^c\nu_c z = 0 \tag{11}$$

for the right null-vectors $z = U'$. Without loss of generality, (11) can be studied in a co-moving frame, in which $u^b = (1,0,0,0)$. In this event, $\Gamma = 1$ and $\partial\Gamma/\partial v^s = 0$. Furthermore, the x-axis of the local coordinate system can be aligned with the magnetic field, so that $h^b = (0,H,0,0)$. Given the two orientations u^s and h^b, the wave-structure is rotationally symmetric about the x axis, and hence ν_y and ν_z act symmetrically as $\sqrt{\nu_y^2 + \nu_z^2}$; we will put $\nu_z = 0$. For $A^c\nu_c$, we have

$$\begin{bmatrix} \rho\nu_1 & 0 & 0 & -\nu_1 H & -H\nu_2 & -H\nu_3 & 0 & \dfrac{\gamma P\nu_2}{r} \\ 0 & \rho\nu_1 & 0 & 0 & H\nu_3 & -H\nu_2 & 0 & \dfrac{\gamma P\nu_3}{r} \\ 0 & 0 & \rho\nu_1 & 0 & 0 & 0 & -H\nu_2 & 0 \\ \nu_1 H & 0 & 0 & -\nu_1 & -\nu_2 & -\nu_3 & 0 & 0 \\ -H\nu_2 & H\nu_3 & 0 & \nu_2 & \nu_1 & 0 & 0 & 0 \\ -H\nu_3 & -H\nu_2 & 0 & \nu_3 & 0 & \nu_1 & 0 & 0 \\ 0 & 0 & -H\nu_2 & 0 & 0 & 0 & \nu_1 & 0 \\ r\nu_2 & r\nu_3 & 0 & 0 & 0 & 0 & 0 & \nu_1 \end{bmatrix}. \tag{12}$$

Note that the lower diagonal block is ν_1 times the 4×4 indentity matrix. *This results from the sign choice in the given combination of Faraday's equations and the constraint in (5) and (10).* Furthermore, notice that the third and seventh rows and columns act independently to give rise to the Alfvén waves. The remaining waves are described by the reduced problem

$$(A^c\nu_c)'z' = 0, \tag{13}$$

where $(A^c\nu_c)'$ is obtained from $A^c\nu_c$ by deleting the third and seventh rows and columns, thereby obtaining a problem in the six-dimensional variable z'. Introducing

$$z' = \begin{pmatrix} x \\ y \end{pmatrix}, \tag{14}$$

(11) takes the form of a coupled system of 3×3 equations

$$\nu_1 Z x + X y = 0, \quad Y x + \nu_1 y = 0, \tag{15}$$

in which

$$Z=\begin{bmatrix}\rho & 0 & -H\\ 0 & \rho & 0\\ H & 0 & -1\end{bmatrix},$$

$$X=\begin{bmatrix}-H\nu_2 & -H\nu_3 & \dfrac{\gamma P\nu_2}{r}\\ H\nu_3 & -H\nu_2 & \dfrac{\gamma P\nu_3}{r}\\ -\nu_2 & -\nu_3 & 0\end{bmatrix}, \tag{16}$$

$$Y=\begin{bmatrix}-H\nu_2 & H\nu_3 & \nu_2\\ -H\nu_3 & -H\nu_2 & \nu_3\\ r\nu_2 & r\nu_3 & 0\end{bmatrix}.$$

This obtains a *single* 3×3 eigenvalue problem in x, given by

$$XYx=\nu_1^2 Zx\Leftrightarrow Z^{-1}XYx=\nu_1^2 x. \tag{17}$$

Here, $Z^{-1}XY-\nu_1^2$ is given by the matrix

$$\begin{bmatrix}W_{1,1} & W_{1,2} & 0\\ W_{2,1} & W_{2,2} & 0\\ \dfrac{H(\gamma P\nu_2^2-rf\nu_2^2-rf\nu_3^2)}{rf} & \dfrac{H\gamma P\nu_2\nu_3}{rf} & \nu_2^2+\nu_3^2-\nu_1^2\end{bmatrix}, \tag{18}$$

where the upper diagonal 2×2 matrix W is given by

$$W=\begin{bmatrix}\dfrac{\gamma P\nu_2^2}{rf}-\nu_1^2 & \dfrac{\gamma P\nu_2\nu_3}{rf}\\ \dfrac{\gamma P\nu_2\nu_3}{rf+H^2} & \dfrac{H^2\nu_3^2+H^2\nu_2^2+\gamma P\nu_3^2}{rf+H^2}-\nu_1^2\end{bmatrix}. \tag{19}$$

The two zeros in the third column of (18) result from $\lambda=1$. Upon substitution $\nu_3^2=\nu^2+\nu_1^2-\nu_2^2$, the determinant assumes the covariant expression

$$\rho\det W=(rf-\gamma P)(u^c\nu_c)^4-(h^2+\gamma P)\nu^2(u^c\nu_c)^2+\frac{\gamma P}{rf}(h^c\nu_c)^2\nu^2. \tag{20}$$

Alfvén waves. The eigenvalues for the Alfvén waves are given by

$$\nu_1=\pm\frac{|h^c\nu_c|}{\sqrt{\rho}} \tag{21}$$

with null-vector

$$z=(0,0,H\nu_2,0,0,0,\rho\nu_1,0)^T, \tag{22}$$

associated with Alfvén waves; covariantly,

$$U^A=(v^a,\pm\sqrt{\rho}v^a,0,0)^T, \tag{23}$$

where v_a may be taken to be

$$H(0,0,\nu_4,-\nu_3)=\epsilon_{abcd}u^b h^c \nu^d \equiv v_a . \tag{24}$$

Thus, the Alfvén wave is transversal in which h^2 is conserved (δh^b is orthogonal to h^b).

Magnetohydrodynamic waves. The eigenvalues for the magnetohydrodynamic waves are given by the roots of the characteristic determinant (20). Writing

$$n^b=\nu^b+(u^c\nu_c)u^c, \tag{25}$$

we have $\nu^2=-t^2+n^2$, $t=u^c\nu_c$, $n^2=n^c n_c$. Let $\alpha=rf/\gamma P$ and $\beta=h^2/\gamma P$. Then

$$\frac{(h^c\nu_c)^2}{rfn^2}=\frac{\beta}{\alpha}\frac{(h^c n_c)^2}{h^2 n^2}\equiv\frac{\beta}{\alpha}\cos^2\phi. \tag{26}$$

Consequently, (20) becomes

$$(\alpha-1)v^4-(1+\beta)v^2(1-v^2)+\beta\alpha^{-1}\cos^2\phi(1-v^2)=0, \tag{27}$$

where $v^2=t^2/n^2$. Equation (27) has real solutions v for any given n^b, whenever

$$(\alpha+\beta)v^4-(1+\beta+\beta\alpha^{-1})v^2+\beta\alpha^{-1}=0 \tag{28}$$

has real solutions v. But (28) has discriminant

$$D=(\alpha+\beta-\alpha\beta)^2\geqslant 0. \tag{29}$$

Weak magnetic fields are described by small β expansions as follows.

Proposition 3.1: Fast magnetosonic waves are a regular perturbation of sound waves in pure hydrodynamics, while the Alfvén and slow magnetosonic waves bifurcate from entropy waves (contact discontinuities), whose propagation velocities satisfy

$$v_f^2/v_h^2\sim 1+\beta\frac{\alpha-1}{\alpha}\sin^2\phi+O(\beta^2),$$

$$v_A^2/v_h^2\sim\beta\cos^2\phi[1-\beta\alpha^{-1}+O(\beta^2)], \tag{30}$$

$$v_s^2/v_h^2\sim\beta\cos^2\phi\left[1-\beta\left(1-\frac{\alpha-1}{\alpha}\cos^2\phi\right)+O(\beta^2)\right],$$

where $v_h^2=\alpha^{-1}$ *is the square of the hydrodynamical velocity, and which obey the inequalities*

$$v_s^2\leqslant v_A^2\leqslant v_f^2 . \tag{31}$$

Inequalities (31) remain valid for general β (e.g., Bazer and Ericson, 1959; Lichnerowicz, 1967; Anile, 1989).

IV. RIGHT NULLVECTORS

Inspection of (19), together with (15), shows the null-vector

$$z=\begin{pmatrix} \nu_1\nu_2\nu_3^2 \\ -\nu_1\nu_3(\nu_2^2-\alpha\nu_1^2) \\ 0 \\ H\nu_1\nu_2\nu_3^2 \\ H\nu_3^2(\nu_2^2-\alpha\nu_1^2) \\ -H\nu_2\nu_3(\nu_2^2-\alpha\nu_1^2) \\ 0 \\ -\alpha r\nu_3^2\nu_1^2 \end{pmatrix}. \tag{32}$$

Of course, (32) can be stated covariantly by noting that $H^2=h^2$, $H\nu_2=h^c\nu_c$, $\nu_1=u^c\nu_c$,

$$H^2(\nu_2^2-\alpha\nu_1^2)=(h^c\nu_c)^2-\alpha h^2(u^c\nu_c)^2\equiv h^2k_1, \tag{33}$$

and introducing

$$H(0,\nu_4^2+\nu_3^2,-\nu_2\nu_3,-\nu_2\nu_4)^T=\epsilon_{abcd}u^b\nu^cv^d\equiv w_a. \tag{34}$$

Since $-\alpha r\nu_3^2\nu_1^2$ is a scalar, ν^3 is to be treated as

$$H^2(\nu_3^2+\nu_4^2)=h^2n^2-(h^c\nu_c)^2\equiv h^2k_2, \tag{35}$$

where $n_a=\nu_a+(u^c\nu_c)u_a$. Note that

$$k_1=n^2(\cos^2\phi-\alpha v^2),\quad k_2=n^2\sin^2\phi, \tag{36}$$

where $v=v_s$, v_f. Clearly, z is formed from

$$\begin{aligned} \delta u^b&=-t(k_1n^b-(k_2+k_1)(\hat{h}^cn_c)\hat{h}^b), \\ \delta h^b&=k_1w^b+k_2t(h^cn_c)u^b, \\ \delta r&=-\alpha rk_2t^2, \\ \delta P&=-rfk_2t^2, \end{aligned} \tag{37}$$

where $\hat{h}^b=h^b/|h|$, and

$$v_a=\epsilon_{abcd}u^bh^c\nu^d,\quad w_a=\epsilon_{abcd}u^b\nu^cv^d. \tag{38}$$

We thus have the following.

Proposition 3.2: Given a unit vector n^b orthogonal to u^b, and a root $\nu^b=n^b+vu^b$, $v=u^c\nu_c$ of (28), the right nullvectors for the hydrodynamical waves of (11), $U^A=(\delta u^b,\delta h^b,\delta r,\delta P)$, are

$$\begin{aligned} \delta u^b&=v[\sin^2\phi n^b-(1-\alpha v^2)(n^b-\cos\phi\,\hat{h}^b)], \\ \delta h^b&=|h|[(\cos^2\phi-\alpha v^2)\tilde{w}^b+v\sin^2\phi\cos\phi u^b], \\ \delta r&=-v^2\alpha r\sin^2\phi, \\ \delta P&=-v^2rf\sin^2\phi. \end{aligned} \tag{39}$$

where $\tilde{w}^b = w^b/|h|$.

Anile (1989) gives a different form of these right nullvectors. By Proposition 3.1, our weak magnetic field limits show that

$$\cos^2\phi - \alpha v_f^2 < 0 \tag{40}$$

for fast magnetosonic waves, while

$$\cos^2\phi - \alpha v_s^2 > 0 \tag{41}$$

for slow magnetosonic waves. Inspection of (34) shows that therefore the tangential component of the magnetic field is strengthened in fast magnetosonic waves, while it is weakened in slow magnetosonic waves. This distinguishing aspect of fast and slow magnetosonic waves was first noted by Bazer and Ericson (1959) in their analysis of shocks in nonrelativistic MHD.

The limit of small β is of particular interest to computation. For example, in various settings a magnetized fluid streams into a nearly unmagnetized environment. A characteristics based scheme must therefore reliably treat a large dynamic range in β. Clearly, a full set of nullvectors (including those of contact discontinuities) obtains for nonzero β. However, the behavior of these nullvectors is somewhat nontrivial as β becomes small. In what follows, we consider the small β limit, in the sense of small $|h|/\sqrt{\gamma P}$, while keeping the direction $\hat{h}^b$ constant. In this limit,

$$\begin{aligned} 1-\alpha v^2 &\sim -\beta\frac{\alpha-1}{\alpha}\sin^2\phi + O(\beta^2), \\ 1-\alpha v^2 &\sim 1 + O(\beta) \end{aligned} \tag{42}$$

for the fast and slow magnetosonic speeds, respectively.

Corollary 4.1: In the limit of low magnetic field strength, the fast magnetosonic waves are described by the right nullvectors

$$\begin{aligned} \delta u^b &= v_f n^b + \beta\frac{\alpha-1}{\alpha}(n^b - \cos\phi\hat{h}^b)v_f + O(\beta^2), \\ \delta h^b &= |h|(-\tilde{w}^b + v_f\cos\phi u^b) + \beta\frac{\alpha-1}{\alpha}w^b + O(\beta^2), \\ \delta r &= -v_f^2\alpha r, \\ \delta P &= -v_f^2 r f, \end{aligned} \tag{43}$$

and the slow magnetosonic waves by

$$\begin{aligned} \delta u^b &= \cos\phi(\hat{h}^b - \cos\phi n^b) + O(\beta), \\ \delta h^b &= \sqrt{\gamma P}(\cos\phi\tilde{w}^b + v_s\sin^2\phi u^b) + O(\beta), \\ \delta r &= -v_s\alpha r\sin^2\phi, \\ \delta P &= -v_s\alpha r f\sin^2\phi. \end{aligned} \tag{44}$$

The small β limit of the nullvectors can now be normalized.

A. Bifurcations from entropy waves

The behavior of the nullvectors in the limit of weak magnetic fields can be derived from (23) and Corollary 4.1. To this end, note that

$$v^a = |h|\tilde{v}^a = \sin\phi |h|\hat{v}^a, \tag{45}$$

where $\hat{v}^c\hat{v}_c = 1$, and ϕ denotes the angle between n^c and h^c,

$$n^b = \cos\phi \hat{h}^b + \sin\phi y^b, \tag{46}$$

$y^c u_c = h^c y_c = 0$, $y^c y_c = 1$ (n^b is normalized to be unit, as in the assumptions of Proposition 3.2). It follows that the Alfvén nullvectors may be normalized to

$$\delta\hat{U}^A = (\hat{v}^a, \pm\sqrt{\rho}\hat{v}^a, 0, 0). \tag{47}$$

In the limit of vanishingly small β, the pair of slow magnetosonic waves collapse to the single normalized nullvector

$$\delta\hat{U}^A = (y^b, \sqrt{\gamma P}y^b, 0, 0). \tag{48}$$

Note that $y^c\hat{v}_c = 0$, so that (47) and (48) are independent. Division by $\sin\phi$ thus provides a normalization of the original expressions (23) and (44).

The nullvector associated with entropy waves ($u^c\nu_c = 0$) is

$$\delta U^A = (0, 0, \delta r, 0) \tag{49}$$

if $h^c\nu_c \neq 0$, and

$$(0, \delta h^c, \delta r, \delta P), \quad (\delta u^c, 0, 0, 0) \tag{50}$$

if $h^c\nu_c = 0$, subject to

$$\delta P + h_c\delta h^c = 0, \quad \nu_c\delta h^c = 0, \quad \nu_c\delta u^c = 0. \tag{51}$$

The second case refers to transverse MHD for which continuity must hold of total pressure, zero orthogonal magnetic field and transverse velocity. Note that transverse MHD has two nullvectors, and corresponds to the case of pure hydrodynamics. With the exception of transverse MHD, therefore, the contact discontinuity provides one nullvector.

Transverse MHD or pure hydrodynamics allows for shear along contact discontinuities, which is responsible for the two independent nullvectors. Whenever magnetic field lines cross a contact discontinuity, however, the persistent coupling to the magnetic field lines in ideal MHD prohibits shear. In ideal MHD, the response to the original two-dimensional degree of freedom in shear is two new wave-modes. These wave-modes are the Alfvén wave and the slow magnetosonic wave. These two wave-modes are indeed different, as (47) and (48) show. The Alfvén and slow magnetosonic wave may be regarded as one pair, bifurcating from the contact discontinuity. This has been illustrated in Fig. 6 of van Putten (1993a). Indeed, *the limit of vanishing β recovers the two shear modes from the independent Alfvén and slow magnetosonic waves*. Of course, the Alfvén wave is purely rotational, while the slow magnetosonic wave is slightly helical, including a longitudinal variation of $\pm v_s\sin^2\phi = \pm\beta\sin^2\phi\cos\phi$. The fast magnetosonic wave remains a regular perturbation of the ordinary sound wave.

The weak magnetic field limit thus obtains two nullvectors from the fast magnetosonic waves, two from the Alfvén waves, one from the slow magnetosonic waves and generally one from the contact discontinuity, a total of six. This leaves an apparent degeneracy of one.

The degeneracy stems from the neighboring to order v_s of the two nullvectors of the slow magnetosonic waves. This would suggest ill-posedness to this order in projections. However,

characteristic based methods consider the product of the projections on the nullvectors *and* the associated eigenvectors. In the present case, therefore, the order of the degeneracy is precisely cancelled by multiplication with the eigenvalue v_s, which is computationally stable. The limit of arbitrarily small β *in the application of characteristic based methods* is computationally well-posed.

V. WELL-POSEDNESS

The theory of ideal relativistic MHD was first shown to be well-posed by Friedrichs (1974), using the Friedrichs–Lax symmetrization procedure. The problem of constraints was circumvented by a reduction of variables. The symmetrization procedure of Fredrichs and Friedrichs and Lax (1971) applies to hyperbolic systems of equations of the form

$$\nabla_a F^{aB} = f^B, \tag{52}$$

which satisfy a certain convexity condition. The presence of conserved constraints, however, can be treated also by an extension of the Friedrichs–Lax symmetrization procedure, with no need for an additional reduction of variables, developed in earlier work on Yang–Mills magnetohydrodynamics in SU(N) (van Putten, 1994c, d). Once in symmetric hyperbolic form, well-posedness results from standard energy arguments (e.g., Fisher and Marsden, 1972). The main arguments of symmetrization in the presence of constraints are briefly recalled here, to highlight the same linear combination of (5), now from the point of view of well-posedness.

A. Symmetrization with constraints

Variations δV^A of (u^b, h^b, r, P) can be unconstraint (with respect to all ten degrees of freedom), and constraint, i.e., those obeying the constraints. For example, $\delta c \neq 0$ results from a total variation, while $\delta c = 0$ is a constraint variation. Symmetrization in the presence of constraints follows if there exists a vector field W_A which produces a total derivative in the modified main dependency relation

$$\text{YI:} \quad W_A \delta F^{aA} \equiv \delta z^a, \tag{53}$$

and which obtains constraint positive definiteness in

$$\text{YII:} \quad \delta W_A \delta F^{aA} \xi_a > 0 \tag{54}$$

for some timelike vector ξ^a. Of course, the source terms f^B must satisfy the consistency condition

$$W_A f^A = 0 \tag{55}$$

whenever the constraints are satisfied. Allowing a possible nonzero total derivative in YI defines an extension (van Putten, 1994c, d) to the Friedrichs–Lax (1971) symmetrization procedure.

Differentiation by V^C of the unconstraint identity YI obtains

$$\frac{\partial W_A}{\partial V^C} \frac{\partial F^{aA}}{\partial V^D} \nabla_a V^D + \frac{W_A \partial^2 F^{aA}}{\partial V^C \partial V^D} \nabla_a V^D = \frac{\partial^2 z}{\partial V^C \partial V^D} \nabla_a V^D. \tag{56}$$

This establishes symmetry of the matrices

$$A^a_{CD} = \frac{\partial W_A}{\partial V^C} \frac{\partial F^{aA}}{\partial V^D}. \tag{57}$$

Also,

$$\delta V^C A^a_{CD} \xi_a \delta V^D = \left(\delta V^C \frac{\partial W_A}{\partial V^C} \right) \left(\frac{\partial F^{aA} \xi_a}{\partial V^D} \delta V^D \right) = \delta W_A \delta F^{aA} \xi_a > 0 \tag{58}$$

for all constraint variations δV^A. Of course, given V^A, the constraint variations δV^A define a linear subspace $\mathcal{V}$ of dimension $N-m$, where m is the number of constraints $c=0$, each giving rise to

$$0=\delta c=\frac{\partial c}{\partial V^A}\,\delta V^A. \tag{59}$$

We have the following construction (van Putten, 1994c, d).

Lemma 5.1: Given a real-symmetric $A\epsilon\mathcal{L}(\mathrm{R}^n,\mathrm{R}^n)$ which is positive definite on a linear subspace $\mathcal{V}\subset\mathrm{R}^n$, there exists a real-symmetric, positive definite $A^*\epsilon\mathcal{L}(\mathrm{R}^n,\mathrm{R}^n)$ such that

$$A^*y=Ay \quad (y\epsilon\mathcal{V}). \tag{60}$$

This may be seen as follows. Consider $A^*=A+\mu x^Tx$, where x is a unit element from $V^\perp$. Then A^* is symmetric positive definite on $V'=\{z=y+\lambda x|y\epsilon V,\lambda\epsilon R\}$: $z^TA^Tz\geqslant c'\|z\|^2=c'(\|y\|^2+\lambda^2\|x\|^2)$ with $c'>0$ upon choosing $\mu>M$, where $M=\|A\|$ denotes the norm of A. This construction may be repeated until $V^\perp$ is exhausted, leaving A^* symmetric positive definite on R^n as an embedding of A on V.

The real-symmetric matrix $A^a_{CD}\xi_a$ is positive definite on the subspace of constraint variations $\mathcal{V}$; let $(A^a_{CD}\xi_a)^*$ be the positive definite, symmetric matrix obtained from the lemma. It follows that solutions to (52) (and its constraints) satisfy the *symmetric positive definite* system of equations

$$-(A^{aAB})^*\xi_a(\xi^c\nabla_c)V_A+A^{aAB}(\nabla_\Sigma)_aV_A=f^B, \tag{61}$$

where

$$\nabla_a=-\xi_a(\xi^c\nabla_c)+(\nabla_\Sigma)_a\,. \tag{62}$$

It remains to show that ideal MHD satisfies properties YI and YII.

B. Symmetrization of hydrodynamics

Relativistic hydrodynamics has been shown to be symmetrizable by Friedrichs (1974), Ruggeri and Strumia (1981), and Anile (1989). This uses the equations in the form

$$\nabla_aF^{aA}_f=\begin{cases}\nabla_a(rfu^au^b+Pg^{ab})=0,\\ \nabla_a(ru^a)=0,\\ \nabla_a(rSu^a)=0\end{cases} \tag{63}$$

away from entropy generating shocks. Then $W^f_A=(u_a,f-TS,T)$ and $V^f_C=(v_\alpha,T,f)$ with a reduction of variables on the velocity four-vector by $u^b=\Gamma(1,v^\alpha)$, where Γ is the Lorentz factor. With F^{aA}_f denoting the fluid dynamical equations $\nabla_aT^{ab}_f=0$, $T^{ab}_f=rfu^au^b+Pg^{ab}$ with f the specific enthalpy, and $\nabla_a(ru^a)=0$, it has been shown that (Ruggeri and Strumia, 1981; Anile, 1989)

$$W^f_A\delta F^{aA}_f\equiv 0, \quad Q_f=\delta W_A\delta F^{aA}_f\xi_a>0, \tag{64}$$

provided that the free enthalpy $G(T,P)=f-TS-1$ is concave, and the sound velocity is less than the speed of light. Under these conditions, the hydrodynamical equations alone, therefore, satisfy YI and YII, and in fact the original Friedrichs–Lax conditions CI and CII of Friedrichs and Lax (1971), so that they satisfy a symmetric hyperbolic system of equations.

C. Symmetrization of ideal MHD

In what follows, we set

$$\omega_{ab}=h^a u^b-u^a h^b+g^{ab}u^c h_c,$$
$$T_m^{ab}=h^2 u^a u^b+\tfrac{1}{2}h^2 g^{ab}-h^a h^b. \tag{65}$$

We then have the expansions

$$\begin{aligned} u_b\delta T_m^{ab}&=u_b(h^2u^a\delta u^b+h^2u^b\delta u^a+2u^a u^b h_c\delta h^c+g^{ab}h_c\delta h^c-h^a\delta h^b-h^b\delta h^a)\\ &=-h^2\delta u^a-u^a(h_c\delta h^c)-h^a(u_c\delta h^c)-c\,\delta h^a,\\ h_b\delta\omega^{ab}&=h_b(h^a\delta u^b+u^b\delta h^a-h^b\delta u^a-u^a\delta h^b+g^{ab}\delta c)\\ &=h^a(h_c\delta u^c)+c\,\delta h^a-h^2\delta u^a-u^a(h_c\delta h^c)+h^a\delta c. \end{aligned} \tag{66}$$

We hereby arrive at the identity

$$u_b\delta T_m^{ab}-h_b\delta\omega^{ab}\equiv\delta z^a, \tag{67}$$

where $z^a=-2h^a c$. *The total derivative in (67) follows by the unique linear combination* $\omega^{ab}=h^a u^b-h^b u^a+g^{ab}c$, *as in (5).* With $W_A=(u_a,h_a,f-TS,S)$ and F^{aA} given by (5) [rewritten according to (63)], it follows that

$$W_A\delta(F_f^{aA}+F_m^{aA})\equiv\delta z^a. \tag{68}$$

A similar calculation (van Putten, 1994c, d) shows that quadratic of constraint variations Q_m given by

$$\delta u_b\delta T_m^{ab}\xi_a-\delta h_b\delta\omega^{ab}\xi_a=(u^c\xi_c)[h^2(\delta u)^2+(\delta h)^2]+2[(\xi_c\delta u^c)(h_c\delta h^c)-(h^c\xi_c)(\delta u_c\delta h^c)] \tag{69}$$

is positive definite (for $\delta h^a\neq 0$). Therefore, the sum

$$Q=\delta W_A\delta F^{aA}\xi_a=Q_f+Q_m \tag{70}$$

is constraint positive definite, whenever Q_f is such (with respect to the fluid dynamical variables). It follows that both YI and YII are satisfied [with $W_A=(u_a,h_a,f-TS,S)$ and $V_A=(v_\alpha,h_a,T,f)$], and hence physical solutions to (5) satisfy the symmetric hyperbolic system (61) with $f^B=0$.

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Four-particle decay of the Bethe–Salpeter kernel in the high-temperature Ising model

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In this article we study the four-particle decay of the Bethe–Salpeter (B-S) kernel for the high-temperature Ising model. We use the hyperplane decoupling method [T. Spencer, Commun. Math. Phys. **44**, 143 (1975); R. S. Schor, Nucl. Phys. B **222**, 71 (1983)] to prove exponential decay in a set of variables particularly adapted to the methods of Spencer and Zirilli [Commun. Math. Phys. **49**, 1 (1976)] for the analysis of scattering and bound states in QFT, transcribed to lattice theories by Auil and Barata [Ann. Henri Poincare **2**, 1065 (2001)]. We study arbitrary derivatives of the general n-point correlation functions with respect to the interpolating variables, and we are able to obtain, in some cases, information about the third derivatives of the B-S kernel. As a later consequence, we have two-body asymptotic completeness for the (massive) Euclidean lattice field theory implemented by this model. This allows us to analyze the Ornstein–Zernike behavior of four-point functions, related to the specific heat of the model. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1510176]

I. INTRODUCTION AND MAIN RESULT

The exponential decay properties of the Bethe–Salpeter (B-S) kernel are used in the analysis of the energy-momentum (e-m) spectrum in the low energy range for weakly coupled models. The methods employed to prove these decay properties are basically lattice analogous of the techniques originally introduced in Euclidean QFT. The work of Spencer[1] introduced new procedures, namely, the decoupling of hyperplane method, then used, in the sequel, in a program about the investigation of the e-m spectrum of $P(\phi)_2$ models.[2–7] The hyperplane decoupling method was introduced in lattice theories in Ref. 8. Several results have been developed recently along the same ideas to analyze e-m spectrum for a wide class of lattice models. Those results focalize basically the existence (or not) of bound states[9–14] and two-body asymptotic completeness (a.c.)[15] in Euclidean lattice theories.

In the present article we verify the four-particle exponential decay, in the sense of Spencer,[1] of the B-S kernel for the ferromagnetic Ising model (IM) at high-temperatures ($\beta \ll 1$). Our analysis is mainly based in polymer expansion and the ''hyperplane decoupling'' method, following closely Ref. 1. Using the results of Ref. 15, this decay property actually proves the two-particle a.c. of the model, because Gaussian domination inequalities hold in this case and exclude bound states from the spectrum, as remarked in Ref. 12. One relevant fact for the standpoint of statistical mechanics is that two-particle a.c. allows us to study the Ornstein–Zernike behavior of four-point functions related to the specific heat of the model. In fact, the exponent in the polynomial correction to the exponential decay is twice that in the presence of bound states, as we remark below in more detail.

We give a more precise description of the method and the model. In the lattice of integers in $d+1$ dimensions $\mathbb{Z}^{d+1}$, with $d \geqslant 1$, the sites will be denoted by $x=(x_0,x_1,\ldots,x_d)$ or $(x_0,\mathbf{x})$ for short. Finite subsets of sites will be denoted generically by Λ. The decoupling method is applicable to hyperplanes perpendicular to any fixed direction parallel to the coordinate axis. To fix

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ideas, and for sake of brevity, here we consider only the x_0 direction, but it is important to have in mind that the method and all results below are equally applicable to the other directions independently. For this aim, we introduce the IM with an anisotropy in the x_0 direction; the boundary conditions are free. Explicitly, the local states are given by

$$\mu_\Lambda(f) := \frac{\Sigma_{\sigma\in S^\Lambda} f(\sigma)\exp(\beta\Sigma_{\langle ij\rangle} J_{ij}\sigma(i)\sigma(j))}{\Sigma_{\sigma\in S^\Lambda}\exp(\beta\Sigma_{\langle ij\rangle} J_{ij}\sigma(i)\sigma(j))}, \tag{1.1}$$

for functions f on the configurations $S^\Lambda=\{\sigma/\sigma:\Lambda\to\{-1,+1\}\}$, where the sum in the exponents is over all the nearest-neighbor, or bounds, and

$$J_{ij} := \begin{cases} J & \text{if } \{i,j\}=\{(n,\mathbf{x}),(n,\mathbf{y})\}, \\ J_m & \text{if } \{i,j\}=\{(m,\mathbf{x}),(m+1,\mathbf{x})\}; \end{cases}$$

being J and J_m strictly positive numbers. The first of them gives the coupling between nearest-neighbor lying in the same hyperplane defined by $x_0=\text{const}=n$, while the J_m's give the coupling between nearest-neighbor lying in two different of such hyperplanes. The isotropic ferromagnetic IM is obtained taking $J_m=J$, $\forall m\in\mathbb{Z}$. In our study we consider the J_{ij}'s as being complex variables and, for convenience, it is useful to introduce a new variable g_{ij} given by g_{ij} $:=\tanh(\beta J_{ij})$. Just for reference, the g_{ij}'s will be called the *interpolating variables*. The correlations, or (local) n-point Euclidean, functions are given by

$$\mathcal{S}_n^\Lambda(x_1,\ldots,x_n) := \frac{\Sigma_{\sigma\in S^\Lambda}\sigma(x_1)\cdots\sigma(x_n)\Pi_{\langle ij\rangle}e^{\beta J_{ij}\sigma(i)\sigma(j)}}{\Sigma_{\sigma\in S^\Lambda}\Pi_{\langle ij\rangle}e^{\beta J_{ij}\sigma(i)\sigma(j)}}. \tag{1.2}$$

The limit $\mathcal{S}_n(x_1,\ldots,x_n) := \lim_{\Lambda\uparrow\mathbb{Z}^{d+1}}\mathcal{S}_n^\Lambda(x_1,\ldots,x_n)$ exists and is translation invariant. As we deal with a model without bound states, we could expect to be compelled to the analysis of derivatives of higher order than in the case of models exhibiting bound states. In our approach, we consider arbitrary derivatives of the n-point correlation functions with respect to the interpolating variables g_{ij}, providing general results and considering lately its particularization for two- and four-point functions. Joining our different particular results, we are able to obtain, in some cases, information about the third (and lower) derivatives of the B-S kernel; see Lemma 4.10 later in this work. Higher derivatives of the two-point function were also considered in Refs. 16 and 17.

We define the connected part of the truncated four-point function as

$$\mathcal{D}(x_1,x_2,x_3,x_4) := \mathcal{S}_4(x_1,x_2,x_3,x_4) - \mathcal{S}_2(x_1,x_2)\mathcal{S}_2(x_3,x_4), \tag{1.3}$$

and the unconnected part as

$$\mathcal{D}_0(x_1,x_2,x_3,x_4) := \mathcal{S}_2(x_1,x_3)\mathcal{S}_2(x_2,x_4) + \mathcal{S}_2(x_1,x_4)\mathcal{S}_2(x_2,x_3). \tag{1.4}$$

We introduce the Bethe–Salpeter (B-S) equation on the lattice

$$\mathcal{D}(x_1,x_2,x_3,x_4) = \mathcal{D}_0(x_1,x_2,x_3,x_4) - \sum_{y_1,y_2,y_3,y_4\in\mathbb{Z}^{d+1}} \mathcal{D}_0(x_1,x_2,y_1,y_2)\mathcal{N}(y_1,y_2,y_3,y_4)\mathcal{D}(y_3,y_4,x_3,x_4), \tag{1.5}$$

or symbolically $\mathcal{D}=\mathcal{D}_0-\mathcal{D}_0\mathcal{N}\mathcal{D}$ for short. Here, the B-S kernel $\mathcal{N}$ is self-defined by this equation. The B-S equation has the formal solution $\mathcal{D}=\mathcal{D}_0(\mathbb{1}+\mathcal{N}\mathcal{D}_0)^{-1}$, provided this inverse exists. Taking formally inverses in this last relation we get $\mathcal{N}=\mathcal{D}^{-1}-\mathcal{D}_0^{-1}$, a convenient expression for the B-S kernel. In fact, this expression allows us to define rigorously the B-S kernel as an operator on the space $\ell_s^2 := \{\{a_{ij}\}_{i,j\in\mathbb{Z}^{d+1}}\in\ell^2(\mathbb{Z}^{d+1}\times\mathbb{Z}^{d+1}): a_{ij}=a_{ji}\}$ of symmetrical quadratically summable se-

quences indexed by pairs of sites. In this space, the inverse $\mathcal{D}_0^{-1}$ is explicitly given by expression (4.1); see Lemma 4.5(c). The inverse $\mathcal{D}^{-1}$ exists and is well-defined as consequence of Lemma 4.7(a) and Lemma 4.8(b); see also expression (4.3).

For sites $i=(i_0,i_1,\ldots,i_d)\in\mathbb{Z}^{d+1}$ we denote $\|i\|=\Sigma_{k=0}^{d}|i_k|$. We can now state our main result as follows.

Theorem 1.1: *For the IM with β sufficiently small there exist $m=m(\beta)$ and $C=C(\beta)$ such that*

$$|\mathcal{N}(i,j,k,l)|\leqslant C\mathrm{e}^{-m(\|i-j\|+\|k-l\|+2\|i+j-k-l\|)}, \tag{1.6}$$

for all $i,j,k,l\in\mathbb{Z}^{d+1}$. □

Note the particular combination of the sites at the exponent in the relation (1.6), becoming analogous to the property proved in Ref. 1 for some $P(\phi)_2$ models in QFT. Theorem 1.1 has the following consequence: the B-S kernel in momentum space $K(k,p,q)$ is analytic in the region

$$|\mathrm{Im}\,k_0|<2m,\quad |\mathrm{Im}\,p_i|<m,\quad |\mathrm{Im}\,q_i|<m\quad (i=0,1,\ldots,d);$$

where K is defined by $\check{K}(i+j-k-l,i-j,k-l)=\mathcal{N}(i,j,k,l)$; see Refs. 15 and 18. As we remark above, these analyticity properties plus the absence of bound states and the upper and lower mass gap imply the two-particle a.c. for the model; see Ref. 15 for details. (See the last remark at the end of Sec. III.)

To state the Ornstein–Zernike behavior of the four-point functions implied by the a.c. condition we introduce before a few definitions. In terms of the new variables

$$\xi:=x_1-x_2,\quad \eta:=x_3-x_4,\quad \tau:=x_1+x_2-(x_3+x_4), \tag{1.7}$$

and expressing, by the translation invariance, the two- and four-point functions in terms of the difference variables $\mathcal{S}_n(x_1,\ldots,x_n)=S_n(x_1-x_n,\ldots,x_{n-1}-x_n)$, we get

$$\mathcal{D}(x_1,x_2,x_3,x_4)=S_4\left(\frac{\tau+\xi+\eta}{2},\frac{\tau-\xi+\eta}{2},\eta\right)-S_2(\xi)S_2(\eta)=:D(\tau,\xi,\eta). \tag{1.8}$$

The change of variables given by (1.7) requires certain care in the lattice context. Here, we remark that for each of the new variables τ, ξ and η are allowed to vary freely in the whole lattice $\mathbb{Z}^{d+1}$ if we redefine D, introduced in (1.8), by D times the characteristic function of the image of the transformation (1.7). The details were extensively discussed in Ref. 15, Appendix A. Denoting by $\hat{}$ the Fourier transform, define $R(k,p,q):=\hat{D}(k,p,q)$, and consider it as a family of integral operators indexed by k, acting as $[R(k)f](p)=\int_{\mathbb{T}^{d+1}}R(k,p,q)f(q)dq$. For fixed f belonging to a suitable set, denote the map $k_0\mapsto\langle f,R(k)f\rangle$ by R, for abuse of notation, and $D=\check{R}$. From the a.c. condition and under suitable hypothesis on the dispersion curve, it is possible to establish (see Ref. 19) the following Ornstein–Zernike behavior for $|D(\tau)|$:

$$|D(\tau)|\leqslant k_1\mathrm{e}^{-m|\tau_0|}\left[\frac{1}{|\tau_0|^d}+O^*(|\tau_0|^{-(d+1)/2})\right]+k_2\mathrm{e}^{-m''|\tau_0|}, \tag{1.9}$$

for $\tau_0\to\infty$, where k_1, k_2 are positive constants and $m''>m$. Here, $O^*(K^{-p})$ means $O(K^{-p+\delta})$ for all $\delta>0$. Note that the τ coordinate in (1.7) is *twice* the center of mass coordinate, so the exponential decay in (1.9) is the expected for a four-point function. The relation (1.9) is valid under reasonably general hypothesis, and not exclusively for the IM. As remarked in Ref. 19, a relation analogous to (1.9) can be derived assuming the existence of two-particle bound states, but in this case with the exponential decay corrected by $|\tau_0|^{-d/2}$ instead of $|\tau_0|^{-d}$. This last situation is like the case of the two-point function.[20] As the four-point functions are related to the specific heat of the model, we could expect that a.c. condition may have, apparently, some influence on the

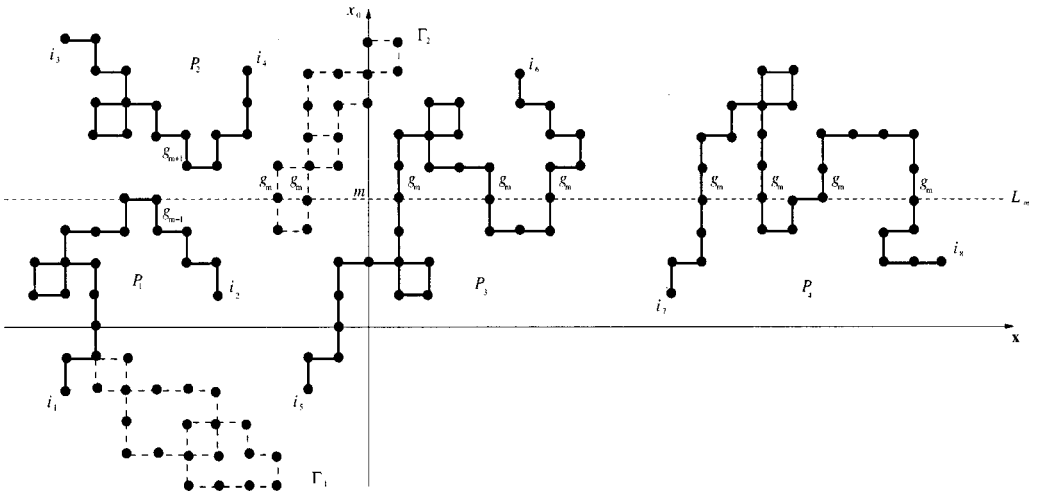


FIG. 1. The P_i's are examples of paths. The Γ_i's are examples of polymers, where Γ_1 is incompatible with the path P_1.

statistical properties of the models. The opposite question could be raised, i.e., to go from Ornstein–Zernike behavior to e-m spectral properties, but this is not our subject here.

This article is organized as follows. In Sec. II we introduce the polymer expansions and prove a general result for arbitrary derivatives of the $2n$-point functions with respect to the interpolating variables g_{ij}, giving a particularization for the case of the first and second derivatives. In Sec. III we perform a detailed study of the two-point function and its convolution inverse. Some of these later results (and main consequences) are known in the literature, but our approach is rather general. In Sec. IV we perform a detailed study of the connected and unconnected parts of the truncated four-point function and its respective inverses, concluding with the proof of Theorem 1.1 in Sec. IV C.

II. HIGH-TEMPERATURE POLYMER EXPANSION

The polymer expansion provides an alternative way to write the the general $2n$-point function (1.2) for the IM. Specifically,

$$\mathcal{S}_{2n}^{\Lambda}(i_1,\ldots,i_{2n})=\sum_{M\in \mathrm{conn}(i_1,\ldots,i_{2n})}\left(\prod_{L\in M} g_L\right)\exp\sum_{\substack{\Gamma\in\mathcal{G}'(\Lambda)\\ \Gamma\not\sim M}} c_\Gamma \mu^\Gamma. \tag{2.1}$$

An element M of $\mathrm{conn}(i_1,\ldots,i_{2n})$ is by definition a set of n paths joining different pairs of sites taken from the set $\{i_1,\ldots,i_{2n}\}$ (a path P is a connected set of bounds, such that an even number of bounds meets at every site except for the initial and final sites, see Fig. 1). The index L denote bounds. The sum in the exponent is basically over the family of set of polymers (i.e., connected sets of bounds, see Fig. 1) with at least one polymer in the set being incompatible with M. Here, c_Γ is a numerical constant and μ^Γ is of the form $\Pi_{\gamma\mathrm{polymer}}(\Pi_{L\in\gamma} g_L)^{n_\gamma}$, where $n_\gamma\in\mathbb{N}\cup\{0\}$. It can be proved that the series in the exponent in (2.1) is absolutely convergent if $|\mu|$ $:=\sup_{\gamma\mathrm{polymer}}|\Pi_{L\in\gamma} g_L|^{1/|\gamma|}$ is sufficiently small; see Refs. 21–23. Note that $|\mu|=|g|$ for the isotropic IM. Polymer expansion allows us to prove that $\mathcal{S}_{2n}(i_1,\ldots,i_{2n})$ is the limit of a convergent net of analytic functions of each g, g_m in a neighborhood of $0\in\mathbb{C}$. For our present aims, the relevant feature about expression (2.1) rests on the fact that it is a sum of a product of two factors $A\mathrm{e}^B$, being A and B products of powers of g_L's.

Denoting $L_m:=\{(x_0,x_1,\ldots,x_d)\in\mathbb{Z}^{d+1}: x_0=m\}$, see Fig. 1, polymer expansions allow to prove the following general result for the $2n$-point functions

Lemma 2.1: Assume that the hyperplane L_m divides the set of sites $\{i_1,\ldots,i_{2n}\}$ in two subsets, let's say $\{i_{k_1},\ldots,i_{k_r}\}$ and $\{i_{k_{r+1}},\ldots,i_{k_{2n}}\}$ (one of them might be eventually empty), in the sense that $\{i_{k_1},\ldots,i_{k_r}\}\subset\{(x_0,x_1,\ldots,x_d)\in\mathbb{Z}^{d+1}:x_0\leqslant m\}$ and $\{i_{k_{r+1}},\ldots,i_{k_{2n}}\}\subset\{(x_0,x_1,\ldots,x_d)\in\mathbb{Z}^{d+1}:x_0\geqslant m+1\}$. Then, we have the following

(a) If r is even, let's say $r=2l$, then $\mathcal{S}_{2n}(i_1,\ldots,i_{2n})|_{g_m=0}$ factorizes as

$$\mathcal{S}_{2n}(i_1,\ldots,i_{2n})|_{g_m=0}=\mathcal{S}_{2l}(i_{k_1},\ldots,i_{k_{2l}})|_{g_m=0}\mathcal{S}_{2n-2l}(i_{k_{2l+1}},\ldots,i_{2n})|_{g_m=0}.$$

For $n\in\mathbb{N}\cup\{0\}$, we have the following.

(b) If r is odd, then $\partial_{g_m}^{2n}\mathcal{S}_{2n}(i_1,\ldots,i_{2n})|_{g_m=0}=0$.

(c) If r is even, then $\partial_{g_m}^{2n+1}\mathcal{S}_{2n}(i_1,\ldots,i_{2n})|_{g_m=0}=0$. □

Proof: For part (a), note that, evaluating $\mathcal{S}_{2n}(i_1,\ldots,i_{2n})$ at $g_m=0$, in the sum in (2.1), only the paths $M\in\mathrm{conn}(i_1,\ldots,i_{2n})$ contribute which are independent of g_m. If there exists an even number of sites lying on both sides of L_m, such paths are the paths joining pairs of sites lying on the same side of the hyperplane and not crossing L_m, as P_1 and P_2 in Fig. 1 (otherwise, the path could lie across L_m and then g_m appears at least one time as a factor, given zero contribution at $g_m=0$). In this case the $2n$-point function factorizes, because the polymers appearing in the exponent in (2.1) are incompatible with at least one of the paths not crossing L_m. [There exists also the case of polymers lying across the hyperplane, as Γ_2 in Fig. 1, but their activities depend on g_m (actually, on g_m^2 or higher even powers, because the connectedness of Γ) and then evaluating at $g_m=0$ their contribution in the exponent is zero, i.e., contribute with a factor 1.] For parts (b) and (c), by (2.1) we have to derivate a sum of a product of two factors. Even derivatives have the form

$$\partial_{g_m}^{2n}\mathcal{S}_{2n}(i_1,\ldots,i_{2n})=\sum_{M\in\mathrm{conn}(i_1,\ldots,i_{2n})}A_1+A_2.$$

Here, A_1 is a sum of terms of the form

$$\text{const}\,\partial_{g_m}^{(\text{even})}\left(\prod_{L\in M}g_L\right)\partial_{g_m}^{(\text{even})}\exp\sum_{\substack{\Gamma\in\mathcal{G}'(\Lambda)\\ \Gamma\not\supset M}}c_\Gamma\mu^\Gamma. \tag{2.2}$$

If there exists an odd number of sites lying on both sides of L_m, then there exists at least one path joining sites lying on different sides of the hyperplane, as P_3 in Fig. 1. Furthermore, such paths would cross L_m an odd number of times and there would exist an odd number of such paths. Thus, in this case, the factor in parentheses in (2.2) depends on odd powers of g_m, and then its derivative vanishes at $g_m=0$, therefore implying $A_1=0$. On the other hand, A_2 is a sum of terms of the form

$$\text{const}\,\partial_{g_m}^{(\text{odd})}\left(\prod_{L\in M}g_L\right)\partial_{g_m}^{(\text{odd})}\exp\sum_{\substack{\Gamma\in\mathcal{G}'(\Lambda)\\ \Gamma\not\supset M}}c_\Gamma\mu^\Gamma$$

that vanish also, because the exponent depends on even powers of g_m since the polymers are connected. Analogously, for part (c) we have

$$\partial_{g_m}^{2n+1}\mathcal{S}_{2n}(i_1,\ldots,i_{2n})=\sum_{M\in\mathrm{conn}(i_1,\ldots,i_{2n})}B_1+B_2.$$

Here, B_1 is a sum of terms of the form

$$\text{const}\,\partial_{g_m}^{(\text{odd})}\left(\prod_{L\in M} g_L\right)\partial_{g_m}^{(\text{even})}\exp\sum_{\substack{\Gamma\in\mathcal{G}'(\Lambda)\\ \Gamma\neq M}} c_\Gamma \mu^\Gamma. \tag{2.3}$$

The paths not crossing the hyperplane are independent of g_m, with a vanishing derivative. The paths that cross L_m joining sites lying on the same side of the hyperplane would cross L_m an even number of times, as P_4 in Fig. 1. The paths that cross L_m joining sites lying on different sides of the hyperplane would cross L_m an odd number of times, as P_3 in Fig. 1, but if r is even, there exists an even number of such paths. So, in both cases, the factor in parentheses in (2.3) depends on even powers of g_m and then its derivative vanishes at $g_m=0$, therefore implying $B_1=0$. On the other hand, B_2 is a sum of terms of the form

$$\text{const}\,\partial_{g_m}^{(\text{even})}\left(\prod_{L\in M} g_L\right)\partial_{g_m}^{(\text{odd})}\exp\sum_{\substack{\Gamma\in\mathcal{G}'(\Lambda)\\ \Gamma\neq M}} c_\Gamma \mu^\Gamma,$$

which vanish also, by the same argument used to prove the vanishing of A_2 above. ■

Lemma 2.2:

$$\partial_{g_m}\mathcal{S}_n(i_1,\ldots,i_n)\big|_{g_m=0}=\sum_{\mathbf{x}\in\mathbb{Z}^d}\mathcal{S}_{n+2}(i_1,\ldots,i_n,(m,\mathbf{x}),(m+1,\mathbf{x}))\big|_{g_m=0}, \tag{2.4}$$

$$\begin{aligned}\partial_{g_m}^2\mathcal{S}_n(i_1,\ldots,i_n)\big|_{g_m=0}=&\sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d}\mathcal{S}_{n+4}(i_1,\ldots,i_n,(m,\mathbf{x}),(m+1,\mathbf{x}),(m,\mathbf{y}),(m+1,\mathbf{y}))\big|_{g_m=0}\\ &-\mathcal{S}_n(i_1,\ldots,i_n)\big|_{g_m=0}\sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d}\mathcal{S}_2((m,\mathbf{x}),(m,\mathbf{y}))\big|_{g_m=0}\\ &\mathcal{S}_2((m+1,\mathbf{x}),(m+1,\mathbf{y}))\big|_{g_m=0}.\end{aligned} \tag{2.5}$$

□

Proof: Recalling that $g_m=\tanh(\beta J_m)$, note that $J_m=(1/\beta)\operatorname{arctanh} g_m$ and therefore $\partial_{g_m}\mathcal{S}_n=(\mathrm{d}J_m/\mathrm{d}g_m)\partial_{J_m}\mathcal{S}_n=[\beta^{-1}/(1-g_m^2)]\partial_{J_m}\mathcal{S}_n$. Using this observation, differentiate (1.2), evaluate at $g_m=0$, and then use Lemma 2.1 to get (2.4). The proof of (2.5) is analogous, differentiating twice (1.2) and using (2.4) to simplify some expressions. ■

III. THE TWO-POINT FUNCTION AND ITS INVERSE

Particularizing the general results of the last section for the case of the two-point function, we have the following lemma.

Lemma 3.3: Consider $i,j\in\mathbb{Z}^{d+1}$ such that $i_0<j_0$ and $n\in\mathbb{N}\cup\{0\}$.

(a) If $i_0\leqslant m<j_0$, then $\partial_{g_m}^{2n}\mathcal{S}_2(i,j)\big|_{g_m=0}=0$.

(b) If $m<i_0$, then

$$\begin{aligned}\partial_{g_m}^2\mathcal{S}_2(i,j)\big|_{g_m=0}=&\sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d}\mathcal{S}_2((m,\mathbf{x}),(m,\mathbf{y}))\big|_{g_m=0}\mathcal{S}_4((m+1,\mathbf{x}),(m+1,\mathbf{y}),i,j)\big|_{g_m=0}\\ &-\mathcal{S}_2(i,j)\big|_{g_m=0}\sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d}\mathcal{S}_2((m,\mathbf{x}),(m,\mathbf{y}))\big|_{g_m=0}\mathcal{S}_2((m+1,\mathbf{x}),(m+1,\mathbf{y}))\big|_{g_m=0}.\end{aligned}$$

(c) If $j_0\leqslant m$, then

$$\partial_{g_m}^2 \mathcal{S}_2(i,j)\big|_{g_m=0} = \sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d} \mathcal{S}_4(i,j,(m,\mathbf{x}),(m,\mathbf{y}))\big|_{g_m=0} \mathcal{S}_2((m+1,\mathbf{x}),(m+1,\mathbf{y}))\big|_{g_m=0}$$

$$- \mathcal{S}_2(i,j)\big|_{g_m=0} \sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d} \mathcal{S}_2((m,\mathbf{x}),(m,\mathbf{y}))\big|_{g_m=0} \mathcal{S}_2((m+1,\mathbf{x}),(m+1,\mathbf{y}))\big|_{g_m=0}.$$

(d) If $m<i_0$ or $j_0\leqslant m$, then $\partial_{g_m}^{2n+1}\mathcal{S}_2(i,j)\big|_{g_m=0}=0$.

(e) If $i_0\leqslant m<j_0$, then

$$\partial_{g_m}\mathcal{S}_2(i,j)\big|_{g_m=0} = \sum_{\mathbf{x}\in\mathbb{Z}^d} \mathcal{S}_2(i,(m,\mathbf{x}))\big|_{g_m=0} \mathcal{S}_2((m+1,\mathbf{x}),j)\big|_{g_m=0}. \tag{3.1}$$

On other hand, when $i_0=j_0$, we have

(f) $\partial_{g_m}^{2n+1}\mathcal{S}_2(i,j)\big|_{g_m=0}=0$, $\forall m$. □

Lemma 3.3(a) has the following well known consequence: for the high-temperature IM the two-point function decays exponentially with the separation of its arguments, i.e., if β is sufficiently small, there exist $m=m(\beta)$ and $C=C(\beta)$ such that $|\mathcal{S}_2(i,j)|\leqslant C\mathrm{e}^{-m|i_0-j_0|}$ (see, e.g., Refs. 24–27). This fact has relevant corollaries, among them the uniqueness of ground state, the existence of a lower mass gap and the analyticity of the Fourier transform of the two-point function in momentum space (see, e.g., Refs. 28, 18, and 24, and cf. Refs. 29 and 30).

The two-point function considered as a linear operator in $\ell^2(\mathbb{Z}^{d+1})$, via

$$[\mathcal{S}_2(\{a_j\}_{j\in\mathbb{Z}^{d+1}})]_i := \sum_{j\in\mathbb{Z}^{d+1}} \mathcal{S}_2(i,j)a_j,$$

is well defined and exists $\mathcal{S}_2^{-1}=:\Gamma$ (see Ref. 25, p. 606 and Lemma A2, pp. 605–606). Moreover, as a consequence of Lemma 3.3(a), for a given $m\in\mathbb{Z}$, $\mathcal{S}_2\big|_{g_m=0}$ leaves invariant each of the subspaces

$$\ell^2_{\leqslant m} := \{\{a_j\}_{j\in\mathbb{Z}^{d+1}}\in\ell^2(\mathbb{Z}^{d+1}) : a_j=0 \quad \text{if } j_0>m\};$$

$$\ell^2_{>m} := \{\{a_j\}_{j\in\mathbb{Z}^{d+1}}\in\ell^2(\mathbb{Z}^{d+1}) : a_j=0 \quad \text{if } j_0\leqslant m\}.$$

Therefore, $\mathcal{S}_2\big|_{g_m=0}$ is a direct sum of two operators acting separately in each of these subspaces and the same follows for Γ. Note also that Γ is symmetrical, i.e., $\Gamma(i,j)=\Gamma(j,i)$.

Lemma 3.4: Consider $i,j\in\mathbb{Z}^{d+1}$ such that $i_0<j_0$.

(a) If $i_0\leqslant m<j_0$, then $\Gamma(i,j)\big|_{g_m=0}=0$.

(b)

$$\partial_{g_m}\Gamma(i,j)\big|_{g_m=0} = \begin{cases} 0 & \text{if } j_0\leqslant m, \\ 0 & \text{if } i_0\leqslant m<j_0 \text{ when } |i_0-j_0|\geqslant 2, \\ 0 & \text{if } m<i_0. \end{cases}$$

On the other hand, when $i_0=j_0$ we have

(c) $\partial_{g_m}\Gamma(i,j)\big|_{g_m=0}=0$, $\forall m$.

Consider now $i,j\in\mathbb{Z}^{d+1}$ arbitrary. If $n\in\mathbb{N}\cup\{0\}$, then

(d) n even $\Rightarrow \partial_{g_m}^n\Gamma(i,j)\big|_{g_m=0}=0 \forall i_0\leqslant m<j_0$ if $i_0<j_0$;

n odd $\Rightarrow \partial_{g_m}^n\Gamma(i,j)\big|_{g_m=0}=0$ if $m<i_0$ or $j_0\leqslant m$ when $i_0<j_0$ or $\forall m$ when $i_0=j_0$.

□

Proof: Note first that for every $n\in\mathbb{N}$ we have the following simple identity

$$\partial_{g_m}^n \Gamma = -\Gamma(\partial_{g_m}^n(\mathcal{S}_2\Gamma) - \mathcal{S}_2\partial_{g_m}^n\Gamma). \tag{3.2}$$

Although formally trivial (since $\Gamma = \mathcal{S}_2^{-1}$), this expression is useful for the *iterative* computation of the nth derivative of Γ, because the right side of (3.2) contains only derivatives of Γ of order $n-1$ at most. Now, part (a) is a consequence of the invariance of $\ell^2_{>m}$ and $\ell^2_{\leqslant m}$ under Γ, using *reductio ad absurdum*. For part (b) in the case of $i_0 \leqslant m < j_0$, using (3.2) with $n=1$ and Lemma 3.3(d–f) we have

$$\begin{aligned}
\partial_{g_m}\Gamma(i,j)|_{g_m=0} &= -\sum_{a,b\in\mathbb{Z}^{d+1}} \Gamma(i,a)|_{g_m=0}\partial_{g_m}\mathcal{S}_2(a,b)|_{g_m=0}\Gamma(b,j)|_{g_m=0} \\
&= -\sum_{a,b\in\mathbb{Z}^{d+1}} \sum_{\mathbf{x}\in\mathbb{Z}^d} \Gamma(i,a)|_{g_m=0}\mathcal{S}_2(a,(m,\mathbf{x}))|_{g_m=0} \\
&\quad \mathcal{S}_2((m+1,\mathbf{x}),b)|_{g_m=0}\Gamma(b,j)|_{g_m=0} \\
&= -\sum_{\mathbf{x}\in\mathbb{Z}^d} \delta_{i(m,\mathbf{x})}\delta_{(m+1,\mathbf{x})j},
\end{aligned} \tag{3.3}$$

where the last expression is equal to zero if $|i_0 - j_0| \geqslant 2$. The other cases of parts (b) and (c) follow using (3.2) analogously, adding the part (a) already proved and Lemma 3.3(b) and (c). The proof of part (d) is done by induction in n. The case $n=0$ is given in part (a) and the case $n=1$ is given in parts (b) and (c), already proved. Assume that statement of part (d) is valid for every i such that $i \leqslant n-1$. From (3.2) we have

$$\partial_{g_m}^n\Gamma(i,j)|_{g_m=0} = -\sum_{a,b\in\mathbb{Z}^{d+1}} \sum_{k=0}^{n-1} \binom{n}{k} \Gamma(i,a)|_{g_m=0}\partial_{g_m}^{n-k}\mathcal{S}_2(a,b)|_{g_m=0}\partial_{g_m}^k\Gamma(b,j)|_{g_m=0}. \tag{3.4}$$

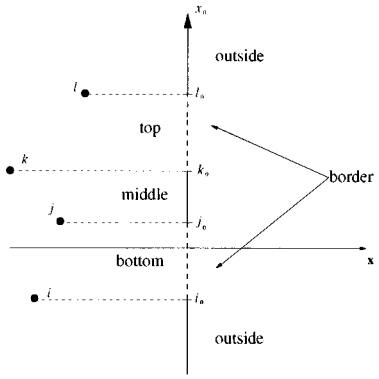
If n is even with $i_0 < j_0$ and $i_0 \leqslant m < j_0$, then, by part (a), the factor $\Gamma(i,a)|_{g_m=0}$ in (3.4) vanishes unless a lays into or below L_m.

(i) Now, when the index k of the second sum in (3.4) is even, the inductive hypothesis implies that the factor $\partial_{g_m}^k\Gamma(b,j)|_{g_m=0}$ in (3.4) vanishes unless b lays above L_m. But in this case $n-k$ is even also and, therefore, by Lemma 3.3(a), the factor $\partial_{g_m}^{n-k}\mathcal{S}_2(a,b)|_{g_m=0}$ vanishes if $a_0 \leqslant m < b_0$.

(ii) On the other hand, when the index k is odd, the inductive hypothesis implies that the factor $\partial_{g_m}^k\Gamma(b,j)|_{g_m=0}$ in (3.4) vanishes unless b lays into or below L_m. But in this case $n-k$ is odd also and, therefore, by Lemma 3.3(b) and (c), the factor $\partial_{g_m}^{n-k}\mathcal{S}_2(a,b)|_{g_m=0}$ vanishes if $a_0,\ b_0 \leqslant m$.

If n is odd with $i_0 < j_0$ and $m < i_0$ (resp. $j_0 \leqslant m$), the proof is analogous, using part (a) and relation (3.4). The case of n odd with $i_0 = j_0$ is also proved analogously, considering the subcases $m < i_0 = j_0$ and $i_0 = j_0 \leqslant m$ separately. ■

Parts (a) and (b) and (d) (with $n=2$) of Lemma 3.4 have the following well known consequence: for the high-temperature IM, if $|i_0 - j_0| \geqslant 2$, then $|\Gamma(i,j)| \leqslant \text{const}\, e^{-3m|i_0-j_0|}$ (see, e.g., Refs. 24–27). [Cf. Remark (1) following Lemma 2.2 in Ref. 25, p. 600.] This fact has as a corollary the analyticity property in momentum space for Γ and allows us to prove for the high-temperature IM the existence of lower and upper mass gaps (or existence of "one-particle states"), i.e., the analogy of Theorem 2.5 in Ref. 24 relative to the Fourier transform of the two-point function.



	A_1	A_2	A_1A_2	B	A_1B	A_2B	A_1A_2B
l ●	l ●	k ●	k ●	j ●	i ●	j ●	i ●
k ●	k ●	l ●	l ●	i ●	j ●	i ●	j ●
j ●	i ●	j ●	i ●	l ●	l ●	k ●	k ●
i ●	j ●	i ●	j ●	k ●	k ●	l ●	l ●
j ○	i ◎	j ○	i ○	l ○	l ◎	k ◎	k ○
k ○	k ○	l ◎	l ○	i ○	j ○	i ◎	j ○
l ○	l ◎	k ◎	k ○	j ○	i ○	j ◎	i ○
i ○	j ◎	i ◎	j ○	k ○	k ◎	l ◎	l ○
l ◎	l ○	k ○	k ◎	j ◎	i ○	j ○	i ◎
j ◎	i ○	j ○	i ◎	l ◎	l ○	k ○	k ◎
k ◎	k ○	l ○	l ◎	i ◎	j ○	i ○	j ◎
i ◎	j ○	i ○	j ◎	k ◎	k ○	l ○	l ◎

● = Type 1 ○ = Type 2 ◎ = Type 3

FIG. 2. *Left:* The top, middle, bottom, border and outside parts are shown in this example of type 1 configuration. *Right:* In the column at left an example of each configuration type. In the columns at right are the configurations obtained from the first at left of the respective row by the application of the operations shown in the top line.

IV. THE FOUR-POINT FUNCTIONS

Given four sites $i,j,k,l \in \mathbb{Z}^{d+1}$ such that $i_0<j_0<k_0<l_0$, the four-tuple $(i_0,j_0,k_0,l_0) \in \mathbb{Z}^4$ will be called the *configuration* determined by these sites. To simplify the statement and proofs of some results, we introduce the following definitions. The sets

$$\{m \in \mathbb{Z}: k_0 \leqslant m < l_0\}, \quad \{m \in \mathbb{Z}: j_0 \leqslant m < k_0\}, \quad \text{and } \{m \in \mathbb{Z}: i_0 \leqslant m < j_0\}$$

will be called respectively the *top*, the *middle* and the *bottom* of the configuration. The complement of the union of these sets will be called the *outside*, and the union of the top and the bottom will be called the *border*. We say that a configuration is of type 1 if the sites i and j are both in the top or in the bottom; see Fig. 2. Analogously, we say that a configuration is of type 2 if the sites i and l are both in the top or in the bottom. Finally, we say that a configuration is of type 3 if the sites i and k are both in the top or in the bottom. See Fig. 2. The configurations of types 1–3, will be relevant for some results, because any statement relative to one of them in the middle is automatically valid for all the others of the same type. In $\ell^2 := \ell^2(\mathbb{Z}^{d+1} \times \mathbb{Z}^{d+1})$ we define the symmetrical and antisymmetrical subspaces respectively by

$$\ell^2_s := \{\{a_{ij}\}_{i,j \in \mathbb{Z}^{d+1}} \in \ell^2 : a_{ij} = a_{ji}\}, \quad \ell^2_a := \{\{a_{ij}\}_{i,j \in \mathbb{Z}^{d+1}} \in \ell^2 : a_{ij} = -a_{ji}\}.$$

A. The unconnected part of truncated four-point function $\mathcal{D}_0$

As a simple consequence of the definition (1.4), we have the following.

Lemma 4.5: (a) $\mathcal{D}_0$ is invariant under the operations $A_1 :=$ exchange $i \leftrightarrow j$,

$$A_2 := \text{exchange } k \leftrightarrow l, \quad B := \text{simultaneous exchange } i \leftrightarrow k \text{ and } j \leftrightarrow l.$$

(b) As an operator in ℓ^2, $\mathcal{D}_0$ vanishes in the antisymmetric space ℓ^2_a.

(c) Considering $\mathcal{D}_0$ as an operator in the symmetric space ℓ^2_s, we have

$$\mathcal{D}_0^{-1}(i,j,k,l) = \tfrac{1}{2}\Gamma(i,k)\Gamma(j,l). \tag{4.1}$$

(d) $\mathcal{D}_0^{-1}$ has the same symmetry properties of part (a) plus the additional symmetry

$$A_3 := \text{exchange } j \leftrightarrow l.$$

□

Note that the set of type 1 configurations is invariant for any of the operations A_1, A_2, A_1A_2, B, A_1B, A_2B and A_1A_2B. In this sense, we say that such configurations are *equivalent*. The union of type 2 and 3 configurations is a set of equivalent configurations also; see Fig. 2. Equivalence of configurations reflects the symmetry properties of $\mathcal{D}_0$ in the following sense: If the value $V_{i,j,k,l}$ of $\mathcal{D}_0(i,j,k,l)$ is known when the sites i,j,k,l determine a given configuration, the value of $\mathcal{D}_0(i,j,k,l)$ when the sites determine another configuration obtained from the original by the application of some of the symmetry operations $C=A_r$, B $(r=1,2,3)$ is given by $V_{C(i,j,k,l)}$. The same considerations apply to derivatives of $\mathcal{D}_0$ with respect to g_m, the inverse $\mathcal{D}_0^{-1}$, and the derivatives of the inverse. Note also that a configuration is of type 2 if and only if it is equivalent to one of type 1 by the application of A_3. Thus, by Lemma 4.5(d), for the study of $\mathcal{D}_0^{-1}$ configurations of types 1 and 2 will be equivalent.

Lemma 4.6: For any configuration we have the following.

(a) $\partial_{g_m}^{2n}\mathcal{D}_0^{-1}(i,j,k,l)|_{g_m=0}=0$ *in the border. Furthermore, in the cases* $n=0,1$ *the corresponding derivative also vanishes in the middle of configuration 1.*

(b) $\partial_{g_m}^{2n-1}\mathcal{D}_0^{-1}(i,j,k,l)|_{g_m=0}=0$ *in the middle. Furthermore, in the case* $n=1$ *the derivative also vanishes in the border of any configuration.* □

Proof: For part (a), by (4.1) we have $\partial_{g_m}^{2n}\mathcal{D}_0^{-1}(i,j,k,l)|_{g_m=0}=A_1+A_2$, where A_1 and A_2 are sums of terms proportional to

$$\partial_{g_m}^{(\text{even})}\Gamma(i,k)|_{g_m=0}\partial_{g_m}^{(\text{even})}\Gamma(j,l)|_{g_m=0} \quad \text{and} \quad \partial_{g_m}^{(\text{odd})}\Gamma(i,k)|_{g_m=0}\partial_{g_m}^{(\text{odd})}\Gamma(j,l)|_{g_m=0},$$

respectively. Using Lemma 3.4(d) such terms have the values

A_1	1 and 2	3
top	0	0
middle	0	A_1
bottom	0	0

and

A_2	1 and 2	3
top	0	0
middle	A_2	0
bottom	0	0

respectively (here, numbers in the first line indicate the configuration type). Note that $A_2=0$ in the case $n=0$ (i.e., without derivative) and that in the case $n=1$ (i.e., the second derivative) the odd derivatives in A_2 are at most of first order, and all are equal to zero from Lemma 3.4(b). For part (b) we have $\partial_{g_m}^{2n-1}\mathcal{D}_0^{-1}(i,j,k,l)|_{g_m=0}=B_1+B_2$, where B_1 and B_2 are sums of terms proportional to

$$\partial_{g_m}^{(\text{odd})}\Gamma(i,k)|_{g_m=0}\partial_{g_m}^{(\text{even})}\Gamma(j,l)|_{g_m=0} \quad \text{and} \quad \partial_{g_m}^{(\text{even})}\Gamma(i,k)|_{g_m=0}\partial_{g_m}^{(\text{odd})}\Gamma(j,l)|_{g_m=0},$$

respectively, both equal to zero in the middle by Lemma 3.4(d). ■

B. The connected part of the truncated four-point function $\mathcal{D}$

It is easy to verify that Lemma 4.5(a) and (b) is also valid for $\mathcal{D}$. The next result is a direct consequence of Definition (1.3) and the general the results of Sec. II plus Lemma 3.3. For part (c) in the following lemma, we assume that the subindexed sites i_{k_m} pertain to the set $\{i,j,k,l\}$ and also we use the following convention: $\widehat{i_{k_m}}$ indicates that site i_{k_m} has to be omitted.

Lemma 4.7: (a) $\mathcal{D}(i,j,k,l)|_{g_m=0}$ *takes the following values*

	1	2	3
top	0	0	0
middle	0	$\mathcal{S}_2(i,l)|_{g_m=0}\mathcal{S}_2(k,j)|_{g_m=0}$	$\mathcal{S}_2(i,k)|_{g_m=0}\mathcal{S}_2(j,l)|_{g_m=0}$
bottom	0	0	0

(b) $\partial_{g_m}\mathcal{D}(i,j,k,l)\big|_{g_m=0}$ *takes the value*

$$\sum_{\mathbf{x}\in\mathbb{Z}^d}\mathcal{S}_4(i_{k_1},\ldots,\widehat{i_{k_r}},\ldots,i_{k_4},(m,\mathbf{x}))\big|_{g_m=0}\mathcal{S}_2((m+1,\mathbf{x}),i_{k_r})\big|_{g_m=0}$$
$$-\mathcal{S}_2(i_{k_1},i_{k_2})\big|_{g_m=0}\partial_{g_m}\mathcal{S}_2(i_{k_3},i_{k_4})\big|_{g_m=0}$$

in the top of any configuration such that $i_{k_r}\in\{i_{k_3},i_{k_4}\}$ *and* $(i_{k_r})_0=\max\{i_0,j_0,k_0,l_0\}$*, and the value*

$$\sum_{\mathbf{x}\in\mathbb{Z}^d}\mathcal{S}_2(i_{k_r},(m,\mathbf{x}))\big|_{g_m=0}\mathcal{S}_4((m+1,\mathbf{x}),i_{k_1},\ldots,\widehat{i_{k_r}},\ldots,i_{k_4})\big|_{g_m=0}$$
$$-\partial_{g_m}\mathcal{S}_2(i_{k_1},i_{k_2})\big|_{g_m=0}\mathcal{S}_2(i_{k_3},i_{k_4})\big|_{g_m=0}$$

in the bottom of any configuration such that $i_{k_r}\in\{i_{k_1},i_{k_2}\}$ *and* $(i_{k_r})_0=\min\{i_0,j_0,k_0,l_0\}$.

(c) In the middle of configuration 1, $\partial_{g_m}^2\mathcal{D}(i,j,k,l)\big|_{g_m=0}$ *is equal to*

$$\sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d}\mathcal{D}(i,j,(m,\mathbf{x}),(m,\mathbf{y}))\big|_{g_m=0}\mathcal{D}((m+1,\mathbf{x}),(m+1,\mathbf{y}),k,l)\big|_{g_m=0}. \tag{4.2}$$

(d) Even derivatives vanish in the border of any configuration.

(e) Odd derivatives vanish in the middle and in the outside of any configuration. □

For a given $m\in\mathbb{Z}$, we define the subspaces

$$\ell^2_{>m}:=\{\{a_{ij}\}_{i,j\in\mathbb{Z}^{d+1}}\in\ell^2: a_{ij}=0 \text{ if } i_0 \text{ or } j_0\leqslant m\},$$

$$\ell^2_{\leqslant m}:=\{\{a_{ij}\}_{i,j\in\mathbb{Z}^{d+1}}\in\ell^2: a_{ij}=0 \text{ if } i_0 \text{ or } j_0> m\},$$

$$\ell^2_{\div m}:=\{\{a_{ij}\}_{i,j\in\mathbb{Z}^{d+1}}\in\ell^2: a_{ij}=0 \text{ if } i_0,j_0\leqslant m \text{ or } i_0,j_0> m\}.$$

Lemma 4.8: (a) *Each of the subspaces above is invariant by* $\mathcal{D}$*, and therefore also under* $\mathcal{D}^{-1}$.

(b) In $\ell^2_{\div m}\cap\ell^2_s$ *we have*

$$\mathcal{D}^{-1}(i,j,k,l)\big|_{g_m=0}=\tfrac{1}{4}[\Gamma(i,k)\big|_{g_m=0}\Gamma(j,l)\big|_{g_m=0}+\Gamma(i,l)\big|_{g_m=0}\Gamma(j,k)\big|_{g_m=0}]. \tag{4.3}$$

(c) In the middle of configuration 1 we have

$$[(\partial_{g_m}\mathcal{D})\mathcal{D}^{-1}\partial_{g_m}\mathcal{D}](i,j,k,l)\big|_{g_m=0}=\partial_{g_m}^2\mathcal{D}(i,j,k,l)\big|_{g_m=0}.$$

□

Proof: Part (a) follows from Lemma 4.7(a), using *reductio ad absurdum*. Part (b) can be proved by direct substitution. For part (c), $(\partial_{g_m}\mathcal{D})\mathcal{D}^{-1}\partial_{g_m}\mathcal{D}\big|_{g_m=0}$ evaluated at (i,j,k,l) is equal to

$$\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\partial_{g_m}\mathcal{D}(i,j,a,b)\big|_{g_m=0}\mathcal{D}^{-1}(a,b,c,d)\big|_{g_m=0}\partial_{g_m}\mathcal{D}(c,d,k,l)\big|_{g_m=0}. \tag{4.4}$$

From Lemma 4.7(e), the third factor in (4.4) considered as a function of index c and d only is in $\ell^2_{\div m}$. Therefore, each term of the summatory in (4.4) vanishes unless the hyperplane L_m separates the pair $\{c,d\}$. Also from Lemma 4.7(e), in the middle of configuration 1 the first factor in (4.4) vanishes unless L_m separates the pair $\{a,b\}$. Thus, we have four cases, depending on the positions of both pairs $\{c,d\}$ and $\{a,b\}$ with respect to the hyperplane L_m. Assume, to fix ideas, that b and d are above L_m and that a and c lie into or below L_m. In any case, sites i,j,a,b determine

configurations with a or b in the top, and the sites c,d,k,l determine configurations with c or d in the bottom. Using Lemma 4.7(b) and (4.3) [note that in this case the second term at right in (4.3) vanishes from Lemma 3.4(a)], expression (4.4) is given by

$$\begin{aligned}
&\frac{1}{4}\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d}\mathcal{S}_4(i,j,a,(m,\mathbf{x}))\big|_{g_m=0}\mathcal{S}_2((m+1,\mathbf{x}),b)\big|_{g_m=0}\Gamma(a,c)\big|_{g_m=0}\\
&\quad\times\Gamma(b,d)\big|_{g_m=0}\mathcal{S}_2(c,(m,\mathbf{y}))\big|_{g_m=0}\mathcal{S}_4((m+1,\mathbf{y}),d,k,l)\big|_{g_m=0}\\
&\quad-\frac{1}{4}\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d}\mathcal{S}_4(i,j,a,(m,\mathbf{x}))\big|_{g_m=0}\mathcal{S}_2((m+1,\mathbf{x}),b)\big|_{g_m=0}\Gamma(a,c)\big|_{g_m=0}\\
&\quad\times\Gamma(b,d)\big|_{g_m=0}\partial_{g_m}\mathcal{S}_2(c,d)\big|_{g_m=0}\mathcal{S}_2(k,l)\big|_{g_m=0}\\
&\quad-\frac{1}{4}\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\sum_{\mathbf{y}\in\mathbb{Z}^d}\mathcal{S}_2(i,j)\big|_{g_m=0}\partial_{g_m}\mathcal{S}_2(a,b)\big|_{g_m=0}\Gamma(a,c)\big|_{g_m=0}\Gamma(b,d)\big|_{g_m=0}\\
&\quad\times\mathcal{S}_2(c,(m,\mathbf{y}))\big|_{g_m=0}\mathcal{S}_4((m+1,\mathbf{y}),d,k,l)\big|_{g_m=0}\\
&\quad+\frac{1}{4}\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\sum_{\mathbf{y}\in\mathbb{Z}^d}\mathcal{S}_2(i,j)\big|_{g_m=0}\partial_{g_m}\mathcal{S}_2(a,b)\big|_{g_m=0}\Gamma(a,c)\big|_{g_m=0}\Gamma(b,d)\big|_{g_m=0}\\
&\quad\times\partial_{g_m}\mathcal{S}_2(c,d)\big|_{g_m=0}\mathcal{S}_2(k,l)\big|_{g_m=0}.
\end{aligned}$$

Using (3.1) to replace the derivatives of the two-point functions in the last three terms above, we get $\frac{1}{4}$ times expression (4.2). The remaining three cases are analogous and give the same result.■

Lemma 4.9: (a) $\mathcal{D}^{-1}(i,j,k,l)\big|_{g_m=0}=0$ *in the border of any configuration and in the middle of the configuration 1. Furthermore,* $\mathcal{D}^{-1}(i,j,k,l)\big|_{g_m=0}=\mathcal{D}_0^{-1}(i,j,k,l)\big|_{g_m=0}$ *in the middle of configurations 2 and 3.*

(b) If $|i_0-j_0|\geqslant 2$ *and* $|k_0-l_0|\geqslant 2$, *then* $\partial_{g_m}\mathcal{D}^{-1}(i,j,k,l)\big|_{g_m=0}=0$ *in the bottom (with* $i_0<m$*), middle, top (with* $m<l_0-1$*) and outside of any configuration.*

(c) $\partial_{g_m}^2\mathcal{D}^{-1}(i,j,k,l)\big|_{g_m=0}=\partial_{g_m}^2\mathcal{D}_0^{-1}(i,j,k,l)\big|_{g_m=0}$ *in the middle of configuration 1.*

If $n\in\mathbb{N}\cup\{0\}$, *then*

(d) n *even* $\Rightarrow\partial_{g_m}^n\mathcal{D}^{-1}(i,j,k,l)\big|_{g_m=0}=0$ *in the border of any configuration.*

n *odd* $\Rightarrow\partial_{g_m}^n\mathcal{D}^{-1}(i,j,k,l)\big|_{g_m=0}$

$=0$ *in the middle and the outside of any configuration.*

□

Proof: Part (a) follows from Lemma 4.7(a) in analogy with the proof Lemma 3.4(a) [note that the second claim of part (a) in $\ell^2_{\div m}\cap\ell^2_s$ follows also from (4.1) and (4.3)]. Once part (b) is proved, the proof of part (d) can be done by induction on n in analogy with the proof of Lemma 3.4(d). To prove (b), using a formula analogous to (3.2) we have that $\partial_{g_m}\mathcal{D}^{-1}(i,j,k,l)\big|_{g_m=0}$ is equal to

$$-\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\mathcal{D}^{-1}(i,j,a,b)\big|_{g_m=0}\partial_{g_m}\mathcal{D}(a,b,c,d)\big|_{g_m=0}\mathcal{D}^{-1}(c,d,k,l)\big|_{g_m=0}. \tag{4.5}$$

Consider first the case of a configuration with $i_0=\min\{i_0,j_0,k_0,l_0\}$. In the bottom, the first factor in (4.5) vanishes, by part (a), unless the hyperplane L_m separates the pair $\{a,b\}$, and by the same argument the third factor vanishes unless the pair $\{c,d\}$ lies above L_m. Thus, with regards to the second factor in (4.5), we are in the bottom of some configuration having a or b in the bottom.

Note that there exist two cases, depending on the positions of a and b with respect to the hyperplane L_m. Assume that b is above and a lies into or below L_m (the argument for the opposite case will be analogous). Note also that by the same argument above, the product of the last two factors in (4.5) considered as a function of a and b only is in $\ell^2_{\div m}$. Using Lemmas 4.8(b) and 4.7(b) to replace the first and second factors in (4.5), respectively, we have that (4.5) can be written as the sum of

$$
\begin{aligned}
&-\frac{1}{4}\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\sum_{\mathbf{x}\in\mathbb{Z}^d}\Gamma(i,a)\big|_{g_m=0}\Gamma(j,b)\big|_{g_m=0}\mathcal{S}_2(a,(m,\mathbf{x}))\big|_{g_m=0}\\
&\quad\mathcal{S}_4((m+1,\mathbf{x}),b,c,d)\big|_{g_m=0}\mathcal{D}^{-1}(c,d,k,l)\big|_{g_m=0}\\
&\quad=-\frac{1}{4}\sum_{b,c,d\in\mathbb{Z}^{d+1}}\sum_{\mathbf{x}\in\mathbb{Z}^d}\delta_{i(m,\mathbf{x})}\Gamma(j,b)\big|_{g_m=0}\\
&\quad\mathcal{S}_4((m+1,\mathbf{x}),b,c,d)\big|_{g_m=0}\mathcal{D}^{-1}(c,d,k,l)\big|_{g_m=0},
\end{aligned}
$$

which vanishes if $i_0<m$, plus

$$
\begin{aligned}
&\frac{1}{4}\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\sum_{\mathbf{x}\in\mathbb{Z}^d}\Gamma(i,a)\big|_{g_m=0}\Gamma(j,b)\big|_{g_m=0}\mathcal{S}_2(a,(m,\mathbf{x}))\big|_{g_m=0}\\
&\quad\mathcal{S}_2((m+1,\mathbf{x}),b)\big|_{g_m=0}\mathcal{S}_2(c,d)\big|_{g_m=0}\mathcal{D}^{-1}(c,d,k,l)\big|_{g_m=0}\\
&\quad=\frac{1}{4}\sum_{c,d\in\mathbb{Z}^{d+1}}\sum_{\mathbf{x}\in\mathbb{Z}^d}\delta_{i(m,\mathbf{x})}\delta_{j(m+1,\mathbf{x})}\mathcal{S}_2(c,d)\big|_{g_m=0}\mathcal{D}^{-1}(c,d,k,l)\big|_{g_m=0},
\end{aligned}
$$

which vanishes if $|i_0-j_0|\geqslant 2$. In the middle we consider two cases separately.

(1) j lie into or below L_m.
From part (a), the first factor in (4.5) vanishes unless the pair $\{a,b\}$ is below L_m, and by the same argument the third factor vanishes unless the pair $\{c,d\}$ is above L_m. But then the second factor vanishes from Lemma 4.7(e).

(2) j lie above L_m.
From part (a), the first factor in (4.5) vanishes unless L_m separates the pair $\{a,b\}$, and by the same argument the third factor vanishes unless L_m separates the pair $\{c,d\}$. But then the second factor vanishes by Lemma 4.7(e).

In the top the analysis is analogous to the bottom part. In the lower (resp. upper) outside part, from part (a) the first and third factors vanish unless the pairs $\{a,b\}$ and $\{c,d\}$ are above (resp. below) L_m. But then the second factor vanishes by Lemma 4.7(e). The proofs for the remainder configurations are analogous.

For part (c), using a formula analogous to (3.2) with $n=1,2$, we have

$$
\partial_{g_m}\mathcal{D}^{-1}=-\mathcal{D}^{-1}[(\partial_{g_m}\mathcal{D})\mathcal{D}^{-1}], \tag{4.6}
$$

$$
\partial^2_{g_m}\mathcal{D}^{-1}=-\mathcal{D}^{-1}[(\partial^2_{g_m}\mathcal{D})\mathcal{D}^{-1}+2(\partial_{g_m}\mathcal{D})(\partial_{g_m}\mathcal{D}^{-1})], \tag{4.7}
$$

respectively. Replacing $\partial_{g_m}\mathcal{D}^{-1}$ in (4.7) by the expression in (4.6), we get

$$
\partial^2_{g_m}\mathcal{D}^{-1}=-\mathcal{D}^{-1}[\partial^2_{g_m}\mathcal{D}-2(\partial_{g_m}\mathcal{D})\mathcal{D}^{-1}\partial_{g_m}\mathcal{D}]\mathcal{D}^{-1}.
$$

As in the proof of part (b), from part (a) each term vanishes unless the sites a,b,c,d determine a type 1 configuration with a and b in the bottom. Evaluating at $g_m=0$ and using Lemma 4.8(c) and (4.2) we have

$$\begin{aligned}\partial_{g_m}^2\mathcal{D}^{-1}(i,j,k,l)\big|_{g_m=0}&=\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\mathcal{D}^{-1}(i,j,a,b)\big|_{g_m=0}\partial_{g_m}^2\mathcal{D}(a,b,c,d)\big|_{g_m=0}\mathcal{D}^{-1}(c,d,k,l)\big|_{g_m=0}\\&=\sum_{a,b,c,d\in\mathbb{Z}^{d+1}}\sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d}\mathcal{D}^{-1}(i,j,a,b)\big|_{g_m=0}\mathcal{D}(a,b,(m,\mathbf{x}),(m,\mathbf{y}))\big|_{g_m=0}\\&\quad\times\mathcal{D}((m+1,\mathbf{x}),(m+1,\mathbf{y}),c,d)\big|_{g_m=0}\mathcal{D}^{-1}(c,d,k,l)\big|_{g_m=0}\\&=\sum_{\mathbf{x},\mathbf{y}\in\mathbb{Z}^d}\delta_{i(m,\mathbf{x})}\delta_{j(m,\mathbf{y})}\delta_{(m+1,\mathbf{x})k}\delta_{(m+1,\mathbf{y})l}\\&=\left(-\sum_{\mathbf{x}\in\mathbb{Z}^d}\delta_{i(m,\mathbf{x})}\delta_{(m+1,\mathbf{x})k}\right)\left(-\sum_{\mathbf{y}\in\mathbb{Z}^d}\delta_{j(m,\mathbf{y})}\delta_{(m+1,\mathbf{y})l}\right)\\&=\partial_{g_m}\Gamma(i,k)\big|_{g_m=0}\partial_{g_m}\Gamma(j,l)\big|_{g_m=0}=\partial_{g_m}^2\mathcal{D}_0^{-1}(i,j,k,l)\big|_{g_m=0}.\end{aligned}$$

In the last line above, we have used (3.3) for the first equality and (4.1) and Lemma 3.4(a) for the second. ■

C. The Bethe–Salpeter kernel

As $\mathcal{N}=\mathcal{D}^{-1}-\mathcal{D}_0^{-1}$, from Lemmas 4.6 and 4.9 we have the following.

Lemma 4.10: (a) If $k=0,1,2,3$, *then* $\partial_{g_m}^k\mathcal{N}(i,j,k,l)\big|_{g_m=0}=0$ *in the middle of configuration 1.*

(b) If $|i_0-j_0|\geq 2$, $|k_0-l_0|\geq 2$ *and* $k=0,1,2$, *then* $\partial_{g_m}^k\mathcal{N}(i,j,k,l)\big|_{g_m=0}=0$ *in the border* (*with* $i_0<m$ *and* $m<l_0-1$) *of all configurations.*

(c) If $k=0,1$, *then* $\partial_{g_m}^k\mathcal{N}(i,j,k,l)\big|_{g_m=0}=0$ *in the middle of configurations 2 and 3.* □

Proof of Theorem 1.1: Consider first the case of configuration 1. From Lemma 4.10 we have

$$\mathcal{N}(i,j,k,l)=(g_{i_0+1}g_{i_0+2}\cdots g_{j_0-1})^3(g_{j_0}g_{j_0+1}\cdots g_{k_0-1})^4(g_{k_0}g_{k_0+1}\cdots g_{l_0-2})^3F(g,g_m),$$

where F is an analytic function. In particular, for the isotropic IM model we have

$$\mathcal{N}(i,j,k,l)=g^{3|j_0-i_0-1|}g^{4|j_0-k_0|}g^{3|l_0-k_0-1|}F(g)=\mathrm{e}^{-m(3|j_0-i_0-1|+4|j_0-k_0|+3|l_0-k_0-1|)}F(g),$$

where $m:=-\ln g>0$ if $0<g<1$. Therefore,

$$|\mathcal{N}(i,j,k,l)|\leq C_1\mathrm{e}^{-m(3|j_0-i_0-1|+4|j_0-k_0|+3|l_0-k_0-1|)}. \tag{4.8}$$

Note that for $a,b\in\mathbb{R}$ we have $|a-b|\leq|a-b-1|+1$, or $|a-b-1|\geq|a-b|-1$. Therefore,

$$3|j_0-i_0-1|+4|j_0-k_0|+3|l_0-k_0-1|\geq 3|i_0-j_0|+4|j_0-k_0|+3|k_0-l_0|-6. \tag{4.9}$$

Note also that $|i_0+j_0-k_0-l_0|\leq|i_0-j_0|+2|j_0-k_0|+|k_0-l_0|$, and, therefore,

$$3|i_0-j_0|+4|j_0-k_0|+3|k_0-l_0|\geq|i_0-j_0|+|k_0-l_0|+2|i_0+j_0-k_0-l_0|. \tag{4.10}$$

Combining (4.8)–(4.10) we have

$$|\mathcal{N}(i,j,k,l)|\leq C_2\mathrm{e}^{-m(|i_0-j_0|+|k_0-l_0|+2|i_0+j_0-k_0-l_0|)}. \tag{4.11}$$

For configuration 2, from Lemma 4.10 we have analogously

$$|\mathcal{N}(i,j,k,l)| \leqslant C_1 \mathrm{e}^{-m(3|l_0-i_0-1|+2|l_0-j_0|+3|k_0-j_0-1|)}, \tag{4.12}$$

and (4.11) follows in this case combining the inequalities

$$3|l_0-i_0-1|+2|l_0-j_0|+3|k_0-j_0-1| \geqslant 3|l_0-i_0|+2|l_0-j_0|+3|k_0-j_0|-6,$$

$$|i_0-l_0|+|j_0-k_0| \geqslant |i_0+j_0-k_0-l_0|,$$

$$|i_0-l_0|+|l_0-j_0| \geqslant |i_0-j_0|,$$

$$|l_0-j_0|+|j_0-k_0| \geqslant |l_0-k_0|.$$

The case of configuration 3 is analogous to this latter case. Finally, Theorem 1.1 follows by the observation that the hyperplane decoupling method is equally applicable in each direction independently. ■

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Central limit theorem for fluctuations in the high temperature region of the Sherrington–Kirkpatrick spin glass model

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In a region above the Almeida–Thouless line, where we are able to control the thermodynamic limit of the Sherrington–Kirkpatrick model and to prove replica symmetry, we show that the fluctuations of the overlaps and of the free energy are Gaussian, on the scale $1/\sqrt{N}$, for large N. The method we employ is based on the idea we recently developed of introducing quadratic coupling between two replicas. The proof makes use of the cavity equations and of concentration of measure inequalities for the free energy. © *2002 American Institute of Physics.*
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I. INTRODUCTION

We consider the mean-field spin glass model, introduced by Sherrington and Kirkpatrick in Refs. 1 and 2, in the regime of high temperature or, equivalently, of large magnetic field. On physical grounds, it is known that in this region the replica symmetric solution holds, as shown for example in Ref. 3, and references quoted therein. However, due to the very large fluctuations present in the model, it is difficult to give a mathematically rigorous description of this region. Rigorous works on this subject include Refs. 4–8. For other rigorous results concerning the model, we refer to Refs. 9–13.

The method developed in Ref. 8 by Talagrand is particularly interesting. The starting point is the very deep physical idea that the phenomenon of replica symmetry breaking can be understood by studying the properties of the model under the application of auxiliary interactions, which explicitly break replica symmetry. In Ref. 8, this idea is employed to prove that the replica symmetric solution holds in a region, which (*probably*) coincides with that found in the theoretical physics literature,[3] i.e., up to the Almeida–Thouless critical line.

Recently,[14] we proposed a different strategy, which consists of coupling two replicas of the system by means of a term proportional to the square of the deviation of the overlap from its replica symmetric value. In this way, we proved that replica symmetry holds in a region above the Almeida–Thouless line. In the same region, we obtained a control of the two-replica system, provided that the coupling parameter is small enough, and we showed that the fluctuations of the overlap are at most of order $1/\sqrt{N}$. In the present paper we prove that, in the same region of parameters, the fluctuations of overlaps and free energy, when suitably rescaled, have a Gaussian distribution when $N\to\infty$. The main ingredients of the proof are the control of the thermodynamic limit obtained in Ref. 14 and concentration of measure techniques inspired by Talagrand's works. Then, by means of the cavity method, one can write self-consistent linear equations for the characteristic functions of the fluctuation variables, which can be easily solved.

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Previous results concerning limit theorems for fluctuations in the high temperature region of mean-field spin glass models include Refs. 4, 6, 15, 9, and 16.

This work is organized as follows: In Sec. II, we recall the main definitions of the model and introduce the overlap distribution structure. In Sec. III, we state the main results. Two useful tools, i.e., exponential inequalities and the cavity method, are briefly outlined in Secs. IV and V. In Secs. VI and VII, we prove the central limit theorem for overlap and free energy fluctuations, respectively. Finally, Sec. VIII is dedicated to a short outlook about open problems and further developments.

II. THE MODEL

The generic configuration of the Sherrington–Kirkpatrick (SK) model is determined by the N Ising variables $\sigma_i = \pm 1$, $i = 1,2,\ldots,N$, and the Hamiltonian is

$$H_N(\sigma,h;J) = -\frac{1}{\sqrt{N}} \sum_{(i,j)} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i, \tag{1}$$

where the sum $\Sigma_{(i,j)}$ runs over all the $N(N-1)/2$ distinct couples of sites. The J_{ij}'s (quenched noise) are independent centered unit Gaussian variables $\mathcal{N}(0,1)$. The first term in (1) is a long-range random two-body interaction, while the second represents the interaction with a fixed external magnetic field h. For a given temperature $1/\beta$ we can introduce the disorder dependent partition function

$$Z_N(\beta,h;J) = \sum_{\{\sigma\}} \exp(-\beta H_N(\sigma,h;J)), \tag{2}$$

and the auxiliary function

$$\alpha_N(\beta,h) = \frac{1}{N} E \ln Z_N(\beta,h;J), \tag{3}$$

where E denotes the average with respect to the external noise J. Note that $\alpha_N(\beta,h)$ is the quenched average of the free energy per spin, apart from the multiplicative factor $-1/\beta$.

For later convenience, it is useful to generalize the model (1) by introducing a quenched random external magnetic field, which at every site is an independent Gaussian variable of strength $x>0$. In other words, the Boltzmann factor of the system becomes

$$\exp\left(\sqrt{\frac{t}{N}} \sum_{(i,j)} J_{ij}\sigma_i\sigma_j + \sum_i (\beta h + \sqrt{x}J_i)\sigma_i \right), \tag{4}$$

where J_i are i.i.d. $\mathcal{N}(0,1)$ random variables, independent of the J_{ij}'s. We let $t=\beta^2$ in the two-body term. In the following, we always regard the system as depending on the parameters $t,x,\beta h$. In analogy with Eqs. (2) and (3), we define the disorder-dependent partition function $Z_N(t,x,h;J)$ and the auxiliary function

$$\alpha_N(t,x,h) = \frac{1}{N} E \ln Z_N(t,x,h;J).$$

Here, E denotes averaging with respect to J_{ij} and J_i. For simplicity of notations, here and in the following we write the argument h instead of βh.

Let us consider a countably infinite number of independent copies (replicas) of the system, whose spin variables σ_i^a are distributed, for fixed J, according to the product state

$$\Omega_J = \Omega_J^1 \Omega_J^2 \ldots,$$

where $\Omega_J \equiv \Omega_J^{N,t,x,h}$ denotes the Gibbs state associated with the Boltzmann factor (4). Each replica is subject to the same quenched noise. The "real replica" approach has already been exploited in a number of papers.[17–20]

The overlap between two replicas a,b is defined as

$$q_{ab}(\sigma^a,\sigma^b)=\frac{1}{N}\sum_i \sigma_i^a\sigma_i^b,$$

with the obvious bounds

$$-1\leqslant q_{ab}\leqslant 1.$$

For a generic smooth function F of the overlaps, we define the $\langle . \rangle$ average as

$$\langle F(q_{12},q_{13},\ldots)\rangle = E\Omega_J(F(q_{12},q_{13},\ldots)).$$

Note that the average over disorder introduces correlations between different groups of replicas, which would be independent under the Boltzmann average Ω_J. For example,

$$\Omega_J(q_{12}q_{34})=\Omega_J(q_{12})\Omega_J(q_{34}),$$

but

$$\langle q_{12}q_{34}\rangle \neq \langle q_{12}\rangle\langle q_{34}\rangle.$$

III. THE HIGH TEMPERATURE REGION AND THE MAIN RESULTS

In this section, we recall the results of Ref. 14 and state limit theorems for fluctuations, in the region where we prove that replica symmetry holds, i.e.,

$$\lim_{N\to\infty}\alpha_N(t,x,h)=\overline{\alpha}(t,x,h).$$

$\overline{\alpha}(t,x,h)$ is the replica-symmetric free energy[1,2]

$$\overline{\alpha}(t,x,h)=\ln 2+\int \ln\cosh(\beta h+z\sqrt{t\overline{q}+x})d\mu(z)+\frac{t}{4}(1-\overline{q})^2,$$

where $\overline{q}$ is the Sherrington–Kirkpatrick order parameter, defined as the unique[17] solution of

$$\overline{q}=\overline{q}(t,x,h)=\int \tanh^2(\beta h+z\sqrt{t\overline{q}+x})d\mu(z),$$

and $d\mu(z)$ is the centered unit Gaussian measure.

In Ref. 14 we proved the following: Consider the auxiliary function $\tilde{\alpha}_N$, dependent on the parameter $\lambda\geqslant 0$

$$\tilde{\alpha}_N(t,x,h;\lambda)=\alpha_N(t,x,h)+\frac{1}{2N}E\ln\Omega_{t,x,h}(e^{N(\lambda/2)(q_{12}-\overline{q})^2})$$

and the trajectory in the (t,x) plane

$$\Gamma=(t',x_{t'})\equiv(t',x+\overline{q}(t-t'))\equiv(t',x_0-\overline{q}t'),\quad 0\leqslant t'\leqslant t \tag{5}$$

where $x_0=x+\overline{q}t$ and $\overline{q}=\overline{q}(t,x,h)=\overline{q}(t',x_{t'},h)$. Notice that $\tilde{\alpha}_N$ equals α_N for $\lambda=0$. Given x_0,h there exists a value $t_c(x_0,h)$, such that

$$|\overline{\alpha}(t',x_{t'},h)-\tilde{\alpha}_N(t',x_{t'},h;\lambda)|\leqslant\frac{k}{N} \tag{6}$$

for some constant k, uniformly in the triangular region

$$0\leqslant t'+\lambda\leqslant\overline{t}<t_c(x_0,h). \tag{7}$$

In the same region, the overlaps self-average around the value $\overline{q}$

$$\langle(q_{ab}-\overline{q})^2\rangle\leqslant\frac{k}{N}. \tag{8}$$

The critical value $t_c(x_0,h)$ is determined in the following way:[14] Let

$$\Delta(x_0,h,\lambda_0)\equiv\frac{1}{2}\max_{\rho\in\mathbb{R}}\left(\int \ln(\cosh\rho+\tanh^2(\beta h+z\sqrt{x_0})\sinh\rho)d\mu(z)-\rho\overline{q}-(\rho^2/2\lambda_0)\right),$$

where $\lambda_0\geqslant 0$. Then, we define $t_c(x_0,h)$ such that, for any $\lambda_0\leqslant t_c(x_0,h)$, one has

$$\Delta(x_0,h,\lambda_0)=0.$$

In the case of vanishing external field $x=h=0$, then also $x_0=\overline{q}=0$ and $t_c=1$, the correct critical value. As discussed in Ref. 14, the region defined by (7) falls short of the Almeida–Thouless line, which is the expected critical line.

In this paper, we investigate more precisely the behavior of fluctuations of physical quantities around the replica symmetric value. First of all, we give a central limit-type theorem for the rescaled overlaps

$$\xi_{ab}^N=\sqrt{N}(q_{ab}-\overline{q}),$$

showing that they behave as centered Gaussian variables characterized by a nondiagonal correlation matrix. Notice that, thanks to (8), one has the following bound for the second moment of the rescaled overlap fluctuations:

$$\langle(\xi_{ab}^N)^2\rangle\leqslant k. \tag{9}$$

Theorem 1: *If $t<t_c(x_0,h)$, the rescaled overlaps ξ_{ab}^N tend in distribution, for $N\to\infty$, to jointly Gaussian variables ξ_{ab}, with covariances*

$$\langle\xi_{ab}^2\rangle=A(t,x,h),$$

$$\langle\xi_{ab}\xi_{ac}\rangle=B(t,x,h),$$

$$\langle\xi_{ab}\xi_{cd}\rangle=C(t,x,h),$$

where a, b, c, d are all different. A, B, and C are explicitly given by

$$A(t,x,h)=(1+2R+4R^2)Y+c_0R^2, \tag{10}$$

$$B(t,x,h)=(1+4R)RY+c_0R^2, \tag{11}$$

$$C(t,x,h)=4R^2Y+c_0R^2, \tag{12}$$

where

$$Y(t,x,h)=\frac{1}{Y_0^{-1}-t},$$

$$R(t,x,h)=\frac{d_0}{Y_0^{-1}+2d_0-t},$$

and $Y_0(x_0,h), c_0(x_0,h)$, *and* $d_0(x_0,h)$ *are chosen in such a way that* A,B,C *satisfy the initial conditions*

$$A(0,x_0,h)=1-\overline{q}^2,$$

$$B(0,x_0,h)=\overline{q}-\overline{q}^2,$$

$$C(0,x_0,h)=\int \tanh^4(z\sqrt{x_0}+\beta h)d\mu(z)-\overline{q}^2.$$

In particular, one has

$$Y_0=\int \cosh^{-4}(z\sqrt{t\overline{q}+x}+\beta h)d\mu(z). \tag{13}$$

Recently, an analogous result was proved independently by Talagrand,[16] who computed the $N\to\infty$ limit for all moments of the ξ variables.

The expressions for $A,B,$ and C were first given by Guerra in Ref. 17. For $h=x=0$, the limit Gaussian variables are not correlated and have variance $1/(1-t)$, which is a well-known result.[4,6]

Let us consider now free-energy fluctuations. Aizenman, Lebowitz, and Ruelle[4] proved that in the case of zero external field and $t<1$, the variable

$$\ln Z_N-\ln EZ_N$$

tends to a shifted Gaussian random variable whose variance diverges at $t=1$. In the general case the situation is quite different and the following theorem holds:

Theorema 2: *Let*

$$\hat{f}_N(t,x,h;J)\equiv\sqrt{N}\left(\frac{\ln Z_N(t,x,h;J)}{N}-\overline{\alpha}(t,x,h)\right).$$

If $t<t_c(x_0,h)$ *then*

$$\hat{f}_N(t,x,h;J)\overset{d}{\to}\mathcal{N}(0,\sigma^2(t,x,h)),$$

where

$$\sigma^2(t,x,h)=Var(\ln\cosh(z\sqrt{t\overline{q}+x}+\beta h))-\frac{\overline{q}^2t}{2}.$$

Here, $Var(.)$ *denotes the variance of a random variable and* $z=\mathcal{N}(0,1)$.

Notice that fluctuations of the extensive free energy $\ln Z_N$ are of order 1 at zero external field and of order $\sqrt{N}$ otherwise.

IV. EXPONENTIAL SUPPRESSION OF OVERLAP FLUCTUATIONS

General arguments based on concentration of measure[9,21,22] show that the fluctuations of the free energy $1/N \ln Z_N$ around its mean value α_N are exponentially suppressed as N grows. Indeed, one has the following:[9]

Theorem 3: *For any* $u>0$,

$$P\left(\left|\frac{1}{N}\ln Z_N(t,x,h;J)-\alpha_N(t,x,h)\right|\geqslant u\right)\leqslant \exp(-NKu^2), \tag{14}$$

where

$$K=\frac{1}{t+2x}.$$

This, in connection with the results of Ref. 14, allows us to obtain a strong control on the fluctuations of the overlaps (we learned this nice argument in Ref. 8): First of all, the same argument leading to Theorem 3 shows that

$$P\left(\left|\frac{1}{2N}\ln \Omega_{t,x,h}(e^{N(\lambda/2)(q_{12}-\bar{q})^2})-\tilde{\alpha}_N(t,x,h,\lambda)+\alpha_N(t,x,h)\right|\geqslant 2u\right)\leqslant \exp(-NKu^2).$$

Therefore, thanks to Eq. (6), with probability at least $1-\exp(-NKu^2)$ one has

$$\Omega_{t,x,h}(e^{(\lambda/2)\,N(q_{12}-\bar{q})^2})\leqslant e^{4Nu+2C}$$

for $\lambda\leqslant\bar{\lambda}<t_c(x_0,h)-t$. Then, by Tchebysheff's inequality

$$\Omega_{t,x,h}(\chi_{\{|q_{12}-\bar{q}|\geqslant v\}})\leqslant e^{-(\bar{\lambda}/2)\,Nv^2}\Omega_{t,x,h}(e^{(\bar{\lambda}/2)\,N(q_{12}-\bar{q})^2})\leqslant e^{N(4u-(\bar{\lambda}/2)\,v^2)+2C}$$

and, choosing $u=\bar{\lambda}v^2/16$, one has

$$\Omega_{t,x,h}(\chi_{\{|q_{12}-\bar{q}|\geqslant v\}})\leqslant e^{-N(v^2\bar{\lambda}/4)+2C}.$$

The estimate we are looking for easily follows

$$E\Omega_{t,x,h}(\chi_{\{|q_{12}-\bar{q}|\geqslant v\}})\leqslant e^{-N(v^2\bar{\lambda}/4)+2C}+e^{-NK(\bar{\lambda}^2v^4/256)}. \tag{15}$$

Of course, this is much more than just self-averaging of the overlaps.

V. THE CAVITY METHOD

The cavity method allows expression of thermal averages of quantities defined on the N-spin system as functions of averages on the system with $N-1$ spins, at a slightly different temperature. This method has been widely applied both in the theoretical physics literature[3] and in the mathematical physics one (see, for instance, Refs. 5, 16, 10, and 18).

Introduce the following definitions:

$$t'=t(1-N^{-1})$$

$$\sigma^a=(\eta^a,\epsilon^a),\quad \eta^a\in\{-1,1\}^{N-1},\quad \epsilon^a=\sigma_N^a=\pm 1$$

$$J=J_N$$

$$g_i=J_{N\ i},\quad i=1,\ldots,N-1$$

$$\Omega'(.)=\Omega_{N-1}^{t'}(.).$$

The cavity equations consist of the identity

$$\Omega_N^{t,x,h}(f(\sigma^1,\ldots,\sigma^k))=\frac{\Omega'(Av\quad f(\eta^1,\epsilon^1,\ldots,\eta^k,\epsilon^k)\Psi^{(k)})}{\Omega'(Av\quad \Psi^{(k)})},\tag{16}$$

where Av denotes the average over the spin variables ϵ^a and

$$\Psi^{(k)}\equiv\exp\sum_{a=1}^{k}\epsilon^a(\sqrt{t/N}g\,\eta^a+\sqrt{x}J+\beta h).\tag{17}$$

$g\,\eta^a$ denotes the scalar product $\Sigma_{i=1}^{N-1}g_i\eta_i^a$.

VI. LIMIT THEOREM FOR OVERLAP FLUCTUATIONS

To prove Theorem 1, it suffices[23] to show that for any integer s, the characteristic function

$$\phi_N^t(u)=\langle\exp i\quad u\xi^N\rangle\equiv\left\langle\exp i\sum_{(a,b)}u_{ab}\xi_{ab}^N\right\rangle,\quad 1\leqslant a<b\leqslant s$$

converges for $N\to\infty$ to

$$\phi^t(u)=\exp\{-\tfrac{1}{2}(\hat{L}u,u)\},\tag{18}$$

where $(\ldots)$ denotes scalar product and $\hat{L}$ is the $s(s-1)/2\times s(s-1)/2$ dimensional matrix of elements

$$L_{(ab),(ab)}=A(t,x,h),$$

$$L_{(ab),(ac)}=B(t,x,h),$$

$$L_{(ab),(cd)}=C(t,x,h).$$

The idea of the proof is to obtain a set of closed linear differential equations for $\phi_N^t(u)$, which determines uniquely the solution as (18), for $N\to\infty$. Some of the calculations involved in the proof are quite long, although straightforward, and are therefore just sketched.

First of all, we explain how the cavity equations (16) and (17) can be simplified in the region where (15) holds. Following Ref. 10, we introduce some notations, letting $\Omega(.)\equiv\Omega_N^{t,x,h}(.)$ and $\Omega'(.)\equiv\Omega_{N-1}^{t',x,h}(.)$. Moreover, we define

$$b=\Omega'(\eta)\in\mathbb{R}^{N-1},$$

$$\dot{\eta}^a=\eta^a-b,$$

$$X=\sqrt{t/N}gb+\sqrt{x}J+\beta h,$$

$$\Psi_0^{(k)}=\exp\left(X\sum_{a=1}^{k}\epsilon^a\right),$$

$$f(\sigma^1,\ldots,\sigma^k)=f(\eta^1,\epsilon^1,\ldots,\eta^k,\epsilon^k).$$

Then, the following holds:[10]

Theorem 4:

$$E\Omega(f(\sigma^1,\ldots,\sigma^k))=E\frac{1}{\cosh^k X}\Omega'(Av\,f\Psi_0^{(k)}) \tag{19}$$

$$+tE\frac{1}{\cosh^k X}\Omega'\left(Av\,f\Psi_0^{(k)}\sum_{1\leqslant a<c\leqslant k}\epsilon^a\epsilon^c\frac{\dot\eta^a\dot\eta^c}{N}\right) \tag{20}$$

$$+tE\frac{1}{\cosh^k X}\Omega'\left(Av\,f\Psi_0^{(k)}\sum_{1\leqslant a\neq c\leqslant k}\epsilon^a\epsilon^c\frac{\dot\eta^c b}{N}\right) \tag{21}$$

$$-ktE\frac{\tanh X}{\cosh^k X}\Omega'\left(Av\,f\Psi_0^{(k)}\sum_{a=1}^{k}\epsilon^a\frac{\dot\eta^a b}{N}\right)+S, \tag{22}$$

and the "error term" S can be estimated as

$$|S|\leqslant w_k(t,x,h)E\Omega'\left(Av|f|\left(\sum_{a=1}^{k+1}\left(\frac{\dot\eta^a b}{N}\right)^2+\sum_{1\leqslant a<c\leqslant k+2}\left(\frac{\dot\eta^a\dot\eta^c}{N}\right)^2\right)\right),$$

where w is a smooth function of its arguments, independent of N.

Note that, with respect to Theorem 3.2 in Ref. 10, the last sum on the right-hand side is performed on $a<c$ instead of $a\leqslant c$. However, the proof of Theorem 4 proceeds exactly as in Ref. 10.

Theorem 4 is a sort of Taylor expansion of the cavity equations around $\eta^a=b$. This turns out to be particularly useful in the region where Eq. (15) holds, since in this case $\dot\eta_a$ is small with large probability, and S vanishes for $N\to\infty$, as we explain in the following.

In order to prove Theorem 1, we first exploit symmetry between sites to write

$$\partial_{u_{rr'}}\phi_N^t(u)=i\langle\xi_{rr'}^N e^{iu\xi^N}\rangle=i\sqrt{N}\langle(\sigma_N^r\sigma_N^{r'}-\overline{q})e^{iu\xi^N}\rangle, \tag{23}$$

$$\varphi_N^{(a)t}(u)\equiv i\langle\xi_{a,s+1}^N e^{iu\xi^N}\rangle=i\sqrt{N}\langle(\sigma_N^a\sigma_N^{s+1}-\overline{q})e^{iu\xi^N}\rangle, \tag{24}$$

$$\psi_N^t(u)\equiv i\langle\xi_{s+1,s+2}^N e^{iu\xi^N}\rangle=i\sqrt{N}\langle(\sigma_N^{s+1}\sigma_N^{s+2}-\overline{q})e^{iu\xi^N}\rangle, \tag{25}$$

and then employ the cavity equations to express these quantities as functions of ϕ,φ,ψ themselves. For instance, apply Theorem 4 to the right-hand side of Eq. (23) and consider the term arising from (19). After averaging on the dichotomic variables ϵ, one is left with

$$\begin{aligned}
&i\left(\sqrt{N}-i\sum_{(a,b)}u_{ab}\overline{q}\right)E\{(\tanh^2 X-\overline{q})\Omega'\exp(iu'\xi^{N-1})\}\\
&\quad-u_{rr'}E\{(1-\overline{q}\tanh^2 X)\Omega'\exp(iu'\xi^{N-1})\}\\
&\quad-(1-\overline{q})\sum_{a\neq r,r'}(u_{ar}+u_{ar'})E\{\tanh^2 X\Omega'\exp(iu'\xi^{N-1})\}\\
&\quad-\sum_{(c,d)c,d\neq r,r'}u_{cd}E\{\tanh^2 X(\tanh^2 X-\overline{q})\Omega'\exp(iu'\xi^{N-1})\}+o(1),
\end{aligned} \tag{26}$$

where $u'=u\sqrt{1-1/N}$. The term $o(1)$ arises when $\exp(iu/\sqrt{N})$ is expanded around $u=0$ and the terms of order u^2 or higher are neglected. Indeed, one has

$$\left|\sqrt{N}\left\langle (\sigma_N^r\sigma_N^{r'}-\overline{q})e^{iu'\xi^{N-1}}\left(e^{i\Sigma_{(a,b)}(u_{ab}/\sqrt{N})(\sigma_N^a\sigma_N^b-\overline{q})}-1-i\sum_{(a,b)}\frac{u_{ab}}{\sqrt{N}}(\sigma_N^a\sigma_N^b-\overline{q})\right)\right\rangle\right|$$

$$\leqslant 2\sqrt{N}\left|e^{i\Sigma_{(a,b)}(u_{ab}/\sqrt{N})(\sigma_N^a\sigma_N^b-\overline{q})}-1-i\sum_{(a,b)}\frac{u_{ab}}{\sqrt{N}}(\sigma_N^a\sigma_N^b-\overline{q})\right|=O(N^{-1/2}).$$

Now, rewrite E as $E\,E_g$, where E_g denotes the average only with respect to the random variables J and $g_i, i=1,\ldots,N-1$, and notice that J, g_i do not appear in the thermal average Ω'. Computation of $E_g(\ldots)$ would be simpler if, instead of X, there were

$$\overline{X}\equiv\sqrt{t/N}g\overline{b}+\sqrt{x}J+\beta h,$$

where

$$\overline{b}\equiv\frac{b}{||b||}\sqrt{N\overline{q}}.$$

Of course, one has

$$\overline{X}\overset{d}{=}z\sqrt{t\overline{q}+x}+\beta h,$$

where z is a standard unit Gaussian variable and equality holds in distribution so that, for instance,

$$E_g\tanh^2\overline{X}=\overline{q}.$$

The idea is, therefore, to expand around $X=\overline{X}$. As a preliminary fact, notice that the second moment of the random variable $(b-\overline{b})$ is bounded uniformly in N. Indeed,

$$E||b-\overline{b}||^2=E(||b||-\sqrt{N\overline{q}})^2\leqslant\frac{1}{\overline{q}N}E(||b||^2-N\overline{q})^2 \tag{27}$$

$$=\frac{1}{\overline{q}}E\Omega'(\xi_{12}^{N-1}\xi_{34}^{N-1})+O(1/N)=O(1), \tag{28}$$

thanks to Eq. (9). As an example, let us examine in detail the first term in (26), that is,

$$i\sqrt{N}EE_g(\tanh^2 X)\Omega'\exp(iu'\xi^{N-1})-i\overline{q}\sqrt{N}E\Omega'\exp(iu'\xi^{N-1}). \tag{29}$$

By a simple second-order Taylor expansion and an integration by parts on the Gaussian noise g, one finds

$$E_g\tanh^2 X=E_g\tanh^2\overline{X}+\frac{t}{N}(b-\overline{b})\overline{b}E_g\partial_x^2\tanh^2 x|_{x=\overline{X}} \tag{30}$$

$$+\frac{t}{2N}E_g\,\partial_x^2\tanh^2 x|_{x=\overline{X}+\theta(X-\overline{X})}(g(b-\overline{b}))^2 \tag{31}$$

$$=\overline{q}+\frac{t}{2N}(b-\overline{b})(b+\overline{b})E_g\partial_x^2\tanh^2\overline{X} \tag{32}$$

$$+\frac{t}{2N}||b-\overline{b}||^2E_g(\partial_x^2\tanh^2 x|_{x=\overline{X}+\theta(X-\overline{X})}-\partial_x^2\tanh^2\overline{X}) \tag{33}$$

$$+\frac{t^2}{2N^2}E_g\,\partial_x^4\tanh^2 x|_{x=\overline{X}+\theta(X-\overline{X})}[(b-\overline{b})(\overline{b}+\theta(b-\overline{b}))]^2, \tag{34}$$

where $0\leqslant\theta\leqslant 1$. Analyze each term separately. Recalling the definitions of b and $\overline{b}$, the second term in (32) equals

$$\frac{t}{2N}\Omega'(\eta^{s+1}\eta^{s+2}-N\overline{q})\int d\mu(z)\,\partial_x^2\tanh^2(\beta h+z\sqrt{t\overline{q}+x}) \tag{35}$$

$$=\frac{t}{\sqrt{N}}\Omega'(\xi^{N-1}_{s+1,s+2})(3Y_0+2\overline{q}-2)+O(1/N), \tag{36}$$

where Y_0 was defined in (13). Another application of Taylor's expansion and integration by parts, together with Cauchy–Schwarz inequality and the fact that the derivatives of the function $\tanh^2(x)$ are bounded, shows that the terms (33) and (34) can be bounded by

$$\frac{k}{N}||b-\overline{b}||^2.$$

Therefore, using the estimate (28), the expression (29) reduces to

$$it(3Y_0+2\overline{q}-2)E\Omega'[\xi_{s+1,s+2}\exp(iu'\xi^{N-1})]+O(N^{-1/2}),$$

and

$$i\sqrt{N}E\{(\tanh^2 X-\overline{q})\Omega'\exp(iu'\xi^{N-1})\}=t(2\overline{q}-2+3Y_0)\psi'+o(1),$$

where

$$\psi'\equiv\psi^{t'}_{N-1}(u').$$

The other terms in (26) are much simpler than (29), and can be dealt with in the same way. Finally, the whole expression (26) can be rewritten as

$$t(2\overline{q}-2+3Y_0)\psi'-u_{rr'}(1-\overline{q}^2)\phi'-(\overline{q}-\overline{q}^2)\sum_{a\neq r,r'}(u_{ar}+u_{ar'})\phi'$$

$$-(Y_0-(1-\overline{q})^2)\sum_{(c,d)c,d\neq r,r'}u_{cd}\phi'+o(1). \tag{37}$$

The steps leading to expression (37) can be repeated with minor changes for the remaining terms (20) to (22). These terms, although they look more complicated than (19) at first sight, are actually simpler to treat, since a first- (instead of second) order Taylor expansion around $X=\overline{X}$ is sufficient. This is due to the presence of terms like $\dot{\eta}_a\dot{\eta}_b/N$ or $\dot{\eta}_a b/N$, which are with large probability small, thanks to (9). Also in this case, one finds that terms (20) to (22) give quantities linear in $\phi',\partial\phi',\varphi',\psi'$, apart from terms of order $o(1)$. As for the "error term" S which appears in Theorem 4, one can easily check that it vanishes in the thermodynamic limit. This is a consequence of the exponential decay of overlap fluctuations, as expressed by (15).

Next, we show that terms like $\phi^{t'}_{N-1}(u')$ or $\psi^{t'}_{N-1}(u')$ can be substituted by the same functions calculated at N,t,u, apart from negligible error terms. Indeed, for instance

$$\phi^t_N(u)=\langle\exp(iu'\xi^{N-1}+iu(\sigma^1_N\sigma^2_N-\overline{q})/\sqrt{N})\rangle_t=\langle\exp iu'\xi^{N-1}\rangle_t(1+o(1))=\phi'+o(1).$$

In the last step, we used Theorem 4 in order to substitute t with t'. Therefore, Eq. (23) reduces to a linear relation between ϕ,φ, and ψ, apart from a remainder which becomes irrelevant in the thermodynamic limit. In the same way, one sees also that Eqs. (24), (25) yield linear equations for ϕ,φ,ψ. Putting everything together, in the thermodynamic limit one has a set of coupled linear differential equations of the form

$$\mathbf{\Phi}^t(u) = \phi^t(u)\mathbf{v}(u) + t\hat{M}\mathbf{\Phi}^t(u), \tag{38}$$

where $\mathbf{\Phi}^t(u)$ is the vector

$$\mathbf{\Phi}^t(u) = (\partial_{u_{12}}\phi^t(u),\ldots,\partial_{u_{s-1,s}}\phi^t(u),\varphi^{(1)\,t}(u),\ldots,\varphi^{(s)\,t}(u),\psi^t(u)).$$

$\mathbf{v}(u)$ is a vector whose components are homogeneous linear functions of the variables u, while $\hat{M}$ is a real square matrix with elements depending on $\overline{q}, Y_0$ alone. We do not report here the explicit expressions of $\mathbf{v}(u)$ and $\hat{M}$, which are quite complicated. However, it is instructive to check that, for instance, the term (37) is in agreement with this structure. In fact, the coefficient of ϕ' is a homogeneous linear function of the u variables, while the coefficient of ψ' is linear in t and depends only on Y_0 and $\overline{q}$. As will be clear in the following, only the structure (38), and not the specific form of $\mathbf{v}$ and $\hat{M}$, are needed to conclude the proof of the theorem.

Assume at first that the matrix $(1-t\ \hat{M})$ is invertible, which in principle can fail only for a finite number of values of t, since $\hat{M}$ is finite dimensional. In this case, Eq. (38) can be reduced to a first-order differential system in normal form

$$\mathbf{\Phi}^t(u) = \phi^t(u)(1-t\ \ \hat{M})^{-1}\mathbf{v}(u), \tag{39}$$

which can be easily integrated. The most general solution for $\phi^t(u)$, compatible with the initial condition

$$\phi^t(0) = 1,$$

is of the form

$$\phi^t(u) = \exp\{-\tfrac{1}{2}(\hat{K}u,u) + (p,u)\}, \tag{40}$$

where p is some $s(s-1)/2$ dimensional u-independent vector, and $\hat{K}$ is a $s(s-1)/2 \times s(s-1)/2$ real symmetric positive definite matrix. The symmetry and non-negativity of $\hat{K}$ derive from the obvious property of symmetry among replicas, and from the bound

$$|\phi^t(u)| \leqslant 1,$$

which holds for any characteristic function. The quadratic dependence on u of the exponent of $\phi^t(u)$ stems from the linear dependence of the components of $\mathbf{v}(u)$. Clearly, Eq. (40) means that the random variables $\{\xi_{ab}^N\}$ converge to some Gaussian process $\{\xi_{ab}\}$. Moreover, it turns out that the identification

$$p = 0$$

and

$$\hat{K} = \hat{L}$$

are straightforward. Indeed, it was shown by Guerra in Ref. 17 that, if the limit process is Gaussian, then it is centered and its covariance function is exactly $\hat{L}$.

In order to conclude the proof, it remains to show convergence of the characteristic function for those possible values $\tilde{t}$ where $(1-t\,\hat{M})$ is singular. For any $\delta>0$ one can write

$$\phi_N^{\tilde{t}}(u)=\phi_N^{\tilde{t}-\delta}(u)+\delta\partial_t\phi_N^t|_{t=\tilde{t}-\theta_N\delta},$$

where $0<\theta_N<1$. After a straightforward computation, one finds that

$$\partial_t\phi_N^t=\frac{1}{2}\left\langle e^{iu\xi^N}\left(\sum_{(a,b)}(\xi_{ab}^N)^2-s\sum_{a=1}^{s}(\xi_{a,s+1}^N)^2+\frac{s(s+1)}{2}(\xi_{s+1,s+2}^N)^2\right)\right\rangle.$$

By exploiting the uniform bound (9) and the arbitrariness of δ, one finds therefore that the theorem holds also for $t=\tilde{t}$. □

VII. FLUCTUATIONS OF THE FREE ENERGY

In order to prove Theorem 2, we show that the characteristic function of $\hat{f}_N$ converges to that of $\mathcal{N}(0,\sigma^2(t,x,h))$, i.e.,

$$\lim_{N\to\infty}Ee^{iu\hat{f}_N(t,x,h)}=e^{-(u^2/2)\,\sigma^2(t,x,h)}.$$

Define

$$\overline{\alpha}(t')=\overline{\alpha}(t',x_{t'},h)$$

$$\zeta_N(t')=\frac{\ln Z_N(t',x_{t'},h;J)}{N},$$

where $x_{t'}$ is defined in Eq. (5). The characteristic function of $\hat{f}_N$ can be written as

$$Ee^{iu\hat{f}_N(t,x,h)}=Ee^{iu\hat{f}_N(0,x_0,h)}+iuE\int_0^t e^{iu\hat{f}_N(t',x_{t'},h)}\frac{d}{dt'}\hat{f}_N(t',x_{t'},h)dt'. \tag{41}$$

Since

$$\frac{d}{dt'}\overline{\alpha}(t')=\frac{1}{4}(1-\overline{q})^2,$$

$$\frac{d}{dt'}\zeta_N(t')=\frac{1}{2\sqrt{t'}N^{3/2}}\sum_{(i,j)}J_{ij}\Omega_{t'}(\sigma_i\sigma_j)-\frac{\overline{q}}{2N\sqrt{x_{t'}}}\sum_i J_i\Omega_{t'}(\sigma_i),$$

one finds through integration by parts that

$$E\left\{e^{iu\zeta_N(t')}\frac{d}{dt'}\zeta_N(t')\right\}=\frac{1}{4}E\{e^{iu\zeta_N(t')}[1-\Omega_{t'}(q_{12}^2)-2\overline{q}(1-\Omega_{t'}(q_{12}))]\}$$
$$+\frac{iu}{4N}E\{e^{iu\zeta_N(t')}[\Omega_{t'}(q_{12}^2)-2\overline{q}\Omega_{t'}(q_{12})-N^{-1}]\}. \tag{42}$$

By using (42) in Eq. (41), one finds

$$Ee^{iu\hat{f}_N(t,x,h)}=Ee^{iu\hat{f}_N(0,x_0,h)}+\frac{u^2\overrightarrow{q}^2}{4}E\int_0^t e^{iu\hat{f}_N(t')}dt'-\frac{u^2}{4N}\int_0^t Ee^{iu\hat{f}_N(t')}(\Omega_{t'}(\xi_{12}^2)-1)dt'$$

$$-\frac{iu}{4\sqrt{N}}\int_0^t Ee^{iu\hat{f}_N(t')}\Omega_{t'}(\xi_{12}^2)dt'. \tag{43}$$

At $t=0$, all sites are decoupled and the central limit theorem for i.i.d. random variables implies that

$$\hat{f}_N(0,x,h)\overset{d}{\to}\mathcal{N}(0,\sigma^2(0,x,h)). \tag{44}$$

The last two terms in Eq. (43) clearly vanish for $N\to\infty$. For instance,

$$N^{-1/2}|Ee^{iu\hat{f}_N(t')}\Omega_{t'}(\xi_{12}^2)|\leqslant N^{-1/2}E\Omega_{t'}(\xi_{12}^2)=O(N^{-1/2}),$$

since

$$E\Omega_{t'}(\xi_{12}^2)=O(1)$$

for $t'<t_c$. Therefore, Eq. (43) yields the following linear integral equation for the characteristic function:

$$Ee^{iu\hat{f}_N(t,x,h)}=Ee^{iu\hat{f}_N(0,x_0,h)}+\frac{u^2\overrightarrow{q}^2}{4}E\int_0^t e^{iu\hat{f}_N(t',x_{t'},h)}dt'+o(1),$$

whose solution is, keeping into account the initial condition (44)

$$Ee^{iu\hat{f}_N(t,x,h)}=e^{-(u^2/2)\,\sigma^2(t,x,h)}+o(1).$$

□

Before concluding this section, we wish to note that from Eq. (43) one can also obtain in a very simple way a well-known result for free-energy fluctuations at zero external field and $t<1$,[4,6] i.e.,

$$\eta_N^t\equiv\ln Z_N(t)-N\left(\ln 2+\frac{t}{4}\right)\overset{d}{\to}\hat{Y}_t-\frac{1}{4}\ln\frac{1}{1-t}, \tag{45}$$

where Y_t is a centered Gaussian random variable of variance

$$\frac{1}{2}\left(\ln\frac{1}{1-t}-t\right).$$

Indeed, setting $u=\sqrt{N}s$ and $x=h=0$ in Eq. (43), one obtains the equation

$$Ee^{is\eta_N^t}=1-\frac{u^2}{4}\int_0^t Ee^{is\eta_N^{t'}}(\Omega_{t'}(\xi_{12}^2)-1)dt'-\frac{iu}{4}\int_0^t Ee^{is\eta_N^{t'}}\Omega_{t'}(\xi_{12}^2)dt'. \tag{46}$$

Since Theorem 1 implies, for vanishing external field and $t<1$,

$$E(\Omega_t(\xi_{12}^2)-\langle\xi_{12}^2\rangle)^2=\langle\xi_{12}^2\xi_{34}^2\rangle-\langle\xi_{12}^2\rangle^2=o(1),$$

Eq. (46) yields

$$Ee^{is\eta_N^t}=1-\frac{u^2}{4}\int_0^t Ee^{is\eta_N^{t'}}\left(\frac{1}{1-t'}-1\right)dt'-\frac{iu}{4}\int_0^t Ee^{is\eta_N^{t'}}\frac{1}{1-t'}dt'+o(1),$$

from which the result (45) easily follows.

VIII. CONCLUSIONS AND OUTLOOK

We have employed the cavity method to prove a central limit theorem for the fluctuations of overlaps and free energy, in a region above the Almeida–Thouless line. The key ingredient was provided by the control of the coupled two replica system. The open question remains to understand whether and how our method can be extended to the entire physically expected high temperature region.

In the case of vanishing external field, our method can be employed to obtain very detailed information on the system in proximity of the critical point. In particular, one can obtain lower and upper bounds on the overlap fluctuations, at $\beta=1$. We plan to report on this soon.[24]

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Duality and representations for new exotic bialgebras

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We find the exotic matrix bialgebras which correspond to the two nontriangular nonsingular 4×4 R-matrices in the classification of Hietarinta, namely, $R_{S0,3}$ and $R_{S1,4}$. We find two new exotic bialgebras $S03$ and $S14$ which are not deformations of the classical algebras of functions on GL(2) or GL(1|1). With this we finalize the classification of the matrix bialgebras which unital associative algebras generated by four elements. We also find the corresponding dual bialgebras of these new exotic bialgebras and study their representation theory in detail. We also discuss in detail a special case of $R_{S1,4}$ in which the corresponding algebra turns out to be a special case of the two-parameter quantum group deformation $\mathrm{GL}_{p,q}(2)$. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1516845]

I. INTRODUCTION

Until now there was no complete list of the matrix bialgebras which are unital associative algebras generated by four elements. Naturally, since the co-product relations are the classical ones we first mention the two related to GL(2), namely, the standard $\mathrm{GL}_{pq}(2)$ (Ref. 1) and nonstandard (Jordanian) $\mathrm{GL}_{gh}(2)$ (Ref. 2) two-parameter deformations. For the supergroup GL(1|1) there are also two: the standard $\mathrm{GL}_{pq}(1|1)$ (Refs. 3–5) and the hybrid (standard–nonstandard) $\mathrm{GL}_{qh}(1|1)$ (Ref. 6) two-parameter deformations. Recently, in Ref. 7 it was shown that there are no more deformations of GL(2) or GL(1|1). In particular, it was shown that these four deformations match the distinct triangular 4×4 R-matrices from the classification of Ref. 8 which are deformations of the trivial R-matrix [corresponding to undeformed GL(2)].

Naturally, there are matrix bialgebras generated by four elements, which are not deformations of the classical algebra of functions over the group GL(2) or the supergroup GL(1|1). Those should correspond to 4×4 R-matrices which are not deformations of the trivial R-matrix. Studying the classification of Ref. 8 we noticed altogether five nonsingular such R-matrices. The triangular ones were introduced in Ref. 7 and their duals were found and studied in detail in Ref. 9. In the latter paper we called these bialgebras exotic.

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In the present article we finalize the explicit classification of the matrix bialgebras generated by four elements, by studying those that correspond to the two nontriangular nonsingular 4×4 R-matrices of Ref. 8, namely, $R_{S0,3}$ and $R_{S1,4}$ which also are not deformations of the trivial R-matrix.

The article is organized as follows. Section II just introduces general notation. In Sec. III we study the matrix bialgebra $S03$ which corresponds to $R_{S0,3}$. We find the dual bialgebra $s03$ and study the representation theory of $s03$ in detail. In Secs. IV and V we study the matrix bialgebras $S14$ and $S14o$ which correspond to $R_{S1,4}$ for two distinctive regions of the deformation parameter q: $q^2\neq1$ and $q^2=1$, respectively. In both cases we find the corresponding dual bialgebras and their representation theory. In Sec. VI we present our conclusions and outlook.

II. GENERALITIES

In this article we consider matrix bialgebras which are unital associative algebras generated by four elements a,b,c,d. The co-product and co-unit relations are the classical ones:

$$\delta\begin{pmatrix} a & b \\ c & d \end{pmatrix}=\begin{pmatrix} a\otimes a+b\otimes c & a\otimes b+b\otimes d \\ c\otimes a+d\otimes c & c\otimes b+d\otimes d \end{pmatrix}, \tag{2.1a}$$

$$\varepsilon\begin{pmatrix} a & b \\ c & d \end{pmatrix}=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{2.1b}$$

However, the bialgebras under consideration are not Hopf algebras, except one. This shall be discussed separately in each case.

It shall be convenient to make the following change of generators:

$$\tilde a=\tfrac12(a+d),\quad \tilde d=\tfrac12(a-d),\quad \tilde b=\tfrac12(b+c),\quad \tilde c=\tfrac12(b-c). \tag{2.2}$$

With the new generators we have

$$\delta\begin{pmatrix} \tilde a & \tilde b \\ \tilde c & \tilde d \end{pmatrix}=\begin{pmatrix} \tilde a\otimes\tilde a+\tilde b\otimes\tilde b-\tilde c\otimes\tilde c+\tilde d\otimes\tilde d & \tilde a\otimes\tilde b+\tilde b\otimes\tilde a-\tilde c\otimes\tilde d+\tilde d\otimes\tilde c \\ \tilde a\otimes\tilde c+\tilde c\otimes\tilde a-\tilde b\otimes\tilde d+\tilde d\otimes\tilde b & \tilde a\otimes\tilde d+\tilde d\otimes\tilde a-\tilde b\otimes\tilde c+\tilde c\otimes\tilde b \end{pmatrix},$$
$$\varepsilon\begin{pmatrix} \tilde a & \tilde b \\ \tilde c & \tilde d \end{pmatrix}=\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{2.3}$$

III. ALGEBRA $S03$

A. Bialgebra relations

In this section we consider the matrix bialgebra $S03$. We obtain it by applying the RTT relations of Ref. 10:

$$RT_1T_2=T_2T_1R, \tag{3.1}$$

where $T_1=T\otimes\mathbf{1}_2$, $T_2=\mathbf{1}_2\otimes T$, for the case when $R=R_{S0,3}$, where

$$R_{S0,3}\equiv\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}. \tag{3.2}$$

This R-matrix is given in Ref. 8.

The relations which follow from (3.1) and (3.2) are

$$\begin{gathered} b^2+c^2=0, \quad a^2-d^2=0, \\ cd=ba, \quad dc=-ab, \\ bd=ca, \quad db=-ac, \\ da=ad, \quad cb=-bc. \end{gathered} \tag{3.3}$$

In terms of the generators $\tilde{a},\tilde{b},\tilde{c},\tilde{d}$ we have

$$\begin{gathered} \tilde{b}^2=\tilde{c}^2=0, \quad \tilde{a}\tilde{d}=\tilde{d}\tilde{a}=0, \\ \tilde{a}\tilde{b}=0, \quad \tilde{b}\tilde{d}=0, \\ \tilde{d}\tilde{c}=0, \quad \tilde{c}\tilde{a}=0. \end{gathered} \tag{3.4}$$

In view of the above relations we conclude that this bialgebra has no PBW basis. Indeed, the ordering following from (3.4) is cyclic:

$$\tilde{a}>\tilde{c}>\tilde{d}>\tilde{b}>\tilde{a}. \tag{3.5}$$

Thus, the basis consists of building blocks like $\tilde{a}^k\tilde{c}\tilde{d}^\ell\tilde{b}$ and cyclic. Explicitly the basis can be described by the following monomials:

$$\tilde{a}^{k_1}\tilde{c}\tilde{d}^{\ell_1}\tilde{b}\cdots\tilde{a}^{k_n}\tilde{c}\tilde{d}^{\ell_n}\tilde{b}\tilde{a}^{k_{n+1}}, \quad n,k_i,\ell_i\in\mathbb{Z}_+, \tag{3.6a}$$

$$\tilde{d}^{\ell_1}\tilde{b}\tilde{a}^{k_1}\tilde{c}\cdots\tilde{d}^{\ell_n}\tilde{b}\tilde{a}^{k_n}, \quad n,k_i,\ell_i\in\mathbb{Z}_+, \tag{3.6b}$$

$$\tilde{a}^{k_1}\tilde{c}\tilde{d}^{\ell_1}\tilde{b}\cdots\tilde{a}^{k_n}\tilde{c}\tilde{d}^{\ell_n}, \quad n,k_i,\ell_i\in\mathbb{Z}_+, \tag{3.6c}$$

$$\tilde{d}^{\ell_1}\tilde{b}\tilde{a}^{k_1}\tilde{c}\cdots\tilde{d}^{\ell_n}\tilde{b}\tilde{a}^{k_n}\tilde{c}\tilde{d}^{\ell_{n+1}}, \quad n,k_i,\ell_i\in\mathbb{Z}_+. \tag{3.6d}$$

We shall call the elements of the basis ''words.'' The one-letter words are the generators $\tilde{a},\tilde{b},\tilde{c},\tilde{d}$; they are obtained from (3.6a), (3.6b), (3.6c), (3.6d), respectively, for $n=0,k_1=1$, $n=1,k_1=\ell_1=0$, $n=1,k_1=\ell_1=0$, $n=0,\ell_1=1$, respectively The unit element $1_{\mathcal{A}}$ is obtained from (3.6b) or (3.6c) for $n=0$.

B. Dual algebra

Two bialgebras $\mathcal{U}$, $\mathcal{A}$ are said to be *in duality*[11] if there exists a doubly nondegenerate bilinear form

$$\langle,\rangle:\mathcal{U}\times\mathcal{A}\to\mathbb{C},\langle,\rangle:(u,a)\mapsto\langle u,a\rangle, u\in\mathcal{U}, a\in\mathcal{A}, \tag{3.7}$$

such that, for $u,v\in\mathcal{U},a,b\in\mathcal{A}$,

$$\langle u,ab\rangle=\langle\delta_{\mathcal{U}}(u),a\otimes b\rangle,\langle uv,a\rangle=\langle u\otimes v,\delta_{\mathcal{A}}(a)\rangle, \tag{3.8a}$$

$$\langle 1_{\mathcal{U}},a\rangle=\varepsilon_{\mathcal{A}}(a),\langle u,1_{\mathcal{A}}\rangle=\varepsilon_{\mathcal{U}}(u). \tag{3.8b}$$

Two Hopf algebras $\mathcal{U}$, $\mathcal{A}$ are said to be *in duality*[11] if they are in duality as bialgebras and if

$$\langle\gamma_{\mathcal{U}}(u),a\rangle=\langle u,\gamma_{\mathcal{A}}(a)\rangle. \tag{3.9}$$

It is enough to define the pairing (3.7) between the generating elements of the two algebras. The pairing between any other elements of $\mathcal{U}$, $\mathcal{A}$ follows then from relations (3.8) and the standard bilinear form inherited by the tensor product.

The duality between two bialgebras or Hopf algebras may be used also to obtain the unknown dual of a known algebra. For that it is enough to give the pairing between the generating elements of the unknown algebra with arbitrary elements of the basis of the known algebra. Using these initial pairings and the duality properties one may find the unknown algebra. One such possibility is given in Ref. 10. However, their approach is not universal. In particular, it is not enough for the algebras considered here (as will become clear), and will be used only as a consistency check.

Another approach was initiated by Sudbery.[12] He obtained $\mathrm{U}_q(\mathrm{sl}(2))\otimes\mathrm{U}(\mathrm{u}(1))$ as the algebra of tangent vectors at the identity of $\mathrm{GL}_q(2)$. The initial pairings were defined through the tangent vectors at the identity. However, such calculations become very difficult for more complicated algebras. Thus, in Ref. 13 a generalization was proposed in which the initial pairings are postulated to be equal to the classical undeformed results. This generalized method was applied in Ref. 13 to the standard two-parameter deformation $\mathrm{GL}_{p,q}(2)$, (where also Sudbery's method was used), then in Ref. 14 to the multiparameter deformation of $\mathrm{GL}(n)$, in Ref. 15 to the matrix quantum Lorentz group of Ref. 16, in Ref. 17 to the Jordanian two-parameter deformation $\mathrm{GL}_{g,h}(2)$, in Ref. 6 to the hybrid two-parameter deformation of the superalgebra $\mathrm{GL}_{q,h}(1|1)$, in Ref. 18 to the multiparameter deformation of the superalgebra $\mathrm{GL}(m|n)$, and in Ref. 9 to the first discussed three exotic bialgebras. [We note that the dual of $\mathrm{GL}_{p,q}(2)$ was obtained also in Ref. 19 by methods of q-differential calculus.]

Let us denote by $s03$ the unknown yet dual algebra of $S03$, and by $\tilde{A},\tilde{B},\tilde{C},\tilde{D}$ the four generators of $s03$. Like in Ref. 13 we define the pairing $\langle Z,f\rangle$, $Z=\tilde{A},\tilde{B},\tilde{C},\tilde{D}$, f is from (3.6), as the classical tangent vector at the identity:

$$\langle Z,f\rangle\equiv\varepsilon\left(\frac{\partial f}{\partial y}\right), \tag{3.10}$$

where $(Z,y)=(\tilde{A},\tilde{a})$, $(\tilde{B},\tilde{b})$, $(\tilde{C},\tilde{c})$, $(\tilde{D},\tilde{d})$. Explicitly, we get

$$\langle\tilde{A},f\rangle=\varepsilon\left(\frac{\partial f}{\partial\tilde{a}}\right)=\begin{cases}k & \text{for } f=\tilde{a}^k,\\ 0 & \text{otherwise,}\end{cases} \tag{3.11a}$$

$$\langle\tilde{B},f\rangle=\varepsilon\left(\frac{\partial f}{\partial\tilde{b}}\right)=\begin{cases}1 & \text{for } f=\tilde{b}\tilde{a}^k,\\ 0 & \text{otherwise,}\end{cases} \tag{3.11b}$$

$$\langle\tilde{C},f\rangle=\varepsilon\left(\frac{\partial f}{\partial\tilde{c}}\right)=\begin{cases}1 & \text{for } f=\tilde{a}^k\tilde{c},\\ 0 & \text{otherwise,}\end{cases} \tag{3.11c}$$

$$\langle\tilde{D},f\rangle=\varepsilon\left(\frac{\partial f}{\partial\tilde{d}}\right)=\begin{cases}1 & \text{for } f=\tilde{d},\\ 0 & \text{otherwise.}\end{cases} \tag{3.11d}$$

Using the above we obtain the following proposition.

Proposition 1: The generators $\tilde{A},\tilde{B},\tilde{C},\tilde{D}$ introduced above obey the following relations:

$$[\tilde{A},Z]=0,\quad Z=\tilde{B},\tilde{C}, \tag{3.12a}$$

$$\tilde{A}\tilde{D}=\tilde{D}\tilde{A}=\tilde{D}^3=\tilde{B}^2\tilde{D}=\tilde{D}\tilde{B}^2=\tilde{D}, \tag{3.12b}$$

$$[\tilde{B},\tilde{C}]=-2\tilde{D}, \tag{3.12c}$$

$$\tilde{D}\tilde{B} = -\tilde{B}\tilde{D} = \tilde{C}\tilde{D}^2 = \tilde{D}^2\tilde{C}, \tag{3.12d}$$

$$\{\tilde{C},\tilde{D}\} = 0, \tag{3.12e}$$

$$\tilde{B}^2 + \tilde{C}^2 = 0, \tag{3.12f}$$

$$\tilde{B}^3 = \tilde{B}, \tag{3.12g}$$

$$\tilde{C}^3 = -\tilde{C}, \tag{3.12h}$$

$$\tilde{B}^2\tilde{A} = \tilde{A}; \tag{3.12i}$$

$$\delta_{\mathcal{U}}(\tilde{A}) = \tilde{A}\otimes 1_{\mathcal{U}} + 1_{\mathcal{U}}\otimes\tilde{A}, \tag{3.13a}$$

$$\delta_{\mathcal{U}}(\tilde{B}) = \tilde{B}\otimes 1_{\mathcal{U}} + (1_{\mathcal{U}} - \tilde{B}^2)\otimes\tilde{B}, \tag{3.13b}$$

$$\delta_{\mathcal{U}}(\tilde{C}) = \tilde{C}\otimes(1_{\mathcal{U}} - \tilde{B}^2) + 1_{\mathcal{U}}\otimes\tilde{C}, \tag{3.13c}$$

$$\delta_{\mathcal{U}}(\tilde{D}) = \tilde{D}\otimes(1_{\mathcal{U}} - \tilde{B}^2) + (1_{\mathcal{U}} - \tilde{B}^2)\otimes\tilde{D}, \tag{3.13d}$$

$$\varepsilon_{\mathcal{U}}(Z) = 0, \quad Z = \tilde{A},\tilde{B},\tilde{C},\tilde{D}. \tag{3.13e}$$

$\tilde{A}$, $\tilde{B}^2 = -\tilde{C}^2$ and $\tilde{D}^2$ are Casimir operators. The bialgebra $s03$ is not a Hopf algebra.

Proof: Using the assumed duality the algebraic relations (3.12) are shown by calculating their pairings with the basis monomials f from (3.6). In particular, we have (giving only the nonzero pairings)

$$\langle\tilde{A}\tilde{B},f\rangle = \langle\tilde{B}\tilde{A},f\rangle = k+1, \quad \text{for } f = \tilde{b}\tilde{a}^k, \tag{3.14a}$$

$$\langle\tilde{A}\tilde{C},f\rangle = \langle\tilde{C}\tilde{A},f\rangle = k+1, \quad \text{for } f = \tilde{a}^k\tilde{c}, \tag{3.14b}$$

$$\langle\tilde{A}\tilde{D},f\rangle = \langle\tilde{D}\tilde{A},f\rangle = \langle\tilde{D}^3,f\rangle = \langle\tilde{B}^2\tilde{D},f\rangle = \langle\tilde{D}\tilde{B}^2,f\rangle = -\langle\tilde{B}\tilde{C},f\rangle = \langle\tilde{C}\tilde{B},f\rangle = \langle\tilde{D},f\rangle = 1, \quad \text{for } f = \tilde{d} \tag{3.14c}$$

$$\langle\tilde{B}\tilde{C},f\rangle = \langle\tilde{C}\tilde{B},f\rangle = 1, \quad \text{for } f = \tilde{b}\tilde{a}^k\tilde{c}, \tag{3.14d}$$

$$\langle\tilde{D}\tilde{B},f\rangle = -\langle\tilde{B}\tilde{D},f\rangle = \langle\tilde{C}\tilde{D}^2,f\rangle = \langle\tilde{D}^2\tilde{C},f\rangle = 1, \quad \text{for } f = \tilde{c}, \tag{3.14e}$$

$$\langle\tilde{D}\tilde{C},f\rangle = -\langle\tilde{C}\tilde{D},f\rangle = 1, \quad \text{for } f = \tilde{b}, \tag{3.14f}$$

$$\langle\tilde{B}^2,f\rangle = -\langle\tilde{C}^2,f\rangle = 1, \quad \text{for } f = \tilde{a}^k, \tag{3.14g}$$

$$\langle\tilde{B}^3,f\rangle = \langle\tilde{B},f\rangle = 1, \quad \text{for } f = \tilde{b}\tilde{a}^k, \tag{3.14h}$$

$$\langle -\tilde{C}^3,f\rangle = \langle\tilde{C},f\rangle = 1, \quad \text{for } f = \tilde{a}^k\tilde{c}, \tag{3.14i}$$

$$\langle\tilde{B}^2\tilde{A},f\rangle = \langle\tilde{A},f\rangle = k, \quad \text{for } f = \tilde{a}^k. \tag{3.14j}$$

For the proof of (3.14h) and (3.14j), (3.14g) is used. The facts that $\tilde{A}$, $\tilde{B}^2=-\tilde{C}^2$ and $\tilde{D}^2$ are Casimir operators follow easily from (3.12) having in mind also (3.14g) and (3.14j) and that $\langle \tilde{D}^2,\tilde{a}\rangle=1$ is the only nonzero pairing of $\tilde{D}^2$. For the proof of (3.13a)–(3.13d) we use the duality property (3.8a):

$$\langle Z,f_1f_2\rangle=\langle \delta_{\mathcal{U}}(Z),f_1\otimes f_2\rangle$$

for every generator Z of $s03$ and for every $f_1,f_2\in S03$, then we calculate separately the lhs and rhs and compare the results. We also use that

$$\tilde{B}^2Z=Z\ , \quad \text{for } Z=\tilde{A},\tilde{B},\tilde{C},\tilde{D}. \tag{3.15}$$

This is contained in (3.12) except for $Z=\tilde{C}$ for which we use that $\langle \tilde{B}^2\tilde{C},\tilde{a}^k\tilde{c}\rangle=1$ is the only nonzero pairing of $\tilde{B}^2\tilde{C}$. Formulas (3.13e) follow from $\varepsilon_{\mathcal{U}}(Z)=\langle Z,1_{\mathcal{A}}\rangle$, cf. (3.8b), and the defining relations (3.11). To show that $s03$ is not a Hopf algebra we suppose that it is, i.e., there should exist an antipode γ. Then we use one of the Hopf algebra axioms:

$$m\circ(\mathrm{id}\otimes\gamma)\circ\delta=i\circ\varepsilon \tag{3.16}$$

as maps $s03\to s03$, where m maps to the usual product in the algebra: $m(Y\otimes Z)=YZ$, $Y,Z\in s03$ and i is the natural embedding of the number field $\mathbb{C}$ into $s03$: $i(\mu)=\mu 1_{\mathcal{U}},\mu\in\mathbb{C}$. Applying this to the generator $\tilde{B}$ we would get

$$\tilde{B}+(1_{\mathcal{U}}-\tilde{B}^2)\gamma(\tilde{B})=0,$$

which is a contradiction, since $1_{\mathcal{U}}-\tilde{B}^2$ is zero when multiplied by anything except by $1_{\mathcal{U}}$, and in the latter case the product is not equal to $-\tilde{B}$. From this we see that γ can not be defined on $\tilde{C}$ and $\tilde{D}$ since their coproducts involve $\tilde{B}$. The antipode may be introduced only if we restrict to the subalgebra generated by $\tilde{A}$, but the bialgebra $s03$ as a whole is not a Hopf algebra. ■

Corollary 1: The algebra generated by the generator $\tilde{A}$ is a sub-bialgebra of $s03$. The algebra $s03'$ generated by the generators $\tilde{B},\tilde{C},\tilde{D}$ is a nine-dimensional sub-bialgebra of $s03$ with PBW basis:

$$1_{\mathcal{U}},\tilde{B},\tilde{C},\tilde{D},\tilde{B}\tilde{C},\tilde{B}\tilde{D},\tilde{D}\tilde{C},\tilde{B}^2,\tilde{D}^2. \tag{3.17}$$

Proof: The statement follows immediately from relations (3.12) and (3.13). We comment on only the PBW basis of the subalgebra $s03'$. Indeed, a priori it has a PBW basis:

$$\tilde{B}^k\tilde{D}^\ell\tilde{C}^m\ , \quad k,\ell\leqslant 2,\ m\leqslant 1, \tag{3.18}$$

the restrictions following from (3.12b), (3.12f), and (3.12g). Furthermore, it is easy to see that there are no cubic (and consequently higher order) elements of the basis. For some of the cubic elements this is clear from (3.12). For the rest we have

$$\tilde{B}\tilde{D}\tilde{C}=-\tilde{D}^2\tilde{C}^2=\tilde{D}^2\tilde{B}^2=\tilde{D}^2, \tag{3.19a}$$

$$\tilde{B}^2\tilde{C}=-\tilde{C}^3=\tilde{C}, \tag{3.19b}$$

$$\tilde{B}\tilde{D}^2=-\tilde{C}\tilde{D}^3=\tilde{D}\tilde{C}, \tag{3.19c}$$

also using (3.12). Thus, the basis is given by (3.17); the algebra is indeed nine-dimensional. ■

Remark 1: The algebra $s03$ is not the direct sum of the two subalgebras described in the preceding Corollary since both subalgebras have nontrivial action on each other, e.g., $\tilde{B}^2\tilde{A}=\tilde{A}$,

$\tilde{A}\tilde{D}=\tilde{D}$. The algebra $s03$ is a nine-dimensional associative algebra over the central algebra generated by $\tilde{A}$. ■

C. Regular representation

We start with the study of the left regular representation (LRR) of the subalgebra $s03'$. For this we need the left multiplication table:

	1	$\tilde{B}$	$\tilde{C}$	$\tilde{B}^2$	$\tilde{B}\tilde{C}$	$\cdots$
$\tilde{B}$	$\tilde{B}$	$\tilde{B}^2$	$\tilde{B}\tilde{C}$	$\tilde{B}$	$\tilde{C}$	$\cdots$
$\tilde{C}$	$\tilde{C}$	$\tilde{B}\tilde{C}+2\tilde{D}$	$-\tilde{B}^2$	$\tilde{C}$	$-\tilde{B}+2\tilde{D}\tilde{C}$	$\cdots$
$\tilde{D}$	$\tilde{D}$	$-\tilde{B}\tilde{D}$	$\tilde{D}\tilde{C}$	$\tilde{D}$	$-\tilde{D}^2$	$\cdots$

	$\cdots$	$\tilde{D}$	$\tilde{D}^2$	$\tilde{B}\tilde{D}$	$\tilde{D}\tilde{C}$
$\tilde{B}$	$\cdots$	$\tilde{B}\tilde{D}$	$\tilde{D}\tilde{C}$	$\tilde{D}$	$\tilde{D}^2$
$\tilde{C}$	$\cdots$	$-\tilde{D}\tilde{C}$	$-\tilde{B}\tilde{D}$	$\tilde{D}^2$	$\tilde{D}$
$\tilde{D}$	$\cdots$	$\tilde{D}^2$	$\tilde{D}$	$-\tilde{D}\tilde{C}$	$-\tilde{B}\tilde{D}$

The LRR hence contains the subrepresentation generated as a vector space by $\{\tilde{D},\tilde{D}^2,\tilde{B}\tilde{D},\tilde{D}\tilde{C}\}$, which decomposes into two two-dimensional irreps:

$$v_0^1=\tilde{D}+\tilde{D}^2, \quad v_1^1=\tilde{B}\tilde{D}+\tilde{D}\tilde{C}, \tag{3.20}$$

$$\tilde{B}\begin{pmatrix} v_0^1 \\ v_1^1 \end{pmatrix}=\begin{pmatrix} v_1^1 \\ v_0^1 \end{pmatrix}, \quad \tilde{C}\begin{pmatrix} v_0^1 \\ v_1^1 \end{pmatrix}=\begin{pmatrix} -v_1^1 \\ v_0^1 \end{pmatrix}, \quad \tilde{D}\begin{pmatrix} v_0^1 \\ v_1^1 \end{pmatrix}=\begin{pmatrix} v_0^1 \\ -v_1^1 \end{pmatrix}, \tag{3.21}$$

and

$$v_0^2=\tilde{B}\tilde{D}-\tilde{D}\tilde{C}, \quad v_1^2=\tilde{D}-\tilde{D}^2, \tag{3.22}$$

$$\tilde{B}\begin{pmatrix} v_0^2 \\ v_1^2 \end{pmatrix}=\begin{pmatrix} v_1^2 \\ v_0^2 \end{pmatrix}, \quad \tilde{C}\begin{pmatrix} v_0^2 \\ v_1^2 \end{pmatrix}=\begin{pmatrix} -v_1^2 \\ v_0^2 \end{pmatrix}, \quad \tilde{D}\begin{pmatrix} v_0^2 \\ v_1^2 \end{pmatrix}=\begin{pmatrix} v_0^2 \\ -v_1^2 \end{pmatrix}. \tag{3.23}$$

These two irreps are isomorphic by the map $(v_0^1,v_1^1)\to(v_0^2,v_1^2)$. On both of them the Casimirs $\tilde{B}^2$, $\tilde{D}^2$ take the value 1. (Also the Casimir $\tilde{A}$ of $s03$ has the value 1.)

The LRR contains also the trivial one-dimensional representation generated by the vector $v=\tilde{B}^2-1_{\mathcal{U}}$. On this vector all Casimirs and, moreover, all generators of $s03$ take the value 0.

The quotient of the LRR by the above three submodules has the following multiplication table:

	1	$\tilde{B}$	$\tilde{C}$	$\tilde{B}\tilde{C}$
$\tilde{B}$	$\tilde{B}$	$\tilde{B}^2$	$\tilde{B}\tilde{C}$	$\tilde{C}$
$\tilde{C}$	$\tilde{C}$	$\tilde{B}\tilde{C}$	$-\tilde{B}^2$	$-\tilde{B}$
$\tilde{D}$	0	0	0	0

Thus the quotient decomposes into a direct sum of four one-dimensional representations, generated as vector spaces by

$$v_{\epsilon,\epsilon'}=\tilde{B}+\epsilon 1_{\mathcal{U}}-i\epsilon\epsilon'\tilde{C}-i\epsilon'\tilde{B}\tilde{C},\quad \epsilon,\epsilon'=\pm. \tag{3.24}$$

On the latter vectors we have the following action:

$$\tilde{B}v_{\epsilon,\epsilon'}=\epsilon v_{\epsilon,\epsilon'},\quad \tilde{C}v_{\epsilon,\epsilon'}=i\epsilon' v_{\epsilon,\epsilon'},\quad \tilde{D}v_{\epsilon,\epsilon'}=0. \tag{3.25}$$

Obviously, on all of them the Casimirs $\tilde{B}^2$, $\tilde{D}^2$ take the values 1,0, respectively. However, these four representations are not isomorphic to each other.

To summarize, there are seven irreps of $s03'$ which are obtained from the LRR:

(i) one-dimensional trivial (all generators act by zero),
(ii) two-dimensional with both Casimirs $\tilde{B}^2$, $\tilde{D}^2$ having value 1, and
(iii) four one-dimensional with Casimir values 1,0 for $\tilde{B}^2$, $\tilde{D}^2$, respectively.

Turning to the algebra $s03$ we note that it inherits the representation structure of its subalgebra $s03'$. On the representations (3.20) and (3.22) the Casimir $\tilde{A}$ has the value 1, while on the trivial irrep generated by $v=\tilde{B}^2-1_{\mathcal{U}}$ the Casimir $\tilde{A}$ has the value 0. However, on the one-dimensional irreps generated by (3.24) the Casimir $\tilde{A}$ has no fixed value. Thus, the list of the irreps of $s03$ arising from the LRR is

(i) one-dimensional trivial,
(ii) two-dimensional with all Casimirs $\tilde{A}$, $\tilde{B}^2$, $\tilde{D}^2$ having value 1, and
(iii) four one-dimensional with Casimir values μ,1,0 for $\tilde{A}$, $\tilde{B}^2$, $\tilde{D}^2$, respectively, $\mu\in\mathbb{C}$.

Finally, we note that we could have studied also the right regular representation of $s03$. The list of irreps would be the same as the one obtained above.

D. Weight representations

Here we consider *weight representations*. These are representations which are built from the action of the algebra on a *weight vector* with respect to one of the generators. We start with a weight vector v_0 such that

$$\tilde{D}\,v_0=\lambda\,v_0, \tag{3.26}$$

where $\lambda\in\mathbb{C}$ is the weight. As we shall see, the cases $\lambda\neq 0$ and $\lambda=0$ are very different.

We start with $\lambda \neq 0$. In that case from $\tilde{D}^3 = \tilde{D}$ follows that $\lambda^2 = 1$, while from $\tilde{B}^2\tilde{D} = \tilde{D}$ follows that $\tilde{B}^2 v_0 = v_0$. Thus, acting with the elements of $s03$ on v_0 we obtain a two-dimensional representation:

$$v_0, \ \tilde{B}\, v_0, \ \tilde{C}\, v_0, \ \tilde{B}\tilde{C}\, v_0. \tag{3.27}$$

This representation is *irreducible*. The action is given as follows:

	v_0	$\tilde{B}v_0$	$\tilde{C}v_0$	$\tilde{B}\tilde{C}v_0$
$\tilde{B}$	$\tilde{B}v_0$	v_0	$\tilde{B}\tilde{C}v_0$	$\tilde{C}v_0$
$\tilde{C}$	$\tilde{C}v_0$	$(\tilde{B}\tilde{C}+2\lambda)v_0$	$-v_0$	$-(\tilde{B}+2\lambda\tilde{C})v_0$
$\tilde{D}$	λv_0	$-\lambda\tilde{B}v_0$	$-\lambda\tilde{C}v_0$	$\lambda\tilde{B}\tilde{C}v_0$

Both Casimirs $\tilde{B}^2$, $\tilde{D}^2$ take the value 1.

Let now $\lambda = 0$. In this case acting with the elements of $s03$ on v_0 we obtain a five-dimensional representation:

$$v_0, \ \tilde{B}\, v_0, \ \tilde{C}\, v_0, \ \tilde{B}\tilde{C}\, v_0, \ \tilde{B}^2\, v_0. \tag{3.28}$$

This representation is *reducible*. It has a one-dimensional subrepresentation spanned by the vector $w = v\, v_0 = (\tilde{B}^2 - 1_{\mathcal{U}})v_0$. This is the trivial representation since all generators act by zero on it. After we factor out this representation the factor representation splits into four one-dimensional representations spanned by the following vectors, $w_{\epsilon,\epsilon'} = v_{\epsilon,\epsilon'}\, v_0$, where $v_{\epsilon,\epsilon'}$ are from (3.24) and the action of the generators is as given in (3.25). Thus, these irreps are as those obtained from the LRR.

To summarize, there are six irreps of $s03'$ which are obtained as weight irreps of the generator $\tilde{D}$:

(i) one-dimensional trivial,
(ii) one two-dimensional with both Casimirs $\tilde{B}^2$, $\tilde{D}^2$ having value 1, and
(iii) four one-dimensional with Casimir values 1,0 for $\tilde{B}^2$, $\tilde{D}^2$, respectively.

Turning to the algebra $s03$ we note that it inherits the representation structure of its subalgebra $s03'$; however, the value of the Casimir $\tilde{A}$ is not fixed except on the trivial irrep. Thus, the list of the irreps of $s03$ which are obtained as weight irreps of the generator $\tilde{D}$ is

(i) one-dimensional trivial,
(ii) one two-dimensional with Casimir values μ,1,1 for $\tilde{A}$, $\tilde{B}^2$, $\tilde{D}^2$, respectively, $\mu \in \mathbb{C}$, and
(iii) four one-dimensional with Casimir values μ,1,0 for $\tilde{A}$, $\tilde{B}^2$, $\tilde{D}^2$, respectively, $\mu \in \mathbb{C}$.

Finally, we note that it is not possible to construct weight representations w.r.t. generator $\tilde{B}$ (or $\tilde{C}$).

E. Representations of *s*03 on *S*03

Here we shall study the representations of $s03$ obtained by the use of its right regular action (RRA) on the dual bialgebra $S03$. The RRA is defined as follows:

$$\pi_R(Z)f \equiv f_{(1)}\langle Z, f_{(2)}\rangle, \quad Z \in s03, \quad Z \neq 1_{\mathcal{U}}, \quad f \in S03, \tag{3.29a}$$

$$\pi_R(1_{\mathcal{U}})f \equiv f, \quad f \in S03, \tag{3.29b}$$

where we use Sweedler's notation for the co-product: $\delta(f)=f_{(1)}\otimes f_{(2)}$. [Note that we can not use the left regular action since that would be given by the formula $\pi_L(Z)f=\langle \gamma_{\mathcal{U}}(Z), f_{(1)}\rangle f_{(2)}$, and we do not have an antipode.] More explicitly, for the generators of $s03$ we have

$$\pi_R(\tilde{A})\begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{pmatrix} = \begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{pmatrix}, \tag{3.30a}$$

$$\pi_R(\tilde{B})\begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{pmatrix} = \begin{pmatrix} \tilde{b} & \tilde{a} \\ \tilde{d} & \tilde{c} \end{pmatrix}, \tag{3.30b}$$

$$\pi_R(\tilde{C})\begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{pmatrix} = \begin{pmatrix} -\tilde{c} & \tilde{d} \\ \tilde{a} & -\tilde{b} \end{pmatrix}, \tag{3.30c}$$

$$\pi_R(\tilde{D})\begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{pmatrix} = \begin{pmatrix} \tilde{d} & -\tilde{c} \\ -\tilde{b} & \tilde{a} \end{pmatrix}, \tag{3.30d}$$

$$\pi_R(Z)\,1_{\mathcal{A}} = 1_{\mathcal{A}}\langle Z, 1_{\mathcal{A}}\rangle = 1_{\mathcal{A}}\,\varepsilon_{\mathcal{U}}(Z) = 0, \quad Z=\tilde{A},\tilde{B},\tilde{C},\tilde{D}. \tag{3.30e}$$

For the action on the elements (words) of $S03$ we use a corollary of (3.29):

$$\pi_R(Z)fg = \pi_R(\delta_{\mathcal{U}}(Z))(f\otimes g), \tag{3.31}$$

where f,g are arbitrary words from (3.6). Further, we shall need the notion of the "length" $\ell(f)$ of the word f. It is defined naturally as the number of the letters of f; in addition we set $\ell(1_{\mathcal{A}})=0$. Now we obtain from (3.31)

$$\pi_R(\tilde{A})\,f = \ell(f)\,f, \tag{3.32a}$$

$$\pi_R(\tilde{B})\,f\cdot g = (\pi_R(\tilde{B})f)\cdot g, \tag{3.32b}$$

$$\pi_R(\tilde{C})\,f\cdot g = f\cdot(\pi_R(\tilde{C})g), \tag{3.32c}$$

$$\pi_R(\tilde{D})\,f = 0, \quad \text{if } \ell(f)>1. \tag{3.32d}$$

From (3.32b) and (3.32c) it is obvious that the only nonzero action of $\tilde{B}$, $\tilde{C}$ actually is

$$\pi_R(\tilde{B})\begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{pmatrix}\cdot f = \begin{pmatrix} \tilde{b} & \tilde{a} \\ \tilde{d} & \tilde{c} \end{pmatrix}\cdot f, \tag{3.33a}$$

$$\pi_R(\tilde{C})\,f\cdot\begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{pmatrix} = f\cdot\begin{pmatrix} -\tilde{c} & \tilde{d} \\ \tilde{a} & -\tilde{b} \end{pmatrix}. \tag{3.33b}$$

From (3.32a) it is obvious that we can classify the irreps by the value μ_A of the Casimir $\tilde{A}$ which runs over the non-negative integers. For fixed μ_A the basis of the corresponding representations is spanned by the words f such that $\ell(f)=\mu_A$. Thus, we have the following.

(i) $\mu_A=0$: This is the one-dimensional trivial representation spanned by the unit element $1_{\mathcal{A}}$ on which all generators of $s03$ have zero action.

(ii) $\mu_A=1$: This representation is four-dimensional spanned by the four generators $\tilde{a}$, $\tilde{b}$, $\tilde{c}$, $\tilde{d}$ of $S03$. It is reducible and decomposes in two two-dimensional irreps with basis vectors:

$$v_0^1=\tilde{a}+\tilde{d}=a, \quad v_1^1=\tilde{b}+\tilde{c}=b, \tag{3.34a}$$

and

$$v_0^2=\tilde{b}-\tilde{c}=c, \quad v_1^2=\tilde{a}-\tilde{d}=d. \tag{3.34b}$$

The RRA of $\tilde{B}$, $\tilde{C}$, $\tilde{D}$ on these vectors is as (3.21) and (3.23):

$$\pi_R(\tilde{B})\begin{pmatrix} v_0^k \\ v_1^k \end{pmatrix}=\begin{pmatrix} v_1^k \\ v_0^k \end{pmatrix}, \quad \pi_R(\tilde{C})\begin{pmatrix} v_0^k \\ v_1^k \end{pmatrix}=\begin{pmatrix} -v_1^k \\ v_0^k \end{pmatrix}, \quad \pi_R(\tilde{D})\begin{pmatrix} v_0^k \\ v_1^k \end{pmatrix}=\begin{pmatrix} v_0^k \\ -v_1^k \end{pmatrix}. \tag{3.35}$$

These two irreps are isomorphic by the map $(v_0^1,v_1^1)\to(v_0^2,v_1^2)$. On both of them the Casimirs $\tilde{B}^2$, $\tilde{D}^2$ take the value 1.

(iii) $\mu_A=2$: This representation is eight-dimensional spanned by $\tilde{a}^2$, $\tilde{a}\tilde{c}$, $\tilde{b}\tilde{a}$, $\tilde{b}\tilde{c}$, $\tilde{c}\tilde{b}$, $\tilde{c}\tilde{d}$, $\tilde{d}^2$, $\tilde{d}\tilde{b}$. It is reducible and decomposes in eight one-dimensional irreps with basis vectors:

$$v^1_{\epsilon,\epsilon'}=(\tilde{a}+\epsilon\tilde{b})(\tilde{a}+i\epsilon'\tilde{c}), \tag{3.36a}$$

$$v^2_{\epsilon,\epsilon'}=(\tilde{d}+\epsilon\tilde{c})(\tilde{d}+i\epsilon'\tilde{b}), \tag{3.36b}$$

$$\epsilon,\epsilon'=\pm.$$

The RRA of $\tilde{B}$, $\tilde{C}$, $\tilde{D}$ on these vectors is as (3.25):

$$\pi_R(\tilde{B})v^k_{\epsilon,\epsilon'}=\epsilon v^k_{\epsilon,\epsilon'}, \quad \pi_R(\tilde{C})v^k_{\epsilon,\epsilon'}=i\epsilon' v^k_{\epsilon,\epsilon'}, \quad \pi_R(\tilde{D})v^k_{\epsilon,\epsilon'}=0. \tag{3.37}$$

The irrep with vector $v^1_{\epsilon,\epsilon'}$ is isomorphic to the irrep with vector $v^2_{\epsilon,\epsilon'}$. Thus, there are only four distinct irreps parametrized by ϵ,ϵ'. On all of them the Casimirs $\tilde{B}^2$, $\tilde{D}^2$ take the values 1,0, respectively.

(iv) $\mu_A=N>2$: These representations are reducible and decompose in one-dimensional irreps with basis vectors:

$$v^1_{\epsilon,\epsilon'}=(\tilde{a}+\epsilon\tilde{b})\cdot f_1\cdot(\tilde{a}+i\epsilon'\tilde{c}), \tag{3.38a}$$

$$v^2_{\epsilon,\epsilon'}=(\tilde{d}+\epsilon\tilde{c})\cdot f_2\cdot(\tilde{d}+i\epsilon'\tilde{b}), \tag{3.38b}$$

$$v^3_{\epsilon,\epsilon'}=(\tilde{a}+\epsilon\tilde{b})\cdot f_3\cdot(\tilde{d}+i\epsilon'\tilde{b}), \tag{3.38c}$$

$$v^4_{\epsilon,\epsilon'}=(\tilde{d}+\epsilon\tilde{c})\cdot f_4\cdot(\tilde{a}+i\epsilon'\tilde{c}), \tag{3.38d}$$

$$\epsilon,\epsilon'=\pm, \quad \ell(f_k)=N-2.$$

The RRA of $\tilde{B}$, $\tilde{C}$, $\tilde{D}$ on these vectors is as exactly as (3.25). The irrep with vector $v^k_{\epsilon,\epsilon'}$ is isomorphic to the irrep with vector $v^n_{\epsilon,\epsilon'}$. Thus, there are only four distinct irreps as in the case above. On all of them the Casimirs $\tilde{B}^2$, $\tilde{D}^2$ take the values 1,0, respectively.

To summarize the list of irreps of $s03'$ is the same as given in Sec. III C. The list of irreps of $s03$ here is smaller since the Casimir $\tilde{A}$ can take only non-negative integer values. Thus, the list of the irreps of $s03$ using the dual bialgebra $S03$ as carrier space is

(i) one-dimensional trivial,
(ii) two-dimensional with all Casimirs $\tilde{A}$, $\tilde{B}^2$, $\tilde{D}^2$ having value 1, and
(iii) four one-dimensional with Casimir values μ,1,0 for $\tilde{A}$, $\tilde{B}^2$, $\tilde{D}^2$, respectively, $\mu \in \mathbb{N}+1$.

The difference in the two lists is natural since here more structure (the co-product) is involved. Speaking more loosely, the irreps here may be looked upon as ''integrals'' of the irreps obtained in Sec. III C.

IV. ALGEBRA *S*14

A. Bialgebra relations

In this section we consider the matrix bialgebra $S14$. We obtain it by applying the RTT relations (3.1) for the case $R=R_{S1,4}$, when $q^2\neq 1$ where

$$R_{S1,4}\equiv\begin{pmatrix} 0 & 0 & 0 & q \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ q & 0 & 0 & 0 \end{pmatrix}. \tag{4.1}$$

This R-matrix is given in Ref. 8.

The relations which follow from (3.1) and (4.1) when $q^2\neq 1$ are

$$\begin{aligned} &b^2-c^2=0, \quad a^2-d^2=0, \\ &ab=ba=0, \quad ac=ca=0, \\ &bd=db=0, \quad cd=dc=0. \end{aligned} \tag{4.2}$$

In terms of the generators $\tilde{a}$, $\tilde{b}$, $\tilde{c}$, $\tilde{d}$,

$$\begin{aligned} &\tilde{b}\tilde{c}+\tilde{c}\tilde{b}=0, \quad \tilde{a}\tilde{d}+\tilde{d}\tilde{a}=0, \\ &\tilde{a}\tilde{b}=\tilde{b}\tilde{a}=0, \quad \tilde{a}\tilde{c}=\tilde{c}\tilde{a}=0, \\ &\tilde{b}\tilde{d}=\tilde{d}\tilde{b}=0, \quad \tilde{c}\tilde{d}=\tilde{d}\tilde{c}=0. \end{aligned} \tag{4.3}$$

From the above relations it is clear that the PBW basis of $S14$ is

$$\tilde{a}^k\tilde{d}^\ell, \quad \tilde{b}^k\tilde{c}^\ell. \tag{4.4}$$

B. Dual algebra

Let us denote by $s14$ the unknown yet dual algebra of $S14$, and by $\tilde{A}$, $\tilde{B}$, $\tilde{C}$, $\tilde{D}$ the four generators of $s14$. We define the pairing $\langle Z,f\rangle$, $Z=\tilde{A}$, $\tilde{B}$, $\tilde{C}$, $\tilde{D}$, f is from (4.4), as (3.10). Explicitly, we obtain

$$\langle \tilde{A}, \ f\rangle=\varepsilon\left(\frac{\partial f}{\partial \tilde{a}}\right)=\begin{cases} k\delta_{\ell 0}, & f=\tilde{a}^k\tilde{d}^\ell, \\ 0, & f=\tilde{b}^k\tilde{c}^\ell, \end{cases} \tag{4.5a}$$

$$\langle \tilde{B}, \ f\rangle=\varepsilon\left(\frac{\partial f}{\partial \tilde{b}}\right)=\begin{cases} 0, & f=\tilde{a}^k\tilde{d}^\ell, \\ \delta_{k1}\delta_{\ell 0}, & f=\tilde{b}^k\tilde{c}^\ell, \end{cases} \tag{4.5b}$$

$$\langle \tilde{C},\ f\rangle = \varepsilon\left(\frac{\partial f}{\partial \tilde{c}}\right) = \begin{cases} 0, & f = \tilde{a}^k \tilde{d}^\ell, \\ \delta_{k0}\delta_{\ell 1}, & f = \tilde{b}^k \tilde{c}^\ell, \end{cases} \tag{4.5c}$$

$$\langle \tilde{D},\ f\rangle = \varepsilon\left(\frac{\partial f}{\partial \tilde{d}}\right) = \begin{cases} \delta_{\ell 1}, & f = \tilde{a}^k \tilde{d}^\ell, \\ 0, & f = \tilde{b}^k \tilde{c}^\ell. \end{cases} \tag{4.5d}$$

We shall need (as in Ref. 9) the auxilliary operator E such that

$$\langle E, f\rangle = \begin{cases} 1 & \text{for } f = 1_{\mathcal{A}}, \\ 0 & \text{otherwise.} \end{cases} \tag{4.6}$$

Using the above we obtain the following.

Proposition 2: The generators $\tilde{A}$, $\tilde{B}$, $\tilde{C}$, $\tilde{D}$ introduced above obey the following relations:

$$\tilde{C} = \tilde{D}\tilde{B} = -\tilde{B}\tilde{D}, \tag{4.7a}$$

$$[\tilde{A}, \tilde{D}] = 0, \tag{4.7b}$$

$$\tilde{A}\tilde{B} = \tilde{B}\tilde{A} = \tilde{D}^2\tilde{B} = \tilde{B}^3 = \tilde{B}, \tag{4.7c}$$

$$EZ = ZE = 0, \quad Z = \tilde{A}, \tilde{B}, \tilde{D}; \tag{4.7d}$$

$$\delta_{\mathcal{U}}(\tilde{A}) = \tilde{A} \otimes 1_{\mathcal{U}} + 1_{\mathcal{U}} \otimes \tilde{A}, \tag{4.8a}$$

$$\delta_{\mathcal{U}}(\tilde{B}) = \tilde{B} \otimes E + E \otimes \tilde{B}, \tag{4.8b}$$

$$\delta_{\mathcal{U}}(\tilde{D}) = \tilde{D} \otimes K + 1_{\mathcal{U}} \otimes \tilde{D}, \quad K \equiv (-1)^{\tilde{A}}, \tag{4.8c}$$

$$\delta(E) = E \otimes E; \tag{4.8d}$$

$$\varepsilon_{\mathcal{U}}(Z) = 0, \quad Z = \tilde{A}, \tilde{B}, \tilde{D}, \tag{4.9a}$$

$$\varepsilon_{\mathcal{U}}(E) = 1. \tag{4.9b}$$

$\tilde{A}$, $\tilde{B}^2$ and $\tilde{D}^2$ are Casimir operators. The bialgebra $s14$ is not a Hopf algebra.

Proof: Using the assumed duality the algebraic relations (4.7) are shown by calculating their pairings with the basis monomials f from (4.4). In particular, we have (giving only the nonzero pairings)

$$\langle \tilde{D}\tilde{B},\ f\rangle = -\langle \tilde{B}\tilde{D},\ f\rangle = \langle \tilde{C},\ f\rangle = 1, \quad \text{for } f = \tilde{c}, \tag{4.10a}$$

$$\langle \tilde{A}\tilde{D},\ f\rangle = \langle \tilde{D}\tilde{A},\ f\rangle = k+1, \quad \text{for } f = \tilde{a}^k\tilde{d}, \tag{4.10b}$$

$$\langle \tilde{A}\tilde{B},\ f\rangle = \langle \tilde{B}\tilde{A},\ f\rangle = \langle \tilde{D}^2\tilde{B},\ f\rangle = \langle \tilde{B}^3,\ f\rangle = \langle \tilde{B},\ f\rangle = 1, \quad \text{for } f = \tilde{b}. \tag{4.10c}$$

The facts that $\tilde{A}$, $\tilde{B}^2$ and $\tilde{D}^2$ are Casimir operators follow easily from (4.7). The proof of (4.8) is done as the proof of (3.13). We also use that

$$\langle \tilde{A}^n,\ \tilde{a}^k\tilde{d}^\ell\rangle = k^n \delta_{\ell 0}, \tag{4.11}$$

and hence

$$\langle K,\ \tilde{a}^k\tilde{d}^\ell\rangle=(-1)^k\delta_{\ell 0}. \tag{4.12}$$

There is no antipode for the bialgebra $s14$. Indeed, suppose that there was such. Then, by applying the Hopf algebra axiom (3.16) to the operator E, we would get

$$E\ \gamma(E)=1_{\mathcal{U}},$$

which would lead to contradiction after multiplication from the left with $Z=\tilde{A},\ \tilde{B},\ \tilde{D}$ (we would get $0=Z$). From this follows also that the generator $\tilde{B}$ does not have an antipode, since from (3.16) to the $\tilde{B}$ we would get

$$\tilde{B}\ \gamma(E)+E\ \gamma(\tilde{B})=0.$$

Thus, the bialgebra $s14$ is not a Hopf algebra. ■

Corollary 2: The algebra generated by the generator $\tilde{A}$ is a sub-bialgebra of $s14$. The algebra $s14'$ generated by $\tilde{B},\tilde{D}$ is a subalgebra of $s14$, but is not a sub-bialgebra [cf. (4.8b) and (4.8c)]. It has the following PBW basis:

$$\tilde{B},\ \tilde{B}^2,\ \tilde{D}\tilde{B},\ \tilde{D}\tilde{B}^2,\ \tilde{D}^\ell,\quad \ell=0,1,2,\ldots, \tag{4.13}$$

where we use the convention $\tilde{D}^0=1_{\mathcal{U}}$. ■

C. Regular representation

We start with the study of the right regular representation of the subalgebra $s14'$. For this we use the right multiplication table:

	$\tilde{B}$	$\tilde{B}^2$	$\tilde{D}\tilde{B}$	$\tilde{D}\tilde{B}^2$	$\tilde{D}^{2k}$	$\tilde{D}^{2k+1}$
$\tilde{B}$	$\tilde{B}^2$	$\tilde{B}$	$\tilde{D}\tilde{B}^2$	$\tilde{D}\tilde{B}$	$\tilde{B}$	$\tilde{D}\tilde{B}$
$\tilde{D}$	$-\tilde{D}\tilde{B}$	$\tilde{D}\tilde{B}^2$	$-\tilde{B}$	$\tilde{B}^2$	$\tilde{D}^{2k+1}$	$\tilde{D}^{2k+2}$

From the above table follows that there is a four-dimensional subspace spanned by $\tilde{B},\tilde{B}^2,\tilde{D}\tilde{B},\tilde{D}\tilde{B}^2$. It is reducible and decomposes into four one-dimensional representations spanned by

$$v_{\epsilon,\epsilon'}=\tilde{B}+\epsilon\tilde{B}^2-\epsilon'\tilde{D}\tilde{B}+\epsilon\epsilon'\tilde{D}\tilde{B}^2. \tag{4.14}$$

The action of $\tilde{B},\tilde{D}$ on these vectors is

$$\tilde{B}v_{\epsilon,\epsilon'}=\epsilon v_{\epsilon,\epsilon'},\quad \tilde{D}v_{\epsilon,\epsilon'}=\epsilon' v_{\epsilon,\epsilon'}. \tag{4.15}$$

The value of the Casimirs $\tilde{B}^2,\tilde{D}^2$ on these vectors is 1.

The quotient of the RRR by the above submodules has the following multiplication table:

	$\tilde{D}^{2k}$	$\tilde{D}^{2k+1}$
$\tilde{B}$	0	0
$\tilde{D}$	$\tilde{D}^{2k+1}$	$\tilde{D}^{2k+2}$

This representation is reducible. It contains an infinite set of nested submodules $V^n \supset V^{n+1}$, $n=0,1,\ldots$, where V^n is spanned by $\tilde{D}^{n+\ell}$, $\ell=0,1,\ldots$. Correspondingly there is an infinite set of one-dimensional irreducible factor-modules $F^n \equiv V^n/V^{n+1}$, (generated by $\tilde{D}^n$) which are all isomorphic to the trivial representation since the generators $\tilde{B},\tilde{D}$ act as zero on them. Thus there are five irreps arising from the RRR of $s14'$:

(i) one-dimensional trivial and
(ii) four one-dimensional with both Casimirs $\tilde{B}^2,\tilde{D}^2$ having value 1.

Turning to the algebra $s14$ we note that it inherits the representation structure of its subalgebra $s14'$. On the representations (4.14) the Casimir $\tilde{A}$ has the value 1. However, on the one-dimensional irreps F^n the Casimir $\tilde{A}$ has no fixed value. Thus, the list of the irreps arising from the RRR of $s14$ is

(i) one-dimensional with Casimir values $\mu,0,0$ for $\tilde{A},\tilde{B}^2,\tilde{D}^2$, respectively, $\mu \in \mathbb{C}$, and
(ii) four one-dimensional with all Casimirs $\tilde{A},\tilde{B}^2,\tilde{D}^2$ having value 1.

D. Weight representations

Here we study weight representations, first w.r.t. $\tilde{D}$, as in (3.26). The resulting representation of $s14'$ is three-dimensional:

$$v_0,\ \tilde{B}v_0,\tilde{B}^2v_0. \tag{4.16}$$

It is reducible and contains one one-dimensional and one two-dimensional irrep:

(i) One-dimensional:

$$w_0=(\tilde{B}^2-1_{\mathcal{U}})v_0, \tag{4.17}$$

$$\tilde{B}w_0=0,\quad \tilde{D}w_0=\lambda w_0, \tag{4.18}$$

$\lambda \in \mathbb{C}$.

(ii) Two-dimensional:

$$\{v_0,v_1=\tilde{B}v_0\}, \tag{4.19}$$

$$\tilde{B}\begin{pmatrix} v_0 \\ v_1 \end{pmatrix}=\begin{pmatrix} v_1 \\ v_0 \end{pmatrix},\quad \tilde{D}\begin{pmatrix} v_0 \\ v_1 \end{pmatrix}=\lambda\begin{pmatrix} v_0 \\ -v_1 \end{pmatrix}, \tag{4.20}$$

with $\lambda=\pm 1$.

Turning to the algebra $s14$ we note that it inherits the representation structure of its subalgebra $s14'$. On the one-dimensional irrep (4.17) the Casimir $\tilde{A}$ has no fixed value since $\tilde{B}$ is trivial, and $[\tilde{A},\tilde{D}]=0$. On the two-dimensional irrep (4.19) the Casimir $\tilde{A}$ has the value 1 since $\tilde{A}\tilde{B}=\tilde{B}$.

Thus, there are the following irreps of $s14$ which are obtained as weight irreps of the generator $\tilde{D}$:

(i) one-dimensional with Casimir values $\mu,0,\lambda^2$ for $\tilde{A},\tilde{B}^2,\tilde{D}^2$, respectively, $\mu,\lambda\in\mathbb{C}$, and
(ii) two two-dimensional with all Casimirs $\tilde{A},\tilde{B}^2,\tilde{D}^2$ having the value 1.

Next we consider weight representations w.r.t. $\tilde{B}$:

$$\tilde{B}\ v_0=\nu\ v_0, \tag{4.21}$$

with $\nu\in\mathbb{C}$. From $\tilde{B}^3=\tilde{B}$ follows that $\nu=0,\pm 1$. Acting with the generators we obtain the following representation vectors: $v_\ell=\tilde{D}^\ell v_0$. We have that $\tilde{D}v_\ell=v_{\ell+1}$.

Further, we consider first the case $\nu^2=1$. Then we apply the relation $\tilde{D}^2\tilde{B}=\tilde{B}$ to v_ℓ and we get

$$\tilde{D}^2\tilde{B}v_\ell=(-1)^\ell\nu v_{\ell+2}=\tilde{B}v_\ell=(-1)^\ell\nu v_\ell$$

from which follows that we have to identify $v_{\ell+2}$ with v_ℓ. Thus the representation is given as follows:

$$\{v_0,v_1=\tilde{D}v_0\}, \tag{4.22}$$

$$\tilde{B}\begin{pmatrix}v_0\\v_1\end{pmatrix}=\nu\begin{pmatrix}v_0\\-v_1\end{pmatrix},\quad \tilde{D}\begin{pmatrix}v_0\\v_1\end{pmatrix}=\begin{pmatrix}v_1\\v_0\end{pmatrix}. \tag{4.23}$$

On this irrep both Casimirs $\tilde{B}^2,\tilde{D}^2$ have value 1 ($\nu^2=1$).

Further, we consider the case $\nu=0$. This representation is reducible. It contains an infinite set of nested submodules $V^n\supset V^{n+1}$, $n=0,1,\ldots$, where V^n is spanned by $\tilde{D}^{n+\ell}v_0$, $\ell=0,1,\ldots$. Correspondingly, there is an infinite set of one-dimensional irreducible factor-modules $F^n\equiv V^n/V^{n+1}$ (generated by $\tilde{D}^n v_0$), which are all isomorphic to the trivial representation since the generators $\tilde{B},\tilde{D}$ act as zero on them.

Turning to the algebra $s14$ we note that it inherits the representation structure of its subalgebra $s14'$, with the value of the Casimir $\tilde{A}$ being not fixed if $\tilde{B}$ acts trivially, and being 1, if $\tilde{B}$ acts nontrivially.

Thus, there are the following irreps of $s14$ which are obtained as weight irreps of the generator $\tilde{B}$:

(i) one-dimensional with Casimir values $\mu,0,0$ for $\tilde{A},\tilde{B}^2,\tilde{D}^2$, respectively, $\mu\in\mathbb{C}$, and
(ii) two two-dimensional with all Casimirs $\tilde{A},\tilde{B}^2,\tilde{D}^2$ having the value 1.

E. Representations of $s14$ on $S14$

Here we shall study the representations of $s14$ obtained by the use of its right regular action (RRA) on the dual bialgebra $S14$. The RRA is defined as in (3.29). For the generators of $s14$ we have

$$\pi_R(\tilde{A})\begin{pmatrix}\tilde{a}&\tilde{b}\\\tilde{c}&\tilde{d}\end{pmatrix}=\begin{pmatrix}\tilde{a}&\tilde{b}\\\tilde{c}&\tilde{d}\end{pmatrix}, \tag{4.24a}$$

$$\pi_R(\tilde{B})\begin{pmatrix}\tilde{a}&\tilde{b}\\\tilde{c}&\tilde{d}\end{pmatrix}=\begin{pmatrix}\tilde{b}&\tilde{a}\\\tilde{d}&\tilde{c}\end{pmatrix}, \tag{4.24b}$$

$$\pi_R(\tilde{D})\begin{pmatrix}\tilde{a} & \tilde{b}\\ \tilde{c} & \tilde{d}\end{pmatrix}=\begin{pmatrix}\tilde{d} & -\tilde{c}\\ -\tilde{b} & \tilde{a}\end{pmatrix}, \tag{4.24c}$$

$$\pi_R(E)\begin{pmatrix}\tilde{a} & \tilde{b}\\ \tilde{c} & \tilde{d}\end{pmatrix}=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix}, \tag{4.24d}$$

$$\pi_R(Z)1_{\mathcal{A}}=1_{\mathcal{A}}\langle Z,1_{\mathcal{A}}\rangle=1_{\mathcal{A}}\varepsilon_{\mathcal{U}}(Z)=\begin{cases}0, & Z=\tilde{A},\tilde{B},\tilde{D},\\ 1, & Z=E.\end{cases} \tag{4.24e}$$

For the action on the basis of $S14$ we use formula (3.31). We obtain

$$\pi_R(A)\tilde{a}^n\tilde{d}^k=(n+k)\tilde{a}^n\tilde{d}^k,\quad \pi_R(A)\tilde{b}^n\tilde{c}^k=(n+k)\tilde{b}^n\tilde{c}^k, \tag{4.25a}$$

$$\pi_R(B)\tilde{a}^n\tilde{d}^k=\delta_{k0}\delta_{n1}\tilde{b}+\delta_{n0}\delta_{k1}\tilde{c},\quad \pi_R(B)\tilde{b}^n\tilde{c}^k=\delta_{k0}\delta_{n1}\tilde{a}+\delta_{n0}\delta_{k1}\tilde{d}, \tag{4.25b}$$

$$\pi_R(D)\tilde{a}^k\tilde{d}^\ell=(-1)^{\ell+1}\ell\tilde{a}^{k+1}\tilde{d}^{\ell-1}+(-1)^\ell k\tilde{a}^{k-1}\tilde{d}^{\ell+1}, \tag{4.25c}$$

$$\pi_R(D)\tilde{b}^k\tilde{c}^\ell=(-1)^\ell\ell\tilde{b}^{k+1}\tilde{c}^{\ell-1}+(-1)^{\ell+1}k\tilde{b}^{k-1}\tilde{c}^{\ell+1}. \tag{4.25d}$$

We see that similarly to Sec. III E, the Casimir $\tilde{A}$ acts as the length of the elements of $S14$, i.e., (3.30) holds. Thus, also here we classify the irreps by the value μ_A of the Casimir $\tilde{A}$ which runs over the non-negative integers. For fixed μ_A the basis of the corresponding representations is spanned by the elements f such that $\ell(f)=\mu_A$. The dimension of each such representation is

$$\dim(\mu_A)=\begin{cases}2(\mu_A+1) & \text{for } \mu_A\geqslant 1,\\ 1 & \text{for } \mu_A=0.\end{cases} \tag{4.26}$$

The classification goes as follows:

(i) $\mu_A=0$: This is the one-dimensional trivial representation spanned by $1_{\mathcal{A}}$.

(ii) $\mu_A=1$: This representation is four-dimensional spanned by the four generators $\tilde{a},\tilde{b},\tilde{c},\tilde{d}$ of $S14$. It decomposes in two two-dimensional, isomorphic to each other irrep with basis vectors as in (3.34)—this is due to the fact that the action (4.24b) and (4.24c) is the same as the action (3.30). The value of the Casimirs $\tilde{B}^2,\tilde{D}^2$ is 1.

(iii) Each representation for fixed $\mu_A\geqslant 2$ is reducible and decomposes in two isomorphic representations: one built on the basis $\tilde{a}^k\tilde{d}^\ell$, and the other built on the basis $\tilde{b}^k\tilde{c}^\ell$, each of dimension μ_A+1. Thus, for $\mu_A\geqslant 2$ we shall consider only the representations built on the basis $\tilde{a}^k\tilde{d}^\ell$. These representations are also reducible and they all decompose in one-dimensional irreps. Further, the action of $\tilde{B}$ is zero, thus, we speak only about the action of $\tilde{D}$.

(iv) $\mu_A=2n$, $n=1,2,\ldots$: For fixed n the representation decomposes into $2n+1$ one-dimensional irreps. On one of these, which is spanned by the element

$$w_0=\sum_{k=0}^{n}\binom{n}{k}\tilde{a}^{2n-2k}\tilde{d}^{2k}, \tag{4.27}$$

the generator $\tilde{D}$ acts by zero. The rest of the irreps are enumerated by the parameters $\pm$, τ, where $\tau=2,4,\ldots,2n=\mu_A$, and are spanned by the vectors

$$u_\tau^\pm=u_0\pm\pi u_1,$$

$$u_0=\sum_{k=0}^{n}\alpha_k\tilde{a}^{2n-2k}\tilde{d}^{2k},\quad \alpha_0=1, \tag{4.28}$$

$$u_1=\sum_{k=0}^{n-1}\beta_k\tilde{a}^{2n-2k-1}\tilde{d}^{2k+1},\quad \beta_0=1,$$

on which $\tilde{D}$ acts by

$$\pi_R(\tilde{D})u_\tau^{\pm}=\pm\tau u_\tau^{\pm}, \tag{4.29}$$

which follows from

$$\pi_R(\tilde{D})\begin{pmatrix}u_0\\u_1\end{pmatrix}=\begin{pmatrix}\tau^2u_1\\u_0\end{pmatrix}. \tag{4.30}$$

Note that the value of the Casimir $\tilde{D}^2$ is equal to τ^2. The coefficients α_k,β_k depend on τ and are fixed from the two recursive equations which follow from (4.30):

$$\tau^2\beta_k=2(n-k)\alpha_k-2(k+1)\alpha_{k+1},\quad k=0,\ldots,n-1, \tag{4.31a}$$

$$\alpha_k=(2k+1)\beta_k-(2n-2k+1)\beta_{k-1},\quad k=0,\ldots,n, \tag{4.31b}$$

where we set $\beta_{-1}\equiv 0$, $\beta_n\equiv 0$.

(v) $\mu_A=2n+1$, $n=1,2,\ldots$: For fixed n the representation is $(2n+2)$-dimensional and decomposes into $2n+2$ irreps which are enumerated by two parameters: $\pm$, τ, where $\tau=1,3,5,\ldots,2n+1=\mu_A$, and are spanned by the vectors

$$w_\tau^{\pm}=w_0\pm\tau w_1,$$

$$w_0=\sum_{k=0}^{n}\alpha_k'\tilde{a}^{2n-2k+1}\tilde{d}^{2k},\quad \alpha_0'=1, \tag{4.32}$$

$$w_1=\sum_{k=0}^{n}\beta_k'\tilde{a}^{2n-2k}\tilde{d}^{2k+1},\quad \beta_0'=1,$$

on which $\tilde{D}$ acts by (4.29). Note that the value of the Casimir $\tilde{D}^2$ is equal to τ^2. The coefficients α_k',β_k' are fixed from the two recursive equations which follow from (4.29):

$$\tau^2\beta_k'=(2n-2k+1)\alpha_k'-2(k+1)\alpha_{k+1}',\quad k=0,\ldots,n, \tag{4.33}$$

$$\alpha_k'=(2k+1)\beta_k'-2(n-k+1)\beta_{k-1}',\quad k=0,\ldots,n, \tag{4.34}$$

where we set $\alpha_{n+1}'\equiv 0$, $\beta_{-1}'\equiv 0$.

To summarize the list of irreps of $s14$ on $S14$ is

(i) one-dimensional trivial;

(ii) two two-dimensional with all Casimirs $\tilde{A},\tilde{B}^2,\tilde{D}^2$ having the value 1;

(iii) one-dimensional enumerated by $n=1,2,\ldots$, which for fixed n have Casimir values $2n,0,0$ for $\tilde{A},\tilde{B}^2,\tilde{D}^2$, respectively;

(iv) pairs of one-dimensional irreps enumerated by $n=1,2,\ldots$, $\tau=2,4,\ldots,2n$, which have Casimir values $2n,0,\tau^2$ for $\tilde{A},\tilde{B}^2,\tilde{D}^2$, respectively; and

(v) pairs of one-dimensional irreps enumerated by $n=1,2,\ldots$, $\tau=1,3,\ldots,(2n+1)$, which have Casimir values $2n+1,0,\tau^2$ for $\tilde{A},\tilde{B}^2,\tilde{D}^2$, respectively.

Finally, we note in the irreps of $s14$ on $S14$ all Casimirs can take only non-negative integer values.

V. ALGEBRA *S*14*o*

A. Bialgebra relations

In this section we consider the matrix bialgebra $S14o$. We obtain it by applying the RTT relations (3.1) for the case $R=R_{S1,4}$, cf. (4.1), when $q^2=1$. We shall consider the case $q=1$ (the case $q=-1$ is equivalent, cf. below). For $q=1$ the relations following from (3.1) and (4.1) are

$$a^2=d^2,\ \ b^2=c^2=0,\quad ab=ba=ac=ca=bd=db=cd=dc=0, \tag{5.1}$$

or, in terms of the generators $\tilde{a},\tilde{b},\tilde{c},\tilde{d}$,

$$\tilde{b}\tilde{a}=\tilde{a}\tilde{b},\ \ \tilde{c}\tilde{a}=-\tilde{a}\tilde{c},\ \ \tilde{d}\tilde{a}=-\tilde{a}\tilde{d},\ \ \tilde{c}\tilde{b}=-\tilde{b}\tilde{c},\ \ \tilde{d}\tilde{b}=-\tilde{b}\tilde{d},\ \ \tilde{d}\tilde{c}=\tilde{c}\tilde{d}. \tag{5.2}$$

(The case $q=-1$ is obtained from the above through the exchange $\tilde{b}\leftrightarrow\tilde{c}$.)

From the above relations it is clear that we can choose any ordering of the PBW basis. For definiteness we choose for the PBW basis of $S14o$

$$\tilde{a}^k\tilde{b}^\ell\tilde{c}^m\tilde{d}^n. \tag{5.3}$$

B. Dual algebra

Let us denote by $s14o$ the unknown yet dual algebra of $S14o$, and by $\tilde{A},\tilde{B},\tilde{C},\tilde{D}$ the four generators of $s14o$. We define the pairing $\langle Z,f\rangle$, $Z=\tilde{A},\tilde{B},\tilde{C},\tilde{D}$, f is from (5.3), as (3.10). Explicitly, we obtain

$$\langle\tilde{A},f\rangle=\varepsilon\left(\frac{\partial f}{\partial\tilde{a}}\right)=\begin{cases}k & \text{for } f=\tilde{a}^k,\\ 0 & \text{otherwise,}\end{cases} \tag{5.4a}$$

$$\langle\tilde{B},f\rangle=\varepsilon\left(\frac{\partial f}{\partial\tilde{b}}\right)=\begin{cases}1 & \text{for } f=\tilde{a}^k\tilde{b},\\ 0 & \text{otherwise,}\end{cases} \tag{5.4b}$$

$$\langle\tilde{C},f\rangle=\varepsilon\left(\frac{\partial f}{\partial\tilde{c}}\right)=\begin{cases}1 & \text{for } f=\tilde{a}^k\tilde{c},\\ 0 & \text{otherwise,}\end{cases} \tag{5.4c}$$

$$\langle\tilde{D},f\rangle=\varepsilon\left(\frac{\partial f}{\partial\tilde{d}}\right)=\begin{cases}1 & \text{for } f=\tilde{a}^k\tilde{d},\\ 0 & \text{otherwise.}\end{cases} \tag{5.4d}$$

Using the above we obtain the following proposition.

Proposition 3: The generators $\tilde{A},\tilde{B},\tilde{C},\tilde{D}$ introduced above obey the following relations:

$$[\tilde{A},Z]=0,\quad Z=\tilde{B},\tilde{C},\tilde{D}, \tag{5.5a}$$

$$[\tilde{B},\tilde{C}]=-2\tilde{D},\quad [\tilde{B},\tilde{D}]=-2\tilde{C},\quad [\tilde{C},\tilde{D}]=-2\tilde{B}, \tag{5.5b}$$

$$\delta_{\mathcal{U}}(\tilde{A})=\tilde{A}\otimes 1_{\mathcal{U}}+1_{\mathcal{U}}\otimes\tilde{A}, \tag{5.6a}$$

$$\delta_{\mathcal{U}}(\tilde{B})=\tilde{B}\otimes 1_{\mathcal{U}}+1_{\mathcal{U}}\otimes\tilde{B}, \tag{5.6b}$$

$$\delta_{\mathcal{U}}(\tilde{C})=\tilde{C}\otimes K+1_{\mathcal{U}}\otimes\tilde{C},\quad K=(-1)^{\tilde{A}}, \tag{5.6c}$$

$$\delta_{\mathcal{U}}(\tilde{D})=\tilde{D}\otimes K+1_{\mathcal{U}}\otimes\tilde{D}, \tag{5.6d}$$

$$\varepsilon_{\mathcal{U}}(Z)=0, \quad Z=\tilde{A},\tilde{B},\tilde{C},\tilde{D}, \tag{5.7}$$

$$\gamma_{\mathcal{U}}(\tilde{A})=-\tilde{A}, \gamma_{\mathcal{U}}(\tilde{B})=-\tilde{B}, \quad \gamma_{\mathcal{U}}(\tilde{C})=-\tilde{C}K, \quad \gamma_{\mathcal{U}}(\tilde{D})=-\tilde{D}K. \tag{5.8}$$

Proof: The proof of (5.5) goes as the standard duality between the classical U(gl(2)) and GL(2), cf. e.g., Ref. 13. The proof of (5.6)–(5.8) is also standard, except the factor K which appears while calculating:

$$\langle \tilde{C},\tilde{c}\tilde{a}^k\rangle=(-1)^k\langle \tilde{C},\tilde{a}^k\tilde{c}\rangle=(-1)^k,$$

which on the other hand is equal to (supposing an unknown yet K)

$$\langle \delta_{\mathcal{U}}(\tilde{C}),\tilde{c}\otimes\tilde{a}^k\rangle=\langle \tilde{C}\otimes K+1_{\mathcal{U}}\otimes\tilde{C},\tilde{c}\otimes\tilde{a}^k\rangle=\langle K,\tilde{a}^k\rangle.$$

Comparing the two rhs's we conclude that $K=(-1)^{\tilde{A}}$. The same follows from calculating $\langle \tilde{D},\tilde{d}\tilde{a}^k\rangle$. ■

Corollary 3: The auxiliary generator $K=(-1)^{\tilde{A}}$ is central and $K^{-1}=K$. Its co-algebra relations are

$$\delta_{\mathcal{U}}(K)=K\otimes K, \quad \varepsilon_{\mathcal{U}}(K)=1, \quad \gamma_{\mathcal{U}}(K)=K. \tag{5.9}$$

■

Corollary 4: The algebra generated by the generator $\tilde{A}$ is a Hopf subalgebra of $s14o$. The algebra $s14o'$ generated by $\tilde{B},\tilde{C},\tilde{D}$ is a subalgebra of $s14o$, but is not a Hopf subalgebra because of the operator K in the co-algebra structure. The algebras $s14o,s14o'$ are isomorphic to U(gl(2)),U(sl(2)), respectively. The latter is seen from the following:

$$X^{\pm}\equiv\tfrac{1}{2}(\tilde{D}\mp\tilde{C}), \tag{5.10a}$$

$$[\tilde{B},X^{\pm}]=\pm 2X^{\pm}, \quad [X^{+},X^{-}]=\tilde{B}. \tag{5.10b}$$

Indeed the last line presents the standard sl(2) commutation relations. However, the generators $X^{\pm}$ inherit the K dependence in the coalgebra operations:

$$\delta_{\mathcal{U}}(X^{\pm})=X^{\pm}\otimes K+1_{\mathcal{U}}\otimes X^{\pm}, \tag{5.11a}$$

$$\varepsilon_{\mathcal{U}}(X^{\pm})=0, \tag{5.11b}$$

$$\gamma_{\mathcal{U}}(X^{\pm})=-X^{\pm}K. \tag{5.11c}$$

The algebra $s14o$ is graded:

$$\deg\ X^{\pm}=\pm 1, \quad \deg\ \tilde{A}=\deg\ \tilde{B}=0, \quad (\Rightarrow \deg\ K=0). \tag{5.12}$$

■

Based on the above corollary we are able to make the following important observation. The algebra $s14o$ may be identified with a special case of the Hopf algebra $\mathcal{U}_{p,q}$ which was found in Ref. 13 as the dual of $\mathrm{GL}_{p,q}(2)$. To make direct contact with Ref. 13 we need to replace their $(p^{1/2},q^{1/2})\to(p,q)$, then set $q=p^{-1}$, and at the end set $p=-1$. [The necessity to set values in such order is clear from, e.g., the formula for the co-product in (5.21) of Ref. 13]. The generators from Ref. 13 $K,p^{K},H,X^{\pm}$ correspond to $\tilde{A},K,\tilde{B},X^{\pm}$ in our notation.

More than this, it turns out that the corresponding algebras in duality, namely, $S14o$ and $\mathrm{GL}_{p,q}(2)$, may be identified setting q,p as above. To make this evident we make the following change of generators:

$$\hat{a}=\tilde{a}+\tilde{b},\quad \hat{b}=\tilde{d}-\tilde{c},\quad \hat{c}=\tilde{c}+\tilde{d},\quad \hat{d}=\tilde{a}-\tilde{b}. \tag{5.13}$$

For these generators the commutation relations are

$$\hat{b}\hat{a}=-\hat{a}\hat{b},\quad \hat{c}\hat{a}=-\hat{a}\hat{c},\quad \hat{d}\hat{a}=\hat{a}\hat{d},\quad \hat{c}\hat{b}=\hat{b}\hat{c},\quad \hat{b}\hat{d}=-\hat{d}\hat{b},\quad \hat{c}\hat{d}=-\hat{d}\hat{c}, \tag{5.14}$$

i.e., exactly those of $\mathrm{GL}_{p,q}(2)$ (cf. Ref. 1) for $p=q=-1$. Furthermore, the co-product and co-unit are as for $\mathrm{GL}_{p,q}(2)$ or $\mathrm{GL}(2)$, i.e., as in (2.1). For the antipode we have to suppose that the determinant $ad-p^{-1}bc$ from Ref. 1, which here becomes (cf. $p=-1$)

$$\omega=\hat{a}\hat{d}+\hat{b}\hat{c}, \tag{5.15}$$

is invertible, or that $\omega\neq 0$, and we extend the algebra by an element ω^{-1} so that

$$\omega\omega^{-1}=\omega^{-1}\omega=1_{\mathcal{A}},\quad \delta_{\mathcal{U}}(\omega^{\pm 1})=\omega^{\pm 1}\otimes\omega^{\pm 1},\ \ \varepsilon_{\mathcal{U}}(\omega^{\pm 1})=1,\ \ \gamma_{\mathcal{U}}(\omega^{\pm 1})=\omega^{\mp 1}. \tag{5.16}$$

Then the antipode is given by

$$\gamma_{\mathcal{U}}\begin{pmatrix}\hat{a} & \hat{b}\\ \hat{c} & \hat{d}\end{pmatrix}=\omega^{-1}\begin{pmatrix}\hat{d} & \hat{b}\\ \hat{c} & \hat{a}\end{pmatrix}, \tag{5.17}$$

or in a more compact notation

$$\gamma_{\mathcal{U}}(M)=M^{-1}. \tag{5.18}$$

Indeed, we have

$$\begin{pmatrix}\hat{a} & \hat{b}\\ \hat{c} & \hat{d}\end{pmatrix}\begin{pmatrix}\hat{d} & \hat{b}\\ \hat{c} & \hat{a}\end{pmatrix}=\begin{pmatrix}\hat{d} & \hat{b}\\ \hat{c} & \hat{a}\end{pmatrix}\begin{pmatrix}\hat{a} & \hat{b}\\ \hat{c} & \hat{d}\end{pmatrix}=\omega\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{5.19}$$

This relation between $s14o$, $S14o$ and $\mathcal{U}_{p,q}$, $\mathrm{GL}_{p,q}(2)$ was not anticipated since the corresponding R-matrices $R_{S1,4}$ and $R_{S2,1}$ are listed in Ref. 8 as different and, furthermore, nonequivalent. It turns out that this is indeed the case, except in the case we have stumbled upon. To show this we first recall

$$R_{S2,1}=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & p & 1-pq & 0\\ 0 & 0 & q & 0\\ 0 & 0 & 0 & 1\end{pmatrix}, \tag{5.20}$$

which for $q=p^{-1}=-1$ becomes

$$R_0\equiv(R_{S2,1})_{q=p^{-1}=-1}=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}. \tag{5.21}$$

Further, we need

$$R_{\pm}\equiv(R_{S1,4})_{q=\pm 1}=\begin{pmatrix} 0 & 0 & 0 & \pm 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ \pm 1 & 0 & 0 & 0 \end{pmatrix}. \tag{5.22}$$

Now we can show that $R_{\pm}$ can be transformed by "gauge transformations" to R_0. Namely, we have

$$R_0=(U_{\pm}\otimes U_{\pm})R_{\pm}(U_{\pm}\otimes U_{\pm})^{-1}, \tag{5.23a}$$

$$U_{+}=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad U_{-}=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}. \tag{5.23b}$$

In accord with this we have

$$\hat{T}\equiv\begin{pmatrix} \hat{a} & \hat{b} \\ \hat{c} & \hat{d} \end{pmatrix}, \quad T\equiv\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad \hat{T}=U_{+}T(U_{+})^{-1} \tag{5.24}$$

$$\Rightarrow \quad \begin{aligned} &\hat{a}=\tfrac{1}{2}(a+b+c+d), \quad \hat{b}=\tfrac{1}{2}(a-b+c-d), \\ &\hat{c}=\tfrac{1}{2}(a+b-c-d), \quad \hat{d}=\tfrac{1}{2}(a-b-c+d), \end{aligned} \tag{5.25}$$

which is equivalent to substituting (2.2) in (5.13).

The use of U_{-} would lead to different relations between hatted and unhatted generators, which, however, would not affect the algebra relations. Indeed,

$$\hat{T}'\equiv\begin{pmatrix} \hat{a}' & \hat{b}' \\ \hat{c}' & \hat{d}' \end{pmatrix}, \quad T'\equiv\begin{pmatrix} a' & b' \\ c' & d' \end{pmatrix}, \quad \hat{T}'=U_{-}T'(U_{-})^{-1} \tag{5.26}$$

$$\Rightarrow \quad \begin{aligned} &\hat{a}'=\tfrac{1}{2}(a'-ib'+ic'+d'), \quad \hat{b}'=\tfrac{1}{2}(-ia'+b'+c'+id'), \\ &\hat{c}'=\tfrac{1}{2}(ia'+b'+c'-id'), \quad \hat{d}'=\tfrac{1}{2}(a'+ib'-ic'+d'). \end{aligned} \tag{5.27}$$

But this becomes equivalent to (5.25) with the changes

$$(\hat{a}',i\hat{b}',-i\hat{c}',\hat{d}')\mapsto(\hat{a},\hat{b},\hat{c},\hat{d}), \quad (a',-ib',ic',d')\mapsto(a,b,c,d), \tag{5.28}$$

while the (inverse) changes (5.28) do not affect (5.14) and (5.1).

C. Representations of *s*14*o* on *S*14*o*

The regular representation of $s14o$ ($s14o'$) on itself and its weight representations are the same as those of $U(gl(2))$ ($U(sl(2))$) due to (5.10). The situation is different for the representations of $s14o$ on $S14o$ since these involve the coalgebra structure. However, the deviation from the trivial coalgebra structure is only via the sign operator K, and as we shall see in some representations there remains no trace of this.

In treating the representations of $s14o$ on $S14o$ we shall use the known construction for the induced representations of $\mathcal{U}_{p,q}$ on $\mathrm{GL}_{p,q}(2)$ from Ref. 20 and the relation between $s14o$,$S14o$

and $\mathcal{U}_{p,q}$, $\mathrm{GL}_{p,q}(2)$ that we established in the previous subsection. For the comparison with Ref. 20 we should note the parametrization used there: $p=ts^{1/2}$, $q=ts^{-1/2}$. Thus, using $q=p^{-1}$, $p=-1$ we need to substitute $t\to 1$, $\sqrt{s}\mapsto -1$. Further, one should substitute the operator h from Ref. 20 with $t^{\tilde{B}/2}$, and expand in order to get the action of $\tilde{B}$. Finally, one should substitute the operator r from Ref. 20 with $\sqrt{s}^{\tilde{A}}=(-1)^{\tilde{A}}=K$. In fact, it is easier to derive the necessary formulas directly, which we shall proceed to do in a compact way.

Here we shall employ both the left action and the right action. We start by calculating the left action using

$$\pi_L(Z)f\equiv\langle \gamma_{\mathcal{U}}(Z),f_{(1)}\rangle f_{(2)},\quad Z\in s14,\ Z\neq 1_{\mathcal{U}},\quad f\in S14, \tag{5.29a}$$

$$\pi_L(1_{\mathcal{U}})f\equiv f,\quad f\in S14, \tag{5.29b}$$

using for the PBW basis

$$\hat{a}^j\hat{d}^k\hat{b}^\ell\hat{c}^n. \tag{5.30}$$

For the left action on the elements of $S14o$ we use a corollary of (5.29):

$$\pi_L(Z)fg=\pi_L(\delta'_{\mathcal{U}}(Z))(f\otimes g), \tag{5.31}$$

where is used the *opposite comultiplication* $\delta'_{\mathcal{U}}\equiv\sigma\circ\delta_{\mathcal{U}}$, where σ is the permutation in $\mathcal{U}\otimes\mathcal{U}$. We find

$$\pi_L(A)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=-k\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}, \tag{5.32a}$$

$$\pi_L(K)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=(-1)^k\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}, \tag{5.32b}$$

$$\pi_L(B)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=k\begin{pmatrix}-\hat{a}^k & -\hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}, \tag{5.32c}$$

$$\pi_L(X^+)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=k\begin{pmatrix}(-1)^{k-1}\hat{a}^{k-1}\hat{c} & \hat{d}\hat{b}^{k-1}\\ 0 & 0\end{pmatrix}, \tag{5.32d}$$

$$\pi_L(X^-)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=k\begin{pmatrix}0 & 0\\ \hat{a}\hat{c}^{k-1} & (-1)^{k-1}\hat{d}^{k-1}\hat{b}\end{pmatrix}, \tag{5.32e}$$

$$\pi_L(K)1_{\mathcal{A}}=1,\quad \pi_L(Z)1_{\mathcal{A}}=0,\quad Z=\tilde{A},\tilde{B},\tilde{C},\tilde{D}. \tag{5.32f}$$

(We give also the action of K though it follows from that of $\tilde{A}$.)

Next we calculate the right action as in (3.29) to find

$$\pi_R(A)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=k\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}, \tag{5.33a}$$

$$\pi_R(K)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=(-1)^k\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}, \tag{5.33b}$$

$$\pi_R(B)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=k\begin{pmatrix}\hat{a}^k & -\hat{b}^k\\ \hat{c}^k & -\hat{d}^k\end{pmatrix}, \tag{5.33c}$$

$$\pi_R(X^+)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=k\begin{pmatrix}0 & (-1)^{k-1}\hat{a}\hat{b}^{k-1}\\ 0 & \hat{d}^{k-1}\hat{c}\end{pmatrix}, \tag{5.33d}$$

$$\pi_R(X^-)\begin{pmatrix}\hat{a}^k & \hat{b}^k\\ \hat{c}^k & \hat{d}^k\end{pmatrix}=k\begin{pmatrix}\hat{a}^{k-1}\hat{b} & 0\\ (-1)^{k-1}\hat{d}\hat{c}^{k-1} & 0\end{pmatrix}, \tag{5.33e}$$

$$\pi_R(K)1_{\mathcal{A}}=1,\quad \pi_R(Z)1_{\mathcal{A}}=0,\quad Z=\tilde{A},\tilde{B},\tilde{C},\tilde{D}. \tag{5.33f}$$

By (5.29) and (5.33) we have defined left and right actions of $s14o$ on $S14o$. As in the classical case the left and right actions commute, and we shall use the right action to reduce the left regular representation. Following Ref. 21 we would like the right action to mimic some properties of a lowest weight module, i.e., annihilation by the lowering (negative grade) generator X^- and scalar action by the (exponent of the) Cartan (zero grade) generators $\tilde{A}$ (or K) and $\tilde{B}$. Such action is the reason we call these representations induced. We start with functions which are formal power series in the PBW basis:

$$f=\sum_{j,k,\ell,m\in\mathbb{Z}_+}\mu_{j,k,\ell,m}\hat{a}^j\hat{d}^k\hat{b}^\ell\hat{c}^m. \tag{5.34}$$

The right-action conditions we mentioned are

$$\pi_R(X^-)f=0, \tag{5.35a}$$

$$\pi_R(\tilde{A})f=\rho f,\quad \pi_R(\tilde{B})f=-\nu f. \tag{5.35b}$$

From (5.35a) follows that our functions would not depend on $\hat{a}$ and $\hat{c}$, except through the determinant ω, since $\pi_R(X^-)\omega=0$. We also have

$$\pi_R(\tilde{A})\omega^n=2n\omega^n,\quad \pi_R(K)\omega^n=\omega^n,\quad \pi_R(B)\omega^n=0,\quad \pi_R(X^\pm)\omega^n=0. \tag{5.36}$$

Thus, we continue with

$$f=\sum_{\substack{k,\ell,n\in\mathbb{Z}_+\\ n\in\mathbb{Z}}}\mu_{k,\ell}\hat{d}^k\hat{b}^\ell\omega^n, \tag{5.37}$$

on which conditions (5.35b) lead to $k+\ell+2n=\rho\in\mathbb{Z}$, $k+\ell=\nu\in\mathbb{Z}_+$, $\rho-\nu\in2\mathbb{Z}$, and the summation becomes single:

$$f=\sum_{\ell\in\mathbb{Z}_+}\mu_\ell u_\ell,\quad u_\ell\equiv\hat{b}^\ell\hat{d}^{\nu-\ell}\omega^{(\rho-\nu)/2}, \tag{5.38}$$

(where we changed the ordering since this would give simpler formulas for the action). Now if neither $\hat{b}$ nor $\hat{d}$ has an inverse the representations will be finite-dimensional, in contrast to the classical case. However, these finite-dimensional representations we shall obtain also if we suppose that either $\hat{b}$ or $\hat{d}$ has an inverse (see below), and at the same time we shall have infinite-dimensional representations. Thus, further, we shall suppose that $\hat{d}$ has an inverse. This means that we can allow k in (5.38) to take any integer values, and then the same is true for ν.

Now we shall work out the representation (left) action for the basis u_ℓ for which we need first the left action on ω:

$$\pi_L(A)\omega^n=-2n\omega^n,\quad \pi_L(K)\omega^n=\omega^n,\quad \pi_L(B)\omega^n=0,\quad \pi_L(X^\pm)\omega^n=0. \tag{5.39}$$

We also remark that the action on $\hat{d}^k$, ω^n for negative k, n is given again by (5.32) and (5.39). [This can be checked, e.g., by calculating $\pi_L(Z)\hat{d}^{-k}\hat{d}^k=\pi_L(Z)1_{\mathcal{A}}$ in two different ways: (5.31) for the lhs, and (5.32) for the rhs.] Then the rules are

$$\pi_{\nu,\rho}(\tilde{A})u_\ell=-\rho u_\ell, \tag{5.40a}$$

$$\pi_{\nu,\rho}(\tilde{B})u_\ell=(\nu-2\ell)u_\ell, \tag{5.40b}$$

$$\pi_{\nu,\rho}(X^+)u_\ell=(-1)^{\ell-1}\ell u_{\ell-1}, \tag{5.40c}$$

$$\pi_{\nu,\rho}(X^-)u_\ell=(-1)^{\ell+1}(\ell-\nu)u_{\ell+1}, \tag{5.40d}$$

where $\pi_{\nu,\rho}$ denotes π_L with the parameter dependence made explicit.

Thus, we have obtained infinite-dimensional representations of $s14o$ parametrized by two integers ν, ρ. We shall denote by $\mathcal{C}_{\nu,\rho}$ the corresponding representation space. Note that these representations are highest weight representations since we have $\pi_L(X^+)u_0=0$. If the parameter ν is non-negative, $\nu\in\mathbb{Z}_+$, then the corresponding representation is reducible, due to the fact that $\pi_L(X^-)u_\nu=0$. Thus, the vectors $u_0,\ldots,u_\nu$ form an invariant subspace, of dimension $\nu+1$, which shall denote by $\mathcal{E}_{\nu,\rho}$, $\nu\in\mathbb{Z}_+$. Thus, if $\nu\in\mathbb{Z}_+$ we have two irreducible representations with representation spaces isomorphic to $\mathcal{E}_{\nu,\rho}$ and to $\mathcal{C}_{\nu,\rho}/\mathcal{E}_{\nu,\rho}$ (the latter is infinite-dimensional). If $\nu\notin\mathbb{Z}_+$ the representation $\mathcal{C}_{\nu,\rho}$ is irreducible.

From the above we are prompted to use the variable $\eta\equiv\hat{b}\hat{d}^{-1}$. This is also related to the following Gauss decomposition of $S14o$:

$$\begin{pmatrix}\hat{a} & \hat{b}\\ \hat{c} & \hat{d}\end{pmatrix}=\begin{pmatrix}1 & \hat{b}\hat{d}^{-1}\\ 0 & 1\end{pmatrix}\begin{pmatrix}\omega\hat{d}^{-1} & 0\\ 0 & \hat{d}\end{pmatrix}\begin{pmatrix}1 & 0\\ \hat{d}^{-1}\hat{c} & 1\end{pmatrix}, \tag{5.41}$$

i.e., from here the natural variables are η, $\hat{d}$, ω. Thus, we use also the functions

$$\varphi=\sum_{\ell\in\mathbb{Z}_+}\alpha_\ell v_\ell,\quad v_\ell\equiv\eta^\ell\hat{d}^\nu\omega^{(\rho-\nu)/2}. \tag{5.42}$$

The action of the generators on the variable η is

$$\begin{pmatrix}\tilde{A} & K\\ \tilde{B} & X^\pm\end{pmatrix}\eta^\ell=\begin{pmatrix}0 & \eta^\ell\\ -2\ell\,\eta^\ell & \pm\ell\,\eta^{\ell\mp1}\end{pmatrix}, \tag{5.43}$$

and the action on the basis is as for u_ℓ except for $X^\pm$:

$$\pi_{\nu,\rho}(X^+)v_\ell=\ell v_{\ell-1}, \tag{5.44a}$$

$$\pi_{\nu,\rho}(X^-)v_\ell=(\nu-\ell)v_{\ell+1}. \tag{5.44b}$$

Thus, in this basis there is no trace of the nontriviality of the co-product of $X^\pm$. More than this we can reduce the representations directly to the classical U(gl(2)) if we introduce the restricted functions $\hat{\varphi}(\eta)$ by the operators

$$\hat{A}_{\nu,\rho}:\mathcal{C}_{\nu,\rho}\to\hat{C}_{\nu,\rho},\quad \hat{\varphi}(\eta)=(\hat{A}_{\nu,\rho}\varphi)(\eta)\equiv\varphi(\eta,1_{\mathcal{A}},1_{\mathcal{A}}),$$
$$\hat{A}^{-1}_{\nu,\rho}:\hat{C}_{\nu,\rho}\to\mathcal{C}_{\nu,\rho},\quad \varphi(\eta,\hat{d},\omega)=(\hat{A}^{-1}_{\nu,\rho}\hat{\varphi})(\eta,\hat{d},\omega)\equiv\hat{\varphi}(\eta)\hat{d}^{\nu}\omega^{(\rho-\nu)/2}. \tag{5.45}$$

We denote the representation space of $\hat{\varphi}(\eta)$ by $\hat{C}_{\nu,\rho}$ and the representation acting in $\hat{C}_{\nu,\rho}$ by $\hat{\pi}_{\nu,\rho}$. The properties of $\hat{C}_{\nu,\rho}$ follow from the intertwining requirements:[21]

$$\hat{\pi}_{\nu,\rho}\circ\hat{A}_{\nu,\rho}=\hat{A}_{\nu,\rho}\circ\pi_{\nu,\rho},\quad \pi_{\nu,\rho}\circ\hat{A}^{-1}_{\nu,\rho}=\hat{A}^{-1}_{\nu,\rho}\circ\hat{\pi}_{\nu,\rho}. \tag{5.46}$$

In particular, the representation action of $\hat{\pi}_{\nu,\rho}$ on η^{ℓ} is given by the same formulas as the action of $\pi_{\nu,\rho}$ on v_{ℓ}.

At this moment, we should note that since we have functions of one variable η we can treat it as complex variable z. In these terms we recover from the action of $\hat{\pi}_{\nu,\rho}$ the classical vector-field representation of gl(2) (with $\partial_z\equiv d/dz$):

$$\tilde{A}\hat{\varphi}=-\rho\hat{\varphi},\quad \tilde{B}\hat{\varphi}=(\nu-2z\partial_z)\hat{\varphi},\quad X^{+}\hat{\varphi}=\partial_z\hat{\varphi},\quad X^{-}\hat{\varphi}=(\nu z-z^2\partial_z)\hat{\varphi}. \tag{5.47}$$

Of course, the importance of the nontrivial co-product for $X^{\pm}$ will be felt in the construction of the tensor products of the representations.

VI. CONCLUSIONS AND OUTLOOK

In this article we have found the exotic matrix bialgebras which correspond to the two nontriangular nonsingular 4×4 R-matrices of Ref. 8, namely, $R_{S0,3}$ and $R_{S1,4}$, which are not deformations of the trivial R-matrix. We study three bialgebras denoted by $S03$, $S14$, $S14o$, the latter two cases corresponding to $R_{S1,4}$ for deformation parameter $q^2\neq1$ and $q^2=1$, respectively. We have found the corresponding dual bialgebras $s03$, $s14$, $s14o$, and studied their representation theory.

For the bialgebras $s03$ and $s14$ we have studied the regular representation (the algebra acting on itself), the weight representations, and the representations in which the algebra acts on the dual matrix bialgebra. The representation theory is degenerate: the irreps are finite-dimensional of maximal dimension 4 and 2 for $s03$ and $s14$, respectively. For future use we shall say that the bialgebras $s03$, $S03$ and $s14$, $S14$ are *exotic* (adding to the list of exotic bialgebras termed so in Ref. 9).

The algebras $s14o$, $S14o$ turned out to be Hopf algebras and to be special cases of the two-parameter deformations $\mathcal{U}_{p,q}$, $\mathrm{GL}_{p,q}(2)$, namely, they would be obtained from the latter by setting $q=p^{-1}$ and then $p=-1$. This was not anticipated since the corresponding R-matrices were different and seemingly nonequivalent cases of the classification of Ref. 8. Thus, this became a case study important methodologically, and so we have made the exposition according to the way we proceeded. In fact, the algebra $s14o$ is equivalent even to U(gl(2)), and the only nontriviality is in the Hopf algebra structure. Thus, the regular and weight representations are as those of U(gl(2)). The induced representations of $s14o$ on $S14o$ could also be extracted from the equivalence with the two-parameter p, q deformations, but their consideration is also important methodologically.

To conclude, we should stress that with this article we finalize the explicit classification of the matrix bialgebras generated by four elements. There are altogether *nine* such bialgebras, four of which are quantum groups and are deformations of the classical algebras of functions on GL(2) and GL(1|1) (two in each case), and the other five bialgebras, which we call exotic, are not such deformations.

Further, we would like to study the spectral decomposition and Baxterization of these exotic algebras and associated noncommutative geometries, cf. Ref. 22.

Note added in proof: Note that the four-dimensional representation of Sec. III D, formula (3.27), actually reduces to a two-dimensional one, since $\tilde{C}v_0=-\lambda\tilde{B}v_0$.

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Geometric coupling thresholds in a two-dimensional strip

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We consider the Laplacian in a strip $\mathbb{R}\times(0,d)$ with the boundary condition which is Dirichlet except at the segment of a length $2a$ of one of the boundaries where it is switched to Neumann. This operator is known to have a non-empty and simple discrete spectrum for any $a>0$. There is a sequence $0<a_1<a_2<\cdots$ of critical values at which new eigenvalues emerge from the continuum when the Neumann window expands. We find the asymptotic behavior of these eigenvalues around the thresholds showing that the gap is in the leading order proportional to $(a-a_n)^2$ with an explicit coefficient expressed in terms of the corresponding threshold-energy resonance eigenfunction. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Spectra of Dirichlet Laplacians in infinitely stretched regions such as planar strips or layers with local perturbations were studied recently in numerous papers. The motivation for this work came from applications in condensed matter physics, and also from the fact that it was itself an interesting mathematical problem.

One of the simplest systems of this type is a free quantum particle confined to a pair of straight parallel strips with Dirichlet boundary conditions coupled laterally by a window in the common boundary. If they are of the same width d, one can employ the mirror symmetry and concentrate on the nontrivial part which is equivalent to the analysis of the Laplacian in a single strip with the Dirichlet boundary condition switched to Neumann at a finite segment of one of the boundaries.

Such a system has at least one bound state for any ''window'' length $2a>0$ as it was found in Ref. 1 and independently in Ref. 2. The discrete spectrum is simple, the eigenvalues $\lambda_n, n=0,1,\ldots,$ are continuously decreasing as functions of a and their number is linear in a up to an error term as the window is widening.[1] These properties follow from a simple bracketing argument which allows to squeeze the eigenvalues between those of a box covering the ''coupled'' part with Dirichlet and Neumann conditions at $x_1=\pm a$. It shows, in particular, that there are critical values a_n, $n=0,1,\ldots,$ at which new eigenvalues emerge from the continuum. By Refs. 1 and 2 we have $a_0=0$ while generally we know only that

$$a_n\in\left(\frac{nd}{\sqrt{3}},\frac{(n+1)d}{\sqrt{3}}\right),\quad n=1,2,\ldots\ . \tag{1.1}$$

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This tells us nothing about the behavior of the eigenvalues around the critical points.

The weak coupling asymptotics was studied for the ground state. A variational method of Ref. 3 yields for small a a two-sided estimate of $\lambda_0(a)$ between two multiples of a^4. This is indeed the leading term: using the matching method of Refs. 4 and 5 Popov derived in Ref. 6 the expansion

$$\lambda_0(a)=\left(\frac{\pi}{d}\right)^2-\left(\frac{\pi^3}{2d^3}\right)^2 a^4+\mathcal{O}(a^5). \tag{1.2}$$

While his argument is not fully rigorous because an estimate of the error term is missing, the formula itself raises no doubts, in particular, because of its excellent agreement with the numerical result of Ref. 1. The result is subtle: recall that (1.2) differs substantially from the asymptotics corresponding to a local change in *mixed* boundary conditions, where the Birman–Schwinger technique is applicable and the leading term is a multiple of the window width *squared*.[7]

In the present paper we address the question about the behavior of the higher eigenvalues λ_n, $n=1,2,\ldots$, in the vicinity of the critical points a_n. It is a natural counterpart of the coupling constant threshold problem of Ref. 8. Our main result is that the gap between an eigenvalue λ_n and the continuum is proportional to $(a-a_n)^2$ with a coefficient given explicitly in terms of the corresponding threshold-energy resonance eigenfunction. This fits well into the analogy between our problem and spectral properties of one-dimensional Schrödinger operators. The latter extends to higher dimensions, but the argument becomes more complicated and we leave that to another paper.

To finish the introduction, let us say something about the method. We deal with a perturbative problem with respect to the parameter ε defined as the excess of the window halfwidth a over the critical value a_n. Since the latter is positive for $n\geqslant 1$, the problem in question is a regular one. This fact makes it possible to map the problem into an equivalent one with a small and local perturbation of the equation and the boundary condition fixed, i.e., independent of ε. This is what we are going to do. We employ the technique introduced in Ref. 9 for calculations of the eigenfunctions for one-dimensional perturbed Schrödinger operator; its advantage is that we arrive at the sought asymptotic formula in a straightforward and reasonably simple way.

II. THE MAIN RESULT

To formulate the result we need first to introduce some notation and recall a few simple facts about the problem in question. We employ Cartesian coordinates, $x=(x_1,x_2)$, in which $\Sigma=\{x:0<x_2<d\}$. The upper strip boundary is $\Gamma=\{x:x_2=d\}$, while the lower decomposes into the union of $\gamma^a=\{x:|x_1|<a,x_2=0\}$ and $\Gamma^a=\{x:|x_1|>a,x_2=0\}$. The operator H_a we are going to consider is the Laplacian, $H_a\psi=-\Delta\psi$, in $L^2(\Sigma)$ with the Dirichlet boundary condition on $\Gamma^a\cup\Gamma$ and Neumann on γ^a; it is a well-defined self-adjoint operator, cf. Ref. 10, Chap. 7.[11]

Proposition 2.1: The discrete part of $\sigma(H_a)$ is simple and the eigenvalues $\lambda_n(a):(\pi/2d)^2<\lambda_0(a)<\lambda_1(a)<\cdots<(\pi/d)^2$ are continuous and monotonously decreasing with respect to a. There are numbers $0=a_0<a_1<a_2<\cdots$ satisfying (1.1) such that (a) for $a\in(a_{n-1},a_n]$ the operator H_a has exactly n eigenvalues, (b) for $a>a_n$ we denote $\varepsilon:=a-a_n$, then the eigenfunction $\psi_n^{(\varepsilon)}$ associated with $\lambda_n(a)$ has a definite parity with respect to x_1, namely

$$\psi_n^{(\varepsilon)}(-x_1,x_2)=(-1)^n\psi_n^{(\varepsilon)}(x_1,x_2),$$

(c) for $a=a_n$ the equation $-\Delta\psi=(\pi/d)^2\psi$ with given boundary conditions has a solution $\psi_n^{(0)}\in H^1_{\mathrm{loc}}(\Sigma)$, unique up to a multiplicative constant, which behaves like

$$\psi_n^{(0)}(x)=c_1(\pm 1)^n\sin\left(\frac{\pi x_2}{d}\right)+\mathcal{O}(\mathrm{e}^{-\delta|x_1|}) \tag{2.1}$$

as $x_1\to\pm\infty$, where $\delta:=\pi\sqrt{3}/d$ (in what follows we set $c_1:=\sqrt{2/\pi}$ for the sake of definiteness).

Proof: Most part was demonstrated in Ref. 1, it remains to check the claim (c). Any solution can be expanded in terms of the transverse eigenfunction bases

$$\chi_j(x_2) := \sqrt{\frac{2}{d}}\sin\left(\frac{\pi j x_2}{d}\right),$$

$$\phi_j(x_2) := \sqrt{\frac{2}{d}}\sin\left(\frac{\pi(2j-1)(d-x_2)}{d}\right)$$

with $j=1,2,\ldots$. Since the problem has a mirror symmetry with respect to $x_1=0$, it is sufficient to discuss the halfstrip part, $x_1\geq 0$, with the appropriate boundary condition at $x_1=0$. Let us consider the even case. A solution of energy $\epsilon(\pi/d)^2$ expresses as

$$\begin{aligned}\psi(x) &= \sum_{j=1}^{\infty} c_j e^{q_j(a-x_1)}\chi_j(x_2),\\ \psi(x) &= \sum_{j=1}^{\infty} b_j \frac{\cosh(p_j x_1)}{\cosh(p_j a)}\phi_j(x_2)\end{aligned} \tag{2.2}$$

for $|x_1|\geq a$ and $|x_1|\leq a$, respectively, where $q_j := (\pi/d)\sqrt{j^2-\epsilon}$ and $p_j := (\pi/d)\sqrt{(j-\frac{1}{2})^2-\epsilon}$. The coefficients in the above relation are determined by the requirement of smoothness of ψ at the segment $x_1=a$; we have

$$\begin{aligned}c_j &= \sum_{k=1}^{\infty} b_k(\chi_j,\phi_k),\\ (\chi_j,\phi_k) &= \frac{(-1)^{j-k}}{\pi}\frac{2j}{j^2-(k-\frac{1}{2})^2},\end{aligned} \tag{2.3}$$

and $b=\{b_j\}$ is given as solution of an infinite system of equations which can be written concisely in the operator form

$$Cb=0 \tag{2.4}$$

with

$$C_{jk} := [q_j + p_k\tanh(p_k a)](\chi_j,\phi_k).$$

The odd case is similar, just cosh and tanh are replaced by sinh and coth, respectively. The allowed values of ϵ are those for which a solution to the system (2.4) exists.

We know from Ref. 1 that the sequence corresponding to an isolated eigenvalue of H_a, i.e., $\epsilon\in(1/4,1)$, belongs to $\ell^2(j^{-r})$ for any $r\geq 1$, and that $C=C(a,\epsilon)$ is Hilbert–Schmidt on $\ell^2(j^{-r})$ with r large enough independently of a and ϵ. Choosing such an r it is straightforward to check that $(a,\epsilon)\mapsto C(a,\epsilon)$ is jointly continuous in the corresponding Hilbert–Schmidt norm. Take $a>a_n$ and $\epsilon_n(a) := (d/\pi)^2\lambda_n(a)$, clearly $\epsilon_n(a)\to 1$ as $a\to a_n+$. The said continuity implies that the equation (2.4) has for $C(a_n,1)$ a unique solution in $\ell^2(j^{-r})$, and by (2.3) it determines a sequence $b\in\ell^2(j^{-r})$. Together they yield the sought threshold resonance solution for $a=a_n$ with the asymptotics (2.1) following from the first one of the relations (2.2). ■

Remark 2.2: The function $\psi_n^{(0)}$ described in Proposition 2.1 has the following smoothness properties. It is infinitely differentiable everywhere in $\overline{\Sigma}$ except the endpoints of the segment γ^{a_n}. At these points the asymptotic formula

$$\psi_n^{(0)}(x)=(\pm 1)^n \alpha_n r_\pm^{1/2} \sin\frac{\theta_\pm}{2}+\mathcal{O}(r_\pm), \quad r_\pm\to 0, \tag{2.5}$$

is valid, where $(r_\pm,\theta_\pm)$ are polar coordinates associated with the variables $(\pm x_1-a_n,x_2)$ and α_n is a some number (a unique one provided we fix c_1). These asymptotics formulas can be verified in two easy steps. First, one should extend the function $\psi_n^{(0)}$ to the mirrored strip $\{x:-d<x_2<0\}$ in the even way. This leads to solution of the equation $-\Delta\psi_n^{(0)}=(\pi/d)^2\psi_n^{(0)}$ in the double strip $\{x:|x_2|<d\}\backslash\{x:|x_1|>a,x_2=0\}$ with the Dirichlet boundary condition at the outer boundary and at the cut $\{x:|x_1|>a,x_2=\pm 0\}$, and it is sufficient to employ the results established in Ref. 12 for such elliptic problems.

Now we can state our main result:

Theorem 2.3: *The eigenvalue $\lambda_n(a)$ of H_a with $n\geqslant 1$ has the following asymptotic behavior,*

$$\lambda_n(a)=\left(\frac{\pi}{d}\right)^2-\mu_n^2(a-a_n)^2+\mathcal{O}((a-a_n)^3) \tag{2.6}$$

as $a\to a_n+$, where the coefficient is given by

$$\mu_n:=\frac{1}{a_n}\int_\Sigma\left|\frac{\partial\psi_n^{(0)}}{\partial x_1}\right|^2 dx_1\,dx_2, \tag{2.7}$$

or alternatively by

$$\mu_n:=\frac{\pi\alpha_n^2}{4}, \tag{2.8}$$

where α_n is the number appearing in (2.5). The associated eigenfunction $\psi_n^{(\varepsilon)}$ can be normalized in such a way that it satisfies the relation

$$\psi_n^{(\varepsilon)}=\psi_n^{(0)}+\mathcal{O}(\varepsilon), \tag{2.9}$$

in $H^1((-R,R)\times(0,d))$ for any $R>0$ behaving asymptotically as

$$\psi_n^{(\varepsilon)}(x)=c_1(\pm 1)^n e^{-\varepsilon\mu_n|x_1|}\sin\left(\frac{\pi x_2}{d}\right)+\mathcal{O}(\mathrm{e}^{-\delta|x_1|}) \tag{2.10}$$

when $x_1\to\pm\infty$, with δ defined in Proposition 2.1.

Remark 2.4: The function $\psi_n^{(\varepsilon)}$ belongs, of course, to $L^2(\Sigma)$, but it does not have a limit in this space as $\varepsilon\to 0+$ since the norm $\|\psi_n^{(\varepsilon)}\|_{L^2(\Sigma)}$ explodes in the limit. Furthermore, α_n is nonzero for any $n\geqslant 1$. This fact can be easily deduced from the assertion (2.7). Indeed, the assumption $\alpha_n=0$ implies immediately that $\psi_n^{(0)}$ is independent on x_1. However, this contradicts to the boundary value problems that $\psi_n^{(0)}$ satisfies to. The coefficient α_n being nonzero, the formula (2.8) shows that the asymptotics of each λ_n is nontrivial in the leading order.

III. PROOF OF THEOREM 2.2

The rest of the paper is devoted to the proof of Theorem 2.3. With the scaling behavior of the spectrum in mind we can put $d=\pi$ without loss of generality in the following. Furthermore, the mirror symmetry with respect to $x_1=0$ makes it possible to consider the half-strip problem with the Dirichlet or Neumann condition at the cut.

We need to introduce some notations. Let $\mathbb{R}^2_+=\{x:x_1>0\}$ be the open right half-plane. As indicated above, we will work in the half-strip $\Pi:=\Sigma\cap\mathbb{R}^2_+$, similarly we introduce γ_ε

$:=\gamma^{a_n+\varepsilon}\cap\mathbb{R}^2_+$, $\Gamma_+:=\Gamma\cap\mathbb{R}^2_+$, and $\Gamma_\varepsilon:=\Gamma^{a_n+\varepsilon}\cap\mathbb{R}^2_+$. Moreover, we need a symbol for the cut at the symmetry axis, $\gamma:=\{x:x_1=0,\ 0<x_2<\pi\}$. Since we consider a fixed eigenvalue, we shall omit the index n when there is no danger of misunderstanding.

Let us outline the strategy of the proof. In the first step we are going to analyze the problem

$$\begin{gathered}(\Delta+1)u=m^2u+f,\quad x\in\Pi,\\ l_xu=0,\quad x\in\gamma,\\ u=0,\quad x\in\Gamma_0\cup\Gamma_+,\\ \frac{\partial u}{\partial x_2}=0,\quad x\in\gamma_0,\end{gathered}\tag{3.1}$$

with a fixed function f at the right-hand side of the equation. The trace operator l_x in the boundary conditions is defined as $(l_xu)(x_1,x_2)=u(0,x_2)$ if n is odd and $(l_xu)(x_1,x_2)=(\partial u/\partial x_1)(0,x_2)$ if n is even. The parameter m is assumed to be complex and to lie in a (sufficiently small) neighborhood of zero (we indicate this neighborhood by $\mathcal{D}$). We also suppose that f is an arbitrary function from $L^2(\Pi)$ with a compact support. We will construct a solution of the problem (3.1), meromorphic with respect to m, with the following asymptotic behavior far from the cut of the half-strip:

$$u(x,m)=c(m)e^{-mx_1}\sin x_2+\mathcal{O}(e^{-\sqrt{3+m^2}x_1}),\quad x_1\to+\infty,\tag{3.2}$$

where $c(m)$ is a constant determined by the function f. In the second step we will transform the original boundary value problem for the eigenfunction $\psi^{(\varepsilon)}$ to another one with an equation the coefficients of which depend smoothly on ε and the boundary condition is independent of ε. What is important is that the reformulated problem will be of the form (3.1) with a particular right-hand side $f=f_\varepsilon$ for which we deduce a sufficient explicit representation. Combining the latter with properties of the solution to (3.1) will finally obtain the announced results concerning λ_ε and $\psi^{(\varepsilon)}$. Since the proof of Theorem 2.3 divides in this way naturally into two steps, we shall discuss them separately in the following two sections.

A. Solution of the problem (3.1)

As we have indicated our aim is to construct a solution of (3.1) which is meromorphic in $m\in\mathcal{D}$. Let us say more explicitly what we mean by that. It is easy to see that there is a unique solution for $m\in\mathcal{D}\cap\{m:\mathrm{Re}\,m>0\}$ which decays as $x_1\to\infty$. We shall check that as a function of m it is analytic in $\mathcal{D}\cap\{m:\mathrm{Re}\,m>0\}$ and extend it to the remaining part of $\mathcal{D}$. The extension will be for $\mathrm{Re}\,m<0$ again a solution to (3.1) with the asymptotics (3.2), and in addition, it will be meromorphic in $m\in\mathcal{D}$ with just one simple pole at $m=0$. Of course, the extension will be bounded at large distances if $\mathrm{Re}\,m=0$ and will be increasing for $\mathrm{Re}\,m<0$. Speaking about solutions everywhere in the following we mean always such analytic continuations.

Recall that a function F with values in some Banach space X is said to be holomorphic in $\mathcal{D}$ if it is differentiable (in the sense of the norm of X) at each point $m\in\mathcal{D}$. If this function is holomorphic in $\mathcal{D}$ everywhere except a discrete set of points which are poles of F, i.e., Laurent's series of F at such a point has at most a finite number of negative terms, then F is said to be meromorphic.

We introduce some notations. Let $\mathcal{L}(X,Y)$ be the Banach space of bounded linear operators from a Banach space X into a Banach space Y. We will use the symbol $\mathcal{H}(X)$ for the class of functions with values in X which are holomorphic with respect to $m\in\mathcal{D}$, and $\mathcal{M}(X)$ for the class of meromorphic on $m\in\mathcal{D}$ functions with values in X. For the sake of brevity we also introduce the notations $\mathcal{H}(X,Y):=\mathcal{H}(\mathcal{L}(X,Y))$, $\mathcal{M}(X,Y):=\mathcal{M}(\mathcal{L}(X,Y))$.

We will treat the problem (3.1) by the technique introduced in Ref. 13, Sec. XVI.4. Let R be a fixed number larger than a_n, $\Pi_R := \Pi \cap \{x : x_1 < R\}$, and g a function from $L^2(\Pi_R)$ which can be also regarded as an element of $L^2(\Pi)$ if we set it equal to zero for $x_1 > R$. The problem

$$(\Delta + 1)v = m^2 v + g, \quad x \in \Pi, \quad v = 0, \quad x \in \partial\Pi, \tag{3.3}$$

can be easily solved by separation of variables, the solution being

$$\begin{gathered} v(x,m) = -\sum_{k=1}^{\infty} \frac{1}{\pi M_k} \int_{\Pi} G_k(x,t,m) g(t) d^2 t, \\ G_k(x,t,m) = (e^{-M_k|x_1 - t_1|} - e^{-M_k(x_1 + t_1)}) \sin kt_2 \sin kx_2, \end{gathered} \tag{3.4}$$

where $M_1 = m$ and $M_k = \sqrt{k^2 - 1 + m^2}$ for $k \geqslant 2$. For the sake of brevity we use the notation $d^2 t = dt_1\, dt_2$. Obviously, the formula (3.4) is valid for all $m \in \mathcal{D}$, not only for $\operatorname{Re} m > 0$. The function v can be represented as $v = T_1(m) g$, where $T_1(m) : L^2(\Pi_R) \to H^2(\Pi_{\tilde{R}})$ is a bounded linear operator for any positive $\tilde{R}$. It is straightforward to check that $v \in \mathcal{H}(H^2(\Pi_{\tilde{R}}))$ and $T_1(\cdot) \in \mathcal{H}(L^2(\Pi_R), H^2(\Pi_{\tilde{R}}))$ in $\mathcal{D}$ for any positive $\tilde{R}$.

In the next step we consider another boundary value problem for an unknown function w, namely

$$\begin{gathered} \Delta w = \Delta v, \quad x \in \Pi_R, \\ w = 0, \quad x \in (\Gamma_+ \cup \Gamma_0) \cap \partial\Pi_R, \\ w = v, \quad x_1 = R, \\ \frac{\partial w}{\partial x_2} = 0, \quad x \in \gamma_0, \\ l_x w = 0, \quad x \in \gamma. \end{gathered} \tag{3.5}$$

Since $v \in H^2(\Pi_R)$ we have $\Delta v \in L^2(\Pi_R)$, and thus the problem (3.5) has a unique solution $w \in H^1(\Pi_R)$, see, e.g., Ref. 14, Sec. 2.5, Rem. 5.1. Using the standard theorem on smoothness of solutions of elliptic boundary value problems we can conclude that $w \in H^2(\Pi_{R,s})$ holds for each $s > 0$, where $\Pi_{R,s} := \Pi_R \setminus D_s$ with $D_s := \{x : x_2 > 0, (x_1 - a_n)^2 + x_2^2 < s^2\}$. Hence we can define the linear operator T_2 by $w =: T_2 v$ which is a linear bounded map from $H^2(\Pi_R)$ into $H^1(\Pi_R)$, and from $H^2(\Pi_R)$ into $H^2(\Pi_{R,s})$ for each fixed s.

Let $\chi_R(x_1)$ be an infinitely differentiable mollifier function equal to one for $x_1 \leqslant R - 1$ and vanishing for $x_1 \geqslant R$. We take the two functions considered above and construct u as a smooth interpolation between them,

$$u(x,m) := \chi_R(x_1) w(x,m) + (1 - \chi_R(x_1)) v(x,m). \tag{3.6}$$

Since $w(x,m) = T_2 T_1(m) g$, we have $w \in \mathcal{H}(H^1(\Pi_R)) \cap \mathcal{H}(H^2(\Pi_{R,s}))$ as a function of m for each $s > 0$. Thus we can introduce the operator $T_3(m)$ which maps a function $g \in L^2(\Pi_R)$ to the function u determined by (3.6), where v and w are the solutions of (3.3) and (3.5), respectively, for this g. It easy to see that $T_3(\cdot) \in \mathcal{H}(L^2(\Pi_R), H^1(\Pi_{\tilde{R}}))$ and $T_3(\cdot) \in \mathcal{H}(L^2(\Pi_R), H^2(\Pi_{\tilde{R},s}))$ in $\mathcal{D}$ for any pair of positive $\tilde{R}$, s.

According to the definition of v and w, the function u satisfies all the boundary condition of (3.1). Applying the operator $(\Delta + 1 - m^2)$ to this function, we obtain

$$(\Delta + 1 - m^2) u = g + (w - v)(\Delta + 1 - m^2)\chi_R + 2(\nabla_x \chi_R, \nabla_x (w - v))_{\mathbb{R}^2},$$

where we have used in the calculation the equations which v and w satisfy. This result shows that the function u solves the problem (3.1) if and only if g satisfies the following equation:

$$g+T_4(m)g=f, \tag{3.7}$$

where

$$T_4(m)g:=(w-v)(\Delta+1-m^2)\chi_R+2(\nabla_x\chi_R,\nabla_x(w-v))_{\mathbb{R}^2};$$

recall that both w and v are obtained from g by actions of the operators specified above.

Proposition 3.1: The operator $T_4(m)$ is compact for any $R>0$ as an element of $\mathcal{L}(L^2(\Pi_R),L^2(\Pi_R))$ and the function $m\mapsto T_4(m)$ belongs to $\mathcal{H}(L^2(\Pi_R),L^2(\Pi_R))$ in $\mathcal{D}$.

Proof: We denote

$$T_{41}(m)g:=(w-v)(\Delta+1-m^2)\chi_R,$$

$$T_{42}(m)g:=2(\nabla_x\chi_R,\nabla_x(w-v))_{\mathbb{R}^2}+(w-v)\Delta\chi_R.$$

Using the described properties of $T_1(m)$ and T_2 it is easy to see that $T_{41}(m)$ is a bounded linear map from $L^2(\Pi_R)$ into $H^1(\Pi_R)$. The operator-valued function $T_{41}(\cdot)$ belongs to $\mathcal{H}(L^2(\Pi_R),H^1(\Pi_R))$. The function χ_R' is smooth and its support lies in $\Pi_R\backslash\overline{\Pi}_{R-1}$. Using this together with the fact that the function $w-v$ belongs to $H^2(\Pi_R\backslash\overline{\Pi}_{R-1})$, we conclude that $T_{42}(m):L^2(\Pi_R)\to H^1(\Pi_R)$ is a linear bounded operator belonging to $\mathcal{H}(L^2(\Pi_R),H^1(\Pi_R))$ as a function of m. Hence $T_4(\cdot)=T_{41}(\cdot)+T_{42}(\cdot)\in\mathcal{H}(L^2(\Pi_R),H^1(\Pi_R))$, and therefore $T_4(m)$ is compact when considered as an operator from $L^2(\Pi_R)$ to $L^2(\Pi_R)$, belonging to $\mathcal{H}(L^2(\Pi_R),L^2(\Pi_R))$ with respect to m. ■

Proposition 3.1 shows that Eq. (3.7) can be studied using Fredholm theorems. This will help us to solve our original problem: to construct the solution of (3.1) we have to solve the equation (3.7), then by the procedure described above its solution gives rise to the solution u of the boundary value problem (3.1): $u=T_3(m)g$.

Proposition 3.2: The problems (3.7) and (3.1) are equivalent: to each solution g of (3.7) there is a unique solution $u=T_3(m)g$ of (3.1), and vice versa, for each solution of (3.1) there exists a unique g solving (3.7) such that $u=T_3(m)g$. The equivalence holds for any $m\in\mathcal{D}$.

Proof: The first part has been proved above, it remains to check invertibility of the operator T_3. Let u be a solution of the problem (3.1). Notice that the function u is infinitely differentiable outside the support of f since there it is a solution of a homogeneous equation. We have to construct the solution g of (3.7) such that $u=T_3g$. Let us first determine the functions v and w. By U we denote a solution of the following problem:

$$\begin{aligned}&\Delta U=0, \quad x\in\Pi_R,\\ &U=0, \quad x\in\partial\Pi_R\backslash\overline{\gamma_0\cup\gamma},\\ &U=u, \quad x\in\gamma_0\cup\gamma,\end{aligned} \tag{3.8}$$

which is unique in $H^1(\Pi_R)$, and moreover, it belongs to $C^\infty(\Pi_R)$ by a standard result on the smoothness of solutions of elliptic equations. We set

$$v(x,m):=u(x,m)-\chi_R(x_1)U(x,m),$$

$$w(x,m):=u(x,m)+(1-\chi_R(x_1))U(x,m).$$

One checks easily that the functions $u=\chi_Rw+(1-\chi_R)v$, w and v satisfy all the required boundary conditions and that $\Delta w=\Delta v$ holds in Π_R. Now it suffices to use the equation of the problem (3.3) to determine the function g by

$$g(x,m) := (\Delta + 1 - m^2)v(x,m) = (\Delta + 1 - m^2)(u(x,m) - \chi_R(x_1)U(x,m))$$
$$= f(x) - (\Delta + 1 - m^2)(\chi_R(x_1)U(x,m)).$$

Let us check that this g solves (3.7). Using the definition of U, v, and w, we compute directly the action of $T_4(m)$ on g obtaining

$$T_4(m)g = U(\Delta + 1 - m^2)\chi_R + 2(\nabla_x \chi_R, \nabla_x U)$$
$$= U(\Delta + 1 - m^2)\chi_R + 2(\nabla_x \chi_R, \nabla_x U) + \chi_R \Delta U = (\Delta + 1 - m^2)(\chi_R U).$$

The last two relations show that g is a solution of Eq. (3.7). Let us check the uniqueness: suppose that there are two solutions g_1 and g_2 of (3.7) leading to the same function $u^{(1)} = u^{(2)}$. Then $g := g_1 - g_2 \neq 0$ gives rise to $u := u^{(1)} - u^{(2)} = 0$. Let v and w be the solutions of (3.3) and (3.5), respectively, associated with u, and set $U := w - v$. Then it easy to see that this U solves (3.8), where the boundary condition on $\gamma_0 \cup \gamma$ is homogeneous. Such a solution of (3.8) is unique, $U = 0$. Thus $w = v = u = 0$ holds in Π_R, and therefore $g = (\Delta + 1 - m^2)v = 0$ in Π_R, which is a contradiction. ■

The solution of Eq. (3.7) depends on m, i.e., $g = g(x,m)$. Our next aim is to clarify a nature of this dependence and to look what this implies for the solution of the problem (3.1). We employ the following result borrowed from Ref. 13, Sec. XV.7:

Theorem 3.3: *Let $\mathcal{D}$ be an open connected domain of the complex plane of the variable m and $\{T(m): m \in \mathcal{D}\}$ be a bounded holomorphic family of compact operators from the Banach space X into itself. Moreover, assume that there exists a point $m_* \in D$ such that $(I + T(m_*))^{-1} \in \mathcal{L}(X,X)$. Then $m \mapsto (I + T(m))^{-1}$ is a meromorphic function in $\mathcal{D}$ with values in $\mathcal{L}(X,X)$.*

In our case the Banach space mentioned in Theorem 3.3 is $L^2(\Pi_R)$ and $T(m) = T_4(m)$. The existence of m_* is easy to establish: since the equation (3.7) is equivalent to the boundary-value problem (3.1) by Proposition 3.2, it is sufficient to prove the existence of m_* for which the problem (3.1) has no nontrivial solution for $f = 0$ and $m = m_*$ with the asymptotics (3.2). This is true for $m_* > 0$ which is sufficiently small, because assuming the contrary would lead us to the conclusion that H_{a_n} has the eigenvalue $(1 - m_*^2)$, and this in turn would contradict to the claims (a) and (c) of Proposition 2.1. The compactness of $T_4(m)$ and its holomorphic dependence on m follow from Proposition 3.1.

Thus we may apply Theorem 3.3 to the equation (3.7). We imply that $(I + T_4(m))^{-1}$ exists and it is meromorphic as an operator-valued function in $\mathcal{D}$, $(I + T_4(\cdot))^{-1} \in \mathcal{M}(L^2(\Pi_R), L^2(\Pi_R))$. Poles of this function are the values of m for which the equation (3.7) with the vanishing right-hand side has a nontrivial solution. The value $m_0 := 0$ has this property as it follows from the claim (c) of Proposition 2.1. Let ϕ_0 be a solution of the equation (3.7) for $f = 0$ and $m = m_0$. The function ϕ_0 is unique up to a multiplicative constant, the uniqueness being implied by Proposition 2.1(c) and Proposition 3.1. The remaining ambiguity is removed if we set $\psi^{(0)} = T_3(0)\phi_0$. Making the domain $\mathcal{D}$ smaller if necessary we can achieve that zero is the only pole of the function $(I + T_4(\cdot))^{-1}$ contained in $\mathcal{D}$. In such a case the solution $g = (I + T_4(m))^{-1}$ of the equation (3.7) can be for any nonzero $m \in \mathcal{D}$ represented as

$$g = g(m) = \frac{g_{-k}}{m^k} + \tilde{g}(m), \tag{3.9}$$

where the integer $k \geqslant 1$ is the order of the pole, the functions $g_{-k}, \tilde{g}(m)$ belong to $L^2(\Pi_R)$ for nonzero $m \in \mathcal{D}$, and $\tilde{g}(\cdot) \in \mathcal{M}(L^2(\Pi_R))$ may have a pole at zero of order not exceeding $k - 1$.

Let us stress that Theorem 3.3 says nothing about the order of this pole. Next we are going to prove that the pole in (3.9) is simple, i.e., $k = 1$. Substituting (3.9) into (3.7) and comparing the leading terms in m we see that $g_{-k} = K_0[f]\phi_0$, where $K_0[f]$ is a constant depending on f. The representation (3.9) in turn yields the following expression for u:

$$u = T_3(m)g = \frac{K_0[f]\psi^{(0)}}{m^k} + \tilde{u}(m). \tag{3.10}$$

Here $\tilde{u}(\cdot)$ is a function belonging to $\mathcal{M}(H^1(\Pi_{\tilde{R}})) \cap \mathcal{M}(H^2(\Pi_{\tilde{R},s}))$ for any positive $\tilde{R}$, s which again may have pole at zero of order not exceeding $k-1$. Multiplying the equation in the problem (3.1) by $\psi^{(0)}$ and integrating by parts we see that

$$\int_{\Pi_{\tilde{R}}} f\psi^{(0)}\, d^2x = -m^2 \int_{\Pi_{\tilde{R}}} \psi^{(0)} u\, d^2x + \int_0^\pi \left(\psi^{(0)} \frac{\partial u}{\partial x_1} - u \frac{\partial \psi^{(0)}}{\partial x_1} \right)\Bigg|_{x_1=\tilde{R}} dx_2. \tag{3.11}$$

For d sufficiently large we have

$$u|_{x_1=\tilde{R}} = \sum_{j=1}^{\infty} C_j(m) \sin jx_2, \quad \psi^{(0)}|_{x_1=\tilde{R}} = \sum_{j=1}^{\infty} c_j \sin jx_2,$$

$$\frac{\partial u}{\partial x_1}\bigg|_{x_1=\tilde{R}} = -\sum_{j=1}^{\infty} \sqrt{j^2-1+m^2}\, C_j(m) \sin jx_2,$$

$$\frac{\partial \psi^{(0)}}{\partial x_1}\bigg|_{x_1=\tilde{R}} = -\sum_{j=2}^{\infty} c_j \sqrt{j^2-1}\, \sin jx_2,$$

where the functions C_j in view of (3.10) behave as

$$C_j(m) = \frac{K_0[f]c_j}{m^k} + \mathcal{O}(m^{-k+1}).$$

Combining the above relations and using the normalization condition $c_1 = \sqrt{2/\pi}$ we deduce that

$$\int_0^\pi \left(\psi^{(0)} \frac{\partial u}{\partial x_1} - u \frac{\partial \psi^{(0)}}{\partial x_1} \right)\Bigg|_{x_1=\tilde{R}} dx_2 = -\frac{K_0[f]}{m^{k-1}} + \mathcal{O}(m^{-k+2}).$$

The first integral on the right-hand side of (3.11) behaves as

$$-m^2 \int_{\Pi_{\tilde{R}}} \psi^{(0)} u\, d^2x = -\frac{K_0[f]}{m^{k-2}} \int_{\Pi_{\tilde{R}}} |\psi^{(0)}|^2 d^2x + \mathcal{O}(m^{-k+3})$$

in the limit $m \to 0$. Substituting the expressions obtained above into (3.11) and comparing the coefficients at the powers of m, we conclude that $k=1$, and furthermore, that

$$K_0[f] = -\int_{\Pi_{\tilde{R}}} f\psi^{(0)}\, d^2x = -\int_{\Pi} f\psi^{(0)}\, d^2x. \tag{3.12}$$

To get the last relation we have used the fact that f has a compact support by assumption which therefore lies in $\Pi_{\tilde{R}}$ for $\tilde{R}$ sufficient large.

Next we denote $A(m) = T_3(m)(I + T_4(m))^{-1}$. It follows from the relations (3.10) and (3.12) that

$$\begin{aligned} u = A(m)f =: A_0(m)f + A_1(m)f = K_0[f]\frac{\psi^{(0)}}{m} + A_1(m)f, \\ A_1(\cdot) \in \mathcal{H}(L^2(\Pi_R), \mathcal{H}(H^1(\Pi_{\tilde{R}})) \cap \mathcal{H}(L^2(\Pi_R), H^2(\Pi_{\tilde{R},s})), \end{aligned} \tag{3.13}$$

where $\tilde{R}$ and s are arbitrary positive.

It is convenient to summarize all the conclusions made above in a single theorem which represents the main result of this subsection.

Theorem 3.4: *Let $f\in L^2(\Pi_R)$, and assume that $\tilde{R}$, s are arbitrary positive numbers, $m\in\mathcal{D}$. Then for $m\in\mathcal{D}\backslash\{0\}$ there exists a unique solution of the boundary value problem (3.1) given by $u=A(m)f$. As a function on m this solution belongs to $\mathcal{M}(H^1(\Pi_{\tilde{R}}))\cap\mathcal{M}(H^2(\Pi_{\tilde{R},s}))$. The neighborhood $\mathcal{D}$ can be chosen in such a way that the function $A(\cdot)\in\mathcal{M}(L^2(\Pi_R),H^1(\Pi_{\tilde{R}}))\cap\mathcal{M}(L^2(\Pi_R),H^2(\Pi_{\tilde{R},s}))$ has just one pole $m_0=0$ which is simple. The operator $A(m)$ can be decomposed into the sum $A(m)=A_0(m)+A_1(m)$, where the operators $A_i(m)$ are defined by (3.13). Finally, the relation (3.12) holds true.*

B. The asymptotic analysis

To find the behavior of the quantity $\lambda_n(a)$ around the threshold we will analyze m_ε defined as $m_\varepsilon^2:=1-\lambda_n(a_n+\varepsilon)$, which satisfies $m_\varepsilon\to 0$ as $\varepsilon\to 0$. Let $y=(y_1,y_2)$ be the Cartesian coordinates of a point in the strip. The boundary value problem for the eigenfunction $\psi^{(\varepsilon)}$ can be then written as

$$\begin{gathered}(\Delta_y+1)\psi^{(\varepsilon)}=m_\varepsilon^2\psi^{(\varepsilon)},\quad y\in\Pi,\\ l_y\psi^{(\varepsilon)}=0,\quad y\in\gamma,\\ \psi^{(\varepsilon)}=0,\quad y\in\Gamma_\varepsilon\cup\Gamma_+,\\ \frac{\partial\psi^{(\varepsilon)}}{\partial y_2}=0,\quad y\in\gamma_\varepsilon.\end{gathered}\tag{3.14}$$

As we have announced, we want to get rid of the ε-dependent boundary condition passing to one independent on ε, while the corresponding equation will have coefficients which depend smoothly on ε. To construct the appropriate transformation we use an infinitely differentiable mollifier function χ of the variable y_1 which is equal to one for $y_1\in[\beta_2,\beta_3]$ and vanishes for $y_1\leqslant\beta_1$ and $y_1\geqslant\beta_4$. Here β_i, $i=1,\ldots,4$, are positive constants, $\beta_1<\beta_2<\beta_3<\beta_4$, such that $\beta_2<a_n+\varepsilon<\beta_3$ holds for all ε from a fixed neighborhood of zero. We consider the function $x_1:\mathbb{R}_+\to\mathbb{R}_+$ defined as

$$x_1: x_1(y_1,\varepsilon)=y_1-\varepsilon\ \chi(y_1).$$

It is easy to see, in particular, that $x_1=a_n$ as $y_1=a_n+\varepsilon$. Taking the first two derivatives we get

$$\frac{dx_1}{dy_1}=1-\varepsilon\chi'(y_1),\quad \frac{d^2x_1}{dy_1^2}=-\varepsilon\chi''(y_1)$$

from where it follows that for all sufficiently small ε the first derivative of x_1, with respect to y_1, is nonzero everywhere in $\mathbb{R}_+$. Thus the map x_1 is bijective and can be used to define a change of the variable, $y_1\mapsto x_1(y_1,\varepsilon)$. The problem (3.14) expressed in the variables $x=(x_1,x_2)$, $x_2:=y_2$, becomes

$$\begin{gathered}(\Delta_x+\varepsilon L_\varepsilon+1)\psi^{(\varepsilon)}=m_\varepsilon^2\psi^{(\varepsilon)},\quad x\in\Pi,\\ l_x\psi^{(\varepsilon)}=0,\quad x\in\gamma,\\ \psi^{(\varepsilon)}=0,\quad x\in\Gamma_0\cup\Gamma_+,\end{gathered}\tag{3.15}$$

$$\frac{\partial\psi^{(\varepsilon)}}{\partial x_2}=0, \quad x\in\gamma_0.$$

The operator L_ε appearing in the transformed equation is defined by

$$L_\varepsilon := b_{11}(x_1,\varepsilon)\frac{\partial^2}{\partial x_1^2}+b_1(x_1,\varepsilon)\frac{\partial}{\partial x_1},$$

$$b_{11}(x_1,\varepsilon) := -2\chi'(y_1(x_1,\varepsilon))+\varepsilon(\chi'(y_1(x_1,\varepsilon)))^2, \tag{3.16}$$

$$b_1(x_1,\varepsilon) := -\chi''(y_1(x_1,\varepsilon)).$$

The functions b_{11} and b_1 are obviously infinitely differentiable, they vanish for $y_1\notin[\beta_1,\beta_2]\cup[\beta_3,\beta_4]$ and satisfy in the limit $\varepsilon\to 0$ the asymptotic formulas

$$b_{11}(x_1,\varepsilon)=-2\chi'(x_1)+\mathcal{O}(\varepsilon), \quad b_1(x_1,\varepsilon)=-\chi''(x_1)+\mathcal{O}(\varepsilon)$$

uniformly in the variable x_1.

Now we can proceed to the calculation of m_ε and $\psi^{(\varepsilon)}$. Proposition 2.1 ensures that the eigenfunction and eigenvalue exist. The function $\psi^{(\varepsilon)}$ decays as $|x_1|\to\infty$ and $\lambda_n(a_n+\varepsilon)$ is real. These two facts imply that m_ε is real and positive. It is obvious that $\psi^{(\varepsilon)}$ solves the problem (3.1) for $m=m_\varepsilon$ and $f=-\varepsilon L_\varepsilon\psi^{(\varepsilon)}$. This allows us to seek for the solution of (3.15) in the form

$$\psi^{(\varepsilon)}=A(m_\varepsilon)f_\varepsilon, \tag{3.17}$$

where the function f_ε is assumed to an unknown element of $L^2(\Pi_R)$ with $R>\beta_4$. This may appear strange at a glance, because we know that $f_\varepsilon=-\varepsilon L_\varepsilon\psi^{(\varepsilon)}$, however, we want to obtain another formula for f_ε not involving $\psi^{(\varepsilon)}$. The function $\psi^{(\varepsilon)}$ defined by (3.17) satisfies all the boundary condition of the problem (3.15). In order to be a solution of (3.15), it is necessary and sufficient for $\psi^{(\varepsilon)}$ to be a solution of the corresponding equation. Substituting into the latter the formula for $\psi^{(\varepsilon)}$, we arrive at the equation for f_ε which reads

$$(I+\varepsilon L_\varepsilon A(m_\varepsilon))f_\varepsilon=0. \tag{3.18}$$

In view of (3.13) we have

$$A(m_\varepsilon)f_\varepsilon=K_0[f_\varepsilon]\frac{\psi^{(0)}}{m_\varepsilon}+A_1(m_\varepsilon)f_\varepsilon. \tag{3.19}$$

We substitute this representation for $A(m_\varepsilon)f_\varepsilon$ into (3.18) obtaining

$$f_\varepsilon+\frac{\varepsilon}{m_\varepsilon}K_0[f_\varepsilon]L_\varepsilon\psi^{(0)}+\varepsilon L_\varepsilon A_1(m_\varepsilon)f_\varepsilon=0. \tag{3.20}$$

It is clear that $L_\varepsilon A_1(\cdot)\in\mathcal{H}(L^2(\Pi_R),L^2(\Pi_R))$ and as a function of (m,ε) the operator $L_\varepsilon A_1(m)$ is jointly continuous. Thus for sufficiently small ε the inverse operator $B(m,\varepsilon)=(I+\varepsilon L_\varepsilon A_1(m))^{-1}:L^2(\Pi_R)\to L^2(\Pi_R)$ exists and converges to the identity map as $\varepsilon\to 0$ uniformly in m. It is also obvious that $B(\cdot,\varepsilon)\in\mathcal{H}(L^2(\Pi_R),L^2(\Pi_R))$. Applying now $B(m_\varepsilon,\varepsilon)$ to the equation (3.20) we find

$$f_\varepsilon+\frac{\varepsilon}{m_\varepsilon}K_0[f_\varepsilon]B(m_\varepsilon,\varepsilon)L_\varepsilon\psi^{(0)}=0. \tag{3.21}$$

Applying further K_0 to (3.21), we get one more equation,

$$K_0[f_\varepsilon]+\frac{\varepsilon}{m_\varepsilon}K_0[f_\varepsilon]K_0[B(m_\varepsilon,\varepsilon)L_\varepsilon\psi^{(0)}]=0.$$

Notice that $K_0[f_\varepsilon]$ cannot be zero, because otherwise (3.21) would imply $f_\varepsilon=0$ which yields $\psi^{(\varepsilon)}=0$. The last equation induces the relation

$$m_\varepsilon=-\varepsilon K_0[B(m_\varepsilon,\varepsilon)L_\varepsilon\psi^{(0)}], \tag{3.22}$$

which can be regarded as an equation for m_ε. It is easy to see that $B(\cdot,\varepsilon)L_\varepsilon\psi^{(0)}\in\mathcal{H}(L^2(\Pi_R))$ and the function $(m,\varepsilon)\mapsto B(m,\varepsilon)L_\varepsilon\psi^{(0)}$ is jointly continuous. This immediately implies that $K_0[B(m,\varepsilon)L_\varepsilon\psi^{(0)}]$ is a holomorphic with respect to m and jointly continuous as a function of (m,ε). Consequently, for all ε small enough the estimate

$$\varepsilon|[K_0[B(m,\varepsilon)L_\varepsilon\psi^{(0)}]|<|\ m|,\quad m\in\partial\mathcal{D},$$

holds true. Using this inequality in combination with the Rouché theorem we conclude that the functions $h_1:h_1(m)=m$ and $h_2:h_2(m)=m+[K_0[B(m,\varepsilon)L_\varepsilon\psi^{(0)}]$ have the same numbers of zeroes inside $\mathcal{D}$. This means that the equation (3.22) has a unique solution in $\mathcal{D}$ for all sufficient small ε. On the other hand, due to Proposition 2.1 we know that there is a root of equation (3.22) that converges to zero, namely

$$m_\varepsilon=\sqrt{\lambda_n(a_n+\varepsilon)-1}>0.$$

Consequently, it is the only root of (3.22). Thus the function

$$f_\varepsilon=-\varepsilon B(m_\varepsilon,\varepsilon)L_\varepsilon\psi^{(0)}, \tag{3.23}$$

where m_ε is the solution of (3.22), solves the equation (3.18). It means that the function f_ε defined by (3.23) gives rise to the eigenfunction $\psi^{(\varepsilon)}=A(m_\varepsilon)f_\varepsilon$ corresponding to the eigenvalue $\lambda_n(a_n+\varepsilon)=1-m_\varepsilon^2$. In fact, we have also proved that there is just one value of $m=m_\varepsilon$ tending to zero as $\varepsilon\to0$, for which the boundary value problem (3.14) has a nontrivial solution. This solution decays as $|x_1|\to\infty$, i.e., there are no nondecaying or even increasing solutions.

The equation (3.22) allows us to calculate the asymptotic expansion for m_ε. Since $B(m,\varepsilon)L_\varepsilon\psi^{(0)}$ is holomorphic with respect to m and jointly continuous in (m,ε), and since m_ε tends to zero as $\varepsilon\to0$, then by the equation (3.22) we have

$$m_\varepsilon=\varepsilon\mu+O(\varepsilon m_\varepsilon),\quad \varepsilon\to0,$$

$$\mu=-K_0[L_0\psi^{(0)}],$$

$$L_0=-2\chi'(x_1)\frac{\partial^2}{\partial x_1^2}-\chi''(x_1)\frac{\partial}{\partial x_1}.$$

Combining these relations, we can rewrite the error term as follows:

$$m_\varepsilon=\varepsilon\mu+O(\varepsilon^2),\quad \varepsilon\to0. \tag{3.24}$$

Next we want to express the coefficient μ,

$$\mu=-\int_\Pi\psi^{(0)}\left(2\chi'(x_1)\frac{\partial^2}{\partial x_1^2}+\chi''(x_1)\frac{\partial}{\partial x_1}\right)\psi^{(0)}\,d^2x. \tag{3.25}$$

Using the equation which the function $\psi^{(0)}$ satisfies we find

$$\left(2\chi'(x_1)\frac{\partial^2}{\partial x_1^2}+\chi''(y_1)\frac{\partial}{\partial x_1}\right)\psi^{(0)}=(\Delta+1)\left(\chi(x_1)\frac{\partial\psi^{(0)}}{\partial x_1}\right).$$

Integrating then by parts and taking into account properties of $\psi^{(0)}$ together with the definition of the mollifier χ we have

$$\mu=-\lim_{s\to 0}\int_{\Pi\setminus D_s}\psi^{(0)}(\Delta+1)\left(\chi(x_1)\frac{\partial\psi^{(0)}}{\partial x_1}\right)d^2x=\lim_{s\to 0}\int_{\partial D_s}\left(\psi^{(0)}\frac{\partial^2\psi^{(0)}}{\partial r\,\partial x_1}-\frac{\partial\psi^{(0)}}{\partial x_1}\frac{\partial\psi^{(0)}}{\partial r}\right)ds.$$

In order to evaluate the last integral along ∂D_s we replace $\psi^{(0)}$ by its asymptotics (2.5) and pass to limit $s\to 0$ obtaining

$$\mu=\frac{1}{2}\alpha^2\int_0^\pi\sin^2\frac{\theta_+}{2}\,d\theta_+=\frac{\pi\alpha^2}{4},$$

which proves (2.8) with $\mu=\mu_n$. In the same way we get

$$0=\int_\Pi x_1\frac{\partial\psi_n^{(0)}}{\partial x_1}(\Delta+1)\psi_n^{(0)}d^2x=a_n\frac{\pi\alpha^2}{4}+2\int_\Pi\psi_n^{(0)}\frac{\partial^2\psi_n^{(0)}}{\partial x_1^2}d^2x=a_n\mu_n-2\int_\Pi\left|\frac{\partial\psi_n^{(0)}}{\partial x_1}\right|^2d^2x,$$

which yields the representation (2.7) for μ,

$$\mu_n=\frac{2}{a_n}\int_\Pi\left|\frac{\partial\psi_n^{(0)}}{\partial x_1}\right|^2d^2x=\frac{1}{a_n}\int_\Sigma\left|\frac{\partial\psi_n^{(0)}}{\partial x_1}\right|^2d^2x.$$

In the last relation we employed the fact that $\psi_n^{(0)}$ has a definite parity.

Let us finally pass to discussion of the eigenfunction. In view of (3.19), (3.23) we find that $\psi^{(\varepsilon)}$ is equal to

$$A(m_\varepsilon)f_\varepsilon=-\frac{\varepsilon K_0[B(m_\varepsilon,\varepsilon)L_\varepsilon\psi^{(0)}]}{m_\varepsilon}\psi^{(0)}-\varepsilon A_1(m_\varepsilon)B(m_\varepsilon,\varepsilon)L_\varepsilon\psi^{(0)}.$$

Using now the equation (3.22) together with the fact that the function $A_1(m)B(m,\varepsilon)L_\varepsilon\psi^{(0)}$ is holomorphic and continuous as a function of the respective variables, we conclude that the relation

$$\psi^{(\varepsilon)}=\psi^{(0)}-\varepsilon A_1(m_\varepsilon)B(m_\varepsilon,\varepsilon)L_\varepsilon\psi^{(0)}$$

is valid in $H^1(\Pi_R)$ for each R. This yields the relation (2.9) and the asymptotic behavior (2.10) concluding thus the proof of Theorem 2.3.

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Continuous spin representations of the Poincaré and super-Poincaré groups

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We construct Wigner's continuous spin representations of the Poincaré algebra for massless particles in higher dimensions. The states are labeled both by the length of a spacelike translation vector and the Dynkin indices of the *short little group* $\mathrm{SO}(d-3)$, where d is the space–time dimension. Continuous spin representations are in one-to-one correspondence with representations of the short little group. We also demonstrate how combinations of the bosonic and fermionic representations form supermultiplets of the super-Poincaré algebra. If the light-cone translations are nilpotent, these representations become finite dimensional, but contain zero or negative norm states, and their supersymmetry algebra contains a central charge in four and ten dimensions. © *2002 American Institute of Physics.*
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I. INTRODUCTION

The Poincaré group is an essential ingredient of relativistic quantum field theories. Its representations in four space–time dimensions were first studied by E. Wigner.[1] Some of its representations describe quantum states found in local field theory: massless particles of fixed helicity and massive particles with or without spin. In string theory, the ''front form'' construction of the Poincaré group generators[2,3] has been particularly useful in describing the 26-dimensional bosonic string.[4]

Other representations do not seem to be realized by nature. One is the tachyon representation with negative mass-squared which appears in theories as indicator of instabilities, for instance in spontaneous symmetry breaking. The others are the ''continuous spin representations'' (CSRs), which describe a massless object with an infinity number of helicities. Wigner himself has argued[5] against their use in physics since they lead to infinite heat capacity of the vacuum. All attempts to associate these representations with physical systems have failed. Several authors[6,7] have shown their naive quantization implies either nonlocality or a breakdown of causality. More recently, Zoller[8] showed how they could arise from a higher-derivative Lagrangian such as the length of the acceleration. In addition, massless theories with helicities greater than two have special problems,[9,10] unless perhaps for theories with an infinite number of degrees of freedom. Not surprisingly, these representations have been forgotten.

Yet, the idea of an infinite number of massless spins has some attractions. Indeed, Vasiliev[11] among others has argued for the existence of such theories. A particular lure is the zero tension (infinite slope) limit of string theories which suggests (classically) an infinite number of massless states with unbounded helicities.

The object of this article is to study these representations in higher dimensions, and show that they can be assembled in representations of supersymmetry.

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II. THE POINCARÉ ALGEBRA

The Poincaré generators satisfy the commutation relations,

$$[P^\mu,P^\nu]=0,$$

$$[M^{\mu\nu},P^\sigma]=i(\eta^{\mu\sigma}P^\nu-\eta^{\nu\sigma}P^\mu),$$

$$[M^{\mu\nu},M^{\alpha\beta}]=i(\eta^{\mu\alpha}M^{\nu\beta}+\eta^{\alpha\nu}M^{\beta\mu}+\eta^{\nu\beta}M^{\mu\alpha}+\eta^{\beta\mu}M^{\alpha\nu}),$$

where $\eta_{\mu\nu}=(-1,1,\ldots,1)$. Its representations are characterized by the values of the Casimir operators which are the squared mass $P_\mu P^\mu$, and the squares of the Pauli–Lubanski forms built out of the Levi-Civitá symbols. In d space–time dimensions, the Pauli–Lubanski n-forms are,

$$W_{\mu_1\cdots\mu_n}=\frac{\epsilon_{\mu_1\cdots\mu_n\mu_{n+1}\cdots\mu_d}P^{\mu_d}M^{\mu_{n+1}\mu_{n+2}}\cdots M^{\mu_{d-2}\mu_{d-1}}}{\sqrt{n!2^{(d-n+1)/2}((d-n-1)/2)((d-n-1)/2)!}},\tag{1}$$

where $n=1,3,\ldots,(d-3)$ for d even and $n=0,2,\ldots,(d-3)$ for d odd.

It is convenient to express the Poincaré generators in Dirac's[2] front form, derived long ago for spin in four dimensions by Bacry and Chang.[3] For a particle of mass m, the Poincaré generators are expressed in terms of transverse positions and momenta

$$[x^i,p^j]=i\delta^{ij},\quad i,j=1,2,\ldots,d-2;\quad [x^-,p^+]=-i,\tag{2}$$

and

$$x^\pm=\frac{1}{\sqrt{2}}(x^0\pm x^{d-1}),\quad p^\pm=\frac{1}{\sqrt{2}}(p^0\pm p^{d-1}).\tag{3}$$

The translations are given by

$$P^-=\frac{p^ip^i+m^2}{2p^+},\quad P^+=p^+,\quad P^i=p^i,\tag{4}$$

where P^- is the light-cone Hamiltonian. The Lorentz generators break up into those which transform the transverse plane into itself, and those which transform out of that plane (called ''kinematic'' and ''Hamiltonian,'' respectively by Dirac). The kinematic generators are given by

$$M^{+i}=-x^ip^+,\quad M^{+-}=-x^-p^+,\quad M^{ij}=x^ip^j-x^jp^i+S^{ij},\tag{5}$$

where S^{ij} obey the SO$(d-2)$ Lie algebra of the transverse little group

$$[S^{ij},S^{kl}]=i(\delta^{ik}S^{jl}+\delta^{jl}S^{ik}-\delta^{il}S^{jk}-\delta^{jk}S^{il}).\tag{6}$$

The Hamiltonian-like boosts are

$$M^{-i}=x^-p^i-\frac{1}{2}\{x^i,P^-\}+\frac{1}{p^+}(T^i-p^jS^{ij}),\tag{7}$$

where the T^i transform as SO$(d-2)$ vectors

$$[S^{ij},T^k]=i\delta^{ik}T^j-i\delta^{jk}T^i,\tag{8}$$

and satisfy

$$[T^i,T^j]=im^2S^{ij}.\tag{9}$$

When $m\neq 0$, T^i/m are the generators of $\mathrm{SO}(d-1)/\mathrm{SO}(d-2)$, which, together with S^{ij}, complete the massive little group $\mathrm{SO}(d-1)$.

When $m=0$, the T^i commute with one another, acting as light-cone translations, and the algebra can be satisfied in two ways:

(i) $T^i=0$. This corresponds to the familiar massless representations which describe particles with a finite number of degrees of freedom, realized on states that satisfy

$$T^i|p^+,p^i;(a_1,\ldots,a_r)\rangle=0, \tag{10}$$

where $(a_1,\ldots,a_r)$ are the Dynkin labels of $\mathrm{SO}(d-2)$ representations and r is the rank of the little group. These label the different helicity states of the massless particle. In four dimensions, the Pauli–Lubanski vector is lightlike.

(ii) $T^i\neq 0$. In this case, T^i are the c-number components of a transverse vector. The states on which the Poincaré algebra is realized are

$$T^i|p^+,p^i;\xi^i,(a_1,\ldots,a_r)\rangle=\xi^i|p^+,p^i;\xi^i,(a_1,\ldots,a_r)\rangle, \tag{11}$$

which have additional labels, in the form of a little group vector ξ^i. There is an important difference from the previous case, since $(a_1,\ldots,a_r)$ now labels the $\mathrm{SO}(d-3)$ subgroup of the transverse little group $\mathrm{SO}(d-2)$. In four dimensions, there is no such group and the states are simply labeled by an additional spacelike vector of constant magnitude. These span two distinct representations, called ''continuous spin representations'' by Wigner in his original work.[1] They are characterized by a spacelike Pauli–Lubanski vector, and describe a massless state with an infinite number of integer-spaced helicities.

In the following, we construct these representations in higher dimensions, as well as their supersymmetric generalizations.

A. Continuous spin representations

These representations are characterized by the fact that the light-cone translations T^i do not vanish, even though $m=0$. It follows that a finite boost creates an infinite number of integer-spaced helicities. To see this, consider a ket that represents a state with lightlike momentum aligned along the z direction. In $(3+1)$-dimensions, a rotation in the transverse plane yields

$$e^{i\phi M^{12}}|p^+,p^i=0;\Xi,\alpha\rangle=|p^+,p^i=0;\Xi,\alpha+\phi\rangle, \tag{12}$$

where Ξ is the length of the transverse light-cone translation vector with components

$$\xi^1=\Xi\cos\alpha,\quad \xi^2=\Xi\sin\alpha,$$

which enables us to set

$$S^{12}=-i\frac{\partial}{\partial\alpha}.$$

Since $[S^{12},\xi^i]\neq 0$ for $i=1,2$, S^{12} (helicity) is no longer a good quantum number; instead it acts on periodic or antiperiodic functions of the angle α

$$|\alpha\rangle=\sum_{\lambda} e^{2\pi i\lambda\alpha}|f_\lambda\rangle,$$

where λ are either integer-spaced integers or half-odd integers. Another way to see the infinite number of helicities is to apply the infinitesimal boost M^{-i} on any state

$$M^{-i}|p^+,p^i=0;\Xi,\alpha\rangle=\frac{T^i}{p^+}|p^+,p^i=0;\Xi,\alpha\rangle, \tag{13}$$

which produces a state which has picked up plus or minus one unit of helicity. In a finite boost, this action is repeated an infinite amount, resulting in states with possible helicities ranging from minus to plus infinity in integer steps. There are (in four dimensions only) two types of representations, those with all integer (single-valued) and those with all half-odd integer (double-valued) helicities. The square of the Pauli–Lubanski vector (Casimir) is the squared length of the translation vector

$$W^\mu W_\mu = \vec{T}\cdot\vec{T} = \Xi^2. \tag{14}$$

As we have stated in the Introduction, the CSRs have no obvious physical applications, explicitly in local field theories, but the appearance of an infinite number of states may indicate a connection with nonlocal theories of extended objects. This motivates their study in more general contexts. We explicitly construct these representations in higher dimensions, then proceed to show that they sustain supersymmetry and build continuous spin representations of supersymmetry. Finally, we show that if the light-cone translations are nilpotent, the CSRs become finite-dimensional, but at the expense of negative or zero-norm state, and the supersymmetric generalizations yield central charges for these massless representations.

1. Higher dimensions

The front-form of the Poincaré generators shows that CSRs in any dimensions correspond to representations of the Galilean little group

$$[T^i, T^j] = 0, \quad [S^{ij}, T^k] = i\delta^{ik}T^j - i\delta^{jk}T^i, \tag{15}$$

where the T^i *do not vanish* and the S^{ij} generate the light-cone little group SO$(d-2)$. Consider $(4+1)$-dimensions, where the light-cone little group is SO(3). In the frame $p^- = \vec{p} = 0$, the Pauli–Lubanski two-form is

$$W_{ij} = \frac{1}{\sqrt{2}}\epsilon_{ijk}T^k,$$

so that one Casimir is

$$W_{ij}W_{ij} = \Xi^2, \tag{16}$$

as in the four-dimensional case. The other Casimir is the Pauli–Lubanski zero-form

$$W = \frac{1}{\sqrt{2}}\epsilon_{ijk}T^iS^{jk},$$

which is the projection of the generator S^{jk} along T^i. The vector T^i then acts as a "quantization axis," along which W assumes the values

$$\frac{W}{\sqrt{2}\Xi} = 0, \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \cdots. \tag{17}$$

It follows that there are two types of representations corresponding to integer and half-odd integer values of $W/\sqrt{2}\Xi$. For each value of $W/\sqrt{2}\Xi$, there corresponds one infinite-dimensional representation. Unlike $(3+1)$-dimensions, there are infinite numbers of CSRs in higher dimensions. The states are no longer characterized by the light-cone little group but by its subgroup orthogonal to T^i, which we call the short little group, SO(2) in this case. Each CSR is labeled by a value of SO(2) (integer or half-odd integer) as well as by the length of T^i.

It is straightforward to find the CSR representations in terms of $|j,m\rangle$, the eigenstates of SO(3), the full little group. Its states are required to be eigenstates of $\vec{T}$, the SO(2) rotations about it, and of the Casimir $\epsilon_{ijk}T^iS^{jk}$. As the action of T^i on each $|j,m\rangle$ yields a linear combination of $j=j,j\pm1$ states, its eigenstates are infinite linear combinations of eigenstates of the full little group SO(3). To see this in detail, take the light-cone vector in the z direction, so that $\vec{T}$ is like the tensor operator $T^1_0\equiv Y^1_0$,

$$T^1_0|j,m\rangle=\alpha^{(jm)}_+|j+1,m\rangle+\alpha^{(jm)}_0|j,m\rangle+\alpha^{(jm)}_-|j-1,m\rangle,$$

where the α's are proportional to Clebsch–Gordan (C-G) coefficients

$$\alpha^{(jm)}_0=\Xi\sqrt{(j+m)(j-m+1)},\quad -j<m<j,$$

$$\alpha^{(jm)}_\pm=\Xi\sqrt{(j'+m)(j'-m+1)},\quad j'=j\pm1,\quad -j'<m<j'.$$

The state of the form

$$|F\rangle=\sum_{j=|M|}^{\infty}f^{(M)}_j|j,M\rangle$$

is an eigenstate of the Casimir

$$\tfrac{1}{2}\epsilon_{ijk}T^iS^{jk}|F\rangle=\Xi M|F\rangle,\quad M=0,\pm\tfrac{1}{2},\pm1,\ldots,$$

and of T^3, as long as the coefficients satisfy the recursion relations

$$\alpha^{(|M|+p,M)}_-f^{(M)}_{|M|+p}+\alpha^{(|M|+p-2,M)}_+f^{(M)}_{|M|+p-2}+(\alpha^{(|M|+p-1,M)}_0-\Xi)f^{(M)}_{|M|+p-1}=0,$$

with $p=2,3,\ldots$ and

$$\alpha^{(|M|+1,M)}_-f^{(M)}_{|M|+1}+(\alpha^{(|M|,M)}_0-\Xi)f^{(M)}_{|M|}=0,$$

since $f^{(M)}_{|M|-1}=0$. The other states of the CSR are determined by acting the SO(3) raising and lowering operators on $|F\rangle$. Unlike the usual case, their action does not terminate, producing an infinite number of SO(3) representations. This is similar to Wigner's CSR which contains an infinite number of integer spaced helicities. The difference in higher dimensions is that there is an infinite number of CSRs, each labeled by M.

In $(5+1)$-dimensions the light-cone little group is SO(4), and there are two Pauli–Lubanski forms,

$$\text{one-form:}\quad W_i=\frac{1}{\sqrt{2}}\epsilon_{ijkl}T^jS^{kl},$$

$$\text{three-form:}\quad W_{ijk}=\frac{1}{\sqrt{6}}\epsilon_{ijkl}T^l.$$

The square of the highest form is Ξ^2, a general feature in any dimensions. The square of the one-form is the other Casimir,

$$W_iW_i=-\Xi^2S^2_\perp,$$

where $S^{ij}_\perp$ are the generators of the SO(3) subgroup of SO(4) perpendicular to T^i, and $S^2_\perp\equiv S^{kl}_\perp S^{lk}_\perp(k,l=1,2,3)$ is its Casimir operator. Thus

$$W_i W_i = \Xi^2 j(j+1), \quad j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \cdots . \tag{18}$$

There are an infinite number of distinct CSRs, one for each value of j. The states of the CSR can be labeled by finite rotations of SO(3) and vector $\vec{T}$ characterized by length, Ξ, and three angles,

$$|p^+, p^i = 0; \Xi, \Omega_3; j, m\rangle,$$

where m ranges from $-j$ to $+j$ in integer steps.

In $(6+1)$-dimensions the little group is SO(5) and the Pauli–Lubanski forms are

$$\text{zero-form:} \quad W = \frac{1}{2\sqrt{2}} \epsilon_{ijklm} T^i S^{jk} S^{lm},$$

$$\text{two-form:} \quad W_{ij} = \frac{1}{2} \epsilon_{ijklm} T^k S^{lm},$$

$$\text{four-form:} \quad W_{ijkl} = \frac{1}{2\sqrt{6}} \epsilon_{ijklm} T^m.$$

The two Casimirs of the short little group $\mathrm{SO}(4) \approx \mathrm{SU}(2) \times \mathrm{SU}(2)$ are given by

$$W^2_{(\text{two-form})} = -\Xi^2 S_\perp^2, \tag{19}$$

where here $S_\perp^{ij}$ are the generators of the SO(4) subgroup of SO(5) which leave $\vec{T}$ invariant, and the zero-form which gives the projection of the vector $\epsilon_{ijklm} S^{jk} S^{lm}$ along $\vec{T}$. The CSR states, characterized by four angles Ω_4, and the (j_1, j_2) representations of $\mathrm{SU}(2) \times \mathrm{SU}(2)$, are of the form

$$|p^+, p^i; \Xi, \Omega_4; j_1, m_1; j_2, m_2\rangle,$$

where $-j_{1(2)} \leqslant m_{1(2)} \leqslant j_{1(2)}$. There are an infinite number of CSRs, each labeled by j_1 and j_2.

The pattern is now clear: the CSRs are labeled by the length of a vector and by the irreps of the short little group $\mathrm{SO}(d-3)$ which leaves it invariant. Its Casimirs are directly related to the squares of the Pauli–Lubanski n-forms and the zero-form. There are infinitely many such representations, fermionic and bosonic.

The case of 11 space–time dimensions is particularly interesting because of M-theory and supergravity. Its CSRs are labeled by SO(8), with its magic triality property which acts on its vector representation, $\mathbf{8}_v$, and two inequivalent spinor representations, $\mathbf{8}_s$ and $\mathbf{8}_s'$.

We conclude this section by writing the general expressions for the Casimir operators of the Poincaré algebra in terms of those of the short little group. The Pauli–Lubanski n-form for the light-cone little group $\mathrm{SO}(d-2)$ is given by Eq. (1),

$$W_{i_1 \cdots i_n} = \frac{\epsilon_{i_1 \cdots i_n i_{n+1} \cdots i_{d-2}} T^{i_{d-2}} S^{i_{n+1} i_{n+2}} \cdots S^{i_{d-4} i_{d-3}}}{\sqrt{n! 2^{(d-n-3)/2} ((d-n-3)/2)!}}.$$

The Casimir operators are simplest to calculate in a frame where only $T^{i_{d-2}} \neq 0$, and the square of the highest form is the squared length of the vector $\vec{T}$. The Casimir operators for $n \geqslant 1$ are given by the following.

(i) For little group SO(6) and SO(7),

$$W^2_{i_1 \cdots i_n} = \Xi^2 \{ (S_\perp^2)^{(d-n-3)/2} - 2(S_\perp^{(d-n-3)}) \}; \quad 5 \geqslant d-n-2 > 1.$$

(ii) For little group SO(8) and SO(9),

$$W^2_{i_1\cdots i_n}=\Xi^2\begin{cases}(S_\perp^2)^{(d-n-3)/2}-2(S_\perp^{(d-n-3)}); & 1<d-n-2<7,\\ -(S_\perp^2)^3+2S_\perp^2S_\perp^4-2S_\perp^6; & d-n=9.\end{cases}$$

(*iii*) In general for the little group SO(d),

$$W^2_{i_1\cdots i_n}=\Xi^2\sum_{p=0}^{k}(A_{2p}S_\perp^{2p}S_\perp^{2(k-p)}+B_{2p}(S_\perp^2)^k+C_{2p}(S_\perp^2)^pS_\perp^{2(k-p)}),$$

where $k=\frac{1}{2}(d-n-3)$, and A_{2p}, B_{2p} and C_{2p}'s are numerical constants. In the above, $S_\perp^{ij}$ are the generators of SO($d-3$) subgroup of SO($d-2$) perpendicular to $T^{i_{d-2}}$ and

$$S_\perp^m\equiv S_\perp^{i_1i_2}S_\perp^{i_2i_3}\cdots S_\perp^{i_{m-1}i_m}S_\perp^{i_mi_1}.$$

In odd dimensions, the extra Casimir operator is provided by the Pauli–Lubanski zero-form

$$W=\frac{1}{\sqrt{2^{(d-3)/2}((d-3)/2)!}}\epsilon_{ijk\cdots mn}T^iS_\perp^{ij}\cdots S_\perp^{mn}.$$

In higher dimensions, the CSR states are labeled by Ξ and the solid angle in $(d-3)$-dimensions, Ω_{d-3}, which give the length and direction of $\vec{T}$, respectively, as well as by $(a_1,\ldots,a_r)$, the Dynkin labels of SO($d-3$),

$$|p^+,p^i;\Xi,\Omega_{d-3};(a_1,\ldots,a_r)\rangle.$$

These differ from the usual massless representations in that they are characterized by a spacelike vector, and contain an infinite number of states.

III. SUPER-POINCARÉ ALGEBRA

A. Super-charges in light-cone form

The continuous spin representations can be generalized to include supersymmetry. Indeed, Wigner originally found two CSRs, one single-valued with integer helicities, the other double-valued with half-odd integer helicities. As we shall see, they are related by supersymmetry.

The super-Poincaré algebra includes the spinor generators which satisfy

$$[Q_A,p^\mu]=0, \tag{20}$$

$$[M^{\mu\nu},Q_A]=-\tfrac{1}{2}(\Sigma^{\mu\nu}Q)_A, \tag{21}$$

$$\{Q_A,Q_B^\dagger\}=(\gamma^\mu p_\mu\gamma^0)_{AB}, \tag{22}$$

where A,B are spinor indices. In the above,

$$\Sigma^{\mu\nu}=-\frac{i}{2}[\gamma^\mu,\gamma^\nu],$$

where the γ matrices satisfy the anticommutation relation,

$$\{\gamma^\mu,\gamma^\nu\}=2\eta^{\mu\nu};\quad \mu,\nu=0,\ldots,d.$$

We first consider these relations in four space–time dimensions. The supercharges do not commute with the Pauli–Lubanski vector, as

$$[W_\mu, Q_A] = \frac{i}{2} p^\nu (\Sigma_{\mu\nu}\gamma_5 Q)_A,$$

using

$$\tfrac{1}{2}\epsilon_{\mu\nu\rho\sigma}\Sigma^{\rho\sigma} = -i\Sigma_{\mu\nu}\gamma_5,$$

and $\gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3$ is the chirality matrix. The supercharges can be realized linearly using Grassmann variables and their derivatives as[12]

$$Q_A = \partial_A + \tfrac{1}{2}(\gamma^\mu p_\mu \gamma^0)_{AB}\overline{\theta^B}, \tag{23}$$

and its conjugate as

$$Q_C^\dagger = \overline{\partial_C} + \tfrac{1}{2}(\gamma^\mu p_\mu \gamma^0)_{DC}\theta^D, \tag{24}$$

where we used

$$\gamma^0\gamma^{\mu\dagger}\gamma^0 = \gamma^\mu,$$

and $\partial_A = \partial/\partial\theta^A$, $\overline{\partial_A} = \partial/\partial\overline{\theta^A}$, and $\overline{\theta_A}$ is the complex conjugate of θ_A with $A,\ldots,D$ running over the spinor indices. θ, $\overline{\theta}$, ∂ and $\overline{\partial}$ are anticommuting Grassmann parameters. We use the light-cone projectors to split the supercharge into two-component spinors,

$$Q = Q_+ + Q_-, \quad \text{where} \quad Q_\pm \equiv \mathcal{P}_\pm Q,$$

with $\mathcal{P}_\pm = \frac{1}{2}\gamma^\mp\gamma^\pm$. In the Weyl representation, from Eqs. (22)–(24), we can now read off the various anticommutation relations, namely,

$$\{Q_{+a}, Q_{+b}^\dagger\} = \sqrt{2}p^+\delta_{ab},$$

$$\{Q_{-a}, Q_{-b}^\dagger\} = \sqrt{2}p^-\delta_{ab} \equiv \sqrt{2}\frac{p\overline{p}}{p^+}\delta_{ab},$$

$$\{Q_{-1}, Q_{+1}^\dagger\} = -\sqrt{2}\overline{p}, \quad \{Q_{+1}, Q_{-1}^\dagger\} = -\sqrt{2}p,$$

$$\{Q_{+2}, Q_{-2}^\dagger\} = \sqrt{2}\overline{p}, \quad \{Q_{-2}, Q_{+2}^\dagger\} = \sqrt{2}p,$$

where $p(\overline{p}) = (1/\sqrt{2})(p^1 \pm ip^2)$ and $a,b = 1,2$, all other anticommutators being zero. This shows that the supercharge splits up into two disconnected sets of anticommutators, corresponding to the left and right projections $[\mathcal{P}_{L,R} = \frac{1}{2}(1 \pm \gamma_5)]$

$$\mathcal{Q}_\pm^R \equiv \mathcal{P}_R Q_\pm, \quad \mathcal{Q}_\pm^L \equiv \mathcal{P}_L Q_\pm. \tag{25}$$

One could also think of these as representing $N = 2$ supersymmetry.

There is further reducibility, indicated by the fact that the supercharge anticommutes with the covariant derivative

$$\mathcal{D}_A = \partial_A - \tfrac{1}{2}(\gamma^\mu p_\mu \gamma^0)_{AB}\overline{\theta^B}, \tag{26}$$

and their Hermitian conjugates, which give the following relations,

$$\mathcal{Q}_-^L = -\frac{\overline{p}}{p^+}\mathcal{Q}_+^L, \quad \mathcal{Q}_-^R = \frac{p}{p^+}\mathcal{Q}_+^R, \tag{27}$$

together with their conjugates

$$\mathcal{Q}_-^{L\dagger}=-\frac{p}{p^+}\mathcal{Q}_+^{L\dagger},\quad \mathcal{Q}_-^{R\dagger}=\frac{\overline{p}}{p^+}\mathcal{Q}_+^{R\dagger},\tag{28}$$

without affecting the anticommutation relations. From now on we concentrate on the right-handed projections of the algebra. On (right-handed) superfields, the constraint becomes

$$\mathcal{P}_R\mathcal{D}\Phi=0,\tag{29}$$

and after using mass-shell condition, we are left with only one supercharge, $\mathcal{Q}_+$ (henceforth we drop the superscript R). It is expressed in terms of one Grassmann variable $\theta_3\equiv\theta$ and its conjugate, as we can drop the θ_4 variable altogether since its derivative is now expressed in terms of the derivative with respect to θ_3. Hence

$$\mathcal{Q}_+=\frac{\partial}{\partial\theta}+\frac{1}{\sqrt{2}}p^+\overline{\theta},\quad \mathcal{Q}_+^\dagger=\frac{\partial}{\partial\overline{\theta}}+\frac{1}{\sqrt{2}}p^+\theta.\tag{30}$$

Since

$$[M^{+-},\mathcal{Q}_\pm]=\pm\frac{i}{2}\mathcal{Q}_\pm,\tag{31}$$

we must extend the Bacry–Chang representation of M^{+-} to

$$M^{+-}=-x^-p^+-\frac{i}{2}\left(\theta\frac{\partial}{\partial\theta}+\overline{\theta}\frac{\partial}{\partial\overline{\theta}}\right).\tag{32}$$

In order to satisfy the other commutation relations,

$$[M^{+i},M^{-j}]=i\delta^{ij}M^{+-}-iM^{ij},\quad [M^{12},\mathcal{Q}_\pm]=\mp\tfrac{1}{2}\mathcal{Q}_\pm,\tag{33}$$

the generators M^{12} and M^{-i} now include the θ-dependent terms,

$$M^{12}=x^1p^2-x^2p^1+\hat{S}^{12},\tag{34}$$

as well as

$$M^{-i}=x^-p^i-\frac{1}{2}\{x^i,P^-\}+\frac{1}{p^+}(T^i-p^j\hat{S}^{ij})+i\frac{p^i}{2p^+}\left(\theta\frac{\partial}{\partial\theta}+\overline{\theta}\frac{\partial}{\partial\overline{\theta}}\right),\tag{35}$$

where now

$$\hat{S}^{12}=S^{12}+\frac{1}{2}\left(\theta\frac{\partial}{\partial\theta}-\overline{\theta}\frac{\partial}{\partial\overline{\theta}}\right).\tag{36}$$

The generator M^{+i} remains unchanged. The other relevant commutators in light-cone form are

$$[M^{\pm i},\mathcal{Q}_\pm]=0.\tag{37}$$

In the frame where $p^i=0$, we have

$$\mathcal{Q}_-=0,\quad M^{-i}=T^i/p^+,\tag{38}$$

so that the commutators

$$[M^{-1},\mathcal{Q}_+]=-\frac{i}{\sqrt{2}}\mathcal{Q}_-,\quad [M^{-2},\mathcal{Q}_+]=-\frac{1}{\sqrt{2}}\mathcal{Q}_-, \tag{39}$$

$$[M^{+1},\mathcal{Q}_-]=-\frac{i}{\sqrt{2}}\mathcal{Q}_+,\quad [M^{+2},\mathcal{Q}_-]=\frac{1}{\sqrt{2}}\mathcal{Q}_+, \tag{40}$$

imply that

$$[T^i,\mathcal{Q}_+]=0. \tag{41}$$

Since the vector that characterizes the CSRs commutes with the supercharge, we can implement supersymmetry on the continuous spin representations without having to change the supercharges.

Thus in $(3+1)$-dimension, we obtain the *unique* representation of supersymmetry which contains all integer and half-odd integer helicities. This of course does not alleviate the problems associated with the CSRs.

B. Higher dimensions

In higher dimensions, Eqs. (20)–(24) still hold, but the number and nature of independent Grassmann parameters, i.e., whether these are Dirac, Weyl or Majorana type, depend on the number of space-time dimensions.[13] In d-dimensions, there are $2^{d/2}(2^{(d-1)/2})$ complex spinor components for d even(odd). Using the anticommutativity between supercharge and covariant derivative, these numbers can be further reduced by a factor of 2. Let a, b run over the independent spinor indices, i.e., $a,b=1,2,\ldots,2^{d/2-m}(2^{(d-1)/2-m})$, for d even(odd), respectively, where m is the number of independent constraints. Using all reducibility conditions, we can always express the super-Poincaré algebra in the light-cone form,

$$M^{ij}=x^ip^j-x^jp^i+\hat{S}^{ij}, \tag{42}$$

$$M^{+-}=-x^-p^++S^{+-}, \tag{43}$$

$$M^{-i}=x^-p^i-\frac{1}{2}\{x^i,P^-\}+\frac{1}{p^+}(T^i-p^j\hat{S}^{ij})-\frac{p^i}{p^+}S^{+-}, \tag{44}$$

where

$$\hat{S}^{ij}=S^{ij}+(\tfrac{1}{2}\theta^a(\gamma^{ij})_{ab}\partial^b+\text{c.c.}), \tag{45}$$

$$S^{+-}=(\tfrac{1}{2}\theta^a(\gamma^{+-})_{ab}\partial^b+\text{c.c.}), \tag{46}$$

and γ^{ij} and γ^{+-} are the reduced Dirac submatrices consistent with the constraints. M^{+i} remain the same as before. The indices i, j run over transverse space. The supercharges can be irreducibly expressed as

$$\mathcal{Q}^a_+=\frac{\partial}{\partial\theta^a}+\frac{1}{\sqrt{2}}p^+\overline{\theta^a},\quad \mathcal{Q}^{\dagger a}_+=\frac{\partial}{\partial\overline{\theta^a}}+\frac{1}{\sqrt{2}}p^+\theta^a, \tag{47}$$

and $\mathcal{Q}^a_-$ can be expressed in terms of $\mathcal{Q}^a_+$. To illustrate this construction, we now show how supersymmetric CSRs arise in 5 and 11 dimensions.

1. (4+1)*-dimensions*

In five dimensions, the spinors have four complex components which can be reduced to two using the covariant derivative constraint. Using the light-cone projectors, $\mathcal{P}_{\pm}=-\frac{1}{2}\gamma^{\mp}\gamma^{\pm}$ in the representation,

$$\gamma^0=i\sigma^1\otimes I,\quad \gamma^i=\sigma^3\otimes\sigma^i,\quad i=1,2,3;\quad \text{and}\quad \gamma^4=\sigma^2\otimes I, \tag{48}$$

and Eq. (22), we find

$$\{\mathcal{Q}_{+a},\mathcal{Q}^{\dagger}_{+b}\}=\sqrt{2}p^{+}\delta_{ab}, \tag{49}$$

$$\{\mathcal{Q}_{-a},\mathcal{Q}^{\dagger}_{-b}\}=\sqrt{2}p^{-}\delta_{ab}=\frac{\vec{p}\cdot\vec{p}}{\sqrt{2}p^{+}}\delta_{ab}, \tag{50}$$

$$\{\mathcal{Q}_{+a},\mathcal{Q}^{\dagger}_{-b}\}=i(\vec{\sigma}\cdot\vec{p})_{ab}, \tag{51}$$

$$\{\mathcal{Q}_{-a},\mathcal{Q}^{\dagger}_{+b}\}=-i(\vec{\sigma}\cdot\vec{p})_{ab}, \tag{52}$$

where $a,b=1,2$ and also we used the on-shell condition $p^{-}=p^{i}p^{i}/2p^{+}$. From Eq. (26) and $\mathcal{D}\Phi=0$, we find

$$\frac{\partial}{\partial\theta^{2+a}}=-i\left(\frac{\vec{\sigma}\cdot\vec{p}}{\sqrt{2}p^{+}}\right)_{ab}\frac{\partial}{\partial\theta^{b}},$$

and similarly for their complex conjugates, allowing us to set $(\theta^3,\theta^4)=0$. The supercharges, Eqs. (23) and (24), reduce to the irreducible form as in Eq. (47) with $a,b=1,2$, and

$$Q_{-a}=-i\left(\frac{\vec{\sigma}\cdot\vec{p}}{\sqrt{2}p^{+}}Q_{+}\right)_{a}\quad\text{and hence}\quad Q^{\dagger}_{-a}=i\left(Q^{\dagger}_{+}\frac{\vec{\sigma}\cdot\vec{p}}{\sqrt{2}p^{+}}\right)_{a}. \tag{53}$$

The Lorentz generators remain the same as in Eqs. (42)–(44) with the following irreducible representations of S^{ij} and S^{+-} [in Eqs. (45) and (46)],

$$S^{+-}=-\frac{i}{2}\left(\theta\frac{\partial}{\partial\theta}+\overline{\theta}\frac{\partial}{\partial\overline{\theta}}\right), \tag{54}$$

$$\hat{S}^{ij}=S^{ij}+\frac{1}{2}\epsilon^{ijk}\left(\theta\sigma^{k}\frac{\partial}{\partial\theta}+\text{c.c.}\right), \tag{55}$$

where $\theta=(\theta^1,\theta^2)$ and $\partial/\partial\theta=(\partial/\partial\theta^1,\partial/\partial\theta^2)$. The supercharges transform as SO(3) spinors,

$$[M^{ij},\mathcal{Q}_{+a}]=-\tfrac{1}{2}\epsilon^{ijk}(\sigma^{k}\mathcal{Q}_{+})_{a}. \tag{56}$$

These charges can be made to act on the CSRs, for which the relevant group is that of the short little group SO(2) which leaves the light-cone translation vector invariant. Aligning $\vec{T}$ along the z-axis, the supercharges split into two components, $\mathcal{Q}_{+1}$ and $\mathcal{Q}^{\dagger}_{+2}$, that lower the value of M^{12} by half a unit, and two components, $\mathcal{Q}_{+2}$ and $\mathcal{Q}^{\dagger}_{+1}$ that raise it.

In terms of M, the eigenvalue of $\hat{S}^{12}$, the supermultiplet consists of

$$|M\rangle_{\text{CSR}}\sim|M\rangle_{\text{CSR}},$$

$$\mathcal{Q}_{+1}|M\rangle_{\text{CSR}},\quad \mathcal{Q}^{\dagger}_{+2}|M\rangle_{\text{CSR}}\sim|M-\tfrac{1}{2}\rangle_{\text{CSR}},$$

$$\mathcal{Q}_{+1}\mathcal{Q}^{\dagger}_{+2}|M\rangle_{\mathrm{CSR}} \sim |M-1\rangle_{\mathrm{CSR}}.$$

It contains two bosonic and two fermionic CSRs, with the same structure as the ordinary ($\vec{T}=0$) massless $N=2$ supermultiplet in four dimensions. The important difference is that it contains not only the ordinary states but their copies under the boosts proportional to $\vec{T}$. This yields as usual an infinite number of SO(3) polarization states. The action of supersymmetry is the same as in the normal case, but the CSR supermultiplets contain an infinite number of ordinary massless supermultiplets of ever-increasing spin.

2. (10+1)*-dimensions*

The case of 11 dimensions is particularly interesting because it is shrouded in mystery, as it contains not only local supergravity but also the elusive M-theory. What we know of M-theory is that its compactifications to lower dimensions yields supersymmetric theories and that its long distance limit is the supergravity theory.

In 11 dimensions, the spinors have 32 complex components, which, upon using the Majorana condition and the covariant derivative constraint, reduce to 16 real components. The supercharge splits as

$$Q=\begin{pmatrix} Q^A \\ Q^{16+A}\end{pmatrix} \equiv \begin{pmatrix} Q^A_+ \\ Q^A_-\end{pmatrix}, \quad A=1,\ldots,16.$$

The Majorana condition implies,

$$Q^A_+ = Q^{\dagger A}_+ \quad \text{and} \quad Q^A_- = -Q^{\dagger A}_-.$$

In the representation

$$\gamma^0 = i\sigma^1\otimes I, \quad \gamma^i = \sigma^3\otimes\tilde{\gamma}^i, \quad \gamma^{10}=\sigma^2\otimes I, \tag{57}$$

where $i=1,\ldots,9$ and $\tilde{\gamma}^i$'s are 16×16 and real, symmetric matrices which satisfy the following algebra

$$\{\tilde{\gamma}^i,\tilde{\gamma}^j\}=2\delta^{ij},$$

the super-Poincaré algebra becomes

$$\{Q^A_+,Q^B_+\}=\sqrt{2}p^+\delta^{AB},$$

$$\{Q^A_-,Q^B_-\}=-\sqrt{2}p^-\delta^{AB}=-\frac{\vec{p}\cdot\vec{p}}{\sqrt{2}p^+}\delta^{AB},$$

$$\{Q^A_+,Q^B_-\}=-i\tilde{\gamma}^{AB}_i p^i,$$

$$[M^{ij},Q^A_\pm]=\frac{i}{2}(\tilde{\gamma}_{ij}Q_\pm)^A,$$

$$[M^{+-},Q^A_\pm]=\pm\frac{i}{2}Q^A_\pm,$$

$$[M^{\pm i},Q^A_\pm]=0, \quad [M^{\pm i},Q^A_\mp]=\pm\frac{i}{\sqrt{2}}(\tilde{\gamma}_i Q_\pm)^A.$$

Using $\mathcal{D}\Phi=0$ and Eq. (26), we find

$$\frac{\partial}{\partial\theta^{16+A}}=-i\left(\frac{\tilde{\gamma}^i p^i}{\sqrt{2}p^+}\frac{\partial}{\partial\theta}\right)_A,$$

allowing us to set $\theta^{16+A}=0$ for $A=1,\ldots,16$. The remaining real Q_+^A's can be expressed in terms of 16 real Grassmann parameters,

$$Q_+^A=\frac{\partial}{\partial\theta^A}+\frac{1}{\sqrt{2}}p^+\theta^A \quad \text{and} \quad Q_-^A=-i\left(\frac{\tilde{\gamma}^i p^i}{\sqrt{2}p^+}Q_+\right)^A.$$

Similarly, in this representation, Eqs. (45) and (46) reduce to

$$S^{+-}=-\frac{i}{2}\theta^A\frac{\partial}{\partial\theta^A},$$

$$\hat{S}^{ij}=S^{ij}-\frac{i}{2}\theta^A\tilde{\gamma}^{ij}_{AB}\frac{\partial}{\partial\theta^B},$$

which together with Eqs. (42)–(44) give the Lorentz generators, where $\tilde{\gamma}^{ij}=\tilde{\gamma}^i\tilde{\gamma}^j$ for $i\neq j$ and zero otherwise.

We can let these charges act onto CSRs, remembering that they are labeled by the short little group SO(8) that leaves the light-cone translation vector $\vec{T}$ invariant. We decompose the supercharges into two eight-component supercharges, $\mathcal{Q}_+^a$ and $\mathcal{Q}_+^{\dot{a}}$, by the SO(8) chirality matrix,

$$Q_+^A=\begin{pmatrix}\mathcal{Q}_+^a\\ \mathcal{Q}_+^{\dot{a}}\end{pmatrix}, \quad a=1,\ldots,8,$$

where

$$\mathcal{Q}_+^a=\tfrac{1}{2}(1+\tilde{\gamma}^{(9)}) \quad \text{and} \quad \mathcal{Q}_+^{\dot{a}}=\tfrac{1}{2}(1-\tilde{\gamma}^{(9)}),$$

and the chirality matrix of SO(8) subgroup is

$$\tilde{\gamma}^{(9)}\equiv\tilde{\gamma}^1\tilde{\gamma}^2\tilde{\gamma}^3\tilde{\gamma}^4\tilde{\gamma}^5\tilde{\gamma}^6\tilde{\gamma}^7\tilde{\gamma}^8.$$

These two eight-component supercharges furnish two inequivalent spinor representations of SO(8), $\mathbf{8}_s$ and $\mathbf{8}_s'$, characterized by opposite SO(8) chirality and $\mathcal{Q}_+^a\sim\mathbf{8}_s$, $\mathcal{Q}_+^{\dot{a}}\sim\mathbf{8}_s'$.

The (16×16) $\tilde{\gamma}^i$ matrices can be written in terms of 8×8 block form

$$\tilde{\gamma}^i=\begin{pmatrix}0 & \tilde{\gamma}^i_{a\dot{a}}\\ \tilde{\gamma}^i_{\dot{b}b} & 0\end{pmatrix},$$

where $\tilde{\gamma}^i_{a\dot{a}}$ is the transpose of $\tilde{\gamma}^i_{\dot{a}a}$. The Clifford algebra for $\tilde{\gamma}^i$ is satisfied if

$$\tilde{\gamma}^i_{a\dot{a}}\tilde{\gamma}^j_{\dot{a}b}+\tilde{\gamma}^j_{a\dot{a}}\tilde{\gamma}^i_{\dot{a}b}=2\,\delta^{ij}\delta_{ab}, \quad \text{for } i,j,a,b=1,\ldots,8,$$

and similarly with undotted and dotted indices interchanged. We also define

$$\tilde{\gamma}^{ij}_{ab}=\tfrac{1}{2}(\tilde{\gamma}^i_{a\dot{a}}\tilde{\gamma}^j_{\dot{a}b}-\tilde{\gamma}^j_{a\dot{a}}\tilde{\gamma}^i_{\dot{a}b}),$$

and similarly for $\tilde{\gamma}^{ij}_{\dot{a}\dot{b}}$. The (8×8) $\tilde{\gamma}^i_{a\dot{a}}$ matrices couple the vector and spinor representations. In this chiral subspace, the supercharges, $\hat{S}^{ij}$ and S^{+-} take the following irreducible forms

$$\mathcal{Q}_+^a = \frac{\partial}{\partial \theta^a} + \frac{1}{\sqrt{2}} p^+ \theta^a, \tag{58}$$

$$\mathcal{Q}_+^{\dot{a}} = \frac{\partial}{\partial \theta^{\dot{a}}} + \frac{1}{\sqrt{2}} p^+ \theta^{\dot{a}},$$

$$\mathcal{Q}_-^a = -\frac{ip^i}{\sqrt{2}p^+} \tilde{\gamma}^i_{a\dot{a}} \mathcal{Q}_+^{\dot{a}}, \tag{59}$$

$$\mathcal{Q}_-^{\dot{a}} = -\frac{ip^i}{\sqrt{2}p^+} \tilde{\gamma}^i_{\dot{a}a} \mathcal{Q}_+^a,$$

as well as

$$S^{+-} = -\frac{i}{2} \theta^a \frac{\partial}{\partial \theta^a}, \quad \hat{S}^{ij} = S^{ij} - \frac{i}{2} \theta^a \tilde{\gamma}^{ij}_{ab} \frac{\partial}{\partial \theta^b}. \tag{60}$$

We have two supersymmetries, each transforming as a different SO(8) spinor, and the basic supermultiplet is of the form $(\mathbf{8}_v + \mathbf{8}_s)_{\mathrm{CSR}} \times (\mathbf{8}_v + \mathbf{8}'_s)_{\mathrm{CSR}}$, with 128 bosonic and 128 fermionic states,

$$(\mathbf{8}_v + \mathbf{8}_s)_{\mathrm{CSR}} \times (\mathbf{8}_v + \mathbf{8}'_s)_{\mathrm{CSR}} = (\mathbf{1} + \mathbf{28} + \mathbf{35} + \mathbf{8} + \mathbf{56})_{v,\mathrm{CSR}} + (\mathbf{8}' + \mathbf{56}' + \mathbf{8} + \mathbf{56})_{s,\mathrm{CSR}}. \tag{61}$$

This supermultiplet (without CSR) is of course that of the massless states of IIA string theory, obtained by dimensional reduction from 11-dimensional supergravity.

As we found in the five-dimensional case, there is a one-to-one correspondence between the labels of the ordinary massless representation for $N=2$ supersymmetry in ten dimensions and those of the massless CSR for $N=1$ supersymmetry in 11 dimensions. However, the CSR supermultiplet contains the states of $N=1$ supergravity as well as an infinite number of massless supermultiplets obtained by boosting along $\vec{T}$.

C. Dimensional reduction

The characteristic feature of the CSRs is the transverse space vector T^i. A nonzero value implies an infinite number of polarization states while a zero value requires a finite number of polarizations. In covariant terms, this vector is written in terms of the Pauli–Lubanski $(d-3)$-form, its magnitude unchanged by Poincaré transformations.

This suggests several ways in which CSRs might play a role in physics. One is to enlarge the invariance group to include transformations capable of changing the length. The other is to view the CSR in the context of dimensional reduction by limiting transformations to rotations perpendicular to $\vec{T}$.

The former approach requires a study of the representations of the larger groups. Of prime interest are the conformal group (since we are dealing with massless representations) and perhaps the de Sitter groups. In particular we need to identify how CSRs and normal massless representations reside in unitary irreducible representations of these groups.

In physical terms we may view the length as an order parameter (as in the Higgs mechanism with a vector representation). For this we need to give it a dynamical meaning and couple it to an external field; it is amusing to note that in 11 dimensions it naturally couples to an eight-form, which is dual to a three-form.

As we let the length tend to zero, we cannot *a priori* determine which normal representation will be singled out in the transition. This is reminiscent of Dashen's theorem in chiral theories where an external additional tag is required; otherwise it points to a first-order phase transition.

In the context of dimensional reduction, the translation vector $\vec{T}$ naturally singles out a subspace perpendicular to its direction. It follows that group operations restricted to that subspace span normal representations of the Poincaré and super-Poincaré algebras. Thus it might be possible to start with a problematic theory and dimensionally reduce it to a well-defined one.

D. Nilpotent light-cone translations

We have seen that CSRs necessarily contain massless states of unbounded spins related by finite boosts, raising many objections for their use in the description of pointlike objects. On the other hand, the extension of Poincaré invariance to supersymmetry introduces nilpotent Grassmann variables, which suggests the construction of the light-cone translations out of these Grassmann parameters. The translations would be nilpotent, and therefore generate a finite number of helicities with finite boosts.

In $(3+1)$-dimensions, we need two complex Grassmann variables, θ_1, θ_2, in order to build an SO(2) vector. We set

$$T^1+iT^2=\sqrt{2}\overline{z}p^+\theta_1\theta_2, \quad T^1-iT^2=\sqrt{2}zp^+\overline{\theta_1}\,\overline{\theta_2}, \tag{62}$$

where z is a complex variable, and we have added the appropriate power of p^+ to ensure proper commutation with M^{+-}. S^{12} now becomes

$$\hat{S}^{12}\equiv S^{12}+\tfrac{1}{2}(\theta^a\partial_a-\overline{\theta}^a\overline{\partial}_a), \tag{63}$$

and the Poincaré Casimir operator is now a nilpotent Grassmann number,

$$W^2=W^\mu W_\mu=-2|z|^2(p^+)^2\theta_1\theta_2\overline{\theta}_1\overline{\theta}_2. \tag{64}$$

With two Grassmann variables, we can construct two supercharges, corresponding to $N=2$ supersymmetry. The kinematic supersymmetries are unaltered

$$\mathcal{Q}^a_+=\frac{\partial}{\partial\theta_a}+\frac{1}{\sqrt{2}}p^+\overline{\theta}_a; \quad \mathcal{Q}^{a\dagger}_+=\frac{\partial}{\partial\overline{\theta}_a}+\frac{1}{\sqrt{2}}p^+\theta_a, \tag{65}$$

where $a=1,2$. However, the light-cone translations no longer commute with these supercharges. To restore the super-Poincaré algebra, the dynamic supersymmetries must be altered to the new form

$$\mathcal{Q}^a_-=\frac{p}{p^+}\mathcal{Q}^a_+-i\overline{z}\epsilon^{ab}\theta_b, \quad \mathcal{Q}^{a\dagger}_-=\frac{\overline{p}}{p^+}\mathcal{Q}^{a\dagger}_++iz\epsilon^{ab}\overline{\theta}_b, \tag{66}$$

which ensures the commutation relations of $\mathcal{Q}^a_+$ with the boosts M^{-i}. The resulting supersymmetry algebra,

$$\{\mathcal{Q}^a_+,\mathcal{Q}^b_-\}=i\epsilon^{ab}\overline{z}, \quad \{\mathcal{Q}^{a\dagger}_+,\mathcal{Q}^{b\dagger}_-\}=-i\epsilon^{ab}z, \tag{67}$$

acquires central charges, even though we are in a massless representation.

This leads to zero or negative norm states. The positive norm states are of the form $|\cdots\rangle$, and $\mathcal{Q}^{a\dagger}_+|\cdots\rangle$, and $\mathcal{Q}^{1\dagger}_+\mathcal{Q}^{2\dagger}_+|\cdots\rangle$, where $|\cdots\rangle$ is annihilated by $\mathcal{Q}^a_+$. However, with central charges, in the frame where only $p^+\neq 0$,

$$\langle\cdots|\mathcal{Q}^1_+\mathcal{Q}^2_-|\cdots\rangle=iz\langle\cdots|\cdots\rangle, \tag{68}$$

and a similar argument with 1,2 interchanged, which shows that the states $\mathcal{Q}^a_-|0\rangle$ do not vanish. Yet from

$$\{\mathcal{Q}_-^a, \mathcal{Q}_-^{b\dagger}\} = 0, \tag{69}$$

their norms must satisfy

$$|\mathcal{Q}_-^a|\cdots\rangle|^2 + |\mathcal{Q}_-^{a\dagger}|\cdots\rangle|^2 = 0, \tag{70}$$

for $a=1,2$, implying that one is negative, or both are zero. This reproduces general arguments[13] based on the absence of negative or zero norm states, which show that central charges are limited to massive representations. In the frame where only $p^+ \neq 0$, the dynamic generators of massless supersymmetry anticommute with one another. If they do not, negative or zero-norm states are generated.

This construction does not seem to generalize to odd dimensions. We have shown this explicitly in 11 dimensions by starting with $\vec{T}$ quadratic in the Grassmann numbers. There a quadratic product of a Grassmann spinor transforms as two- and three-forms, so that to make a vector we need some c-number tensors, either a one- or two-form, but the commutation with the supercharge does not have the right form.

On the other hand, the construction in $(9+1)$-dimensions is straighforward. We consider two supercharges

$$\mathcal{Q}_+^{(1)} = \frac{\partial}{\partial\theta} + \frac{1}{\sqrt{2}} p^+ \theta; \quad \mathcal{Q}_+^{(2)} = \frac{\partial}{\partial\eta} + \frac{1}{\sqrt{2}} p^+ \eta,$$

where $\theta \sim \mathbf{8}_s$, $\eta \sim \mathbf{8}_s'$. We take the light-cone translation vector to be

$$T^i = i p^+ z\, \theta \tilde{\gamma}^i \eta \sim \mathbf{8}_v, \quad z \text{ real},$$

so that this corresponds to type IIA supersymmetry. The dynamic boosts are

$$S^{-i} = i z\, \theta \tilde{\gamma}^i \eta - \frac{p^j}{p^+} \hat{S}^{ij} - \frac{p^i}{p^+} S^{+-},$$

with

$$\hat{S}^{ij} = S^{ij} - \frac{i}{2}\left(\theta \tilde{\gamma}^{ij} \frac{\partial}{\partial\theta} + \eta \tilde{\gamma}^{ij} \frac{\partial}{\partial\eta} \right), \quad \text{and} \quad S^{+-} = -\frac{i}{2}\left(\theta \frac{\partial}{\partial\theta} + \eta \frac{\partial}{\partial\eta} \right).$$

The dynamic supercharges are now

$$\mathcal{Q}_-^{(2)} = -\frac{i p^i}{\sqrt{2} p^+} \tilde{\gamma}^i \mathcal{Q}_+^{(2)} + i\sqrt{2} z\, \theta,$$

$$\mathcal{Q}_-^{(1)} = -\frac{i p^i}{\sqrt{2} p^+} \tilde{\gamma}^i \mathcal{Q}_+^{(1)} - i\sqrt{2} z\, \eta.$$

The resulting supersymmetry algebra now includes central charge

$$\{\mathcal{Q}_+^{(1)}, \mathcal{Q}_-^{(2)}\} = -\{\mathcal{Q}_+^{(2)}, \mathcal{Q}_-^{(1)}\} = i\sqrt{2} z.$$

We have seen that our construction leads to supersymmetry but the representations necessarily contain negative and zero-norm states. Although it is interesting to note that central charges occur naturally whenever the light-cone translations are built out of the Grassmann variables, the representations contain negative and zero-norm states; at best they could be used as ghost compensators of some unknown theory.

IV. CONCLUSION

In this article, we considered nonzero light-cone translations to construct the continuous spin representations of both Poincaré and super-Poincaré algebra. We started with the Poincaré algebra in four space–time dimensions and generalized it to higher dimensions. The light-cone translation vector, $\vec{T}$, is represented by spherical harmonics in $(d-2)$-dimensions for the light-cone little group $\mathrm{SO}(d-2)$. We find that the states can be represented by p^+, the length Ξ and $(d-3)$ number of angles of the $\mathrm{SO}(d-2)$ spherical harmonics, and the Dynkin labels $(a_1,\ldots,a_r)$ of $\mathrm{SO}(d-3)$ the short little group, with r being the rank. There is one CSR for each representation $(a_1,\ldots,a_r)$.

If $\vec{T}$ is nilpotent, a finite number of states are generated by the light-cone boost, instead of infinite number of states, but the resulting CSR contains zero or negative norm states, and its supersymmetric extension (in four and ten dimensions) has a central charge. The nilpotent construction of T^i in higher dimensions is not so evident. These CSRs may be useful in conjunction with theories where the invariances force overcounting, as in ghost states in gauge theories.

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Analytical expressions for some multiplicity-free isoscalar factors of $S_f \supset S_{f-1}$

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An algebraic routine for the evaluation of analytical expressions for isoscalar factors (ISFs) of $S_f \supset S_{f-1}$ is formulated based on the linear equation method (LEM) and the analytical continuation of the rank f. As examples, ISFs of $S_f \supset S_{f-1}$ for the coupling $[f-1,1]\cdot[f-1,1]$, $[f-1,1]\cdot[f-2,2]$, $[f-2,1,1]\cdot[f-2,1,1]$ are tabulated. The results demonstrate that the number of ISF tables can be greatly reduced compared with corresponding numerical results produced using other methods. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1517169]

I. INTRODUCTION

Clebsch–Gordan Coefficients (CGCs) of the symmetric groups S_f are very important. First of all, by definition, they are transformation coefficients between uncoupled basis vectors of two irreducible representations (irreps) and a coupled inner product irrep of those two irreps.[1] Next, it has been shown[2–5] that the CGCs of S_f can be used to evaluate coupling coefficients for the $U(mn)\supset U(m)\times U(n)$, $SU(mn)\supset SU(m)\times SU(n)$ coefficients of fractional parentage (CFP), and so on, due to the Schur–Weyl duality relation between the symmetric group S_f and the unitary group $U(n)$.

There are many different ways to evaluate the CGCs of S_f.[6–11] Vanagas studied an extension of the tensor algebraic approach to the symmetric groups.[6] In this approach, one- and two-body operators are expressed in terms of irreducible tensor operators of symmetric groups. Hence, the Wigner–Racah tensor operator technique can be applied for evaluating matrix elements of the operators with CGCs and Racah coefficients of S_f. Analytical expressions of the isoscalar factors (ISFs) for the inner product $[f-1]\cdot[f-1]$ were derived based on this method. However, this approach is not practical for deriving analytical expressions of other ISFs due to the fact that the order of the symmetric group S_f increases dramatically with f and more complex Young shapes. As a consequence, numerical algorithms have been developed based on various routines for $f \leqslant 6$. The Schindler and Mirman method for computing the CGCs of S_f is based on the fact that the CG vectors of S_f are the simultaneous eigenvectors of the two-cycle class operators of its subgroups.[10,11] Chen *et al.* proposed the eigenfunction method,[7,8] and pointed out that the CG vectors of S_f can be much more easily obtained by diagonalizing a single matrix rather than by diagonalizing simultaneously the $f-1$ representation matrices of the $f-1$ two-cycle class operators used by Schindler and Mirman. Based on these considerations, two sets of tables of CGCs of S_f for $f \leqslant 6$ have been published; one was generated using the Schindler and Mirman algorithm,[11] while another was produced by Chen *et al.* based on the eigenfunction method.[7,8] Very recently, ISFs of $S_f \supset S_{f-1}$ for $f \leqslant 6$ have been calculated[12] based on Hamermesh's recursion relation.[1]

CGCs or ISFs of the symmetric groups calculated by any of these methods quickly become intractable with increasing rank f. Furthermore, these methods only yield CGCs and ISFs for a specific f, implying the need for a large number of tables. But, upon close examination of the results one finds that many of the tables have common structures, suggesting that an analytical continuation in the rank f may be possible.

In this paper, the linear equation method (LEM) is used to evaluate ISFs of $S_f \supset S_{f-1}$. The LEM has proven to be an effective method for dealing with coupling and recoupling coefficients of Hecke, Brauer, and Birman–Wenzl algebras in analytical form.[13–17] In Ref. 17, tensor product reduction coefficients of Hecke algebras $H_f(q)$ are also discussed within the LEM framework. The tensor product reduction coefficients reduce to CGCs of S_f when $q \to 1$. In Sec. II, the LEM for evaluating ISFs of $S_f \supset S_{f-1}$ will be outlined. Analytical expressions of ISFs of $S_f \supset S_{f-1}$ for the coupling $[f-1,1]\cdot[f-1,1]$, $[f-1,1]\cdot[f-2,2]$, $[f-2,1,1]\cdot[f-2,1,1]$ are tabulated in Sec. III.

II. THE LINEAR EQUATION METHOD

The symmetric group S_f can be defined by $f-1$ generators $\{g_i;\ i=1,2,\ldots,f-1\}$, which are nothing but adjacent permutations that satisfy the following relations:

$$g_i g_{i+1} g_i = g_{i+1} g_i g_{i+1},$$
$$g_i g_j = g_j g_i \quad \text{for} \quad |i-j| \geqslant 2, \tag{1}$$

and the constraint

$$g_i^2 = 1. \tag{2}$$

Consider two symmetric groups of the same rank $S_f^{(k)}$, $k=1,2$. The inner product $S_f^{(1)} \cdot S_f^{(2)}$ can be defined in terms of the generators of $g_i^{(k)} \in S_f^{(k)}$ with

$$G_i = g_i^{(1)} g_i^{(2)} \quad \in S_f^{(1)} \cdot S_f^{(2)}, \tag{3}$$

where $i=1,2,\ldots,f-1$. It can be verified easily that the new generators G_i with $i=1,2,\ldots,f-1$ satisfy (1) and (2). Therefore, the $\{G_i\}$ generate the symmetric group S_f.

The reduction, or CG series of the symmetric group, is designated

$$[\nu_1]\cdot[\nu_2] = \sum_{\nu} \{\nu_1 \nu_2 \nu\}[\nu], \tag{4}$$

where $[\nu_1]$ and $[\nu_2]$ are irreps of $S_f^{(1)}$ and $S_f^{(2)}$, respectively, $[\nu]$ is an irrep of S_f, and $\{\nu_1 \nu_2 \nu\}$ is multiplicity of $[\nu]$ in the reduction.

Let $|Y_{m_k}^{[\nu_k]}\rangle$ with $k=1$, 2 be basis vectors of the symmetric groups S_f^k. Then, uncoupled basis vectors of $S_f^1 \cdot S_f^2$ can be denoted as

$$|Y_{m_1}^{[\nu_1]}\rangle |Y_{m_2}^{[\nu_2]}\rangle, \tag{5}$$

where $Y_m^{[\nu]}$ denotes a standard Young tableau and the $|Y_m^{[\nu]}\rangle$ orthogonal basis vectors, that is, the $|Y_m^{[\nu]}\rangle$ satisfy $\langle Y_m^{[\nu]} | Y_{m'}^{[\nu]} \rangle = \delta_{mm'}$, $[\nu] \equiv [\nu_1 \nu_2 \cdots \nu_f]$ with $\nu_1 \geqslant \nu_2 \geqslant \cdots \geqslant \nu_f$ and $\Sigma_i \nu_i = f$. Here, f denotes an irrep of S_f, and the Yamanouchi basis $[\nu]m$ operates on the indices of the basis vectors in the so-called decreasing page order of the Yamanouchi symbol.[13] There exist unitary transformations between the uncoupled basis vectors (5) and basis vectors for an irrep $[\nu]$ of S_f, namely

$$|Y_m^{[\nu]}; \tau\rangle = \sum_{m_1 m_2} C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2} |Y_{m_1}^{[\nu_1]}\rangle |Y_{m_2}^{[\nu_2]}\rangle, \tag{6}$$

where τ is a multiplicity label needed in the decomposition $S_f^{(1)}\cdot S_f^{(2)}\downarrow S_f$. The coefficients $C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2}$ appearing in (6) are the CGCs of $S_f^{(1)}\cdot S_f^{(2)}\downarrow S_f$. The CGCs satisfy unitary conditions

$$\sum_{m_1m_2} C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2}C^{[\nu']m';\tau'}_{[\nu_1]m_1;[\nu_2]m_2}=\delta_{\nu\nu'}\delta_{mm'}\delta_{\tau\tau'}, \tag{7a}$$

$$\sum_{m\tau} C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2}C^{[\nu]m;\tau}_{[\nu_1]m_1';[\nu_2]m_2'}=\delta_{m_1m_1'}\delta_{m_2m_2'}, \tag{7b}$$

and the following symmetry property:

$$C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2}=\epsilon(\nu_1\nu_2\nu)C^{[\nu]m;\tau}_{[\nu_2]m_2;[\nu_1]m_1}, \tag{8}$$

where $\epsilon(\nu_1\nu_2\nu)$ is a phase factor that will be determined later.

We can use the linear equation method (LEM),[17] i.e., the intertwining relations among the CGCs derived from generators of S_f, to evaluate the CGCs of $S_f\cdot S_f\downarrow S_f$. Let $g_iY_m^{[\nu]}$ be the Young tableau obtained by interchanging the numbers i and $i+1$ in $Y_m^{[\nu]}$. It is understood that if the resultant tableau is not a standard one, the corresponding basis vector $|g_iY_m^{[\nu]}\rangle$ is set to zero. First of all, the results of generators $\{g_i^{(k)},\ i=1,2,\ldots,f-1;\ k=1,2\}$ acting on the uncoupled basis vectors $|Y^{[\nu_1]}_{m_1}\rangle|Y^{[\nu_2]}_{m_2}\rangle$ can be known directly from the standard results of the symmetric group given by

$$g_i|Y_m^{[\nu]}\rangle=\frac{1}{d_i}|Y_m^{[\nu]}\rangle+\left(\frac{(d_i+1)(d_i-1)}{d_i^2}\right)^{1/2}|(g_iY_m^{[\nu]})\rangle, \tag{9}$$

where d_i is the axial distance from the box i to the box $i+1$ in the Young tableau $Y_m^{[\lambda]}$ with movement upward and to the right being counted as positive.

Applying $G_i=g_i^{(1)}g_i^{(2)}$ with $i=1,2,\ldots,f-1$ to (6), the left-hand side of (6) becomes

$$\sum_{m';m_1'm_2'}(G_i)^{[\nu]}_{m'm}C^{[\nu]m';\tau}_{[\nu_1]m_1';[\nu_2]m_2'}|Y^{[\nu_1]}_{m_1'}\rangle|Y^{[\nu_2]}_{m_2'}\rangle, \tag{10}$$

where $(G_i)_{m'm}$ is a matrix element of G_i in the standard basis given by (9). On the other hand, the right-hand side of (6) becomes

$$\sum_{m_1m_2m_1'm_2'}C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2}(g_i^{(1)})_{m_1'm_1}(g_i^{(2)})_{m_2'm_2}|Y^{[\nu_1]}_{m_1'}\rangle|Y^{[\nu_2]}_{m_2'}\rangle, \tag{11}$$

where $(g_i^{(k)})_{m_i'm_i}$ with $k=1,2$ are matrix elements of $g_i^{(k)}$ in the standard basis vectors of $S_f^{(k)}$, which can also be obtained by using Eq. (9). Combining (10) and (11), we can establish linear relations among the CGCs $C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2}$

$$\sum_{m'}(G_i)^{[\nu]}_{m'm}C^{[\nu]m';\tau}_{[\nu_1]m_1';[\nu_2]m_2'}=\sum_{m_1m_2}C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2}(g_i^{(1)})_{m_1'm_1}(g_i^{(2)})_{m_2'm_2}. \tag{12}$$

These relations, together with unitary conditions (7), are sufficient to determine the $C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2}$ up to an overall phase factor, which can be fixed by requiring that the CGCs with smallest m and m_1 be positive

$$(C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2})\big|_{(m,m_1)=\min}\rangle 0, \tag{13}$$

where $(m,m_1)=\min$ means taking the index m as small as possible followed by taking m_1 as small as possible for which the CGC $C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2}$ is nonzero. Then, it can easily be seen that

$$\epsilon(\nu_1\nu_2\nu)=\mathrm{Sign}((C^{[\nu]m;\tau}_{[\nu_1]m_1;[\nu_2]m_2})|_{(m_2,m_1)=\min}). \tag{14}$$

Using this method, one can easily deduce the following simple results.

(1) If both $[\nu_1]$ and $[\nu_2]$ are symmetric, $[\nu_1]=[\nu_2]=[\nu]$,

$$C^{[\nu]}_{[\nu][\nu]}=1, \tag{15a}$$

(2) If $[\nu_1]$ is symmetric, while $[\nu_2]$ is neither symmetric nor antisymmetric

$$C^{[\nu]m}_{[\nu_1][\nu_2]m_2}=\delta_{\nu\nu_2}\delta_{mm_2}, \tag{15b}$$

(3) If $[\nu_1]$ is antisymmetric, while $[\nu_2]$ is symmetric

$$C^{[\nu]}_{[\nu_1][\nu_2]}=\delta_{\nu\nu_1}. \tag{15c}$$

The LEM stated above, however, can only be used to evaluate CGCs of S_f for specific f. According to the Racah factorization lemma,[18,19] the CGCs of S_f can be written as

$$C^{[\nu]\tau m}_{[\nu_1]m_1;[\nu_2]m_2}=\sum_{\tau'}\left\langle\begin{matrix}[\nu_1] & [\nu_2]\\ [\nu_1'] & [\nu_2']\end{matrix}\middle|\begin{matrix}\tau[\nu]\\ \tau'[\nu']\end{matrix}\right\rangle C^{\tau'[\nu']m'}_{[\nu_1']m_1';[\nu_2']m_2'}, \tag{16}$$

where $[\nu_1']$, $[\nu_2']$, and $[\nu']$, are possible irreps occurring in the reductions $[\nu_1]\downarrow[\nu_1']$, $[\nu_2]\downarrow[\nu_2']$, and $[\nu]\downarrow[\nu']$ of $S_f\supset S_{f-1}$, respectively,

$$\left\langle\begin{matrix}[\nu_1] & [\nu_2]\\ [\nu_1'] & [\nu_2']\end{matrix}\middle|\begin{matrix}\tau[\nu]\\ \tau'[\nu']\end{matrix}\right\rangle$$

is the ISF of $S_f\supset S_{f-1}$ and $C^{\tau'[\nu']m'}_{[\nu_1']m_1';[\nu_2']m_2'}$ is the CGCs of S_{f-1}, similar to S_f, $[\nu_1']m_1'$, $[\nu_2']m_2'$, $[\nu']m'$ denote Yamanouchi basis of S_{f-1}, and τ' is the multiplicity label for the inner product $[\nu_1']\cdot[\nu_2']\downarrow[\nu']$. In the multiplicity-free case, the multiplicity labels τ and τ' are redundant; one simply gets

$$C^{[\nu]m}_{[\nu_1]m_1;[\nu_2]m_2}=\left\langle\begin{matrix}[\nu_1] & [\nu_2]\\ [\nu_1'] & [\nu_2']\end{matrix}\middle|\begin{matrix}[\nu]\\ [\nu']\end{matrix}\right\rangle C^{[\nu']m'}_{[\nu_1']m_1';[\nu_2']m_2'}. \tag{17}$$

The ISFs of $S_f\supset S_{f-1}$ satisfy the unitary conditions

$$\sum_{\nu_1'\nu_2'\tau'}\left\langle\begin{matrix}[\nu_1] & [\nu_2]\\ [\nu_1'] & [\nu_2']\end{matrix}\middle|\begin{matrix}\tau[\nu]\\ \tau'[\nu']\end{matrix}\right\rangle\left\langle\begin{matrix}[\nu_1] & [\nu_2]\\ [\nu_1'] & [\nu_2']\end{matrix}\middle|\begin{matrix}\overline{\tau}[\overline{\nu}]\\ \tau'[\nu']\end{matrix}\right\rangle=\delta_{\nu\overline{\nu}}\delta_{\tau\overline{\tau}}, \tag{18a}$$

$$\sum_{\tau\nu}\left\langle\begin{matrix}[\nu_1] & [\nu_2]\\ [\nu_1'] & [\nu_2']\end{matrix}\middle|\begin{matrix}\tau[\nu]\\ \tau'[\nu']\end{matrix}\right\rangle\left\langle\begin{matrix}[\nu_1] & [\nu_2]\\ [\overline{\nu}_1'] & [\overline{\nu}_2']\end{matrix}\middle|\begin{matrix}\tau[\nu]\\ \overline{\tau}'[\nu']\end{matrix}\right\rangle=\delta_{\overline{\nu}_1'\nu_1'}\delta_{\overline{\nu}_2'\nu_2'}\delta_{\tau'\overline{\tau}'}. \tag{18b}$$

Our method for evaluating analytical expressions of the ISFs of $S_f\supset S_{f-1}$ can be summarized as follows. First, we use linear relations among the CGCs of S_f provided by (12) for inner product $[\nu_1]\cdot[\nu_2]\downarrow[\nu]$ with smallest f, as long as the irreps $[\nu_1]$, $[\nu_2]$, and $[\nu]$ exist. For example, irreps $[f]$, $[f-1,1]$ exist when $f\geqslant 2$, while irrep $[f-2,1,1]$ only exists when $f\geqslant 3$, and $[f-2,2]$ only exists when $f\geqslant 4$. Then, in the multiplicity-free cases, we use (17) together with (12) to get linear

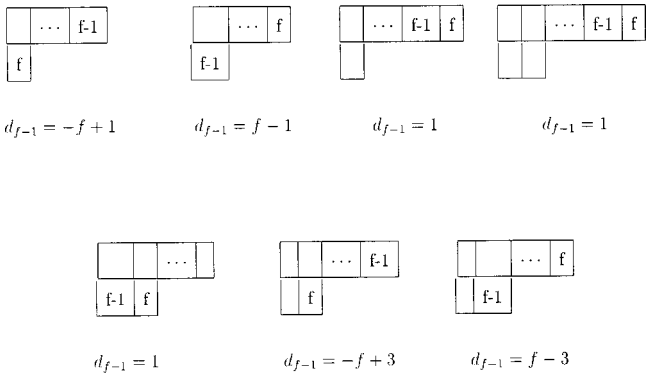

FIG. 1. Axial distance d_{f-1} for $[f-1,1]$ and $[f-2,2]$ with different possible locations of the final two numbers $f-1$ and f in the corresponding Young tableau.

relations of the corresponding ISFs of $S_f \supset S_{f-1}$. The ISFs of $S_f \supset S_{f-1}$ are f-dependent. One can replace the ISFs of $S_f \supset S_{f-1}$ for the specific f by those with general f. Actually, it can be shown that the relations among the ISFs of the same coupling are the same for any f value. Therefore, one can get analytical expressions for ISFs of $S_f \supset S_{f-1}$ from those for specific f. To do this, one has to use analytical expressions of the axial distance d_{f-1} in (12). Values of d_{f-1} for some irreps with different reductions of $S_f \supset S_{f-1}$ are shown in Fig. 1. Finally, one can use the linear relations obtained together with the unitary condition

$$\sum_{\nu_1' \nu_2'} \left\langle \begin{matrix} [\nu_1] & [\nu_2] \\ [\nu_1'] & [\nu_2'] \end{matrix} \middle| \begin{matrix} [\nu] \\ [\nu'] \end{matrix} \right\rangle^2 = 1, \tag{19}$$

to derive all ISFs involved in these linear relations up to an overall phase. The phase convention used here is consistent with that chosen for the CGCs of S_f shown in Ref. 20. We will use the symbol $[\nu]_p$ to denote $[\nu][\nu']$ for the reduction $[\nu]\downarrow[\nu']$ of $S_f \supset S_{f-1}$, where p denotes the last number f in the pth row of the Young diagram $[\nu]$. For example, $[f-1,1][f-1] \equiv [f-1,1]_2$, $[f-1,1][f-2,1] \equiv [f-1,1]_1$, etc. This labeling scheme greatly simplifies the final results. In the following, we give an example to show how the method works.

A. Example 1. Deriving ISFs of $S_f \supset S_{f-1}$ for the inner product $[f-1,1]\cdot[f-1,1]\downarrow[f]_1$

In this case, we need to work with $f=3$ because there are two reductions in $S_f \supset S_{f-1}$ for irrep $[f-1,1]$, namely $[f-1,1]\downarrow[f-2,1]$ and $[f-1]$, and the smallest f allowed for $[f-2,1]$ is $f \geqslant 3$. Hence, we need to consider the following expansion:

$$|[3]_1\rangle = \sum_{m_1 m_2} C^{[3]_1}_{m_1 m_2} |Y^{[21]}_{m_1} Y^{[21]}_{m_2}\rangle. \tag{20a}$$

Step 1. Acting with $G_1 = g_1^{(1)} g_1^{(2)}$ on (20a), one gets

$$|[3]_1\rangle = c_1 |Y^{[21]}_1 Y^{[21]}_1\rangle + c_2 |Y^{[21]}_2 Y^{[21]}_2\rangle. \tag{20b}$$

Other CGCs are obviously zero in this case according to the linear relations obtained from the results of the G_1 action.

Step 2. We need first to extend $[3] \to [f]$, and $[21] \to [f-1,1]$. Hence, (20b) becomes

$$|[f]_1\rangle = c_1 |[f-1,1]_1 [f-1,1]_1\rangle + c_2 |[f-1,1]_2 [f-1,1]_2\rangle. \tag{20c}$$

Step 3. By acting with $G_2 \to G_{f-1}$ on (20c), the left-hand side of (20c) is

$$c_1|[f-1,1]_1[f-1,1]_1\rangle+c_2|[f-1,1]_2[f-1,1]_2\rangle, \tag{20d}$$

while the right-hand side of (20c) becomes

$$\begin{aligned}
&c_1\Bigg(\frac{1}{(f-1)^2}|[f-1,1]_1[f-1,1]_1\rangle+\frac{f(f-2)}{(f-1)^2}|[f-1,1]_2[f-1,1]_2\rangle\\
&\quad+\frac{\sqrt{f(f-2)}}{(f-1)^2}(|[f-1,1]_1[f-1,1]_2\rangle+|[f-1,1]_2[f-1,1]_1\rangle\Bigg)\\
&\quad+c_2\Bigg(\frac{1}{(f-1)^2}|[f-1,1]_2[f-1,1]_2\rangle+\frac{f(f-2)}{(f-1)^2}|[f-1,1]_1[f-1,1]_1\rangle\\
&\quad-\frac{\sqrt{f(f-2)}}{(f-1)^2}(|[f-1,1]_1[f-1,1]_2\rangle+|[f-1,1]_2[f-1,1]_1\rangle\Bigg).
\end{aligned} \tag{20e}$$

Combining (20d) and (20e), we obtain

$$c_1=c_2. \tag{20f}$$

Because of analyticity, (20f) should hold for $f\geqslant 3$. Hence, for general f, (20c) should be written as

$$\begin{aligned}
|[f]_1\rangle&=C_f|[f-1,1]_2[f-1,1]_2\rangle+C_f\sum_{m_1m_2}|Y^{[f-1,1]_1}_{m_1}Y^{[f-1,1]_1}_{m_2}\rangle\\
&=C_f|[f-1,1]_2[f-1,1]_2\rangle+\frac{C_f}{C_{f-1}}(|[f-1,1]_1[f-1,1]_1\rangle)^{[f]_1},
\end{aligned} \tag{20g}$$

where

$$C_f=c_1=\langle[f-1,1]_2[f-1,1]_2|[f]_1\rangle,\quad c_2=\frac{C_f}{C_{f-1}}=\langle[f-1,1]_1[f-1,1]_1|[f]_1\rangle \tag{21}$$

are the ISFs involved in the coupling.

Step 4. Finally, using the unitary condition (19), we obtain the recursion relation for C_f^2 with

$$C_f^2=\frac{C_{f-1}^2}{C_{f-1}^2+1}. \tag{22}$$

Starting with $C_2^2=1$, we finally get

$$\langle[f-1,1]_2[f-1,1]_2|[f]_1\rangle=+\sqrt{\frac{1}{f-1}},\quad \langle[f-1,1]_1[f-1,1]_1|[f]_1\rangle=+\sqrt{\frac{f-2}{f-1}}, \tag{23}$$

where the overall phase is fixed with $C_f>0$ which is consistent with the phase convention for the CGCs of S_f set in Ref. 20. ISFs of $[f-1,1]\cdot[f-1,1]\downarrow[f-1,1]_2$ can be obtained by the unitary condition

$$\sum_{[\nu]_p}\langle[\nu_1]_{p_1}[\nu_2]_{p_2}|[\nu]_p\rangle^2=1 \tag{24}$$

or by the similar procedure. The results are shown in Table III.

TABLE I. Some inner product reduction rules of S_f.

$$
\begin{aligned}
&[f-1,1]\cdot[f-1,1]=[f]+[f-1,1]+[f-2,1,1]+[f-2,2]\\
&[f-1,1]\cdot[f-2,2]=[f-1,1]+[f-2,2]+[f-2,1,1]\\
&\qquad\qquad+[f-3,3]+[f-3,2,1]\\
&[f-2,1,1]\cdot[f-1,1]=[f-1,1]+[f-2,2]+[f-2,1,1]\\
&\qquad\qquad+[f-3,2,1]+[f-3,1^3]\\
&[f-2,2]\cdot[f-2,2]=[f]+[f-1,1]+2[f-2,2]+[f-2,1,1]\\
&\qquad\qquad+[f-3,3]+2[f-3,2,1]+[f-3,1^3]\\
&\qquad\qquad+[f-4,4]+[f-4,3,1]+[f-4,2,2]\\
&[f-2,1,1]\cdot[f-2,2]=[f-1,1]+[f-2,2]+2[f-2,1,1]\\
&\qquad\qquad+[f-3,3]+2[f-3,2,1]+[f-3,1^3]\\
&\qquad\qquad+[f-4,3,1]+[f-4,2,1^2]\\
&[f-2,1,1]\cdot[f-2,1,1]=[f]+[f-1,1]+2[f-2,2]+[f-2,1,1]\\
&\qquad\qquad+[f-3,3]+2[f-3,2,1]+[f-3,1^3]\\
&\qquad\qquad+[f-4,2,2]+[f-4,2,1^2]+[f-4,1^4]
\end{aligned}
$$

B. Example 2. Deriving ISFs of $S_f \supset S_{f-1}$ for the inner product $[f-1,1]\cdot[f-1,1]\downarrow[f-1,1]_1$

In this example, we choose to work with $f=4$. After acting with $G_1=g_1^{(1)}g_1^{(2)}$ on an expansion similar to (20a), we get

$$
\left|\begin{matrix}124\\3\end{matrix}\right\rangle = a_1\left|\begin{matrix}124\\3\end{matrix}\right\rangle\left|\begin{matrix}123\\4\end{matrix}\right\rangle + a_2\left|\begin{matrix}123\\4\end{matrix}\right\rangle\left|\begin{matrix}124\\3\end{matrix}\right\rangle + a_3\left(-\sqrt{\frac{1}{f-2}}\left|\begin{matrix}134\\2\end{matrix}\right\rangle\left|\begin{matrix}134\\2\end{matrix}\right\rangle + \sqrt{\frac{f-3}{f-2}}\left|\begin{matrix}124\\3\end{matrix}\right\rangle\left|\begin{matrix}124\\3\end{matrix}\right\rangle\right), \tag{25}
$$

where $C^{[21]_1}_{[21]_1[21]_1}$ and $C^{[21]_1}_{[21]_2[21]_2}$ have been replaced by $C^{[f-1,1]_1}_{[f-1,1]_1[f-1,1]_1}$ and $C^{[f-1,1]_1}_{[f-1,1]_2[f-1,1]_2}$, respectively, of which the analytical expressions derived in the example 1 are used, and

$$
a_1=\langle[f-1,1]_1[f-1,1]_2|[f-1,1]_1\rangle,\quad a_2=\langle[f-1,1]_2[f-1,1]_1|[f-1,1]_1\rangle,
$$

$$
a_3=\langle[f-1,1]_1[f-1,1]_1|[f-1,1]_1\rangle \tag{26}
$$

are the corresponding ISFs. Similarly, we have

$$
\left|\begin{matrix}123\\4\end{matrix}\right\rangle = \sqrt{\frac{f-2}{f-1}}\left|\begin{matrix}123\\4\end{matrix}\right\rangle\left|\begin{matrix}123\\4\end{matrix}\right\rangle - \sqrt{\frac{1}{(f-1)(f-2)}}\left|\begin{matrix}124\\3\end{matrix}\right\rangle\left|\begin{matrix}124\\3\end{matrix}\right\rangle - \sqrt{\frac{f-3}{(f-1)(f-2)}}\left|\begin{matrix}134\\2\end{matrix}\right\rangle\left|\begin{matrix}134\\2\end{matrix}\right\rangle. \tag{27}
$$

By acting with $G_3\to G_{f-1}=g_{f-1}^{(1)}g_{f-1}^{(2)}$ on (25), the left-hand side of (25) becomes

TABLE II. Dimensions of some irreps of S_f.

$$
\begin{aligned}
&\dim([f])=1\\
&\dim([f-1,1])=f-1\\
&\dim([f-2,2])=f(f-3)/2\\
&\dim([f-2,1^2])=(f-1)(f-2)/2\\
&\dim([f-3,2,1])=f(f-2)(f-4)/3\\
&\dim([f-3,1^3])=(f-1)(f-2)(f-3)/6\\
&\dim([f-3,3])=f(f-1)(f-5)/6\\
&\dim([f-4,4])=f(f-1)(f-2)(f-7)/24\\
&\dim([f-4,2,1^2])=f(f-2)(f-3)(f-5)/8\\
&\dim([f-4,2^2])=f(f-1)(f-4)(f-5)/12\\
&\dim([f-4,3,1])=f(f-1)(f-3)(f-6)/8\\
&\dim([f-4,1^4])=(f-1)(f-2)(f-3)(f-4)/24
\end{aligned}
$$

TABLE III. ISFs of $[f-1,1]\cdot[f-1,1]\downarrow[f]+[f-1,1]$.

	$[f]_1$	$[f-1,1]_2$
$[f-1,1]_2[f-1,1]_2$	$\sqrt{\frac{1}{f-1}}$	$\sqrt{\frac{f-2}{f-1}}$
$[f-1,1]_1[f-1,1]_1$	$\sqrt{\frac{f-2}{f-1}}$	$-\sqrt{\frac{1}{f-1}}$

$$G_{f-1}\left|\begin{matrix}124\\3\end{matrix}\right\rangle=\frac{1}{f-1}\left|\begin{matrix}124\\3\end{matrix}\right\rangle+\sqrt{\frac{f(f-2)}{(f-1)^2}}\left|\begin{matrix}123\\4\end{matrix}\right\rangle, \tag{28}$$

while the right-hand side of (25) becomes

$$\begin{aligned}&\left(-\frac{a_1}{(f-1)^2}+a_2\frac{f(f-2)}{(f-1)^2}+a_3\sqrt{\frac{f(f-3)}{(f-1)^4}}\right)\left|\begin{matrix}124\\3\end{matrix}\right\rangle\left|\begin{matrix}123\\4\end{matrix}\right\rangle\\&\quad+\left(a_1\frac{f(f-2)}{(f-1)^2}-\frac{a_2}{(f-1)^2}+a_3\sqrt{\frac{f(f-3)}{(f-1)^4}}\right)\left|\begin{matrix}123\\4\end{matrix}\right\rangle\left|\begin{matrix}124\\3\end{matrix}\right\rangle\\&\quad+\left(-a_1\sqrt{\frac{f(f-2)}{(f-1)^4}}-a_2\sqrt{\frac{f(f-2)}{(f-1)^4}}+a_3\frac{\sqrt{f(f-2)(f-3)}}{(f-1)^2}\right)\left|\begin{matrix}123\\4\end{matrix}\right\rangle\left|\begin{matrix}123\\4\end{matrix}\right\rangle\\&\quad+\left(a_1\sqrt{\frac{f(f-2)}{(f-1)^4}}+a_2\sqrt{\frac{f(f-2)}{(f-1)^4}}+\frac{a_3}{(f-1)^2}\sqrt{\frac{f-3}{f-2}}\right)\left|\begin{matrix}124\\3\end{matrix}\right\rangle\left|\begin{matrix}124\\3\end{matrix}\right\rangle-a_3\sqrt{\frac{1}{f-2}}\left|\begin{matrix}134\\2\end{matrix}\right\rangle\left|\begin{matrix}134\\2\end{matrix}\right\rangle.\end{aligned} \tag{29}$$

Combining (25) and (27)–(29), we get

$$a_1=a_2=-\sqrt{\frac{1}{(f-1)(f-2)}},\quad a_3=\sqrt{\frac{f(f-3)}{(f-1)(f-2)}}. \tag{30}$$

Using this procedure, one can obtain all the ISFs of $S_f\supset S_{f-1}$ with smallest f as long as the couplings and the reductions exist with the specific f value. In the evaluation, the unitary condition for the ISFs given in (24) and

$$\sum_{p_1p_2}\langle[\nu_1]_{p_1}[\nu_2]_{p_2}|[\nu]_p\rangle^2=1 \tag{31}$$

are always helpful. Some examples will be given in the next section.

TABLE IV. ISFs of $[f-1,1]\cdot[f-1,1]\downarrow[f-1,1]+[f-2,2]+[f-2,1,1]$.

	$[f-1,1]_1$	$[f-2,2]_2$	$[f-2,1,1]_3$
$[f-1,1]_2[f-1,1]_1$	$-\sqrt{\frac{1}{(f-1)(f-2)}}$	$\sqrt{\frac{f(f-3)}{2(f-1)(f-2)}}$	$\sqrt{\frac{1}{2}}$
$[f-1,1]_1[f-1,1]_2$	$-\sqrt{\frac{1}{(f-1)(f-2)}}$	$\sqrt{\frac{f(f-3)}{2(f-1)(f-2)}}$	$-\sqrt{\frac{1}{2}}$
$[f-1,1]_1[f-1,1]_1$	$\sqrt{\frac{f(f-3)}{(f-1)(f-2)}}$	$\sqrt{\frac{2}{(f-1)(f-2)}}$	0

TABLE V. ISFs of $[f-1,1]\cdot[f-2,1,1]\downarrow[f-1,1]+[f-2,2]+[f-2,1,1]$.

	$[f-1,1]_2$	$[f-2,2]_2$	$[f-2,1,1]_3$
$[f-1,1]_2[f-2,1,1]_3$	$\sqrt{\frac{1}{f-2}}$	$\sqrt{\frac{f(f-3)}{2(f-1)(f-2)}}$	$\sqrt{\frac{f-3}{2(f-1)}}$
$[f-1,1]_1[f-2,1,1]_3$	0	$-\sqrt{\frac{f-2}{2(f-1)}}$	$\sqrt{\frac{f}{2(f-1)}}$
$[f-1,1]_1[f-2,1,1]_1$	$-\sqrt{\frac{f-3}{f-2}}$	$\sqrt{\frac{f}{2(f-1)(f-2)}}$	$\sqrt{\frac{1}{2(f-1)}}$

TABLE VI. ISFs of $[f-1,1]\cdot[f-2,1,1]\downarrow[f-2,2]+[f-3,2,1]$.

	$[f-2,2]_1$	$[f-3,2,1]_3$
$[f-1,1]_1[f-2,1,1]_3$	$-\sqrt{\frac{1}{(f-1)^2}}$	$\sqrt{\frac{f(f-2)}{(f-1)^2}}$
$[f-1,1]_1[f-2,1,1]_1$	$-\sqrt{\frac{f(f-2)}{(f-1)^2}}$	$-\sqrt{\frac{1}{(f-1)^2}}$

TABLE VII. ISFs of $[f-1,1]\cdot[f-2,1,1]\downarrow[f-2,1,1]+[f-3,2,1]+[f-3,1^3]$.

	$[f-2,1,1]_1$	$[f-3,2,1]_2$	$[f-3,1^3]_3$
$[f-1,1]_2[f-2,1,1]_1$	$-\sqrt{\frac{f-3}{2(f-1)}}$	$\sqrt{\frac{f(f-3)}{2(f-1)(f-2)}}$	$\sqrt{\frac{1}{f-2}}$
$[f-1,1]_1[f-2,1,1]_3$	$-\sqrt{\frac{1}{2(f-1)}}$	$\sqrt{\frac{f}{2(f-1)(f-2)}}$	$-\sqrt{\frac{f-3}{f-2}}$
$[f-1,1]_1[f-2,1,1]_1$	$-\sqrt{\frac{f}{2(f-1)}}$	$-\sqrt{\frac{f-2}{2(f-1)}}$	0

TABLE VIII. ISFs of $[f-1,1]\cdot[f-2,2]\downarrow[f-1,1]+[f-2,2]+[f-2,1,1]$.

	$[f-1,1]_1$	$[f-2,2]_2$	$[f-2,1,1]_3$
$[f-1,1]_2[f-2,2]_2$	$\sqrt{\frac{1}{f-2}}$	$\sqrt{\frac{f-4}{2(f-2)}}$	$\sqrt{\frac{1}{2}}$
$[f-1,1]_1[f-2,2]_2$	$\sqrt{\frac{4}{f(f-2)(f-3)}}$	$\sqrt{\frac{f(f-4)}{2(f-2)(f-3)}}$	$-\sqrt{\frac{(f-2)^2}{2\,f(f-3)}}$
$[f-1,1]_1[f-2,2]_1$	$\sqrt{\frac{(f-1)^2(f-4)}{f(f-2)(f-3)}}$	$-\sqrt{\frac{f}{2(f-2)(f-3)}}$	$-\sqrt{\frac{f-4}{2\,f(f-3)}}$

TABLE IX. ISFs of $[f-1,1]\cdot[f-2,2]\downarrow[f-2,1,1]+[f-3,2,1]$.

	$[f-2,1,1]_1$	$[f-2,2]_2$
$[f-1,1]_1[f-2,2]_2$	$-\sqrt{\frac{1}{(f-3)^2}}$	$\sqrt{\frac{(f-2)(f-4)}{(f-3)^2}}$
$[f-1,1]_1[f-2,2]_1$	$\sqrt{\frac{(f-2)(f-4)}{(f-3)^2}}$	$\sqrt{\frac{1}{(f-3)^2}}$

III. SOME MULTIPLICITY-FREE ISFS OF $S_f \supset S_{f-1}$

In this section, ISFs of $S_f \supset S_{f-1}$ for the inner products $[f-1,1]\cdot[f-1,1]$, $[f-1,1]\cdot[f-2,2]$, and $[f-2,1,1]\cdot[f-1,1]$, all of which are multiplicity-free, will be tabulated using the procedure outlined in Sec. II. Actually, we do not need the inner product reduction rule of (4) in the calculation because the LEM will automatically generate the product irreps. Some inner product reduction rules of S_f are listed in Table I. One can check their validity by using the dimension formulas shown in Table II. The ISFs are tabulated in Tables III–IX. It should be noted that Table III should be evaluated with $f=3$ and the f-continuation by the LEM; Tables IV and V should be evaluated with $f=4$; Tables VI–IX with $f=5$; and Table X with $f=6$. The phase is chosen to be consistent with that of the CGCs of S_f given in Ref. 20. It is clear that one needs to work with higher rank cases for most other irreps. For example, one needs to work with $f=7$ for the inner product reduction $[f-2,2]\cdot[f-2,2]\downarrow[f-4,3,1]$, and with $f=8$ for $[f-2,2]\cdot[f-2,2]\downarrow[f-4,4]$. For any $f\geqslant 3$, one can always derive some ISFs of $S_f \supset S_{f-1}$ analytically by using the LEM outlined in Sec. II. Some trivial ISFs involved in the inner product reduction considered are

$$\langle[f-1,1]_1[f-1,1]_1|[f-2,2]_1\rangle=1,\quad \langle[f-1,1]_1[f-1,1]_1|[f-2,1,1]_1\rangle=1,$$

$$\langle[f-1,1]_1[f-2,2]_2|[f-1,1]_2\rangle=1,\quad \langle[f-1,1]_1[f-2,2]_1|[f-3,3]_1\rangle=1,$$

$$\langle[f-1,1]_1[f-2,2]_1|[f-3,2,1]_1\rangle=1,\quad \langle[f-2,1,1]_3[f-1,1]_1|[f-1,1]_2\rangle=-1,$$

$$\langle[f-2,1,1]_1[f-1,1]_1|[f-3,2,1]_1\rangle=1,\quad \langle[f-2,1,1]_1[f-1,1]_1|[f-3,1,1]_1\rangle=1.$$

IV. CONCLUSIONS

In this paper, an algebraic routine for the evaluation of analytical expressions for isoscalar factors (ISFs) of $S_f \supset S_{f-1}$ is formulated based on the linear equation method (LEM) and the analytical continuation of the rank f. As examples, ISFs of $S_f \supset S_{f-1}$ for the coupling $[f-1,1]\cdot[f-1,1]$, $[f-1,1]\cdot[f-2,2]$ and $[f-2,1,1]\cdot[f-2,1,1]$ are tabulated. It is obvious that the number of ISF tables is greatly reduced in comparison with numerical results calculated using other

TABLE X. $[f-1,1]\cdot[f-2,2]\downarrow[f-2,2]+[f-3,3]+[f-3,2,1]$.

	$[f-2,2]_1$	$[f-3,3]_2$	$[f-3,2,1]_3$
$[f-1,1]_2[f-2,2]_1$	$-\sqrt{\frac{2(f-2)}{(f-1)^2(f-4)}}$	$\sqrt{\frac{f(f-5)}{3(f-1)(f-4)}}$	$\sqrt{\frac{2f(f-2)}{3(f-1)^2}}$
$[f-1,1]_1[f-2,2]_2$	$-\sqrt{\frac{f}{(f-1)(f-3)(f-4)}}$	$\sqrt{\frac{2(f-5)}{3(f-3)(f-4)}}$	$-\sqrt{\frac{(f-2)^2}{3(f-1)(f-3)}}$
$[f-1,1]_1[f-2,2]_1$	$\sqrt{\frac{f(f-5)(f-2)^2}{(f-1)^2(f-3)(f-4)}}$	$\sqrt{\frac{8(f-2)}{3(f-1)(f-3)(f-4)}}$	$\sqrt{\frac{f-5}{3(f-1)^2(f-3)}}$

methods. Though the method is only illustrated for multiplicity-free cases, the method can also be applied to cases with multiplicity. Similar to the LEM applied to the Hecke algebra case,[13] the same linear relation given by (12) hold for ISFs with different multiplicity labels in the case with multiplicity. The ISFs of $S_f \supset S_{f-1}$ with different multiplicity labels should be chosen to be orthogonal to each other. Therefore, the solution to the ISFs of $S_f \supset S_{f-1}$ will not be unique and depends on the phase convention and symmetry properties imposed on the ISFs.[13,20] However, one can use the procedure with smallest f and f-continuation outlined in this paper to derive the ISFs with multiplicity. It can be seen from Table I that the multiplicity case occurs for $f \geqslant 6$. Hence, one needs to work at least with $f \geqslant 6$ for ISFs with multiplicity, which will be studied in our next paper.

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Metrics on the real quantum plane

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Using the frame formalism we determine some possible metrics and metric-compatible connections on the noncommutative differential geometry of the real quantum plane. By definition, a metric maps the tensor product of two 1-forms into a ''function'' on the quantum plane. It is symmetric in a modified sense, namely in the definition of symmetry one has to replace the permutator map with a deformed map σ fulfilling some suitable conditions. Correspondingly, also the definition of the Hermitian conjugate of the tensor product of two 1-forms is modified (but reduces to the standard one if σ coincides with the permutator). The metric is real with respect to such modified $*$-structure. © *2002 American Institute of Physics.*
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I. INTRODUCTION AND NOTATION

It is an old idea[1,2] that a noncommutative modification of the algebraic structure of space–time could provide a regularization of the divergences of quantum field theory, because the representations of noncommutative ''spaces'' have a lattice-like structure. The main aim of noncommutative geometry[3] is to endow such an algebra with additional structures (starting from a differential calculus), so as to build a bridge between the algebra and its ''geometrical'' interpretation. Since there is no unique prescription how to do this, it is useful to test possible prescriptions first on simpler models.

In this paper we choose as a noncommutative space(time) algebra model the so-called real quantum or Manin plane,[4] and as a differential calculus upon it the so-called Wess–Zumino calculus.[5,6] The latter is charaterized by the property that the relations defining the module of 1-forms are covariant under the action of the quantum group $SL_q(2)$ and homogeneous in the generators. We adopt the noncommutative geometry formalism of Refs. 7–11.

We start with a brief description of the latter. Let $\mathcal{A}$ be an algebra with differential calculus $\{\Omega^*(\mathcal{A}),d\}$[3] [here, $\Omega^*(\mathcal{A})$ denotes the algebra of differential forms on $\mathcal{A}$ and d the exterior derivative acting on the latter] and suppose that the calculus has a *frame*,[7,10] i.e., a basis of 1-forms θ^i $(i=1,2,\ldots,n)$ which commutes with the elements of the algebra

$$\theta^i f = f\theta^i. \tag{1.1}$$

The relation

$$df = \theta^i e_i f \tag{1.2}$$

(with $f \in \mathcal{A}$) defines a set of derivations e_i dual to θ^i, from which it follows that the module structure of $\Omega^1(\mathcal{A})$ is given by

$$f\,dg = \theta^i f e_i g, \quad dg\,f = \theta^i (e_i g) f.$$

We see that the $\mathcal{A}$-bimodule $\Omega^1(\mathcal{A})$ is free of rank n as a left or right module. It can therefore be identified with the direct sum

$$\Omega^1(\mathcal{A}) = \bigoplus_1^n \mathcal{A}, \tag{1.3}$$

of n copies of $\mathcal{A}$. In this representation θ^i is given by the element of the direct sum with the unit in the ith position and zero elsewhere. We shall refer to the integer n as the dimension of the geometry.

The wedge product π in $\Omega^*(\mathcal{A})$ fulfills relations of the form

$$\theta^i \theta^j \equiv \pi(\theta^i \otimes_{\mathcal{A}} \theta^j) = P^{ij}_{kl} \theta^k \theta^l \tag{1.4}$$

(we omit the symbol $\wedge$ of the wedge product), where P is a projector

$$P^{ij}_{mn} P^{mn}_{kl} = P^{ij}_{kl}, \tag{1.5}$$

with entries $P^{ij}_{kl} \in \mathcal{Z}(\mathcal{A})$. If in particular the wedge product is such that the θ^i anticommute, then P is the antisymmetric projector

$$P^{ij}_{kl} = \tfrac{1}{2}(\delta^i_k \delta^j_l - \delta^j_k \delta^i_l).$$

From (1.3) it follows immediately that the algebra and its differential calculus are related in a simple manner. Let $\wedge^*_P$ be the exterior algebra over $\mathbb{C}^n$ with the wedge product defined by (1.4). Then, with the identification (1.3) it follows that one can write

$$\Omega^*(\mathcal{A}) = \mathcal{A} \otimes \wedge^*_P. \tag{1.6}$$

Since the exterior derivative of θ^i is a 2-form, it can necessarily be written as

$$d\theta^i = -\tfrac{1}{2} C^i_{jk} \theta^j \theta^k,$$

where, because of (1.4), the structure elements can be chosen to satisfy the constraints

$$C^i_{jk} P^{jk}_{lm} = C^i_{lm}.$$

It will also be convenient to introduce the quantities

$$C^{ij}_{kl} = \delta^i_k \delta^j_l - 2P^{ij}_{kl}. \tag{1.7}$$

Then, from (1.5) we find that

$$C^{ij}_{kl} C^{kl}_{mn} = \delta^i_m \delta^j_n. \tag{1.8}$$

For simplicity, we shall further assume that the e_i are inner derivations: $e_i f = [\lambda_i, f]$, $\lambda_i \in \mathcal{A}$. From the θ^i we can construct a 1-form

$$\theta = -\lambda_i \theta^i \tag{1.9}$$

in $\Omega^1(\mathcal{A})$ which plays the role of a Dirac operator[3]

$$df = -[\theta, f]. \tag{1.10}$$

One can show that from the general consistency of the differential calculus it follows that

$$2P^{ij}_{kl}\lambda_i\lambda_j - F^i_{kl}\lambda_i - K_{kl} = 0, \tag{1.11}$$

for some array of elements $F^i_{jk}, K_{kl} \in \mathcal{Z}(\mathcal{A})$. In the cases which interest us here, the latter vanish.

In order to consistently define a covariant derivative, we need to introduce[8] a flip σ, i.e., a $\mathcal{A}$-bilinear map

$$\Omega^1(\mathcal{A}) \otimes_{\mathcal{A}} \Omega^1(\mathcal{A}) \overset{\sigma}{\to} \Omega^1(\mathcal{A}) \otimes_{\mathcal{A}} \Omega^1(\mathcal{A}). \tag{1.12}$$

In the case of the De-Rham calculus on the commutative algebra of functions on an ordinary manifold, it reduces to $\sigma(\omega \otimes_{\mathcal{A}} \omega') = \omega' \otimes_{\mathcal{A}} \omega$. In terms of the frame it is given by $S^{ij}_{kl} \in \mathcal{Z}(\mathcal{A})$, defined by

$$\sigma(\theta^i \otimes_{\mathcal{A}} \theta^j) = S^{ij}_{kl}\theta^k \otimes_{\mathcal{A}} \theta^l.$$

A covariant derivative on the module $\Omega^1(\mathcal{A})$ is a map

$$\Omega^1(\mathcal{A}) \overset{D}{\to} \Omega^1(\mathcal{A}) \otimes_{\mathcal{A}} \Omega^1(\mathcal{A}), \tag{1.13}$$

satisfying both a left and a right Leibniz rule. We use the ordinary left Leibniz rule and define the right Leibniz rule as

$$D(\xi f) = \sigma(\xi \otimes_{\mathcal{A}} df) + (D\xi) f, \tag{1.14}$$

for arbitrary $f \in \mathcal{A}$ and $\xi \in \Omega^1(\mathcal{A})$. The connection 1-form $\omega^i_k \equiv \omega^i_{jk}\theta^j$ is defined by

$$D\theta^i = \omega^i_k \otimes_{\mathcal{A}} \theta^k. \tag{1.15}$$

We shall impose the condition

$$\pi \circ (\sigma + 1) = 0, \tag{1.16}$$

so that the antisymmetric part of a symmetric tensor vanishes. This can be considered as a condition on the product or on the flip. In ordinary geometry it is the definition of π; a 2-form can be considered as an antisymmetric tensor. Because of this condition the torsion is a bilinear map.[11] The most general solution can be written in the form

$$1 + \sigma = (1 - \pi) \circ \tau, \tag{1.17}$$

where τ is an an arbitrary $\mathcal{A}$-bilinear map. Suppose that τ is invertible. Then, because of the identity

$$1 = \pi + (1 + \sigma) \circ \tau^{-1},$$

one can identify the second term on the right-hand side as the projection onto the symmetric part of the tensor product. The choice $\tau = 2$ yields the value $\sigma = 1 - 2\pi$. If τ is not invertible there arises the possibility that part of the tensor product is neither symmetric nor antisymmetric. Condition (1.16) applied to the tensor product $\theta^i \otimes_{\mathcal{A}} \theta^j$ becomes

$$P^{ij}_{lm} + S^{ij}_{hk}P^{hk}_{lm} = 0. \tag{1.18}$$

If the flip is such that in (1.11) $F^i_{jk} = K_{kl} = 0$, one possible linear connection is

$$\omega^i_{jk} = \lambda_l (S^{il}_{jk} - \delta^l_j \delta^i_k). \tag{1.19}$$

The corresponding connection 1-form is given by

$$\omega^i_k = \lambda_l S^{il}_{jk} \theta^j + \delta^i_k \theta. \tag{1.20}$$

The curvature of the covariant derivative D defined in (1.19) can be readily calculated. One finds the expression

$$\tfrac{1}{2} R^i_{jkl} = S^{im}_{rn} S^{np}_{sj} P^{rs}_{kl} \lambda_m \lambda_p . \tag{1.21}$$

This can also be written in the form

$$\tfrac{1}{2} R^i_{jkl} = - S^{im}_{rn} S^{np}_{sj} S^{rs}_{uv} P^{uv}_{kl} \lambda_m \lambda_p .$$

In complete analogy with the commutative case, a metric g can be defined as an $\mathcal{A}$-bilinear, nondegenerate map[11]

$$\Omega^1(\mathcal{A}) \otimes_{\mathcal{A}} \Omega^1(\mathcal{A}) \overset{g}{\to} \mathcal{A}, \tag{1.22}$$

and as such it can[12] be used to define a ''distance'' between ''points.'' It is important to notice here that the bilinearity is an alternative way of expressing locality. In ordinary differential geometry, if ξ and η are 1-forms then the value of $g(\xi \otimes \eta)$ at a given point depends only on the values of ξ and η at that point. Bilinearity

$$g(f\xi \otimes_{\mathcal{A}} \eta h) = f\, g(\xi \otimes_{\mathcal{A}} \eta)\, h \quad \forall f, h \in \mathcal{A},$$

is an exact expression of this fact. In general the algebra introduces a certain amount of nonlocality via its nontrivial commutation relations, and it is important to assure that all geometric quantities be just that nonlocal and not more. Without the bilinearity condition it is not possible to distinguish, for example, in ordinary space–time a metric which assigns a function to a vector field in such a way that the value at a given point depends only on the vector at that point from one which is some sort of convolution over the entire manifold.

We define frame components of the metric by

$$g^{ij} = g(\theta^i \otimes_{\mathcal{A}} \theta^j).$$

They lie necessarily in the center $\mathcal{Z}(\mathcal{A})$ of the algebra. The condition that (1.19) be metric-compatible can be written as[10]

$$S^{im}_{ln} g^{np} S^{jk}_{mp} = g^{ij} \delta^k_l . \tag{1.23}$$

As a way to remember this seemingly odd condition, introduce a ''covariant derivative'' $D_i X^j$ of a ''vector'' X^j. The covariant derivative $D_i(X^j Y)$ of the product of X^j by a ''field'' Y must then be defined as

$$D_i(X^j Y) = D_i X^j Y + S^{jl}_{im} X^m D_l Y,$$

since there is a ''flip'' as the index on the derivation crosses the index on the first ''vector.'' If we apply this rule again to $Y = Y^k Z$, with Y^k also a vector and Z another field, we find

$$D_i(X^j Y^k Z) = D_i(X^j Y^k) Z + S^{jl}_{im} X^m Y^p S^{kn}_{lp} D_n Z.$$

Since g^{jk} is a ''tensor,'' the ''crossing rule'' is the same as for $X^j Y^k$

$$D_i(g^{jk}Z)=(D_i g^{jk})Z+S_{im}^{jl}g^{mp}S_{lp}^{kn}D_n Z.$$

Therefore, (1.23) is equivalent to the usual condition

$$D_i g^{jk}=0,$$

that the connection be compatible with the metric.

We shall require that the metric be symmetric in the sense

$$g\circ\pi=0, \tag{1.24}$$

that it annihilates the 2-forms. This condition applied to the tensor product $\theta^i\otimes_{\mathcal{A}}\theta^j$ becomes

$$P_{lm}^{ij}g^{lm}=0. \tag{1.25}$$

Let us now briefly summarize the additional conditions which arise from the requirement of existence of $*$-structures. Assume $\mathcal{A}$ is a $*$-algebra. If[13,14] the $*$-structure of $\mathcal{A}\equiv\Omega^0(\mathcal{A})$ can be extended to a $*$-structure of $\Omega^*(\mathcal{A})$, and

$$(df)^*=df^*, \tag{1.26}$$

the differential calculus is said to be real. A sufficient condition for (1.26) to hold[15] is that the λ_i are anti-Hermitian (with respect to the $*$ of $\mathcal{A}$) and the θ^i are Hermitian [with respect to the extension of $*$ to $\Omega^*(\mathcal{A})$], so that the ''Dirac operator'' θ is anti-Hermitian.

To obtain a real covariant derivative it is necessary first of all that the flip σ satisfies a reality constraint (see Ref. 15), which takes the simple form

$$(S_{kl}^{ji})^*S_{mn}^{lk}=\delta_m^i\delta_n^j, \tag{1.27}$$

if $(\theta^i)^*=\theta^i$. Moreover, the connection 1-form ω_k^i and the flip σ must satisfy a condition[15] involving both, which we do not report here because it is automatically satisfied in the case of the connection (1.19). In order to define a real metric, one has to use σ to impose the reality condition of Ref. 15, which takes the simple form

$$S_{kl}^{ij}g^{kl}=(g^{ji})^*, \tag{1.28}$$

in the case of a real frame. This is a combination of a ''twisted'' symmetry condition and the ordinary condition of reality on a complex matrix. It can also be written as an ordinary condition of symmetry and a twisted definition of reality. The map σ is also involved[15] in the reality condition for the curvature or for the covariant derivative acting on tensor powers of $\Omega^1(\mathcal{A})$. The latter implies the former, and takes the form of the braid equation

$$S_{12}S_{23}S_{12}=S_{23}S_{12}S_{23}, \tag{1.29}$$

where

$$(S_{12})_{def}^{abc}:=S_{de}^{ab}\delta_f^c, \quad (S_{23})_{def}^{abc}:=\delta_d^a S_{ef}^{bc}.$$

The ''infinitesimal distance'' ds corresponding to the metric g is introduced through the relation

$$ds^2=g_{ij}\theta^i\otimes_{\mathcal{A}}\theta^j, \tag{1.30}$$

where $g_{ij}\in\mathcal{A}$ are the matrix elements of the inverse matrix of $\|g^{ij}\|$. Every representation of $\mathcal{A}$ yields a distance between ''points'' because of (1.6). Let $dt=\xi_i\theta^i\in\Omega^1(\mathcal{A})$ be an exact form, which we can think of as an infinitesimal displacement along an axis t, and suppose that $|p\rangle$ is a

common eigenvector of all the ξ_i: $\xi_i|p\rangle=\tilde{\xi}_i|p\rangle$. This would be the case, for example, if only one of them is not equal to zero. We define the element of distance δs along the "coordinate" t at the state $|p\rangle$ by the equation

$$(\delta s)^2=\langle p|ds^2|p\rangle=g^{ij}\tilde{\xi}_i\tilde{\xi}_j.$$

Let $\hbar$ be the length scale at which points become fuzzy and K^{-1} the scale at which the curvature effects become important. The definition of g which we have given is unambiguous but the interpretation of the norm $|\delta s|^2$ of an infinitesimal displacement as a distance can be only made within the range

$$\hbar\ll|\delta s|^2\ll K^{-1}.$$

If the displacement is too small then the points are not defined; if it is too large then an integral must be taken. The second problem was solved by Leibniz/Newton; the first is a feature, not a bug, of noncommutative geometry. We are especially interested in the region $|\delta s|^2\simeq\hbar$ where the noncommutative effects become of interest.

There exist other definitions of distance. One proposal[16–18] uses the Dirac operator to define distance on the space of pure states. Several authors[19,20] do not consider the bilinearity condition we have imposed as important and several[21–27] consider the invariance under the coaction of a quantum group as essential.

It is sometimes convenient to write the metric as a sum

$$g^{ij}=g_S^{ij}+g_A^{ij},$$

of a symmetric and an antisymmetric part (in the usual sense of the word). The inverse matrix we write as a sum

$$g_{ij}=\eta_{ij}+B_{ij},$$

of a symmetric and an antisymmetric term. We shall choose as normalization when possible the condition that η_{ij} be the standard Minkowski or Euclidean form.

II. THE WESS–ZUMINO CALCULUS

The extended real quantum plane is the $*$-algebra $\mathcal{A}$ generated by Hermitian elements $(x^i)=(x,y)$

$$x^*=x \quad y^*=y, \tag{2.1}$$

together with their inverses, fulfilling the relation

$$xy=\tilde{q}yx, \tag{2.2}$$

with $|\tilde{q}|=1$ and $q\neq\pm1$, as well as the usual relations between inverses. We call it *extended* because in the original version[4] the inverses x^{-1},y^{-1} were not included; the word *real* refers to the $*$-structure (2.1). The center of $\mathcal{A}$ is trivial, $\mathcal{Z}(\mathcal{A})=\mathbb{C}$. We now show how the Wess–Zumino calculus[5] fits in the scheme described in the previous section. We define, for $\tilde{q}^4\neq1$

$$\lambda_1=-\epsilon_1\frac{\tilde{q}^4}{\tilde{q}^4-1}x^{-2}y^2, \quad \lambda_2=\epsilon_2\frac{\tilde{q}^2}{\tilde{q}^4-1}x^{-2}.$$

There is an ambiguity in this definition due to the fact that the defining relations (2.2) are homogeneous and which we reduce to a sign: $\epsilon_a = \pm 1$. The extra minus is a "historical convenience." The important fact is that the λ_a are singular in the limit $\tilde{q} \to 1$ and that they are anti-Hermitian if $\tilde{q}$ is of unit modulus, as we are assuming. We find for $\tilde{q}^2 \neq -1$

$$e_1 x = \epsilon_1 \frac{\tilde{q}^2}{(\tilde{q}^2+1)} x^{-1} y^2, \quad e_1 y = \epsilon_1 \frac{\tilde{q}^4}{\tilde{q}^2+1} x^{-2} y^3,$$
$$e_2 x = 0, \quad e_2 y = -\epsilon_2 \frac{\tilde{q}^2}{\tilde{q}^2+1} x^{-2} y. \tag{2.3}$$

These derivations are again extended to arbitrary polynomials in the generators by the Leibniz rule. Using them and (1.9), (1.10), we find

$$dx = \frac{\tilde{q}^2}{(\tilde{q}^2+1)} x^{-1} y^2 \epsilon_1 \theta^1, \quad dy = \frac{\tilde{q}^2}{\tilde{q}^2+1} x^{-2} y (\tilde{q}^2 y^2 \epsilon_1 \theta^1 - \epsilon_2 \theta^2), \tag{2.4}$$

and solving for the θ^i we obtain

$$\epsilon_1 \theta^1 = (\tilde{q}^2+1) x y^{-2} dx, \quad \epsilon_2 \theta^2 = -(\tilde{q}^2+1) x (x y^{-1} dy - dx).$$

The module structure which follows from the condition (1.1) that the θ^i commute with the elements of the algebra is equivalent to the Wess–Zumino relations[5]

$$x dx = \tilde{q}^2 dx\, x, \quad x\, dy = \tilde{q}\, dy\, x + (\tilde{q}^2 - 1) dx\, y,$$
$$y dx = \tilde{q}\, dx\, y, \quad y\, dy = \tilde{q}^2 dy\, y. \tag{2.5}$$

One can show that they are invariant under the coaction of the quantum group $SL_q(2,\mathbb{C})$. This invariance was encoded in the choice of λ_a.

Consider the elements

$$u := \epsilon_2 \tilde{q}^{-2} x^2, \quad v := \epsilon_1 x^2 y^{-2}. \tag{2.6}$$

We shall see that each of the four possible choices of sign pairs corresponds to an identification of x and y as the coordinates of one of the four regions on $\mathbb{R}^2$ defined by the light cone of a metric with Minkowski signature. The u, v fulfill the quadratic commutation relation

$$uv = qvu, \tag{2.7}$$

where $q := \tilde{q}^{-4}$. They and their inverses generate a slightly smaller algebra than $\mathcal{A}$. One also finds that (2.5) becomes

$$u du = q^{-1} du u, \quad u dv = q dv u,$$
$$v du = q^{-1} du v, \quad v dv = q dv v. \tag{2.8}$$

In terms of the new generators, the θ^i become

$$\theta^1 = q^{-1} v u^{-1} du, \quad \theta^2 = u v^{-1} dv. \tag{2.9}$$

What we have done in fact is use the λ_a^{-1} as generators of the algebra and the differential calculus; otherwise, nothing has been changed. The form θ is most conveniently expressed in terms of the λ_a. Since

$$\lambda_1=\frac{1}{1-q^{-1}}v^{-1},\quad \lambda_2=-\frac{1}{1-q^{-1}}u^{-1}, \tag{2.10}$$

we find that

$$\theta=\frac{1}{1-q}(u^{-1}du-qv^{-1}dv).$$

It is an anti-Hermitian closed form with vanishing square

$$d\theta=0,\quad (\theta)^2=0. \tag{2.11}$$

The volume element is a product of two exact forms

$$\theta^1\theta^2=du\,dv.$$

The structure of the exterior algebra is given by the relations

$$(\theta^1)^2=0,\quad (\theta^2)^2=0,\quad \theta^1\theta^2+q\theta^2\theta^1=0. \tag{2.12}$$

This can be written in the form (1.4) with

$$P=\tfrac{1}{2}\begin{pmatrix}0&0&0&0\\0&1&-q&0\\0&-q^{-1}&1&0\\0&0&0&0\end{pmatrix}. \tag{2.13}$$

If we reorder the indices $(11,12,21,22)=(1,2,3,4)$, then the C^{ij}_{kl} introduced in (1.7) is given by the expression

$$C=\begin{pmatrix}1&0&0&0\\0&0&q&0\\0&q^{-1}&0&0\\0&0&0&1\end{pmatrix}.$$

That is, $C^{12}_{21}=q$ and $C^{21}_{12}=q^{-1}$.

The reality of the differential implies that the structure elements must satisfy the conditions

$$((C^i_{jk})^*+C^i_{jk})P^{jk}_{lm}=0,$$

from which it follows that

$$(C^i_{21})^*=-C^i_{12}=q^{-1}C^i_{21},\quad (C^i_{12})^*=-C^i_{21}=qC^i_{12}.$$

More precisely, the independent coefficients are given by

$$C^1_{12}=(q^{-1}-1)\lambda_2,\quad C^2_{12}=(q^{-1}-1)\lambda_1. \tag{2.14}$$

The C^i_{jk} do not depend on the sign ambiguities. With the generators

$$t=\frac{1}{\sqrt{2}}(u+v),\quad r=\frac{1}{\sqrt{2}}(u-v), \tag{2.15}$$

the four possible sign combinations can be written as

$$\epsilon_1=\epsilon_2:\quad \mathrm{sgn}(t)=\epsilon_1,\quad \epsilon_1=-\epsilon_2:\quad \mathrm{sgn}(r)=\epsilon_2.$$

We shall later in Sec. V introduce a light-cone and interpret these relations in terms of space-like and time-like.

Introduce the notation

$$X=\begin{pmatrix} t \\ r \end{pmatrix},\quad \Xi=\begin{pmatrix} dt \\ dr \end{pmatrix},\quad Q=\begin{pmatrix} \cos(\pi\gamma) & i\sin(\pi\gamma) \\ i\sin(\pi\gamma) & \cos(\pi\gamma) \end{pmatrix}\quad q=e^{2\pi i\gamma}.$$

Then, Q is unitary. The commutation relations in $\Omega^*(\mathcal{A})$ can be written in the form

$$X^t(Q\sigma_2)X=0,\quad X\Xi^t=\Xi(Q^2X)^t,\quad \Xi^tQ\Xi=0. \tag{2.16}$$

The σ_2 is the second Pauli matrix.

There are alternative $*$-structures which require a real q. One can impose the conditions $u^*=v$, $v^*=u$. In terms of the original variables x and y, this implies that

$$x^*=\pm\tilde{q}^{1/2}xy^{-1},\quad y^*=y.$$

It follows that the frame satisfies

$$(\theta^1)^*=\theta^2,\quad (\theta^1)^*=\theta^2,$$

and so one can introduce a real frame by taking the real and imaginary parts or consider the resulting structure as a q-deformed complex line. This is better with the change of generators

$$t=\frac{1}{\sqrt{2}}(u+v),\quad r=\frac{i}{\sqrt{2}}(u-v). \tag{2.17}$$

It is equivalent to a replacement $\gamma\mapsto i\gamma$ in the formula (2.16).

III. REPRESENTATIONS

An extensive discussion of the $*$-representations of the algebra $\mathcal{A}$ for $|\tilde{q}|=1$ and $q\neq\pm1$ has been given.[28] We recall parts of it to illustrate our interpretation of the geometry. It is easy to see that there can be no normed basis with u or v diagonal. Suppose in fact that there is a basis with $v|j\rangle=v_j|j\rangle$. Since v is Hermitian the eigenvalue $v_j\in\mathbb{R}$. Using the commutation relations one sees that $v(u|j\rangle)=q^{-1}v_j(u|j\rangle)$, and so $u|j\rangle$ is also an eigenvector with eigenvalue $q^{-1}v_j\notin\mathbb{R}$. One concludes, therefore, that $u|j\rangle\notin\mathcal{H}$. More specifically, one can consider $\mathcal{H}=L^2(\mathbb{R})$ with the plane-wave basis $|k\rangle=e^{ikx}$. The operator $u=-i\partial_x$ is Hermitian on a dense subspace of $\mathcal{H}$ and diagonal: $u|k\rangle=k|k\rangle$. We can formally set

$$v|k\rangle=|qk\rangle=e^{-iqkx}$$

in order to have the correct commutation relations, but u is not properly defined on the plane-wave basis.

As solution to this problem we restrict our representation space to the positive real line $\mathbb{R}^+$ with free boundary condition at $x=0$. The Laplace transform replaces the Fourier transform and so we choose as basis $|k\rangle=e^{-kx}$ for $k\in\mathbb{C}$ with $\Re k>0$. We need in fact represent only one (at a time) of the four regions defined by the light "cone" and we choose the one defined by $\epsilon_1=\epsilon_2=1$. Our sign conventions were partly dictated by the desire that this be the forward light cone. We choose[28] then two positive real numbers α and β with $\alpha\beta=\gamma$, and we define on the Hilbert space $L^2(\mathbb{R}^+)$

$$(uf)(x)=f(x+i\beta),\quad (vf)(x)=e^{-2\pi\alpha x}f(x).$$

Both u and v are formally Hermitian and bounded. It is more convenient to express them in terms of the Laplace transform, which we recall is given by

$$F(k)=(Lf)(k)=\int_0^\infty f(x)e^{-kx}dx, \quad f(x)=(L^{-1}F)(x)=\frac{1}{2\pi i}\int_{a+i\infty}^{a-i\infty}F(k)e^{kx}dk,$$

where a depends on the growth rate of the function. We have then

$$(uF)(k)\equiv(L(uf))(k)=e^{i\beta k}F(k), \quad (vF)(k)\equiv(L(vf))(k)=F(k+2\pi\alpha).$$

In particular, these transformation formulas are valid on the basis $|k\rangle=e^{-kx}$. The operators u and v are well-defined and positive for $\Re k>0$.

IV. THE METRICS AND THEIR CONNECTIONS

We now determine some possible metrics and metric-compatible connections on the real quantum plane. We require them to fulfill all or at least part of the conditions listed in Sec. I, namely (1.18), (1.29), (1.25), (1.23), (1.27), (1.28).

To shorten the notation, we shall often perform the following change of index notation: $(11,12,21,22)\to(1,2,3,4)$. Then, the condition (1.23) can be written in the matrix form

$$\begin{pmatrix} S_1^1 & S_2^1 & S_3^1 & S_4^1 \\ S_1^2 & S_2^2 & S_3^2 & S_4^2 \\ S_1^3 & S_2^3 & S_3^3 & S_4^3 \\ S_1^4 & S_2^4 & S_3^4 & S_4^4 \end{pmatrix}\times(S_{(g)})=\begin{pmatrix} g^1 & 0 & g^3 & 0 \\ 0 & g^1 & 0 & g^3 \\ g^2 & 0 & g^4 & 0 \\ 0 & g^2 & 0 & g^4 \end{pmatrix}, \tag{4.1}$$

where we have introduced the matrix $S_{(g)}$ defined by

$$S_{(g)}=\begin{pmatrix} S_1^1g^1+S_2^1g^3 & S_3^1g^1+S_4^1g^3 & S_1^3g^1+S_2^3g^3 & S_3^3g^1+S_4^3g^3 \\ S_1^1g^2+S_2^1g^4 & S_3^1g^2+S_4^1g^4 & S_1^3g^2+S_2^3g^4 & S_3^3g^2+S_4^3g^4 \\ S_1^2g^1+S_2^2g^3 & S_3^2g^1+S_4^2g^3 & S_1^4g^1+S_2^4g^3 & S_3^4g^1+S_4^4g^3 \\ S_1^2g^2+S_2^2g^4 & S_3^2g^2+S_4^2g^4 & S_1^4g^2+S_2^4g^4 & S_3^4g^2+S_4^4g^4 \end{pmatrix}. \tag{4.2}$$

Using the expression (2.13) for P, the condition (1.25) becomes

$$g^2=qg^3. \tag{4.3}$$

The consistency condition (1.16) is equivalent to the conditions

$$S_3^1=qS_2^1, \quad S_3^2=q(S_2^2+1), \quad S_3^3=qS_2^3-1, \quad S_3^4=qS_2^4. \tag{4.4}$$

The equations to be solved then are Eqs. (4.1), (4.3), and (4.4). We are especially interested in real solutions, which satisfy therefore also (1.27) and (1.28). We have found that there are several types of solutions, four of which we shall describe in the following subsections. One can show that there are no solutions with $\tau=2$. A complete classification has been given[29] of the solutions to the braid equation as well[30,31] as of those which satisfy a weaker modified equation.

If one considers locality as of importance only in the commutative limit, then there is no restriction on the coefficients of the metric, except that they be local functions in this limit. If one considers locality as of importance even before the limit but is willing to accept a metric which is real and symmetric only in the commutative limit, then the most general line element one can write is of the form

$$ds^2=g_{ij}\theta^i\otimes\theta^j.$$

The g_{ij} is a real symmetric matrix (in the sense we have defined it) and the moving frame θ^i is defined by

$$\theta^1 = v u^{-1} du, \quad \theta^2 = u v^{-1} dv.$$

The line element (1.30) then becomes

$$ds^2 = g_1 v^2 u^{-2}\, du^2 + 2 g_2 du\, dv + g_4 u^2 v^{-2}\, dv^2. \tag{4.5}$$

The product here is the symmetrized tensor product; not the exterior product.

The associated metric connection is given by the structure functions

$$C^1_{12} = u^{-1}, \quad C^2_{12} = -v^{-1}.$$

If we interpret the matrix g_{ij} as the components of the Killing metric on $SO(2)$ or $SO(1,1)$ then we can use it to calculate the connection form. The result will be of the form

$$\omega^i_j = A^i_{jk} u^{-1} \theta^k + B^i_{jk} v^{-1} \theta^k,$$

with $g_{ik}\omega^k_j$ antisymmetric in the two indices. The Gaussian curvature K is a second-order homogeneous polynomial in the variables u^{-1} and v^{-1}

$$K = \kappa_{11} u^{-2} + 2\kappa_{12} u^{-1} v^{-1} + \kappa_{22} v^{-2}.$$

A. Solution I

A one-parameter family of solutions of conditions (1.18), (1.25), (1.23), can be found with a Minkowski-signature metric. For the particular value $\zeta = 0$ of the parameter also the braid relation (1.29) and the reality conditions (1.27), (1.28) are fulfilled. These are the most interesting solutions.

With the convenient normalization of the metric so that $g^3 = q^{-1/2}$ the flip is given by the matrix

$$S = \begin{pmatrix} q & -q^{-1/2}\zeta & -q^{1/2}\zeta & q^{-1}(q^2-1)^{-1}\zeta^2(q^2+1) \\ 0 & 0 & q & -q^{-1/2}\zeta \\ 0 & q^{-1} & 0 & q^{-3/2}\zeta \\ 0 & 0 & 0 & q^{-1} \end{pmatrix},$$

where $\zeta \in \mathbb{C}$. It tends to the ordinary flip as $q \to 1$ if $\zeta = 0$; only for $\zeta = 0$ it is a solution to the braid equation (1.29). The corresponding metric is given by

$$g^{ij} = \begin{pmatrix} (q-1)^{-1}\zeta & q^{1/2} \\ q^{-1/2} & 0 \end{pmatrix}. \tag{4.6}$$

From (4.3) one sees that it is σ-symmetric for all g^1 and real if $g^1 = 0$ (i.e., $\zeta = 0$). In this case S is given by

$$S = \begin{pmatrix} q & 0 & 0 & 0 \\ 0 & 0 & q & 0 \\ 0 & q^{-1} & 0 & 0 \\ 0 & 0 & 0 & q^{-1} \end{pmatrix}. \tag{4.7}$$

The σ and π are related as in (1.17) with $T^{ij} := \tau(\theta^i \otimes_{\mathcal{A}} \theta^j)$

$$T=\begin{pmatrix} 1+q & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1+q^{-1} \end{pmatrix}. \tag{4.8}$$

The fact that T is not proportional to the identity is due to the fact that the map $(1+\sigma)/2$ is not a projector and that we would like it to act as such and be the complement to π. The metric matrix is of indefinite signature and in ''light-cone'' coordinates. If we use the expression $q=e^{2\pi i\eta}$, we find that

$$g_S^{ij}=\cos(\pi\eta)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad g_A^{ij}=i\sin(\pi\eta)\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{4.9}$$

The inverse metric components are defined by the equation

$$g_{ij}g^{jk}=\delta_i^k.$$

This matrix also can be split. If we rescale so that the symmetric part is of the standard form, we find

$$(\eta_{ij})=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (B_{ij})=i\tan(\pi\zeta)\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

For the choice (4.7) of the flip (i.e., for $\zeta=0$) the metric connection (1.20) is given by

$$(\omega_j^i)=(1-q)\begin{pmatrix} 1 & 0 \\ 0 & -q^{-1} \end{pmatrix}\theta,$$

and has vanishing curvature, because of the identities (2.11) and (1.29). This can be shown by an argument already used in Refs. 32 and 33. In other words, in this case the quantum plane is flat. In the commutative limit the line element is given by

$$ds^2=g_{ij}\theta^i\otimes\theta^j=2\,\theta^1\otimes\theta^2=2\,du\otimes dv=dt^2-dr^2.$$

The frame is singular along the light cone through the origin [see (2.9)]. Suppose $\epsilon_1=\epsilon_2=1$. If in a representation one forces x and y to be Hermitian, then the u and v must be positive operators. One concludes then that $t>|r|$; the geometry describes only the forward light cone through the origin. The other three regions are given by the other three possible combinations of signs.

B. Solution II

A family of solutions defined by flips which are solutions to (1.18), (1.27), but not to the braid equation (1.29) is given by

$$S=\begin{pmatrix} -q^2 & 0 & 0 & 0 \\ 0 & 0 & q & 0 \\ 0 & -q^{-2} & -1-q^{-1} & 0 \\ 0 & 0 & 0 & q^{-1} \end{pmatrix}. \tag{4.10}$$

The metric is given again by (4.6) with $\zeta=0$, and fulfills (1.23), (1.25), but not (1.28). The metric connection (1.20) is

$$(\omega_j^i)=(1+q^2)\begin{pmatrix}1 & 0\\ 0 & q^{-2}\end{pmatrix}\quad\theta+(1+q^{-1})\begin{pmatrix}0 & 0\\ -1 & 0\end{pmatrix}\quad\lambda_1\theta^2+(q+1)\begin{pmatrix}q & 0\\ 0 & q^{-2}\end{pmatrix}\quad\lambda_2\theta^2.$$

The curvature is equal to

$$\Omega_j^i=-(q^2-1)q^{-3}(1+q+q^2)\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}(\lambda_1)^2\theta^1\theta^2.$$

It diverges as $(q-1)^{-1}$ when $q\to 1$. This is then the case of a regular metric which has a singular metric connection.

C. Solution III

A third family

$$S=\frac{1}{q^2+1}\begin{pmatrix}2q & 0 & 0 & 1-q^2\\ 0 & 1-q^2 & 2q & 0\\ 0 & 2q & q^2-1 & 0\\ q^2-1 & 0 & 0 & 2q\end{pmatrix},\tag{4.11}$$

$$g^{ij}=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},$$

fulfills (1.18), (1.25), (1.23), the reality condition (1.27) but not the one (1.28) nor the braid relation (1.29). The latter are fulfilled for $q=\pm 1$. For $q=-1$ this means the connection form is imaginary in the usual sense of the word (since so are the λ_i).

The compatible connection (1.20) form is

$$(\omega_j^i)=\frac{(q-1)^2}{q^2+1}\delta_j^i\theta+\frac{q^2-1}{q^2+1}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\quad(\lambda_2\theta^1+\lambda_1\theta^2).$$

The curvature 2-form is

$$(\Omega_j^i)=\frac{(q^2-1)}{(q^2+1)^2}\left\{-q^{-1}(q^2-1)^2\delta_j^i\lambda_1\lambda_2+2(q-1)\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\quad((\lambda_1)^2+(\lambda_2)^2)\right\}\theta^1\theta^2.$$

In the limit $q\to 1$ this becomes

$$(\Omega_j^i)=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\quad(u^{-2}+v^{-2})\theta^1\theta^2.$$

D. The $\hat{R}$-matrix "solution"

Finally, one might ask whether one can find a solution (S,g) using the formalism of Faddeev *et al.*,[34] as has been done[32,33] for the q-Euclidean spaces $\mathbb{R}_q^n$ with $n>2$. This would imply an S proportional to the braid matrix $\hat{R}$ of $SL_q(2)$ or to its inverse. One can show that there is a solution only if one admits nonsymmetry metrics.

We recall that the braid matrix which defines the Hopf algebra $SL_q(2)$

$$\hat{R}_q=\begin{pmatrix} q & 0 & 0 & 0 \\ 0 & q-q^{-1} & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & q \end{pmatrix},$$

fulfills the braid relation, admits the projector decomposition

$$\hat{R}_q=qP_{s,q}-q^{-1}P_{a,q},$$

and fulfills the (1.29) relations

$$\hat{R}_q^{\pm 1}{}^{ij}_{hk}\varepsilon_q^{kl}\hat{R}_q^{\pm 1}{}^{rs}_{jl}=q^{\mp 1}\varepsilon_q^{ir}\delta_h^s, \quad \hat{R}_q^{\pm 1}{}^{ij}_{hk}\varepsilon_q^{hk}=-q^{\mp 1}\varepsilon_q^{ij}, \tag{4.12}$$

where ε_q^{ij} is the q-deformed epsilon tensor

$$\varepsilon_q^{ij}=\begin{pmatrix} 0 & -q^{-1/2} \\ q^{1/2} & 0 \end{pmatrix}.$$

So, one finds

$$P^{ij}_{a,qhk}=(\varepsilon^{lm}\varepsilon_{lm})^{-1}(\varepsilon^{ij}\varepsilon_{hk})=\frac{1}{q+q^{-1}}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & q^{-1} & -1 & 0 \\ 0 & -1 & q & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

By a straightforward computation, one can check that (2.12) can be given the form (1.4) by setting

$$P=P_{a,q^{-1}}.$$

The first relation in (4.12) suggests that we make the ansatz $S\propto\hat{R}^{\pm 1}_{q^{-1}}$, $g^{ij}\propto\varepsilon^{ij}_{q^{-1}}$, so that we can fulfill (1.23) at least up to a conformal factor. Equation (1.16) fixes the first proportionality constant to be either

$$S=q^{-1}\hat{R}_{q^{-1}} \quad \text{or} \quad S=q(\hat{R}_{q^{-1}})^{-1},$$

which respectively implies that

$$S^{im}_{ln}g^{np}S^{jk}_{mp}=q^{-1}g^{ij}\delta^k_l, \quad S^{im}_{ln}g^{np}S^{jk}_{mp}=qg^{ij}\delta^k_l, \tag{4.13}$$

i.e., we indeed fulfill (1.23) only up to a conformal factor $q^{\pm 1}$, and

$$S^{ij}_{hk}g^{hk}=-g^{ij}. \tag{4.14}$$

This ''antisymmetry'' relation is to be contrasted with Eq. (1.24), which, with the above choice of S, amounts to replacing at the right-hand side of (4.14) -1, respectively, by q^{-2} or q^2, as can be seen writing P as a combination of S and of the identity matrix. Using the fact that $|q|=1$ and $\hat{R}^{ij}_{q^{-1}hk}=\hat{R}_q^{-1}{}^{ji}_{kh}$,[34] one can easily see that the reality conditions (1.27) and (1.28) are satisfied. The curvature (1.21) can easily be calculated to be zero using the conditions $K^{ij}=0$ and $F^h_{ij}=0$ as well as the fact that P_q is a polynomial in S, which it turn fulfills the braid equation.

E. Other "solutions"

There are a certain number of partial solutions which are unsatisfactory for some reason or other. As an example, to underline the possibility of exotic metrics which are both symmetric and antisymmetric according to our definitions, we consider σ defined by the matrix

$$S=\begin{pmatrix} 0 & 0 & 0 & \zeta \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \zeta^{-1} & 0 & 0 & 0 \end{pmatrix},$$

where $\zeta \in \mathbb{R}$ is a parameter. This value of S is a solution to the braid equation. The σ and π are related as in (1.17) with (using the same conventions)

$$\mathbf{1}+S=T=\begin{pmatrix} 1 & 0 & 0 & \zeta \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \zeta^{-1} & 0 & 0 & 1 \end{pmatrix}. \tag{4.15}$$

This means that τ is not invertible and the case is degenerate. The unpleasant thing here is that $(1+\sigma)/2$ and π do not add up to the identity map. The metric is given by

$$g^{ij}=i\begin{pmatrix} 1 & 0 \\ 0 & -\zeta^{-1} \end{pmatrix}. \tag{4.16}$$

One has $\tau=1+\sigma$ and the flip is degenerate. Instead of interchanging g^2 and g^3, as does the ordinary flip, it interchanges g^1 and g^4. It also changes the sign, which accounts for the i in the metric components. Also, $g\bigcirc(1+\sigma)=0$ so in a certain sense the metric has vanishing symmetric as well as antisymmetric parts. We refer to σ nonetheless as a flip because it satisfies (1.16).

The linear connection (1.19) is given by

$$\omega^i_j=\delta^i_j\theta+\begin{pmatrix} 0 & 1 \\ -\zeta^{-1} & 0 \end{pmatrix} \quad (\zeta\lambda_1\theta^2-\lambda_2\theta^1).$$

The curvature is given by

$$\Omega^i_j=q^{-1}(q^2-1)\,\delta^i_j\lambda_1\lambda_2\theta^1\theta^2.$$

The connection is singular in the commutative limit as is the curvature. Because of (1.24) it cannot be satisfied for any curvature which is proportional to the metric.

V. JORDANIAN DEFORMATION

It has been shown recently (See, for example, Aneva *et al.*[31]) that the Jordanian deformation is a singular limit of a family of q deformations. The transformation from the set of generators of one algebra to the other has also been studied in some detail.[35] We can now discuss to what extent the limit can be understood in a geometric manner. We recall that the Jordanian deformation is defined using a parameter h and that the generators (x',y') satisfy the commutation relations $[x',y']=hy'^2$. The differential calculus is given by two elements λ'_a similar to the λ_a which satisfy the $SL(2,\mathbb{R})$ relation $[\lambda'_1,\lambda'_2]=\lambda'_1$, a relation which is not quadratic. This must be compared with the quadratic relation $\lambda_1\lambda_2=q^{-1}\lambda_2\lambda_1$ satisfied by the elements (2.10). We must find a smooth map from one algebra into the other, that is, one which respects the commutation relations between the elements which define the derivations dual to the frame. Consider[35] the map

$$\lambda_1' = h_0^{-1}\lambda_1, \quad \lambda_2' = h_0^{-1}\lambda_2 - \frac{1}{2}h^{-1}h_0, \quad h_0 = \frac{2h}{1-q}. \tag{5.1}$$

This change defines a deformation of the differential calculus. From the commutation relations of the λ_i, we deduce that

$$[\lambda_1', \lambda_2'] = h_0^{-2}[\lambda_1, \lambda_2] = h_0^{-2}(1-q)\lambda_1\lambda_2 = \lambda_1' + (1-q)\lambda_1'\lambda_2'.$$

In the (singular) limit when $q \to 1$ the differential calculus tends to that of the Jordanian deformation.

The relations between the two calculi can be written in terms of a diagram

$$\begin{array}{ccc} (x,\ y) & \to & (u,\ v) = (\epsilon_2 q^{1/2} x^2,\ \epsilon_1 x^2 y^{-2}). \\ \downarrow & & \downarrow \\ (x',\ y') & \to & (u',\ v') = (x' y'^{-1} + \frac{1}{2}h,\ y'^{-2}). \end{array} \tag{5.2}$$

The two horizontal arrows are changes of generators. The two vertical ones define a map between the two deformations. In terms of the generators u and v and their analogs[36] u' and v' for the Jordanian deformation, the map (5.1) can be written as

$$u' = qu^{-1} - h_0, \quad v' = -qv^{-1}$$

with $h_0 \to \infty$. It has been shown[36] that the local metric on the Jordanian deformation is that of Lobachevsky. This must be a limit of one of the family of metrics (4.5). The Lobachevsky metric can be described with the line element $ds'^2 = v'^{-2}(du'^2 + dv'^2)$. To compare, we write (4.5) in the primed variables

$$ds^2 = (u' + h_0)^{-2} v'^{-2}[q^2 g_1 du'^2 - 2g_2 du'\, dv' + q^{-2} g_4 dv'^2].$$

We see then that we must choose $g_2 = 0$ and let $g_1, g_4 \to \infty$ with the constraint

$$g_1 h_0^{-2} = g_4 h_0^{-2} = 1.$$

The quantum-plane metric belongs to the family III. Another interesting metric obtained in the same limit is with $g_1 = g_4 = 0$ and $g_2 \to \infty$ so that $g_2 h_0^{-2} = 1$

$$ds^2 = -2v'^{-2} du'\, dv' = -2du'\, dv.$$

This solution belongs to the family I.

VI. PATCHING

Let us consider now the solutions *I* found in Sec. IV A. To each of the four regions defined by the light cone through the origin in two dimensions we have associated an algebra, a differential calculus, and a metric, but none is complete as ''manifold.'' From the form of the metric we see that this can be done using the generators (t,r) or (u,v), but that the generators (x,y) are singular on the cone.

The patching is done[28] by extending the domain of definition of u for example to negative eigenvalues. The frame θ^i is also singular on the cone, but the equivalent frame du^i is quite regular. We can write $\theta^i = \Lambda^i_j\, du^j$, where

$$\Lambda^i_j = \sqrt{q}\begin{pmatrix} vu^{-1} & 0 \\ 0 & uv^{-1} \end{pmatrix}$$

is a local Lorentz transformation in the commutative limit.

VII. DISCUSSION

We have given a partial classification of the solutions to the three conditions of metric compatibility (1.23), symmetry (1.24), and the consistency condition (1.16), as well as the reality conditions (1.27), (1.28), and the braid relation (1.29), without due regard to quantum covariance. In fact, we could show that there was no solution which respected a coaction of the quantum group. A similar problem was found by Cotta-Ramusino and Rinaldi in trying to construct holonomy groups.[37] Written in terms of the components in the frame basis, one sees that S^{ij}_{kl} has 16 unknowns and g^{ij} has 4 unknowns. The condition (1.16) gives 4 equations and metric compatibility gives 16 equations. So, a naive computation would say that the solution is unique up to a rescaling of g^{ij}, which is not fixed by the equation. We have indeed found a finite set of solutions.

Another conclusion concerns the uniqueness of the vacuum. It has been claimed[38] that within the context of the present formalism there is essentially a unique differential calculus which has associated with it a given metric, unique that is up to a choice of norm on the frame. This statement needs qualification since we have shown here that the quantum plane is naturally endowed with the Lorentz-signature flat metric and it is known that the same is true of the Heisenberg algebra with its natural differential calculus.

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N coupled nonlinear Schrödinger equations: Special set and applications to *N*=3

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Analytic solutions for a special set of N coupled nonlinear Schrödinger equations characterized by 2^N interaction types are presented for $N=1-3$. They provide an overview of the important role played by nonlinear couplings. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1521238]

I. INTRODUCTION

There are many physical processes that are described by the nonlinear Schrödinger equations. Because of problems of mathematical interest and a growing interest in nonlinear phenomena in optical fibers,[1] systems of coupled nonlinear Schrödinger (CNLS) equations involving two and generally N components have attracted a great deal of attention. The complex wavefunction $\phi_m(z,t)$ of the mth component as a function of position z and time t is assumed to satisfy the following N CNLS equations:

$$i\phi_{mz}+\varepsilon_m\phi_{mtt}+\kappa_m\phi_m+\left(\sum_{j=1}^{N}\lambda_{mj}|\phi_j|^2\right)\phi_m=0, \quad m=1,\ldots,N, \tag{1}$$

where ε_m, κ_m and λ_{mj} are real parameters characteristic of the medium and interaction, and where the subscripts in z and t denote derivatives with respect to z and t, and the subscript m is for different components. Although the term $\kappa_m\phi_m$ can be eliminated by a substitution $\phi_m \rightarrow \phi_m e^{i\kappa_m z}$, we shall keep the term for the purpose of ordering the N equations that will become clear later.

Soliton[1–4] and solitary-wave solutions[4–6] have been presented for special sets of parameters ε_m, κ_m and λ_{mj}. In particular, Lakshmanan and his collaborators[7] have studied a special set of ''mixed'' interaction cases using the Painlevé analysis.

In a recent paper, Hioe and Salter[8] showed that there is a special set that can be characterized by 2^N specific arrays of interaction parameters for which the N CNLS equations possess special analytic solutions. For this special set, the N components of the CNLS equations can be expressed in terms of N Lamé functions,[9] and every Lamé function of order $n \leqslant N$ is a solution for one or more components for one or more interaction types of this special set. In particular, they presented simple rules that (a) identify a given combination of Lamé functions to be a solution to one or more specific interaction types, and (b) give all the possible combinations of Lamé functions as solutions of a specific interaction type. These CNLS equations that have these Lamé functions as solutions were called the L-set. It was pointed out that the L-set coincides with the set of CNLS equations that pass the Painlevé test identified by Radhakrishnan *et al.*[7] In a separate development, Hioe and Carroll[10] showed that N coupled Gross–Pitaevskii (CGP) equations in D-dimensions with a square-well and Coulomb potential can be transformed into N CNLS equations, and solutions in terms of same or different Lamé functions can be used to suggest possible ways of making multiple Bose–Einstein condensates overlap each other or separate.

In this article, we first review briefly the L-set and the subsets of it that consist of what are called the weakly and strongly mixed interaction types. We then present and consider analytic

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solutions particularly for $N=3$. The use of two or three coupled waves can play a very important role in optical communication with unexpected results. For example, a wave that cannot be solitary by itself when it propagates through an anomalous group-velocity dispersion (GVD) region[1] can be made to do so when it is coupled to a second appropriate wave, and two waves that cannot be solitary by themselves when they propagate through an anomalous GVD region can be made to do so when they are coupled to a third appropriate wave. For the many analytic solutions presented in this article, besides their theoretical and mathematical interest, the true test of their practical usefulness could be realized if and when a general recognizable pattern would emerge that would strongly suggest the robustness of certain combinations of waveforms.

II. THE L-SET FOR *N* CNLS EQUATIONS

We first review the L-set for a general value of N. The L-set of N CNLS equations (1) is defined to be a special subset of Eq. (1) given by the following,[8]

$$i\phi_{mz}\pm\beta_m\phi_{mtt}+\kappa_m\phi_m\pm\left(\sum_{j=1}^{N}\beta_m\beta_j|\phi_j|^2\right)\phi_m=0,\quad m=1,\ldots,N, \tag{2}$$

where $\beta_j=+1$ or -1, for $j=1,\ldots,N$. That is, the L-set of N CNLS equations (1) has those coefficients ε_m and λ_{mj} which are expressible as in Eq. (2).

Consider the stationary-wave solution of the form

$$\phi_m(z,t)=\psi_m(t)\exp(i\omega z), \tag{3}$$

where ω is a real constant and $\psi_m(t)$'s are real functions of t only. Substitution of Eq. (3) into Eq. (2) gives the following N equations for $\psi_m(t)$:

$$\psi_{mtt}+c_m\psi_m+\left(\sum_{j=1}^{N}\beta_j\psi_j^2\right)\psi_m=0,\quad m=1,\ldots,N, \tag{4}$$

where

$$c_m=\pm\beta_m(\kappa_m-\omega). \tag{5}$$

To eliminate the permutation symmetry, Eq. (4) is arranged such that

$$c_1\geqslant c_2\geqslant\cdots\geqslant c_N, \tag{6}$$

so that only one of the two choices (the upper or lower sign) in Eq. (2) gives Eq. (4). The traveling waves, if required, can be constructed by substituting the solutions ψ_m from Eq. (4) into Eq. (2), and replacing $\phi_m(z,t)$ by $\phi_m(z,t-z/v)\exp\{i[t-z/(2v)]/(2v)\}$, where v is the common velocity of the waves.

The interaction parameters of Eq. (2) [and Eq. (4)] are now characterized by the array $(\beta_1,\beta_2,\ldots,\beta_N)$, where $\beta_j=+1$ or -1, and each of the 2^N arrays is referred to as an interaction type. The two special cases are the normal GVD region characterized by $(--\ldots-)$ and the anomalous GVD region characterized by $(++\ldots+)$. Note that the 2^N interaction types constitute only a subset of the symmetric λ_{mn} that can take on values $+1$ or -1, because the λ_{mn}'s are constrained to be only those given by $\lambda_{mn}=+\beta_m\beta_n$ or $-\beta_m\beta_n$. This special set of CNLS equations that consists of the 2^N interaction types is the L-set.

A Lamé equation of order n can be written in the form[9]

$$d^2f/d\tau^2+[h-n(n+1)k^2sn^2(\tau,k)]f=0. \tag{7}$$

Only the polynomial solutions of the Lamé equation are used here and are referred to as Lamé functions, and the $2n+1$ Lamé functions of order n, $f_1^{(n)},f_2^{(n)},\ldots,f_{2n+1}^{(n)}$, are numbered in the

order of numbering their corresponding eigenvalues $h_m^{(n)}$ arranged in descending order $h_1^{(n)} > h_2^{(n)} > \cdots > h_{2n+1}^{(n)}$. These Lamé functions and their corresponding eigenvalues, which will be needed later for our analytic solutions, are given in Appendix A for $n=1-3$. An N-combination $(f_{p_1}^{(n)}, f_{p_2}^{(n)}, \ldots, f_{p_N}^{(n)})$ that gives an analytic solution for the N components $(\psi_1, \psi_2, \ldots, \psi_N)$ will be represented simply by $(p_1, p_2, \ldots, p_N)_n$, where Eq. (6) implies $p_1 \leqslant p_2 \leqslant \cdots \leqslant p_N$. The $2n+1$ eigenvalues of the Lamé equation $h_1^{(n)}, h_2^{(n)}, \ldots, h_{2n+1}^{(n)}$ are renumbered as $h_1^{(n)}, h_2^{(n)}, h_{2'}^{(n)}, \ldots, h_{n+1}^{(n)}, h_{(n+1)'}^{(n)}$, and the corresponding Lamé functions $f_1^{(n)}$, $f_2^{(n)}$, $\ldots$, $f_{2n+1}^{(n)}$ as $f_1^{(n)}, f_2^{(n)}, f_{2'}^{(n)}, \ldots, f_{n+1}^{(n)}, f_{(n+1)'}^{(n)}$, i.e., they are grouped in pairs except the first one. The use of Lamé function ansatz described in Ref. 4 gives the required specific values for the c_m of Eq. (4) and the amplitude C_m for the mth component, thus giving, for combination $(p_1, p_2, \ldots, p_N)_n$, the solution

$$\psi_m(t) = C_m f_{p_m}^{(n)}(t), \quad m = 1, \ldots, N. \tag{8}$$

Two separate cases of representing the solutions in terms of Lamé functions may be distinguished: case (I) is in terms of Lamé functions of order $n=N$, and case (II) in terms of Lamé functions of order $n<N$.

(I) For $n=N$, the N Lamé functions for the N components must necessarily be different Lamé functions. The number of N combinations that can be chosen from $2n+1$ distinct Lamé functions of order $n=N$, with no repetition allowed, is $M=\binom{2n+1}{N}$.

Every one of the M combinations is a solution of one and only one particular interaction type, and every interaction type has one or more combinations as solutions. More specifically,

(a) Combination $(p_1, p_2+1, p_3+2, \ldots, p_N+N-1)_n$ is a solution of interaction type $((-1)^{p_1}, (-1)^{p_2}, (-1)^{p_3}, \ldots, (-1)^{p_N})$, and

(b) an interaction type $((-1)^{p_1}, (-1)^{p_2}, (-1)^{p_3}, \ldots, (-1)^{p_N})$ has solutions given by all possible combinations $(m_1, m_2, m_3, \ldots, m_N)_n$, that can be obtained by setting $m_1 = p_1$, $m_2 = p_2+1$, $m_3 = p_3+2, \ldots$, $m_N = p_N+N-1$, and by increasing or decreasing m_j by any multiple of 2 subject to the condition that $m_1 < m_2 < m_3 < \cdots < m_N$, where m_j can take on values $1, 2, 2', 3, 3', \ldots, n+1, (n+1)'$ with the understanding that $r < r'$.

(II) For $n<N$, two or more of the Lamé functions for the N components may be the same function. The number of N combinations that can be chosen from $2n+1$ distinct Lamé functions of order $n<N$ each of which may appear from 0 to N times is $M' = \binom{2n+N}{N}$.

A total of M' combinations $(m_1, m_2, \ldots, m_N)_n$ are possible where $m_1 \leqslant m_2 \leqslant m_3 \leqslant \ldots \leqslant m_N$ can be chosen, with repetition allowed, from 1, 2, 2′, 3, 3′, $\ldots$, $n+1$, $(n+1)'$, and in general, these combinations are possible solutions for each of the 2^N interaction types, but with a number of exceptions, some specific and some general. The following restrictions apply generally:

(a) A combination $(m_1, m_2, \ldots, m_N)_n$ must have at least n distinct m's for it to be a solution; and

(b) combination $(m_1, m_2, \ldots, m_N)_n$ is disallowed for interaction type $((-1)^{m_1+n}, (-1)^{m_2+n}, \ldots, (-1)^{m_N+n})$.

III. COMBINATIONS AND INTERACTION TYPES

For the case of $N>n$ for which combinations with repetitions are allowed, a combination in which two or more of the m's in the combination $(m_1, m_2, \ldots, m_N)_n$ are equal is referred to as a degenerate combination, and one in which all the m's are distinct as a nondegenerate combination.

For the case of $n=N$, all combinations must be nondegenerate (for $0<k^2<1$) to be solutions of N CNLS equations (4). It is useful to divide the $M=\binom{2n+1}{N}$ combinations of Lamé functions that can be obtained from $2n+1$ Lamé functions of order n (with no repetition allowed) into two kinds: the degenerative combination is one in which at least two of the m's in the combination $(m_1, m_2, \ldots, m_N)_n$ involve a pair p and p', where p is one of the numbers from 2 to $n+1$; the

nondegenerative combination is one that is not degenerative. Of the M combinations, the number of degenerative combinations is $M_d = n(2n-1)!/\{(N-2)!(2n-N+1)!\}$ and the number of nondegenerative combinations is $M_{nd} = M - M_d$.

The 2^N interaction types are divided into two subsets: (1) the interaction types in which all the $-$'s precede the $+$'s belong to the "weakly" mixed type or subset that includes the "pure" type in which the signs are all $-$'s or all $+$'s, as two special cases; and (2) the interaction types in which the $-$'s that appear before *and* after the $+$'s belong to the "strongly" mixed type or subset. The weakly mixed subset consists of $N+1$ interaction types, and the strongly mixed subset consists of the remaining $2^N - N - 1$ interaction types.

The nondegenerative combinations are found to be solutions of only the weakly mixed interaction type. The degenerative combinations can be solutions of the strongly mixed as well as the weakly mixed interaction types excepting the pure type. Division into degenerative and nondegenerative combinations aside, every one of the M possible combinations (for $n=N$) of Lamé functions is a solution to one and only one of the 2^N interaction types.

In Appendix B, we present, for $N=1-3$, the combinations of Lamé functions that give analytic solutions for each of the 2^N interaction types, the Lamé functions being those given in Appendix A. The grouping can be verified to be in agreement with the rules given above. To complete the analytic solutions, we need the explicit expressions for the amplitudes C's for Eq. (8) and the required c's for Eq. (4). Some solutions given previously[6,11–13] were for the pure type only. For $N=1$ and 2, the solutions for the entire set were given in Ref. 14. For $N=3$, the number of possible combinations for $n=3$ alone is 35, and there are many combinations that are solutions for $n=1$ and 2. We present, in Appendix C, the complete analytic solutions for five specific combinations, pure and mixed, with examples from $n=1$, 2 and 3, for which the Lamé functions given in Appendix A are used and Eq. (8) applies.

The complete analytic solutions for $N=3$ for the case of $k^2=1$, for which the $2n+1$ Lamé functions of order n coalesce into $n+1$ associated Legendre functions of order n, will be presented later. Indeed, for the case $k^2=1$, two special cases allow very compact expressions for a general N which we shall discuss in the next section.

The division of combinations into degenerative and nondegenerative is consistent with consideration of Lamé functions as k^2 becomes equal to 1. In that case, the $2n+1$ eigenvalues, except for the first one, become pairwise degenerate, i.e., $h_2^{(n)} = h_{2'}^{(n)}, h_3^{(n)} = h_{3'}^{(n)}, \ldots, h_{n+1}^{(n)} = h_{(n+1)'}^{(n)}$, and the corresponding Lamé functions of order n become $n+1$ associated Legendre functions of order n, $P_n^m(x)$, $m=0,1,2,\ldots,n$, where $x=\tanh(\alpha t)$. These (unnormalized) Legendre functions are presented in Appendix D.

IV. ANALYTIC SOLUTIONS FOR $k^2=1$

We shall present in this section all analytic solutions for $N=1-3$ for $k^2=1$ for all 2^N interaction types. For the weakly mixed interaction type, we have compact closed-form expressions of analytic solutions for a general value of N for two special cases that are derived from studying the equations obtained with the use of the ansatz.[5]

We first define our normalized associated Legendre functions $P_n^m(x)$ as follows:

$$P_n^m(x) = (1-x^2)^{m/2} d^m P_n(x)/dx^m,$$

where $P_n(x) = (2^{-n}/n!) d^n (x^2-1)^n / dx^n$.

Consider the following $(N+1)$ CNLS equations involving ψ_j, $j=1,2,\ldots,N+1$:

$$\psi_{mtt} + c_m \psi_m + \left(\sum_{j=1}^{s} - \psi_j^2 + \sum_{j=s+1}^{N+1} \psi_j^2 \right) \psi_m = 0, \quad m = 1, \ldots, N+1, \tag{9}$$

where s can take the value from 0 to $N+1$. It can be verified that the following analytic solution for ψ_j satisfies Eq. (9):

$$\psi_j = C_j P_N^{j-1}(\tanh \alpha t), \quad j=1,\ldots,N+1, \tag{10}$$

$$C_1 = \pm c_1, \quad + \text{for } s \geqslant 1, \quad - \text{for } s=0,$$

$$C_j = \pm\{[(N-j+1)!][c_1 - 2(j-1)^2\alpha^2]/(N+j-1)!\}^{1/2},$$

where $+$ for $j=2,...,s$, $s \geqslant 2$, $-$ for $j=s+1,\ldots,N+1$, $N \geqslant s$,

$$c_j = c_1 - (j-1)^2\alpha^2, \quad j=1,\ldots,N+1,$$

$$c_1 < 0 \quad \text{for } s=0,$$

$$2s^2\alpha^2 > c_1 > 2(s-1)^2\alpha^2 \quad \text{for } N+1 > s \geqslant 1,$$

$$c_1 > 2N^2\alpha^2 \quad \text{for } s=N+1.$$

We now consider the above $(N+1)$ CNLS equations involving ψ_j, $j=1,2,\ldots,N+1$ with $j=r$ missing (or $\psi_r=0$), where r can be any one of the $N+1$ components. Written explicitly, we have the following equations:

$$\psi_{mtt} + c_m\psi_m + \left(\sum_{j=1}^{r-1} -\psi_j^2 + \sum_{j=r+1}^{N+1} \psi_j^2\right)\psi_m = 0, \quad m=1,\ldots,N+1. \tag{11}$$

We find the following analytic solutions ψ_j with amplitudes C_j and the required c_j given by

$$\psi_j = C_j P_N^{j-1}(\tanh \alpha t), \quad j=1,\ldots,N+1, \quad j \neq r, \tag{12}$$

$$C_1 = [2(r-1)^2]^{1/2}\alpha,$$

$$C_j = \{4[(N-j+1)!]|(r-1)^2 - (j-1)^2|/(N+j-1)!\}^{1/2}\alpha, \quad \text{for } j>1,$$

$$c_j = [2(r-1)^2 - (j-1)^2]\alpha^2, \quad j=1,\ldots,N+1, \quad j \neq r,$$

where the specification $j \neq r$ is not really necessary since setting $j=r$ would give C_j and c_j equal to zero anyway. However, the specification $j \neq r$ is a reminder that there are N and not N+1 coupled components of CNLS equations considered.

Equation (12) gives a compact expression for the analytic solution for the L-set of N CNLS equations for the weakly mixed interaction type in terms of a combination of (different) associated Legendre functions of order $n=N$. It can be checked that for $r=1$, i.e., when the nonlinear coupling parameters in Eq. (11) are all equal to $+1$, the above results coincide with those given previously in Refs. 4–6, and for $r=N+1$, i.e., when the nonlinear coupling parameters are all equal to -1, the above results coincide with those given previously in Ref. 12. Thus our above results given by Eq. (12) generalize the previous results to the weakly mixed type where the first $r-1$ of the β's in Eqs. (11) are equal to -1, and the remaining β's are equal to $+1$. It may be noted that the ''generalized'' dark solitary wave is $P_n^0(\tanh \alpha t)$ and the ''generalized'' bright solitary wave is $P_n^n(\tanh \alpha t)$; they become the familiar dark solitary wave $\tanh \alpha t$ and the familiar bright solitary wave $\operatorname{sech} \alpha t$, respectively, for $n=1$. The generalized dark solitary waves $P_n^0(\tanh \alpha t)$, unlike the rest of the set $P_n^m(\tanh \alpha t)$, $m=1,\ldots,n$, do not become zero when $t \to \pm\infty$.

By replacing N by $N-1$, Eq. (10) can be seen to provide a compact expression for a particular analytic solution for the L-set of N CNLS equations for the weakly mixed interaction type in terms of N different associated Legendre functions of order $n=N-1$. Unlike the analytic solution given by Eq. (12) for Eq. (11) which is the only analytic solution in terms of associated Legendre

functions of order $n=N$, there is generally more than one analytic solution in terms of Legendre functions of order $n=N-1$ for $n<N$ generally: the other possibilities include combinations in which the same Legendre functions represent different components.

For the strongly mixed interaction type, the ansatz and procedure given in Ref. 5 are used to obtain the analytic solutions. The complete analytic solutions for $N=1-3$ in terms of associated Legendre functions of order $n\leqslant N$ are presented in Appendix E for all 2^N interaction types. To use these results, the solution of Eq. (4) for N CNLS equations characterized by the interaction type $(\beta_1,\ldots,\beta_N)$ for combination $(p_1,\ldots,p_N)$ is expressed in the form

$$\psi_m(t)=C_m f_{p_m}^{(n)}(x), \quad m=1,\ldots,N, \tag{13}$$

where the associated Legendre functions f's used are those given in Appendix D, the C's for Eq. (13) and the required c's for Eq. (4) are given in Appendix E, and where $x\equiv\tanh(\alpha t)$, α being a scaling parameter. Note that the $f_q^{(n)}(x)$ used for Eq. (13) differs from the normalized associated Legendre function $P_n^{(q-1)}(x)$ used for Eqs. (10) and (12) by a normalization constant. The solutions for $\psi_m(t)$ obtained from Eqs. (13) must of course be the same as those obtained from Eqs. (10) or (12) for the corresponding cases. Notice that combinations of associated Legendre functions of order $n=N$ are absent for the strongly mixed interaction type for $k^2=1$, which can be understood from the rules described in Secs. II and III (see also Appendix B for $0<k^2<1$).

The important role played by coupling a wave to another wave or to two other waves can now be seen in full view in Appendix E. For example, the wave $f_1^{(1)}$ that can by itself be a solitary wave only in the normal GVD region $[(1)_1$ in $(-)]$ can be a solitary wave in the anomalous GVD region if it is coupled with another wave $f_2^{(1)}$ $[(1,2)_1$ in $(++)]$; and the coupled waves $f_1^{(2)}$ and $f_2^{(2)}$ that can be a solitary-wave pair only in the normal GVD region $[(1,2)_2$ in $(--)]$ can be made into solitary waves in the anomalous GVD region if the pair is coupled to a third wave $f_3^{(2)}$ $[(1,2,3)_2$ in $(+++)]$.

V. SUMMARY

We have reviewed the L-set for N CNLS equations that possess analytic solutions in terms of N combinations of Lamé functions of order $n\leqslant N$ for 2^N interaction types. That every combination of Lamé functions of order $n=N$ is a solution for *one and only one* interaction type, and that every interaction type has *at least one* combination of Lamé functions of order $n=N$ as solution, as were first presented in Ref. 8, clearly tie the Lamé functions of order $n=N$ very intimately with the L-set for N CNLS equations, and may indicate a relationship of a deeper significance to be uncovered. The relationship between the weakly mixed interaction type and the nondegenerative combinations of Lamé functions order $n=N$ is another curiously interesting result.

For $k^2=1$, the weakly mixed interaction type allows the analytic solution in a combination of associated Legendre functions of order $n=N$ to be expressed in a compact closed-form expression for a general N, and likewise for a combination of associated Legendre functions of order $n=N-1$. Generally for $0<k^2\leqslant 1$ and every possible interaction type, however, the analytic solutions must be obtained individually, for which the ansatz and procedure prescribed in Ref. 5 can be used efficiently.

The complete analytic solutions presented for $N=1-3$ in Appendix E for $k^2=1$, for combinations of associated Legendre functions of order $n\leqslant N$, and for all 2^N interaction types, provide an excellent overview of the important role played by nonlinear couplings. For example, it enables one to easily see that coupling another wave or two other waves to a given wave can make all partners propagate as solitary waves in certain GVD regions when the individual waves cannot propagate as solitary waves by themselves. The robustness of the combinations must await experimental testing which hopefully will be used also to discover the required general pattern for certain combinations to be robust and practically useful. There is another useful application of our results. As presented in a recent communication,[10] they provide the analytic forms of stationary distributions of coupled Bose–Einstein condensates that can be used to suggest possible ways of making condensates overlap each other (i.e., same functions appearing in the combination) or

separated (i.e. different functions in the combination). The mixed interaction types, which make the L-set complete in terms of its relationship to Lamé functions of order $n=N$, are clearly important mathematically, but their physical applications still await experimental explorations.

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APPENDIX A: LAMÉ FUNCTIONS FOR $n=1-3$

The $2n+1$ Lamé functions $f_m^{(n)}(\tau)$ and their eigenvalues $h_m^{(n)}$ satisfy the Lamé equations (7), and we list them for $n=1-3$ according to the subscript $m=1,2,2',3,3',\ldots,n+1,(n+1)'$ in the following.

1. $n=1$

$$h_1^{(1)}=1+k^2,\quad h_2^{(1)}=1,\quad h_{2'}^{(1)}=k^2,$$

$$f_1^{(1)}=sn(\tau),\quad f_2^{(1)}=cn(\tau),\quad f_{2'}^{(1)}=dn(\tau).$$

2. $n=2$

$$h_{1,3'}^{(2)}=2(1+k^2)\pm 2\sqrt{1-k^2+k^4},$$

$$h_2^{(2)}=4+k^2,\quad h_{2'}^{(2)}=1+4k^2,\quad h_3^{(2)}=1+k^2,$$

$$f_{1,3'}^{(2)}=\frac{1}{3}(1+k^2\mp\sqrt{1-k^2+k^4})-k^2sn^2(\tau),$$

$$f_2^{(2)}=sn(\tau)cn(\tau),\quad f_{2'}^{(2)}=sn(\tau)dn(\tau),\quad f_3^{(2)}=cn(\tau)dn(\tau).$$

3. $n=3$

$$h_{1,3'}^{(3)}=5(1+k^2)\pm 2\sqrt{4-7k^2+4k^4},$$

$$h_{2,4}^{(3)}=5+2k^2\pm 2\sqrt{4-k^2+k^4},$$

$$h_{2',4'}^{(3)}=2+5k^2\pm 2\sqrt{1-k^2+4k^4},$$

$$h_3^{(3)}=4(1+k^2),$$

$$f_{1,3'}^{(3)}=sn(\tau)\{1-a_{1,3'}sn^2(\tau)\},$$

$$f_{2,4}^{(3)}=cn(\tau)\{1-a_{2,4}sn^2(\tau)\},$$

$$f_{2',4'}^{(3)}=dn(\tau)\{1-a_{2',4'}sn^2(\tau)\},$$

$$f_3^{(3)}=sn(\tau)cn(\tau)dn(\tau),$$

where

$$a_{1,3'}=\frac{1}{3}[2+2k^2\pm\sqrt{4-7k^2+4k^4}],$$

$$a_{2,4}=2+k^2\pm\sqrt{4-k^2+k^4},$$

$$a_{2',4'}=1+2k^2\pm\sqrt{1-k^2+4k^4}.$$

APPENDIX B: COMBINATIONS AND INTERACTION TYPES FOR $N=1-3$

A collection of N Lamé functions $(f^{(n)}_{m_1},f^{(n)}_{m_2},\ldots,f^{(n)}_{m_N})$ or $(m_1,m_2,\ldots,m_N)_n$ chosen from $2n+1$ Lamé functions $f^{(n)}_m$ of order n that can serve as an analytic solution for the N components ψ_m, $m=1,\ldots,N$, of Eqs. (4) is referred to as a combination. In this Appendix, we list, for every one of the 2^N possible interaction types $(\beta_1,\beta_2,\ldots,\beta_N)$, where β_j can be $+1$ or -1, for Eq. (4), all the possible combinations for Lamé functions of order $n=N$, for $N=1-3$ [the subscript n in the combination $(m_1,m_2,\ldots,m_N)_n$ is dropped as it is understood that $n=N$]. The total number M of possible combinations for $N=1,2,3$ are 3, 10, and 35, respectively.

We list only the ''principal'' combinations with the number of total possible combinations that can be obtained from them by changing, say, 2 to $2'$, 3 to $3'$, etc., given in the square brackets that follow, remembering the restriction that for any combination $(m_1,m_2,\ldots,m_N)_n$ for the case $n=N$, $m_1<m_2<\ldots<m_N$. For example, (2)[2] represents two combinations $(2)_1$ and $(2')_1$, and (1,2,3)[4] represents four combinations $(1,2,3)_3$, $(1,2,3')_3$, $(1,2',3)_3$ and $(1,2',3')_3$.

Interaction type	Combination
$N=1$	
$(-)$	(1)[1]
$(+)$	(2)[2]
$N=2$	
$(--)$	(1,2)[2]
$(-+)$	(1,3)[2],(3,3′)[1]
$(+-)$	(2,2′)[1]
$(++)$	(2,3)[4]
$N=3$	
$(---)$	(1,2,3)[4]
$(--+)$	(1,2,2′)[1],(1,2,4)[4],(1,4,4′)[1], (3,4,4′)[2]
$(-+-)$	(1,3,3′)[1]
$(-++)$	(1,3,4)[4],(3,3′,4)[2]
$(+--)$	(2,2′,3)[2]
$(+-+)$	(2,2′,4)[2],(2,4,4′)[2]
$(++-)$	(2,3,3′)[2]
$(+++)$	(2,3,4)[8]

APPENDIX C: SOLUTIONS FOR FIVE COMBINATIONS FOR $N=3$

In this Appendix, we give some representative examples of analytic solutions for $N=3$ of Eq. (4) for various interaction types: three combinations consist of Lamé functions of order 3, and one combination each consists of Lamé functions of orders 1 and 2. For combination $(p_1,p_2,p_3)_n$, the analytic solution is $\psi_m=C_m f^{(n)}_{p_m}$, $m=1,2,3$, where f's are given in Appendix A, and C's and the required c's for Eq. (4) are given in this Appendix.

1. *N*=3

(*i*) Combination $(1,2,3)_3$ for interaction type $(---)$.

$$C_j=(\Delta_j/\Delta)^{1/2},$$

where

$$\Delta_1=108k^2\alpha^2(8-k^2+4\sqrt{4-k^2+k^4}),$$

$$\Delta_2=12k^2\alpha^2\{8-3k^2-3k^4+8k^6+2(2+k^2+2k^4)\sqrt{4-7k^2+4k^4}\},$$

$$\Delta_3=12k^4\alpha^2\{-80+57k^2+18k^4+16k^6+(-50+26k^2+16k^4)\sqrt{4-k^2+k^4}+(50+16k^2+8k^4)\sqrt{4-7k^2+4k^4}+(20+8k^2)\sqrt{(4-7k^2+4k^4)(4-k^2+k^4)}\},$$

$$\Delta=32-90k^2+78k^4-16k^6+4(5-11k^2+8k^4)\sqrt{4-k^2+k^4}+2(-10+16k^2-4k^4)\sqrt{4-7k^2+4k^4}+8(-1+2k^2)\sqrt{(4-7k^2+4k^4)(4-k^2+k^4)},$$

$$c_j=\Delta_j/\Delta+h_j^{(3)}\alpha^2.$$

(*ii*) Combination $(1,3,3')_3$ for interaction type $(--+)$.

$$C_{1,3}=\sqrt{3}k'^{-2}k\alpha\left(2+k^2+2k^4\mp\frac{(1+k^2)(8-11k^2+8k^4)}{2\sqrt{4-7k^2+4k^4}}\right)^{1/2},$$

$$C_2=\sqrt{30}k'^{-2}k\alpha,$$

$$c_{1,3}=\{5(1+k^2)\pm2\sqrt{4-7k^2+4k^4}\}\alpha^2,\quad c_2=4(1+k^2)\alpha^2.$$

(*iii*) Combination $(2,3,4)_3$ for interaction type $(+++)$.

$$C_{1,3}=\sqrt{3}k\alpha\left(2\mp\frac{8-k^2}{2\sqrt{4-k^2+k^4}}\right)^{1/2},\quad C_2=\sqrt{30}k^2\alpha,$$

$$c_{1,3}=\{5(1-2k^2)\pm2\sqrt{4-k^2+k^4}\}\alpha^2,\quad c_2=4(1-2k^2)\alpha^2.$$

(*iv*) Combination $(1,2,3)_2$ for interaction type $(\beta_1,\beta_2,\beta_3)$, excluding $(-+-)$ and $(+-+)$.

$$C_1=(D_1/D)^{1/2},\quad C_2=(D_2/D)^{1/2}+6k^4\alpha^2,\quad C_3=(D_3/D)^{1/2}+6k^2\alpha^2,$$

where

$$D_1=9\beta_1\{-c_1+[2(1-2k^2)+2\sqrt{1-k^2+k^4}]\alpha^2\},$$

$$D_2=3\beta_2k^4(1+k^2+2\sqrt{1-k^2+k^4})\{-c_1+[2(1-2k^2)+2\sqrt{1-k^2+k^4}]\alpha^2\},$$

$$D_3=3\beta_3k^2(-2+k^2+2\sqrt{1-k^2+k^4})\{-c_1+[2(1-2k^2)+2\sqrt{1-k^2+k^4}]\alpha^2\},$$

$$D=2-5k^2+5k^4-2(1-2k^2)\sqrt{1-k^2+k^4},$$

$$c_1-c_2=-2+k^2+2\sqrt{1-k^2+k^4},\quad c_1-c_3=1+k^2+2\sqrt{1-k^2+k^4}.$$

(v) Combination $(1,2,2)_1$ for interaction type $(\beta_1,\beta_2,\beta_3)$, excluding $(+--)$.

$$C_1=\beta_1\{-c_1+(1-k^2)\alpha^2\},$$

$$\beta_2C_2^2+\beta_3C_3^2=-c_1+(1+k^2)\alpha^2,$$

$$c_1-c_2=k^2\alpha^2, \quad c_2=c_3,$$

$$\text{and for } \beta_1=+1, \quad c_1<(1-k^2)\alpha^2,$$

$$\text{and for } \beta_1=-1, \quad c_1>(1-k^2)\alpha^2.$$

APPENDIX D: ASSOCIATED LEGENDRE FUNCTIONS FOR $n=1-3$

In this Appendix, we list the $n+1$ associated Legendre functions of order $n=1-3$ that are to be used for Eq. (13) in conjunction with Appendix E.

1. $n=1$

$$f_1^{(1)}=\tanh(\alpha t)\equiv x, \quad f_2^{(1)}=\operatorname{sech}(\alpha t)=(1-x^2)^{1/2}.$$

2. $n=2$

$$f_1^{(2)}=\operatorname{sech}^2(\alpha t)-\frac{2}{3}=\frac{1}{3}-x^2,$$

$$f_2^{(2)}=\tanh(\alpha t)\operatorname{sech}(\alpha t)=x(1-x^2)^{1/2},$$

$$f_3^{(2)}=\operatorname{sech}^2(\alpha t)=1-x^2.$$

3. $n=3$

$$f_1^{(3)}=\tanh(\alpha t)\left\{\operatorname{sech}^2(\alpha t)-\frac{2}{5}\right\}=x\left(\frac{3}{5}-x^2\right),$$

$$f_2^{(3)}=\operatorname{sech}(\alpha t)\left\{\operatorname{sech}^2(\alpha t)-\frac{4}{5}\right\}=(1-x^2)^{1/2}\left(\frac{1}{5}-x^2\right),$$

$$f_3^{(3)}=\tanh(\alpha t)\operatorname{sech}^2(\alpha t)=x(1-x^2),$$

$$f_4^{(3)}=\operatorname{sech}^3(\alpha t)=(1-x^2)^{3/2}.$$

APPENDIX E: SPECIAL SOLUTIONS FOR $N=1-3$

In this Appendix, we give all analytic solutions of Eq. (4) for 2^N interaction types in terms of combinations of associated Legendre functions given in Appendix D, for $N=1-3$. See Eq. (13) for applications of the parameters given here.

1. $N=1$

$\underline{(-)}$ $(1)_1$ $C_1=\sqrt{2}\alpha, \quad c_1=2\alpha^2.$

$\underline{(+)}$ $(2)_1$ $C_1=\sqrt{2}\alpha, \quad c_1=-\alpha^2.$

2. *N*=2

$(--)$

$(1,2)_2 \quad C_1=C_2=3\sqrt{2}\alpha, \quad c_1=8\alpha^2, \quad c_2=7\alpha^2.$

$(1,1)_1 \quad C_1^2+C_2^2=2\alpha^2, \quad c_1=c_2=2\alpha^2.$

$(1,2)_1 \quad C_1^2=c_1, \quad C_2^2=c_1-2\alpha^2, \quad c_1-c_2=\alpha^2, \quad c_1>2\alpha^2.$

$(-+)$

$(1,3)_2 \quad C_1=C_2=3\sqrt{2}\alpha/2, \quad c_1=2\alpha^2, \quad c_2=-2\alpha^2.$

$(1,1)_1 \quad C_1^2-C_2^2=2\alpha^2, \quad c_1=c_2=2\alpha^2.$

$(1,2)_1 \quad C_1^2=c_1, \quad C_2^2=-c_1+2\alpha^2, \quad c_1-c_2=\alpha^2, \quad 2\alpha^2>c_1>0.$

$(2,2)_1 \quad -C_1^2+C_2^2=2\alpha^2, \quad c_1=c_2=-\alpha^2.$

$(+-)$

$(1,1)_1 \quad -C_1^2+C_2^2=2\alpha^2, \quad c_1=c_2=2\alpha^2.$

$(2,2)_1 \quad C_1^2-C_2^2=2\alpha^2, \quad c_1=c_2=-\alpha^2.$

$(++)$

$(2,3)_2 \quad C_1=C_2=\sqrt{6}\alpha, \quad c_1=-\alpha^2, \quad c_2=-4\alpha^2.$

$(1,2)_1 \quad C_1^2=-c_1, \quad C_2^2=-c_1+2\alpha^2, \quad c_1-c_2=\alpha^2, \quad c_1<0.$

3. *N*=3

$(---)$

$(1,2,3)_3 \quad C_1=15\sqrt{2}\alpha/2, \quad C_2=5\sqrt{6}\alpha, \quad C_3=5\sqrt{6}\alpha/2, \quad c_1=18\alpha^2, \quad c_2=17\alpha^2, \quad c_3=14\alpha^2.$

$(1,1,2)_2 \quad C_1^2+C_2^2=C_3^2=18\alpha^2, \quad c_1=c_2=8\alpha^2, \quad c_3=7\alpha^2.$

$(1,2,2)_2 \quad C_1^2=C_2^2+C_3^2=18\alpha^2, \quad c_1=8\alpha^2, \quad c_2=c_3=7\alpha^2.$

$(1,2,3)_2 \quad C_1^2=9c_1/4, \quad C_2^2=3(c_1-2\alpha^2), \quad C_3^2=3(c_1-8\alpha^2)/4, \quad c_1>4\alpha^2,$

$c_2=c_1-\alpha^2, \quad c_3=c_1-4\alpha^2.$

$(1,1,1)_1 \quad C_1^2+C_2^2+C_3^2=2\alpha^2, \quad c_1=c_2=c_3=2\alpha^2.$

$(1,1,2)_1 \quad C_1^2+C_2^2=c_1, \quad C_3^2=c_1-2\alpha^2, \quad c_1>2\alpha^2, \quad c_1=c_2, \quad c_1-c_3=\alpha^2.$

$(1,2,2)_1 \quad C_1^2=c_1, \quad C_2^2+C_3^2=c_1-2\alpha^2, \quad c_1>2\alpha^2.$

$(--+)$

$(1,2,4)_3 \quad C_1=5\sqrt{2}\alpha, \quad C_2=15\alpha/2, \quad C_3=5\alpha/2, \quad c_1=8\alpha^2, \quad c_2=7\alpha^2, \quad c_3=-\alpha^2.$

$(1,1,3)_2 \quad C_1^2+C_2^2=C_3^2=9\alpha^2/2, \quad c_1=c_2=2\alpha^2, \quad c_3=-2\alpha^2.$

$(1,2,2)_2 \quad C_1^2=C_2^2-C_3^2=18\alpha^2, \quad c_1=8\alpha^2, \quad c_2=c_3=7\alpha^2.$

$(1,2,3)_2 \quad C_1^2=9c_1/4, \quad C_2^2=3(c_1-2\alpha^2), \quad C_3^2=3(-c_1+8\alpha^2)/4, \quad 8\alpha^2>c_1>2\alpha^2,$

$c_2=c_1-\alpha^2, \quad c_3=c_1-4\alpha^2.$

$(1,3,3)_2 \quad C_1^2=-C_2^2+C_3^2=9\alpha^2/2, \quad c_1=2\alpha^2, \quad c_2=c_3=-2\alpha^2.$

$(1,1,1)_1 \quad C_1^2+C_2^2-C_3^2=2\alpha^2, \quad c_1=c_2=c_3=2\alpha^2.$

$(1,1,2)_1 \quad C_1^2+C_2^2=c_1, \quad C_3^2=-c_1+2\alpha^2, \quad 0<c_1<2\alpha^2, \quad c_1=c_2, \quad c_1-c_3=\alpha^2.$

$(1,2,2)_1 \quad C_1^2=c_1, \quad -C_2^2+C_3^2=-c_1+2\alpha^2, \quad c_1>0, \quad c_2=c_3, \quad c_1-c_2=\alpha^2.$

$(2,2,2)_1 \quad C_1^2+C_2^2-C_3^2=-2\alpha^2, \quad c_1=c_2=c_3=-\alpha^2.$

$(-+-)$

$(1,1,2)_2 \quad C_1^2-C_2^2=C_3^2=18\alpha^2, \quad c_1=c_2=8\alpha^2, \quad c_3=7\alpha^2.$

$(1,2,2)_2 \quad C_1^2=-C_2^2+C_3^2=18\alpha^2, \quad c_1=8\alpha^2, \quad c_2=c_3=7\alpha^2.$

$(1,3,3)_2 \quad C_1^2=C_2^2-C_3^2=9\alpha^2/2, \quad c_1=2\alpha^2, \quad c_2=c_3=-2\alpha^2.$

$(1,1,1)_1 \quad C_1^2-C_2^2+C_3^2=2\alpha^2, \quad c_1=c_2=c_3=2\alpha^2.$

$(1,1,2)_1 \quad -C_1^2+C_2^2=c_1, \quad C_3^2=c_1-2\alpha^2, \quad c_1>2\alpha^2, \quad c_1=c_2, \quad c_1-c_3=\alpha^2.$

$(1,2,2)_1 \quad C_1^2=c_1, \quad C_2^2-C_3^2=-c_1+2\alpha^2, \quad c_1>0, \quad c_2=c_3, \quad c_1-c_2=\alpha^2.$

$(2,2,2)_1 \quad C_1^2-C_2^2+C_3^2=-2\alpha^2, \quad c_1=c_2=c_3=-\alpha^2.$

$(-++)$

$(1,3,4)_3 \quad C_1=5\sqrt{2}\alpha/2, \quad C_2=3\sqrt{10}\alpha/2, \quad C_3=\sqrt{10}\alpha, \quad c_1=2\alpha^2, \quad c_2=-2\alpha^2, \quad c_3=-7\alpha^2.$

$(1,1,3)_2 \quad C_1^2-C_2^2=C_3^2=9\alpha^2/2, \quad c_1=c_2=2\alpha^2, \quad c_3=-2\alpha^2.$

$(1,2,3)_2 \quad C_1^2=9c_1/4, \quad C_2^2=3(-c_1+2\alpha^2), \quad C_3^2=3(-c_1+8\alpha^2)/4, \quad 2\alpha^2>c_1>0,$

$c_2=c_1-\alpha^2, \quad c_3=c_1-4\alpha^2.$

$(1,3,3)_2 \quad C_1^2=C_2^2+C_3^2=9\alpha^2/2, \quad c_1=2\alpha^2, \quad c_2=c_3=-2\alpha^2.$

$(2,2,3)_2 \quad -C_1^2+C_2^2=C_3^2=6\alpha^2, \quad c_1=c_2=-\alpha^2, \quad c_3=-4\alpha^2.$

$(1,1,1)_1 \quad C_1^2-C_2^2-C_3^2=2\alpha^2, \quad c_1=c_2=c_3=2\alpha^2.$

$(1,1,2)_1 \quad C_1^2-C_2^2=c_1, \quad C_3^2=-c_1+2\alpha^2, \quad c_1<2\alpha^2, \quad c_1=c_2, \quad c_1-c_3=\alpha^2.$

$(1,2,2)_1 \quad C_1^2=c_1, \quad C_2^2+C_3^2=-c_1+2\alpha^2, \quad 2\alpha^2>c_1>0, \quad c_2=c_3, \quad c_1-c_2=\alpha^2.$

$(2,2,2)_1 \quad C_1^2-C_2^2-C_3^2=-2\alpha^2, \quad c_1=c_2=c_3=-\alpha^2.$

$(+--)$

$(1,1,2)_2 \quad -C_1^2+C_2^2=C_3^2=18\alpha^2, \quad c_1=c_2=8\alpha^2, \quad c_3=7\alpha^2.$

$(1,1,1)_1 \quad -C_1^2+C_2^2+C_3^2=2\alpha^2, \quad c_1=c_2=c_3=2\alpha^2.$

$(1,1,2)_1 \quad C_1^2-C_2^2=-c_1, \quad C_3^2=c_1-2\alpha^2, \quad c_1>2\alpha^2, \quad c_1=c_2, \quad c_1-c_3=\alpha^2.$

$(2,2,2)_1 \quad -C_1^2+C_2^2+C_3^2=-2\alpha^2, \quad c_1=c_2=c_3=-\alpha^2.$

$(+-+)$

$(1,1,3)_2 \quad -C_1^2+C_2^2=C_3^2=9\alpha^2/2, \quad c_1=c_2=2\alpha^2, \quad c_3=-2\alpha^2.$

$(2,2,3)_2 \quad C_1^2-C_2^2=C_3^2=6\alpha^2, \quad c_1=c_2=-\alpha^2, \quad c_3=-4\alpha^2.$

$(2,3,3)_2 \quad C_1^2=-C_2^2+C_3^2=6\alpha^2, \quad c_1=-\alpha^2, \quad c_2=c_3=-4\alpha^2.$

$(1,1,1)_1 \quad -C_1^2+C_2^2-C_3^2=2\alpha^2, \quad c_1=c_2=c_3=2\alpha^2.$

$(1,1,2)_1 \quad C_1^2-C_2^2=-c_1, \quad C_3^2=-c_1+2\alpha^2, \quad c_1<2\alpha^2, \quad c_1=c_2, \quad c_1-c_3=\alpha^2.$

$(1,2,2)_1 \quad C_1^2=-c_1, \quad -C_2^2+C_3^2=-c_1+2\alpha^2, \quad c_1<0, \quad c_2=c_3, \quad c_1-c_2=\alpha^2.$

$(2,2,2)_1 \quad -C_1^2+C_2^2-C_3^2=-2\alpha^2, \quad c_1=c_2=c_3=-\alpha^2.$

$(++-)$

$(2,2,3)_2 \quad C_1^2=C_2^2-C_3^2=6\alpha^2, \quad c_1=-\alpha^2, \quad c_2=c_3=-4\alpha^2.$

$(1,1,1)_1 \quad -C_1^2-C_2^2+C_3^2=2\alpha^2, \quad c_1=c_2=c_3=2\alpha^2.$

$(1,2,2)_1 \quad C_1^2=-c_1, \quad C_2^2-C_3^2=-c_1+2\alpha^2, \quad c_1<0, \quad c_1-c_2=\alpha^2, \quad c_1=c_3.$

$(2,2,2)_1 \quad -C_1^2-C_2^2+C_3^2=-2\alpha^2, \quad c_1=c_2=c_3=-\alpha^2.$

$(+++)$

$(2,3,4)_3 \quad C_1=5\sqrt{3}\alpha/2, \quad C_2=\sqrt{30}\alpha, \quad C_3=3\sqrt{5}\alpha/2, \quad c_1=-\alpha^2, \quad c_2=-4\alpha^2, \quad c_3=-9\alpha^2.$

$(1,2,3)_2 \quad C_1^2=-9c_1/4, \quad C_2^2=3(-c_1+2\alpha^2), \quad C_3^2=3(-c_1+8\alpha^2)/4,$

$c_1<0, \quad c_2=c_1-\alpha^2, \quad c_3=c_1-4\alpha^2.$

$(2,2,3)_2 \quad C_1^2+C_2^2=C_3^2=6\alpha^2, \quad c_1=c_2=-\alpha^2, \quad c_3=-4\alpha^2.$

$(2,3,3)_2 \quad C_1^2=C_2^2+C_3^2=6\alpha^2, \quad c_1=-\alpha^2, \quad c_2=c_3=-4\alpha^2.$

$(1,1,2)_1 \quad C_1^2+C_2^2=-c_1, \quad C_3^2=-c_1+2\alpha^2, \quad c_1<0, \quad c_1=c_2, \quad c_1-c_3=\alpha^2.$

$(1,2,2)_1 \quad C_1^2=-c_1, \quad C_2^2+C_3^2=-c_1+2\alpha^2, \quad c_1<0, \quad c_2=c_3, \quad c_1-c_2=\alpha^2.$

$(2,2,2)_1 \quad C_1^2+C_2^2+C_3^2=2\alpha^2, \quad c_1=c_2=c_3=-\alpha^2.$

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De Rham–Wu decomposition of holomorphic Riemannian manifolds

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It is shown that a de Rham–Wu decomposition for holomorphic Riemannian manifolds is obtained easily from the underlying real geometry of holomorphic Riemannian manifolds by appealing to H. Wu's extension to pseudo-Riemannian manifolds of de Rham's decomposition theorem. © *2002 American Institute of Physics.*
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I. INTRODUCTION

A holomorphic Riemannian manifold is a complex manifold M, of complex dimension n say, together with a holomorphic tensor field h that is a complex scalar product (i.e., nondegenerate, symmetric, **C**-bilinear form) on each holomorphic tangent space T'_pM, $p \in M$.

Holomorphic Riemannian geometry has many formal analogies with pseudo-Riemannian geometry and so has not required special study to elaborate its basic features. Nevertheless, it has attracted considerable interest in the context of general relativity, arising initially from the fact that the Hodge star operator provides a complex structure J on $\Lambda^2(\mathbf{R}^{1,3})$ so that the notion of self-duality in Lorentzian geometry involves complex-valued objects. In fact, $\Lambda^2(\mathbf{R}^{1,3}) \cong \mathbf{R}^{3,3}$ and the Hodge star operator is an *anti*-orthogonal complex structure J with respect to the neutral scalar product g on $\Lambda^2(\mathbf{R}^{1,3})$. Defining $\mu(\ ,\ ) := g(J\ ,\ )$, then $g - i\mu$ defines a complex scalar product on $(\Lambda^2(\mathbf{R}^{1,3}), J)$. This linear algebra plays a role in the well-known Petrov classification and underlies the associated proof that $\mathbf{SO}^+(\mathbf{1},\mathbf{3}) \cong \mathbf{SO}(\mathbf{3},\mathbf{C})$, (cf., Ref. 10). Complex geometry also occurs in general relativity in the form of complex space–times, i.e., four-(complex-)dimensional holomorphic Riemannian manifolds, of special interest in Penrose's twistor theory and Newman's theory of $\mathcal{H}$-space, cf., e.g., Ref. 7. Specifically, half-flat complex space–times provide a nonlinear analog of (anti-)self-dual objects in the linear theory. These applications inspired further work on complex Riemannian geometry itself, e.g., Ref. 6.

Typically, holomorphic Riemannian geometry is regarded as arising most naturally via complexification of real analytic Riemannian geometry. But, as in the linear theory, holomorphic Riemannian geometry possesses an underlying real geometry consisting of a pseudo-Riemannian metric of neutral signature for which the (integrable) almost complex structure tensor is anti-orthogonal. The latter approach is more natural in a geometrical setting, can include the weaker case of almost complex manifolds, and also indicates the significance of neutral signature amongst the various indefinite signatures. Rózga[9] and Woodhouse[11] appear to be have been the first to employ the real geometry of complex space–times, in applications to real slices of complex space–time. Recently, Robinson[8] has employed the real geometry to study half-flat complex space–times. The real geometry of holomorphic Riemannian manifolds has also been considered for its own sake, e.g., Ref. 2.

Much differential geometry of a holomorphic Riemannian manifold (M,h) may be developed simply by analogy with pseudo-Riemannian geometry. The notion of holonomy, however, would appear to be an exception. One approach is to utilize the underlying real geometry of (M,h). In this paper, I employ this approach to formulate for (M,h) an analog of Wu's[12–14] generalization to pseudo-Riemannian geometry of the de Rham decomposition theorem of Riemannian geometry,

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see, e.g., Ref. 4. This result further demonstrates the utility of the real geometric approach to holomorphic Riemannian manifolds, not only for elucidating the holomorphic Riemannian geometry but also for suggesting how to adapt concepts (such as holonomy) from the real to the complex context.

II. HOLOMORPHIC RIEMANNIAN GEOMETRY

Briefly, consider a real, orientable, $2n$-dimensional manifold M, equipped with a neutral metric g, i.e., a pseudo-Riemannian metric of signature type (n,n), and an almost complex structure J which is compatible with g in the sense that J acts as an anti-orthogonal transformation of each tangent space T_pM:

$$g(J(v),J(w))=-g(v,w),$$

$v,\ w\in T_pM$. Extend g $\mathbf{C}$-bilinearly and J $\mathbf{C}$-linearly to the complexified tangent space $\mathbf{C}T_pM$. As usual, let $T_p^{1,0}M$ and $T_p^{0,1}M$ be, respectively, the eigenspaces of the eigenvalues i and $-i$ of J acting on $\mathbf{C}T_pM$. The compatability of J with g entails that $\mathbf{C}T_pM=T_p^{1,0}M\oplus T_p^{0,1}M$ is an orthogonal decomposition with respect to g. Moreover, the restriction, h, of g to $T_p^{1,0}M$ is a complex scalar product. If the Levi-Civita connection ∇_g of g is almost complex, $\nabla_g J=0$, then it turns out that J is integrable and h is holomorphic, i.e., (M,h) is a holomorphic Riemannian manifold. Conversely, every holomorphic Riemannian manifold can be seen to arise in this manner. Thus, one may refer to such (M,g,J) as a holomorphic Riemannian manifold. Note that one defines $\mu(\ ,\ ):=g(J\ ,\ )$ (by analogy with the Kähler form in Hermitian geometry), which is another neutral metric on M. Then ∇_g is almost complex iff $\nabla_g=\nabla_\mu$, where the latter is the Levi-Civita connection of μ. These results appear in Woodhouse[11] and Robinson[8] and are easy analogs of familiar results in Hermitian/Kähler geometry. Indeed, one may now develop holomorphic differential geometry in purely real terms by analogy with the development of Hermitian and Kähler geometry in, for example, Ref. 5, Chap. IX.

Let U be a holomorphic chart domain for a holomorphic Riemannian manifold $(M,h)=(M,g,J)$ equipped with holomorphic coordinates $\{z_1,\ldots,z_n\}$ and write $Z^i:=\partial/\partial z_i$ so that $\{Z_1,\ldots,Z_n\}$ is a basis for $T_p^{1,0}$, $p\in U$. Adopting the notation of Ref. 5, Chap. IX, Sec. 5, $\{Z_A:A=1,\ldots,n,\overline{1},\ldots,\overline{n}\}=\{Z_\alpha,Z_{\overline{\alpha}}:\alpha=1,\ldots,n\}$ denotes the associated basis of the complexified tangent space $\mathbf{C}T_pM$. Introduce Christoffel symbols as follows:

$$\nabla_{Z_B}Z_C=\Gamma_{BC}^A Z_A,$$

where ∇ is the $\mathbf{C}$-linear extension of ∇_g to $\mathbf{C}TM$. As ∇_g is almost complex and torsion free, then (cf., Ref. 5, p. 156)

$$\Gamma_{\beta\gamma}^{\alpha}=\Gamma_{\gamma\beta}^{\alpha},\quad \Gamma_{\beta\overline{\gamma}}^{\overline{\alpha}}=\overline{\Gamma_{\beta\gamma}^{\alpha}}\quad \text{all other } \Gamma_{BC}^A \text{ vanish.}$$

Hence, $\nabla_{Z_\beta}Z_\gamma=\Gamma_{\beta\gamma}^{\alpha}Z_\alpha$. Adaptation of a standard argument shows that

$$\Gamma_{BC}^A=\tfrac{1}{2}g^{DA}(\partial_B g_{DC}+\partial_C g_{DB}-\partial_D g_{BC}),$$

where $g_{AB}:=g(Z_A,Z_B)$, and g^{AB} are the entries of the matrix inverse to (g_{AB}). With $h_{\alpha\beta}:=h(Z_\alpha,Z_\beta)$, and $h^{\alpha\beta}$ the entries of the matrix inverse to the matrix $(h_{\alpha\beta})$, one finds

$$\Gamma_{\beta\gamma}^{\alpha}=\tfrac{1}{2}h^{\delta\alpha}(\partial_\beta h_{\delta\gamma}+\partial_\gamma h_{\delta\beta}-\partial_\delta h_{\beta\gamma}),$$

i.e., the Christoffel symbols of h with respect to the coordinates $\{z_\alpha\}$ are just $\Gamma_{\beta\gamma}^{\alpha}$. In a similar fashion, one may, for example, obtain the holomorphic Riemann curvature tensor of h from the (complexification) of the Riemann curvature tensor of g.

Turning to the matter of holonomy, it turns out that ∇_g is almost complex iff the Levi-Civita connection, as a connection on the frame bundle, reduces to the bundle of complex frames (analog of Ref. 5, (4.8), p. 152). Thus, taking the holonomy for (M,h) to be that of the connection ∇_g yields holonomy in

$$\mathbf{O}(\mathbf{n};\mathbf{C}) = \mathbf{GL}(\mathbf{n};\mathbf{C}) \cap \mathbf{O}(\mathbf{n},\mathbf{n}),$$

as is appropriate. The holonomy of neutral metrics is the subject of Refs. 1 and 3 though with an emphasis upon the four (real)-dimensional case.

III. THE DE RHAM–WU DECOMPOSITION

The possibility of obtaining a de Rham-like decomposition theorem for (M,h), when M is simply connected, is now accessible through Wu's[12–14] extension to pseudo-Riemannian geometry of de Rham's result by applying Wu's result directly to (M,g).

Let $\Psi(p)$ be the linear holonomy group of ∇_g at $p \in M$ acting on T_pM, and T_0 the subspace of tangent vectors fixed under this action. Suppose T_0 is nondegenerate, which I shall refer to as *Wu's condition*. Then, there is a decomposition $T_pM = \oplus_{i=0}^{k} T_i$ into mutually g-orthogonal, $\Psi(p)$-invariant, weakly irreducible (i.e., no nontrivial, nondegenerate, $\Psi(p)$-invariant subspaces) subspaces T_i. The decomposition is unique up to order and $\Psi(p)$ is a direct product $\Psi_0 \times \cdots \times \Psi_k$ of normal subgroups, with Ψ_i acting trivially on T_j, $j \neq i$, and weakly irreducibly on T_i, and $\Psi_0 = \langle 1 \rangle$. The subspaces T_i may be parallely propagated to yield involutive distributions.

If M is complete, one obtains a global decomposition: M is isometric to a product $M_0 \times \cdots \times M_k$, where each factor M_i is a simply connected, complete pseudo-Riemannian manifold with weakly irreducible holonomy Ψ_i, and is totally geodesic as a submanifold of M. Furthermore, M_0 is flat (in fact pseudo-Euclidean since it is a simply connected space form). Call such a decomposition a *de Rham–Wu decomposition*.

Given a de Rham–Wu decomposition of a manifold with neutral metric, then presumably the factors need not, in general, be neutral. Nevertheless, one still has:

Theorem: Let (M,g,J) be a simply connected, complete, holomorphic Riemannian manifold of real dimension $2n$ satisfying Wu's condition. Then M has a de Rham–Wu decomposition $M_0 \times \cdots \times M_k$, where each factor is holomorphic Riemannian in a natural manner and the isometry $M \simeq M_0 \times \cdots \times M_k$ is biholomorphic. $M_0 \simeq \mathbf{R}^{m,m}$, some $m \leqslant n$.

Proof: The essentials of the argument of Ref. 5, Theorem 8.1, p. 172, carry over to the present circumstances. In particular, the argument there establishes that J restricts to each T_i as an anti-orthogonal complex structure, whence each factor *is* neutral. The remainder of the argument in Ref. 5, Theorem 8.1 confirms the assertions in the theorem.

Completeness in the Theorem refers to the geodesics of g, but it is clear from the discussion of complex geodesics in Ref. 6 that the obvious notion of *completeness* for the complex geodesics of h is equivalent to completeness of the geodesics of g.

Note that the notion of nondegeneracy introduced on p. 173 of Ref. 5 is not relevant to holomorphic Riemannian manifolds as J, being anti-orthogonal, cannot belong to $\Psi(x)$.

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Pseudo-Hermiticity for a class of nondiagonalizable Hamiltonians

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We give two characterization theorems for pseudo-Hermitian (possibly nondiagonalizable) Hamiltonians with a discrete spectrum that admit a block-diagonalization with finite-dimensional diagonal blocks. In particular, we prove that for such an operator H the following statements are equivalent: (1) H is pseudo-Hermitian; (2) the spectrum of H consists of real and/or complex-conjugate pairs of eigenvalues and the geometric multiplicity and the dimension of the diagonal blocks for the complex-conjugate eigenvalues are identical; (3) H is Hermitian with respect to a positive-semidefinite inner product. We further discuss the relevance of our findings for the merging of a complex-conjugate pair of eigenvalues of diagonalizable pseudo-Hermitian Hamiltonians in general, and the PT-symmetric Hamiltonians and the effective Hamiltonian for a certain closed FRW minisuperspace quantum cosmological model in particular. © *2002 American Institute of Physics.*
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I. INTRODUCTION

In Refs. 1–5 we developed the notion of a pseudo-Hermitian operator and investigated its various consequences in particular in connection with PT-symmetric quantum systems[6] and two-component formulation of the FRW minisuperspace quantum cosmology.[7] Since the announcement of the results of Ref. 1 several authors have explored the implications of pseudo-Hermiticity.[8] The main results reported in Refs. 1–5 were, however, based on the assumption that the Hamiltonian of the system is diagonalizable and has a discrete spectrum. As demonstrated in Ref. 5, the latter condition can be easily relaxed. Moreover, in Ref. 9 we showed, without making any assumption about the diagonalizability of the Hamiltonian or discreteness of its spectrum, that the results of Refs. 1 and 3 generalized to the class of all PT-symmetric standard Hamiltonians having $\mathbb{R}$ as their configuration space. This suggests that these results may be valid under more general conditions. Our purpose in the present article is to generalize the results of Ref. 1 to the class of possibly nondiagonalizable Hamiltonians that admit a block-diagonalization with finite-dimensional diagonal blocks. This, in particular, includes all the matrix Hamiltonians. It is also relevant to the accidental loss of diagonalizability due to the pseudo-Hermiticity-preserving variations of diagonalizable pseudo-Hermitian Hamiltonians that lead to the merging of complex-conjugate pairs of eigenvalues.

The organization of the article is as follows. In Sec. II, we discuss the basic properties of the class of the Hamiltonians admitting a block-diagonalization with finite-dimensional diagonal blocks. In Sec. III, we present two characterization theorems for pseudo-Hermitian Hamiltonians belonging to this class. In Sec. IV, we study general 2×2 matrix Hamiltonians. In Sec. V, we discuss an application of our results in quantum cosmology. Finally, in Sec. VI, we present our concluding remarks.

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II. BLOCK-DIAGONALIZABLE HAMILTONIANS WITH FINITE-DIMENSIONAL DIAGONAL BLOCKS

Consider a linear operator $H:\mathcal{H}\to\mathcal{H}$ acting in a (separable) Hilbert space $\mathcal{H}$ and having a discrete spectrum. Suppose that for every eigenvalue E_n, there are positive integers $g_n, p_n \in \mathbb{Z}^+$ such that for all $l \in \mathbb{Z}^+$,

$$d_{n,l} := \dim[\ker(H-E_n 1)^l] = g_n, \text{ if and only if } l \geqslant p_n. \tag{1}$$

This in particular means that

$$d_{n,1} \leqslant d_{n,2} \leqslant \cdots \leqslant d_{n,p_n-1} \leqslant d_{n,p_n} = g_n. \tag{2}$$

The integer $d_{n,1}$ is just the degree of degeneracy or the geometric multiplicity of E_n. In what follows, we shall use the abbreviated notation d_n for $d_{n,1}$ and denote the degeneracy labels $1,2,\ldots,d_n$ by the letters from the beginning of the Latin alphabet.

The integer g_n is called the algebraic multiplicity of E_n. The condition (1) means that all the eigenvalues of H have finite algebraic multiplicity. Throughout this paper we shall assume that this condition is satisfied and that there is a basis of the Hilbert space in which H is block-diagonal with diagonal blocks being finite-dimensional. In this case, we can always find a basis in which the diagonal blocks have the canonical Jordan form,[10] i.e., there is an invertible operator $A:\mathcal{H}\to\mathcal{H}$ and an orthonormal basis $\{|n,a,i\rangle\}$ with n being the spectral label, $a \in \{1,2,\ldots,d_n\}$, $i \in \{1,2,\ldots,p_{n,a}\}$, and $p_{n,a} \in \mathbb{Z}^+$, such that

$$A^{-1}HA = H_b := \sum_n \sum_{a=1}^{d_n} \left(E_n \sum_{i=1}^{p_{n,a}} |n,a,i\rangle\langle n,a,i| + \sum_{i=1}^{p_{n,a}-1} |n,a,i\rangle\langle n,a,i+1| \right). \tag{3}$$

Alternatively, letting

$$|\psi_n,a,i\rangle := A|n,a,i\rangle, \quad |\phi_n,a,i\rangle := A^{-1\dagger}|n,a,i\rangle, \tag{4}$$

we have

$$\langle \psi_n,a,i|\phi_m,b,j\rangle = \delta_{mn}\delta_{ab}\delta_{ij}, \quad \sum_i \sum_{a=1}^{d_n} \sum_{i=1}^{p_{n,a}} |\psi_n,a,i\rangle\langle\phi_n,a,i| = 1, \tag{5}$$

$$H = AH_bA^{-1} = \sum_n \sum_{a=1}^{d_n} \left(E_n \sum_{i=1}^{p_{n,a}} |\psi_n,a,i\rangle\langle\phi_n,a,i| + \sum_{i=1}^{p_{n,a}-1} |\psi_n,a,i\rangle\langle\phi_n,a,i+1| \right). \tag{6}$$

Note that according to Eqs. (5) and (6), $\{|\psi_n,a,i\rangle, |\phi_n,a,i\rangle\}$ is a complete biorthonormal system for the Hilbert space and

$$H|\psi_n,a,1\rangle = E_n|\psi_n,a,1\rangle, \tag{7}$$

$$H^\dagger|\phi_n,a,p_{n,a}\rangle = E_n^*|\phi_n,a,p_{n,a}\rangle. \tag{8}$$

Hence $|\psi_n,a,1\rangle$ are the eigenvectors of H and $|\phi_n,a,p_{n,a}\rangle$ are the eigenvectors of $H^\dagger$.

The numbers $p_{n,a}$ represent the dimension of the Jordan block associated with the spectral label n and the degeneracy label a. We shall refer to them as the Jordan dimensions. For a given eigenvalue E_n, the number of the corresponding Jordan blocks (which is equal to the geometric multiplicity of E_n) and the Jordan dimensions are uniquely determined by the integers $d_{n,l}$ of (1) up to the permutations of the degeneracy labels.[10] Note also that the algebraic multiplicity is the sum of the Jordan dimensions, $g_n := \sum_{a=1}^{d_n} p_{n,a}$.

III. CONSEQUENCES OF PSEUDO-HERMITICITY

Theorem 1: Let $H:\mathcal{H}\to\mathcal{H}$ be a linear operator acting in a (separable) Hilbert space $\mathcal{H}$. Suppose that the spectrum of H is discrete, its eigenvalues have finite algebraic multiplicity, and that (6) holds. Then, H is pseudo-Hermitian if and only if the eigenvalues of H are either real or come in complex-conjugate pairs and the geometric multiplicity and the Jordan dimensions of the complex-conjugate eigenvalues coincide.

Proof: Suppose that H is pseudo-Hermitian. Then, by definition,[1] there is a Hermitian automorphism (linear bijection mapping $\mathcal{H}$ onto $\mathcal{H}$) $\eta:\mathcal{H}\to\mathcal{H}$ such that $H^\dagger=\eta H\eta^{-1}$. Now let E_n be an arbitrary element of the spectrum of H. Then, by virtue of Eqs. (7) and (8), for each $a\in\{1,2,\ldots,d_n\}$, $|\psi_n,a,1\rangle$ is an eigenvector of H with eigenvalue E_n and $|\phi_n,a,p_{n,a}\rangle$ is an eigenvector of $H^\dagger$ with eigenvalue E_n^*. This in turn implies $H\eta^{-1}|\phi_n,a,p_{n,a}\rangle=\eta^{-1}H^\dagger|\phi_n,a,p_{n,a}\rangle=E_n^*\eta^{-1}|\phi_n,a,p_{n,a}\rangle$. As η^{-1} is an invertible operator, $\eta^{-1}|\phi_n,a,p_{n,a}\rangle\neq 0$. Hence E_n^* also belongs to the spectrum of H. Next, note that because the eigenvalues of H and consequently $H^\dagger$ have finite algebraic multiplicity, for every $l\in\mathbb{Z}^+$, $\text{kernel}(H-E_n)^l$, $\text{kernel}(H-E_n^*)^l$, and $\text{kernel}(H^\dagger-E_n^*)^l$ are finite-dimensional subspaces of $\mathcal{H}$. Clearly, as a result of (6), H and $H^\dagger$ have essentially the same Jordan block-diagonalization. In particular, the geometric multiplicity and the Jordan dimensions of E_n^* as an eigenvalue of $H^\dagger$ is the same as the geometric multiplicity and the Jordan dimensions of E_n as an eigenvalue of H. This implies that $\text{kernel}(H^\dagger-E_n^*)^l$ and $\text{kernel}(H-E_n)^l$ have the same dimension. Thus they are isomorphic. Furthermore, using the fact that η is an automorphism, $\text{kernel}(H^\dagger-E_n^*)^l$ is also isomorphic to

$$\text{kernel}[\,\eta^{-1}(H^\dagger-E_n^*)^l\eta]=\text{kernel}(\,\eta^{-1}H^\dagger\eta-E_n^*)^l=\text{kernel}(H-E_n^*)^l.$$

Therefore, for every $l\in\mathbb{Z}^+$, $\text{kernel}(H-E_n)^l$ and $\text{kernel}(H-E_n^*)^l$ are isomorphic and consequently have the same dimension. This in turns implies that the number of the Jordan blocks associated with E and their dimensions are identical with those of E_n^*, i.e., E_n and E_n^* have the same geometric multiplicity, and up to permutations of the degeneracy labels they have identical Jordan dimensions as well. Conversely, suppose that the eigenvalues of H are either real or come in complex-conjugate pairs and the geometric multiplicity d_n and the Jordan dimensions $p_{n,a}$ of the complex conjugate pairs of eigenvalues are identical. We shall set $n=\nu_0,\nu,\nu-$ depending on whether imaginary part of E_n is zero, positive, or negative. Then $E_{\nu-}=E_\nu^*$, $d_{\nu-}=d_\nu$, for all $a\in\{1,2,\ldots,d_n\}$, $p_{\nu-,a}=p_{\nu,a}$, and Eq. (6) takes the form

$$\begin{aligned}H=&\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}}\Bigg(E_{\nu_0}\sum_{i=1}^{p_{\nu_0,a}}|\psi_{\nu_0},a,i\rangle\langle\phi_{\nu_0},a,i|+\sum_{i=1}^{p_{\nu_0,a}-1}|\psi_{\nu_0},a,i\rangle\langle\phi_{\nu_0},a,i+1|\Bigg)\\&+\sum_{\nu}\sum_{a=1}^{d_\nu}\Bigg[\sum_{i=1}^{p_{\nu,a}}(E_\nu|\psi_\nu,a,i\rangle\langle\phi_\nu,a,i|+E_\nu^*|\psi_{\nu-},a,i\rangle\langle\phi_{\nu-},a,i|)\\&+\sum_{i=1}^{p_{\nu,a}-1}(|\psi_\nu,a,i\rangle\langle\phi_\nu,a,i+1|+|\psi_{\nu-},a,i\rangle\langle\phi_{\nu-},a,i+1|)\Bigg].\end{aligned}\tag{9}$$

Next, let

$$\begin{aligned}\eta(x,\xi):=&\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}}\sum_{i=1}^{p_{\nu_0,a}}\sum_{j=p_{\nu_0,a}+1-i}^{p_{\nu_0,a}}x_{\nu_0,a,i+j}|\phi_{\nu_0},a,i\rangle\langle\phi_{\nu_0},a,j|\\&+\sum_{\nu}\sum_{a=1}^{d_\nu}\sum_{i=1}^{p_{\nu,a}}\sum_{j=p_{\nu,a}+1-i}^{p_{\nu,a}}(\xi_{\nu,a,i+j}|\phi_\nu,a,i\rangle\langle\phi_{\nu-},a,j|+\xi_{\nu,a,i+j}^*|\phi_{\nu-},a,j\rangle\langle\phi_\nu,a,i|),\end{aligned}\tag{10}$$

where $x_{\nu_0,a,k}\in\mathbb{R}$, $\xi_{\nu,a,k}\in\mathbb{C}$,

$$x_{\nu_0,a,p_{\nu_0,a}+1}\neq 0\neq \xi_{\nu,a,p_{\nu,a}+1}, \tag{11}$$

and x and ξ, respectively, stand for the sequences $\{x_{\nu_0,a,k}\}$ and $\{\xi_{\nu,a,k}\}$. It is not difficult to check that, for all $n=\nu_0,\nu,\nu-$, $m=\mu_0,\mu,\mu-$, and the corresponding degeneracy labels a,b and Jordan block labels i,j,

$$\langle\psi_{\nu_0},a,i|\,\eta(x,\xi)\,|\psi_{\mu_0},b,j\rangle=\begin{cases}\delta_{\nu_0,\mu_0}\delta_{ab}x_{\nu_0,a,i+j}, & \text{for } i+j>p_{\nu_0,a}\\ 0, & \text{otherwise;}\end{cases}$$

$$\begin{aligned}\langle\psi_{\nu},a,i|\,\eta(x,\xi)\,|\psi_{\mu-},b,j\rangle&=\langle\psi_{\mu-},a,i|\,\eta(x,\xi)\,|\psi_{\nu},b,j\rangle^*\\&=\begin{cases}\delta_{\nu,\mu}\delta_{ab}\xi_{\nu,a,i+j}, & \text{for } i+j>p_{\nu,a}\\ 0, & \text{otherwise;}\end{cases}\end{aligned} \tag{13}$$

and that the other matrix elements of $\eta:=\eta(x,\xi)$, in the basis $\{|\psi_n,a,j\rangle\}$, vanish. In view of Eqs. (12), (13), and (11), η is a Hermitian automorphism. Furthermore, using Eqs. (5) and (9)–(11), one can check that it satisfies $\eta H=H^\dagger\eta$. Hence, $H^\sharp:=\eta^{-1}H^\dagger\eta=H$, and H is η-pseudo-Hermitian.□

An immediate consequence of this theorem is the following

Corollary 1: Let H be as in Theorem 1. Then the pseudo-Hermiticity of H is a necessary condition for the reality of its spectrum.

Note that (10) is not the most general expression for an η with respect to which H is η-pseudo-Hermitian. One can obtain more general expressions by performing appropriate basis transformations. (These are the transformations that mix the basis vectors with different degeneracy labels a but identical spectral label n and the Jordan dimension $p_{n,a}$). Similarly to the diagonalizable case,[4] one can also perform a change of basis to set $x_{\nu_0,a,k}=\pm 1$ and $\xi_{\nu,a,k}=1$. This is, however not the simplest choice for η. It is not difficult to check that the following simpler choice works as well:

$$x_{\nu_0,a,k}=\begin{cases}\pm 1, & \text{for } k=p_{\nu_0,a}+1,\\ 0, & \text{otherwise,}\end{cases}\qquad \xi_{\nu,a,k}=\begin{cases}1, & \text{for } k=p_{\nu,a}+1,\\ 0, & \text{otherwise.}\end{cases} \tag{14}$$

In this way one obtains the following set of simple canonical automorphisms with respect to which H is η-pseudo-Hermitian:

$$\begin{aligned}\eta(\sigma):=&\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}}\sigma_{\nu_0,a}\left(\sum_{i=1}^{p_{\nu_0,a}}|\phi_{\nu_0},a,i\rangle\langle\phi_{\nu_0},a,p_{\nu_0,a}+1-i|\right)\\&+\sum_{\nu}\sum_{a=1}^{d_\nu}\sum_{i=1}^{p_{\nu,a}}(|\phi_\nu,a,i\rangle\langle\phi_{\nu-},a,p_{\nu,a}+1-i|+|\phi_{\nu-},a,p_{\nu,a}+1-i\rangle\langle\phi_\nu,a,i|),\end{aligned} \tag{15}$$

with $\sigma:=\{\sigma_{\nu_0,a}\}$ being a sequence of signs. A straightforward calculation shows that

$$\begin{aligned}\eta(\sigma)^{-1}:=&\sum_{\nu_0}\sum_{a=1}^{d_{\nu_0}}\sigma_{\nu_0,a}\left(\sum_{i=1}^{p_{\nu_0,a}}|\psi_{\nu_0},a,i\rangle\langle\psi_{\nu_0},a,p_{\nu_0,a}+1-i|\right)\\&+\sum_{\nu}\sum_{a=1}^{d_\nu}\sum_{i=1}^{p_{\nu,a}}(|\psi_\nu,a,i\rangle\langle\psi_{\nu-},a,p_{\nu,a}+1-i|+|\psi_{\nu-},a,p_{\nu,a}+1-i\rangle\langle\psi_\nu,a,i|).\end{aligned} \tag{16}$$

If H is diagonalizable, $p_{n,a}=1$ and (15) yields the expression for the canonical automorphisms given in Ref. 4. Again choosing all the signs $\sigma_{\nu_0,a}$ to be positive yields a positive-semidefinite (non-negative) η and a positive-semidefinite inner product,

$$\langle\langle\psi,\phi\rangle\rangle_\eta := \langle\psi|\,\eta\,|\phi\rangle. \tag{17}$$

However, even if the complex eigenvalues are absent this choice does not lead to a positive-definite inner product on the Hilbert space unless H is diagonalizable. This is because in general there are defective (real) eigenvalues E_{ν_0}; at least one of the Jordan dimensions $p_{\nu_0,a}$ is greater than 1; and according to (12) and (13), $\langle\langle\psi_{\nu_0},a,1|\psi_{\nu_0},a,1\rangle\rangle_\eta=\langle\psi_{\nu_0},a,1|\,\eta\,|\psi_{nu_0},a,1\rangle=0$. Hence the corresponding eigenvector $|\psi_{\nu_0},a,1\rangle$ is null, and the inner product (17) is not positive-definite.

Theorem 2: Let H be as in Theorem 1. Then H is pseudo- Hermitian if and only if it is Hermitian with respect to a positive-semidefinite inner product $\langle\langle\,,\rangle\rangle:\mathcal{H}^2\to\mathbb{C}$, i.e., for all $\phi,\psi\in\mathcal{H}$, $\langle\langle\phi,H\psi\rangle\rangle=\langle\langle H\phi,\psi\rangle\rangle$.

Proof: Suppose H is pseudo-Hermitian, then according to Theorem 1 it has real and/or complex-conjugate pairs of eigenvalues with identical geometric multiplicity and Jordan dimensions. According to the proof of this theorem, this implies that H is pseudo-Hermitian with respect to the automorphism (15) with $\sigma_{\nu_0,a}=1$ for all ν_0 and $a\in\{1,2,\ldots,d_{\nu_0}\}$. The latter yields the positive-semidefinite inner product (17) which satisfies, for all $\psi,\phi\in\mathcal{H}$,

$$\langle\langle\phi,H\psi\rangle\rangle_\eta=\langle\phi|\,\eta H\,|\psi\rangle=\langle\phi|H^\dagger\,\eta\,|\psi\rangle=\langle H\phi|\,\eta\,|\psi\rangle=\langle\langle H\phi,\psi\rangle\rangle_\eta.$$

Hence H is Hermitian with respect to the inner product (17). Conversely, let H be Hermitian with respect to a positive-semidefinite inner product $\langle\langle\,,\rangle\rangle$. Let $\eta:\mathcal{H}\to\mathcal{H}$ be defined in terms of its matrix elements according to, for all $\psi,\phi\in\mathcal{H}$,

$$\langle\psi|\,\eta\,|\phi\rangle := \langle\langle\psi,\phi\rangle\rangle.$$

Then, because $\langle\langle\,,\rangle\rangle$ is a sesquilinear, Hermitian, nondegenerate quadratic form,[11] η is a linear, Hermitian, automorphism. Furthermore, because H is Hermitian with respect to $\langle\langle\,,\rangle\rangle$ we have, for all $\psi,\phi\in\mathcal{H}$,

$$\langle\phi|\,\eta H\psi\rangle=\langle\langle\phi,H\psi\rangle\rangle=\langle\langle H\phi,\psi\rangle\rangle=\langle H\phi|\,\eta\,|\psi\rangle=\langle\phi|H^\dagger\,\eta\psi\rangle.$$

Therefore, $\eta H=H^\dagger\,\eta$ or $H^\sharp:=\eta^{-1}H^\dagger\,\eta=H$, i.e., H is pseudo-Hermitian. □

IV. 2×2 MATRIX HAMILTONIANS

In Ref. 3, we showed that the pseudo-Hermiticity of a diagonalizable Hamiltonian is equivalent to the presence of antilinear symmetries. The PT-symmetry studied in the literature[6] is a primary example. In general, such a Hamiltonian depends on certain continuous parameters whose variation does not destroy the symmetry but changes the spectrum. In particular, it is possible that under such variations complex-conjugate pairs of eigenvalues merge and produce real eigenvalues or a real eigenvalue splits into a complex-conjugate pair of eigenvalues. This is a generic behavior observed in the numerical studies of PT-symmetric Hamiltonians[6] and naturally applies in the case of general pseudo-Hermitian Hamiltonians. Now consider a diagonalizable pseudo-Hermitian Hamiltonian with a discrete spectrum that undergoes a continuous pseudo-Hermiticity-preserving perturbation. In general, such a perturbation may not preserve the diagonalizability of the Hamiltonian.[12] In particular, at the critical values of the perturbation parameter when two nondegenerate complex-conjugate eigenvalues merge to produce a real eigenvalue, there is no guarantee that the resulting eigenvalue is doubly degenerate. This observation underlies the importance of the results of Sec. III in the study of the behavior of diagonalizable pseudo-Hermitian operators undergoing arbitrary pseudo-Hermiticity-preserving perturbations.

Consider the case that under such a perturbation a pair of complex-conjugate nondegenerate eigenvalues cross while no other level-crossing occurs. In the vicinity of this level-crossing, one can approximate the behavior of the Hamiltonian by a traceless 2×2 matrix Hamiltonian. In Ref. 4, we have studied the properties of general complex, traceless, diagonalizable, pseudo-Hermitian 2×2 matrix Hamiltonians. A traceless 2×2 matrix H with two nondegenerate eigenvalues is pseudo-Hermitian if its determinant is a nonzero real number.[4] As we explain below the converse of this statement is also true. In particular, $\det(H)<0$ or $\det(H)>0$ depending on whether the eigenvalues are real or imaginary. This means that the moduli space $\mathcal{M}$ of traceless pseudo-Hermitian 2×2 matrices with two nondegenerate eigenvalues is a 5-dimensional subspace of the 8-dimensional space $M(2,\mathbb{C})$ of all complex 2×2 matrices. The latter has the manifold structure of $\mathbb{C}^4=\mathbb{R}^8$. If we, respectively, denote the subsets of complex traceless 2×2 matrices, complex traceless pseudo-Hermitian 2×2 matrices, and traceless Hermitian 2×2 matrices by M_0, $\mathcal{M}'$, and $\mathcal{M}_0$, we have

$$\begin{array}{ccccccccc} \mathcal{M}_0 & \subset & \mathcal{M} & \subset & \mathcal{M}' & \subset & M_0 & \subset & M(2,\mathbb{C}) \\ || & & & & & & || & & || \\ \mathbb{R}^3 & & & & & & \mathbb{R}^6 & & \mathbb{R}^8. \end{array}$$

We can identify $\mathcal{M}$ with the inverse image of $\mathbb{R}-\{0\}\subset\mathbb{R}^2=\mathbb{C}$ under the continuous function $\det: M(2,\mathbb{C})\to\mathbb{C}=\mathbb{R}^2$. Noting that $\mathbb{R}^+$ and $\mathbb{R}^-$ are disjoint, open, connected subsets of $\mathbb{C}$ and det is continuous, we infer that $\mathcal{M}$ consists of two open connected components, namely

$$\mathcal{M}^{\pm}:=\{H\in\mathcal{M}|\det H\in\mathbb{R}^{\pm}\}.$$

This in turn implies that at a critical point of the parameters of H where a level-crossing happens, H fails to stay in $\mathcal{M}$. This is also easily seen by realizing that because H is traceless, a level-crossing can occur only if $\det H$ vanishes. Therefore, at the level-crossing either $H=0$ or it is nondiagonalizable.

In fact, it is not difficult to see that an element $X_{\pm}$ of $\mathcal{M}^{\pm}$ has the general form

$$X_{\pm}=\sqrt{\pm 1}Eg^{-1}\sigma_3 g, \tag{18}$$

where E is a nonzero real number, g is an element of the special linear group $SL(2,\mathbb{C})$, and σ_3 is the diagonal Pauli matrix $\mathrm{diag}(1,-1)$. The form (18) indicates that the moduli spaces $\mathcal{M}^+$ and $\mathcal{M}^-$ have the manifold structure of $F\times(\mathbb{R}-\{0\})$ where F is the 4-dimensional homogeneous space:

$$F:=SL(2,\mathbb{C})/U_{\mathbb{C}}(1),$$

and

$$U_{\mathbb{C}}(1):=\{e^{z\sigma_3}|z\in\mathbb{C}\}=\left\{\left(\begin{array}{cc} w & 0 \\ 0 & w^{-1}\end{array}\right)\middle| w\in\mathbb{C}-\{0\}\right\}.$$

Furthermore, according to (18) the group elements g that are uniquely parametrized by the points of F play the same role for both X_+ and X_-. It is the factor $\sqrt{\pm 1}\,E$ in (18) that differentiates X_+ and X_-. This suggests that we can identify $\mathcal{M}^{\pm}$ by $F\times L^{\pm}$, where

$$L^+:=\{z\in\mathbb{C}-\{0\}|\mathrm{Re}(z)=0\}=\text{imaginary axis in the complex plane with 0 removed,}$$

$$L^-:=\{z\in\mathbb{C}-\{0\}|\mathrm{Im}(z)=0\}=\text{real axis in the complex plane with 0 removed,}$$

and ''Re'' and ''Im'' stand for the ''real'' and the ''imaginary'' part of the corresponding complex variable, respectively.

The above picture of $\mathcal{M}$ confirms our earlier remark that at a level-crossing a traceless pseudo-Hermitian 2×2 matrix,

$$H=\begin{pmatrix} a & b \\ c & -a \end{pmatrix}, \tag{19}$$

either vanishes identically:

$$a=b=c=0, \tag{20}$$

or becomes nondiagonalizable:

$$a=\pm i\sqrt{bc}, \quad |a|^2+|b|^2+|c|^2\neq 0, \tag{21}$$

where $i:=\sqrt{-1}$. In the latter case, according to (6), H has the form $H=|\psi_1\rangle\langle\phi_2|$ where $\{|\psi_a\rangle,|\phi_a\rangle\}$ with $a=\{1,2\}$ is a complete biorthonormal system in $\mathbb{C}^2$. In particular, we have the following.

Proposition 1: Every traceless nondiagonalizable 2×2 matrix H is pseudo-Hermitian.

Proof: Because H is both traceless and nondiagonalizable, zero is the only eigenvalue of H. Hence according to Theorem 1, it must be pseudo-Hermitian. □

Theorem 3: A traceless 2×2 matrix H is pseudo-Hermitian if and only if it has a real determinant, i.e.,

$$\mathcal{M}'=\{H\in M_0|\det H\in\mathbb{R}\}.$$

Proof: If H is not diagonalizable, then according to Proposition 1 it is pseudo-Hermitian, and the statement of Theorem 3 is trivially satisfied. If H is diagonalizable, it is either identically zero, in which case it is pseudo-Hermitian and has a real (zero) determinant, or it has two nondegenerate eigenvalues. In the latter case, in view of a proposition proven in Ref. 4, the reality of the determinant of H implies its pseudo-Hermiticity. The converse is also true. For if H is pseudo-Hermitian, then its eigenvalues are either both real or they are complex-conjugate of one another. Because H has a vanishing trace, in the latter case the eigenvalues must be imaginary. This in turn implies that in both cases the determinant of H is real. □

In light of Theorem 3, the possibility (20) that at a level-crossing a traceless pseudo-Hermitian 2×2 matrix Hamiltonian remains diagonalizable corresponds to a single point in the uncountably infinite set of traceless nondiagonalizable pseudo-Hermitian 2×2 matrices $\mathcal{M}'-\mathcal{M}$. To make this observation more transparent, consider the pseudo-Hermitian matrix Hamiltonians (19) corresponding to the choice $c=0$. Then $\det H=-a^2$, $a\in L^{\pm}$, and $H\in\mathcal{M}^{\pm}$. Now suppose that a and b are analytic functions of a real perturbation parameter λ and that a level-crossing occurs at $\lambda=0$. Then at the vicinity of the level-crossing, i.e., for $|\lambda|<\epsilon$ for some sufficiently small $\epsilon\in\mathbb{R}^+$,

$$a(\lambda)\approx\begin{cases} a_{\rm r}\lambda, & \text{for} \quad -\epsilon<\lambda\leqslant 0 \\ ia_{\rm i}\lambda, & \text{for} \quad 0\leqslant\lambda<\epsilon \end{cases}, \quad b(\lambda)\approx b_0+b_1\lambda,$$

where $a_{\rm r}$ and $a_{\rm i}$ are nonzero real constants, and b_0 and b_1 are complex constants. At $\lambda=0$, H vanishes identically provided that $b_0=b(0)=0$. This is the only way in which H can maintain its diagonalizability. Clearly, for $b_0\neq 0$, H becomes nondiagonalizable at $\lambda=0$. In both cases $a(0)=0\in\mathbb{R}$ is the only eigenvalue (alternatively $\det H=0$). Hence, according to Corollary 1 (respectively, Theorem 3), H remains pseudo-Hermitian at $\lambda=0$. This example clearly shows that the loss of diagonalizability at the crossing of the complex-conjugate eigenvalues is a generic behavior.

V. APPLICATION

Consider the Wheeler–DeWitt equation for the closed FRW minisuperspace model with a real massive scalar field,

$$\left[-\frac{\partial^2}{\partial\alpha^2}+\frac{\partial^2}{\partial\varphi^2}+e^{4\alpha}-m^2e^{6\alpha}\varphi^2\right]\psi(\alpha,\varphi)=0, \tag{22}$$

where $\alpha:=\ln a$, "a" is the scale factor, φ is a real scalar field of mass m, and we have chosen a particularly simple factor ordering and the natural units.[13,14] The Wheeler–DeWitt equation (22) can be written in the Schrödinger form $i\dot{\Psi}=H\Psi$ where Ψ is the two-component wave function,[7]

$$\Psi:=\frac{1}{\sqrt{2}}\begin{pmatrix}\psi+i\dot{\psi}\\ \psi-i\dot{\psi}\end{pmatrix},$$

H is the effective Hamiltonian,

$$H:=\frac{1}{2}\begin{pmatrix}1+D & -1+D\\ 1-D & -1-D\end{pmatrix}, \tag{23}$$

a dot means a derivative with respect to α, and

$$D:=-\frac{\partial^2}{\partial\varphi^2}+m^2e^{6\alpha}\varphi^2-e^{4\alpha}. \tag{24}$$

The eigenvalue problem for the Hamiltonian (23) may be easily solved.[7] The eigenvectors $\Psi_{n\pm}$ and the corresponding eigenvalues $E_{n\pm}$ have the form

$$\Psi_{n\pm}=\frac{1}{\sqrt{2}}\begin{pmatrix}1+E_{n\pm}\\ 1-E_{n\pm}\end{pmatrix}\phi_n,\quad E_{n\pm}=\pm\sqrt{me^{3\alpha}(2n+1)-e^{4\alpha}}=\pm a\sqrt{a[m(2n+1)-a]}, \tag{25}$$

where $n=0,1,2,\ldots$, $\phi_n:=N_nH_n(m^{1/2}e^{3\alpha/2}\varphi)e^{-me^{3\alpha}\varphi^2/2}$, H_n are Hermite polynomials, and $N_n:=[me^{3\alpha}/(\pi 2^{2n}n!^2)]^{1/4}$ are normalization constants.

As seen from (25), for $a\leqslant m$ the spectrum of H is real, and for $a>m$ it consists of real and complex-conjugate pairs of eigenvalues. In general H is pseudo-Hermitian, because $H^\dagger=\sigma_3H\sigma_3$. For $a\neq(2n+1)m$, it is also diagonalizable. But at the critical values $a=(2n+1)m$ where a real (namely the zero) eigenvalue splits into a complex-conjugate pair of eigenvalues or the converse happens, H fails to be diagonalizable. The situation is precisely like the one discussed in Sec. IV. Here the perturbation parameter has the form $\lambda:=a-(2n+1)m$. At the vicinity of a level-crossing where $\lambda\to0$, the operator D and its eigenvectors do not undergo any discontinuous changes. Therefore, one can approximate the span of the eigenvectors Ψ_{n-} and Ψ_{n+} for $\lambda\neq0$ with the span of the vectors,

$$|1\rangle=\begin{pmatrix}\phi_n\\ 0\end{pmatrix},\quad |2\rangle=\begin{pmatrix}0\\ \phi_n\end{pmatrix},$$

where ϕ_n is evaluated at $\alpha=\ln a=\ln[(2n+1)m]$, i.e., $\lambda=0$. Clearly, we can study the level-crossing by confining our attention to this subspace. The above approximation becomes exact in the limit $\lambda\to0$. In the subspace spanned by $|1\rangle$ and $|2\rangle$ the operator D is identically zero. Therefore, we can approximate D by a constant that tends to zero as $\lambda\to0$. Therefore, the Hamiltonian (23) takes the form of the matrix Hamiltonian (19) with $a=(1+D)/2$,$b=(-1+D)/2$, and $c=(1-D)/2$. In the limit $\lambda\to0$, D approaches zero, and the conditions (21) hold. Hence, as expected, H becomes nondiagonalizable at the level-crossing.

The above argument implies that in general H is diagonalizable for all values of the scale factor except the critical values $a=(2n+1)m$. At these values H becomes nondiagonalizable as one of its eigenvalues, namely the zero eigenvalue, becomes defective. The algebraic multiplicity of this eigenvalue is two. In fact, the effective Hamiltonian (23) belongs to the class of block-diagonalizable Hamiltonians discussed in Secs. II and III. Its canonical Jordan form consists of a 2×2 Jordan block corresponding to the zero eigenvalue and an infinite number of trivial (1×1) blocks corresponding to nonzero eigenvalues. The fact that this Hamiltonian is pseudo-Hermitian for all values of the scale factor, its spectrum consists of real and complex- conjugate eigenvalues, and its complex eigenvalues are not defective is consistent with the general results of Sec. III.

VI. SUMMARY AND CONCLUSION

In this article we generalized our earlier results on diagonalizable pseudo-Hermitian Hamiltonians to a broad class of nondiagonalizable Hamiltonians. We showed that if a pseudo-Hermitian Hamiltonian may be mapped to a block-diagonal operator with finite-dimensional blocks via a similarity transformation, then the characterization theorems of Ref. 1 apply provided that the number and size of the Jordan blocks for the complex-conjugate pairs of eigenvalues are identical.

We also discussed the implications of our findings for the phenomenon of the loss of diagonalizability at the crossing of the complex-conjugate pairs of eigenvalues of diagonalizable pseudo-Hermitian Hamiltonians. For the latter, pseudo-Hermiticity is known to be equivalent to the presence of an antilinear symmetry.[3] This in particular means that our results are relevant in the description of the PT-symmetric systems that are diagonalizable except in the case of level-crossings of the complex-conjugate eigenvalues due to perturbations of the Hamiltonian. If at the critical values of the perturbation parameter each level-crossing involves a finite number of levels, then our results apply generally. This seems to be the case for various PT-symmetric models studied in the literature. Specifically, at the critical values of the parameters of the PT-symmetric systems that undergo a spontaneous PT-symmetry breaking, a pair of real eigenvalues merge and a loss of diagonalizability similar to the one discussed in Sec. V occurs.

As a final note, we wish to emphasize that the results of this paper rely on the basic assumption that the quantum system has a genuine separable Hilbert space in which the Hamiltonian acts. For many PT-symmetric Hamiltonians the (inner product) structure of the function space in which one solves for the eigenfunctions is not clear. In this context, the assumption of considering non-Hermitian Hamiltonians acting in a separable Hilbert space may seem too restrictive. Nevertheless, we believe that this assumption provides a framework for exploring some of the intriguing properties of a class of non-Hermitian Hamiltonians. This class includes many PT-symmetric Hamiltonians as well as all the matrix Hamiltonians and the non-Hermitian Hamiltonians appearing in the two-component formulation of the Klein–Gordon and Wheeler–DeWitt equations.

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The eight fine gradings of sl(4, $\mathbb{C}$) and o(6, $\mathbb{C}$)

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A grading of a Lie algebra is called fine if it cannot be further refined. Fine gradings provide basic information about the structure of the algebra. There are eight fine gradings of the simple Lie algebra of type A_3 over the complex number field. One of them (root decomposition) is the main tool of the theory and applications in working with A_3 and with its representations; one other has also been used in the literature, and the rest have apparently not been recognized so far. An explicit description of all the fine gradings of A_3 is given in terms of the four-dimensional [sl(4, $\mathbb{C}$)] and six-dimensional orthogonal [o(6, $\mathbb{C}$)] representations of the algebra. These results should be useful generally for choosing bases which reflect structural properties of the Lie algebra, for defining various sets of additive quantum numbers for systems with such symmetries, and for systematic study of grading preserving contractions of this Lie algebra. © *2002 American Institute of Physics.*
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I. INTRODUCTION

Decomposition of a Lie algebra, considered as a linear space, into the direct sum of subspaces of lower dimension is a simple problem which obviously has many solutions. However, if in addition one requires that such a decomposition is a grading, severe limitations are imposed on the possible decompositions so that the problem of classification of all the gradings becomes a difficult task. Its solution has not been published for any simple Lie algebra of rank >1. Indeed, grading is a requirement involving the multiplication (i.e., commutation) in the algebra. It is natural to consider two decompositions (grading or not) equivalent if one can be transformed into the other by an automorphism of the Lie algebra.

A finite dimensional Lie algebra can be decomposed into a finite number of nonempty subspaces. (We disregard the decompositions which would introduce additional subspaces of dimension 0.) A coarse grading decomposes the Lie algebra into a small number of grading subspaces. The coarsest trivial one leaves the Lie algebra in one subspace. The coarsest nontrivial gradings decompose the algebra into two subspaces. Every simple Lie algebra over $\mathbb{C}$ admits several gradings of this kind. It is well known that the real forms of the algebra are in one-to-one correspondence with such gradings.

The *fine grading* was introduced in Ref. 1 as a grading which decomposes the Lie algebra into a maximal number of subspaces. By definition such a decomposition cannot be further refined while remaining a grading. The best known example of a fine grading of simple Lie algebra over $\mathbb{C}$ is the root (also called Cartan) decomposition. There a Lie algebra of rank r and dimension rk is decomposed into the r-dimensional Cartan subalgebra and $r(k-1)$ one-dimensional root spaces. There is no grading which would further split the Catran subalgebra.

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The present article is very similar to Ref. 2, where an explicit description of fine gradings of a rank two Lie algebra of type B_2 [equivalently sp(4, $\mathbb{C}$) and o(5, $\mathbb{C}$)] is given. There are eight nonequivalent fine gradings of the simple Lie algebra A_3.[3] Their description is provided in this article for the first time. More precisely, we consider the lowest representations of A_3 of dimension 4 and 6, calling them respectively sl(4, $\mathbb{C}$) and o(6, $\mathbb{C}$), and present the eight gradings in both representations. Only one of them is well known (root decomposition) and one other for each representation can also be found in the literature. We refer to Ref. 2 also for general motivation for studying fine gradings of semisimple Lie algebras. Let us point out here only the following: A fine grading goes a long way in defining a basis of the Lie algebra (up to a normalization). A graded basis exploits structural properties of the Lie algebra such as the simplicity of commutation relations of the generators. The most difficult step in describing all the gradings of an algebra is to find its fine gradings. Many important properties of simple Lie algebras and computing tools are related to their root systems. Therefore it is natural to ask whether the grading labels of other fine gradings could possibly play an analogous role. In particular, an important class of subalgebras are the regular ones. They are all displayed by the root decomposition. Other fine gradings display other subalgebras.

Consider a simple Lie algebra L with complex parameters. In Ref. 3 maximal subgroups of the automorphism group Aut L with Abelian diagonalizable action on L were classified (so called MAD-groups). Decomposition of L into eigenspaces of a given MAD-group is a fine grading. The eigenspaces (grading subspaces) of such a decomposition are naturally labeled by the eigenvalues of the elements of the MAD-group. Practically a small number of elements of the MAD-group provides enough eigenvalues to label the subspaces. Choice of the labeling elements is far from unique but the grading subspaces of a fine grading do not depend on that choice. In physics the eigenvalues labeling the grading subspaces are interpreted as maximal sets of simultaneously admissible quantum numbers describing a system with the symmetry of the Lie algebra L. Different choices of the labeling elements reflect the fact that there are several possible choices of quantum numbers describing the systems with the same symmetry algebra L.

Once the explicit fine gradings are written down, it is easy to verify that among them there are no equivalent pairs. Indeed, one can proceed, for example, as follows: (i) Compare the dimensions of grading subspaces. If they do not coincide, gradings are not equivalent. It there are coincidences, then (ii) compare the number of one-dimensional grading subspaces which consist of semisimple and nilpotent elements. Again, if those numbers do not coincide, the two gradings are not equivalent. Finally, if previous tests failed to provide a definite answer, (iii) compare the number of commuting pairs of one-dimensional grading subspaces. The three simple criteria above may not be sufficient for all the simple Lie algebras, but they suffice to verify the nonequivalence of the eight gradings of sl(4, $\mathbb{C}$). It is taken from Ref. 3 that there are precisely eight such gradings. One of the motivations for the present article is the fact that the way from the MAD-groups to actual gradings is rather laborious and that the properties of the fine gradings are not easily detectable from its MAD-group.

In this article we say that a subalgebra L' of a Lie algebra L is *displayed* by a grading of L, if L' consists of several grading subspaces of the grading decomposition. There are four maximal reductive subalgebras in sl(4, $\mathbb{C}$), namely the following ones:

$$\mathrm{sp}(4,\mathbb{C}),\quad \mathrm{o}(4,\mathbb{C})\simeq\mathrm{sl}(2,\mathbb{C})\times\mathrm{sl}(2,\mathbb{C}),\quad \mathrm{gl}(3,\mathbb{C})\simeq\mathrm{sl}(3,\mathbb{C})\times\mathrm{u}(1),\quad \mathrm{sl}(2,\mathbb{C})\times\mathrm{sl}(2,\mathbb{C})\times\mathrm{u}(1). \tag{1}$$

Here we have noted the well known isomorphisms; u(1) stands for a one-dimensional ideal of the subalgebra. The presence of a displayed maximal reductive subalgebra for each of the fine gradings is pointed out in the article. There is an inherent ambiguity in the traditional notations for subalgebras (1). Thus, for example, the two subalgebras denoted sl(2, $\mathbb{C}$)$\times$sl(2, $\mathbb{C}$) are very different [see (6) in Sec. II].

In Sec. II preliminary useful information is recalled and some notations are fixed. Section III contains a description of the fine gradings of sl(4, $\mathbb{C}$) in terms of 4×4 matrices. Maximal reductive subalgebras of A_3 are described in Sec. IV. The fine gradings of o(6, $\mathbb{C}$) are presented in Sec. V in terms of 6×6 matrices. The last section contains comments and conclusions.

II. PRELIMINARIES

Since the task we have set forth in this article is to describe eight rather complicated cases in two versions each, it makes sense to collect in this section common notations, facts, and as much as possible of the repetitive pertinent properties, besides the introductory mathematics that one typically expects here. The economy of space one gains in this way does not come without a price: the section becomes a collection of little connected and/or motivated facts which need to be frequently consulted later on.

(1) The defining or natural representation of the simple Lie algebra sl(4, $\mathbb{C}$) has 15 complex valued parameters which are denoted by $a,b,\ldots,p$. Thus the (complex) dimension of the algebra is 15:

$$\mathrm{sl}(4,\mathbb{C})=\{X\in\mathbb{C}^{4\times4}|\mathrm{tr}X=0\}=\left\{X=\begin{pmatrix} a & b & c & d\\ e & f & g & h\\ j & k & l & m\\ n & o & p & -a-f-l\end{pmatrix}\middle|\, a,\ldots,p\in\mathbb{C}\right\}. \tag{2}$$

In a number of applications one needs to consider only the Lie algebras of orthogonal transformations. It is one of the coincidences which happen among small rank simple Lie algebras, that sl(4, $\mathbb{C}$) of (2) is isomorphic to the Lie algebra o(6, $\mathbb{C}$):

$$\mathrm{o}(6,\mathbb{C})=\{X\in\mathbb{C}^{6\times6}|XK+KX^T=0\},\quad K=K^T,\quad \det K=1. \tag{3}$$

Different choices of the matrix K define equivalent representations of the algebra. The two following representations are widely used:

$$K=\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 0 & 1\end{pmatrix}:$$

$$\mathrm{o}(6,\mathbb{C})=\left\{\begin{pmatrix} 0 & a & b & c & d & e\\ -a & 0 & f & g & h & j\\ -b & -f & 0 & k & l & m\\ -c & -g & -k & 0 & n & o\\ -d & -h & -l & -n & 0 & p\\ -e & -j & -m & -o & -p & 0\end{pmatrix}\middle|\, a,\ldots,p\in\mathbb{C}\right\}, \tag{4}$$

$$K=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}:$$

$$\mathrm{o}(6,\mathbb{C})=\left\{ \begin{pmatrix} a & b & c & d & e & 0 \\ f & g & h & j & 0 & -e \\ k & l & m & 0 & -j & -d \\ n & o & 0 & -m & -h & -c \\ p & 0 & -o & -l & -g & -b \\ 0 & -p & -n & -k & -f & -a \end{pmatrix} \middle| \; a,\ldots,p\in\mathbb{C} \right\}. \tag{5}$$

One simple way how to choose a basis, also called the generators, of the Lie algebra, is to put one parameter equal to 1 and all others equal to 0. The bases chosen in this way from (2) and (4) or (5) are in no particular correspondence. In our study of gradings, the normalization of the generators is of no importance, therefore we are often being guided by the simplicity of the corresponding matrices.

In general, the equality of the normalizations in (2) and (4), (5) can be fixed by using the Killing form with the second indices of the representations involved. More precisely, suppose $\phi(x)$ and $\psi(x)$ represent the element $x\in A_3$ in two different representations, say ϕ and ψ. Denoting the second indices of the representations respectively by l_ϕ and l_ψ, one has the Killing form (x,y) given (up to a suitable constant) by

$$(x,y)=l_\phi \mathrm{tr}(\phi(x)\phi(y))=l_\psi \mathrm{tr}(\psi(x)\psi(y)),$$

which fixes the relative normalization in the representations ϕ and ψ. In particular, let ϕ and ψ stand for the representations (2) and (3), respectively. Then we have

$$\mathrm{tr}(\phi(x)\phi(y))=2\,\mathrm{tr}(\psi(x)\psi(y)).$$

The values of the indices can be found, for example, in Ref. 4 for many representations.

(2) Grading of a Lie algebra L implies that, as a linear space, the algebra can be decomposed into the direct sum of several nontrivial subspaces, $L=\oplus_{k\in\mathcal{I}}L_k$ in such a way that for every choice of $x\in L_k$ and $y\in L_j$ we have $[x,y]\in L_{k+j}$. Symbolically we note this property as

$$0\neq[L_k,L_j]\subseteq L_{k+j}. \tag{6}$$

If $j+k\notin\mathcal{I}$ for some $j,k\in\mathcal{I}$, then necessarily the subspaces L_j, L_k commute.

The grading labels $k,j,\ldots$ are far from uniquely defined. However, the decomposition into the direct sum of subspaces is determined up to an automorphism of L. Natural requirements of simplicity reduce the wide choice of grading labels to a very few. In general the grading labels are multi-component.

A grading is determined if a basis for each subspace L_k is given. Practically a grading is obtained as an eigenspace decomposition of suitably chosen elements of the automorphism group $Aut\ L$ of L. It follows that the grading subspaces are orthogonal with respect to the Killing form.

The result that we present in this article is the list of all nonequivalent *fine* gradings of the Lie algebra sl(4, $\mathbb{C}$). A grading $L=\oplus_{k\in\mathcal{I}}L_k$ of a Lie algebra is called fine when none of its subspaces L_k can be further split into several nontrivial subspaces in such a way that the new decomposition would still be a grading of L.

It is useful to introduce two operations on gradings of a Lie algebra L, namely *refinement* and *coarsening* of a grading. A given grading $L=\oplus_{k\in\mathcal{I}}L_k$ is refined when some of its subspaces L_k are split and the resulting decomposition is a grading. Thus a fine grading is an end of the process of successive refinements of a grading. In the opposite direction, the ultimate end of coarsening a grading is the whole Lie algebra forming just one grading subspace.

(3) For a simple Lie algebra $L/\ \mathbb{C}$ there is a one-to-one correspondence between fine gradings of L and maximal Abelian groups of diagonalizable automorphisms on L (so-called MAD-groups). The list of MAD-groups used in this article was obtained from Ref. 3.

In order to obtain all the nonequivalent fine gradings of sl(4, $\mathbb{C}$) we first rewrite the pertinent MAD-groups of Ref. 3 as subgroups of the group of automorphisms Aut sl(4, $\mathbb{C}$). Subsequently, we have to use also the MAD-groups of Aut o(6, $\mathbb{C}$). They are described in Sec. V. The correspondence between the two sets of MAD-groups is not entirely obvious.

We use the Lie group SL(4, $\mathbb{C}$)$=\{A\in\ \mathbb{C}^{4\times4}|\det A=1\}$ to describe the set $\mathcal{A}ut$ sl(4, $\mathbb{C}$) of all automorphisms on sl(4, $\mathbb{C}$). In general, $\mathcal{A}ut$ sl(4, $\mathbb{C}$) contains both inner and outer automorphisms. These act on an element X of the Lie algebra sl(4, $\mathbb{C}$) in the following way:

$$\text{inner automorphism}\quad Ad_A:\ Ad_AX=A^{-1}XA, \tag{7}$$

$$\text{outer automorphism}\quad Out_C:\ Out_CX=-(C^{-1}XC)^T. \tag{8}$$

Notice that for any $\alpha\neq0$ the description for $Ad_{\alpha A}$ and Ad_A coincide. Therefore the condition $\det A=1$ can be released to $\det A\neq0$. A compact description of the set $\mathcal{A}ut$ sl(4, $\mathbb{C}$) is then

$$\mathcal{A}ut\ \text{sl}(4,\mathbb{C})=\{Ad_A|\det A\neq0\}\cup\{Out_C|\det C\neq0\}.$$

(4) Two of the MAD-groups of Aut sl(4, $\mathbb{C}$) consist of inner automorphisms only, the remaining six involve also outer automorphisms. In our list of the MAD-groups we always characterize a MAD-group $\mathcal{G}$ by the set G_{Ad} of matrices A of the inner automorphisms Ad_A and by the set G_{Out} of matrices C for outer automorphisms Out_C. Actually when G_{Out} is nonempty, we mention only one of its elements denoted C, because all other elements F of G_{Out} can be written as $F=AC$, where $A\in G_{Ad}$. The outer automorphism $Out_F=Out_{AC}$ is just a composition of Out_C and Ad_A, respectively: $Out_{AC}=Out_C\circ Ad_A$.

The list of MAD-groups $\mathcal{G}_1,\ldots,\mathcal{G}_8$ in Aut sl(4, $\mathbb{C}$) is found in Table I. The symbols σ_k, $k=0,1,2,3$, stand for 2×2 Pauli matrices:

$$\sigma_0=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&1\\-1&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

Our convention as to how the tensor product $\otimes$ is understood is explained by the following example, where A is an arbitrary matrix:

$$\sigma_1\otimes A=\begin{pmatrix}0&1\\1&0\end{pmatrix}\otimes A=\begin{pmatrix}0&A\\A&0\end{pmatrix}.$$

(5) It is convenient to introduce the constant $n\times n$ matrices E_{jk}, M_{jk}, and N_{jk}, and to recall their commutation rules:

$$(E_{jk})_{lm}=\delta_{jl}\delta_{km},\quad M_{jk}=E_{jk}-E_{kj},\quad N_{jk}=E_{jk}-E_{(n+1-k)(n+1-j)}, \tag{9}$$

$$[E_{jk},E_{lm}]=\delta_{kl}E_{jm}-\delta_{jm}E_{lk}, \tag{10}$$

$$[M_{jk},M_{lm}]=\delta_{kl}M_{jm}-\delta_{jm}M_{lk}-\delta_{jl}M_{km}+\delta_{km}M_{lj}, \tag{11}$$

$$[N_{jk},N_{lm}]=\delta_{kl}N_{jm}-\delta_{jm}N_{lk}-\delta_{j(n+1-l)}N_{(n+1-k)m}+\delta_{k(n+1-m)}N_{l(n+1-j)}. \tag{12}$$

TABLE I. The full list of nonconjugate maximal Abelian groups of diagonalizable automorphisms (MAD-groups) on sl(4, $\mathbb{C}$).

	G_{Ad}	G_{Out}
$\mathcal{G}_1$	$\{A=\mathrm{diag}(d_1,d_2,d_3,1),\ d_j\in\mathbb{C}, d_j\neq 0\}$	$\emptyset$
$\mathcal{G}_2$	$\left\{A=P^jQ^k, j,k=0,1,2,3, P=\begin{pmatrix}0&1&0&0\\0&0&1&0\\0&0&0&1\\1&0&0&0\end{pmatrix},\ Q=\mathrm{diag}(1,i,-1,-i)\right\}$	$\emptyset$
$\mathcal{G}_3$	$\{A=\mathrm{diag}(\varepsilon_1,\varepsilon_2,\varepsilon_3,1),\ \varepsilon_i=\pm 1\}$	$C=I_4$
$\mathcal{G}_4$	$\{A=\mathrm{diag}(1,\varepsilon,\alpha,\alpha^{-1}),\ \varepsilon=\pm 1,\alpha\in\mathbb{C},\alpha\neq 0\}$	$C=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}$
$\mathcal{G}_5$	$\{A=\mathrm{diag}(\alpha,\alpha^{-1},\beta,\beta^{-1}),\ \alpha,\beta\in\mathbb{C},\alpha,\beta\neq 0\}$	$C=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}$
$\mathcal{G}_6$	$\{A=\sigma_j\otimes\mathrm{diag}(\alpha,\alpha^{-1}),\ \alpha\in\mathbb{C},\alpha\neq 0, j=0,1,2,3\}$	$C=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}$
$\mathcal{G}_7$	$\{A=\sigma_j\otimes\sigma_k,\ j,k=0,1,2,3\}$	$C=I_4$
$\mathcal{G}_8$	$\left\{A\in(G_0\otimes I_2)\cup(RG_0\otimes\sigma_3)\cup(G_0\otimes\sigma_1)\cup(RG_0\otimes\sigma_2),\ G_0=\left\{\begin{pmatrix}1&0\\0&1\end{pmatrix},\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right\}, R=\begin{pmatrix}1&0\\0&i\end{pmatrix}\right\}$	$C=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}$

(6) A simple way to avoid the ambiguity of traditional notations for maximal reductive subalgebras (1) is to provide the branching rule for one of the representations, usually of very low dimension. In this article we encounter three irreducible representations of A_3. Therefore it is useful to provide the corresponding branching rules. For that we use the notations of Ref. 4 for representations of the semisimple algebras (by their highest weight relative to the basis of fundamental weights). Irreducible representations of u(1) are all one-dimensional. The nonequivalent ones are labeled by an integer (positive and negative). In order to distinguish the representations of u(1), we write them as $[k]$.

Branching rules for the four-dimensional representation (1,0,0) of A_3:

$$(1)(1) \quad \text{for} \quad \mathrm{o}(4,\mathbb{C})\simeq\mathrm{sl}(2,\mathbb{C})\times\mathrm{sl}(2,\mathbb{C}), \tag{13}$$

$$(1,0) \quad \text{for} \quad \mathrm{sp}(4,\mathbb{C}), \tag{14}$$

$$(1,0)[1]+(0,0)[-3] \quad \text{for} \quad \mathrm{gl}(3,\mathbb{C})\simeq\mathrm{sl}(3,\mathbb{C})\times\mathrm{u}(1), \tag{15}$$

$$(1)(0)[1]+(0)(1)[-1] \quad \text{for} \quad \mathrm{sl}(2,\mathbb{C})\times\mathrm{sl}(2,\mathbb{C})\times\mathrm{u}(1). \tag{16}$$

Branching rules for the six-dimensional representation (0,1,0) of A_3:

$$(2)(0)+(0)(2) \quad \text{for } o(4,\mathbb{C})\simeq sl(2,\mathbb{C})\times sl(2,\mathbb{C}), \tag{17}$$

$$(1,0)+(0,0) \quad \text{for } sp(4,\mathbb{C}), \tag{18}$$

$$(1,0)[-2]+(0,1)[2] \quad \text{for } gl(3,\mathbb{C})\simeq sl(3,\mathbb{C})\times u(1), \tag{19}$$

$$(1)(1)[0]+(0)(0)[2]+(0)(0)[-2] \quad \text{for } sl(2,\mathbb{C})\times sl(2,\mathbb{C})\times u(1). \tag{20}$$

Branching rules for the 15-dimensional representation (1,0,1) of A_3:

$$(2)(2)+(2)(0)+(0)(2) \quad \text{for } o(4,\mathbb{C})\simeq sl(2,\mathbb{C})\times sl(2,\mathbb{C}), \tag{21}$$

$$(2,0)+(0,1) \quad \text{for } sp(4,\mathbb{C}), \tag{22}$$

$$(1,1)[0]+(0,1)[-4]+(1,0)[4] \quad \text{for } gl(3,\mathbb{C})\simeq sl(3,\mathbb{C})\times u(1), \tag{23}$$

$$(1)(1)[2]+(1)(1)[-2]+(2)(0)[0]+(0)(2)[0]+(+(0)(0)[0] \text{ for } sl(2,\mathbb{C})\times sl(2,\mathbb{C})\times u(1). \tag{24}$$

(7) *Example*. Consider an example of the automorphism $g(X)=F^{-1}XF$ of a general 4×4 matrix X [an element of gl(4, $\mathbb{C}$)]. Let the automorphism be realized by the diagonal matrix $F=\mathrm{diag}(\omega^3,\omega,\omega^{-1},\omega^{-3})$, where $\omega=\exp 2\pi i/8$. Corresponding eigenspace decomposition of gl(4, $\mathbb{C}$) is a grading by the cyclic group of order four generated by $g=Ad_F$. The adjoint action of this group is of order 4 while F is of order eight. Indeed, the equation $F^{-1}XF=\lambda X$ has four eigenvalues $\pm1,\pm i$ and four eigenspaces,

$$L_0=\begin{pmatrix} a & 0 & 0 & 0\\ 0 & f & 0 & 0\\ 0 & 0 & l & 0\\ 0 & 0 & 0 & q \end{pmatrix}, \quad L_1=\begin{pmatrix} 0 & b & 0 & 0\\ 0 & 0 & g & 0\\ 0 & 0 & 0 & m\\ n & 0 & 0 & 0 \end{pmatrix}, \quad L_2=\begin{pmatrix} 0 & 0 & c & 0\\ 0 & 0 & 0 & h\\ j & 0 & 0 & 0\\ 0 & o & 0 & 0 \end{pmatrix},$$

$$L_3=\begin{pmatrix} 0 & 0 & 0 & d\\ e & 0 & 0 & 0\\ 0 & k & 0 & 0\\ 0 & 0 & p & 0 \end{pmatrix}, \tag{25}$$

which we are labeling additively (subscripts read mod 4), rather than multiplicatively by the eigenvalues. Clearly the grading property (6) is satisfied. The grading decomposition gl(4, $\mathbb{C}$) $=L_0+L_1+L_2+L_3$ displays two subalgebras: L_0 of dimension 4 and L_0+L_2 of dimension 8. The latter subalgebra consists of four ideals, thus it can be written as a direct sum of four commuting subspaces. The ideals can be given by the generic 4×4 matrices which represent them:

$$\begin{pmatrix} a & 0 & c & 0\\ 0 & 0 & 0 & 0\\ j & 0 & -a & 0\\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 & 0\\ 0 & f & 0 & h\\ 0 & 0 & 0 & 0\\ 0 & o & 0 & -f \end{pmatrix}, \quad \begin{pmatrix} b & 0 & 0 & 0\\ 0 & -b & 0 & 0\\ 0 & 0 & b & 0\\ 0 & 0 & 0 & -b \end{pmatrix}, \quad \begin{pmatrix} l & 0 & 0 & 0\\ 0 & l & 0 & 0\\ 0 & 0 & l & 0\\ 0 & 0 & 0 & l \end{pmatrix}. \tag{26}$$

Note that the ideals are not displayed by the grading (25) Indeed, the subspace L_0 is split between all four ideals. Consequently, the four ideals could not be displayed in any refinement of the grading (25).

Putting $q=-a-f-l$, one restricts gl(4, $\mathbb{C}$) in this example to sl(4, $\mathbb{C}$) considered in this article. With that additional restriction, L_0 becomes three-dimensional, the last of the ideals (26) is eliminated, so that the remaining three ideals then form the subalgebra sl(2, $\mathbb{C}$)$\times$sl(2, $\mathbb{C}$) $\times$u(1). In the branching rule (24) the subalgebra is shown as its adjoint representation, namely $(2)(0)[0]+(0)(2)[0]+(0)(0)[0]$, corresponding to the first three ideals in (26). The remaining two terms of (24) are two irreducible representations of dimension 4 each which differ just by the representation of u(1). Again one could investigate whether the representations are displayed by the grading. The answer is negative in this example. The two representations are found within L_1+L_3 but not within L_1 or L_3 separately. Using the three diagonal generators of the subalgebra (one from each ideal) and remembering that their spectrum is either $\pm1,\pm1,2$ or $\pm1,\pm1,-2$ on the two representations, respectively, one finds directly the generic matrices of the two representations:

$$(1)(1)[2]\Leftrightarrow\begin{pmatrix}0&b&0&d\\0&0&0&0\\0&k&0&m\\0&0&0&0\end{pmatrix},\quad (1)(1)[-2]\Leftrightarrow\begin{pmatrix}0&0&0&0\\e&0&g&0\\0&0&0&0\\n&0&p&0\end{pmatrix}.$$

III. FINE GRADINGS OF THE COMPLEX LIE ALGEBRA sl(4, $\mathbb{C}$)

In this section we list all nonequivalent fine gradings of the Lie algebra sl(4, $\mathbb{C}$). Corresponding results for o(6, $\mathbb{C}$) are found in Sec. V.

A fine grading is a decomposition of the Lie algebra into eigenspaces (grading subspaces) of a MAD-group. It suffices to characterize a fine grading using a small subset of the MAD-group whose elements provide enough eigenvalues so that one can distinguish the eigenspaces–subspaces of the grading. There is a table shown for each fine grading. In this table one finds the eigenspaces (grading subspaces) labeled additively, the eigenvalues, and a basis for each subspaces. If the eigenvalues turn out to be functions of continuous parameters, we show as well their fixed values used for the grading.

A. Fine grading of sl(4, $\mathbb{C}$) corresponding to $\mathcal{G}_1$

In order to produce the grading, we just take a generic element of $\mathcal{G}_1$, namely the automorphism Ad_A with $A=\mathrm{diag}(d_1,d_2,d_3,1)$. It decomposes sl(4, $\mathbb{C}$) into 13 subspaces: one three-dimensional (Cartan subalgebra) and 12 one-dimensional (root) subspaces. Results of this case are summarized in Table II.

The eigenvectors $X_1,\ldots,X_{15}$ of Ad_A are given in terms of matrices E_{jk} of (9):

$$\begin{gathered}X_1=E_{11}-E_{22},\quad X_2=E_{22}-E_{33},\quad X_3=E_{33}-E_{44},\\ X_4=E_{23},\quad X_5=E_{12},\quad X_6=E_{13},\\ X_7=E_{34},\quad X_8=E_{24},\quad X_9=E_{41},\\ X_{10}=E_{14},\quad X_{11}=E_{42},\quad X_{12}=E_{43},\\ X_{13}=E_{31},\quad X_{14}=E_{21},\quad X_{15}=E_{32}.\end{gathered}\tag{27}$$

In Table II we identify the grading subspaces L_j by their basis vectors X_k and by the corresponding eigenvalues. Two sets of eigenvalues are shown. The first one involves continuous parameters d_1,d_2,d_3. In the second set the values of the parameters are fixed to take some convenient values. Clearly there are many ways this could be done.

This grading is the well known root or Cartan decomposition of sl(4, $\mathbb{C}$). The grading group $\mathcal{G}_1$ is a fixed maximal torus of the Lie group SL(4, $\mathbb{C}$). The three-dimensional grading space L_0, spanned by X_1,X_2,X_3, is the Cartan subalgebra, the remaining 12 one-dimensional grading spaces

TABLE II. $\mathcal{G}_1$: The correspondence between eigenvectors X_k from (27) and the eigenvalue λ of Ad_A. Fixing the values of $d_1=\omega^6$, $d_2=\omega^8$, and $d_3=\omega^9$, where $\omega=\exp(2\pi i/13)$, the maximal torus is restricted to its cyclic subgroup $\mathbb{Z}_{13}$.

	Eigenvector	$\lambda=\lambda(d_1,d_2,d_3)$	$\lambda=\lambda(\omega^6,\omega^8,\omega^9)$
L_0	X_1	1	
	X_2	1	ω^0
	X_3	1	
L_1	X_4	$\frac{d_3}{d_2}$	ω^1
L_2	X_5	$\frac{d_2}{d_1}$	ω^2
L_3	X_6	$\frac{d_3}{d_1}$	ω^3
L_4	X_7	$\frac{1}{d_3}$	ω^4
L_5	X_8	$\frac{1}{d_2}$	ω^5
L_6	X_9	d_1	ω^6
L_7	X_{10}	$\frac{1}{d_1}$	ω^7
L_8	X_{11}	d_2	ω^8
L_9	X_{12}	d_3	ω^9
L_{10}	X_{13}	$\frac{d_1}{d_3}$	ω^{10}
L_{11}	X_{14}	$\frac{d_1}{d_2}$	ω^{11}
L_{12}	X_{15}	$\frac{d_2}{d_3}$	ω^{12}

are the root spaces of that decomposition. Let $\alpha_1,\alpha_2,\alpha_3$ denote the three simple roots. Matrices representing the root spaces can be chosen, for example, as follows: $E_{\alpha_1}=E_{12}$, $E_{\alpha_2}=E_{23}$, $E_{\alpha_3}=E_{34}$, $E_{\alpha_1+\alpha_2}=E_{13}$, $E_{\alpha_2+\alpha_3}=E_{24}$, $E_{\alpha_1+\alpha_2+\alpha_3}=E_{14}$. Then for the negative roots one has $E_{-\alpha_1}=E_{21}$, $E_{-\alpha_2}=E_{32}$, $E_{-\alpha_3}=E_{43}$, $E_{-\alpha_1-\alpha_2}=E_{31}$, $E_{-\alpha_2-\alpha_3}=E_{42}$, $E_{-\alpha_1-\alpha_2-\alpha_3}=E_{41}$.

Any further decomposition of sl(4, $\mathbb{C}$), which can split the Cartan subalgebra into lower dimensional subspaces while preserving the root spaces, is not a grading.

B. The fine grading of sl(4, $\mathbb{C}$) corresponding to $\mathcal{G}_2$

Inner automorphisms Ad_{A_1} and Ad_{A_2}, where

$$A_1=Q=\begin{pmatrix}1&0&0&0\\0&i&0&0\\0&0&-1&0\\0&0&0&-i\end{pmatrix},\quad A_2=P=\begin{pmatrix}0&1&0&0\\0&0&1&0\\0&0&0&1\\1&0&0&0\end{pmatrix},$$

decompose the Lie algebra sl(4, $\mathbb{C}$) into 15 one-dimensional subspaces. Results of this case are summarized in Table III. The eigenvectors $X_1,\ldots,X_{15}$ can be given as powers of P and Q:

$$X_1=P^0Q^3,\quad X_2=P^0Q^2,\quad X_3=P^0Q^1,$$

TABLE III. $\mathcal{G}_2$: The correspondence between eigenvectors X_k from (28) and the eigenvalues λ_1,λ_2 of $Ad_{A_1}=Ad_Q$, $Ad_{A_2}=Ad_P$.

	Eigenvector	λ_1	λ_2
$L_{(0,1)}$	X_1	1	i
$L_{(0,2)}$	X_2	1	-1
$L_{(0,3)}$	X_3	1	$-i$
$L_{(1,0)}$	X_4	i	1
$L_{(1,1)}$	X_5	i	i
$L_{(1,2)}$	X_6	i	-1
$L_{(1,3)}$	X_7	i	$-i$
$L_{(2,0)}$	X_8	-1	1
$L_{(2,1)}$	X_9	-1	i
$L_{(2,2)}$	X_{10}	-1	-1
$L_{(2,3)}$	X_{11}	-1	$-i$
$L_{(3,0)}$	X_{12}	$-i$	1
$L_{(3,1)}$	X_{13}	$-i$	i
$L_{(3,2)}$	X_{14}	$-i$	-1
$L_{(3,3)}$	X_{15}	$-i$	$-i$

$$\begin{aligned} &X_4=P^1Q^0, \quad X_5=P^1Q^3, \quad X_6=P^1Q^2, \quad X_7=P^1Q^1,\\ &X_8=P^2Q^0, \quad X_9=P^2Q^3, \quad X_{10}=P^2Q^2, \quad X_{11}=P^2Q^1,\\ &X_{12}=P^3Q^0, \quad X_{13}=P^3Q^3, \quad X_{14}=P^3Q^2, \quad X_{15}=P^3Q^1. \end{aligned} \tag{28}$$

In terms of subspaces $L_{(j,k)}$ denoted by indices from the additive group $\mathbb{Z}_4\times\mathbb{Z}_4$ this can be briefly written as $L_{(j,k)}=\mathbb{C}(P^jQ^{-k})$, and the pair (λ_1,λ_2) of eigenvalues of elements from $L_{(j,k)}$ is equal to $(\lambda_1,\lambda_2)=(i^j,i^k)$.

Properties of the associative algebra generated by $n\times n$ matrices analogous to P and Q have been noted a long time ago.[5] The corresponding grading of $\mathrm{sl}(n,\mathbb{C})$ was studied in Ref. 6.

C. The fine grading of sl(4, $\mathbb{C}$) corresponding to $\mathcal{G}_3$

Results of this case are summarized in Table IV. Using $A_1=\mathrm{diag}(-1,1,1,1)$, $A_2=\mathrm{diag}(-1,-1,1,1)$, $A_3=\mathrm{diag}(-1,-1,-1,1)$ for Ad_A and $C=I_4$ for Out_C the Lie algebra

TABLE IV. $\mathcal{G}_3$: The correspondence between eigenvectors X_k from (29) and the eigenvalues $\lambda_0,\lambda_1,\lambda_2,\lambda_3$ of $Out_C, Ad_{A_1}, Ad_{A_2}, Ad_{A_3}$. Indices of the subspaces $L_{(j,k,l,m)}$ are elements of the additive group $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$.

	Eigenvector	λ_0	λ_1	λ_2	λ_3
$L_{(1,1,1,1)}$	X_1	-1	-1	-1	-1
$L_{(0,1,1,1)}$	X_2	1	-1	-1	-1
$L_{(1,0,1,1)}$	X_3	-1	1	-1	-1
$L_{(0,0,1,1)}$	X_4	1	1	-1	-1
$L_{(1,0,0,1)}$	X_5	-1	1	1	-1
$L_{(0,0,0,1)}$	X_6	1	1	1	-1
$L_{(1,1,1,0)}$	X_7	-1	-1	-1	1
$L_{(0,1,1,0)}$	X_8	1	-1	-1	1
$L_{(1,0,1,0)}$	X_9	-1	1	-1	1
$L_{(0,0,1,0)}$	X_{10}	1	1	-1	1
$L_{(1,1,0,0)}$	X_{11}	-1	-1	1	1
$L_{(0,1,0,0)}$	X_{12}	1	-1	1	1
$L_{(1,0,0,0)}$	X_{13}	-1	1	1	1
	X_{14}	-1	1	1	1
	X_{15}	-1	1	1	1

TABLE V. $\mathcal{G}_4$: The correspondence between eigenvectors X_k from (30) and the eigenvalues λ_0, λ_1 of Out_C, Ad_A. Denoting $\eta = \exp(2\pi i/8)$ and appointing the value $\alpha = \eta$ to the parameter α, the indices of subspaces become elements of $\mathbb{Z}_2 \times \mathbb{Z}_8$.

	Eigenvector	λ_0	$\lambda_1 = \lambda_1(\alpha)$	$\lambda_1 = \lambda_1(\eta)$
$L_{(0,0)}$	X_1	1	1	η^0
$L_{(1,0)}$	X_2	-1	1	η^0
	X_3	-1	1	
$L_{(0,1)}$	X_4	1	α	η^1
$L_{(1,1)}$	X_5	-1	α	η^1
$L_{(1,2)}$	X_6	-1	α^2	η^2
$L_{(0,3)}$	X_7	1	$-\alpha^{-1}$	η^3
$L_{(1,3)}$	X_8	-1	$-\alpha^{-1}$	η^3
$L_{(0,4)}$	X_9	1	-1	η^4
$L_{(1,4)}$	X_{10}	-1	-1	η^4
$L_{(0,5)}$	X_{11}	1	$-\alpha$	η^5
$L_{(1,5)}$	X_{12}	-1	$-\alpha$	η^5
$L_{(1,6)}$	X_{13}	-1	α^{-2}	η^6
$L_{(0,7)}$	X_{14}	1	α^{-1}	η^7
$L_{(1,7)}$	X_{15}	-1	α^{-1}	η^7

sl(4, $\mathbb{C}$) is decomposed into one three-dimensional and 12 one-dimensional subspaces which are described by simultaneous eigenvectors $X_1, \ldots, X_{15}$:

$$\begin{gathered} X_1 = E_{14} + E_{41}, \quad X_2 = E_{14} - E_{41}, \quad X_3 = E_{24} + E_{42}, \quad X_4 = E_{24} - E_{42}, \\ X_5 = E_{34} + E_{43}, \quad X_6 = E_{34} - E_{43}, \quad X_7 = E_{13} + E_{31}, \quad X_8 = E_{13} - E_{31}, \\ X_9 = E_{23} + E_{32}, \quad X_{10} = E_{23} - E_{32}, \quad X_{11} = E_{12} + E_{21}, \quad X_{12} = E_{12} - E_{21}, \\ X_{13} = E_{11} - E_{22}, \quad X_{14} = E_{22} - E_{33}, \quad X_{15} = E_{33} - E_{44}. \end{gathered} \tag{29}$$

One can see that the present grading is not conjugate to the root decomposition, e.g., because all grading subspaces are spanned by semisimple elements of the Lie algebra, as opposed to the root decomposition, where only the Cartan subalgebra consists of such elements.

Clearly the six skew-symmetric matrices in this grading display the subalgebra o(4, $\mathbb{C}$). The simplest way to examine the grading is the following: Consider the four subalgebras which consist of the subspaces of the form $L_{(0,*,*,*)}$, $L_{(*,0,*,*)}$, $L_{(*,*,0,*)}$, $L_{(*,*,*,0)}$. Here $*$ stands for any admissible value of the corresponding label. Then identify each subalgebra. In this way one finds here respectively o(4, $\mathbb{C}$), gl(3, $\mathbb{C}$), sl(2, $\mathbb{C}$) $\times$ sl(2, $\mathbb{C}$) $\times$ u(1), and gl(3, $\mathbb{C}$).

D. The fine grading of sl(4, $\mathbb{C}$) corresponding to $\mathcal{G}_4$

Results of this case are summarized in Table V. To obtain a fine grading by $\mathcal{G}_4$ one only needs to use the inner automorphism Ad_A with matrix $A = \mathrm{diag}(1, -1, \alpha, \alpha^{-1})$ and the outer automorphism Out_C with

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

TABLE VI. $\mathcal{G}_5$: The correspondence between eigenvectors X_k from (31) and the eigenvalues λ_0, λ_1 of Out_C, Ad_A. In order to embed the index set into the additive group $\mathbb{Z}_2 \times \mathbb{Z}_9$ we put $\alpha = \nu^2$ and $\beta = \nu^8$, where $\nu = \exp(2\pi i/9)$.

	Eigenvector	λ_0	$\lambda_1 = \lambda_1(\alpha, \beta)$	$\lambda_1 = \lambda_1(\nu^2, \nu^8)$
$L_{(0,0)}$	X_1	1	1	ν^0
	X_2	1	1	
$L_{(1,0)}$	X_3	-1	1	ν^0
$L_{(0,1)}$	X_4	1	$\alpha\beta$	ν^1
$L_{(1,1)}$	X_5	-1	$\alpha\beta$	ν^1
$L_{(1,2)}$	X_6	-1	β^{-2}	ν^2
$L_{(0,3)}$	X_7	1	$\alpha\beta^{-1}$	ν^3
$L_{(1,3)}$	X_8	-1	$\alpha\beta^{-1}$	ν^3
$L_{(1,4)}$	X_9	-1	α^2	ν^4
$L_{(1,5)}$	X_{10}	-1	α^{-2}	ν^5
$L_{(0,6)}$	X_{11}	1	$\alpha^{-1}\beta$	ν^6
$L_{(1,6)}$	X_{12}	-1	$\alpha^{-1}\beta$	ν^6
$L_{(1,7)}$	X_{13}	-1	β^2	ν^7
$L_{(0,8)}$	X_{14}	1	$\alpha^{-1}\beta^{-1}$	ν^8
$L_{(1,8)}$	X_{15}	-1	$\alpha^{-1}\beta^{-1}$	ν^8

There are one two-dimensional and 13 one-dimensional subspaces, and we list them in terms of eigenvectors $X_1, \ldots, X_{15}$:

$$
\begin{gathered}
X_1 = E_{33} - E_{44}, \quad X_2 = E_{11} + E_{22} - E_{33} - E_{44}, \quad X_3 = E_{11} - E_{22}, \\
X_4 = E_{13} - E_{41}, \quad X_5 = E_{13} + E_{41}, \quad X_6 = E_{43}, \\
X_7 = E_{24} - E_{32}, \quad X_8 = E_{24} + E_{32}, \quad X_9 = E_{12} - E_{21}, \\
X_{10} = E_{12} + E_{21}, \quad X_{11} = E_{23} - E_{42}, \quad X_{12} = E_{23} + E_{42}, \\
X_{13} = E_{34}, \quad X_{14} = E_{14} - E_{31}, \quad X_{15} = E_{14} + E_{31}.
\end{gathered} \tag{30}
$$

The presence of the parameter α indicates that a one-parametric subgroup of the torus remains a part of the grading group. It can be identified with the subgroup $\mathrm{SL}(2, \mathbb{C}) \subset \mathrm{SL}(4, \mathbb{C})$ corresponding to one of the simple roots of $\mathrm{sl}(4, \mathbb{C})$. This decomposition of $\mathrm{sl}(4, \mathbb{C})$ displays $\mathrm{sl}(2, \mathbb{C})$ spanned by $\{X_1, X_6, X_{13}\}$. Equivalently one may identify it as one of the $\mathrm{sl}(2, \mathbb{C})$ ideals in $\mathrm{sl}(2, \mathbb{C}) \times \mathrm{sl}(2, \mathbb{C}) \times \mathrm{u}(1)$. Indeed, the exponents of α in Table V are the weights of the $\mathrm{sl}(2, \mathbb{C})$-representation. Thus one obtains the direct sum of one three-dimensional, four two-dimensional, and four one-dimensional representations. That is what one finds from (24) when it is reduced further to the subalgebra $\mathrm{sl}(2, \mathbb{C}) \subset \mathrm{sl}(2, \mathbb{C}) \times \mathrm{sl}(2, \mathbb{C}) \times \mathrm{u}(1)$.

E. The fine grading of sl(4, $\mathbb{C}$) corresponding to $\mathcal{G}_5$

Results of this case are summarized in Table VI. Here, again, we only need one (general) inner automorphism $Ad_A \in \mathcal{G}_5$ with $A = \mathrm{diag}(\alpha, \alpha^{-1}, \beta, \beta^{-1})$ and the outer automorphism Out_C,

$$
C = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.
$$

TABLE VII. $\mathcal{G}_6$: The correspondence between eigenvectors X_k from (32) and the eigenvalues $\lambda_0,\lambda_1,\lambda_2$ of $Out_C, Ad_{A_1}, Ad_{A_2}$. With the choice of $\alpha = \xi^{1/2}$, where $\xi = \exp(2\pi i/6)$, the additive group for subspace indices is $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_6$.

	Eigenvector	λ_0	λ_1	$\lambda_2=\lambda_2(\alpha)$	$\lambda_2=\lambda_2(\xi^{1/2})$
$L_{(0,0,0)}$	X_1	1	1	1	ξ^0
$L_{(0,1,0)}$	X_2	1	−1	1	ξ^0
$L_{(1,1,0)}$	X_3	−1	−1	1	ξ^0
$L_{(1,0,1)}$	X_4	−1	1	α^2	ξ^1
$L_{(1,1,1)}$	X_5	−1	−1	α^2	ξ^1
$L_{(0,1,2)}$	X_6	1	−1	$-\alpha^{-2}$	ξ^2
$L_{(1,0,2)}$	X_7	−1	1	$-\alpha^{-2}$	ξ^2
$L_{(0,0,3)}$	X_8	1	1	−1	ξ^3
$L_{(0,1,3)}$	X_9	1	−1	−1	ξ^3
$L_{(1,0,3)}$	X_{10}	−1	1	−1	ξ^3
$L_{(1,1,3)}$	X_{11}	−1	−1	−1	ξ^3
$L_{(0,1,4)}$	X_{12}	1	−1	$-\alpha^2$	ξ^4
$L_{(1,0,4)}$	X_{13}	−1	1	$-\alpha^2$	ξ^4
$L_{(1,0,5)}$	X_{14}	−1	1	α^{-2}	ξ^5
$L_{(1,1,5)}$	X_{15}	−1	−1	α^{-2}	ξ^5

The Lie algebra sl(4, $\mathbb{C}$) is decomposed into one two-dimensional and 13 one-dimensional subspaces, whose bases are given in terms of vectors E_{jk}:

$$
\begin{gathered}
X_1=E_{11}-E_{22}, \quad X_6=E_{34}, \quad X_{11}=E_{13}-E_{42}, \\
X_2=E_{33}-E_{44}, \quad X_7=E_{24}-E_{31}, \quad X_{12}=E_{13}+E_{42}, \\
X_3=E_{11}+E_{22}-E_{33}-E_{44}, \quad X_8=E_{24}+E_{31}, \quad X_{13}=E_{43}, \\
X_4=E_{23}-E_{41}, \quad X_9=E_{21}, \quad X_{14}=E_{14}-E_{32}, \\
X_5=E_{23}+E_{41}, \quad X_{10}=E_{12}, \quad X_{15}=E_{14}+E_{32}.
\end{gathered}
\tag{31}
$$

The parameters α and β indicate that a two-parametric subgroup of the maximal torus belongs to the grading group. The parameters can be identified with two orthogonal simple roots of sl(4, $\mathbb{C}$). Hence the grading displays two commuting sl(2, $\mathbb{C}$) subalgebras spanned by $\{X_1,X_9,X_{10}\}$ and $\{X_2,X_6,X_{13}\}$.

F. The fine grading of sl(4, $\mathbb{C}$) corresponding to $\mathcal{G}_6$

Results of this case are summarized in Table VII. This time it is necessary to use two inner automorphisms Ad_A, e.g., those with matrices $A_1=\sigma_1\otimes\mathrm{diag}(1,1)$, $A_2=\sigma_3\otimes\mathrm{diag}(\alpha,\alpha^{-1})$, and also the outer automorphism Out_C,

$$
C=\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.
$$

We obtain a decomposition into 15 one-dimensional subspaces—linear hulls of eigenvectors $X_1,\ldots,X_{15}$:

TABLE VIII. $\mathcal{G}_7$: The correspondence between eigenvectors X_k from (33) and the eigenvalues $\lambda_1,\lambda_2,\lambda_3,\lambda_4$ of $Ad_{A_1},Ad_{A_2},Ad_{A_3},Ad_{A_4}$. The additive group is $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$.

	Eigenvector	λ_1	λ_2	λ_3	λ_4
$L_{(0,0,0,1)}$	X_1	1	1	1	−1
$L_{(0,0,1,0)}$	X_2	1	1	−1	1
$L_{(0,0,1,1)}$	X_3	1	1	−1	−1
$L_{(0,1,0,0)}$	X_4	1	−1	1	1
$L_{(0,1,0,1)}$	X_5	1	−1	1	−1
$L_{(0,1,1,0)}$	X_6	1	−1	−1	1
$L_{(0,1,1,1)}$	X_7	1	−1	−1	−1
$L_{(1,0,0,0)}$	X_8	−1	1	1	1
$L_{(1,0,0,1)}$	X_9	−1	1	1	−1
$L_{(1,0,1,0)}$	X_{10}	−1	1	−1	1
$L_{(1,0,1,1)}$	X_{11}	−1	1	−1	−1
$L_{(1,1,0,0)}$	X_{12}	−1	−1	1	1
$L_{(1,1,0,1)}$	X_{13}	−1	−1	1	−1
$L_{(1,1,1,0)}$	X_{14}	−1	−1	−1	1
$L_{(1,1,1,1)}$	X_{15}	−1	−1	−1	−1

$$
\begin{gathered}
X_1=E_{11}-E_{22}+E_{33}-E_{44},\quad X_2=E_{11}-E_{22}-E_{33}+E_{44},\\
X_3=E_{11}+E_{22}-E_{33}-E_{44},\quad X_4=E_{21}+E_{43},\\
X_5=E_{21}-E_{43},\quad X_6=E_{14}-E_{32},\\
X_7=E_{14}+E_{32},\quad X_8=E_{13}-E_{24}+E_{31}-E_{42},\\
X_9=E_{13}+E_{24}-E_{31}-E_{42},\quad X_{10}=E_{13}+E_{24}+E_{31}+E_{42},\\
X_{11}=E_{13}-E_{24}-E_{31}+E_{42},\quad X_{12}=E_{23}-E_{41},\\
X_{13}=E_{23}+E_{41},\quad X_{14}=E_{12}+E_{34},\\
X_{15}=E_{12}-E_{34}.
\end{gathered}
\tag{32}
$$

The single parameter here cannot be identified with a root of sl(2, $\mathbb{C}$) as in the previous cases. Nevertheless, its presence identifies a one-parametric subgroup of the sl(2, $\mathbb{C}$)-torus and hence an sl(2, $\mathbb{C}$) subalgebra of sl(4, $\mathbb{C}$). The simple root of the subalgebra divides the angle between the two orthogonal roots of sl(4, $\mathbb{C}$) and it is $\sqrt{2}$ shorter than the roots of sl(4, $\mathbb{C}$). Practically it amounts to putting $\alpha=\beta$ in the previous grading.

G. The fine grading of sl(4, $\mathbb{C}$) corresponding to $\mathcal{G}_7$

Results of this case are summarized in Table VIII. To reach the complete decomposition of sl(4, $\mathbb{C}$) by the MAD-group $\mathcal{G}_7$, four inner automorphisms Ad_A must be used. The outer automorphism does not supply any of them, so we do not use it this time although it belongs to the MAD-group.

The matrices A for the inner automorphisms are the following: $A_1=\sigma_3\otimes\sigma_3$, $A_2=\sigma_0\otimes\sigma_3$, $A_3=\sigma_2\otimes\sigma_2$, and $A_4=\sigma_2\otimes\sigma_3$. Those 15 one-dimensional subspaces $L_{(j,k,l,m)}$ are linear hulls of eigenvectors $X_1,\ldots,X_{15}$; the set of indices is equal to the additive group $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$; the subspace $L_{(0,0,0,0)}$ is empty:

TABLE IX. $\mathcal{G}_8$: The correspondence between eigenvectors X_k from (34) and the eigenvalues $\lambda_0,\lambda_1,\lambda_2$ of $Out_C, Ad_{A_1}, Ad_{A_2}$. The additive group in this case is $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_4$.

	Eigenvector	λ_0	λ_1	λ_2
$L_{(0,1,0)}$	X_1	1	−1	1
$L_{(1,0,0)}$	X_2	−1	1	1
$L_{(1,1,0)}$	X_3	−1	−1	1
$L_{(0,0,1)}$	X_4	1	1	i
$L_{(0,1,1)}$	X_5	1	−1	i
$L_{(1,0,1)}$	X_6	−1	1	i
$L_{(1,1,1)}$	X_7	−1	−1	i
$L_{(0,1,2)}$	X_8	1	−1	−1
$L_{(1,0,2)}$	X_9	−1	1	−1
	X_{10}	−1	1	−1
$L_{(1,1,2)}$	X_{11}	−1	−1	−1
$L_{(0,0,3)}$	X_{12}	1	−1	$-i$
$L_{(0,1,3)}$	X_{13}	1	−1	$-i$
$L_{(1,0,3)}$	X_{14}	−1	1	$-i$
$L_{(1,1,3)}$	X_{15}	−1	1	$-i$

$$
\begin{aligned}
&X_1=E_{11}-E_{22}-E_{33}+E_{44}, \quad X_2=E_{11}-E_{22}+E_{33}-E_{44},\\
&X_3=E_{11}+E_{22}-E_{33}-E_{44}, \quad X_4=E_{14}+E_{23}+E_{32}+E_{41},\\
&X_5=E_{14}-E_{23}-E_{32}+E_{41}, \quad X_6=E_{14}-E_{23}+E_{32}-E_{41},\\
&X_7=E_{14}+E_{23}-E_{32}-E_{41}, \quad X_8=E_{13}+E_{24}-E_{31}-E_{42},\\
&X_9=E_{13}-E_{24}+E_{31}-E_{42}, \quad X_{10}=E_{13}-E_{24}-E_{31}+E_{42},\\
&X_{11}=E_{13}+E_{24}+E_{31}+E_{42}, \quad X_{12}=E_{12}+E_{21}-E_{34}-E_{43},\\
&X_{13}=E_{12}-E_{21}+E_{34}-E_{43}, \quad X_{14}=E_{12}-E_{21}-E_{34}+E_{43},\\
&X_{15}=E_{12}+E_{21}+E_{34}+E_{43}.
\end{aligned}
\tag{33}
$$

The eigenvectors $X_j, j=1,\ldots,15$, can be written as $\sigma_k\otimes\sigma_l$, where $k,l\in\{0,1,2,3\}$, except for $k=l=0$.

H. The fine grading of sl(4, $\mathbb{C}$) corresponding to $\mathcal{G}_8$

Results of this case are summarized in Table IX. To obtain a fine grading by $\mathcal{G}_8$, one outer and two inner automorphisms are used, namely those with $A_1=I_2\otimes\sigma_1$, $A_2=R\otimes\sigma_3$ for Ad_A, and

$$
C=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}
$$

for Out_C. The fine grading of sl(4, $\mathbb{C}$) consists of one two-dimensional and 13 one-dimensional subspaces, which are described by the following set of eigenvectors:

TABLE X. Subalgebra gl(3, $\mathbb{C}$) displayed by fine gradings of sl(4, $\mathbb{C}$).

MAD-group of sl(4, $\mathbb{C}$)	Displayed gl(3, $\mathbb{C}$) in terms of $L_k \subset$ sl(4, $\mathbb{C}$)
$\mathcal{G}_1$	$L_{(0)} \oplus L_{(1)} \oplus L_{(2)} \oplus L_{(3)} \oplus L_{(10)} \oplus L_{(11)} \oplus L_{(12)}$
$\mathcal{G}_3$	$L_{(1,0,1,1)} \oplus L_{(0,0,1,1)} \oplus L_{(1,0,0,1)} \oplus L_{(0,0,0,1)} \oplus L_{(1,0,1,0)} \oplus L_{(0,0,1,0)} \oplus L_{(1,0,0,0)}$
$\mathcal{G}_4$	$L_{(0,0)} \oplus L_{(1,0)} \oplus L_{(1,2)} \oplus L_{(0,3)} \oplus L_{(1,3)} \oplus L_{(0,5)} \oplus L_{(1,5)} \oplus L_{(1,6)}$

$$
\begin{gathered}
X_1 = E_{33} - E_{44}, \quad X_2 = E_{11} + E_{22} - E_{33} - E_{44}, \\
X_3 = E_{11} - E_{22}, \quad X_4 = E_{13} + E_{24} - E_{32} - E_{41}, \\
X_5 = E_{13} - E_{24} + E_{32} - E_{41}, \quad X_6 = E_{13} + E_{24} + E_{32} + E_{41}, \\
X_7 = E_{13} - E_{24} - E_{32} + E_{41}, \quad X_8 = E_{12} - E_{21}, \\
X_9 = E_{12} + E_{21}, \quad X_{10} = E_{34} + E_{43}, \\
X_{11} = E_{34} - E_{43}, \quad X_{12} = E_{14} + E_{23} - E_{31} - E_{42}, \\
X_{13} = E_{14} - E_{23} - E_{31} + E_{42}, \quad X_{14} = E_{14} + E_{23} + E_{31} + E_{42}, \\
X_{15} = E_{14} - E_{23} + E_{31} - E_{42}.
\end{gathered}
\tag{34}
$$

IV. MAXIMAL SUBALGEBRAS OF sl(4, $\mathbb{C}$) DISPLAYED BY THE FINE GRADINGS OF sl(4, $\mathbb{C}$)

Recall that a subalgebra is said to be displayed by a grading if it is a sum of several grading subspaces of the grading (cf. example in Sec. II). Having described the fine gradings, it is curious to know which of the maximal subalgebras of A_3 are preferred by each grading. The root grading displays so called regular subalgebras. (A subalgebra of L is regular if its roots can be chosen as a subset of roots of L.)

We are interested here in the four maximal reductive subalgebras (1) of sl(4, $\mathbb{C}$). There are ways how to characterize the subalgebras in a representation independent way, but our aim is to be as specific as possible. Hence we describe the subalgebras by explicit 4×4 matrices.

A. gl(3, $\mathbb{C}$) as a subalgebra of sl(4, $\mathbb{C}$)

The subalgebra gl(3, $\mathbb{C}$) $\subset$ sl(4, $\mathbb{C}$) spans a nine-dimensional subspace in (2). It can be realized as the set of matrices

$$
\text{gl}(3, \mathbb{C}) = \begin{pmatrix} a & b & c & 0 \\ e & f & g & 0 \\ j & k & l & 0 \\ 0 & 0 & 0 & -a-f-l \end{pmatrix}. \tag{35}
$$

There are just three MAD-groups in $\mathcal{A}ut$ sl(4, $\mathbb{C}$) providing fine gradings of sl(4, $\mathbb{C}$) which display the subalgebra gl(3, $\mathbb{C}$). These are the MAD-groups $\mathcal{G}_1$, $\mathcal{G}_3$, and $\mathcal{G}_4$. In each of these cases the subalgebra gl(3, $\mathbb{C}$) can be picked out as an eigensubspace of $Ad_A \in \mathcal{G}_j$ corresponding to the eigenvalue $+1$. [$A = \text{diag}(-1,-1,-1,1)$ for $\mathcal{G}_1$ and $\mathcal{G}_3$, $A = \text{diag}(1,-1,-1,-1)$ for $\mathcal{G}_4$.] Table X depicts the subspaces L_k of fine gradings by $\mathcal{G}_1, \mathcal{G}_3, \mathcal{G}_4$ that make up the subalgebra gl(3, $\mathbb{C}$).

TABLE XI. Gradings of o(4, $\mathbb{C}$) displayed by fine gradings of sl(4, $\mathbb{C}$). These gradings are all fine, with the only exception of the one by $\mathcal{G}_5$.

MAD-group on sl(4, $\mathbb{C}$)	Grading of o(4, $\mathbb{C}$) in terms of $L_k \subset$ sl(4, $\mathbb{C}$)
$\mathcal{G}_3$	$L_{(0,1,1,1)} \oplus L_{(0,0,1,1)} \oplus L_{(0,0,0,1)} \oplus L_{(0,1,1,0)} \oplus L_{(0,0,1,0)} \oplus L_{(0,1,0,0)}$
$\mathcal{G}_4$	$L_{(0,0)} \oplus L_{(0,1)} \oplus L_{(0,3)} \oplus L_{(0,4)} \oplus L_{(0,5)} \oplus L_{(0,7)}$
$\mathcal{G}_5$	$L_{(0,0)} \oplus L_{(0,1)} \oplus L_{(0,3)} \oplus L_{(0,6)} \oplus L_{(0,8)}$
$\mathcal{G}_6$	$L_{(0,0,0)} \oplus L_{(0,1,0)} \oplus L_{(0,1,2)} \oplus L_{(0,0,3)} \oplus L_{(0,1,3)} \oplus L_{(0,1,4)}$
$\mathcal{G}_7$	$L_{(0,1,1,0)} \oplus L_{(0,1,1,1)} \oplus L_{(1,0,0,0)} \oplus L_{(1,0,1,0)} \oplus L_{(1,1,0,1)} \oplus L_{(1,1,1,0)}$
$\mathcal{G}_8$	$L_{(0,1,0)} \oplus L_{(0,0,1)} \oplus L_{(0,1,1)} \oplus L_{(0,1,2)} \oplus L_{(0,0,3)} \oplus L_{(0,1,3)}$

B. o(4, $\mathbb{C}$) subalgebra of sl(4, $\mathbb{C}$)

This is the six-dimensional subalgebra which is most simply realized in sl(4, $\mathbb{C}$) as the subset of all matrices antisymmetric with respect to transposition (skew-symmetric). A general definition is the following:

$$\mathrm{o}(n, \mathbb{C}) = \{X \in \mathbb{C}^{n\times n} | XK + KX^T = 0\}, \quad K \in \mathbb{C}^{n\times n}, \det K = 1, K = K^T. \tag{36}$$

[With $K = I$, o(n, $\mathbb{C}$) is the set of all skew-symmetric matrices.]

A simple rule to decide whether a particular fine grading of sl(n, $\mathbb{C}$) displays o(n, $\mathbb{C}$) is found in Ref. 3.

Theorem 4.1: (*I*) *Let* $\mathcal{G} = \{Ad_A | A \in G_{Ad}\} \cup \{Out_C | C \in G_{Out}\}$ *be a MAD-group on* sl(n, $\mathbb{C}$). *A fine grading of* sl(n, $\mathbb{C}$) *produced by the MAD-group* $\mathcal{G}$ *(i.e., consisting of simultaneous eigensubspaces of automorphisms from* $\mathcal{G}$*) displays the subalgebra* o(n, $\mathbb{C}$) *iff there exists a matrix* $A \in G_{Ad}$ *such that* AC *is symmetric.*

If such $A \in G_{Ad}$ *exists, then* $\{Ad_A | A \in G_{Ad}\}$ *is a MAD-group on the displayed subalgebra* o(n, $\mathbb{C}$).

(*II*) *A MAD-group* $\mathcal{H}$ on sl(n, $\mathbb{C}$) *which does not contain any outer automorphism* Out_C *does not display the subalgebra* o(n, $\mathbb{C}$).

Once we have found the matrix $A \in G_{Ad}$ such that AC is symmetric, we put $K = AC$, and then pick out all the subspaces L_k that are eigensubspaces corresponding to eigenvalue $+1$ for Out_{AC}. These subspaces build up the subalgebra o(n, $\mathbb{C}$). Indeed, for an element X fulfilling $Out_{AC}X = X$ one can write

$$X = Out_{AC}X = -((AC)^{-1}X(AC))^T = -(K^{-1}XK)^T,$$

$$-X^T = K^{-1}XK,$$

$$-KX^T = XK,$$

$$0 = XK + KX^T.$$

The matrix $K = AC$ is symmetric (i.e., $K = K^T$), and $\det K = \det(AC) = \det A \cdot \det C = 1 \cdot 1 = 1$ [since $A, C \in$ SL(4, $\mathbb{C}$)], so matrices from the extracted subspaces correspond to the definition (36) of o(n, $\mathbb{C}$).

According to part II of Theorem 4.1, the MAD-groups $\mathcal{G}_1$ and $\mathcal{G}_2$ do not come into consideration any more. But all the remaining MAD-groups $\mathcal{G}_3, \ldots, \mathcal{G}_8$ contain an outer automorphism Out_C, even with C symmetric (i.e., AC is symmetric for $A = I$). So, each of the fine gradings of sl(4, $\mathbb{C}$) produced by MAD-groups $\mathcal{G}_3, \ldots, \mathcal{G}_8$ displays the subalgebra o(4, $\mathbb{C}$) in the following way (see Table XI):

$$\mathrm{o}(4, \mathbb{C}) = \{X \in \mathbb{C}^{4\times 4} | XC + CX^T = O\} \tag{37}$$

$$o(4,\mathbb{C}) = \oplus_{k\in\mathcal{S}} L_k, \tag{38}$$

where $\mathcal{S}=\{j|(\forall X\in L_j)(Out_C X = X)\}$, with $Out_C \in \mathcal{G}_j$, $j=3,\ldots,8$.

But not only it holds that the fine gradings by $\mathcal{G}_3,\ldots,\mathcal{G}_8$ display the subalgebra o(4, $\mathbb{C}$). The sum (38) is a fine grading of o(4, $\mathbb{C}$) for all $j=3,4,6,7,8$. For $j=5$ the subspace $L_{(0,0)}$ can be split into two to get a fine grading. In this way each fine grading of o(4, $\mathbb{C}$) is displayed by exactly one fine grading of sl(4, $\mathbb{C}$) by $\mathcal{G}_j$, $j=3,\ldots,8$. [Indeed, the algebra o(4, $\mathbb{C}$) has six fine gradings.]

Note the zero value in the first index of all the subspaces L_k (with the exception of the grading by $\mathcal{G}_7$). It stands for the eigenvalue $+1$ of Out_C. In the $\mathcal{G}_7$-grading we did not use the eigenvalues of Out_C in the indices.

The Lie algebra o(4, $\mathbb{C}$) is isomorphic to sl(2, $\mathbb{C}$)$\times$sl(2, $\mathbb{C}$). Suppose one has $C=I$. Then, according to (37) o(4, $\mathbb{C}$) is formed by 4×4 skew-symmetric matrices. In that case the two commuting sl(2, $\mathbb{C}$)-subalgebras can be written in the form

$$\begin{pmatrix} 0 & a & b & c \\ -a & 0 & c & -b \\ -b & -c & 0 & a \\ -c & b & -a & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & f & e & d \\ -f & 0 & -d & e \\ -e & d & 0 & -f \\ -d & -e & f & 0 \end{pmatrix}. \tag{39}$$

Again, this is just one of the basis dependent forms of the subalgebra o(4, $\mathbb{C}$)$\simeq$sl(2, $\mathbb{C}$)$\times$sl(2, $\mathbb{C}$). Therefore, even if the subalgebra is displayed by a grading, it may not be displayed in the form of (39)

In order to get the subalgebra o(4, $\mathbb{C}$) in terms of skew-symmetric matrices one only needs to introduce a change of coordinates: $\tilde{X}=S^{-1}XS$, with $S=\left(\begin{smallmatrix}1 & 0\\ 0 & 1\end{smallmatrix}\right)\oplus\left(\begin{smallmatrix}1/2 & -i/2\\ 1 & i\end{smallmatrix}\right)$ for the cases of $\mathcal{G}_4$, $\mathcal{G}_8$, and $S=\left(\begin{smallmatrix}1/2 & -i/2\\ 1 & i\end{smallmatrix}\right)\oplus\left(\begin{smallmatrix}1/2 & -i/2\\ 1 & i\end{smallmatrix}\right)$ for the cases $\mathcal{G}_5$, $\mathcal{G}_6$. The fine gradings by $\mathcal{G}_3$ and $\mathcal{G}_7$ already display o(4, $\mathbb{C}$) as skew-symmetric matrices (because here $C=I$).

C. sp(4, $\mathbb{C}$) subalgebra of sl(4, $\mathbb{C}$)

The ten-dimensional Lie algebra sp(4, $\mathbb{C}$) can be realized as the complex vector space of matrices

$$\begin{aligned} sp(4,\mathbb{C}) &= \left\{ X \,\middle|\, X\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} X^T = 0 \right\} \\ &= \begin{pmatrix} a & b & c & d \\ e & -a & g & h \\ -h & d & l & m \\ g & c & p & -l \end{pmatrix}. \end{aligned} \tag{40}$$

But also here it is useful to write down the general definition:

$$sp(n,\mathbb{C}) = \{X\in \mathbb{C}^{n\times n} | XK + KX^T = 0\}, \quad K\in \mathbb{C}^{n\times n}, \det K = 1, K = -K^T. \tag{41}$$

In particular, with $n=4$,

$$K = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix},$$

one arrives at (40).

As well as in the case of o(4, $\mathbb{C}$), theory from Ref. 3 provides us with a tool to decide whether a fine grading of sl(4, $\mathbb{C}$) displays sp(4, $\mathbb{C}$) or not. Actually one just replaces o(n, $\mathbb{C}$) with sp(n, $\mathbb{C}$),

TABLE XII. Fine gradings of sp(4, $\mathbb{C}$) displayed by fine gradings of sl(4, $\mathbb{C}$).

MAD-group on sl(4, $\mathbb{C}$)	Fine grading of sp(4, $\mathbb{C}$) in terms of $L_k \subset$ sl(4, $\mathbb{C}$)
$\mathcal{G}_5$	$L_{(0,0)} \oplus L_{(1,1)} \oplus L_{(1,2)} \oplus L_{(0,3)} \oplus L_{(1,4)} \oplus L_{(1,5)} \oplus L_{(0,6)} \oplus L_{(1,7)} \oplus L_{(1,8)}$
$\mathcal{G}_6$	$L_{(0,0,0)} \oplus L_{(0,1,0)} \oplus L_{(1,0,1)} \oplus L_{(1,1,1)} \oplus L_{(1,0,2)} \oplus L_{(0,0,3)} \oplus L_{(0,1,3)} \oplus L_{(1,0,4)} \oplus L_{(1,0,5)} \oplus L_{(1,1,5)}$
$\mathcal{G}_7$	$L_{(0,0,0,1)} \oplus L_{(0,0,1,0)} \oplus L_{(0,1,0,0)} \oplus L_{(0,1,1,0)} \oplus L_{(1,0,0,0)} \oplus L_{(1,0,0,1)} \oplus L_{(1,1,0,0)} \oplus L_{(1,1,0,1)} \oplus L_{(1,1,1,0)} \oplus L_{(1,1,1,1)}$

and AC symmetric with AC skew-symmetric in Theorem 4.1. Fine gradings by $\mathcal{G}_1$ and $\mathcal{G}_2$ are again out of discussion, and so we restrict ourselves to $\mathcal{G}_3,\ldots,\mathcal{G}_8$, more precisely to matrices AC, $A \in G_{Ad}$. And again, once we find such a matrix $A \in G_{Ad}$ that AC is skew-symmetric, $Out_C \in \mathcal{G}_j$, the same reasoning as for o(4, $\mathbb{C}$) leads to the conclusion that the subalgebra sp(4, $\mathbb{C}$) displayed by the fine grading of sl(4, $\mathbb{C}$) is the eigensubspace of Out_{AC} corresponding to the eigenvalue $+1$. (Dimension of such an eigensubspace is 10.) Since the Lie algebra sp(4, $\mathbb{C}$) is simple, it is guaranteed by the sp(n, $\mathbb{C}$)-modification of Theorem 4.1 that this subalgebra displayed by a fine grading of sl(4, $\mathbb{C}$) is already in the form of its fine grading. All fine gradings of sp(4, $\mathbb{C}$) have been described in Ref. 2 and they are all displayed by exactly one fine grading of sl(4, $\mathbb{C}$)—see Table XII. [Indeed, the Lie algebra sp(4, $\mathbb{C}$) has three fine gradings.] All the fine gradings by $\mathcal{G}_j, j=5,6,7$ display sp(4, $\mathbb{C}$) in the form described in (40).

D. sl(2, $\mathbb{C}$)×sl(2, $\mathbb{C}$)×u(1) subalgebra of sl(4, $\mathbb{C}$)

There is another maximal reductive subalgebra in sl(4, $\mathbb{C}$). It has dimension 7 and can be realized as follows:

$$\mathrm{sl}(2,\mathbb{C})\times\mathrm{sl}(2,\mathbb{C})\times\mathrm{u}(1)=\begin{pmatrix} a+g & b & 0 & 0 \\ c & -a+g & 0 & 0 \\ 0 & 0 & d-g & e \\ 0 & 0 & f & -d-g \end{pmatrix}. \tag{42}$$

Here u(1) denotes a one-dimensional subalgebra, its parameter is denoted by g. The semisimple part sl(2, $\mathbb{C}$)×sl(2, $\mathbb{C}$) of the subalgebra is not maximal among semisimple subalgebras of sl(4, $\mathbb{C}$). Indeed, one has sl(2, $\mathbb{C}$)×sl(2, $\mathbb{C}$)⊂sp(4, $\mathbb{C}$)⊂sl(4, $\mathbb{C}$).

The algebra sl(2, $\mathbb{C}$)×sl(2, $\mathbb{C}$)×u(1) is displayed by five fine gradings of sl(4, $\mathbb{C}$), namely by those corresponding to MAD-groups $\mathcal{G}_j$, $j=1,3,4,5,8$. Fine gradings produced by MAD-groups $\mathcal{G}_2$, $\mathcal{G}_6$, and $\mathcal{G}_7$ do not display sl(2, $\mathbb{C}$)×sl(2, $\mathbb{C}$)×u(1). Table XIII gives the list of subspaces that form the subalgebra sl(2, $\mathbb{C}$)×sl(2, $\mathbb{C}$)×u(1) in terms of subspaces of the fine gradings of sl(4, $\mathbb{C}$).

TABLE XIII. Subalgebra sl(2, $\mathbb{C}$)×sl(2, $\mathbb{C}$)×u(1) displayed by fine gradings of sl(4, $\mathbb{C}$).

MAD-group on sl(4, $\mathbb{C}$)	Subalgebra sl(2, $\mathbb{C}$)×sl(2, $\mathbb{C}$)×u(1) in terms of $L_k \subset$ sl(4, $\mathbb{C}$)
$\mathcal{G}_1$	$L_{(0)} \oplus L_{(2)} \oplus L_{(4)} \oplus L_{(9)} \oplus L_{(11)}$
$\mathcal{G}_3$	$L_{(1,0,0,1)} \oplus L_{(0,0,0,1)} \oplus L_{(1,1,0,0)} \oplus L_{(0,1,0,0)} \oplus L_{(1,0,0,0)}$
$\mathcal{G}_4$	$L_{(0,0)} \oplus L_{(1,0)} \oplus L_{(1,2)} \oplus L_{(0,4)} \oplus L_{(1,4)} \oplus L_{(1,6)}$
$\mathcal{G}_5$	$L_{(0,0)} \oplus L_{(1,0)} \oplus L_{(1,2)} \oplus L_{(1,4)} \oplus L_{(1,5)} \oplus L_{(1,7)}$
$\mathcal{G}_8$	$L_{(0,1,0)} \oplus L_{(1,0,0)} \oplus L_{(1,1,0)} \oplus L_{(0,1,2)} \oplus L_{(1,0,2)} \oplus L_{(1,1,2)}$

TABLE XIV. The full list of nonconjugate MAD-groups on o(6, $\mathbb{C}$).

	H_{Ad}
$\mathcal{H}_1$	$\left\{A=\begin{pmatrix}\cos\varphi_1 & \sin\varphi_1\\ -\sin\varphi_1 & \cos\varphi_1\end{pmatrix}\oplus\begin{pmatrix}\cos\varphi_2 & \sin\varphi_2\\ -\sin\varphi_2 & \cos\varphi_2\end{pmatrix}\oplus\begin{pmatrix}\cos\varphi_3 & \sin\varphi_3\\ -\sin\varphi_3 & \cos\varphi_3\end{pmatrix},\ \varphi_i\in\mathbb{C}\right\}$
$\mathcal{H}_2$	$\{A\in D^{-1}\{(H_0\otimes I_2)\cup(TH_0\otimes\sigma_3)\cup(UH_0\otimes\sigma_1)\cup(TUH_0\otimes\sigma_2)\}D.$ $D=\mathrm{diag}(1,1,1,i)\oplus\frac{1}{\sqrt{2}}\begin{pmatrix}1 & i\\ 1 & -i\end{pmatrix},$ $H_0=\{\mathrm{diag}(1,\varepsilon_1,\varepsilon_2)\mid\varepsilon_i=\pm1\},$ $T=\mathrm{diag}(1,1,i),\ U=\mathrm{diag}(1,i,1)\}$
$\mathcal{H}_3$	$\{A=\sigma_k\otimes\mathrm{diag}(1,\varepsilon_1,\varepsilon_2),t\varepsilon_i=\pm1,k=0,1,2,3\}$
$\mathcal{H}_4$	$\left\{A=\sigma_k\otimes\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\varphi & \sin\varphi\\ 0 & -\sin\varphi & \cos\varphi\end{pmatrix},\ \varphi\in\mathbb{C},\ k=0,1,2,3\right\}$
$\mathcal{H}_5$	$\left\{A=\mathrm{diag}(1,\varepsilon)\oplus\begin{pmatrix}\cos\varphi_1 & \sin\varphi_1\\ -\sin\varphi_1 & \cos\varphi_1\end{pmatrix}\oplus\begin{pmatrix}\cos\varphi_2 & \sin\varphi_2\\ -\sin\varphi_2 & \cos\varphi_2\end{pmatrix},\ \varepsilon=\pm1,\varphi_j\in\mathbb{C}\right\}$
$\mathcal{H}_6$	$\left\{A=\mathrm{diag}(1,\varepsilon_1,\varepsilon_2,\varepsilon_3)\oplus\begin{pmatrix}\cos\varphi & \sin\varphi\\ -\sin\varphi & \cos\varphi\end{pmatrix},\ \varepsilon_i=\pm1,\varphi\in\mathbb{C}\right\}$
$\mathcal{H}_7$	$\{A=\mathrm{diag}(1,\varepsilon_1,\varepsilon_2,\varepsilon_3,\varepsilon_4,\varepsilon_5),\ \varepsilon_i=\pm1\}$
$\mathcal{H}_8$	$\{A\in E^{-1}\{(H_0\otimes I_2)\cup(H_0\otimes\sigma_3)\cup(VH_0\otimes\sigma_1)\cup(VH_0\otimes\sigma_2)\}E,$ $E=\mathrm{diag}(1,1,1,1,1,i),\ H_0=\{\mathrm{diag}(1,\varepsilon_1,\varepsilon_2)\mid\varepsilon_i=\pm1\},$ $V=\mathrm{diag}(1,1,i)\}$

V. FINE GRADINGS OF THE LIE ALGEBRA o(6, $\mathbb{C}$)

In this section we consider the analogous objects, MAD-groups, gradings, eigenvalues and eigenvectors, as in Sec. III. The difference here is that the Lie algebra A_3 is represented by 6×6 matrices and called traditionally o(6, $\mathbb{C}$). It is useful because in a number of applications one works only with the Lie algebra of the orthogonal group O(6, $\mathbb{C}$), and because the correspondence between the two representations is not always straightforward. Indeed, take for example the center of SL(4, $\mathbb{C}$) which is of order 4. In the six-dimensional representation, half of it coalesces, so that the center of O(6, $\mathbb{C}$) is of order 2.

The list of MAD-groups $\mathcal{H}_1,\ldots,\mathcal{H}_8$ in Aut o(6, $\mathbb{C}$) follows in Table XIV [they are ordered in such a way that $\mathcal{H}_j$ produces a fine grading of o(6, $\mathbb{C}$) which is isomorphic to the fine grading of sl(4, $\mathbb{C}$) by $\mathcal{G}_j$ in Sec. III]. Note, however, that the generators are generally not normalized to the same values. Within grading subspaces of dimension greater than 1, the basis is chosen by convenience, no particular correspondence between the four- and six-dimensional representations is maintained.

A. The fine grading of o(6, $\mathbb{C}$) corresponding to $\mathcal{H}_1$

In this case the MAD-group is the maximal torus of the Lie group represented by 6×6 matrices. Its generic element is A,

$$A=\begin{pmatrix}\cos\varphi_1 & \sin\varphi_1\\ -\sin\varphi_1 & \cos\varphi_1\end{pmatrix}\oplus\begin{pmatrix}\cos\varphi_2 & \sin\varphi_2\\ -\sin\varphi_2 & \cos\varphi_2\end{pmatrix}\oplus\begin{pmatrix}\cos\varphi_3 & \sin\varphi_3\\ -\sin\varphi_3 & \cos\varphi_3\end{pmatrix}.$$

Using A and (4) in (7) the Lie algebra o(6, $\mathbb{C}$) is decomposed into 13 subspaces: one three-dimensional (Cartan subalgebra) and 10 one-dimensional (root) subspaces.

The eigenvectors $Z_1,\ldots,Z_{15}$ are given in terms of matrices M_{jk} of (9):

$$
\begin{gathered}
Z_1=M_{34}-M_{56}, \quad Z_2=M_{12}-M_{34}, \\
Z_3=M_{34}+M_{56}, \quad Z_4=(M_{13}+M_{24})+i(M_{14}-M_{23}), \\
Z_5=(M_{35}+M_{46})+i(M_{36}-M_{45}), \quad Z_6=(M_{15}+M_{26})+i(M_{16}-M_{25}), \\
Z_7=(M_{35}-M_{46})+i(-M_{36}-M_{45}), \quad Z_8=(M_{15}-M_{26})+i(-M_{16}-M_{25}), \\
Z_9=(M_{13}-M_{24})+i(M_{14}+M_{23}), \quad Z_{10}=(M_{13}-M_{24})+i(-M_{14}-M_{23}), \\
Z_{11}=(M_{15}-M_{26})+i(M_{16}+M_{25}), \quad Z_{12}=(M_{35}-M_{46})+i(M_{36}+M_{45}), \\
Z_{13}=(M_{15}+M_{26})+i(-M_{16}+M_{25}), \quad Z_{14}=(M_{35}+M_{46})+i(-M_{36}+M_{45}), \\
Z_{15}=(M_{13}+M_{24})+i(-M_{14}+M_{23}).
\end{gathered}
\tag{43}
$$

The eigenvalues of Z_j coincide with those of X_j of $\mathcal{G}_1$ (Table II), after the values d_1, d_2, d_3 are replaced by $\exp(-i(\varphi_1+\varphi_2))$, $\exp(-i(\varphi_1+\varphi_3))$, and $\exp(-i(\varphi_2+\varphi_3))$. Clearly the additive group is again $\mathbb{Z}_{13}$. The Cartan subalgebra is spanned by the generators Z_1, Z_2, and Z_3.

Rather complicated expressions for the nilpotent generators of the root spaces $Z_4, \ldots, Z_{13}$ are the result of our choice of $\{M_{jk}\}$ of (9) as the basis of o(6, $\mathbb{C}$), in which we write the basis $\{Z_m\}$. Had we started with the representation (5) of o(6, $\mathbb{C}$), the expressions for $\{Z_m\}$ would have been simpler in terms of N_{jk} (see Table XVI).

B. The fine grading of o(6, $\mathbb{C}$) corresponding to $\mathcal{H}_2$

With $A_1=D^{-1}(TU\otimes\sigma_2)D, A_2=D^{-1}(T\otimes\sigma_3)D$ the Lie algebra o(6, $\mathbb{C}$) is decomposed into 15 one-dimensional subspaces—linear hulls of the eigenvectors Z_j:

$$
\begin{gathered}
Z_1=(M_{35}-M_{46})+i(M_{36}-M_{45}), \quad Z_2=M_{12}, \\
Z_3=(M_{35}-M_{46})+i(-M_{36}+M_{45}), \quad Z_4=M_{13}+iM_{24}, \\
Z_5=(M_{15}+M_{25})+i(M_{16}-M_{26}), \quad Z_6=M_{14}+iM_{23}, \\
Z_7=(M_{15}-M_{25})+i(-M_{16}-M_{26}), \quad Z_8=M_{56}, \\
Z_9=(M_{35}+M_{46})+i(M_{36}+M_{45}), \quad Z_{10}=M_{34}, \\
Z_{11}=(M_{35}+M_{46})+i(-M_{36}-M_{45}), \quad Z_{12}=M_{13}-iM_{24}, \\
Z_{13}=(M_{15}-M_{25})+i(M_{16}+M_{26}), \quad Z_{14}=M_{14}-iM_{23}, \\
Z_{15}=(M_{15}+M_{25})+i(-M_{16}+M_{26}).
\end{gathered}
\tag{44}
$$

The additive group ($\mathbb{Z}_4\times\mathbb{Z}_4$) and the table of eigenvalues are the same as for $\mathcal{G}_2$ (Table III).

C. The fine grading of o(6, $\mathbb{C}$) corresponding to $\mathcal{H}_3$

With $A_1=\sigma_0\otimes\mathrm{diag}(1,1,-1)$, $A_2=\sigma_3\otimes\mathrm{diag}(1,1,1)$, $A_3=\sigma_2\otimes\mathrm{diag}(1,1,-1)$, and $A_4=\sigma_1\otimes\mathrm{diag}(1,-1,1)$ the Lie algebra o(6, $\mathbb{C}$) is decomposed into one three-dimensional and 12 one-dimensional subspaces whose bases consist of the eigenvectors Z_j:

TABLE XV. $\mathcal{H}_3$: The correspondence between eigenvectors Z_k from (45) and the eigenvalues $\lambda_1,\lambda_2,\lambda_3,\lambda_4$ of $Ad_{A_1},Ad_{A_2},Ad_{A_3},Ad_{A_4}$.

	Eigenvector	λ_1	λ_2	λ_3	λ_4
$L_{(0,0,0,1)}$	Z_1	1	1	1	−1
$L_{(0,0,1,0)}$	Z_2	1	1	−1	1
$L_{(0,1,0,0)}$	Z_3	1	−1	1	1
$L_{(0,1,0,1)}$	Z_4	1	−1	1	−1
	Z_5	1	−1	1	−1
	Z_6	1	−1	1	−1
$L_{(0,1,1,1)}$	Z_7	1	−1	−1	−1
$L_{(1,0,0,0)}$	Z_8	−1	1	1	1
$L_{(1,0,0,1)}$	Z_9	−1	1	1	−1
$L_{(1,0,1,0)}$	Z_{10}	−1	1	−1	1
$L_{(1,0,1,1)}$	Z_{11}	−1	1	−1	−1
$L_{(1,1,0,0)}$	Z_{12}	−1	−1	1	1
$L_{(1,1,0,1)}$	Z_{13}	−1	−1	1	−1
$L_{(1,1,1,0)}$	Z_{14}	−1	−1	−1	1
$L_{(1,1,1,1)}$	Z_{15}	−1	−1	−1	−1

$$
\begin{gathered}
Z_1=M_{12}+M_{45},\quad Z_2=M_{12}-M_{45},\quad Z_3=M_{15}+M_{24},\quad Z_4=M_{36},\\
Z_5=M_{25},\quad Z_6=M_{14},\quad Z_7=M_{15}-M_{24},\quad Z_8=M_{23}-M_{56},\\
Z_9=M_{13}-M_{46},\quad Z_{10}=M_{13}+M_{46},\quad Z_{11}=M_{23}+M_{56},\quad Z_{12}=M_{16}-M_{34},\\
Z_{13}=M_{26}-M_{35},\quad Z_{14}=M_{26}+M_{35},\quad Z_{15}=M_{16}+M_{34}.
\end{gathered}
\tag{45}
$$

The table of eigenvalues follows (Table XV); and the indices of eigensubspaces are elements of $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$.

D. The fine grading of o(6, $\mathbb{C}$) corresponding to $\mathcal{H}_4$

With

$$
A_1=\sigma_1\otimes\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\quad A_2=\sigma_2\otimes\begin{pmatrix}1&0&0\\0&\cos\varphi&\sin\varphi\\0&-\sin\varphi&\cos\varphi\end{pmatrix}
$$

the Lie algebra o(6, $\mathbb{C}$) is decomposed into one two-dimensional and 13 one-dimensional subspaces. The eigenvectors $Z_1,\ldots,Z_{15}$ describing the subspaces are

$$
\begin{gathered}
Z_1=M_{23}+M_{56},\quad Z_2=M_{14},\\
Z_3=M_{25}+M_{36},\quad Z_4=(M_{12}+M_{45})+i(-M_{13}-M_{46}),\\
Z_5=(M_{15}+M_{24})+i(-M_{16}-M_{34}),\quad Z_6=(M_{25}-M_{36})+i(-M_{26}-M_{35}),\\
Z_7=(M_{15}-M_{24})+i(M_{16}-M_{34}),\quad Z_8=(M_{12}-M_{45})+i(M_{13}-M_{46})\\
Z_9=M_{26}-M_{35},\quad Z_{10}=M_{23}-M_{56}\\
Z_{11}=(M_{15}-M_{24})+i(-M_{16}+M_{34}),\quad Z_{12}=(M_{12}-M_{45})+i(-M_{13}+M_{46}),\\
Z_{13}=(M_{25}-M_{36})+i(M_{26}+M_{35}),\quad Z_{14}=(M_{12}+M_{45})+i(M_{13}+M_{46}),\\
Z_{15}=(M_{15}+M_{24})+i(M_{16}+M_{34}).
\end{gathered}
\tag{46}
$$

As in the case of $\mathcal{G}_4$, the set of indices is a subset of $\mathbb{Z}_2\times\mathbb{Z}_8$. The eigenvalues are the same as in Table V with $\alpha=\exp(i\varphi)$.

E. The fine grading of o(6, $\mathbb{C}$) corresponding to $\mathcal{H}_5$

Using the two matrices

$$A_1=\mathrm{diag}(1,-1)\oplus\begin{pmatrix}-1&0\\0&-1\end{pmatrix}\oplus\begin{pmatrix}1&0\\0&1\end{pmatrix},$$

$$A_2=\mathrm{diag}(1,1)\oplus\begin{pmatrix}\cos\varphi_1&\sin\varphi_1\\-\sin\varphi_1&\cos\varphi_1\end{pmatrix}\oplus\begin{pmatrix}\cos\varphi_2&\sin\varphi_2\\-\sin\varphi_2&\cos\varphi_2\end{pmatrix}$$

for Ad_A, the Lie algebra o(6, $\mathbb{C}$) is decomposed into 13 one-dimensional and one two-dimensional subspaces with bases consisting of eigenvectors $Z_1,\ldots,Z_{15}$:

$$\begin{gathered}
Z_1=M_{34},\quad Z_2=M_{56},\\
Z_3=M_{12},\quad Z_4=M_{15}-iM_{16},\\
Z_5=M_{25}-iM_{26},\quad Z_6=(M_{35}+M_{46})+i(M_{36}-M_{45}),\\
Z_7=M_{23}-iM_{24},\quad Z_8=M_{13}-iM_{14},\\
Z_9=(M_{35}-M_{46})+i(-M_{36}-M_{45}),\quad Z_{10}=(M_{35}-M_{46})+i(M_{36}+M_{45}),\\
Z_{11}=M_{23}+iM_{24},\quad Z_{12}=M_{13}+iM_{14},\\
Z_{13}=(M_{35}+M_{46})+i(-M_{36}+M_{45}),\quad Z_{14}=M_{15}+iM_{16},\\
Z_{15}=M_{25}+iM_{26}.
\end{gathered}\tag{47}$$

Replacing α with $\exp((i/2)(\varphi_1+\varphi_2))$ and β with $\exp((i/2)(-\varphi_1+\varphi_2))$ in Table VI we get the pairs of eigenvalues of Ad_{A_1} and Ad_{A_2}; these are then embedded into the additive group $\mathbb{Z}_2\times\mathbb{Z}_9$.

F. The fine grading of o(6, $\mathbb{C}$) corresponding to $\mathcal{H}_6$

Three inner automorphisms Ad_A, $A_1=\mathrm{diag}(1,1,-1,1,-1,-1)$, $A_2=\mathrm{diag}(1,-1,-1,1,1,1)$, and

$$A_3=\mathrm{diag}(1,1,-1,-1)\oplus\begin{pmatrix}\cos\varphi&\sin\varphi\\-\sin\varphi&\cos\varphi\end{pmatrix},$$

split the Lie algebra o(6, $\mathbb{C}$) into 15 one-dimensional subspaces—linear hull of matrices Z_j:

$$\begin{gathered}
Z_1=M_{56},\quad Z_2=M_{12},\quad Z_3=M_{34},\quad Z=M_{15}-iM_{16},\\
Z_5=M_{25}-iM_{26},\quad Z_6=M_{35}+iM_{36},\quad Z_7=M_{45}+iM_{46},\quad Z_8=M_{14},\\
Z_9=M_{24},\quad Z_{10}=M_{23},\quad Z_{11}=M_{13},\quad Z_{12}=M_{35}-iM_{36},\\
Z_{13}=M_{45}-iM_{46},\quad Z_{14}=M_{15}+iM_{16},\quad Z_{15}=M_{25}+iM_{26}.
\end{gathered}\tag{48}$$

The table of eigenvalues (elements of $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_6$) can be obtained from Table VII, just with the value $\exp(i\varphi/2)$ in the place of α.

G. The fine grading of o(6, $\mathbb{C}$) corresponding to $\mathcal{H}_7$

With four specimen of $A=\mathrm{diag}(1,\varepsilon_1,\varepsilon_2,\varepsilon_3,\varepsilon_4,\varepsilon_5)$, namely $A_1=\mathrm{diag}(1,1,-1,-1,-1,-1)$, $A_2=\mathrm{diag}(1,-1,1,-1,-1,-1)$, $A_3=\mathrm{diag}(1,-1,-1,1,-1,-1)$, and $A_4=\mathrm{diag}(1,-1,-1,-1,1,-1)$, the Lie algebra o(6, $\mathbb{C}$) is decomposed into 15 one-dimensional subspaces, whose bases are the eigenvectors Z_j:

$$\begin{gathered}Z_1=M_{56},\quad Z_2=M_{46},\quad Z_3=M_{45},\quad Z_4=M_{36},\\ Z_5=M_{35},\quad Z_6=M_{34},\quad Z_7=M_{12},\quad Z_8=M_{26},\\ Z_9=M_{25},\quad Z_{10}=M_{24},\quad Z_{11}=M_{13},\quad Z_{12}=M_{23},\\ Z_{13}=M_{14},\quad Z_{14}=M_{15},\quad Z_{15}=M_{16}.\end{gathered}\tag{49}$$

See Table VIII for the eigenvalues $(j,k,l,m)\in\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$.

H. The fine grading of o(6, $\mathbb{C}$) corresponding to $\mathcal{H}_8$

Using $A_1=E^{-1}(I_3\otimes\sigma_3)E$, $A_2=E^{-1}(\mathrm{diag}(1,-1,1)\otimes\sigma_0)E$, and $A_3=E^{-1}(I_3\otimes\sigma_1)E$ in Ad_A, the Lie algebra o(6, $\mathbb{C}$) is decomposed into fourteen subspaces, one being two-dimensional and the rest one-dimensional. The eigenvectors $Z_1,\ldots,Z_{15}$ are again given in terms of M_{ij}:

$$\begin{gathered}Z_1=M_{13}+M_{24},\quad Z_2=M_{56},\quad Z_3=M_{14}+M_{23},\quad Z_4=M_{15}+iM_{26},\\ Z_5=M_{35}+iM_{46},\quad Z_6=M_{16}-iM_{25},\quad Z_7=M_{36}-iM_{45},\quad Z_8=M_{13}-M_{24},\\ Z_9=M_{12},\quad Z_{10}=M_{34},\quad Z_{11}=M_{14}-M_{23},\quad Z_{12}=M_{15}-iM_{26},\\ Z_{13}=M_{35}-iM_{46},\quad Z_{14}=M_{16}+iM_{25},\quad Z_{15}=M_{36}+iM_{45}.\end{gathered}\tag{50}$$

The grading subspaces generated by $Z_1,\ldots,Z_{12}$ are labeled by the eigenvalues of $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_4$ given in Table IX.

VI. CONCLUDING REMARKS

Having seen the eight fine gradings of A_3 in this article, the four fine gradings of A_2 in Ref. 3, the two such gradings of A_1 (the root decomposition and the grading spanned by the Pauli matrices), as well as the four fine gradings of the simple Lie algebra $C_2\simeq B_2$ in Ref. 2, it appears unlikely that it will ever be practical to describe all fine gradings of sl(n, $\mathbb{C}$) or other simple Lie algebras for much higher ranks in an explicit way similarly as it is done in this article. There are, however, other interesting questions one may want to address, once particular fine gradings are known or can be found. Let us mention some of them.

(i) There are many intermediate gradings of a Lie algebra between the two grading extremes, the finest gradings (which we call fine) and the coarsest one. It would be useful to know them. Indeed, our original motivation for studying fine gradings came from the need to know the intermediate ones in order to use them for contractions of Lie algebras which preserve a chosen grading (cf. Ref. 7 and references therein). Typically in physics applications one requires that a subalgebra L' of L should be left intact, while contractions of the rest of L are admitted. An appropriate grading for such a problem would have L' displayed.

The most difficult part in finding all the nonequivalent gradings is to determine the fine ones. One can visualize information about all gradings of a given algebra, for example, as

a graph with nodes, representing different gradings, ordered by levels which are given by the number of grading subspaces in each grading, and with edges linking nodes/gradings related by a minimal refinement/coarsening. A complete list of gradings is simple to make for A_1, but it is considerably more difficult for all higher rank algebras. In fact, a description of all nonequivalent gradings is not available even for rank two algebras.

(ii) In this article we have introduced the notion of a subalgebra $L' \subset L$ which is displayed by a grading of L. In general, such a grading may not be a fine one. It is unlikely that for any $L' \subset L$ one can find a grading of L which would display L'. An interesting problem is to recognize the subalgebras which are displayed by some grading of L. We have seen in this article that all maximal reductive subalgebras are displayed by some grading, usually more than one. That includes the subalgebras o(4, $\mathbb{C}$) and sp(4, $\mathbb{C}$) which are of rank 2 and which are not displayed by the root grading.

(iii) Besides the fine gradings by the maximal torus, well known for all simple Lie algebras, there is also another family of fine gradings of all sl(n, $\mathbb{C}$). The corresponding MAD-group $\mathcal{P}_n$ is finite, is of order n^3, and is generated by the $n \times n$ Pauli matrices.[6] In this article such a grading is produced by the MAD-group $\mathcal{G}_2$ in four dimensions and by $\mathcal{H}_2$ in six dimensions.

Furthermore, for each sl(n, $\mathbb{C}$) with $n = n_1 \times n_2$, where the factors n_1 and n_2 have a nontrivial common divisor, there is another MAD-group $\mathcal{P}_{n_1} \times \mathcal{P}_{n_2}$ containing the tensor products of Pauli matrices $n_1 \times n_1$ and $n_2 \times n_2$. It is the case of MAD-groups $\mathcal{G}_7$ for $n_1 = n_2 = 2$ in this article. The group $\mathcal{H}_7$ is a six-dimensional representation of $\mathcal{G}_7$. If n_1 and n_2 have no common divisor, $\mathcal{P}_{n_1} \times \mathcal{P}_{n_2}$ is isomorphic to $\mathcal{P}_n$.

(iv) The fine gradings of the real forms of A_3 and the maximal reductive subalgebras they display are considered in our subsequent paper. Given the classification of the corresponding MAD-groups,[8] it is a natural continuation of this work.

(v) The Lie algebra A_3 has two independent Casimir operators, of degree 2 and 3. The degree 2 operator and its eigenvalues on irreducible representations are well known for simple Lie algebras of all types. The operator of degree 3 was written for all sl(n, $\mathbb{C}$) by I. M. Gelfand some 50 years ago. Its eigenvalues apparently were never given in a closed form for all irreducible representations.

It would be interesting to write the operators in terms of other bases than that given by the root decomposition. It is conceivable that an easier description of their eigenvalues would then be possible.

(vi) Ubiquity of the weight decomposition of the representations of simple Lie algebras, which is the decomposition of the representation spaces into eigenspaces of the maximal torus, is well known as the workhorse of the applications of the standard representation theory of these Lie algebras.

Eigenspace decomposition of representation spaces of A_3 by other MAD-groups is a well defined problem which would be interesting to consider even before a fine grading turns out to be particularly useful: Such a decomposition may suggest useful applications of the grading. There is a technical complication arising in all but the root decomposition. It is related to the fact that the MAD-groups involve automorphisms of finite order. Such automorphisms, in general, behave differently in representations belonging to different congruence classes.[9] Their order may be different in representations belonging to different congruence classes.

(vii) Finally, let us point out an interesting new application of the fine gradings outside the Lie theory proper. The well known Drinfeld–Jimbo quantum algebra is a q-deformation of the universal enveloping algebra U(so(n)) in the basis given by the root decomposition. In Refs. 10 and 11 a new deformation of U(so(n)) is based on another fine grading of so(n), namely on the grading generated by the MAD-group $\mathcal{G} = \{Ad_A | A = \mathrm{diag}(\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n), \varepsilon_i = \pm 1\}$. This new deformation is nonisomorphic to the Drifeld–Jimbo deformation. It is quite natural to ask the question about q-deformations for every fine grading of so(n), not only for the two mentioned in Ref. 10.

TABLE XVI. Matrices representing the root spaces e_{α_1}, e_{α_2}, e_{α_3} of A_3 in terms of matrices E_{jk}, N_{jk}, and M_{jk} defined in (9), and normalized so that corresponding structure constants coincide.

	sl(4, $\mathbb{C}$)	o(6, $\mathbb{C}$)	
e_{α_1}	E_{12}	N_{23}	$\frac{1}{2}[(M_{35}+M_{46})+i(M_{36}-M_{45})]$
e_{α_2}	E_{23}	N_{12}	$\frac{1}{2}[(M_{13}+M_{24})+i(M_{14}-M_{23})]$
e_{α_3}	E_{34}	N_{24}	$\frac{1}{2}[(M_{35}-M_{46})-i(M_{36}+M_{45})]$

(viii) Occasionally one needs bases/generators of the Lie algebra chosen in different representations in such a way that the corresponding structure constants coincide. In Table XVI one finds such a choice of the matrices representing the root vectors of the three simple roots e_{α_1}, e_{α_2}, and e_{α_3} in the four- and six-dimensional representations of A_3. For the latter we show them in both realizations (4) and (5). The root vectors of the negative simple roots roots, $e_{-\alpha_j}, j=1,2,3$, are obtained from the positive ones by matrix transposition in the cases (2) and (5): $e_{-\alpha_j}=e_{\alpha_j}^T$, whereas for o(6, $\mathbb{C}$), represented by skew-symmetric matrices (4), one uses Hermitian conjugation (transposition and complex conjugation): $e_{-\alpha_j}=\overline{e_{\alpha_j}^T}=\overline{-e_{\alpha_j}}$. From the six root vectors $e_{\pm\alpha_j}, j=1,2,3$, the rest of the basis is generated by repeated commutations. In all three cases the structure constants are the same.

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Comment on: " 'Massive' vector field in de Sitter space" [J. Math. Phys. 41, 5920 (2000)]

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Equation (3.26) and the sentence below it should be replaced by

$$K_{2\alpha}(z)=\mathcal{E}^{*(\lambda)}_{\alpha}(z^*,\xi)(Hz\cdot\xi)^{-3/2-i\nu}, \tag{3.26}$$

in which $z,z^*\in X_H^{(c)}$ and $\xi\in\mathcal{C}^+$.

Equations (4.8) and (4.9) should be replaced by

$$K_2^{\xi,\lambda}(z)=(Hz\cdot\xi)^{-3/2-i\nu}\mathcal{E}^{*\lambda}(z^*,\xi), \tag{4.8}$$

$$W^{\nu}_{\alpha\alpha'}(z,z')=c_{\nu}\int_T (z.\xi)^{-3/2-i\nu}(z'.\xi)^{-3/2+i\nu}\sum_{\lambda=1}^{3}\mathcal{E}^{\lambda}_{\alpha}(z,\xi)\mathcal{E}^{*\lambda}_{\alpha'}(z'^*,\xi)d\mu_T(\xi). \tag{4.9}$$

Equations (4.14) and (4.16) should be replaced by

$$\overline{\partial'}\mathcal{W}^{\nu}_2(x,x')=\frac{1}{\nu^2+\frac{1}{4}}[\theta'\cdot\overline{\partial}\mathcal{W}^{\nu}_1(x,x')+2H^2\theta'\cdot x\mathcal{W}^{\nu}_1(x,x')]. \tag{4.14}$$

$$D_{\alpha\alpha'}=\theta_{\alpha}\cdot\theta'_{\alpha'}+\frac{1}{H^2(\nu^2+\frac{1}{4})}\overline{\partial}_{\alpha}[\theta'_{\alpha'}\cdot\overline{\partial}+2H^2\theta'_{\alpha'}\cdot x]. \tag{4.16}$$

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A note on a series of papers on relativistic δ-sphere interactions in quantum mechanics published by M. N. Hounkonnou and G. Y. H. Avossevou in the Journal of Mathematical Physics

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In this note, we show that the definitions proposed in J. Math. Phys. **41**, 24 (2000); **41**, 1718 (2000); **41**, 1735 (2000) for the description of relativistic δ-sphere interactions and its various generalizations are not correct. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1518786]

I. INTRODUCTION

In the last two decades, several researchers were attracted by the study of δ-sphere interactions in quantum mechanics both from the mathematical point of view and for their applications in modelling various physical phenomena.

For a long time, most of the studies were focusing on nonrelativistic interactions. The first rigorous mathematical definition and analysis of relativistic δ-sphere interactions were provided in Refs. 1 and 2.

More recently, Hounkonnou and Avossevou[3–5] published a series of papers on relativistic δ, δ' and finitely many δ-sphere interactions in quantum mechanics. Although they refer to Refs. 1 and 2, the definitions proposed in Refs. 3–5 for the description of relativistic δ-sphere interactions are not correct. Furthermore, the papers contain several other mistakes related to a misunderstanding of some basic concepts of the theory of self-adjoint extensions of symmetric operators in Hilbert spaces.

The purpose of this note is to show that the definitions proposed in Refs. 3–5 do not correspond to any relativistic δ-sphere interaction.

In Secs. II and III we review the definitions proposed in Refs. 1 and 2 and 3–5, respectively, and in Sec. IV we carry out a comprehensive critical analysis of the boundary conditions of the models introduced in Refs. 3–5.

II. THE DEFINITION OF DITTRICH, EXNER, AND SEBA (Ref. 1)

Using the theory of self-adjoint extensions of symmetric operators in Hilbert spaces, Dittrich *et al.*[1] introduced the Dirac Hamiltonian with a δ-sphere interaction, formally given in three dimensions by

$$H_{\underline{\underline{G}}} = H_D + \underline{\underline{G}}\,\delta(|x|-R); \quad x \in \mathbb{R}^3, \quad R \in (0,\infty), \tag{1}$$

where H_D is the free Dirac Hamiltonian and $\underline{\underline{G}}$ is a real 4×4 matrix of the form $\underline{\underline{G}} = \left(\begin{smallmatrix} A & 0 \\ 0 & B \end{smallmatrix}\right)$.

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For the construction of the self-adjoint operator corresponding to $H_{\underline{G}}$ the authors proceed as follows. First, they consider the operator

$$H = H_D,$$
$$\mathcal{D}(H) = C_0^\infty(\mathbb{R}^3 \backslash \{S_R\}) \otimes \mathbb{C}^4, \tag{2}$$

where S_R is the closed ball of radius R centered at the origin in $\mathbb{R}^3$ and look for those self-adjoint extensions of H which are rotationally and space reflection symmetric.

Next they decompose the state Hilbert space $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ with respect to radial and angular variables and introduce a unitary operator in order to remove the weight factor r^2 from the integration measure.

With these transformations, the analysis of $H_{\underline{G}}$ in Eq. (1) is reduced to that of the radial Dirac Hamiltonian h_D with a δ-interaction formally given by

$$h_G = h_D + G\,\delta(r-R), \tag{3}$$

where G is a real 2×2 matrix of the form $G = \left(\begin{smallmatrix} A & 0 \\ 0 & B \end{smallmatrix}\right)$ and

$$h_D = \begin{pmatrix} \dfrac{c^2}{2} & -c\dfrac{d}{dr} + c\dfrac{\kappa_{jl}}{r} \\ c\dfrac{d}{dr} + c\dfrac{\kappa_{jl}}{r} & -\dfrac{c^2}{2} \end{pmatrix} \equiv \tau, \quad \mathcal{D}(h_D) = H^{1,2}((0,\infty)) \otimes \mathbb{C}^2. \tag{4}$$

In Eq. (4), c denotes the velocity of the light, $H^{1,2}((0,\infty))$, the Sobolev space of indices (1,2) and $\kappa_{jl} = (-1)^{j-l+\frac{1}{2}}(j+\frac{1}{2})$.

The construction of the self-adjoint operator corresponding to h_G is performed as follows. Fisrt, one considers the closure of the radial part of the operator H which is defined by

$$h_{jl} = \tau,$$
$$D(h_{jl}) = \{\psi \in L^2((0,\infty)) \otimes \mathbb{C}^2 \,|\, \psi \in \mathrm{AC}_{\mathrm{loc}}((0,\infty)), \psi(R\pm) = 0;$$
$$\tau\psi \in L^2((0,\infty)) \otimes \mathbb{C}^2\}, \tag{5}$$

where $\mathrm{AC}_{\mathrm{loc}}(\Omega)$ denotes the set of locally absolutely continuous functions on Ω and

$$\psi(x\pm) = \lim_{\epsilon \to 0+} \psi(x \pm \epsilon).$$

The adjoint h_{jl}^* of h_{jl} reads

$$h_{jl}^* = \tau,$$
$$D(h_{jl}^*) = \{\psi \in L^2((0,\infty)) \otimes \mathbb{C}^2 \,|\, \psi \in \mathrm{AC}_{\mathrm{loc}}((0,\infty) \backslash \{R\}),$$
$$\tau\psi \in L^2((0,\infty)) \otimes \mathbb{C}^2\}. \tag{6}$$

The following theorem was proved in Ref. 1

Theorem 1:

Any self-adjoint extension $\hat{h}_{jl}$ of h_{jl} reads

$$\hat{h}_{jl} = \tau,$$
$$\mathcal{D}(\hat{h}_{jl}) = \{\psi \in \mathcal{D}(h_{jl}^*) \,|\, C\psi(R-) + D\psi(R+) = 0\}, \tag{7}$$

where C and D are 2×2 matrices such that the 2×4 matrix (C,D) has rank 2.

Conversely any operator of this form is a self-adjoint extension of h_{jl}.

Definition:

According to Ref. 1, Eqs. (4.3) and (4.6), the operator h_G in Eq. (3) is defined in $L^2((0,\infty))\otimes\mathbb{C}^2$ by

$$h_G=\tau,$$

$$D(h_G)=\left\{\psi\in\mathcal{D}(h_{jl}^*)\left|\begin{pmatrix}1 & \frac{B}{2c}\\ -\frac{A}{2c} & 1\end{pmatrix}\psi(R+)-\begin{pmatrix}1 & -\frac{B}{2c}\\ \frac{A}{2c} & 1\end{pmatrix}\psi(R-)=0\right.\right\}. \tag{8}$$

The particular cases $A\neq0$, $B=0$ and $A=0$, $B\neq0$ yield the relativistic δ-sphere interactions of the first and second type, respectively, with the domains

$$\mathcal{D}(h_A)=\left\{\psi=\begin{pmatrix}f\\ g\end{pmatrix}\in\mathcal{D}(h_{jl}^*)\left|f(R-)=f(R+)\equiv f(R),g(R+)-g(R-)=\frac{A}{c}f(R)\right.\right\}, \tag{9}$$

$$\mathcal{D}(h_B)=\left\{\psi=\begin{pmatrix}f\\ g\end{pmatrix}\in\mathcal{D}(h_{jl}^*)\left|g(R-)=g(R+)\equiv g(R),f(R+)-f(R-)=-\frac{B}{c}g(R)\right.\right\}. \tag{10}$$

III. THE DEFINITIONS OF HOUNKONNOU AND AVOSSEVOU (Refs. 3–5)

Recently, Hounkonnou and Avossevou published a series of papers on relativistic δ-interactions of the type

$$h_\alpha=h_D+\alpha\,\delta(r-R), \tag{11}$$

$$h_{\alpha,\{R\}}=h_D+\sum_{m=1}^{N}\alpha_m\delta(r-R_m), \tag{12}$$

$$\tilde{h}_{\alpha,\{R\}}=h_D+\sum_{m=1}^{N}\tilde{\alpha}_m\delta'(r-R_m), \tag{13}$$

where h_D is the radial Dirac Hamiltonian defined by Eq. (4).

The authors define these interactions in Ref. 3, Eqs. (2.21)–(2.25), Ref. 5, Eqs. (2.21)–(2.24), and Ref. 4, Eqs. (2.18)–(2.21), respectively.

In this note we focus our analysis on the model given by Eq. (11). Our argumentation applies as well to the models defined by Eqs. (12) and (13).

The following two definitions were proposed in Ref. 3, Eqs. (2.21)–(2.25) for the formal expression (11),

(i)

$$h_{\alpha,1}=\tau,$$

$$\mathcal{D}(h_{\alpha,1})=\left\{\psi=\begin{pmatrix}f\\ g\end{pmatrix}\in L^2((0,\infty))\otimes\mathbb{C}^2\left|f'(R+)=f'(R-),\right.\right.$$

$$g'\in\mathrm{AC}_{\mathrm{loc}}((0,\infty)\backslash\{R\}),g'(R+)-g'(R-)$$

$$\left.\left.=\frac{\alpha}{c}f'(R)+\tilde{A},\quad \tau\psi\in L^2((0,\infty))\otimes\mathbb{C}^2,\quad \tilde{A}\neq0,-\infty<\alpha\leqslant+\infty\right\}; \right. \tag{14}$$

(ii)

$$h_{\alpha,2}=\tau,$$

$$\mathcal{D}(h_{\alpha,2})=\left\{\psi=\begin{pmatrix} f \\ g \end{pmatrix}\in L^2((0,\infty))\otimes\mathbb{C}^2 \,\middle|\, g'(R+)=g'(R-),\right.$$

$$f'\in \mathrm{AC}_{loc}((0,\infty)\backslash\{R\}), f'(R+)-f'(R-)$$

$$\left.=-\frac{\alpha}{c}g'(R)+\tilde{B}, \tau\psi\in L^2((0,\infty))\otimes\mathbb{C}^2, \tilde{B}\neq 0, -\infty<\alpha\leqslant+\infty\right\}. \tag{15}$$

IV. DISCUSSION

In this section we carry out a comprehensive critical analysis of the model introduced in Ref. 3. As indicated in Sec. III, our argumentation applies as well to the models discussed in Refs. 4 and 5.

(1) Obviously the operators defined by Eqs. (14) and (15) are different from the operators h_A and h_B given by Eqs. (9) and (10). Therefore (14) and (15) do not define any relativistic δ-sphere interaction.

Moreover, since H_β and H_γ in Ref. 3, Eqs. (2.22) and (2.25) are defined through Eqs. (14) and (15), it follows that they do not correspond to the relativistic δ-sphere interaction given by Ref. 3, Eq. (2.1). Furthermore, since the operator $h_{\alpha,\{R\}}$ in Eq. (12) is defined through h_α, it follows that $h_{\alpha,\{R\}}$ does not correspond to any radial Dirac Hamiltonian with finitely many δ-sphere interactions supported by concentric spheres.

(2) The boundary conditions given in Eqs. (14) and (15) cannot be written in the form

$$C\psi(R-)+D\psi(R+)=0. \tag{16}$$

Therefore, according to theorem 1, the corresponding operators are not self-adjoint and consequently the conditions required for the application of Krein's formula and Weyl's theorem for the computation of the resolvent equation and the analysis of spectral properties of the Hamiltonians are not fulfilled.

Furthemore, the domain $\mathcal{D}(h_{\alpha,1})$ is not a linear manifold unless the quantity $\tilde{A}$ entering the boundary conditions in (14) is a linear functional on $\mathcal{D}(h_{jl}^*)$. Since this assumption was not explicitely stated, it follows that $h_{\alpha,1}$ is not a linear operator.

(3) The paper contains several other mistakes related to a misunderstanding of some basic concepts of the theory of self-adjoint extensions of symmetric operators in Hilbert spaces. In this note we just point out the following mistakes.

(i) The domain $\mathcal{D}(\dot{h}_{jl})$ in Ref. 3, Eq. (2.13) should read

$$D(\dot{h}_{jl})=\{\psi\in L^2((0,\infty))\otimes\mathbb{C}^2 | \psi\in \mathrm{AC}_{loc}((0,\infty)), \psi(R\pm)=0;$$

$$\tau\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\}. \tag{17}$$

Moreover, contrary to the statement following Ref. 3, Eq. (2.11), $\dot{h}_{jl}$ is not a self-adjoint operator.

(ii) The operator $\dot{h}_{jl}^*$ in Ref. 3, Eq. (2.14) has not been introduced. Since the definition of $\dot{h}_{jl}$ in Ref. 3, Eq. (2.13) is wrong, we assume that the definition of $\dot{h}_{jl}^*$ in Ref. 3, Eq. (2.14) is also wrong.

(iii) In Ref. 3, Eq. (2.21), the case $\beta_{jl}=0$ leads to the boundary conditions $f'_{jl}\in \mathrm{AC_{loc}}((0,\infty))$ and $g'_{jl}(k,R+)-g'_{jl}(k,R-)=\tilde{A}$. These boundary conditions do not define the radial Dirac Hamiltonian given by (4).

(iv) In Ref. 3, Eq. (2.11) the boundary conditions are defined on $(0,\infty)$. Therefore the case $\beta_{jl}=\infty$ can not lead to any boundary condition on the sphere S_R in $\mathbb{R}^3$. Furthemore, the case

$\beta_{jl}=\infty$ leads to the boundary condition $g'_{jl}(R)=0$ and not $g'_{jl}(k,R+)-g'_{jl}(k,R-)=0$. Therefore, $\beta_{jl}=\infty$ does not coincide with the radial Dirac Hamiltonian with a Neumann boundary condition at R.

(v) The definition of H_{γ_0} in Ref. 3, Eq. (3.2) is wrong. H_{γ_0} should read

$$H_{\gamma_0}=H_D+\frac{\gamma_0}{|x|};\quad x\in\mathbb{R}^3. \tag{18}$$

Moreover, as in the case $\gamma_0=0$, one can show that Ref. 3, Eq. (3.5) is wrong and that Ref. 3, Eqs. (3.11)–(3.13) do not define any relativistic δ-sphere plus a Coulomb interaction.

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The second line of Eq. (7.22a) should read "$\times(l-q)(l+q+N-3)$" and the second line of Eq. (7.22b) should read "$\times(l-q+1)(l+q+N-2)$."

The first line of the right-hand side of Eq. (7.24a) should read

$$\frac{(l-r)(l+1)}{(l-m)(l-m+1)}$$

and that of Eq. (7.24b) should read

$$-\frac{(l+N+r-2)(l+N-3)}{(l+N+m-2)(L+N+m-3)}.$$

In the line between Eqs. (8.12) and (8.13) "replacing r, L, l, and N by m, l, q, and $N-1$" should read "replacing m, l, q, and $N-1$ by r, L, l, and N."

In Eqs. (9.12) and (9.17), the factor of π should be replaced by 2.

